wwPDB EM Validation Summary Report

Jul 9, 2026 – 06:43 PM JST

PDB ID	:	9JJ8 / pdb_00009jj8
EMDB ID	:	EMD-61519
Title	:	Structural insights into the PSI-FCPI supercomplex from the coccolithophore Emiliania huxleyi
Authors	:	Shen, L.L.; Li, Z.H.; Wang, W.D.
Deposited on	:	2024-09-13
Resolution	:	2.79 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

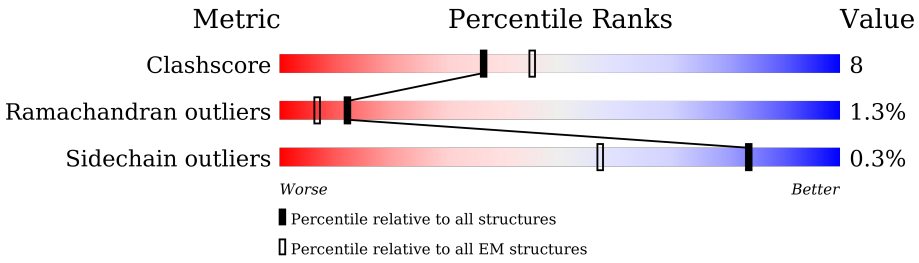
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

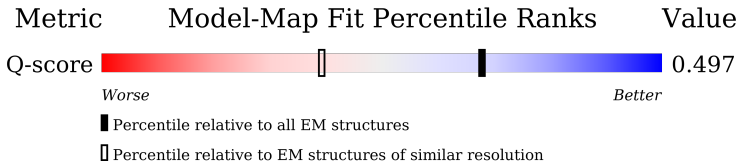
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	752	84% 15%
2	b	734	88% 12%
3	c	81	85% 12%
4	d	142	87% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	e	131	46% 52%
6	f	184	79% 8% 12%
7	i	36	78% 14% 8%
8	j	40	78% 22%
9	l	145	86% 13%
10	m	30	80% 20%
11	k	145	40% 10% 50%
12	o	123	7% 32% 7% 61%
13	A	201	77% 14% 9%
14	B	177	24% 78% 19%
15	C	233	6% 65% 10% 24%
16	D	231	71% 11% 18%
17	E	217	73% 13% 14%
18	F	239	59% 18% 21%
19	G	204	68% 16% 16%
20	H	210	5% 66% 14% 20%
21	J	251	13% 53% 15% 32%
22	K	198	75% 7% 15%
23	L	244	6% 76% 9% 14%
24	M	224	71% 15% 14%
24	P	224	71% 15% 14%
24	W	224	72% 12% 14%
25	O	219	6% 57% 12% 29%
26	Q	257	63% 18% 16%
27	5	219	67% 14% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	R	219	69% 11% 19%
27	V	219	69% 16% 14%
27	X	219	67% 14% 19%
28	4	255	76% 13% 11%
28	7	255	16% 80% 10% 11%
28	S	255	74% 14% 11%
28	x	255	60% 87% 11%
28	y	255	47% 87% 11%
28	z	255	56% 86% 11%
29	T	211	78% 15% 7%
30	U	198	63% 16% 20%
31	0	254	70% 15% 14%
32	1	253	27% 67% 12% 21%
33	3	268	18% 74% 14% 12%
34	6	250	53% 84% 6% 10%
34	8	250	22% 82% 7% 10%
35	9	245	14% 76% 9% 15%
36	I	209	65% 10% 25%
37	h	133	64% 35%
38	2	260	53% 75% 12% 14%
38	Y	260	85% 82% 5% 13%
38	Z	260	82% 83% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	LMG	4	326	-	-	X	-
48	A86	Q	304	-	-	X	-
49	KC2	5	313	-	-	X	-
51	A1ECV	0	321	X	-	-	-
51	A1ECV	1	318	X	-	-	-
51	A1ECV	2	311	X	-	-	-
51	A1ECV	4	315	X	-	-	-
51	A1ECV	4	321	X	-	-	-
51	A1ECV	5	309	X	-	-	-
51	A1ECV	5	312	X	-	-	-
51	A1ECV	6	320	X	-	-	-
51	A1ECV	7	317	X	-	-	-
51	A1ECV	7	323	X	-	-	-
51	A1ECV	9	314	X	-	-	-
51	A1ECV	9	317	X	-	-	-
51	A1ECV	E	311	X	-	-	-
51	A1ECV	G	316	X	-	-	-
51	A1ECV	L	318	X	-	-	-
51	A1ECV	M	316	X	-	-	-
51	A1ECV	O	315	X	-	-	-
51	A1ECV	P	315	X	-	-	-
51	A1ECV	Q	316	X	-	-	-
51	A1ECV	Q	319	X	-	-	-
51	A1ECV	R	310	X	-	-	-
51	A1ECV	R	313	X	-	-	-
51	A1ECV	S	312	X	-	-	-
51	A1ECV	S	318	X	-	-	-
51	A1ECV	T	317	X	-	-	-
51	A1ECV	V	317	X	-	-	-
51	A1ECV	W	317	X	-	-	-
51	A1ECV	X	310	X	-	-	-
51	A1ECV	X	313	X	-	-	-
51	A1ECV	Y	306	X	-	-	-
51	A1ECV	Y	312	X	-	-	-
51	A1ECV	Z	308	X	-	-	-
51	A1ECV	Z	314	X	-	-	-
51	A1ECV	x	310	X	-	-	-
51	A1ECV	x	316	X	-	-	-
51	A1ECV	y	311	X	-	-	-
51	A1ECV	y	317	X	-	-	-
51	A1ECV	z	310	X	-	-	-
51	A1ECV	z	316	X	-	-	-

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 114135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	741	5835	3817	993	995	30	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	733	5818	3828	982	987	21	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	80	598	365	105	117	11	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	140	1103	710	184	206	3	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	63	491	314	86	90	1	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	161	1232	797	207	224	4	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	33	Total	C	N	O	S	0	0
			254	176	34	43	1		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			318	211	47	57	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	143	Total	C	N	O	S	0	0
			1084	716	172	195	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	30	Total	C	N	O	S	0	0
			224	149	35	38	2		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	73	Total	C	N	O	S	0	0
			533	347	87	93	6		

- Molecule 12 is a protein called Linker-protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	48	Total	C	N	O	S	0	0
			360	231	61	66	2		

- Molecule 13 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	183	Total	C	N	O	S	0	0
			1419	916	229	264	10		

- Molecule 14 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	172	Total	C	N	O	S	0	0
			1255	805	212	231	7		

- Molecule 15 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	176	Total	C	N	O	S	0	0
			1329	857	221	242	9		

- Molecule 16 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	189	Total	C	N	O	S	0	0
			1424	921	226	271	6		

- Molecule 17 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	187	Total	C	N	O	S	0	0
			1384	896	222	258	8		

- Molecule 18 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	188	Total	C	N	O	S	0	0
			1411	907	244	251	9		

- Molecule 19 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	171	Total	C	N	O	S	0	0
			1340	875	226	232	7		

- Molecule 20 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	168	Total	C	N	O	S	0	0
			1263	810	206	235	12		

- Molecule 21 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	171	Total	C	N	O	S	0	0
			1270	810	223	230	7		

- Molecule 22 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	168	Total	C	N	O	S	0	0
			1251	806	206	231	8		

- Molecule 23 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	210	Total	C	N	O	S	0	0
			1626	1064	273	281	8		

- Molecule 24 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	P	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	W	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		

- Molecule 25 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	155	Total	C	N	O	S	0	0
			1133	717	200	209	7		

- Molecule 26 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	215	Total	C	N	O	S	0	0
			1666	1094	273	294	5		

- Molecule 27 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	188	Total	C	N	O	S	0	0
			1353	872	227	248	6		
27	X	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		
27	5	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

- Molecule 28 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	4	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	7	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	x	228	Total	C	N	O		0	0
			1113	657	228	228			
28	y	228	Total	C	N	O		0	0
			1113	657	228	228			
28	z	228	Total	C	N	O		0	0
			1113	657	228	228			

- Molecule 29 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	197	Total	C	N	O	S	0	0
			1482	973	246	257	6		

- Molecule 30 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	158	Total	C	N	O	S	0	0
			1240	801	207	226	6		

- Molecule 31 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	0	218	Total	C	N	O	S	0	0
			1706	1114	278	309	5		

- Molecule 32 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	201	Total	C	N	O	S	0	0
			1255	794	223	237	1		

- Molecule 33 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3	236	Total	C	N	O	S	0	0
			1775	1155	294	318	8		

- Molecule 34 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	224	Total	C	N	O	S	0	0
			1415	892	255	261	7		
34	6	224	Total	C	N	O	S	0	0
			1326	825	249	250	2		

- Molecule 35 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	209	Total	C	N	O	S	0	0
			1490	970	246	267	7		

- Molecule 36 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	I	156	Total	C	N	O	S	0	0
			1203	780	201	213	9		

- Molecule 37 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	87	Total	C	N	O	S	0	0
			650	425	104	120	1		

- Molecule 38 is a protein called Light harvesting protein.

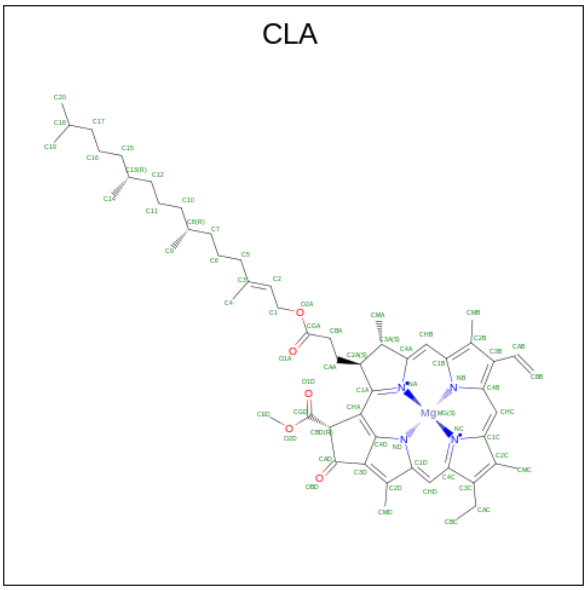
Mol	Chain	Residues	Atoms				AltConf	Trace
38	Y	225	Total	C	N	O	0	0
			1099	649	225	225		
38	Z	225	Total	C	N	O	0	0
			1099	649	225	225		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	224	Total	C	N	O	S	0	0
			1383	858	256	263	6		

- Molecule 39 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	j	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	k	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	o	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	o	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	o	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	o	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
39	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	L	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	M	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	R	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	S	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	W	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	X	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	x	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	y	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Y	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

Continued on next page...

Continued from previous page...

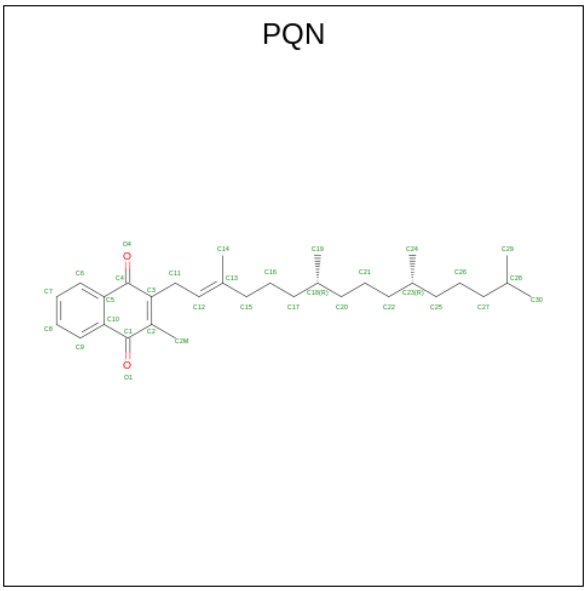
Mol	Chain	Residues	Atoms					AltConf
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	Z	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			52	44	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

Continued on next page...

Continued from previous page...

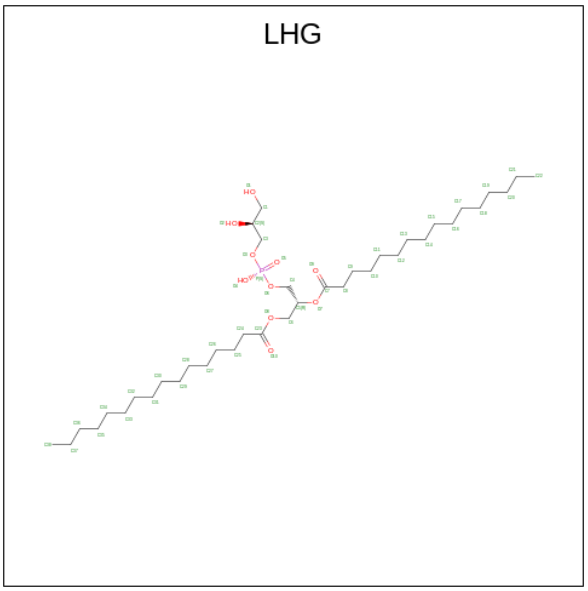
Mol	Chain	Residues	Atoms					AltConf
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 40 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



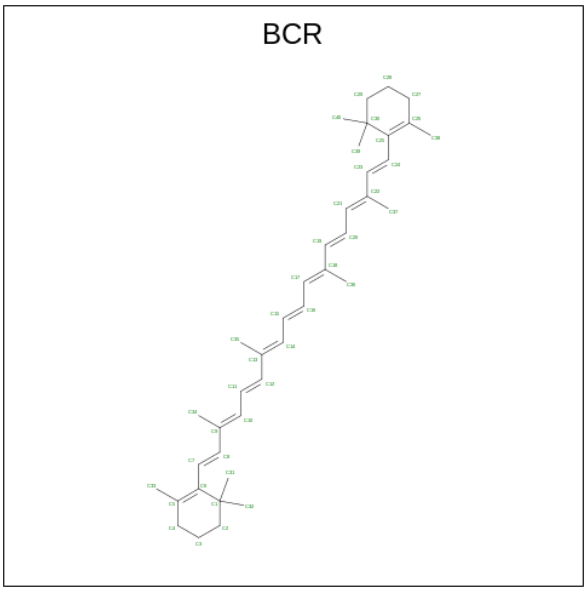
Mol	Chain	Residues	Atoms			AltConf
40	a	1	Total	C	O	0
			33	31	2	
40	b	1	Total	C	O	0
			33	31	2	

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
41	a	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			27	16	10	1	
41	j	1	Total	C	O	P	0
			30	19	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	H	1	Total	C	O	P	0
			35	24	10	1	
41	X	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 42 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



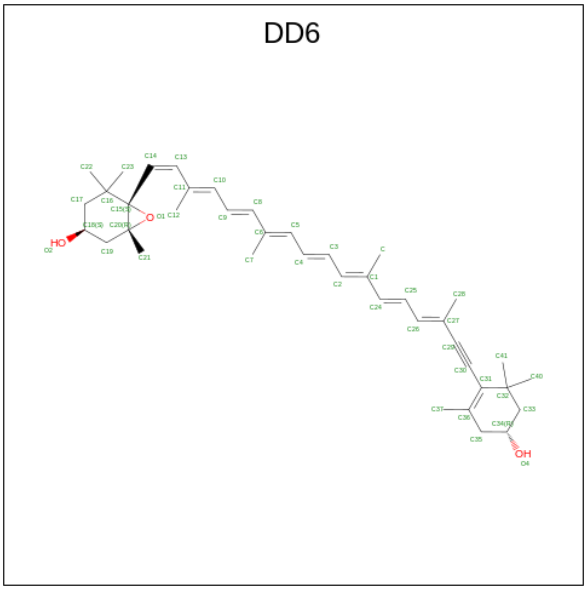
Mol	Chain	Residues	Atoms	AltConf
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	a	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	b	1	Total C 40 40	0
42	f	1	Total C 40 40	0
42	f	1	Total C 40 40	0
42	i	1	Total C 40 40	0
42	j	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	m	1	Total C 40 40	0
42	k	1	Total C 40 40	0
42	h	1	Total C 40 40	0

- Molecule 43 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
43	a	1	Total C O 43 40 3	0
43	j	1	Total C O 43 40 3	0
43	o	1	Total C O 43 40 3	0
43	A	1	Total C O 43 40 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
43	A	1	Total C O 43 40 3	0
43	A	1	Total C O 43 40 3	0
43	A	1	Total C O 43 40 3	0
43	B	1	Total C O 43 40 3	0
43	C	1	Total C O 43 40 3	0
43	D	1	Total C O 43 40 3	0
43	D	1	Total C O 43 40 3	0
43	D	1	Total C O 43 40 3	0
43	E	1	Total C O 43 40 3	0
43	E	1	Total C O 43 40 3	0
43	E	1	Total C O 43 40 3	0
43	F	1	Total C O 43 40 3	0
43	F	1	Total C O 43 40 3	0
43	G	1	Total C O 43 40 3	0
43	G	1	Total C O 43 40 3	0
43	H	1	Total C O 43 40 3	0
43	H	1	Total C O 43 40 3	0
43	J	1	Total C O 43 40 3	0
43	J	1	Total C O 43 40 3	0
43	J	1	Total C O 43 40 3	0
43	K	1	Total C O 43 40 3	0

Continued on next page...

Continued from previous page...

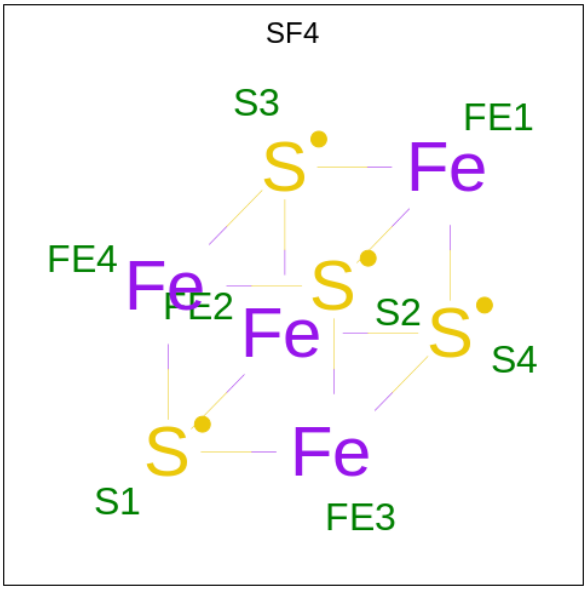
Mol	Chain	Residues	Atoms			AltConf
43	M	1	Total	C	O	0
			43	40	3	
43	O	1	Total	C	O	0
			43	40	3	
43	O	1	Total	C	O	0
			43	40	3	
43	O	1	Total	C	O	0
			43	40	3	
43	P	1	Total	C	O	0
			43	40	3	
43	Q	1	Total	C	O	0
			43	40	3	
43	Q	1	Total	C	O	0
			43	40	3	
43	R	1	Total	C	O	0
			43	40	3	
43	S	1	Total	C	O	0
			43	40	3	
43	T	1	Total	C	O	0
			43	40	3	
43	U	1	Total	C	O	0
			43	40	3	
43	V	1	Total	C	O	0
			43	40	3	
43	W	1	Total	C	O	0
			43	40	3	
43	X	1	Total	C	O	0
			43	40	3	
43	1	1	Total	C	O	0
			43	40	3	
43	3	1	Total	C	O	0
			43	40	3	
43	3	1	Total	C	O	0
			43	40	3	
43	4	1	Total	C	O	0
			43	40	3	
43	4	1	Total	C	O	0
			43	40	3	
43	5	1	Total	C	O	0
			43	40	3	
43	7	1	Total	C	O	0
			43	40	3	

Continued on next page...

Continued from previous page...

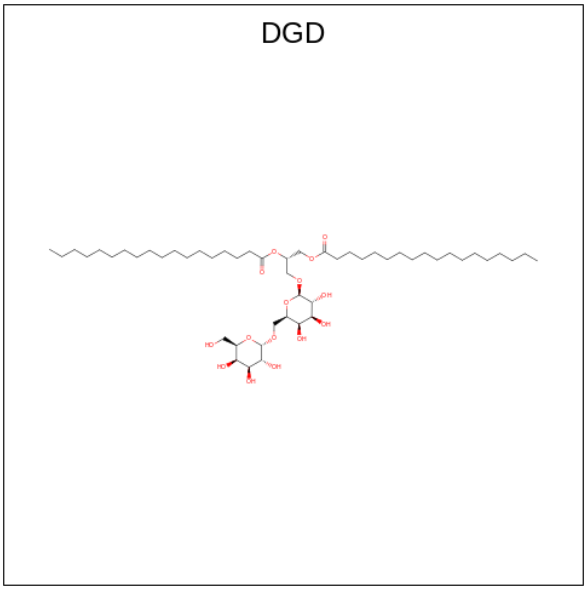
Mol	Chain	Residues	Atoms	AltConf
43	7	1	Total C O 43 40 3	0
43	I	1	Total C O 43 40 3	0
43	I	1	Total C O 43 40 3	0
43	I	1	Total C O 43 40 3	0
43	x	1	Total C O 43 40 3	0
43	x	1	Total C O 43 40 3	0
43	y	1	Total C O 43 40 3	0
43	y	1	Total C O 43 40 3	0
43	z	1	Total C O 43 40 3	0
43	z	1	Total C O 43 40 3	0
43	Z	1	Total C O 43 40 3	0
43	2	1	Total C O 43 40 3	0

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



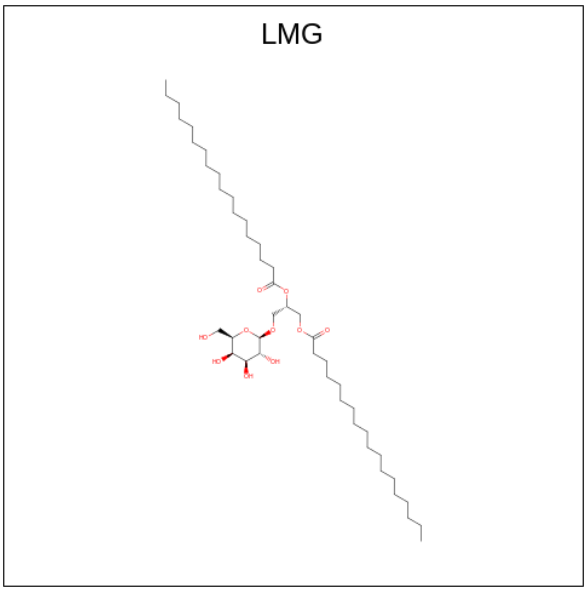
Mol	Chain	Residues	Atoms	AltConf
44	b	1	Total Fe S 8 4 4	0
44	c	1	Total Fe S 8 4 4	0
44	c	1	Total Fe S 8 4 4	0

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
45	b	1	Total C O 60 45 15	0
45	C	1	Total C O 40 25 15	0

- Molecule 46 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



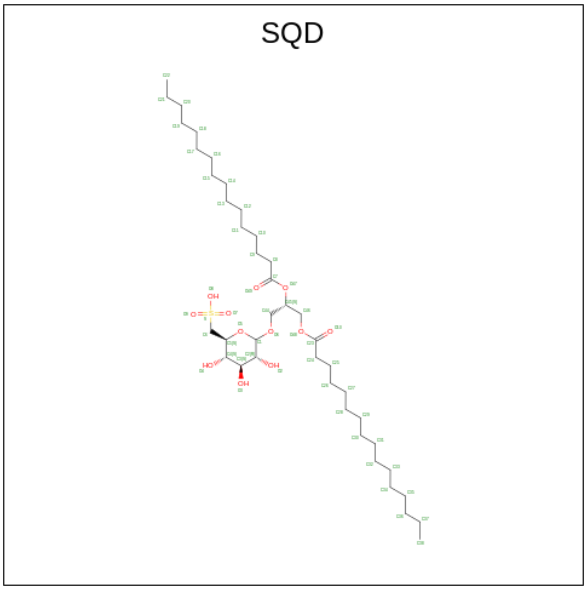
Mol	Chain	Residues	Atoms	AltConf
46	l	1	Total C O 39 29 10	0
46	A	1	Total C O 29 19 10	0
46	D	1	Total C O 37 27 10	0
46	F	1	Total C O 39 29 10	0
46	F	1	Total C O 34 24 10	0
46	M	1	Total C O 39 29 10	0
46	M	1	Total C O 33 23 10	0
46	P	1	Total C O 39 29 10	0
46	Q	1	Total C O 28 18 10	0
46	S	1	Total C O 32 22 10	0
46	S	1	Total C O 46 36 10	0
46	W	1	Total C O 39 29 10	0
46	W	1	Total C O 33 23 10	0
46	0	1	Total C O 27 17 10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
46	4	1	Total C O 32 22 10	0
46	4	1	Total C O 46 36 10	0
46	7	1	Total C O 46 36 10	0
46	7	1	Total C O 32 22 10	0
46	9	1	Total C O 36 26 10	0
46	I	1	Total C O 42 32 10	0

- Molecule 47 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



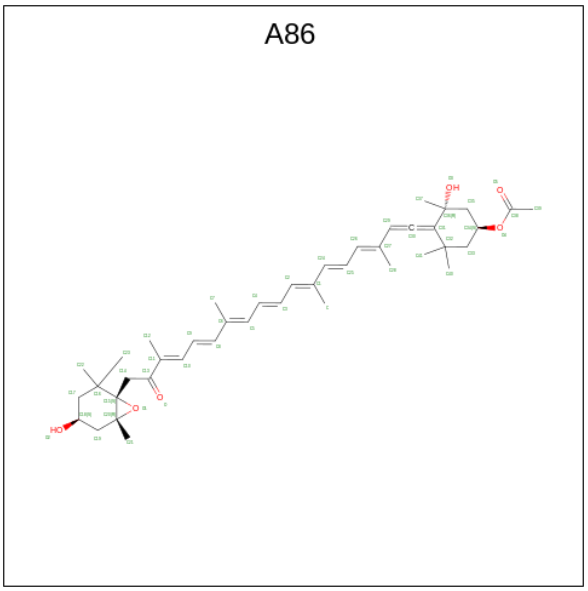
Mol	Chain	Residues	Atoms	AltConf
47	k	1	Total C O S 38 25 12 1	0
47	D	1	Total C O S 38 25 12 1	0
47	D	1	Total C O S 37 24 12 1	0
47	D	1	Total C O S 39 26 12 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
47	E	1	Total	C	O	S	0
			35	22	12	1	
47	F	1	Total	C	O	S	0
			42	29	12	1	
47	F	1	Total	C	O	S	0
			37	24	12	1	
47	H	1	Total	C	O	S	0
			38	25	12	1	
47	M	1	Total	C	O	S	0
			39	26	12	1	
47	P	1	Total	C	O	S	0
			38	25	12	1	
47	S	1	Total	C	O	S	0
			39	26	12	1	
47	T	1	Total	C	O	S	0
			36	23	12	1	
47	W	1	Total	C	O	S	0
			28	15	12	1	
47	4	1	Total	C	O	S	0
			39	26	12	1	
47	7	1	Total	C	O	S	0
			39	26	12	1	
47	9	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 48 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
48	k	1	Total C O 48 42 6	0
48	B	1	Total C O 48 42 6	0
48	C	1	Total C O 48 42 6	0
48	D	1	Total C O 48 42 6	0
48	E	1	Total C O 48 42 6	0
48	F	1	Total C O 48 42 6	0
48	F	1	Total C O 48 42 6	0
48	G	1	Total C O 48 42 6	0
48	G	1	Total C O 48 42 6	0
48	H	1	Total C O 48 42 6	0
48	J	1	Total C O 48 42 6	0
48	J	1	Total C O 48 42 6	0
48	K	1	Total C O 48 42 6	0
48	L	1	Total C O 48 42 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	
48	M	1	Total	C	O	0
			48	42	6	
48	M	1	Total	C	O	0
			48	42	6	
48	M	1	Total	C	O	0
			48	42	6	
48	O	1	Total	C	O	0
			48	42	6	
48	O	1	Total	C	O	0
			48	42	6	
48	O	1	Total	C	O	0
			48	42	6	
48	P	1	Total	C	O	0
			48	42	6	
48	P	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	Q	1	Total	C	O	0
			48	42	6	
48	R	1	Total	C	O	0
			48	42	6	
48	R	1	Total	C	O	0
			48	42	6	
48	R	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
48	S	1	Total	C	O	0
			48	42	6	
48	S	1	Total	C	O	0
			48	42	6	
48	S	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	U	1	Total	C	O	0
			48	42	6	
48	U	1	Total	C	O	0
			48	42	6	
48	V	1	Total	C	O	0
			48	42	6	
48	V	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	X	1	Total	C	O	0
			48	42	6	
48	X	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	1	1	Total	C	O	0
			48	42	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
48	1	1	Total C O 48 42 6	0
48	1	1	Total C O 48 42 6	0
48	1	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	3	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	4	1	Total C O 48 42 6	0
48	5	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	7	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0

Continued on next page...

Continued from previous page...

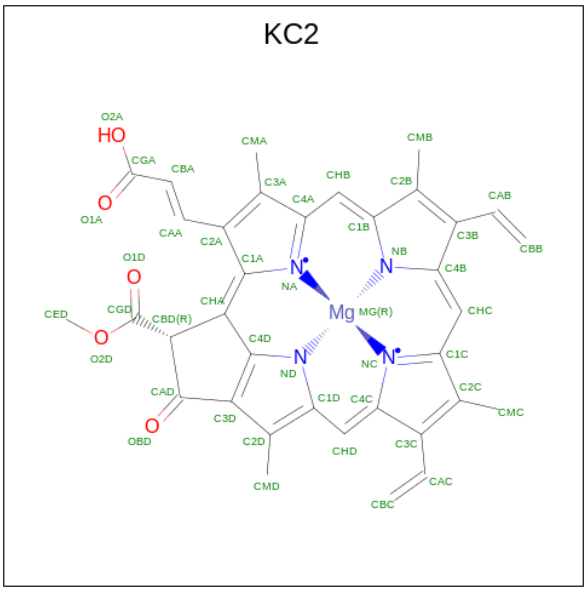
Mol	Chain	Residues	Atoms	AltConf
48	8	1	Total C O 48 42 6	0
48	8	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	9	1	Total C O 48 42 6	0
48	I	1	Total C O 48 42 6	0
48	x	1	Total C O 48 42 6	0
48	y	1	Total C O 48 42 6	0
48	y	1	Total C O 48 42 6	0
48	z	1	Total C O 48 42 6	0
48	Y	1	Total C O 48 42 6	0
48	Z	1	Total C O 48 42 6	0
48	Z	1	Total C O 48 42 6	0
48	2	1	Total C O 48 42 6	0
48	2	1	Total C O 48 42 6	0
48	2	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
48	6	1	Total C O 48 42 6	0
48	6	1	Total C O 48 42 6	0

- Molecule 49 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
49	A	1	Total C Mg N O 45 35 1 4 5	0
49	A	1	Total C Mg N O 45 35 1 4 5	0
49	B	1	Total C Mg N O 45 35 1 4 5	0
49	C	1	Total C Mg N O 45 35 1 4 5	0
49	C	1	Total C Mg N O 45 35 1 4 5	0
49	F	1	Total C Mg N O 45 35 1 4 5	0
49	F	1	Total C Mg N O 44 35 1 4 4	0
49	G	1	Total C Mg N O 45 35 1 4 5	0
49	G	1	Total C Mg N O 45 35 1 4 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
49	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	M	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	O	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	P	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
49	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Q	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
49	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	W	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	0	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	5	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
49	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	I	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

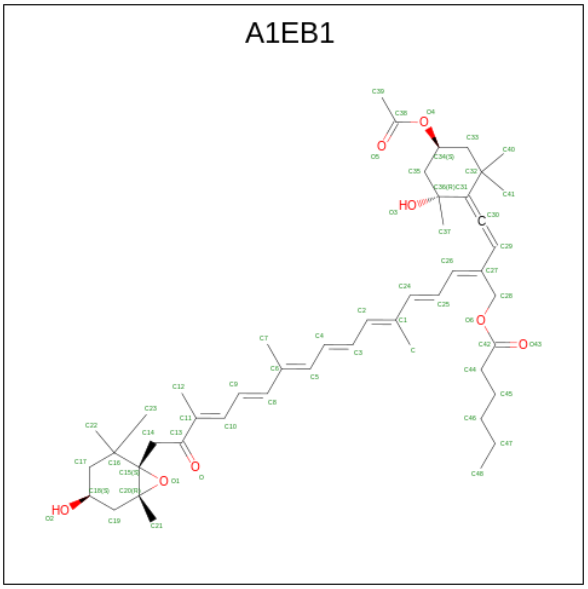
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
49	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	z	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
49	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
49	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
49	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 50 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-2-[2-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]ethenyl]-6,11,15-trimethyl-16-oxidanylidene-17-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]heptadec

a-2,4,6,8,10,12,14-heptaenyl] hexanoate (CCD ID: A1EB1) (formula: $C_{48}H_{68}O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
50	C	1	Total C O 56 48 8	0
50	D	1	Total C O 56 48 8	0
50	E	1	Total C O 56 48 8	0
50	F	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	G	1	Total C O 56 48 8	0
50	H	1	Total C O 56 48 8	0
50	H	1	Total C O 56 48 8	0
50	J	1	Total C O 56 48 8	0
50	K	1	Total C O 56 48 8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
50	K	1	Total C O 56 48 8	0
50	K	1	Total C O 56 48 8	0
50	L	1	Total C O 56 48 8	0
50	O	1	Total C O 56 48 8	0
50	Q	1	Total C O 56 48 8	0
50	Q	1	Total C O 56 48 8	0
50	R	1	Total C O 56 48 8	0
50	S	1	Total C O 56 48 8	0
50	S	1	Total C O 56 48 8	0
50	T	1	Total C O 56 48 8	0
50	T	1	Total C O 56 48 8	0
50	U	1	Total C O 56 48 8	0
50	U	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	V	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0
50	0	1	Total C O 56 48 8	0

Continued on next page...

Continued from previous page...

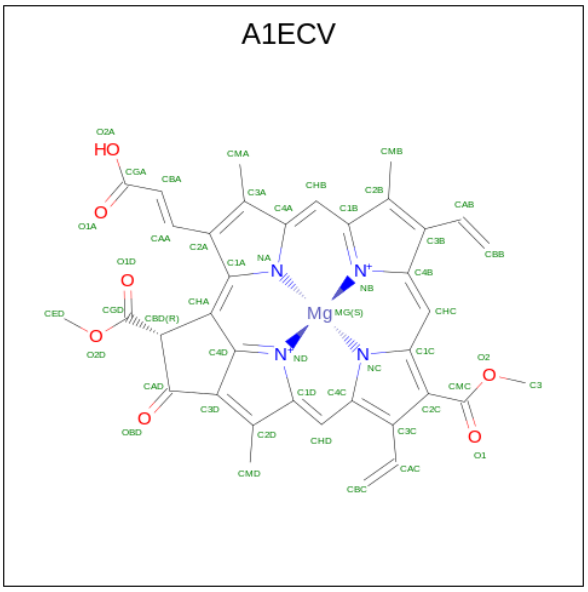
Mol	Chain	Residues	Atoms	AltConf
50	1	1	Total C O 56 48 8	0
50	1	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	3	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	4	1	Total C O 56 48 8	0
50	5	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	7	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	8	1	Total C O 56 48 8	0
50	9	1	Total C O 56 48 8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
50	h	1	Total C O 56 48 8	0
50	x	1	Total C O 56 48 8	0
50	x	1	Total C O 56 48 8	0
50	y	1	Total C O 56 48 8	0
50	y	1	Total C O 56 48 8	0
50	z	1	Total C O 48 42 6	0
50	z	1	Total C O 56 48 8	0
50	2	1	Total C O 56 48 8	0
50	2	1	Total C O 56 48 8	0
50	6	1	Total C O 56 48 8	0
50	6	1	Total C O 53 45 8	0
50	6	1	Total C O 48 42 6	0
50	6	1	Total C O 56 48 8	0

- Molecule 51 is Chlorophyll C3 (CCD ID: A1ECV) (formula: $C_{36}H_{28}MgN_4O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
51	E	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	G	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	L	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	M	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	O	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	P	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	T	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	V	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

Continued on next page...

Continued from previous page...

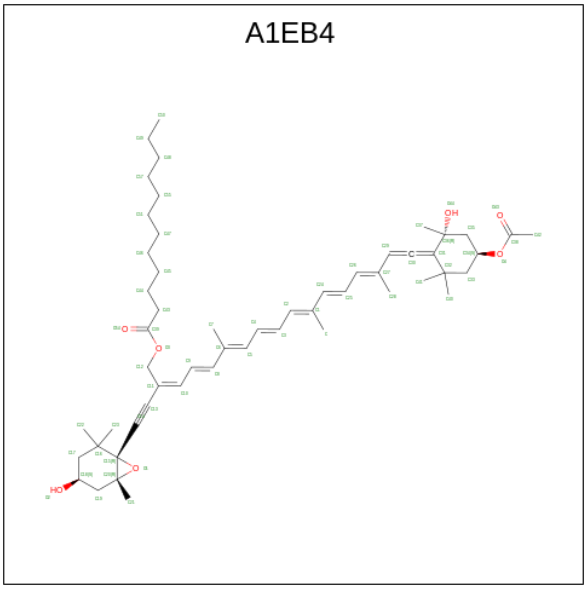
Mol	Chain	Residues	Atoms					AltConf
51	W	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	X	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	X	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	0	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	1	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	4	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	4	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	5	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	5	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	7	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	7	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	9	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	9	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	x	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	x	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Y	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	2	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	6	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

- Molecule 52 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[2-[(1 {R},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethynyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] dodecanoate (CCD ID: A1EB4) (formula: $C_{54}H_{78}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	C	O	0
			58	51	7	
52	M	1	Total	C	O	0
			57	50	7	
52	P	1	Total	C	O	0
			56	49	7	
52	P	1	Total	C	O	0
			54	47	7	
52	P	1	Total	C	O	0
			57	50	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			57	50	7	
52	T	1	Total	C	O	0
			55	48	7	
52	W	1	Total	C	O	0
			56	49	7	
52	W	1	Total	C	O	0
			57	50	7	
52	X	1	Total	C	O	0
			57	50	7	
52	5	1	Total	C	O	0
			57	50	7	

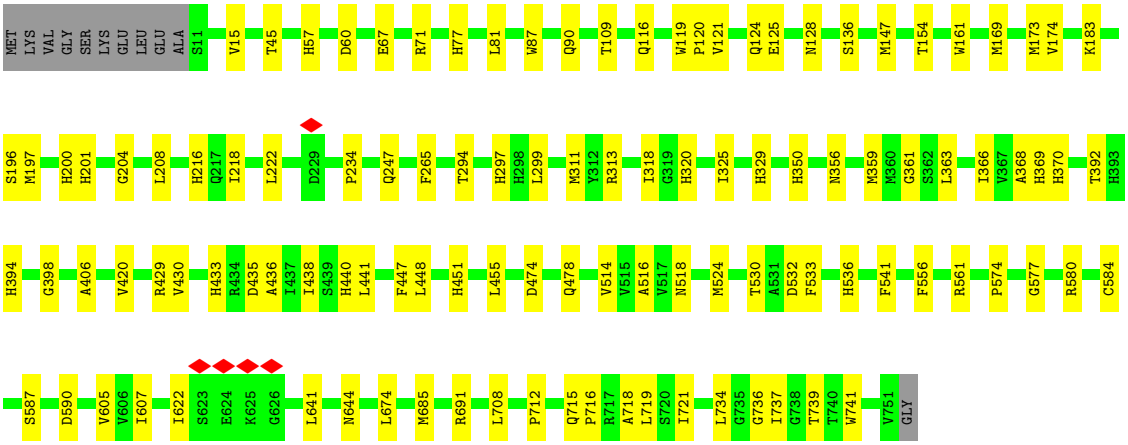
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:

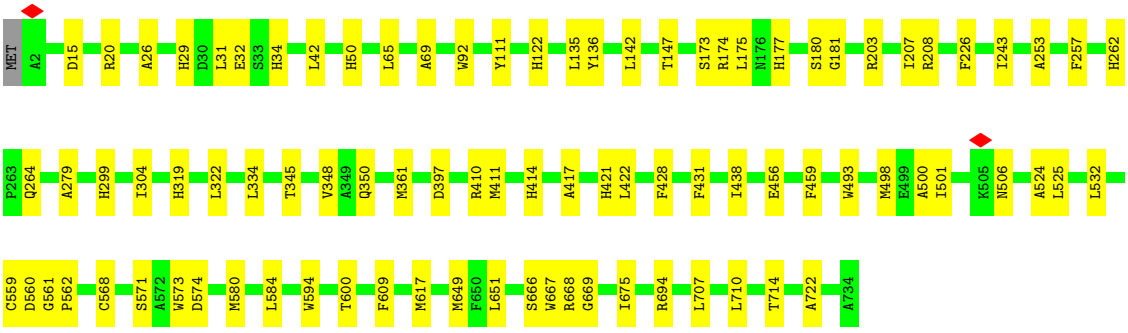




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:

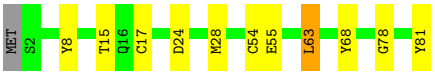




• Molecule 3: Photosystem I iron-sulfur center

Chain c:





• Molecule 4: Photosystem I reaction center subunit II

Chain d:





• Molecule 5: Photosystem I reaction center subunit IV

Chain e:

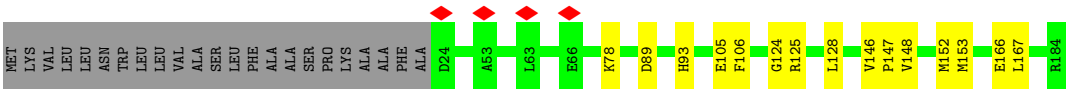




• Molecule 6: Photosystem I reaction center subunit III

Chain f:

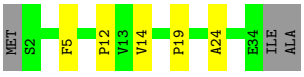




• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:

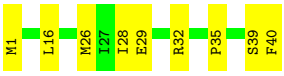




• Molecule 8: Photosystem I reaction center subunit IX

Chain j:

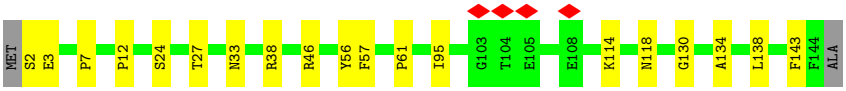




• Molecule 9: Photosystem I reaction center subunit XI

Chain l:

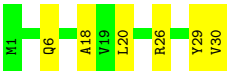




• Molecule 10: Photosystem I reaction center subunit XII

Chain m:

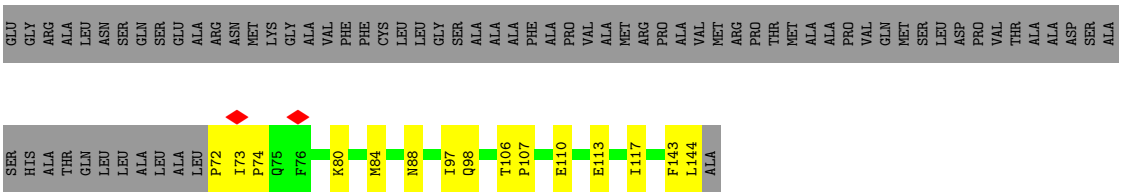




• Molecule 11: PSI-K

Chain k:

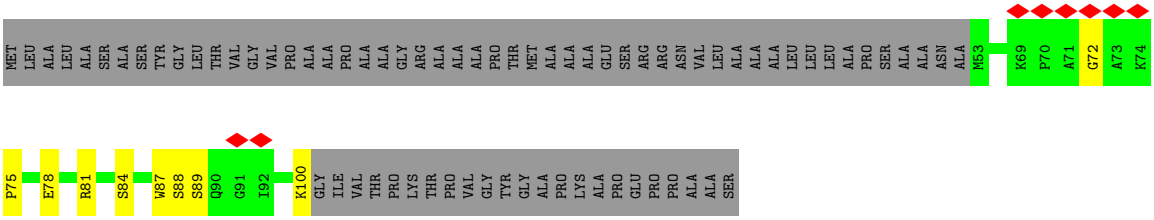




• Molecule 12: Linker-protein

Chain o:

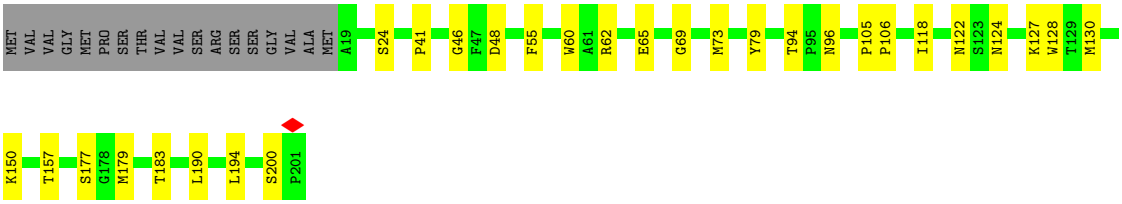




• Molecule 13: Light harvesting protein

Chain A:

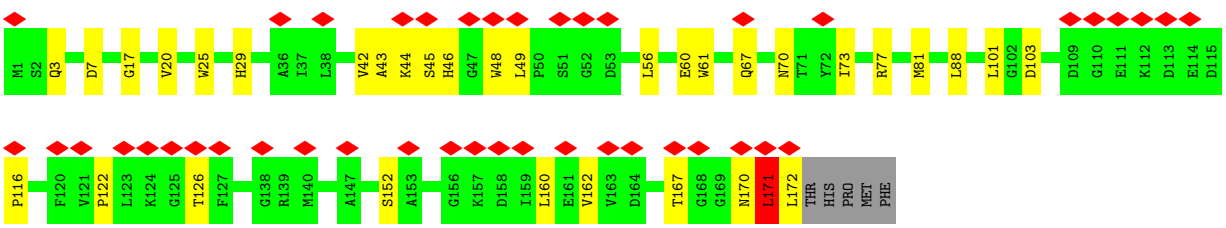




• Molecule 14: Light harvesting protein

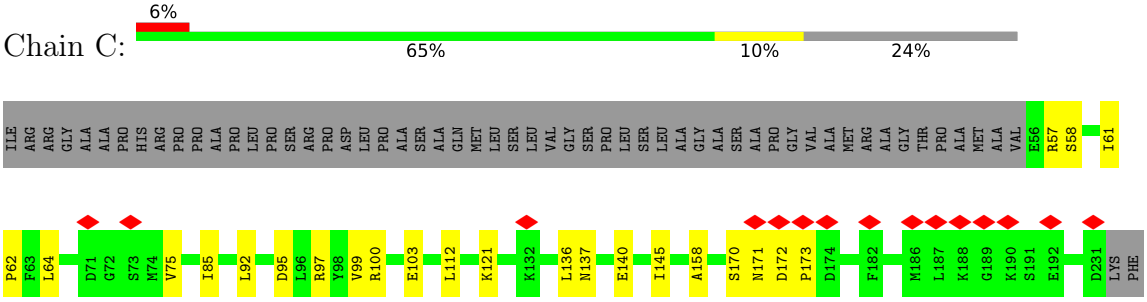
Chain B:





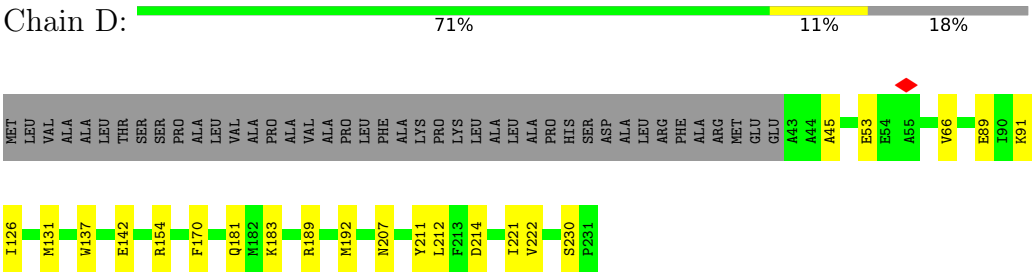
• Molecule 15: Light harvesting protein

Chain C:



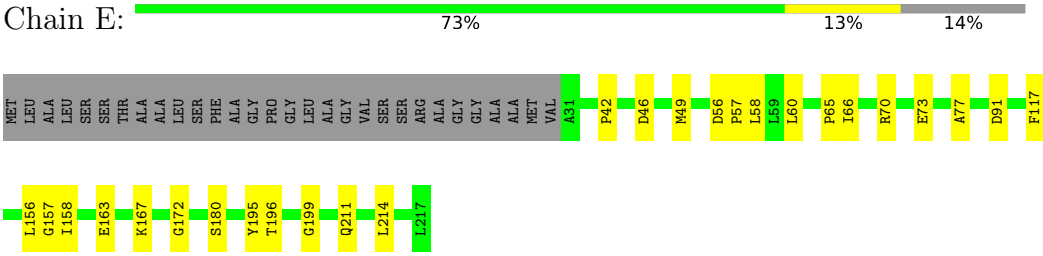
• Molecule 16: Light harvesting protein

Chain D:



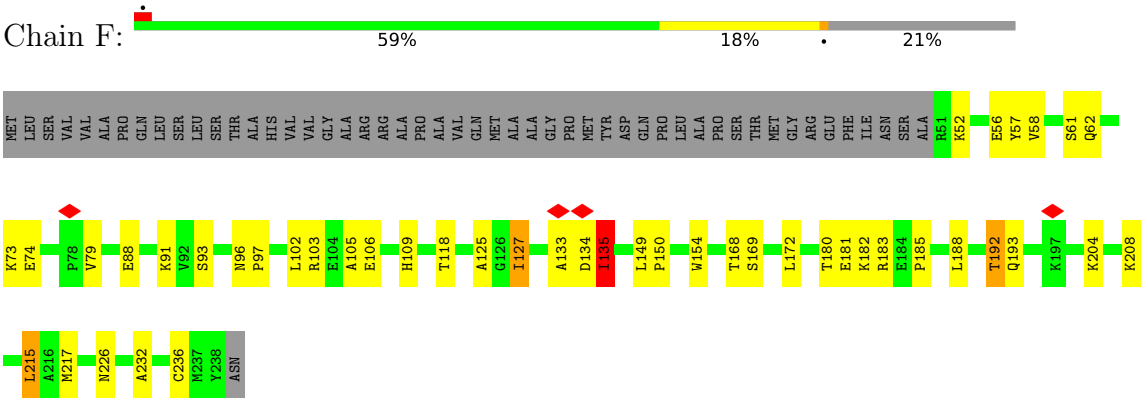
• Molecule 17: Light harvesting protein

Chain E:



• Molecule 18: Light harvesting protein

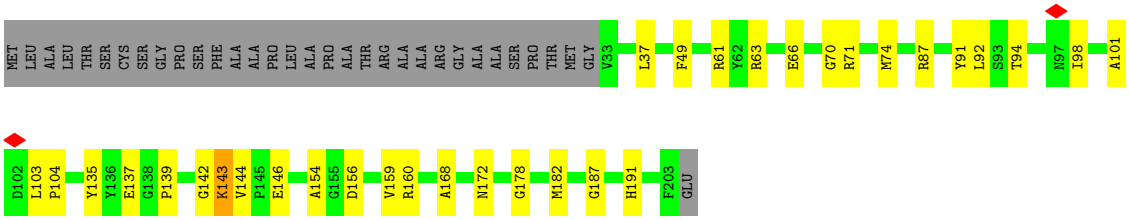
Chain F:



• Molecule 19: Light harvesting protein

Chain G:

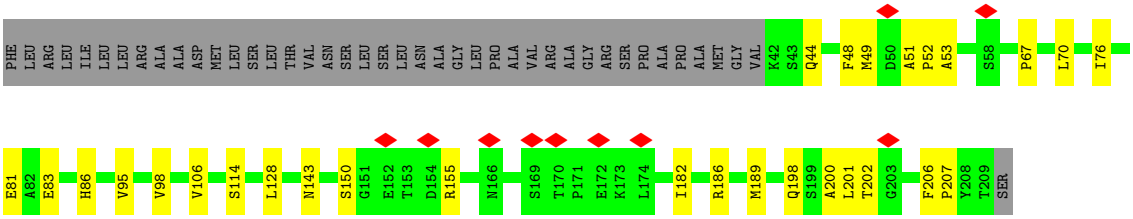




• Molecule 20: Light harvesting protein

Chain H:

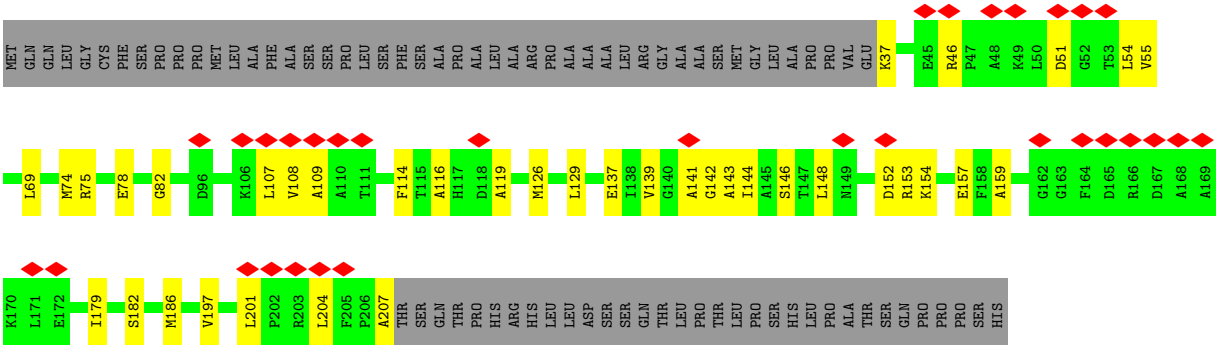




• Molecule 21: Light harvesting protein

Chain J:

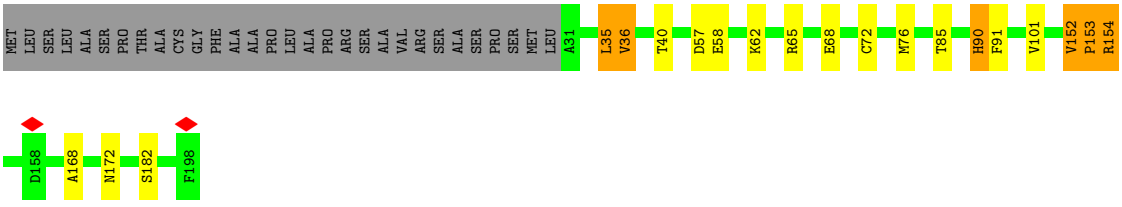




• Molecule 22: Light harvesting protein

Chain K:

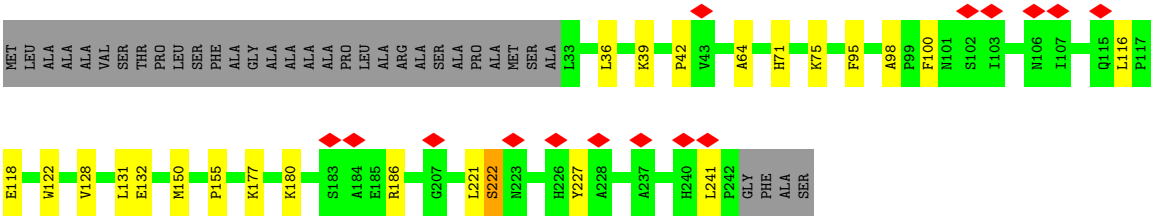




• Molecule 23: Light harvesting protein

Chain L:

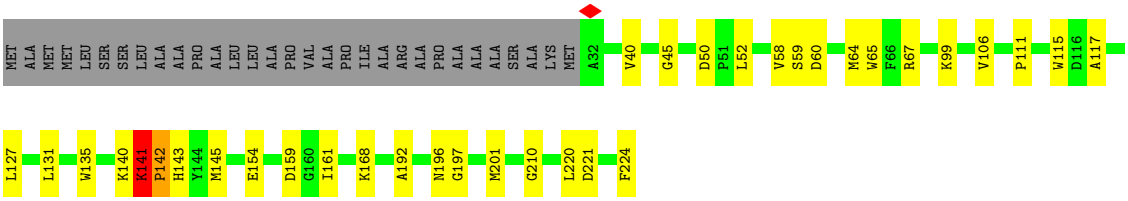




• Molecule 24: Light harvesting protein

Chain M:

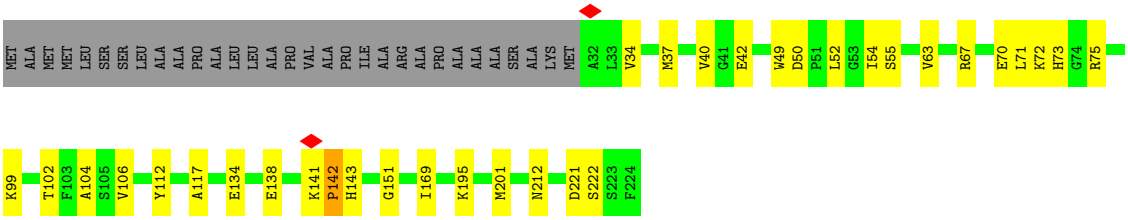




• Molecule 24: Light harvesting protein

Chain P:

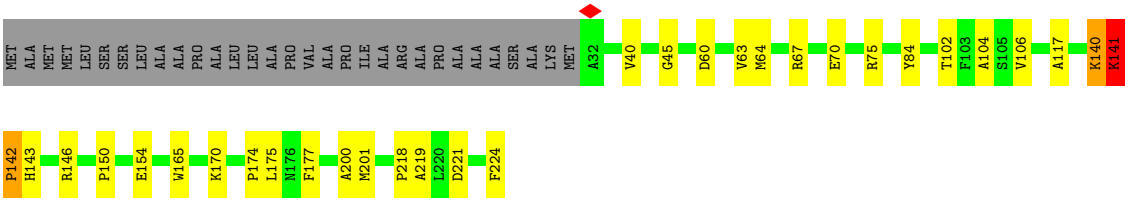




• Molecule 24: Light harvesting protein

Chain W:

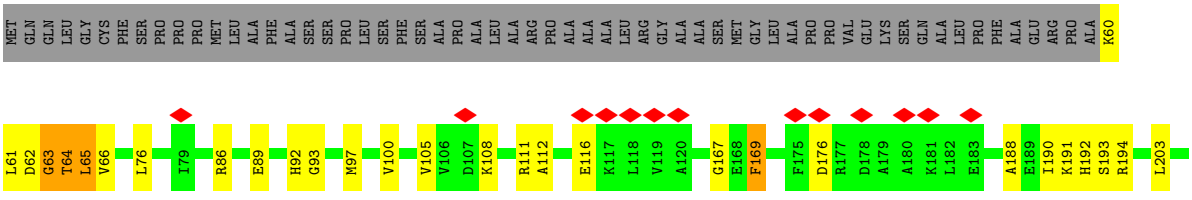


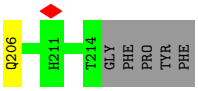


• Molecule 25: Light harvesting protein

Chain O:



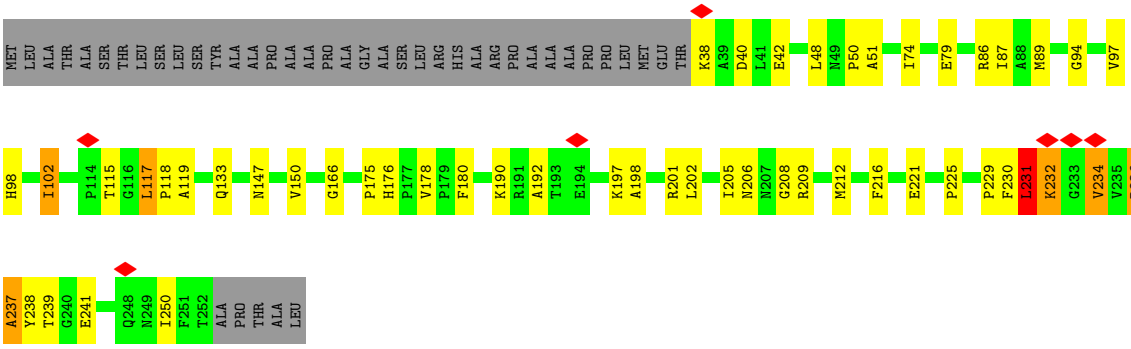




• Molecule 26: Light harvesting protein

Chain Q:

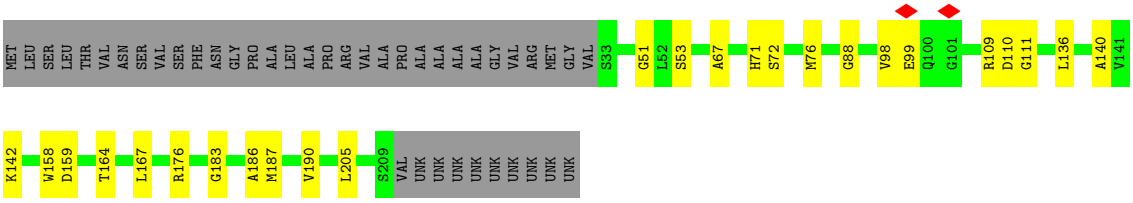




• Molecule 27: Light harvesting protein

Chain R:

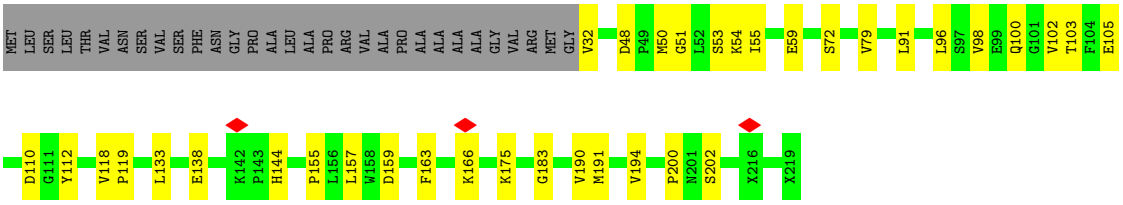




• Molecule 27: Light harvesting protein

Chain V:

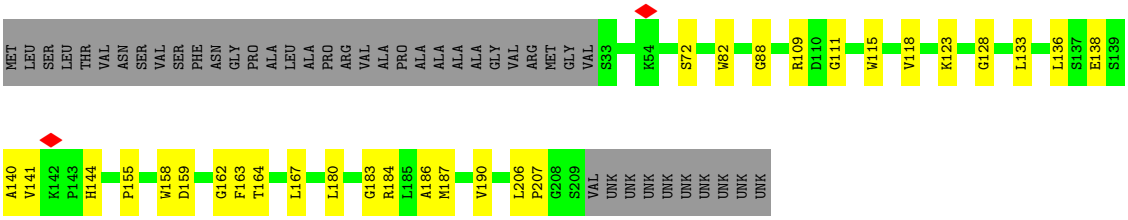




• Molecule 27: Light harvesting protein

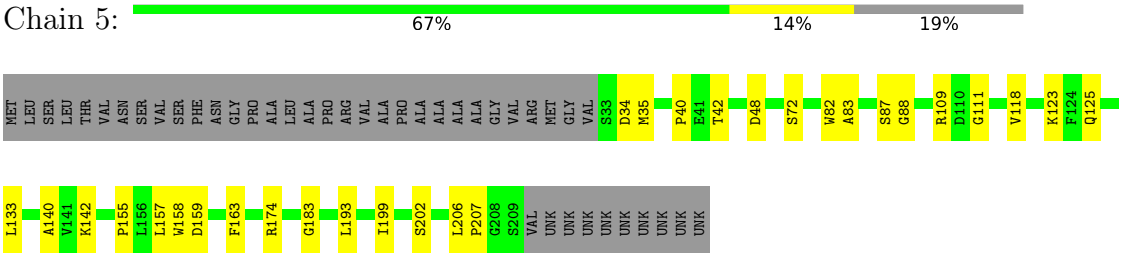
Chain X:





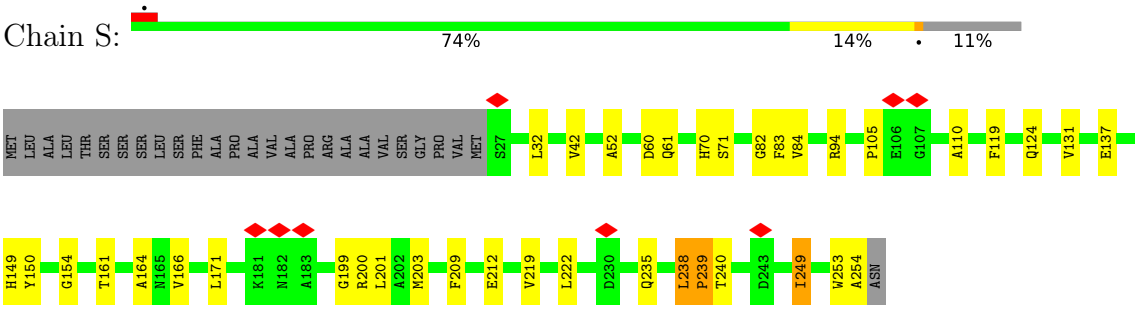
• Molecule 27: Light harvesting protein

Chain 5:



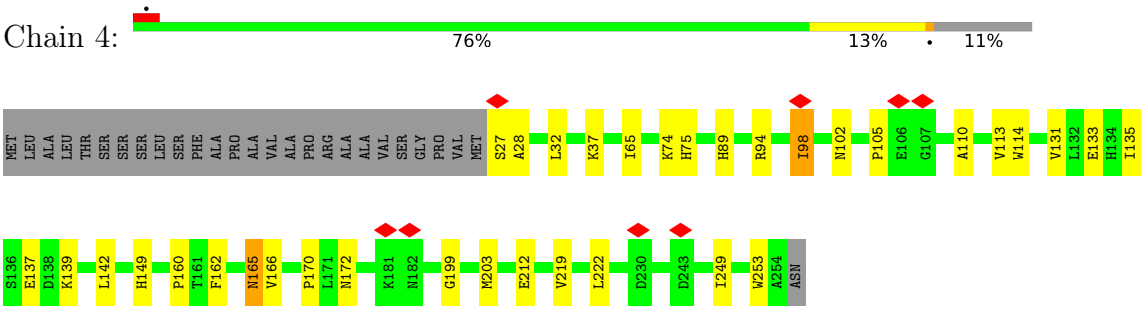
• Molecule 28: Light harvesting protein

Chain S:



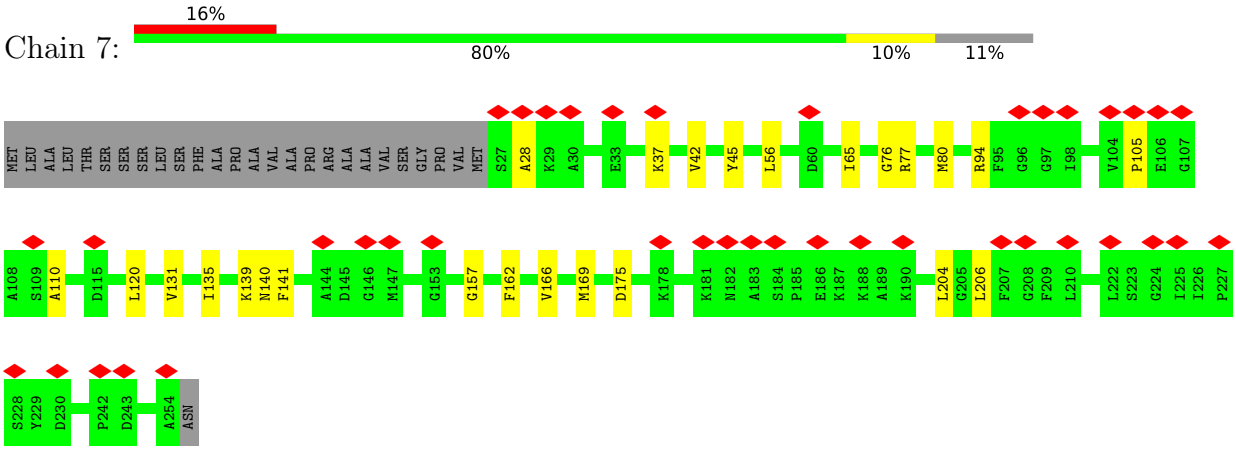
• Molecule 28: Light harvesting protein

Chain 4:



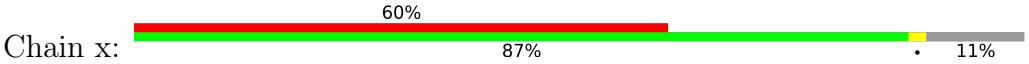
• Molecule 28: Light harvesting protein

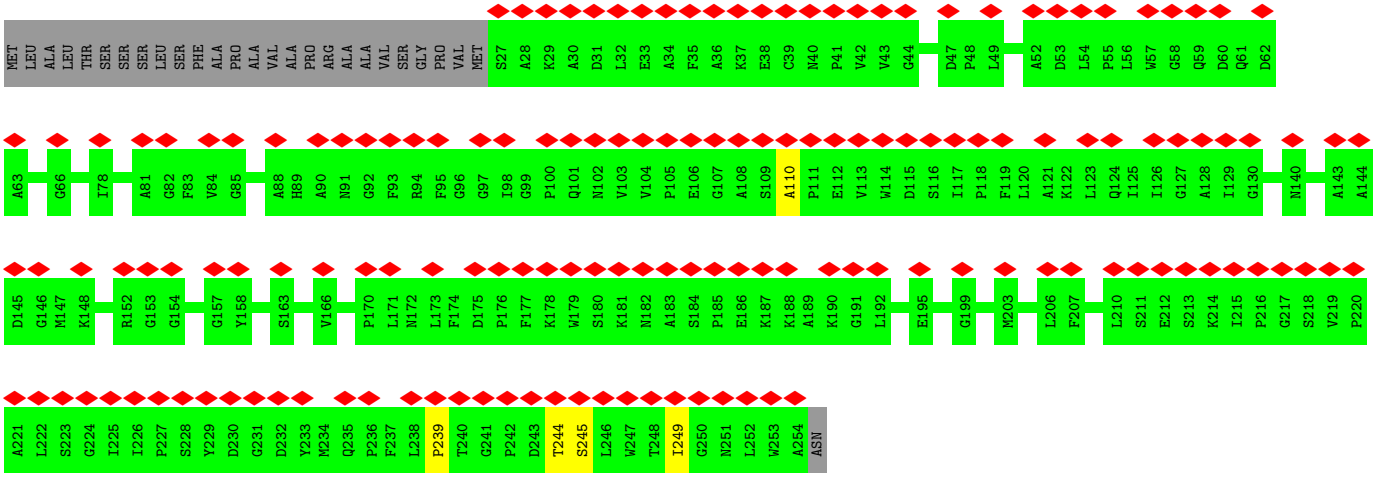
Chain 7:



• Molecule 28: Light harvesting protein

Chain x:

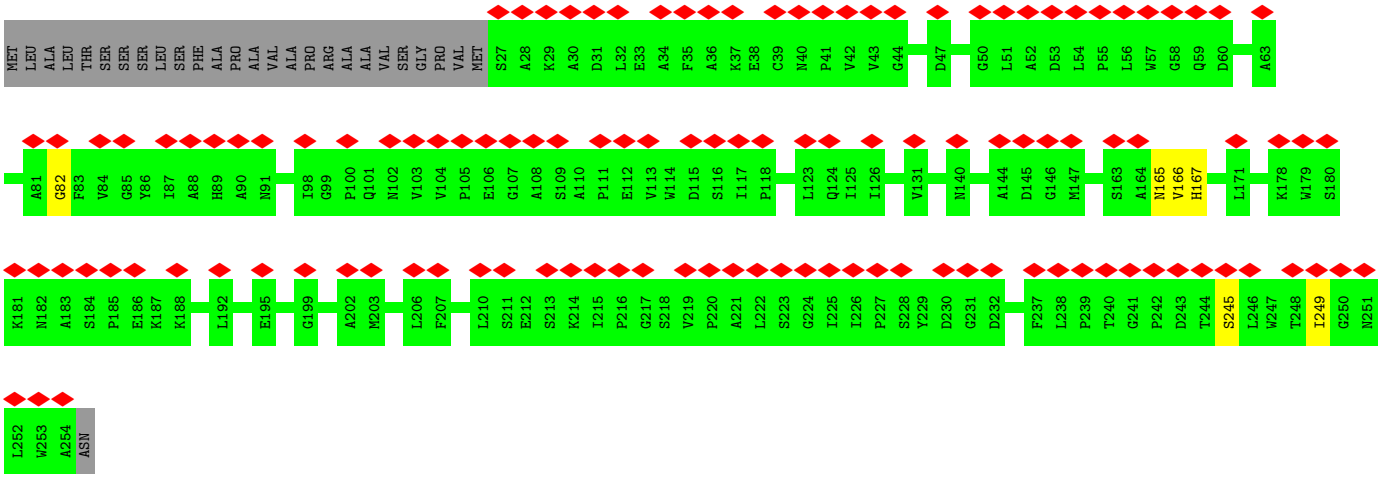




• Molecule 28: Light harvesting protein

Chain y:

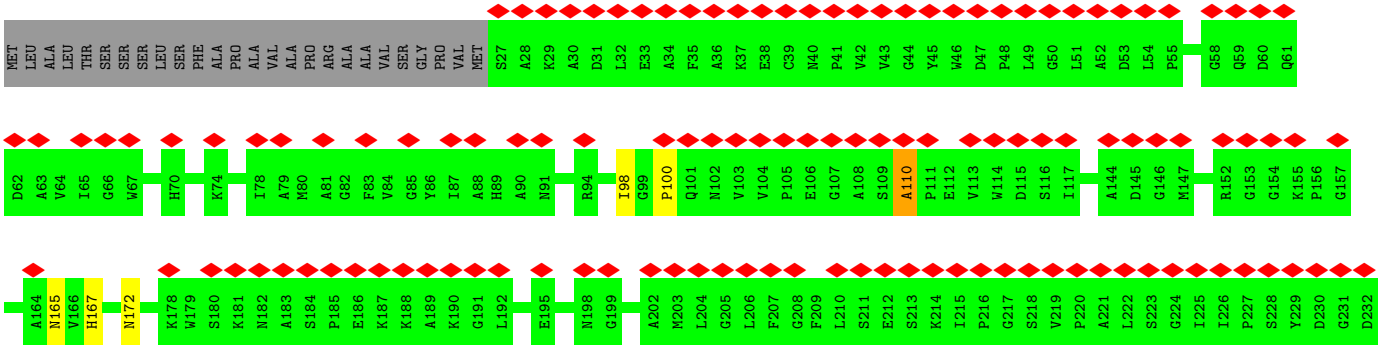


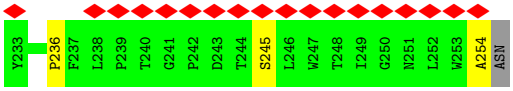


• Molecule 28: Light harvesting protein

Chain z:

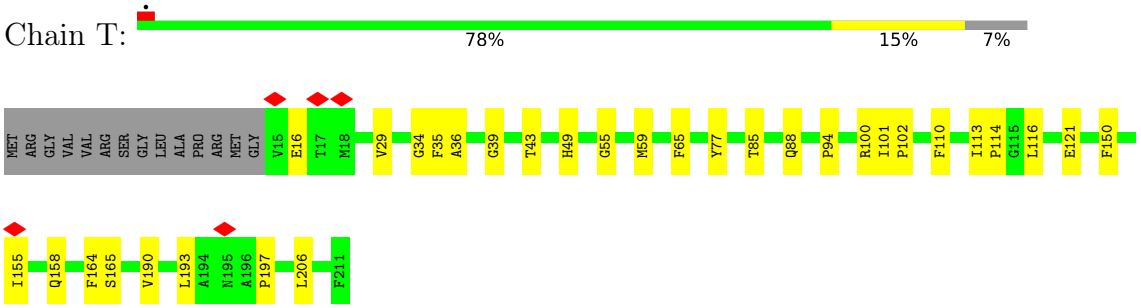






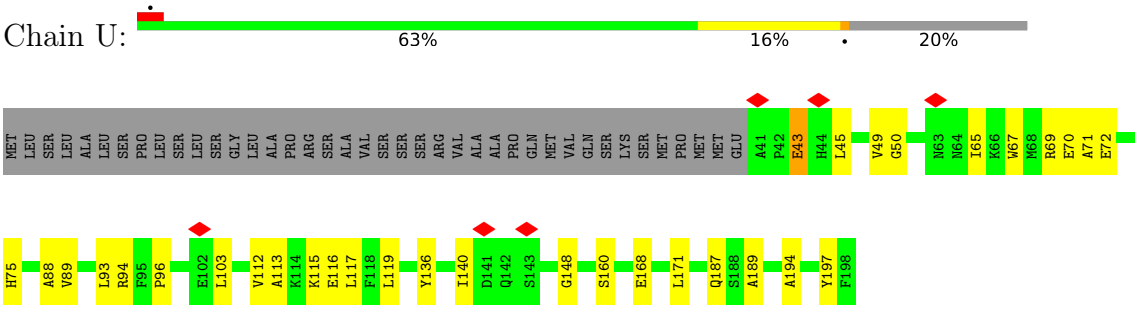
• Molecule 29: Light harvesting protein

Chain T:



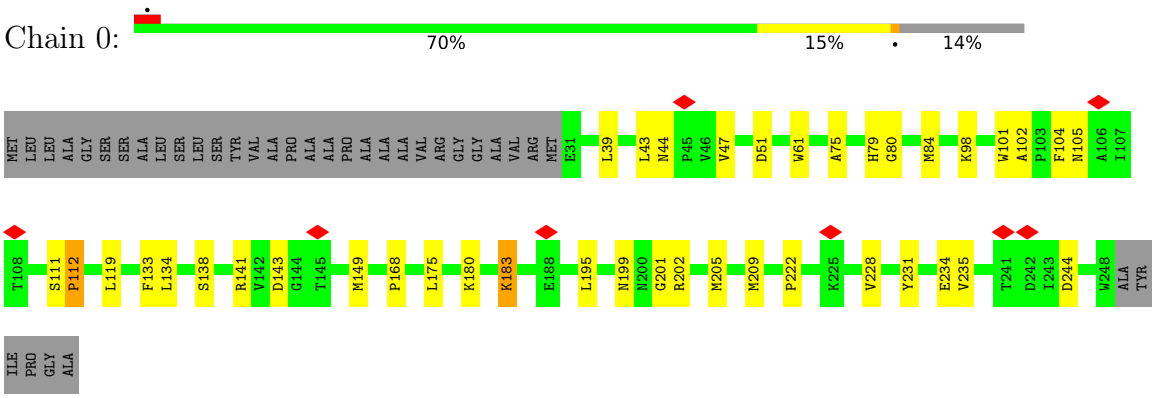
• Molecule 30: Light harvesting protein

Chain U:



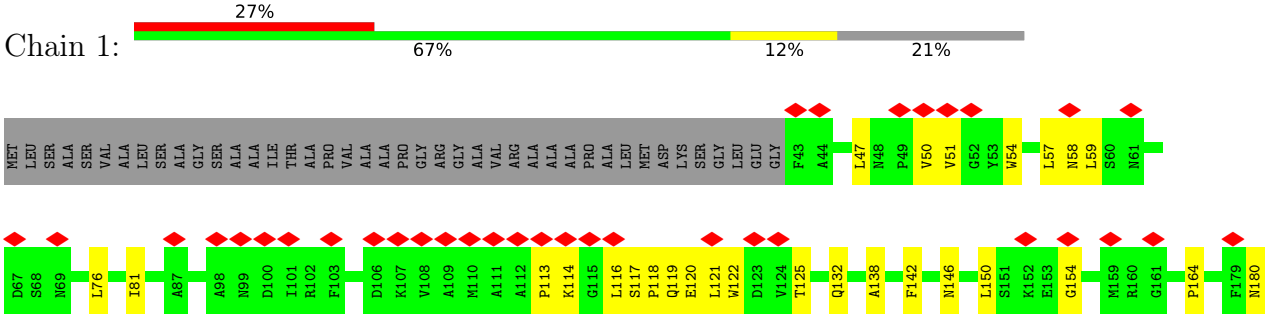
• Molecule 31: Light harvesting protein

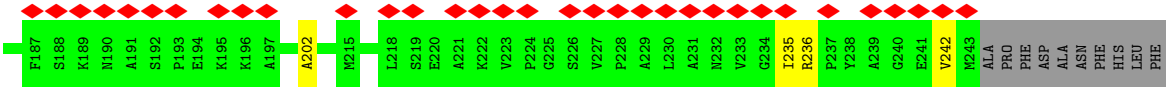
Chain 0:



• Molecule 32: Light harvesting protein

Chain 1:

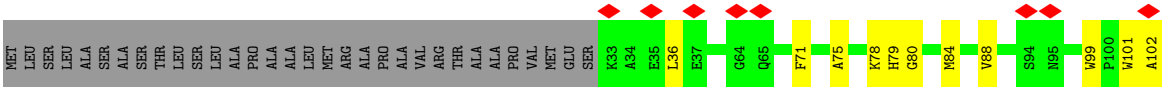


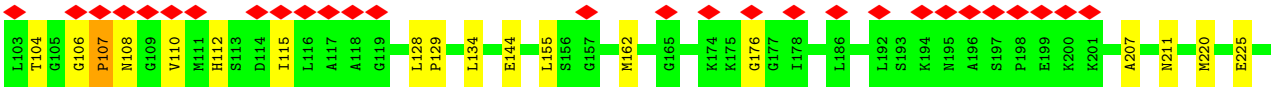


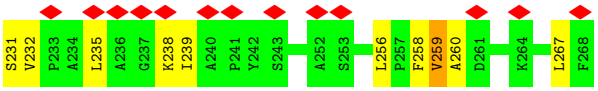
• Molecule 33: Light harvesting protein

Chain 3:





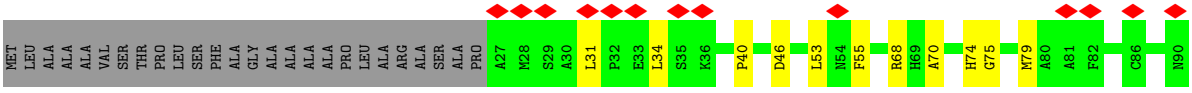


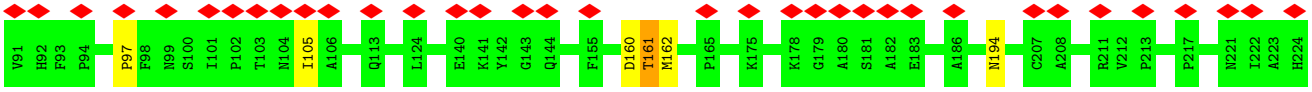


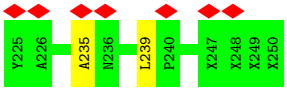
• Molecule 34: Light harvesting protein

Chain 8:



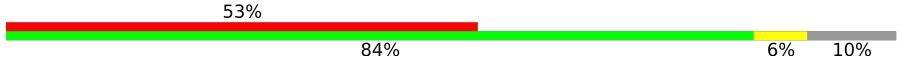


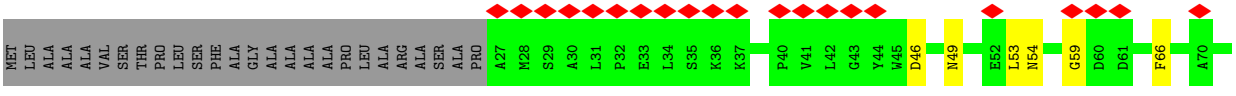


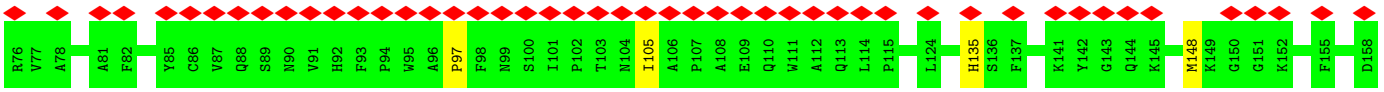


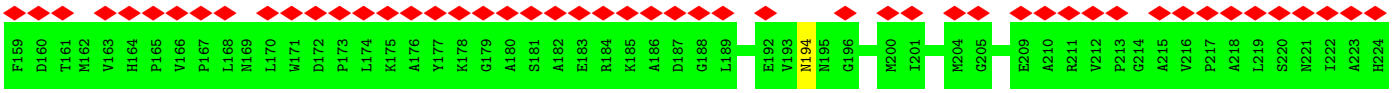
• Molecule 34: Light harvesting protein

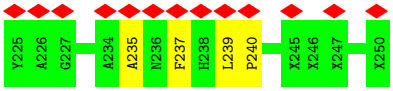
Chain 6:







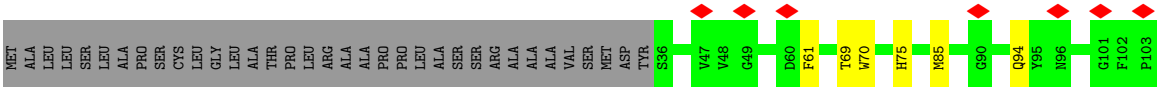


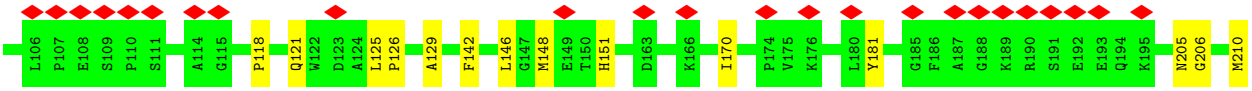


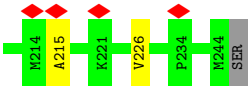
• Molecule 35: Light harvesting protein

Chain 9:





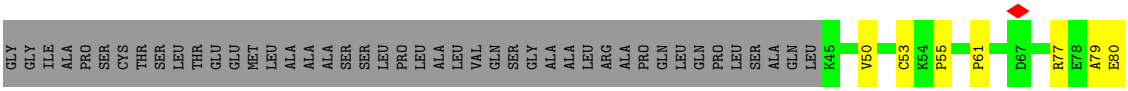


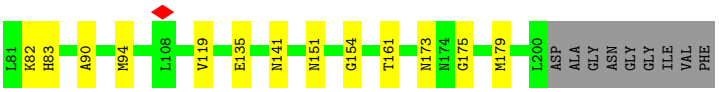


• Molecule 36: Light harvesting protein

Chain I:



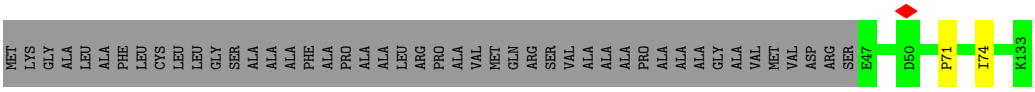




• Molecule 37: PsaR

Chain h:

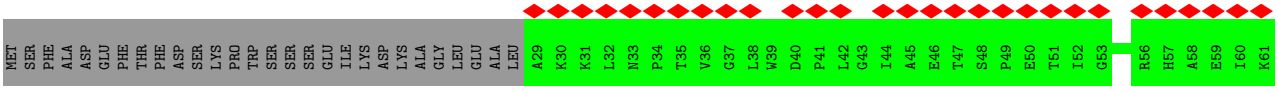


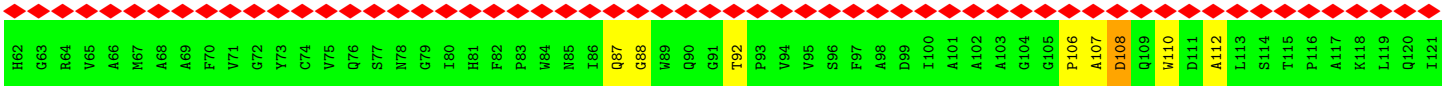


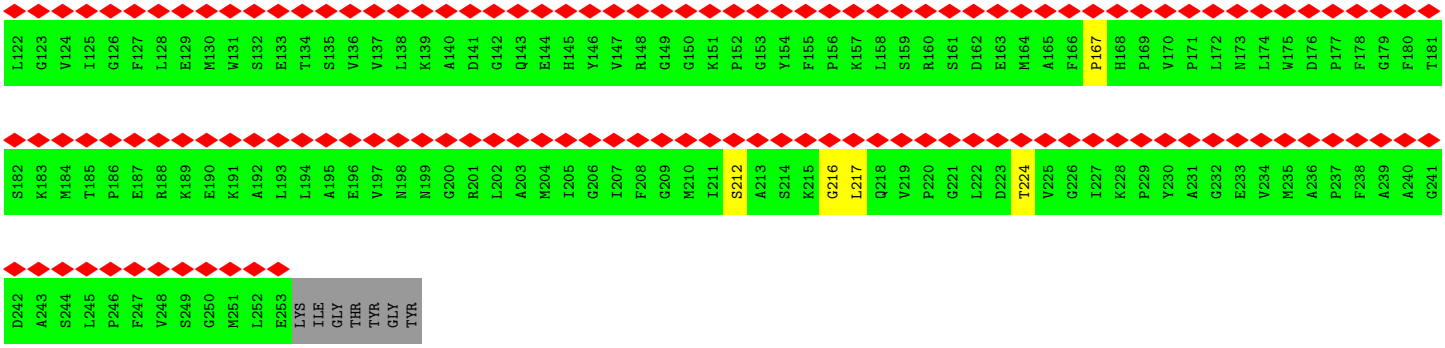
• Molecule 38: Light harvesting protein

Chain Y:





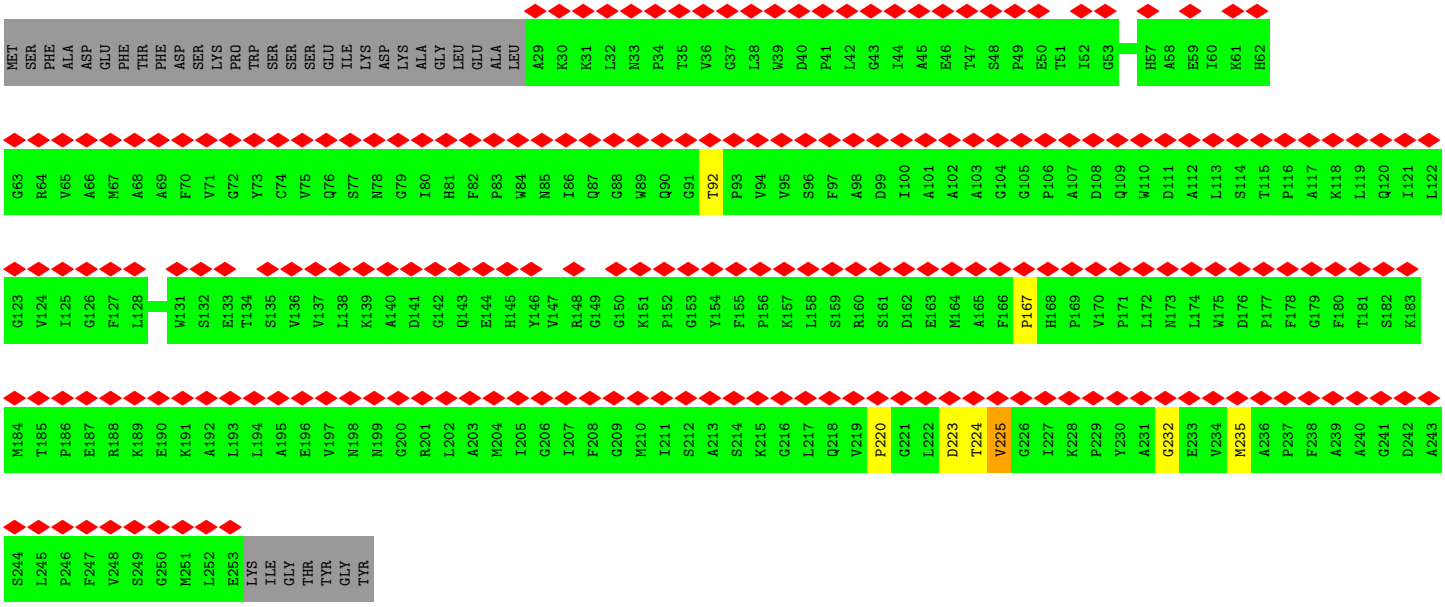




• Molecule 38: Light harvesting protein

Chain Z:

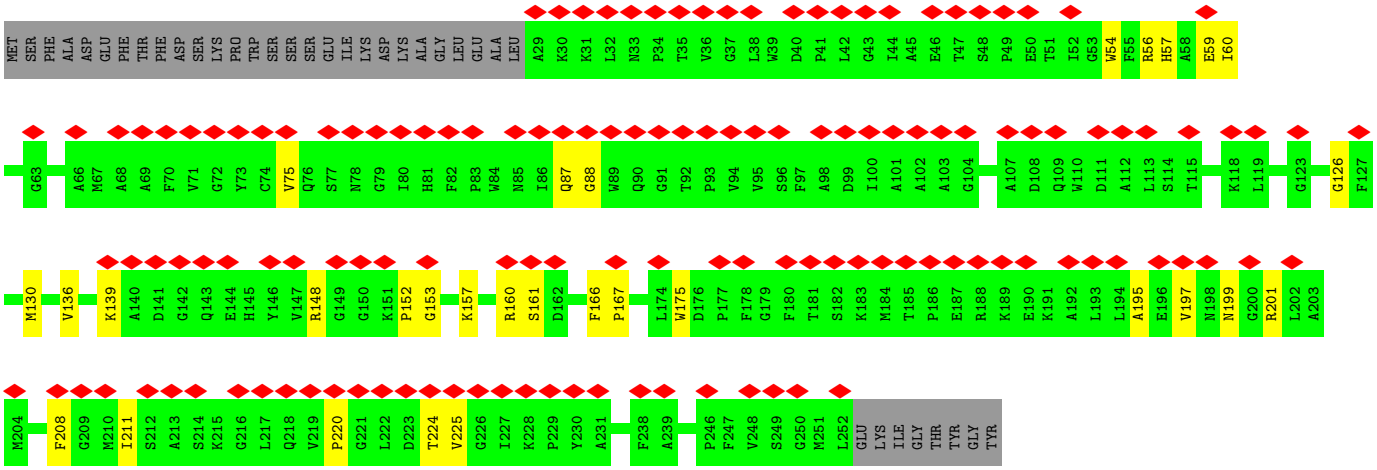




• Molecule 38: Light harvesting protein

Chain 2:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.066	Depositor
Map size (Å)	533.28, 533.28, 533.28	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.808, 0.808, 0.808	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1EB4, PQN, DGD, CLA, BCR, A86, SF4, LMG, A1EB1, KC2, A1ECV, LHG, SQD, DD6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	a	0.18	0/6028	0.40	0/8207
2	b	0.22	0/6028	0.46	1/8222 (0.0%)
3	c	0.16	0/608	0.54	0/824
4	d	0.18	0/1128	0.47	0/1525
5	e	0.24	0/503	0.45	0/683
6	f	0.18	0/1263	0.45	0/1714
7	i	0.30	0/261	0.56	0/357
8	j	0.14	0/325	0.33	0/438
9	l	0.19	0/1113	0.41	0/1513
10	m	0.21	0/226	0.62	0/306
11	k	0.19	0/545	0.43	0/737
12	o	0.21	0/371	0.59	0/503
13	A	0.18	0/1458	0.43	0/1979
14	B	0.20	0/1285	0.49	0/1750
15	C	0.21	0/1357	0.48	0/1836
16	D	0.19	0/1462	0.47	0/1988
17	E	0.22	0/1417	0.51	0/1933
18	F	0.28	0/1449	0.64	3/1967 (0.2%)
19	G	0.22	0/1386	0.55	2/1885 (0.1%)
20	H	0.25	0/1296	0.54	0/1757
21	J	0.23	0/1294	0.54	0/1749
22	K	0.24	0/1281	0.56	1/1744 (0.1%)
23	L	0.20	0/1684	0.49	0/2298
24	M	0.21	0/1491	0.42	0/2020
24	P	0.18	0/1491	0.42	0/2020
24	W	0.21	0/1491	0.45	0/2020
25	O	0.25	0/1152	0.60	0/1555
26	Q	0.26	0/1719	0.60	0/2340
27	5	0.24	0/1346	0.60	0/1830
27	R	0.22	0/1346	0.57	0/1830
27	V	0.23	0/1339	0.57	0/1820
27	X	0.23	0/1346	0.54	0/1830

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
28	4	0.21	0/1801	0.51	2/2451 (0.1%)
28	7	0.20	0/1801	0.48	0/2451
28	S	0.21	0/1801	0.49	0/2451
28	x	0.17	0/1112	0.43	0/1539
28	y	0.16	0/1112	0.38	0/1539
28	z	0.15	0/1112	0.41	0/1539
29	T	0.24	0/1534	0.55	1/2091 (0.0%)
30	U	0.21	0/1274	0.48	0/1726
31	0	0.24	0/1764	0.59	2/2410 (0.1%)
32	1	0.26	0/1284	0.56	0/1770
33	3	0.21	0/1828	0.54	3/2483 (0.1%)
34	6	0.16	0/1317	0.42	0/1813
34	8	0.20	0/1413	0.48	0/1941
35	9	0.25	0/1537	0.57	0/2106
36	I	0.23	0/1233	0.50	0/1666
37	h	0.17	0/669	0.37	0/915
38	2	0.23	0/1401	0.64	0/1911
38	Y	0.19	0/1098	0.59	1/1520 (0.1%)
38	Z	0.18	0/1098	0.58	0/1520
All	All	0.21	0/72678	0.50	16/99022 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	668	ARG	N-CA-C	10.45	123.65	111.11
22	K	36	VAL	N-CA-C	-6.07	107.94	113.71
28	4	165	ASN	CA-C-N	5.99	132.74	121.97
28	4	165	ASN	C-N-CA	5.99	132.74	121.97
33	3	231	SER	CA-C-N	5.66	132.60	122.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5835	0	5733	90	0
2	b	5818	0	5640	71	0
3	c	598	0	581	7	0
4	d	1103	0	1113	20	0
5	e	491	0	480	1	0
6	f	1232	0	1231	13	0
7	i	254	0	262	5	0
8	j	318	0	333	7	0
9	l	1084	0	1090	15	0
10	m	224	0	243	7	0
11	k	533	0	547	11	0
12	o	360	0	363	6	0
13	A	1419	0	1408	20	0
14	B	1255	0	1223	28	0
15	C	1329	0	1352	16	0
16	D	1424	0	1361	20	0
17	E	1384	0	1399	22	0
18	F	1411	0	1407	41	0
19	G	1340	0	1303	17	0
20	H	1263	0	1232	23	0
21	J	1270	0	1295	33	0
22	K	1251	0	1249	16	0
23	L	1626	0	1560	19	0
24	M	1455	0	1468	40	0
24	P	1455	0	1468	26	0
24	W	1455	0	1468	29	0
25	O	1133	0	1141	28	0
26	Q	1666	0	1649	69	0
27	5	1311	0	1326	19	0
27	R	1311	0	1326	18	0
27	V	1353	0	1332	22	0
27	X	1311	0	1326	20	0
28	4	1744	0	1703	23	0
28	7	1744	0	1703	19	0
28	S	1744	0	1703	34	0
28	x	1113	0	529	2	0
28	y	1113	0	529	3	0
28	z	1113	0	529	4	0
29	T	1482	0	1457	22	0
30	U	1240	0	1212	22	0
31	0	1706	0	1662	24	0
32	1	1255	0	932	19	0
33	3	1775	0	1765	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	6	1326	0	910	8	0
34	8	1415	0	1126	9	0
35	9	1490	0	1326	17	0
36	I	1203	0	1215	15	0
37	h	650	0	636	1	0
38	2	1383	0	1078	18	0
38	Y	1099	0	529	4	0
38	Z	1099	0	529	2	0
39	0	457	0	379	18	0
39	1	384	0	279	6	0
39	2	385	0	275	5	0
39	3	477	0	425	12	0
39	4	460	0	454	14	0
39	5	339	0	320	7	0
39	6	345	0	258	3	0
39	7	410	0	353	19	0
39	8	353	0	266	7	0
39	9	347	0	258	10	0
39	A	531	0	527	12	0
39	B	287	0	228	7	0
39	C	470	0	474	13	0
39	D	685	0	725	25	0
39	E	728	0	683	20	0
39	F	551	0	512	13	0
39	G	280	0	257	3	0
39	H	479	0	430	13	0
39	I	520	0	512	12	0
39	J	576	0	506	15	0
39	K	418	0	427	13	0
39	L	420	0	364	7	0
39	M	444	0	424	11	0
39	O	423	0	332	8	0
39	P	352	0	358	8	0
39	Q	437	0	399	13	0
39	R	339	0	320	7	0
39	S	456	0	452	18	0
39	T	406	0	330	15	0
39	U	498	0	410	8	0
39	V	357	0	357	22	0
39	W	398	0	391	13	0
39	X	339	0	320	11	0
39	Y	374	0	265	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Z	374	0	265	3	0
39	a	2327	0	2356	90	0
39	b	2553	0	2635	106	0
39	f	120	0	121	2	0
39	h	55	0	49	0	0
39	i	130	0	144	10	0
39	j	65	0	72	5	0
39	k	162	0	141	3	0
39	l	229	0	222	13	0
39	o	258	0	219	6	0
39	x	337	0	240	5	0
39	y	339	0	244	2	0
39	z	335	0	240	2	0
40	a	33	0	46	4	0
40	b	33	0	46	3	0
41	D	70	0	80	3	0
41	H	35	0	40	3	0
41	X	41	0	55	2	0
41	a	76	0	98	3	0
41	j	30	0	30	1	0
42	a	160	0	224	16	0
42	b	240	0	336	23	0
42	f	80	0	112	6	0
42	h	40	0	56	4	0
42	i	40	0	56	6	0
42	j	40	0	56	1	0
42	k	40	0	56	2	0
42	l	120	0	168	10	0
42	m	40	0	56	5	0
43	1	43	0	0	2	0
43	2	43	0	0	1	0
43	3	86	0	0	3	0
43	4	86	0	0	1	0
43	5	43	0	0	1	0
43	7	86	0	0	5	0
43	A	172	0	0	1	0
43	B	43	0	0	0	0
43	C	43	0	0	0	0
43	D	129	0	0	1	0
43	E	129	0	0	1	0
43	F	86	0	0	7	0
43	G	86	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	H	86	0	0	1	0
43	I	129	0	0	1	0
43	J	129	0	0	1	0
43	K	43	0	0	0	0
43	M	43	0	0	2	0
43	O	129	0	0	2	0
43	P	43	0	0	2	0
43	Q	86	0	0	5	0
43	R	43	0	0	0	0
43	S	43	0	0	1	0
43	T	43	0	0	0	0
43	U	43	0	0	1	0
43	V	43	0	0	0	0
43	W	43	0	0	0	0
43	X	43	0	0	0	0
43	Z	43	0	0	0	0
43	a	43	0	0	0	0
43	j	43	0	0	0	0
43	o	43	0	0	0	0
43	x	86	0	0	0	0
43	y	86	0	0	0	0
43	z	86	0	0	1	0
44	b	8	0	0	0	0
44	c	16	0	0	0	0
45	C	40	0	38	0	0
45	b	60	0	81	3	0
46	0	27	0	23	4	0
46	4	78	0	93	35	0
46	7	78	0	93	22	0
46	9	36	0	42	0	0
46	A	29	0	28	1	0
46	D	37	0	44	1	0
46	F	73	0	84	21	0
46	I	42	0	54	1	0
46	M	72	0	82	10	0
46	P	39	0	46	5	0
46	Q	28	0	25	2	0
46	S	78	0	93	23	0
46	W	72	0	82	14	0
46	l	39	0	47	4	0
47	4	39	0	42	1	0
47	7	39	0	42	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	9	36	0	36	1	0
47	D	114	0	119	6	0
47	E	35	0	34	0	0
47	F	79	0	86	1	0
47	H	38	0	40	3	0
47	M	39	0	42	3	0
47	P	38	0	40	1	0
47	S	39	0	42	4	0
47	T	36	0	35	1	0
47	W	28	0	20	1	0
47	k	38	0	40	2	0
48	0	240	0	0	1	0
48	1	192	0	0	1	0
48	2	144	0	0	1	0
48	3	192	0	0	0	0
48	4	240	0	0	0	0
48	5	48	0	0	2	0
48	6	240	0	0	0	0
48	7	192	0	0	1	0
48	8	288	0	0	0	0
48	9	240	0	0	1	0
48	B	48	0	0	0	0
48	C	48	0	0	0	0
48	D	48	0	0	1	0
48	E	48	0	0	1	0
48	F	96	0	0	9	0
48	G	96	0	0	0	0
48	H	48	0	0	0	0
48	I	48	0	0	1	0
48	J	96	0	0	0	0
48	K	48	0	0	0	0
48	L	288	0	0	4	0
48	M	144	0	0	0	0
48	O	144	0	0	0	0
48	P	96	0	0	0	0
48	Q	240	0	0	31	0
48	R	144	0	0	2	0
48	S	144	0	0	0	0
48	T	144	0	0	0	0
48	U	96	0	0	1	0
48	V	96	0	0	0	0
48	W	144	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	X	96	0	0	0	0
48	Y	48	0	0	0	0
48	Z	96	0	0	1	0
48	k	48	0	0	0	0
48	x	48	0	0	0	0
48	y	96	0	0	0	0
48	z	48	0	0	0	0
49	0	179	0	0	2	0
49	1	135	0	0	0	0
49	2	134	0	0	1	0
49	3	180	0	0	1	0
49	4	180	0	0	1	0
49	5	179	0	0	27	0
49	6	180	0	0	1	0
49	7	135	0	0	1	0
49	8	225	0	0	1	0
49	9	180	0	0	0	0
49	A	90	0	0	0	0
49	B	45	0	0	0	0
49	C	90	0	0	0	0
49	F	89	0	0	8	0
49	G	180	0	0	0	0
49	H	90	0	0	0	0
49	I	89	0	0	0	0
49	J	45	0	0	0	0
49	K	90	0	0	0	0
49	L	225	0	0	1	0
49	M	179	0	0	1	0
49	O	44	0	0	1	0
49	P	224	0	0	3	0
49	Q	134	0	0	1	0
49	R	179	0	0	16	0
49	S	135	0	0	0	0
49	T	180	0	0	2	0
49	V	270	0	0	1	0
49	W	179	0	0	3	0
49	X	224	0	0	20	0
49	Y	90	0	0	1	0
49	Z	90	0	0	0	0
49	x	135	0	0	1	0
49	y	135	0	0	0	0
49	z	134	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	0	224	0	0	4	0
50	1	112	0	0	0	0
50	2	112	0	0	1	0
50	3	280	0	0	0	0
50	4	224	0	0	1	0
50	5	56	0	0	0	0
50	6	213	0	0	0	0
50	7	224	0	0	1	0
50	8	224	0	0	0	0
50	9	56	0	0	1	0
50	C	56	0	0	0	0
50	D	56	0	0	0	0
50	E	56	0	0	0	0
50	F	56	0	0	4	0
50	G	224	0	0	0	0
50	H	112	0	0	1	0
50	J	56	0	0	0	0
50	K	168	0	0	0	0
50	L	56	0	0	0	0
50	O	56	0	0	0	0
50	Q	112	0	0	0	0
50	R	56	0	0	0	0
50	S	112	0	0	1	0
50	T	112	0	0	0	0
50	U	112	0	0	0	0
50	V	224	0	0	0	0
50	h	56	0	0	0	0
50	x	112	0	0	2	0
50	y	112	0	0	0	0
50	z	104	0	0	1	0
51	0	48	0	0	2	0
51	1	48	0	0	1	0
51	2	48	0	0	1	0
51	4	96	0	0	0	0
51	5	96	0	0	0	0
51	6	48	0	0	0	0
51	7	96	0	0	6	0
51	9	96	0	0	2	0
51	E	48	0	0	0	0
51	G	48	0	0	0	0
51	L	48	0	0	0	0
51	M	48	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	O	48	0	0	0	0
51	P	48	0	0	0	0
51	Q	96	0	0	0	0
51	R	96	0	0	0	0
51	S	96	0	0	0	0
51	T	48	0	0	1	0
51	V	48	0	0	0	0
51	W	48	0	0	0	0
51	X	96	0	0	0	0
51	Y	96	0	0	1	0
51	Z	96	0	0	0	0
51	x	96	0	0	1	0
51	y	96	0	0	1	0
51	z	96	0	0	1	0
52	5	57	0	0	1	0
52	M	115	0	0	0	0
52	P	167	0	0	5	0
52	R	57	0	0	1	0
52	T	55	0	0	0	0
52	W	113	0	0	5	0
52	X	57	0	0	0	0
All	All	114135	0	89288	1556	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1556 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:4:326:LMG:H311	49:5:313:KC2:C3A	1.15	1.56
49:X:314:KC2:C3A	46:7:301:LMG:H311	1.26	1.55
46:4:326:LMG:C31	49:5:313:KC2:C3A	2.03	1.35
46:4:326:LMG:C32	49:5:313:KC2:C4A	2.09	1.30
46:4:326:LMG:C31	49:5:313:KC2:C4A	2.12	1.27

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	739/752 (98%)	706 (96%)	33 (4%)	0	100	100
2	b	731/734 (100%)	698 (96%)	32 (4%)	1 (0%)	48	77
3	c	78/81 (96%)	74 (95%)	3 (4%)	1 (1%)	9	31
4	d	138/142 (97%)	125 (91%)	12 (9%)	1 (1%)	18	47
5	e	61/131 (47%)	58 (95%)	2 (3%)	1 (2%)	7	27
6	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
7	i	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	l	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
10	m	28/30 (93%)	27 (96%)	0	1 (4%)	2	10
11	k	71/145 (49%)	69 (97%)	1 (1%)	1 (1%)	9	30
12	o	46/123 (37%)	36 (78%)	9 (20%)	1 (2%)	5	19
13	A	181/201 (90%)	167 (92%)	13 (7%)	1 (1%)	21	51
14	B	170/177 (96%)	153 (90%)	15 (9%)	2 (1%)	10	34
15	C	174/233 (75%)	164 (94%)	9 (5%)	1 (1%)	21	51
16	D	187/231 (81%)	172 (92%)	14 (8%)	1 (0%)	24	55
17	E	185/217 (85%)	169 (91%)	16 (9%)	0	100	100
18	F	186/239 (78%)	157 (84%)	23 (12%)	6 (3%)	3	11
19	G	169/204 (83%)	148 (88%)	16 (10%)	5 (3%)	3	12
20	H	166/210 (79%)	147 (89%)	18 (11%)	1 (1%)	21	51
21	J	169/251 (67%)	150 (89%)	18 (11%)	1 (1%)	21	51
22	K	166/198 (84%)	149 (90%)	12 (7%)	5 (3%)	3	12
23	L	208/244 (85%)	182 (88%)	24 (12%)	2 (1%)	12	38
24	M	191/224 (85%)	170 (89%)	18 (9%)	3 (2%)	7	27
24	P	191/224 (85%)	175 (92%)	14 (7%)	2 (1%)	12	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
24	W	191/224 (85%)	176 (92%)	12 (6%)	3 (2%)	7 27
25	O	153/219 (70%)	135 (88%)	13 (8%)	5 (3%)	3 11
26	Q	213/257 (83%)	178 (84%)	24 (11%)	11 (5%)	1 5
27	5	175/219 (80%)	153 (87%)	22 (13%)	0	100 100
27	R	175/219 (80%)	151 (86%)	24 (14%)	0	100 100
27	V	178/219 (81%)	147 (83%)	24 (14%)	7 (4%)	2 8
27	X	175/219 (80%)	157 (90%)	18 (10%)	0	100 100
28	4	226/255 (89%)	202 (89%)	21 (9%)	3 (1%)	9 31
28	7	226/255 (89%)	201 (89%)	24 (11%)	1 (0%)	30 60
28	S	226/255 (89%)	204 (90%)	18 (8%)	4 (2%)	6 23
28	x	226/255 (89%)	203 (90%)	20 (9%)	3 (1%)	9 31
28	y	226/255 (89%)	211 (93%)	13 (6%)	2 (1%)	14 41
28	z	226/255 (89%)	203 (90%)	19 (8%)	4 (2%)	6 23
29	T	195/211 (92%)	169 (87%)	23 (12%)	3 (2%)	8 28
30	U	156/198 (79%)	138 (88%)	16 (10%)	2 (1%)	9 31
31	0	216/254 (85%)	186 (86%)	25 (12%)	5 (2%)	5 18
32	1	199/253 (79%)	163 (82%)	29 (15%)	7 (4%)	3 10
33	3	234/268 (87%)	204 (87%)	26 (11%)	4 (2%)	7 25
34	6	217/250 (87%)	182 (84%)	31 (14%)	4 (2%)	6 23
34	8	217/250 (87%)	186 (86%)	25 (12%)	6 (3%)	4 14
35	9	207/245 (84%)	173 (84%)	32 (16%)	2 (1%)	12 38
36	I	154/209 (74%)	142 (92%)	12 (8%)	0	100 100
37	h	85/133 (64%)	83 (98%)	2 (2%)	0	100 100
38	2	222/260 (85%)	186 (84%)	31 (14%)	5 (2%)	5 18
38	Y	223/260 (86%)	186 (83%)	31 (14%)	6 (3%)	4 15
38	Z	223/260 (86%)	191 (86%)	26 (12%)	6 (3%)	4 15
All	All	9768/11553 (84%)	8765 (90%)	873 (9%)	130 (1%)	12 31

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	101	PRO
13	A	200	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	C	171	ASN
18	F	135	ILE
18	F	181	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	608/616 (99%)	608 (100%)	0	100 100
2	b	591/592 (100%)	591 (100%)	0	100 100
3	c	68/69 (99%)	68 (100%)	0	100 100
4	d	120/122 (98%)	118 (98%)	2 (2%)	53 83
5	e	51/91 (56%)	51 (100%)	0	100 100
6	f	126/144 (88%)	126 (100%)	0	100 100
7	i	29/32 (91%)	29 (100%)	0	100 100
8	j	36/36 (100%)	36 (100%)	0	100 100
9	l	114/115 (99%)	114 (100%)	0	100 100
10	m	23/23 (100%)	23 (100%)	0	100 100
11	k	56/107 (52%)	56 (100%)	0	100 100
12	o	40/85 (47%)	40 (100%)	0	100 100
13	A	155/170 (91%)	155 (100%)	0	100 100
14	B	120/131 (92%)	119 (99%)	1 (1%)	73 90
15	C	140/181 (77%)	140 (100%)	0	100 100
16	D	140/171 (82%)	140 (100%)	0	100 100
17	E	146/163 (90%)	146 (100%)	0	100 100
18	F	140/180 (78%)	138 (99%)	2 (1%)	59 85
19	G	132/153 (86%)	132 (100%)	0	100 100
20	H	131/163 (80%)	131 (100%)	0	100 100
21	J	128/194 (66%)	128 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	K	127/149 (85%)	126 (99%)	1 (1%)	73 90
23	L	161/183 (88%)	160 (99%)	1 (1%)	78 92
24	M	146/165 (88%)	145 (99%)	1 (1%)	76 91
24	P	146/165 (88%)	146 (100%)	0	100 100
24	W	146/165 (88%)	144 (99%)	2 (1%)	59 85
25	O	112/160 (70%)	111 (99%)	1 (1%)	70 89
26	Q	171/199 (86%)	167 (98%)	4 (2%)	44 78
27	5	134/157 (85%)	134 (100%)	0	100 100
27	R	134/157 (85%)	134 (100%)	0	100 100
27	V	132/157 (84%)	132 (100%)	0	100 100
27	X	134/157 (85%)	134 (100%)	0	100 100
28	4	179/199 (90%)	179 (100%)	0	100 100
28	7	179/199 (90%)	179 (100%)	0	100 100
28	S	179/199 (90%)	177 (99%)	2 (1%)	65 87
29	T	150/161 (93%)	150 (100%)	0	100 100
30	U	128/162 (79%)	128 (100%)	0	100 100
31	0	177/198 (89%)	177 (100%)	0	100 100
32	1	74/194 (38%)	74 (100%)	0	100 100
33	3	181/204 (89%)	181 (100%)	0	100 100
34	6	58/183 (32%)	58 (100%)	0	100 100
34	8	91/183 (50%)	89 (98%)	2 (2%)	45 78
35	9	126/188 (67%)	126 (100%)	0	100 100
36	I	126/163 (77%)	126 (100%)	0	100 100
37	h	67/94 (71%)	67 (100%)	0	100 100
38	2	82/204 (40%)	82 (100%)	0	100 100
All	All	6434/7883 (82%)	6415 (100%)	19 (0%)	84 95

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	S	240	THR
34	8	160	ASP
34	8	161	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	W	141	LYS
25	O	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
33	3	54	ASN
34	6	195	ASN
33	3	210	ASN
28	7	140	ASN
13	A	82	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

869 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
42	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.78	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	A86	0	304	-	44,50,50	1.20	2 (4%)	51,76,76	1.94	15 (29%)
49	KC2	T	316	-	49,53,53	1.76	9 (18%)	62,89,89	2.13	16 (25%)
49	KC2	R	306	-	49,53,53	1.81	10 (20%)	62,89,89	2.08	14 (22%)
39	CLA	Y	311	-	45,49,73	1.52	6 (13%)	54,84,113	1.57	6 (11%)
48	A86	Q	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.35	19 (37%)
39	CLA	a	838	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	5 (6%)
39	CLA	W	316	24	45,49,73	1.51	8 (17%)	54,84,113	1.57	9 (16%)
48	A86	Q	308	-	44,50,50	1.15	2 (4%)	51,76,76	2.25	15 (29%)
49	KC2	8	319	34	49,53,53	1.79	10 (20%)	62,89,89	2.14	17 (27%)
39	CLA	O	311	-	46,50,73	1.56	7 (15%)	55,85,113	1.48	6 (10%)
39	CLA	P	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
46	LMG	7	326	-	32,32,55	0.93	1 (3%)	40,40,63	1.23	3 (7%)
39	CLA	a	822	-	69,73,73	1.25	7 (10%)	83,113,113	1.34	7 (8%)
39	CLA	W	313	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
39	CLA	2	310	-	46,50,73	1.51	7 (15%)	55,85,113	1.53	5 (9%)
49	KC2	V	314	-	49,53,53	1.77	9 (18%)	62,89,89	2.14	19 (30%)
39	CLA	b	817	-	63,67,73	1.31	6 (9%)	75,105,113	1.36	7 (9%)
49	KC2	3	315	-	49,53,53	1.81	10 (20%)	62,89,89	2.14	15 (24%)
39	CLA	U	207	-	64,68,73	1.30	8 (12%)	77,107,113	1.33	5 (6%)
50	A1EB1	S	302	-	51,58,58	1.30	3 (5%)	60,85,85	1.97	17 (28%)
50	A1EB1	3	310	-	51,58,58	1.27	4 (7%)	60,85,85	2.05	17 (28%)
50	A1EB1	z	302	-	51,58,58	1.28	3 (5%)	60,85,85	2.12	20 (33%)
39	CLA	y	309	-	50,54,73	1.47	7 (14%)	60,90,113	1.43	5 (8%)
39	CLA	J	317	-	46,50,73	1.53	8 (17%)	55,85,113	1.48	4 (7%)
39	CLA	A	311	-	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
46	LMG	F	320	49	34,34,55	1.14	2 (5%)	42,42,63	1.20	6 (14%)
39	CLA	S	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.49	6 (11%)
50	A1EB1	y	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	20 (33%)
50	A1EB1	2	304	-	51,58,58	1.26	4 (7%)	60,85,85	2.16	20 (33%)
50	A1EB1	0	305	-	51,58,58	1.27	3 (5%)	60,85,85	2.03	17 (28%)
43	DD6	J	306	-	39,45,45	1.99	3 (7%)	52,67,67	2.16	12 (23%)
39	CLA	V	319	-	56,60,73	1.40	8 (14%)	67,97,113	1.36	5 (7%)
48	A86	1	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.20	18 (35%)
39	CLA	K	307	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	4 (4%)
39	CLA	S	313	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	Y	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.40	5 (9%)
39	CLA	a	820	-	55,59,73	1.43	9 (16%)	66,96,113	1.35	5 (7%)
43	DD6	Q	303	-	39,45,45	2.12	3 (7%)	52,67,67	2.59	17 (32%)
39	CLA	D	318	-	69,73,73	1.26	6 (8%)	83,113,113	1.31	5 (6%)
49	KC2	7	319	-	49,53,53	1.76	10 (20%)	62,89,89	2.18	17 (27%)
50	A1EB1	Q	323	-	51,58,58	1.24	3 (5%)	60,85,85	2.08	15 (25%)
49	KC2	O	317	46	48,52,53	1.80	10 (20%)	59,87,89	2.06	13 (22%)
42	BCR	a	844	-	41,41,41	0.72	0	56,56,56	1.91	17 (30%)
43	DD6	y	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	15 (28%)
39	CLA	V	311	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	4 (4%)
39	CLA	b	851	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
39	CLA	D	309	16	53,57,73	1.43	8 (15%)	62,93,113	1.53	7 (11%)
48	A86	7	308	-	44,50,50	1.19	2 (4%)	51,76,76	2.06	16 (31%)
43	DD6	7	309	-	39,45,45	1.99	3 (7%)	52,67,67	1.87	15 (28%)
51	A1ECV	5	312	27	47,56,56	3.35	19 (40%)	32,93,93	3.13	12 (37%)
39	CLA	F	321	-	69,73,73	1.26	7 (10%)	83,113,113	1.33	8 (9%)
39	CLA	J	318	-	50,54,73	1.45	8 (16%)	60,90,113	1.48	7 (11%)
46	LMG	4	325	-	32,32,55	0.90	0	40,40,63	1.25	4 (10%)
39	CLA	6	321	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	5 (9%)
48	A86	0	308	51	44,50,50	1.27	3 (6%)	51,76,76	2.18	19 (37%)
39	CLA	2	309	-	50,54,73	1.47	9 (18%)	60,90,113	1.42	6 (10%)
39	CLA	D	315	-	69,73,73	1.25	7 (10%)	83,113,113	1.26	5 (6%)
39	CLA	a	812	-	49,53,73	1.49	8 (16%)	59,89,113	1.47	8 (13%)
49	KC2	F	307	-	49,53,53	1.77	10 (20%)	62,89,89	2.19	18 (29%)
39	CLA	K	306	-	65,69,73	1.31	9 (13%)	78,108,113	1.35	7 (8%)
39	CLA	5	307	-	64,68,73	1.32	7 (10%)	77,107,113	1.30	6 (7%)
39	CLA	z	309	-	45,49,73	1.52	7 (15%)	54,84,113	1.54	6 (11%)
39	CLA	S	310	-	46,50,73	1.51	7 (15%)	55,85,113	1.59	6 (10%)
39	CLA	6	310	-	46,50,73	1.53	7 (15%)	55,85,113	1.44	5 (9%)
39	CLA	9	315	-	45,49,73	1.53	8 (17%)	54,84,113	1.53	5 (9%)
48	A86	Q	304	-	44,50,50	1.19	3 (6%)	51,76,76	2.14	17 (33%)
48	A86	8	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.04	15 (29%)
39	CLA	1	309	-	46,50,73	1.52	9 (19%)	55,85,113	1.46	5 (9%)
49	KC2	z	315	-	49,53,53	1.76	10 (20%)	62,89,89	2.20	18 (29%)
50	A1EB1	C	302	-	51,58,58	1.24	3 (5%)	60,85,85	1.81	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	a	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
39	CLA	a	801	-	69,73,73	1.27	9 (13%)	83,113,113	1.35	7 (8%)
49	KC2	L	315	-	49,53,53	1.78	10 (20%)	62,89,89	2.18	15 (24%)
39	CLA	z	306	-	45,49,73	1.54	7 (15%)	54,84,113	1.52	5 (9%)
52	A1EB4	M	322	-	52,59,63	2.81	6 (11%)	61,85,89	2.80	22 (36%)
39	CLA	U	201	-	50,54,73	1.44	9 (18%)	60,90,113	1.49	7 (11%)
49	KC2	0	317	31	49,53,53	1.79	10 (20%)	62,89,89	2.15	18 (29%)
39	CLA	l	201	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	6 (7%)
49	KC2	x	312	-	49,53,53	1.76	10 (20%)	62,89,89	2.11	17 (27%)
48	A86	Z	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.18	19 (37%)
39	CLA	D	316	-	69,73,73	1.25	7 (10%)	83,113,113	1.26	5 (6%)
39	CLA	Q	320	-	51,55,73	1.44	7 (13%)	61,91,113	1.41	4 (6%)
39	CLA	Z	312	-	45,49,73	1.52	6 (13%)	54,84,113	1.51	5 (9%)
49	KC2	G	315	-	49,53,53	1.81	10 (20%)	62,89,89	2.19	19 (30%)
39	CLA	E	317	-	56,60,73	1.39	6 (10%)	67,97,113	1.43	6 (8%)
39	CLA	Y	305	-	45,49,73	1.53	6 (13%)	54,84,113	1.54	5 (9%)
39	CLA	3	322	-	55,59,73	1.40	8 (14%)	66,96,113	1.45	6 (9%)
39	CLA	H	307	-	49,53,73	1.50	6 (12%)	59,89,113	1.48	4 (6%)
51	A1ECV	6	320	-	47,56,56	3.37	20 (42%)	32,93,93	3.14	11 (34%)
39	CLA	Z	306	-	50,54,73	1.46	7 (14%)	60,90,113	1.46	5 (8%)
48	A86	3	305	-	44,50,50	1.19	2 (4%)	51,76,76	1.79	10 (19%)
39	CLA	0	312	31	57,61,73	1.36	9 (15%)	68,98,113	1.41	7 (10%)
51	A1ECV	5	309	27	47,56,56	3.32	19 (40%)	32,93,93	3.31	12 (37%)
39	CLA	G	312	-	56,60,73	1.39	6 (10%)	67,97,113	1.47	6 (8%)
39	CLA	M	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	4 (4%)
50	A1EB1	K	304	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	18 (30%)
48	A86	9	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.38	15 (29%)
50	A1EB1	6	304	-	48,55,58	1.32	3 (6%)	57,82,85	2.32	19 (33%)
50	A1EB1	h	203	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	19 (31%)
48	A86	4	305	-	44,50,50	1.16	2 (4%)	51,76,76	1.94	11 (21%)
52	A1EB4	R	305	-	52,59,63	2.56	4 (7%)	61,85,89	1.92	21 (34%)
48	A86	J	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.28	18 (35%)
39	CLA	L	316	-	45,49,73	1.51	7 (15%)	54,84,113	1.60	6 (11%)
49	KC2	X	315	-	49,53,53	1.77	10 (20%)	62,89,89	2.15	17 (27%)
39	CLA	l	205	-	54,58,73	1.41	8 (14%)	65,95,113	1.44	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	a	808	-	60,64,73	1.34	8 (13%)	72,102,113	1.39	4 (5%)
39	CLA	b	830	-	69,73,73	1.27	8 (11%)	83,113,113	1.40	7 (8%)
48	A86	R	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.06	16 (31%)
51	A1ECV	Y	312	-	47,56,56	3.33	19 (40%)	32,93,93	3.26	11 (34%)
47	SQD	E	320	-	34,35,54	1.17	5 (14%)	43,46,65	1.98	11 (25%)
39	CLA	W	310	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
39	CLA	F	314	18	59,63,73	1.36	6 (10%)	71,101,113	1.48	10 (14%)
39	CLA	C	306	-	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
47	SQD	D	320	39	36,37,54	1.16	5 (13%)	45,48,65	1.86	10 (22%)
39	CLA	F	312	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
39	CLA	x	311	-	49,53,73	1.49	6 (12%)	59,89,113	1.46	4 (6%)
39	CLA	a	815	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
39	CLA	O	310	-	64,68,73	1.32	9 (14%)	77,107,113	1.39	10 (12%)
50	A1EB1	E	301	-	51,58,58	1.31	4 (7%)	60,85,85	1.91	19 (31%)
39	CLA	b	818	-	59,63,73	1.35	7 (11%)	71,101,113	1.39	8 (11%)
48	A86	6	303	-	44,50,50	1.15	3 (6%)	51,76,76	2.21	15 (29%)
39	CLA	1	320	-	45,49,73	1.53	6 (13%)	54,84,113	1.56	7 (12%)
39	CLA	a	809	-	66,70,73	1.27	7 (10%)	79,109,113	1.32	5 (6%)
47	SQD	9	322	-	35,36,54	1.16	5 (14%)	44,47,65	1.65	9 (20%)
39	CLA	H	309	20	56,60,73	1.40	8 (14%)	67,97,113	1.40	6 (8%)
48	A86	Q	302	-	44,50,50	1.21	3 (6%)	51,76,76	2.27	18 (35%)
48	A86	X	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.10	18 (35%)
42	BCR	l	206	-	41,41,41	0.69	0	56,56,56	1.76	13 (23%)
39	CLA	J	314	-	69,73,73	1.27	7 (10%)	83,113,113	1.22	6 (7%)
39	CLA	F	308	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
39	CLA	A	305	13	53,57,73	1.44	8 (15%)	62,93,113	1.41	5 (8%)
40	PQN	a	839	-	34,34,34	1.60	2 (5%)	42,45,45	1.10	2 (4%)
39	CLA	H	306	-	52,56,73	1.44	8 (15%)	62,92,113	1.44	5 (8%)
50	A1EB1	7	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.22	18 (30%)
48	A86	J	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.13	18 (35%)
39	CLA	J	312	-	50,54,73	1.48	8 (16%)	60,90,113	1.47	4 (6%)
39	CLA	K	309	-	66,70,73	1.28	6 (9%)	79,109,113	1.30	5 (6%)
48	A86	V	304	-	44,50,50	1.18	3 (6%)	51,76,76	2.02	17 (33%)
39	CLA	a	825	-	66,70,73	1.27	7 (10%)	79,109,113	1.34	8 (10%)
39	CLA	0	320	-	49,53,73	1.50	6 (12%)	59,89,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	M	308	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
46	LMG	l	208	49	39,39,55	1.06	2 (5%)	47,47,63	1.23	5 (10%)
49	KC2	1	315	-	49,53,53	1.80	10 (20%)	62,89,89	2.09	15 (24%)
39	CLA	F	309	-	56,60,73	1.39	7 (12%)	67,97,113	1.40	4 (5%)
43	DD6	K	303	-	39,45,45	1.95	3 (7%)	52,67,67	1.73	11 (21%)
48	A86	V	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.45	17 (33%)
39	CLA	F	313	-	61,65,73	1.34	9 (14%)	73,103,113	1.35	6 (8%)
39	CLA	7	321	-	45,49,73	1.52	7 (15%)	54,84,113	1.59	6 (11%)
43	DD6	A	304	-	39,45,45	2.00	2 (5%)	52,67,67	1.75	13 (25%)
39	CLA	U	212	-	50,54,73	1.48	7 (14%)	60,90,113	1.42	5 (8%)
39	CLA	x	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.48	8 (14%)
39	CLA	I	311	-	69,73,73	1.24	7 (10%)	83,113,113	1.35	5 (6%)
48	A86	Z	303	-	44,50,50	1.16	3 (6%)	51,76,76	2.27	18 (35%)
49	KC2	H	311	-	49,53,53	1.78	10 (20%)	62,89,89	2.12	15 (24%)
43	DD6	O	304	-	39,45,45	2.10	4 (10%)	52,67,67	1.91	15 (28%)
48	A86	O	307	-	44,50,50	1.17	2 (4%)	51,76,76	2.35	19 (37%)
51	A1ECV	x	316	-	47,56,56	3.36	19 (40%)	32,93,93	3.12	13 (40%)
39	CLA	8	313	-	45,49,73	1.51	7 (15%)	54,84,113	1.51	6 (11%)
48	A86	T	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.33	17 (33%)
49	KC2	V	308	27	49,53,53	1.77	10 (20%)	62,89,89	2.20	18 (29%)
49	KC2	P	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.17	19 (30%)
50	A1EB1	H	304	-	51,58,58	1.22	3 (5%)	60,85,85	1.63	11 (18%)
50	A1EB1	T	302	-	51,58,58	1.27	3 (5%)	60,85,85	2.04	12 (20%)
39	CLA	L	308	-	65,69,73	1.31	7 (10%)	78,108,113	1.37	6 (7%)
39	CLA	k	201	-	56,60,73	1.37	9 (16%)	67,97,113	1.39	5 (7%)
43	DD6	Z	302	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
50	A1EB1	V	307	-	51,58,58	1.26	4 (7%)	60,85,85	2.09	21 (35%)
42	BCR	m	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.34	7 (12%)
39	CLA	6	313	-	46,50,73	1.50	6 (13%)	55,85,113	1.48	4 (7%)
49	KC2	5	311	-	49,53,53	1.78	10 (20%)	62,89,89	2.25	19 (30%)
50	A1EB1	T	307	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	19 (31%)
43	DD6	G	306	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
39	CLA	O	309	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)
39	CLA	R	308	-	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
50	A1EB1	y	301	-	51,58,58	1.23	4 (7%)	60,85,85	2.16	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	LMG	A	316	-	29,29,55	1.00	0	37,37,63	1.23	4 (10%)
51	A1ECV	Z	308	-	47,56,56	3.34	20 (42%)	32,93,93	3.27	13 (40%)
39	CLA	S	320	-	69,73,73	1.28	9 (13%)	83,113,113	1.29	6 (7%)
39	CLA	b	819	-	63,67,73	1.32	8 (12%)	75,105,113	1.36	5 (6%)
39	CLA	7	318	28	50,54,73	1.44	8 (16%)	60,90,113	1.38	4 (6%)
39	CLA	9	309	-	45,49,73	1.51	8 (17%)	54,84,113	1.58	5 (9%)
49	KC2	4	318	28	49,53,53	1.79	10 (20%)	62,89,89	2.14	16 (25%)
39	CLA	b	828	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
39	CLA	b	834	-	62,66,73	1.33	7 (11%)	74,104,113	1.37	6 (8%)
39	CLA	D	310	47	65,69,73	1.31	8 (12%)	78,108,113	1.33	7 (8%)
49	KC2	0	314	46,31	48,52,53	1.72	9 (18%)	59,87,89	2.23	17 (28%)
51	A1ECV	y	311	-	47,56,56	3.30	20 (42%)	32,93,93	3.33	12 (37%)
49	KC2	M	314	-	49,53,53	1.78	9 (18%)	62,89,89	2.11	19 (30%)
48	A86	9	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.01	14 (27%)
48	A86	9	305	-	44,50,50	1.19	3 (6%)	51,76,76	1.91	17 (33%)
39	CLA	E	314	-	60,64,73	1.35	9 (15%)	72,102,113	1.36	4 (5%)
39	CLA	6	315	-	45,49,73	1.52	8 (17%)	54,84,113	1.57	7 (12%)
39	CLA	7	314	-	60,64,73	1.36	7 (11%)	72,102,113	1.47	10 (13%)
39	CLA	F	310	-	58,62,73	1.37	6 (10%)	69,99,113	1.39	6 (8%)
39	CLA	X	311	27	54,58,73	1.41	6 (11%)	65,95,113	1.42	7 (10%)
39	CLA	G	318	-	53,57,73	1.43	8 (15%)	62,93,113	1.36	5 (8%)
50	A1EB1	0	302	-	51,58,58	1.22	3 (5%)	60,85,85	2.11	19 (31%)
49	KC2	9	311	-	49,53,53	1.79	10 (20%)	62,89,89	2.10	15 (24%)
48	A86	7	312	-	44,50,50	1.21	2 (4%)	51,76,76	2.29	18 (35%)
43	DD6	A	302	-	39,45,45	1.97	3 (7%)	52,67,67	1.84	11 (21%)
39	CLA	b	824	-	64,68,73	1.30	8 (12%)	77,107,113	1.33	4 (5%)
39	CLA	L	310	23	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
39	CLA	X	316	-	51,55,73	1.45	8 (15%)	61,91,113	1.48	6 (9%)
49	KC2	7	322	-	49,53,53	1.78	10 (20%)	62,89,89	2.11	17 (27%)
47	SQD	F	318	-	41,42,54	1.07	5 (12%)	50,53,65	1.70	10 (20%)
39	CLA	5	308	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
43	DD6	A	303	-	39,45,45	2.03	3 (7%)	52,67,67	2.88	20 (38%)
49	KC2	z	313	-	46,50,53	1.98	11 (23%)	49,80,89	2.25	12 (24%)
42	BCR	a	845	-	41,41,41	0.75	0	56,56,56	2.14	15 (26%)
43	DD6	4	308	-	39,45,45	2.06	3 (7%)	52,67,67	2.04	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	KC2	T	315	29	49,53,53	1.76	10 (20%)	62,89,89	2.10	19 (30%)
50	A1EB1	G	308	-	51,58,58	1.22	3 (5%)	60,85,85	2.28	16 (26%)
48	A86	1	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.29	18 (35%)
49	KC2	C	312	-	49,53,53	1.76	10 (20%)	62,89,89	2.14	17 (27%)
46	LMG	S	322	49	46,46,55	0.95	2 (4%)	54,54,63	1.32	5 (9%)
39	CLA	V	309	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
51	A1ECV	G	316	-	47,56,56	3.30	19 (40%)	32,93,93	3.24	12 (37%)
48	A86	M	306	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	17 (33%)
49	KC2	S	314	-	49,53,53	1.78	9 (18%)	62,89,89	2.11	17 (27%)
39	CLA	U	214	-	50,54,73	1.47	7 (14%)	60,90,113	1.42	4 (6%)
43	DD6	U	204	-	39,45,45	2.04	4 (10%)	52,67,67	1.72	12 (23%)
48	A86	9	304	-	44,50,50	1.16	3 (6%)	51,76,76	2.06	16 (31%)
39	CLA	b	839	-	51,55,73	1.45	8 (15%)	61,91,113	1.37	6 (9%)
39	CLA	U	211	-	64,68,73	1.31	7 (10%)	77,107,113	1.36	8 (10%)
42	BCR	b	846	-	41,41,41	0.74	0	56,56,56	2.13	16 (28%)
39	CLA	0	311	-	59,63,73	1.38	9 (15%)	71,101,113	1.39	10 (14%)
39	CLA	a	818	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
52	A1EB4	5	304	-	52,59,63	2.56	4 (7%)	61,85,89	1.93	19 (31%)
39	CLA	U	215	-	45,49,73	1.55	7 (15%)	54,84,113	1.56	6 (11%)
39	CLA	b	832	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
52	A1EB4	P	305	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)
39	CLA	a	803	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
43	DD6	P	304	-	39,45,45	2.10	3 (7%)	52,67,67	2.77	14 (26%)
48	A86	R	302	-	44,50,50	1.15	2 (4%)	51,76,76	2.19	13 (25%)
39	CLA	L	313	-	54,58,73	1.40	8 (14%)	65,95,113	1.40	4 (6%)
51	A1ECV	9	317	-	47,56,56	3.32	20 (42%)	32,93,93	3.25	12 (37%)
39	CLA	Z	304	-	45,49,73	1.53	8 (17%)	54,84,113	1.56	5 (9%)
39	CLA	S	308	-	65,69,73	1.30	7 (10%)	78,108,113	1.32	6 (7%)
43	DD6	G	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.82	11 (21%)
43	DD6	x	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.89	16 (30%)
48	A86	U	202	-	44,50,50	1.17	3 (6%)	51,76,76	2.30	20 (39%)
39	CLA	a	807	1	69,73,73	1.27	9 (13%)	83,113,113	1.29	5 (6%)
39	CLA	2	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.58	5 (9%)
49	KC2	A	310	13	49,53,53	1.81	9 (18%)	62,89,89	2.04	12 (19%)
49	KC2	Q	313	46	48,52,53	1.81	11 (22%)	59,87,89	2.24	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	o	203	12	59,63,73	1.35	7 (11%)	71,101,113	1.38	5 (7%)
48	A86	W	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.29	18 (35%)
51	A1ECV	E	311	-	47,56,56	3.42	20 (42%)	32,93,93	3.59	12 (37%)
49	KC2	4	324	-	49,53,53	1.78	10 (20%)	62,89,89	2.23	17 (27%)
46	LMG	4	326	49	46,46,55	0.96	2 (4%)	54,54,63	1.28	6 (11%)
48	A86	8	323	-	44,50,50	1.19	3 (6%)	51,76,76	2.21	16 (31%)
42	BCR	f	804	-	41,41,41	0.68	0	56,56,56	1.98	14 (25%)
39	CLA	a	805	-	69,73,73	1.24	8 (11%)	83,113,113	1.34	9 (10%)
49	KC2	1	314	-	49,53,53	1.78	10 (20%)	62,89,89	2.09	16 (25%)
49	KC2	z	312	-	49,53,53	1.78	10 (20%)	62,89,89	2.04	15 (24%)
39	CLA	1	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.54	5 (9%)
39	CLA	B	205	-	46,50,73	1.52	6 (13%)	55,85,113	1.51	6 (10%)
51	A1ECV	W	317	-	47,56,56	3.34	19 (40%)	32,93,93	3.00	10 (31%)
39	CLA	Y	302	-	45,49,73	1.53	7 (15%)	54,84,113	1.56	5 (9%)
39	CLA	x	309	-	45,49,73	1.53	8 (17%)	54,84,113	1.55	6 (11%)
48	A86	8	309	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	19 (37%)
50	A1EB1	V	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.09	17 (28%)
49	KC2	W	308	-	49,53,53	1.77	10 (20%)	62,89,89	2.21	17 (27%)
39	CLA	b	808	-	49,53,73	1.48	7 (14%)	59,89,113	1.51	6 (10%)
43	DD6	o	204	-	39,45,45	1.99	2 (5%)	52,67,67	1.88	12 (23%)
39	CLA	X	307	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	6 (7%)
45	DGD	C	314	-	41,41,67	1.10	2 (4%)	55,55,81	1.38	6 (10%)
39	CLA	4	322	-	56,60,73	1.40	9 (16%)	67,97,113	1.44	7 (10%)
39	CLA	a	824	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
48	A86	4	328	-	44,50,50	1.14	2 (4%)	51,76,76	2.28	15 (29%)
49	KC2	R	314	46	48,52,53	1.74	9 (18%)	59,87,89	2.20	16 (27%)
48	A86	0	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.25	17 (33%)
48	A86	H	302	-	44,50,50	1.15	3 (6%)	51,76,76	2.29	17 (33%)
39	CLA	b	801	-	69,73,73	1.23	10 (14%)	83,113,113	1.33	8 (9%)
39	CLA	1	311	-	45,49,73	1.53	7 (15%)	54,84,113	1.47	5 (9%)
39	CLA	K	311	-	69,73,73	1.24	6 (8%)	83,113,113	1.27	5 (6%)
39	CLA	Z	316	-	45,49,73	1.52	6 (13%)	54,84,113	1.61	6 (11%)
39	CLA	B	203	-	50,54,73	1.45	7 (14%)	60,90,113	1.44	5 (8%)
48	A86	G	301	-	44,50,50	1.18	2 (4%)	51,76,76	2.46	19 (37%)
39	CLA	T	319	29	50,54,73	1.47	7 (14%)	60,90,113	1.48	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	B	204	-	50,54,73	1.47	8 (16%)	60,90,113	1.45	6 (10%)
39	CLA	D	313	-	69,73,73	1.24	7 (10%)	83,113,113	1.29	8 (9%)
48	A86	1	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.05	13 (25%)
42	BCR	l	207	-	41,41,41	0.69	0	56,56,56	1.81	11 (19%)
43	DD6	1	304	-	39,45,45	2.22	3 (7%)	52,67,67	3.19	18 (34%)
48	A86	L	302	-	44,50,50	1.13	3 (6%)	51,76,76	2.99	22 (43%)
39	CLA	a	847	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	5 (6%)
39	CLA	O	314	-	59,63,73	1.37	8 (13%)	71,101,113	1.35	6 (8%)
39	CLA	a	836	-	69,73,73	1.24	7 (10%)	83,113,113	1.32	4 (4%)
48	A86	M	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.16	19 (37%)
48	A86	3	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.40	20 (39%)
39	CLA	W	319	-	50,54,73	1.47	6 (12%)	60,90,113	1.44	4 (6%)
39	CLA	x	318	-	45,49,73	1.54	8 (17%)	54,84,113	1.57	8 (14%)
50	A1EB1	6	301	-	51,58,58	1.28	3 (5%)	60,85,85	2.00	16 (26%)
48	A86	L	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.32	18 (35%)
48	A86	7	311	-	44,50,50	1.19	3 (6%)	51,76,76	2.16	16 (31%)
39	CLA	G	310	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	6 (7%)
51	A1ECV	L	318	-	47,56,56	3.35	20 (42%)	32,93,93	3.16	12 (37%)
39	CLA	C	308	-	64,68,73	1.30	8 (12%)	77,107,113	1.35	6 (7%)
49	KC2	1	312	-	49,53,53	1.83	11 (22%)	62,89,89	2.02	15 (24%)
51	A1ECV	y	317	-	47,56,56	3.38	20 (42%)	32,93,93	3.14	13 (40%)
50	A1EB1	G	304	-	51,58,58	1.31	4 (7%)	60,85,85	2.04	20 (33%)
39	CLA	I	314	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
39	CLA	A	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	8 (9%)
49	KC2	H	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.13	18 (29%)
49	KC2	I	312	46	48,52,53	1.73	9 (18%)	59,87,89	2.31	19 (32%)
49	KC2	S	317	-	49,53,53	1.75	10 (20%)	62,89,89	2.17	17 (27%)
42	BCR	h	202	-	41,41,41	0.74	0	56,56,56	1.87	17 (30%)
49	KC2	W	314	-	49,53,53	1.76	9 (18%)	62,89,89	2.14	17 (27%)
49	KC2	9	316	35	49,53,53	1.79	10 (20%)	62,89,89	2.11	16 (25%)
39	CLA	1	310	-	49,53,73	1.50	7 (14%)	59,89,113	1.48	4 (6%)
39	CLA	9	310	-	45,49,73	1.51	8 (17%)	54,84,113	1.57	8 (14%)
51	A1ECV	M	316	-	47,56,56	3.32	19 (40%)	32,93,93	3.06	12 (37%)
49	KC2	P	310	46	48,52,53	1.72	9 (18%)	59,87,89	2.21	18 (30%)
39	CLA	a	806	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	BCR	j	103	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
49	KC2	W	312	46,24	48,52,53	1.72	9 (18%)	59,87,89	2.21	18 (30%)
39	CLA	b	822	2	54,58,73	1.42	8 (14%)	65,95,113	1.42	5 (7%)
39	CLA	o	206	-	62,66,73	1.32	6 (9%)	74,104,113	1.36	5 (6%)
39	CLA	y	312	-	46,50,73	1.52	7 (15%)	55,85,113	1.46	4 (7%)
49	KC2	5	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.16	18 (29%)
39	CLA	E	319	17	53,57,73	1.43	7 (13%)	62,93,113	1.40	5 (8%)
48	A86	B	201	-	44,50,50	1.19	3 (6%)	51,76,76	2.49	19 (37%)
39	CLA	J	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
48	A86	k	206	-	44,50,50	1.18	3 (6%)	51,76,76	2.00	13 (25%)
47	SQD	k	205	-	37,38,54	1.13	5 (13%)	46,49,65	1.66	9 (19%)
39	CLA	b	809	-	69,73,73	1.24	6 (8%)	83,113,113	1.28	7 (8%)
46	LMG	W	320	-	33,33,55	0.94	1 (3%)	41,41,63	1.21	4 (9%)
49	KC2	P	313	24	49,53,53	1.82	11 (22%)	62,89,89	2.21	19 (30%)
48	A86	0	301	-	44,50,50	1.26	3 (6%)	51,76,76	2.19	19 (37%)
48	A86	6	309	-	44,50,50	1.18	2 (4%)	51,76,76	2.22	17 (33%)
51	A1ECV	S	318	-	47,56,56	3.38	20 (42%)	32,93,93	3.02	11 (34%)
39	CLA	S	311	-	69,73,73	1.26	8 (11%)	83,113,113	1.26	5 (6%)
39	CLA	T	318	-	51,55,73	1.44	7 (13%)	61,91,113	1.47	5 (8%)
39	CLA	U	208	-	50,54,73	1.47	9 (18%)	60,90,113	1.39	5 (8%)
50	A1EB1	5	302	-	51,58,58	1.26	3 (5%)	60,85,85	2.12	16 (26%)
39	CLA	M	321	24	50,54,73	1.46	7 (14%)	60,90,113	1.47	5 (8%)
39	CLA	Z	307	-	45,49,73	1.52	8 (17%)	54,84,113	1.54	6 (11%)
49	KC2	Q	315	-	49,53,53	1.75	10 (20%)	62,89,89	2.13	18 (29%)
39	CLA	b	826	-	69,73,73	1.28	10 (14%)	83,113,113	1.26	7 (8%)
49	KC2	A	313	-	49,53,53	1.79	10 (20%)	62,89,89	2.14	19 (30%)
39	CLA	b	825	-	69,73,73	1.27	9 (13%)	83,113,113	1.34	8 (9%)
46	LMG	7	301	49	46,46,55	0.95	2 (4%)	54,54,63	1.28	6 (11%)
49	KC2	y	313	-	49,53,53	1.76	10 (20%)	62,89,89	2.13	17 (27%)
42	BCR	f	801	-	41,41,41	0.68	0	56,56,56	1.92	14 (25%)
43	DD6	4	307	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	15 (28%)
50	A1EB1	G	307	-	51,58,58	1.29	4 (7%)	60,85,85	1.87	17 (28%)
39	CLA	0	310	-	65,69,73	1.32	8 (12%)	78,108,113	1.33	7 (8%)
50	A1EB1	0	307	-	51,58,58	1.25	3 (5%)	60,85,85	2.24	17 (28%)
39	CLA	M	310	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	b	840	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
39	CLA	0	322	-	55,59,73	1.42	10 (18%)	66,96,113	1.44	5 (7%)
49	KC2	G	311	19	49,53,53	1.78	10 (20%)	62,89,89	2.17	16 (25%)
49	KC2	8	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.12	17 (27%)
39	CLA	C	305	-	65,69,73	1.30	6 (9%)	78,108,113	1.29	5 (6%)
50	A1EB1	R	303	-	51,58,58	1.31	5 (9%)	60,85,85	2.18	19 (31%)
48	A86	T	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.22	19 (37%)
39	CLA	E	312	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	6 (7%)
43	DD6	A	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.88	12 (23%)
39	CLA	l	204	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	8 (9%)
39	CLA	F	306	-	50,54,73	1.46	7 (14%)	60,90,113	1.43	5 (8%)
39	CLA	X	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
39	CLA	S	319	-	56,60,73	1.39	9 (16%)	67,97,113	1.53	9 (13%)
42	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
39	CLA	a	817	1	49,53,73	1.50	9 (18%)	59,89,113	1.49	4 (6%)
39	CLA	J	313	-	50,54,73	1.47	7 (14%)	60,90,113	1.44	4 (6%)
39	CLA	8	312	-	49,53,73	1.49	7 (14%)	59,89,113	1.49	4 (6%)
39	CLA	Z	305	-	45,49,73	1.54	7 (15%)	54,84,113	1.53	6 (11%)
43	DD6	W	305	-	39,45,45	1.91	3 (7%)	52,67,67	1.78	12 (23%)
49	KC2	P	312	-	49,53,53	1.79	10 (20%)	62,89,89	2.17	16 (25%)
39	CLA	V	316	-	54,58,73	1.42	7 (12%)	65,95,113	1.44	9 (13%)
48	A86	2	301	-	44,50,50	1.18	3 (6%)	51,76,76	2.31	17 (33%)
39	CLA	2	312	-	45,49,73	1.51	9 (20%)	54,84,113	1.56	6 (11%)
41	LHG	D	301	-	34,34,48	0.72	0	37,40,54	1.25	3 (8%)
50	A1EB1	x	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	14 (23%)
49	KC2	G	313	-	49,53,53	1.79	10 (20%)	62,89,89	2.23	20 (32%)
49	KC2	L	312	-	49,53,53	1.81	10 (20%)	62,89,89	1.99	14 (22%)
39	CLA	A	308	-	55,59,73	1.42	8 (14%)	66,96,113	1.33	5 (7%)
39	CLA	V	313	27	69,73,73	1.23	9 (13%)	83,113,113	1.27	4 (4%)
43	DD6	5	303	-	39,45,45	1.90	3 (7%)	52,67,67	1.73	12 (23%)
39	CLA	H	315	-	45,49,73	1.51	8 (17%)	54,84,113	1.50	6 (11%)
39	CLA	Y	314	-	45,49,73	1.53	6 (13%)	54,84,113	1.61	6 (11%)
39	CLA	y	308	-	49,53,73	1.49	8 (16%)	59,89,113	1.51	7 (11%)
48	A86	R	317	-	44,50,50	1.17	2 (4%)	51,76,76	2.06	12 (23%)
47	SQD	7	302	-	38,39,54	1.13	5 (13%)	47,50,65	1.69	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	o	202	-	46,50,73	1.51	7 (15%)	55,85,113	1.52	6 (10%)
39	CLA	9	307	-	45,49,73	1.54	8 (17%)	54,84,113	1.51	6 (11%)
48	A86	K	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.15	18 (35%)
39	CLA	J	311	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
39	CLA	b	814	-	59,63,73	1.36	8 (13%)	71,101,113	1.36	6 (8%)
39	CLA	U	210	-	64,68,73	1.32	9 (14%)	77,107,113	1.31	7 (9%)
48	A86	Y	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	15 (29%)
50	A1EB1	F	304	-	51,58,58	1.30	4 (7%)	60,85,85	2.12	18 (30%)
39	CLA	T	313	-	55,59,73	1.44	7 (12%)	66,96,113	1.27	7 (10%)
39	CLA	9	308	-	59,63,73	1.34	8 (13%)	71,101,113	1.51	11 (15%)
49	KC2	V	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.25	18 (29%)
43	DD6	z	305	-	39,45,45	2.02	2 (5%)	52,67,67	1.89	16 (30%)
49	KC2	3	321	-	49,53,53	1.74	9 (18%)	62,89,89	2.12	18 (29%)
48	A86	F	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.23	15 (29%)
49	KC2	L	317	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	18 (29%)
39	CLA	5	315	-	51,55,73	1.44	8 (15%)	61,91,113	1.44	6 (9%)
49	KC2	9	318	-	49,53,53	1.82	9 (18%)	62,89,89	2.03	14 (22%)
51	A1ECV	T	317	-	47,56,56	3.32	20 (42%)	32,93,93	3.13	11 (34%)
39	CLA	D	311	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
49	KC2	Y	308	-	49,53,53	1.83	9 (18%)	62,89,89	2.02	14 (22%)
49	KC2	2	313	-	48,52,53	1.80	10 (20%)	62,88,89	2.19	19 (30%)
43	DD6	E	305	-	39,45,45	1.99	3 (7%)	52,67,67	1.92	14 (26%)
39	CLA	H	308	-	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
39	CLA	4	316	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
39	CLA	J	308	-	54,58,73	1.42	6 (11%)	65,95,113	1.41	6 (9%)
39	CLA	b	802	-	69,73,73	1.26	8 (11%)	83,113,113	1.25	5 (6%)
47	SQD	P	301	-	37,38,54	1.11	5 (13%)	46,49,65	1.73	12 (26%)
39	CLA	6	318	-	45,49,73	1.52	8 (17%)	54,84,113	1.55	5 (9%)
48	A86	L	305	-	44,50,50	1.22	3 (6%)	51,76,76	2.17	16 (31%)
39	CLA	A	314	-	69,73,73	1.25	6 (8%)	83,113,113	1.35	7 (8%)
39	CLA	a	835	-	69,73,73	1.26	8 (11%)	83,113,113	1.32	8 (9%)
43	DD6	X	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.87	16 (30%)
51	A1ECV	Z	314	-	47,56,56	3.36	20 (42%)	32,93,93	3.28	11 (34%)
39	CLA	L	311	23	56,60,73	1.39	8 (14%)	67,97,113	1.38	7 (10%)
39	CLA	A	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	KC2	V	312	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	18 (29%)
39	CLA	l	203	-	53,57,73	1.44	8 (15%)	62,93,113	1.45	7 (11%)
52	A1EB4	P	319	-	52,59,63	2.81	6 (11%)	61,85,89	2.79	21 (34%)
39	CLA	S	309	-	69,73,73	1.29	9 (13%)	83,113,113	1.36	10 (12%)
48	A86	W	303	-	44,50,50	1.19	2 (4%)	51,76,76	2.16	19 (37%)
51	A1ECV	Y	306	-	47,56,56	3.33	19 (40%)	32,93,93	3.28	13 (40%)
46	LMG	P	317	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
50	A1EB1	8	306	-	51,58,58	1.28	3 (5%)	60,85,85	2.08	19 (31%)
39	CLA	a	810	-	58,62,73	1.37	8 (13%)	69,99,113	1.37	7 (10%)
43	DD6	z	304	-	39,45,45	2.05	4 (10%)	52,67,67	1.88	14 (26%)
42	BCR	b	845	-	41,41,41	0.72	0	56,56,56	1.96	17 (30%)
50	A1EB1	2	306	-	51,58,58	1.24	3 (5%)	60,85,85	2.09	20 (33%)
50	A1EB1	8	304	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	17 (28%)
39	CLA	E	313	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	9 (10%)
39	CLA	7	324	-	45,49,73	1.53	8 (17%)	54,84,113	1.64	8 (14%)
49	KC2	y	314	-	49,53,53	1.81	9 (18%)	62,89,89	2.05	14 (22%)
39	CLA	6	312	-	55,59,73	1.39	8 (14%)	65,95,113	1.39	5 (7%)
48	A86	8	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.24	19 (37%)
39	CLA	C	307	-	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
46	LMG	M	319	49	39,39,55	1.08	2 (5%)	47,47,63	1.56	8 (17%)
39	CLA	b	820	-	64,68,73	1.31	9 (14%)	77,107,113	1.29	4 (5%)
49	KC2	P	306	24	49,53,53	1.82	12 (24%)	62,89,89	2.19	17 (27%)
48	A86	9	301	-	44,50,50	1.20	3 (6%)	51,76,76	2.14	15 (29%)
48	A86	z	303	-	44,50,50	1.14	2 (4%)	51,76,76	1.90	11 (21%)
49	KC2	8	316	-	49,53,53	1.77	10 (20%)	62,89,89	2.20	16 (25%)
39	CLA	a	830	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	4 (4%)
39	CLA	H	316	-	50,54,73	1.47	8 (16%)	60,90,113	1.49	4 (6%)
52	A1EB4	W	321	-	52,59,63	2.65	5 (9%)	61,85,89	2.25	20 (32%)
39	CLA	Z	309	-	45,49,73	1.53	6 (13%)	54,84,113	1.46	4 (7%)
39	CLA	7	325	-	54,58,73	1.43	7 (12%)	65,95,113	1.44	7 (10%)
50	A1EB1	0	303	-	51,58,58	1.26	3 (5%)	60,85,85	2.23	17 (28%)
49	KC2	T	312	-	49,53,53	1.81	10 (20%)	62,89,89	2.19	17 (27%)
48	A86	D	305	-	44,50,50	1.21	3 (6%)	51,76,76	2.71	21 (41%)
50	A1EB1	3	324	-	51,58,58	1.29	3 (5%)	60,85,85	2.03	18 (30%)
50	A1EB1	7	303	-	51,58,58	1.33	3 (5%)	60,85,85	2.01	20 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	A1EB1	O	301	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	18 (30%)
41	LHG	j	104	-	29,29,48	0.74	1 (3%)	32,35,54	1.23	3 (9%)
48	A86	x	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.26	17 (33%)
39	CLA	1	313	32	45,49,73	1.51	8 (17%)	54,84,113	1.51	5 (9%)
48	A86	5	301	-	44,50,50	1.21	2 (4%)	51,76,76	2.19	16 (31%)
39	CLA	J	310	-	59,63,73	1.37	8 (13%)	71,101,113	1.36	7 (9%)
49	KC2	8	314	-	49,53,53	1.79	10 (20%)	62,89,89	2.07	15 (24%)
39	CLA	a	819	-	53,57,73	1.41	7 (13%)	62,93,113	1.44	7 (11%)
49	KC2	K	313	22	49,53,53	1.79	10 (20%)	62,89,89	2.19	18 (29%)
49	KC2	2	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.16	18 (29%)
48	A86	3	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.24	13 (25%)
47	SQD	D	304	-	37,38,54	1.14	5 (13%)	46,49,65	1.74	10 (21%)
48	A86	4	306	-	44,50,50	1.18	2 (4%)	51,76,76	1.99	15 (29%)
43	DD6	7	310	-	39,45,45	2.06	3 (7%)	52,67,67	2.49	14 (26%)
48	A86	7	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.22	17 (33%)
50	A1EB1	S	303	-	51,58,58	1.25	3 (5%)	60,85,85	2.14	21 (35%)
39	CLA	b	831	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	8 (12%)
49	KC2	4	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.17	17 (27%)
49	KC2	S	315	28	49,53,53	1.81	10 (20%)	62,89,89	2.15	18 (29%)
39	CLA	b	811	-	69,73,73	1.23	10 (14%)	83,113,113	1.40	7 (8%)
49	KC2	F	311	46	48,52,53	1.73	9 (18%)	59,87,89	2.31	19 (32%)
50	A1EB1	8	308	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	18 (30%)
39	CLA	M	318	24	50,54,73	1.47	7 (14%)	60,90,113	1.50	4 (6%)
49	KC2	6	319	-	49,53,53	1.82	11 (22%)	62,89,89	2.05	13 (20%)
43	DD6	O	305	-	39,45,45	1.99	2 (5%)	52,67,67	1.62	12 (23%)
50	A1EB1	1	305	-	51,58,58	1.25	4 (7%)	60,85,85	2.08	16 (26%)
39	CLA	P	308	24	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
39	CLA	a	833	1	49,53,73	1.48	7 (14%)	59,89,113	1.49	5 (8%)
50	A1EB1	K	305	-	51,58,58	1.25	3 (5%)	60,85,85	2.22	18 (30%)
39	CLA	C	309	-	50,54,73	1.47	6 (12%)	60,90,113	1.40	4 (6%)
39	CLA	b	807	-	69,73,73	1.24	8 (11%)	83,113,113	1.43	8 (9%)
39	CLA	x	314	-	45,49,73	1.52	7 (15%)	54,84,113	1.56	5 (9%)
49	KC2	L	314	-	49,53,53	1.75	9 (18%)	62,89,89	2.17	19 (30%)
39	CLA	L	320	-	50,54,73	1.47	6 (12%)	60,90,113	1.56	7 (11%)
50	A1EB1	6	308	-	51,58,58	1.29	4 (7%)	60,85,85	2.25	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	LHG	D	302	-	34,34,48	0.70	0	37,40,54	1.27	3 (8%)
43	DD6	2	303	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
51	A1ECV	Q	319	-	47,56,56	3.32	19 (40%)	32,93,93	3.17	12 (37%)
39	CLA	M	317	-	55,59,73	1.40	9 (16%)	66,96,113	1.41	4 (6%)
39	CLA	y	307	-	45,49,73	1.53	8 (17%)	54,84,113	1.54	5 (9%)
39	CLA	0	318	-	45,49,73	1.54	6 (13%)	54,84,113	1.50	5 (9%)
39	CLA	E	316	-	56,60,73	1.39	9 (16%)	67,97,113	1.43	6 (8%)
48	A86	y	306	-	44,50,50	1.16	2 (4%)	51,76,76	2.50	18 (35%)
39	CLA	J	316	-	50,54,73	1.46	7 (14%)	60,90,113	1.49	4 (6%)
39	CLA	I	309	-	69,73,73	1.27	7 (10%)	83,113,113	1.29	4 (4%)
52	A1EB4	M	305	-	53,60,63	2.51	4 (7%)	62,86,89	2.08	16 (25%)
48	A86	S	307	-	44,50,50	1.19	2 (4%)	51,76,76	2.32	18 (35%)
39	CLA	b	812	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
49	KC2	I	303	-	49,53,53	1.77	10 (20%)	62,89,89	2.33	21 (33%)
39	CLA	H	313	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
39	CLA	x	317	-	45,49,73	1.53	6 (13%)	54,84,113	1.53	6 (11%)
41	LHG	a	840	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	7 (13%)
49	KC2	0	316	-	49,53,53	1.75	10 (20%)	62,89,89	2.13	19 (30%)
50	A1EB1	L	303	-	51,58,58	1.29	3 (5%)	60,85,85	2.24	19 (31%)
39	CLA	b	821	-	69,73,73	1.27	8 (11%)	83,113,113	1.31	7 (8%)
48	A86	F	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.12	15 (29%)
39	CLA	b	806	-	69,73,73	1.23	7 (10%)	83,113,113	1.25	7 (8%)
39	CLA	9	320	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	8 (14%)
39	CLA	T	310	29	56,60,73	1.39	9 (16%)	67,97,113	1.39	5 (7%)
49	KC2	X	314	46	48,52,53	1.75	9 (18%)	59,87,89	2.20	17 (28%)
50	A1EB1	Q	307	-	51,58,58	1.31	5 (9%)	60,85,85	2.01	15 (25%)
39	CLA	T	320	-	56,60,73	1.39	8 (14%)	67,97,113	1.36	5 (7%)
44	SF4	b	804	-	0,12,12	-	-	-		
49	KC2	X	312	-	49,53,53	1.76	9 (18%)	62,89,89	2.20	19 (30%)
49	KC2	4	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.12	17 (27%)
48	A86	Q	305	-	44,50,50	1.14	3 (6%)	51,76,76	2.03	14 (27%)
50	A1EB1	4	304	-	51,58,58	1.28	3 (5%)	60,85,85	2.17	21 (35%)
39	CLA	E	318	17	50,54,73	1.46	8 (16%)	60,90,113	1.42	5 (8%)
39	CLA	Y	304	-	50,54,73	1.46	6 (12%)	60,90,113	1.47	4 (6%)
51	A1ECV	4	321	-	47,56,56	3.37	20 (42%)	32,93,93	3.09	13 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	3	312	-	69,73,73	1.27	7 (10%)	83,113,113	1.36	8 (9%)
43	DD6	M	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.71	12 (23%)
50	A1EB1	z	301	-	44,50,58	1.15	2 (4%)	51,76,85	1.70	12 (23%)
39	CLA	C	311	-	69,73,73	1.25	6 (8%)	83,113,113	1.29	4 (4%)
48	A86	2	305	-	44,50,50	1.12	2 (4%)	51,76,76	2.43	15 (29%)
39	CLA	a	813	1	54,58,73	1.42	7 (12%)	65,95,113	1.50	6 (9%)
50	A1EB1	1	301	-	51,58,58	1.22	3 (5%)	60,85,85	1.92	17 (28%)
39	CLA	H	310	-	61,65,73	1.32	8 (13%)	73,103,113	1.36	4 (5%)
49	KC2	5	313	46	48,52,53	1.74	9 (18%)	59,87,89	2.19	16 (27%)
50	A1EB1	x	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.07	19 (31%)
49	KC2	2	317	-	49,53,53	1.78	11 (22%)	62,89,89	2.24	19 (30%)
39	CLA	O	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.58	5 (9%)
39	CLA	6	311	-	43,48,73	1.56	7 (16%)	51,83,113	1.53	7 (13%)
49	KC2	7	320	-	49,53,53	1.79	9 (18%)	62,89,89	2.06	15 (24%)
49	KC2	x	315	-	49,53,53	1.79	9 (18%)	62,89,89	2.05	15 (24%)
39	CLA	E	306	17	53,57,73	1.42	8 (15%)	62,93,113	1.43	5 (8%)
51	A1ECV	X	313	-	47,56,56	3.38	20 (42%)	32,93,93	3.26	12 (37%)
49	KC2	Y	309	-	49,53,53	1.77	9 (18%)	62,89,89	2.11	17 (27%)
39	CLA	G	314	19	62,66,73	1.31	7 (11%)	74,104,113	1.45	6 (8%)
49	KC2	R	318	-	49,53,53	1.78	10 (20%)	62,89,89	2.13	17 (27%)
51	A1ECV	7	317	-	47,56,56	3.42	20 (42%)	32,93,93	3.31	13 (40%)
39	CLA	6	322	-	50,54,73	1.47	6 (12%)	60,90,113	1.46	4 (6%)
39	CLA	b	838	-	69,73,73	1.25	6 (8%)	83,113,113	1.33	8 (9%)
49	KC2	K	310	-	49,53,53	1.77	10 (20%)	62,89,89	2.19	17 (27%)
39	CLA	0	315	31	54,58,73	1.39	7 (12%)	65,95,113	1.42	9 (13%)
43	DD6	I	307	-	39,45,45	2.01	3 (7%)	52,67,67	1.90	10 (19%)
39	CLA	M	315	-	45,49,73	1.51	7 (15%)	54,84,113	1.55	9 (16%)
46	LMG	9	321	-	36,36,55	0.91	0	44,44,63	1.20	3 (6%)
39	CLA	8	310	-	49,53,73	1.51	6 (12%)	59,89,113	1.51	7 (11%)
47	SQD	S	301	-	38,39,54	1.14	5 (13%)	47,50,65	1.67	10 (21%)
39	CLA	a	802	-	59,63,73	1.35	7 (11%)	71,101,113	1.39	8 (11%)
50	A1EB1	7	306	-	51,58,58	1.26	3 (5%)	60,85,85	2.11	22 (36%)
47	SQD	D	321	-	38,39,54	1.10	5 (13%)	47,50,65	1.70	11 (23%)
39	CLA	b	841	2	69,73,73	1.28	6 (8%)	83,113,113	1.29	6 (7%)
43	DD6	I	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	a	816	-	69,73,73	1.27	8 (11%)	83,113,113	1.34	10 (12%)
48	A86	L	306	-	44,50,50	1.16	3 (6%)	51,76,76	2.15	15 (29%)
39	CLA	y	310	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	5 (9%)
39	CLA	R	315	-	51,55,73	1.45	8 (15%)	61,91,113	1.49	8 (13%)
46	LMG	F	317	49	39,39,55	1.05	2 (5%)	47,47,63	1.23	6 (12%)
39	CLA	i	101	-	69,73,73	1.25	7 (10%)	83,113,113	1.25	5 (6%)
39	CLA	T	308	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	6 (10%)
43	DD6	C	301	-	39,45,45	2.32	4 (10%)	52,67,67	2.51	14 (26%)
49	KC2	R	312	-	49,53,53	1.75	11 (22%)	62,89,89	2.18	19 (30%)
42	BCR	b	850	-	41,41,41	0.68	0	56,56,56	1.86	12 (21%)
47	SQD	W	301	-	27,28,54	1.22	4 (14%)	36,39,65	1.79	9 (25%)
49	KC2	6	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	19 (30%)
42	BCR	i	102	-	41,41,41	0.72	0	56,56,56	2.26	19 (33%)
51	A1ECV	X	310	-	47,56,56	3.32	19 (40%)	32,93,93	3.28	11 (34%)
39	CLA	b	823	-	50,54,73	1.46	6 (12%)	60,90,113	1.46	5 (8%)
48	A86	W	307	-	44,50,50	1.23	4 (9%)	51,76,76	1.94	13 (25%)
39	CLA	Y	313	-	45,49,73	1.53	8 (17%)	54,84,113	1.54	5 (9%)
43	DD6	3	304	-	39,45,45	2.05	3 (7%)	52,67,67	3.25	19 (36%)
50	A1EB1	H	301	-	51,58,58	1.27	3 (5%)	60,85,85	2.10	17 (28%)
39	CLA	h	201	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	6 (8%)
39	CLA	b	829	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
39	CLA	b	836	-	49,53,73	1.50	8 (16%)	59,89,113	1.51	8 (13%)
39	CLA	3	313	-	57,61,73	1.40	8 (14%)	68,98,113	1.35	5 (7%)
43	DD6	S	306	-	39,45,45	2.01	2 (5%)	52,67,67	1.92	16 (30%)
46	LMG	Q	322	49	28,28,55	1.26	2 (7%)	36,36,63	1.44	6 (16%)
39	CLA	8	311	-	59,63,73	1.35	7 (11%)	71,101,113	1.40	6 (8%)
39	CLA	8	321	-	46,50,73	1.51	7 (15%)	55,85,113	1.46	4 (7%)
39	CLA	W	318	-	55,59,73	1.41	8 (14%)	66,96,113	1.42	4 (6%)
39	CLA	3	320	-	49,53,73	1.49	6 (12%)	59,89,113	1.53	6 (10%)
48	A86	S	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.02	14 (27%)
39	CLA	D	319	16	69,73,73	1.26	6 (8%)	83,113,113	1.31	7 (8%)
39	CLA	E	310	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
39	CLA	Y	303	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	6 (11%)
49	KC2	6	317	-	49,53,53	1.76	9 (18%)	62,89,89	2.13	18 (29%)
39	CLA	B	209	-	60,64,73	1.36	8 (13%)	72,102,113	1.29	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	k	203	-	59,63,73	1.36	7 (11%)	71,101,113	1.37	5 (7%)
39	CLA	f	802	-	69,73,73	1.27	7 (10%)	83,113,113	1.26	7 (8%)
43	DD6	E	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.77	8 (15%)
48	A86	P	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.25	18 (35%)
42	BCR	b	847	-	41,41,41	0.71	0	56,56,56	2.01	16 (28%)
49	KC2	L	321	-	49,53,53	1.80	11 (22%)	62,89,89	2.06	15 (24%)
50	A1EB1	D	308	-	51,58,58	1.28	3 (5%)	60,85,85	2.34	20 (33%)
39	CLA	8	322	-	45,49,73	1.54	7 (15%)	54,84,113	1.63	8 (14%)
39	CLA	a	837	-	69,73,73	1.27	7 (10%)	83,113,113	1.26	5 (6%)
39	CLA	z	308	-	50,54,73	1.46	7 (14%)	60,90,113	1.42	4 (6%)
47	SQD	T	321	-	35,36,54	1.15	5 (14%)	44,47,65	1.80	10 (22%)
39	CLA	b	835	-	69,73,73	1.26	7 (10%)	83,113,113	1.24	5 (6%)
42	BCR	k	204	-	41,41,41	0.71	0	56,56,56	1.90	15 (26%)
39	CLA	Z	315	-	45,49,73	1.53	7 (15%)	54,84,113	1.53	5 (9%)
43	DD6	H	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	10 (19%)
47	SQD	H	318	-	37,38,54	1.13	5 (13%)	46,49,65	1.64	8 (17%)
39	CLA	B	207	-	59,63,73	1.39	8 (13%)	71,101,113	1.42	7 (9%)
44	SF4	c	101	-	0,12,12	-	-	-		
39	CLA	T	309	-	60,64,73	1.37	7 (11%)	72,102,113	1.34	9 (12%)
48	A86	P	302	-	44,50,50	1.23	2 (4%)	51,76,76	2.31	17 (33%)
46	LMG	D	322	-	37,37,55	0.91	0	45,45,63	1.21	5 (11%)
50	A1EB1	U	203	-	51,58,58	1.25	3 (5%)	60,85,85	2.17	19 (31%)
39	CLA	Q	312	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	4 (4%)
39	CLA	0	323	-	50,54,73	1.43	8 (16%)	60,90,113	1.48	5 (8%)
39	CLA	E	308	-	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
39	CLA	L	319	-	55,59,73	1.41	6 (10%)	66,96,113	1.40	4 (6%)
39	CLA	O	318	-	50,54,73	1.47	7 (14%)	60,90,113	1.50	7 (11%)
43	DD6	j	102	-	39,45,45	1.96	2 (5%)	52,67,67	1.85	12 (23%)
48	A86	L	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	14 (27%)
43	DD6	T	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.87	13 (25%)
49	KC2	T	314	-	49,53,53	1.75	10 (20%)	62,89,89	2.18	18 (29%)
39	CLA	I	315	-	56,60,73	1.39	6 (10%)	67,97,113	1.45	8 (11%)
39	CLA	W	309	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	5 (6%)
39	CLA	I	316	36	45,49,73	1.51	6 (13%)	54,84,113	1.50	6 (11%)
52	A1EB4	P	318	-	49,56,63	2.77	5 (10%)	58,82,89	2.27	18 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	o	201	-	55,59,73	1.40	8 (14%)	66,96,113	1.40	5 (7%)
39	CLA	W	311	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
39	CLA	x	308	-	45,49,73	1.51	7 (15%)	54,84,113	1.61	6 (11%)
48	A86	6	307	-	44,50,50	1.15	3 (6%)	51,76,76	2.11	17 (33%)
39	CLA	Q	317	-	50,54,73	1.48	7 (14%)	60,90,113	1.40	5 (8%)
49	KC2	y	316	-	49,53,53	1.75	10 (20%)	62,89,89	2.15	18 (29%)
39	CLA	4	313	-	50,54,73	1.45	7 (14%)	60,90,113	1.41	4 (6%)
48	A86	M	302	-	44,50,50	1.18	2 (4%)	51,76,76	2.19	17 (33%)
47	SQD	F	319	-	36,37,54	1.14	5 (13%)	45,48,65	1.72	10 (22%)
43	DD6	Q	306	-	39,45,45	2.01	3 (7%)	52,67,67	1.83	14 (26%)
43	DD6	J	304	-	39,45,45	2.23	5 (12%)	52,67,67	2.35	14 (26%)
52	A1EB4	X	305	-	52,59,63	2.59	4 (7%)	61,85,89	1.90	19 (31%)
39	CLA	K	314	-	45,49,73	1.52	7 (15%)	54,84,113	1.52	7 (12%)
39	CLA	C	310	-	69,73,73	1.23	8 (11%)	83,113,113	1.33	5 (6%)
48	A86	I	304	-	44,50,50	1.13	3 (6%)	51,76,76	2.14	14 (27%)
39	CLA	Q	309	-	65,69,73	1.29	8 (12%)	78,108,113	1.32	4 (5%)
39	CLA	U	213	-	45,49,73	1.52	7 (15%)	54,84,113	1.56	5 (9%)
39	CLA	K	312	-	69,73,73	1.24	8 (11%)	83,113,113	1.34	6 (7%)
43	DD6	D	306	-	39,45,45	2.66	4 (10%)	52,67,67	2.39	12 (23%)
39	CLA	X	308	-	64,68,73	1.31	8 (12%)	77,107,113	1.36	8 (10%)
39	CLA	R	307	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
48	A86	G	305	-	44,50,50	1.19	2 (4%)	51,76,76	2.29	16 (31%)
50	A1EB1	K	302	-	51,58,58	1.29	4 (7%)	60,85,85	2.12	21 (35%)
39	CLA	R	316	-	56,60,73	1.41	9 (16%)	67,97,113	1.45	5 (7%)
49	KC2	V	318	-	49,53,53	1.78	9 (18%)	62,89,89	2.15	17 (27%)
39	CLA	z	314	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	5 (9%)
39	CLA	b	827	-	69,73,73	1.26	7 (10%)	83,113,113	1.31	4 (4%)
39	CLA	E	309	-	57,61,73	1.38	8 (14%)	68,98,113	1.37	6 (8%)
48	A86	T	306	-	44,50,50	1.19	2 (4%)	51,76,76	2.35	15 (29%)
51	A1ECV	R	313	-	47,56,56	3.40	20 (42%)	32,93,93	3.32	12 (37%)
39	CLA	X	317	-	56,60,73	1.40	9 (16%)	67,97,113	1.45	6 (8%)
41	LHG	a	841	39	26,26,48	0.85	1 (3%)	29,32,54	1.33	3 (10%)
39	CLA	A	307	-	64,68,73	1.32	8 (12%)	77,107,113	1.30	6 (7%)
39	CLA	3	319	-	45,49,73	1.52	6 (13%)	54,84,113	1.57	7 (12%)
43	DD6	D	303	-	39,45,45	2.10	2 (5%)	52,67,67	2.77	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	LMG	0	324	49	27,27,55	1.31	2 (7%)	35,35,63	1.47	4 (11%)
50	A1EB1	J	302	-	51,58,58	1.26	4 (7%)	60,85,85	2.25	23 (38%)
51	A1ECV	0	321	48	47,56,56	3.35	19 (40%)	32,93,93	3.32	14 (43%)
39	CLA	I	310	-	58,62,73	1.36	8 (13%)	69,99,113	1.39	5 (7%)
39	CLA	b	815	-	69,73,73	1.27	8 (11%)	83,113,113	1.28	7 (8%)
39	CLA	A	315	-	54,58,73	1.41	6 (11%)	65,95,113	1.42	6 (9%)
49	KC2	J	315	-	49,53,53	1.79	9 (18%)	62,89,89	2.11	20 (32%)
39	CLA	4	319	-	45,49,73	1.53	7 (15%)	54,84,113	1.56	5 (9%)
43	DD6	a	846	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	12 (23%)
39	CLA	O	313	-	54,58,73	1.40	8 (14%)	65,95,113	1.45	5 (7%)
49	KC2	Z	311	-	49,53,53	1.75	9 (18%)	62,89,89	2.16	17 (27%)
51	A1ECV	1	318	-	47,56,56	3.33	20 (42%)	32,93,93	3.34	11 (34%)
39	CLA	b	833	-	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
39	CLA	P	316	-	55,59,73	1.41	8 (14%)	66,96,113	1.43	5 (7%)
48	A86	6	302	-	44,50,50	1.16	3 (6%)	51,76,76	2.16	15 (29%)
50	A1EB1	3	309	-	51,58,58	1.28	4 (7%)	60,85,85	1.97	15 (25%)
39	CLA	z	318	-	45,49,73	1.52	7 (15%)	54,84,113	1.58	7 (12%)
39	CLA	J	307	21	53,57,73	1.43	7 (13%)	62,93,113	1.45	5 (8%)
49	KC2	9	313	-	49,53,53	1.78	12 (24%)	62,89,89	2.11	15 (24%)
49	KC2	M	311	46	48,52,53	1.72	9 (18%)	59,87,89	2.20	17 (28%)
39	CLA	Y	310	-	45,49,73	1.54	6 (13%)	54,84,113	1.55	5 (9%)
48	A86	E	304	-	44,50,50	1.26	3 (6%)	51,76,76	2.41	19 (37%)
39	CLA	Q	321	-	57,61,73	1.42	7 (12%)	68,98,113	1.33	8 (11%)
48	A86	S	304	-	44,50,50	1.13	2 (4%)	51,76,76	1.98	11 (21%)
49	KC2	M	307	-	49,53,53	1.76	10 (20%)	62,89,89	2.21	19 (30%)
50	A1EB1	7	304	-	51,58,58	1.23	4 (7%)	60,85,85	2.03	19 (31%)
51	A1ECV	R	310	-	47,56,56	3.31	19 (40%)	32,93,93	3.55	11 (34%)
39	CLA	2	319	-	50,54,73	1.46	7 (14%)	60,90,113	1.67	9 (15%)
39	CLA	a	814	-	65,69,73	1.28	8 (12%)	78,108,113	1.35	6 (7%)
39	CLA	o	205	-	56,60,73	1.40	7 (12%)	67,97,113	1.39	5 (7%)
39	CLA	A	306	-	65,69,73	1.30	9 (13%)	78,108,113	1.35	6 (7%)
39	CLA	Q	311	-	50,54,73	1.45	9 (18%)	60,90,113	1.53	6 (10%)
49	KC2	x	313	-	49,53,53	1.77	9 (18%)	62,89,89	2.13	17 (27%)
39	CLA	Q	310	-	69,73,73	1.27	8 (11%)	83,113,113	1.27	10 (12%)
42	BCR	a	842	-	41,41,41	0.67	0	56,56,56	1.82	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	A86	0	309	-	44,50,50	1.20	2 (4%)	51,76,76	2.35	18 (35%)
48	A86	3	308	-	44,50,50	1.25	3 (6%)	51,76,76	2.33	18 (35%)
39	CLA	O	308	-	41,46,73	1.60	7 (17%)	51,80,113	2.03	11 (21%)
43	DD6	E	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.84	11 (21%)
39	CLA	E	315	-	50,54,73	1.48	8 (16%)	60,90,113	1.45	4 (6%)
49	KC2	M	313	-	49,53,53	1.79	9 (18%)	62,89,89	2.17	17 (27%)
49	KC2	6	316	-	49,53,53	1.76	9 (18%)	62,89,89	2.14	19 (30%)
39	CLA	H	312	20	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
39	CLA	P	311	-	69,73,73	1.26	6 (8%)	83,113,113	1.28	5 (6%)
39	CLA	U	209	-	56,60,73	1.39	8 (14%)	67,97,113	1.43	7 (10%)
39	CLA	1	317	-	45,49,73	1.53	6 (13%)	54,84,113	1.53	5 (9%)
48	A86	C	303	-	44,50,50	1.21	2 (4%)	51,76,76	1.92	14 (27%)
50	A1EB1	4	301	-	51,58,58	1.25	3 (5%)	60,85,85	1.93	18 (30%)
43	DD6	F	303	-	39,45,45	1.93	2 (5%)	52,67,67	1.79	10 (19%)
39	CLA	b	803	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
48	A86	O	302	-	44,50,50	1.22	3 (6%)	51,76,76	2.36	20 (39%)
48	A86	6	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	16 (31%)
49	KC2	0	319	-	49,53,53	1.91	11 (22%)	62,89,89	2.01	15 (24%)
51	A1ECV	7	323	-	47,56,56	3.34	20 (42%)	32,93,93	3.48	12 (37%)
49	KC2	5	305	27	49,53,53	1.73	9 (18%)	62,89,89	2.17	16 (25%)
48	A86	8	307	-	44,50,50	1.23	3 (6%)	51,76,76	2.45	23 (45%)
51	A1ECV	9	314	-	47,56,56	3.40	20 (42%)	32,93,93	3.33	12 (37%)
39	CLA	z	307	-	46,50,73	1.51	6 (13%)	55,85,113	1.50	6 (10%)
42	BCR	a	843	-	41,41,41	0.73	0	56,56,56	1.94	17 (30%)
39	CLA	P	307	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	5 (6%)
48	A86	1	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.18	17 (33%)
39	CLA	z	317	-	46,50,73	1.52	6 (13%)	55,85,113	1.48	4 (7%)
39	CLA	3	316	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	6 (9%)
43	DD6	R	304	-	39,45,45	1.95	4 (10%)	52,67,67	1.84	15 (28%)
46	LMG	S	321	-	32,32,55	0.92	0	40,40,63	1.21	5 (12%)
39	CLA	a	829	-	60,64,73	1.35	6 (10%)	72,102,113	1.39	6 (8%)
39	CLA	Q	314	-	58,62,73	1.36	9 (15%)	69,99,113	1.37	5 (7%)
43	DD6	J	305	-	39,45,45	2.05	3 (7%)	52,67,67	2.29	17 (32%)
42	BCR	l	202	-	41,41,41	0.76	0	56,56,56	1.93	13 (23%)
43	DD6	y	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	DD6	3	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	13 (25%)
50	A1EB1	G	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.07	19 (31%)
43	DD6	I	306	-	39,45,45	1.95	3 (7%)	52,67,67	1.76	11 (21%)
39	CLA	E	307	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	8 (9%)
50	A1EB1	8	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	16 (26%)
39	CLA	2	318	-	45,49,73	1.53	7 (15%)	54,84,113	1.53	5 (9%)
39	CLA	O	312	-	50,54,73	1.47	8 (16%)	60,90,113	1.45	4 (6%)
39	CLA	3	311	-	65,69,73	1.30	8 (12%)	78,108,113	1.27	5 (6%)
40	PQN	b	843	-	34,34,34	1.53	2 (5%)	42,45,45	1.26	4 (9%)
39	CLA	Z	313	-	45,49,73	1.55	8 (17%)	54,84,113	1.89	10 (18%)
39	CLA	D	314	-	69,73,73	1.27	8 (11%)	83,113,113	1.23	7 (8%)
39	CLA	a	831	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	5 (6%)
39	CLA	y	318	-	46,50,73	1.51	6 (13%)	55,85,113	1.48	4 (7%)
48	A86	2	302	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	18 (35%)
39	CLA	5	306	-	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
39	CLA	D	312	16	59,63,73	1.35	8 (13%)	71,101,113	1.39	8 (11%)
39	CLA	4	311	-	65,69,73	1.32	9 (13%)	78,108,113	1.37	8 (10%)
39	CLA	R	309	-	69,73,73	1.25	6 (8%)	83,113,113	1.32	7 (8%)
51	A1ECV	S	312	-	47,56,56	3.44	20 (42%)	32,93,93	3.45	11 (34%)
41	LHG	X	301	-	40,40,48	0.67	1 (2%)	43,46,54	1.30	6 (13%)
43	DD6	O	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	13 (25%)
39	CLA	8	318	-	45,49,73	1.53	6 (13%)	54,84,113	1.52	6 (11%)
39	CLA	I	313	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	6 (7%)
39	CLA	b	816	-	64,68,73	1.31	8 (12%)	77,107,113	1.31	6 (7%)
39	CLA	a	827	-	69,73,73	1.28	10 (14%)	83,113,113	1.40	8 (9%)
39	CLA	5	316	-	56,60,73	1.41	9 (16%)	67,97,113	1.42	5 (7%)
39	CLA	G	309	-	60,64,73	1.34	9 (15%)	72,102,113	1.40	6 (8%)
48	A86	L	307	-	44,50,50	1.18	3 (6%)	51,76,76	2.52	20 (39%)
46	LMG	I	302	-	42,42,55	0.89	1 (2%)	50,50,63	1.22	4 (8%)
39	CLA	V	310	-	64,68,73	1.31	8 (12%)	77,107,113	1.43	12 (15%)
39	CLA	9	312	35	46,50,73	1.49	8 (17%)	55,85,113	1.53	6 (10%)
47	SQD	M	301	-	38,39,54	1.11	5 (13%)	47,50,65	1.69	13 (27%)
39	CLA	1	319	-	55,59,73	1.41	9 (16%)	66,96,113	1.43	5 (7%)
39	CLA	9	319	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	5 (8%)
50	A1EB1	9	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.05	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	KC2	Q	318	26	49,53,53	1.75	10 (20%)	62,89,89	2.19	17 (27%)
49	KC2	3	318	-	49,53,53	1.80	10 (20%)	62,89,89	2.13	18 (29%)
39	CLA	i	103	-	69,73,73	1.27	9 (13%)	83,113,113	1.38	10 (12%)
46	LMG	W	302	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
48	A86	X	302	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	17 (33%)
51	A1ECV	Q	316	26	47,56,56	3.37	21 (44%)	32,93,93	3.10	11 (34%)
49	KC2	W	315	-	49,53,53	1.81	9 (18%)	62,89,89	2.05	14 (22%)
48	A86	8	305	-	44,50,50	1.20	3 (6%)	51,76,76	2.63	22 (43%)
39	CLA	C	304	-	47,51,73	1.50	8 (17%)	56,86,113	1.44	5 (8%)
39	CLA	y	315	-	45,49,73	1.52	7 (15%)	54,84,113	1.57	5 (9%)
43	DD6	B	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.99	12 (23%)
49	KC2	3	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.16	19 (30%)
50	A1EB1	3	303	-	51,58,58	1.28	4 (7%)	60,85,85	2.05	18 (30%)
43	DD6	F	305	-	39,45,45	2.14	3 (7%)	52,67,67	2.66	17 (32%)
39	CLA	2	316	-	45,49,73	1.52	7 (15%)	54,84,113	1.58	5 (9%)
39	CLA	a	821	-	59,63,73	1.35	8 (13%)	71,101,113	1.40	5 (7%)
43	DD6	H	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	10 (19%)
45	DGD	b	849	-	61,61,67	0.93	2 (3%)	75,75,81	1.37	8 (10%)
39	CLA	a	804	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
39	CLA	1	308	-	45,49,73	1.54	7 (15%)	54,84,113	1.57	5 (9%)
39	CLA	x	306	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	4 (6%)
48	A86	y	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.00	16 (31%)
39	CLA	K	308	22	63,67,73	1.32	8 (12%)	75,105,113	1.30	5 (6%)
49	KC2	Z	310	-	49,53,53	1.76	10 (20%)	62,89,89	2.15	18 (29%)
50	A1EB1	4	303	-	51,58,58	1.27	3 (5%)	60,85,85	1.84	14 (23%)
39	CLA	f	803	-	59,63,73	1.37	7 (11%)	71,101,113	1.33	6 (8%)
51	A1ECV	O	315	-	47,56,56	3.34	20 (42%)	32,93,93	3.23	11 (34%)
51	A1ECV	P	315	-	47,56,56	3.34	19 (40%)	32,93,93	3.12	12 (37%)
39	CLA	I	308	-	65,69,73	1.27	7 (10%)	78,108,113	1.29	7 (8%)
50	A1EB1	V	302	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	20 (33%)
39	CLA	7	315	-	54,58,73	1.42	8 (14%)	65,95,113	1.43	7 (10%)
39	CLA	b	805	-	69,73,73	1.25	7 (10%)	83,113,113	1.21	6 (7%)
39	CLA	b	837	-	64,68,73	1.31	9 (14%)	77,107,113	1.39	8 (10%)
39	CLA	a	811	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	5 (6%)
43	DD6	V	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.75	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	CLA	L	309	-	57,62,73	1.37	9 (15%)	68,100,113	1.41	7 (10%)
46	LMG	M	320	-	33,33,55	0.94	0	41,41,63	1.19	4 (9%)
47	SQD	4	327	-	38,39,54	1.14	5 (13%)	47,50,65	1.69	11 (23%)
39	CLA	5	310	27	54,58,73	1.40	6 (11%)	65,95,113	1.46	6 (9%)
39	CLA	B	206	-	46,50,73	1.51	8 (17%)	55,85,113	1.47	6 (10%)
49	KC2	X	318	-	49,53,53	1.77	9 (18%)	62,89,89	2.15	16 (25%)
51	A1ECV	x	310	-	47,56,56	3.35	21 (44%)	32,93,93	3.30	11 (34%)
49	KC2	G	317	-	49,53,53	1.77	10 (20%)	62,89,89	2.25	19 (30%)
39	CLA	M	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.35	6 (7%)
39	CLA	b	813	-	58,62,73	1.41	10 (17%)	73,100,113	1.42	6 (8%)
39	CLA	T	311	-	60,64,73	1.35	7 (11%)	72,102,113	1.35	5 (6%)
50	A1EB1	6	306	-	44,50,58	1.15	2 (4%)	51,76,85	1.86	11 (21%)
39	CLA	a	828	1	54,58,73	1.42	9 (16%)	65,95,113	1.40	5 (7%)
39	CLA	7	316	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
48	A86	U	206	-	44,50,50	1.20	3 (6%)	51,76,76	2.39	19 (37%)
48	A86	4	309	-	44,50,50	1.21	3 (6%)	51,76,76	2.13	17 (33%)
49	KC2	X	306	27	49,53,53	1.85	10 (20%)	62,89,89	2.05	15 (24%)
49	KC2	8	320	-	49,53,53	1.77	9 (18%)	62,89,89	2.14	16 (25%)
51	A1ECV	z	310	-	47,56,56	3.33	20 (42%)	32,93,93	3.43	11 (34%)
51	A1ECV	2	311	-	47,56,56	3.35	20 (42%)	32,93,93	3.26	12 (37%)
52	A1EB4	T	304	-	50,57,63	2.65	5 (10%)	59,83,89	2.20	19 (32%)
39	CLA	0	313	-	59,63,73	1.36	7 (11%)	71,101,113	1.38	6 (8%)
39	CLA	8	315	-	47,51,73	1.49	8 (17%)	56,86,113	1.43	4 (7%)
51	A1ECV	z	316	-	47,56,56	3.37	20 (42%)	32,93,93	3.37	11 (34%)
39	CLA	P	314	-	45,49,73	1.53	8 (17%)	54,84,113	1.56	6 (11%)
39	CLA	7	313	-	65,69,73	1.31	8 (12%)	78,108,113	1.33	7 (8%)
44	SF4	c	102	-	0,12,12	-	-	-		
39	CLA	2	315	-	45,49,73	1.53	8 (17%)	54,84,113	1.50	5 (9%)
39	CLA	j	101	-	69,73,73	1.24	7 (10%)	83,113,113	1.33	8 (9%)
39	CLA	b	842	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
50	A1EB1	U	205	-	51,58,58	1.23	4 (7%)	60,85,85	1.99	19 (31%)
39	CLA	D	317	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	8 (9%)
39	CLA	R	311	27	54,58,73	1.40	8 (14%)	65,95,113	1.41	5 (7%)
51	A1ECV	4	315	-	47,56,56	3.42	20 (42%)	32,93,93	3.40	11 (34%)
52	A1EB4	W	306	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	A86	O	306	-	44,50,50	1.18	3 (6%)	51,76,76	2.57	20 (39%)
51	A1ECV	V	317	-	47,56,56	3.38	20 (42%)	32,93,93	3.15	11 (34%)
39	CLA	I	301	41	56,60,73	1.40	7 (12%)	67,97,113	1.38	7 (10%)
39	CLA	k	202	-	59,63,73	1.36	9 (15%)	71,101,113	1.35	6 (8%)
50	A1EB1	3	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.09	18 (30%)
39	CLA	b	810	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	5 (6%)
39	CLA	F	315	18	45,49,73	1.52	6 (13%)	54,84,113	1.66	6 (11%)
49	KC2	C	313	-	49,53,53	1.75	9 (18%)	62,89,89	2.16	18 (29%)
39	CLA	z	311	-	45,49,73	1.53	7 (15%)	54,84,113	1.49	5 (9%)
39	CLA	2	308	-	50,54,73	1.48	8 (16%)	60,90,113	1.46	6 (10%)
39	CLA	F	316	-	55,59,73	1.42	8 (14%)	66,96,113	1.40	5 (7%)
43	DD6	D	307	-	39,45,45	1.97	3 (7%)	52,67,67	1.79	10 (19%)
50	A1EB1	V	306	-	51,58,58	1.25	3 (5%)	60,85,85	1.97	19 (31%)
39	CLA	3	314	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
50	A1EB1	4	302	-	51,58,58	1.24	4 (7%)	60,85,85	2.12	20 (33%)
39	CLA	y	319	-	45,49,73	1.54	8 (17%)	54,84,113	1.59	8 (14%)
43	DD6	x	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.96	16 (30%)
39	CLA	3	323	-	50,54,73	1.46	8 (16%)	60,90,113	1.50	4 (6%)
39	CLA	4	314	-	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
41	LHG	H	317	-	34,34,48	0.71	0	37,40,54	1.19	3 (8%)
49	KC2	B	208	-	49,53,53	1.77	10 (20%)	62,89,89	2.24	19 (30%)
39	CLA	4	323	-	69,73,73	1.29	9 (13%)	83,113,113	1.27	4 (4%)
39	CLA	4	312	-	69,73,73	1.26	8 (11%)	83,113,113	1.37	10 (12%)
39	CLA	a	823	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	10 (12%)
49	KC2	V	315	-	49,53,53	1.79	11 (22%)	62,89,89	2.14	16 (25%)
39	CLA	a	834	-	55,59,73	1.40	8 (14%)	66,96,113	1.45	8 (12%)
48	A86	4	310	-	44,50,50	1.18	2 (4%)	51,76,76	2.34	17 (33%)
39	CLA	a	832	-	54,58,73	1.42	7 (12%)	65,95,113	1.45	6 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	BCR	b	848	-	-	1/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	0	304	-	-	12/34/90/90	0/3/3/3
49	KC2	T	316	-	-	7/15/71/71	-
49	KC2	R	306	-	-	8/15/71/71	-
39	CLA	Y	311	-	-	6/10/86/115	-
48	A86	Q	301	-	-	5/34/90/90	0/3/3/3
39	CLA	a	838	-	-	12/39/115/115	-
39	CLA	W	316	24	-	3/10/86/115	-
48	A86	Q	308	-	-	8/34/90/90	0/3/3/3
49	KC2	8	319	34	-	12/15/71/71	-
39	CLA	O	311	-	-	2/12/88/115	-
39	CLA	P	309	-	-	14/39/115/115	-
46	LMG	7	326	-	-	6/27/47/70	0/1/1/1
39	CLA	a	822	-	-	9/39/115/115	-
39	CLA	W	313	-	-	10/39/115/115	-
39	CLA	2	310	-	-	6/12/88/115	-
49	KC2	V	314	-	-	9/15/71/71	-
39	CLA	b	817	-	-	7/32/108/115	-
49	KC2	3	315	-	-	8/15/71/71	-
39	CLA	U	207	-	-	17/33/109/115	-
50	A1EB1	S	302	-	-	11/42/100/100	0/3/3/3
50	A1EB1	3	310	-	-	11/42/100/100	0/3/3/3
50	A1EB1	z	302	-	-	13/42/100/100	0/3/3/3
39	CLA	y	309	-	-	6/17/93/115	-
39	CLA	J	317	-	-	4/12/88/115	-
39	CLA	A	311	-	-	13/39/115/115	-
46	LMG	F	320	49	-	14/29/49/70	0/1/1/1
39	CLA	S	316	-	-	6/10/86/115	-
50	A1EB1	y	302	-	-	10/42/100/100	0/3/3/3
50	A1EB1	2	304	-	-	16/42/100/100	0/3/3/3
50	A1EB1	0	305	-	-	16/42/100/100	0/3/3/3
43	DD6	J	306	-	-	3/26/80/80	0/3/3/3
39	CLA	V	319	-	-	6/24/100/115	-
48	A86	1	307	-	-	0/34/90/90	0/3/3/3
39	CLA	K	307	-	-	14/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	S	313	-	-	7/39/115/115	-
39	CLA	Y	307	-	-	5/10/86/115	-
39	CLA	a	820	-	-	10/23/99/115	-
43	DD6	Q	303	-	-	4/26/80/80	0/3/3/3
39	CLA	D	318	-	-	16/39/115/115	-
49	KC2	7	319	-	-	7/15/71/71	-
50	A1EB1	Q	323	-	-	9/42/100/100	0/3/3/3
49	KC2	O	317	46	-	7/14/70/71	-
42	BCR	a	844	-	-	0/29/63/63	0/2/2/2
43	DD6	y	304	-	-	0/26/80/80	0/3/3/3
39	CLA	V	311	-	-	17/39/115/115	-
39	CLA	b	851	-	-	13/39/115/115	-
39	CLA	D	309	16	-	8/20/96/115	-
48	A86	7	308	-	-	8/34/90/90	0/3/3/3
43	DD6	7	309	-	-	2/26/80/80	0/3/3/3
51	A1ECV	5	312	27	3/3/17/24	11/19/117/117	-
39	CLA	F	321	-	-	19/39/115/115	-
39	CLA	J	318	-	-	7/17/93/115	-
46	LMG	4	325	-	-	16/27/47/70	0/1/1/1
39	CLA	6	321	-	-	5/10/86/115	-
48	A86	0	308	51	-	2/34/90/90	0/3/3/3
39	CLA	2	309	-	-	6/17/93/115	-
39	CLA	D	315	-	-	9/39/115/115	-
39	CLA	a	812	-	-	4/15/91/115	-
49	KC2	F	307	-	-	9/15/71/71	-
39	CLA	K	306	-	-	13/35/111/115	-
39	CLA	5	307	-	-	5/33/109/115	-
39	CLA	z	309	-	-	5/10/86/115	-
39	CLA	S	310	-	-	4/12/88/115	-
39	CLA	6	310	-	-	6/12/88/115	-
39	CLA	9	315	-	-	3/10/86/115	-
48	A86	Q	304	-	-	2/34/90/90	0/3/3/3
48	A86	8	303	-	-	6/34/90/90	0/3/3/3
39	CLA	1	309	-	-	6/12/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	z	315	-	-	10/15/71/71	-
50	A1EB1	C	302	-	-	10/42/100/100	0/3/3/3
39	CLA	a	826	-	-	18/39/115/115	-
39	CLA	a	801	-	-	16/39/115/115	-
49	KC2	L	315	-	-	9/15/71/71	-
39	CLA	z	306	-	-	4/10/86/115	-
52	A1EB4	M	322	-	-	6/38/99/103	0/3/3/3
39	CLA	U	201	-	-	11/17/93/115	-
49	KC2	0	317	31	-	3/15/71/71	-
39	CLA	l	201	-	-	16/39/115/115	-
49	KC2	x	312	-	-	8/15/71/71	-
48	A86	Z	301	-	-	11/34/90/90	0/3/3/3
39	CLA	D	316	-	-	16/39/115/115	-
39	CLA	Q	320	-	-	8/18/94/115	-
39	CLA	Z	312	-	-	4/10/86/115	-
49	KC2	G	315	-	-	11/15/71/71	-
39	CLA	E	317	-	-	8/24/100/115	-
39	CLA	Y	305	-	-	2/10/86/115	-
39	CLA	3	322	-	-	12/23/99/115	-
51	A1ECV	6	320	-	3/3/17/24	12/19/117/117	-
39	CLA	H	307	-	-	4/15/91/115	-
39	CLA	Z	306	-	-	9/17/93/115	-
48	A86	3	305	-	-	12/34/90/90	0/3/3/3
39	CLA	0	312	31	-	8/25/101/115	-
51	A1ECV	5	309	27	3/3/17/24	11/19/117/117	-
39	CLA	G	312	-	-	12/24/100/115	-
39	CLA	M	312	-	-	14/39/115/115	-
50	A1EB1	K	304	-	-	8/42/100/100	0/3/3/3
48	A86	9	306	-	-	6/34/90/90	0/3/3/3
50	A1EB1	6	304	-	-	11/39/97/100	0/3/3/3
50	A1EB1	h	203	-	-	10/42/100/100	0/3/3/3
48	A86	4	305	-	-	6/34/90/90	0/3/3/3
52	A1EB4	R	305	-	-	10/38/99/103	0/3/3/3
48	A86	J	303	-	-	6/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	L	316	-	-	8/10/86/115	-
49	KC2	X	315	-	-	8/15/71/71	-
39	CLA	l	205	-	-	2/21/97/115	-
39	CLA	a	808	-	-	12/29/105/115	-
51	A1ECV	Y	312	-	3/3/17/24	7/19/117/117	-
39	CLA	b	830	-	-	13/39/115/115	-
48	A86	R	301	-	-	2/34/90/90	0/3/3/3
47	SQD	E	320	-	-	12/30/50/69	0/1/1/1
39	CLA	W	310	-	-	16/39/115/115	-
39	CLA	F	314	18	-	10/27/103/115	-
39	CLA	C	306	-	-	8/39/115/115	-
47	SQD	D	320	39	-	11/32/52/69	0/1/1/1
39	CLA	F	312	-	-	8/39/115/115	-
39	CLA	x	311	-	-	2/15/91/115	-
39	CLA	a	815	-	-	16/39/115/115	-
39	CLA	O	310	-	-	15/33/109/115	-
50	A1EB1	E	301	-	-	9/42/100/100	0/3/3/3
39	CLA	b	818	-	-	11/27/103/115	-
48	A86	6	303	-	-	2/34/90/90	0/3/3/3
39	CLA	1	320	-	-	6/10/86/115	-
39	CLA	a	809	-	-	14/36/112/115	-
47	SQD	9	322	-	-	10/31/51/69	0/1/1/1
39	CLA	H	309	20	-	5/24/100/115	-
48	A86	Q	302	-	-	7/34/90/90	0/3/3/3
48	A86	X	303	-	-	8/34/90/90	0/3/3/3
42	BCR	l	206	-	-	6/29/63/63	0/2/2/2
39	CLA	J	314	-	-	20/39/115/115	-
39	CLA	F	308	-	-	16/39/115/115	-
39	CLA	A	305	13	-	6/20/96/115	-
40	PQN	a	839	-	-	7/23/43/43	0/2/2/2
39	CLA	H	306	-	-	10/19/95/115	-
50	A1EB1	7	305	-	-	16/42/100/100	0/3/3/3
48	A86	J	301	-	-	2/34/90/90	0/3/3/3
39	CLA	J	312	-	-	7/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	K	309	-	-	9/36/112/115	-
48	A86	V	304	-	-	3/34/90/90	0/3/3/3
39	CLA	a	825	-	-	11/36/112/115	-
39	CLA	0	320	-	-	8/15/91/115	-
39	CLA	M	308	-	-	12/39/115/115	-
46	LMG	l	208	49	-	15/34/54/70	0/1/1/1
49	KC2	1	315	-	-	11/15/71/71	-
39	CLA	F	309	-	-	6/24/100/115	-
43	DD6	K	303	-	-	0/26/80/80	0/3/3/3
48	A86	V	301	-	-	2/34/90/90	0/3/3/3
39	CLA	F	313	-	-	12/30/106/115	-
39	CLA	7	321	-	-	6/10/86/115	-
43	DD6	A	304	-	-	3/26/80/80	0/3/3/3
39	CLA	U	212	-	-	7/17/93/115	-
39	CLA	x	307	-	-	4/10/86/115	-
39	CLA	I	311	-	-	15/39/115/115	-
51	A1ECV	x	316	-	3/3/17/24	8/19/117/117	-
48	A86	Z	303	-	-	8/34/90/90	0/3/3/3
43	DD6	O	304	-	-	1/26/80/80	0/3/3/3
48	A86	O	307	-	-	9/34/90/90	0/3/3/3
49	KC2	H	311	-	-	9/15/71/71	-
39	CLA	8	313	-	-	5/10/86/115	-
48	A86	T	301	-	-	2/34/90/90	0/3/3/3
49	KC2	V	308	27	-	8/15/71/71	-
49	KC2	P	320	-	-	9/15/71/71	-
50	A1EB1	H	304	-	-	14/42/100/100	0/3/3/3
50	A1EB1	T	302	-	-	14/42/100/100	0/3/3/3
39	CLA	L	308	-	-	15/35/111/115	-
39	CLA	k	201	-	-	7/24/100/115	-
43	DD6	Z	302	-	-	2/26/80/80	0/3/3/3
50	A1EB1	V	307	-	-	12/42/100/100	0/3/3/3
42	BCR	m	101	-	-	9/29/63/63	0/2/2/2
39	CLA	6	313	-	-	5/12/88/115	-
49	KC2	5	311	-	-	6/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	T	307	-	-	6/42/100/100	0/3/3/3
43	DD6	G	306	-	-	4/26/80/80	0/3/3/3
39	CLA	O	309	-	-	6/15/91/115	-
39	CLA	R	308	-	-	11/33/109/115	-
50	A1EB1	y	301	-	-	11/42/100/100	0/3/3/3
46	LMG	A	316	-	-	13/24/44/70	0/1/1/1
51	A1ECV	Z	308	-	3/3/17/24	11/19/117/117	-
39	CLA	S	320	-	-	15/39/115/115	-
39	CLA	b	819	-	-	11/32/108/115	-
39	CLA	7	318	28	-	5/17/93/115	-
39	CLA	9	309	-	-	3/10/86/115	-
49	KC2	4	318	28	-	9/15/71/71	-
39	CLA	b	828	-	-	15/39/115/115	-
39	CLA	b	834	-	-	7/31/107/115	-
39	CLA	D	310	47	-	19/35/111/115	-
51	A1ECV	y	311	-	3/3/17/24	10/19/117/117	-
49	KC2	0	314	46,31	-	8/14/70/71	-
49	KC2	M	314	-	-	7/15/71/71	-
48	A86	9	303	-	-	7/34/90/90	0/3/3/3
48	A86	9	305	-	-	6/34/90/90	0/3/3/3
39	CLA	E	314	-	-	12/29/105/115	-
39	CLA	6	315	-	-	1/10/86/115	-
39	CLA	7	314	-	-	13/29/105/115	-
39	CLA	F	310	-	-	7/26/102/115	-
39	CLA	X	311	27	-	5/21/97/115	-
39	CLA	G	318	-	-	13/20/96/115	-
50	A1EB1	0	302	-	-	13/42/100/100	0/3/3/3
49	KC2	9	311	-	-	7/15/71/71	-
48	A86	7	312	-	-	4/34/90/90	0/3/3/3
43	DD6	A	302	-	-	0/26/80/80	0/3/3/3
39	CLA	b	824	-	-	10/33/109/115	-
39	CLA	L	310	23	-	14/39/115/115	-
39	CLA	X	316	-	-	9/18/94/115	-
49	KC2	7	322	-	-	12/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SQD	F	318	-	-	17/37/57/69	0/1/1/1
39	CLA	5	308	-	-	14/39/115/115	-
43	DD6	A	303	-	-	5/26/80/80	0/3/3/3
49	KC2	z	313	-	-	6/16/59/71	-
42	BCR	a	845	-	-	4/29/63/63	0/2/2/2
43	DD6	4	308	-	-	1/26/80/80	0/3/3/3
49	KC2	T	315	29	-	7/15/71/71	-
50	A1EB1	G	308	-	-	10/42/100/100	0/3/3/3
48	A86	1	302	-	-	5/34/90/90	0/3/3/3
49	KC2	C	312	-	-	10/15/71/71	-
46	LMG	S	322	49	-	28/41/61/70	0/1/1/1
51	A1ECV	G	316	-	3/3/17/24	11/19/117/117	-
39	CLA	V	309	-	-	11/39/115/115	-
48	A86	M	306	-	-	2/34/90/90	0/3/3/3
49	KC2	S	314	-	-	6/15/71/71	-
39	CLA	U	214	-	-	4/17/93/115	-
43	DD6	U	204	-	-	1/26/80/80	0/3/3/3
48	A86	9	304	-	-	9/34/90/90	0/3/3/3
39	CLA	b	839	-	-	4/18/94/115	-
39	CLA	U	211	-	-	9/33/109/115	-
42	BCR	b	846	-	-	3/29/63/63	0/2/2/2
39	CLA	0	311	-	-	11/27/103/115	-
39	CLA	a	818	-	-	11/39/115/115	-
52	A1EB4	5	304	-	-	5/38/99/103	0/3/3/3
39	CLA	U	215	-	-	7/10/86/115	-
39	CLA	b	832	-	-	15/39/115/115	-
52	A1EB4	P	305	-	-	10/37/98/103	0/3/3/3
39	CLA	a	803	-	-	17/39/115/115	-
43	DD6	P	304	-	-	2/26/80/80	0/3/3/3
48	A86	R	302	-	-	11/34/90/90	0/3/3/3
51	A1ECV	9	317	-	3/3/17/24	7/19/117/117	-
39	CLA	L	313	-	-	3/21/97/115	-
39	CLA	Z	304	-	-	5/10/86/115	-
39	CLA	S	308	-	-	18/35/111/115	-
43	DD6	G	303	-	-	1/26/80/80	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	DD6	x	304	-	-	0/26/80/80	0/3/3/3
48	A86	U	202	-	-	4/34/90/90	0/3/3/3
39	CLA	a	807	1	-	13/39/115/115	-
39	CLA	2	307	-	-	4/10/86/115	-
49	KC2	A	310	13	-	7/15/71/71	-
49	KC2	Q	313	46	-	9/14/70/71	-
39	CLA	o	203	12	-	7/27/103/115	-
48	A86	W	304	-	-	0/34/90/90	0/3/3/3
51	A1ECV	E	311	-	3/3/17/24	8/19/117/117	-
49	KC2	4	324	-	-	8/15/71/71	-
46	LMG	4	326	49	-	23/41/61/70	0/1/1/1
48	A86	8	323	-	-	4/34/90/90	0/3/3/3
42	BCR	f	804	-	-	2/29/63/63	0/2/2/2
39	CLA	a	805	-	-	11/39/115/115	-
49	KC2	1	314	-	-	11/15/71/71	-
49	KC2	z	312	-	-	7/15/71/71	-
39	CLA	1	316	-	-	5/10/86/115	-
39	CLA	B	205	-	-	5/12/88/115	-
51	A1ECV	W	317	-	3/3/17/24	9/19/117/117	-
39	CLA	Y	302	-	-	4/10/86/115	-
39	CLA	x	309	-	-	4/10/86/115	-
48	A86	8	309	-	-	4/34/90/90	0/3/3/3
50	A1EB1	V	305	-	-	12/42/100/100	0/3/3/3
49	KC2	W	308	-	-	6/15/71/71	-
39	CLA	b	808	-	-	7/15/91/115	-
43	DD6	o	204	-	-	2/26/80/80	0/3/3/3
39	CLA	X	307	-	-	10/39/115/115	-
45	DGD	C	314	-	-	15/29/69/95	0/2/2/2
39	CLA	4	322	-	-	7/24/100/115	-
39	CLA	a	824	-	-	7/39/115/115	-
48	A86	4	328	-	-	15/34/90/90	0/3/3/3
49	KC2	R	314	46	-	7/14/70/71	-
48	A86	0	306	-	-	2/34/90/90	0/3/3/3
48	A86	H	302	-	-	6/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	801	-	-	10/39/115/115	-
39	CLA	1	311	-	-	7/10/86/115	-
39	CLA	K	311	-	-	14/39/115/115	-
39	CLA	Z	316	-	-	8/10/86/115	-
39	CLA	B	203	-	-	5/17/93/115	-
48	A86	G	301	-	-	11/34/90/90	0/3/3/3
39	CLA	T	319	29	-	10/17/93/115	-
39	CLA	B	204	-	-	4/17/93/115	-
39	CLA	D	313	-	-	12/39/115/115	-
48	A86	1	306	-	-	9/34/90/90	0/3/3/3
42	BCR	l	207	-	-	2/29/63/63	0/2/2/2
43	DD6	1	304	-	-	4/26/80/80	0/3/3/3
48	A86	L	302	-	-	13/34/90/90	0/3/3/3
39	CLA	a	847	-	-	20/39/115/115	-
39	CLA	O	314	-	-	7/27/103/115	-
39	CLA	a	836	-	-	9/39/115/115	-
48	A86	M	303	-	-	0/34/90/90	0/3/3/3
48	A86	3	307	-	-	6/34/90/90	0/3/3/3
39	CLA	W	319	-	-	8/17/93/115	-
39	CLA	x	318	-	-	8/10/86/115	-
50	A1EB1	6	301	-	-	12/42/100/100	0/3/3/3
48	A86	L	304	-	-	12/34/90/90	0/3/3/3
48	A86	7	311	-	-	3/34/90/90	0/3/3/3
39	CLA	G	310	-	-	12/39/115/115	-
51	A1ECV	L	318	-	3/3/17/24	14/19/117/117	-
39	CLA	C	308	-	-	16/33/109/115	-
49	KC2	1	312	-	-	7/15/71/71	-
51	A1ECV	y	317	-	3/3/17/24	9/19/117/117	-
50	A1EB1	G	304	-	-	8/42/100/100	0/3/3/3
39	CLA	I	314	-	-	14/39/115/115	-
39	CLA	A	309	-	-	13/39/115/115	-
49	KC2	H	314	-	-	11/15/71/71	-
49	KC2	I	312	46	-	7/14/70/71	-
49	KC2	S	317	-	-	7/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A1ECV	M	316	-	3/3/17/24	8/19/117/117	-
42	BCR	h	202	-	-	6/29/63/63	0/2/2/2
49	KC2	W	314	-	-	7/15/71/71	-
39	CLA	1	310	-	-	6/15/91/115	-
39	CLA	9	310	-	-	3/10/86/115	-
49	KC2	9	316	35	-	9/15/71/71	-
49	KC2	P	310	46	-	8/14/70/71	-
39	CLA	a	806	-	-	17/39/115/115	-
42	BCR	j	103	-	-	4/29/63/63	0/2/2/2
49	KC2	W	312	46,24	-	8/14/70/71	-
39	CLA	b	822	2	-	4/21/97/115	-
39	CLA	o	206	-	-	14/31/107/115	-
39	CLA	y	312	-	-	5/12/88/115	-
49	KC2	5	314	-	-	8/15/71/71	-
39	CLA	E	319	17	-	13/20/96/115	-
48	A86	B	201	-	-	5/34/90/90	0/3/3/3
39	CLA	J	309	-	-	17/39/115/115	-
48	A86	k	206	-	-	5/34/90/90	0/3/3/3
47	SQD	k	205	-	-	13/33/53/69	0/1/1/1
39	CLA	b	809	-	-	16/39/115/115	-
46	LMG	W	320	-	-	15/28/48/70	0/1/1/1
49	KC2	P	313	24	-	10/15/71/71	-
51	A1ECV	S	318	-	3/3/17/24	6/19/117/117	-
48	A86	0	301	-	-	4/34/90/90	0/3/3/3
48	A86	6	309	-	-	13/34/90/90	0/3/3/3
39	CLA	S	311	-	-	13/39/115/115	-
39	CLA	T	318	-	-	9/18/94/115	-
39	CLA	U	208	-	-	5/17/93/115	-
50	A1EB1	5	302	-	-	9/42/100/100	0/3/3/3
39	CLA	M	321	24	-	5/17/93/115	-
39	CLA	Z	307	-	-	0/10/86/115	-
49	KC2	Q	315	-	-	8/15/71/71	-
39	CLA	b	826	-	-	9/39/115/115	-
49	KC2	A	313	-	-	11/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	825	-	-	14/39/115/115	-
46	LMG	7	301	49	-	23/41/61/70	0/1/1/1
49	KC2	y	313	-	-	8/15/71/71	-
42	BCR	f	801	-	-	4/29/63/63	0/2/2/2
43	DD6	4	307	-	-	1/26/80/80	0/3/3/3
50	A1EB1	G	307	-	-	17/42/100/100	0/3/3/3
39	CLA	0	310	-	-	25/35/111/115	-
50	A1EB1	0	307	-	-	11/42/100/100	0/3/3/3
39	CLA	M	310	-	-	14/39/115/115	-
39	CLA	b	840	-	-	11/39/115/115	-
39	CLA	0	322	-	-	14/23/99/115	-
49	KC2	G	311	19	-	9/15/71/71	-
49	KC2	8	317	-	-	8/15/71/71	-
39	CLA	C	305	-	-	17/35/111/115	-
50	A1EB1	R	303	-	-	10/42/100/100	0/3/3/3
48	A86	T	305	-	-	6/34/90/90	0/3/3/3
39	CLA	E	312	-	-	23/39/115/115	-
43	DD6	A	301	-	-	0/26/80/80	0/3/3/3
39	CLA	l	204	-	-	11/39/115/115	-
39	CLA	F	306	-	-	6/17/93/115	-
39	CLA	X	309	-	-	14/39/115/115	-
39	CLA	S	319	-	-	10/24/100/115	-
42	BCR	b	844	-	-	6/29/63/63	0/2/2/2
39	CLA	a	817	1	-	6/15/91/115	-
39	CLA	J	313	-	-	9/17/93/115	-
39	CLA	8	312	-	-	8/15/91/115	-
39	CLA	Z	305	-	-	4/10/86/115	-
43	DD6	W	305	-	-	1/26/80/80	0/3/3/3
49	KC2	P	312	-	-	7/15/71/71	-
39	CLA	V	316	-	-	6/21/97/115	-
48	A86	2	301	-	-	3/34/90/90	0/3/3/3
39	CLA	2	312	-	-	7/10/86/115	-
41	LHG	D	301	-	-	8/39/39/53	-
50	A1EB1	x	301	-	-	14/42/100/100	0/3/3/3
49	KC2	G	313	-	-	6/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	L	312	-	-	8/15/71/71	-
39	CLA	A	308	-	-	9/23/99/115	-
39	CLA	V	313	27	-	8/39/115/115	-
43	DD6	5	303	-	-	1/26/80/80	0/3/3/3
39	CLA	H	315	-	-	6/10/86/115	-
39	CLA	Y	314	-	-	8/10/86/115	-
39	CLA	y	308	-	-	9/15/91/115	-
48	A86	R	317	-	-	3/34/90/90	0/3/3/3
47	SQD	7	302	-	-	15/34/54/69	0/1/1/1
39	CLA	o	202	-	-	5/12/88/115	-
39	CLA	9	307	-	-	4/10/86/115	-
48	A86	K	301	-	-	6/34/90/90	0/3/3/3
39	CLA	J	311	-	-	12/39/115/115	-
39	CLA	b	814	-	-	7/27/103/115	-
39	CLA	U	210	-	-	9/33/109/115	-
48	A86	Y	301	-	-	5/34/90/90	0/3/3/3
50	A1EB1	F	304	-	-	11/42/100/100	0/3/3/3
39	CLA	T	313	-	-	6/23/99/115	-
39	CLA	9	308	-	-	17/27/103/115	-
49	KC2	V	320	-	-	8/15/71/71	-
43	DD6	z	305	-	-	1/26/80/80	0/3/3/3
49	KC2	3	321	-	-	10/15/71/71	-
48	A86	F	301	-	-	4/34/90/90	0/3/3/3
49	KC2	L	317	-	-	11/15/71/71	-
39	CLA	5	315	-	-	5/18/94/115	-
51	A1ECV	T	317	-	3/3/17/24	6/19/117/117	-
49	KC2	9	318	-	-	10/15/71/71	-
39	CLA	D	311	-	-	23/39/115/115	-
49	KC2	Y	308	-	-	9/15/71/71	-
49	KC2	2	313	-	-	6/13/69/71	-
43	DD6	E	305	-	-	3/26/80/80	0/3/3/3
39	CLA	H	308	-	-	7/33/109/115	-
39	CLA	4	316	-	-	13/39/115/115	-
39	CLA	J	308	-	-	6/21/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	802	-	-	6/39/115/115	-
47	SQD	P	301	-	-	12/33/53/69	0/1/1/1
39	CLA	6	318	-	-	8/10/86/115	-
48	A86	L	305	-	-	2/34/90/90	0/3/3/3
39	CLA	A	314	-	-	17/39/115/115	-
39	CLA	a	835	-	-	13/39/115/115	-
51	A1ECV	Z	314	-	3/3/17/24	7/19/117/117	-
43	DD6	X	304	-	-	0/26/80/80	0/3/3/3
39	CLA	L	311	23	-	10/24/100/115	-
39	CLA	A	312	-	-	15/39/115/115	-
49	KC2	V	312	-	-	6/15/71/71	-
39	CLA	l	203	-	-	8/20/96/115	-
52	A1EB4	P	319	-	-	6/38/99/103	0/3/3/3
39	CLA	S	309	-	-	19/39/115/115	-
48	A86	W	303	-	-	4/34/90/90	0/3/3/3
51	A1ECV	Y	306	-	3/3/17/24	9/19/117/117	-
46	LMG	P	317	49	-	18/34/54/70	0/1/1/1
50	A1EB1	8	306	-	-	13/42/100/100	0/3/3/3
39	CLA	a	810	-	-	8/26/102/115	-
43	DD6	z	304	-	-	6/26/80/80	0/3/3/3
42	BCR	b	845	-	-	1/29/63/63	0/2/2/2
50	A1EB1	2	306	-	-	16/42/100/100	0/3/3/3
50	A1EB1	8	304	-	-	10/42/100/100	0/3/3/3
39	CLA	E	313	-	-	13/39/115/115	-
39	CLA	7	324	-	-	5/10/86/115	-
49	KC2	y	314	-	-	7/15/71/71	-
39	CLA	6	312	-	-	8/20/96/115	-
48	A86	8	302	-	-	8/34/90/90	0/3/3/3
39	CLA	C	307	-	-	12/39/115/115	-
46	LMG	M	319	49	-	13/34/54/70	0/1/1/1
39	CLA	b	820	-	-	16/33/109/115	-
49	KC2	P	306	24	-	7/15/71/71	-
48	A86	9	301	-	-	9/34/90/90	0/3/3/3
48	A86	z	303	-	-	9/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	8	316	-	-	11/15/71/71	-
39	CLA	a	830	-	-	20/39/115/115	-
39	CLA	H	316	-	-	10/17/93/115	-
52	A1EB4	W	321	-	-	8/38/99/103	0/3/3/3
39	CLA	Z	309	-	-	2/10/86/115	-
39	CLA	7	325	-	-	9/21/97/115	-
50	A1EB1	0	303	-	-	10/42/100/100	0/3/3/3
49	KC2	T	312	-	-	10/15/71/71	-
48	A86	D	305	-	-	8/34/90/90	0/3/3/3
50	A1EB1	3	324	-	-	20/42/100/100	0/3/3/3
50	A1EB1	7	303	-	-	17/42/100/100	0/3/3/3
50	A1EB1	O	301	-	-	16/42/100/100	0/3/3/3
41	LHG	j	104	-	-	22/34/34/53	-
48	A86	x	305	-	-	8/34/90/90	0/3/3/3
39	CLA	1	313	32	-	5/10/86/115	-
48	A86	5	301	-	-	3/34/90/90	0/3/3/3
39	CLA	J	310	-	-	8/27/103/115	-
49	KC2	8	314	-	-	10/15/71/71	-
39	CLA	a	819	-	-	11/20/96/115	-
49	KC2	K	313	22	-	9/15/71/71	-
49	KC2	2	314	-	-	10/15/71/71	-
48	A86	3	306	-	-	8/34/90/90	0/3/3/3
47	SQD	D	304	-	-	8/33/53/69	0/1/1/1
48	A86	4	306	-	-	8/34/90/90	0/3/3/3
43	DD6	7	310	-	-	4/26/80/80	0/3/3/3
48	A86	7	307	-	-	3/34/90/90	0/3/3/3
50	A1EB1	S	303	-	-	14/42/100/100	0/3/3/3
39	CLA	b	831	-	-	7/21/97/115	-
49	KC2	4	320	-	-	10/15/71/71	-
49	KC2	S	315	28	-	7/15/71/71	-
39	CLA	b	811	-	-	10/39/115/115	-
49	KC2	F	311	46	-	7/14/70/71	-
50	A1EB1	8	308	-	-	11/42/100/100	0/3/3/3
39	CLA	M	318	24	-	7/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	6	319	-	-	11/15/71/71	-
43	DD6	O	305	-	-	5/26/80/80	0/3/3/3
50	A1EB1	1	305	-	-	10/42/100/100	0/3/3/3
39	CLA	P	308	24	-	22/39/115/115	-
39	CLA	a	833	1	-	11/15/91/115	-
50	A1EB1	K	305	-	-	7/42/100/100	0/3/3/3
39	CLA	C	309	-	-	13/17/93/115	-
39	CLA	b	807	-	-	14/39/115/115	-
39	CLA	x	314	-	-	7/10/86/115	-
49	KC2	L	314	-	-	7/15/71/71	-
39	CLA	L	320	-	-	10/17/93/115	-
51	A1ECV	Q	319	-	3/3/17/24	13/19/117/117	-
41	LHG	D	302	-	-	21/39/39/53	-
43	DD6	2	303	-	-	2/26/80/80	0/3/3/3
50	A1EB1	6	308	-	-	15/42/100/100	0/3/3/3
39	CLA	M	317	-	-	6/23/99/115	-
39	CLA	y	307	-	-	4/10/86/115	-
39	CLA	0	318	-	-	3/10/86/115	-
39	CLA	E	316	-	-	8/24/100/115	-
48	A86	y	306	-	-	6/34/90/90	0/3/3/3
39	CLA	J	316	-	-	7/17/93/115	-
39	CLA	I	309	-	-	12/39/115/115	-
52	A1EB4	M	305	-	-	9/39/100/103	0/3/3/3
48	A86	S	307	-	-	6/34/90/90	0/3/3/3
39	CLA	b	812	-	-	10/39/115/115	-
49	KC2	I	303	-	-	7/15/71/71	-
39	CLA	H	313	-	-	9/39/115/115	-
39	CLA	x	317	-	-	5/10/86/115	-
41	LHG	a	840	-	-	26/53/53/53	-
49	KC2	0	316	-	-	4/15/71/71	-
50	A1EB1	L	303	-	-	15/42/100/100	0/3/3/3
39	CLA	b	821	-	-	11/39/115/115	-
48	A86	F	302	-	-	2/34/90/90	0/3/3/3
39	CLA	b	806	-	-	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	9	320	-	-	4/10/86/115	-
39	CLA	T	310	29	-	6/24/100/115	-
49	KC2	X	314	46	-	7/14/70/71	-
50	A1EB1	Q	307	-	-	8/42/100/100	0/3/3/3
39	CLA	T	320	-	-	10/24/100/115	-
44	SF4	b	804	-	-	-	0/6/5/5
49	KC2	X	312	-	-	7/15/71/71	-
49	KC2	4	317	-	-	5/15/71/71	-
48	A86	Q	305	-	-	16/34/90/90	0/3/3/3
50	A1EB1	4	304	-	-	9/42/100/100	0/3/3/3
39	CLA	E	318	17	-	10/17/93/115	-
39	CLA	Y	304	-	-	9/17/93/115	-
51	A1ECV	4	321	-	3/3/17/24	10/19/117/117	-
39	CLA	3	312	-	-	22/39/115/115	-
43	DD6	M	304	-	-	0/26/80/80	0/3/3/3
50	A1EB1	z	301	-	-	12/34/90/100	0/3/3/3
39	CLA	C	311	-	-	17/39/115/115	-
48	A86	2	305	-	-	12/34/90/90	0/3/3/3
39	CLA	a	813	1	-	4/21/97/115	-
50	A1EB1	1	301	-	-	11/42/100/100	0/3/3/3
39	CLA	H	310	-	-	7/30/106/115	-
49	KC2	5	313	46	-	7/14/70/71	-
50	A1EB1	x	302	-	-	15/42/100/100	0/3/3/3
49	KC2	2	317	-	-	7/15/71/71	-
39	CLA	O	316	-	-	6/10/86/115	-
39	CLA	6	311	-	-	1/8/84/115	-
49	KC2	7	320	-	-	7/15/71/71	-
49	KC2	x	315	-	-	10/15/71/71	-
39	CLA	E	306	17	-	6/20/96/115	-
51	A1ECV	X	313	-	3/3/17/24	7/19/117/117	-
49	KC2	Y	309	-	-	8/15/71/71	-
39	CLA	G	314	19	-	8/31/107/115	-
49	KC2	R	318	-	-	7/15/71/71	-
51	A1ECV	7	317	-	3/3/17/24	7/19/117/117	-
39	CLA	6	322	-	-	11/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	838	-	-	15/39/115/115	-
49	KC2	K	310	-	-	7/15/71/71	-
39	CLA	0	315	31	-	5/21/97/115	-
43	DD6	I	307	-	-	1/26/80/80	0/3/3/3
39	CLA	M	315	-	-	4/10/86/115	-
46	LMG	9	321	-	-	16/31/51/70	0/1/1/1
39	CLA	8	310	-	-	8/15/91/115	-
47	SQD	S	301	-	-	13/34/54/69	0/1/1/1
39	CLA	a	802	-	-	7/27/103/115	-
50	A1EB1	7	306	-	-	10/42/100/100	0/3/3/3
47	SQD	D	321	-	-	16/34/54/69	0/1/1/1
39	CLA	b	841	2	-	12/39/115/115	-
43	DD6	I	305	-	-	1/26/80/80	0/3/3/3
39	CLA	a	816	-	-	15/39/115/115	-
48	A86	L	306	-	-	12/34/90/90	0/3/3/3
39	CLA	y	310	-	-	7/10/86/115	-
39	CLA	R	315	-	-	7/18/94/115	-
46	LMG	F	317	49	-	20/34/54/70	0/1/1/1
39	CLA	i	101	-	-	10/39/115/115	-
39	CLA	T	308	-	-	10/17/93/115	-
43	DD6	C	301	-	-	3/26/80/80	0/3/3/3
49	KC2	R	312	-	-	8/15/71/71	-
42	BCR	b	850	-	-	6/29/63/63	0/2/2/2
47	SQD	W	301	-	-	8/22/42/69	0/1/1/1
49	KC2	6	314	-	-	8/15/71/71	-
51	A1ECV	X	310	-	3/3/17/24	10/19/117/117	-
42	BCR	i	102	-	-	4/29/63/63	0/2/2/2
39	CLA	b	823	-	-	9/17/93/115	-
48	A86	W	307	-	-	2/34/90/90	0/3/3/3
39	CLA	Y	313	-	-	5/10/86/115	-
43	DD6	3	304	-	-	3/26/80/80	0/3/3/3
50	A1EB1	H	301	-	-	12/42/100/100	0/3/3/3
39	CLA	h	201	-	-	10/27/103/115	-
39	CLA	b	829	-	-	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	836	-	-	3/15/91/115	-
39	CLA	3	313	-	-	5/25/101/115	-
43	DD6	S	306	-	-	4/26/80/80	0/3/3/3
46	LMG	Q	322	49	-	13/23/43/70	0/1/1/1
39	CLA	8	311	-	-	11/27/103/115	-
39	CLA	8	321	-	-	4/12/88/115	-
39	CLA	W	318	-	-	7/23/99/115	-
39	CLA	3	320	-	-	5/15/91/115	-
48	A86	S	305	-	-	6/34/90/90	0/3/3/3
39	CLA	D	319	16	-	22/39/115/115	-
39	CLA	E	310	-	-	9/39/115/115	-
39	CLA	Y	303	-	-	4/10/86/115	-
49	KC2	6	317	-	-	9/15/71/71	-
39	CLA	B	209	-	-	12/29/105/115	-
39	CLA	k	203	-	-	9/27/103/115	-
39	CLA	f	802	-	-	11/39/115/115	-
43	DD6	E	302	-	-	0/26/80/80	0/3/3/3
48	A86	P	303	-	-	0/34/90/90	0/3/3/3
42	BCR	b	847	-	-	4/29/63/63	0/2/2/2
49	KC2	L	321	-	-	7/15/71/71	-
50	A1EB1	D	308	-	-	8/42/100/100	0/3/3/3
39	CLA	8	322	-	-	4/10/86/115	-
39	CLA	a	837	-	-	5/39/115/115	-
39	CLA	z	308	-	-	4/17/93/115	-
47	SQD	T	321	-	-	13/31/51/69	0/1/1/1
39	CLA	b	835	-	-	16/39/115/115	-
42	BCR	k	204	-	-	2/29/63/63	0/2/2/2
39	CLA	Z	315	-	-	4/10/86/115	-
43	DD6	H	305	-	-	2/26/80/80	0/3/3/3
47	SQD	H	318	-	-	9/33/53/69	0/1/1/1
39	CLA	B	207	-	-	14/27/103/115	-
44	SF4	c	101	-	-	-	0/6/5/5
39	CLA	T	309	-	-	11/29/105/115	-
48	A86	P	302	-	-	12/34/90/90	0/3/3/3
46	LMG	D	322	-	-	14/32/52/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	U	203	-	-	9/42/100/100	0/3/3/3
39	CLA	Q	312	-	-	11/39/115/115	-
39	CLA	0	323	-	-	11/17/93/115	-
39	CLA	E	308	-	-	11/39/115/115	-
39	CLA	L	319	-	-	8/23/99/115	-
39	CLA	O	318	-	-	6/17/93/115	-
43	DD6	j	102	-	-	6/26/80/80	0/3/3/3
48	A86	L	301	-	-	7/34/90/90	0/3/3/3
43	DD6	T	303	-	-	1/26/80/80	0/3/3/3
49	KC2	T	314	-	-	7/15/71/71	-
39	CLA	I	315	-	-	6/24/100/115	-
39	CLA	W	309	-	-	12/39/115/115	-
39	CLA	I	316	36	-	2/10/86/115	-
52	A1EB4	P	318	-	-	9/35/96/103	0/3/3/3
39	CLA	o	201	-	-	5/23/99/115	-
39	CLA	W	311	-	-	15/39/115/115	-
39	CLA	x	308	-	-	2/10/86/115	-
48	A86	6	307	-	-	10/34/90/90	0/3/3/3
39	CLA	Q	317	-	-	7/17/93/115	-
49	KC2	y	316	-	-	7/15/71/71	-
39	CLA	4	313	-	-	3/17/93/115	-
48	A86	M	302	-	-	8/34/90/90	0/3/3/3
47	SQD	F	319	-	-	13/32/52/69	0/1/1/1
43	DD6	Q	306	-	-	1/26/80/80	0/3/3/3
43	DD6	J	304	-	-	3/26/80/80	0/3/3/3
52	A1EB4	X	305	-	-	10/38/99/103	0/3/3/3
39	CLA	K	314	-	-	6/10/86/115	-
39	CLA	C	310	-	-	18/39/115/115	-
48	A86	I	304	-	-	11/34/90/90	0/3/3/3
39	CLA	Q	309	-	-	9/35/111/115	-
39	CLA	U	213	-	-	6/10/86/115	-
39	CLA	K	312	-	-	17/39/115/115	-
43	DD6	D	306	-	-	0/26/80/80	0/3/3/3
39	CLA	X	308	-	-	18/33/109/115	-
39	CLA	R	307	-	-	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	G	305	-	-	7/34/90/90	0/3/3/3
50	A1EB1	K	302	-	-	6/42/100/100	0/3/3/3
39	CLA	R	316	-	-	10/24/100/115	-
49	KC2	V	318	-	-	7/15/71/71	-
39	CLA	z	314	-	-	5/10/86/115	-
39	CLA	b	827	-	-	10/39/115/115	-
39	CLA	E	309	-	-	7/25/101/115	-
48	A86	T	306	-	-	6/34/90/90	0/3/3/3
51	A1ECV	R	313	-	3/3/17/24	9/19/117/117	-
39	CLA	X	317	-	-	10/24/100/115	-
41	LHG	a	841	39	-	13/31/31/53	-
39	CLA	A	307	-	-	8/33/109/115	-
39	CLA	3	319	-	-	6/10/86/115	-
51	A1ECV	0	321	48	2/2/17/24	10/19/117/117	-
43	DD6	D	303	-	-	0/26/80/80	0/3/3/3
46	LMG	0	324	49	-	13/21/41/70	0/1/1/1
50	A1EB1	J	302	-	-	9/42/100/100	0/3/3/3
39	CLA	I	310	-	-	10/26/102/115	-
39	CLA	b	815	-	-	14/39/115/115	-
39	CLA	A	315	-	-	8/21/97/115	-
49	KC2	J	315	-	-	10/15/71/71	-
39	CLA	4	319	-	-	4/10/86/115	-
43	DD6	a	846	-	-	5/26/80/80	0/3/3/3
51	A1ECV	1	318	-	3/3/17/24	6/19/117/117	-
39	CLA	O	313	-	-	4/21/97/115	-
49	KC2	Z	311	-	-	10/15/71/71	-
39	CLA	b	833	-	-	15/39/115/115	-
39	CLA	P	316	-	-	7/23/99/115	-
48	A86	6	302	-	-	7/34/90/90	0/3/3/3
50	A1EB1	3	309	-	-	9/42/100/100	0/3/3/3
39	CLA	z	318	-	-	6/10/86/115	-
39	CLA	J	307	21	-	10/20/96/115	-
49	KC2	9	313	-	-	6/15/71/71	-
49	KC2	M	311	46	-	7/14/70/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	Y	310	-	-	4/10/86/115	-
48	A86	E	304	-	-	2/34/90/90	0/3/3/3
39	CLA	Q	321	-	-	6/25/101/115	-
48	A86	S	304	-	-	8/34/90/90	0/3/3/3
49	KC2	M	307	-	-	7/15/71/71	-
50	A1EB1	7	304	-	-	14/42/100/100	0/3/3/3
51	A1ECV	R	310	-	3/3/17/24	12/19/117/117	-
39	CLA	2	319	-	-	13/17/93/115	-
39	CLA	a	814	-	-	15/35/111/115	-
39	CLA	o	205	-	-	12/24/100/115	-
39	CLA	A	306	-	-	11/35/111/115	-
39	CLA	Q	311	-	-	5/17/93/115	-
49	KC2	x	313	-	-	6/15/71/71	-
39	CLA	Q	310	-	-	20/39/115/115	-
42	BCR	a	842	-	-	4/29/63/63	0/2/2/2
48	A86	0	309	-	-	7/34/90/90	0/3/3/3
48	A86	3	308	-	-	6/34/90/90	0/3/3/3
39	CLA	O	308	-	-	4/4/80/115	-
43	DD6	E	303	-	-	1/26/80/80	0/3/3/3
39	CLA	E	315	-	-	12/17/93/115	-
49	KC2	M	313	-	-	6/15/71/71	-
49	KC2	6	316	-	-	10/15/71/71	-
39	CLA	H	312	20	-	19/39/115/115	-
39	CLA	P	311	-	-	10/39/115/115	-
39	CLA	U	209	-	-	8/24/100/115	-
39	CLA	1	317	-	-	6/10/86/115	-
48	A86	C	303	-	-	6/34/90/90	0/3/3/3
50	A1EB1	4	301	-	-	12/42/100/100	0/3/3/3
43	DD6	F	303	-	-	0/26/80/80	0/3/3/3
39	CLA	b	803	-	-	14/39/115/115	-
48	A86	O	302	-	-	2/34/90/90	0/3/3/3
48	A86	6	305	-	-	11/34/90/90	0/3/3/3
51	A1ECV	7	323	-	2/2/17/24	8/19/117/117	-
49	KC2	0	319	-	-	10/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	A1ECV	9	314	-	3/3/17/24	9/19/117/117	-
48	A86	8	307	-	-	12/34/90/90	0/3/3/3
49	KC2	5	305	27	-	7/15/71/71	-
39	CLA	z	307	-	-	3/12/88/115	-
42	BCR	a	843	-	-	0/29/63/63	0/2/2/2
39	CLA	P	307	-	-	12/39/115/115	-
48	A86	1	303	-	-	2/34/90/90	0/3/3/3
39	CLA	z	317	-	-	7/12/88/115	-
39	CLA	3	316	-	-	7/21/97/115	-
43	DD6	R	304	-	-	0/26/80/80	0/3/3/3
46	LMG	S	321	-	-	11/27/47/70	0/1/1/1
39	CLA	a	829	-	-	7/29/105/115	-
39	CLA	Q	314	-	-	6/26/102/115	-
43	DD6	J	305	-	-	3/26/80/80	0/3/3/3
42	BCR	l	202	-	-	4/29/63/63	0/2/2/2
43	DD6	y	303	-	-	1/26/80/80	0/3/3/3
43	DD6	3	301	-	-	2/26/80/80	0/3/3/3
50	A1EB1	G	302	-	-	8/42/100/100	0/3/3/3
43	DD6	I	306	-	-	2/26/80/80	0/3/3/3
39	CLA	E	307	-	-	21/39/115/115	-
50	A1EB1	8	301	-	-	13/42/100/100	0/3/3/3
39	CLA	2	318	-	-	5/10/86/115	-
39	CLA	O	312	-	-	7/17/93/115	-
39	CLA	3	311	-	-	16/35/111/115	-
40	PQN	b	843	-	-	3/23/43/43	0/2/2/2
39	CLA	Z	313	-	-	6/10/86/115	-
39	CLA	D	314	-	-	11/39/115/115	-
39	CLA	a	831	-	-	12/39/115/115	-
39	CLA	y	318	-	-	7/12/88/115	-
48	A86	2	302	-	-	5/34/90/90	0/3/3/3
39	CLA	5	306	-	-	13/39/115/115	-
51	A1ECV	S	312	-	3/3/17/24	9/19/117/117	-
39	CLA	D	312	16	-	9/27/103/115	-
39	CLA	R	309	-	-	13/39/115/115	-
39	CLA	4	311	-	-	19/35/111/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	X	301	-	-	25/45/45/53	-
43	DD6	O	303	-	-	3/26/80/80	0/3/3/3
39	CLA	8	318	-	-	5/10/86/115	-
39	CLA	I	313	-	-	19/39/115/115	-
39	CLA	b	816	-	-	10/33/109/115	-
39	CLA	a	827	-	-	6/39/115/115	-
39	CLA	5	316	-	-	10/24/100/115	-
39	CLA	G	309	-	-	15/29/105/115	-
48	A86	L	307	-	-	3/34/90/90	0/3/3/3
46	LMG	I	302	-	-	23/37/57/70	0/1/1/1
39	CLA	V	310	-	-	10/33/109/115	-
39	CLA	9	312	35	-	5/12/88/115	-
47	SQD	M	301	-	-	15/34/54/69	0/1/1/1
39	CLA	1	319	-	-	12/23/99/115	-
39	CLA	9	319	-	-	8/15/91/115	-
50	A1EB1	9	302	-	-	18/42/100/100	0/3/3/3
49	KC2	Q	318	26	-	6/15/71/71	-
49	KC2	3	318	-	-	6/15/71/71	-
39	CLA	i	103	-	-	17/39/115/115	-
46	LMG	W	302	49	-	18/34/54/70	0/1/1/1
48	A86	X	302	-	-	7/34/90/90	0/3/3/3
51	A1ECV	Q	316	26	3/3/17/24	9/19/117/117	-
49	KC2	W	315	-	-	8/15/71/71	-
48	A86	8	305	-	-	12/34/90/90	0/3/3/3
39	CLA	C	304	-	-	5/13/89/115	-
39	CLA	y	315	-	-	8/10/86/115	-
43	DD6	B	202	-	-	3/26/80/80	0/3/3/3
49	KC2	3	317	-	-	7/15/71/71	-
50	A1EB1	3	303	-	-	8/42/100/100	0/3/3/3
43	DD6	F	305	-	-	1/26/80/80	0/3/3/3
39	CLA	2	316	-	-	6/10/86/115	-
39	CLA	a	821	-	-	13/27/103/115	-
43	DD6	H	303	-	-	1/26/80/80	0/3/3/3
45	DGD	b	849	-	-	27/49/89/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	a	804	-	-	18/39/115/115	-
39	CLA	1	308	-	-	6/10/86/115	-
39	CLA	x	306	-	-	7/15/91/115	-
48	A86	y	305	-	-	0/34/90/90	0/3/3/3
39	CLA	K	308	22	-	13/32/108/115	-
49	KC2	Z	310	-	-	9/15/71/71	-
50	A1EB1	4	303	-	-	12/42/100/100	0/3/3/3
39	CLA	f	803	-	-	11/27/103/115	-
51	A1ECV	O	315	-	3/3/17/24	7/19/117/117	-
51	A1ECV	P	315	-	3/3/17/24	12/19/117/117	-
39	CLA	I	308	-	-	10/35/111/115	-
50	A1EB1	V	302	-	-	12/42/100/100	0/3/3/3
39	CLA	7	315	-	-	6/21/97/115	-
39	CLA	b	805	-	-	9/39/115/115	-
39	CLA	b	837	-	-	10/33/109/115	-
39	CLA	a	811	-	-	17/39/115/115	-
43	DD6	V	303	-	-	0/26/80/80	0/3/3/3
39	CLA	L	309	-	-	11/25/101/115	-
46	LMG	M	320	-	-	10/28/48/70	0/1/1/1
47	SQD	4	327	-	-	17/34/54/69	0/1/1/1
39	CLA	5	310	27	-	6/21/97/115	-
39	CLA	B	206	-	-	6/12/88/115	-
49	KC2	X	318	-	-	7/15/71/71	-
51	A1ECV	x	310	-	3/3/17/24	5/19/117/117	-
49	KC2	G	317	-	-	7/15/71/71	-
39	CLA	M	309	-	-	17/39/115/115	-
39	CLA	b	813	-	-	3/25/101/115	-
39	CLA	T	311	-	-	5/29/105/115	-
50	A1EB1	6	306	-	-	5/34/90/100	0/3/3/3
39	CLA	a	828	1	-	6/21/97/115	-
51	A1ECV	z	310	-	3/3/17/24	11/19/117/117	-
51	A1ECV	2	311	-	3/3/17/24	8/19/117/117	-
39	CLA	7	316	-	-	10/39/115/115	-
48	A86	U	206	-	-	3/34/90/90	0/3/3/3
48	A86	4	309	-	-	1/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	X	306	27	-	10/15/71/71	-
49	KC2	8	320	-	-	8/15/71/71	-
52	A1EB4	T	304	-	-	9/36/97/103	0/3/3/3
39	CLA	0	313	-	-	12/27/103/115	-
39	CLA	8	315	-	-	3/13/89/115	-
51	A1ECV	z	316	-	3/3/17/24	6/19/117/117	-
39	CLA	P	314	-	-	4/10/86/115	-
39	CLA	7	313	-	-	21/35/111/115	-
44	SF4	c	102	-	-	-	0/6/5/5
39	CLA	2	315	-	-	5/10/86/115	-
39	CLA	j	101	-	-	19/39/115/115	-
39	CLA	b	842	-	-	14/39/115/115	-
50	A1EB1	U	205	-	-	11/42/100/100	0/3/3/3
51	A1ECV	4	315	-	3/3/17/24	9/19/117/117	-
39	CLA	D	317	-	-	16/39/115/115	-
39	CLA	R	311	27	-	5/21/97/115	-
52	A1EB4	W	306	-	-	10/37/98/103	0/3/3/3
48	A86	O	306	-	-	6/34/90/90	0/3/3/3
51	A1ECV	V	317	-	3/3/17/24	11/19/117/117	-
39	CLA	I	301	41	-	7/24/100/115	-
39	CLA	k	202	-	-	13/27/103/115	-
50	A1EB1	3	302	-	-	15/42/100/100	0/3/3/3
39	CLA	b	810	-	-	15/39/115/115	-
39	CLA	F	315	18	-	4/10/86/115	-
49	KC2	C	313	-	-	11/15/71/71	-
39	CLA	z	311	-	-	5/10/86/115	-
39	CLA	2	308	-	-	11/17/93/115	-
39	CLA	F	316	-	-	10/23/99/115	-
43	DD6	D	307	-	-	2/26/80/80	0/3/3/3
50	A1EB1	V	306	-	-	7/42/100/100	0/3/3/3
39	CLA	3	314	-	-	18/39/115/115	-
50	A1EB1	4	302	-	-	11/42/100/100	0/3/3/3
39	CLA	y	319	-	-	5/10/86/115	-
43	DD6	x	303	-	-	1/26/80/80	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	3	323	-	-	11/17/93/115	-
39	CLA	4	314	-	-	10/39/115/115	-
41	LHG	H	317	-	-	18/39/39/53	-
49	KC2	B	208	-	-	9/15/71/71	-
39	CLA	4	323	-	-	13/39/115/115	-
39	CLA	4	312	-	-	18/39/115/115	-
39	CLA	a	823	-	-	10/39/115/115	-
49	KC2	V	315	-	-	9/15/71/71	-
39	CLA	a	834	-	-	6/23/99/115	-
48	A86	4	310	-	-	5/34/90/90	0/3/3/3
39	CLA	a	832	-	-	7/21/97/115	-

The worst 5 of 5834 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	M	322	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	319	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	318	A1EB4	C13-C11	-16.98	1.25	1.43
52	W	321	A1EB4	C13-C11	-16.67	1.25	1.43
52	T	304	A1EB4	C13-C11	-16.45	1.25	1.43

The worst 5 of 9304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2	303	DD6	O1-C20-C21	17.30	135.78	115.06
43	Z	302	DD6	O1-C20-C21	17.29	135.77	115.06
43	F	305	DD6	O1-C20-C21	13.19	130.87	115.06
43	D	303	DD6	O1-C20-C21	12.88	130.49	115.06
52	M	322	A1EB4	O1-C20-C21	12.53	130.07	115.06

5 of 115 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
51	E	311	A1ECV	NA
51	E	311	A1ECV	NB
51	E	311	A1ECV	ND
51	G	316	A1ECV	NA
51	G	316	A1ECV	NB

5 of 7546 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	a	801	CLA	CBD-CGD-O2D-CED
39	a	802	CLA	C1A-C2A-CAA-CBA
39	a	803	CLA	CHA-CBD-CGD-O1D
39	a	803	CLA	CHA-CBD-CGD-O2D
39	a	803	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

444 monomers are involved in 929 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	b	848	BCR	5	0
48	0	304	A86	1	0
48	Q	301	A86	1	0
39	a	838	CLA	3	0
39	P	309	CLA	1	0
46	7	326	LMG	2	0
39	a	822	CLA	5	0
39	W	313	CLA	2	0
39	2	310	CLA	1	0
39	b	817	CLA	3	0
39	U	207	CLA	3	0
50	z	302	A1EB1	1	0
39	A	311	CLA	2	0
46	F	320	LMG	7	0
50	2	304	A1EB1	1	0
39	V	319	CLA	1	0
48	1	307	A86	1	0
39	K	307	CLA	1	0
39	S	313	CLA	4	0
39	a	820	CLA	2	0
43	Q	303	DD6	5	0
39	D	318	CLA	5	0
49	7	319	KC2	1	0
49	O	317	KC2	1	0
42	a	844	BCR	3	0
39	V	311	CLA	1	0
39	b	851	CLA	4	0
39	D	309	CLA	1	0
39	F	321	CLA	1	0
39	J	318	CLA	2	0
46	4	325	LMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	6	321	CLA	1	0
39	2	309	CLA	1	0
39	D	315	CLA	1	0
39	a	812	CLA	1	0
49	F	307	KC2	1	0
39	K	306	CLA	6	0
39	6	310	CLA	1	0
48	Q	304	A86	28	0
39	1	309	CLA	1	0
39	a	826	CLA	3	0
39	a	801	CLA	6	0
49	L	315	KC2	1	0
39	z	306	CLA	1	0
39	U	201	CLA	1	0
39	l	201	CLA	3	0
49	x	312	KC2	1	0
39	D	316	CLA	2	0
39	Q	320	CLA	1	0
39	E	317	CLA	3	0
39	Y	305	CLA	1	0
39	3	322	CLA	2	0
39	Z	306	CLA	1	0
39	0	312	CLA	8	0
39	M	312	CLA	4	0
52	R	305	A1EB4	1	0
39	l	205	CLA	7	0
39	a	808	CLA	1	0
39	b	830	CLA	3	0
39	W	310	CLA	7	0
39	F	314	CLA	3	0
39	C	306	CLA	2	0
47	D	320	SQD	2	0
39	F	312	CLA	1	0
39	x	311	CLA	1	0
39	a	815	CLA	4	0
39	O	310	CLA	4	0
39	b	818	CLA	3	0
39	a	809	CLA	3	0
47	9	322	SQD	1	0
39	H	309	CLA	2	0
48	Q	302	A86	2	0
42	l	206	BCR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	J	314	CLA	3	0
39	F	308	CLA	3	0
39	A	305	CLA	1	0
40	a	839	PQN	4	0
39	H	306	CLA	3	0
39	K	309	CLA	1	0
39	a	825	CLA	7	0
39	M	308	CLA	1	0
46	l	208	LMG	4	0
39	F	309	CLA	1	0
39	F	313	CLA	3	0
39	7	321	CLA	1	0
39	x	307	CLA	2	0
39	I	311	CLA	1	0
48	Z	303	A86	1	0
43	O	304	DD6	1	0
39	8	313	CLA	1	0
50	H	304	A1EB1	1	0
39	L	308	CLA	3	0
39	k	201	CLA	2	0
42	m	101	BCR	5	0
39	6	313	CLA	1	0
39	O	309	CLA	1	0
39	R	308	CLA	1	0
46	A	316	LMG	1	0
39	S	320	CLA	3	0
39	b	819	CLA	1	0
39	7	318	CLA	3	0
39	b	828	CLA	6	0
39	b	834	CLA	2	0
39	D	310	CLA	2	0
49	0	314	KC2	2	0
51	y	311	A1ECV	1	0
48	9	303	A86	1	0
39	E	314	CLA	5	0
39	7	314	CLA	5	0
39	F	310	CLA	1	0
39	X	311	CLA	1	0
39	G	318	CLA	1	0
48	7	312	A86	1	0
43	A	302	DD6	1	0
39	b	824	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	L	310	CLA	2	0
39	5	308	CLA	2	0
42	a	845	BCR	5	0
43	4	308	DD6	1	0
49	T	315	KC2	2	0
46	S	322	LMG	20	0
39	V	309	CLA	2	0
43	U	204	DD6	1	0
39	b	839	CLA	3	0
42	b	846	BCR	4	0
39	0	311	CLA	3	0
39	a	818	CLA	3	0
52	5	304	A1EB4	1	0
39	U	215	CLA	1	0
39	b	832	CLA	5	0
39	a	803	CLA	3	0
43	P	304	DD6	2	0
48	R	302	A86	2	0
39	L	313	CLA	1	0
51	9	317	A1ECV	2	0
39	S	308	CLA	2	0
39	a	807	CLA	3	0
48	W	304	A86	5	0
49	4	324	KC2	1	0
46	4	326	LMG	33	0
42	f	804	BCR	3	0
39	b	808	CLA	1	0
39	X	307	CLA	2	0
39	a	824	CLA	5	0
49	R	314	KC2	15	0
39	b	801	CLA	7	0
39	K	311	CLA	1	0
39	Z	316	CLA	1	0
39	T	319	CLA	1	0
39	B	204	CLA	1	0
39	D	313	CLA	1	0
42	l	207	BCR	4	0
43	1	304	DD6	2	0
39	a	847	CLA	2	0
39	a	836	CLA	6	0
48	L	304	A86	4	0
39	G	310	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	C	308	CLA	3	0
39	A	309	CLA	1	0
42	h	202	BCR	4	0
49	W	314	KC2	2	0
39	1	310	CLA	1	0
49	P	310	KC2	1	0
39	a	806	CLA	1	0
42	j	103	BCR	1	0
39	b	822	CLA	2	0
39	o	206	CLA	2	0
39	J	309	CLA	3	0
47	k	205	SQD	2	0
39	b	809	CLA	5	0
39	S	311	CLA	5	0
39	T	318	CLA	1	0
39	U	208	CLA	2	0
49	Q	315	KC2	1	0
39	b	826	CLA	7	0
39	b	825	CLA	2	0
46	7	301	LMG	20	0
42	f	801	BCR	3	0
39	0	310	CLA	2	0
50	0	307	A1EB1	2	0
39	M	310	CLA	3	0
39	b	840	CLA	4	0
39	C	305	CLA	1	0
39	E	312	CLA	3	0
39	l	204	CLA	1	0
39	X	309	CLA	2	0
39	S	319	CLA	2	0
42	b	844	BCR	2	0
39	a	817	CLA	2	0
39	J	313	CLA	1	0
49	P	312	KC2	2	0
39	V	316	CLA	10	0
39	V	313	CLA	5	0
43	5	303	DD6	1	0
47	7	302	SQD	1	0
39	9	307	CLA	1	0
39	J	311	CLA	4	0
39	b	814	CLA	2	0
50	F	304	A1EB1	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	T	313	CLA	2	0
39	9	308	CLA	3	0
43	z	305	DD6	1	0
48	F	301	A86	1	0
39	5	315	CLA	2	0
51	T	317	A1ECV	1	0
39	D	311	CLA	2	0
49	Y	308	KC2	1	0
49	2	313	KC2	1	0
39	H	308	CLA	2	0
39	4	316	CLA	1	0
39	b	802	CLA	1	0
47	P	301	SQD	1	0
39	A	314	CLA	3	0
39	a	835	CLA	3	0
39	L	311	CLA	2	0
39	A	312	CLA	1	0
39	l	203	CLA	2	0
52	P	319	A1EB4	2	0
39	S	309	CLA	2	0
51	Y	306	A1ECV	1	0
46	P	317	LMG	5	0
42	b	845	BCR	3	0
39	E	313	CLA	2	0
39	7	324	CLA	4	0
39	C	307	CLA	2	0
46	M	319	LMG	10	0
39	b	820	CLA	3	0
49	8	316	KC2	1	0
39	a	830	CLA	4	0
39	H	316	CLA	1	0
52	W	321	A1EB4	1	0
39	Z	309	CLA	1	0
39	7	325	CLA	1	0
50	0	303	A1EB1	2	0
48	D	305	A86	1	0
41	j	104	LHG	1	0
39	1	313	CLA	2	0
48	5	301	A86	2	0
39	J	310	CLA	1	0
47	D	304	SQD	2	0
43	7	310	DD6	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	S	303	A1EB1	1	0
39	b	831	CLA	2	0
39	b	811	CLA	2	0
49	F	311	KC2	7	0
43	O	305	DD6	1	0
39	P	308	CLA	5	0
39	b	807	CLA	3	0
41	D	302	LHG	3	0
43	2	303	DD6	1	0
39	M	317	CLA	2	0
39	y	307	CLA	1	0
39	E	316	CLA	1	0
39	I	309	CLA	2	0
39	b	812	CLA	3	0
39	H	313	CLA	2	0
39	x	317	CLA	1	0
41	a	840	LHG	3	0
39	b	821	CLA	2	0
48	F	302	A86	8	0
39	b	806	CLA	1	0
49	X	314	KC2	19	0
39	T	320	CLA	2	0
49	X	312	KC2	1	0
50	4	304	A1EB1	1	0
39	E	318	CLA	1	0
39	3	312	CLA	4	0
43	M	304	DD6	2	0
39	C	311	CLA	1	0
48	2	305	A86	1	0
39	a	813	CLA	3	0
39	H	310	CLA	3	0
49	5	313	KC2	26	0
50	x	302	A1EB1	2	0
39	O	316	CLA	1	0
51	7	317	A1ECV	2	0
39	b	838	CLA	4	0
39	0	315	CLA	2	0
39	8	310	CLA	3	0
47	S	301	SQD	4	0
39	a	802	CLA	2	0
50	7	306	A1EB1	1	0
47	D	321	SQD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	b	841	CLA	4	0
39	a	816	CLA	7	0
39	y	310	CLA	1	0
46	F	317	LMG	14	0
39	i	101	CLA	4	0
39	T	308	CLA	9	0
49	R	312	KC2	1	0
42	b	850	BCR	5	0
47	W	301	SQD	1	0
42	i	102	BCR	6	0
39	b	823	CLA	1	0
48	W	307	A86	1	0
39	Y	313	CLA	1	0
43	3	304	DD6	3	0
39	b	829	CLA	2	0
39	3	313	CLA	1	0
43	S	306	DD6	1	0
46	Q	322	LMG	2	0
39	8	311	CLA	2	0
39	8	321	CLA	1	0
39	W	318	CLA	1	0
39	3	320	CLA	1	0
39	D	319	CLA	3	0
39	E	310	CLA	4	0
39	B	209	CLA	4	0
39	k	203	CLA	1	0
39	f	802	CLA	1	0
42	b	847	BCR	4	0
39	a	837	CLA	1	0
47	T	321	SQD	1	0
39	b	835	CLA	1	0
42	k	204	BCR	2	0
47	H	318	SQD	3	0
39	B	207	CLA	2	0
46	D	322	LMG	1	0
39	Q	312	CLA	1	0
39	0	323	CLA	2	0
39	E	308	CLA	1	0
39	I	315	CLA	1	0
39	W	309	CLA	2	0
52	P	318	A1EB4	3	0
39	o	201	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	W	311	CLA	2	0
39	x	308	CLA	1	0
47	F	319	SQD	1	0
39	K	314	CLA	1	0
39	C	310	CLA	3	0
48	I	304	A86	1	0
39	Q	309	CLA	2	0
39	K	312	CLA	2	0
43	D	306	DD6	1	0
39	X	308	CLA	4	0
39	R	307	CLA	2	0
39	R	316	CLA	2	0
39	b	827	CLA	7	0
39	X	317	CLA	3	0
46	0	324	LMG	4	0
51	0	321	A1ECV	2	0
39	b	815	CLA	4	0
39	A	315	CLA	2	0
39	O	313	CLA	1	0
51	1	318	A1ECV	1	0
39	b	833	CLA	3	0
39	P	316	CLA	1	0
39	J	307	CLA	1	0
48	E	304	A86	1	0
39	Q	321	CLA	3	0
39	a	814	CLA	2	0
39	o	205	CLA	2	0
39	A	306	CLA	3	0
39	Q	311	CLA	3	0
39	Q	310	CLA	3	0
42	a	842	BCR	5	0
39	O	308	CLA	1	0
43	E	303	DD6	1	0
39	E	315	CLA	2	0
49	M	313	KC2	1	0
49	6	316	KC2	1	0
39	H	312	CLA	2	0
39	U	209	CLA	1	0
43	F	303	DD6	6	0
39	b	803	CLA	2	0
51	7	323	A1ECV	4	0
49	5	305	KC2	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	a	843	BCR	4	0
39	P	307	CLA	3	0
46	S	321	LMG	3	0
39	a	829	CLA	2	0
39	Q	314	CLA	2	0
43	J	305	DD6	1	0
42	l	202	BCR	5	0
43	I	306	DD6	1	0
39	2	318	CLA	1	0
39	3	311	CLA	2	0
40	b	843	PQN	3	0
39	Z	313	CLA	1	0
39	D	314	CLA	2	0
39	a	831	CLA	4	0
39	5	306	CLA	2	0
39	D	312	CLA	2	0
39	R	309	CLA	1	0
41	X	301	LHG	2	0
39	I	313	CLA	2	0
39	a	827	CLA	2	0
39	5	316	CLA	2	0
39	G	309	CLA	1	0
46	I	302	LMG	1	0
39	V	310	CLA	5	0
39	9	312	CLA	4	0
47	M	301	SQD	3	0
39	9	319	CLA	2	0
50	9	302	A1EB1	1	0
39	i	103	CLA	6	0
46	W	302	LMG	14	0
49	W	315	KC2	1	0
39	C	304	CLA	1	0
49	3	317	KC2	1	0
43	F	305	DD6	1	0
39	2	316	CLA	1	0
39	a	821	CLA	2	0
43	H	303	DD6	1	0
45	b	849	DGD	3	0
39	a	804	CLA	2	0
39	1	308	CLA	2	0
39	x	306	CLA	1	0
39	K	308	CLA	1	0

Continued on next page...

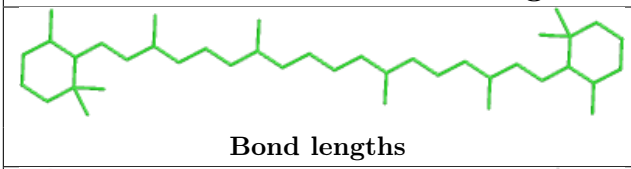
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	f	803	CLA	1	0
39	I	308	CLA	3	0
39	b	805	CLA	3	0
39	b	837	CLA	1	0
39	a	811	CLA	5	0
47	4	327	SQD	1	0
39	B	206	CLA	1	0
51	x	310	A1ECV	1	0
39	M	309	CLA	2	0
39	b	813	CLA	2	0
39	T	311	CLA	1	0
39	7	316	CLA	4	0
48	U	206	A86	1	0
51	2	311	A1ECV	1	0
39	0	313	CLA	2	0
51	z	316	A1ECV	1	0
39	7	313	CLA	2	0
39	j	101	CLA	5	0
39	b	842	CLA	2	0
39	D	317	CLA	5	0
39	R	311	CLA	1	0
52	W	306	A1EB4	4	0
39	I	301	CLA	3	0
39	b	810	CLA	3	0
39	z	311	CLA	1	0
39	2	308	CLA	1	0
39	F	316	CLA	2	0
39	3	314	CLA	3	0
39	4	314	CLA	4	0
41	H	317	LHG	3	0
39	4	323	CLA	7	0
39	4	312	CLA	2	0
39	a	823	CLA	3	0
49	V	315	KC2	1	0
39	a	832	CLA	1	0

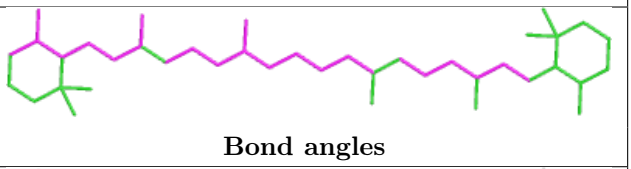
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BCR b 848



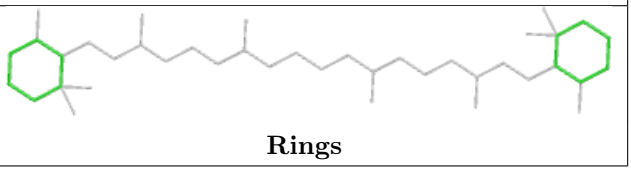
Bond lengths



Bond angles

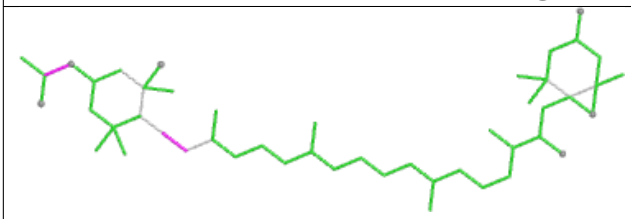


Torsions

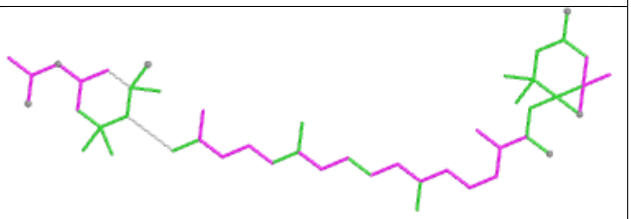


Rings

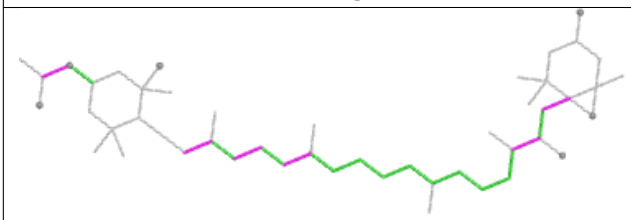
Ligand A86 0 304



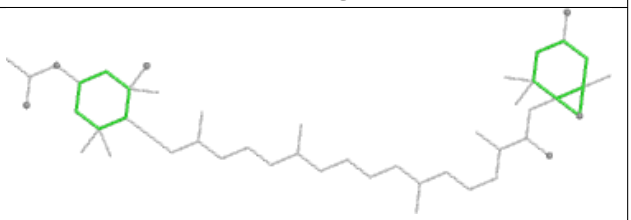
Bond lengths



Bond angles

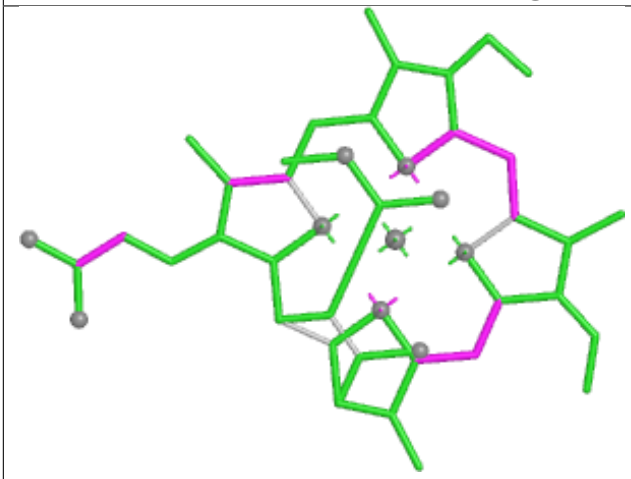


Torsions

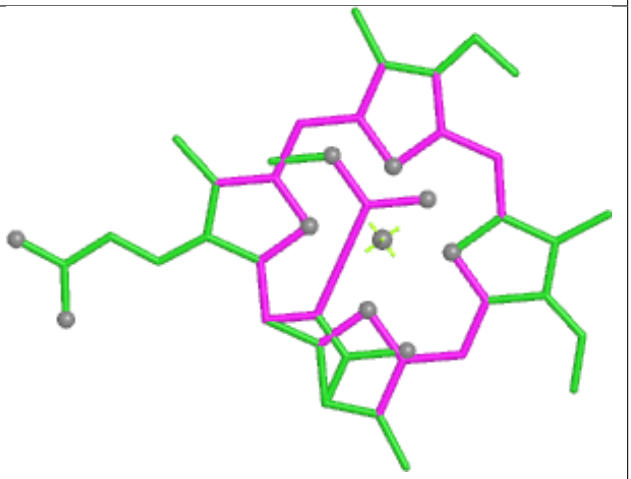


Rings

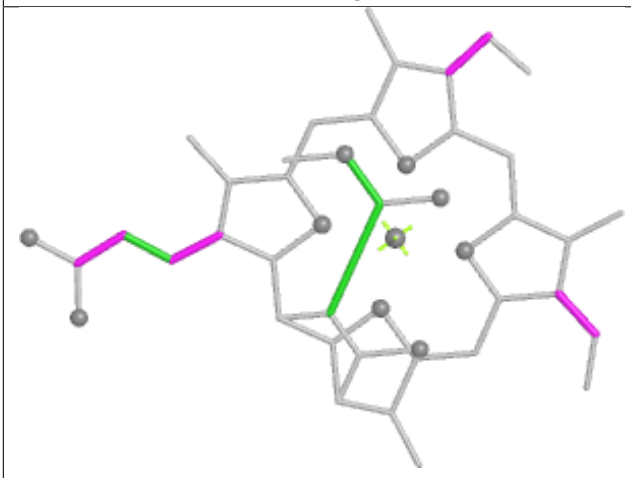
Ligand KC2 T 316



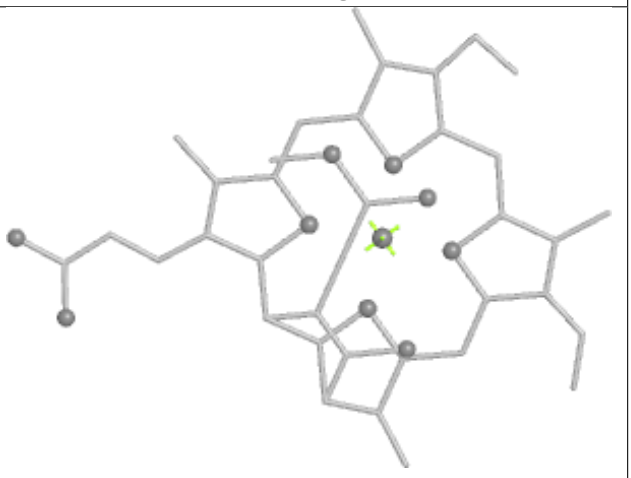
Bond lengths



Bond angles

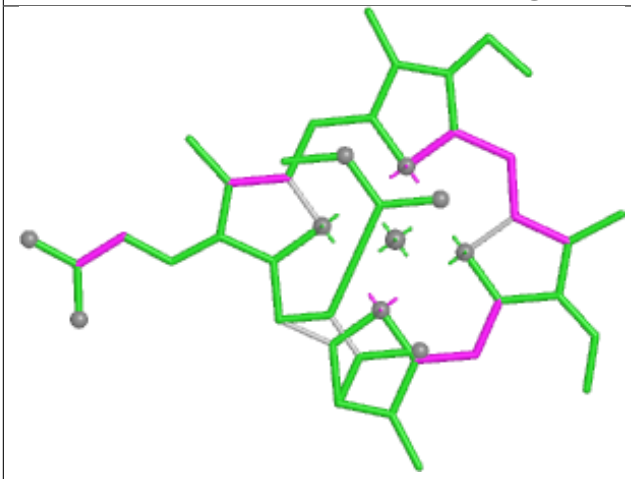


Torsions

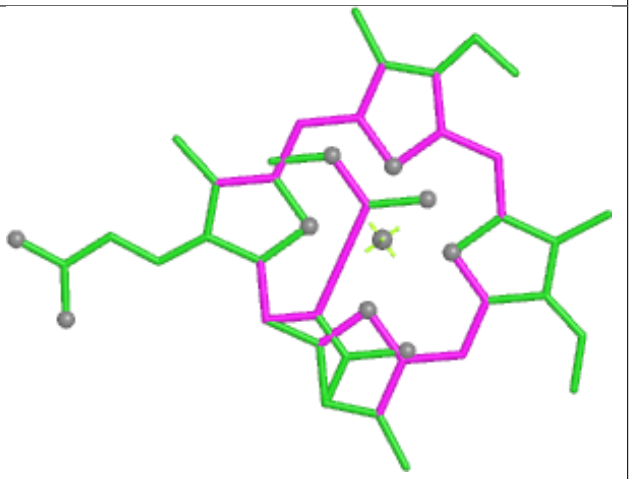


Rings

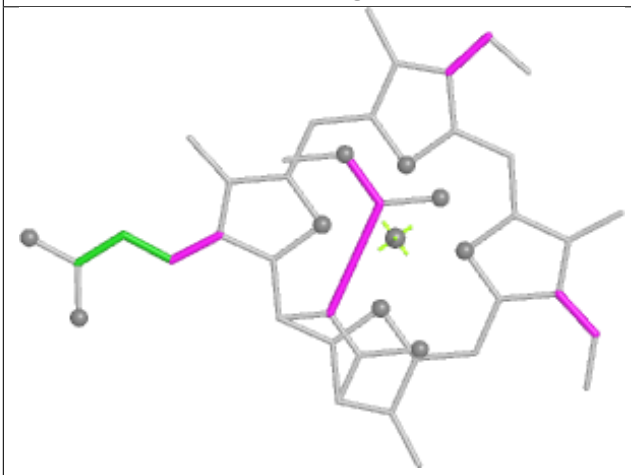
Ligand KC2 R 306



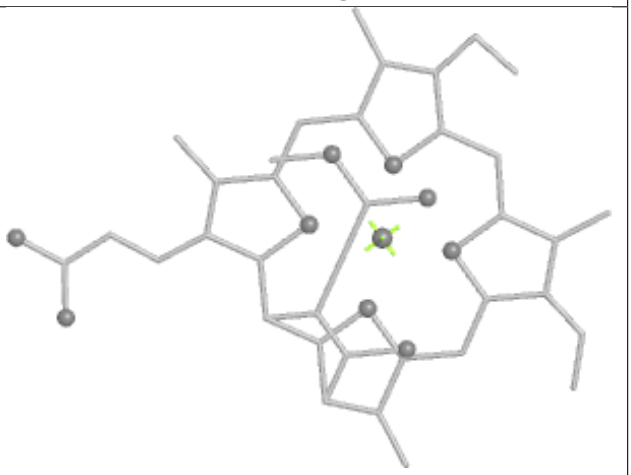
Bond lengths



Bond angles

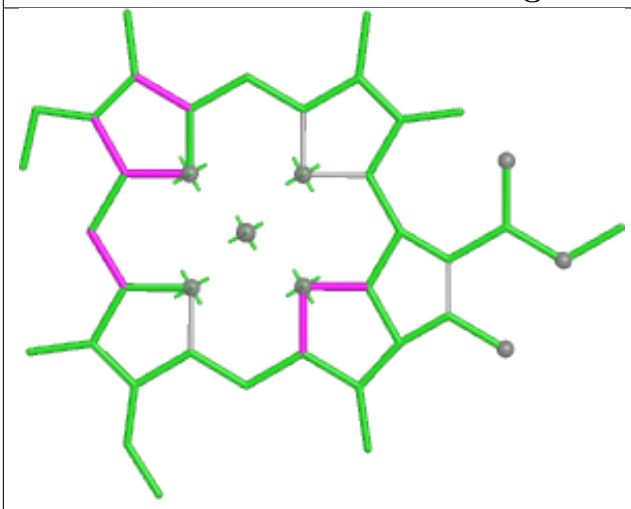


Torsions

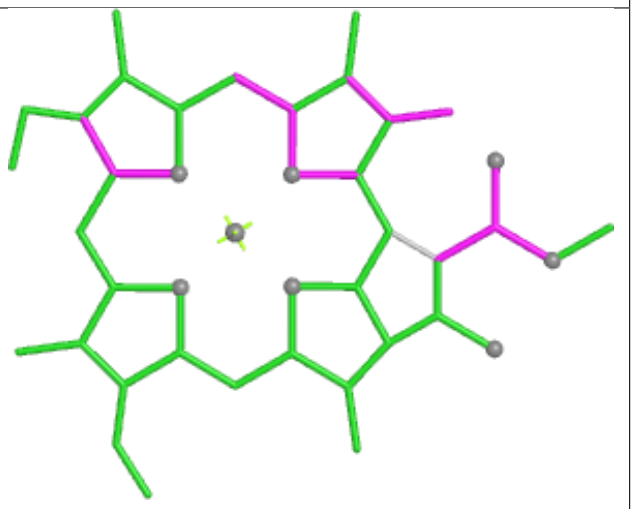


Rings

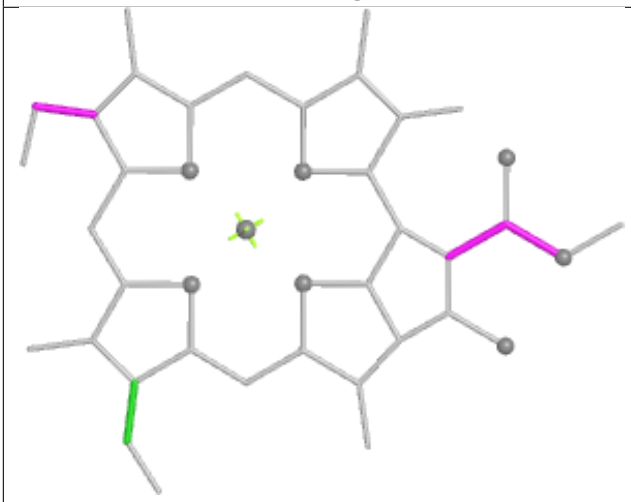
Ligand CLA Y 311



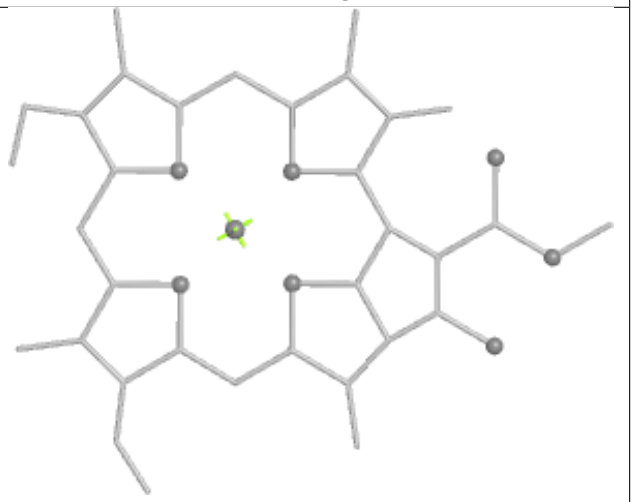
Bond lengths



Bond angles

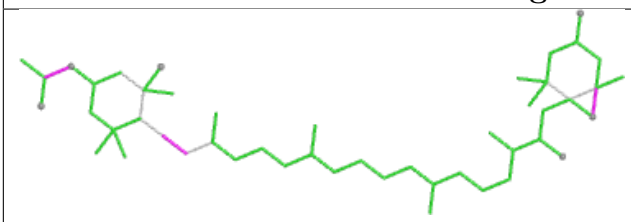


Torsions

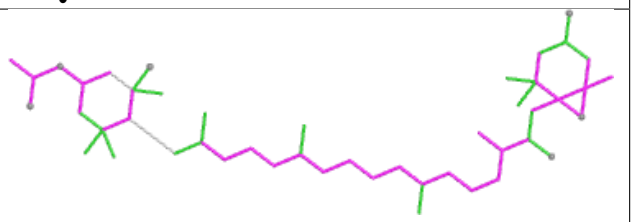


Rings

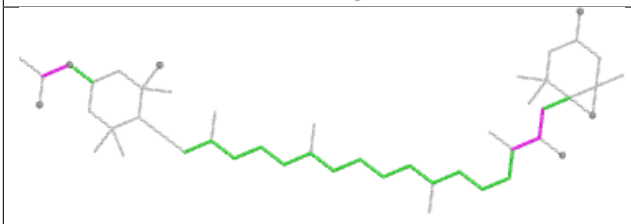
Ligand A86 Q 301



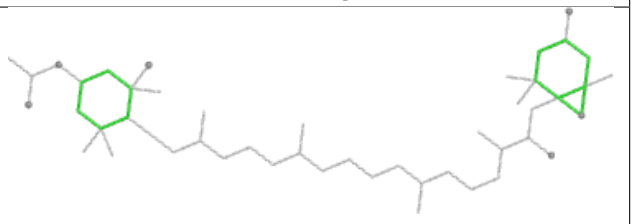
Bond lengths



Bond angles

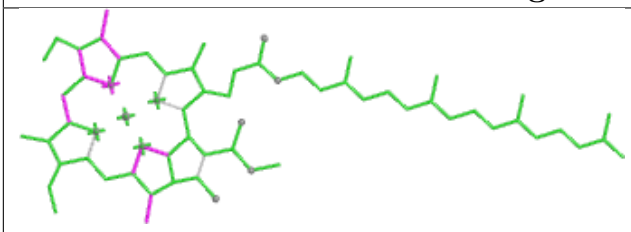


Torsions

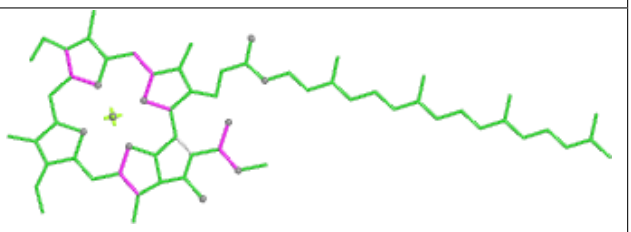


Rings

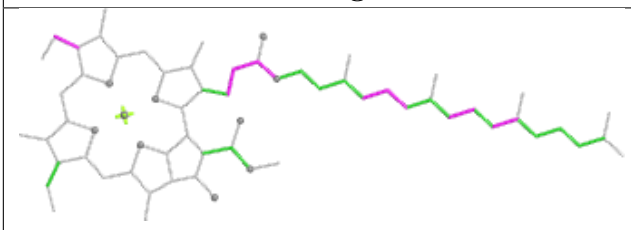
Ligand CLA a 838



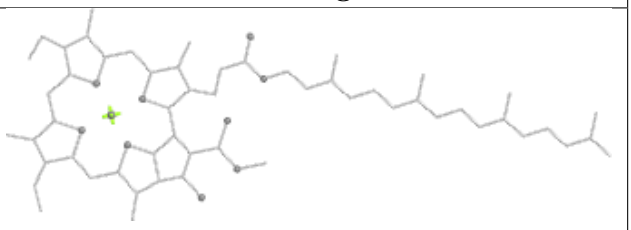
Bond lengths



Bond angles

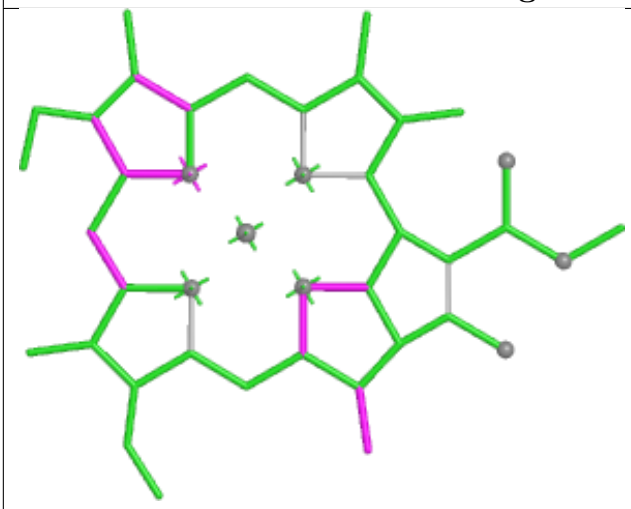


Torsions

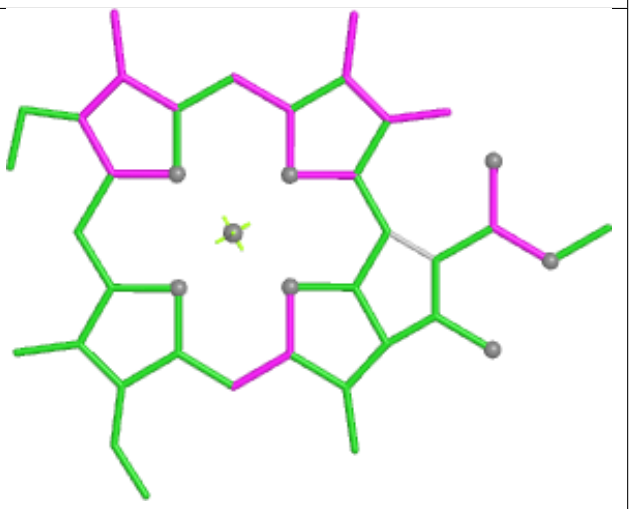


Rings

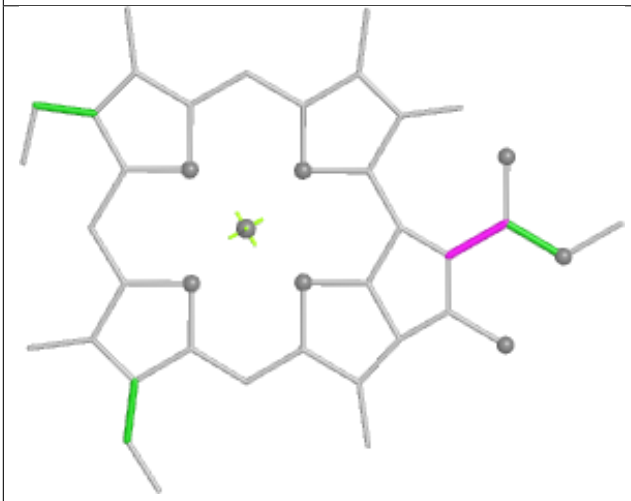
Ligand CLA W 316



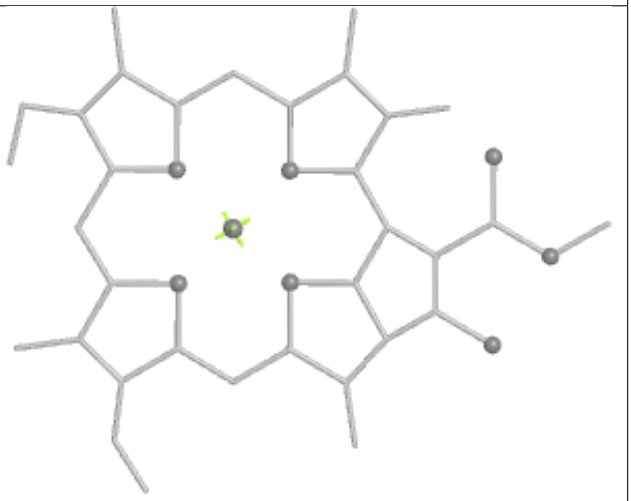
Bond lengths



Bond angles

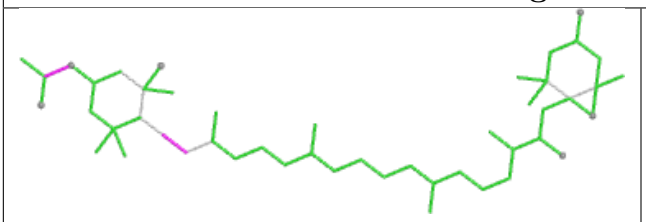


Torsions

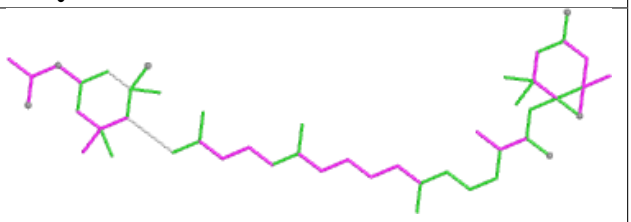


Rings

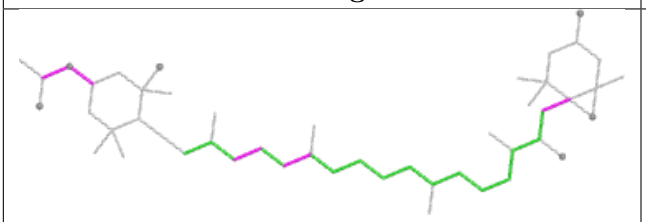
Ligand A86 Q 308



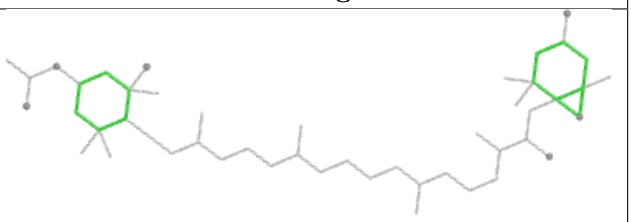
Bond lengths



Bond angles

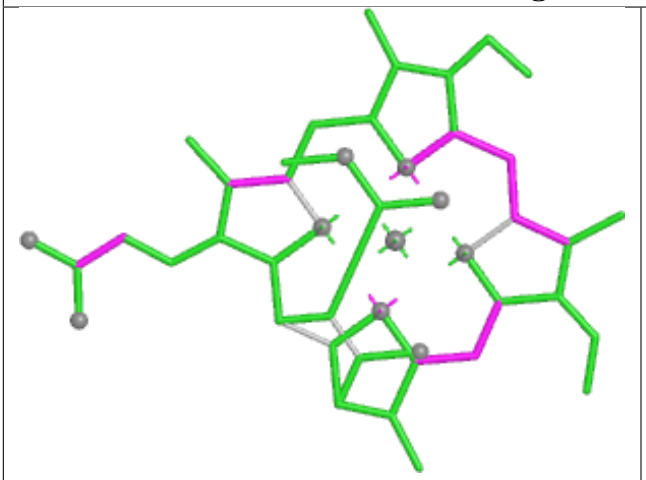


Torsions

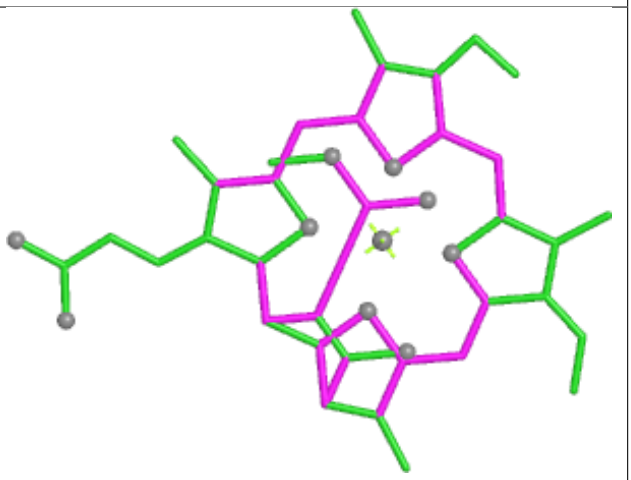


Rings

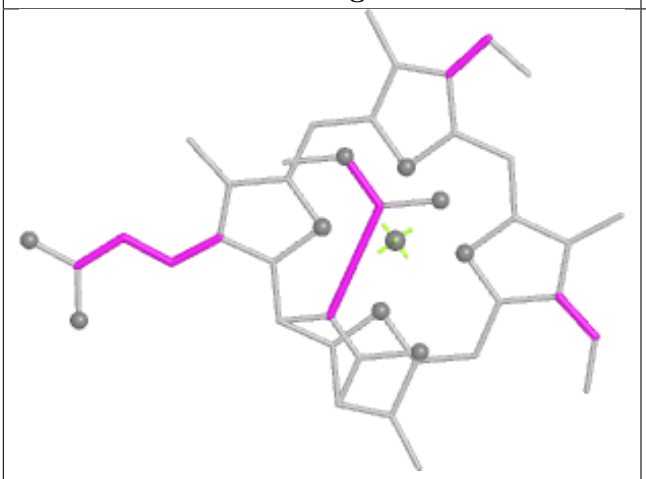
Ligand KC2 8 319



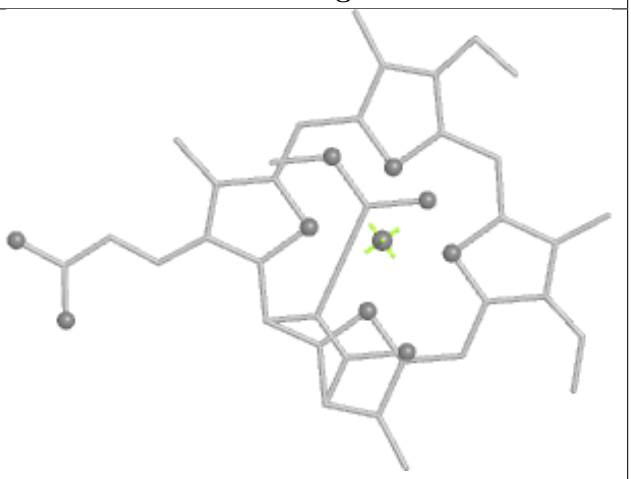
Bond lengths



Bond angles

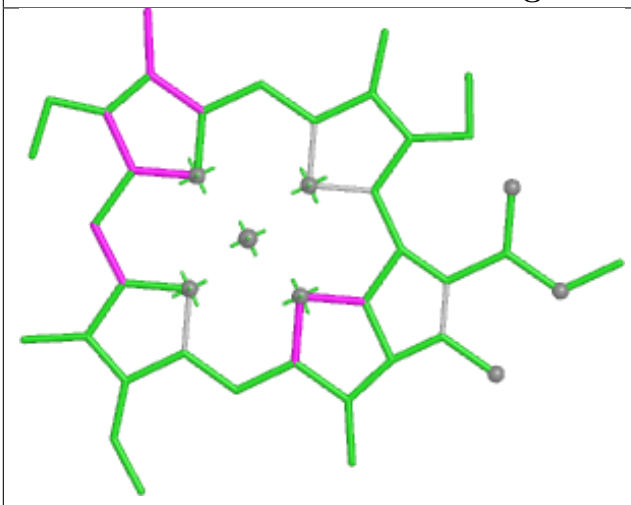


Torsions

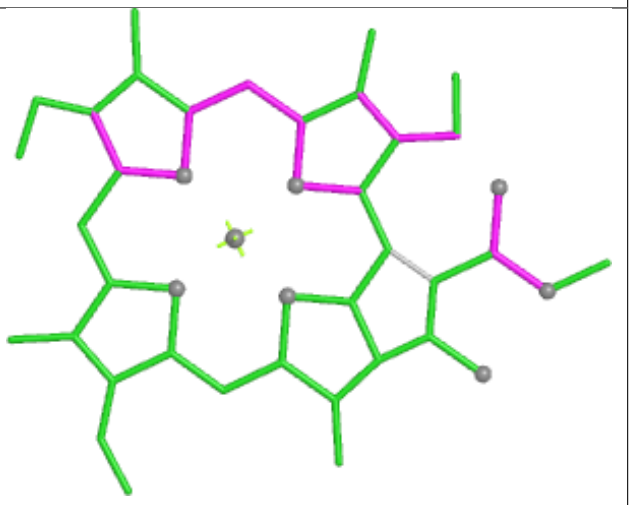


Rings

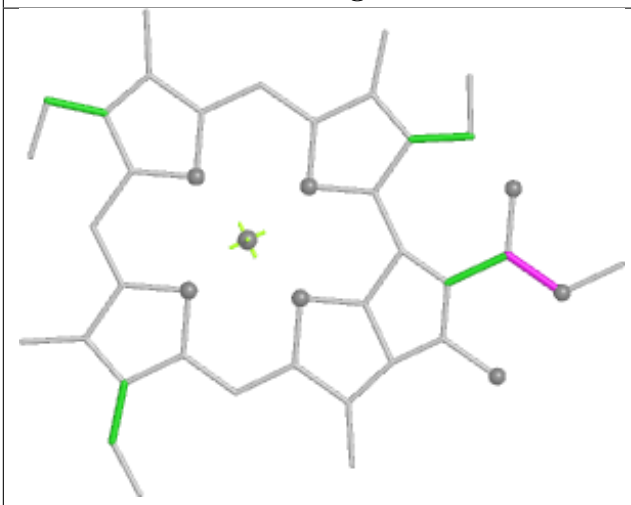
Ligand CLA O 311



Bond lengths



Bond angles

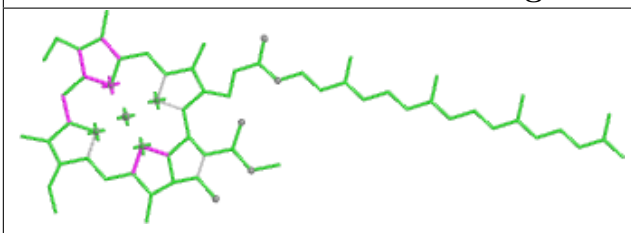


Torsions

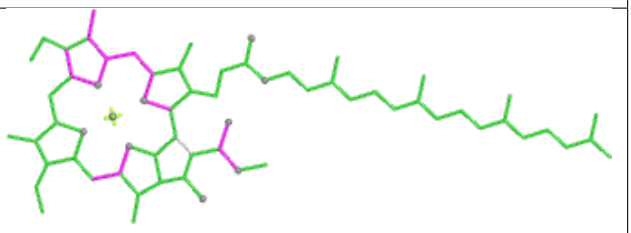


Rings

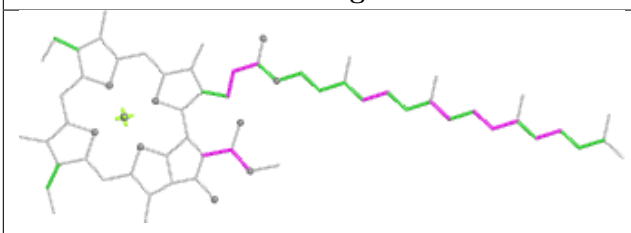
Ligand CLA P 309



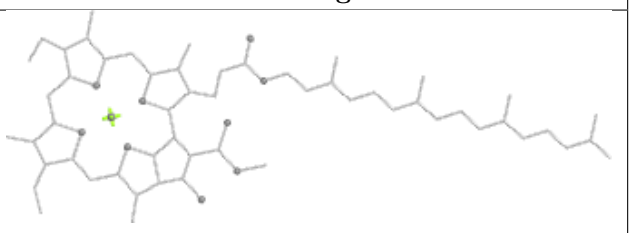
Bond lengths



Bond angles

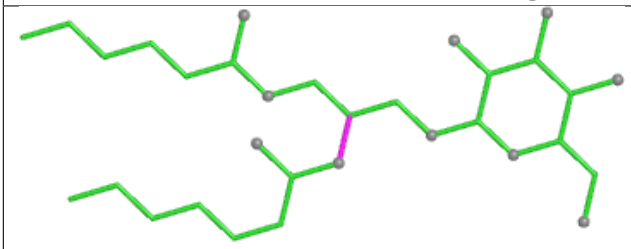


Torsions

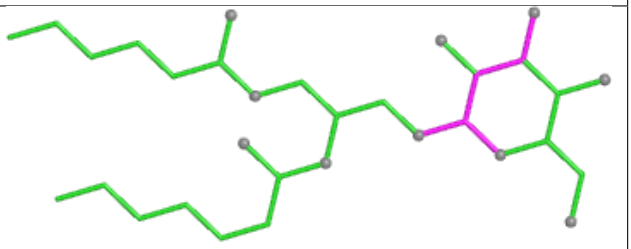


Rings

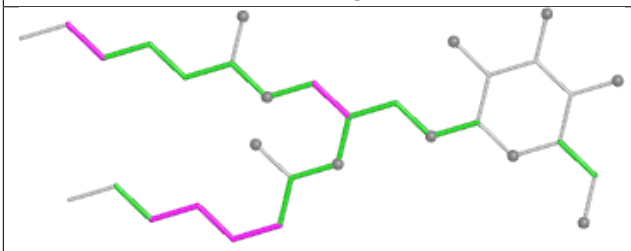
Ligand LMG 7 326



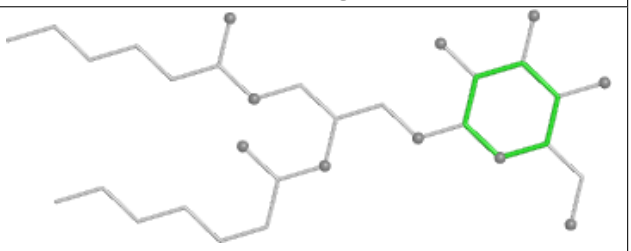
Bond lengths



Bond angles

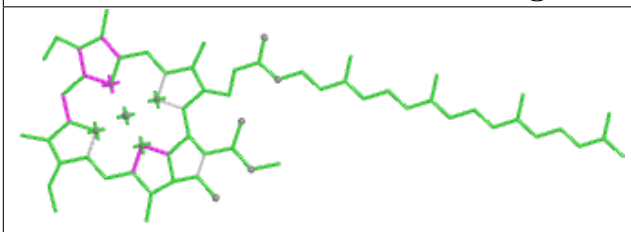


Torsions

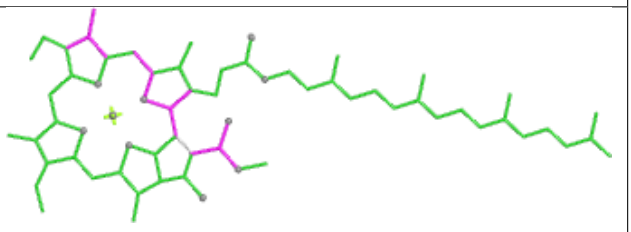


Rings

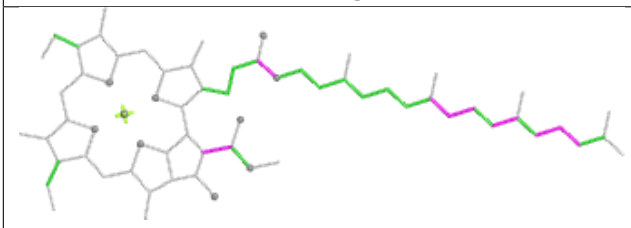
Ligand CLA a 822



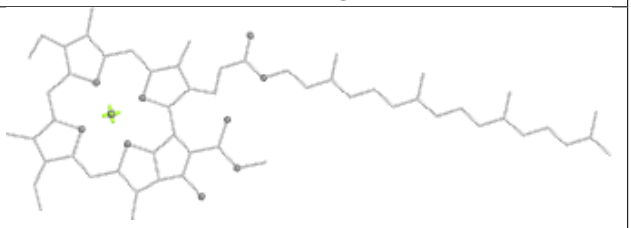
Bond lengths



Bond angles

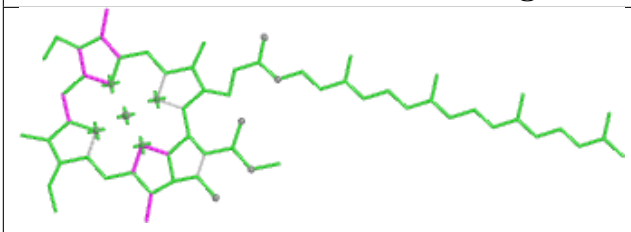


Torsions

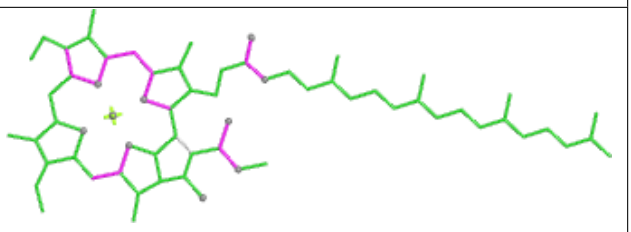


Rings

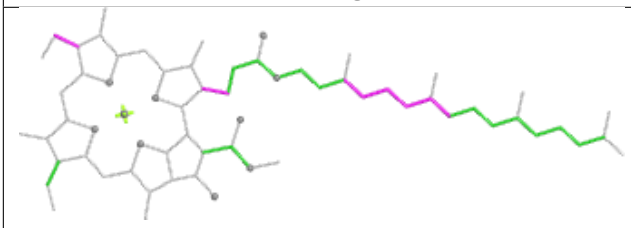
Ligand CLA W 313



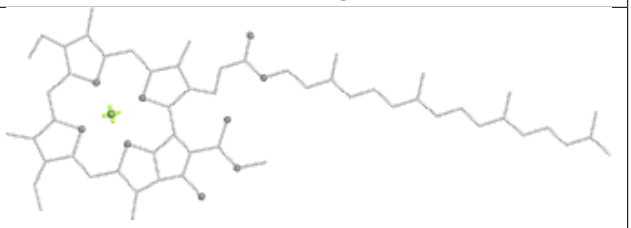
Bond lengths



Bond angles

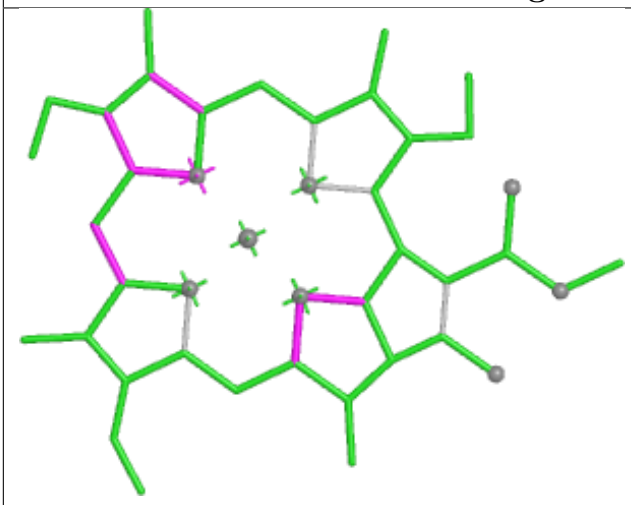


Torsions

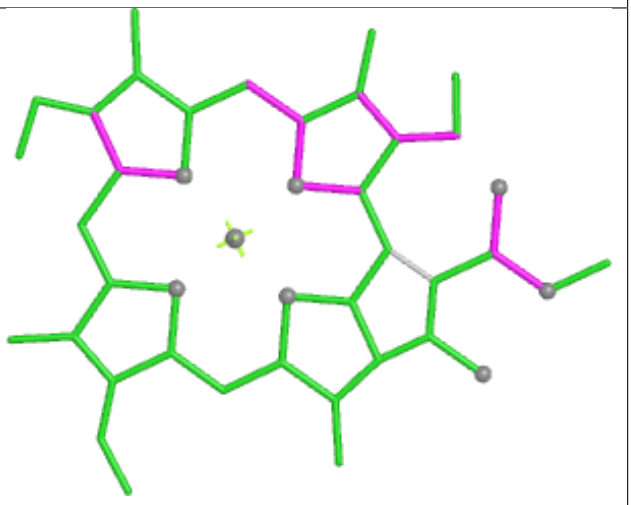


Rings

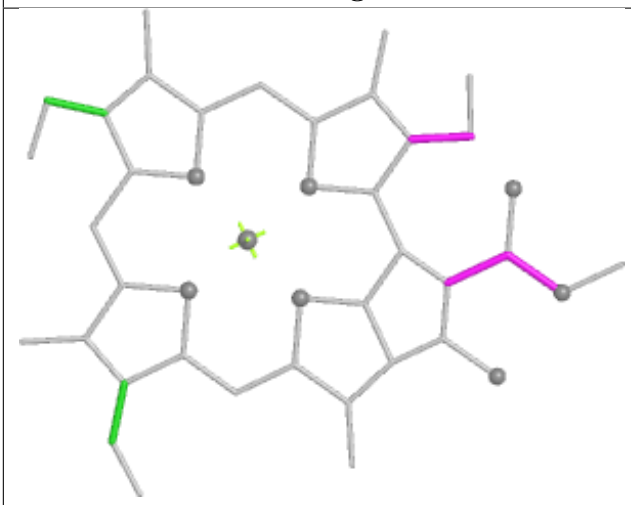
Ligand CLA 2 310



Bond lengths



Bond angles

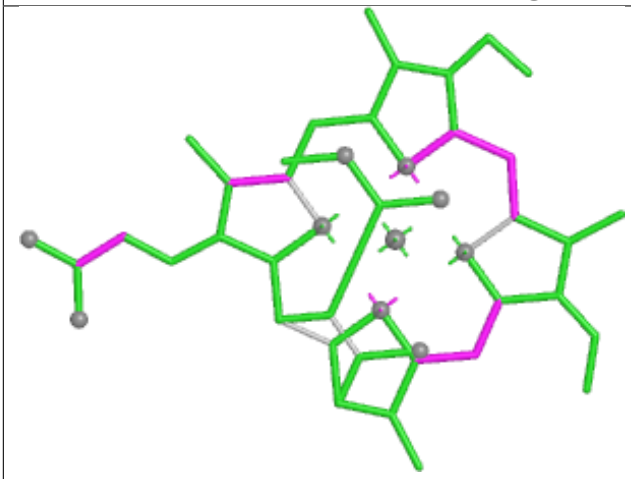


Torsions

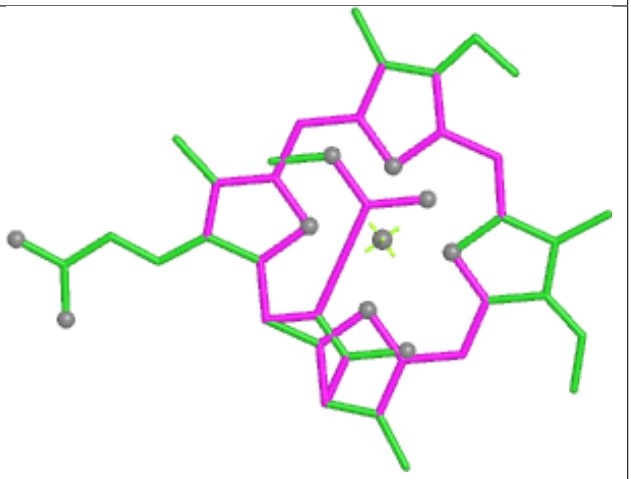


Rings

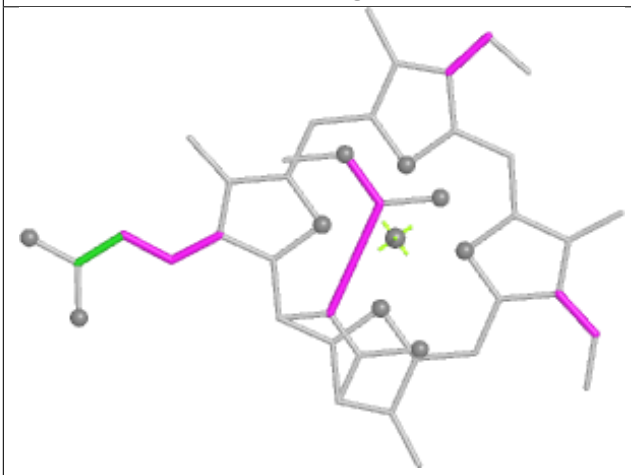
Ligand KC2 V 314



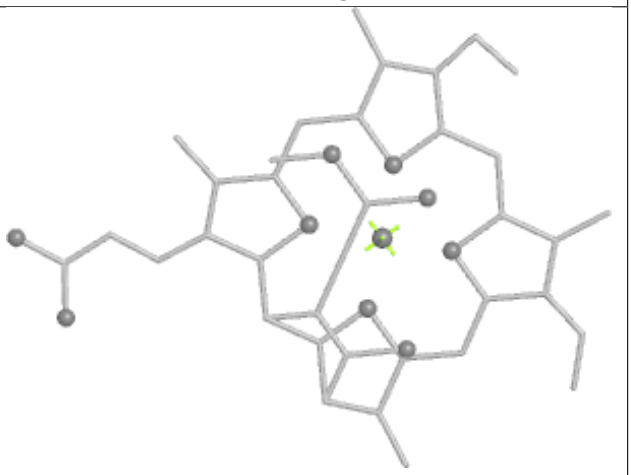
Bond lengths



Bond angles

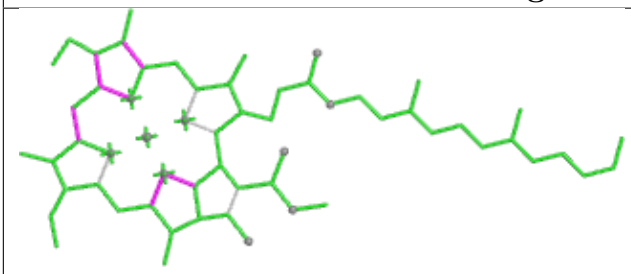


Torsions

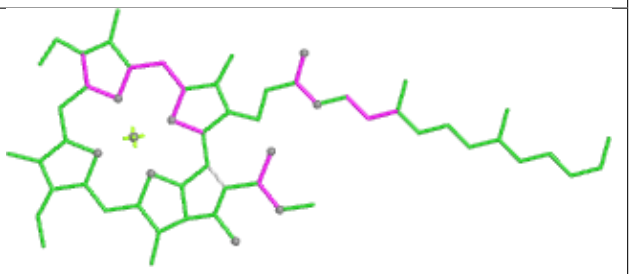


Rings

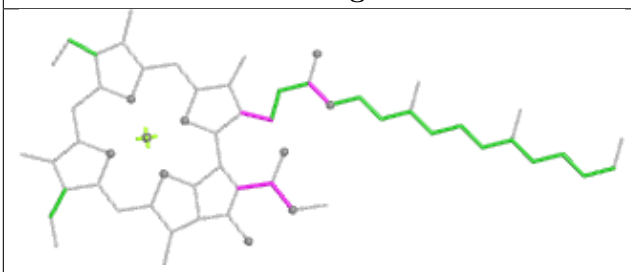
Ligand CLA b 817



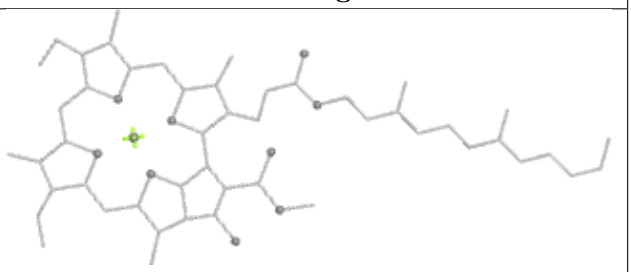
Bond lengths



Bond angles

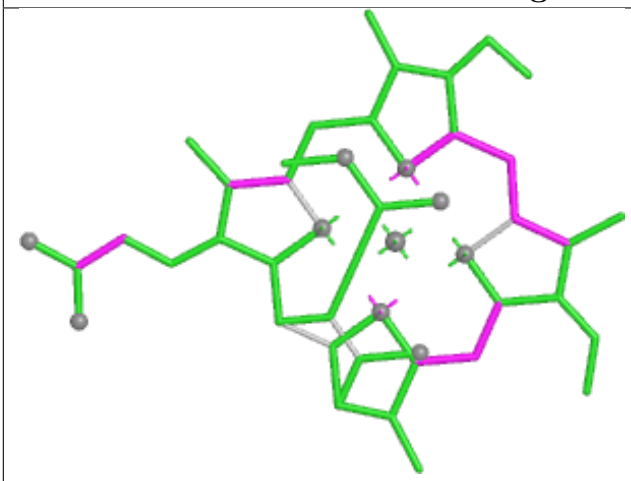


Torsions

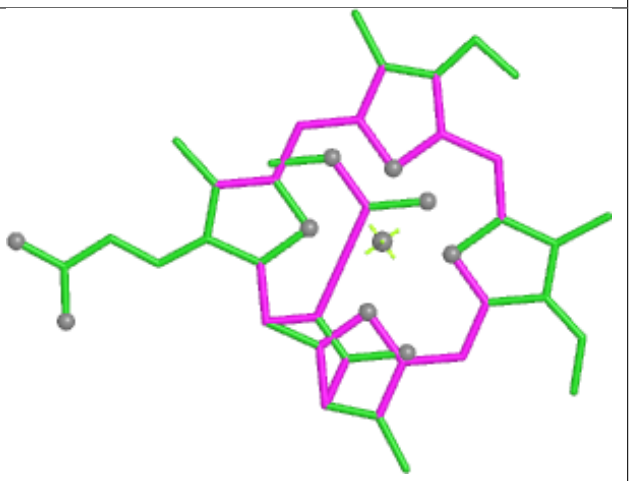


Rings

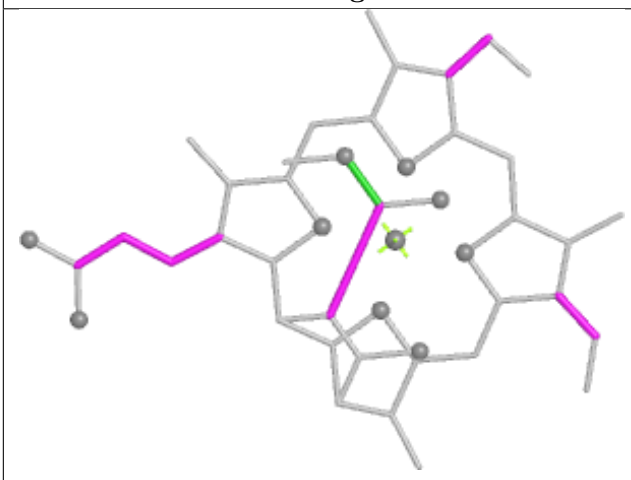
Ligand KC2 3 315



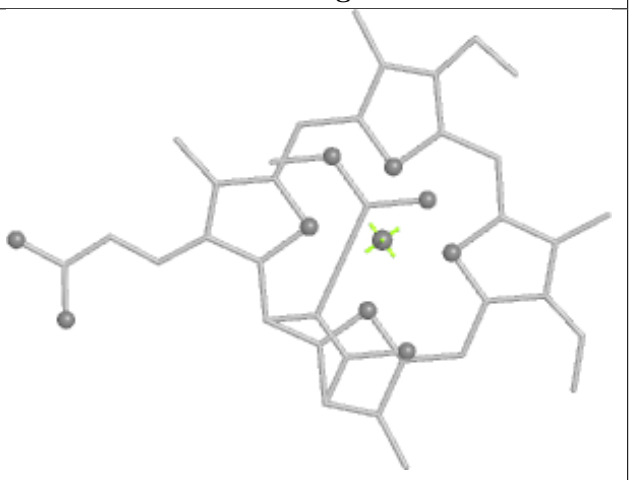
Bond lengths



Bond angles

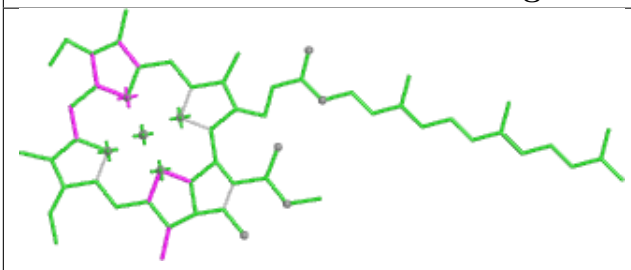


Torsions

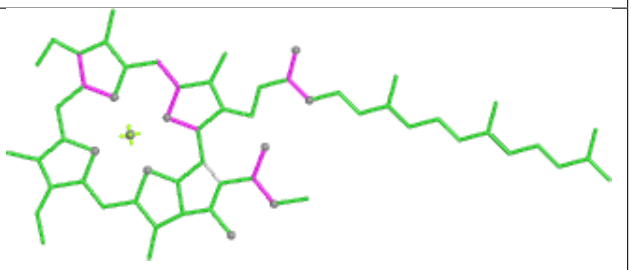


Rings

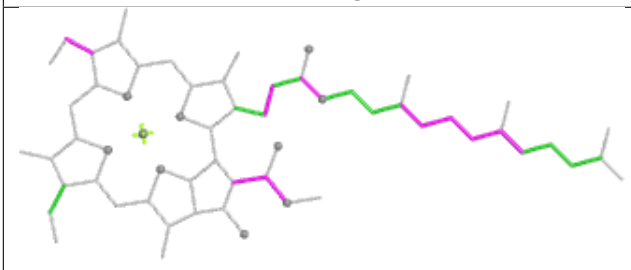
Ligand CLA U 207



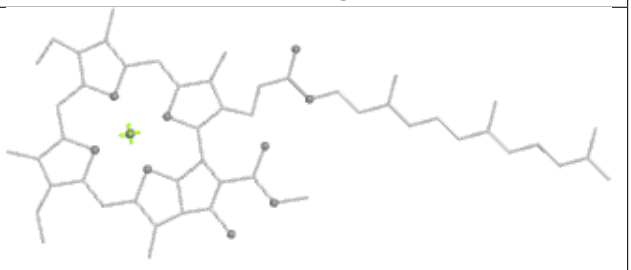
Bond lengths



Bond angles

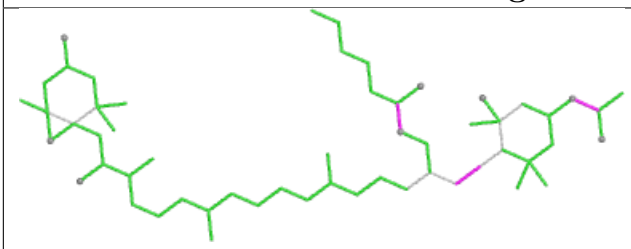


Torsions

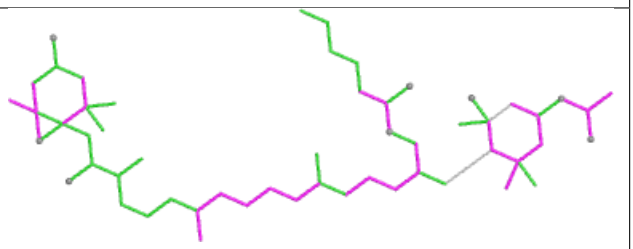


Rings

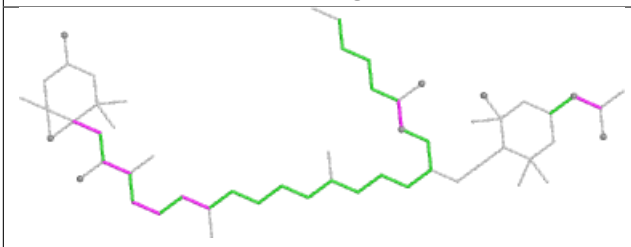
Ligand A1EB1 S 302



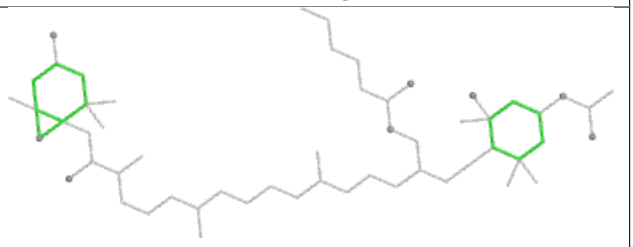
Bond lengths



Bond angles

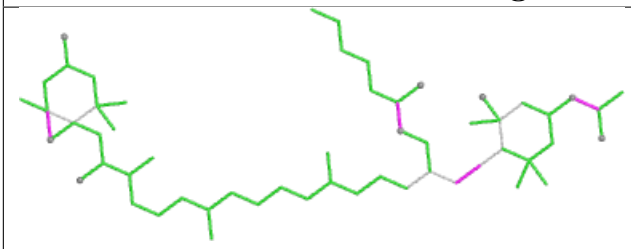


Torsions

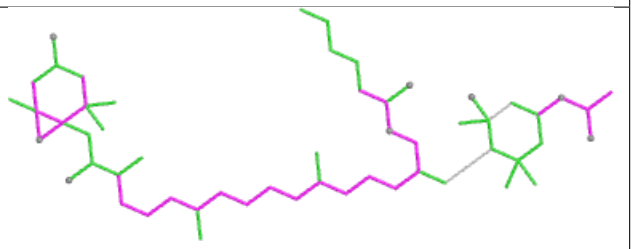


Rings

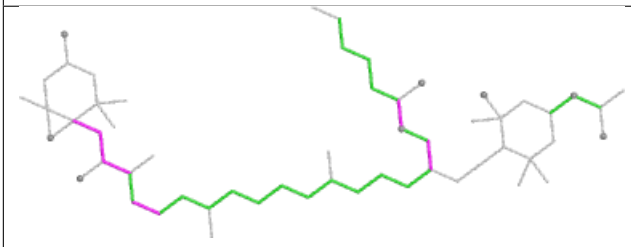
Ligand A1EB1 3 310



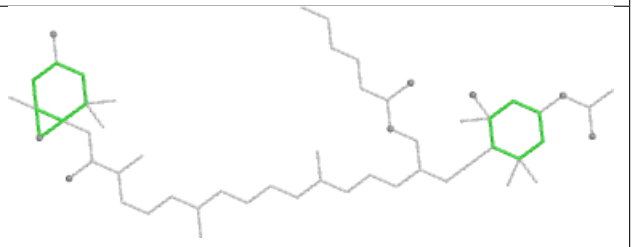
Bond lengths



Bond angles

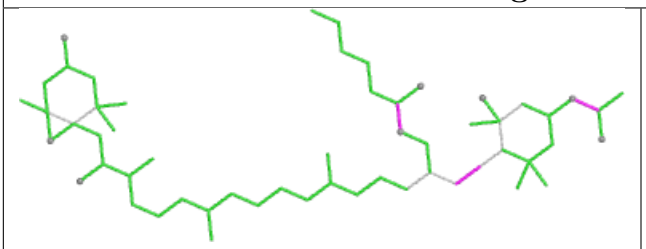


Torsions

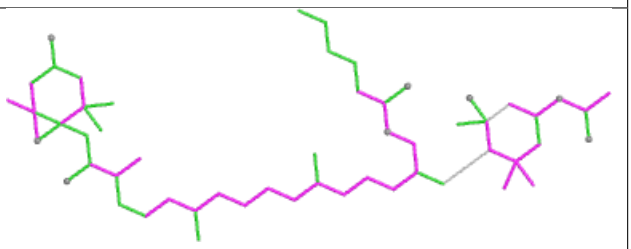


Rings

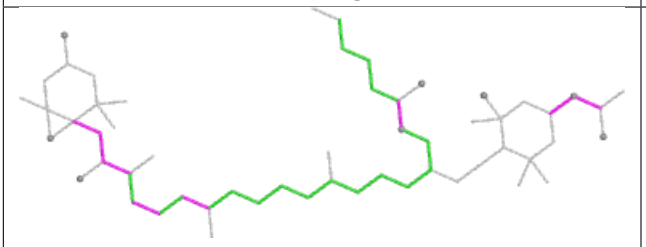
Ligand A1EB1 z 302



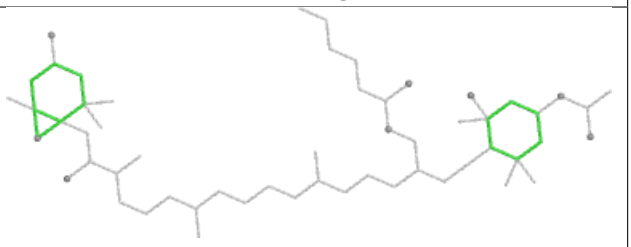
Bond lengths



Bond angles

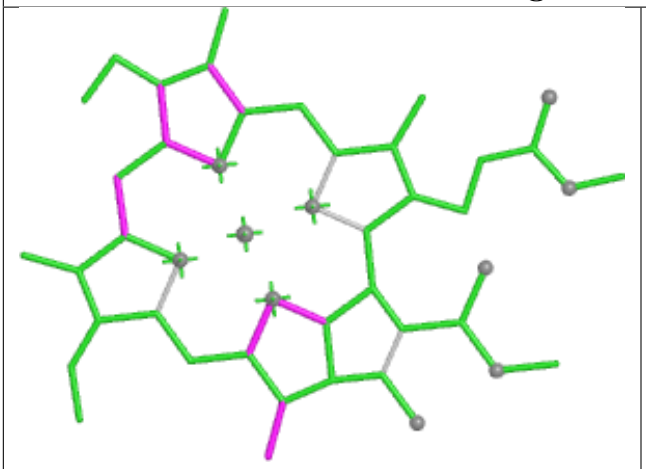


Torsions

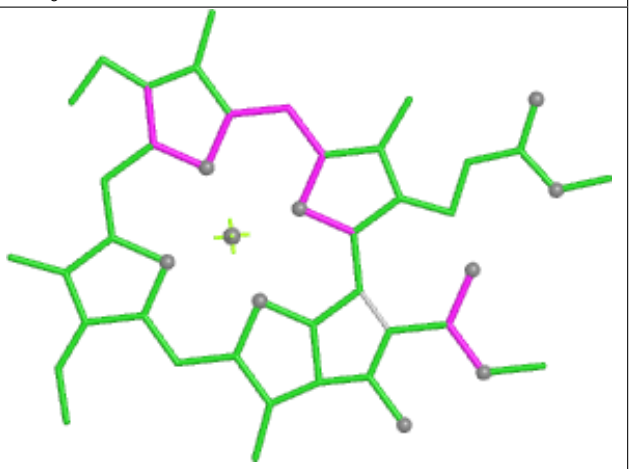


Rings

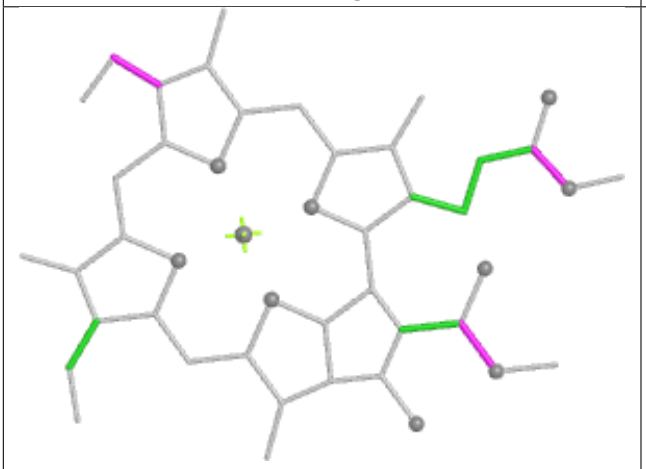
Ligand CLA y 309



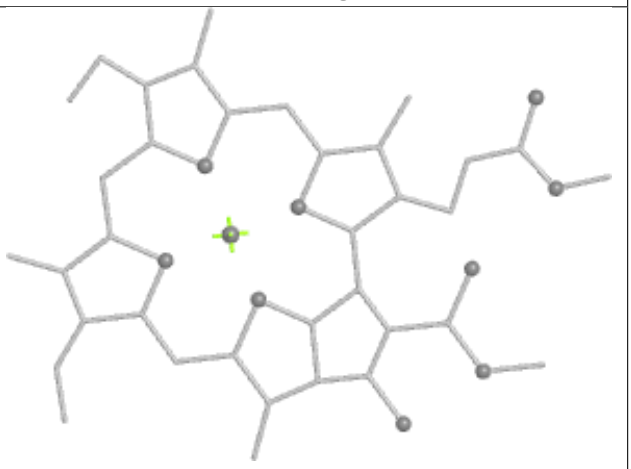
Bond lengths



Bond angles

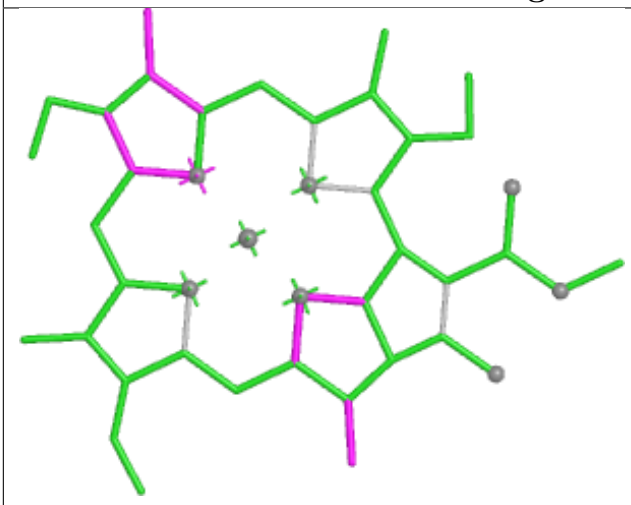


Torsions

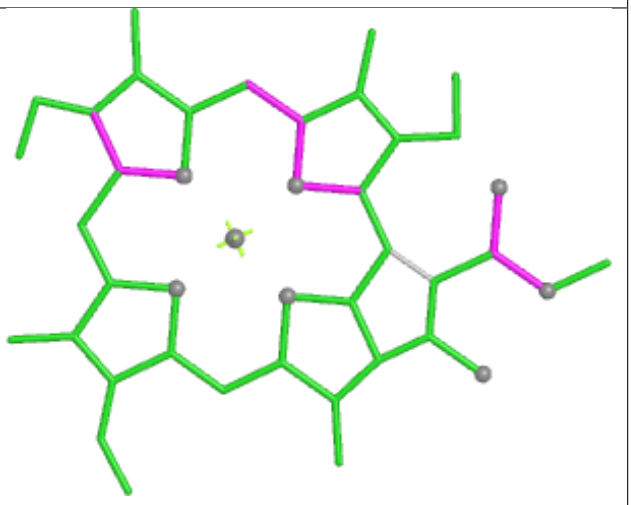


Rings

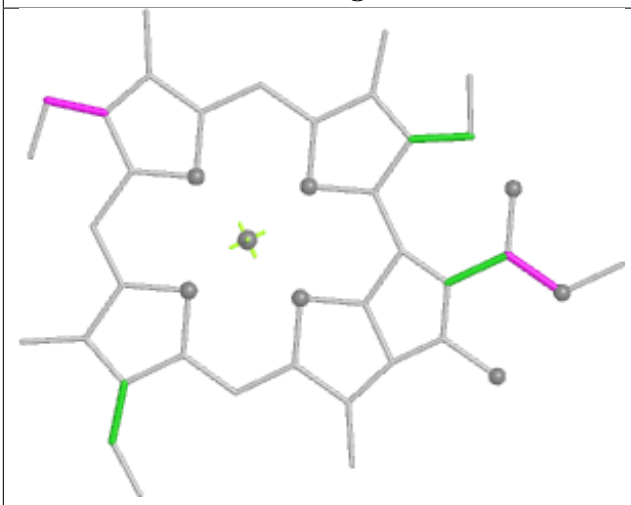
Ligand CLA J 317



Bond lengths



Bond angles

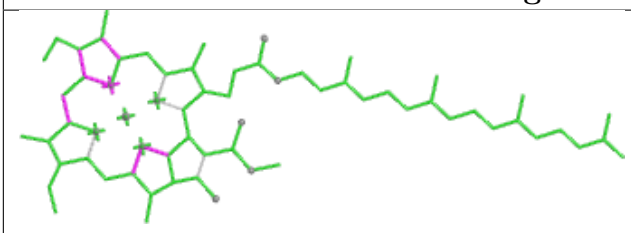


Torsions

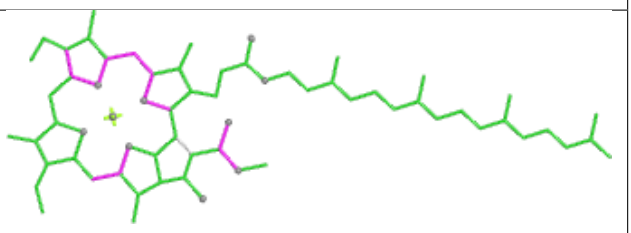


Rings

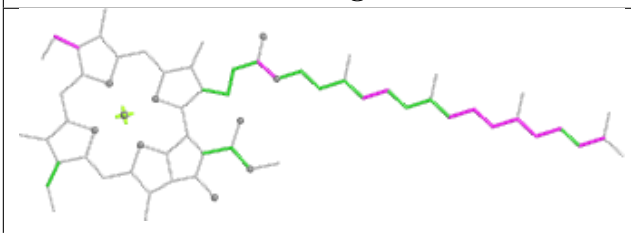
Ligand CLA A 311



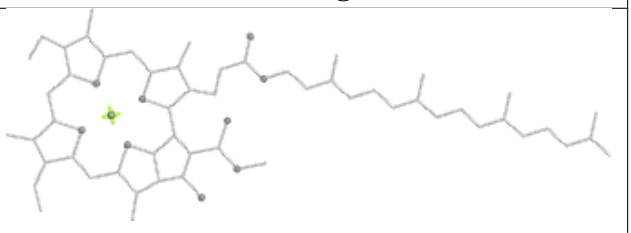
Bond lengths



Bond angles

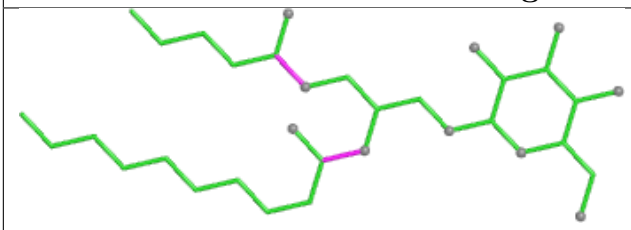


Torsions

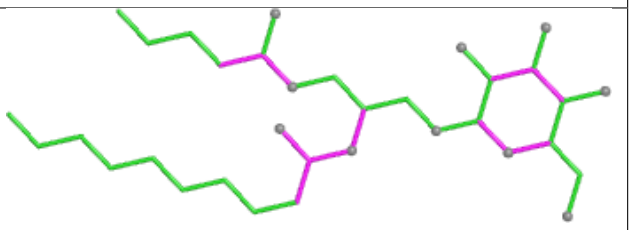


Rings

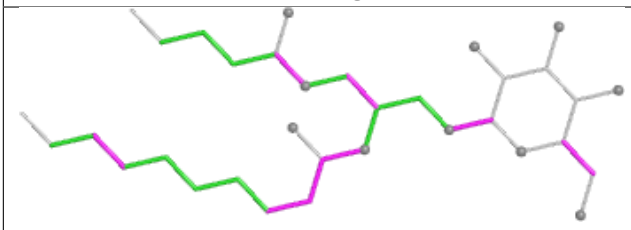
Ligand LMG F 320



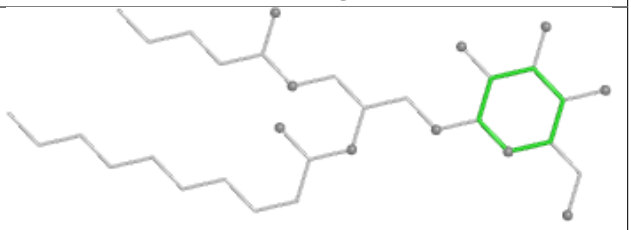
Bond lengths



Bond angles

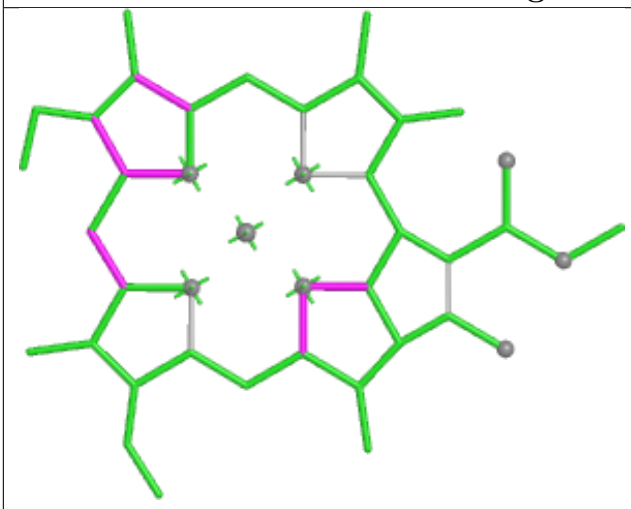


Torsions

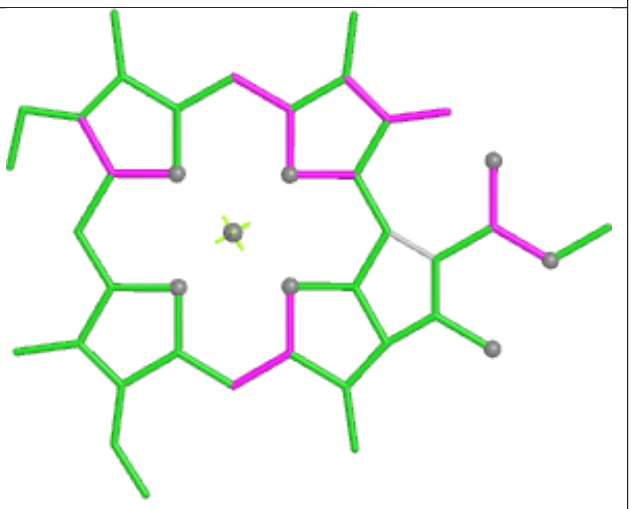


Rings

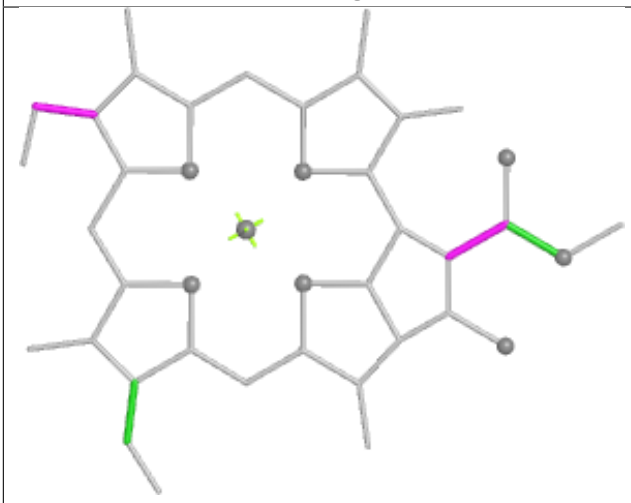
Ligand CLA S 316



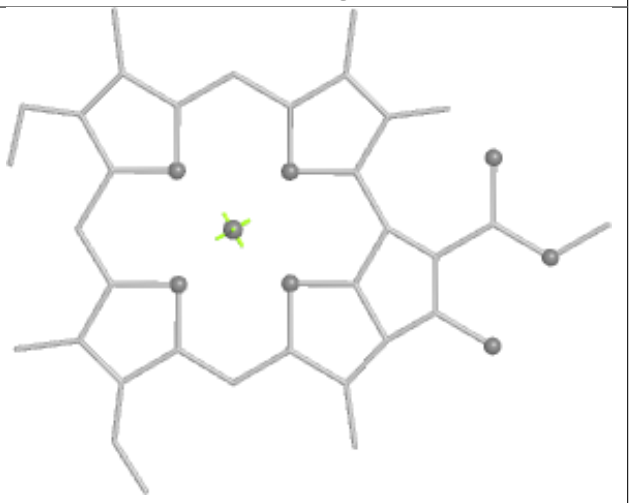
Bond lengths



Bond angles

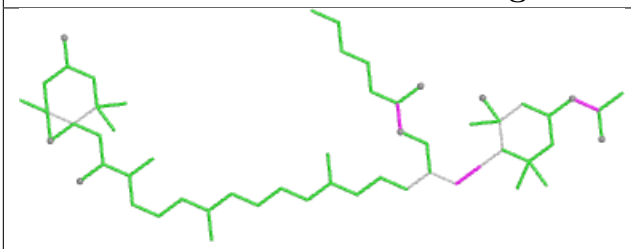


Torsions

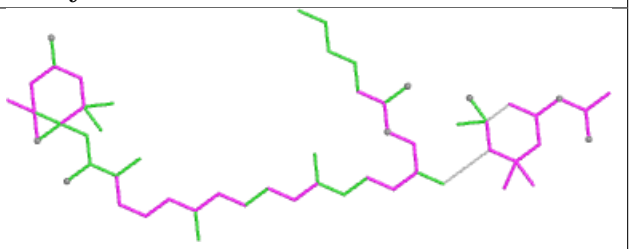


Rings

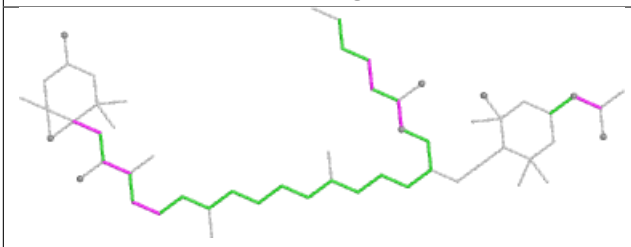
Ligand A1EB1 y 302



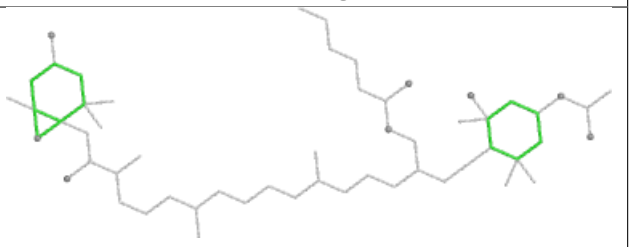
Bond lengths



Bond angles

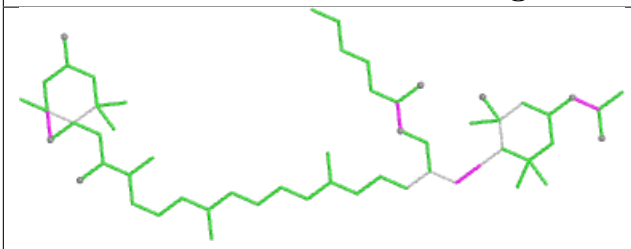


Torsions

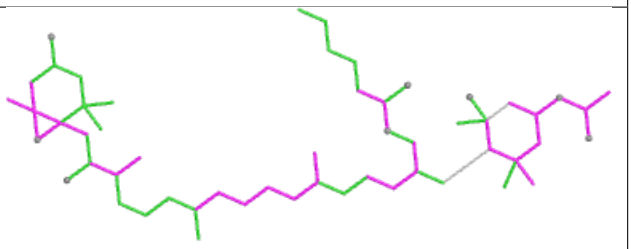


Rings

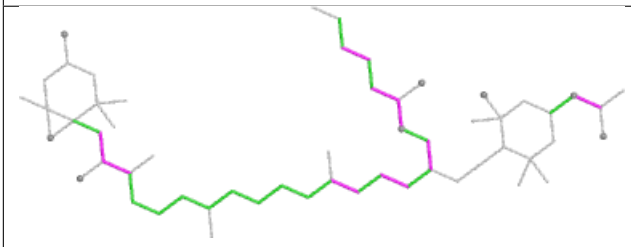
Ligand A1EB1 2 304



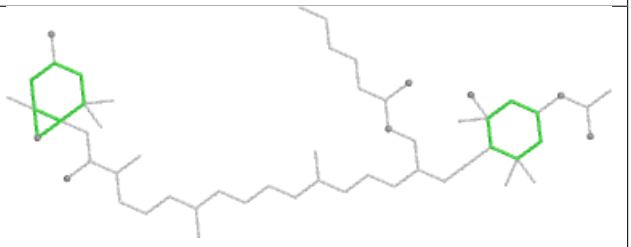
Bond lengths



Bond angles

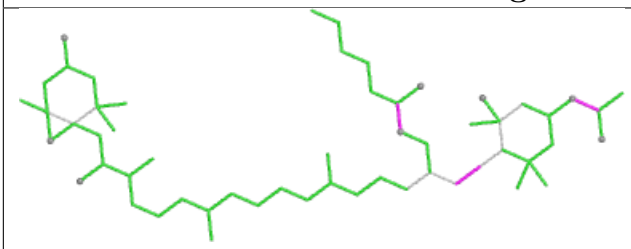


Torsions

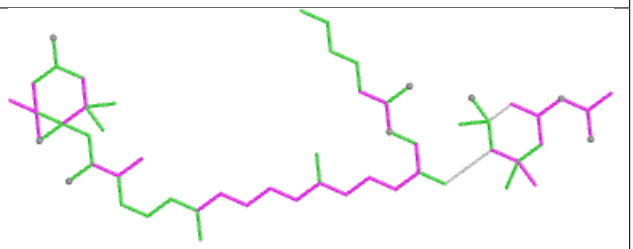


Rings

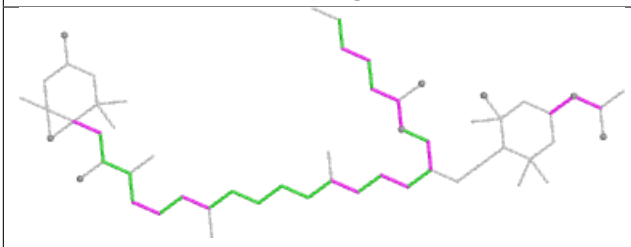
Ligand A1EB1 0 305



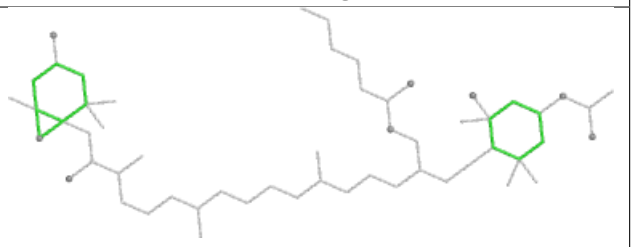
Bond lengths



Bond angles

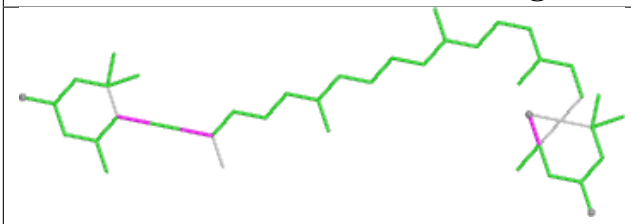


Torsions

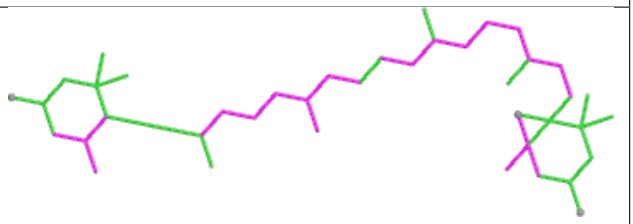


Rings

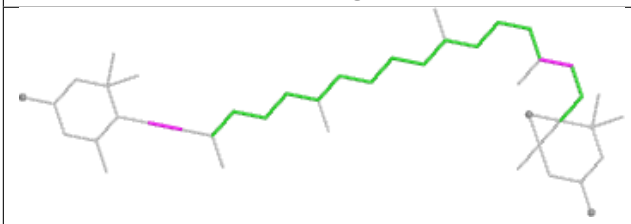
Ligand DD6 J 306



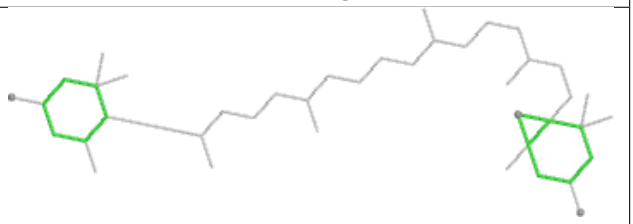
Bond lengths



Bond angles

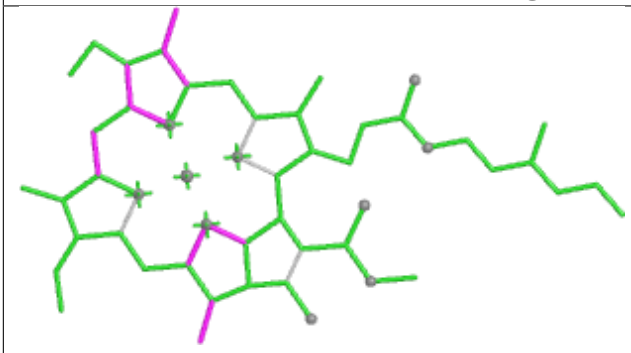


Torsions

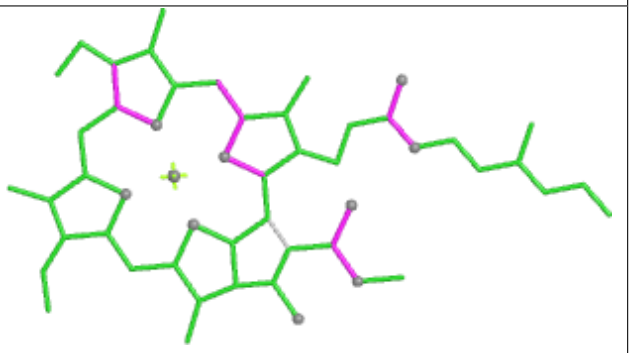


Rings

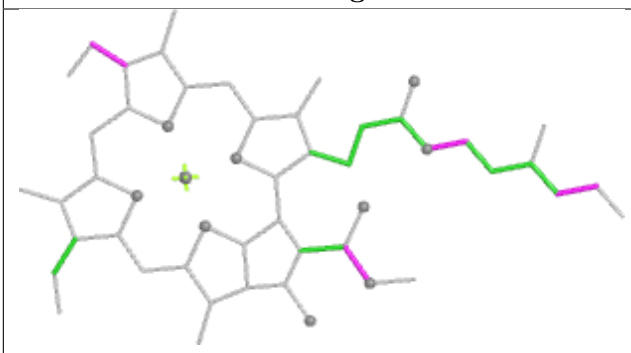
Ligand CLA V 319



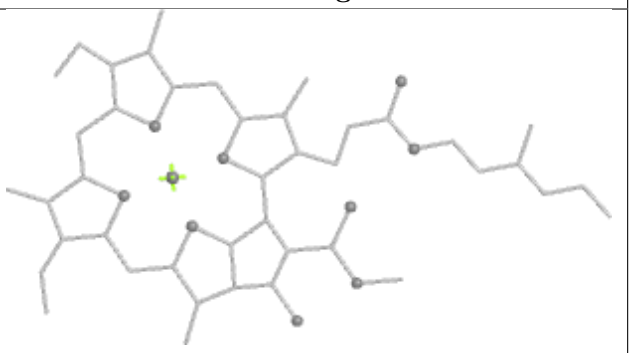
Bond lengths



Bond angles

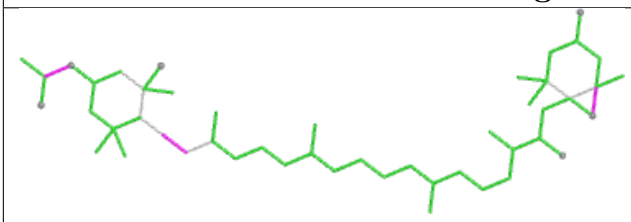


Torsions

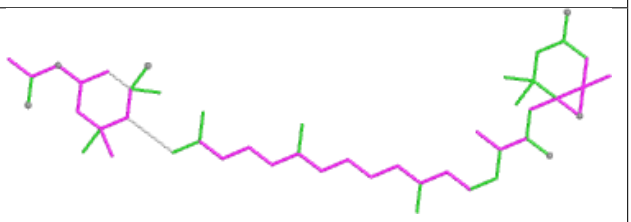


Rings

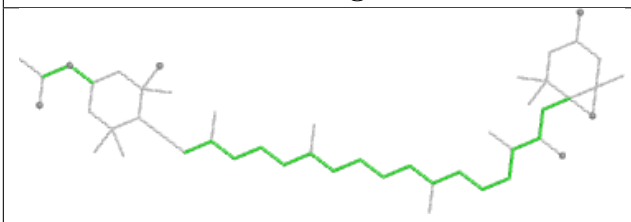
Ligand A86 1 307



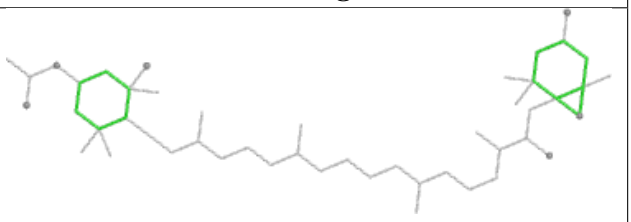
Bond lengths



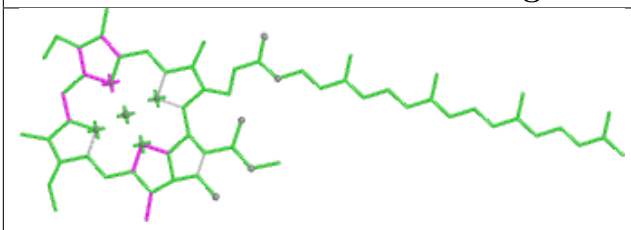
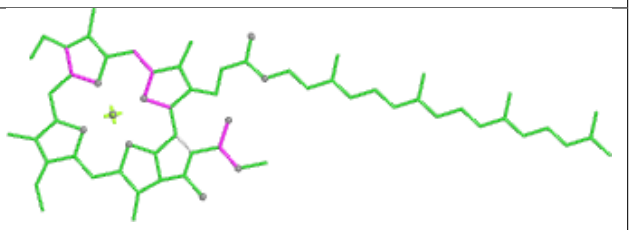
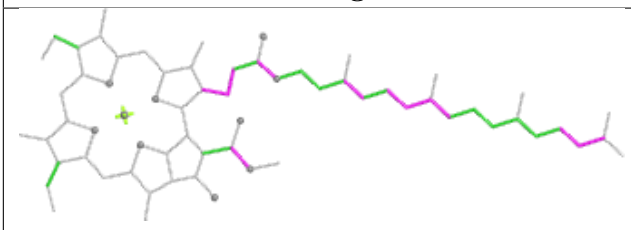
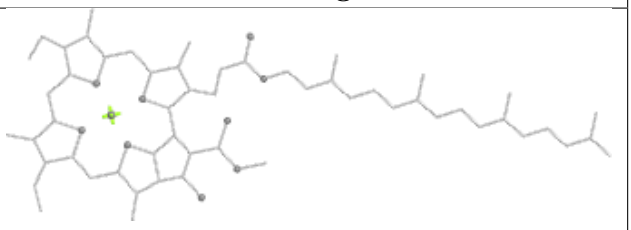
Bond angles

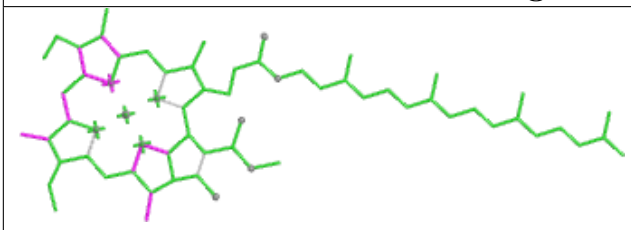
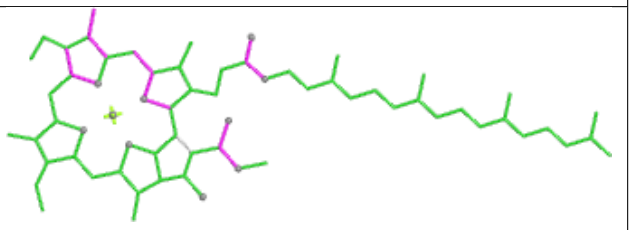
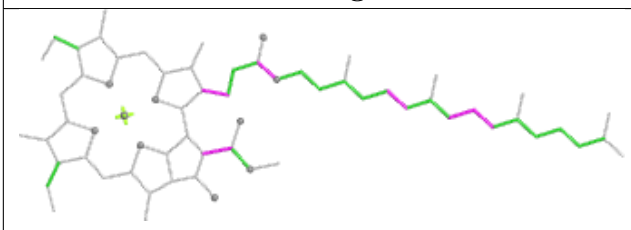
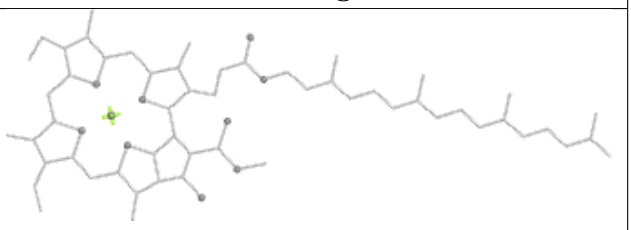


Torsions

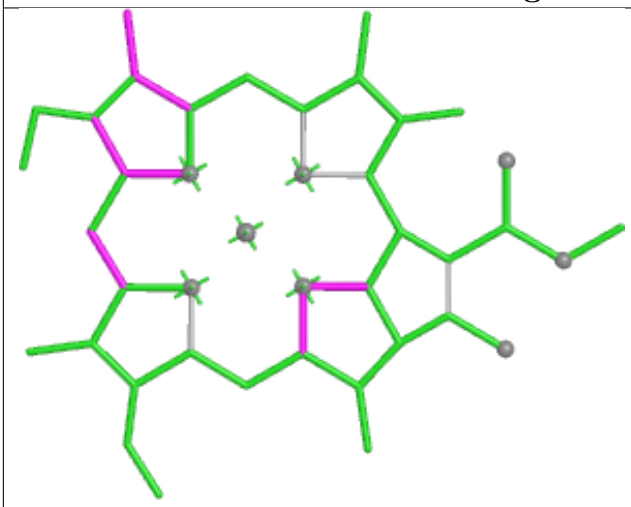


Rings

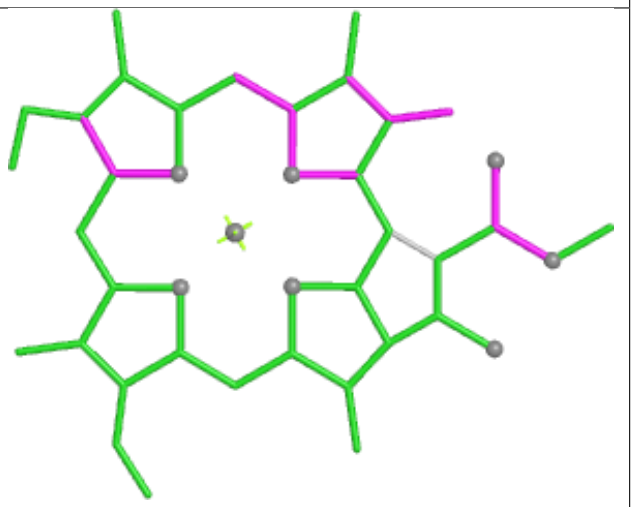
Ligand CLA K 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

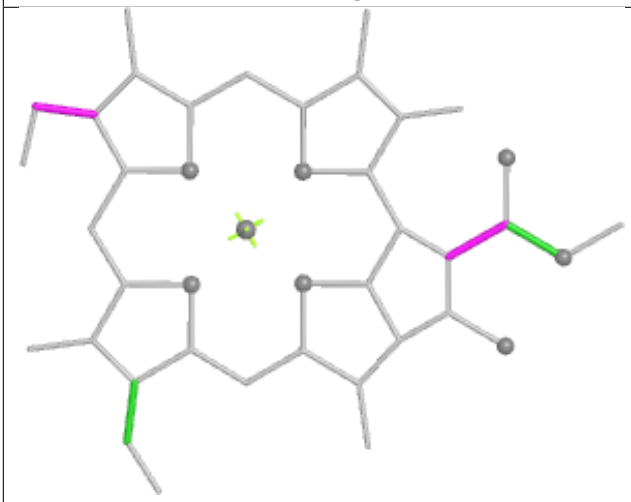
Ligand CLA Y 307



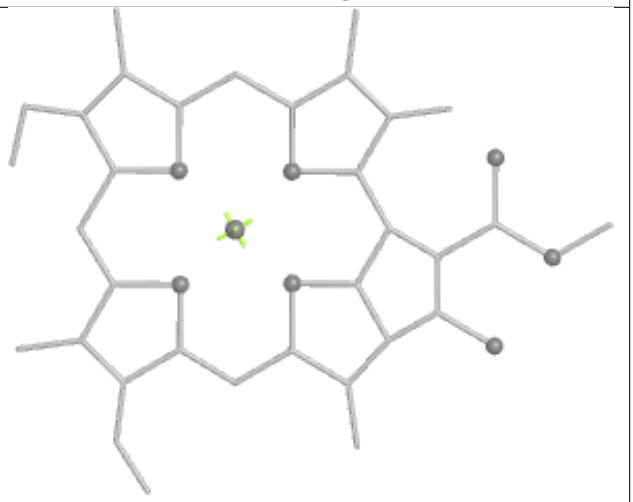
Bond lengths



Bond angles

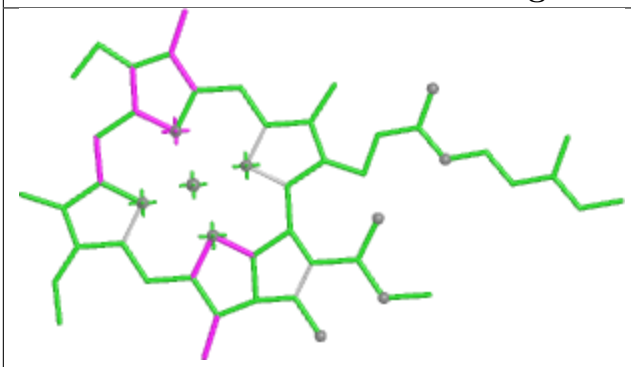


Torsions

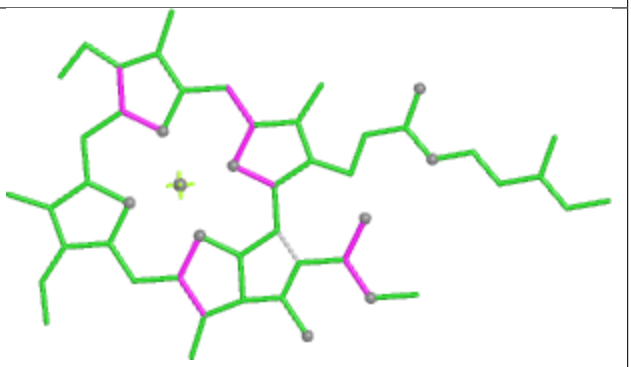


Rings

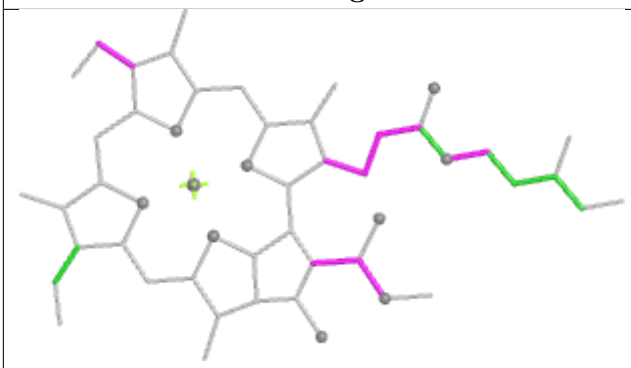
Ligand CLA a 820



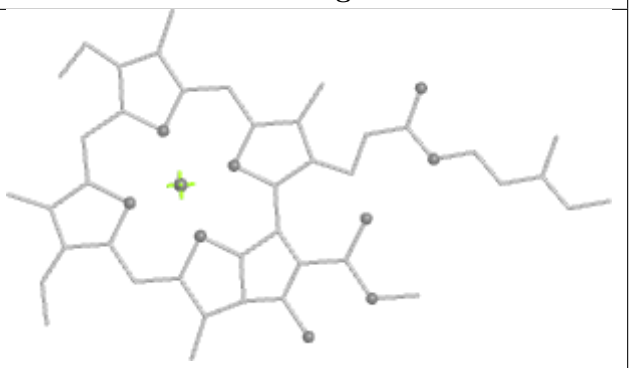
Bond lengths



Bond angles

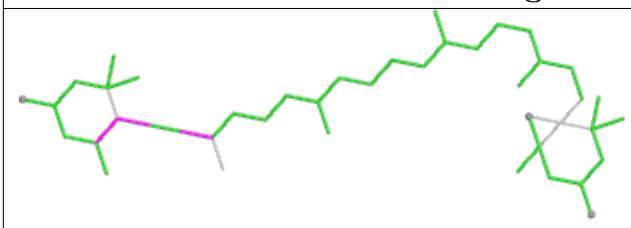


Torsions

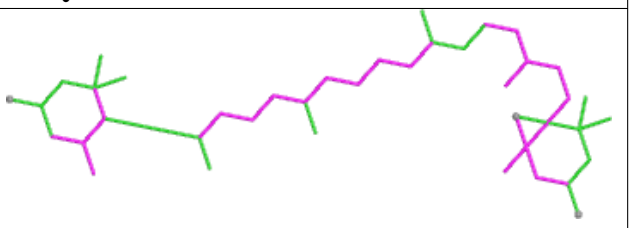


Rings

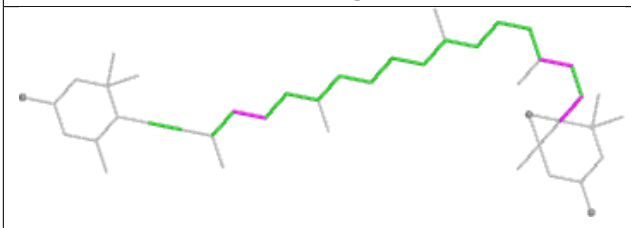
Ligand DD6 Q 303



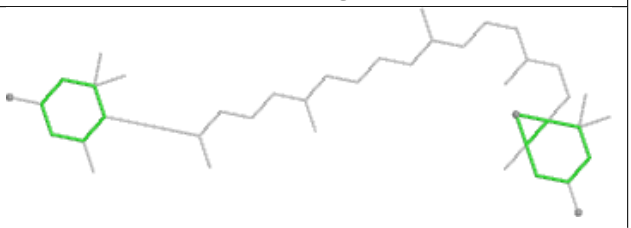
Bond lengths



Bond angles

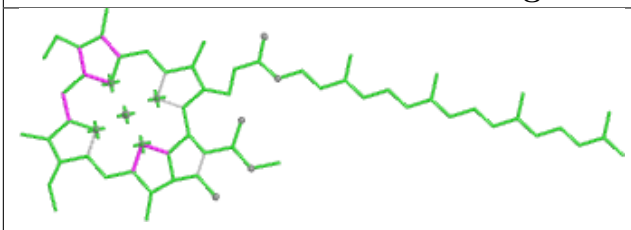


Torsions

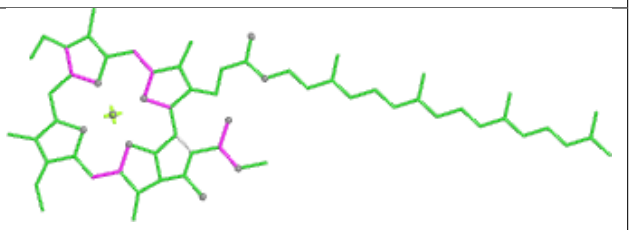


Rings

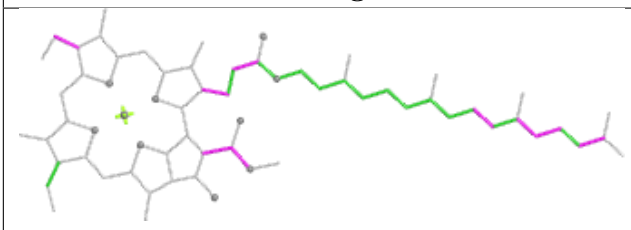
Ligand CLA D 318



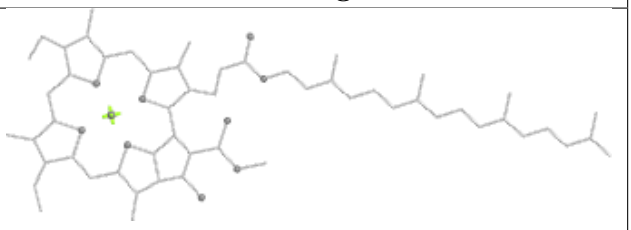
Bond lengths



Bond angles

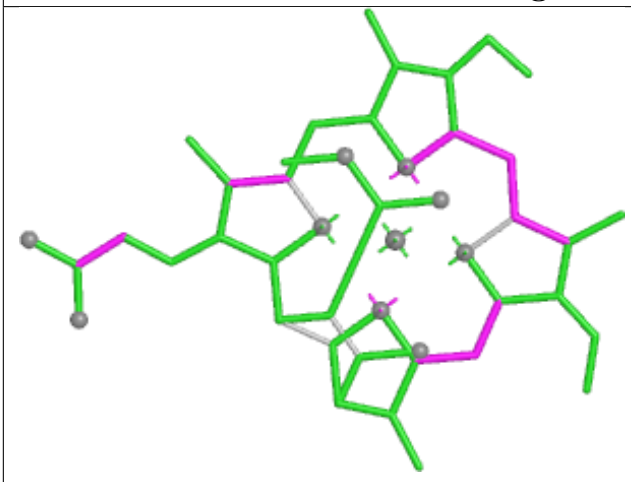


Torsions

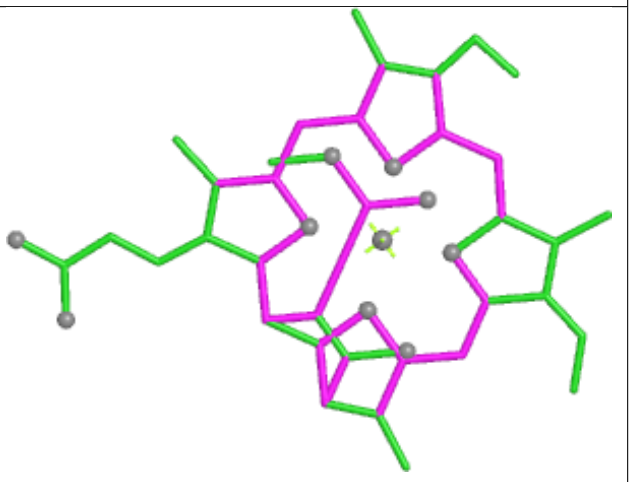


Rings

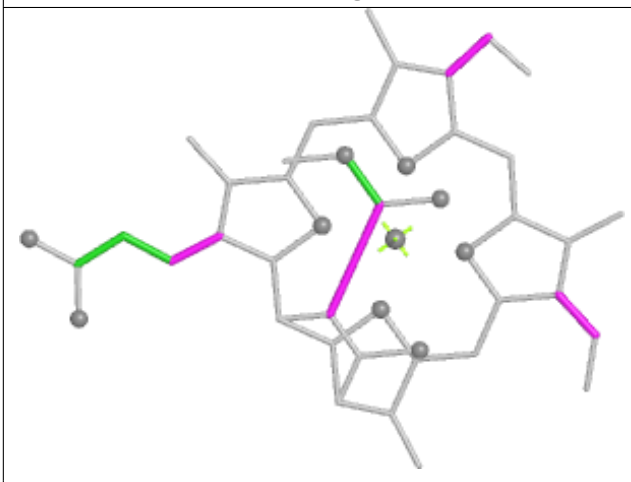
Ligand KC2 7 319



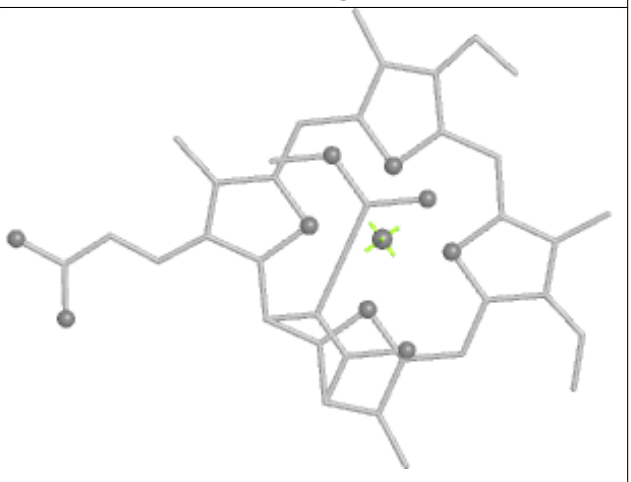
Bond lengths



Bond angles

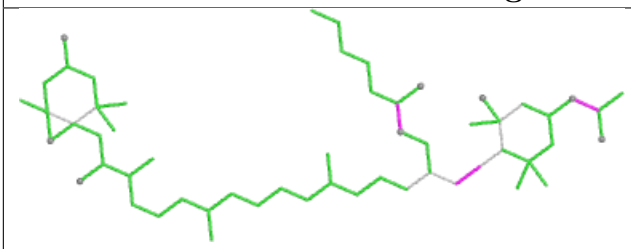


Torsions

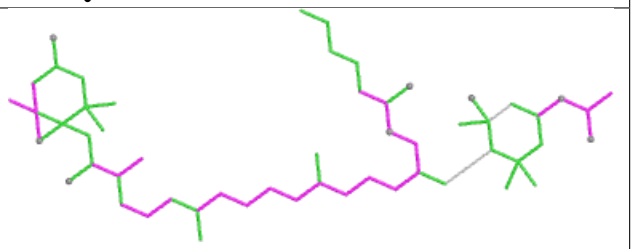


Rings

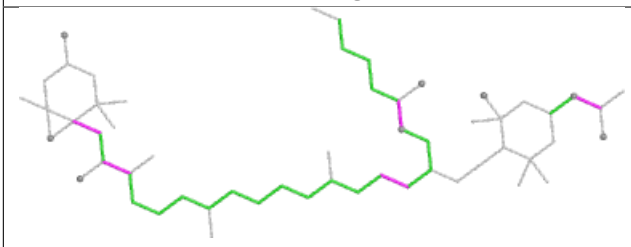
Ligand A1EB1 Q 323



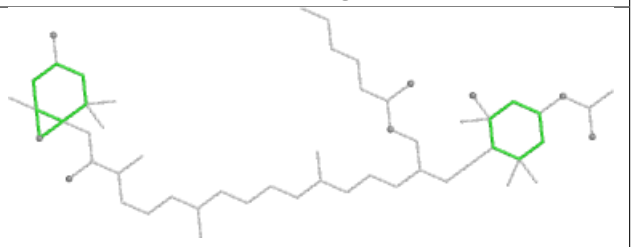
Bond lengths



Bond angles

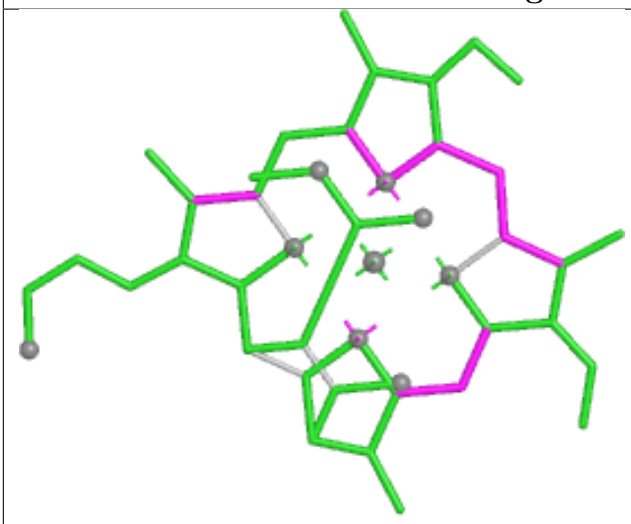


Torsions

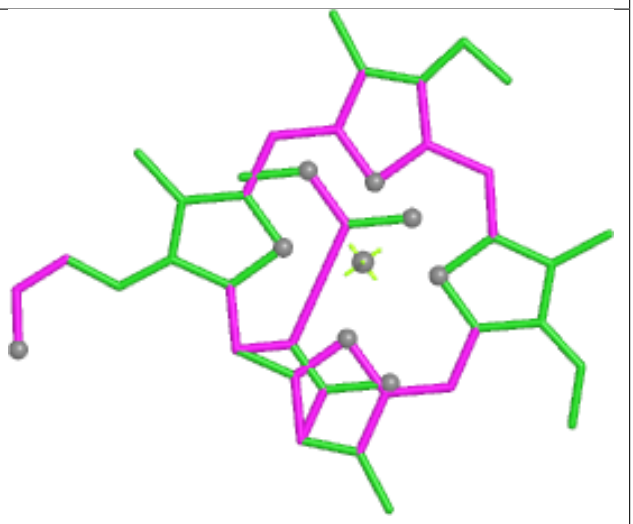


Rings

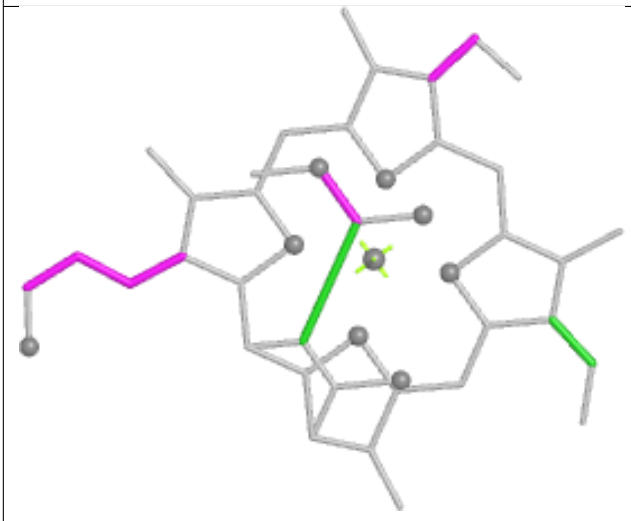
Ligand KC2 O 317



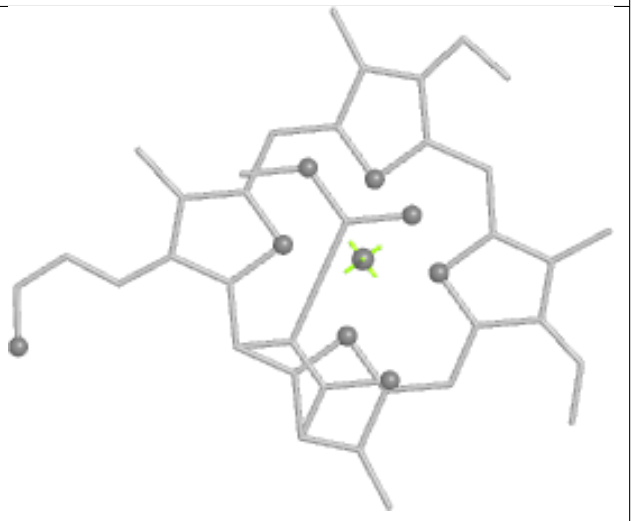
Bond lengths



Bond angles

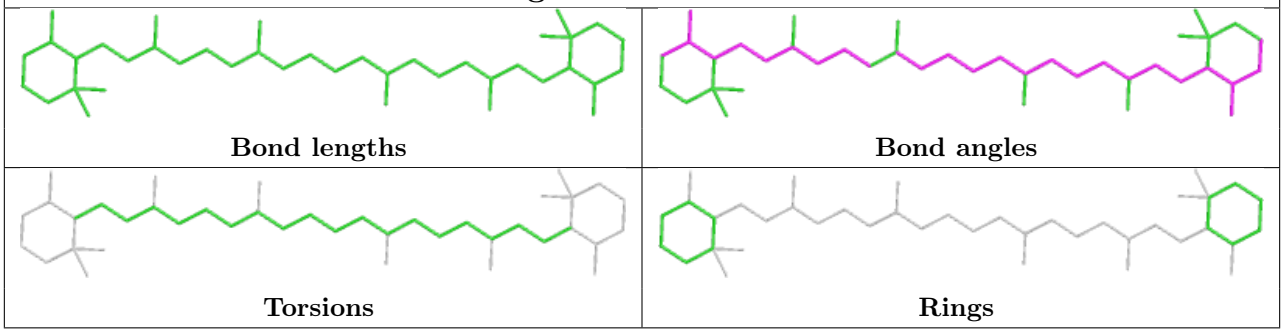


Torsions

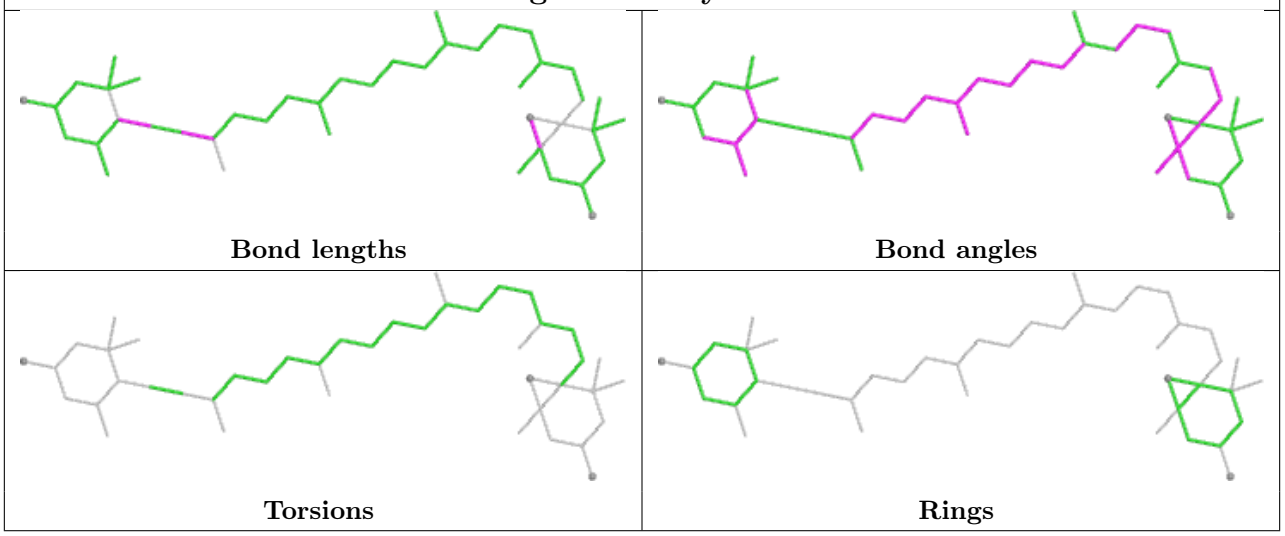


Rings

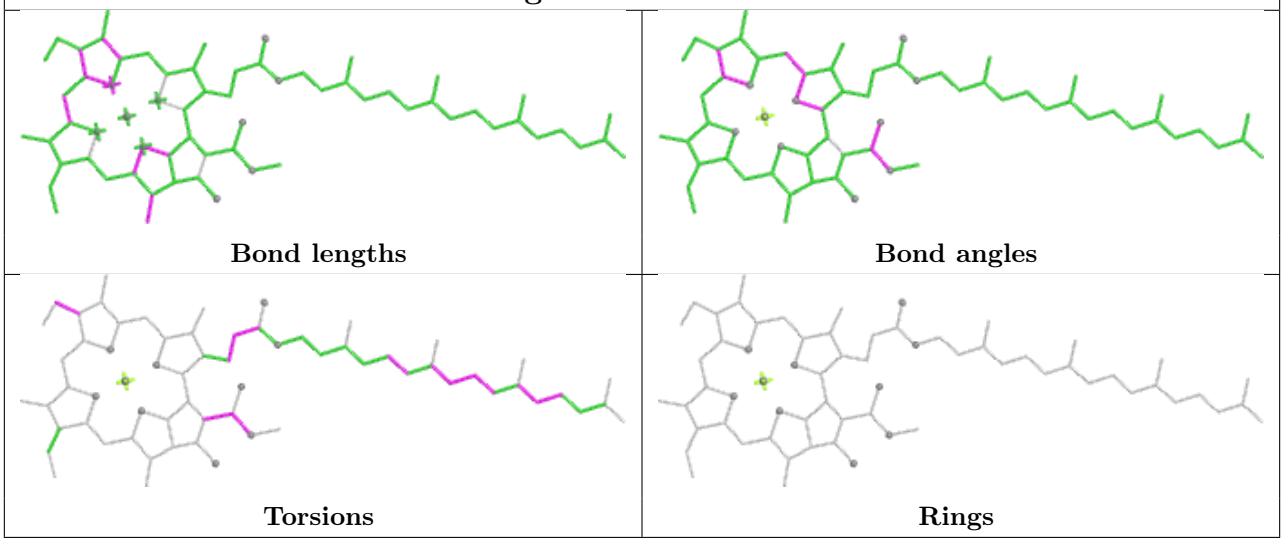
Ligand BCR a 844



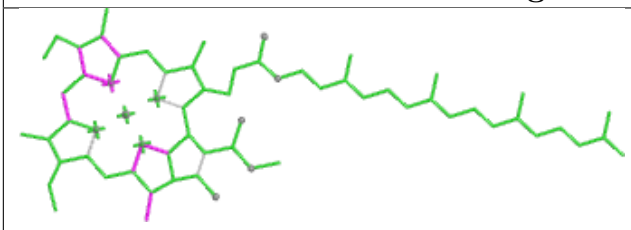
Ligand DD6 y 304



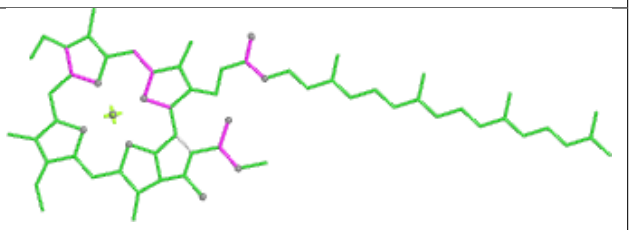
Ligand CLA V 311



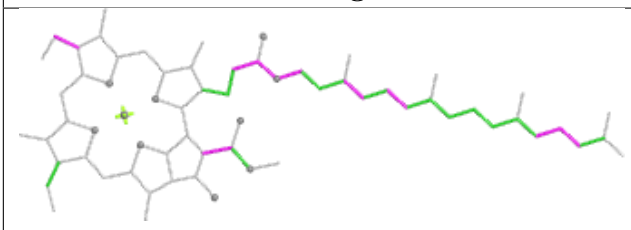
Ligand CLA b 851



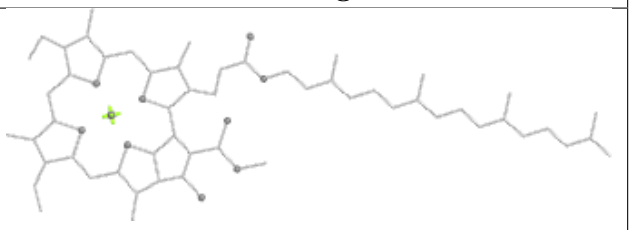
Bond lengths



Bond angles

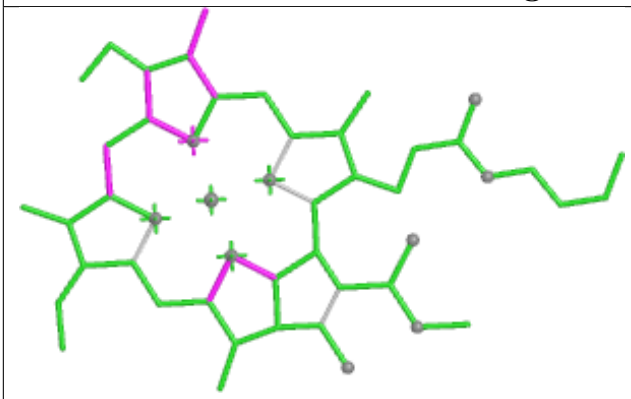


Torsions

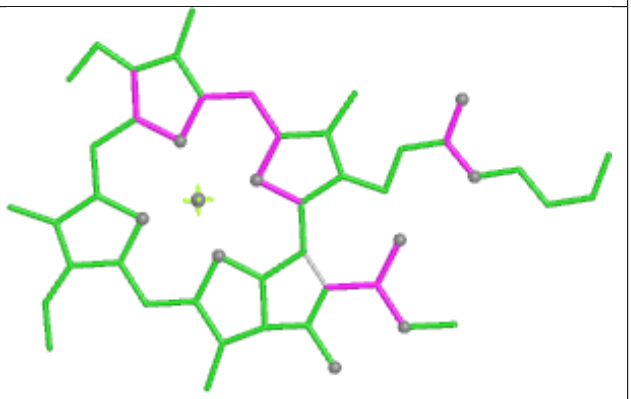


Rings

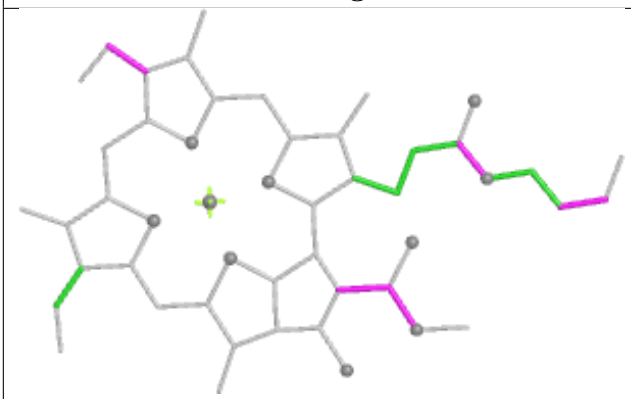
Ligand CLA D 309



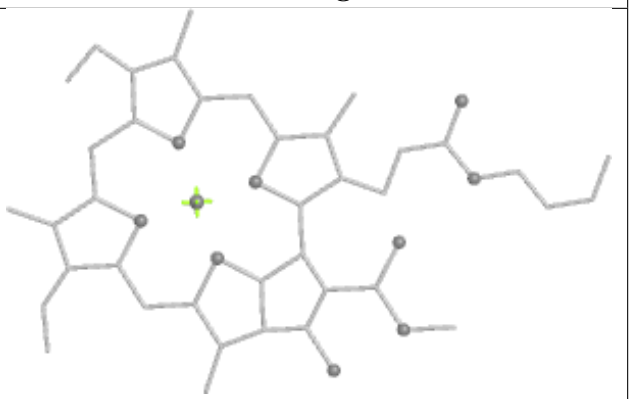
Bond lengths



Bond angles

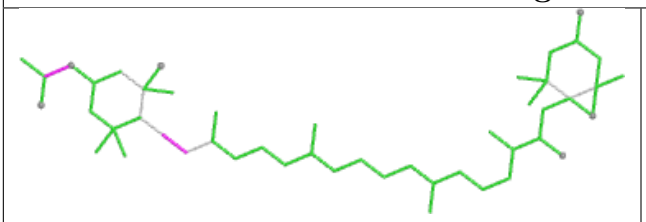


Torsions

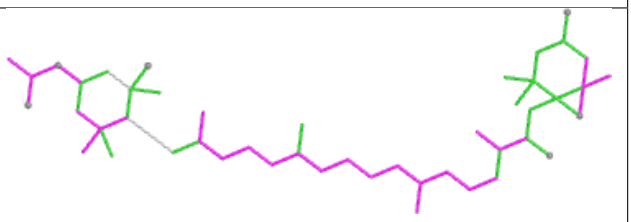


Rings

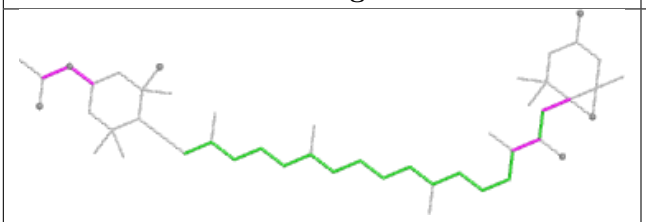
Ligand A86 7 308



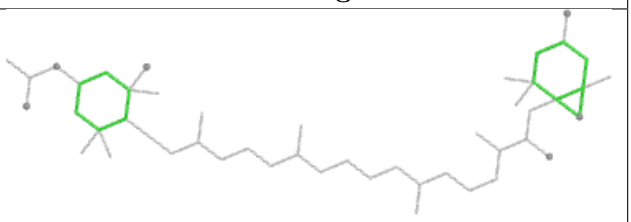
Bond lengths



Bond angles

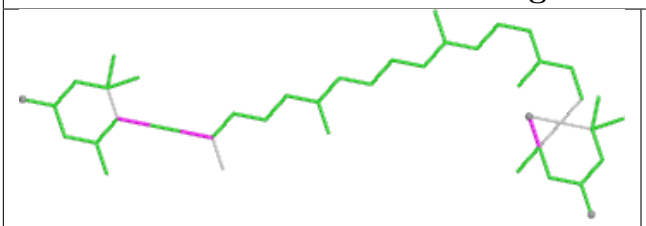


Torsions

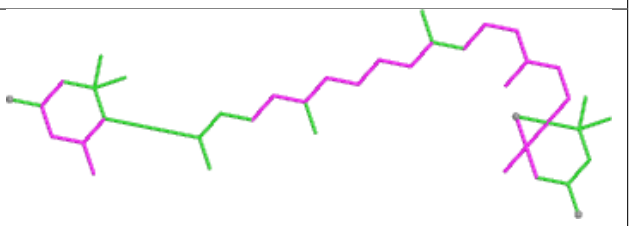


Rings

Ligand DD6 7 309



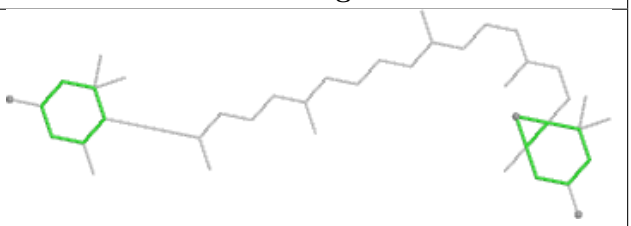
Bond lengths



Bond angles

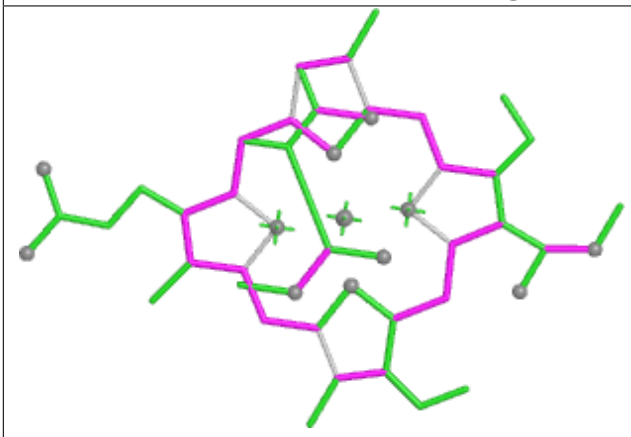


Torsions

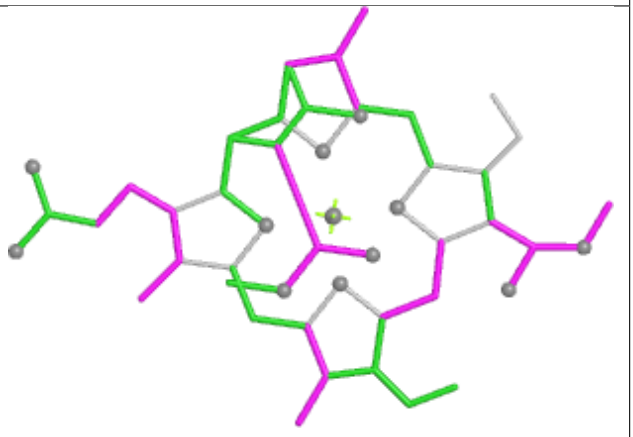


Rings

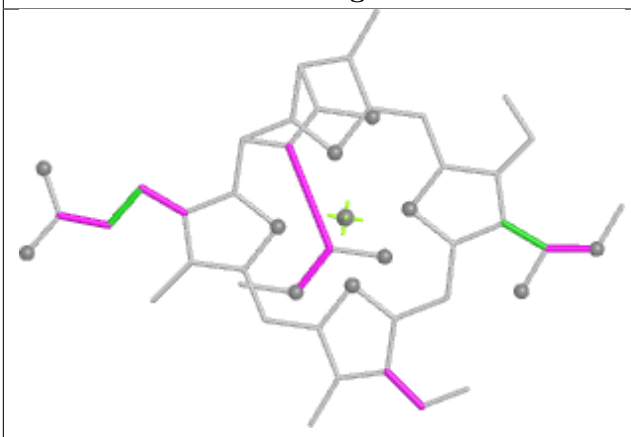
Ligand A1ECV 5 312



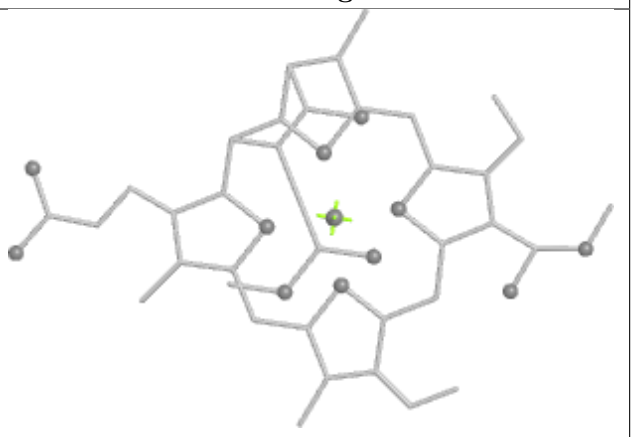
Bond lengths



Bond angles

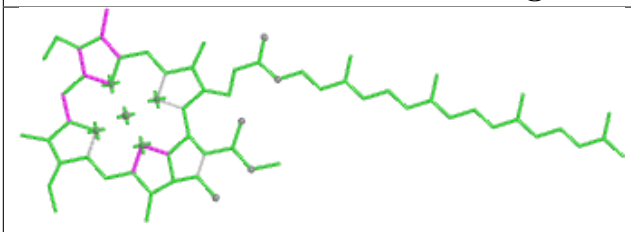


Torsions

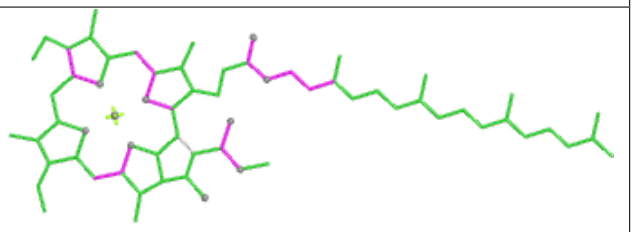


Rings

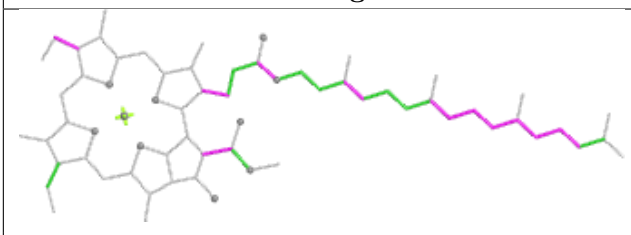
Ligand CLA F 321



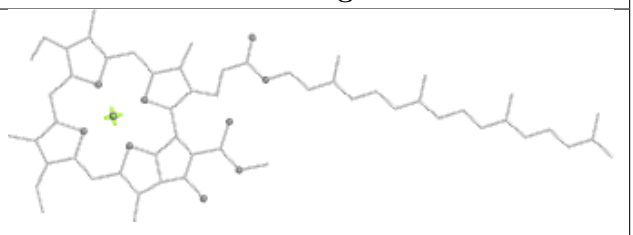
Bond lengths



Bond angles

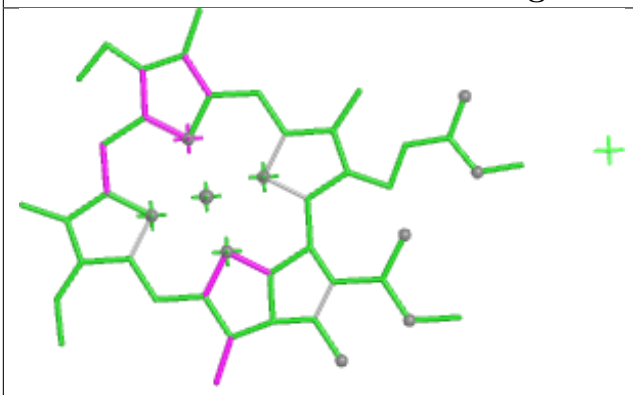


Torsions

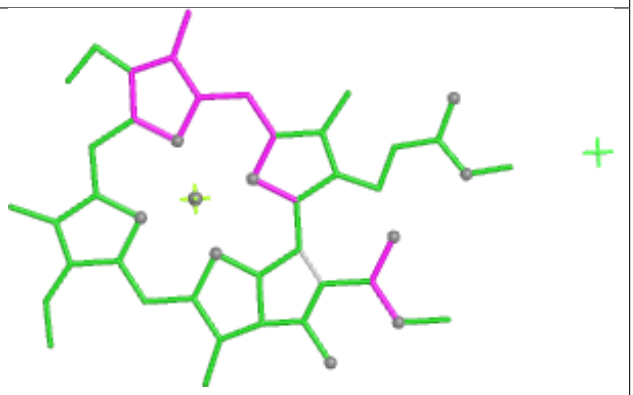


Rings

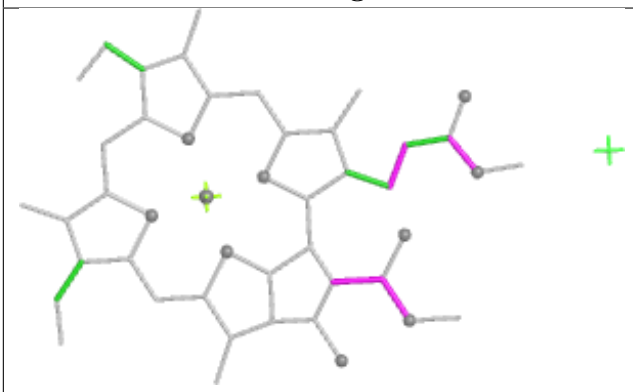
Ligand CLA J 318



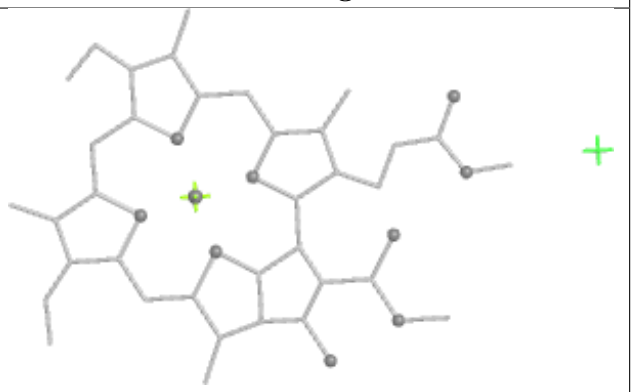
Bond lengths



Bond angles

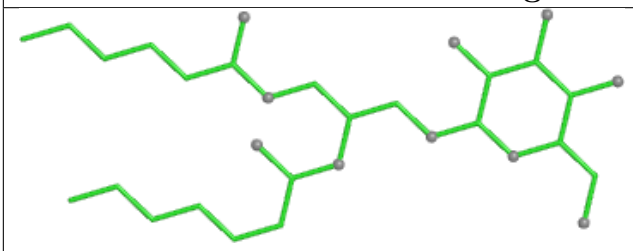


Torsions

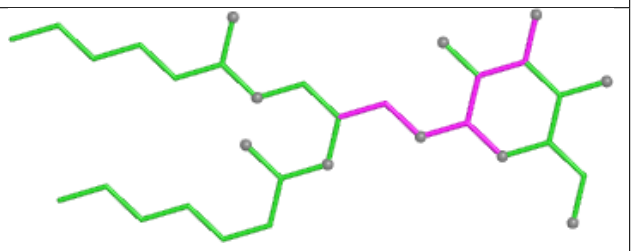


Rings

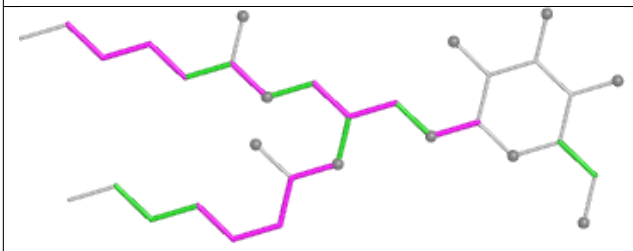
Ligand LMG 4 325



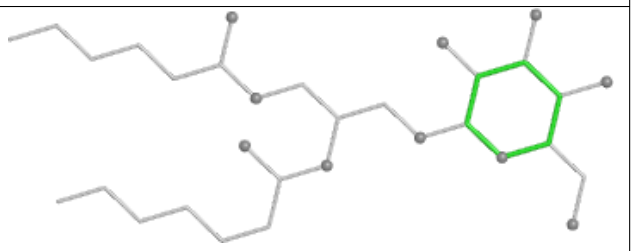
Bond lengths



Bond angles

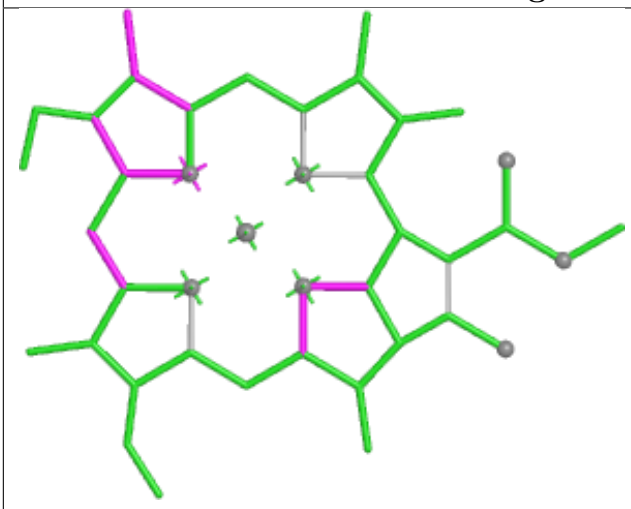


Torsions

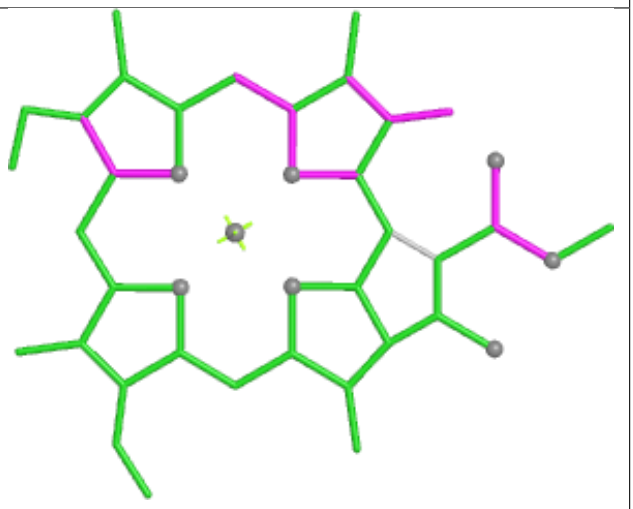


Rings

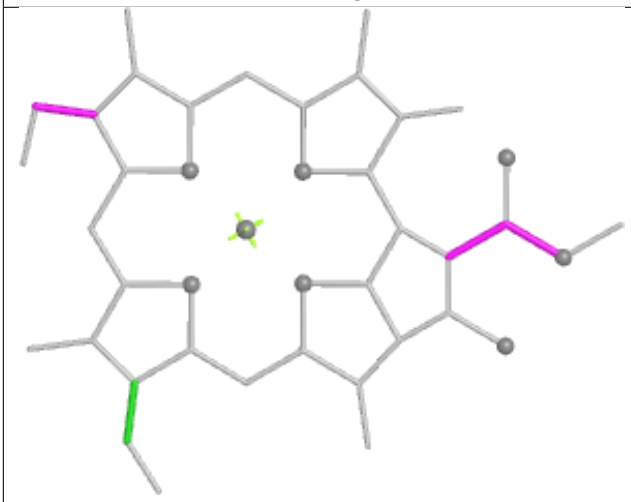
Ligand CLA 6 321



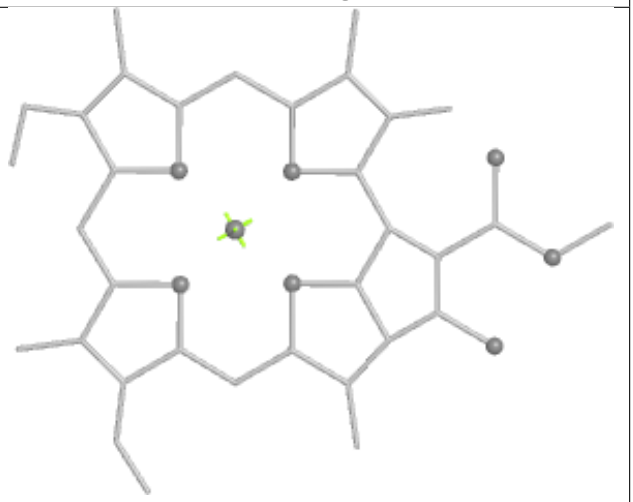
Bond lengths



Bond angles

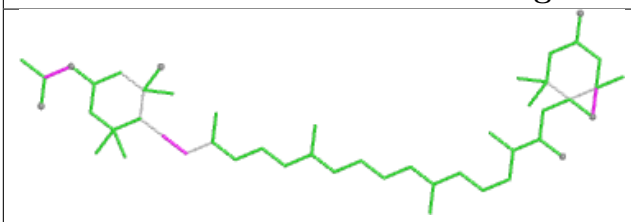


Torsions

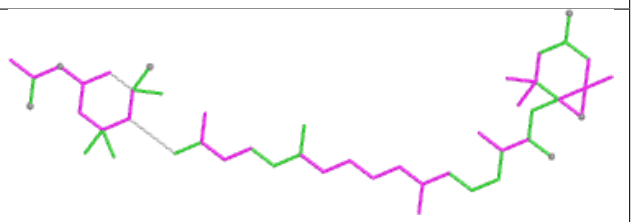


Rings

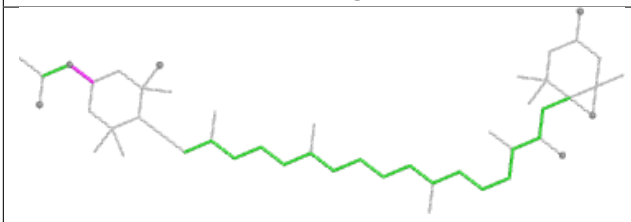
Ligand A86 0 308



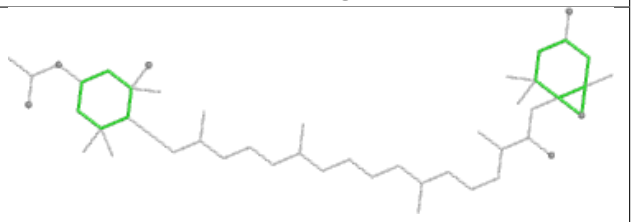
Bond lengths



Bond angles

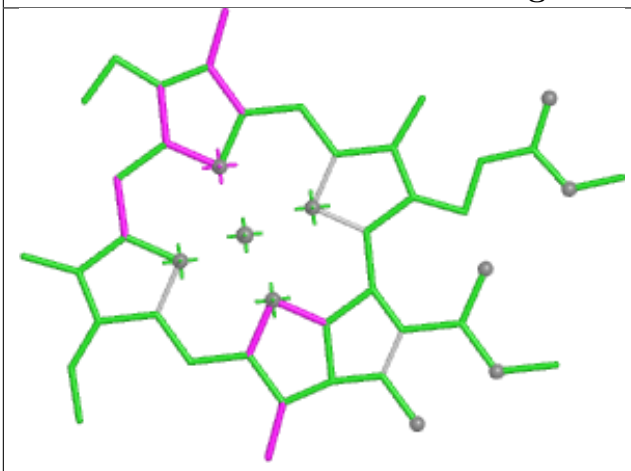


Torsions

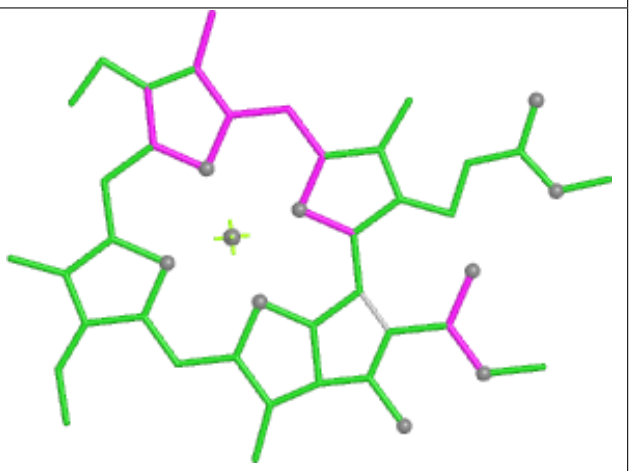


Rings

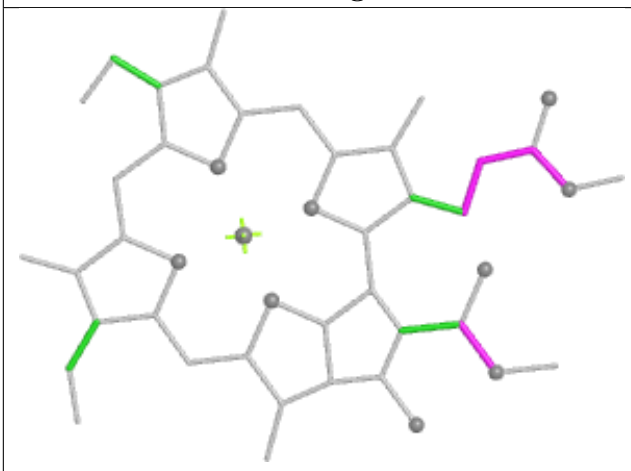
Ligand CLA 2 309



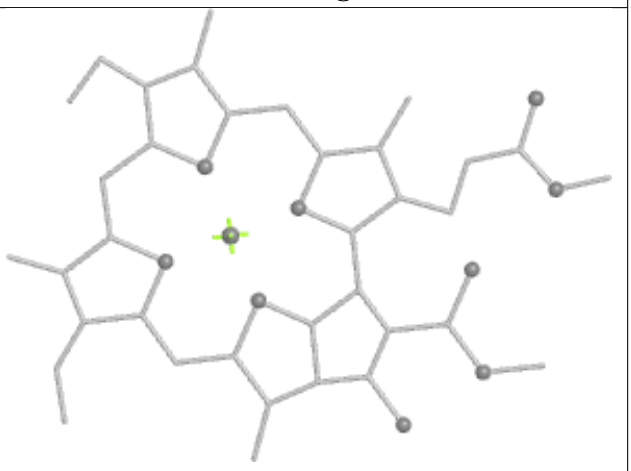
Bond lengths



Bond angles

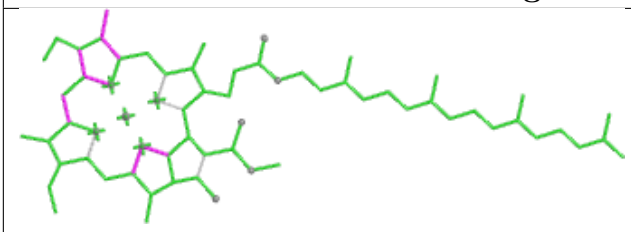


Torsions

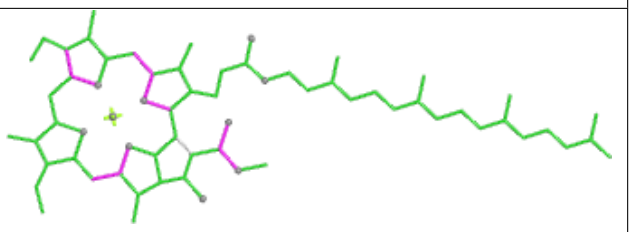


Rings

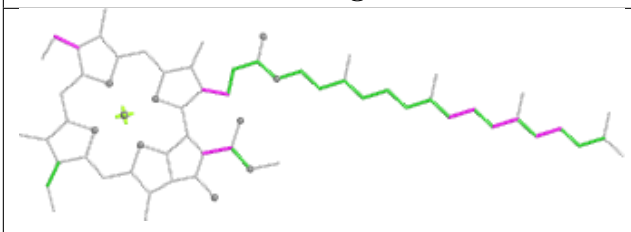
Ligand CLA D 315



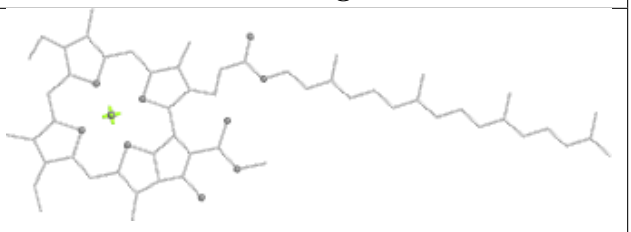
Bond lengths



Bond angles

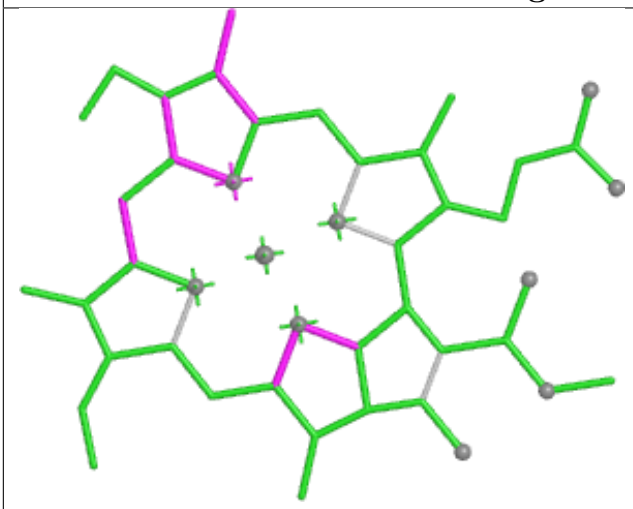


Torsions

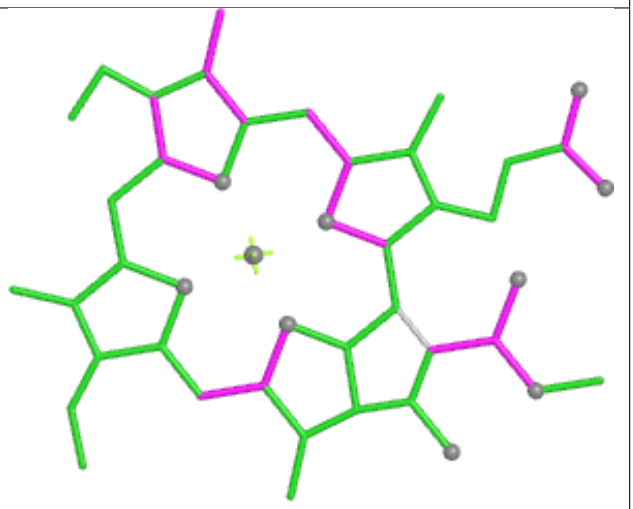


Rings

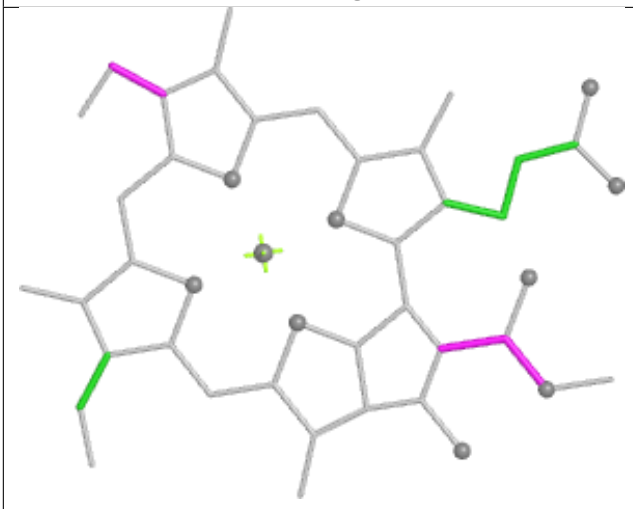
Ligand CLA a 812



Bond lengths



Bond angles

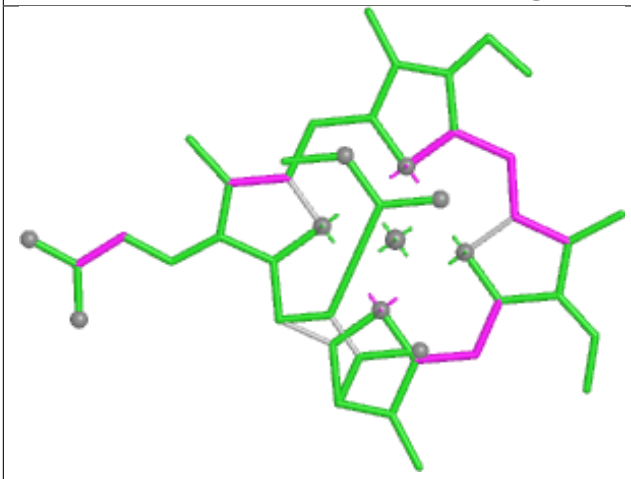


Torsions

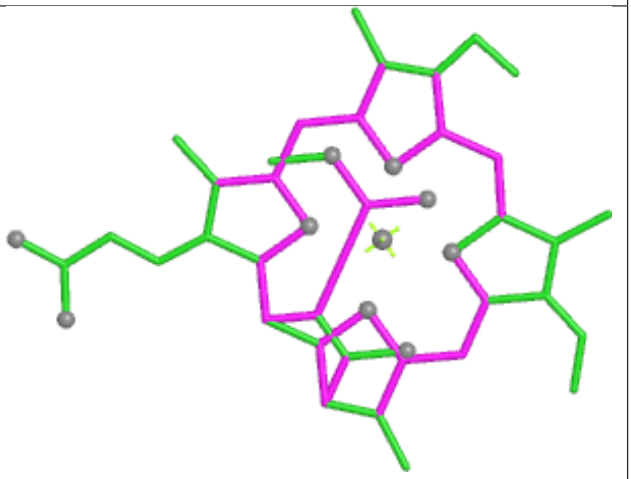


Rings

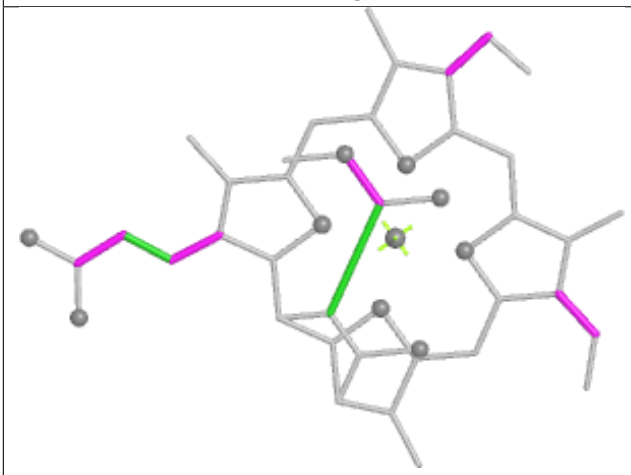
Ligand KC2 F 307



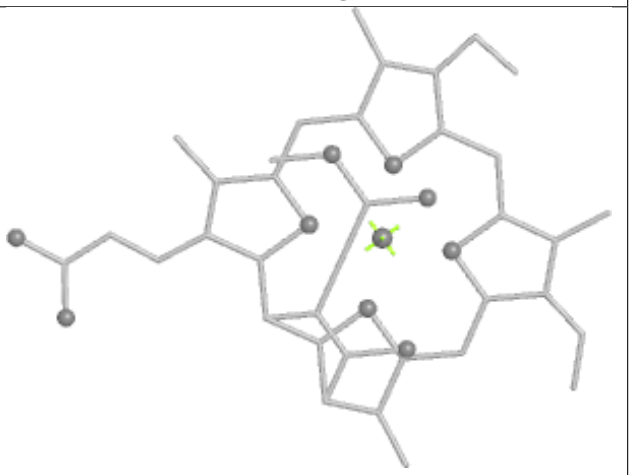
Bond lengths



Bond angles

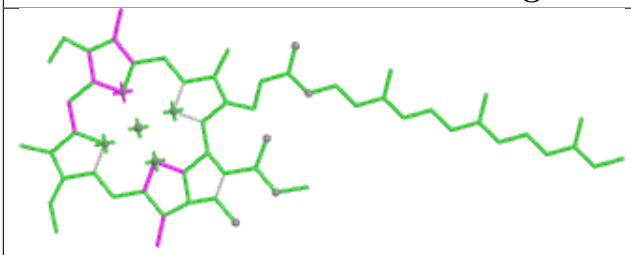


Torsions

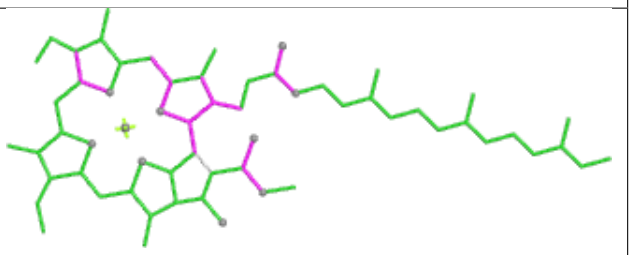


Rings

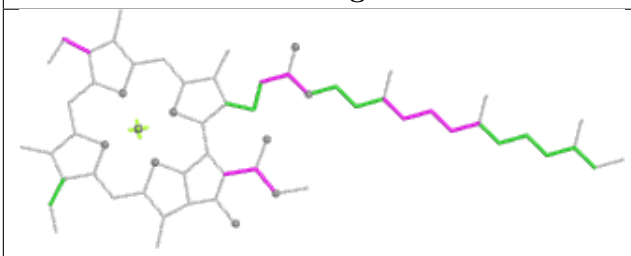
Ligand CLA K 306



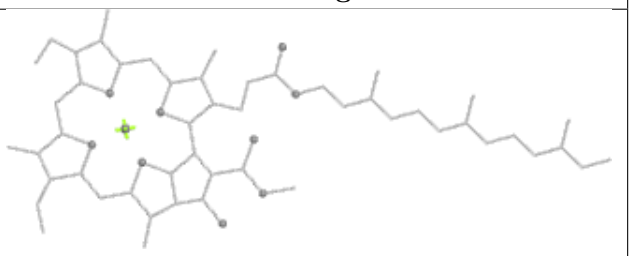
Bond lengths



Bond angles

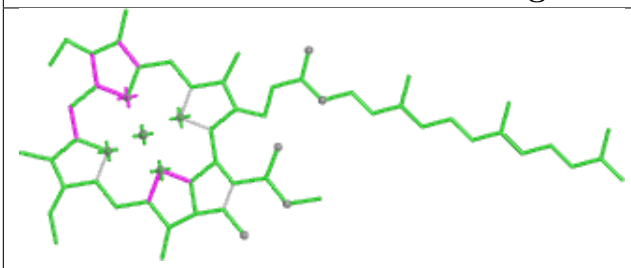


Torsions

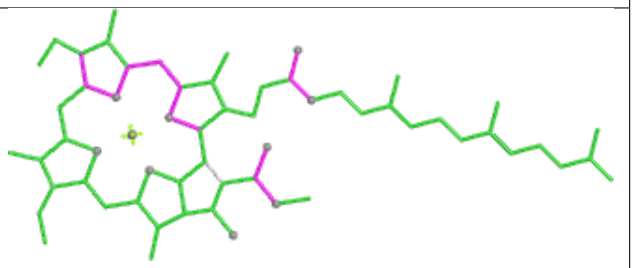


Rings

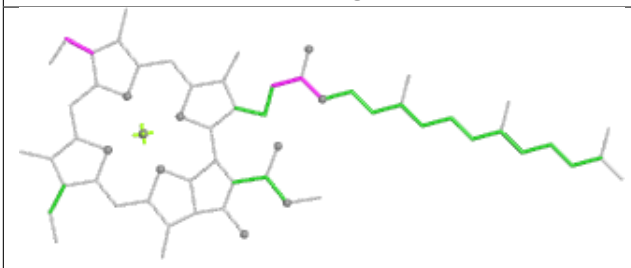
Ligand CLA 5 307



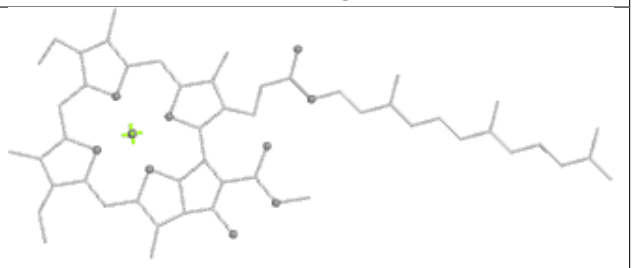
Bond lengths



Bond angles

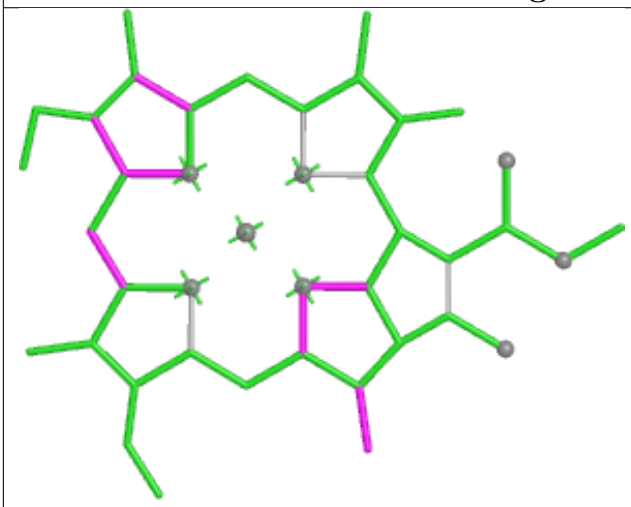


Torsions

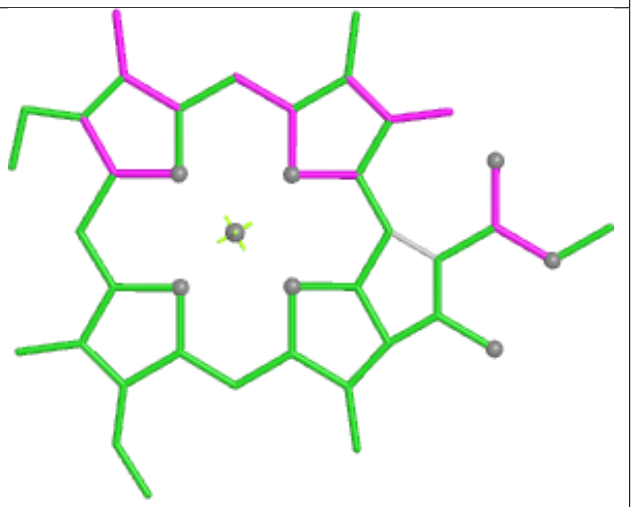


Rings

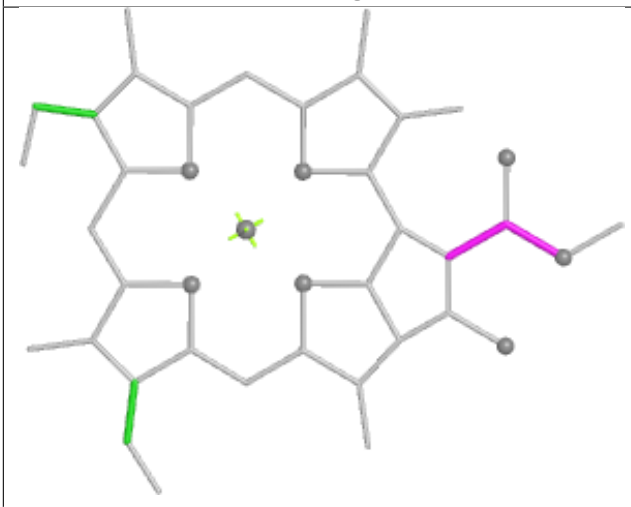
Ligand CLA z 309



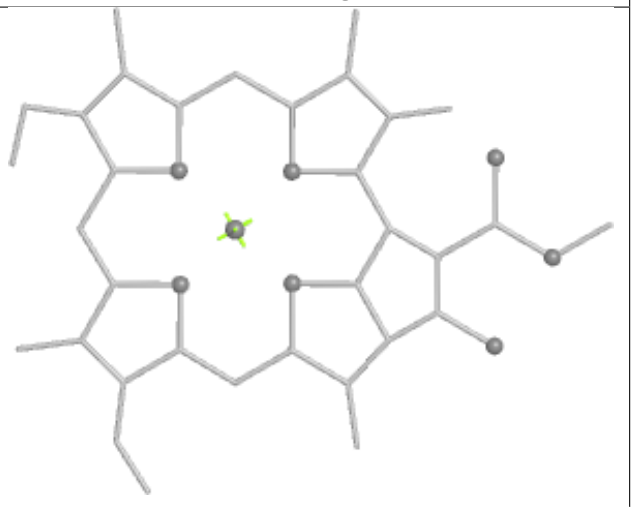
Bond lengths



Bond angles

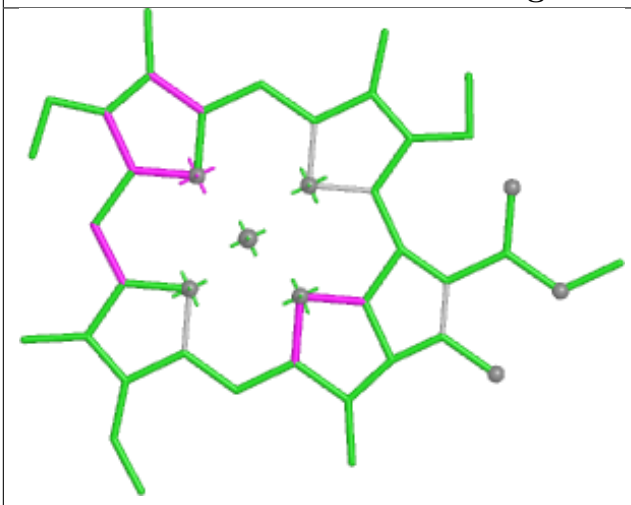


Torsions

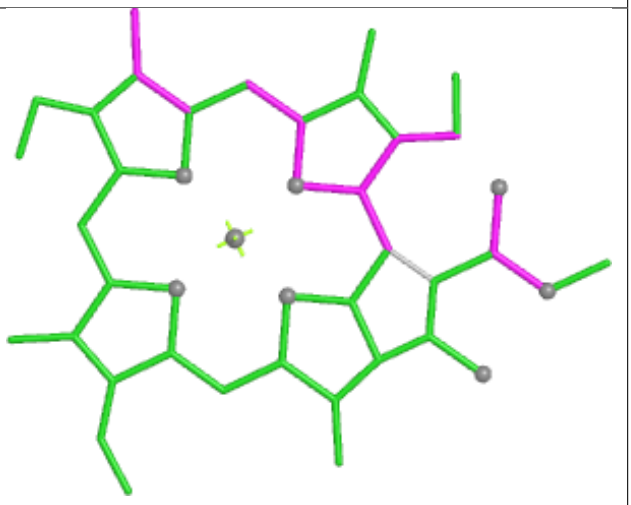


Rings

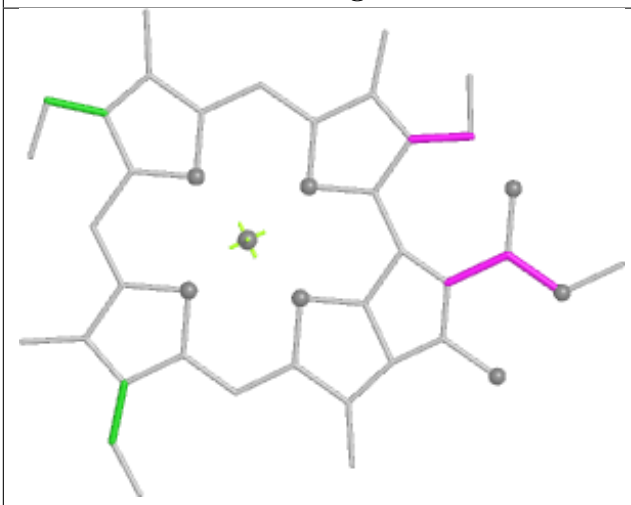
Ligand CLA S 310



Bond lengths



Bond angles

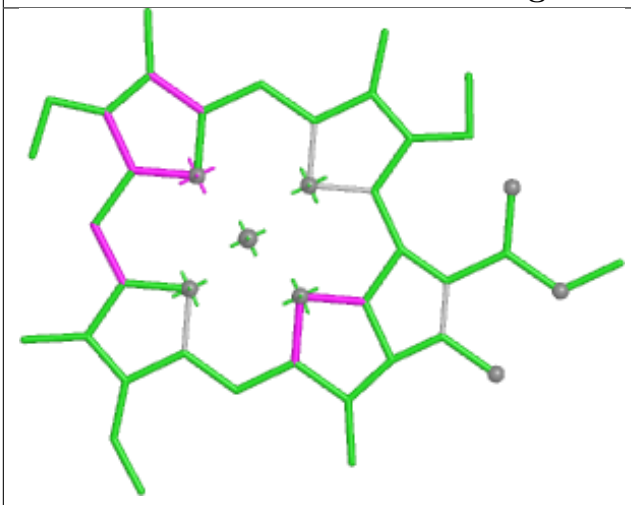


Torsions

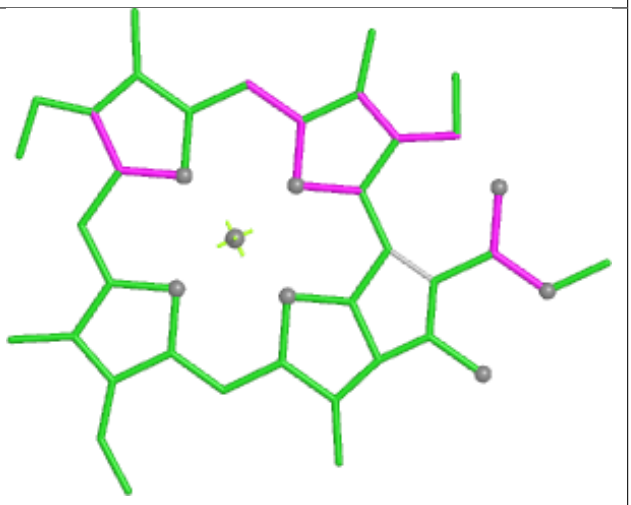


Rings

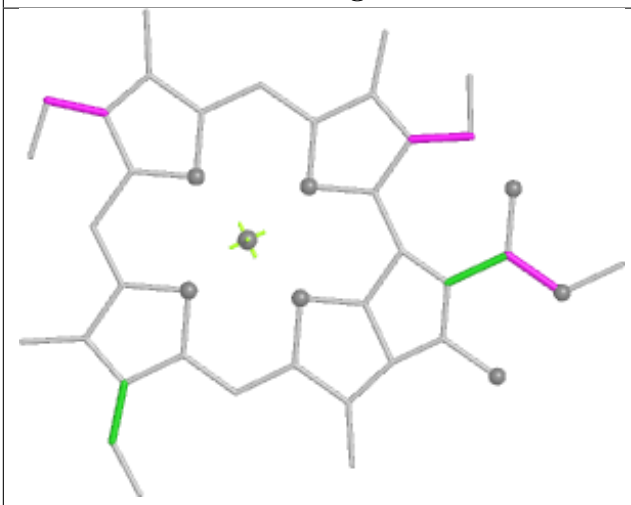
Ligand CLA 6 310



Bond lengths



Bond angles

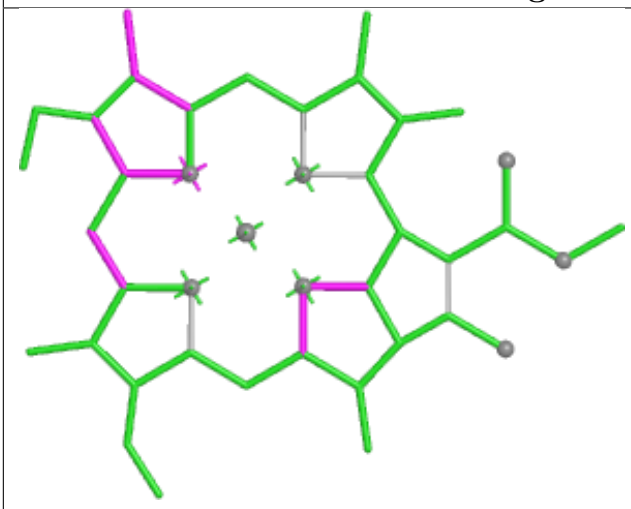


Torsions

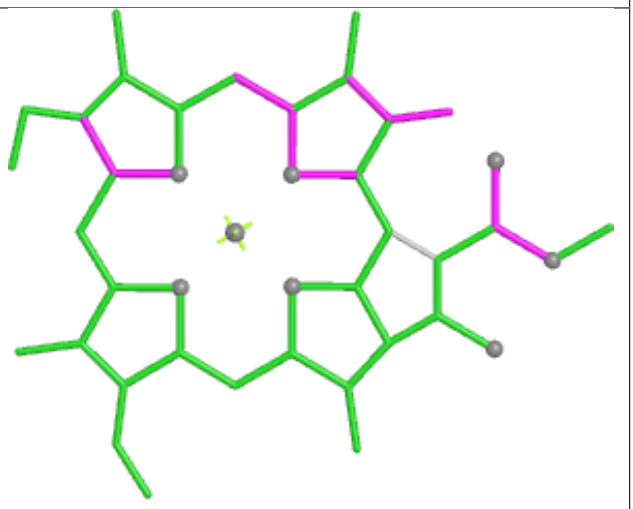


Rings

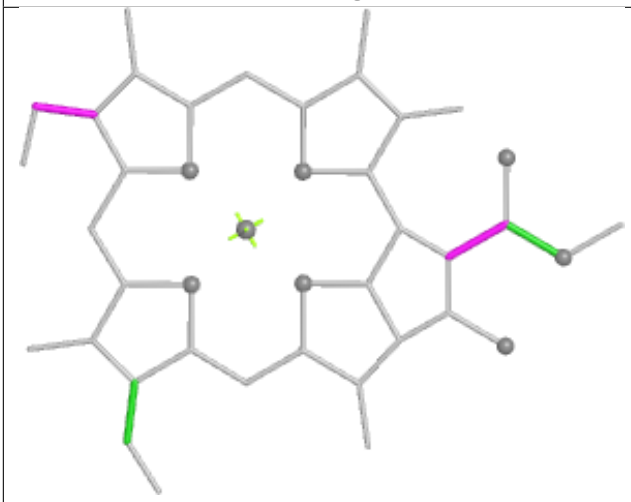
Ligand CLA 9 315



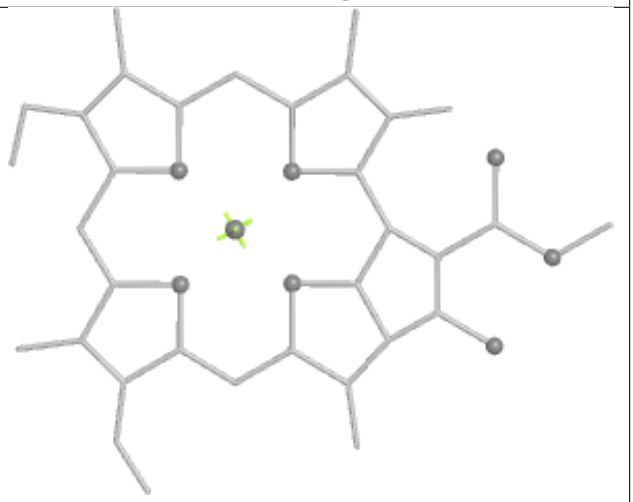
Bond lengths



Bond angles

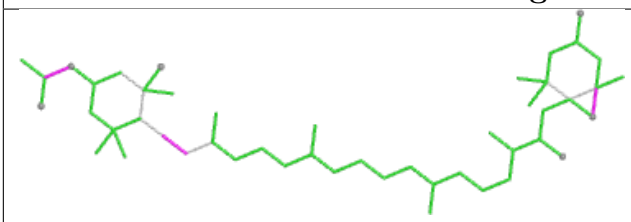


Torsions

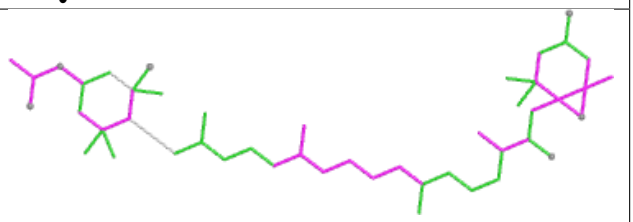


Rings

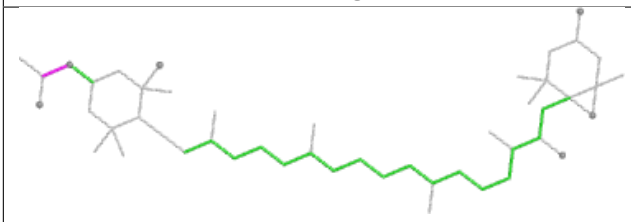
Ligand A86 Q 304



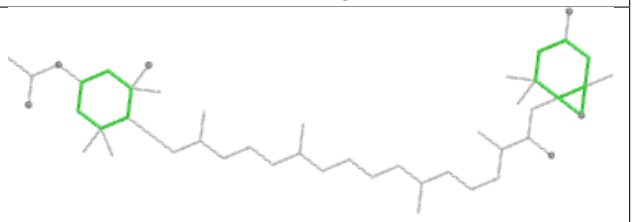
Bond lengths



Bond angles

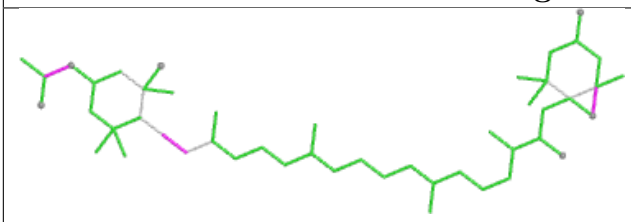


Torsions

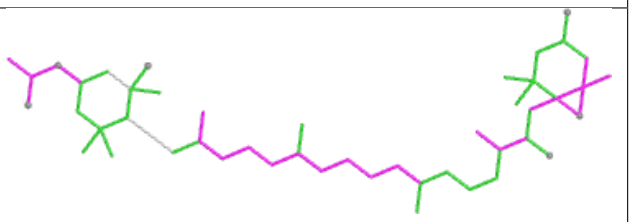


Rings

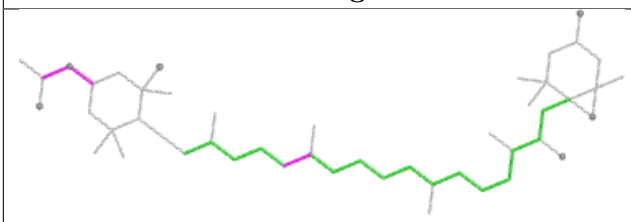
Ligand A86 8 303



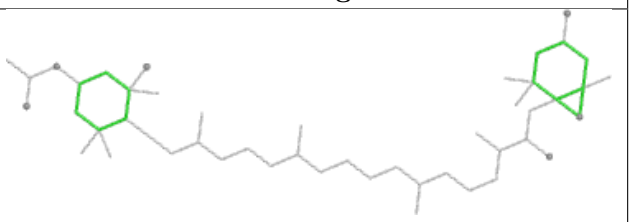
Bond lengths



Bond angles

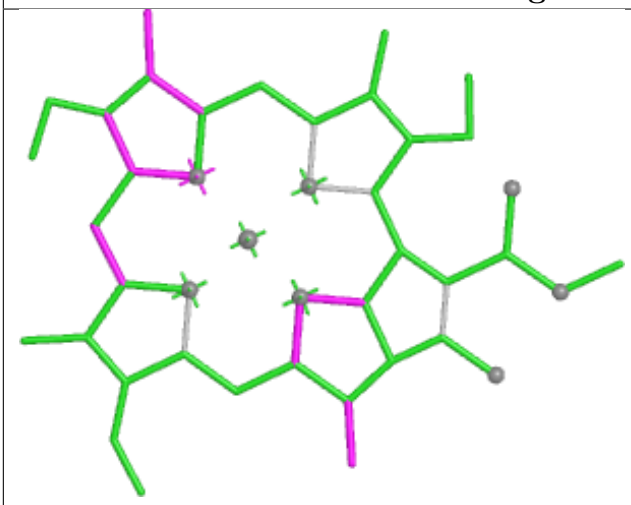


Torsions

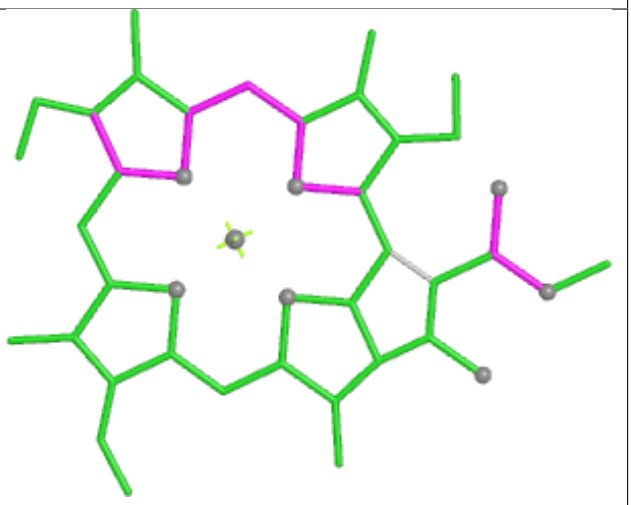


Rings

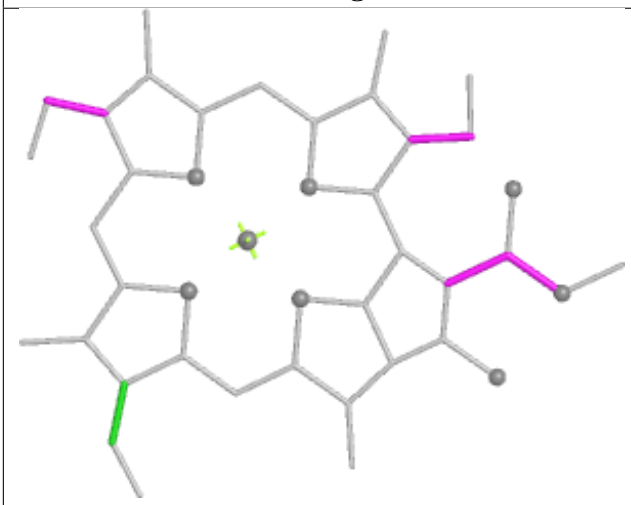
Ligand CLA 1 309



Bond lengths



Bond angles

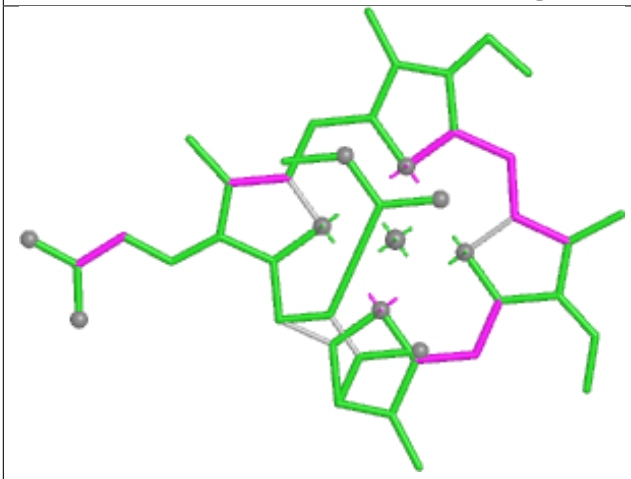


Torsions

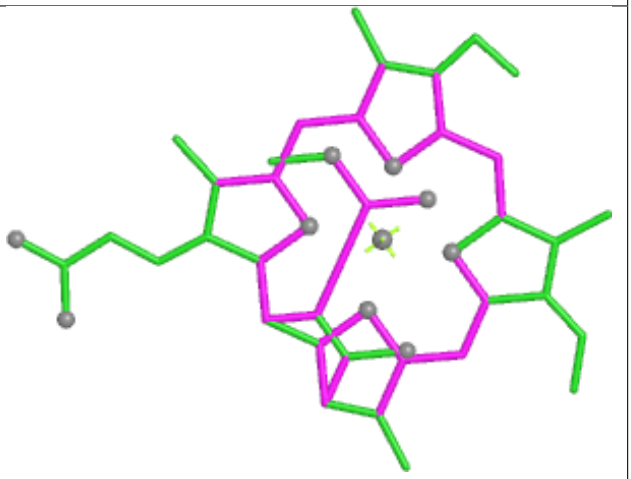


Rings

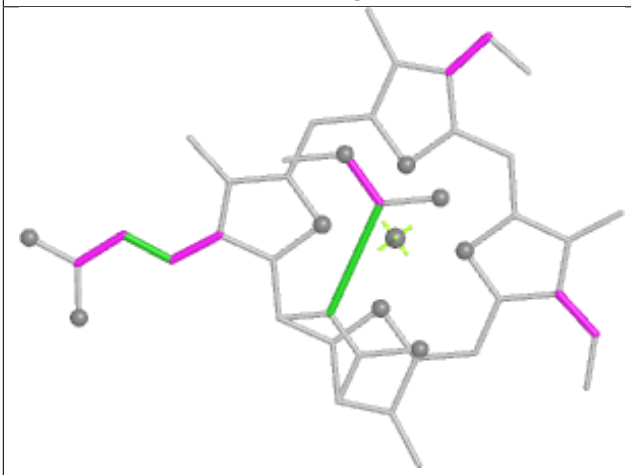
Ligand KC2 z 315



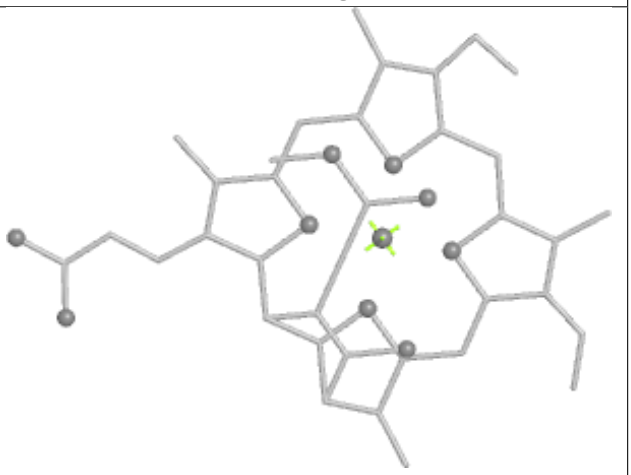
Bond lengths



Bond angles

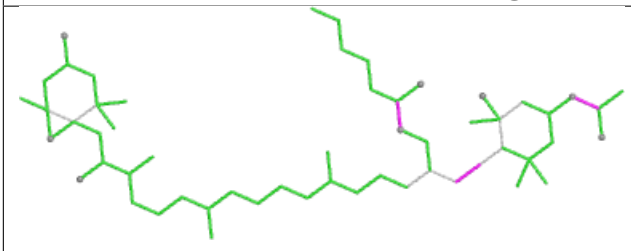


Torsions

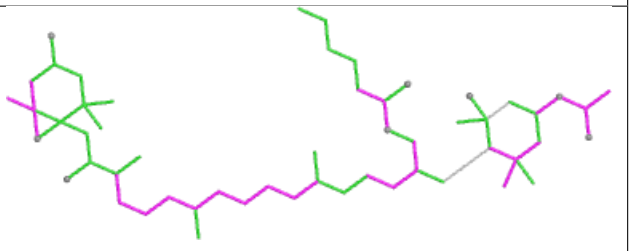


Rings

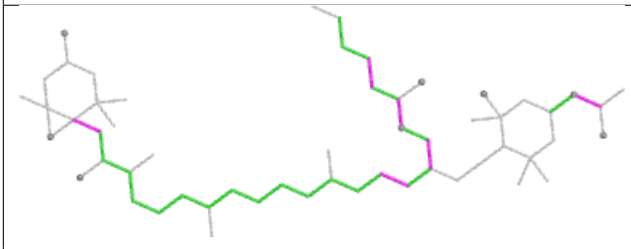
Ligand A1EB1 C 302



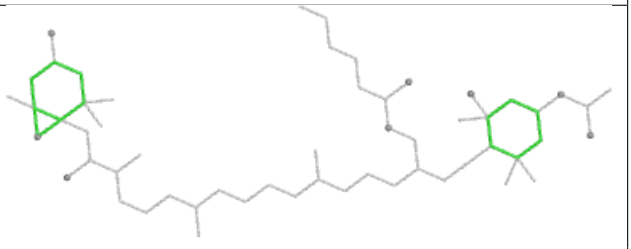
Bond lengths



Bond angles

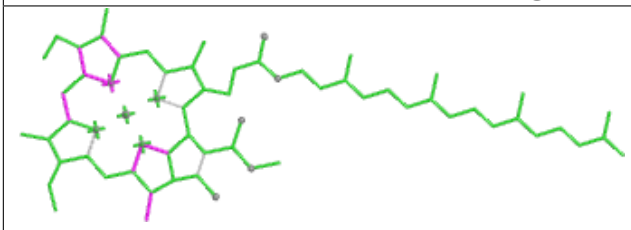


Torsions

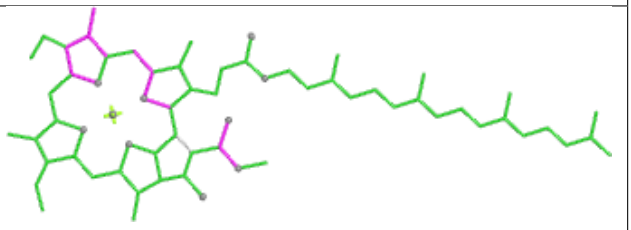


Rings

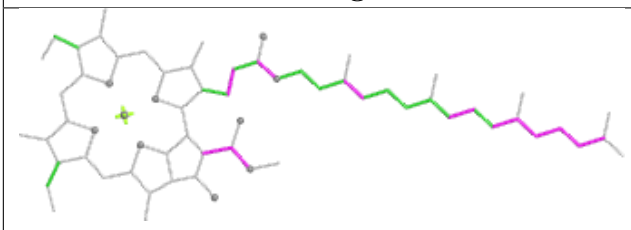
Ligand CLA a 826



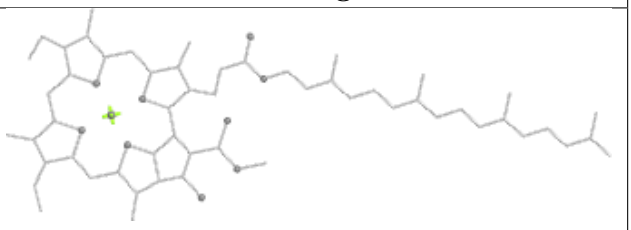
Bond lengths



Bond angles

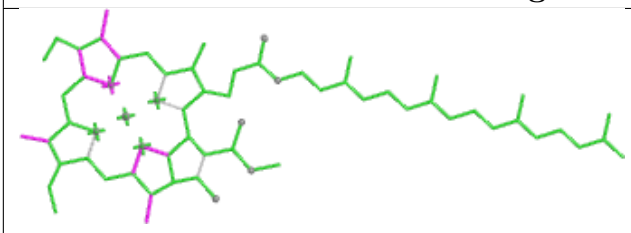


Torsions

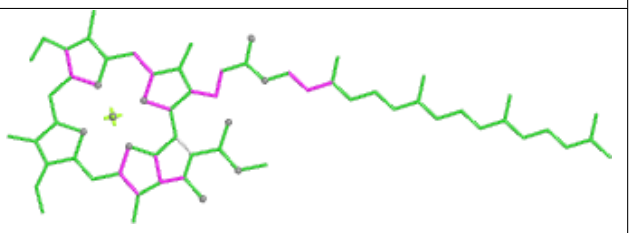


Rings

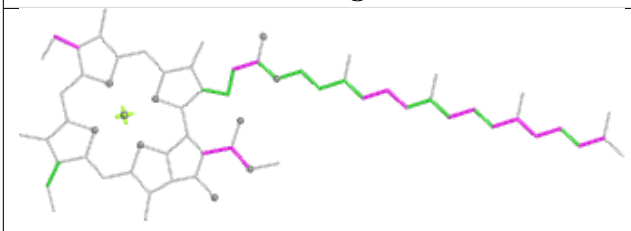
Ligand CLA a 801



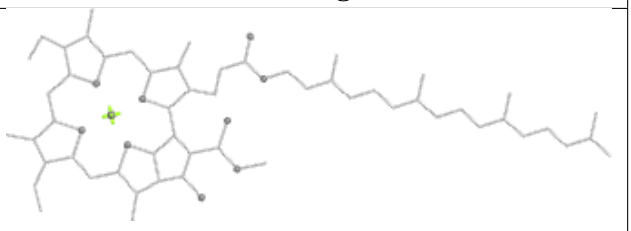
Bond lengths



Bond angles

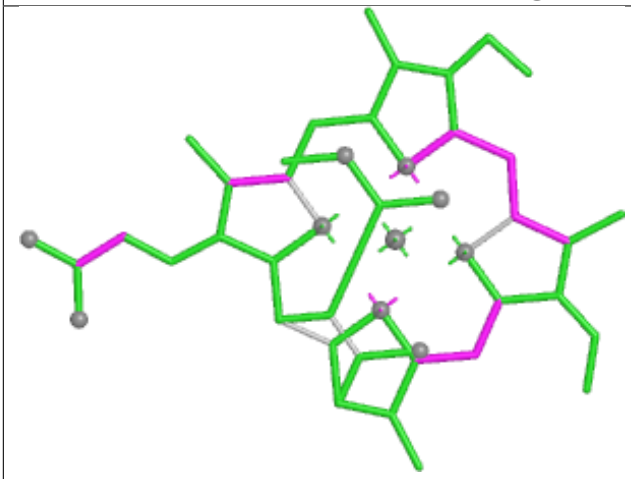


Torsions

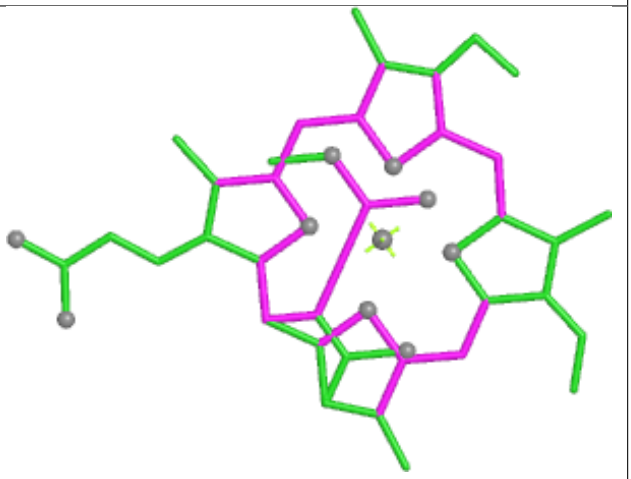


Rings

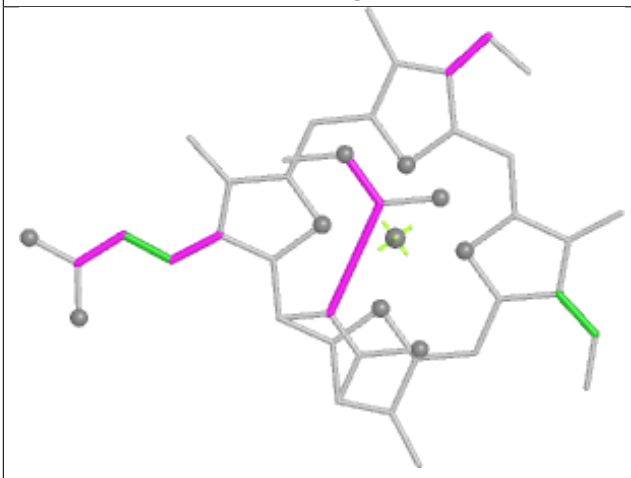
Ligand KC2 L 315



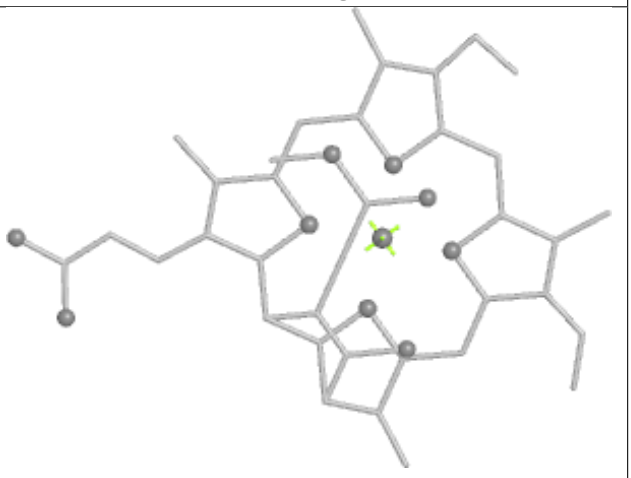
Bond lengths



Bond angles

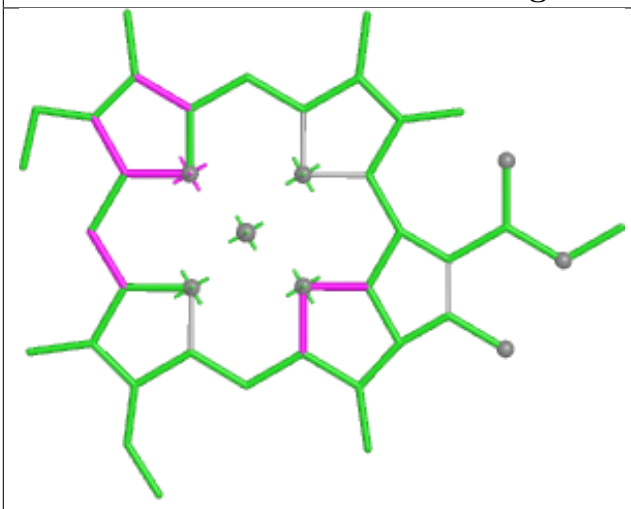


Torsions

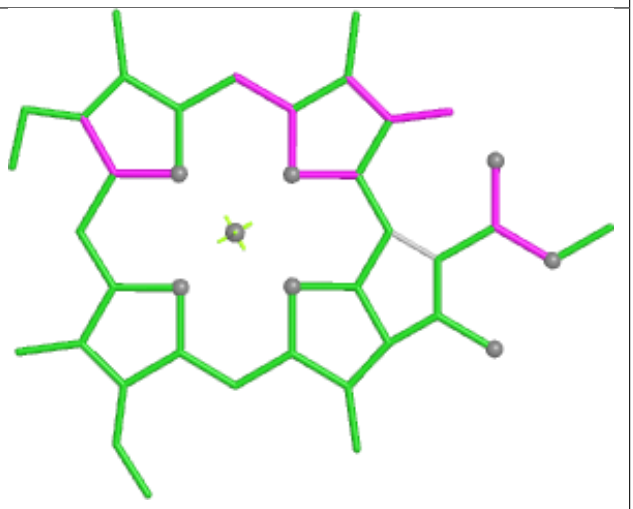


Rings

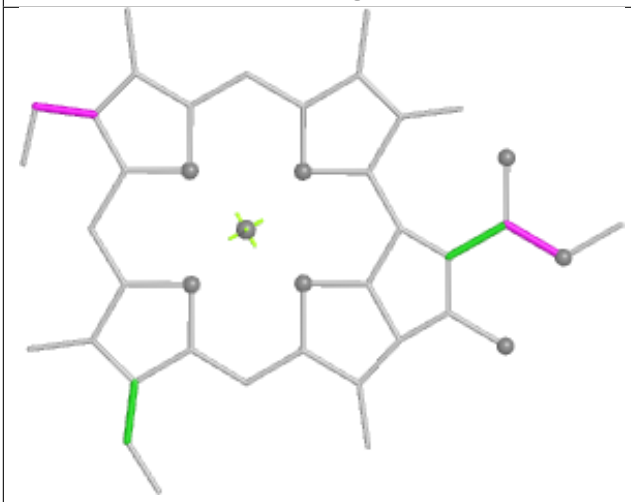
Ligand CLA z 306



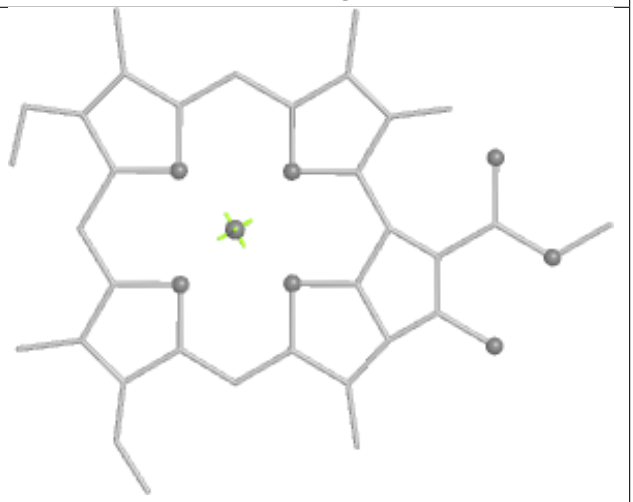
Bond lengths



Bond angles

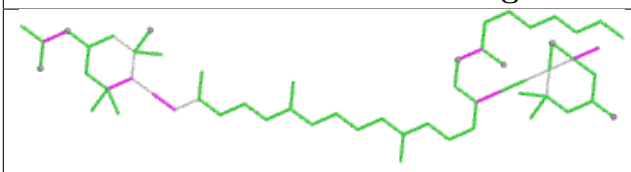


Torsions

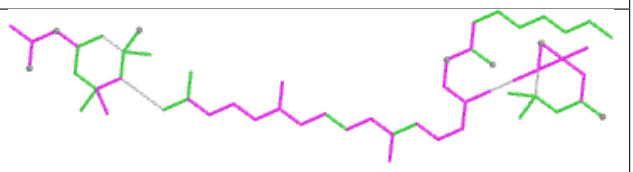


Rings

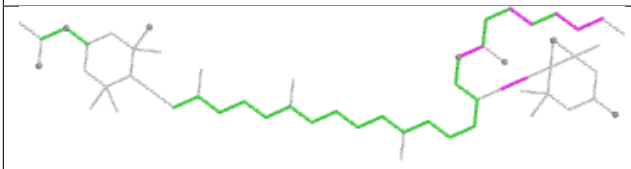
Ligand A1EB4 M 322



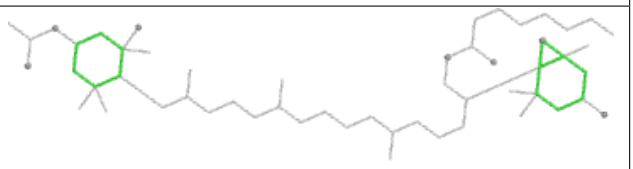
Bond lengths



Bond angles

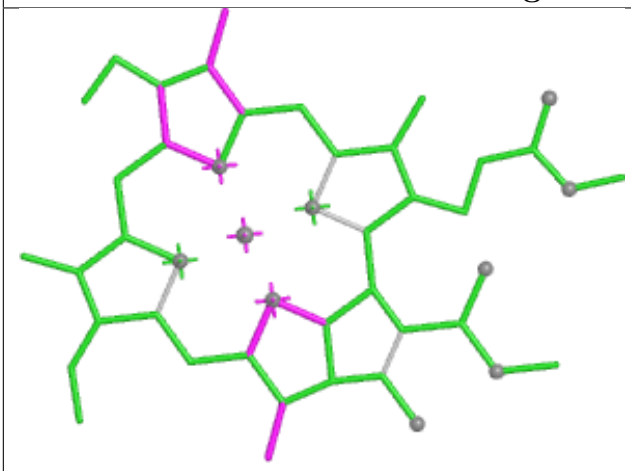


Torsions

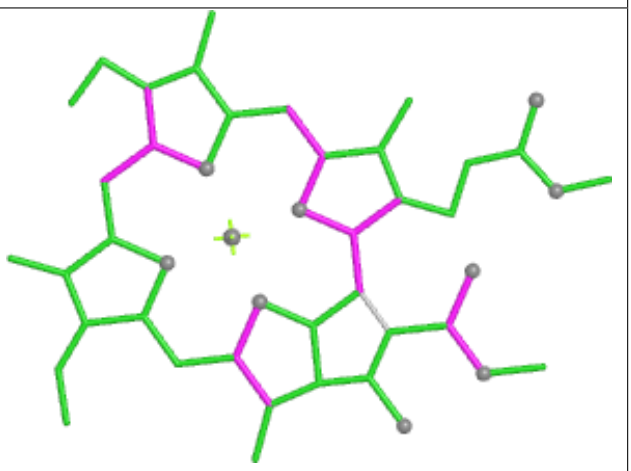


Rings

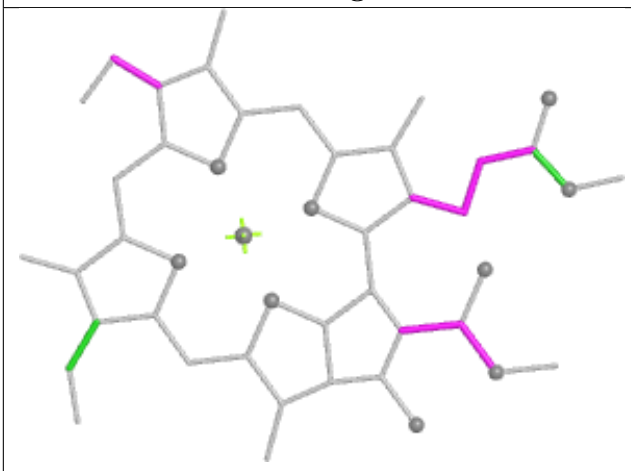
Ligand CLA U 201



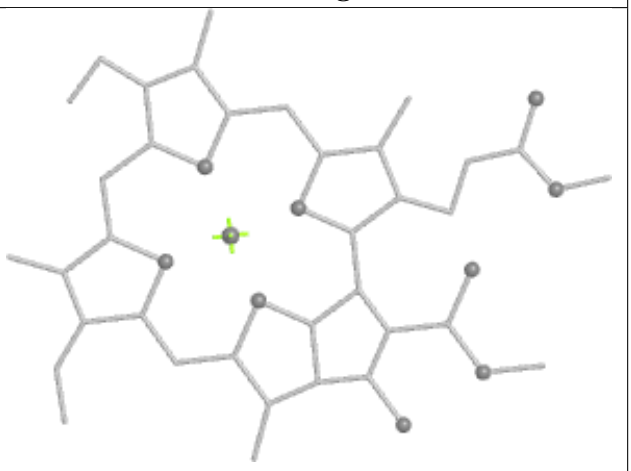
Bond lengths



Bond angles

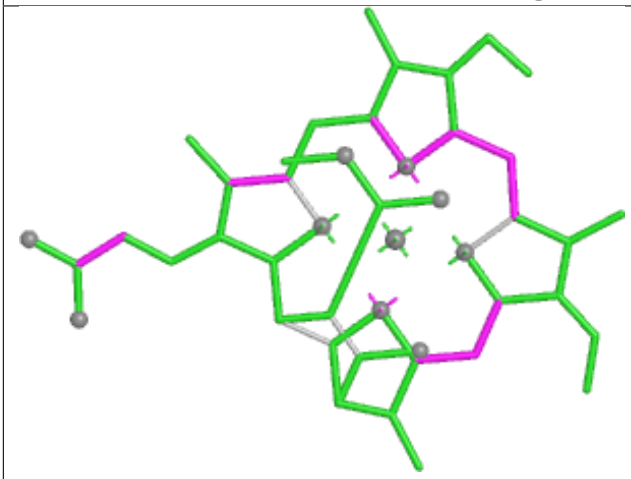


Torsions

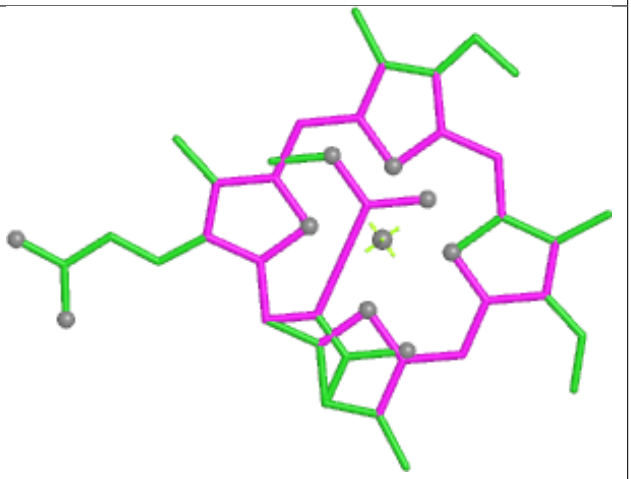


Rings

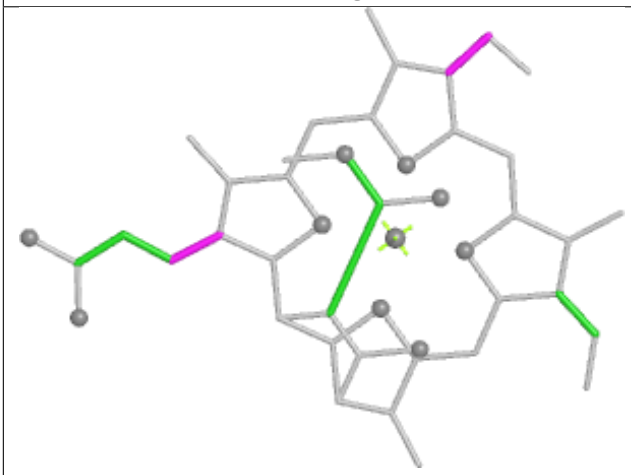
Ligand KC2 0 317



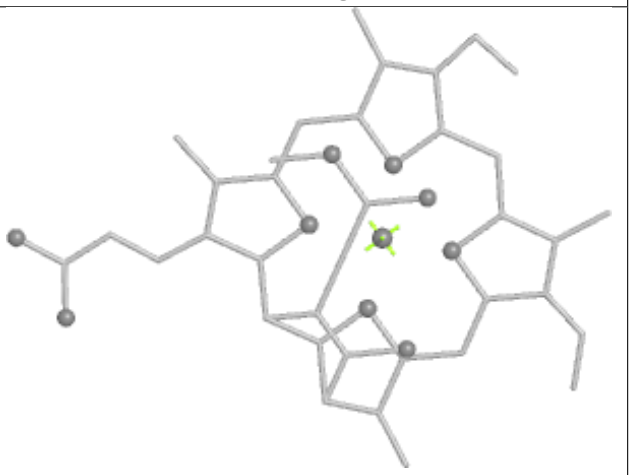
Bond lengths



Bond angles

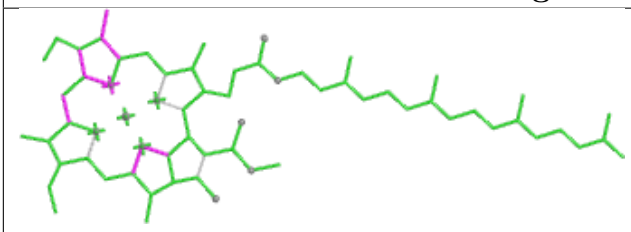


Torsions

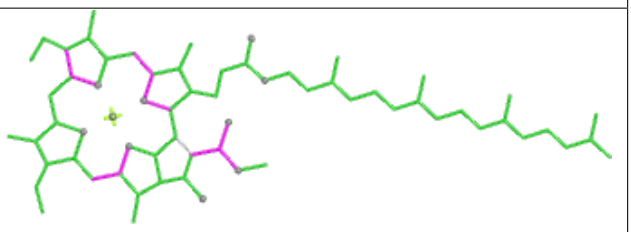


Rings

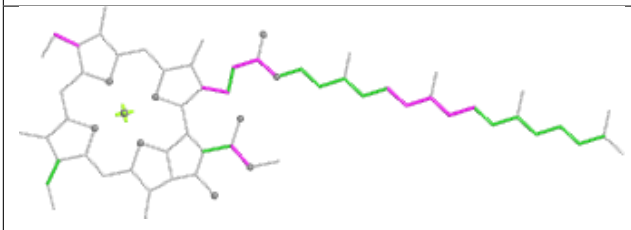
Ligand CLA l 201



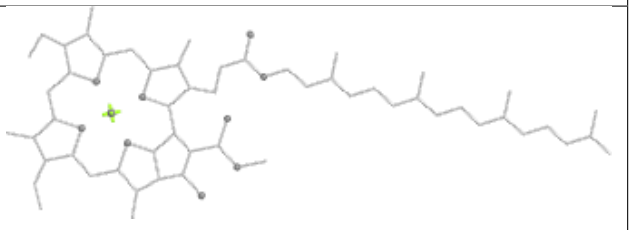
Bond lengths



Bond angles

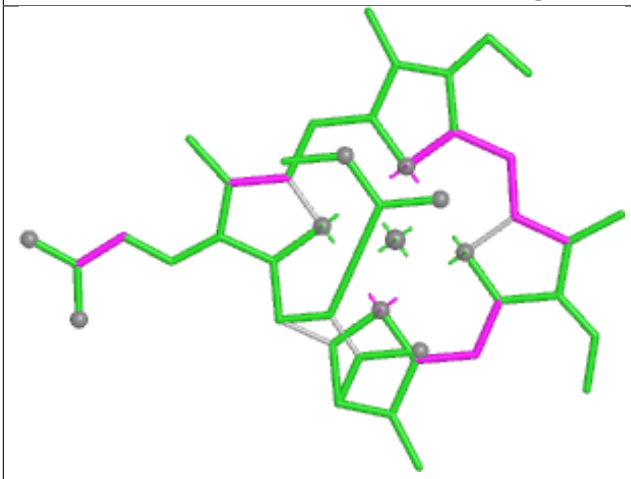


Torsions

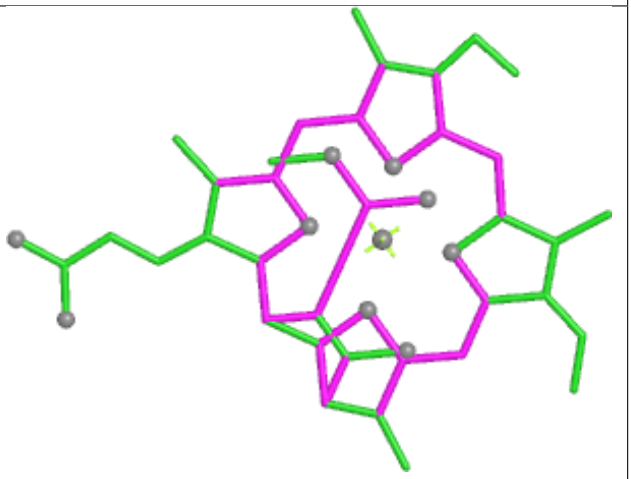


Rings

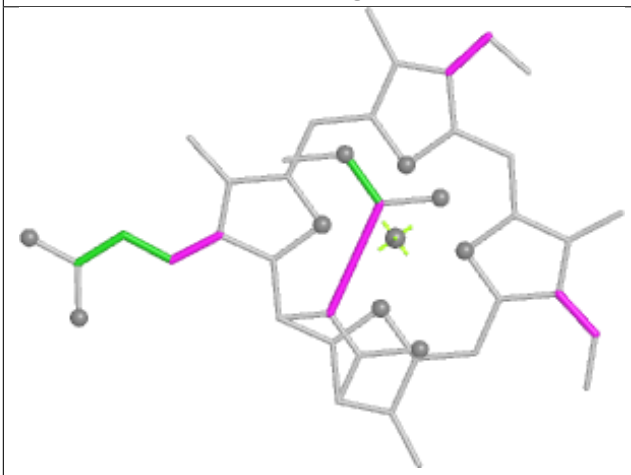
Ligand KC2 x 312



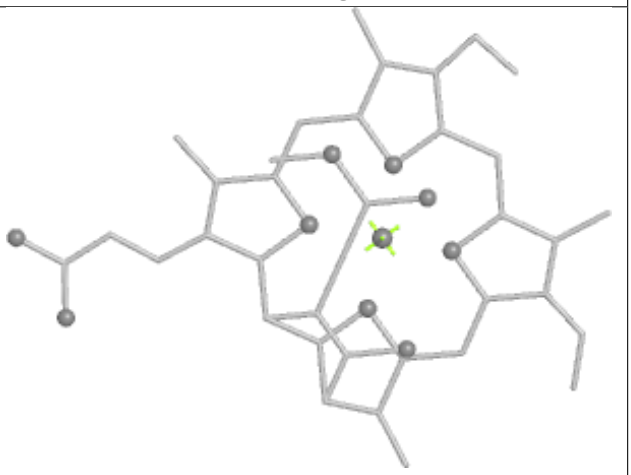
Bond lengths



Bond angles

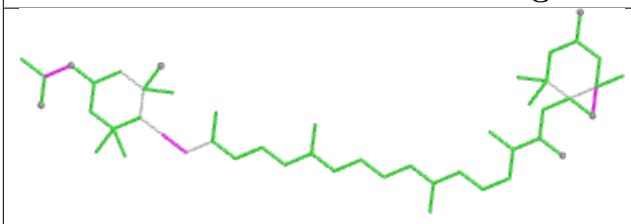


Torsions

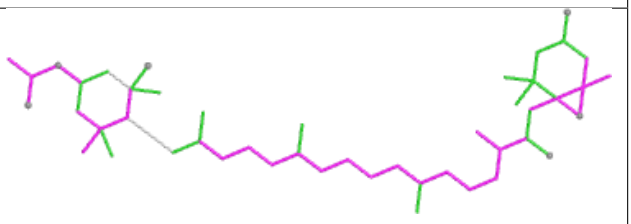


Rings

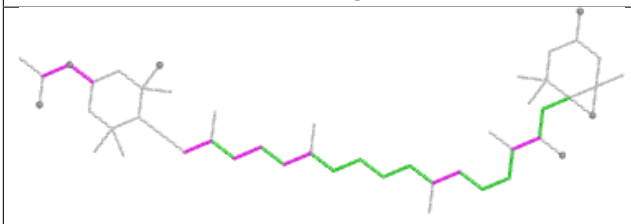
Ligand A86 Z 301



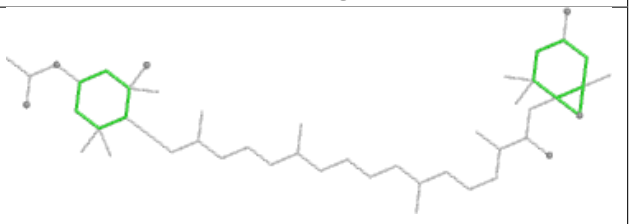
Bond lengths



Bond angles

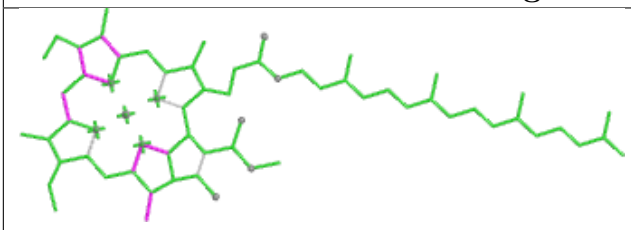


Torsions

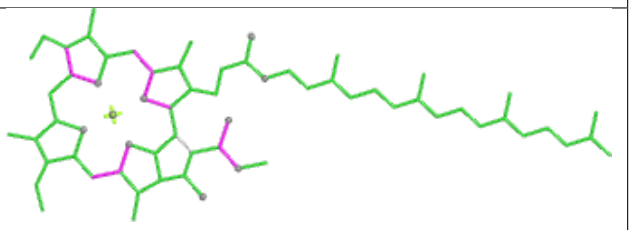


Rings

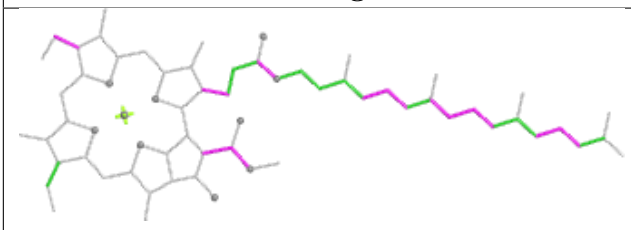
Ligand CLA D 316



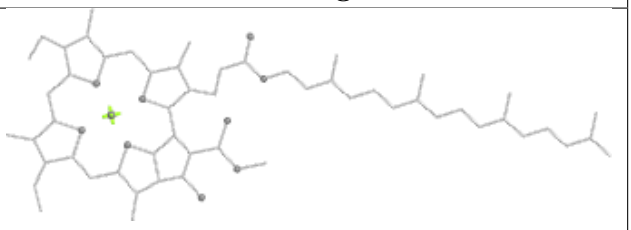
Bond lengths



Bond angles

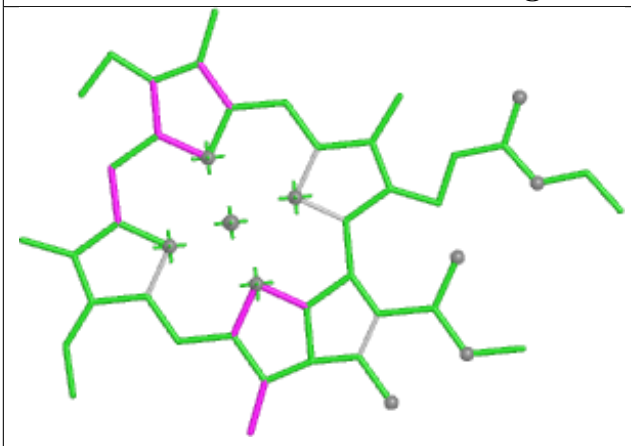


Torsions

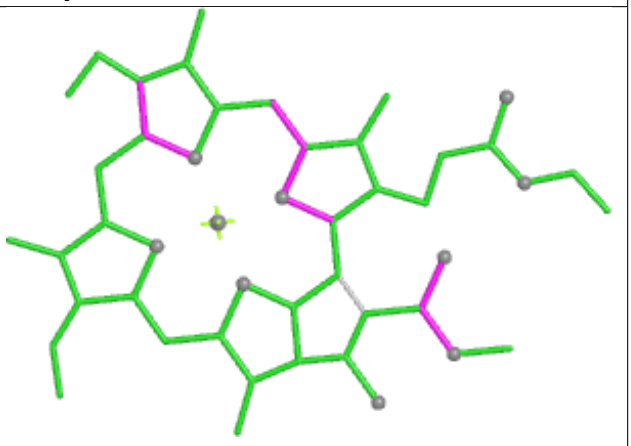


Rings

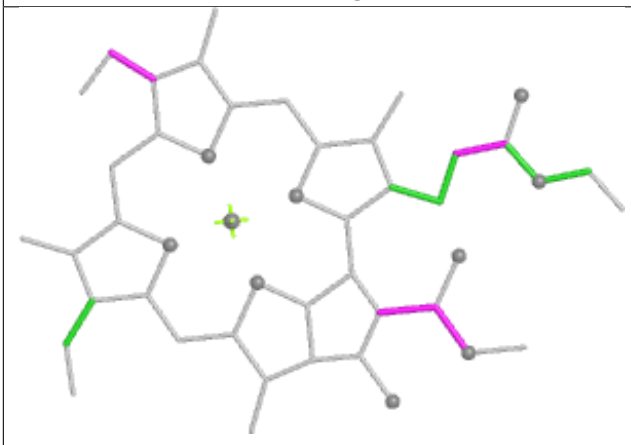
Ligand CLA Q 320



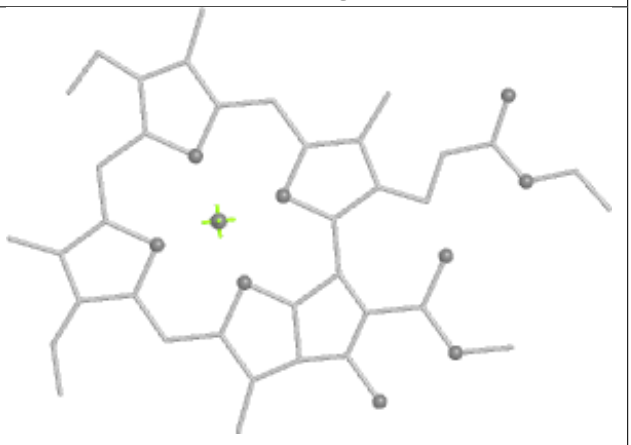
Bond lengths



Bond angles

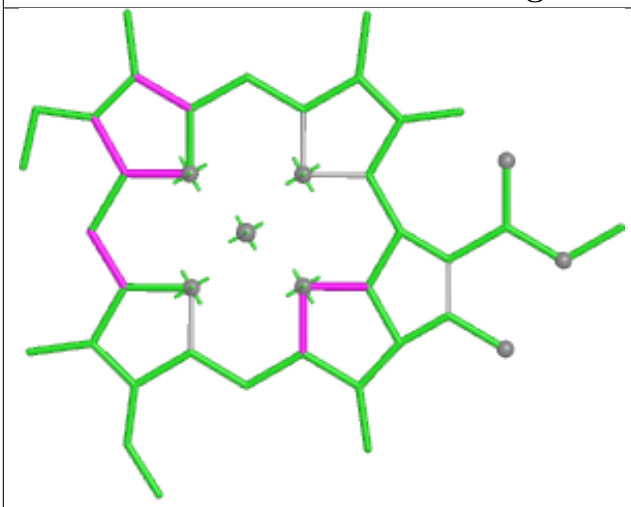


Torsions

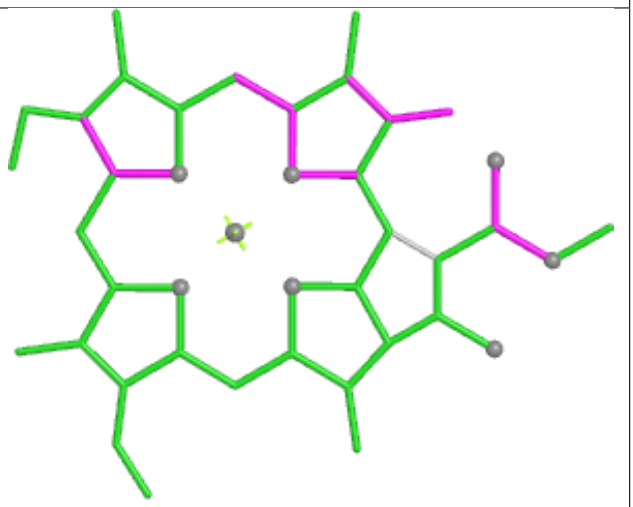


Rings

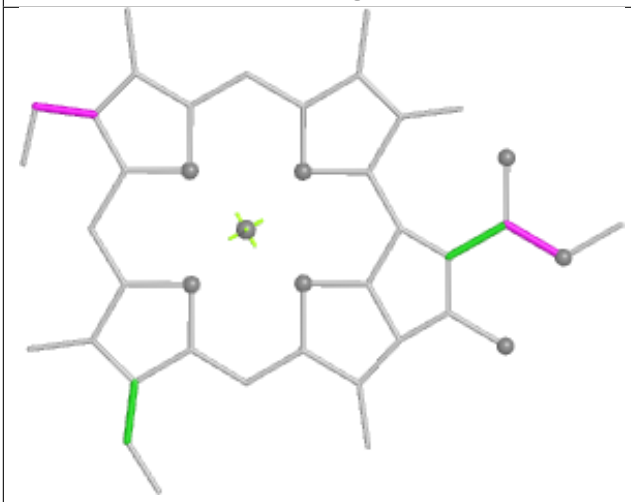
Ligand CLA Z 312



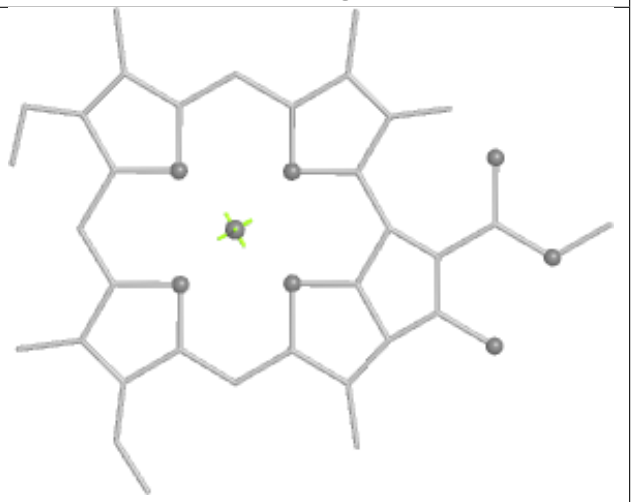
Bond lengths



Bond angles

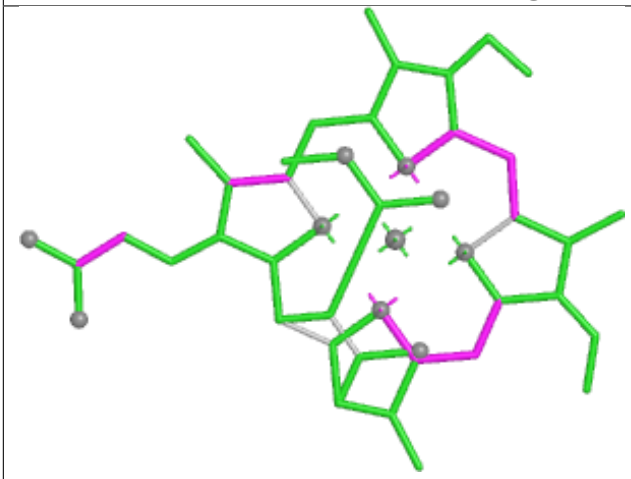


Torsions

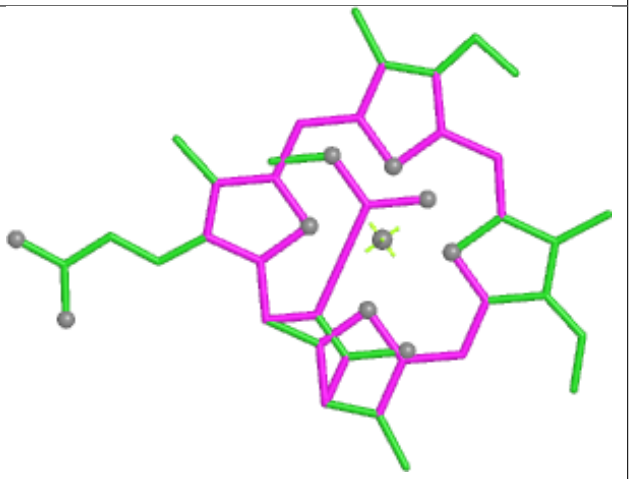


Rings

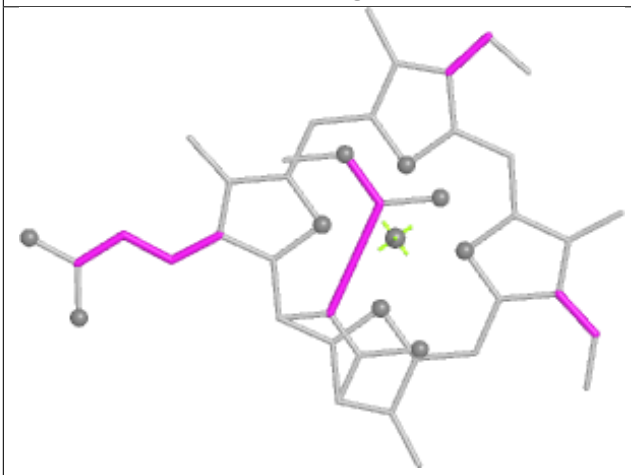
Ligand KC2 G 315



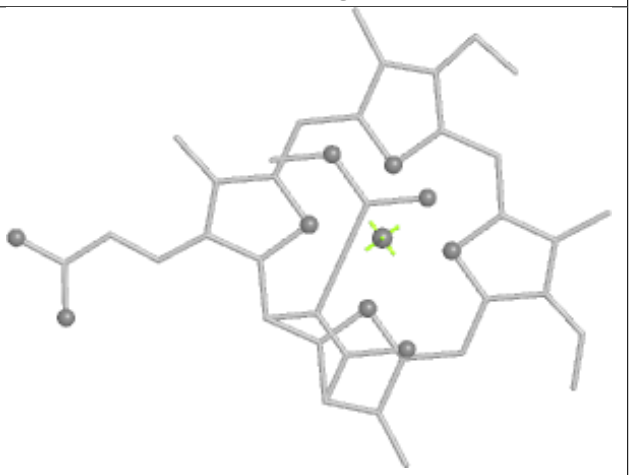
Bond lengths



Bond angles

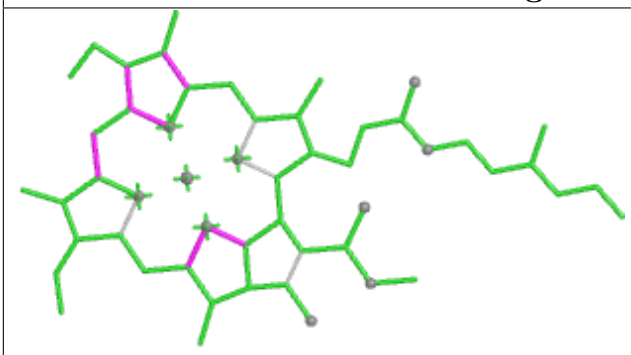


Torsions

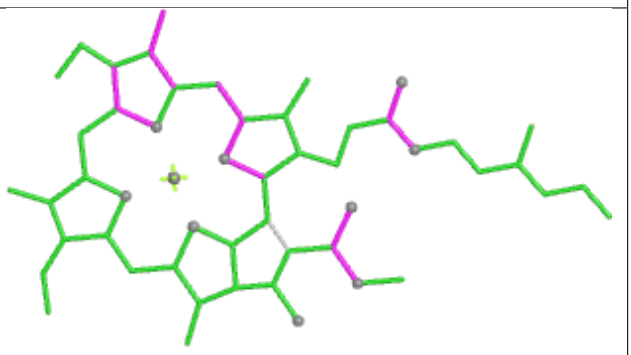


Rings

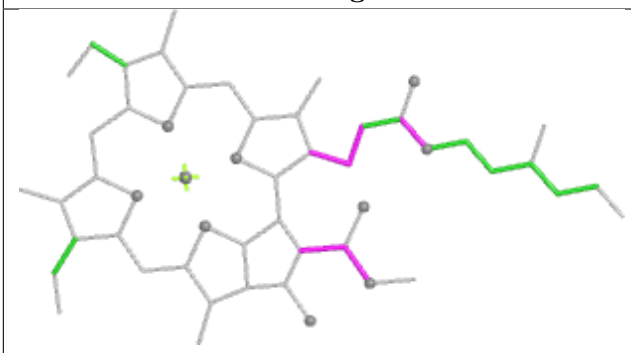
Ligand CLA E 317



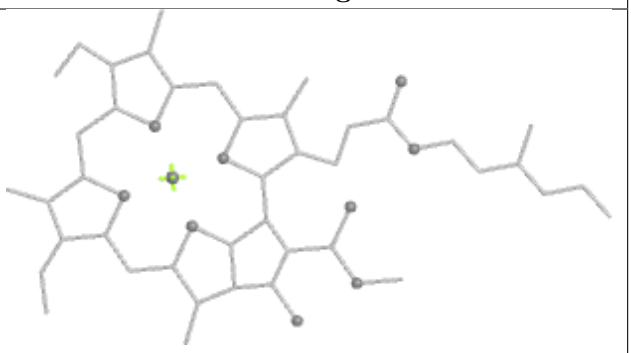
Bond lengths



Bond angles

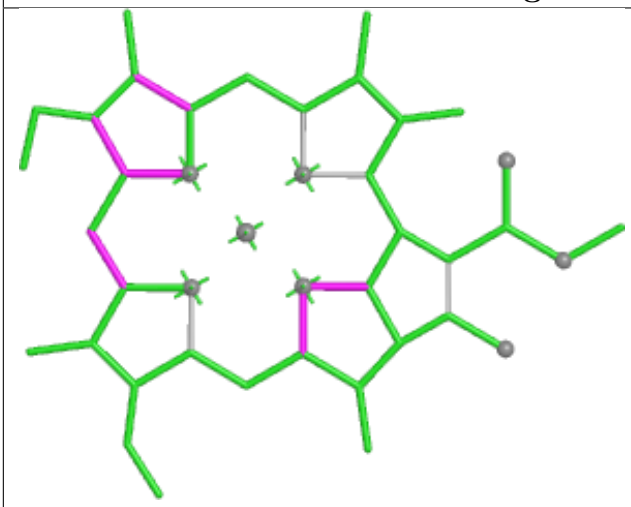


Torsions

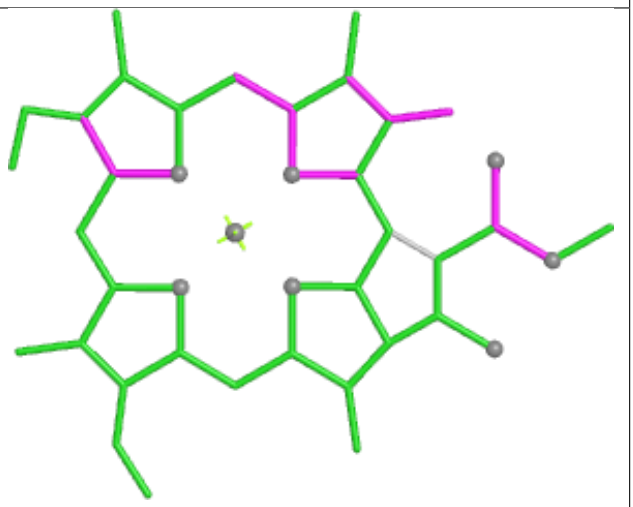


Rings

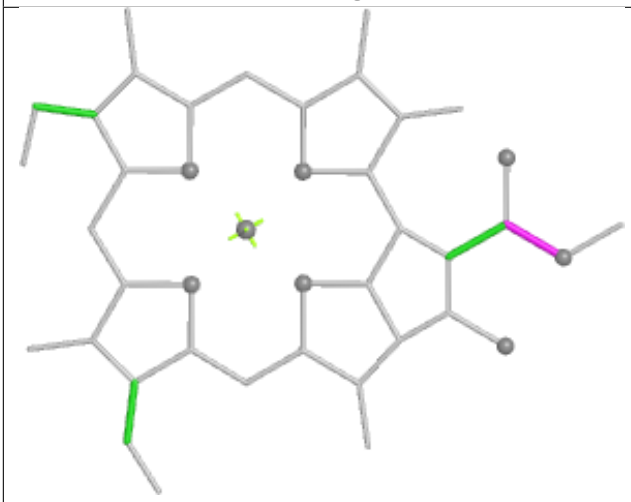
Ligand CLA Y 305



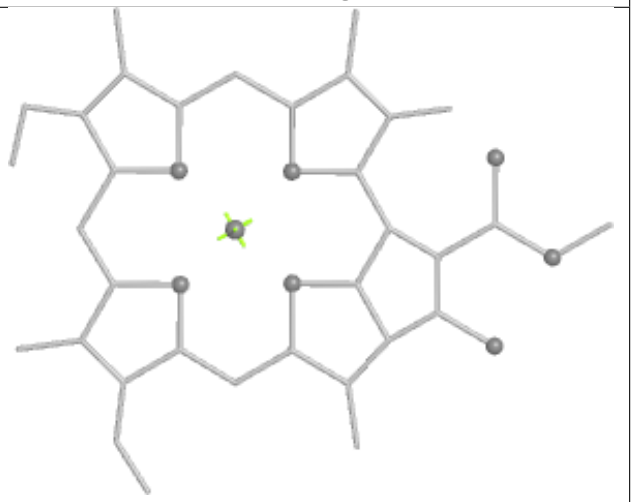
Bond lengths



Bond angles

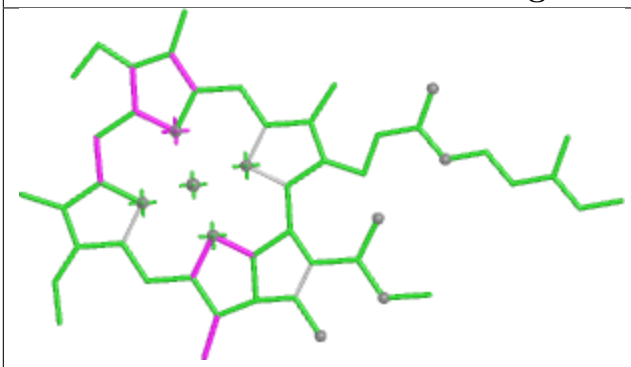


Torsions

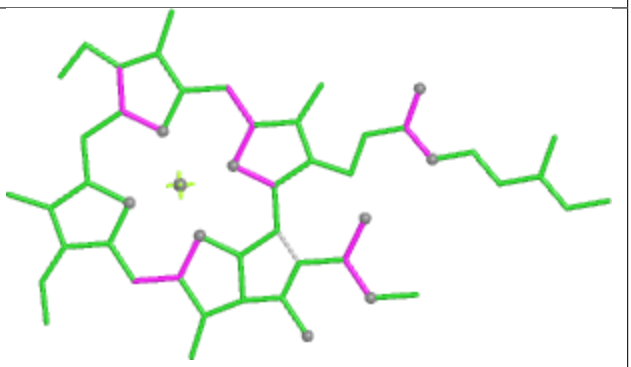


Rings

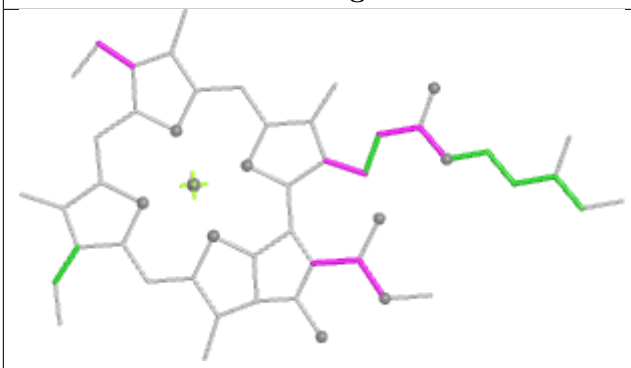
Ligand CLA 3 322



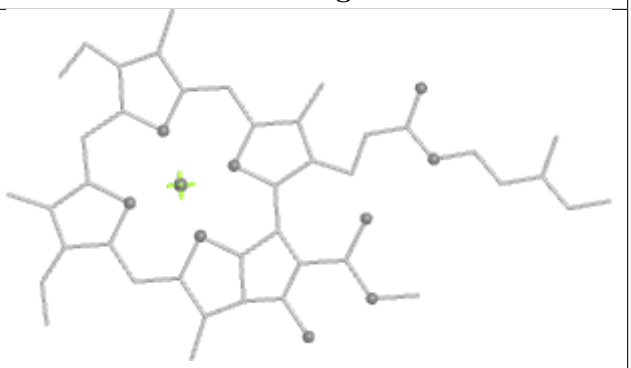
Bond lengths



Bond angles

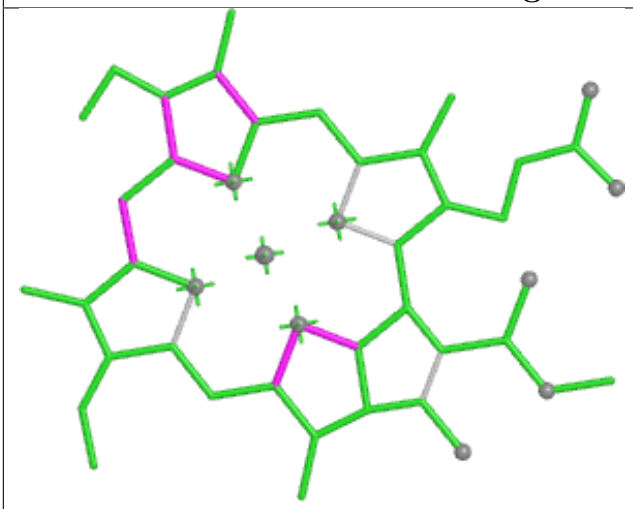


Torsions

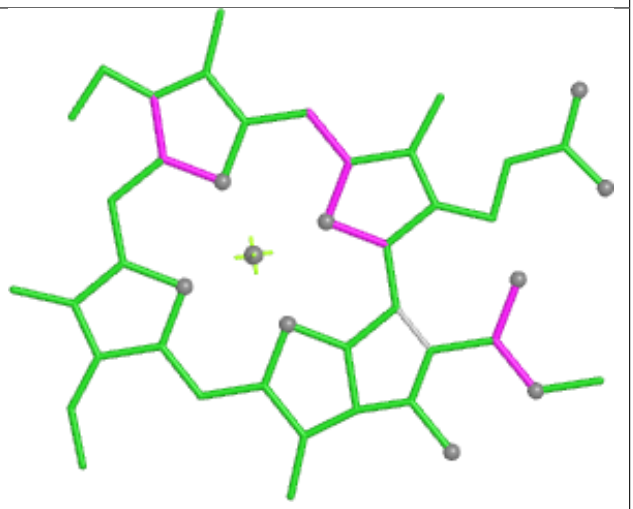


Rings

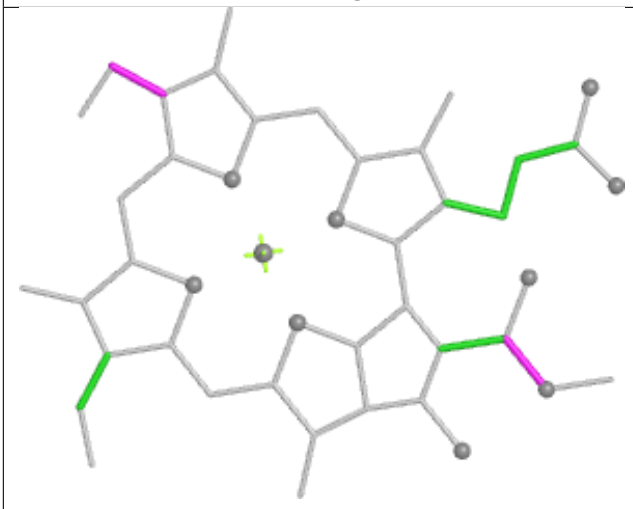
Ligand CLA H 307



Bond lengths



Bond angles

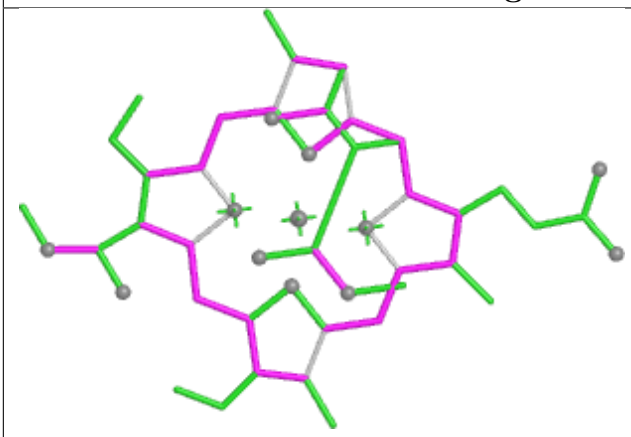


Torsions

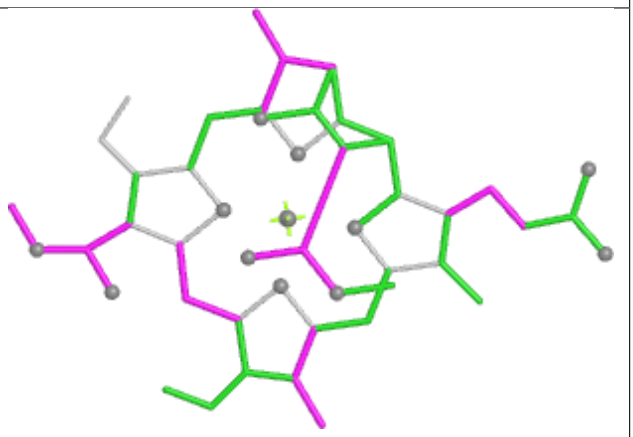


Rings

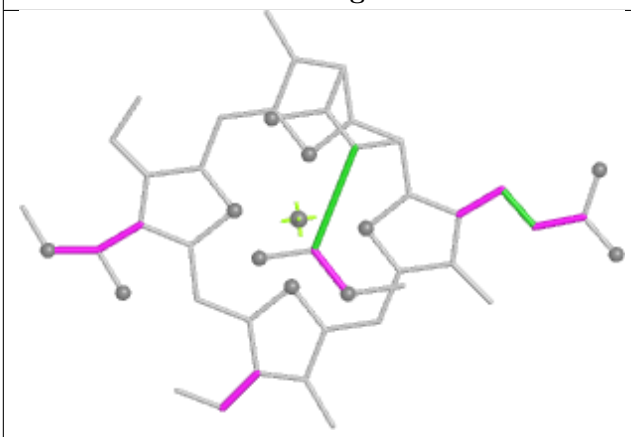
Ligand A1ECV 6 320



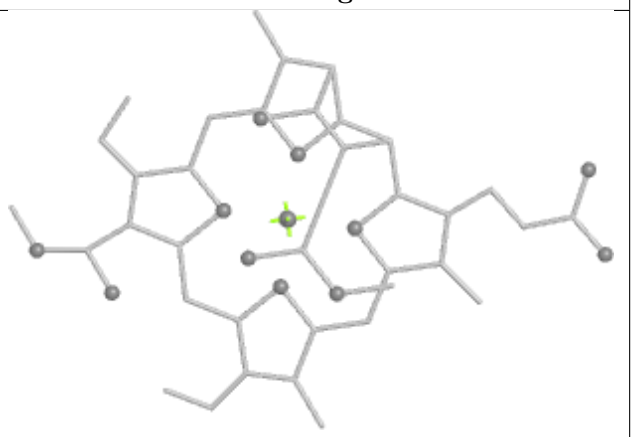
Bond lengths



Bond angles

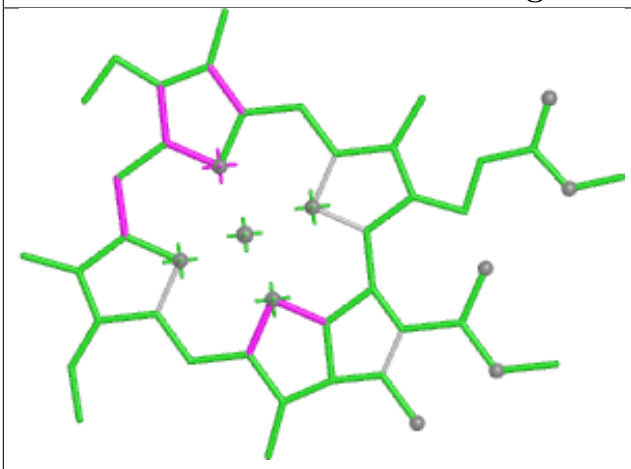


Torsions

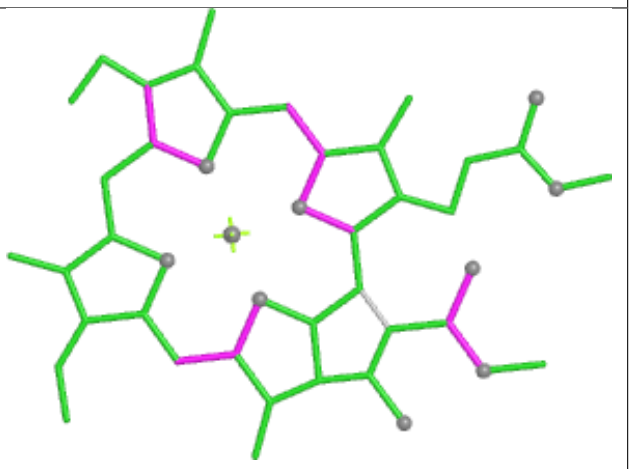


Rings

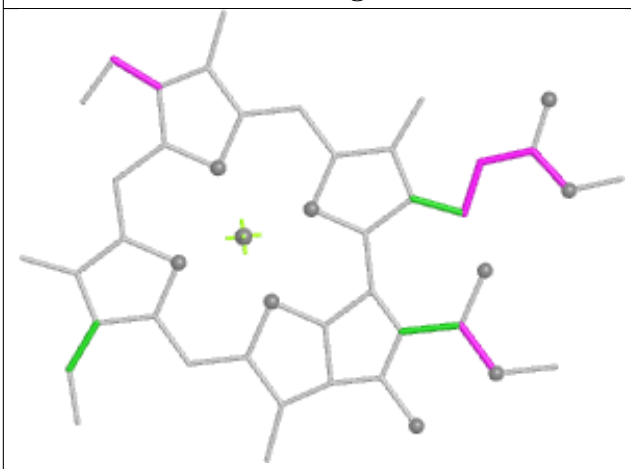
Ligand CLA Z 306



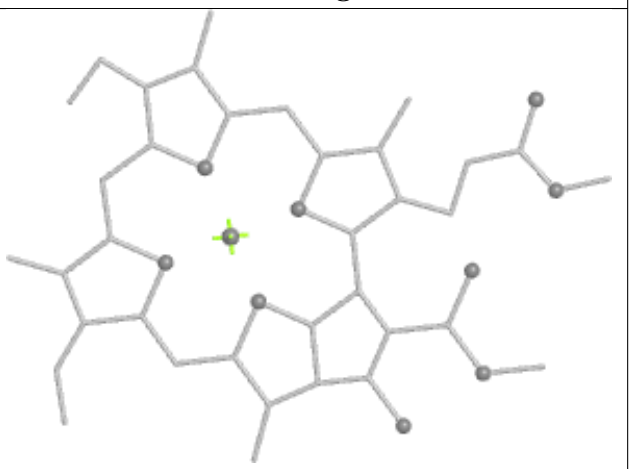
Bond lengths



Bond angles

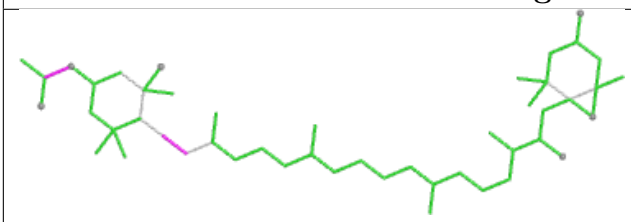


Torsions

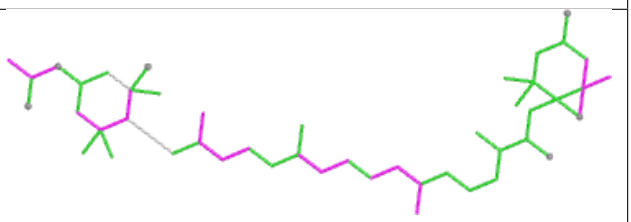


Rings

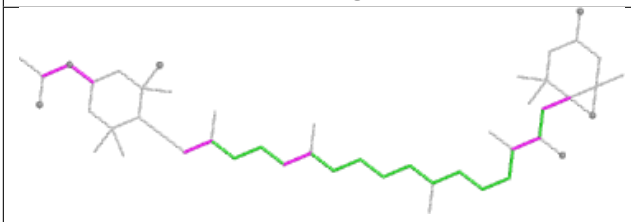
Ligand A86 3 305



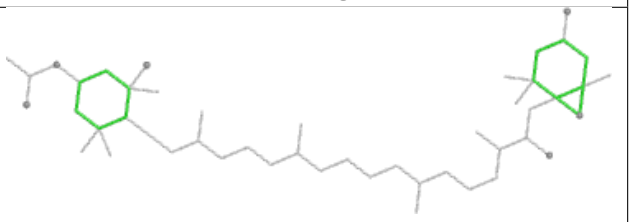
Bond lengths



Bond angles

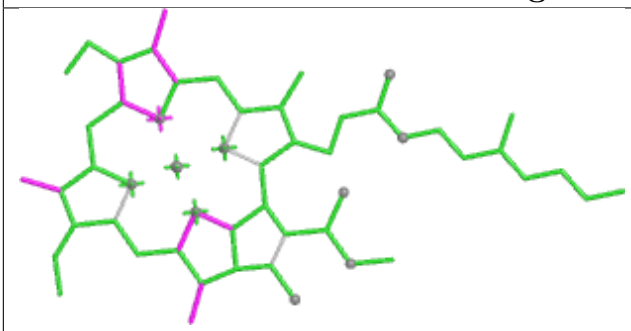


Torsions

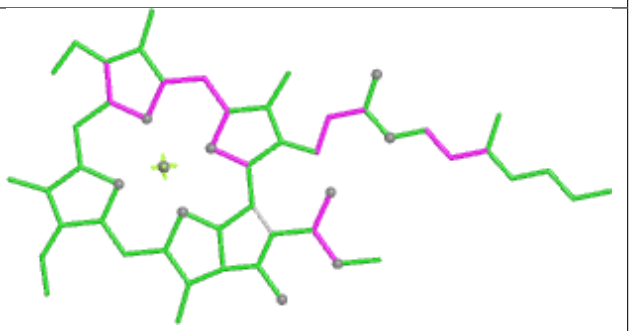


Rings

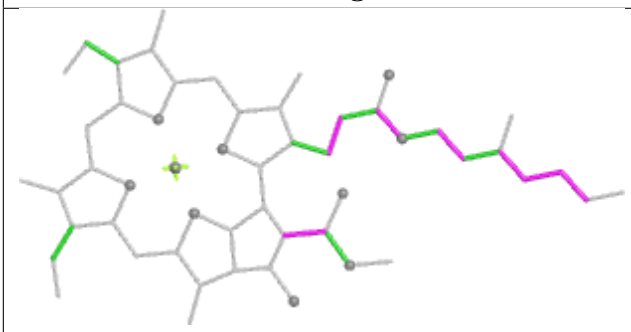
Ligand CLA 0 312



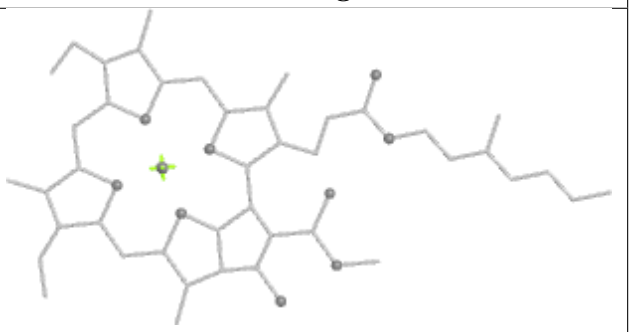
Bond lengths



Bond angles

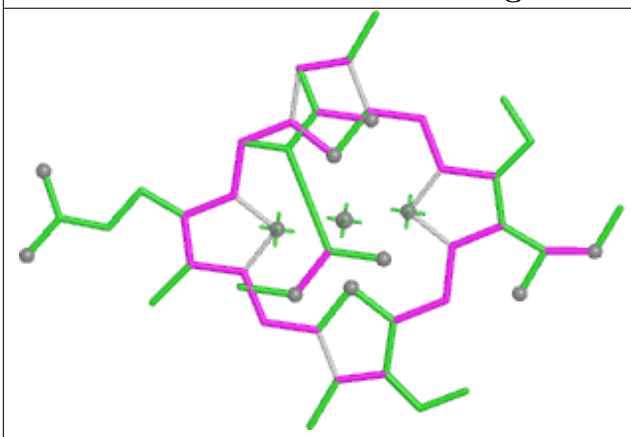


Torsions

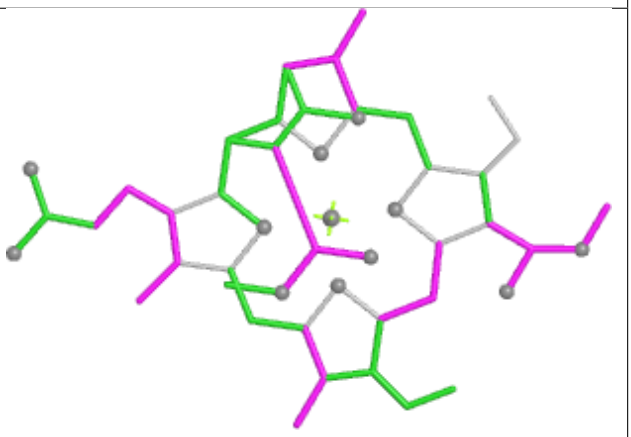


Rings

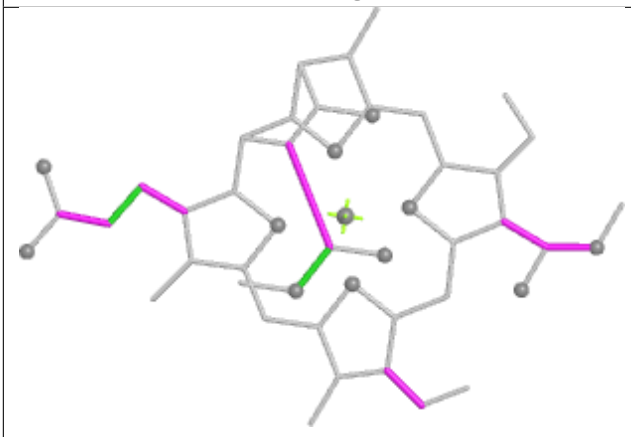
Ligand A1ECV 5 309



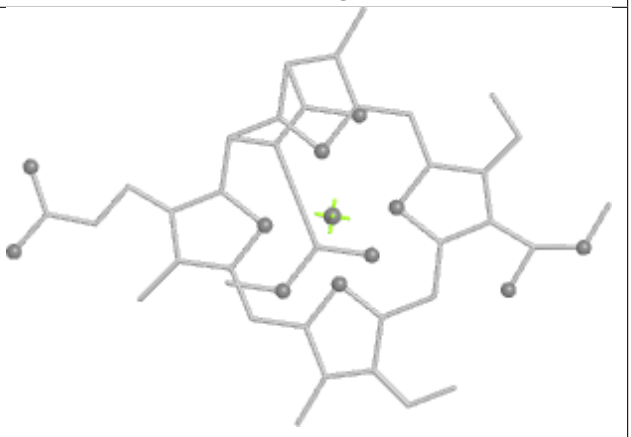
Bond lengths



Bond angles

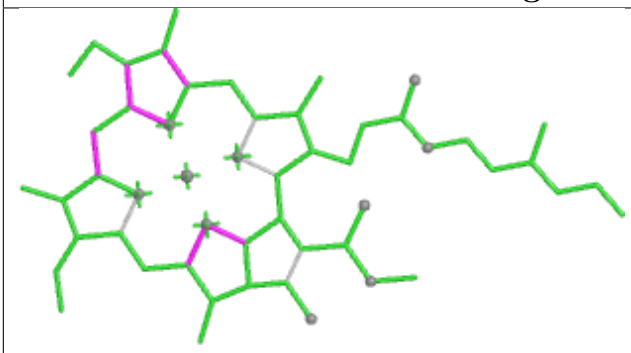


Torsions

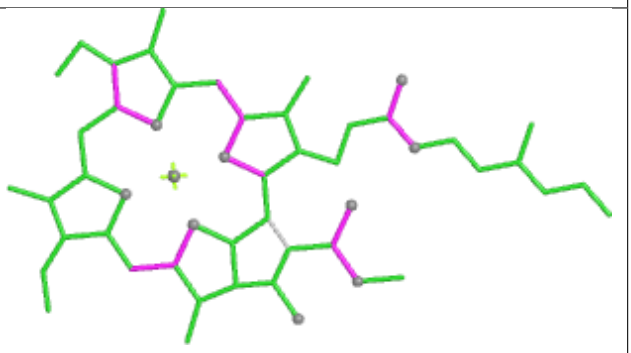


Rings

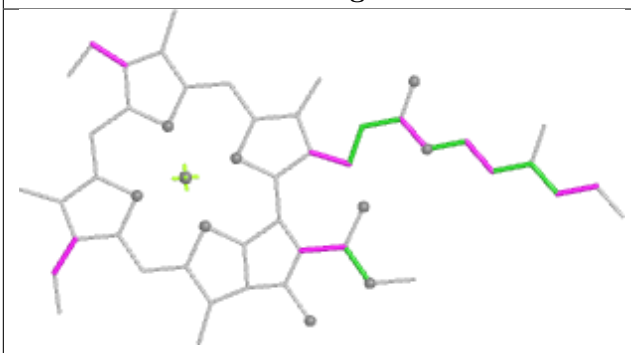
Ligand CLA G 312



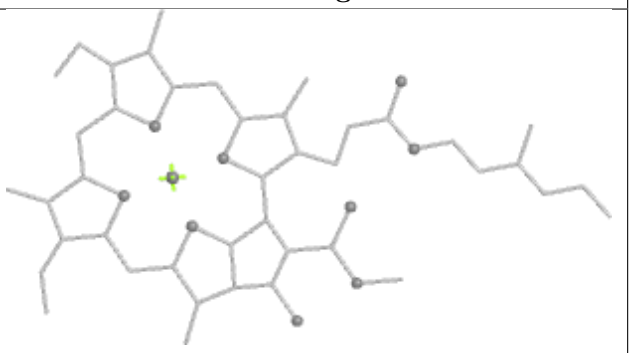
Bond lengths



Bond angles

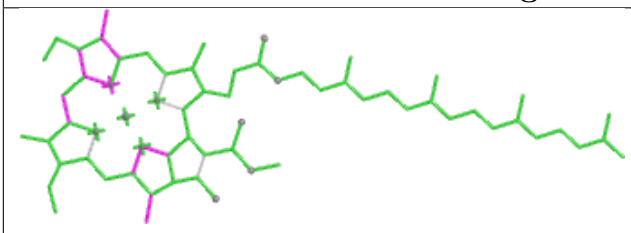


Torsions

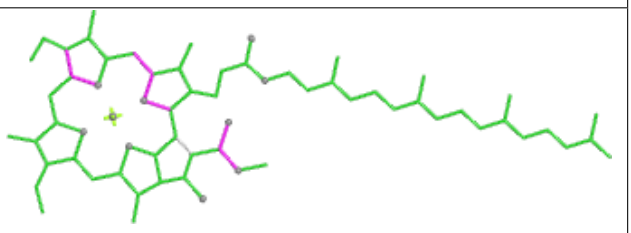


Rings

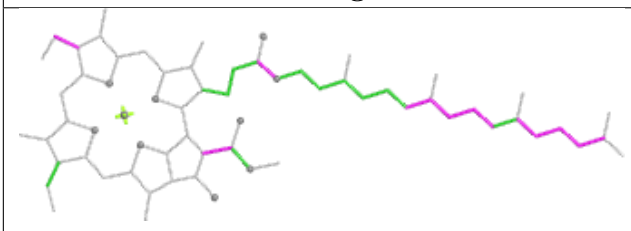
Ligand CLA M 312



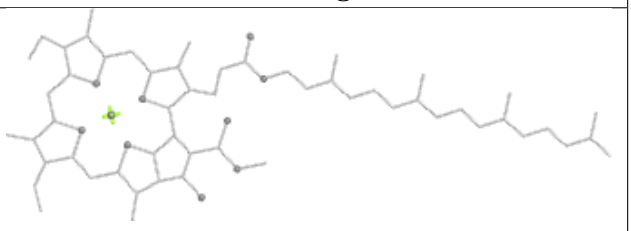
Bond lengths



Bond angles

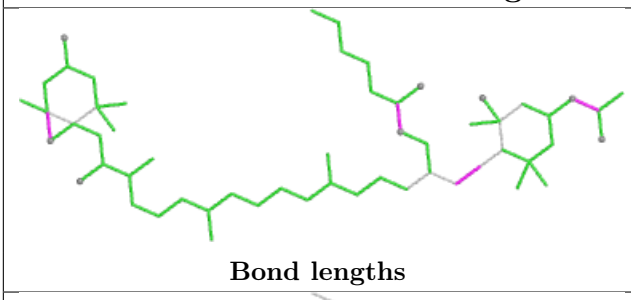


Torsions

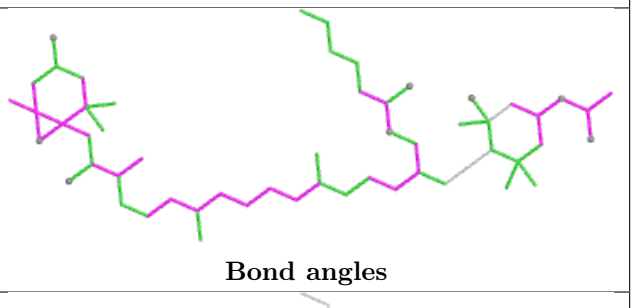


Rings

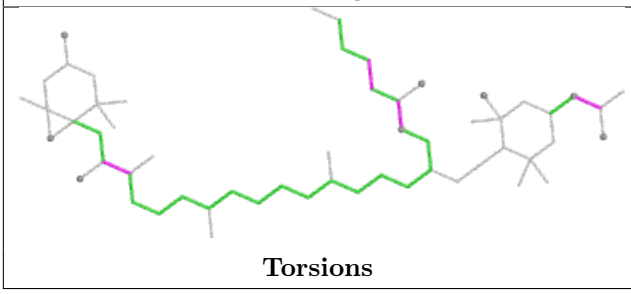
Ligand A1EB1 K 304



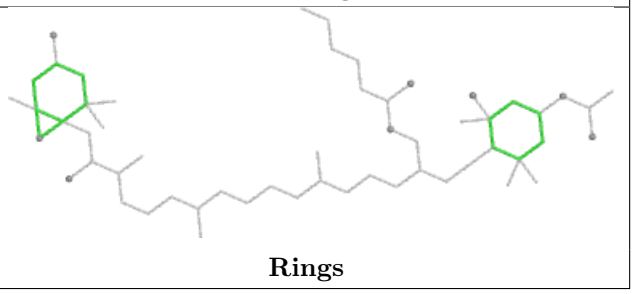
Bond lengths



Bond angles

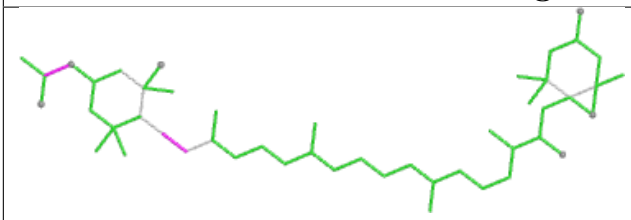


Torsions

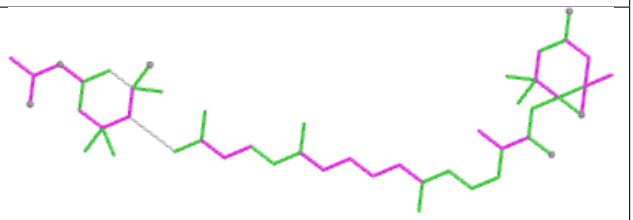


Rings

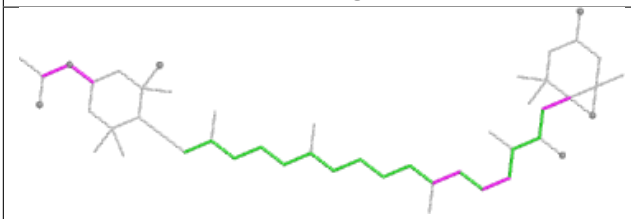
Ligand A86 9 306



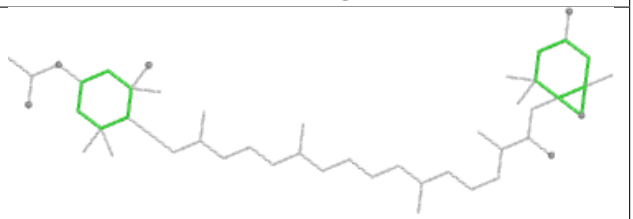
Bond lengths



Bond angles

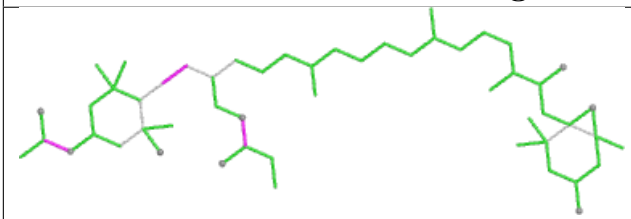


Torsions

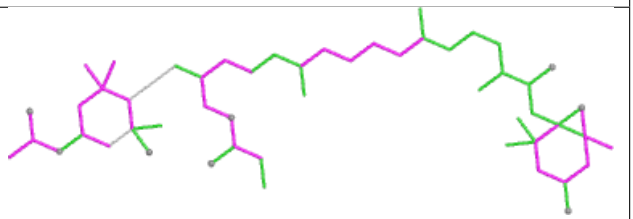


Rings

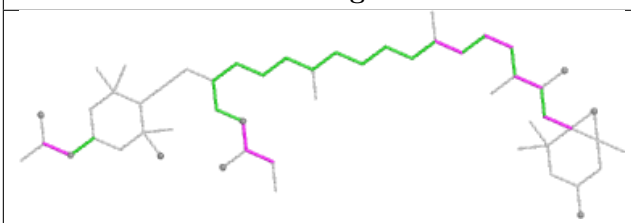
Ligand A1EB1 6 304



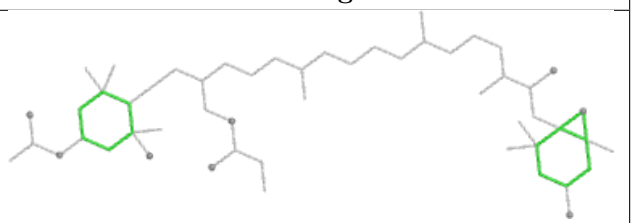
Bond lengths



Bond angles

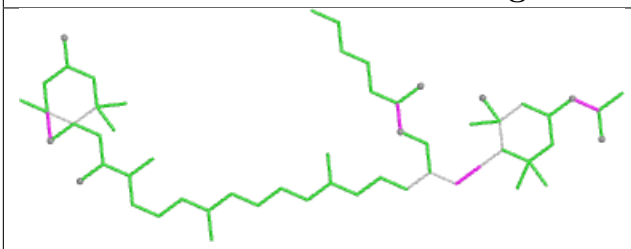


Torsions

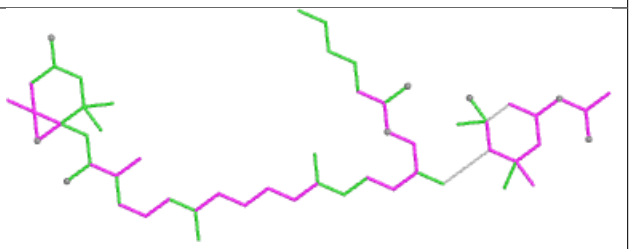


Rings

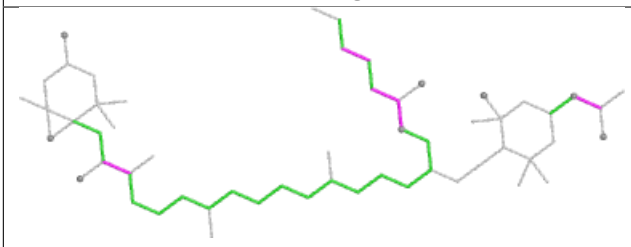
Ligand A1EB1 h 203



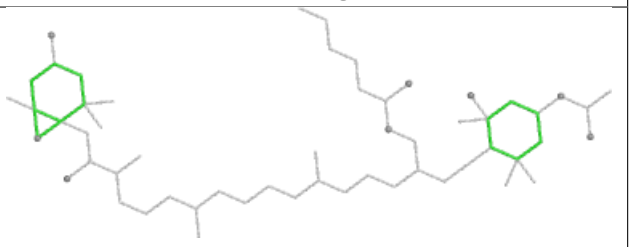
Bond lengths



Bond angles

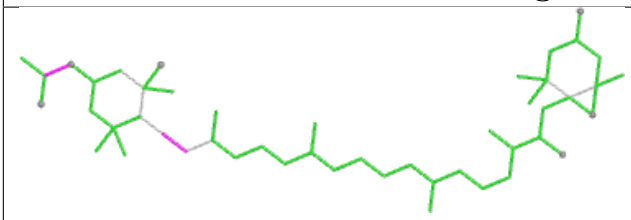


Torsions

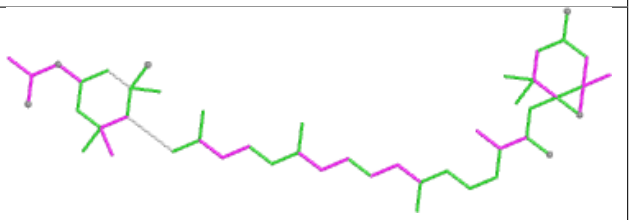


Rings

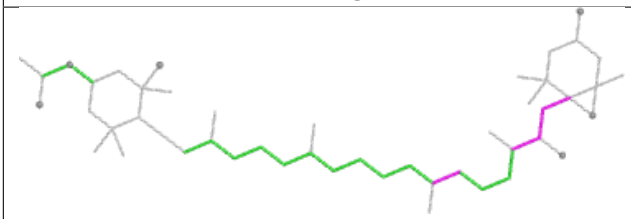
Ligand A86 4 305



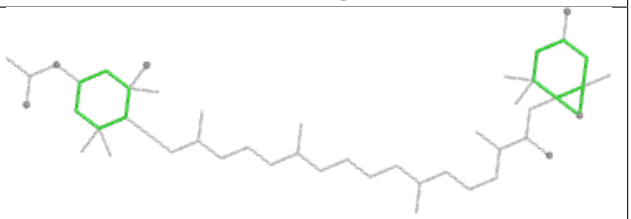
Bond lengths



Bond angles

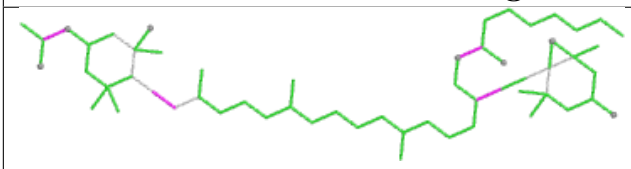


Torsions

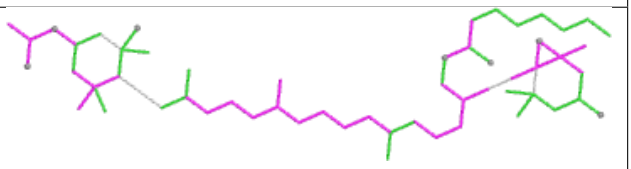


Rings

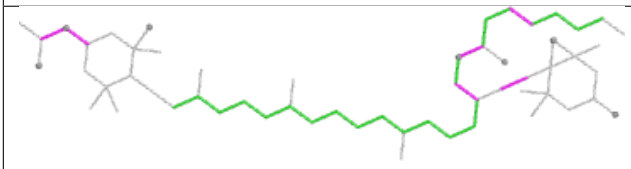
Ligand A1EB4 R 305



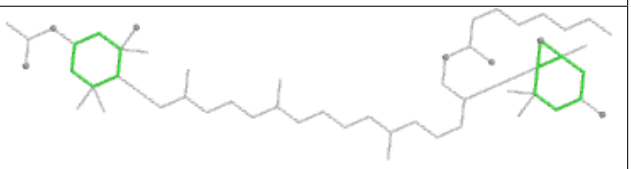
Bond lengths



Bond angles

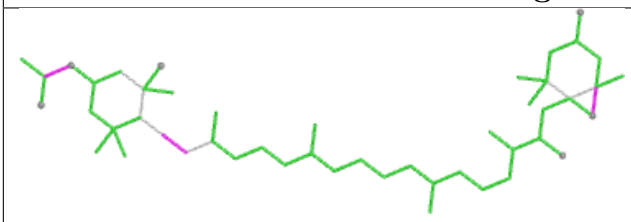


Torsions

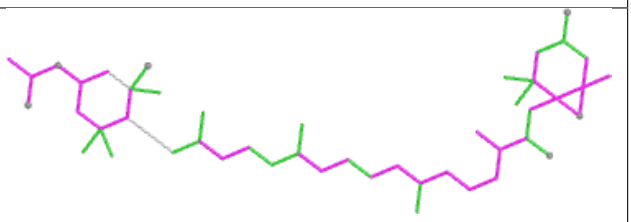


Rings

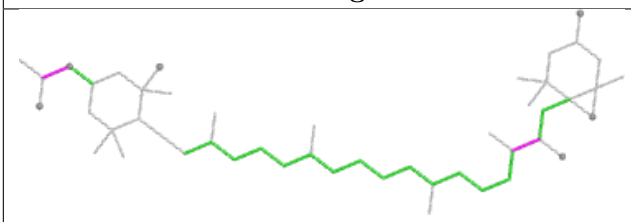
Ligand A86 J 303



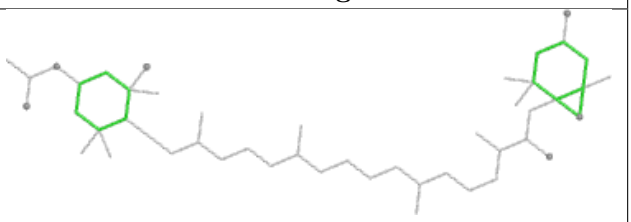
Bond lengths



Bond angles

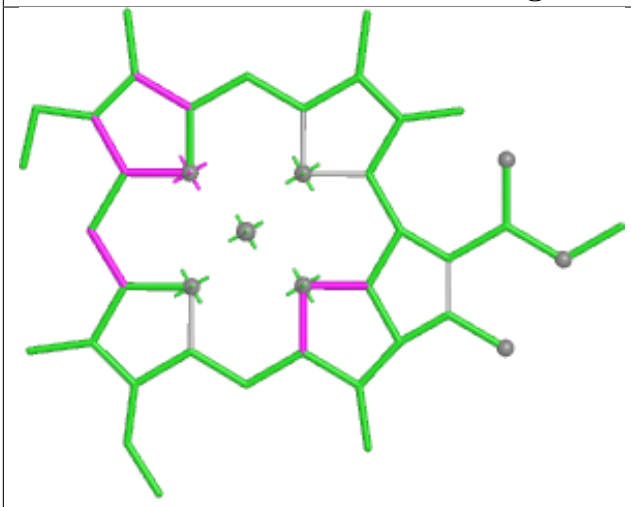


Torsions

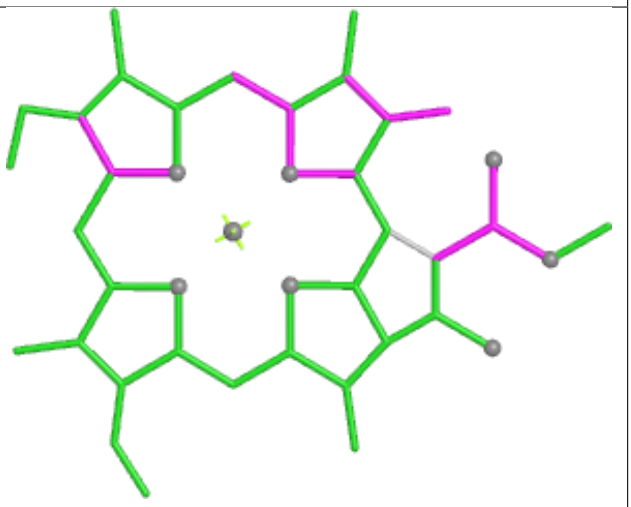


Rings

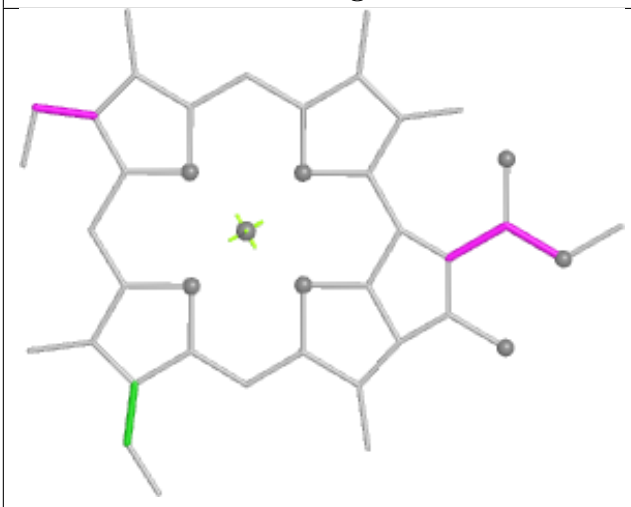
Ligand CLA L 316



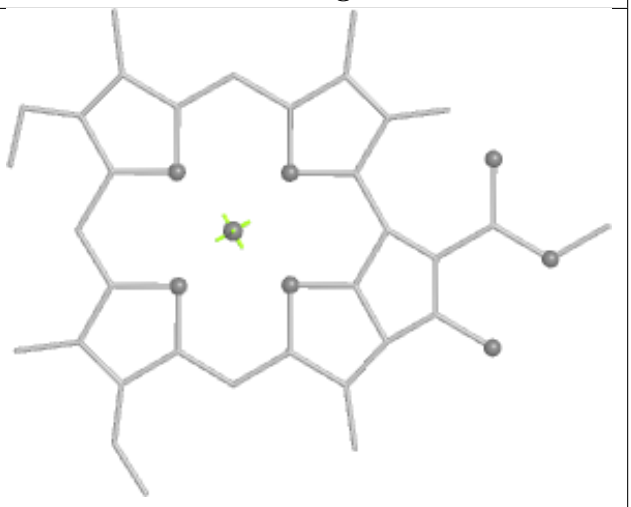
Bond lengths



Bond angles

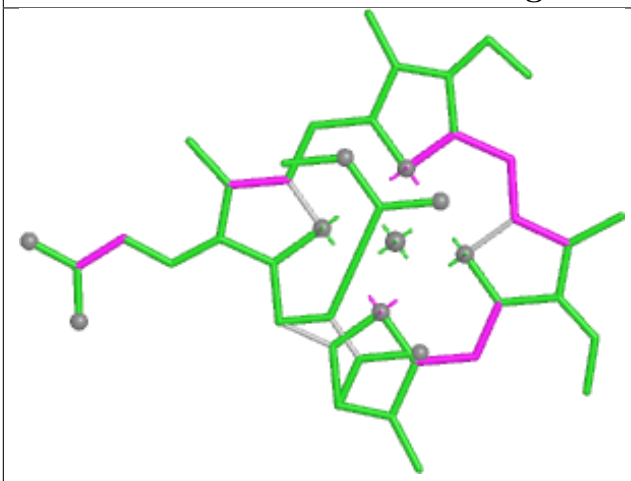


Torsions

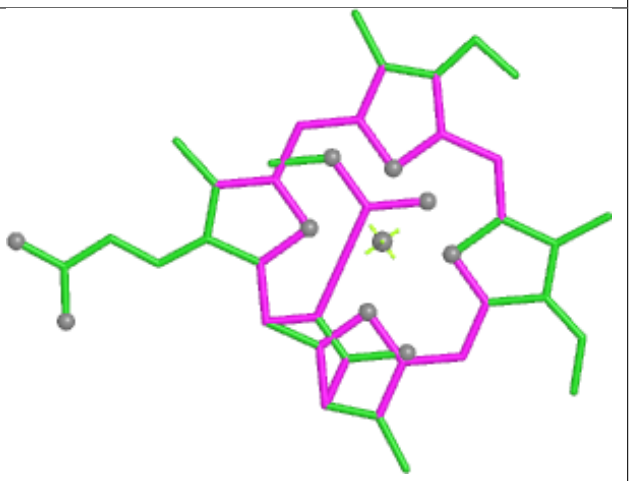


Rings

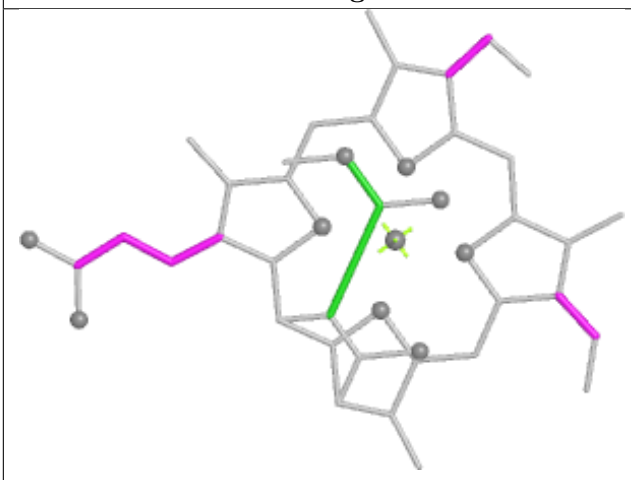
Ligand KC2 X 315



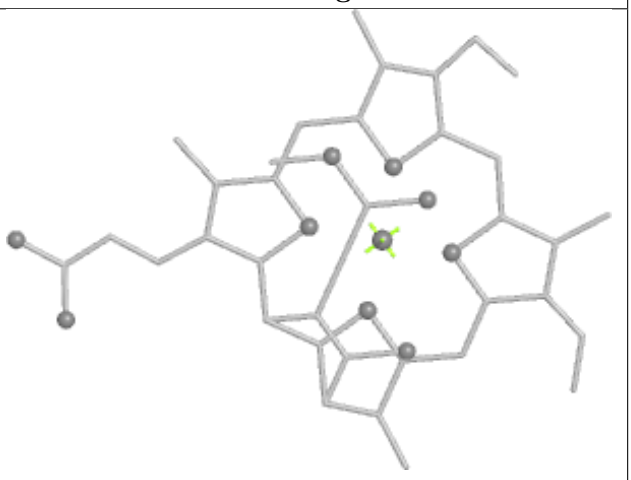
Bond lengths



Bond angles

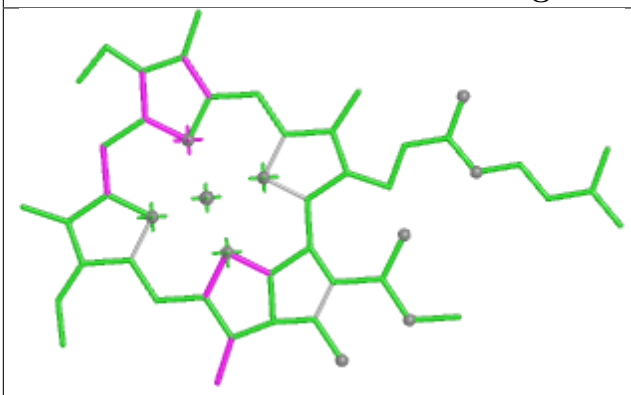


Torsions

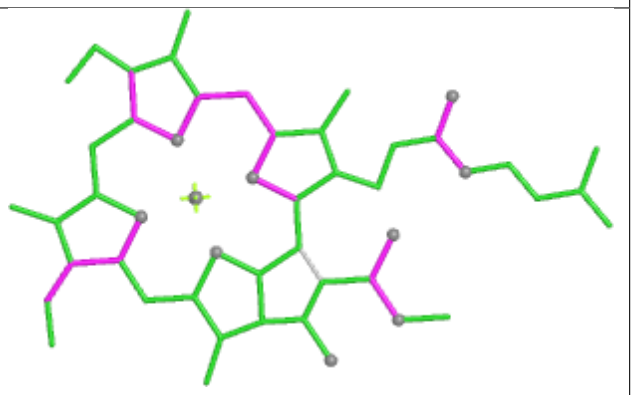


Rings

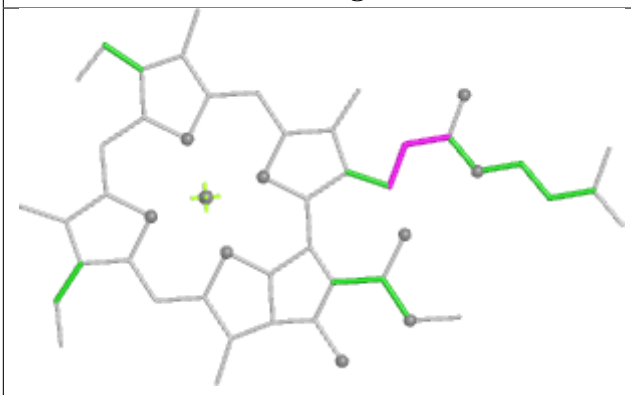
Ligand CLA l 205



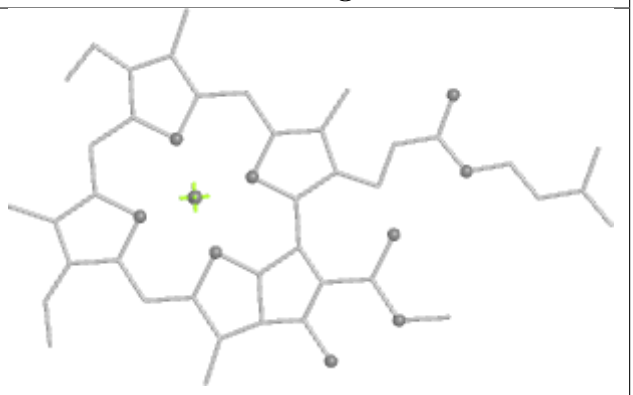
Bond lengths



Bond angles

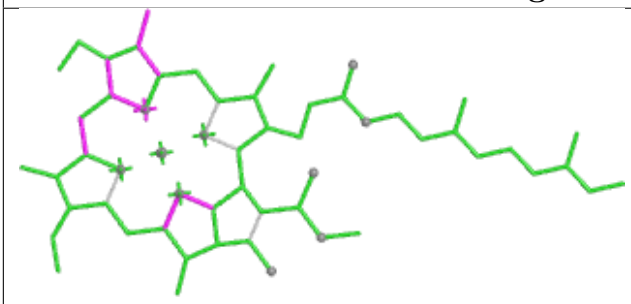


Torsions

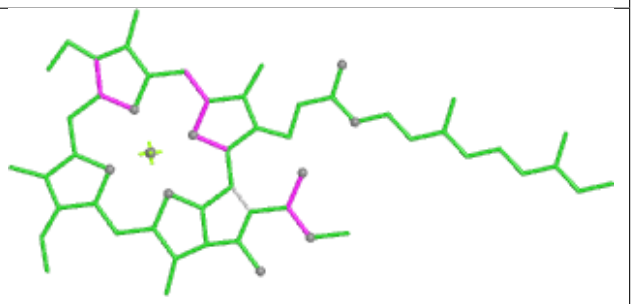


Rings

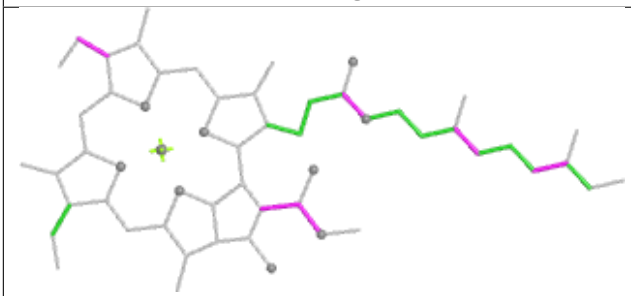
Ligand CLA a 808



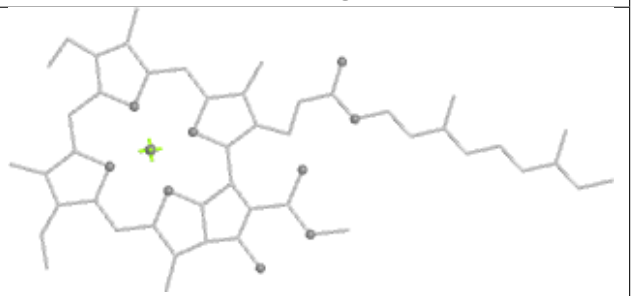
Bond lengths



Bond angles

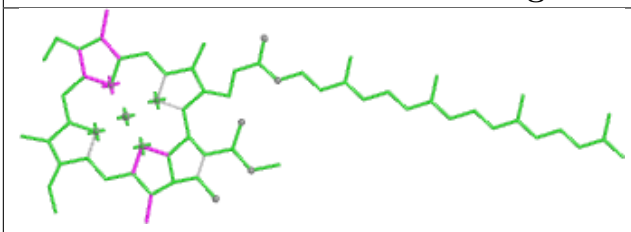


Torsions

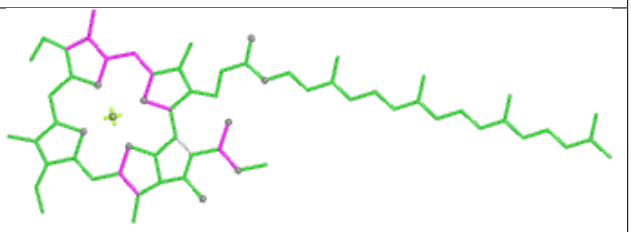


Rings

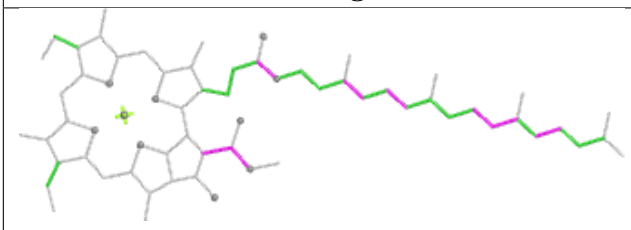
Ligand CLA b 830



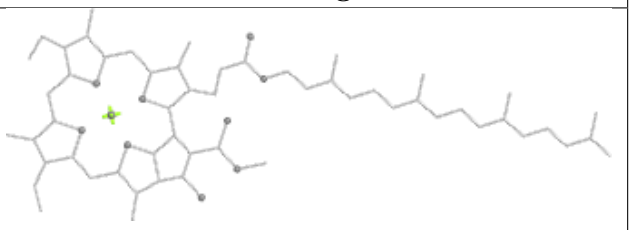
Bond lengths



Bond angles



Torsions

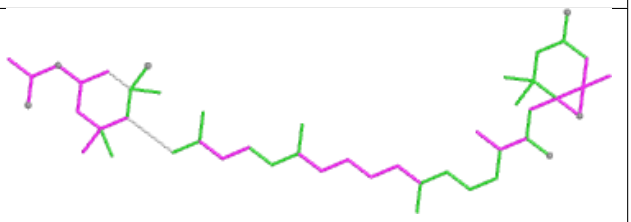


Rings

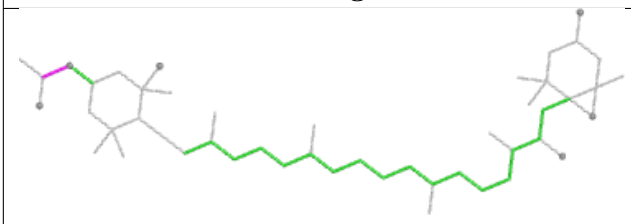
Ligand A86 R 301



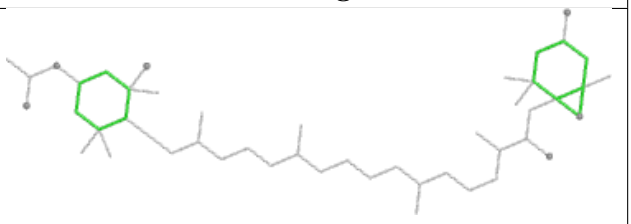
Bond lengths



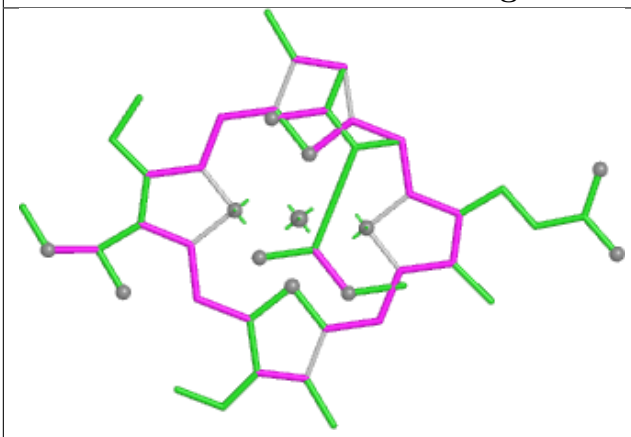
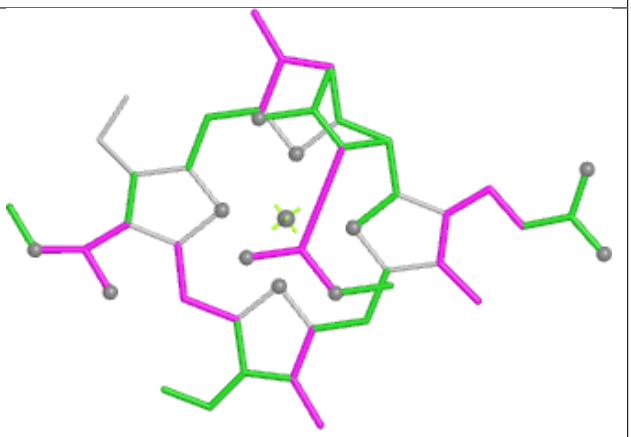
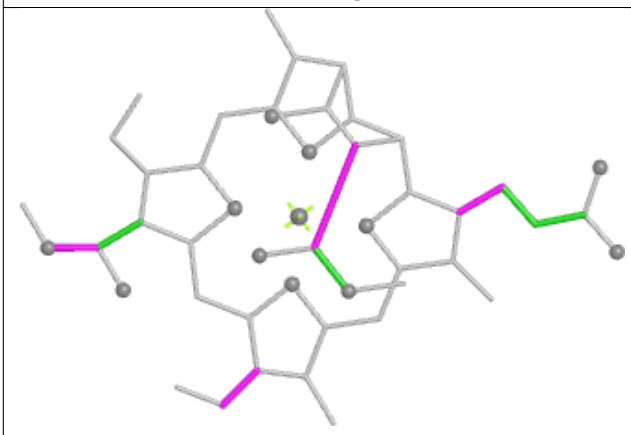
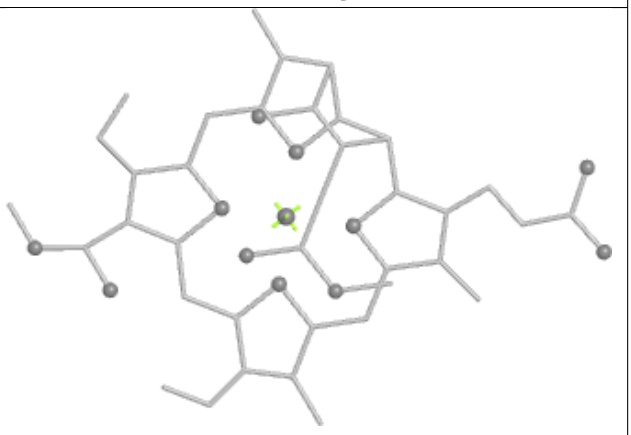
Bond angles



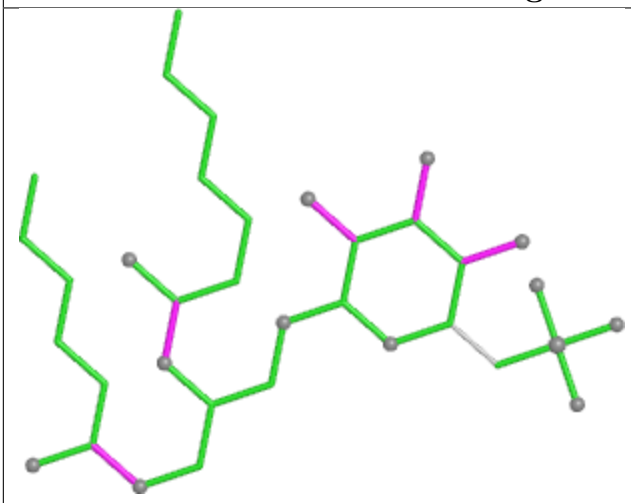
Torsions



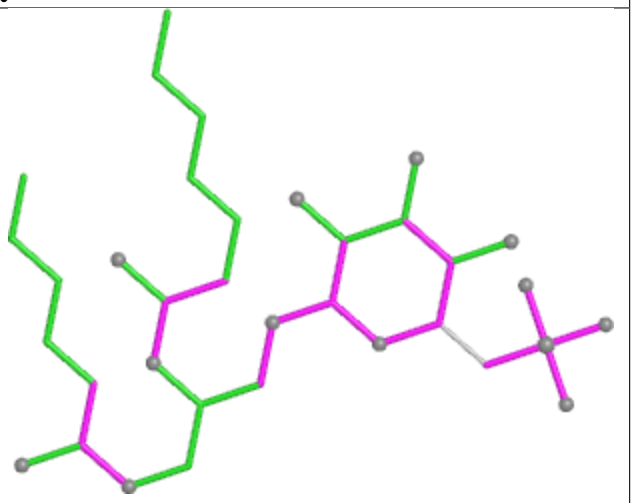
Rings

Ligand A1ECV Y 312	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

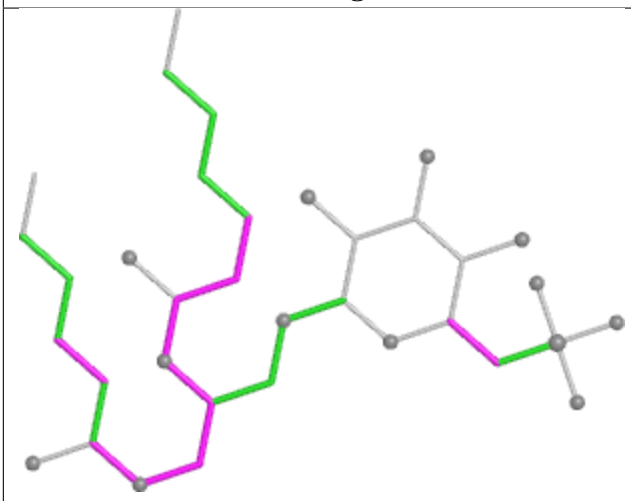
Ligand SQD E 320



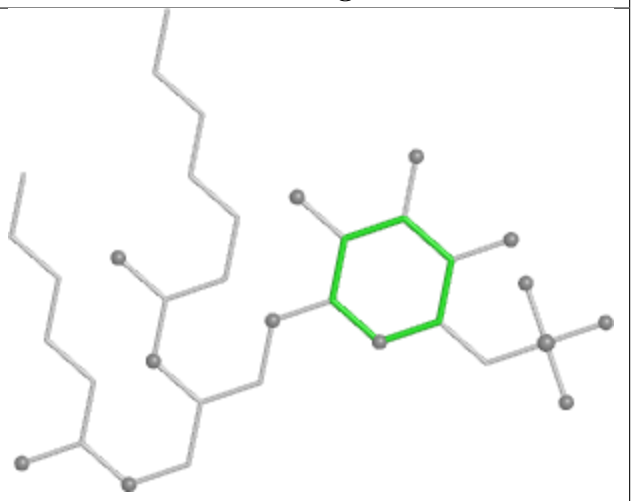
Bond lengths



Bond angles

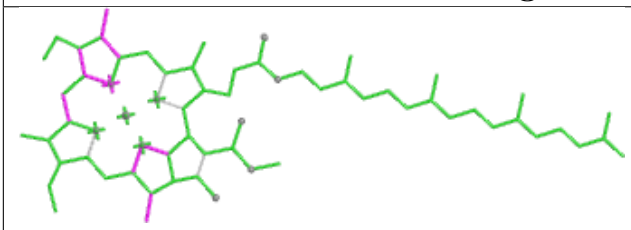


Torsions

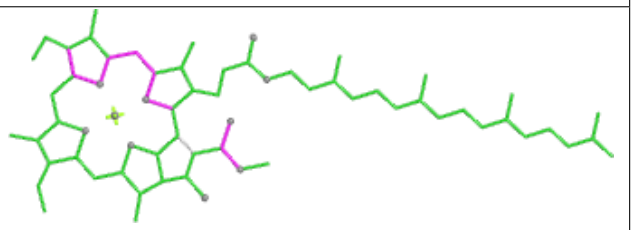


Rings

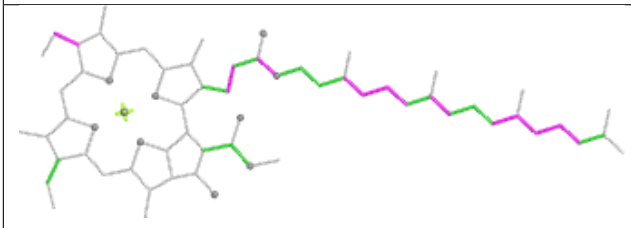
Ligand CLA W 310



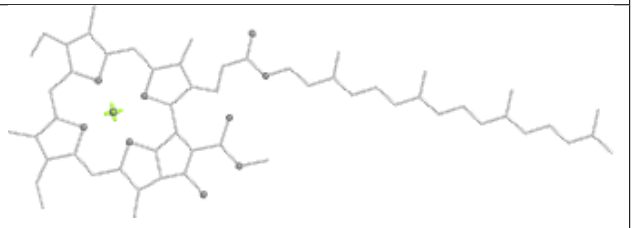
Bond lengths



Bond angles

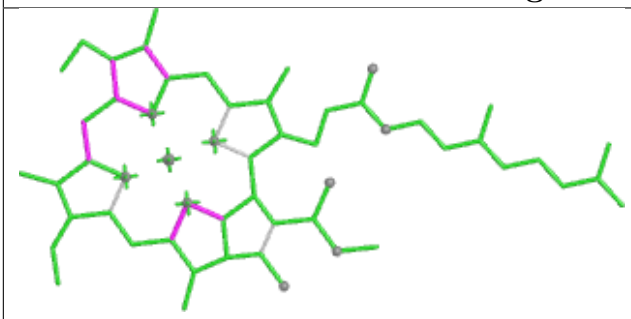


Torsions

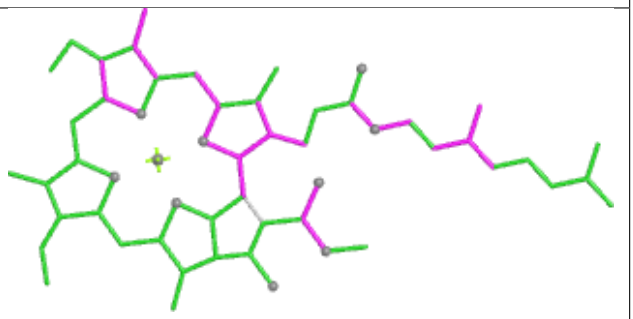


Rings

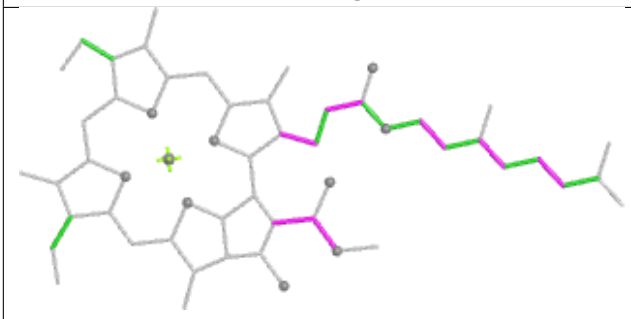
Ligand CLA F 314



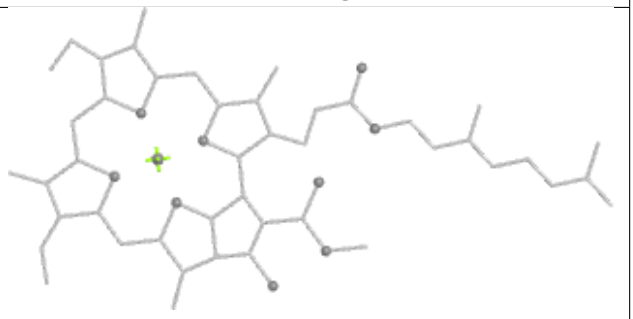
Bond lengths



Bond angles

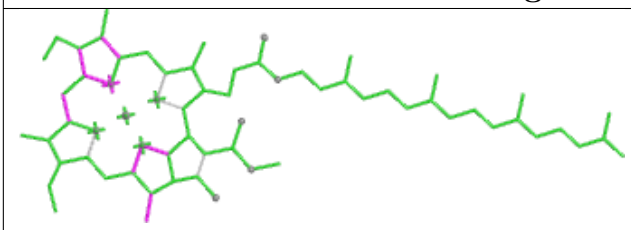


Torsions

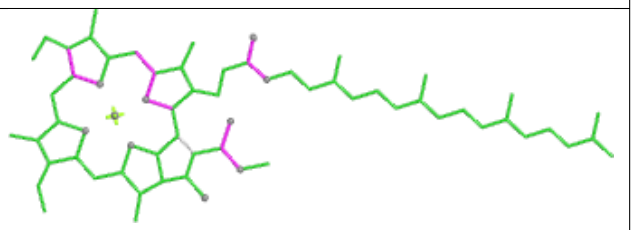


Rings

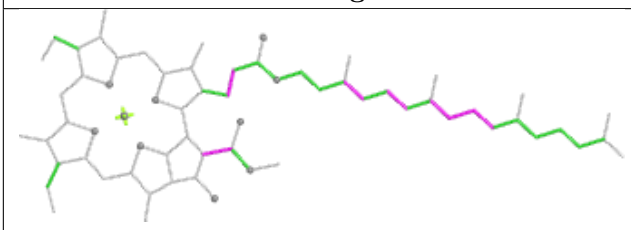
Ligand CLA C 306



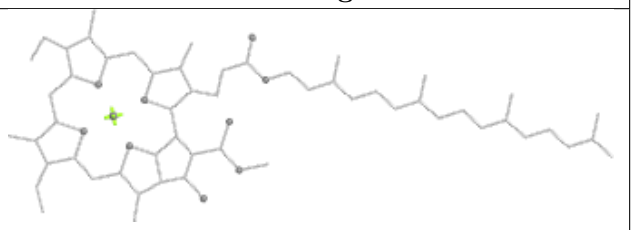
Bond lengths



Bond angles

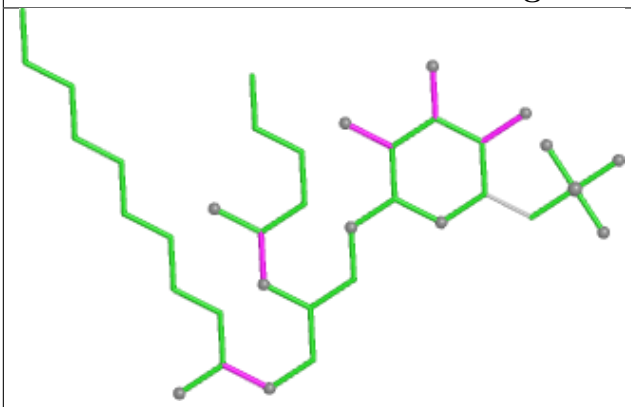


Torsions

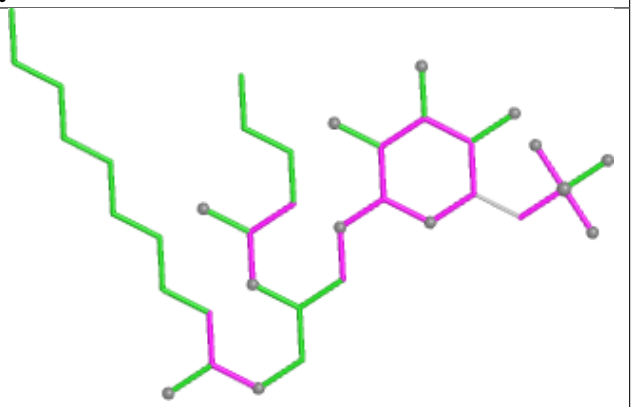


Rings

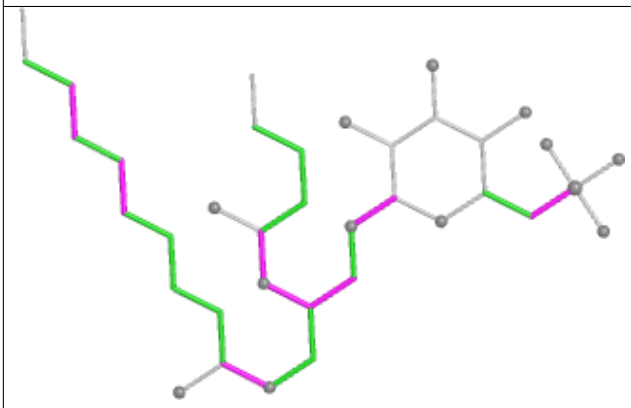
Ligand SQD D 320



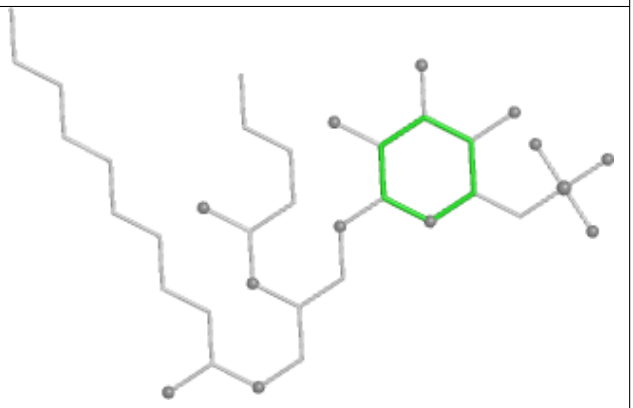
Bond lengths



Bond angles

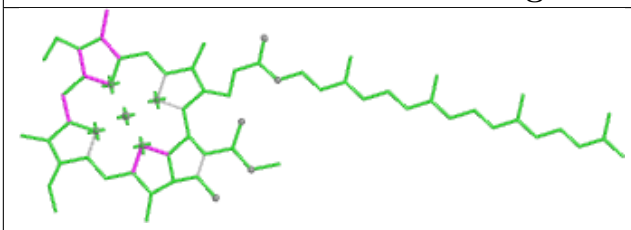


Torsions

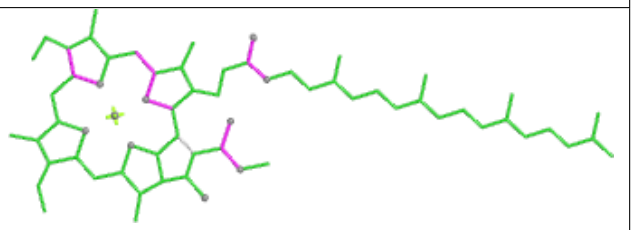


Rings

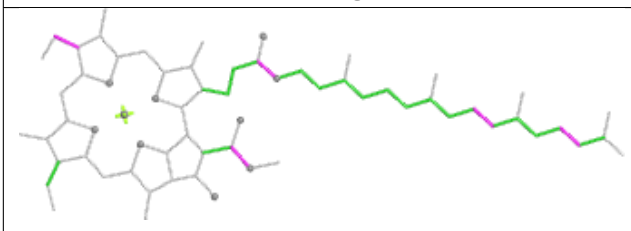
Ligand CLA F 312



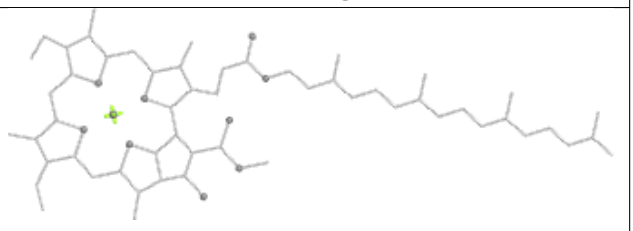
Bond lengths



Bond angles

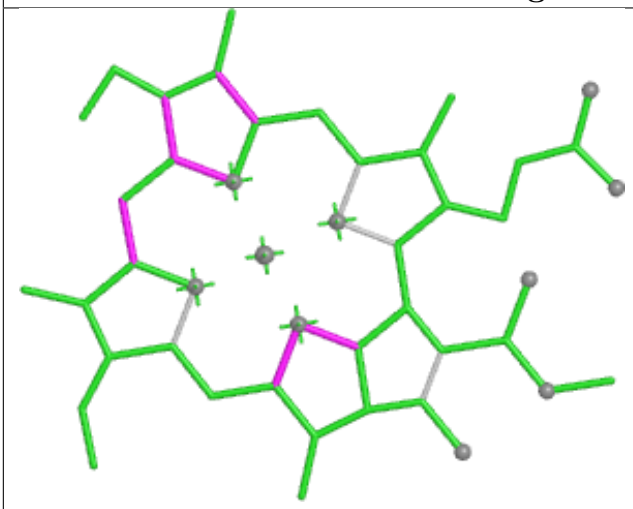


Torsions

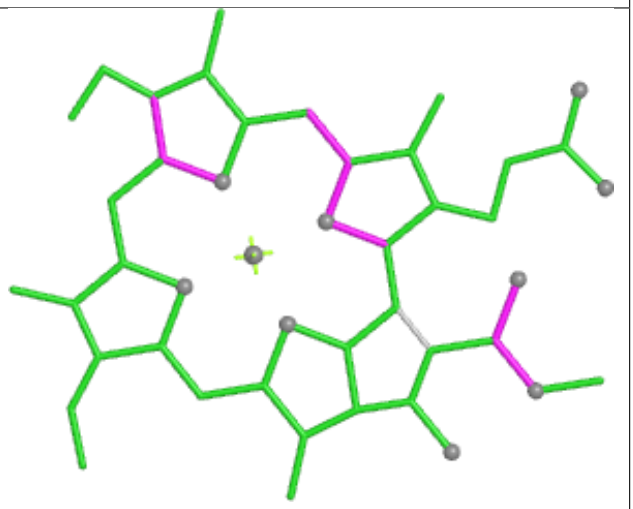


Rings

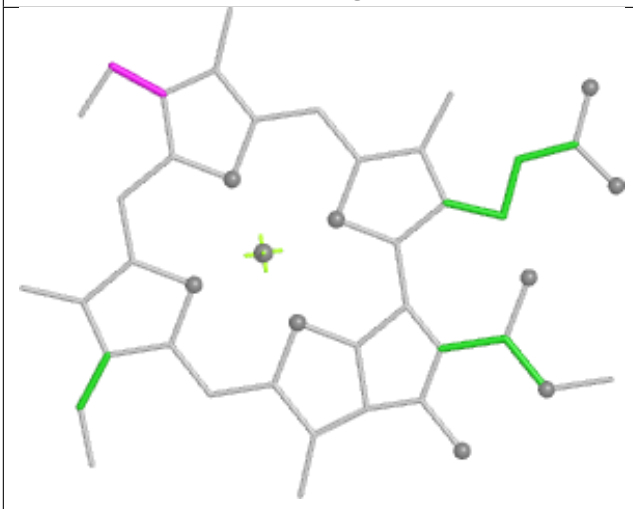
Ligand CLA x 311



Bond lengths



Bond angles

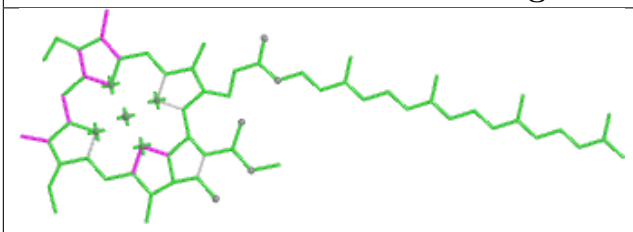


Torsions

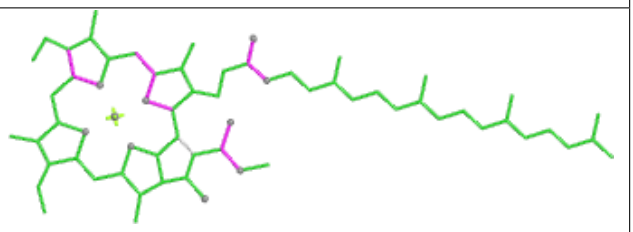


Rings

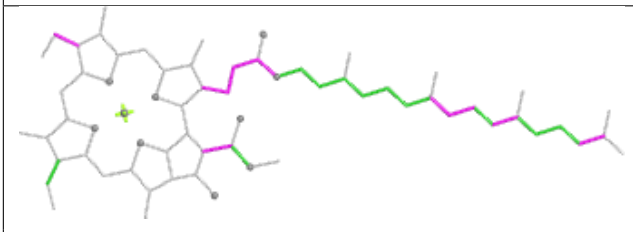
Ligand CLA a 815



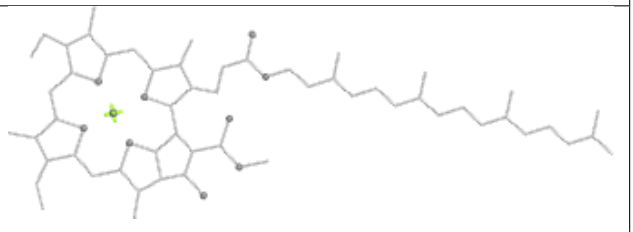
Bond lengths



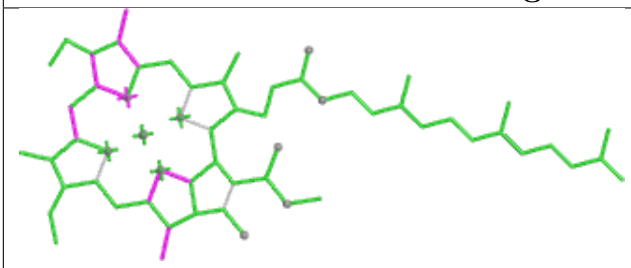
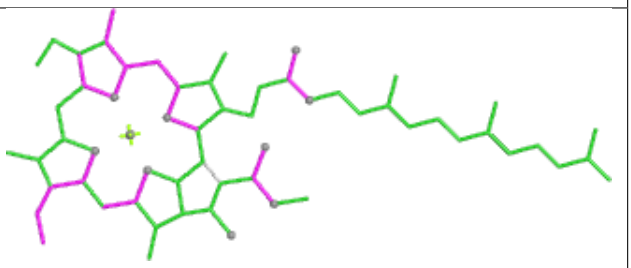
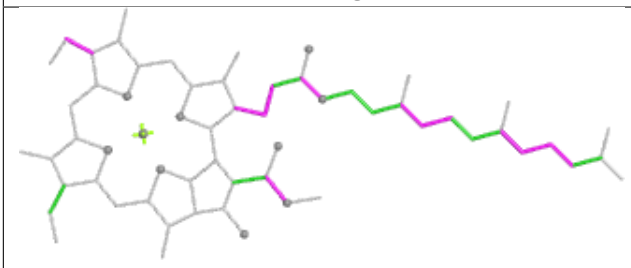
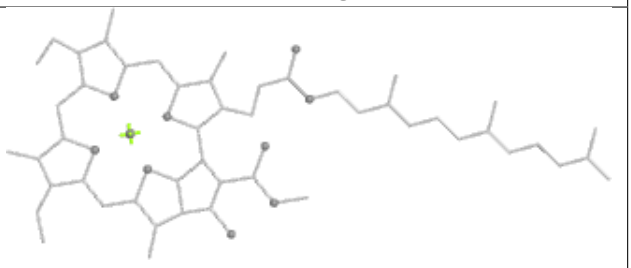
Bond angles

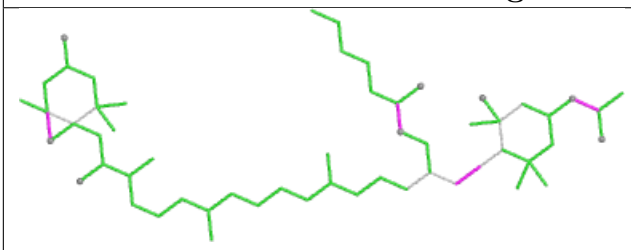
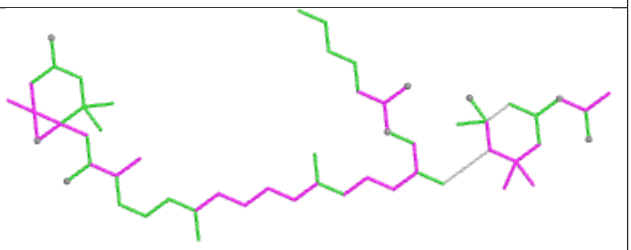
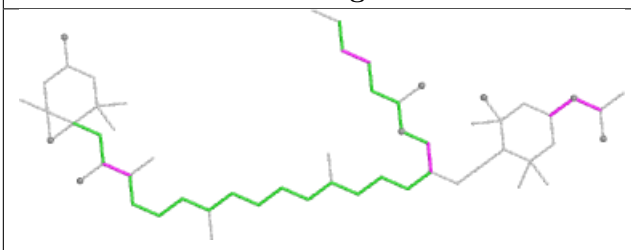
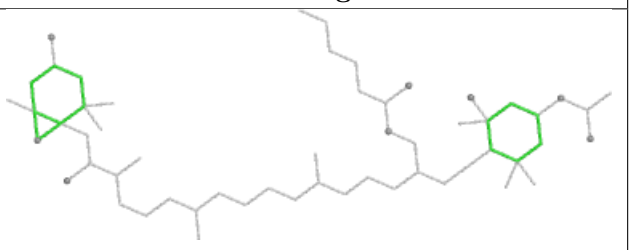


Torsions

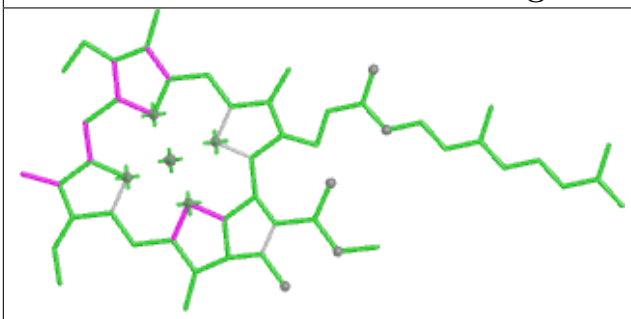


Rings

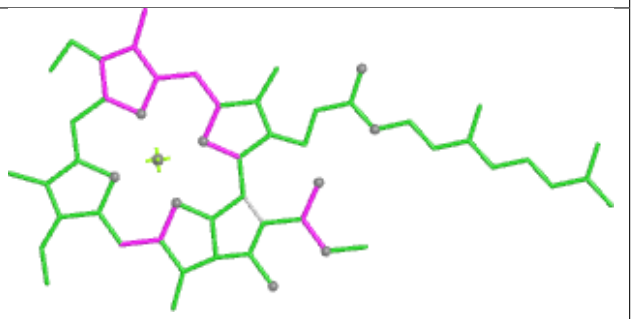
Ligand CLA O 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EB1 E 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

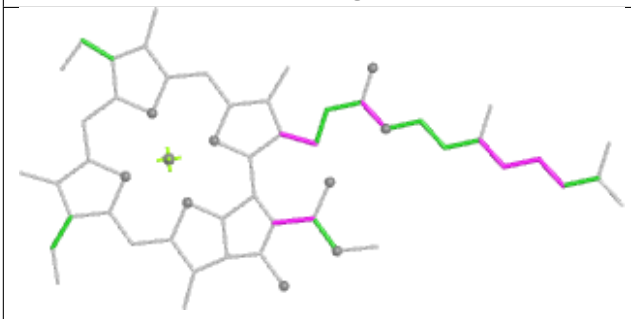
Ligand CLA b 818



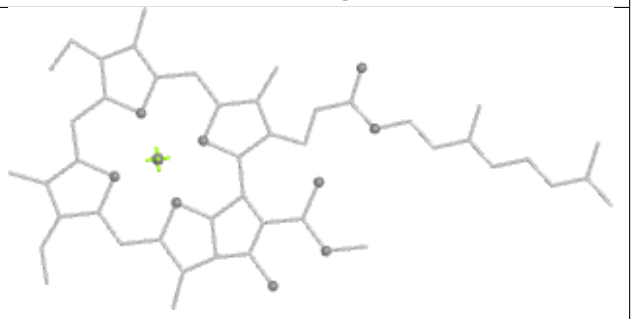
Bond lengths



Bond angles

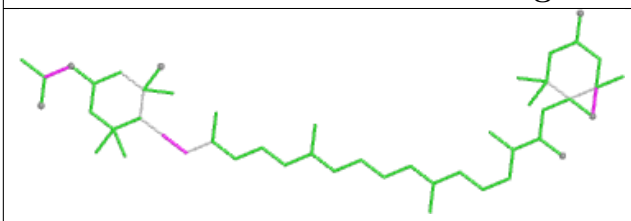


Torsions

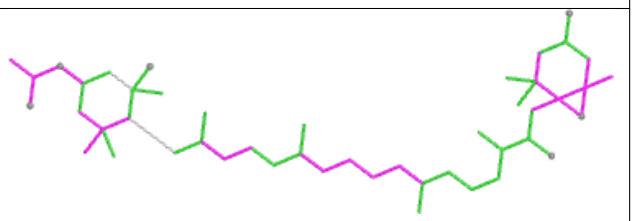


Rings

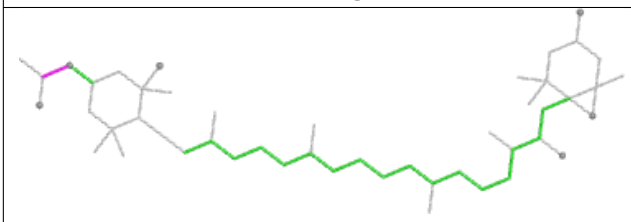
Ligand A86 6 303



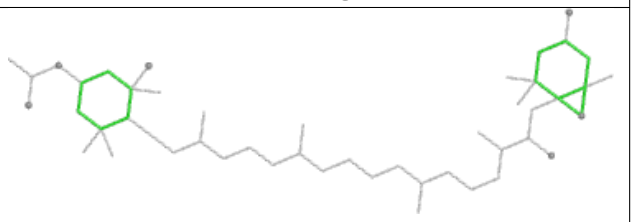
Bond lengths



Bond angles

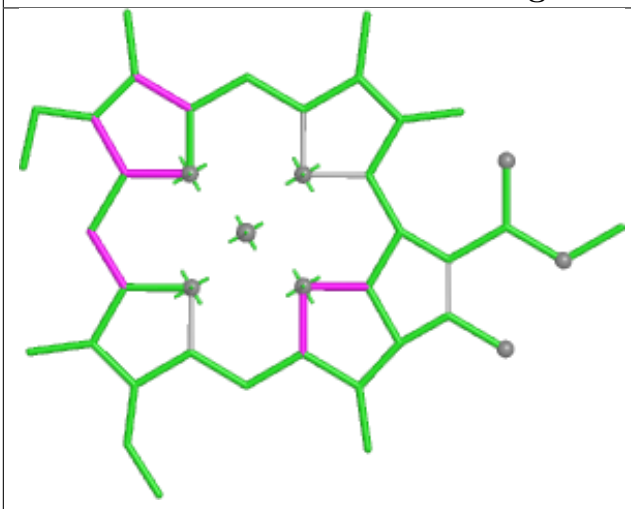


Torsions

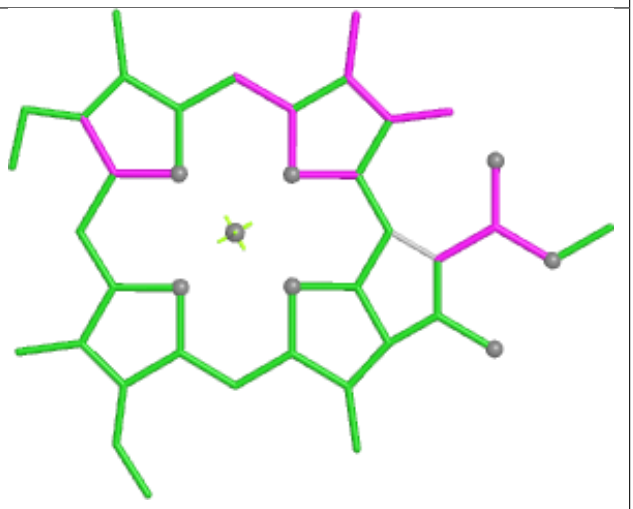


Rings

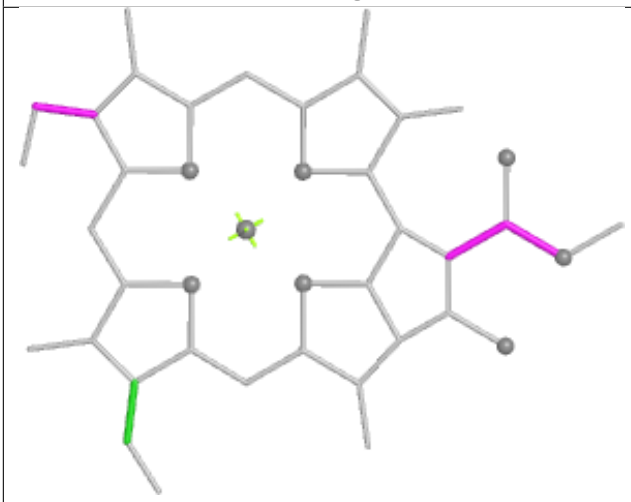
Ligand CLA 1 320



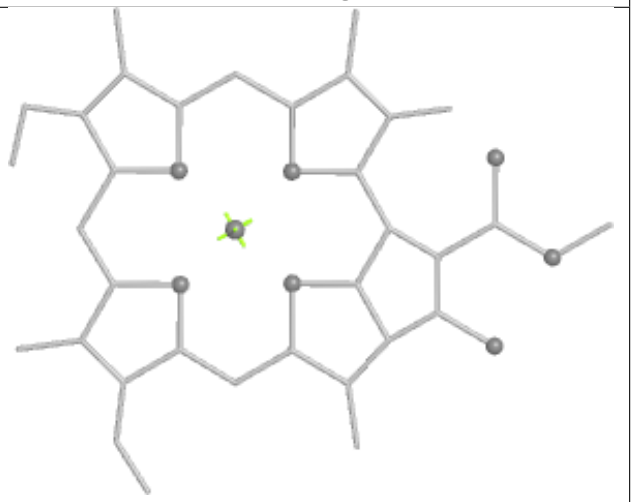
Bond lengths



Bond angles

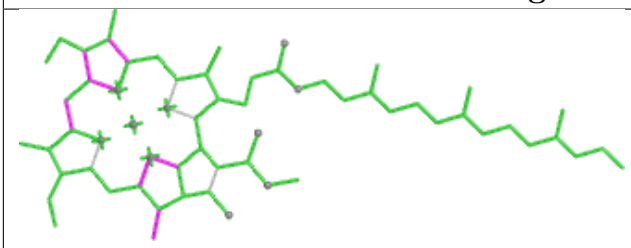


Torsions

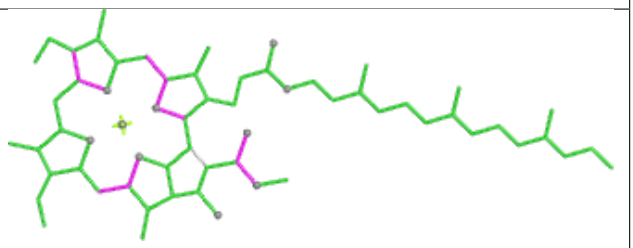


Rings

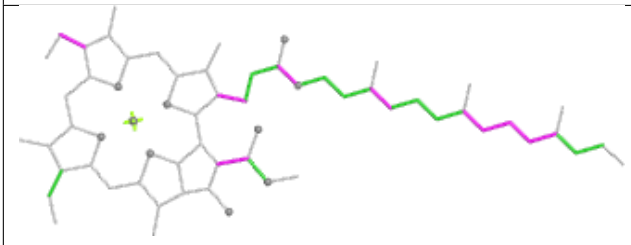
Ligand CLA a 809



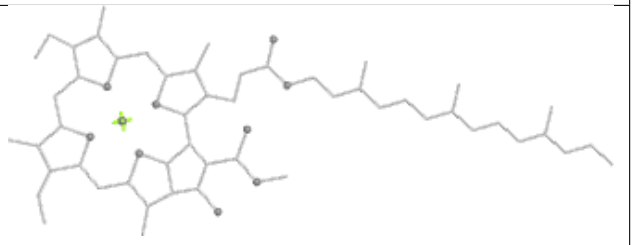
Bond lengths



Bond angles

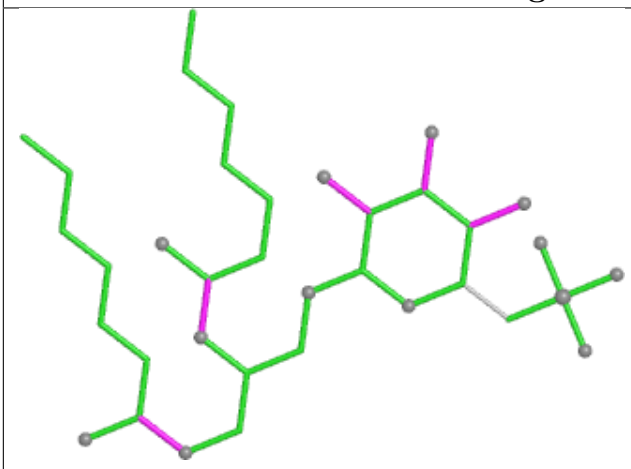


Torsions

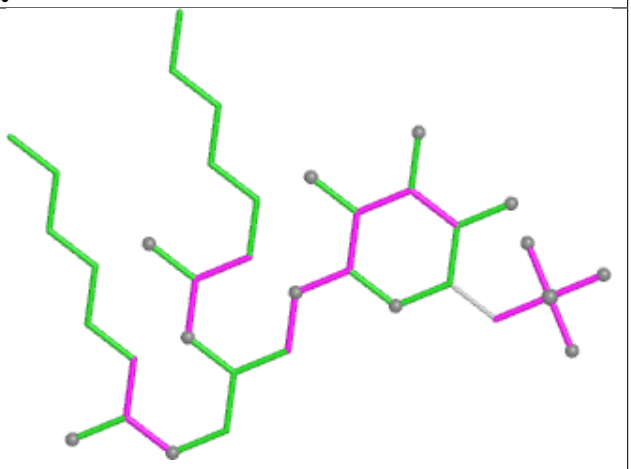


Rings

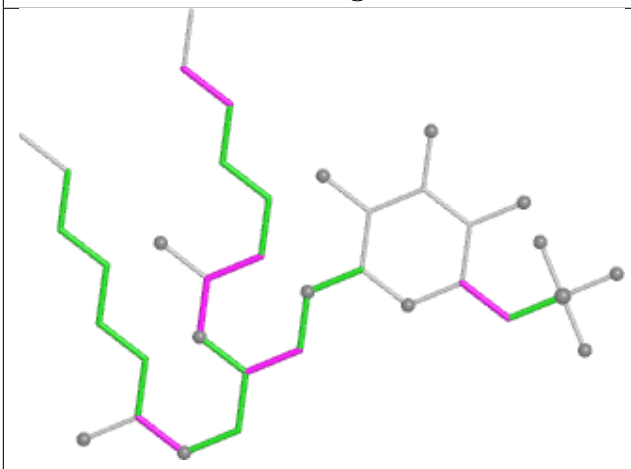
Ligand SQD 9 322



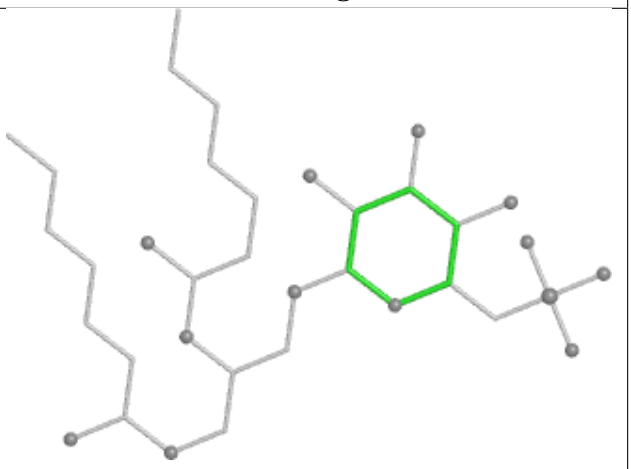
Bond lengths



Bond angles

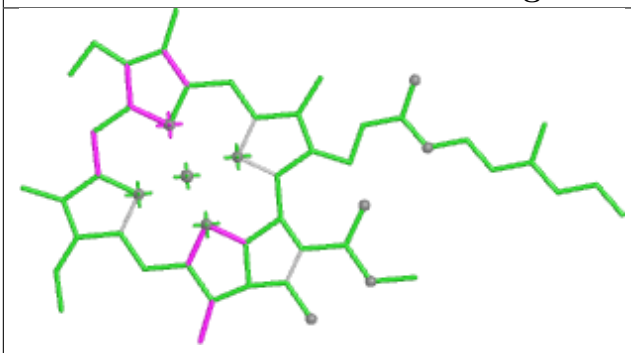


Torsions

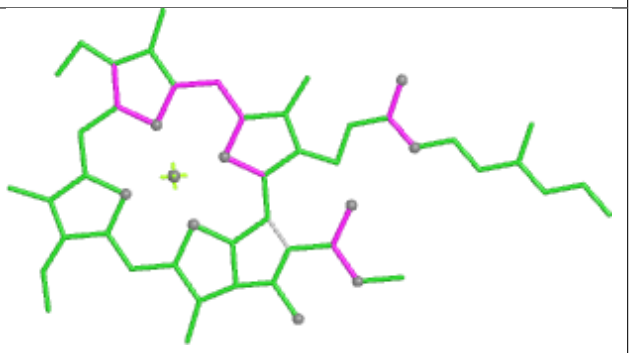


Rings

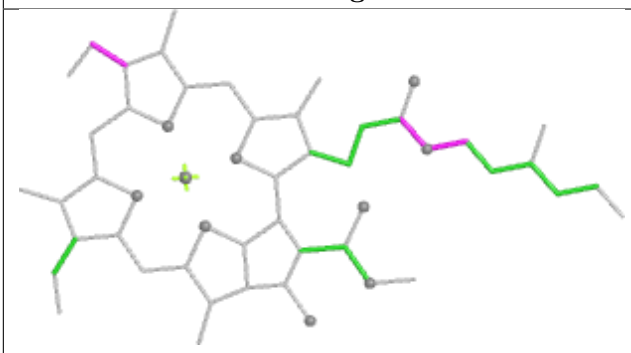
Ligand CLA H 309



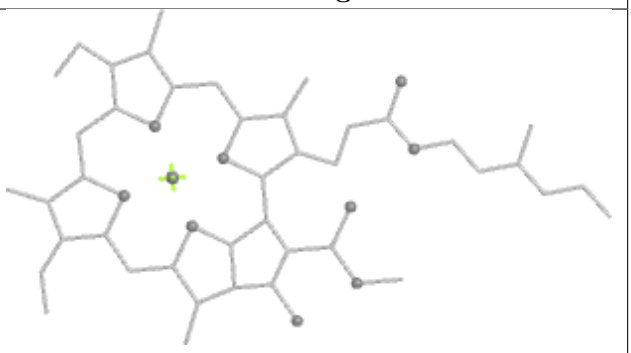
Bond lengths



Bond angles

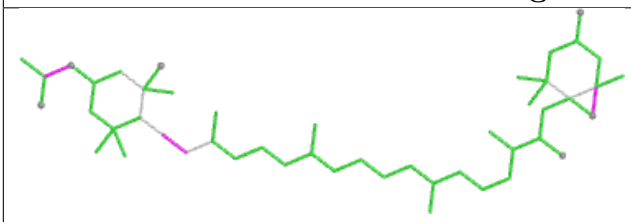


Torsions

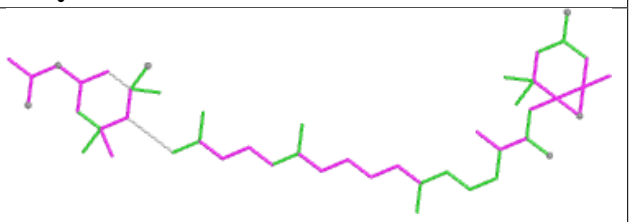


Rings

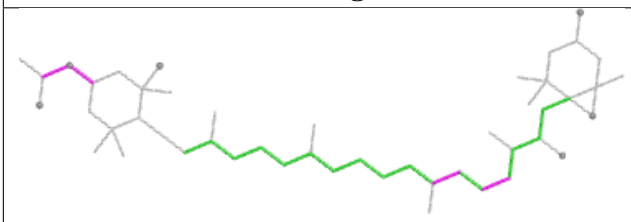
Ligand A86 Q 302



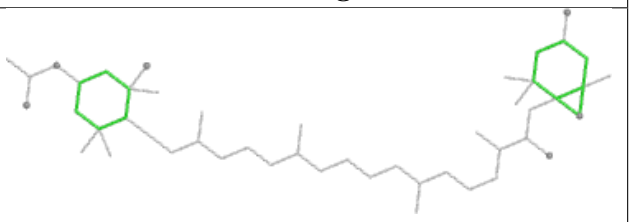
Bond lengths



Bond angles

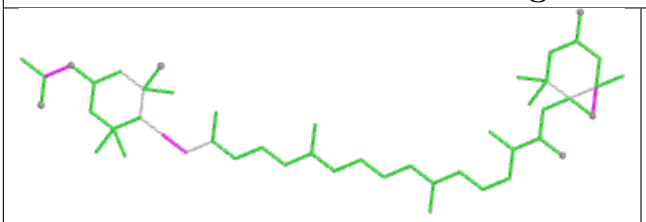


Torsions

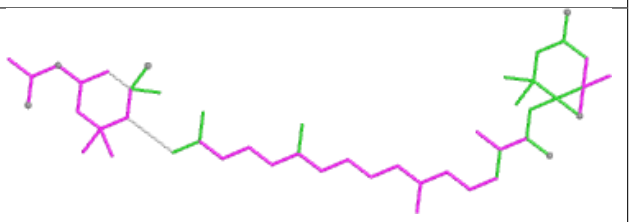


Rings

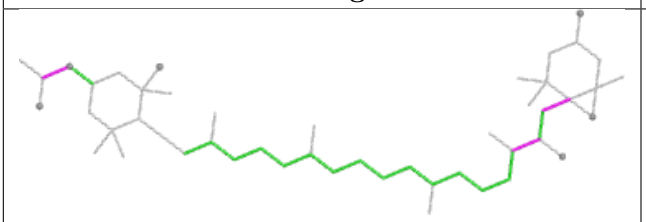
Ligand A86 X 303



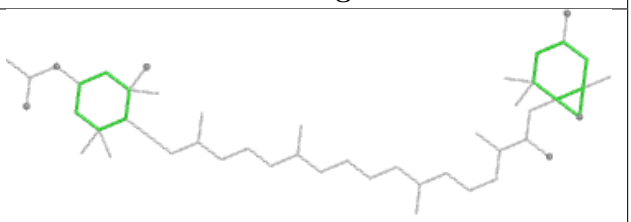
Bond lengths



Bond angles



Torsions

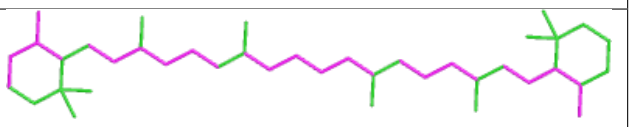


Rings

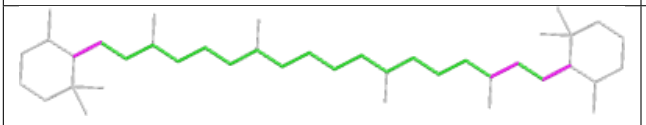
Ligand BCR l 206



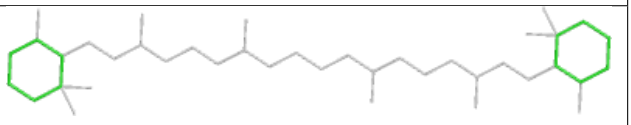
Bond lengths



Bond angles

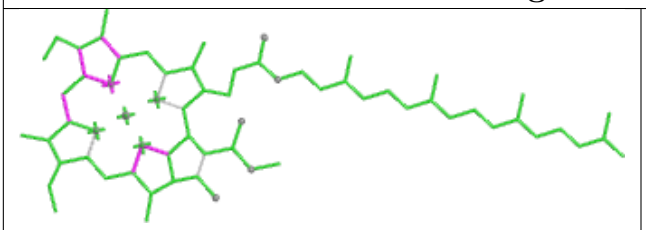


Torsions

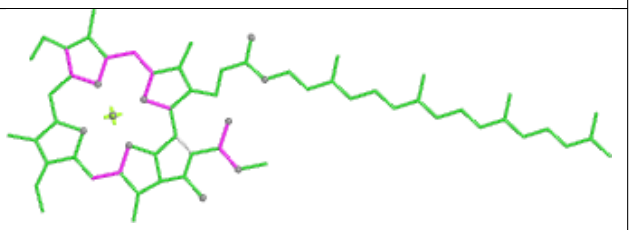


Rings

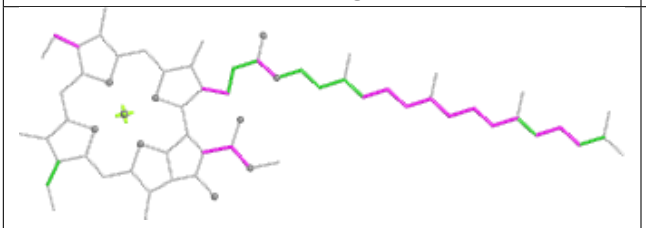
Ligand CLA J 314



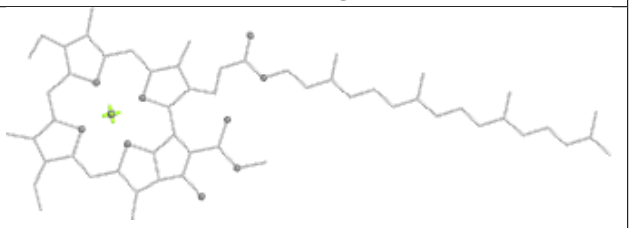
Bond lengths



Bond angles

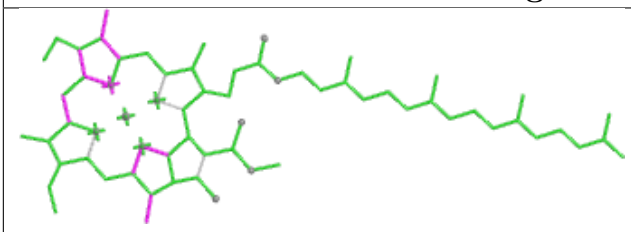


Torsions

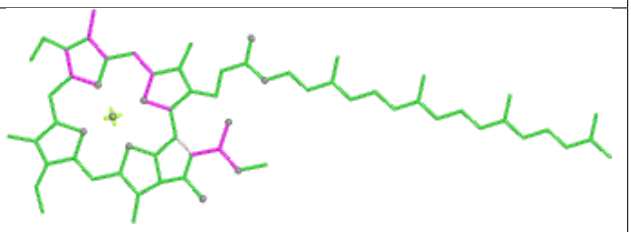


Rings

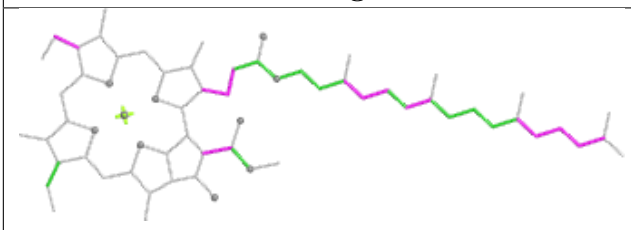
Ligand CLA F 308



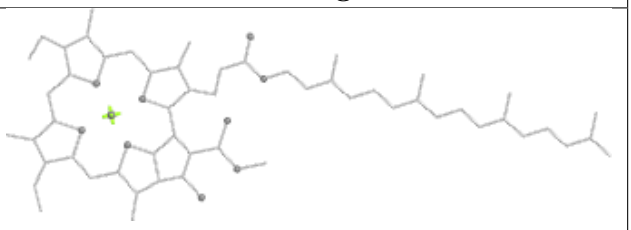
Bond lengths



Bond angles

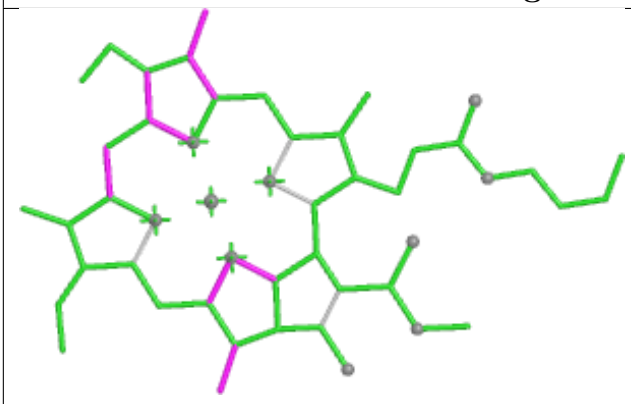


Torsions

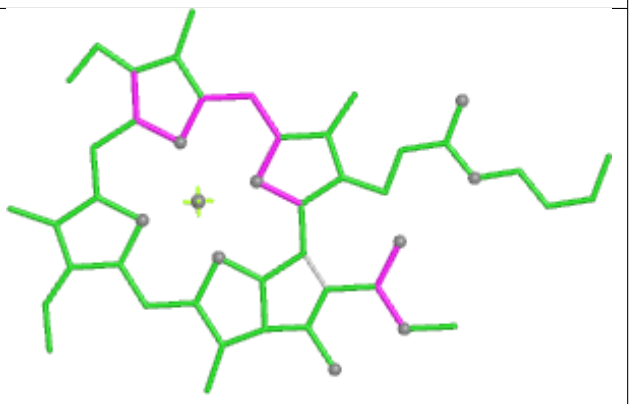


Rings

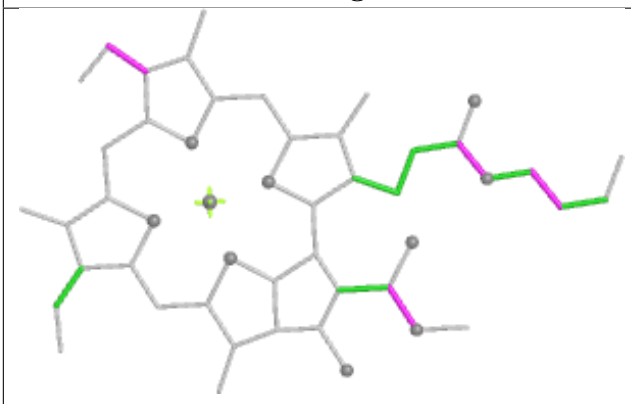
Ligand CLA A 305



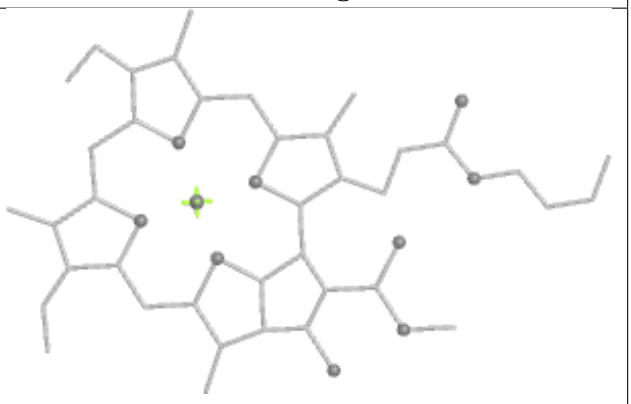
Bond lengths



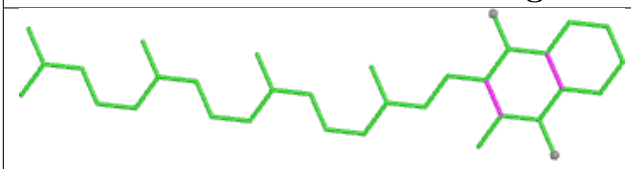
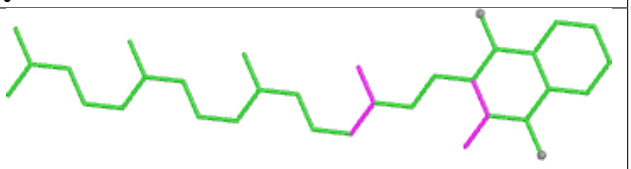
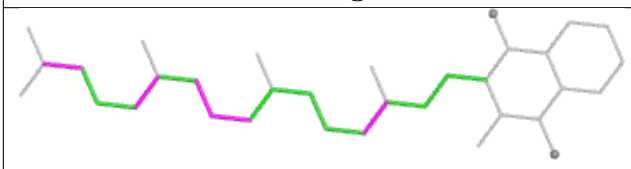
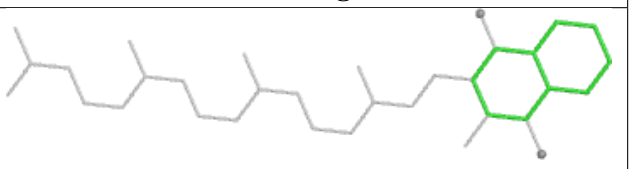
Bond angles

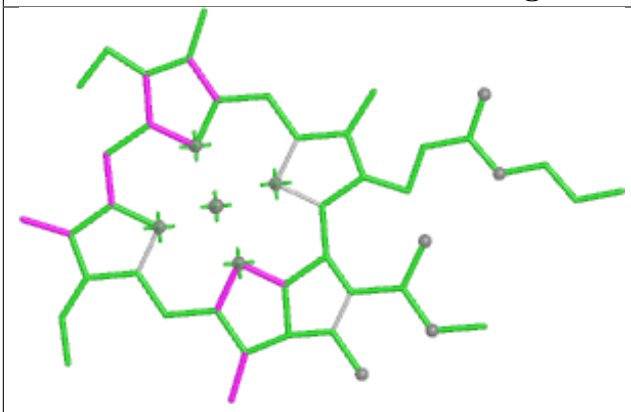
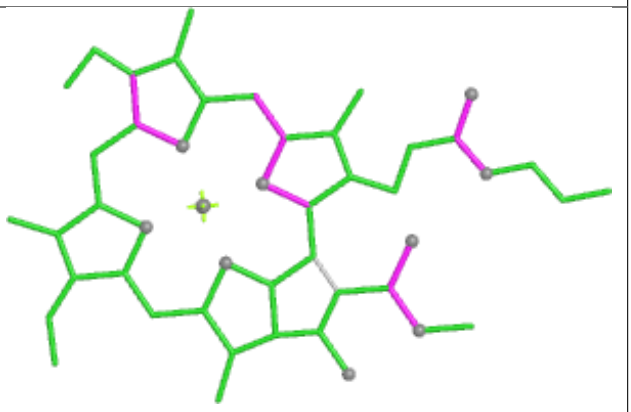
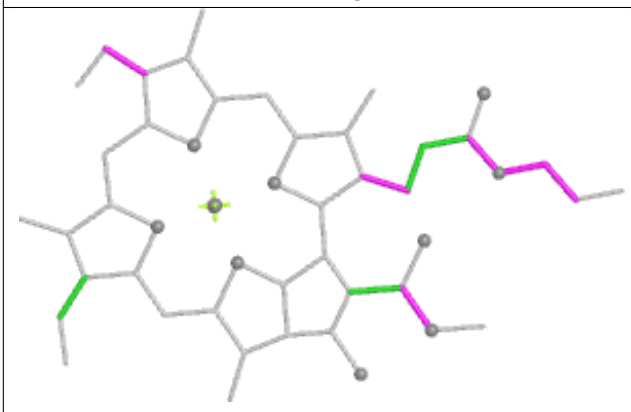
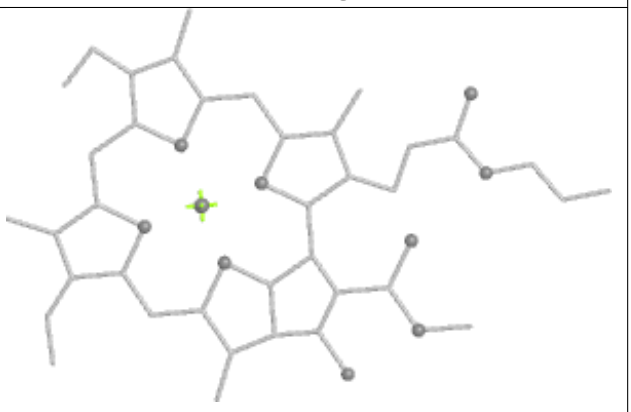


Torsions

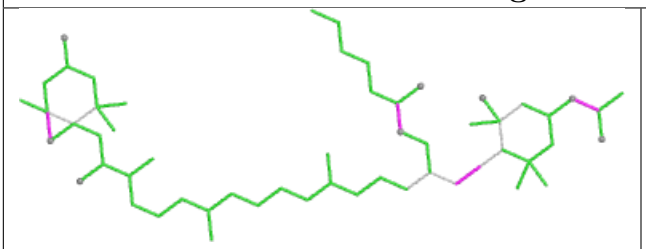


Rings

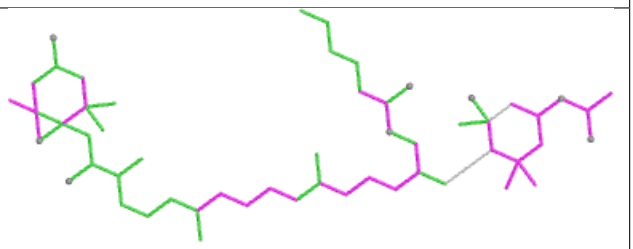
Ligand PQN a 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

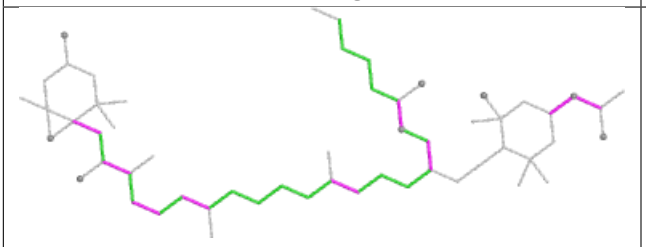
Ligand A1EB1 7 305



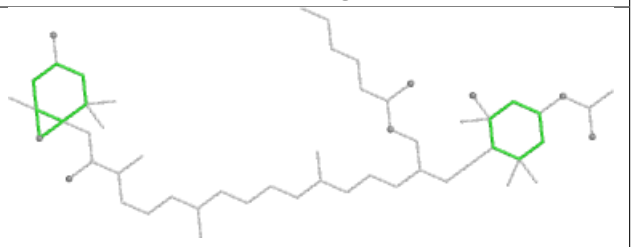
Bond lengths



Bond angles

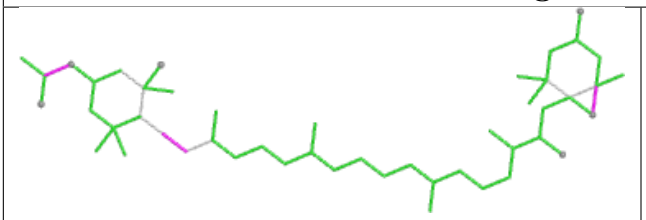


Torsions

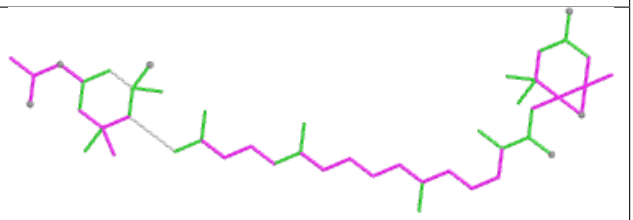


Rings

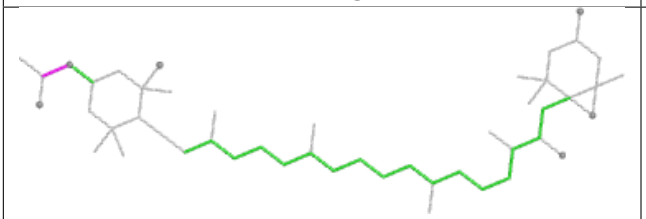
Ligand A86 J 301



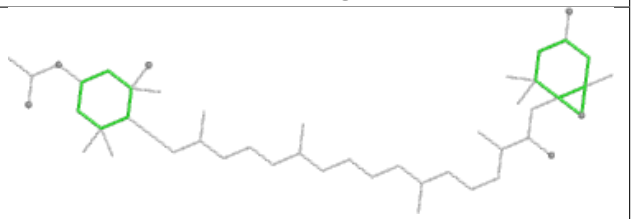
Bond lengths



Bond angles

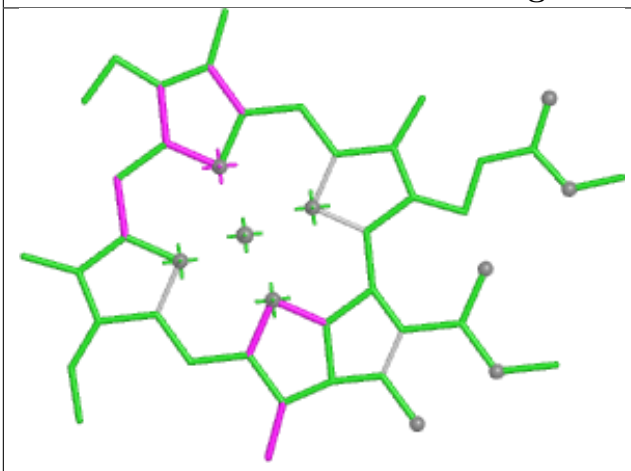


Torsions

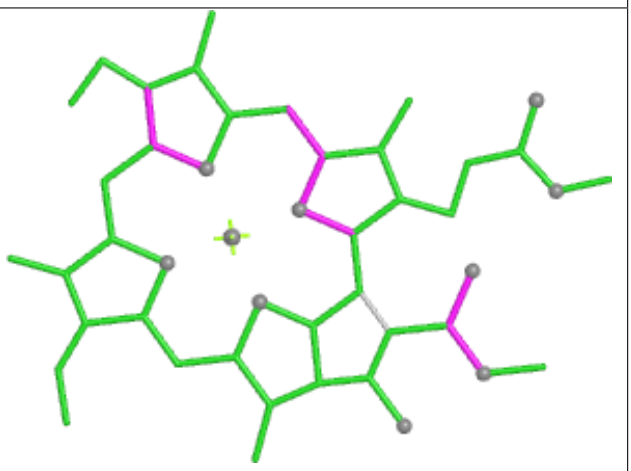


Rings

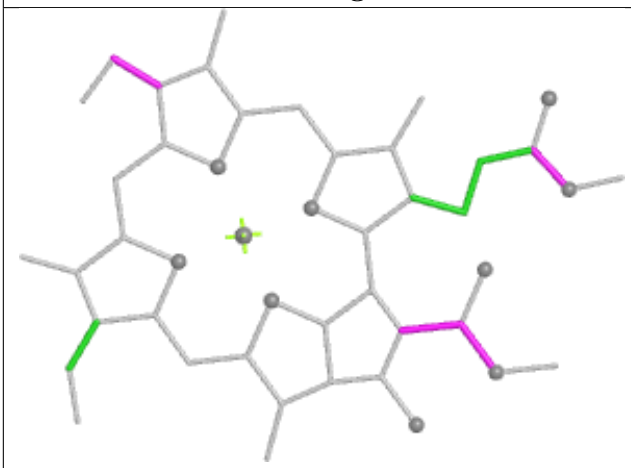
Ligand CLA J 312



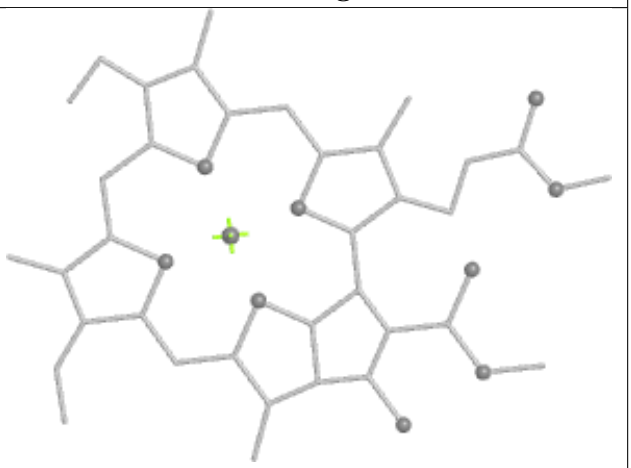
Bond lengths



Bond angles

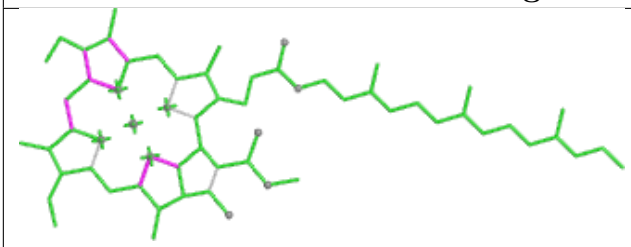


Torsions

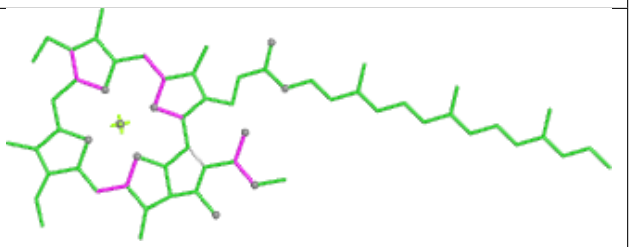


Rings

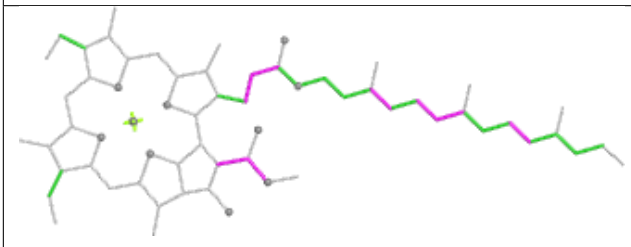
Ligand CLA K 309



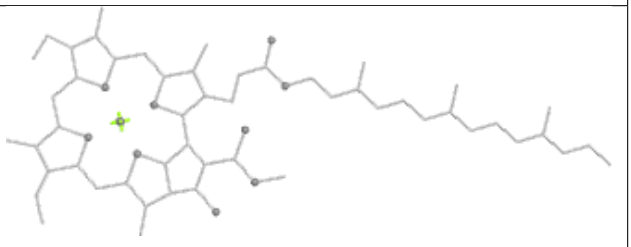
Bond lengths



Bond angles

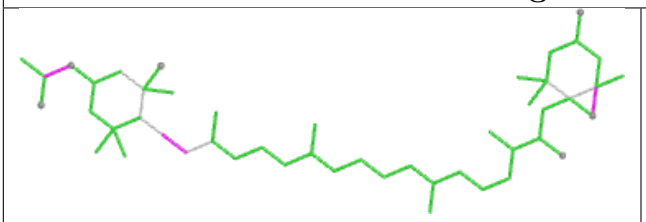


Torsions

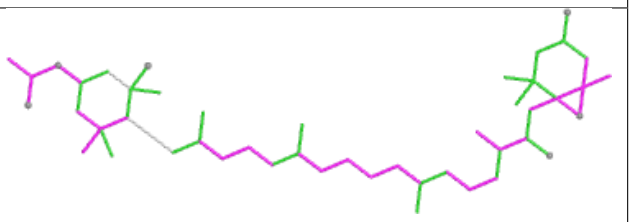


Rings

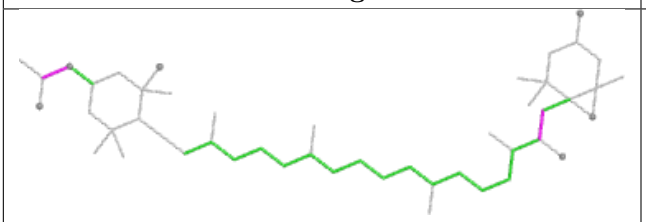
Ligand A86 V 304



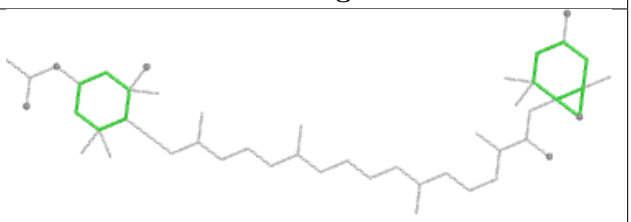
Bond lengths



Bond angles

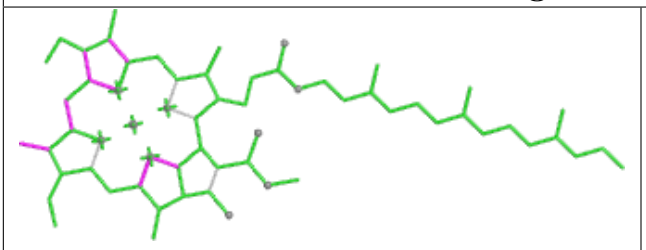


Torsions

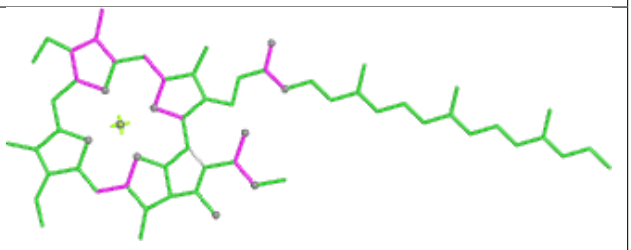


Rings

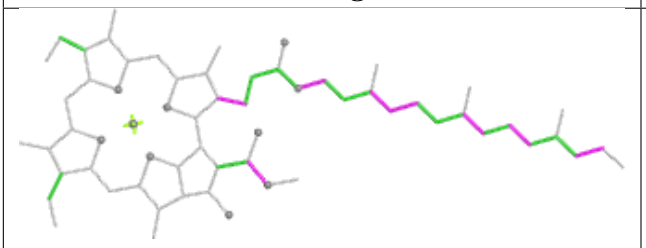
Ligand CLA a 825



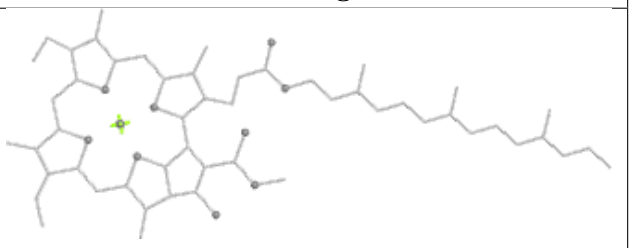
Bond lengths



Bond angles

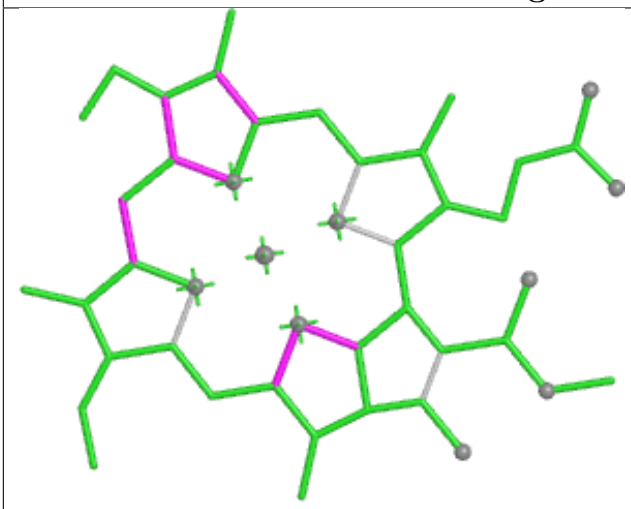


Torsions

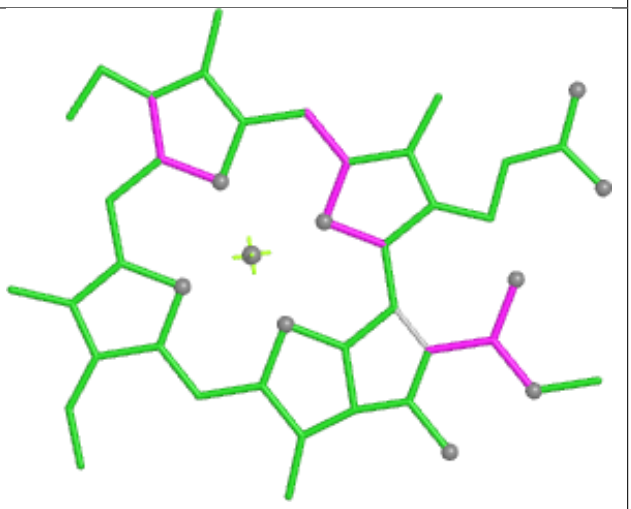


Rings

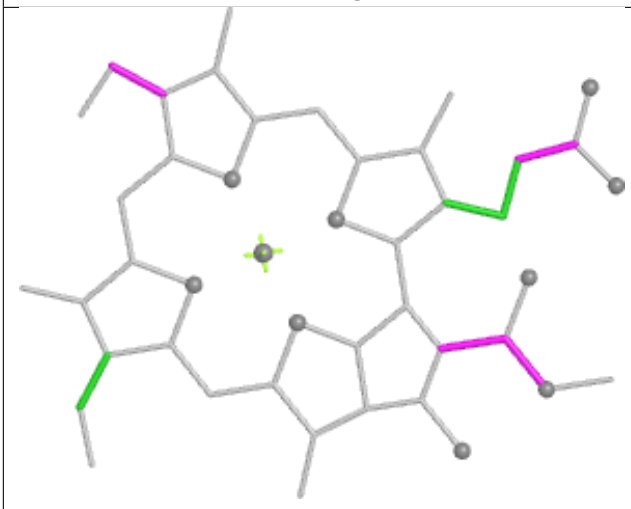
Ligand CLA 0 320



Bond lengths



Bond angles

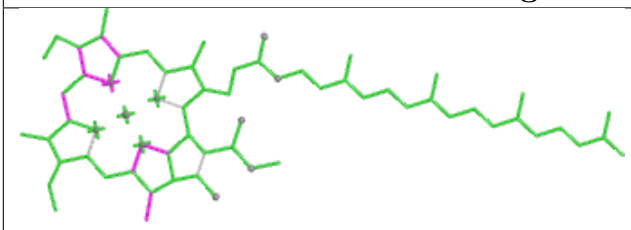


Torsions

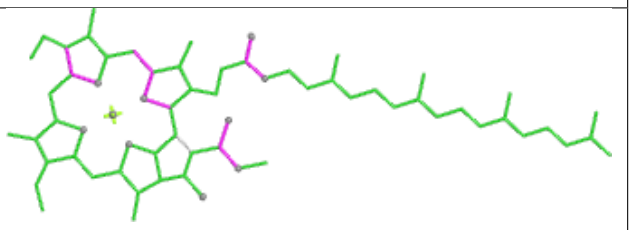


Rings

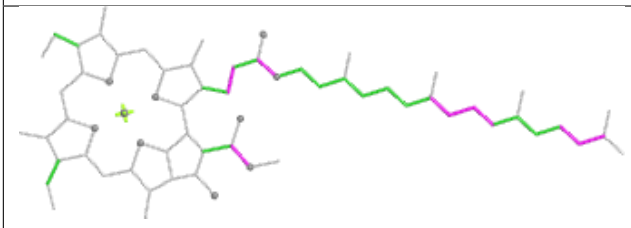
Ligand CLA M 308



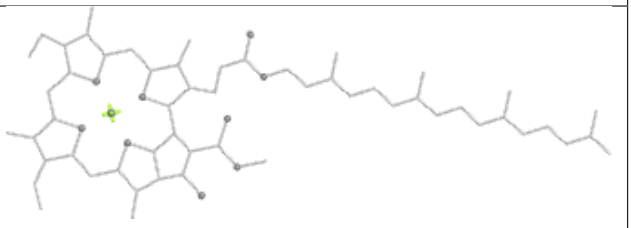
Bond lengths



Bond angles

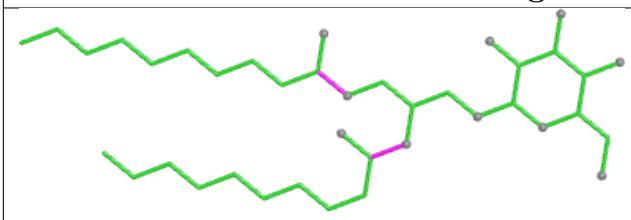


Torsions

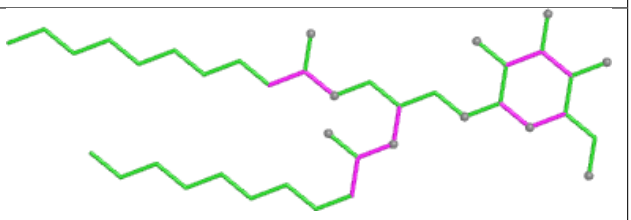


Rings

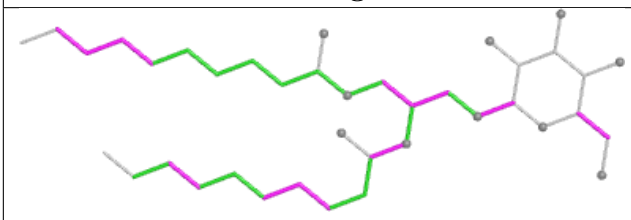
Ligand LMG l 208



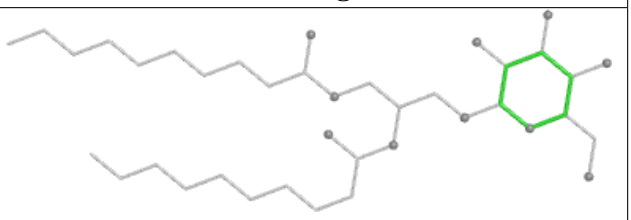
Bond lengths



Bond angles

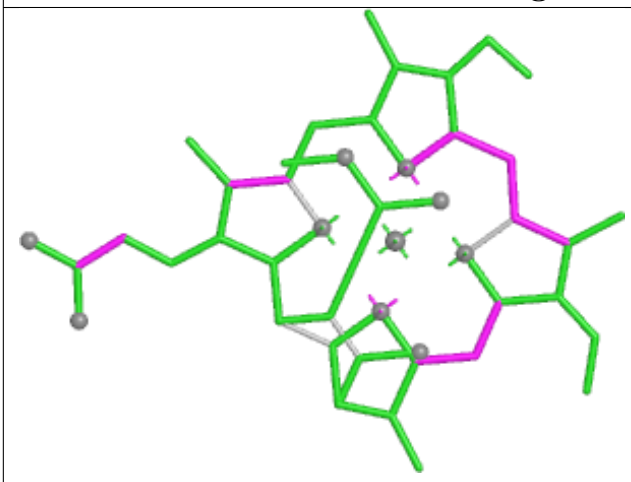


Torsions

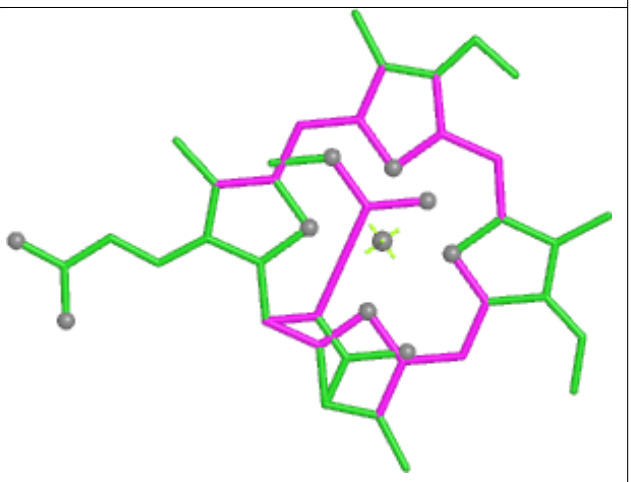


Rings

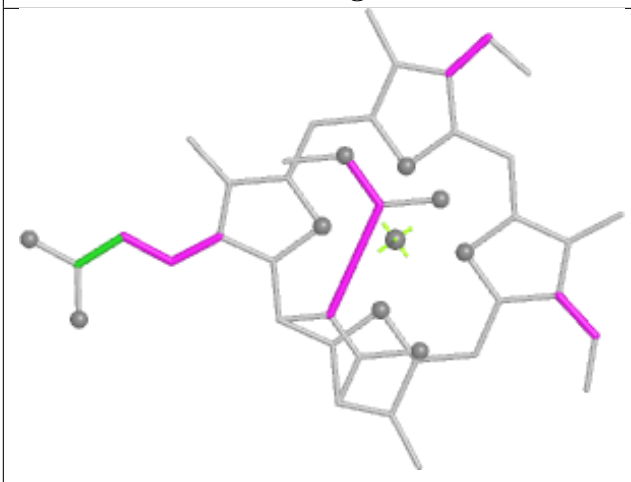
Ligand KC2 1 315



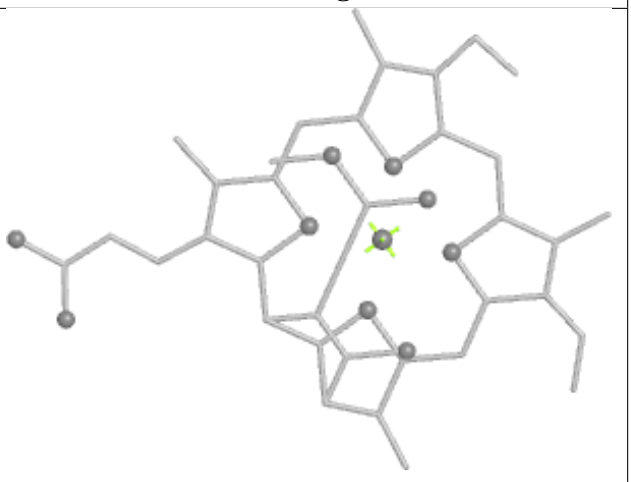
Bond lengths



Bond angles

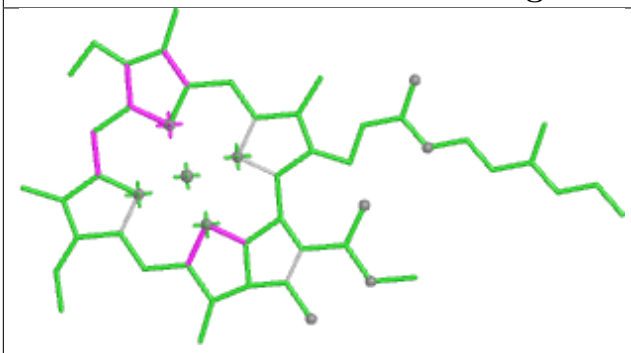


Torsions

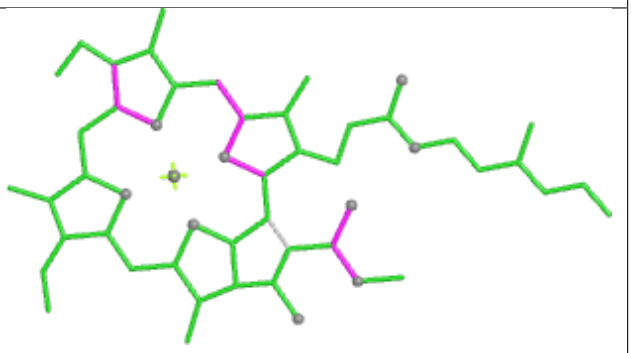


Rings

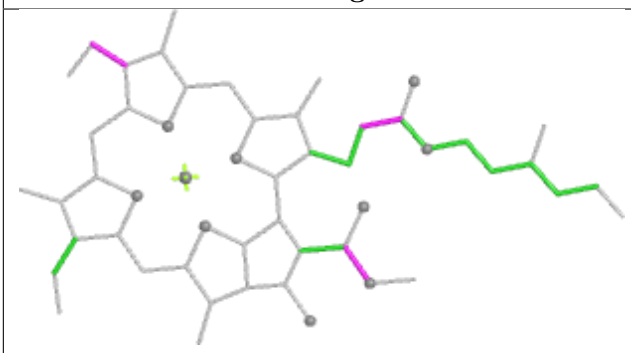
Ligand CLA F 309



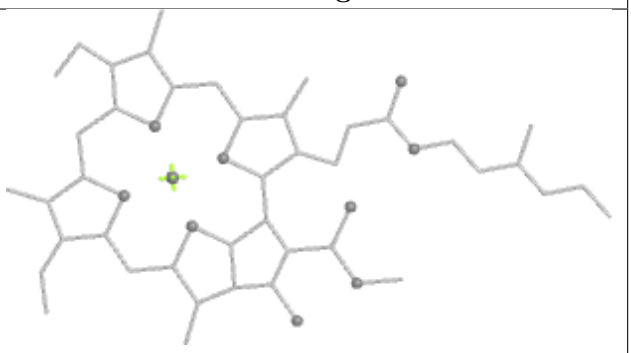
Bond lengths



Bond angles

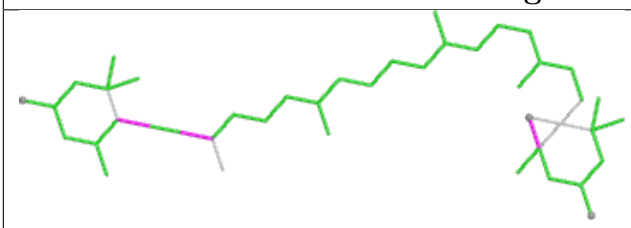


Torsions

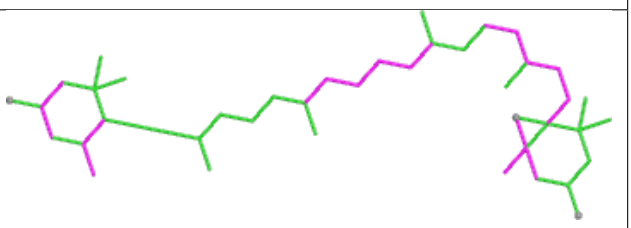


Rings

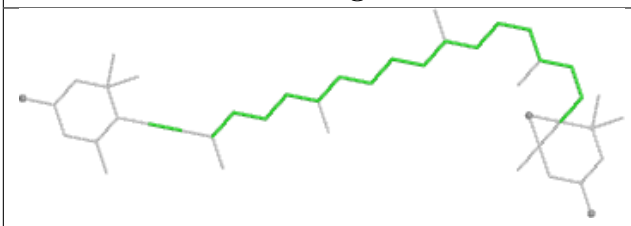
Ligand DD6 K 303



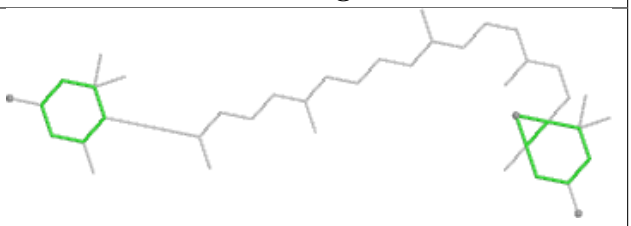
Bond lengths



Bond angles

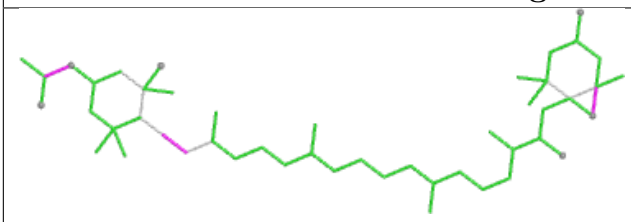


Torsions

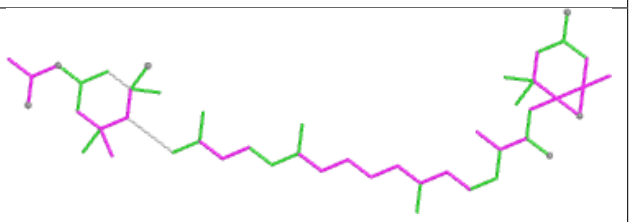


Rings

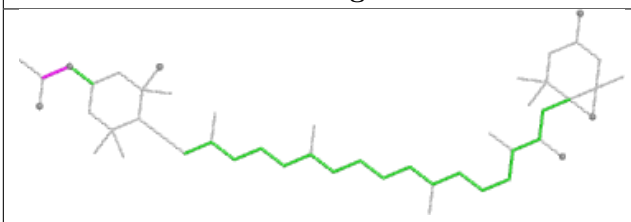
Ligand A86 V 301



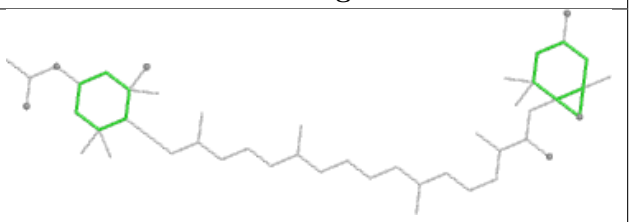
Bond lengths



Bond angles

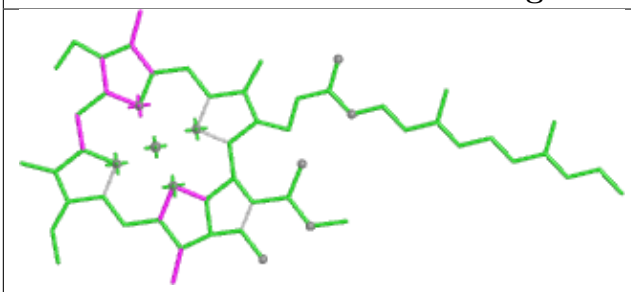


Torsions

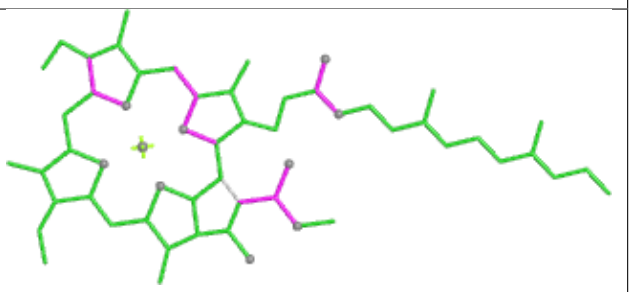


Rings

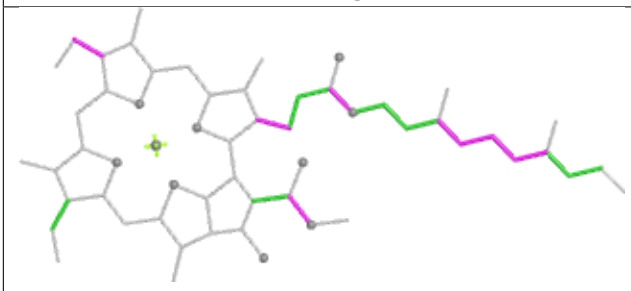
Ligand CLA F 313



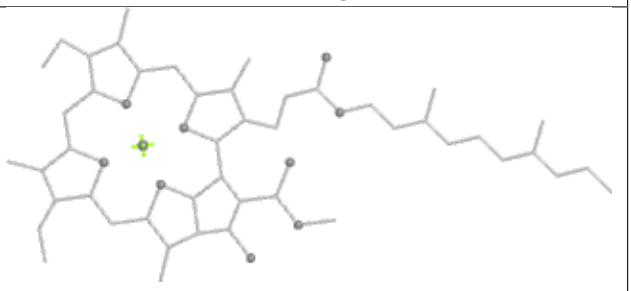
Bond lengths



Bond angles

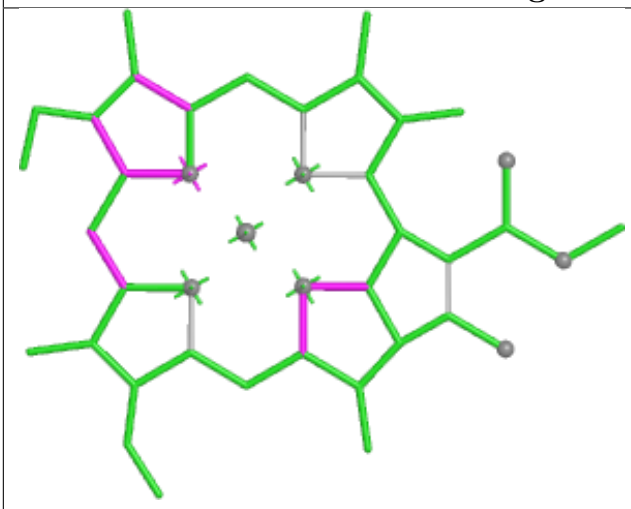


Torsions

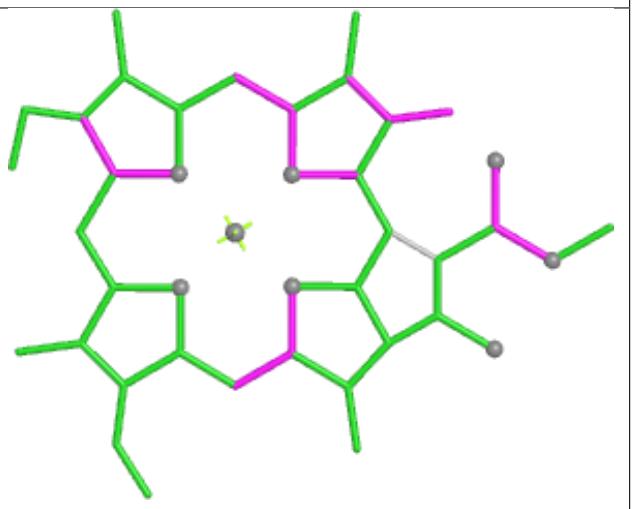


Rings

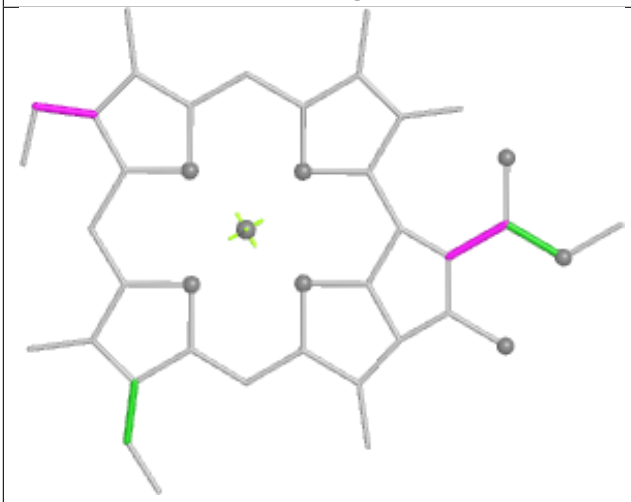
Ligand CLA 7 321



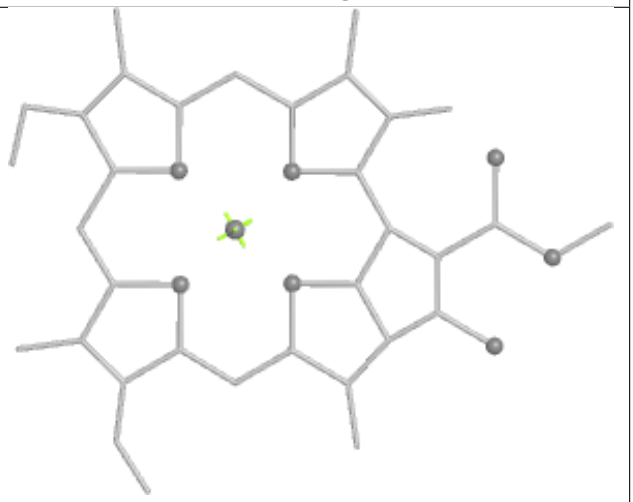
Bond lengths



Bond angles

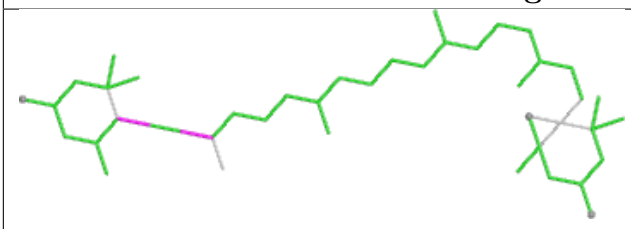


Torsions

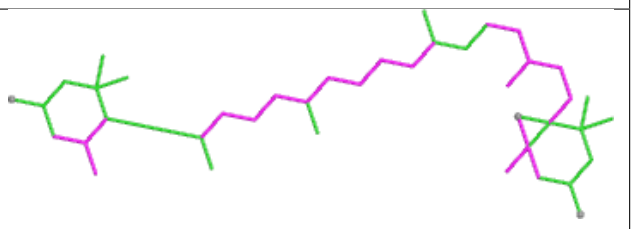


Rings

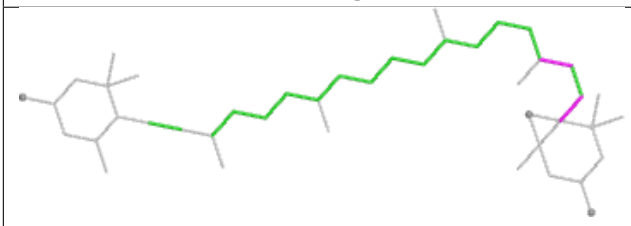
Ligand DD6 A 304



Bond lengths



Bond angles

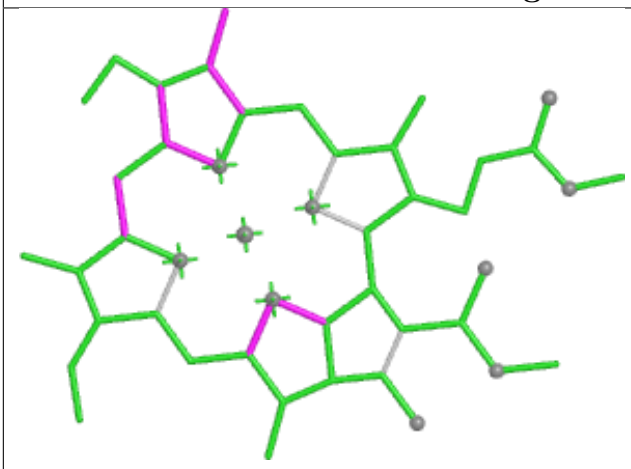


Torsions

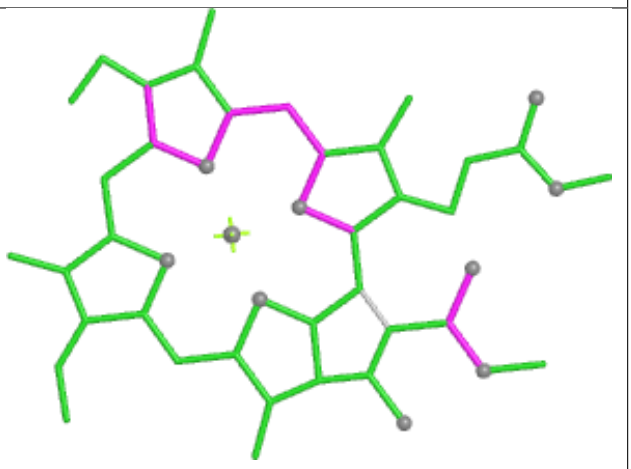


Rings

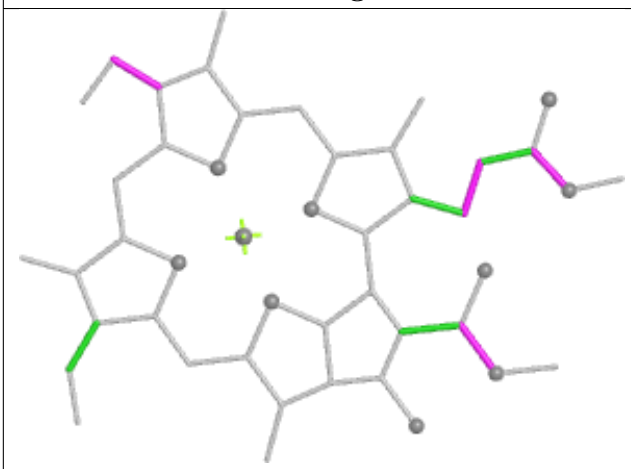
Ligand CLA U 212



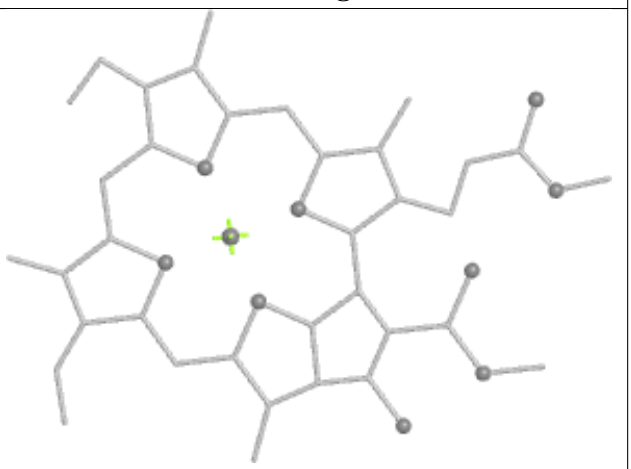
Bond lengths



Bond angles

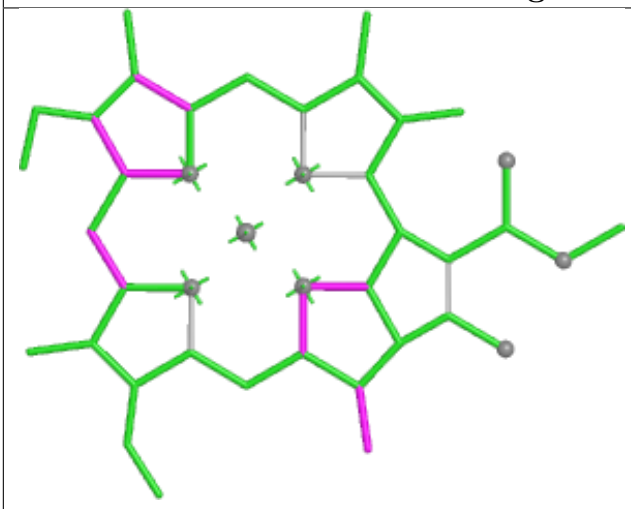


Torsions

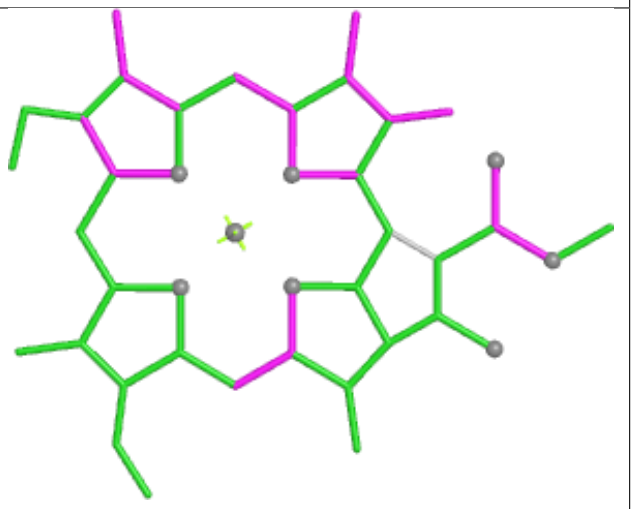


Rings

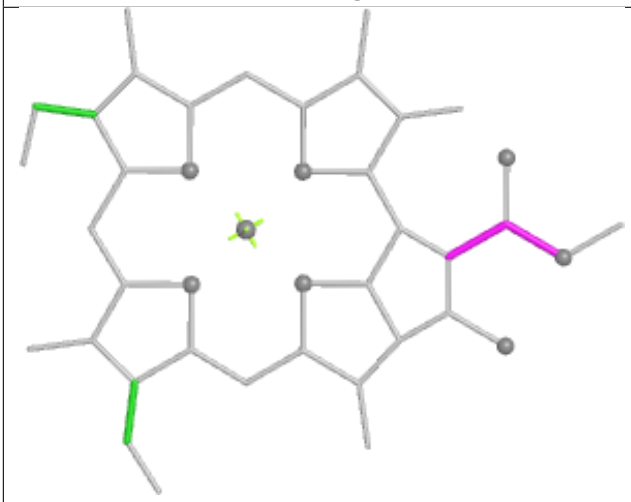
Ligand CLA x 307



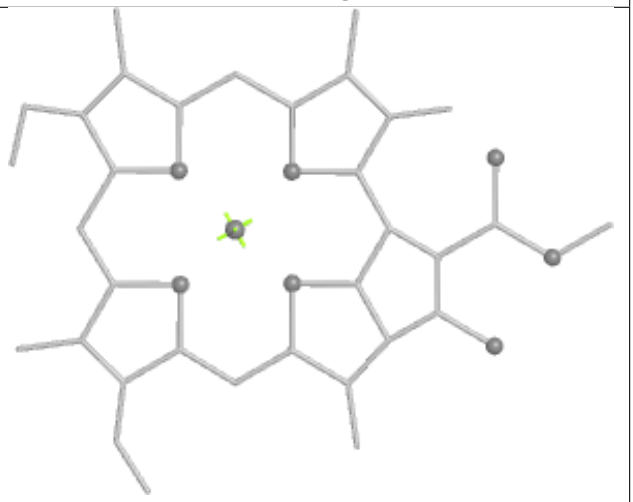
Bond lengths



Bond angles

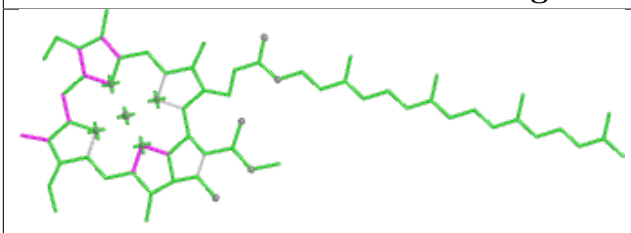


Torsions

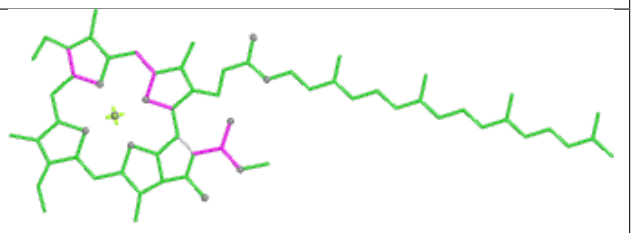


Rings

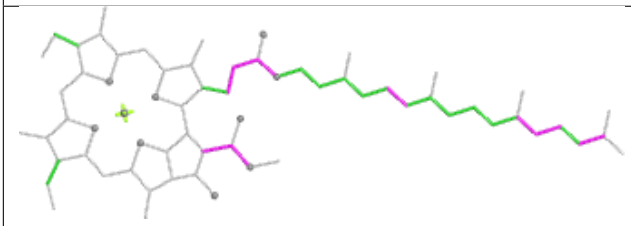
Ligand CLA I 311



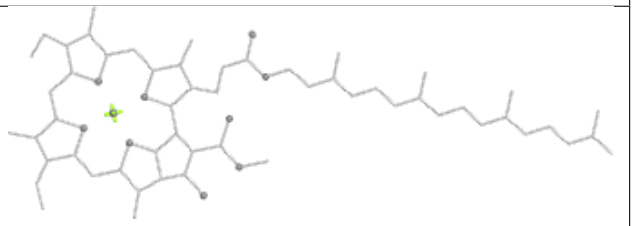
Bond lengths



Bond angles

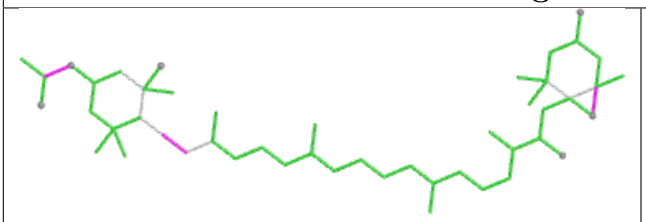


Torsions

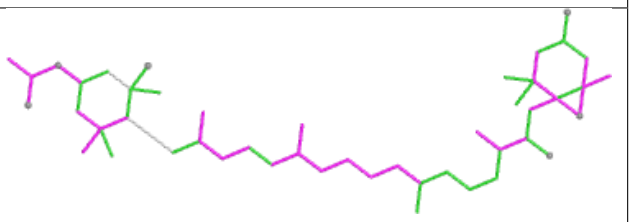


Rings

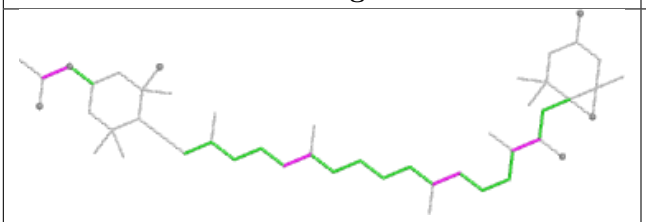
Ligand A86 Z 303



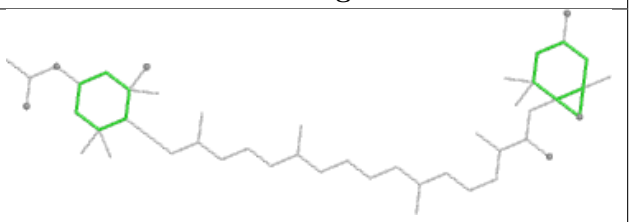
Bond lengths



Bond angles

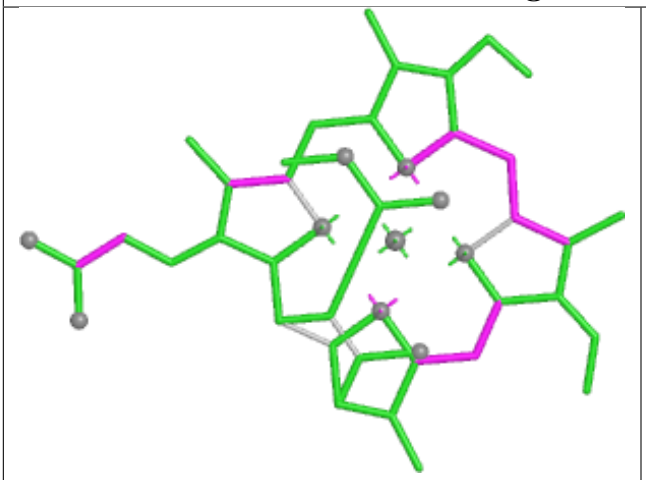


Torsions

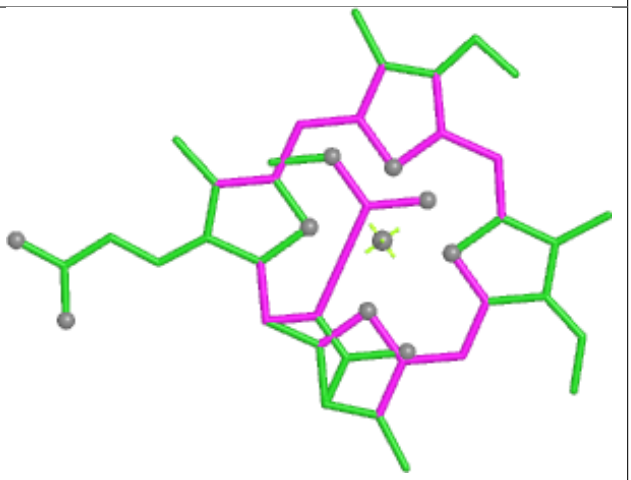


Rings

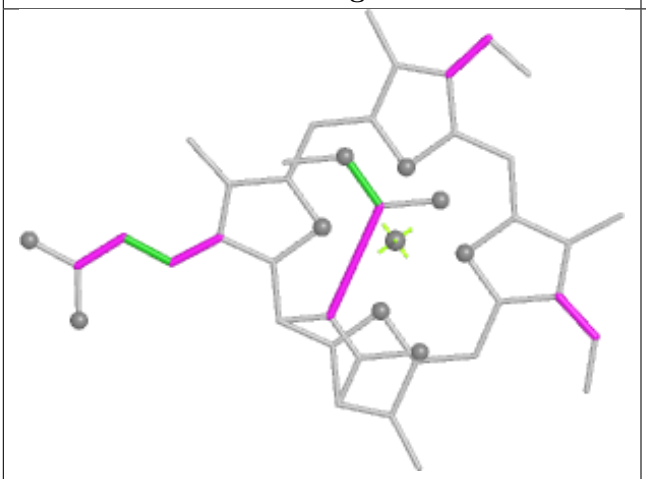
Ligand KC2 H 311



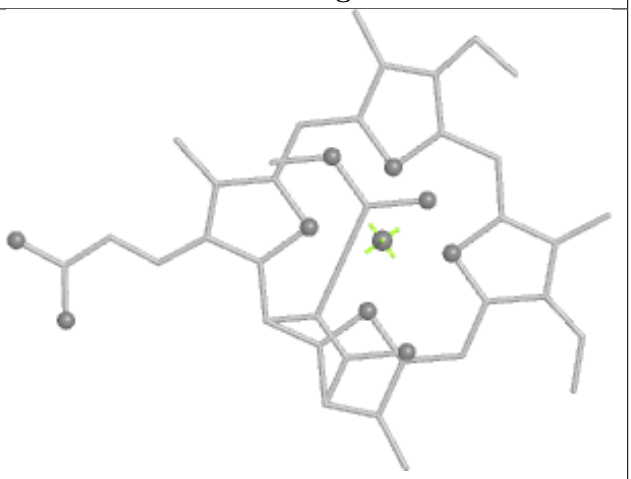
Bond lengths



Bond angles

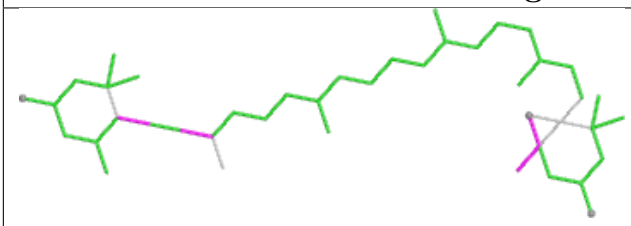


Torsions

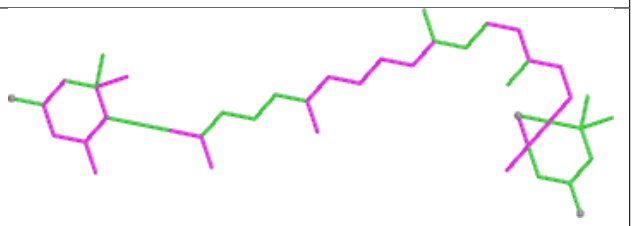


Rings

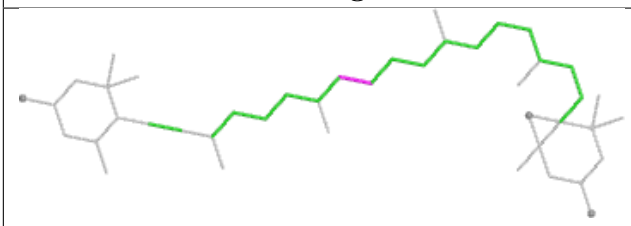
Ligand DD6 O 304



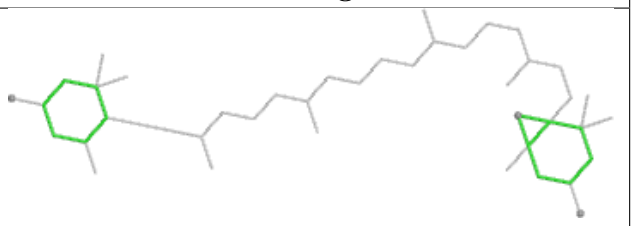
Bond lengths



Bond angles

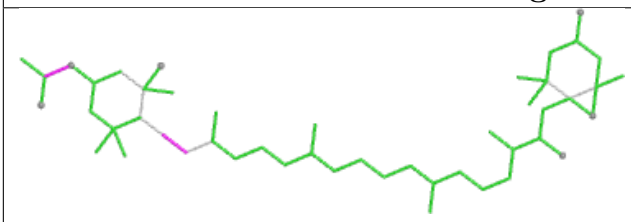


Torsions

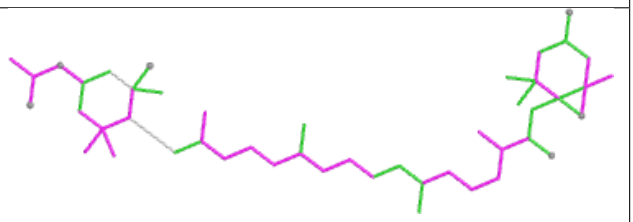


Rings

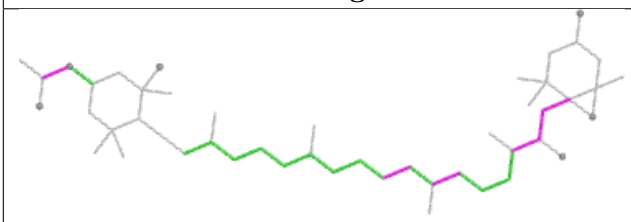
Ligand A86 O 307



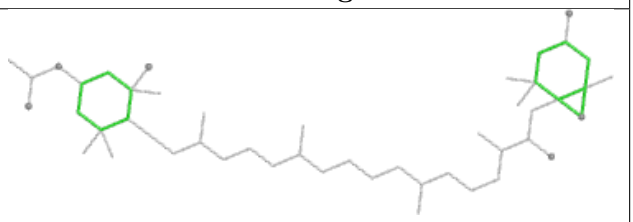
Bond lengths



Bond angles

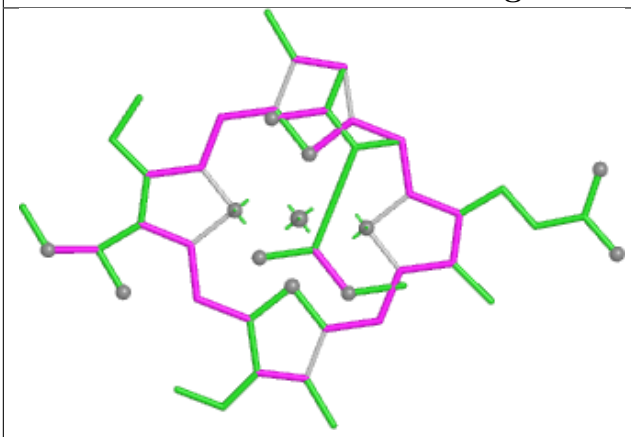


Torsions

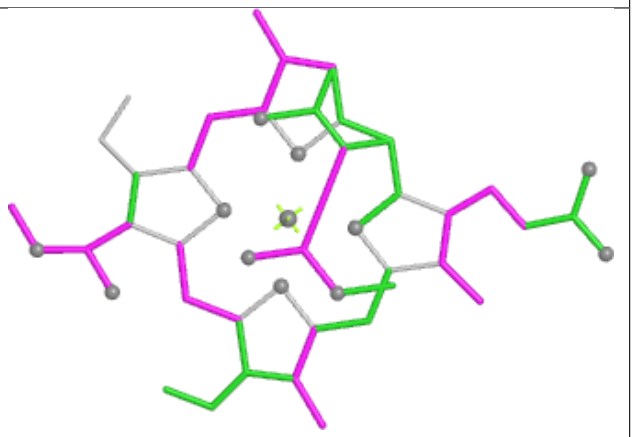


Rings

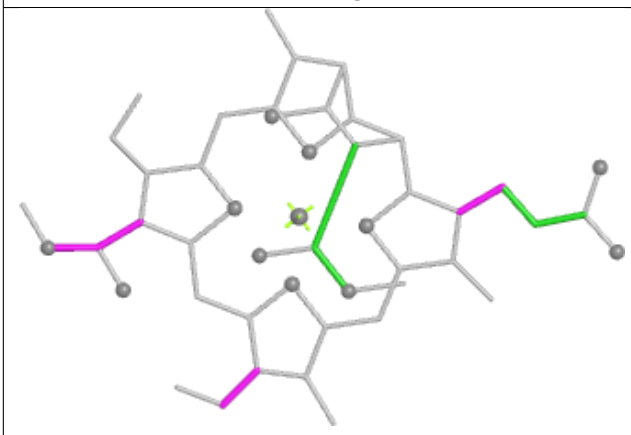
Ligand A1ECV x 316



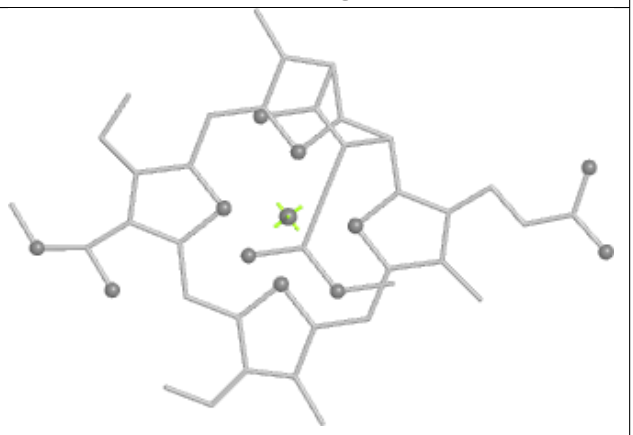
Bond lengths



Bond angles

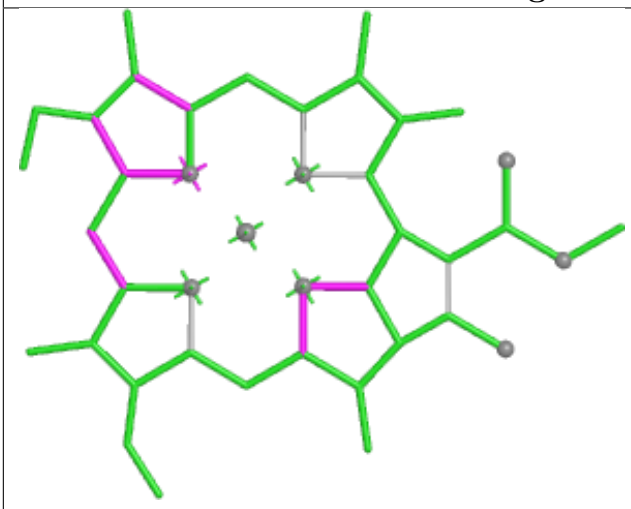


Torsions

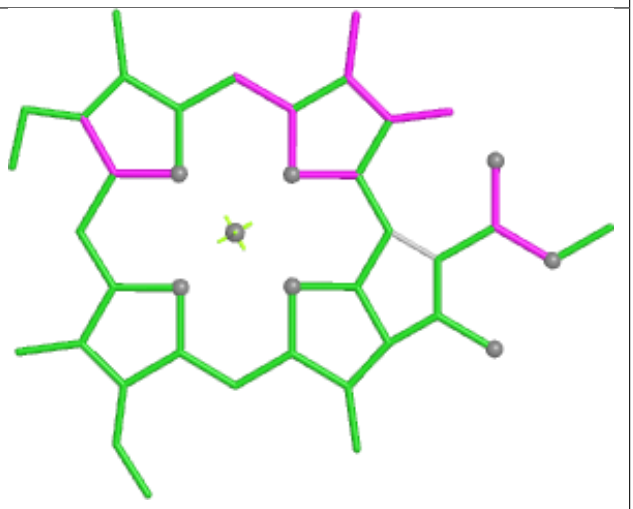


Rings

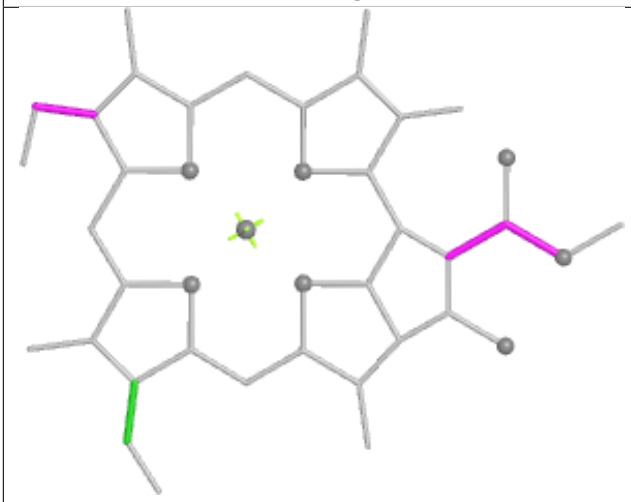
Ligand CLA 8 313



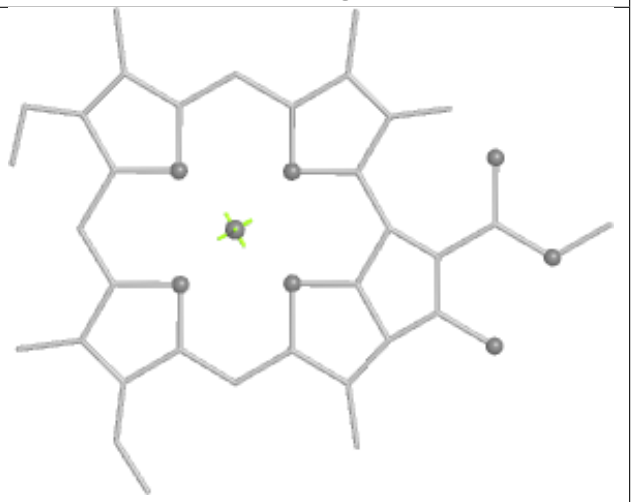
Bond lengths



Bond angles

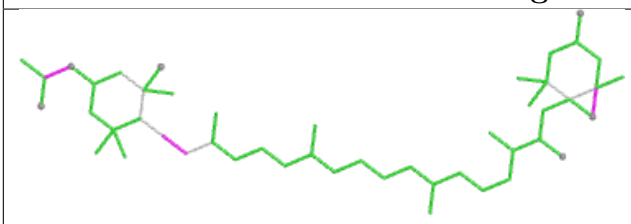


Torsions

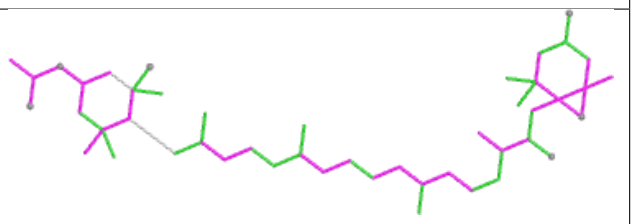


Rings

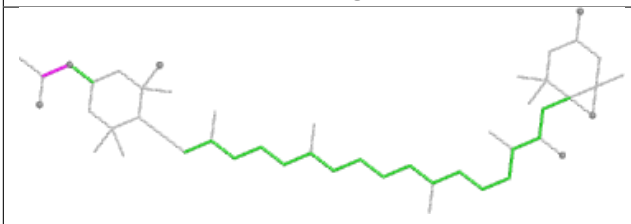
Ligand A86 T 301



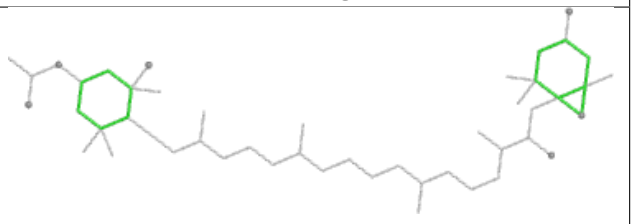
Bond lengths



Bond angles

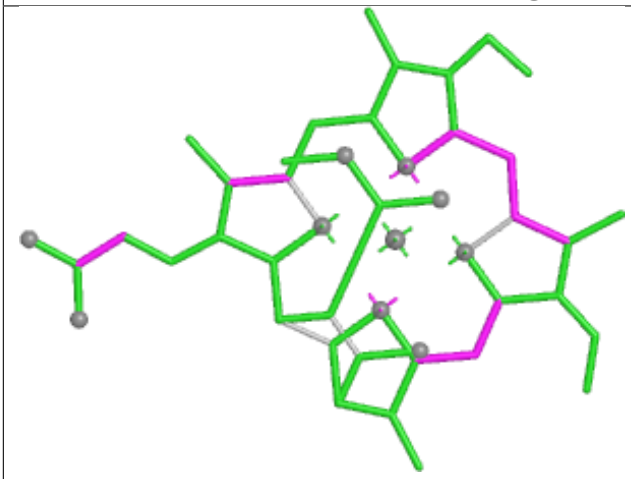


Torsions

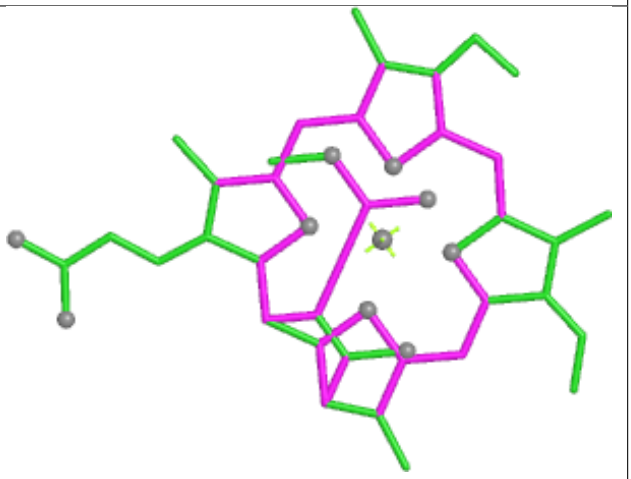


Rings

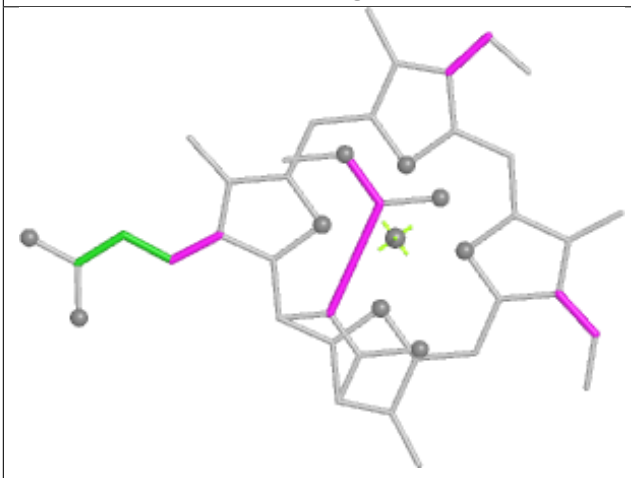
Ligand KC2 V 308



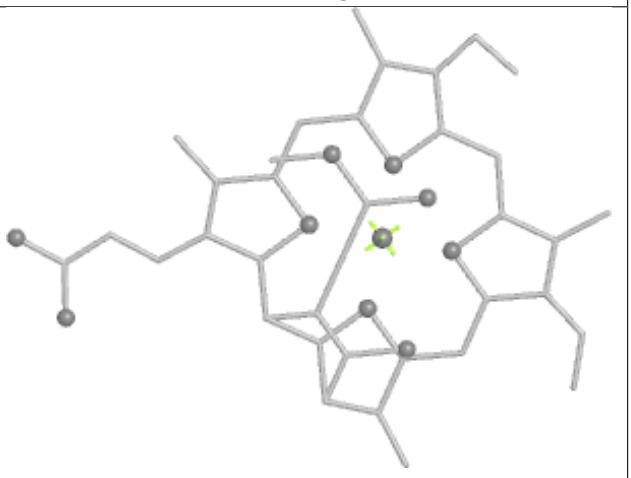
Bond lengths



Bond angles

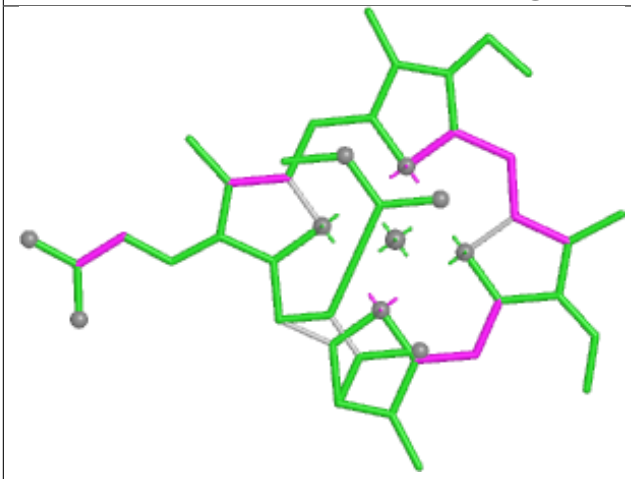


Torsions

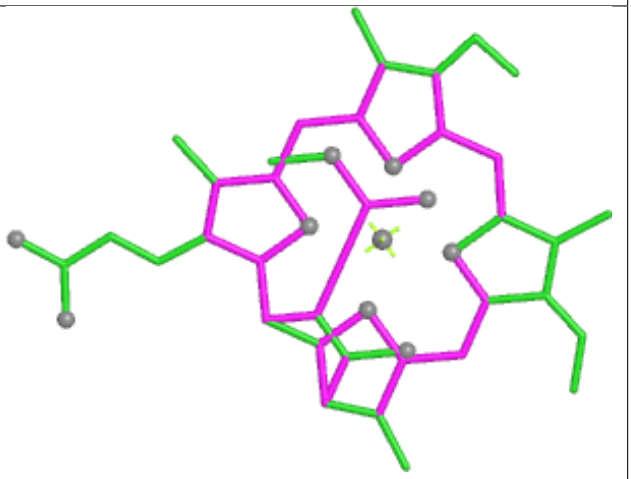


Rings

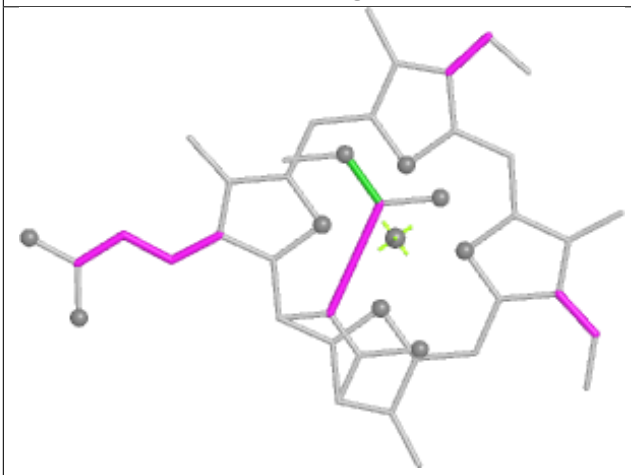
Ligand KC2 P 320



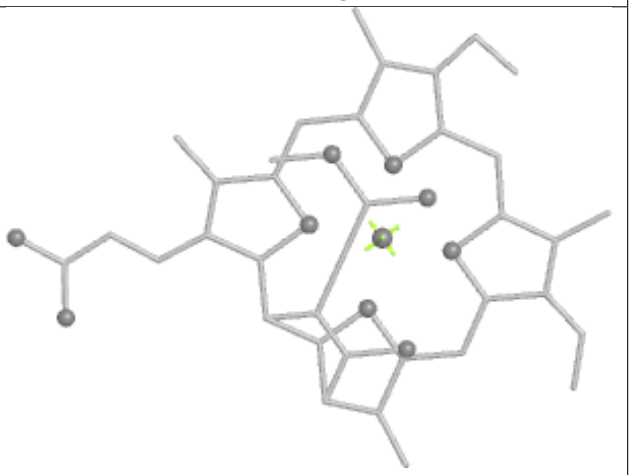
Bond lengths



Bond angles

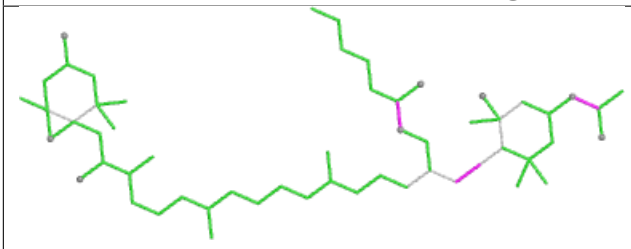


Torsions

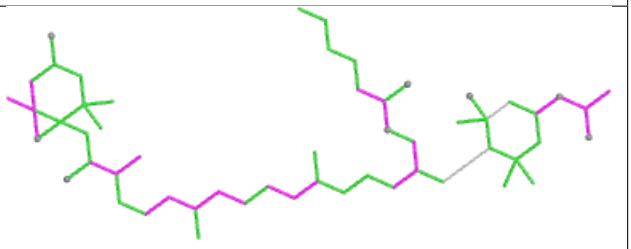


Rings

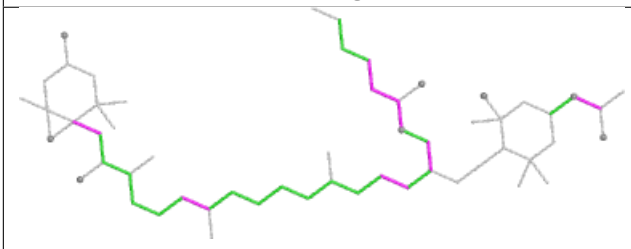
Ligand A1EB1 H 304



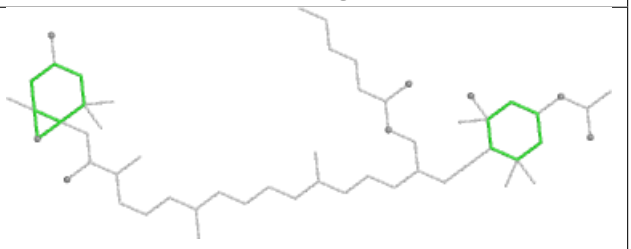
Bond lengths



Bond angles

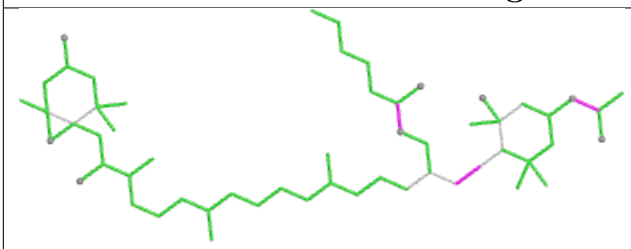


Torsions

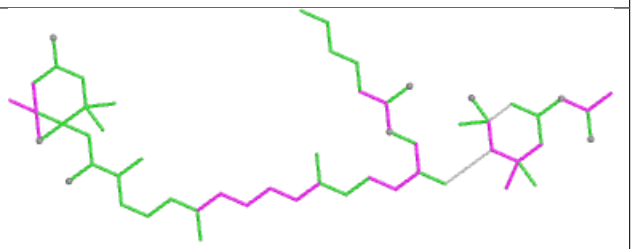


Rings

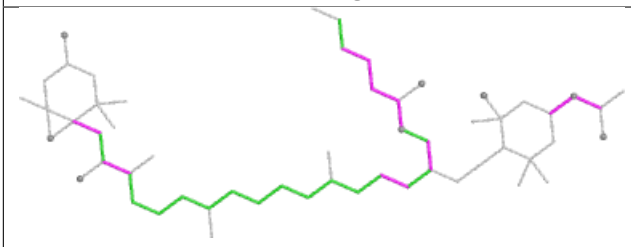
Ligand A1EB1 T 302



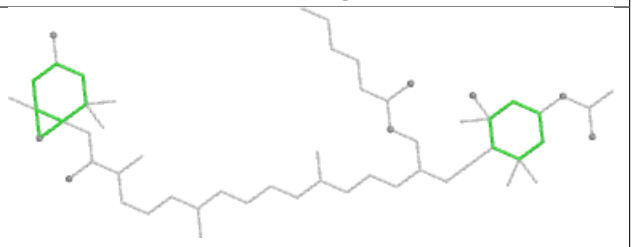
Bond lengths



Bond angles

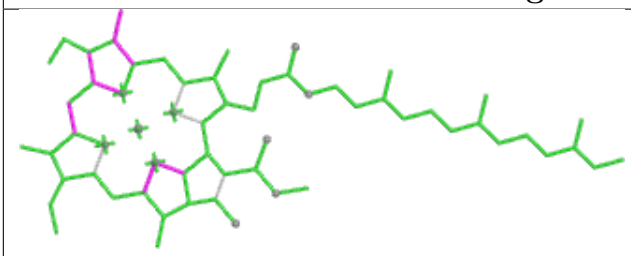


Torsions

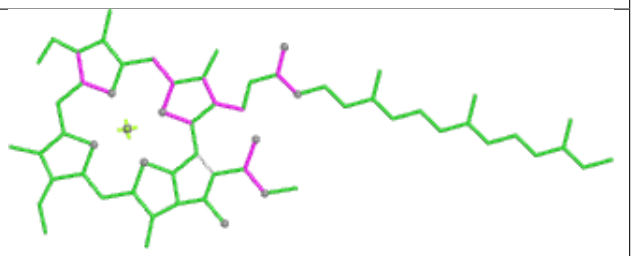


Rings

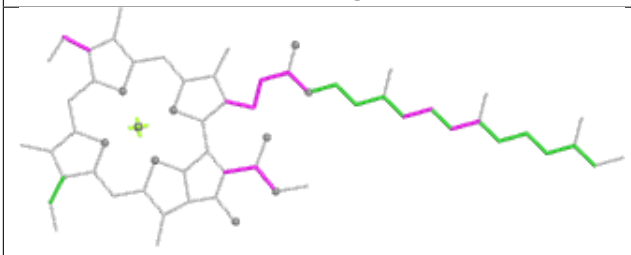
Ligand CLA L 308



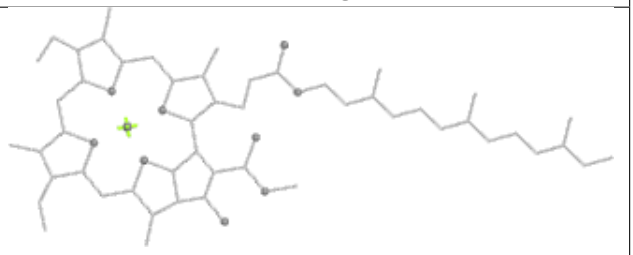
Bond lengths



Bond angles

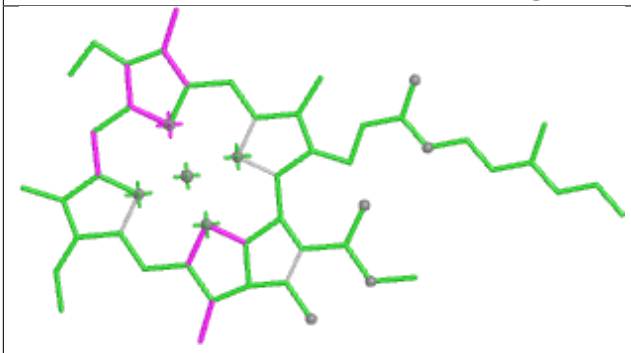


Torsions

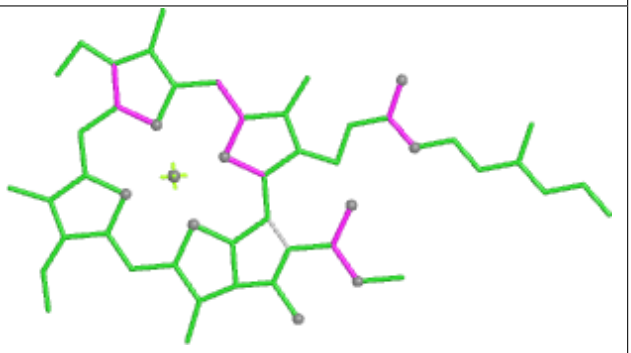


Rings

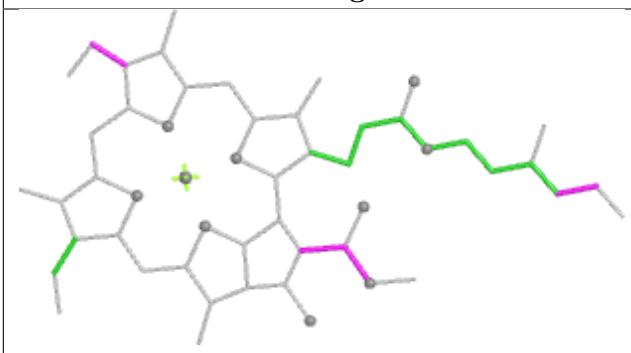
Ligand CLA k 201



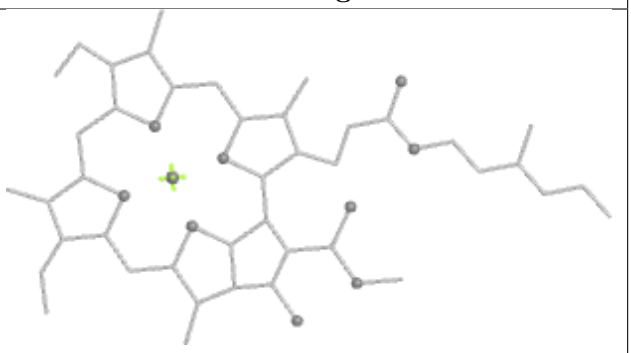
Bond lengths



Bond angles

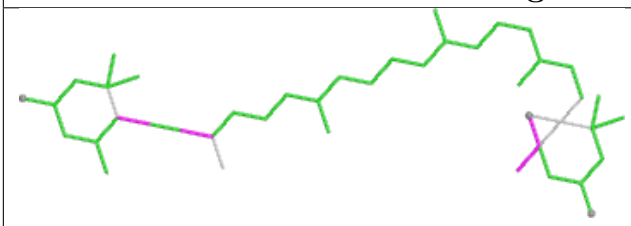


Torsions

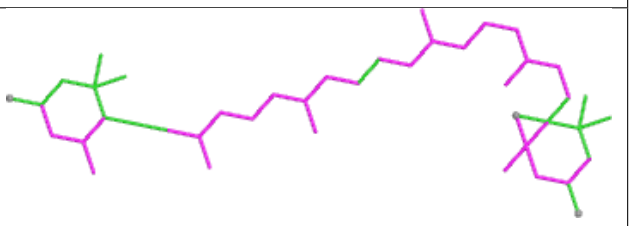


Rings

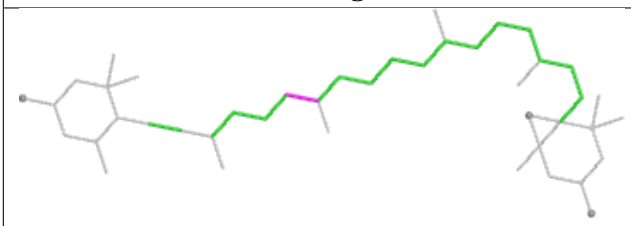
Ligand DD6 Z 302



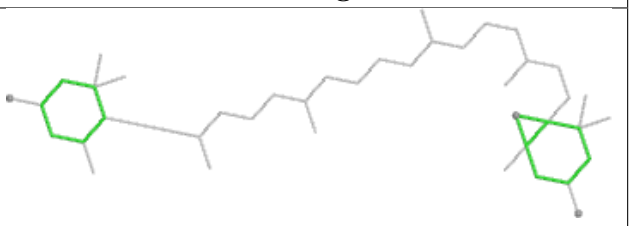
Bond lengths



Bond angles

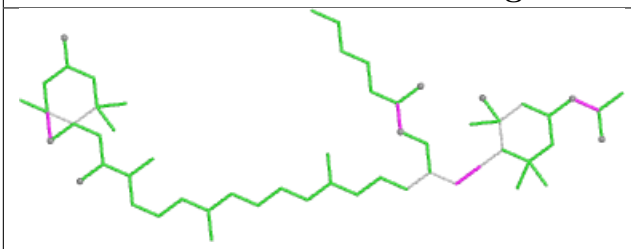


Torsions

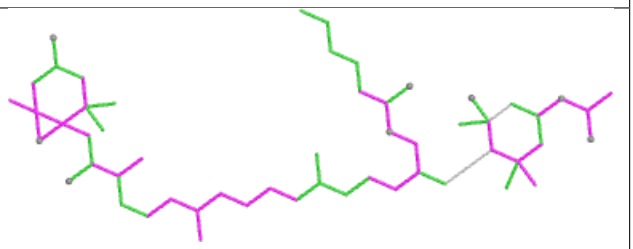


Rings

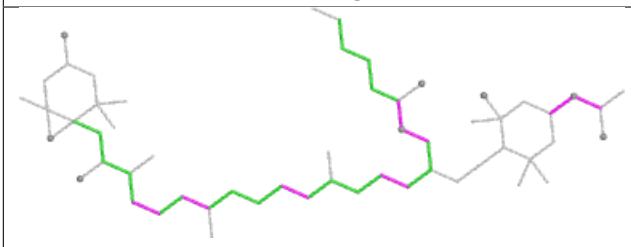
Ligand A1EB1 V 307



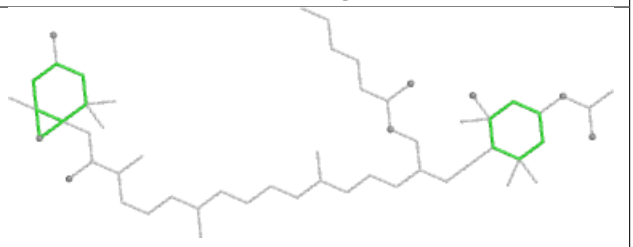
Bond lengths



Bond angles

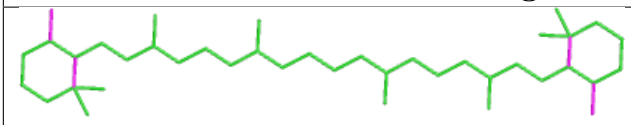


Torsions

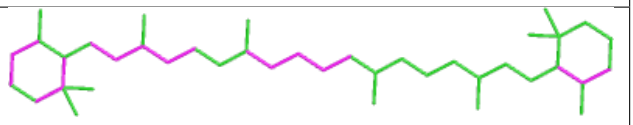


Rings

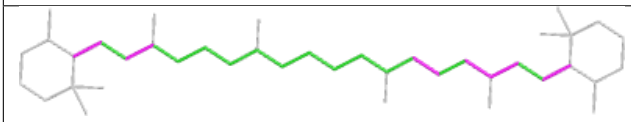
Ligand BCR m 101



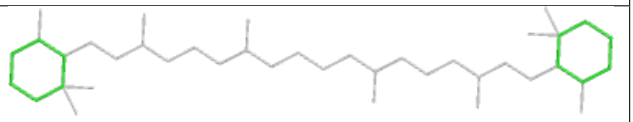
Bond lengths



Bond angles

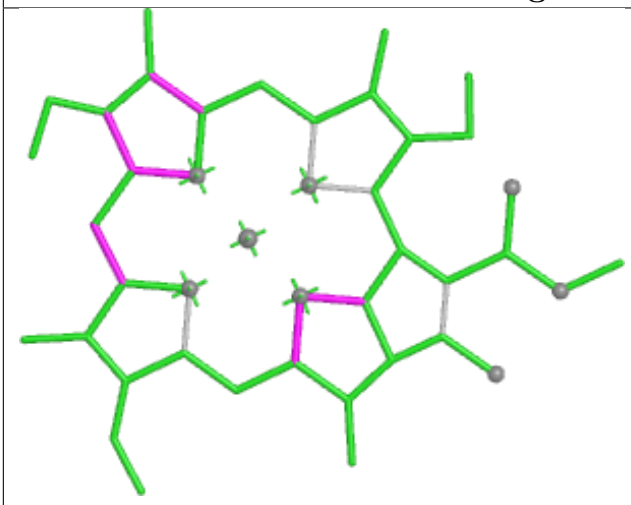


Torsions

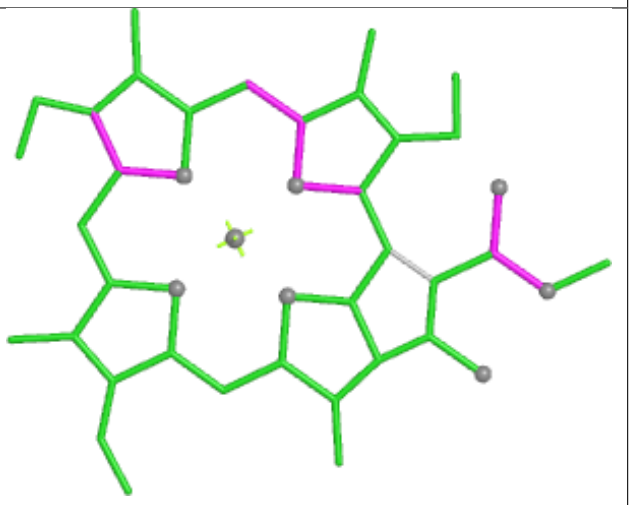


Rings

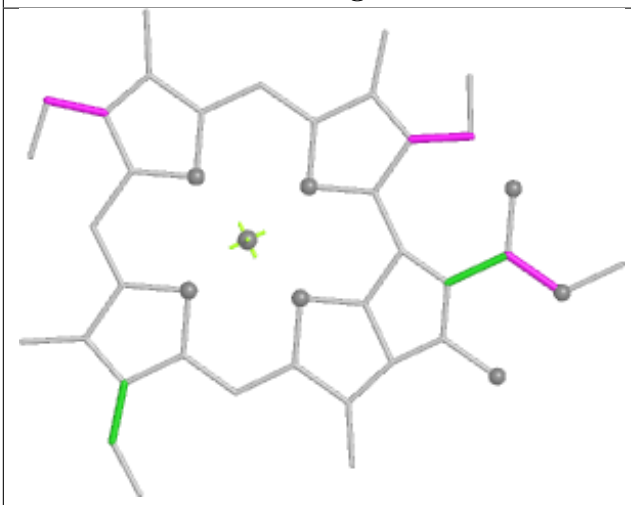
Ligand CLA 6 313



Bond lengths



Bond angles

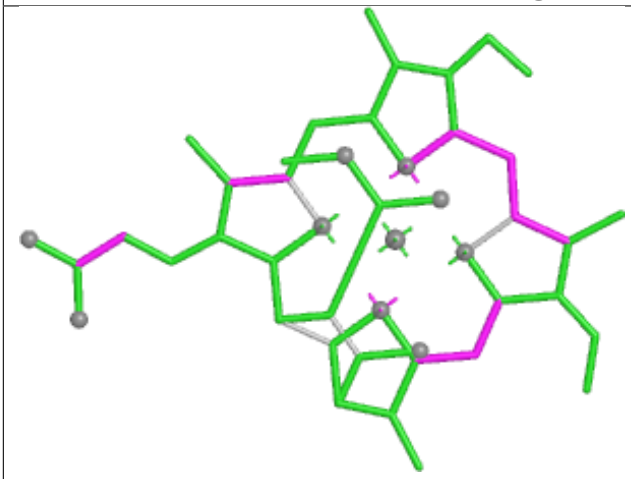


Torsions

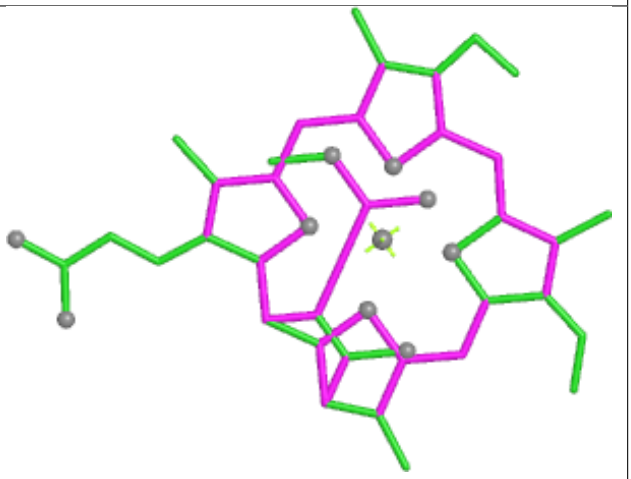


Rings

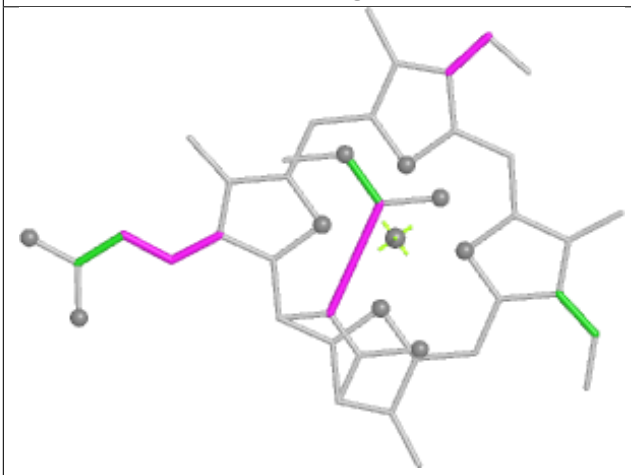
Ligand KC2 5 311



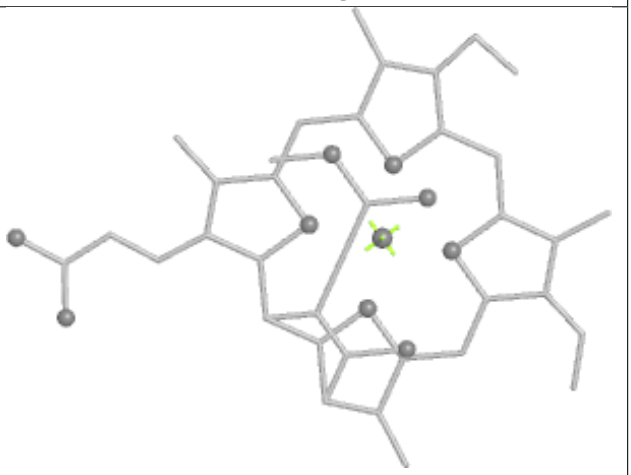
Bond lengths



Bond angles

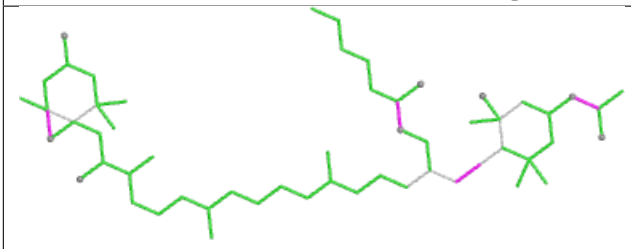


Torsions

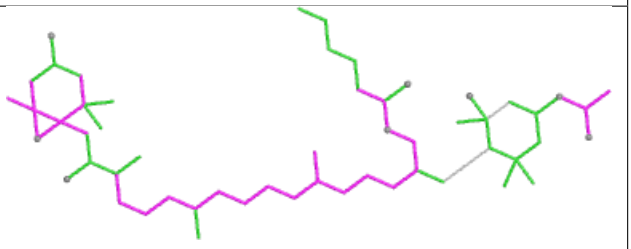


Rings

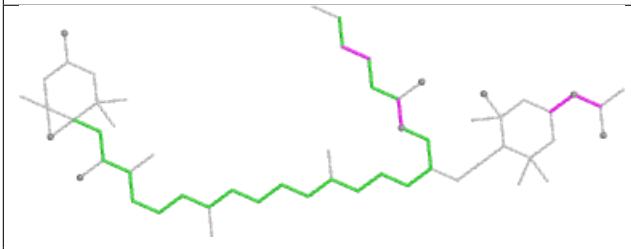
Ligand A1EB1 T 307



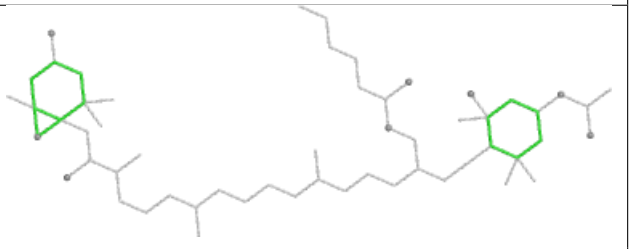
Bond lengths



Bond angles

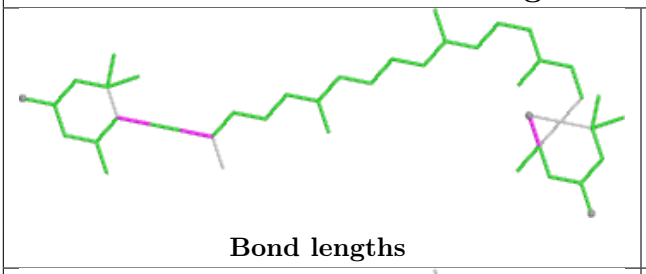


Torsions

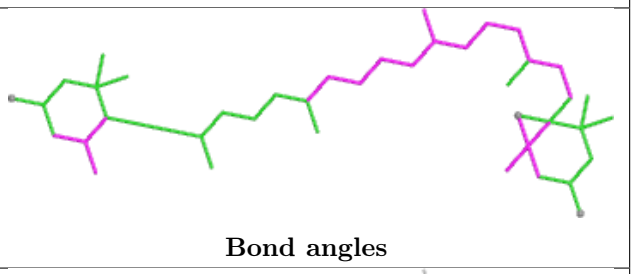


Rings

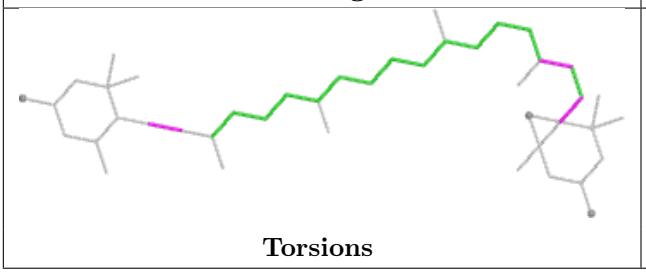
Ligand DD6 G 306



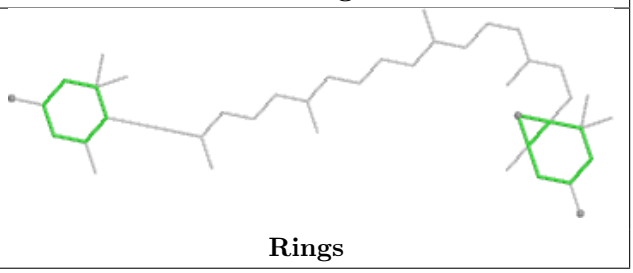
Bond lengths



Bond angles

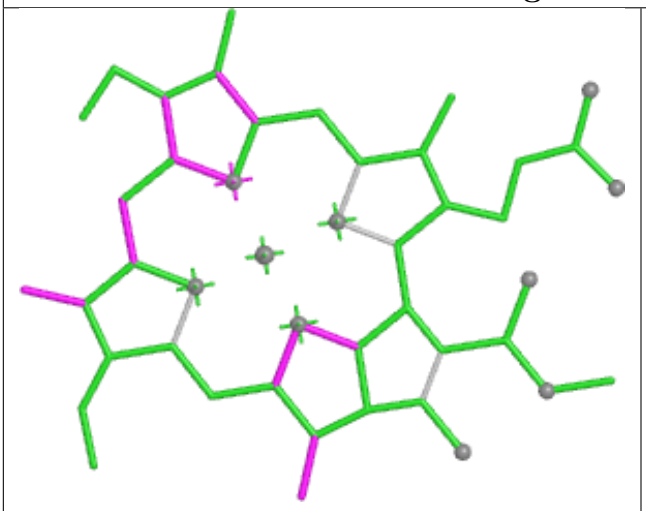


Torsions

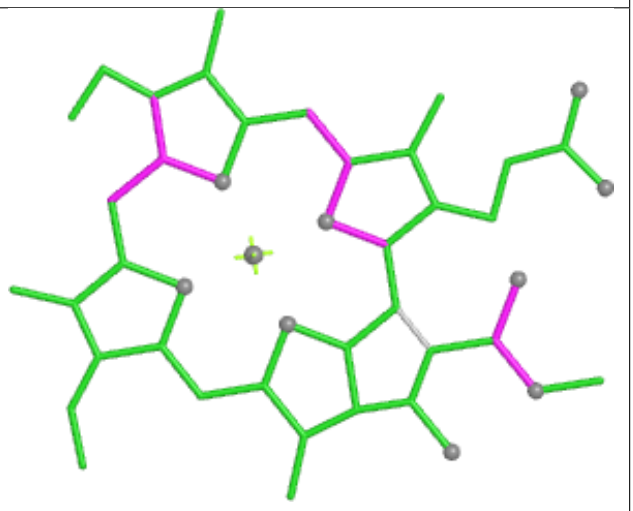


Rings

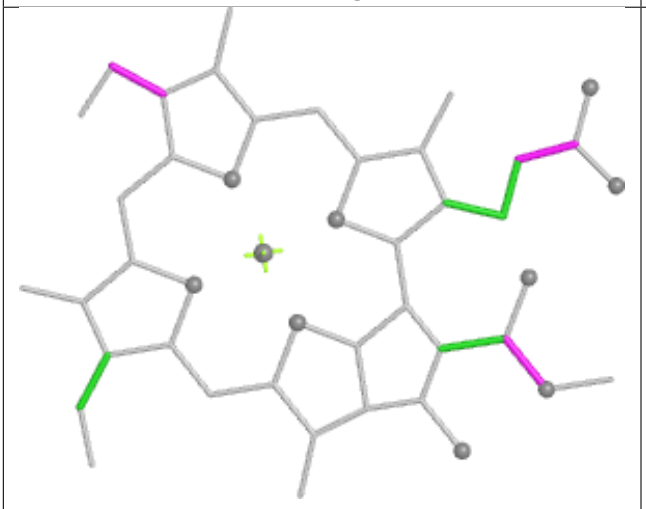
Ligand CLA O 309



Bond lengths



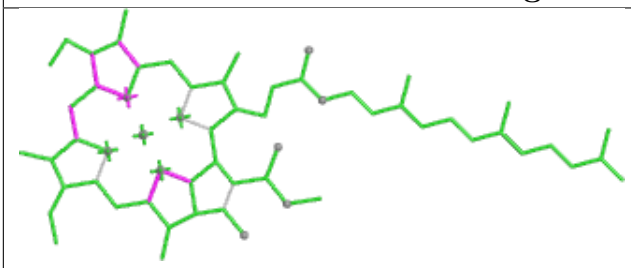
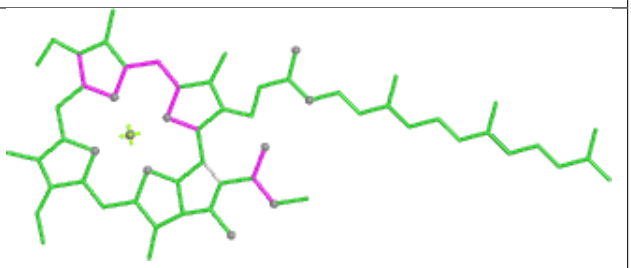
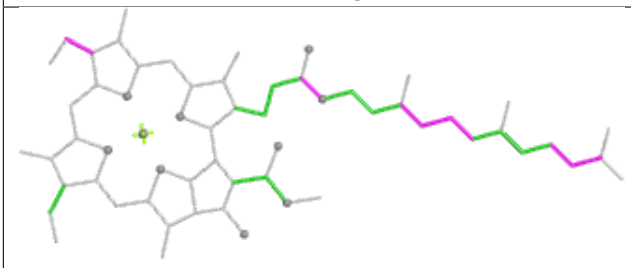
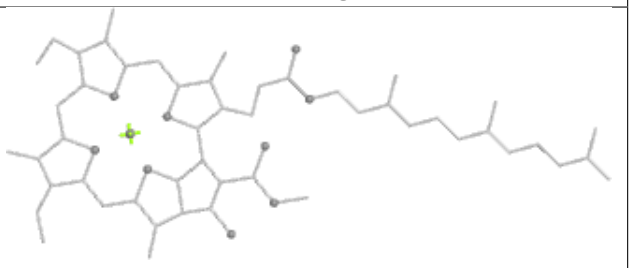
Bond angles

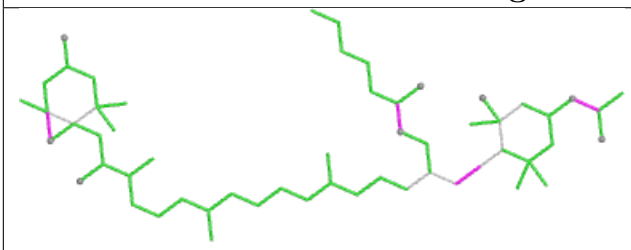
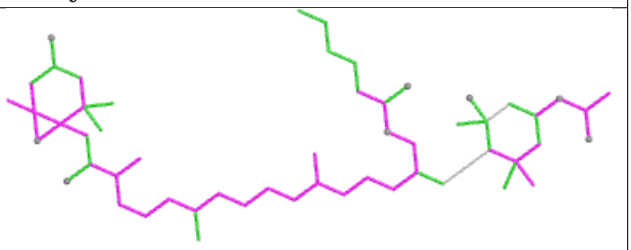
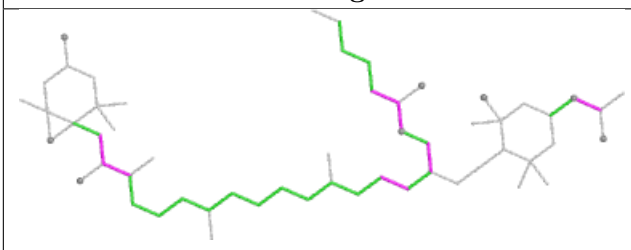
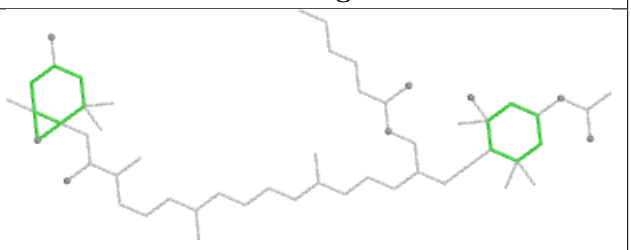


Torsions

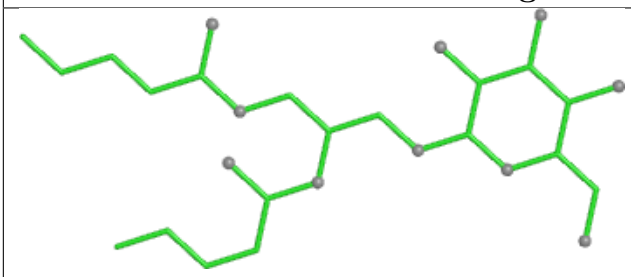


Rings

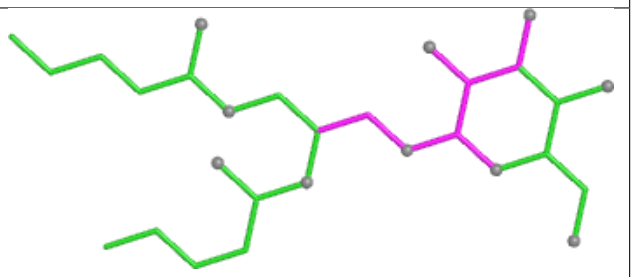
Ligand CLA R 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EB1 y 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

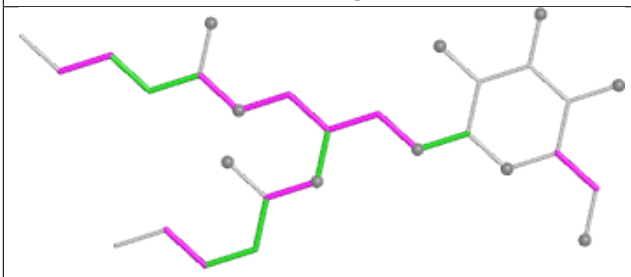
Ligand LMG A 316



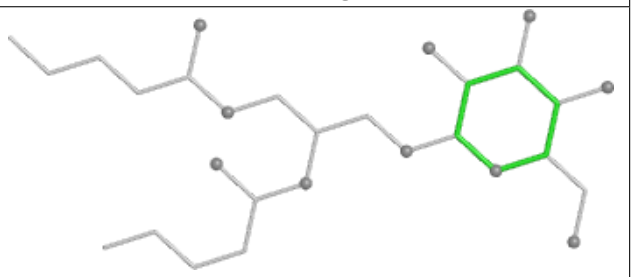
Bond lengths



Bond angles

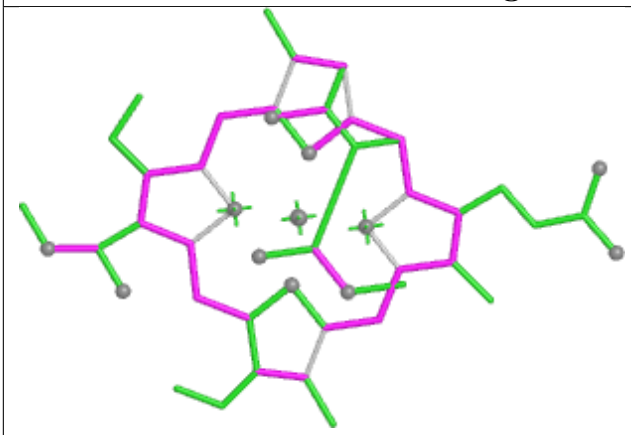


Torsions

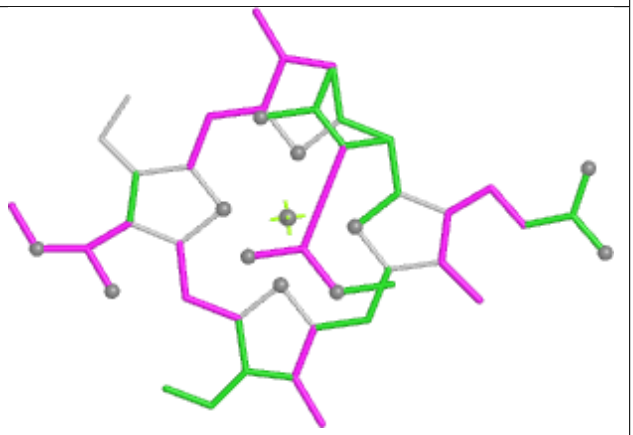


Rings

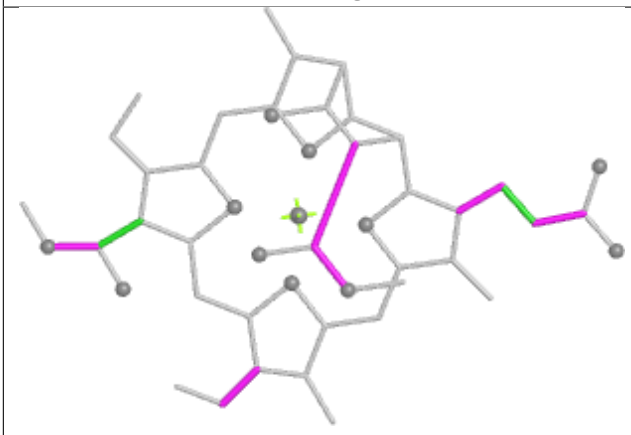
Ligand A1ECV Z 308



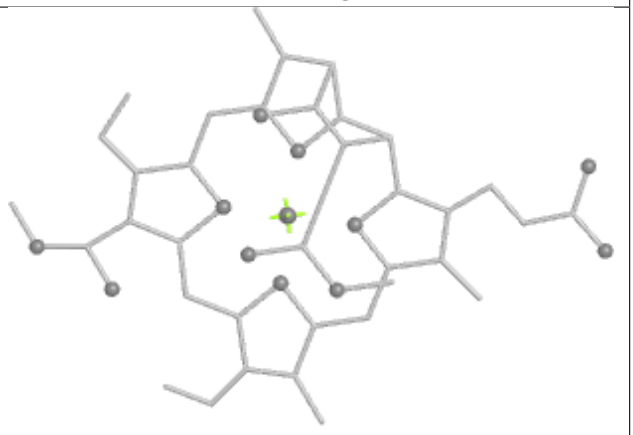
Bond lengths



Bond angles

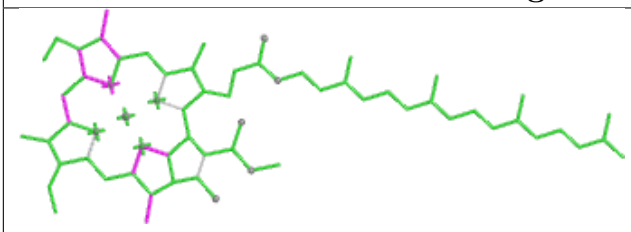


Torsions

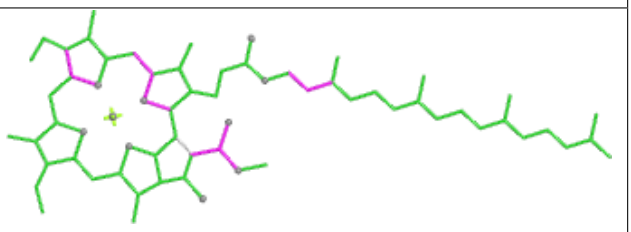


Rings

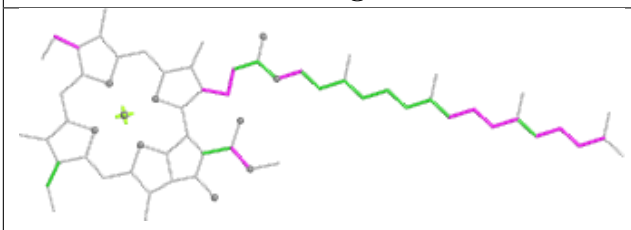
Ligand CLA S 320



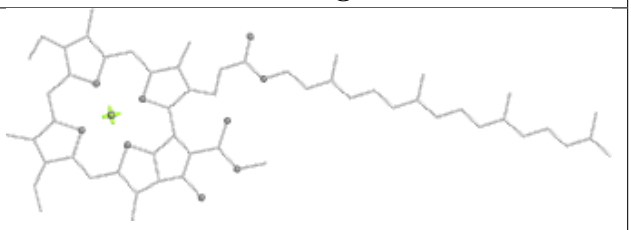
Bond lengths



Bond angles

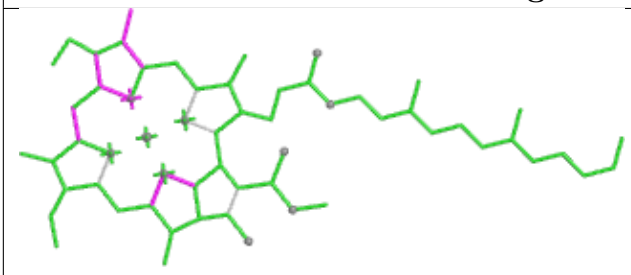


Torsions

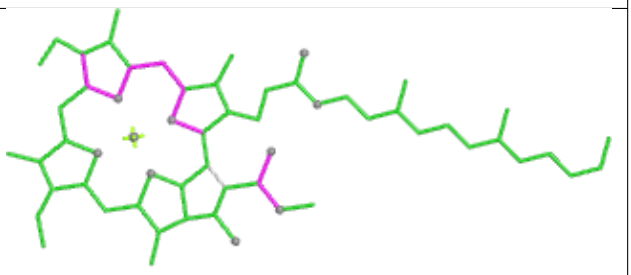


Rings

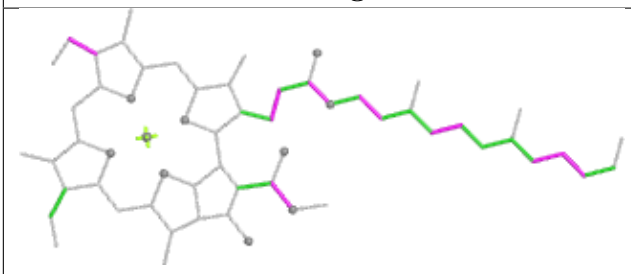
Ligand CLA b 819



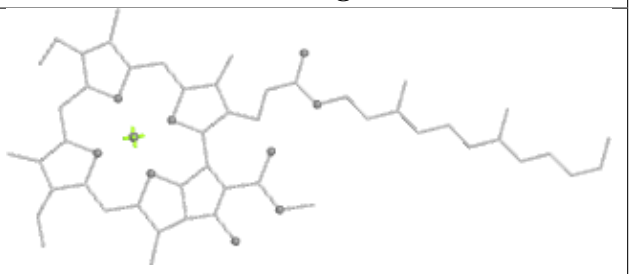
Bond lengths



Bond angles

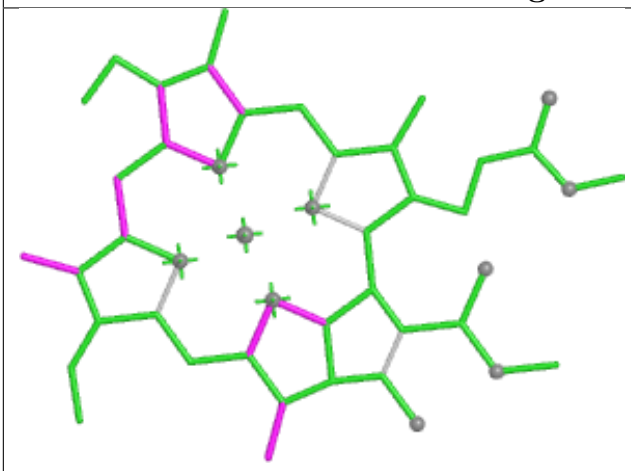


Torsions

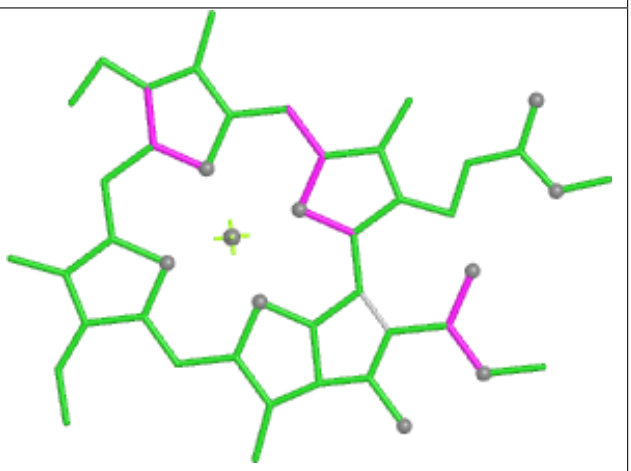


Rings

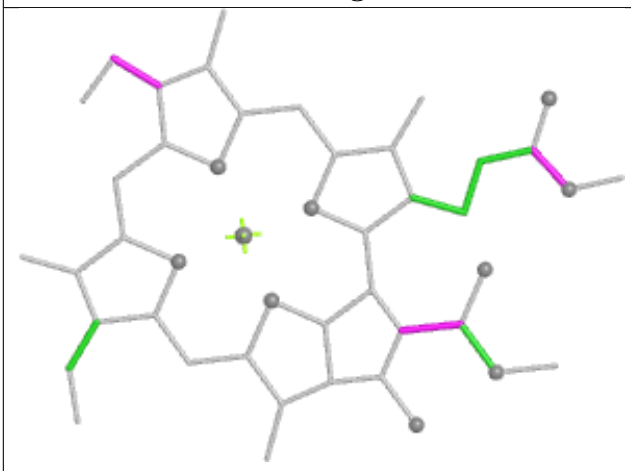
Ligand CLA 7 318



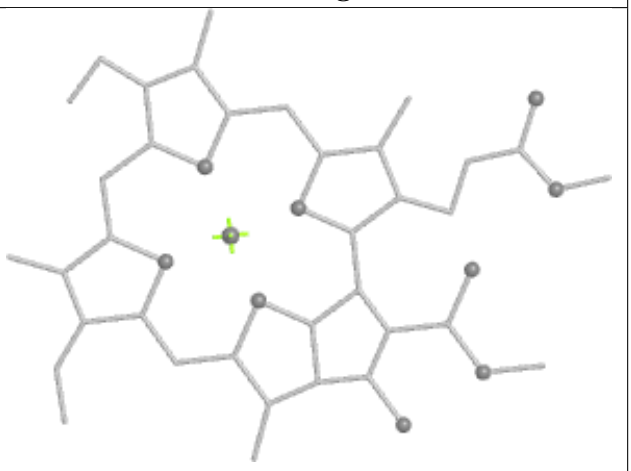
Bond lengths



Bond angles

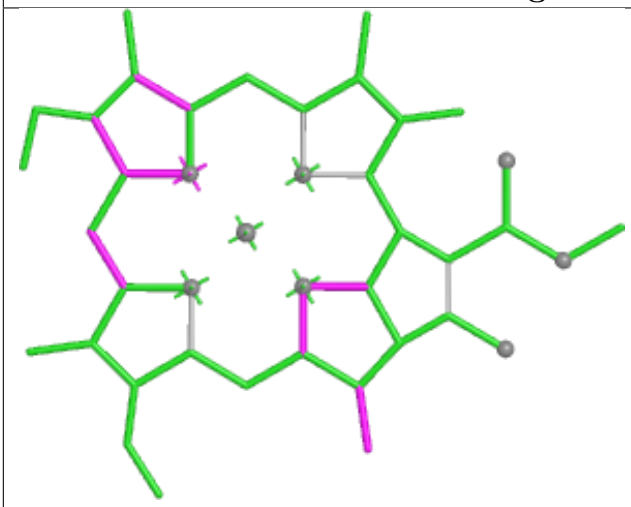


Torsions

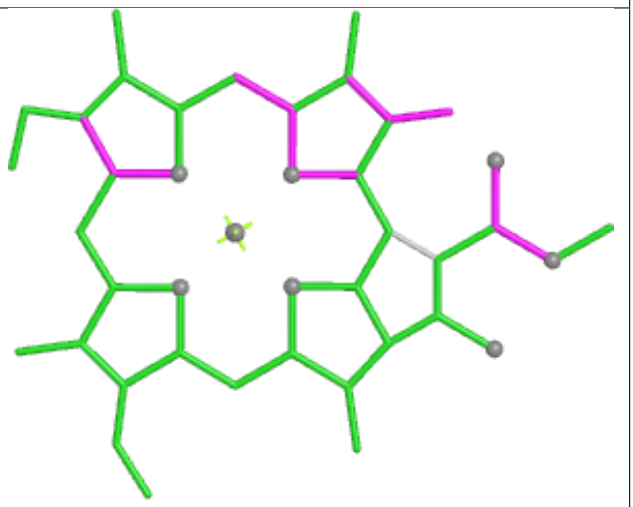


Rings

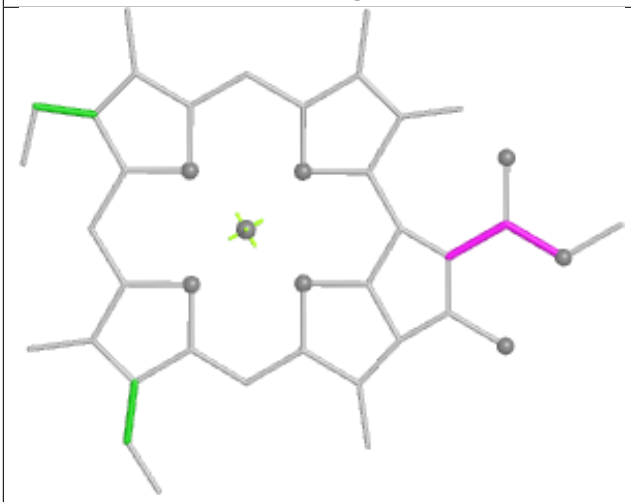
Ligand CLA 9 309



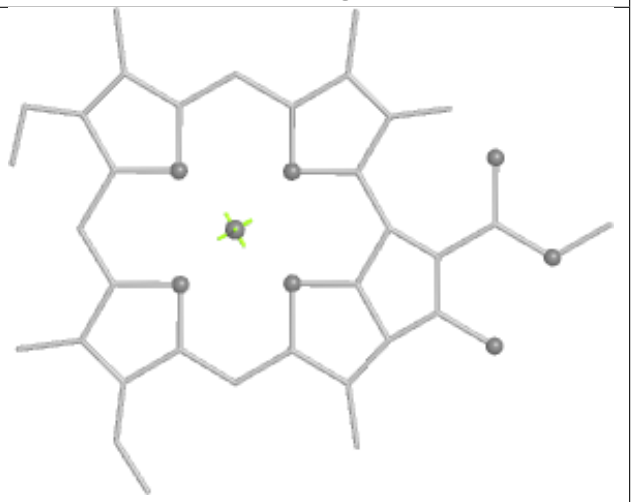
Bond lengths



Bond angles

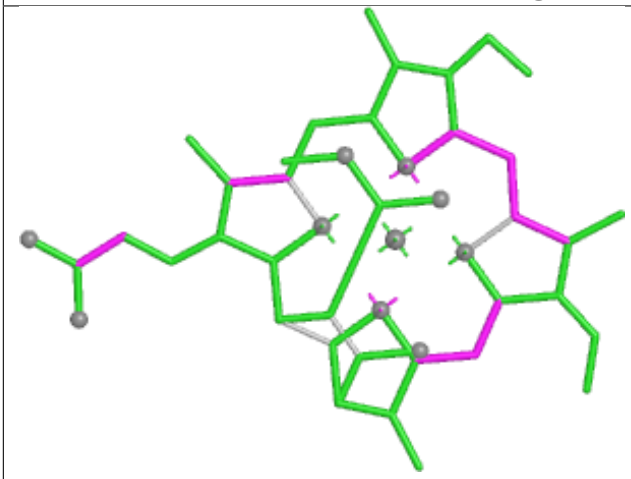


Torsions

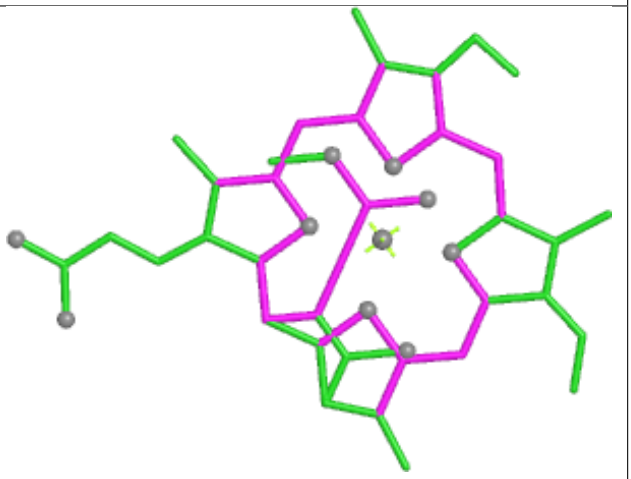


Rings

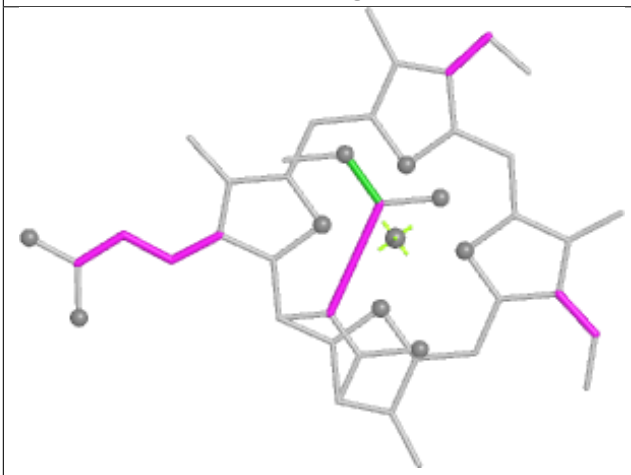
Ligand KC2 4 318



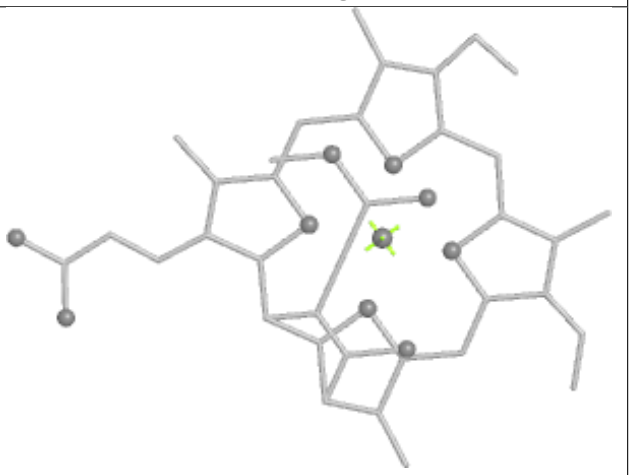
Bond lengths



Bond angles

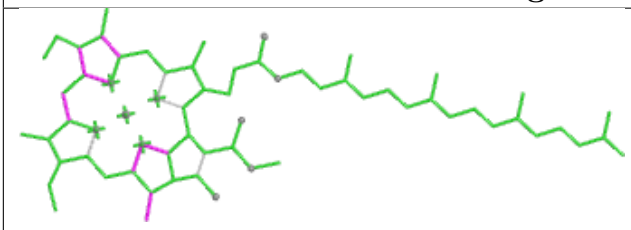


Torsions

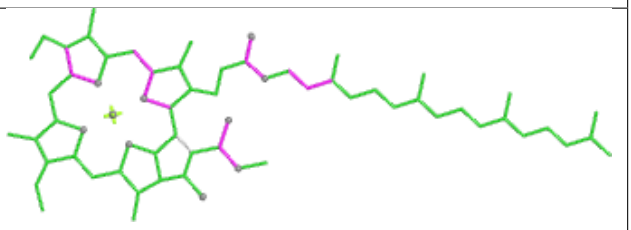


Rings

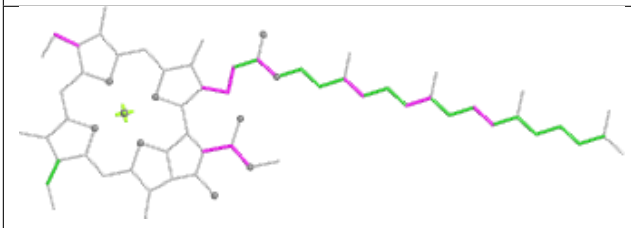
Ligand CLA b 828



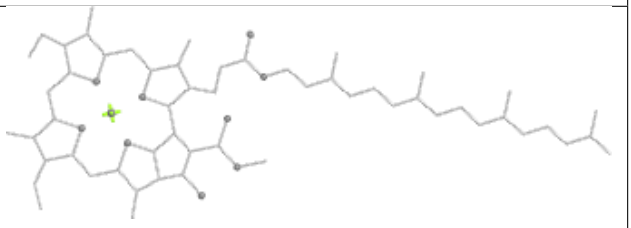
Bond lengths



Bond angles

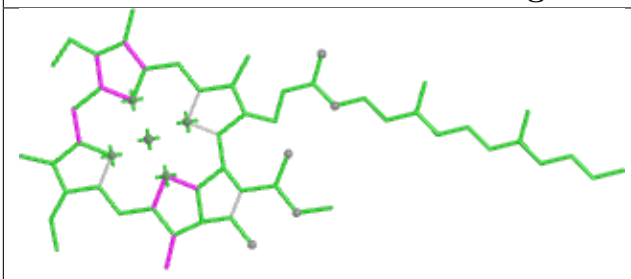


Torsions

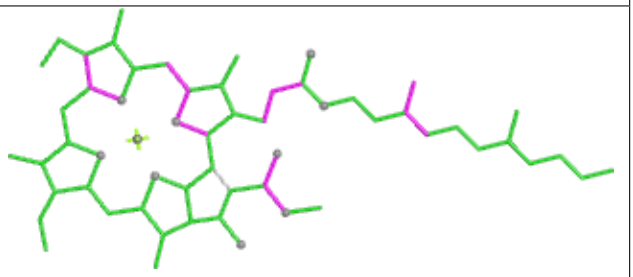


Rings

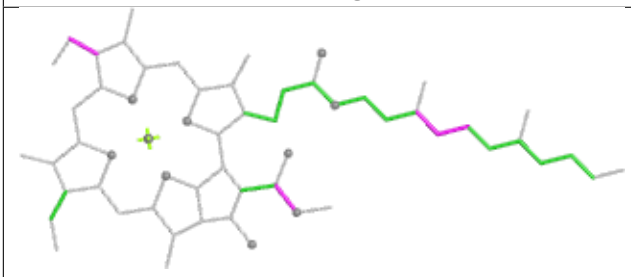
Ligand CLA b 834



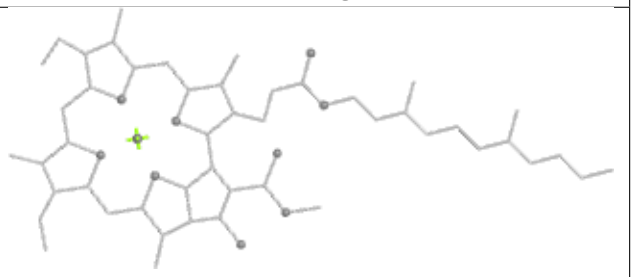
Bond lengths



Bond angles

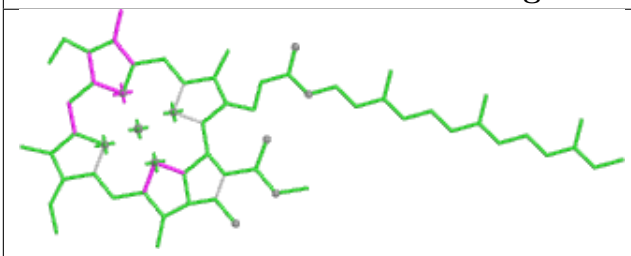


Torsions

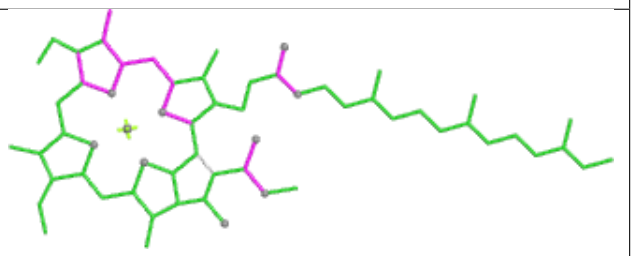


Rings

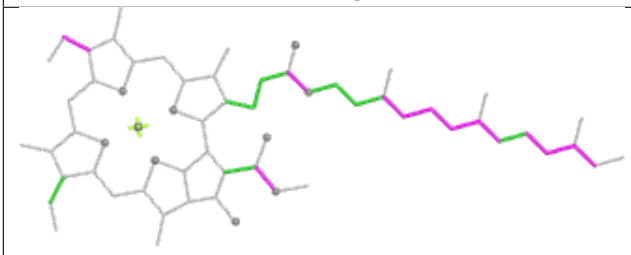
Ligand CLA D 310



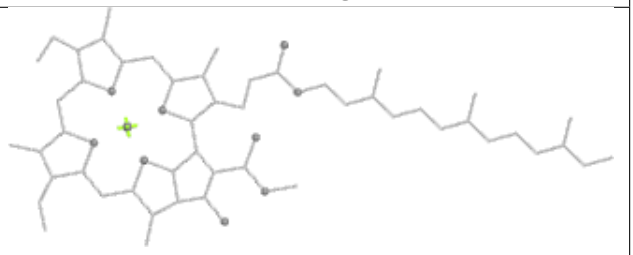
Bond lengths



Bond angles

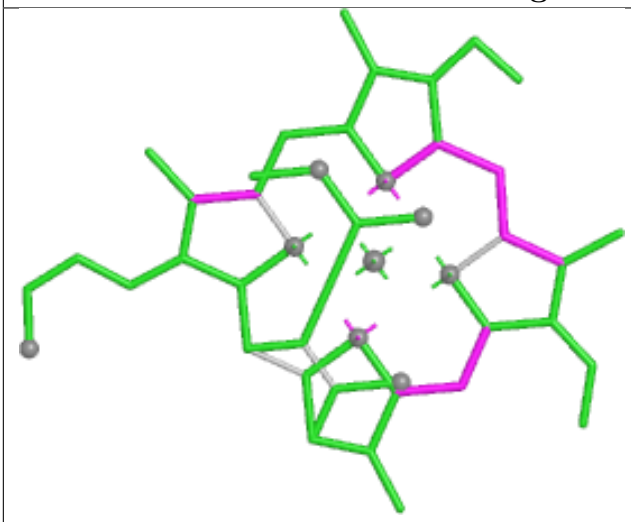


Torsions



Rings

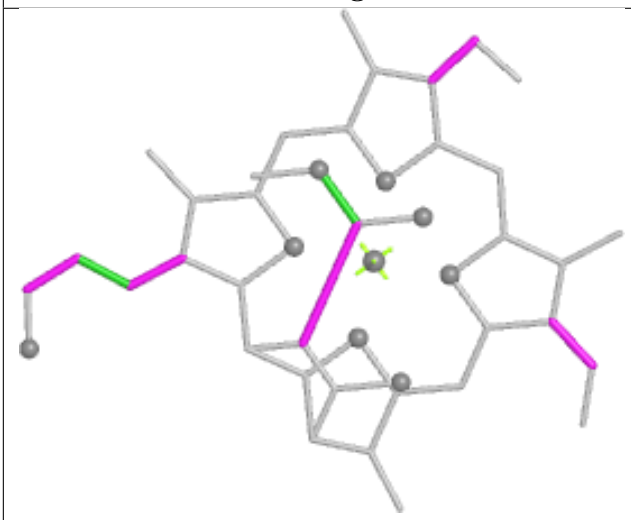
Ligand KC2 0 314



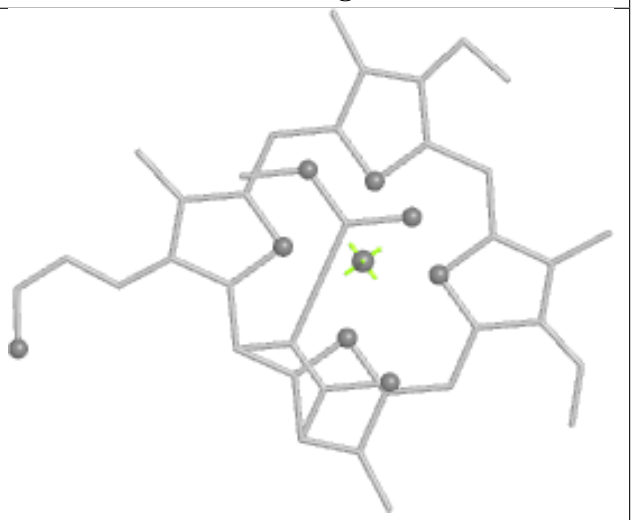
Bond lengths



Bond angles

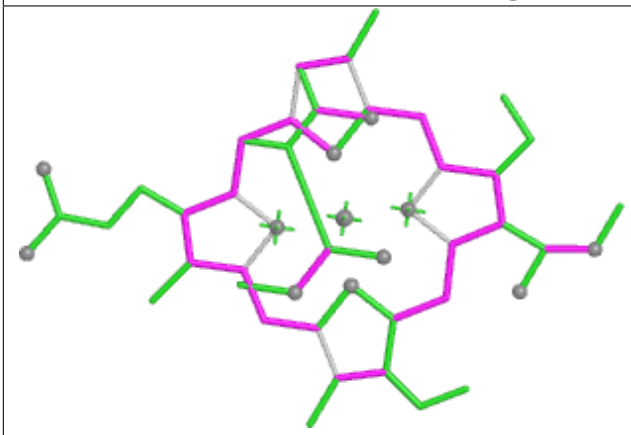


Torsions

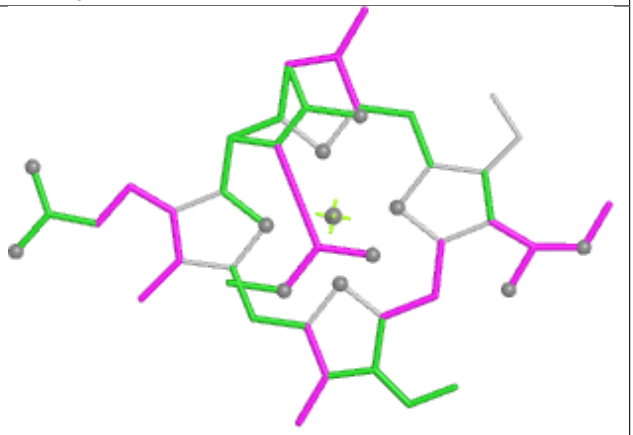


Rings

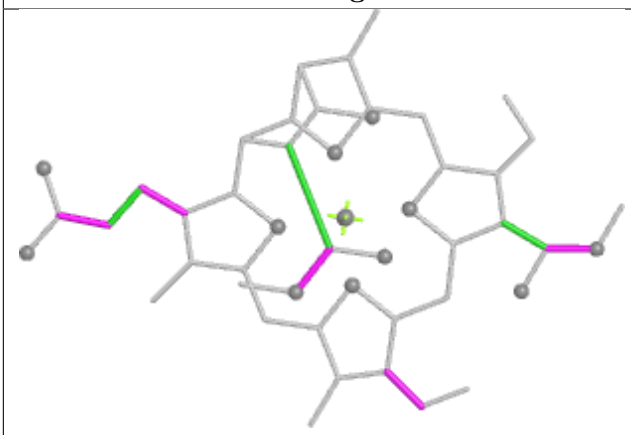
Ligand A1ECV y 311



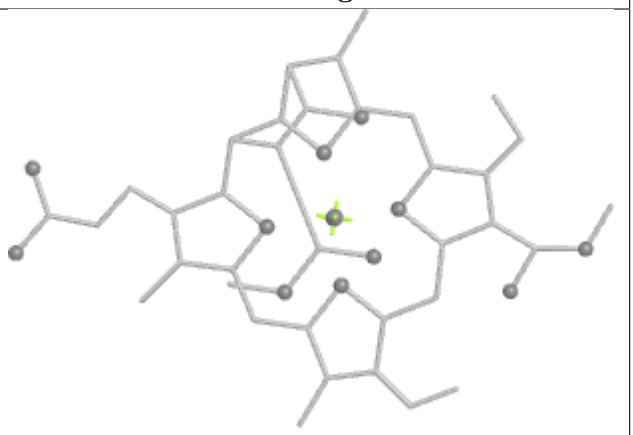
Bond lengths



Bond angles

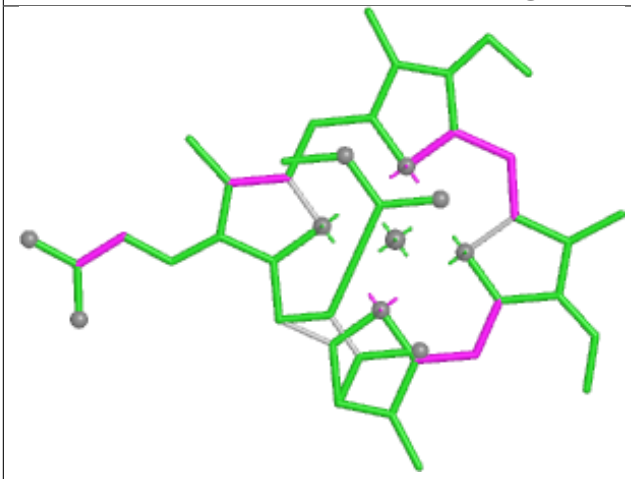


Torsions

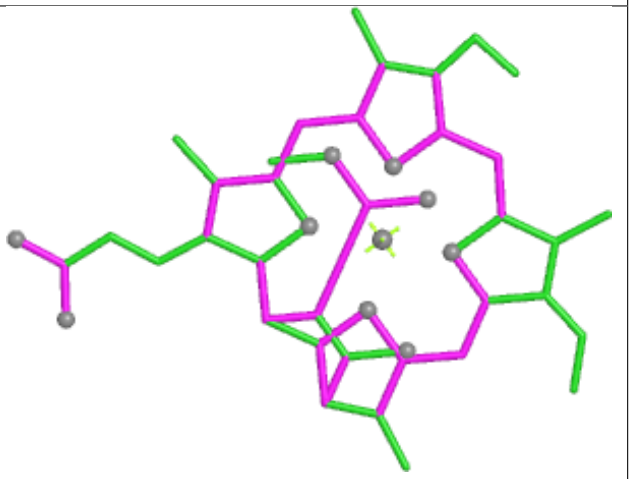


Rings

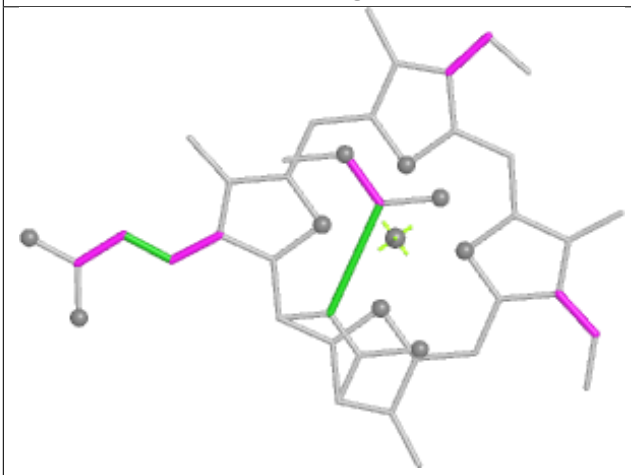
Ligand KC2 M 314



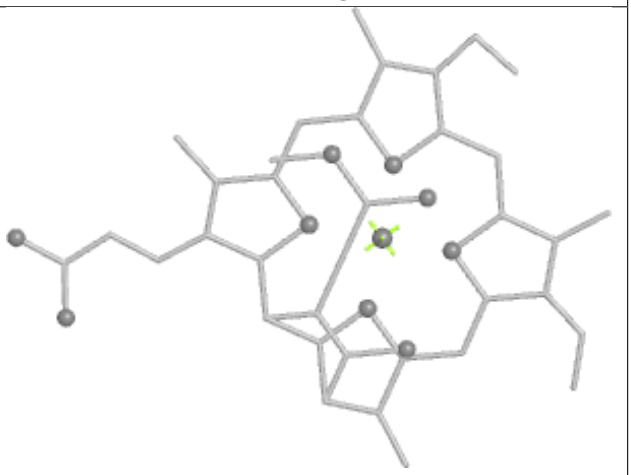
Bond lengths



Bond angles

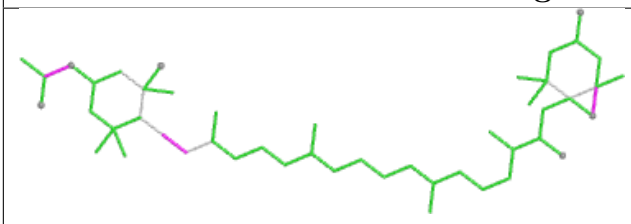


Torsions

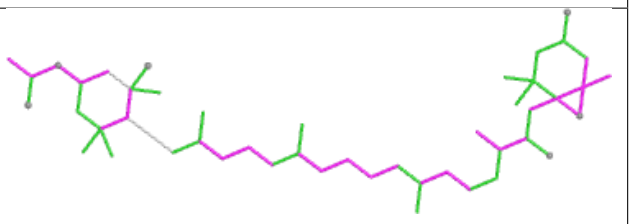


Rings

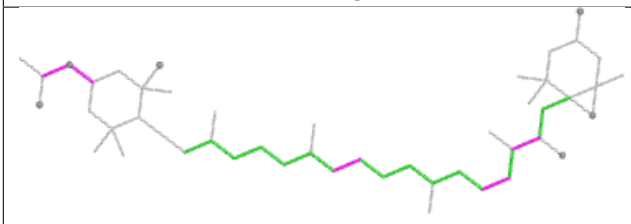
Ligand A86 9 303



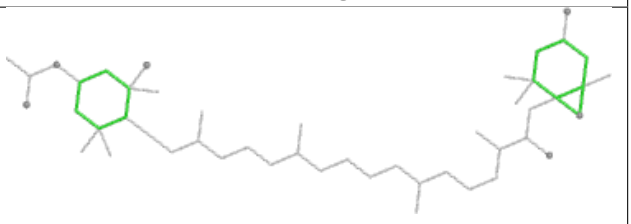
Bond lengths



Bond angles

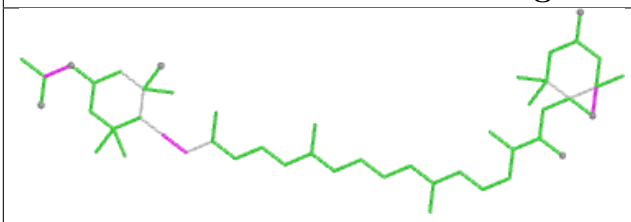


Torsions

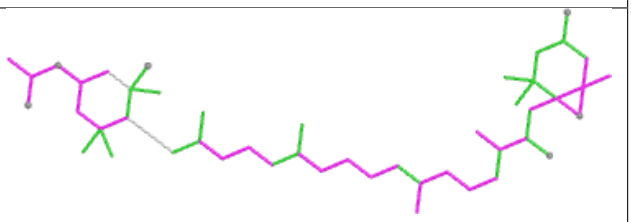


Rings

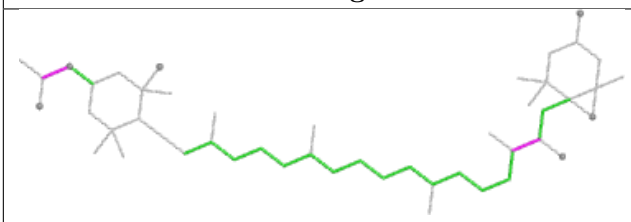
Ligand A86 9 305



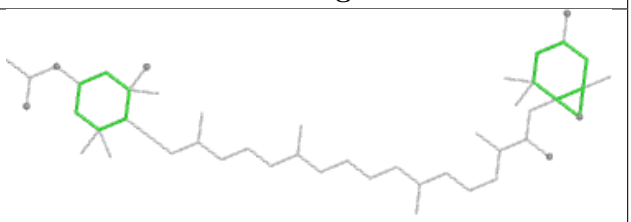
Bond lengths



Bond angles

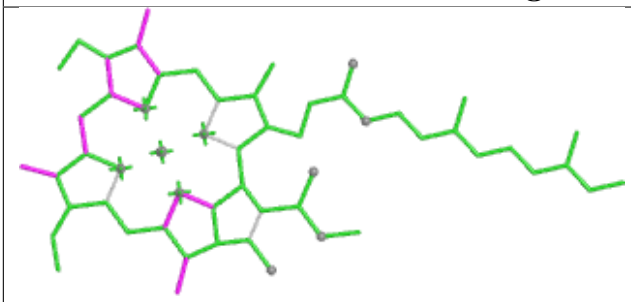


Torsions

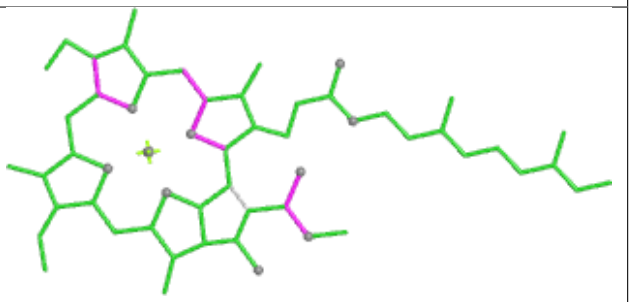


Rings

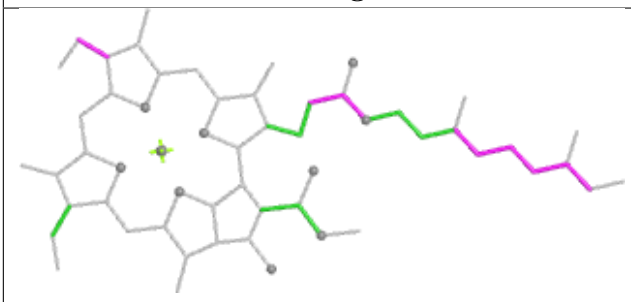
Ligand CLA E 314



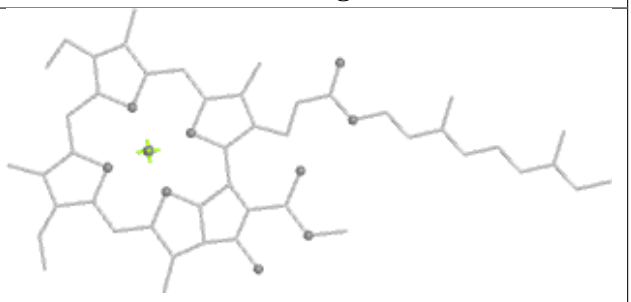
Bond lengths



Bond angles

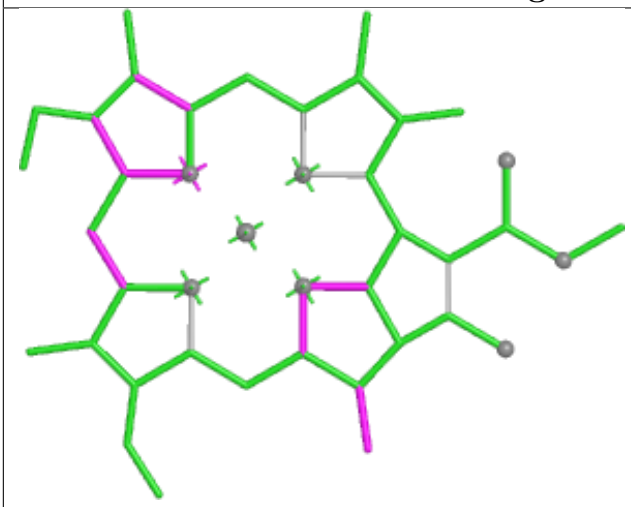


Torsions

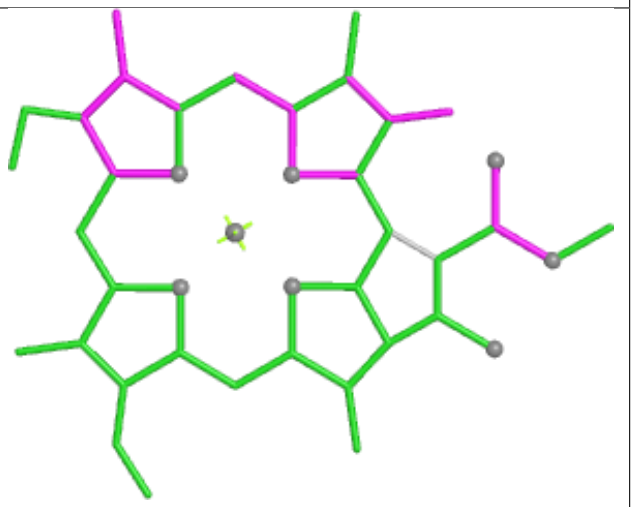


Rings

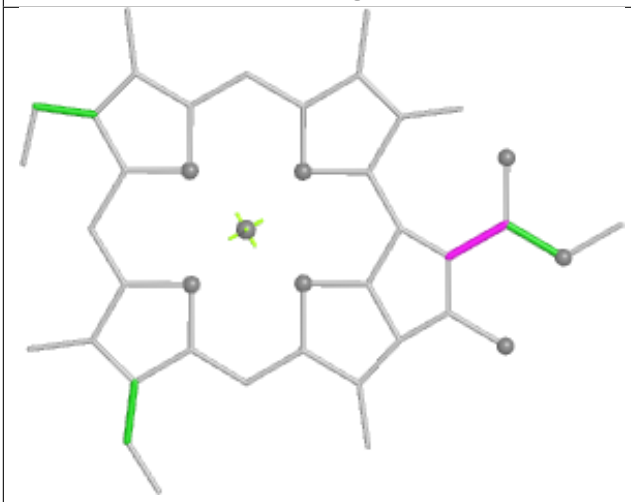
Ligand CLA 6 315



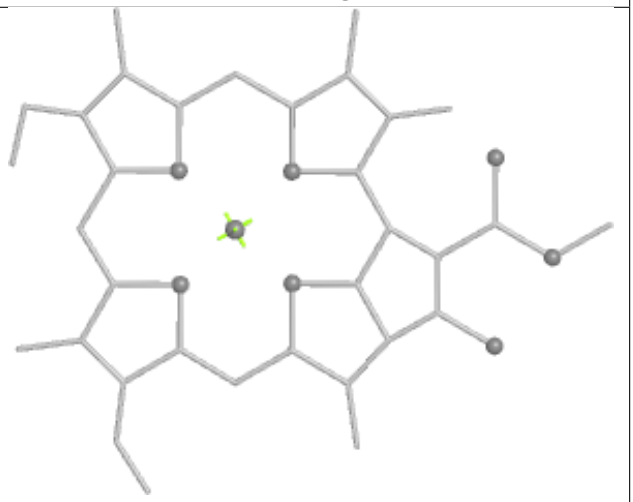
Bond lengths



Bond angles

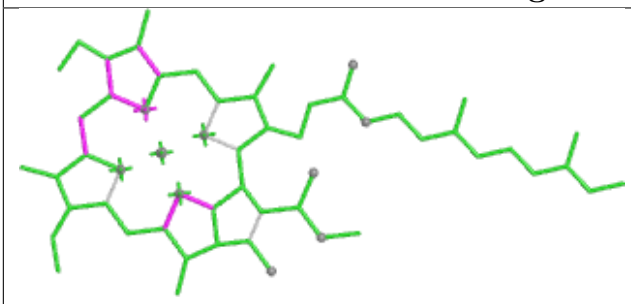


Torsions

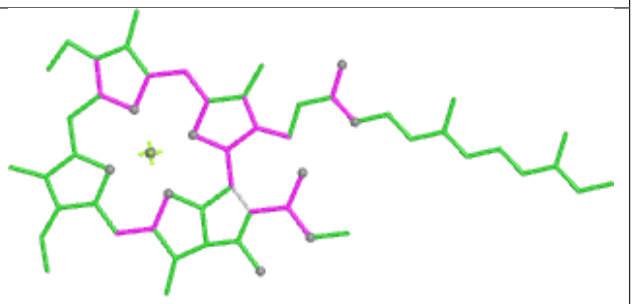


Rings

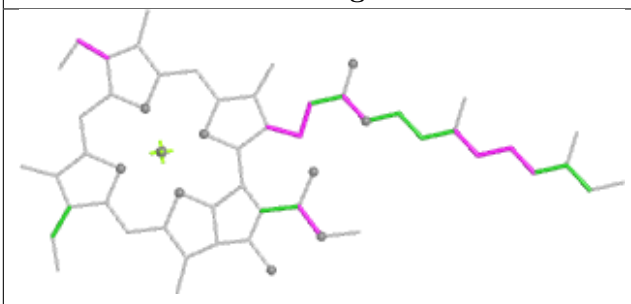
Ligand CLA 7 314



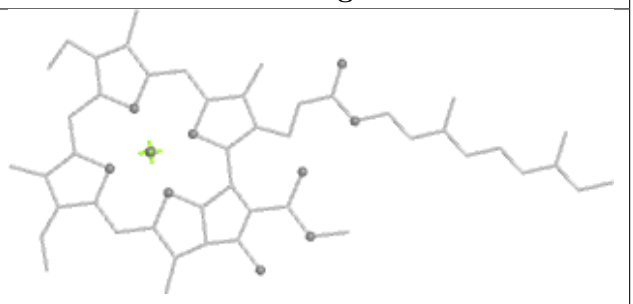
Bond lengths



Bond angles

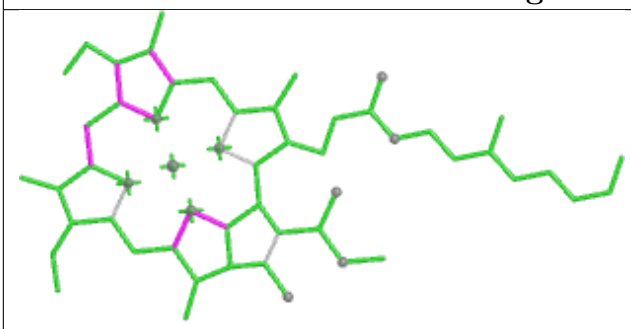


Torsions

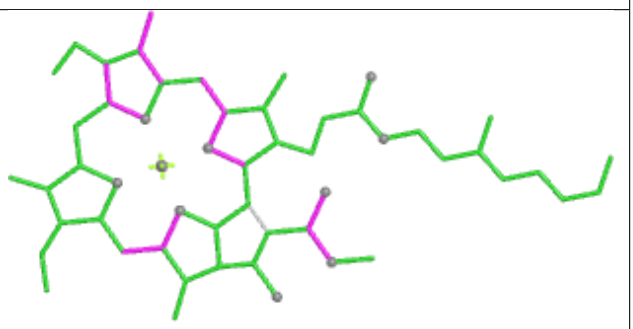


Rings

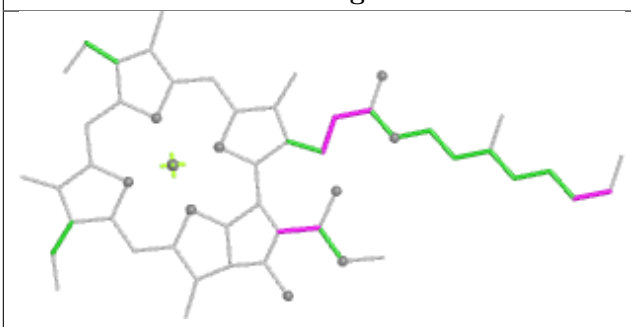
Ligand CLA F 310



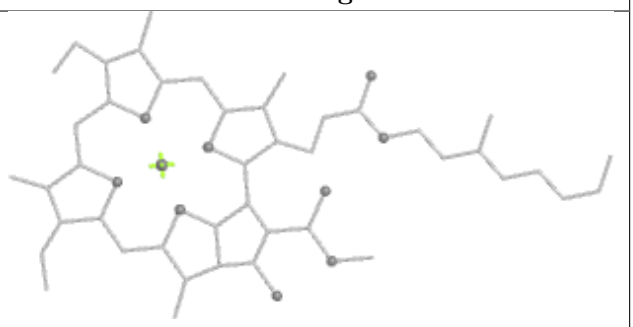
Bond lengths



Bond angles

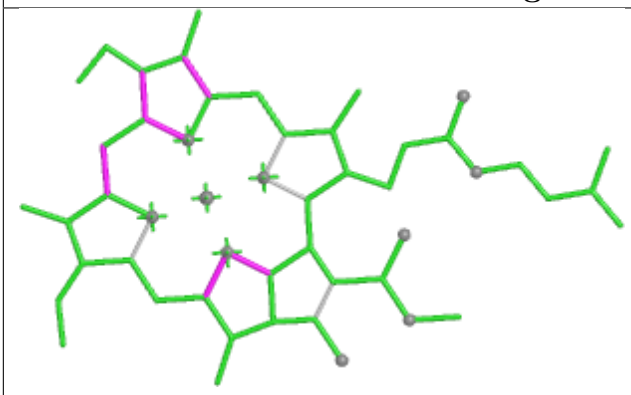


Torsions

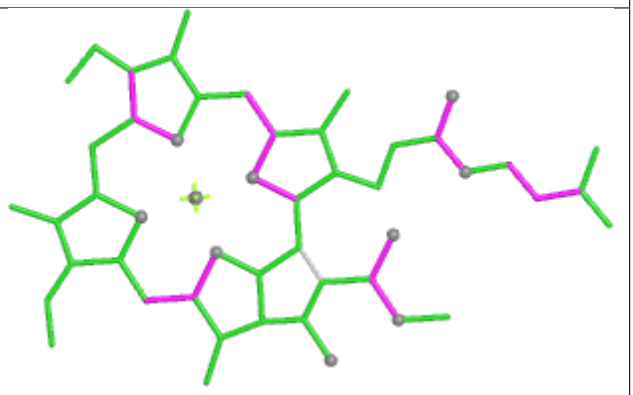


Rings

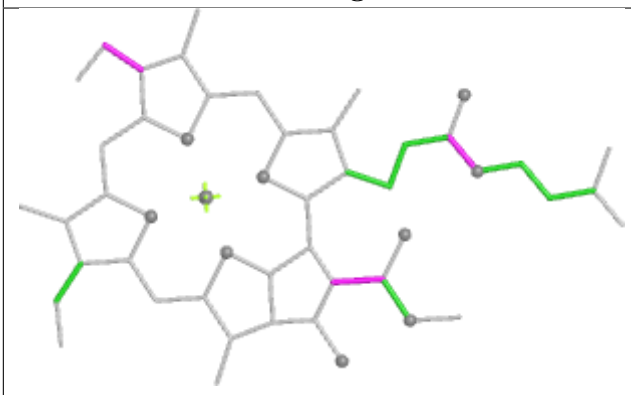
Ligand CLA X 311



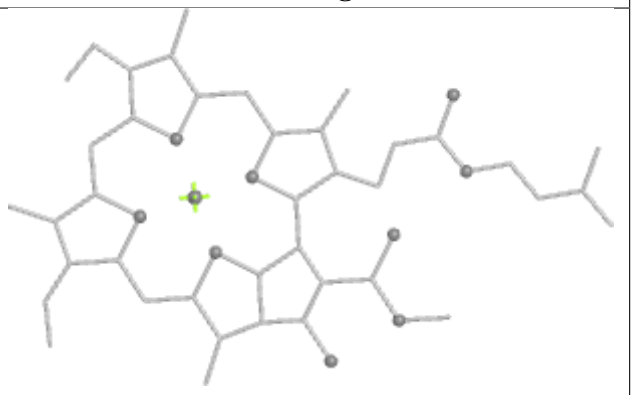
Bond lengths



Bond angles

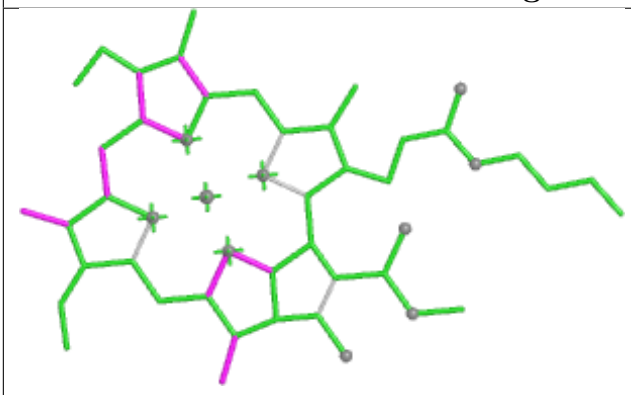


Torsions

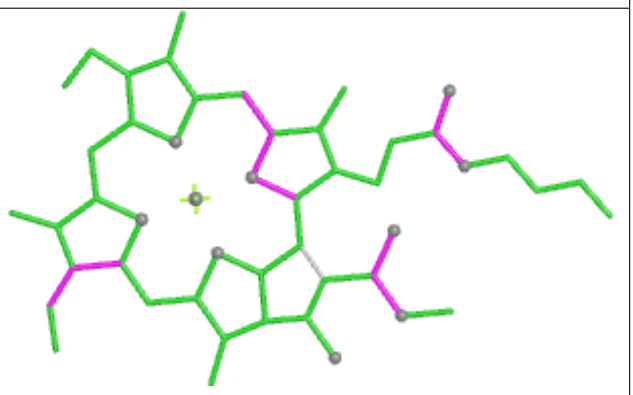


Rings

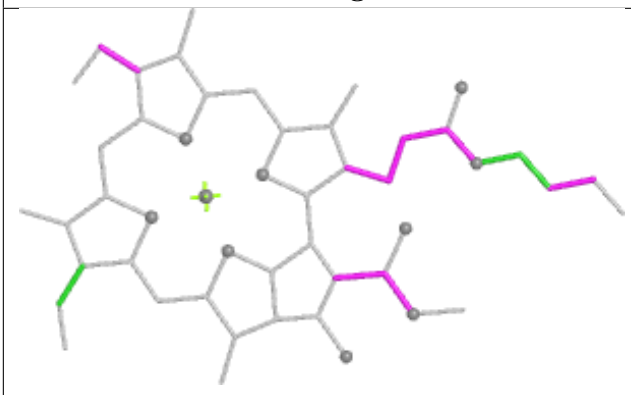
Ligand CLA G 318



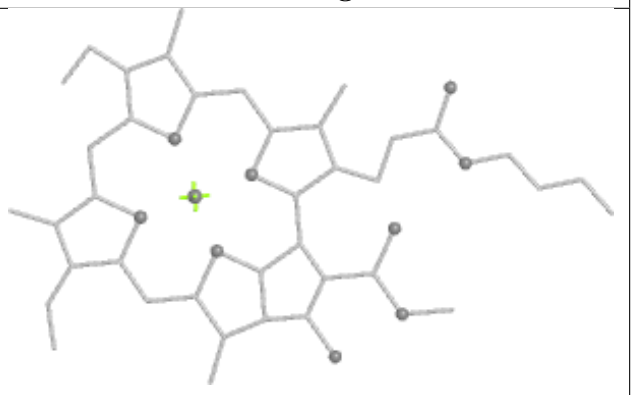
Bond lengths



Bond angles

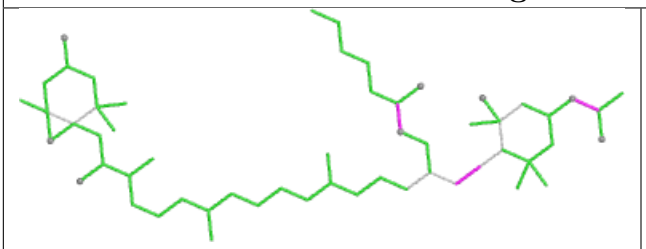


Torsions

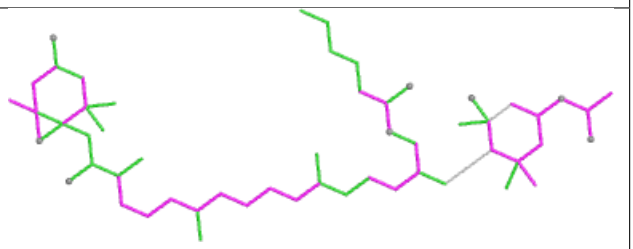


Rings

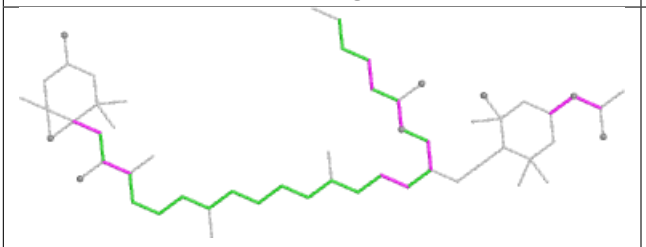
Ligand A1EB1 0 302



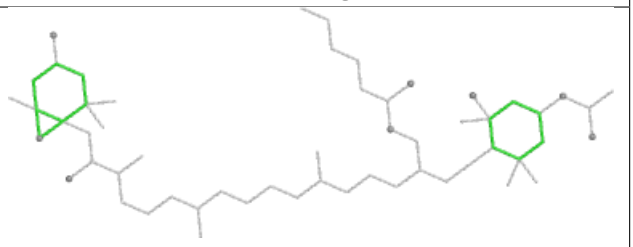
Bond lengths



Bond angles

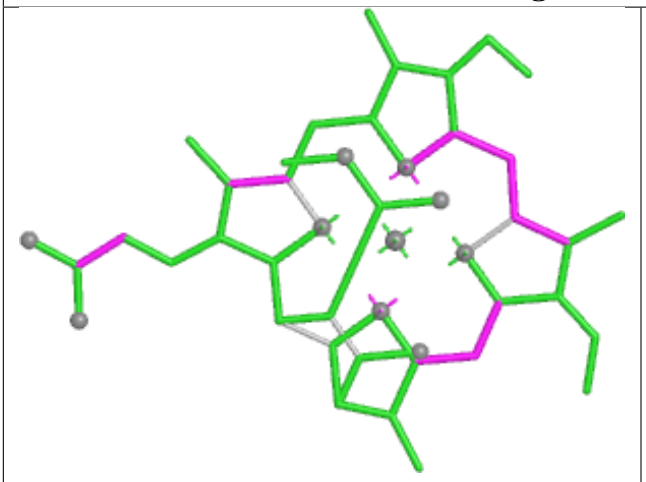


Torsions

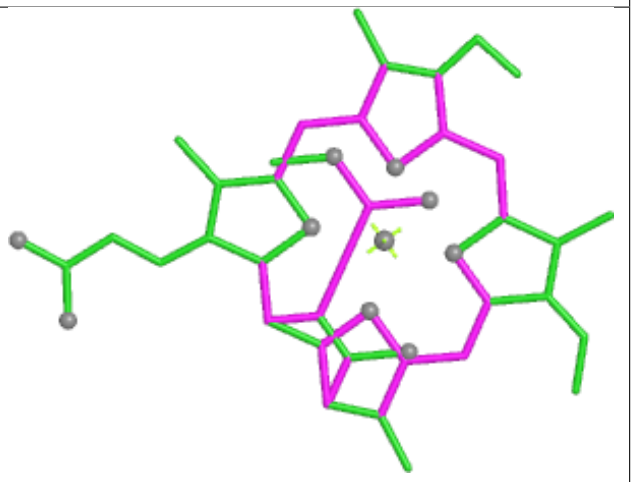


Rings

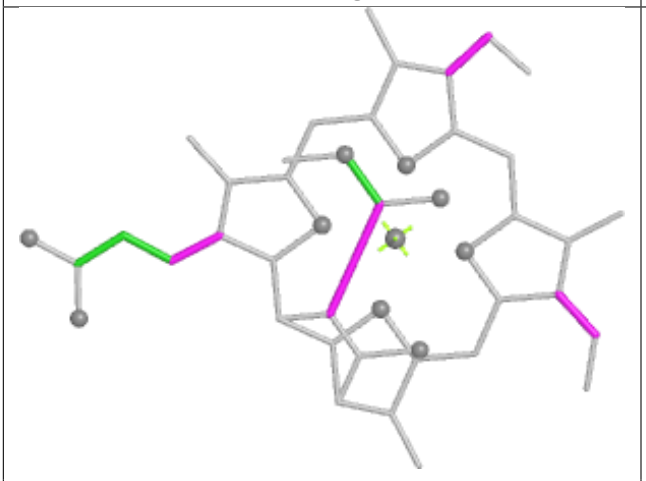
Ligand KC2 9 311



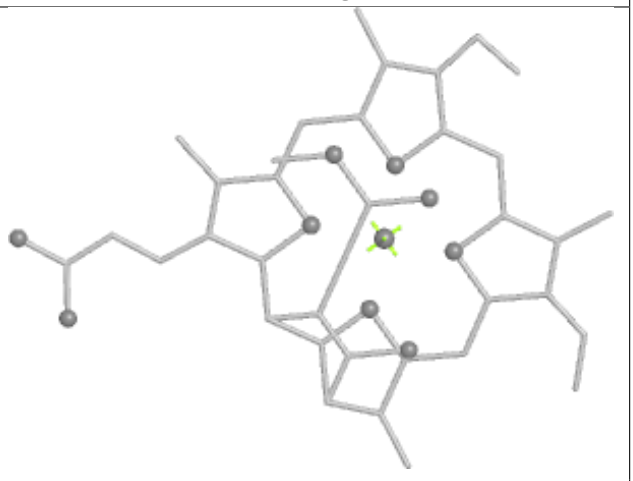
Bond lengths



Bond angles

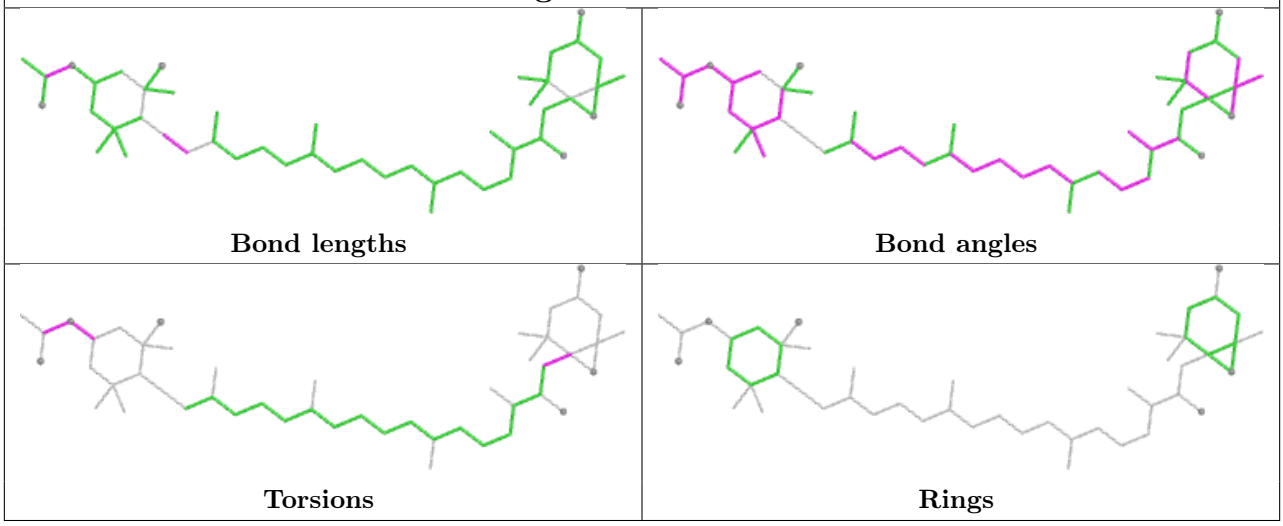


Torsions

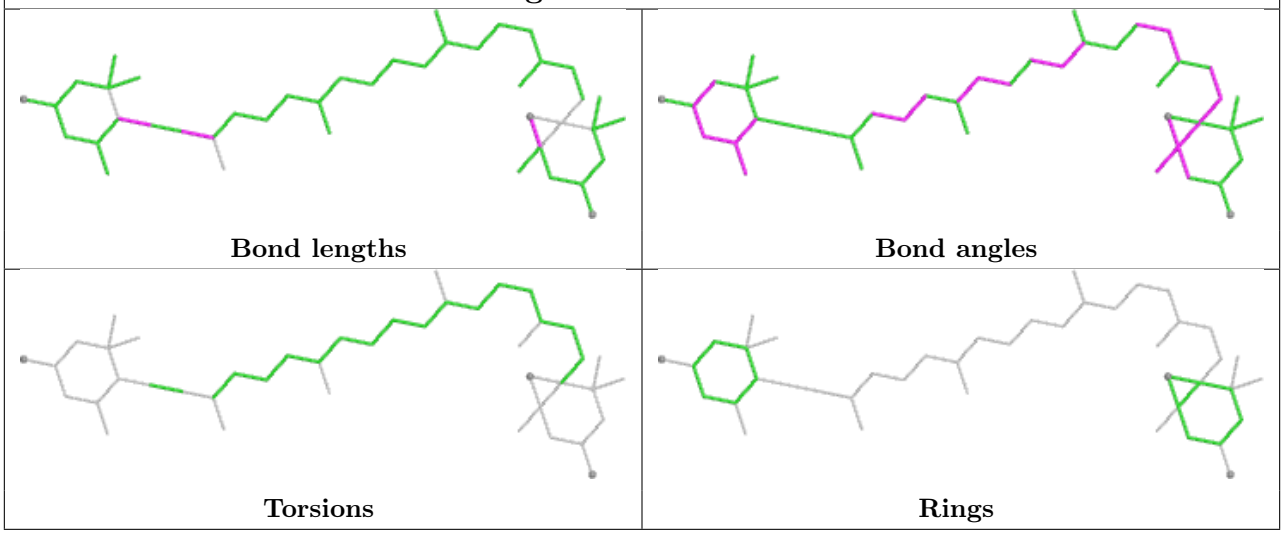


Rings

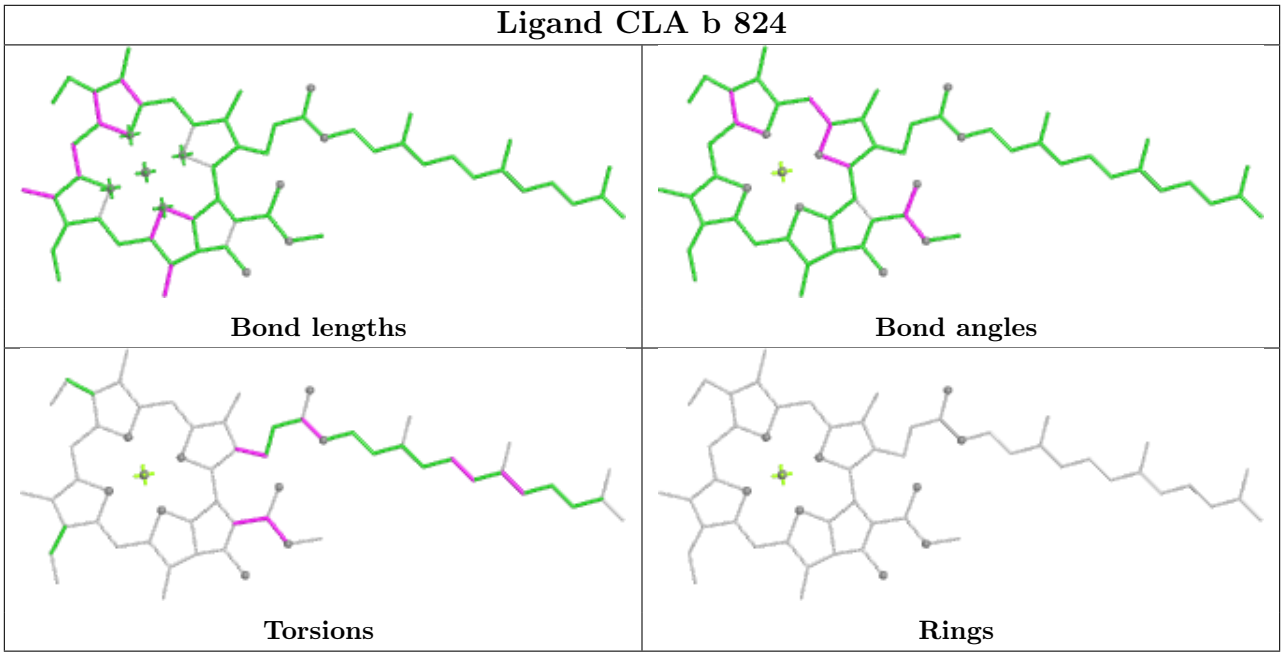
Ligand A86 7 312



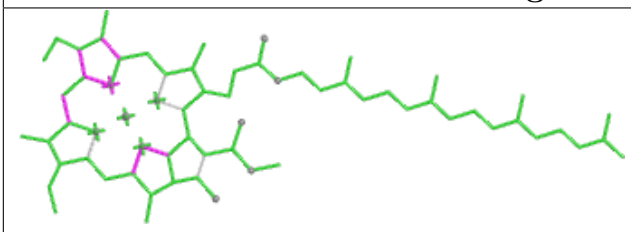
Ligand DD6 A 302



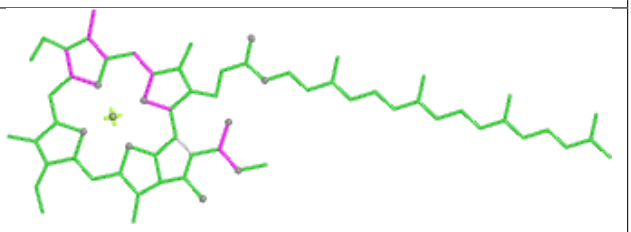
Ligand CLA b 824



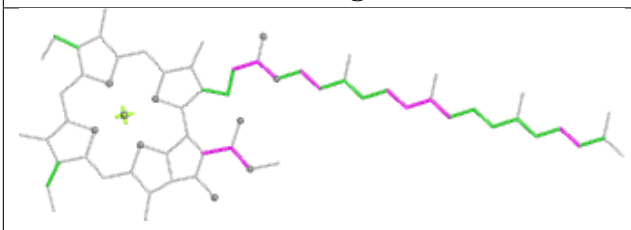
Ligand CLA L 310



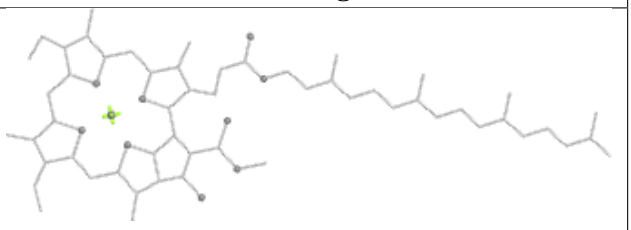
Bond lengths



Bond angles

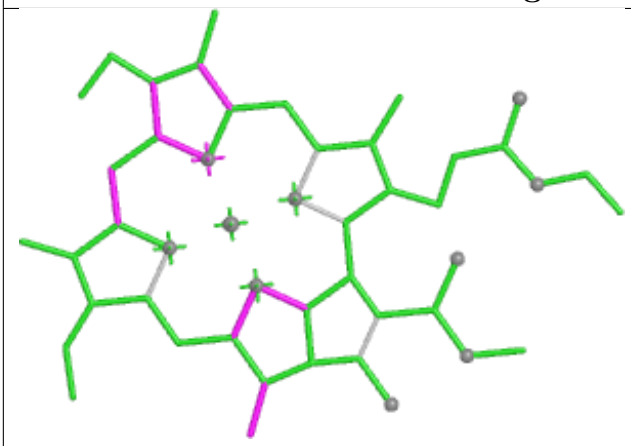


Torsions

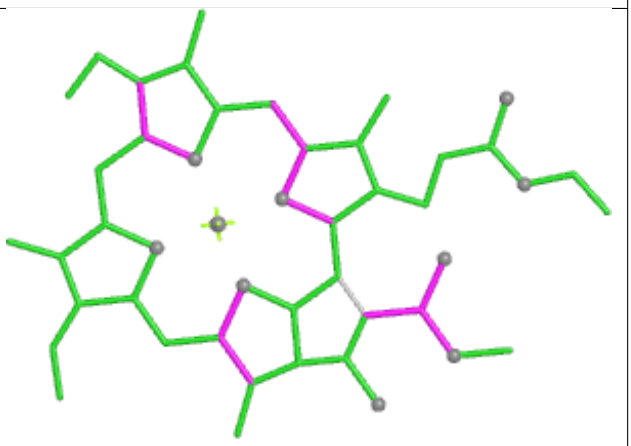


Rings

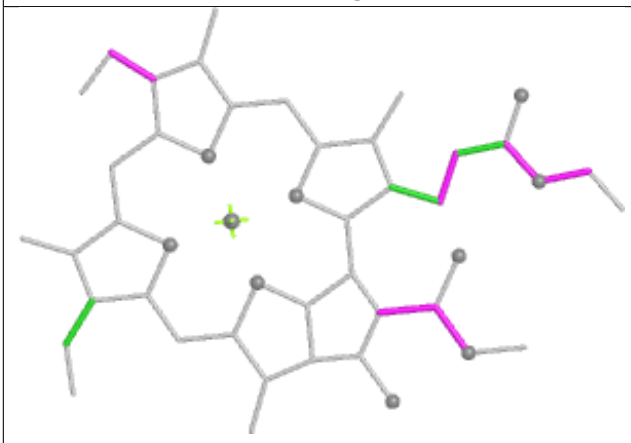
Ligand CLA X 316



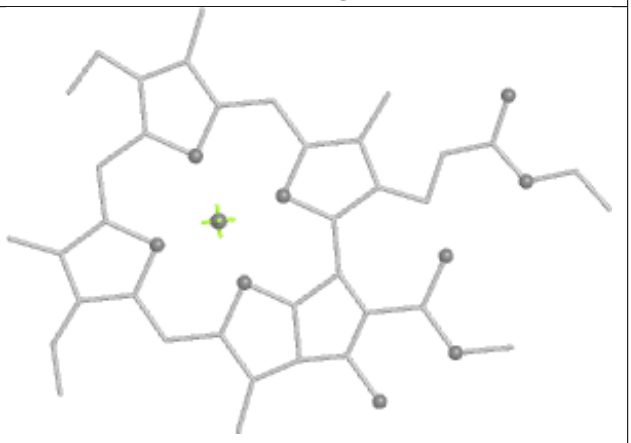
Bond lengths



Bond angles

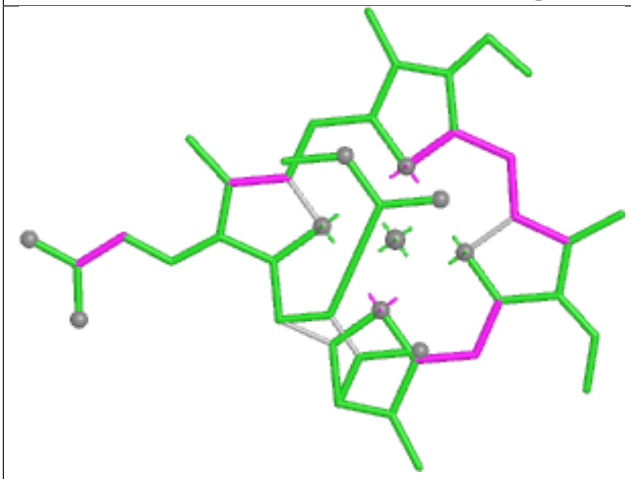


Torsions

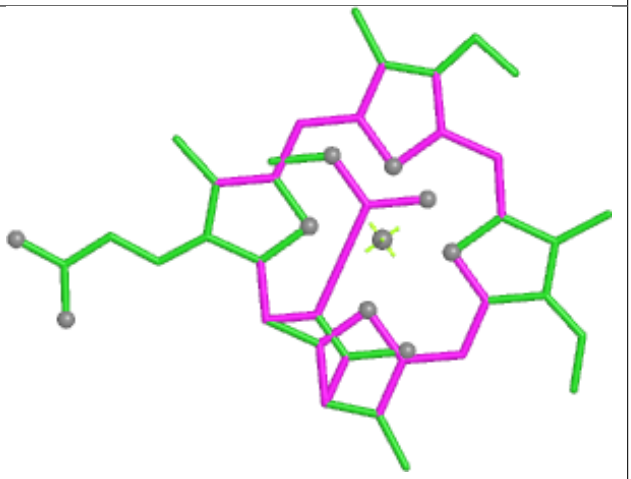


Rings

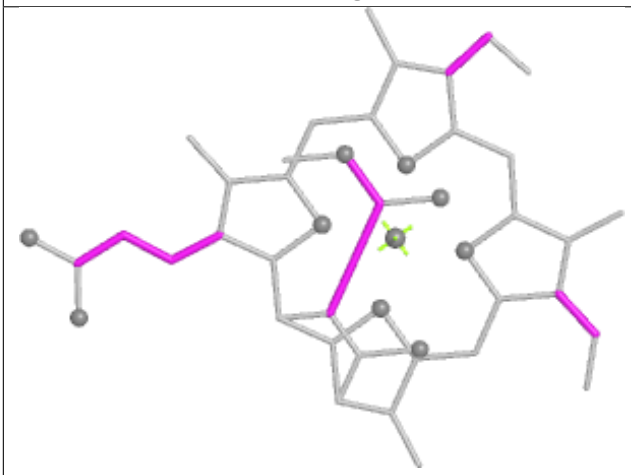
Ligand KC2 7 322



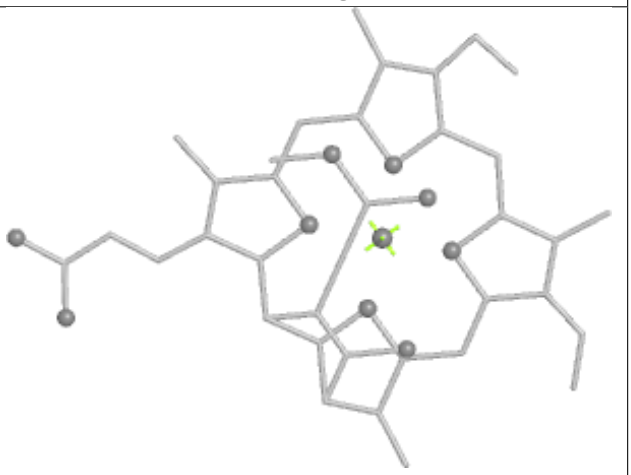
Bond lengths



Bond angles

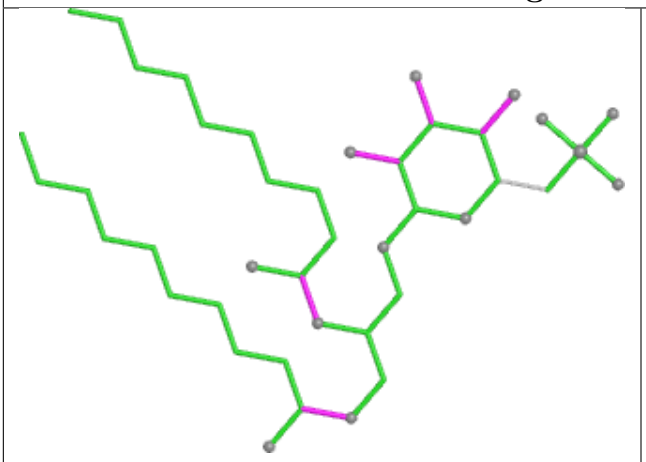


Torsions

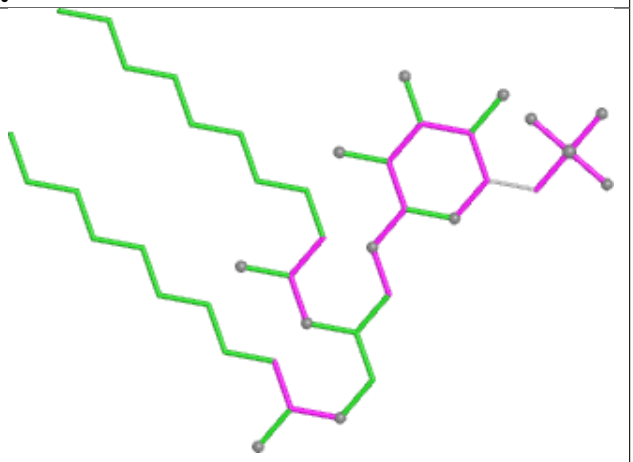


Rings

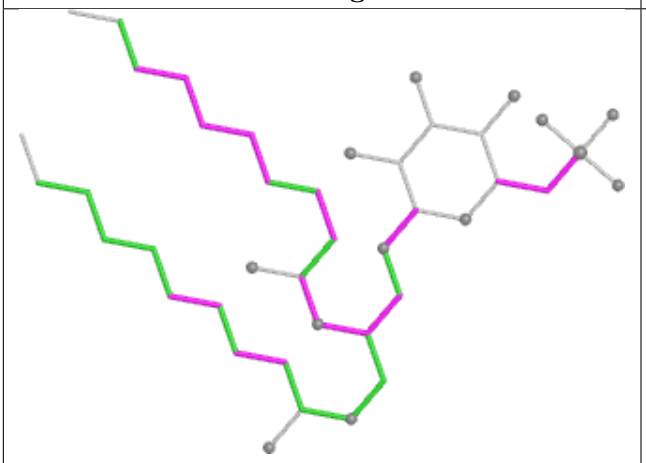
Ligand SQD F 318



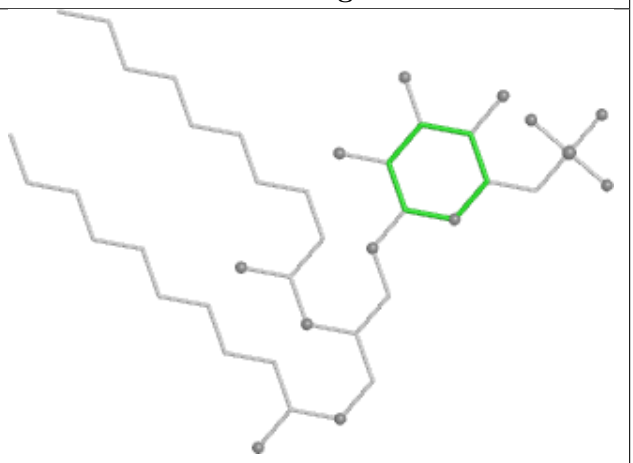
Bond lengths



Bond angles

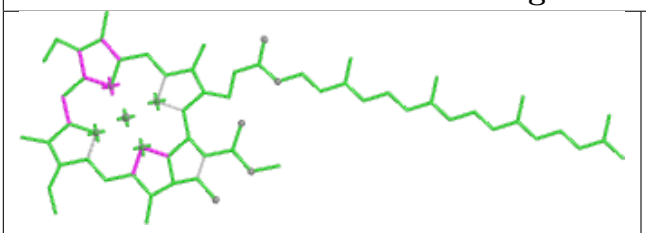


Torsions

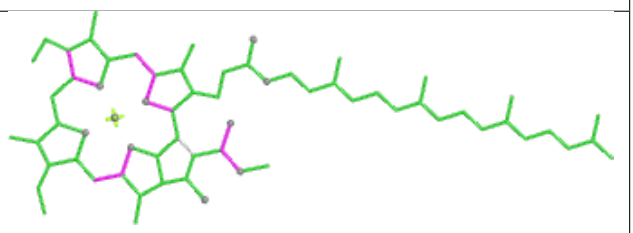


Rings

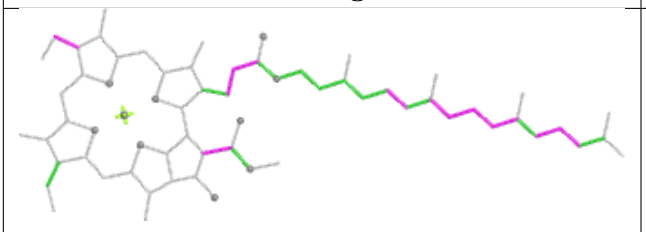
Ligand CLA 5 308



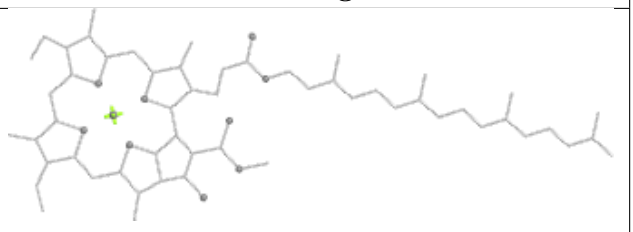
Bond lengths



Bond angles

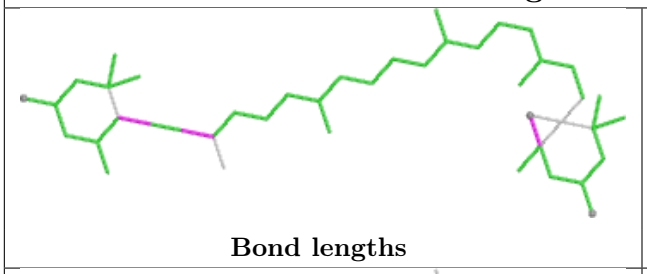


Torsions

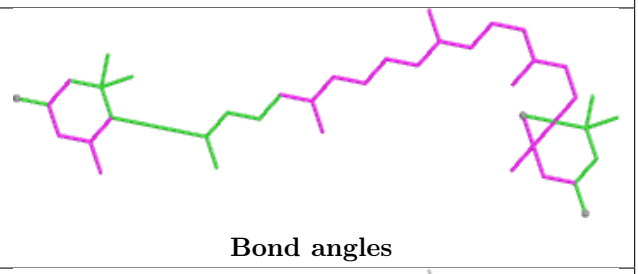


Rings

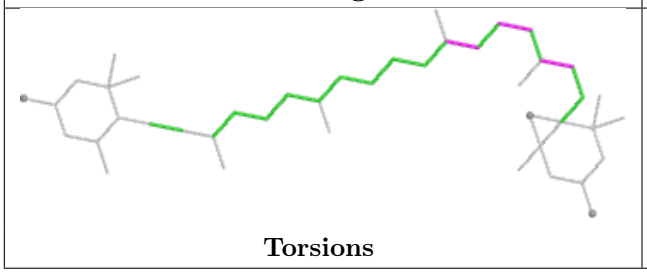
Ligand DD6 A 303



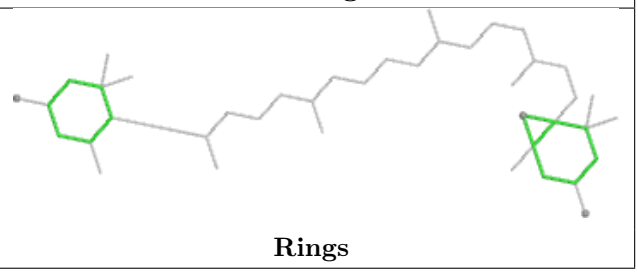
Bond lengths



Bond angles

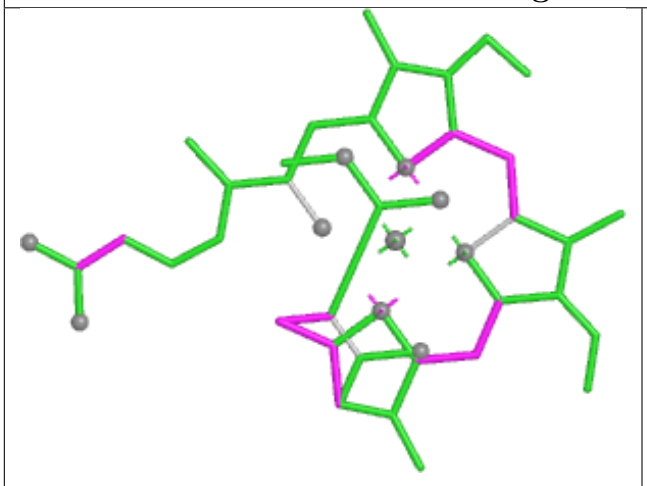


Torsions

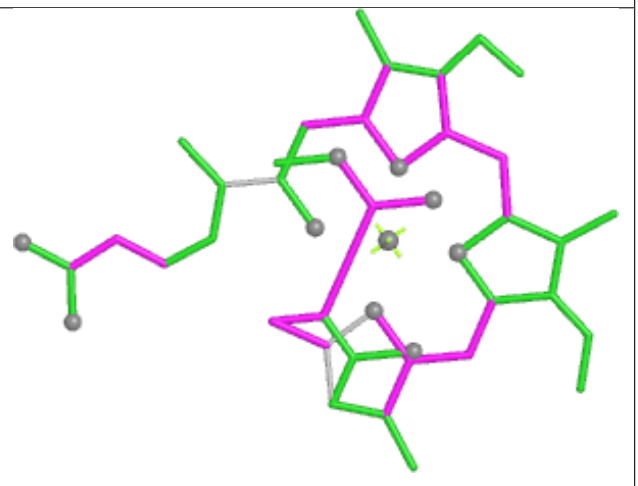


Rings

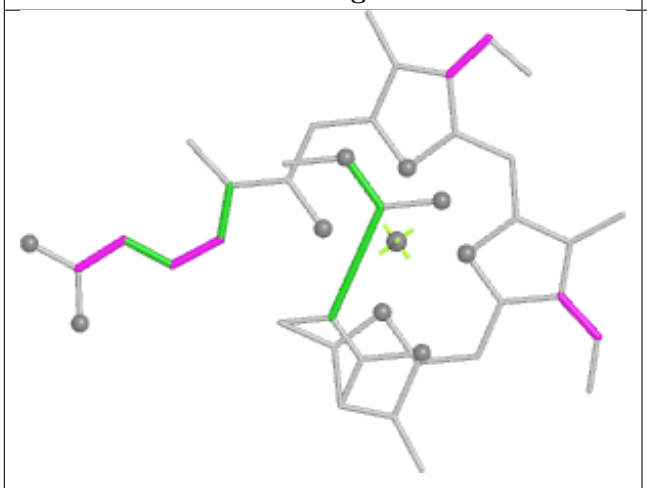
Ligand KC2 z 313



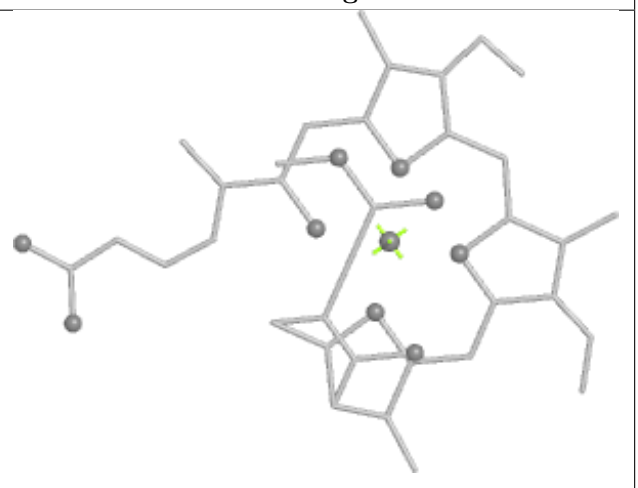
Bond lengths



Bond angles

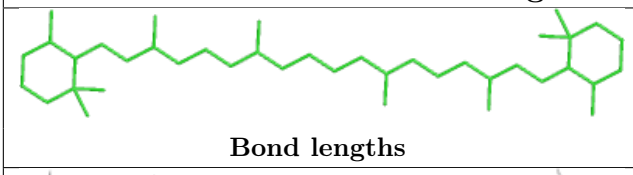


Torsions

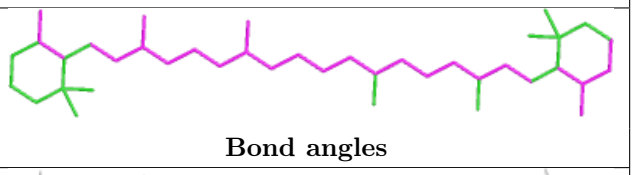


Rings

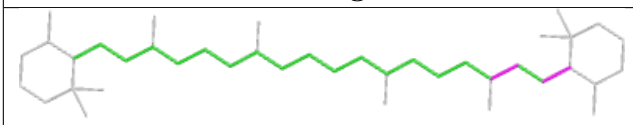
Ligand BCR a 845



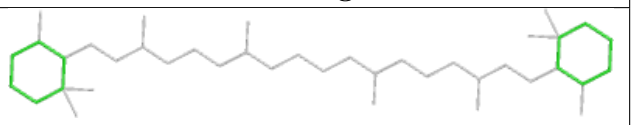
Bond lengths



Bond angles



Torsions

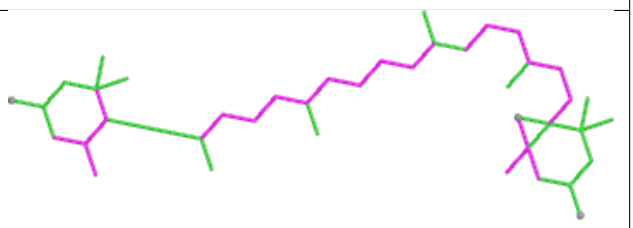


Rings

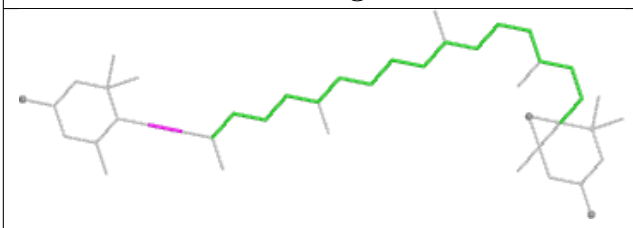
Ligand DD6 4 308



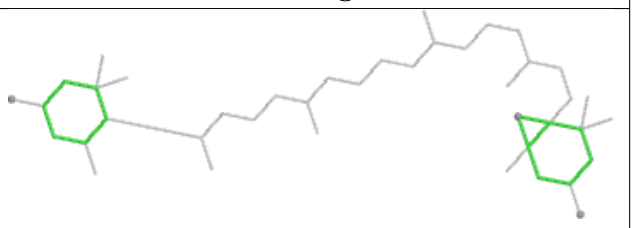
Bond lengths



Bond angles

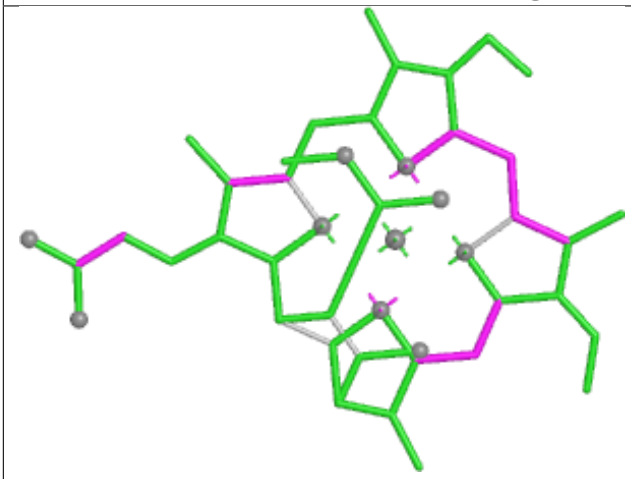


Torsions

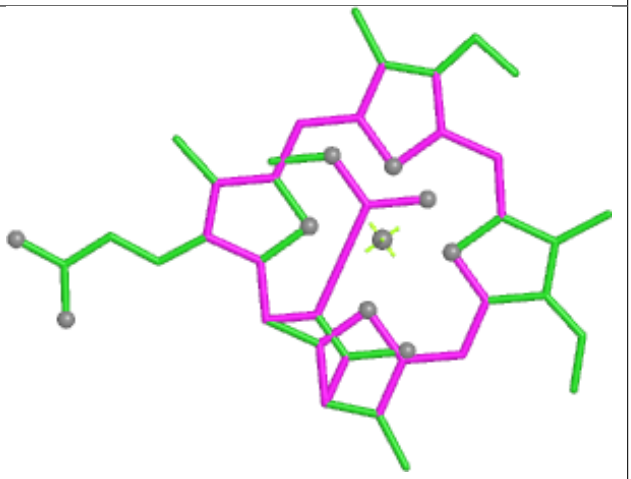


Rings

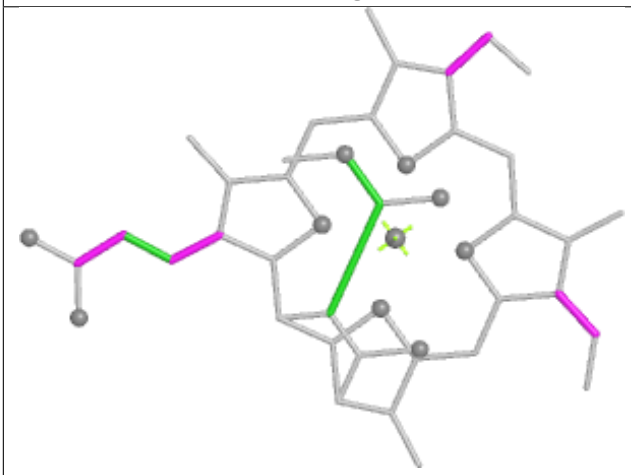
Ligand KC2 T 315



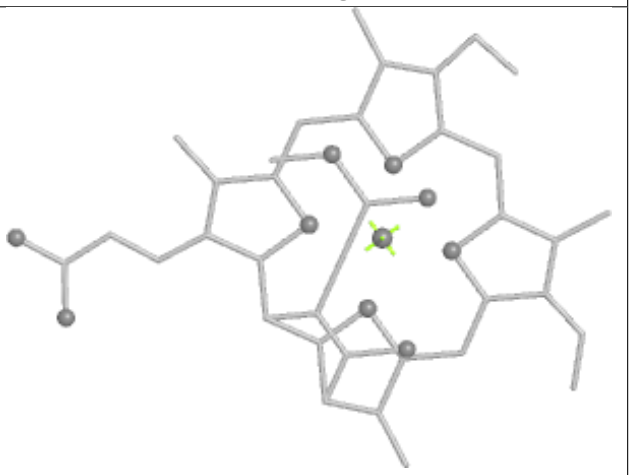
Bond lengths



Bond angles

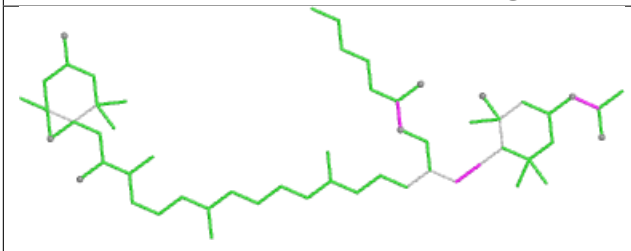


Torsions

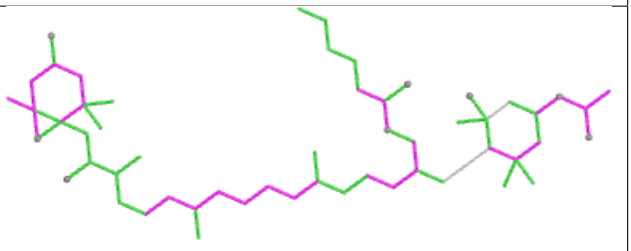


Rings

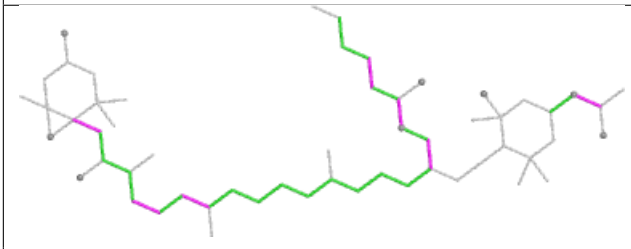
Ligand A1EB1 G 308



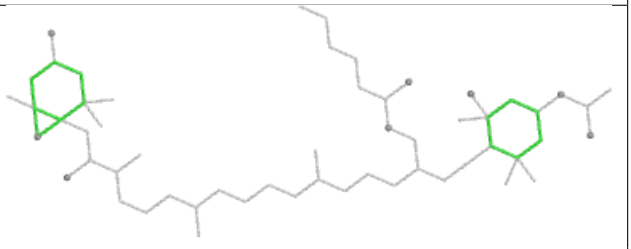
Bond lengths



Bond angles

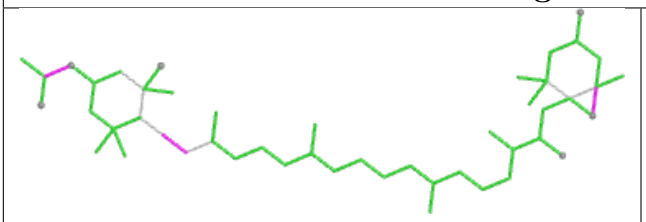


Torsions

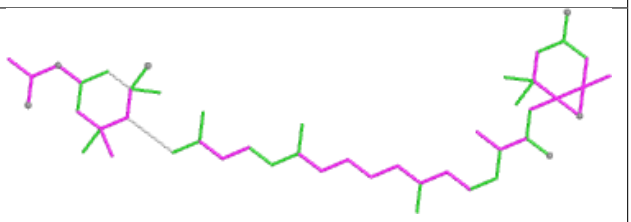


Rings

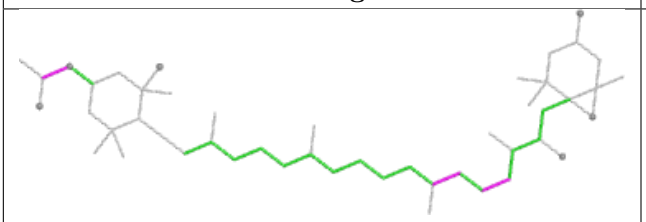
Ligand A86 1 302



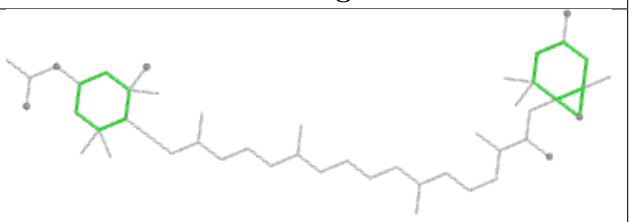
Bond lengths



Bond angles

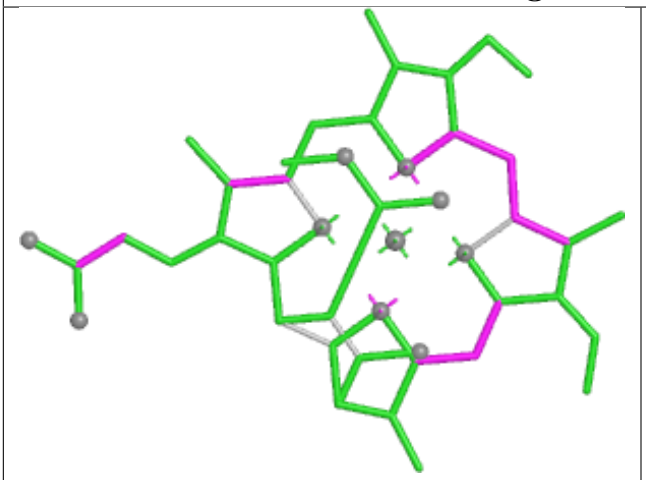


Torsions

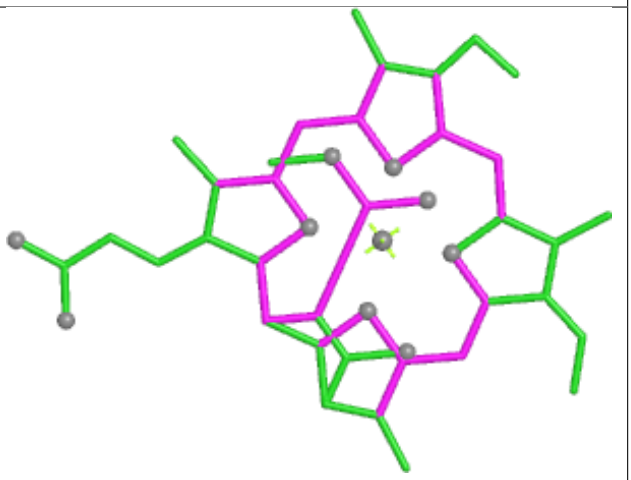


Rings

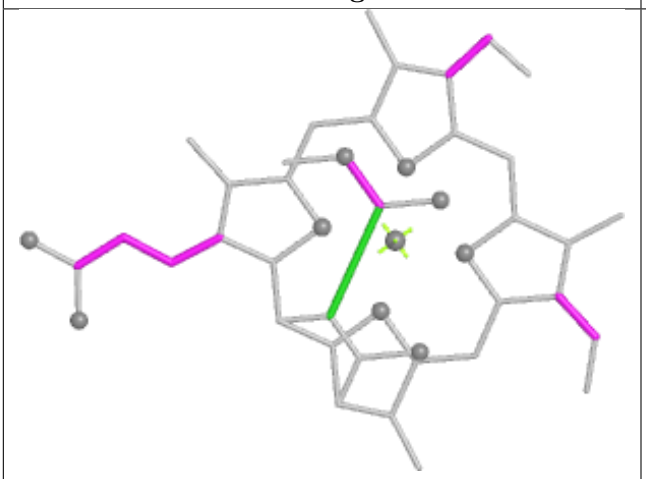
Ligand KC2 C 312



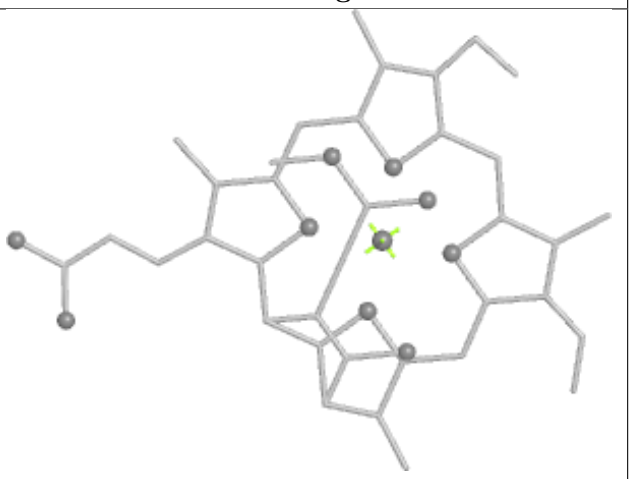
Bond lengths



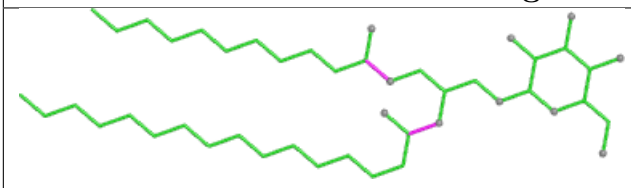
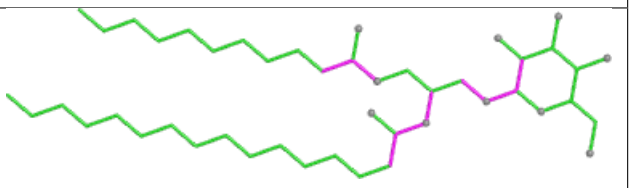
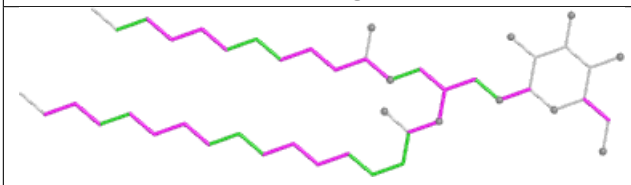
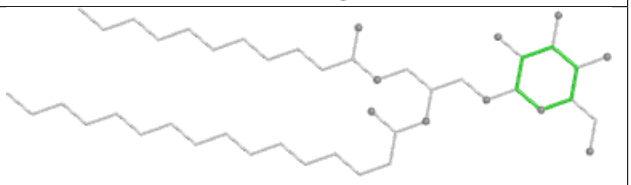
Bond angles

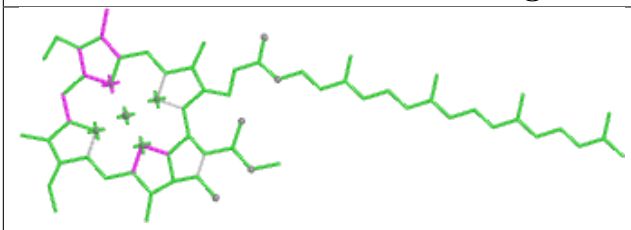
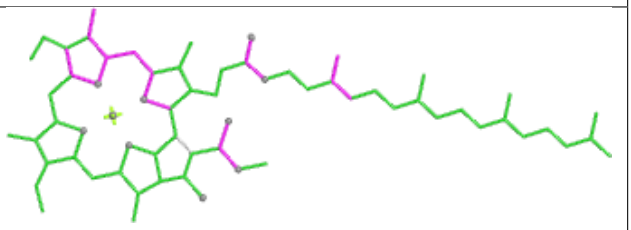
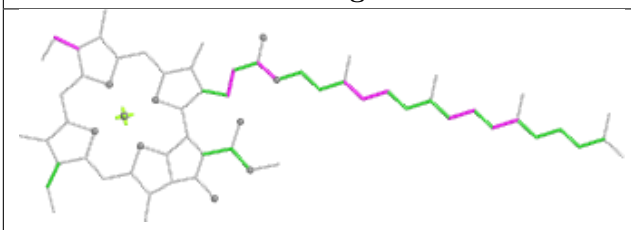
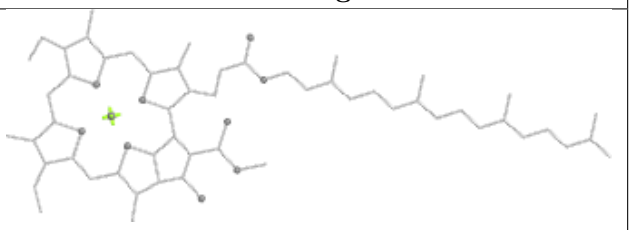


Torsions

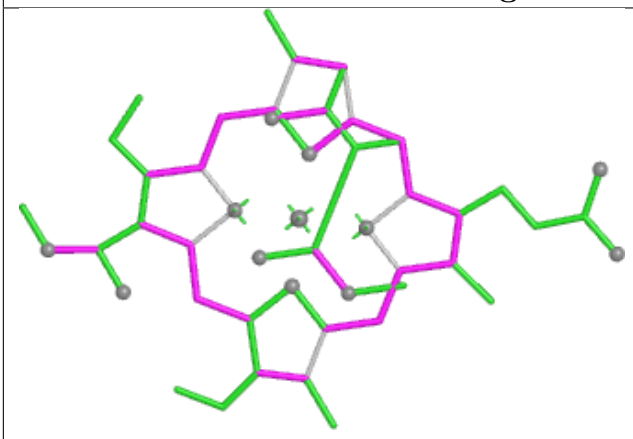


Rings

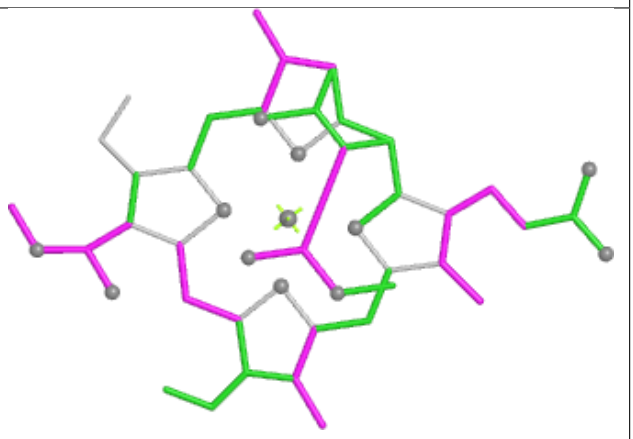
Ligand LMG S 322	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

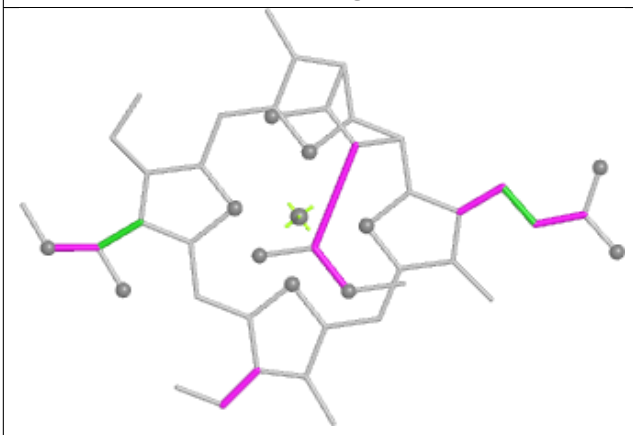
Ligand A1ECV G 316



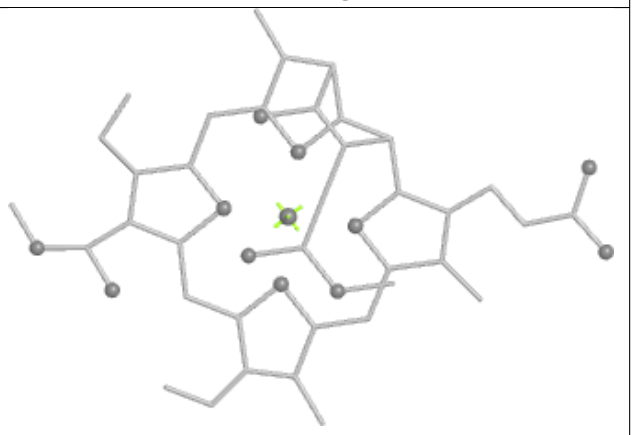
Bond lengths



Bond angles

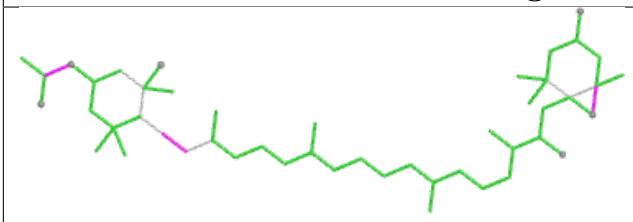


Torsions

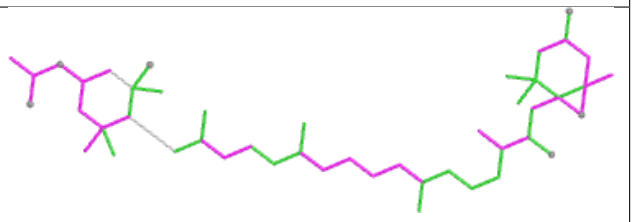


Rings

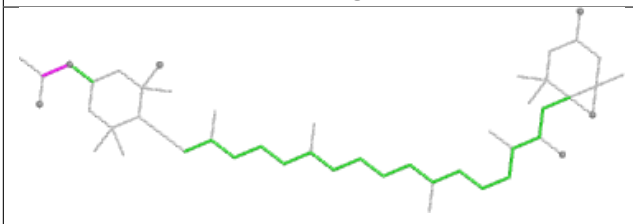
Ligand A86 M 306



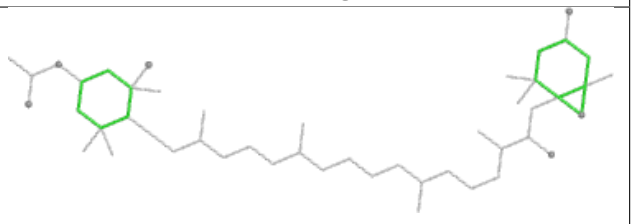
Bond lengths



Bond angles

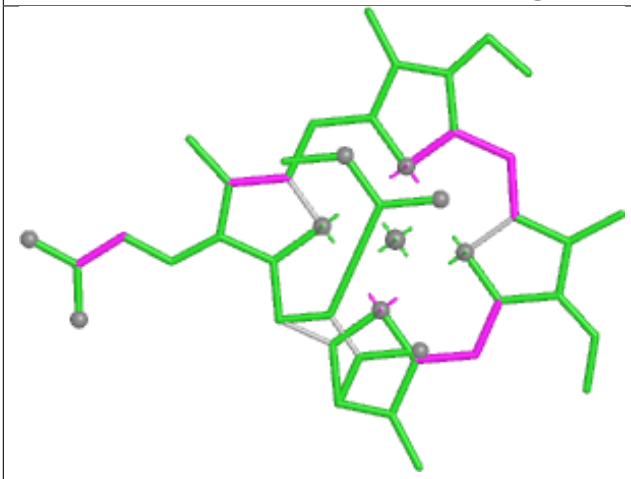


Torsions

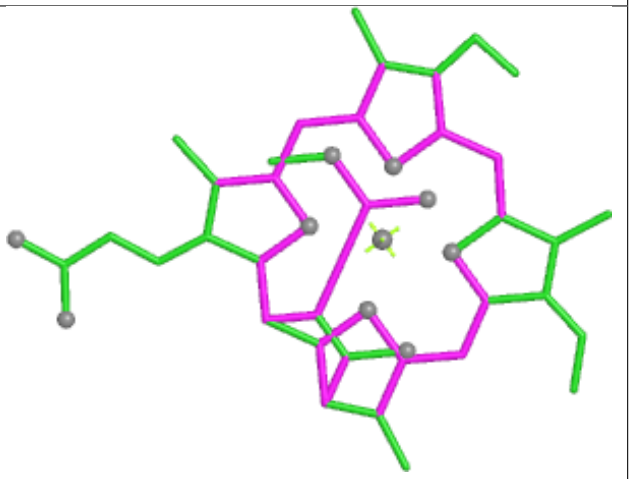


Rings

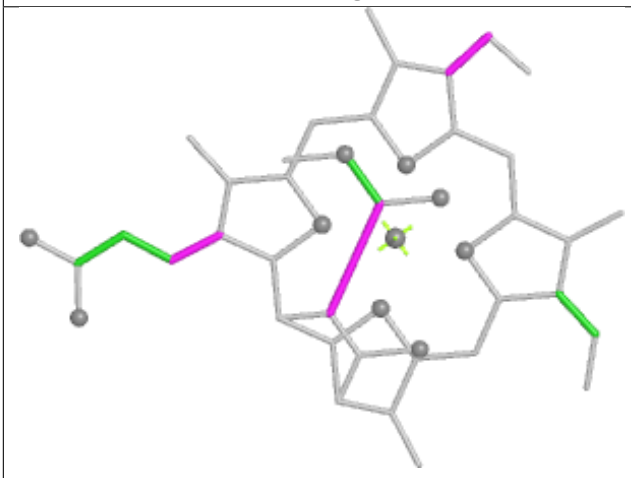
Ligand KC2 S 314



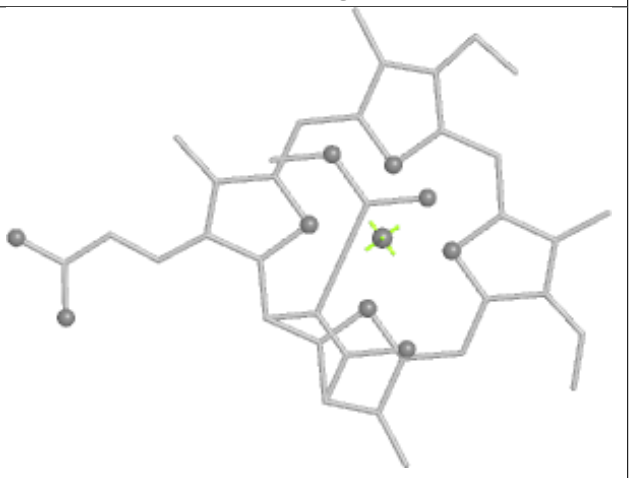
Bond lengths



Bond angles

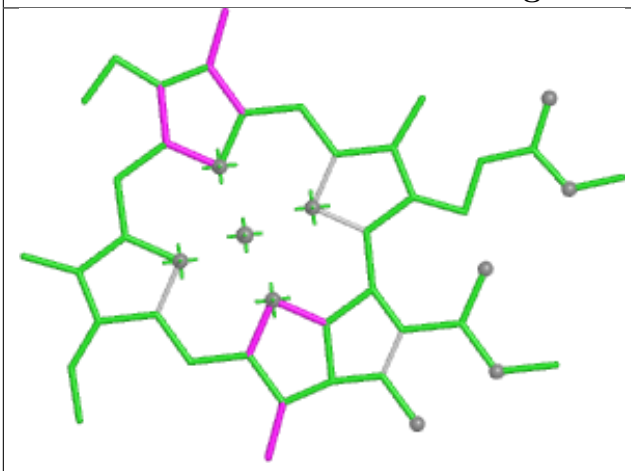


Torsions

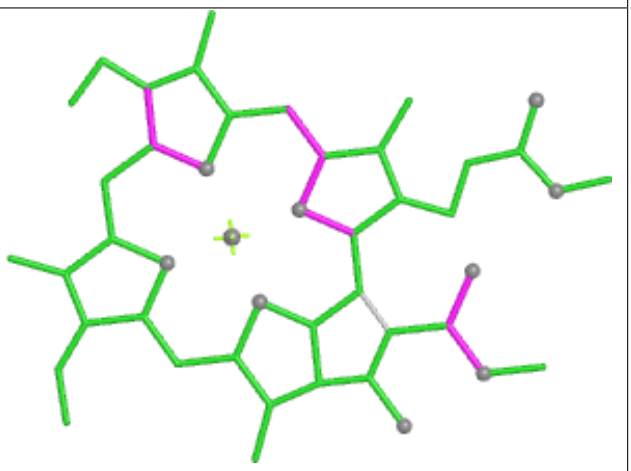


Rings

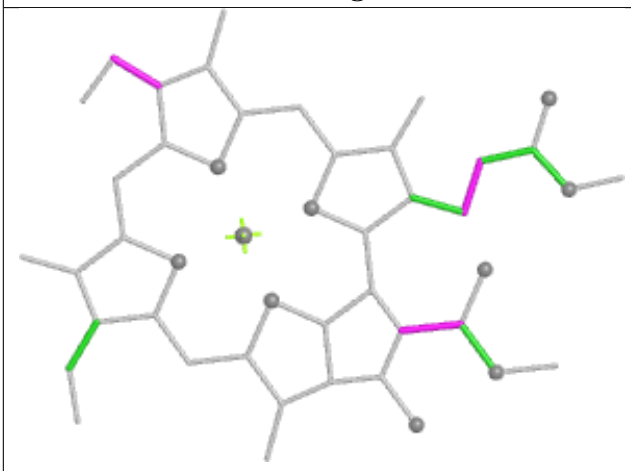
Ligand CLA U 214



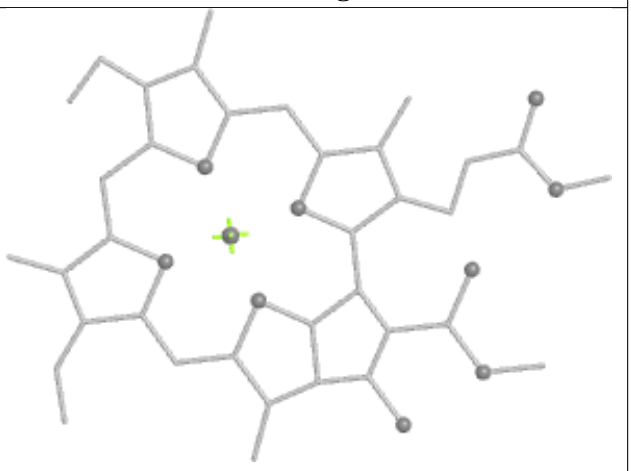
Bond lengths



Bond angles

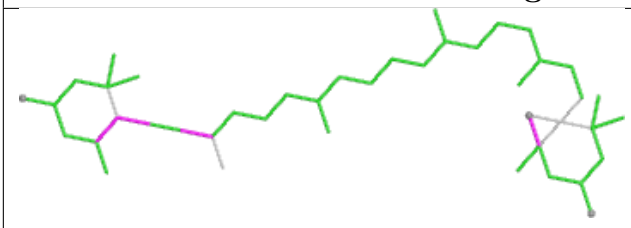


Torsions

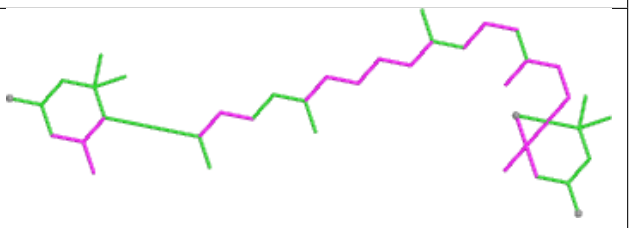


Rings

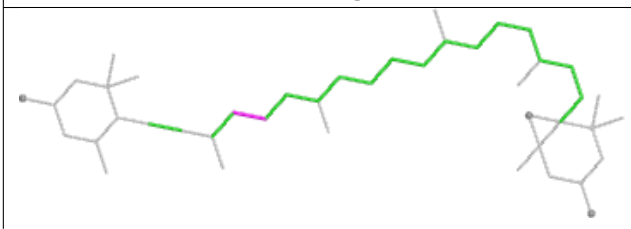
Ligand DD6 U 204



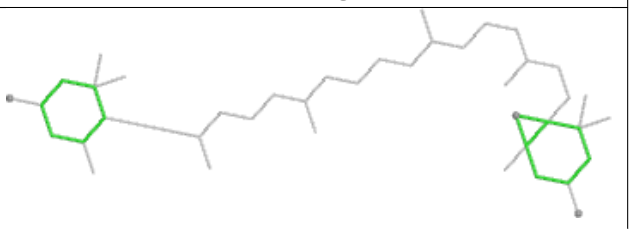
Bond lengths



Bond angles

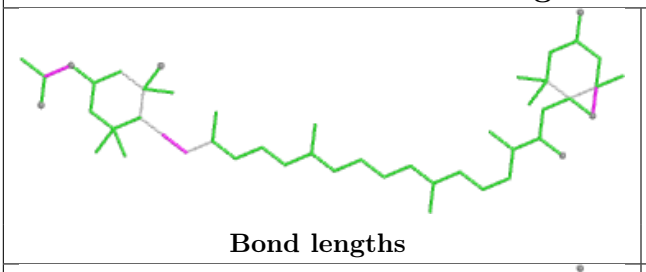


Torsions

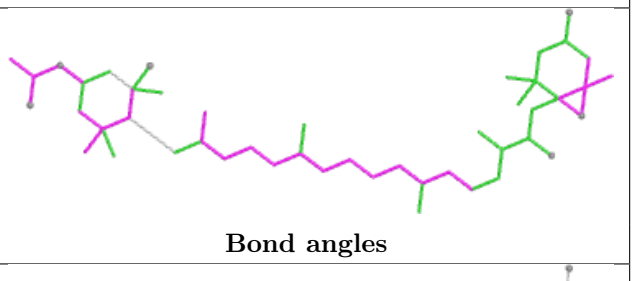


Rings

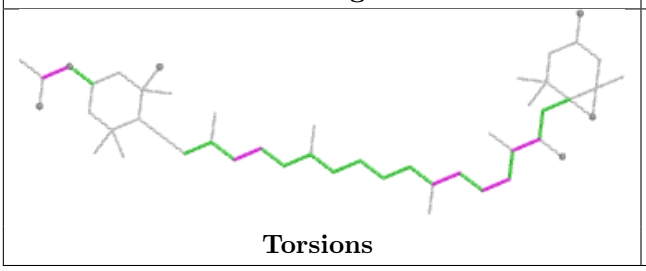
Ligand A86 9 304



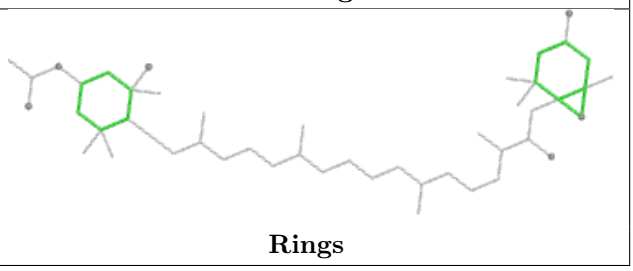
Bond lengths



Bond angles

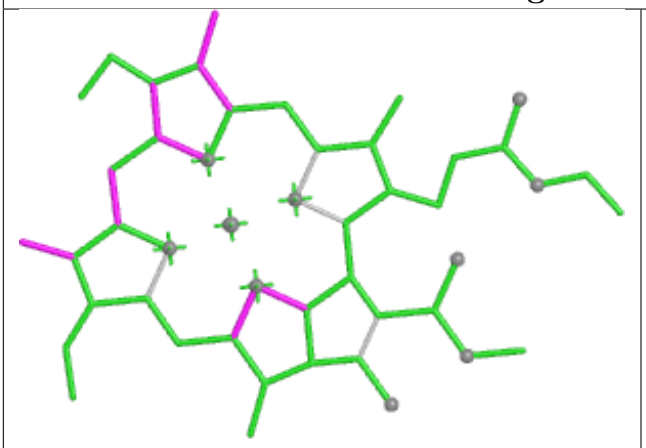


Torsions

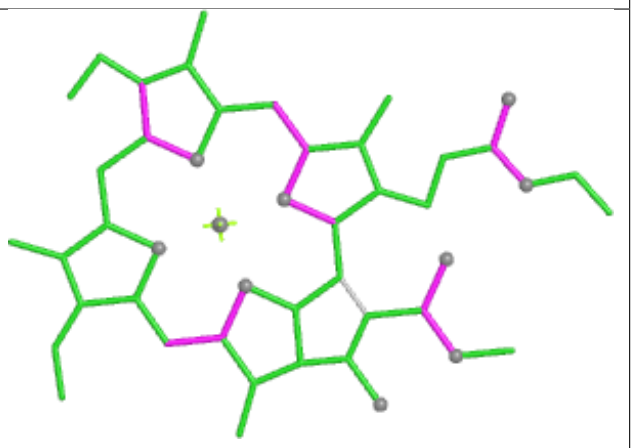


Rings

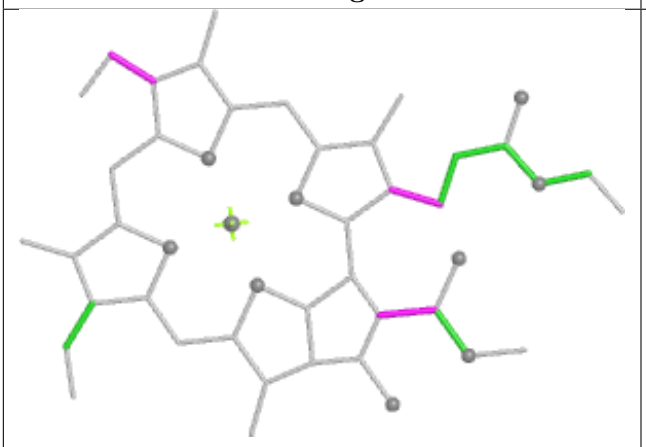
Ligand CLA b 839



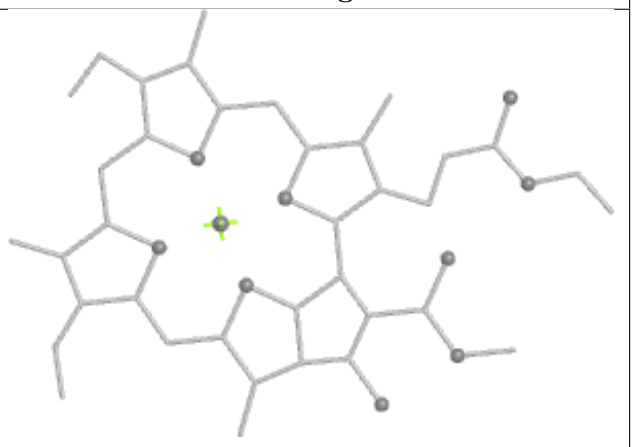
Bond lengths



Bond angles

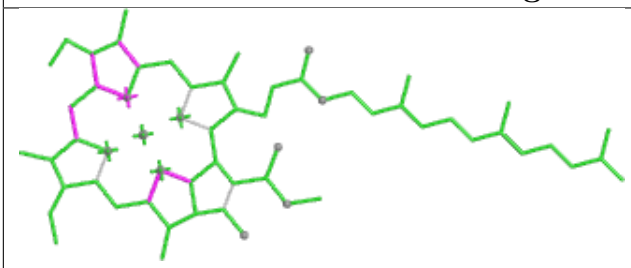


Torsions

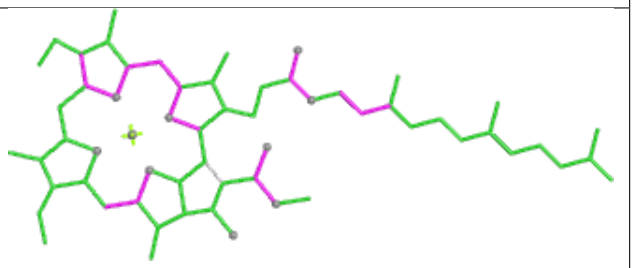


Rings

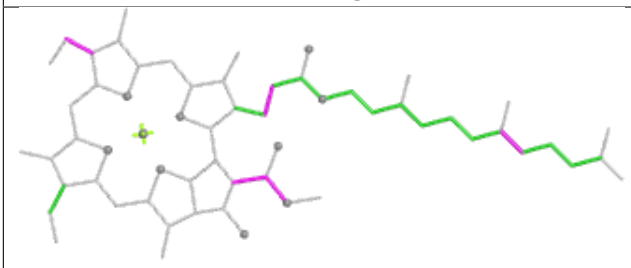
Ligand CLA U 211



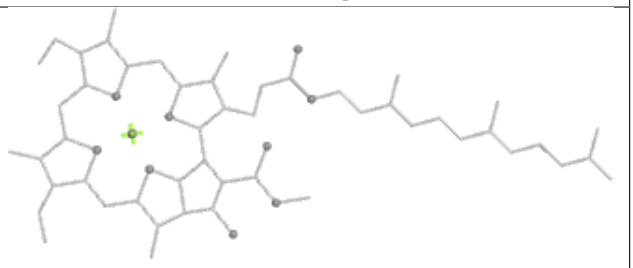
Bond lengths



Bond angles

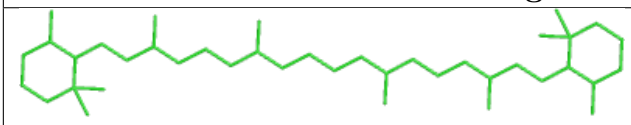


Torsions

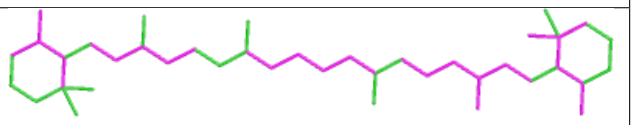


Rings

Ligand BCR b 846



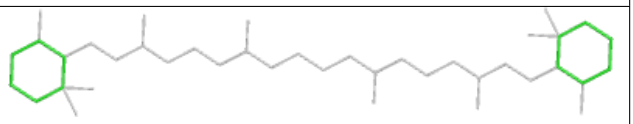
Bond lengths



Bond angles

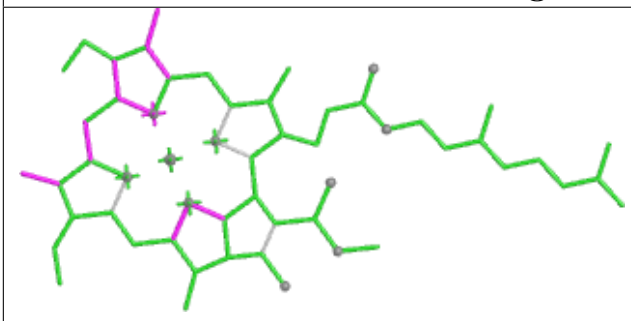


Torsions

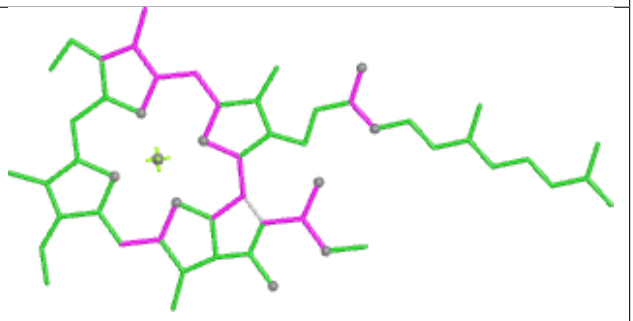


Rings

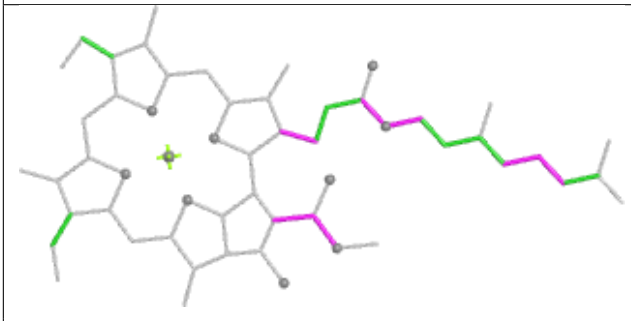
Ligand CLA 0 311



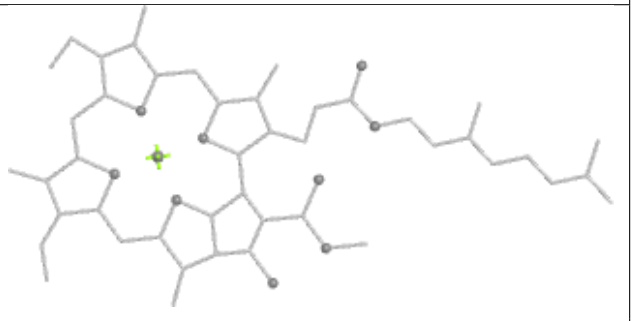
Bond lengths



Bond angles

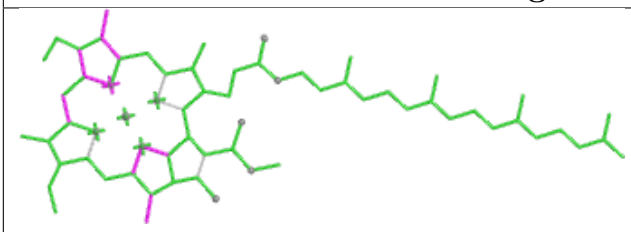


Torsions

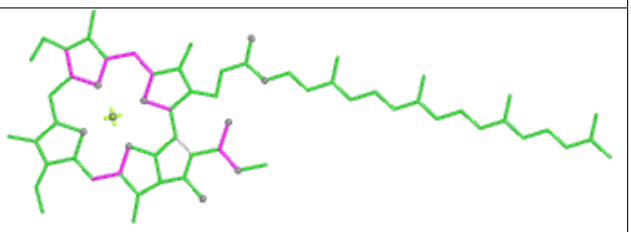


Rings

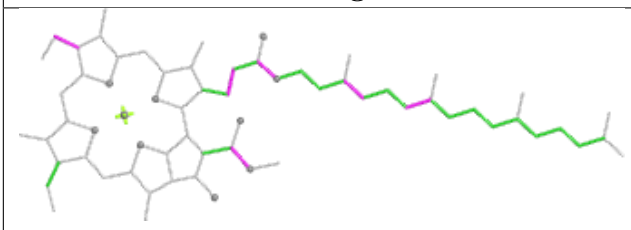
Ligand CLA a 818



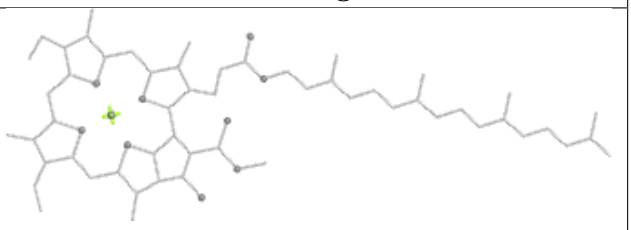
Bond lengths



Bond angles



Torsions

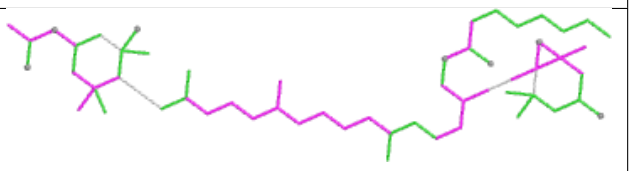


Rings

Ligand A1EB4 5 304



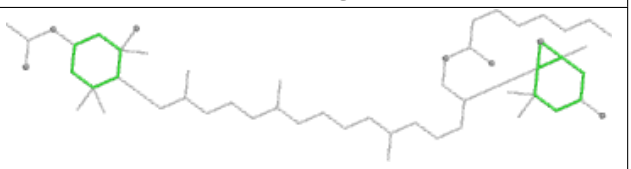
Bond lengths



Bond angles

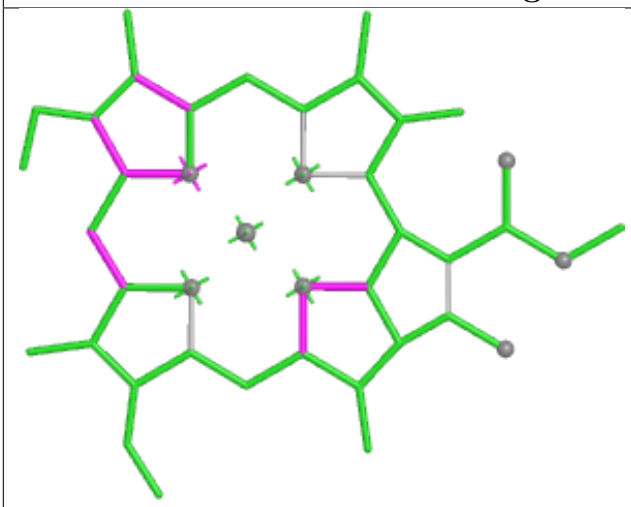


Torsions

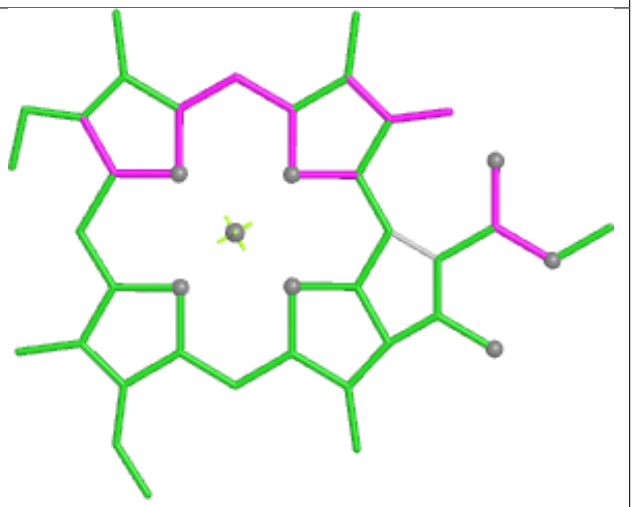


Rings

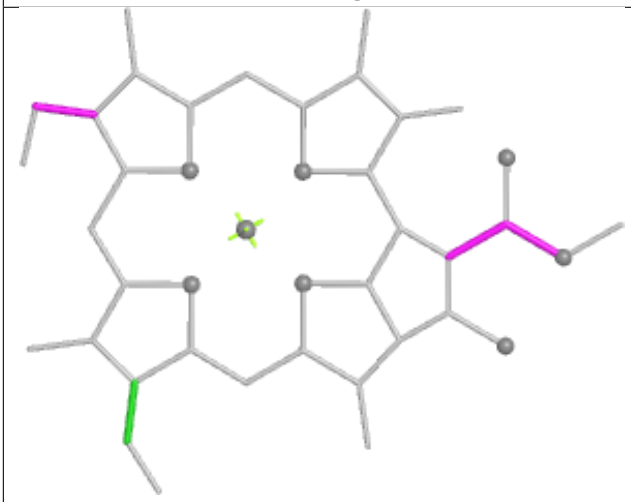
Ligand CLA U 215



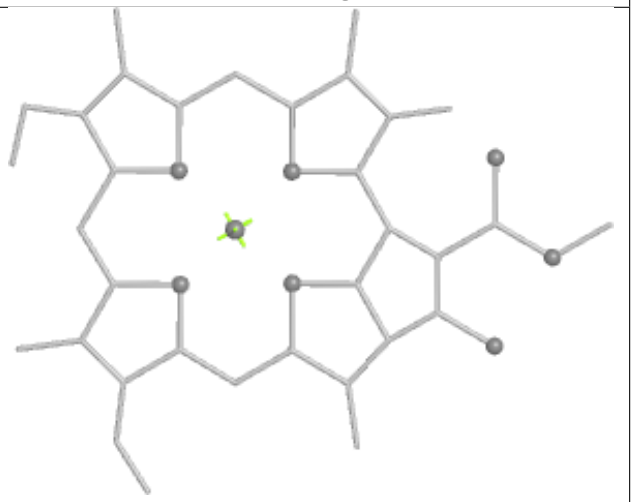
Bond lengths



Bond angles

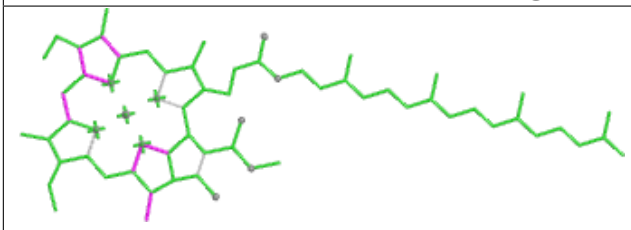


Torsions

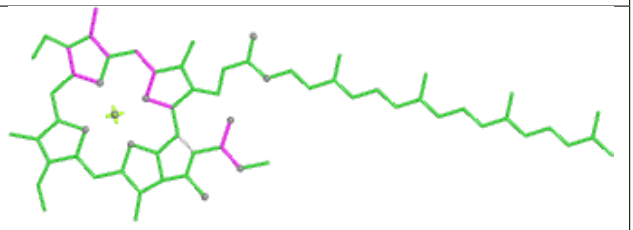


Rings

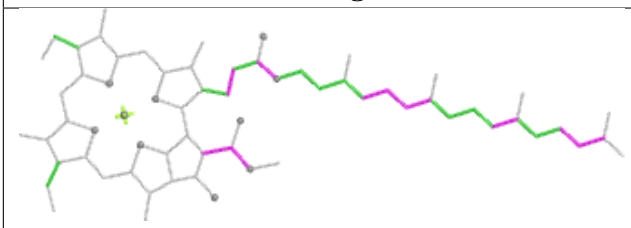
Ligand CLA b 832



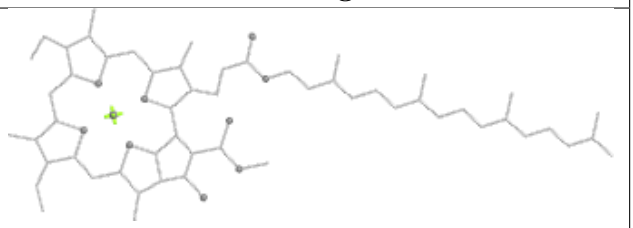
Bond lengths



Bond angles

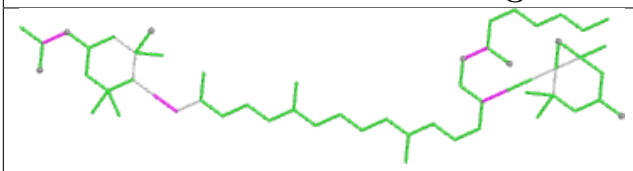


Torsions

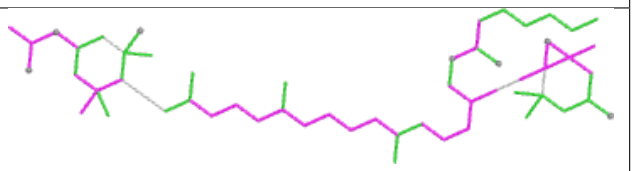


Rings

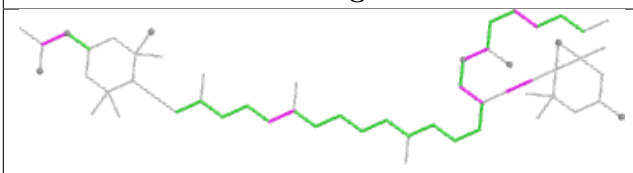
Ligand A1EB4 P 305



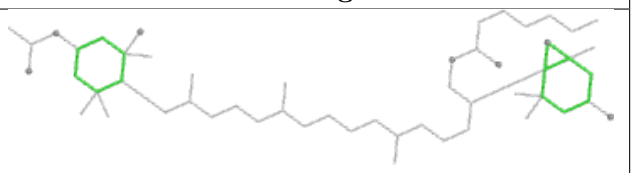
Bond lengths



Bond angles

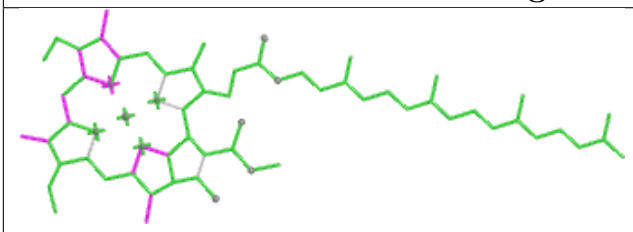


Torsions

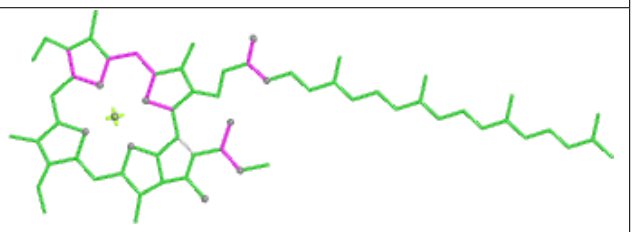


Rings

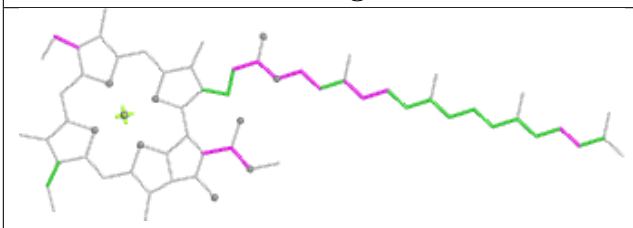
Ligand CLA a 803



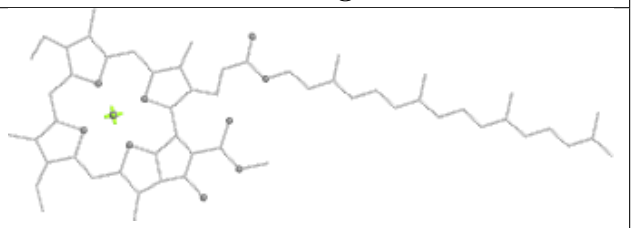
Bond lengths



Bond angles

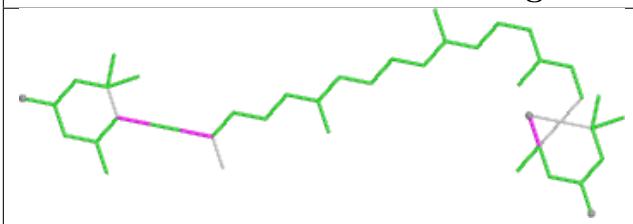


Torsions

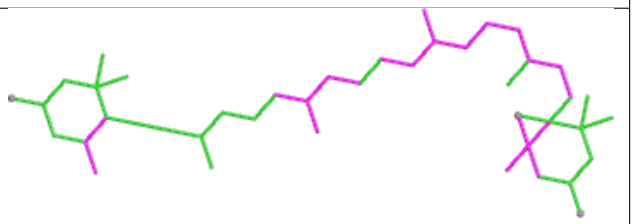


Rings

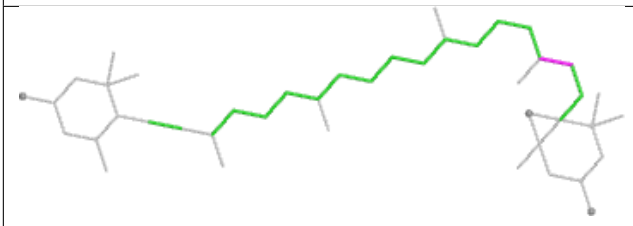
Ligand DD6 P 304



Bond lengths



Bond angles

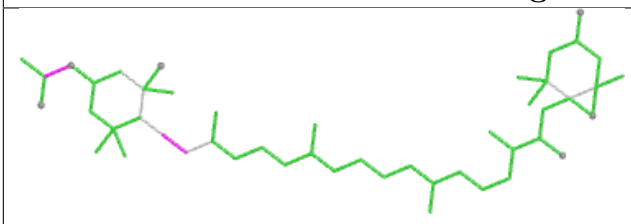


Torsions

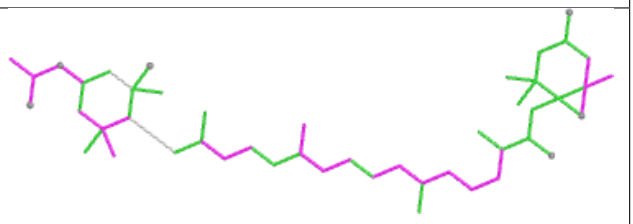


Rings

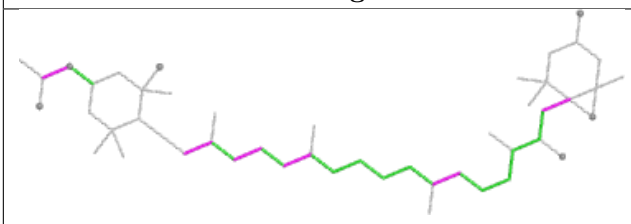
Ligand A86 R 302



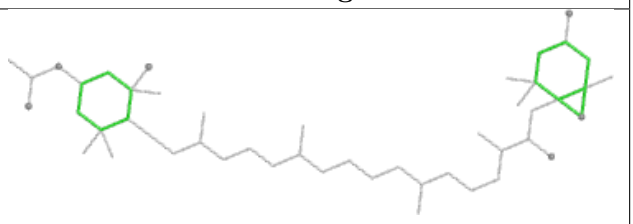
Bond lengths



Bond angles

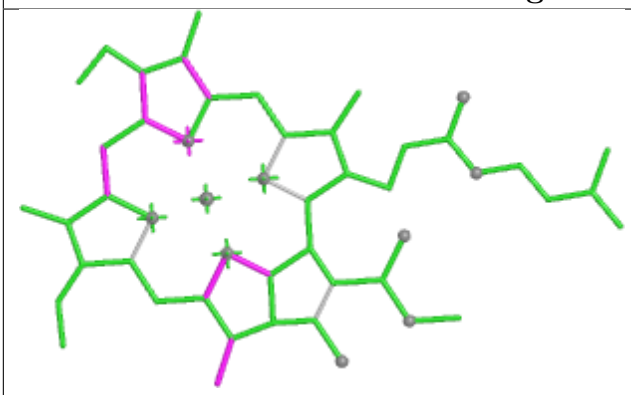


Torsions

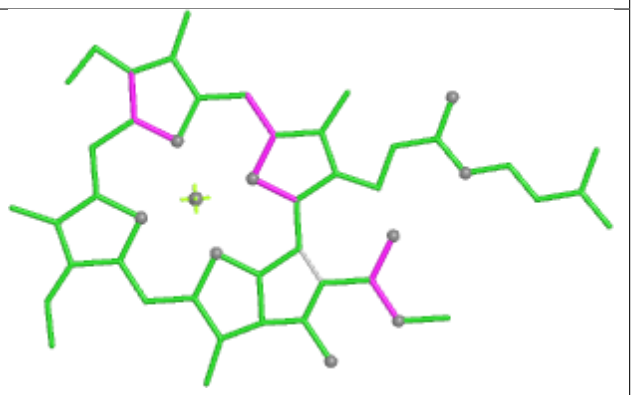


Rings

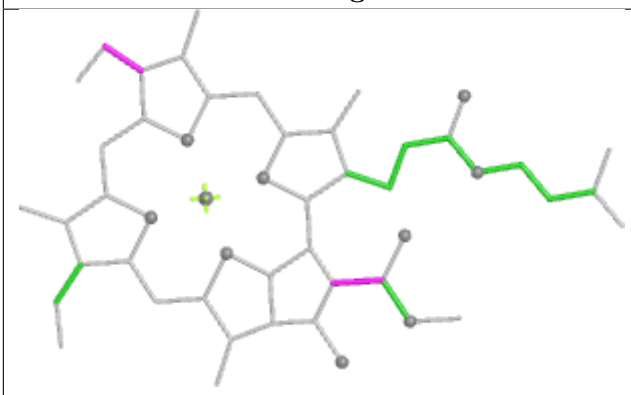
Ligand CLA L 313



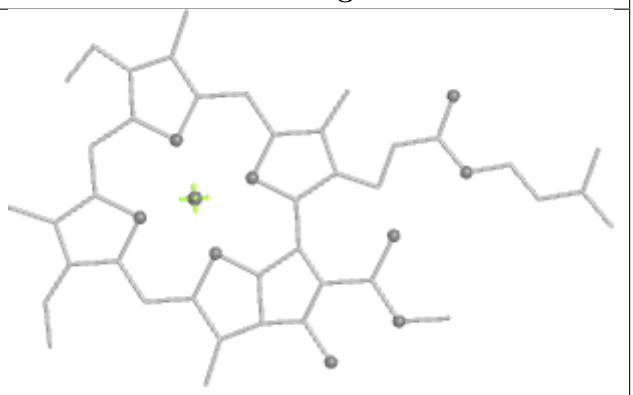
Bond lengths



Bond angles

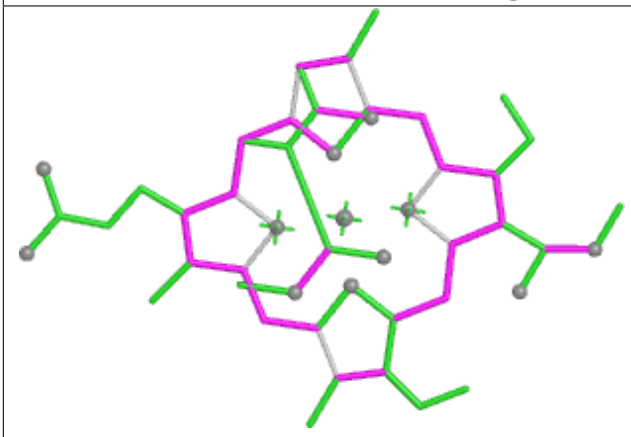


Torsions

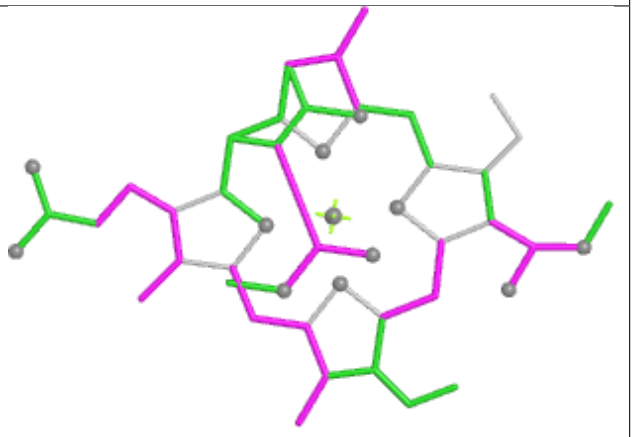


Rings

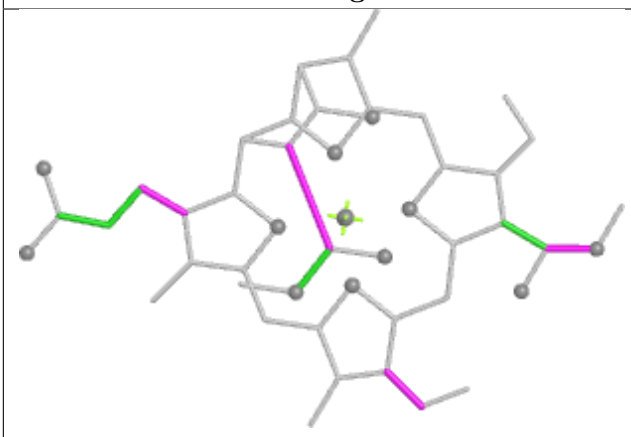
Ligand A1ECV 9 317



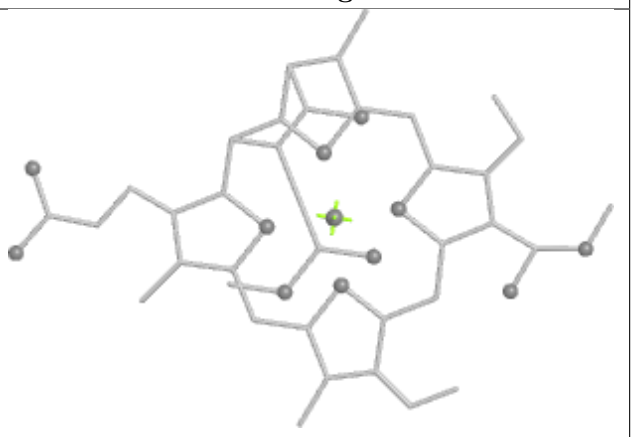
Bond lengths



Bond angles

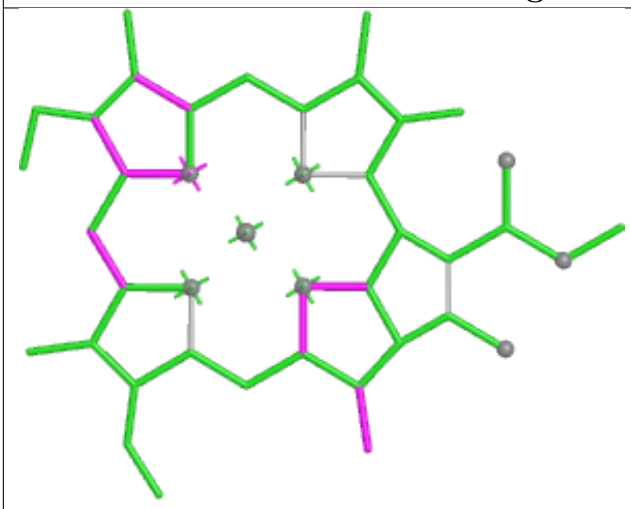


Torsions

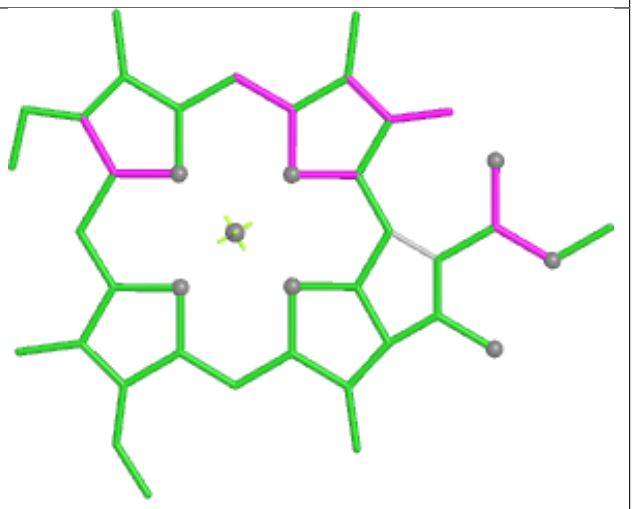


Rings

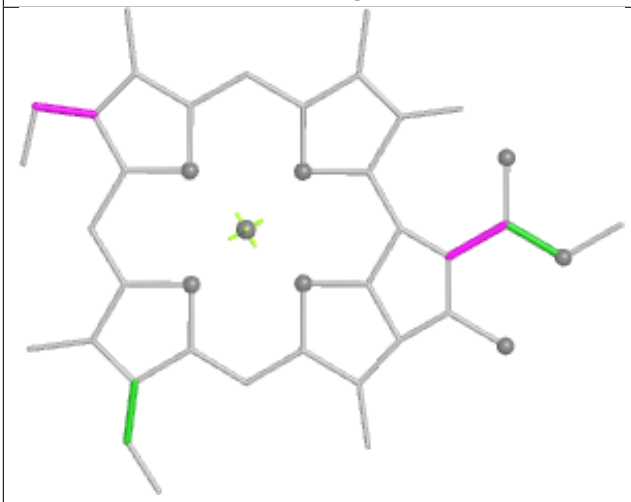
Ligand CLA Z 304



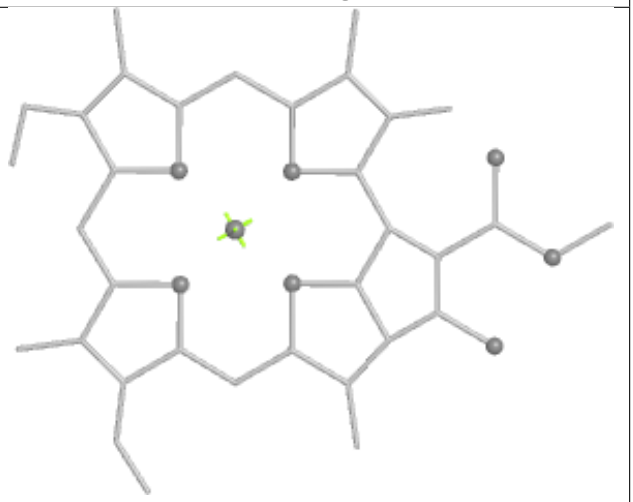
Bond lengths



Bond angles

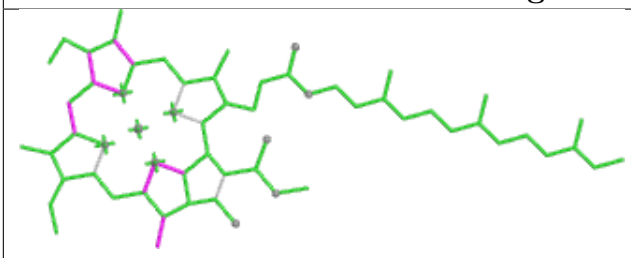


Torsions

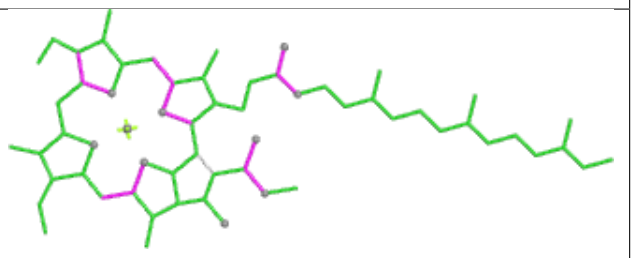


Rings

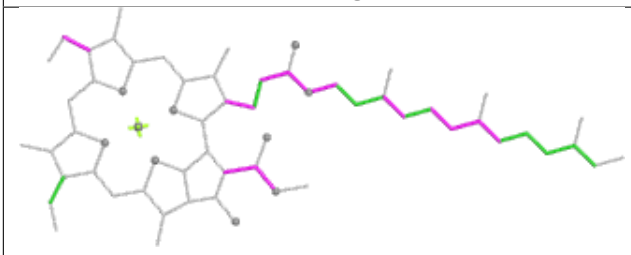
Ligand CLA S 308



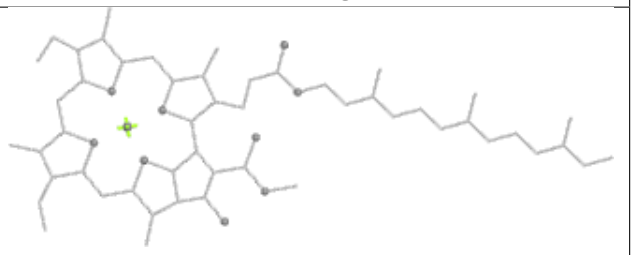
Bond lengths



Bond angles

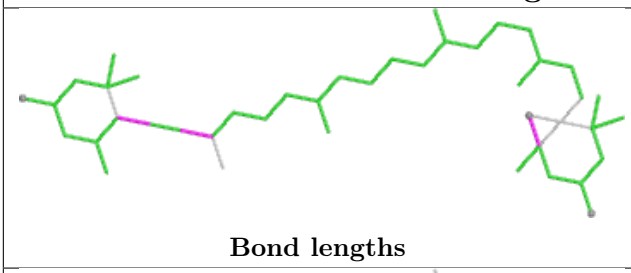


Torsions

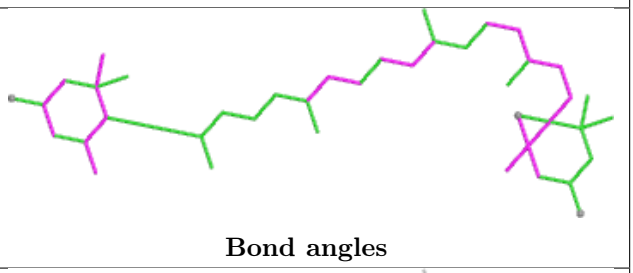


Rings

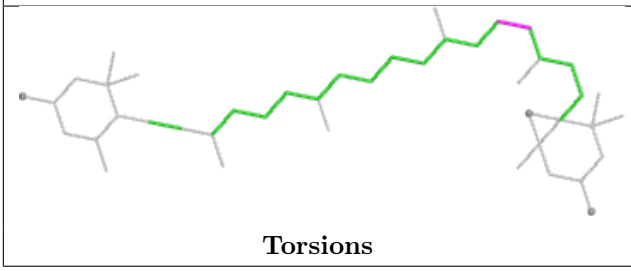
Ligand DD6 G 303



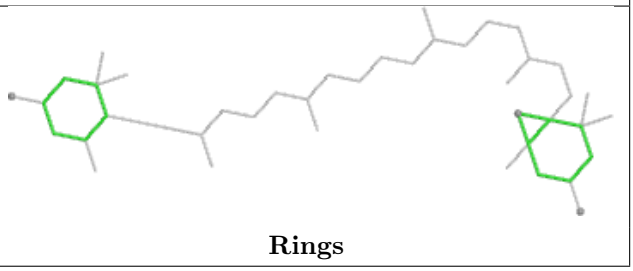
Bond lengths



Bond angles

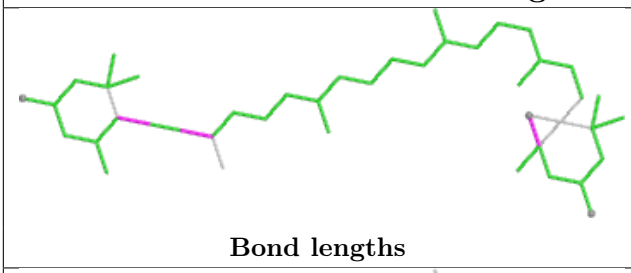


Torsions

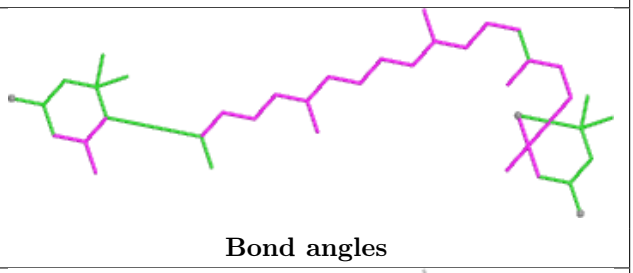


Rings

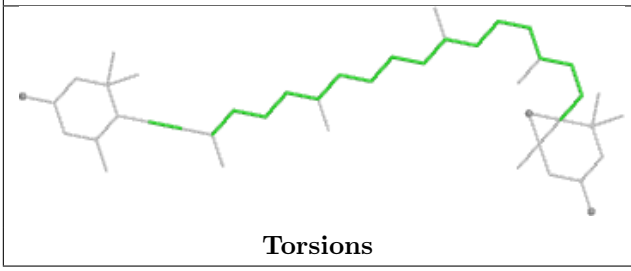
Ligand DD6 x 304



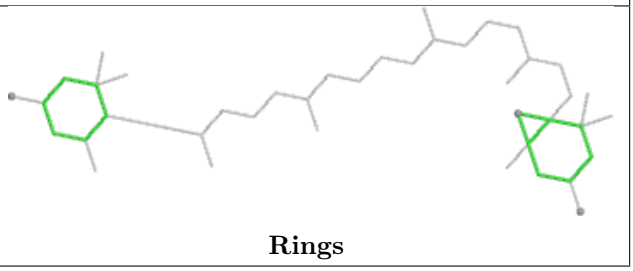
Bond lengths



Bond angles

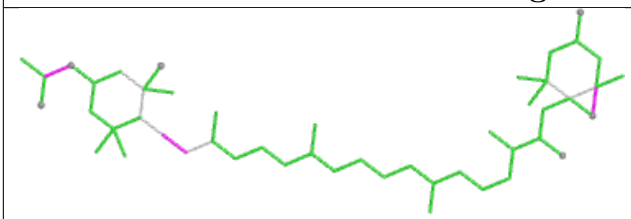


Torsions

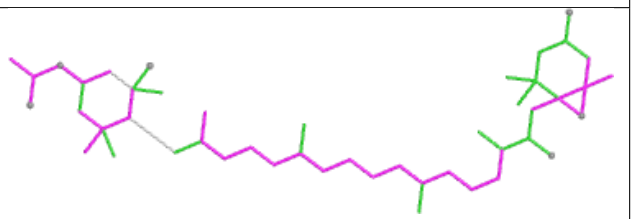


Rings

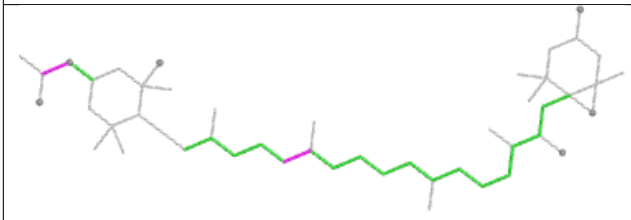
Ligand A86 U 202



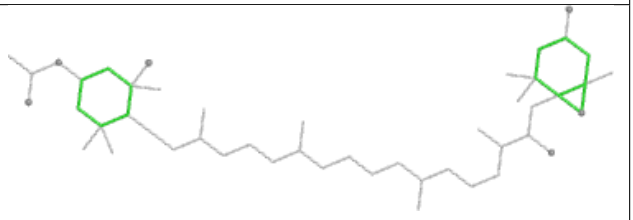
Bond lengths



Bond angles

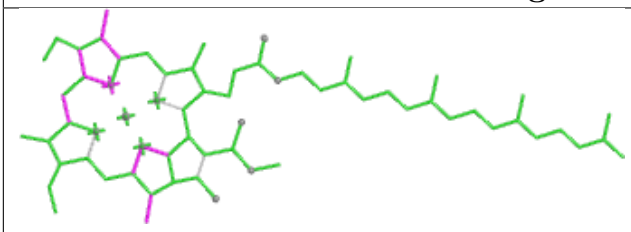


Torsions

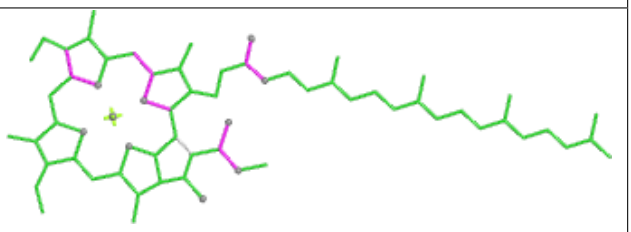


Rings

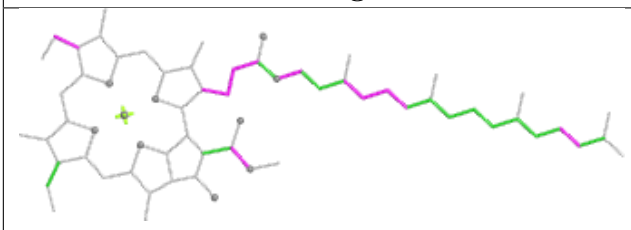
Ligand CLA a 807



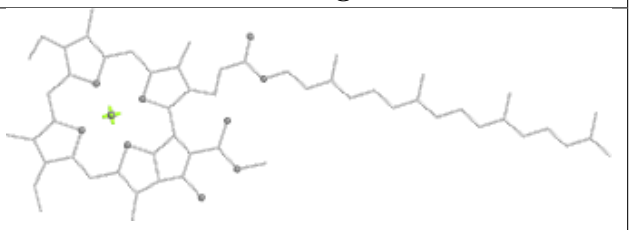
Bond lengths



Bond angles

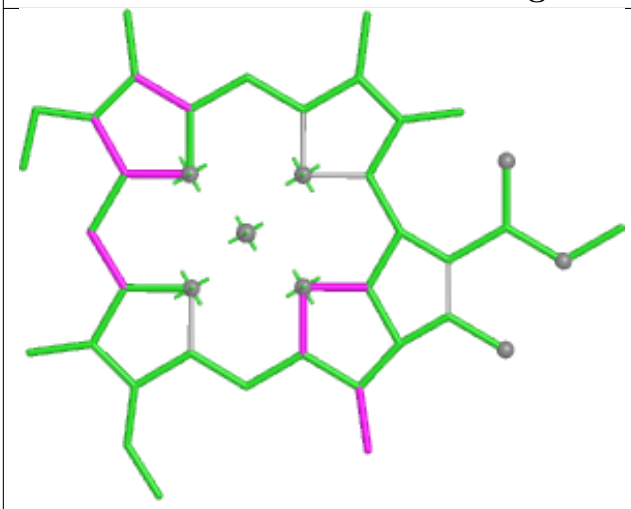


Torsions

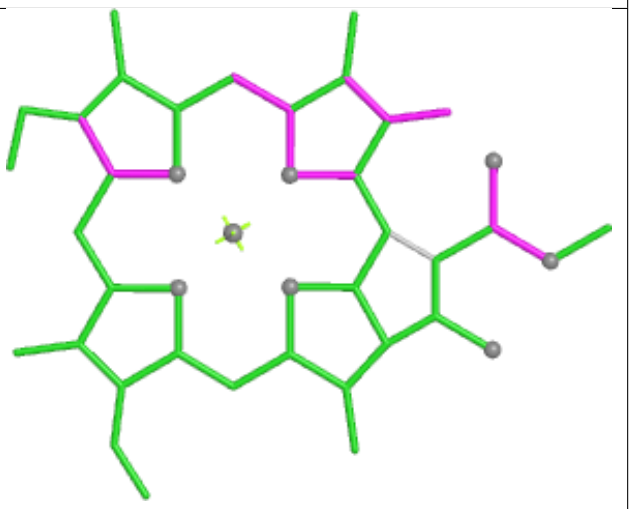


Rings

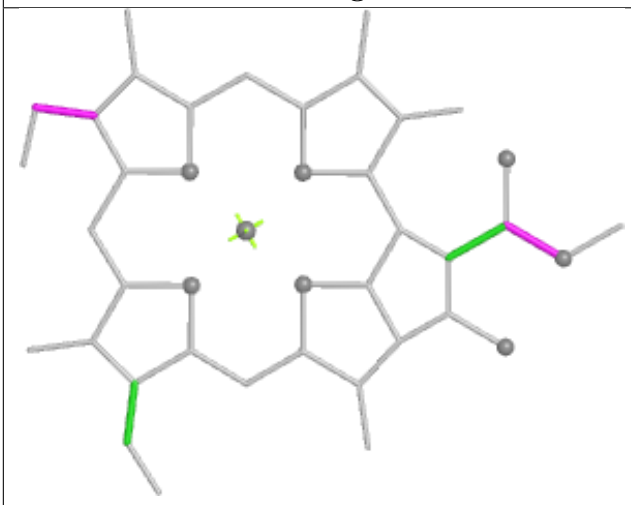
Ligand CLA 2 307



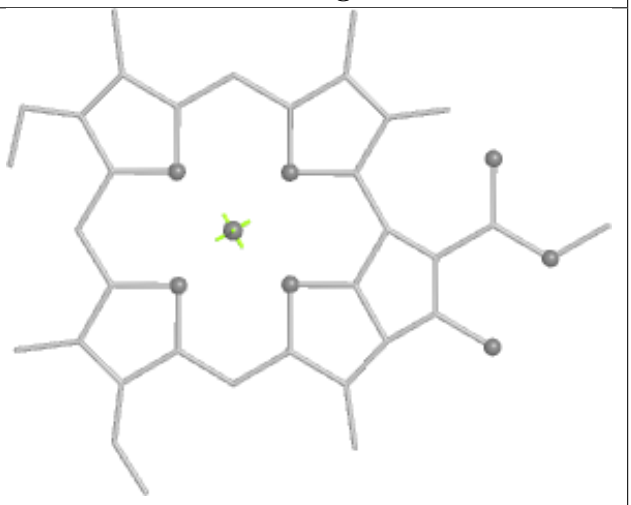
Bond lengths



Bond angles

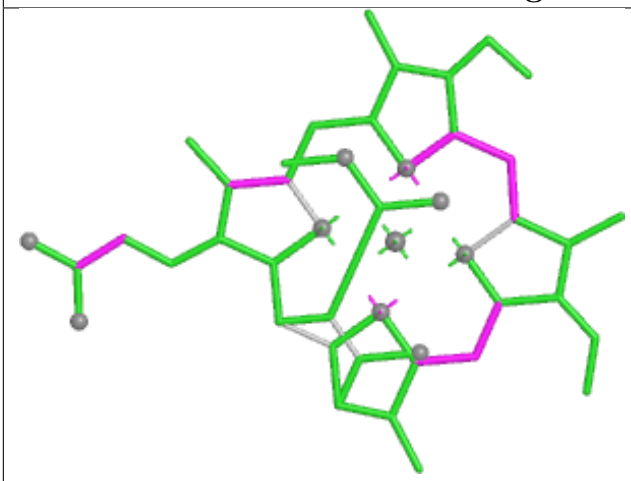


Torsions

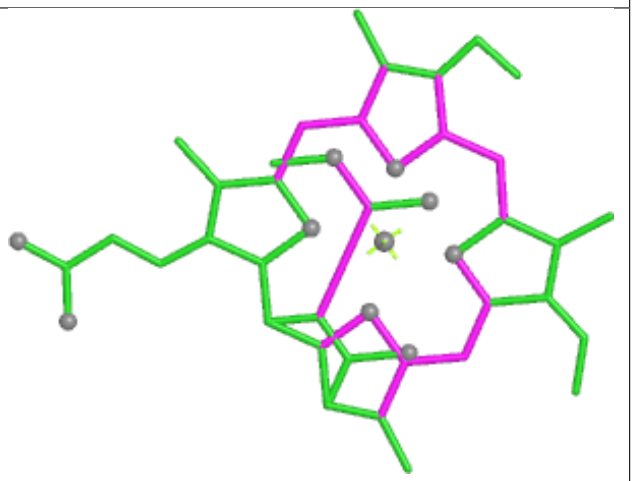


Rings

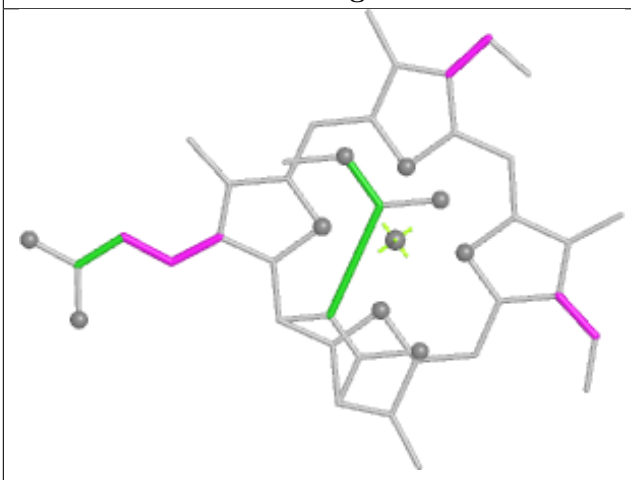
Ligand KC2 A 310



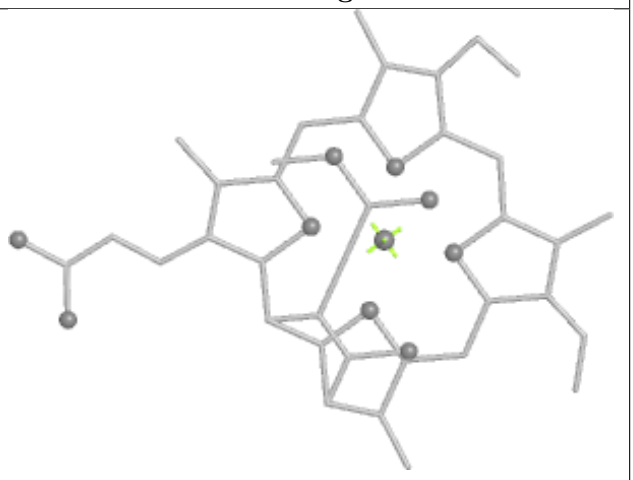
Bond lengths



Bond angles

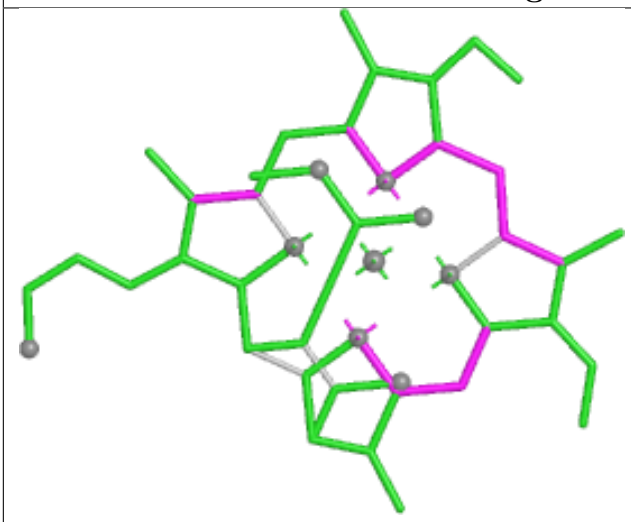


Torsions

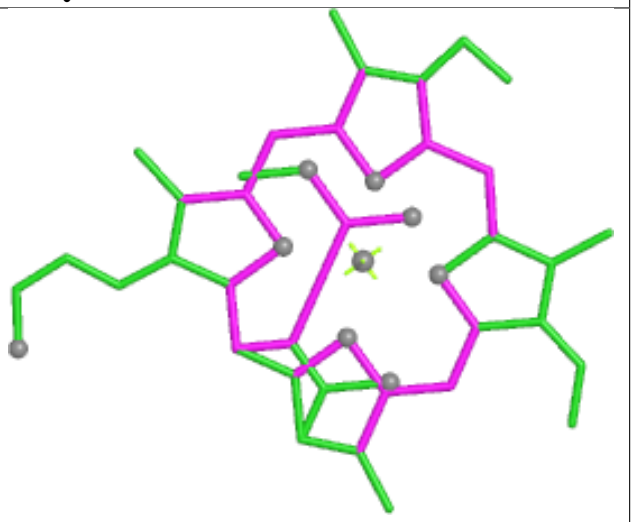


Rings

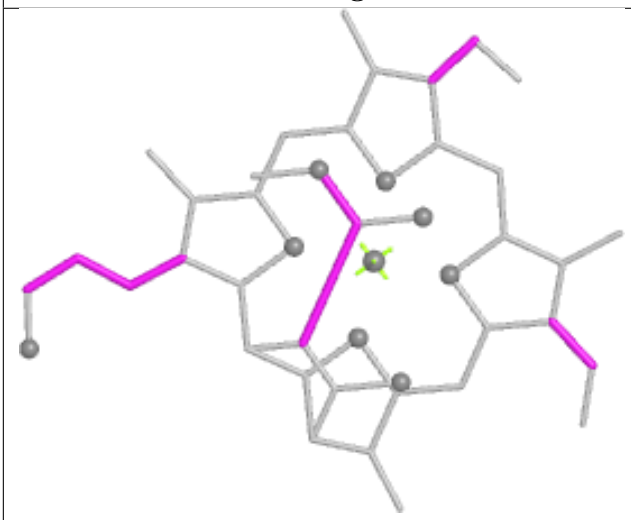
Ligand KC2 Q 313



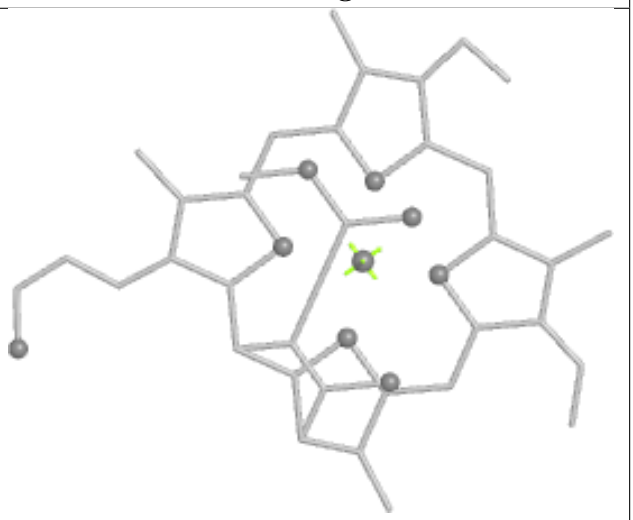
Bond lengths



Bond angles

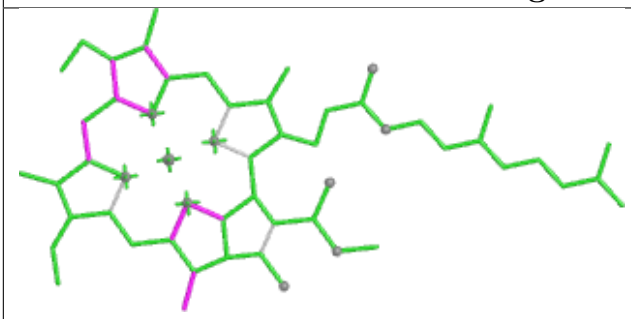


Torsions

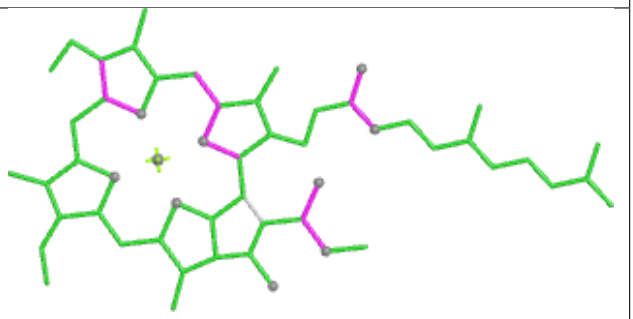


Rings

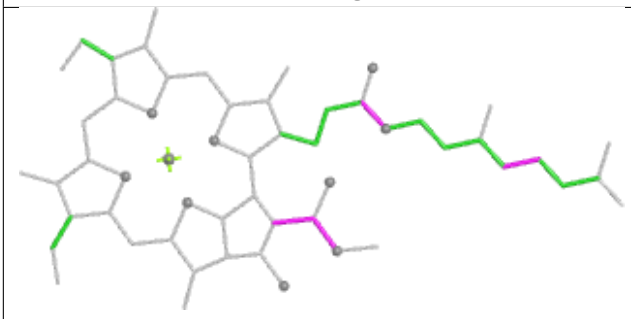
Ligand CLA o 203



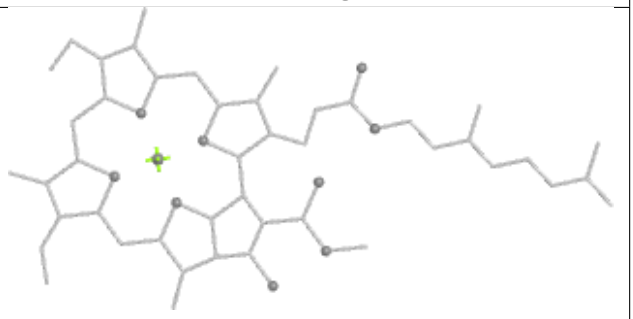
Bond lengths



Bond angles

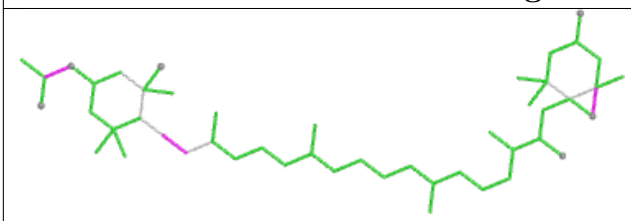


Torsions

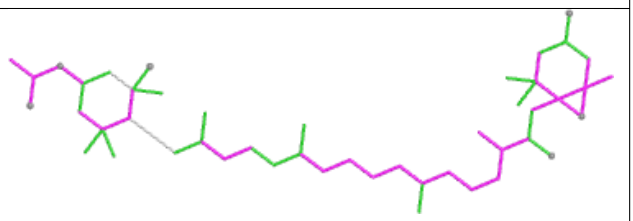


Rings

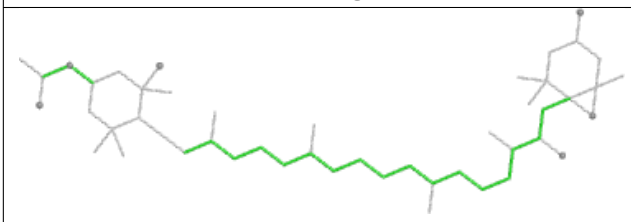
Ligand A86 W 304



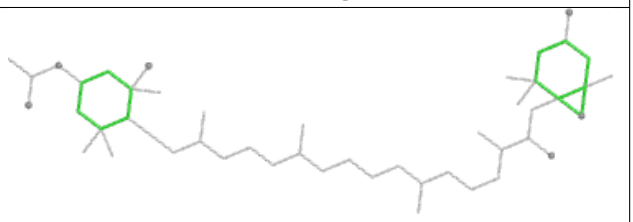
Bond lengths



Bond angles

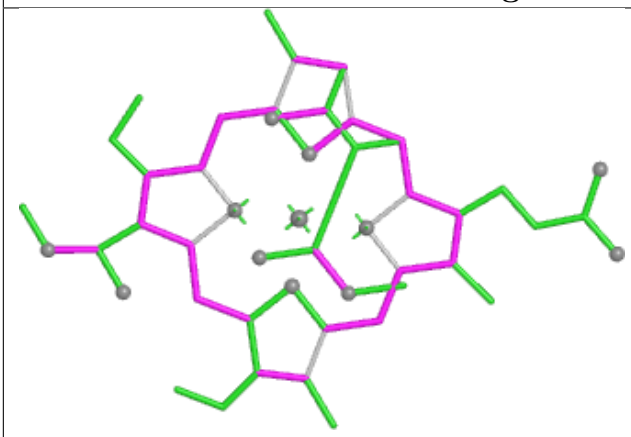


Torsions

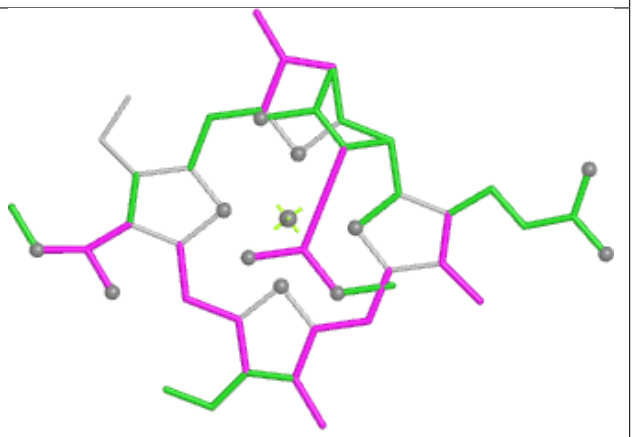


Rings

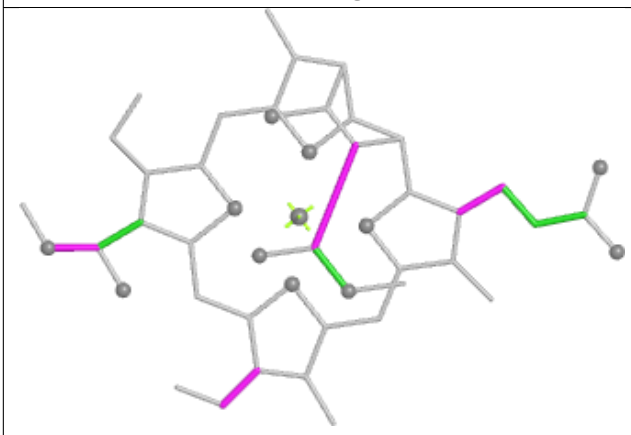
Ligand A1ECV E 311



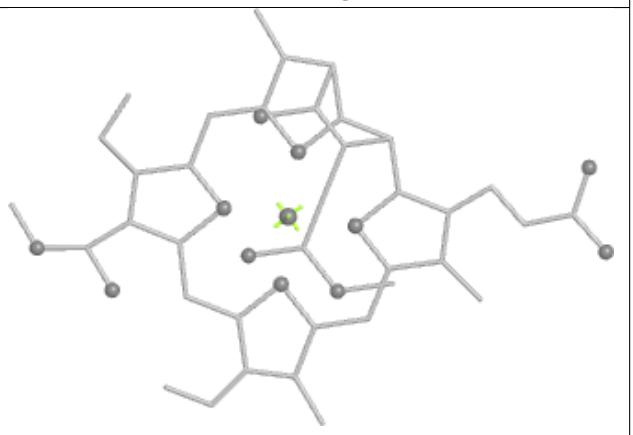
Bond lengths



Bond angles

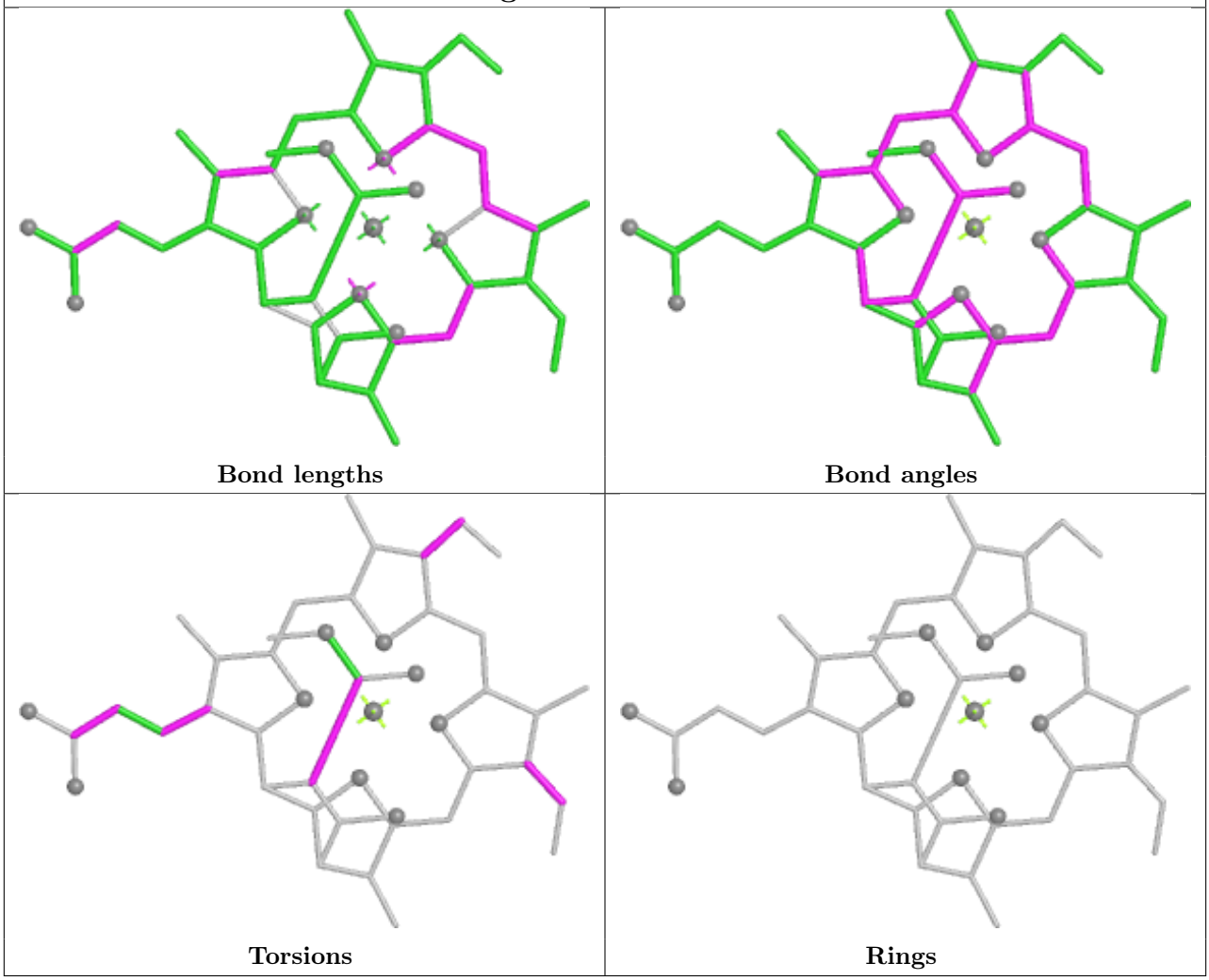


Torsions



Rings

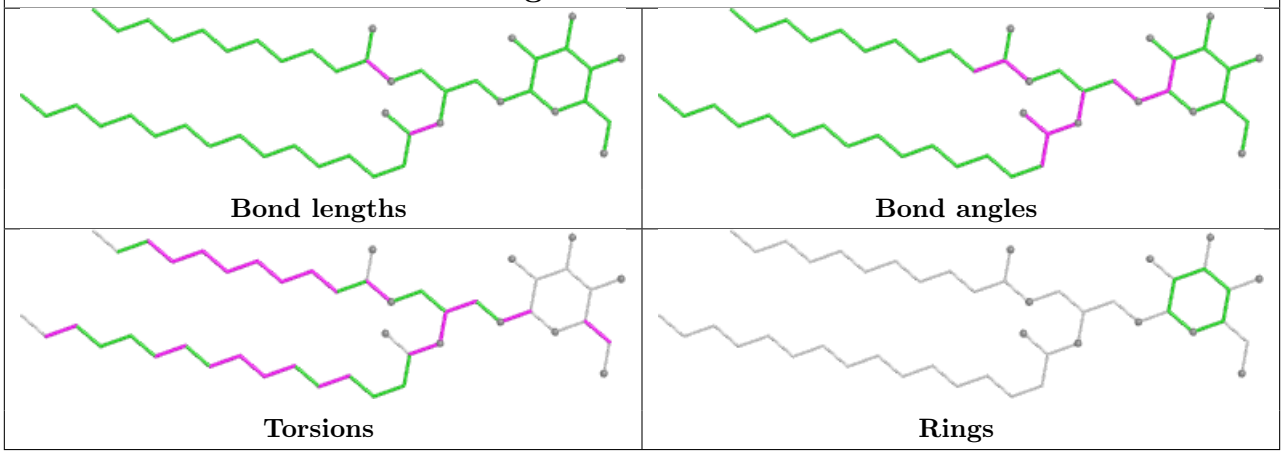
Ligand KC2 4 324



Bond lengths | Bond angles

Torsions | Rings

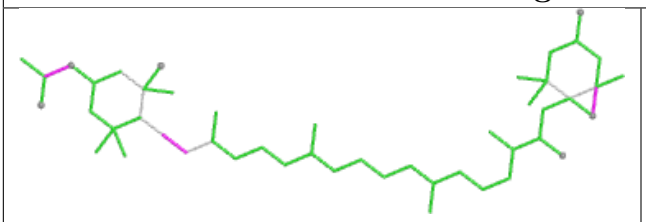
Ligand LMG 4 326



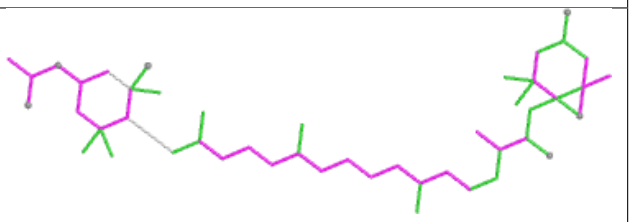
Bond lengths | Bond angles

Torsions | Rings

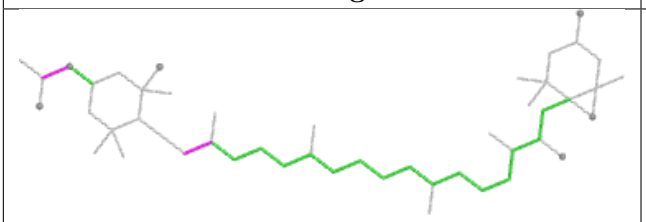
Ligand A86 8 323



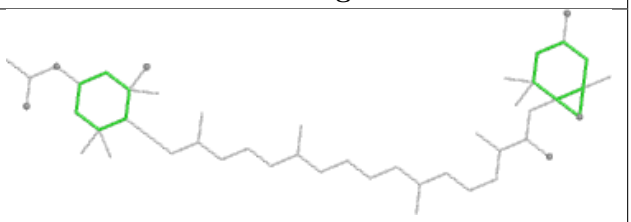
Bond lengths



Bond angles



Torsions

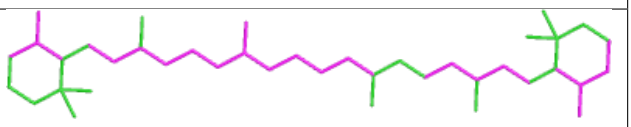


Rings

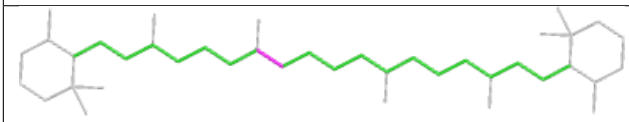
Ligand BCR f 804



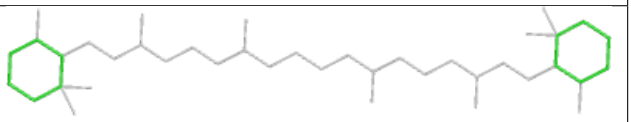
Bond lengths



Bond angles

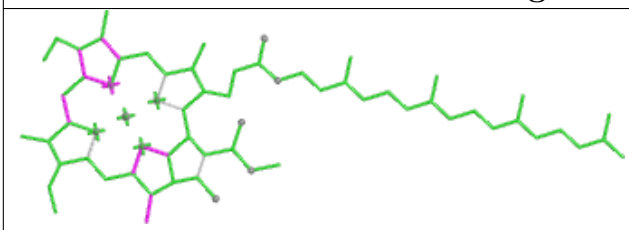


Torsions

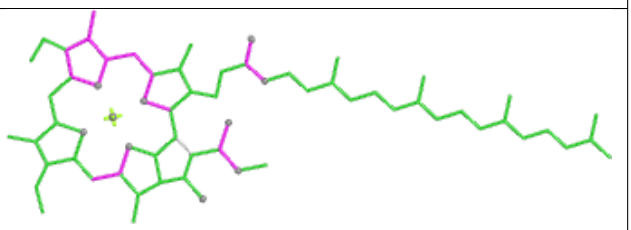


Rings

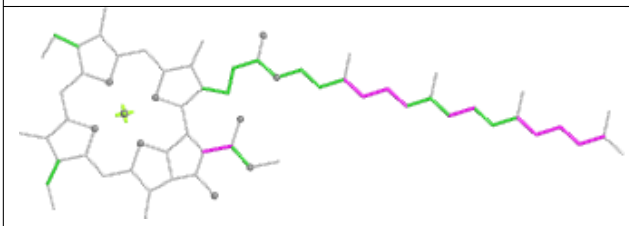
Ligand CLA a 805



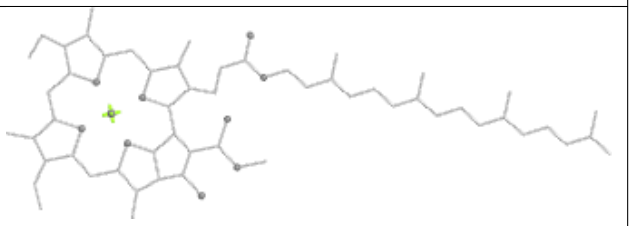
Bond lengths



Bond angles

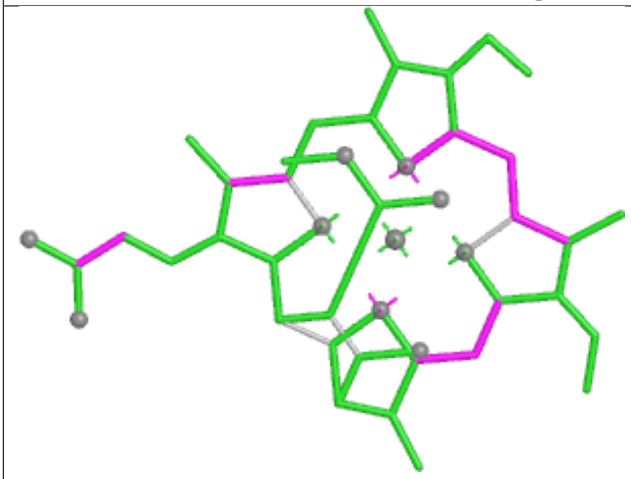


Torsions

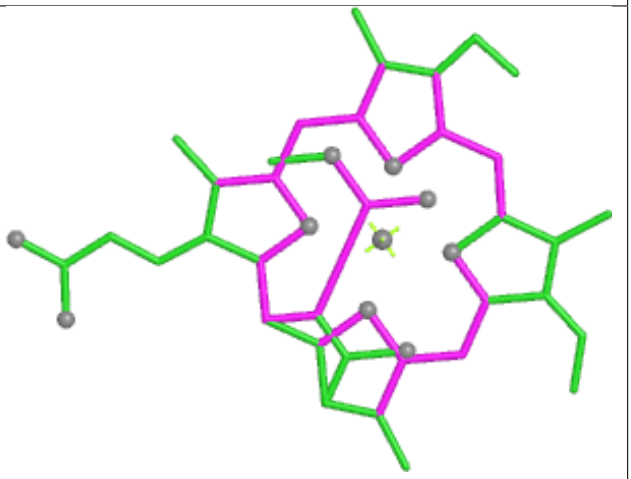


Rings

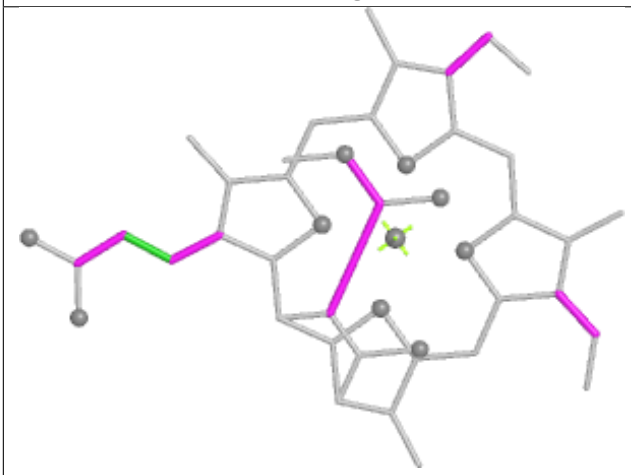
Ligand KC2 1 314



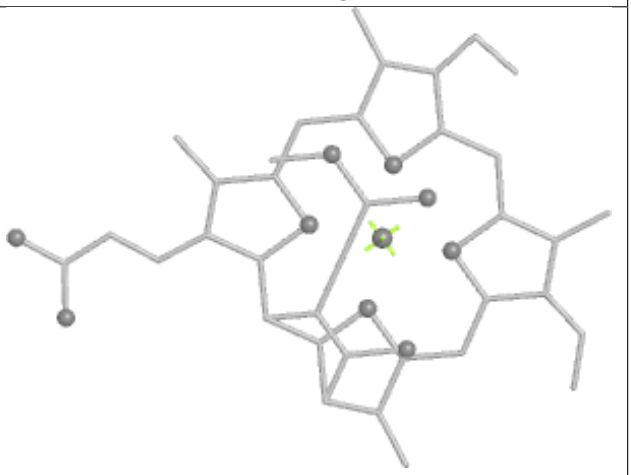
Bond lengths



Bond angles

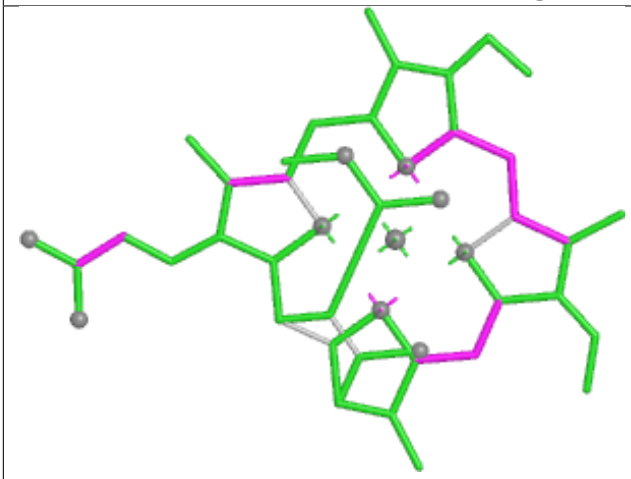


Torsions

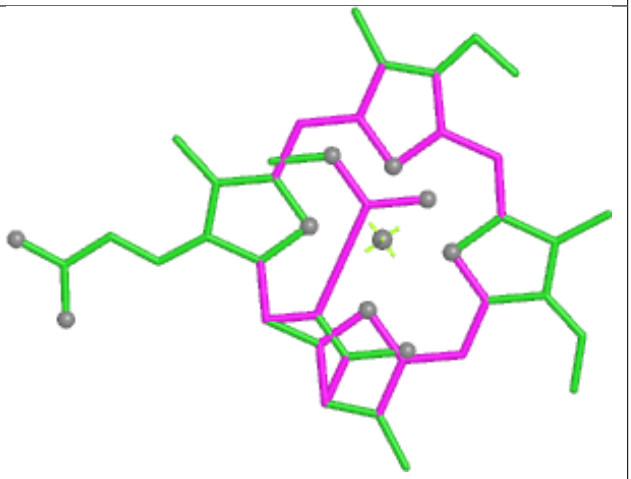


Rings

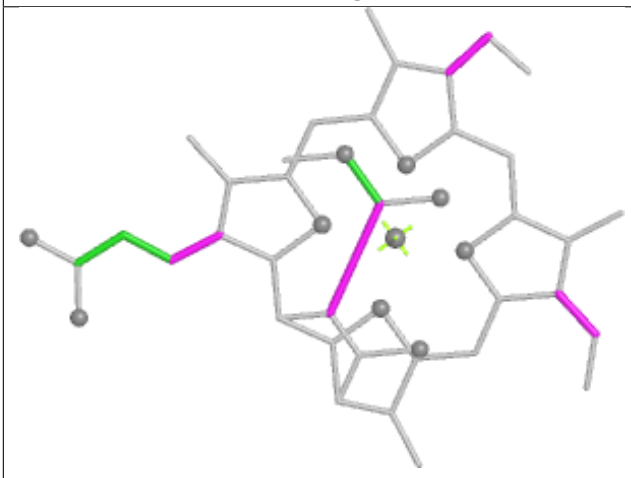
Ligand KC2 z 312



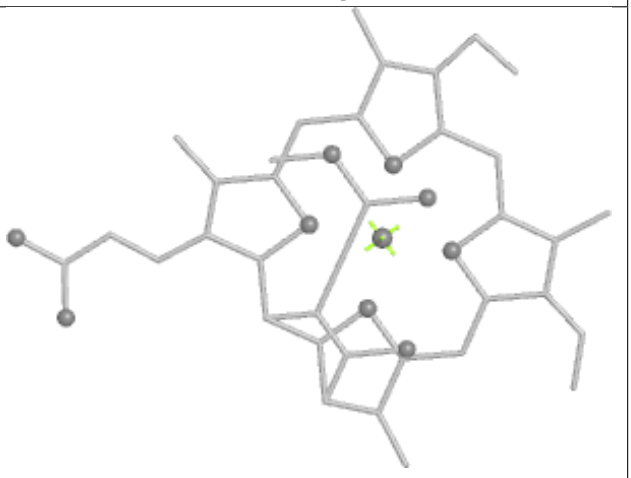
Bond lengths



Bond angles

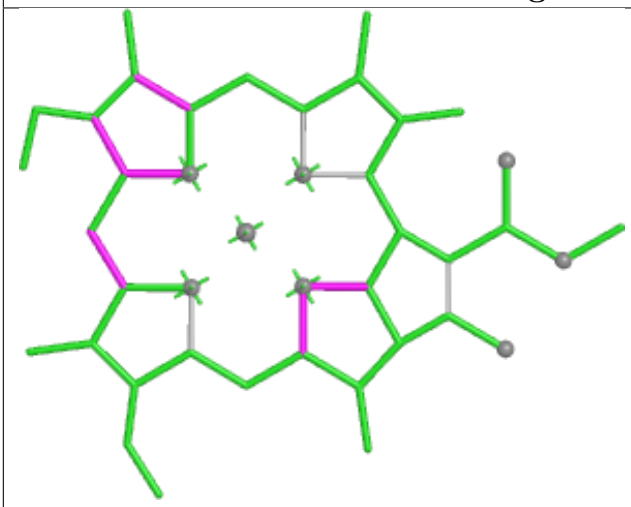


Torsions

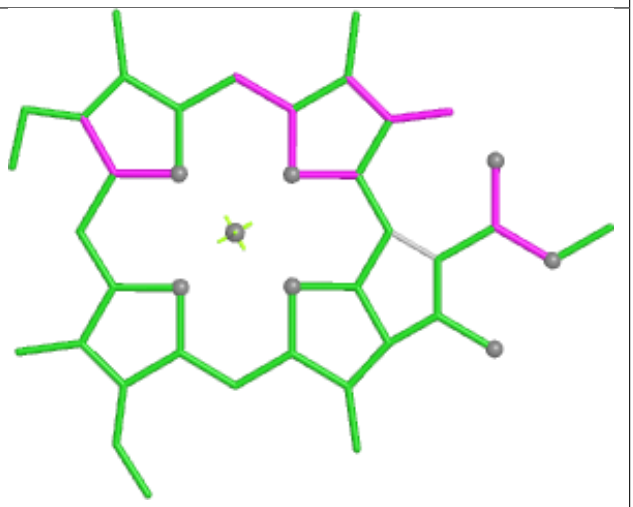


Rings

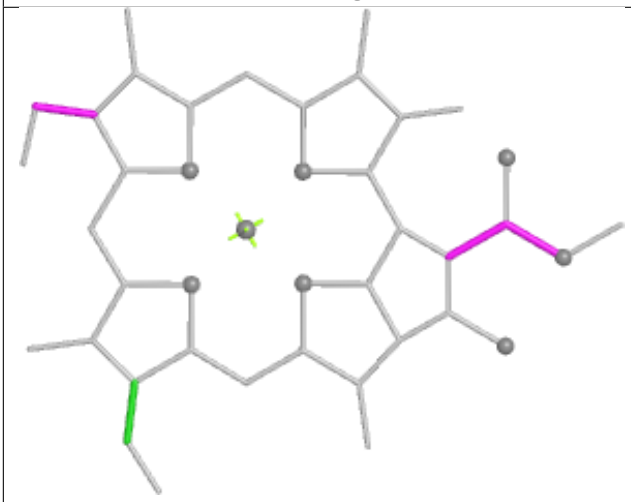
Ligand CLA 1 316



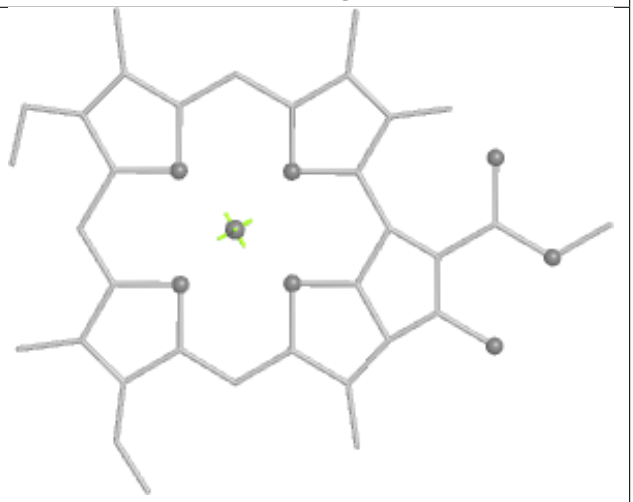
Bond lengths



Bond angles

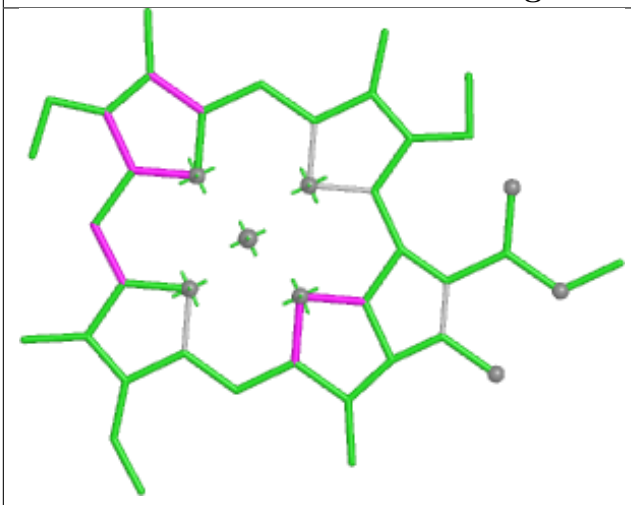


Torsions

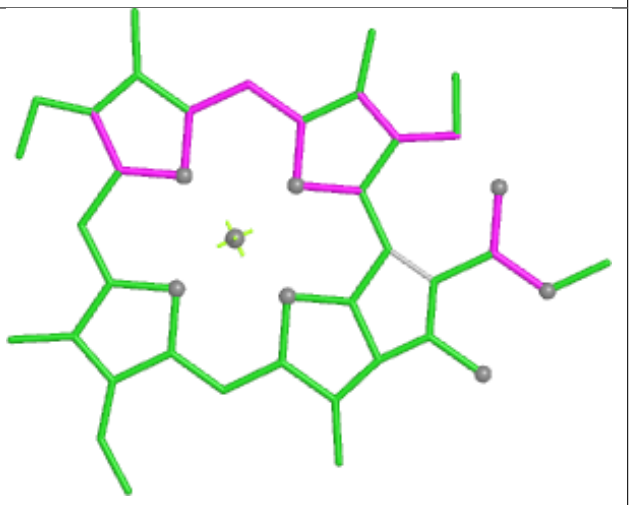


Rings

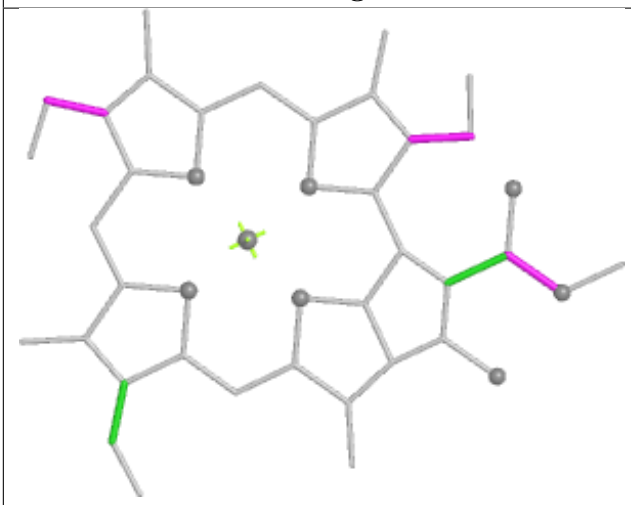
Ligand CLA B 205



Bond lengths



Bond angles

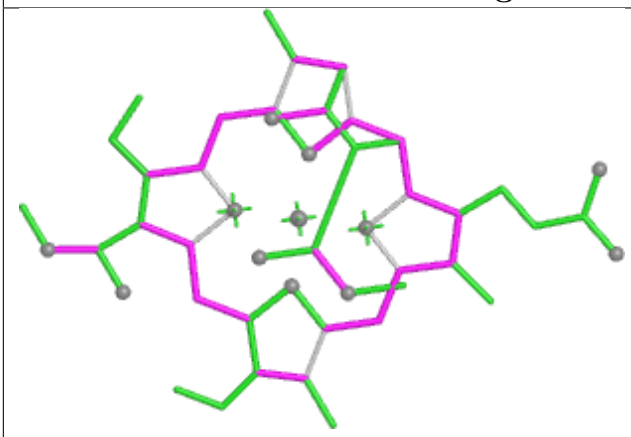


Torsions

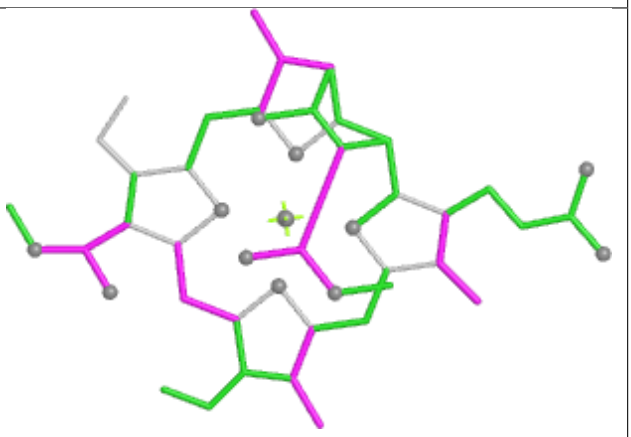


Rings

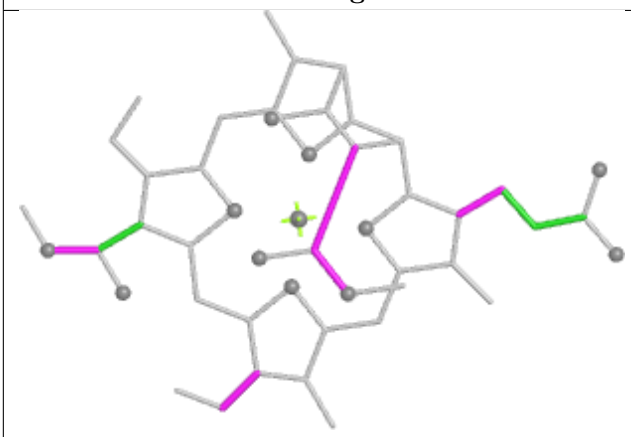
Ligand A1ECV W 317



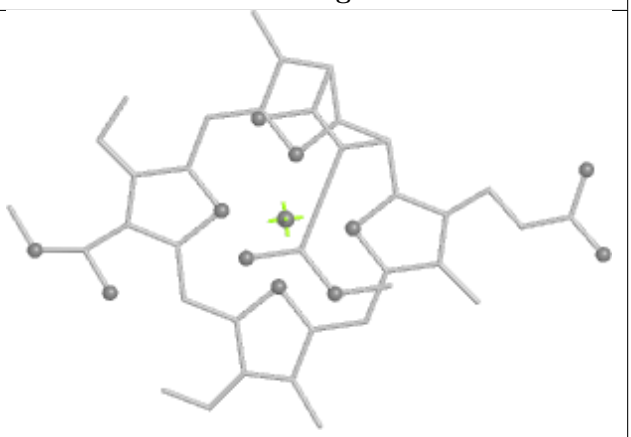
Bond lengths



Bond angles

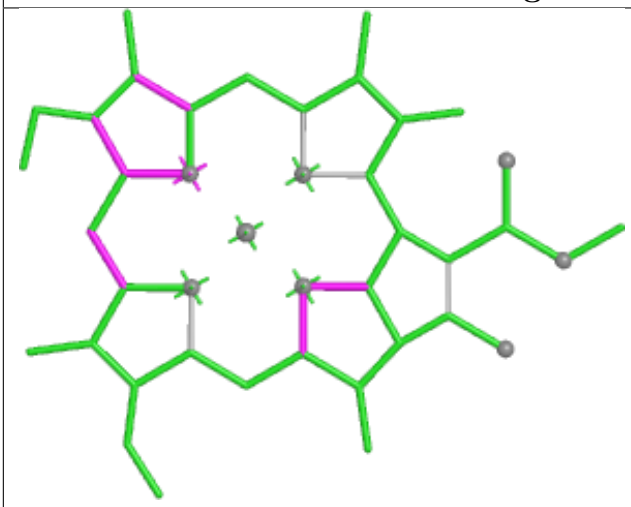


Torsions

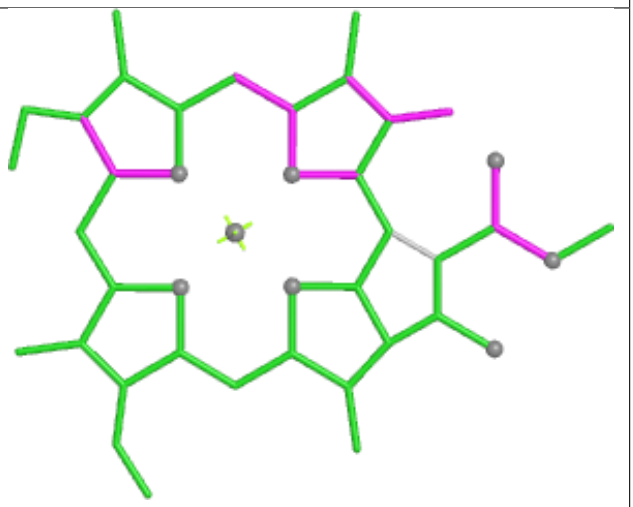


Rings

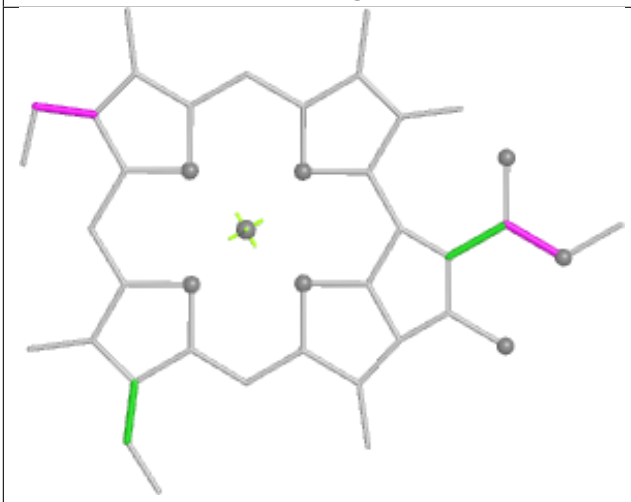
Ligand CLA Y 302



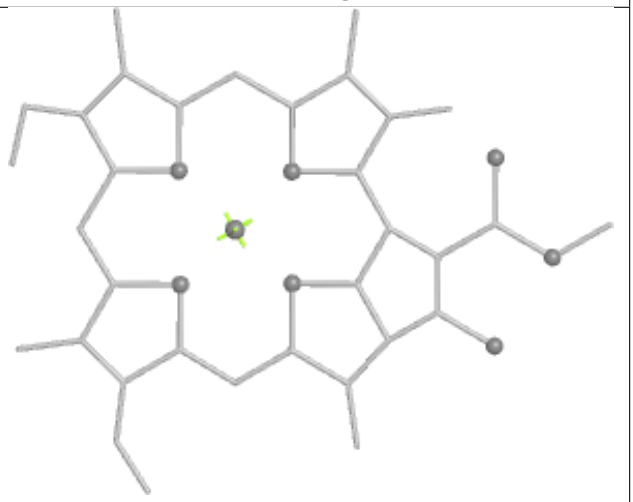
Bond lengths



Bond angles

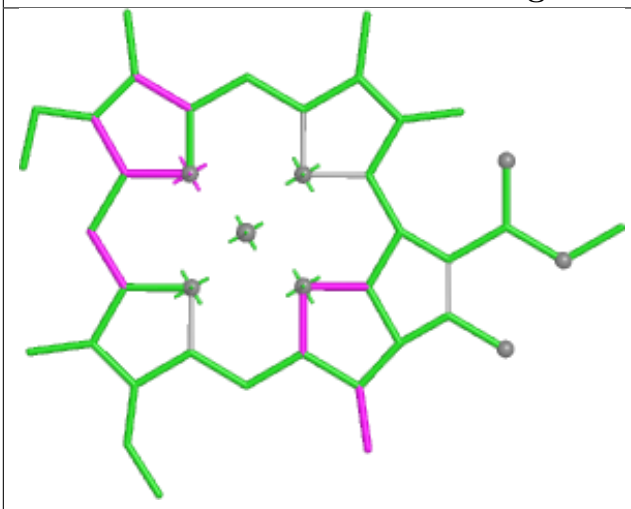


Torsions

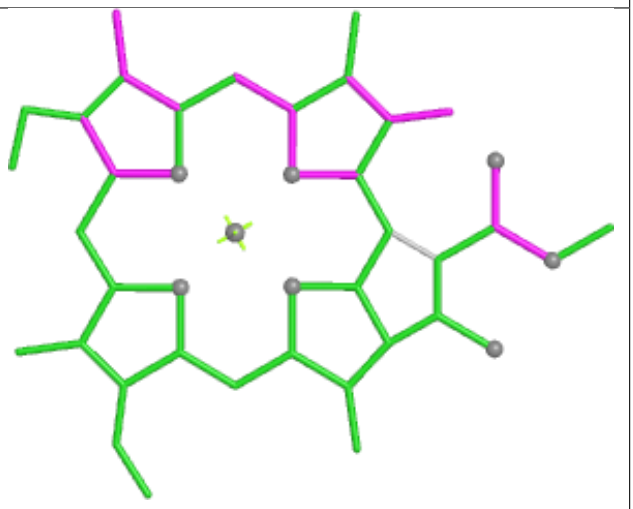


Rings

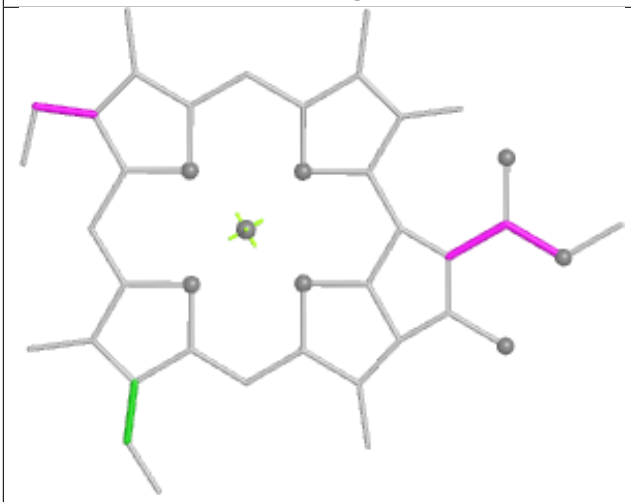
Ligand CLA x 309



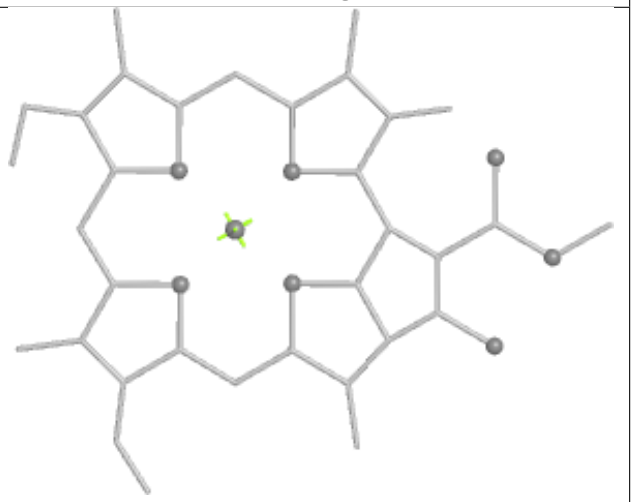
Bond lengths



Bond angles

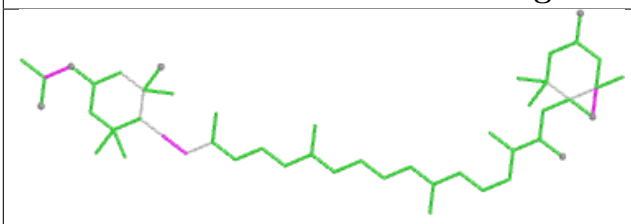


Torsions

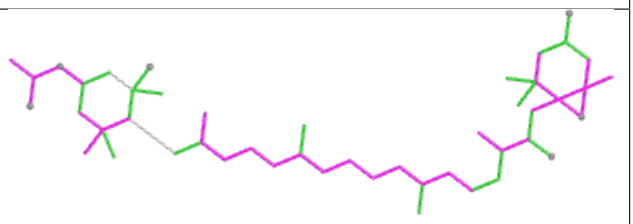


Rings

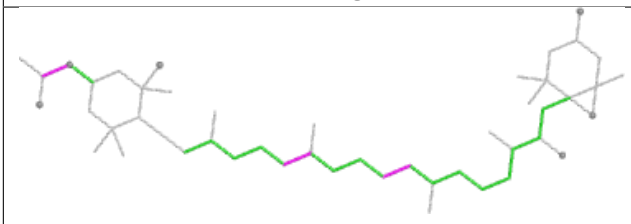
Ligand A86 8 309



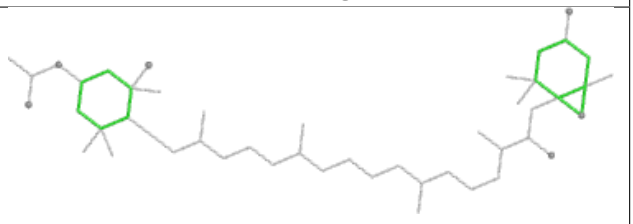
Bond lengths



Bond angles

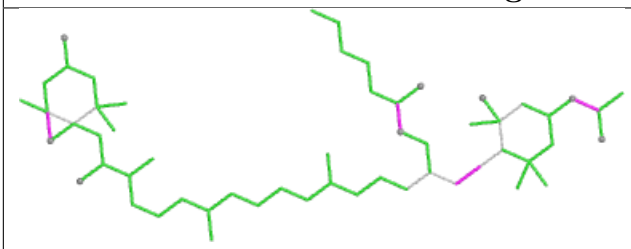


Torsions

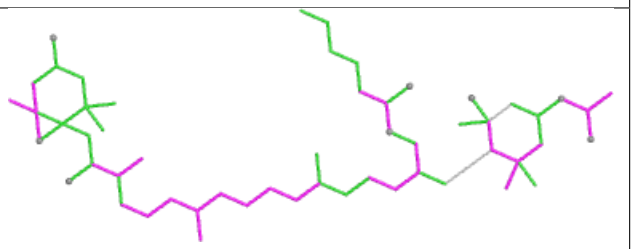


Rings

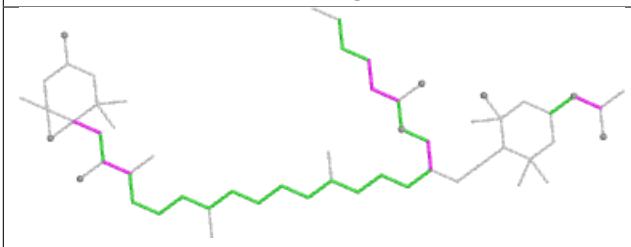
Ligand A1EB1 V 305



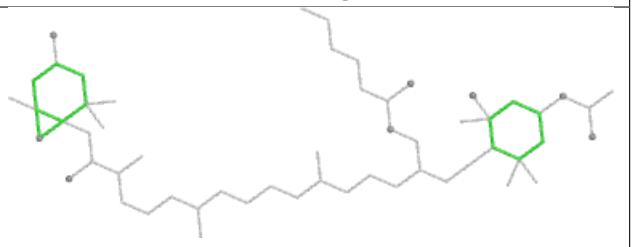
Bond lengths



Bond angles

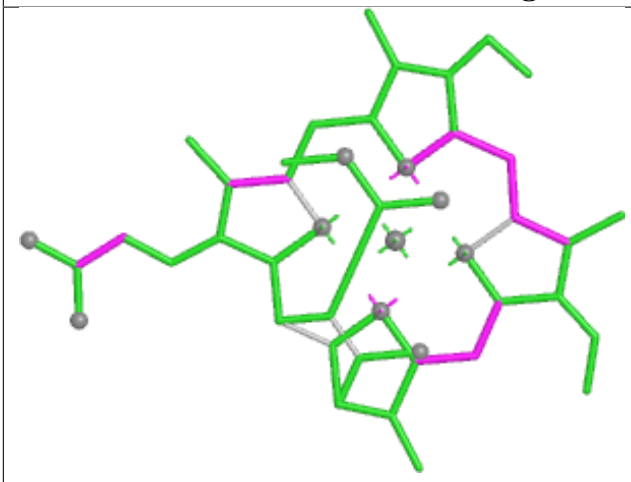


Torsions

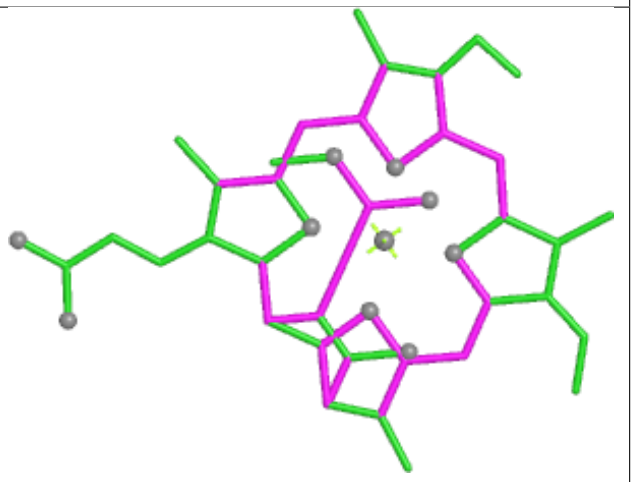


Rings

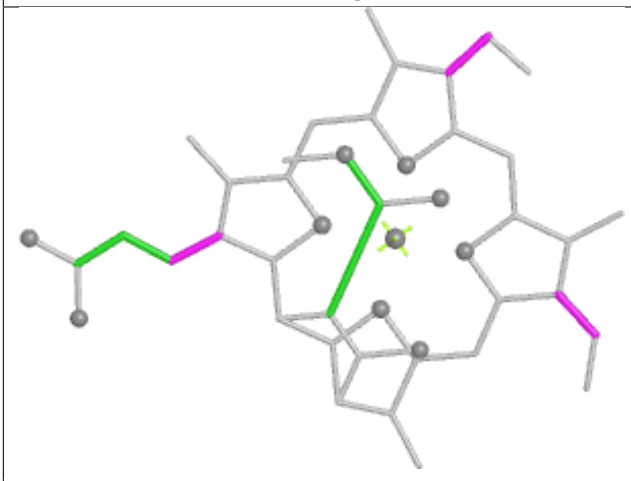
Ligand KC2 W 308



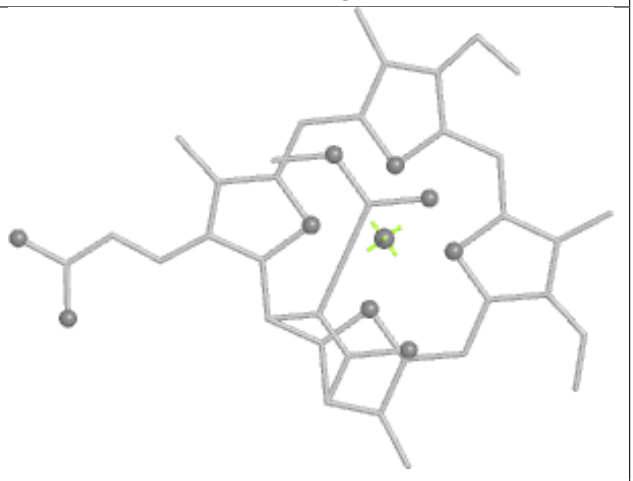
Bond lengths



Bond angles

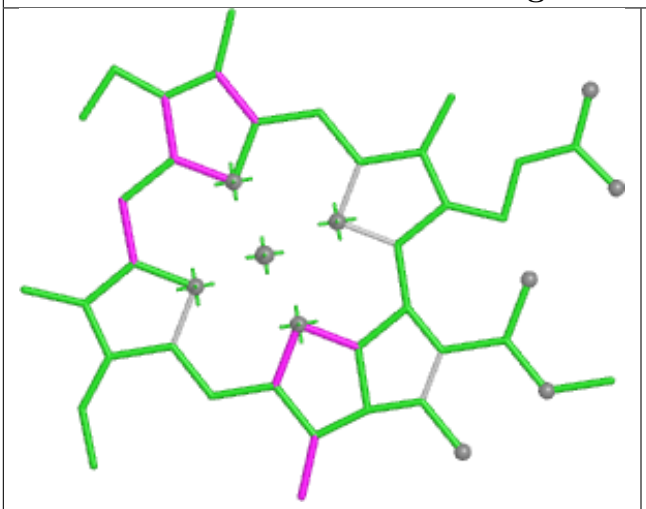


Torsions

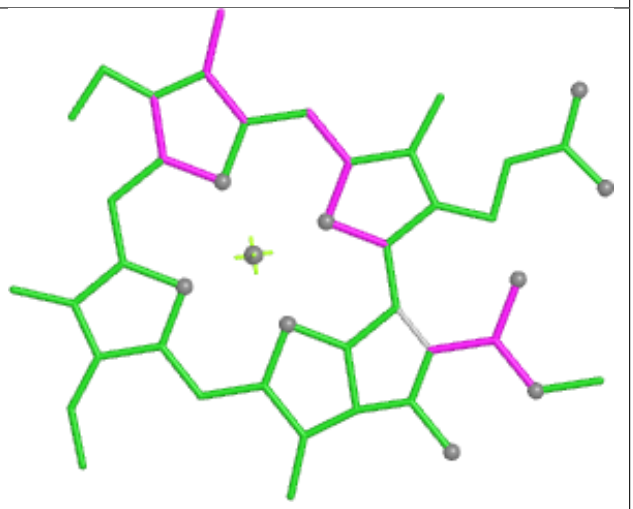


Rings

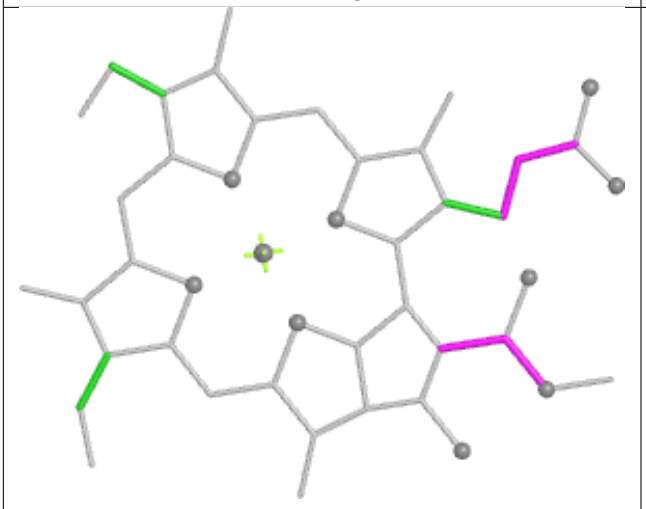
Ligand CLA b 808



Bond lengths



Bond angles

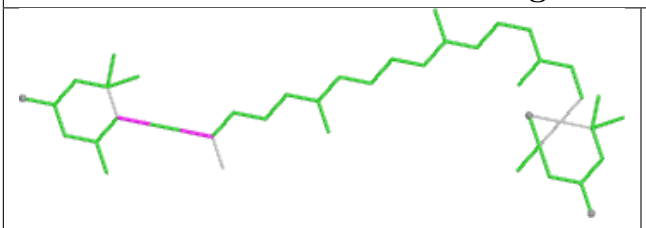


Torsions

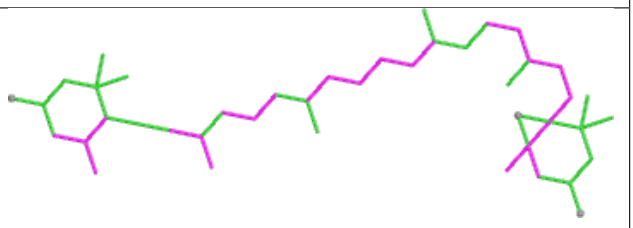


Rings

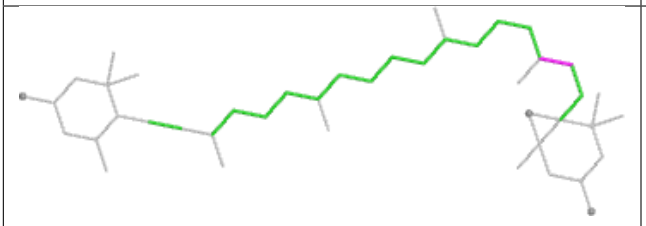
Ligand DD6 o 204



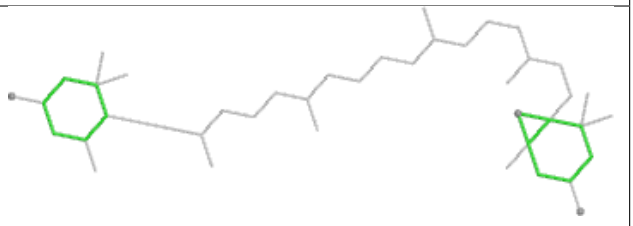
Bond lengths



Bond angles

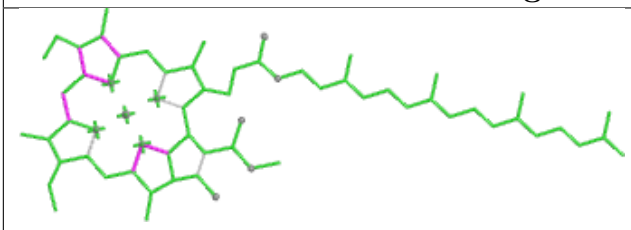


Torsions

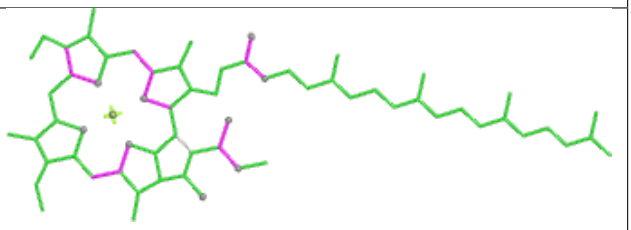


Rings

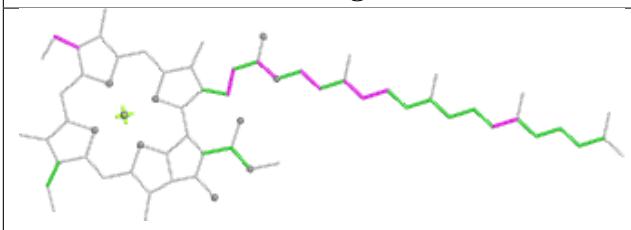
Ligand CLA X 307



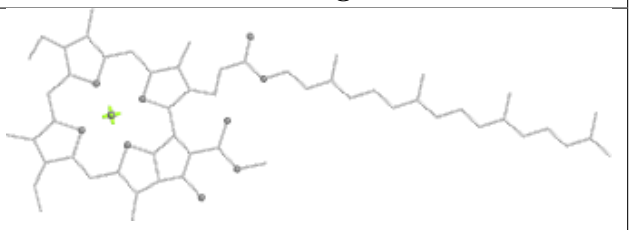
Bond lengths



Bond angles

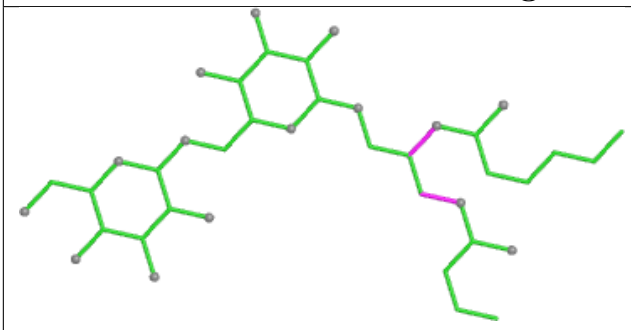


Torsions

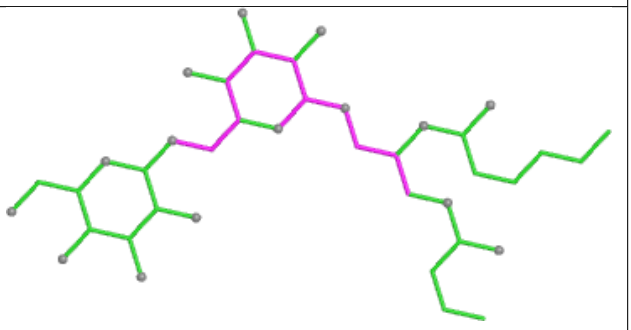


Rings

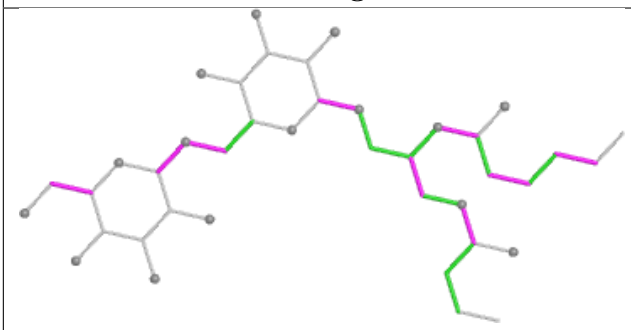
Ligand DGD C 314



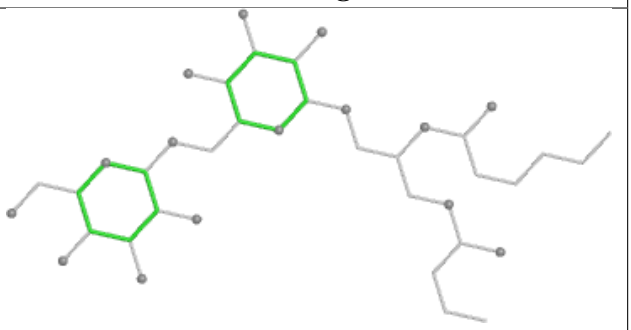
Bond lengths



Bond angles

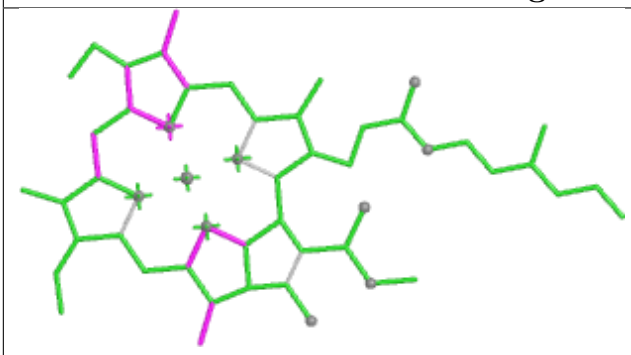


Torsions

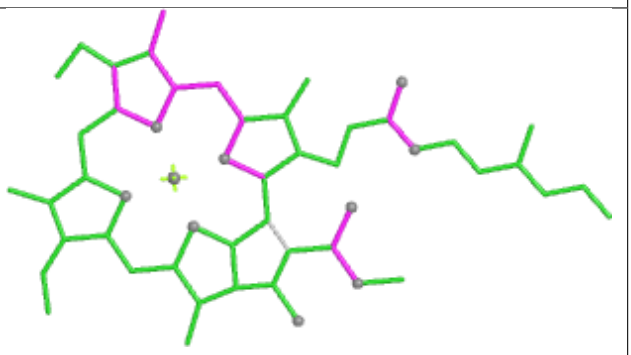


Rings

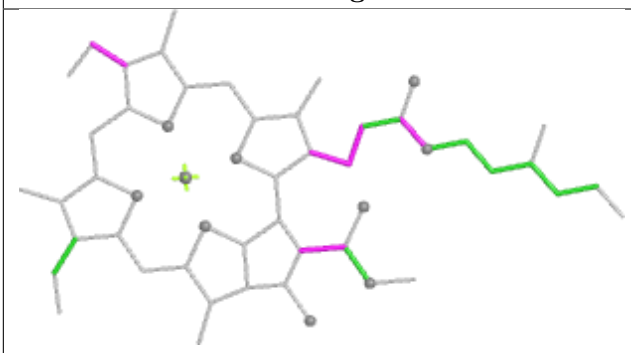
Ligand CLA 4 322



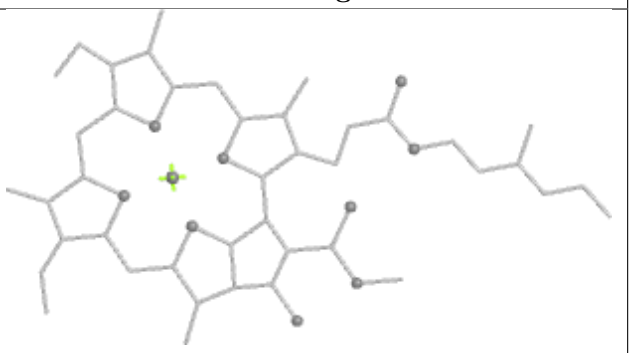
Bond lengths



Bond angles

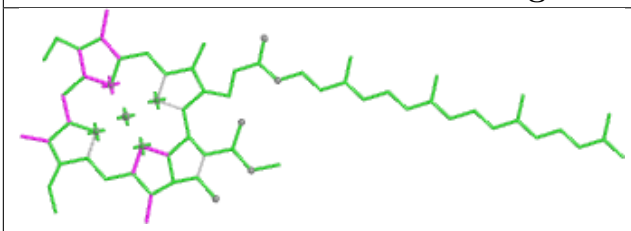


Torsions

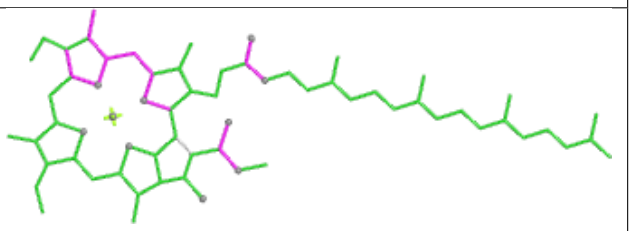


Rings

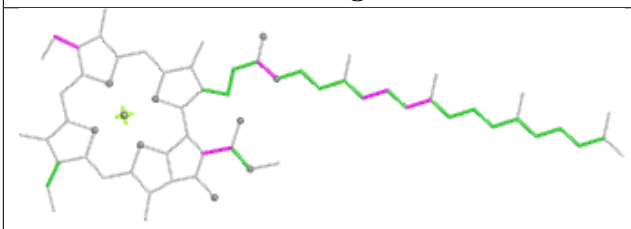
Ligand CLA a 824



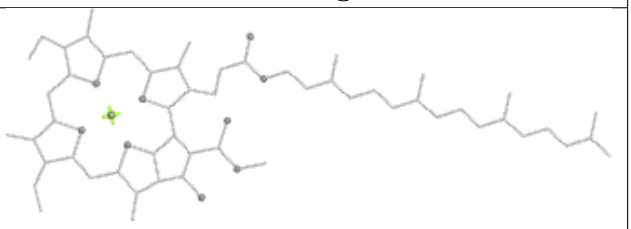
Bond lengths



Bond angles

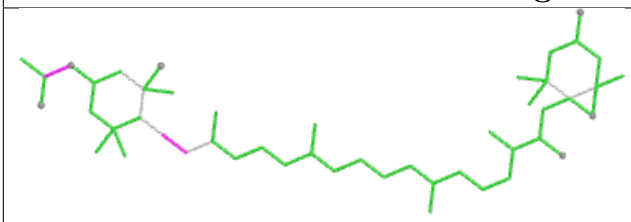


Torsions

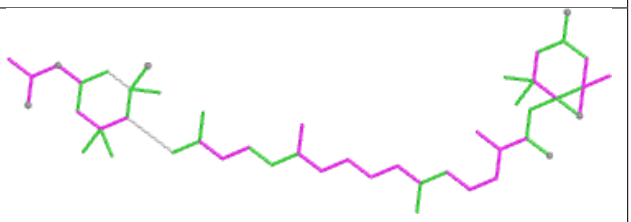


Rings

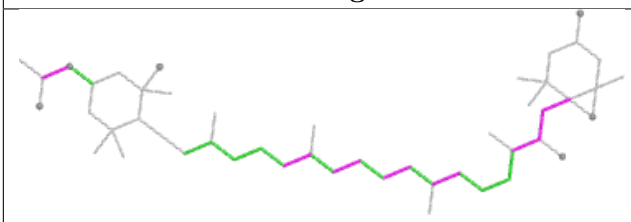
Ligand A86 4 328



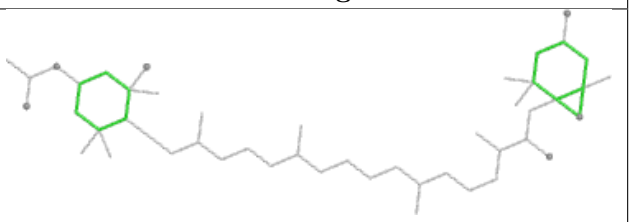
Bond lengths



Bond angles

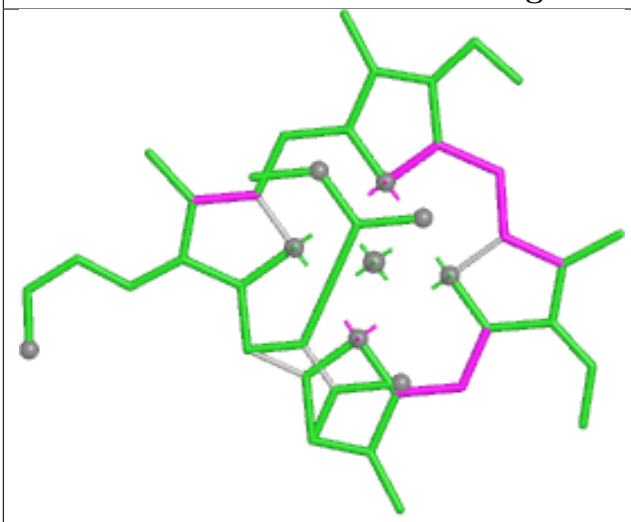


Torsions



Rings

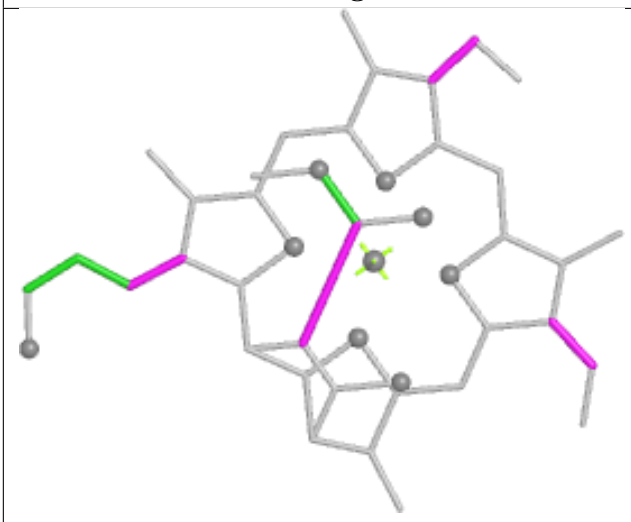
Ligand KC2 R 314



Bond lengths



Bond angles

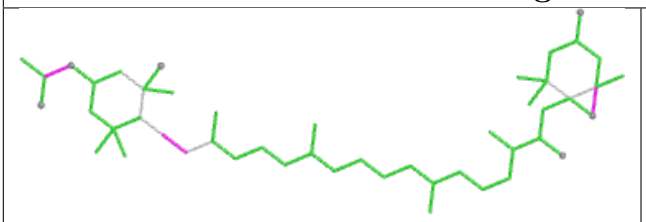


Torsions

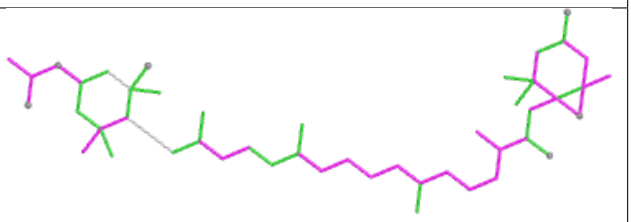


Rings

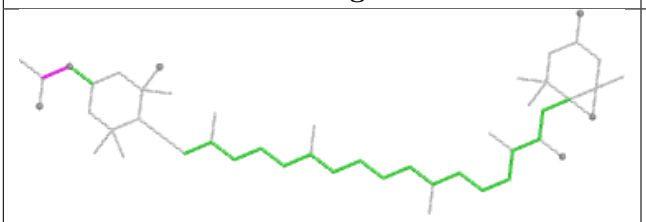
Ligand A86 0 306



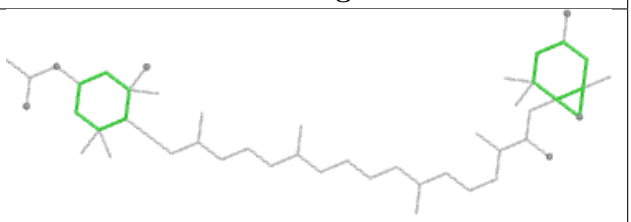
Bond lengths



Bond angles

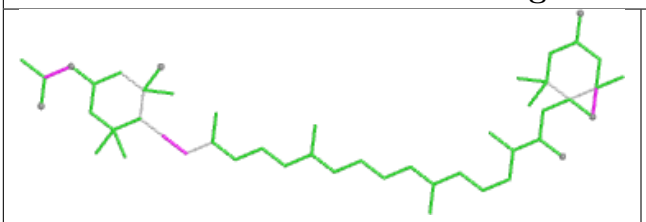


Torsions

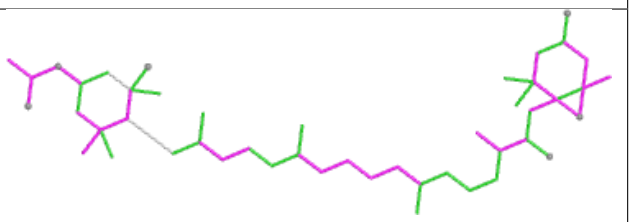


Rings

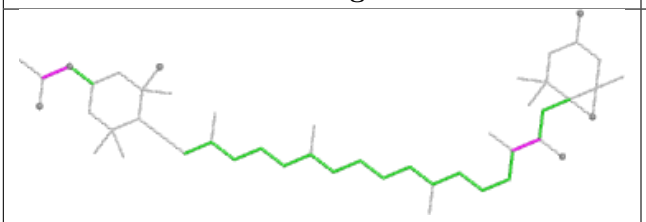
Ligand A86 H 302



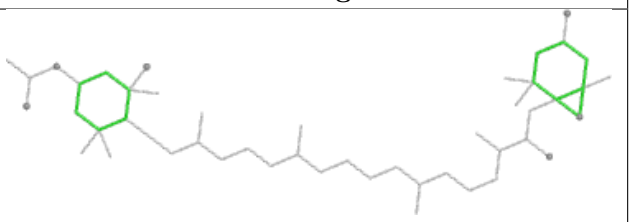
Bond lengths



Bond angles

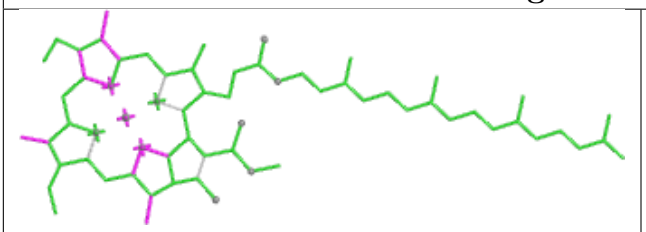


Torsions

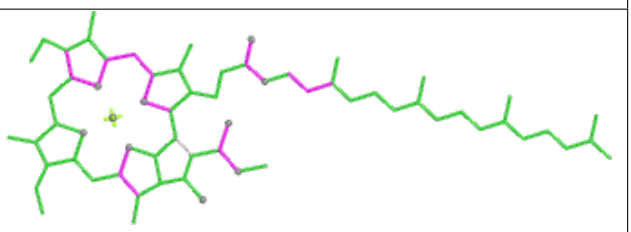


Rings

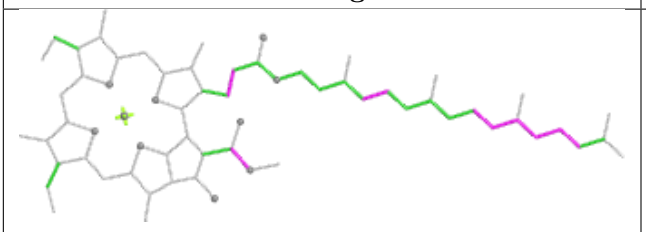
Ligand CLA b 801



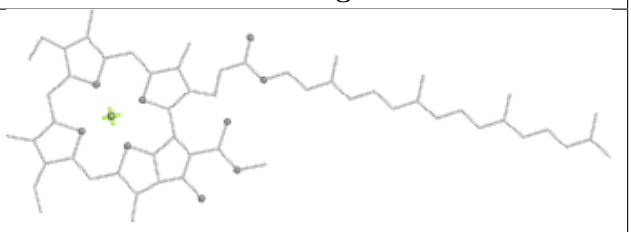
Bond lengths



Bond angles

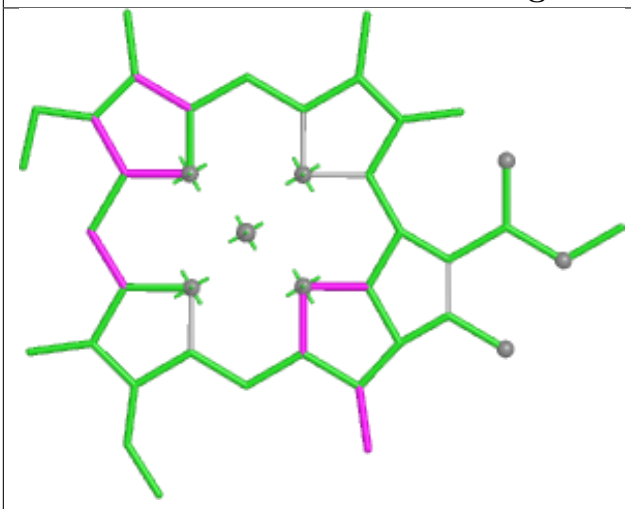


Torsions

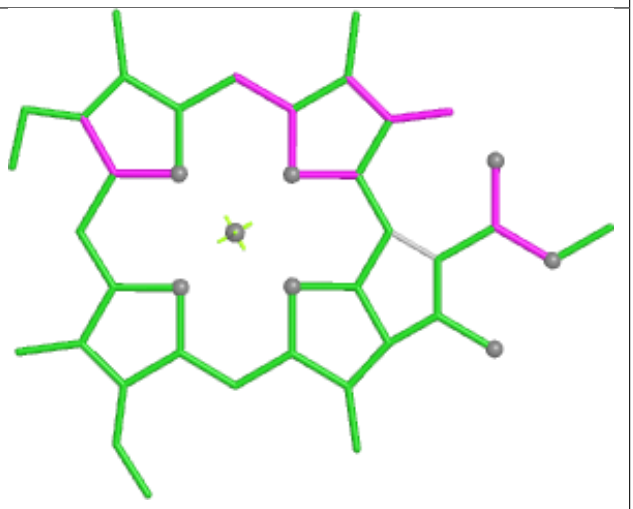


Rings

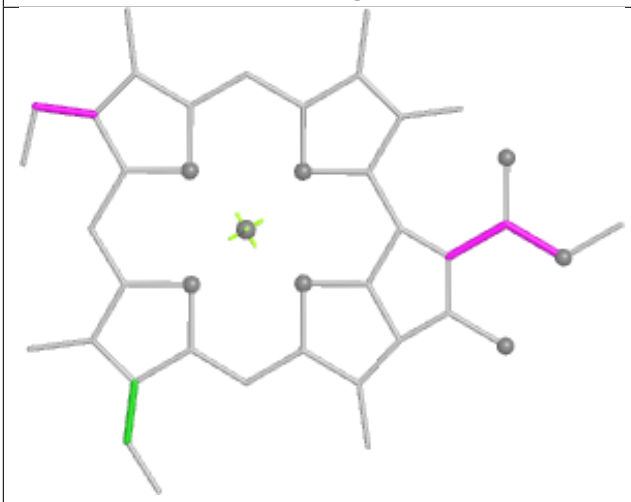
Ligand CLA 1 311



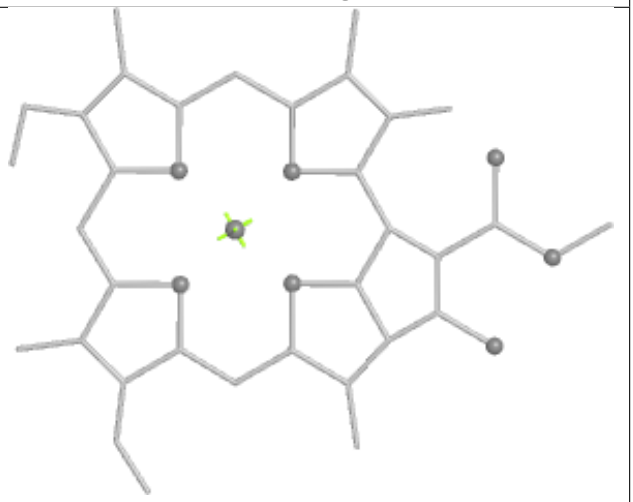
Bond lengths



Bond angles

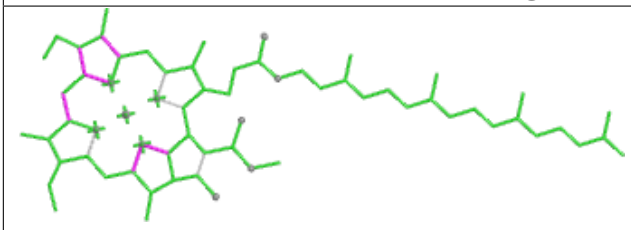


Torsions

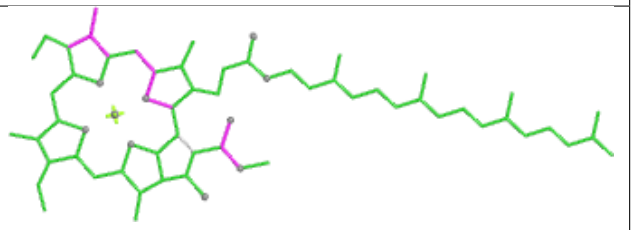


Rings

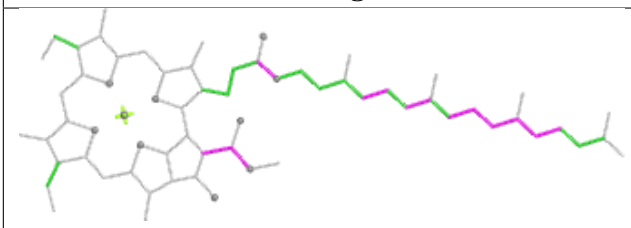
Ligand CLA K 311



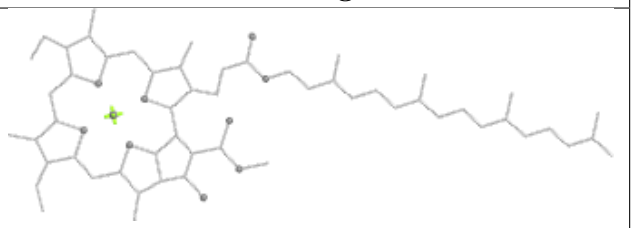
Bond lengths



Bond angles

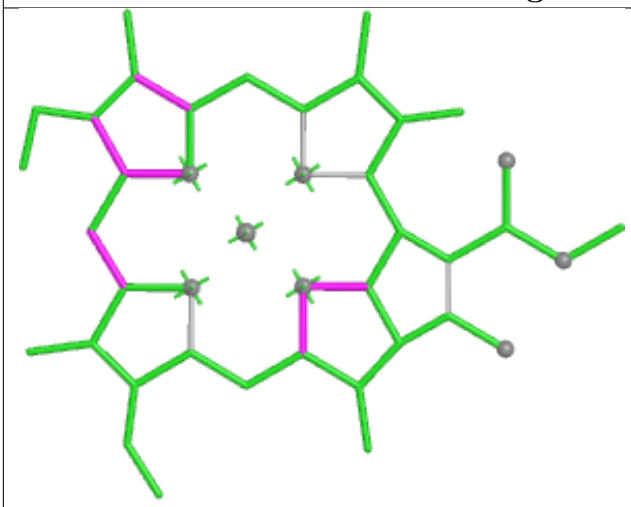


Torsions

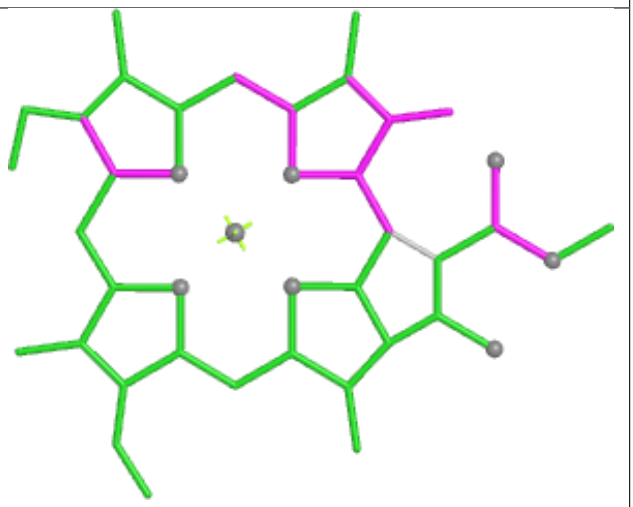


Rings

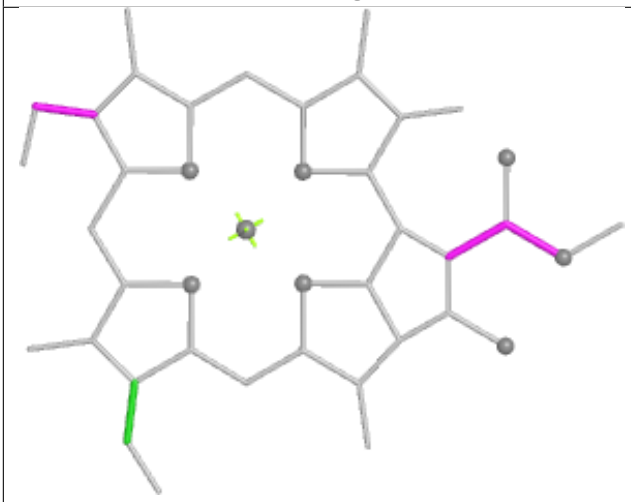
Ligand CLA Z 316



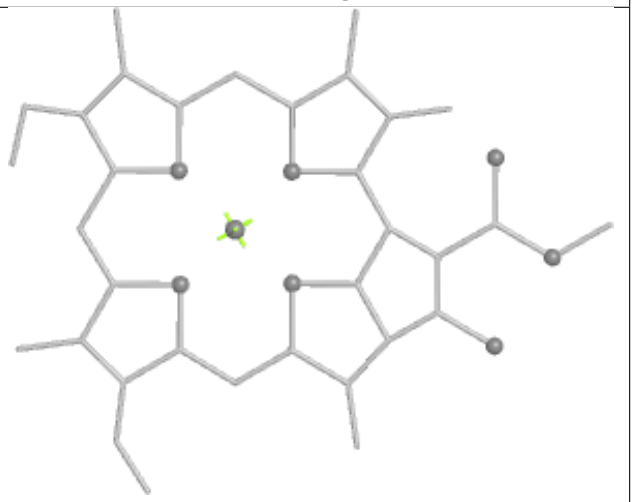
Bond lengths



Bond angles

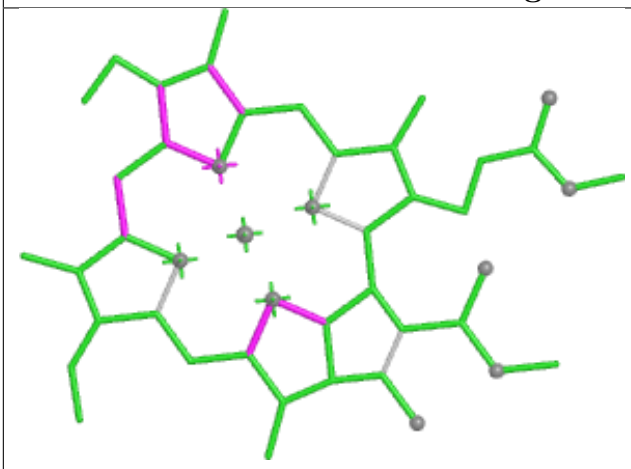


Torsions

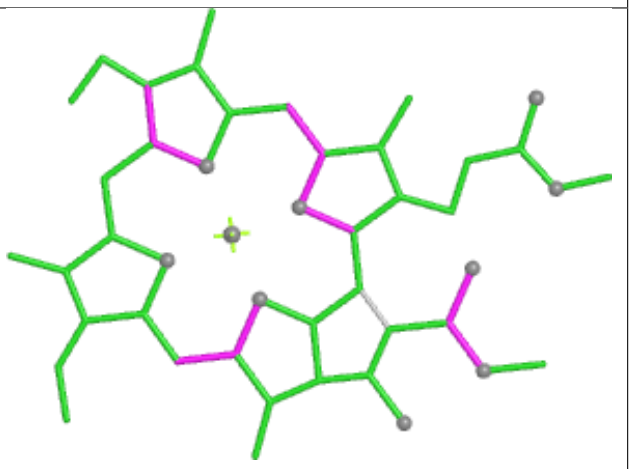


Rings

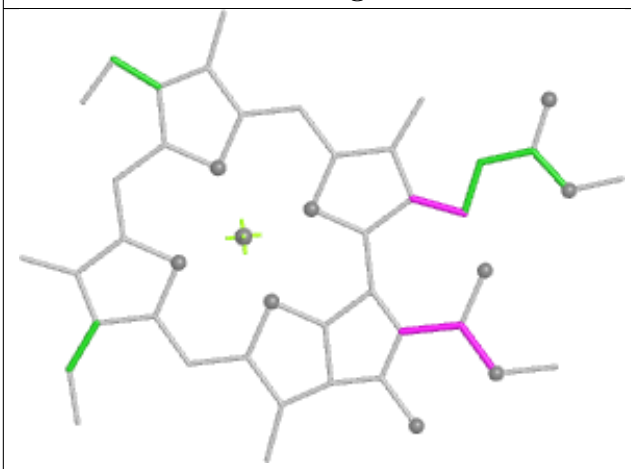
Ligand CLA B 203



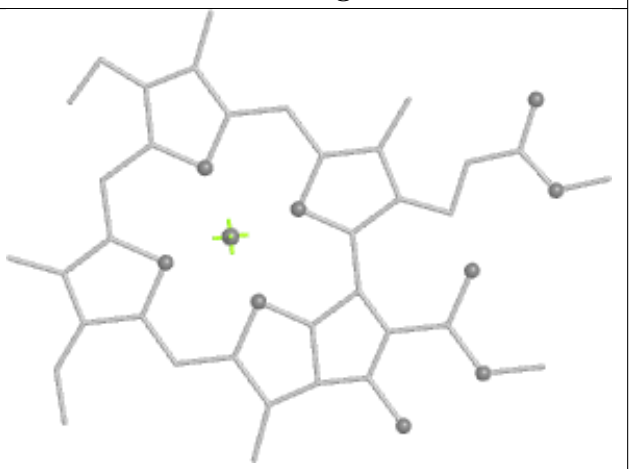
Bond lengths



Bond angles

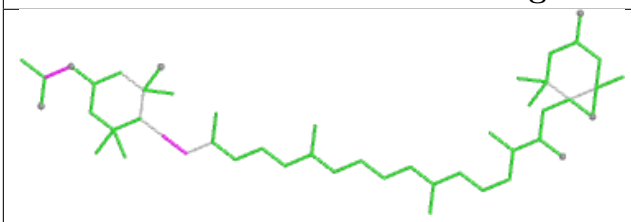


Torsions

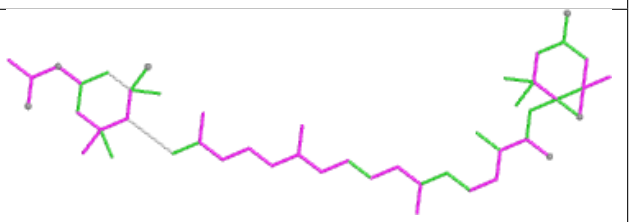


Rings

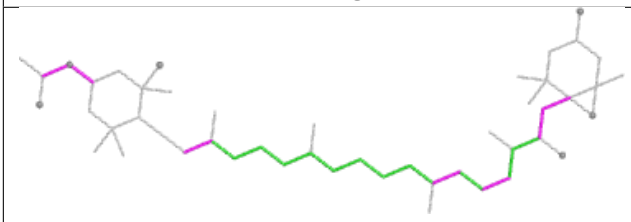
Ligand A86 G 301



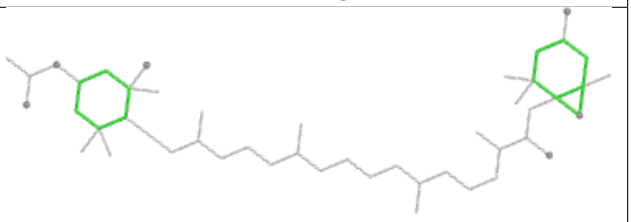
Bond lengths



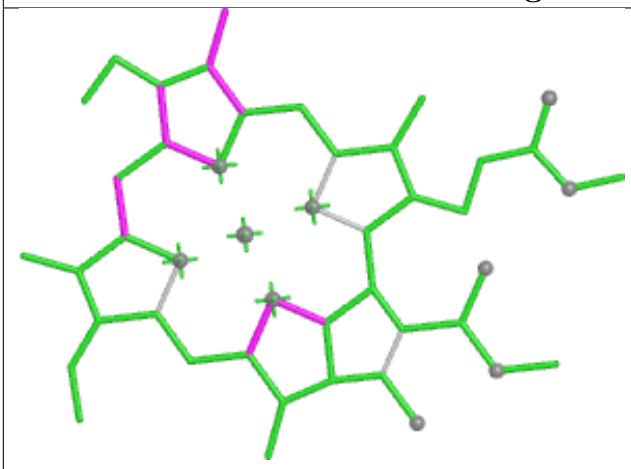
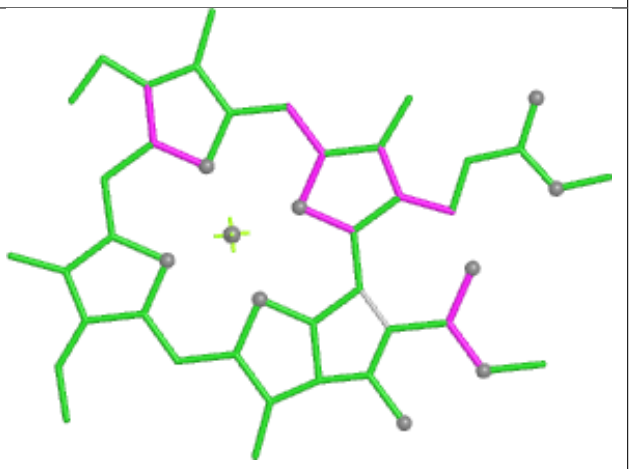
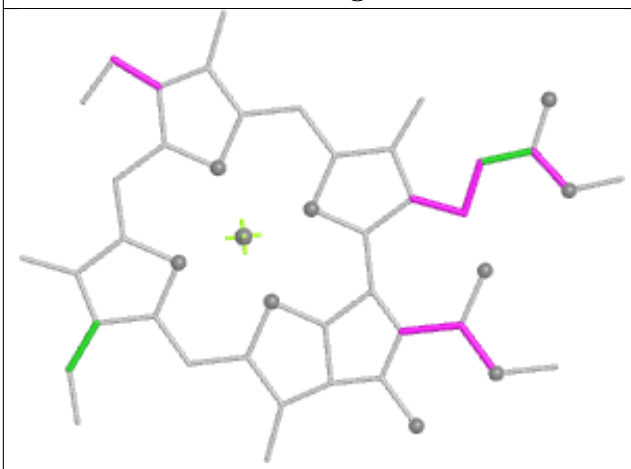
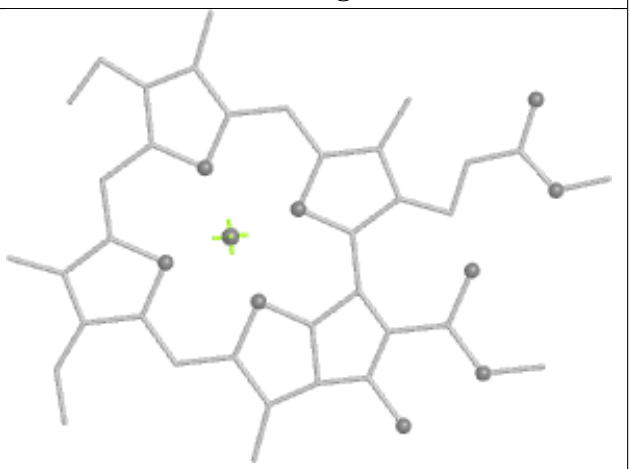
Bond angles



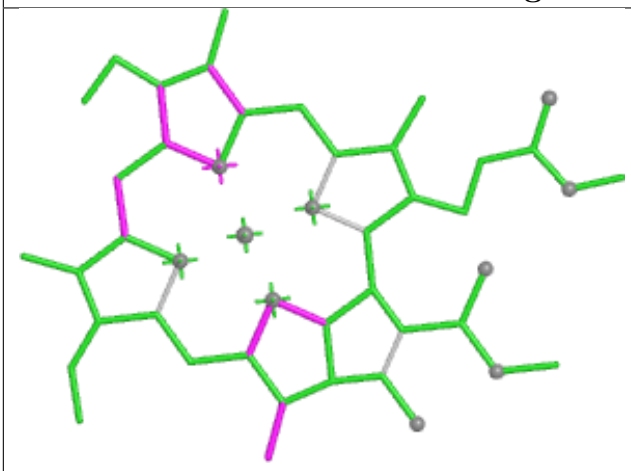
Torsions



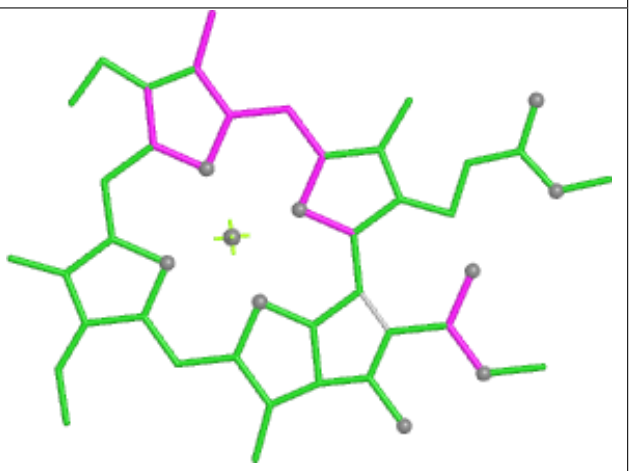
Rings

Ligand CLA T 319	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

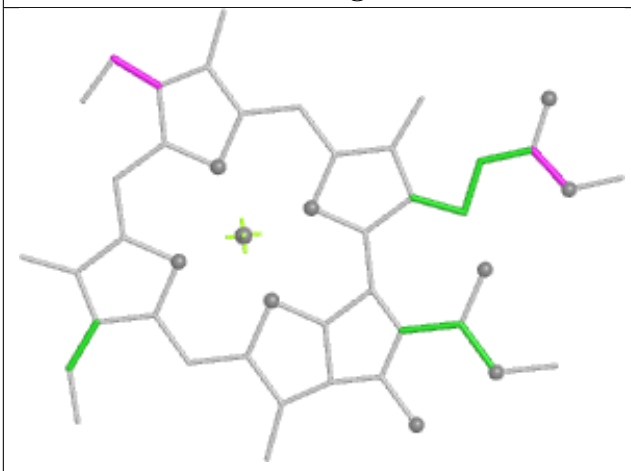
Ligand CLA B 204



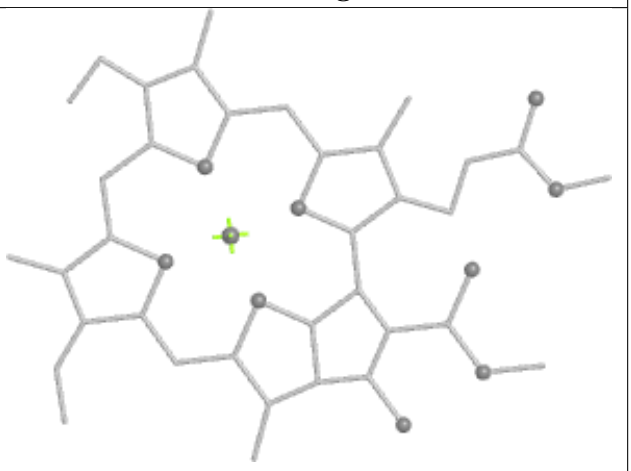
Bond lengths



Bond angles

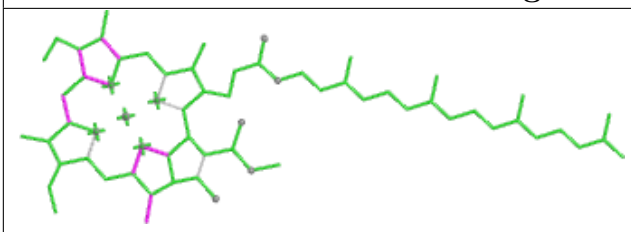


Torsions

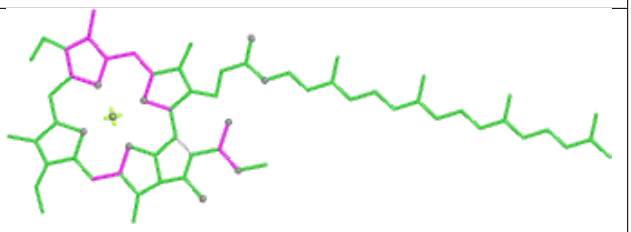


Rings

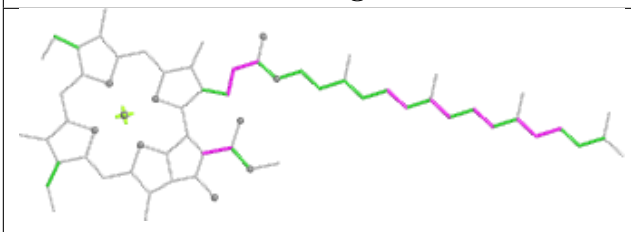
Ligand CLA D 313



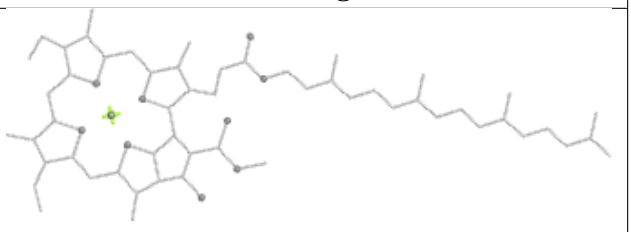
Bond lengths



Bond angles

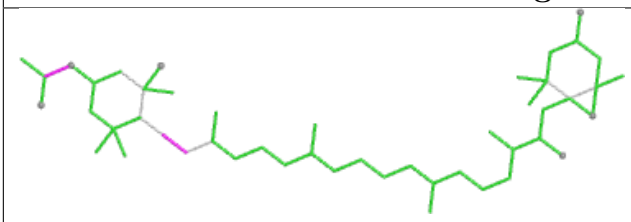


Torsions

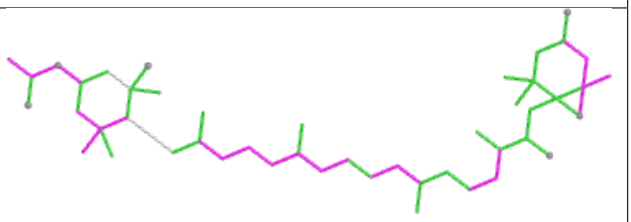


Rings

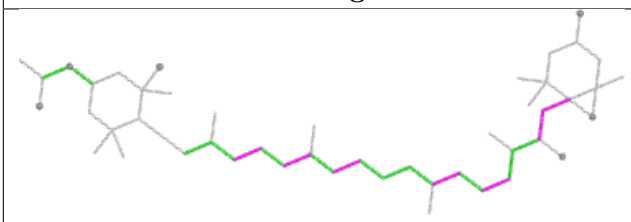
Ligand A86 1 306



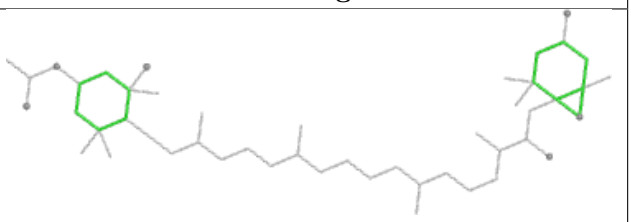
Bond lengths



Bond angles



Torsions

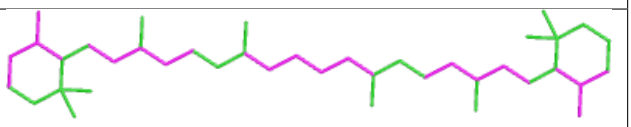


Rings

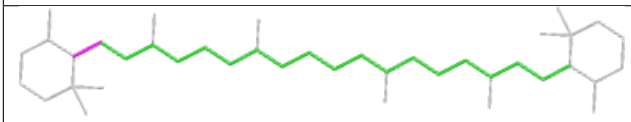
Ligand BCR l 207



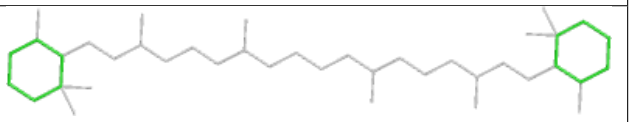
Bond lengths



Bond angles

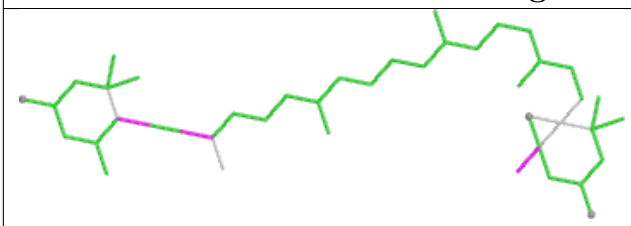


Torsions

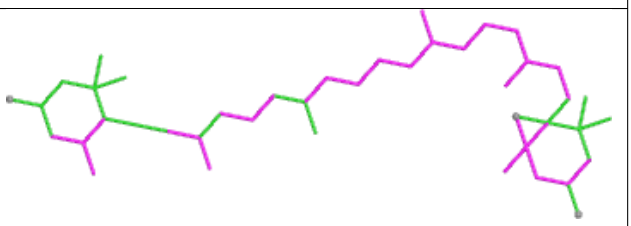


Rings

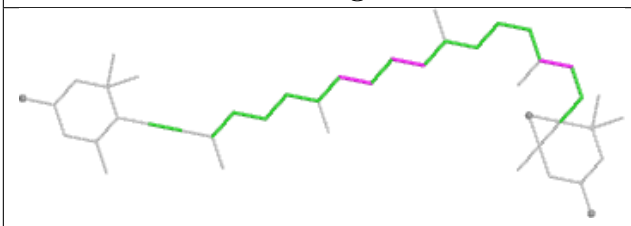
Ligand DD6 1 304



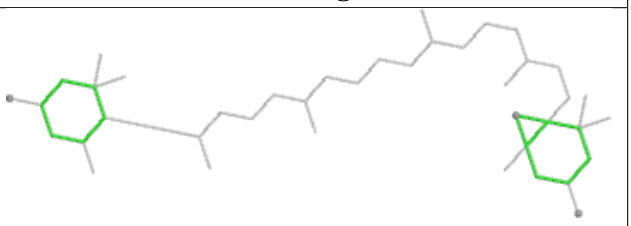
Bond lengths



Bond angles

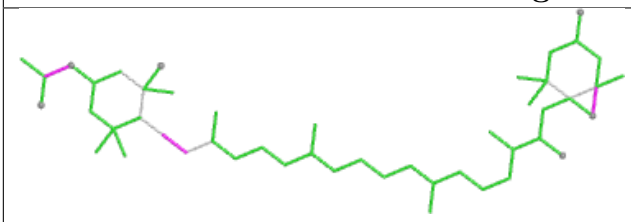


Torsions

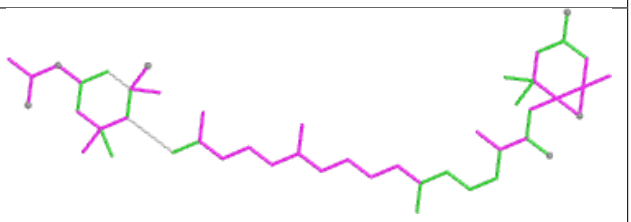


Rings

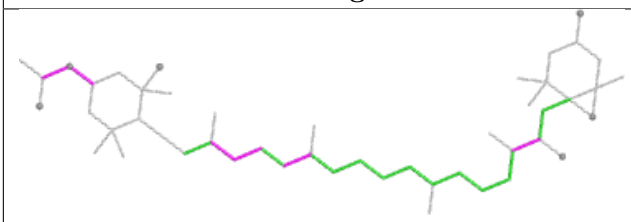
Ligand A86 L 302



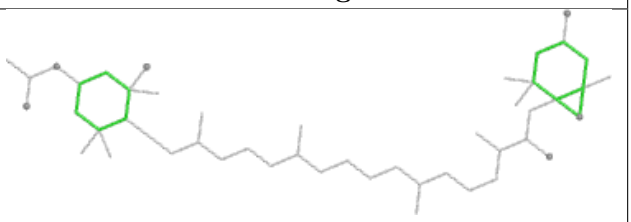
Bond lengths



Bond angles

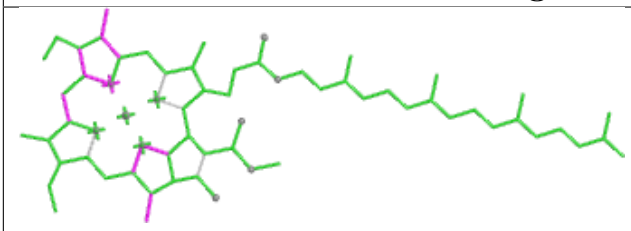


Torsions

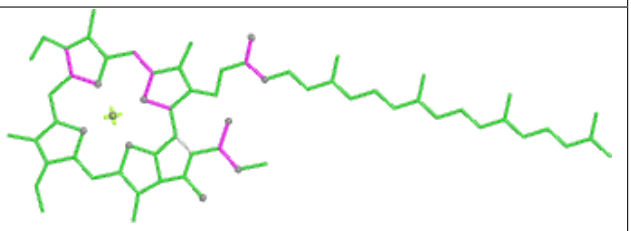


Rings

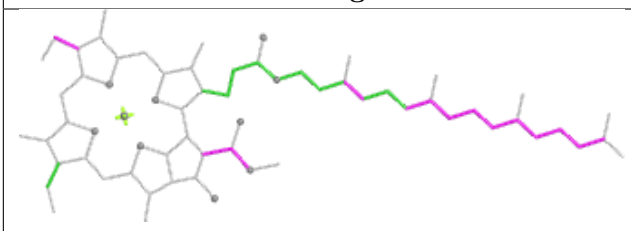
Ligand CLA a 847



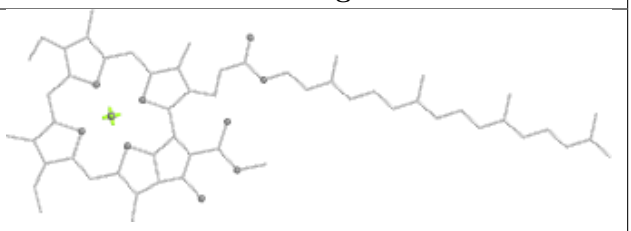
Bond lengths



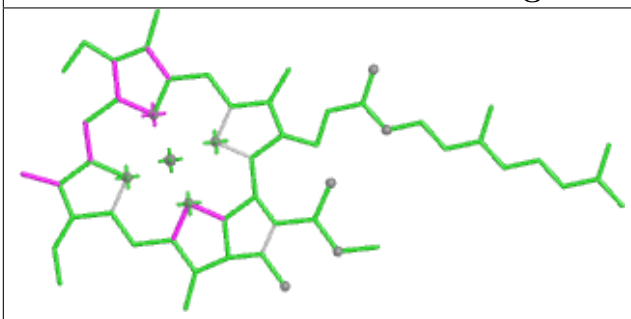
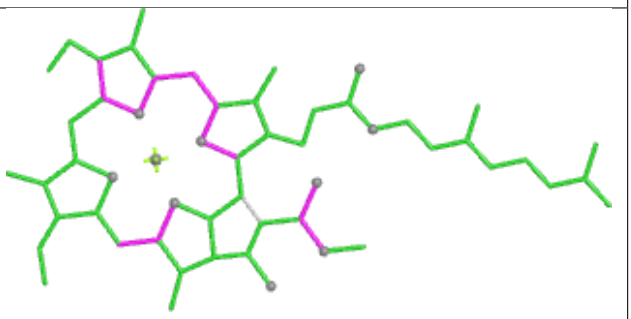
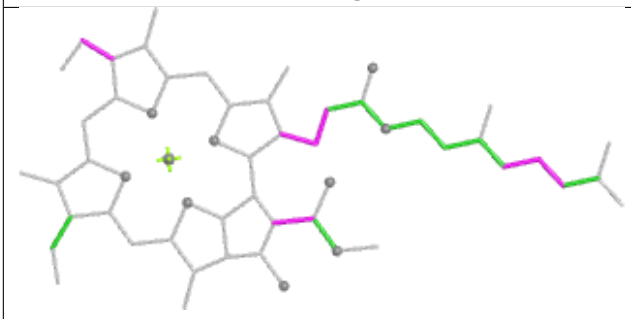
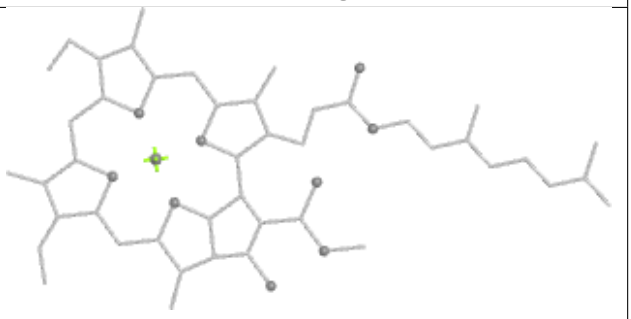
Bond angles

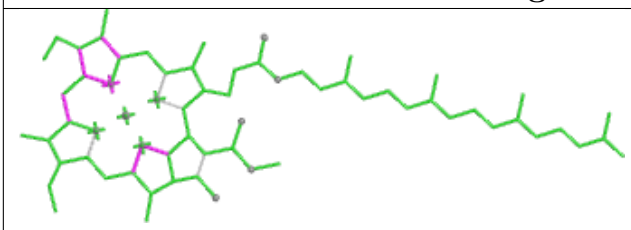
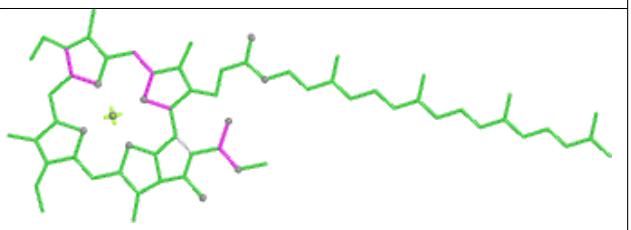
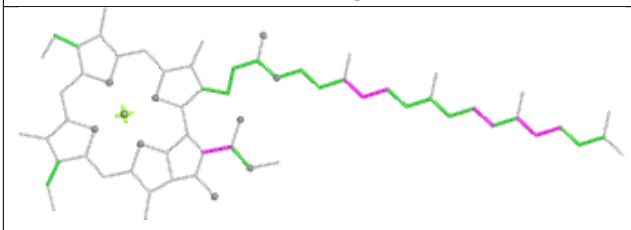
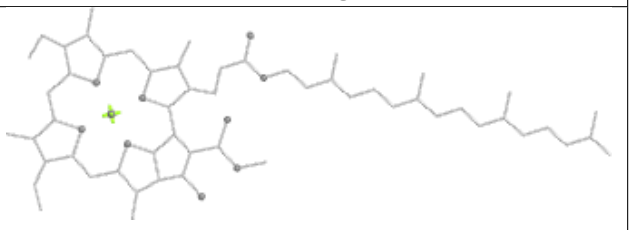


Torsions

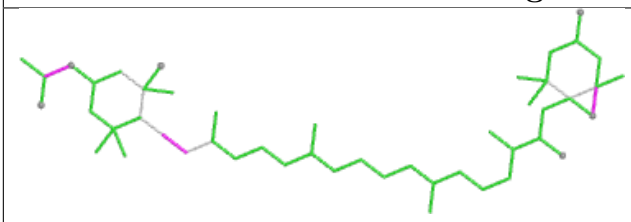


Rings

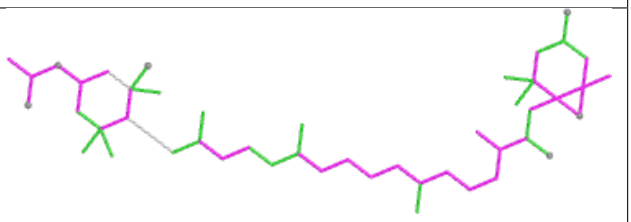
Ligand CLA O 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

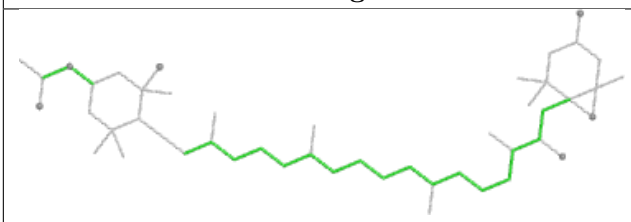
Ligand A86 M 303



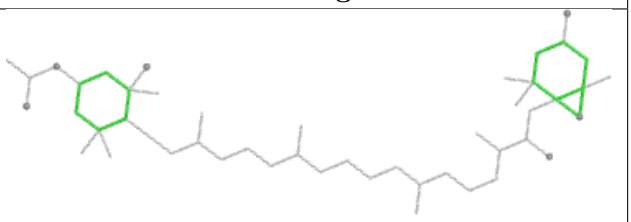
Bond lengths



Bond angles

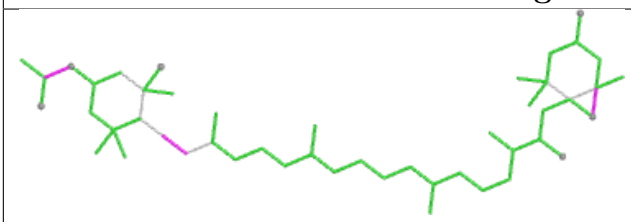


Torsions

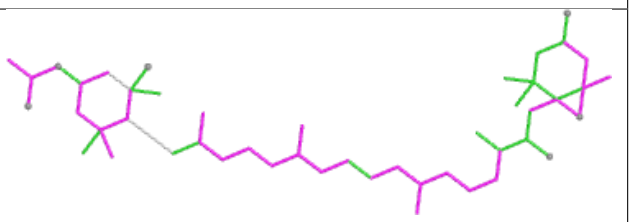


Rings

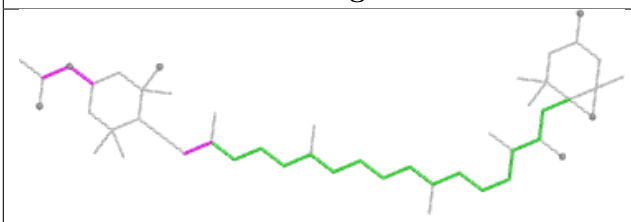
Ligand A86 3 307



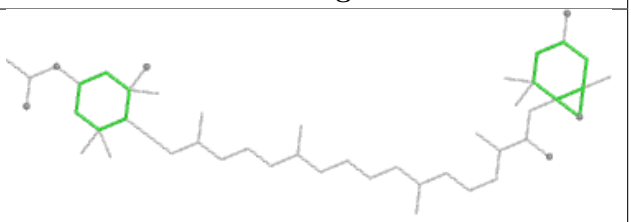
Bond lengths



Bond angles

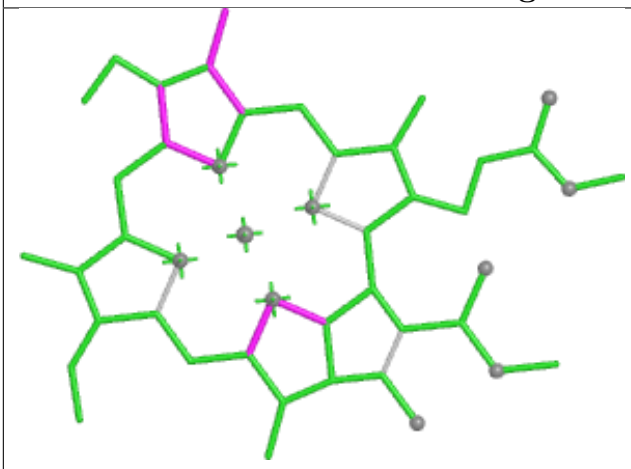


Torsions

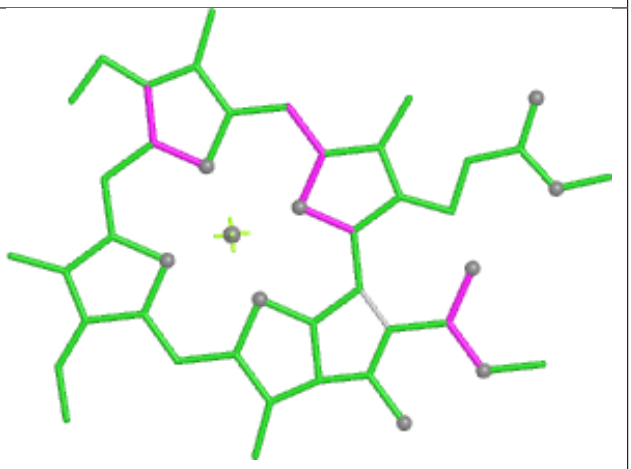


Rings

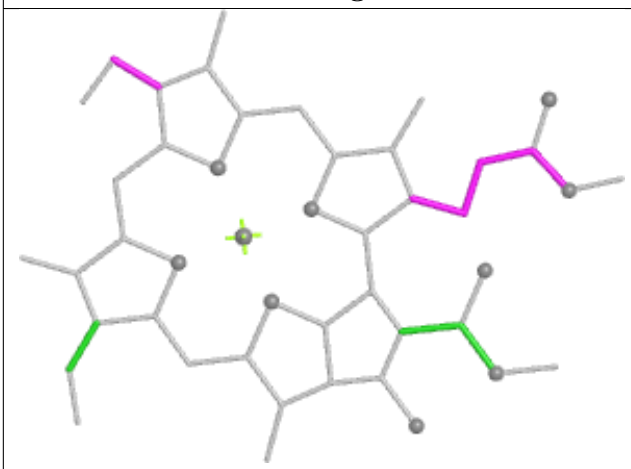
Ligand CLA W 319



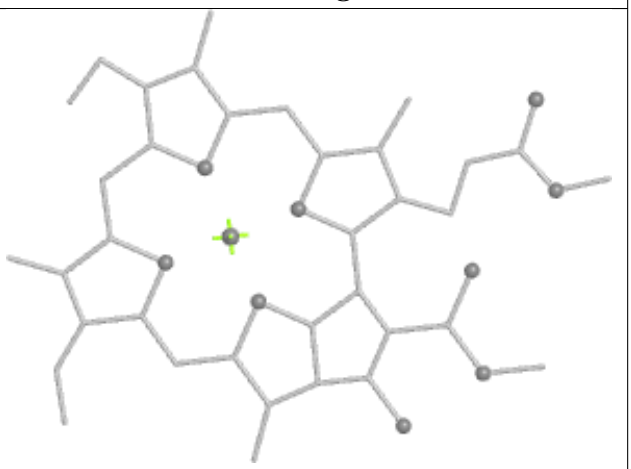
Bond lengths



Bond angles

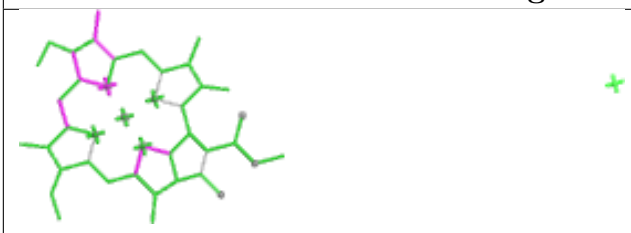


Torsions

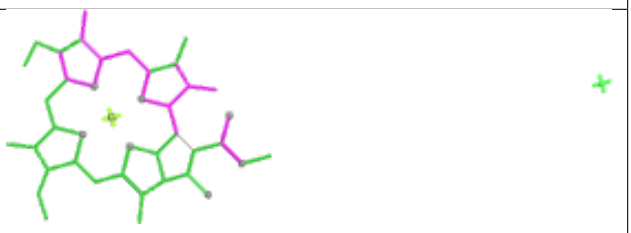


Rings

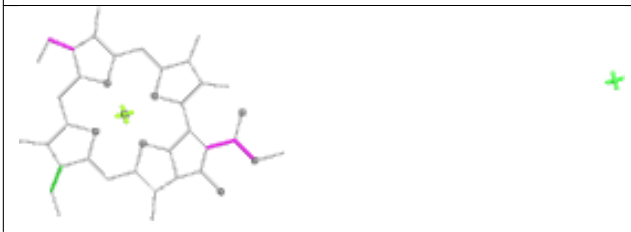
Ligand CLA x 318



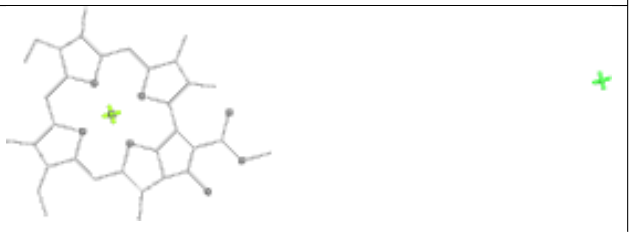
Bond lengths



Bond angles

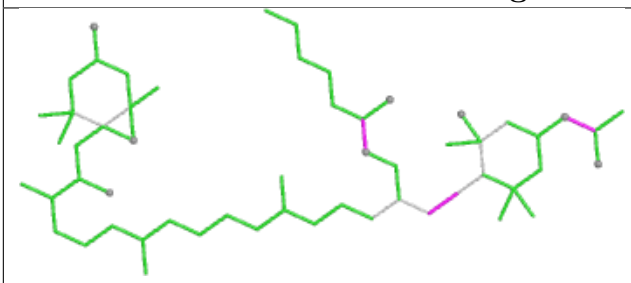


Torsions

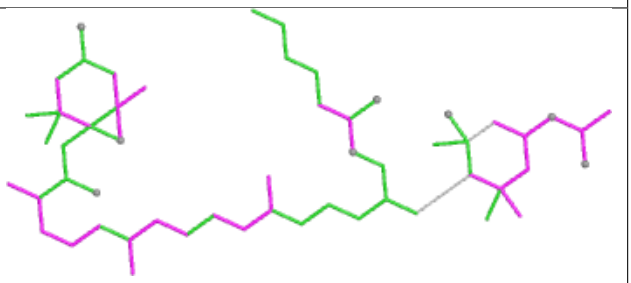


Rings

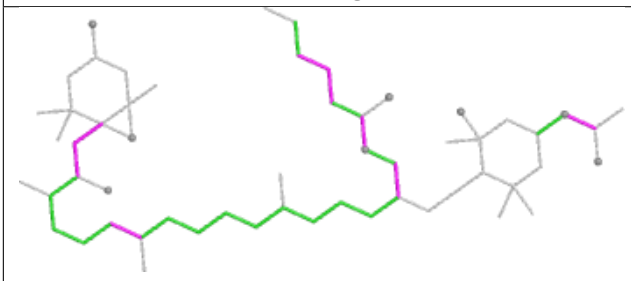
Ligand A1EB1 6 301



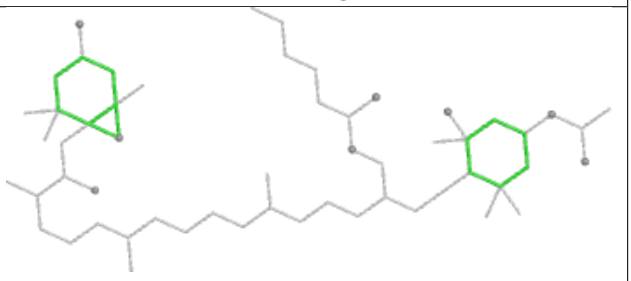
Bond lengths



Bond angles

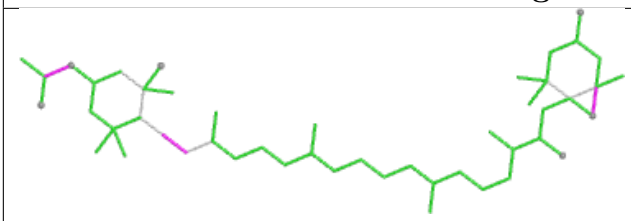


Torsions

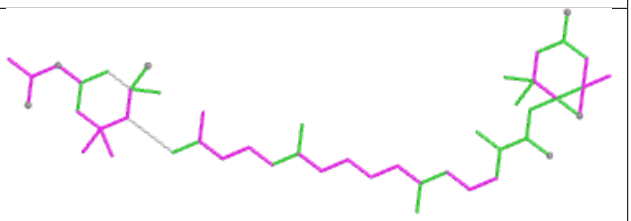


Rings

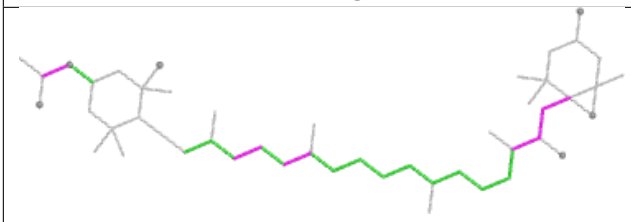
Ligand A86 L 304



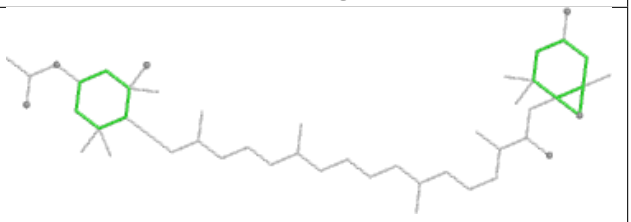
Bond lengths



Bond angles

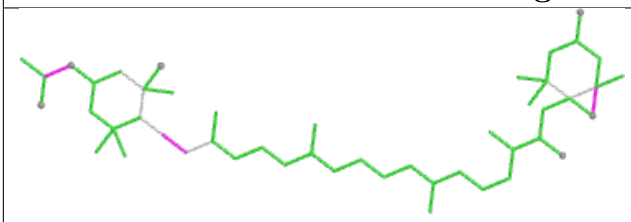


Torsions

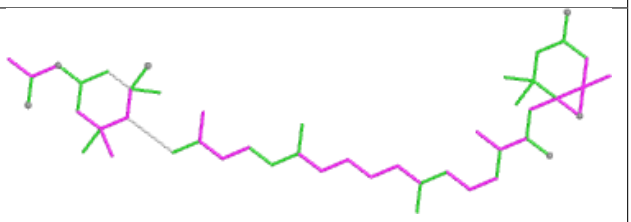


Rings

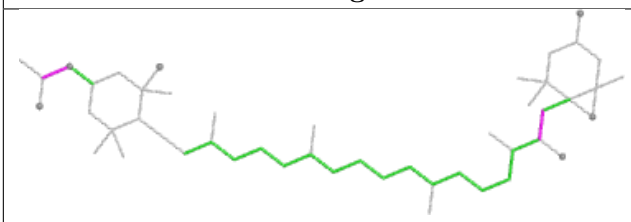
Ligand A86 7 311



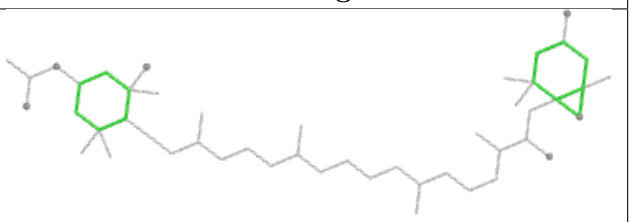
Bond lengths



Bond angles

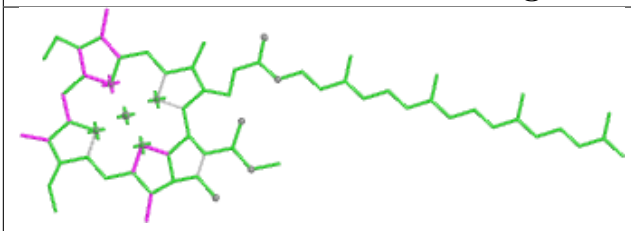


Torsions

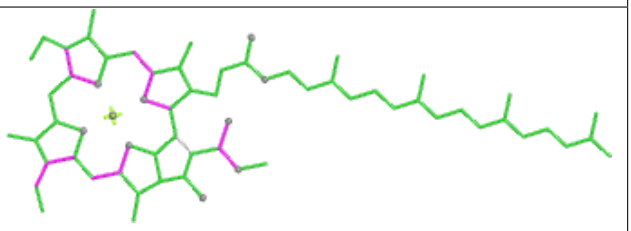


Rings

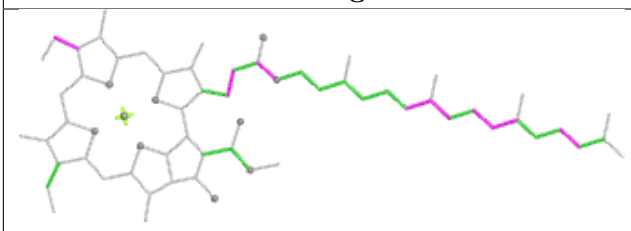
Ligand CLA G 310



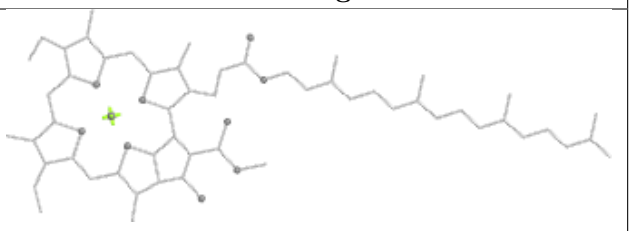
Bond lengths



Bond angles

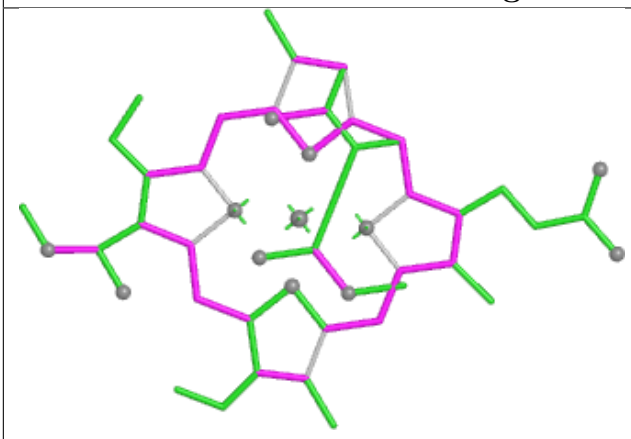


Torsions

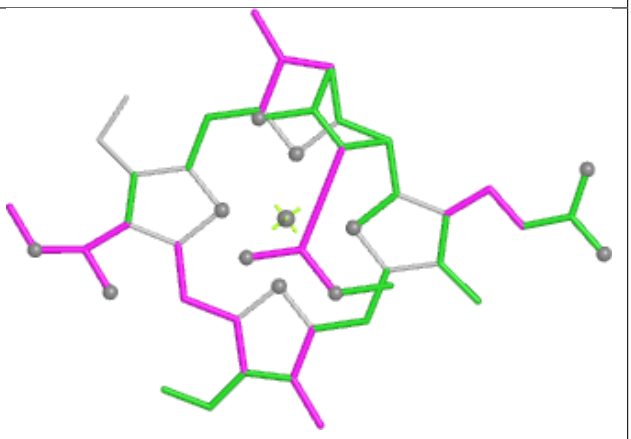


Rings

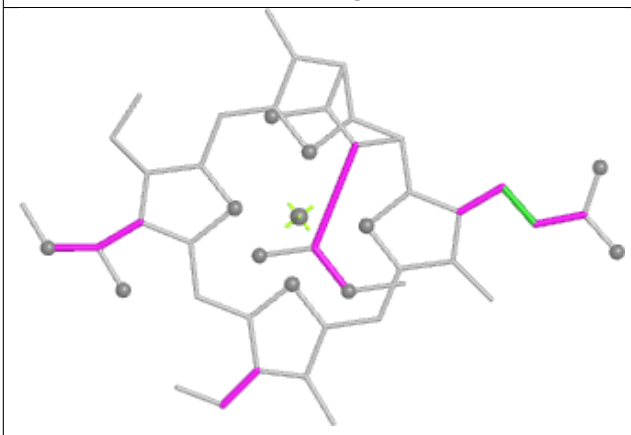
Ligand A1ECV L 318



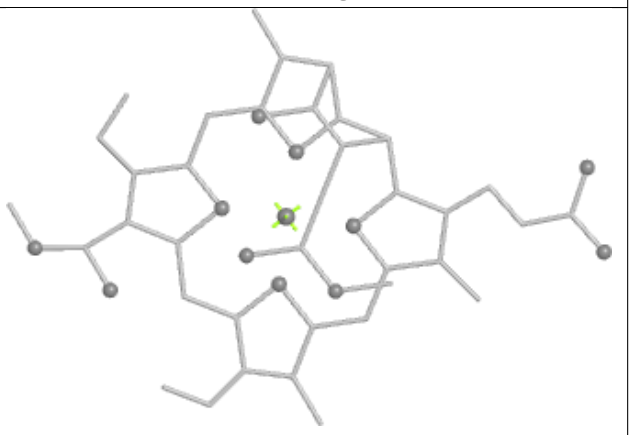
Bond lengths



Bond angles

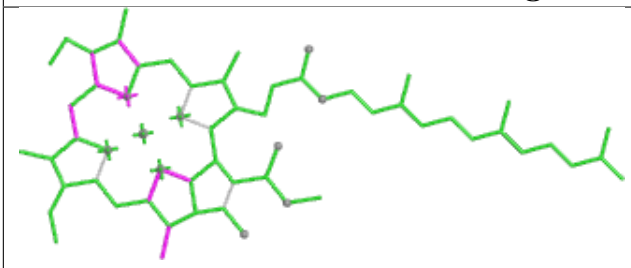


Torsions

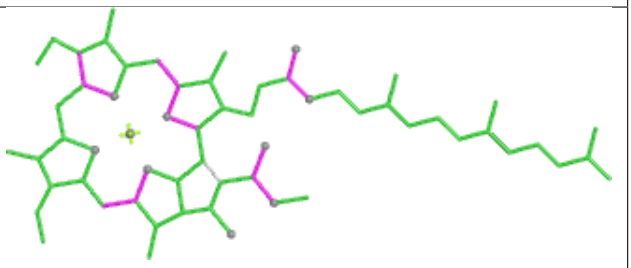


Rings

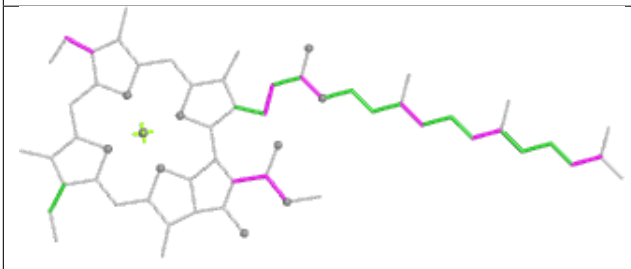
Ligand CLA C 308



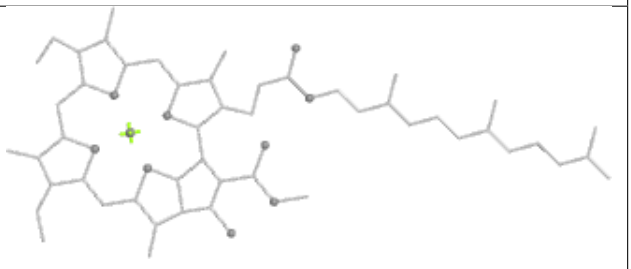
Bond lengths



Bond angles

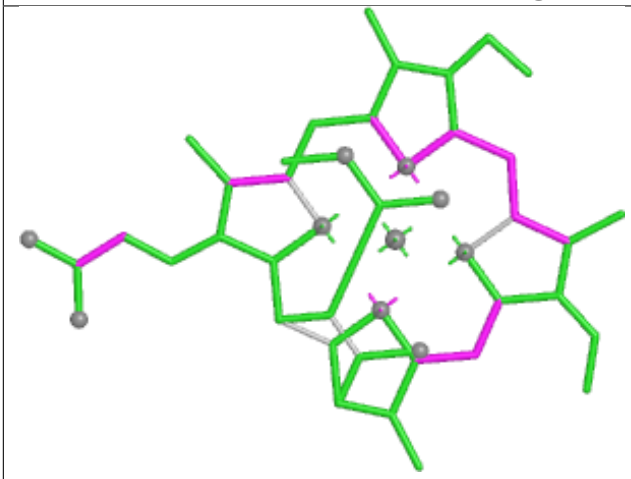


Torsions

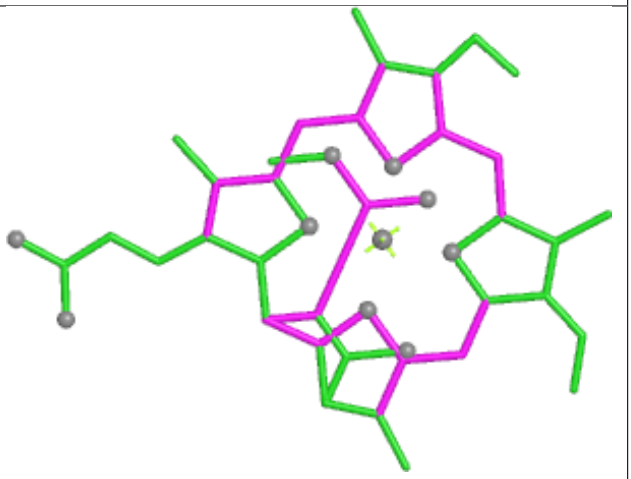


Rings

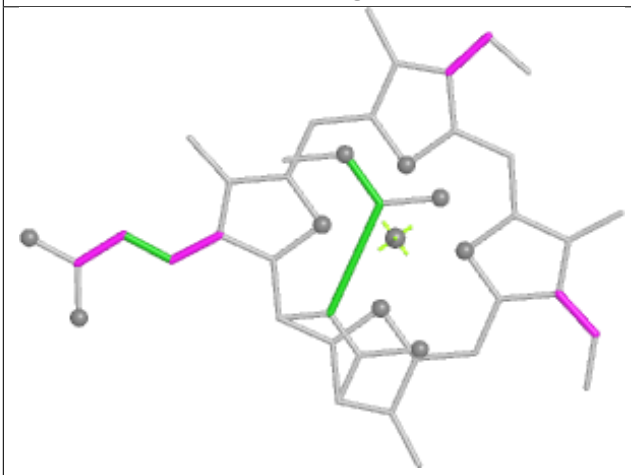
Ligand KC2 1 312



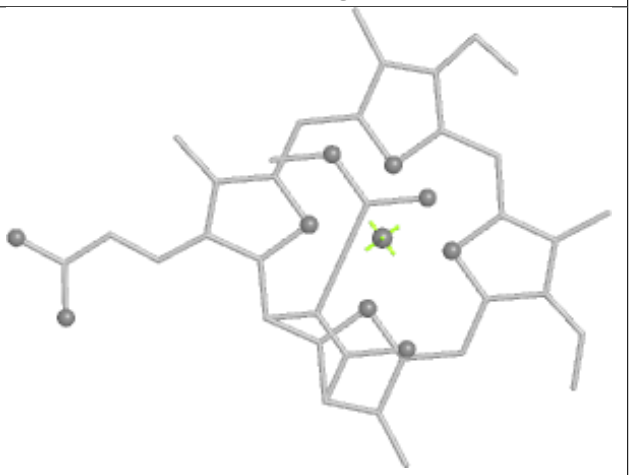
Bond lengths



Bond angles

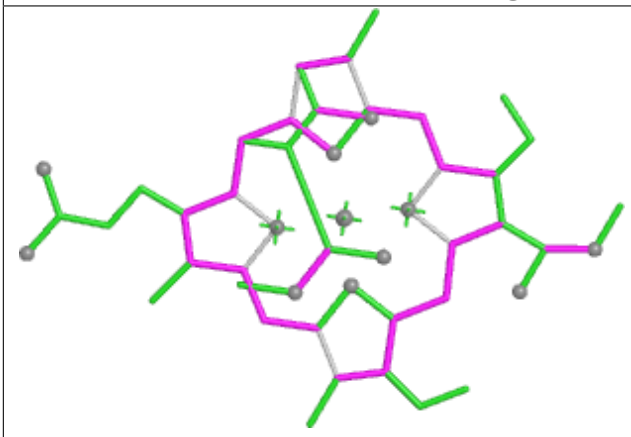


Torsions

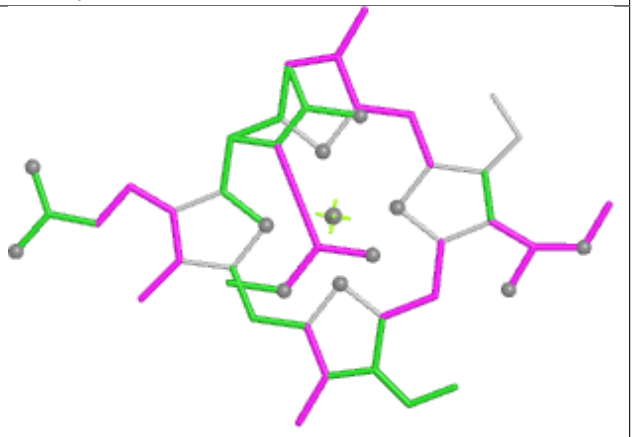


Rings

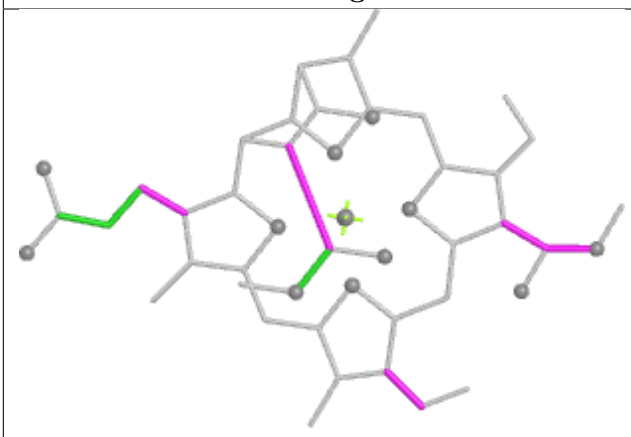
Ligand A1ECV y 317



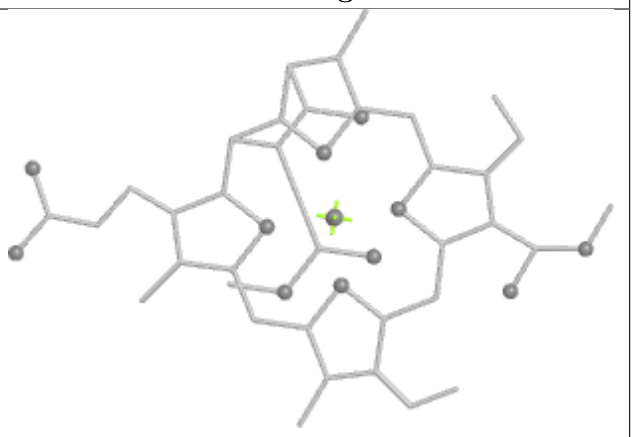
Bond lengths



Bond angles

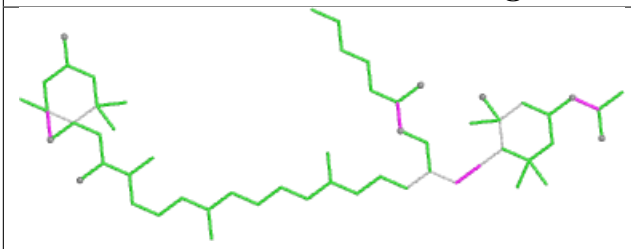


Torsions

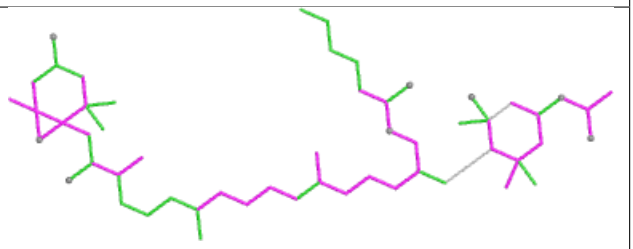


Rings

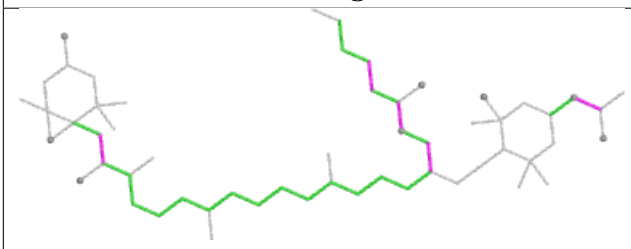
Ligand A1EB1 G 304



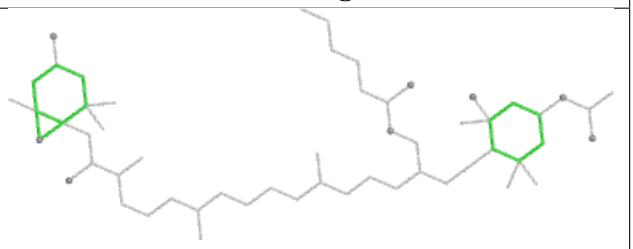
Bond lengths



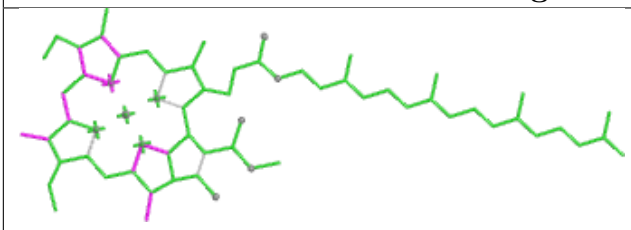
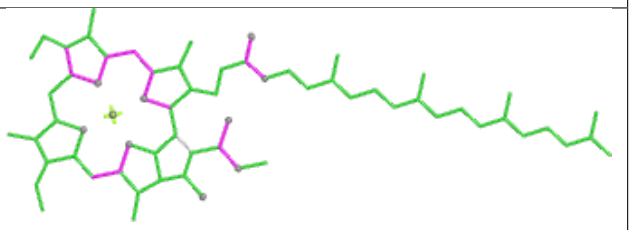
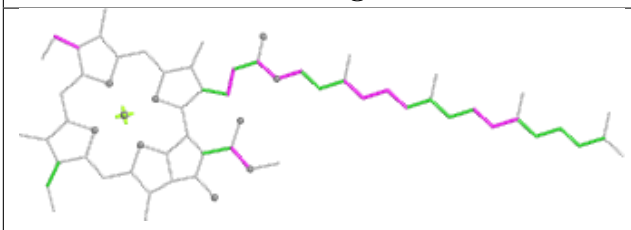
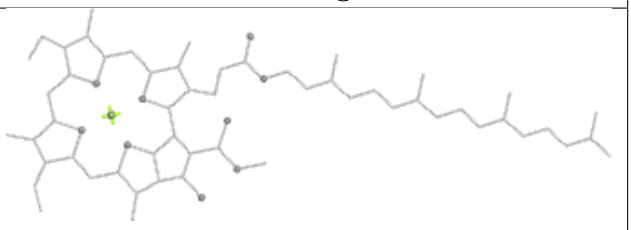
Bond angles

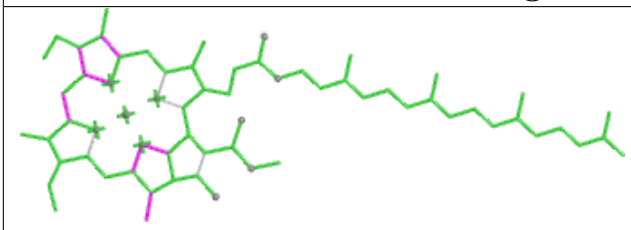
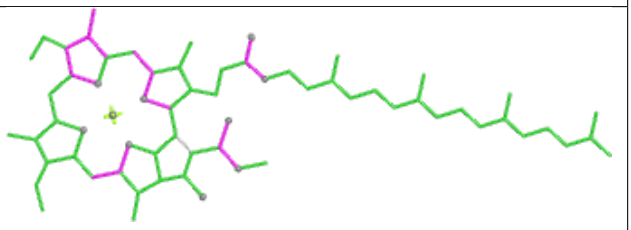
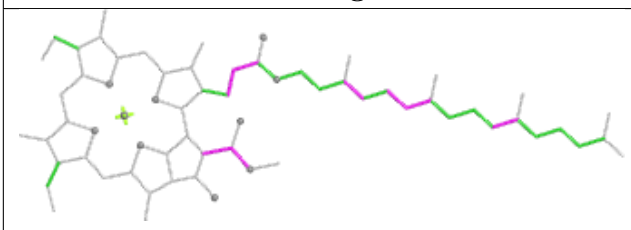
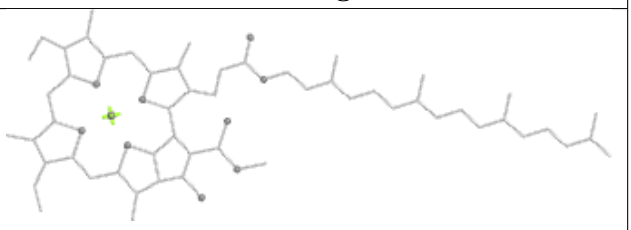


Torsions

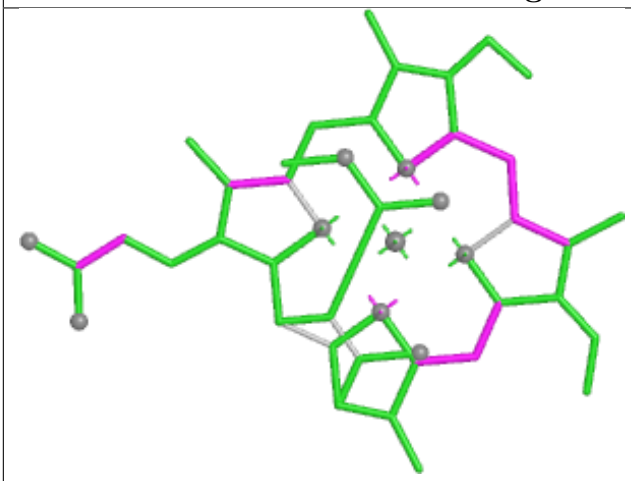


Rings

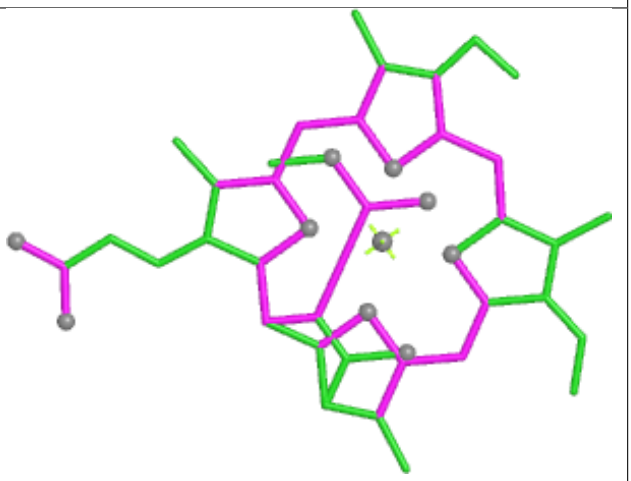
Ligand CLA I 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

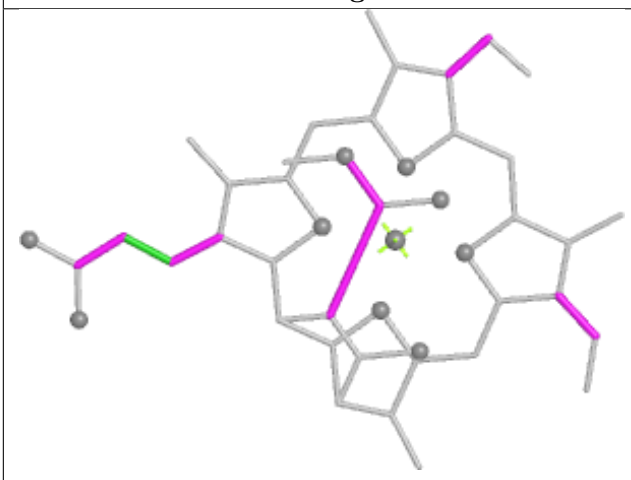
Ligand KC2 H 314



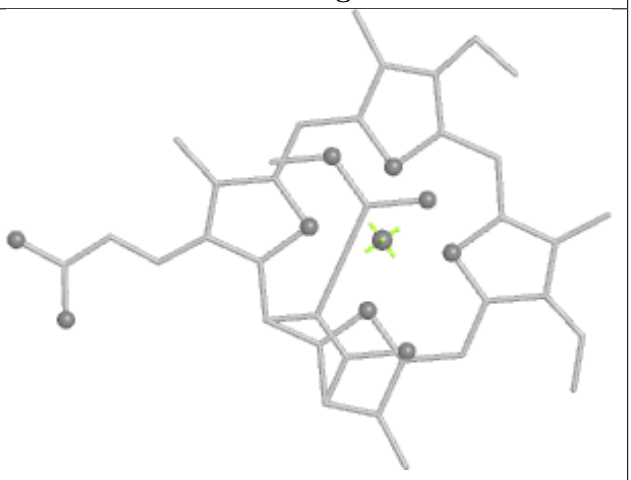
Bond lengths



Bond angles

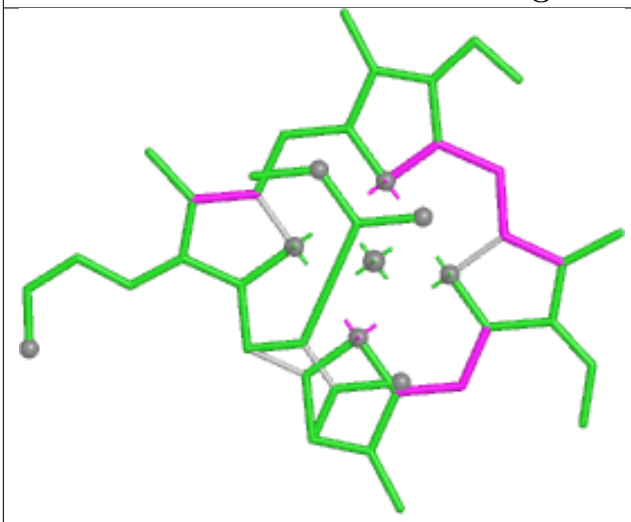


Torsions



Rings

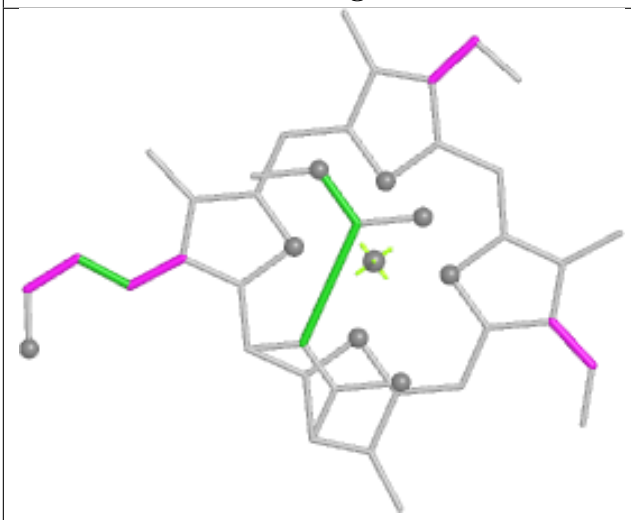
Ligand KC2 I 312



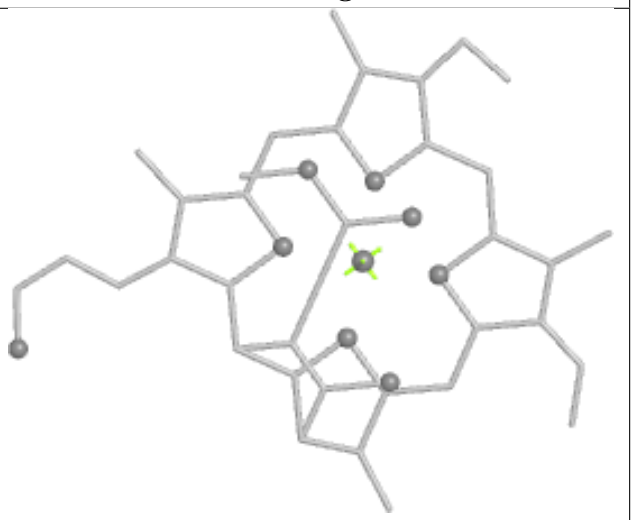
Bond lengths



Bond angles

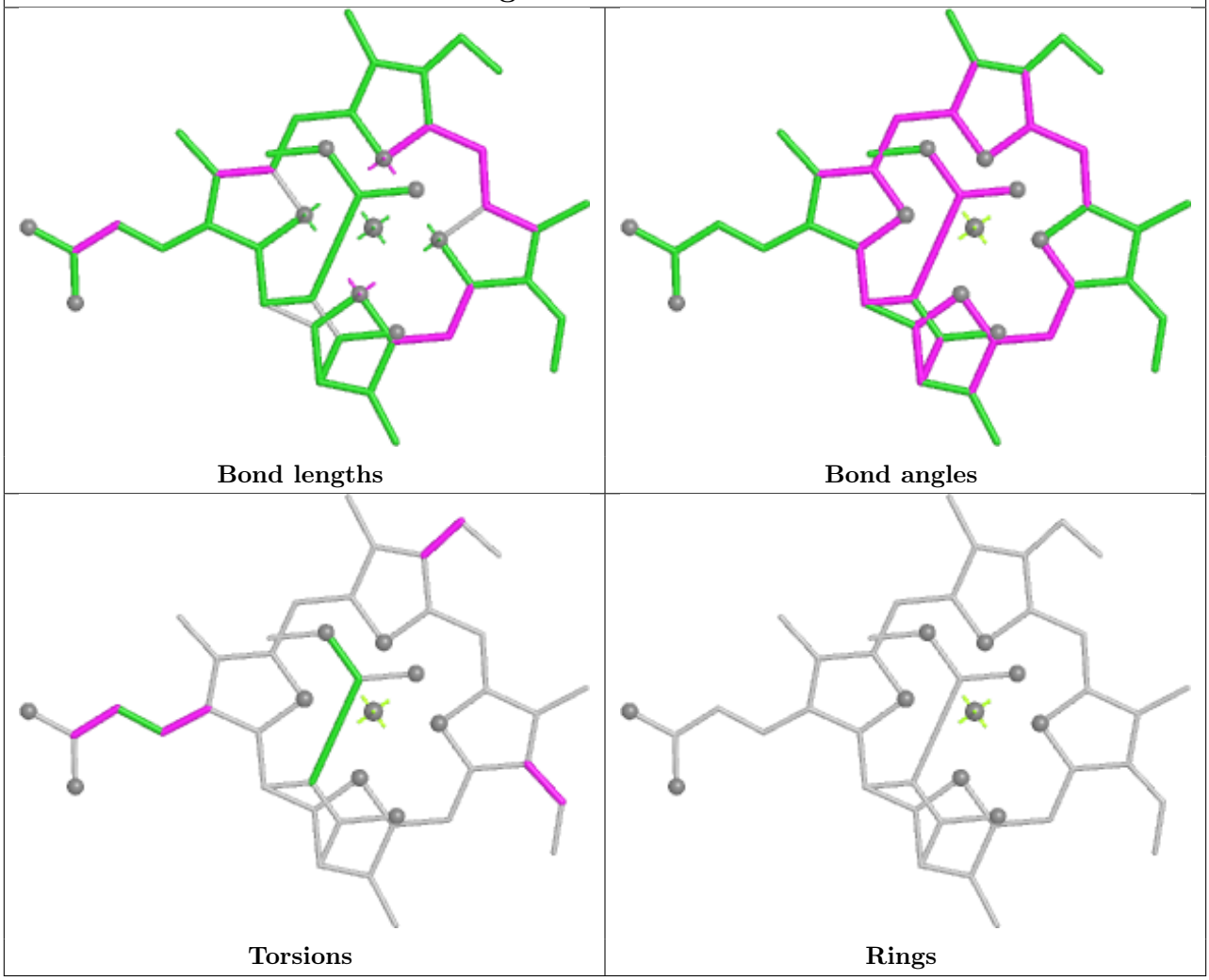


Torsions



Rings

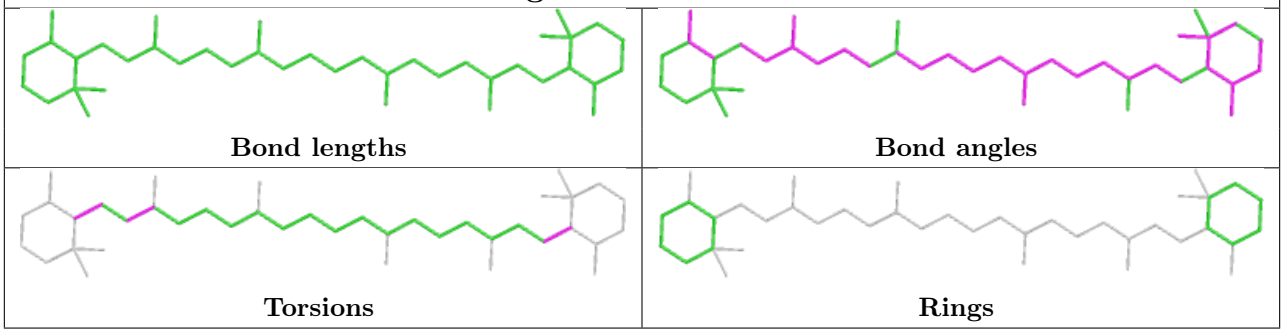
Ligand KC2 S 317



Bond lengths | Bond angles

Torsions | Rings

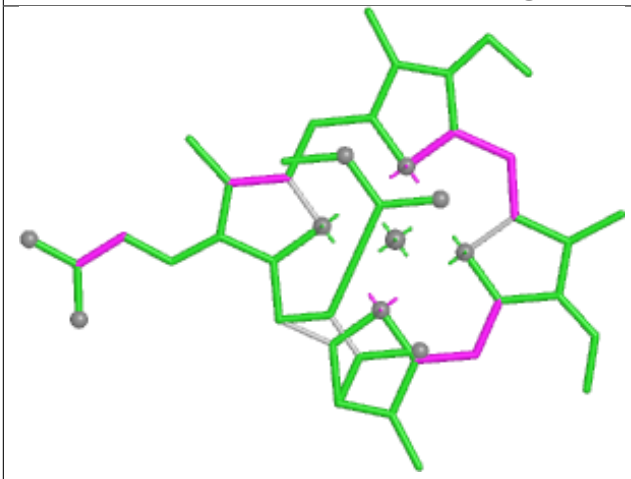
Ligand BCR h 202



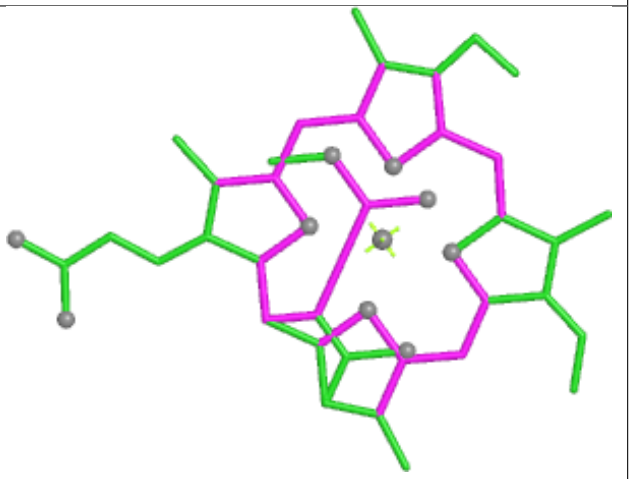
Bond lengths | Bond angles

Torsions | Rings

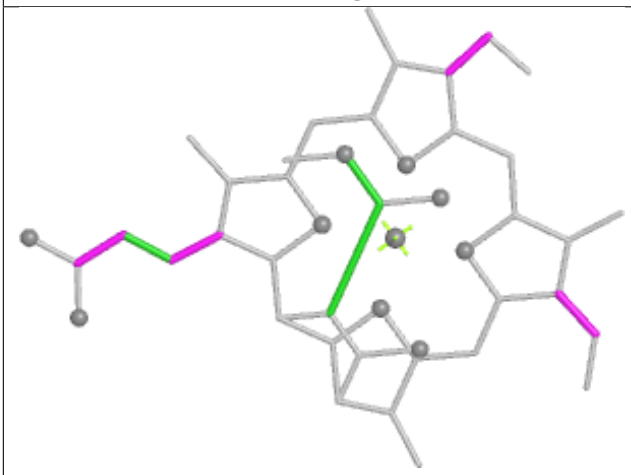
Ligand KC2 W 314



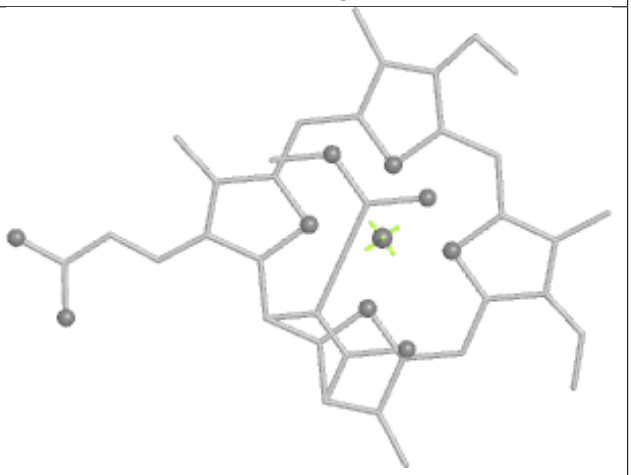
Bond lengths



Bond angles

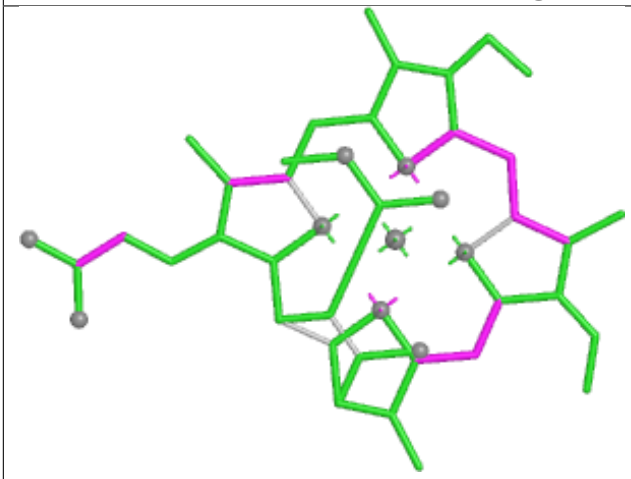


Torsions

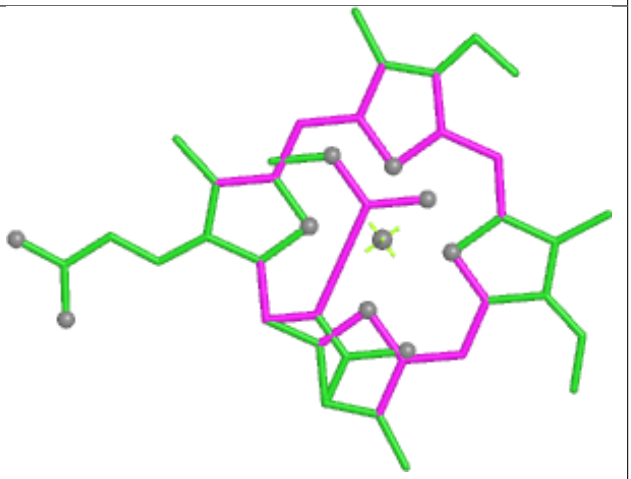


Rings

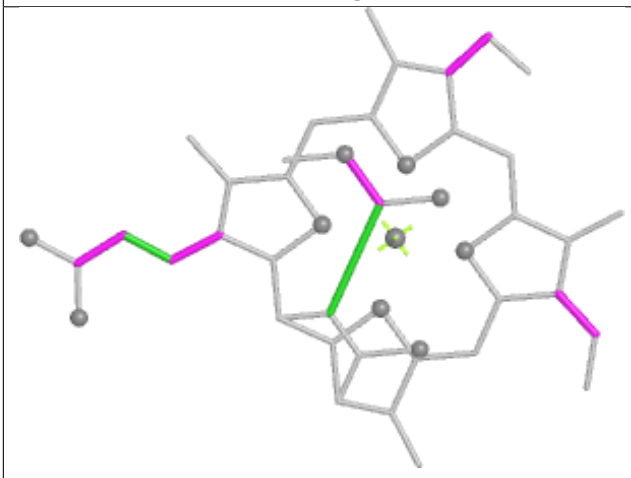
Ligand KC2 9 316



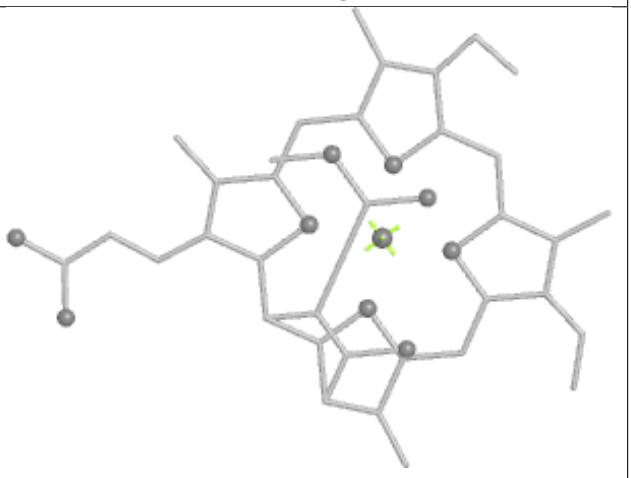
Bond lengths



Bond angles

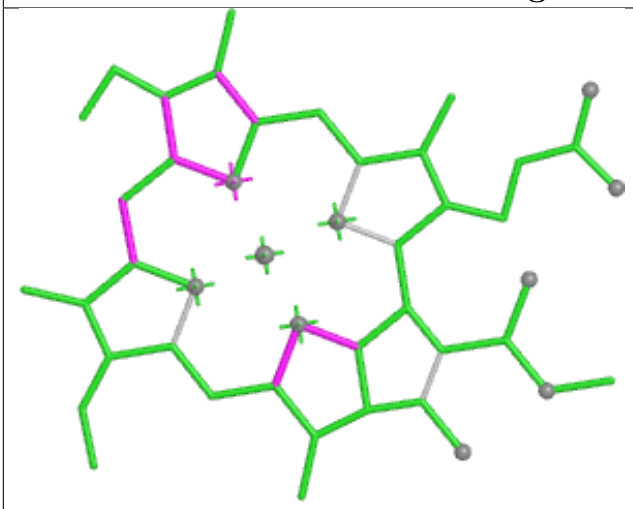


Torsions

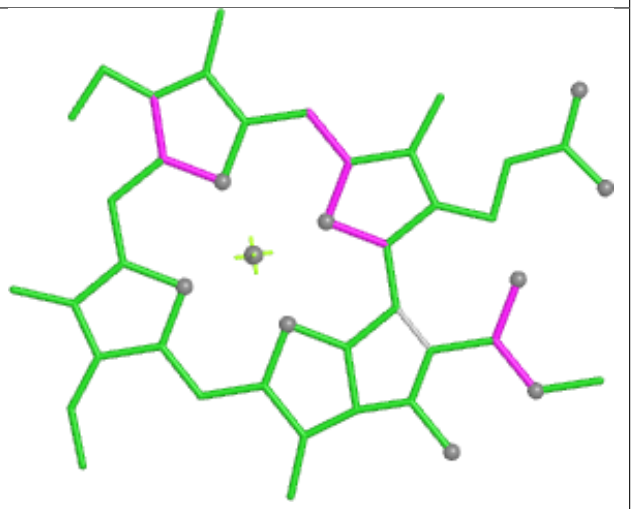


Rings

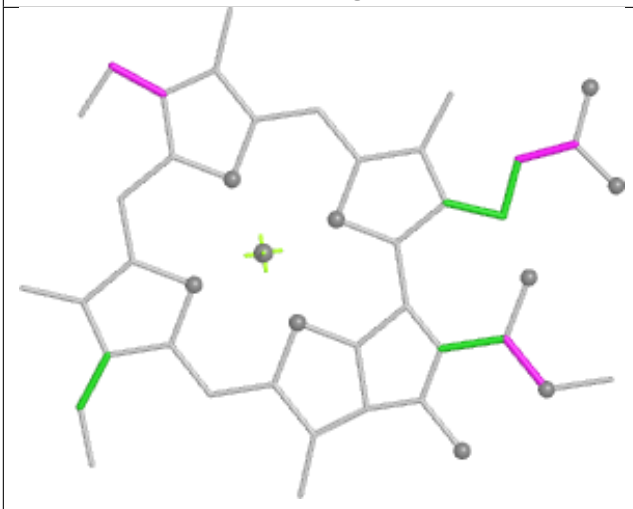
Ligand CLA 1 310



Bond lengths



Bond angles

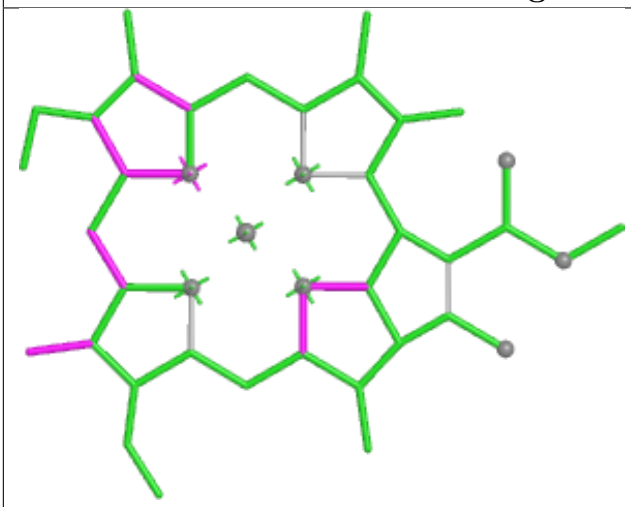


Torsions

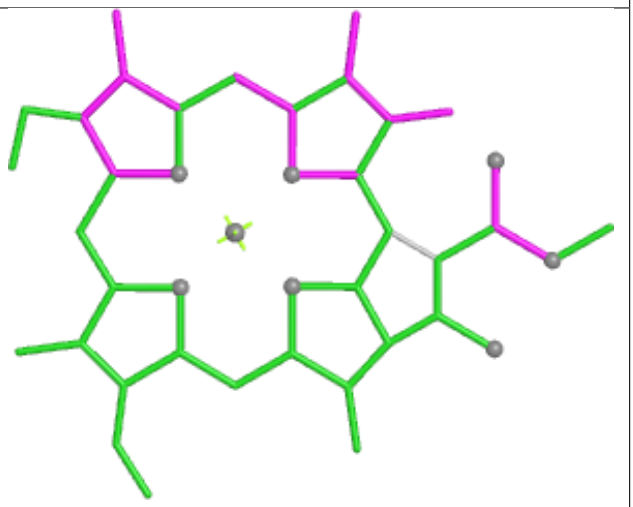


Rings

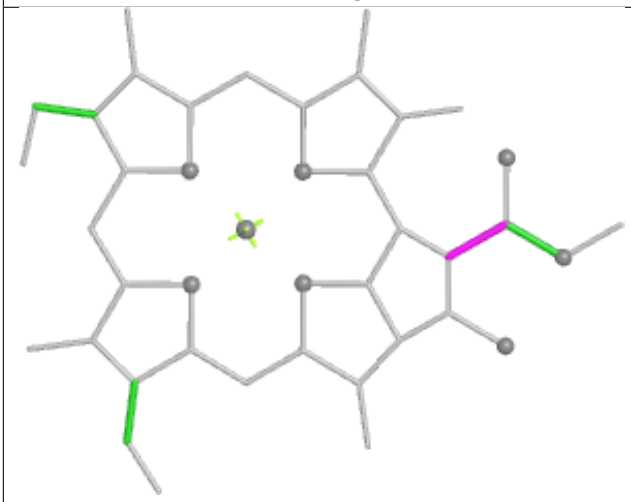
Ligand CLA 9 310



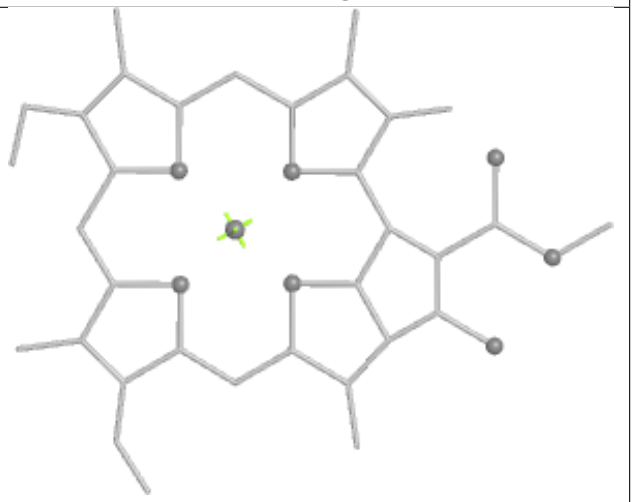
Bond lengths



Bond angles

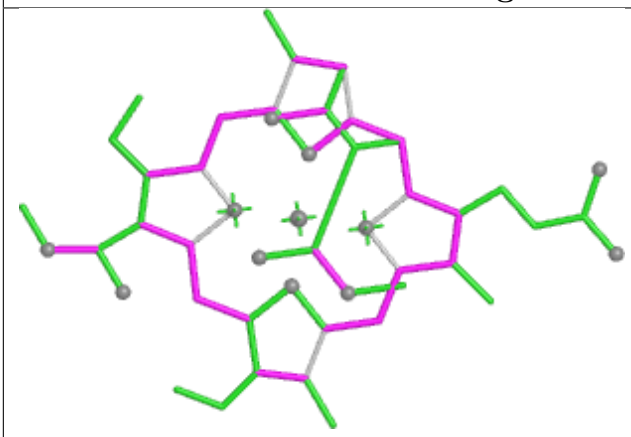


Torsions

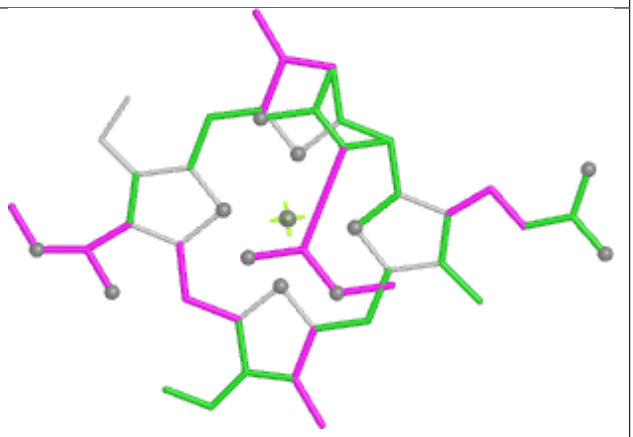


Rings

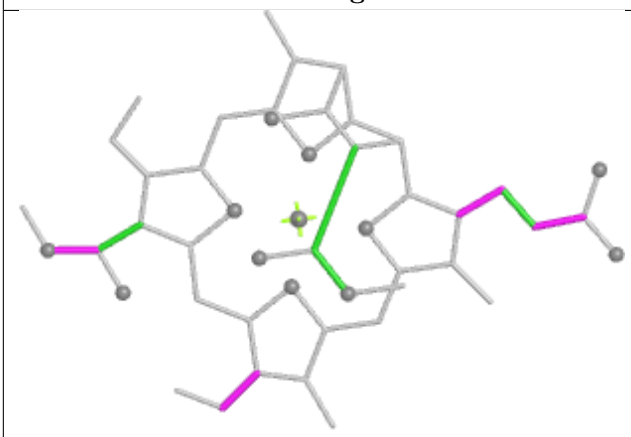
Ligand A1ECV M 316



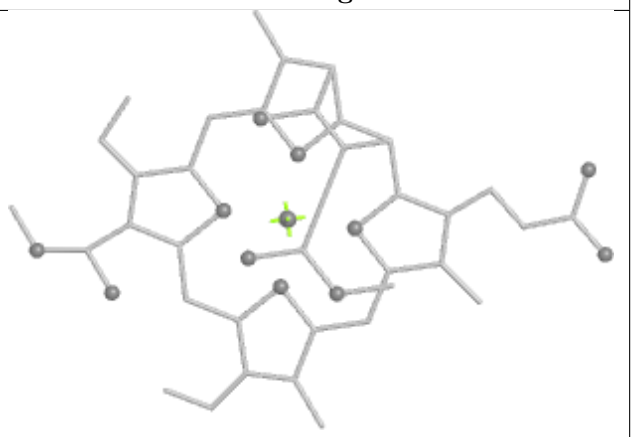
Bond lengths



Bond angles

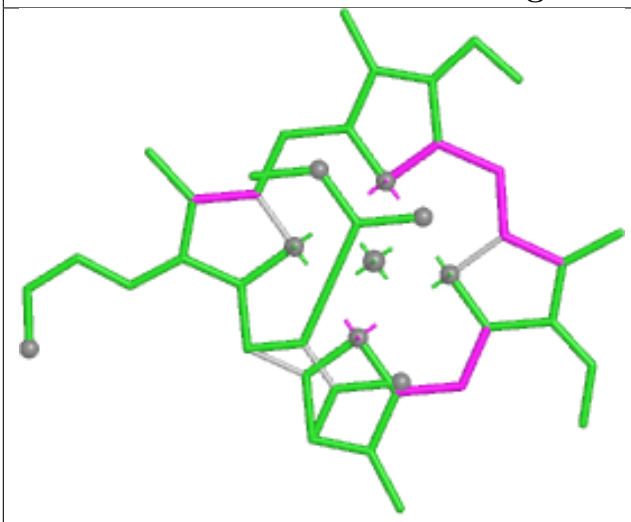


Torsions



Rings

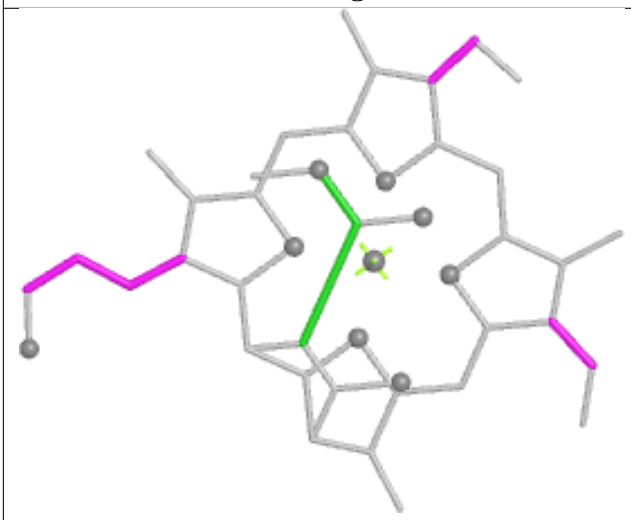
Ligand KC2 P 310



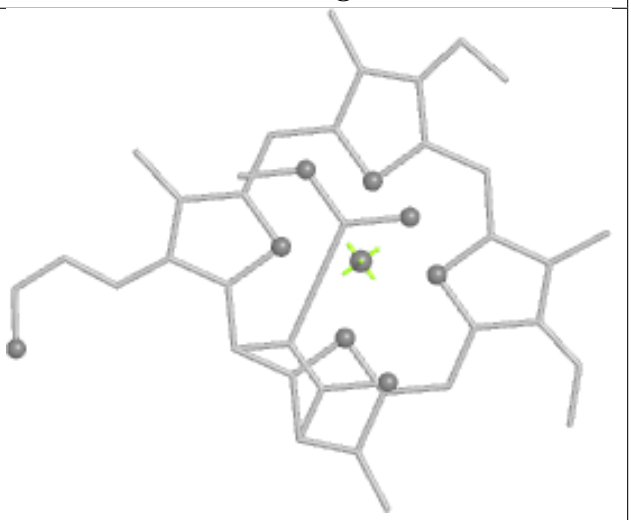
Bond lengths



Bond angles

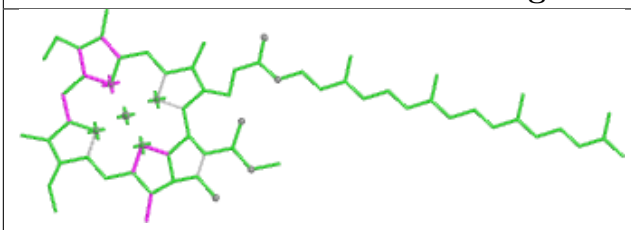


Torsions

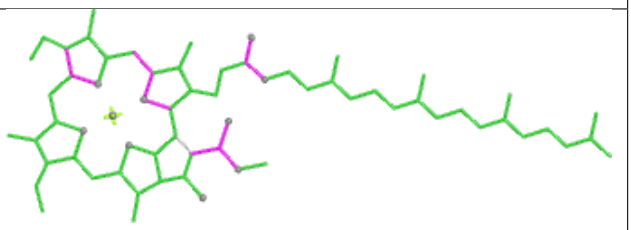


Rings

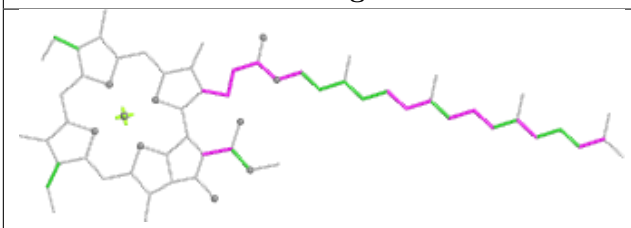
Ligand CLA a 806



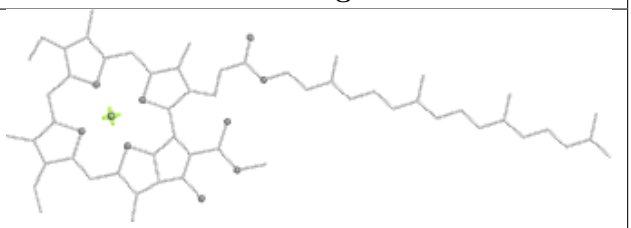
Bond lengths



Bond angles

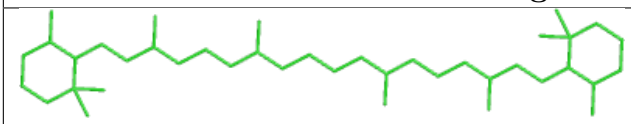


Torsions

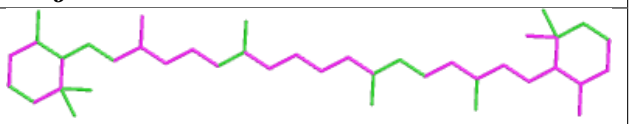


Rings

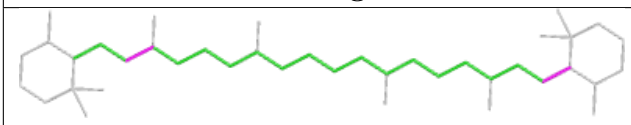
Ligand BCR j 103



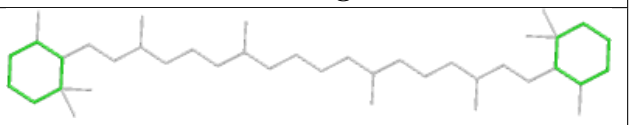
Bond lengths



Bond angles

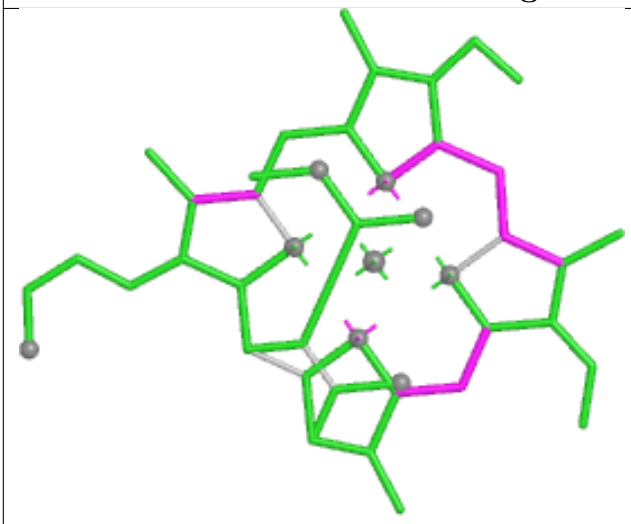


Torsions



Rings

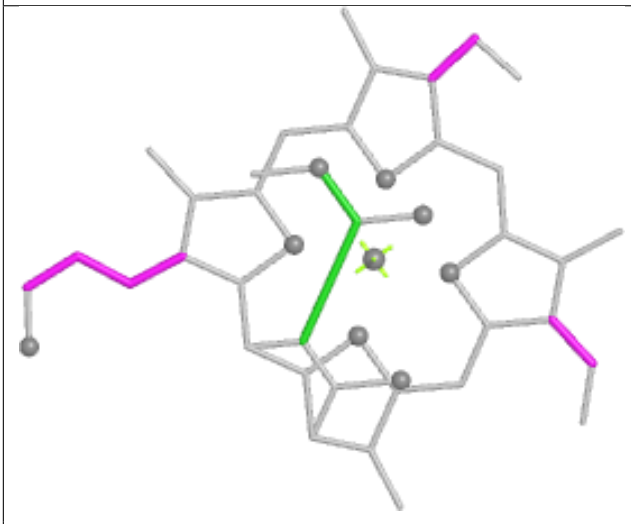
Ligand KC2 W 312



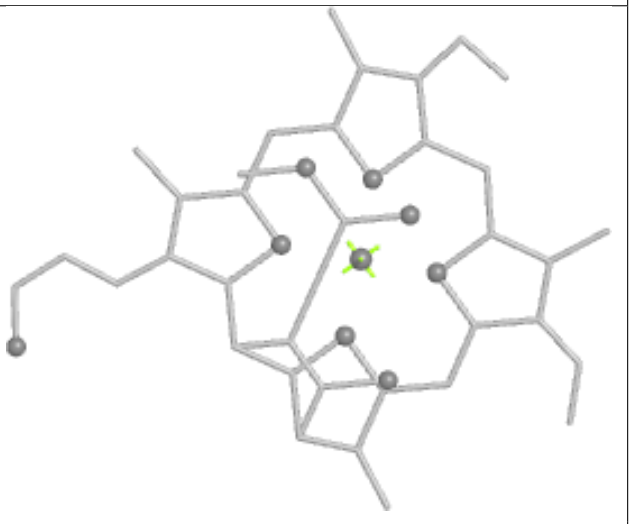
Bond lengths



Bond angles

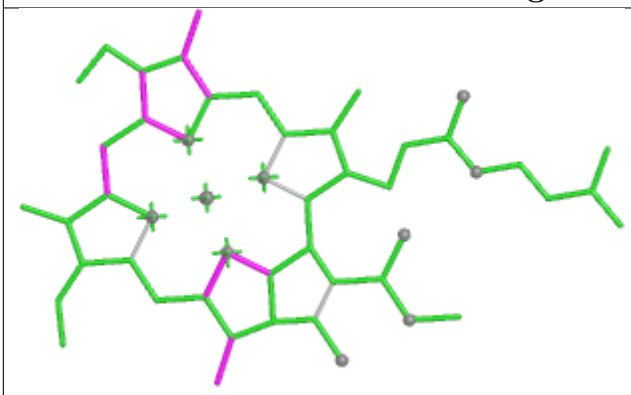


Torsions

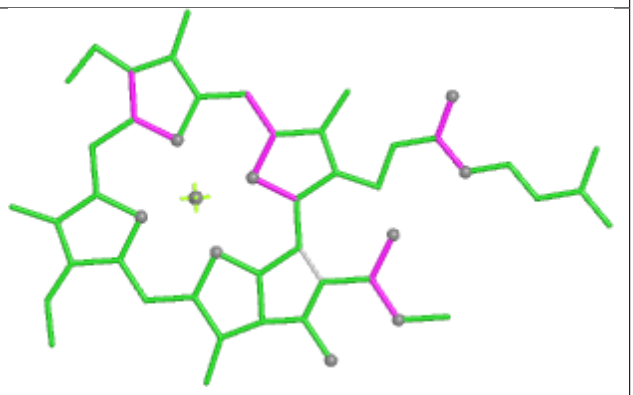


Rings

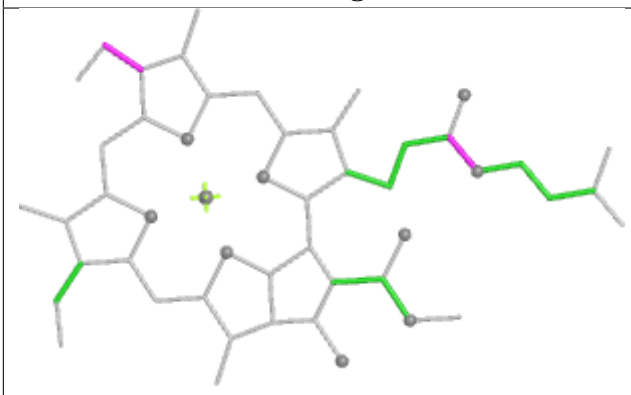
Ligand CLA b 822



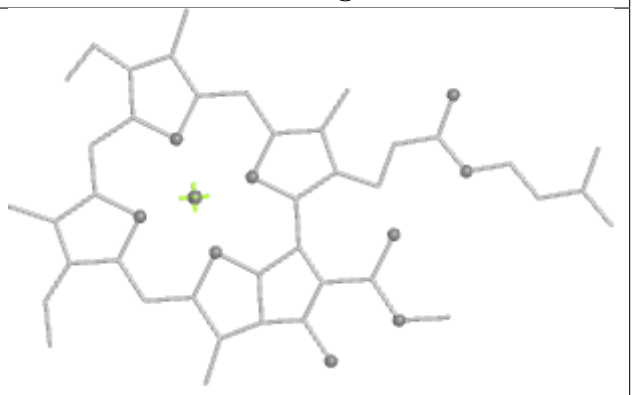
Bond lengths



Bond angles

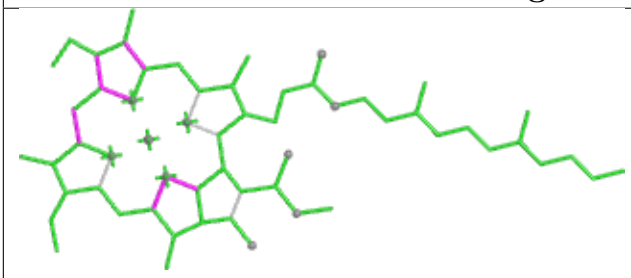


Torsions

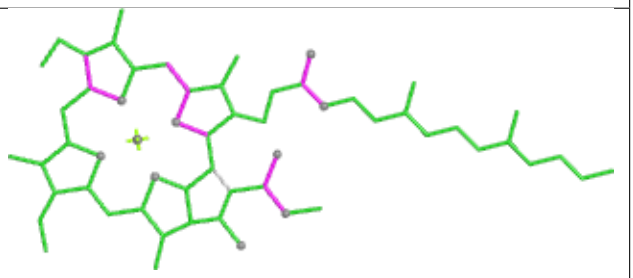


Rings

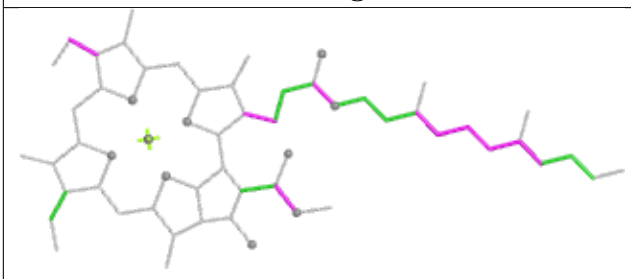
Ligand CLA o 206



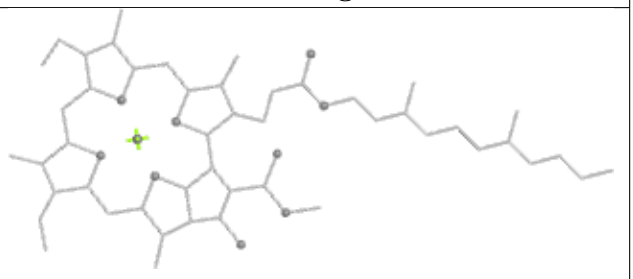
Bond lengths



Bond angles

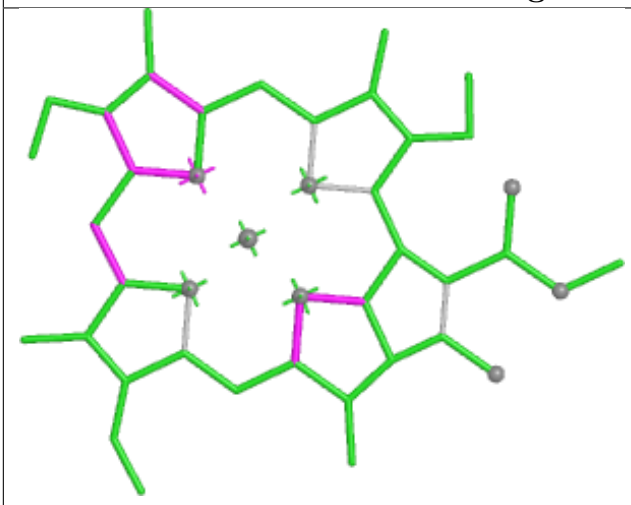


Torsions

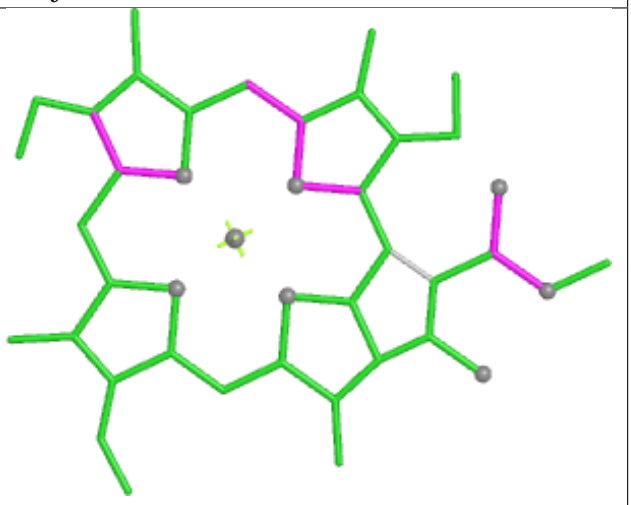


Rings

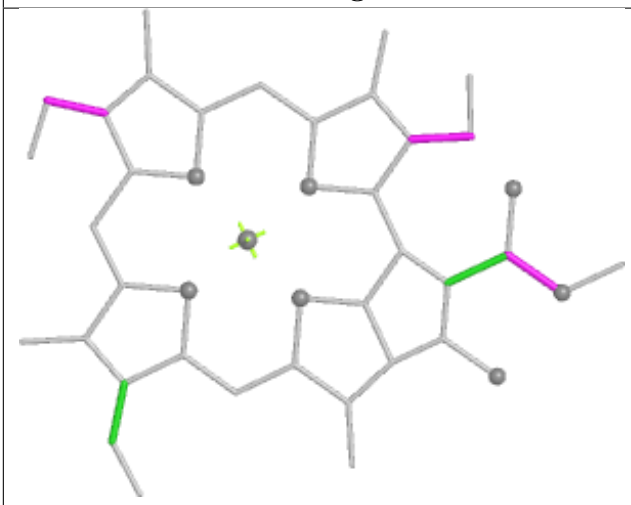
Ligand CLA y 312



Bond lengths



Bond angles

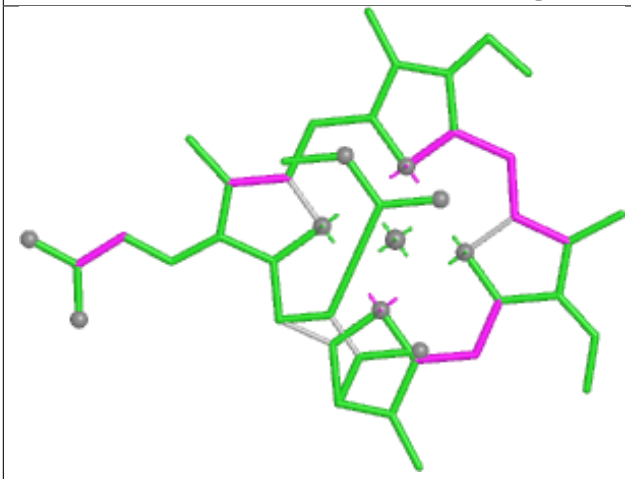


Torsions

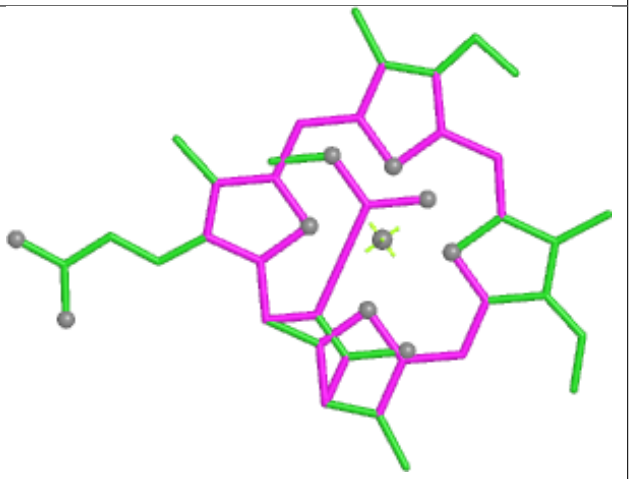


Rings

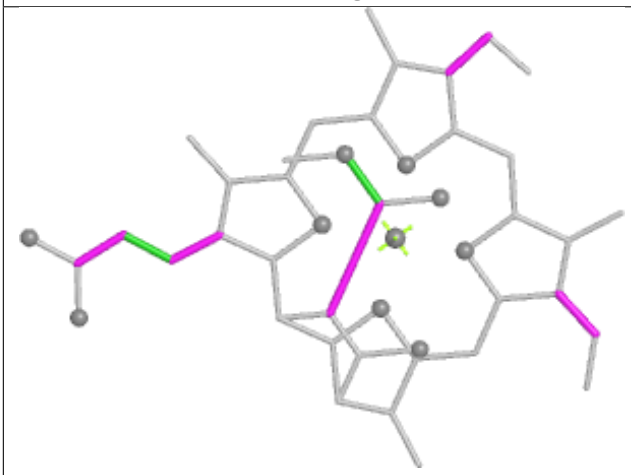
Ligand KC2 5 314



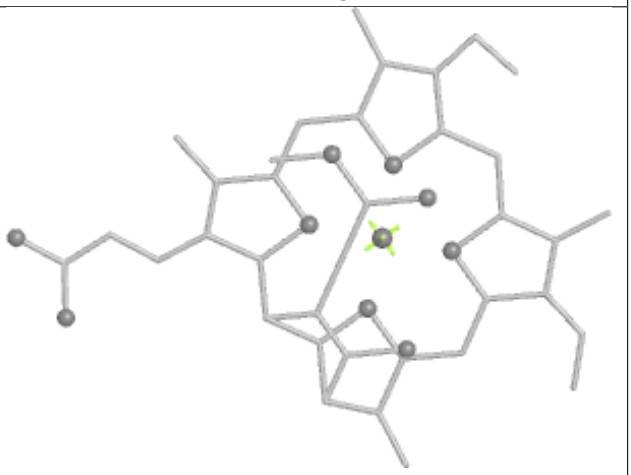
Bond lengths



Bond angles

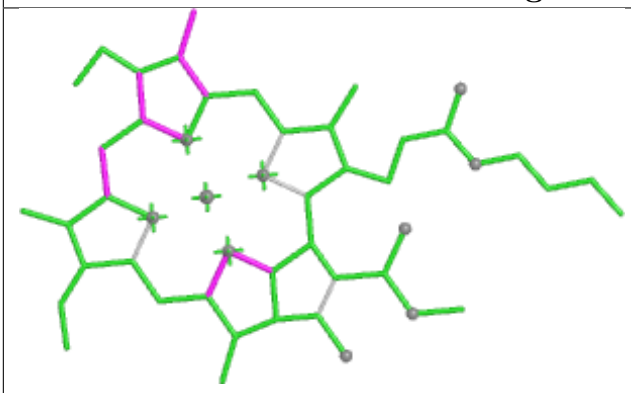


Torsions

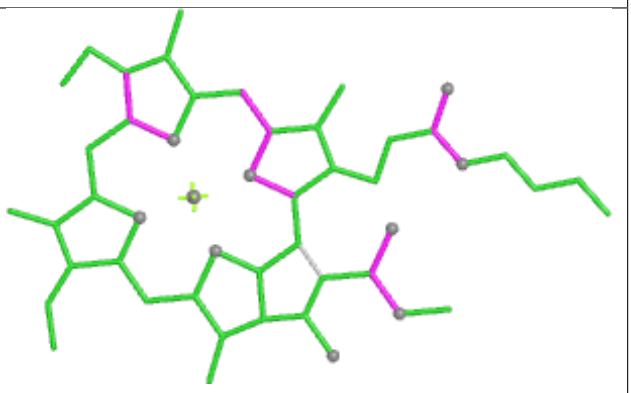


Rings

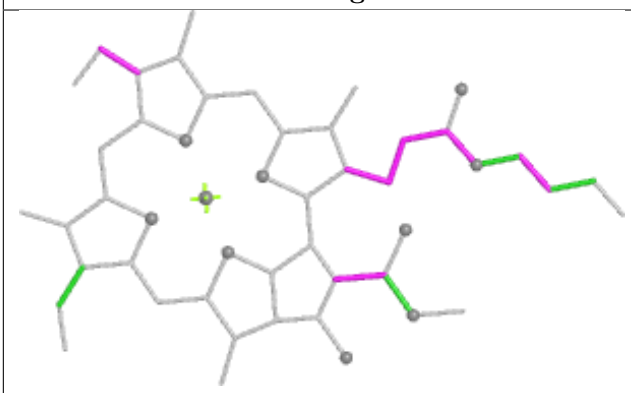
Ligand CLA E 319



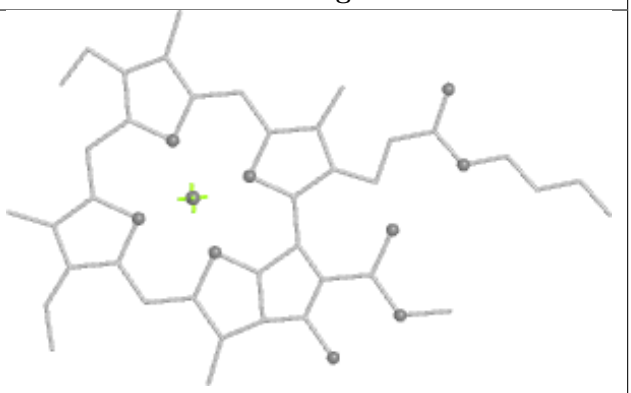
Bond lengths



Bond angles

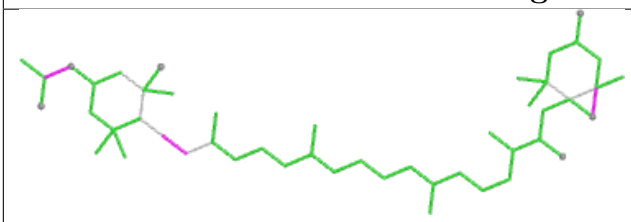


Torsions

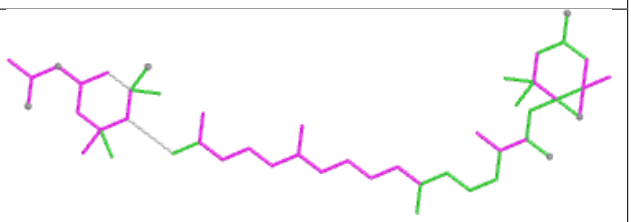


Rings

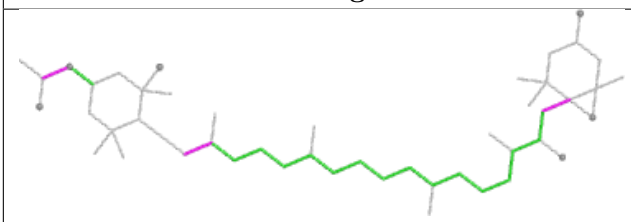
Ligand A86 B 201



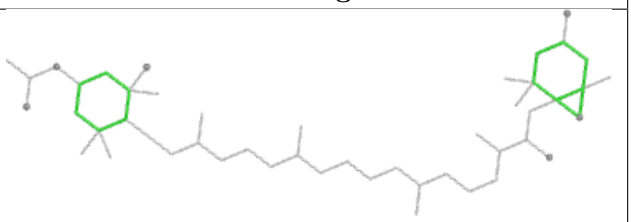
Bond lengths



Bond angles

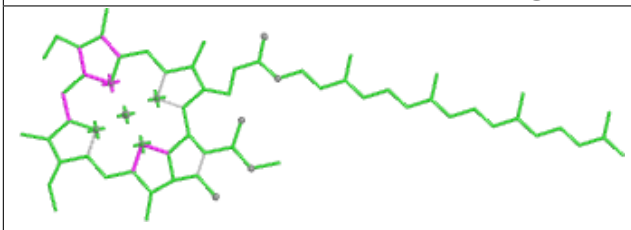


Torsions

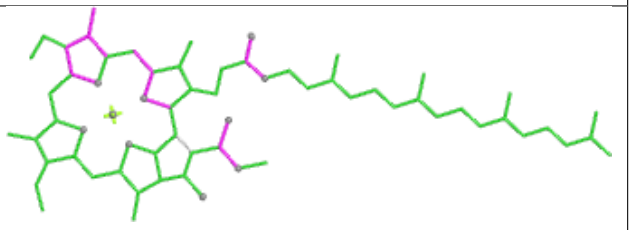


Rings

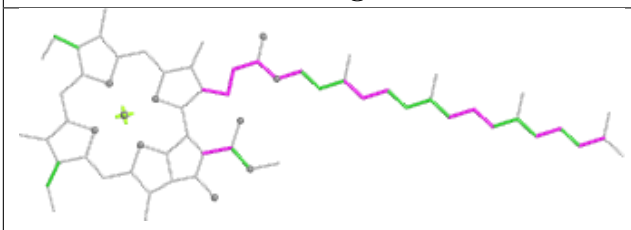
Ligand CLA J 309



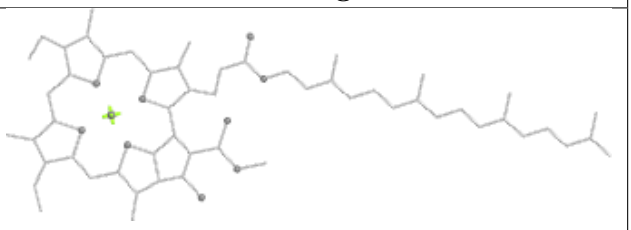
Bond lengths



Bond angles



Torsions

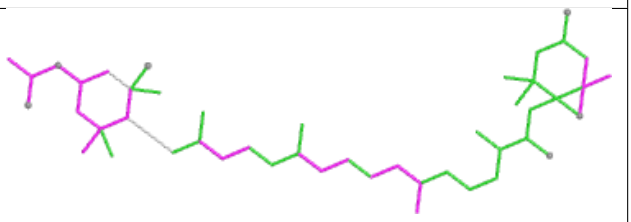


Rings

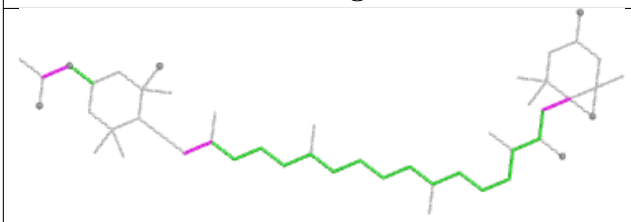
Ligand A86 k 206



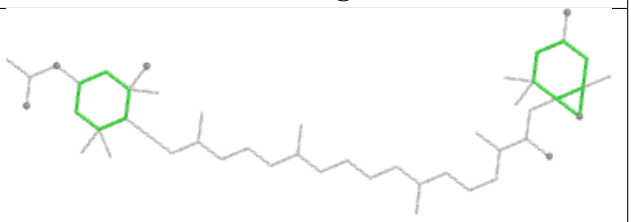
Bond lengths



Bond angles

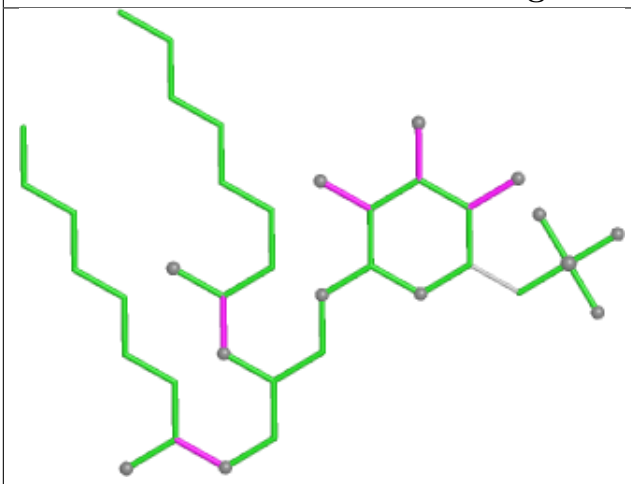


Torsions

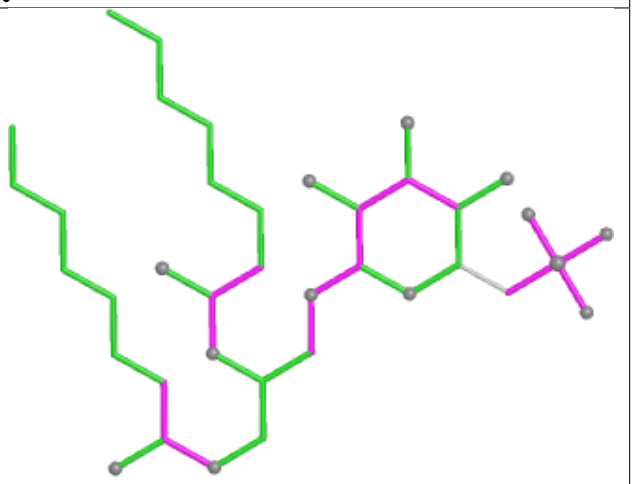


Rings

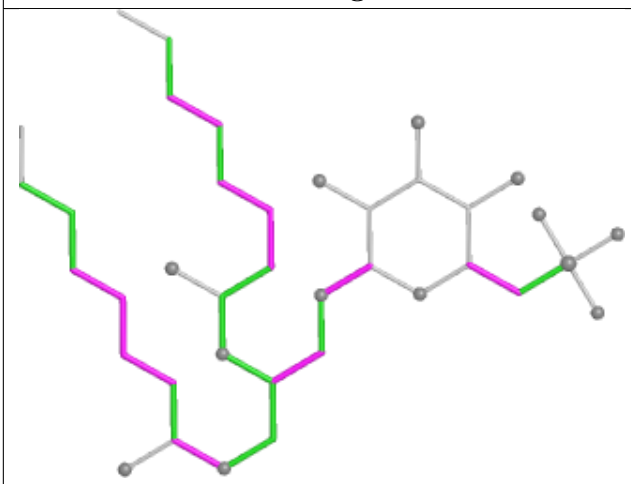
Ligand SQD k 205



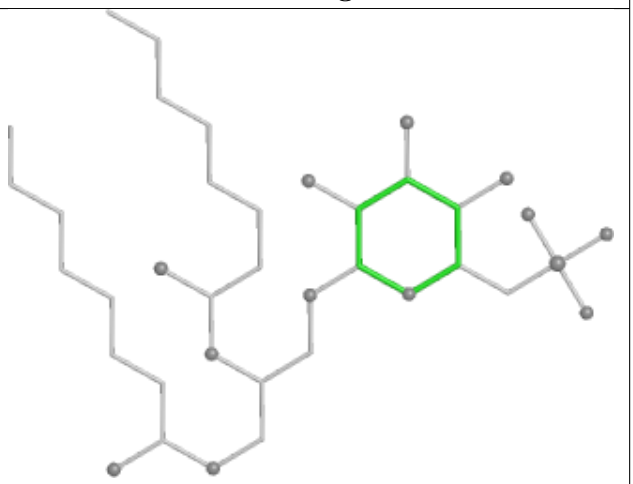
Bond lengths



Bond angles

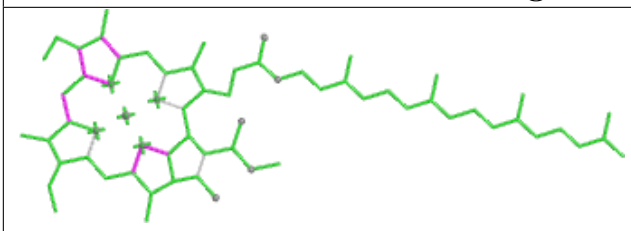


Torsions

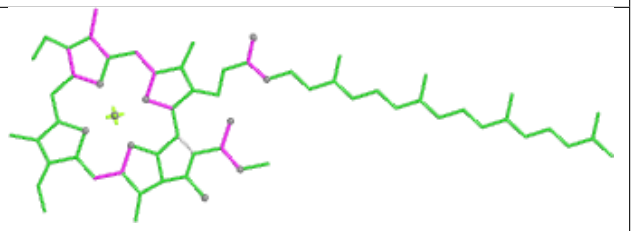


Rings

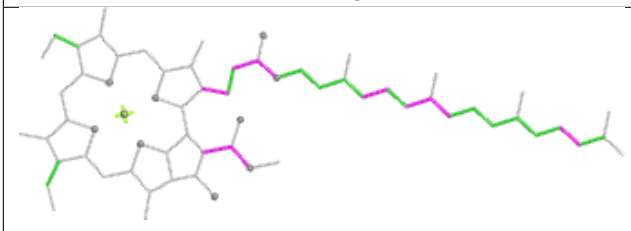
Ligand CLA b 809



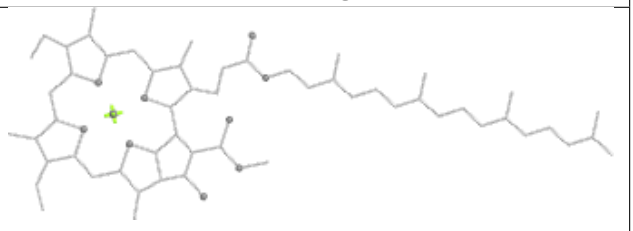
Bond lengths



Bond angles

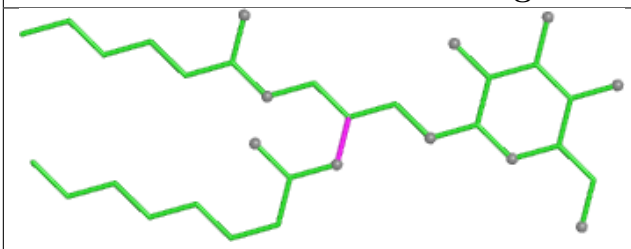


Torsions

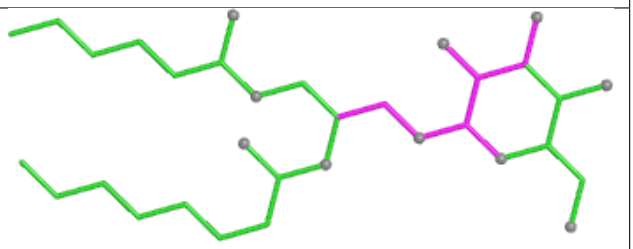


Rings

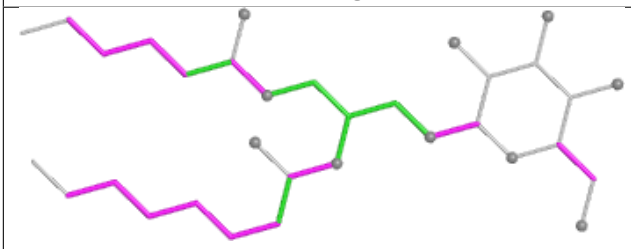
Ligand LMG W 320



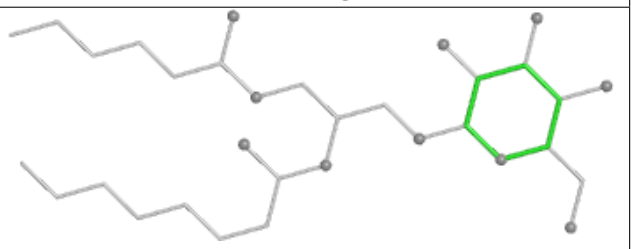
Bond lengths



Bond angles

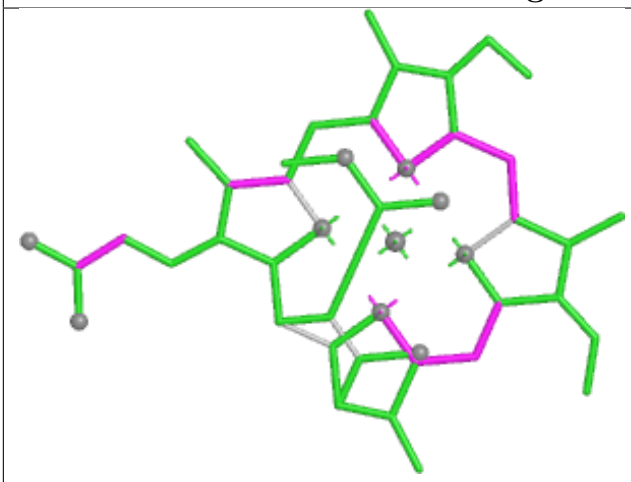


Torsions

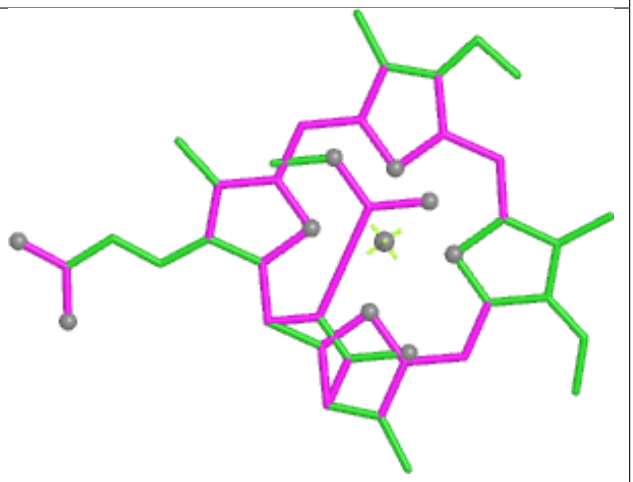


Rings

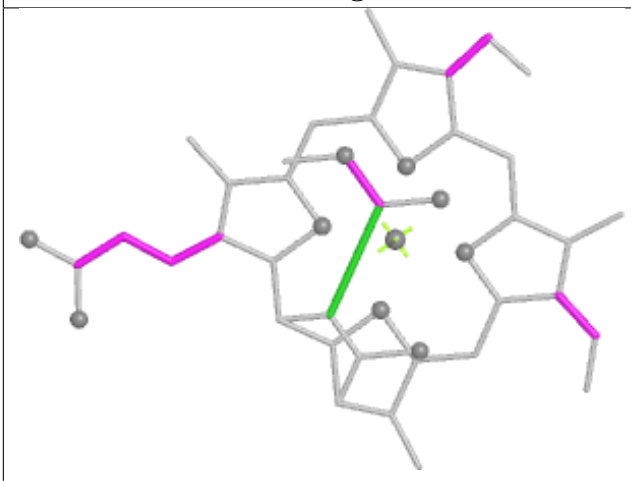
Ligand KC2 P 313



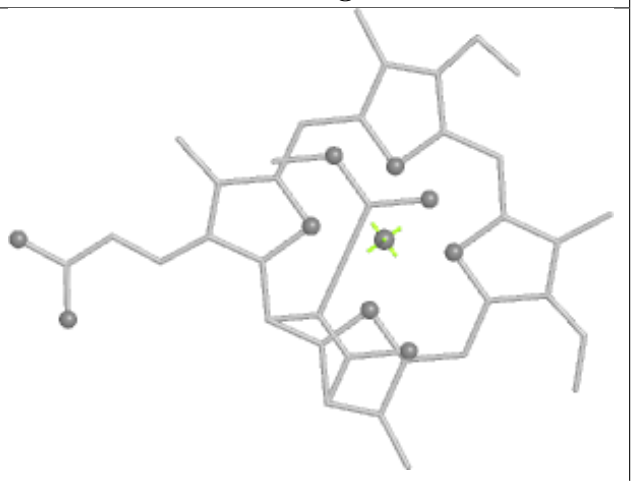
Bond lengths



Bond angles

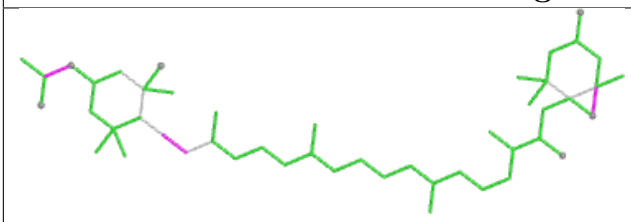


Torsions

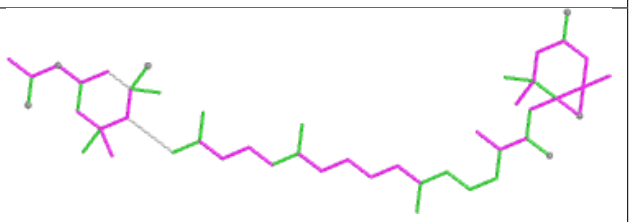


Rings

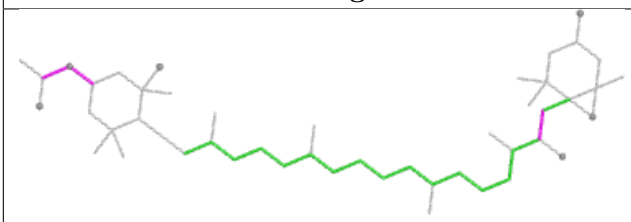
Ligand A86 0 301



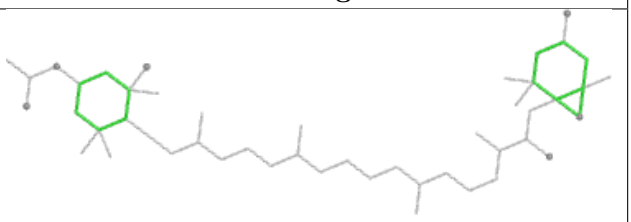
Bond lengths



Bond angles

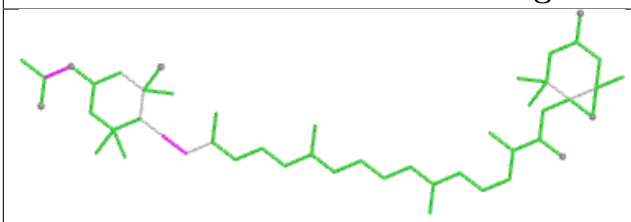


Torsions

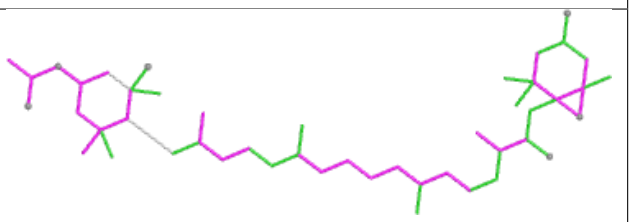


Rings

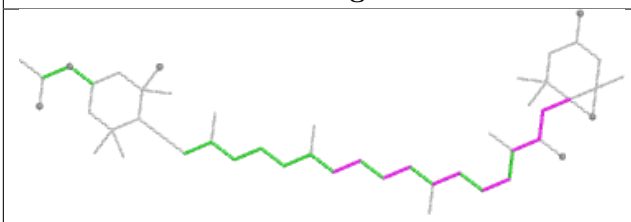
Ligand A86 6 309



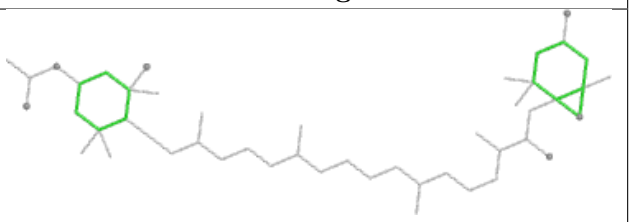
Bond lengths



Bond angles

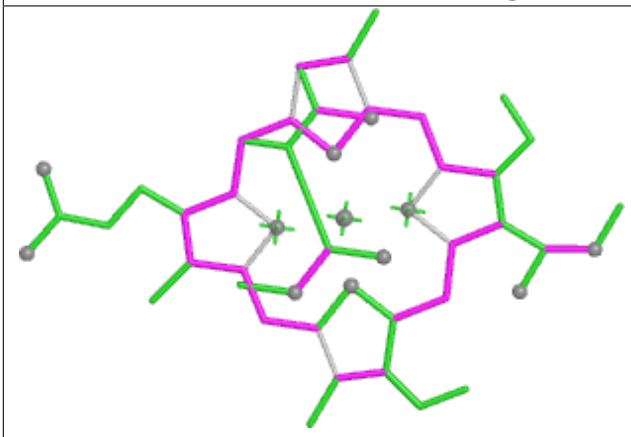


Torsions

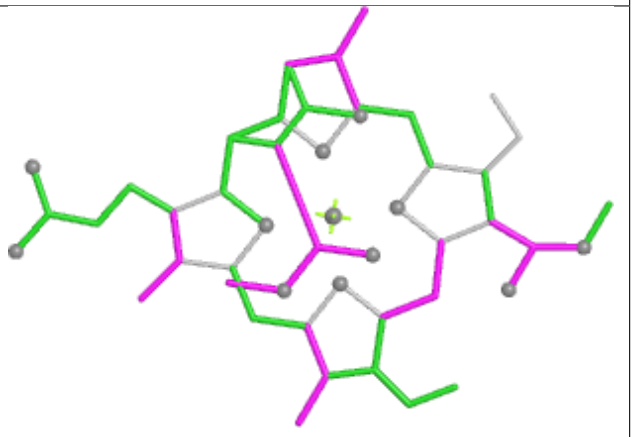


Rings

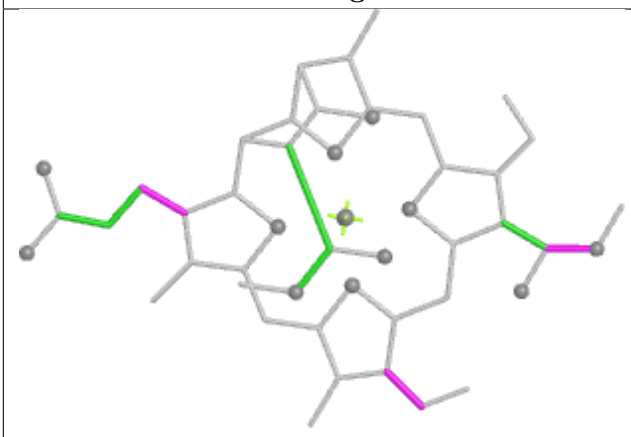
Ligand A1ECV S 318



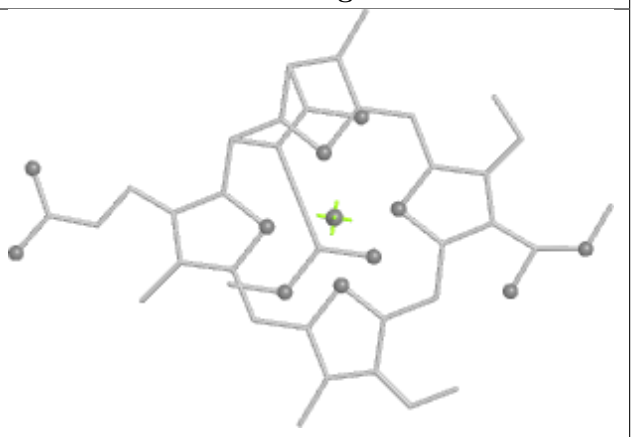
Bond lengths



Bond angles

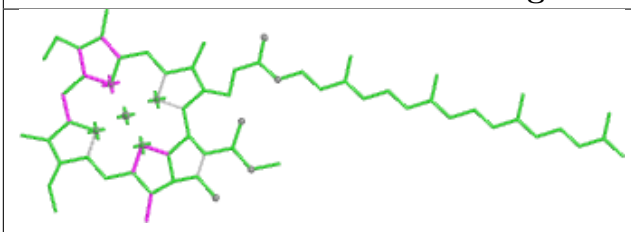


Torsions

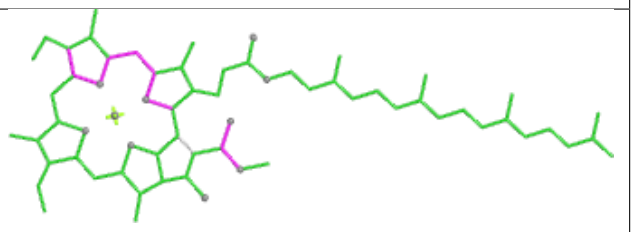


Rings

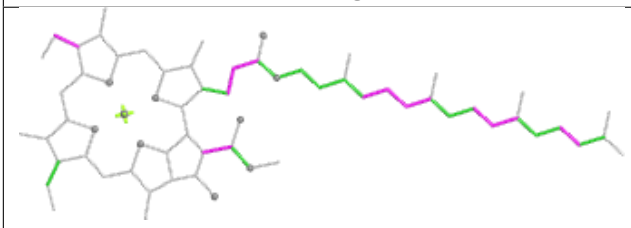
Ligand CLA S 311



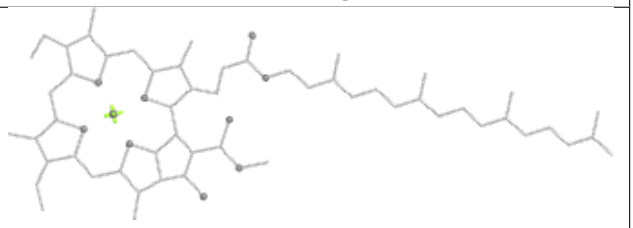
Bond lengths



Bond angles

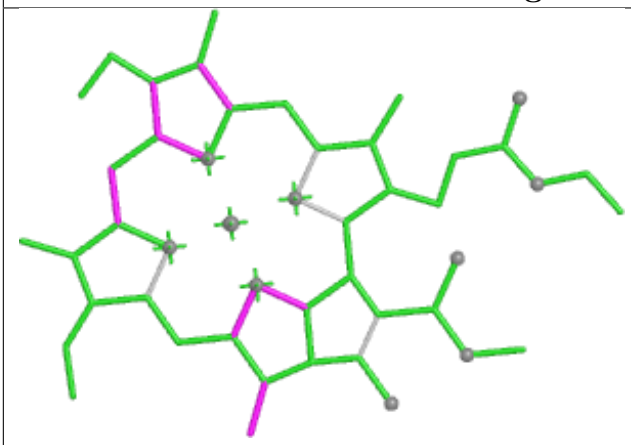


Torsions

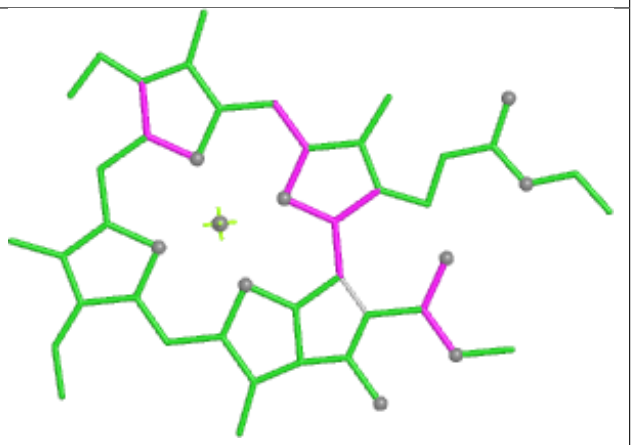


Rings

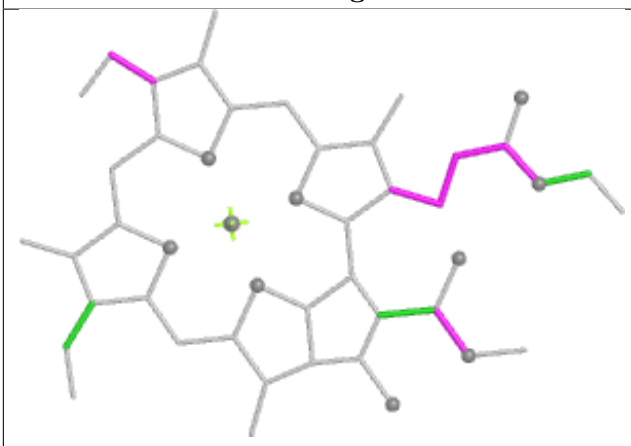
Ligand CLA T 318



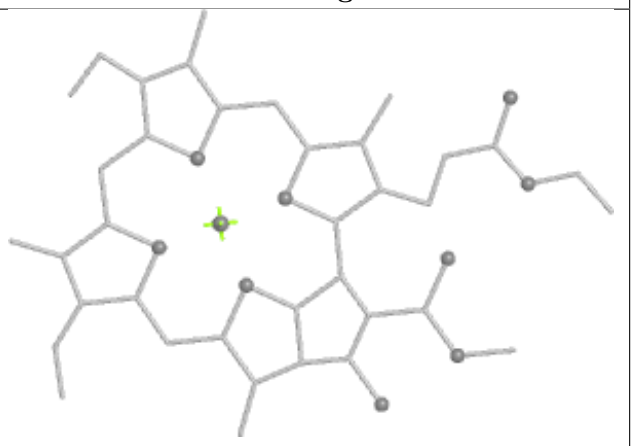
Bond lengths



Bond angles

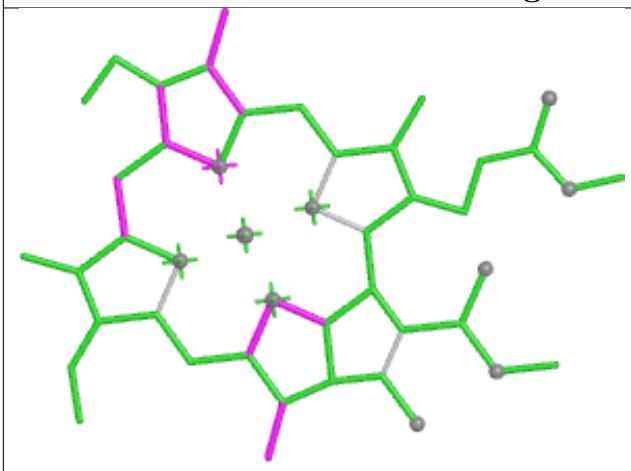


Torsions

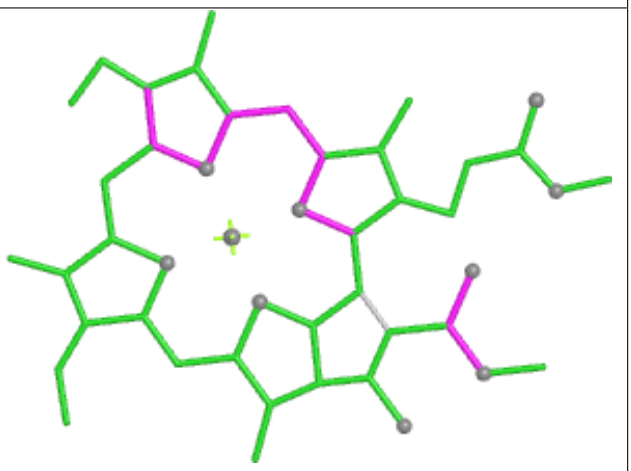


Rings

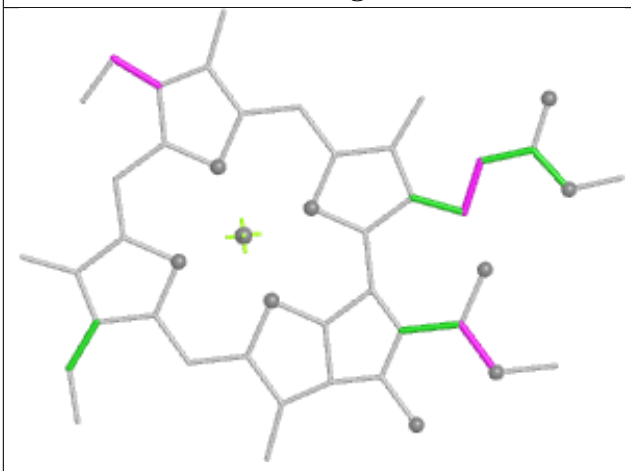
Ligand CLA U 208



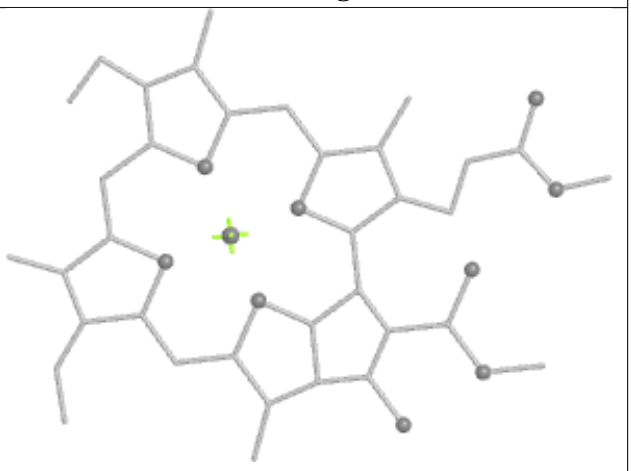
Bond lengths



Bond angles

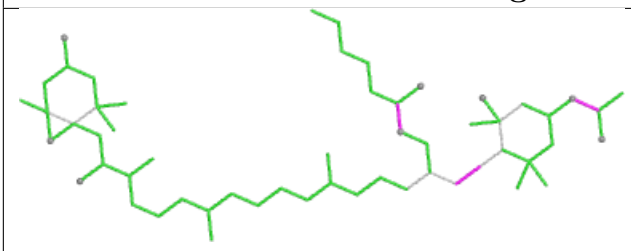


Torsions

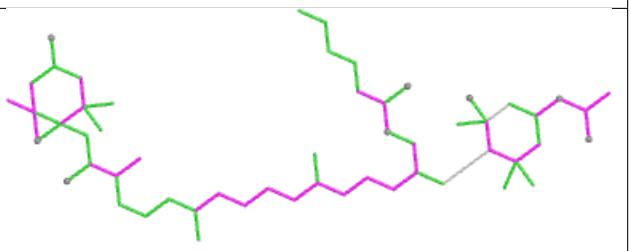


Rings

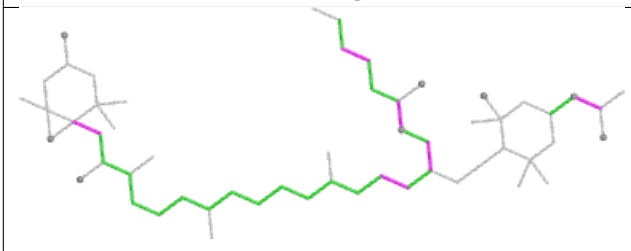
Ligand A1EB1 5 302



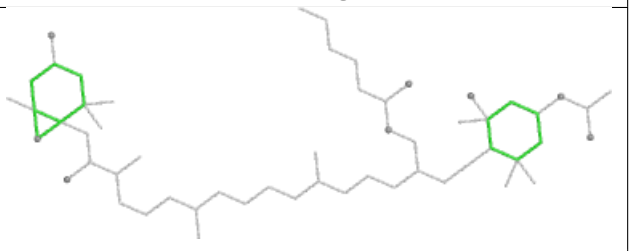
Bond lengths



Bond angles

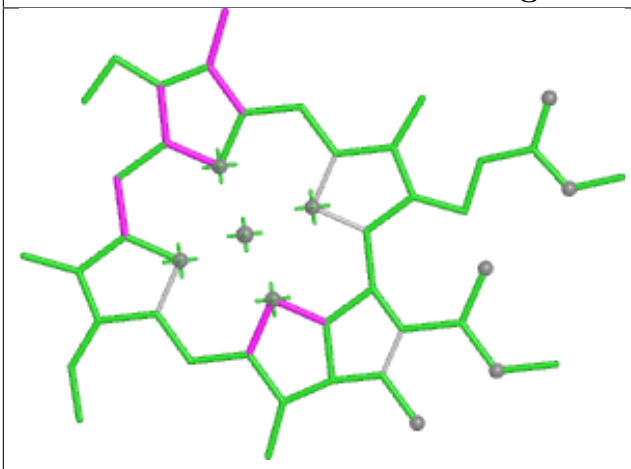


Torsions

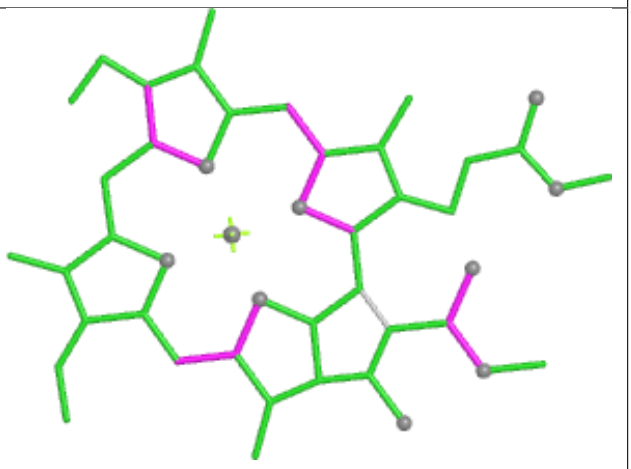


Rings

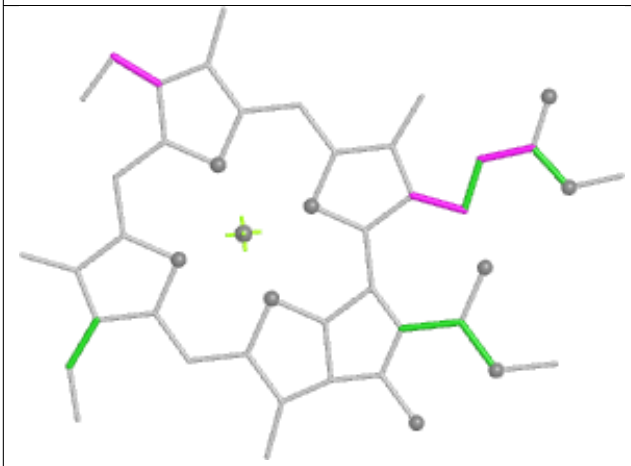
Ligand CLA M 321



Bond lengths



Bond angles

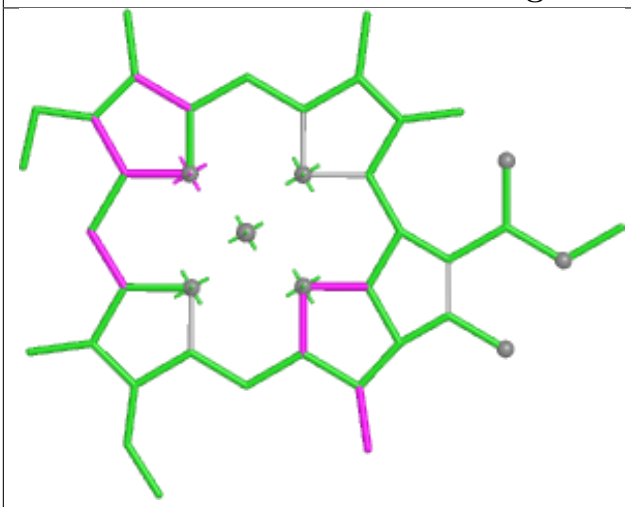


Torsions

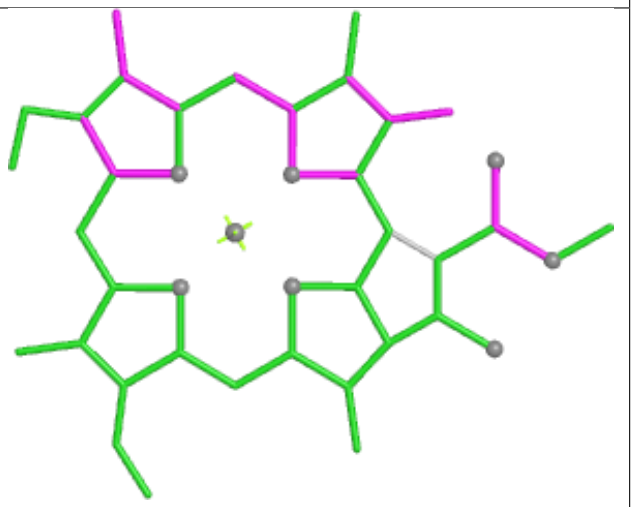


Rings

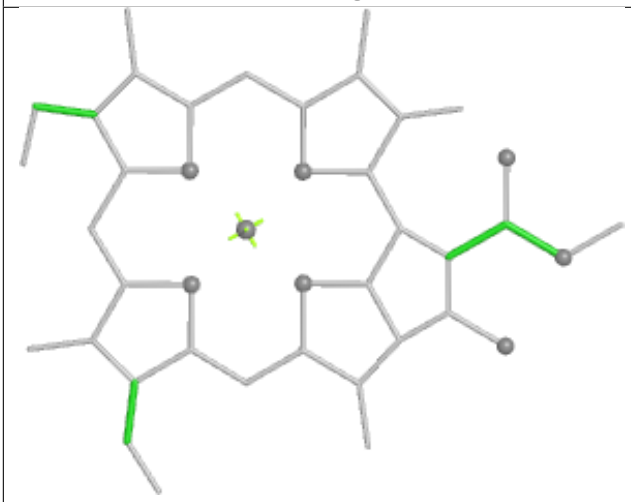
Ligand CLA Z 307



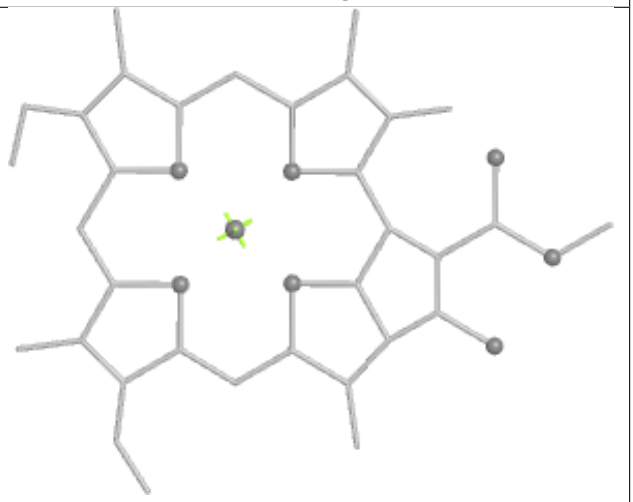
Bond lengths



Bond angles

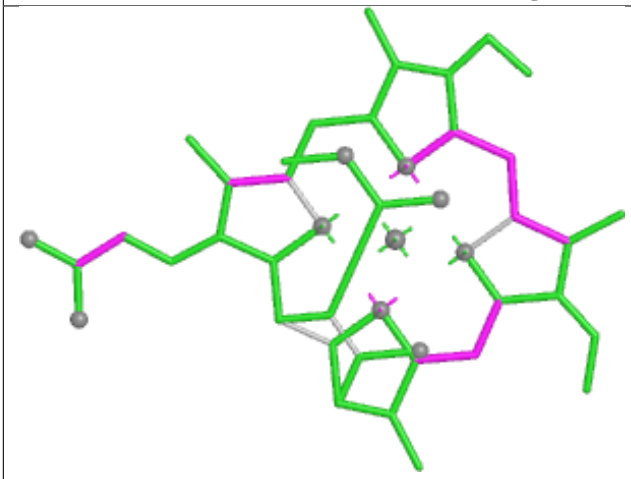


Torsions

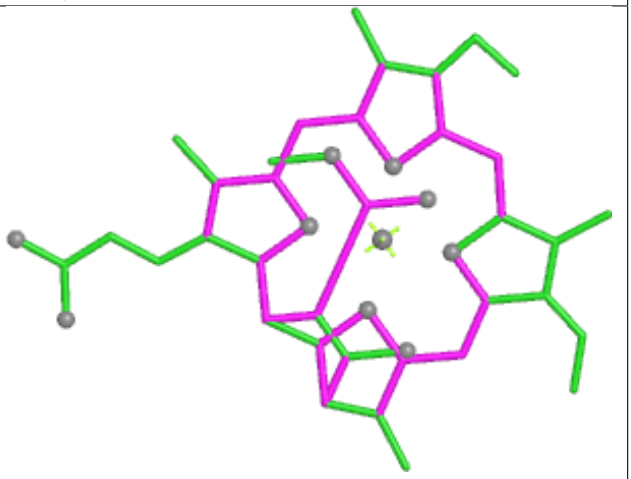


Rings

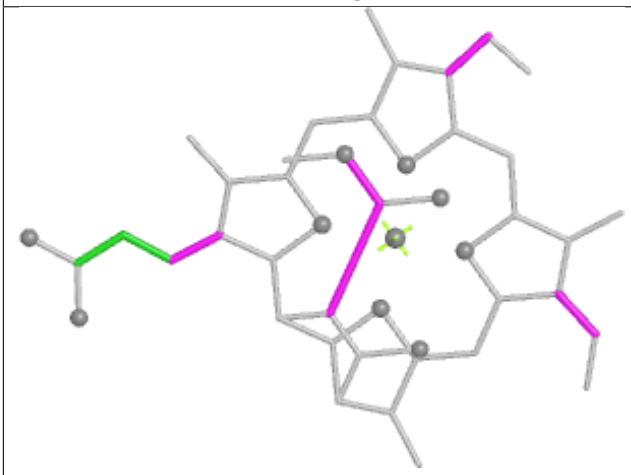
Ligand KC2 Q 315



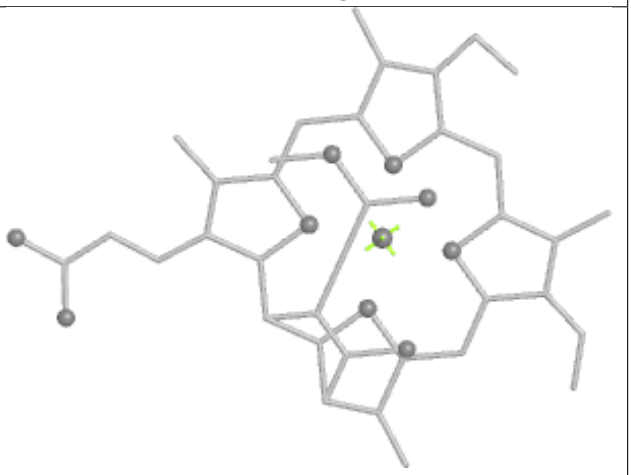
Bond lengths



Bond angles

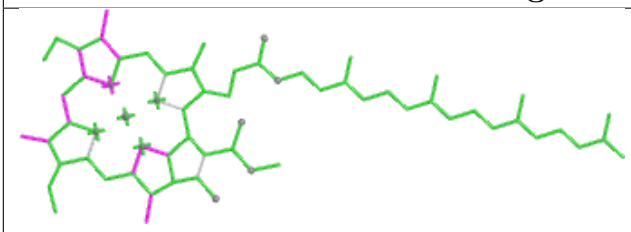


Torsions

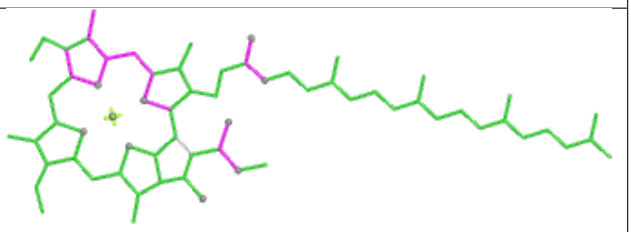


Rings

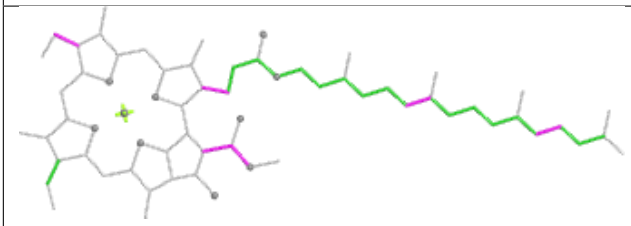
Ligand CLA b 826



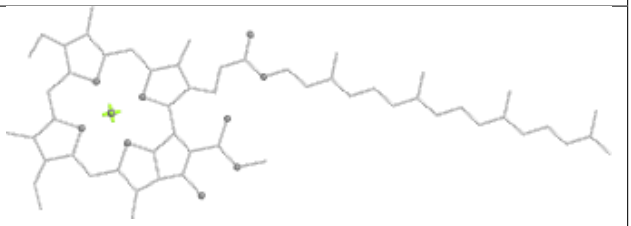
Bond lengths



Bond angles

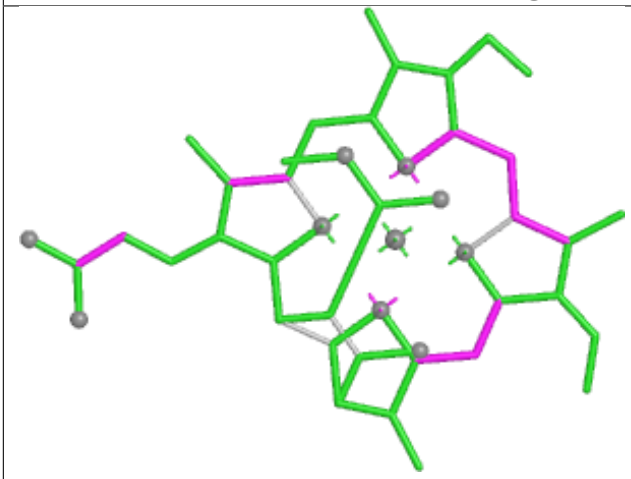


Torsions

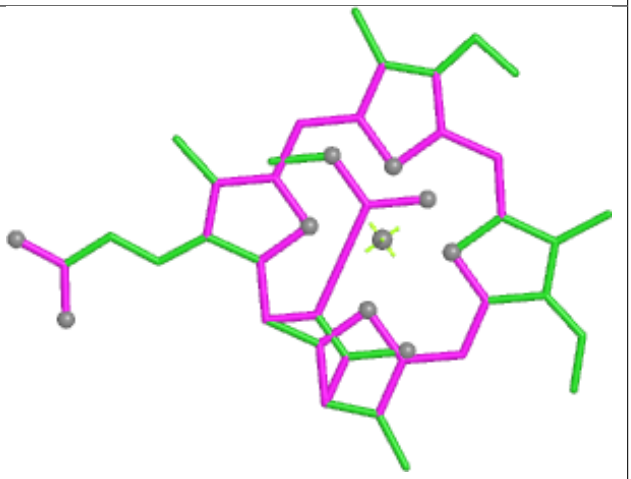


Rings

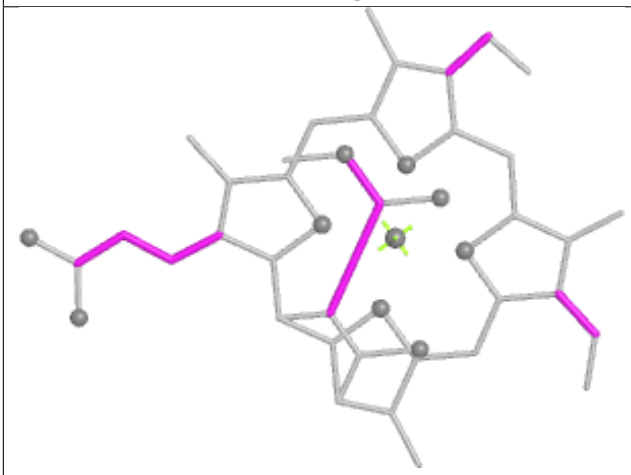
Ligand KC2 A 313



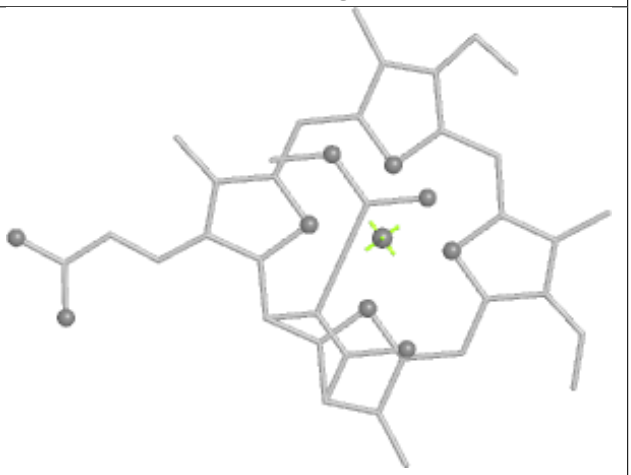
Bond lengths



Bond angles

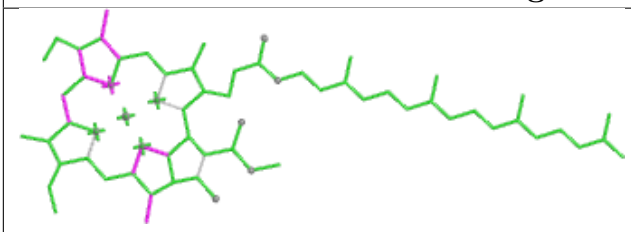


Torsions

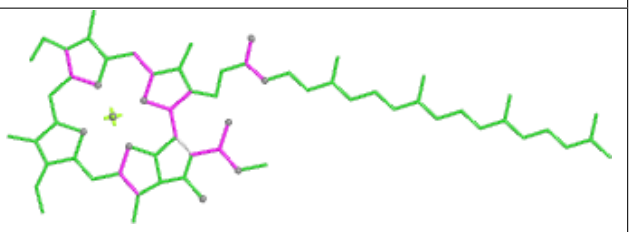


Rings

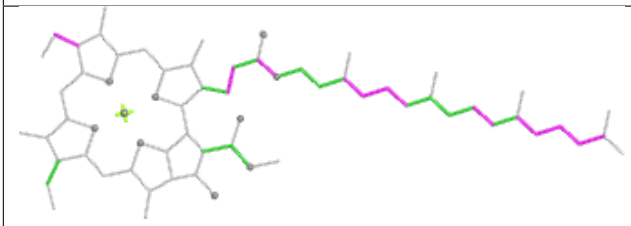
Ligand CLA b 825



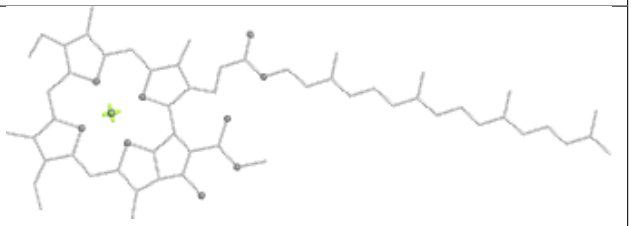
Bond lengths



Bond angles

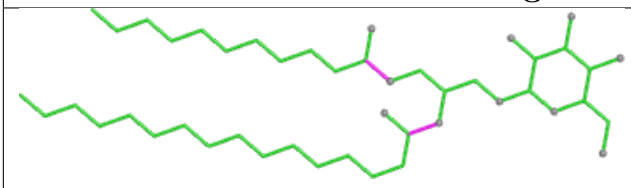


Torsions

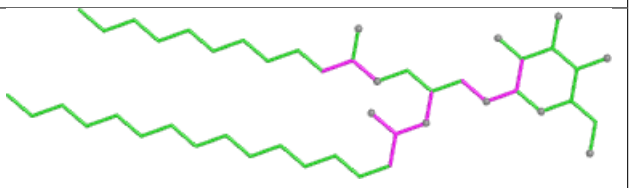


Rings

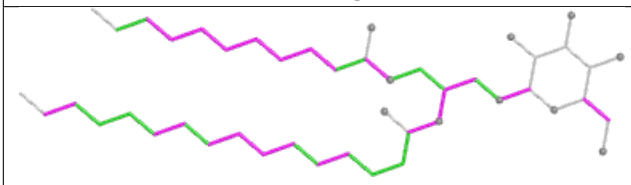
Ligand LMG 7 301



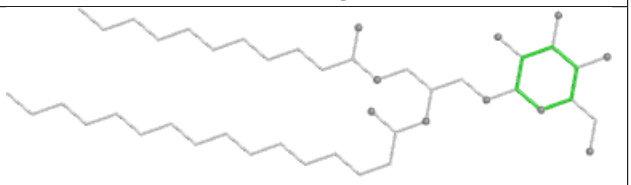
Bond lengths



Bond angles

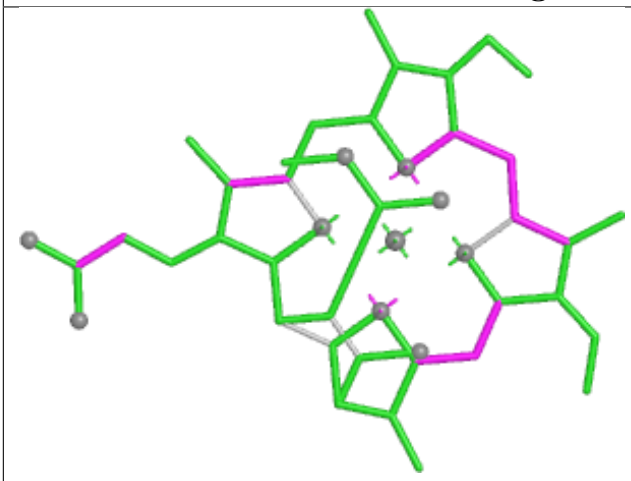


Torsions

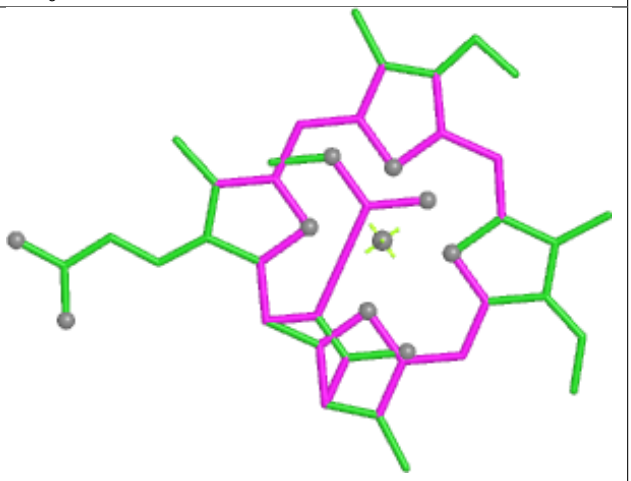


Rings

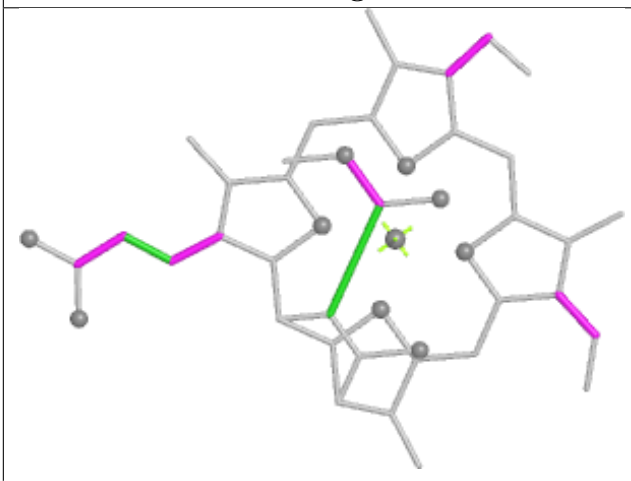
Ligand KC2 y 313



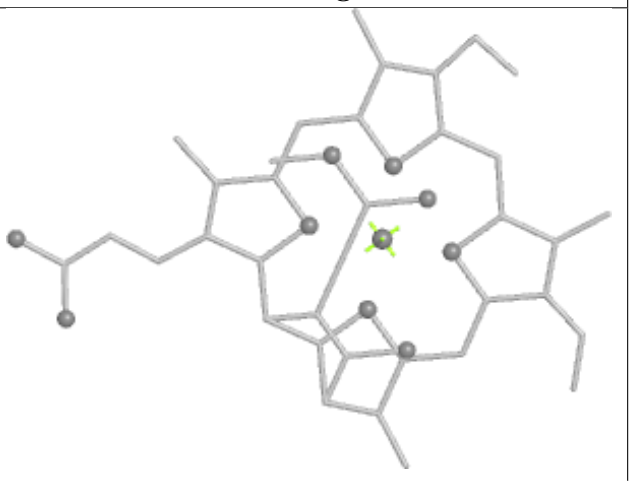
Bond lengths



Bond angles

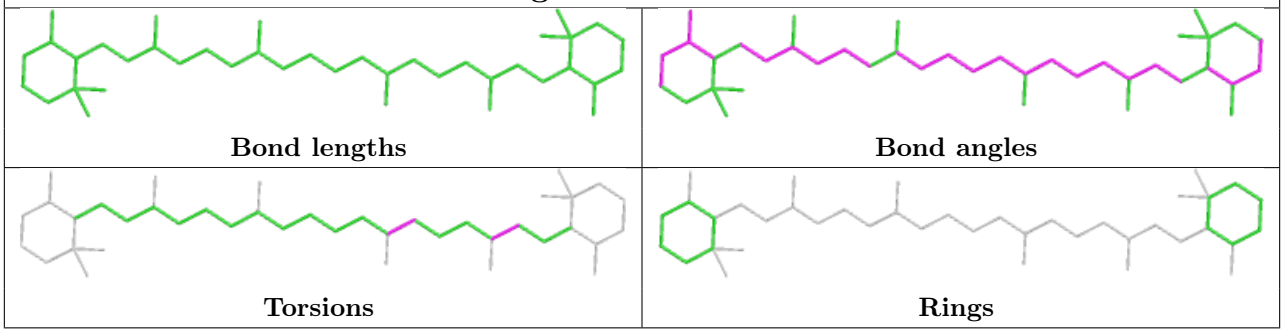


Torsions

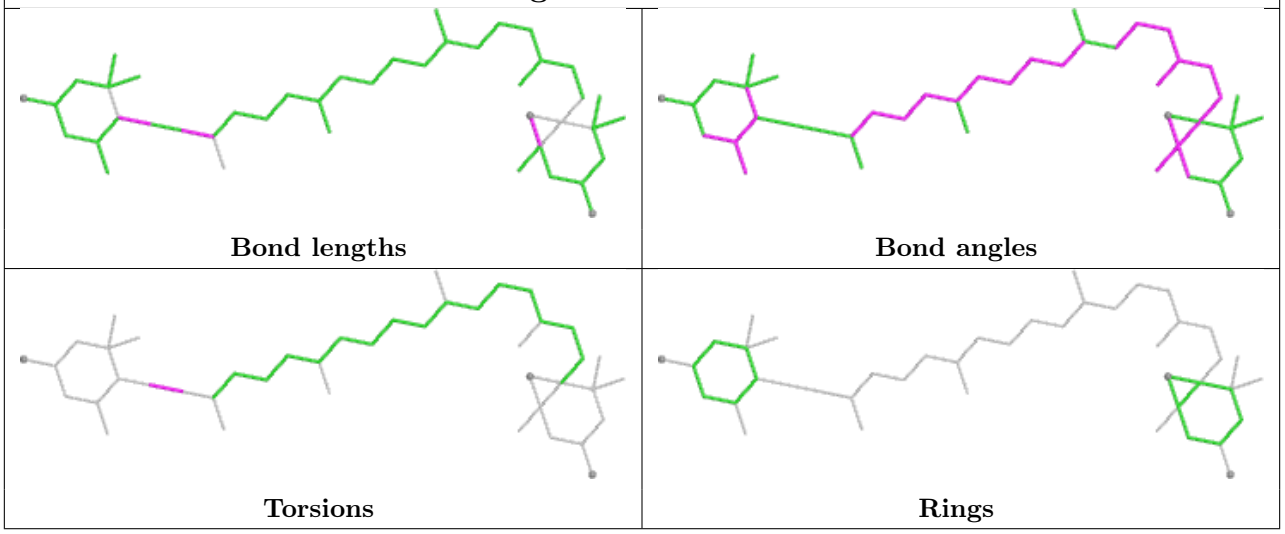


Rings

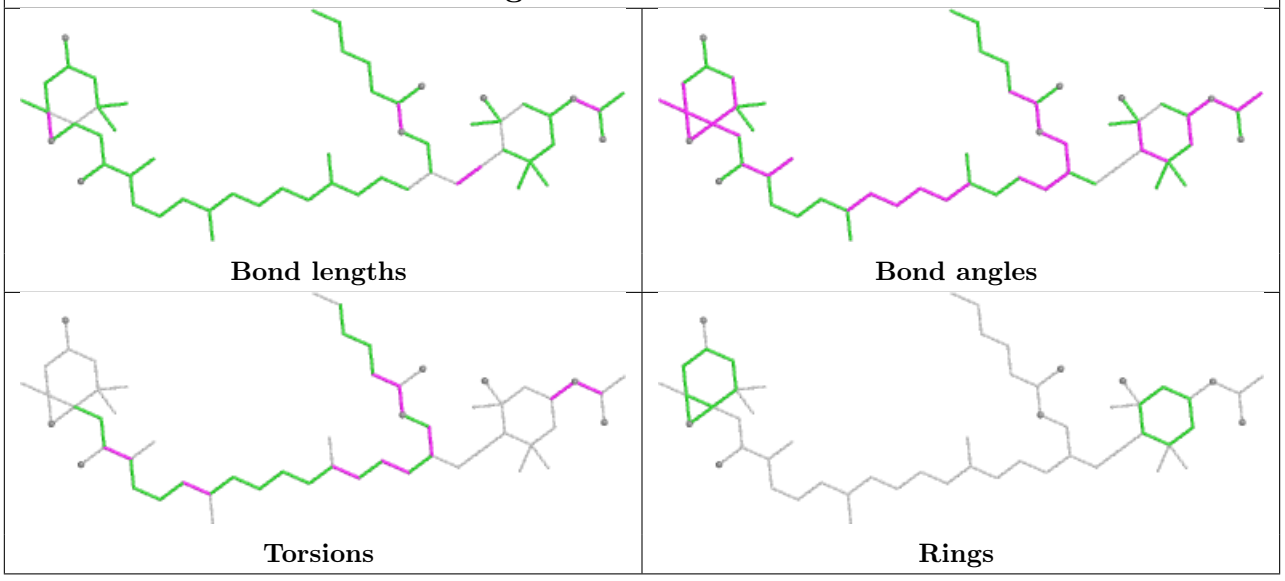
Ligand BCR f 801



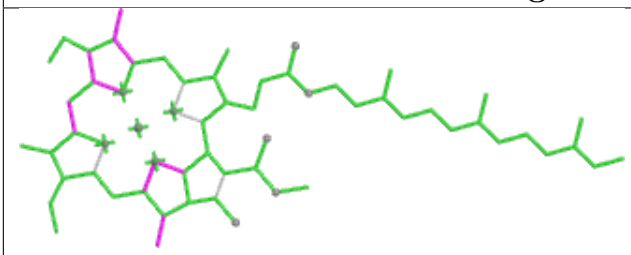
Ligand DD6 4 307



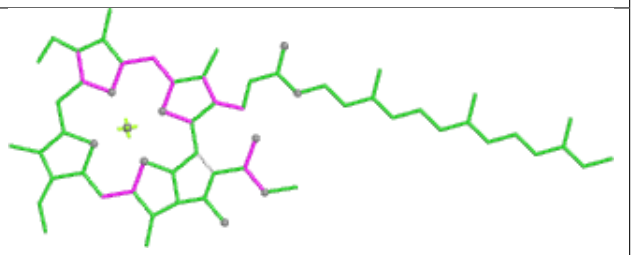
Ligand A1EB1 G 307



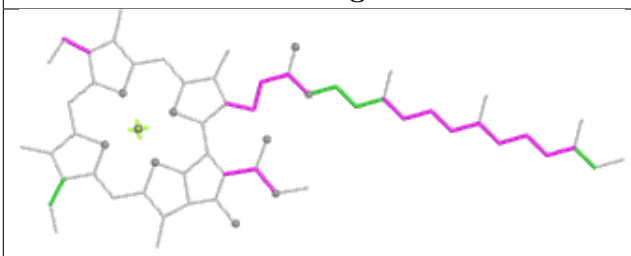
Ligand CLA 0 310



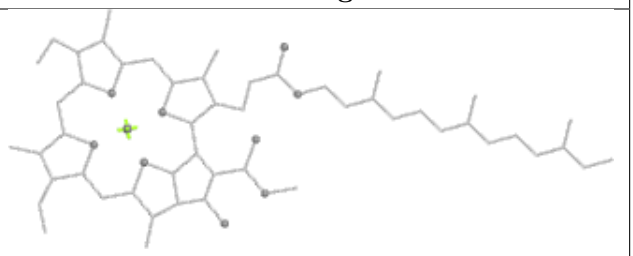
Bond lengths



Bond angles

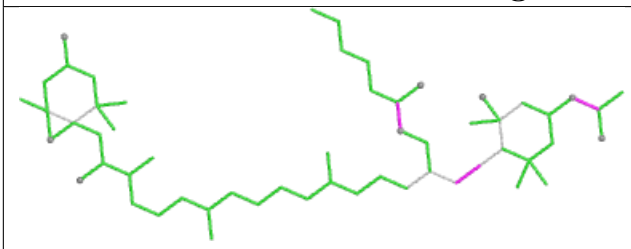


Torsions

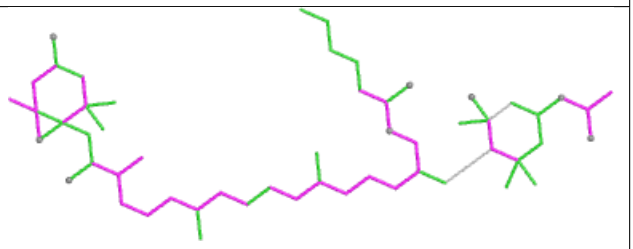


Rings

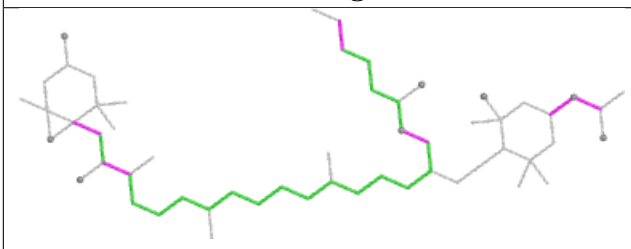
Ligand A1EB1 0 307



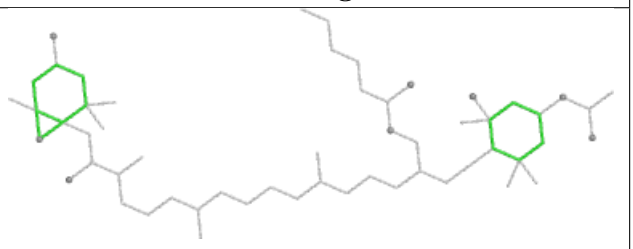
Bond lengths



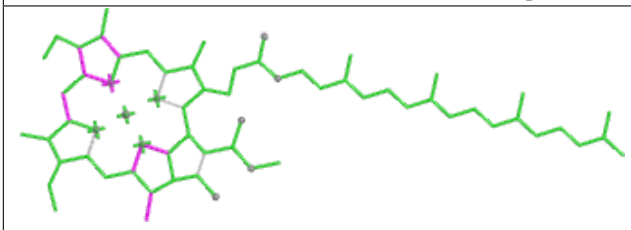
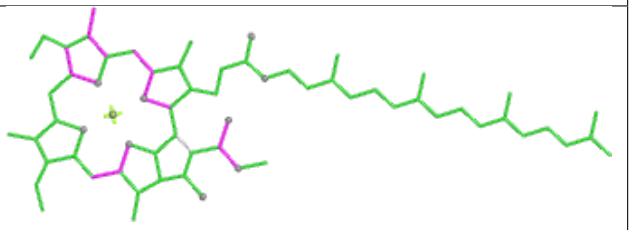
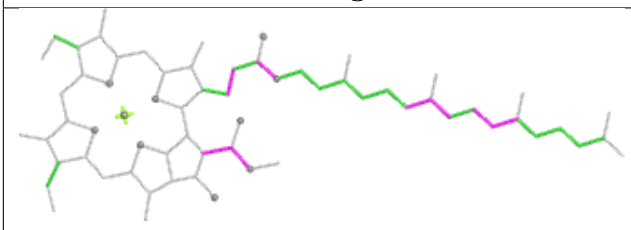
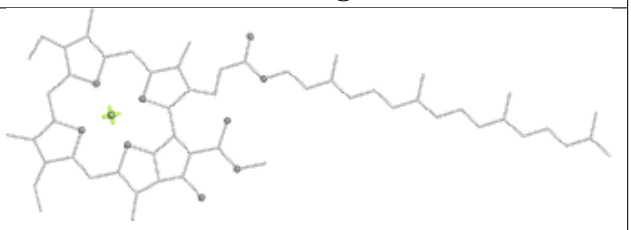
Bond angles

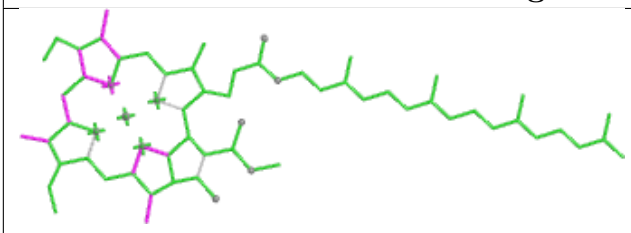
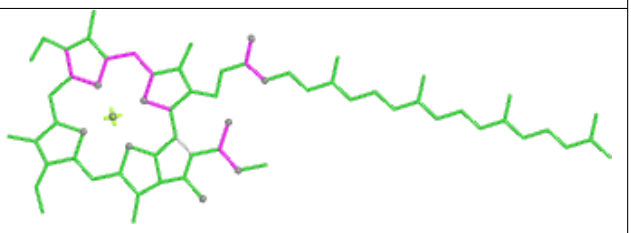
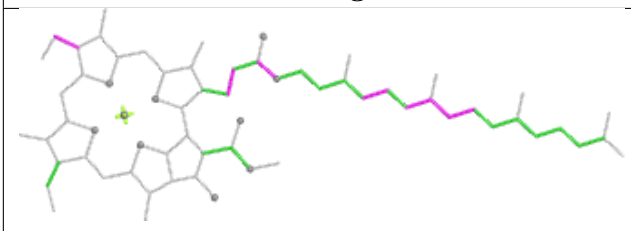
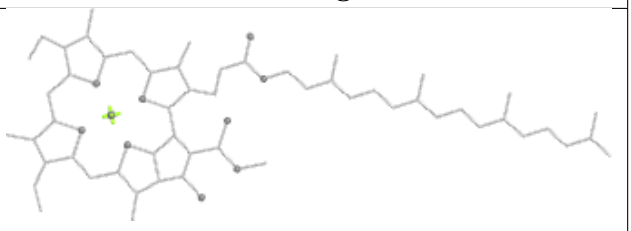


Torsions

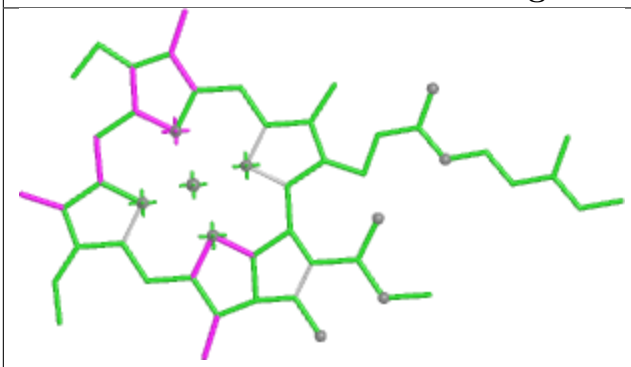


Rings

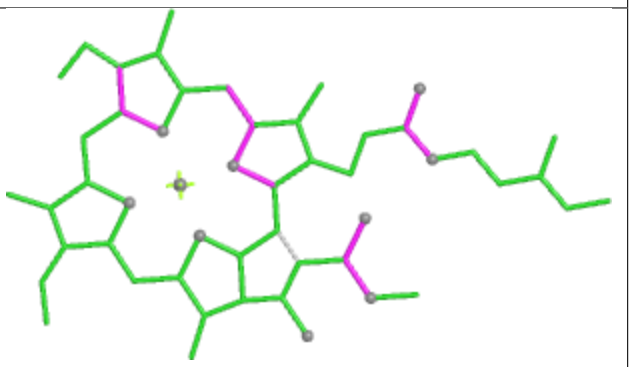
Ligand CLA M 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

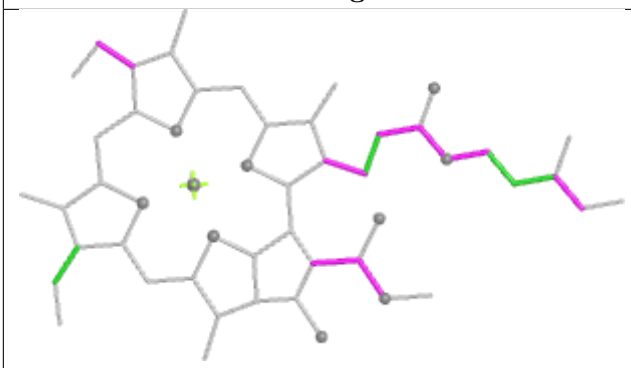
Ligand CLA 0 322



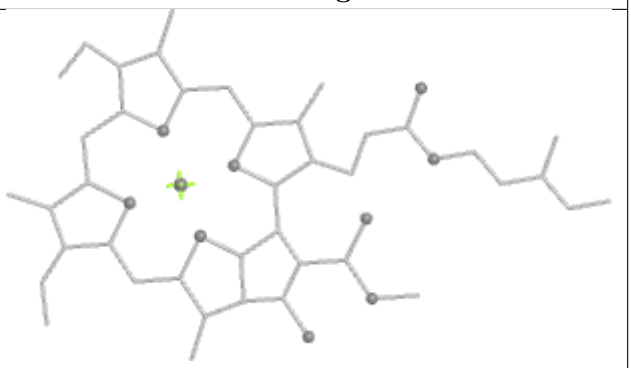
Bond lengths



Bond angles

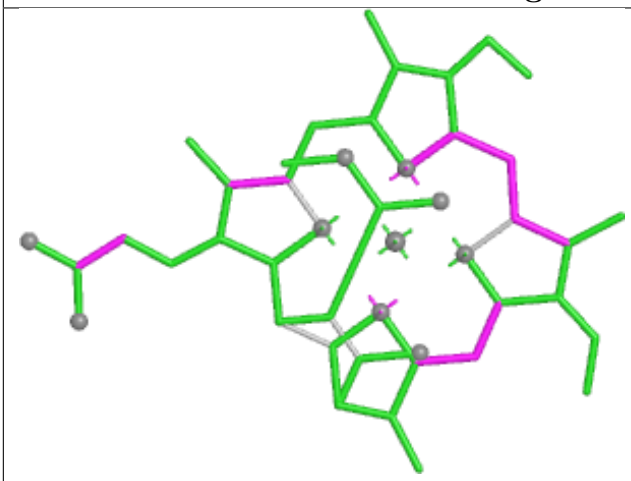


Torsions

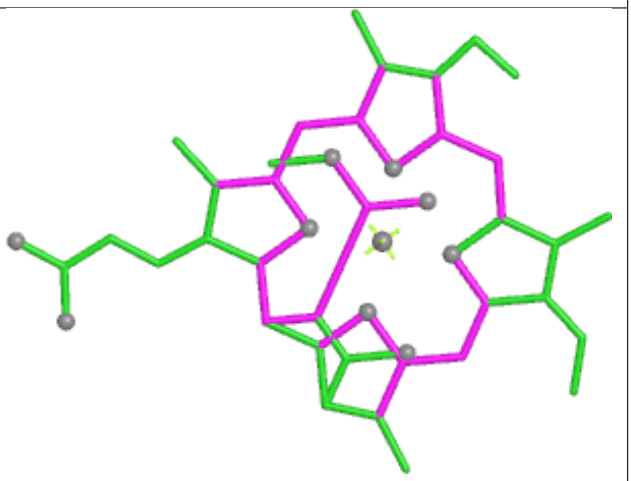


Rings

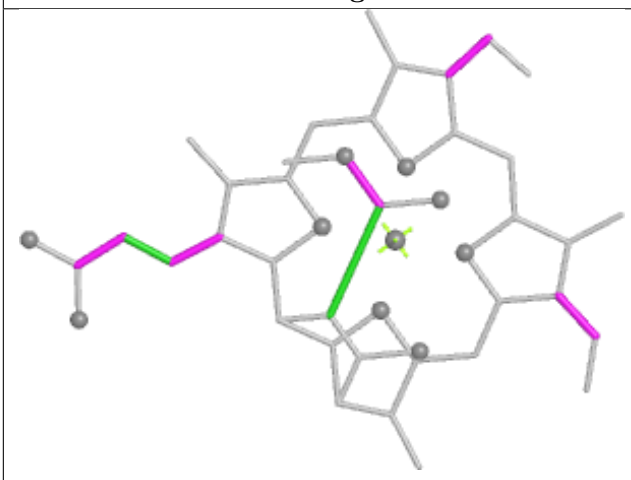
Ligand KC2 G 311



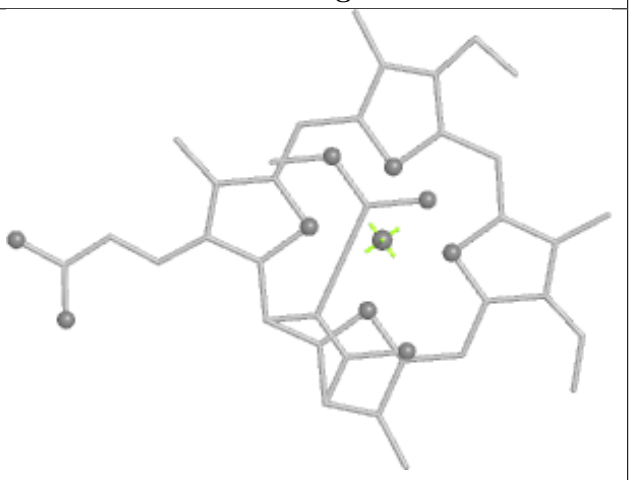
Bond lengths



Bond angles

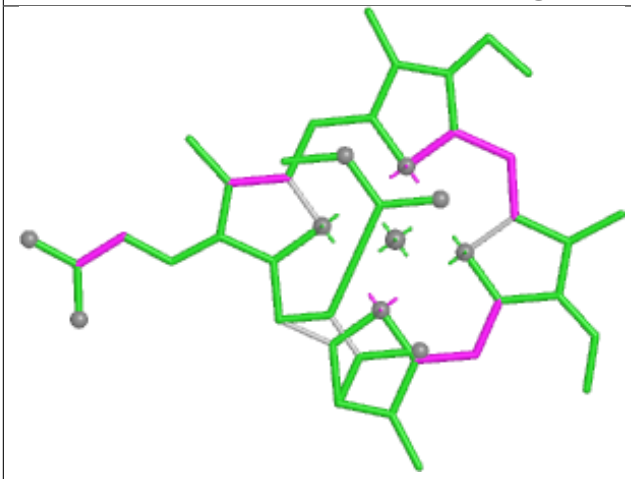


Torsions

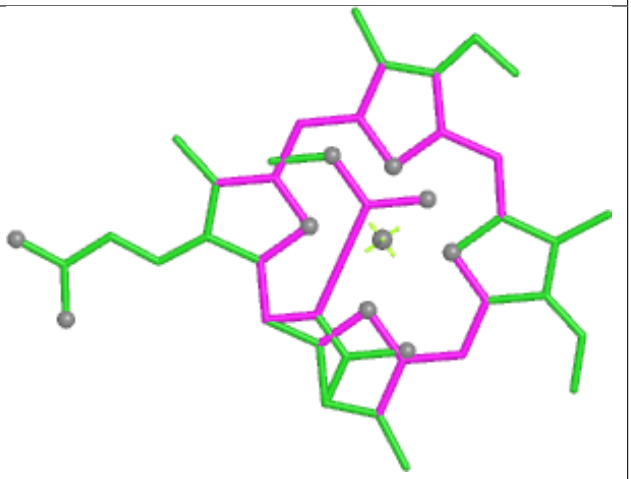


Rings

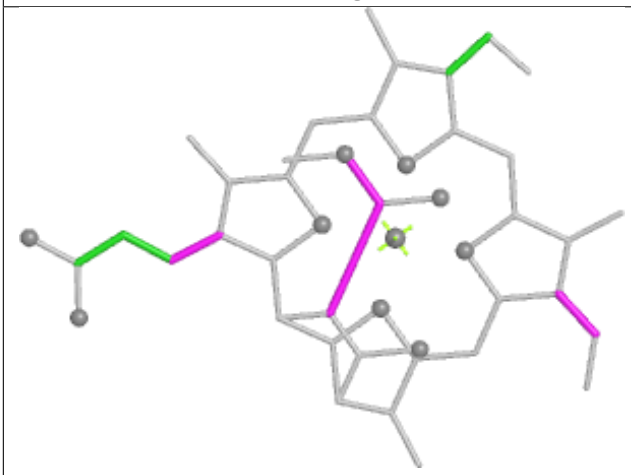
Ligand KC2 8 317



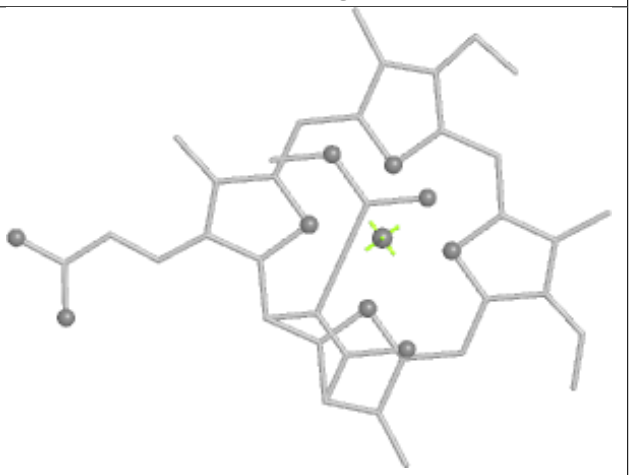
Bond lengths



Bond angles

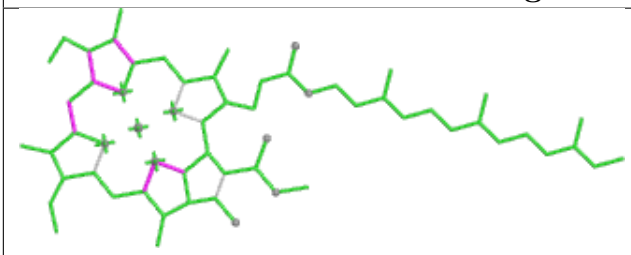


Torsions

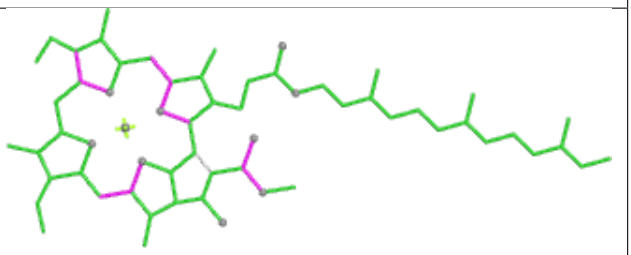


Rings

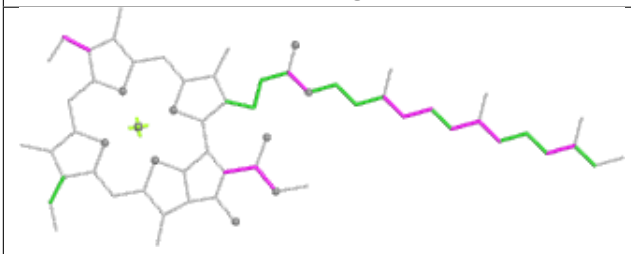
Ligand CLA C 305



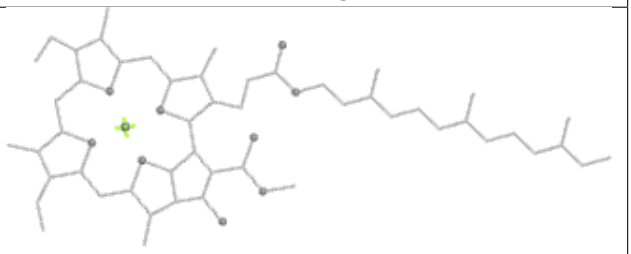
Bond lengths



Bond angles

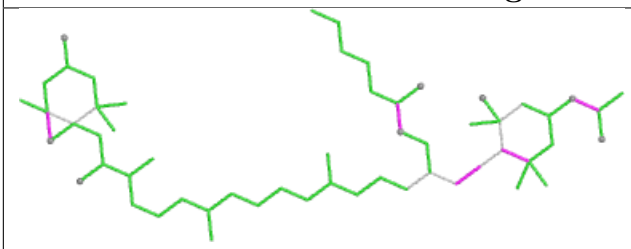


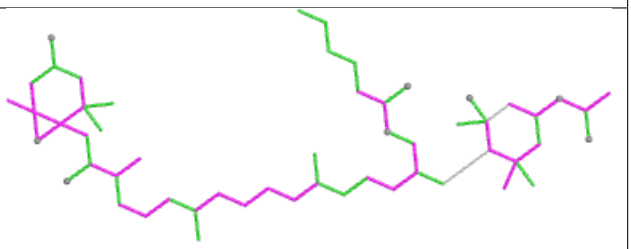
Torsions

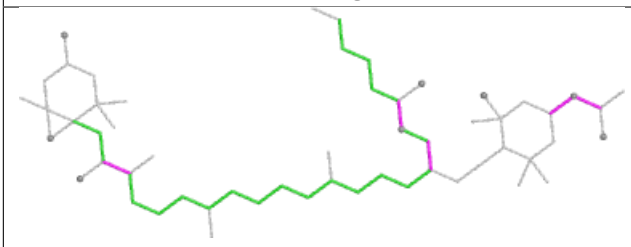


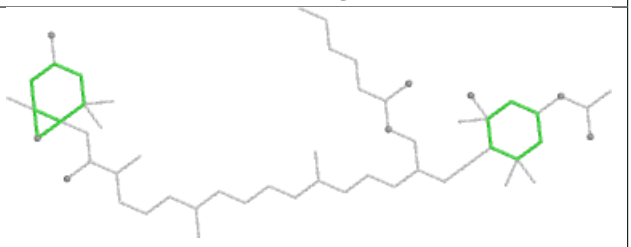
Rings

Ligand A1EB1 R 303

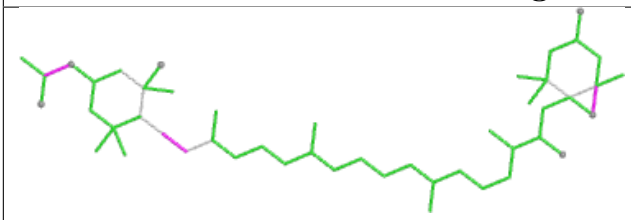

Bond lengths

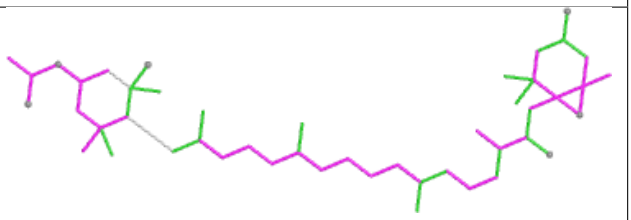

Bond angles

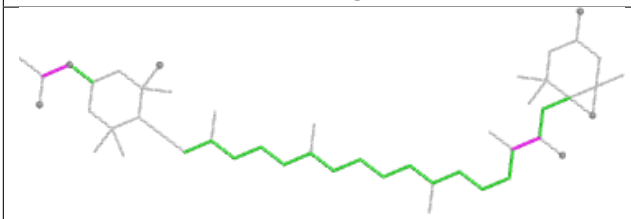

Torsions

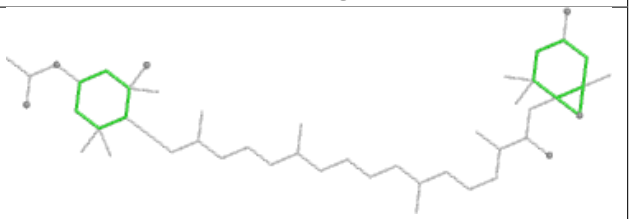

Rings

Ligand A86 T 305

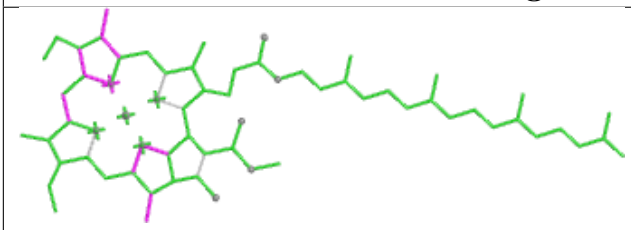

Bond lengths

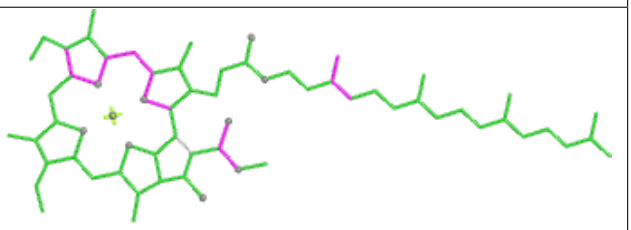

Bond angles

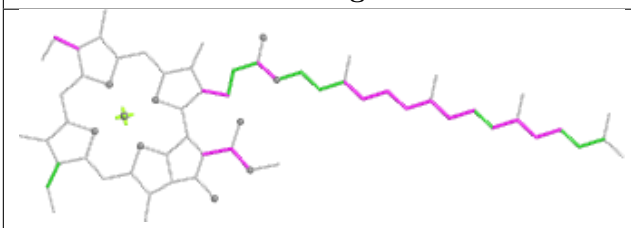

Torsions

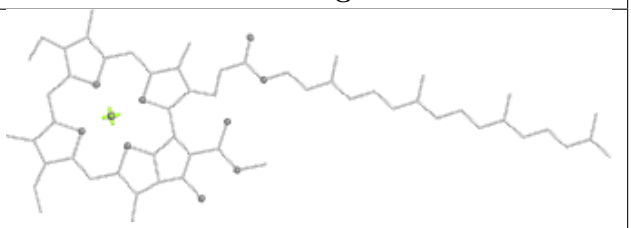

Rings

Ligand CLA E 312

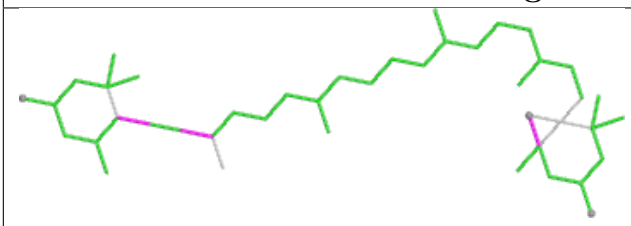

Bond lengths


Bond angles

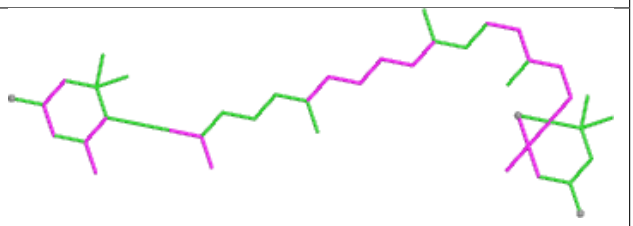

Torsions


Rings

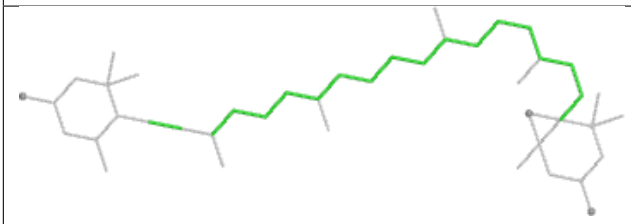
Ligand DD6 A 301



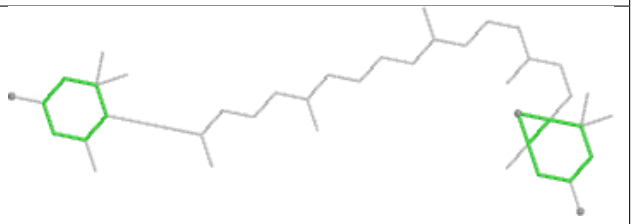
Bond lengths



Bond angles

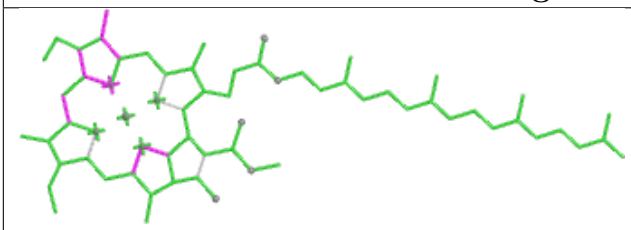


Torsions

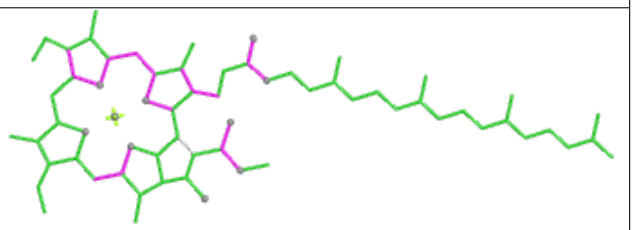


Rings

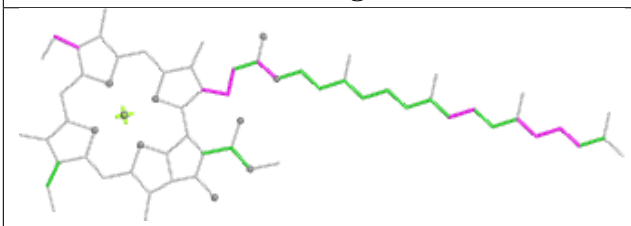
Ligand CLA l 204



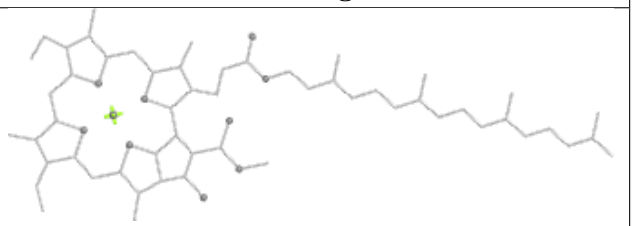
Bond lengths



Bond angles

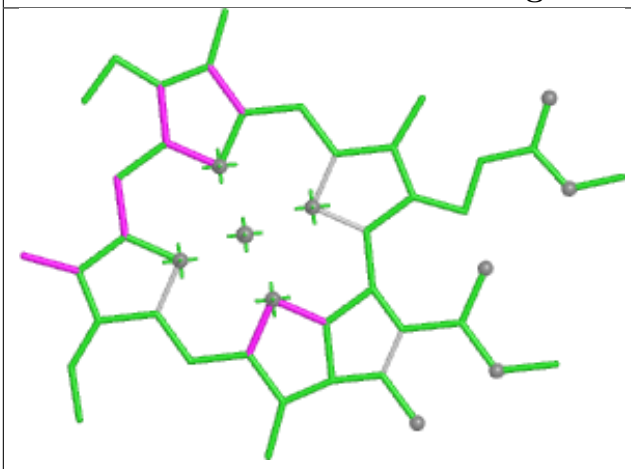


Torsions

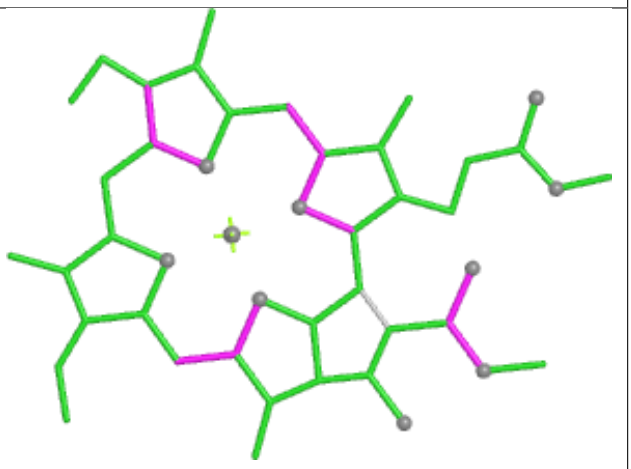


Rings

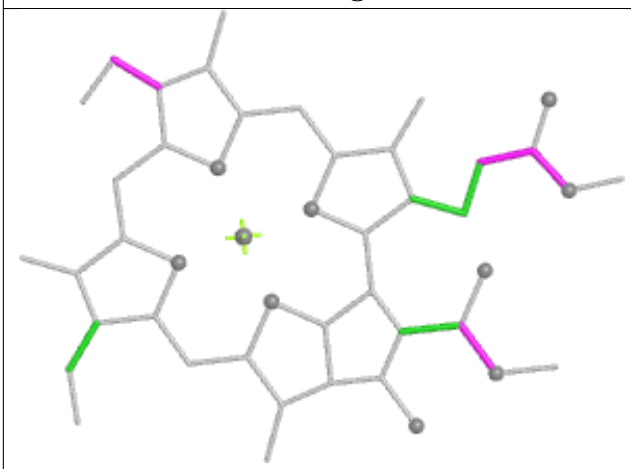
Ligand CLA F 306



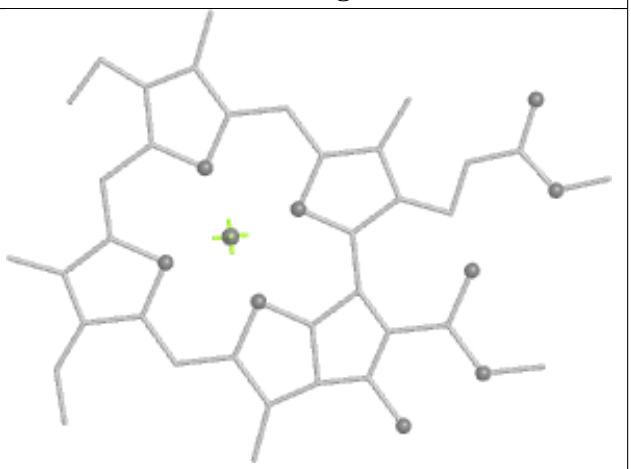
Bond lengths



Bond angles

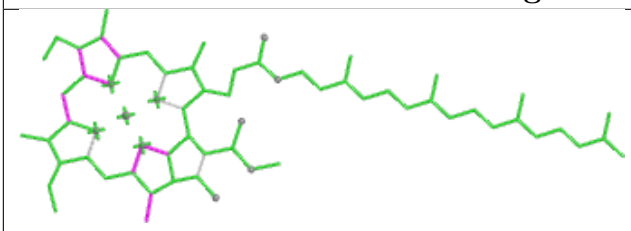


Torsions

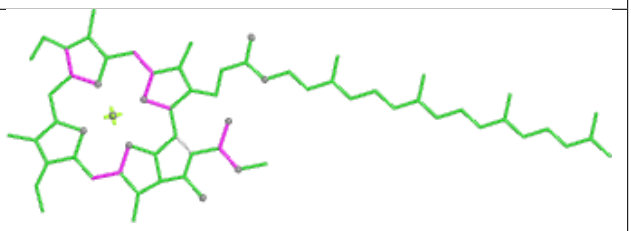


Rings

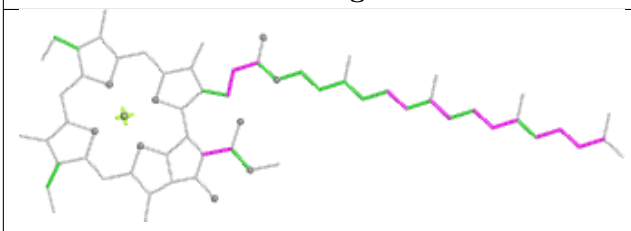
Ligand CLA X 309



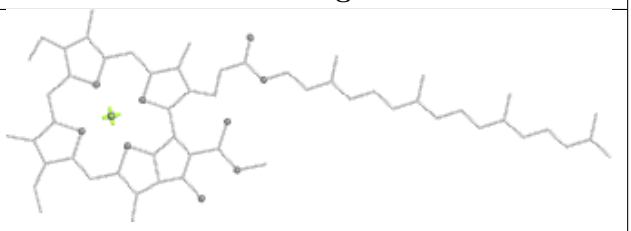
Bond lengths



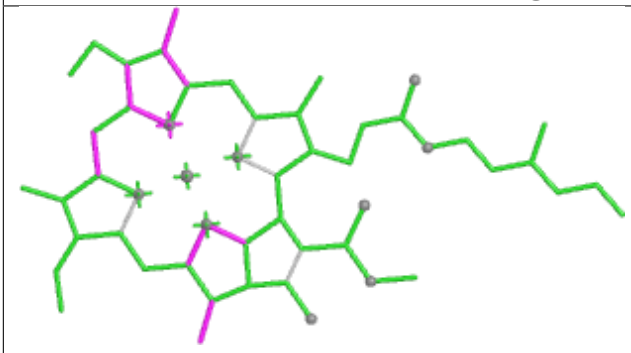
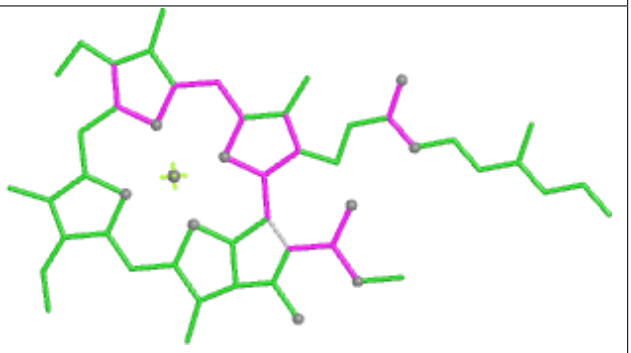
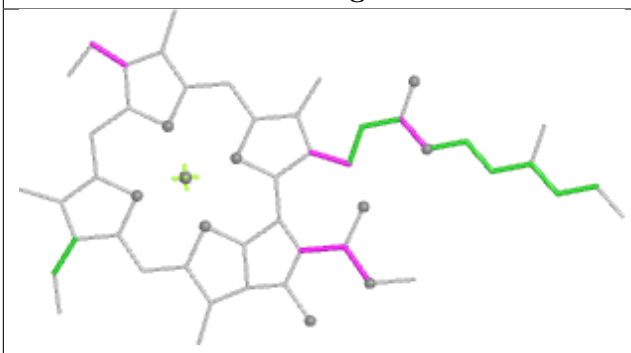
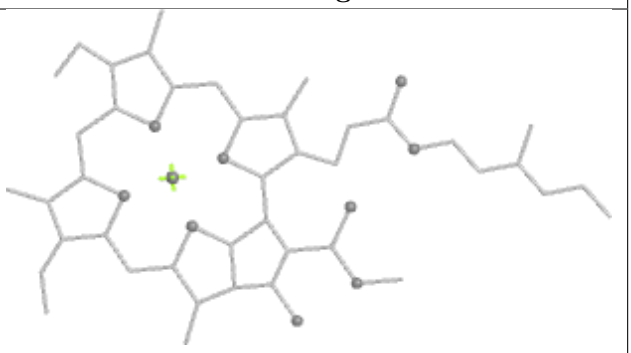
Bond angles

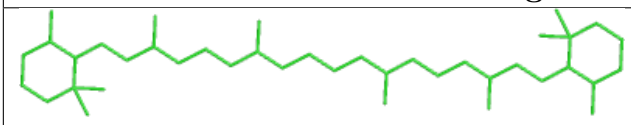
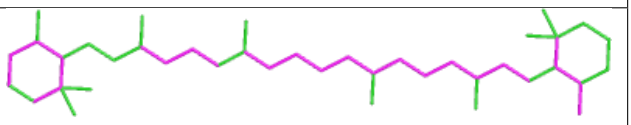
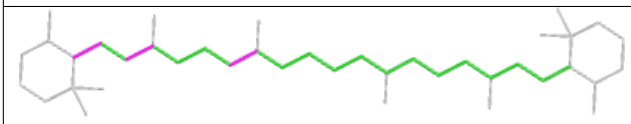
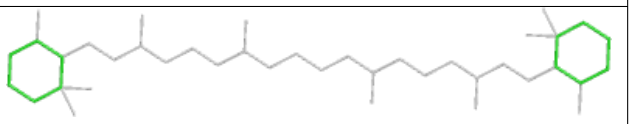


Torsions

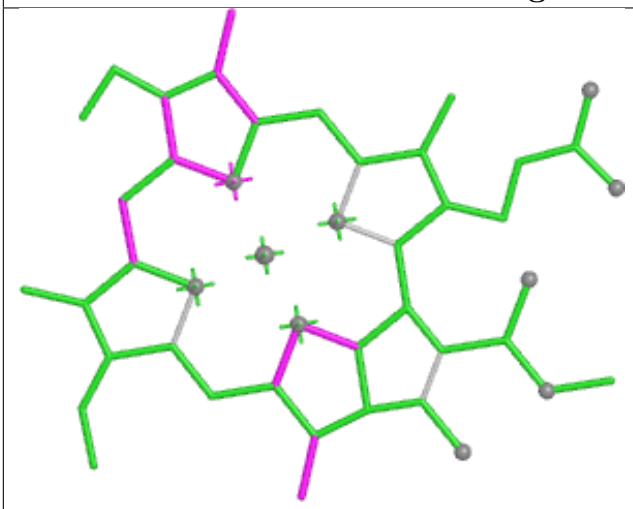


Rings

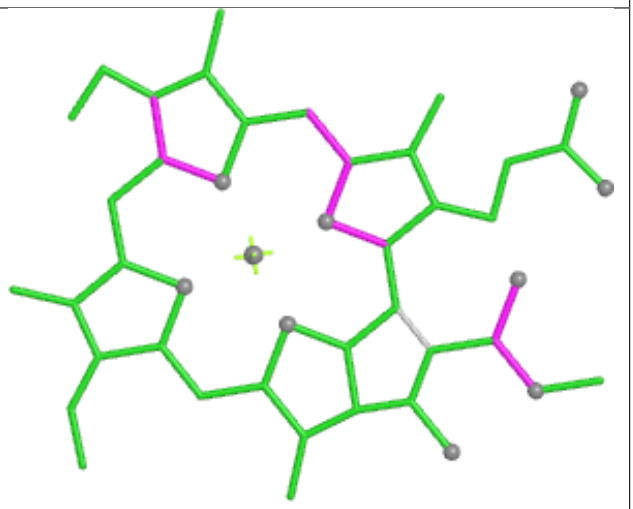
Ligand CLA S 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

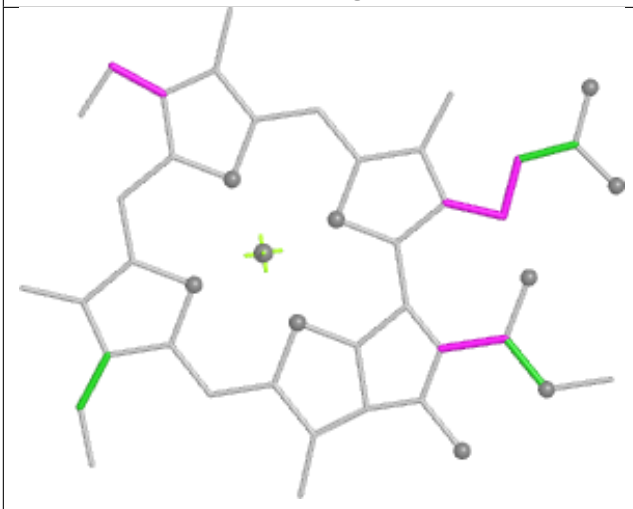
Ligand CLA a 817



Bond lengths



Bond angles

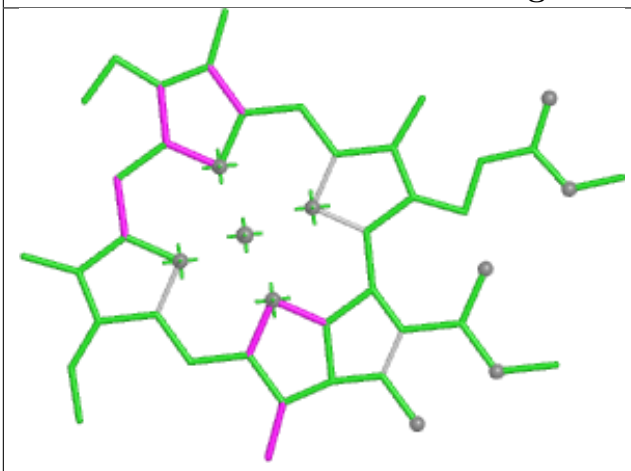


Torsions

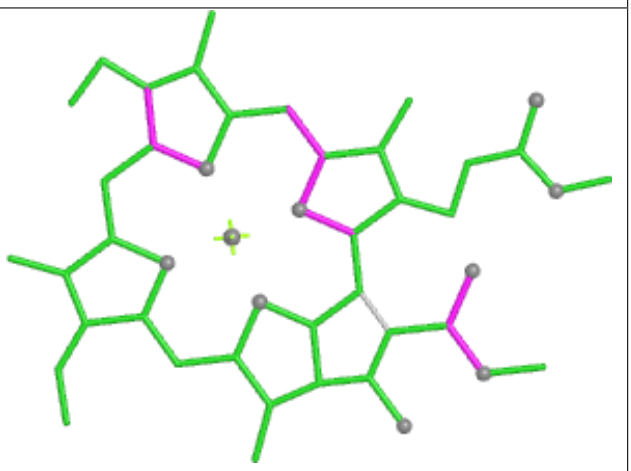


Rings

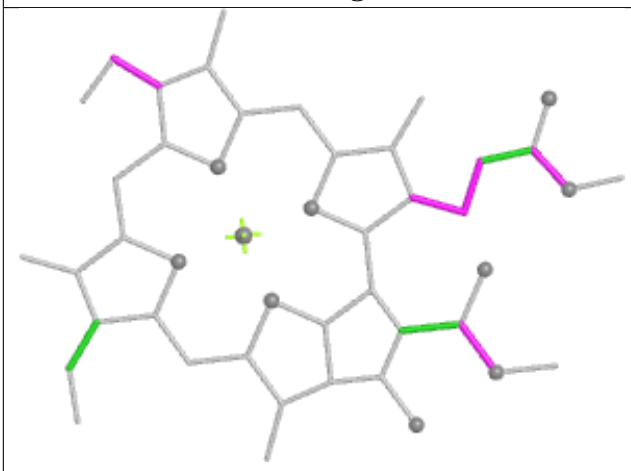
Ligand CLA J 313



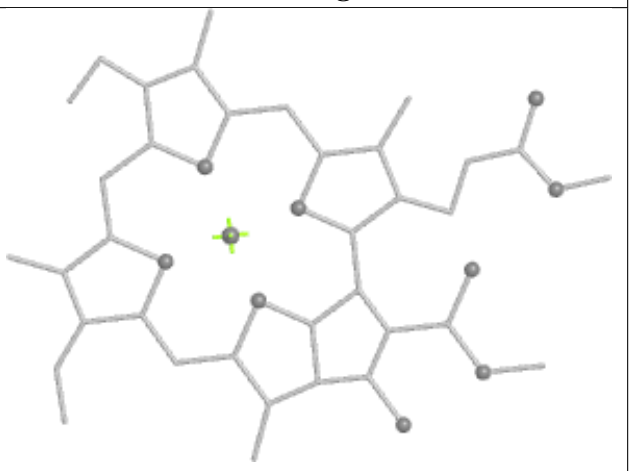
Bond lengths



Bond angles

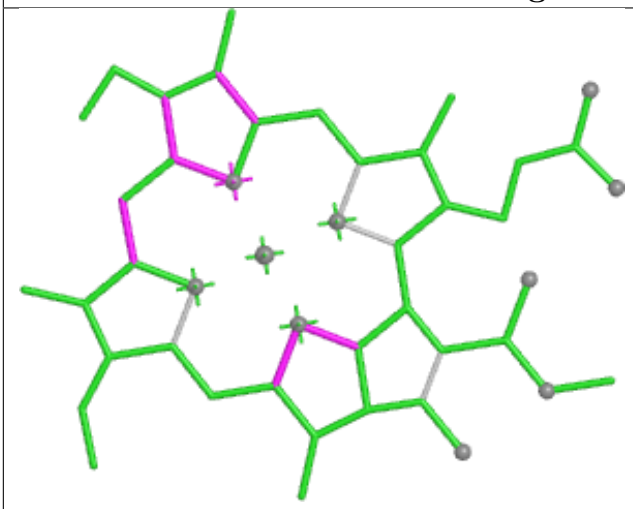


Torsions

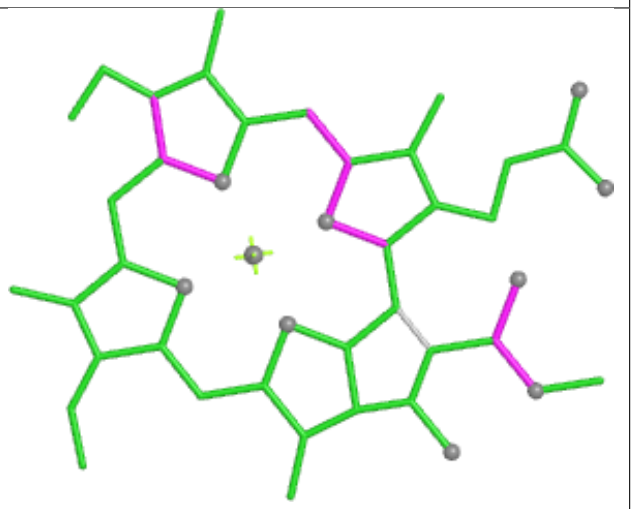


Rings

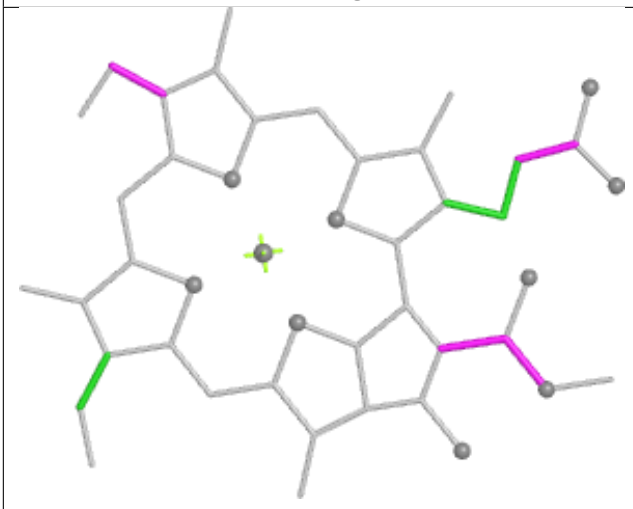
Ligand CLA 8 312



Bond lengths



Bond angles

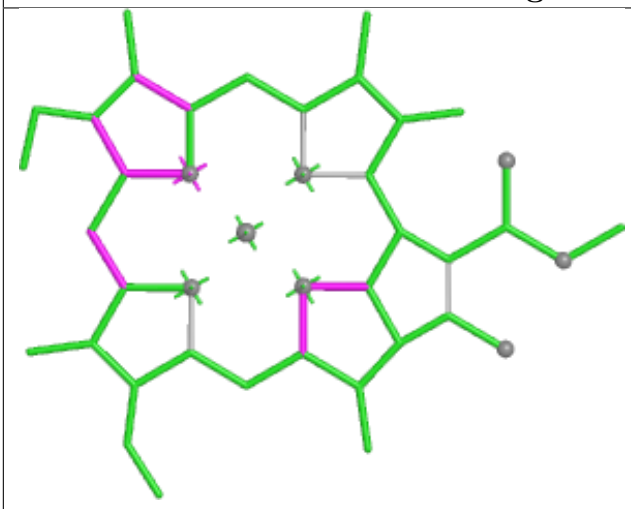


Torsions

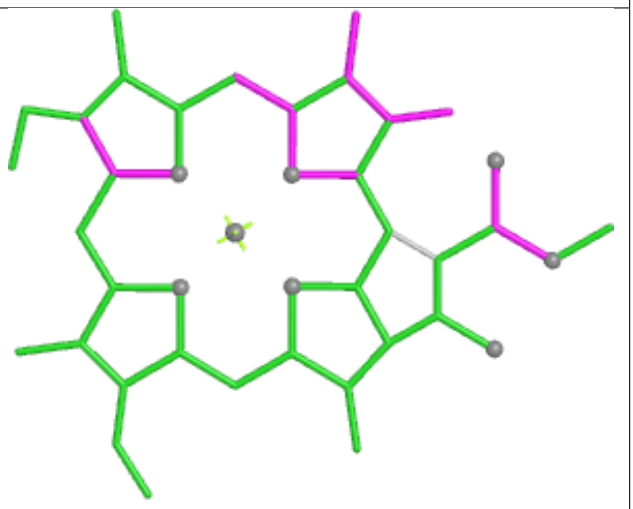


Rings

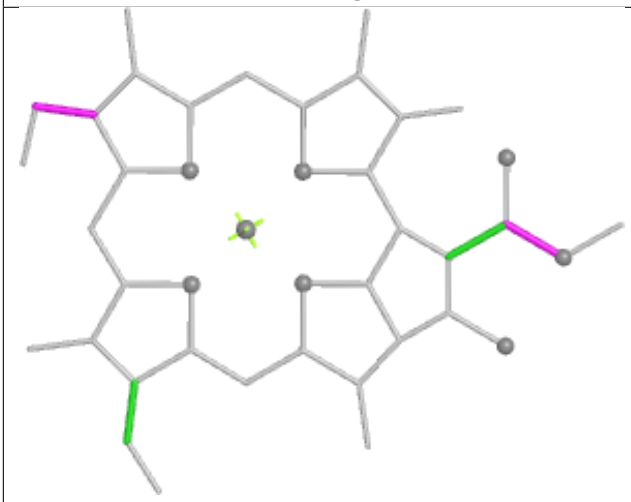
Ligand CLA Z 305



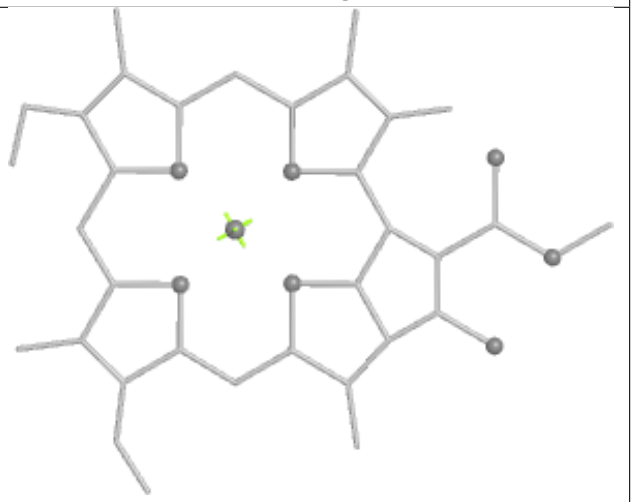
Bond lengths



Bond angles

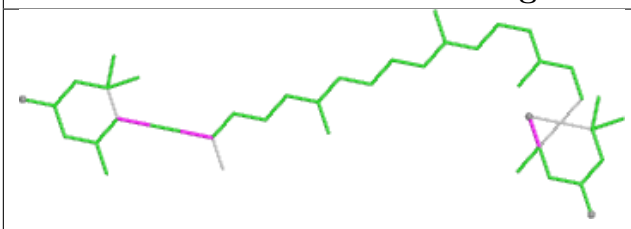


Torsions

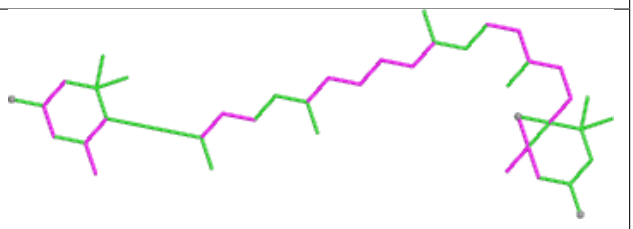


Rings

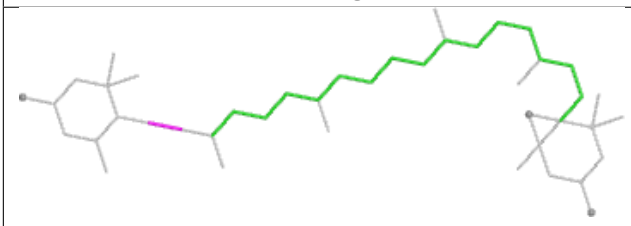
Ligand DD6 W 305



Bond lengths



Bond angles

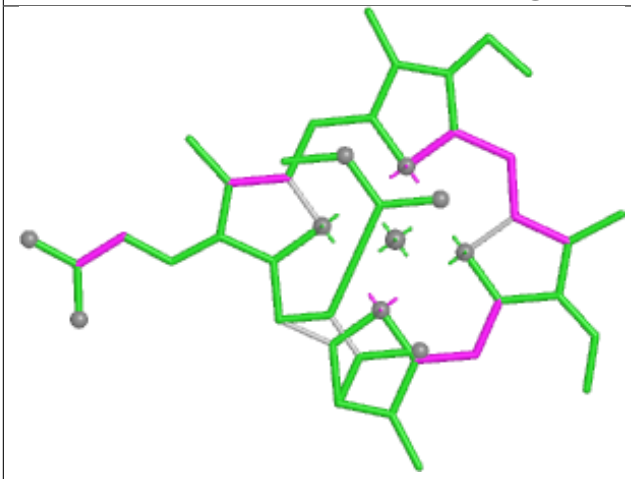


Torsions

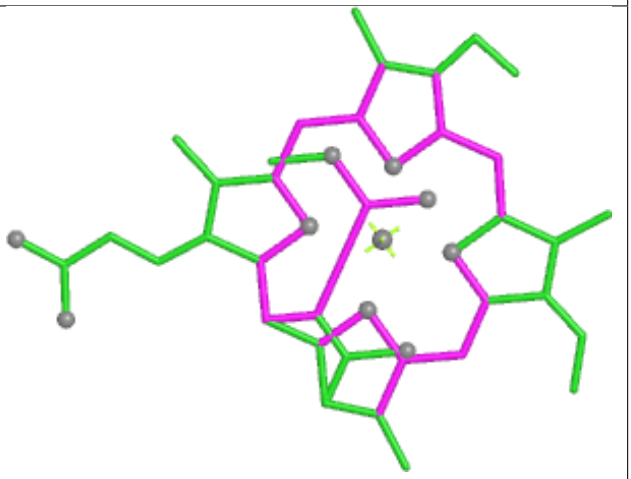


Rings

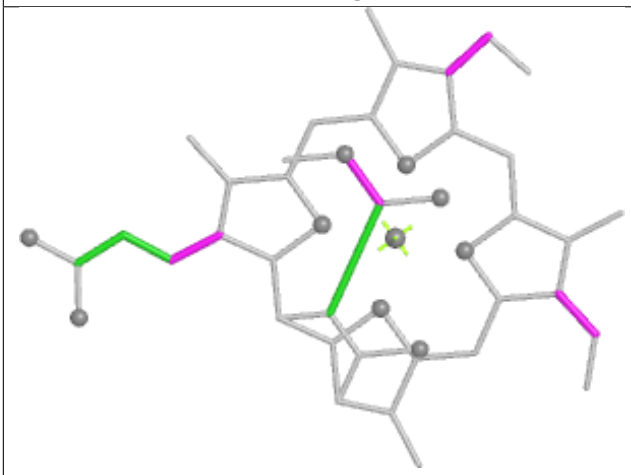
Ligand KC2 P 312



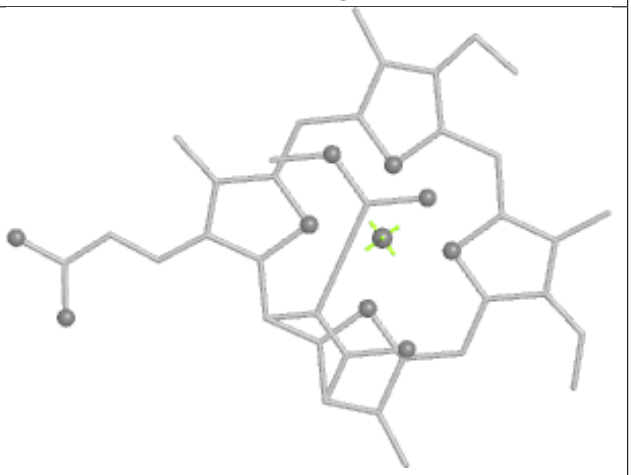
Bond lengths



Bond angles

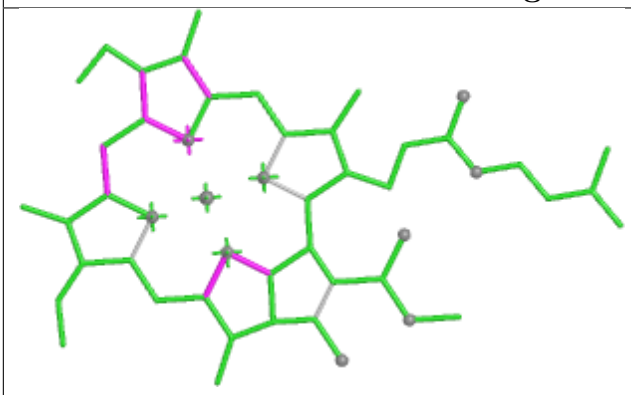


Torsions

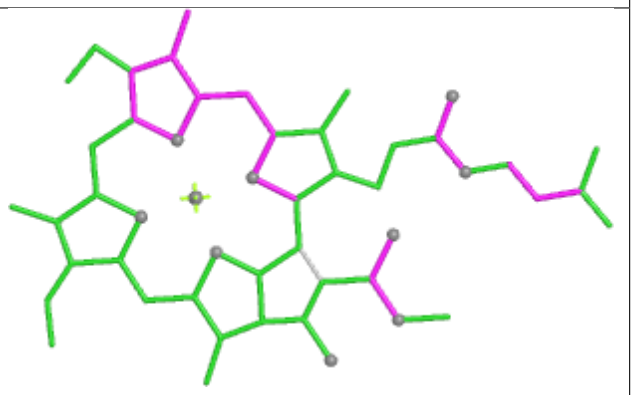


Rings

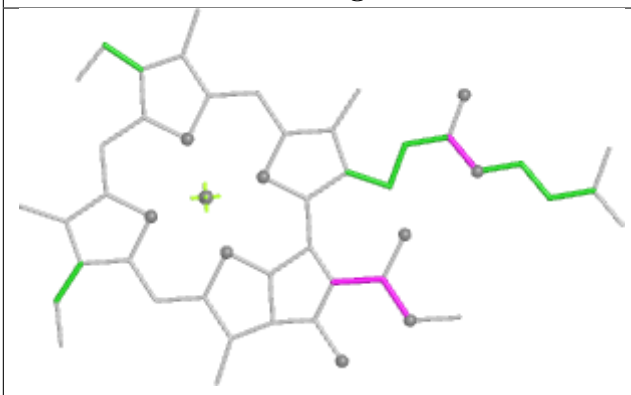
Ligand CLA V 316



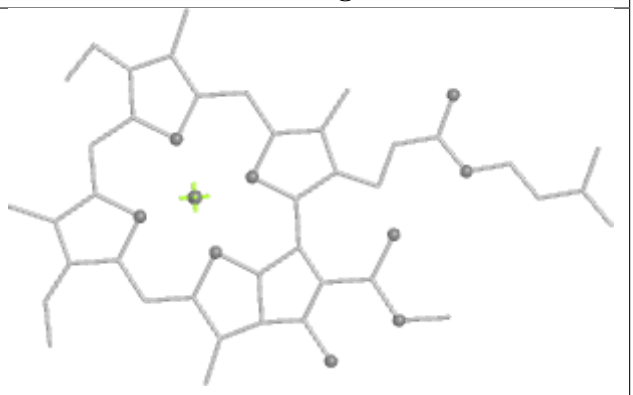
Bond lengths



Bond angles

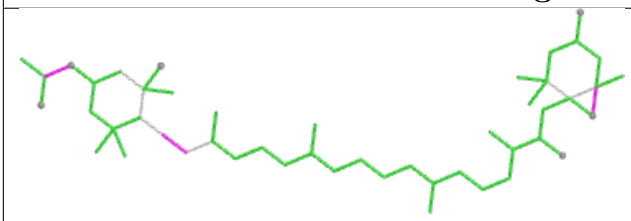


Torsions

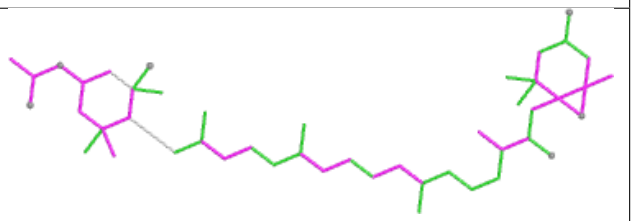


Rings

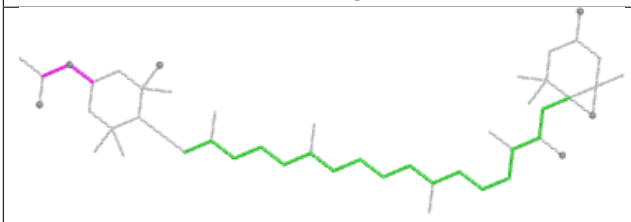
Ligand A86 2 301



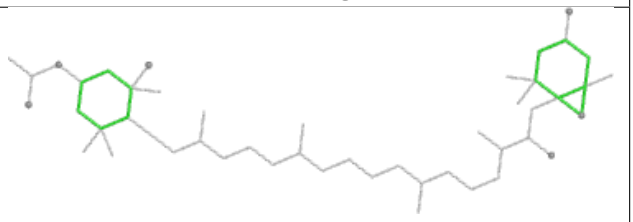
Bond lengths



Bond angles

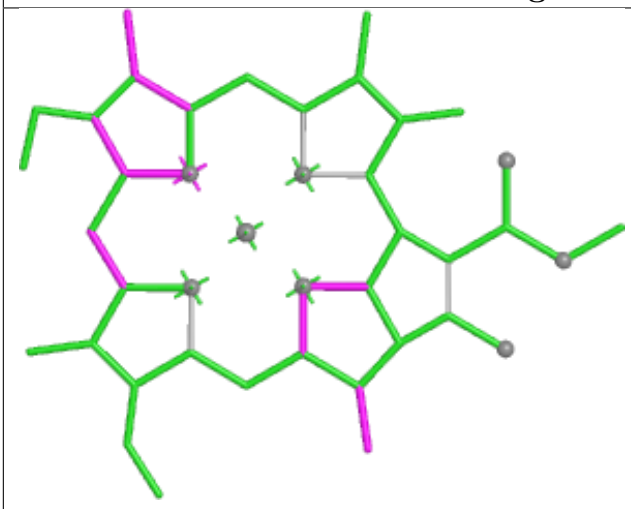


Torsions

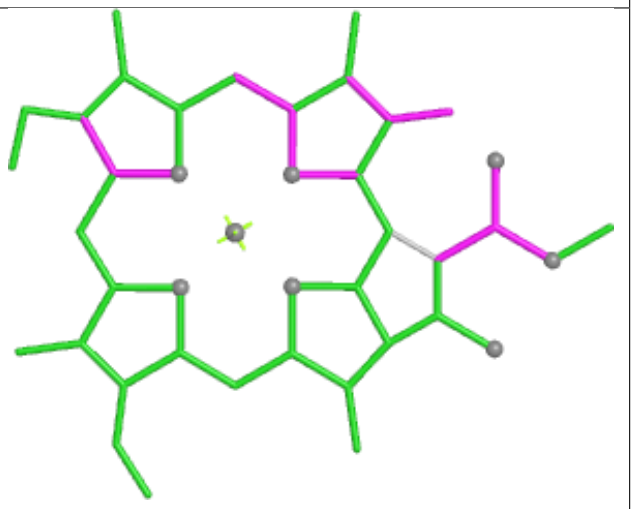


Rings

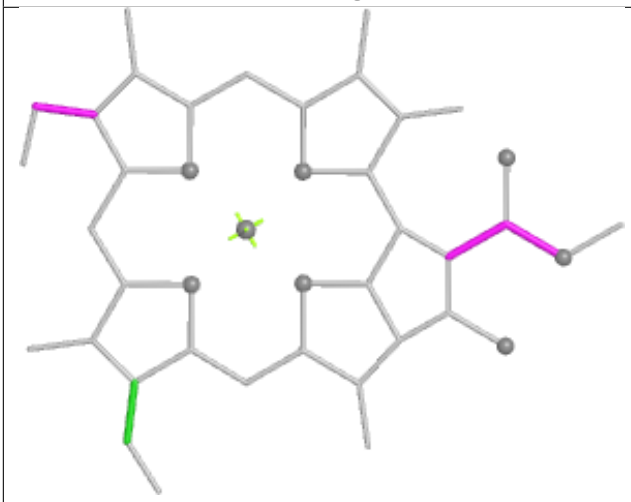
Ligand CLA 2 312



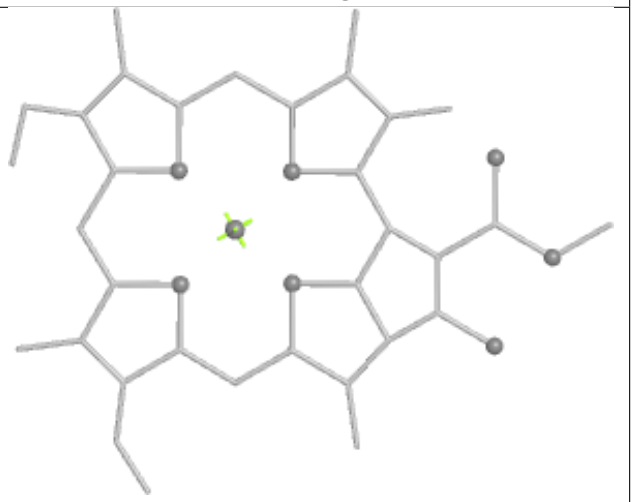
Bond lengths



Bond angles

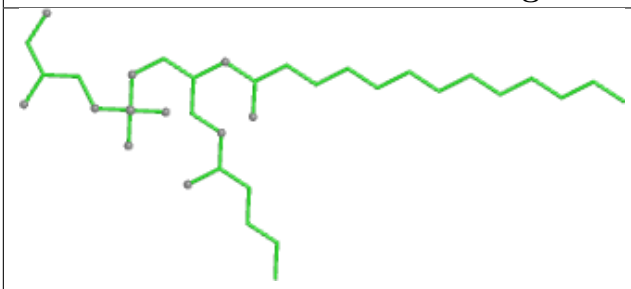


Torsions

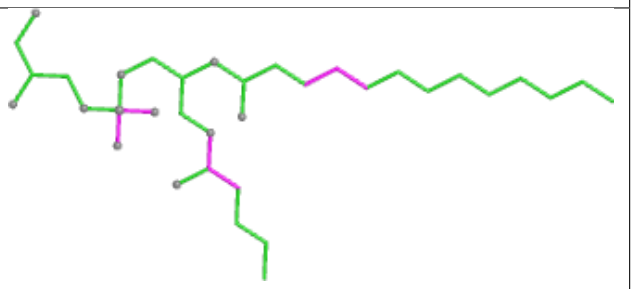


Rings

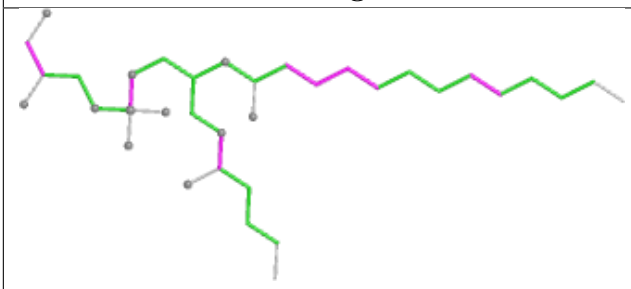
Ligand LHG D 301



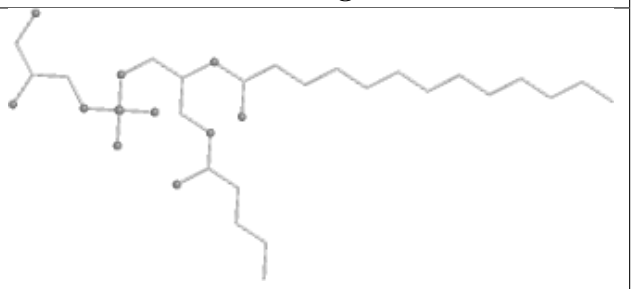
Bond lengths



Bond angles



Torsions

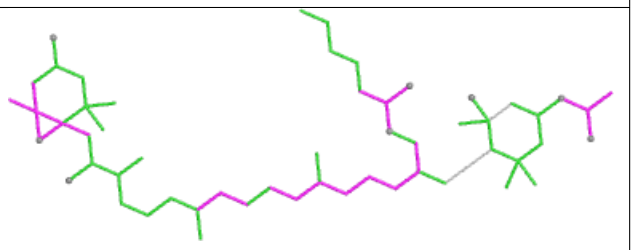


Rings

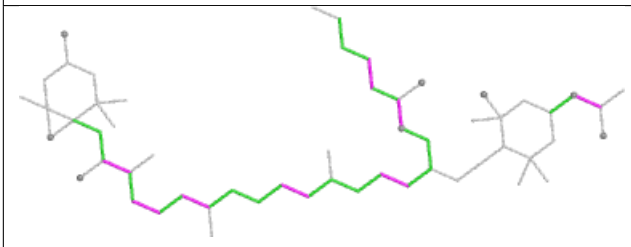
Ligand A1EB1 x 301



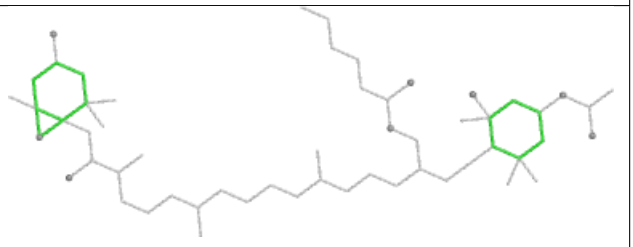
Bond lengths



Bond angles

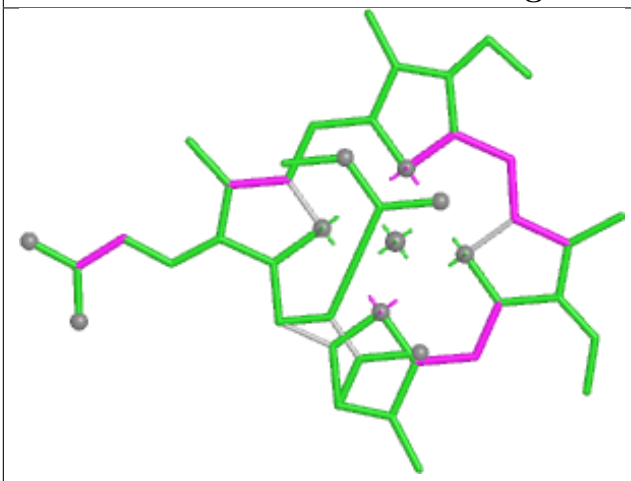


Torsions

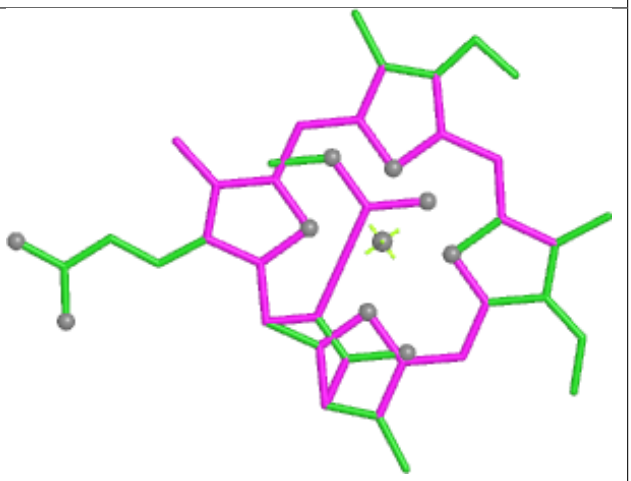


Rings

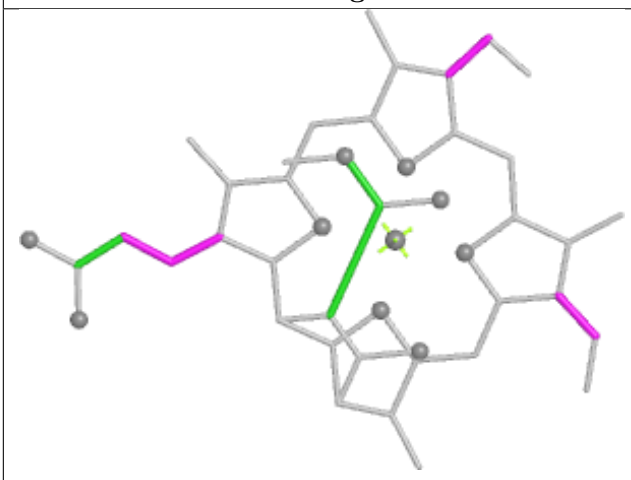
Ligand KC2 G 313



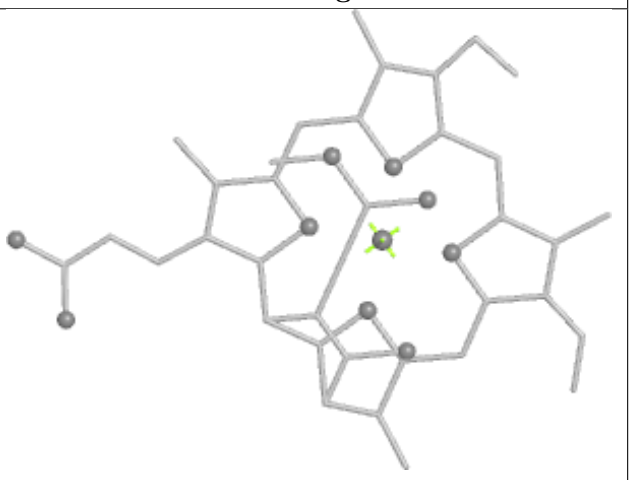
Bond lengths



Bond angles

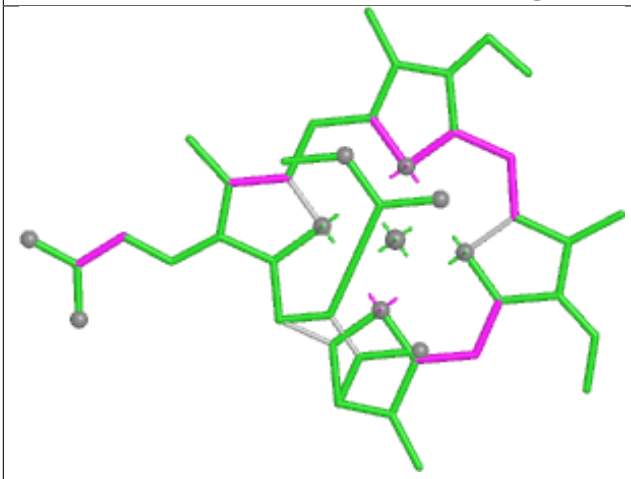


Torsions

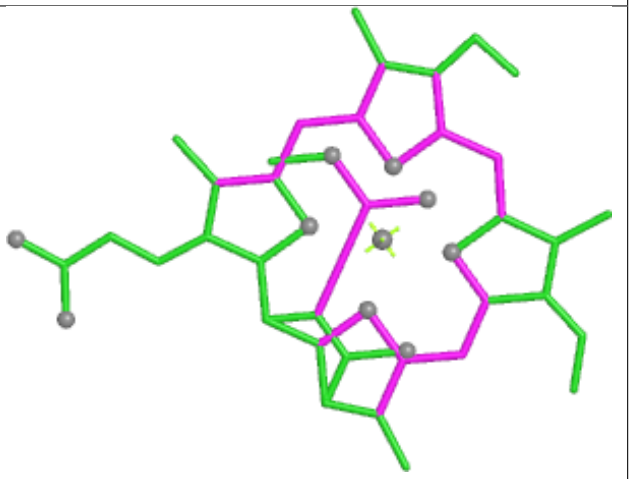


Rings

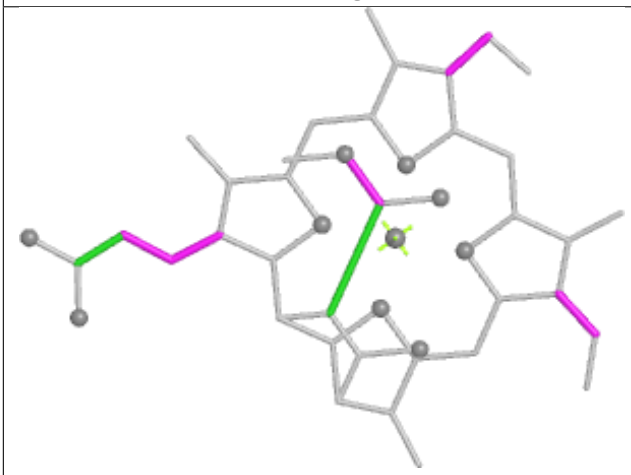
Ligand KC2 L 312



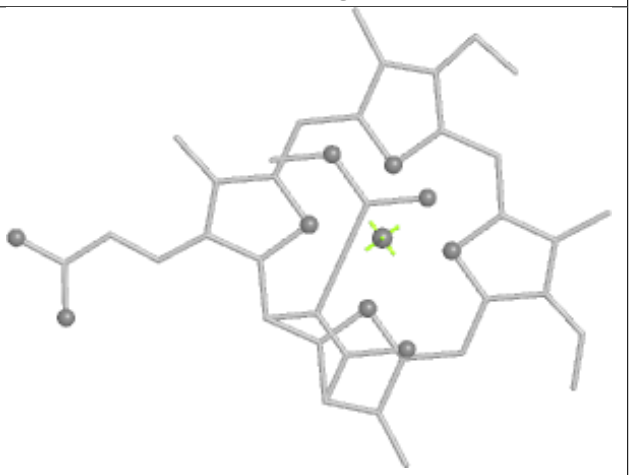
Bond lengths



Bond angles

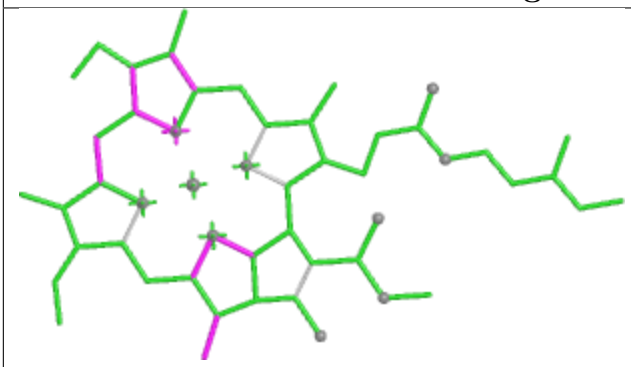


Torsions

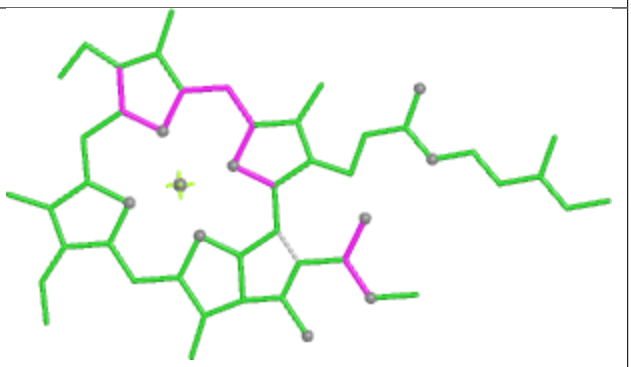


Rings

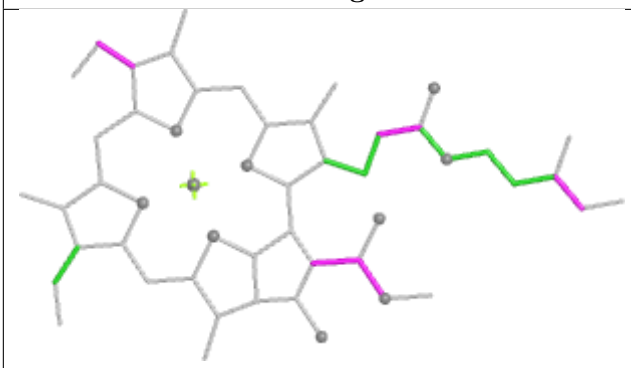
Ligand CLA A 308



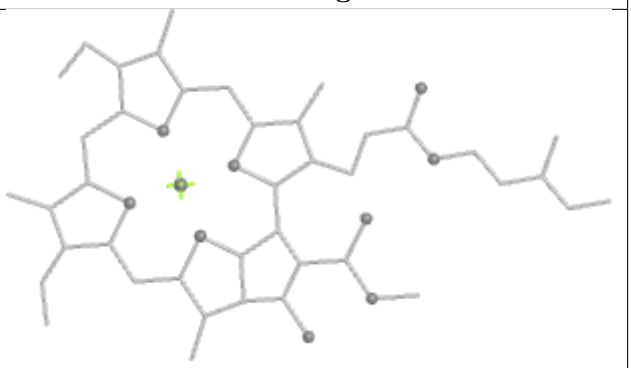
Bond lengths



Bond angles

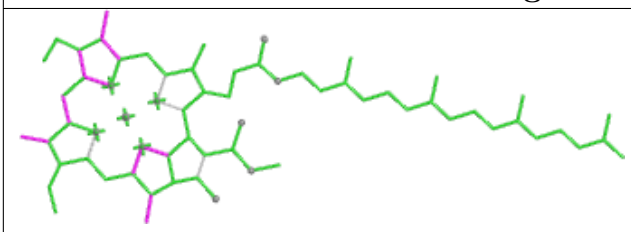


Torsions

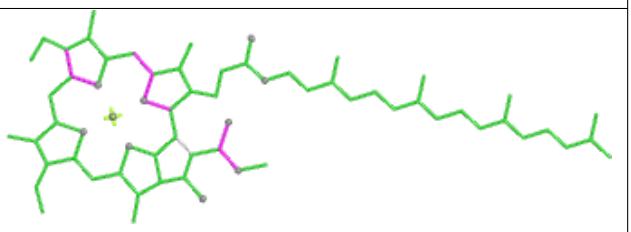


Rings

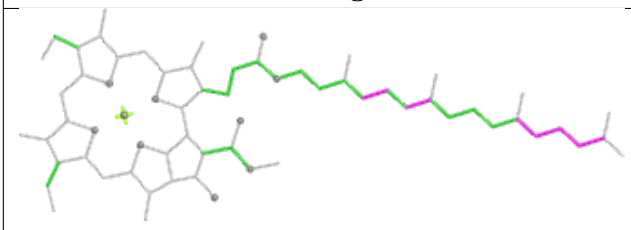
Ligand CLA V 313



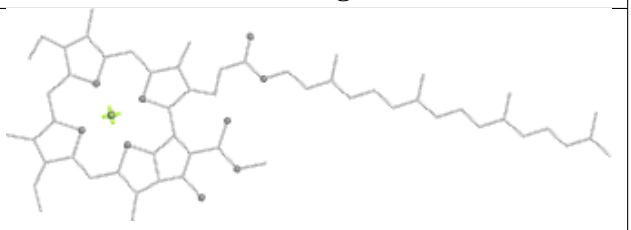
Bond lengths



Bond angles

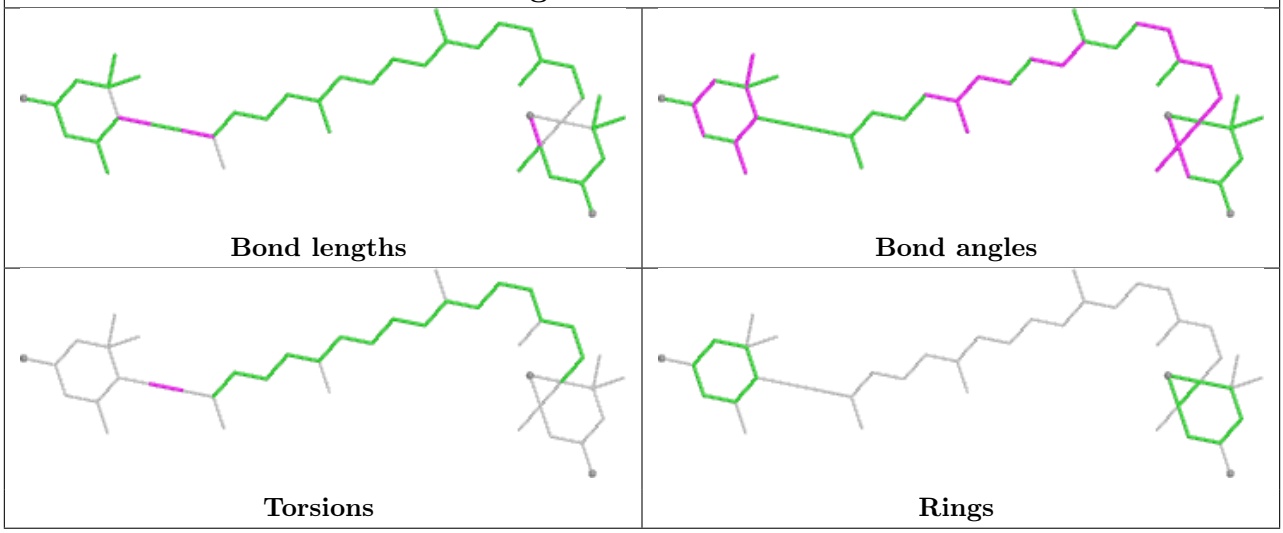


Torsions

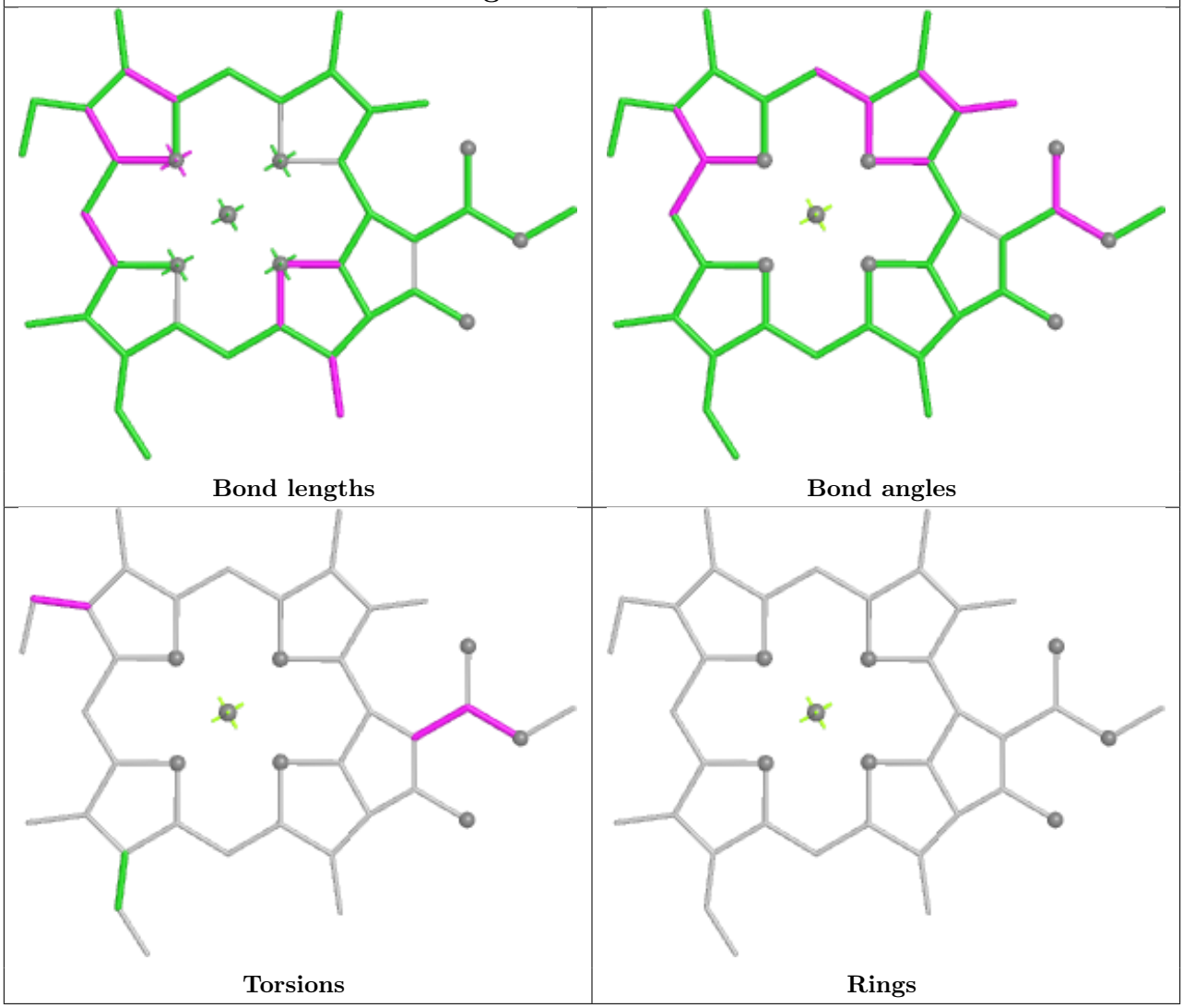


Rings

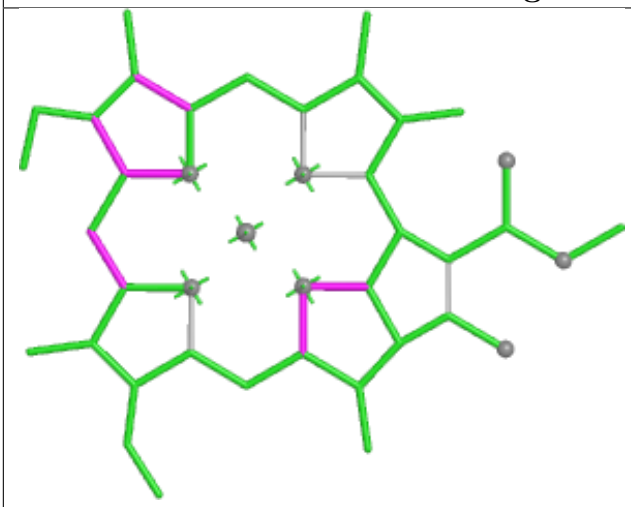
Ligand DD6 5 303



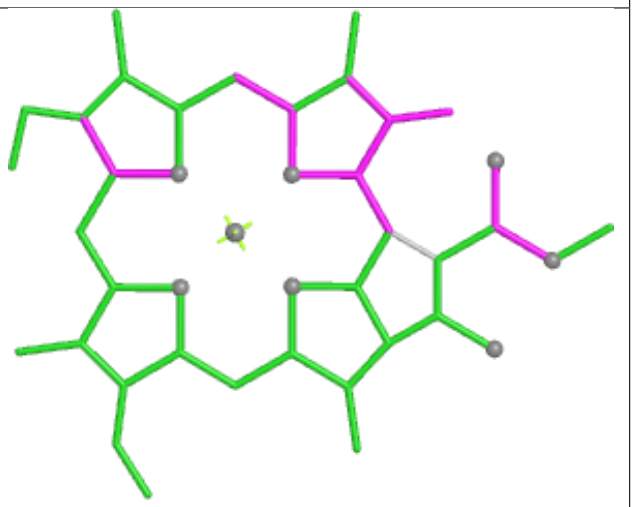
Ligand CLA H 315



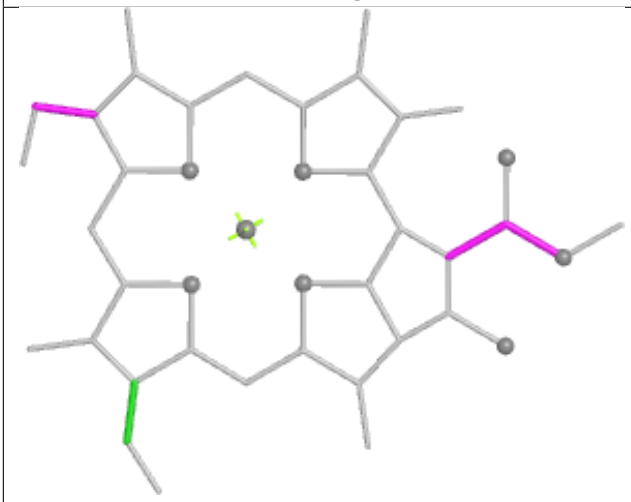
Ligand CLA Y 314



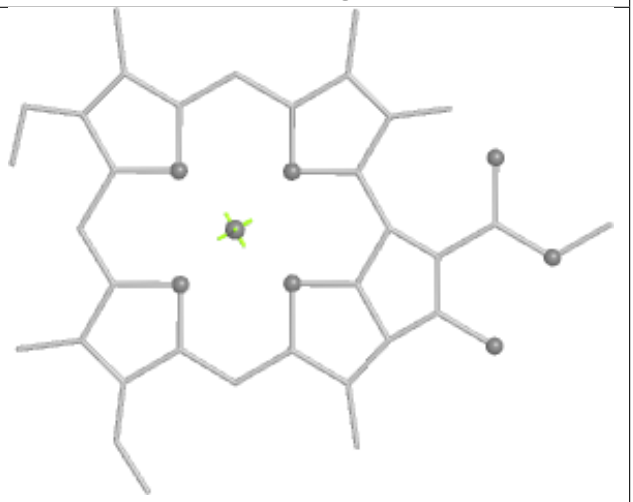
Bond lengths



Bond angles

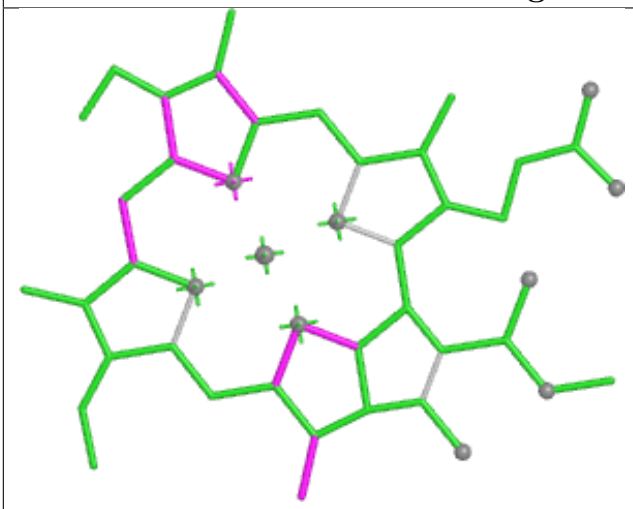


Torsions

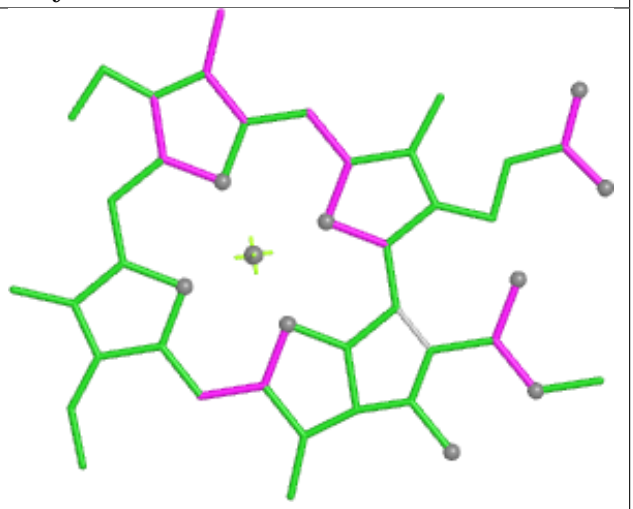


Rings

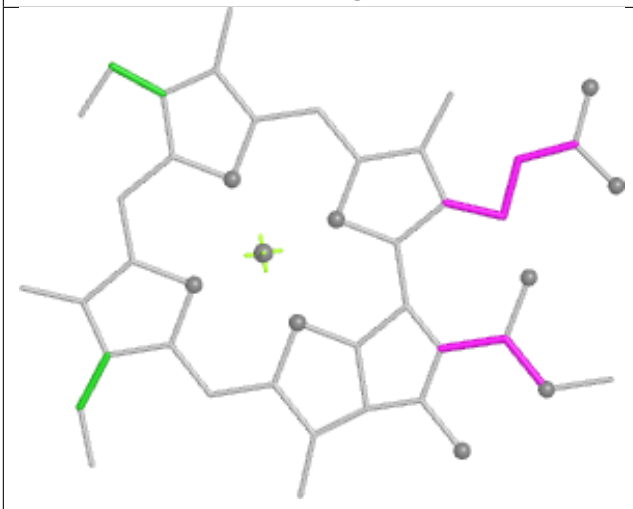
Ligand CLA y 308



Bond lengths



Bond angles

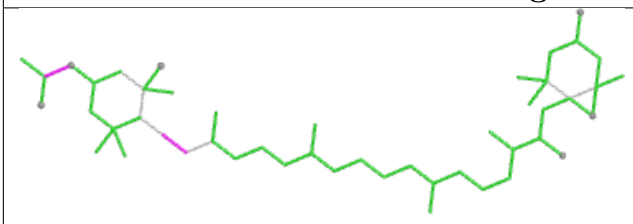


Torsions

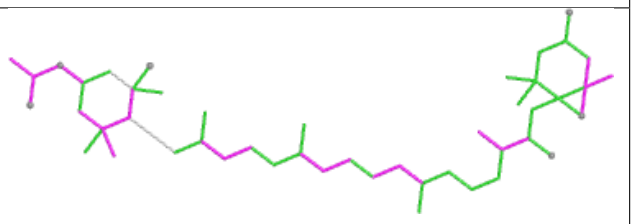


Rings

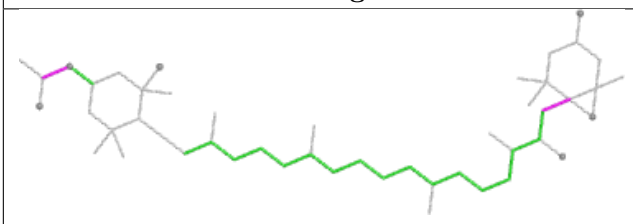
Ligand A86 R 317



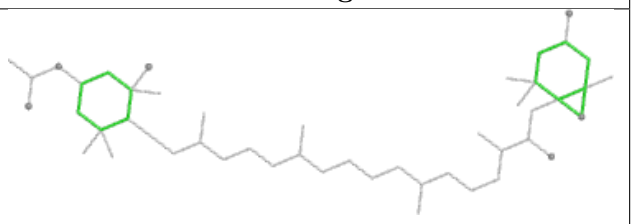
Bond lengths



Bond angles

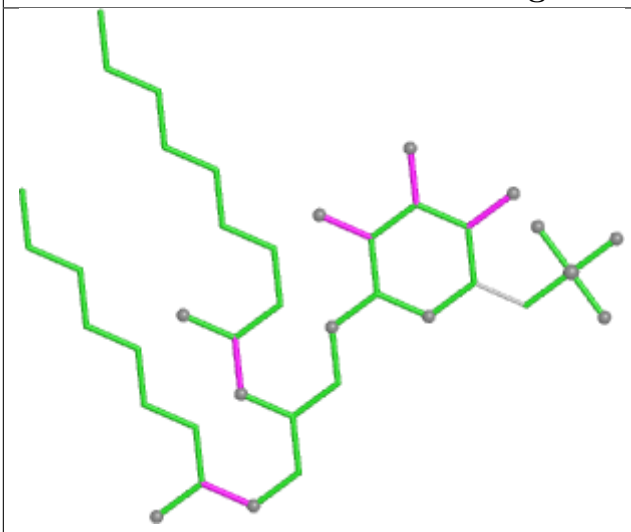


Torsions

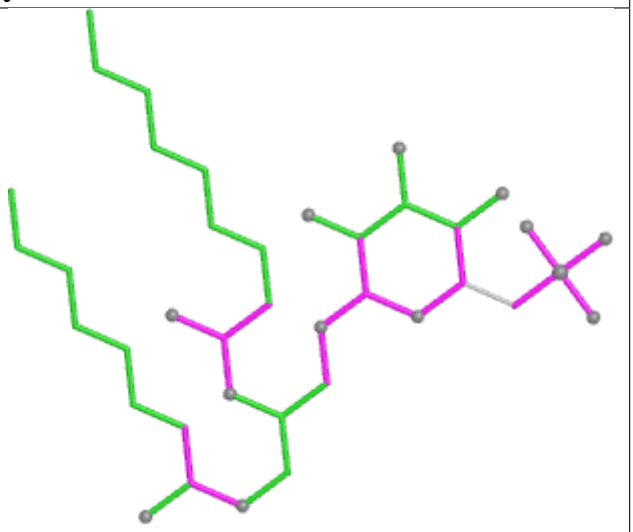


Rings

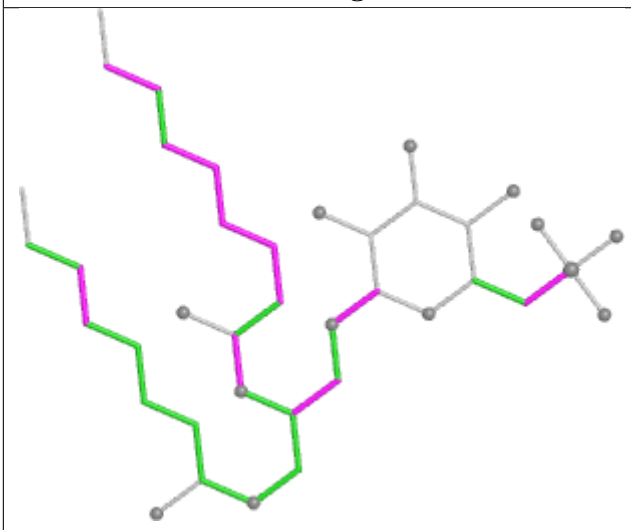
Ligand SQD 7 302



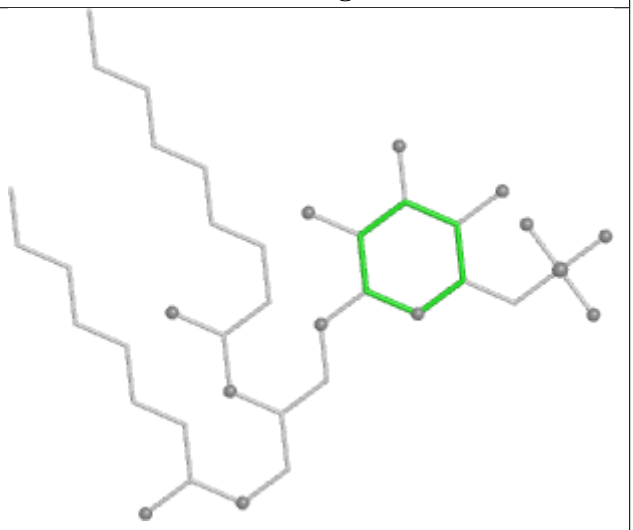
Bond lengths



Bond angles

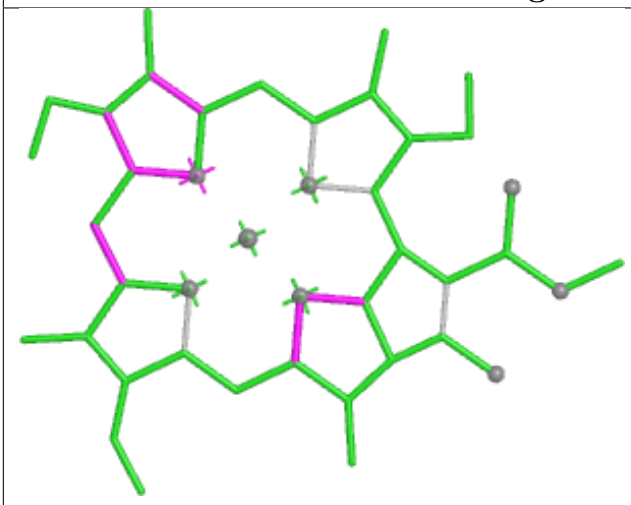


Torsions

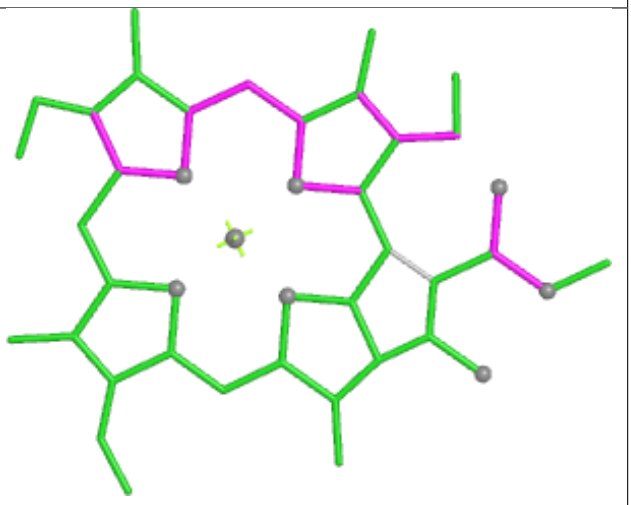


Rings

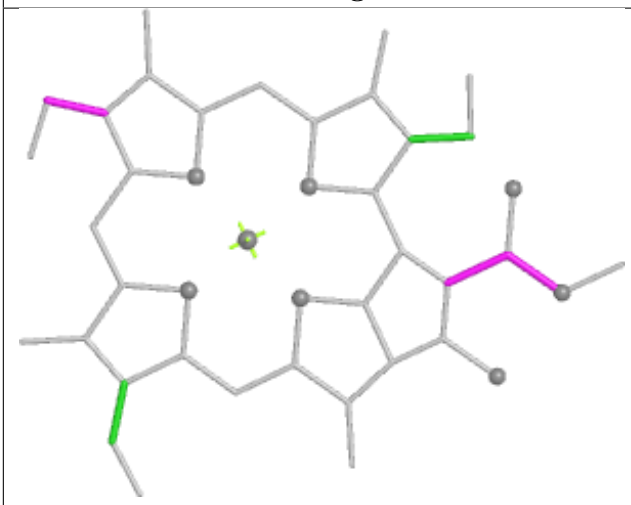
Ligand CLA o 202



Bond lengths



Bond angles

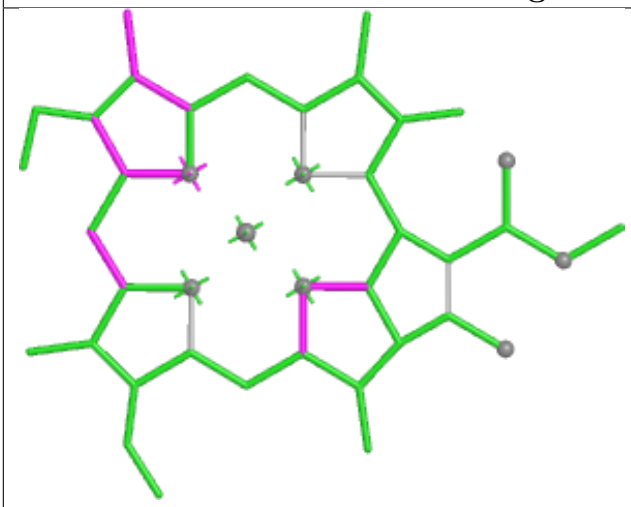


Torsions

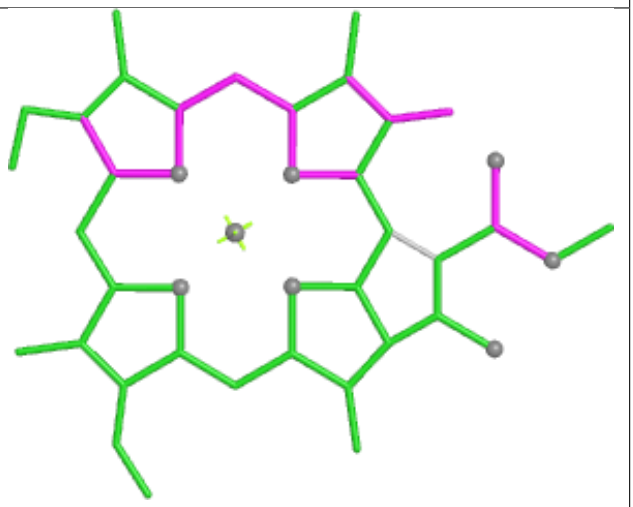


Rings

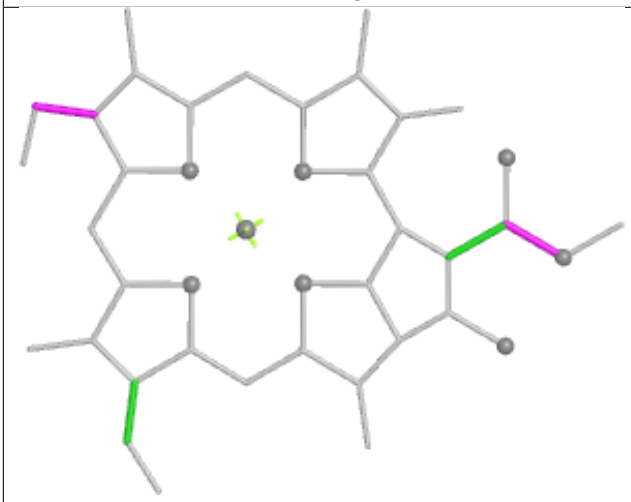
Ligand CLA 9 307



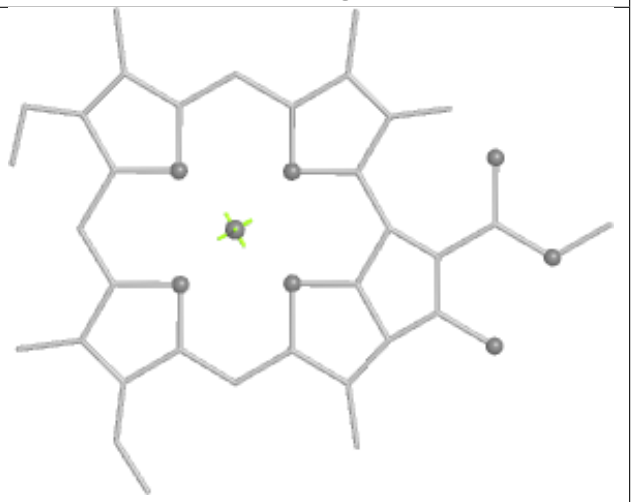
Bond lengths



Bond angles

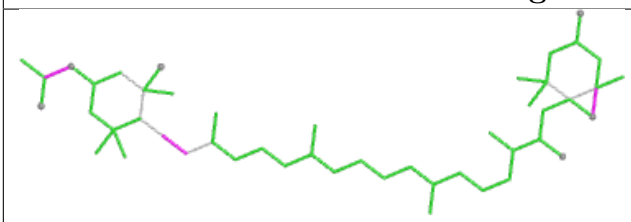


Torsions

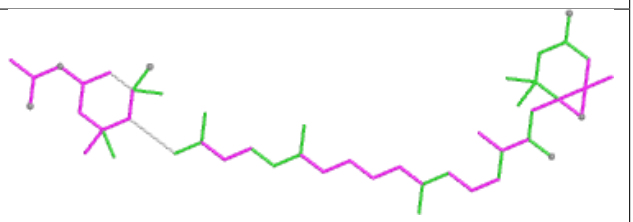


Rings

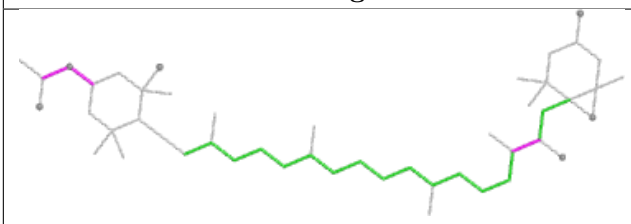
Ligand A86 K 301



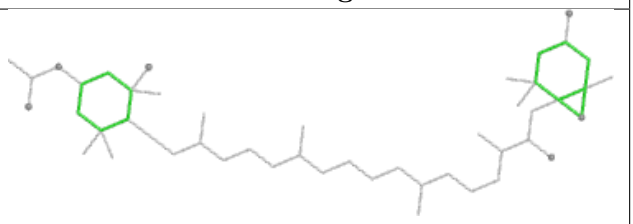
Bond lengths



Bond angles

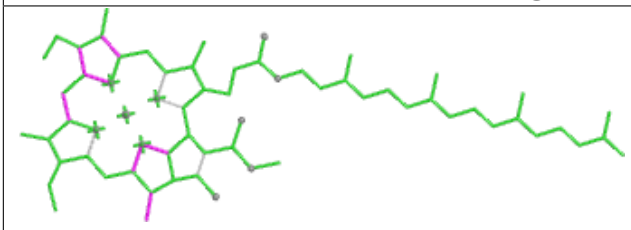


Torsions

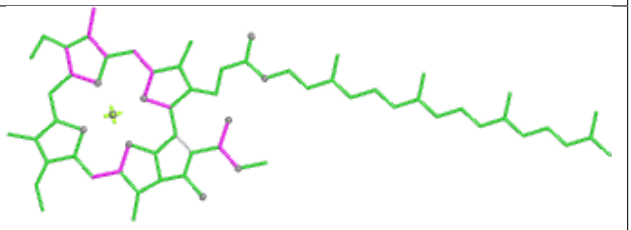


Rings

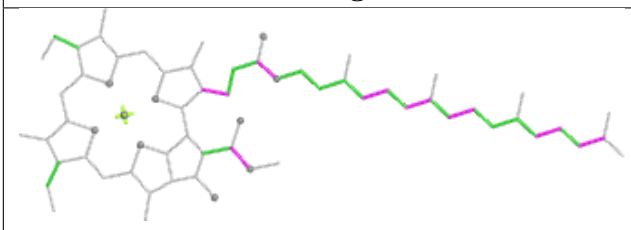
Ligand CLA J 311



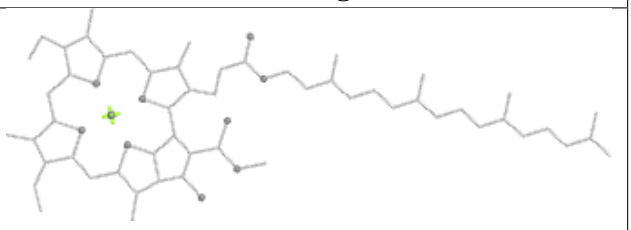
Bond lengths



Bond angles

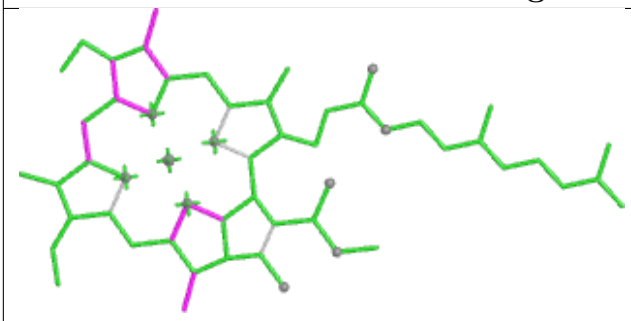


Torsions

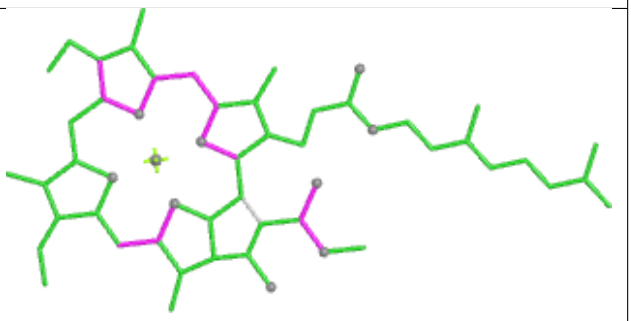


Rings

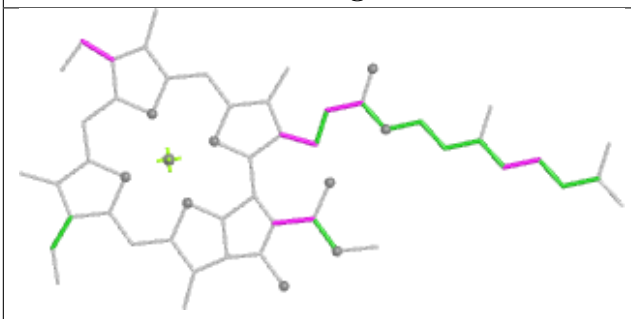
Ligand CLA b 814



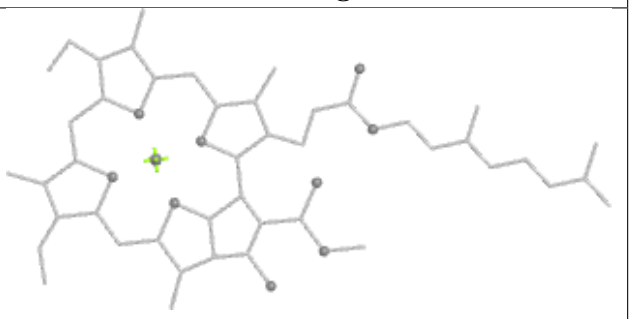
Bond lengths



Bond angles

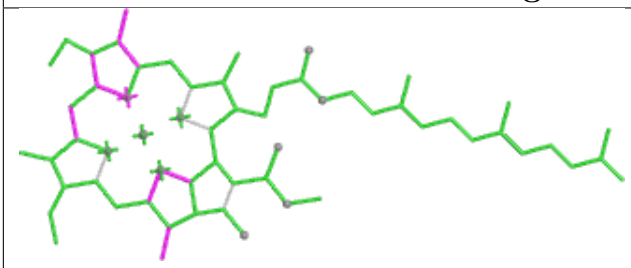


Torsions

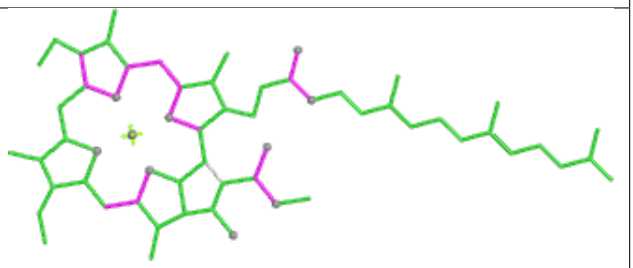


Rings

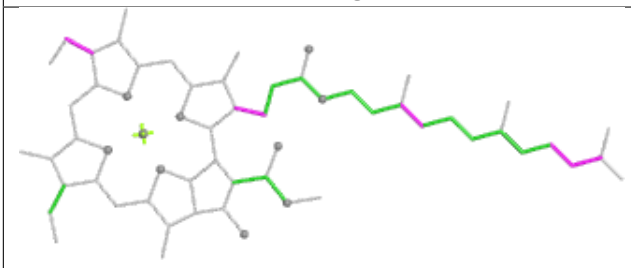
Ligand CLA U 210



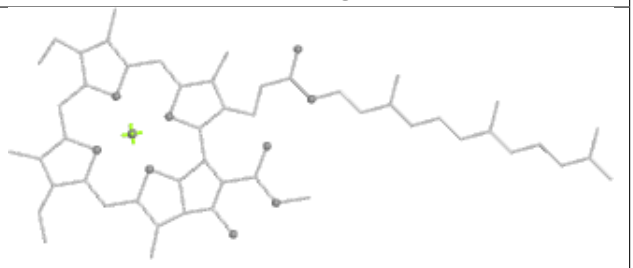
Bond lengths



Bond angles

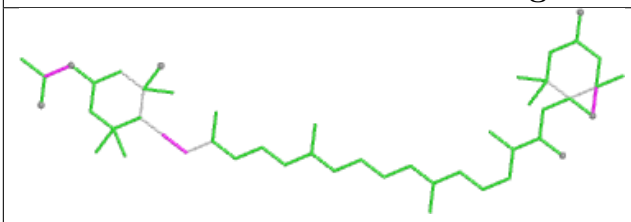


Torsions

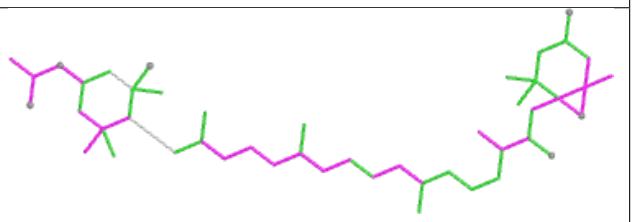


Rings

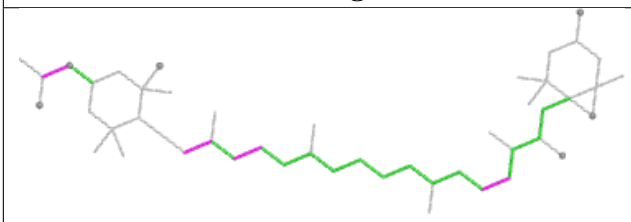
Ligand A86 Y 301



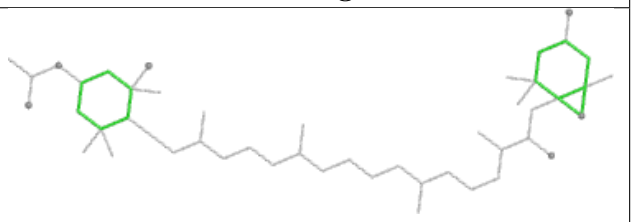
Bond lengths



Bond angles

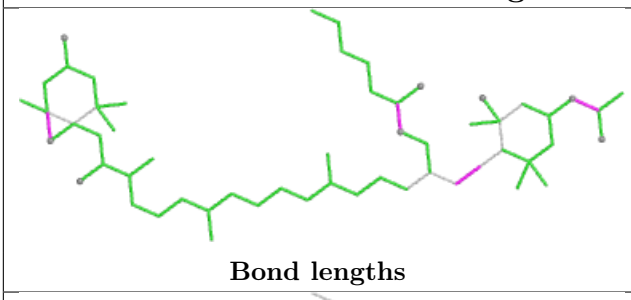


Torsions

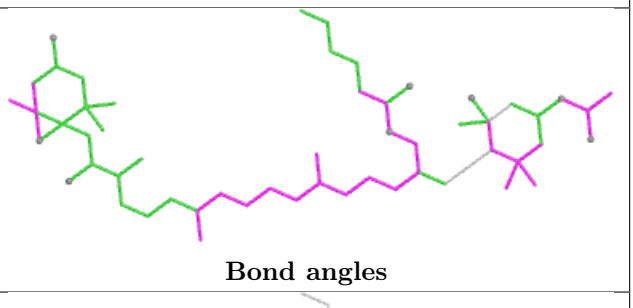


Rings

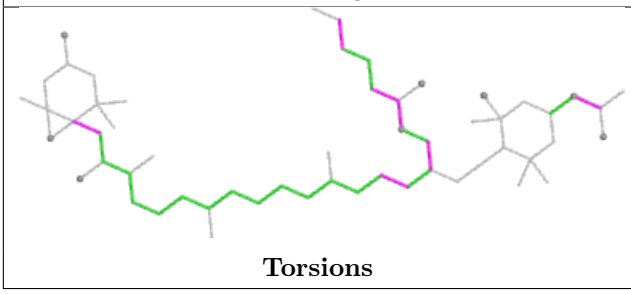
Ligand A1EB1 F 304



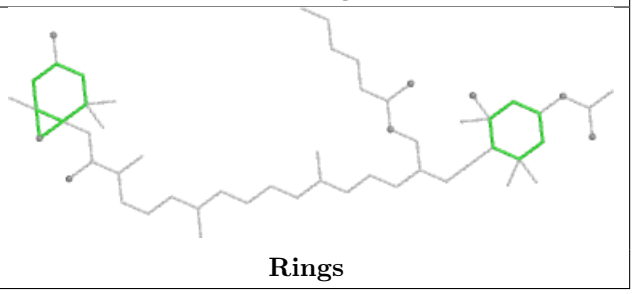
Bond lengths



Bond angles

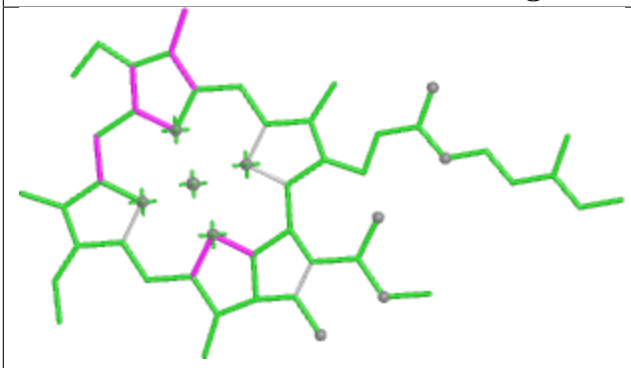


Torsions

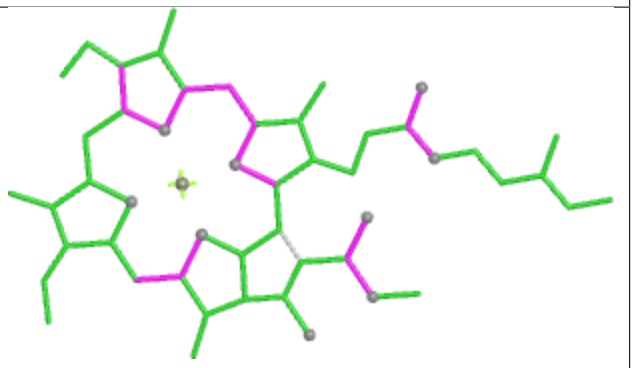


Rings

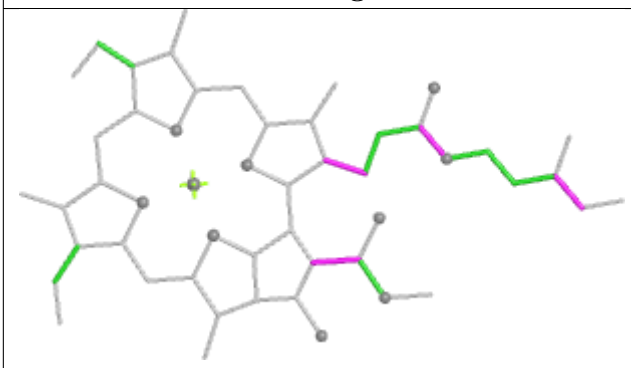
Ligand CLA T 313



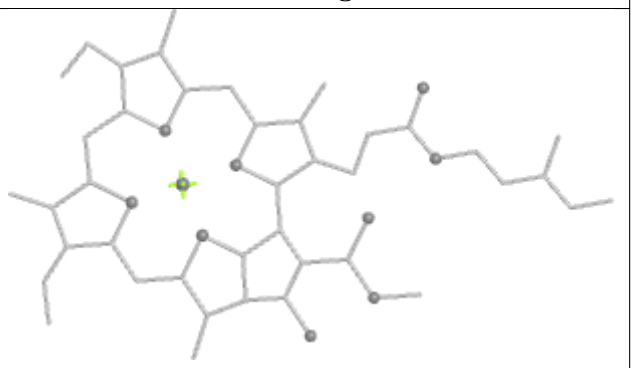
Bond lengths



Bond angles

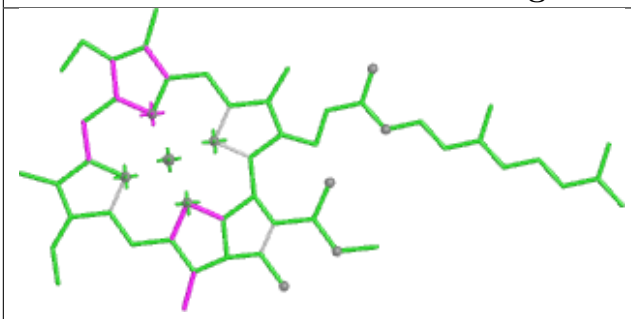


Torsions

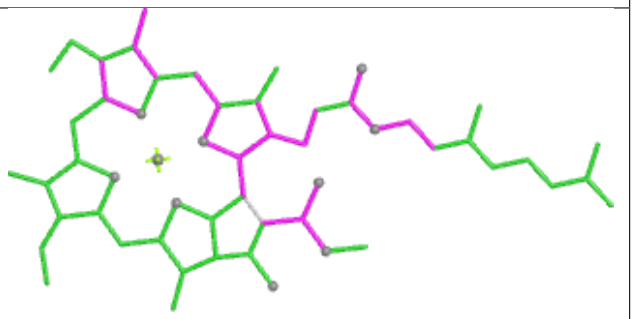


Rings

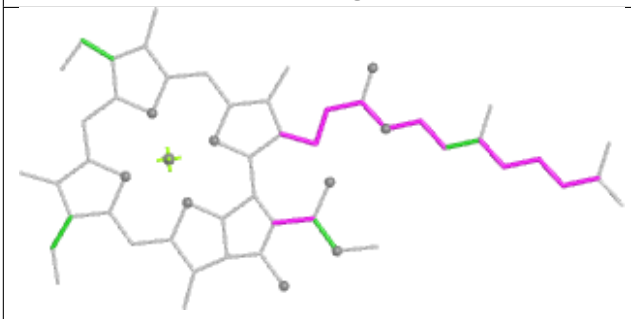
Ligand CLA 9 308



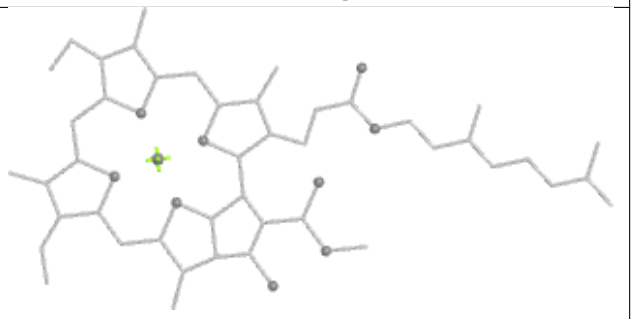
Bond lengths



Bond angles

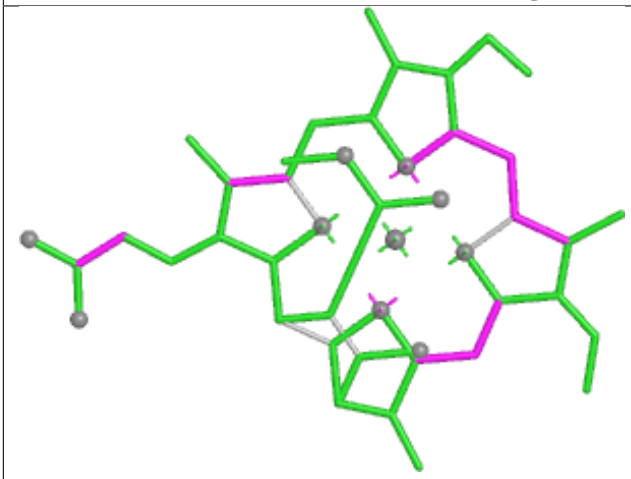


Torsions

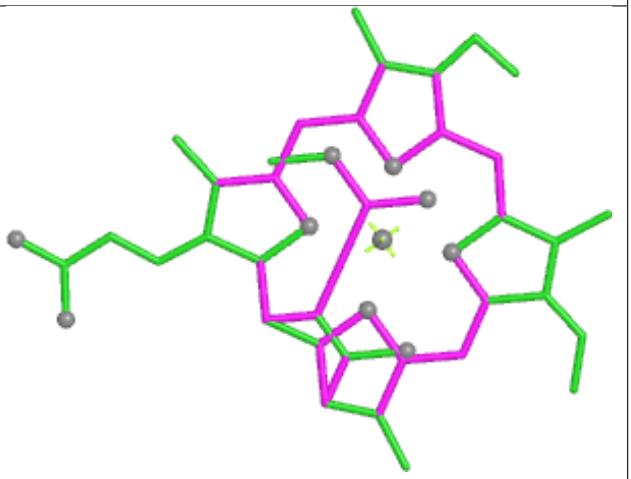


Rings

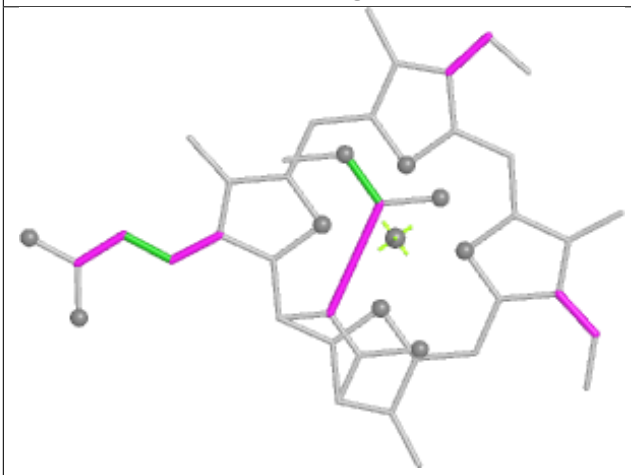
Ligand KC2 V 320



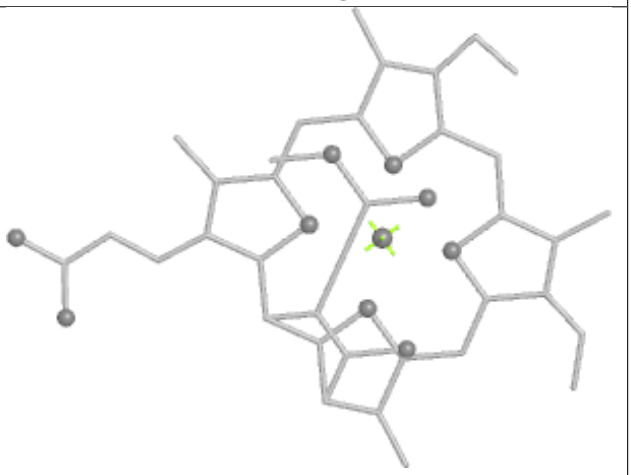
Bond lengths



Bond angles

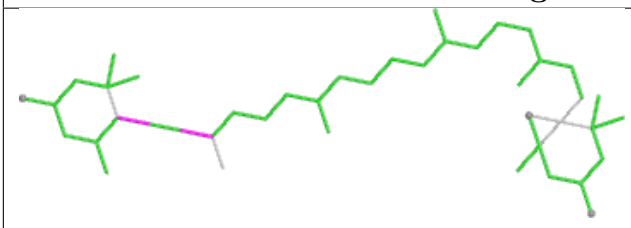


Torsions

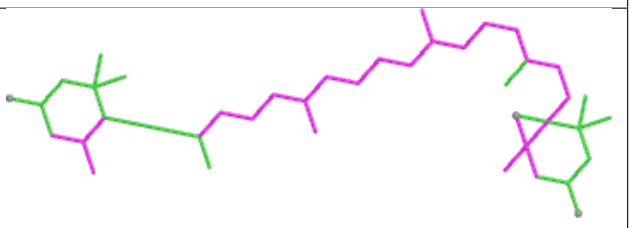


Rings

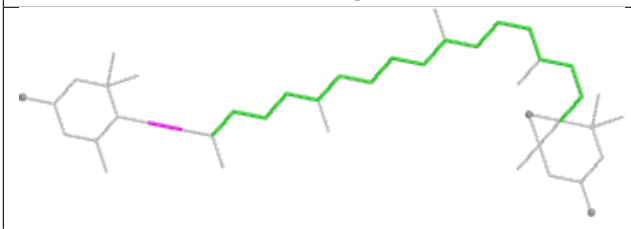
Ligand DD6 z 305



Bond lengths



Bond angles

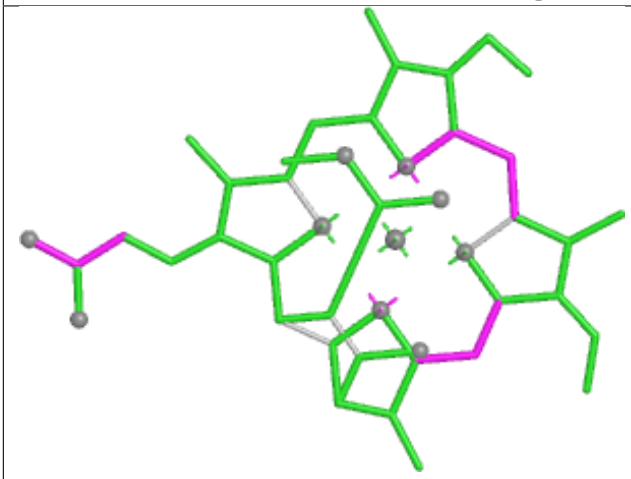


Torsions

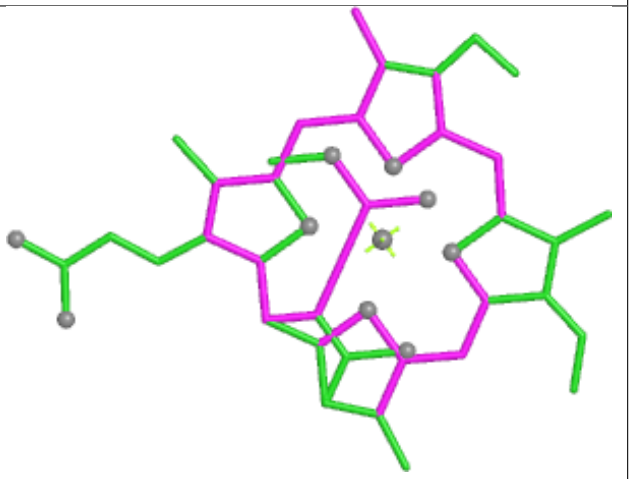


Rings

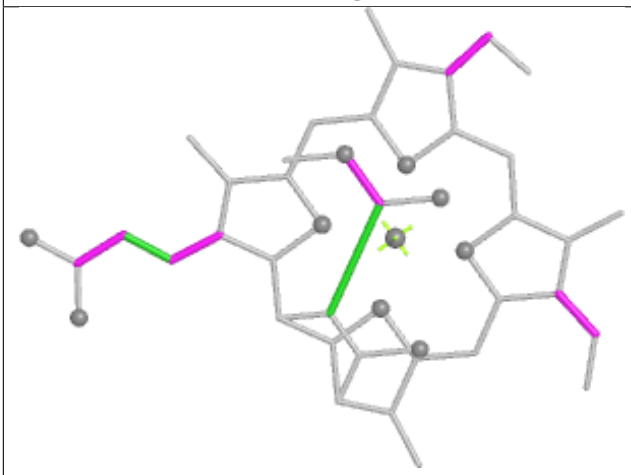
Ligand KC2 3 321



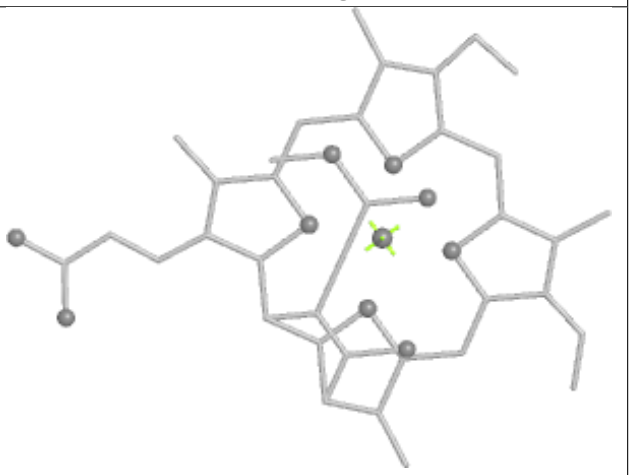
Bond lengths



Bond angles

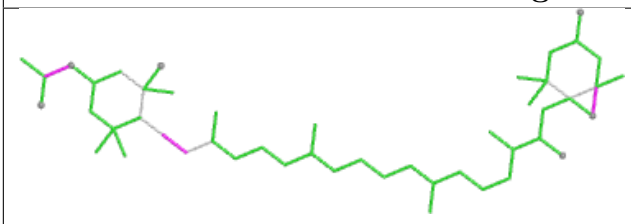


Torsions

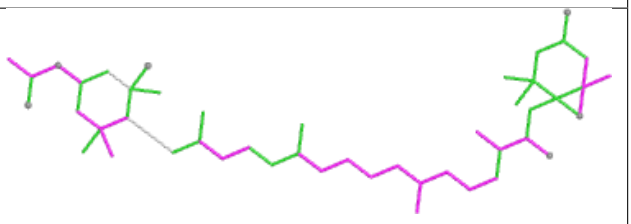


Rings

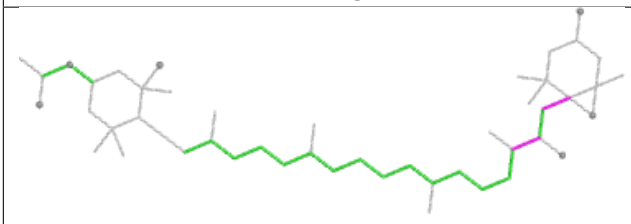
Ligand A86 F 301



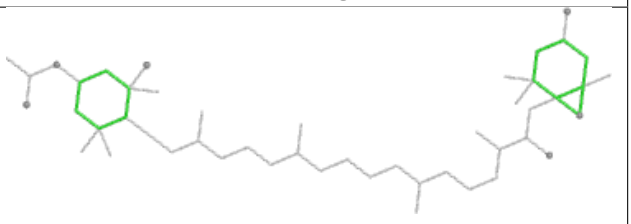
Bond lengths



Bond angles

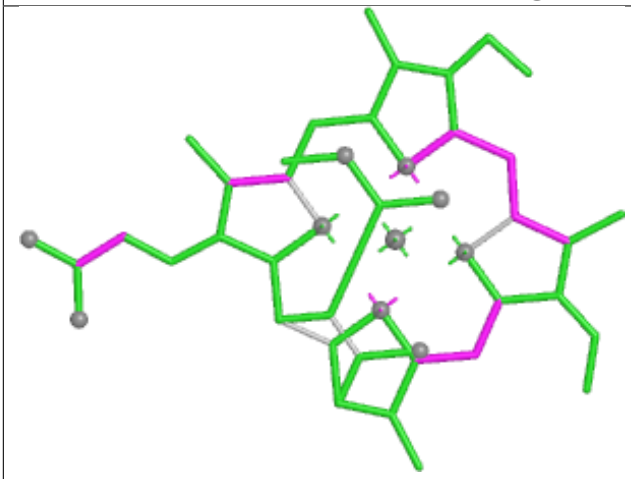


Torsions

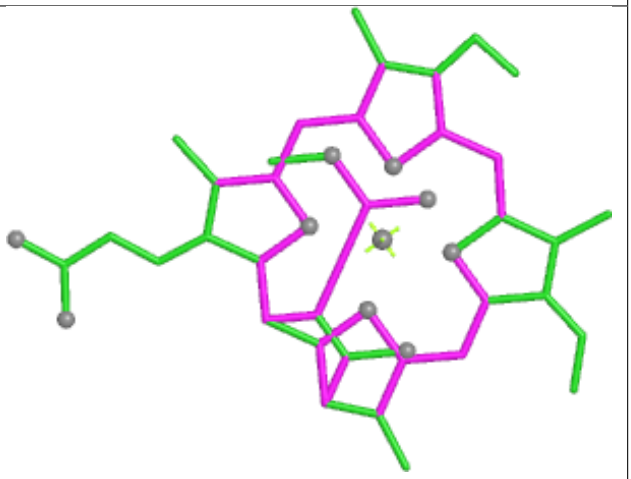


Rings

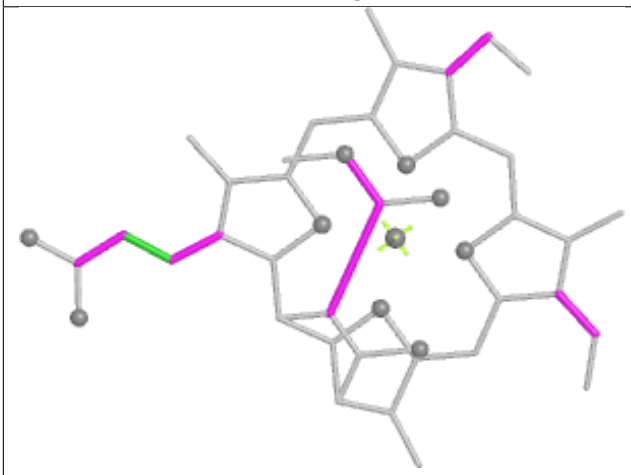
Ligand KC2 L 317



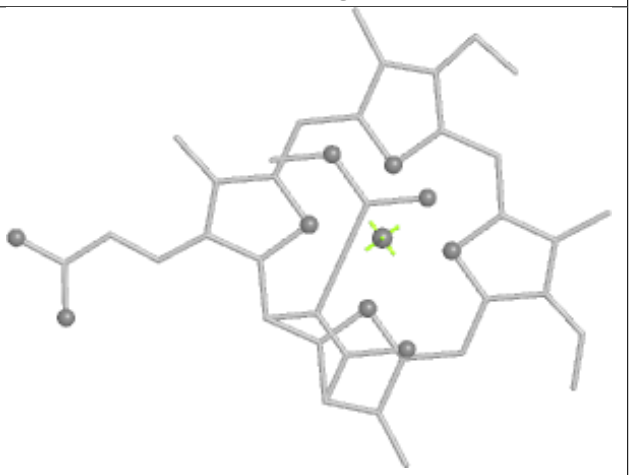
Bond lengths



Bond angles

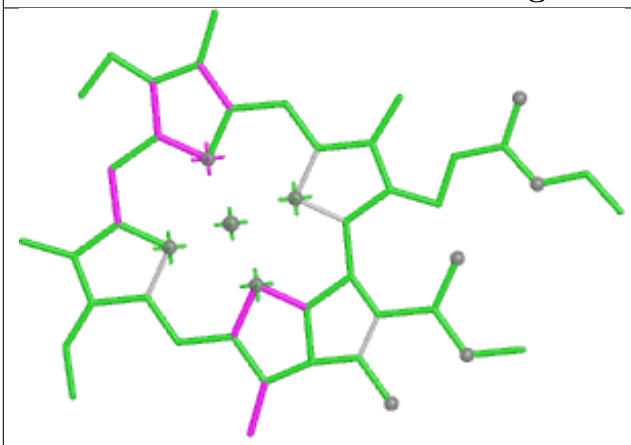


Torsions

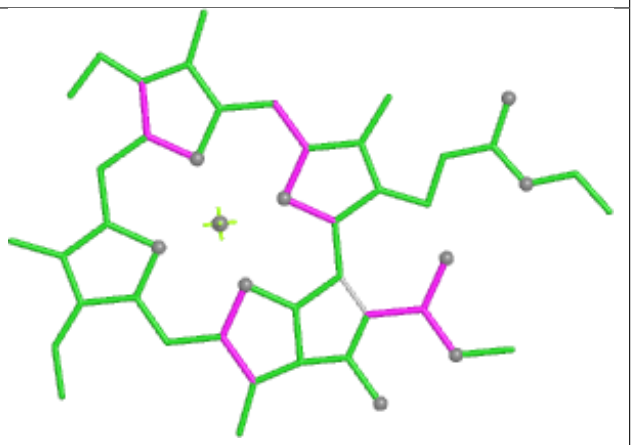


Rings

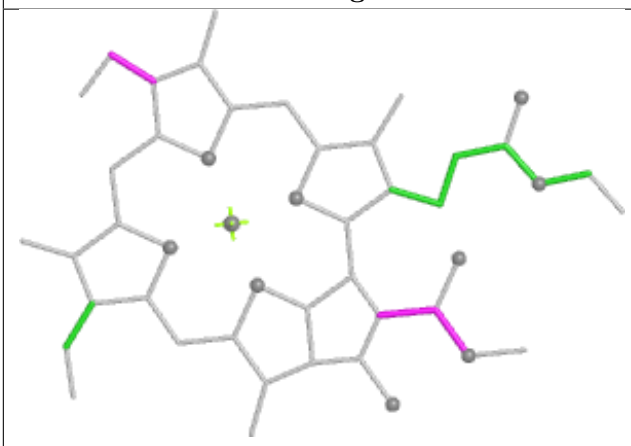
Ligand CLA 5 315



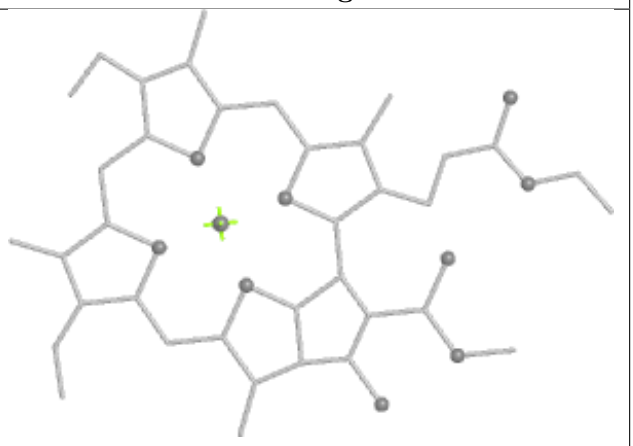
Bond lengths



Bond angles

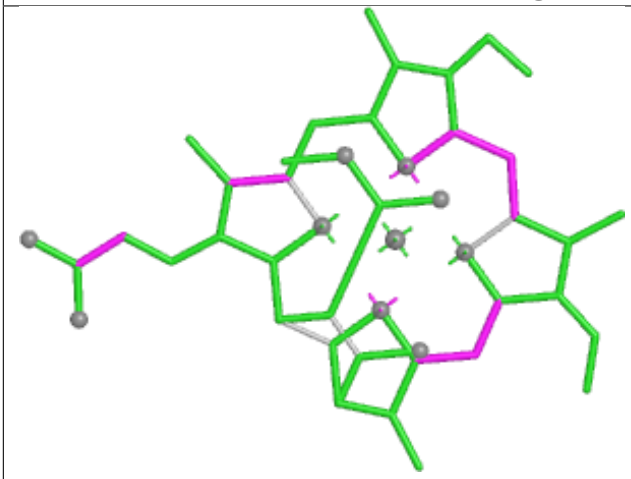


Torsions

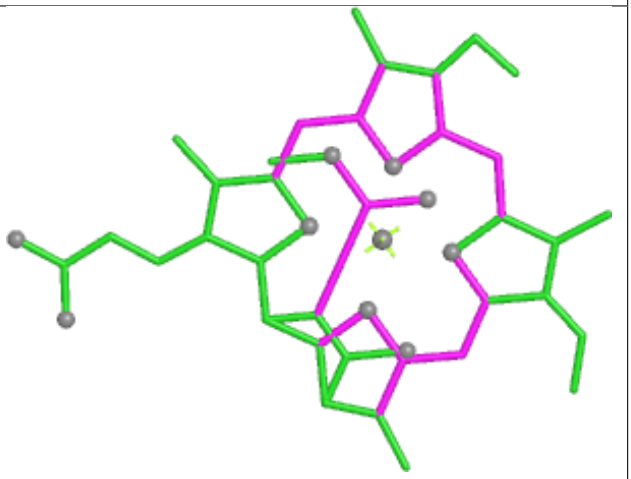


Rings

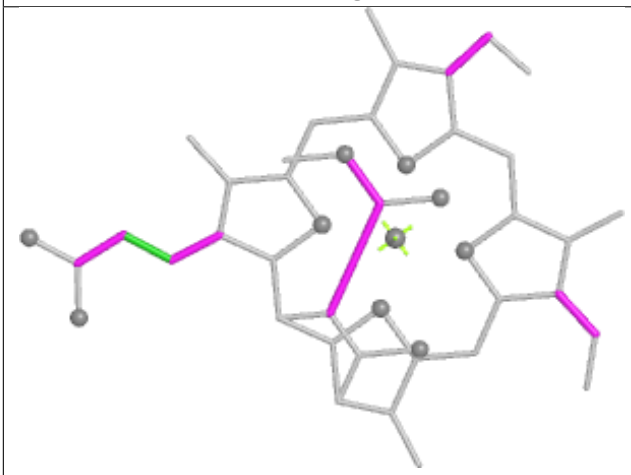
Ligand KC2 9 318



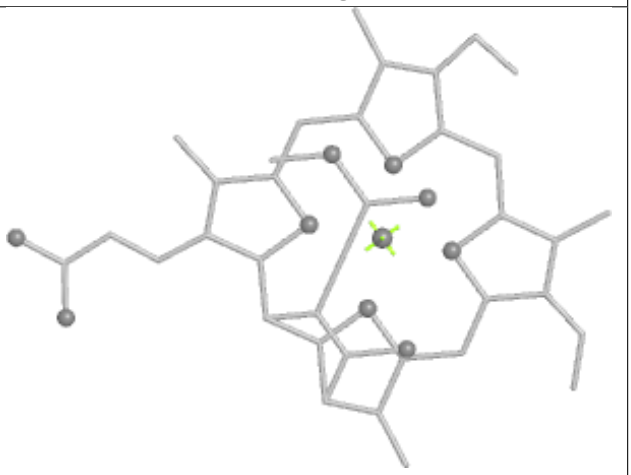
Bond lengths



Bond angles

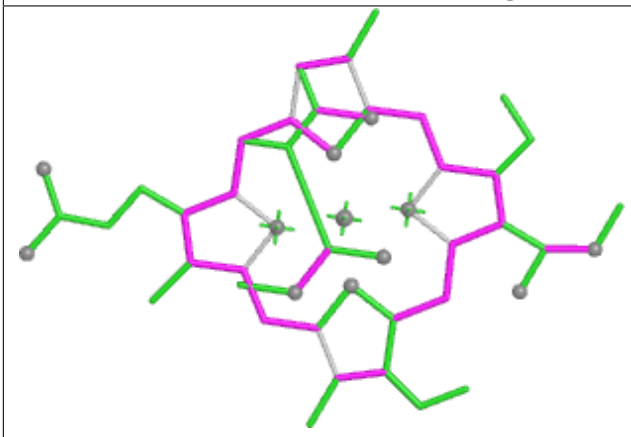


Torsions

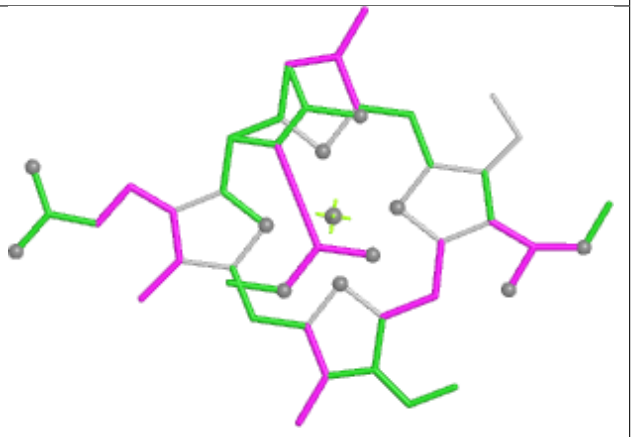


Rings

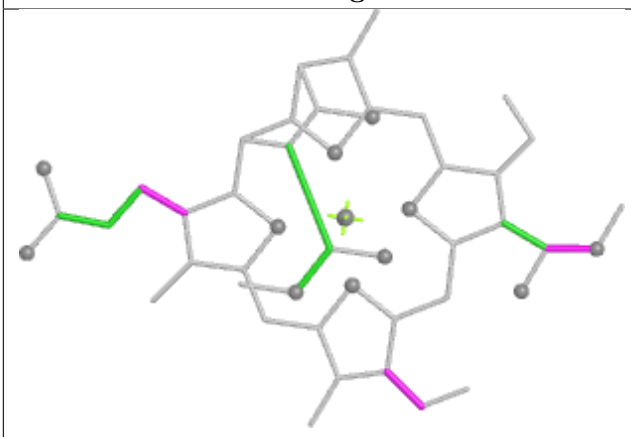
Ligand A1ECV T 317



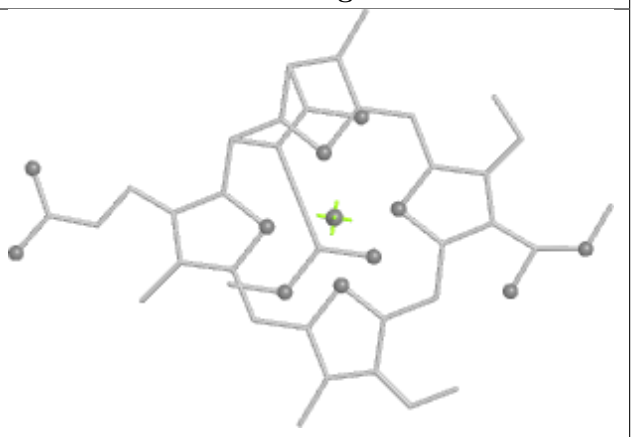
Bond lengths



Bond angles

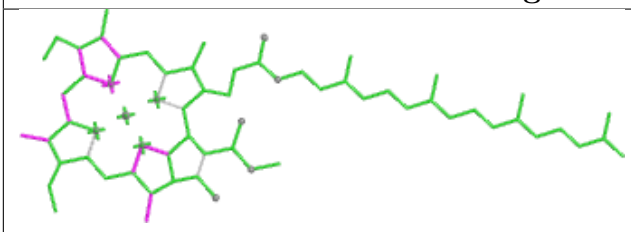


Torsions

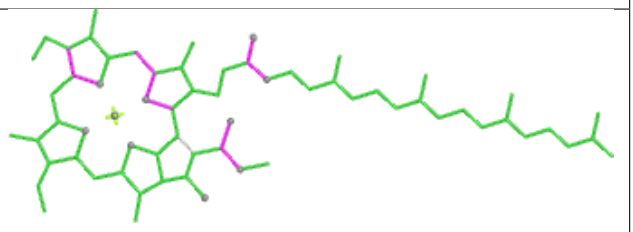


Rings

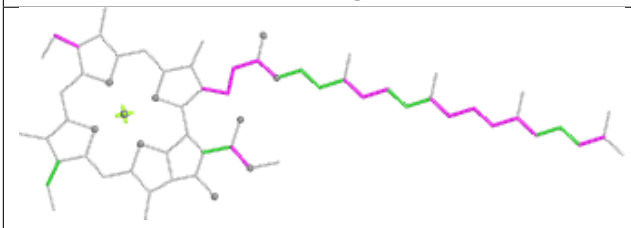
Ligand CLA D 311



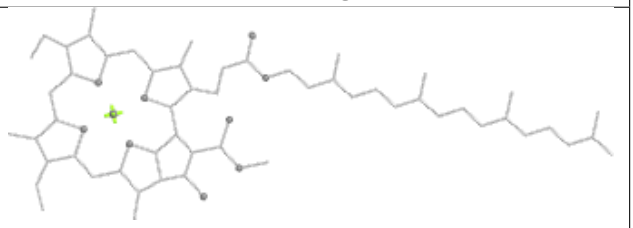
Bond lengths



Bond angles

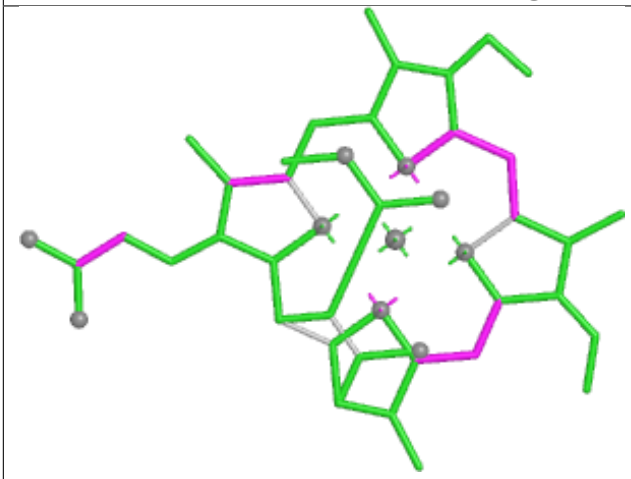


Torsions

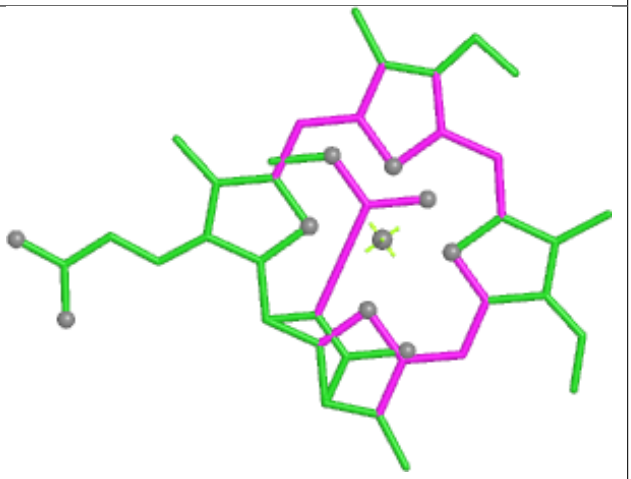


Rings

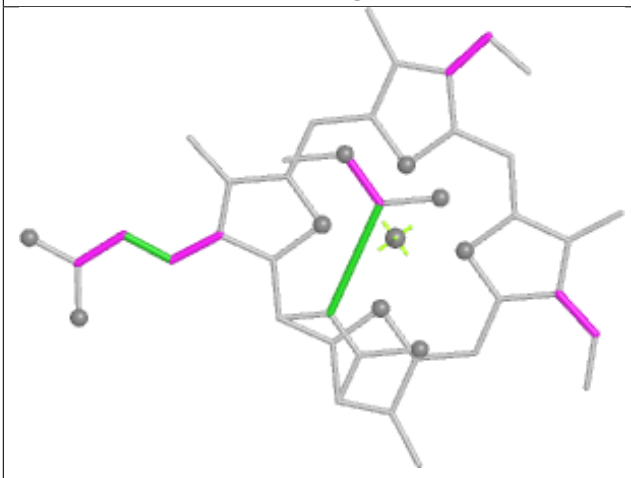
Ligand KC2 Y 308



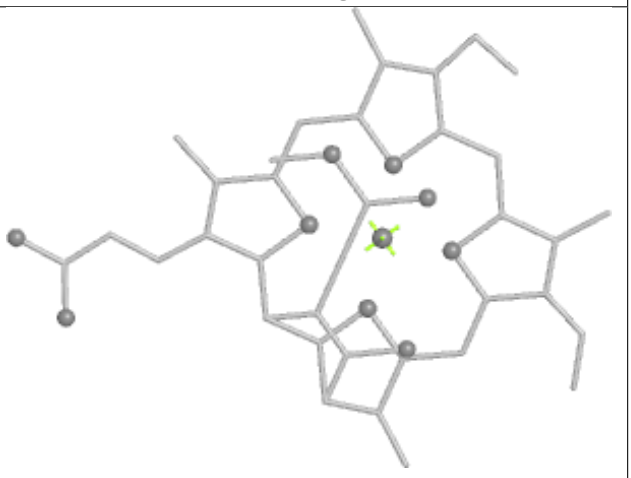
Bond lengths



Bond angles

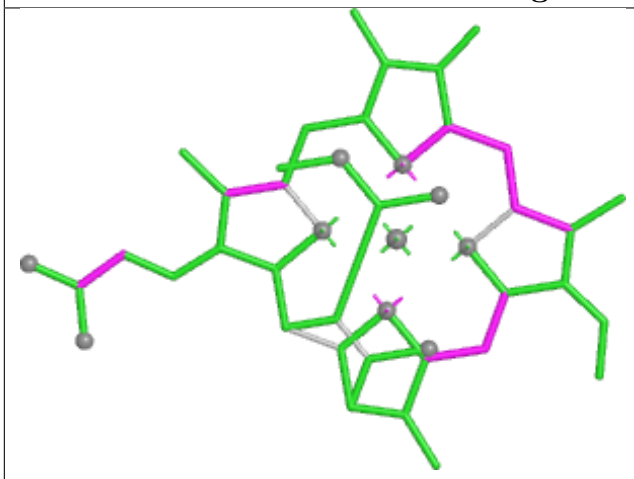


Torsions

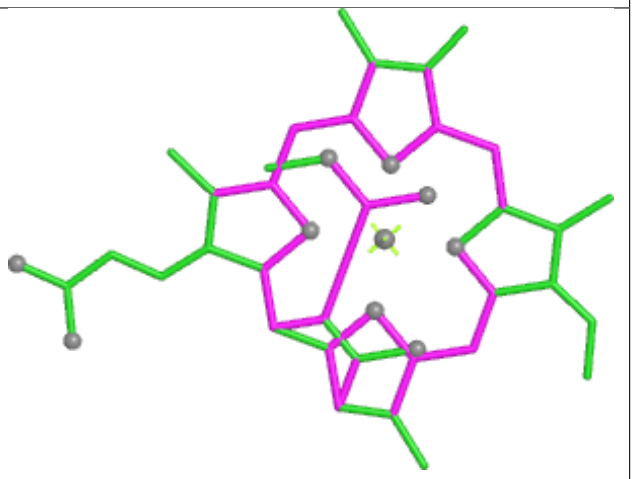


Rings

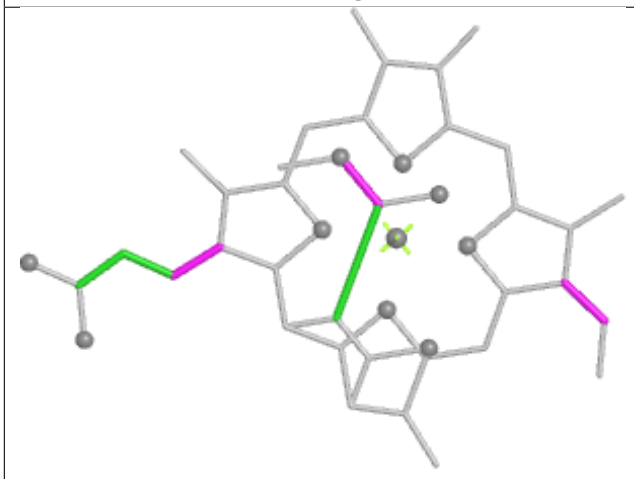
Ligand KC2 2 313



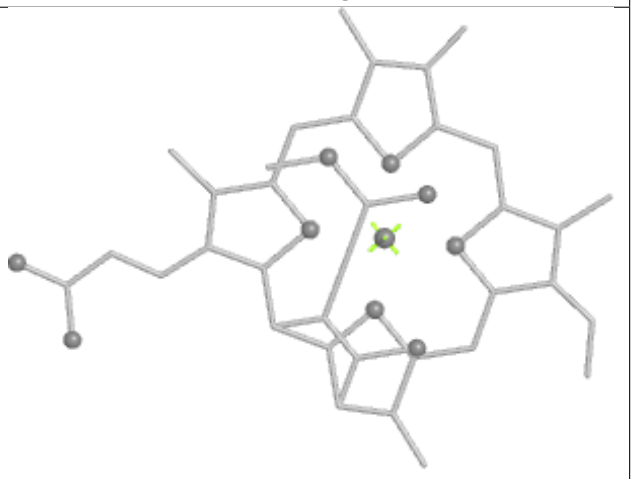
Bond lengths



Bond angles

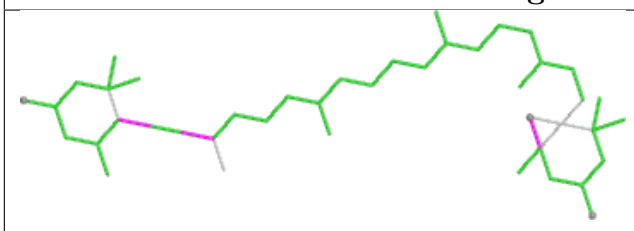


Torsions

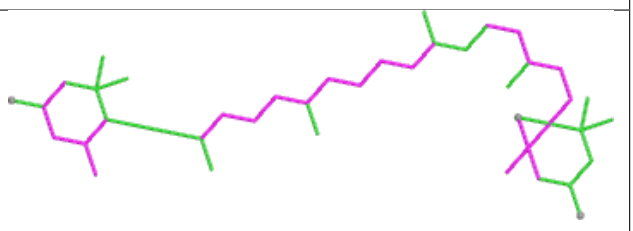


Rings

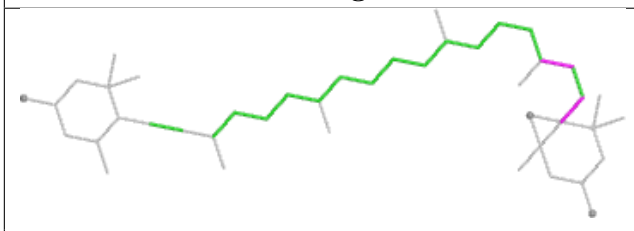
Ligand DD6 E 305



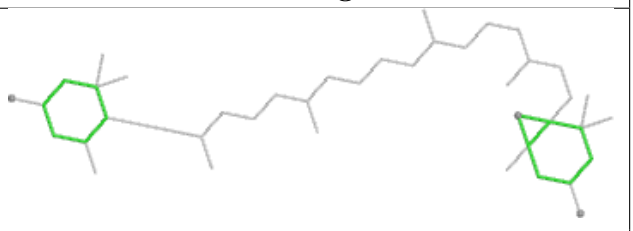
Bond lengths



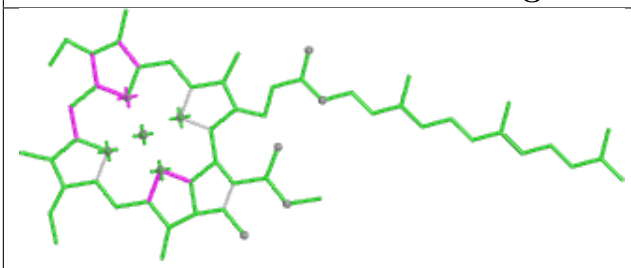
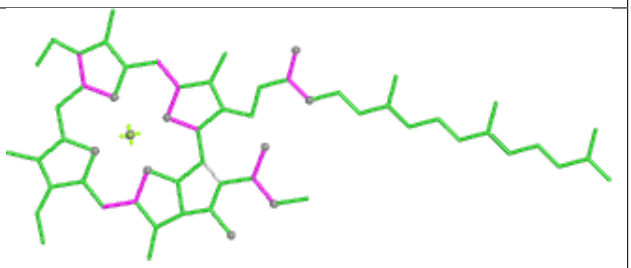
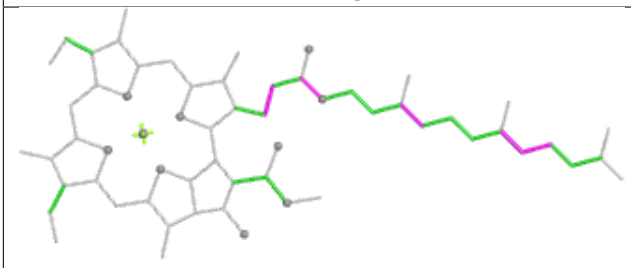
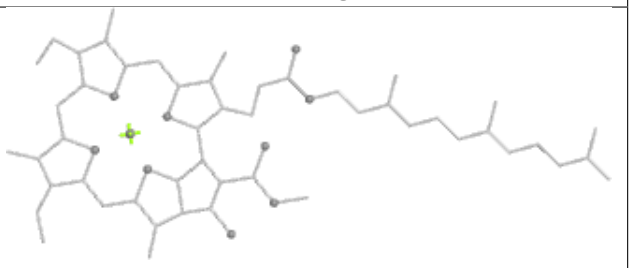
Bond angles

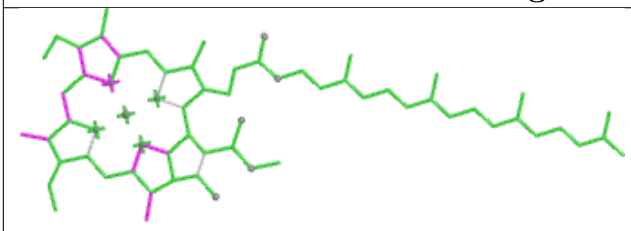
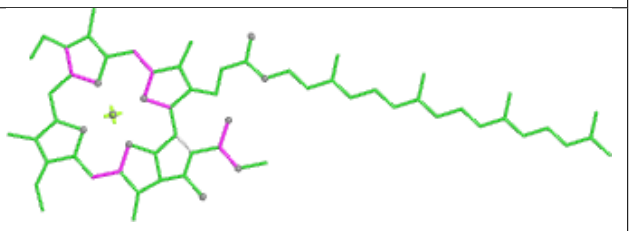
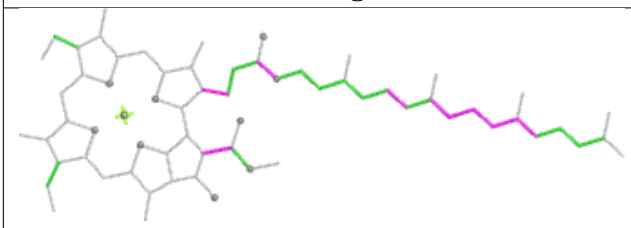
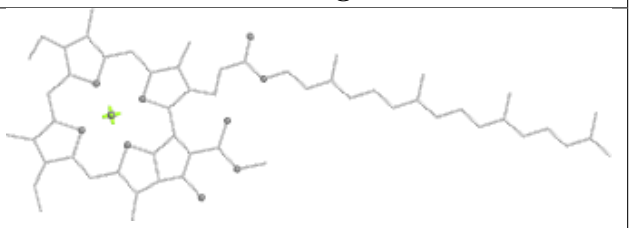


Torsions

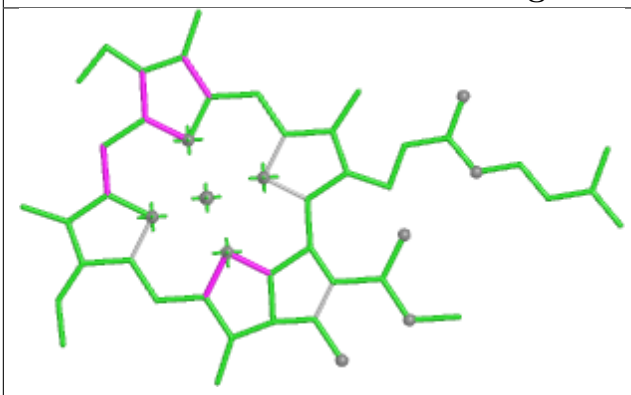


Rings

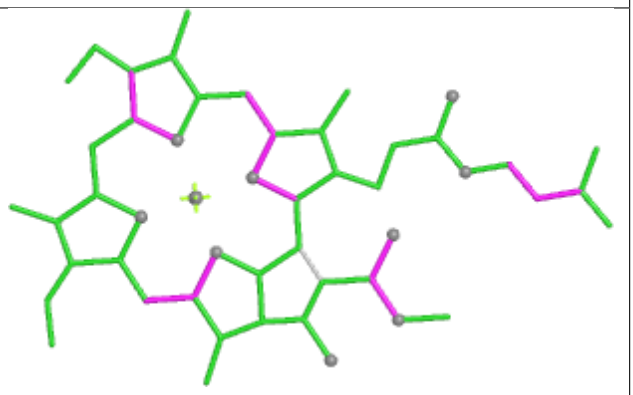
Ligand CLA H 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

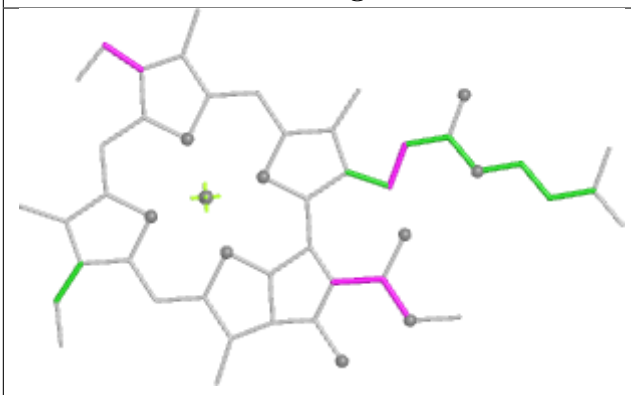
Ligand CLA J 308



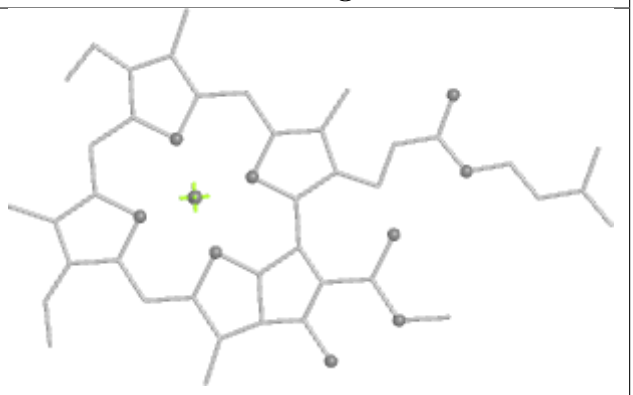
Bond lengths



Bond angles

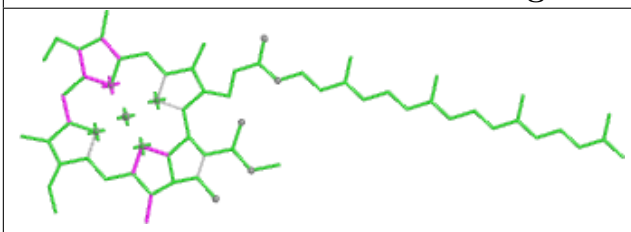


Torsions

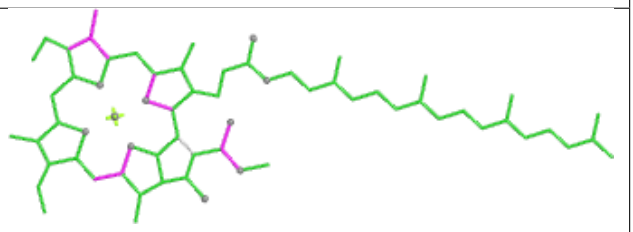


Rings

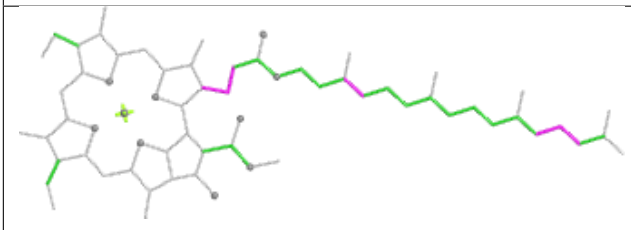
Ligand CLA b 802



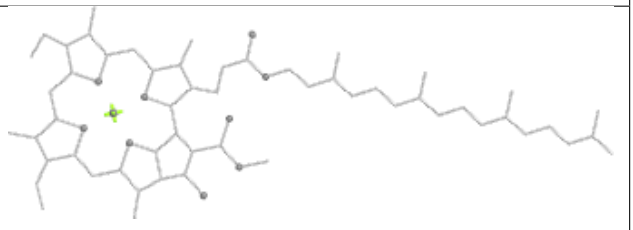
Bond lengths



Bond angles

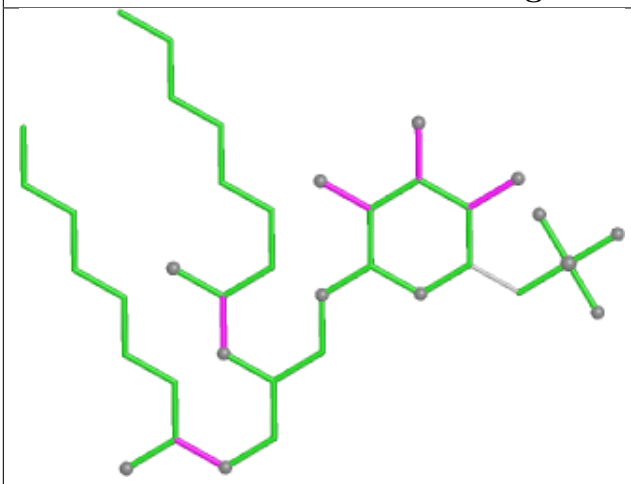


Torsions

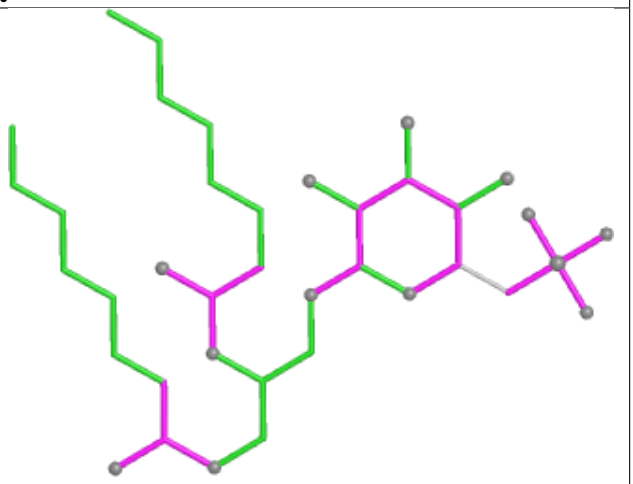


Rings

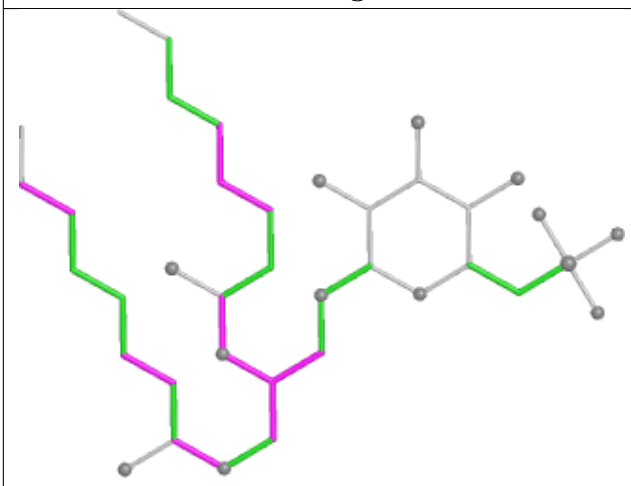
Ligand SQD P 301



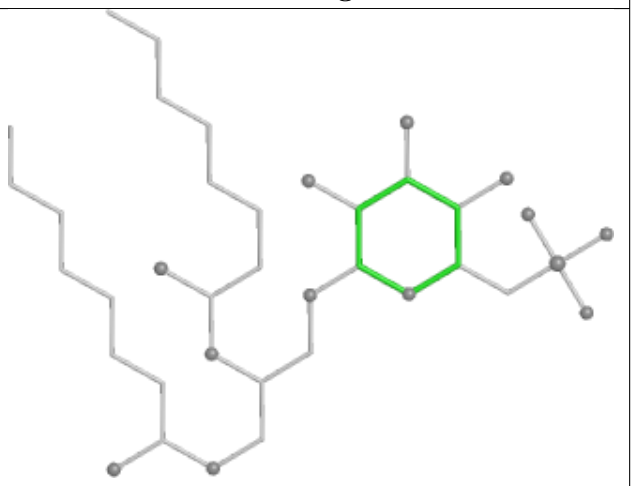
Bond lengths



Bond angles

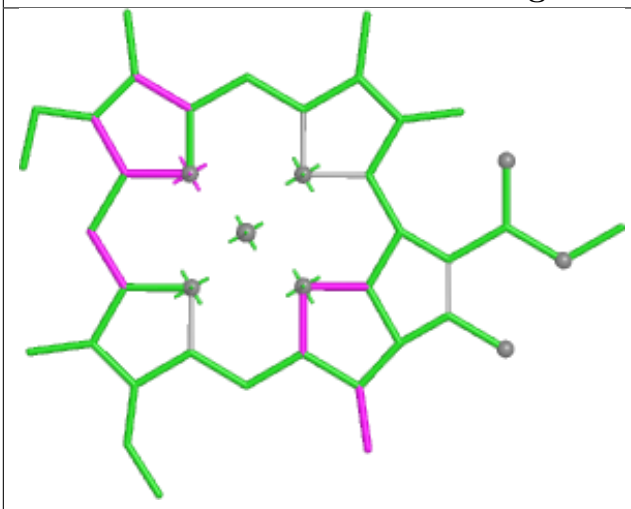


Torsions

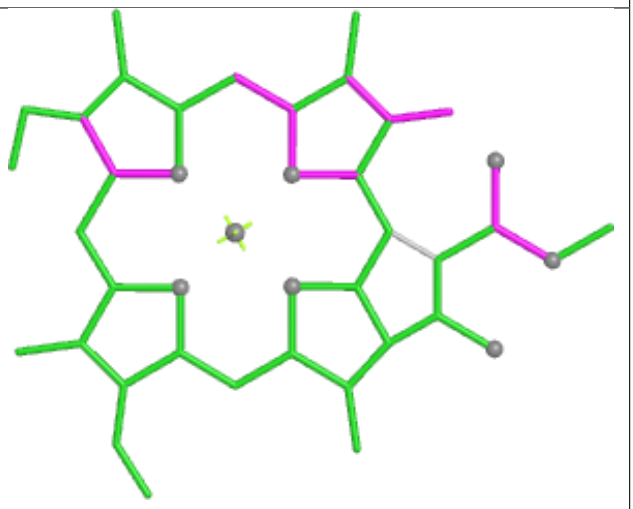


Rings

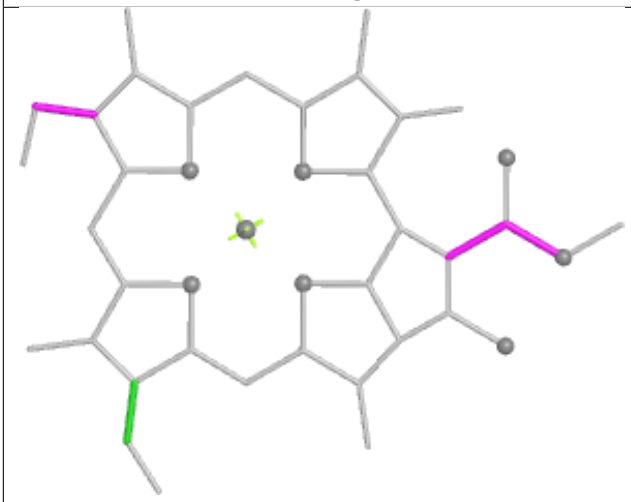
Ligand CLA 6 318



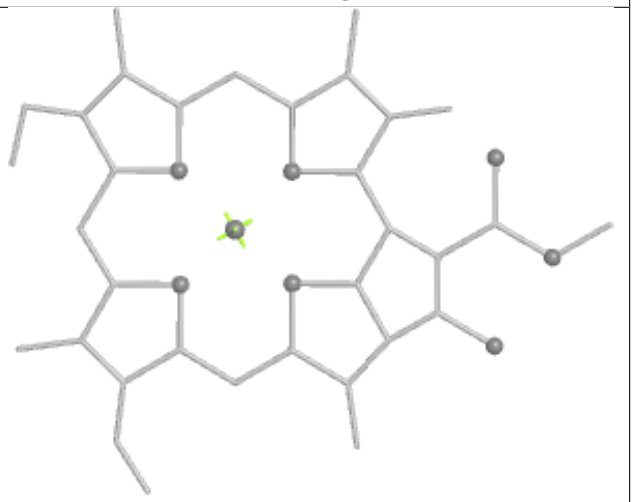
Bond lengths



Bond angles

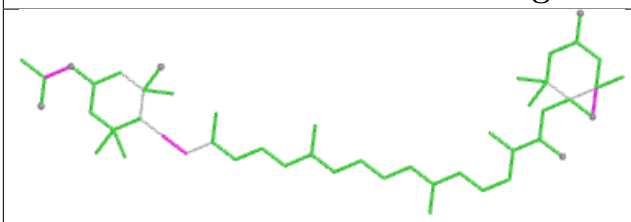


Torsions

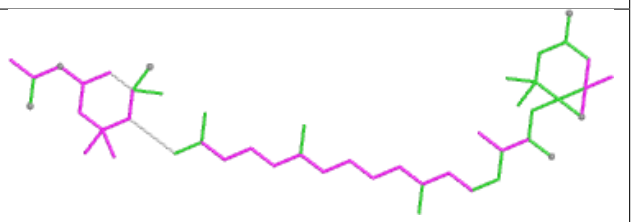


Rings

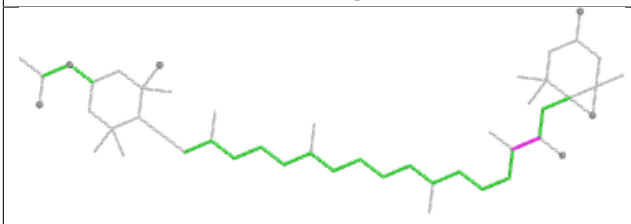
Ligand A86 L 305



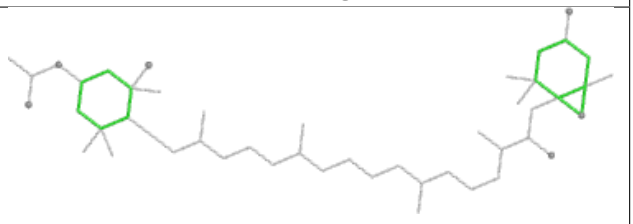
Bond lengths



Bond angles

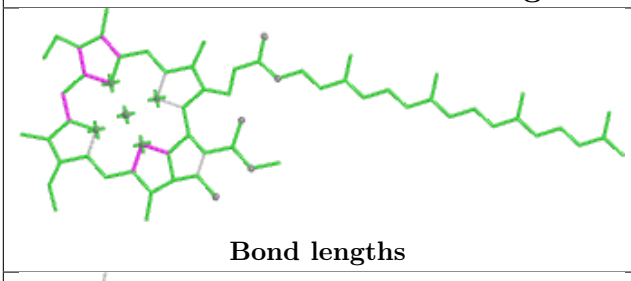


Torsions

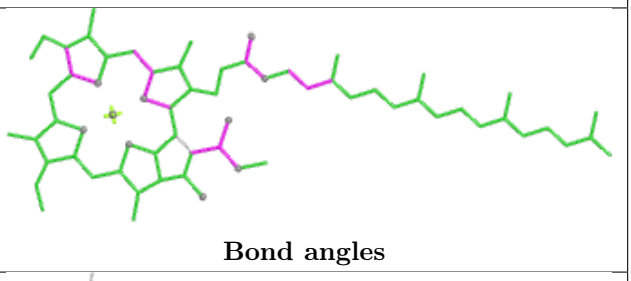


Rings

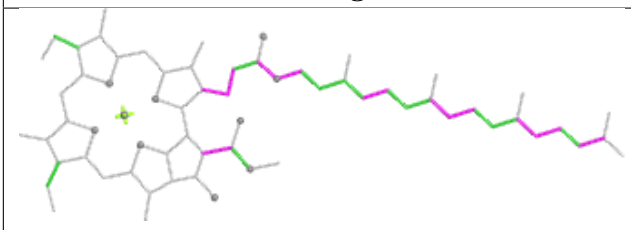
Ligand CLA A 314



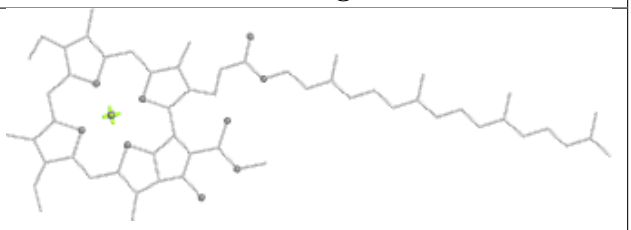
Bond lengths



Bond angles

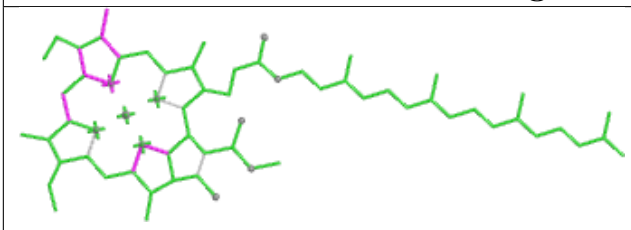


Torsions

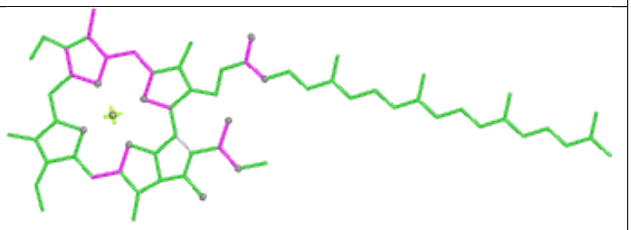


Rings

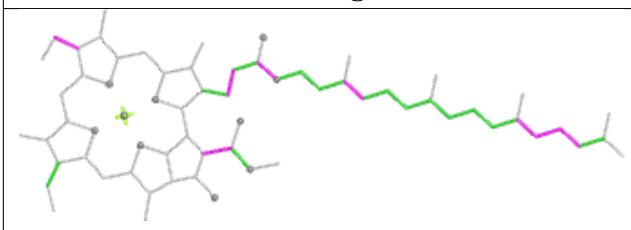
Ligand CLA a 835



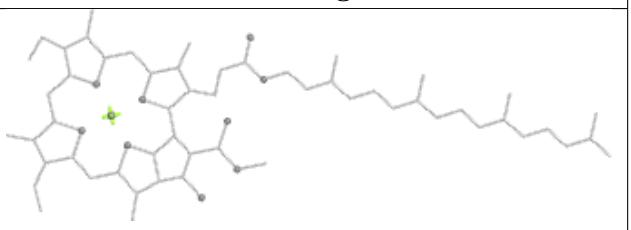
Bond lengths



Bond angles

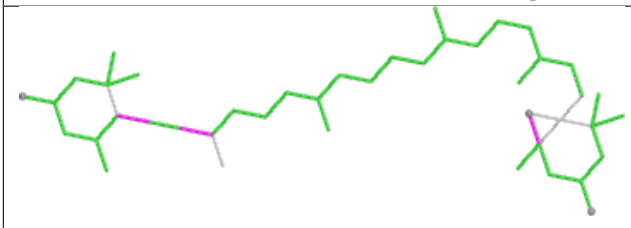


Torsions

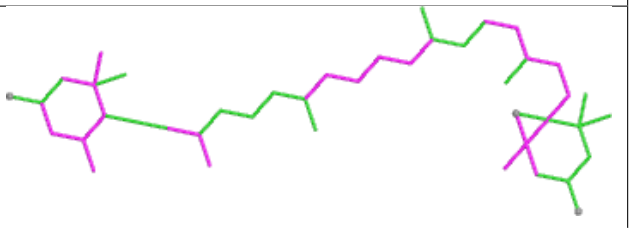


Rings

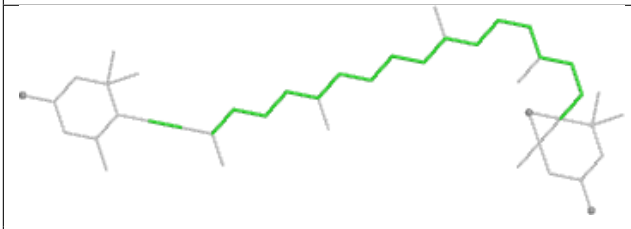
Ligand DD6 X 304



Bond lengths



Bond angles

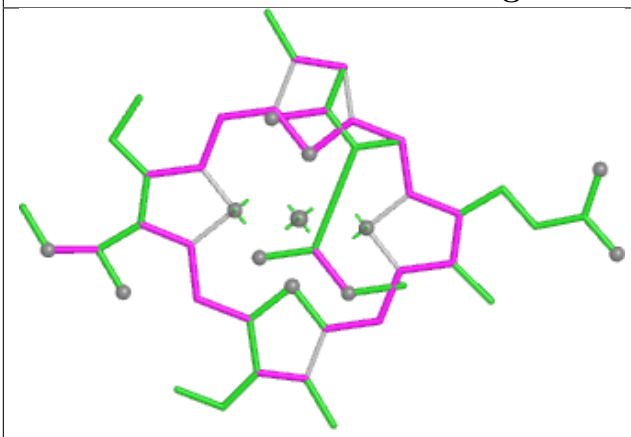


Torsions

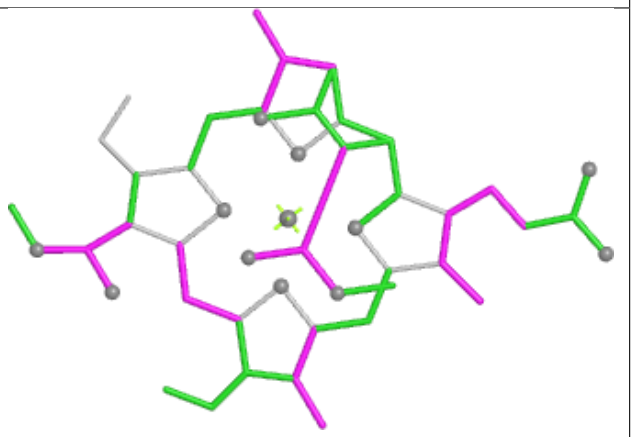


Rings

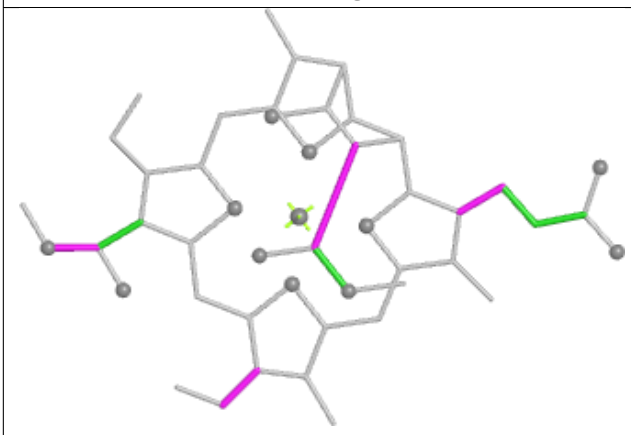
Ligand A1ECV Z 314



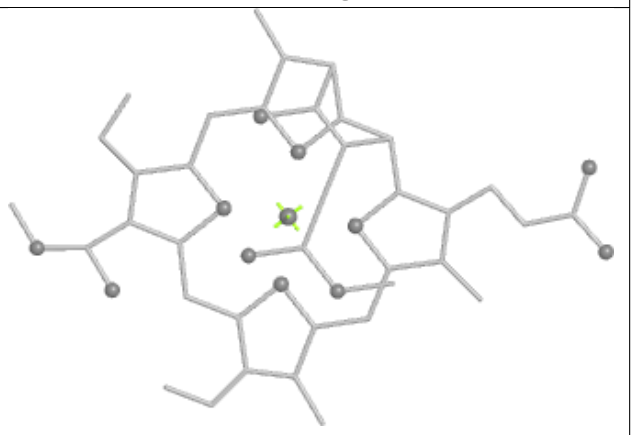
Bond lengths



Bond angles

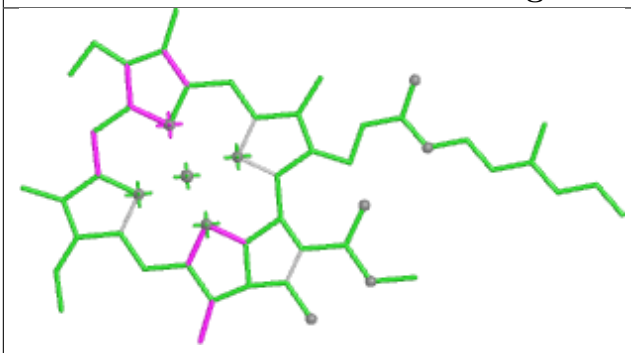


Torsions

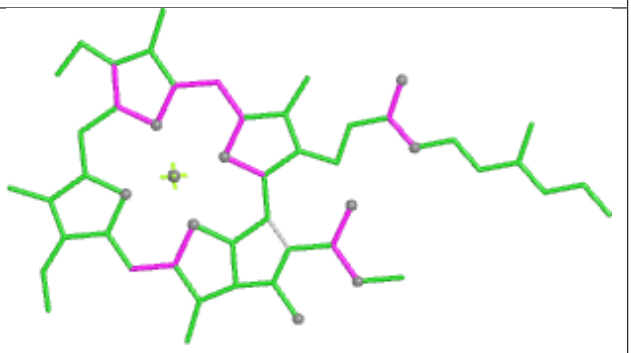


Rings

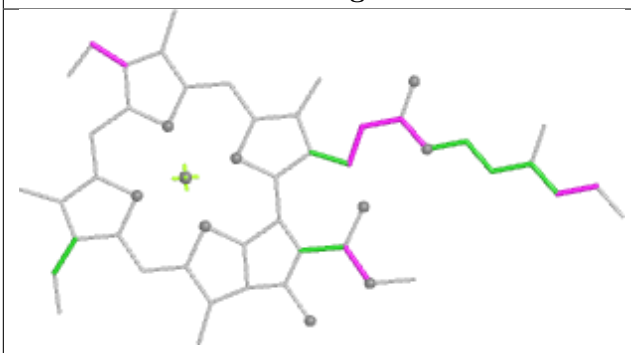
Ligand CLA L 311



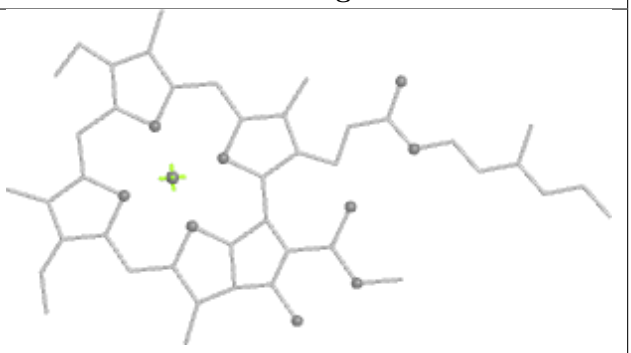
Bond lengths



Bond angles

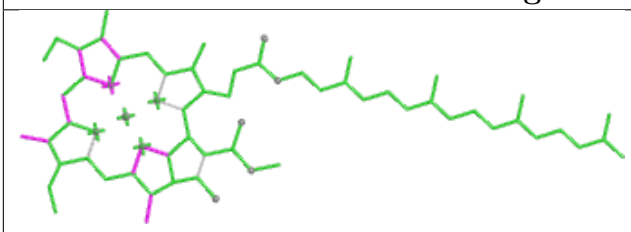


Torsions

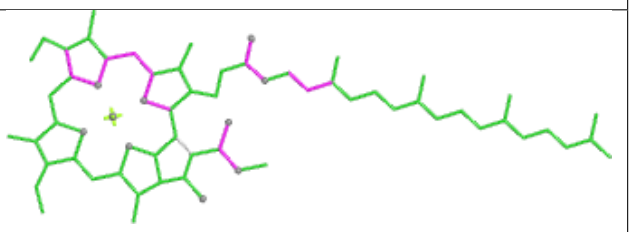


Rings

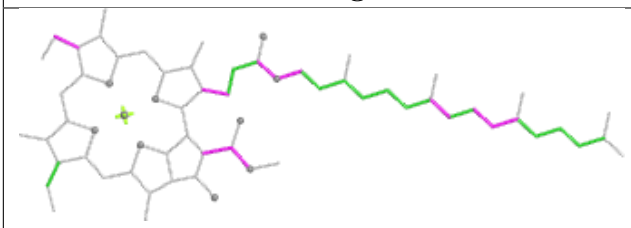
Ligand CLA A 312



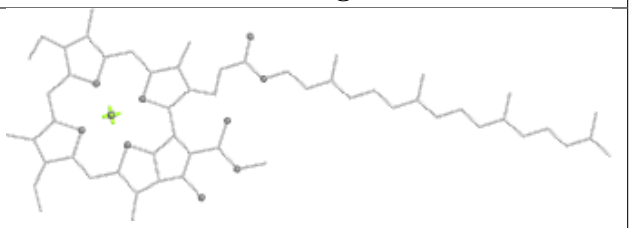
Bond lengths



Bond angles

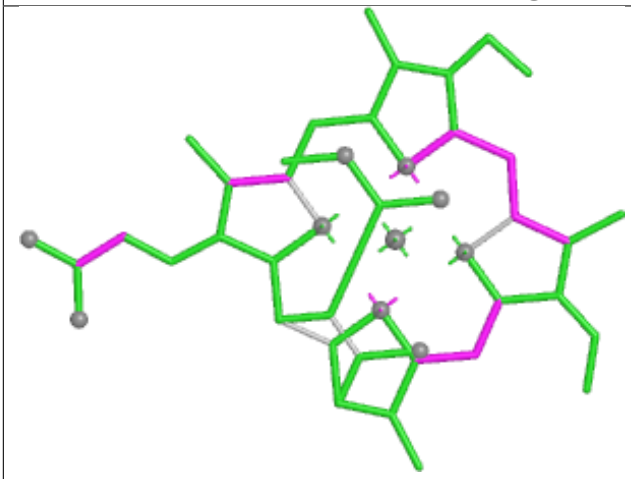


Torsions

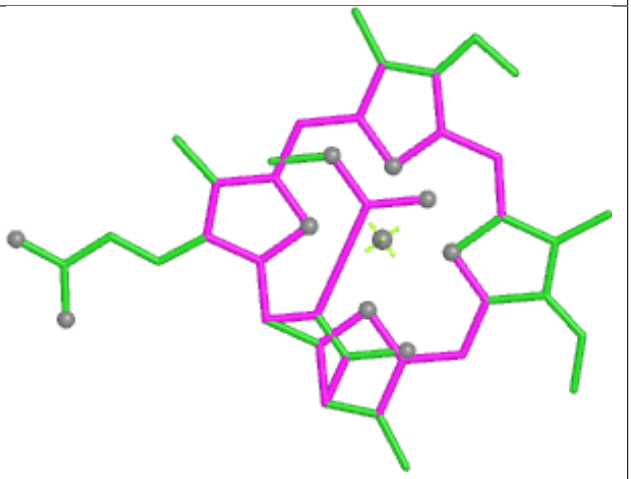


Rings

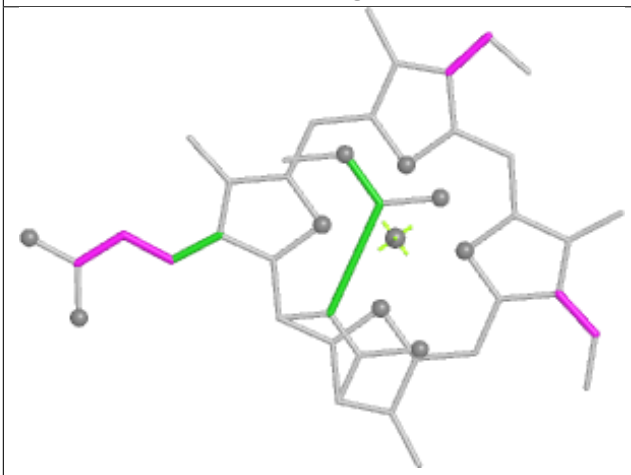
Ligand KC2 V 312



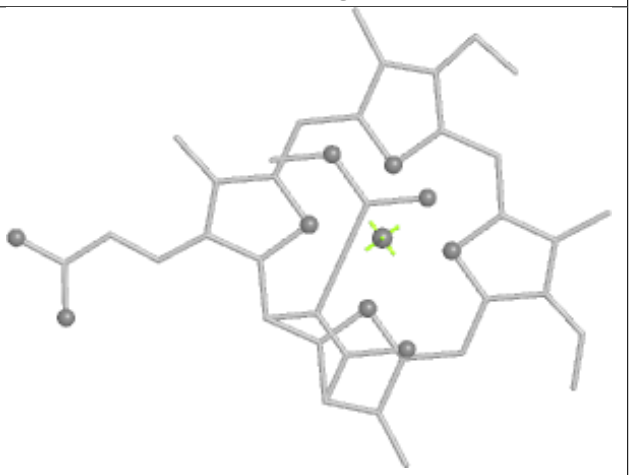
Bond lengths



Bond angles

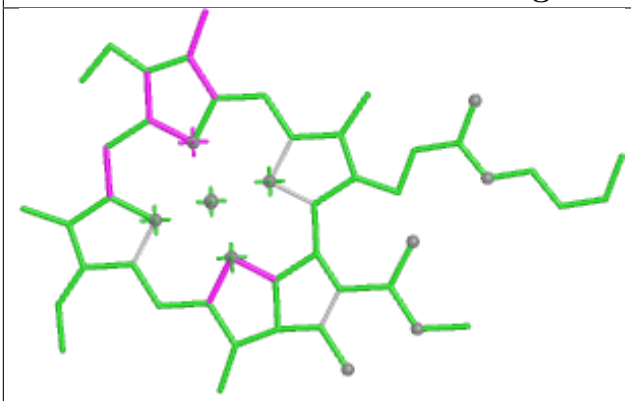


Torsions

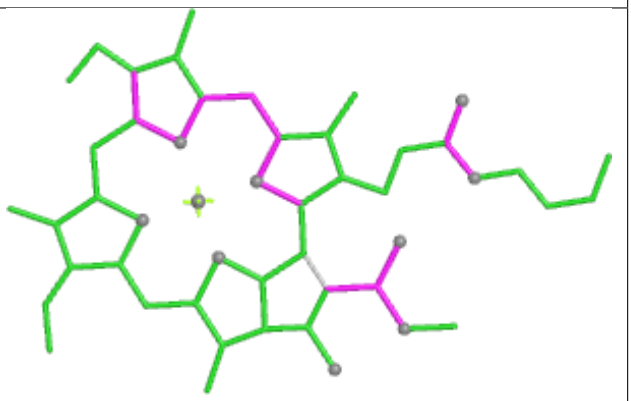


Rings

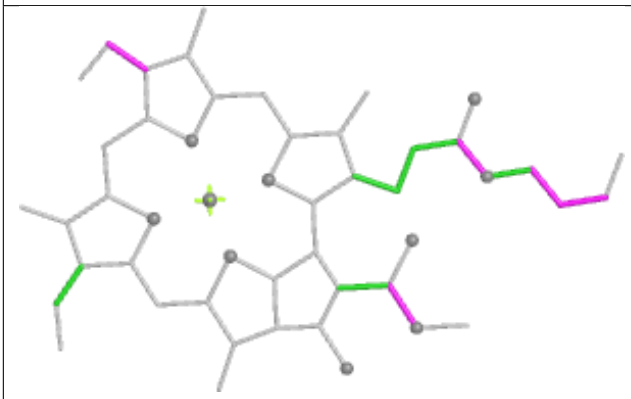
Ligand CLA l 203



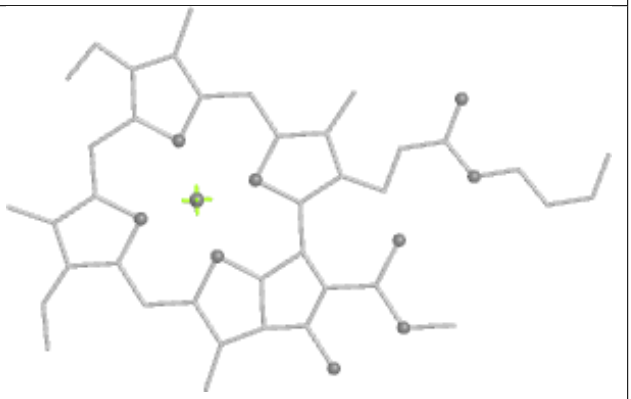
Bond lengths



Bond angles

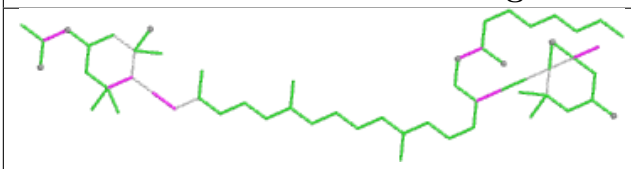


Torsions

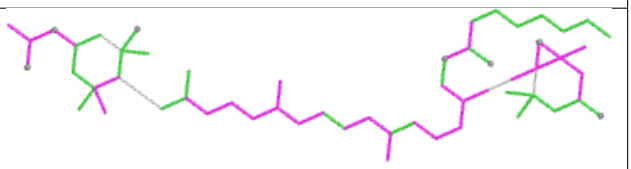


Rings

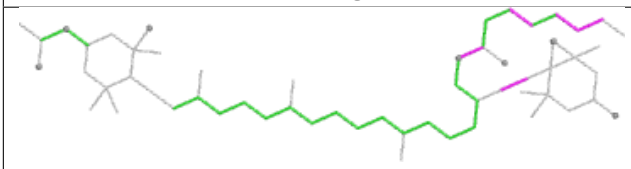
Ligand A1EB4 P 319



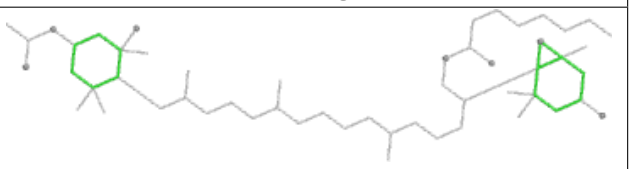
Bond lengths



Bond angles

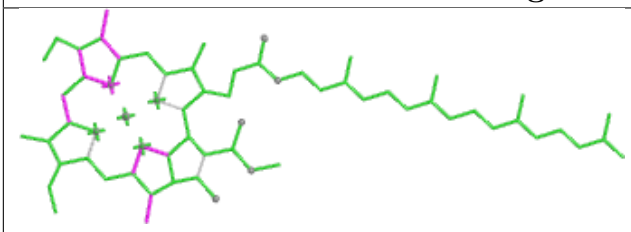


Torsions

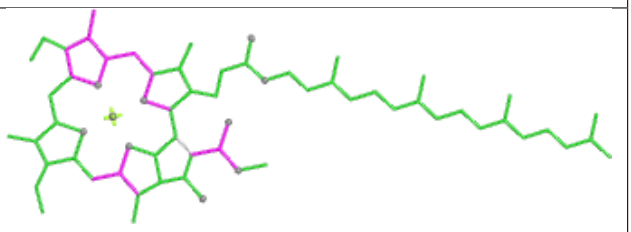


Rings

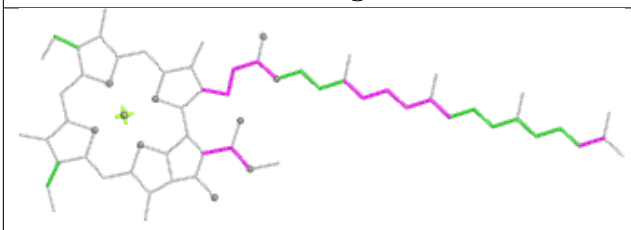
Ligand CLA S 309



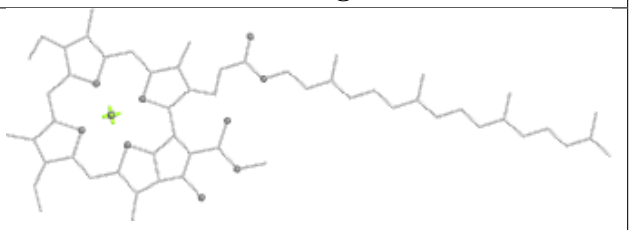
Bond lengths



Bond angles



Torsions

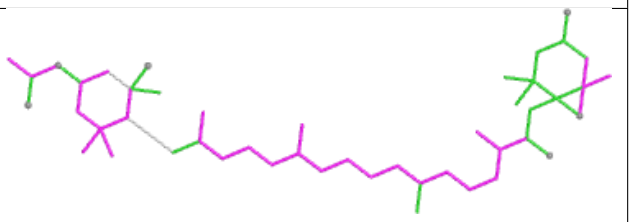


Rings

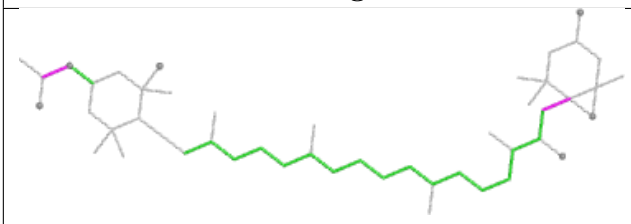
Ligand A86 W 303



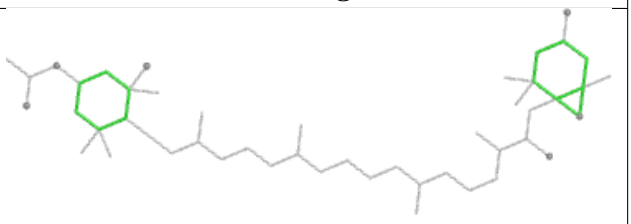
Bond lengths



Bond angles

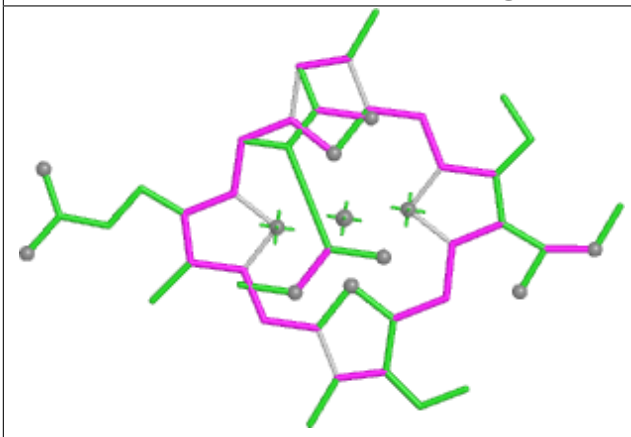


Torsions

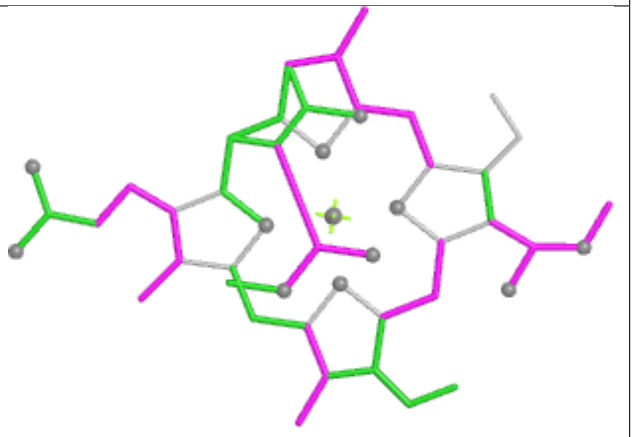


Rings

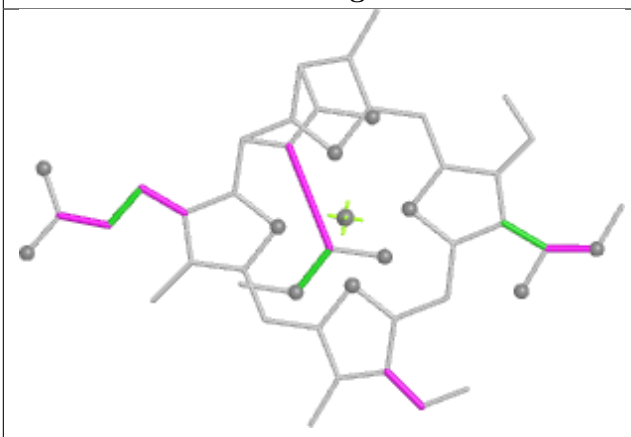
Ligand A1ECV Y 306



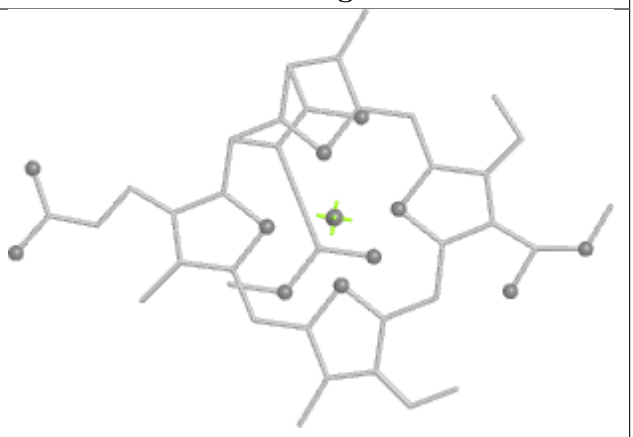
Bond lengths



Bond angles

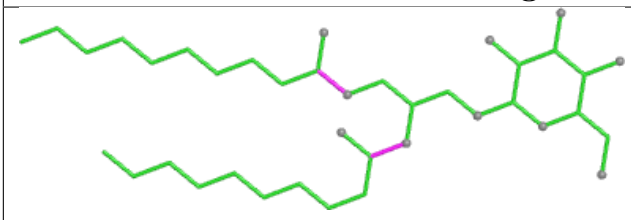


Torsions

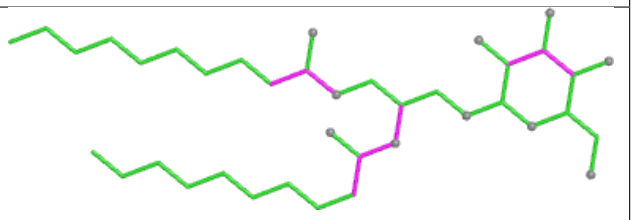


Rings

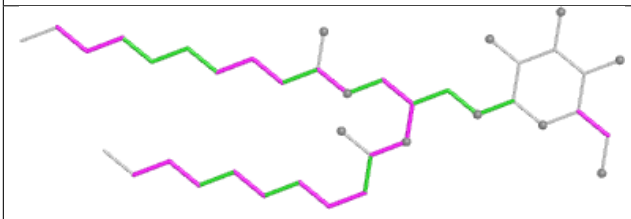
Ligand LMG P 317



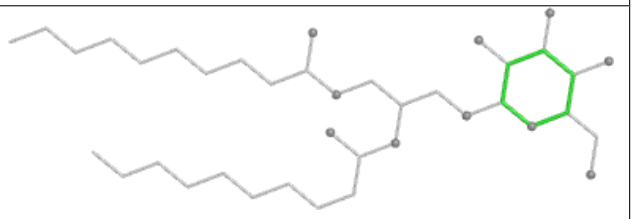
Bond lengths



Bond angles

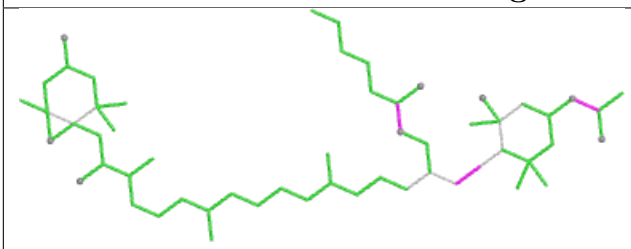


Torsions

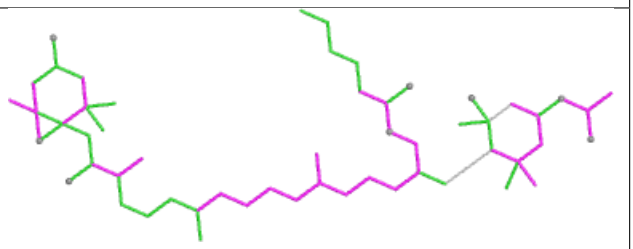


Rings

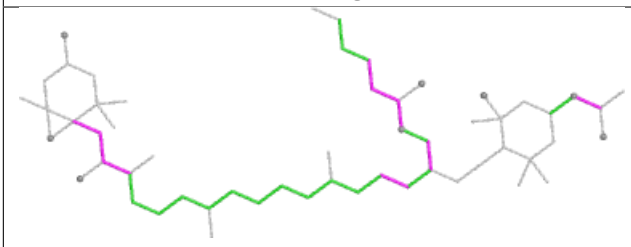
Ligand A1EB1 8 306



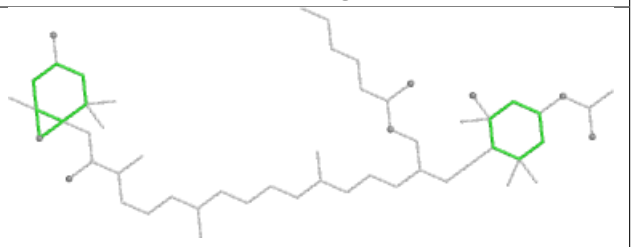
Bond lengths



Bond angles

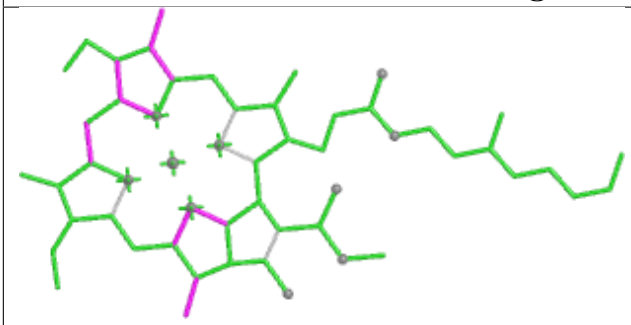


Torsions

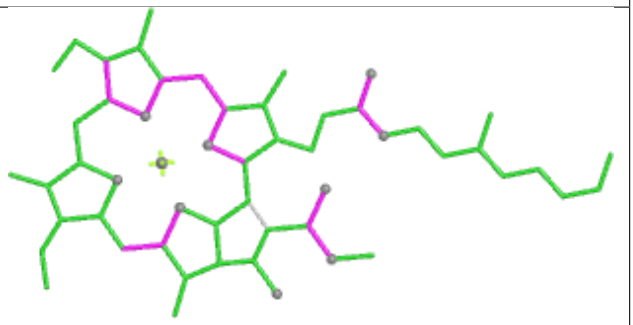


Rings

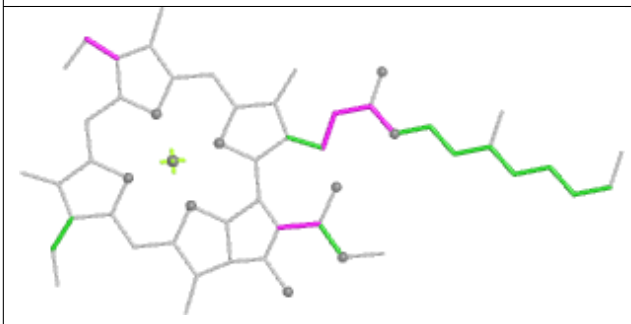
Ligand CLA a 810



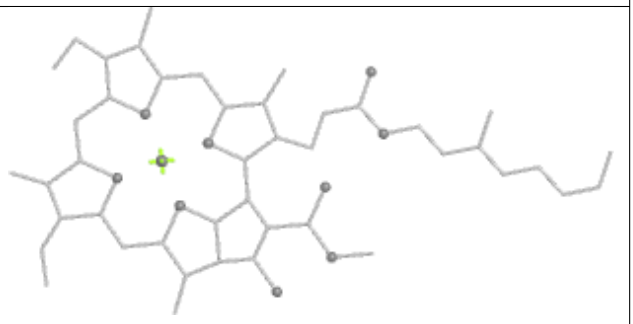
Bond lengths



Bond angles

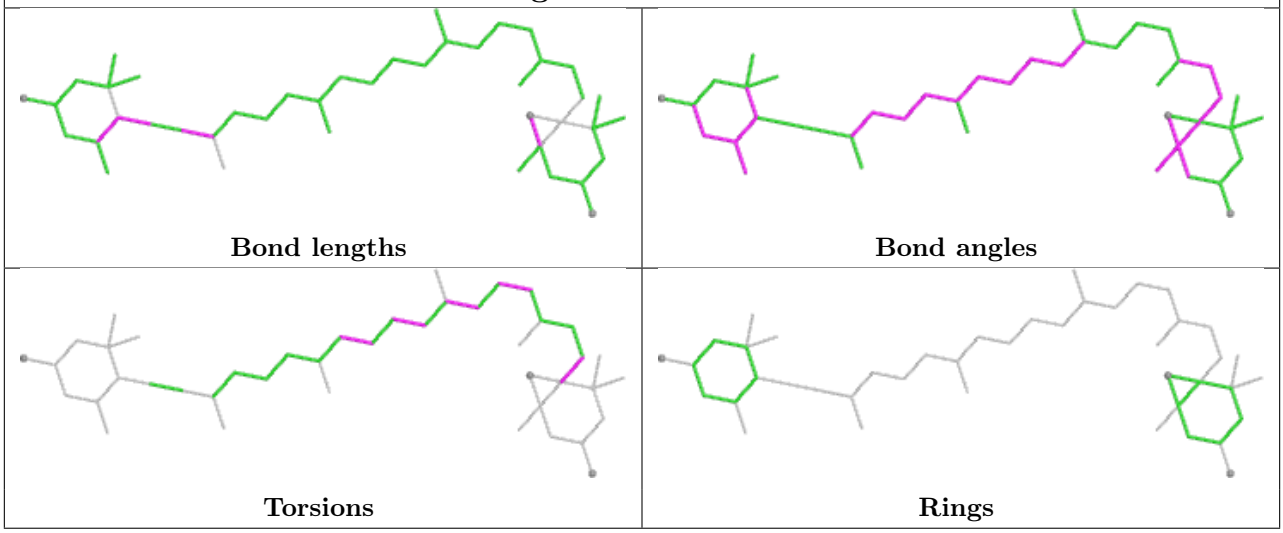


Torsions

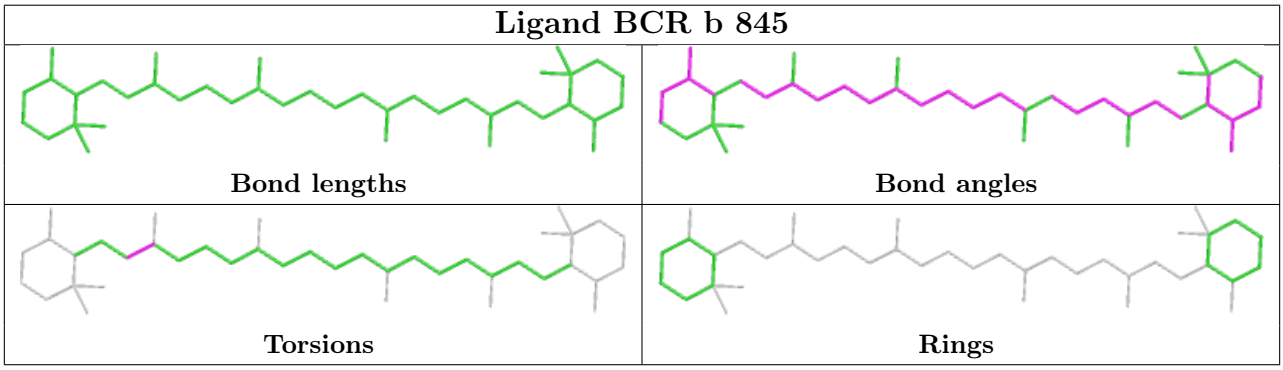


Rings

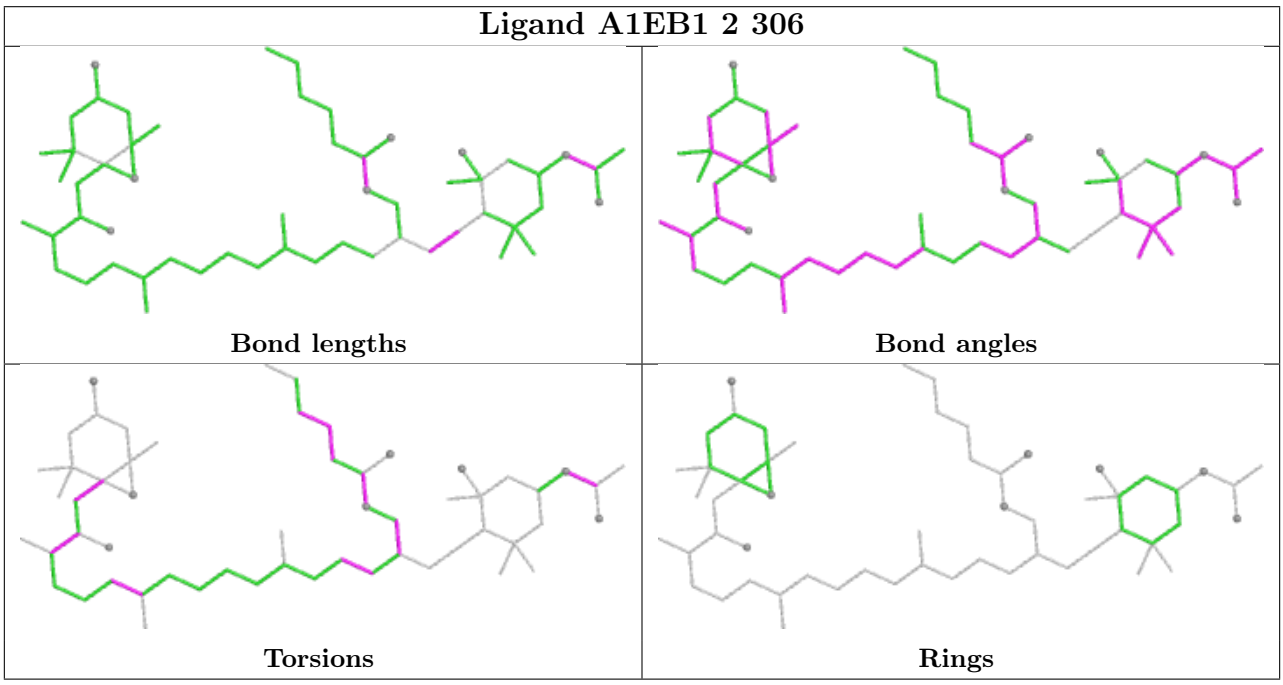
Ligand DD6 z 304



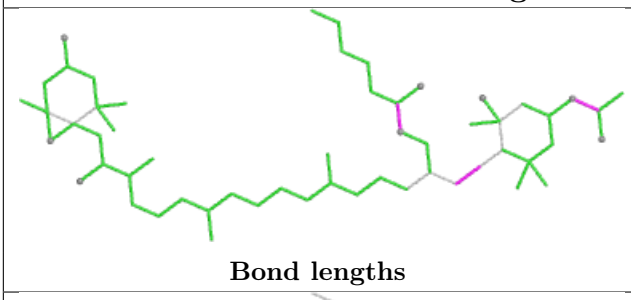
Ligand BCR b 845



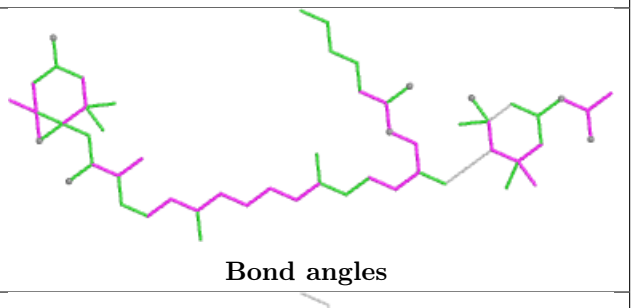
Ligand A1EB1 2 306



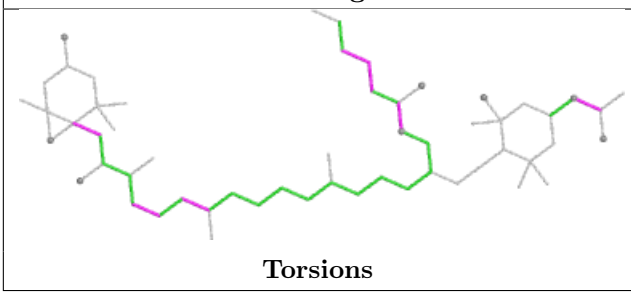
Ligand A1EB1 8 304



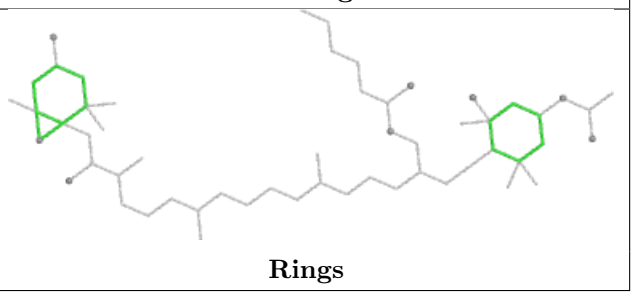
Bond lengths



Bond angles

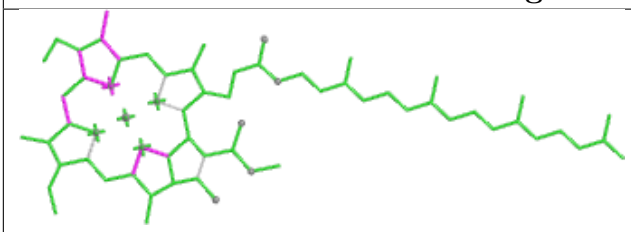


Torsions

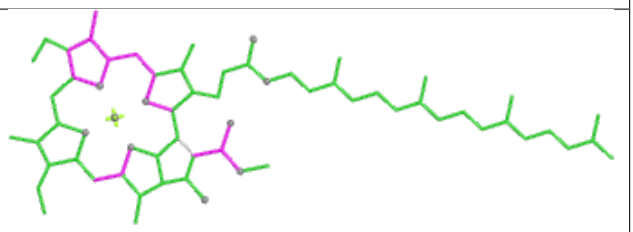


Rings

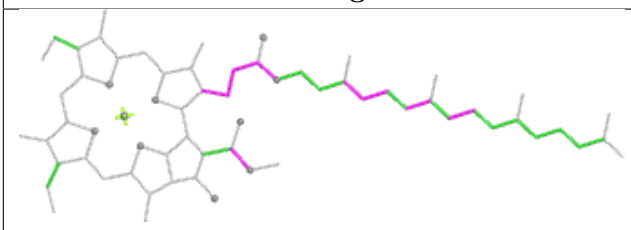
Ligand CLA E 313



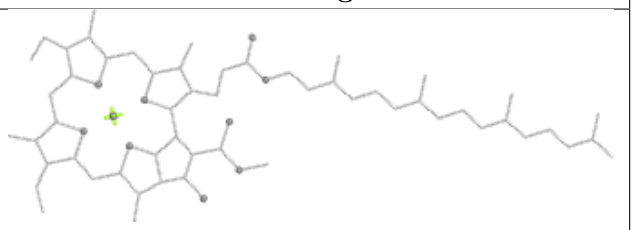
Bond lengths



Bond angles

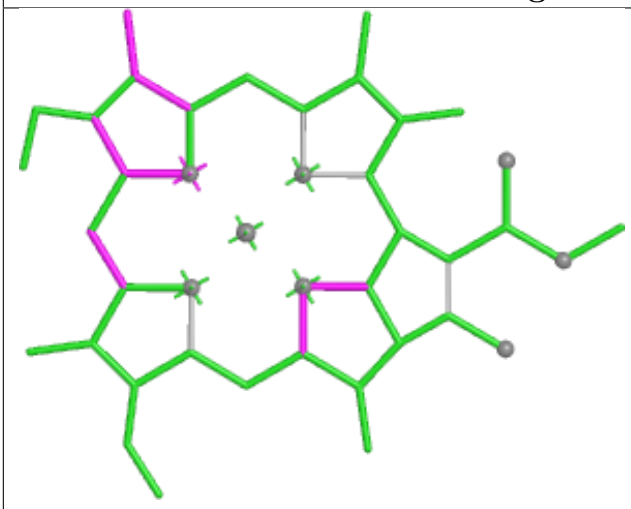


Torsions

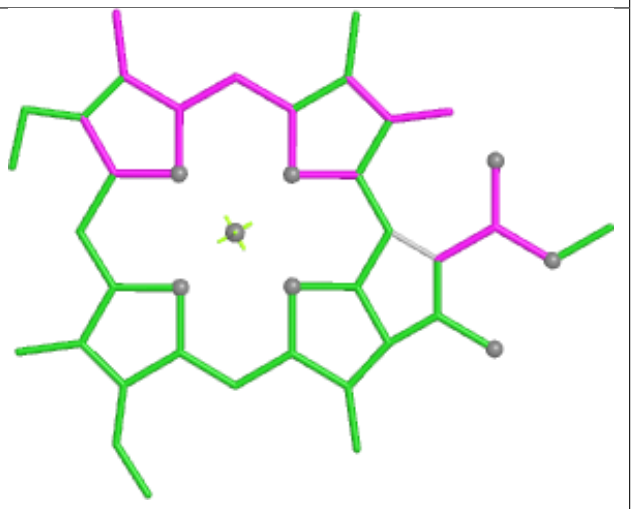


Rings

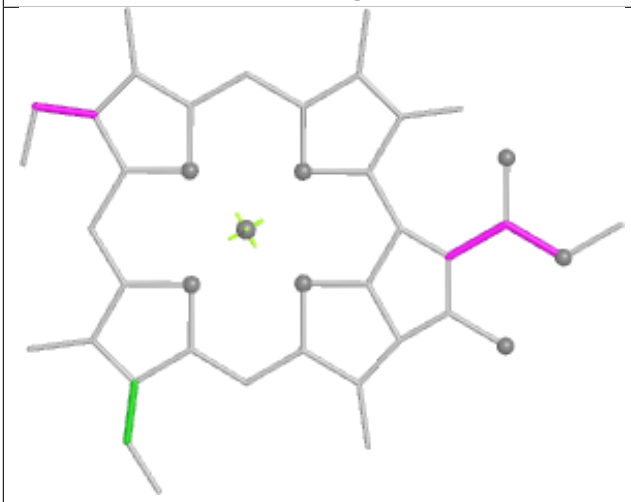
Ligand CLA 7 324



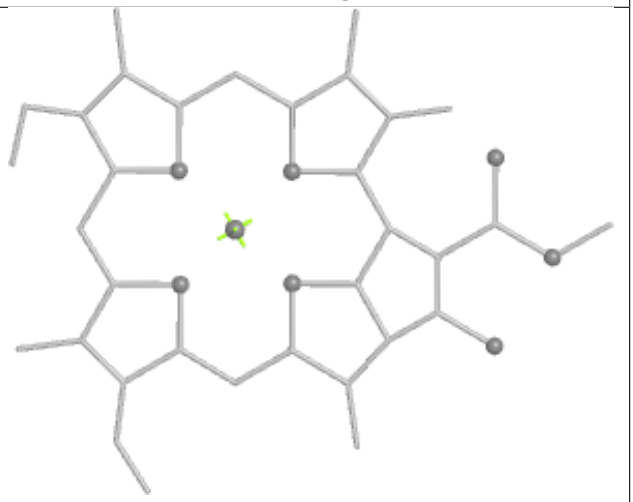
Bond lengths



Bond angles

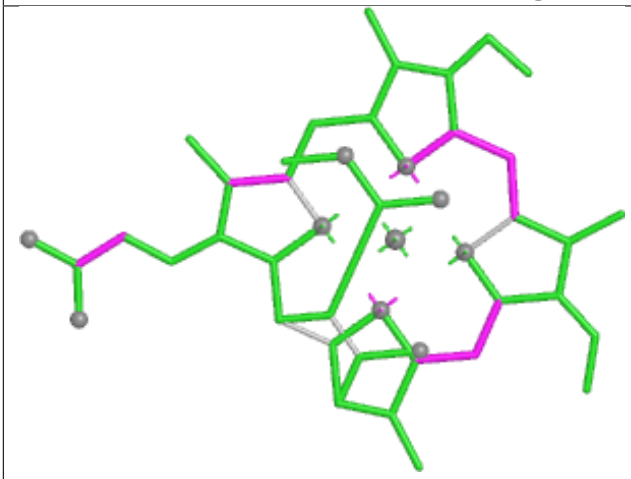


Torsions

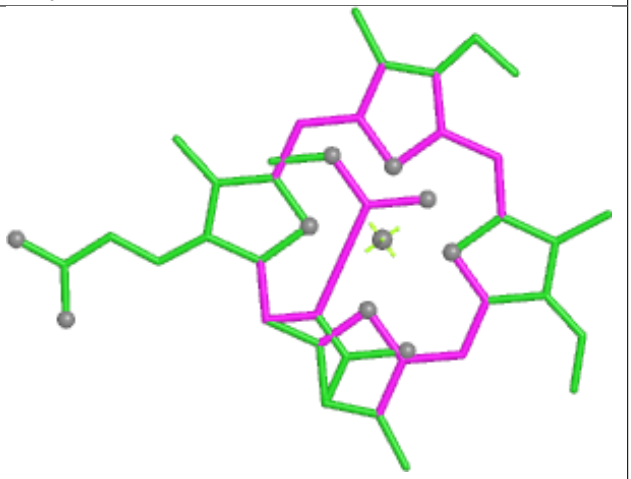


Rings

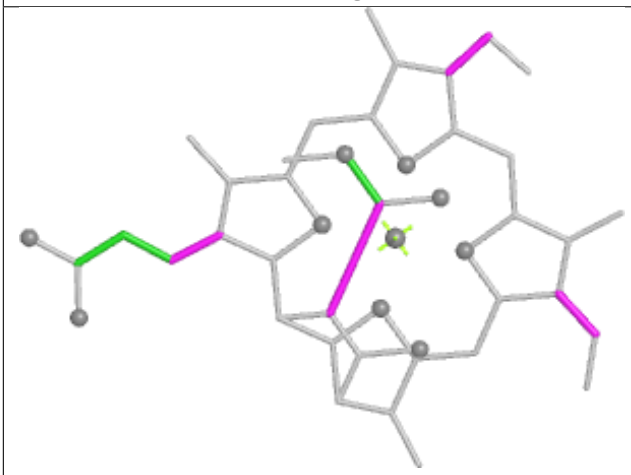
Ligand KC2 y 314



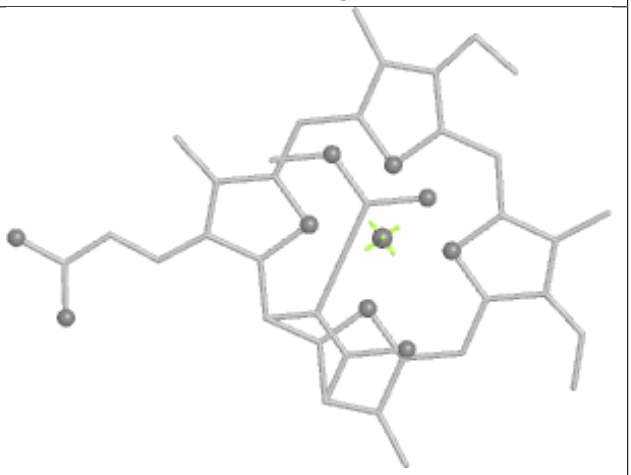
Bond lengths



Bond angles

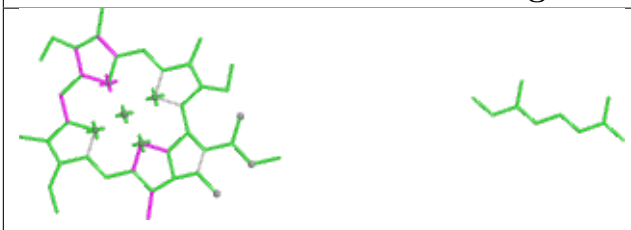


Torsions

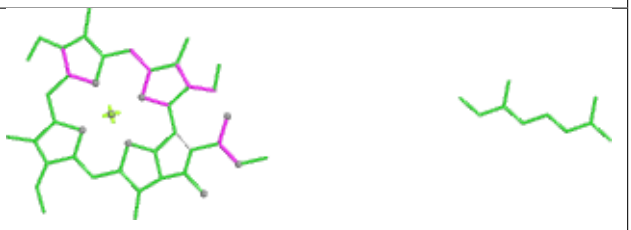


Rings

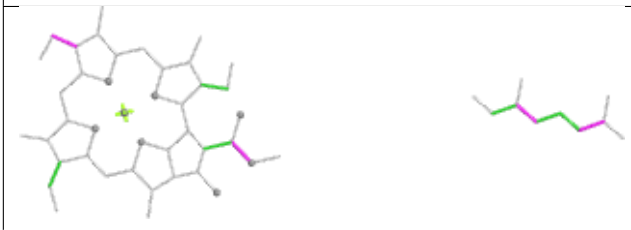
Ligand CLA 6 312



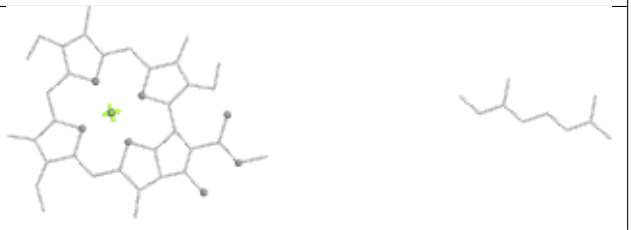
Bond lengths



Bond angles

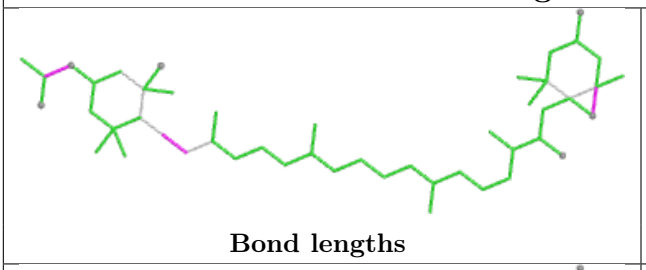


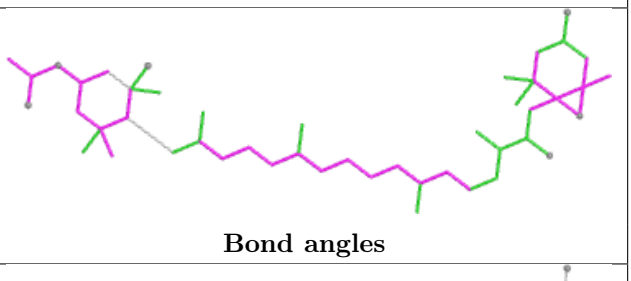
Torsions

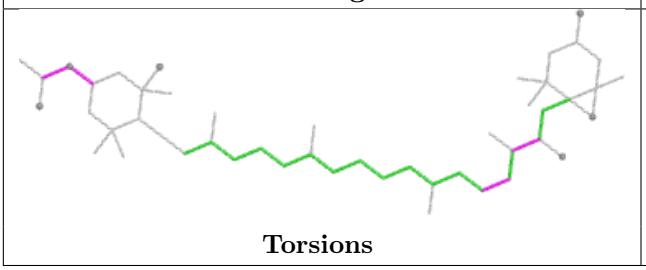


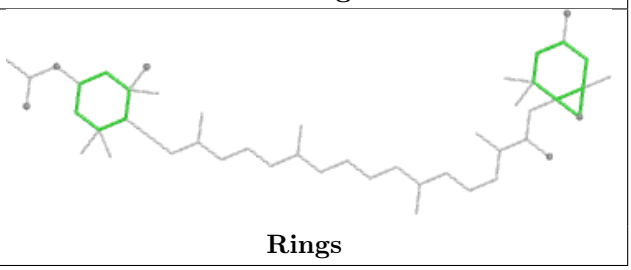
Rings

Ligand A86 8 302

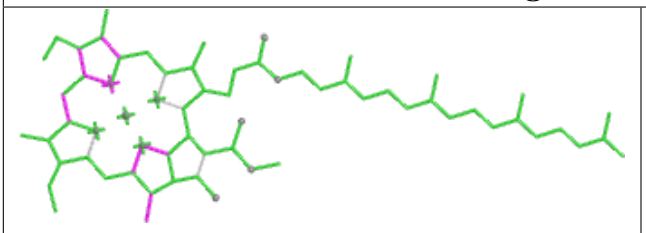

Bond lengths

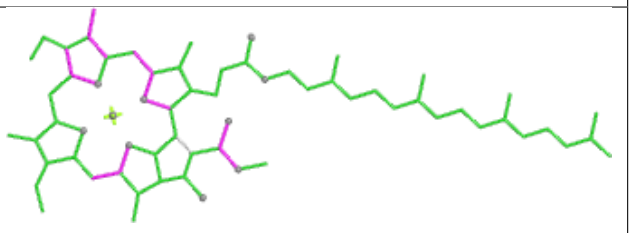

Bond angles

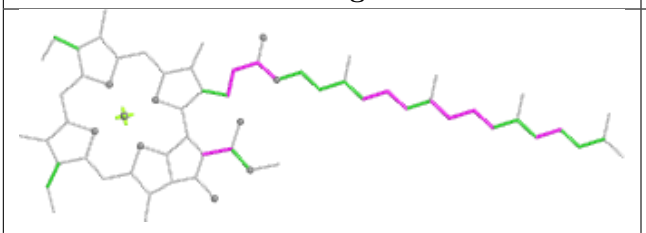

Torsions

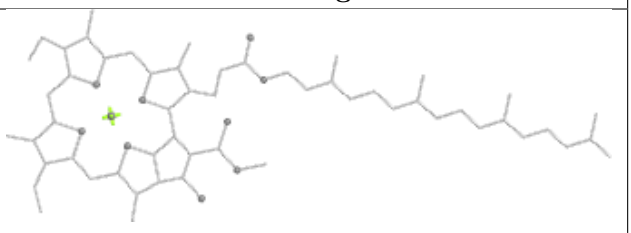

Rings

Ligand CLA C 307

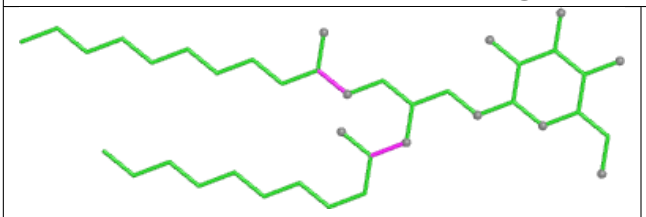

Bond lengths

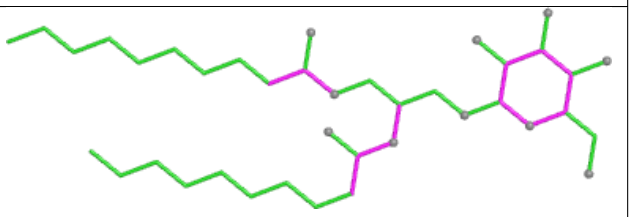

Bond angles

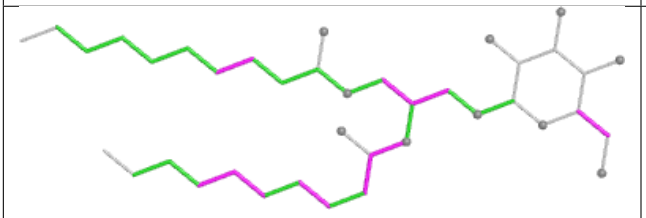

Torsions

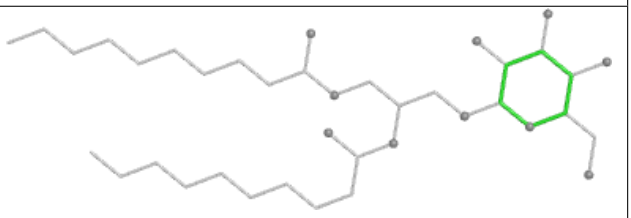

Rings

Ligand LMG M 319

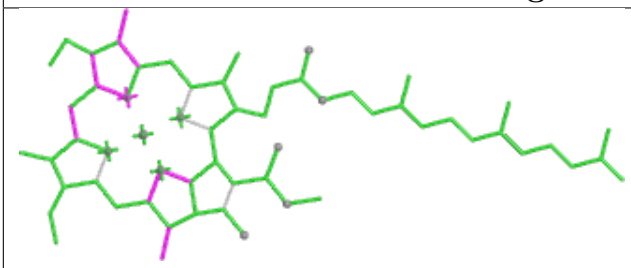

Bond lengths


Bond angles

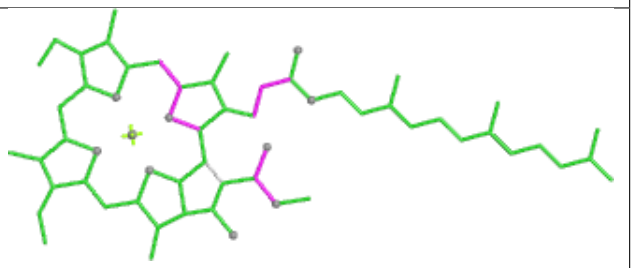

Torsions


Rings

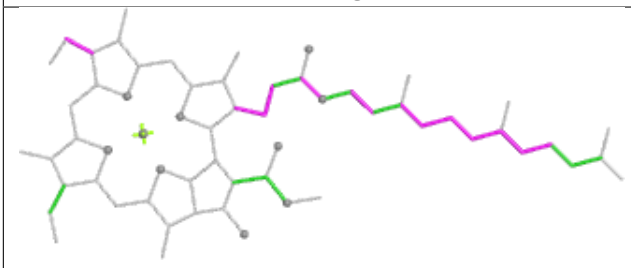
Ligand CLA b 820



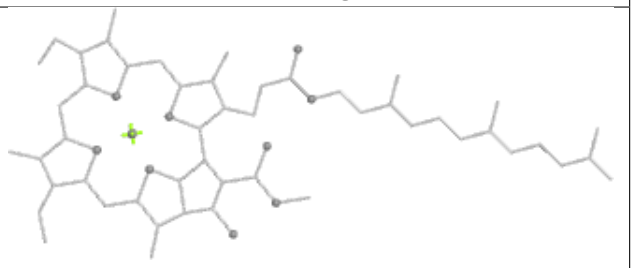
Bond lengths



Bond angles

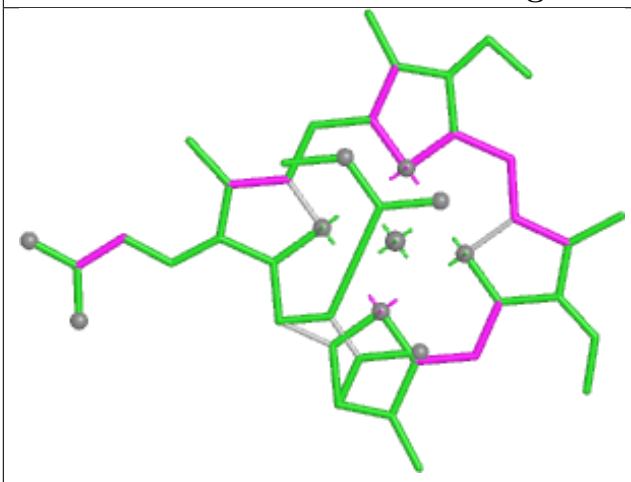


Torsions

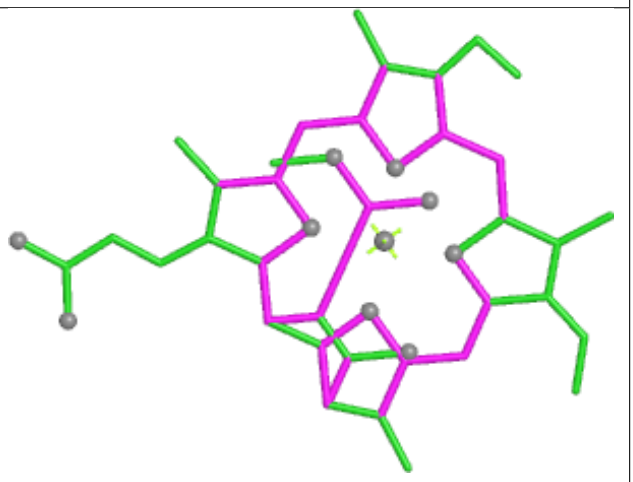


Rings

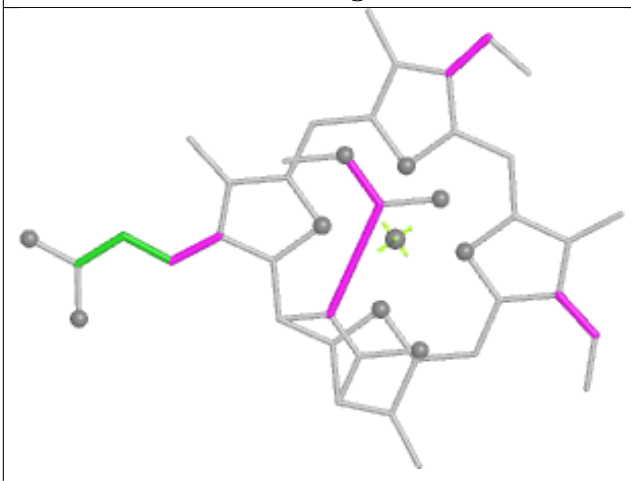
Ligand KC2 P 306



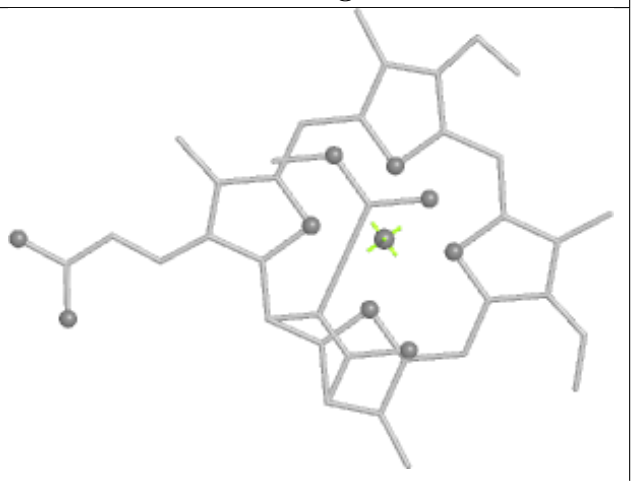
Bond lengths



Bond angles

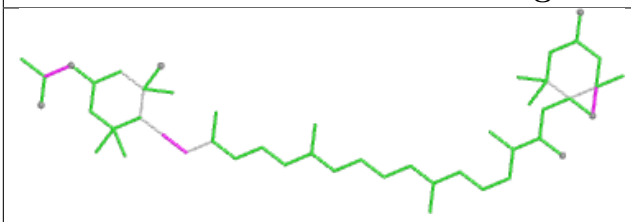


Torsions

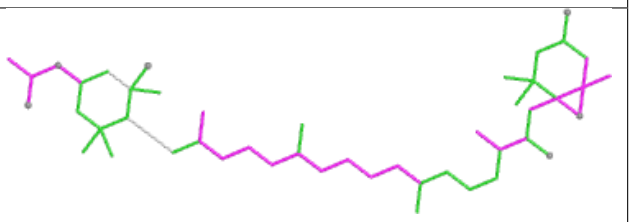


Rings

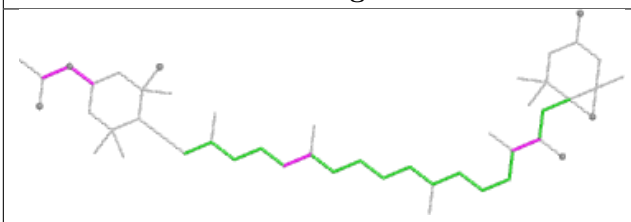
Ligand A86 9 301



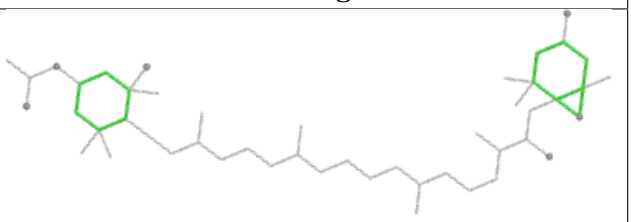
Bond lengths



Bond angles

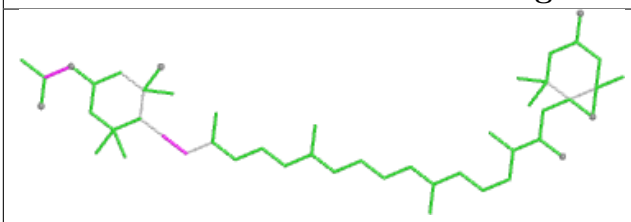


Torsions

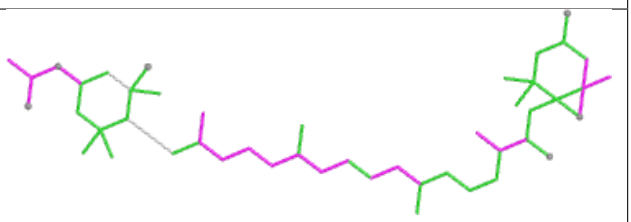


Rings

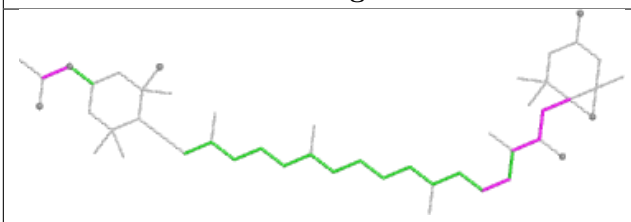
Ligand A86 z 303



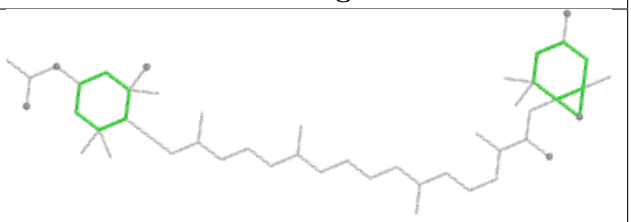
Bond lengths



Bond angles

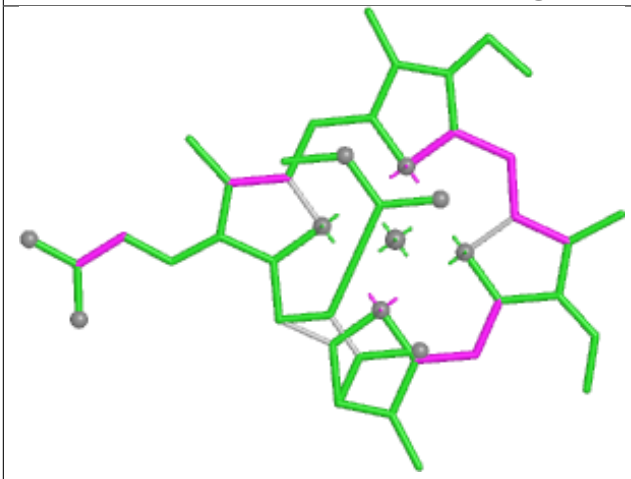


Torsions

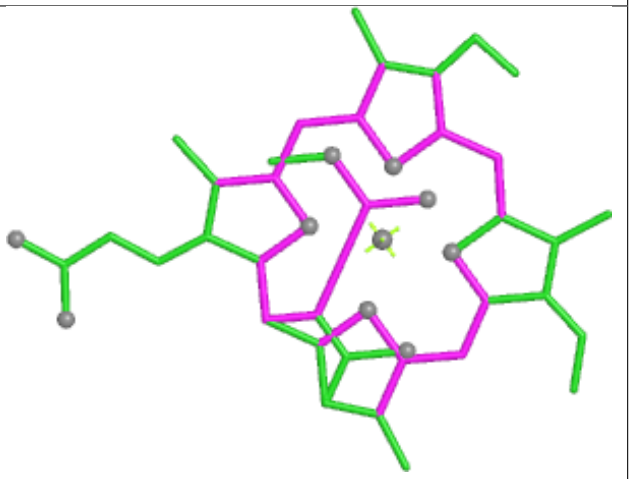


Rings

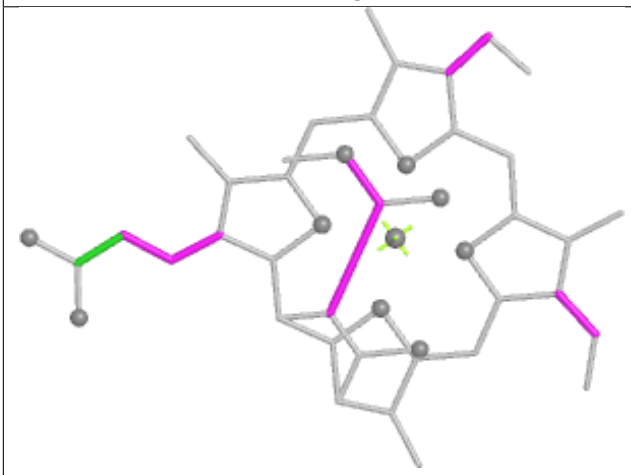
Ligand KC2 8 316



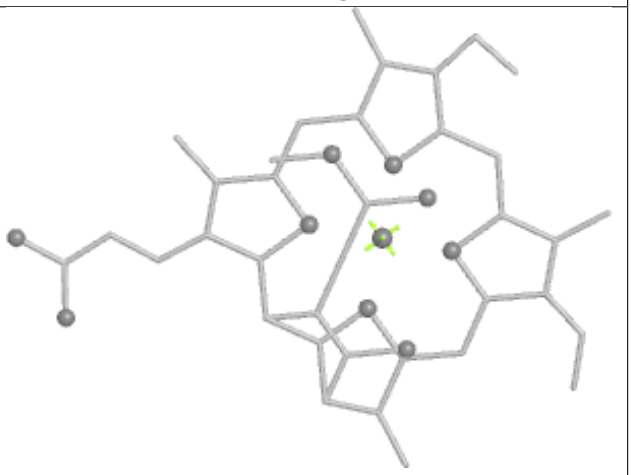
Bond lengths



Bond angles

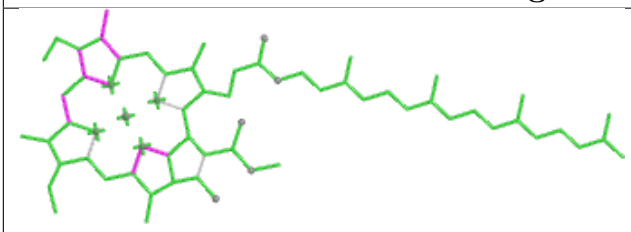


Torsions

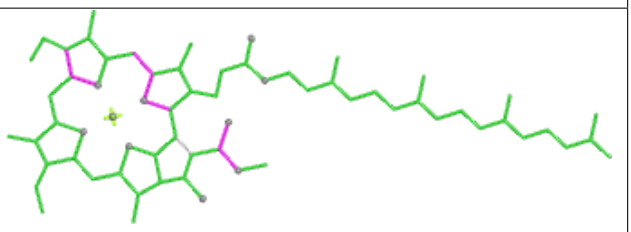


Rings

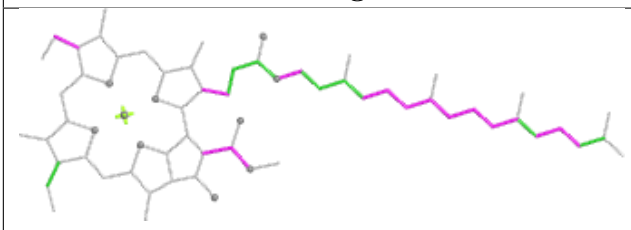
Ligand CLA a 830



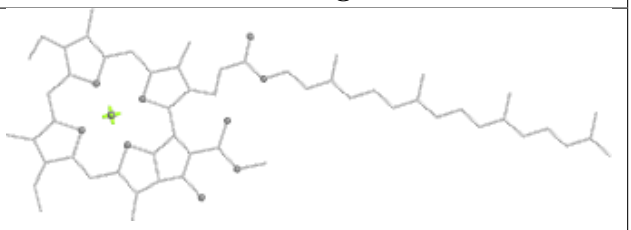
Bond lengths



Bond angles

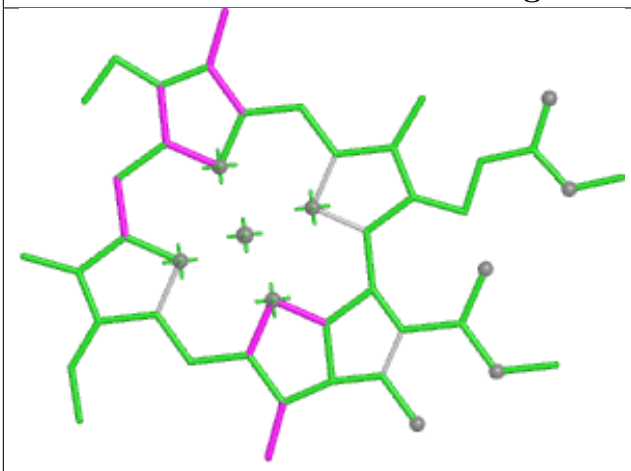


Torsions

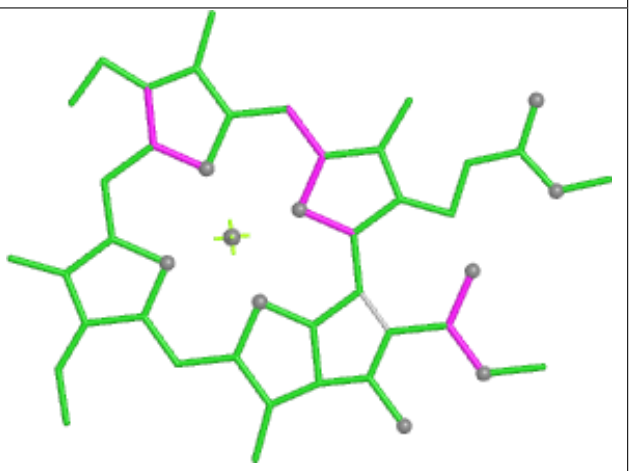


Rings

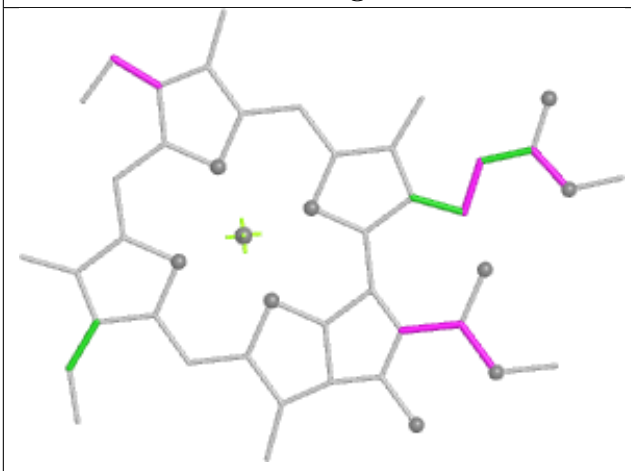
Ligand CLA H 316



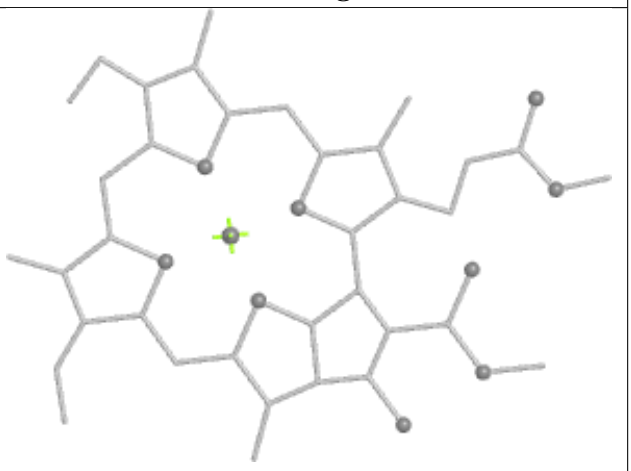
Bond lengths



Bond angles

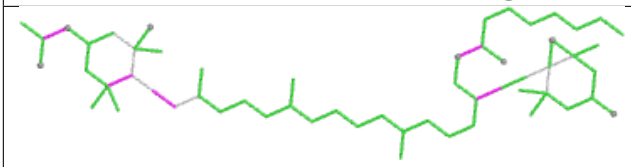


Torsions

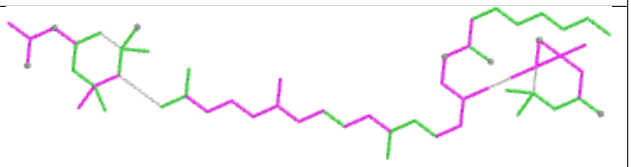


Rings

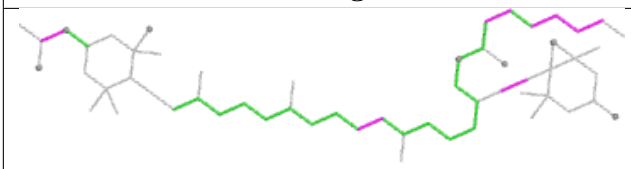
Ligand A1EB4 W 321



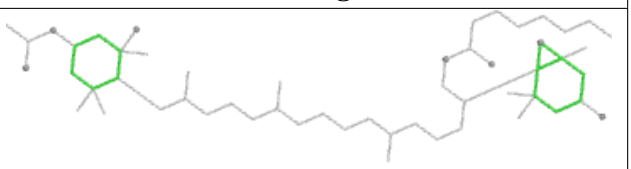
Bond lengths



Bond angles

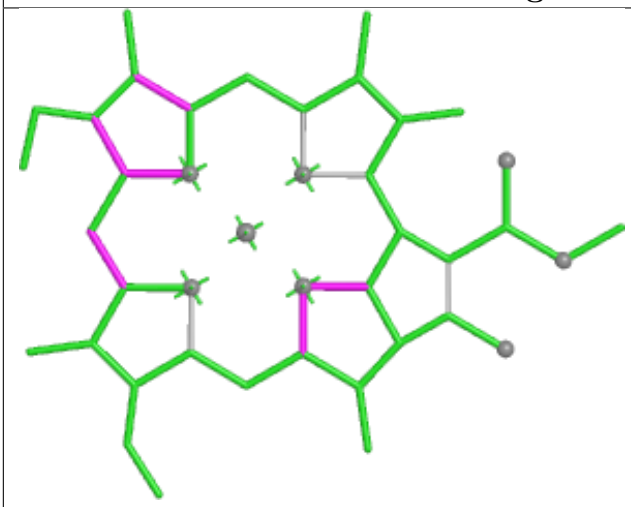


Torsions

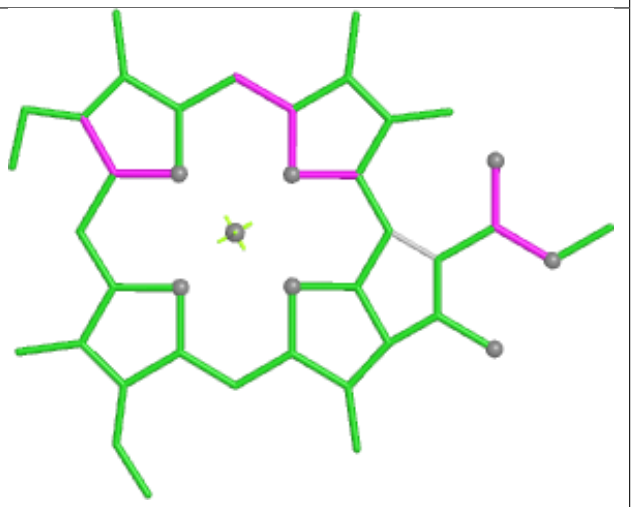


Rings

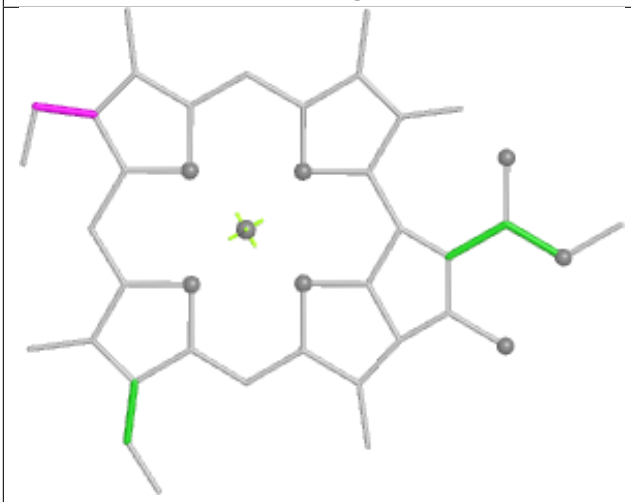
Ligand CLA Z 309



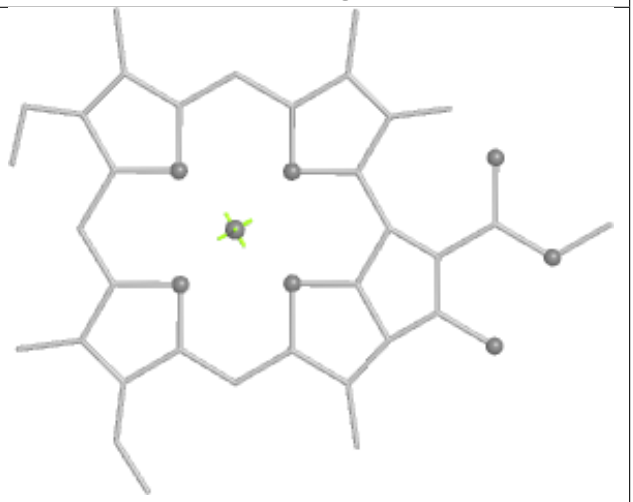
Bond lengths



Bond angles

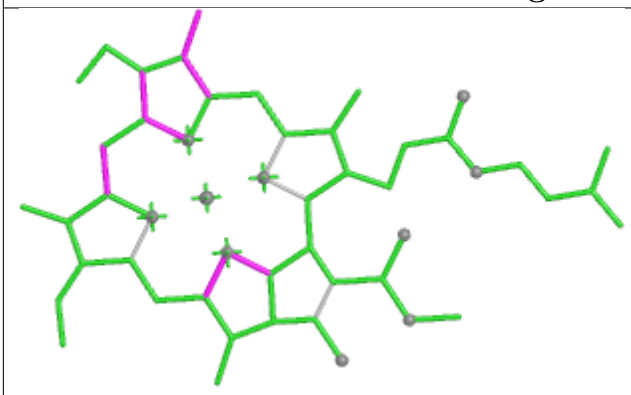


Torsions

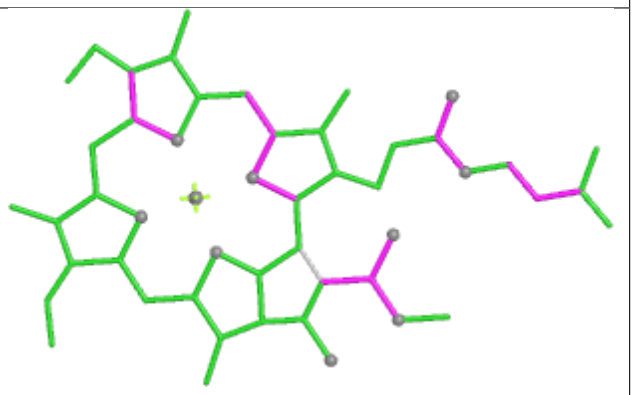


Rings

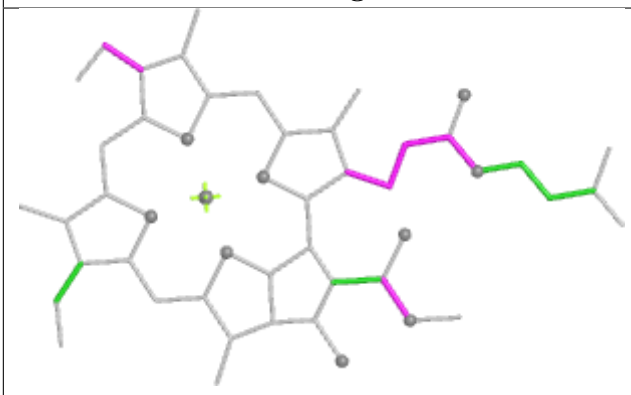
Ligand CLA 7 325



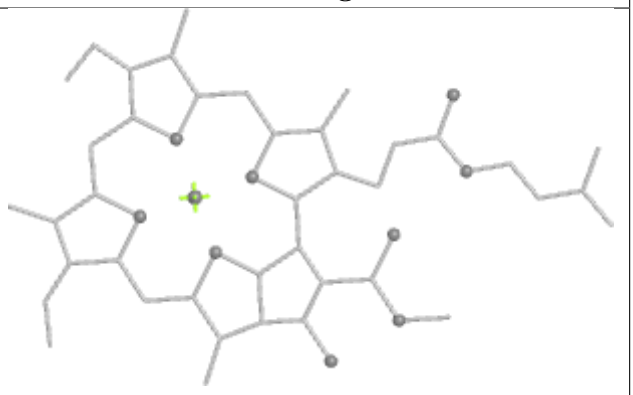
Bond lengths



Bond angles

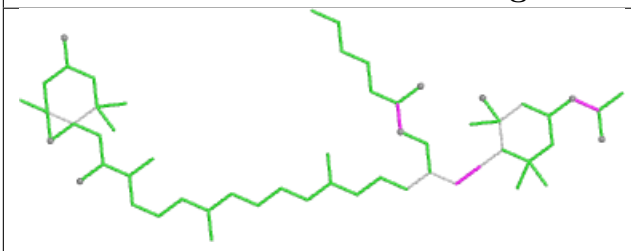


Torsions

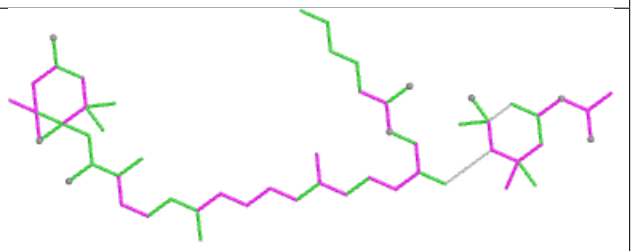


Rings

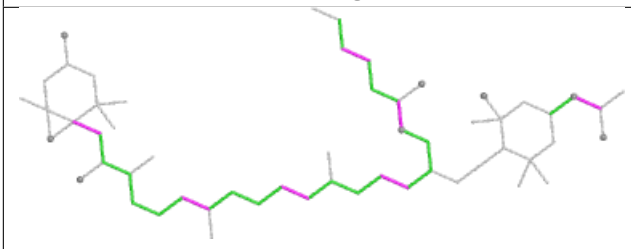
Ligand A1EB1 0 303



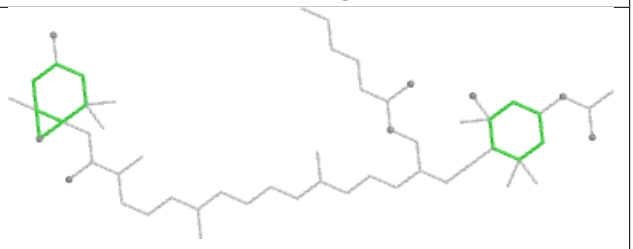
Bond lengths



Bond angles

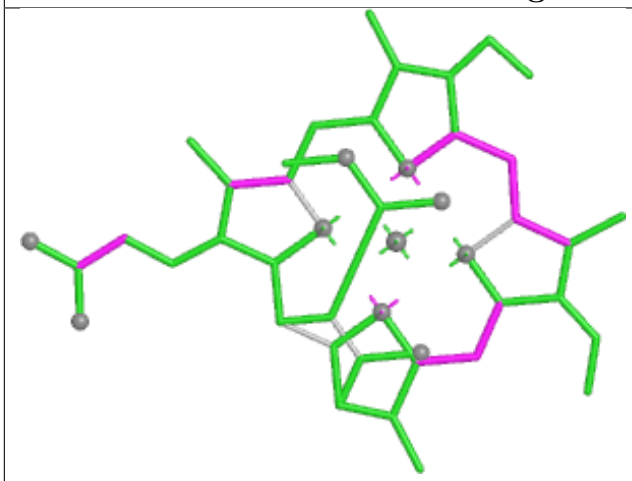


Torsions

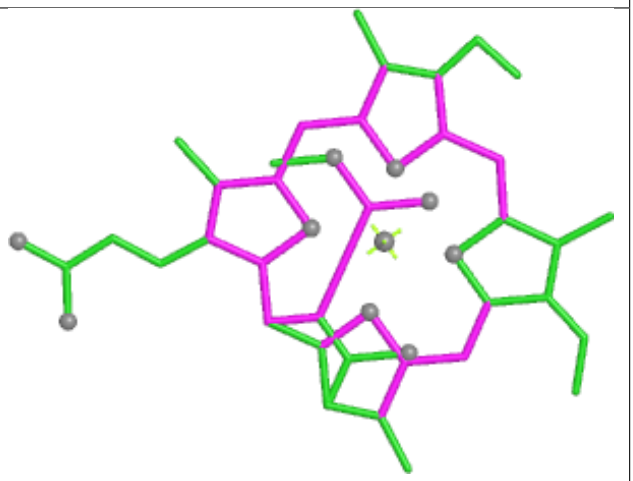


Rings

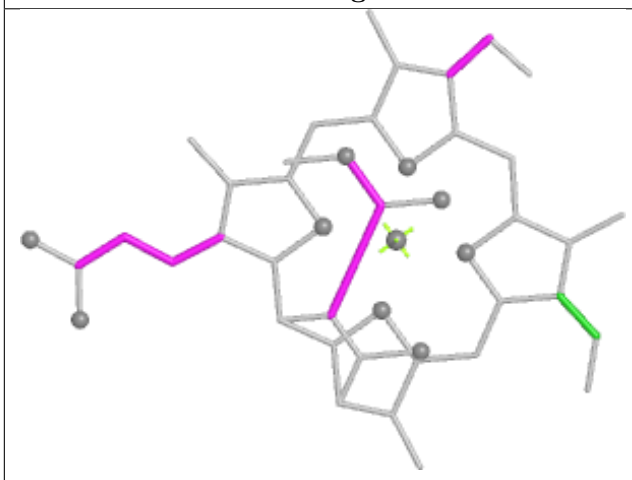
Ligand KC2 T 312



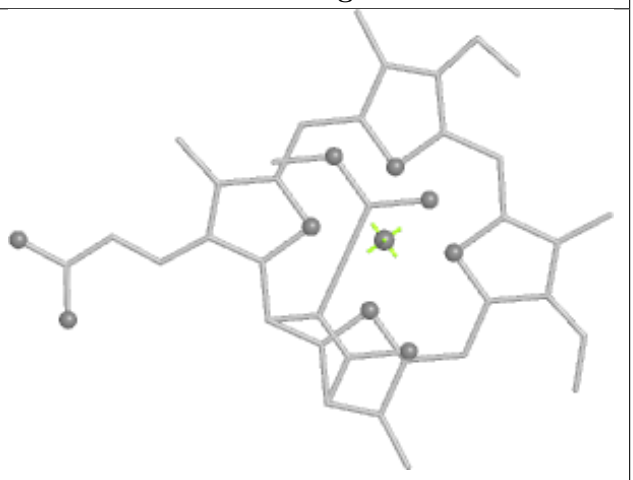
Bond lengths



Bond angles

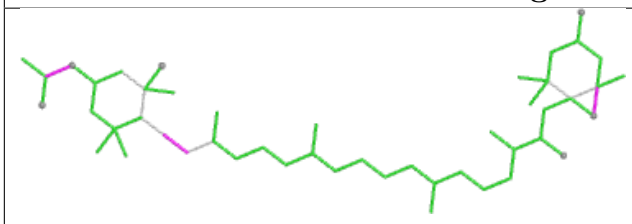


Torsions



Rings

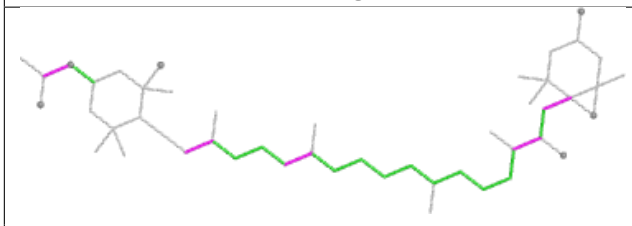
Ligand A86 D 305



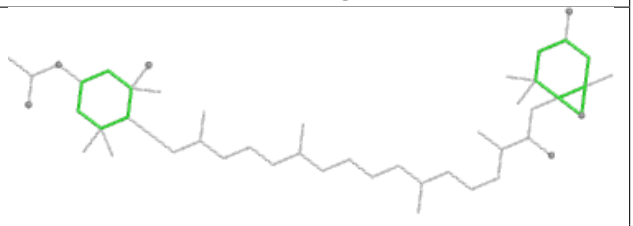
Bond lengths



Bond angles

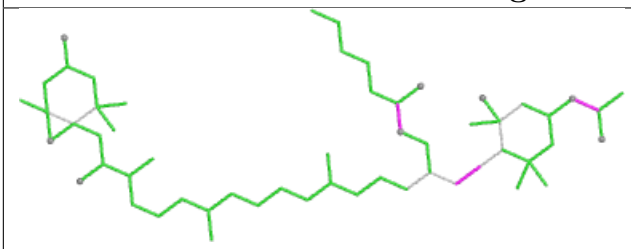


Torsions

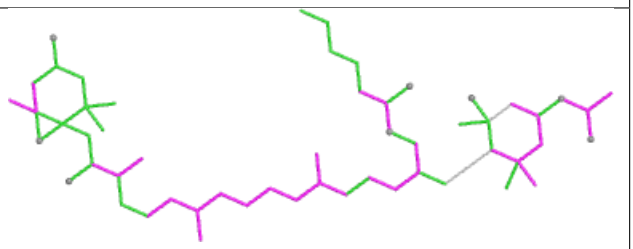


Rings

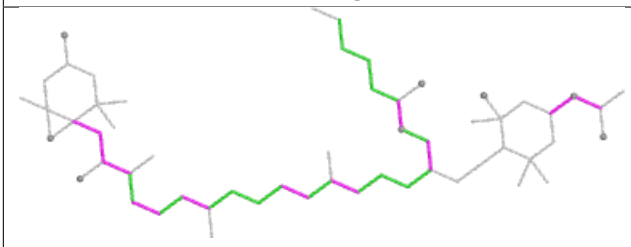
Ligand A1EB1 3 324



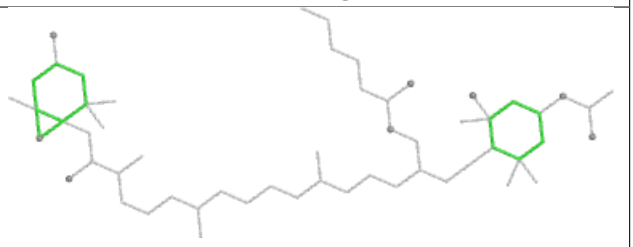
Bond lengths



Bond angles

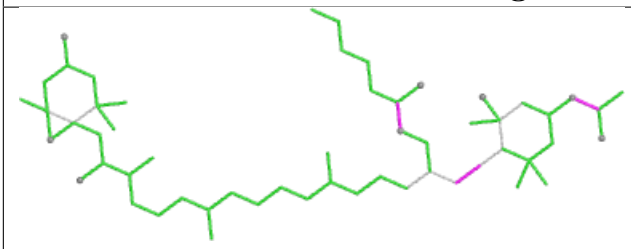


Torsions

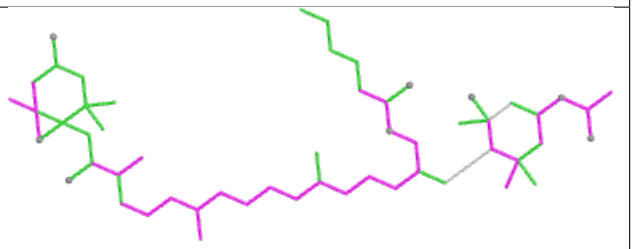


Rings

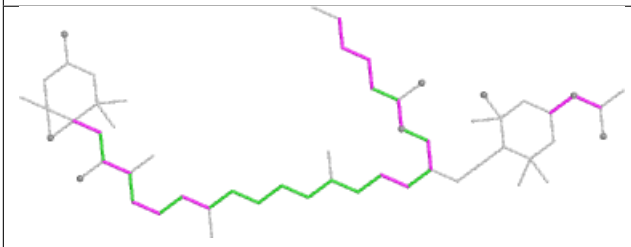
Ligand A1EB1 7 303



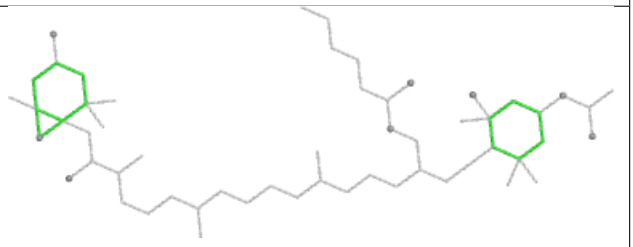
Bond lengths



Bond angles

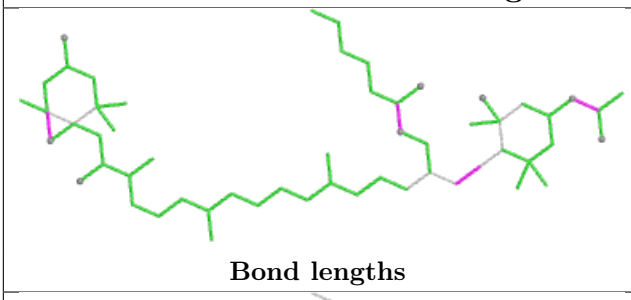


Torsions

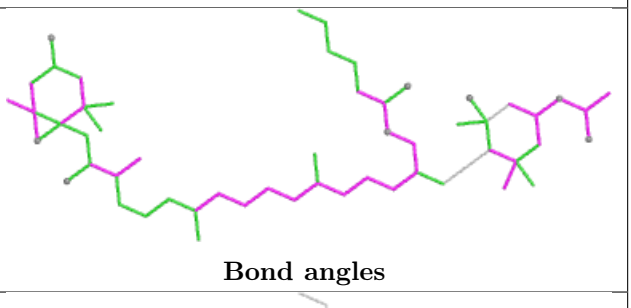


Rings

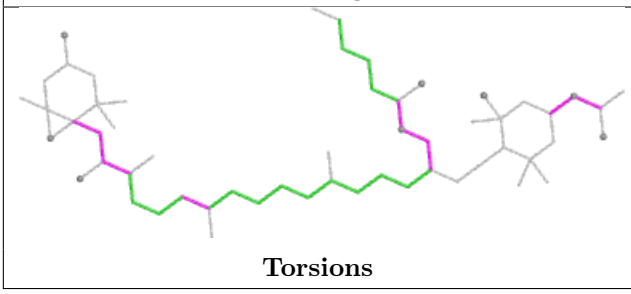
Ligand A1EB1 O 301



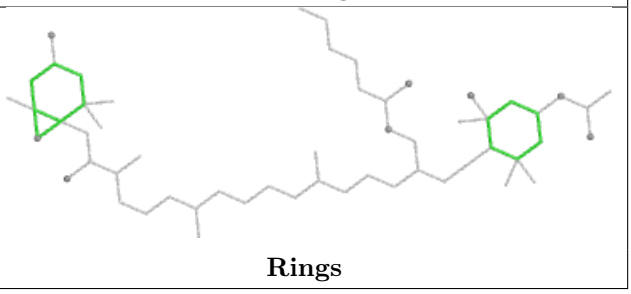
Bond lengths



Bond angles

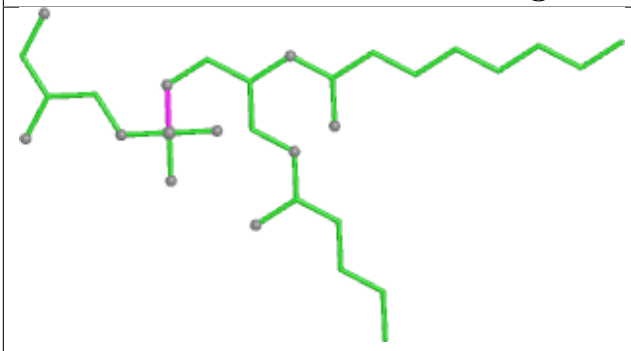


Torsions

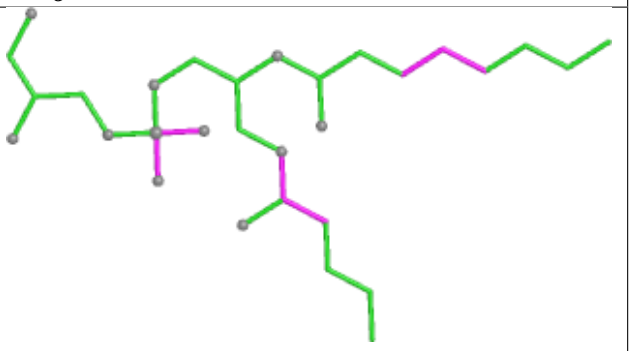


Rings

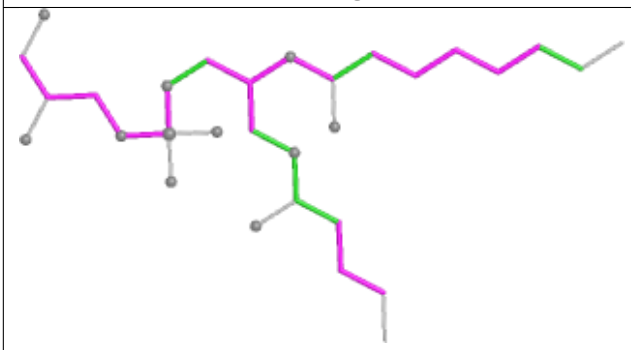
Ligand LHG j 104



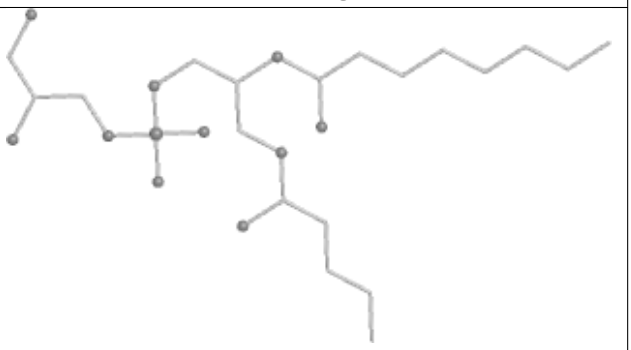
Bond lengths



Bond angles

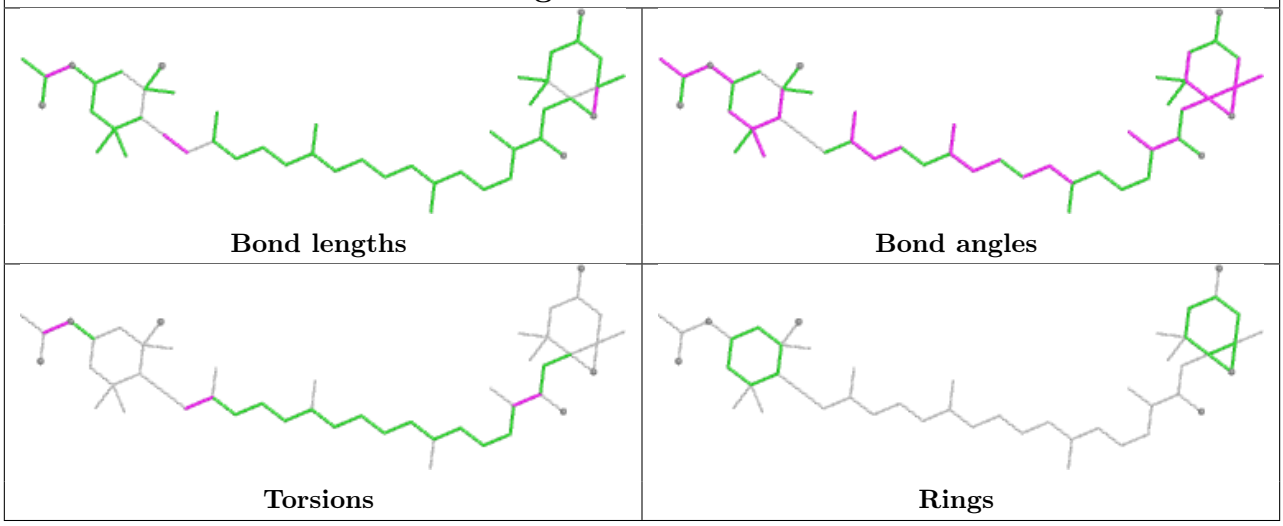


Torsions

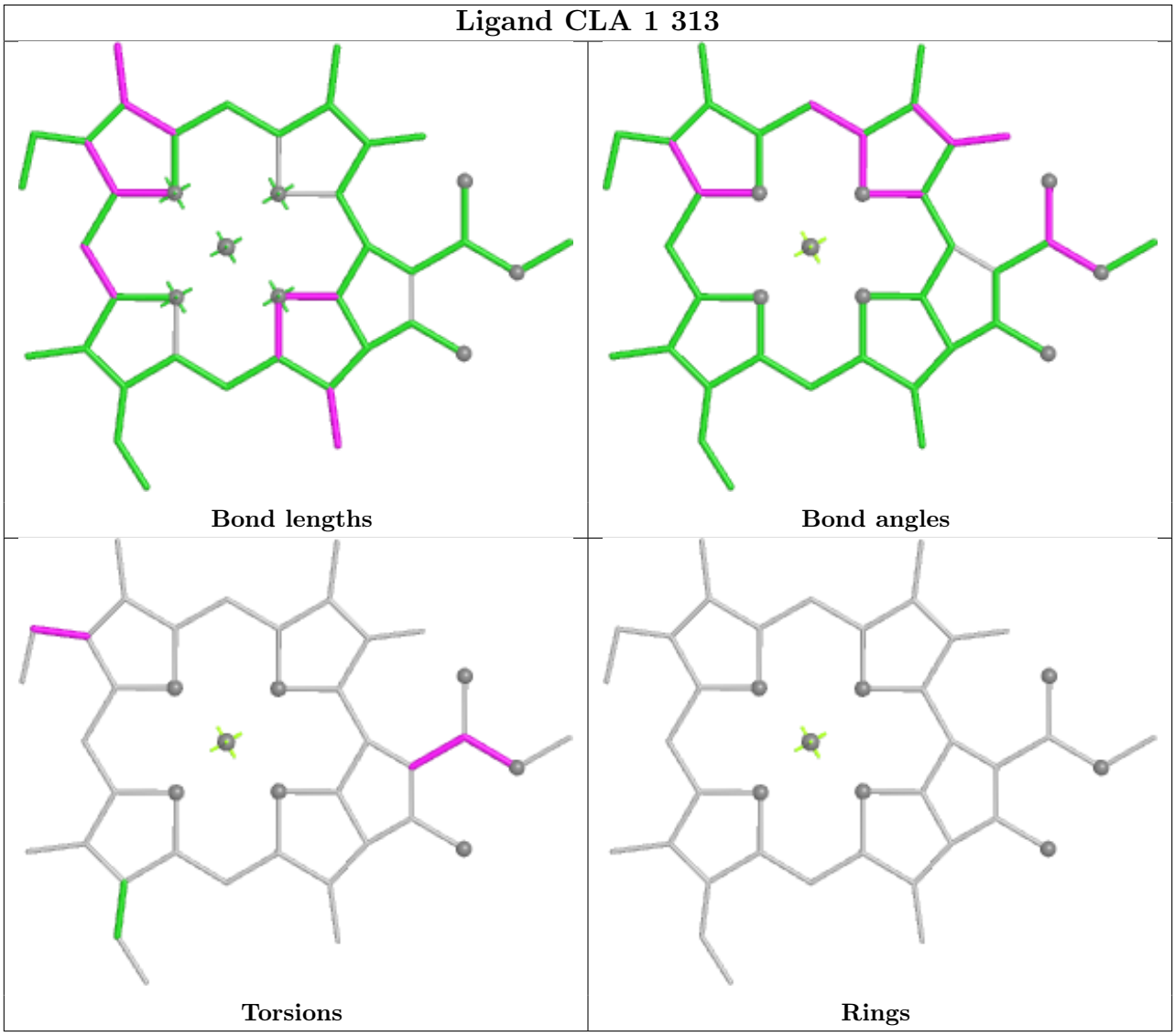


Rings

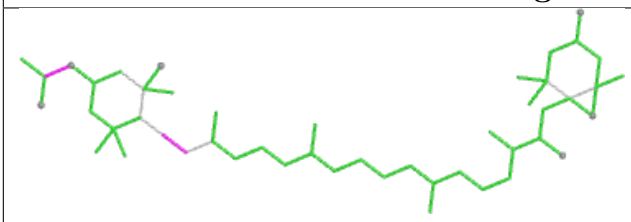
Ligand A86 x 305



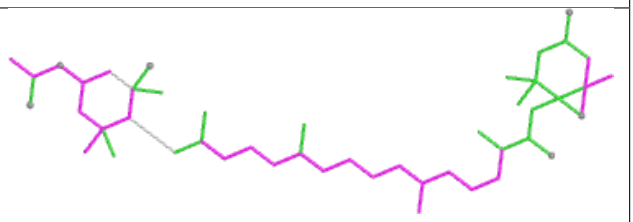
Ligand CLA 1 313



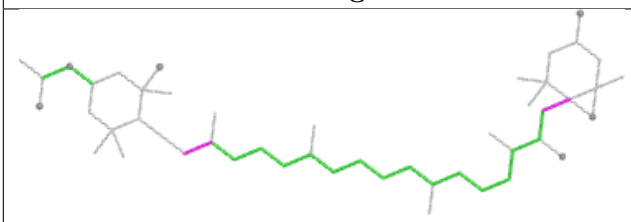
Ligand A86 5 301



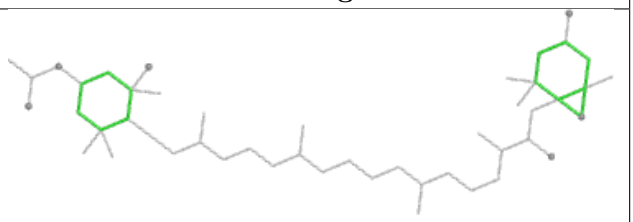
Bond lengths



Bond angles

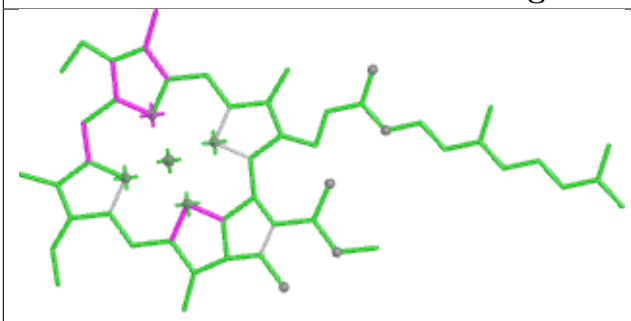


Torsions

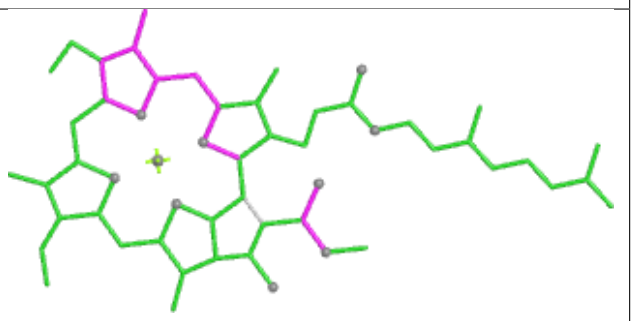


Rings

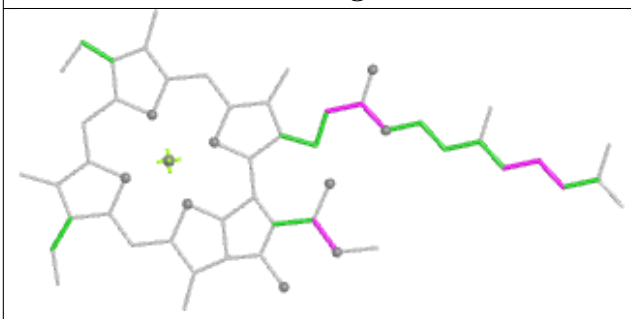
Ligand CLA J 310



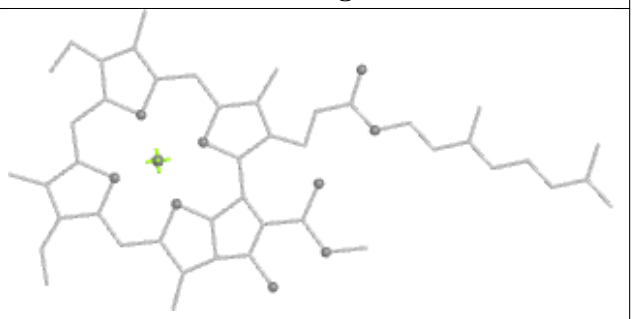
Bond lengths



Bond angles

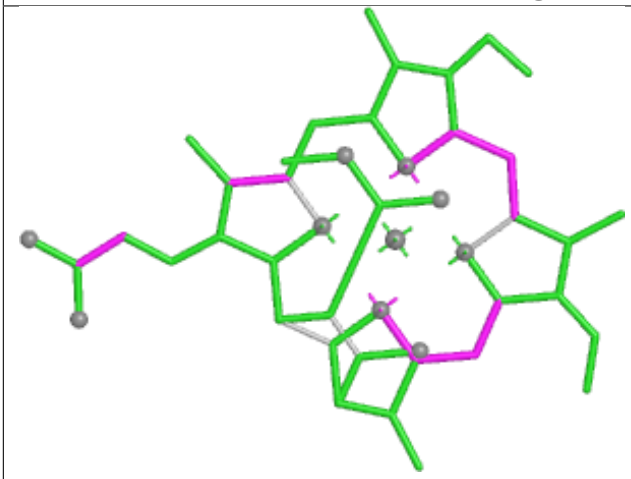


Torsions

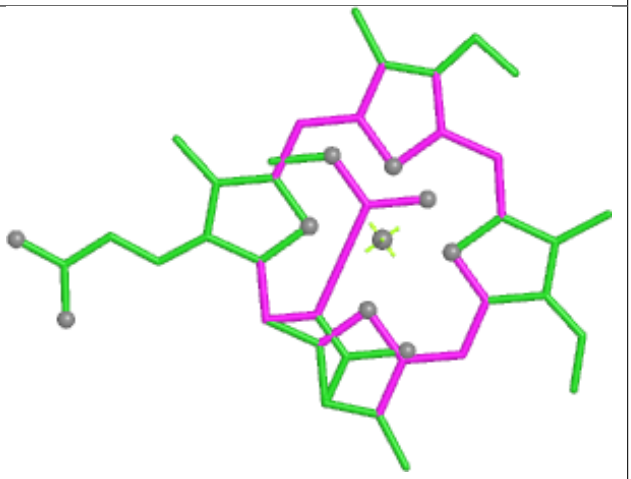


Rings

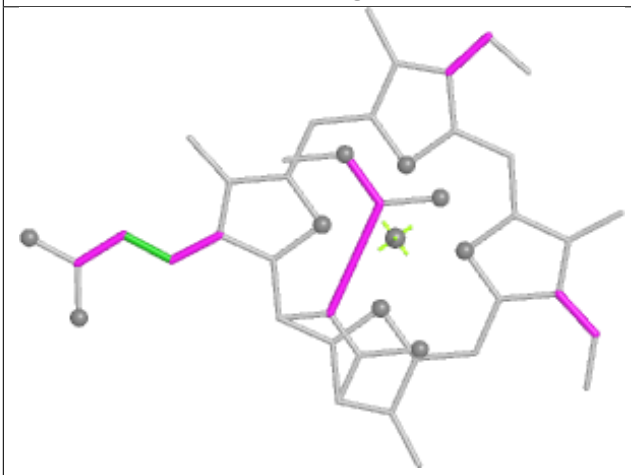
Ligand KC2 8 314



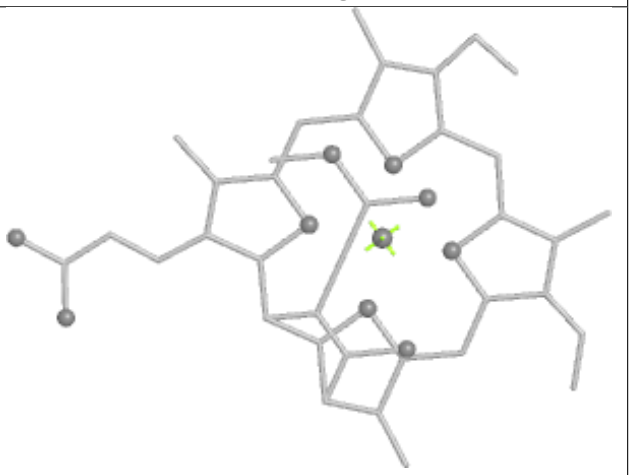
Bond lengths



Bond angles

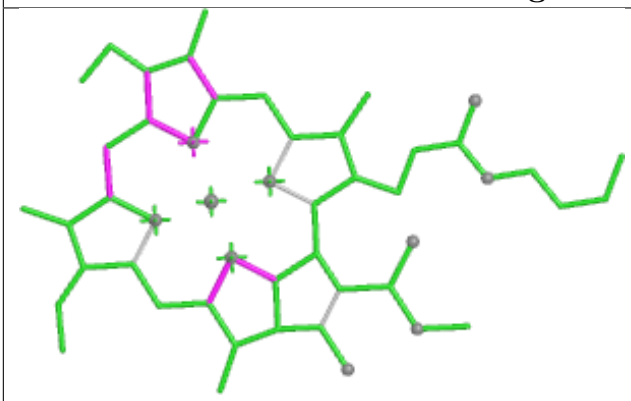


Torsions

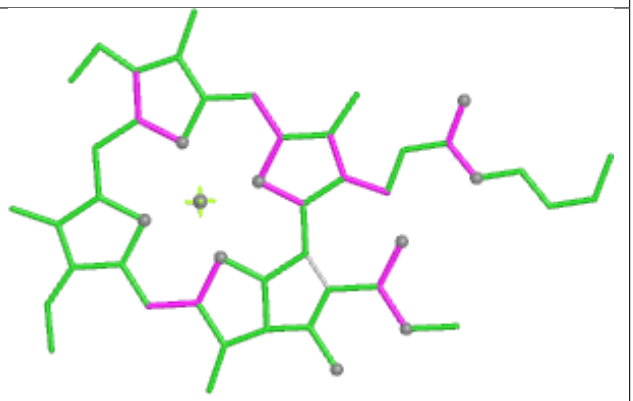


Rings

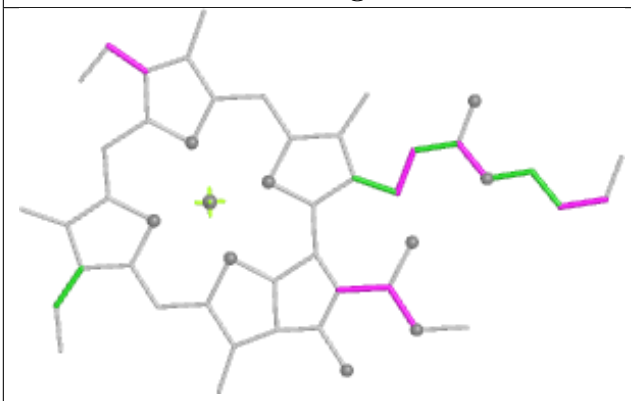
Ligand CLA a 819



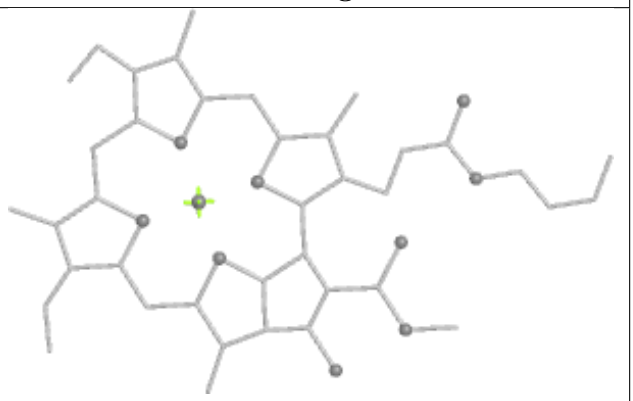
Bond lengths



Bond angles

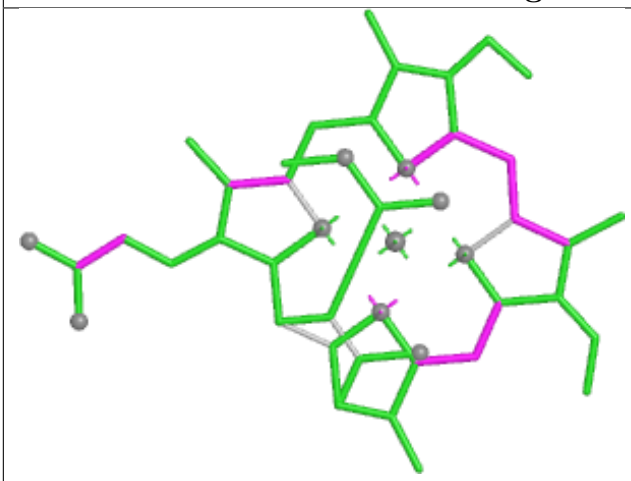


Torsions

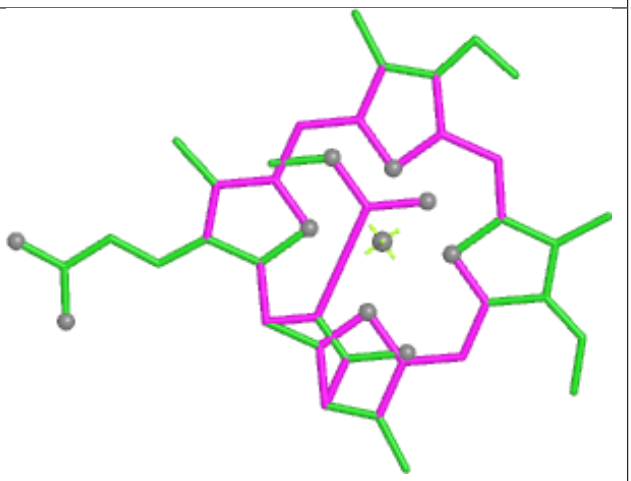


Rings

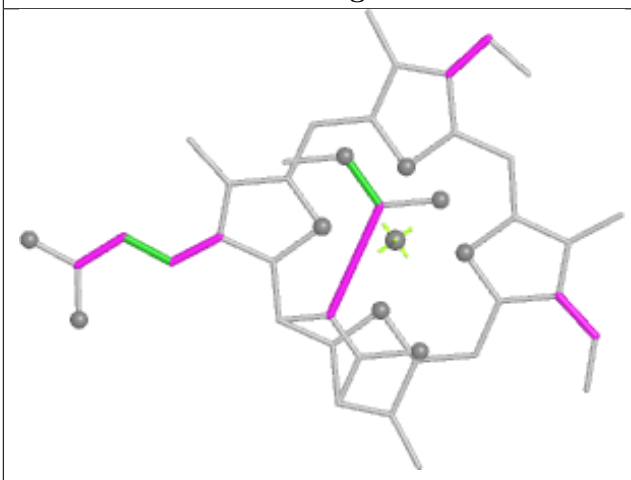
Ligand KC2 K 313



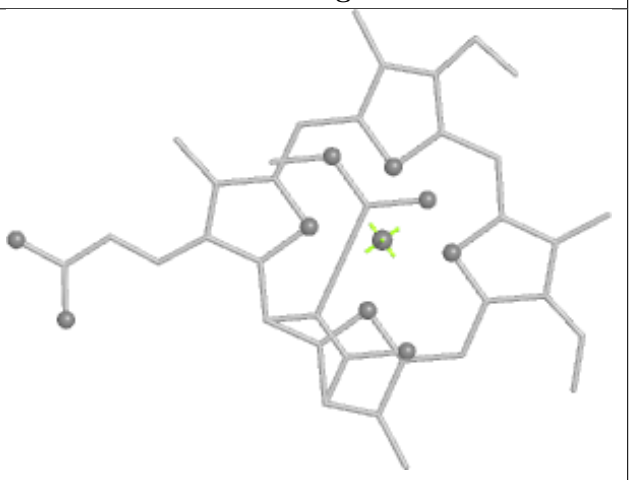
Bond lengths



Bond angles

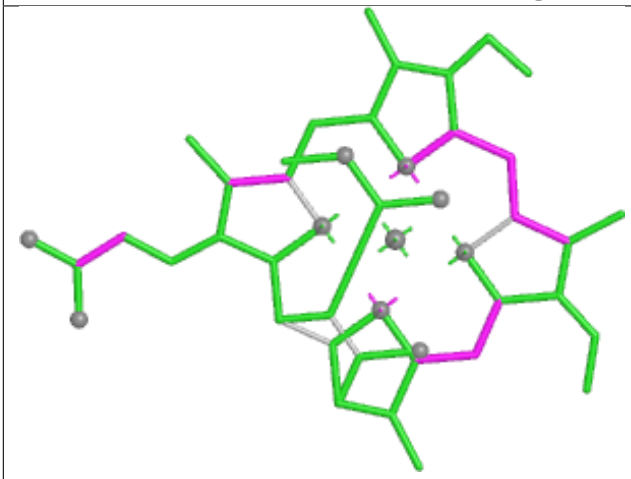


Torsions

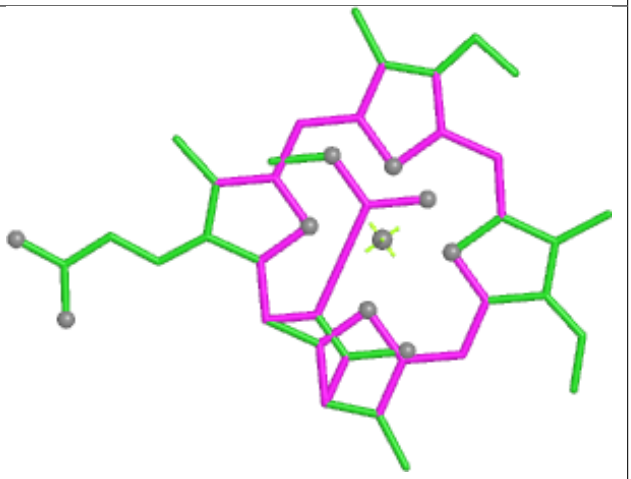


Rings

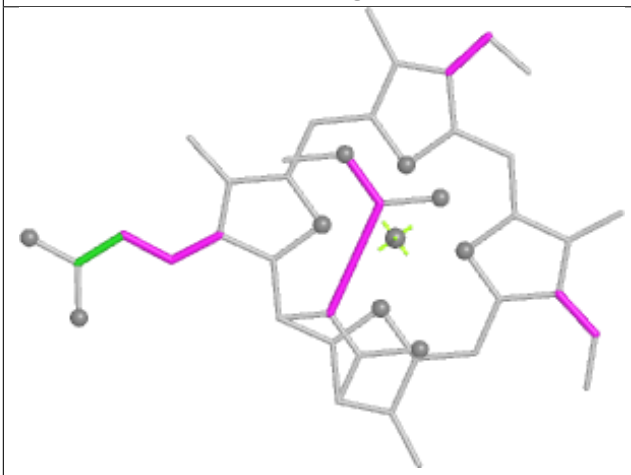
Ligand KC2 2 314



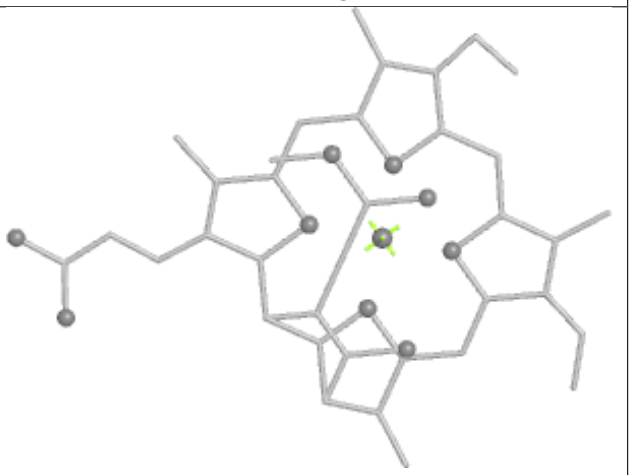
Bond lengths



Bond angles

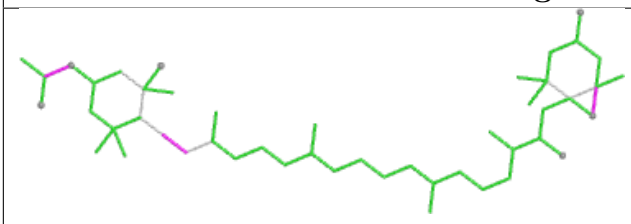


Torsions

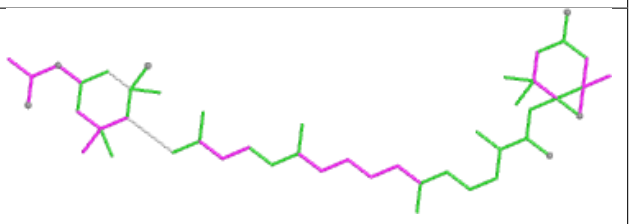


Rings

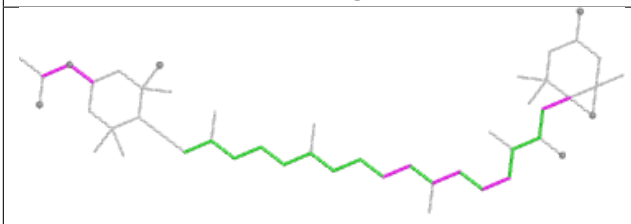
Ligand A86 3 306



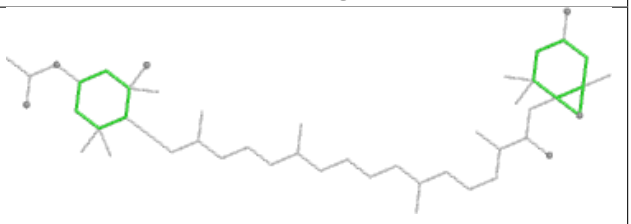
Bond lengths



Bond angles

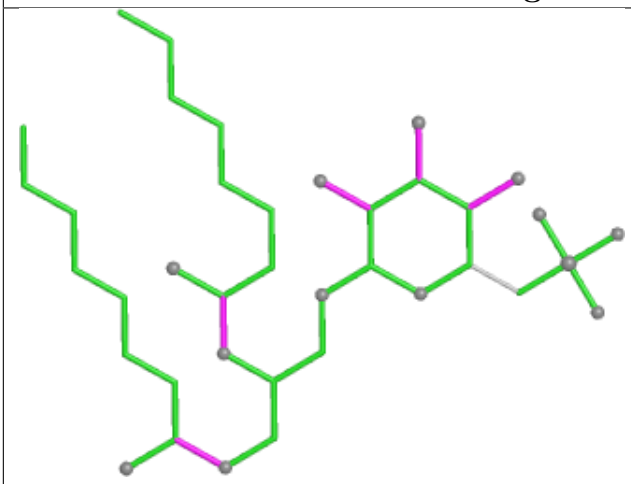


Torsions

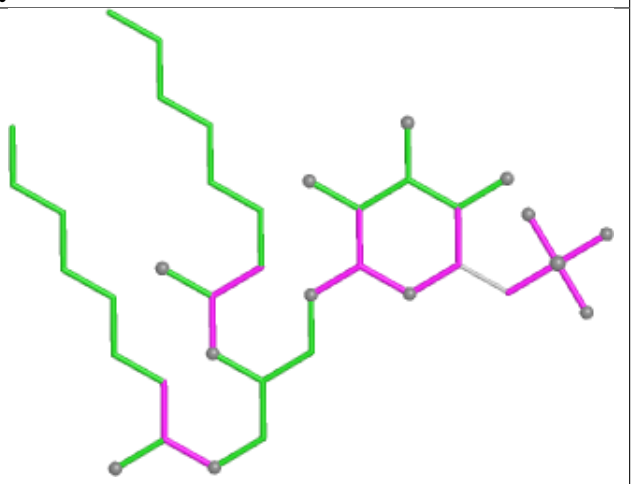


Rings

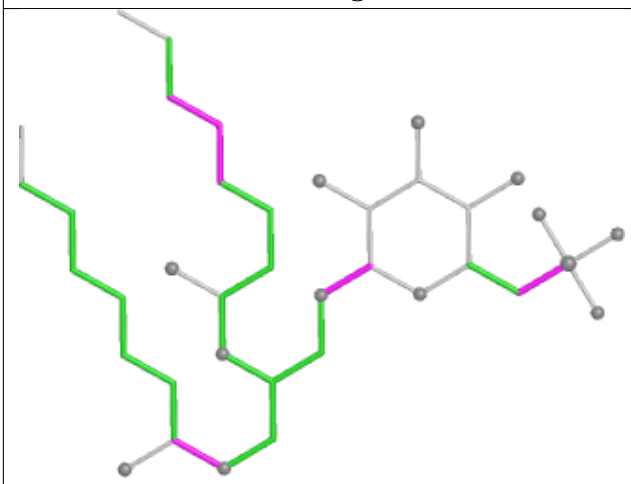
Ligand SQD D 304



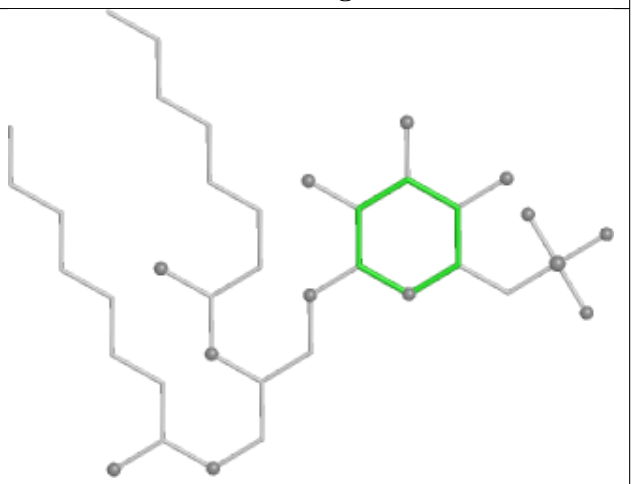
Bond lengths



Bond angles

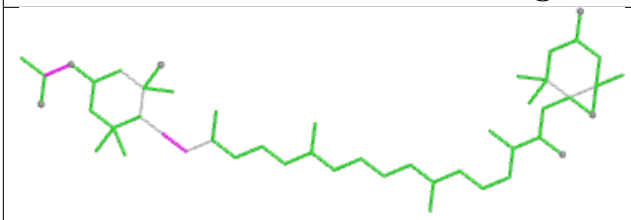


Torsions

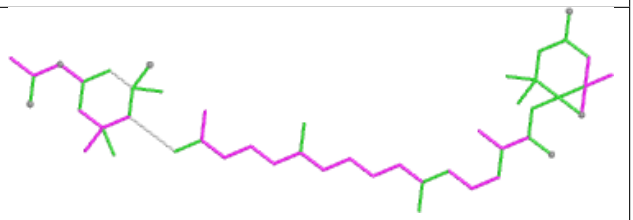


Rings

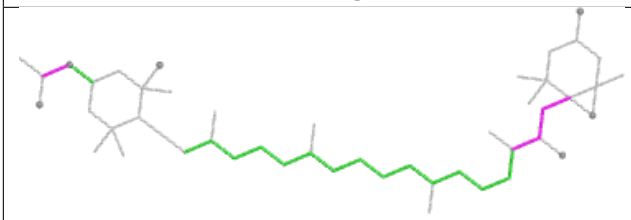
Ligand A86 4 306



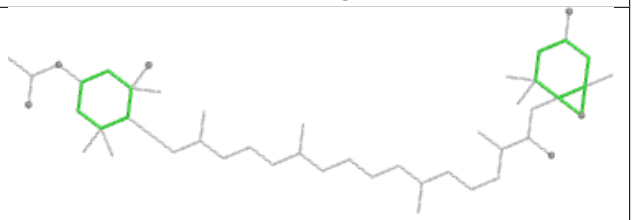
Bond lengths



Bond angles

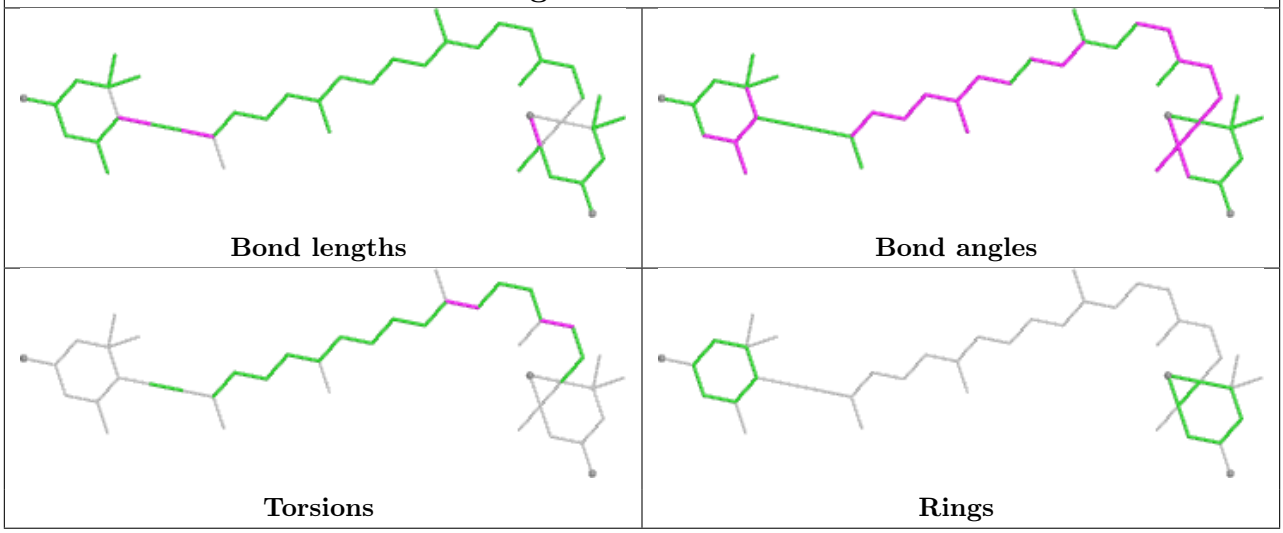


Torsions

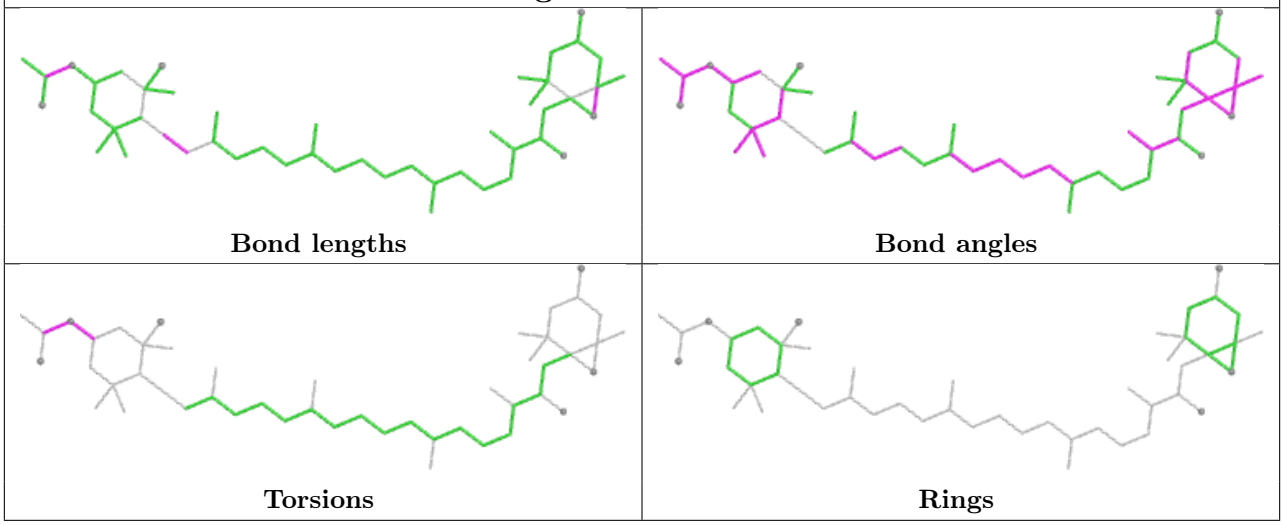


Rings

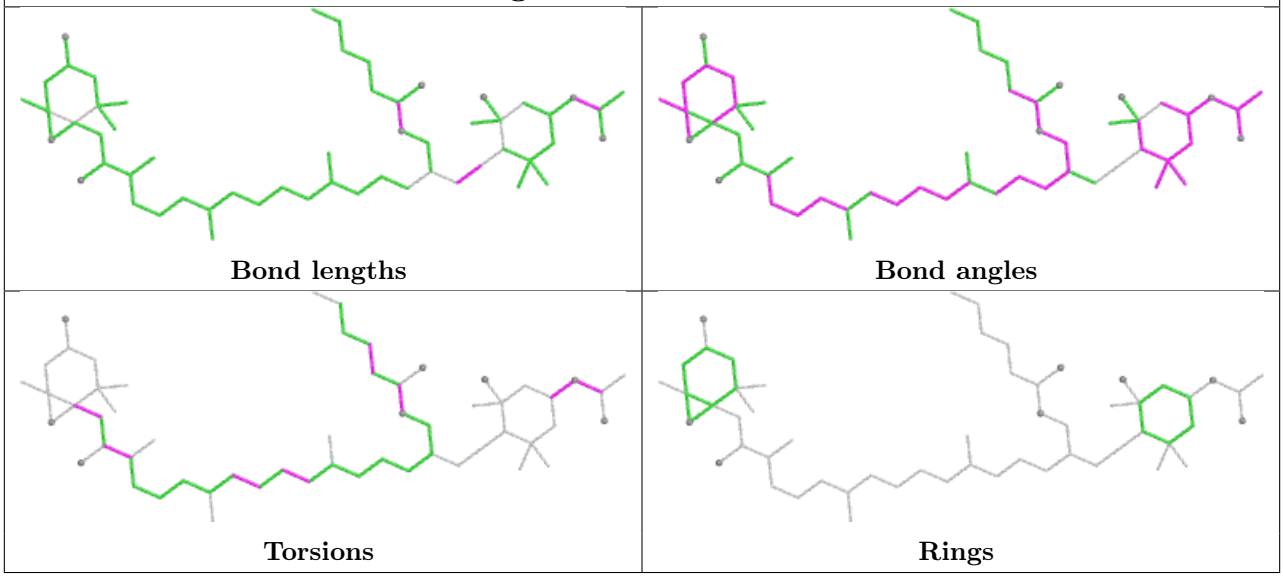
Ligand DD6 7 310



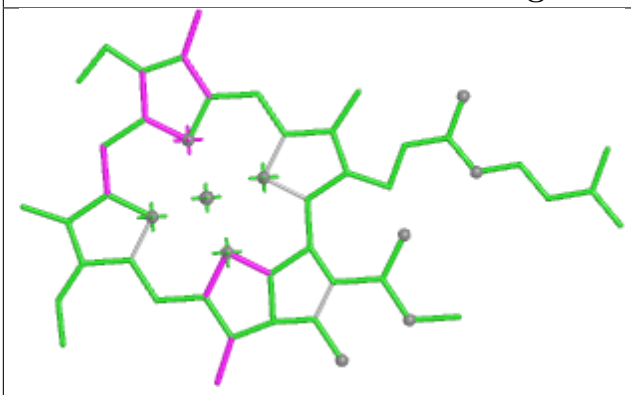
Ligand A86 7 307



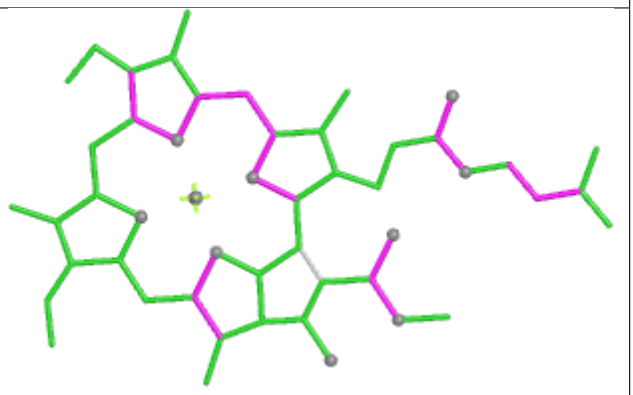
Ligand A1EB1 S 303



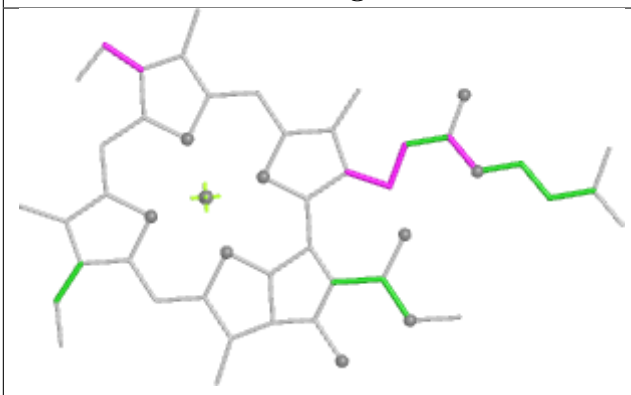
Ligand CLA b 831



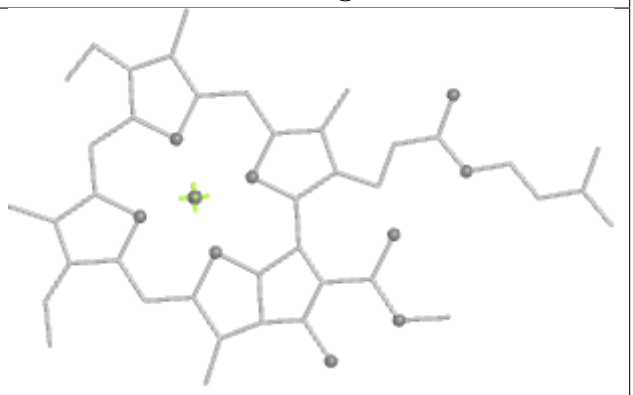
Bond lengths



Bond angles

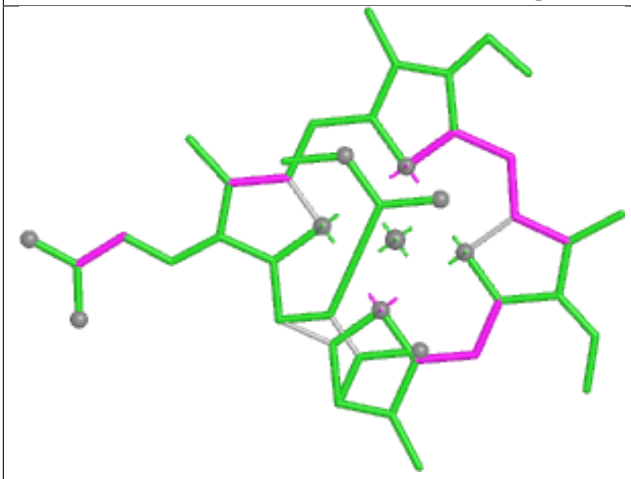


Torsions

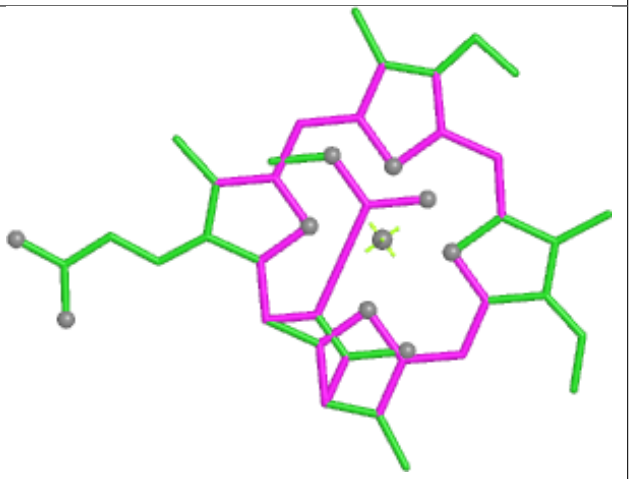


Rings

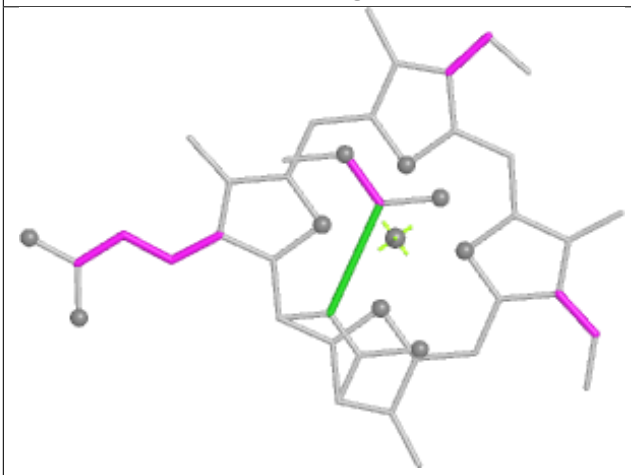
Ligand KC2 4 320



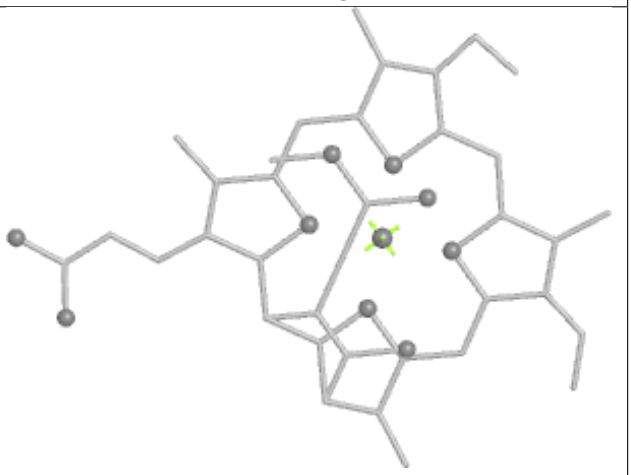
Bond lengths



Bond angles

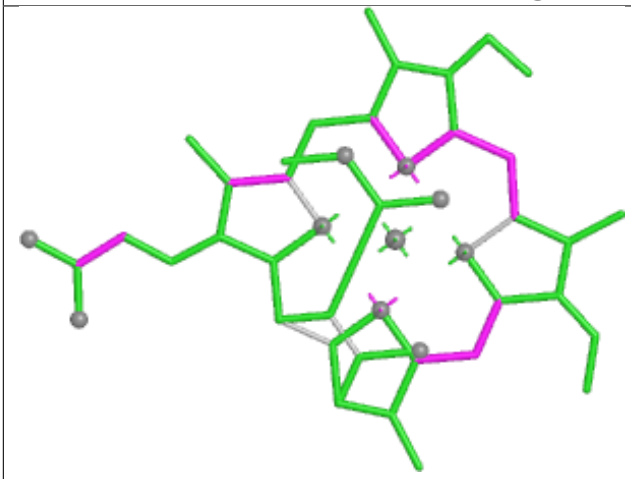


Torsions

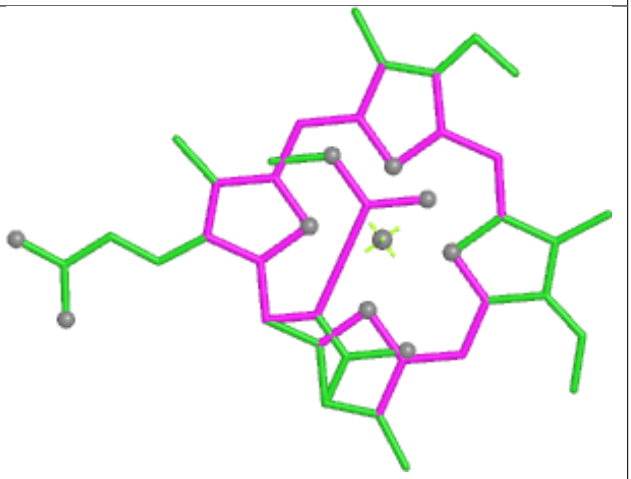


Rings

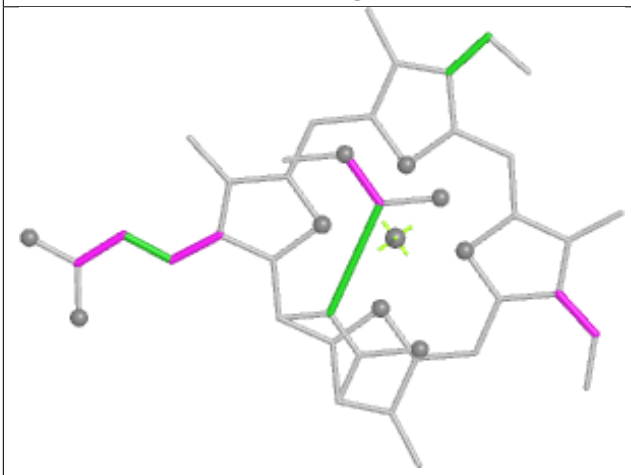
Ligand KC2 S 315



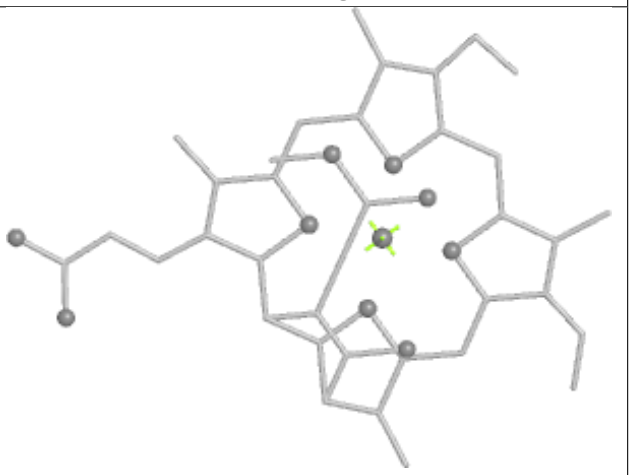
Bond lengths



Bond angles

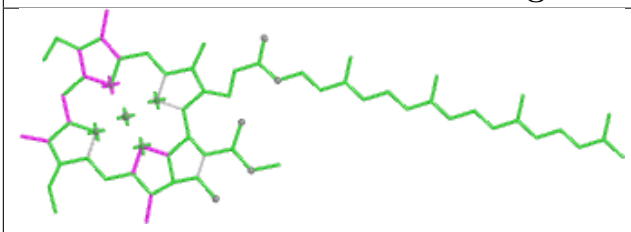


Torsions

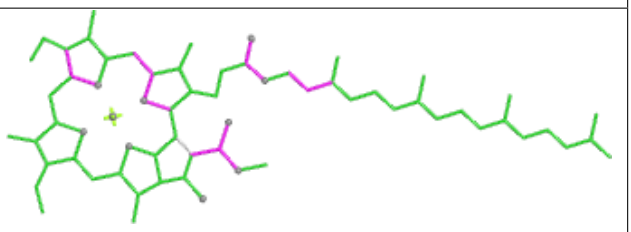


Rings

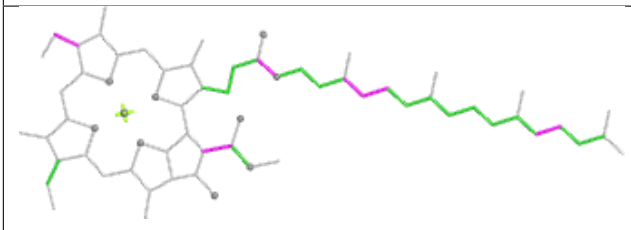
Ligand CLA b 811



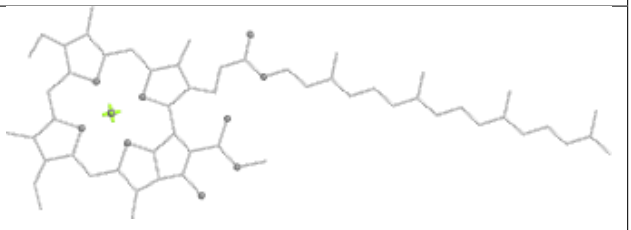
Bond lengths



Bond angles

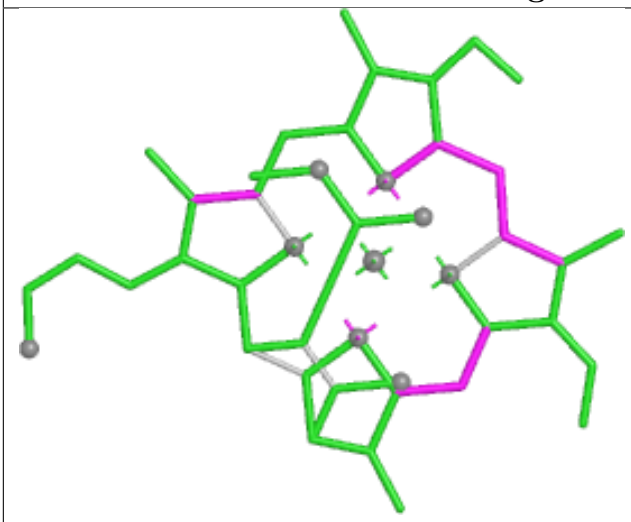


Torsions



Rings

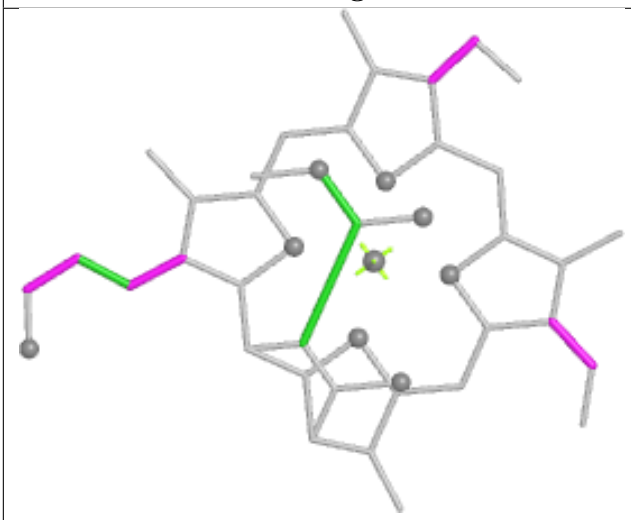
Ligand KC2 F 311



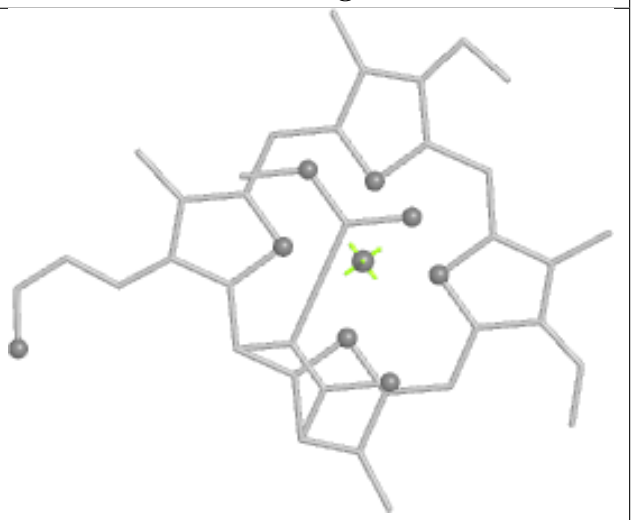
Bond lengths



Bond angles

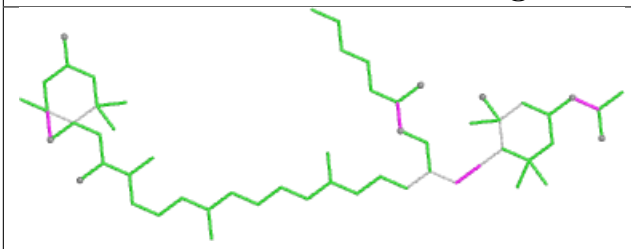


Torsions

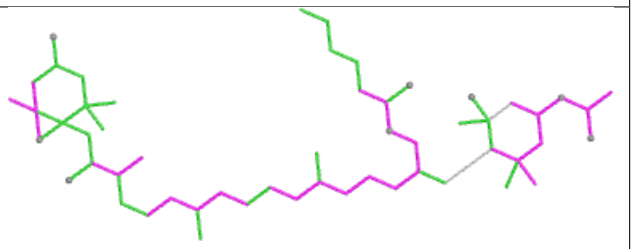


Rings

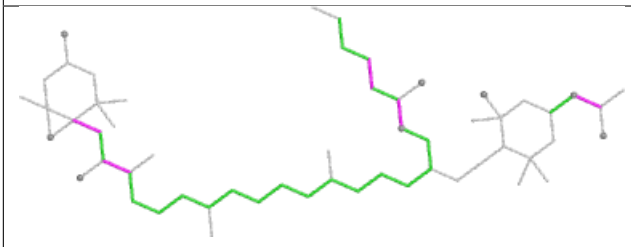
Ligand A1EB1 8 308



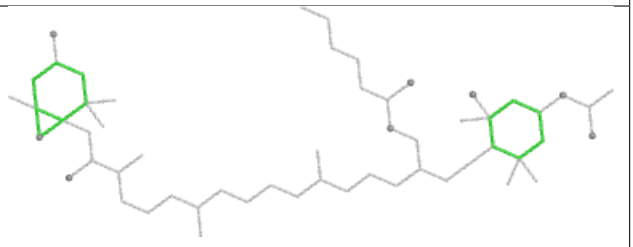
Bond lengths



Bond angles

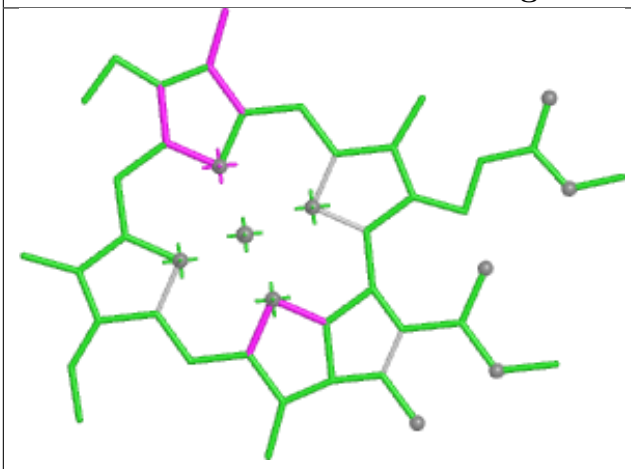


Torsions

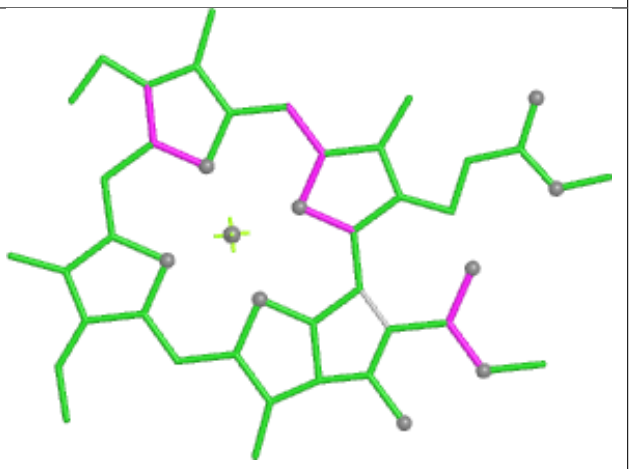


Rings

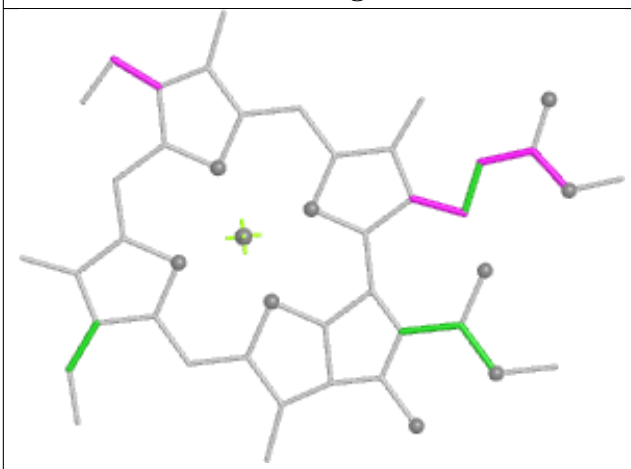
Ligand CLA M 318



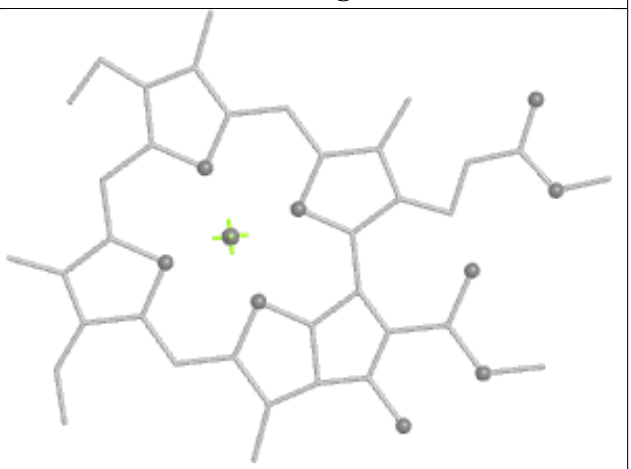
Bond lengths



Bond angles

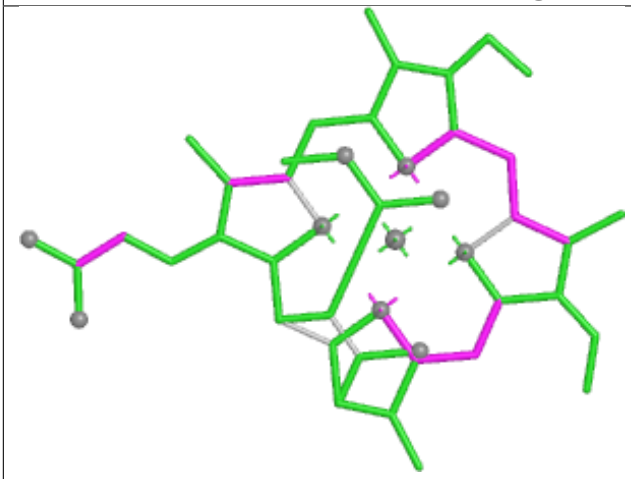


Torsions

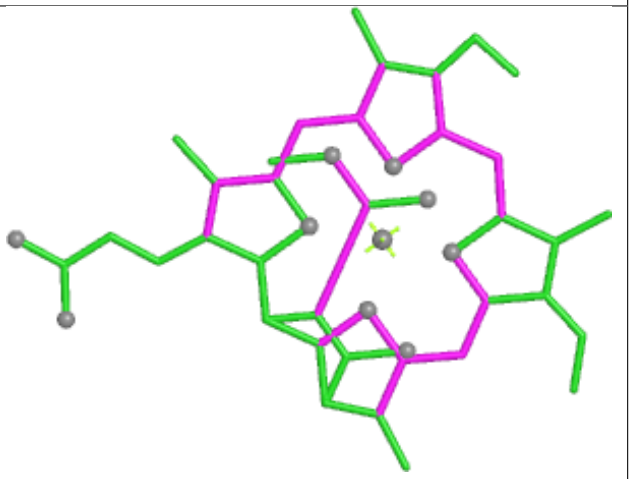


Rings

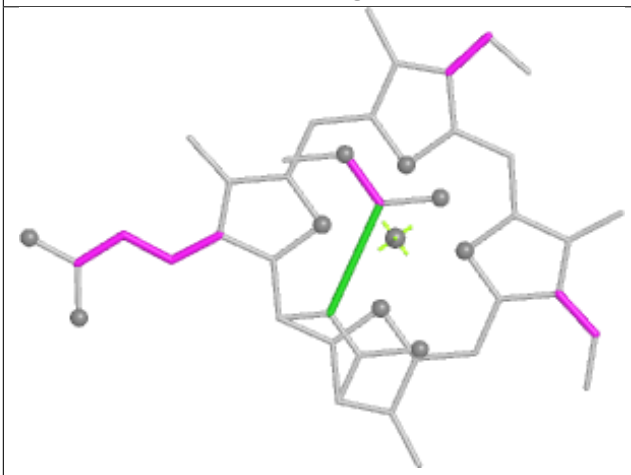
Ligand KC2 6 319



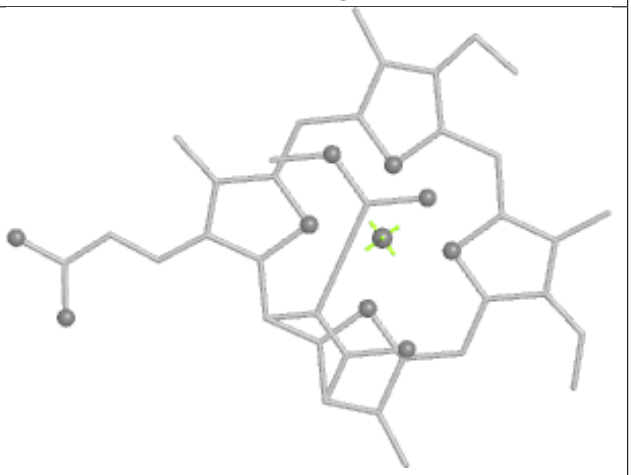
Bond lengths



Bond angles

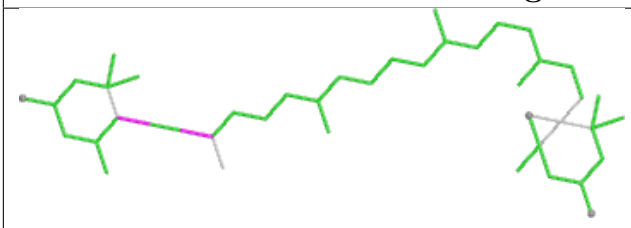


Torsions

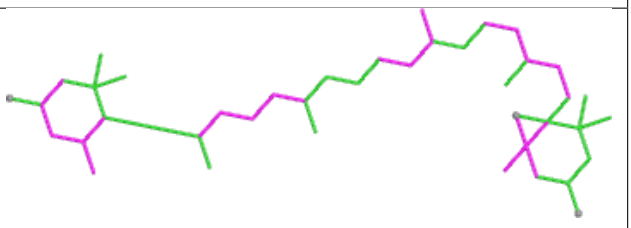


Rings

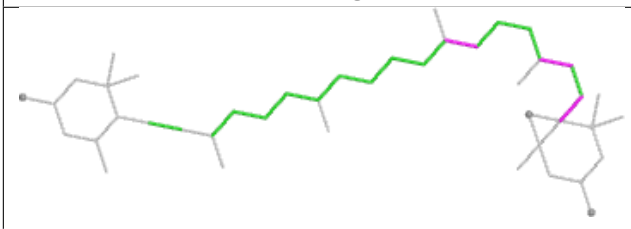
Ligand DD6 O 305



Bond lengths



Bond angles

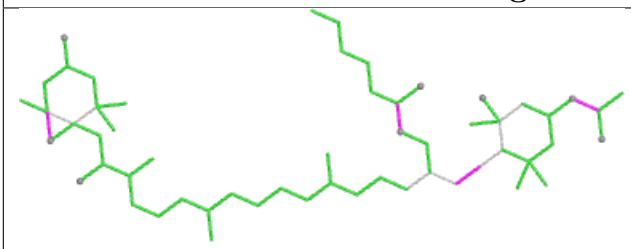


Torsions

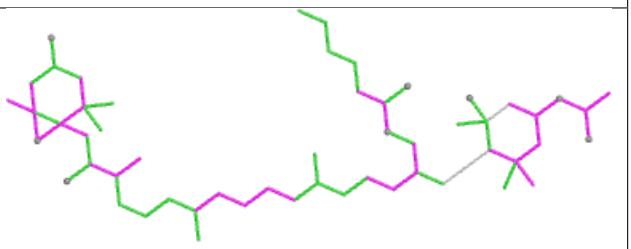


Rings

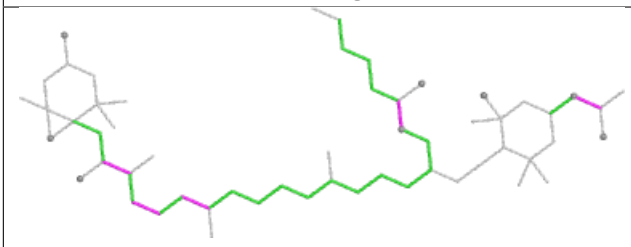
Ligand A1EB1 1 305



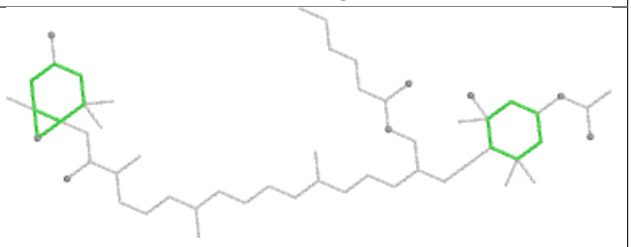
Bond lengths



Bond angles

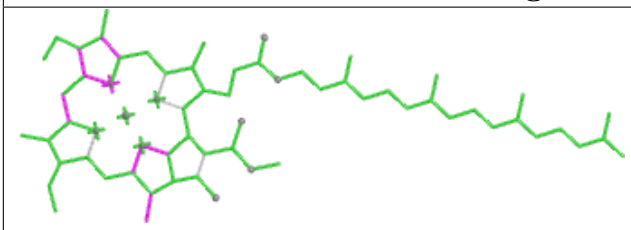


Torsions

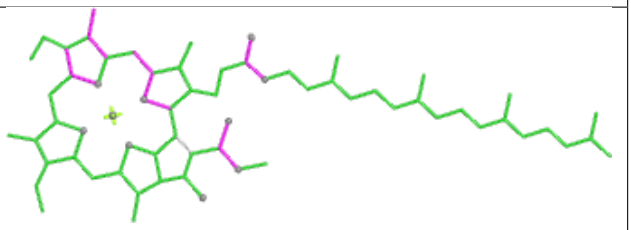


Rings

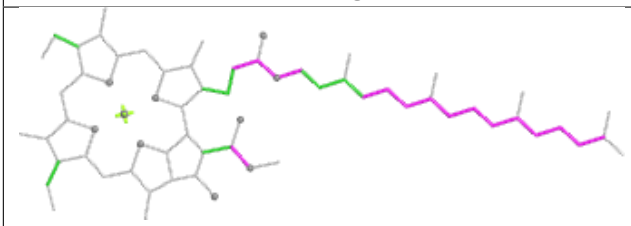
Ligand CLA P 308



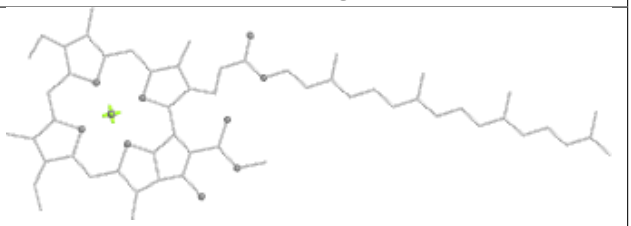
Bond lengths



Bond angles

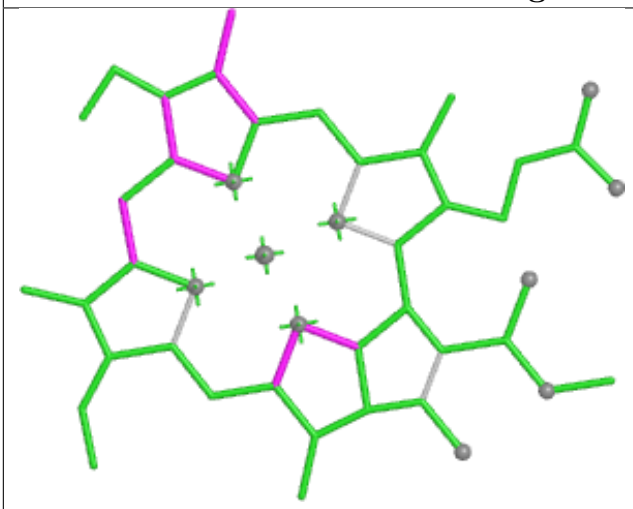


Torsions

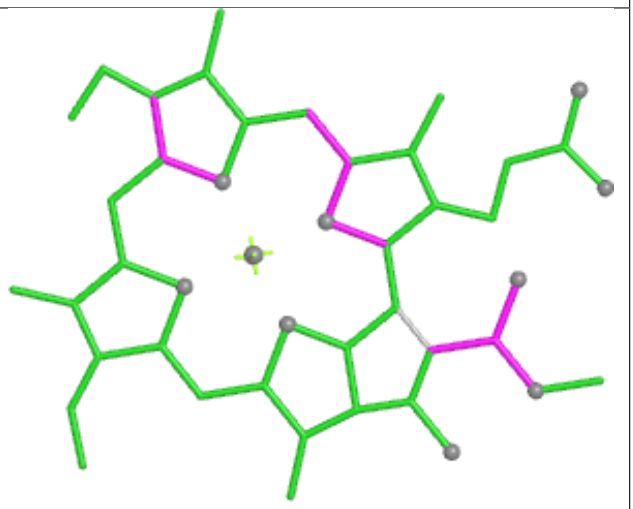


Rings

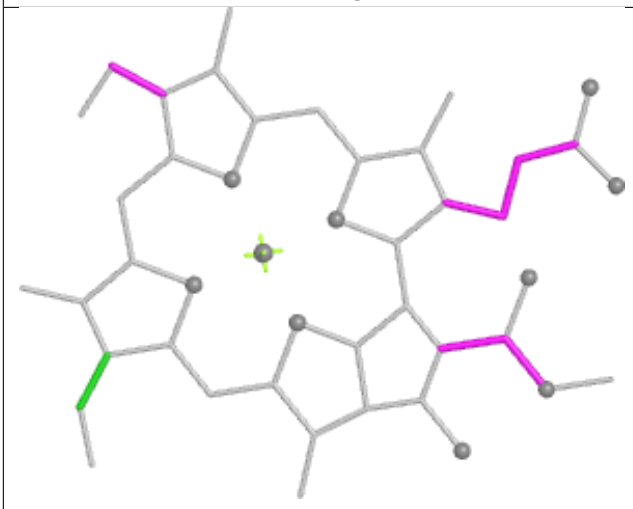
Ligand CLA a 833



Bond lengths



Bond angles

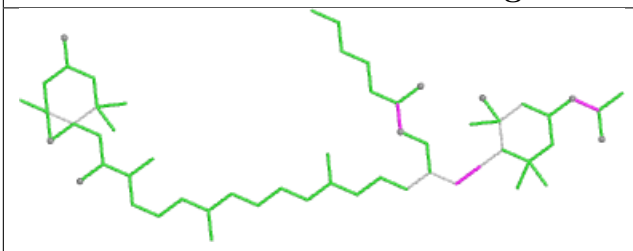


Torsions

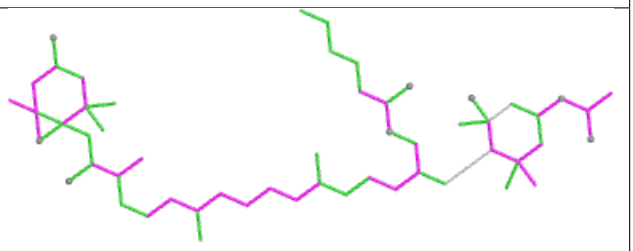


Rings

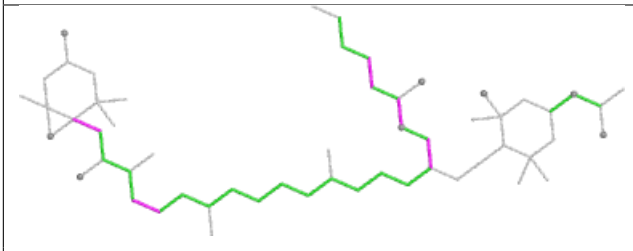
Ligand A1EB1 K 305



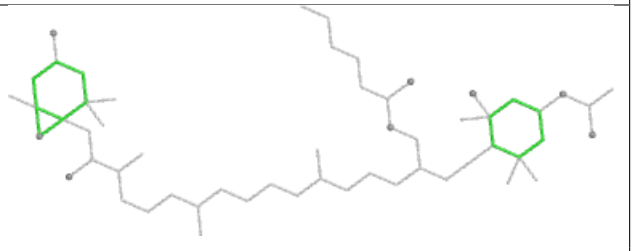
Bond lengths



Bond angles

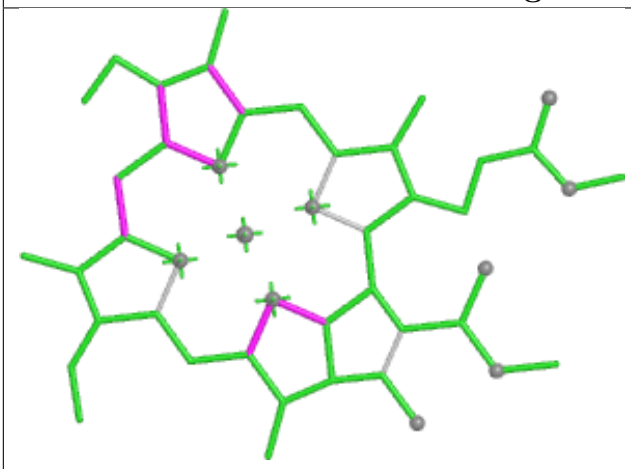


Torsions

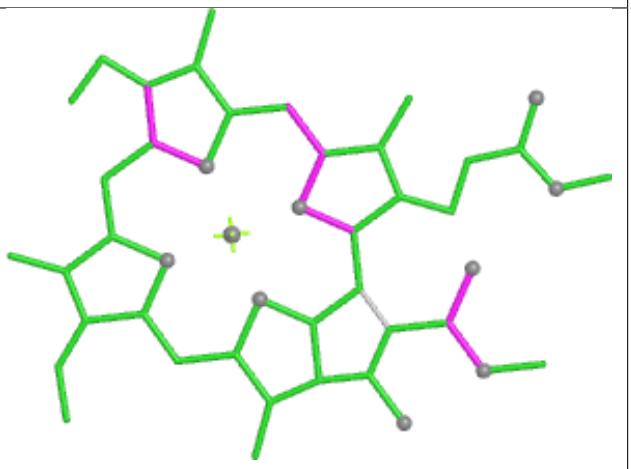


Rings

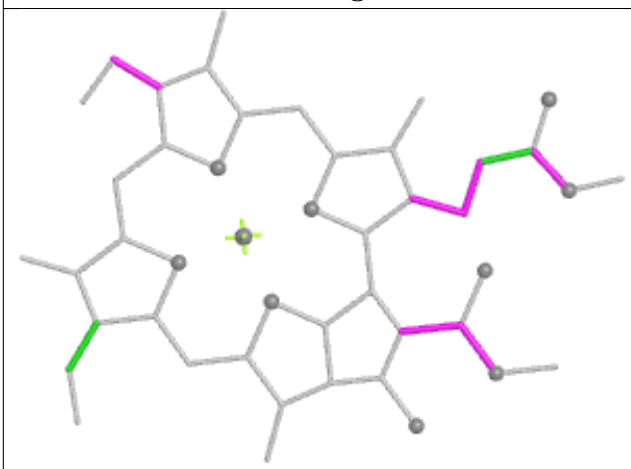
Ligand CLA C 309



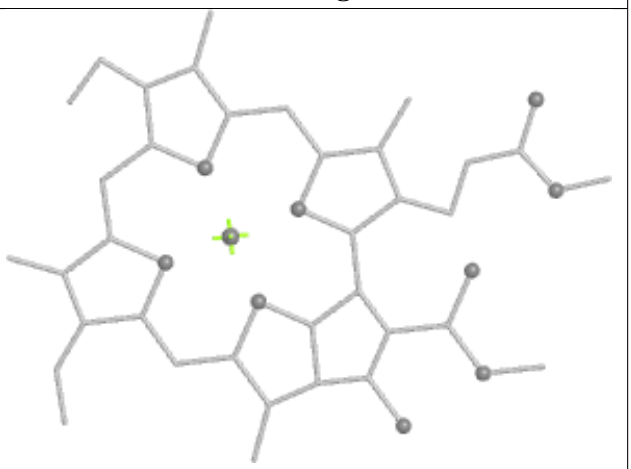
Bond lengths



Bond angles

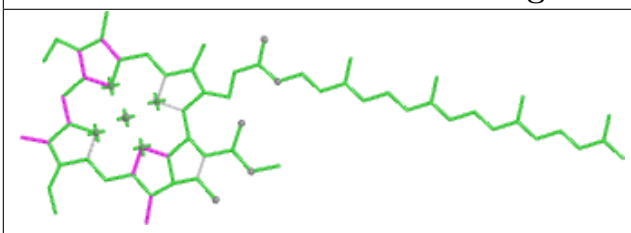


Torsions

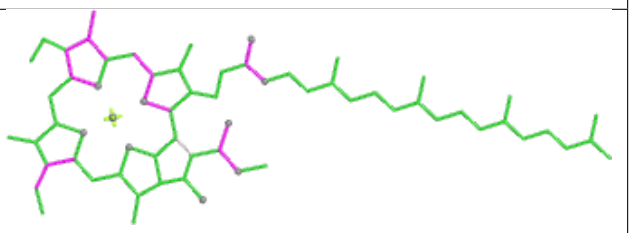


Rings

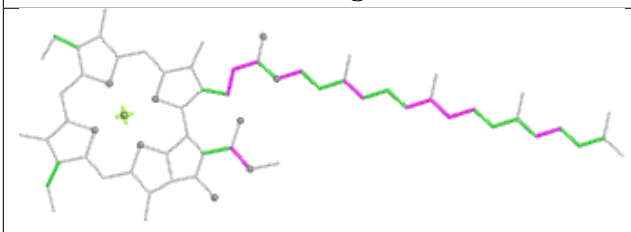
Ligand CLA b 807



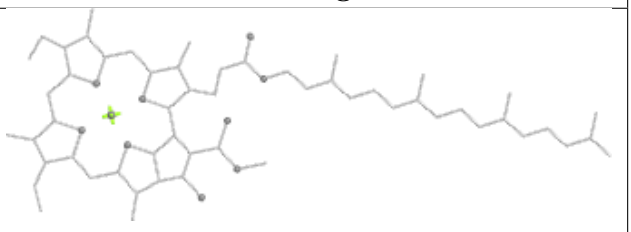
Bond lengths



Bond angles

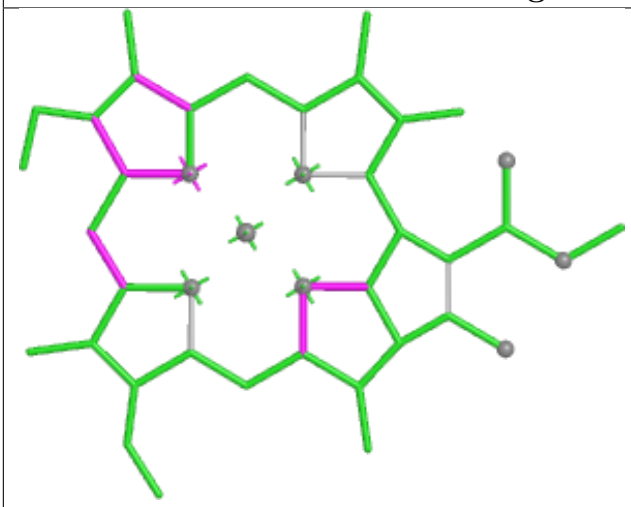


Torsions

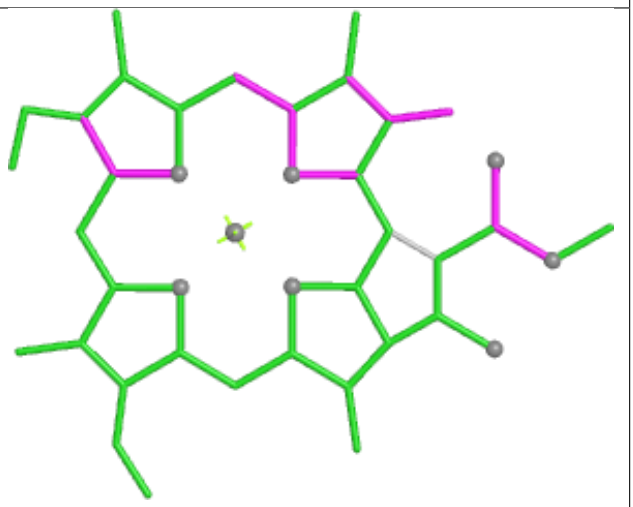


Rings

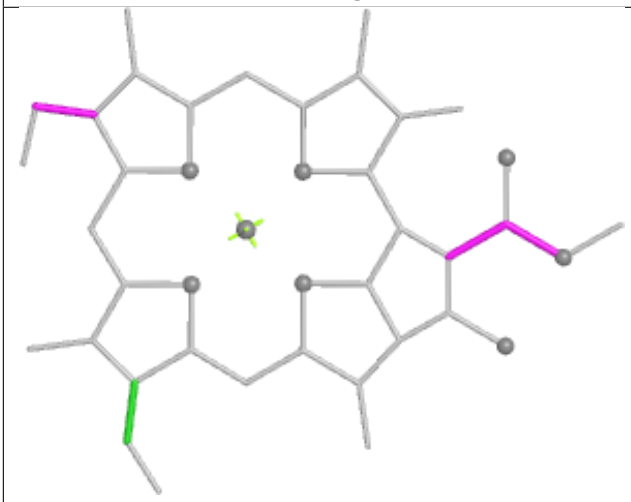
Ligand CLA x 314



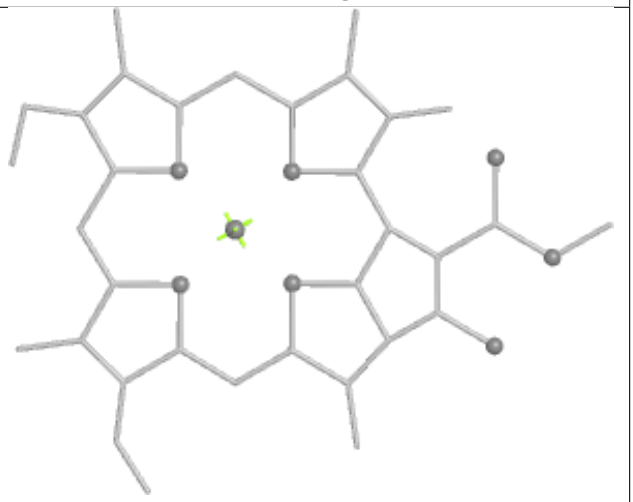
Bond lengths



Bond angles

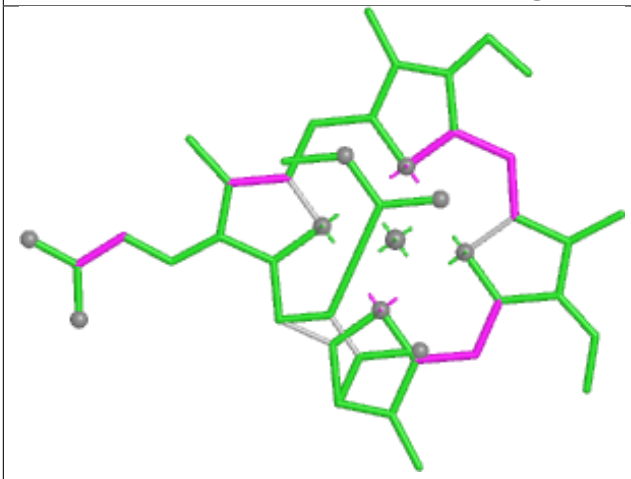


Torsions

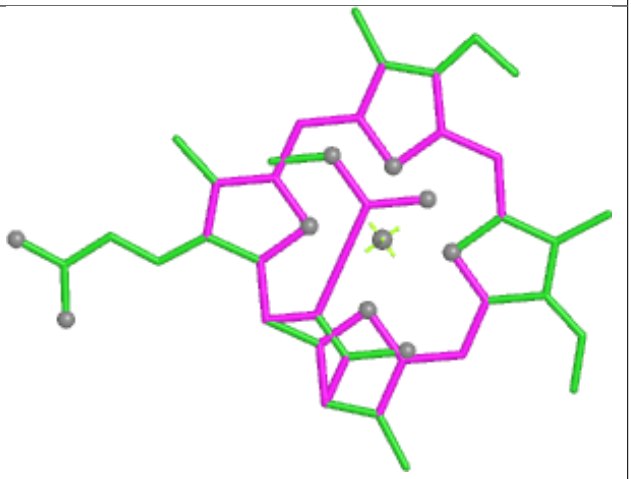


Rings

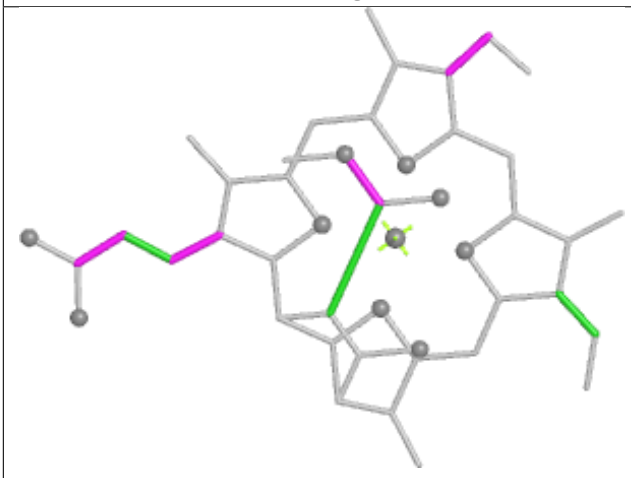
Ligand KC2 L 314



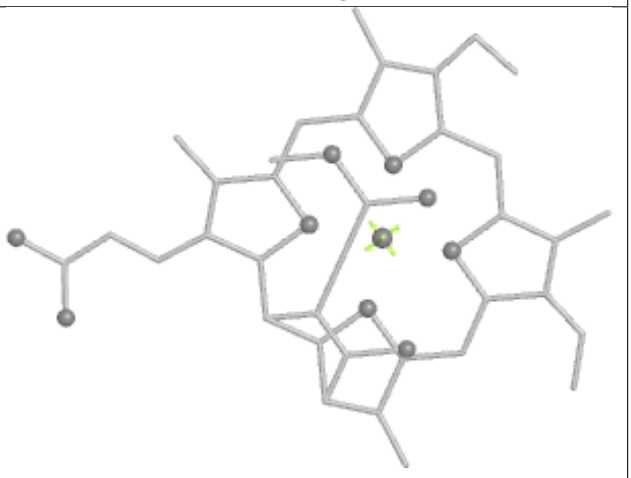
Bond lengths



Bond angles

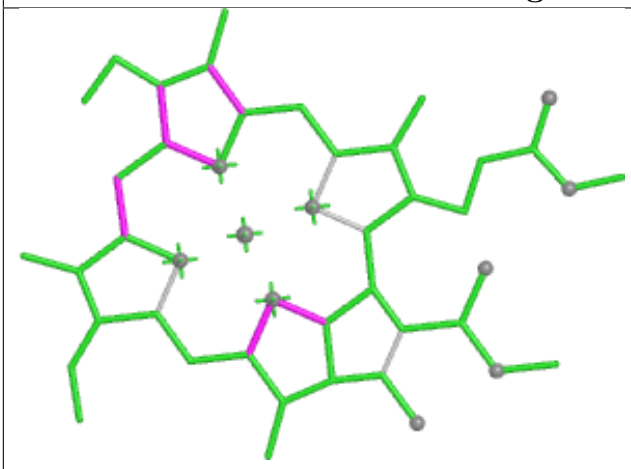


Torsions

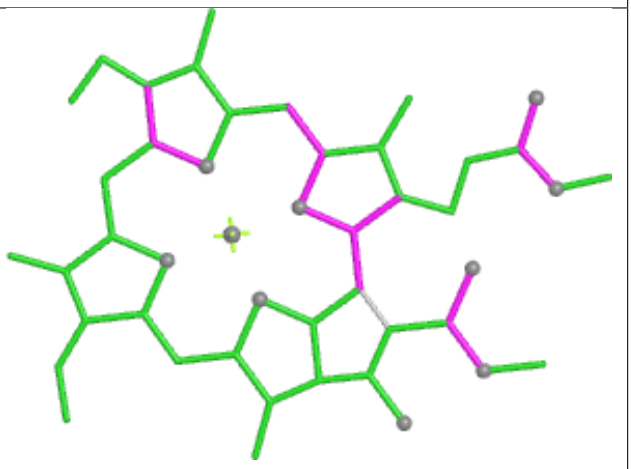


Rings

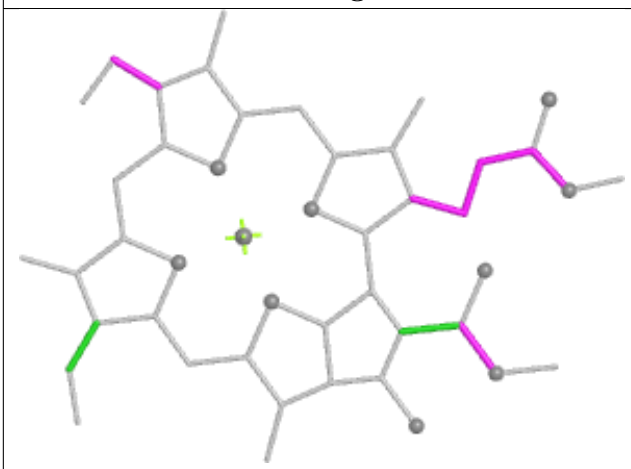
Ligand CLA L 320



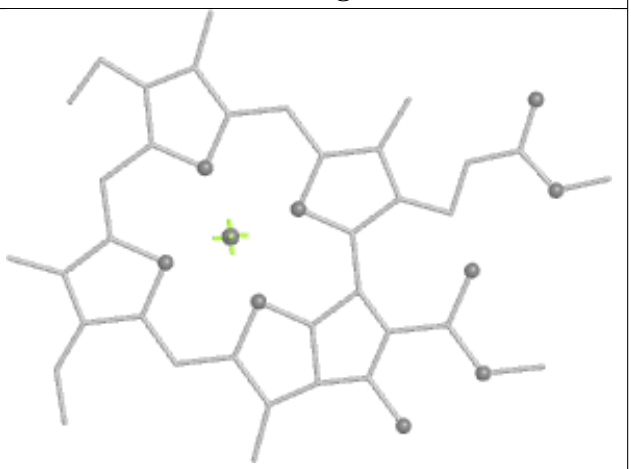
Bond lengths



Bond angles

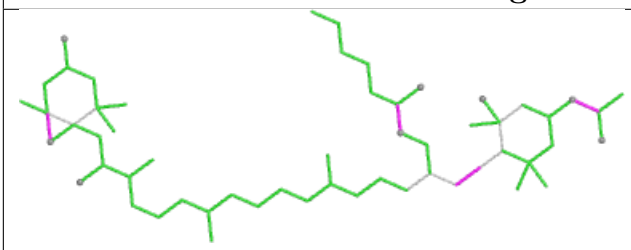


Torsions

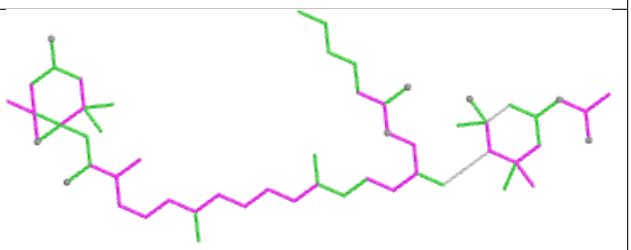


Rings

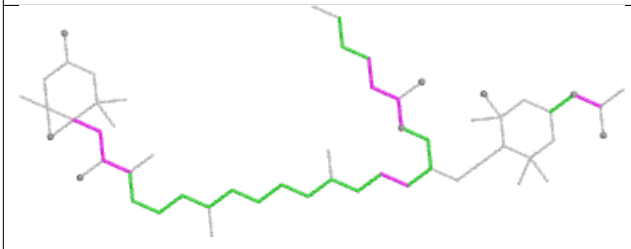
Ligand A1EB1 6 308



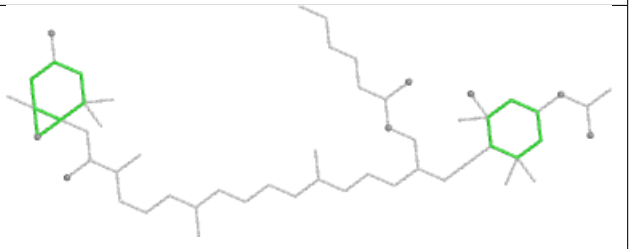
Bond lengths



Bond angles

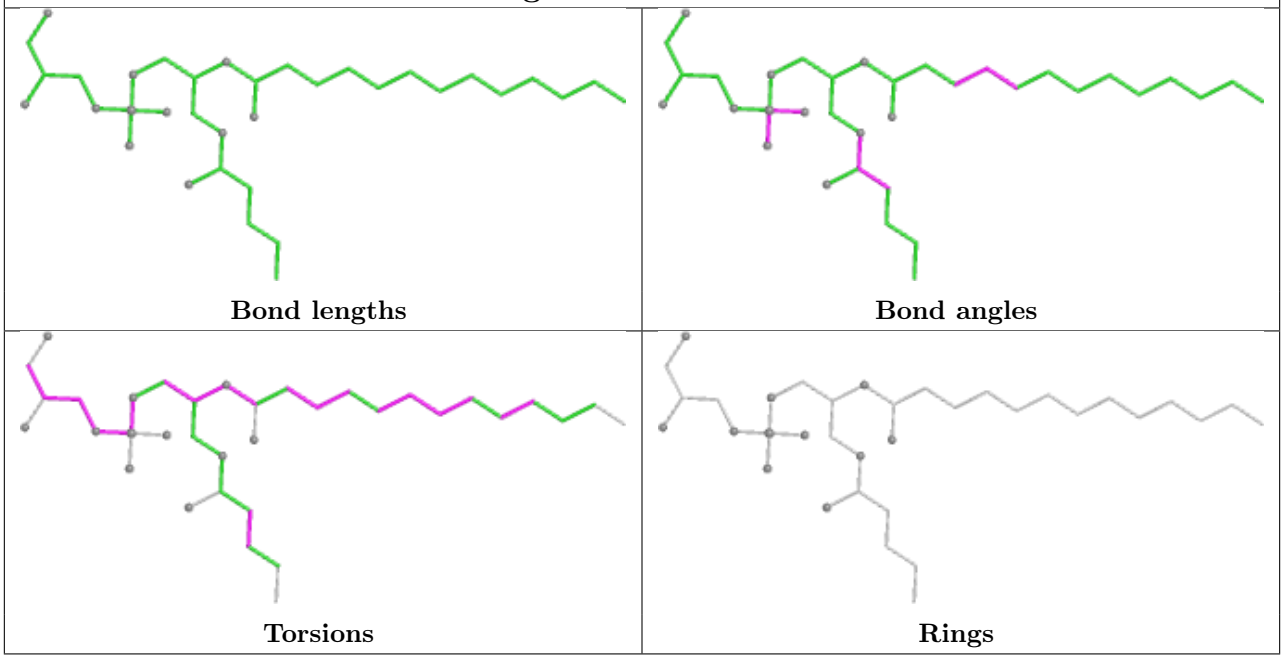


Torsions

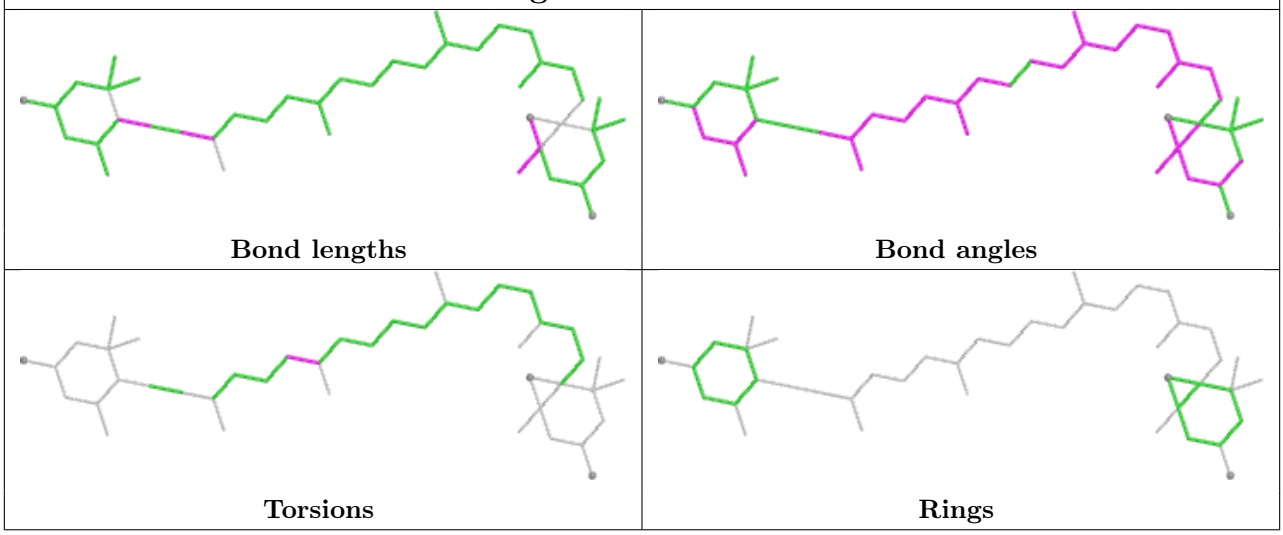


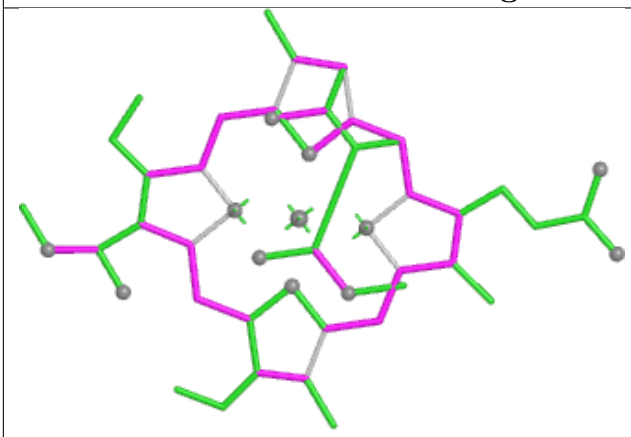
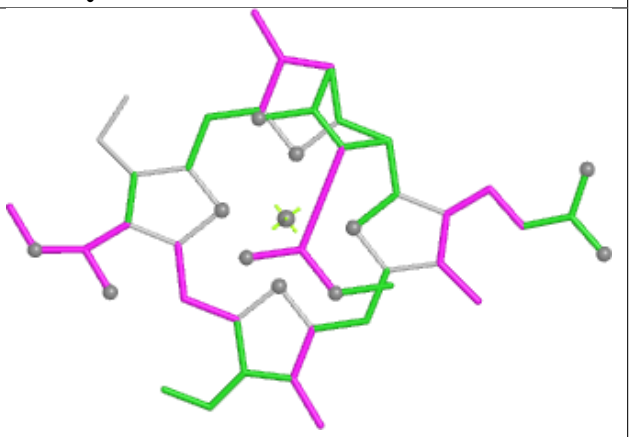
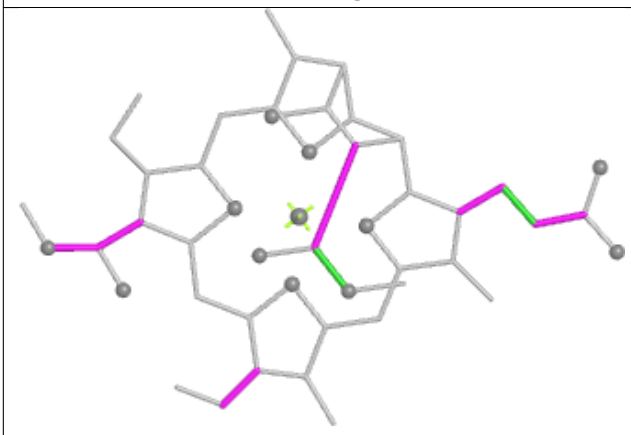
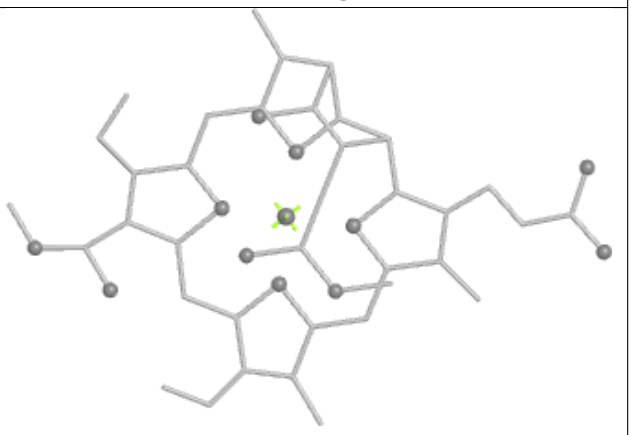
Rings

Ligand LHG D 302

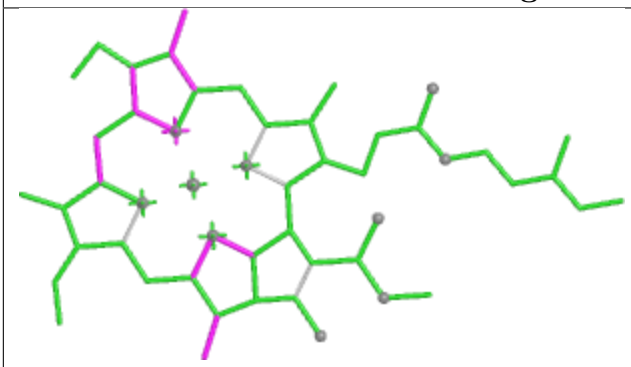


Ligand DD6 2 303

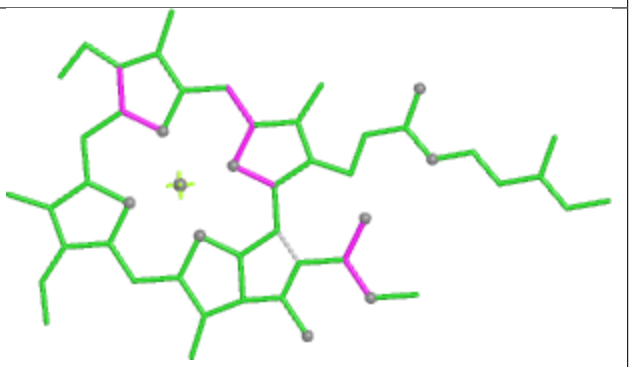


Ligand A1ECV Q 319	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

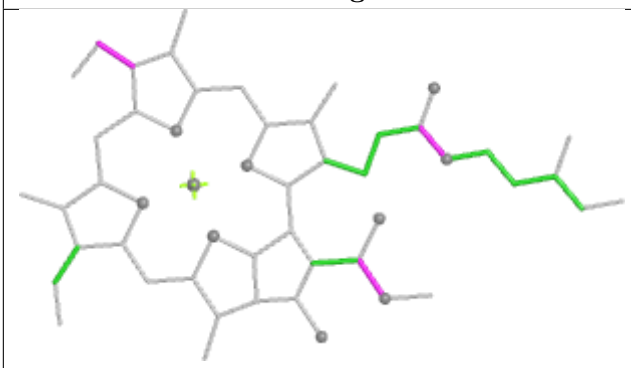
Ligand CLA M 317



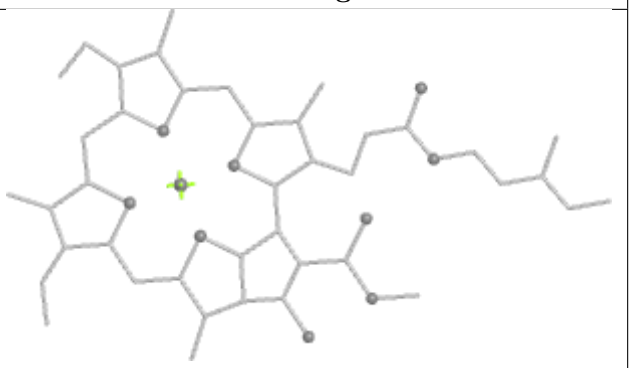
Bond lengths



Bond angles

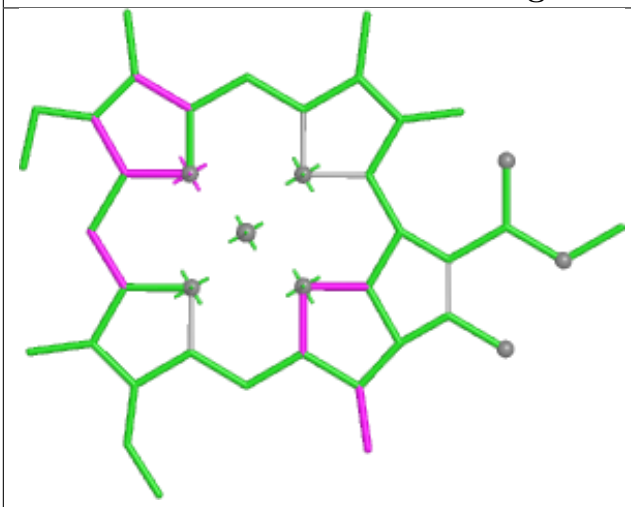


Torsions

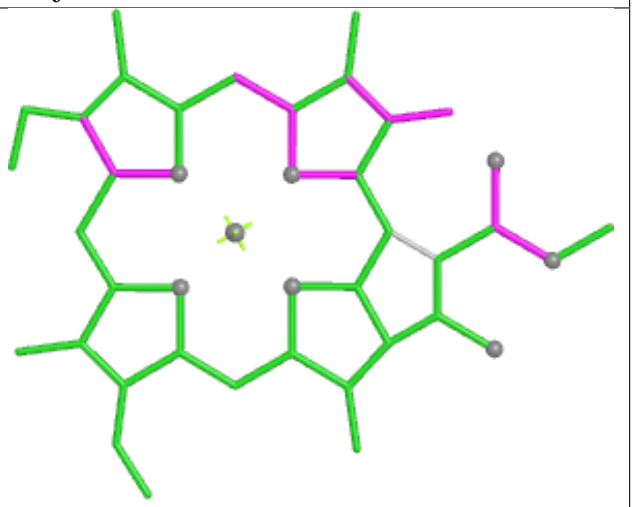


Rings

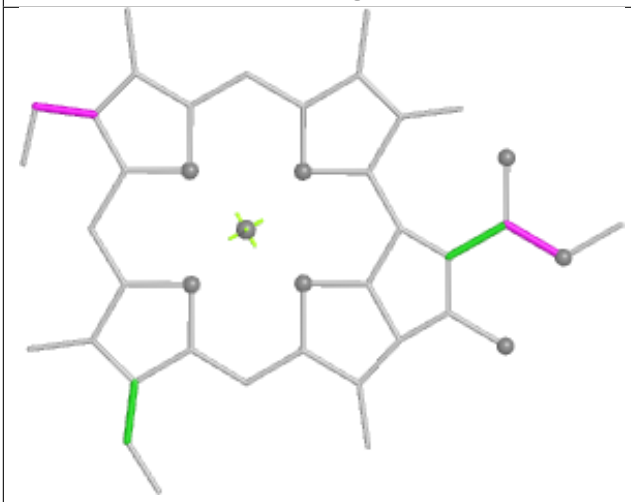
Ligand CLA y 307



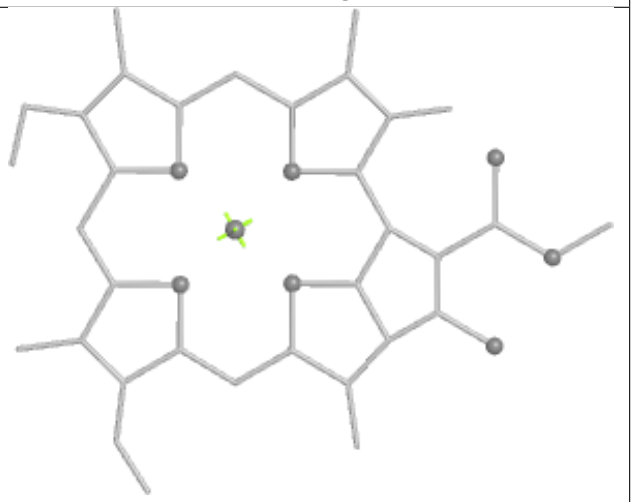
Bond lengths



Bond angles

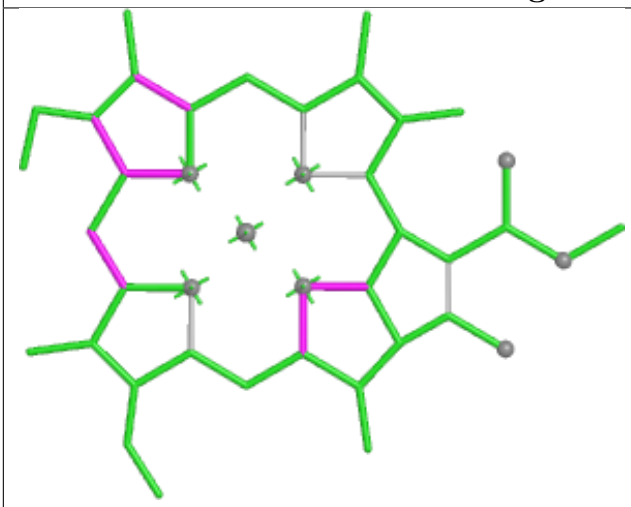


Torsions

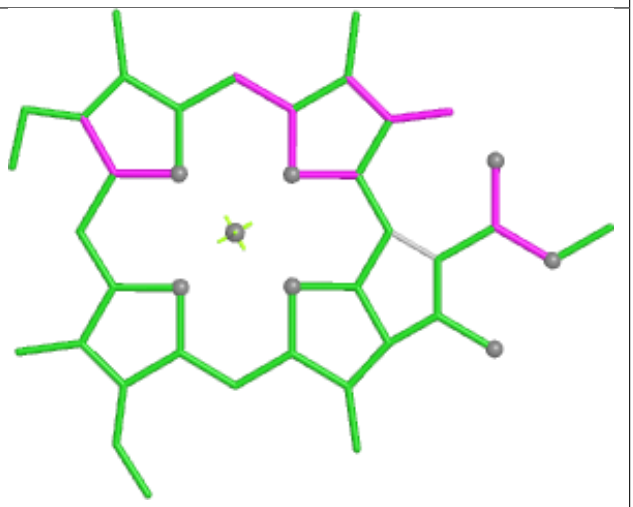


Rings

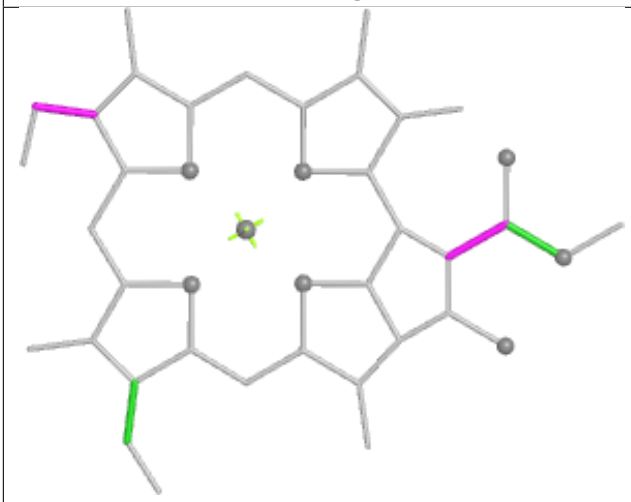
Ligand CLA 0 318



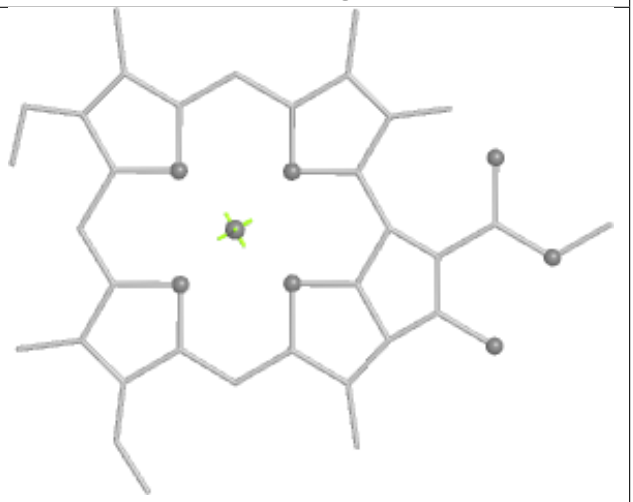
Bond lengths



Bond angles

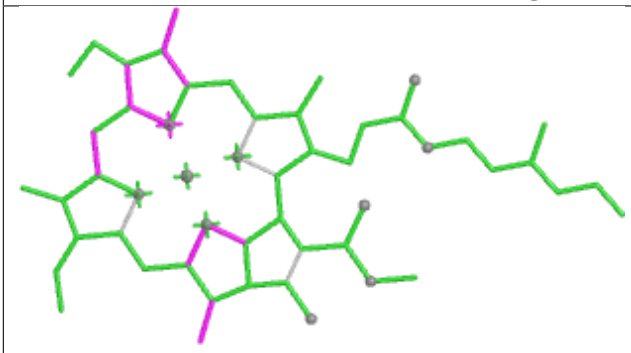


Torsions

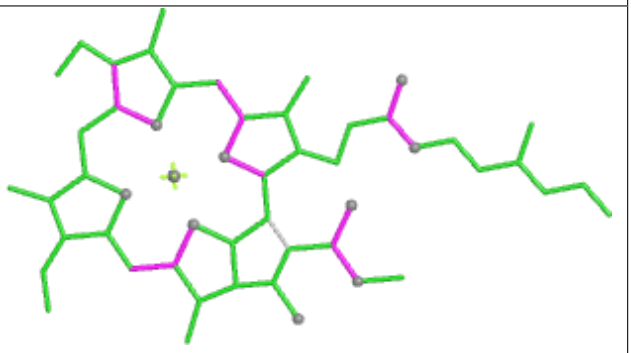


Rings

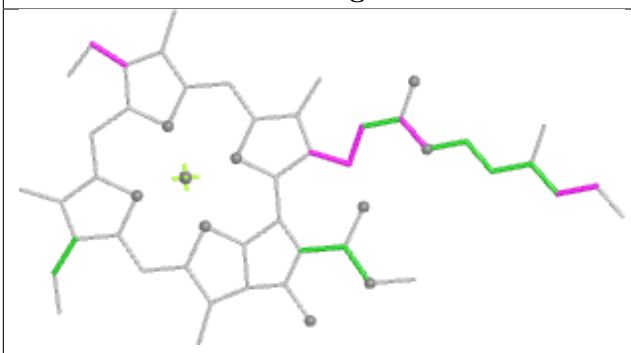
Ligand CLA E 316



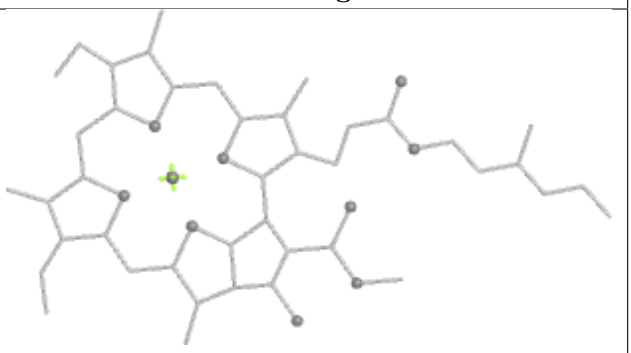
Bond lengths



Bond angles

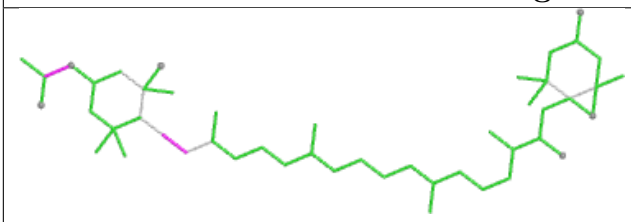


Torsions

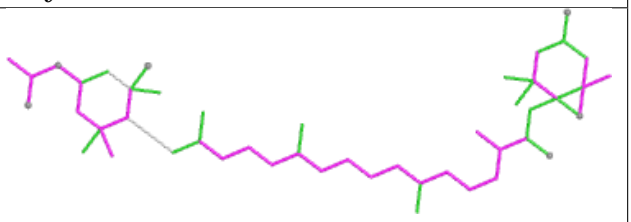


Rings

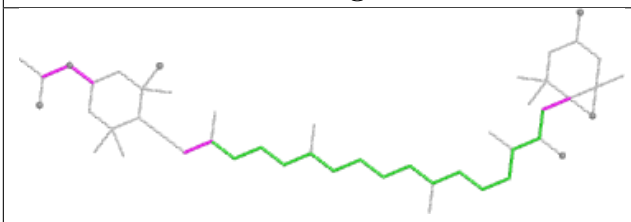
Ligand A86 y 306



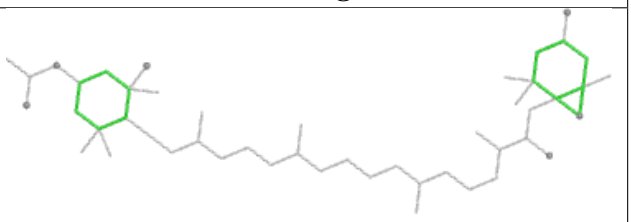
Bond lengths



Bond angles

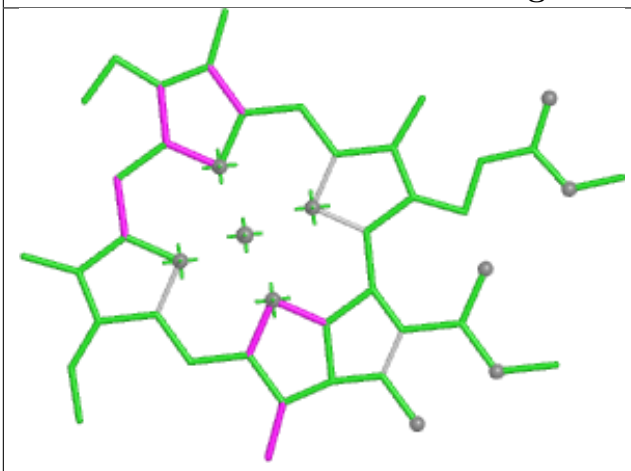


Torsions

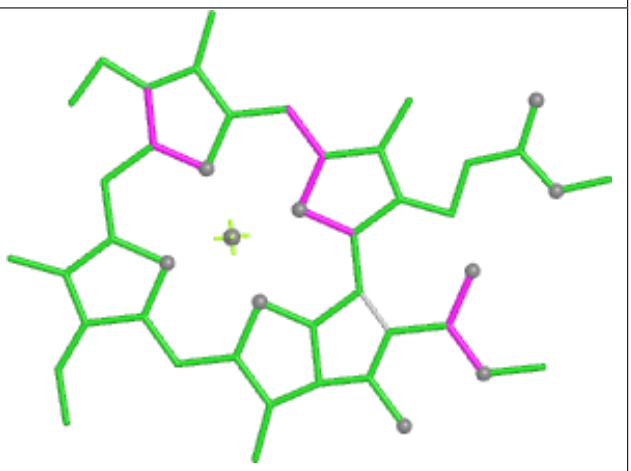


Rings

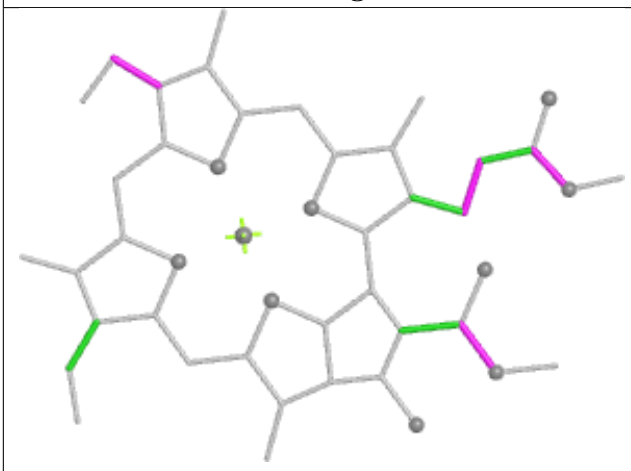
Ligand CLA J 316



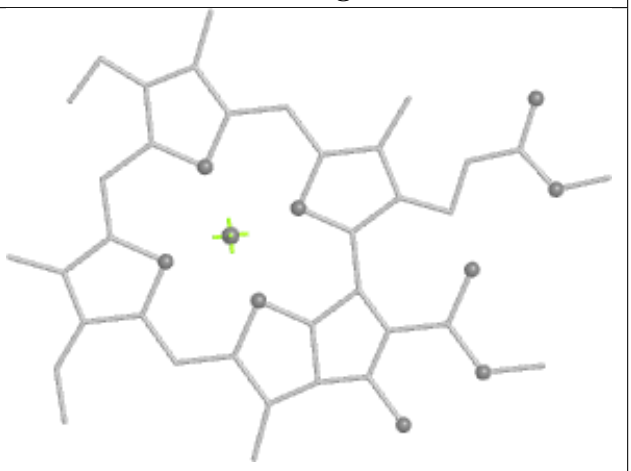
Bond lengths



Bond angles

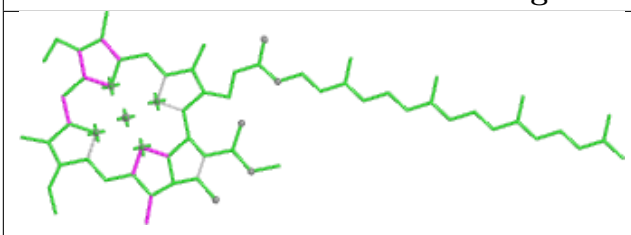


Torsions

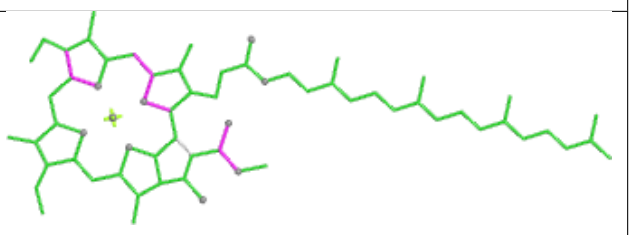


Rings

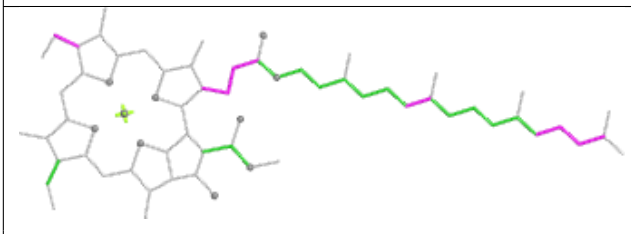
Ligand CLA I 309



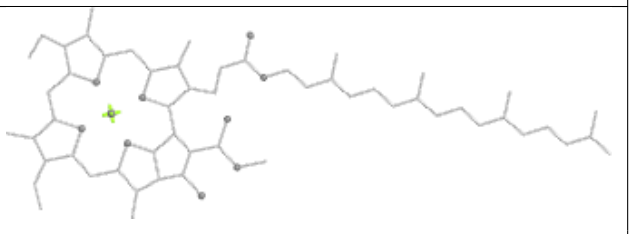
Bond lengths



Bond angles

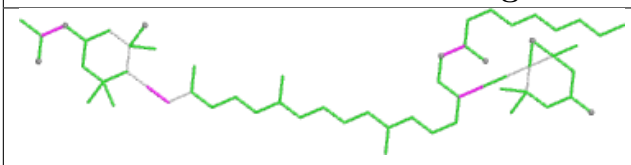


Torsions

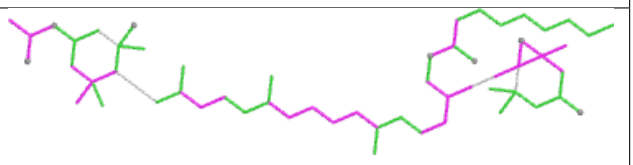


Rings

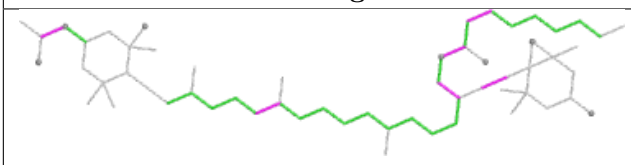
Ligand A1EB4 M 305



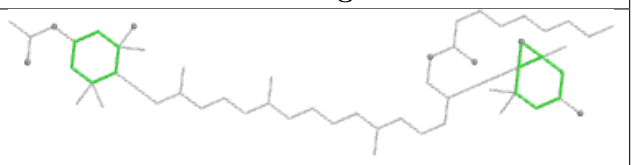
Bond lengths



Bond angles

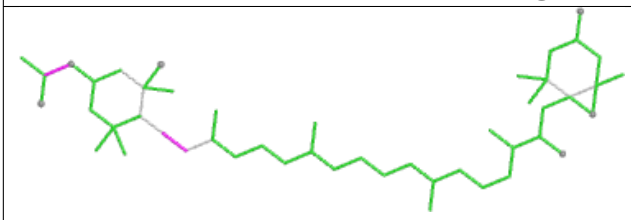


Torsions

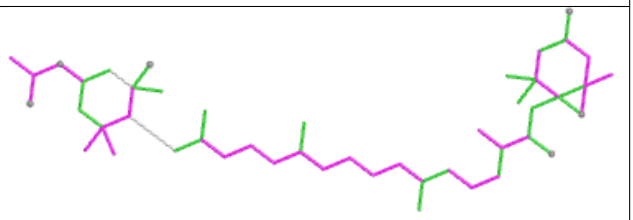


Rings

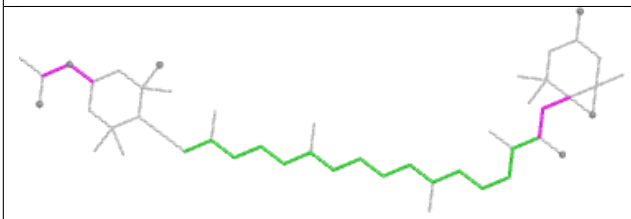
Ligand A86 S 307



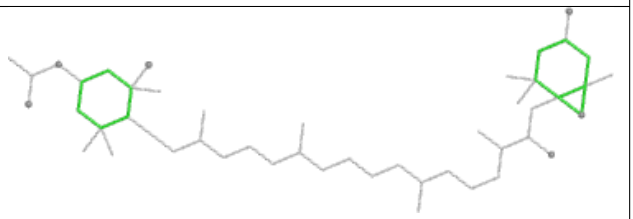
Bond lengths



Bond angles

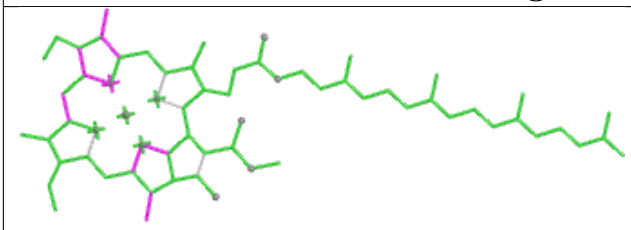


Torsions

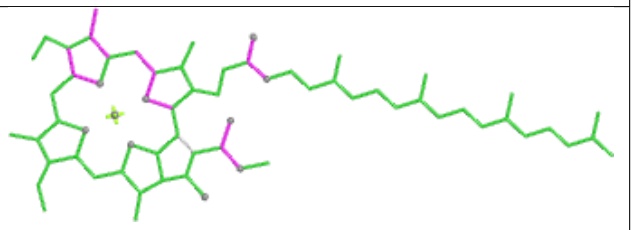


Rings

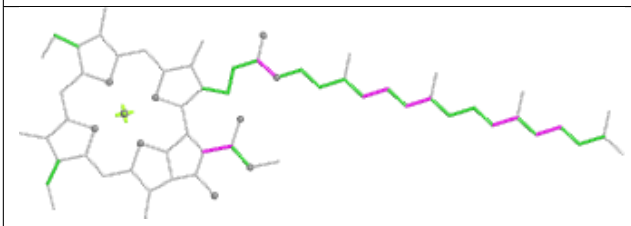
Ligand CLA b 812



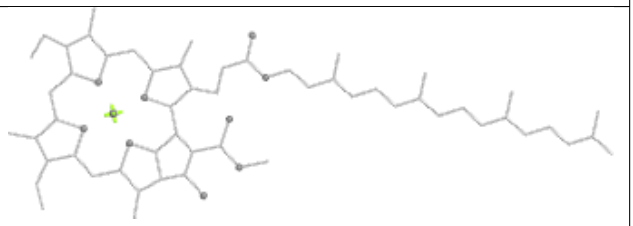
Bond lengths



Bond angles

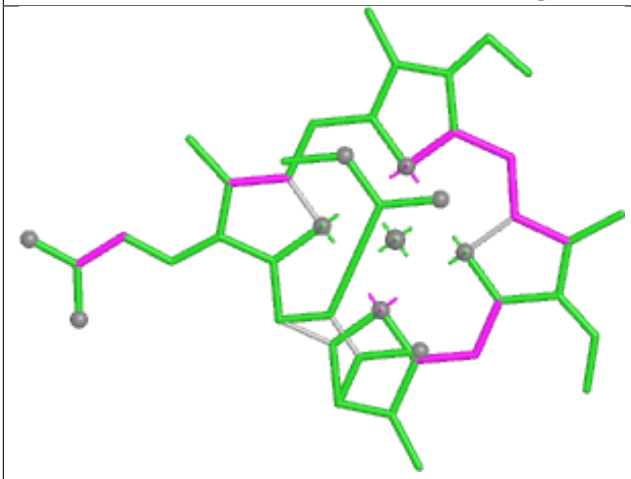


Torsions

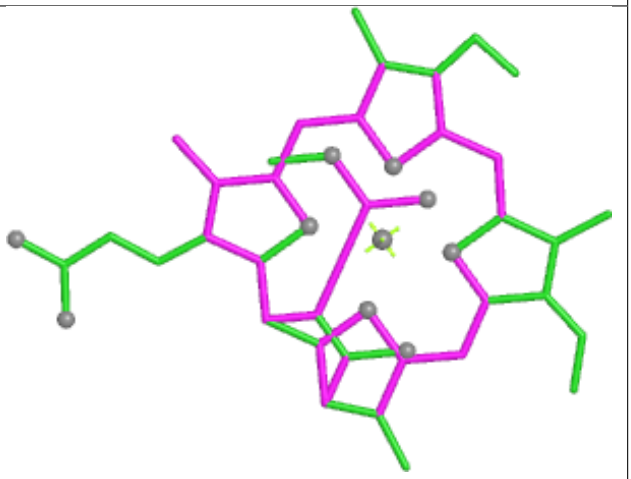


Rings

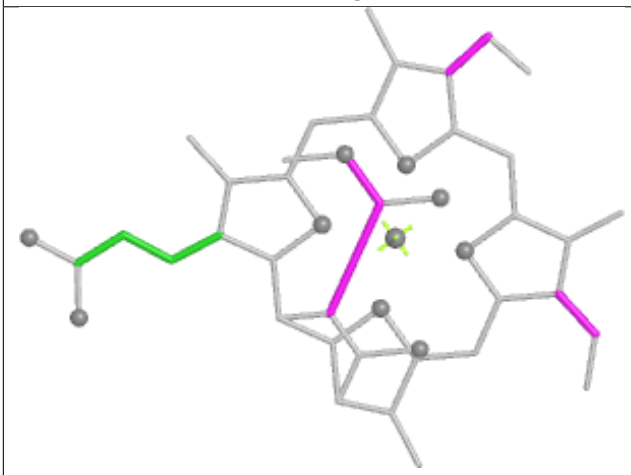
Ligand KC2 I 303



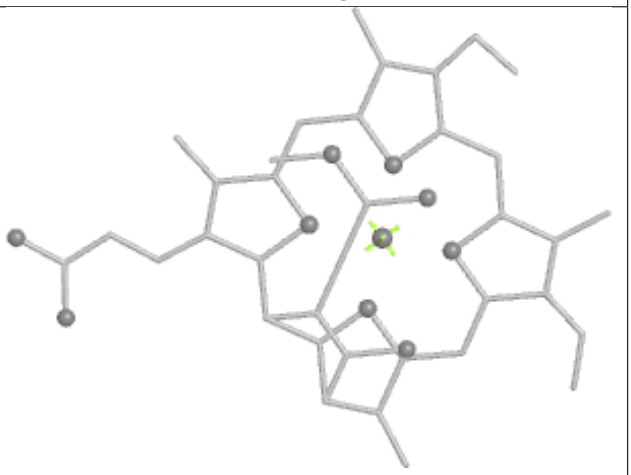
Bond lengths



Bond angles

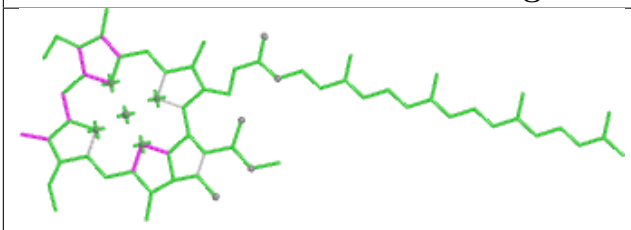


Torsions

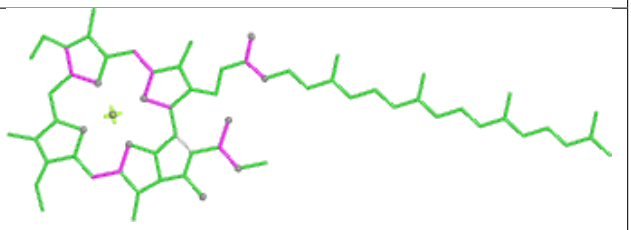


Rings

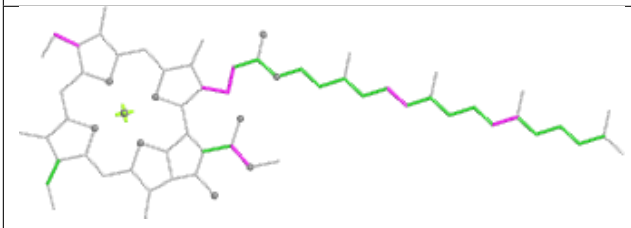
Ligand CLA H 313



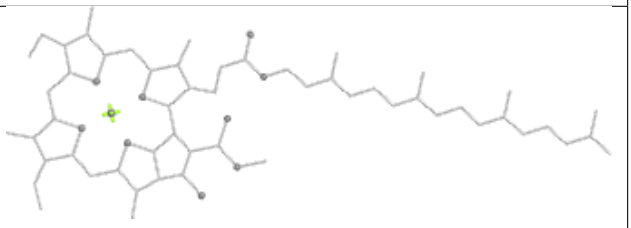
Bond lengths



Bond angles

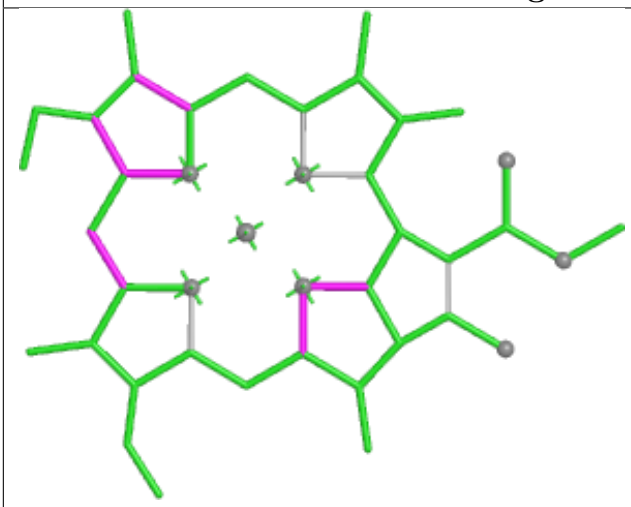


Torsions

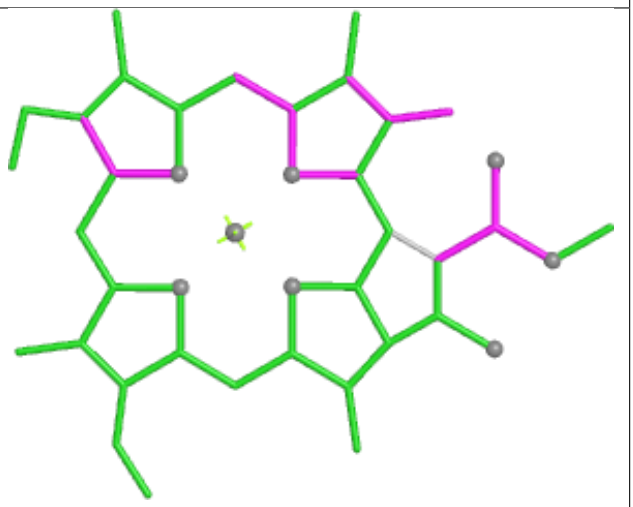


Rings

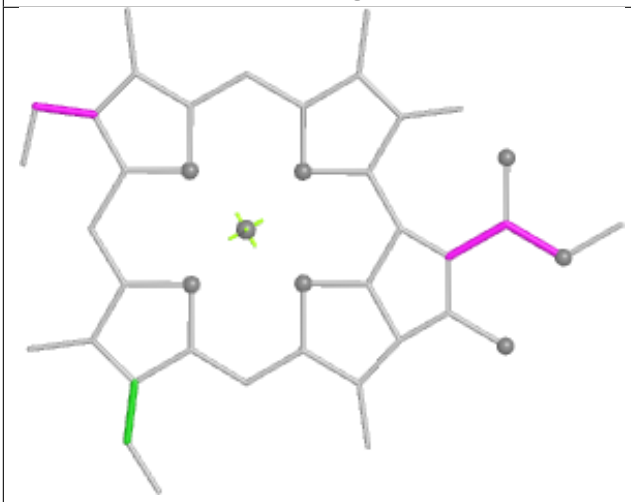
Ligand CLA x 317



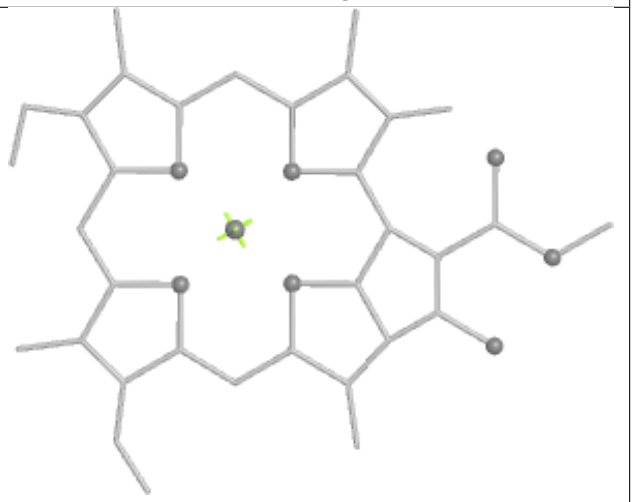
Bond lengths



Bond angles

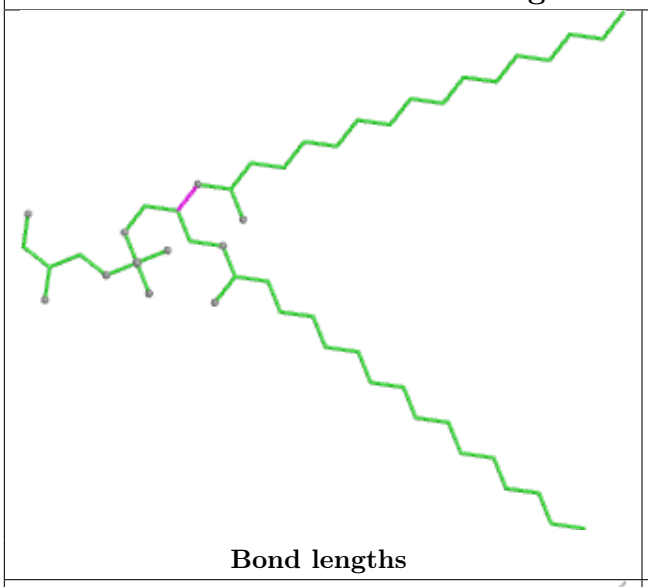


Torsions

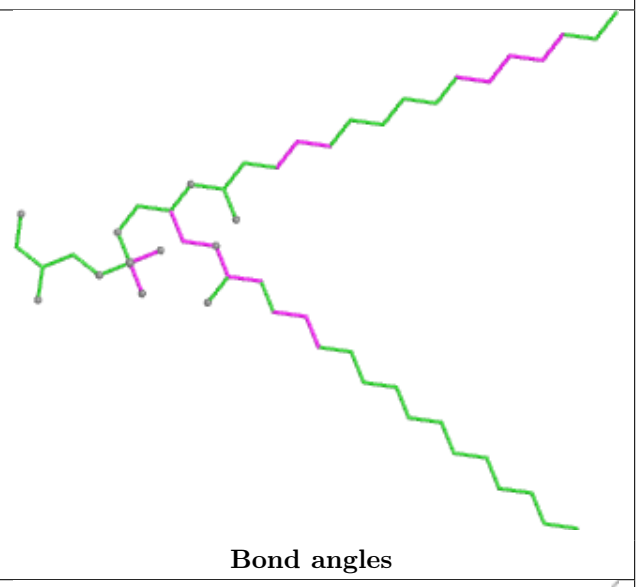


Rings

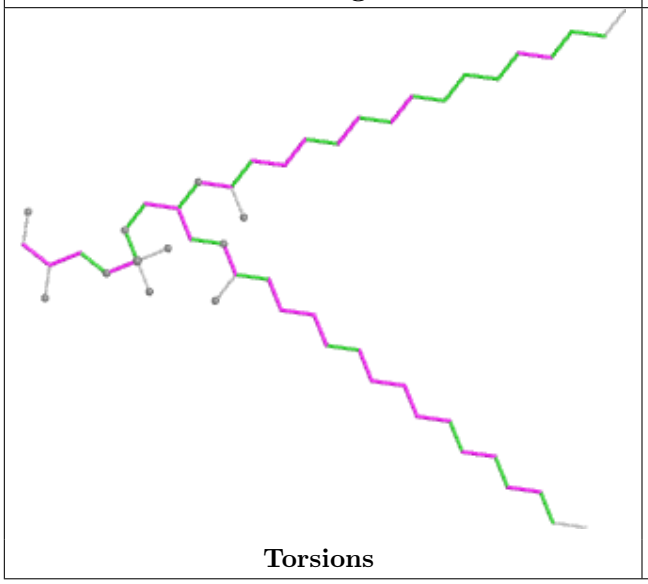
Ligand LHG a 840



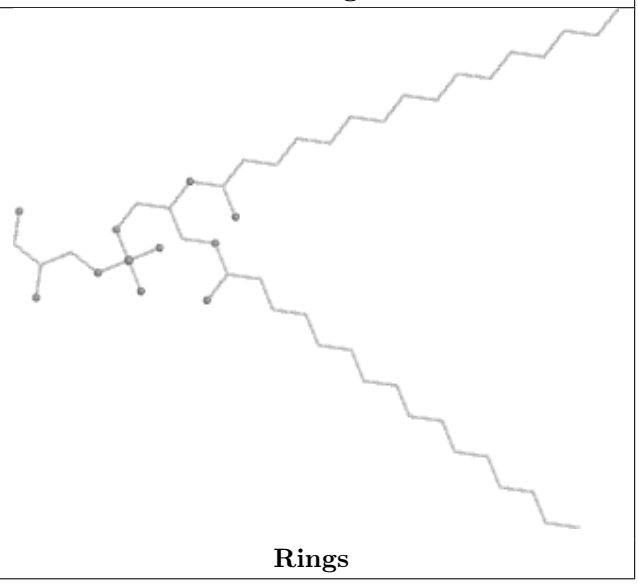
Bond lengths



Bond angles

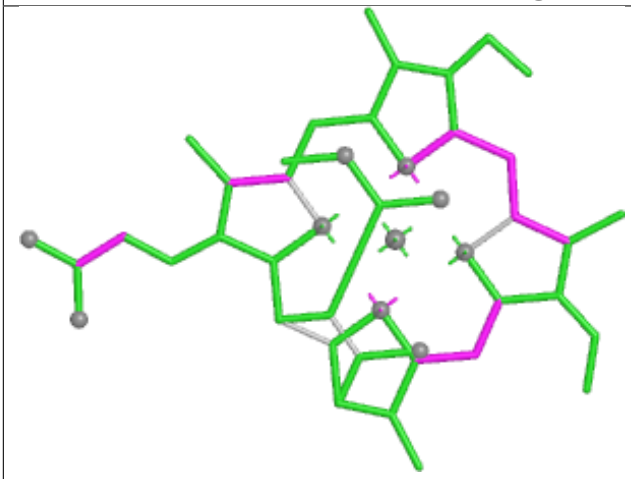


Torsions

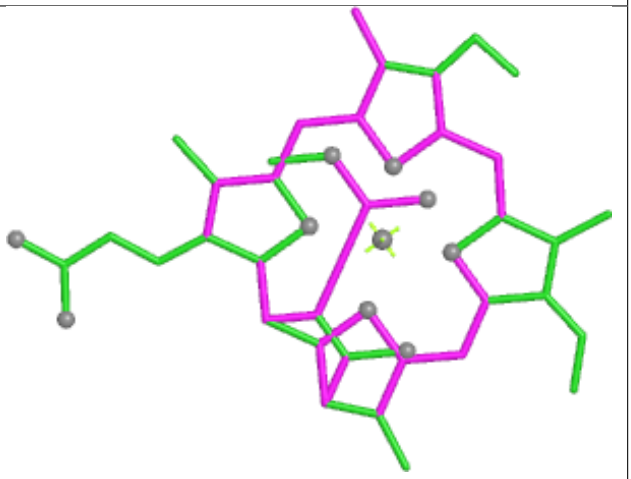


Rings

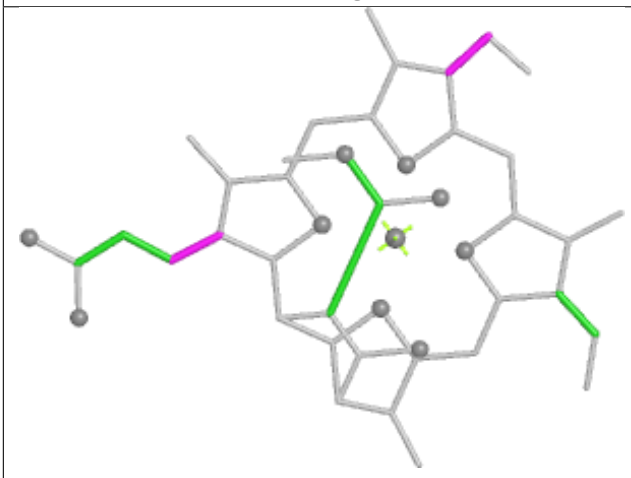
Ligand KC2 0 316



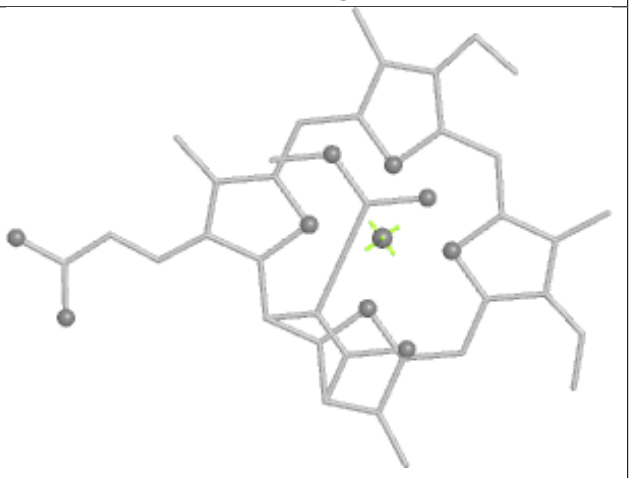
Bond lengths



Bond angles

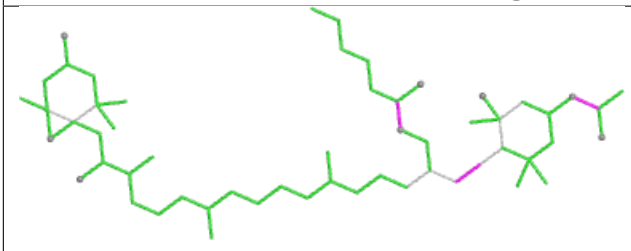


Torsions

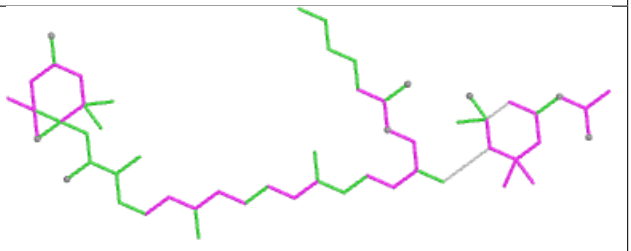


Rings

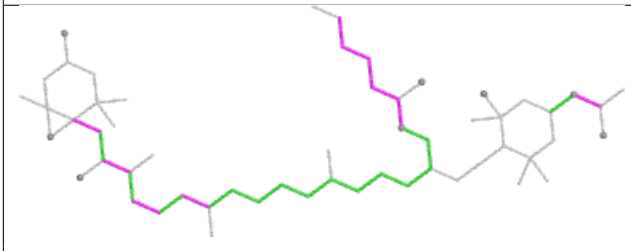
Ligand A1EB1 L 303



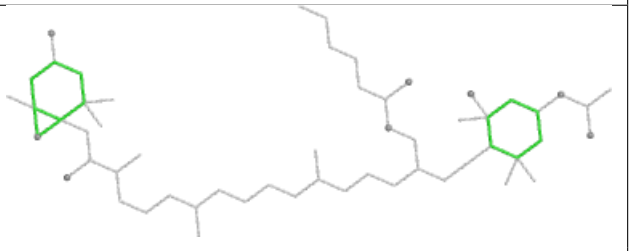
Bond lengths



Bond angles

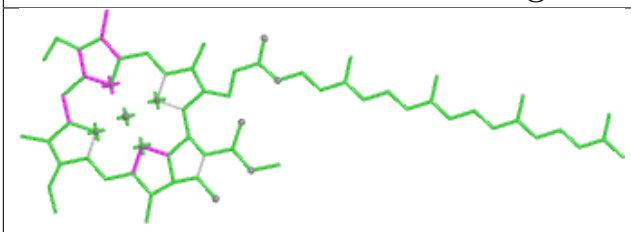


Torsions

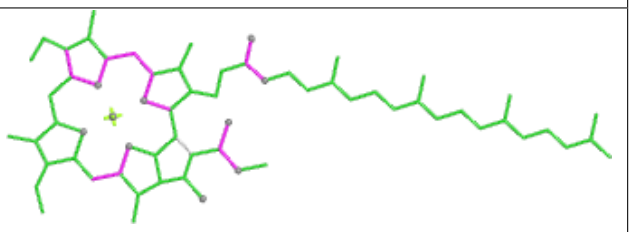


Rings

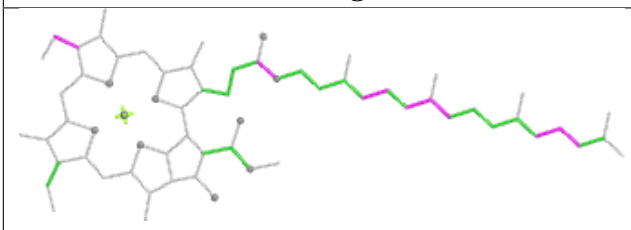
Ligand CLA b 821



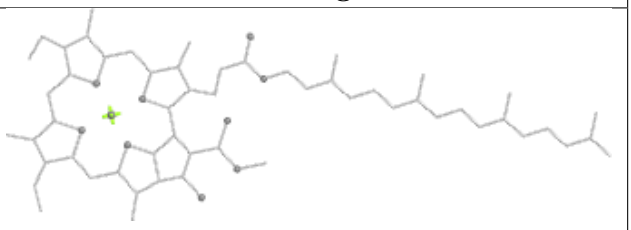
Bond lengths



Bond angles



Torsions

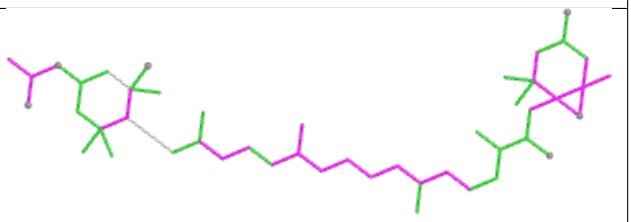


Rings

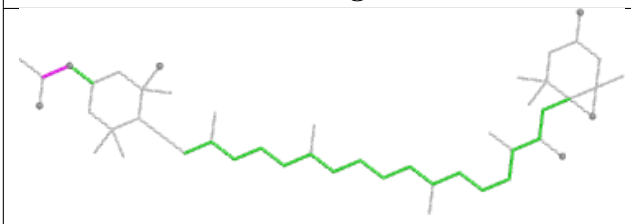
Ligand A86 F 302



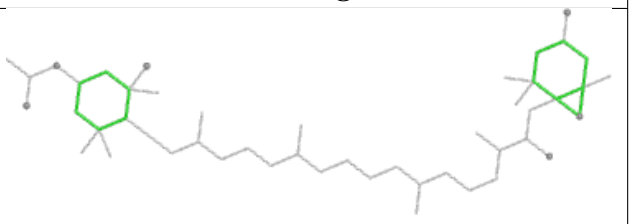
Bond lengths



Bond angles

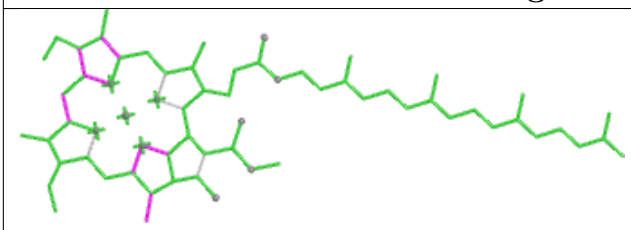


Torsions

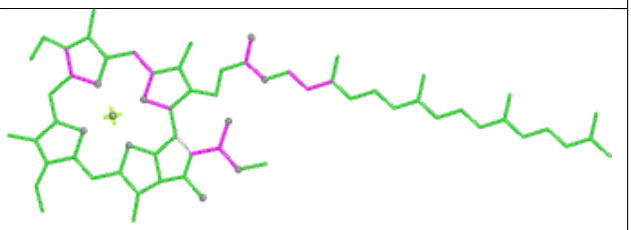


Rings

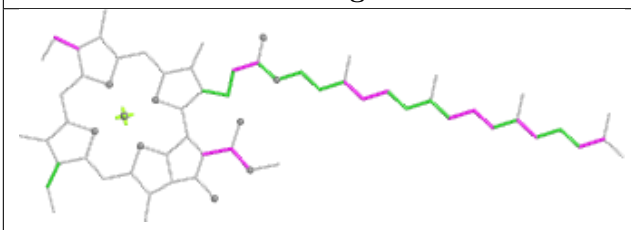
Ligand CLA b 806



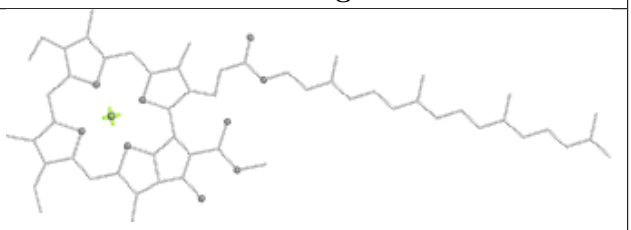
Bond lengths



Bond angles

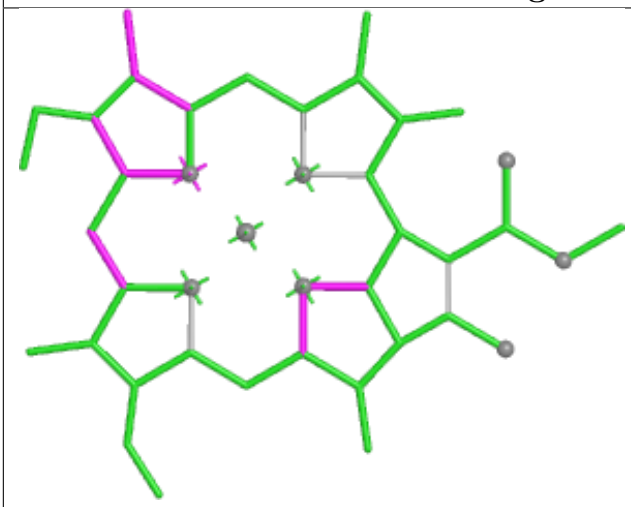


Torsions

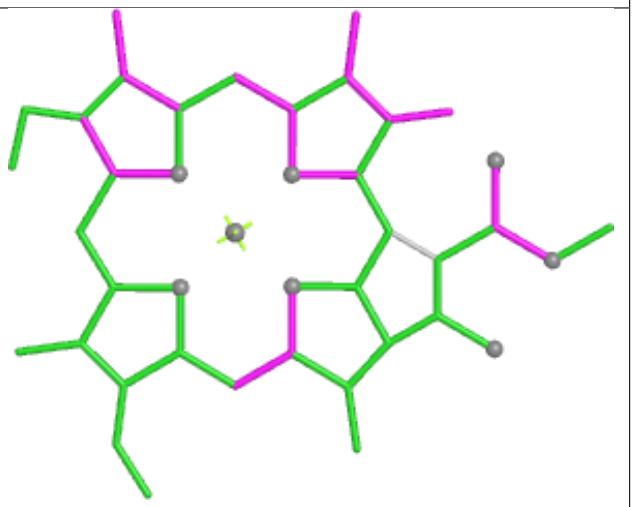


Rings

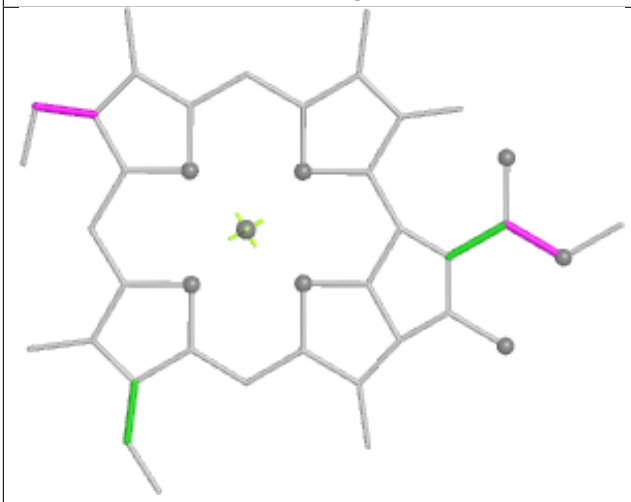
Ligand CLA 9 320



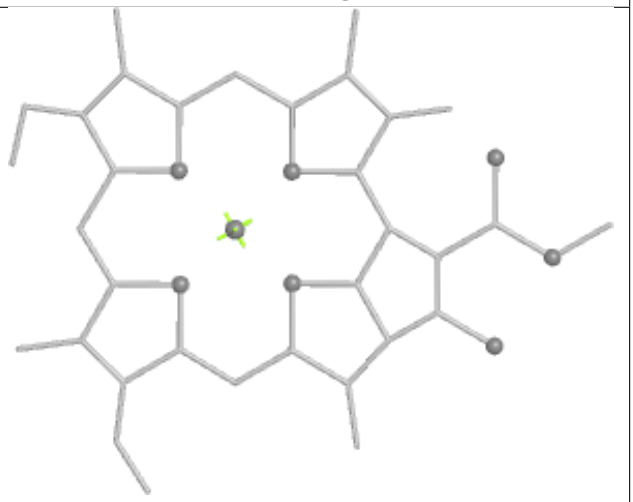
Bond lengths



Bond angles

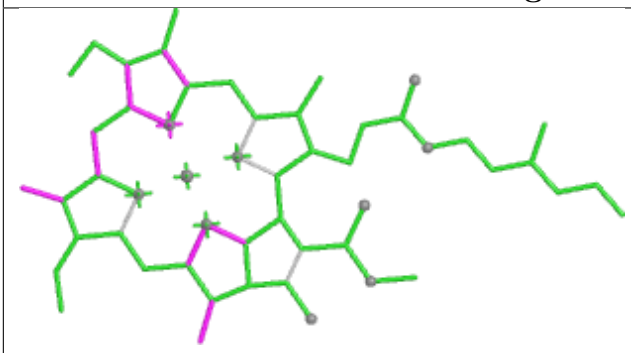


Torsions

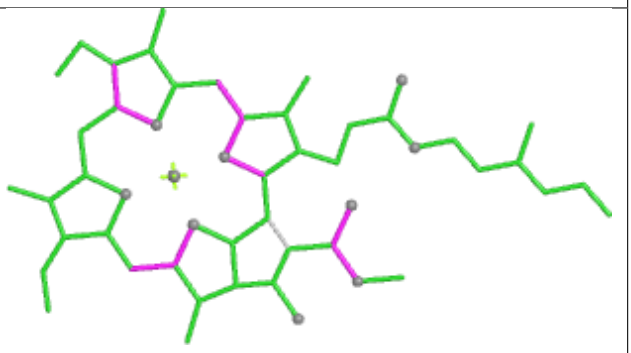


Rings

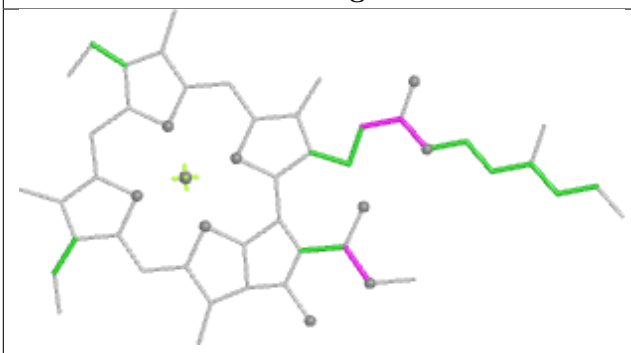
Ligand CLA T 310



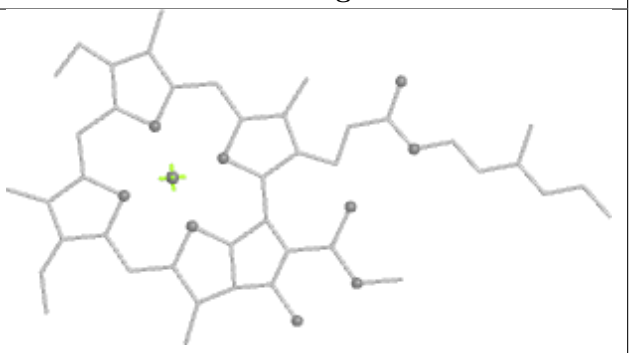
Bond lengths



Bond angles

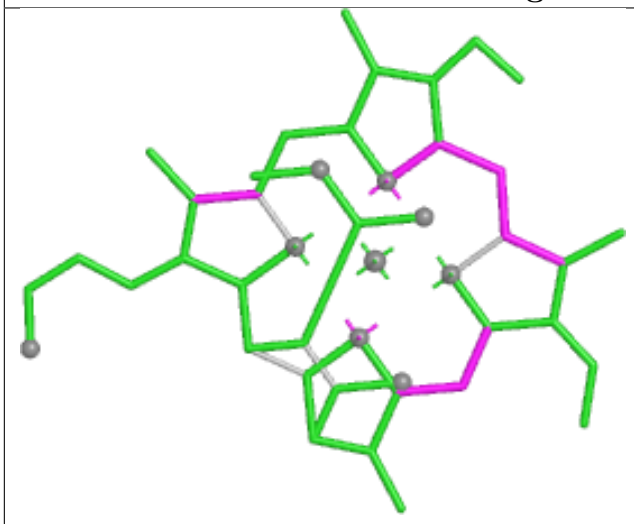


Torsions



Rings

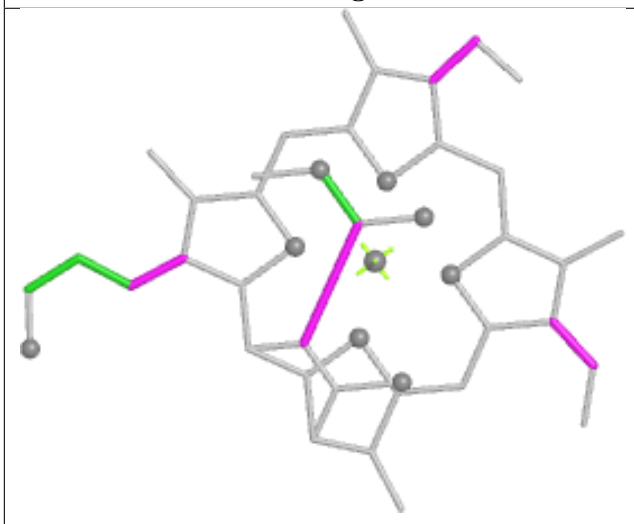
Ligand KC2 X 314



Bond lengths



Bond angles

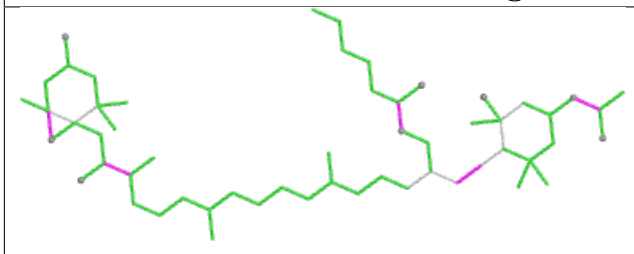


Torsions

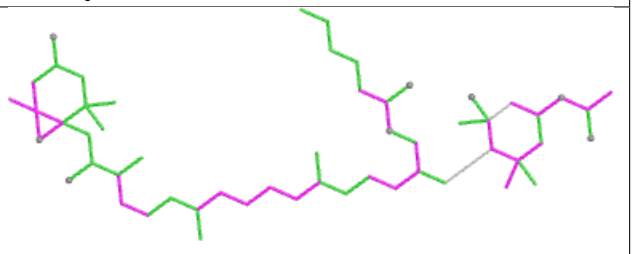


Rings

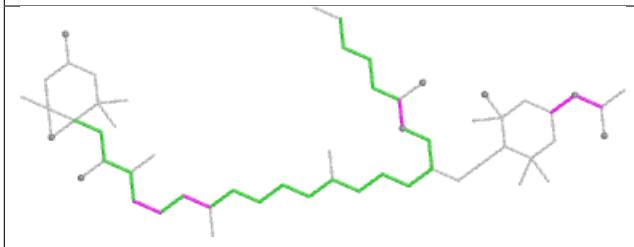
Ligand A1EB1 Q 307



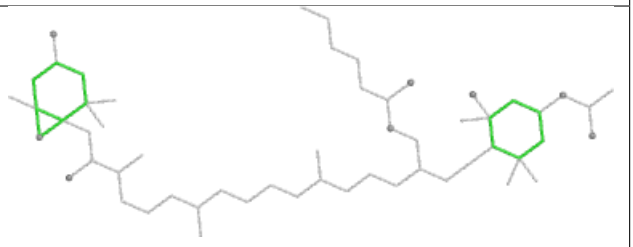
Bond lengths



Bond angles

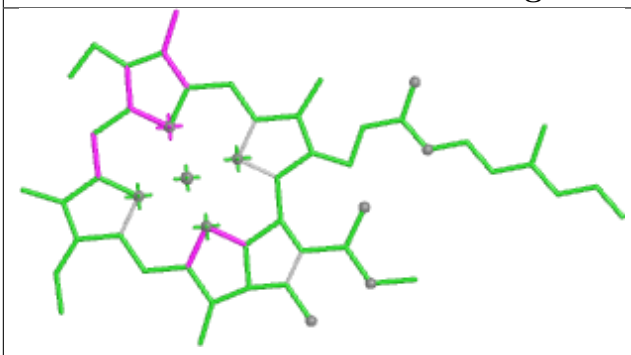


Torsions

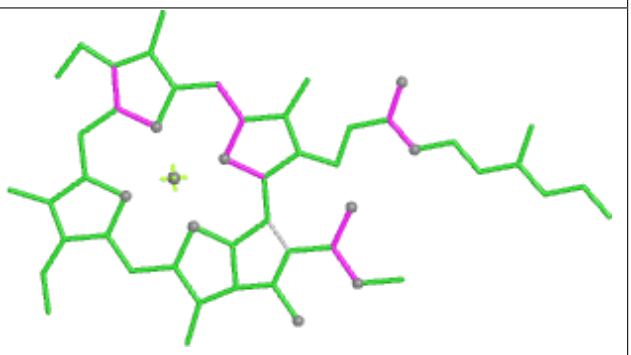


Rings

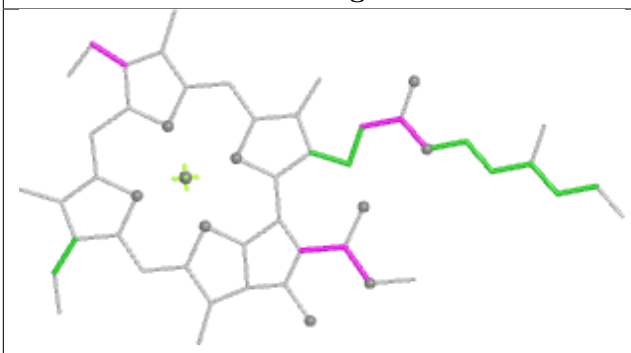
Ligand CLA T 320



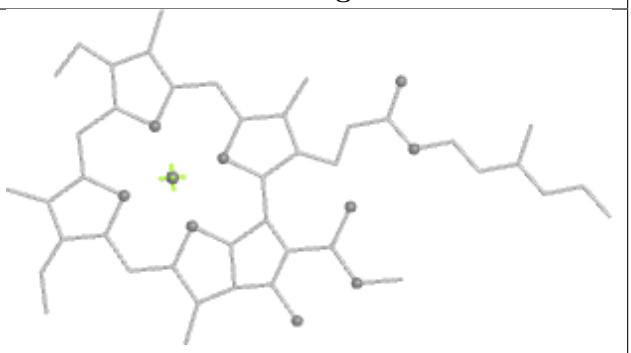
Bond lengths



Bond angles

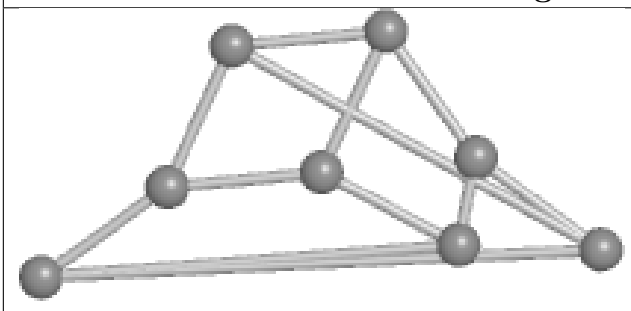


Torsions

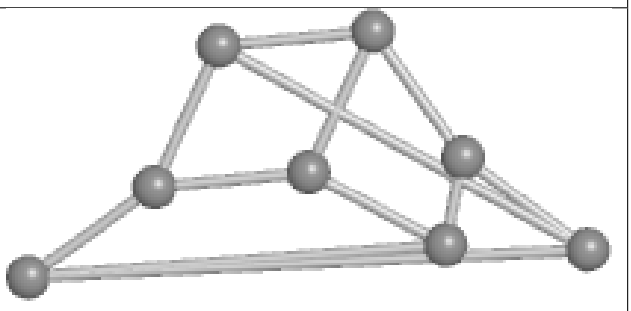


Rings

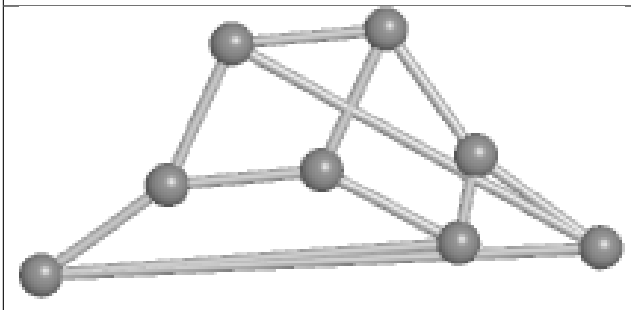
Ligand SF4 b 804



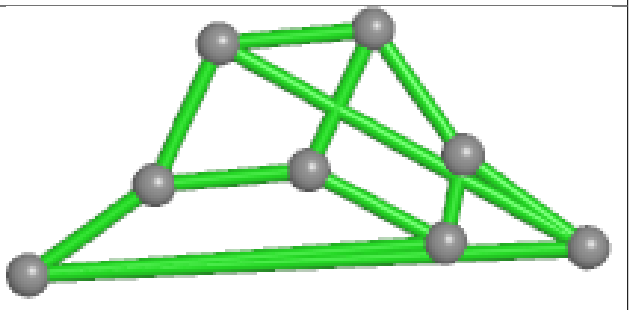
Bond lengths



Bond angles

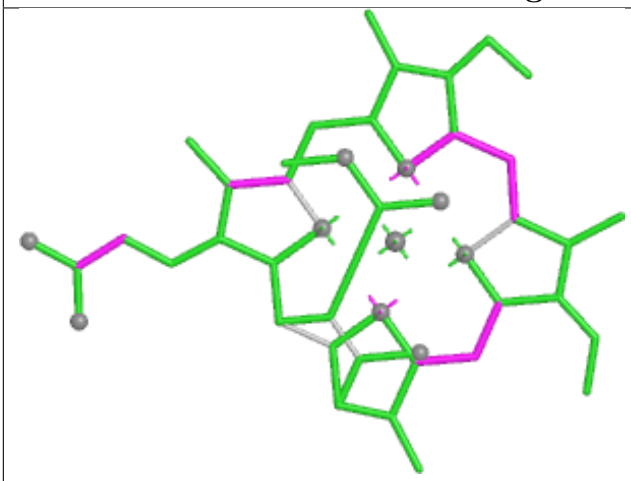


Torsions

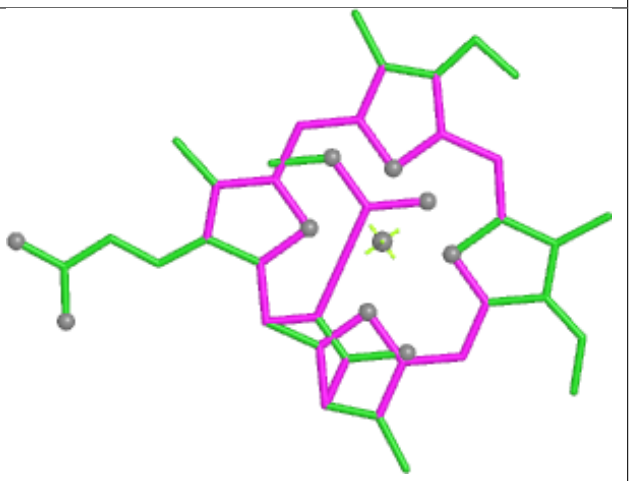


Rings

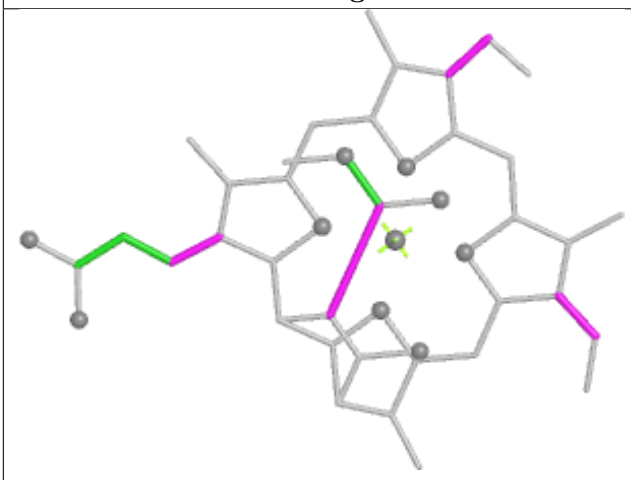
Ligand KC2 X 312



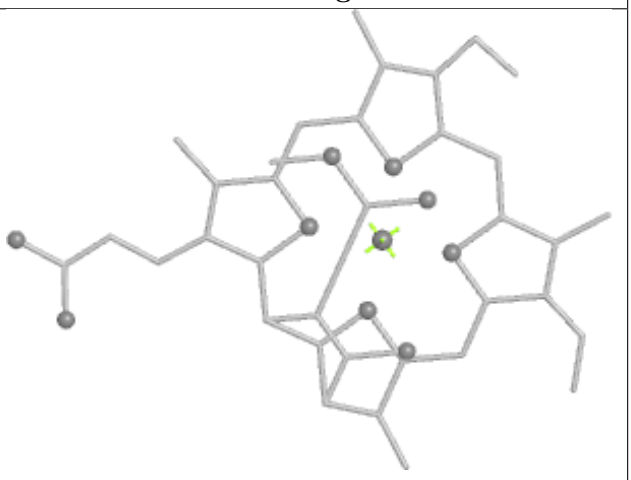
Bond lengths



Bond angles

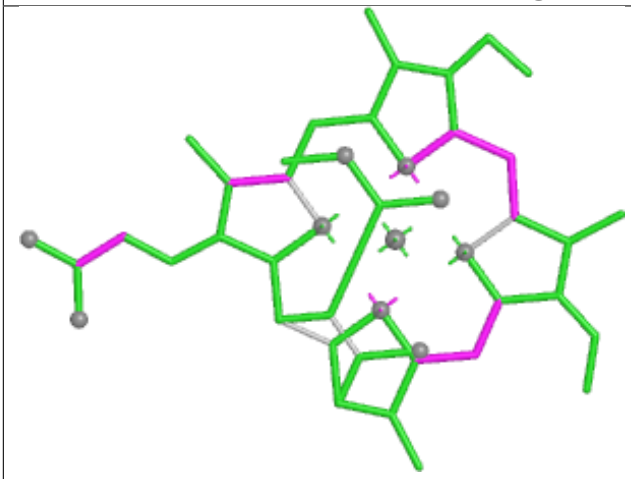


Torsions

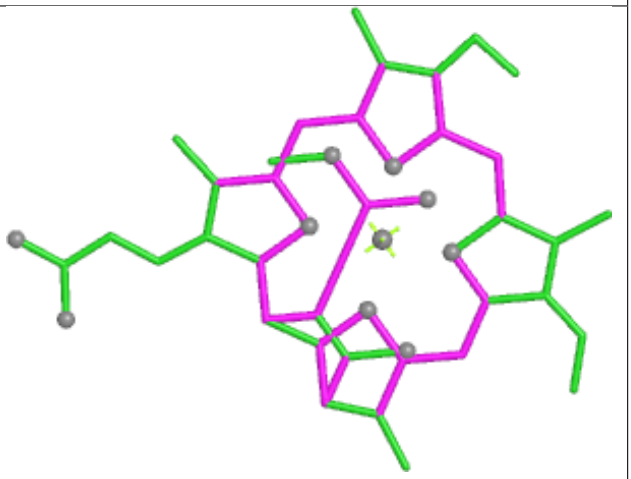


Rings

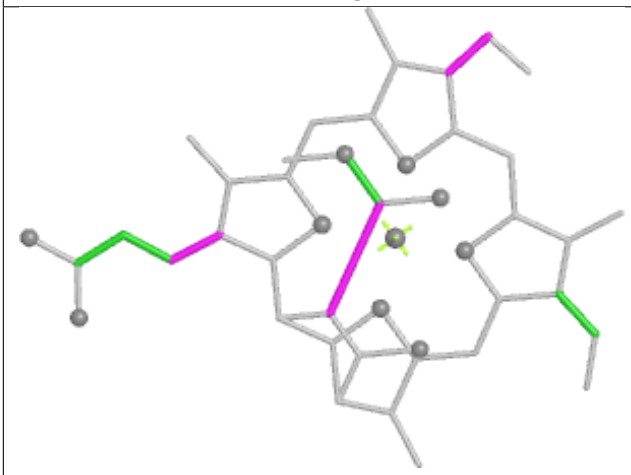
Ligand KC2 4 317



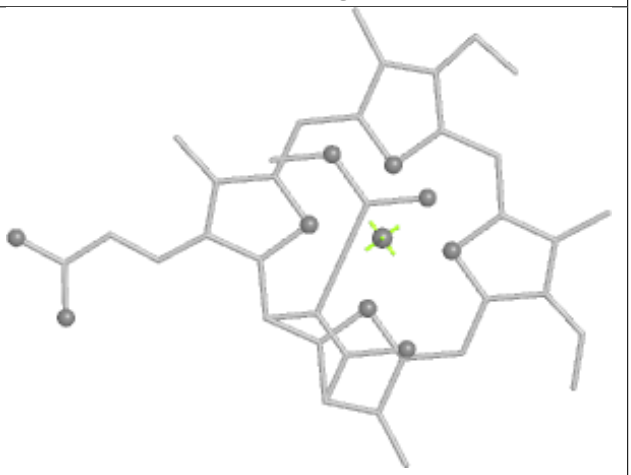
Bond lengths



Bond angles

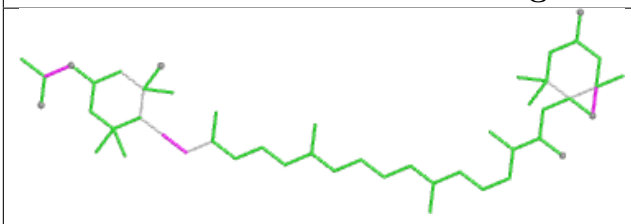


Torsions

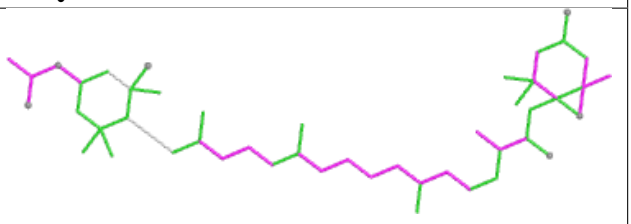


Rings

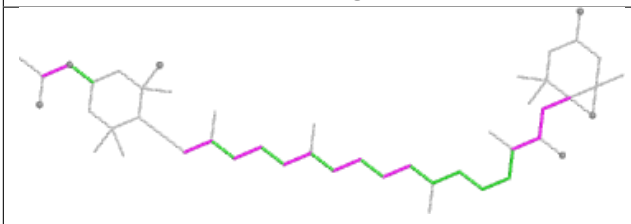
Ligand A86 Q 305



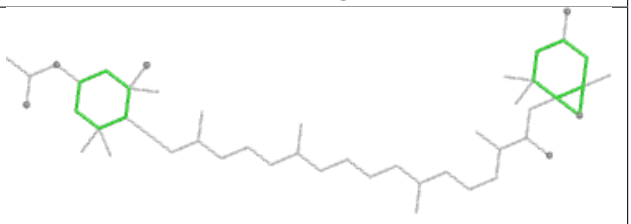
Bond lengths



Bond angles

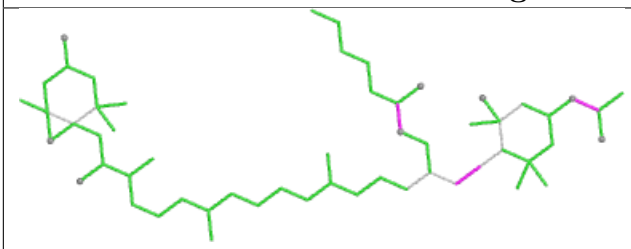


Torsions

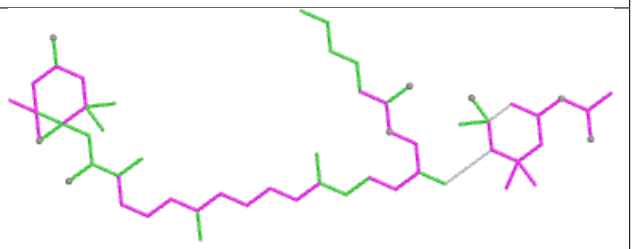


Rings

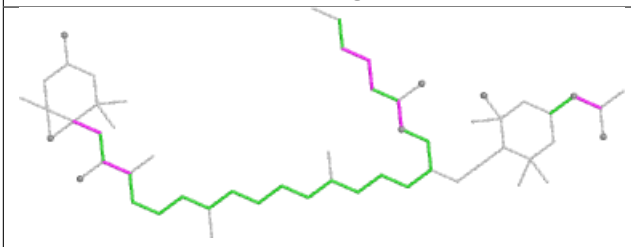
Ligand A1EB1 4 304



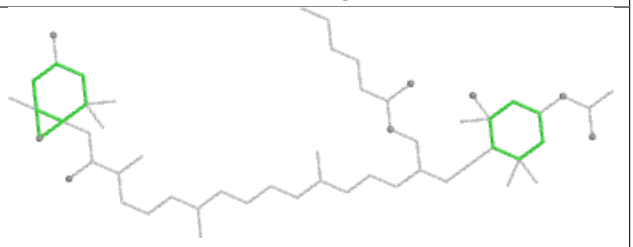
Bond lengths



Bond angles

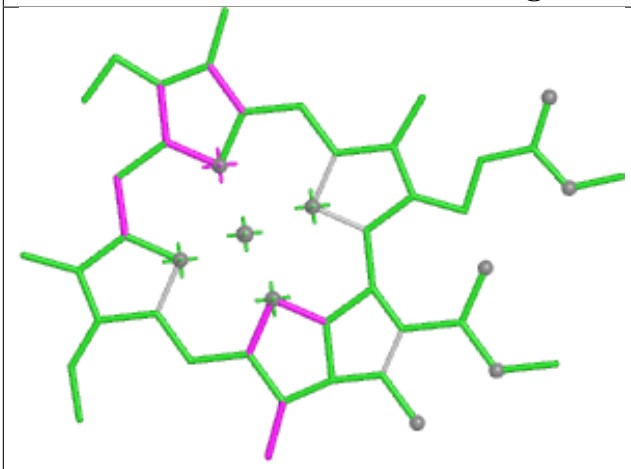


Torsions

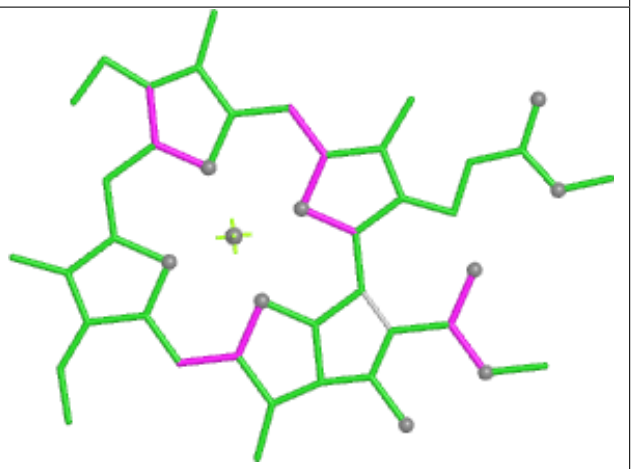


Rings

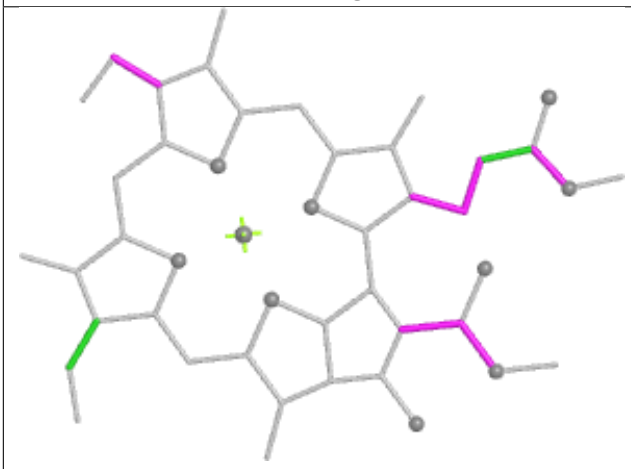
Ligand CLA E 318



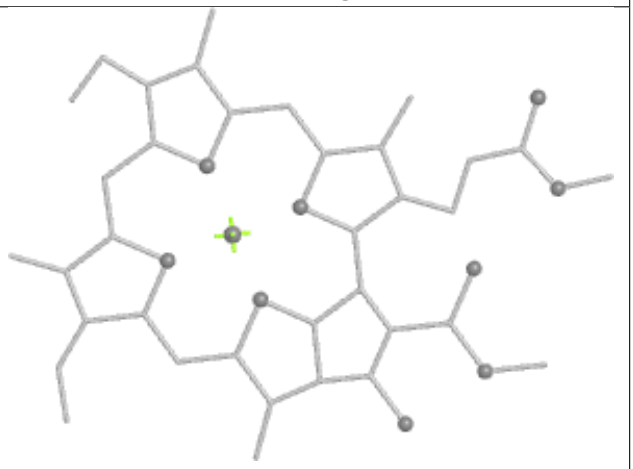
Bond lengths



Bond angles

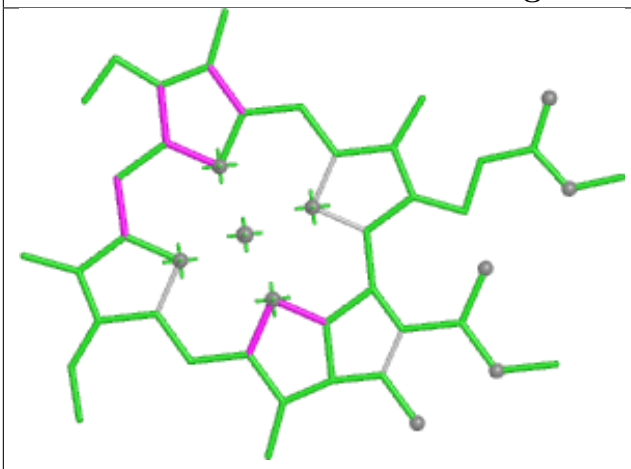


Torsions

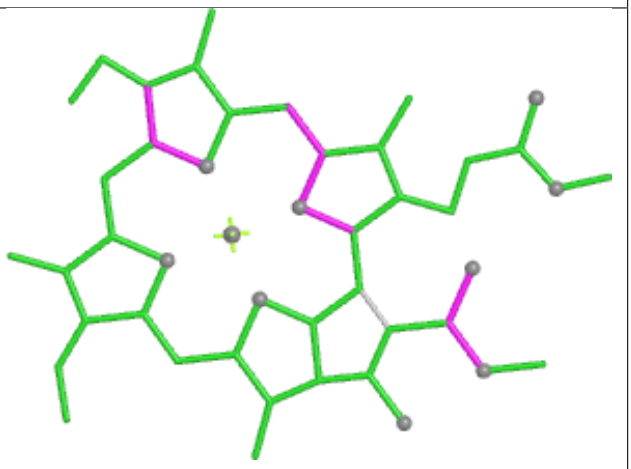


Rings

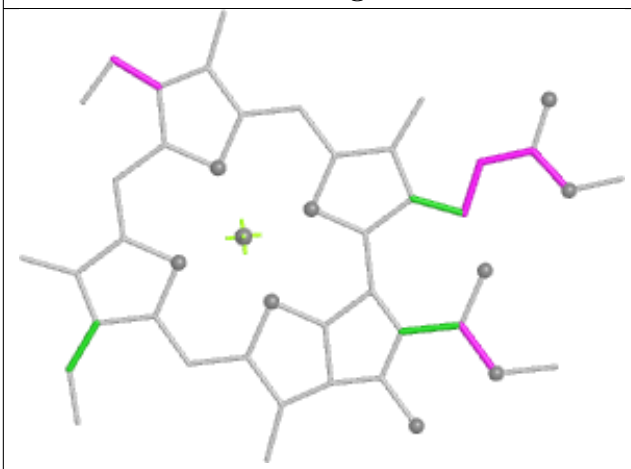
Ligand CLA Y 304



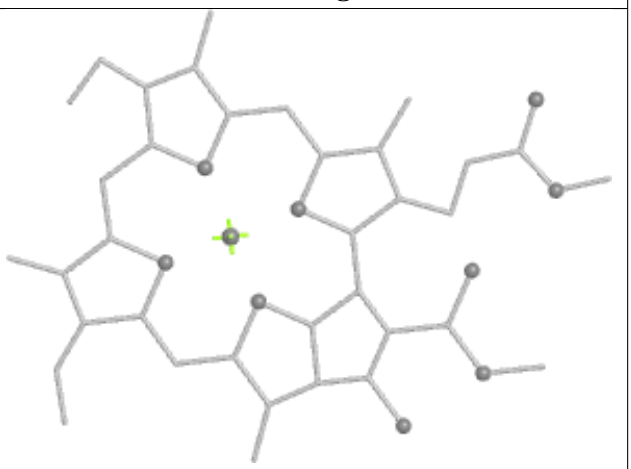
Bond lengths



Bond angles

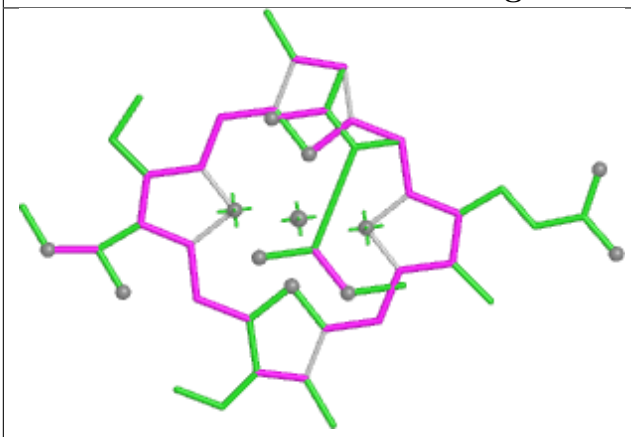


Torsions

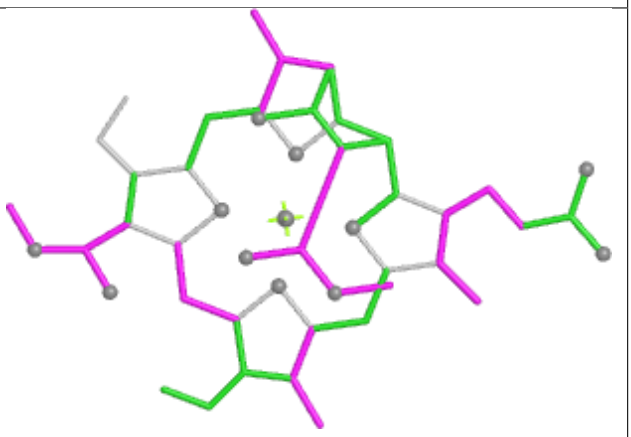


Rings

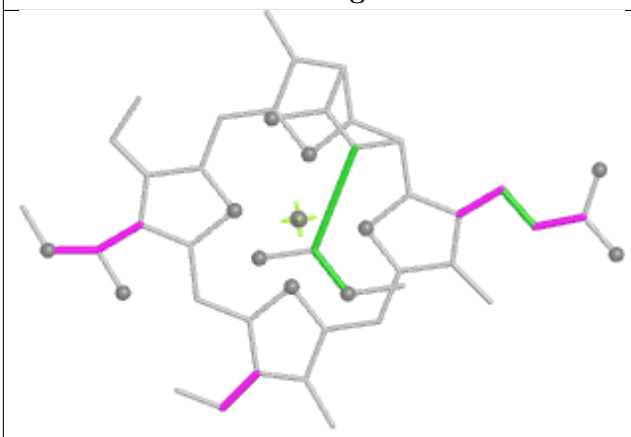
Ligand A1ECV 4 321



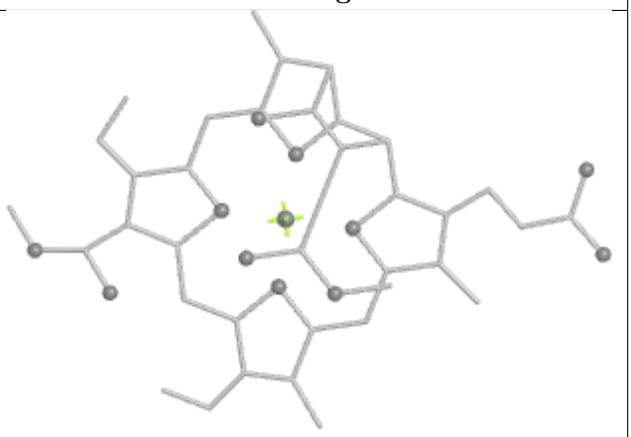
Bond lengths



Bond angles

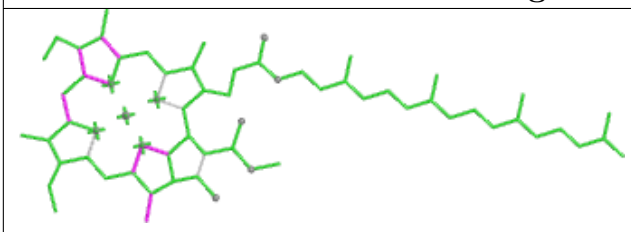


Torsions

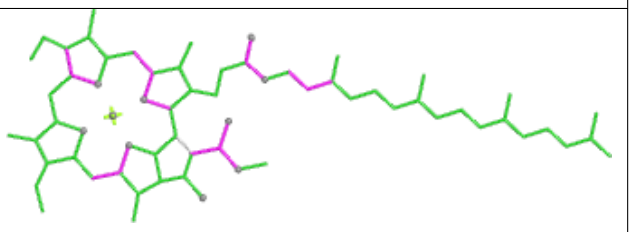


Rings

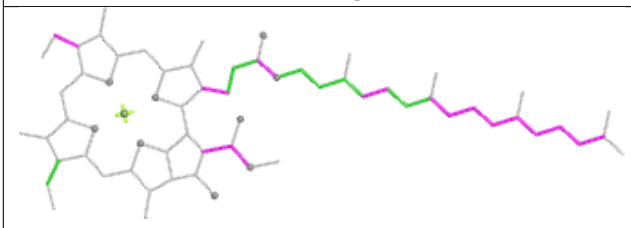
Ligand CLA 3 312



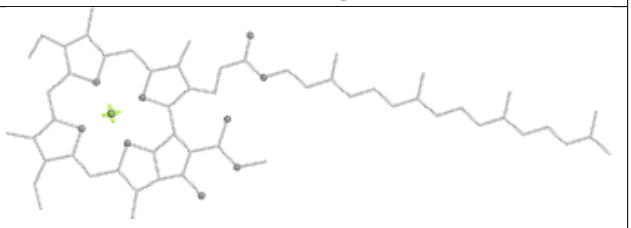
Bond lengths



Bond angles

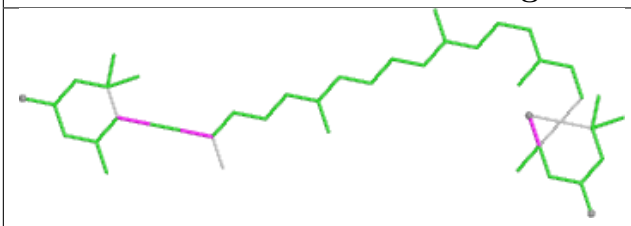


Torsions

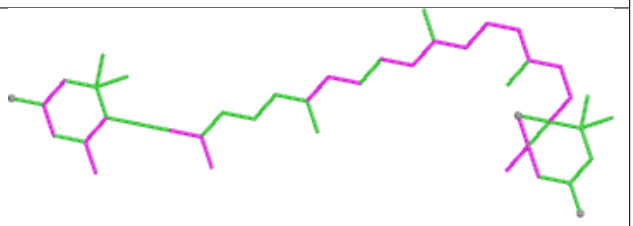


Rings

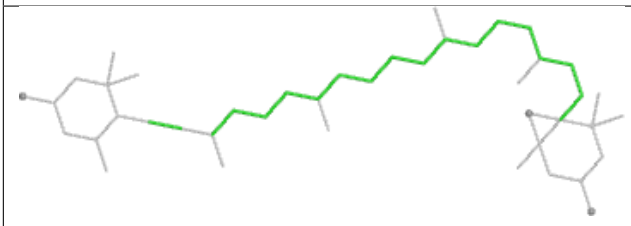
Ligand DD6 M 304



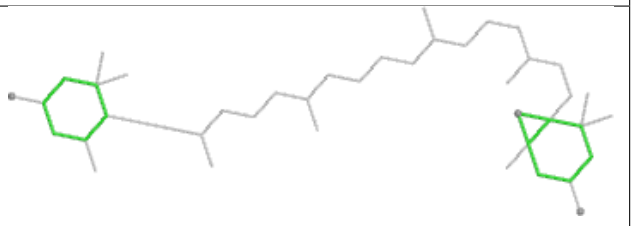
Bond lengths



Bond angles

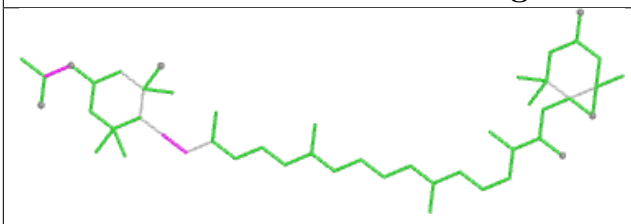


Torsions

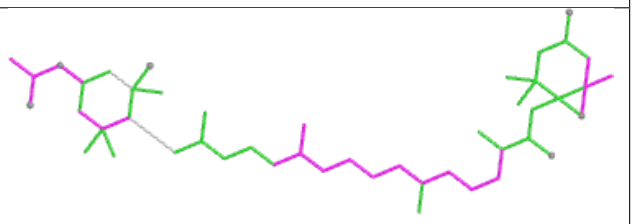


Rings

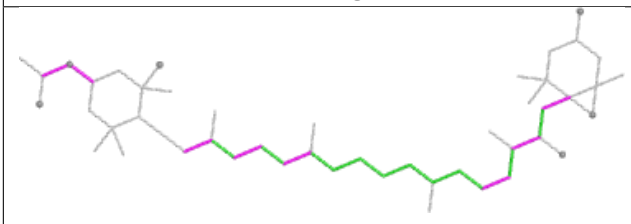
Ligand A1EB1 z 301



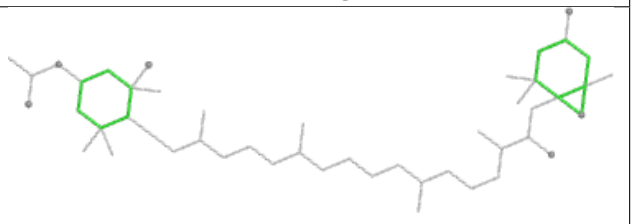
Bond lengths



Bond angles

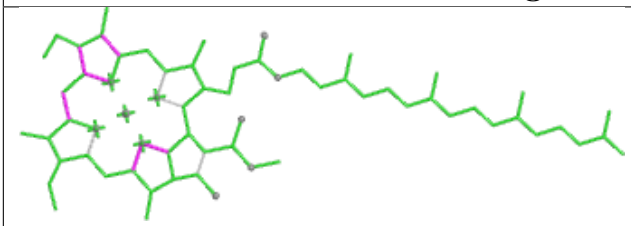


Torsions

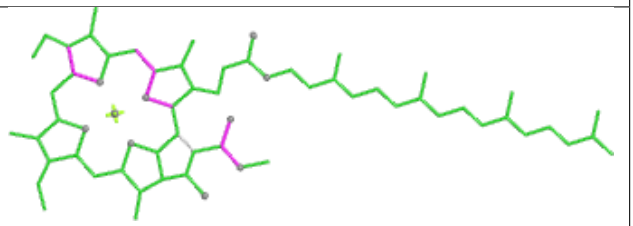


Rings

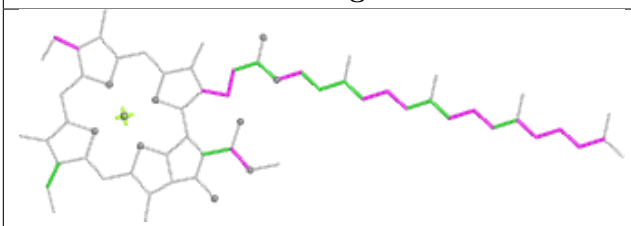
Ligand CLA C 311



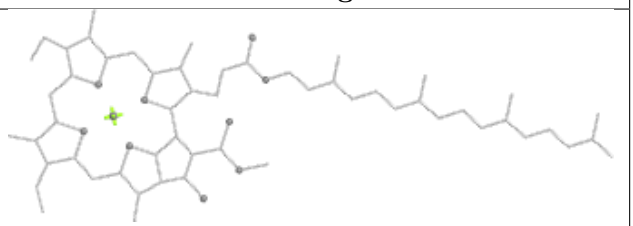
Bond lengths



Bond angles

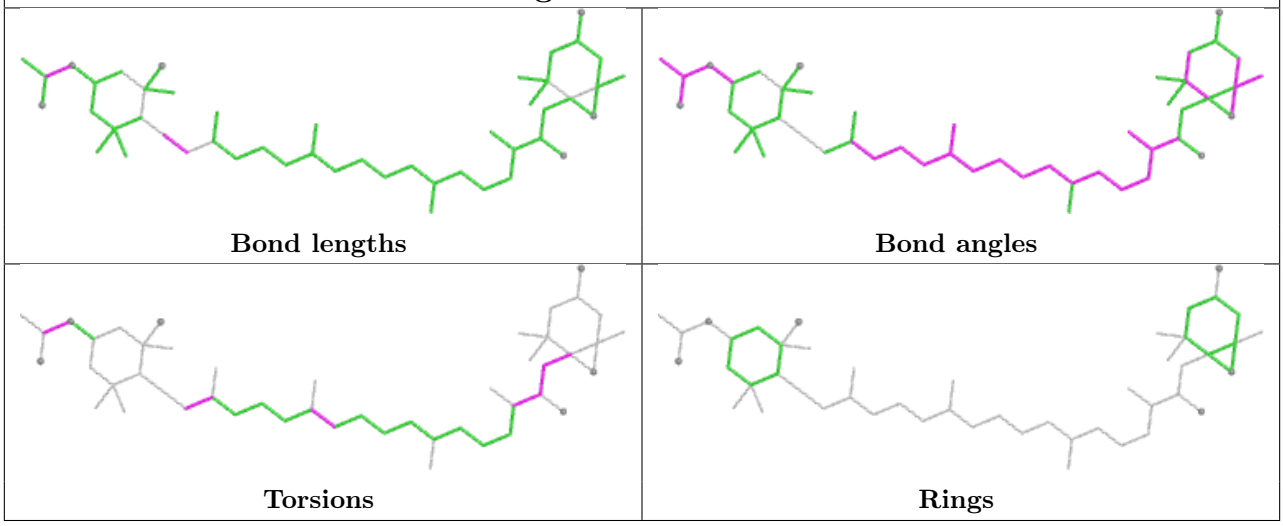


Torsions

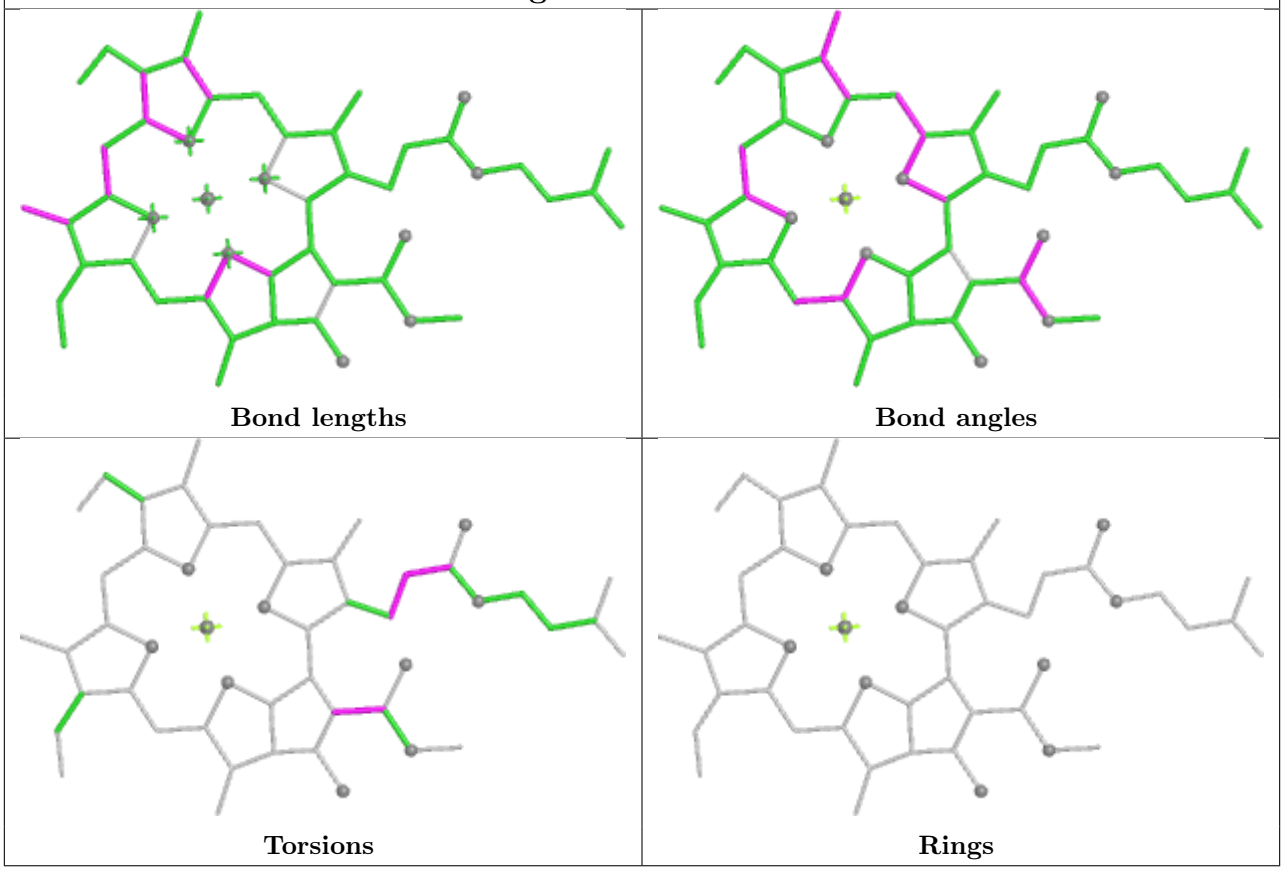


Rings

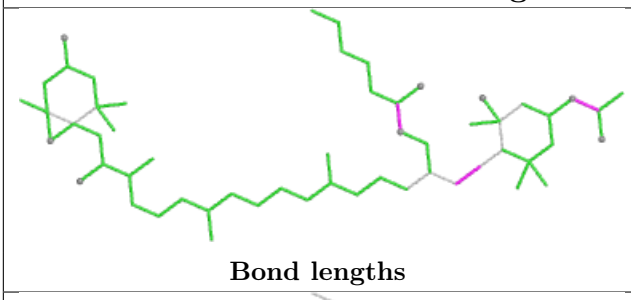
Ligand A86 2 305



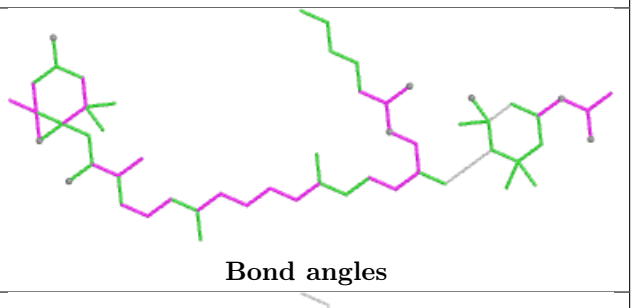
Ligand CLA a 813



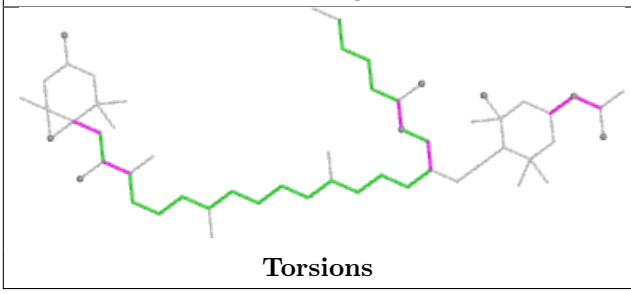
Ligand A1EB1 1 301



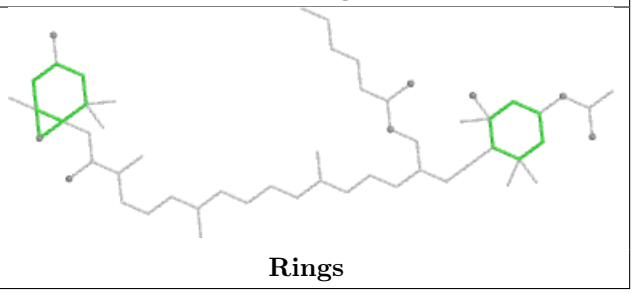
Bond lengths



Bond angles

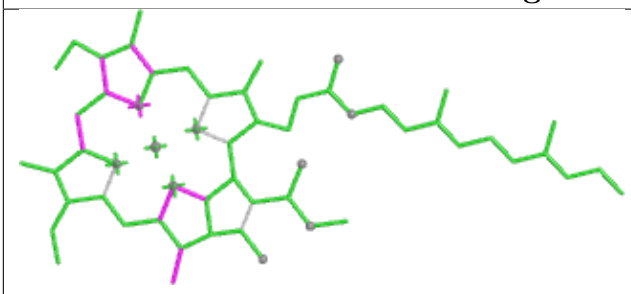


Torsions

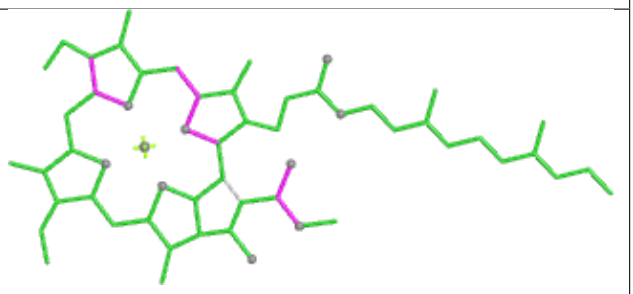


Rings

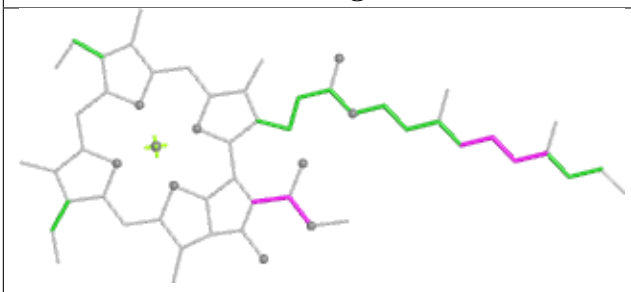
Ligand CLA H 310



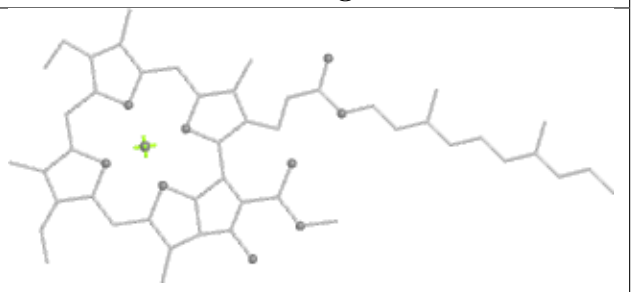
Bond lengths



Bond angles

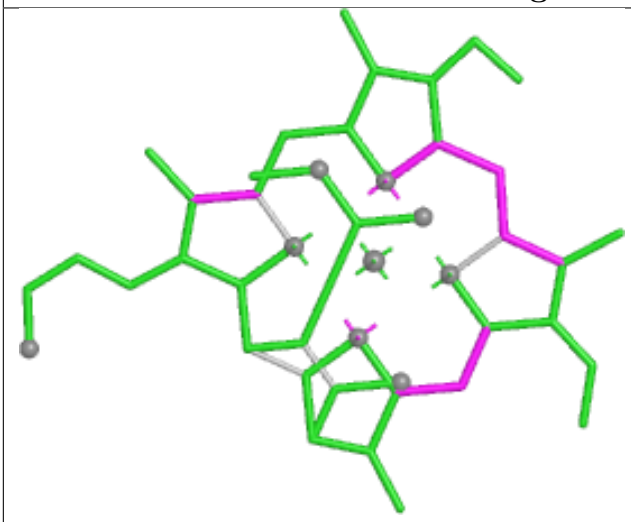


Torsions



Rings

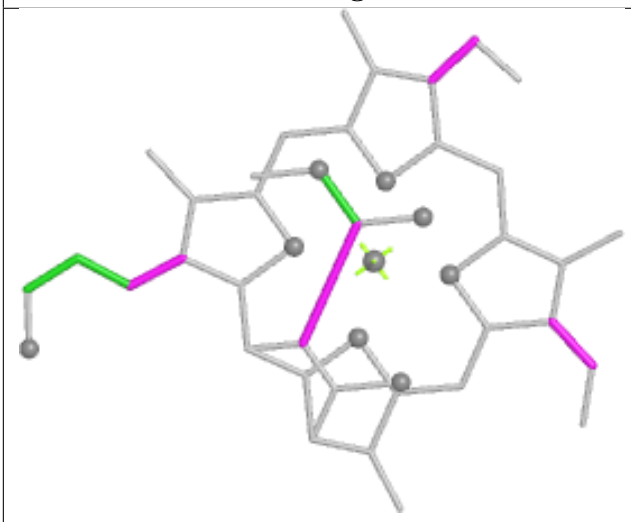
Ligand KC2 5 313



Bond lengths



Bond angles

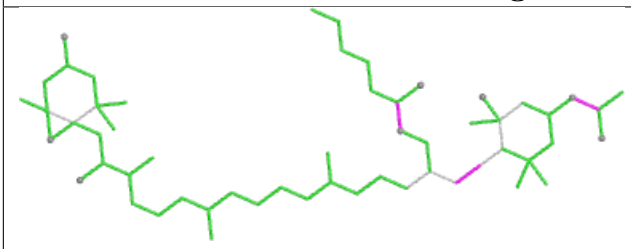


Torsions

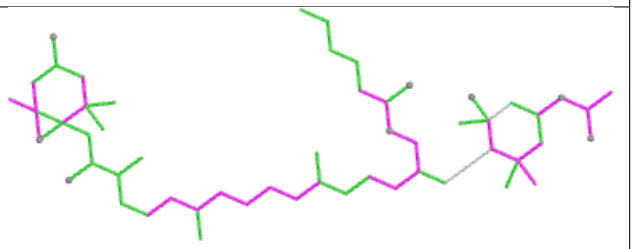


Rings

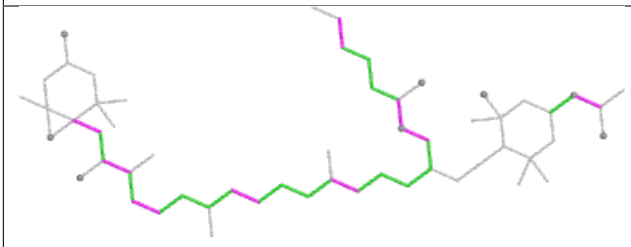
Ligand A1EB1 x 302



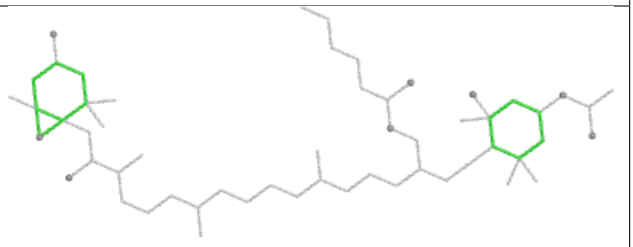
Bond lengths



Bond angles

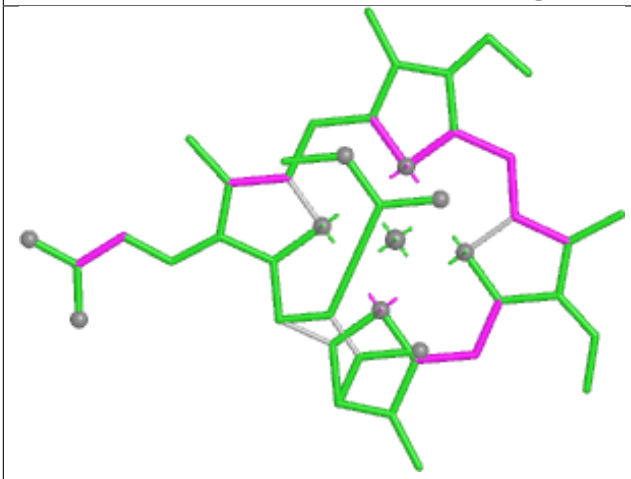


Torsions

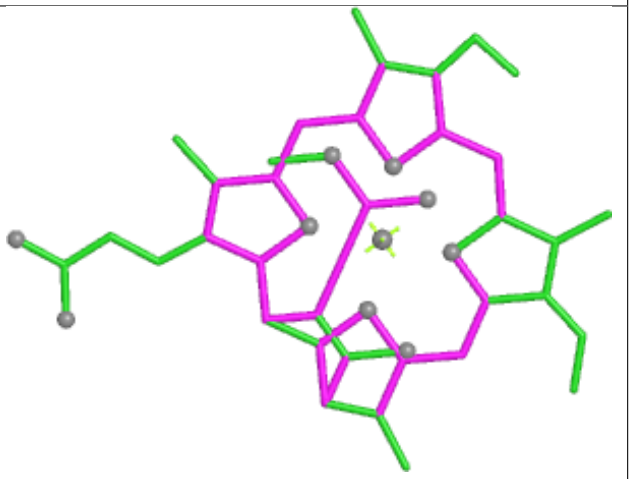


Rings

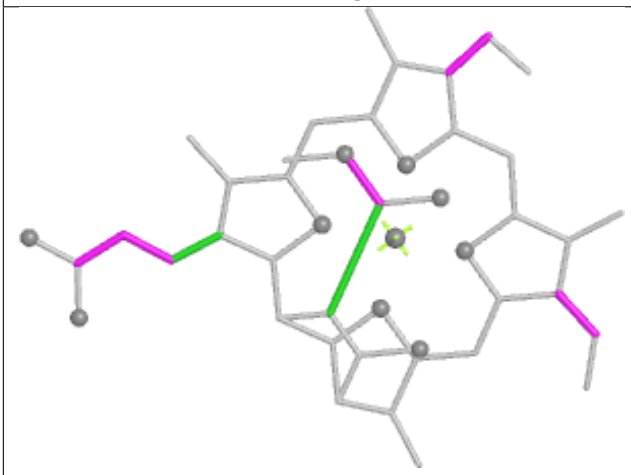
Ligand KC2 2 317



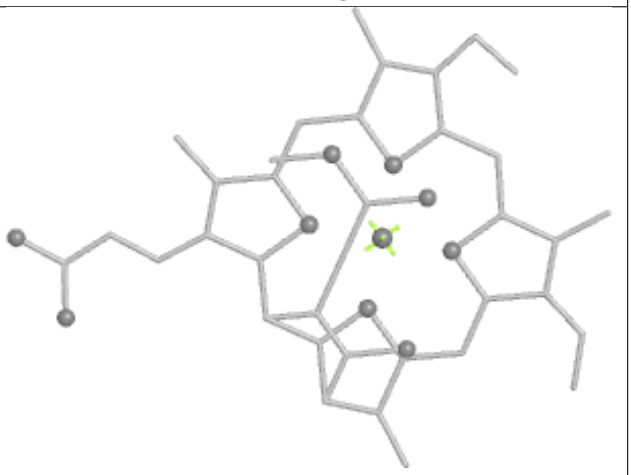
Bond lengths



Bond angles

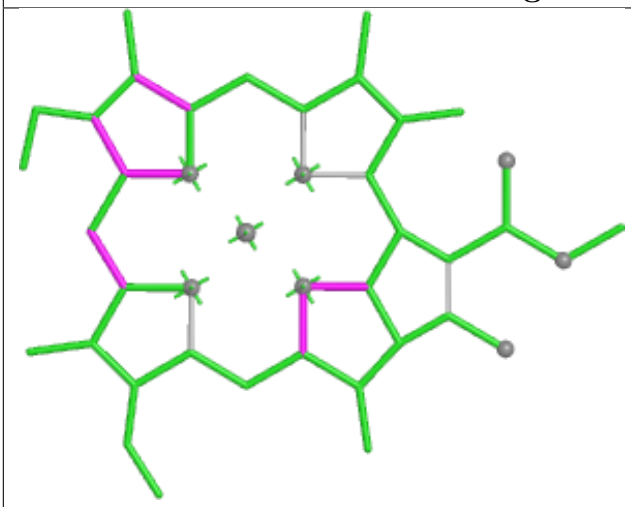


Torsions

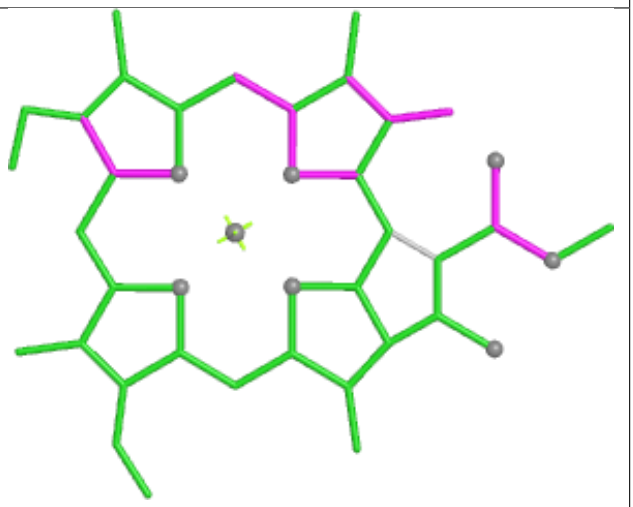


Rings

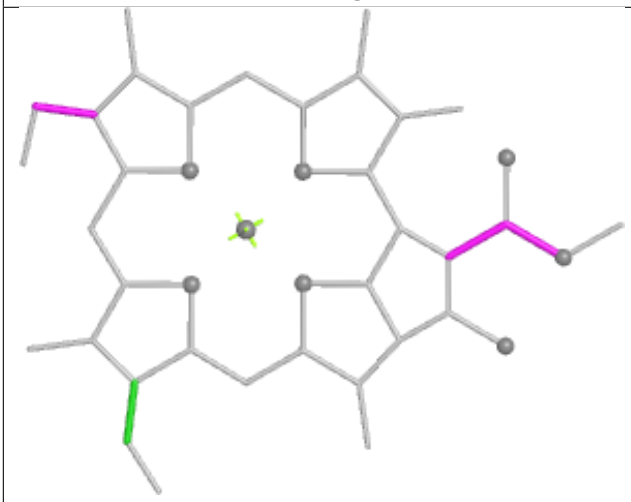
Ligand CLA O 316



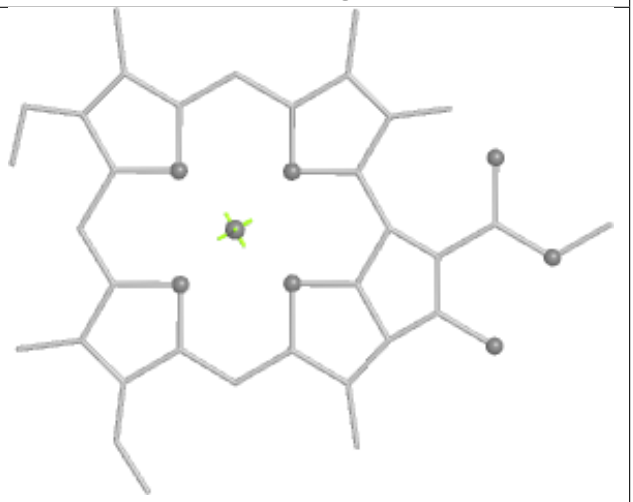
Bond lengths



Bond angles

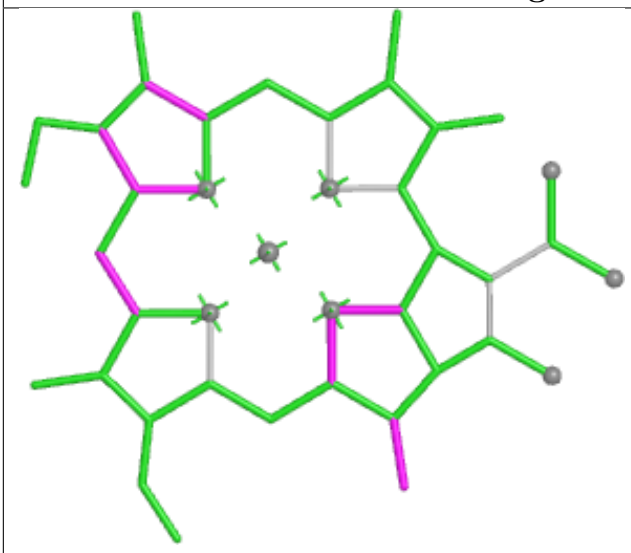


Torsions

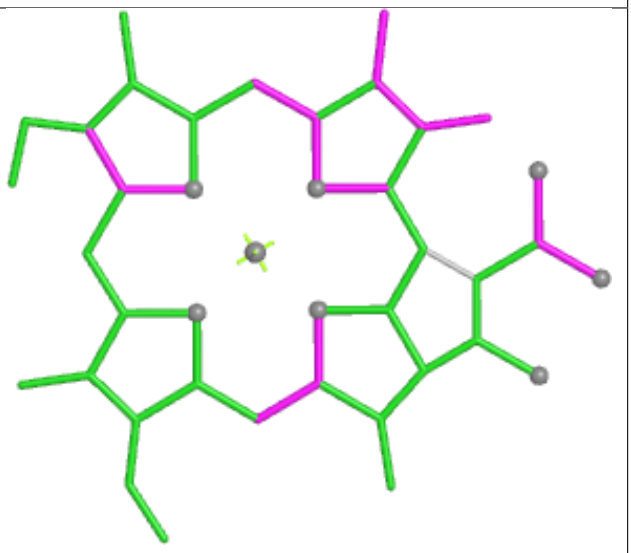


Rings

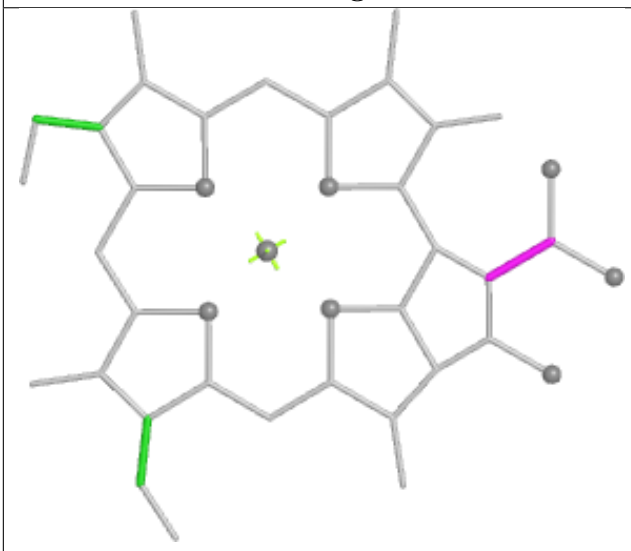
Ligand CLA 6 311



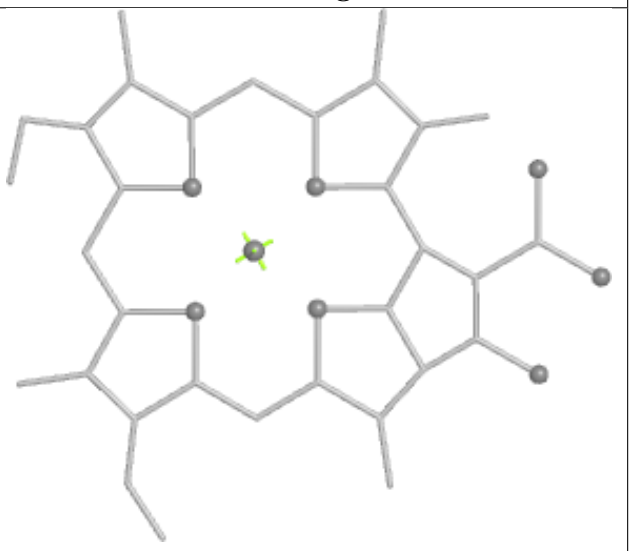
Bond lengths



Bond angles

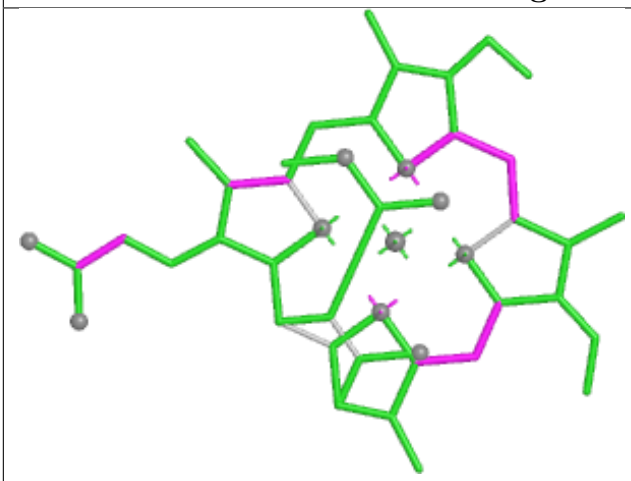


Torsions

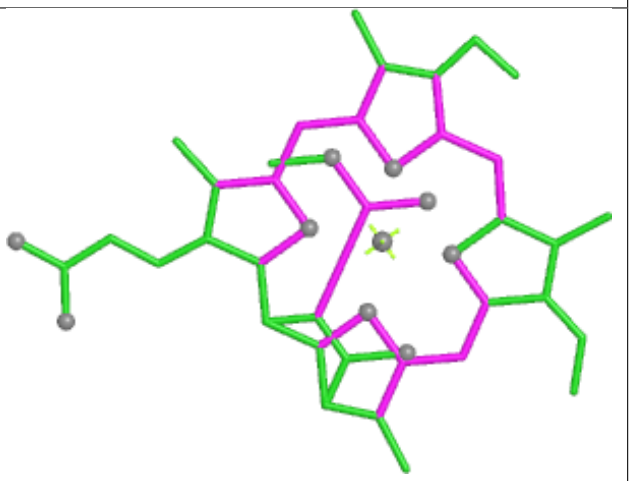


Rings

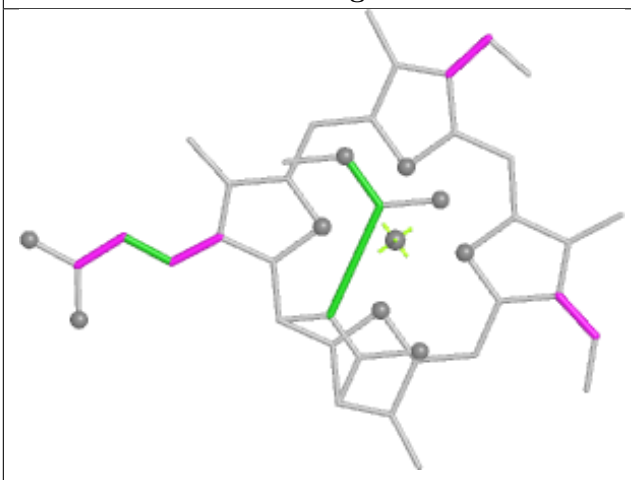
Ligand KC2 7 320



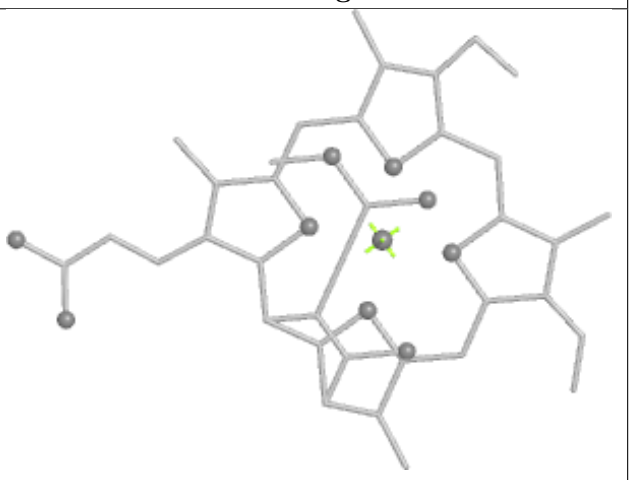
Bond lengths



Bond angles

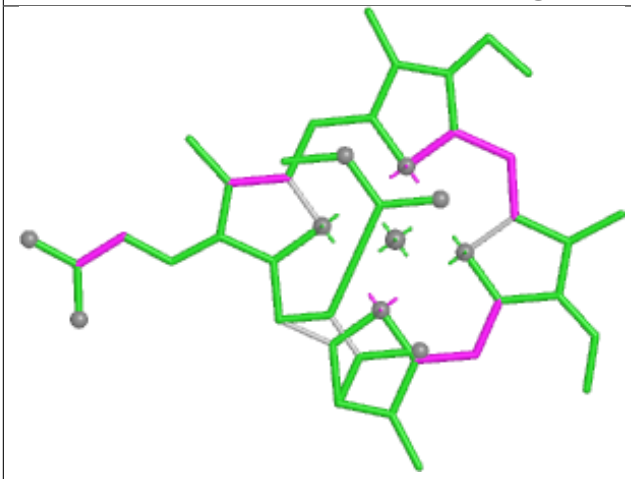


Torsions

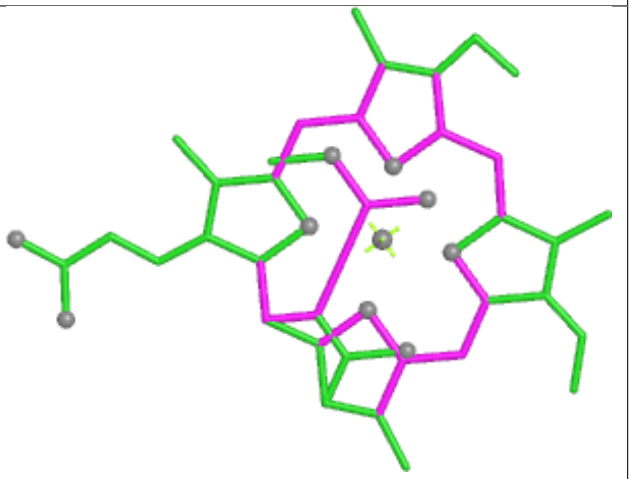


Rings

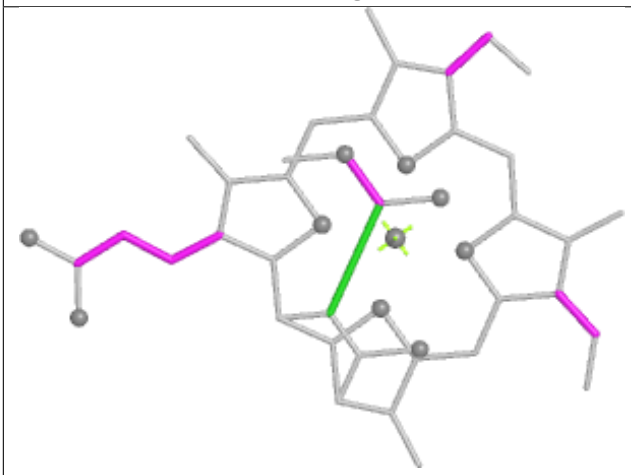
Ligand KC2 x 315



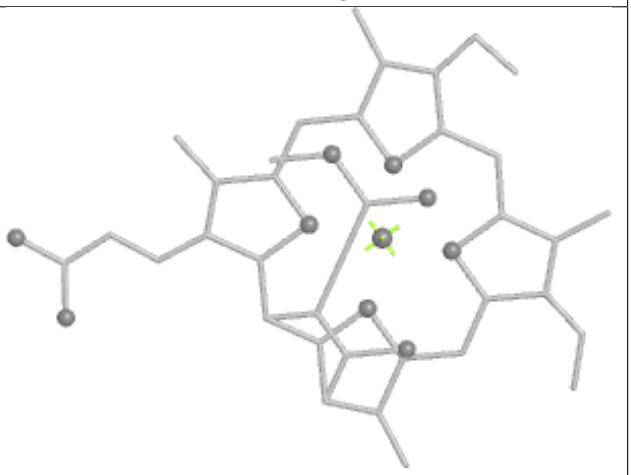
Bond lengths



Bond angles

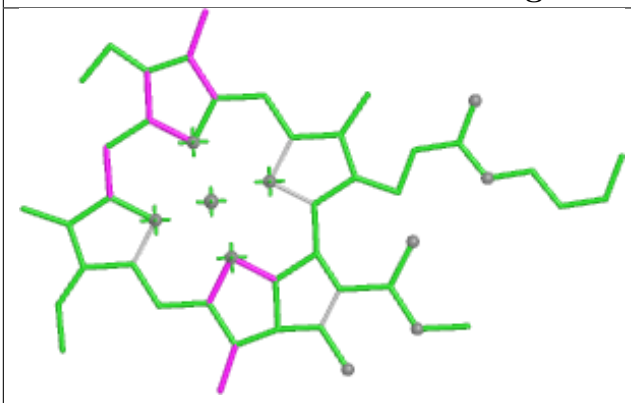


Torsions

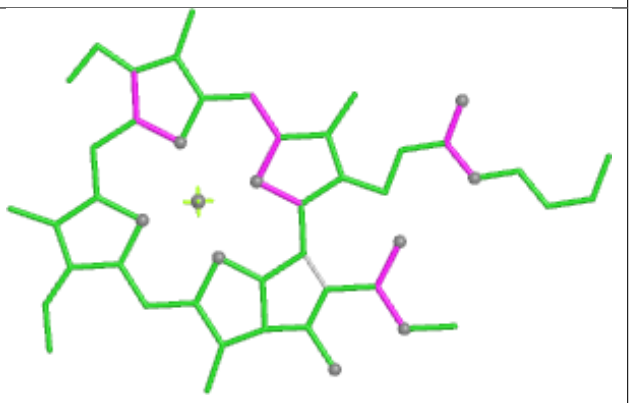


Rings

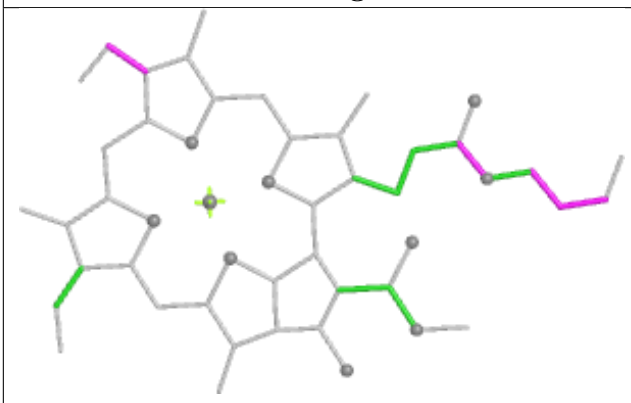
Ligand CLA E 306



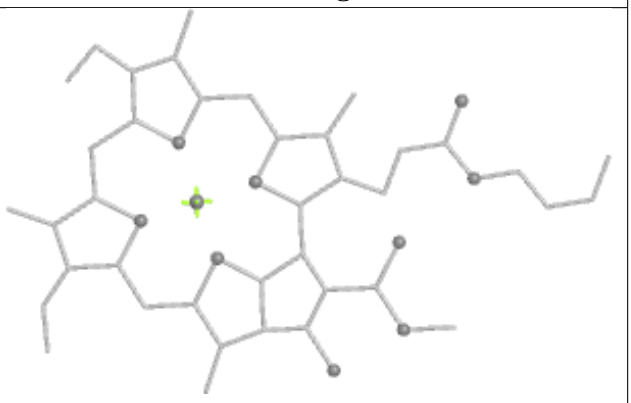
Bond lengths



Bond angles

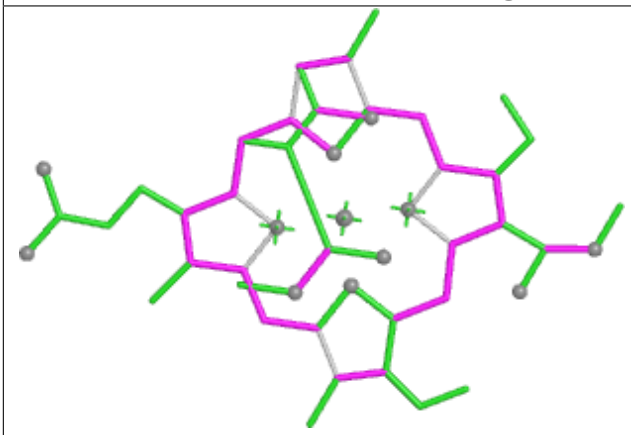


Torsions

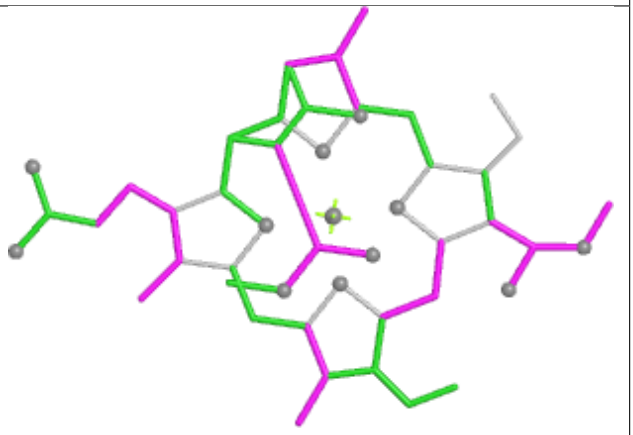


Rings

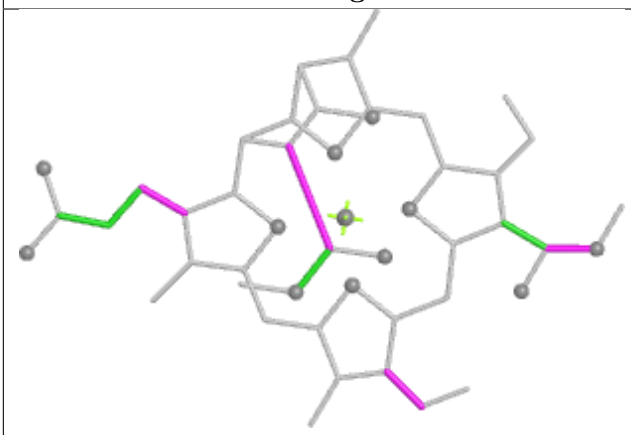
Ligand A1ECV X 313



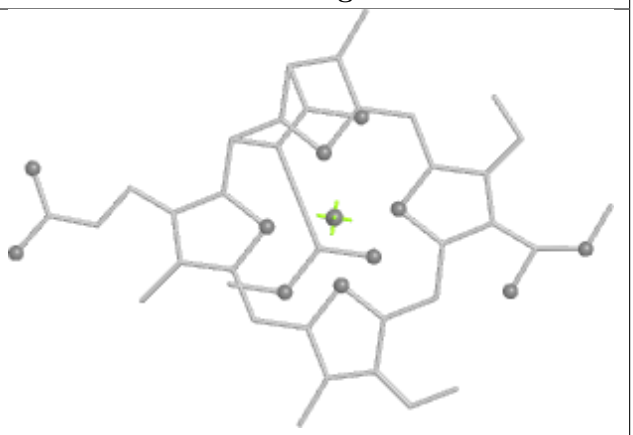
Bond lengths



Bond angles

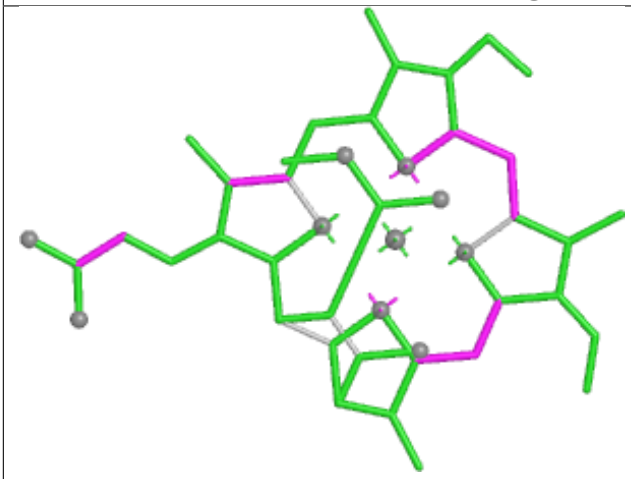


Torsions

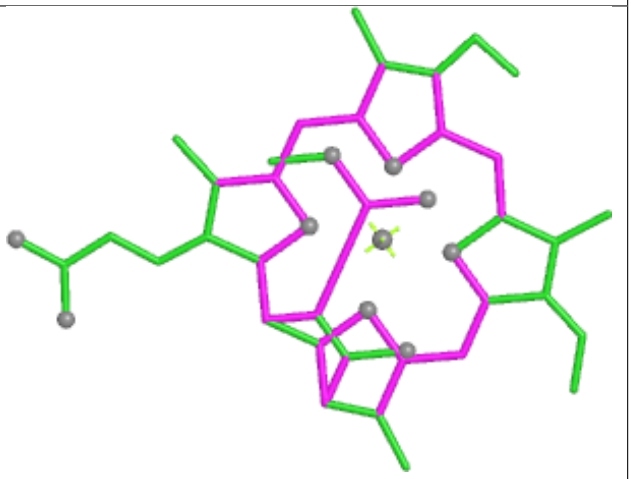


Rings

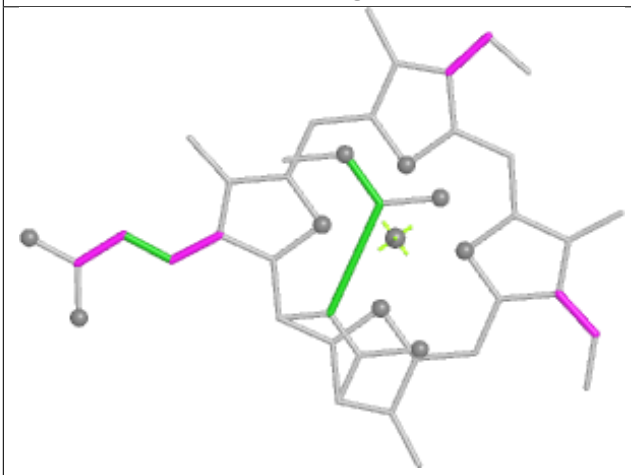
Ligand KC2 Y 309



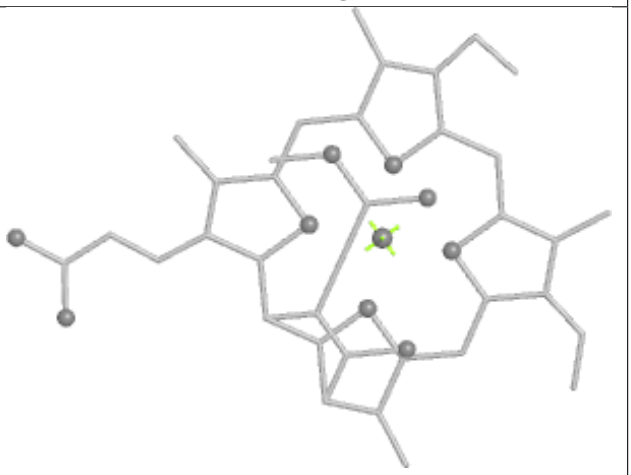
Bond lengths



Bond angles

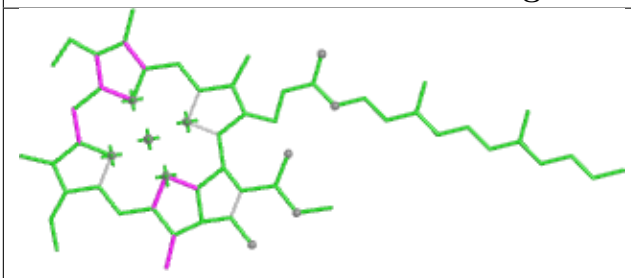


Torsions

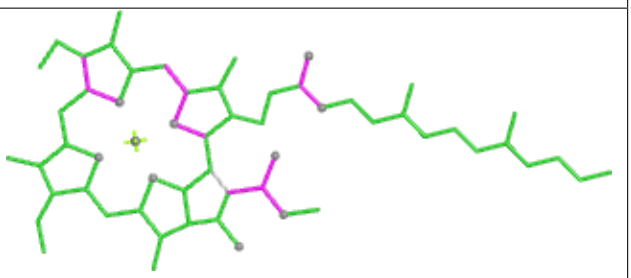


Rings

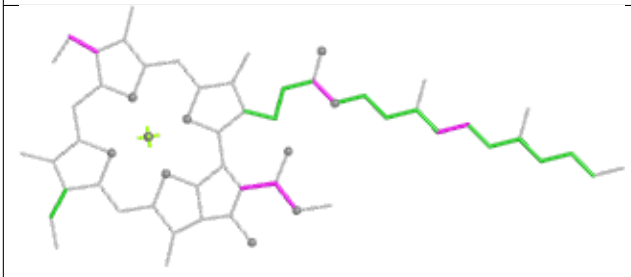
Ligand CLA G 314



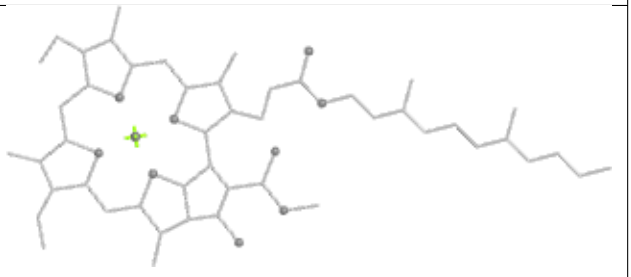
Bond lengths



Bond angles

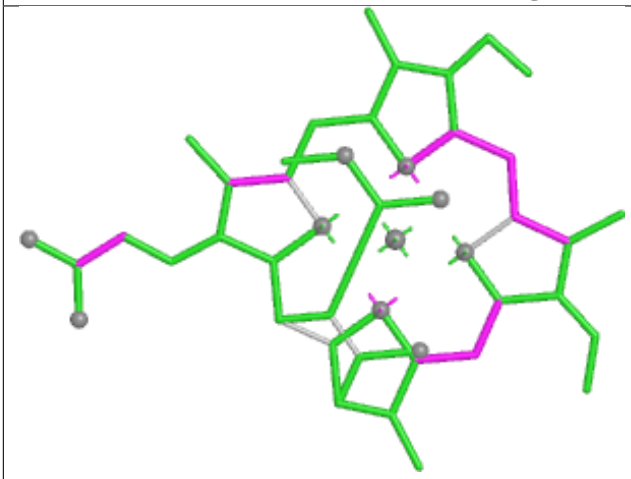


Torsions

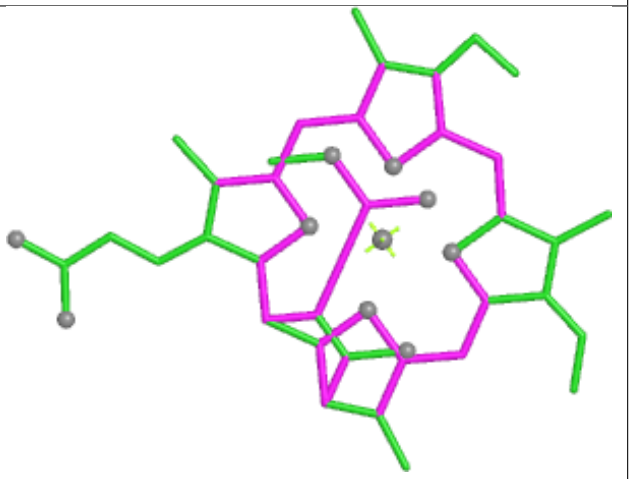


Rings

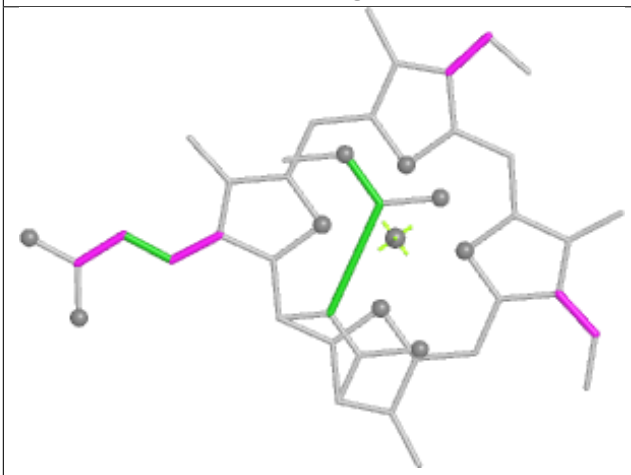
Ligand KC2 R 318



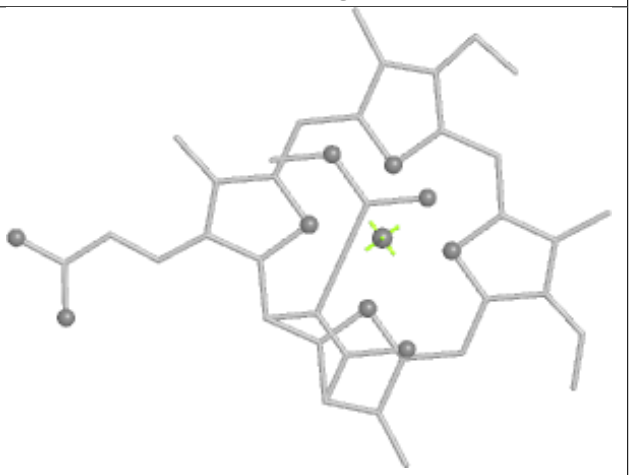
Bond lengths



Bond angles

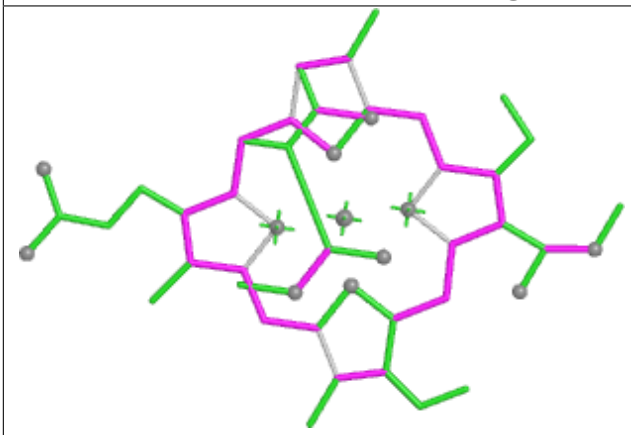


Torsions

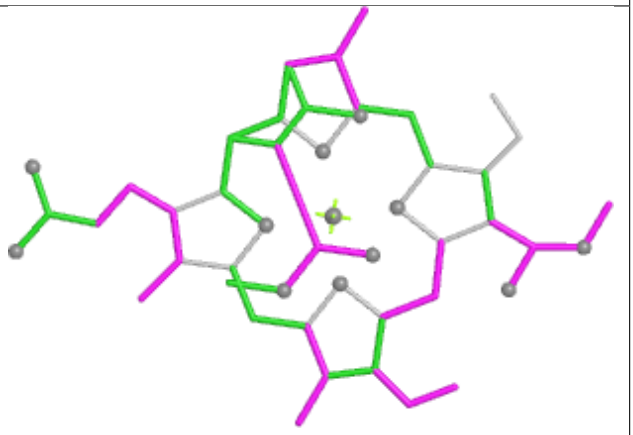


Rings

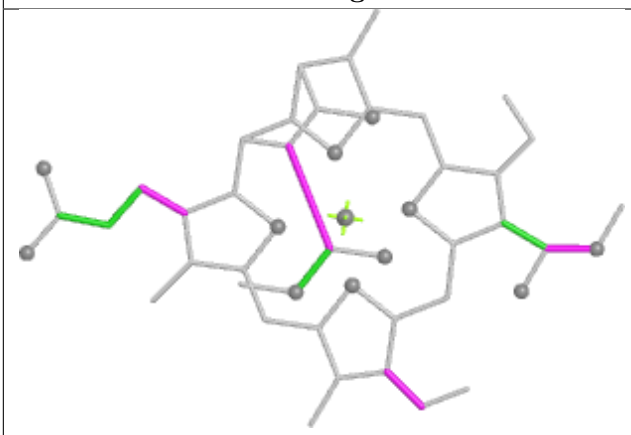
Ligand A1ECV 7 317



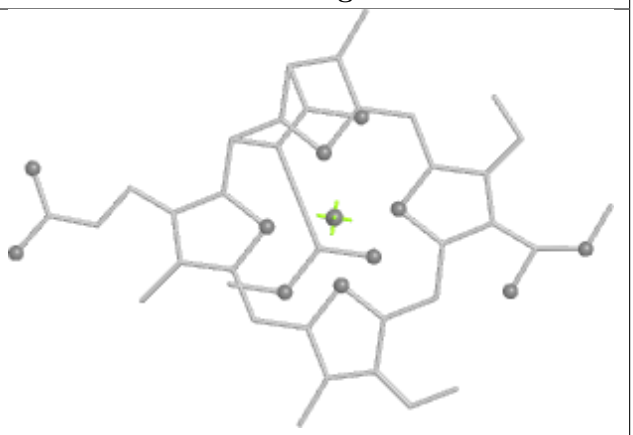
Bond lengths



Bond angles

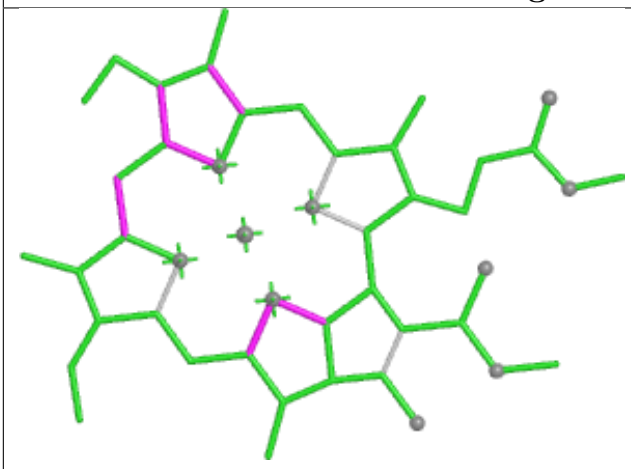


Torsions

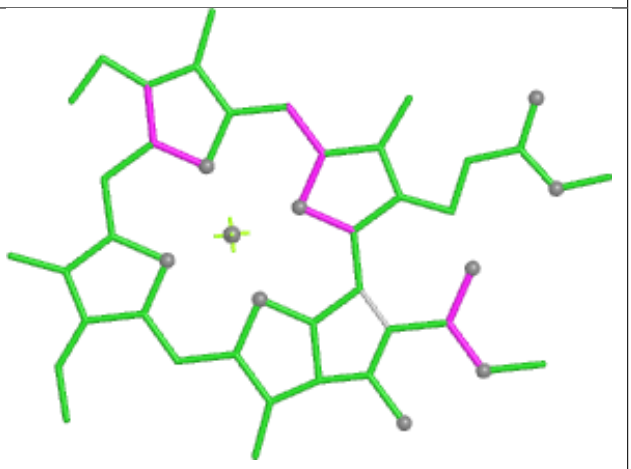


Rings

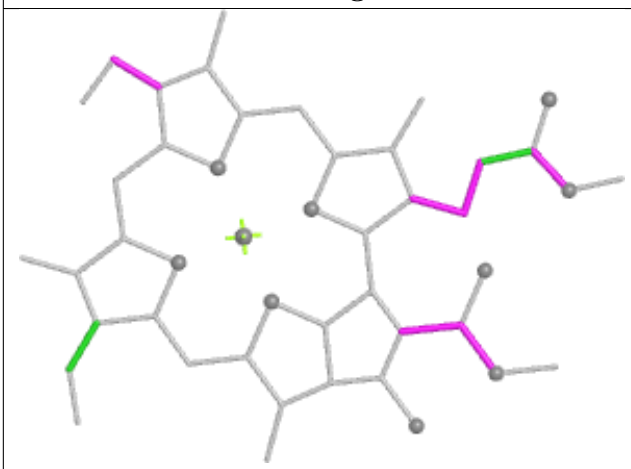
Ligand CLA 6 322



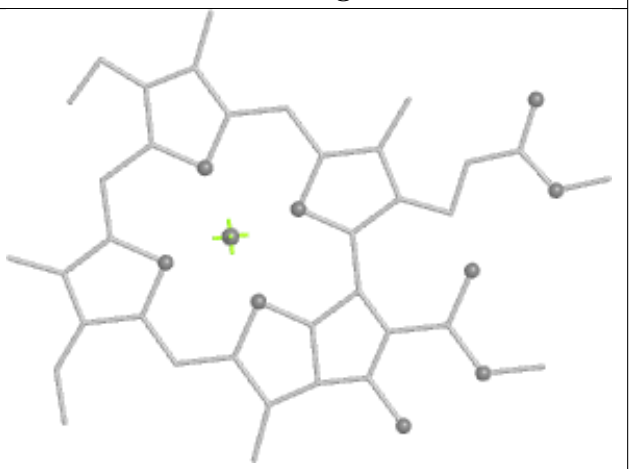
Bond lengths



Bond angles

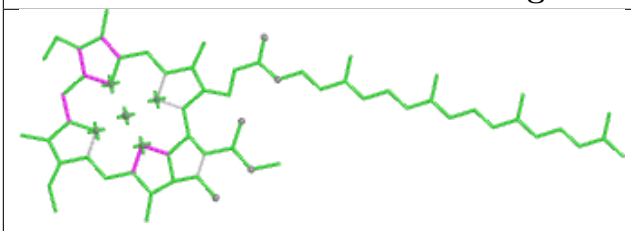


Torsions

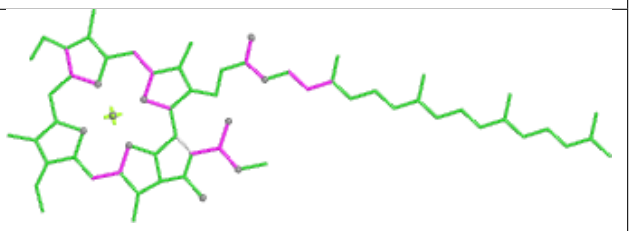


Rings

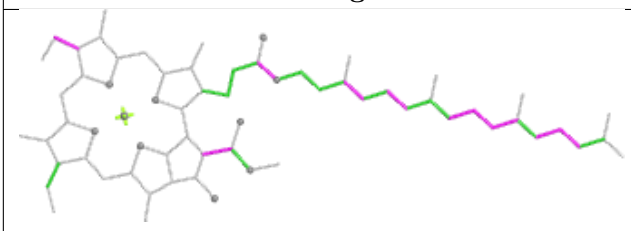
Ligand CLA b 838



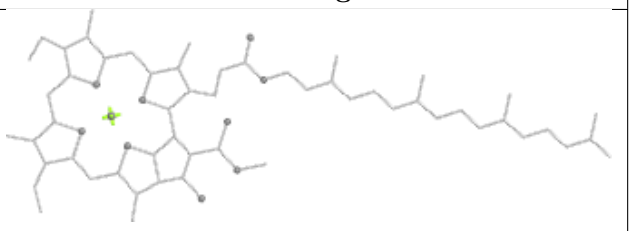
Bond lengths



Bond angles

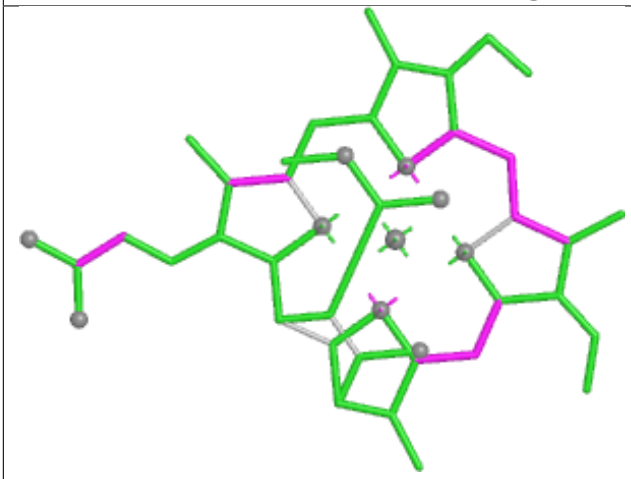


Torsions

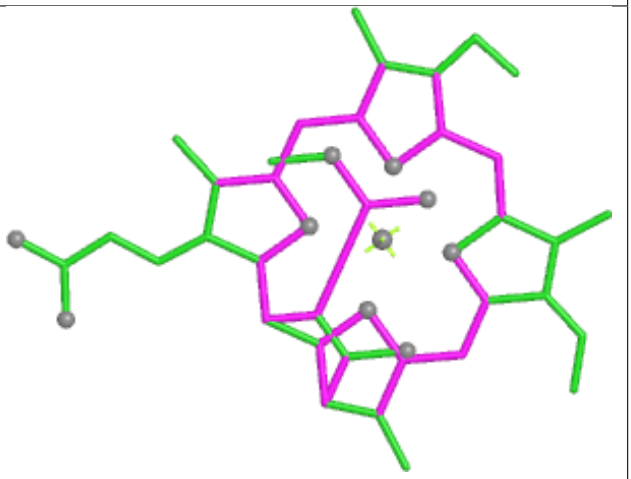


Rings

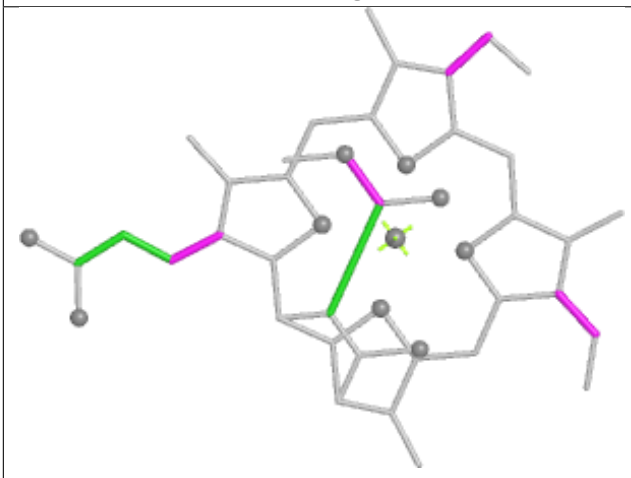
Ligand KC2 K 310



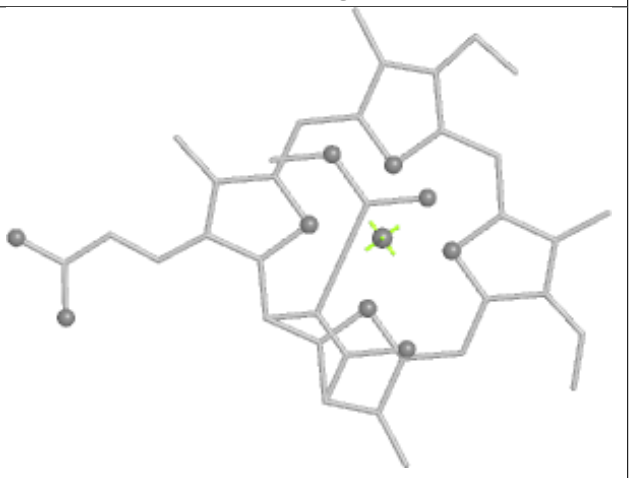
Bond lengths



Bond angles

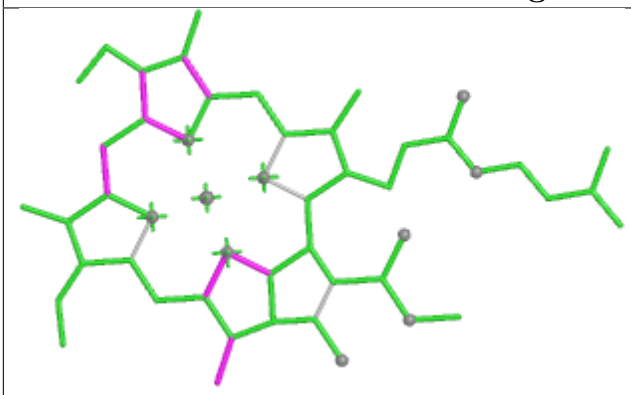


Torsions

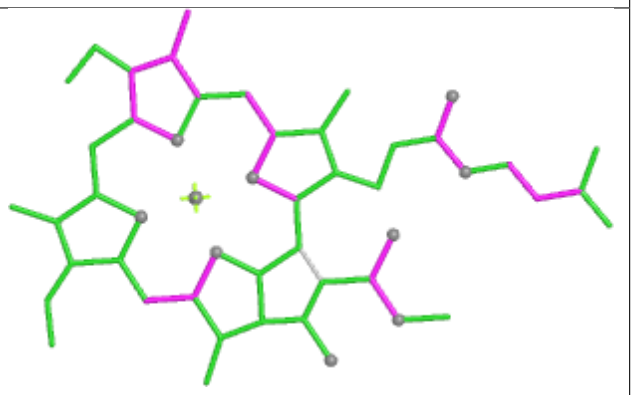


Rings

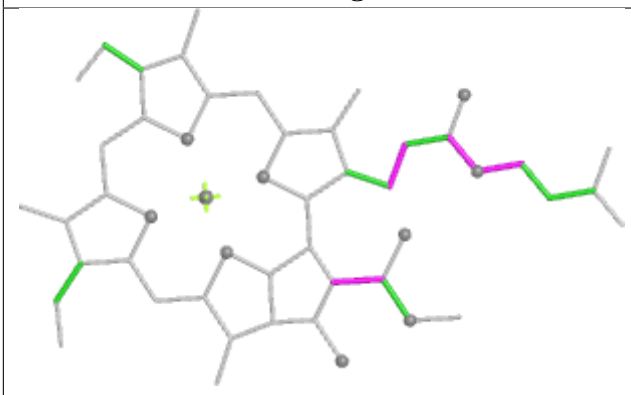
Ligand CLA 0 315



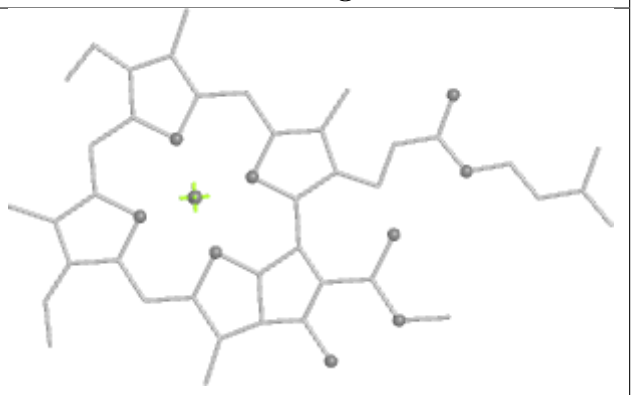
Bond lengths



Bond angles

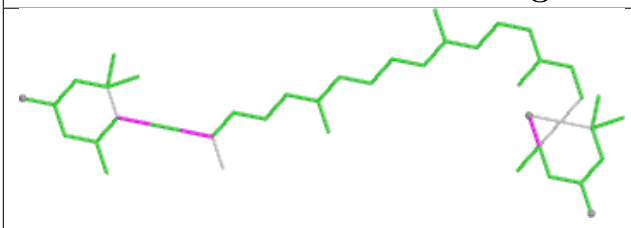


Torsions

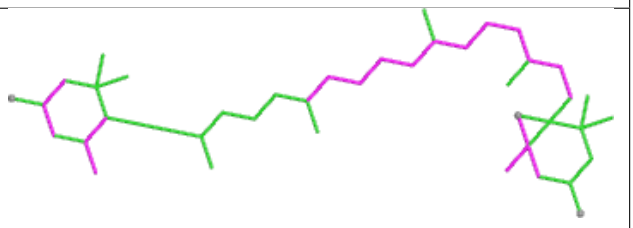


Rings

Ligand DD6 I 307



Bond lengths



Bond angles

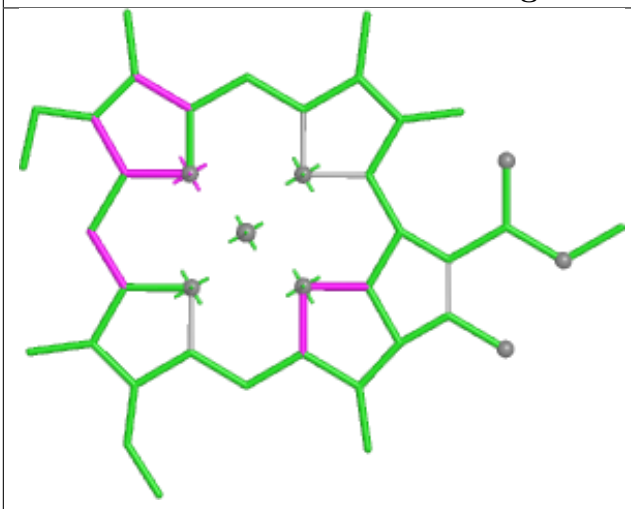


Torsions

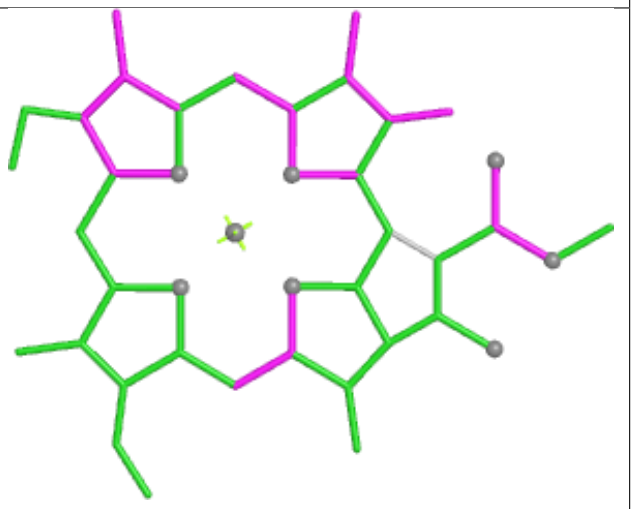


Rings

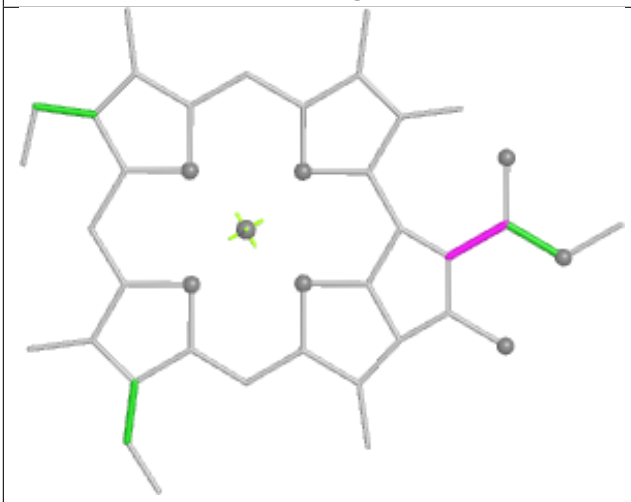
Ligand CLA M 315



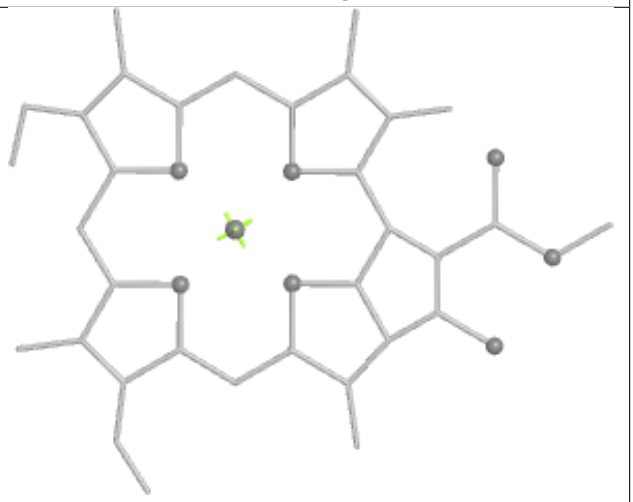
Bond lengths



Bond angles

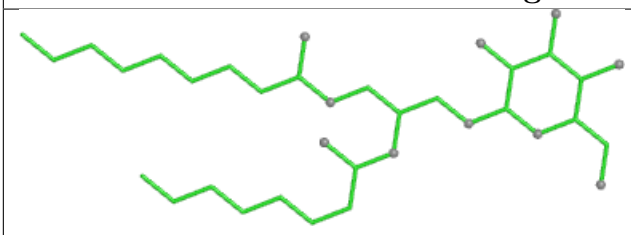


Torsions

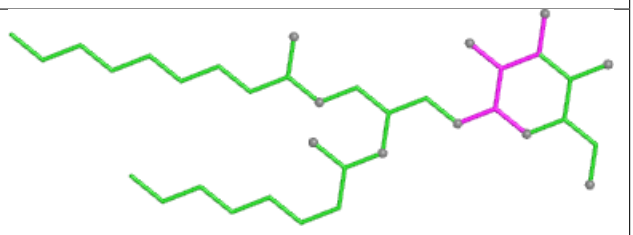


Rings

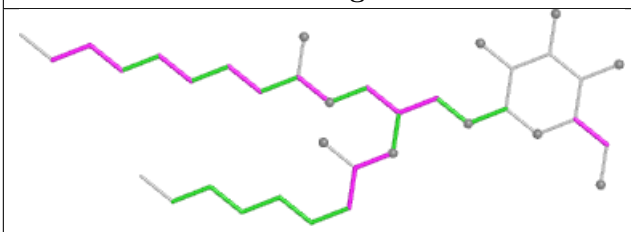
Ligand LMG 9 321



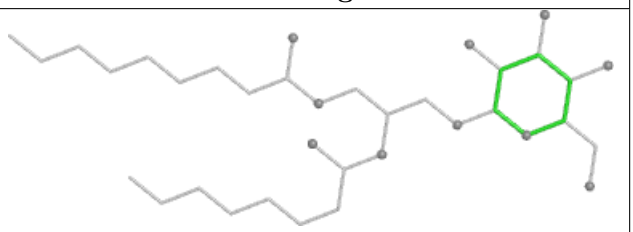
Bond lengths



Bond angles

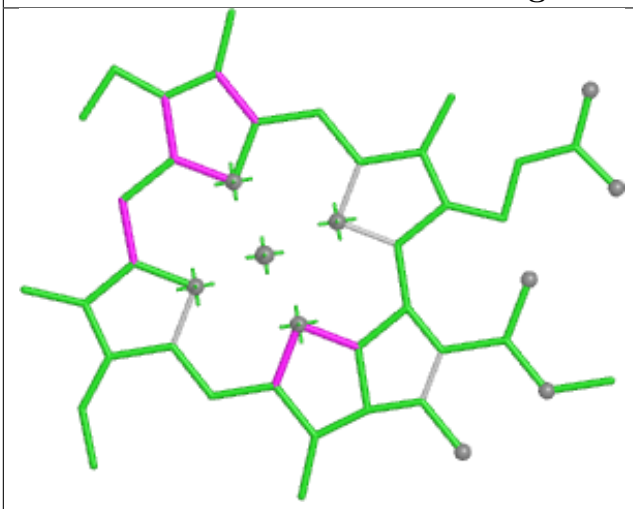


Torsions

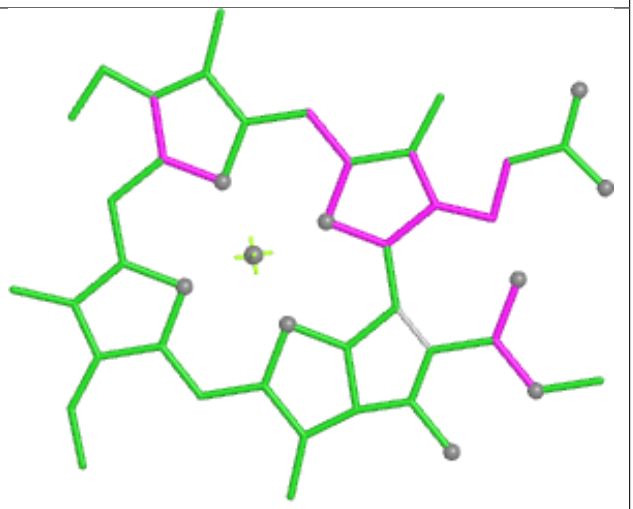


Rings

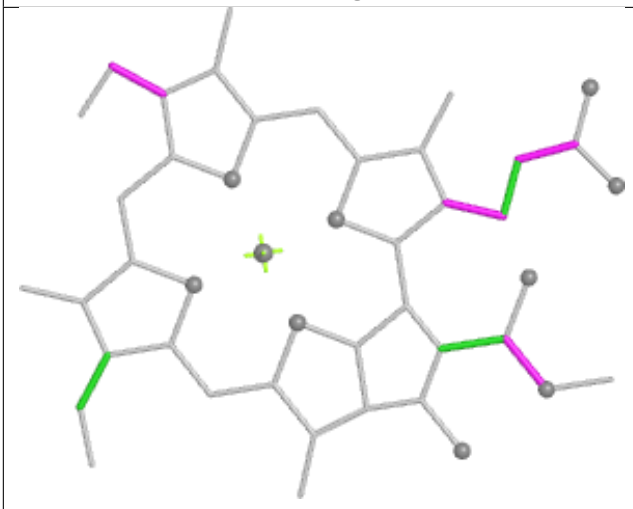
Ligand CLA 8 310



Bond lengths



Bond angles

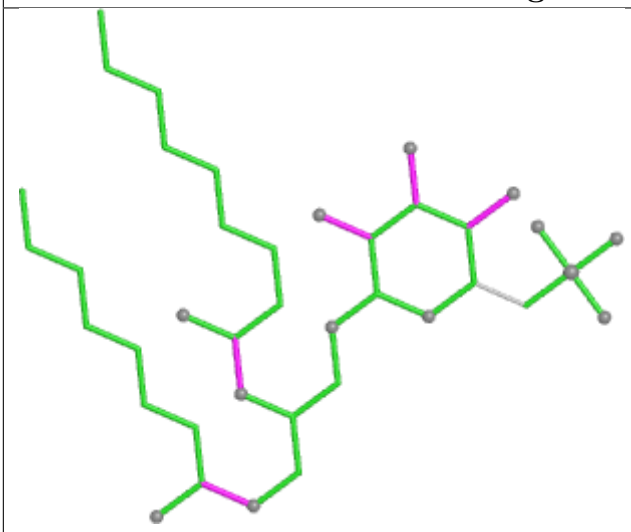


Torsions

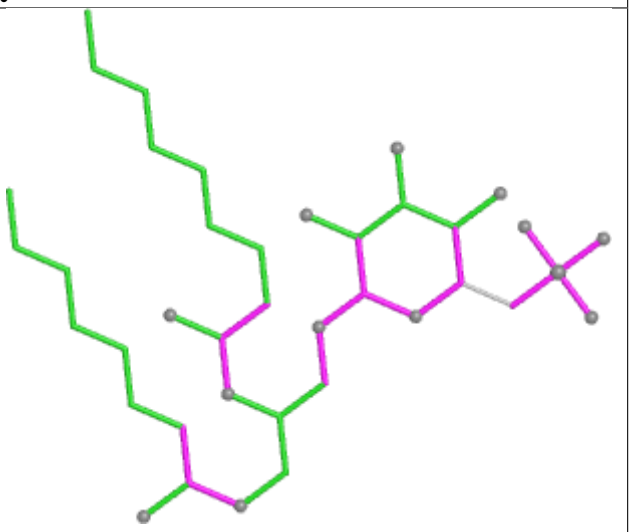


Rings

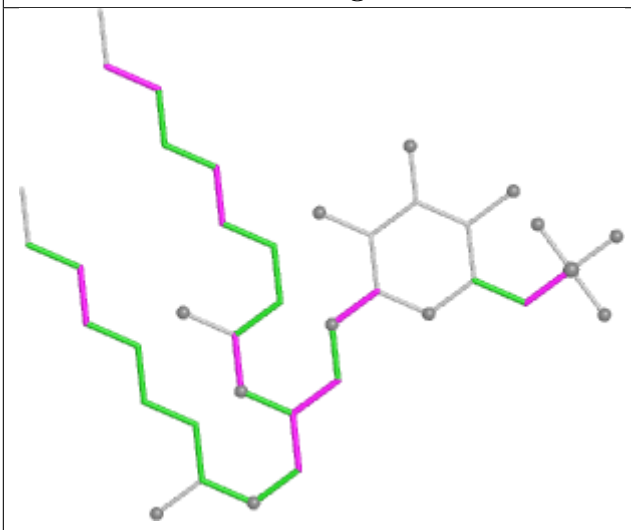
Ligand SQD S 301



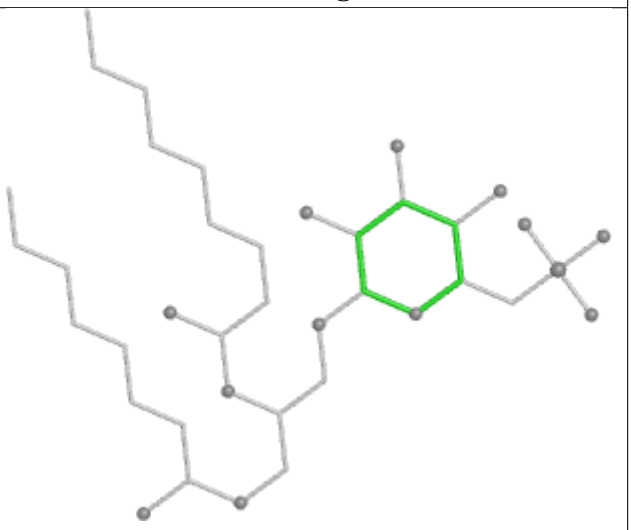
Bond lengths



Bond angles

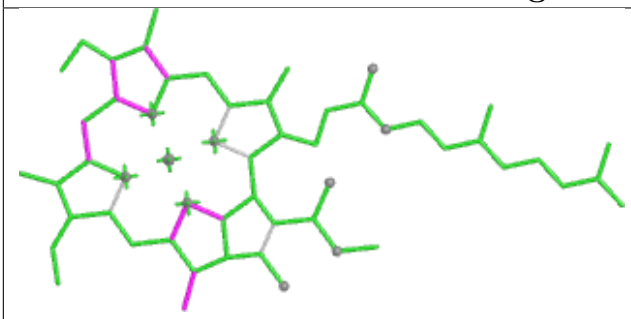


Torsions

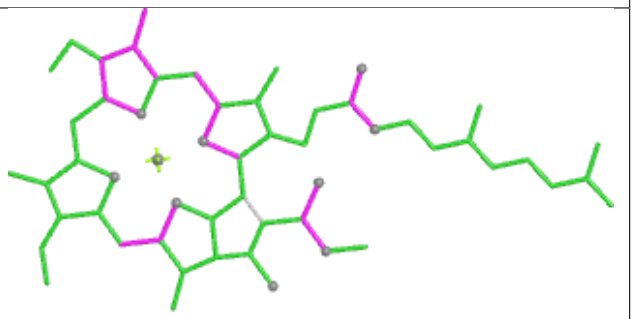


Rings

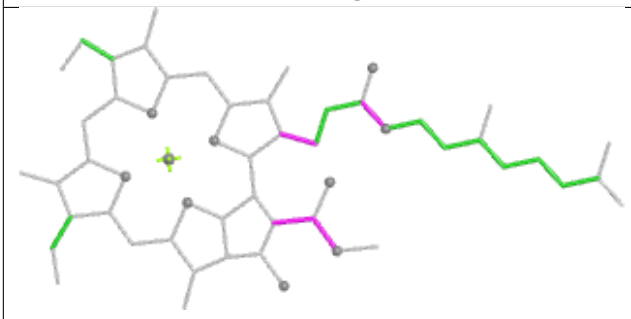
Ligand CLA a 802



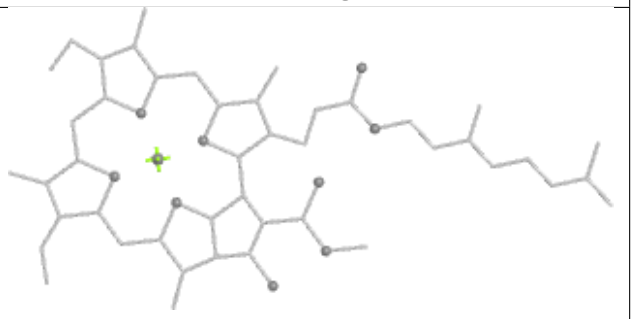
Bond lengths



Bond angles

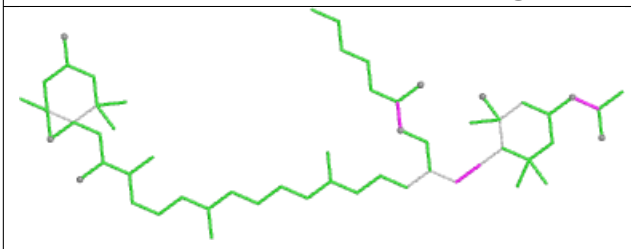


Torsions

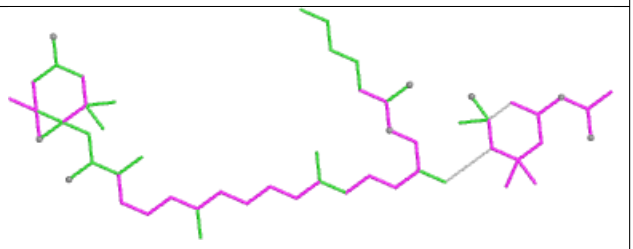


Rings

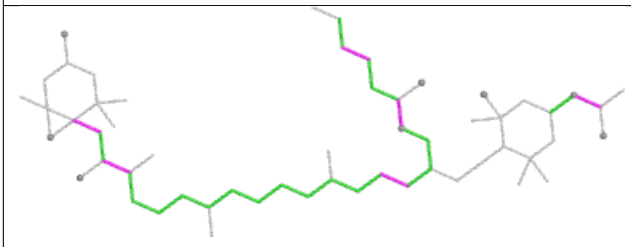
Ligand A1EB1 7 306



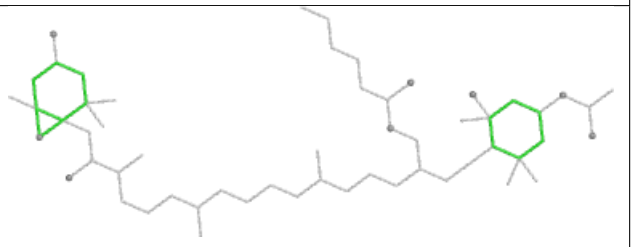
Bond lengths



Bond angles

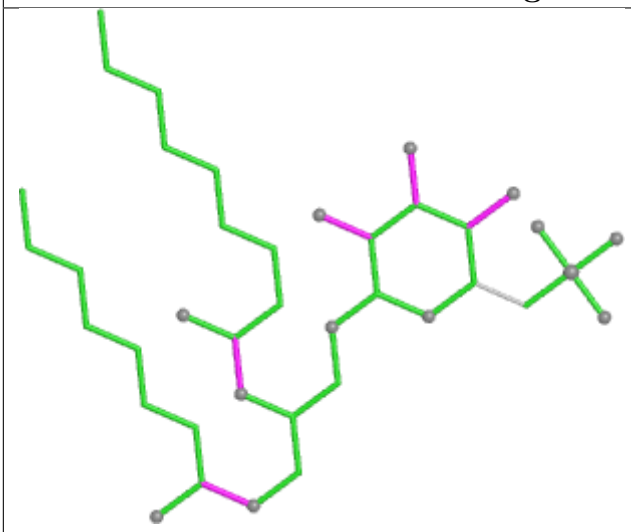


Torsions

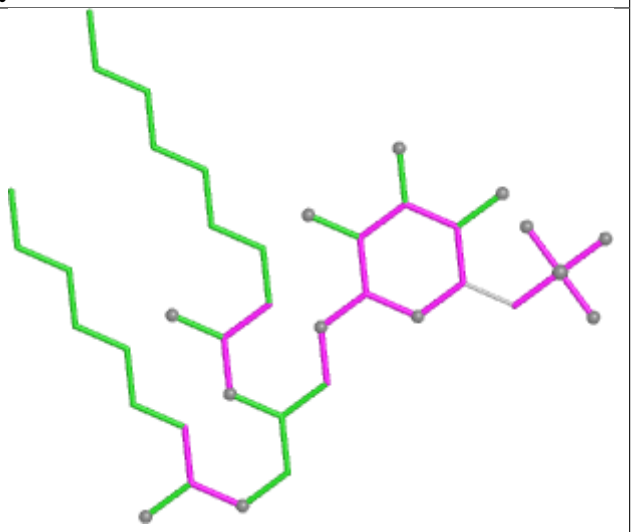


Rings

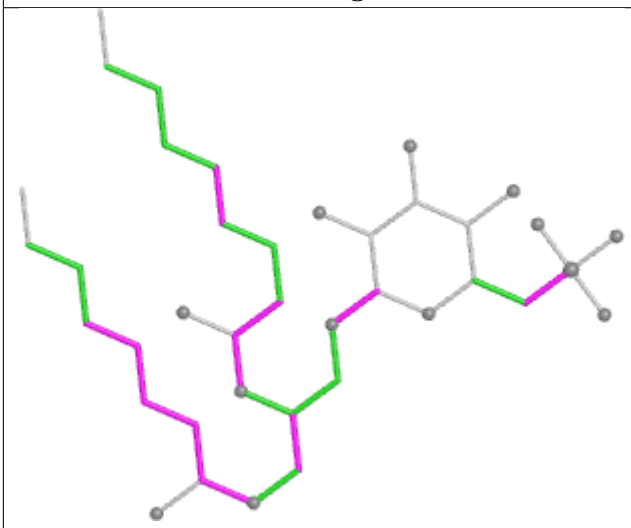
Ligand SQD D 321



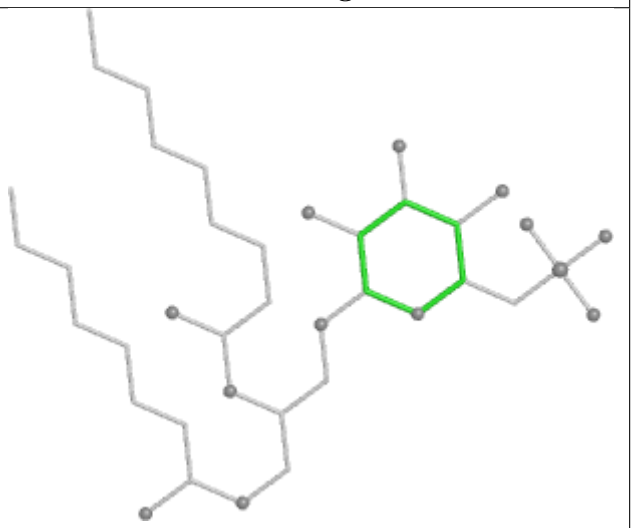
Bond lengths



Bond angles

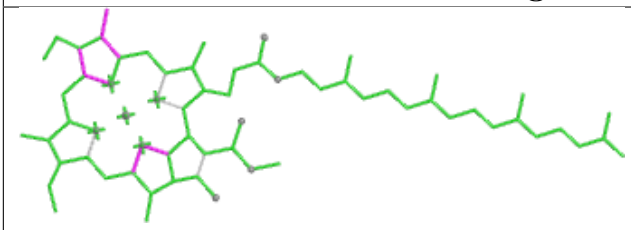


Torsions

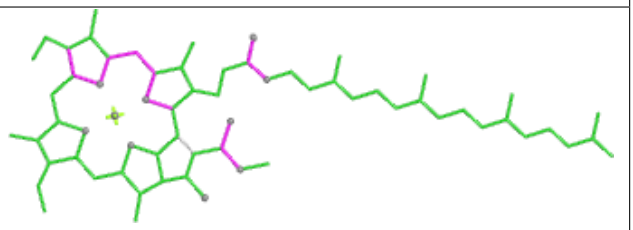


Rings

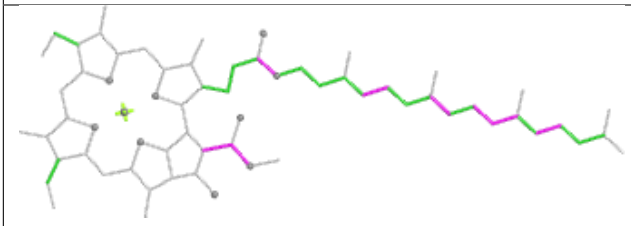
Ligand CLA b 841



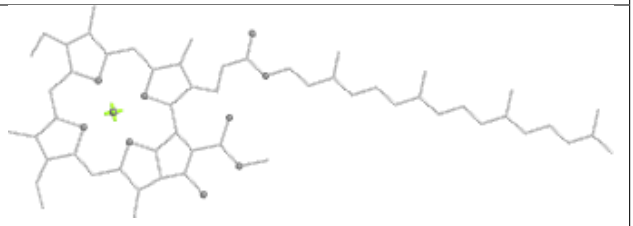
Bond lengths



Bond angles

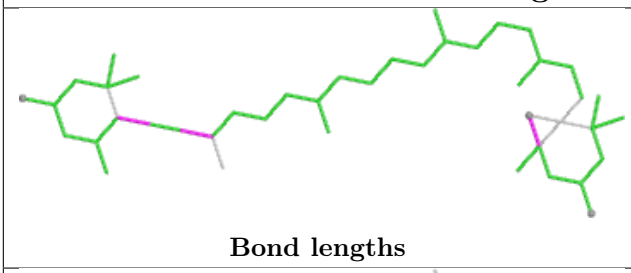


Torsions

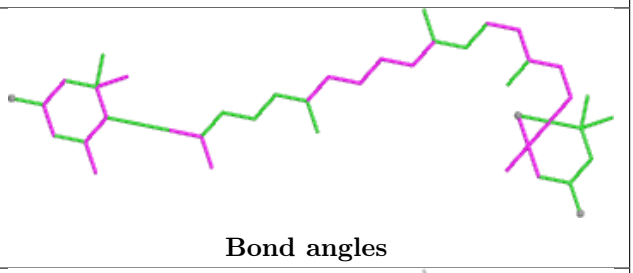


Rings

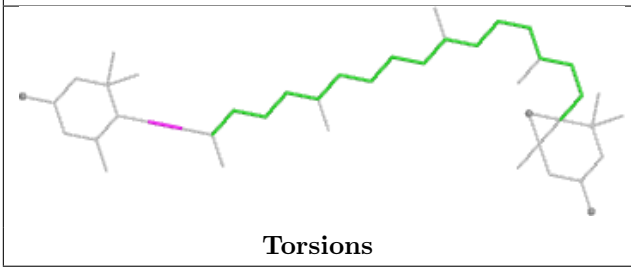
Ligand DD6 I 305



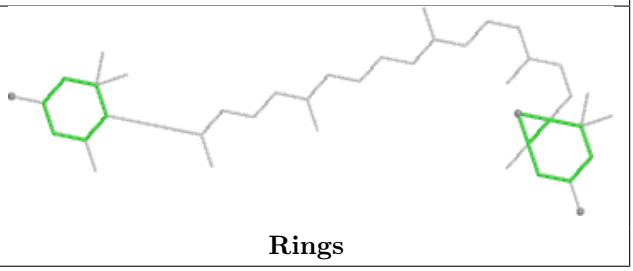
Bond lengths



Bond angles

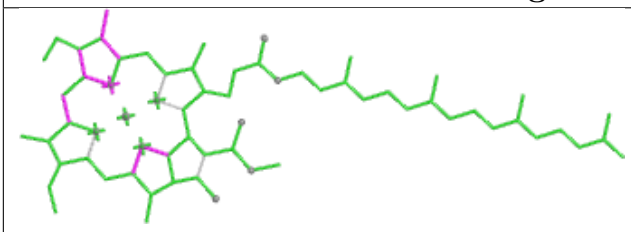


Torsions

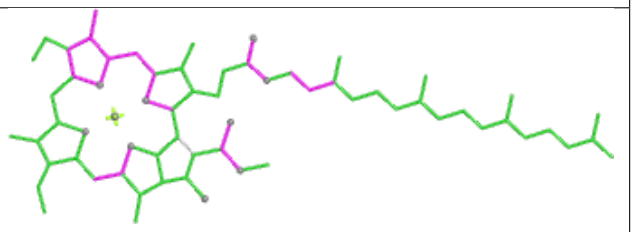


Rings

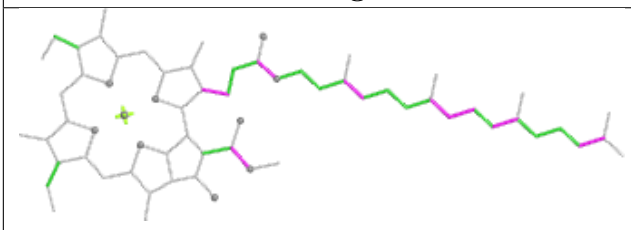
Ligand CLA a 816



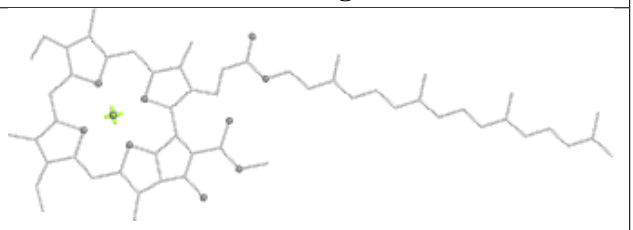
Bond lengths



Bond angles

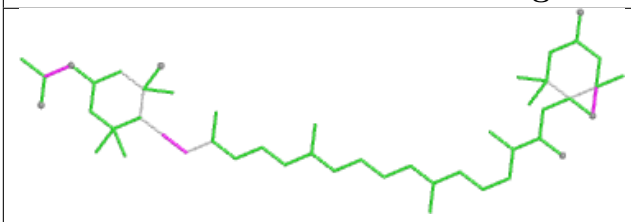


Torsions

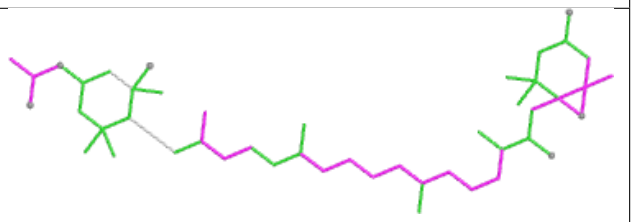


Rings

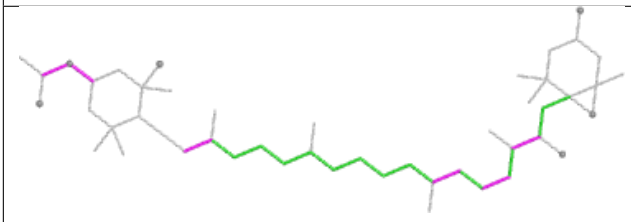
Ligand A86 L 306



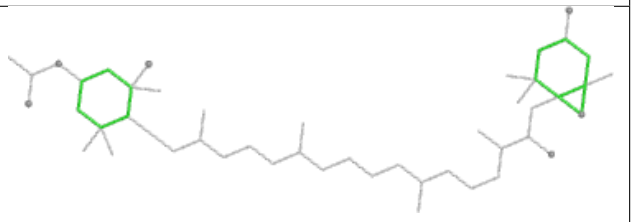
Bond lengths



Bond angles

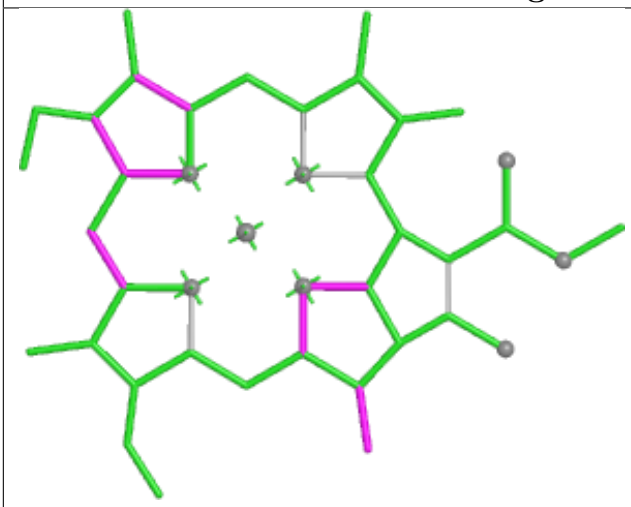


Torsions

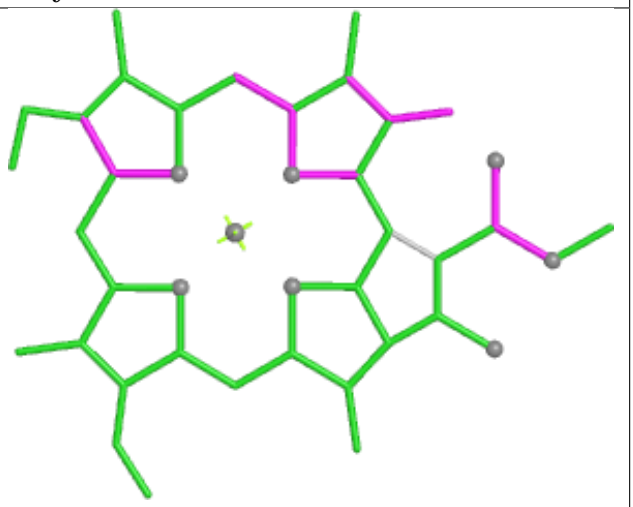


Rings

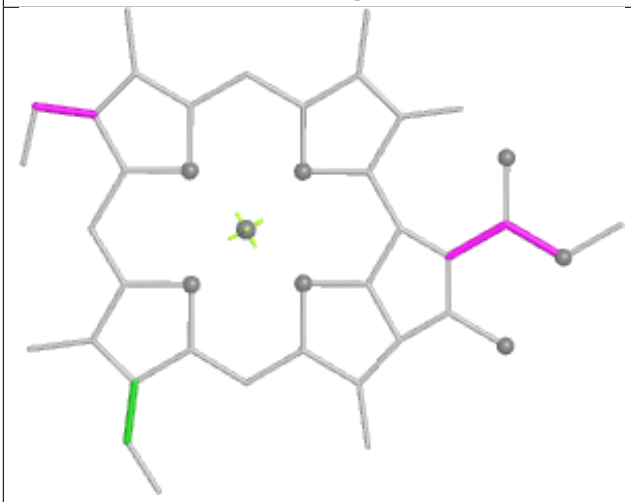
Ligand CLA y 310



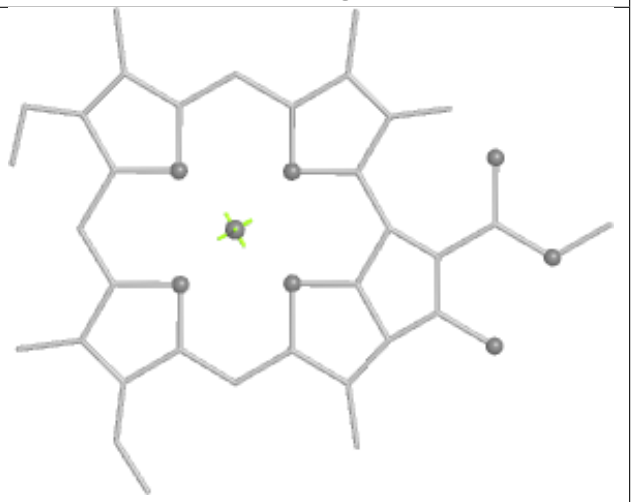
Bond lengths



Bond angles

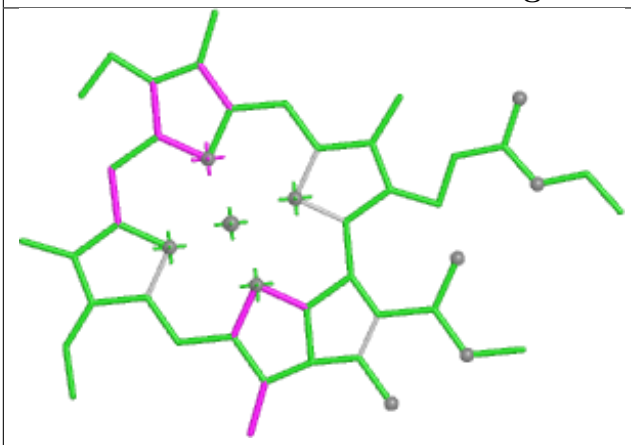


Torsions

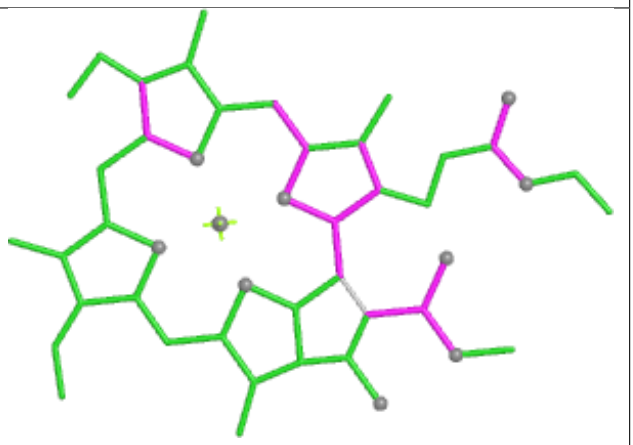


Rings

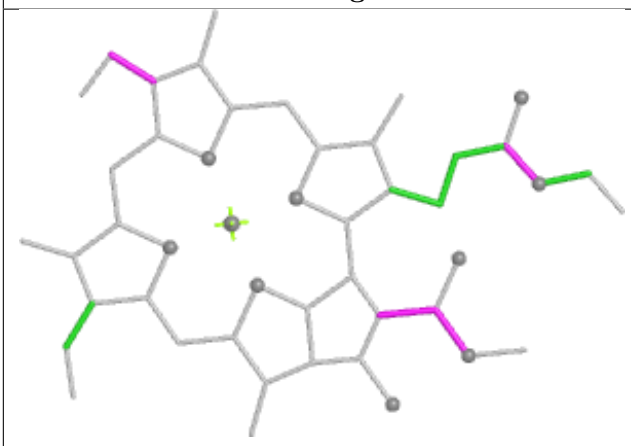
Ligand CLA R 315



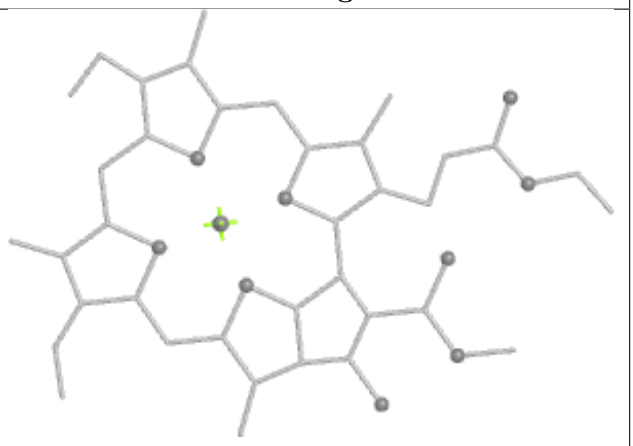
Bond lengths



Bond angles

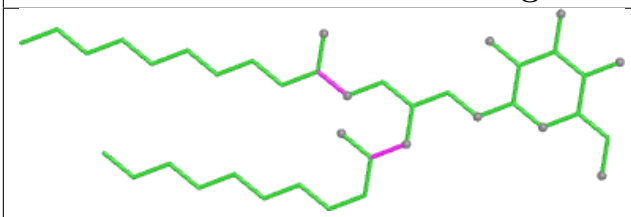


Torsions

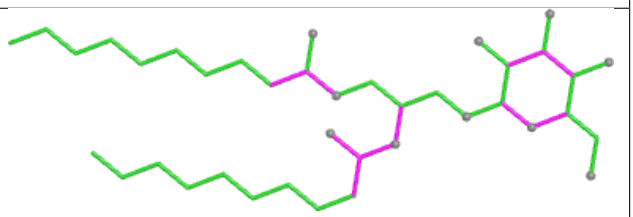


Rings

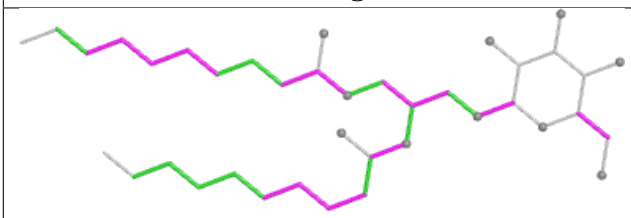
Ligand LMG F 317



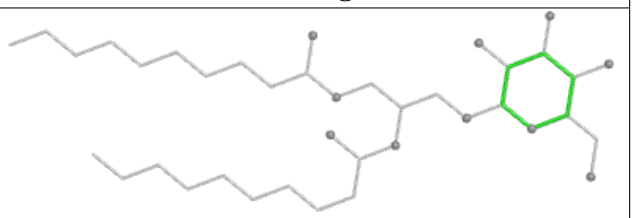
Bond lengths



Bond angles

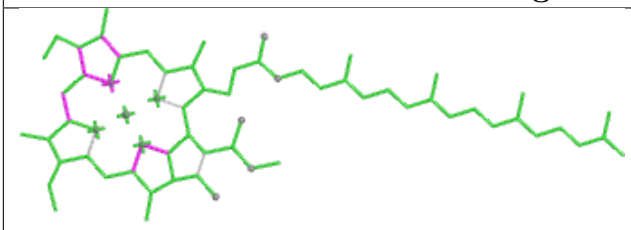


Torsions

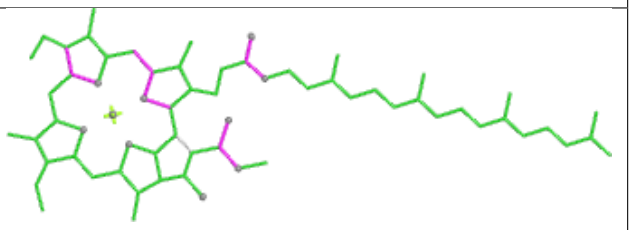


Rings

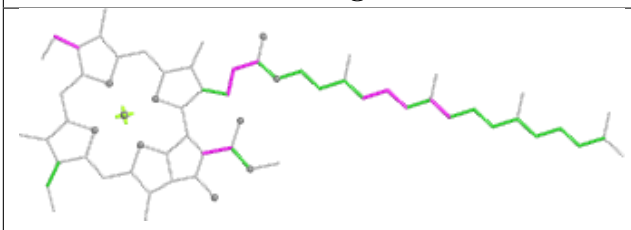
Ligand CLA i 101



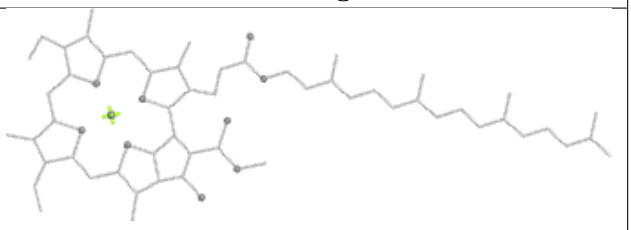
Bond lengths



Bond angles

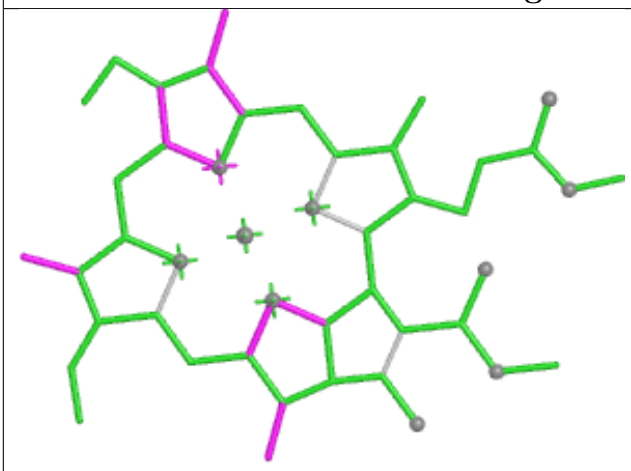


Torsions

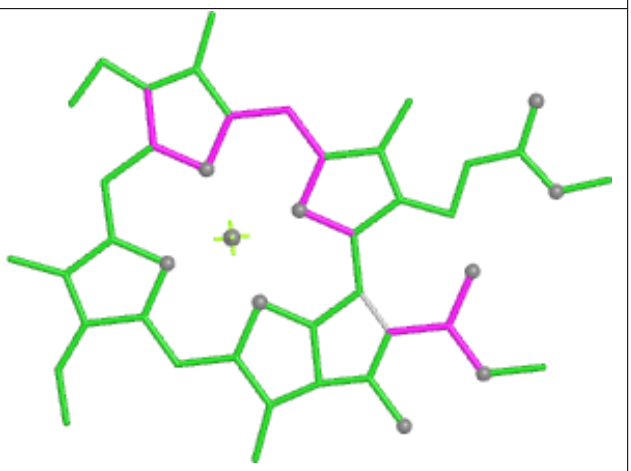


Rings

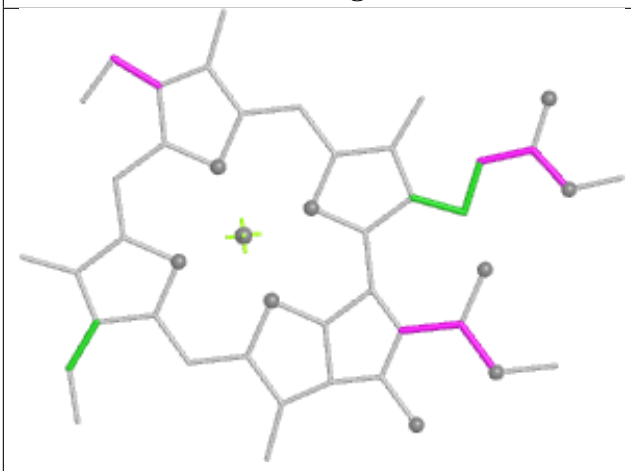
Ligand CLA T 308



Bond lengths



Bond angles

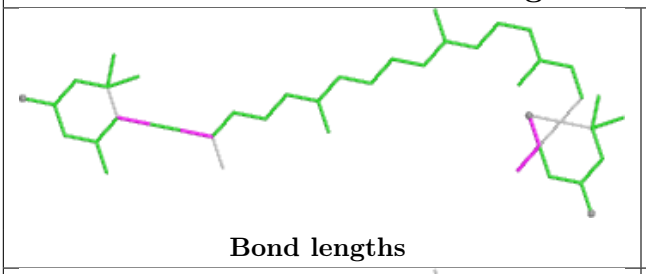


Torsions

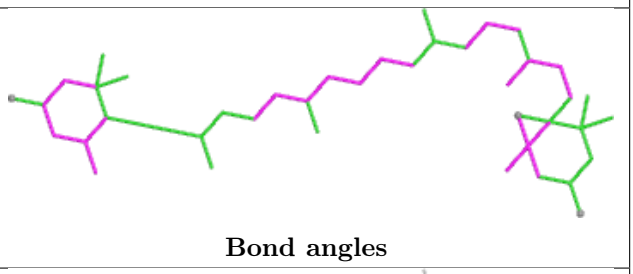


Rings

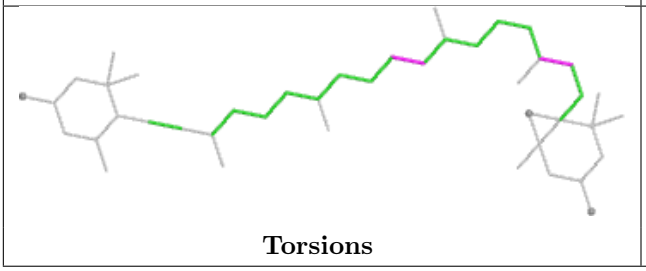
Ligand DD6 C 301



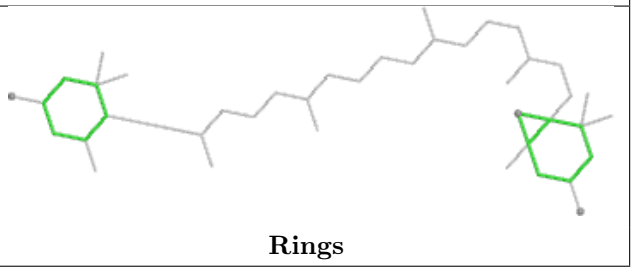
Bond lengths



Bond angles

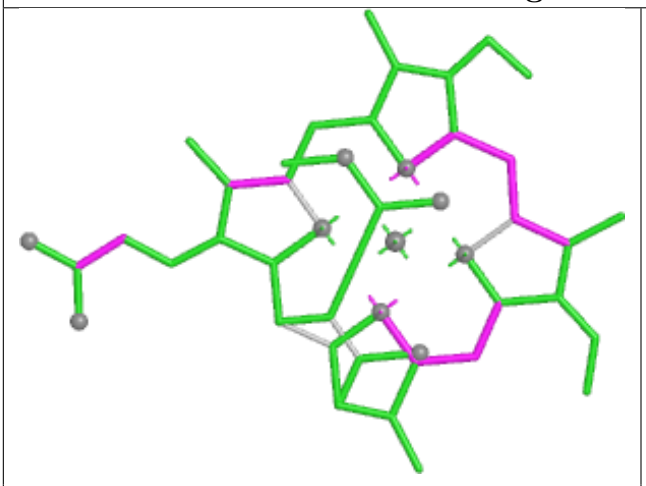


Torsions

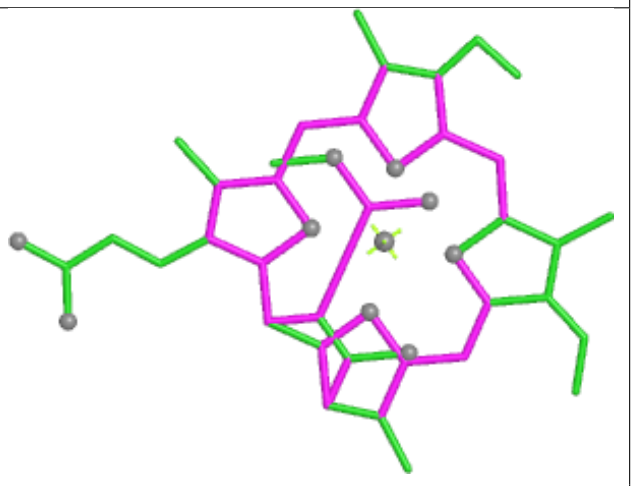


Rings

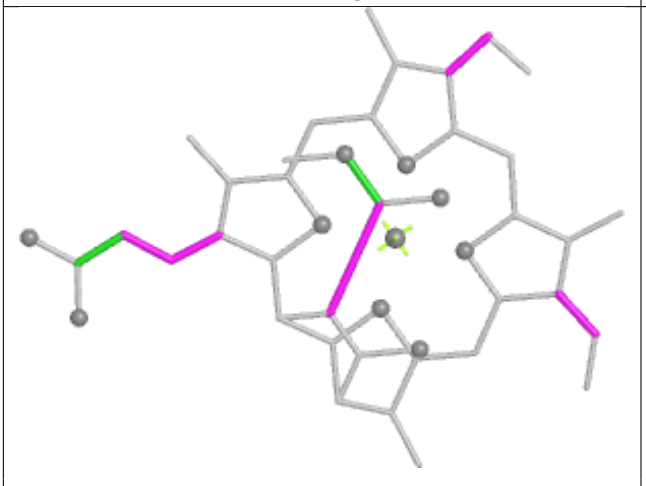
Ligand KC2 R 312



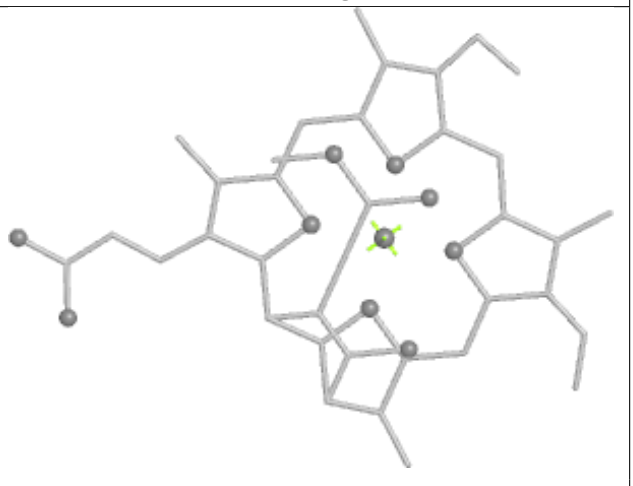
Bond lengths



Bond angles

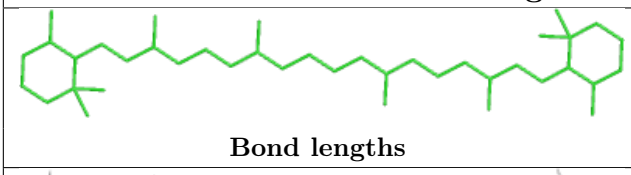


Torsions

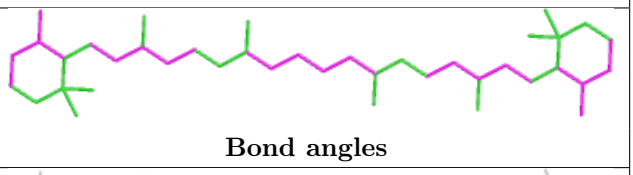


Rings

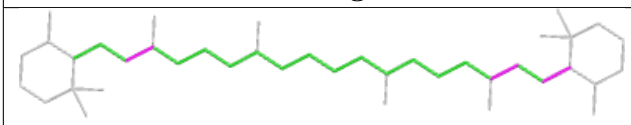
Ligand BCR b 850



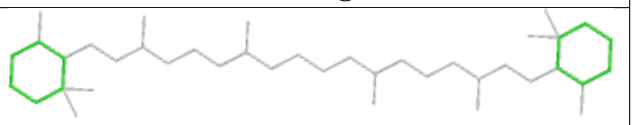
Bond lengths



Bond angles

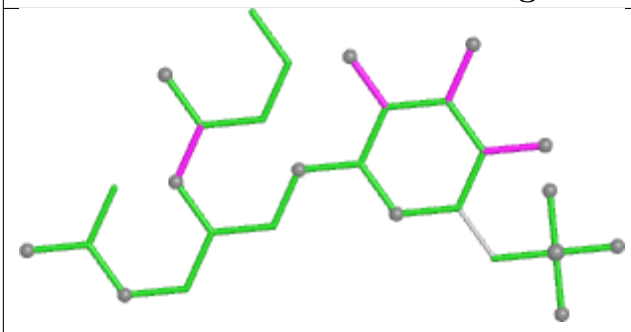


Torsions

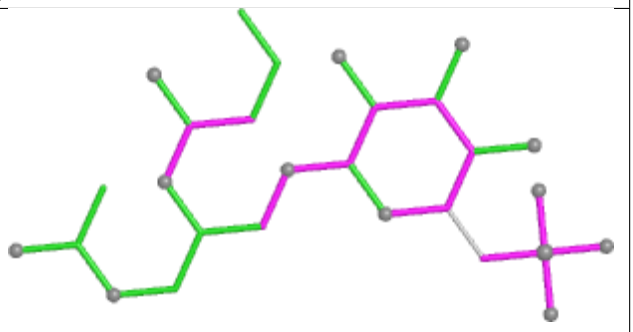


Rings

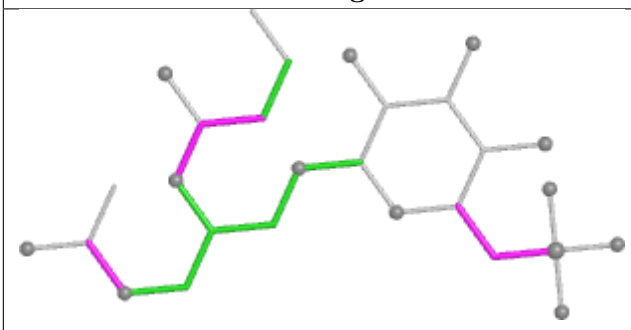
Ligand SQD W 301



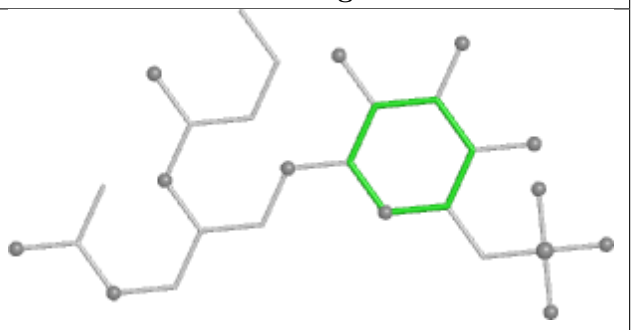
Bond lengths



Bond angles

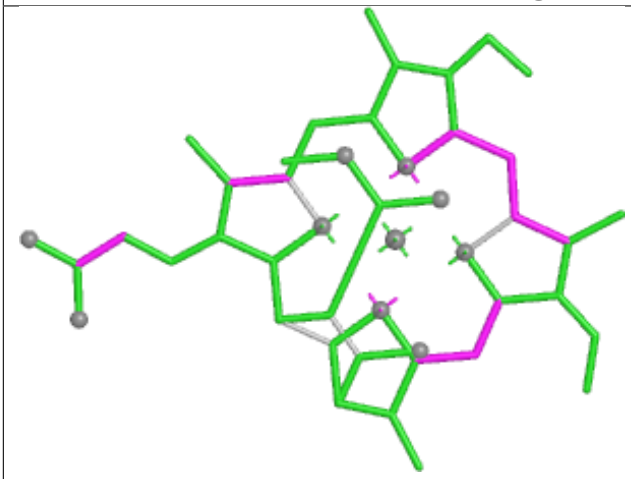


Torsions

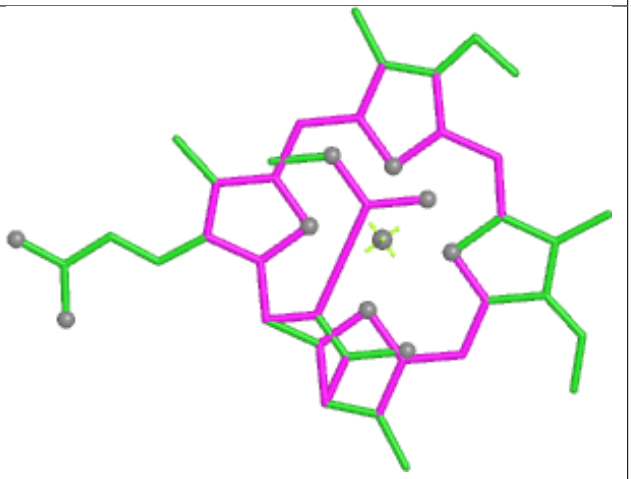


Rings

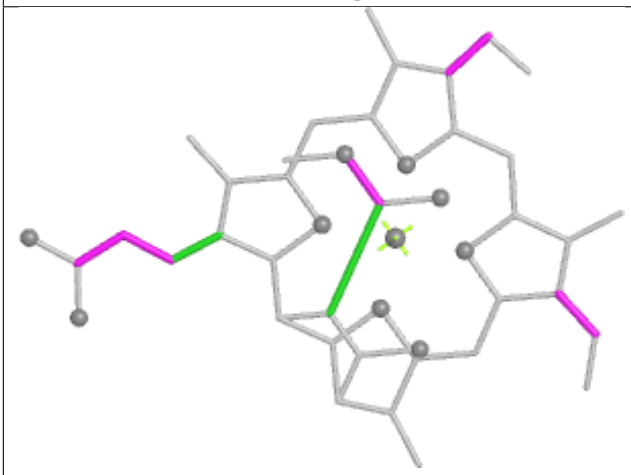
Ligand KC2 6 314



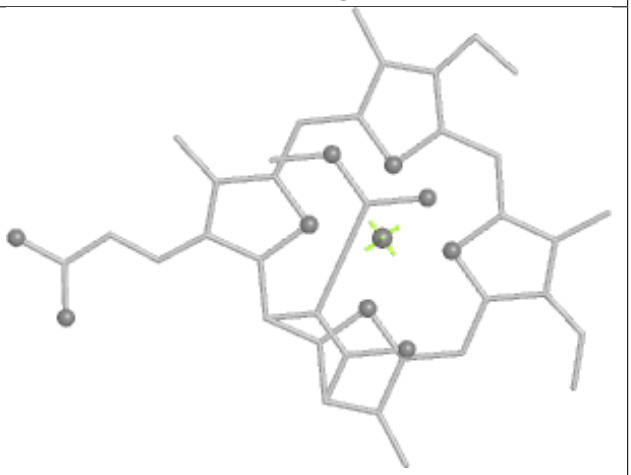
Bond lengths



Bond angles



Torsions

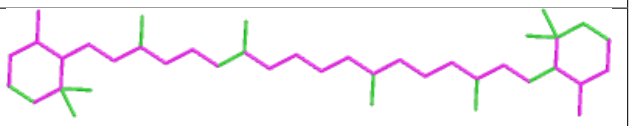


Rings

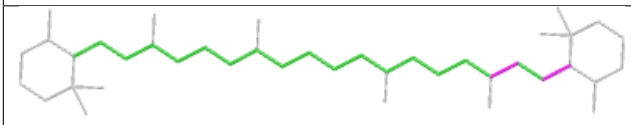
Ligand BCR i 102



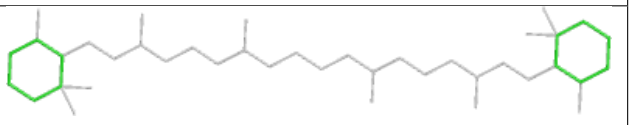
Bond lengths



Bond angles

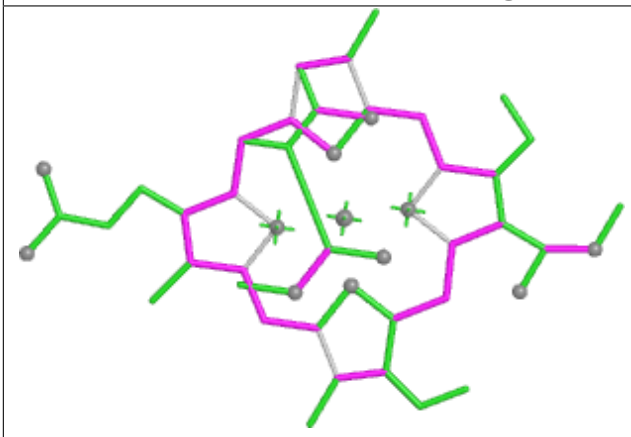


Torsions

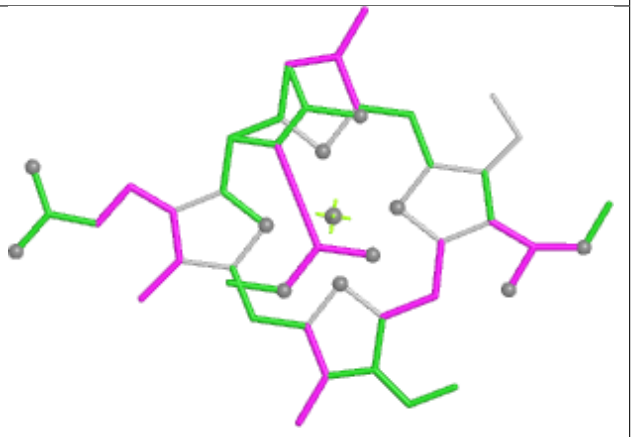


Rings

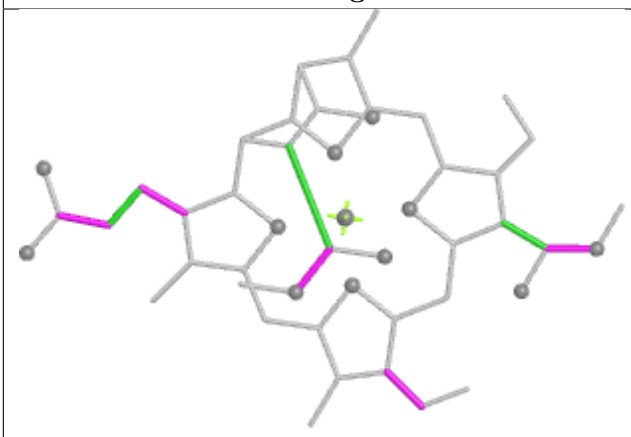
Ligand A1ECV X 310



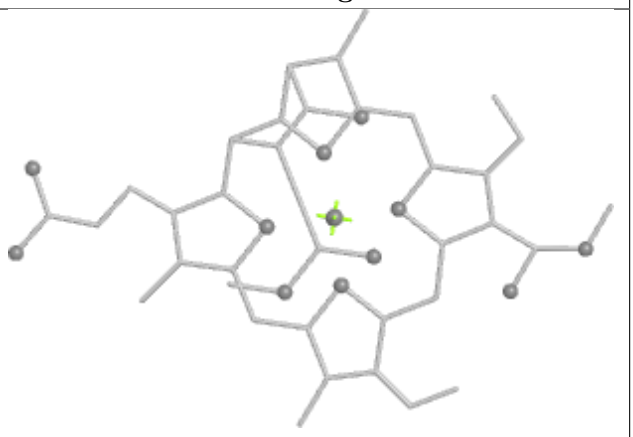
Bond lengths



Bond angles

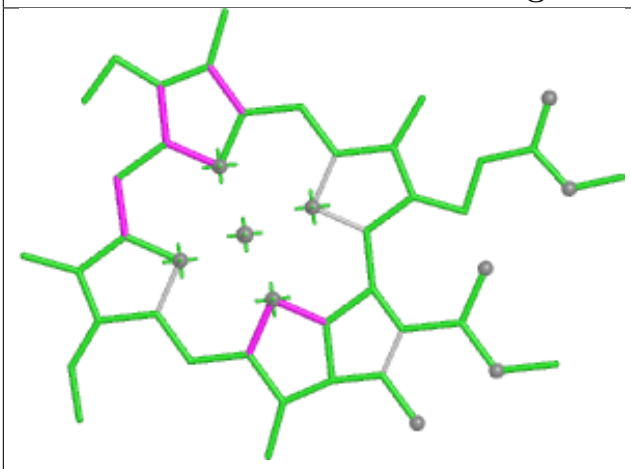


Torsions

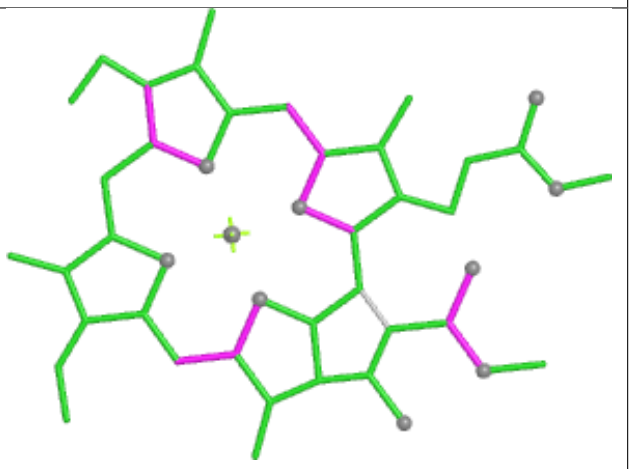


Rings

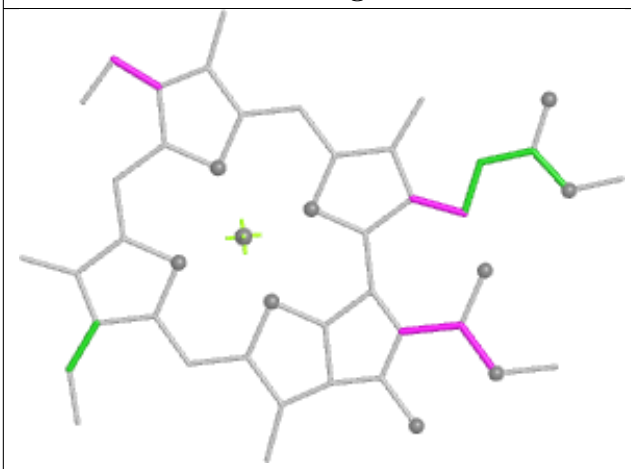
Ligand CLA b 823



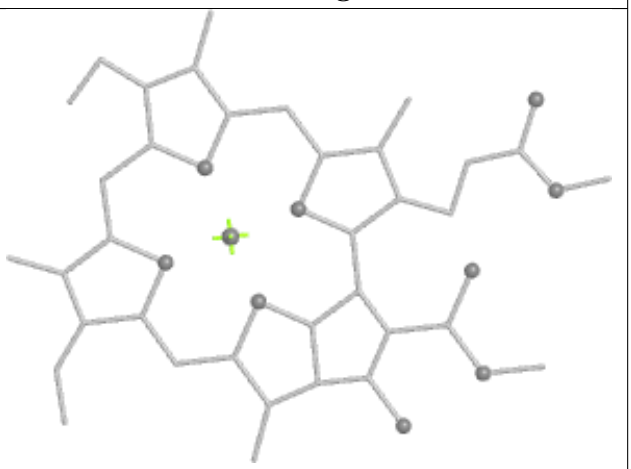
Bond lengths



Bond angles

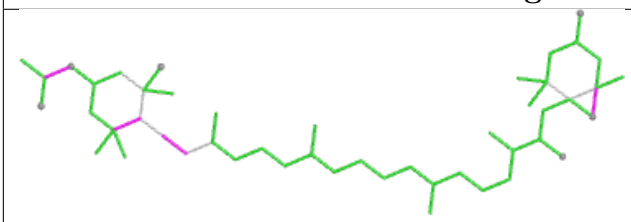


Torsions

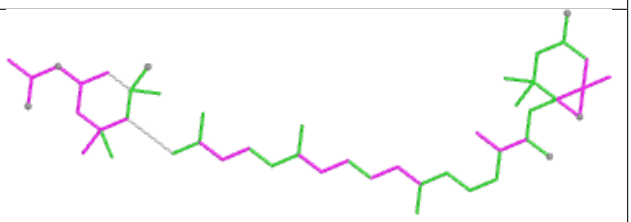


Rings

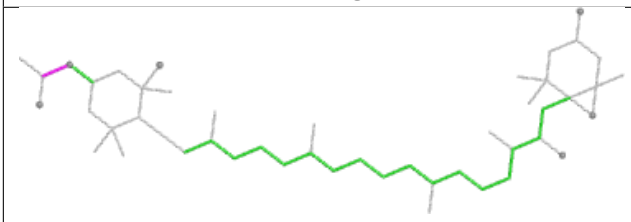
Ligand A86 W 307



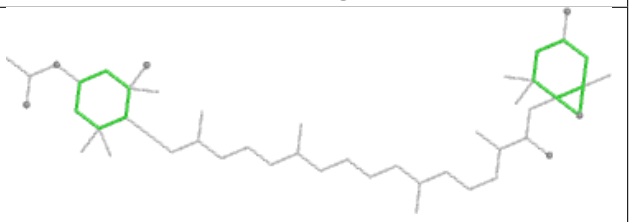
Bond lengths



Bond angles

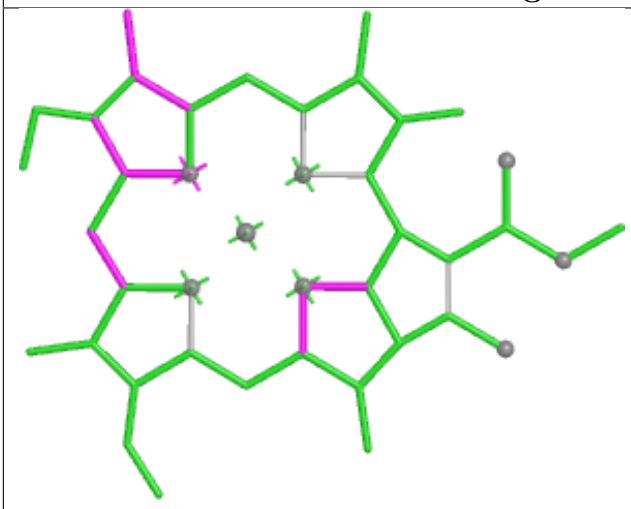


Torsions

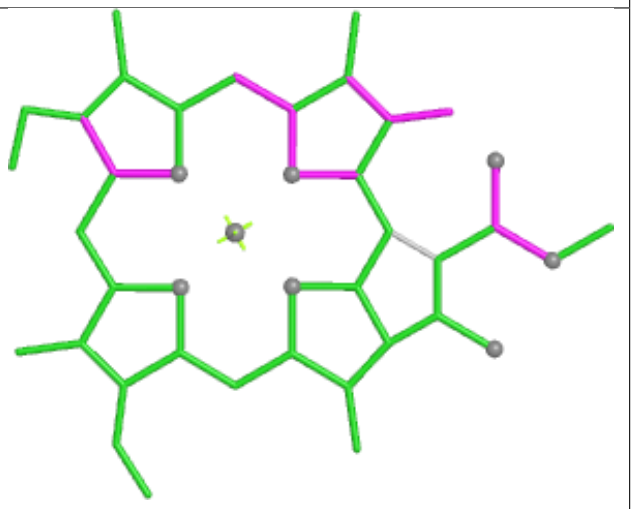


Rings

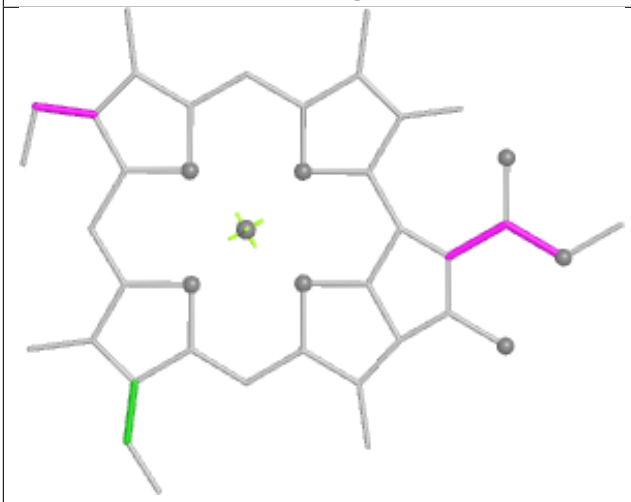
Ligand CLA Y 313



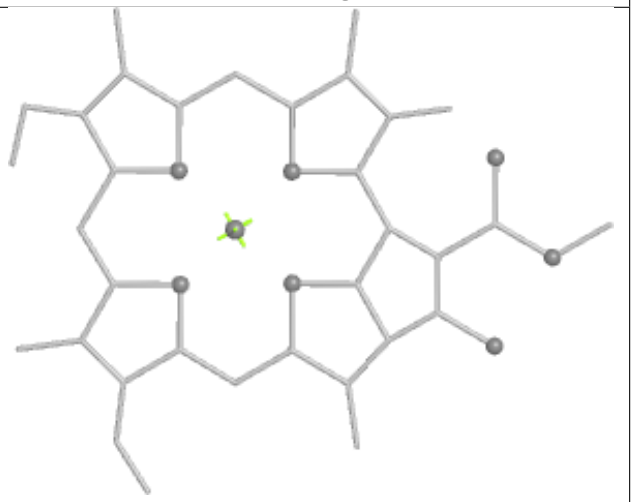
Bond lengths



Bond angles

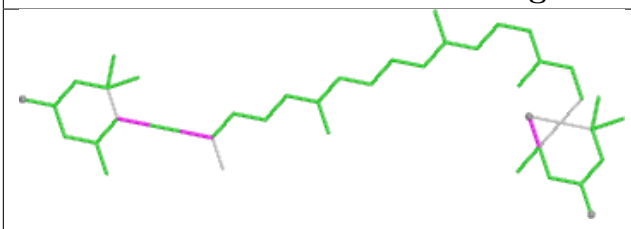


Torsions

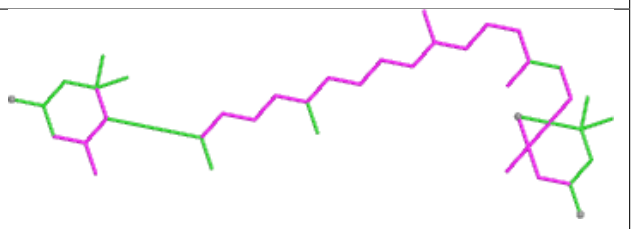


Rings

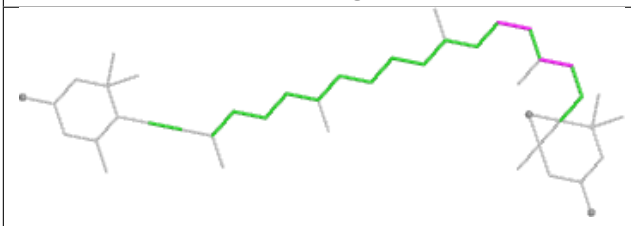
Ligand DD6 3 304



Bond lengths



Bond angles

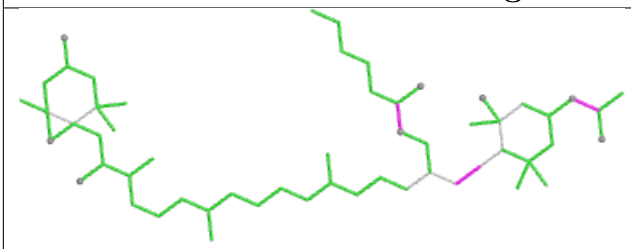


Torsions

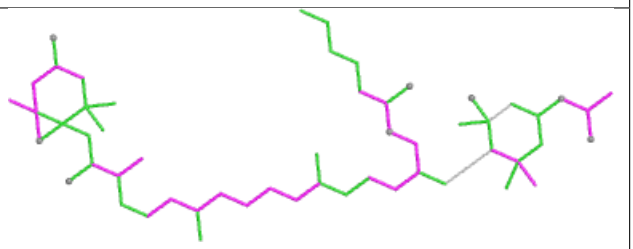


Rings

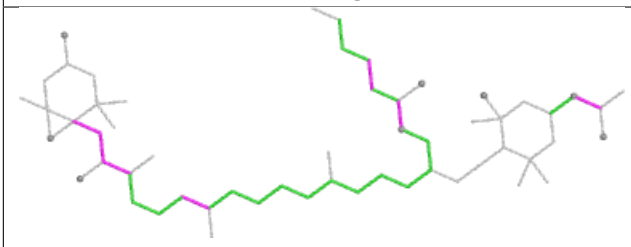
Ligand A1EB1 H 301



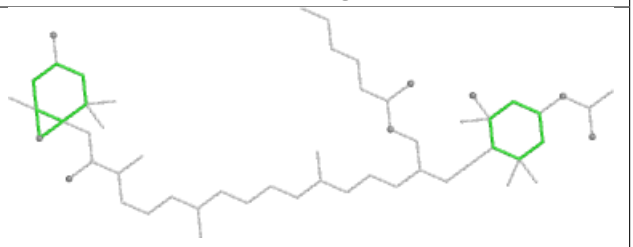
Bond lengths



Bond angles

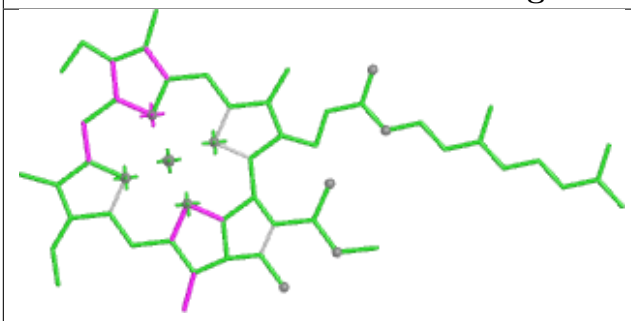


Torsions

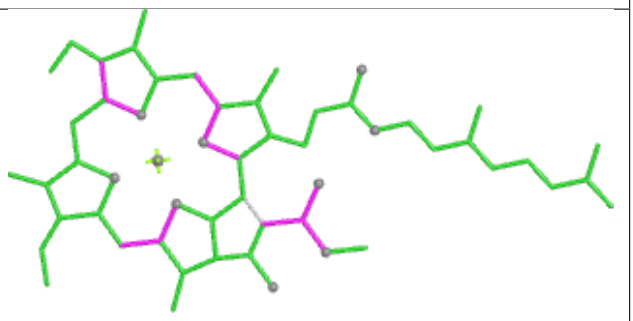


Rings

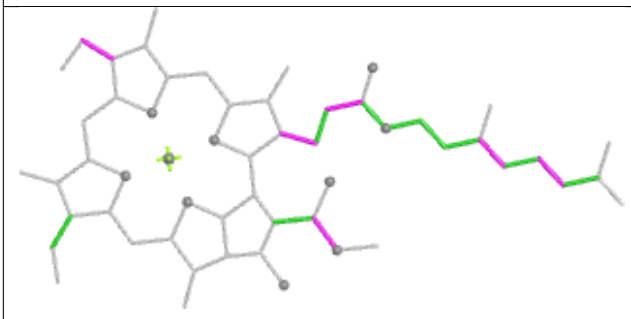
Ligand CLA h 201



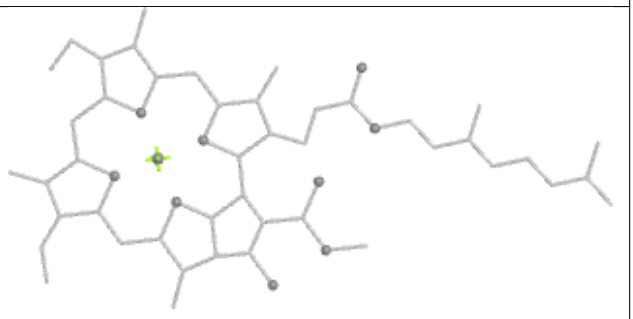
Bond lengths



Bond angles

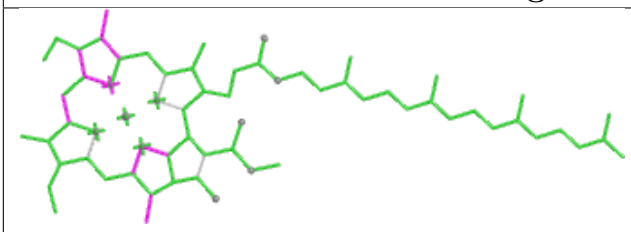


Torsions

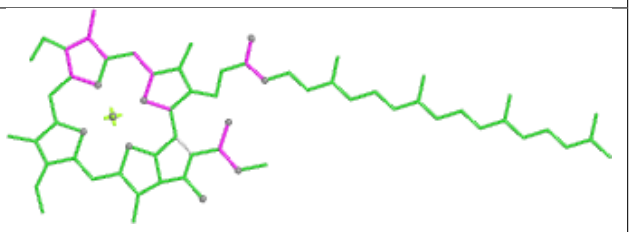


Rings

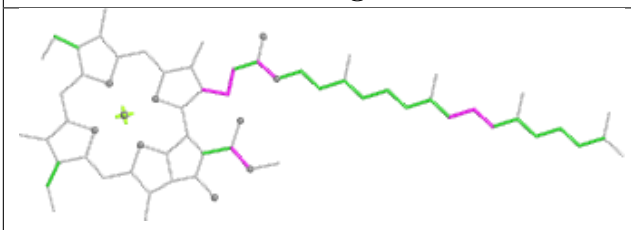
Ligand CLA b 829



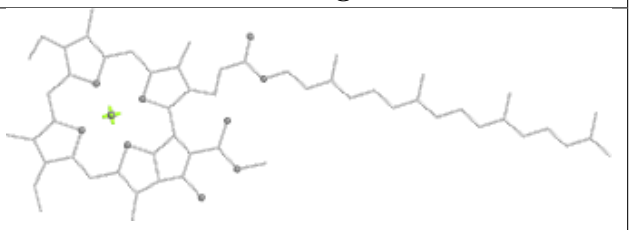
Bond lengths



Bond angles

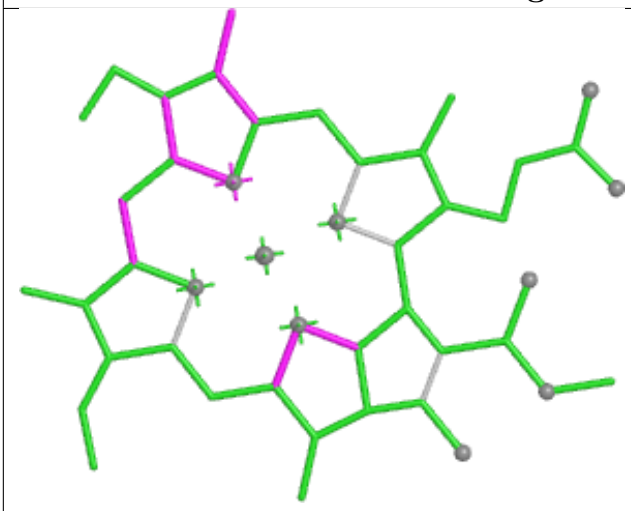


Torsions

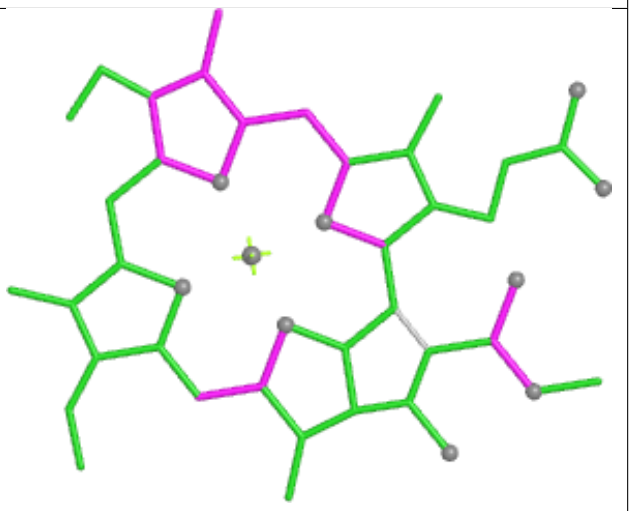


Rings

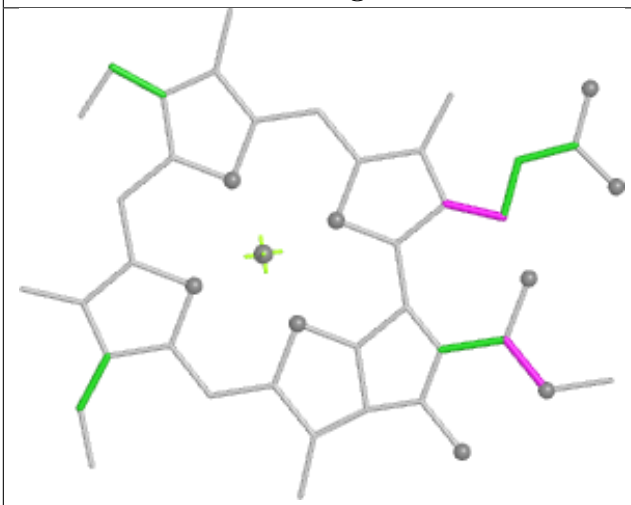
Ligand CLA b 836



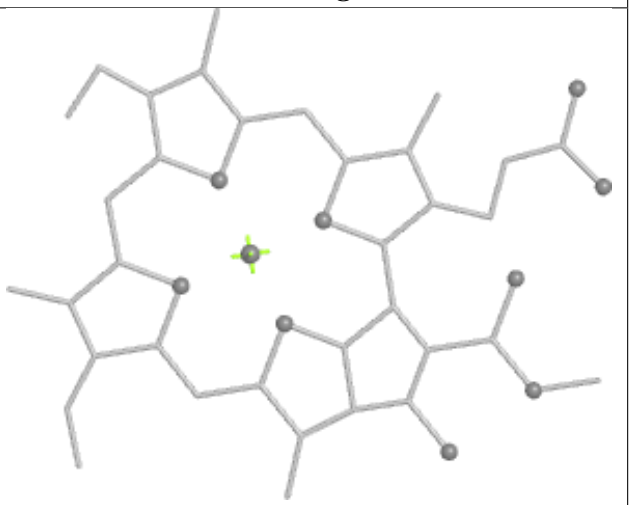
Bond lengths



Bond angles

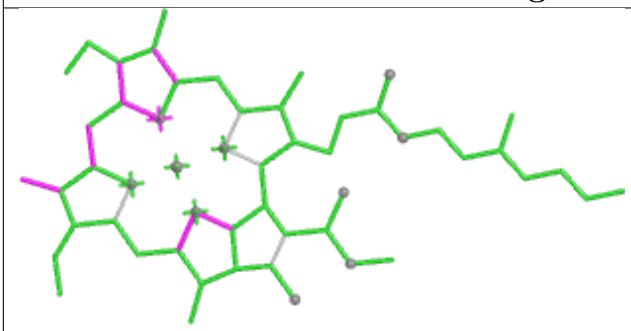


Torsions

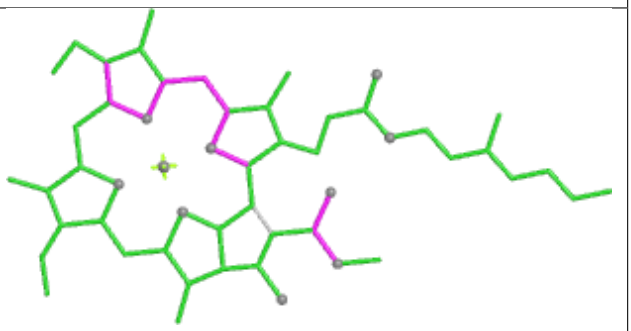


Rings

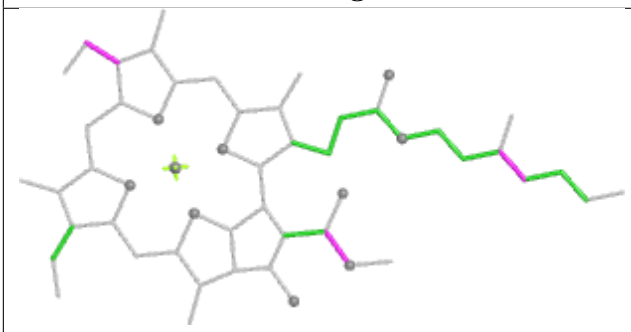
Ligand CLA 3 313



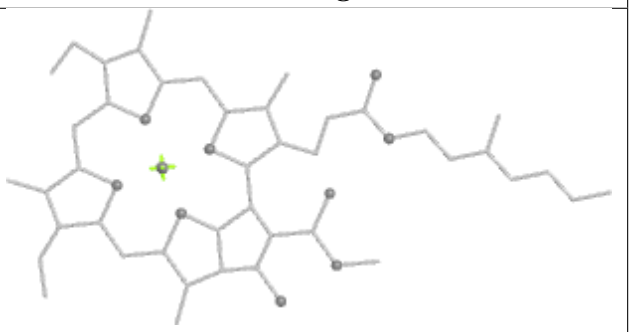
Bond lengths



Bond angles

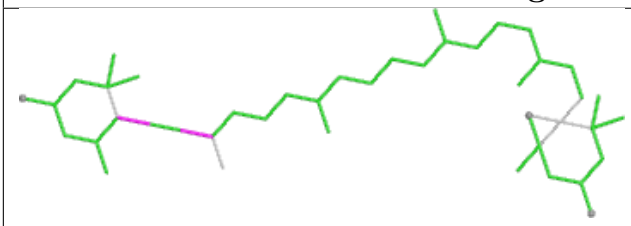


Torsions

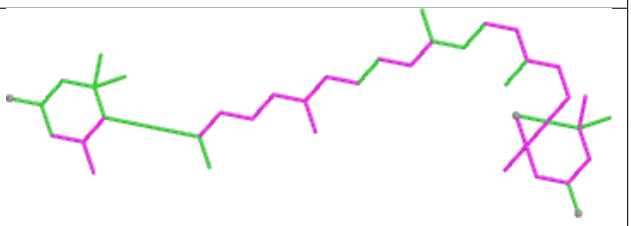


Rings

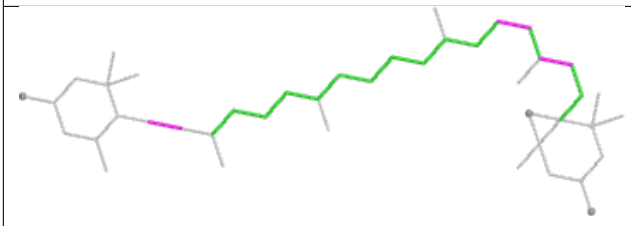
Ligand DD6 S 306



Bond lengths



Bond angles

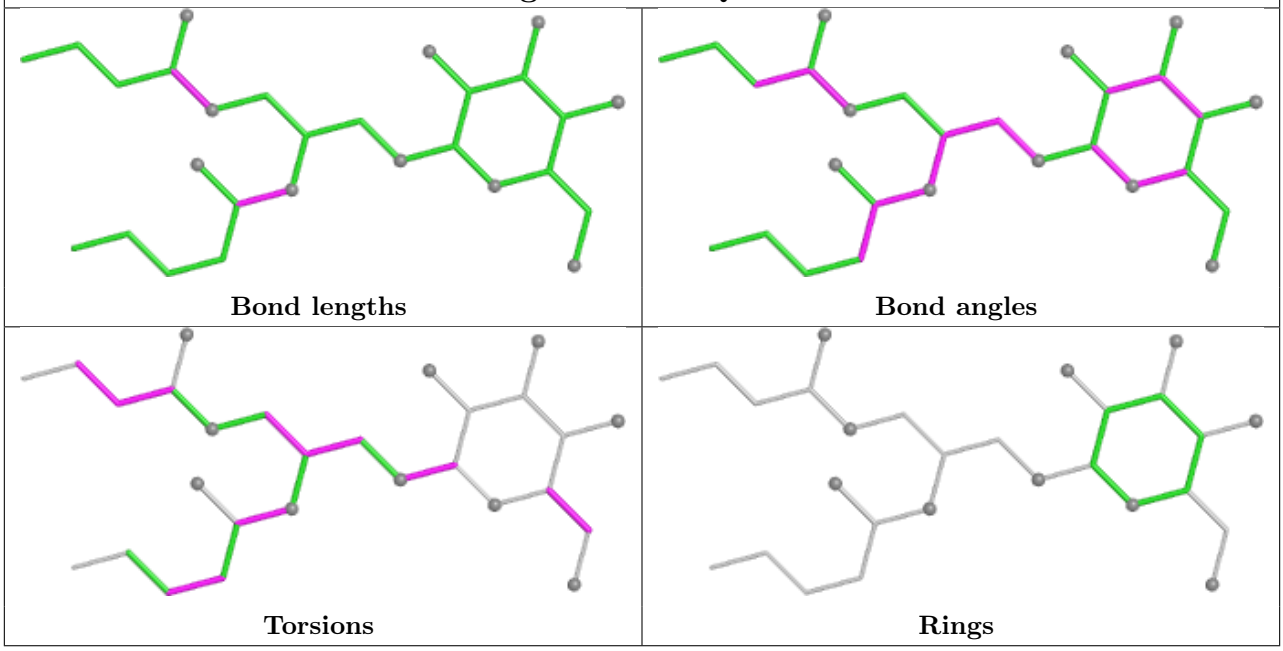


Torsions

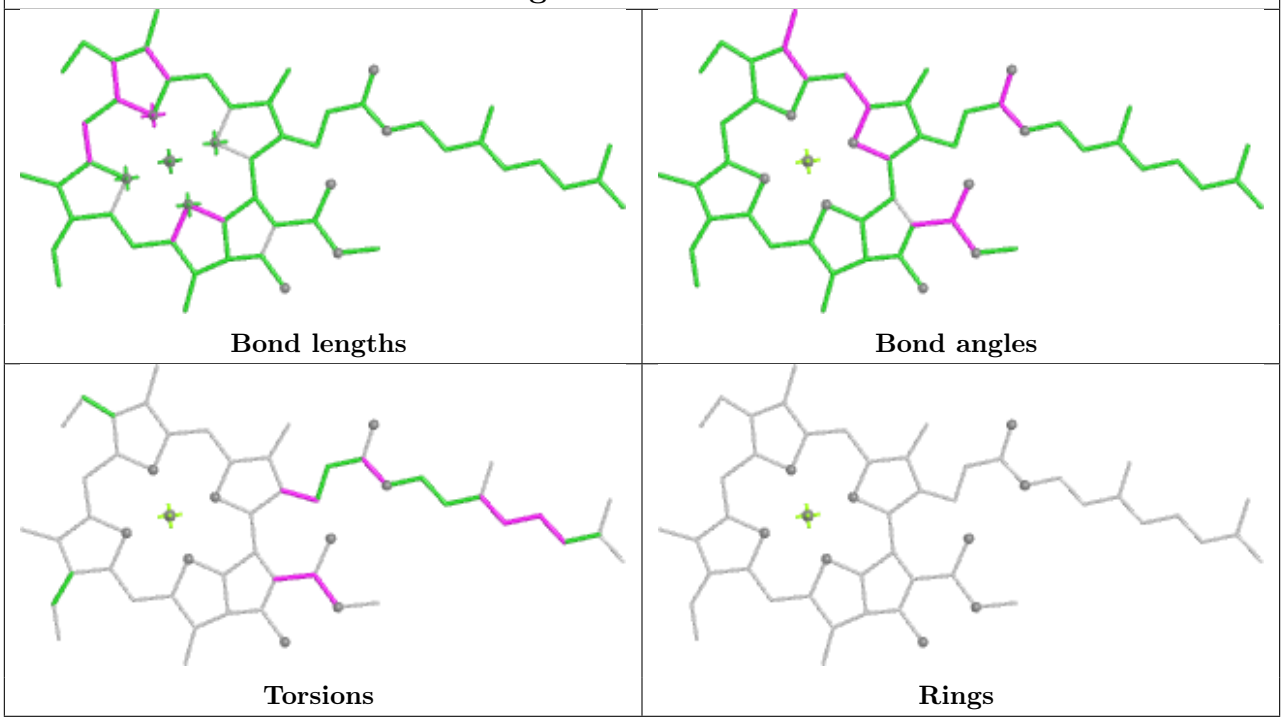


Rings

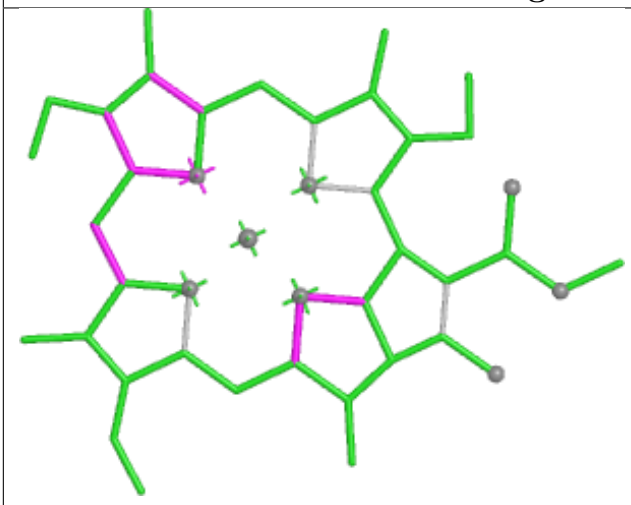
Ligand LMG Q 322



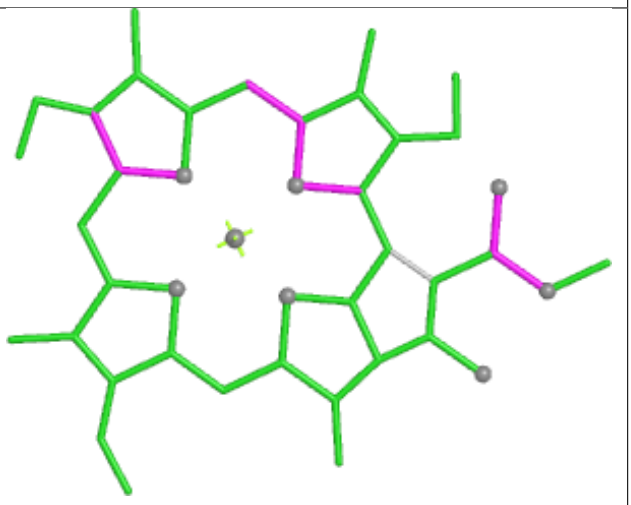
Ligand CLA 8 311



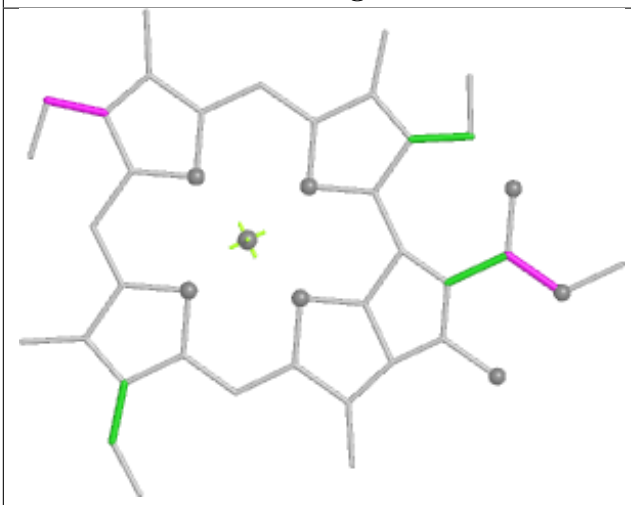
Ligand CLA 8 321



Bond lengths



Bond angles

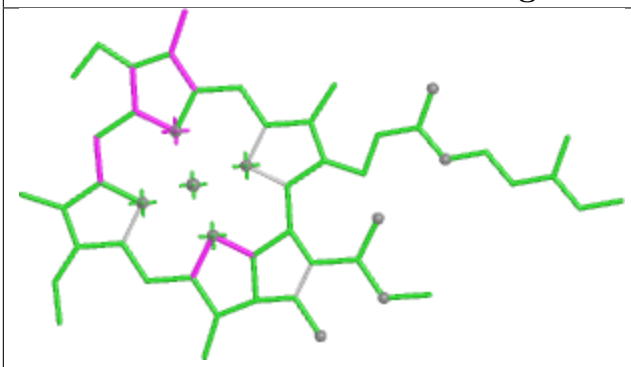


Torsions

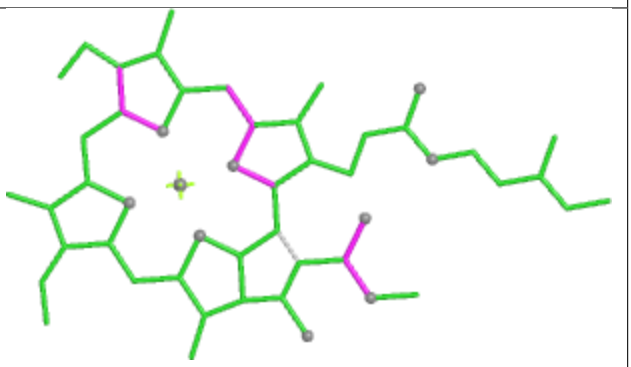


Rings

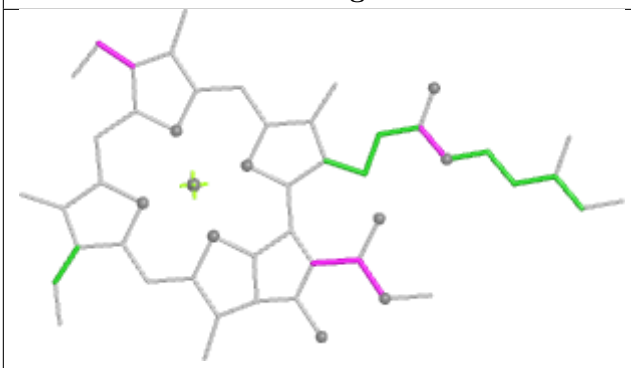
Ligand CLA W 318



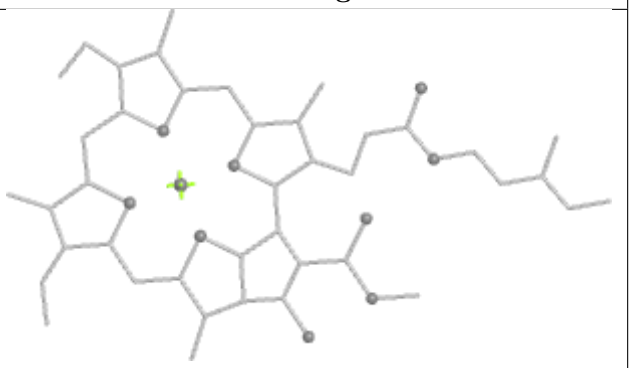
Bond lengths



Bond angles

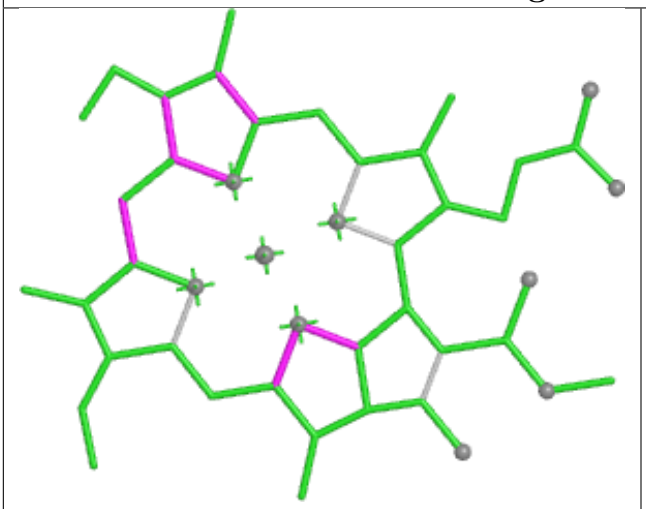


Torsions

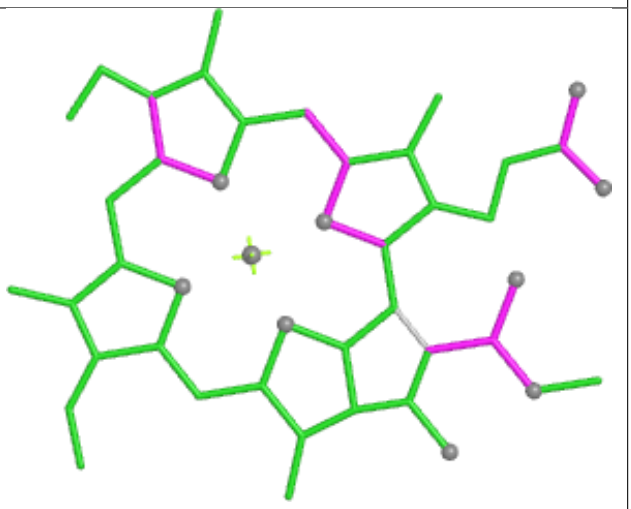


Rings

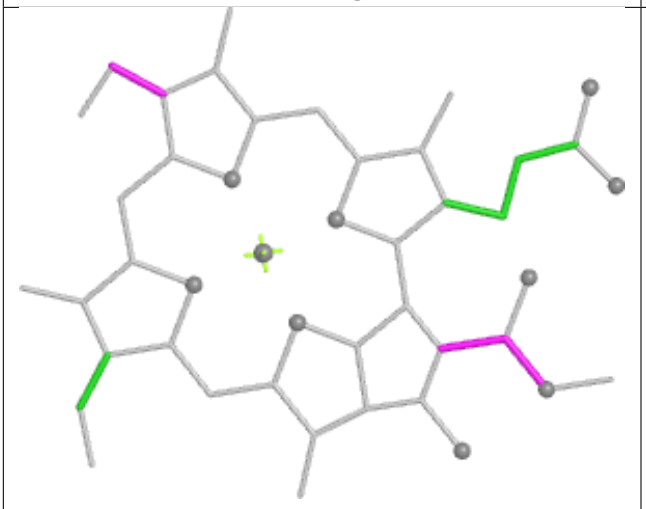
Ligand CLA 3 320



Bond lengths



Bond angles

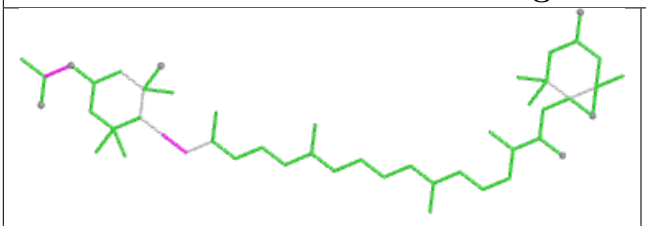


Torsions

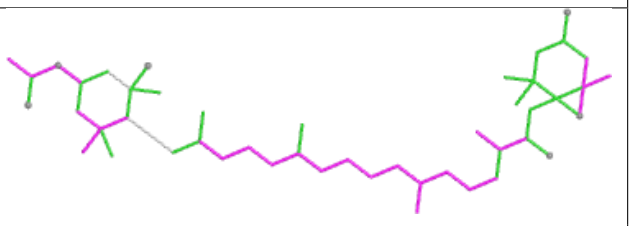


Rings

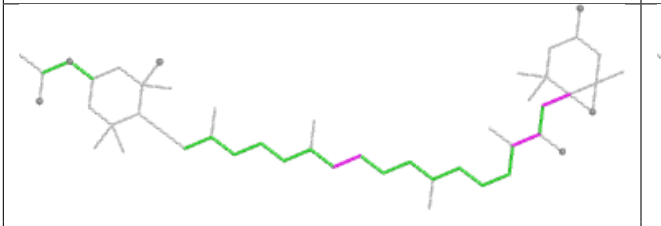
Ligand A86 S 305



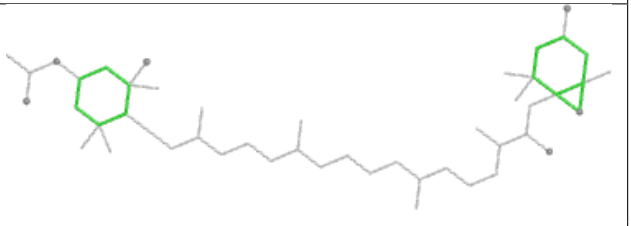
Bond lengths



Bond angles

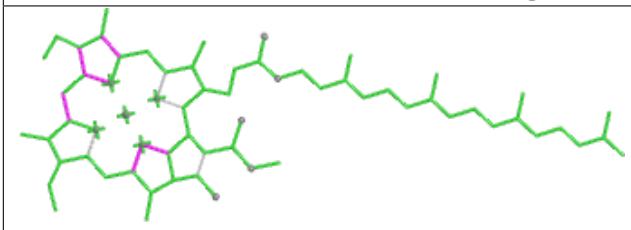


Torsions

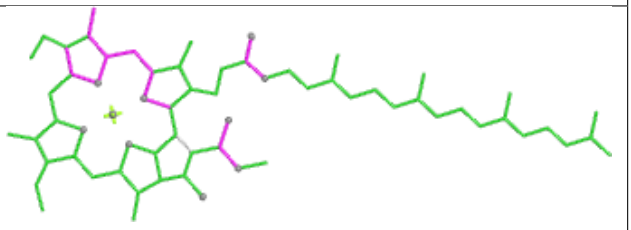


Rings

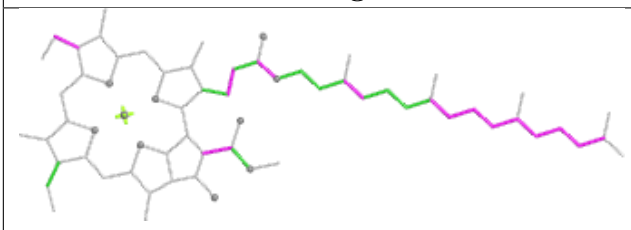
Ligand CLA D 319



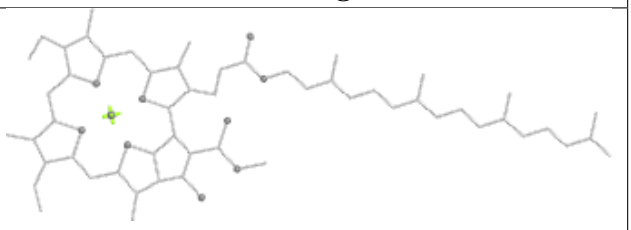
Bond lengths



Bond angles

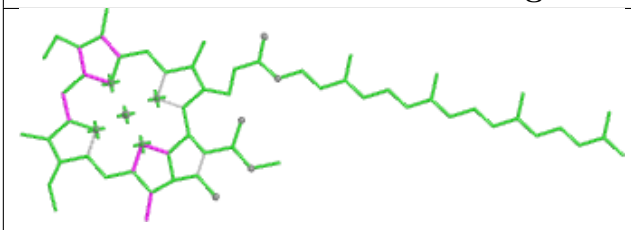


Torsions

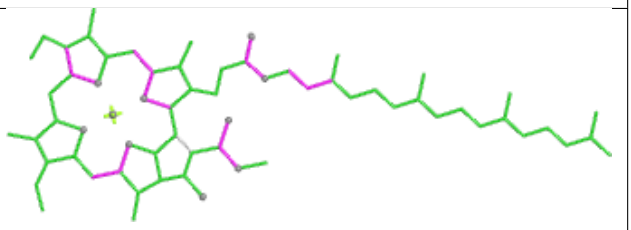


Rings

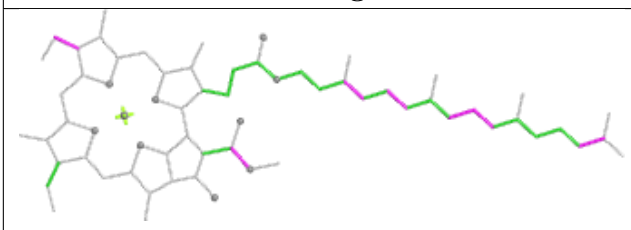
Ligand CLA E 310



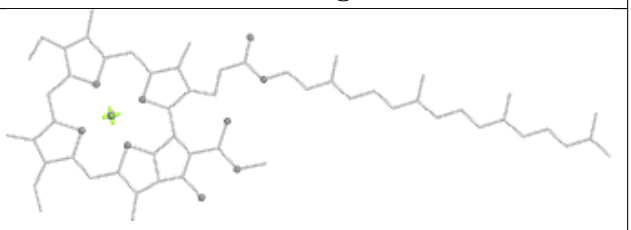
Bond lengths



Bond angles

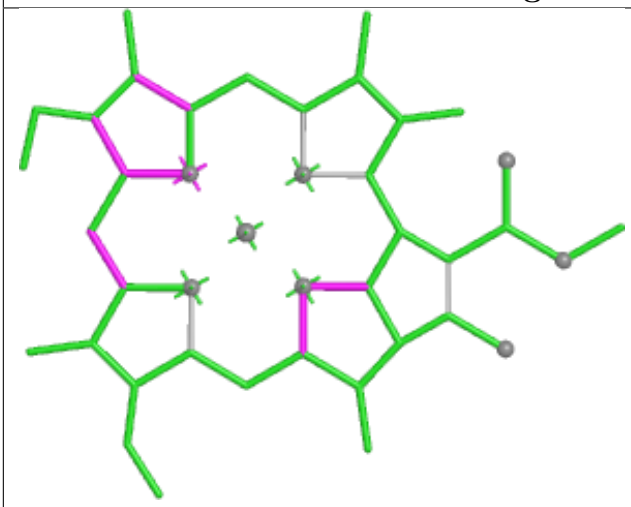


Torsions

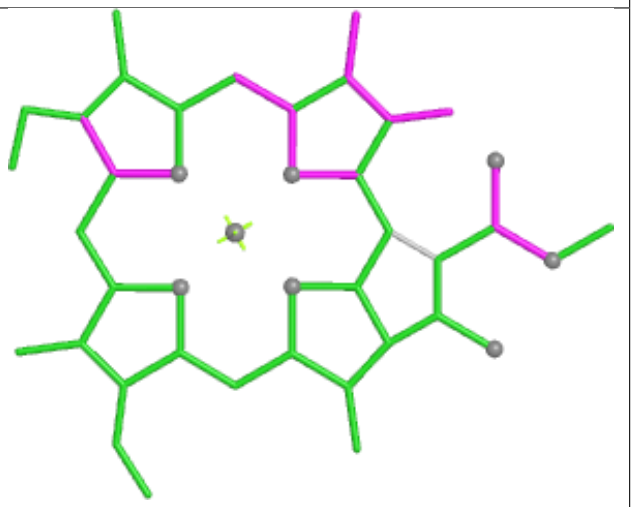


Rings

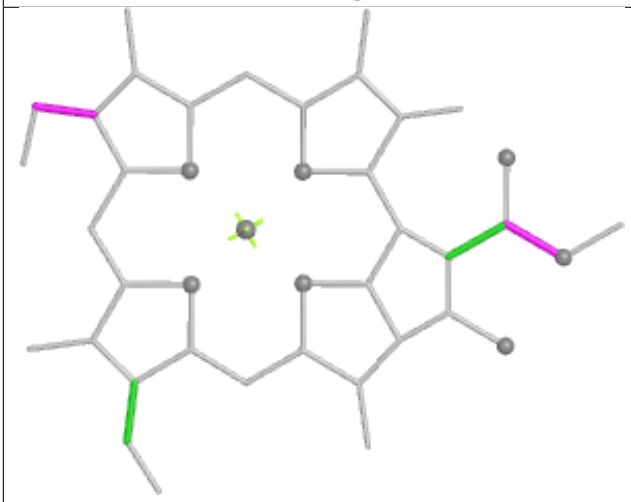
Ligand CLA Y 303



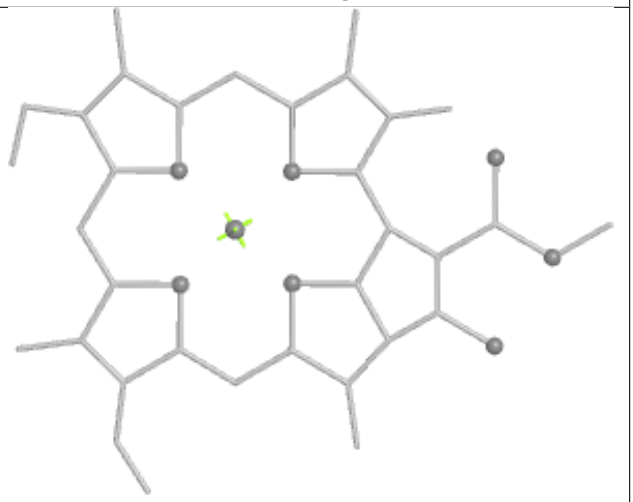
Bond lengths



Bond angles

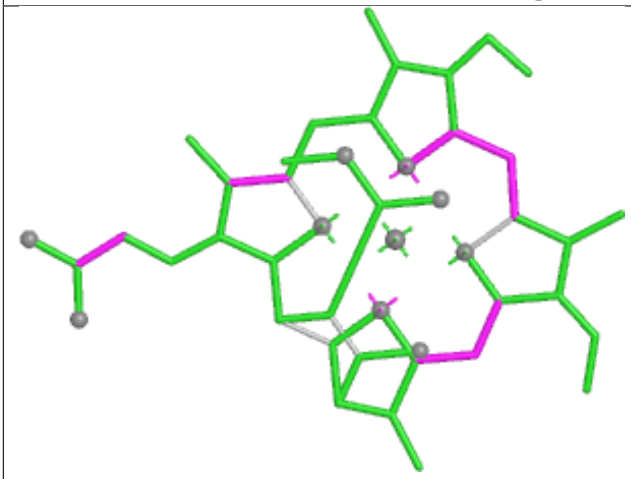


Torsions

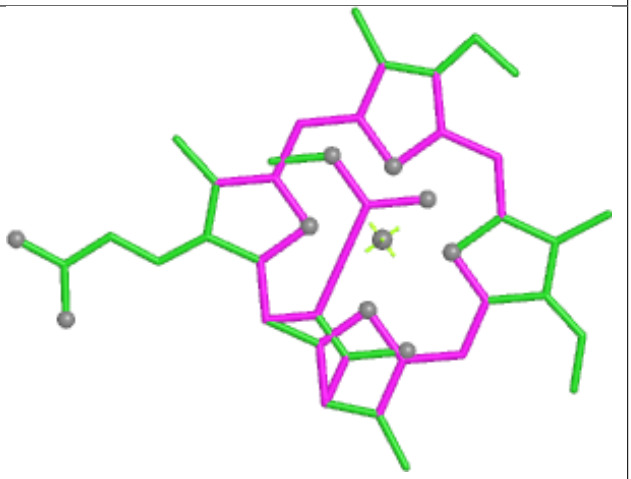


Rings

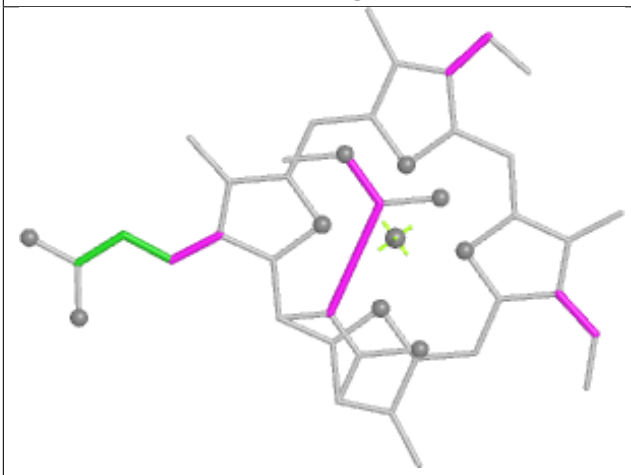
Ligand KC2 6 317



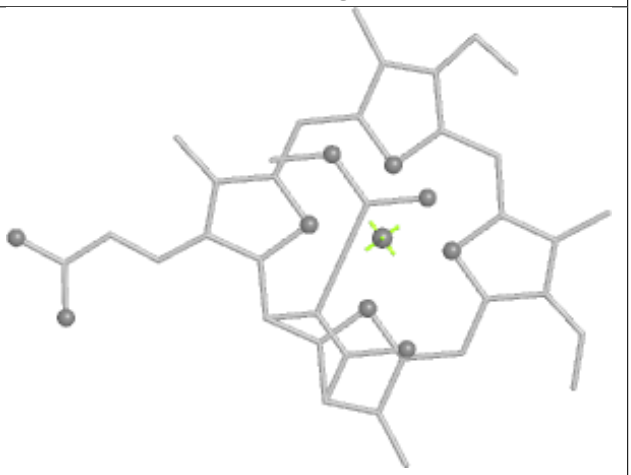
Bond lengths



Bond angles

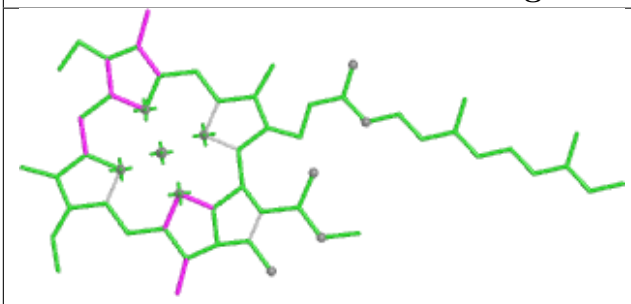


Torsions

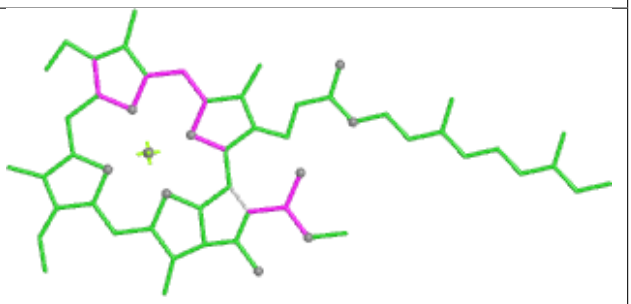


Rings

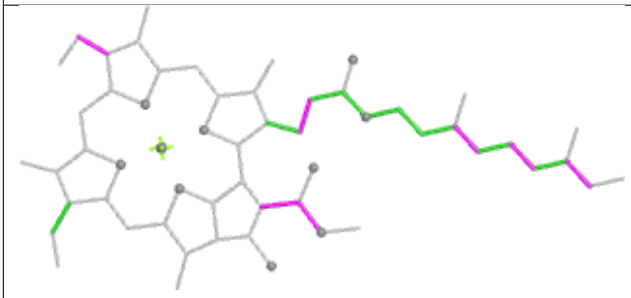
Ligand CLA B 209



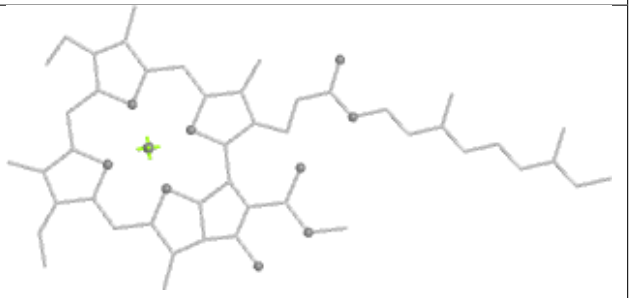
Bond lengths



Bond angles

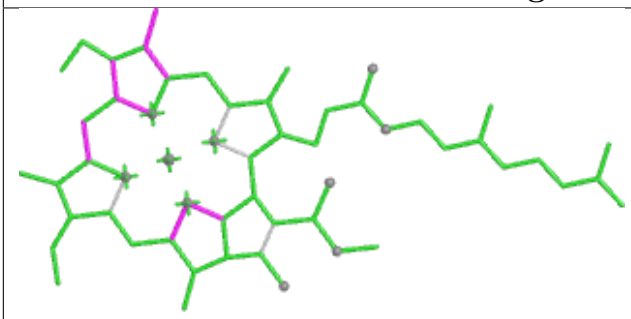


Torsions

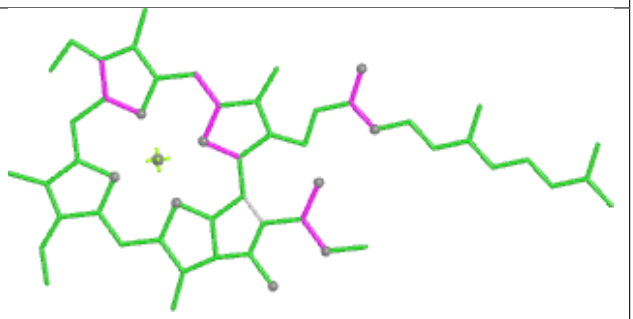


Rings

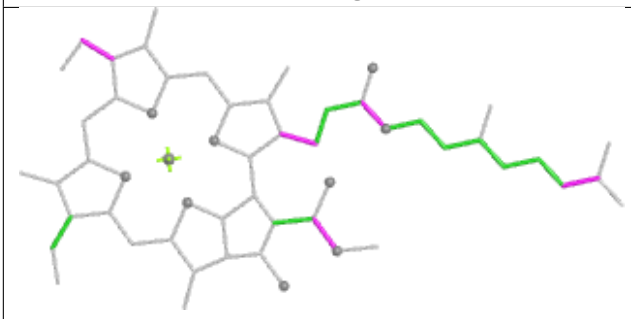
Ligand CLA k 203



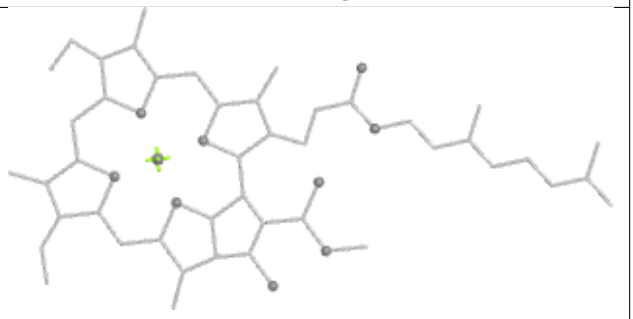
Bond lengths



Bond angles

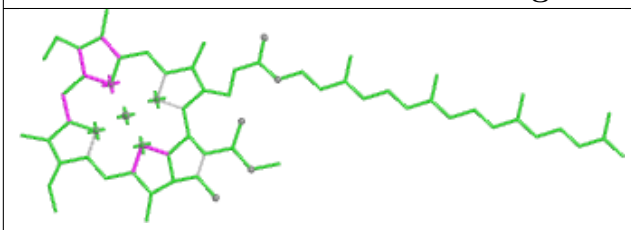


Torsions

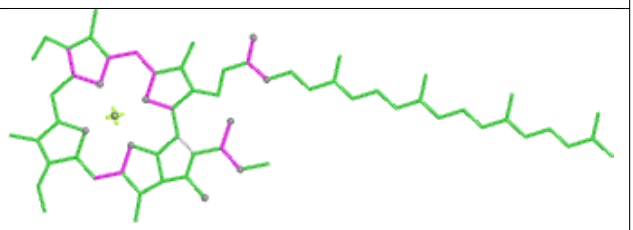


Rings

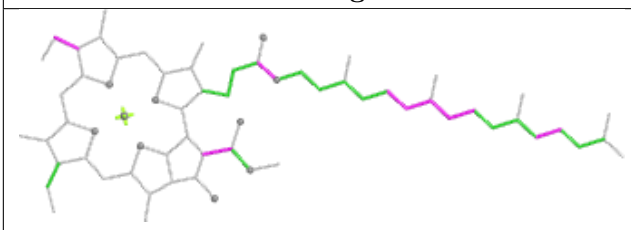
Ligand CLA f 802



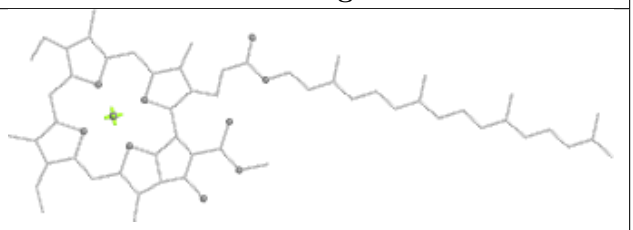
Bond lengths



Bond angles

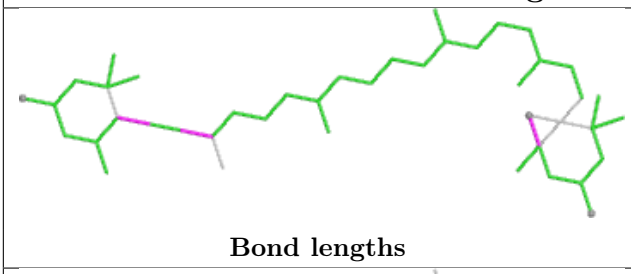


Torsions

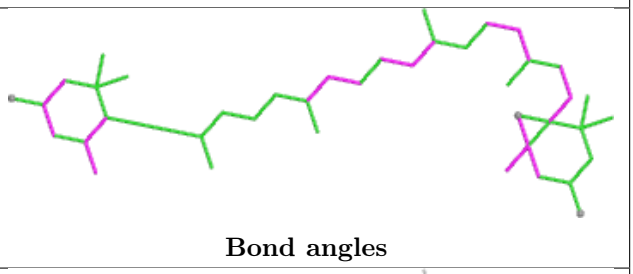


Rings

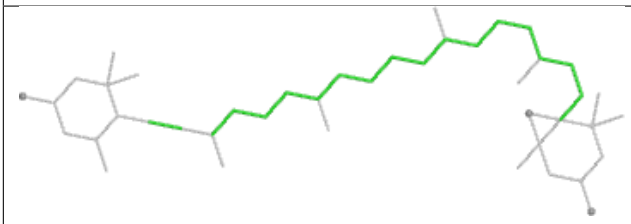
Ligand DD6 E 302



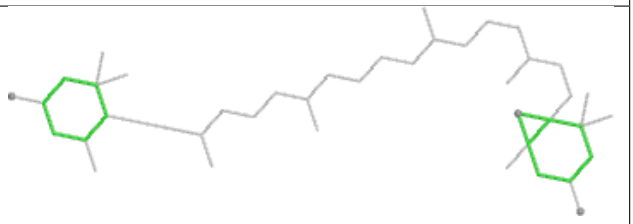
Bond lengths



Bond angles

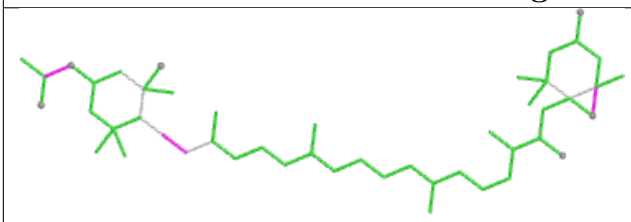


Torsions

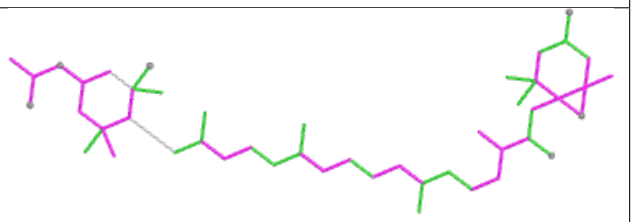


Rings

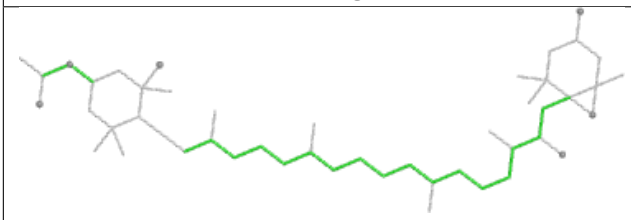
Ligand A86 P 303



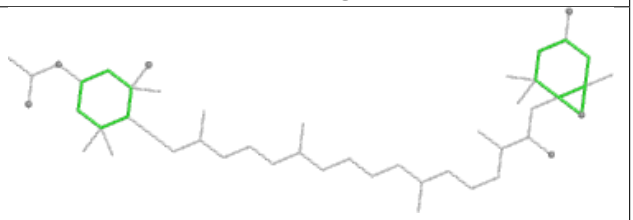
Bond lengths



Bond angles

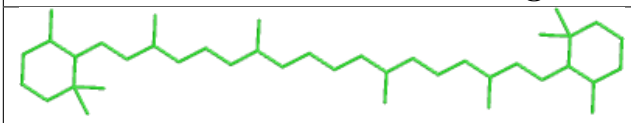


Torsions

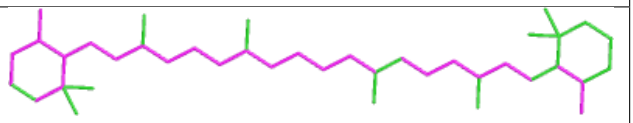


Rings

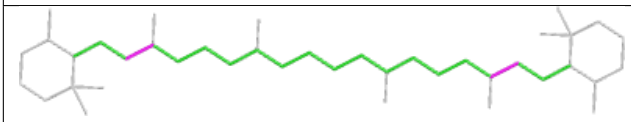
Ligand BCR b 847



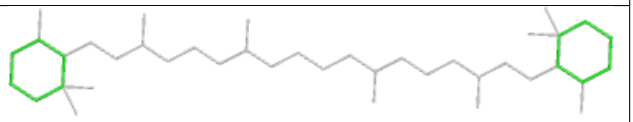
Bond lengths



Bond angles

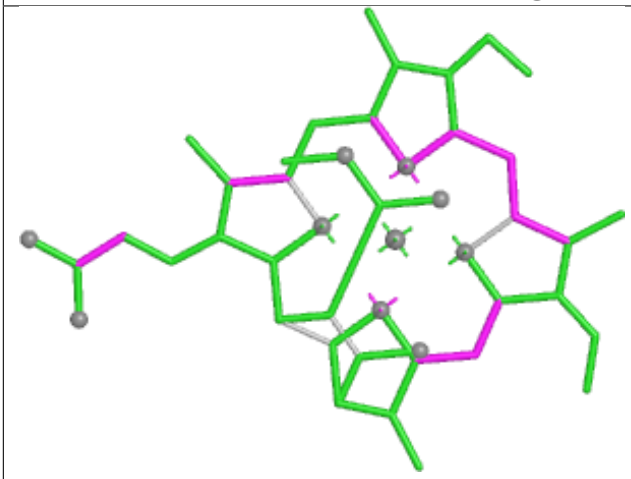


Torsions

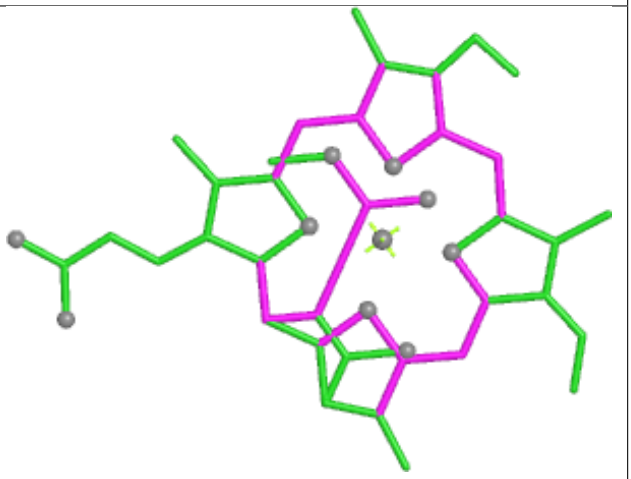


Rings

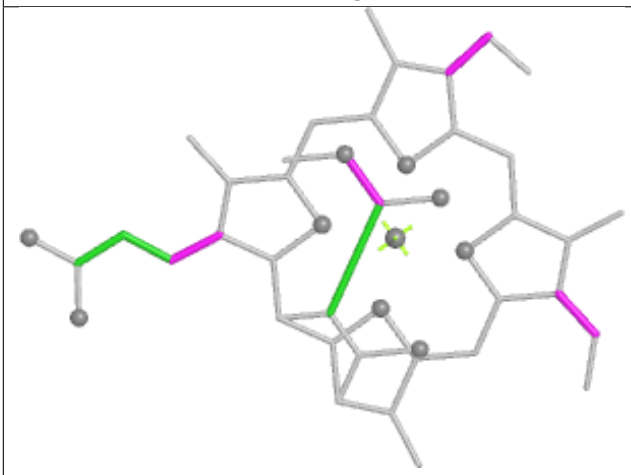
Ligand KC2 L 321



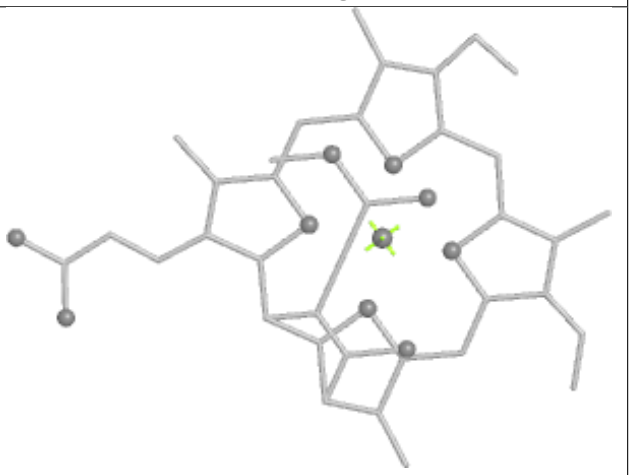
Bond lengths



Bond angles

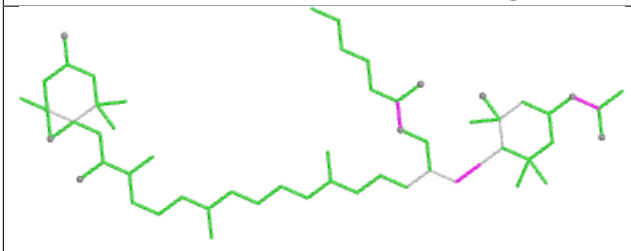


Torsions

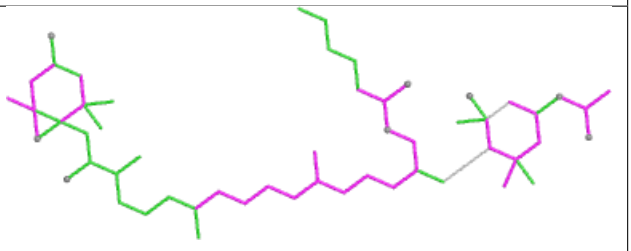


Rings

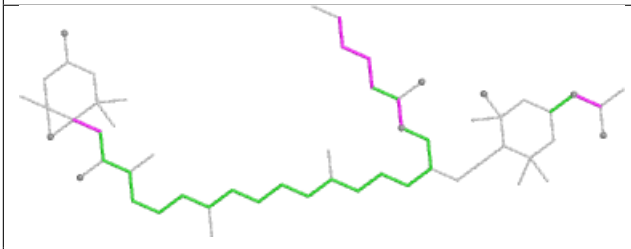
Ligand A1EB1 D 308



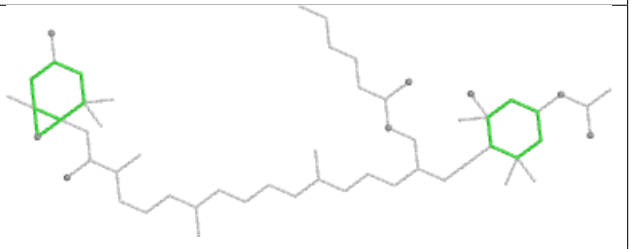
Bond lengths



Bond angles

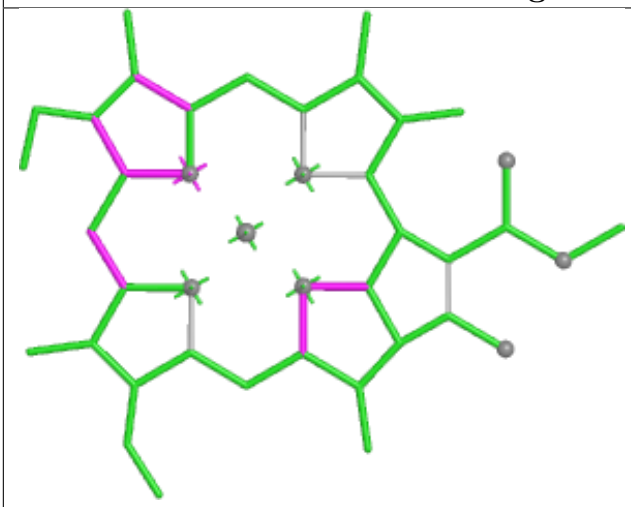


Torsions

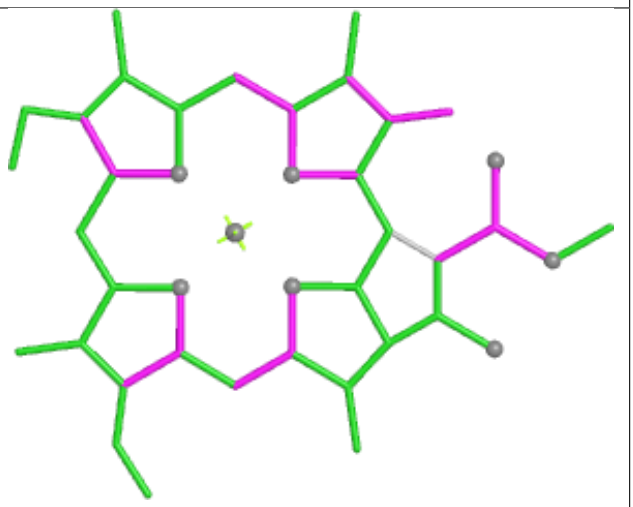


Rings

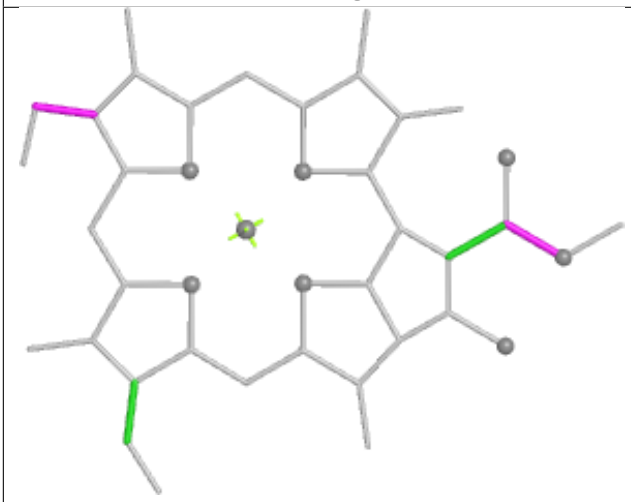
Ligand CLA 8 322



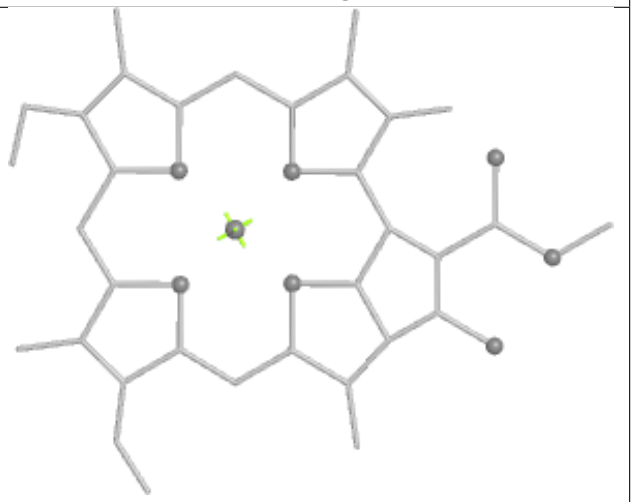
Bond lengths



Bond angles

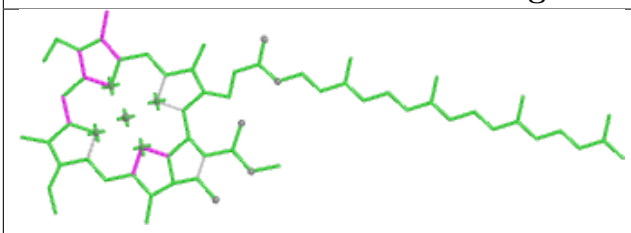


Torsions

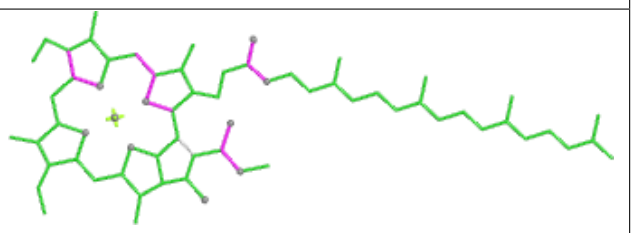


Rings

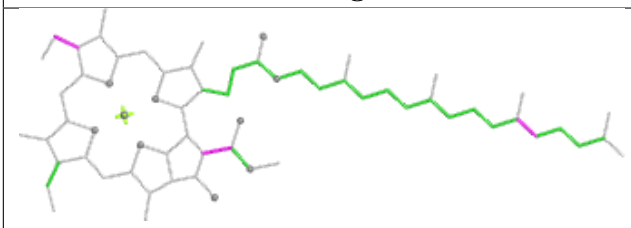
Ligand CLA a 837



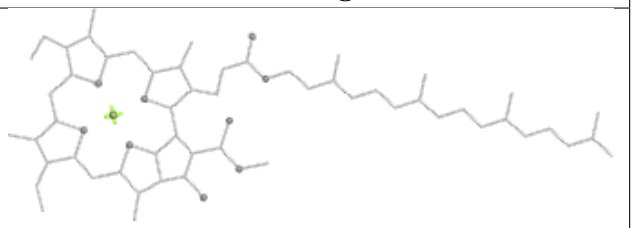
Bond lengths



Bond angles

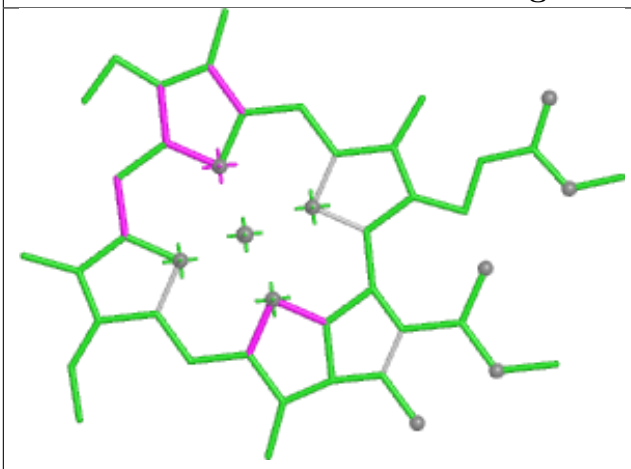


Torsions

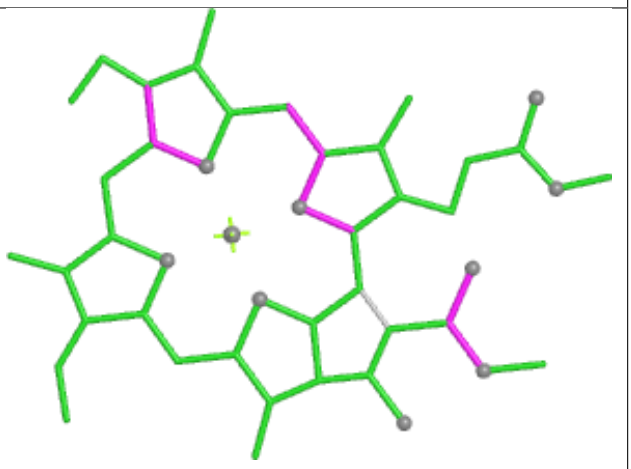


Rings

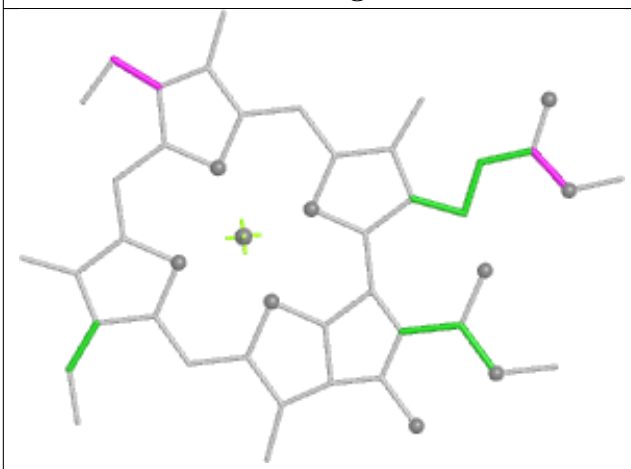
Ligand CLA z 308



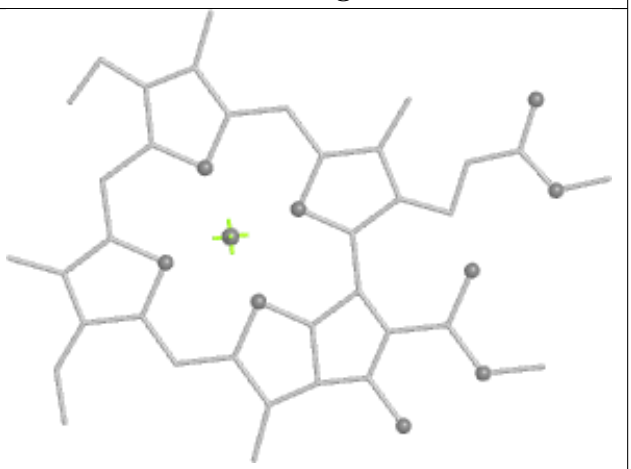
Bond lengths



Bond angles

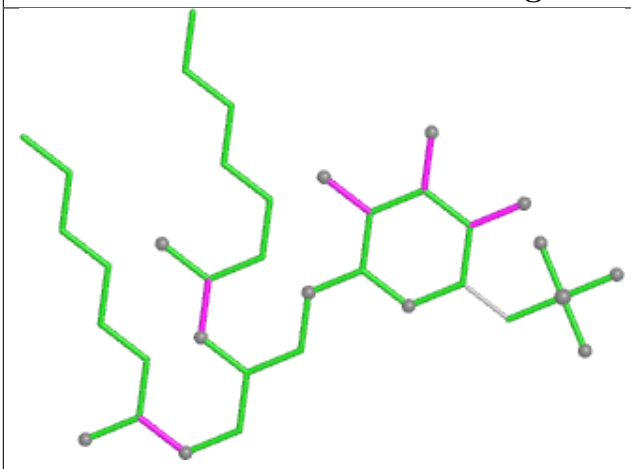


Torsions

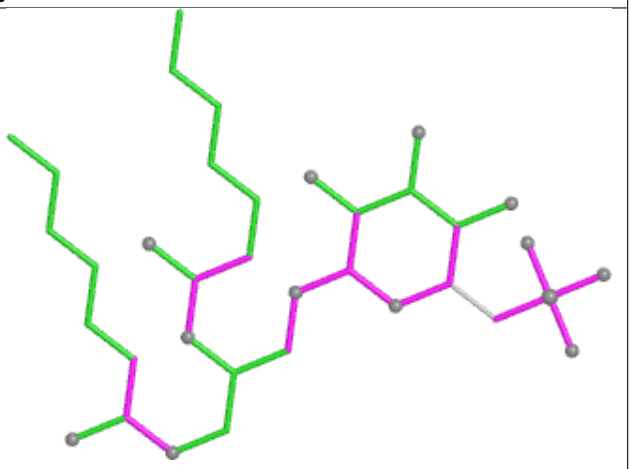


Rings

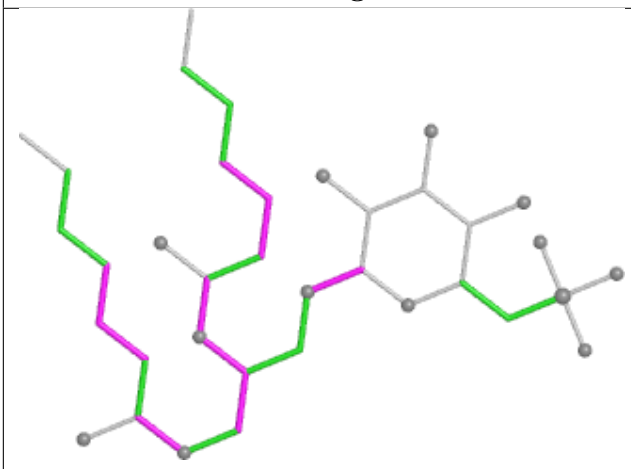
Ligand SQD T 321



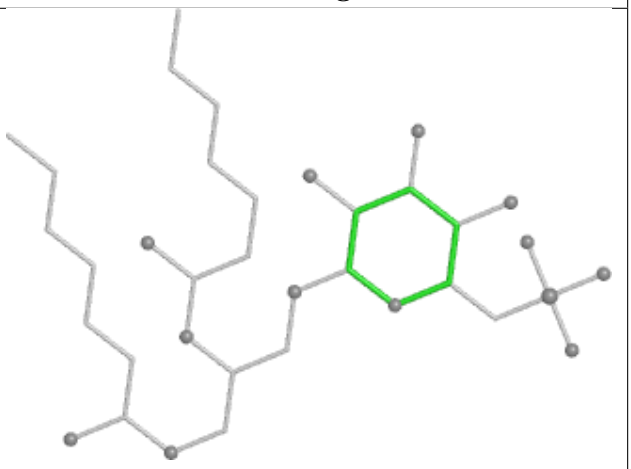
Bond lengths



Bond angles

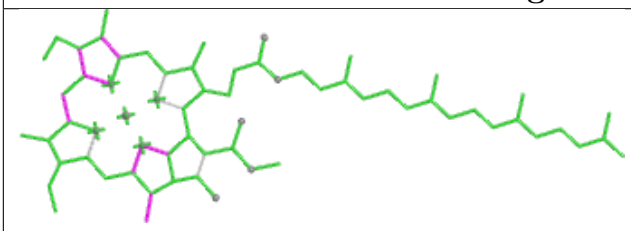


Torsions

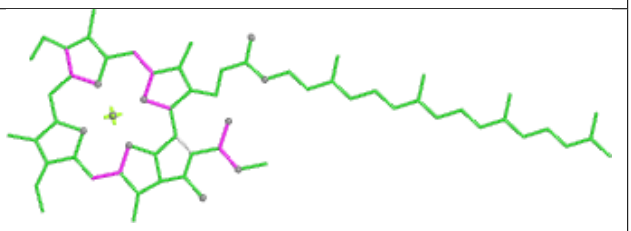


Rings

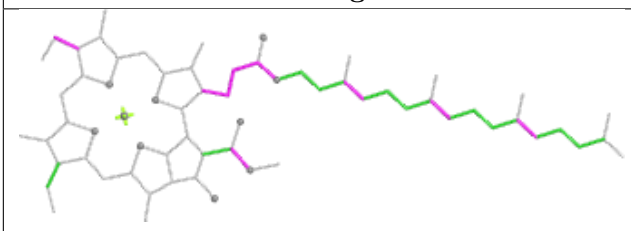
Ligand CLA b 835



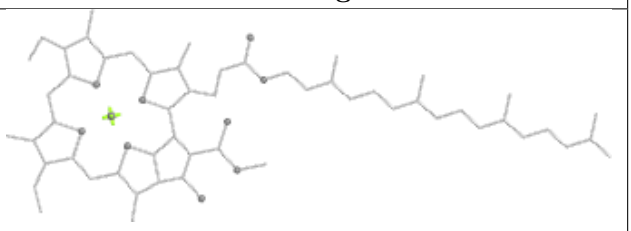
Bond lengths



Bond angles

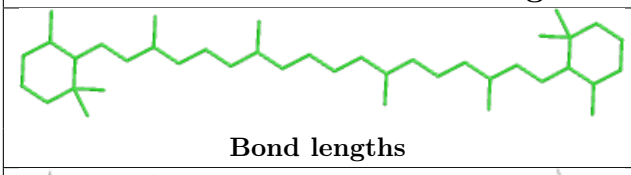


Torsions

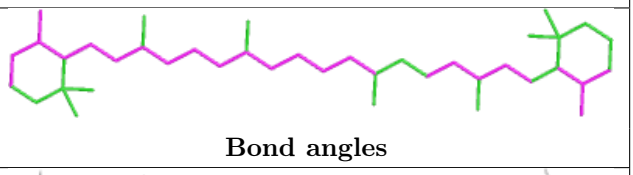


Rings

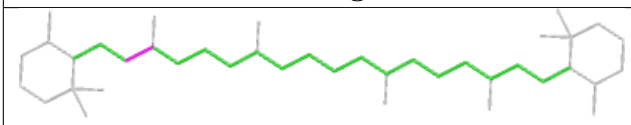
Ligand BCR k 204



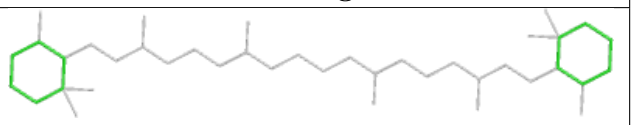
Bond lengths



Bond angles

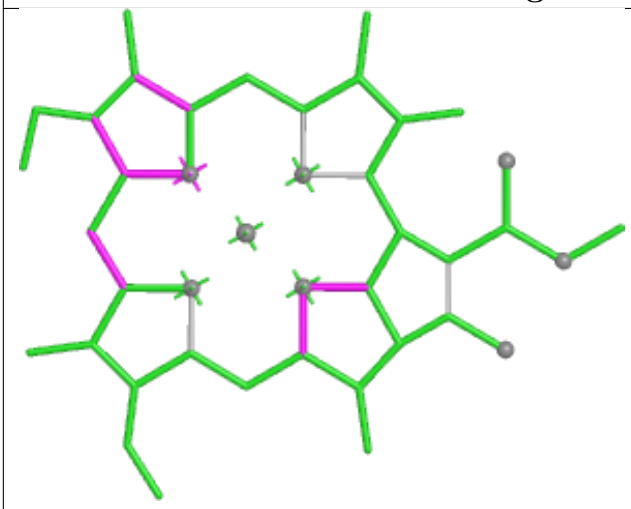


Torsions

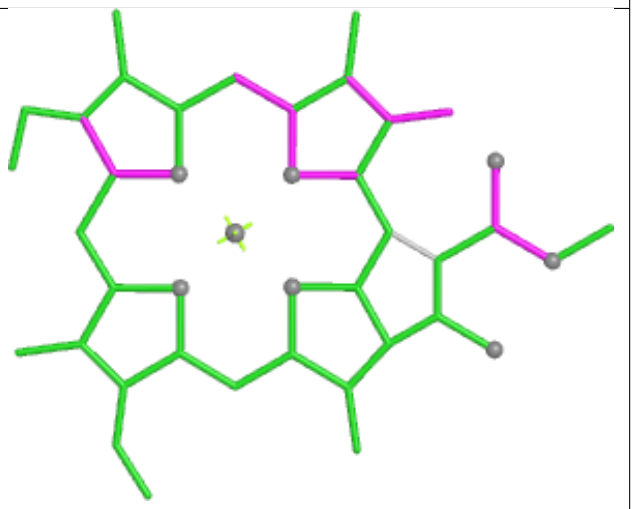


Rings

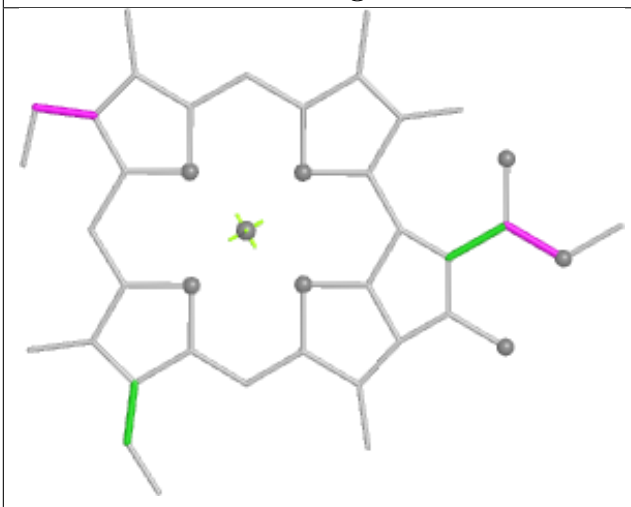
Ligand CLA Z 315



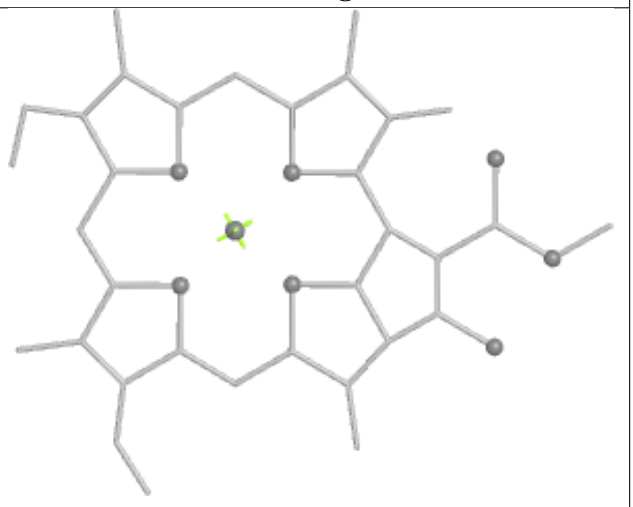
Bond lengths



Bond angles

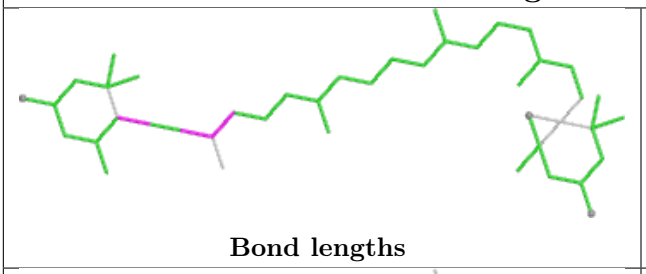


Torsions

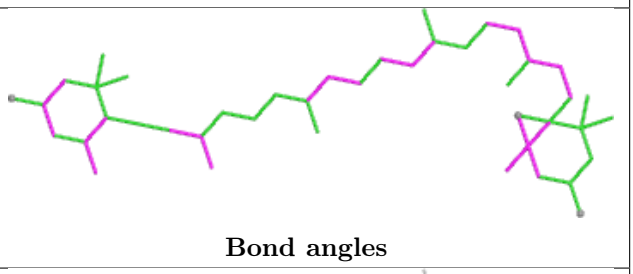


Rings

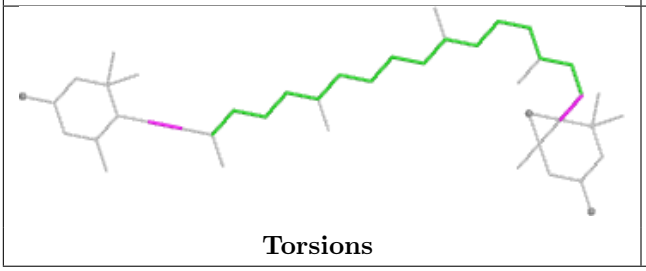
Ligand DD6 H 305



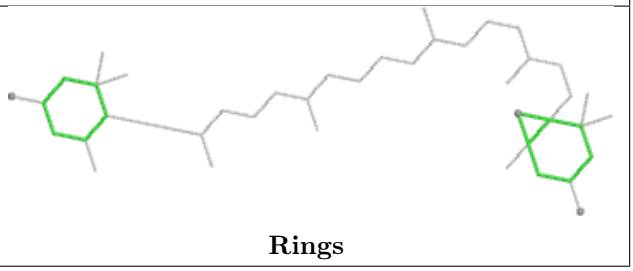
Bond lengths



Bond angles

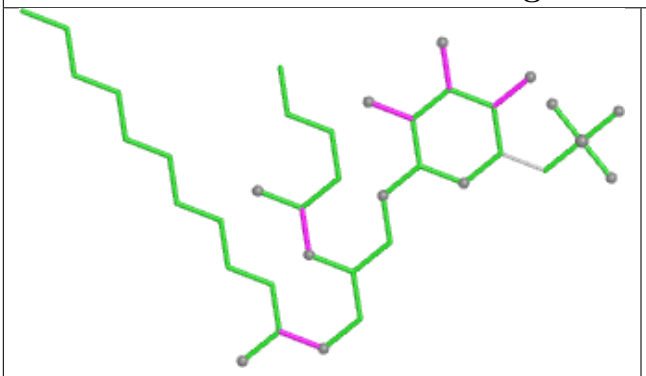


Torsions

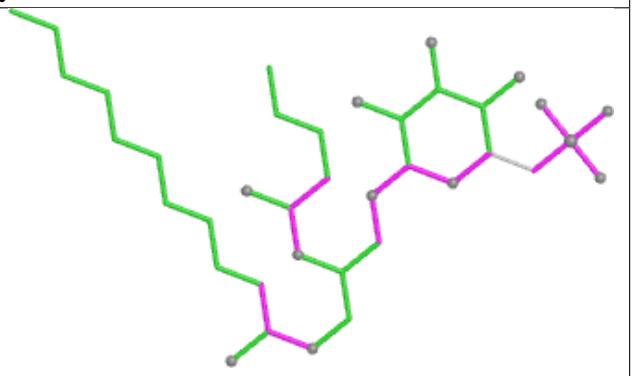


Rings

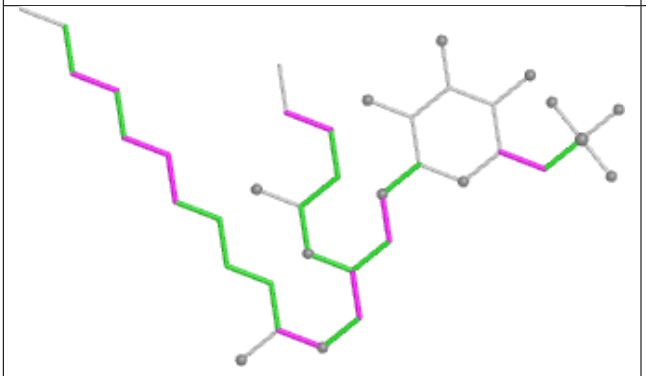
Ligand SQD H 318



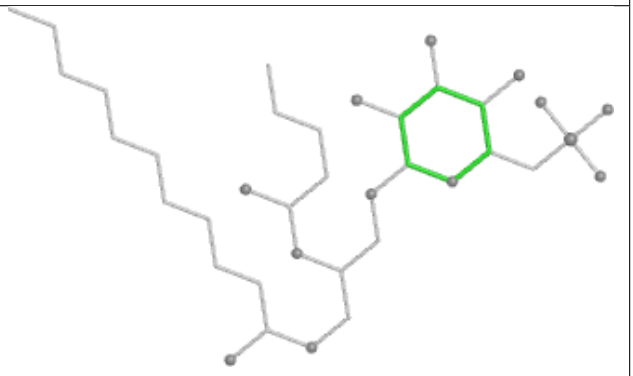
Bond lengths



Bond angles

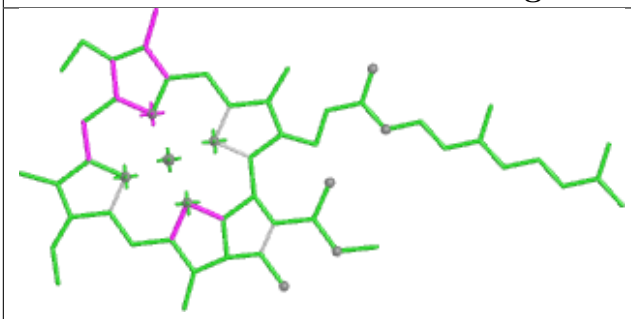


Torsions

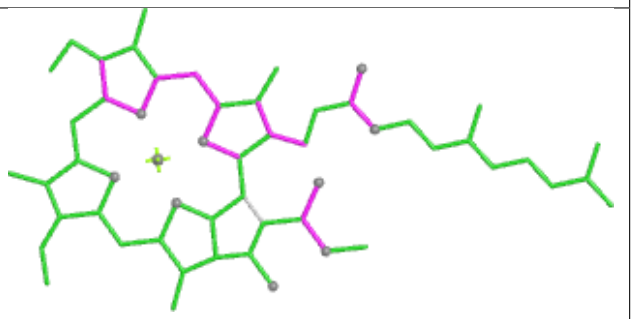


Rings

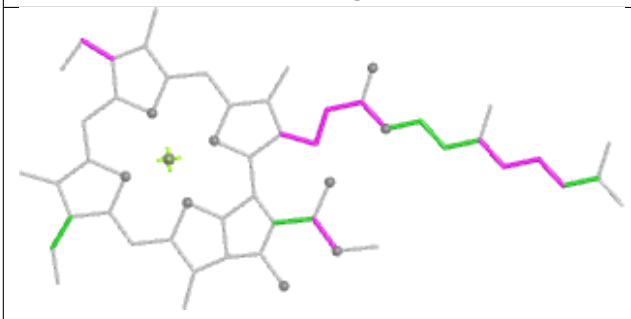
Ligand CLA B 207



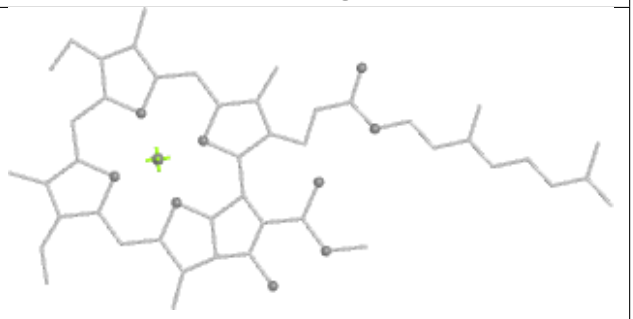
Bond lengths



Bond angles

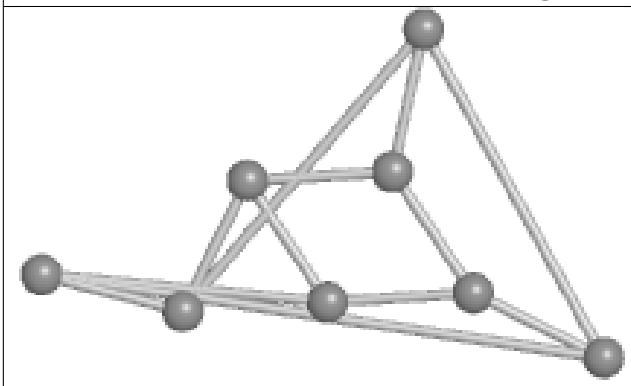


Torsions

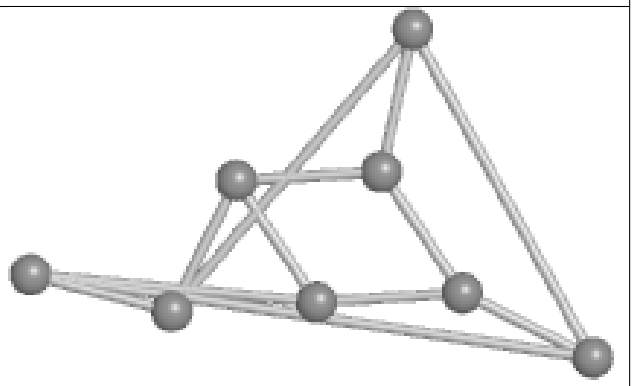


Rings

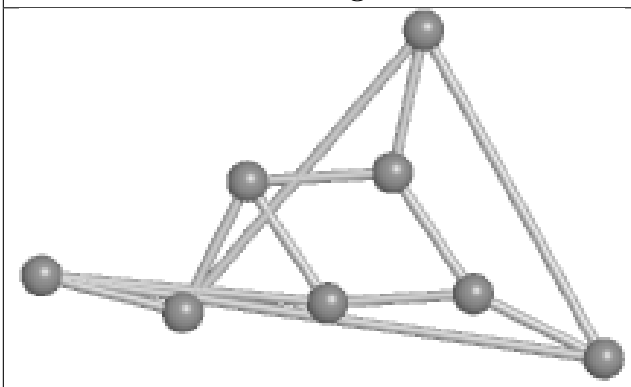
Ligand SF4 c 101



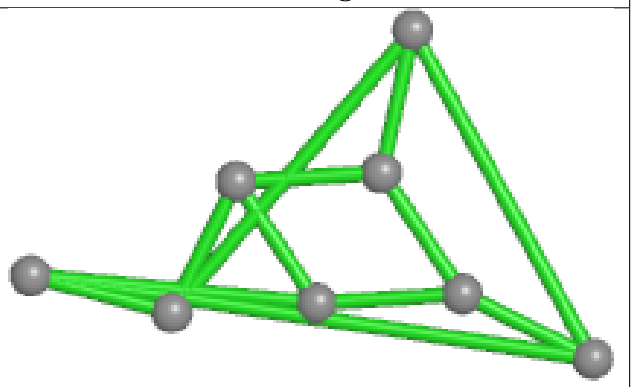
Bond lengths



Bond angles

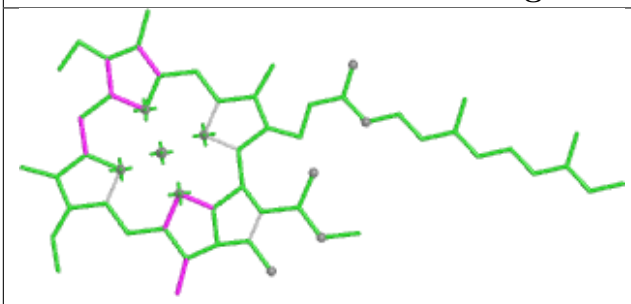


Torsions

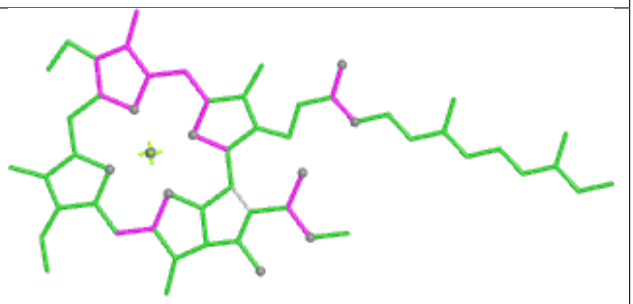


Rings

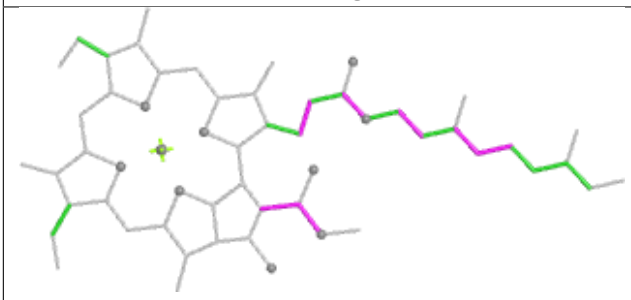
Ligand CLA T 309



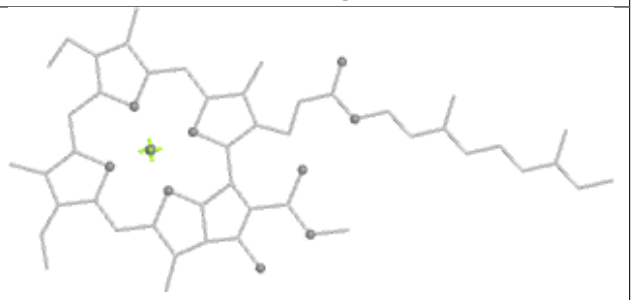
Bond lengths



Bond angles

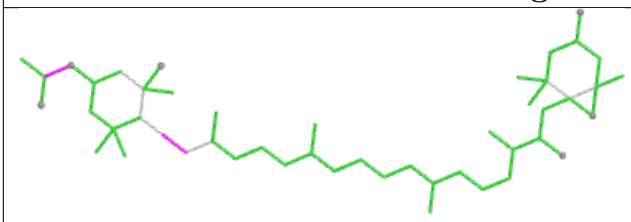


Torsions

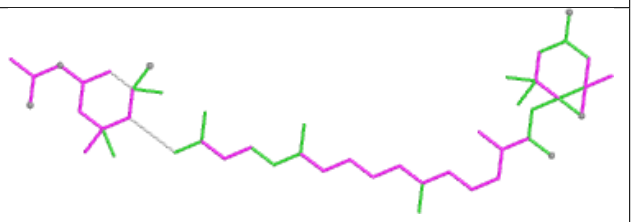


Rings

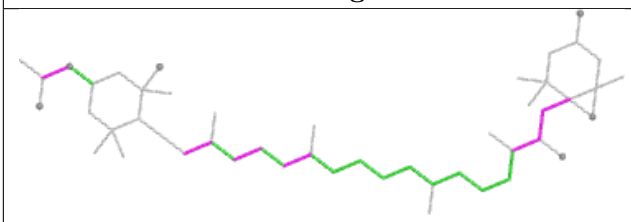
Ligand A86 P 302



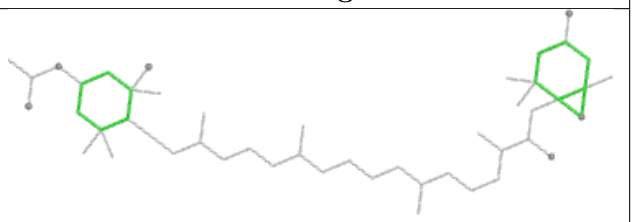
Bond lengths



Bond angles

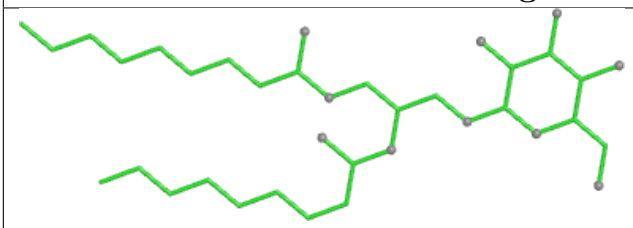


Torsions

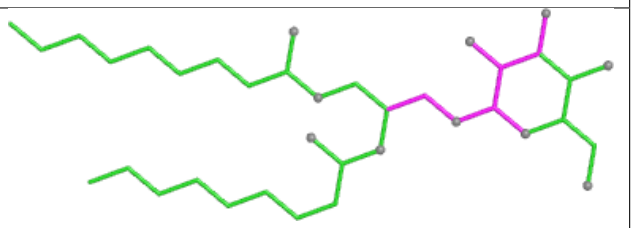


Rings

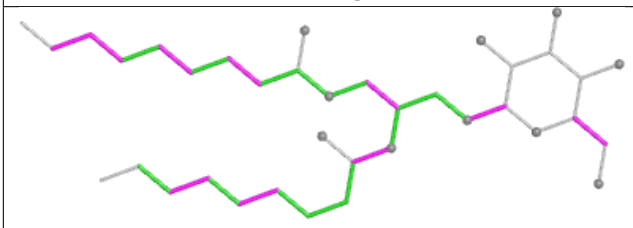
Ligand LMG D 322



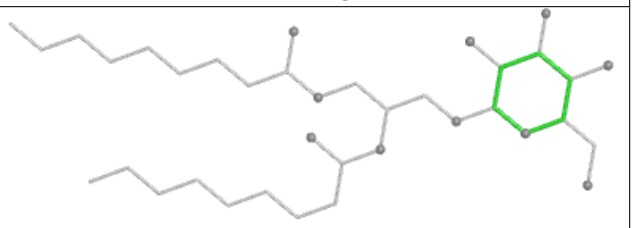
Bond lengths



Bond angles

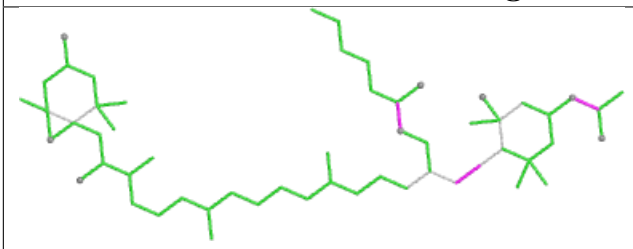


Torsions

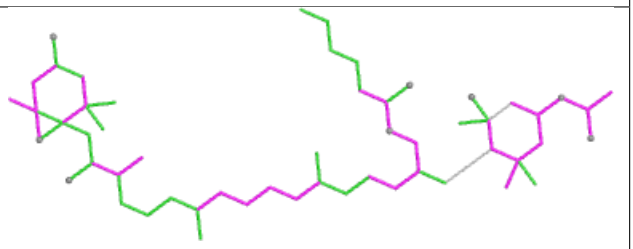


Rings

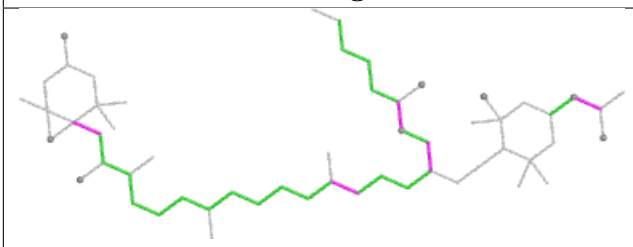
Ligand A1EB1 U 203



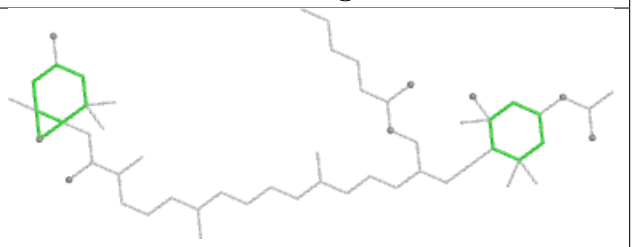
Bond lengths



Bond angles

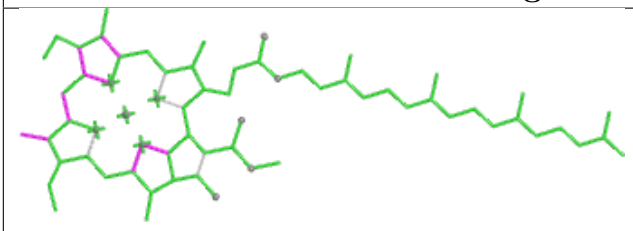


Torsions

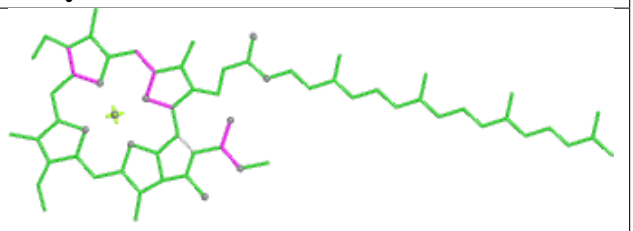


Rings

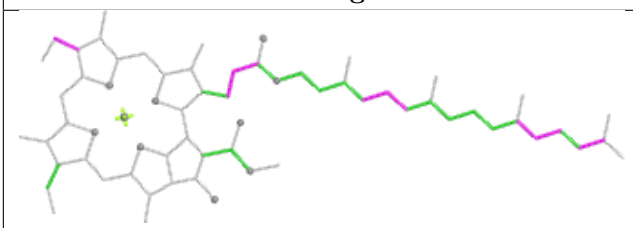
Ligand CLA Q 312



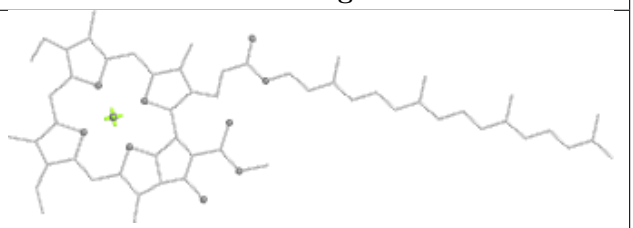
Bond lengths



Bond angles

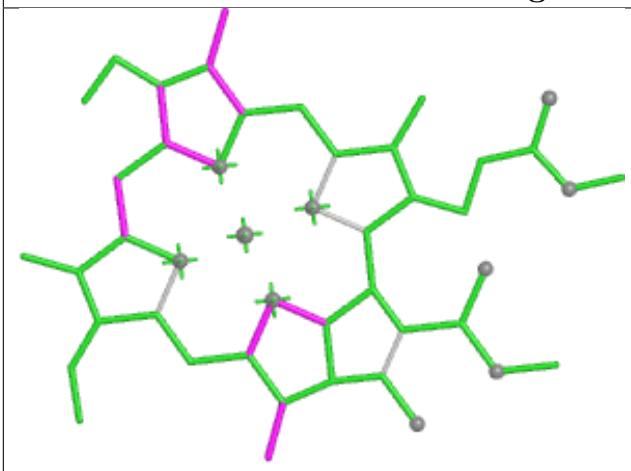


Torsions

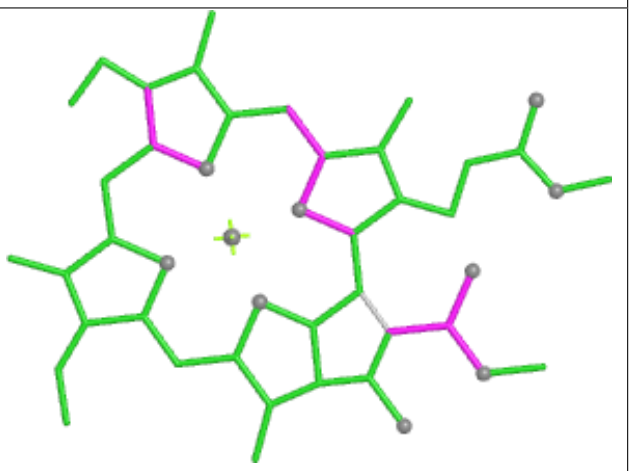


Rings

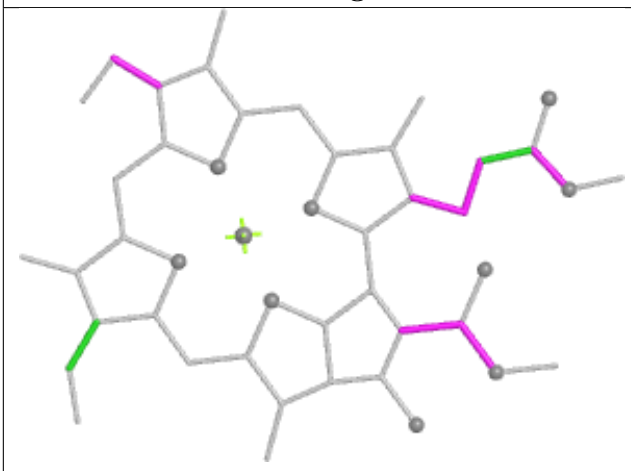
Ligand CLA 0 323



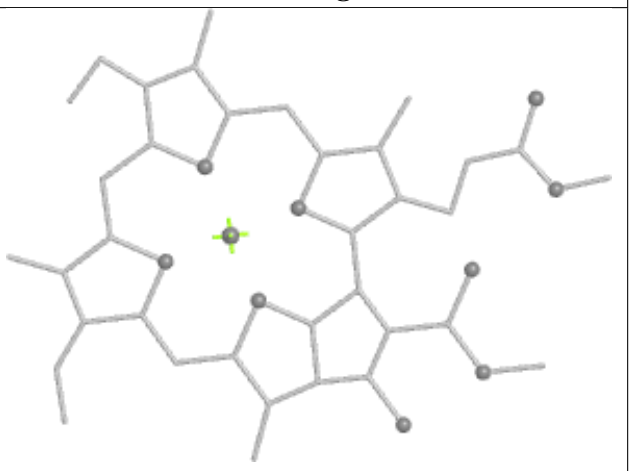
Bond lengths



Bond angles

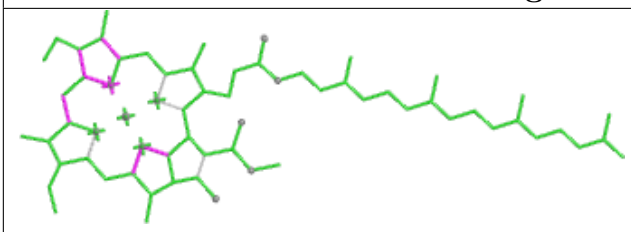


Torsions

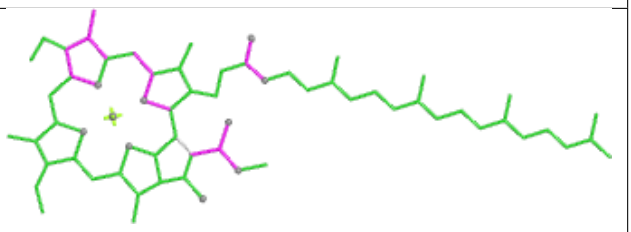


Rings

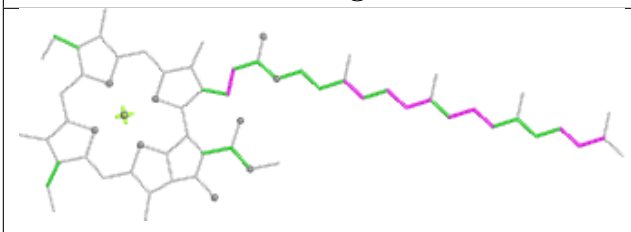
Ligand CLA E 308



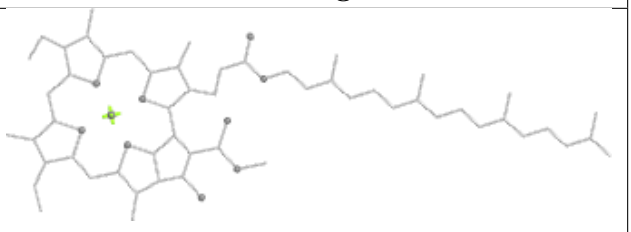
Bond lengths



Bond angles

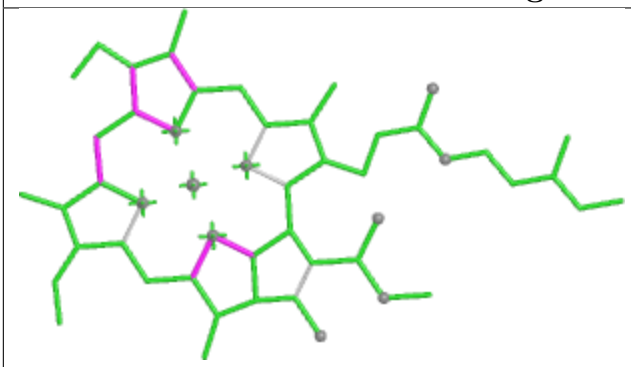


Torsions

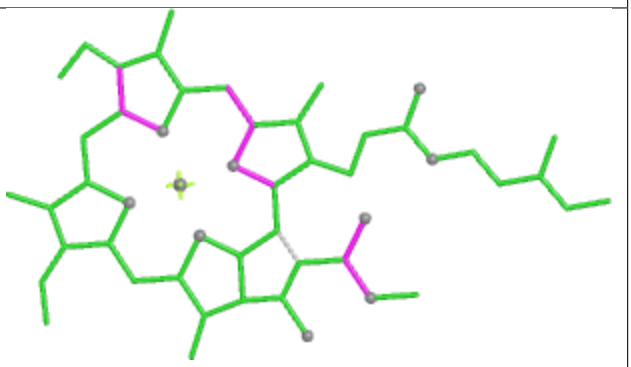


Rings

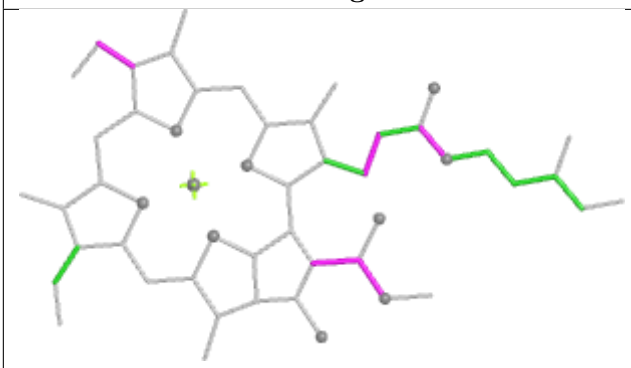
Ligand CLA L 319



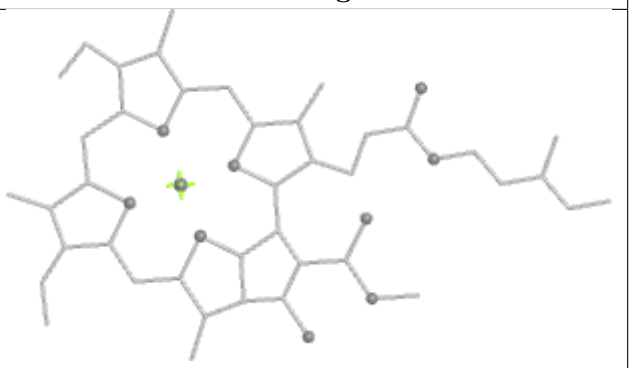
Bond lengths



Bond angles

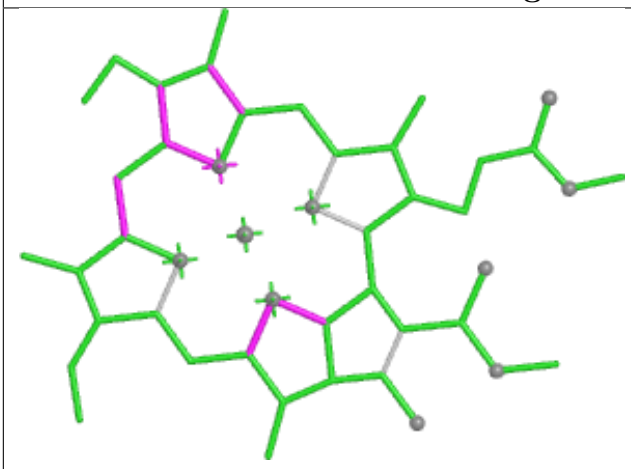


Torsions

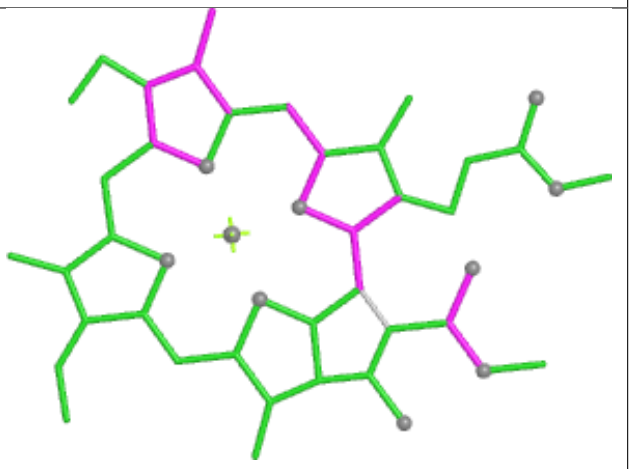


Rings

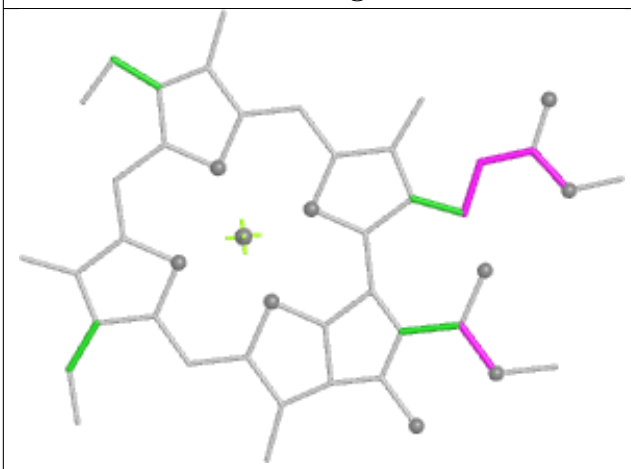
Ligand CLA O 318



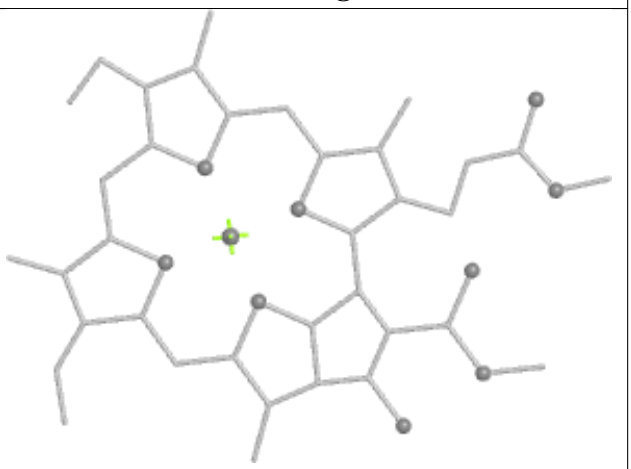
Bond lengths



Bond angles

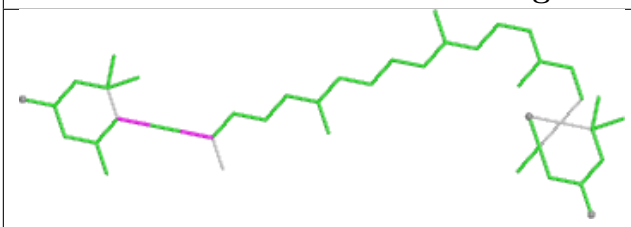


Torsions

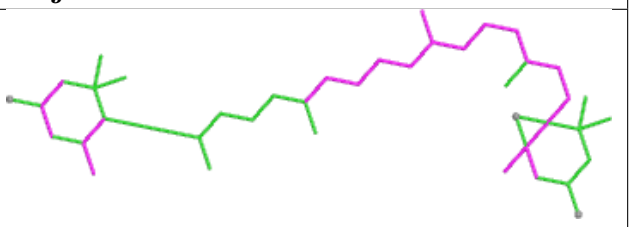


Rings

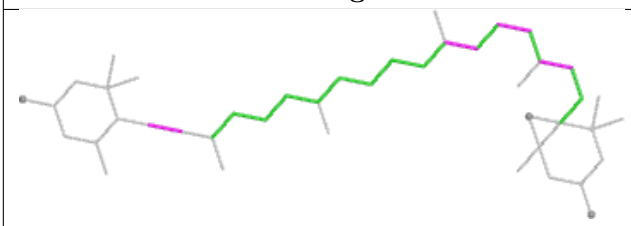
Ligand DD6 j 102



Bond lengths



Bond angles

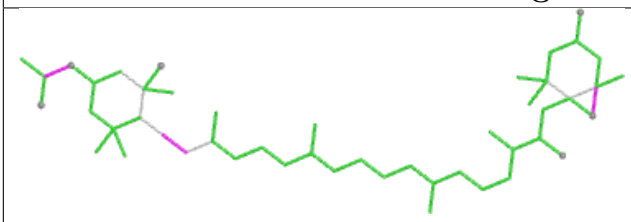


Torsions

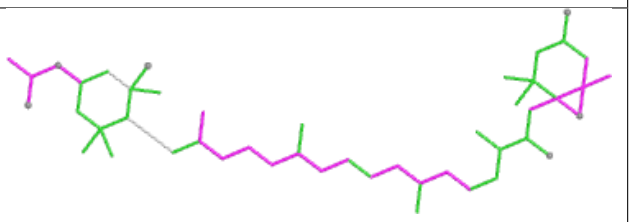


Rings

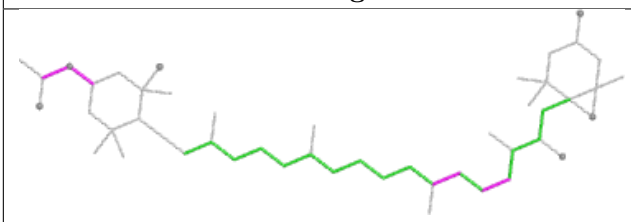
Ligand A86 L 301



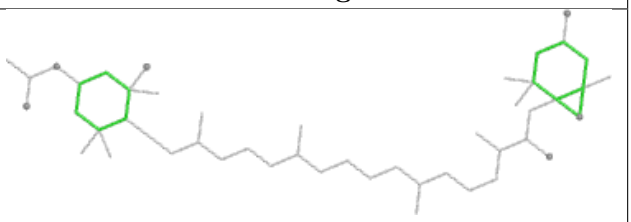
Bond lengths



Bond angles

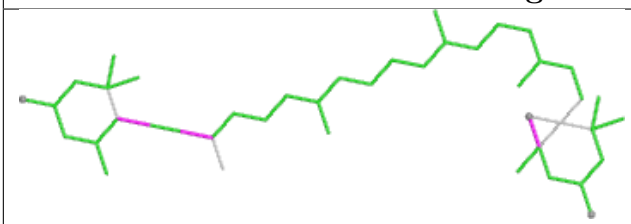


Torsions

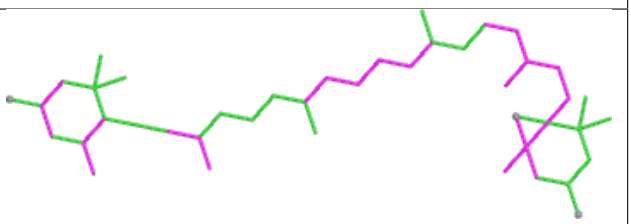


Rings

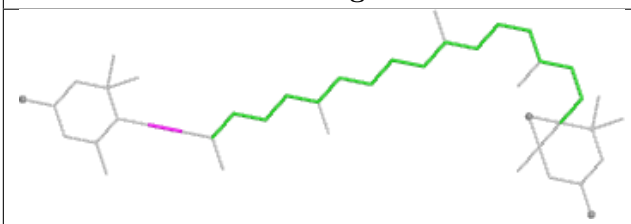
Ligand DD6 T 303



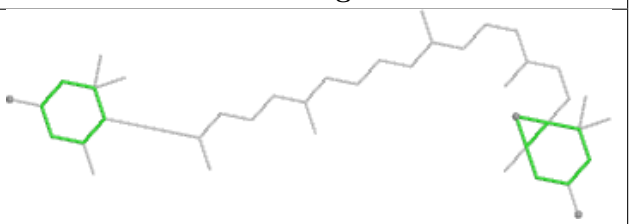
Bond lengths



Bond angles

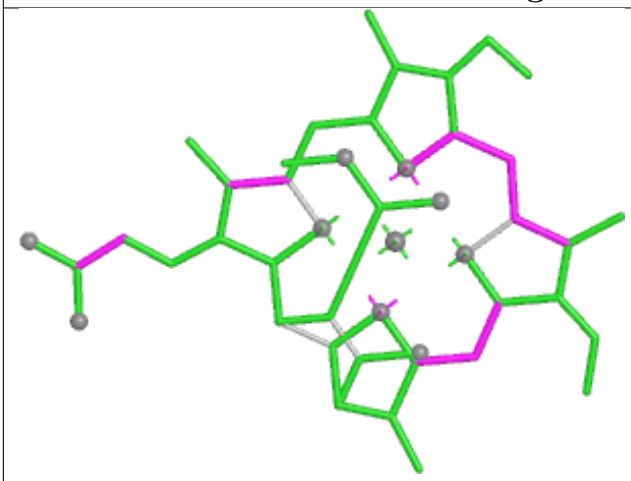


Torsions

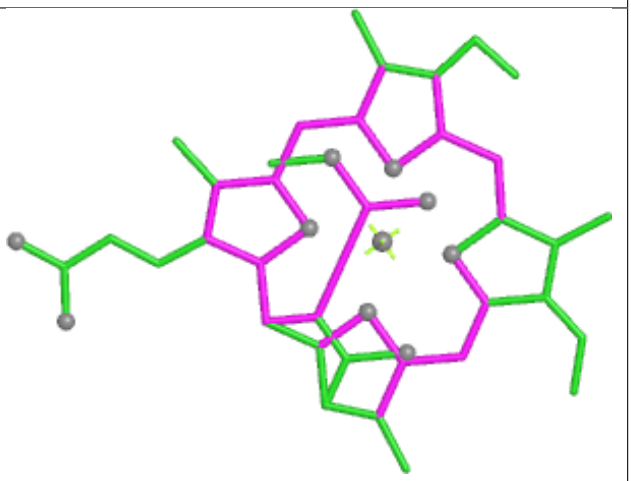


Rings

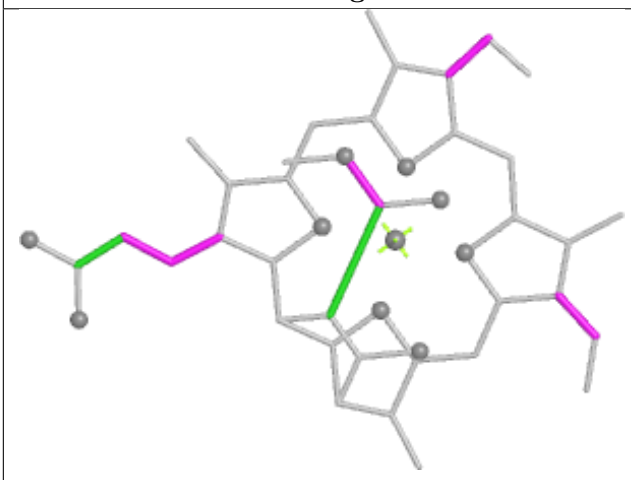
Ligand KC2 T 314



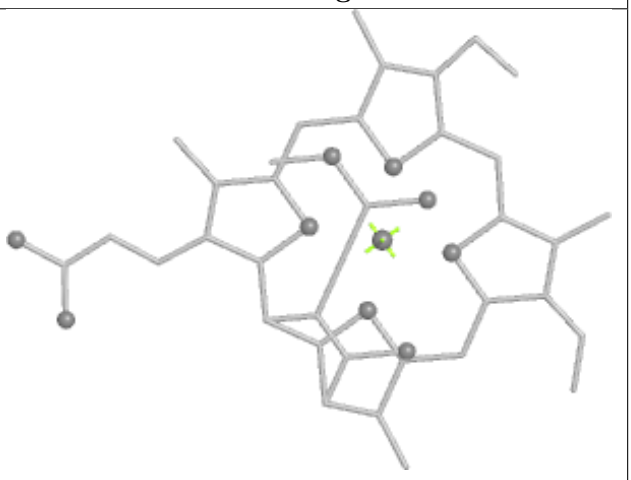
Bond lengths



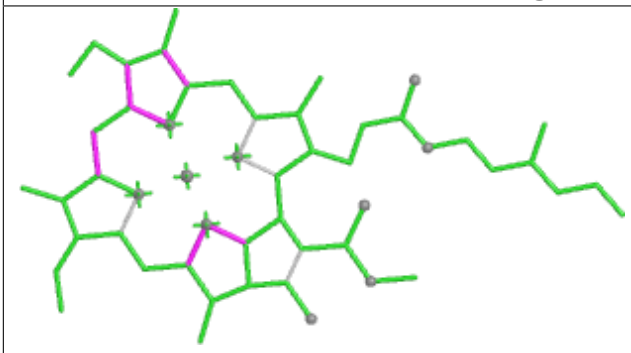
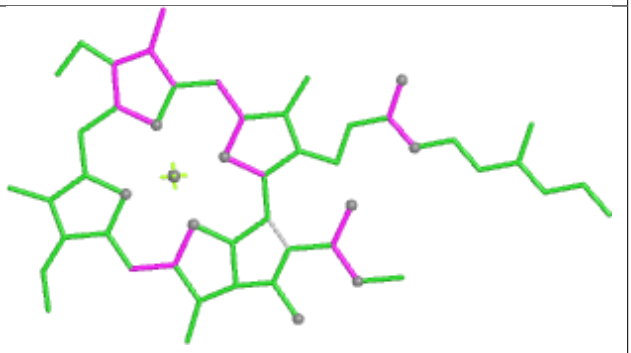
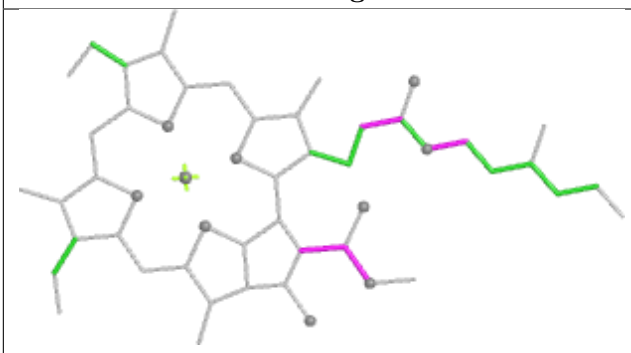
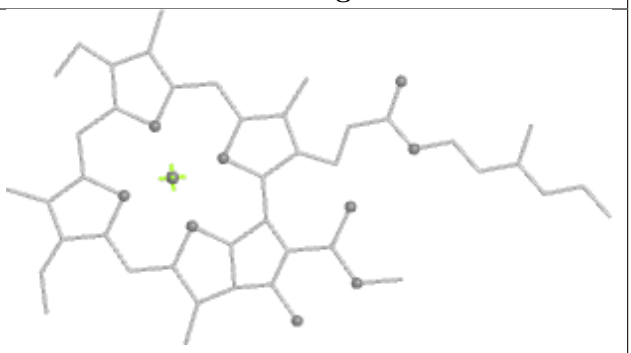
Bond angles

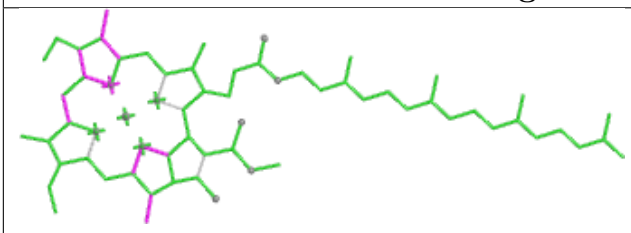
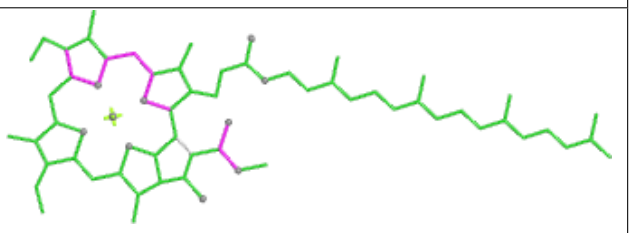
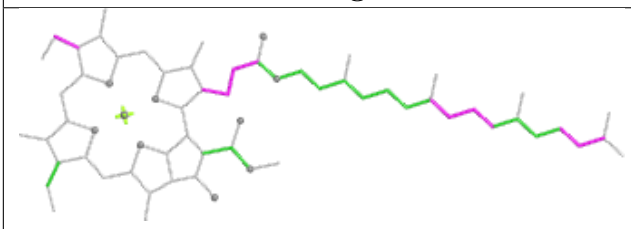
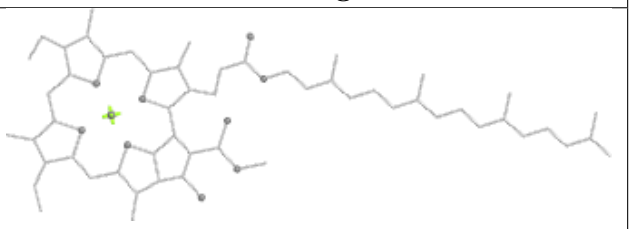


Torsions

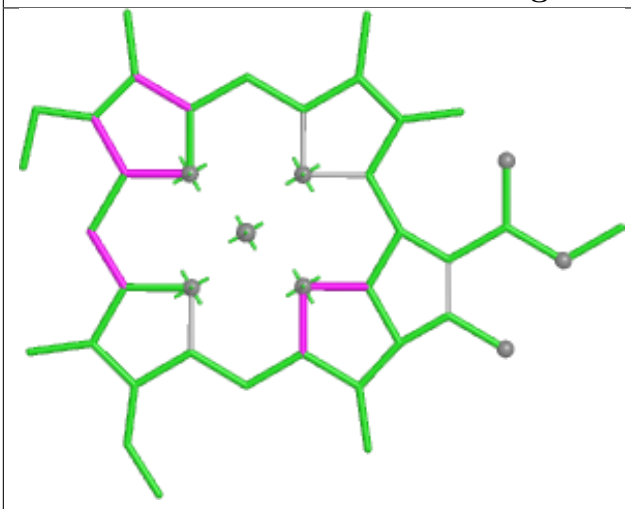


Rings

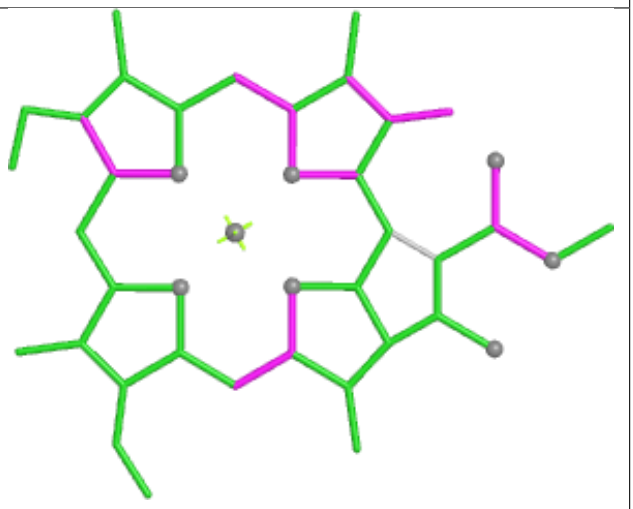
Ligand CLA I 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA W 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

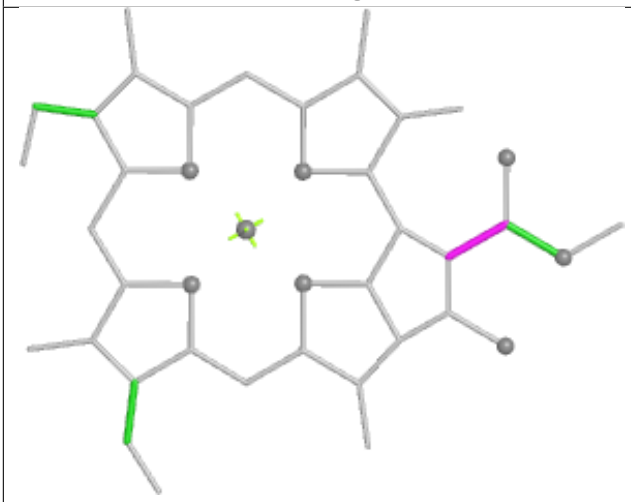
Ligand CLA I 316



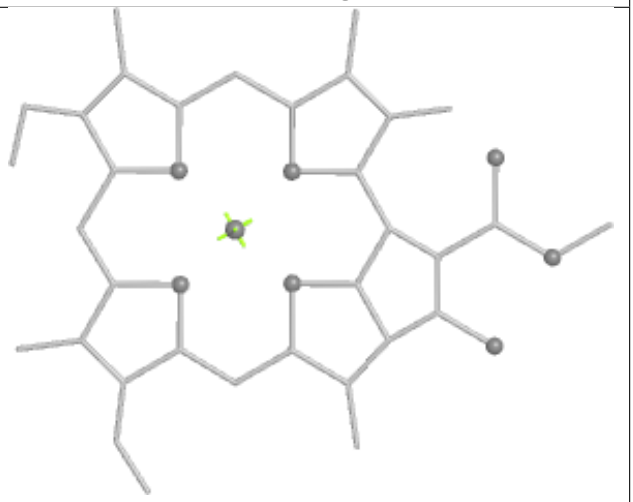
Bond lengths



Bond angles

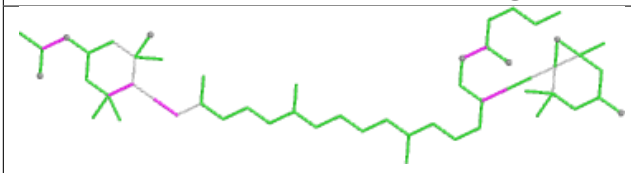


Torsions

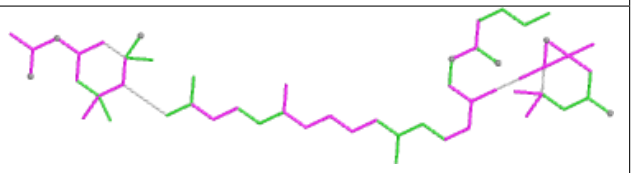


Rings

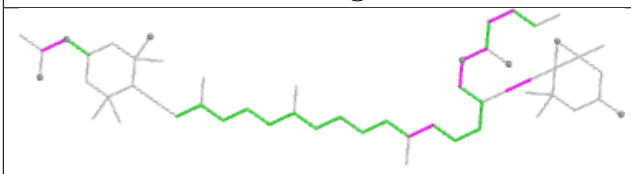
Ligand A1EB4 P 318



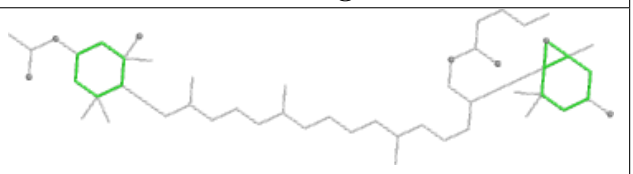
Bond lengths



Bond angles

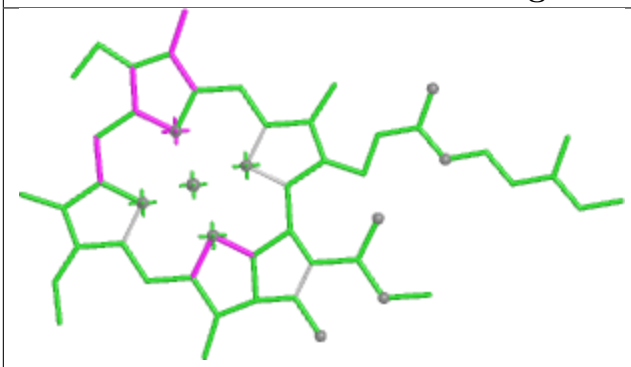


Torsions

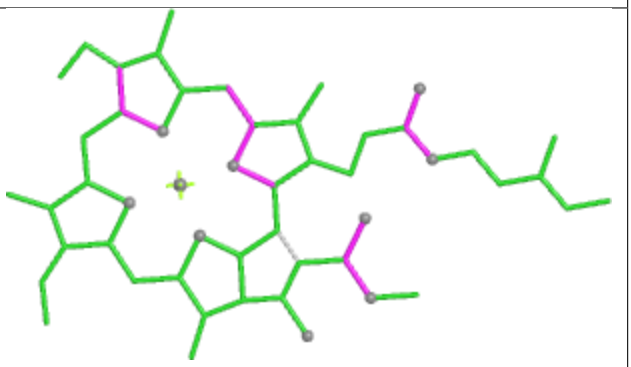


Rings

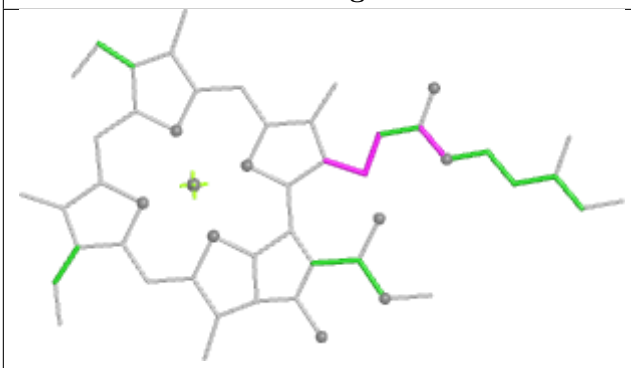
Ligand CLA o 201



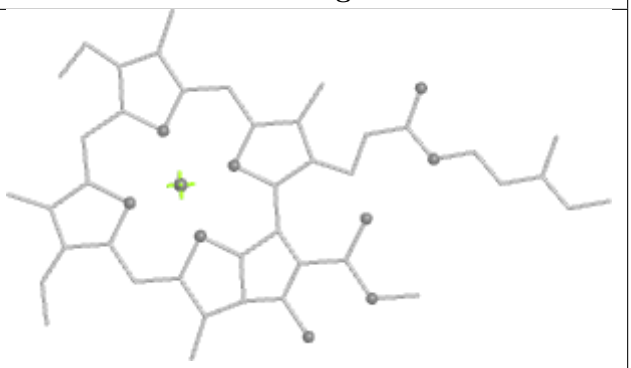
Bond lengths



Bond angles

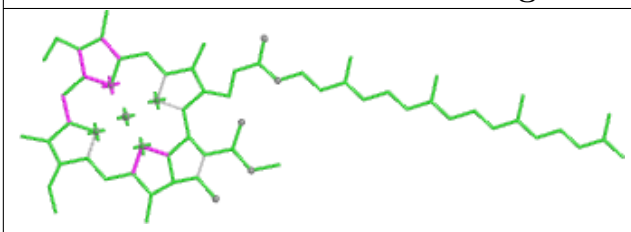


Torsions

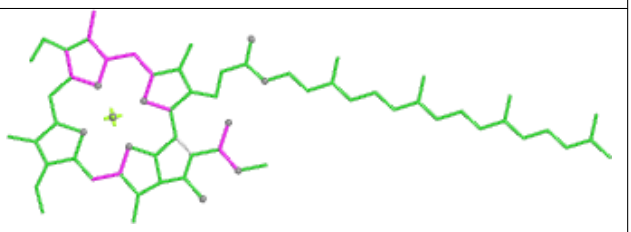


Rings

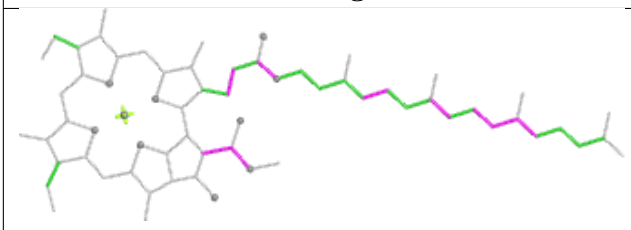
Ligand CLA W 311



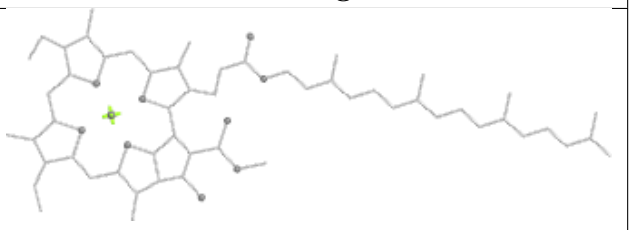
Bond lengths



Bond angles

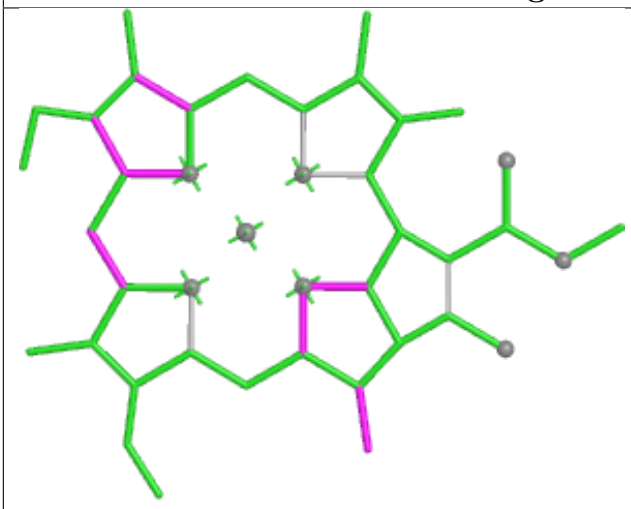


Torsions

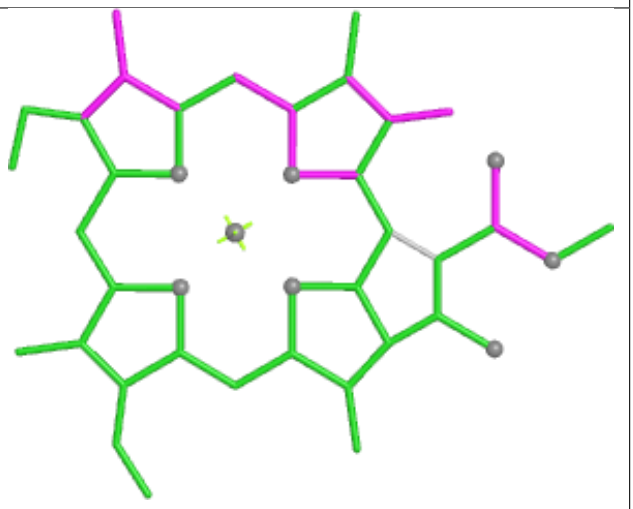


Rings

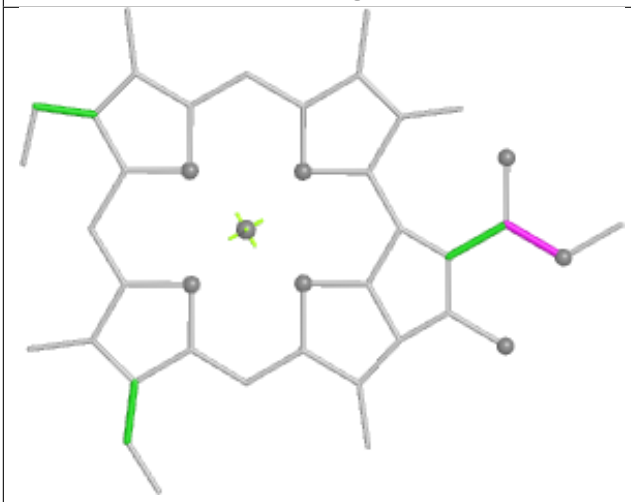
Ligand CLA x 308



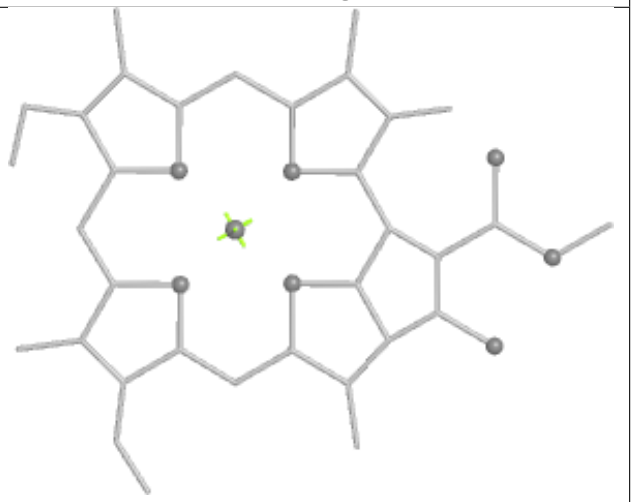
Bond lengths



Bond angles

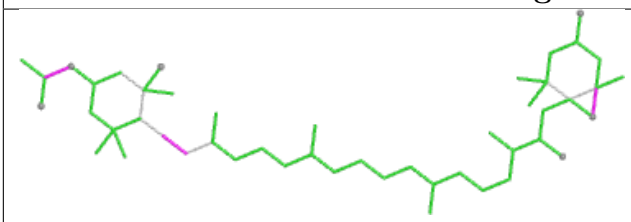


Torsions

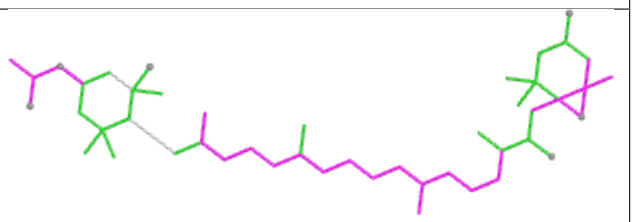


Rings

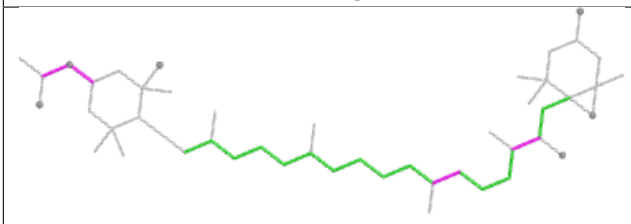
Ligand A86 6 307



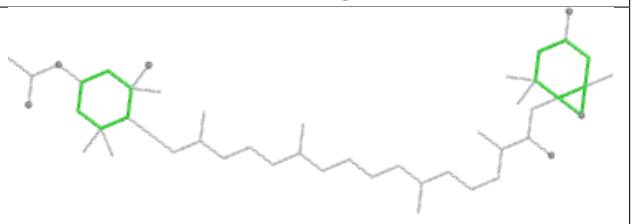
Bond lengths



Bond angles

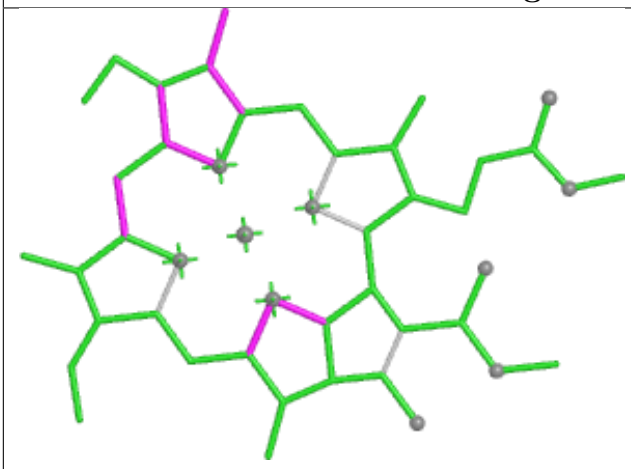


Torsions

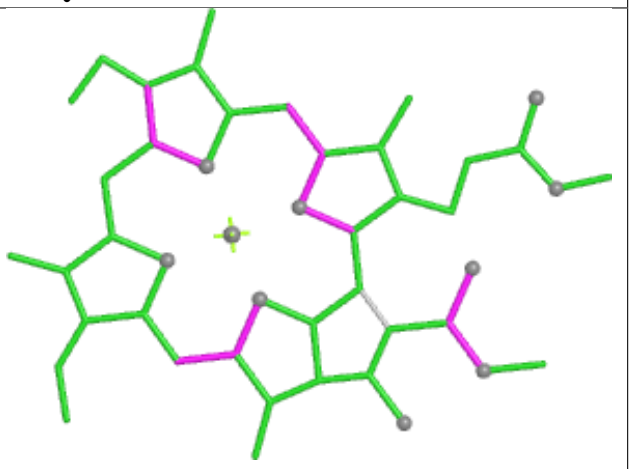


Rings

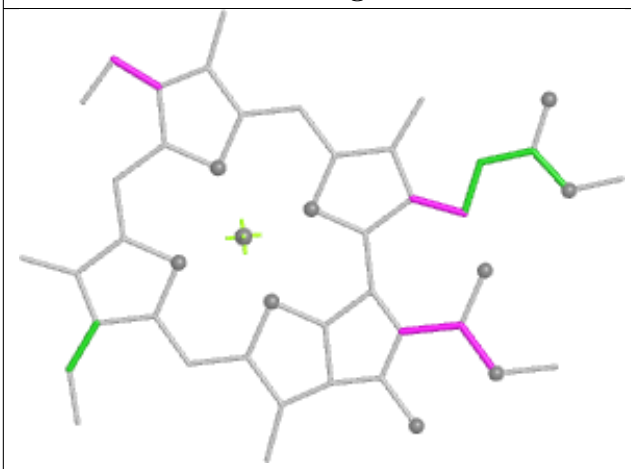
Ligand CLA Q 317



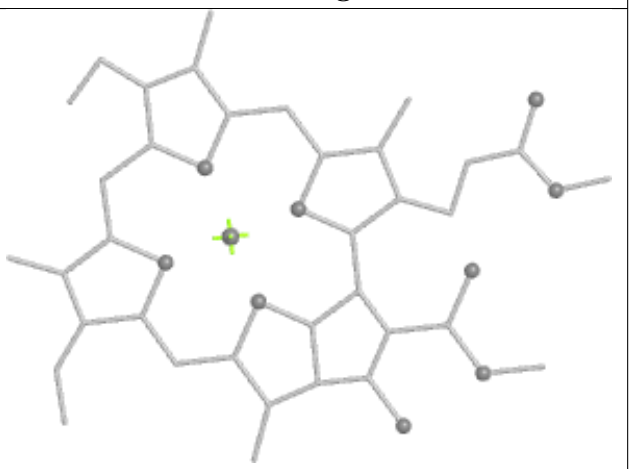
Bond lengths



Bond angles

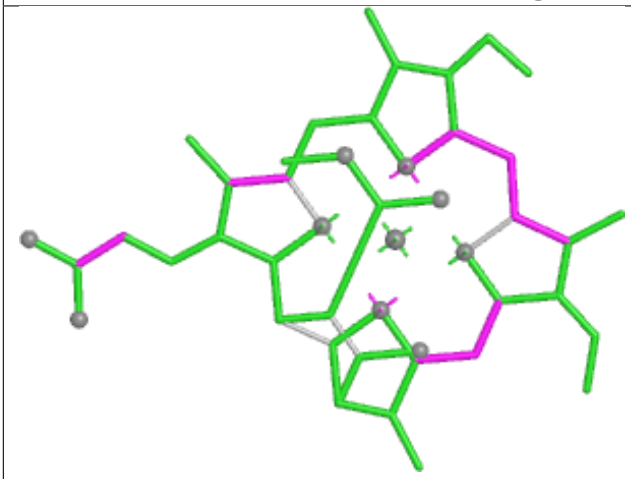


Torsions

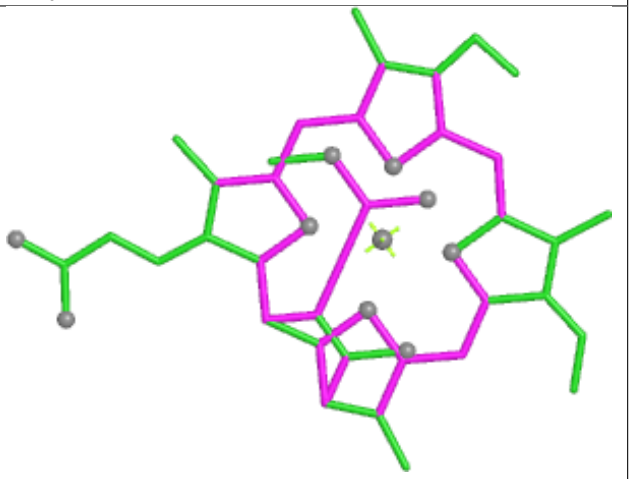


Rings

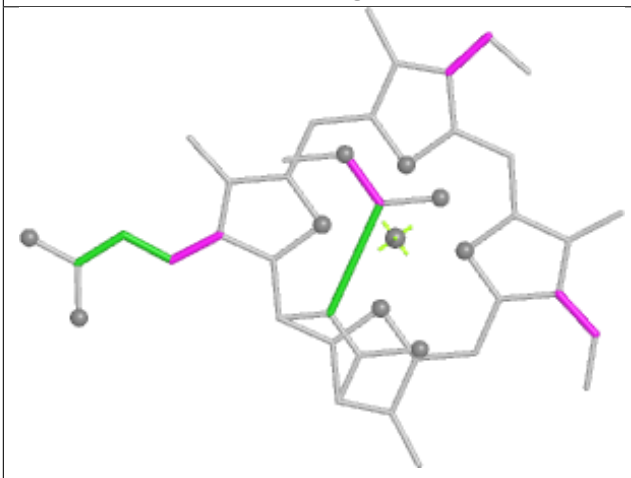
Ligand KC2 y 316



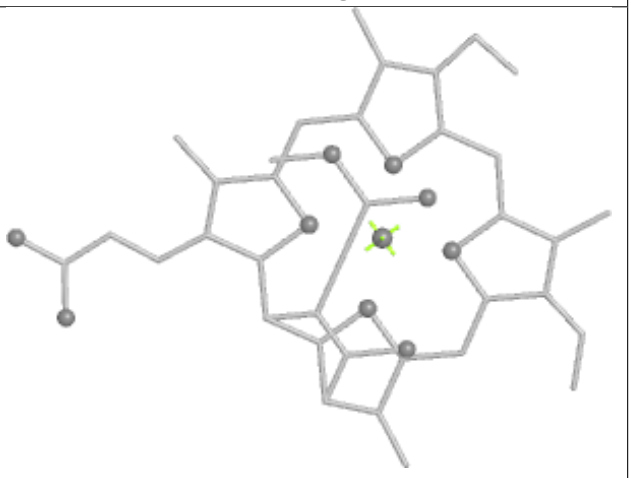
Bond lengths



Bond angles

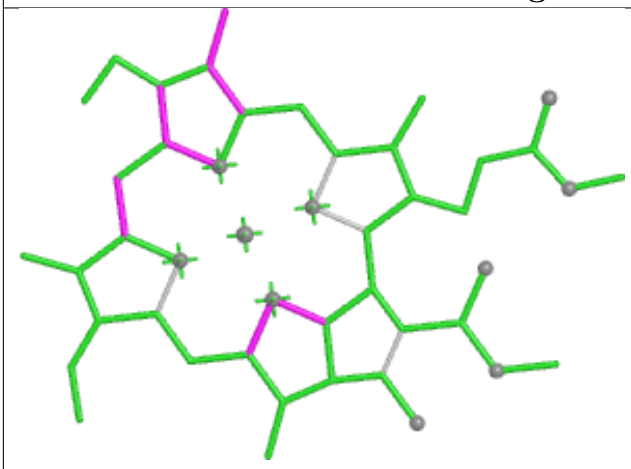


Torsions

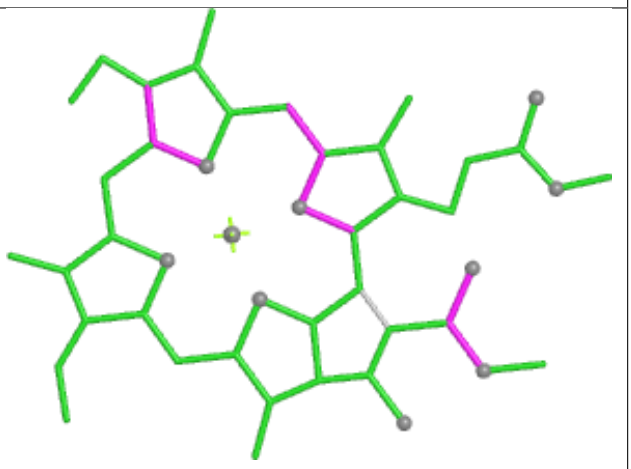


Rings

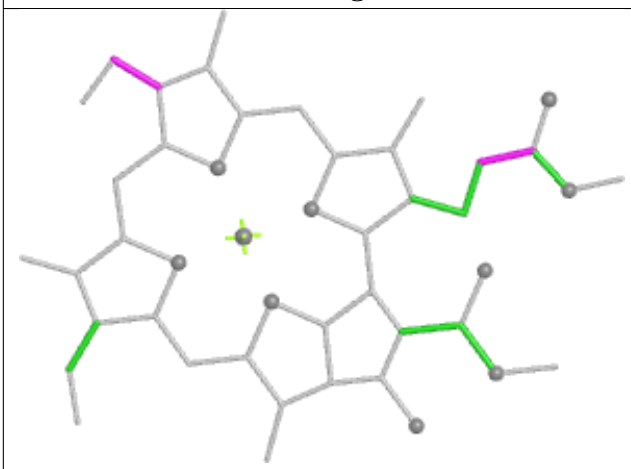
Ligand CLA 4 313



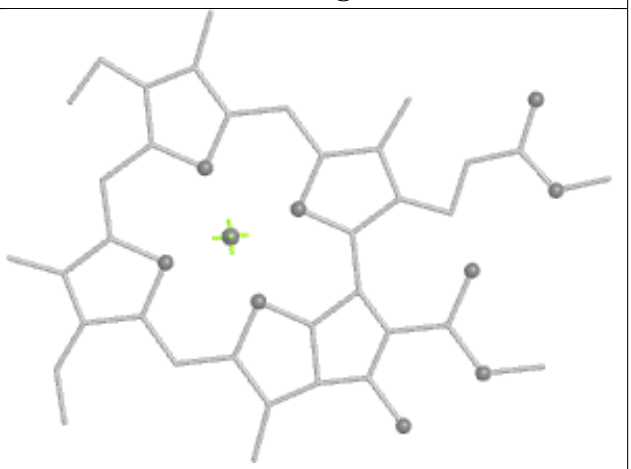
Bond lengths



Bond angles

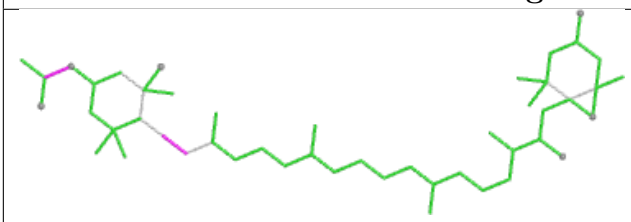


Torsions

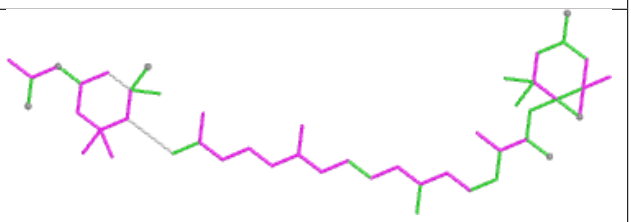


Rings

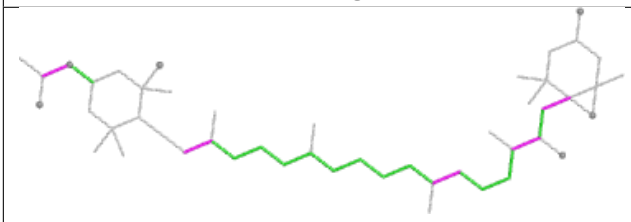
Ligand A86 M 302



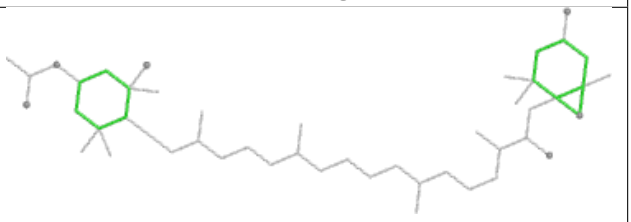
Bond lengths



Bond angles

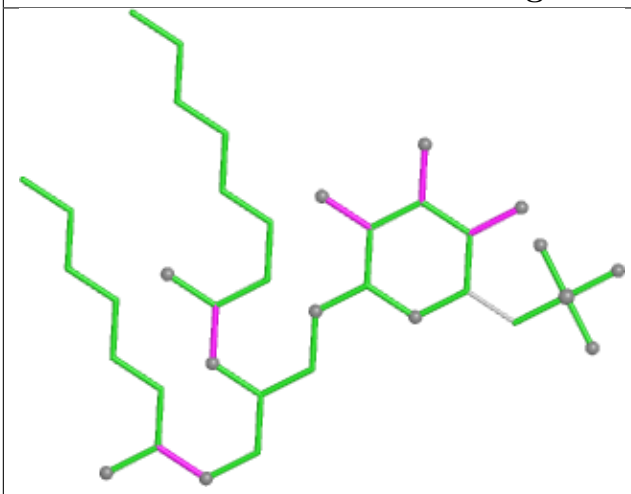


Torsions

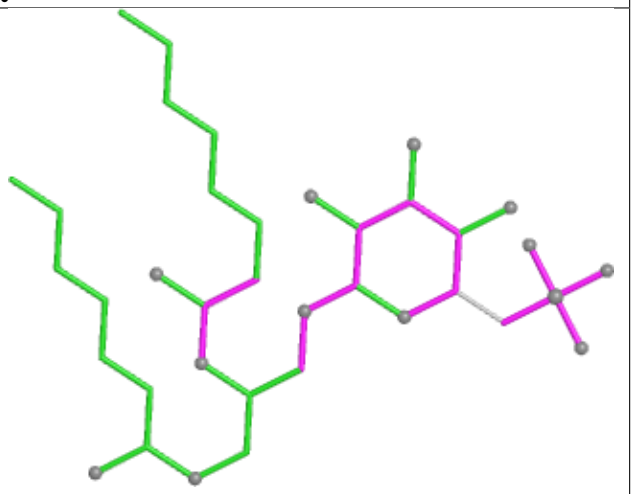


Rings

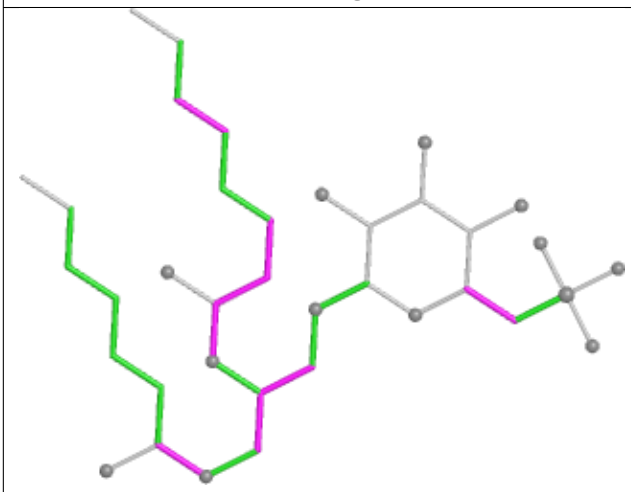
Ligand SQD F 319



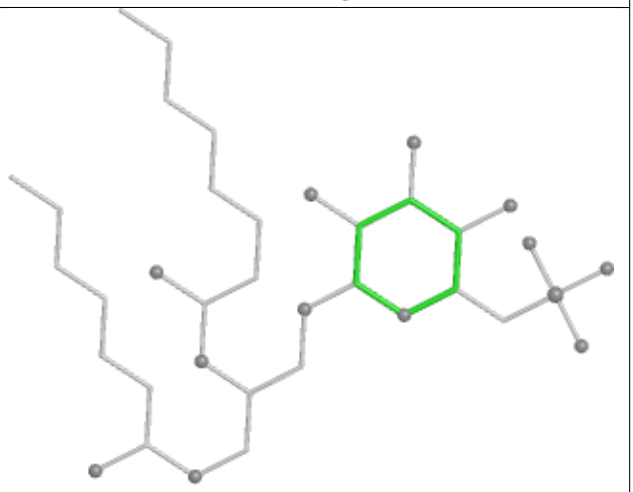
Bond lengths



Bond angles

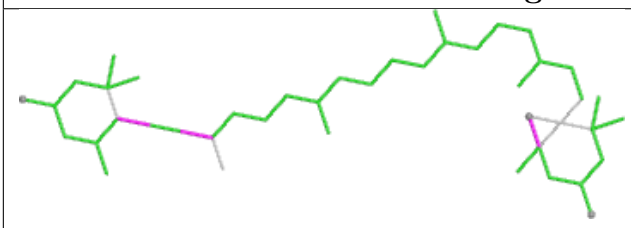


Torsions

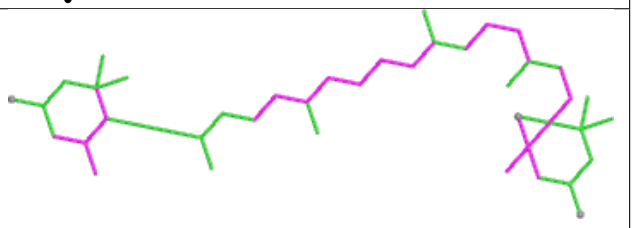


Rings

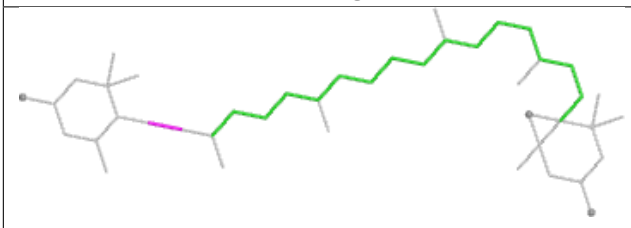
Ligand DD6 Q 306



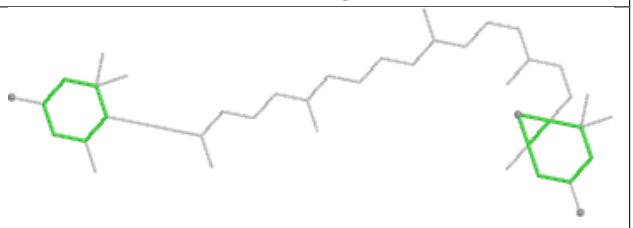
Bond lengths



Bond angles

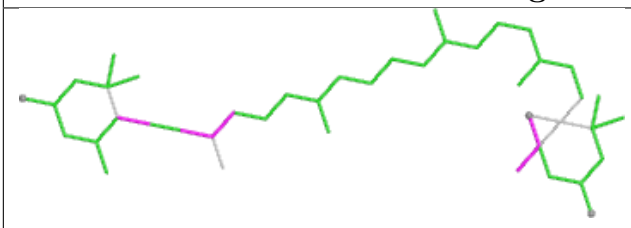


Torsions

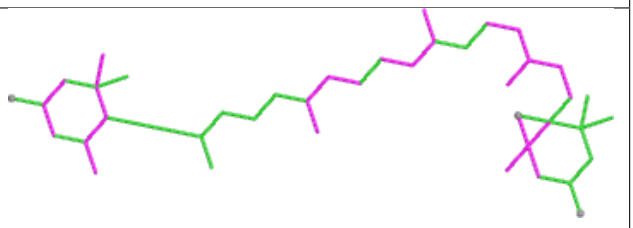


Rings

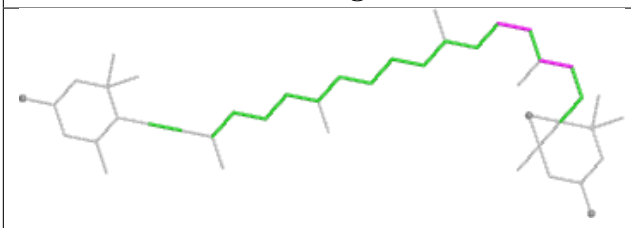
Ligand DD6 J 304



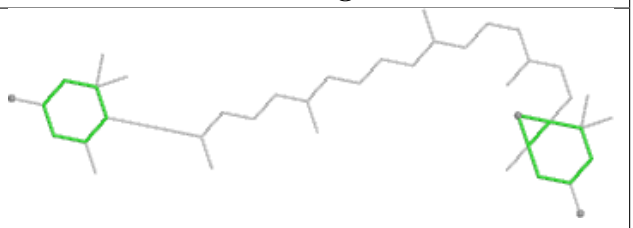
Bond lengths



Bond angles

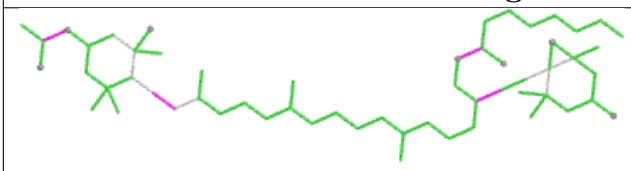


Torsions

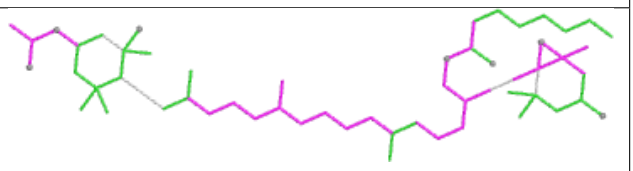


Rings

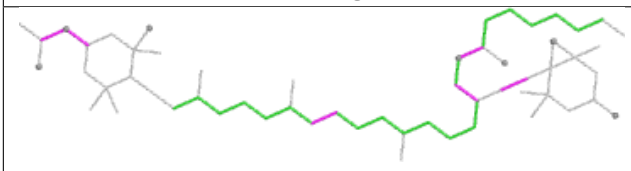
Ligand A1EB4 X 305



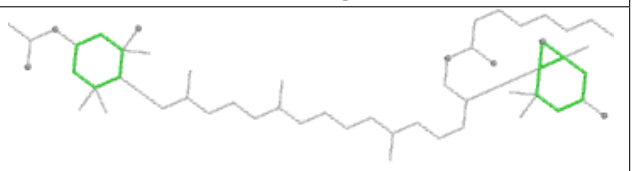
Bond lengths



Bond angles

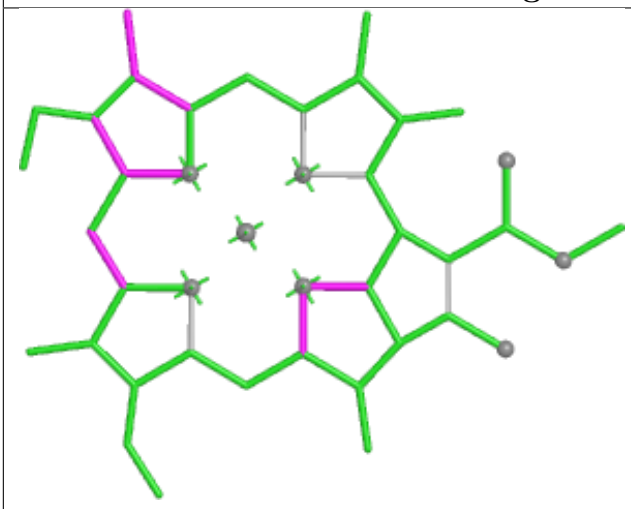


Torsions

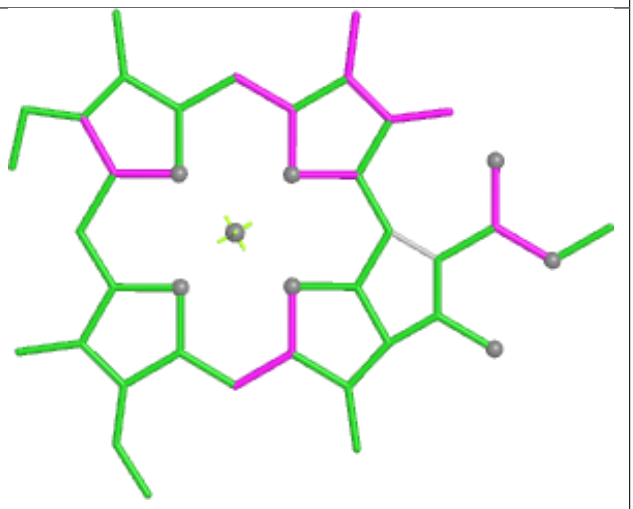


Rings

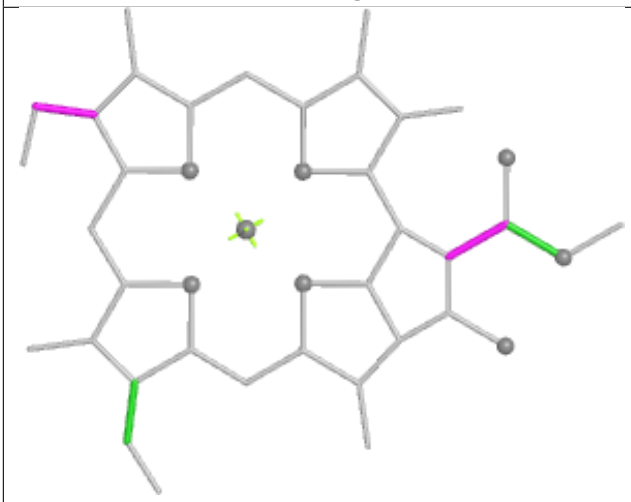
Ligand CLA K 314



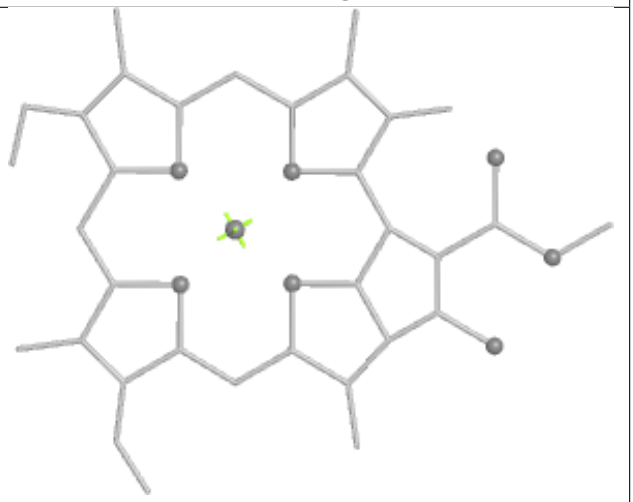
Bond lengths



Bond angles

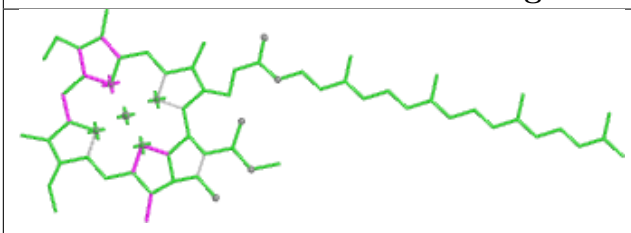


Torsions

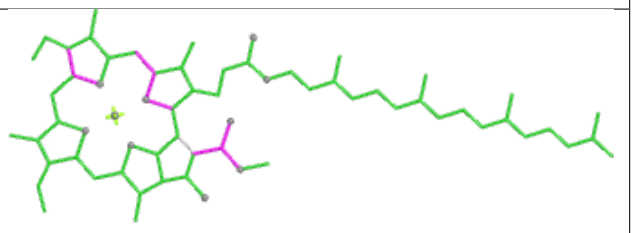


Rings

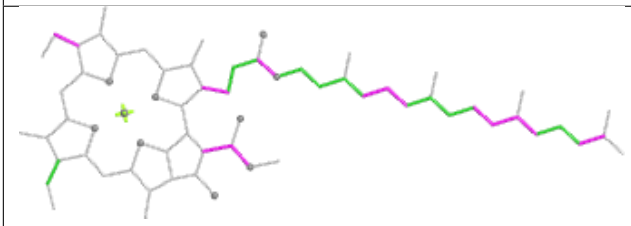
Ligand CLA C 310



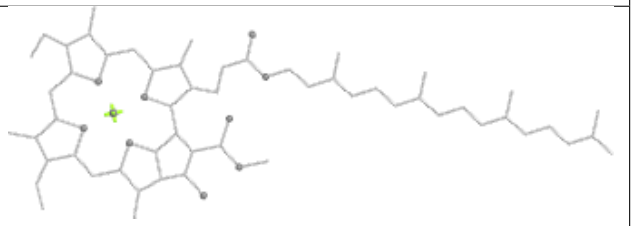
Bond lengths



Bond angles

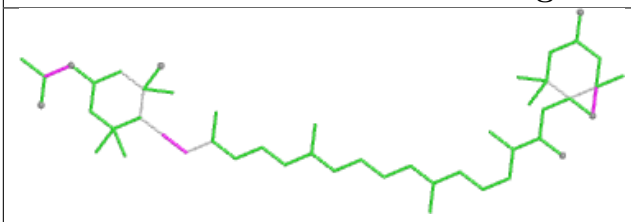


Torsions

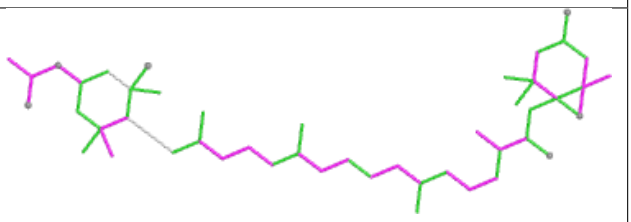


Rings

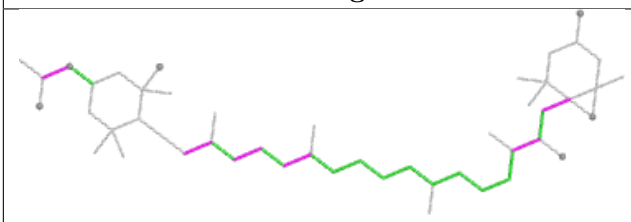
Ligand A86 I 304



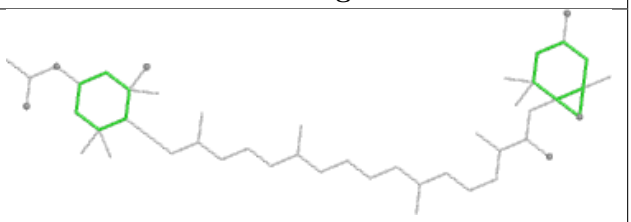
Bond lengths



Bond angles

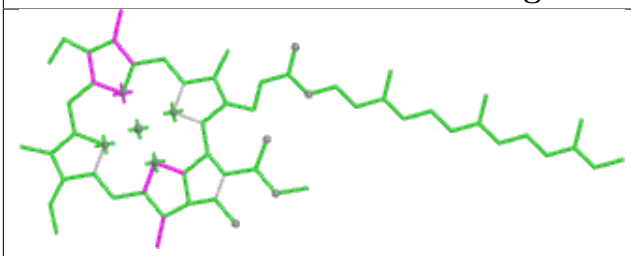


Torsions

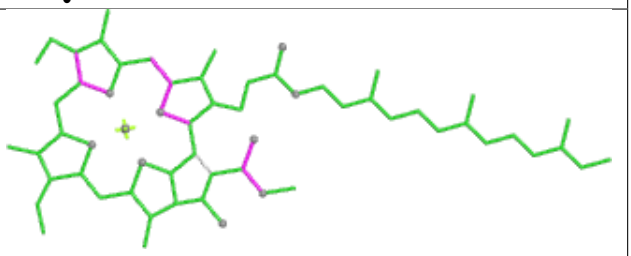


Rings

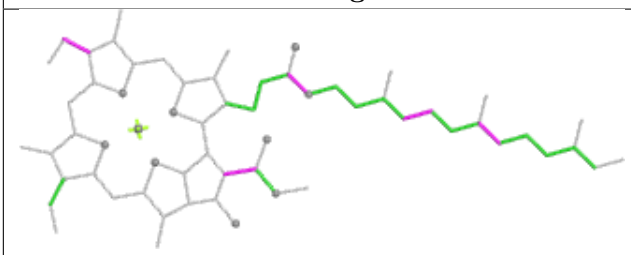
Ligand CLA Q 309



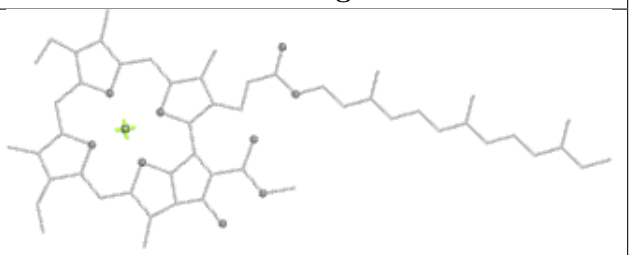
Bond lengths



Bond angles

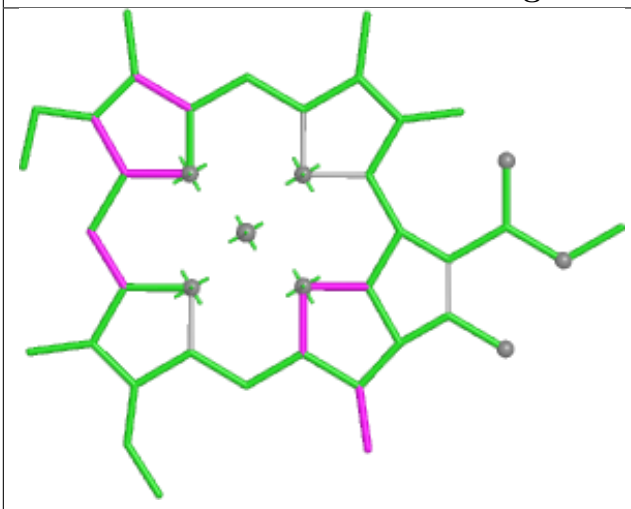


Torsions

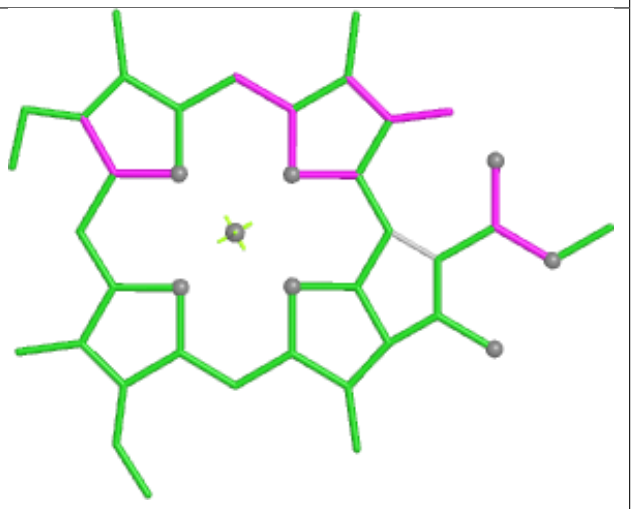


Rings

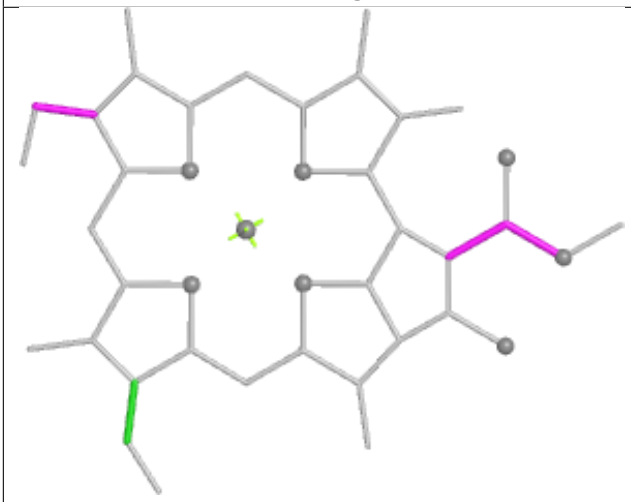
Ligand CLA U 213



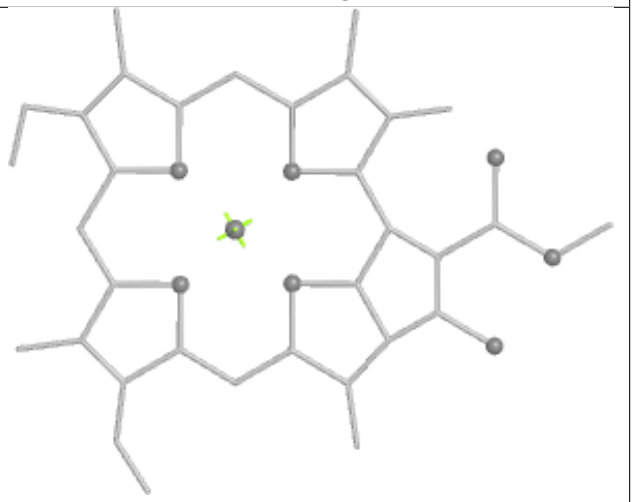
Bond lengths



Bond angles

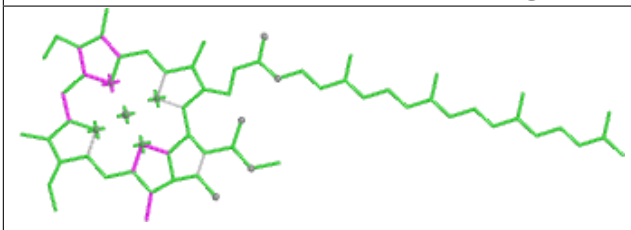


Torsions

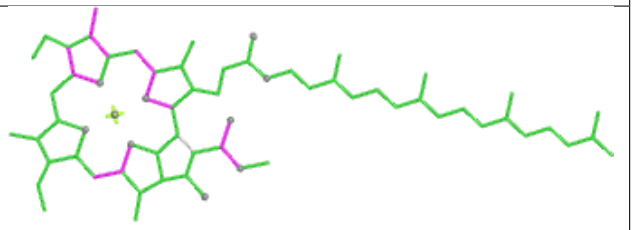


Rings

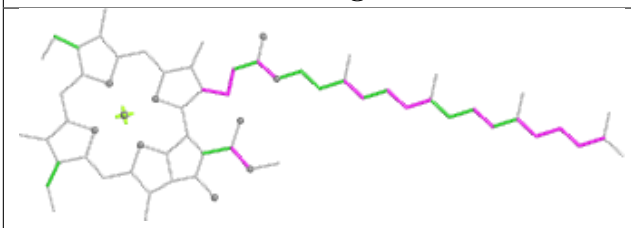
Ligand CLA K 312



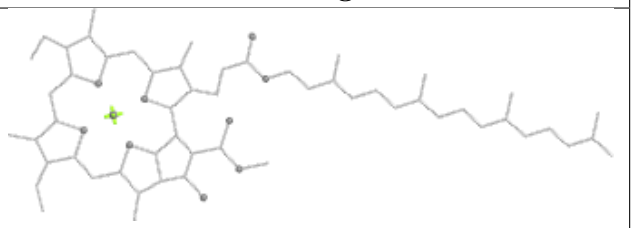
Bond lengths



Bond angles

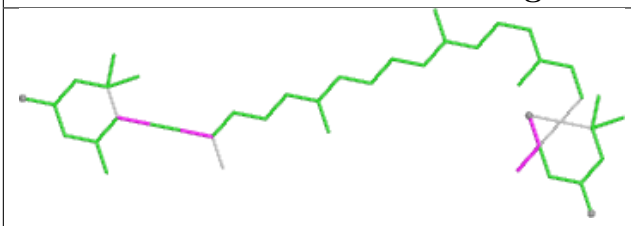


Torsions

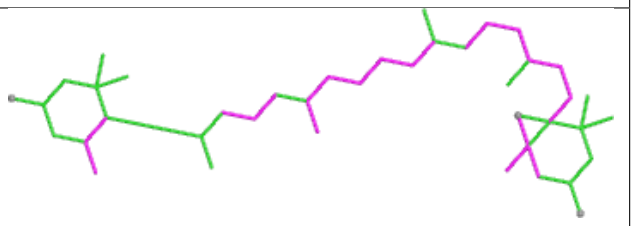


Rings

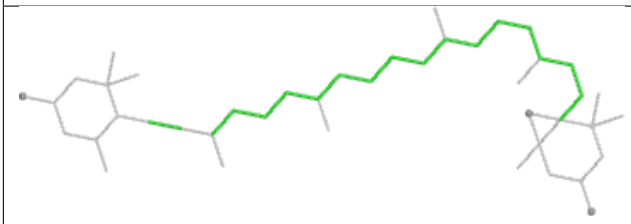
Ligand DD6 D 306



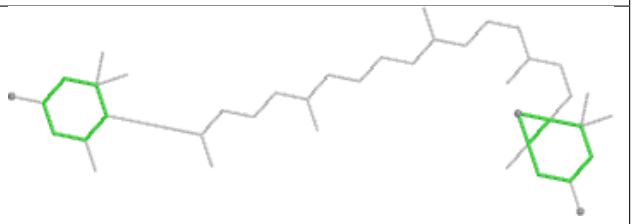
Bond lengths



Bond angles

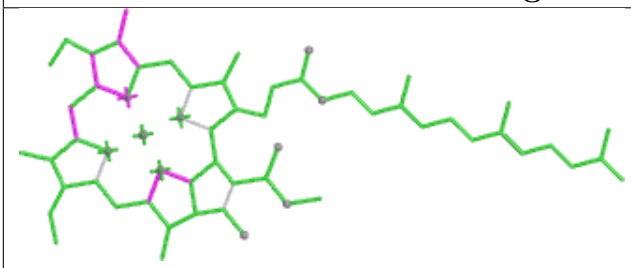


Torsions

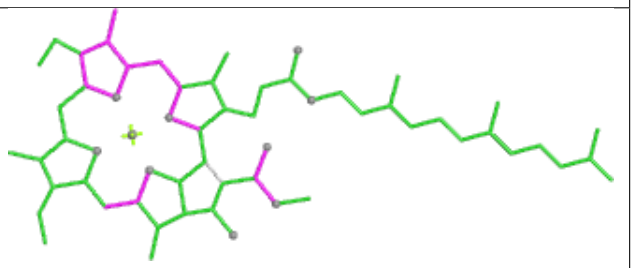


Rings

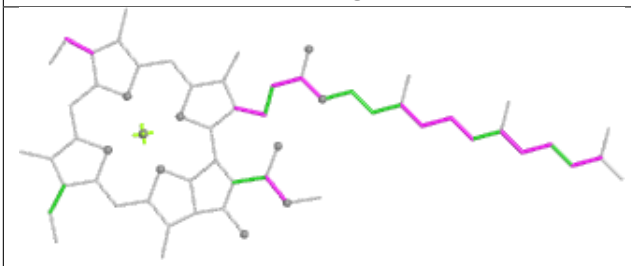
Ligand CLA X 308



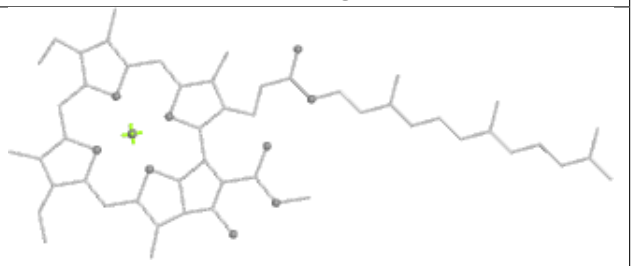
Bond lengths



Bond angles

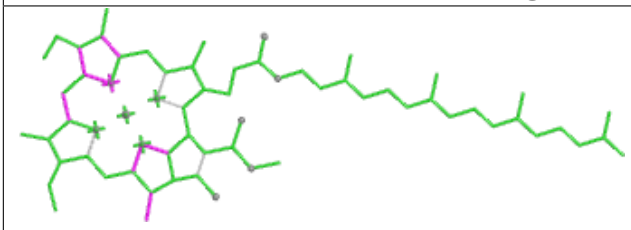


Torsions

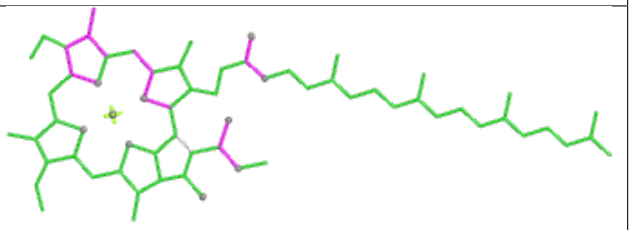


Rings

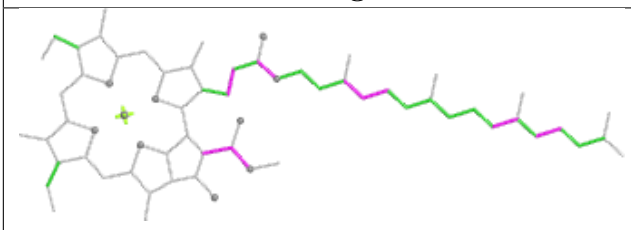
Ligand CLA R 307



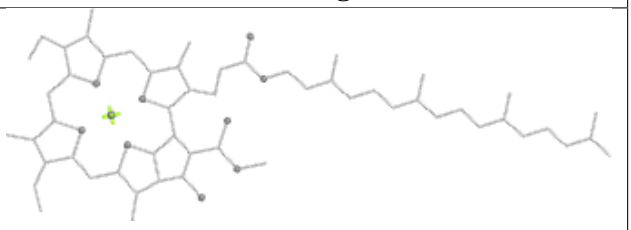
Bond lengths



Bond angles



Torsions

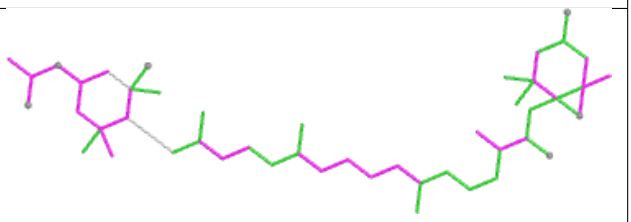


Rings

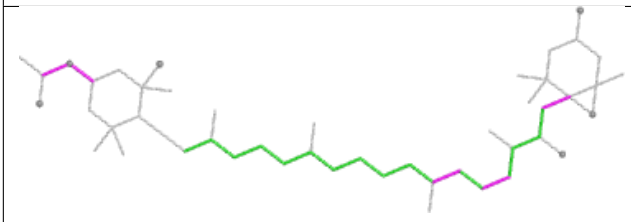
Ligand A86 G 305



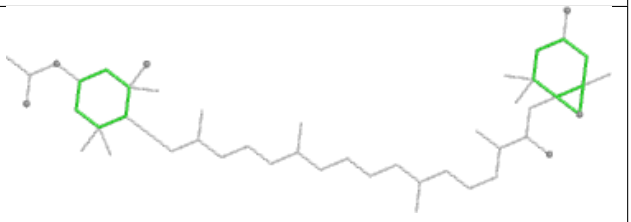
Bond lengths



Bond angles

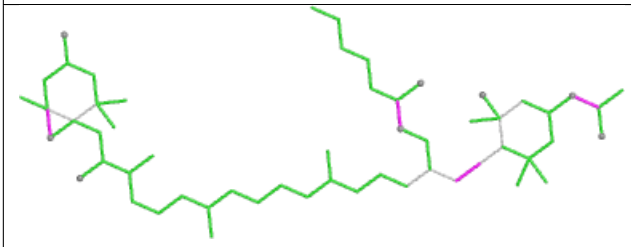


Torsions

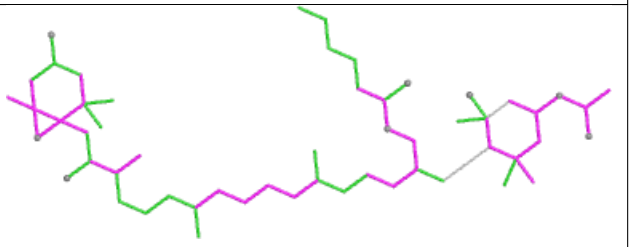


Rings

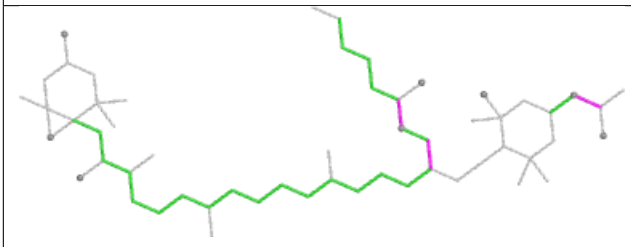
Ligand A1EB1 K 302



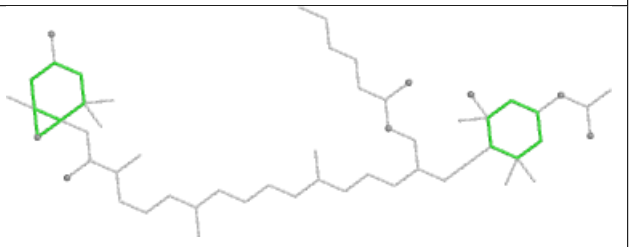
Bond lengths



Bond angles

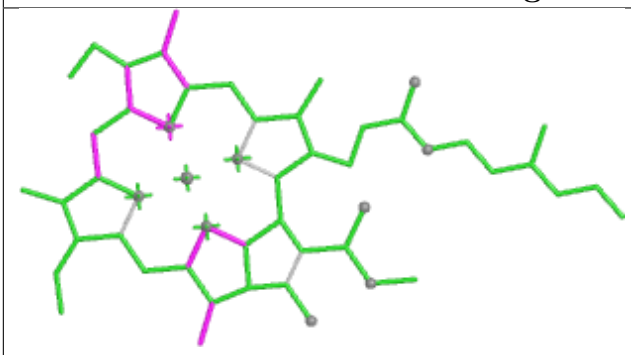


Torsions

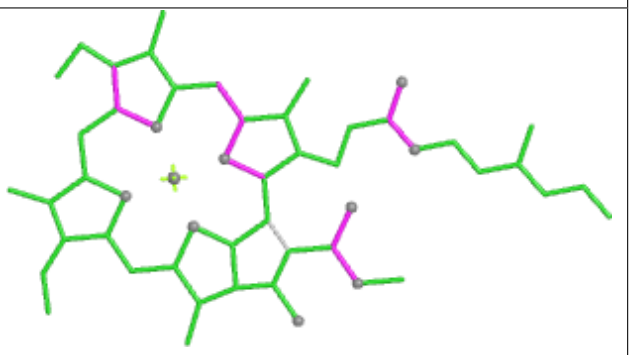


Rings

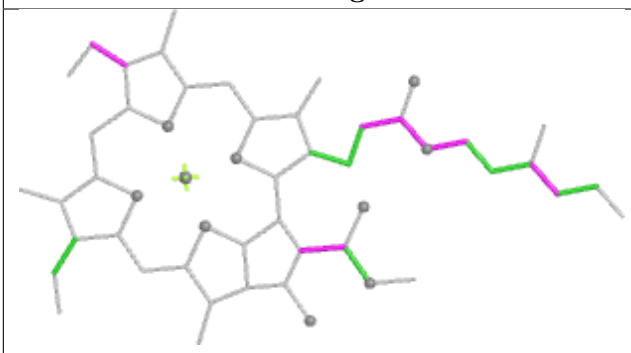
Ligand CLA R 316



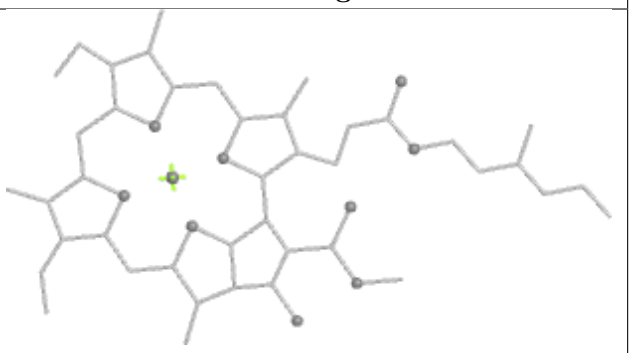
Bond lengths



Bond angles

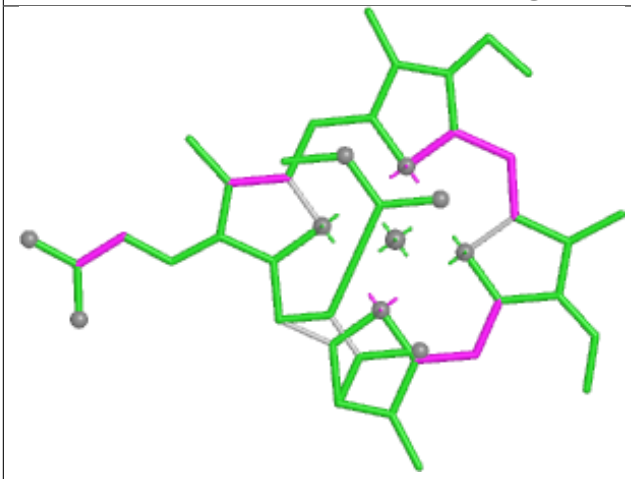


Torsions

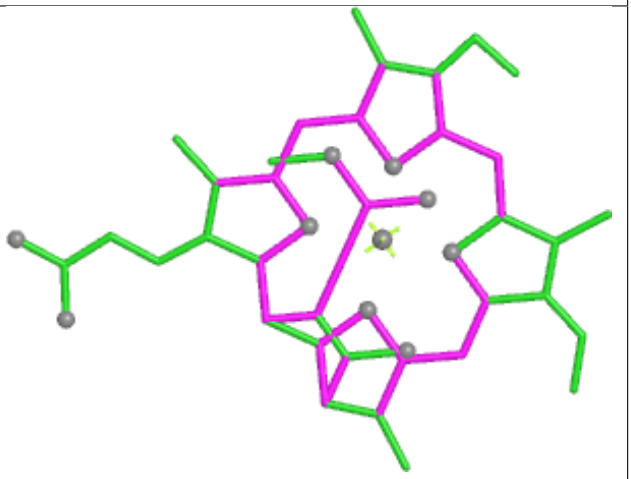


Rings

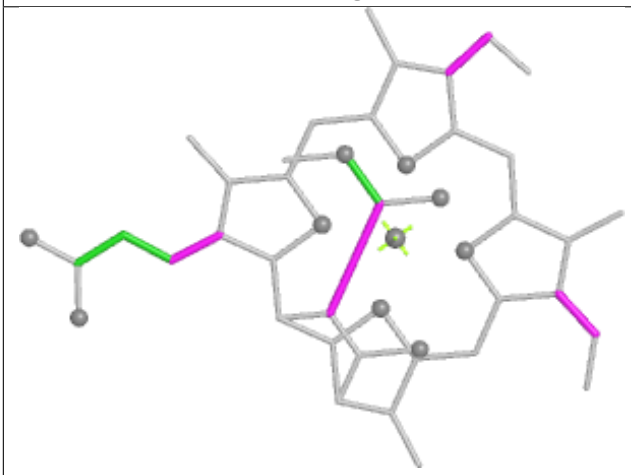
Ligand KC2 V 318



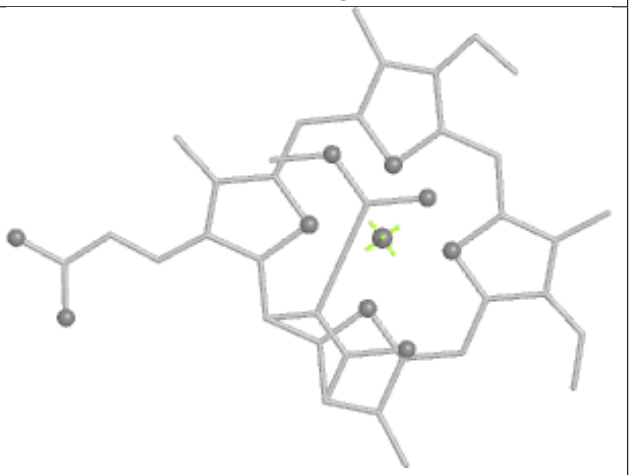
Bond lengths



Bond angles

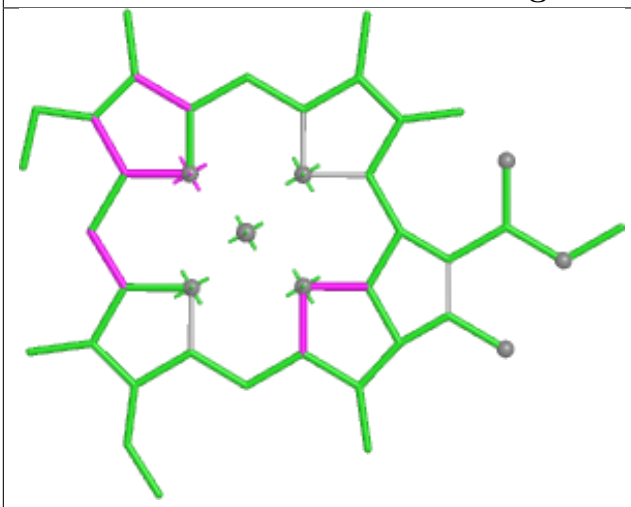


Torsions

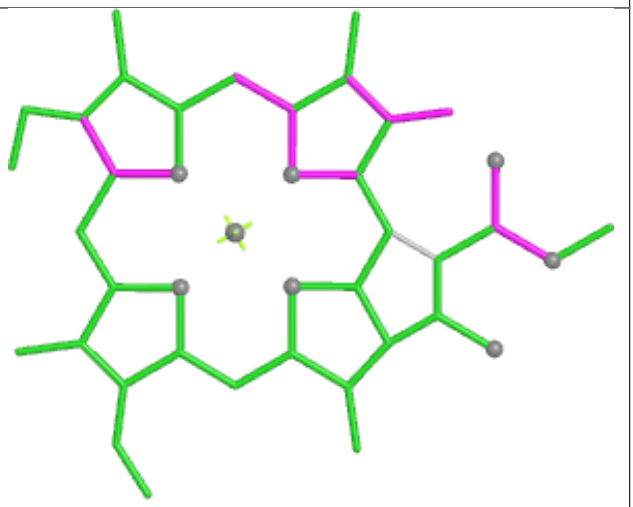


Rings

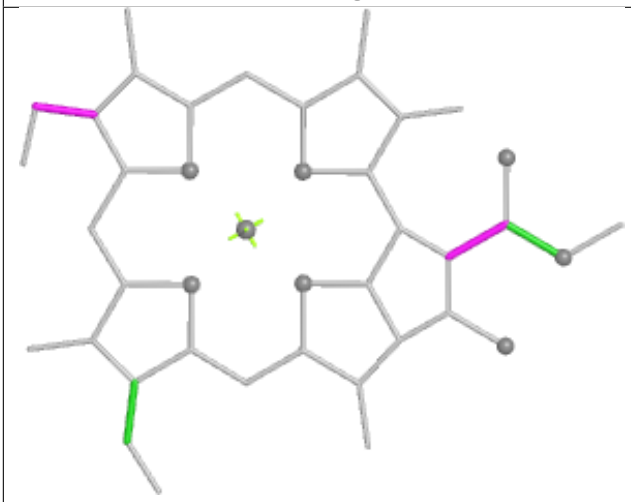
Ligand CLA z 314



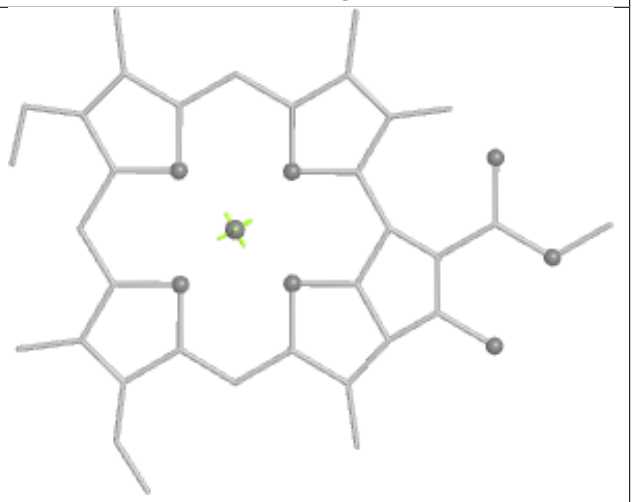
Bond lengths



Bond angles

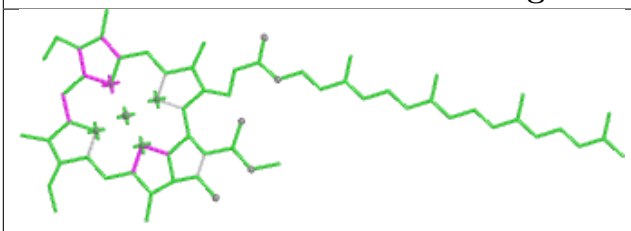


Torsions

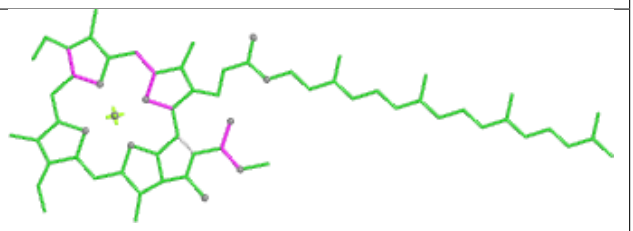


Rings

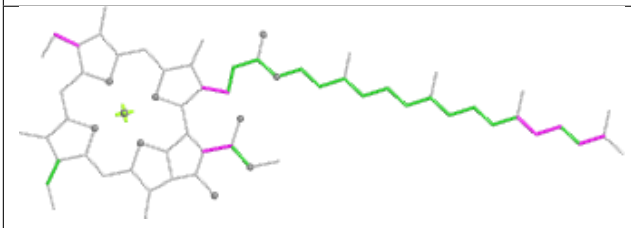
Ligand CLA b 827



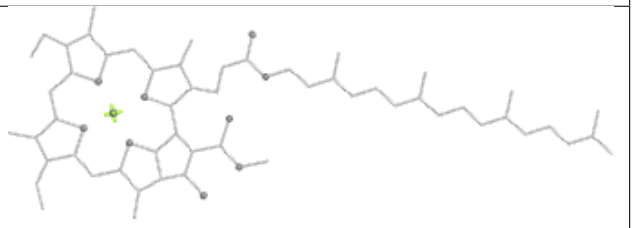
Bond lengths



Bond angles

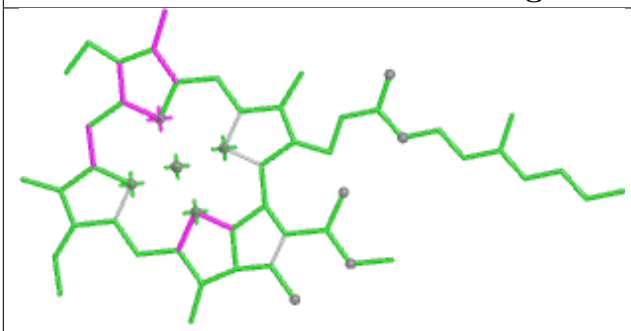


Torsions

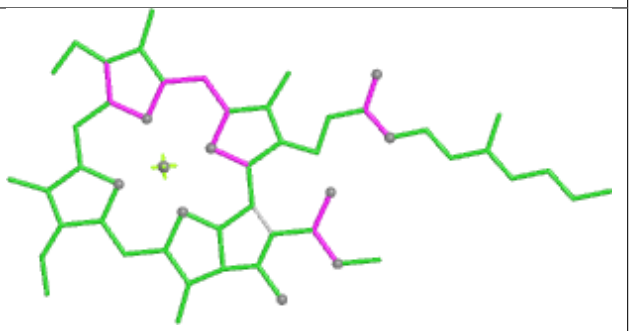


Rings

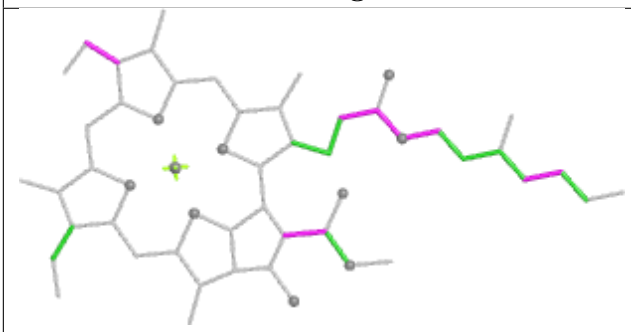
Ligand CLA E 309



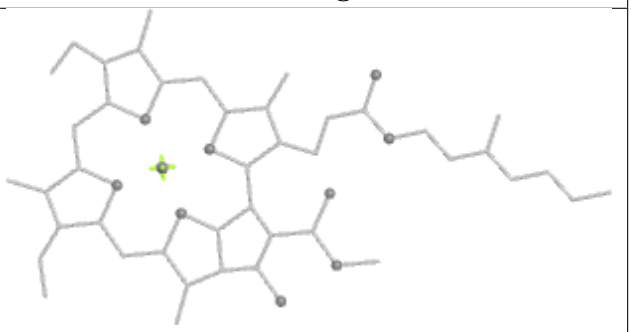
Bond lengths



Bond angles

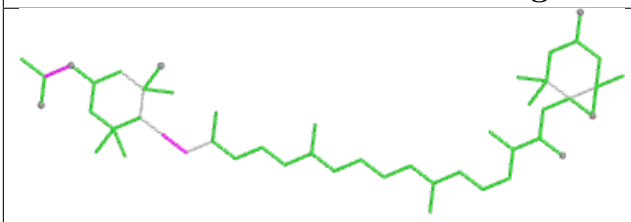


Torsions

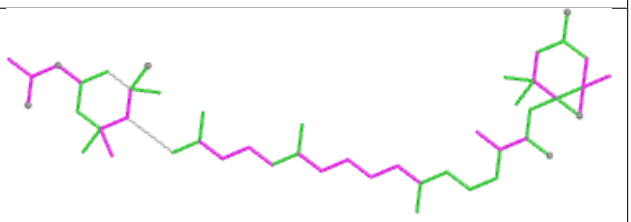


Rings

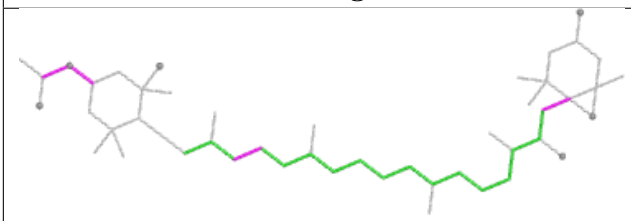
Ligand A86 T 306



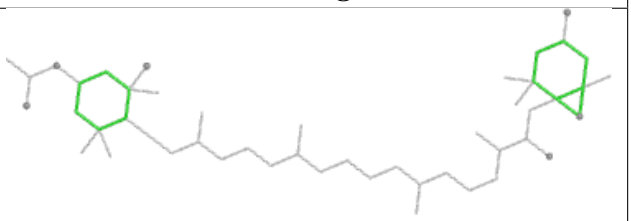
Bond lengths



Bond angles

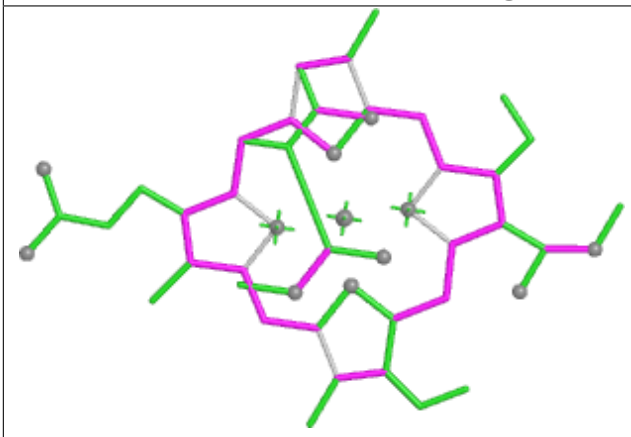


Torsions

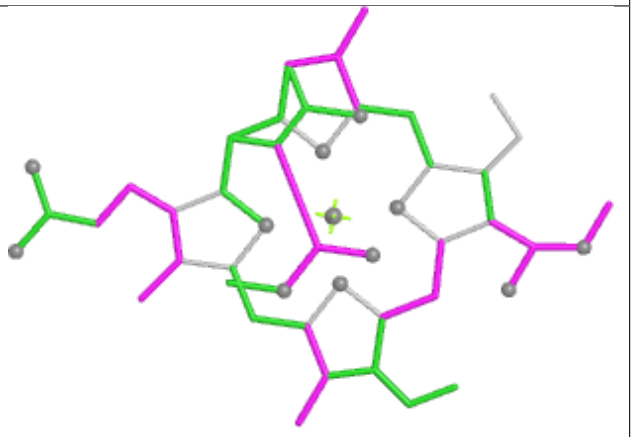


Rings

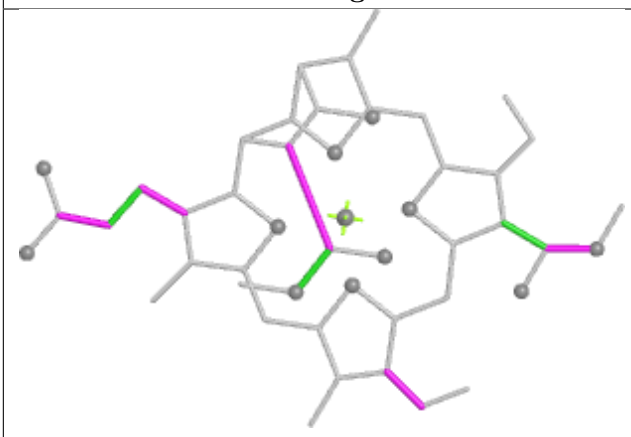
Ligand A1ECV R 313



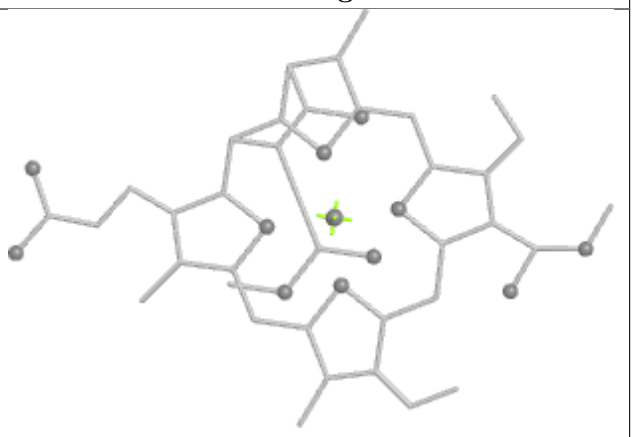
Bond lengths



Bond angles

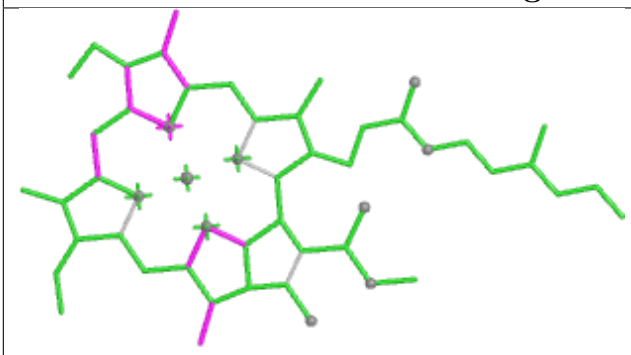


Torsions

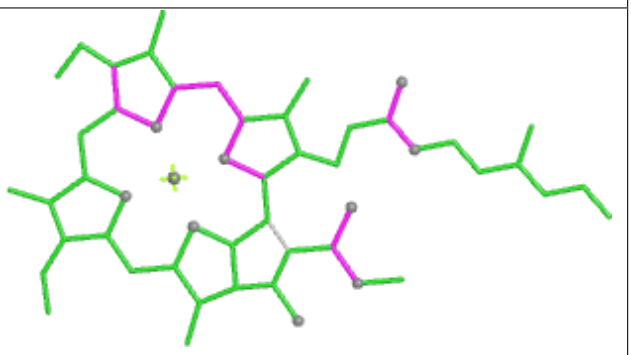


Rings

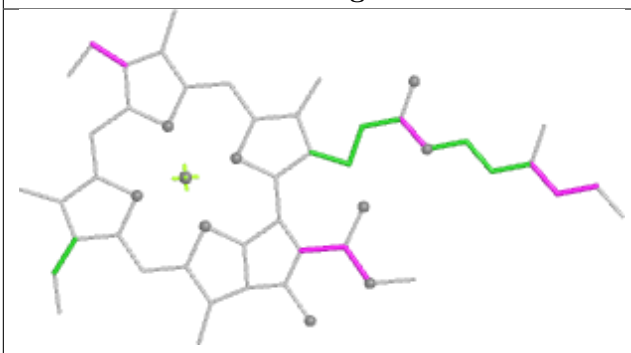
Ligand CLA X 317



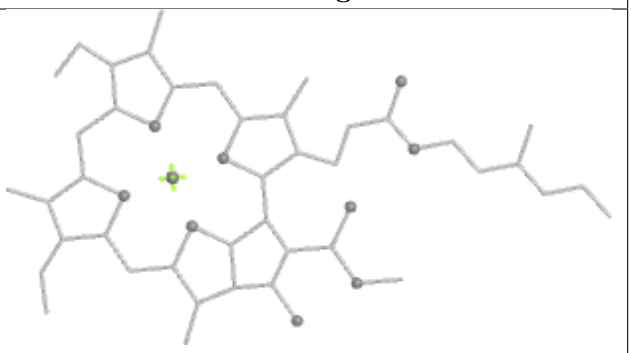
Bond lengths



Bond angles

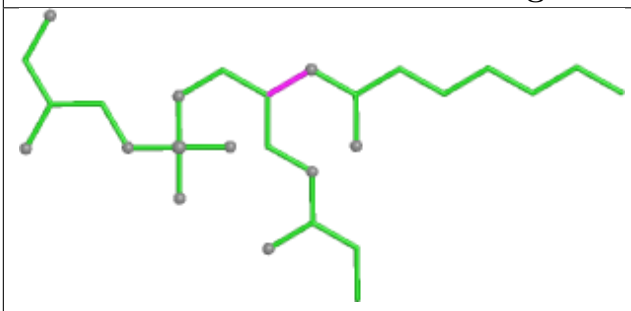


Torsions

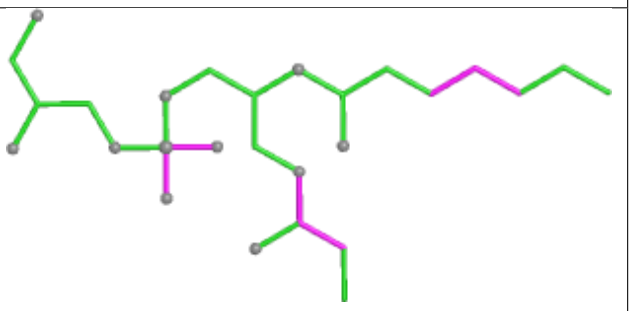


Rings

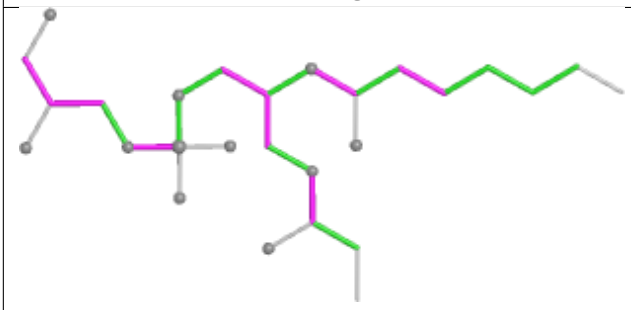
Ligand LHG a 841



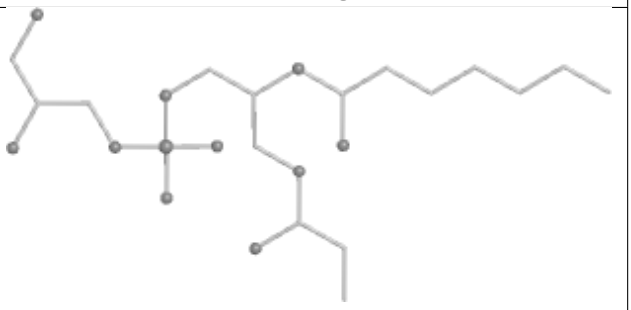
Bond lengths



Bond angles

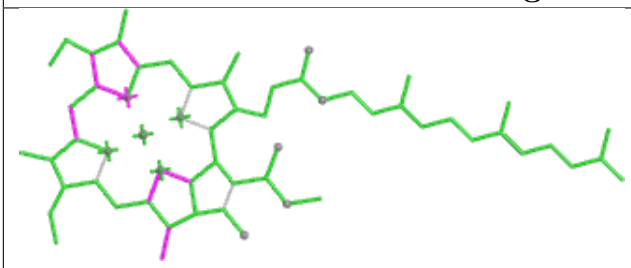


Torsions

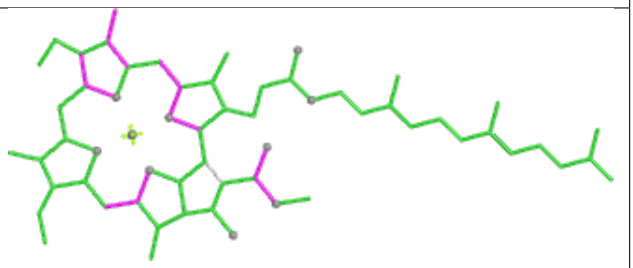


Rings

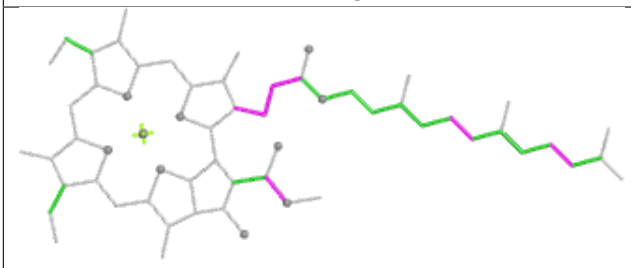
Ligand CLA A 307



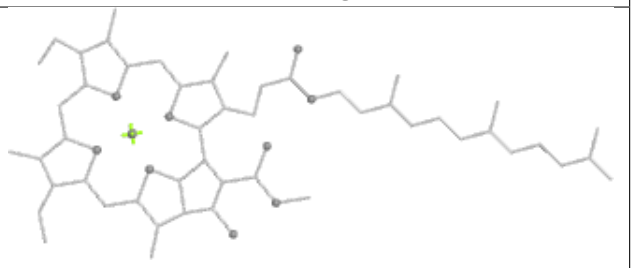
Bond lengths



Bond angles

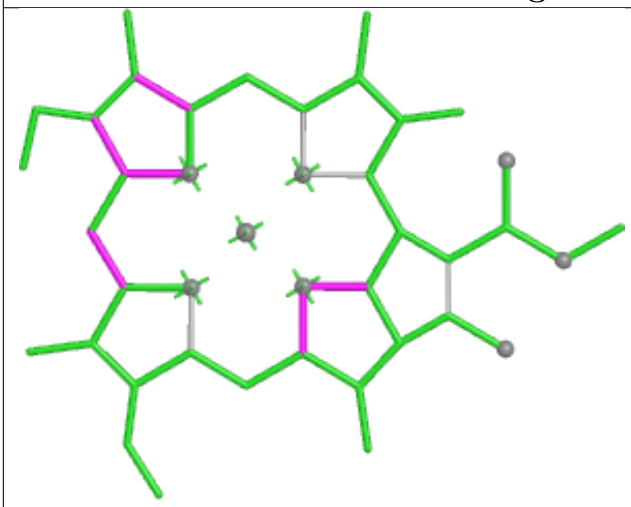


Torsions

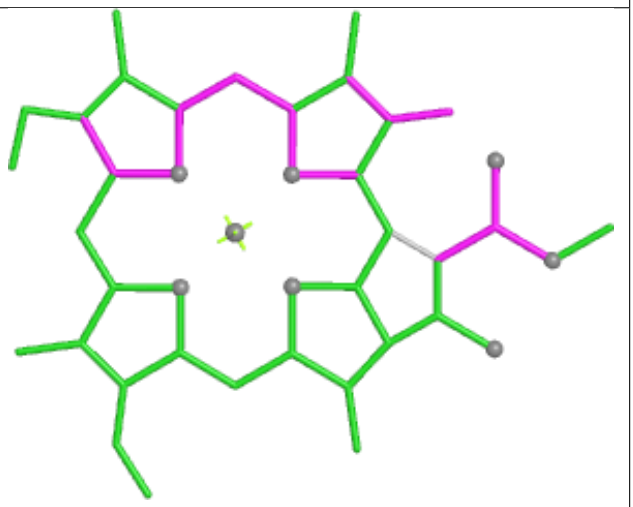


Rings

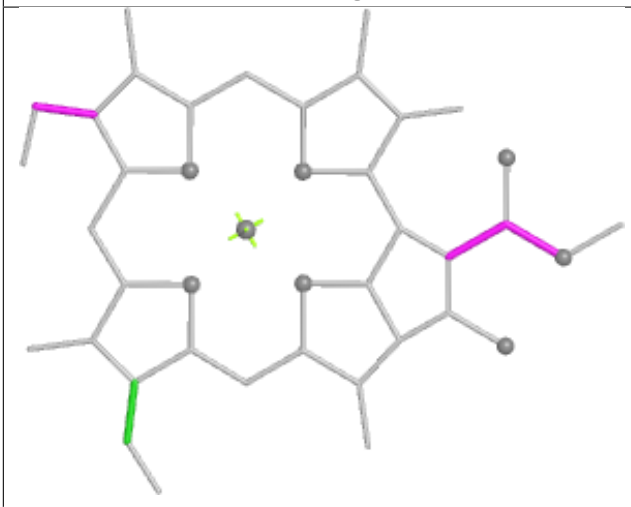
Ligand CLA 3 319



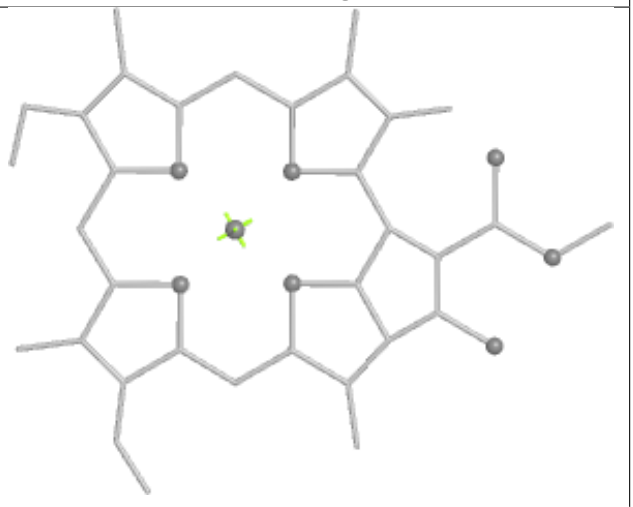
Bond lengths



Bond angles

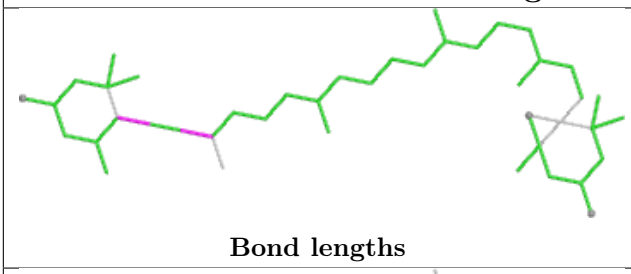


Torsions

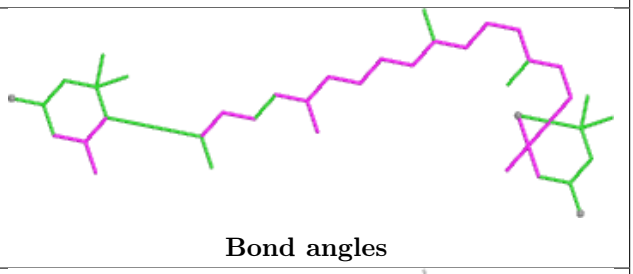


Rings

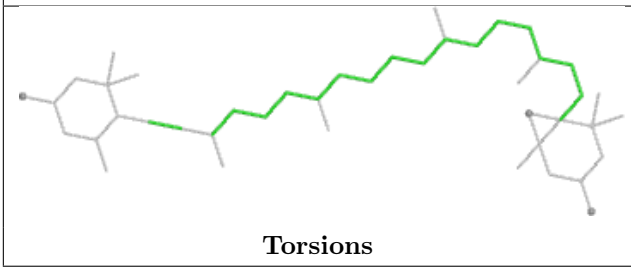
Ligand DD6 D 303



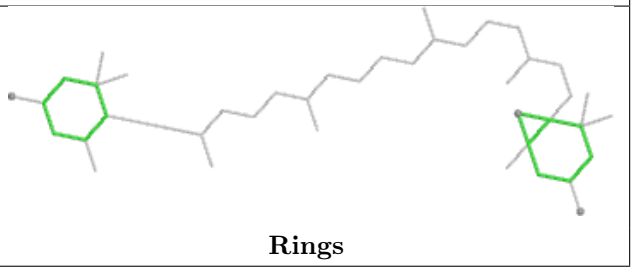
Bond lengths



Bond angles

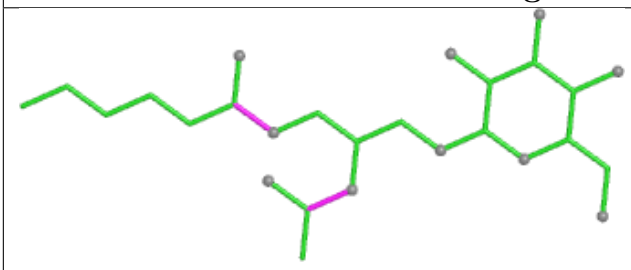


Torsions

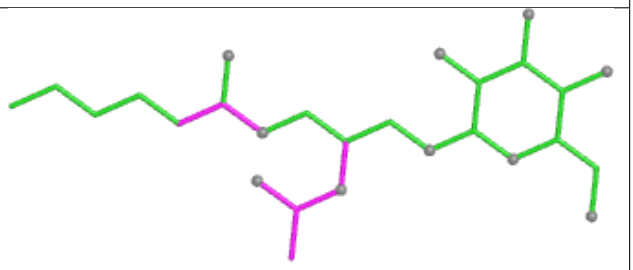


Rings

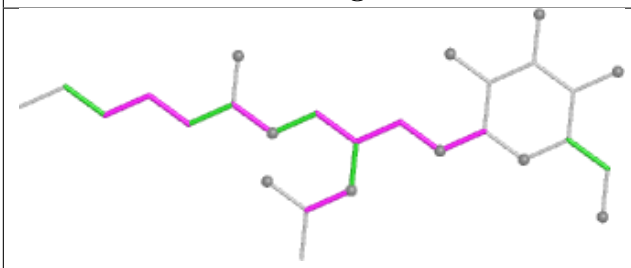
Ligand LMG 0 324



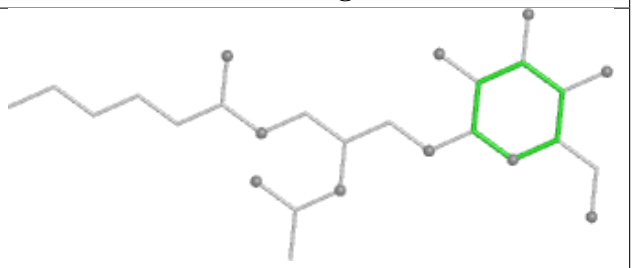
Bond lengths



Bond angles

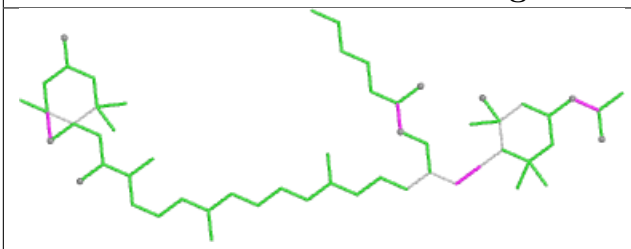


Torsions

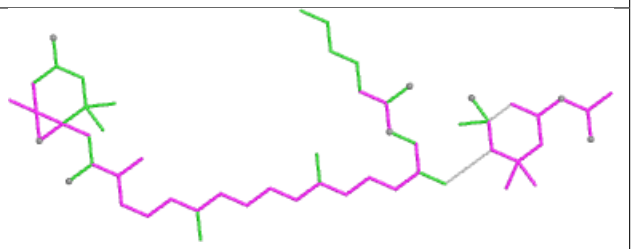


Rings

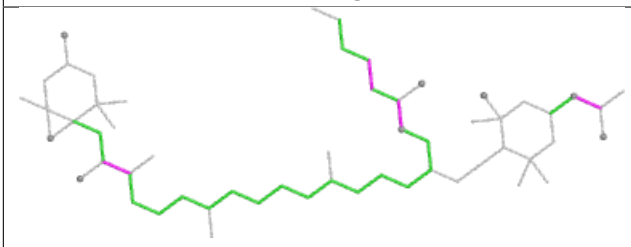
Ligand A1EB1 J 302



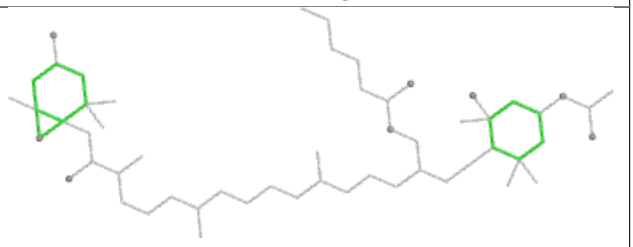
Bond lengths



Bond angles

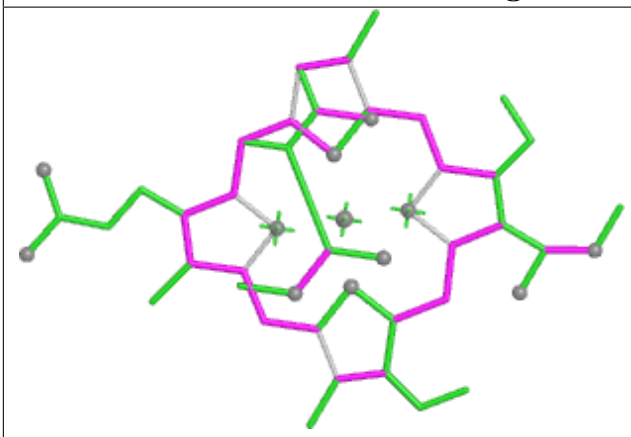


Torsions

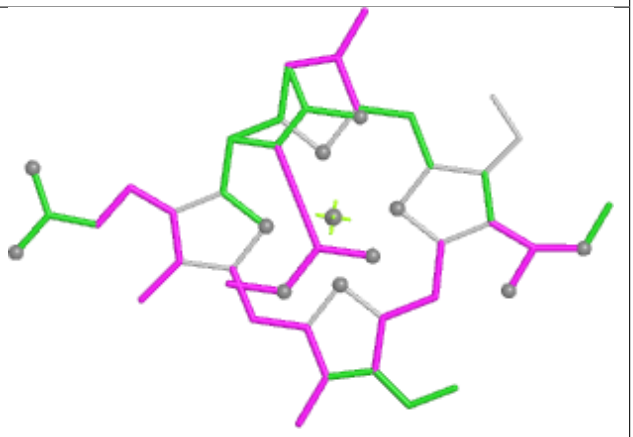


Rings

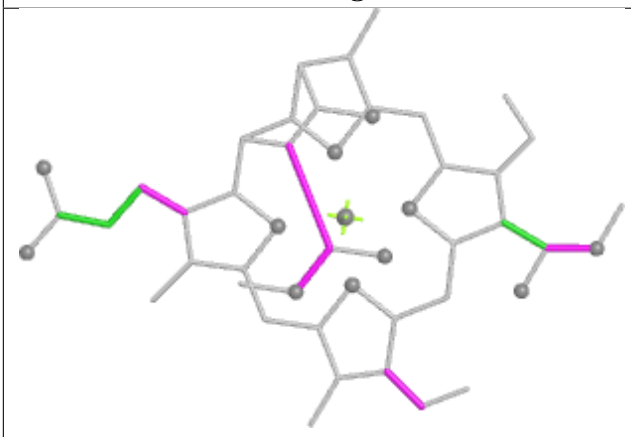
Ligand A1ECV 0 321



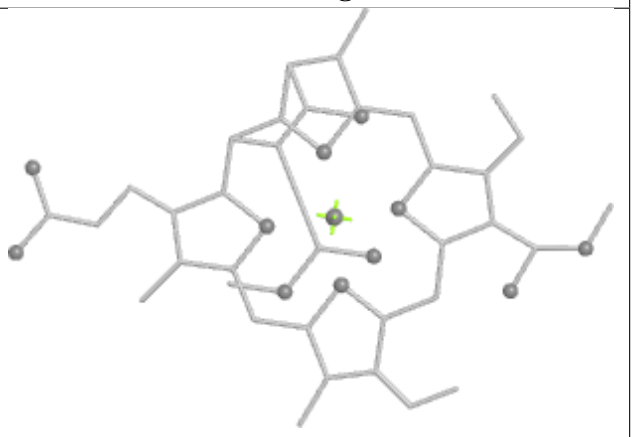
Bond lengths



Bond angles

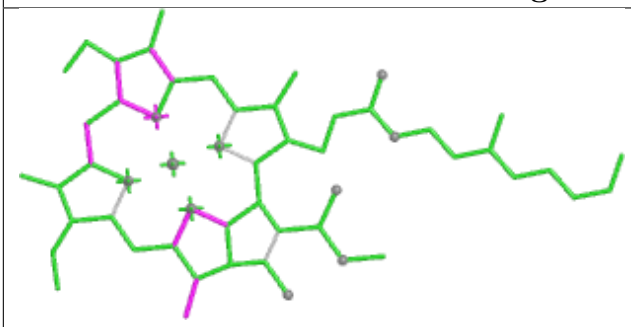


Torsions

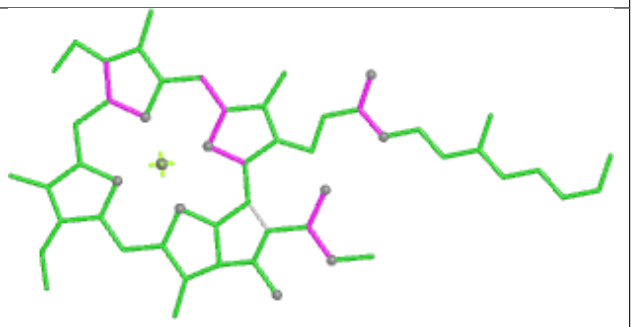


Rings

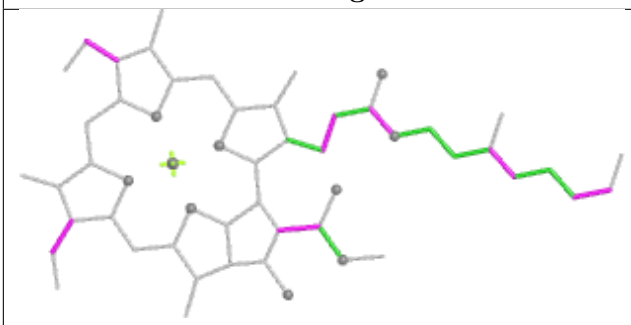
Ligand CLA I 310



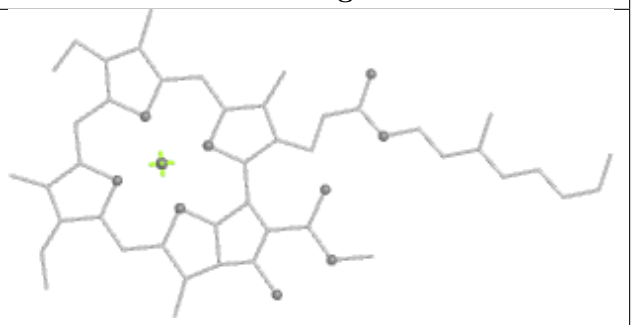
Bond lengths



Bond angles

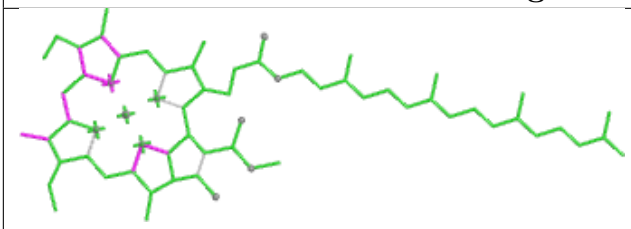


Torsions

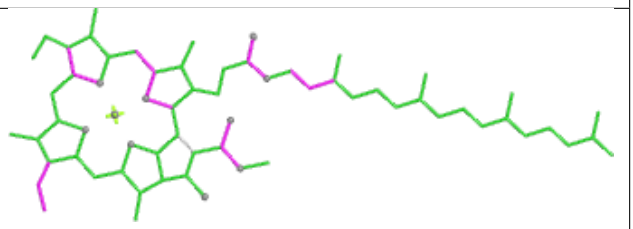


Rings

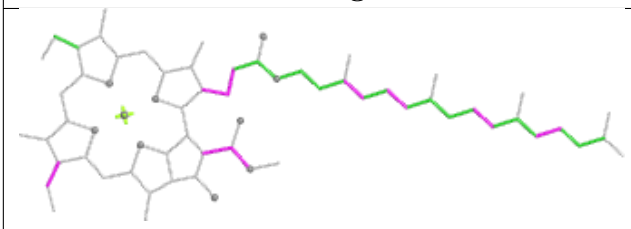
Ligand CLA b 815



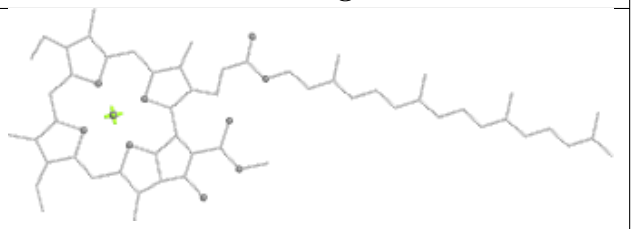
Bond lengths



Bond angles

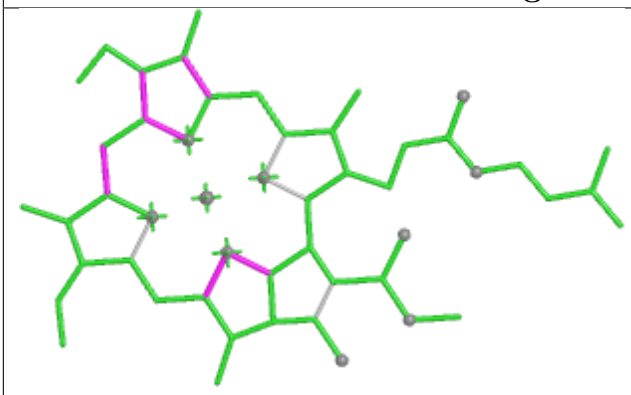


Torsions

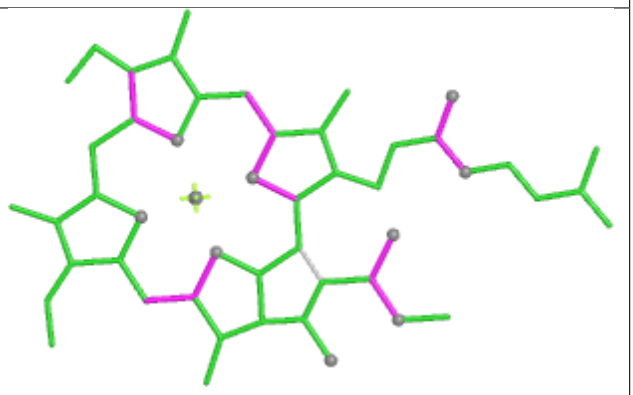


Rings

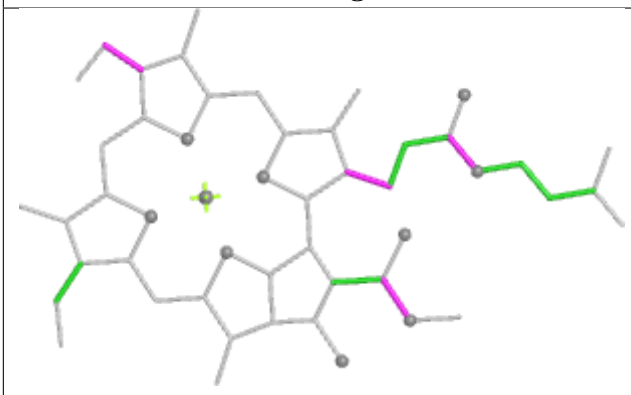
Ligand CLA A 315



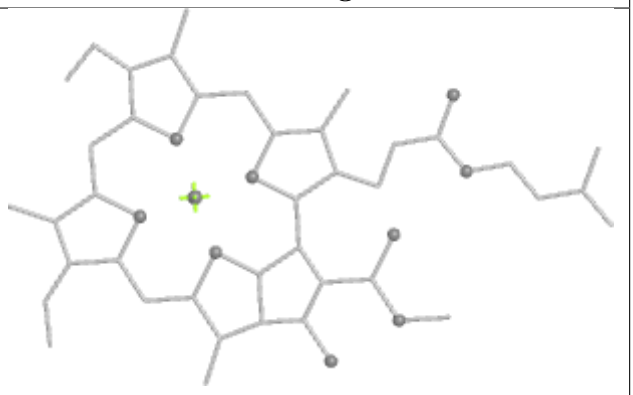
Bond lengths



Bond angles

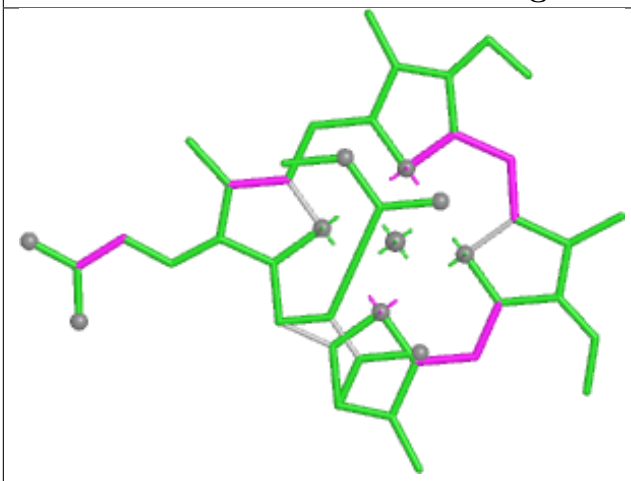


Torsions

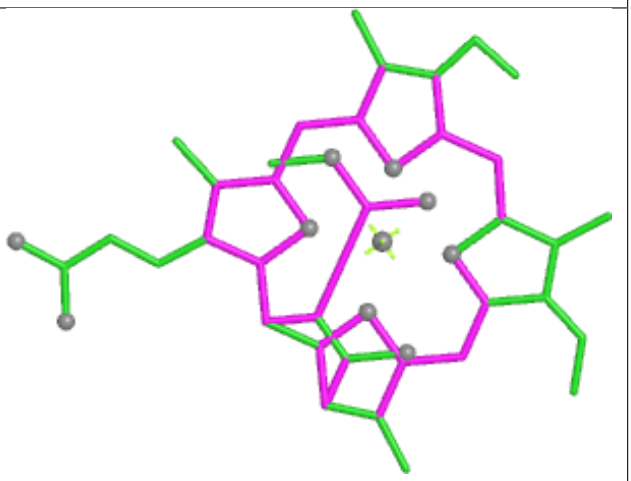


Rings

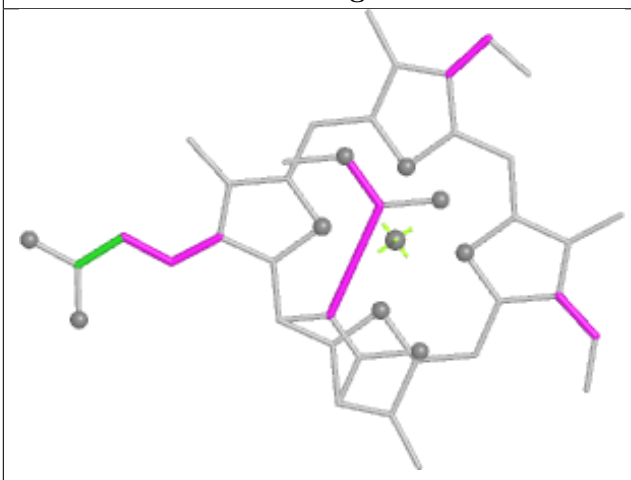
Ligand KC2 J 315



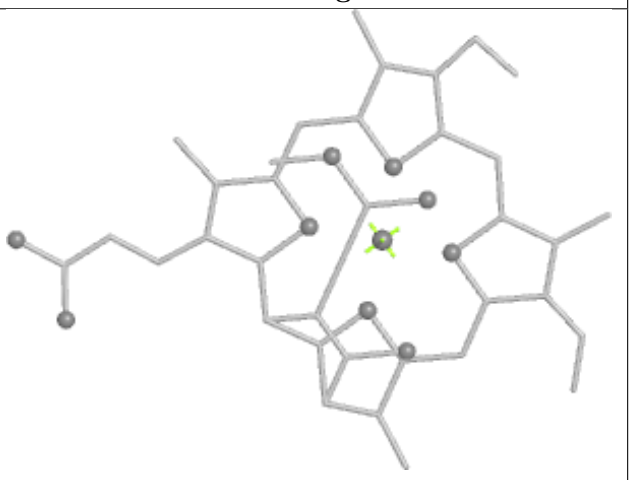
Bond lengths



Bond angles

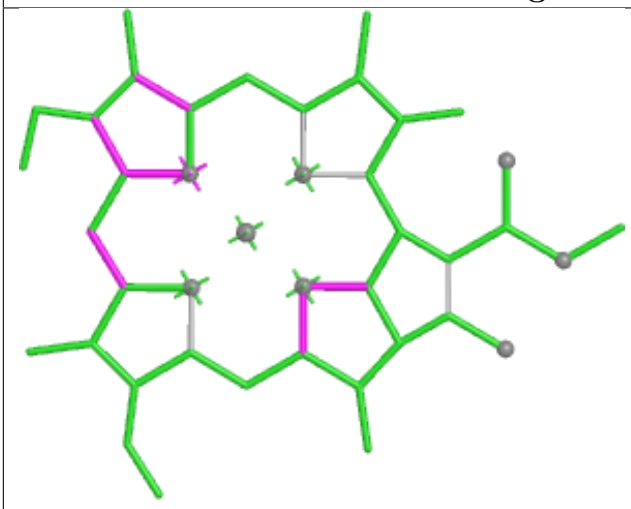


Torsions

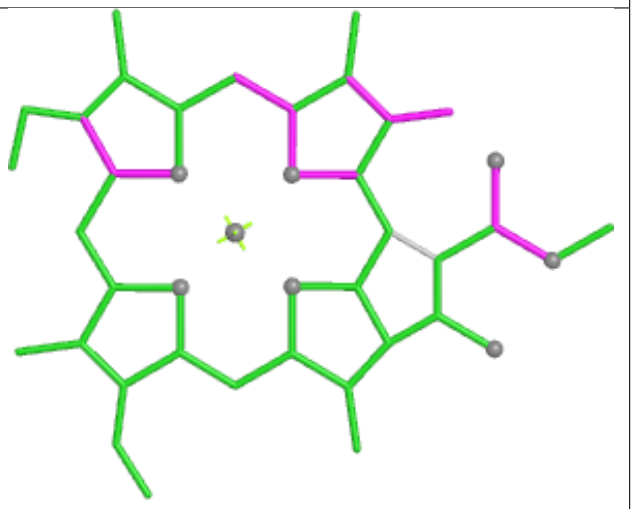


Rings

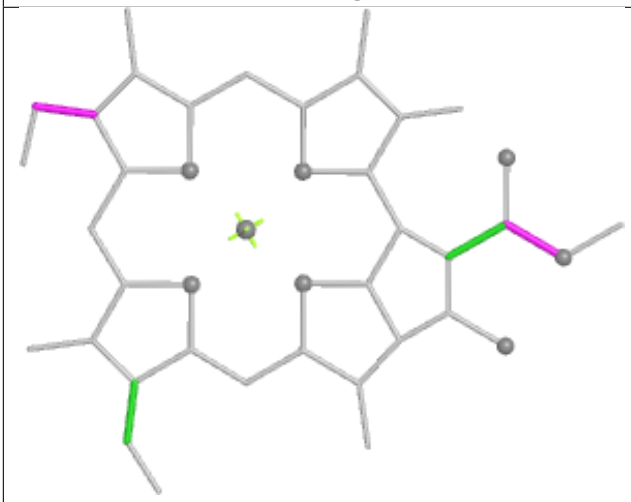
Ligand CLA 4 319



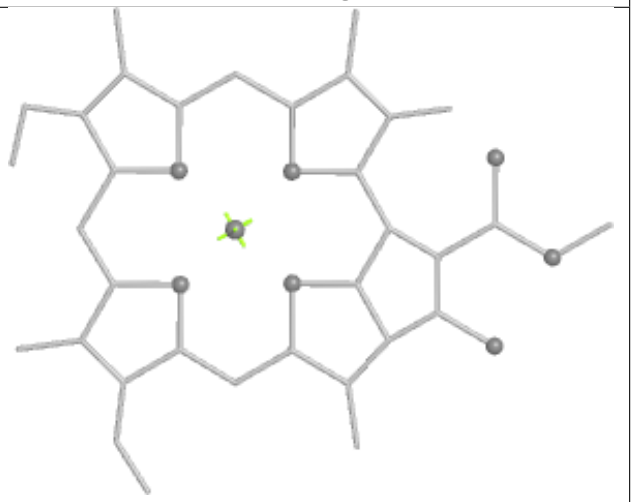
Bond lengths



Bond angles

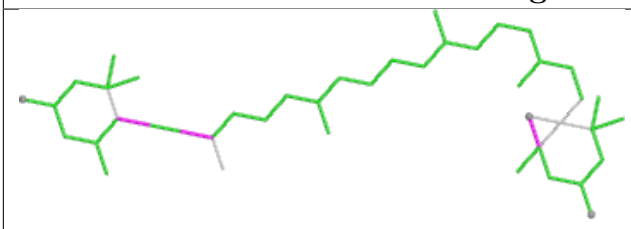


Torsions

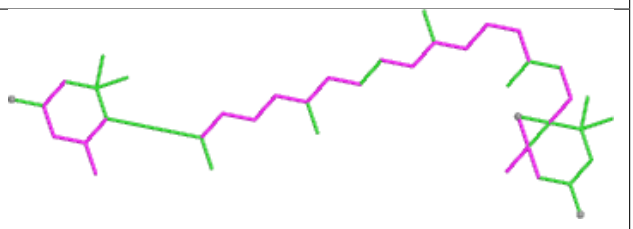


Rings

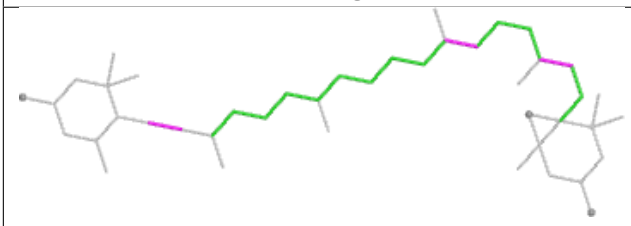
Ligand DD6 a 846



Bond lengths



Bond angles

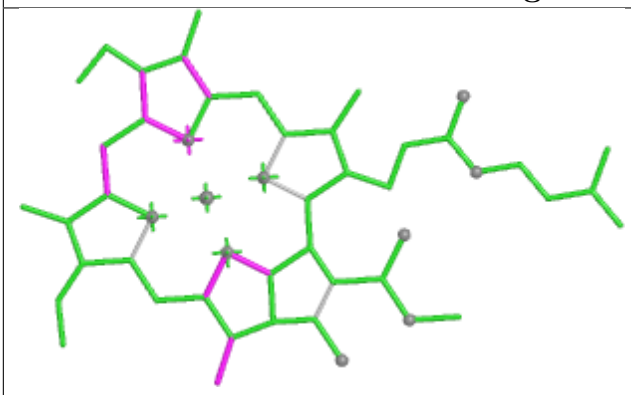


Torsions

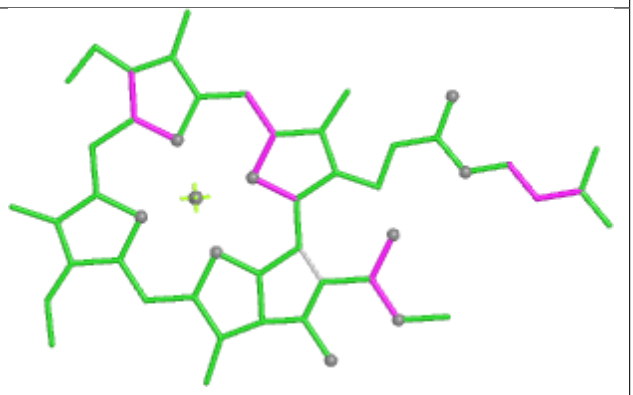


Rings

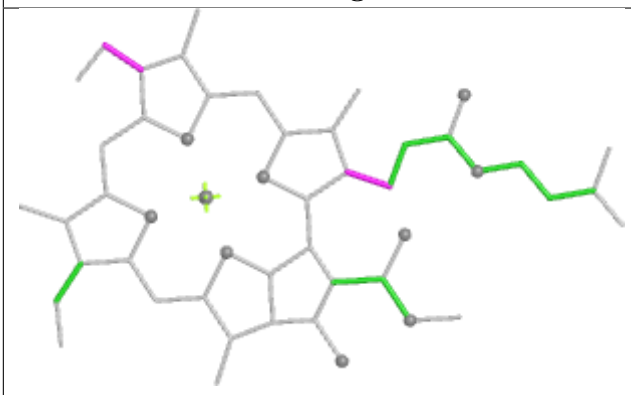
Ligand CLA O 313



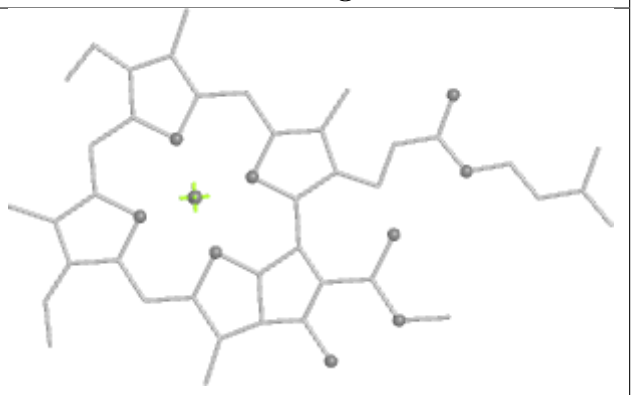
Bond lengths



Bond angles

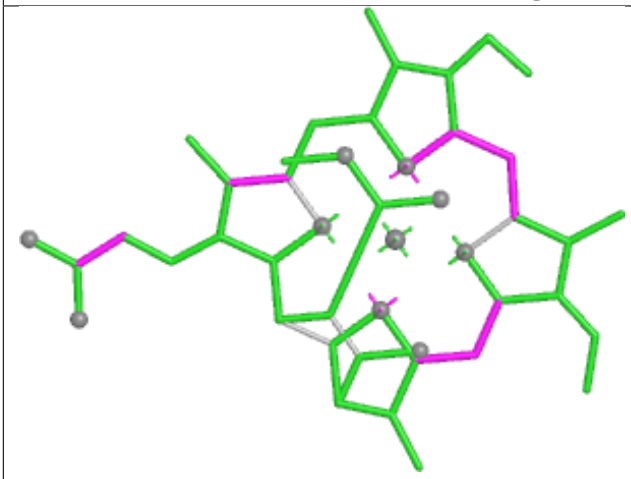


Torsions

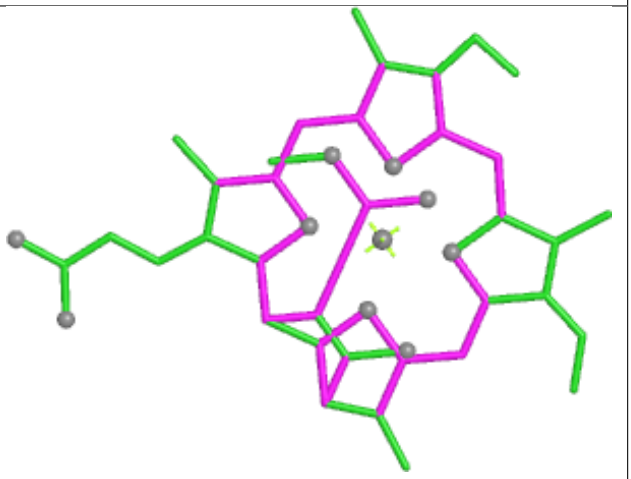


Rings

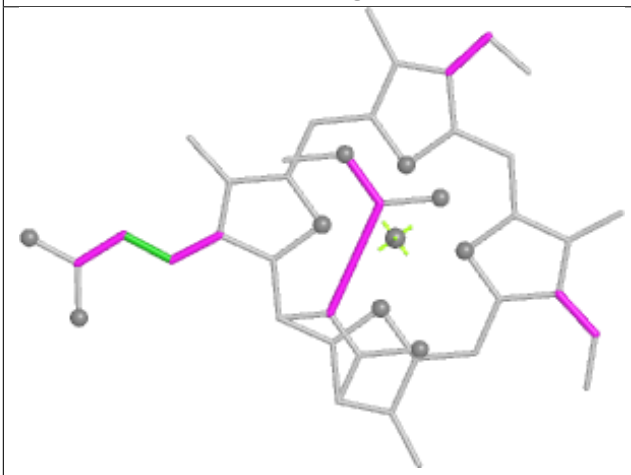
Ligand KC2 Z 311



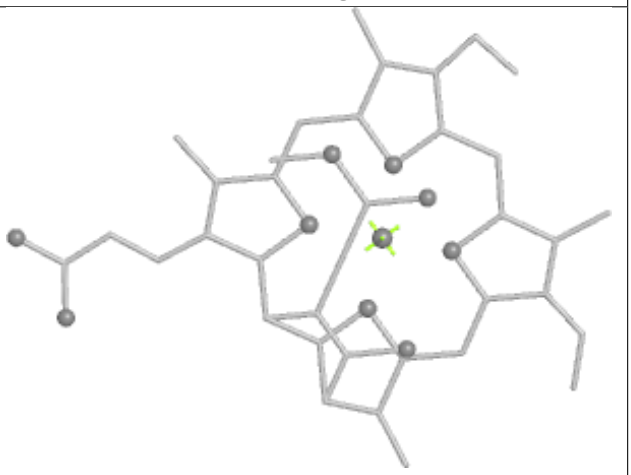
Bond lengths



Bond angles

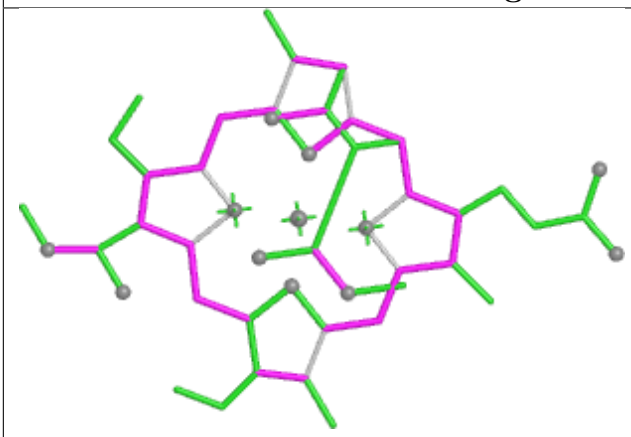


Torsions

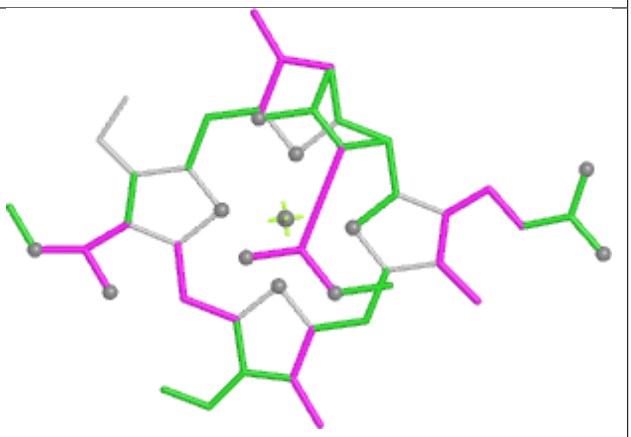


Rings

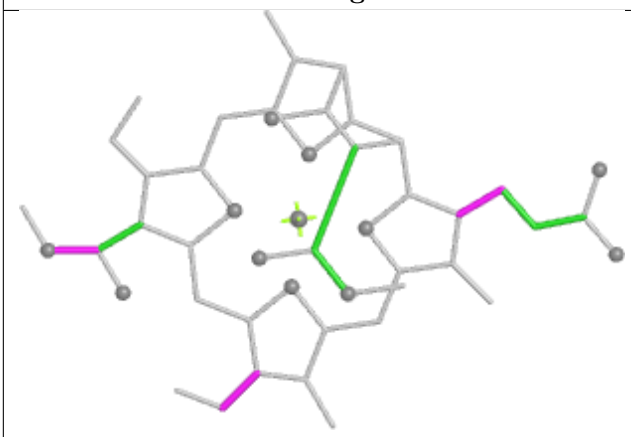
Ligand A1ECV 1 318



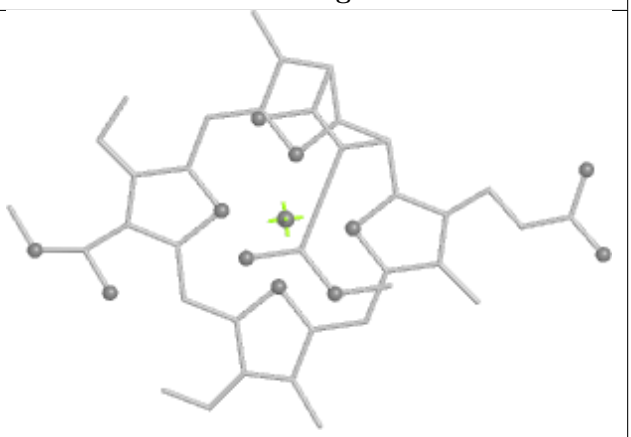
Bond lengths



Bond angles

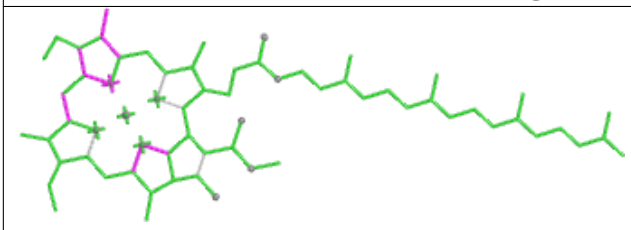


Torsions

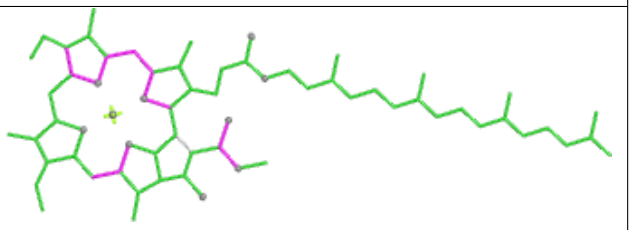


Rings

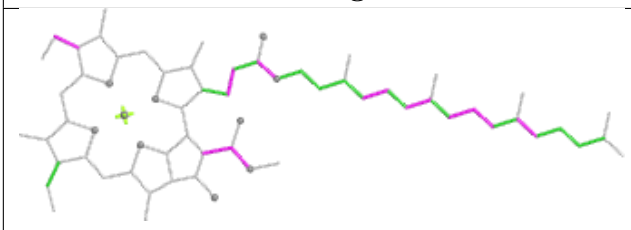
Ligand CLA b 833



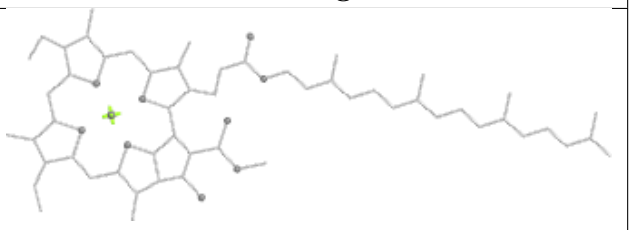
Bond lengths



Bond angles

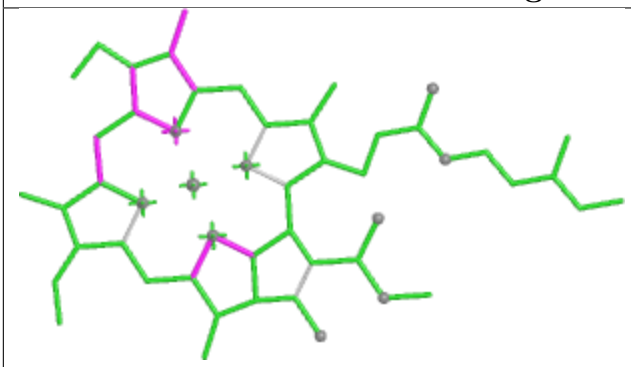


Torsions

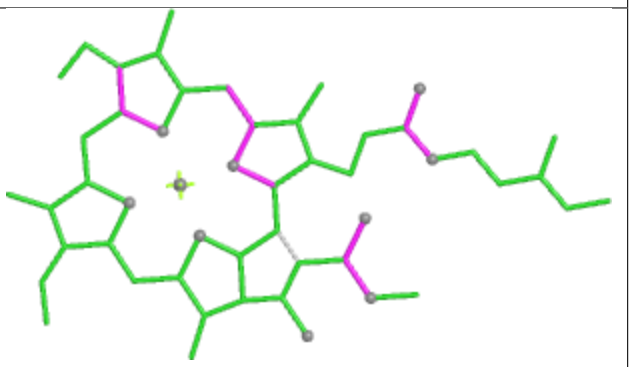


Rings

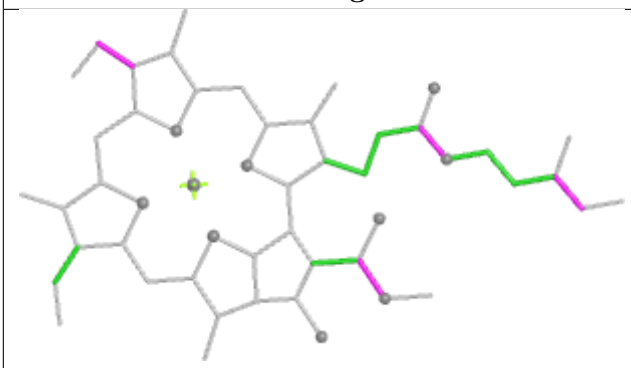
Ligand CLA P 316



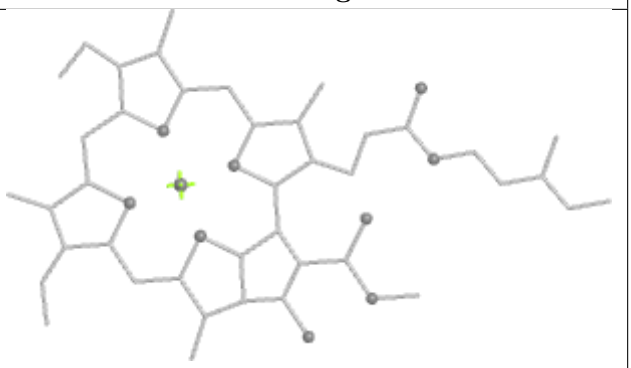
Bond lengths



Bond angles

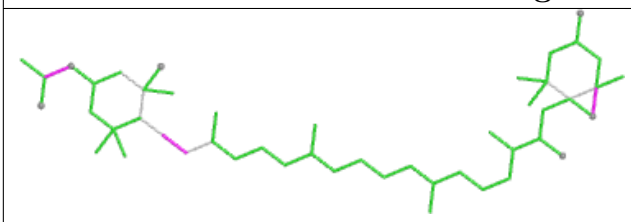


Torsions

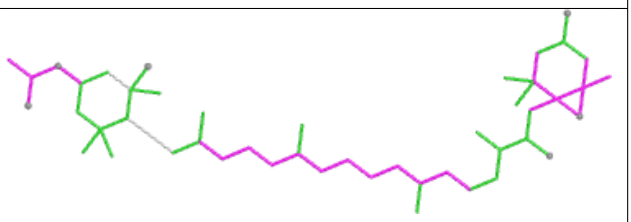


Rings

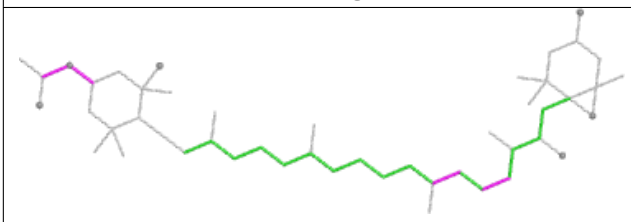
Ligand A86 6 302



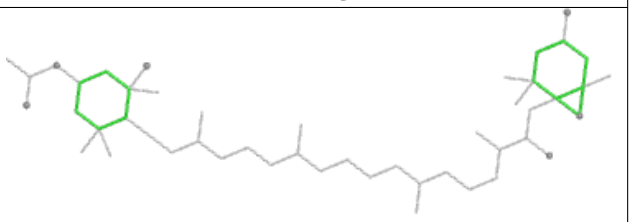
Bond lengths



Bond angles

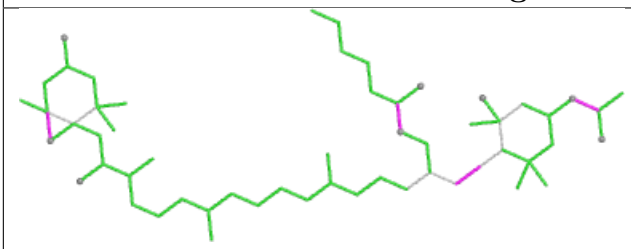


Torsions

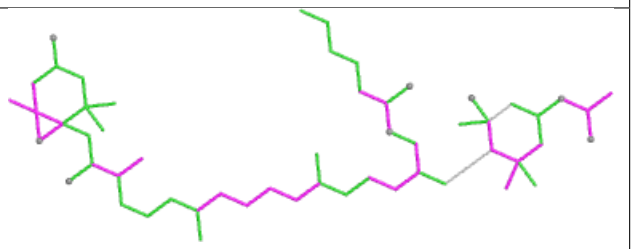


Rings

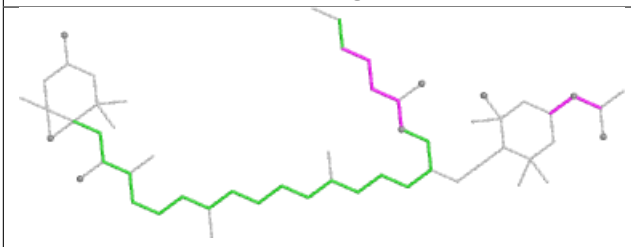
Ligand A1EB1 3 309



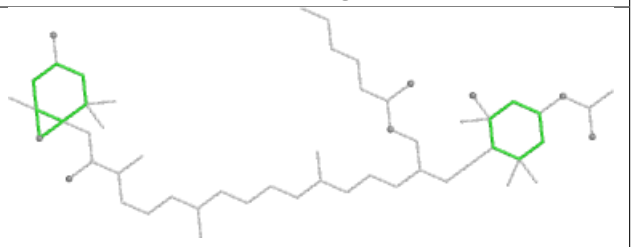
Bond lengths



Bond angles

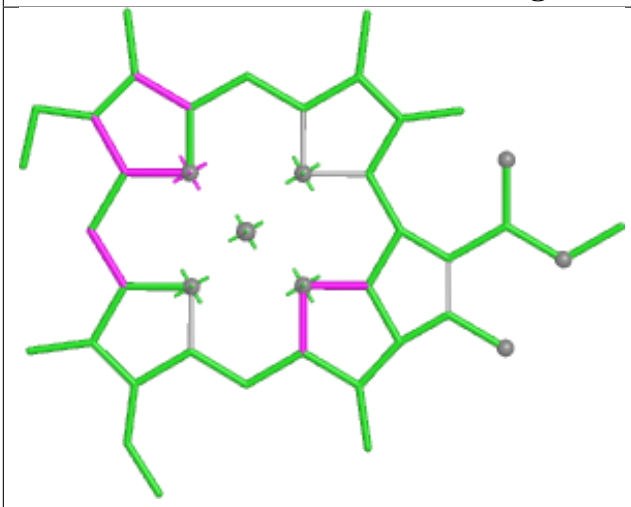


Torsions

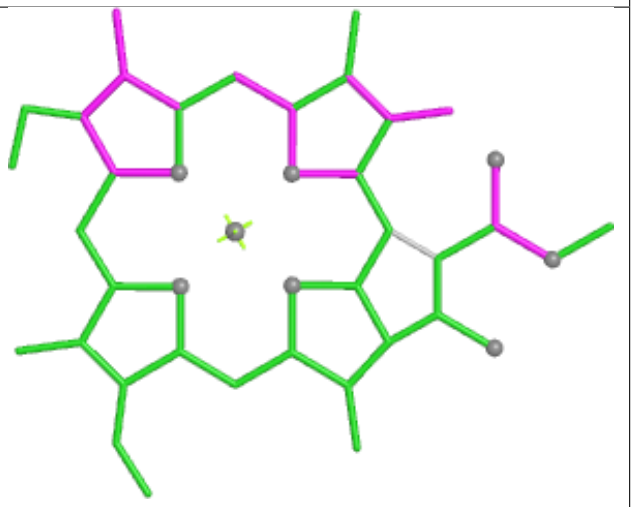


Rings

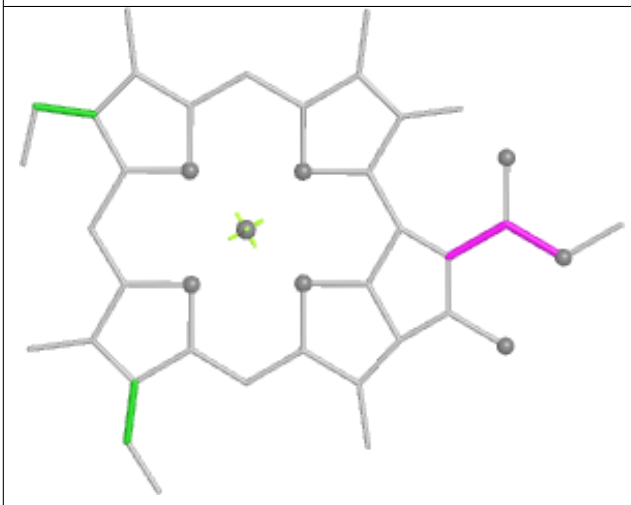
Ligand CLA z 318



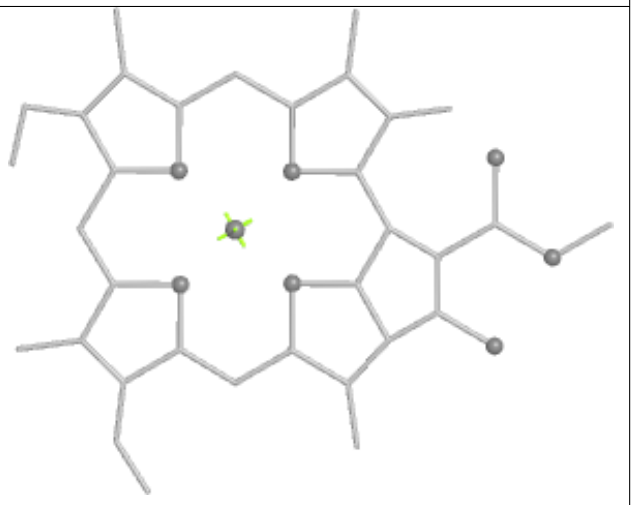
Bond lengths



Bond angles

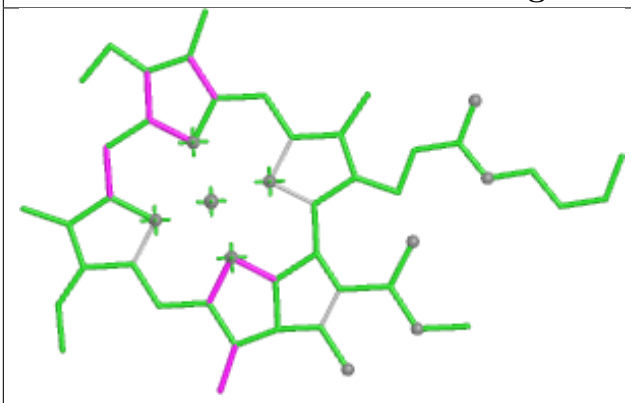


Torsions

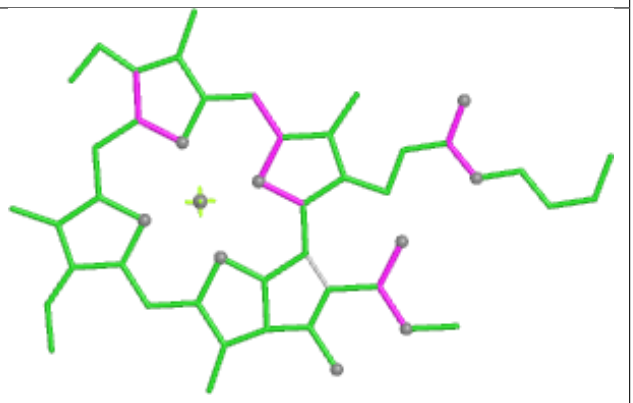


Rings

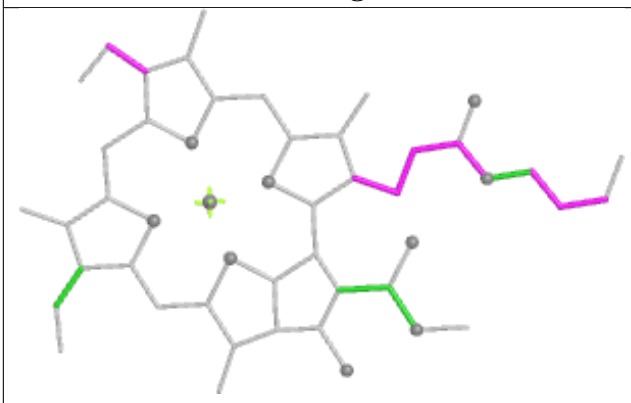
Ligand CLA J 307



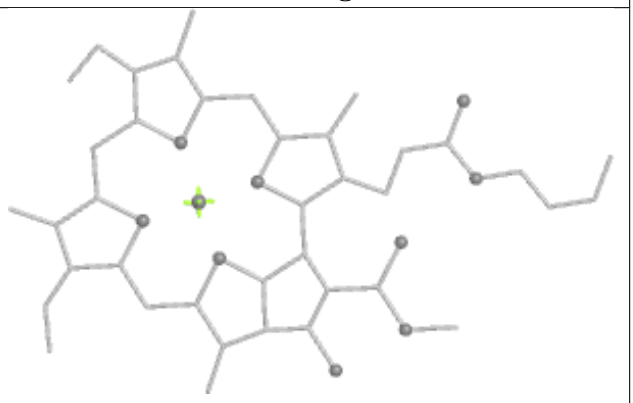
Bond lengths



Bond angles

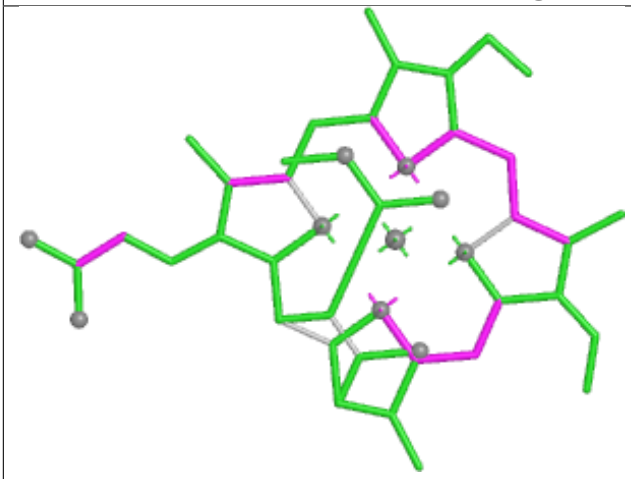


Torsions

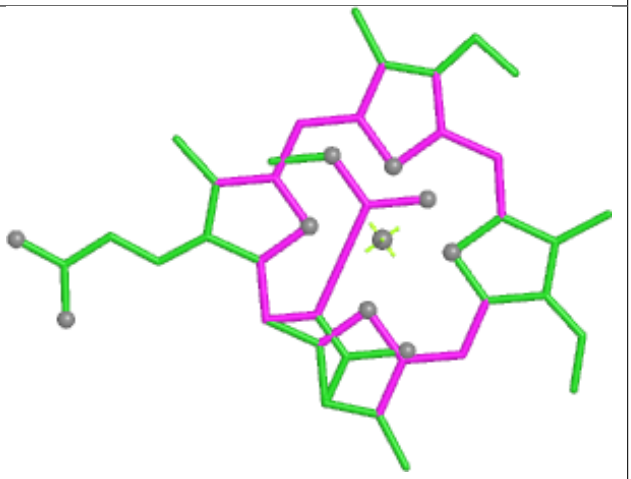


Rings

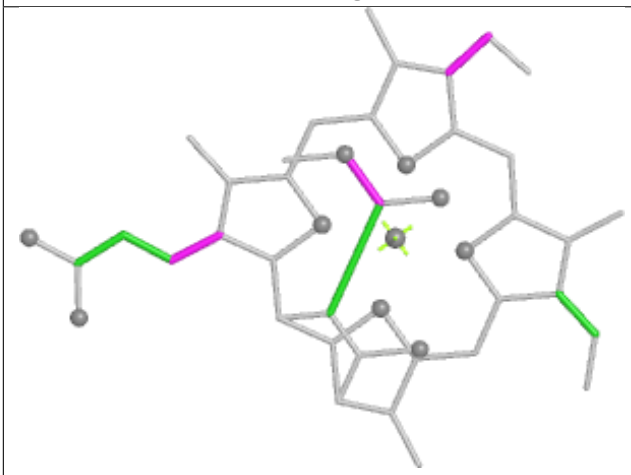
Ligand KC2 9 313



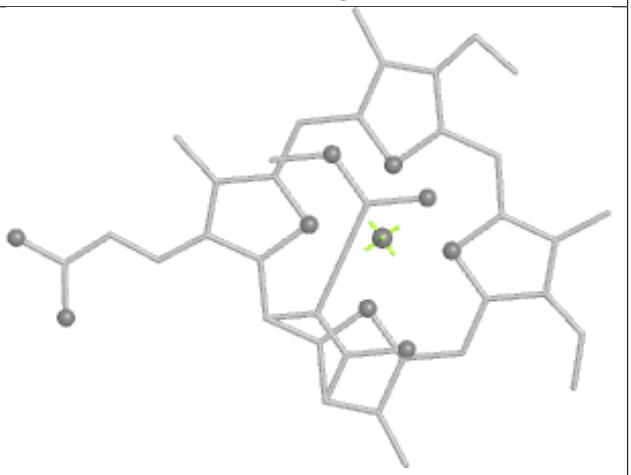
Bond lengths



Bond angles

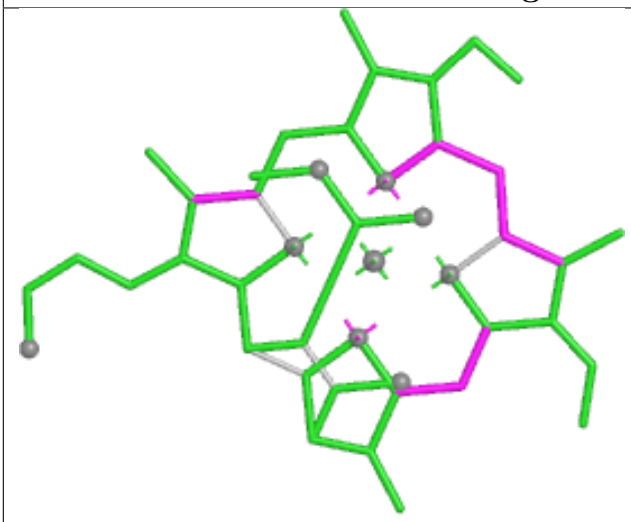


Torsions



Rings

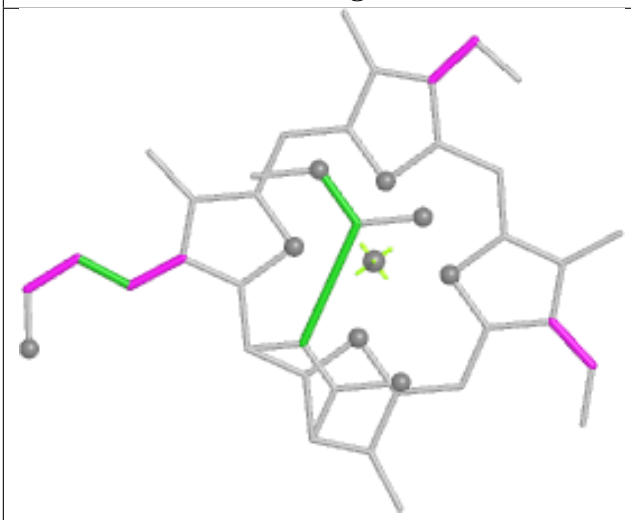
Ligand KC2 M 311



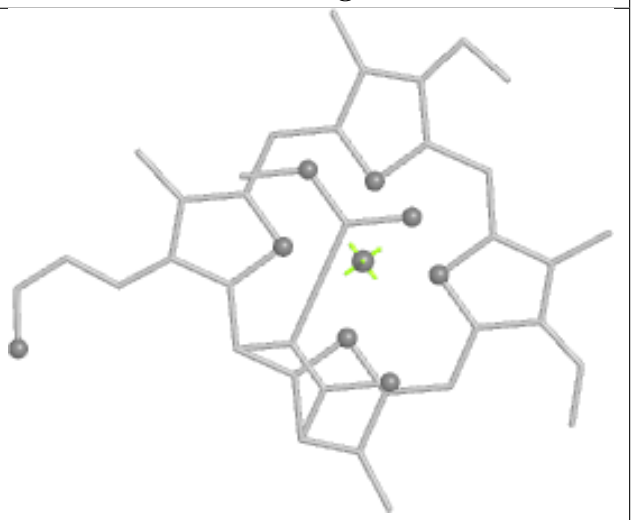
Bond lengths



Bond angles

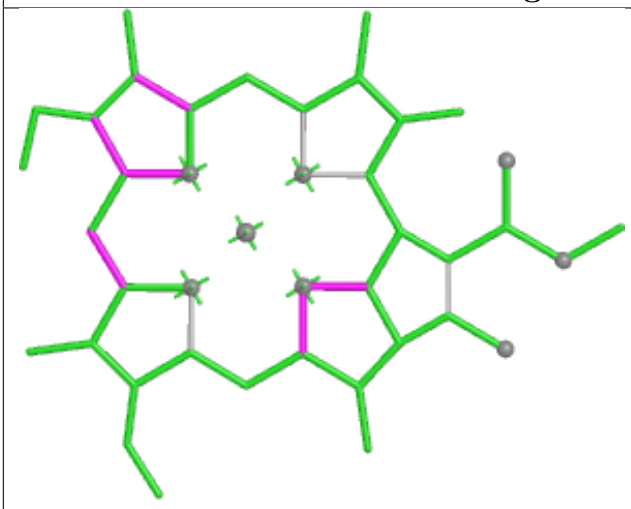


Torsions

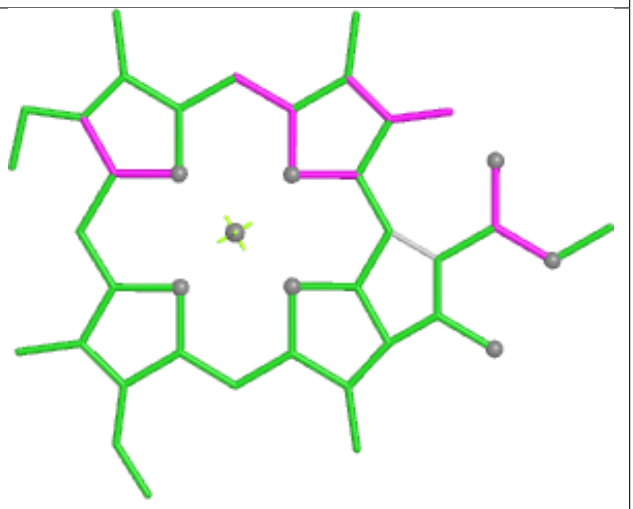


Rings

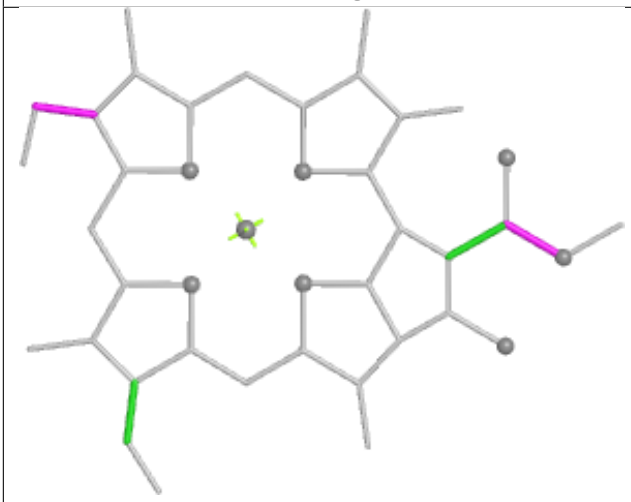
Ligand CLA Y 310



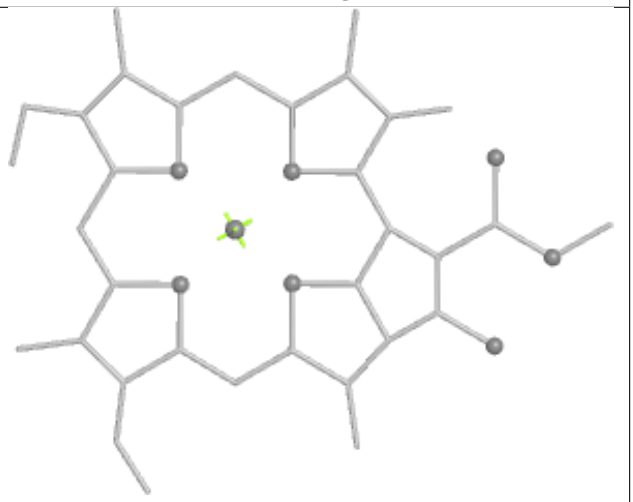
Bond lengths



Bond angles

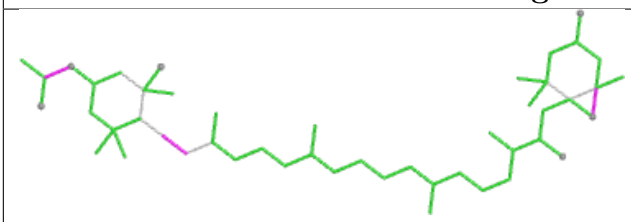


Torsions

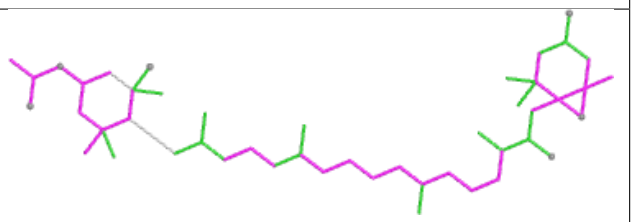


Rings

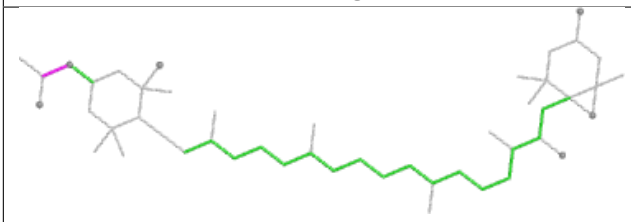
Ligand A86 E 304



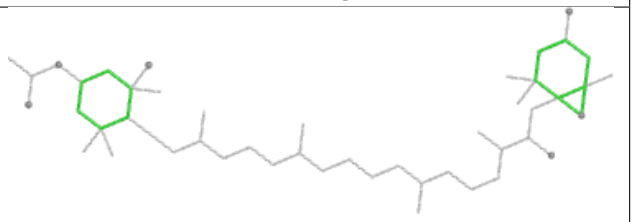
Bond lengths



Bond angles

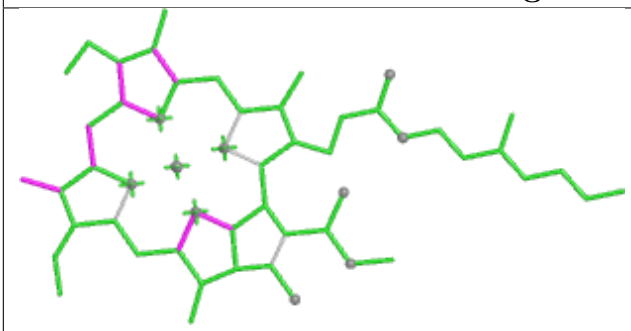


Torsions

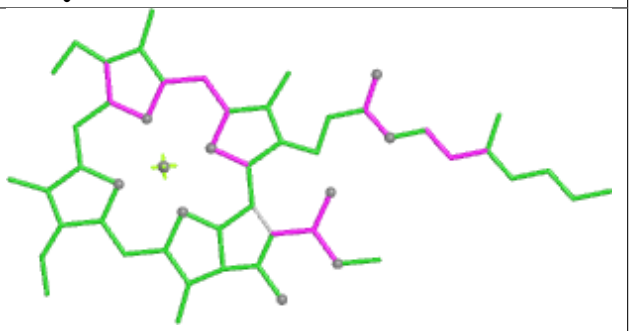


Rings

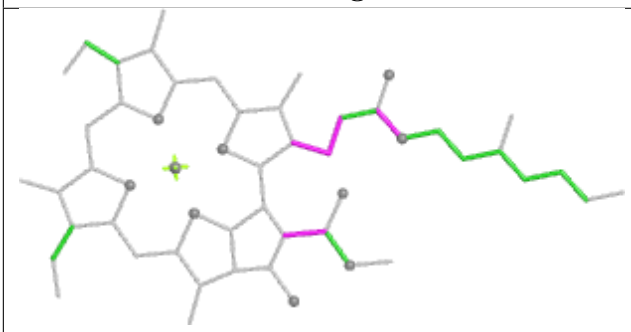
Ligand CLA Q 321



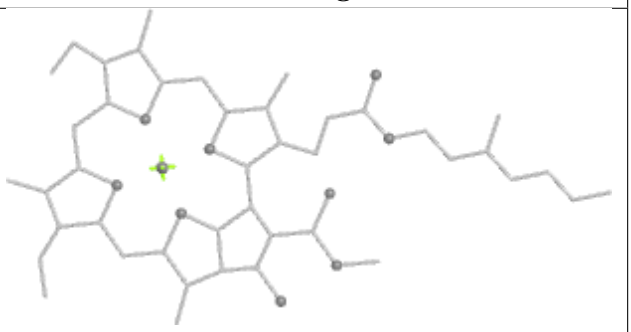
Bond lengths



Bond angles

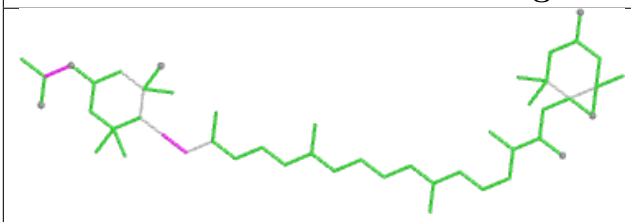


Torsions

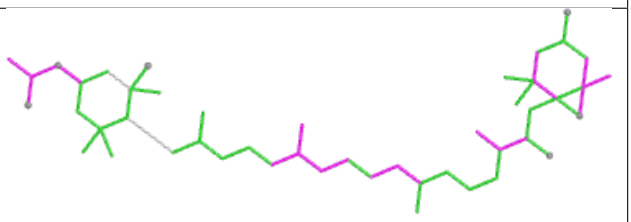


Rings

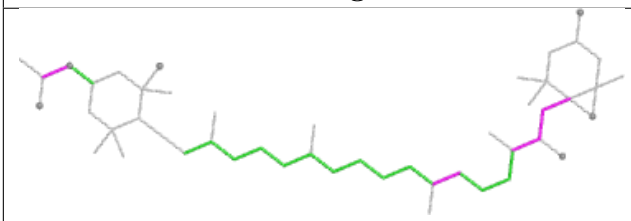
Ligand A86 S 304



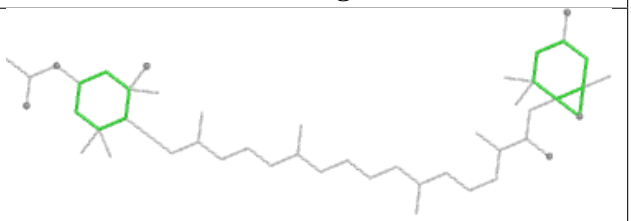
Bond lengths



Bond angles

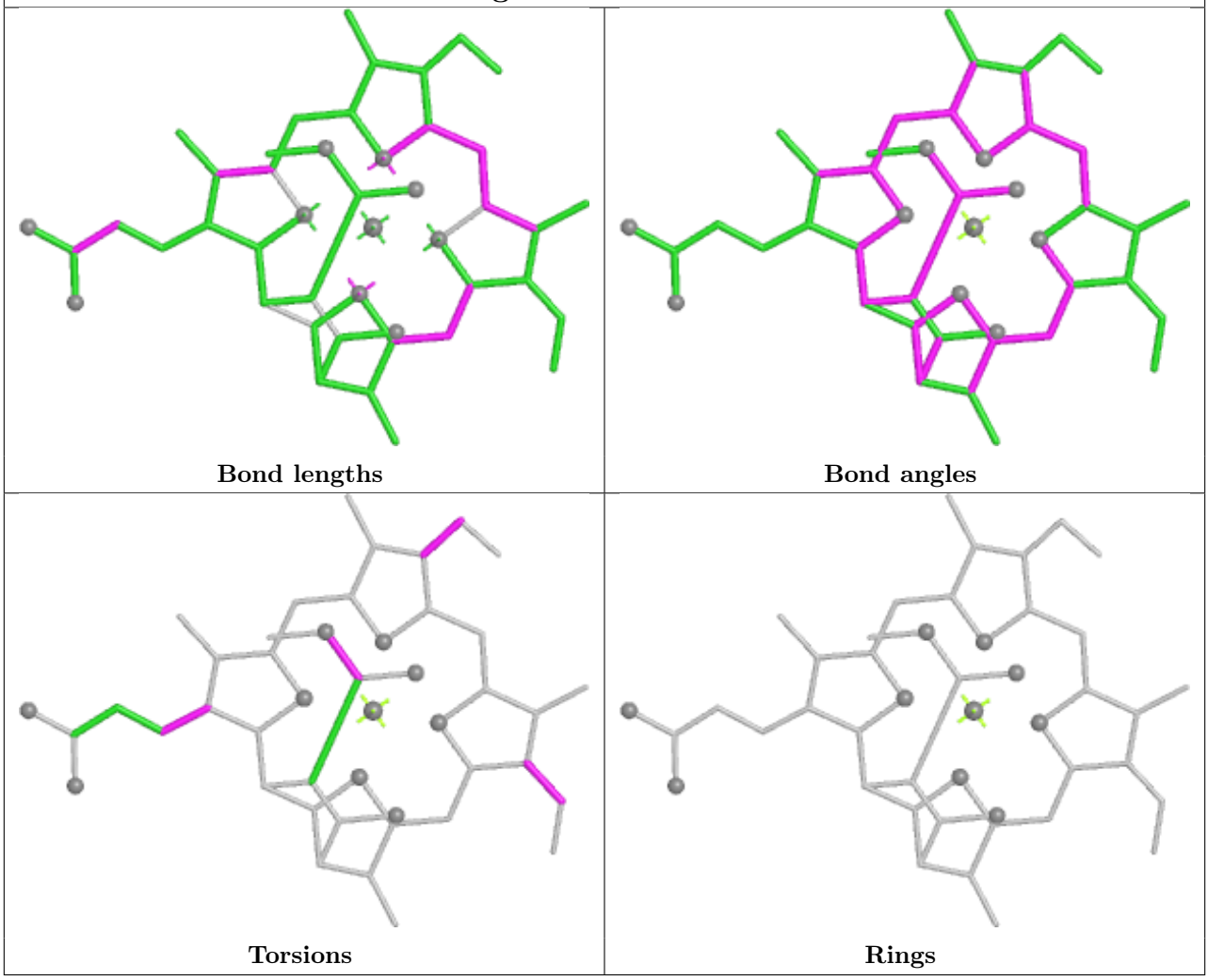


Torsions



Rings

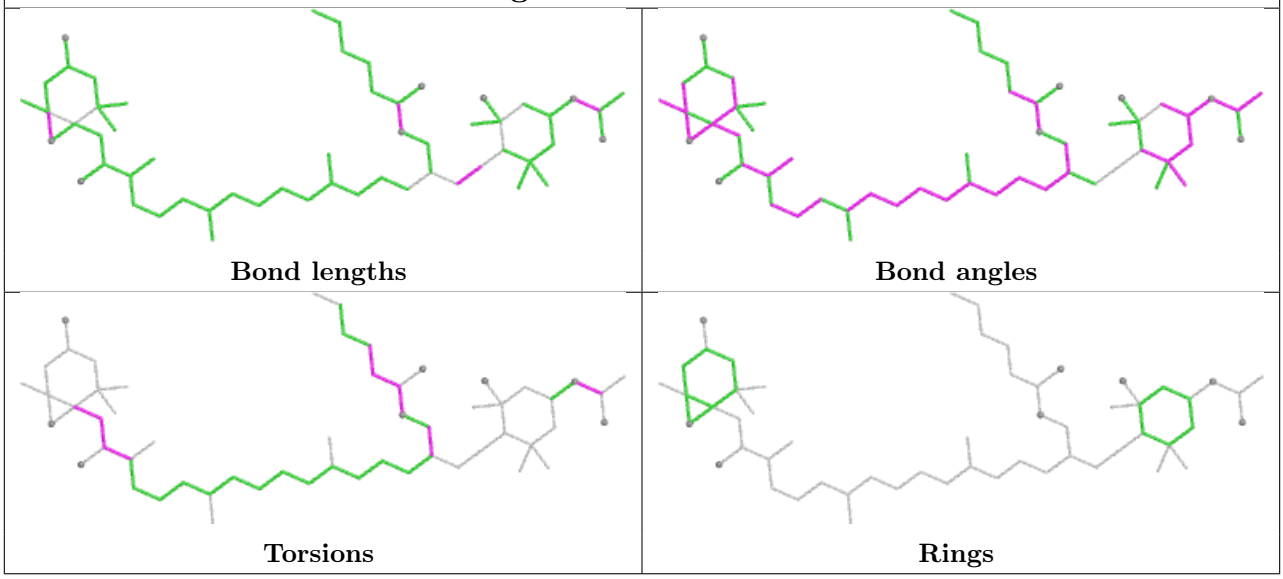
Ligand KC2 M 307



Bond lengths | Bond angles

Torsions | Rings

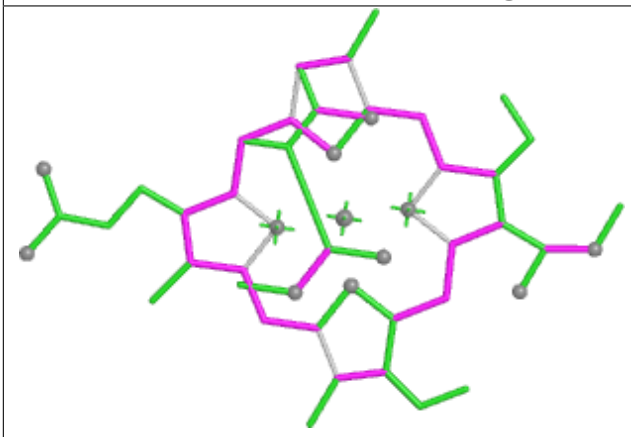
Ligand A1EB1 7 304



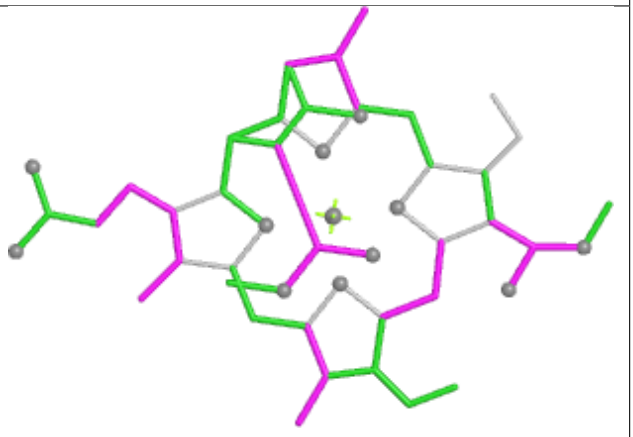
Bond lengths | Bond angles

Torsions | Rings

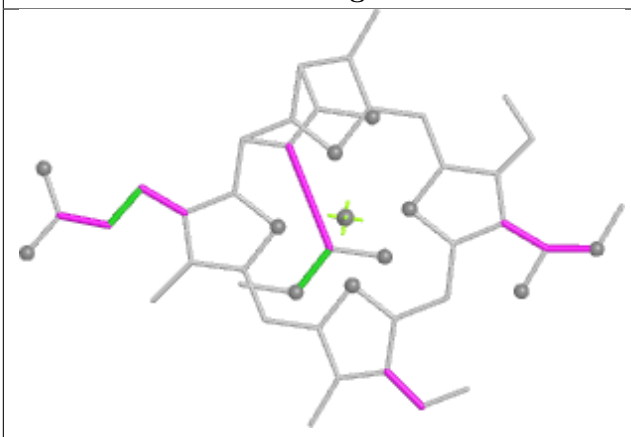
Ligand A1ECV R 310



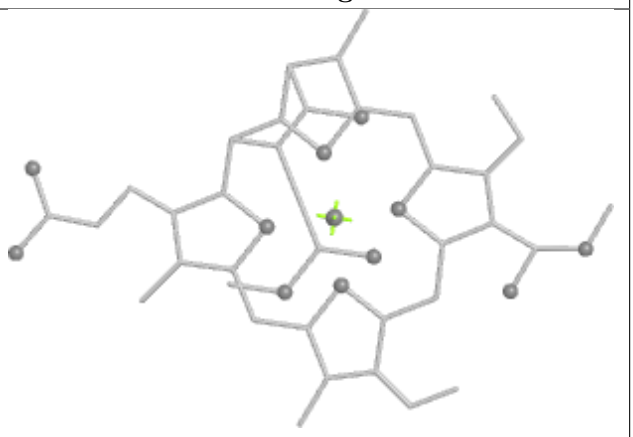
Bond lengths



Bond angles

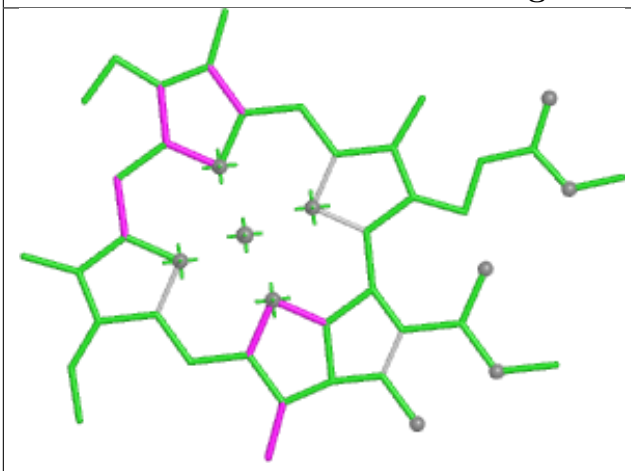


Torsions

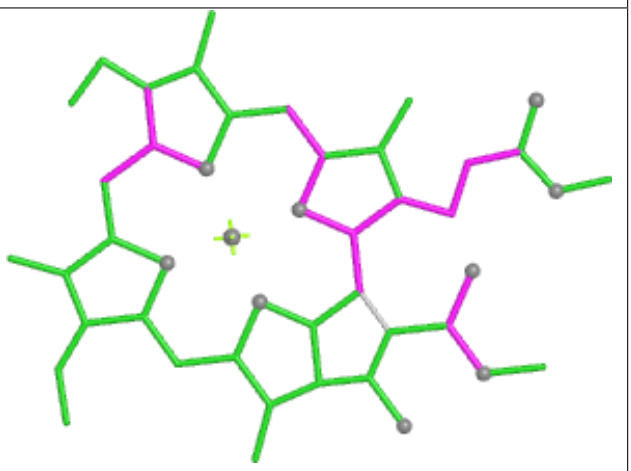


Rings

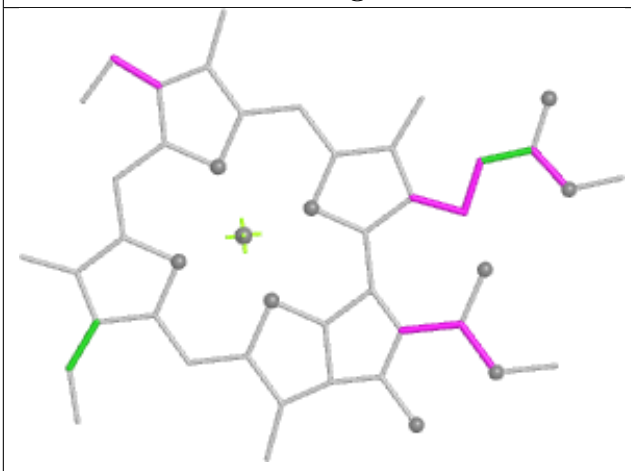
Ligand CLA 2 319



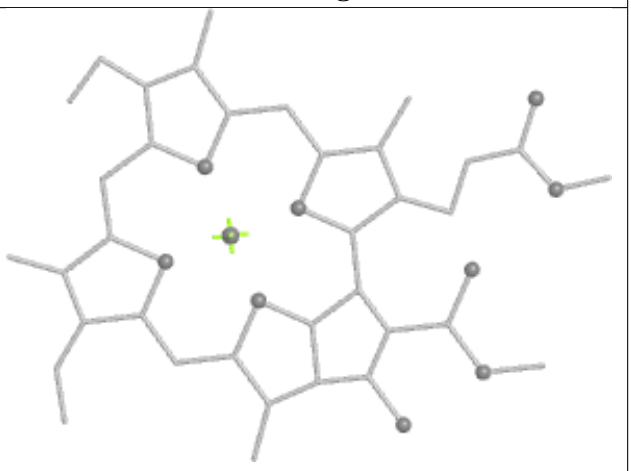
Bond lengths



Bond angles

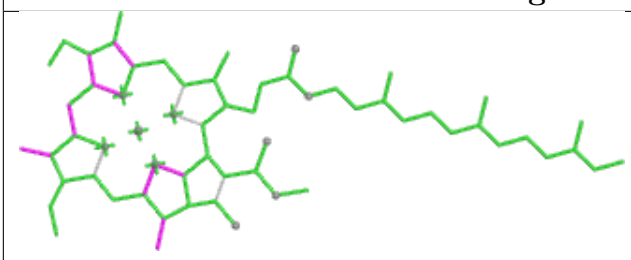


Torsions

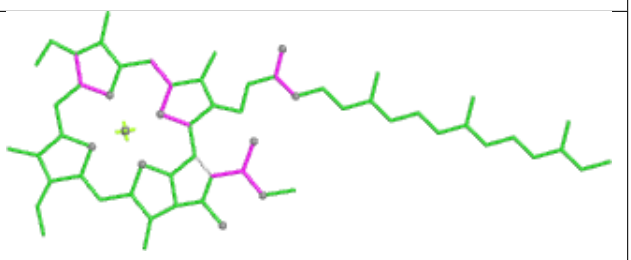


Rings

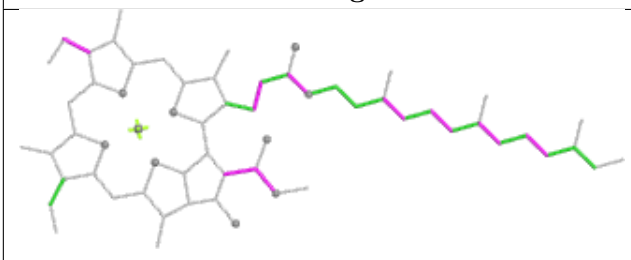
Ligand CLA a 814



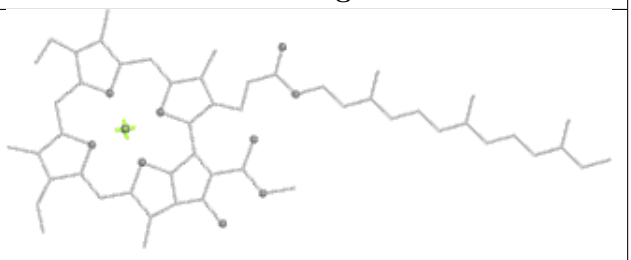
Bond lengths



Bond angles

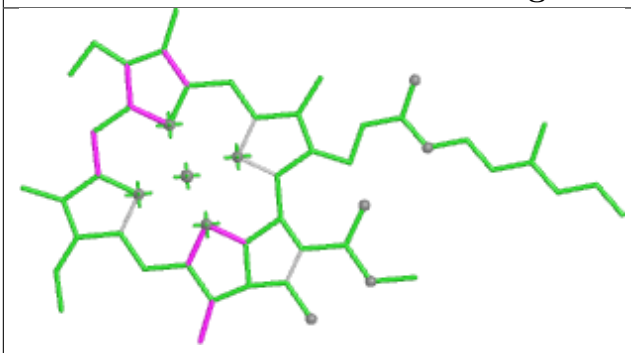


Torsions

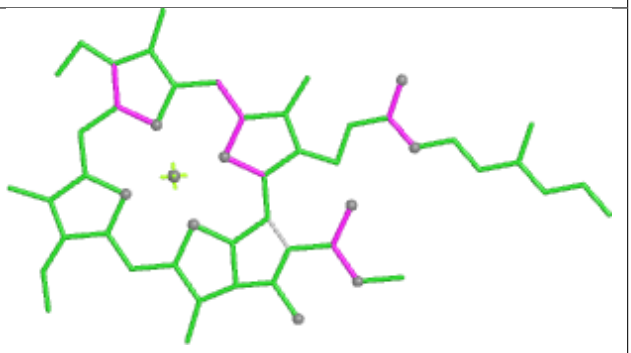


Rings

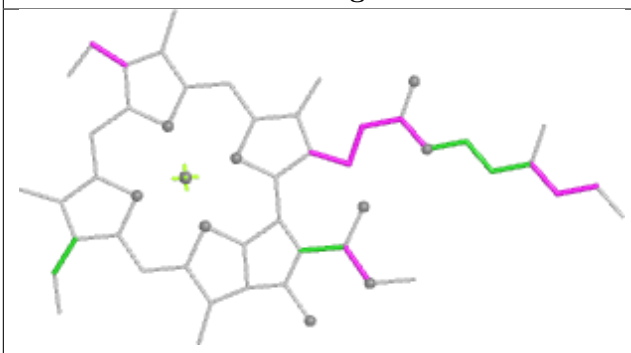
Ligand CLA o 205



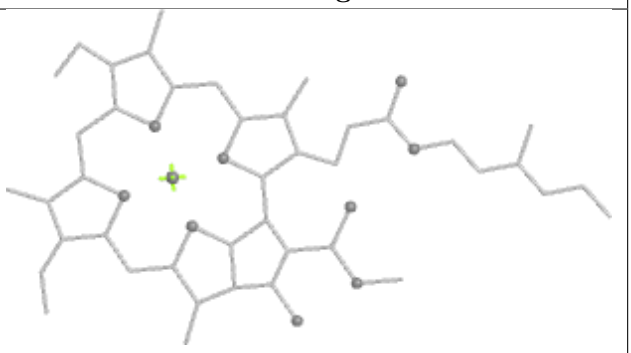
Bond lengths



Bond angles

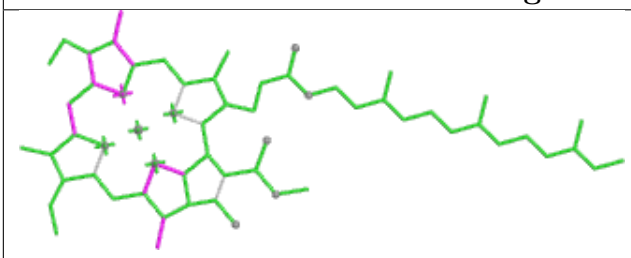


Torsions

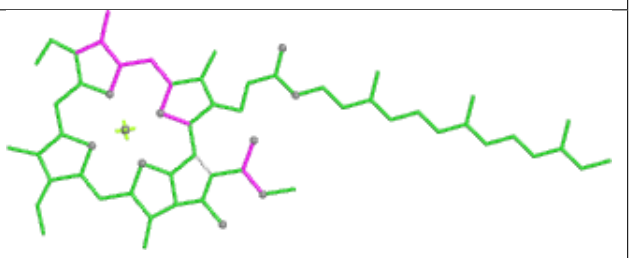


Rings

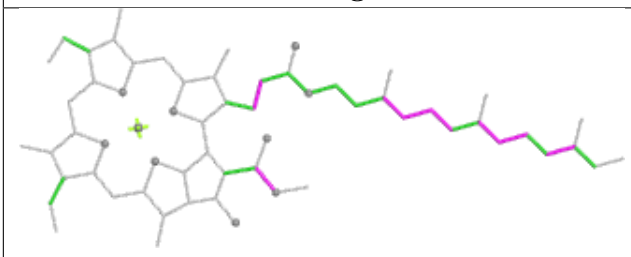
Ligand CLA A 306



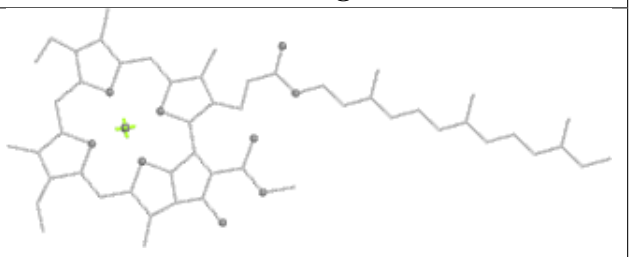
Bond lengths



Bond angles

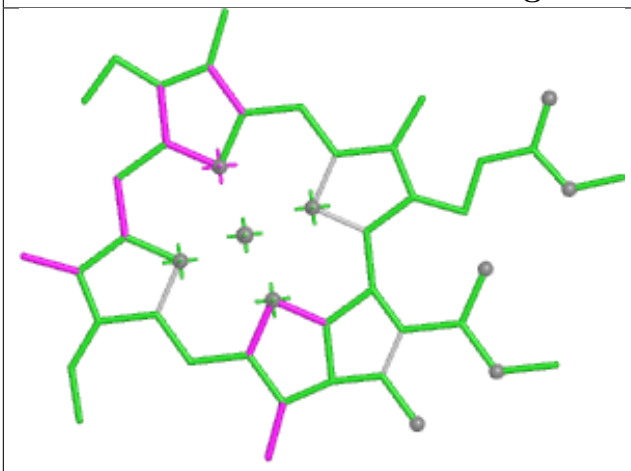


Torsions

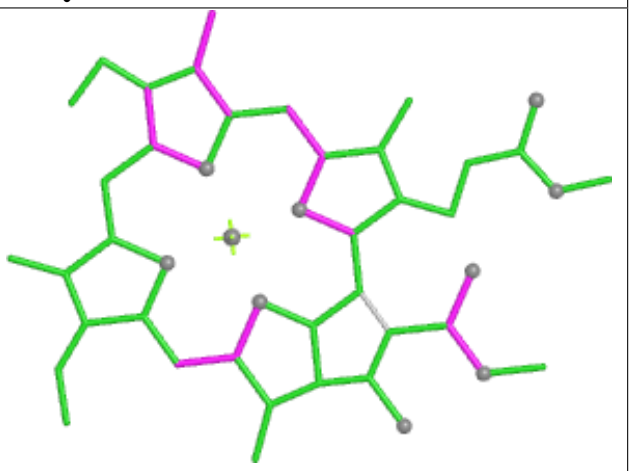


Rings

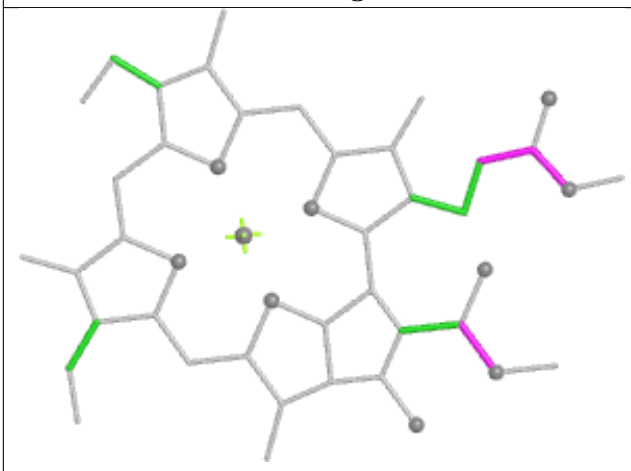
Ligand CLA Q 311



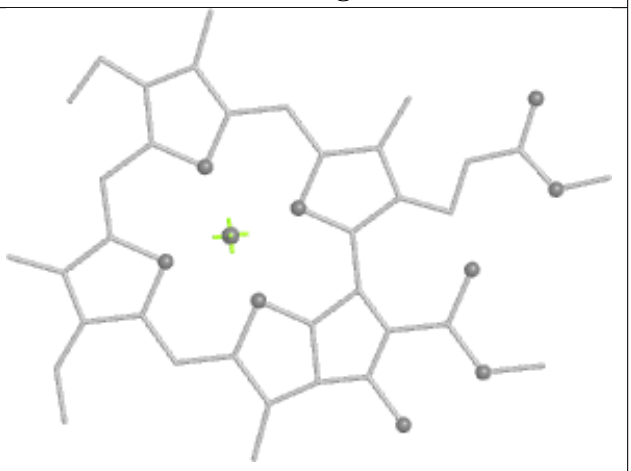
Bond lengths



Bond angles

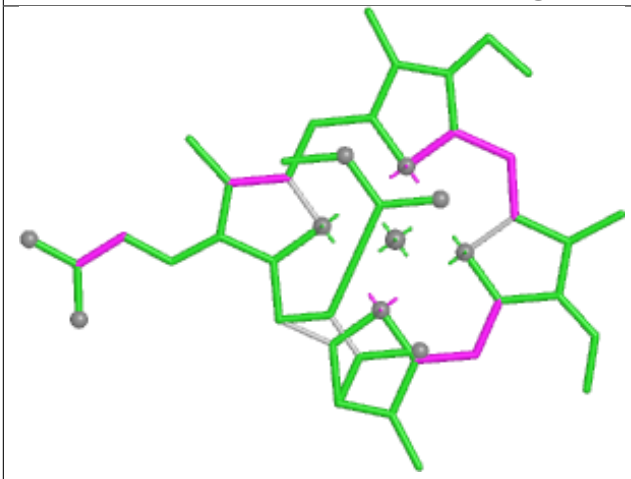


Torsions

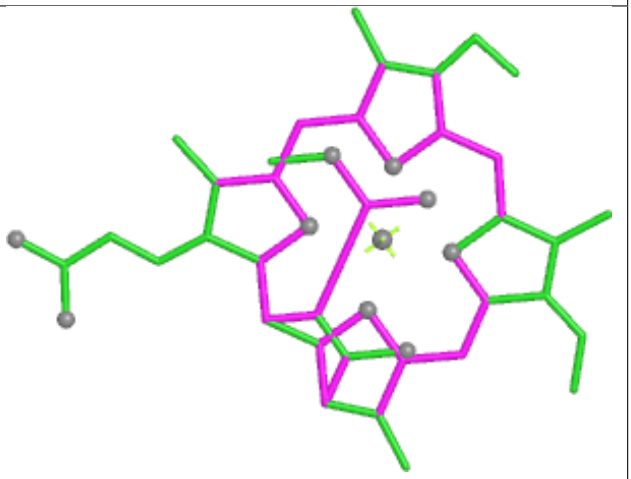


Rings

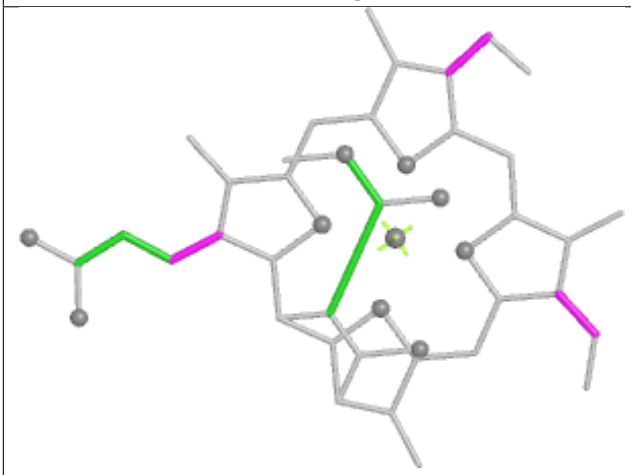
Ligand KC2 x 313



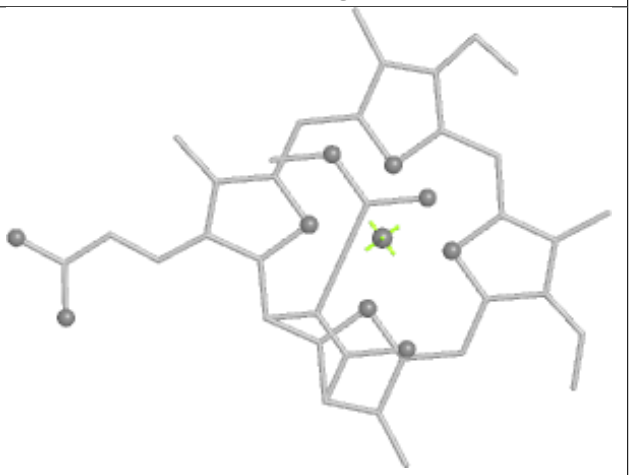
Bond lengths



Bond angles

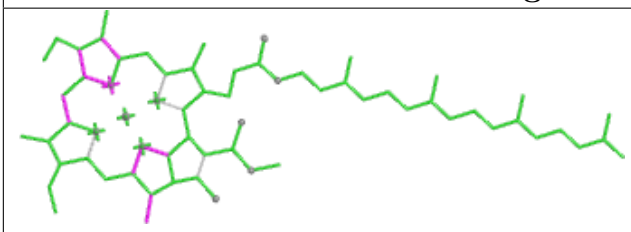


Torsions

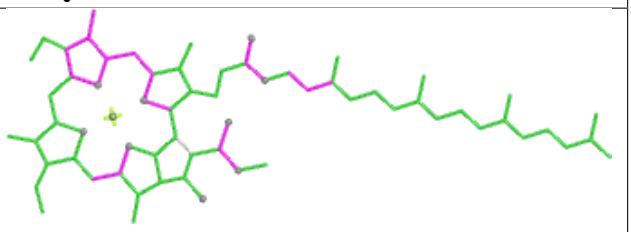


Rings

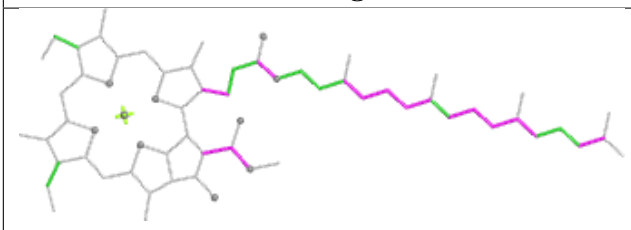
Ligand CLA Q 310



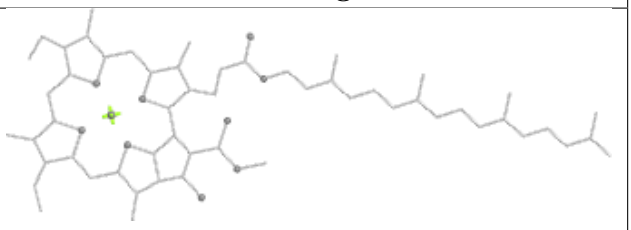
Bond lengths



Bond angles

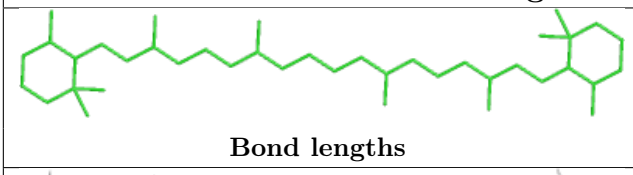


Torsions

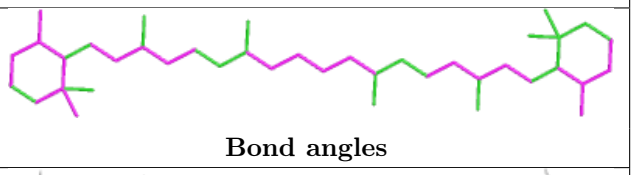


Rings

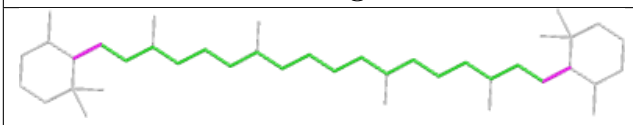
Ligand BCR a 842



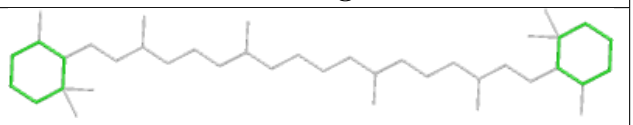
Bond lengths



Bond angles

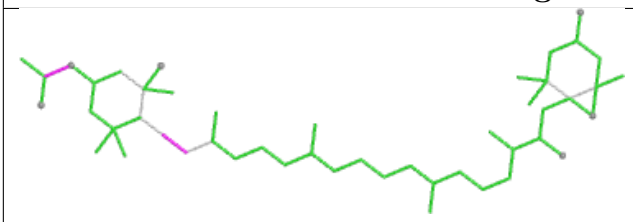


Torsions

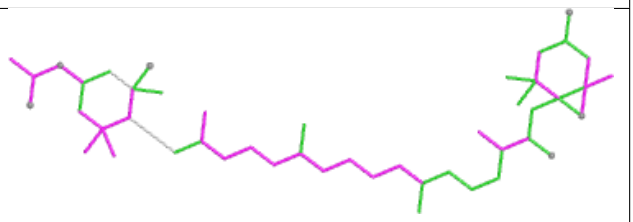


Rings

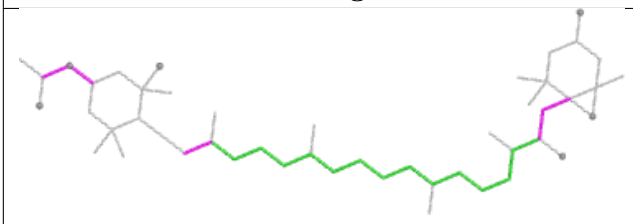
Ligand A86 0 309



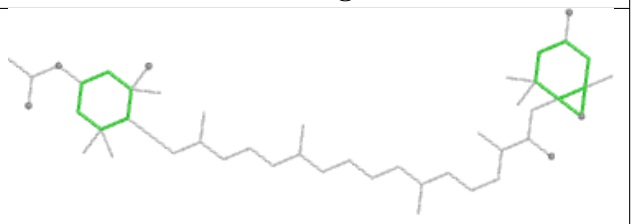
Bond lengths



Bond angles

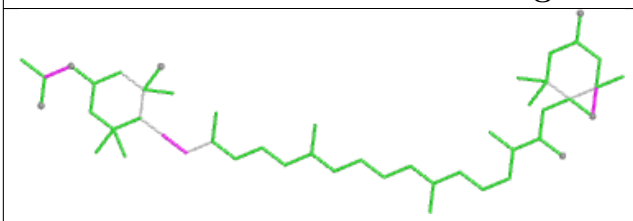


Torsions

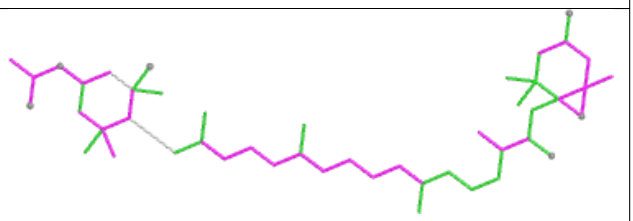


Rings

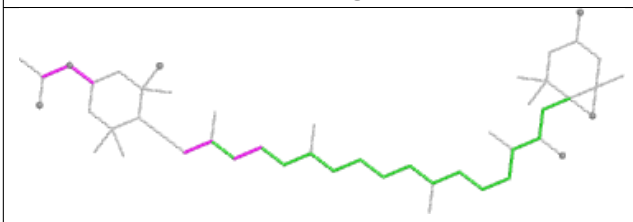
Ligand A86 3 308



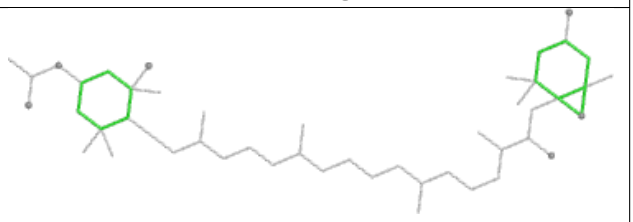
Bond lengths



Bond angles

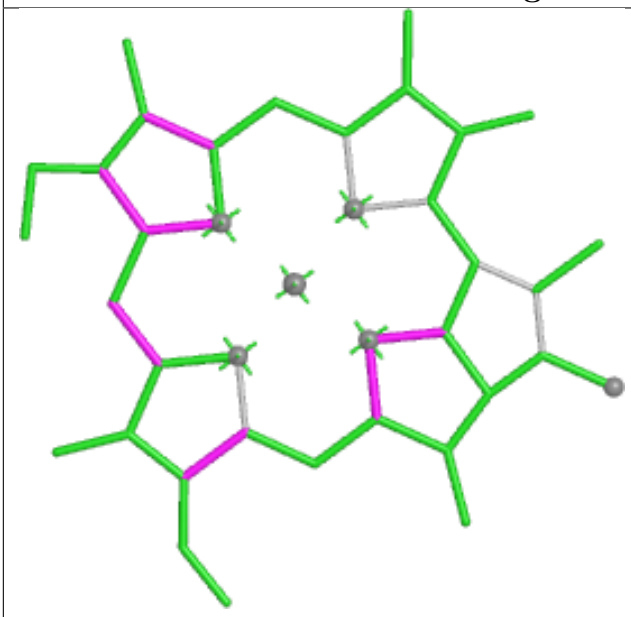


Torsions

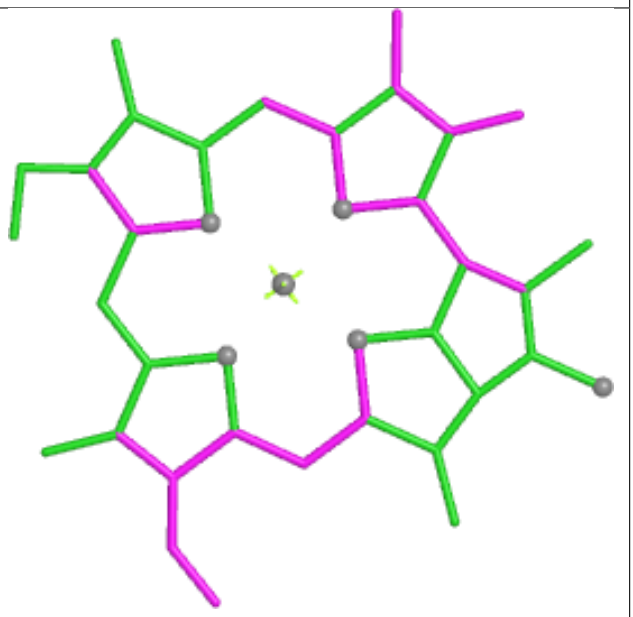


Rings

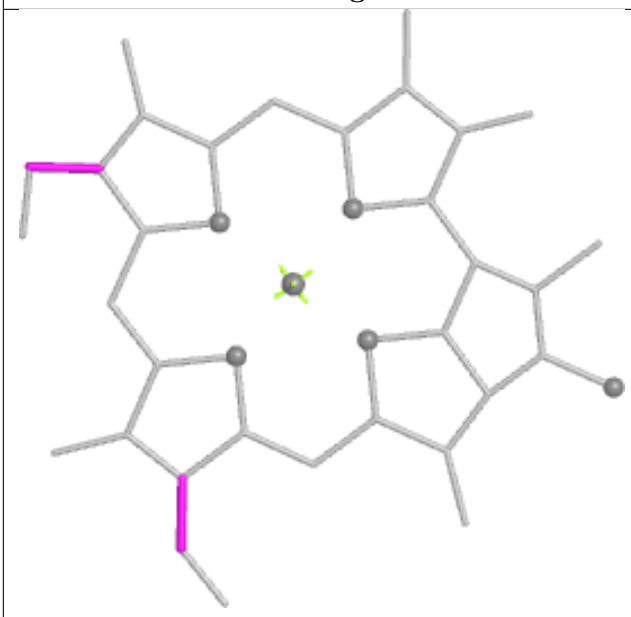
Ligand CLA O 308



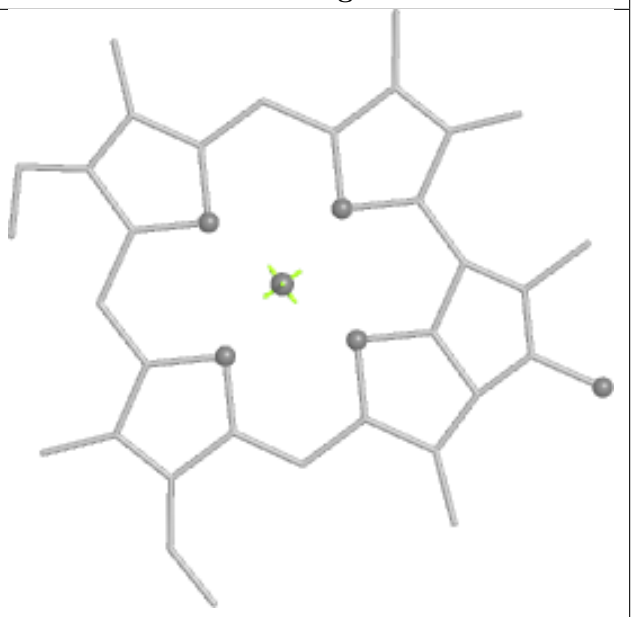
Bond lengths



Bond angles

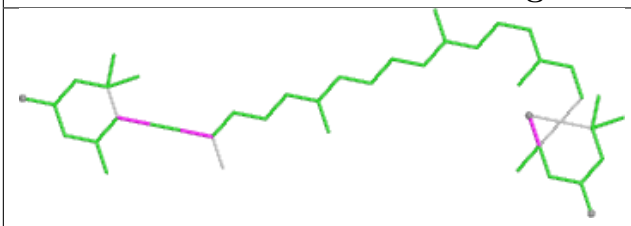


Torsions

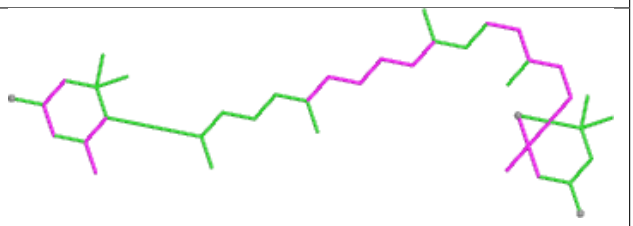


Rings

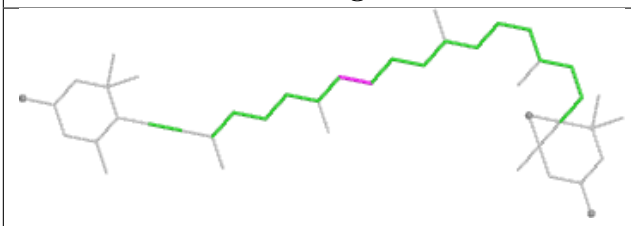
Ligand DD6 E 303



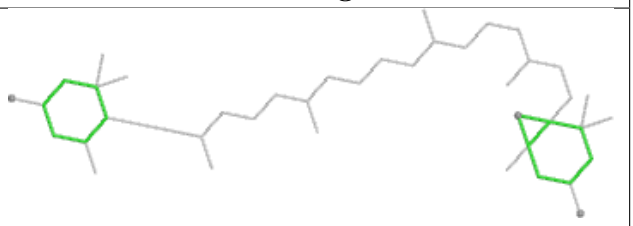
Bond lengths



Bond angles

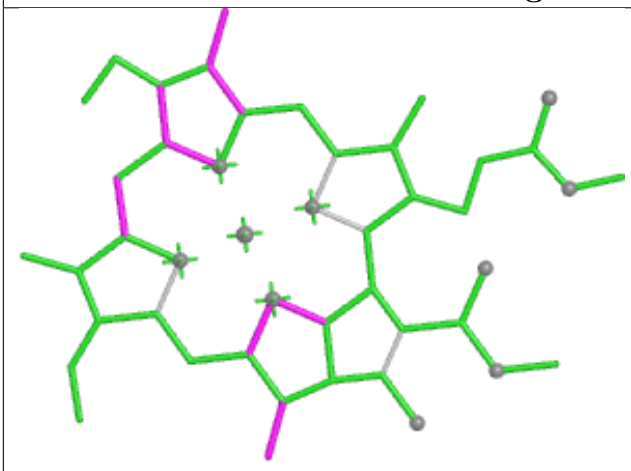


Torsions

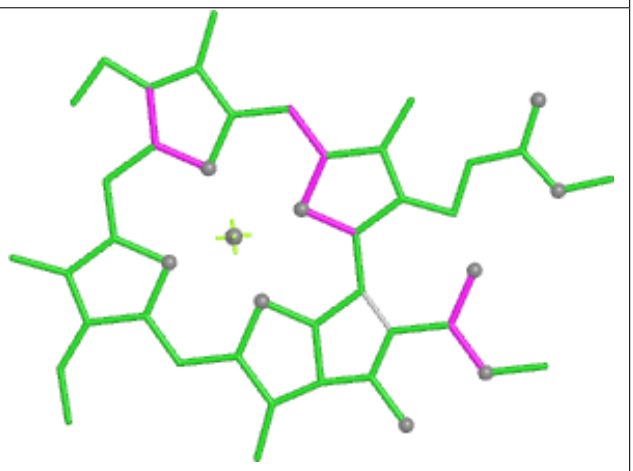


Rings

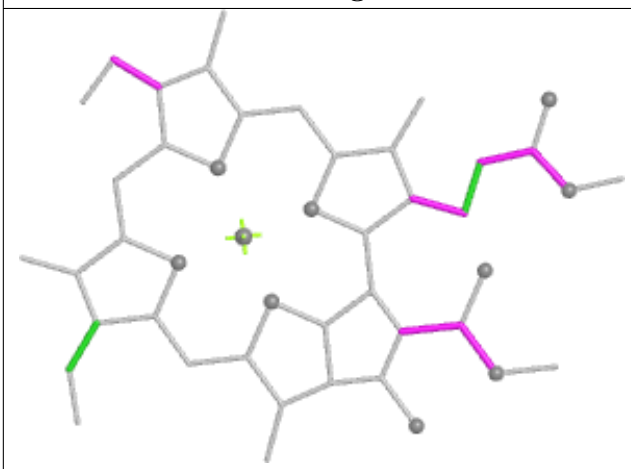
Ligand CLA E 315



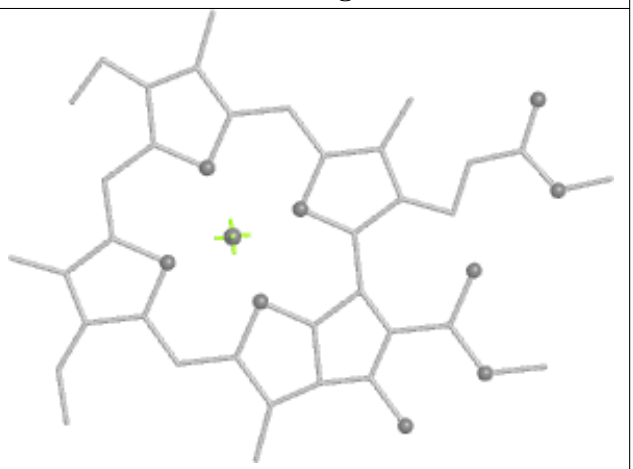
Bond lengths



Bond angles

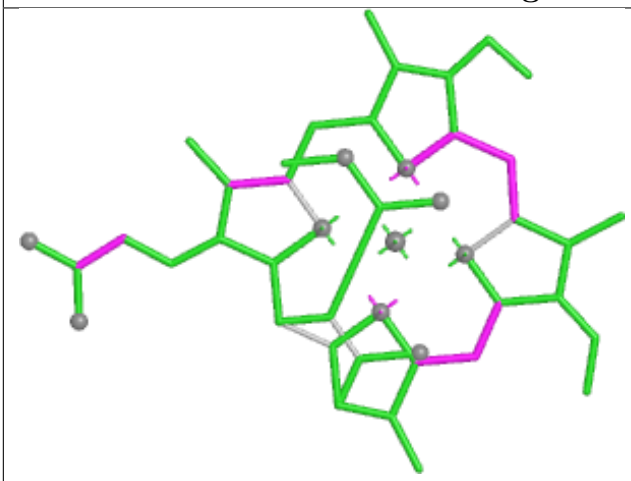


Torsions

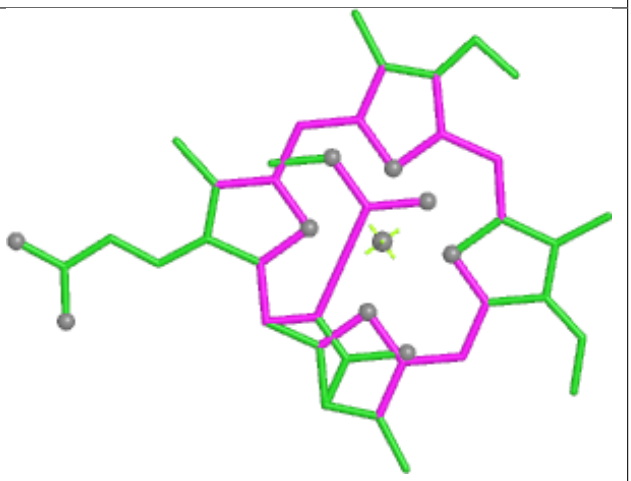


Rings

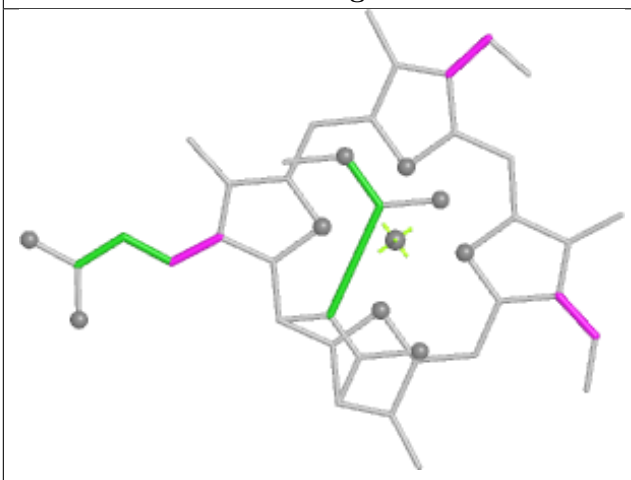
Ligand KC2 M 313



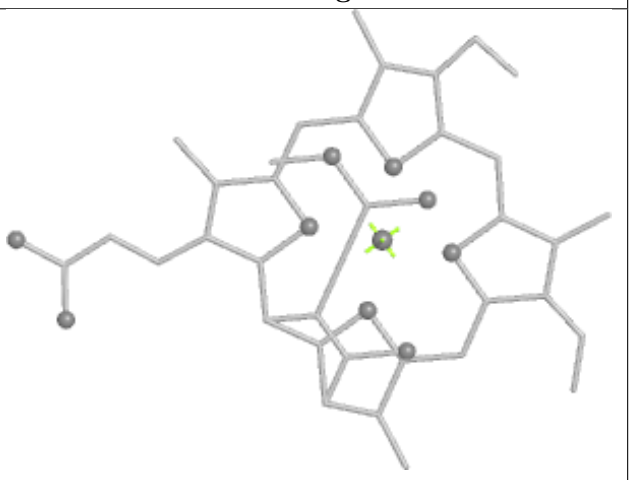
Bond lengths



Bond angles

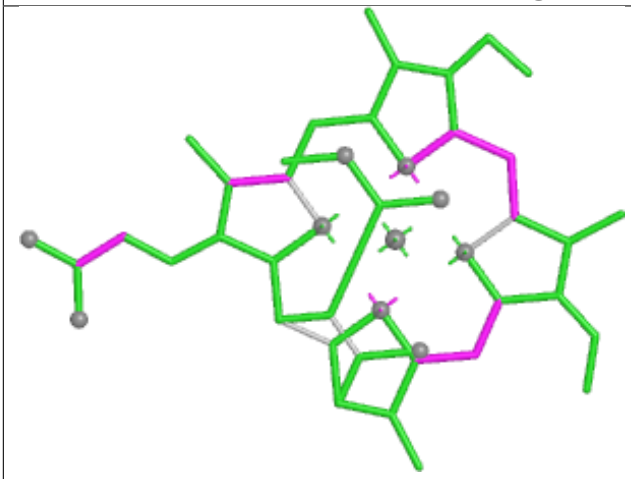


Torsions

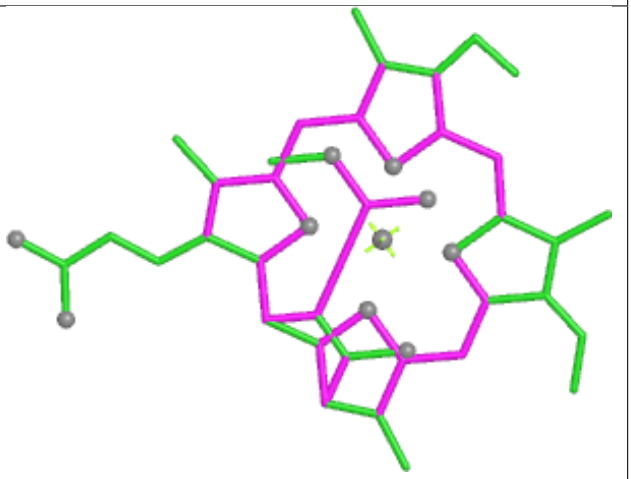


Rings

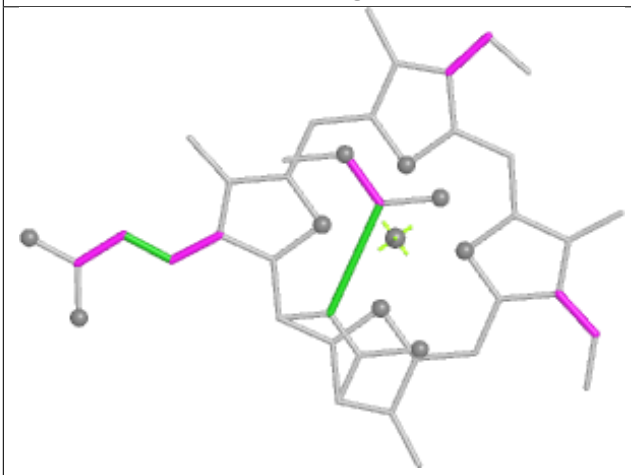
Ligand KC2 6 316



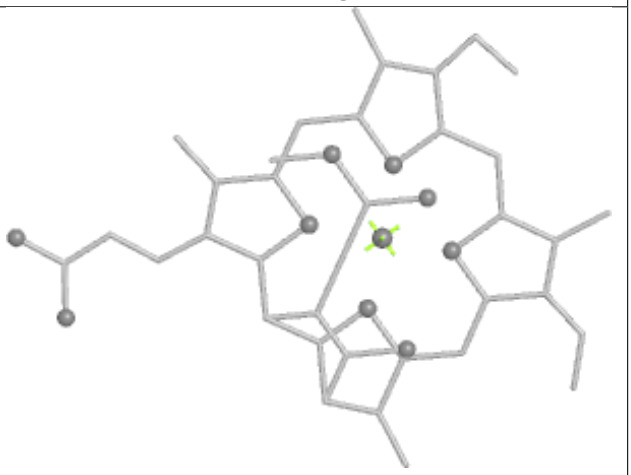
Bond lengths



Bond angles

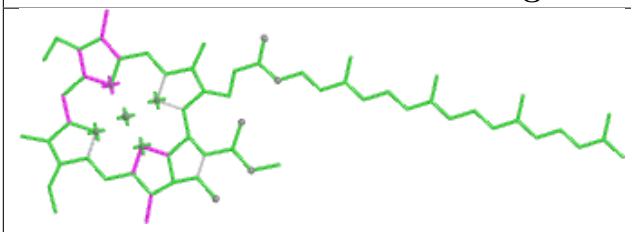


Torsions

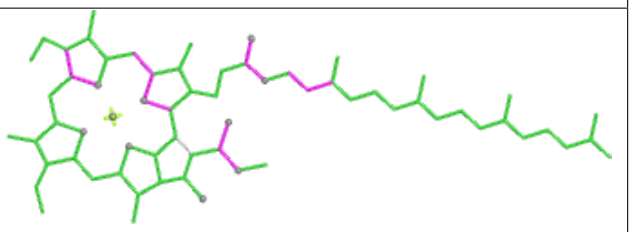


Rings

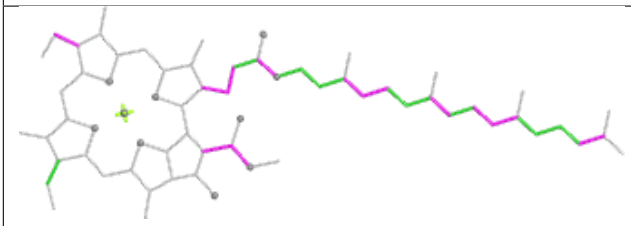
Ligand CLA H 312



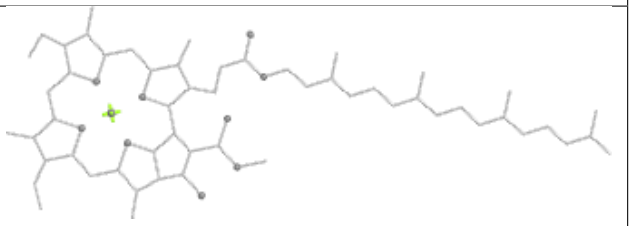
Bond lengths



Bond angles

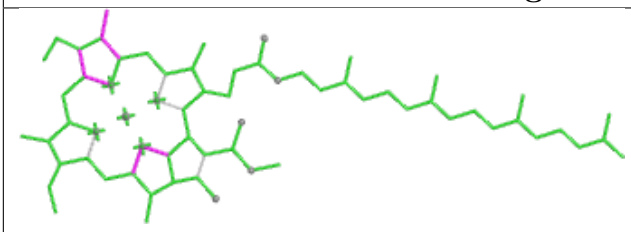


Torsions

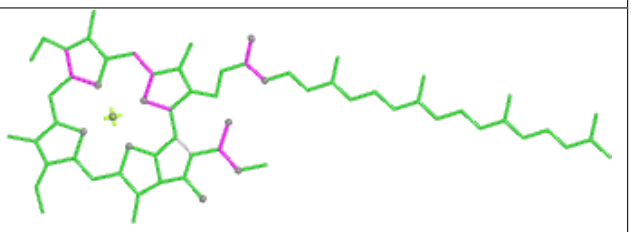


Rings

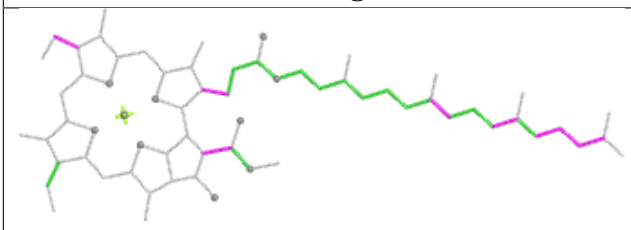
Ligand CLA P 311



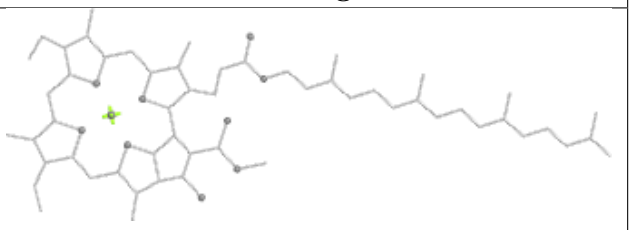
Bond lengths



Bond angles

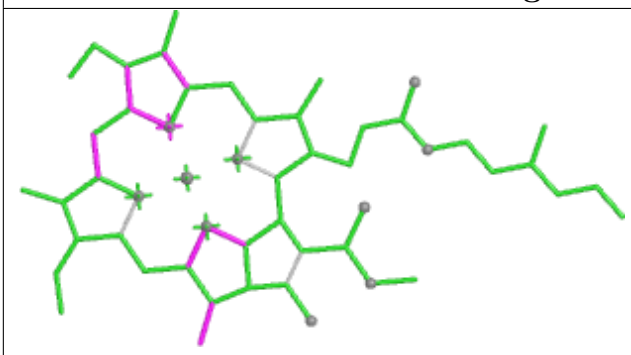


Torsions

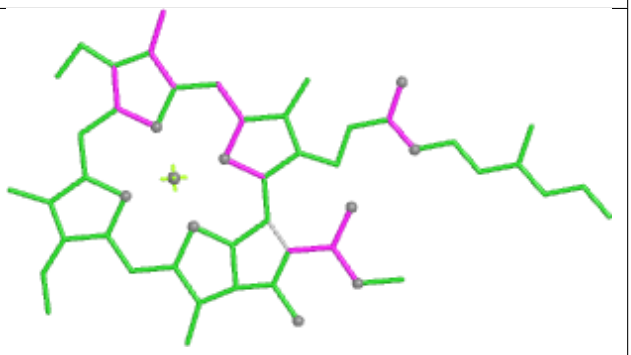


Rings

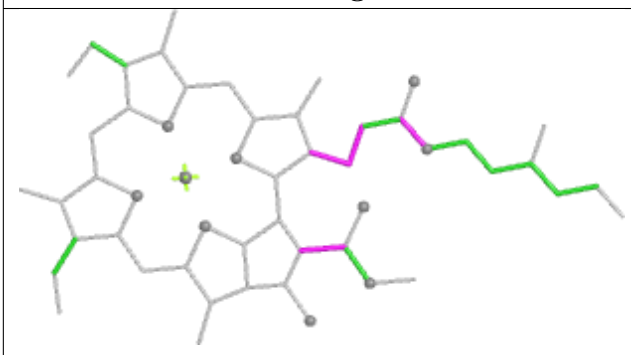
Ligand CLA U 209



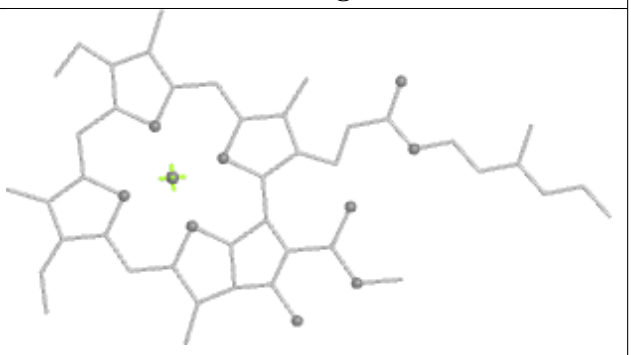
Bond lengths



Bond angles

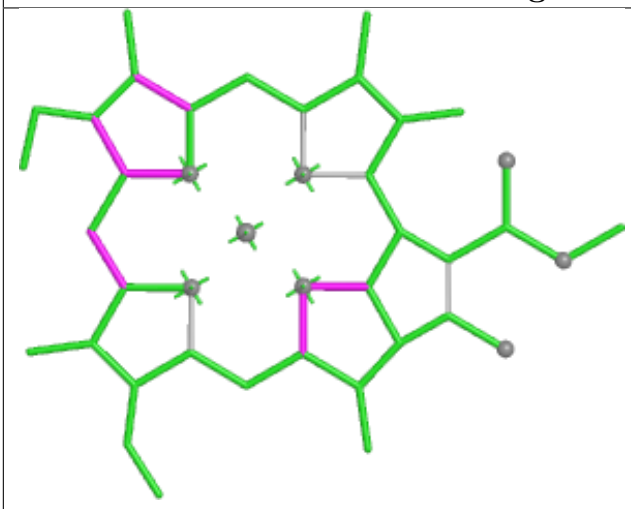


Torsions

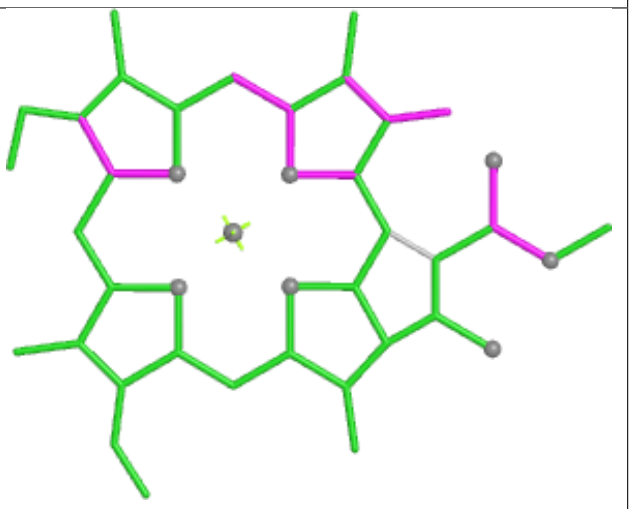


Rings

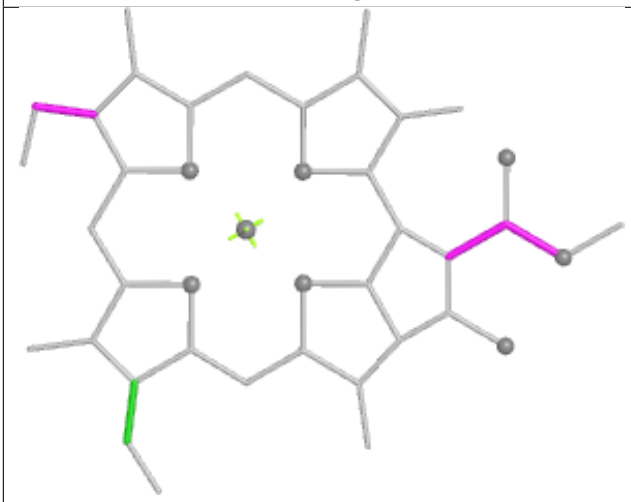
Ligand CLA 1 317



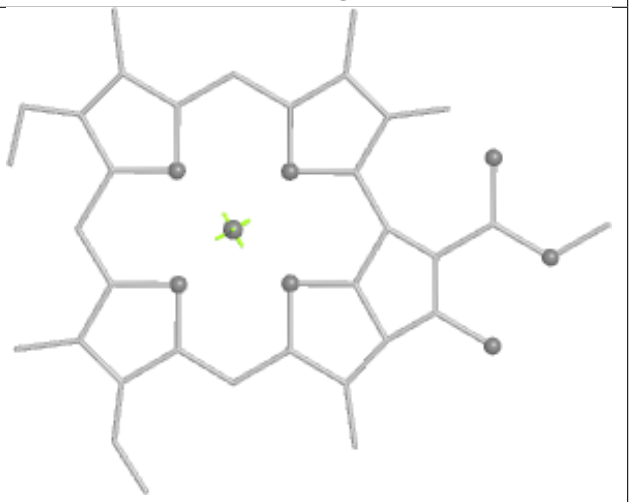
Bond lengths



Bond angles

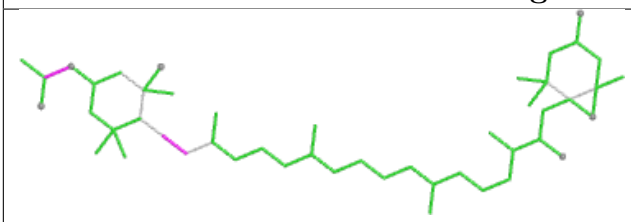


Torsions

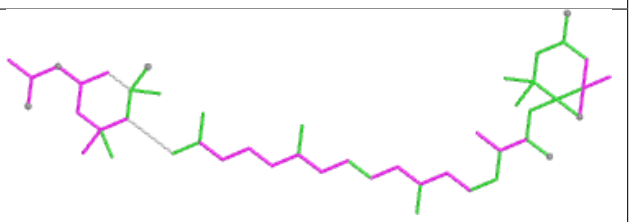


Rings

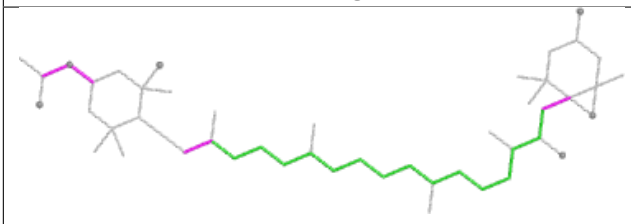
Ligand A86 C 303



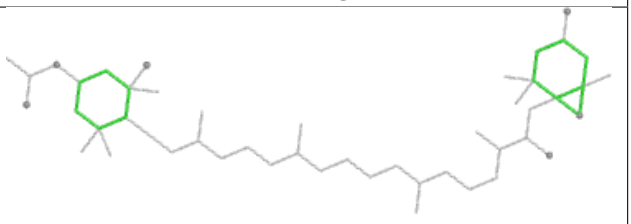
Bond lengths



Bond angles

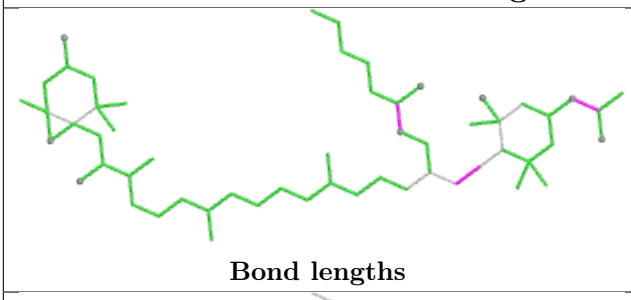


Torsions

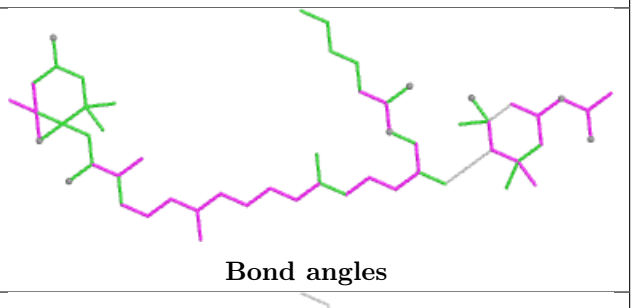


Rings

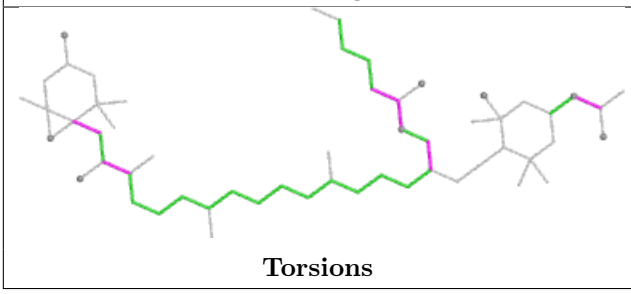
Ligand A1EB1 4 301



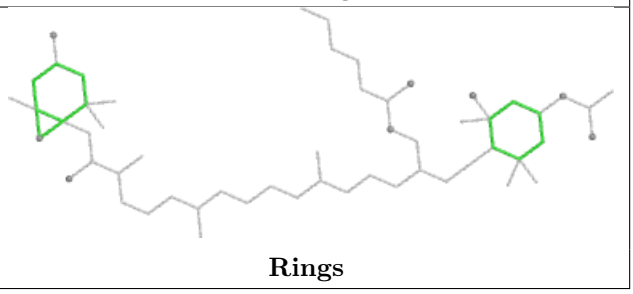
Bond lengths



Bond angles

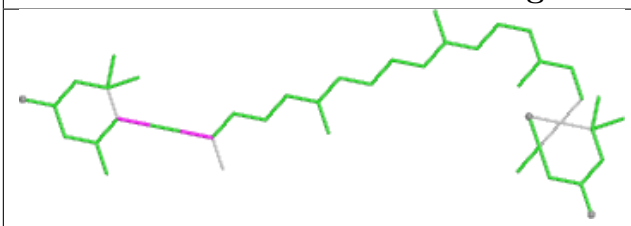


Torsions

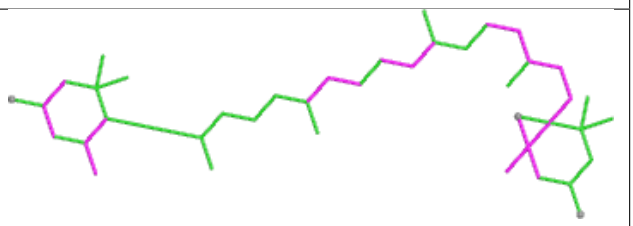


Rings

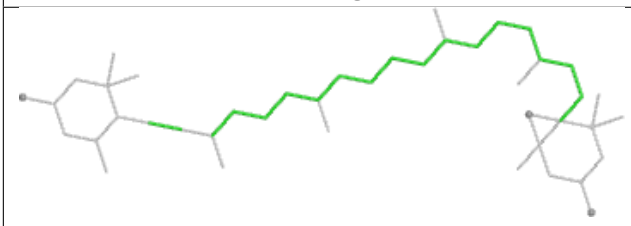
Ligand DD6 F 303



Bond lengths



Bond angles

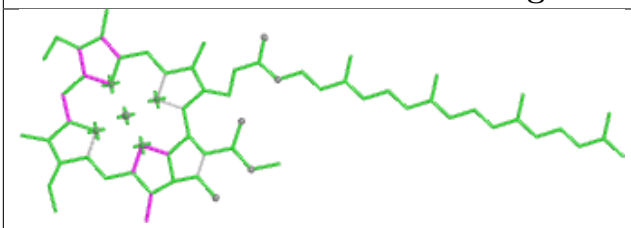


Torsions

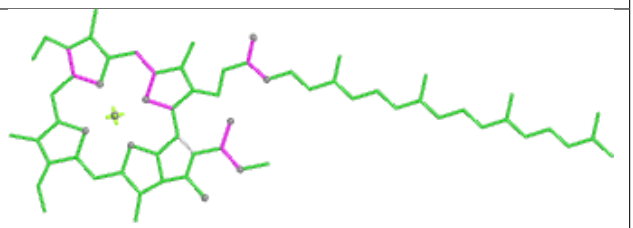


Rings

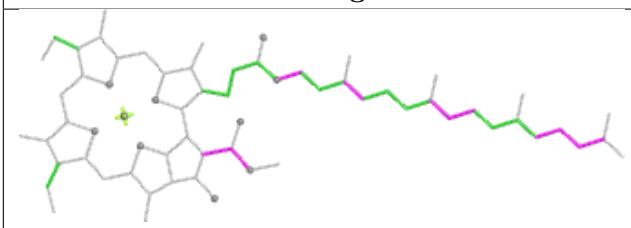
Ligand CLA b 803



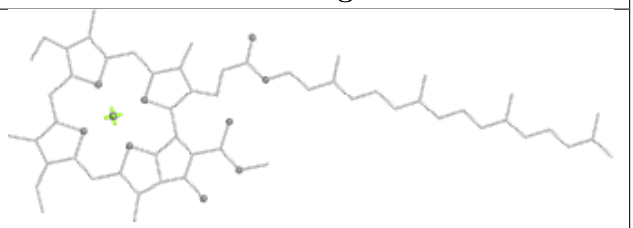
Bond lengths



Bond angles

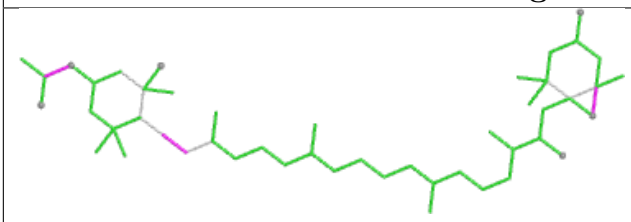


Torsions

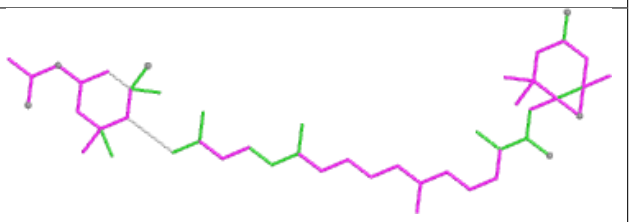


Rings

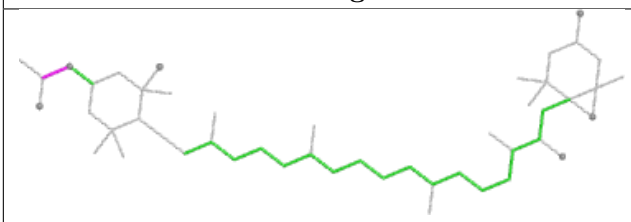
Ligand A86 O 302



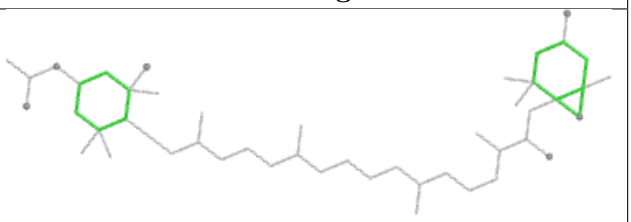
Bond lengths



Bond angles

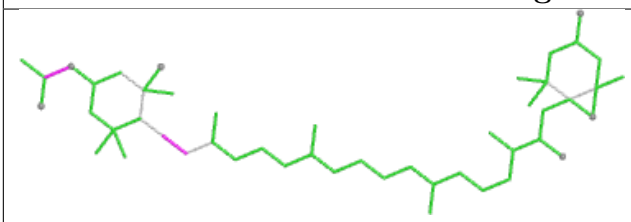


Torsions

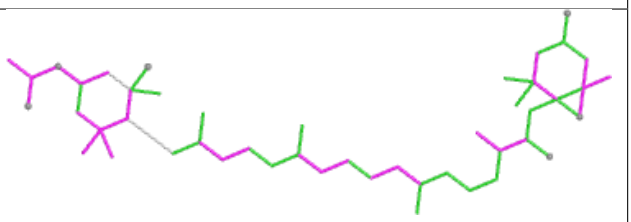


Rings

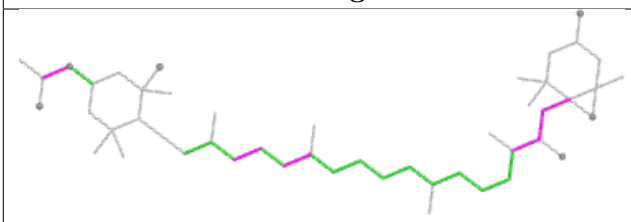
Ligand A86 6 305



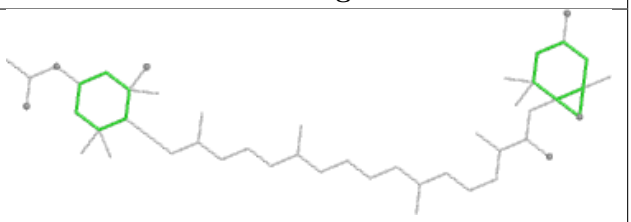
Bond lengths



Bond angles

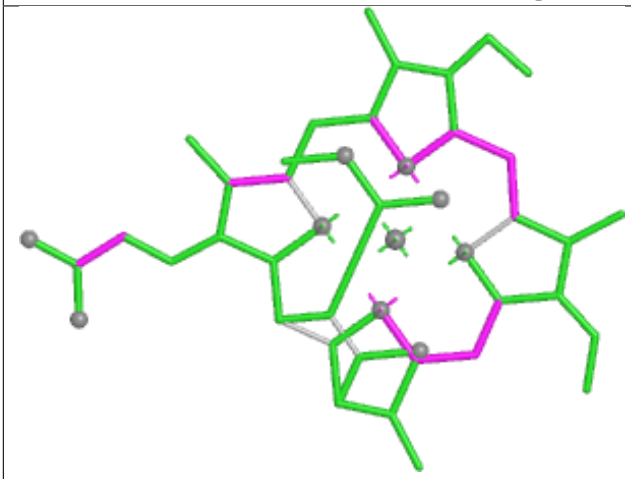


Torsions

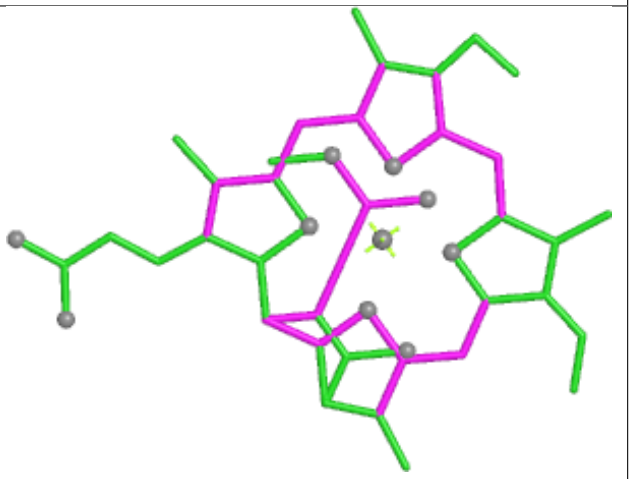


Rings

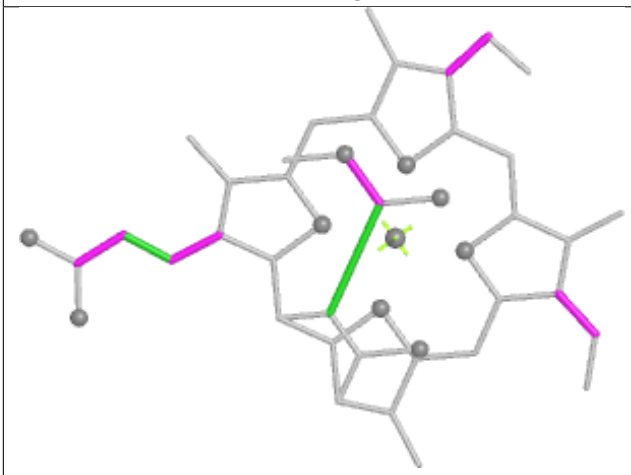
Ligand KC2 0 319



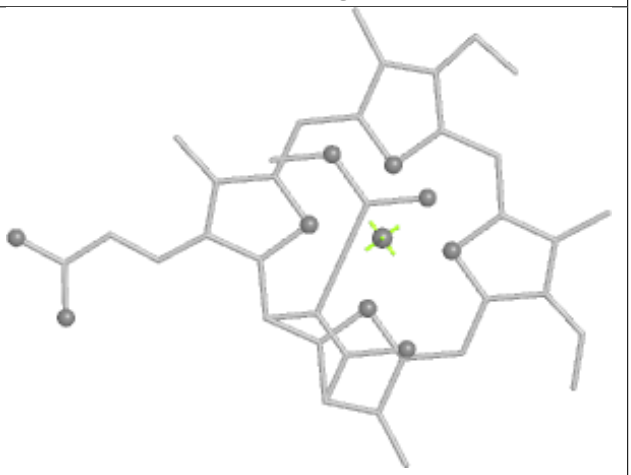
Bond lengths



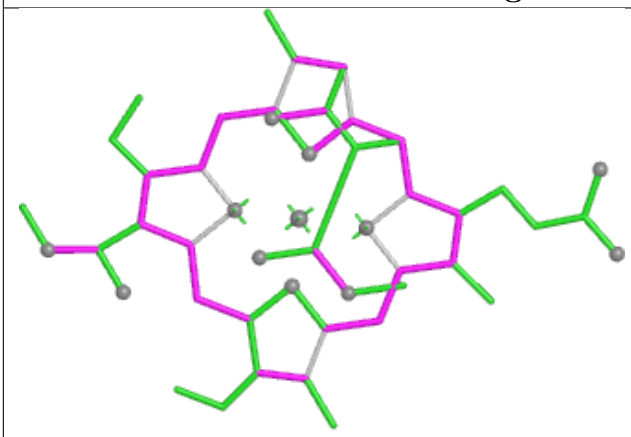
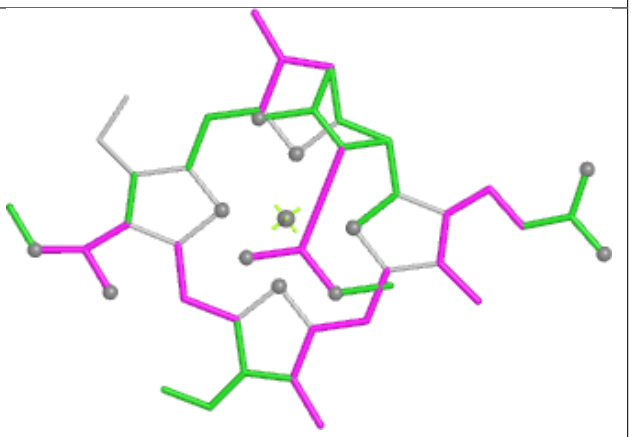
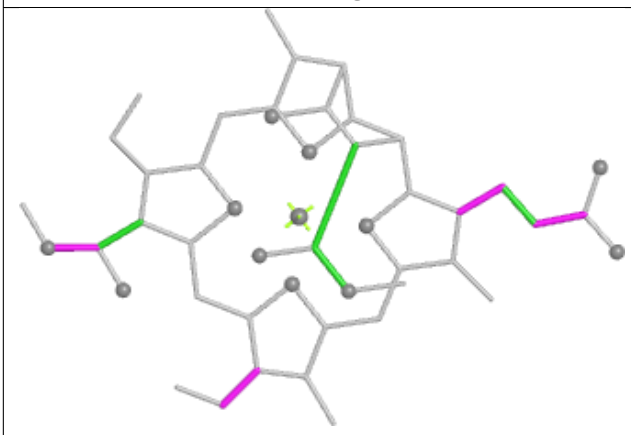
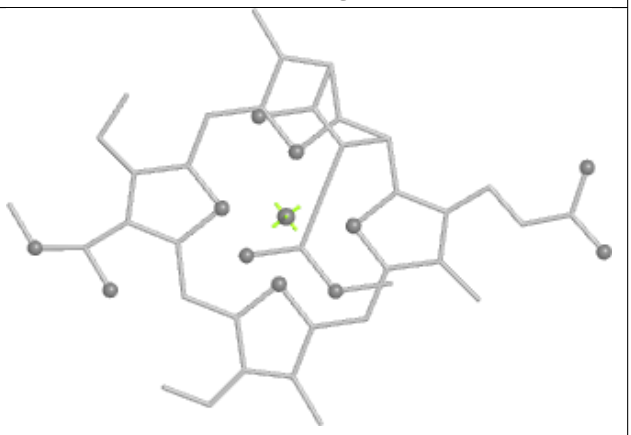
Bond angles



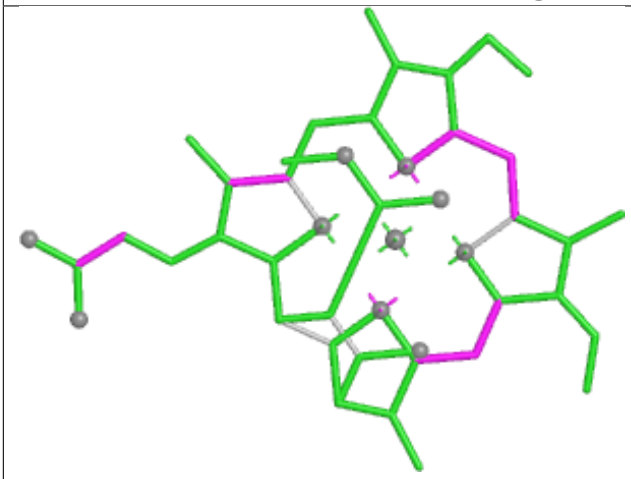
Torsions



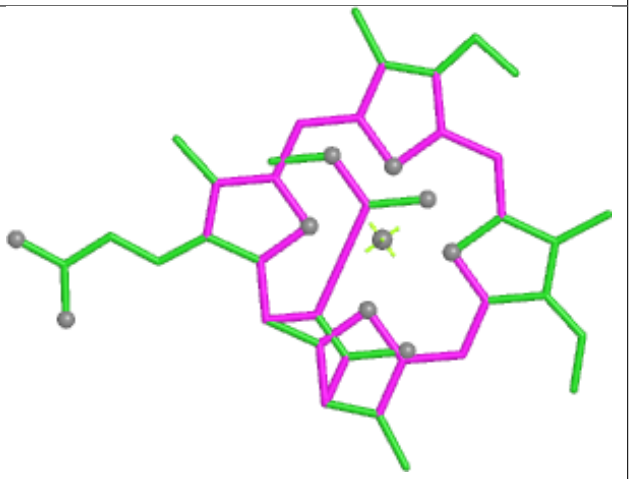
Rings

Ligand A1ECV 7 323	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

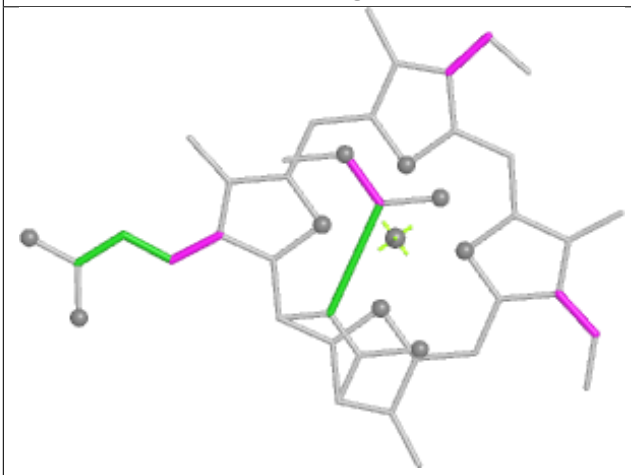
Ligand KC2 5 305



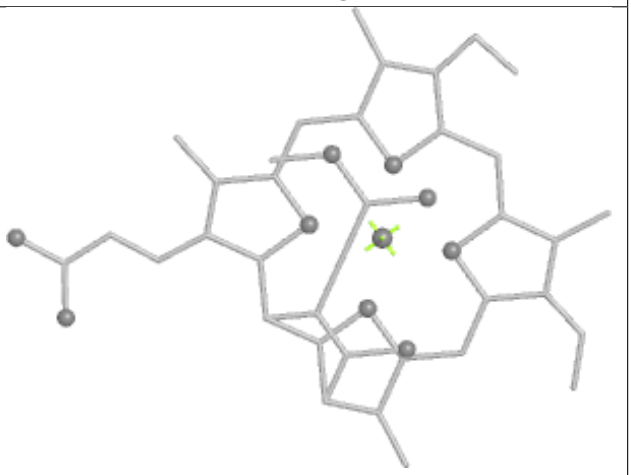
Bond lengths



Bond angles

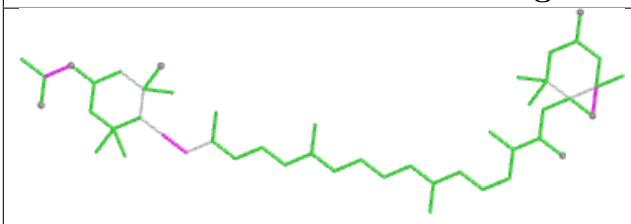


Torsions

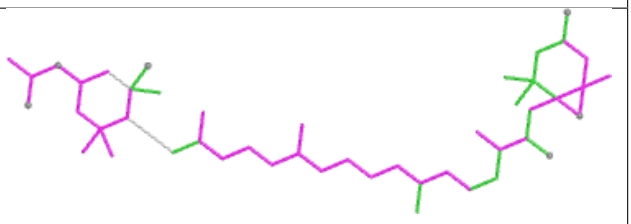


Rings

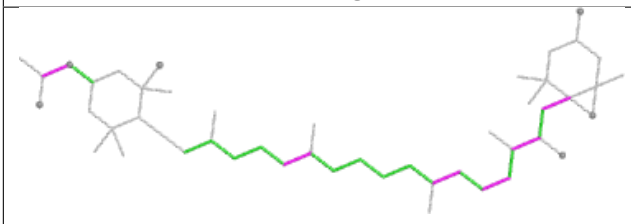
Ligand A86 8 307



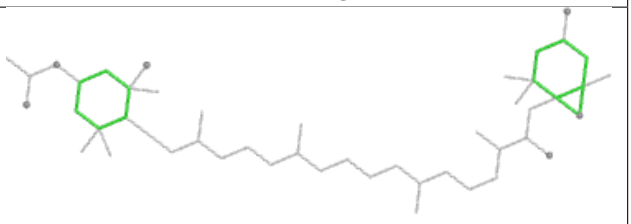
Bond lengths



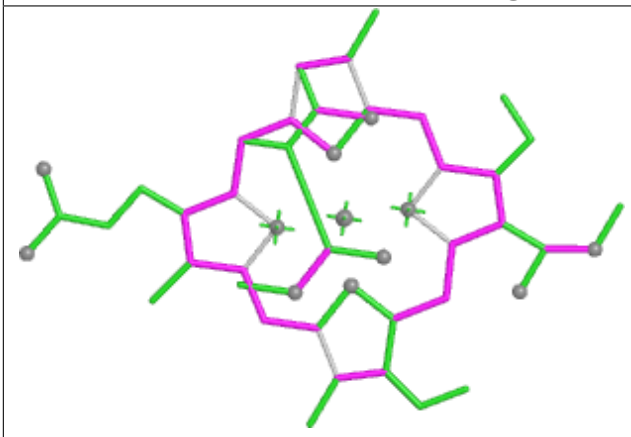
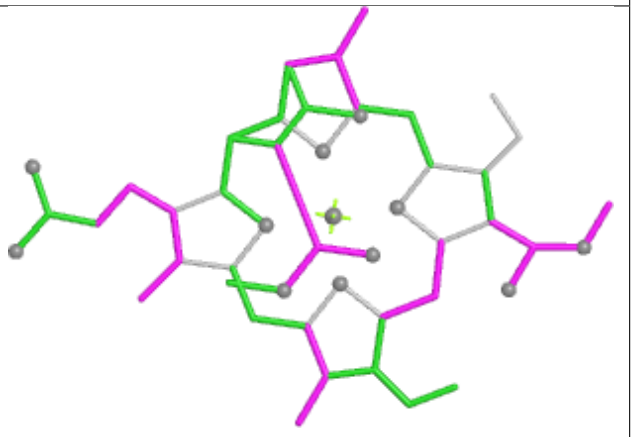
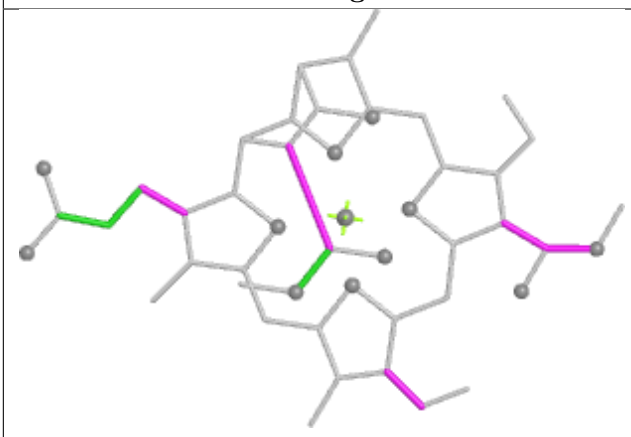
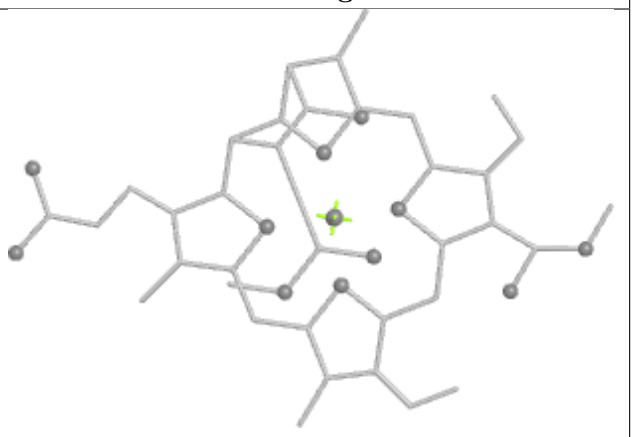
Bond angles



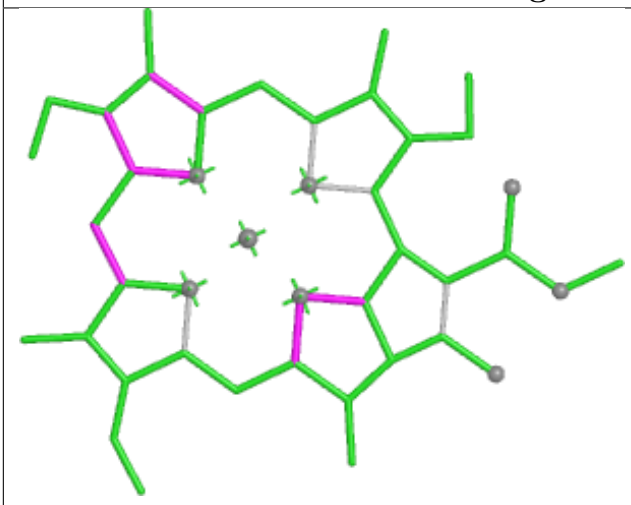
Torsions



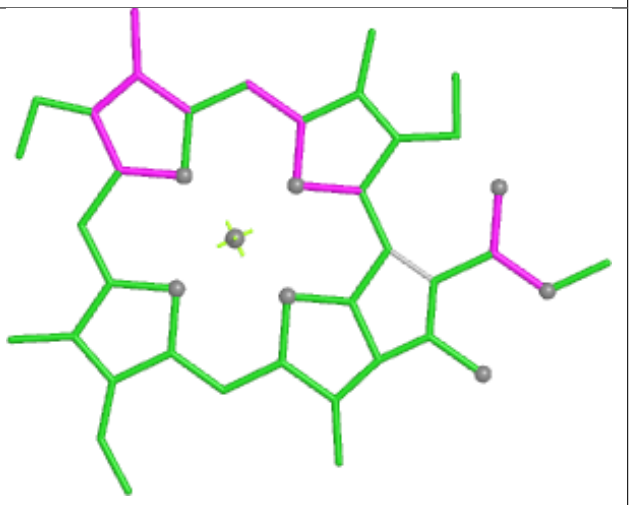
Rings

Ligand A1ECV 9 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

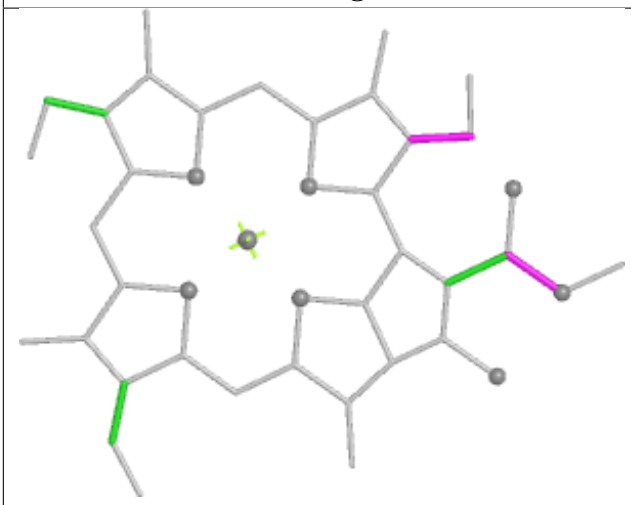
Ligand CLA z 307



Bond lengths



Bond angles



Torsions

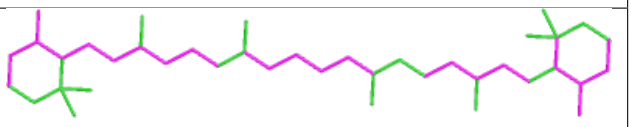


Rings

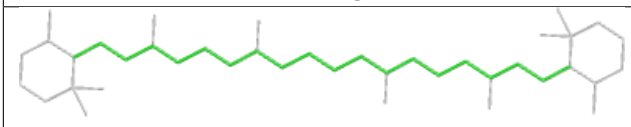
Ligand BCR a 843



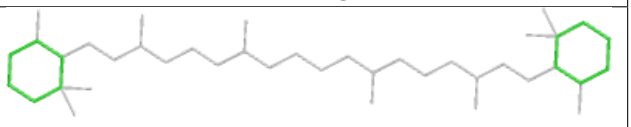
Bond lengths



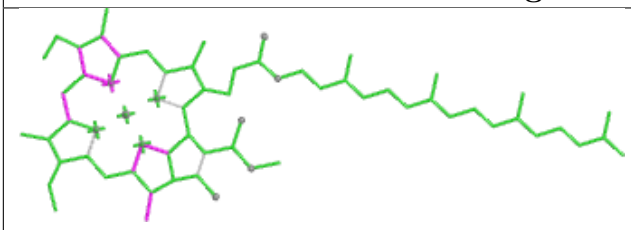
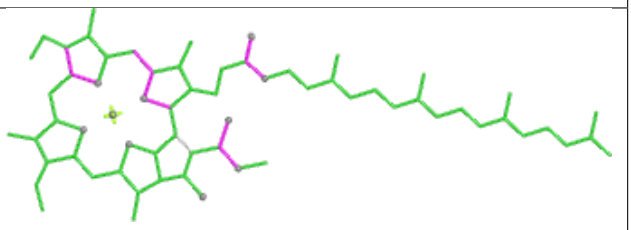
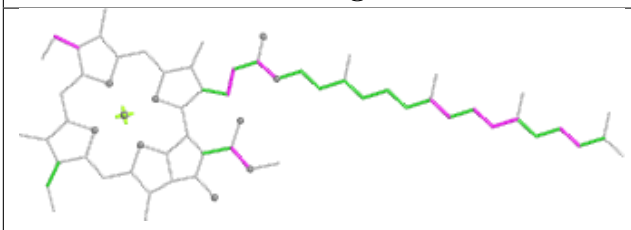
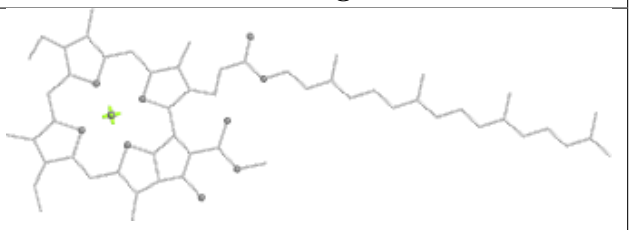
Bond angles

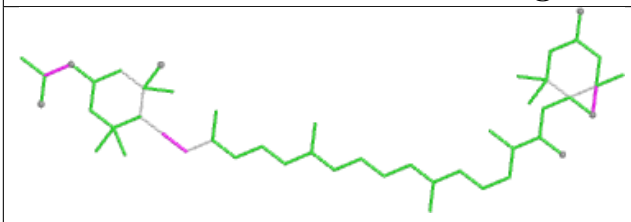
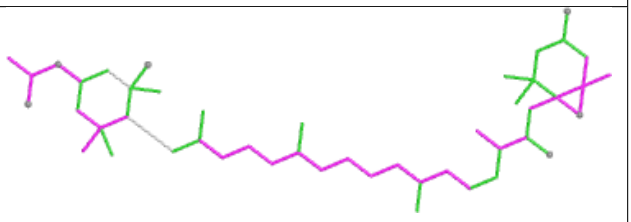
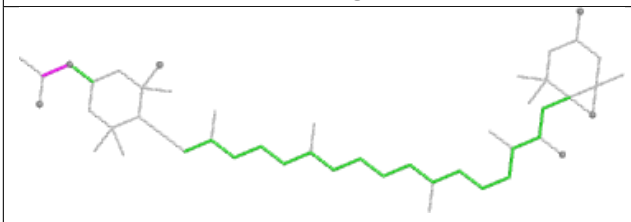
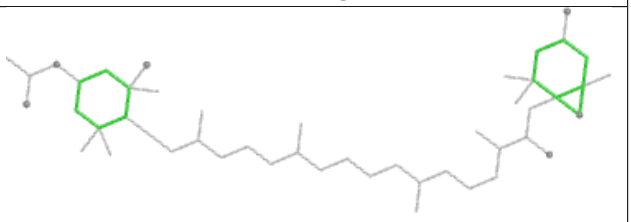


Torsions

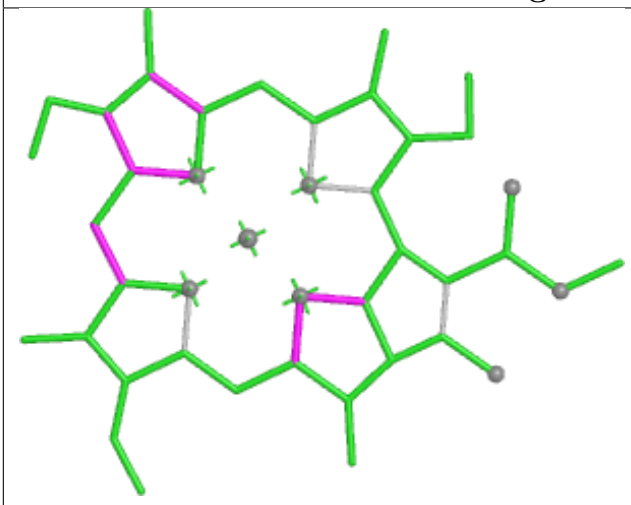


Rings

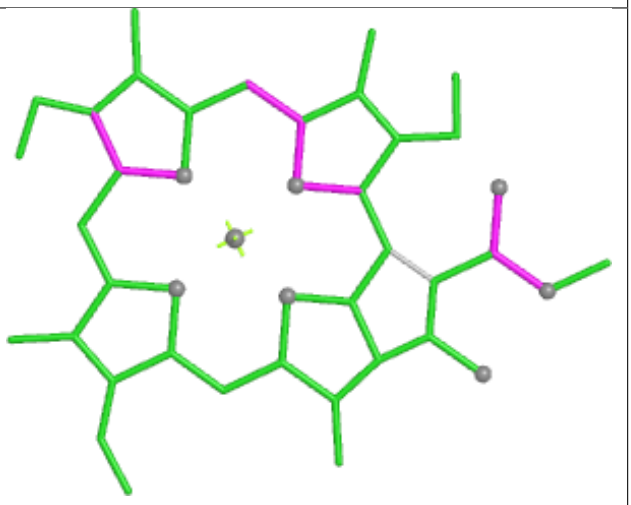
Ligand CLA P 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 1 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

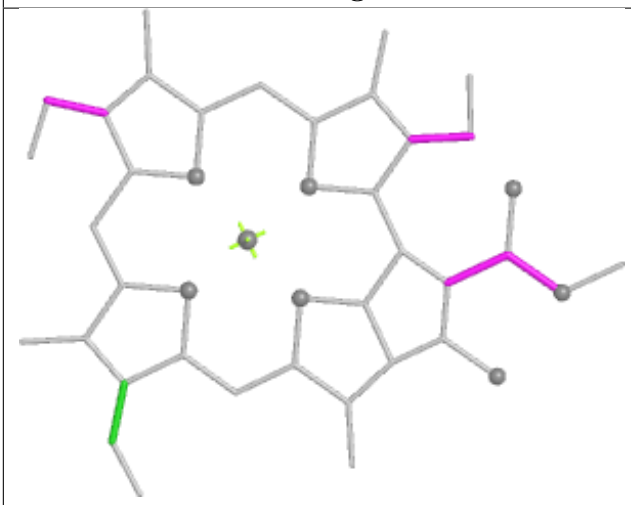
Ligand CLA z 317



Bond lengths



Bond angles

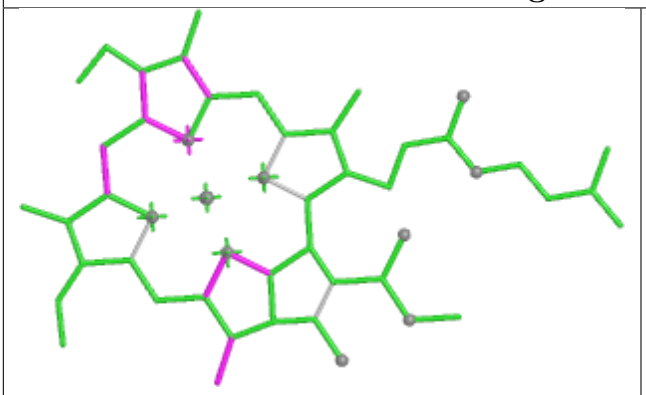


Torsions

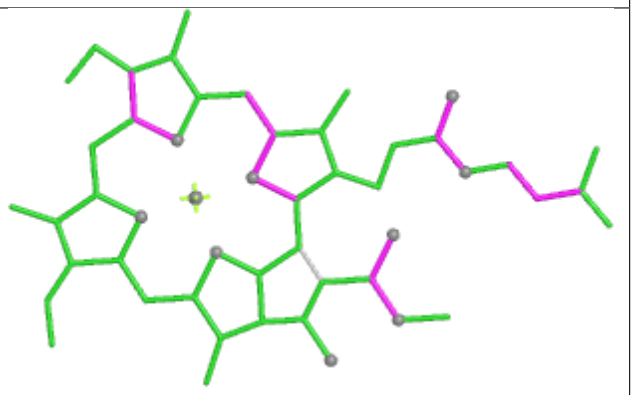


Rings

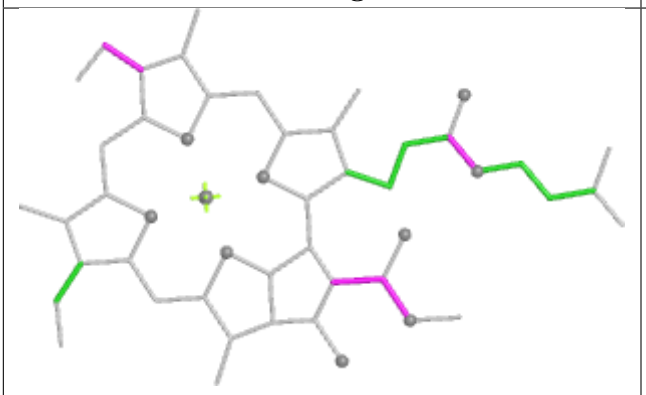
Ligand CLA 3 316



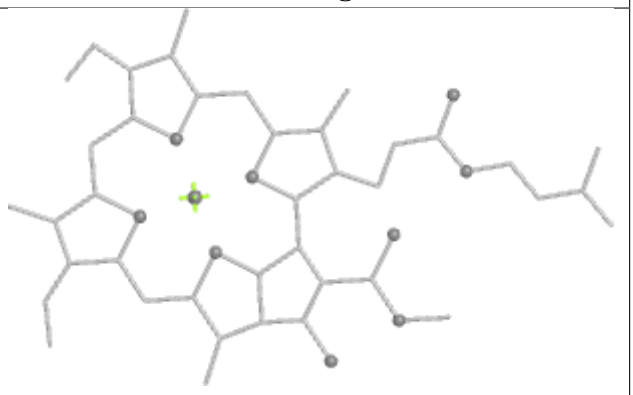
Bond lengths



Bond angles

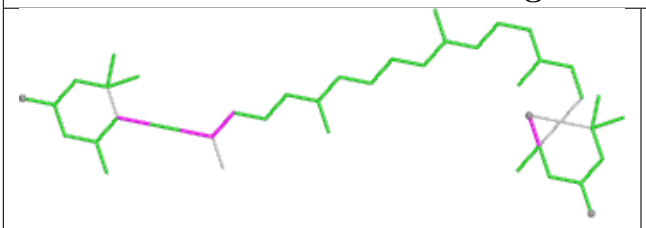


Torsions

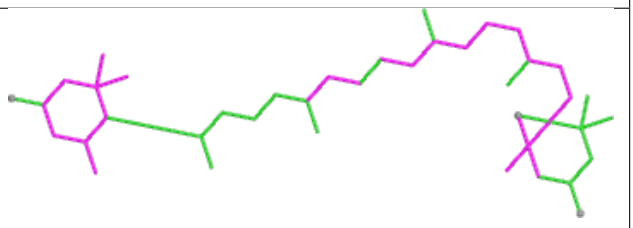


Rings

Ligand DD6 R 304



Bond lengths



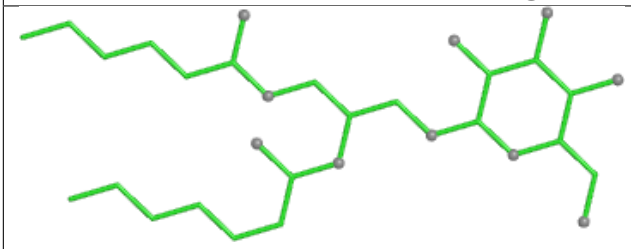
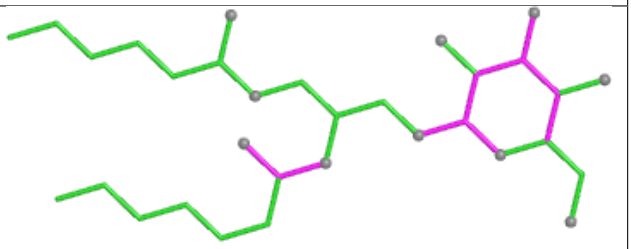
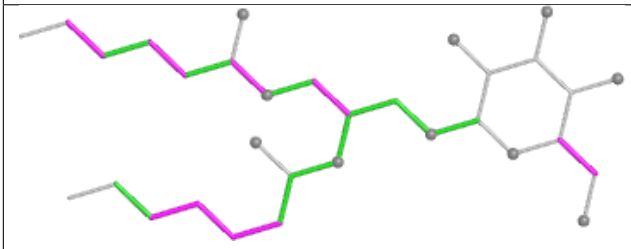
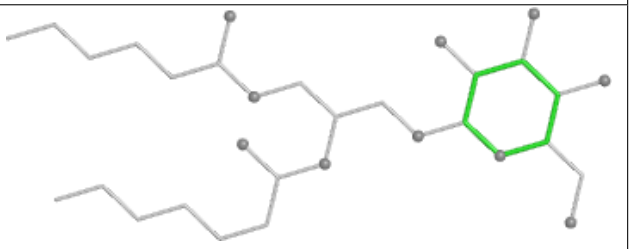
Bond angles

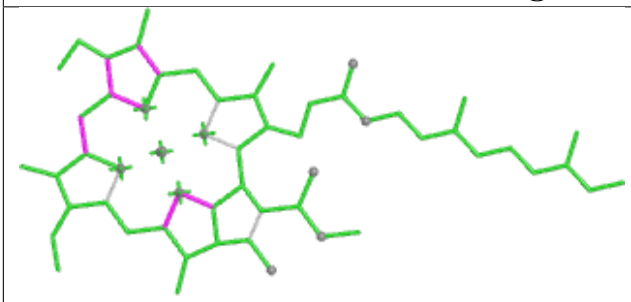
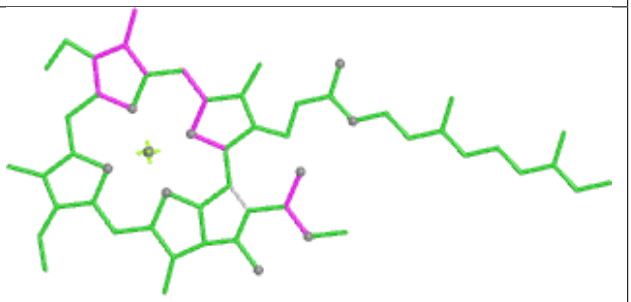
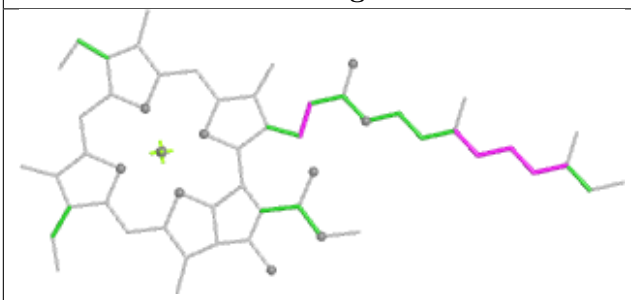
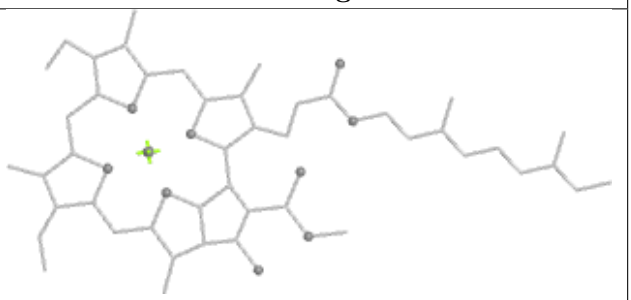


Torsions

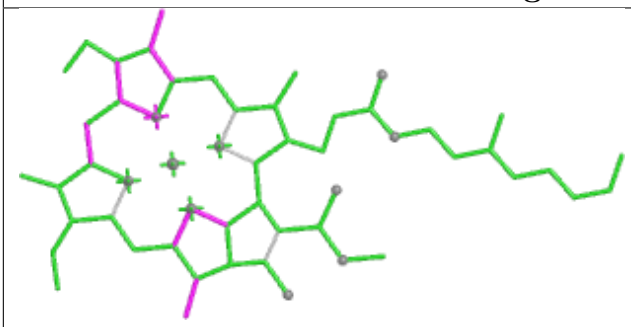


Rings

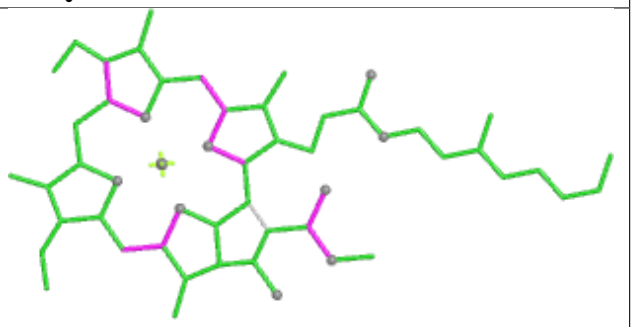
Ligand LMG S 321	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

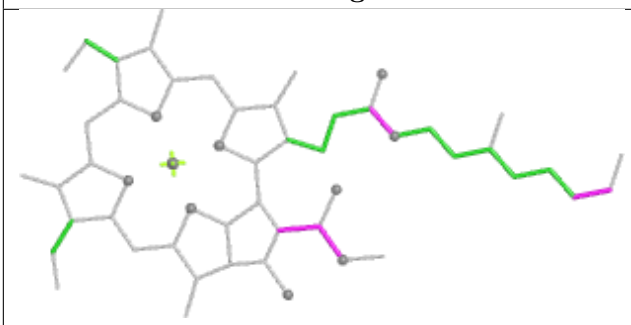
Ligand CLA Q 314



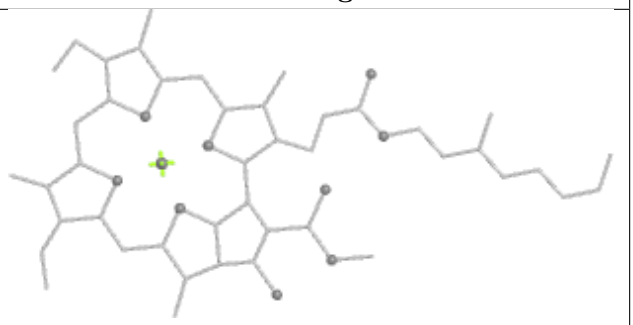
Bond lengths



Bond angles

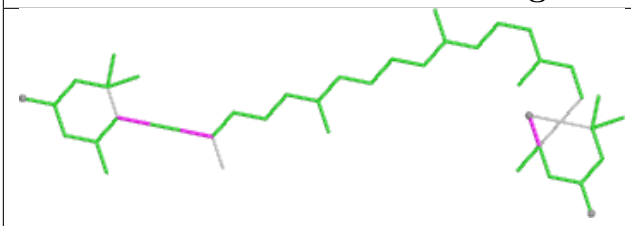


Torsions

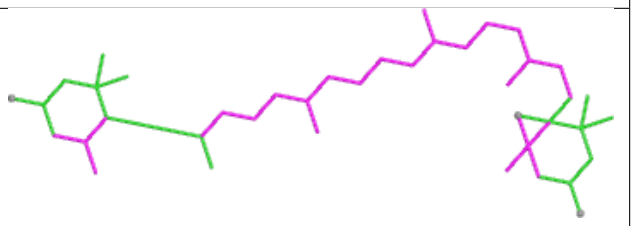


Rings

Ligand DD6 J 305



Bond lengths



Bond angles



Torsions

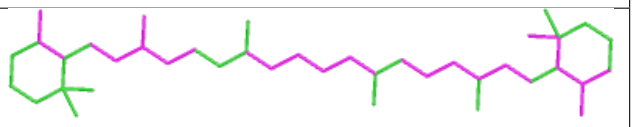


Rings

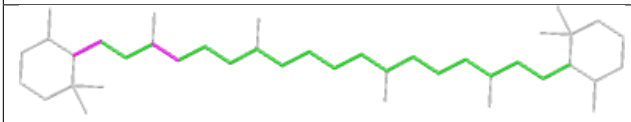
Ligand BCR l 202



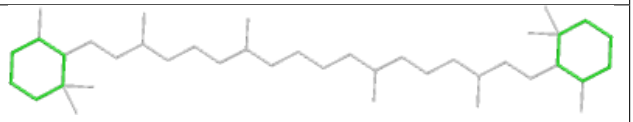
Bond lengths



Bond angles

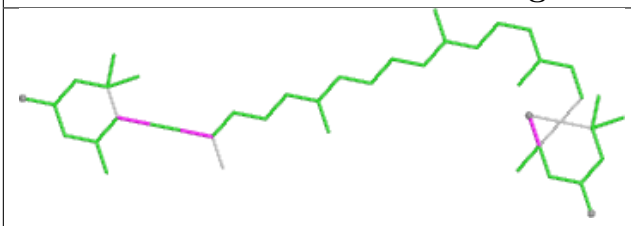


Torsions

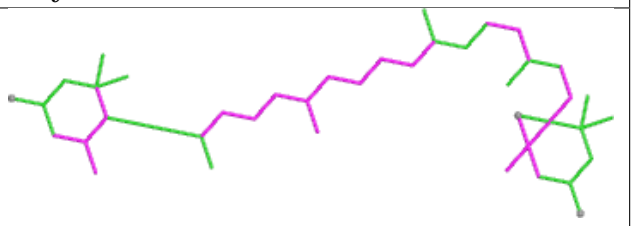


Rings

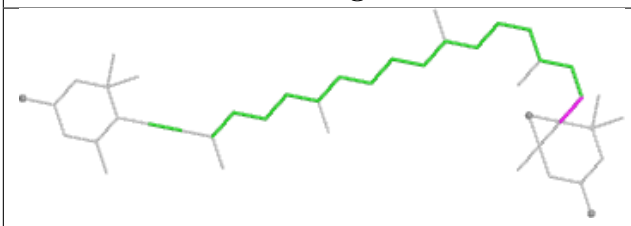
Ligand DD6 y 303



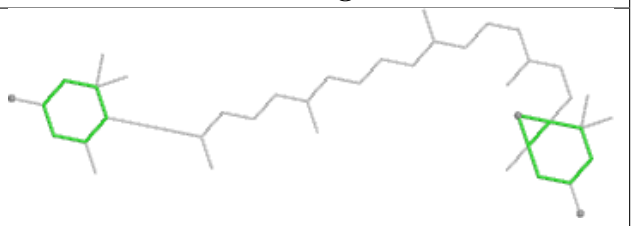
Bond lengths



Bond angles

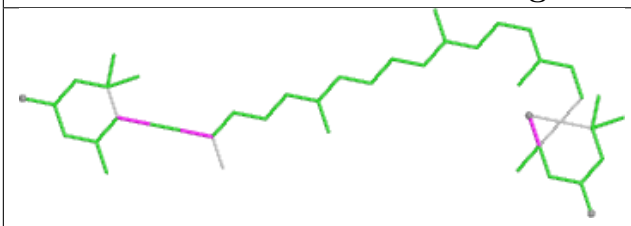


Torsions

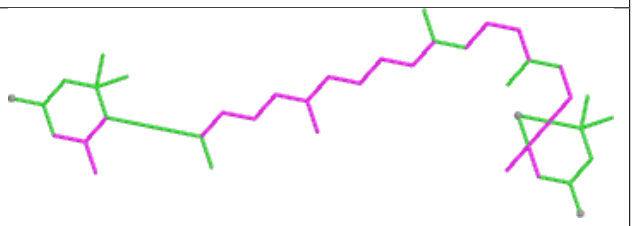


Rings

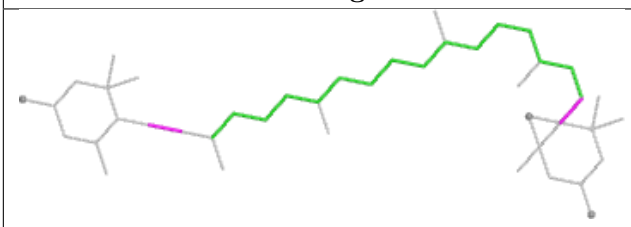
Ligand DD6 3 301



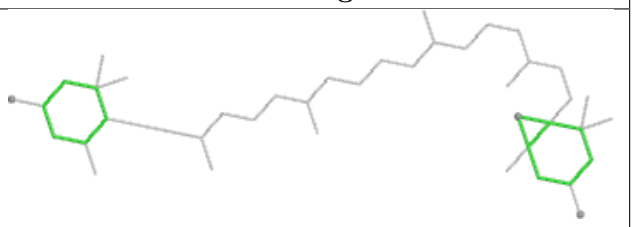
Bond lengths



Bond angles

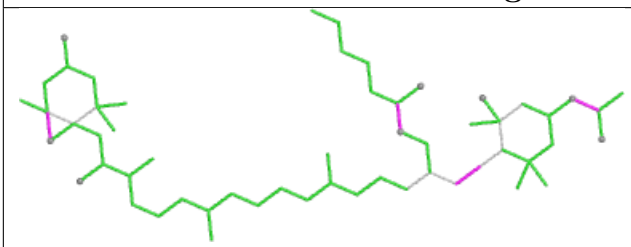


Torsions

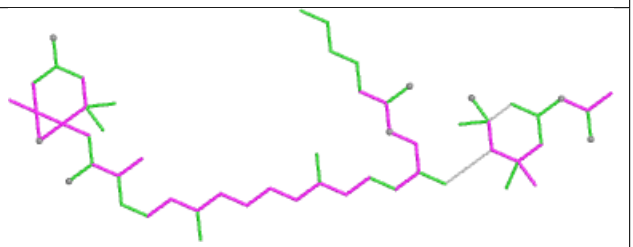


Rings

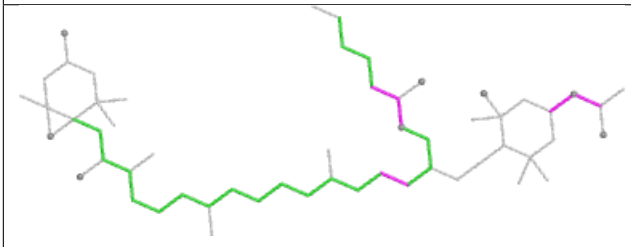
Ligand A1EB1 G 302



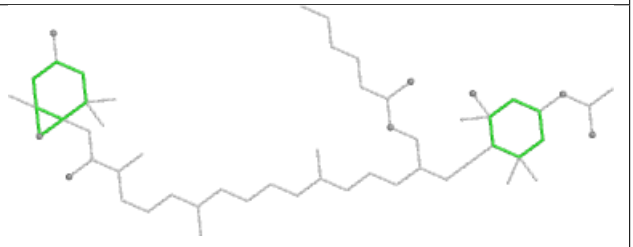
Bond lengths



Bond angles

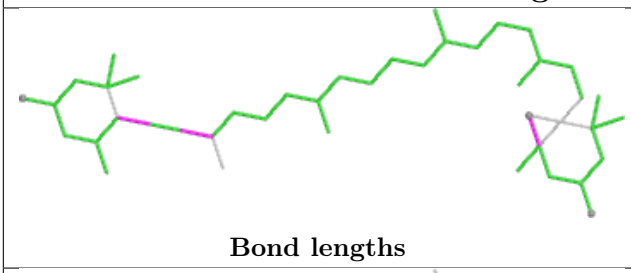


Torsions

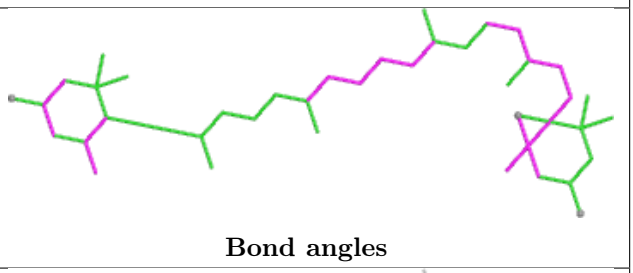


Rings

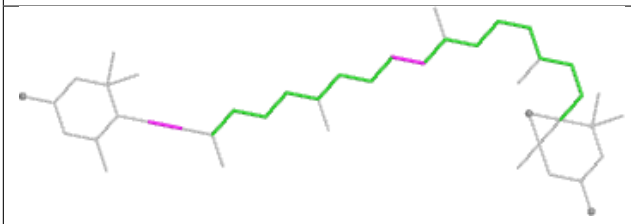
Ligand DD6 I 306



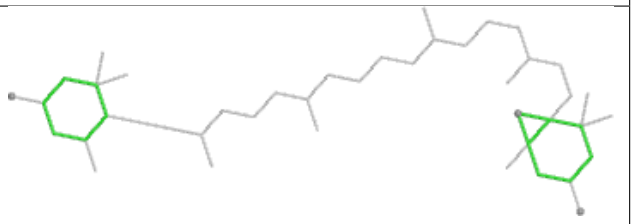
Bond lengths



Bond angles

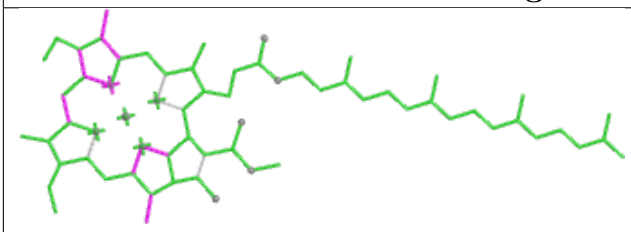


Torsions

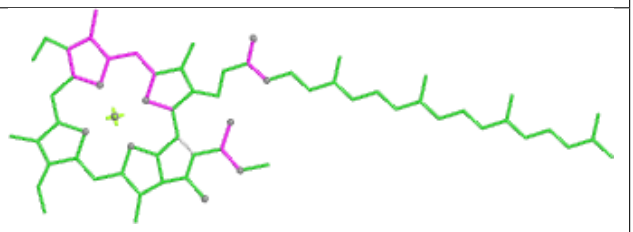


Rings

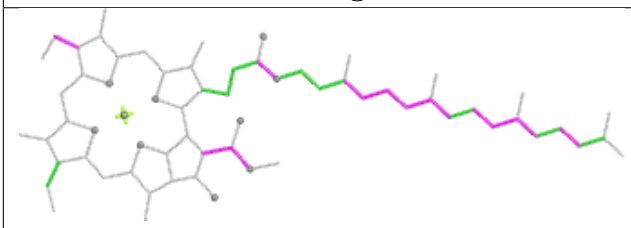
Ligand CLA E 307



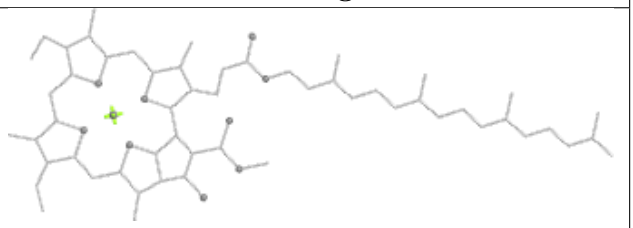
Bond lengths



Bond angles

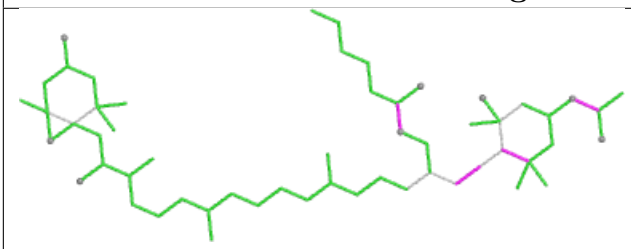


Torsions

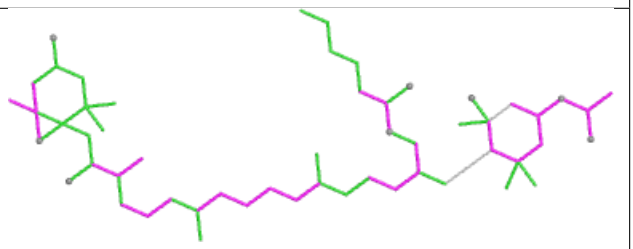


Rings

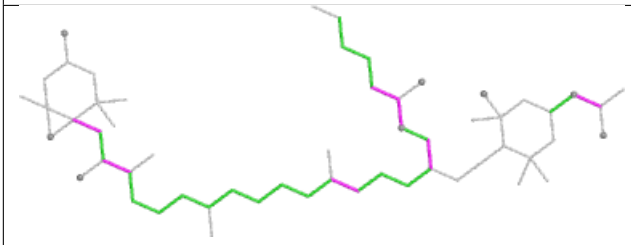
Ligand A1EB1 8 301



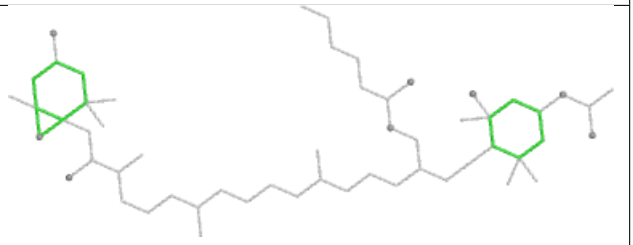
Bond lengths



Bond angles

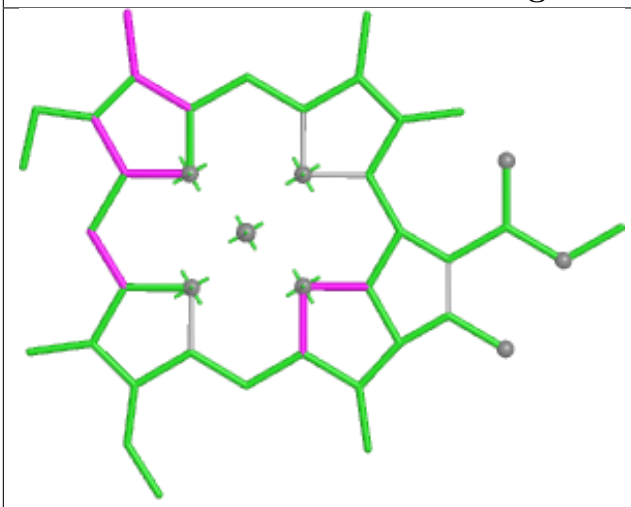


Torsions

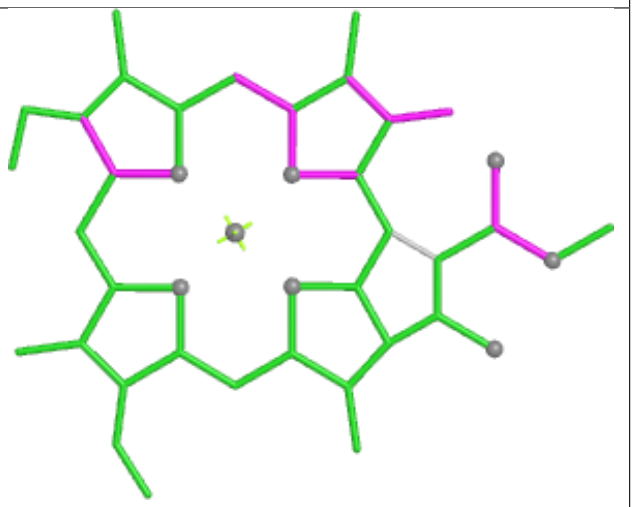


Rings

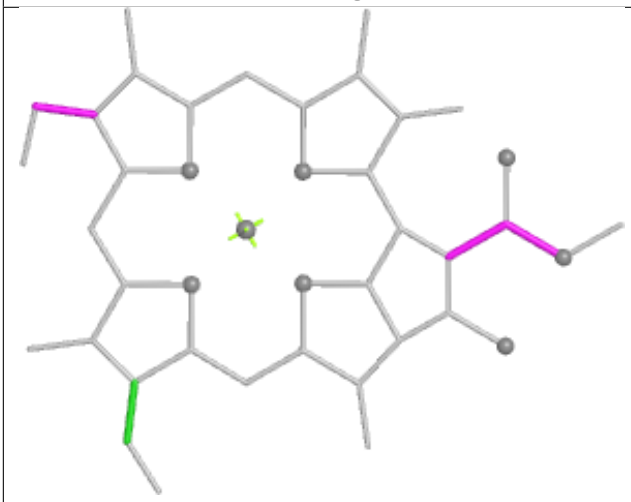
Ligand CLA 2 318



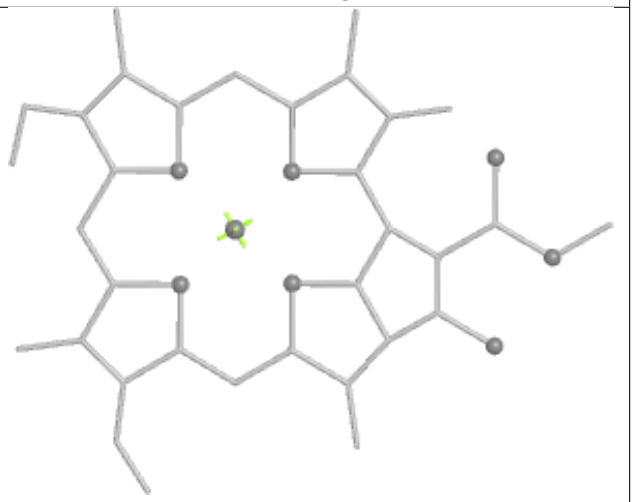
Bond lengths



Bond angles

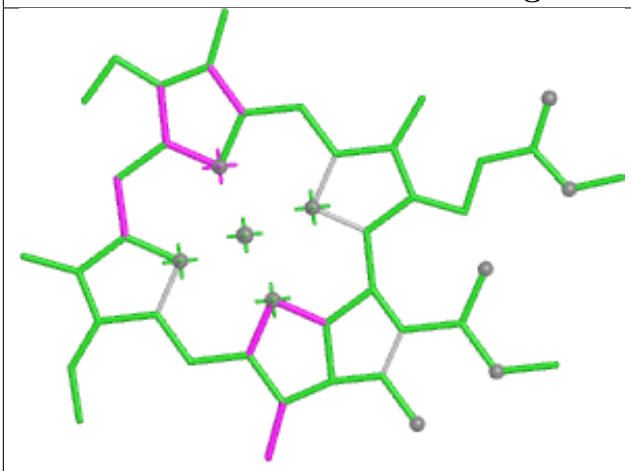


Torsions

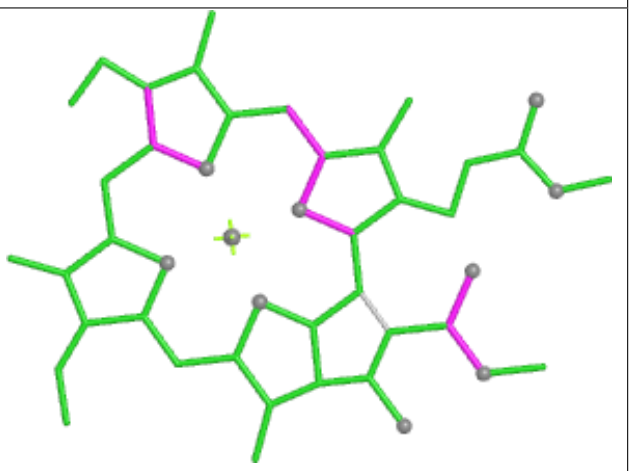


Rings

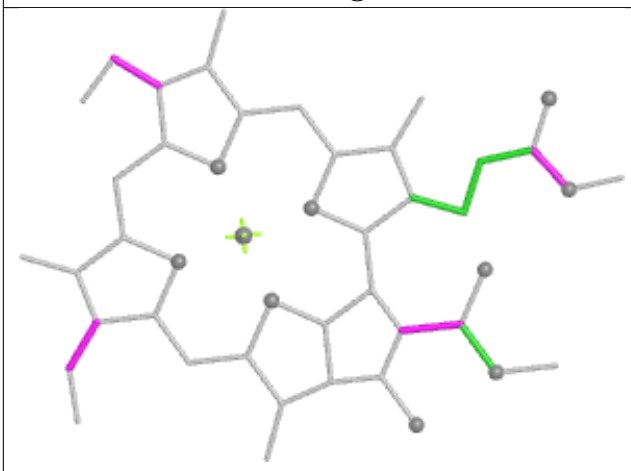
Ligand CLA O 312



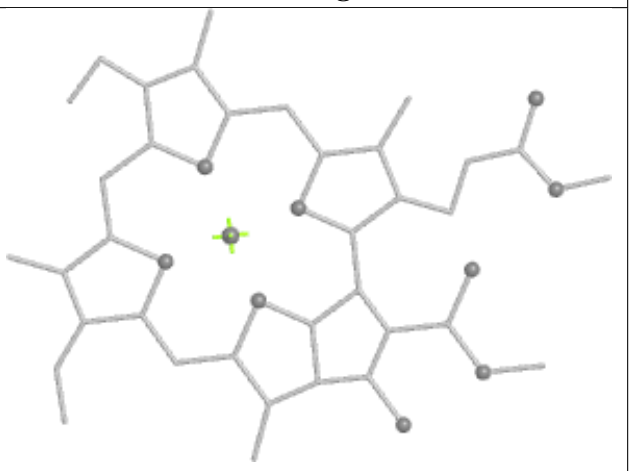
Bond lengths



Bond angles

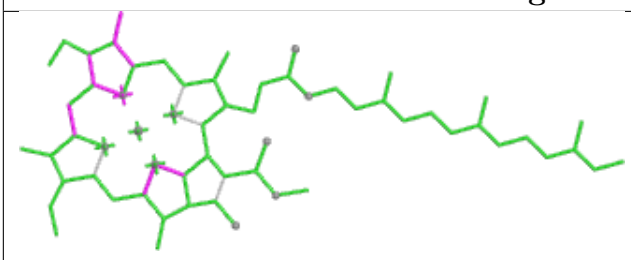


Torsions

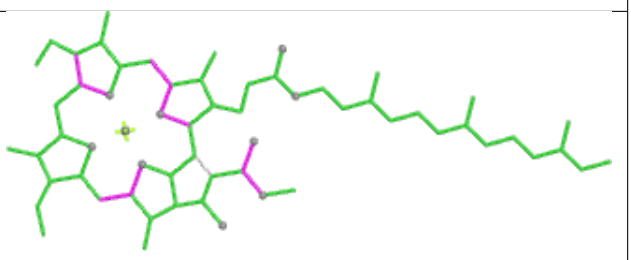


Rings

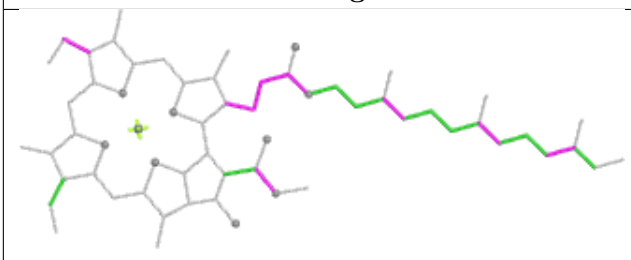
Ligand CLA 3 311



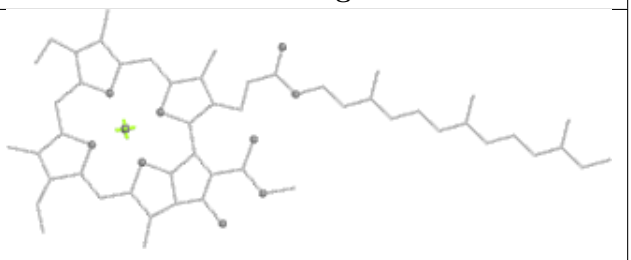
Bond lengths



Bond angles

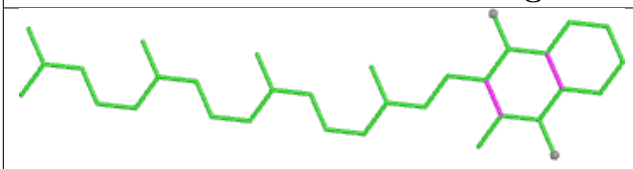


Torsions

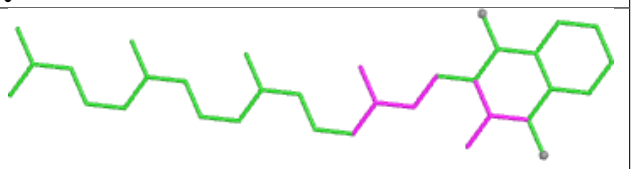


Rings

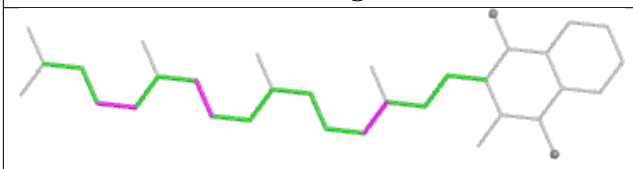
Ligand PQN b 843



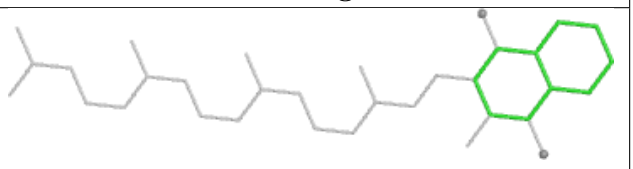
Bond lengths



Bond angles

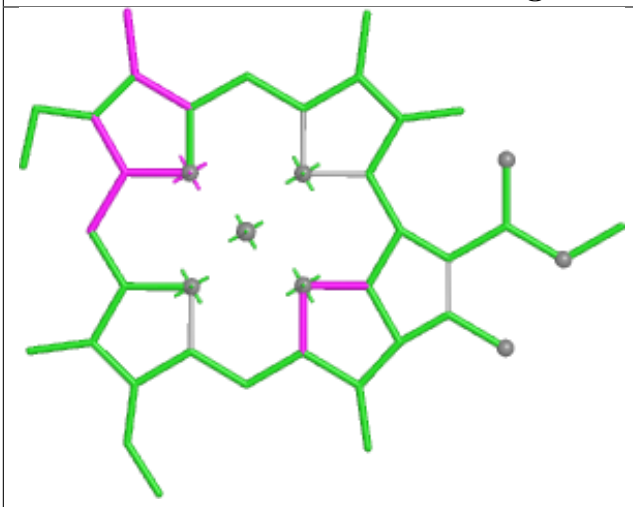


Torsions

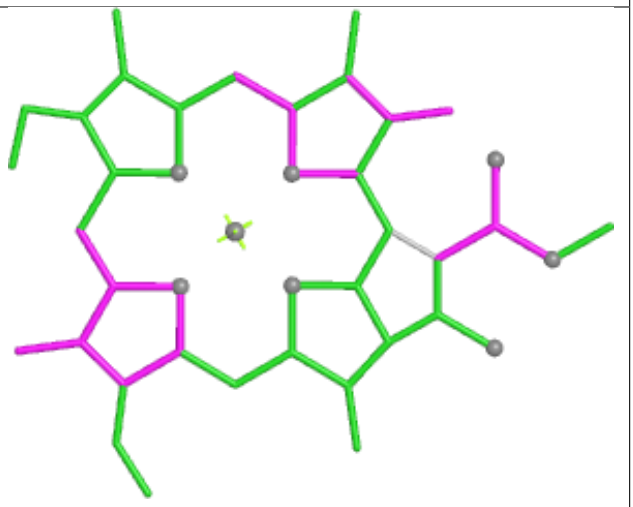


Rings

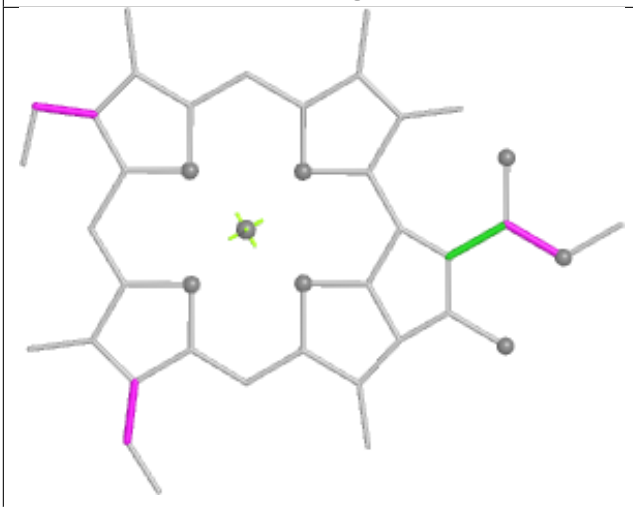
Ligand CLA Z 313



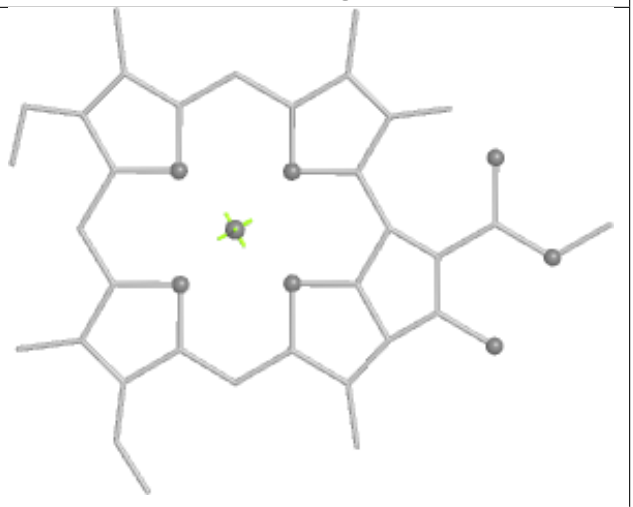
Bond lengths



Bond angles

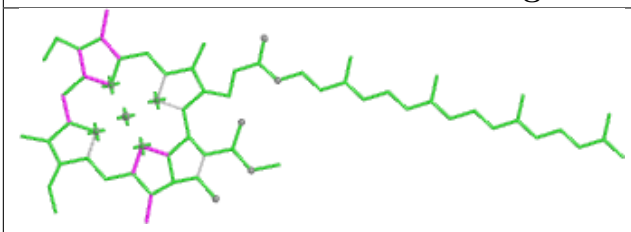


Torsions

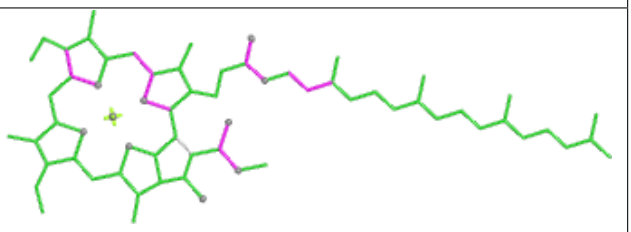


Rings

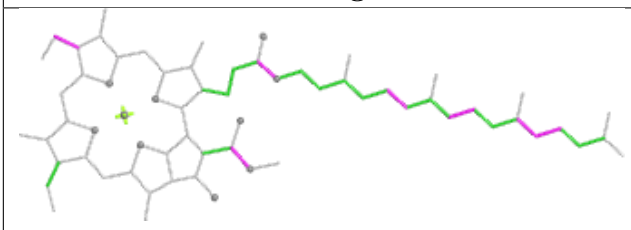
Ligand CLA D 314



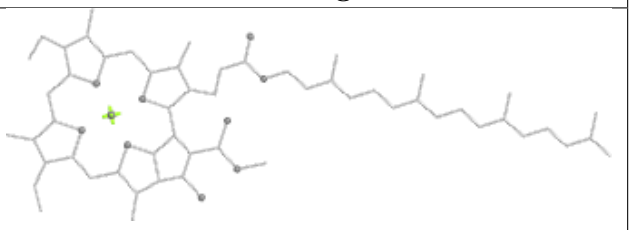
Bond lengths



Bond angles

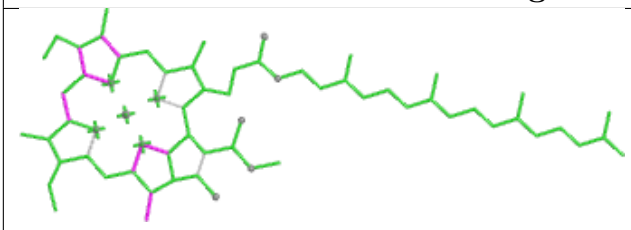


Torsions

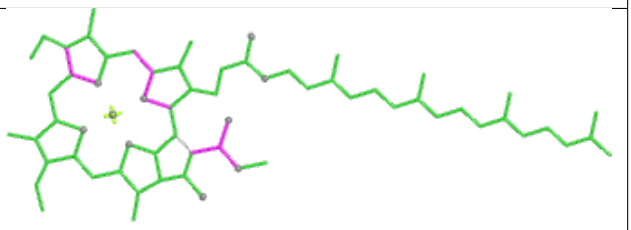


Rings

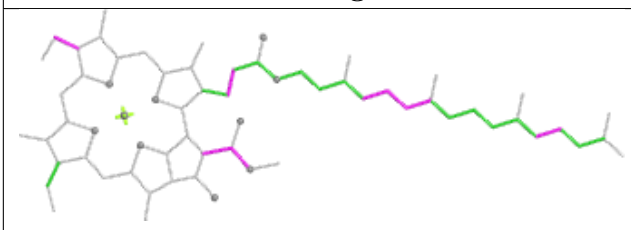
Ligand CLA a 831



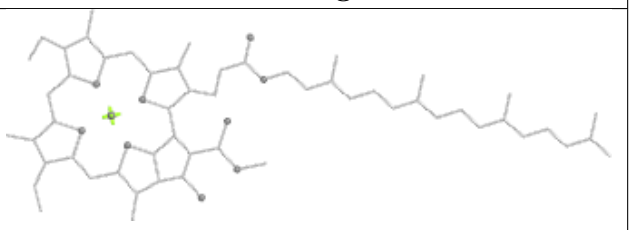
Bond lengths



Bond angles

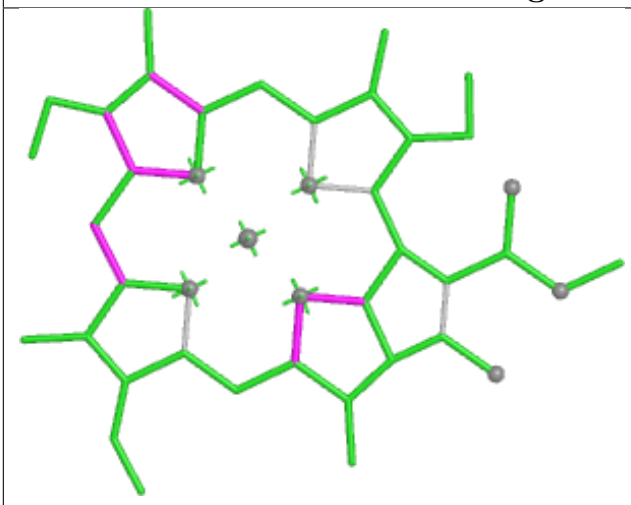


Torsions

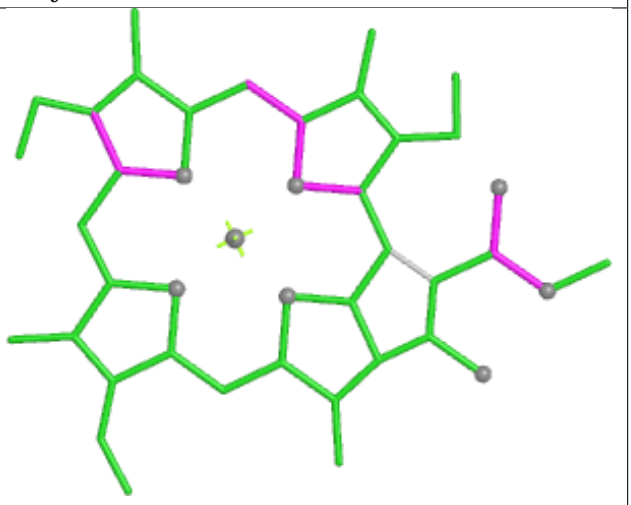


Rings

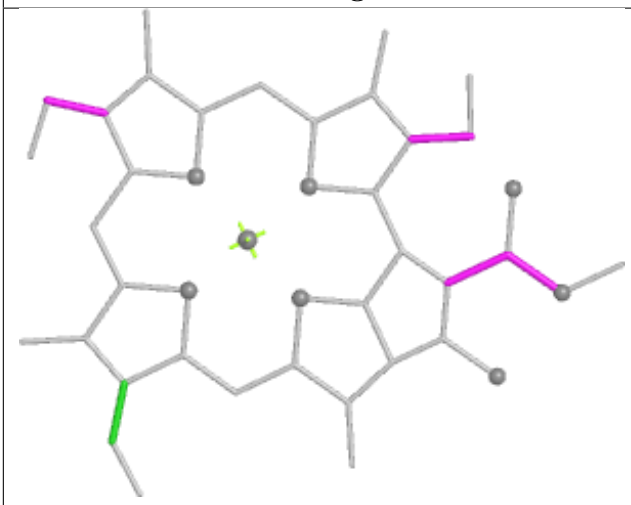
Ligand CLA y 318



Bond lengths



Bond angles

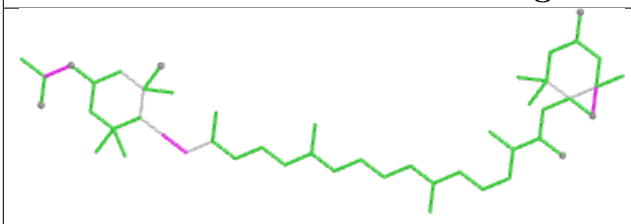


Torsions

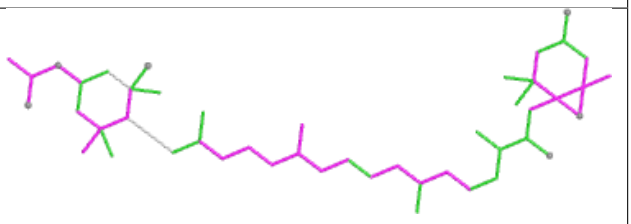


Rings

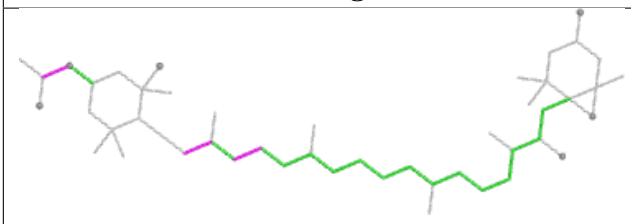
Ligand A86 2 302



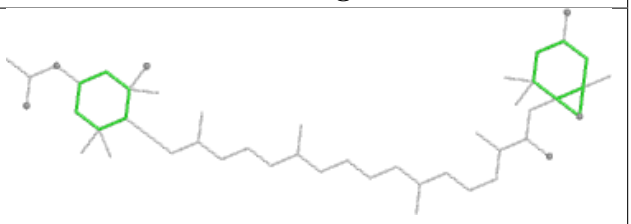
Bond lengths



Bond angles

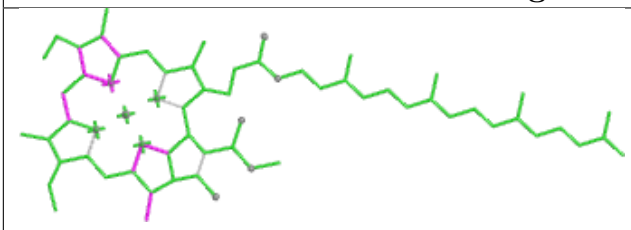


Torsions

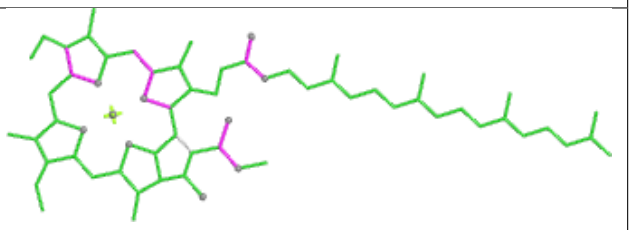


Rings

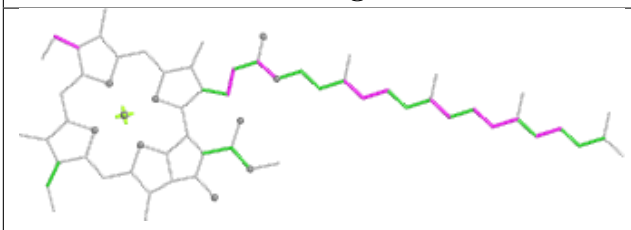
Ligand CLA 5 306



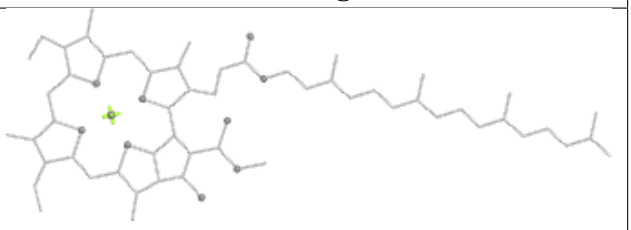
Bond lengths



Bond angles

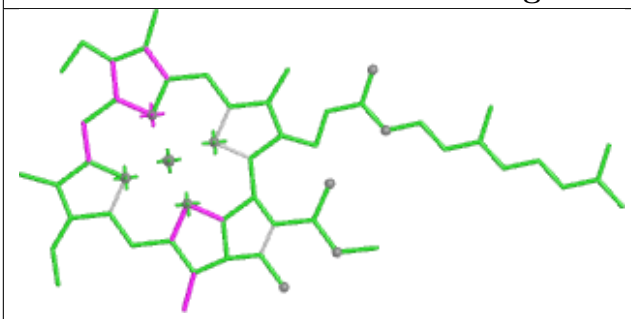


Torsions

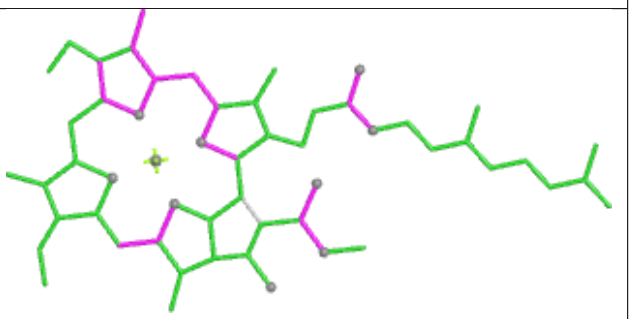


Rings

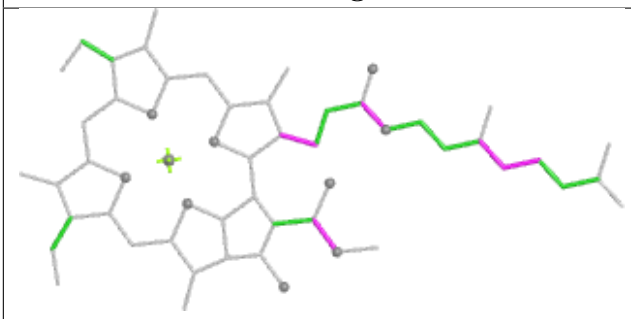
Ligand CLA D 312



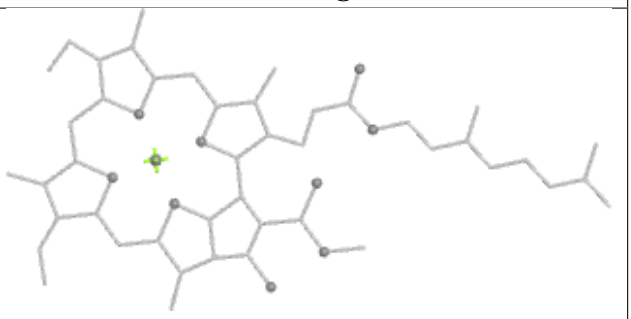
Bond lengths



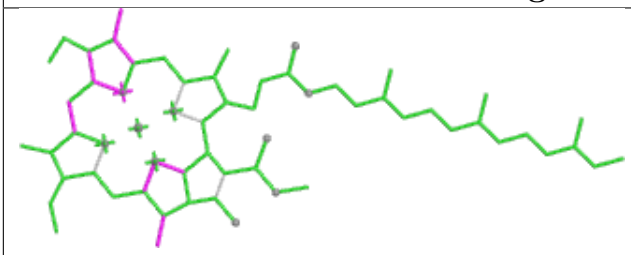
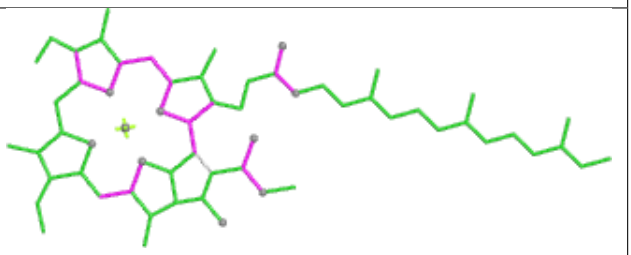
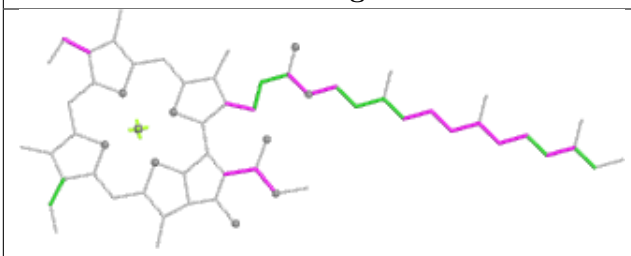
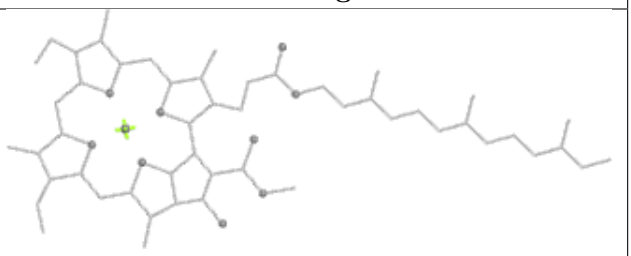
Bond angles

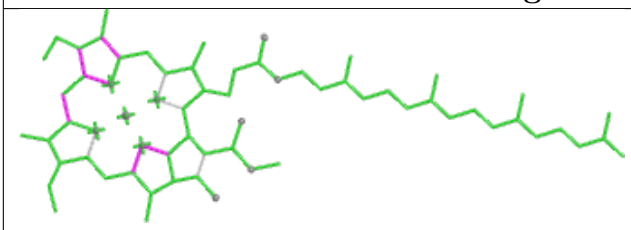
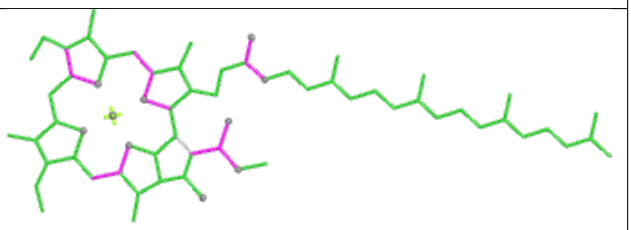
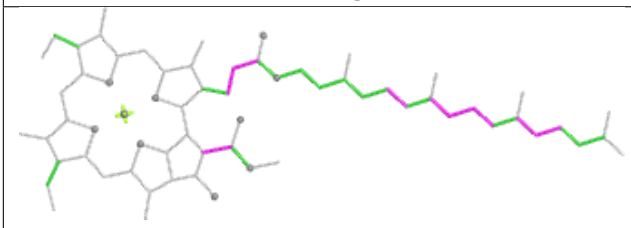
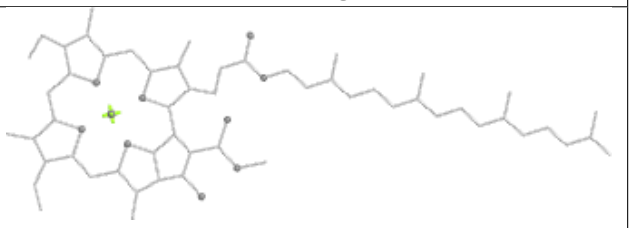


Torsions

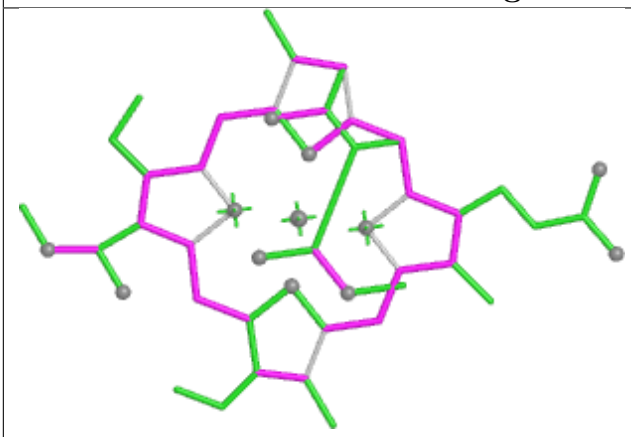


Rings

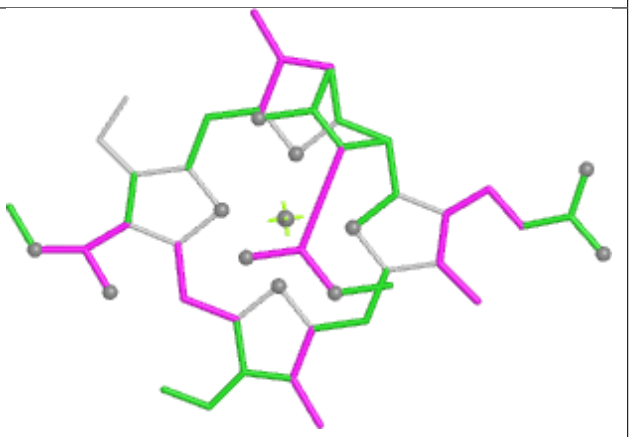
Ligand CLA 4 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

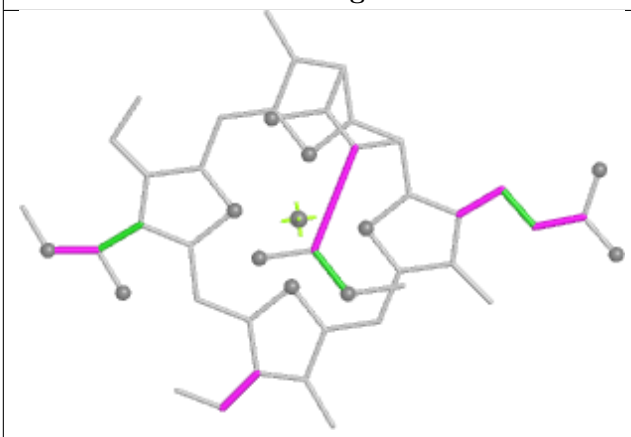
Ligand A1ECV S 312



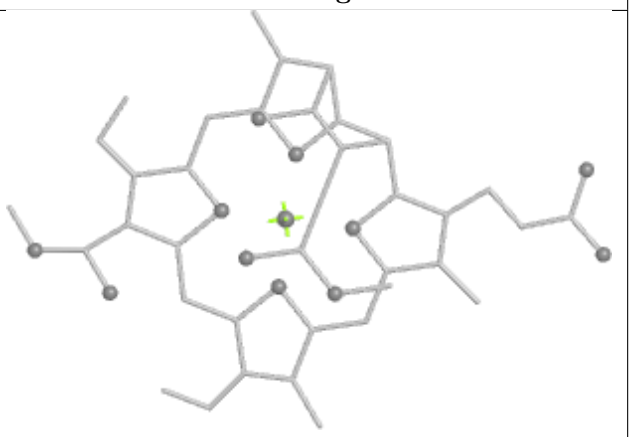
Bond lengths



Bond angles

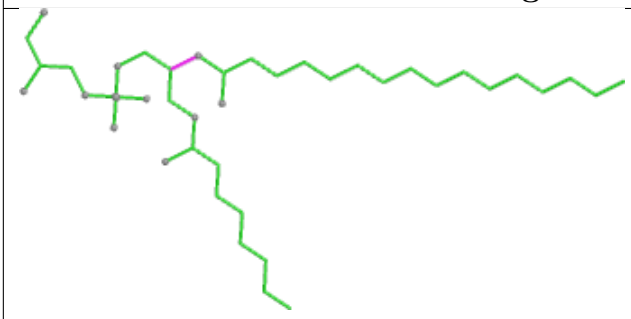


Torsions

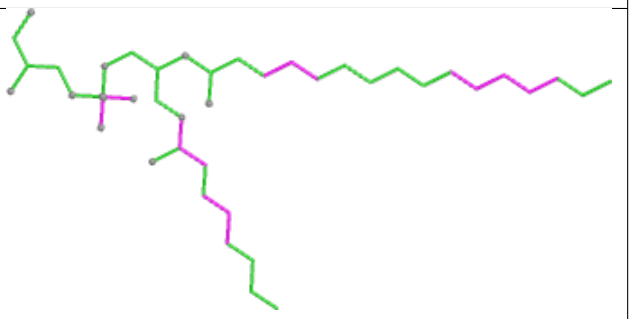


Rings

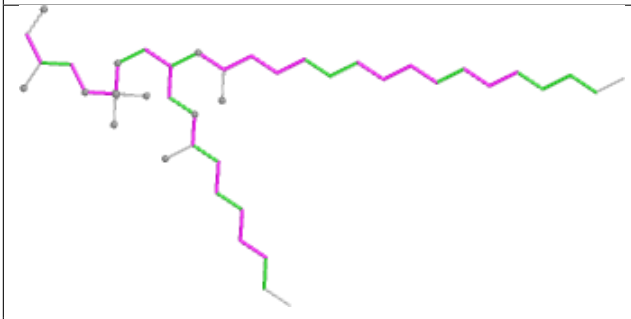
Ligand LHG X 301



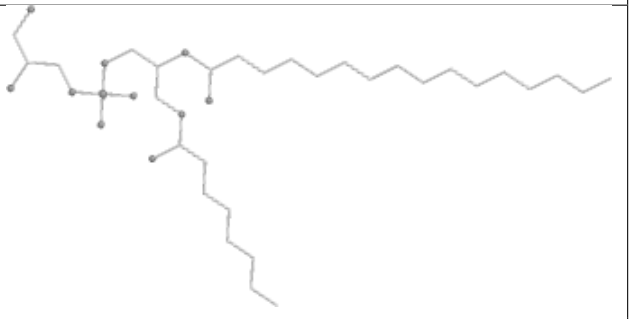
Bond lengths



Bond angles

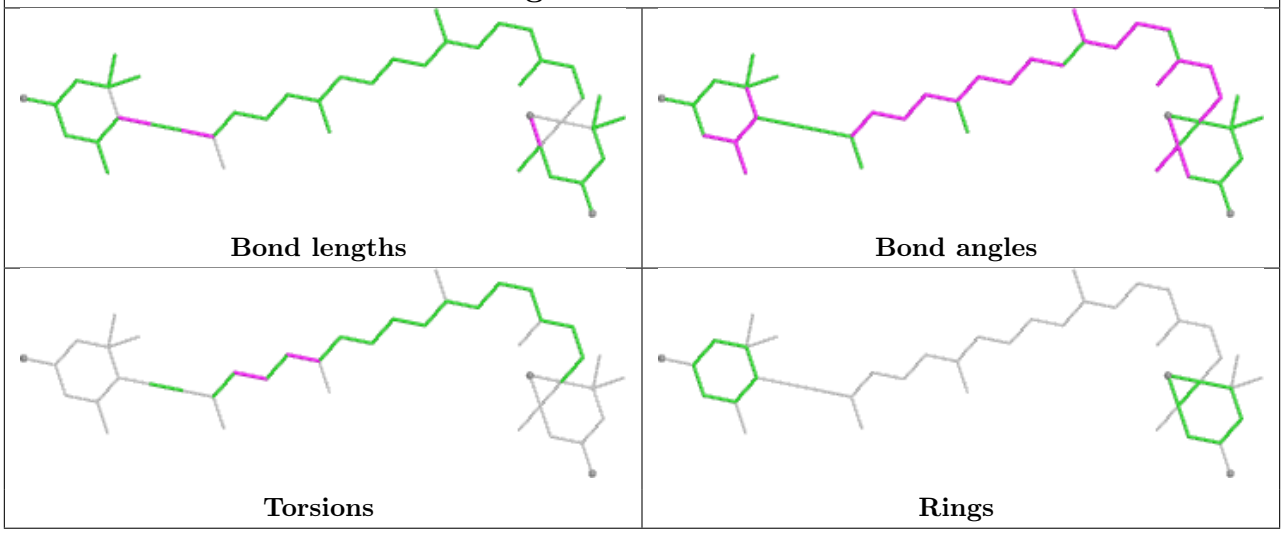


Torsions

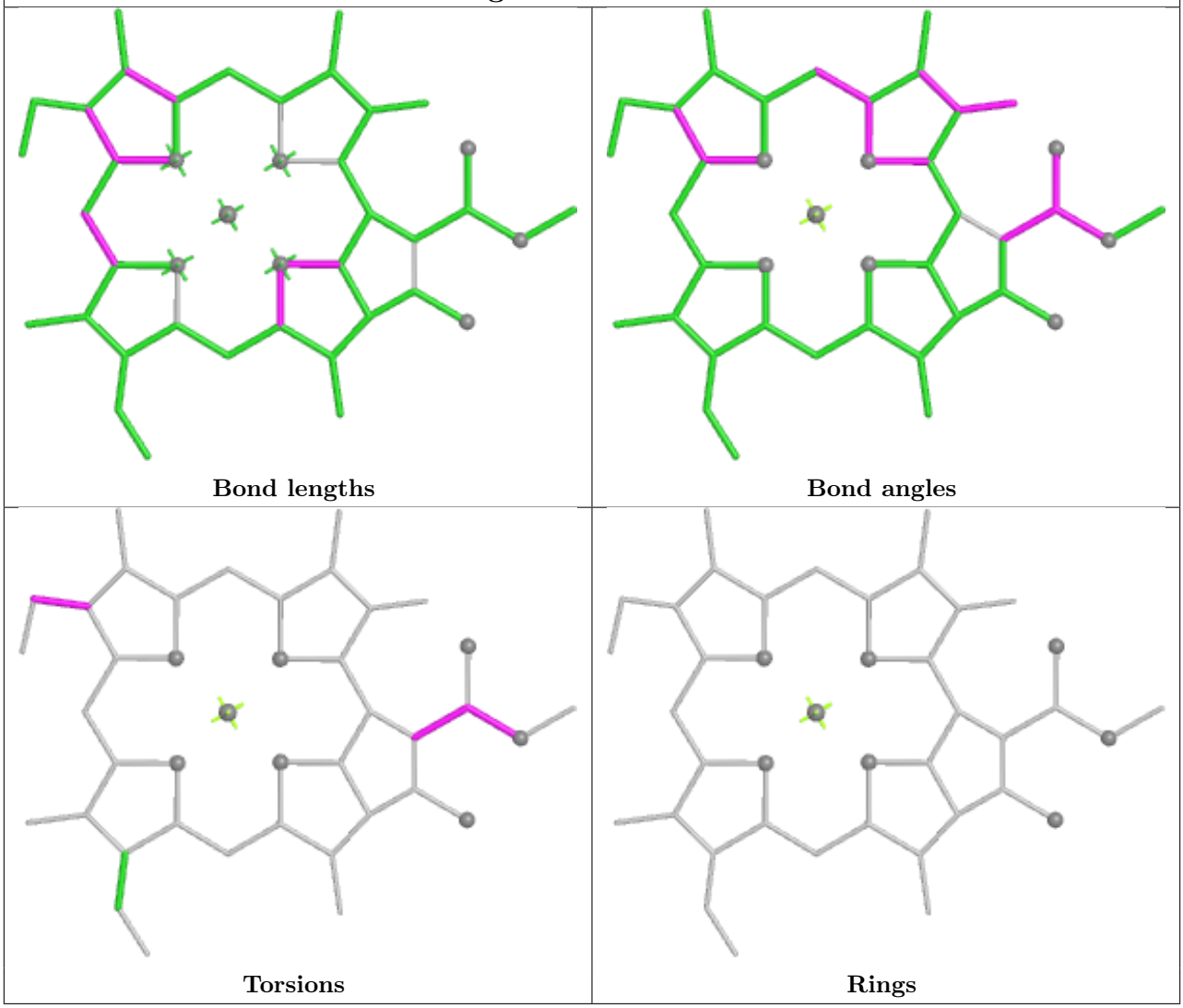


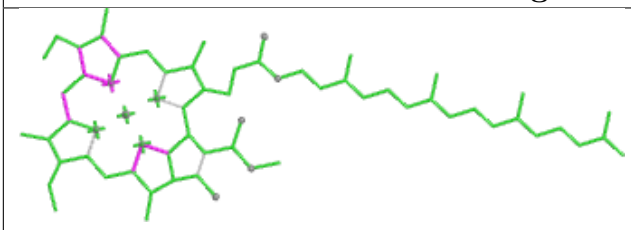
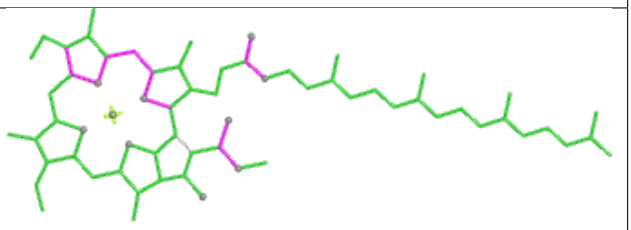
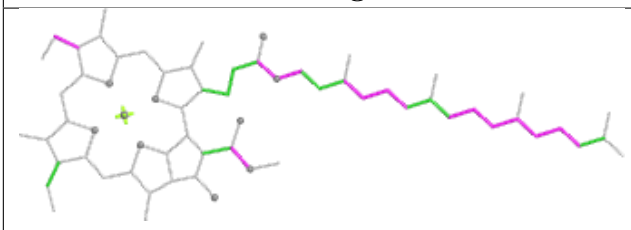
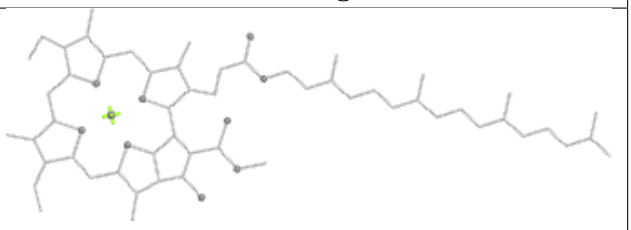
Rings

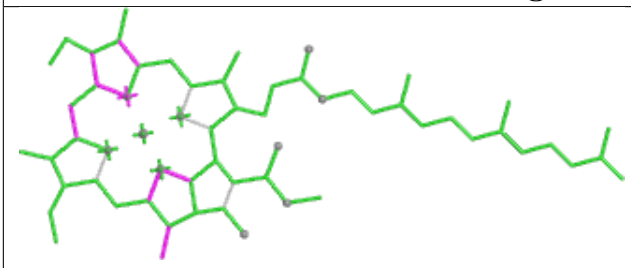
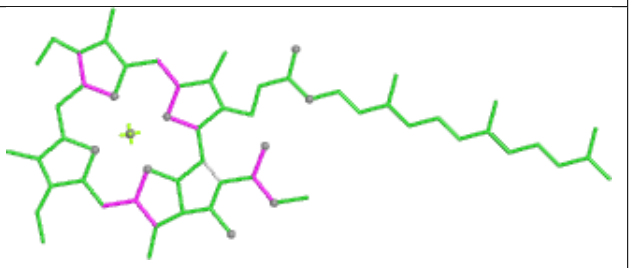
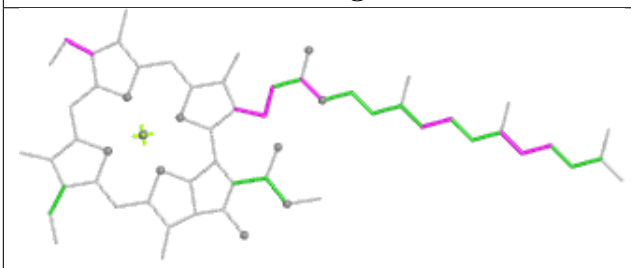
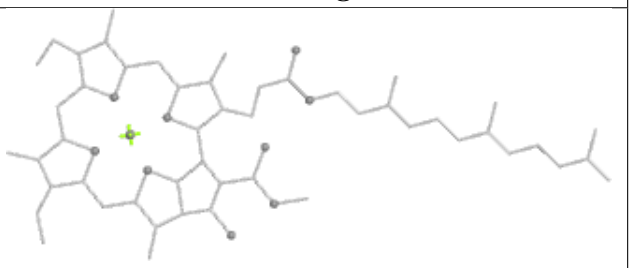
Ligand DD6 O 303



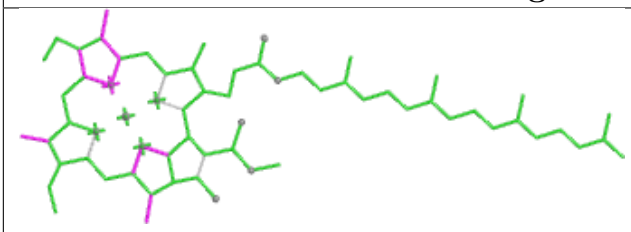
Ligand CLA 8 318



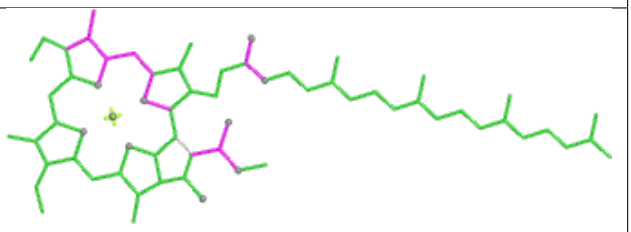
Ligand CLA I 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

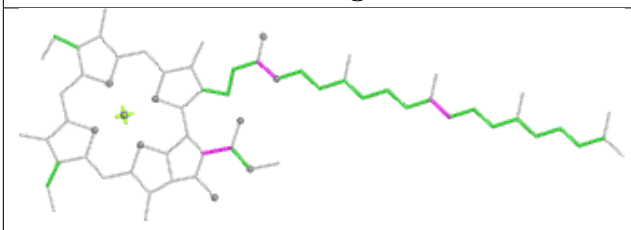
Ligand CLA a 827



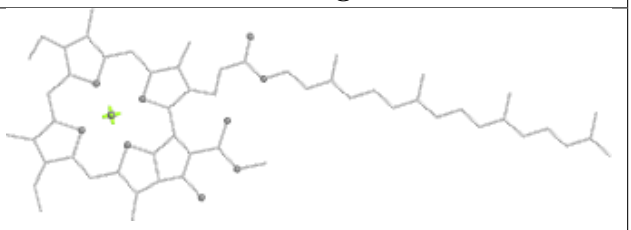
Bond lengths



Bond angles

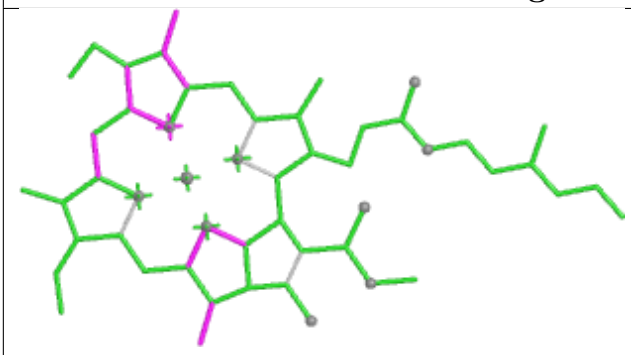


Torsions

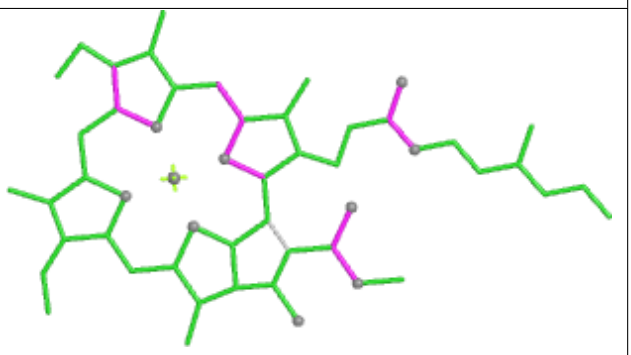


Rings

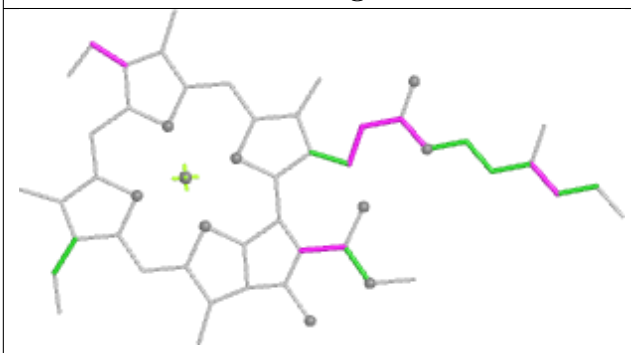
Ligand CLA 5 316



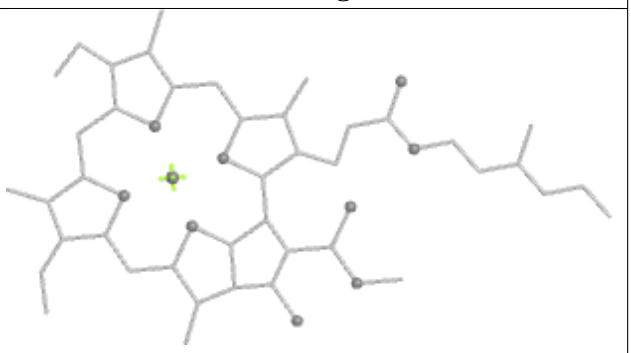
Bond lengths



Bond angles

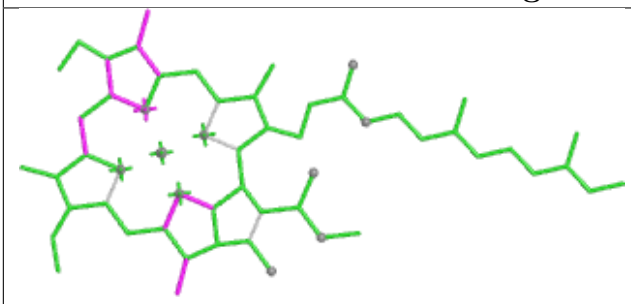


Torsions

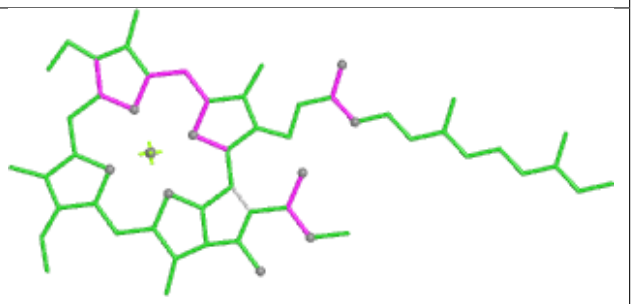


Rings

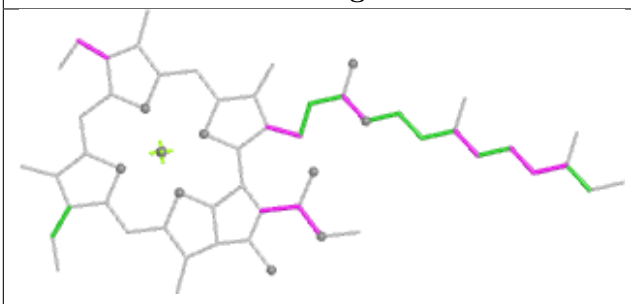
Ligand CLA G 309



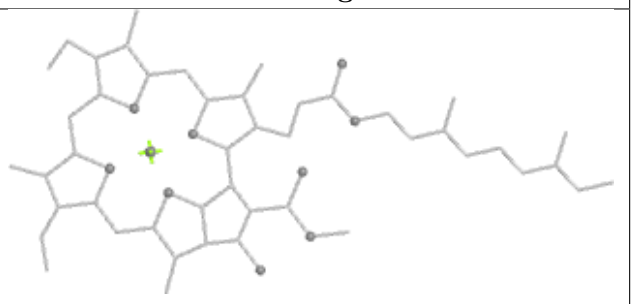
Bond lengths



Bond angles

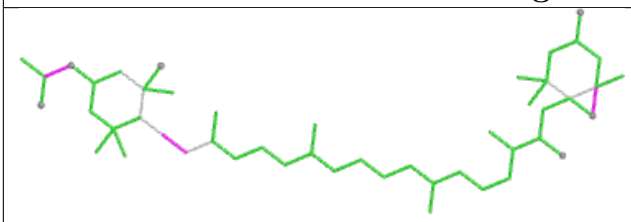


Torsions

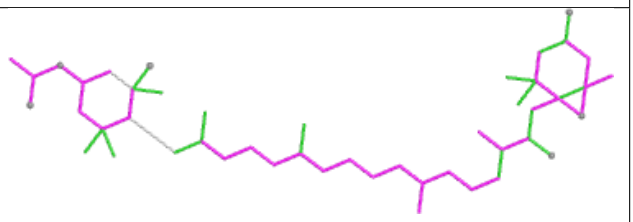


Rings

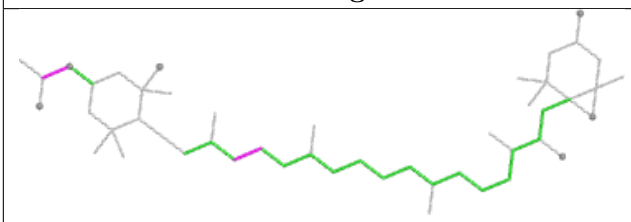
Ligand A86 L 307



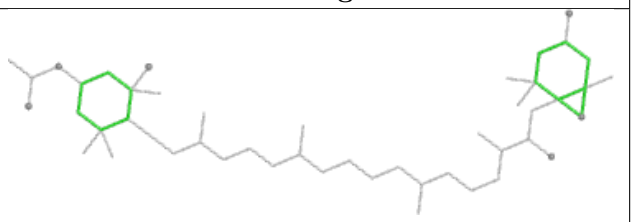
Bond lengths



Bond angles

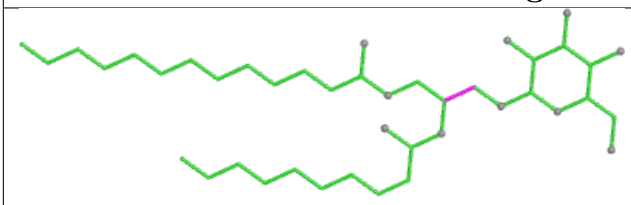


Torsions

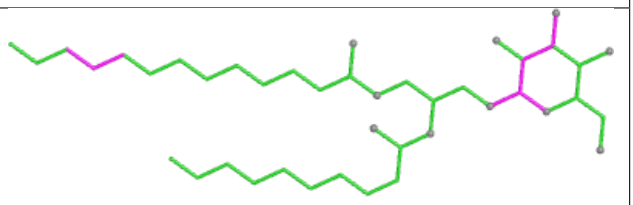


Rings

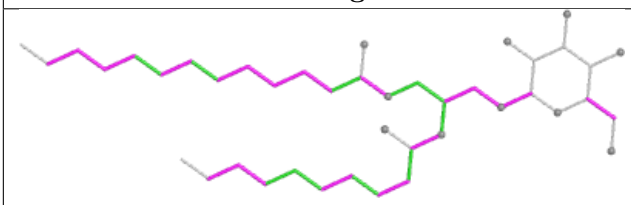
Ligand LMG I 302



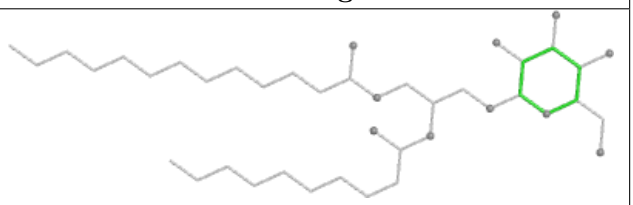
Bond lengths



Bond angles

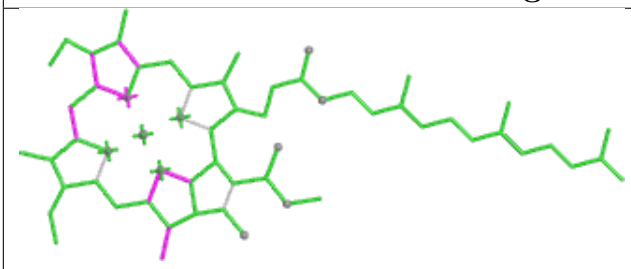


Torsions

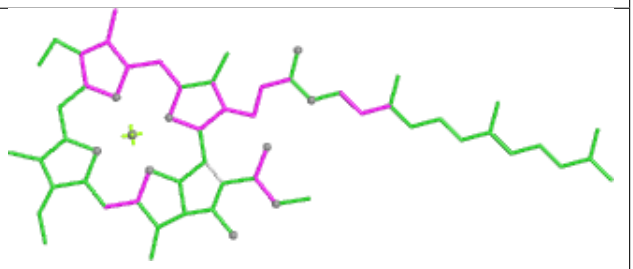


Rings

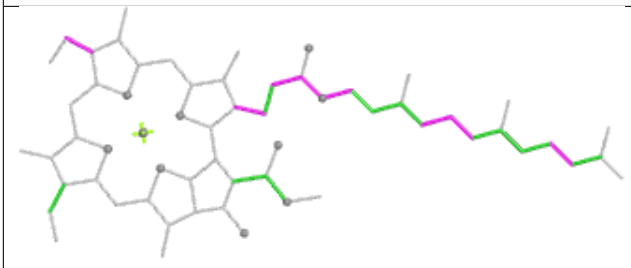
Ligand CLA V 310



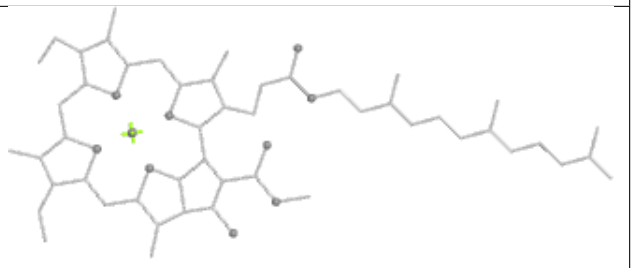
Bond lengths



Bond angles

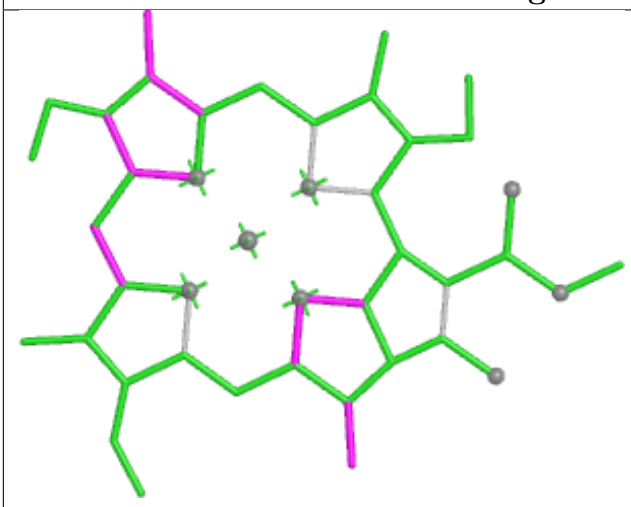


Torsions

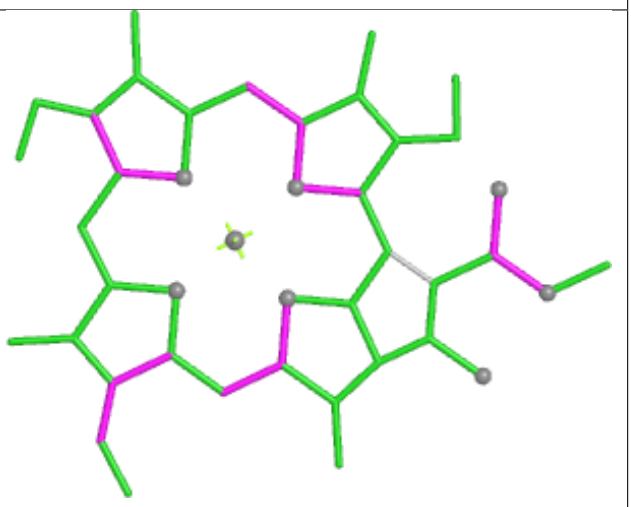


Rings

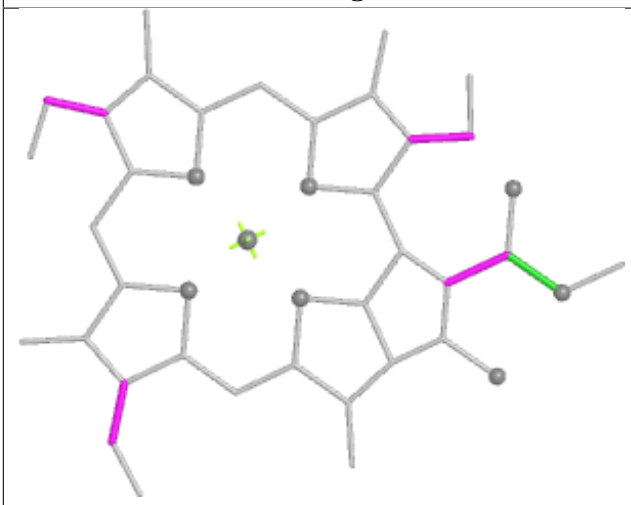
Ligand CLA 9 312



Bond lengths



Bond angles

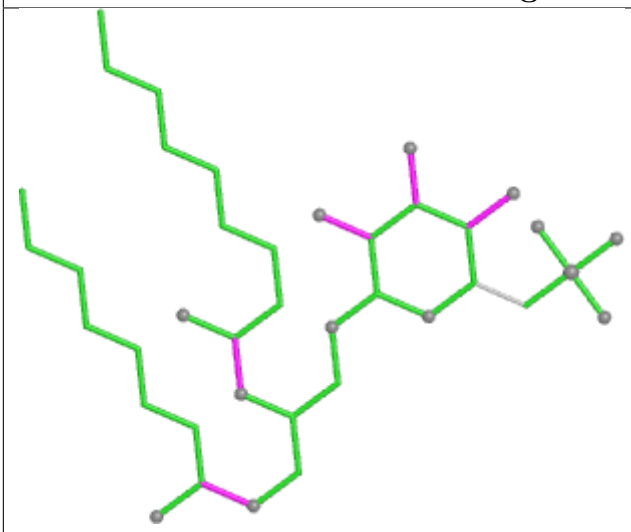


Torsions

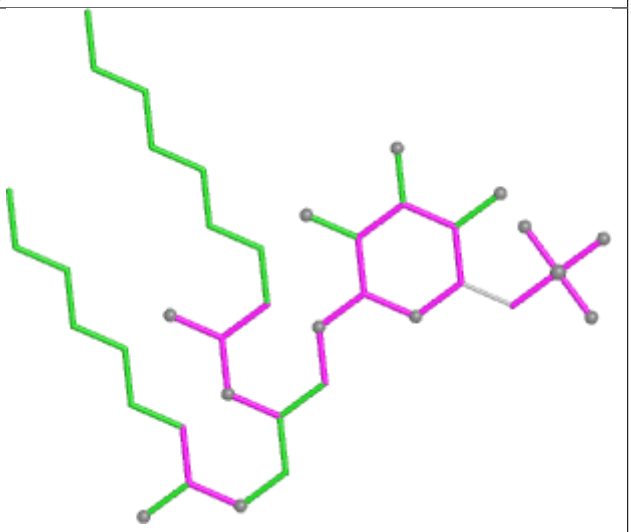


Rings

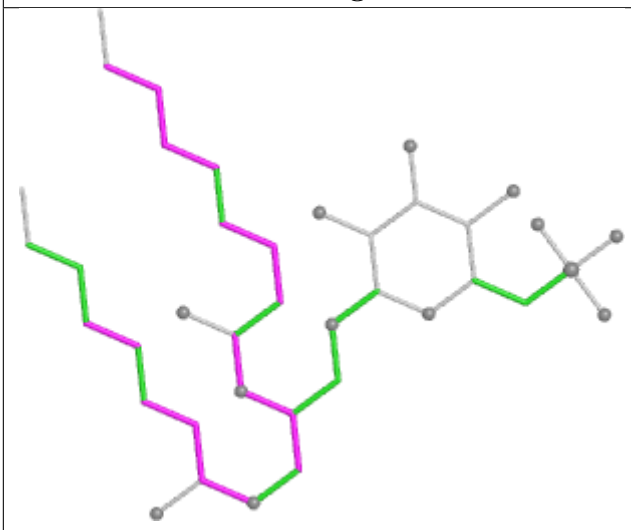
Ligand SQD M 301



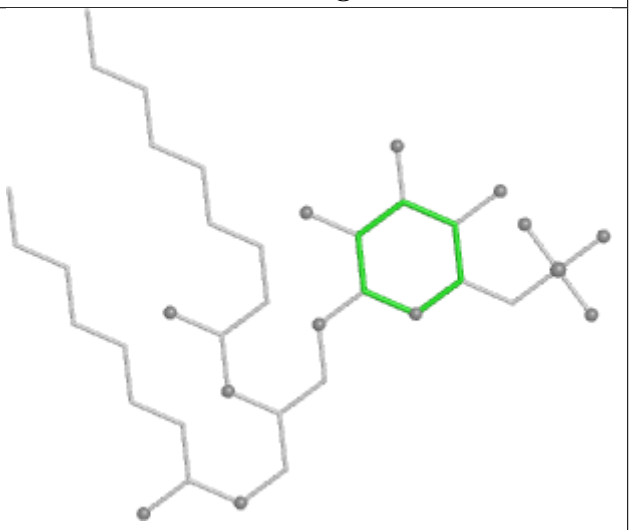
Bond lengths



Bond angles

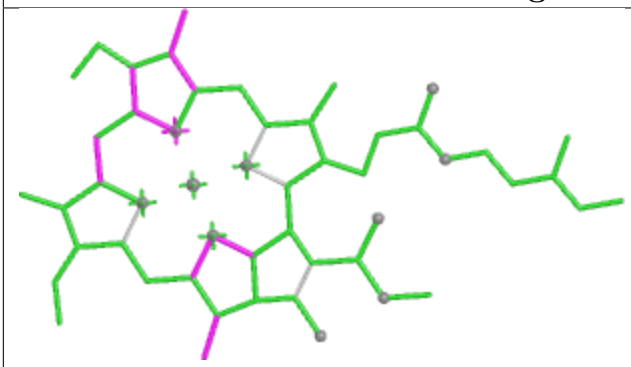


Torsions

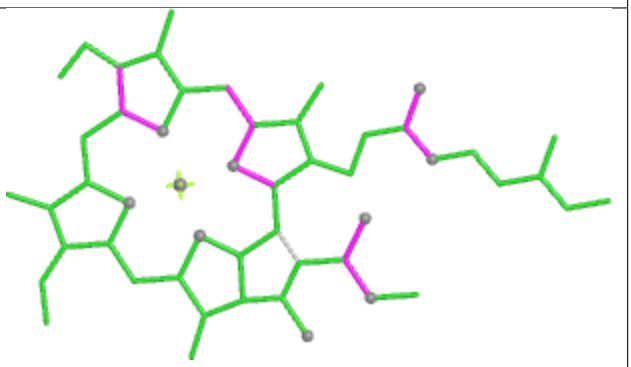


Rings

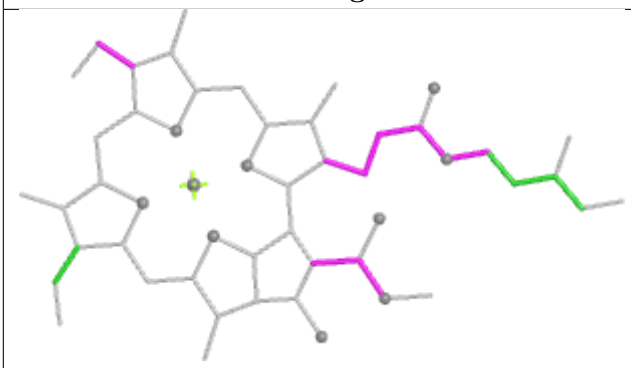
Ligand CLA 1 319



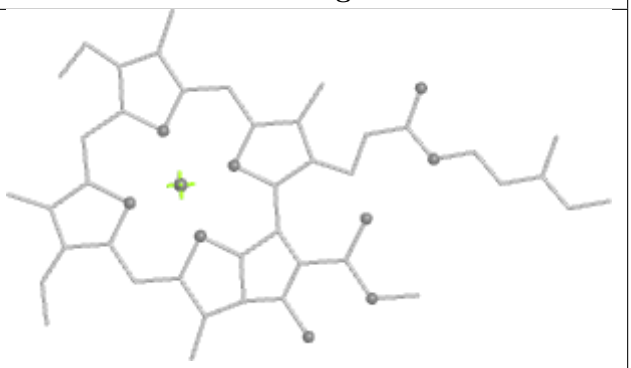
Bond lengths



Bond angles

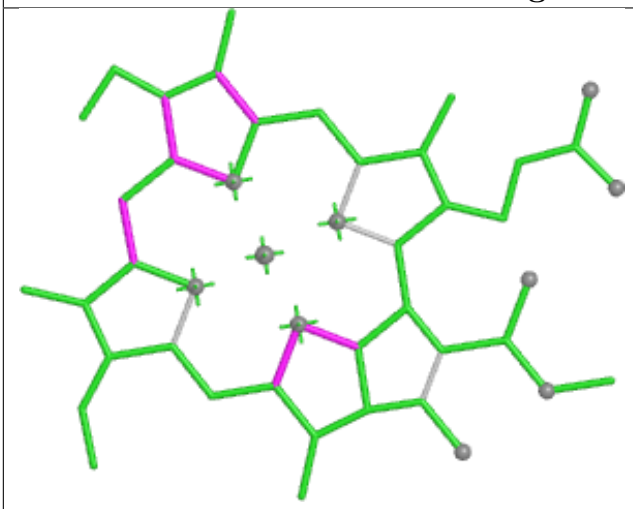


Torsions

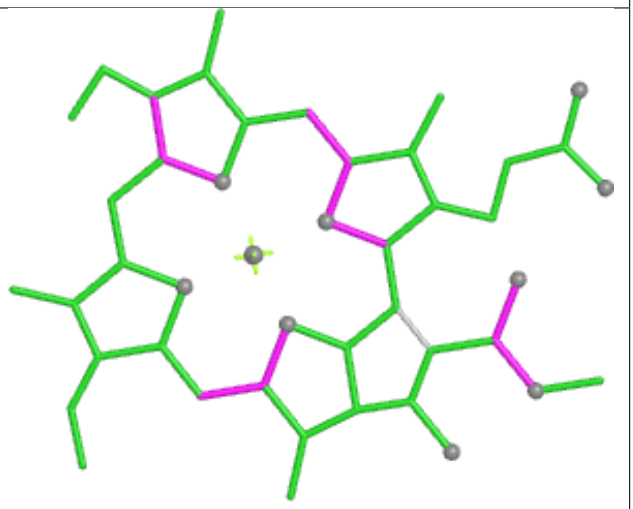


Rings

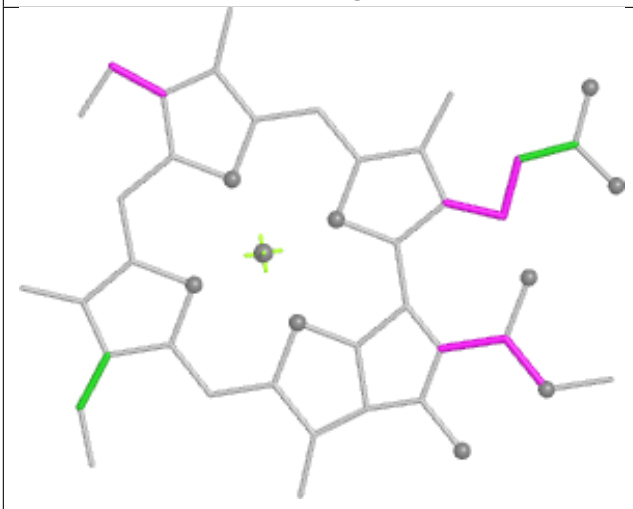
Ligand CLA 9 319



Bond lengths



Bond angles

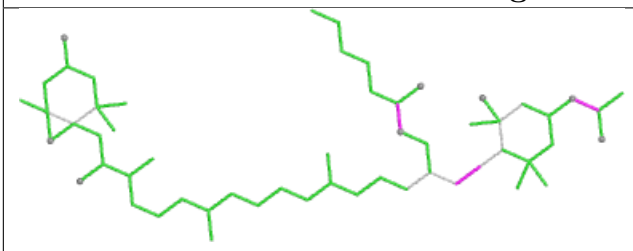


Torsions

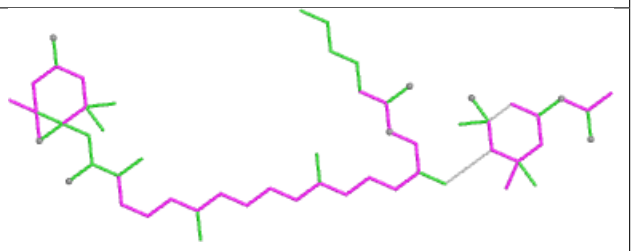


Rings

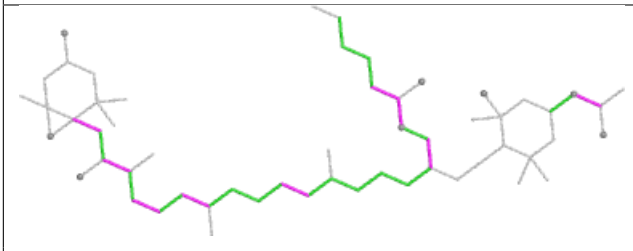
Ligand A1EB1 9 302



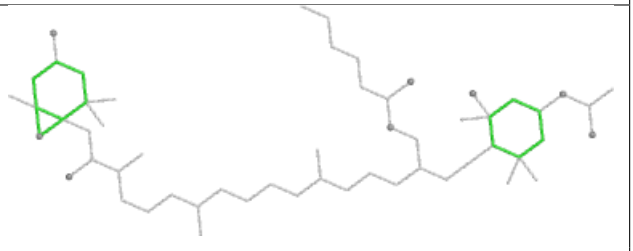
Bond lengths



Bond angles

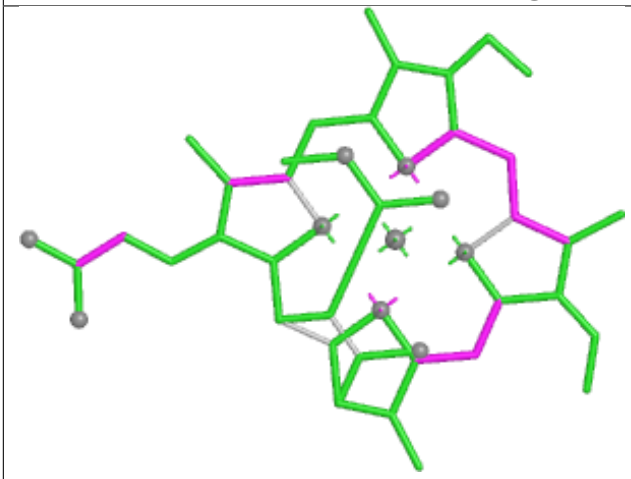


Torsions

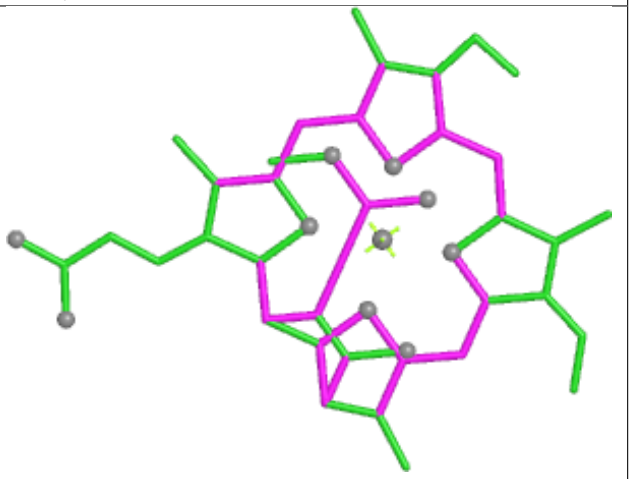


Rings

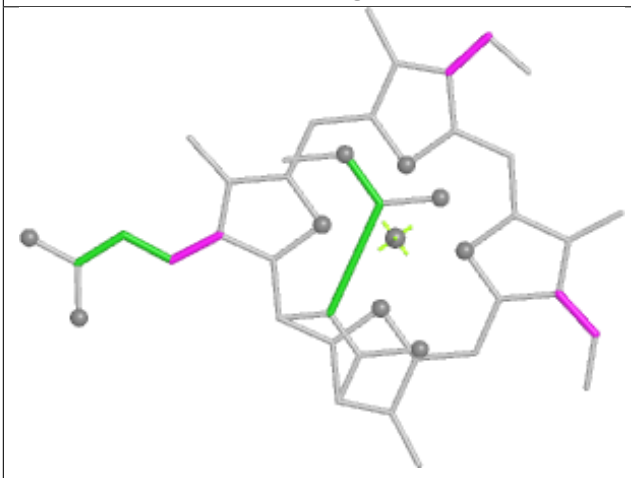
Ligand KC2 Q 318



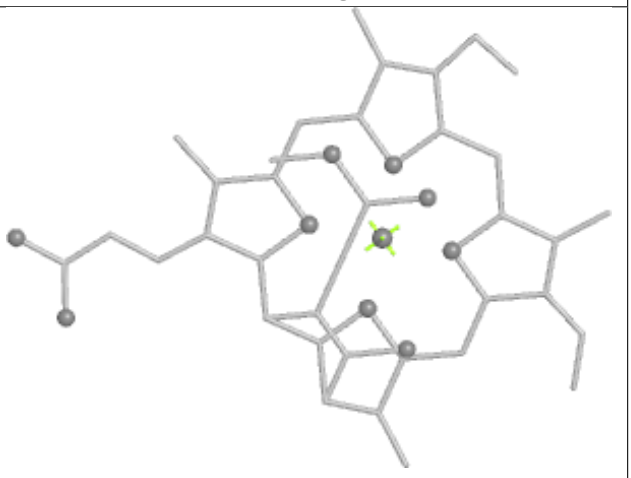
Bond lengths



Bond angles

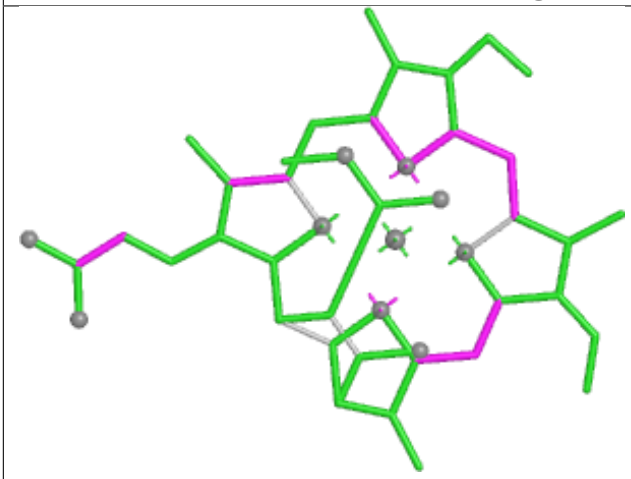


Torsions

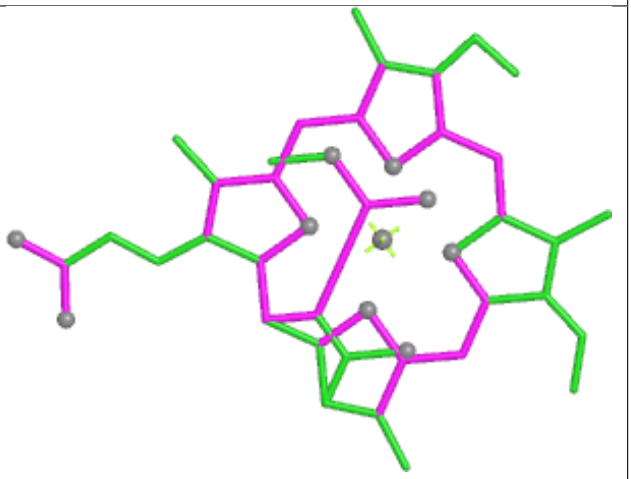


Rings

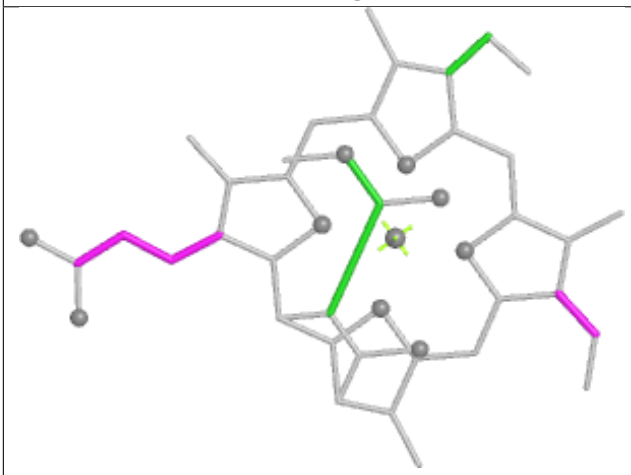
Ligand KC2 3 318



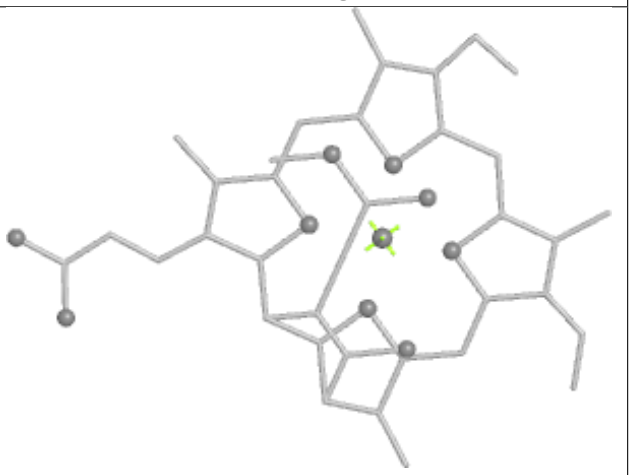
Bond lengths



Bond angles

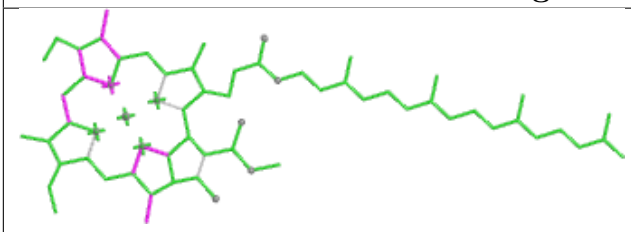


Torsions

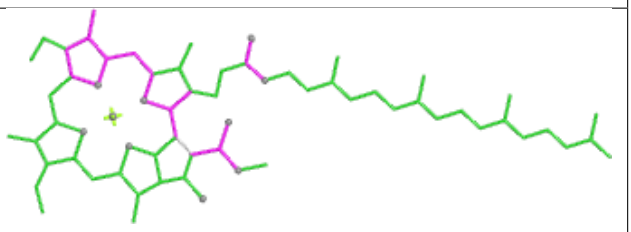


Rings

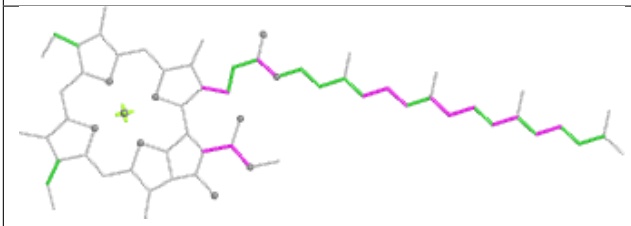
Ligand CLA i 103



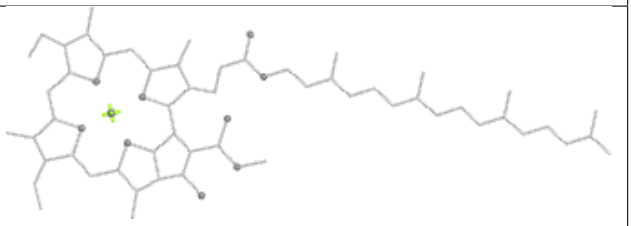
Bond lengths



Bond angles

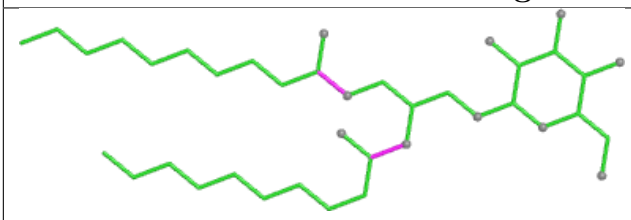


Torsions

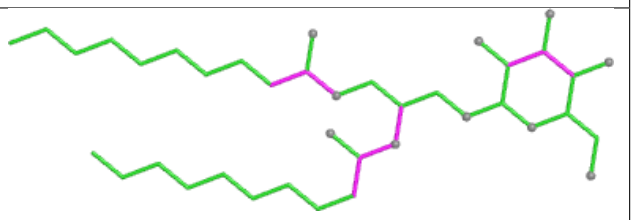


Rings

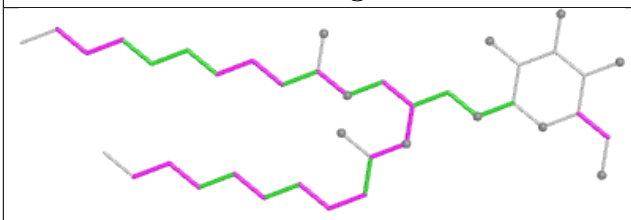
Ligand LMG W 302



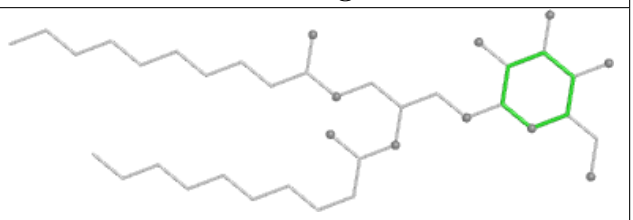
Bond lengths



Bond angles

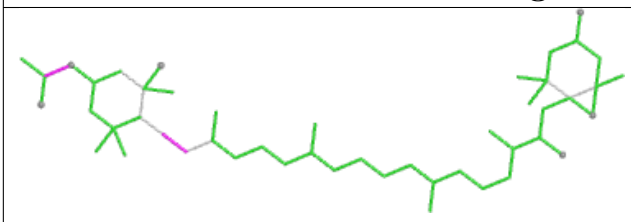


Torsions

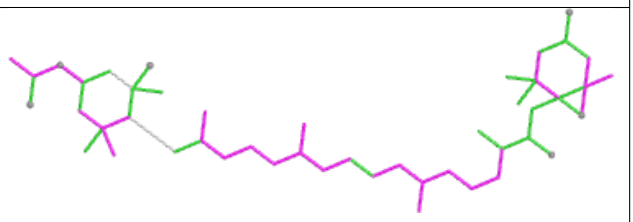


Rings

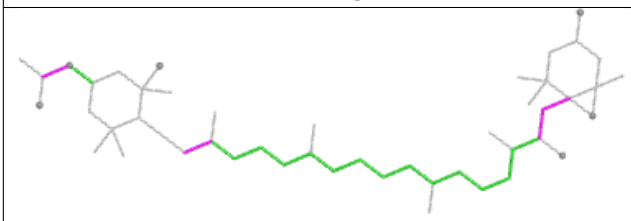
Ligand A86 X 302



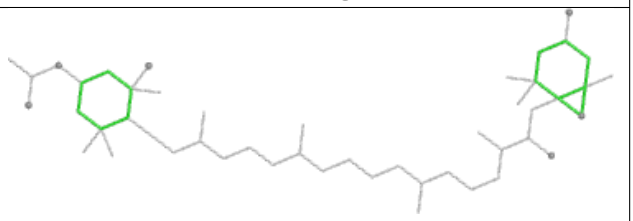
Bond lengths



Bond angles

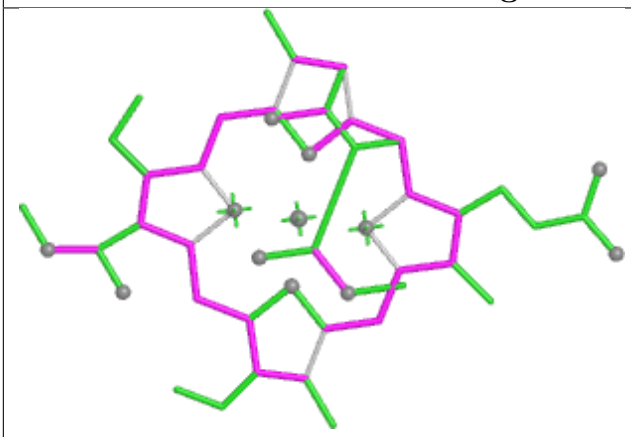


Torsions

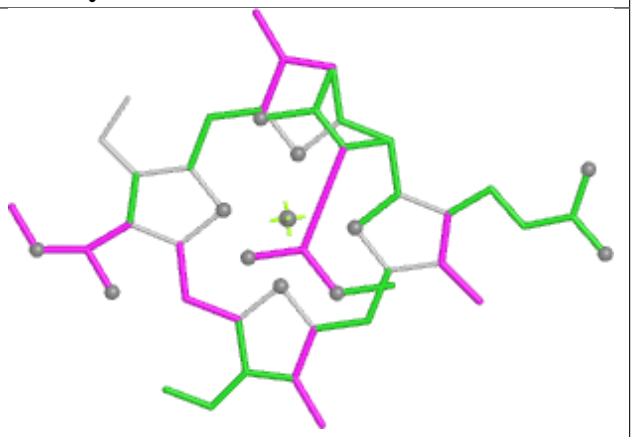


Rings

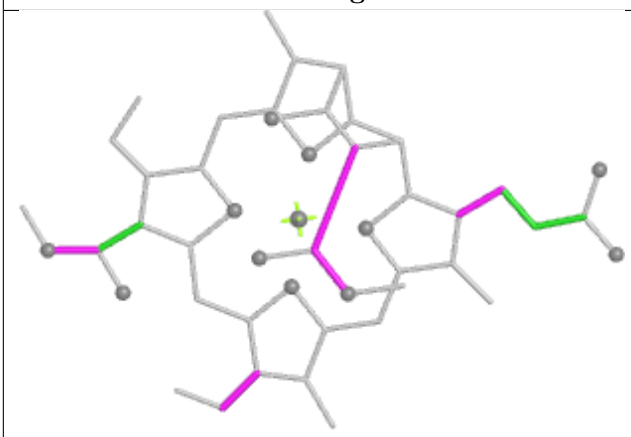
Ligand A1ECV Q 316



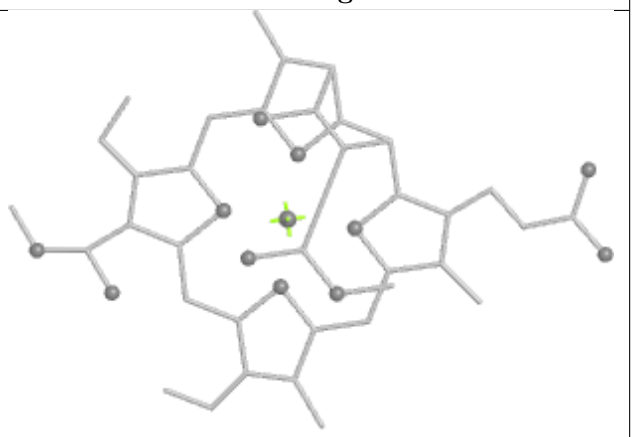
Bond lengths



Bond angles

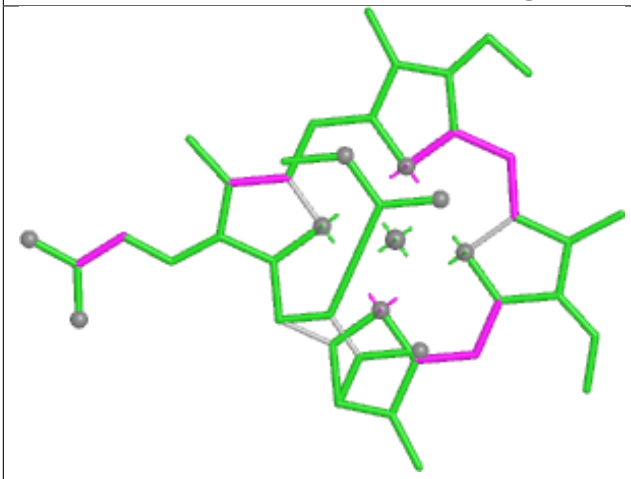


Torsions

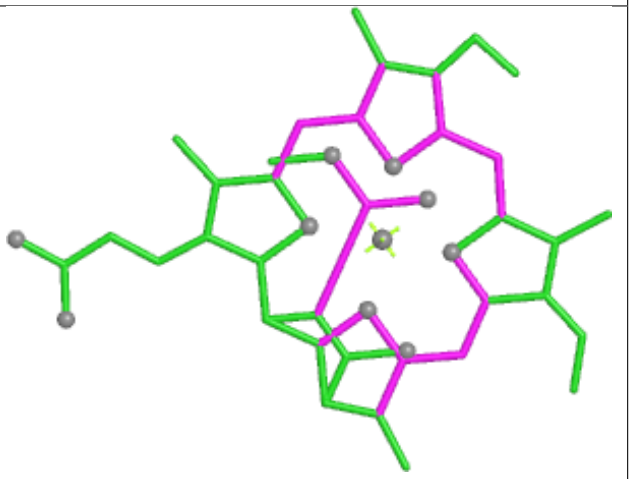


Rings

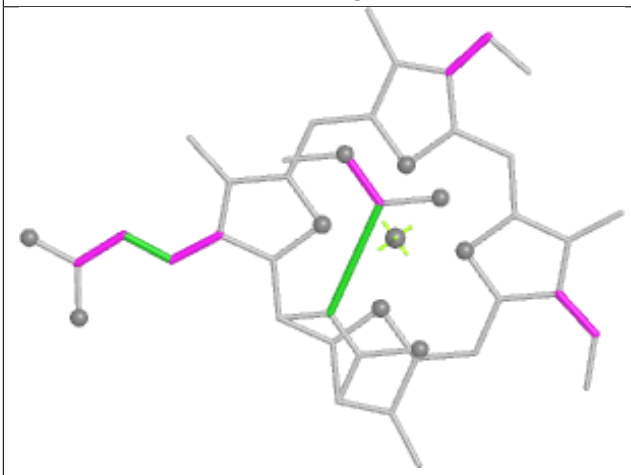
Ligand KC2 W 315



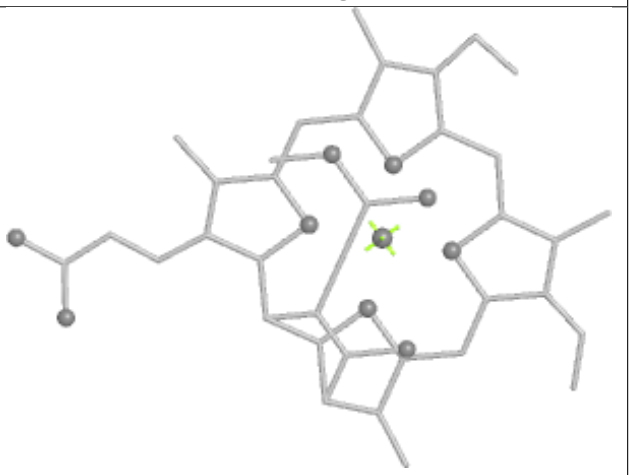
Bond lengths



Bond angles

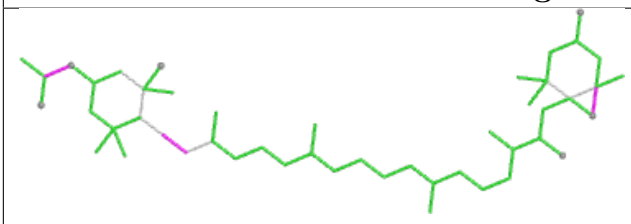


Torsions



Rings

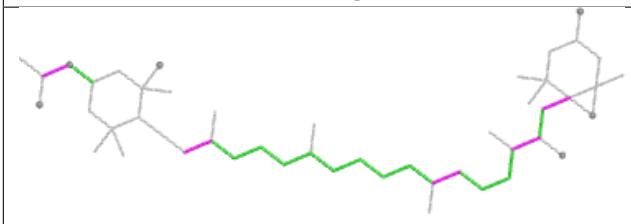
Ligand A86 8 305



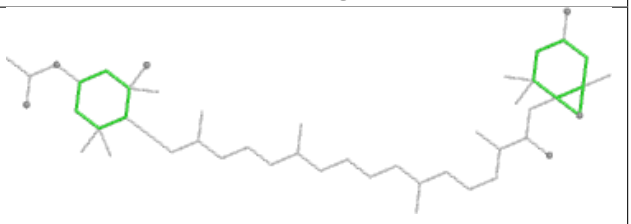
Bond lengths



Bond angles

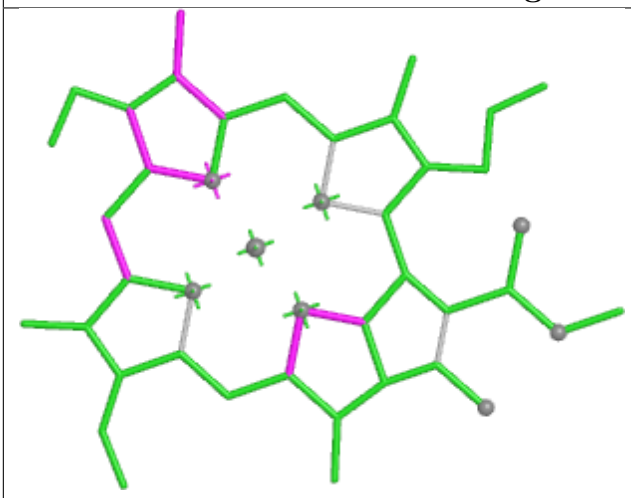


Torsions

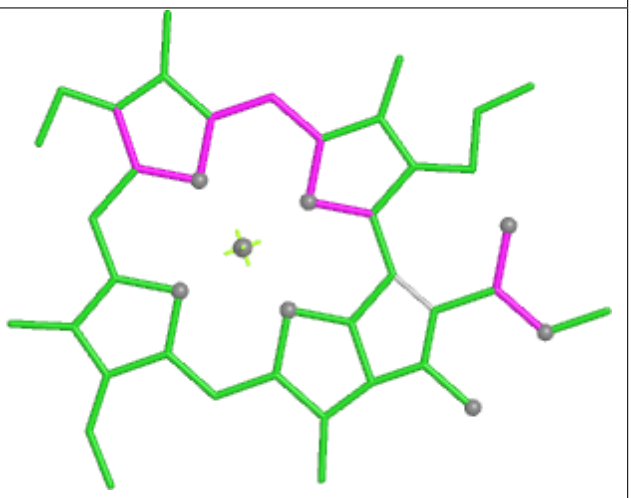


Rings

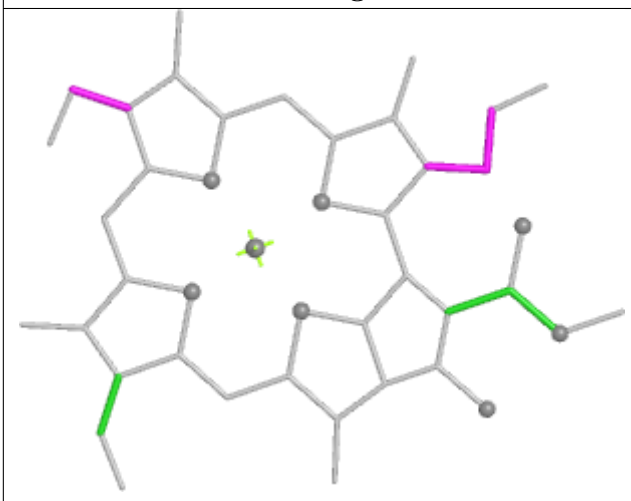
Ligand CLA C 304



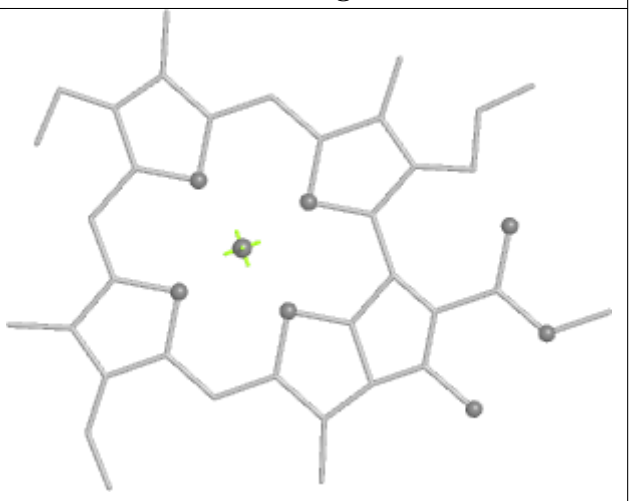
Bond lengths



Bond angles

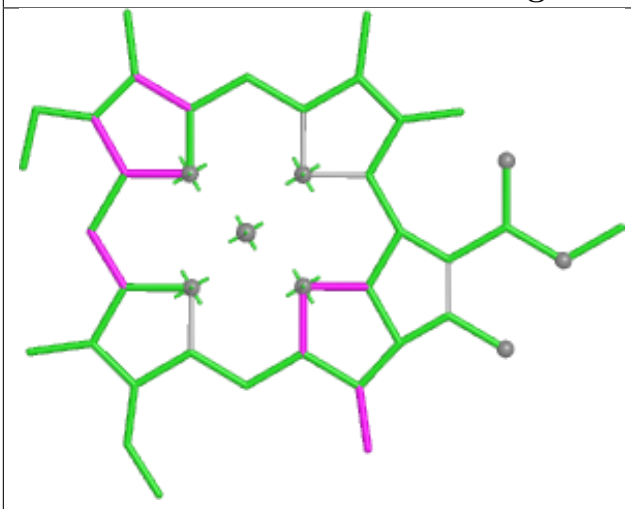


Torsions

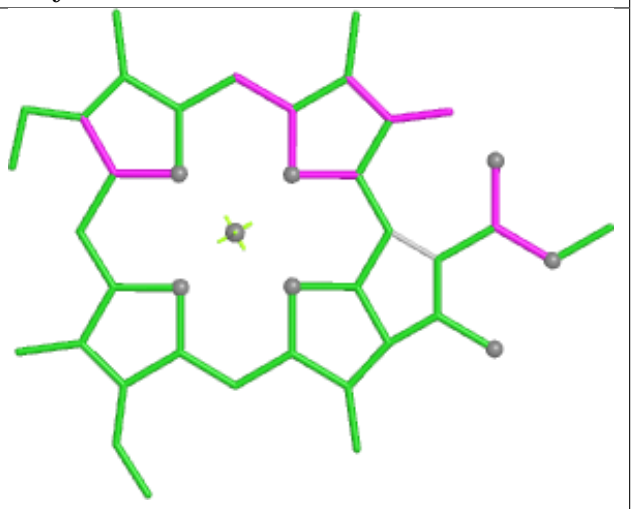


Rings

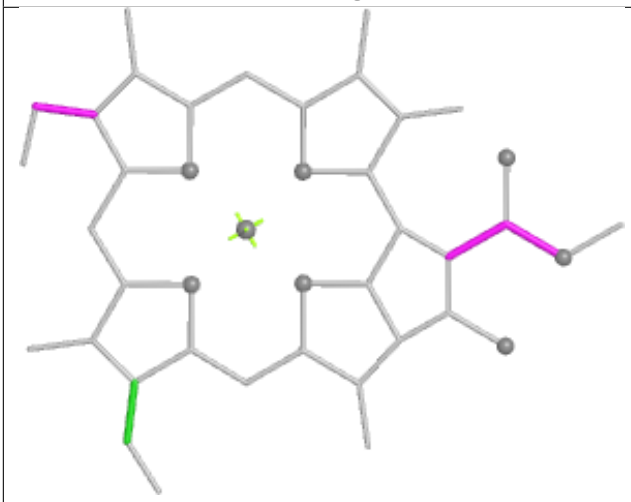
Ligand CLA y 315



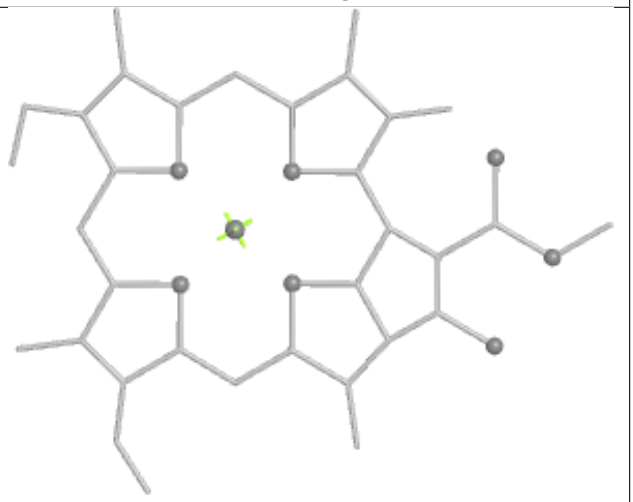
Bond lengths



Bond angles

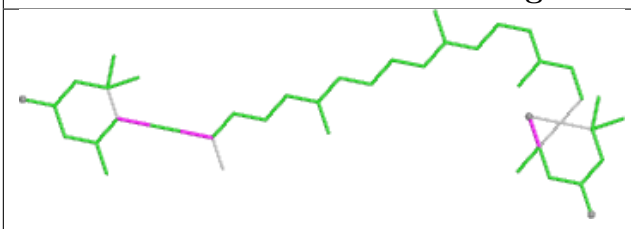


Torsions

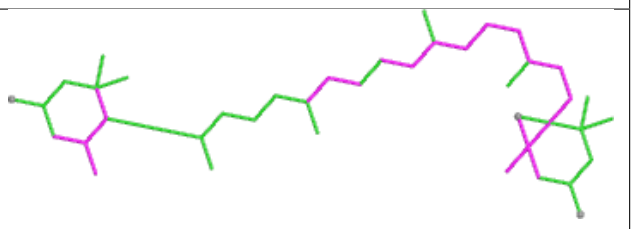


Rings

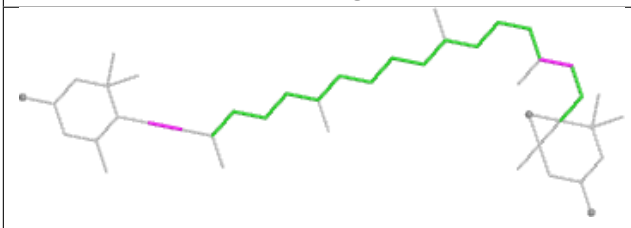
Ligand DD6 B 202



Bond lengths



Bond angles

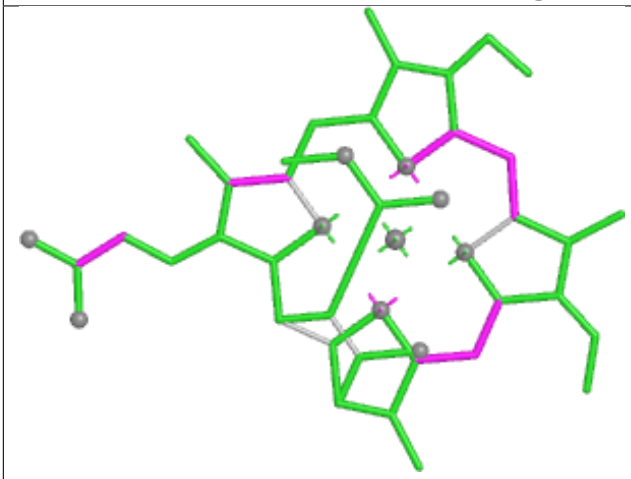


Torsions

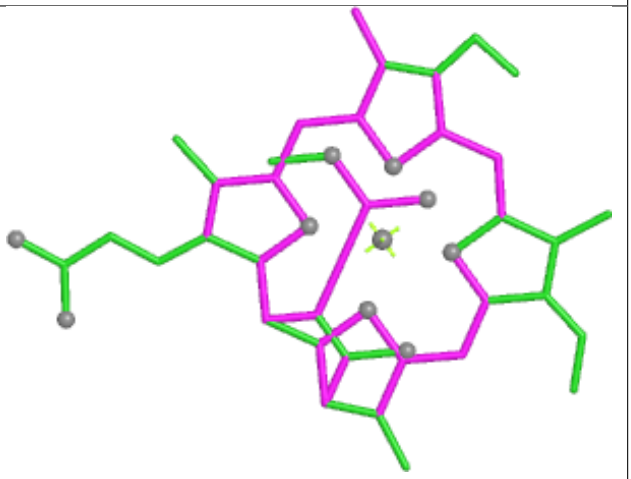


Rings

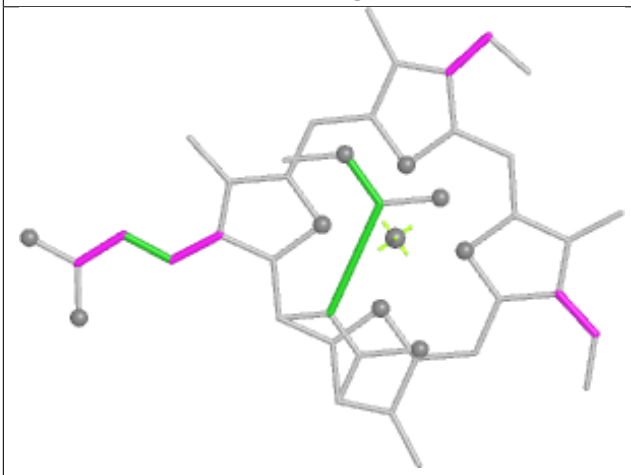
Ligand KC2 3 317



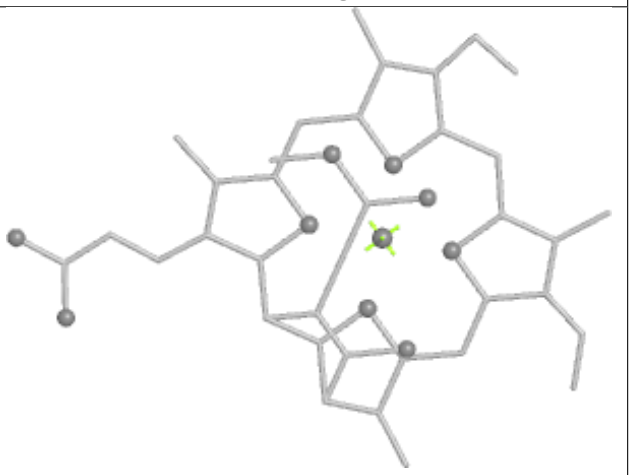
Bond lengths



Bond angles

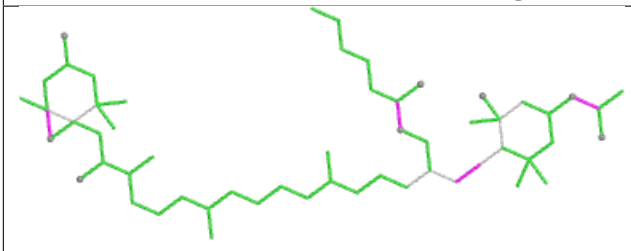


Torsions

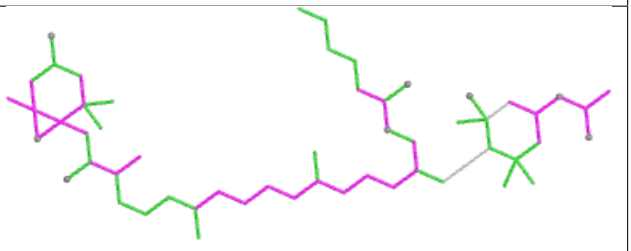


Rings

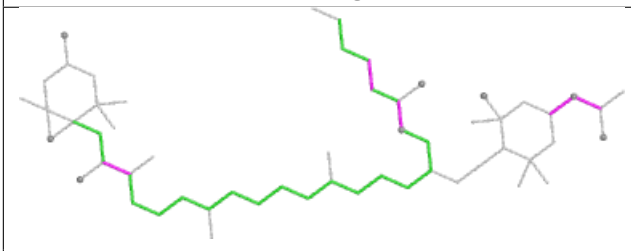
Ligand A1EB1 3 303



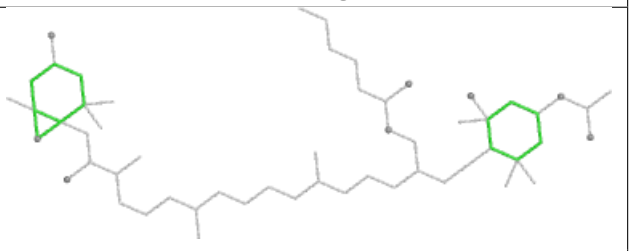
Bond lengths



Bond angles

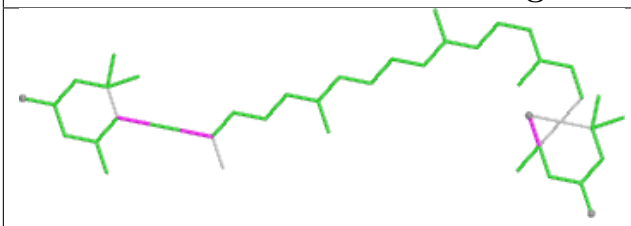


Torsions

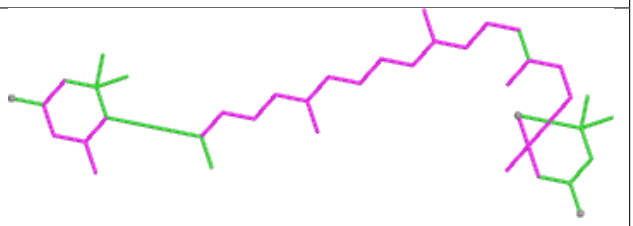


Rings

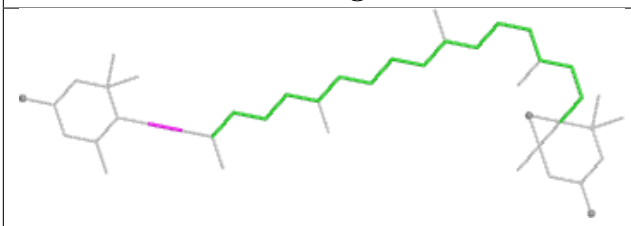
Ligand DD6 F 305



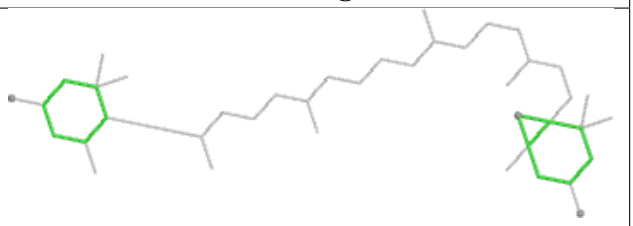
Bond lengths



Bond angles

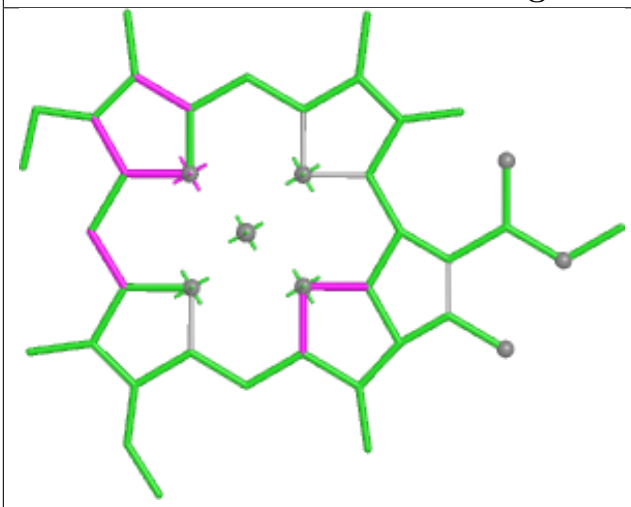


Torsions

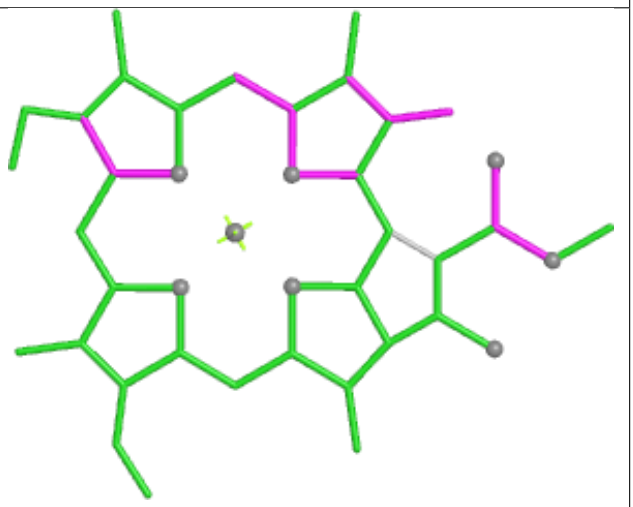


Rings

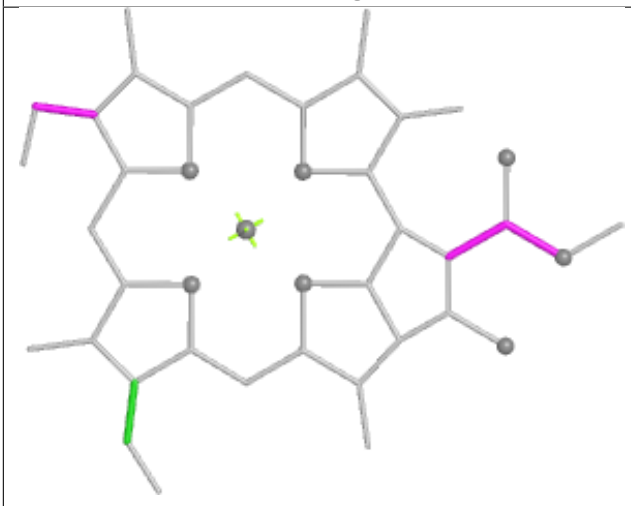
Ligand CLA 2 316



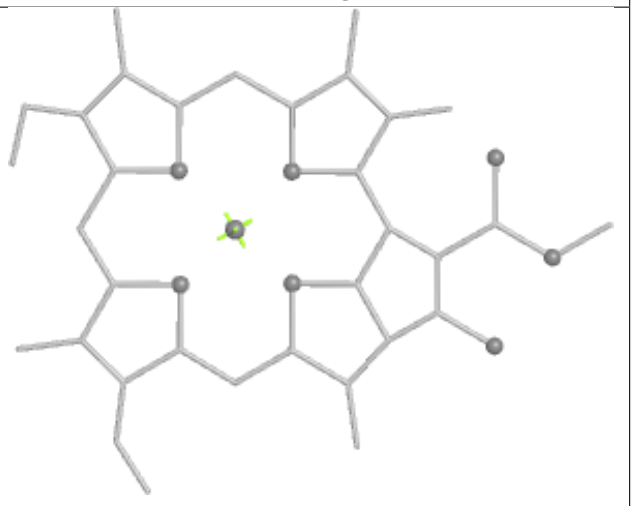
Bond lengths



Bond angles

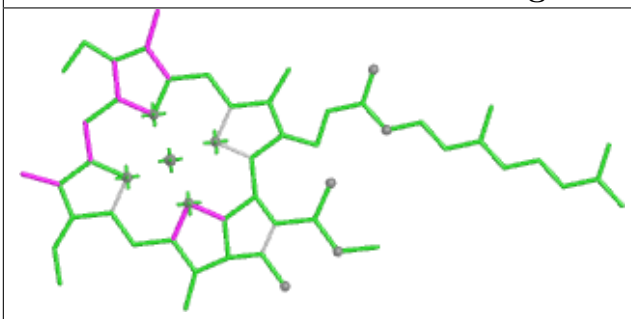


Torsions

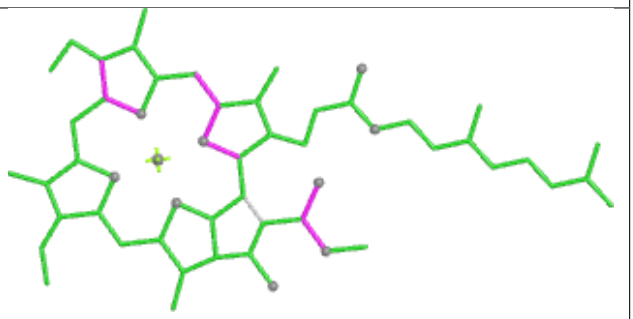


Rings

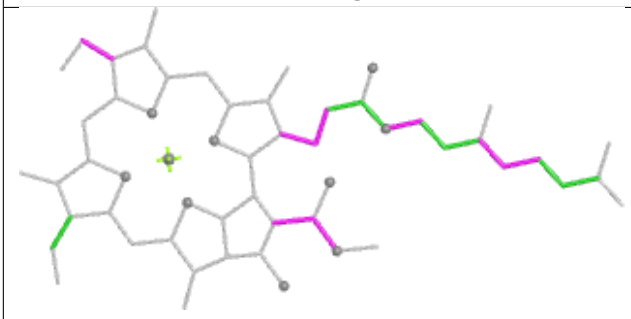
Ligand CLA a 821



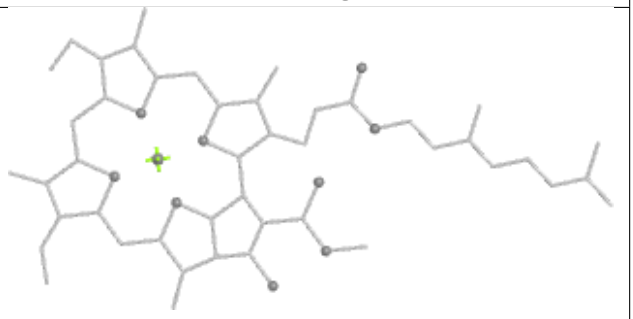
Bond lengths



Bond angles

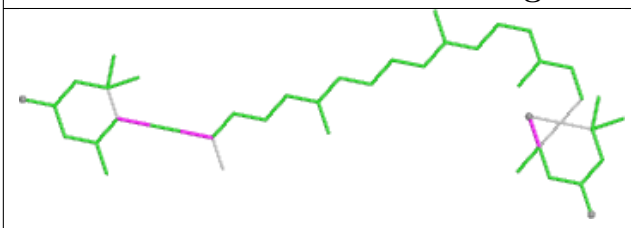


Torsions

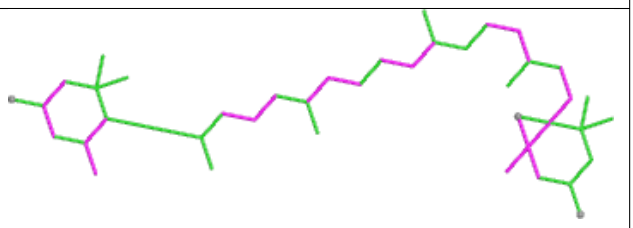


Rings

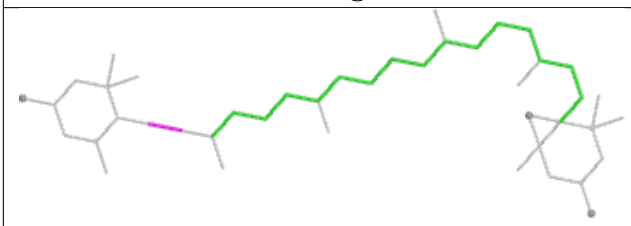
Ligand DD6 H 303



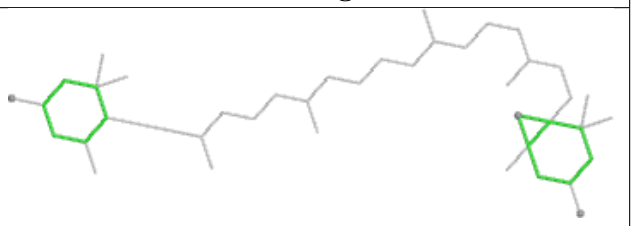
Bond lengths



Bond angles

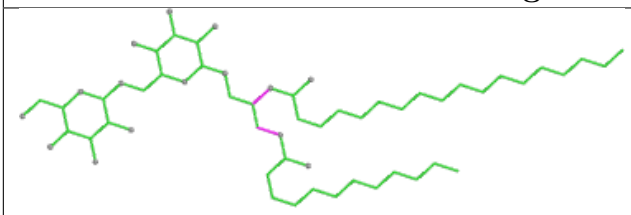


Torsions

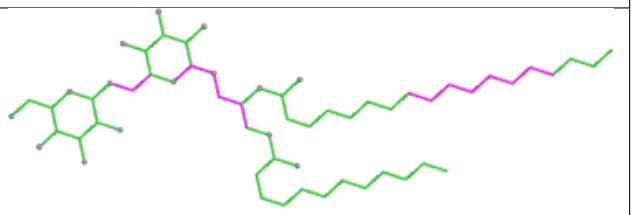


Rings

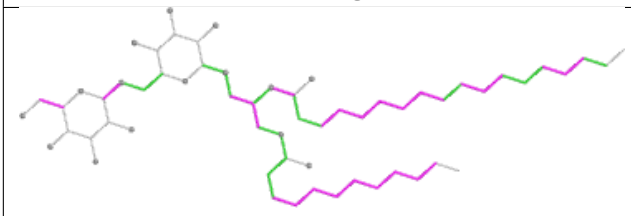
Ligand DGD b 849



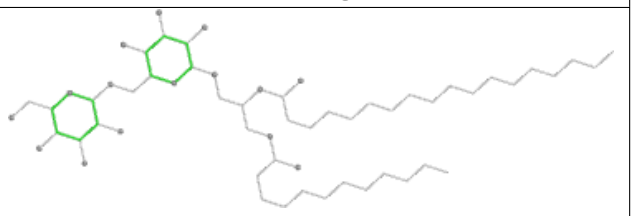
Bond lengths



Bond angles

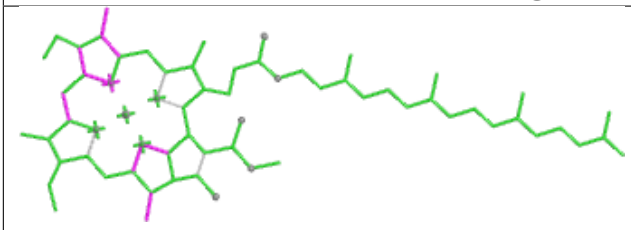


Torsions

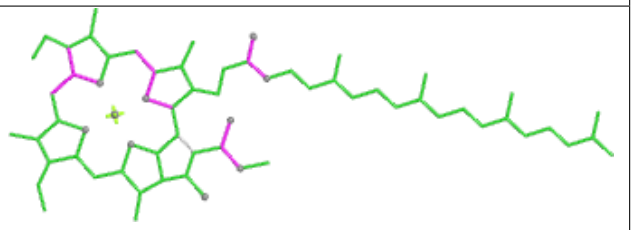


Rings

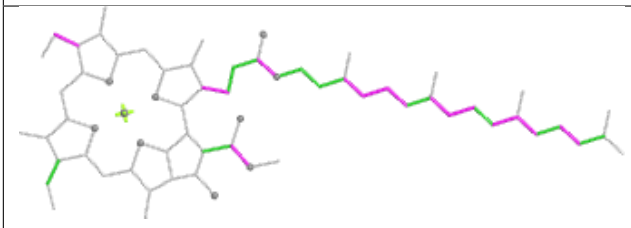
Ligand CLA a 804



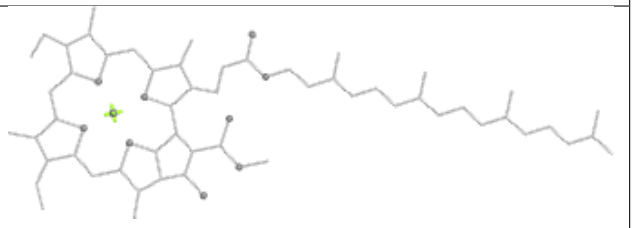
Bond lengths



Bond angles

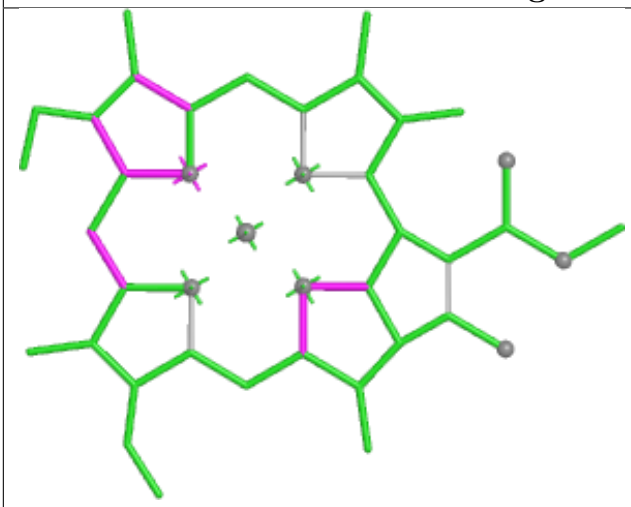


Torsions

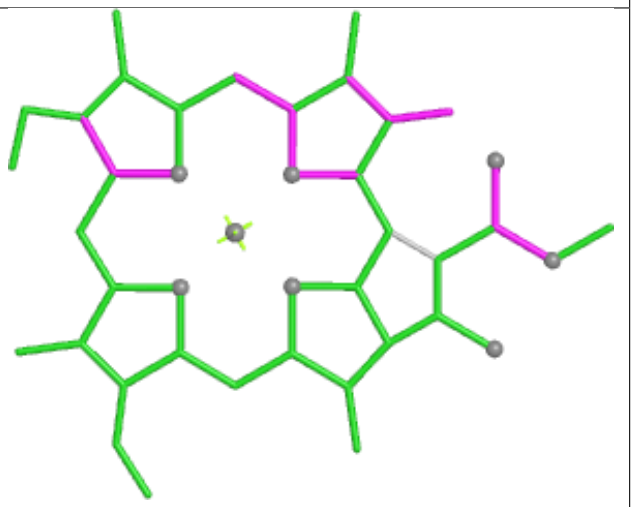


Rings

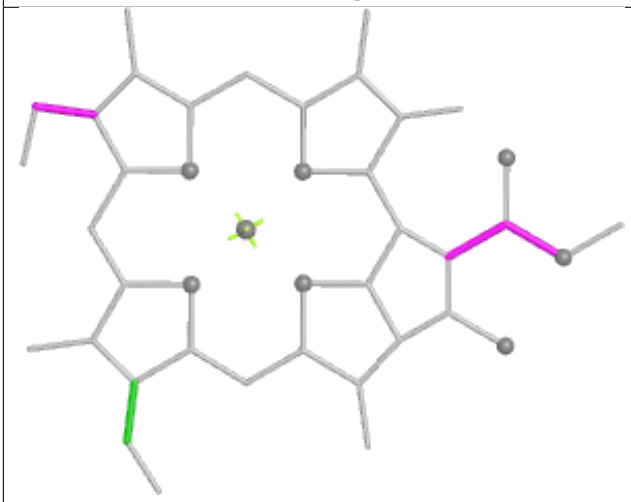
Ligand CLA 1 308



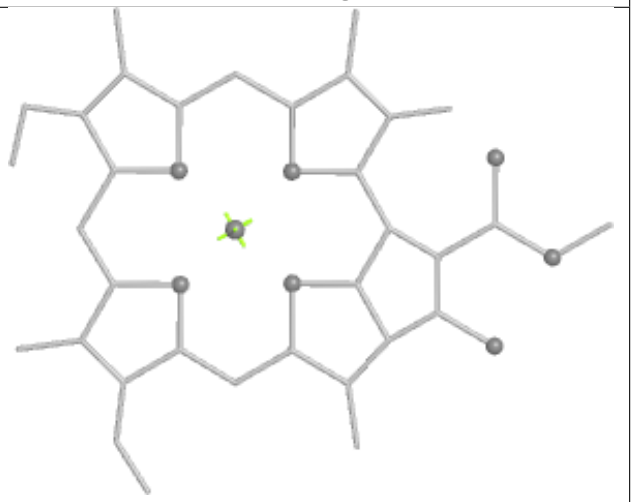
Bond lengths



Bond angles

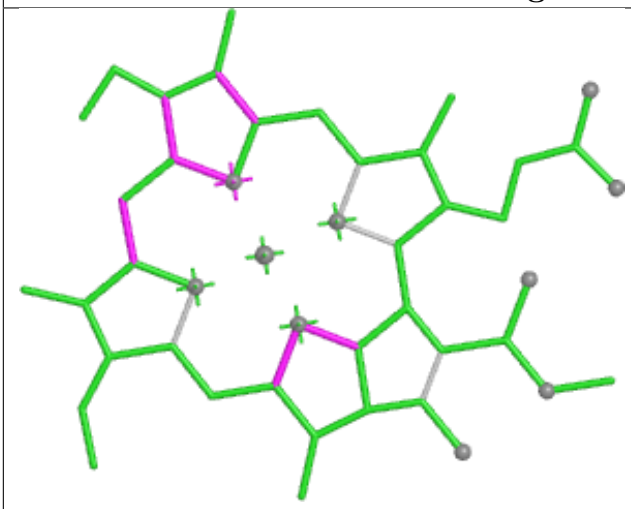


Torsions

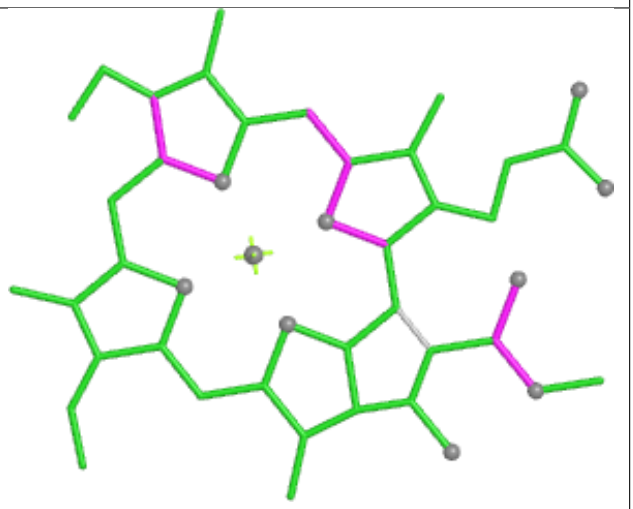


Rings

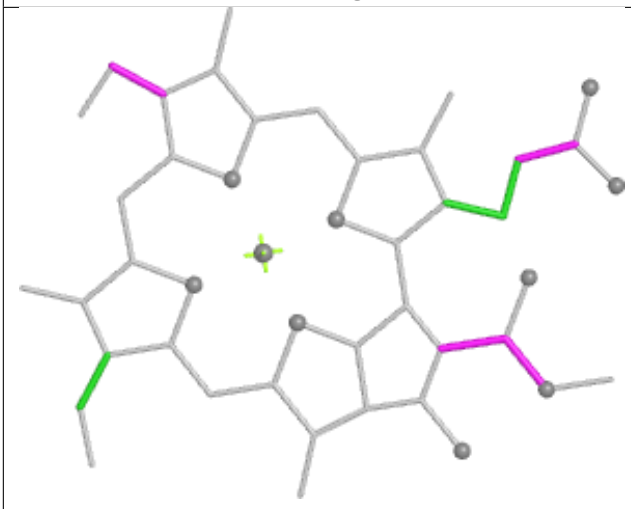
Ligand CLA x 306



Bond lengths



Bond angles

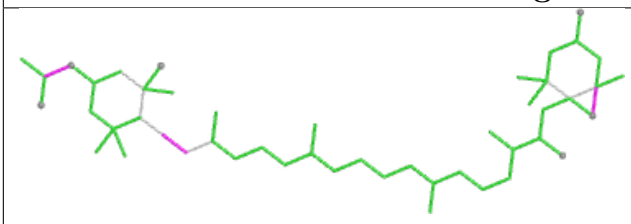


Torsions

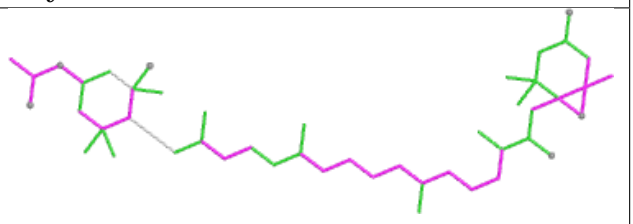


Rings

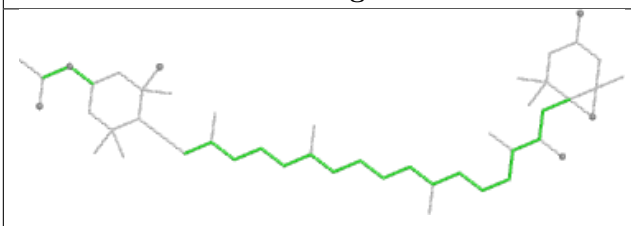
Ligand A86 y 305



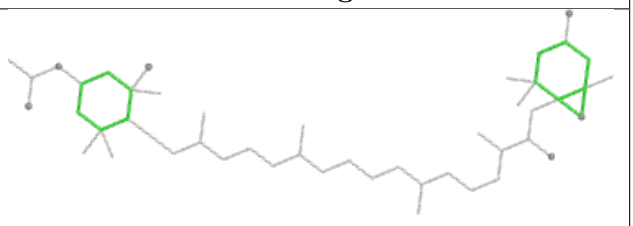
Bond lengths



Bond angles

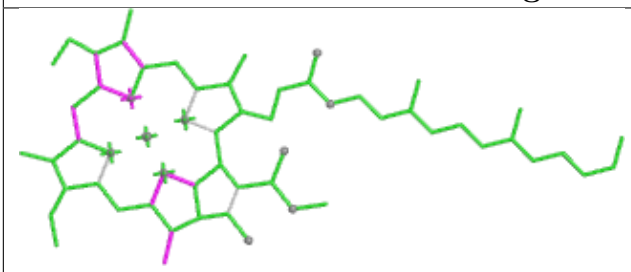


Torsions

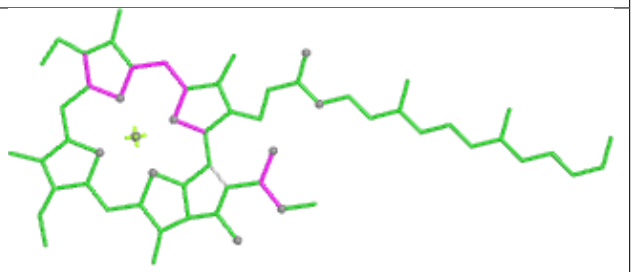


Rings

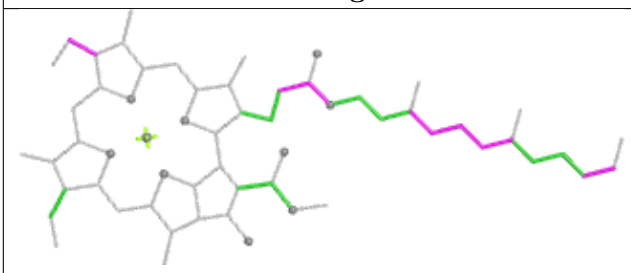
Ligand CLA K 308



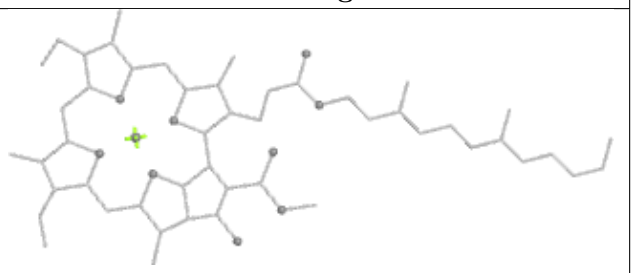
Bond lengths



Bond angles

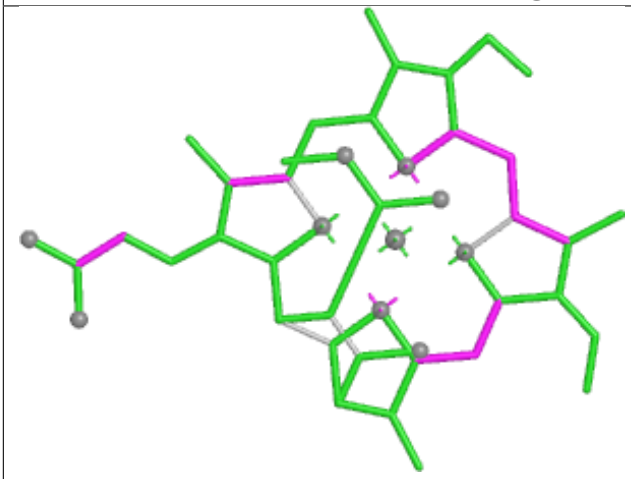


Torsions

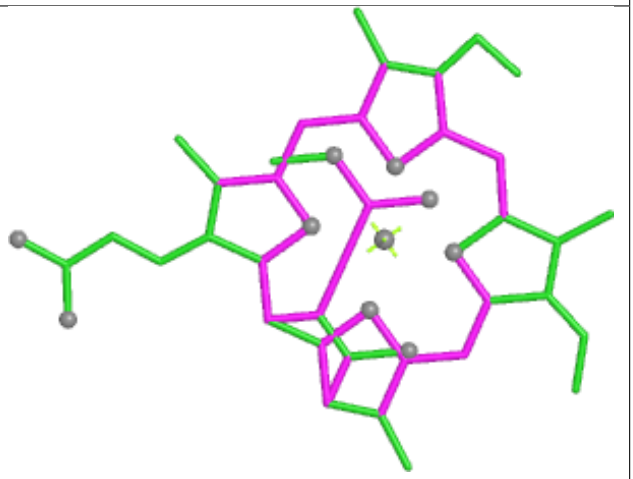


Rings

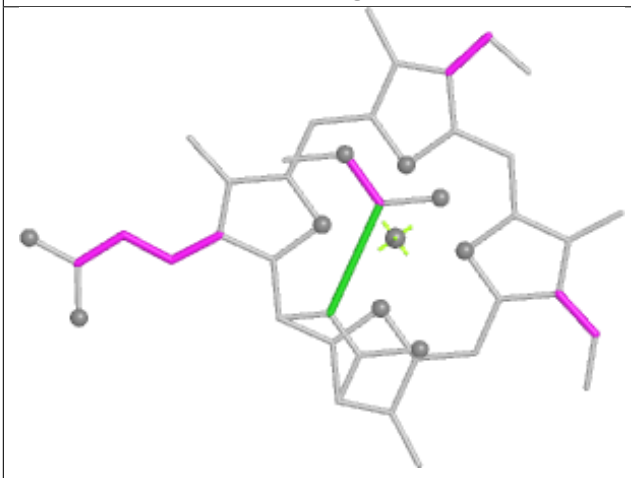
Ligand KC2 Z 310



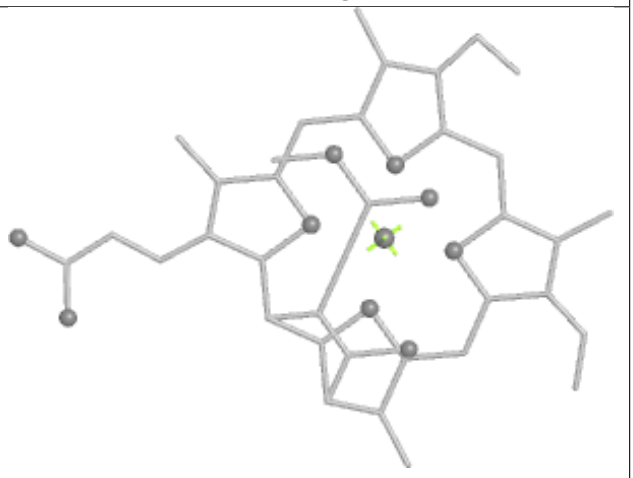
Bond lengths



Bond angles

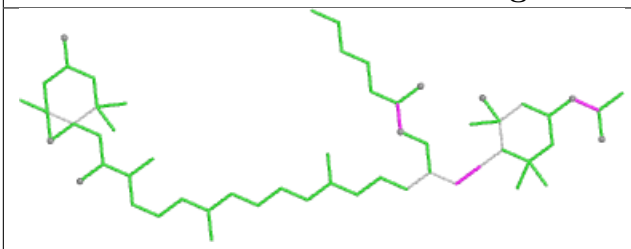


Torsions

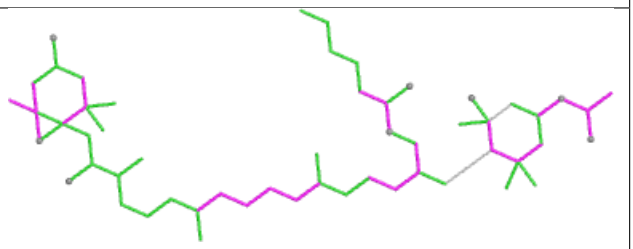


Rings

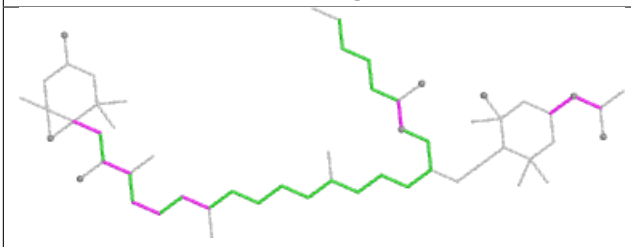
Ligand A1EB1 4 303



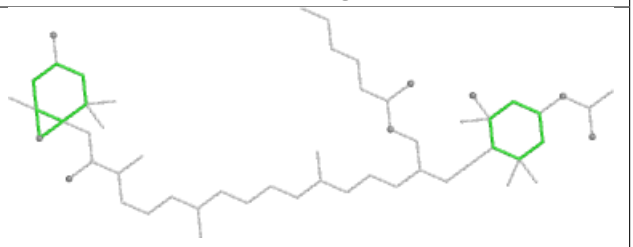
Bond lengths



Bond angles

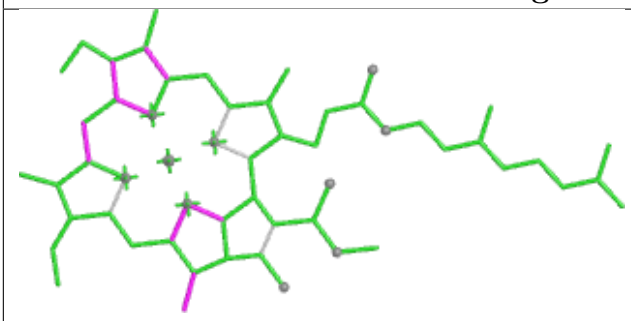


Torsions

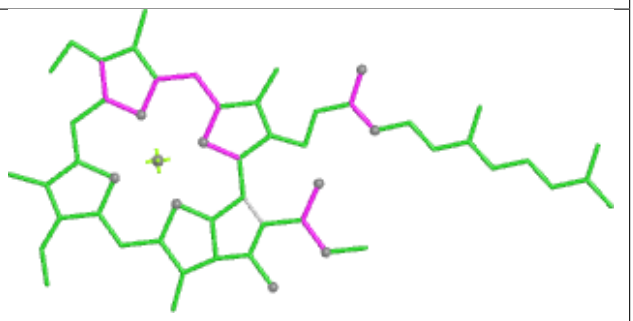


Rings

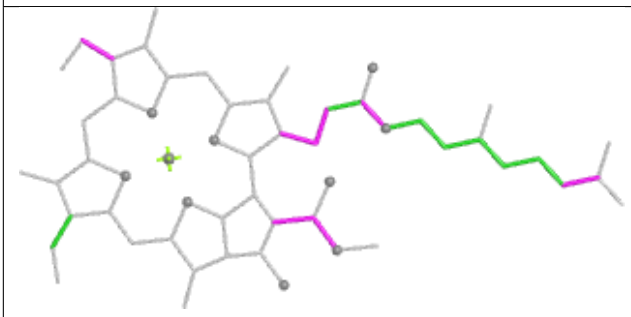
Ligand CLA f 803



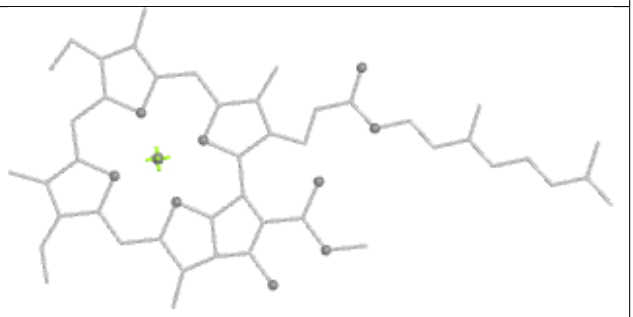
Bond lengths



Bond angles

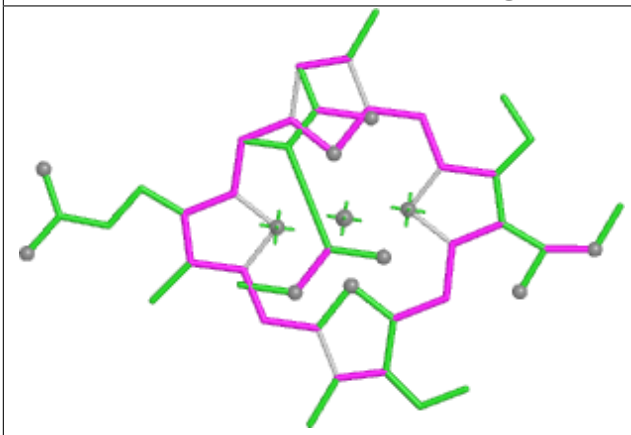


Torsions

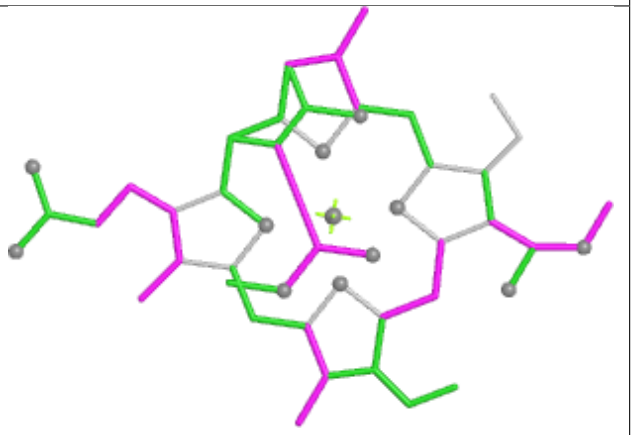


Rings

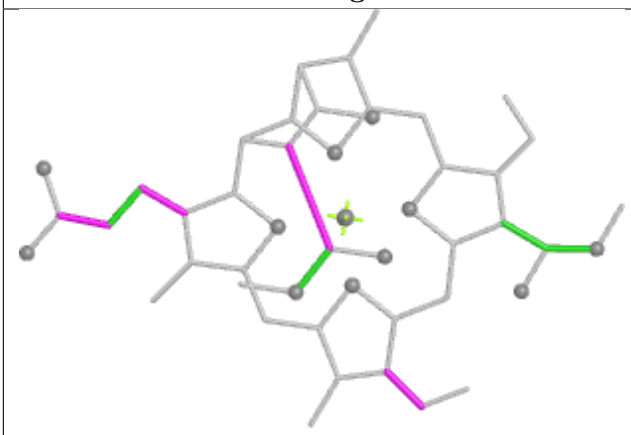
Ligand A1ECV O 315



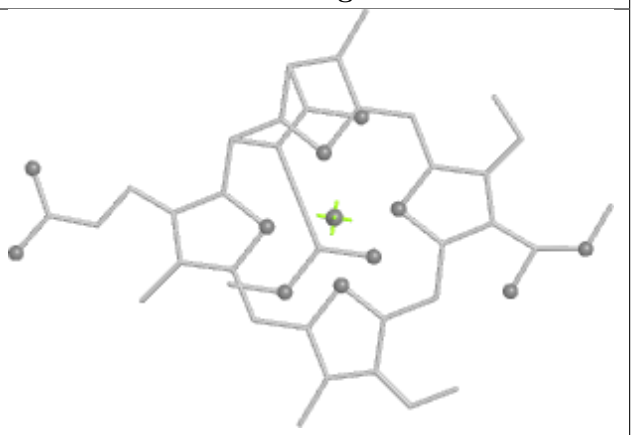
Bond lengths



Bond angles

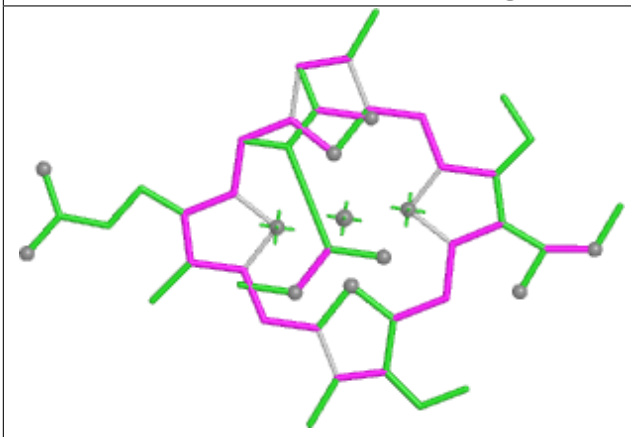


Torsions

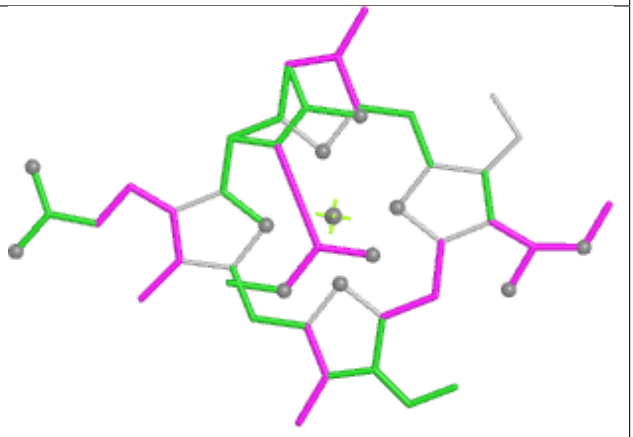


Rings

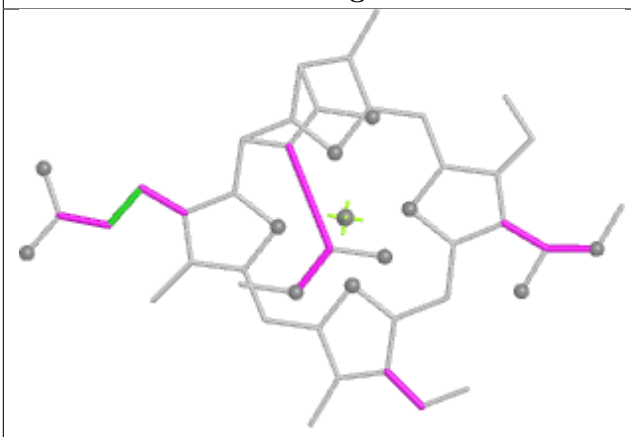
Ligand A1ECV P 315



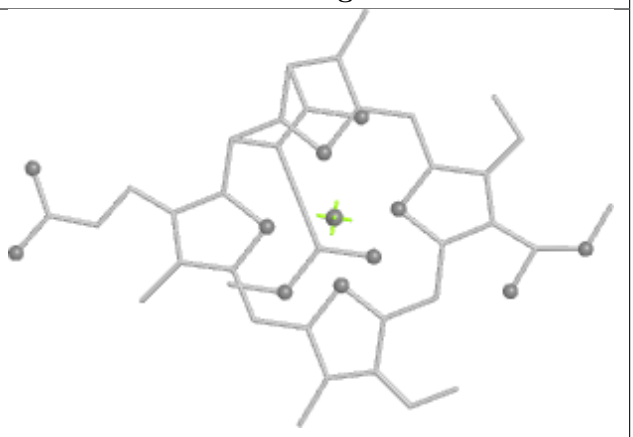
Bond lengths



Bond angles

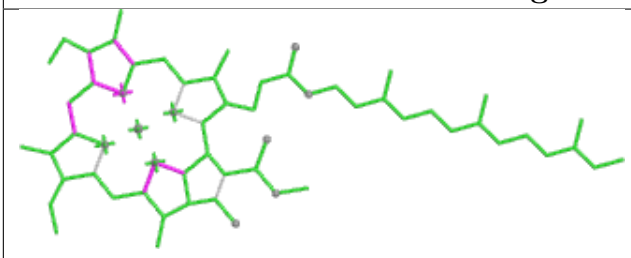


Torsions

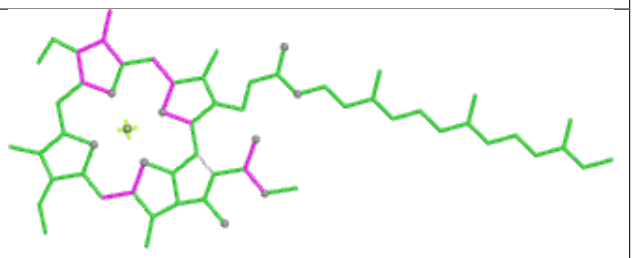


Rings

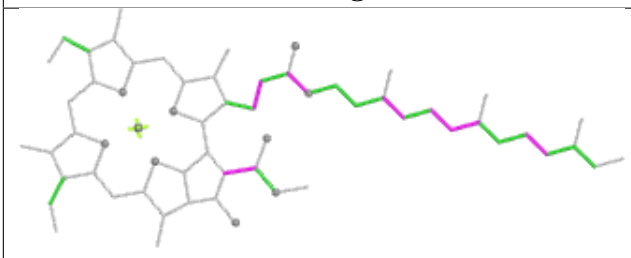
Ligand CLA I 308



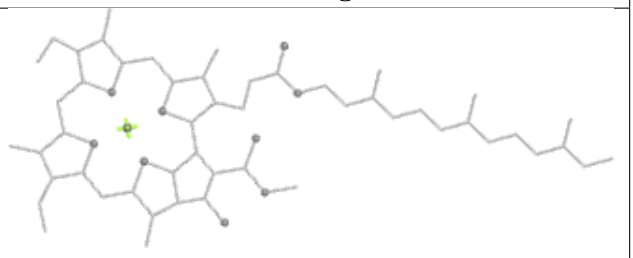
Bond lengths



Bond angles

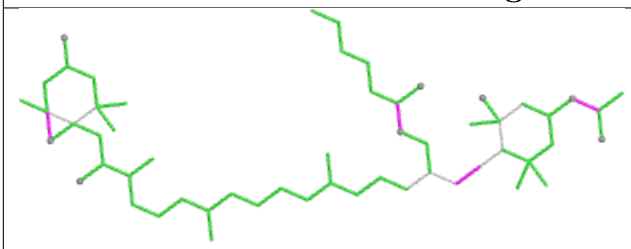


Torsions

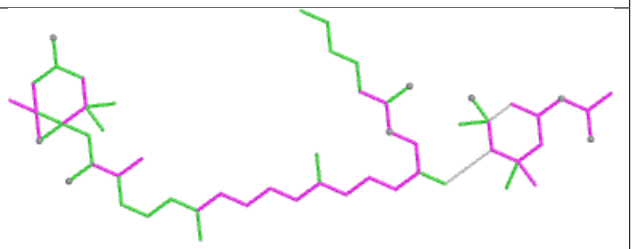


Rings

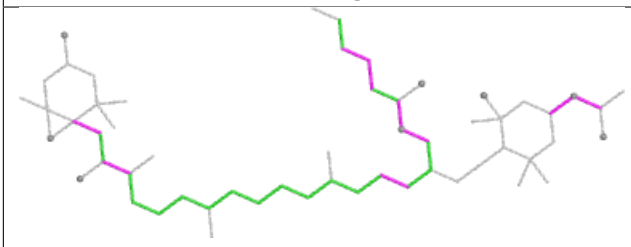
Ligand A1EB1 V 302



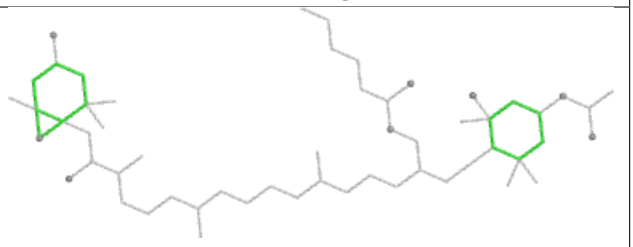
Bond lengths



Bond angles

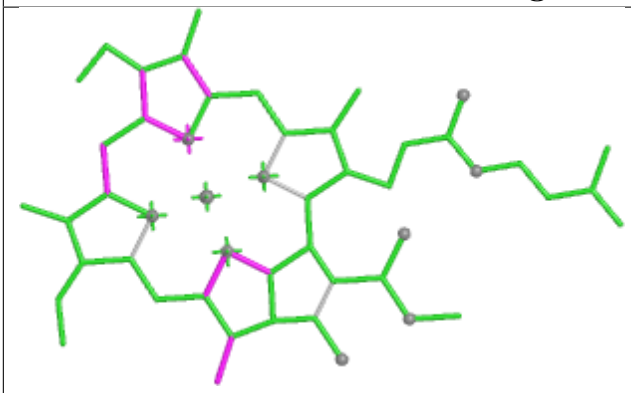


Torsions

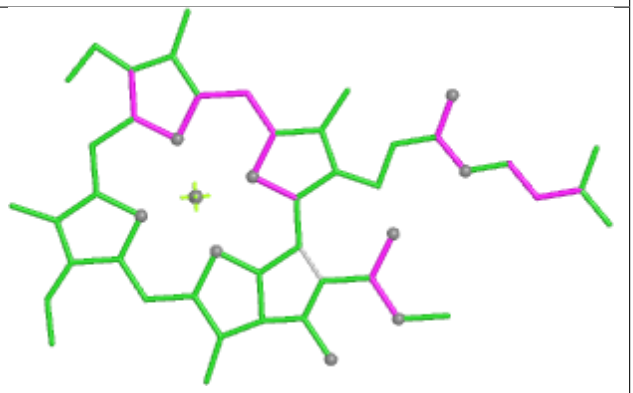


Rings

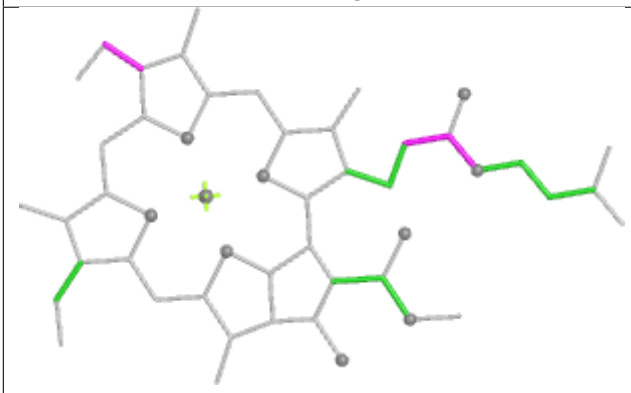
Ligand CLA 7 315



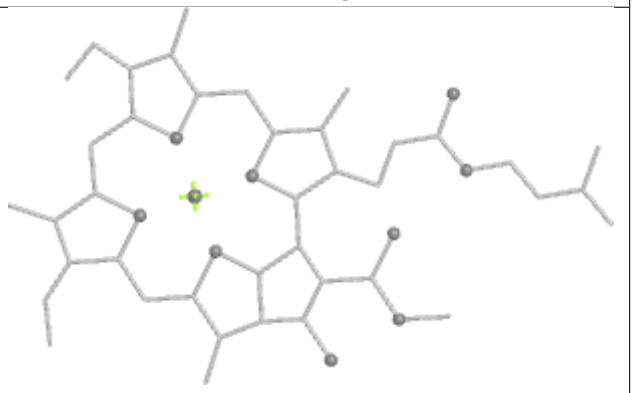
Bond lengths



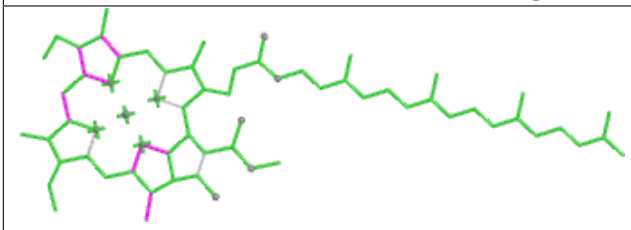
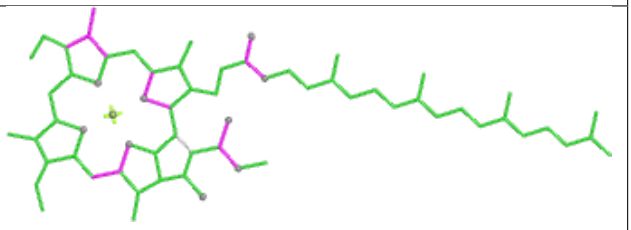
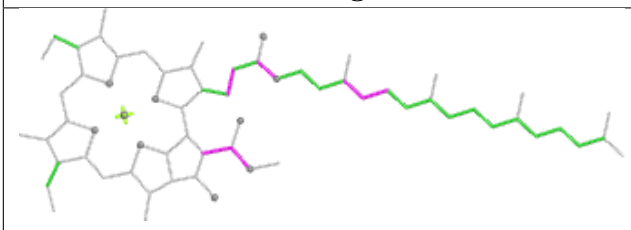
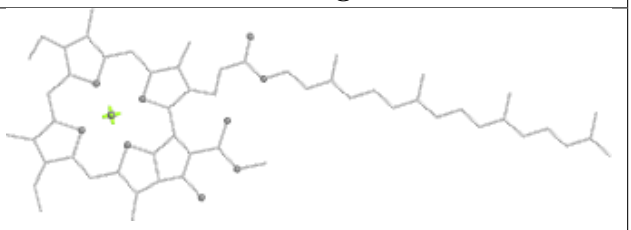
Bond angles

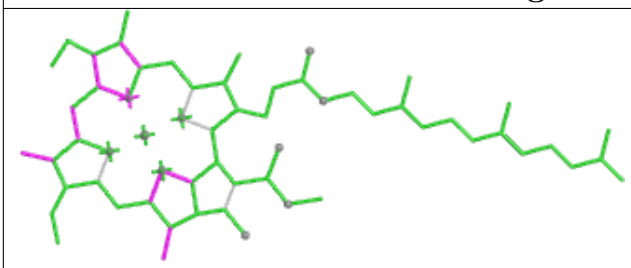
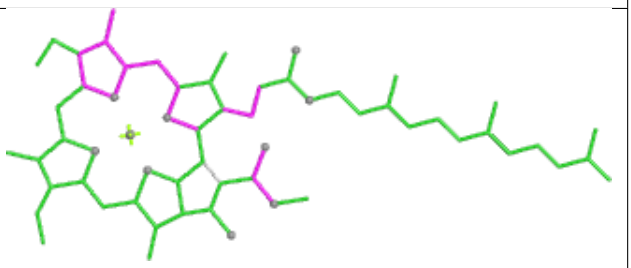
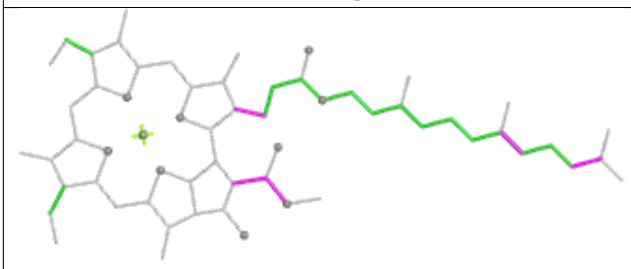
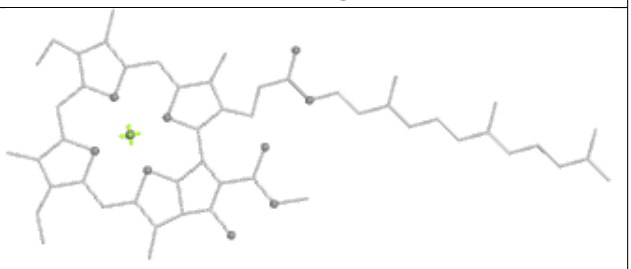


Torsions

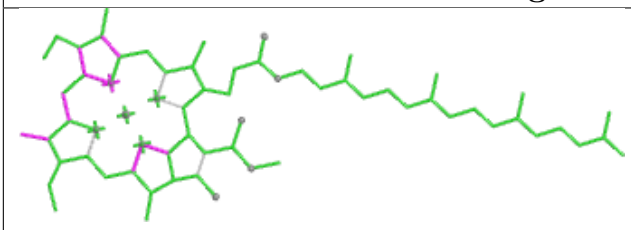


Rings

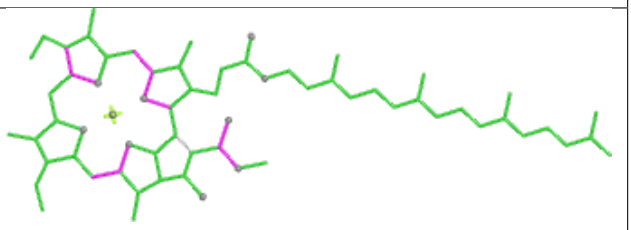
Ligand CLA b 805	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b 837	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

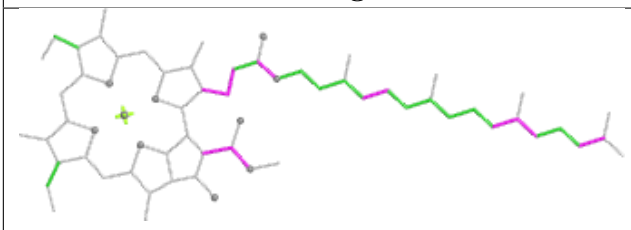
Ligand CLA a 811



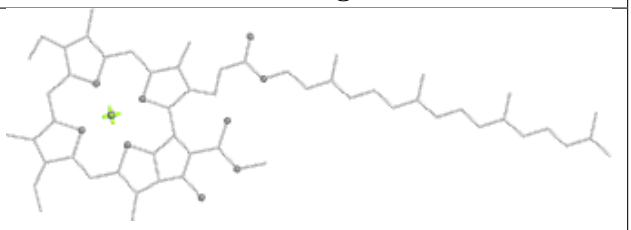
Bond lengths



Bond angles

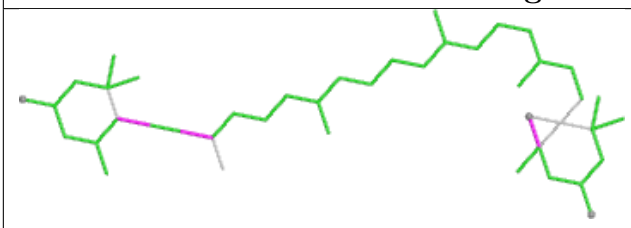


Torsions

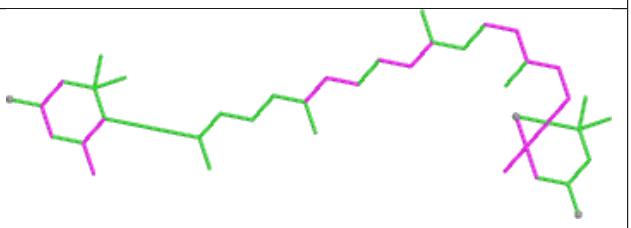


Rings

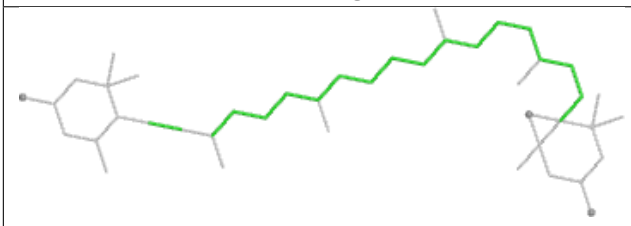
Ligand DD6 V 303



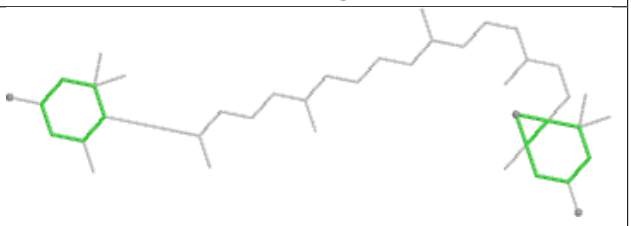
Bond lengths



Bond angles

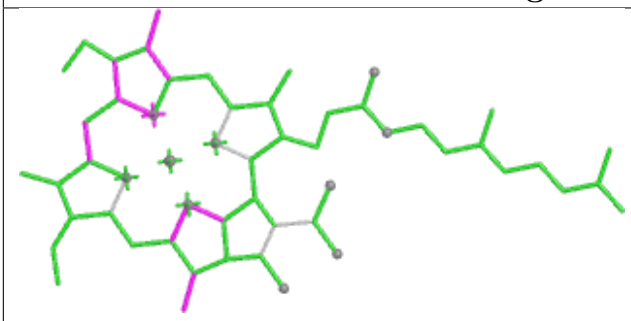


Torsions

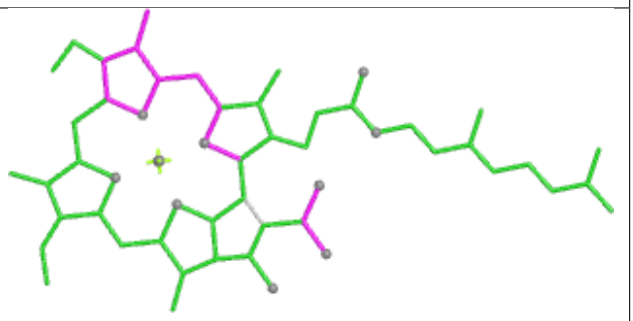


Rings

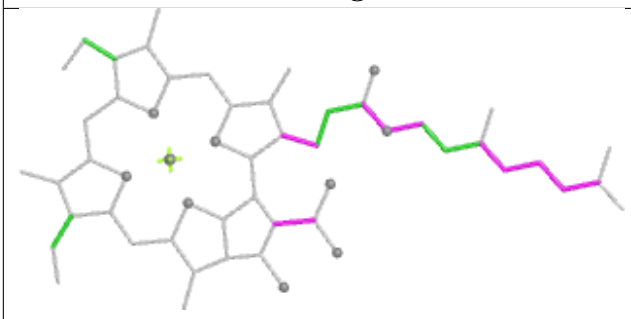
Ligand CLA L 309



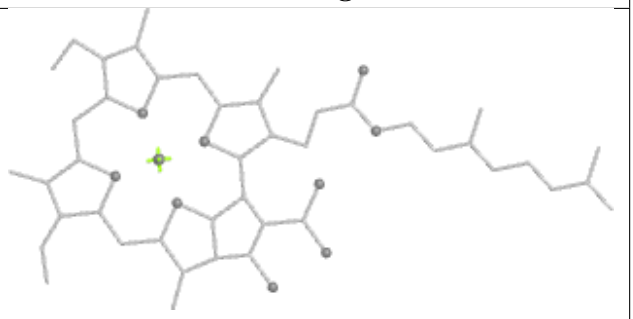
Bond lengths



Bond angles

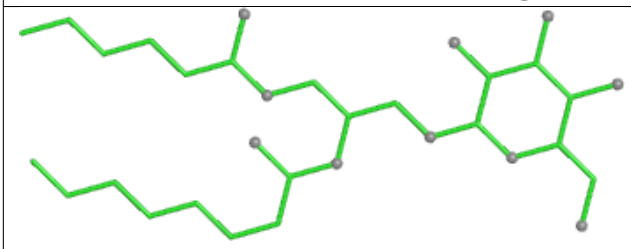


Torsions

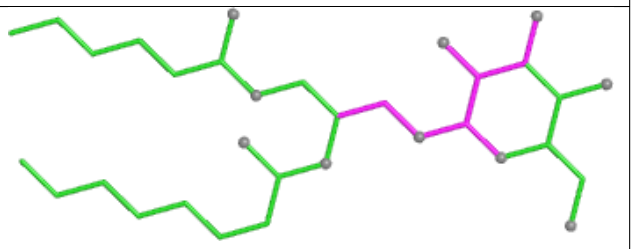


Rings

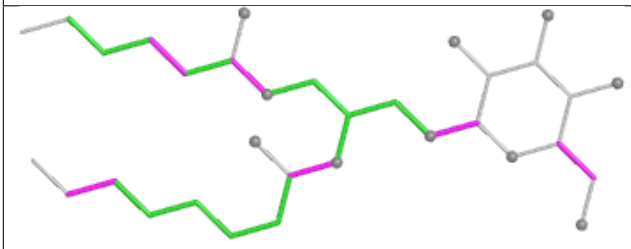
Ligand LMG M 320



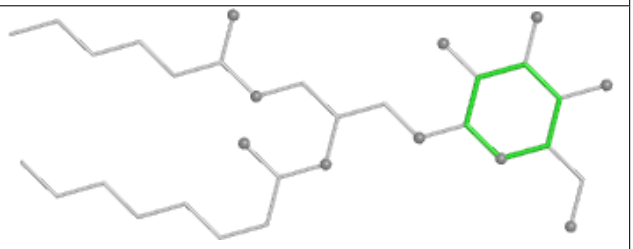
Bond lengths



Bond angles

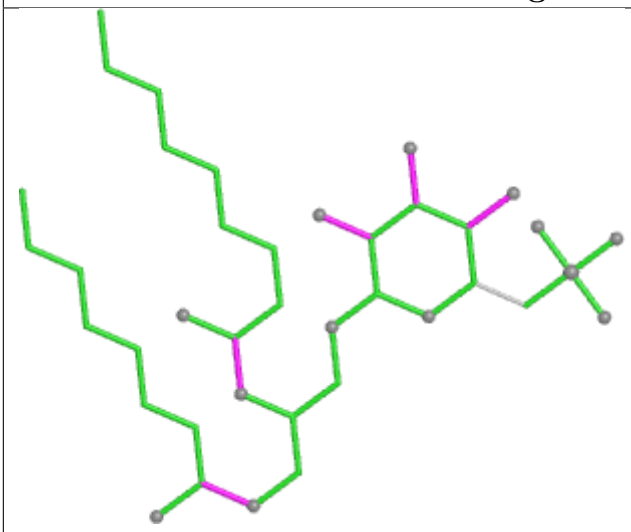


Torsions

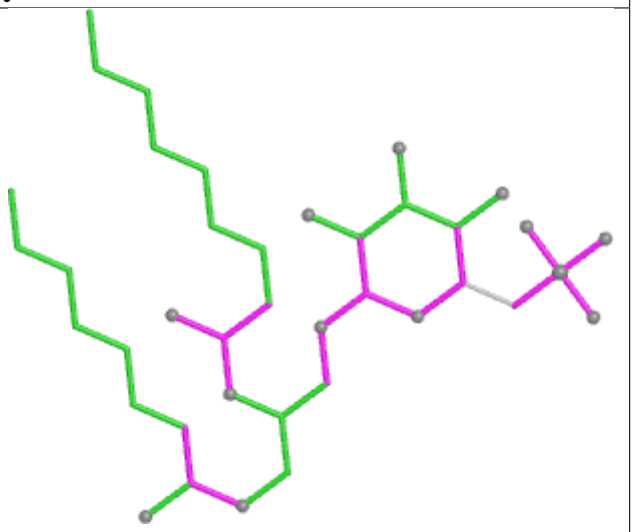


Rings

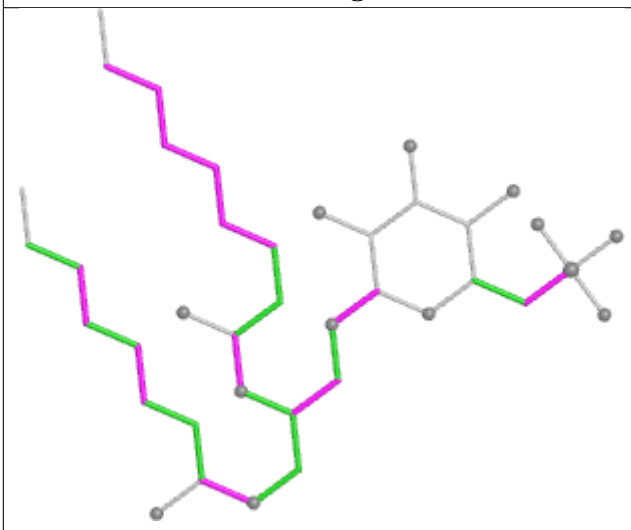
Ligand SQD 4 327



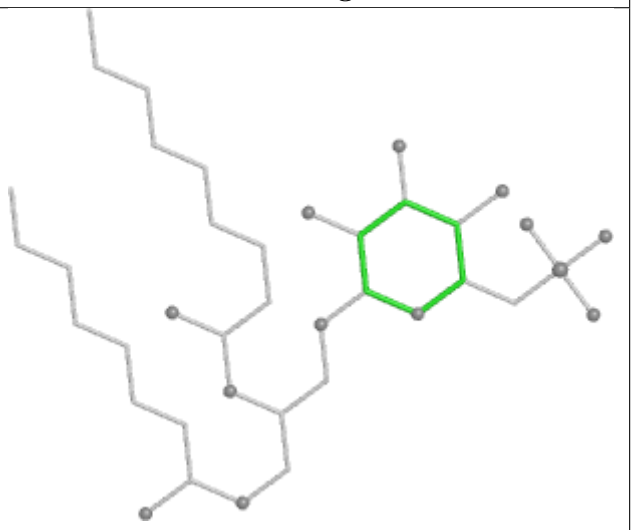
Bond lengths



Bond angles

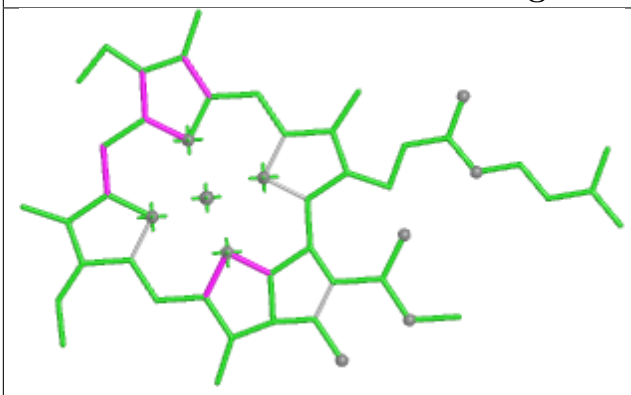


Torsions

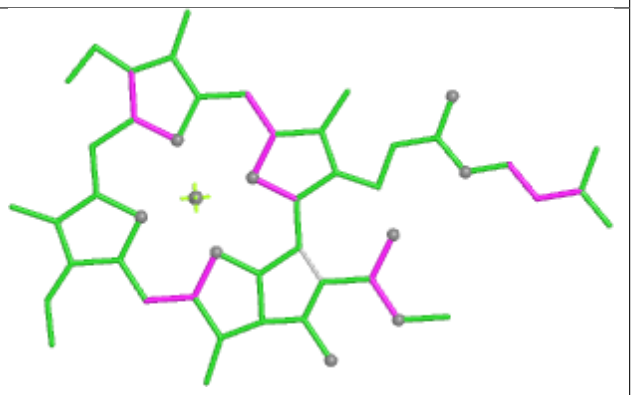


Rings

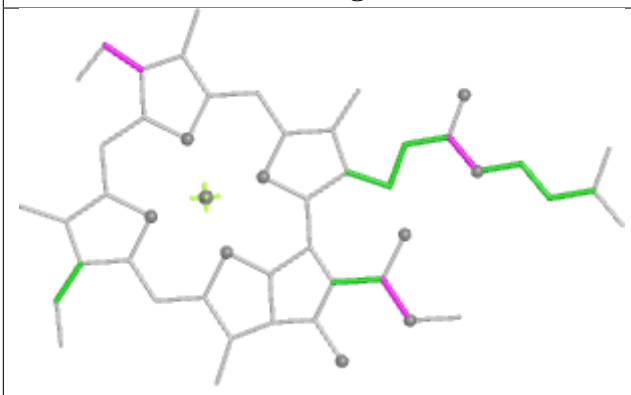
Ligand CLA 5 310



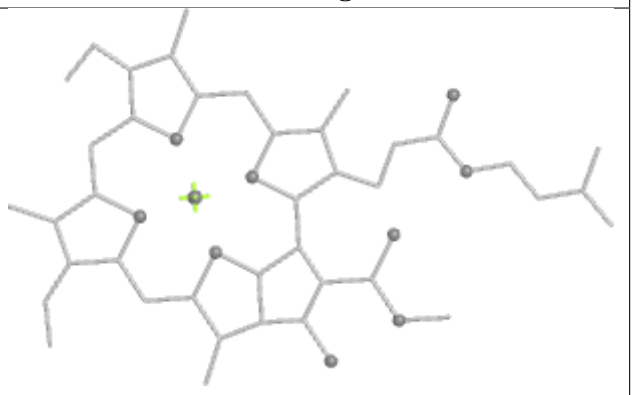
Bond lengths



Bond angles

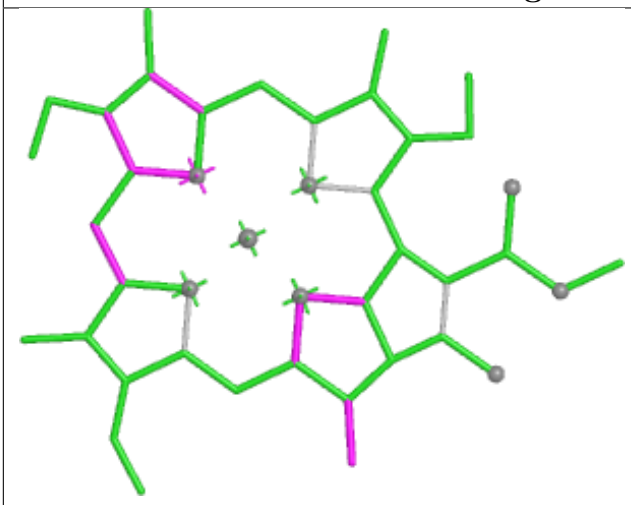


Torsions

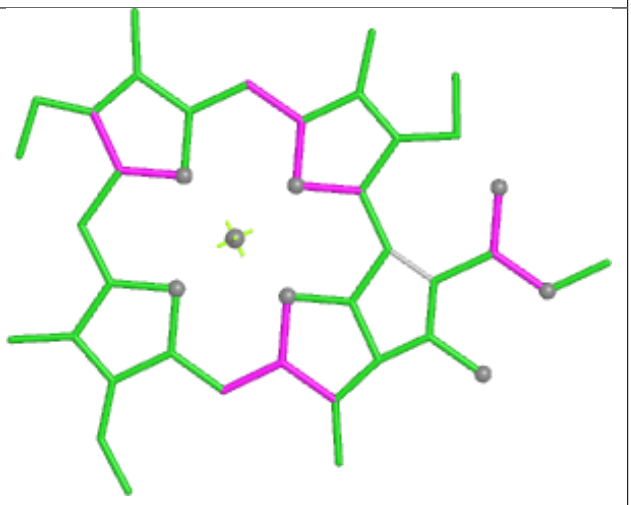


Rings

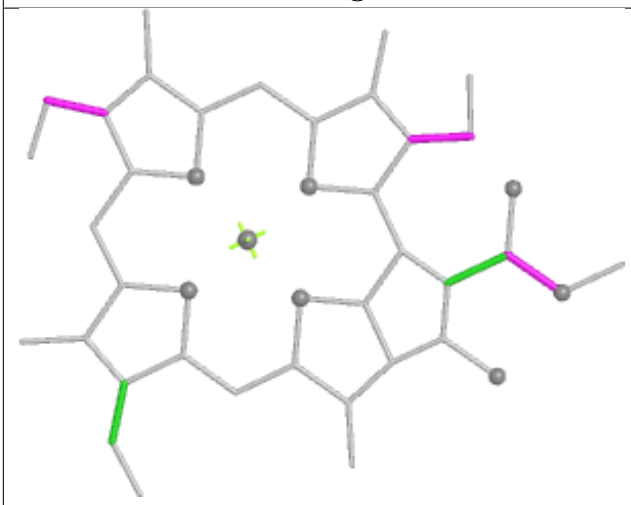
Ligand CLA B 206



Bond lengths



Bond angles

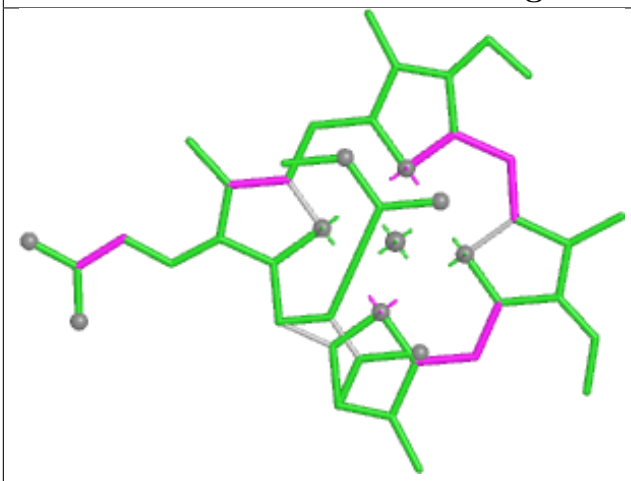


Torsions

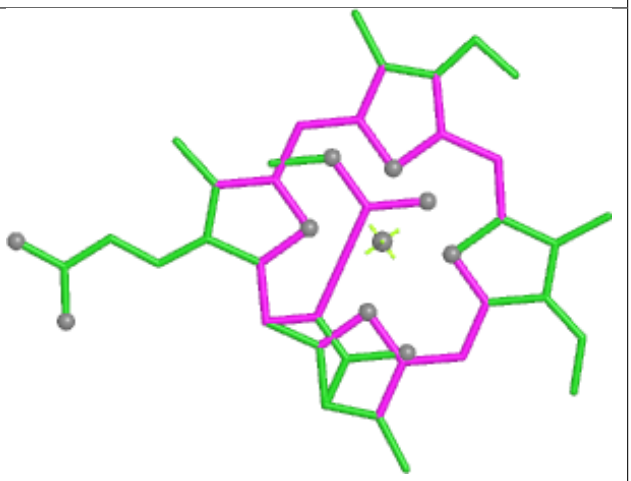


Rings

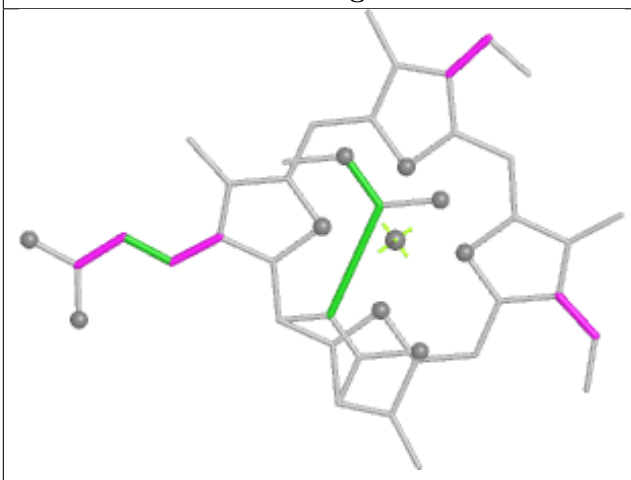
Ligand KC2 X 318



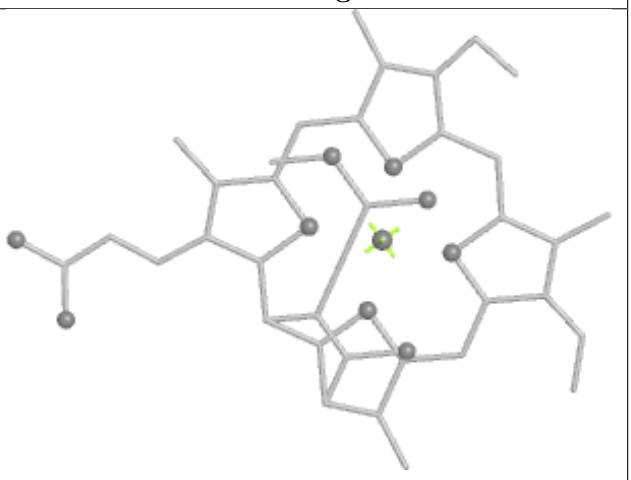
Bond lengths



Bond angles

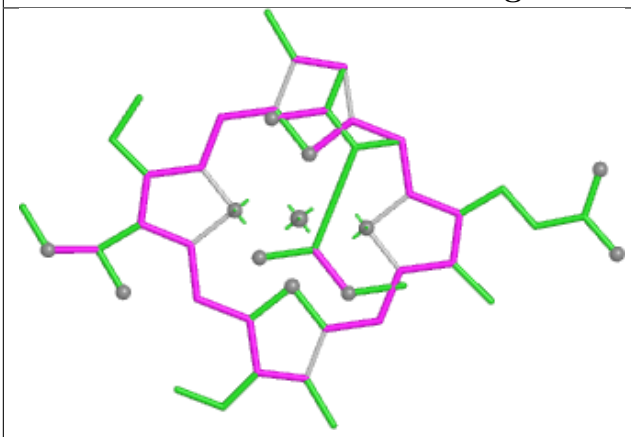


Torsions

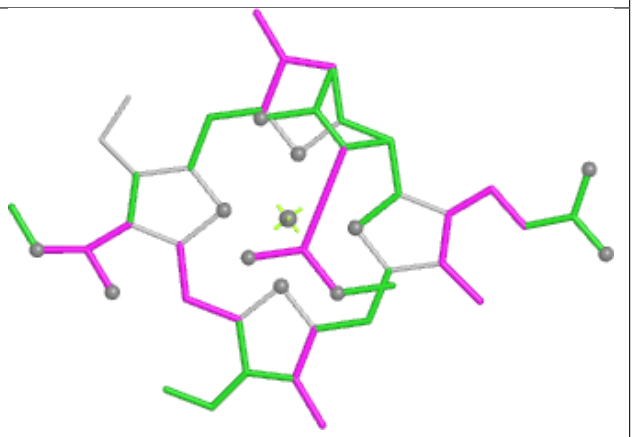


Rings

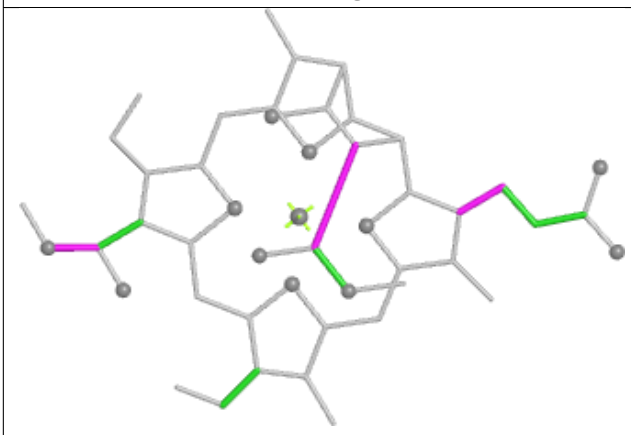
Ligand A1ECV x 310



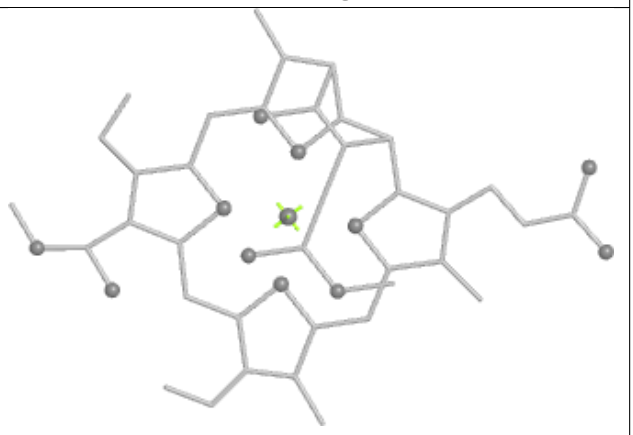
Bond lengths



Bond angles

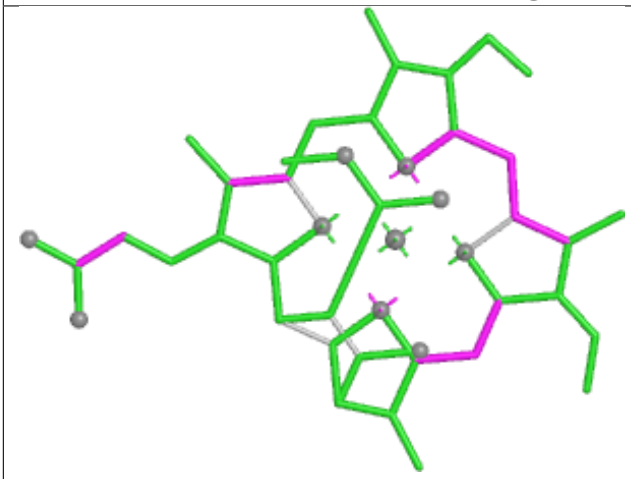


Torsions

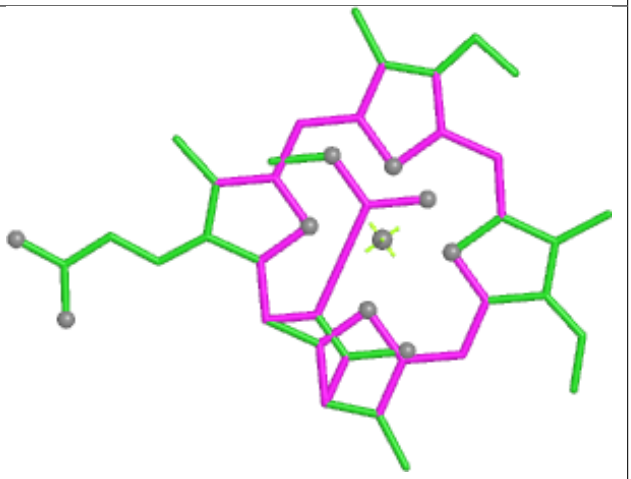


Rings

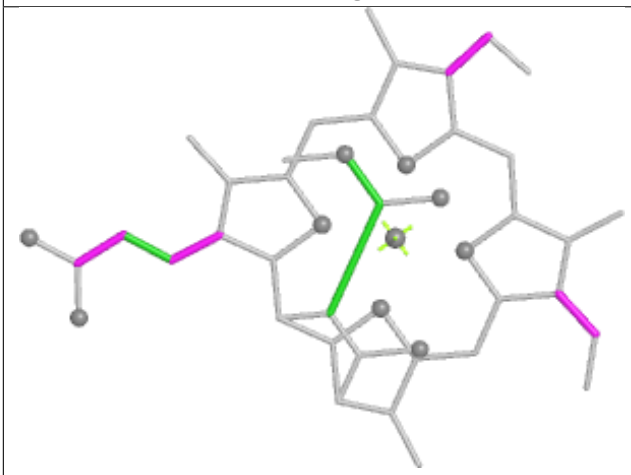
Ligand KC2 G 317



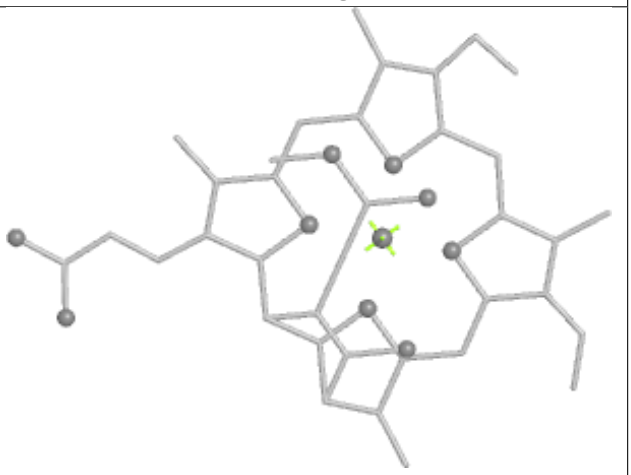
Bond lengths



Bond angles

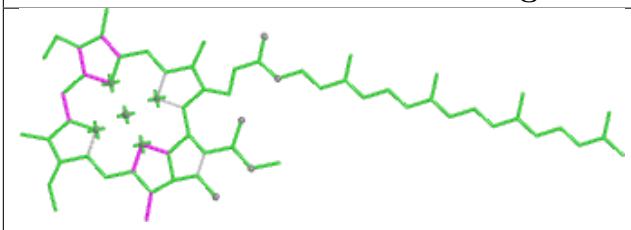


Torsions

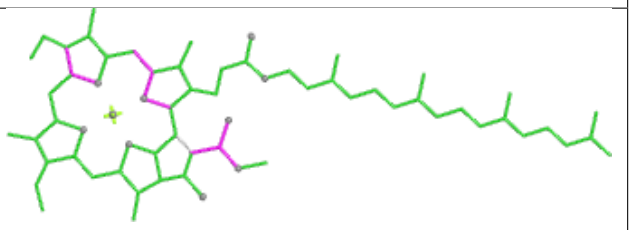


Rings

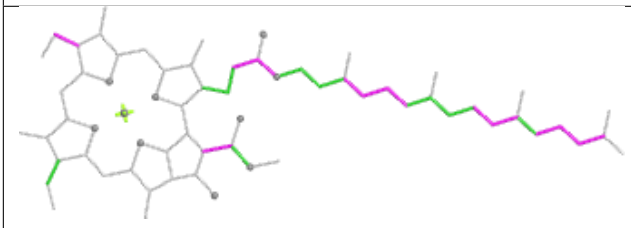
Ligand CLA M 309



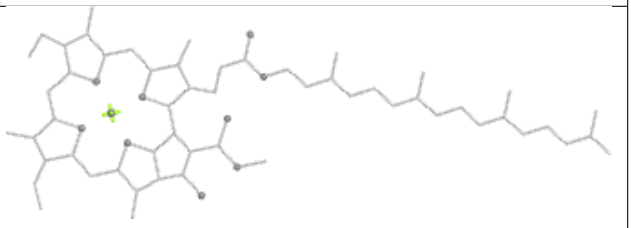
Bond lengths



Bond angles

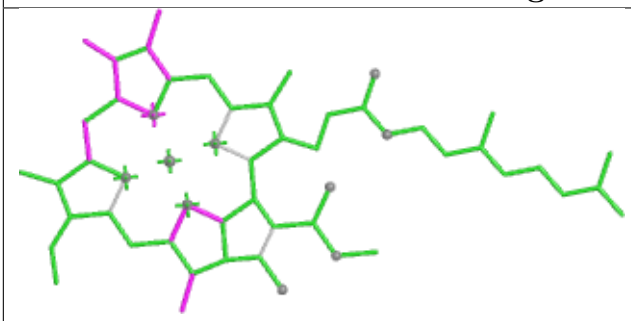


Torsions

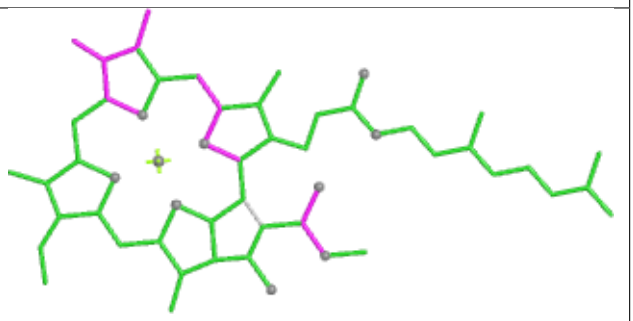


Rings

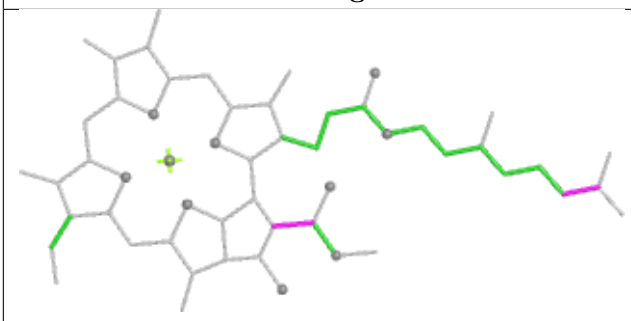
Ligand CLA b 813



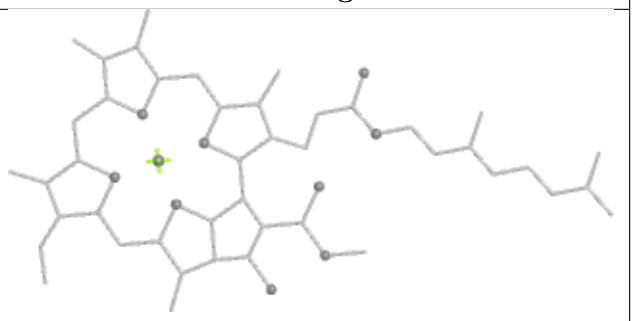
Bond lengths



Bond angles

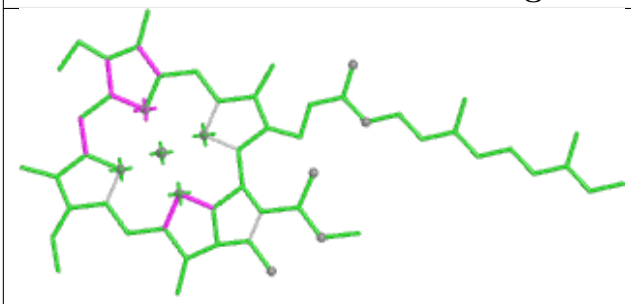


Torsions

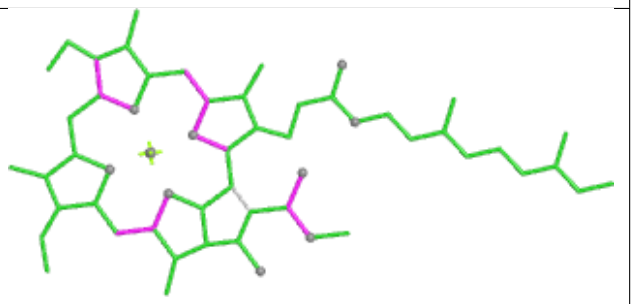


Rings

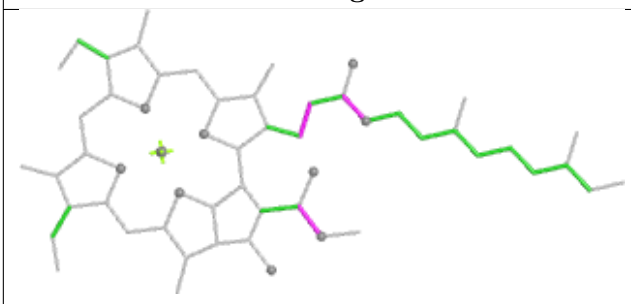
Ligand CLA T 311



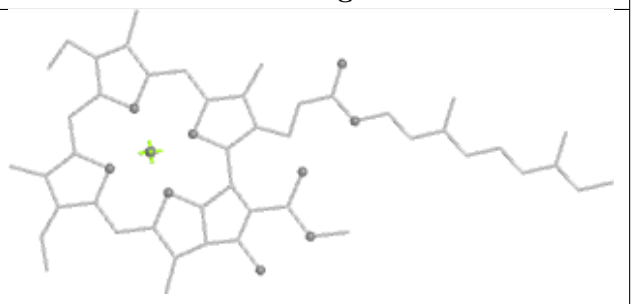
Bond lengths



Bond angles

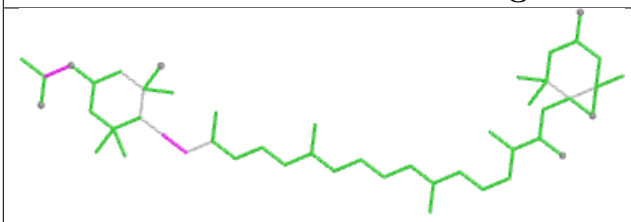


Torsions

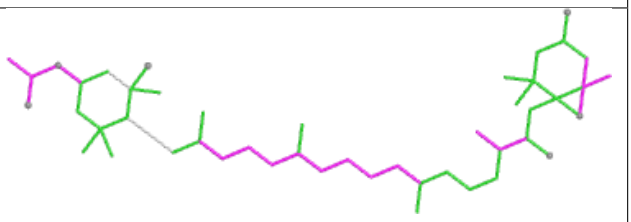


Rings

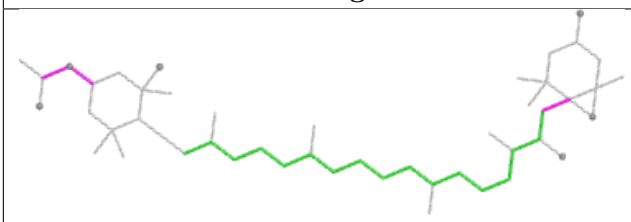
Ligand A1EB1 6 306



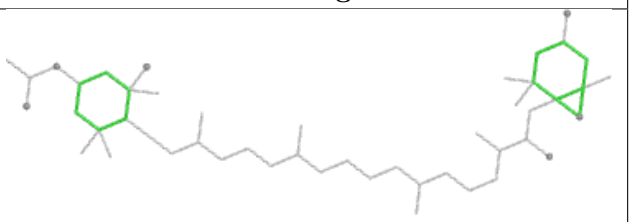
Bond lengths



Bond angles

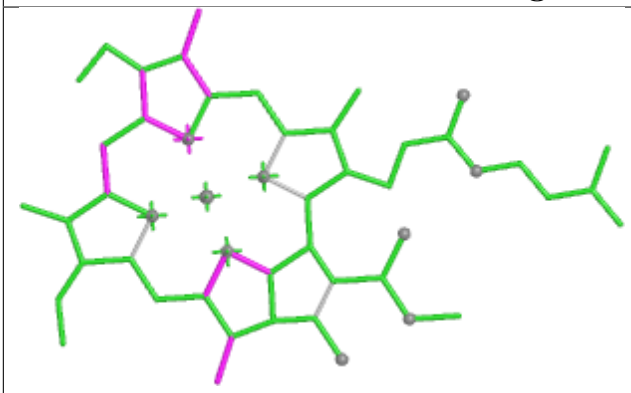


Torsions

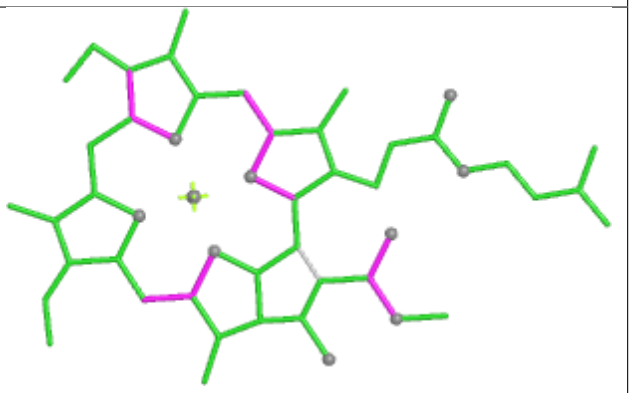


Rings

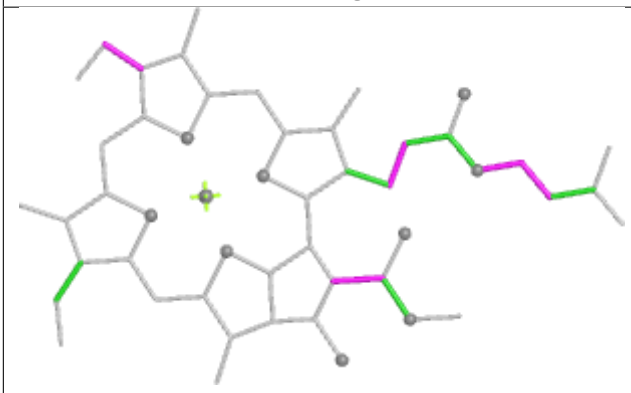
Ligand CLA a 828



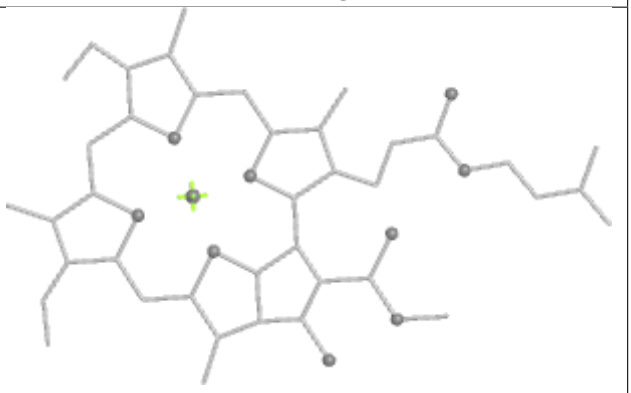
Bond lengths



Bond angles

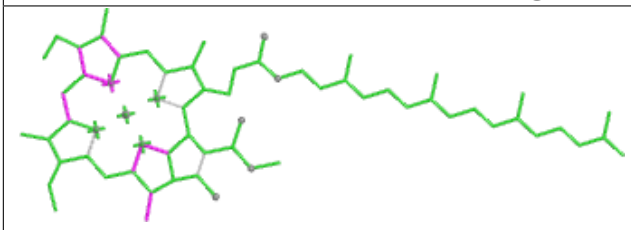


Torsions

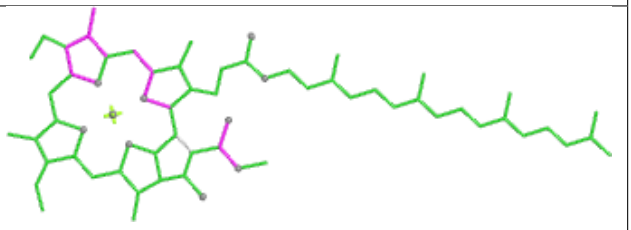


Rings

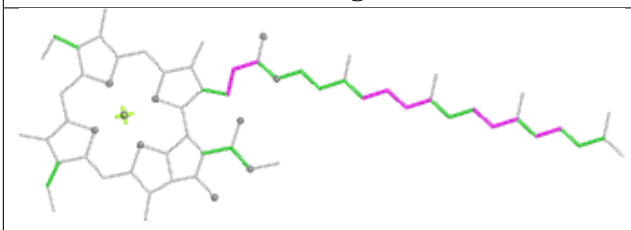
Ligand CLA 7 316



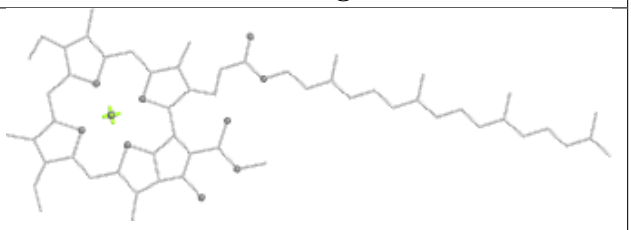
Bond lengths



Bond angles



Torsions

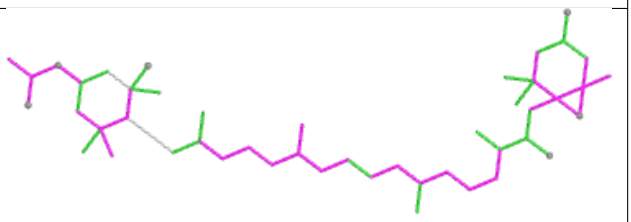


Rings

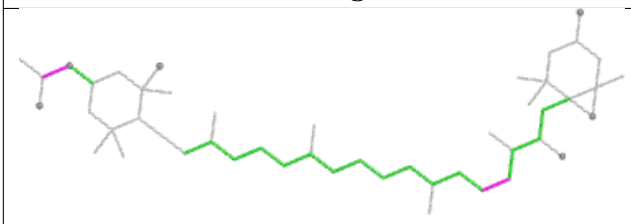
Ligand A86 U 206



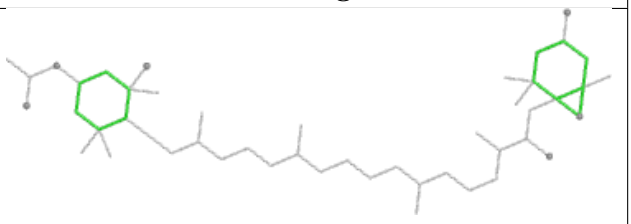
Bond lengths



Bond angles

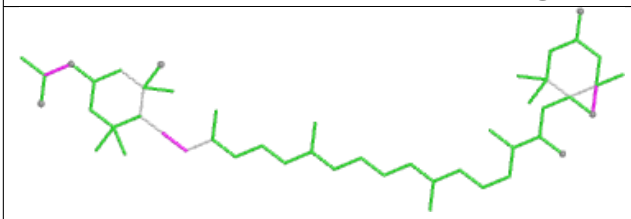


Torsions

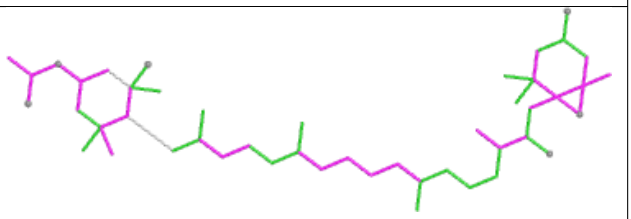


Rings

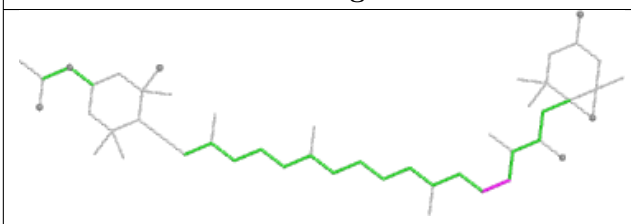
Ligand A86 4 309



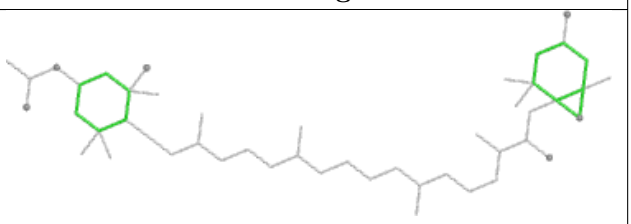
Bond lengths



Bond angles

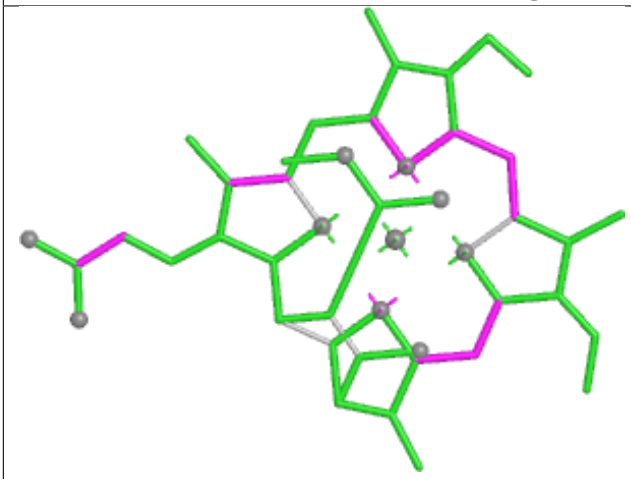


Torsions

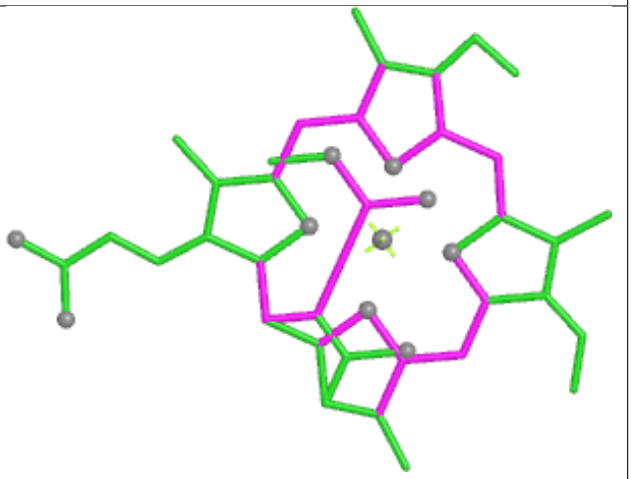


Rings

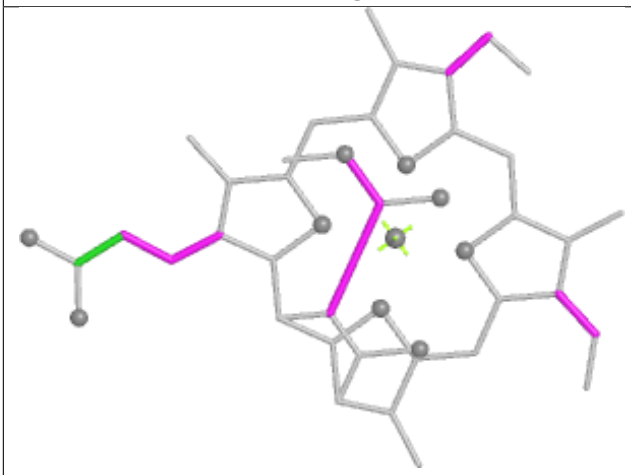
Ligand KC2 X 306



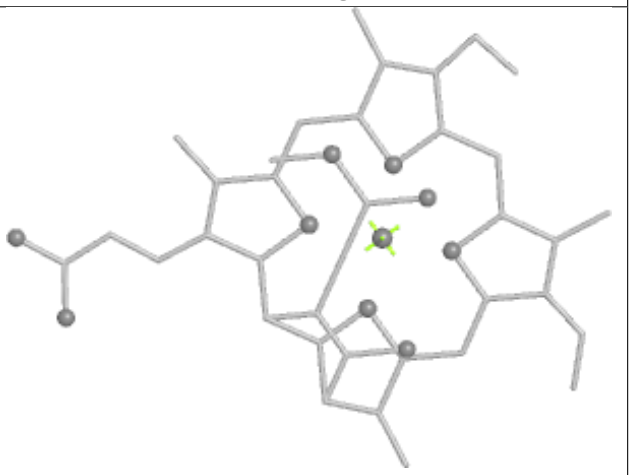
Bond lengths



Bond angles

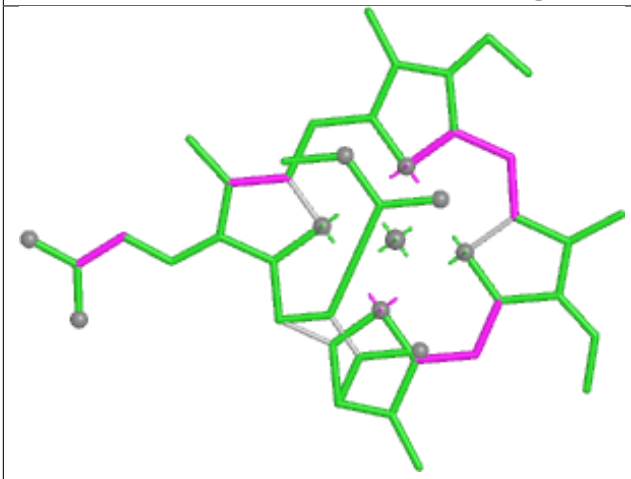


Torsions

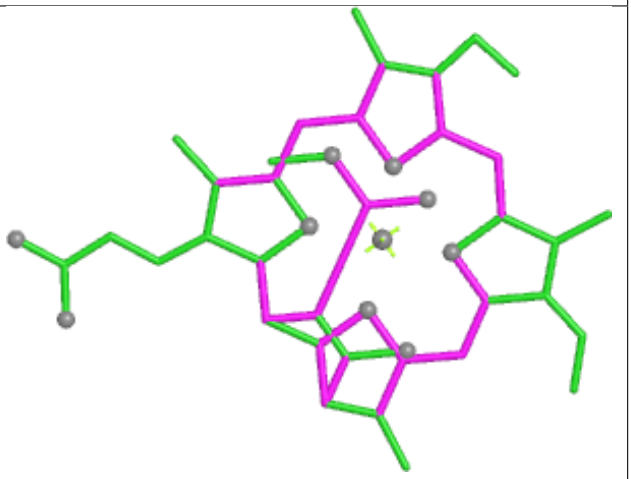


Rings

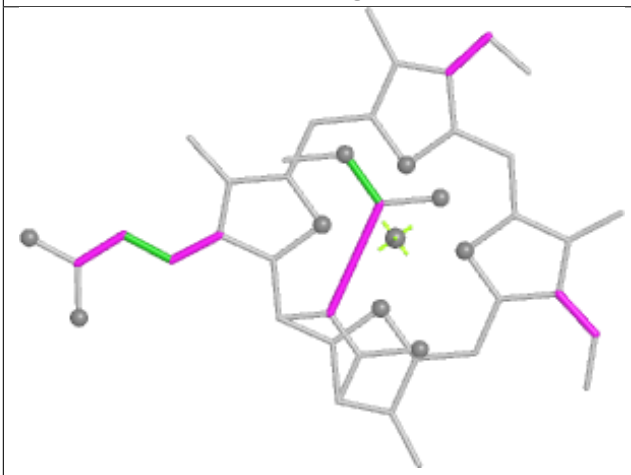
Ligand KC2 8 320



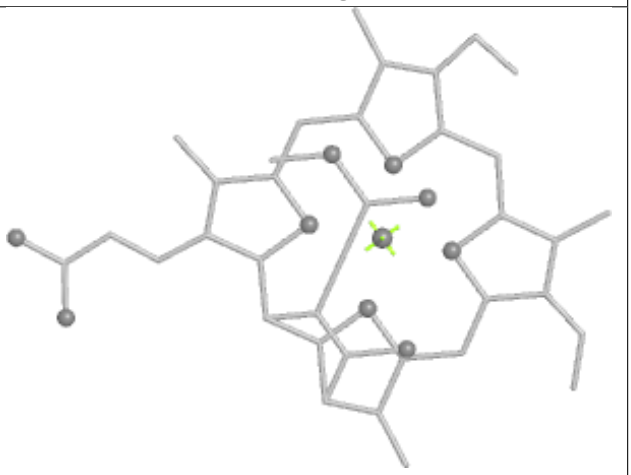
Bond lengths



Bond angles

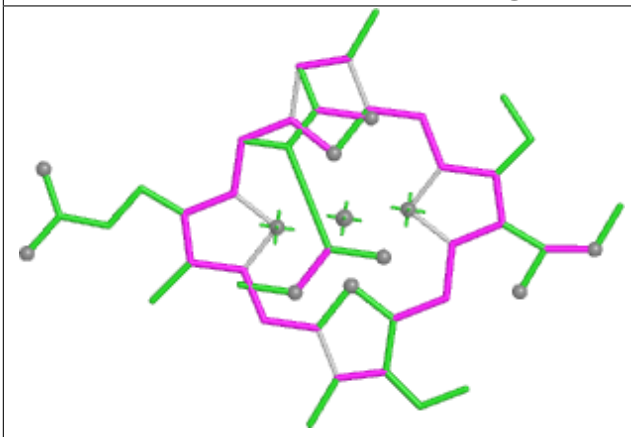


Torsions

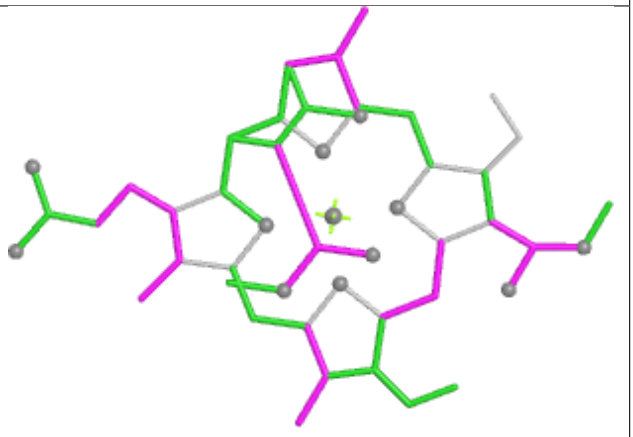


Rings

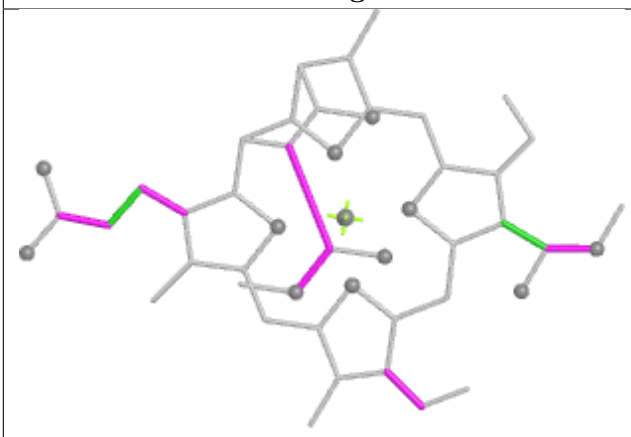
Ligand A1ECV z 310



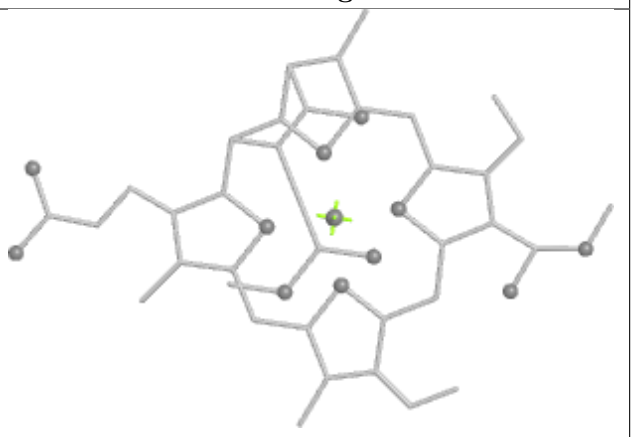
Bond lengths



Bond angles

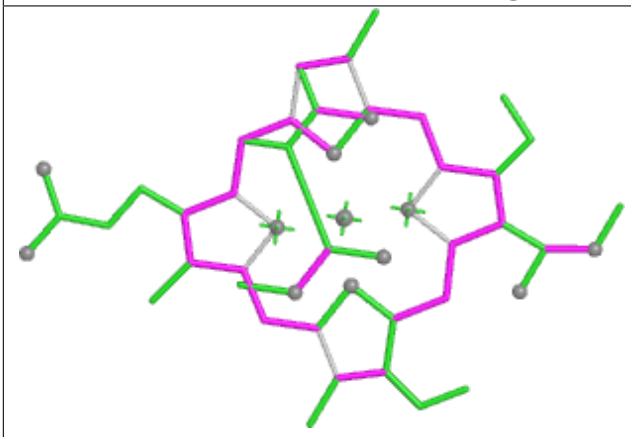


Torsions

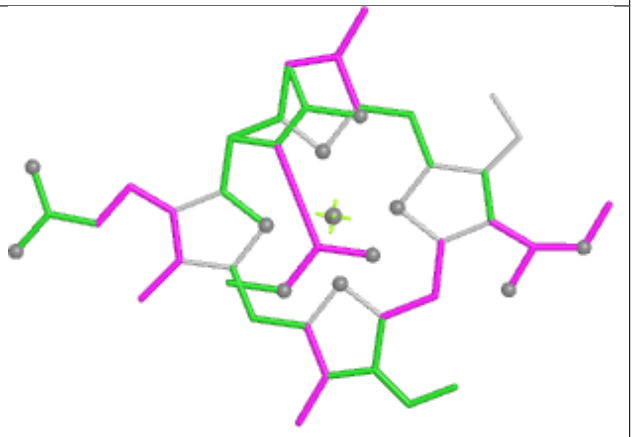


Rings

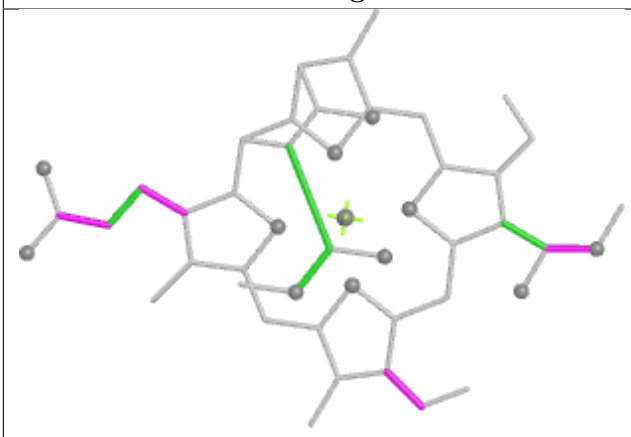
Ligand A1ECV 2 311



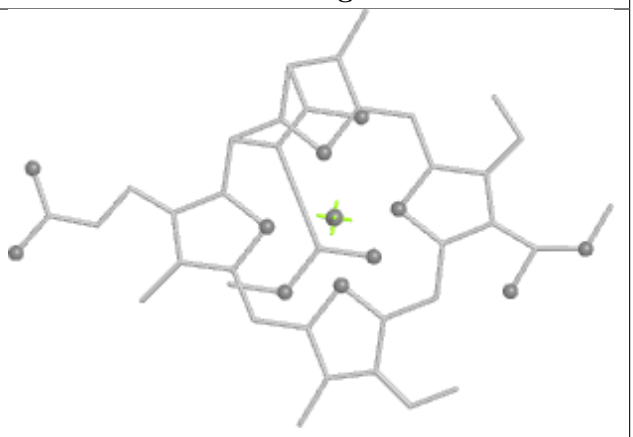
Bond lengths



Bond angles

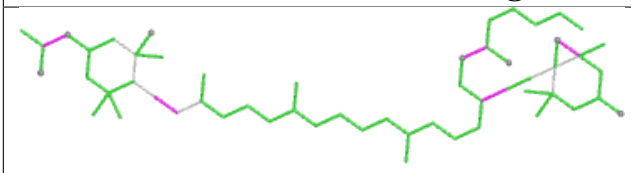


Torsions

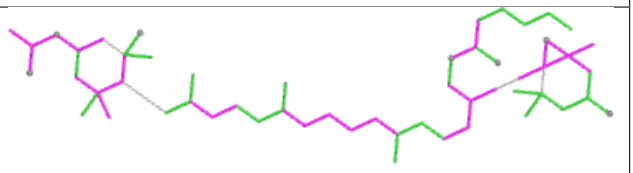


Rings

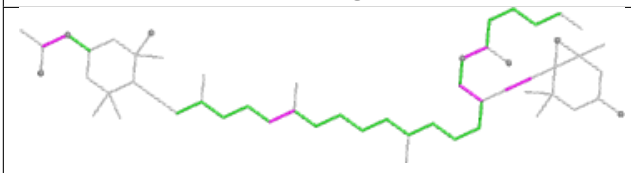
Ligand A1EB4 T 304



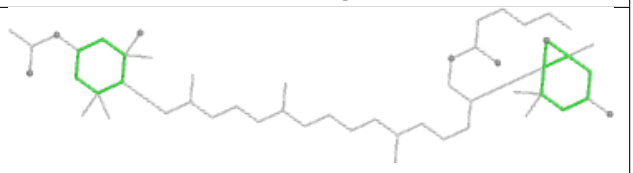
Bond lengths



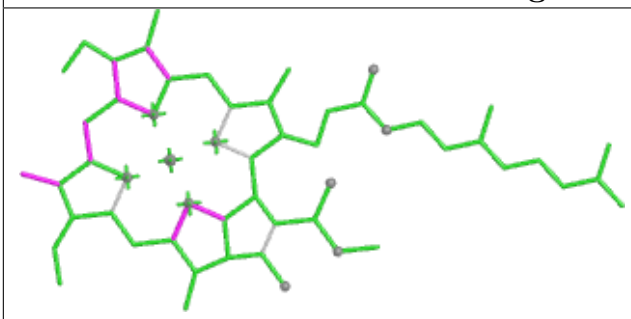
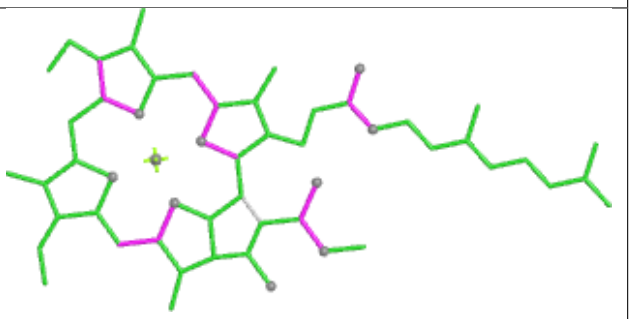
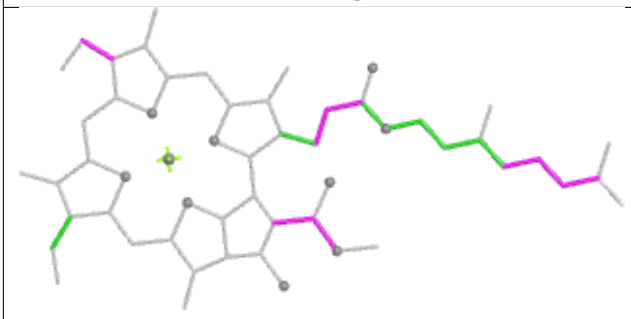
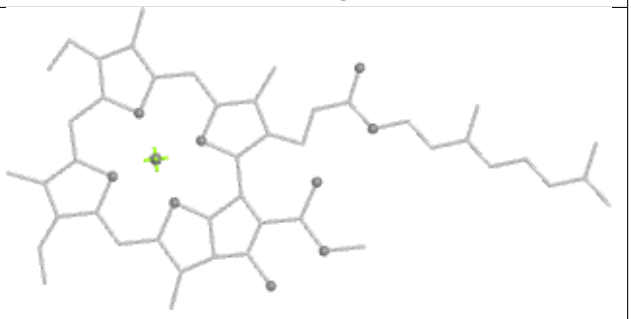
Bond angles



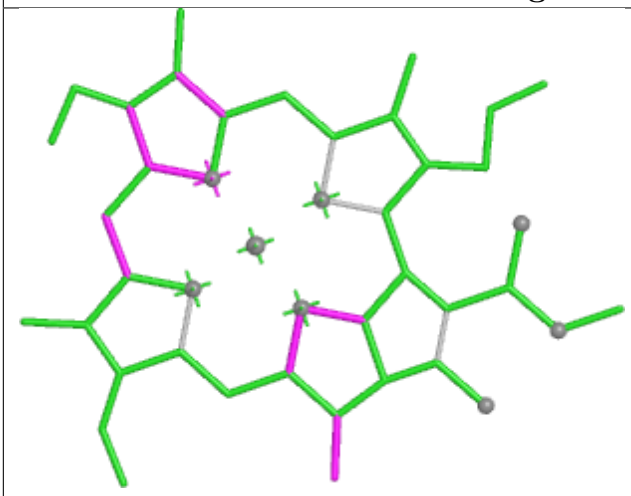
Torsions



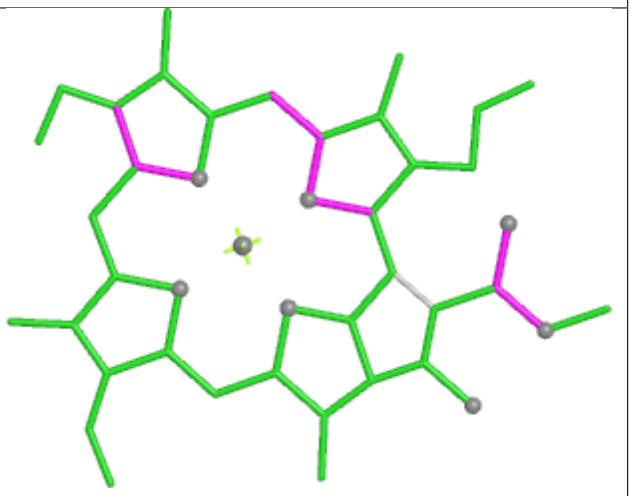
Rings

Ligand CLA 0 313	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

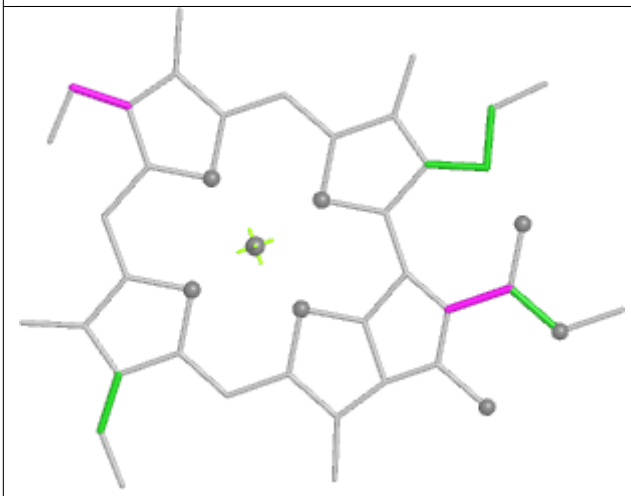
Ligand CLA 8 315



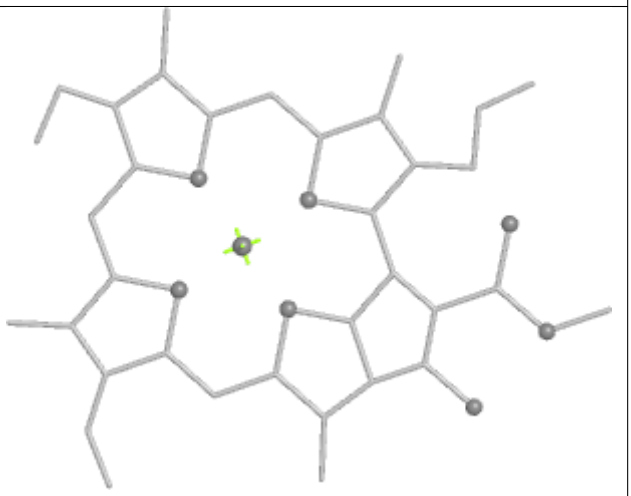
Bond lengths



Bond angles

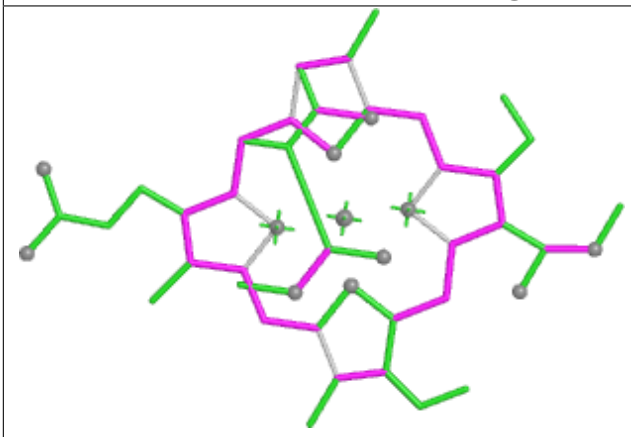


Torsions

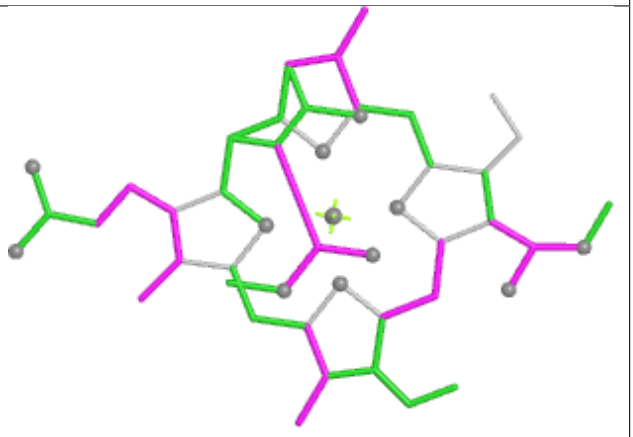


Rings

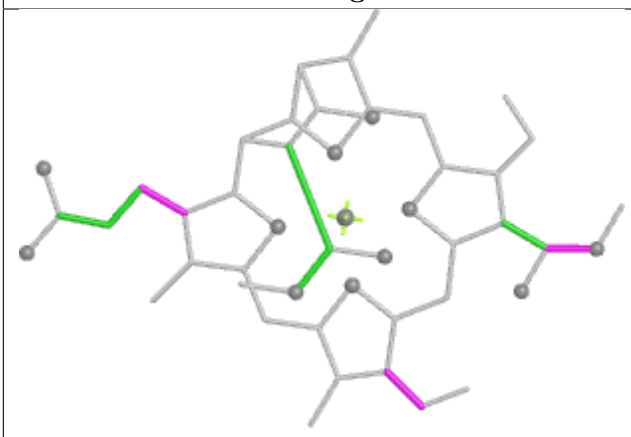
Ligand A1ECV z 316



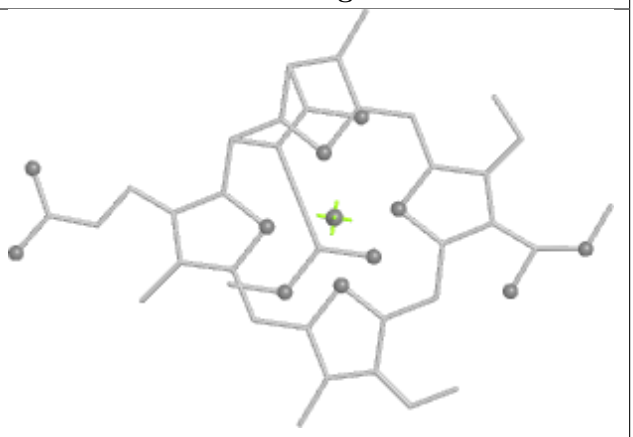
Bond lengths



Bond angles

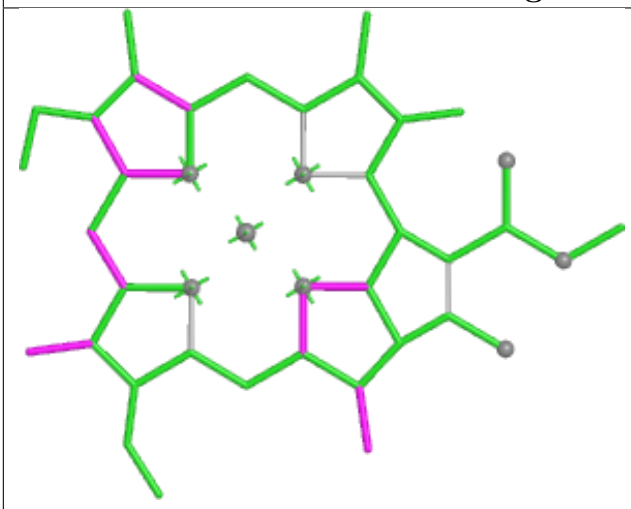


Torsions

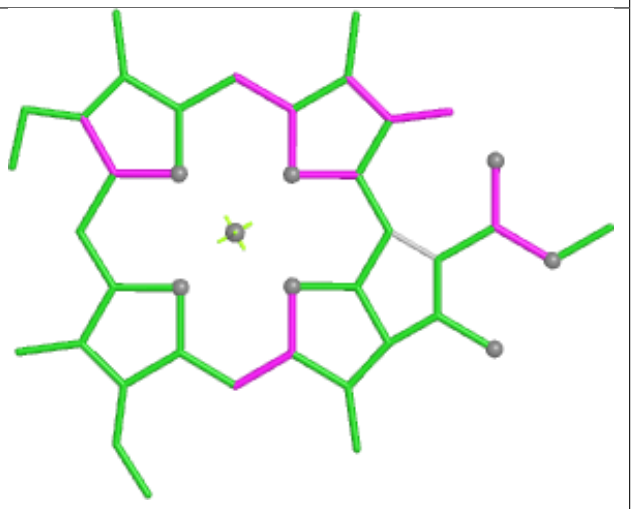


Rings

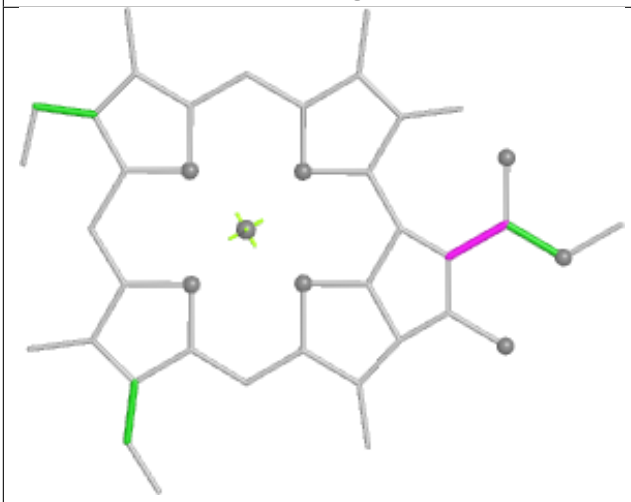
Ligand CLA P 314



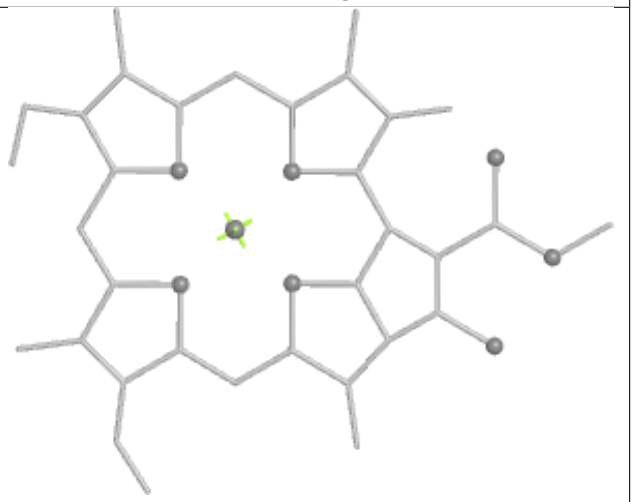
Bond lengths



Bond angles

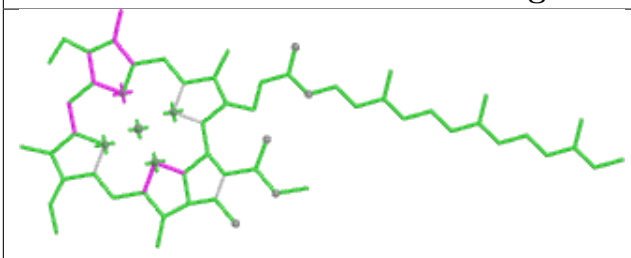


Torsions

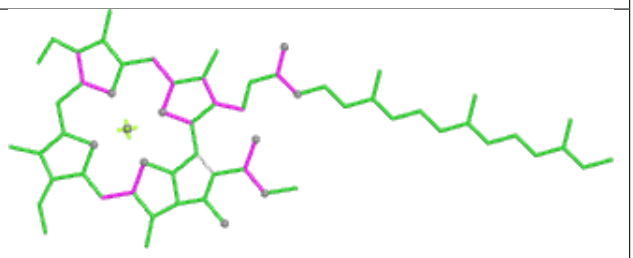


Rings

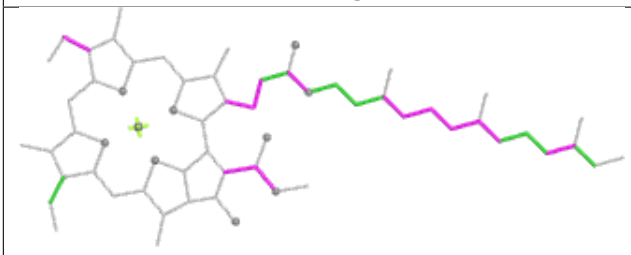
Ligand CLA 7 313



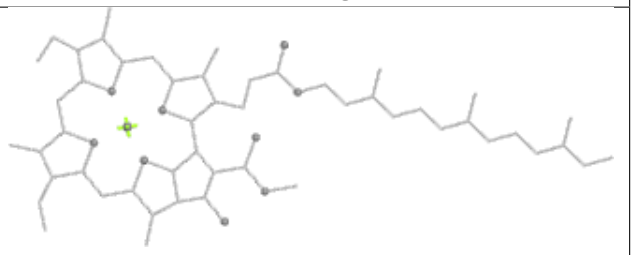
Bond lengths



Bond angles

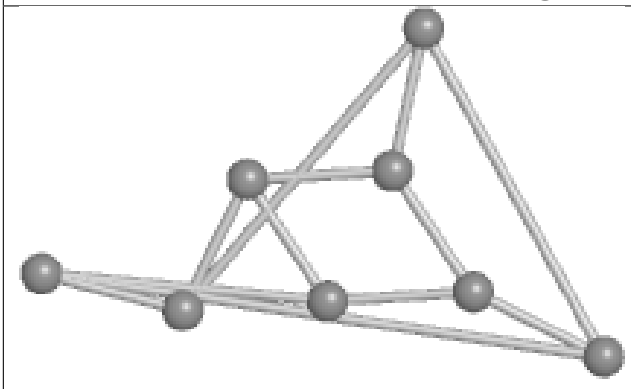


Torsions

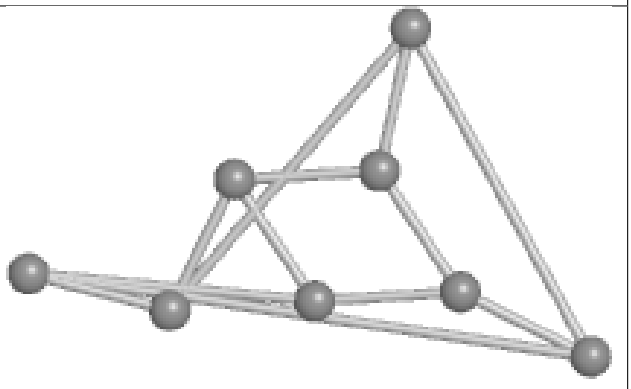


Rings

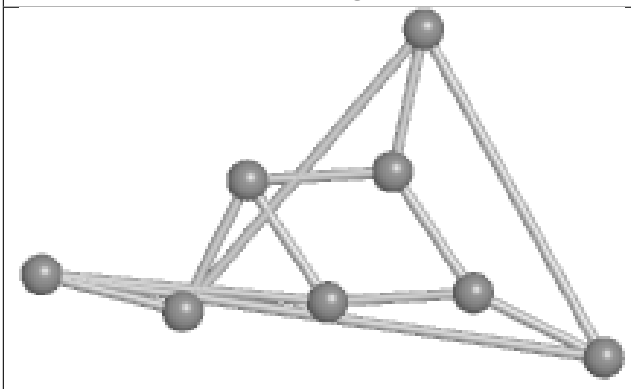
Ligand SF4 c 102



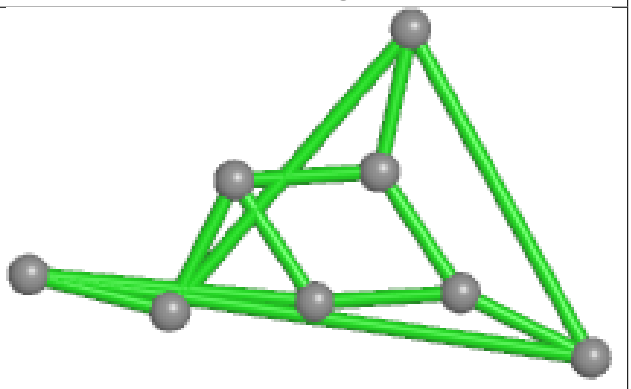
Bond lengths



Bond angles

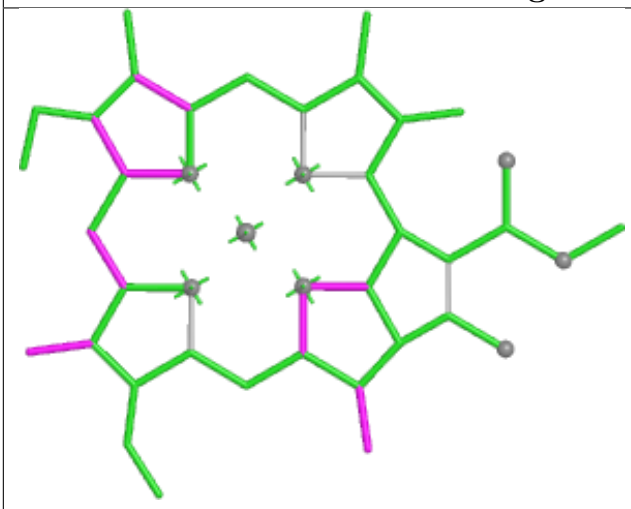


Torsions

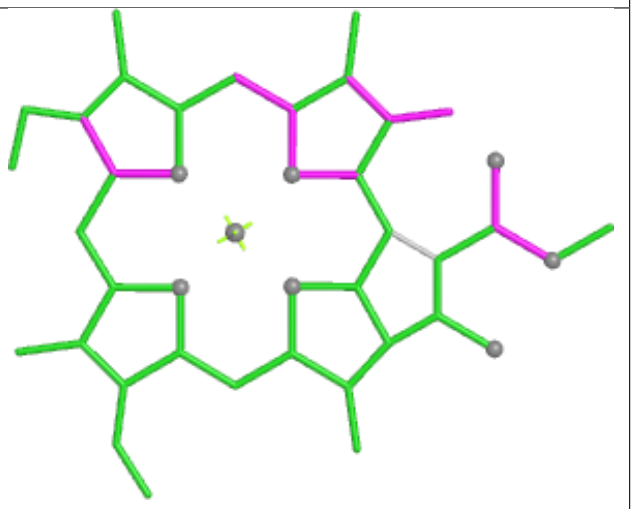


Rings

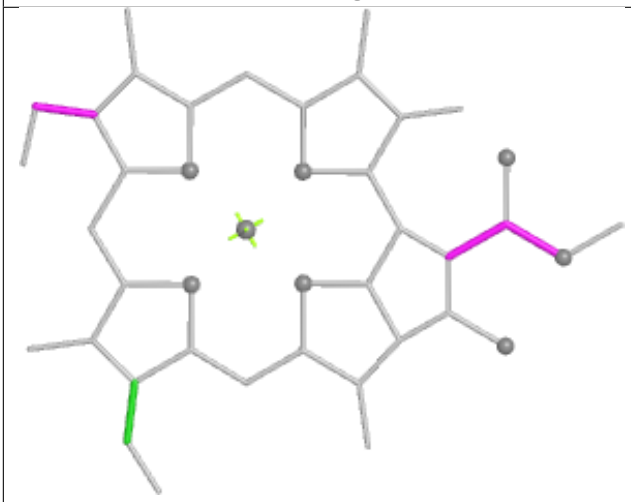
Ligand CLA 2 315



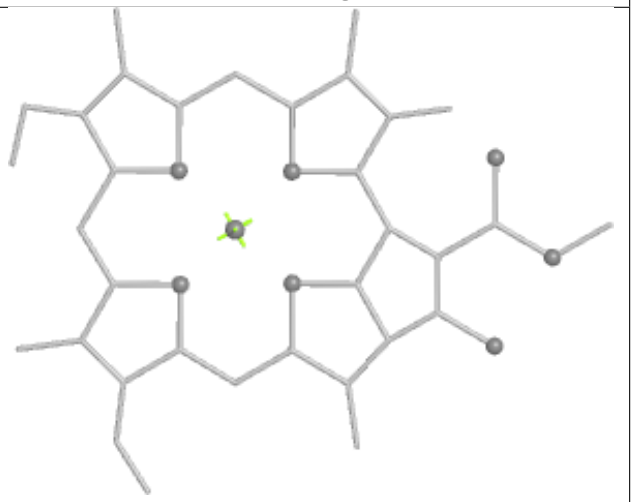
Bond lengths



Bond angles

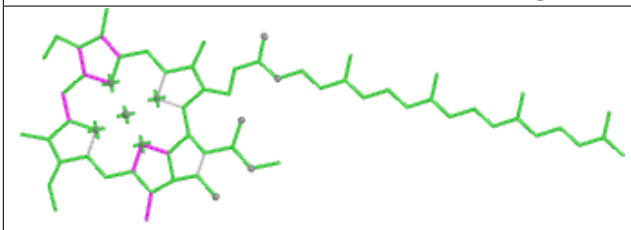


Torsions

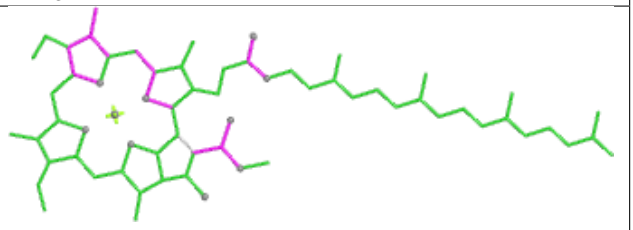


Rings

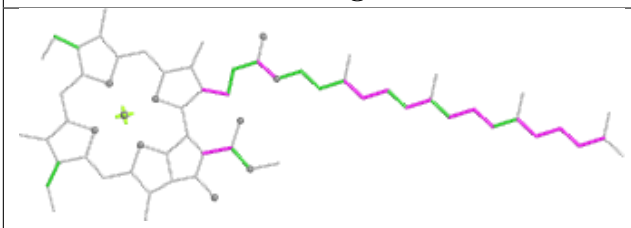
Ligand CLA j 101



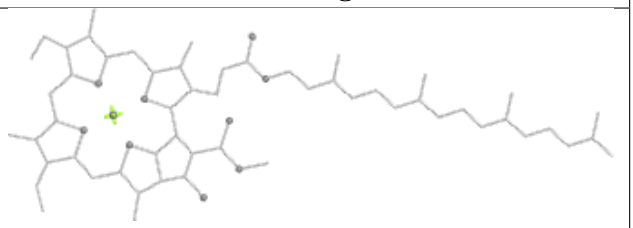
Bond lengths



Bond angles

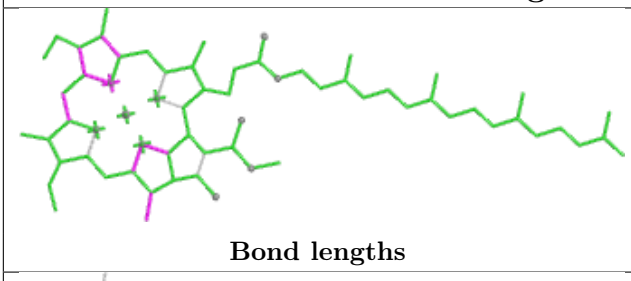


Torsions

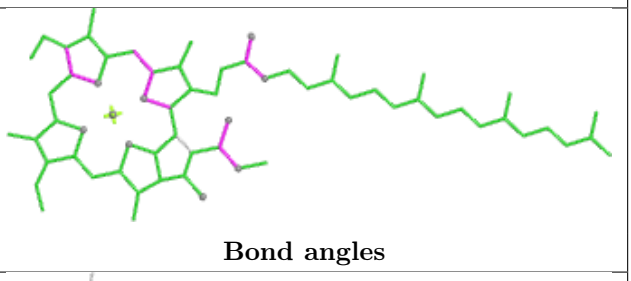


Rings

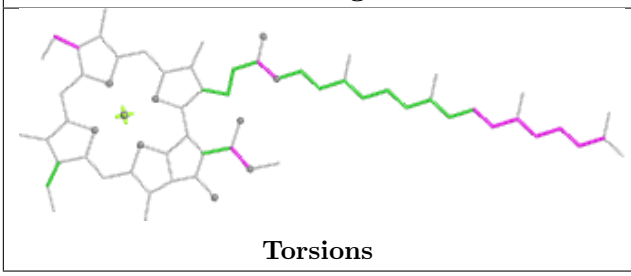
Ligand CLA b 842



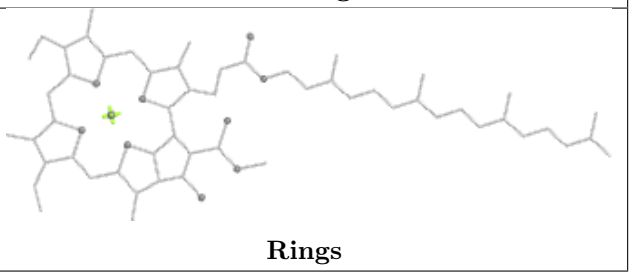
Bond lengths



Bond angles

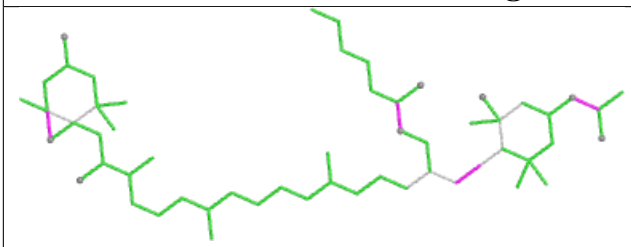


Torsions

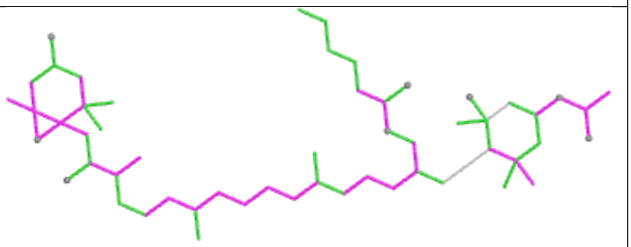


Rings

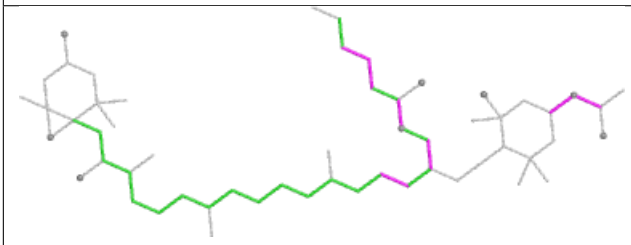
Ligand A1EB1 U 205



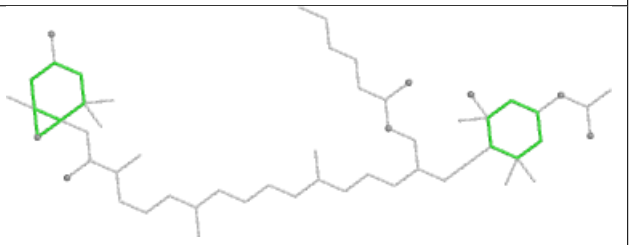
Bond lengths



Bond angles

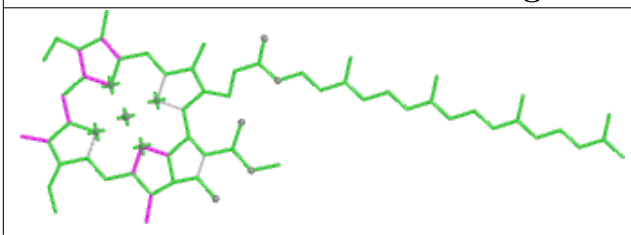


Torsions

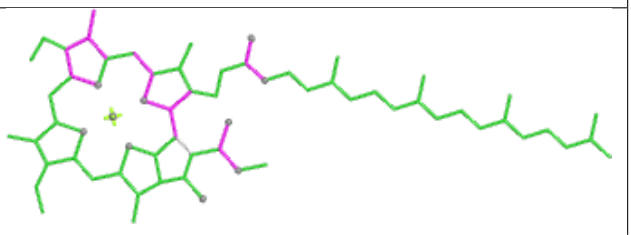


Rings

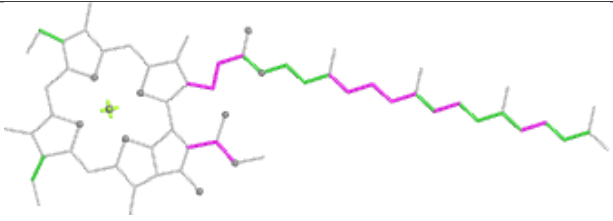
Ligand CLA D 317



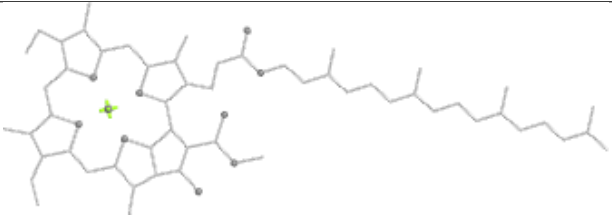
Bond lengths



Bond angles

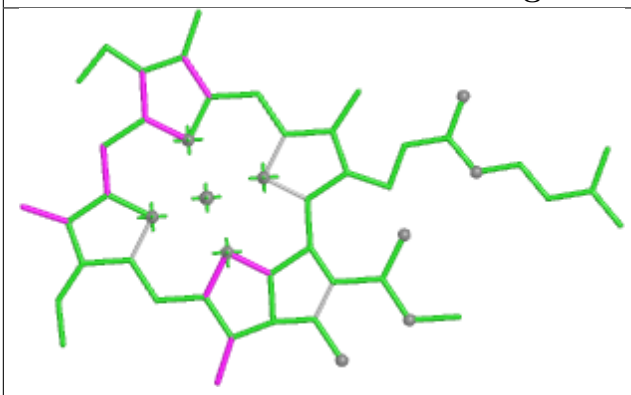


Torsions

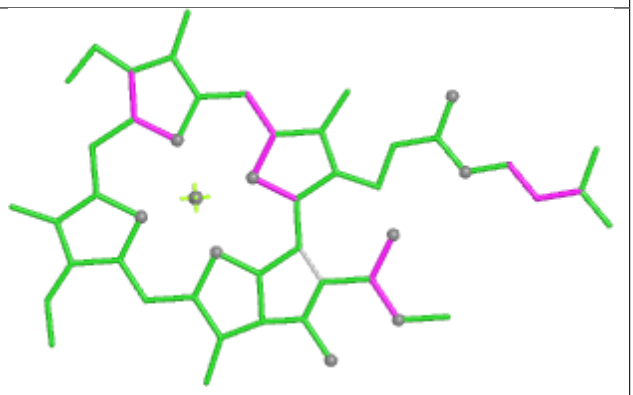


Rings

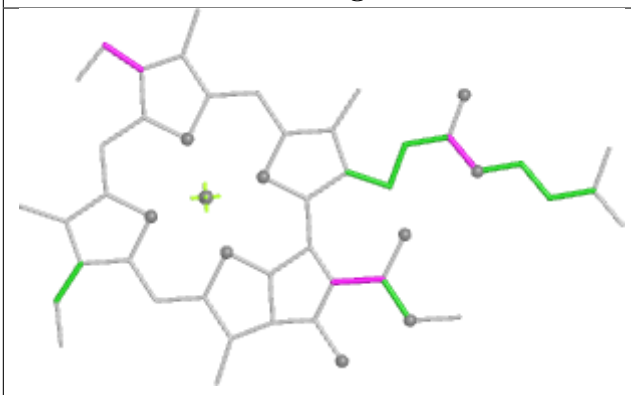
Ligand CLA R 311



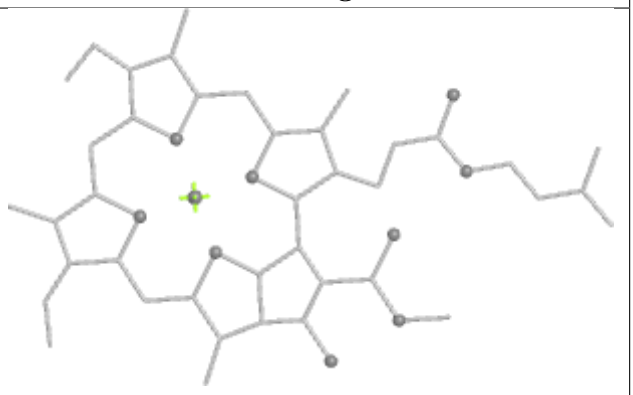
Bond lengths



Bond angles

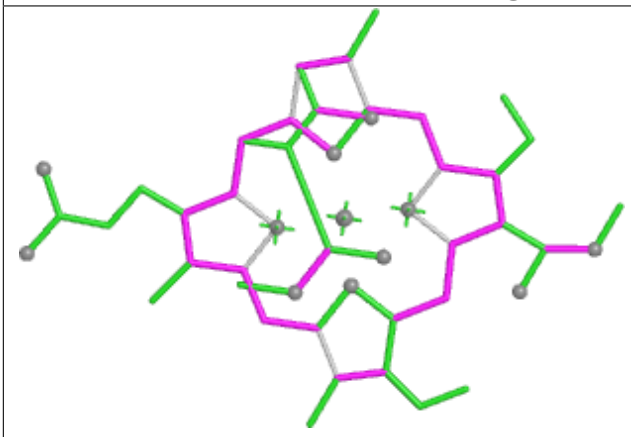


Torsions

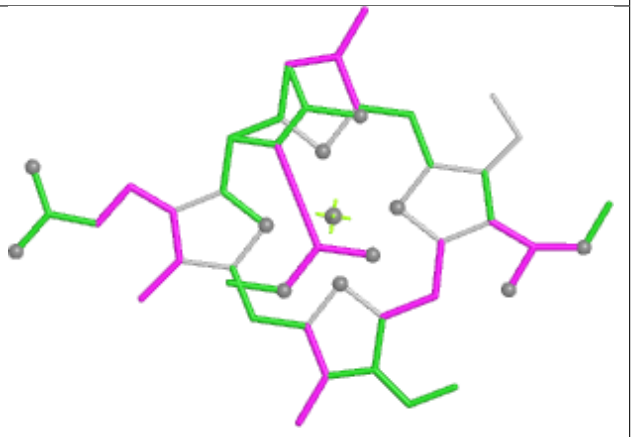


Rings

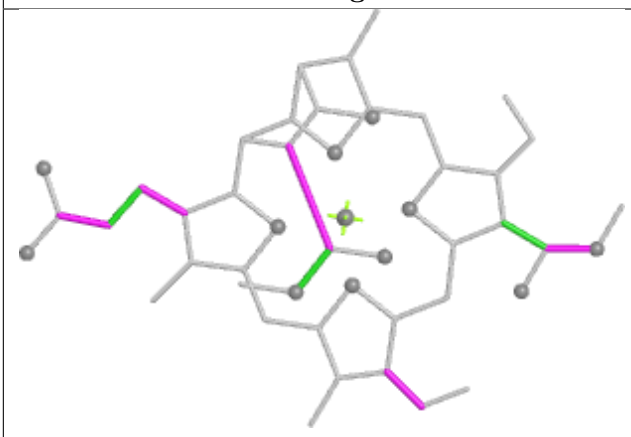
Ligand A1ECV 4 315



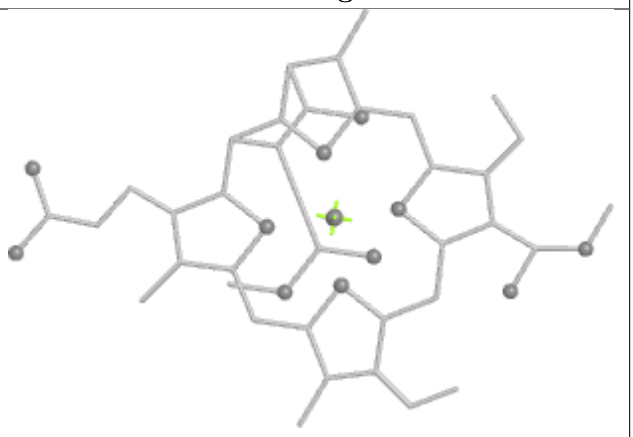
Bond lengths



Bond angles

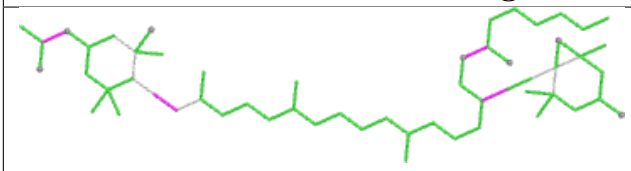


Torsions

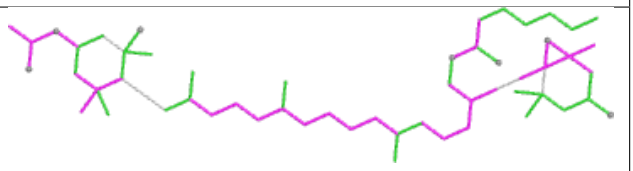


Rings

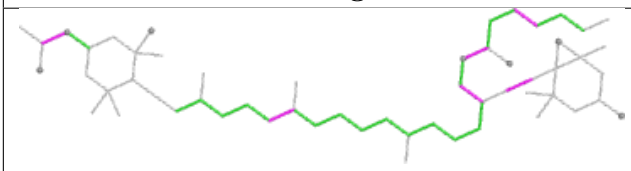
Ligand A1EB4 W 306



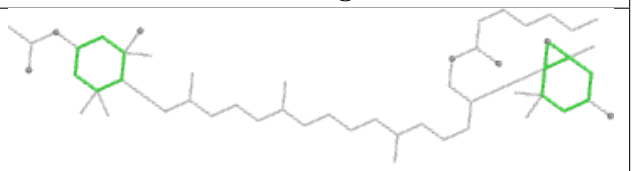
Bond lengths



Bond angles

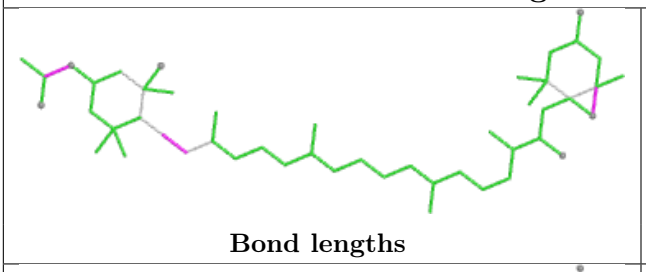


Torsions

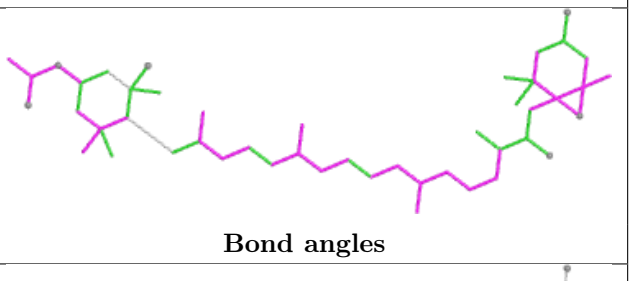


Rings

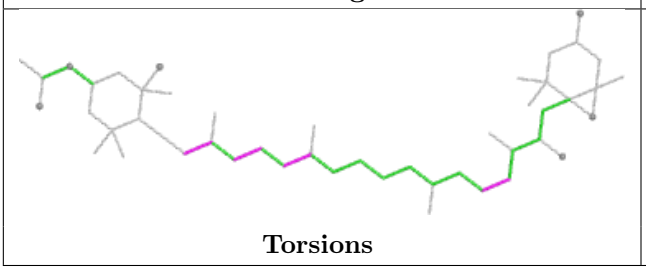
Ligand A86 O 306



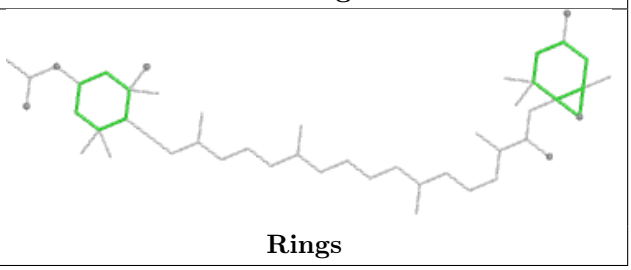
Bond lengths



Bond angles

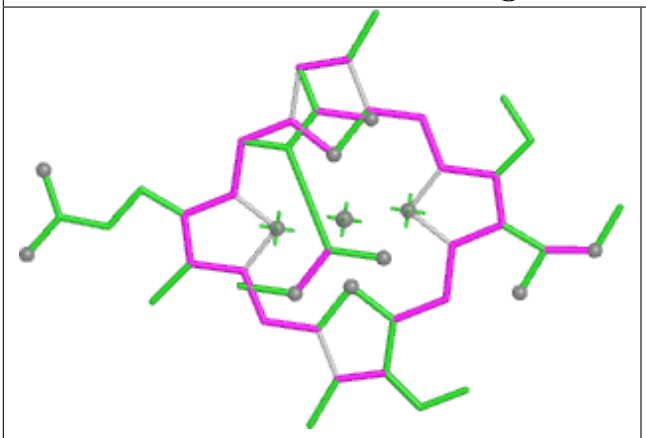


Torsions

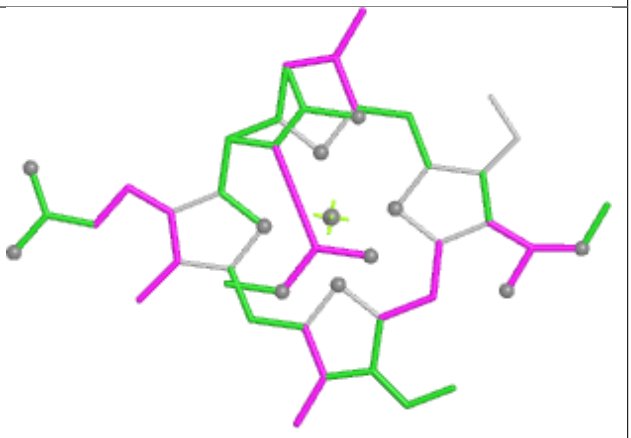


Rings

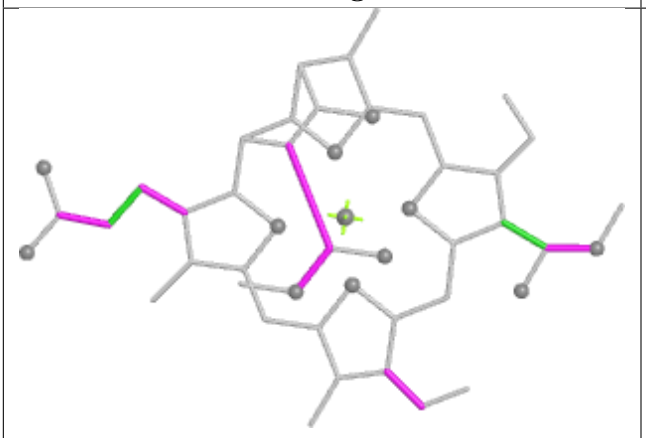
Ligand A1ECV V 317



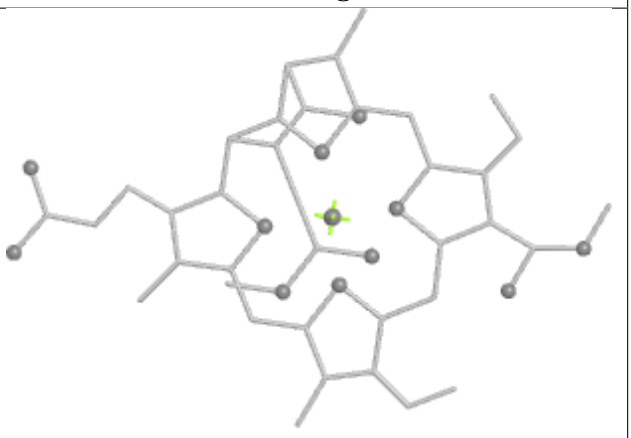
Bond lengths



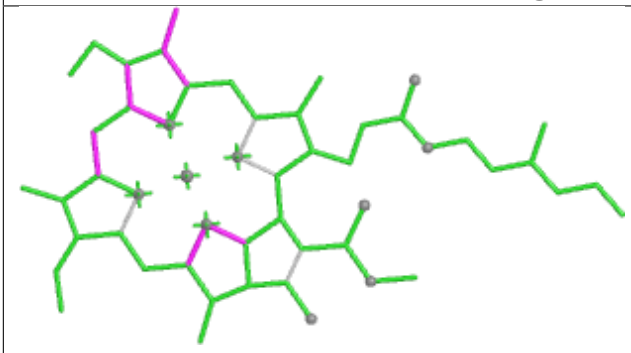
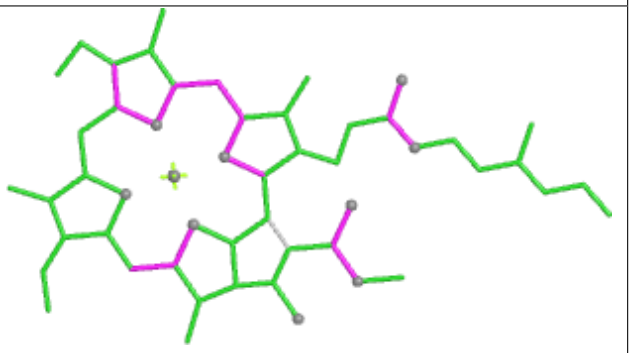
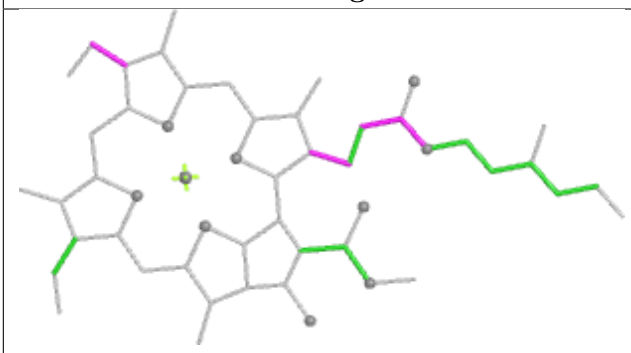
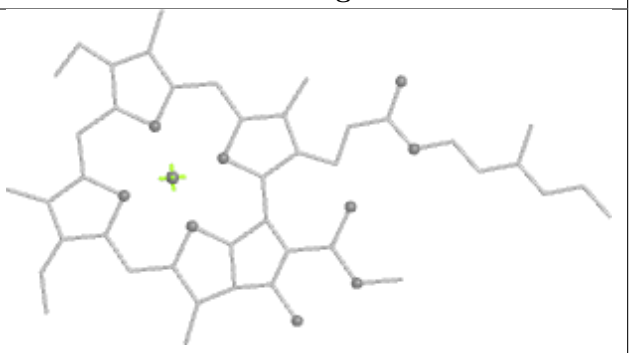
Bond angles

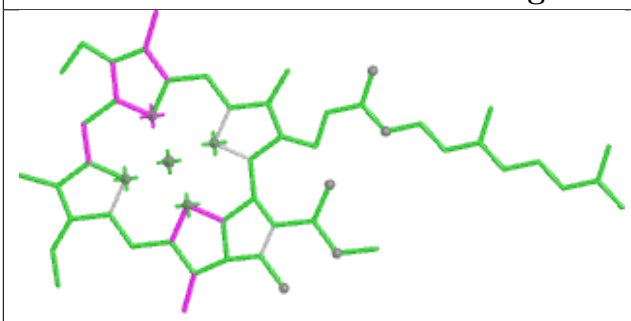
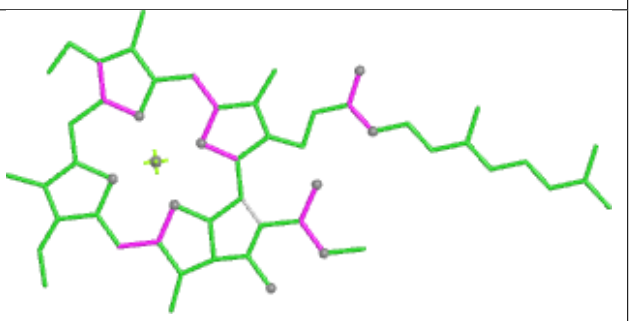
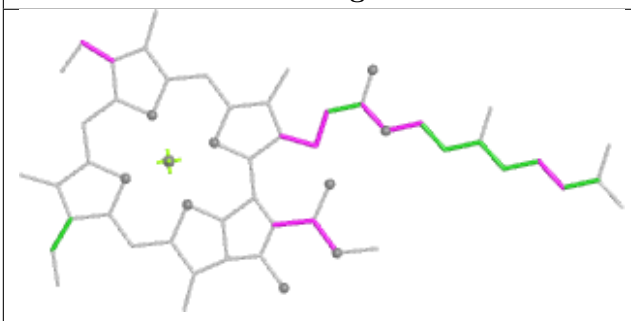
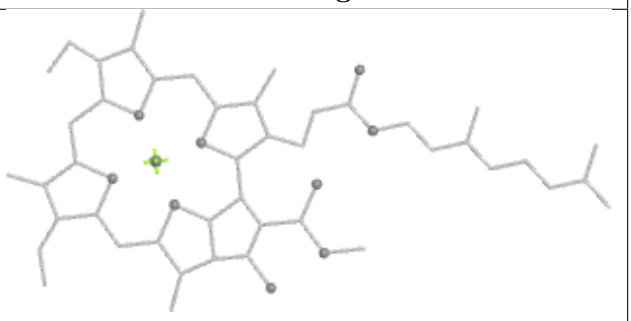


Torsions

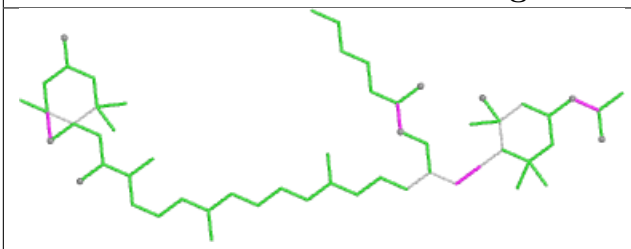


Rings

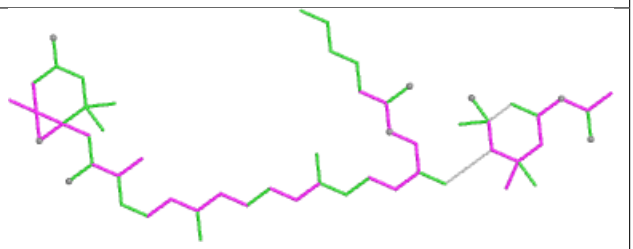
Ligand CLA I 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA k 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

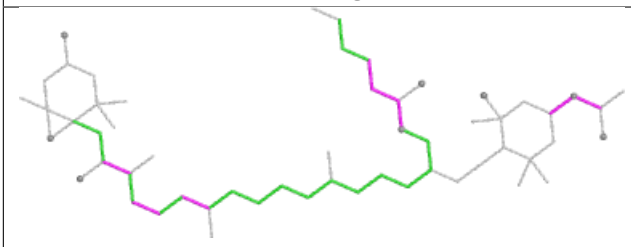
Ligand A1EB1 3 302



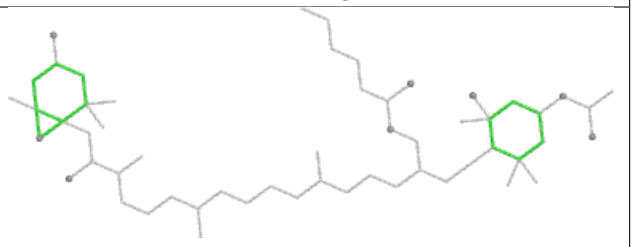
Bond lengths



Bond angles

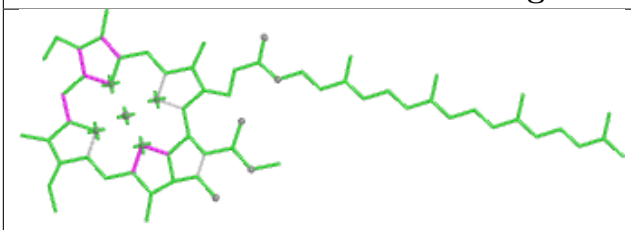


Torsions

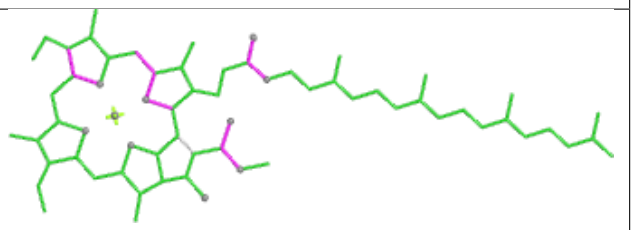


Rings

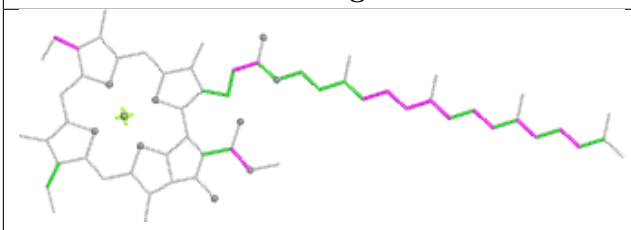
Ligand CLA b 810



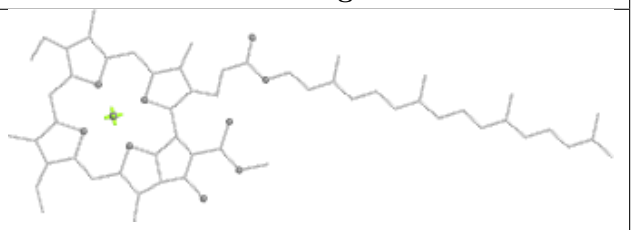
Bond lengths



Bond angles

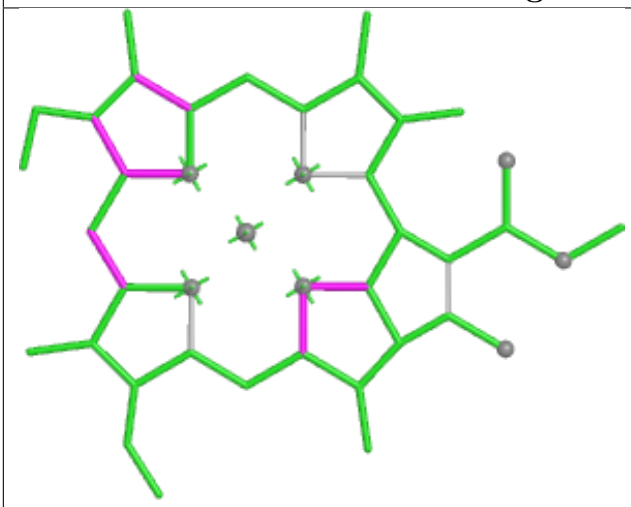


Torsions

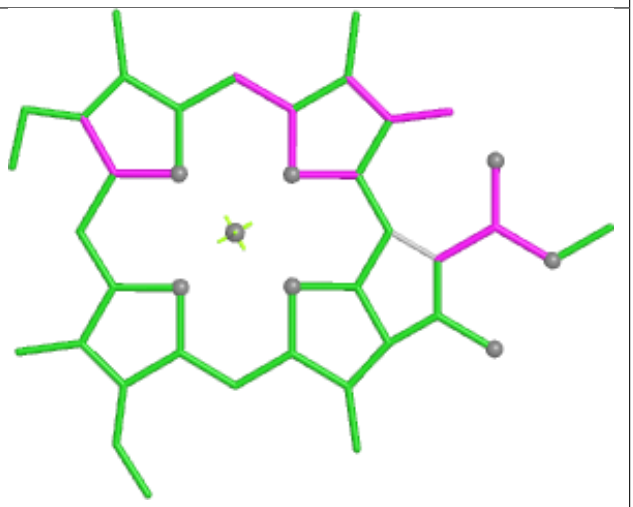


Rings

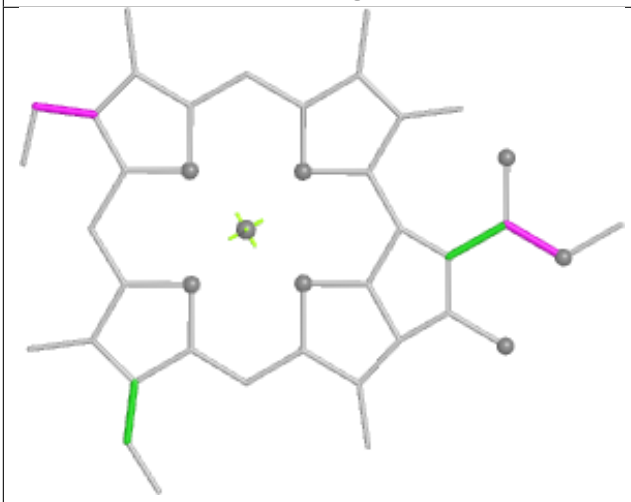
Ligand CLA F 315



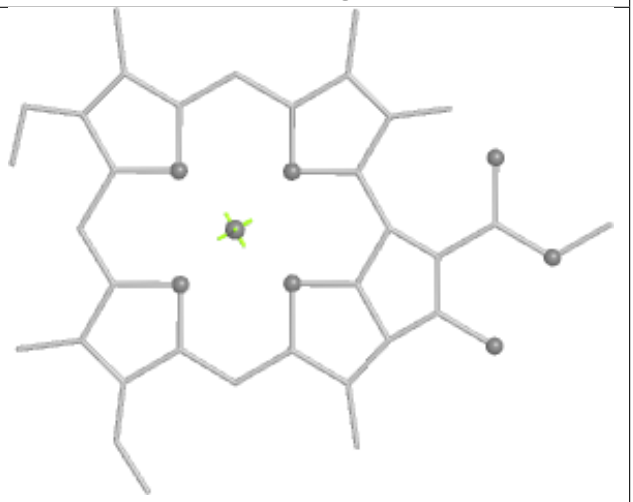
Bond lengths



Bond angles

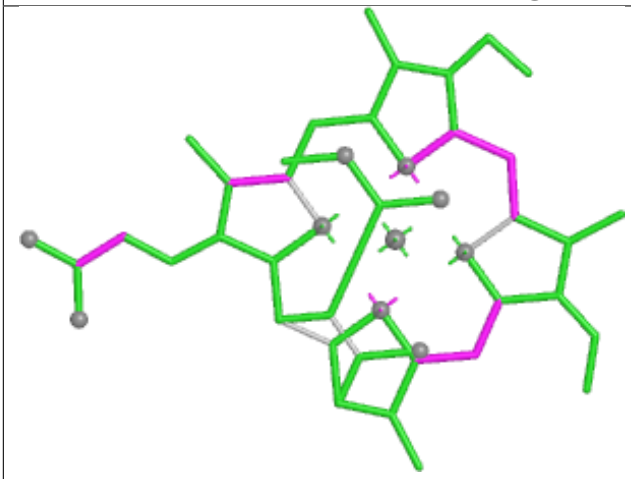


Torsions

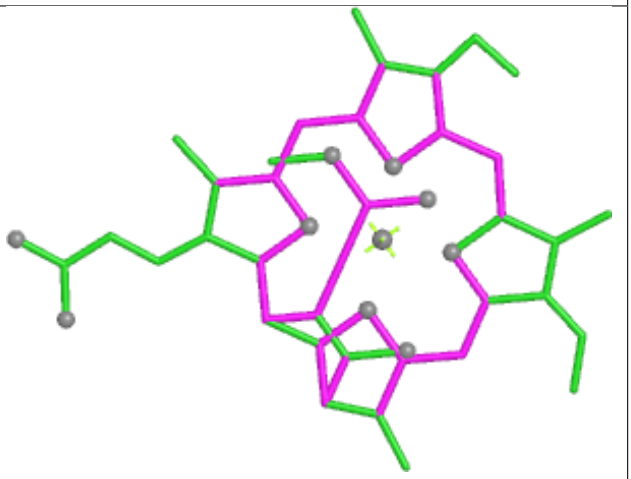


Rings

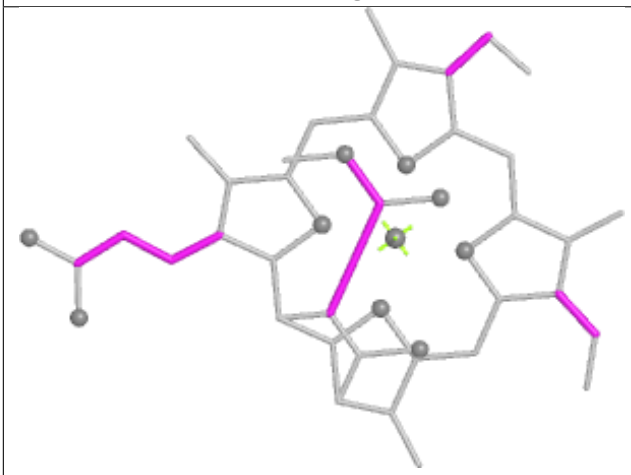
Ligand KC2 C 313



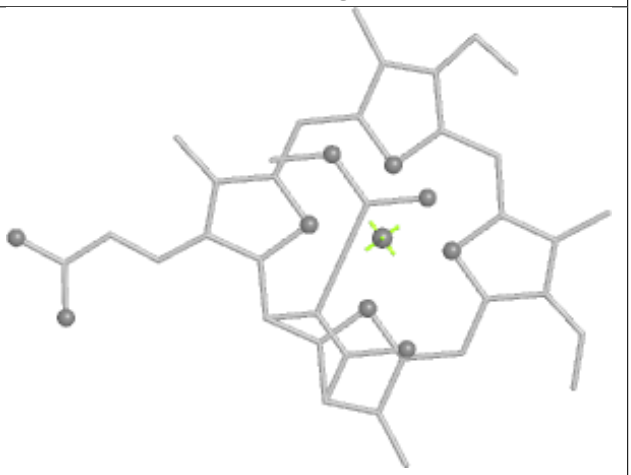
Bond lengths



Bond angles

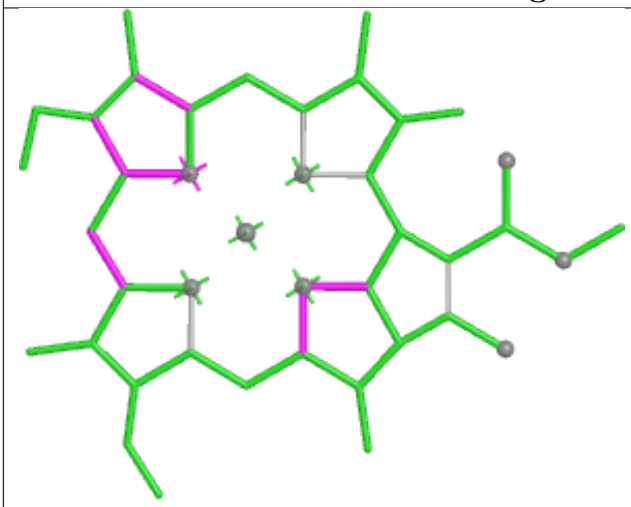


Torsions

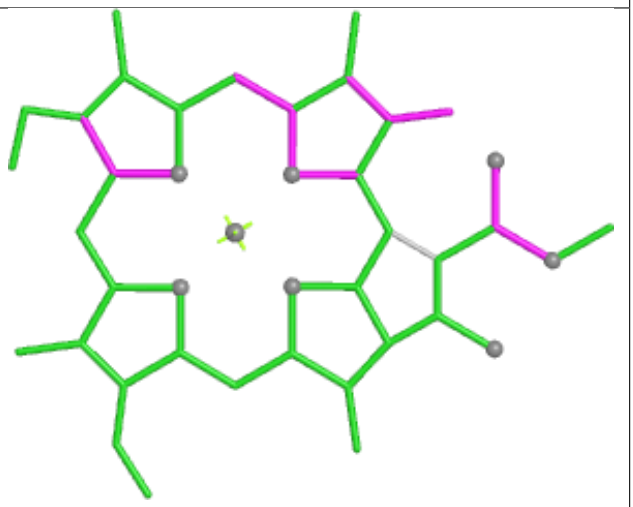


Rings

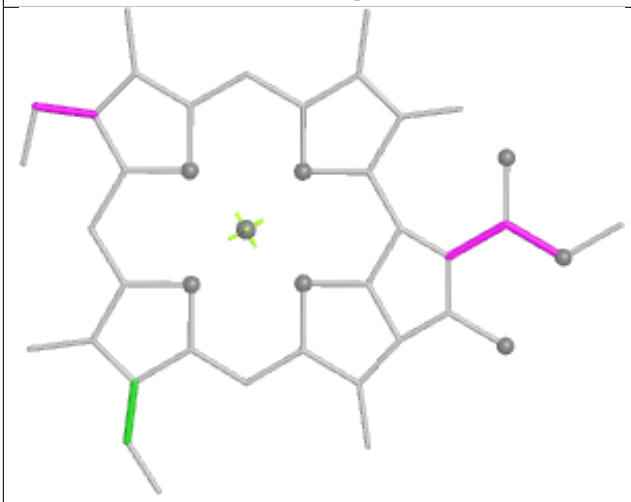
Ligand CLA z 311



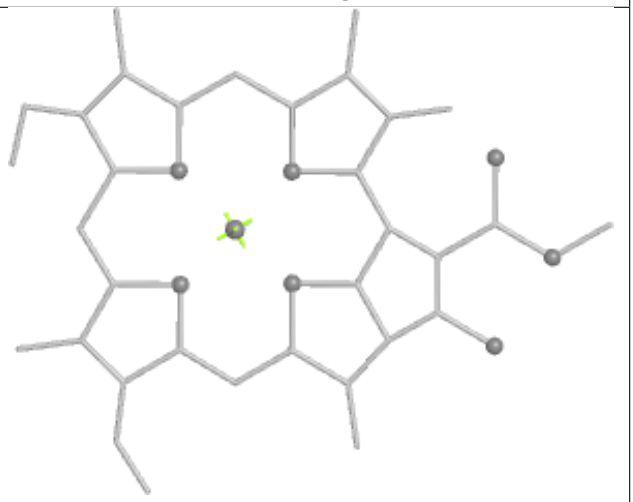
Bond lengths



Bond angles

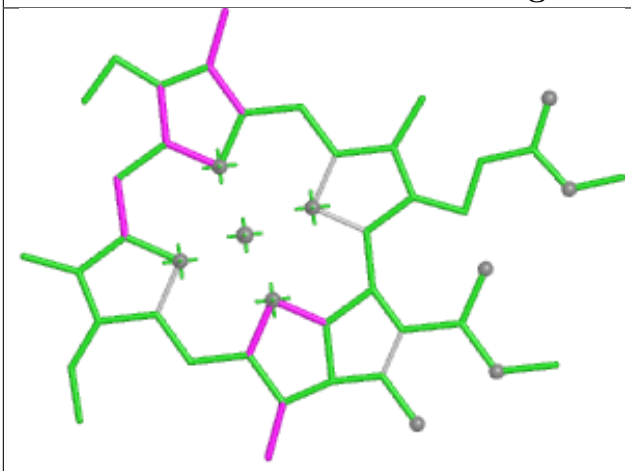


Torsions

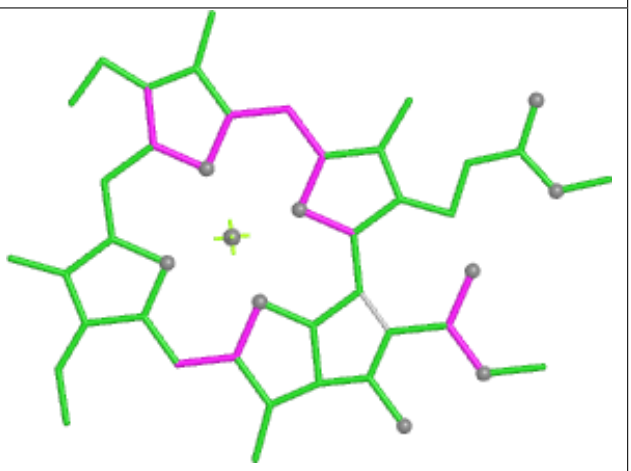


Rings

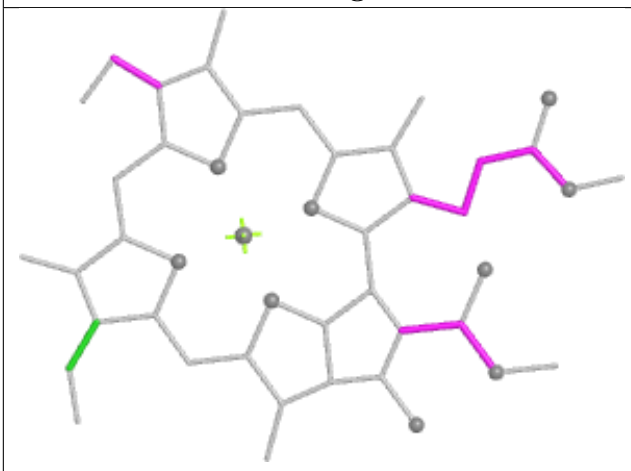
Ligand CLA 2 308



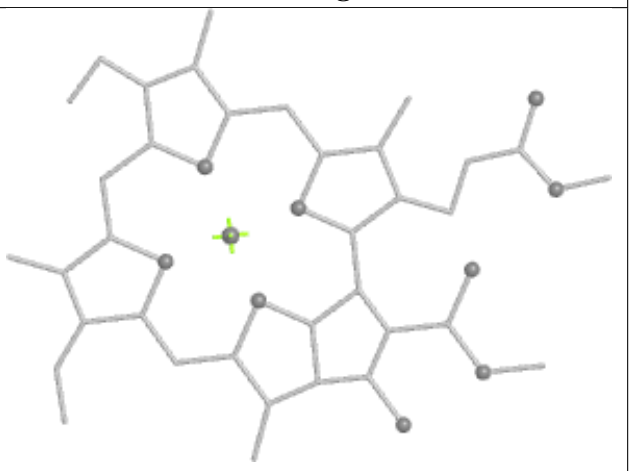
Bond lengths



Bond angles

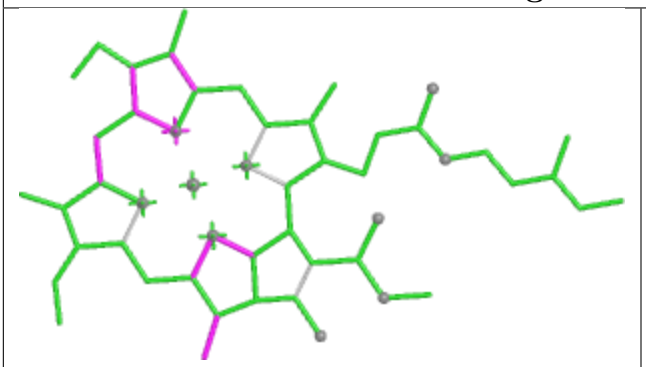


Torsions

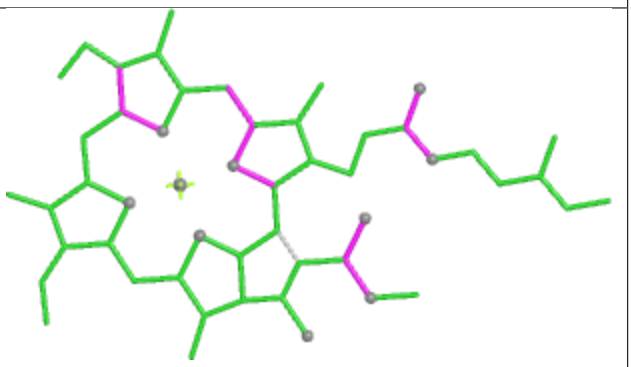


Rings

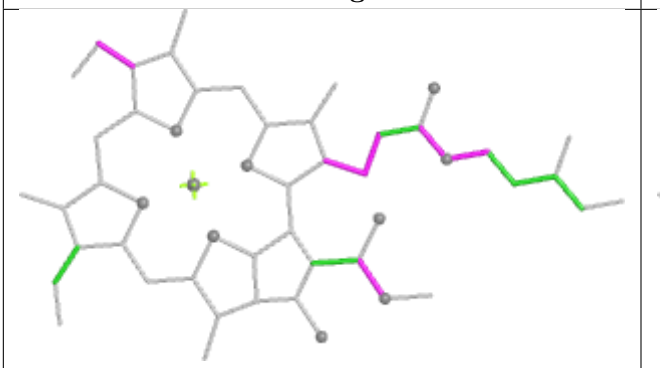
Ligand CLA F 316



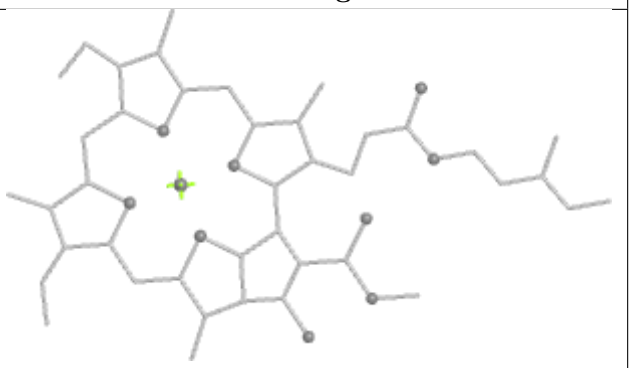
Bond lengths



Bond angles

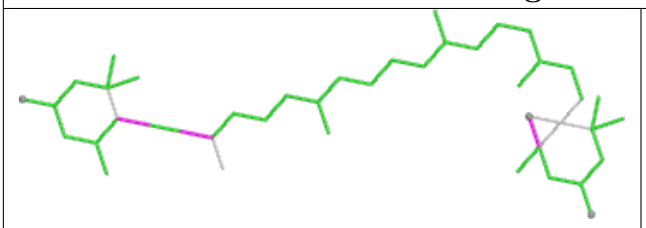


Torsions

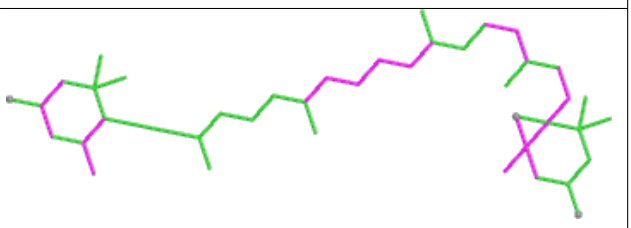


Rings

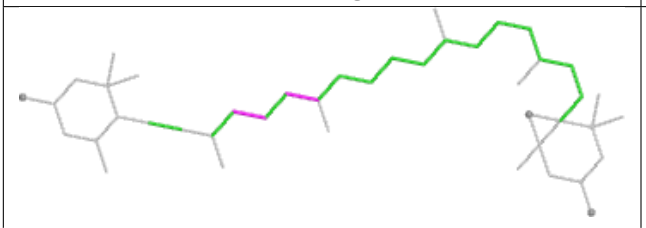
Ligand DD6 D 307



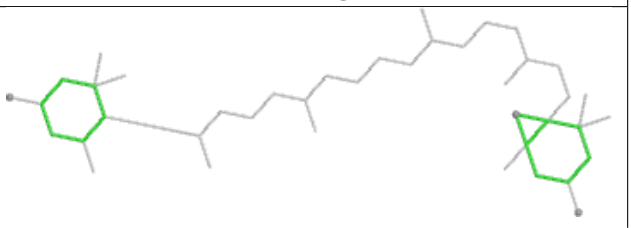
Bond lengths



Bond angles

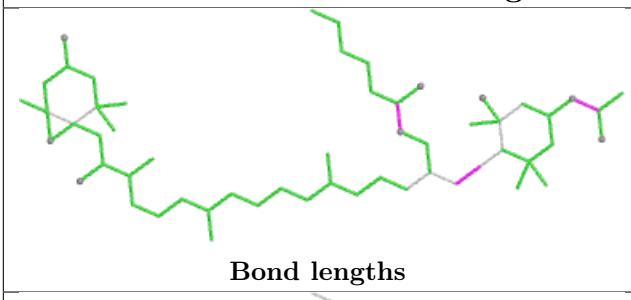


Torsions

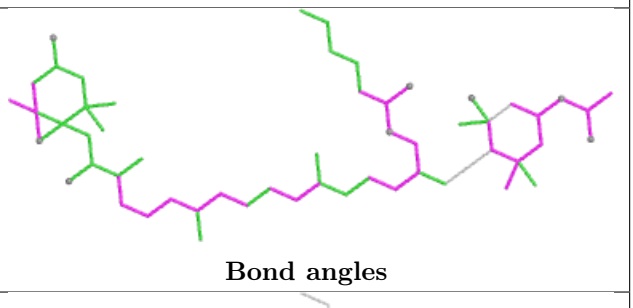


Rings

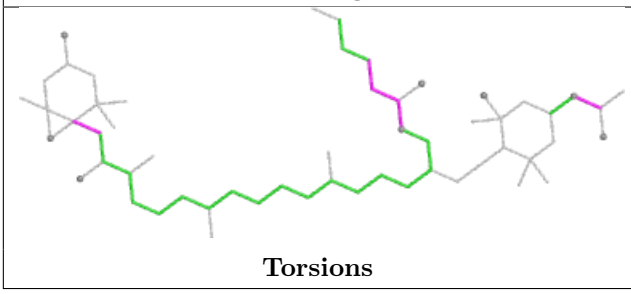
Ligand A1EB1 V 306



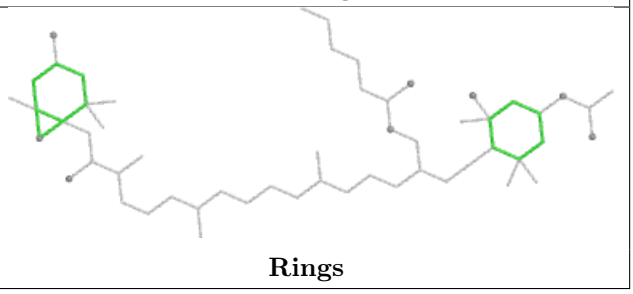
Bond lengths



Bond angles

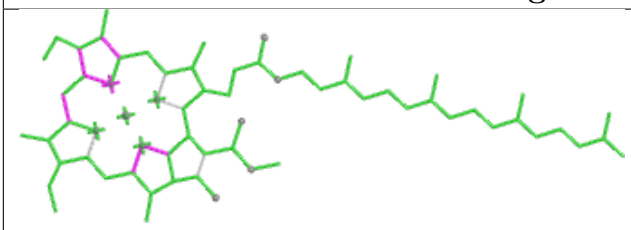


Torsions

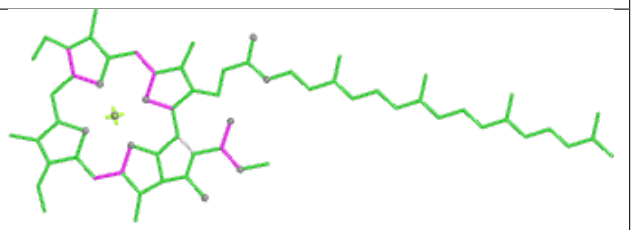


Rings

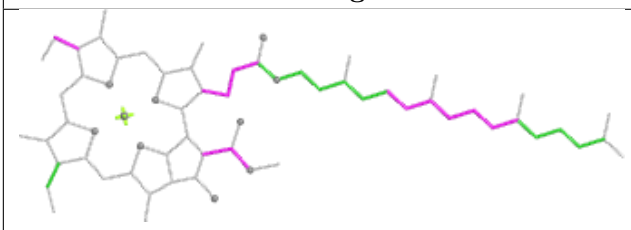
Ligand CLA 3 314



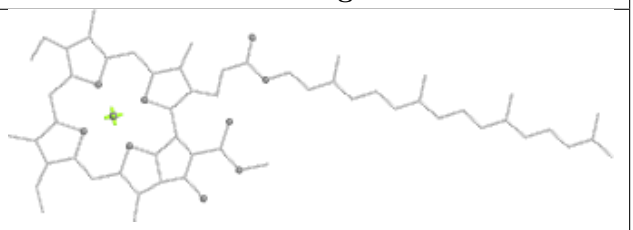
Bond lengths



Bond angles

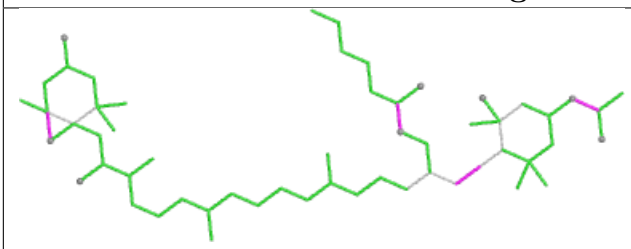


Torsions

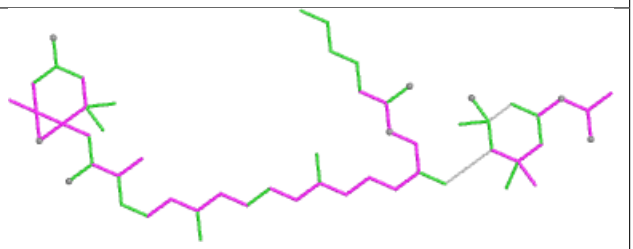


Rings

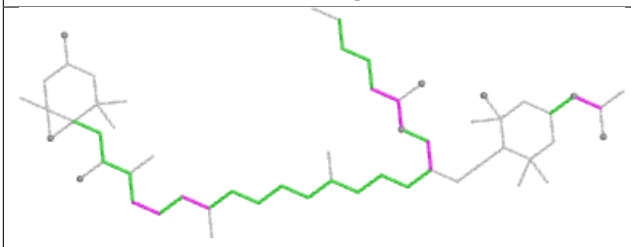
Ligand A1EB1 4 302



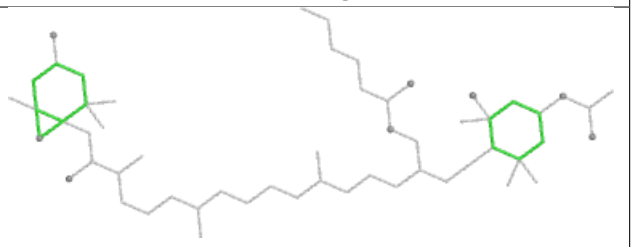
Bond lengths



Bond angles

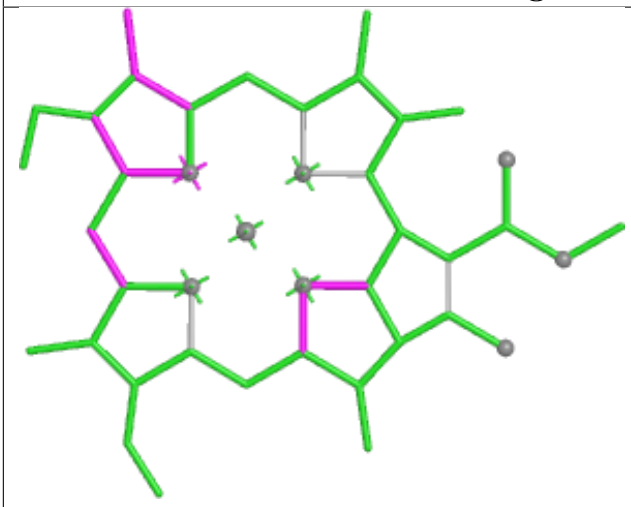


Torsions

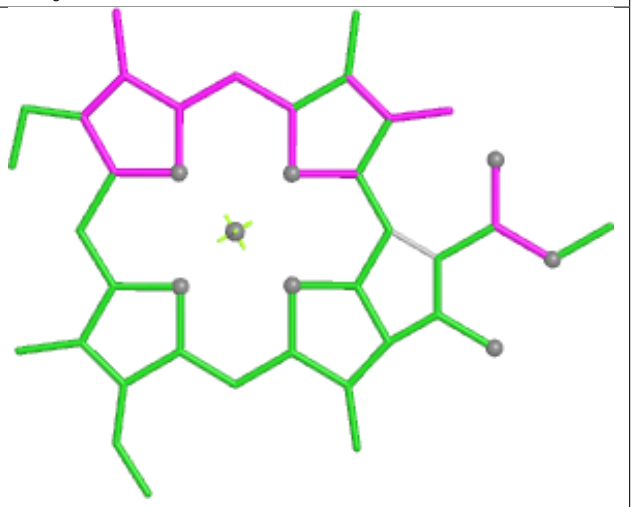


Rings

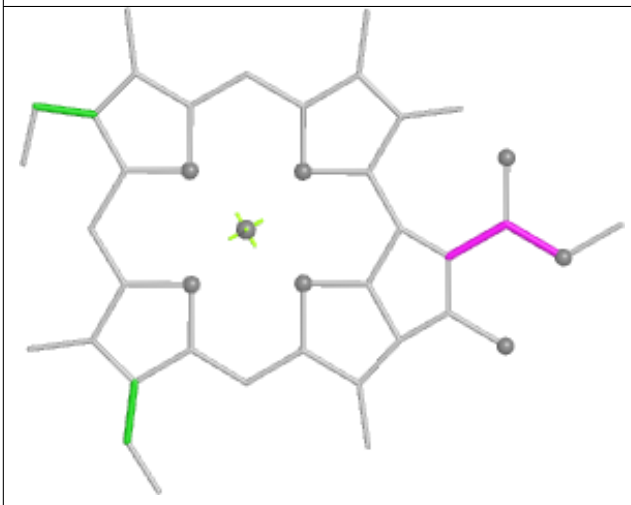
Ligand CLA y 319



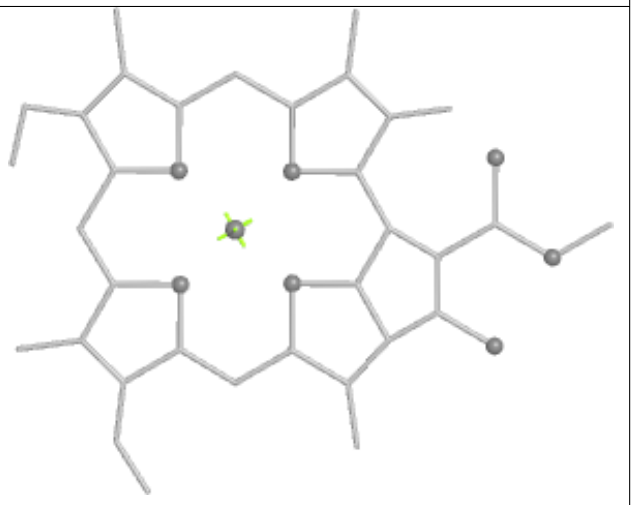
Bond lengths



Bond angles

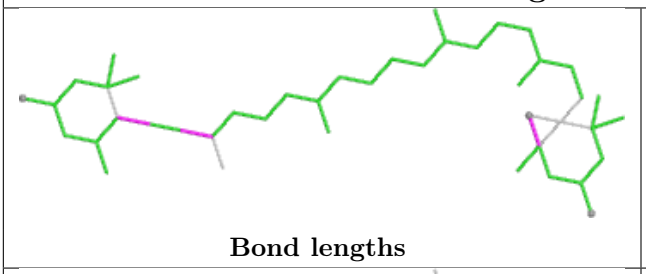


Torsions

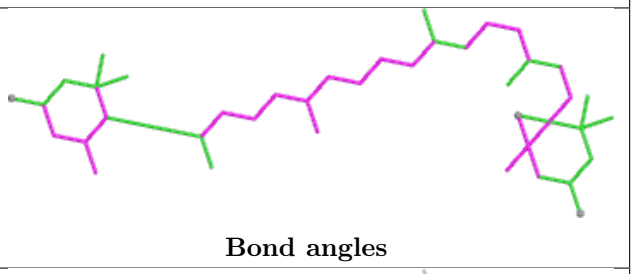


Rings

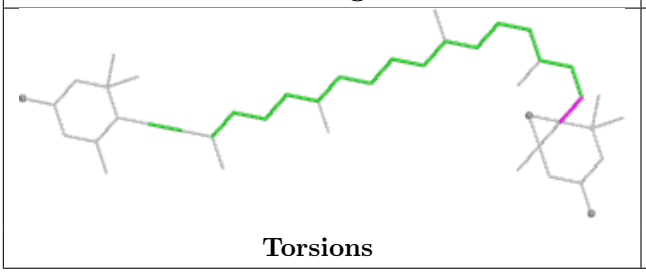
Ligand DD6 x 303



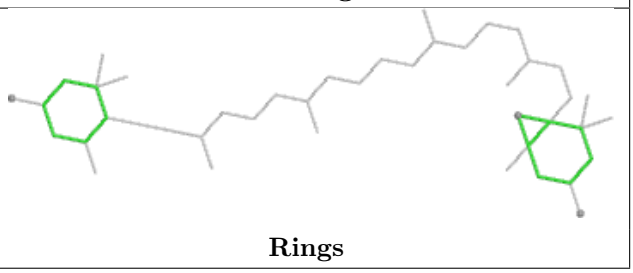
Bond lengths



Bond angles

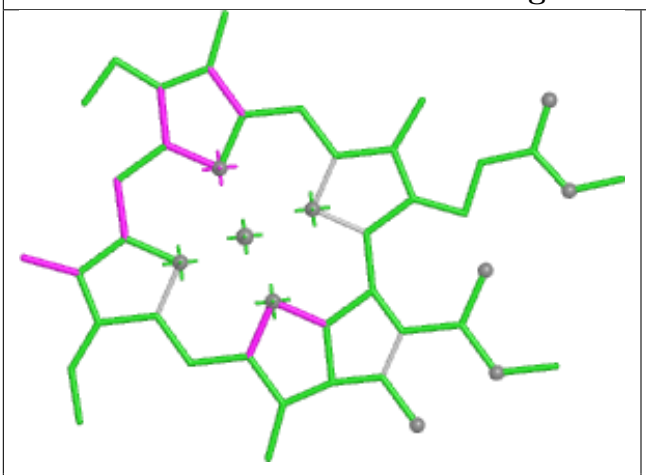


Torsions

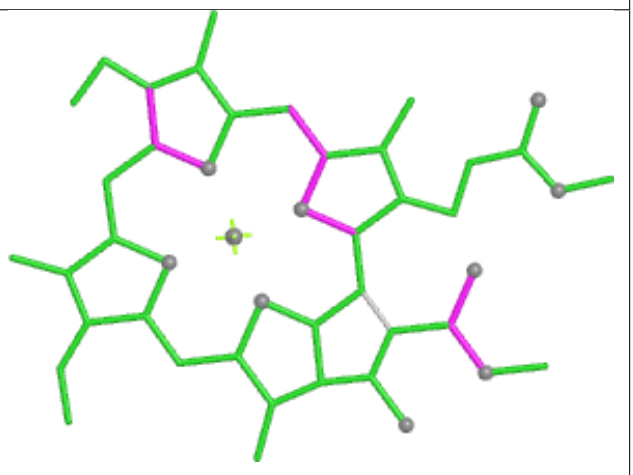


Rings

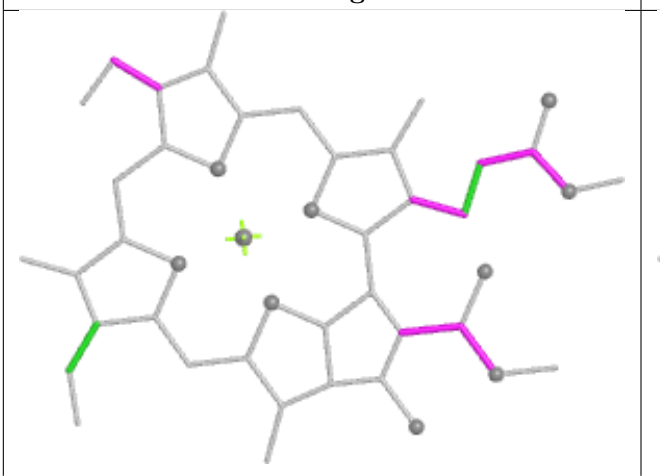
Ligand CLA 3 323



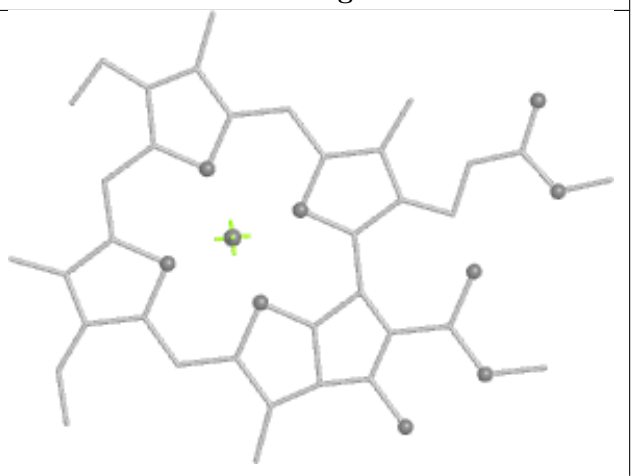
Bond lengths



Bond angles

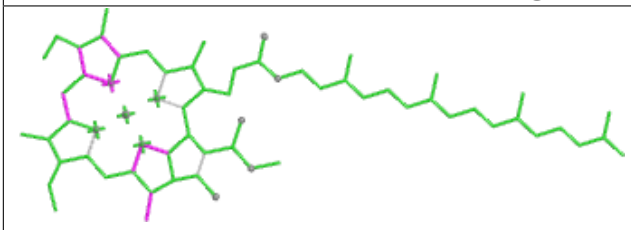


Torsions

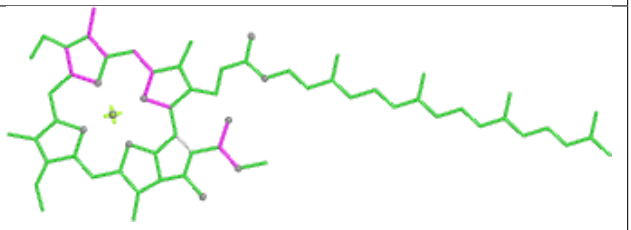


Rings

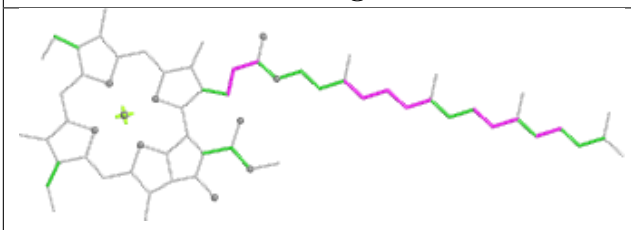
Ligand CLA 4 314



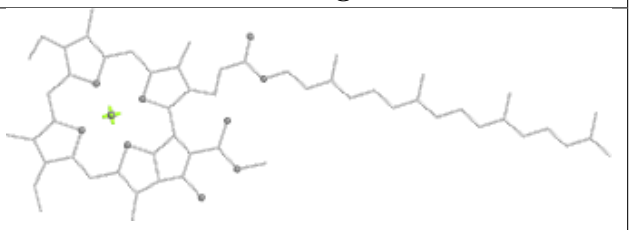
Bond lengths



Bond angles

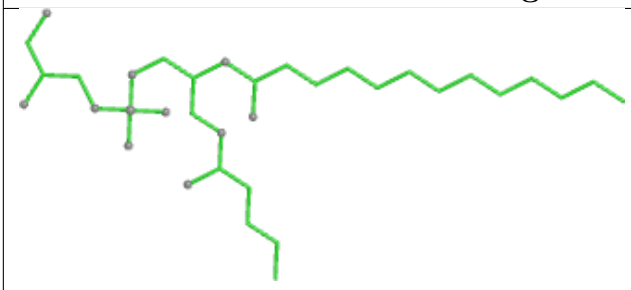


Torsions

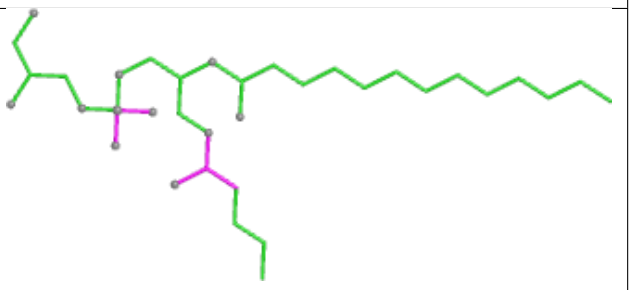


Rings

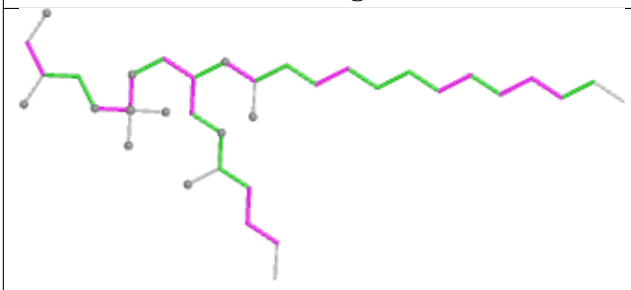
Ligand LHG H 317



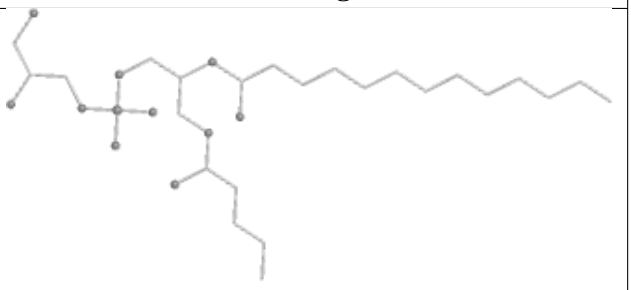
Bond lengths



Bond angles

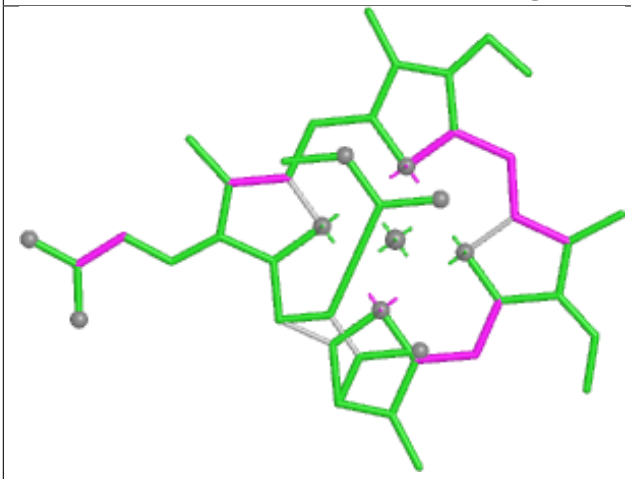


Torsions

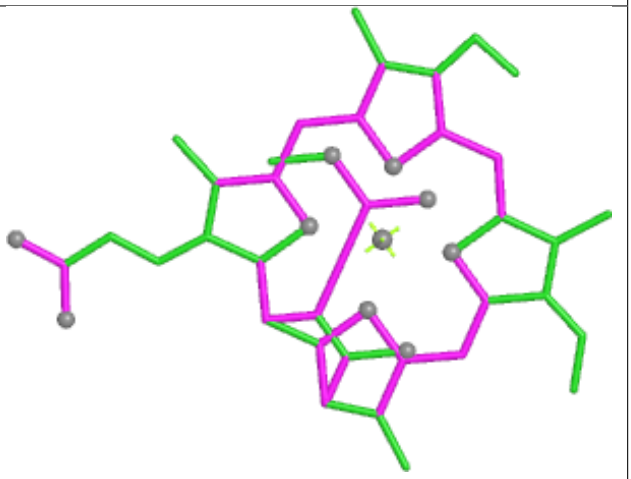


Rings

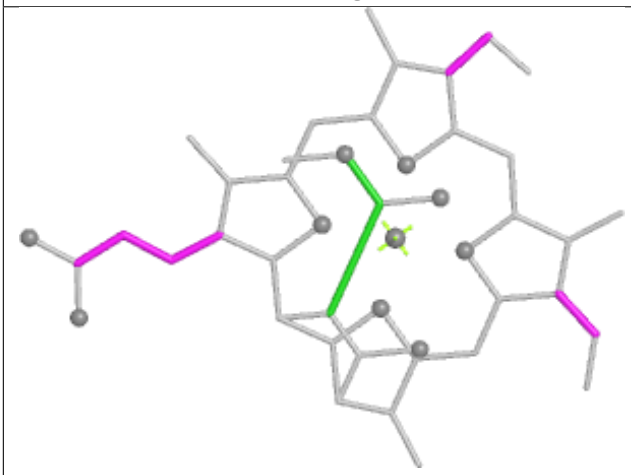
Ligand KC2 B 208



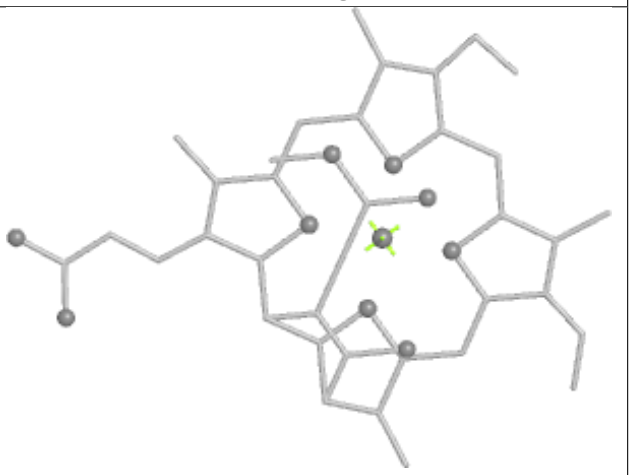
Bond lengths



Bond angles

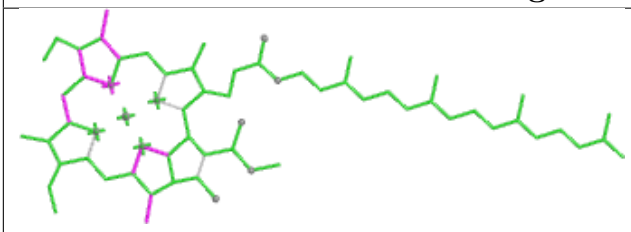


Torsions

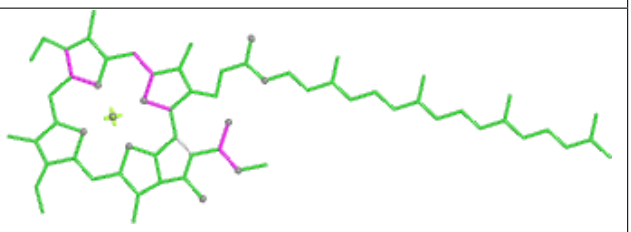


Rings

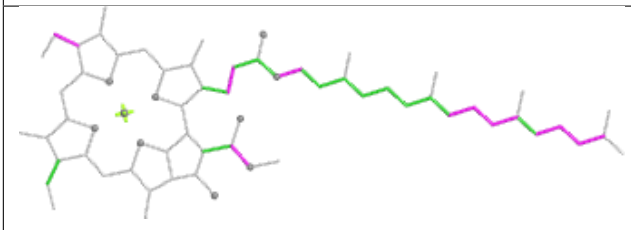
Ligand CLA 4 323



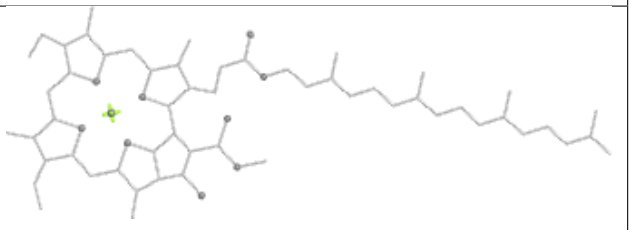
Bond lengths



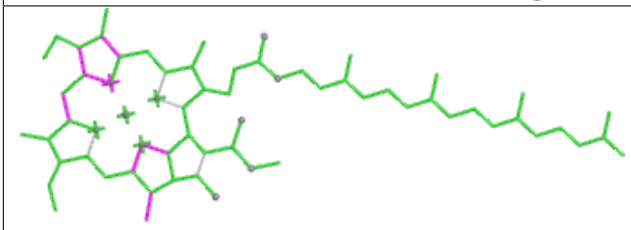
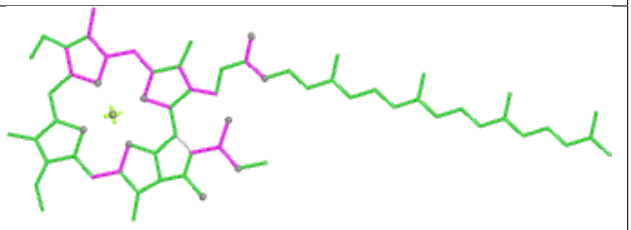
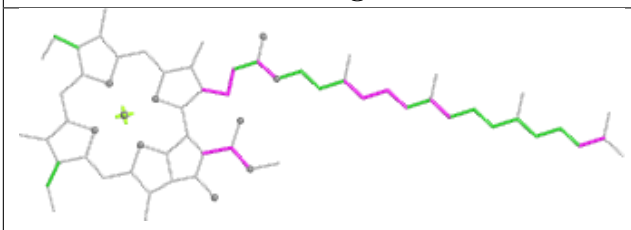
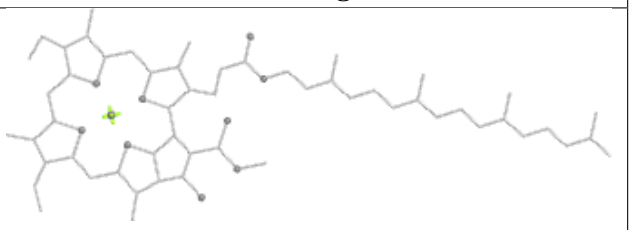
Bond angles

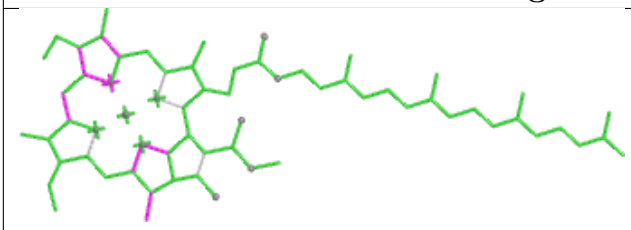
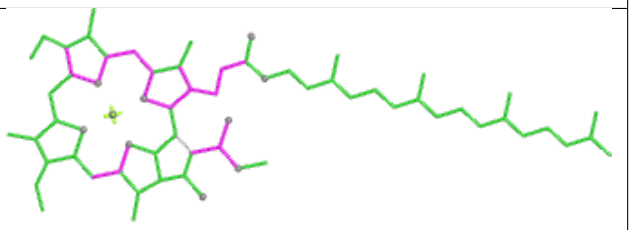
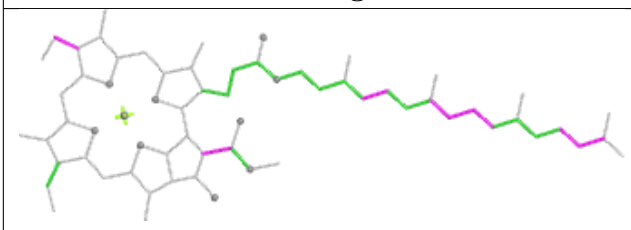
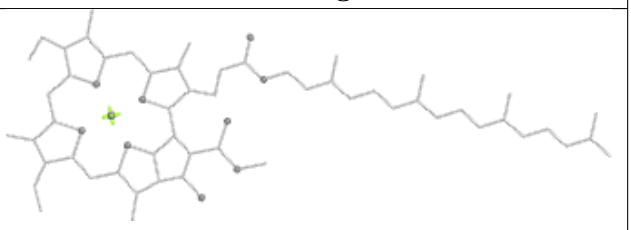


Torsions

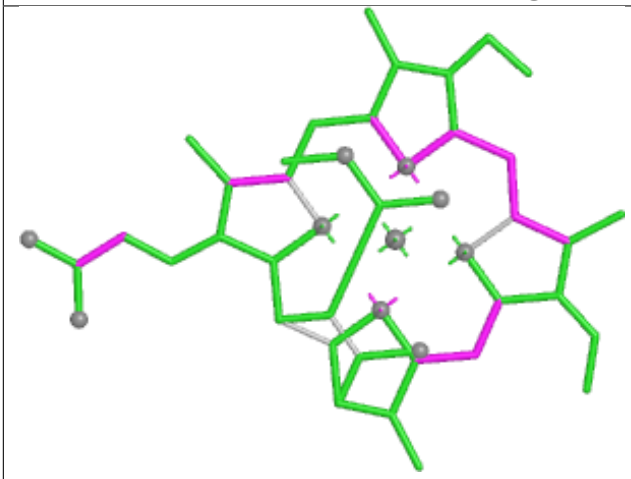


Rings

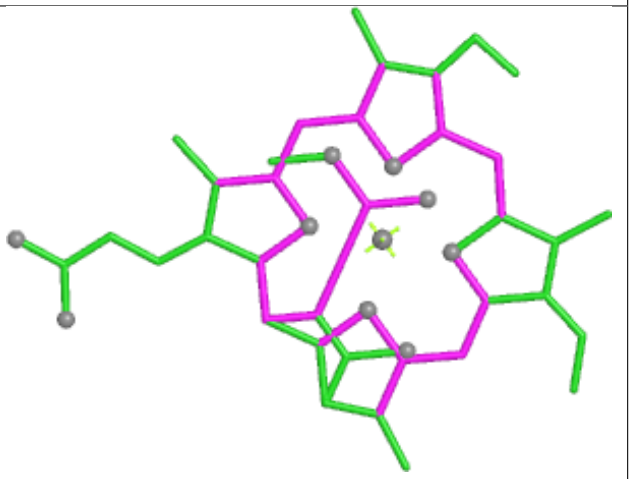
Ligand CLA 4 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

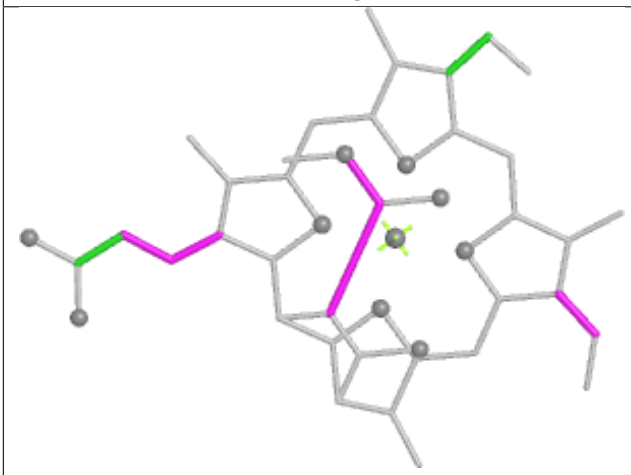
Ligand KC2 V 315



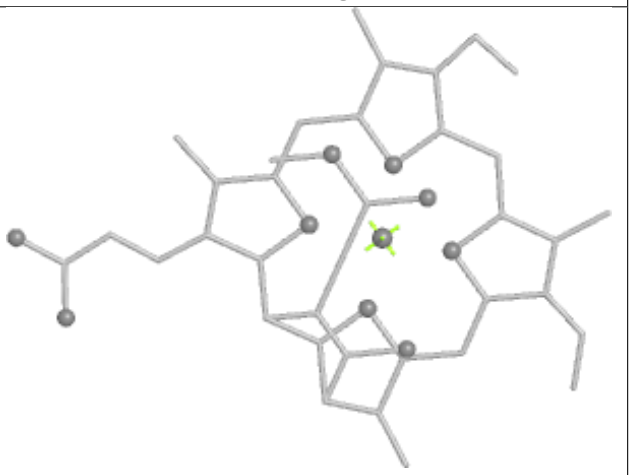
Bond lengths



Bond angles

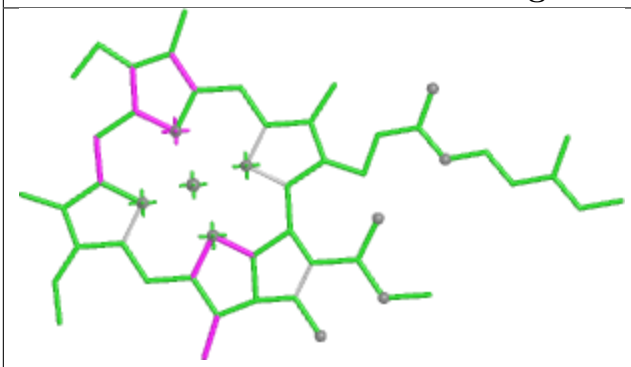


Torsions

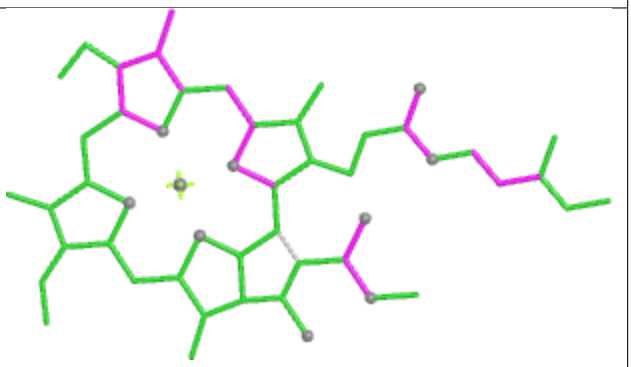


Rings

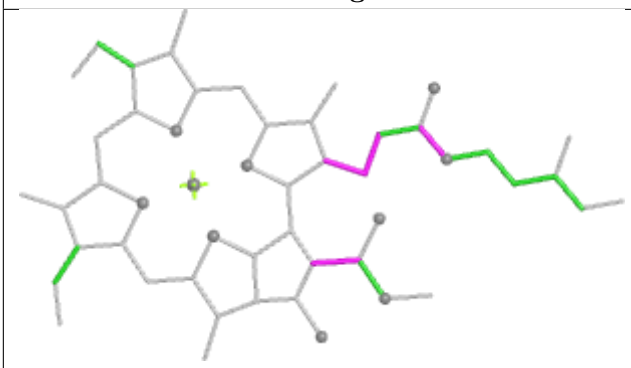
Ligand CLA a 834



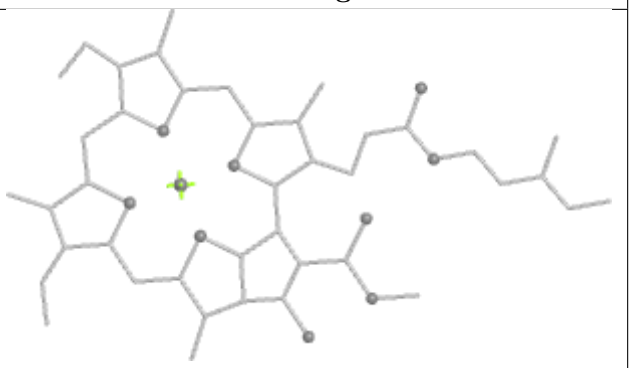
Bond lengths



Bond angles

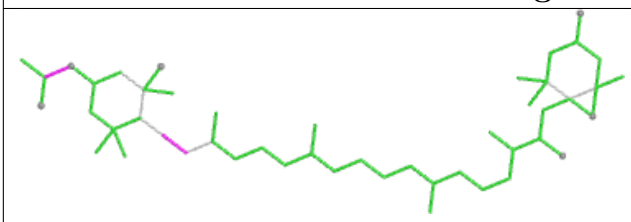


Torsions

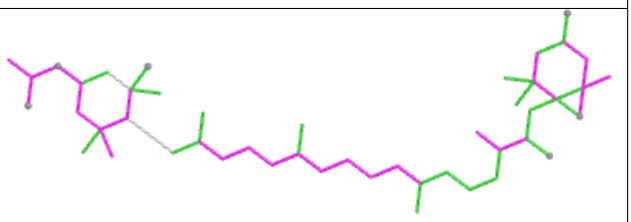


Rings

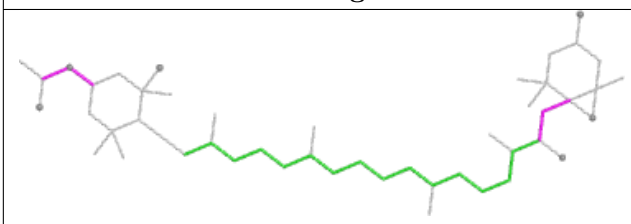
Ligand A86 4 310



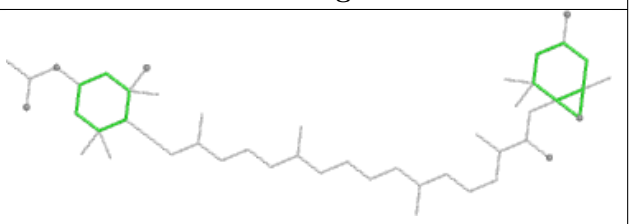
Bond lengths



Bond angles

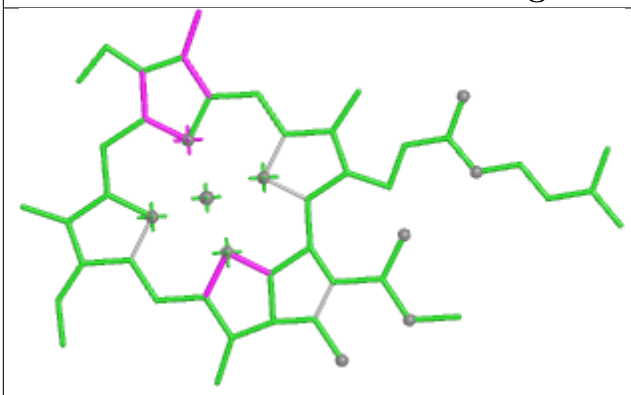


Torsions

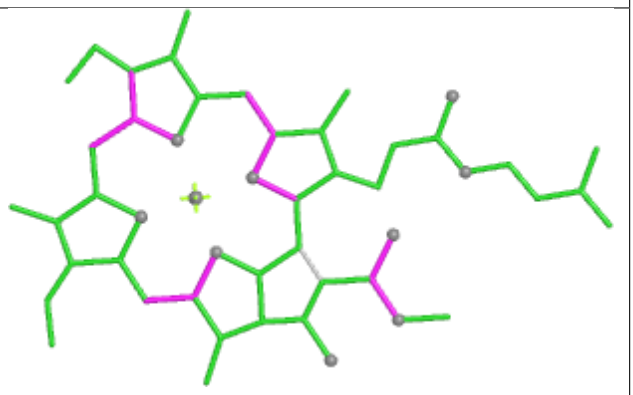


Rings

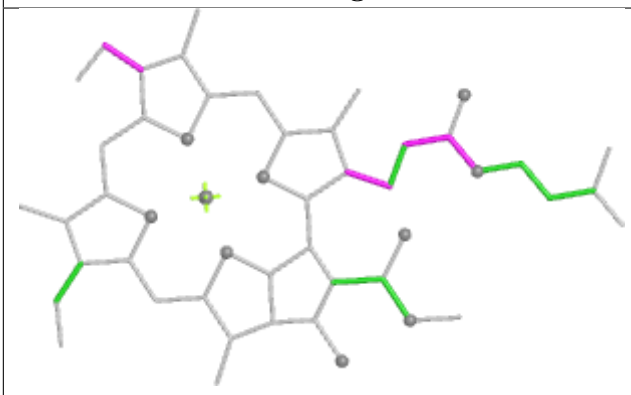
Ligand CLA a 832



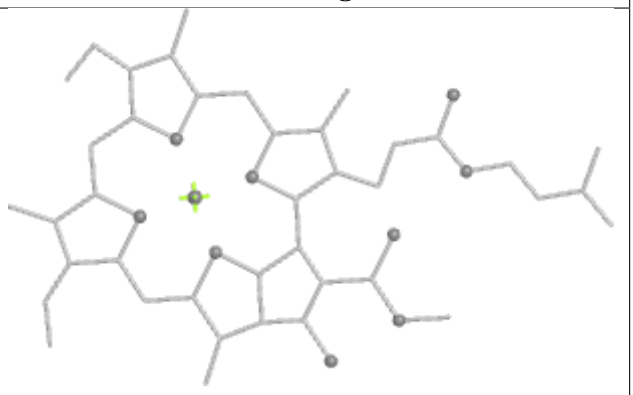
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

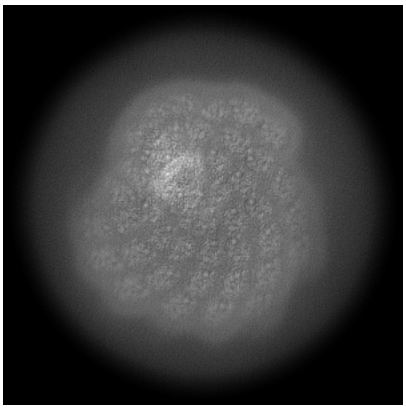
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61519. These allow visual inspection of the internal detail of the map and identification of artifacts.

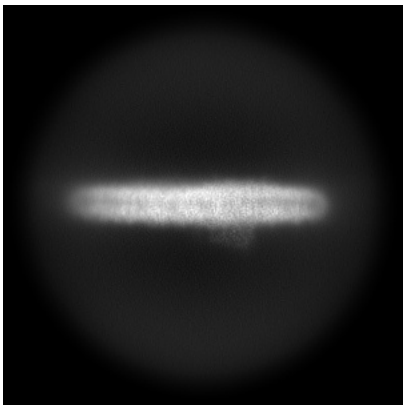
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

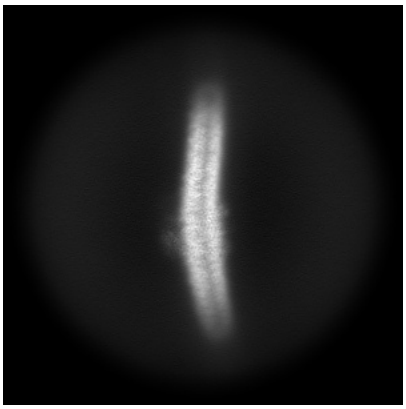
6.1.1 Primary map



X

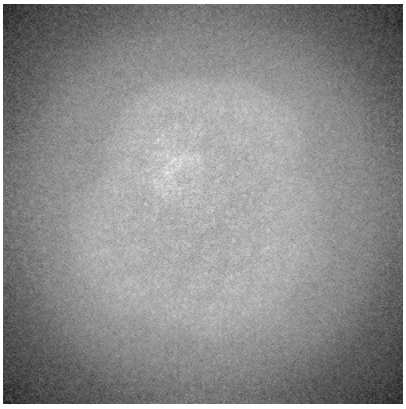


Y

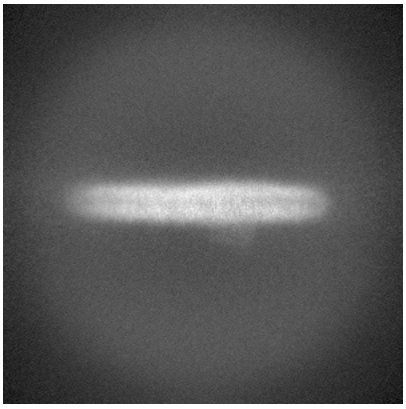


Z

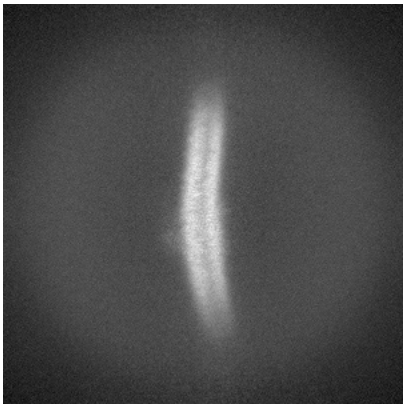
6.1.2 Raw map



X



Y

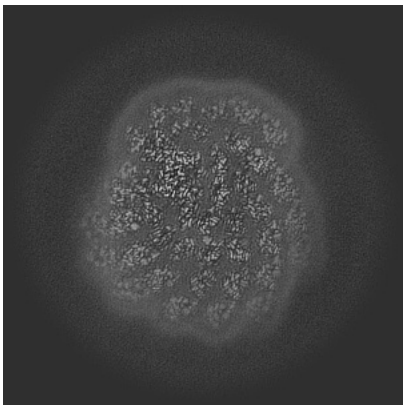


Z

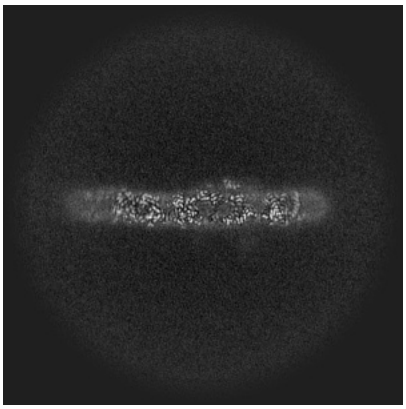
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

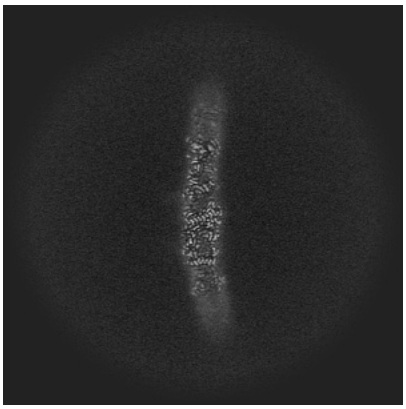
6.2.1 Primary map



X Index: 330

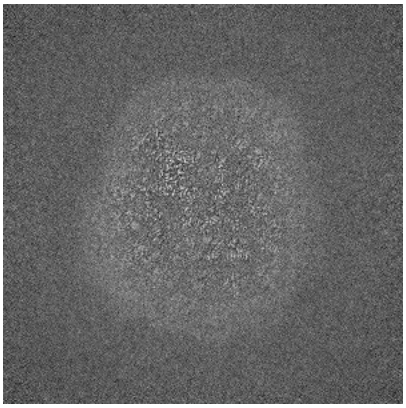


Y Index: 330

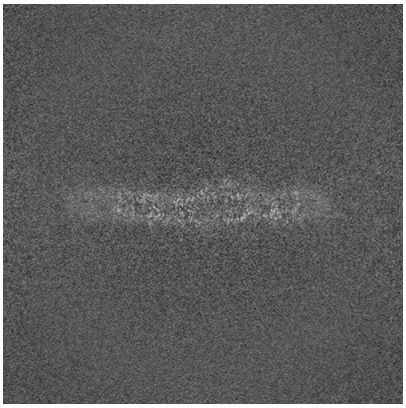


Z Index: 330

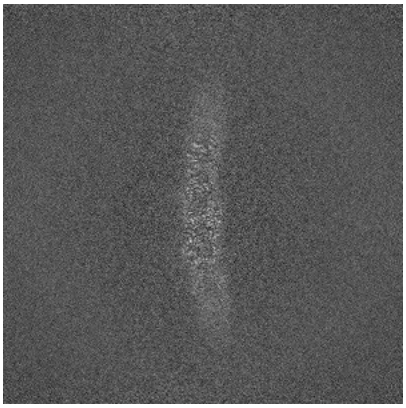
6.2.2 Raw map



X Index: 330



Y Index: 330

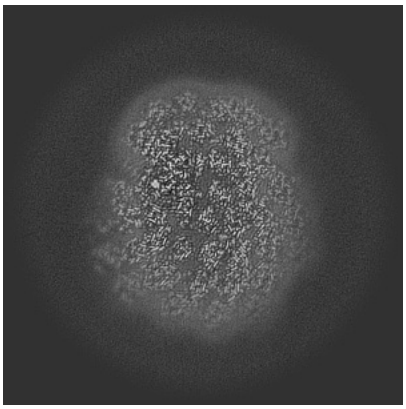


Z Index: 330

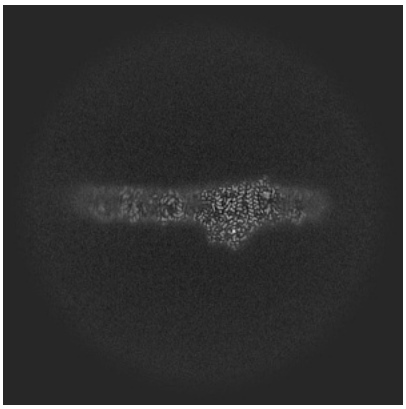
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

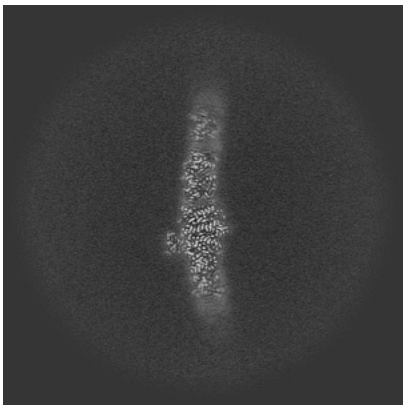
6.3.1 Primary map



X Index: 318

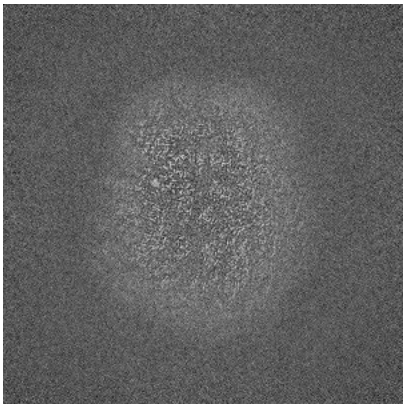


Y Index: 272

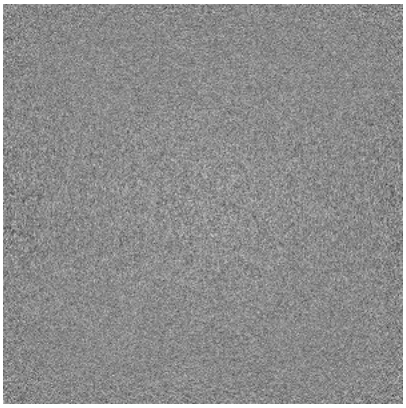


Z Index: 354

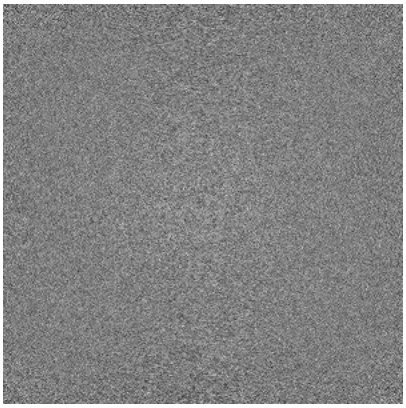
6.3.2 Raw map



X Index: 318



Y Index: 0

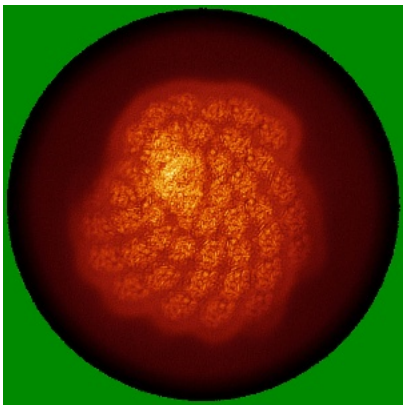


Z Index: 0

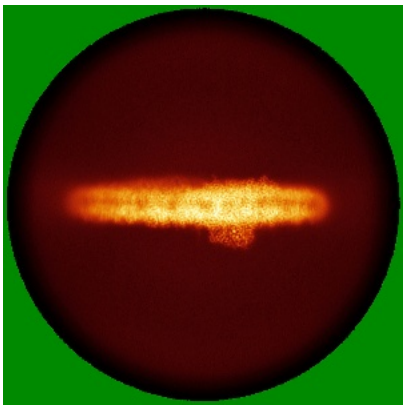
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

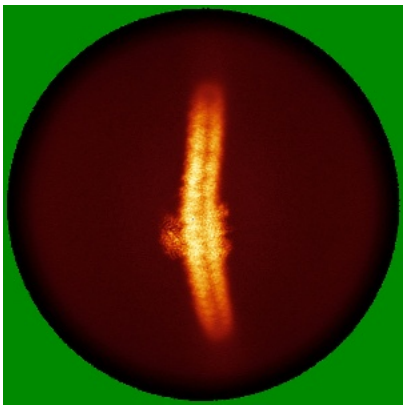
6.4.1 Primary map



X

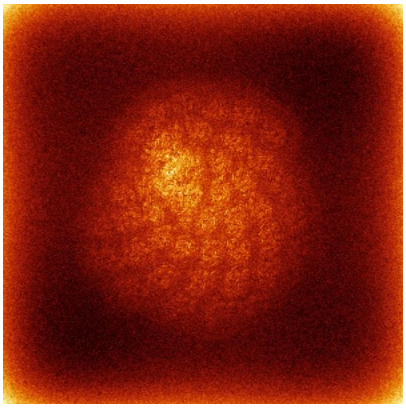


Y

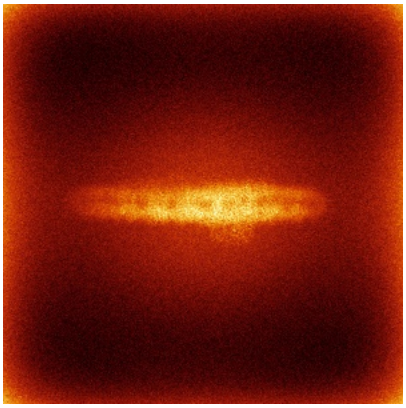


Z

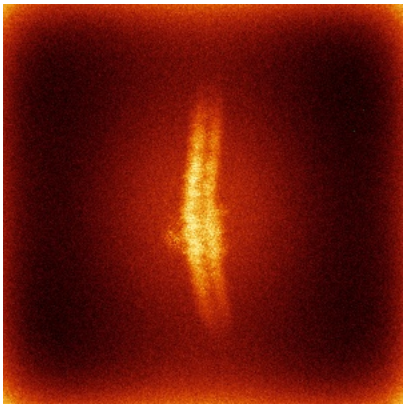
6.4.2 Raw map



X



Y

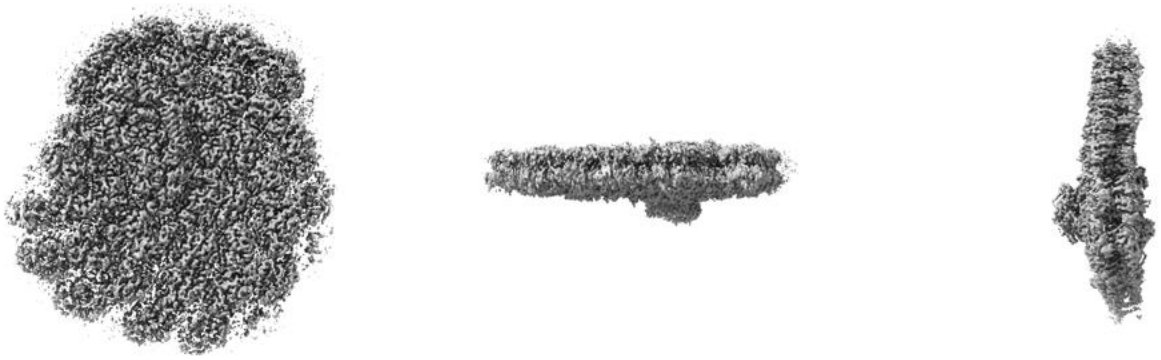


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.066. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

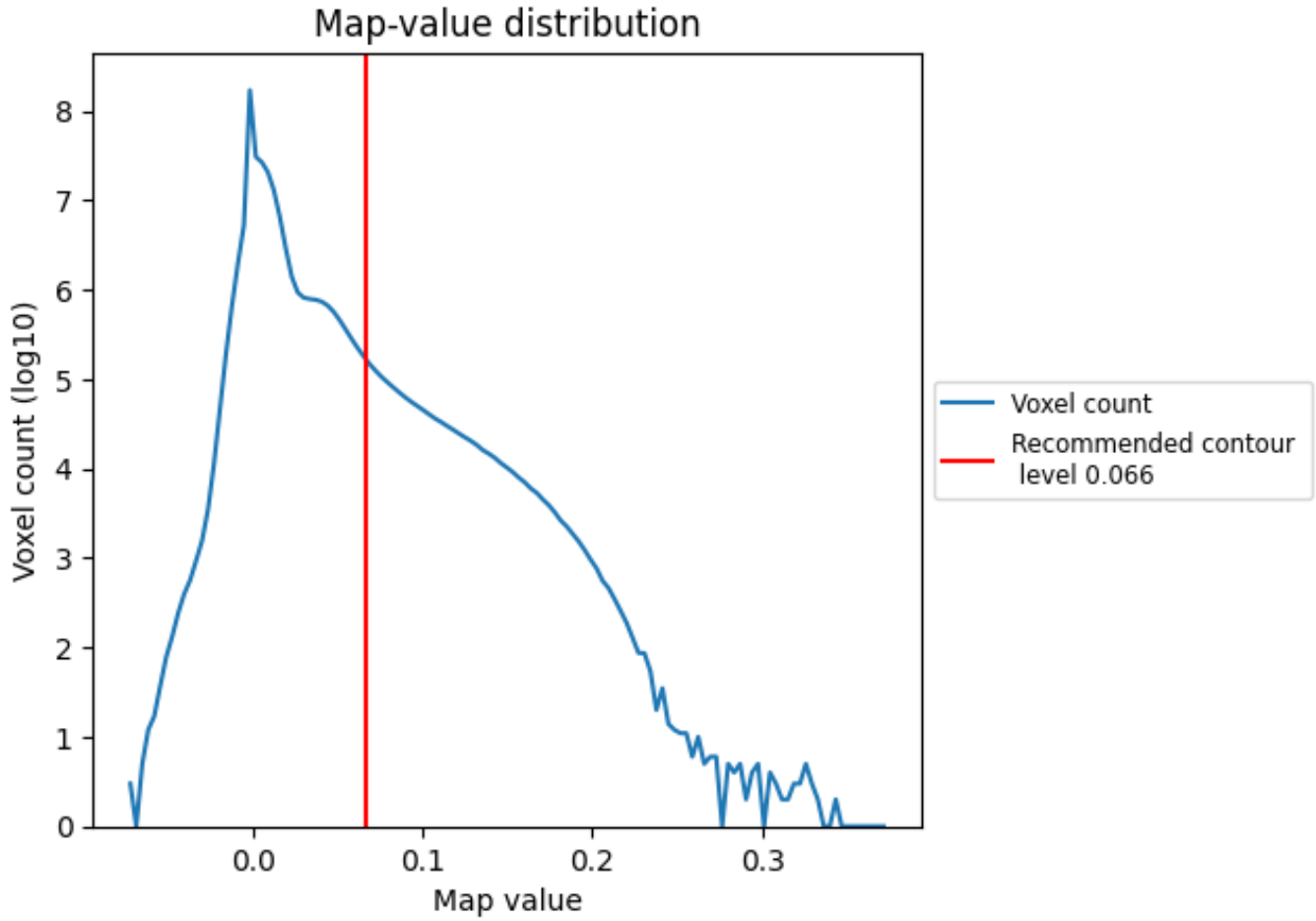
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

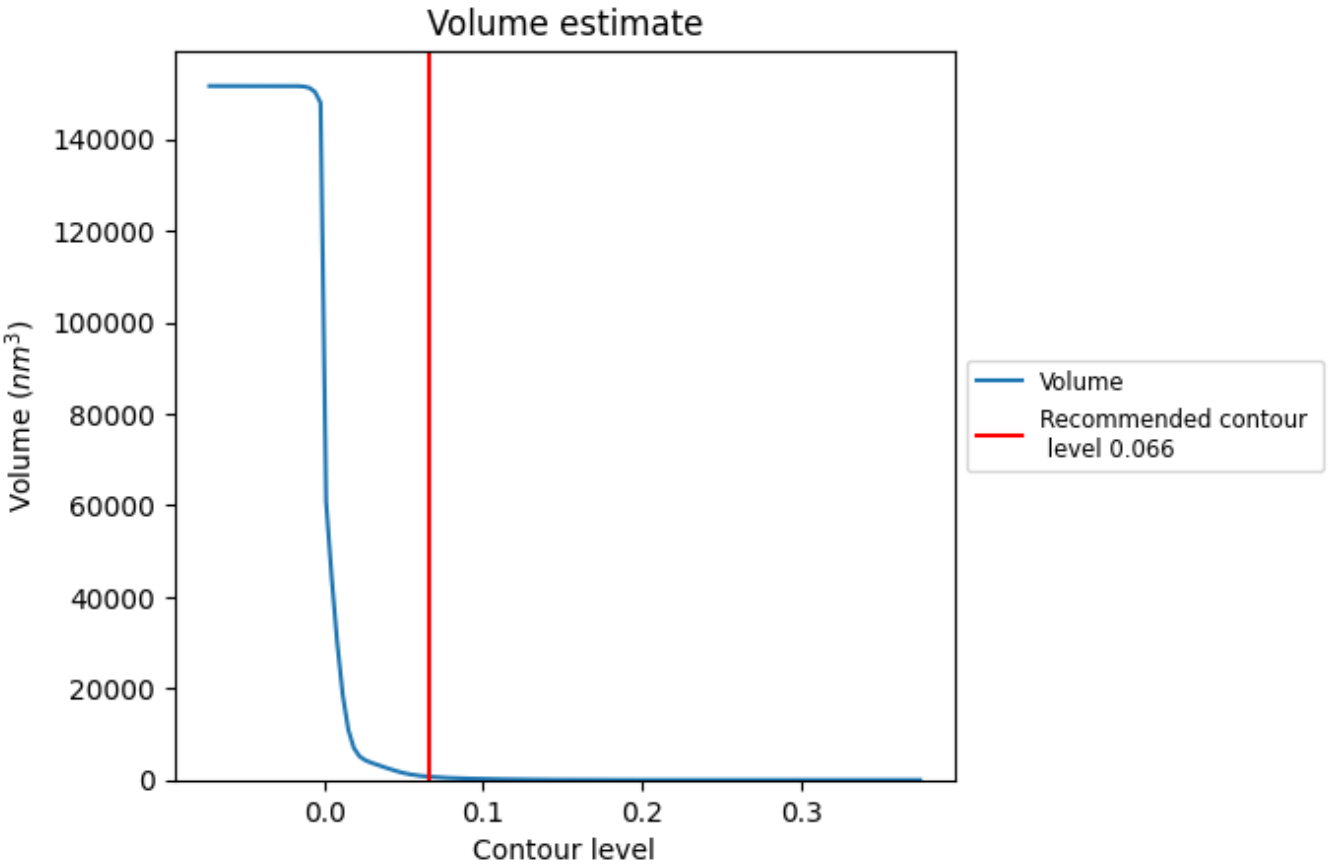
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

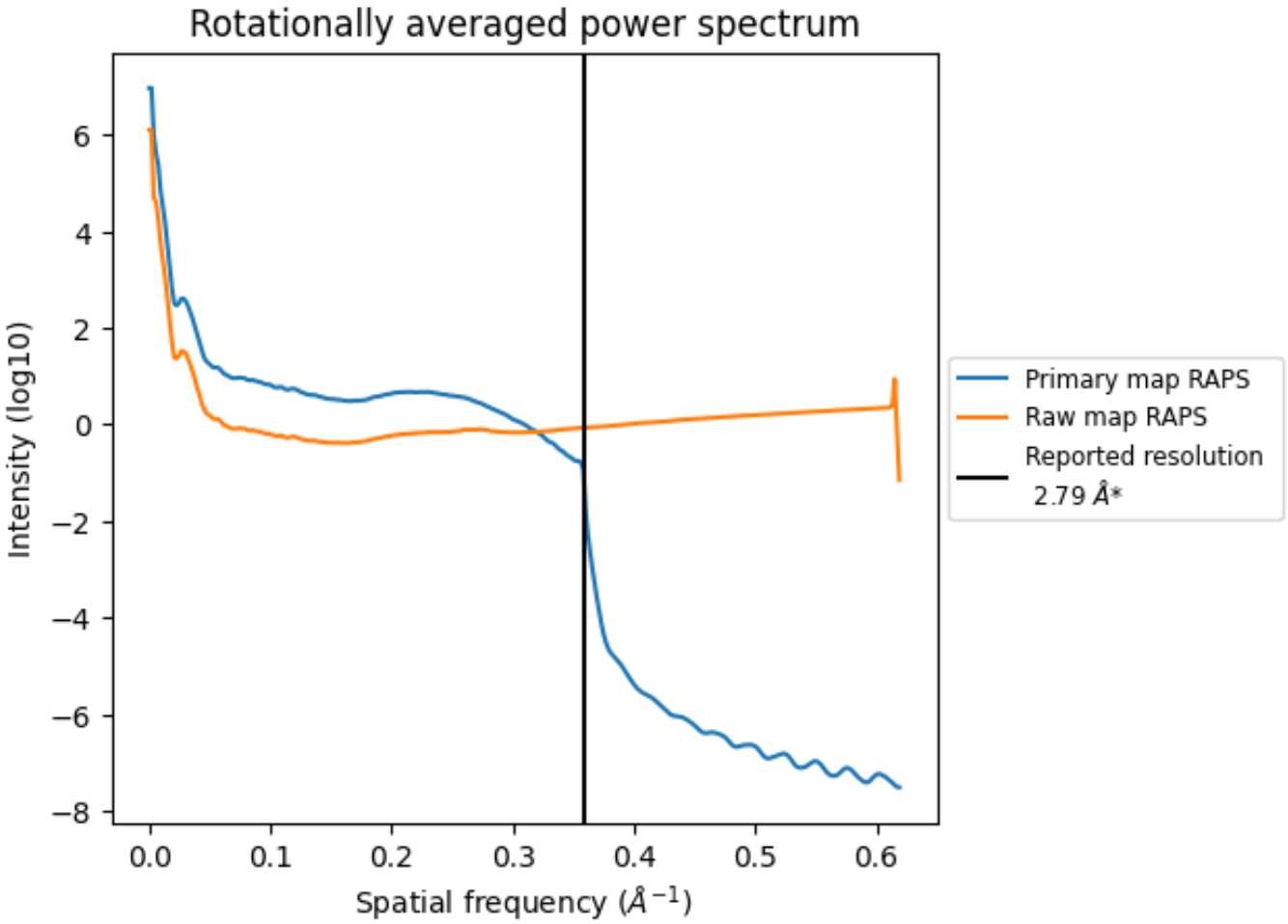
7.2 Volume estimate



The volume at the recommended contour level is 712 nm^3; this corresponds to an approximate mass of 643 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

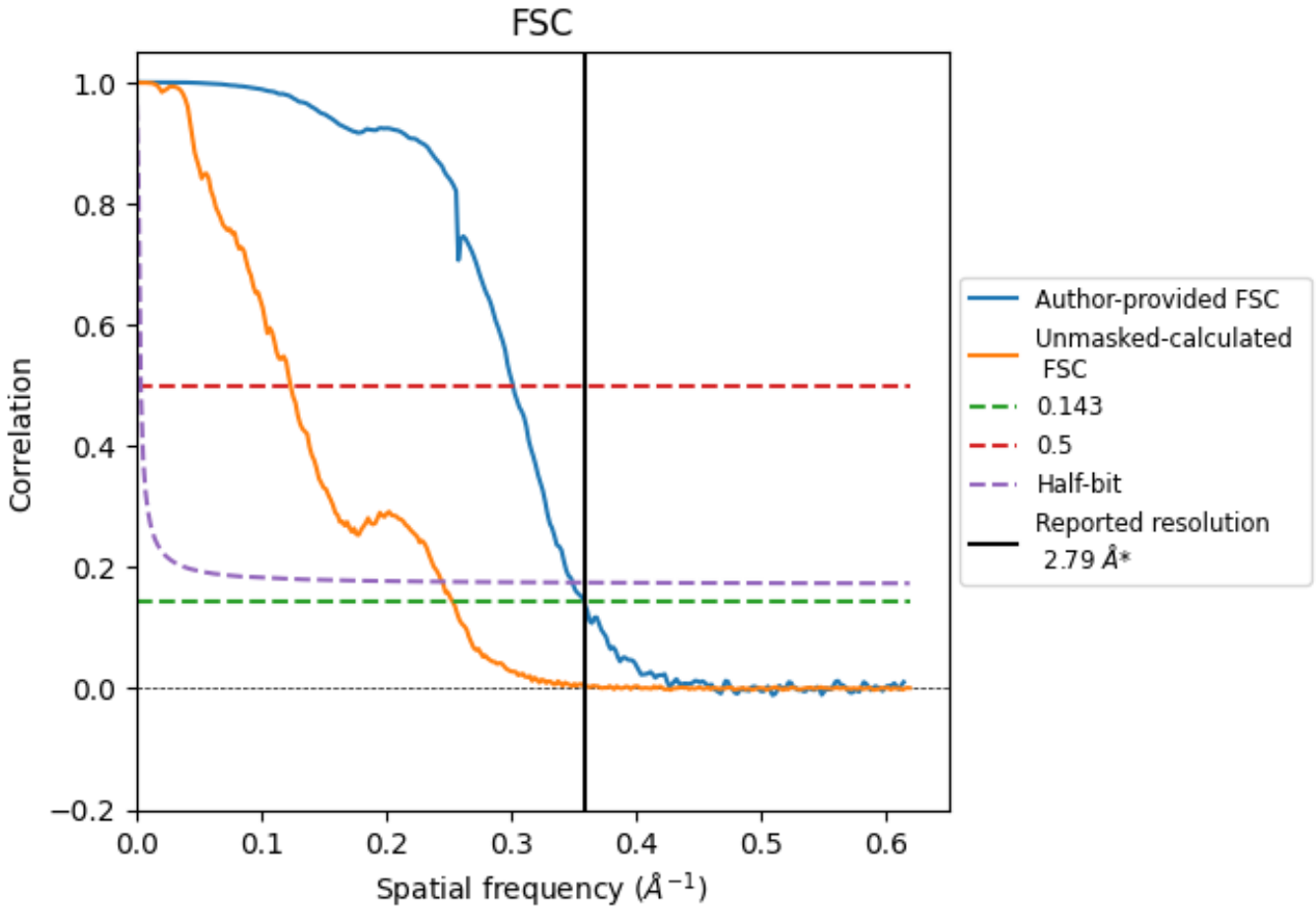


*Reported resolution corresponds to spatial frequency of 0.358 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.358 Å^{-1}

8.2 Resolution estimates (i)

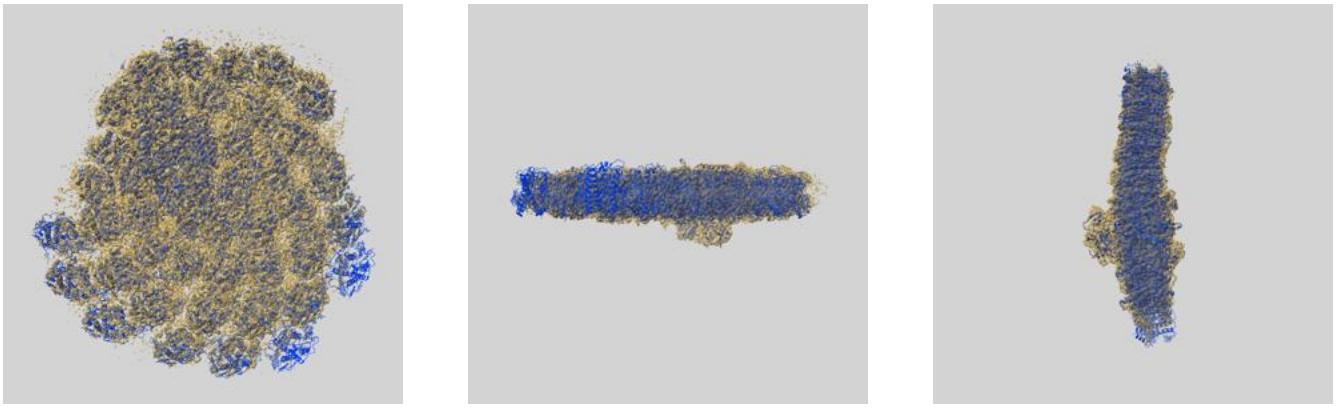
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.32	2.86
Unmasked-calculated*	3.95	8.10	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.79 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61519 and PDB model 9JJ8. Per-residue inclusion information can be found in section 3 on page 62.

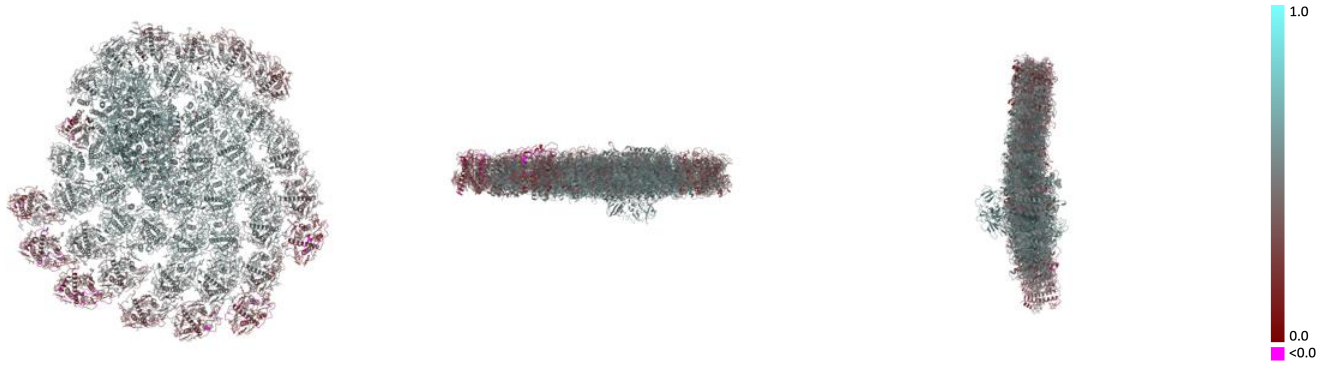
9.1 Map-model overlay



X Y Z

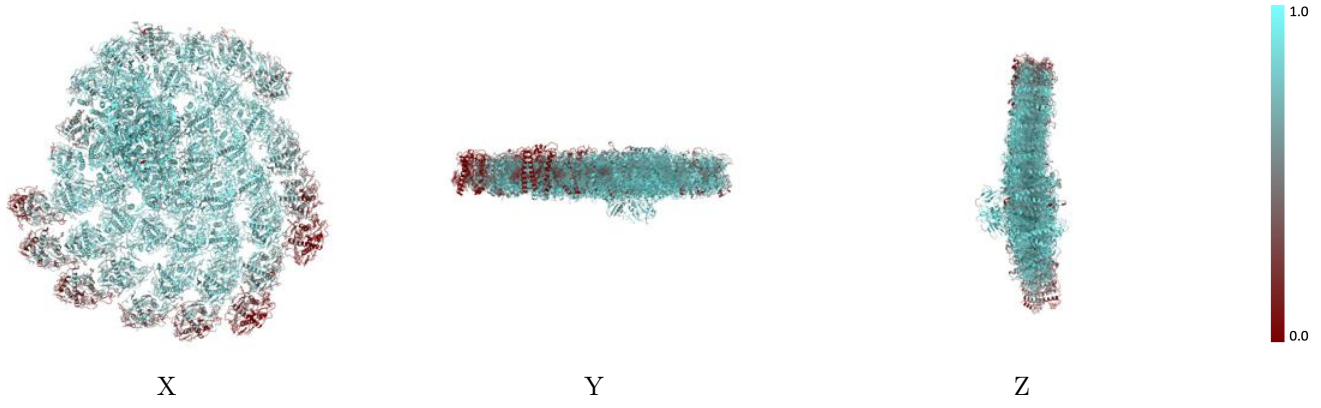
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



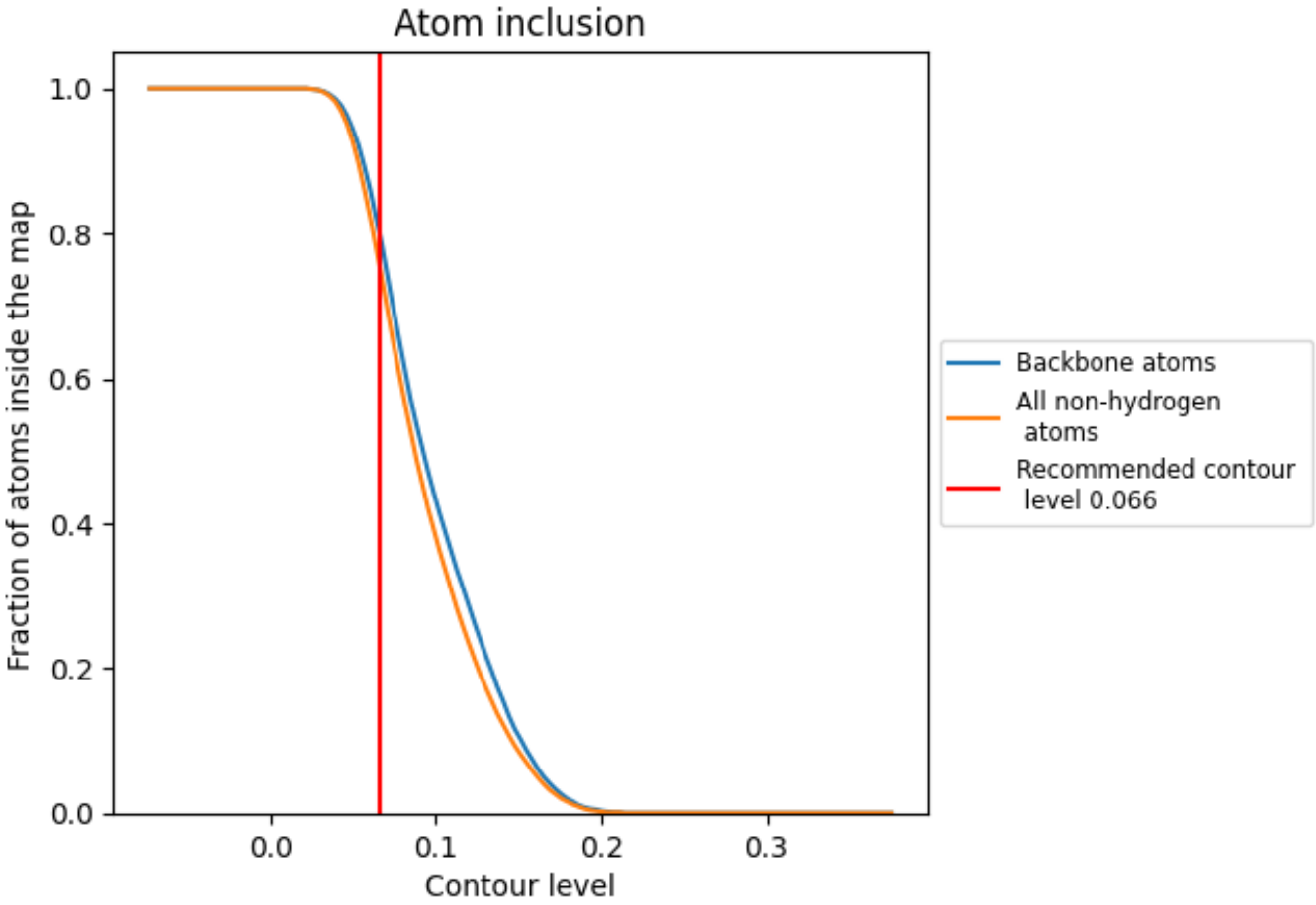
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.066).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.066) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.4970
0	0.7730	0.4850
1	0.5320	0.3590
2	0.3860	0.3210
3	0.6050	0.4440
4	0.7900	0.5080
5	0.8680	0.5370
6	0.4230	0.4270
7	0.6570	0.4750
8	0.6230	0.3800
9	0.7070	0.4130
A	0.8990	0.5670
B	0.6160	0.3650
C	0.7300	0.4910
D	0.9090	0.5770
E	0.9140	0.5810
F	0.8440	0.5350
G	0.8770	0.5490
H	0.7460	0.5100
I	0.9040	0.5730
J	0.6160	0.4410
K	0.8850	0.5630
L	0.7380	0.4540
M	0.9150	0.5810
O	0.7290	0.4320
P	0.8980	0.5700
Q	0.7920	0.4910
R	0.8830	0.5470
S	0.7930	0.5050
T	0.8170	0.5200
U	0.7860	0.5060
V	0.8500	0.5200
W	0.9100	0.5700
X	0.8410	0.5180
Y	0.0510	0.2320



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	0.0890	0.2370
a	0.9340	0.5960
b	0.9310	0.5920
c	0.9500	0.5810
d	0.8370	0.5680
e	0.8070	0.5750
f	0.8570	0.5590
h	0.8640	0.5510
i	0.9040	0.5730
j	0.9040	0.5690
k	0.8880	0.5540
l	0.9100	0.5760
m	0.8620	0.5300
o	0.7770	0.5290
x	0.3510	0.2530
y	0.4260	0.2940
z	0.3600	0.3220