wwPDB EM Validation Summary Report

Mar 9, 2026 – 05:03 PM UTC

PDB ID	:	8J5K / pdb_00008j5k
EMDB ID	:	EMD-35987
Title	:	Structural insights into photosystem II supercomplex and trimeric FCP antennae of a centric diatom Cyclotella meneghiniana
Authors	:	Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on	:	2023-04-23
Resolution	:	2.93 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:

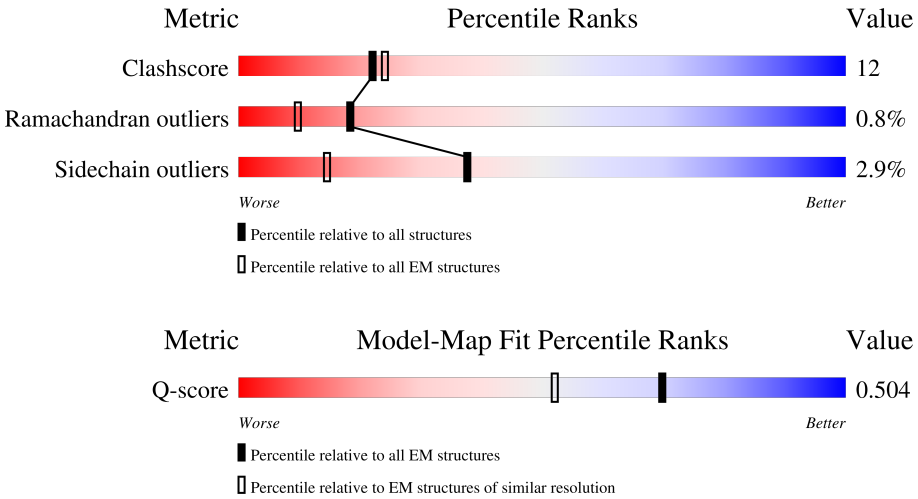
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.93 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.



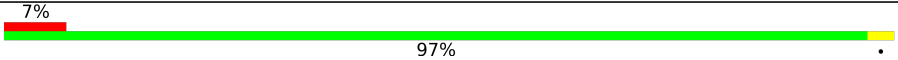
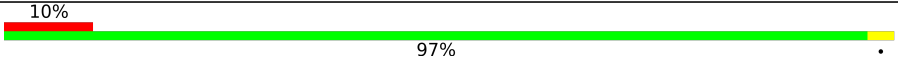
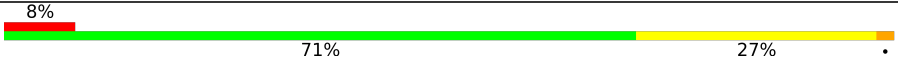
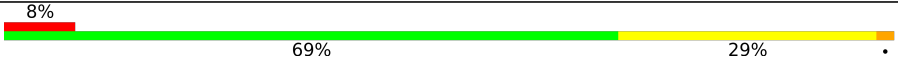
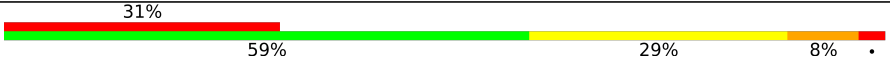
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13037 (2.43 - 3.43)

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	333	80% 20%
1	a	333	81% 18%
2	B	481	81% 18%
2	b	481	81% 18%

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Mol	Chain	Length	Quality of chain
3	C	450	
3	c	450	
4	D	340	
4	d	340	
5	E	75	
5	e	75	
6	F	31	
6	f	31	
7	H	65	
7	h	65	
8	I	34	
8	i	34	
9	J	34	
9	j	34	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	41	
12	m	41	
13	N	30	
13	n	30	
14	O	248	
14	o	248	
15	Q	145	

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Mol	Chain	Length	Quality of chain
15	q	145	33% 60% 28% 8%
16	T	29	83% 17%
16	t	29	83% 17%
17	U	92	78% 18%
17	u	92	78% 18%
18	V	136	72% 26%
18	v	136	72% 26%
19	W	50	8% 68% 22% 8%
19	w	50	8% 68% 20% 10%
20	X	34	74% 24%
20	x	34	65% 32%
21	Y	33	61% 36%
21	y	33	61% 36%
22	Z	59	54% 32% 14%
22	z	59	47% 39% 14%
23	0	169	77% 23%
23	5	169	76% 24%
24	2	164	5% 70% 30%
24	7	164	5% 70% 30%
25	1	164	71% 28%
25	6	164	71% 27%
26	P	214	71% 86% 14%
26	p	214	71% 88% 12%
27	4	153	85% 96%
27	9	153	85% 97%

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Mol	Chain	Length	Quality of chain
28	3	163	77% 84% 16%
28	8	163	77% 85% 15%

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
31	CLA	0	304	X	-	-	-
31	CLA	0	305	X	-	-	-
31	CLA	0	306	X	-	-	-
31	CLA	0	307	X	-	-	-
31	CLA	0	308	X	-	-	-
31	CLA	0	309	X	-	-	-
31	CLA	0	310	X	-	-	-
31	CLA	0	311	X	-	-	-
31	CLA	0	312	X	-	-	-
31	CLA	0	313	X	-	-	-
31	CLA	0	314	X	-	-	-
31	CLA	1	201	X	-	-	-
31	CLA	1	205	X	-	-	-
31	CLA	1	206	X	-	-	-
31	CLA	1	207	X	-	-	-
31	CLA	1	208	X	-	-	-
31	CLA	1	209	X	-	-	-
31	CLA	1	210	X	-	-	-
31	CLA	1	211	X	-	-	-
31	CLA	1	212	X	-	-	-
31	CLA	1	213	X	-	-	-
31	CLA	1	214	X	-	-	-
31	CLA	1	215	X	-	-	-
31	CLA	1	216	X	-	-	-
31	CLA	2	305	X	-	-	-
31	CLA	2	306	X	-	-	-
31	CLA	2	307	X	-	-	-
31	CLA	2	308	X	-	-	-
31	CLA	2	309	X	-	-	-
31	CLA	2	310	X	-	-	-
31	CLA	2	311	X	-	-	-
31	CLA	2	312	X	-	-	-
31	CLA	2	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	2	314	X	-	-	-
31	CLA	2	315	X	-	-	-
31	CLA	2	316	X	-	-	-
31	CLA	3	304	X	-	-	-
31	CLA	3	305	X	-	-	-
31	CLA	3	306	X	-	-	-
31	CLA	3	307	X	-	-	-
31	CLA	3	308	X	-	-	-
31	CLA	3	309	X	-	-	-
31	CLA	3	310	X	-	-	-
31	CLA	3	311	X	-	-	-
31	CLA	3	312	X	-	-	-
31	CLA	3	313	X	-	-	-
31	CLA	3	314	X	-	-	-
31	CLA	4	204	X	-	-	-
31	CLA	4	205	X	-	-	-
31	CLA	4	206	X	-	-	-
31	CLA	4	207	X	-	-	-
31	CLA	4	208	X	-	-	-
31	CLA	4	209	X	-	-	-
31	CLA	4	210	X	-	-	-
31	CLA	4	211	X	-	-	-
31	CLA	4	212	X	-	-	-
31	CLA	4	213	X	-	-	-
31	CLA	5	304	X	-	-	-
31	CLA	5	305	X	-	-	-
31	CLA	5	306	X	-	-	-
31	CLA	5	307	X	-	-	-
31	CLA	5	308	X	-	-	-
31	CLA	5	309	X	-	-	-
31	CLA	5	310	X	-	-	-
31	CLA	5	311	X	-	-	-
31	CLA	5	312	X	-	-	-
31	CLA	5	313	X	-	-	-
31	CLA	5	314	X	-	-	-
31	CLA	6	201	X	-	-	-
31	CLA	6	205	X	-	-	-
31	CLA	6	206	X	-	-	-
31	CLA	6	207	X	-	-	-
31	CLA	6	208	X	-	-	-
31	CLA	6	209	X	-	-	-
31	CLA	6	210	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	6	211	X	-	-	-
31	CLA	6	212	X	-	-	-
31	CLA	6	213	X	-	-	-
31	CLA	6	214	X	-	-	-
31	CLA	6	215	X	-	-	-
31	CLA	6	216	X	-	-	-
31	CLA	7	305	X	-	-	-
31	CLA	7	306	X	-	-	-
31	CLA	7	307	X	-	-	-
31	CLA	7	308	X	-	-	-
31	CLA	7	309	X	-	-	-
31	CLA	7	310	X	-	-	-
31	CLA	7	311	X	-	-	-
31	CLA	7	312	X	-	-	-
31	CLA	7	313	X	-	-	-
31	CLA	7	314	X	-	-	-
31	CLA	7	315	X	-	-	-
31	CLA	7	316	X	-	-	-
31	CLA	8	304	X	-	-	-
31	CLA	8	305	X	-	-	-
31	CLA	8	306	X	-	-	-
31	CLA	8	307	X	-	-	-
31	CLA	8	308	X	-	-	-
31	CLA	8	309	X	-	-	-
31	CLA	8	310	X	-	-	-
31	CLA	8	311	X	-	-	-
31	CLA	8	312	X	-	-	-
31	CLA	8	313	X	-	-	-
31	CLA	8	314	X	-	-	-
31	CLA	9	204	X	-	-	-
31	CLA	9	205	X	-	-	-
31	CLA	9	206	X	-	-	-
31	CLA	9	207	X	-	-	-
31	CLA	9	208	X	-	-	-
31	CLA	9	209	X	-	-	-
31	CLA	9	210	X	-	-	-
31	CLA	9	211	X	-	-	-
31	CLA	9	212	X	-	-	-
31	CLA	9	213	X	-	-	-
31	CLA	A	403	X	-	-	-
31	CLA	A	404	X	-	-	-
31	CLA	A	407	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	B	501	X	-	-	-
31	CLA	B	502	X	-	-	-
31	CLA	B	503	X	-	-	-
31	CLA	B	504	X	-	-	-
31	CLA	B	505	X	-	-	-
31	CLA	B	506	X	-	-	-
31	CLA	B	507	X	-	-	-
31	CLA	B	508	X	-	-	-
31	CLA	B	509	X	-	-	-
31	CLA	B	510	X	-	-	-
31	CLA	B	511	X	-	-	-
31	CLA	B	512	X	-	-	-
31	CLA	B	513	X	-	-	-
31	CLA	B	514	X	-	-	-
31	CLA	B	515	X	-	-	-
31	CLA	B	516	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C	514	X	-	-	-
31	CLA	D	401	X	-	-	-
31	CLA	D	403	X	-	-	-
31	CLA	D	404	X	-	-	-
31	CLA	P	601	X	-	-	-
31	CLA	P	602	X	-	-	-
31	CLA	P	603	X	-	-	-
31	CLA	P	604	X	-	-	-
31	CLA	P	605	X	-	-	-
31	CLA	P	606	X	-	-	-
31	CLA	P	607	X	-	-	-
31	CLA	P	608	X	-	-	-
31	CLA	P	609	X	-	-	-
31	CLA	W	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	Z	101	X	-	-	-
31	CLA	a	403	X	-	-	-
31	CLA	a	404	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	b	502	X	-	-	-
31	CLA	b	503	X	-	-	-
31	CLA	b	504	X	-	-	-
31	CLA	b	505	X	-	-	-
31	CLA	b	506	X	-	-	-
31	CLA	b	507	X	-	-	-
31	CLA	b	508	X	-	-	-
31	CLA	b	509	X	-	-	-
31	CLA	b	510	X	-	-	-
31	CLA	b	511	X	-	-	-
31	CLA	b	512	X	-	-	-
31	CLA	b	513	X	-	-	-
31	CLA	b	514	X	-	-	-
31	CLA	b	515	X	-	-	-
31	CLA	b	516	X	-	-	-
31	CLA	b	517	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-
31	CLA	c	513	X	-	-	-
31	CLA	c	514	X	-	-	-
31	CLA	d	401	X	-	-	-
31	CLA	d	403	X	-	-	-
31	CLA	d	404	X	-	-	-
31	CLA	p	601	X	-	-	-
31	CLA	p	602	X	-	-	-
31	CLA	p	603	X	-	-	-
31	CLA	p	604	X	-	-	-
31	CLA	p	605	X	-	-	-
31	CLA	p	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	p	607	X	-	-	-
31	CLA	p	608	X	-	-	-
31	CLA	p	609	X	-	-	-
31	CLA	w	202	X	-	-	-
31	CLA	z	101	X	-	-	-

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 71446 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 PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2530	1656	421	439	14		
1	a	333	Total	C	N	O	S	0	0
			2530	1656	421	439	14		

- Molecule 2 is a protein called PsbB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	481	Total	C	N	O	S	0	0
			3748	2456	635	646	11		
2	b	481	Total	C	N	O	S	0	0
			3748	2456	635	646	11		

- Molecule 3 is a protein called PsbC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3437	2252	579	595	11		
3	c	450	Total	C	N	O	S	0	0
			3437	2252	579	595	11		

- Molecule 4 is a protein called PsbD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2667	1765	437	455	10		
4	d	340	Total	C	N	O	S	0	0
			2667	1765	437	455	10		

- Molecule 5 is a protein called PsbE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total 602	C 392	N 101	O 109	0	0
5	e	75	Total 602	C 392	N 101	O 109	0	0

- Molecule 6 is a protein called PsbF.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	31	Total 242	C 166	N 41	O 35	0	0
6	f	31	Total 242	C 166	N 41	O 35	0	0

- Molecule 7 is a protein called PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total 499	C 331	N 82	O 85	S 1	0	0
7	h	65	Total 499	C 331	N 82	O 85	S 1	0	0

- Molecule 8 is a protein called PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total 266	C 179	N 40	O 46	S 1	0	0
8	i	34	Total 266	C 179	N 40	O 46	S 1	0	0

- Molecule 9 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	34	Total 247	C 167	N 38	O 42	0	0
9	j	34	Total 247	C 167	N 38	O 42	0	0

- Molecule 10 is a protein called PsbK.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total 294	C 205	N 44	O 45	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total 294	C 205	N 44	O 45	0	0

- Molecule 11 is a protein called PsbL.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	37	Total 294	C 197	N 46	O 51	0	0
11	l	37	Total 294	C 197	N 46	O 51	0	0

- Molecule 12 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	41	Total 295	C 193	N 49	O 53	0	0
12	m	41	Total 295	C 193	N 49	O 53	0	0

- Molecule 13 is a protein called Psb34.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	N	30	Total 150	C 90	N 30	O 30	0	0
13	n	30	Total 150	C 90	N 30	O 30	0	0

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	248	Total 1824	C 1151	N 304	O 362	S 7	0	0
14	o	248	Total 1824	C 1151	N 304	O 362	S 7	0	0

- Molecule 15 is a protein called PsbQ'.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Q	145	Total 1050	C 654	N 182	O 214	0	0
15	q	145	Total 1050	C 654	N 182	O 214	0	0

- Molecule 16 is a protein called PsbT.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			234	164	32	36	2		
16	t	29	Total	C	N	O	S	0	0
			234	164	32	36	2		

- Molecule 17 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	92	Total	C	N	O	S	0	0
			678	436	111	130	1		
17	u	92	Total	C	N	O	S	0	0
			678	436	111	130	1		

- Molecule 18 is a protein called PsbV.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	136	Total	C	N	O	S	0	0
			979	612	169	194	4		
18	v	136	Total	C	N	O	S	0	0
			979	612	169	194	4		

- Molecule 19 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	50	Total	C	N	O	S	0	0
			338	211	56	68	3		
19	w	50	Total	C	N	O	S	0	0
			338	211	56	68	3		

- Molecule 20 is a protein called PsbX.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	34	Total	C	N	O	S	0	0
			233	150	39	43	1		
20	x	34	Total	C	N	O	S	0	0
			233	150	39	43	1		

- Molecule 21 is a protein called PsbY.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	33	Total 216	C 137	N 39	O 40	0	0
21	y	33	Total 216	C 137	N 39	O 40	0	0

- Molecule 22 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	59	Total 413	C 270	N 65	O 77	S 1	0	0
22	z	59	Total 413	C 270	N 65	O 77	S 1	0	0

- Molecule 23 is a protein called FCPII-G, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5	169	Total 1280	C 827	N 211	O 239	S 3	0	0
23	0	169	Total 1280	C 827	N 211	O 239	S 3	0	0

- Molecule 24 is a protein called FCPII-H2, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	7	164	Total 1222	C 808	N 198	O 212	S 4	0	0
24	2	164	Total 1222	C 808	N 198	O 212	S 4	0	0

- Molecule 25 is a protein called FCPII-H1, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	164	Total 1209	C 796	N 210	O 201	S 2	0	0
25	1	164	Total 1209	C 796	N 210	O 201	S 2	0	0

- Molecule 26 is a protein called FCPII-I, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	p	214	Total 1265	C 789	N 230	O 245	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	214	Total	C	N	O	S	0	0
			1265	789	230	245	1		

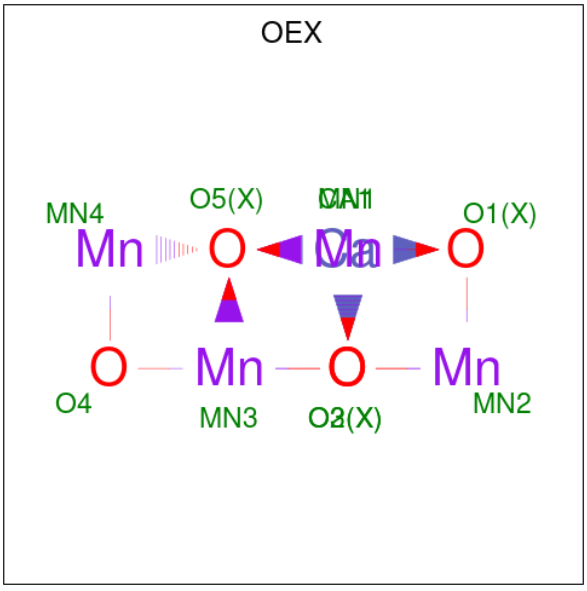
- Molecule 27 is a protein called FCPII-K, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	4	153	Total	C	N	O	0	0
			765	459	153	153		
27	9	153	Total	C	N	O	0	0
			765	459	153	153		

- Molecule 28 is a protein called FCPII-J, fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	3	163	Total	C	N	O	0	0
			992	616	192	184		
28	8	163	Total	C	N	O	0	0
			992	616	192	184		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

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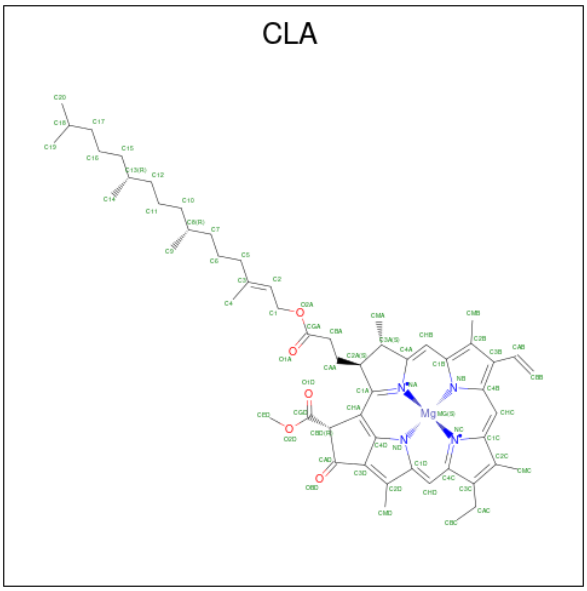
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Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Fe	0
			1	1	
30	a	1	Total	Fe	0
			1	1	

- Molecule 31 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
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	B	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
31	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	Z	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	b	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
31	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
31	c	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	d	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	w	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	z	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	5	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	5	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	7	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	7	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	7	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	7	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	6	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	6	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	6	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	p	1	Total	C	Mg	N	O	0
			36	30	1	4	1	

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Mol	Chain	Residues	Atoms					AltConf
31	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	p	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	p	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	p	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	p	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	p	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	p	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
31	p	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
31	4	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	4	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	4	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	4	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	4	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	4	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
31	4	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	4	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	3	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
31	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	3	1	Total	C	Mg	N	O	0
			33	27	1	4	1	

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Mol	Chain	Residues	Atoms					AltConf
31	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	3	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	3	1	Total	C	Mg	N	O	0
			39	33	1	4	1	
31	3	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	P	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	P	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	P	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	P	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	P	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	P	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	P	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
31	P	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
31	9	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	9	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	9	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
31	9	1	Total	C	Mg	N	O	0
			38	32	1	4	1	

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Mol	Chain	Residues	Atoms					AltConf
31	9	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	9	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	9	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
31	9	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	9	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	8	1	Total	C	Mg	N	O	0
			34	28	1	4	1	
31	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	8	1	Total	C	Mg	N	O	0
			33	27	1	4	1	
31	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	8	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	8	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	8	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	8	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
31	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	8	1	Total	C	Mg	N	O	0
			39	33	1	4	1	
31	8	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
31	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	0	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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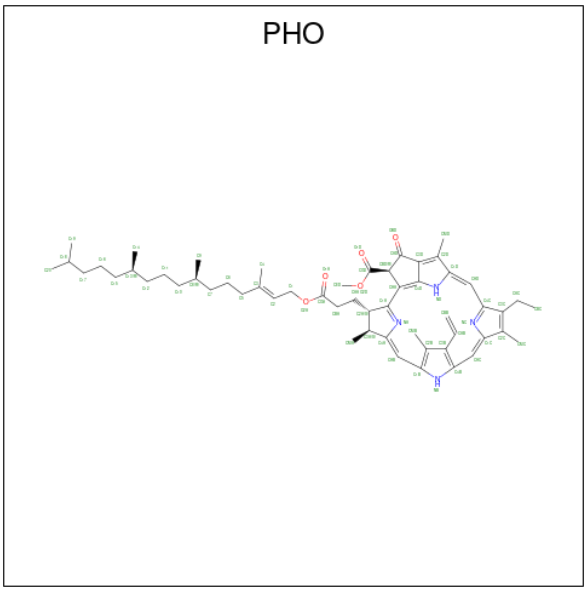
Mol	Chain	Residues	Atoms					AltConf
31	0	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	0	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	0	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	0	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
31	2	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	2	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	2	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
31	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
31	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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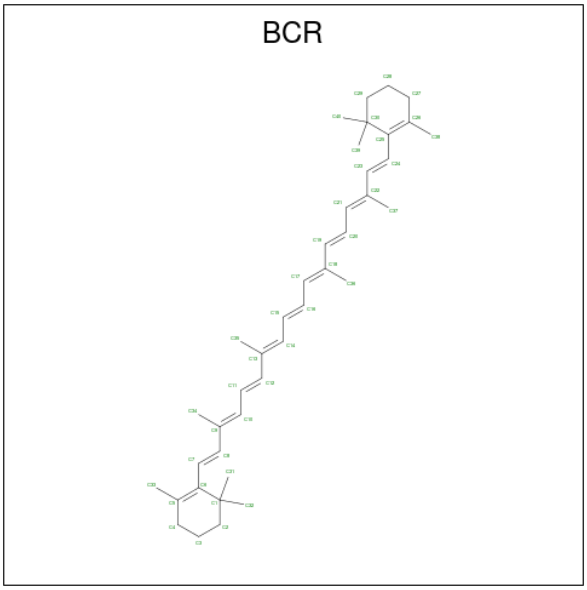
Mol	Chain	Residues	Atoms					AltConf
31	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	1	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
31	1	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	1	1	Total 38	C 32	Mg 1	N 4	O 1	0
31	1	1	Total 38	C 32	Mg 1	N 4	O 1	0

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C N O 64 55 4 5	0
32	A	1	Total C N O 64 55 4 5	0
32	a	1	Total C N O 64 55 4 5	0
32	a	1	Total C N O 64 55 4 5	0

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



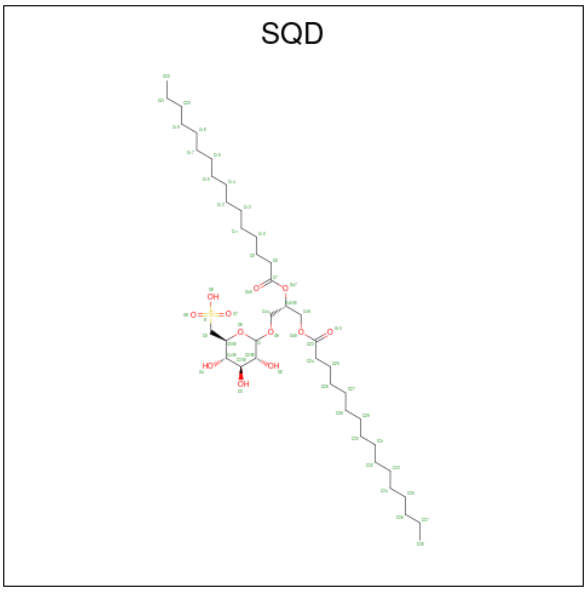
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	C	1	Total C 40 40	0
33	C	1	Total C 40 40	0
33	C	1	Total C 40 40	0
33	D	1	Total C 40 40	0

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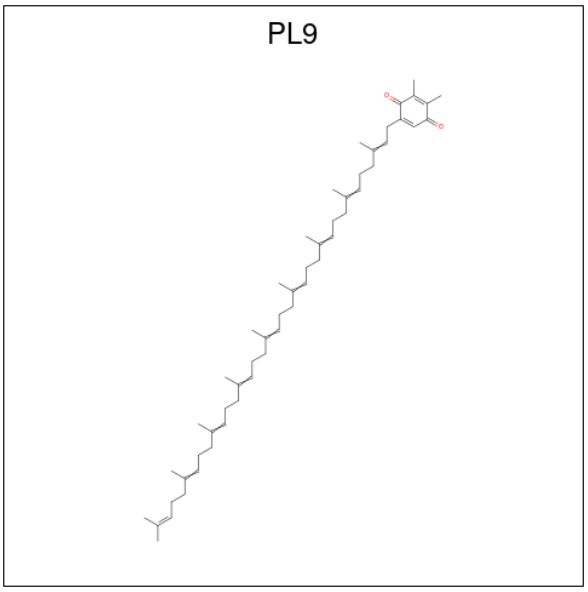
Mol	Chain	Residues	Atoms	AltConf
33	H	1	Total C 40 40	0
33	K	1	Total C 40 40	0
33	a	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	d	1	Total C 40 40	0
33	h	1	Total C 40 40	0
33	k	1	Total C 40 40	0

- Molecule 34 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).



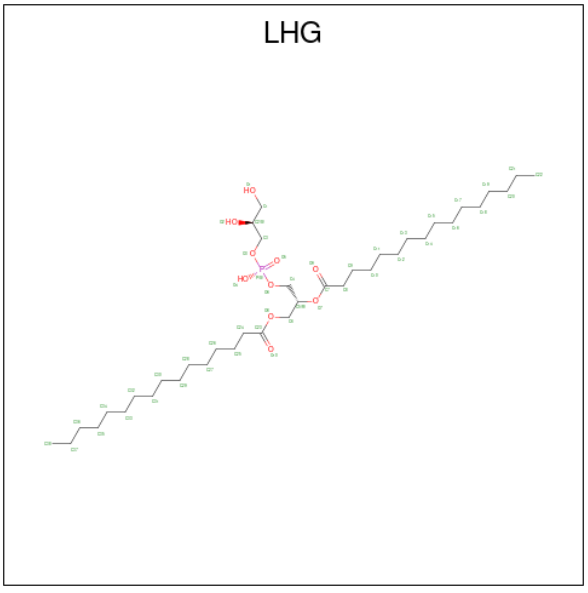
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total 54	C 41	O 12	S 1	0
34	A	1	Total 54	C 41	O 12	S 1	0
34	B	1	Total 54	C 41	O 12	S 1	0
34	B	1	Total 40	C 27	O 12	S 1	0
34	a	1	Total 54	C 41	O 12	S 1	0
34	b	1	Total 40	C 27	O 12	S 1	0
34	5	1	Total 48	C 35	O 12	S 1	0
34	0	1	Total 48	C 35	O 12	S 1	0

- Molecule 35 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



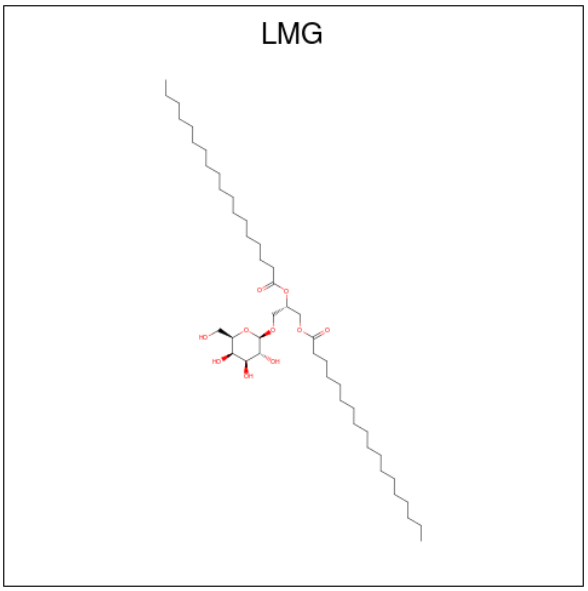
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total C O 32 30 2	0
35	D	1	Total C O 55 53 2	0
35	a	1	Total C O 32 30 2	0
35	d	1	Total C O 55 53 2	0

- Molecule 36 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
36	A	1	Total	C	O	P	0
			43	32	10	1	
36	A	1	Total	C	O	P	0
			26	15	10	1	
36	B	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			48	38	9	1	
36	D	1	Total	C	O	P	0
			34	23	10	1	
36	D	1	Total	C	O	P	0
			28	19	8	1	
36	H	1	Total	C	O	P	0
			42	31	10	1	
36	a	1	Total	C	O	P	0
			43	32	10	1	
36	a	1	Total	C	O	P	0
			26	15	10	1	
36	b	1	Total	C	O	P	0
			49	38	10	1	
36	d	1	Total	C	O	P	0
			48	38	9	1	
36	d	1	Total	C	O	P	0
			34	23	10	1	
36	d	1	Total	C	O	P	0
			28	19	8	1	
36	h	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 37 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
37	B	1	Total C O 28 18 10	0
37	C	1	Total C O 51 41 10	0
37	D	1	Total C O 46 36 10	0
37	D	1	Total C O 37 27 10	0
37	D	1	Total C O 40 30 10	0
37	J	1	Total C O 50 40 10	0
37	M	1	Total C O 51 41 10	0
37	M	1	Total C O 40 30 10	0
37	W	1	Total C O 48 38 10	0
37	Y	1	Total C O 46 36 10	0
37	b	1	Total C O 28 18 10	0
37	c	1	Total C O 51 41 10	0
37	d	1	Total C O 46 36 10	0
37	d	1	Total C O 37 27 10	0

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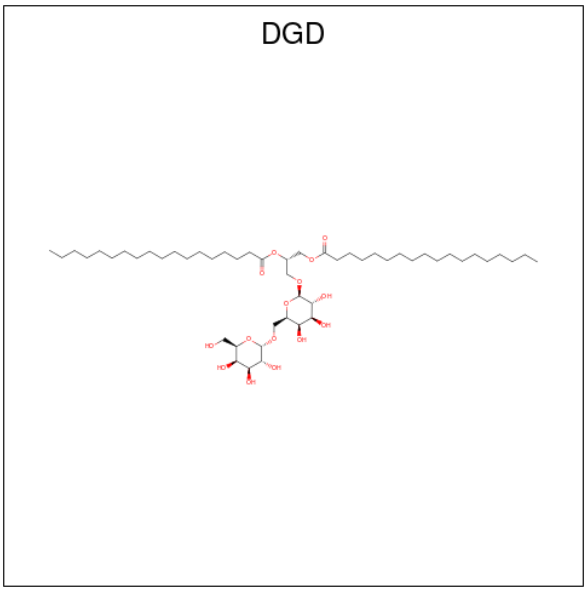
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Mol	Chain	Residues	Atoms	AltConf
37	d	1	Total C O 40 30 10	0
37	j	1	Total C O 50 40 10	0
37	m	1	Total C O 51 41 10	0
37	m	1	Total C O 40 30 10	0
37	w	1	Total C O 48 38 10	0
37	y	1	Total C O 46 36 10	0
37	5	1	Total C O 48 38 10	0
37	0	1	Total C O 48 38 10	0

- Molecule 38 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

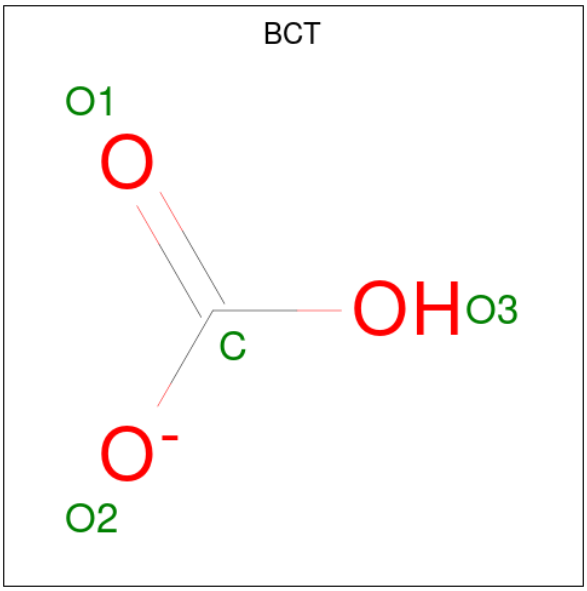
Mol	Chain	Residues	Atoms	AltConf
38	C	1	Total Cl 1 1	0
38	c	1	Total Cl 1 1	0

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



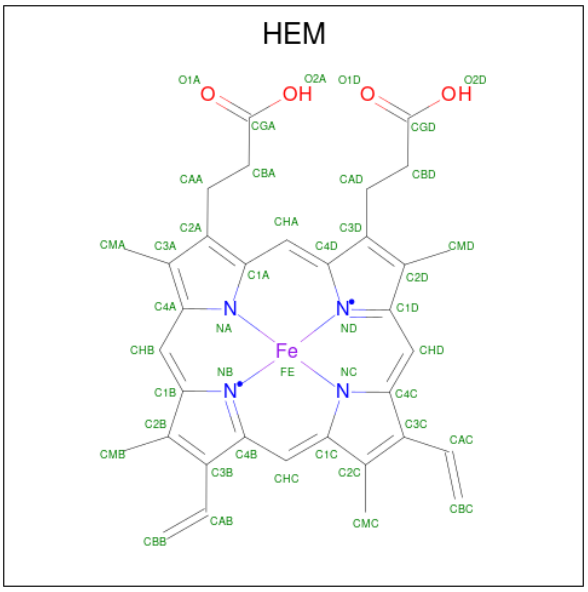
Mol	Chain	Residues	Atoms	AltConf
39	C	1	Total C O 55 40 15	0
39	C	1	Total C O 62 47 15	0
39	C	1	Total C O 62 47 15	0
39	H	1	Total C O 62 47 15	0
39	c	1	Total C O 55 40 15	0
39	c	1	Total C O 62 47 15	0
39	c	1	Total C O 62 47 15	0
39	h	1	Total C O 62 47 15	0

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



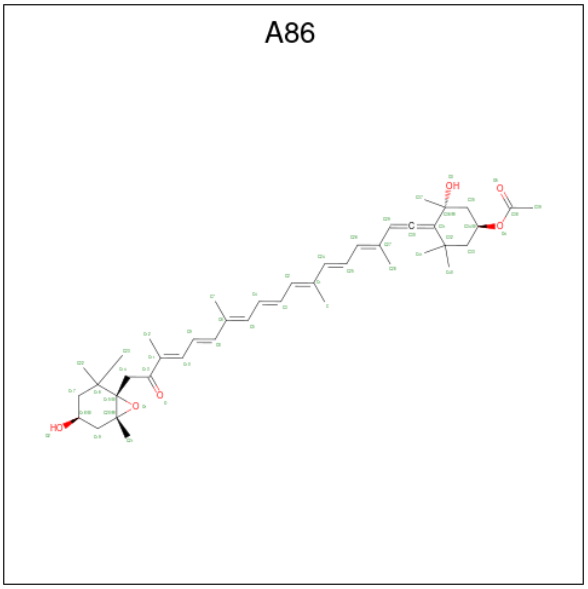
Mol	Chain	Residues	Atoms	AltConf
40	D	1	Total C O 4 1 3	0
40	d	1	Total C O 4 1 3	0

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
41	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 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).



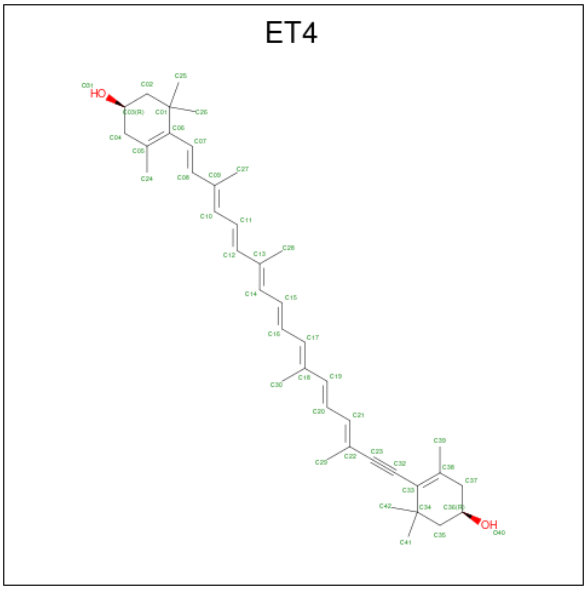
Mol	Chain	Residues	Atoms			AltConf
42	5	1	Total	C	O	0
			48	42	6	
42	5	1	Total	C	O	0
			48	42	6	
42	5	1	Total	C	O	0
			48	42	6	
42	7	1	Total	C	O	0
			48	42	6	
42	7	1	Total	C	O	0
			48	42	6	
42	6	1	Total	C	O	0
			48	42	6	
42	p	1	Total	C	O	0
			48	42	6	
42	4	1	Total	C	O	0
			48	42	6	
42	4	1	Total	C	O	0
			48	42	6	
42	4	1	Total	C	O	0
			48	42	6	
42	3	1	Total	C	O	0
			48	42	6	
42	3	1	Total	C	O	0
			48	42	6	
42	P	1	Total	C	O	0
			48	42	6	
42	9	1	Total	C	O	0
			48	42	6	
42	9	1	Total	C	O	0
			48	42	6	
42	9	1	Total	C	O	0
			48	42	6	
42	8	1	Total	C	O	0
			48	42	6	
42	8	1	Total	C	O	0
			48	42	6	
42	0	1	Total	C	O	0
			48	42	6	
42	0	1	Total	C	O	0
			48	42	6	
42	0	1	Total	C	O	0
			48	42	6	
42	2	1	Total	C	O	0
			48	42	6	

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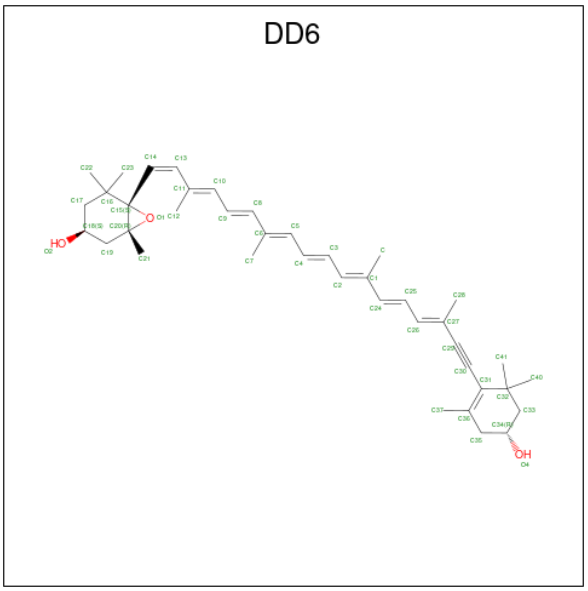
Mol	Chain	Residues	Atoms			AltConf
42	2	1	Total 48	C 42	O 6	0
42	1	1	Total 48	C 42	O 6	0

- Molecule 43 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
43	5	1	Total 42	C 40	O 2	0
43	0	1	Total 42	C 40	O 2	0

- Molecule 44 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
44	7	1	Total	C	O	0
			43	40	3	
44	7	1	Total	C	O	0
			43	40	3	
44	6	1	Total	C	O	0
			43	40	3	
44	6	1	Total	C	O	0
			43	40	3	
44	p	1	Total	C	O	0
			43	40	3	
44	3	1	Total	C	O	0
			43	40	3	
44	P	1	Total	C	O	0
			43	40	3	
44	8	1	Total	C	O	0
			43	40	3	
44	2	1	Total	C	O	0
			43	40	3	
44	2	1	Total	C	O	0
			43	40	3	
44	1	1	Total	C	O	0
			43	40	3	
44	1	1	Total	C	O	0
			43	40	3	

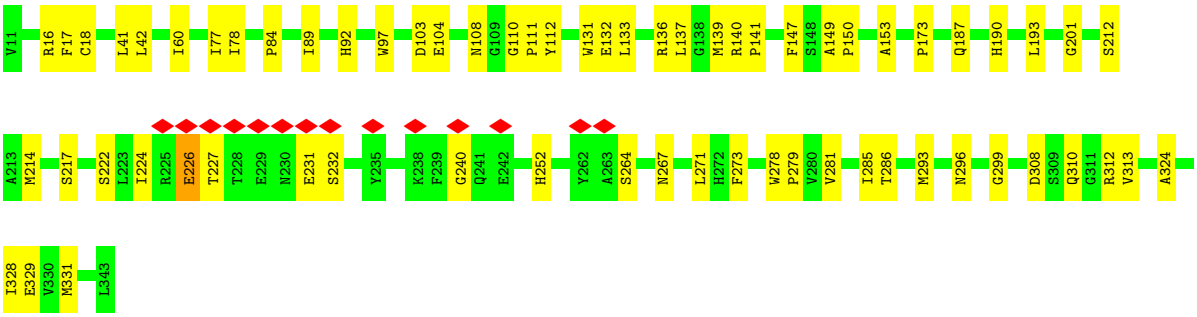
3 Residue-property plots (i)

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: PsbA

Chain A:

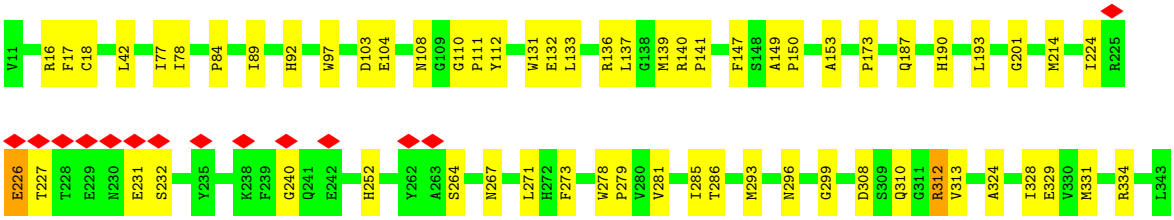




- Molecule 1: PsbA

Chain a:

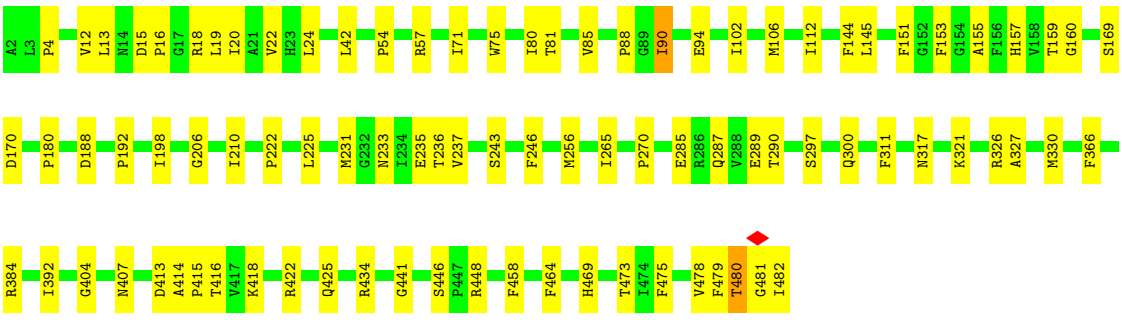




- Molecule 2: PsbB

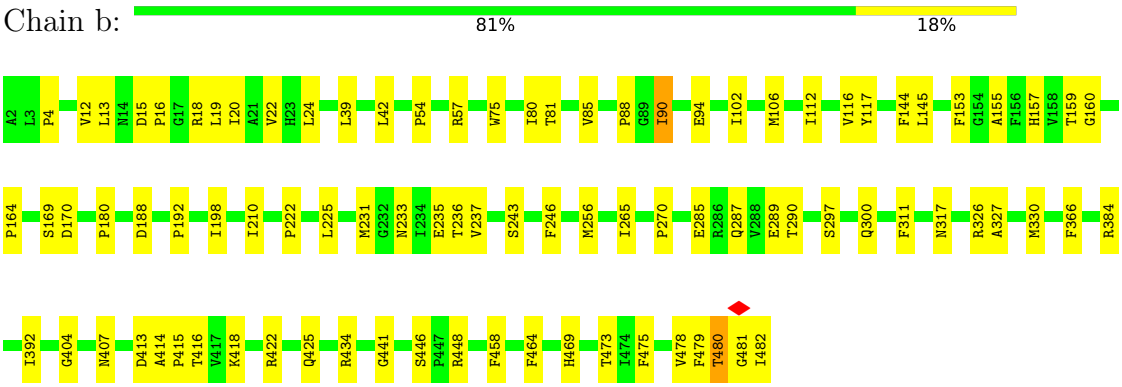
Chain B:





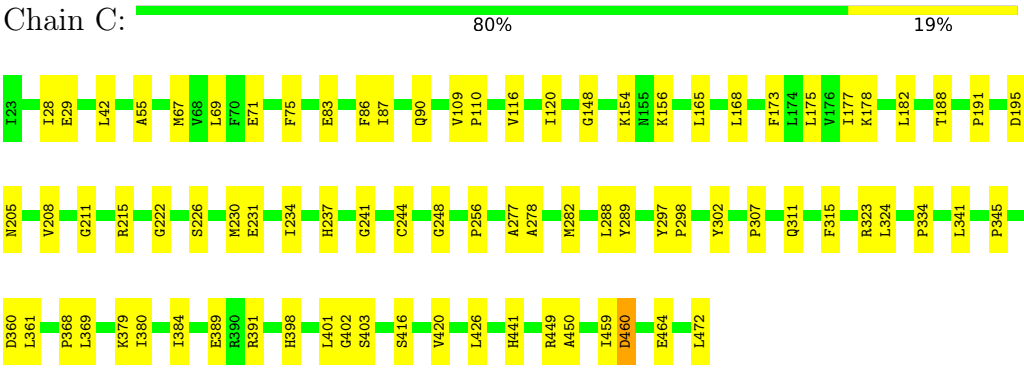
• Molecule 2: PsbB

Chain b:



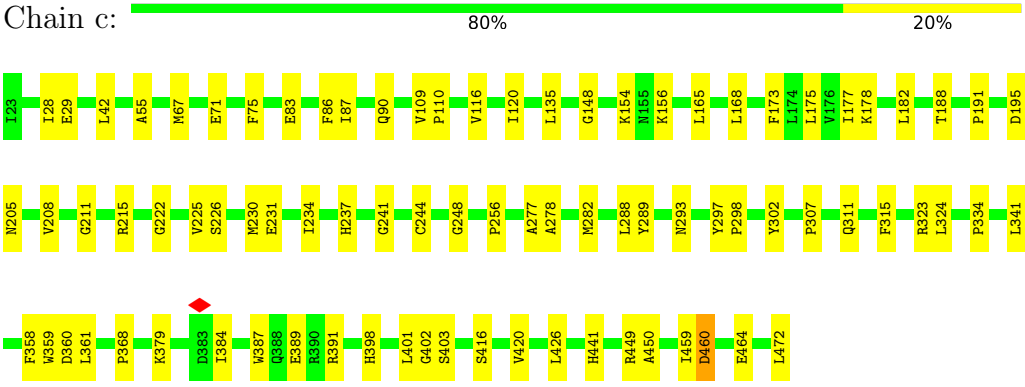
• Molecule 3: PsbC

Chain C:



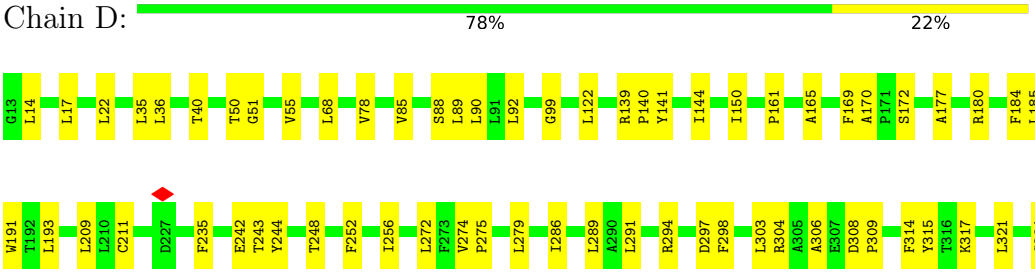
• Molecule 3: PsbC

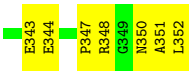
Chain c:



• Molecule 4: PsbD

Chain D:

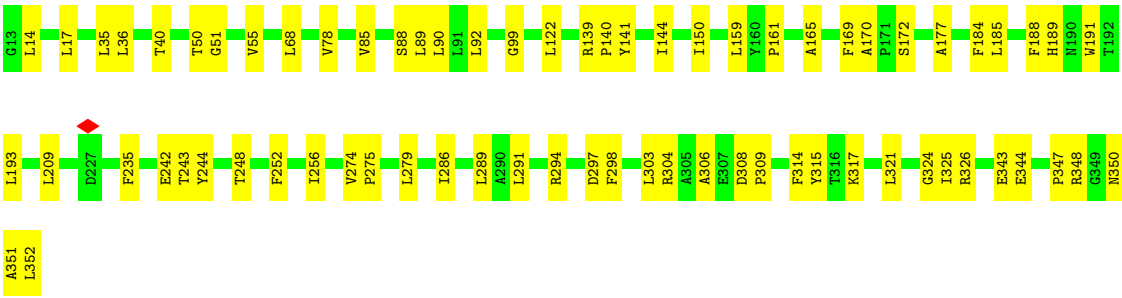




• Molecule 4: PsbD

Chain d:

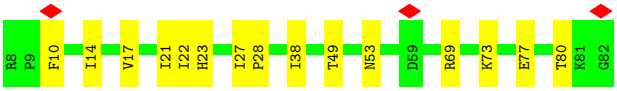




• Molecule 5: PsbE

Chain E:

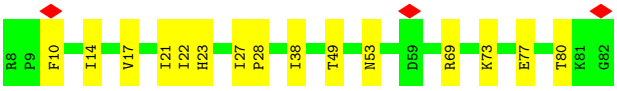




• Molecule 5: PsbE

Chain e:





• Molecule 6: PsbF

Chain F:





• Molecule 6: PsbF

Chain f:

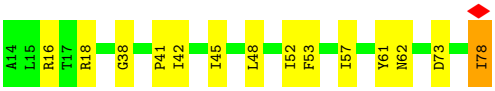




• Molecule 7: PsbH

Chain H:

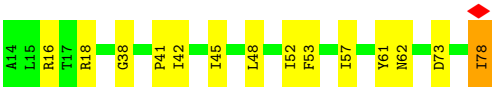




• Molecule 7: PsbH

Chain h:

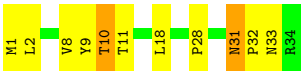




• Molecule 8: PsbI

Chain I:

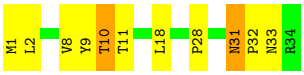




• Molecule 8: PsbI

Chain i:

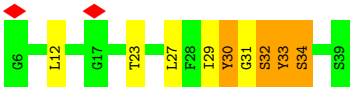




• Molecule 9: PsbJ

Chain J:

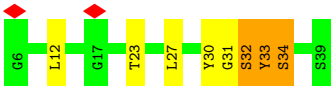




• Molecule 9: PsbJ

Chain j:





• Molecule 10: PsbK

Chain K:





• Molecule 10: PsbK

Chain k:





• Molecule 11: PsbL

Chain L:

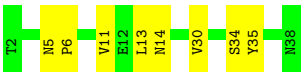




• Molecule 11: PsbL

Chain l:

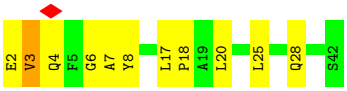




• Molecule 12: PsbM

Chain M:

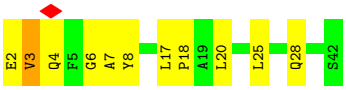




• Molecule 12: PsbM

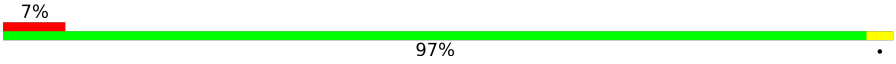
Chain m:

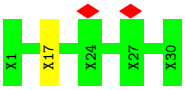




• Molecule 13: Psb34

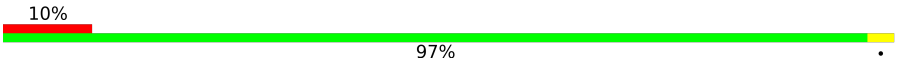
Chain N:

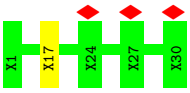




• Molecule 13: Psb34

Chain n:

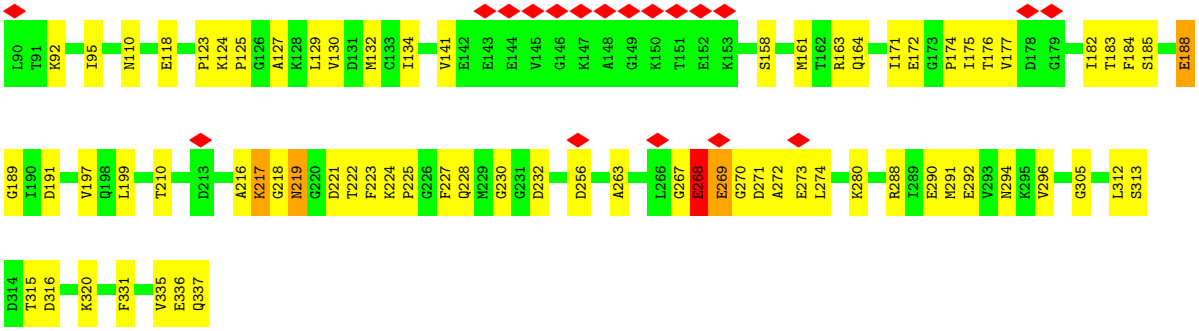




• Molecule 14: PsbO

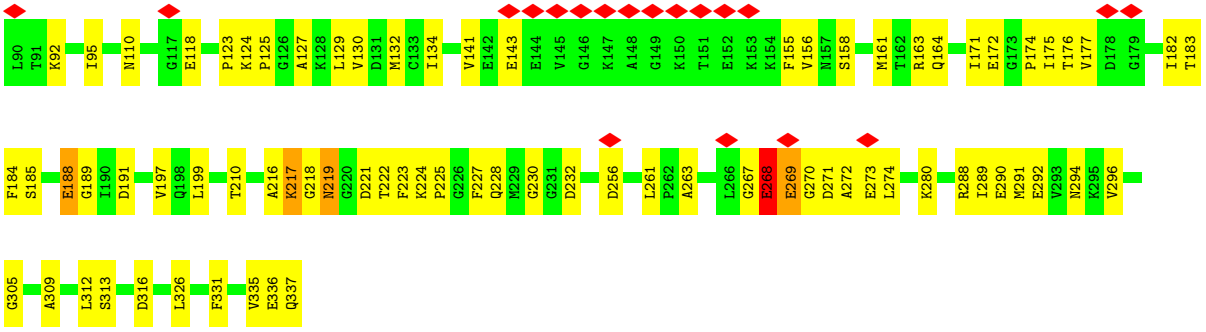
Chain O:





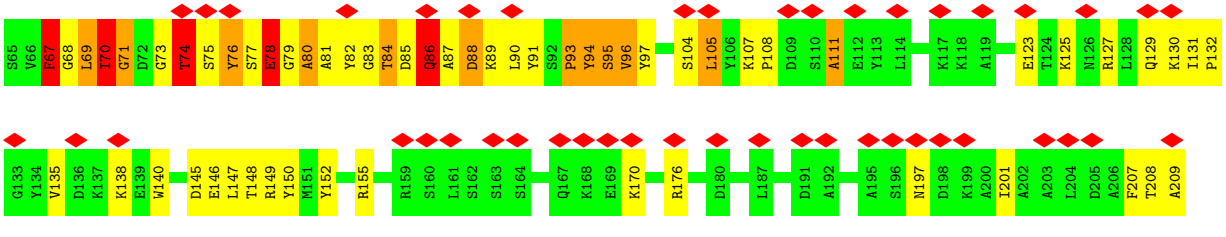
• Molecule 14: PsbO





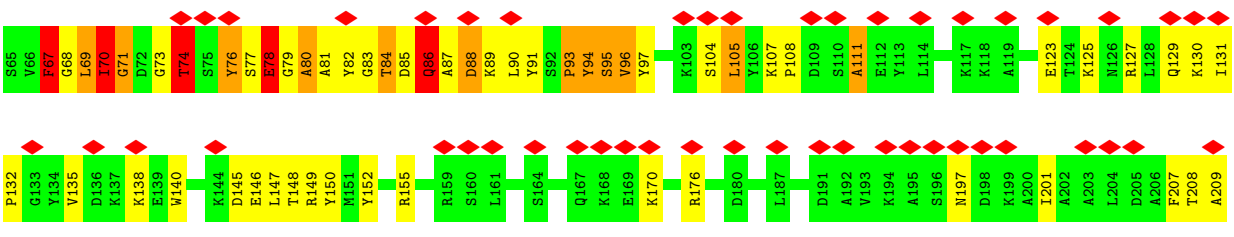
• Molecule 15: PsbQ'



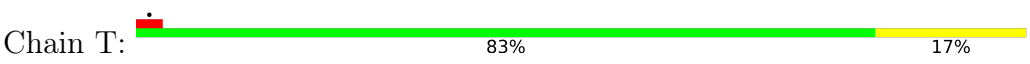


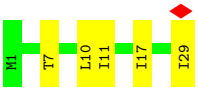
• Molecule 15: PsbQ'





• Molecule 16: PsbT

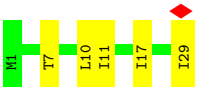




• Molecule 16: PsbT

Chain t:





• Molecule 17: PsbU

Chain U:





• Molecule 17: PsbU

Chain u:





• Molecule 18: PsbV

Chain V:





• Molecule 18: PsbV

Chain v:

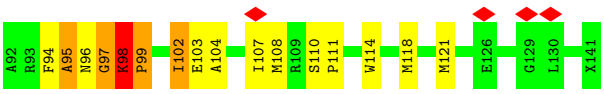




• Molecule 19: PsbW

Chain W:

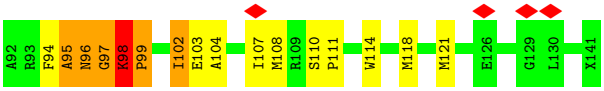




• Molecule 19: PsbW

Chain w:

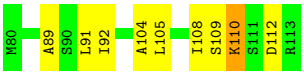




• Molecule 20: PsbX

Chain X:

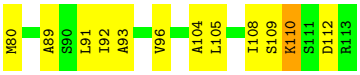




• Molecule 20: PsbX

Chain x:

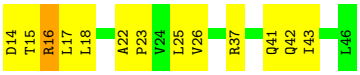




• Molecule 21: PsbY

Chain Y:





• Molecule 21: PsbY

Chain y:

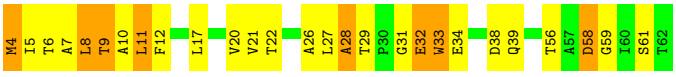




• Molecule 22: PsbZ

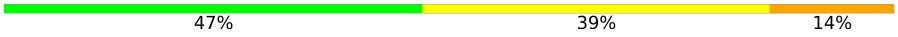
Chain Z:

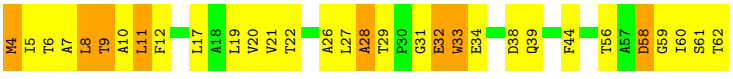




• Molecule 22: PsbZ

Chain z:





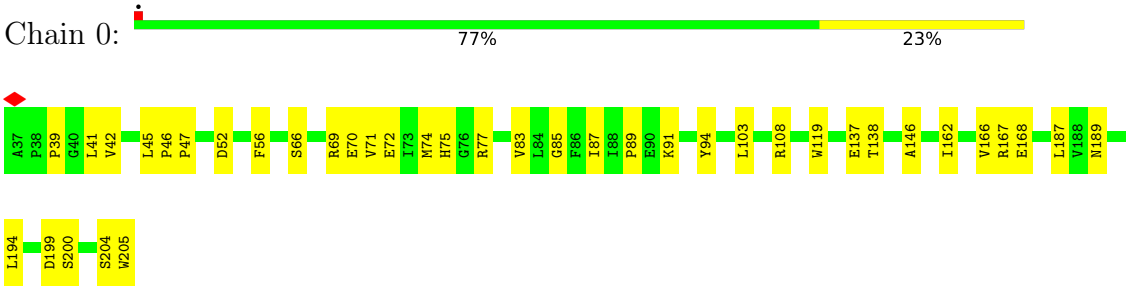
• Molecule 23: FCPII-G, fucoxanthin chlorophyll a/c binding protein

Chain 5:

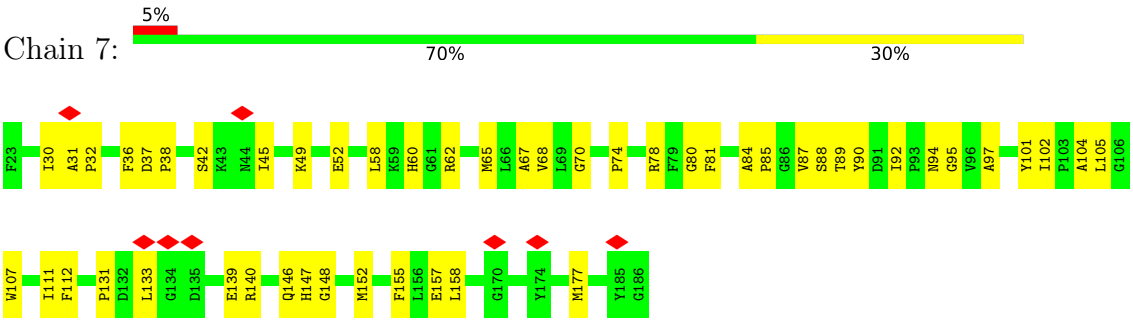




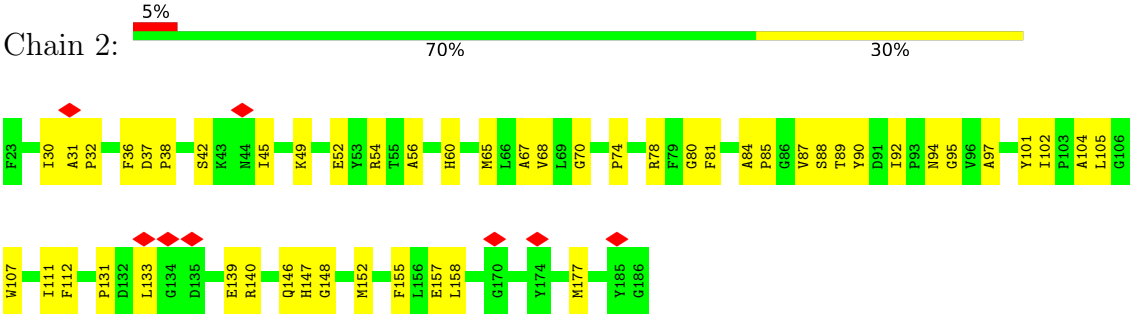
• Molecule 23: FCPII-G, fucoxanthin chlorophyll a/c binding protein



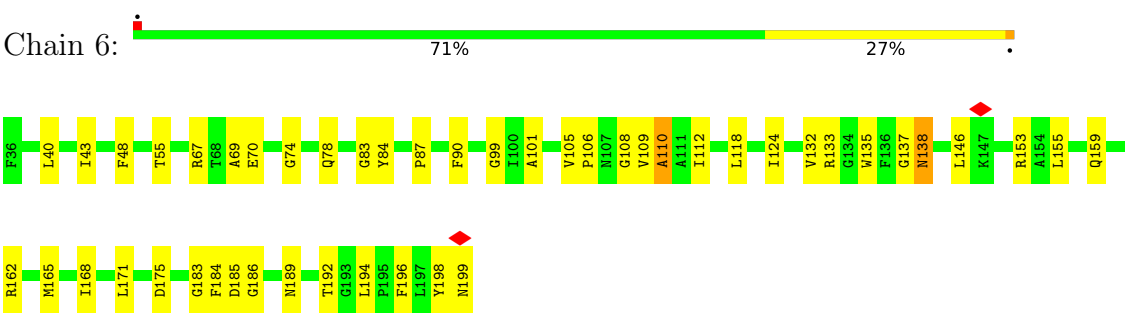
• Molecule 24: FCPII-H2, fucoxanthin chlorophyll a/c binding protein



• Molecule 24: FCPII-H2, fucoxanthin chlorophyll a/c binding protein

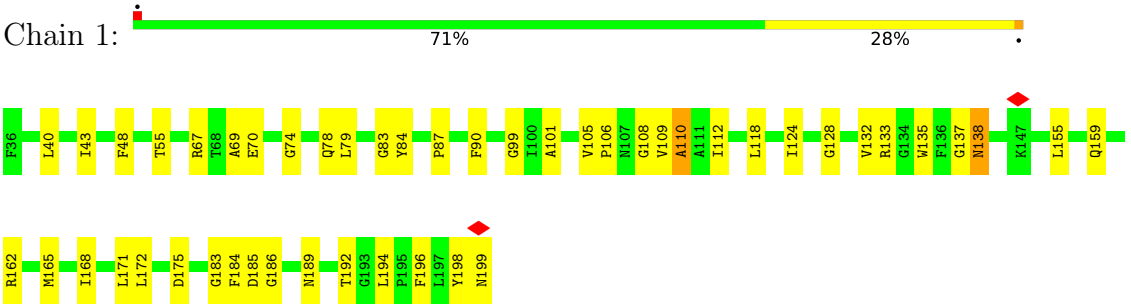


• Molecule 25: FCPII-H1, fucoxanthin chlorophyll a/c binding protein



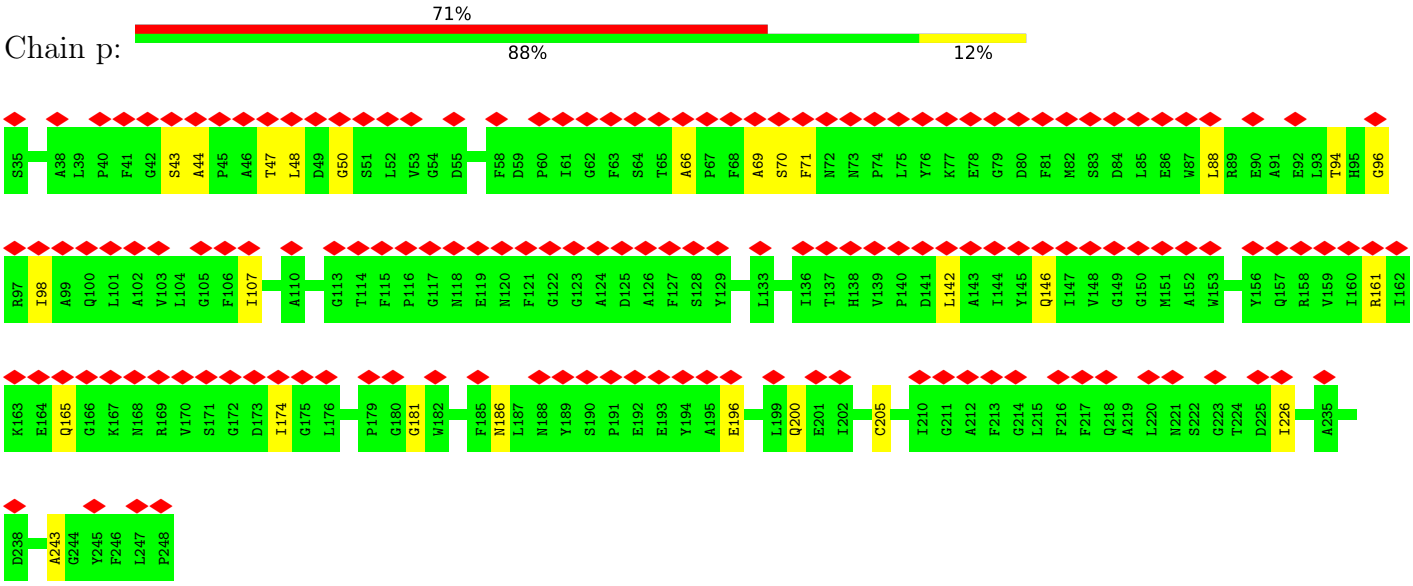
• Molecule 25: FCPII-H1, fucoxanthin chlorophyll a/c binding protein

Chain 1:



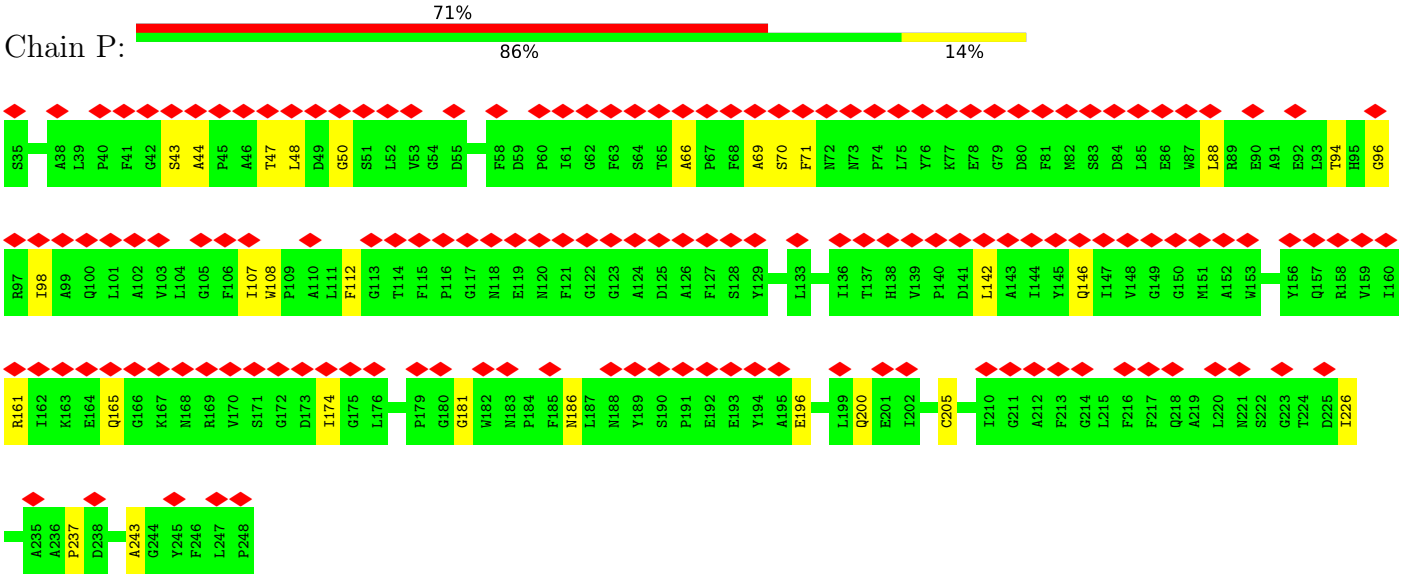
• Molecule 26: FCPII-I, fucoxanthin chlorophyll a/c binding protein

Chain p:



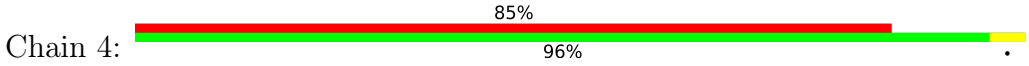
• Molecule 26: FCPII-I, fucoxanthin chlorophyll a/c binding protein

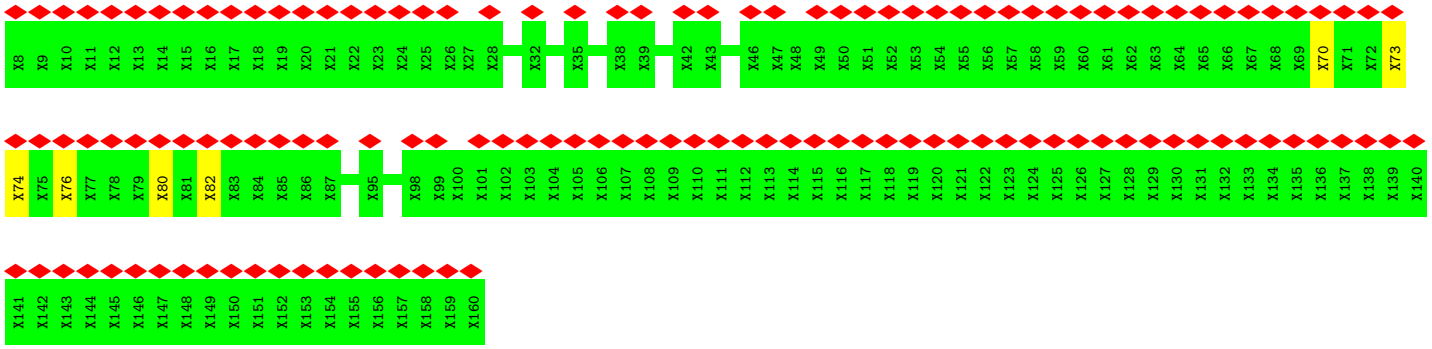
Chain P:



• Molecule 27: FCPII-K, fucoxanthin chlorophyll a/c binding protein

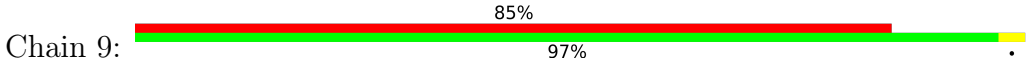
Chain 4:





• Molecule 27: FCPII-K, fucoxanthin chlorophyll a/c binding protein

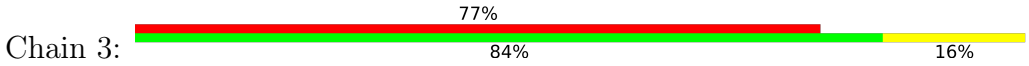
Chain 9:

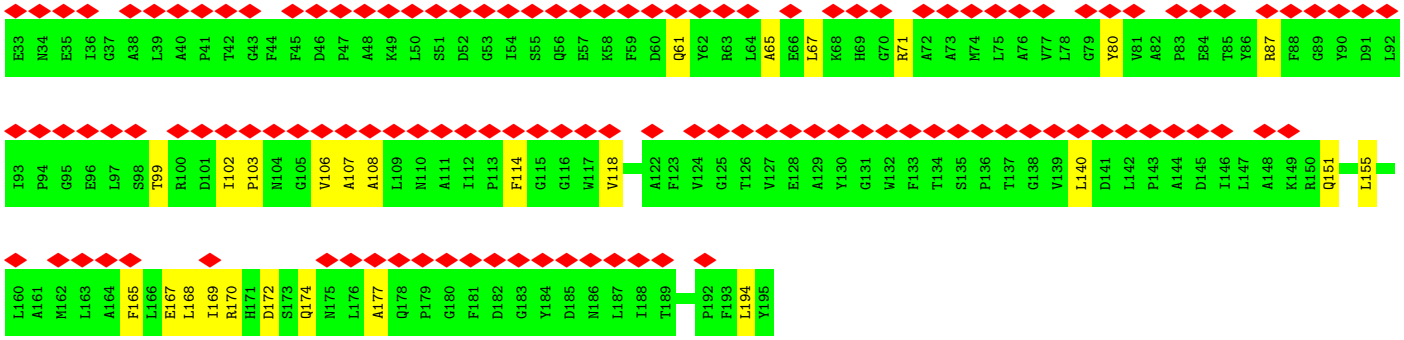




• Molecule 28: FCPII-J, fucoxanthin chlorophyll a/c binding protein

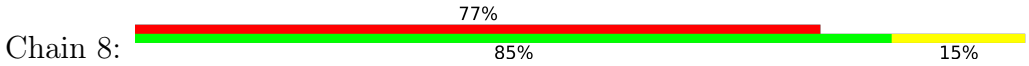
Chain 3:

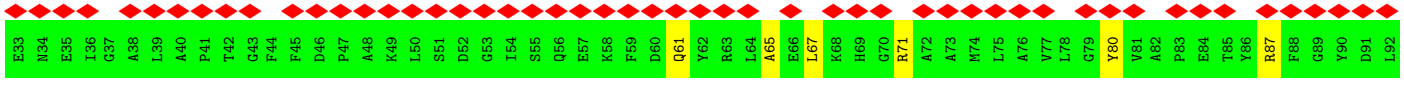


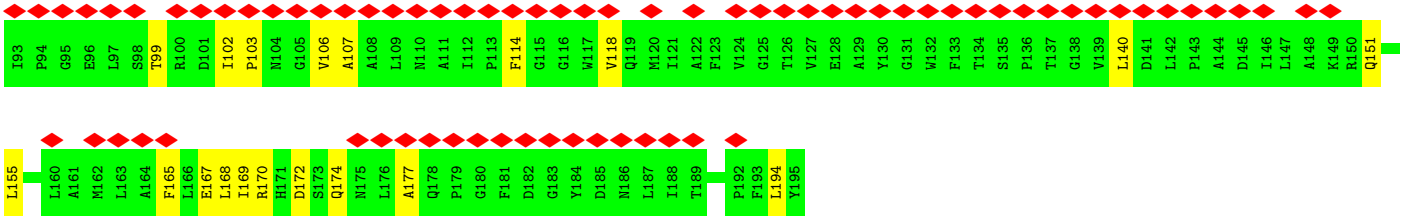


• Molecule 28: FCPII-J, fucoxanthin chlorophyll a/c binding protein

Chain 8:






I93 P94 G95 E96 L97 S98 T99 R100 D101 I102 P103 N104 G105 V106 A107 A108 L109 N110 A111 I112 P113 F114 G115 G116 W117 V118 Q119 M120 I121 A122 F123 V124 G125 T126 V127 E128 A129 Y130 G131 W132 F133 T134 S135 P136 T137 G138 V139 L140 D141 L142 P143 A144 D145 I146 L147 A148 K149 R150 Q151

L155 L160 A161 M162 L163 A164 F165 L166 E167 L168 I169 R170 H171 D172 S173 Q174 N175 L176 A177 Q178 P179 G180 F181 D182 G183 Y184 D185 N186 L187 I188 T189 P192 F193 L194 Y195

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.709	Depositor
Minimum map value	-0.314	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.158	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A86, BCR, OEX, PL9, CLA, BCT, DD6, SQD, HEM, ET4, DGD, CL, PHO, FE2, LMG, LHG

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	0.28	0/2609	0.39	0/3563
1	a	0.28	0/2609	0.40	0/3563
2	B	0.24	0/3878	0.36	0/5282
2	b	0.24	0/3878	0.36	0/5282
3	C	0.21	0/3553	0.35	0/4850
3	c	0.22	0/3553	0.35	0/4850
4	D	0.20	0/2759	0.34	0/3766
4	d	0.20	0/2759	0.34	0/3766
5	E	0.20	0/620	0.33	0/847
5	e	0.20	0/620	0.33	0/847
6	F	0.56	0/250	0.64	0/340
6	f	0.56	0/250	0.64	0/340
7	H	0.34	0/509	0.50	0/696
7	h	0.34	0/509	0.50	0/696
8	I	0.40	0/273	0.51	0/371
8	i	0.40	0/273	0.51	0/371
9	J	0.80	2/253 (0.8%)	0.96	4/344 (1.2%)
9	j	0.79	2/253 (0.8%)	0.96	4/344 (1.2%)
10	K	0.51	0/305	0.59	0/420
10	k	0.51	0/305	0.59	0/420
11	L	0.31	0/303	0.43	0/415
11	l	0.31	0/303	0.43	0/415
12	M	0.33	0/299	0.39	0/404
12	m	0.33	0/299	0.39	0/404
14	O	0.24	0/1853	0.40	0/2505
14	o	0.25	0/1853	0.40	0/2505
15	Q	0.35	0/1065	0.63	1/1439 (0.1%)
15	q	0.35	0/1065	0.63	1/1439 (0.1%)
16	T	0.22	0/240	0.34	0/325
16	t	0.23	0/240	0.34	0/325
17	U	0.21	0/693	0.36	0/945
17	u	0.21	0/693	0.36	0/945

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	V	0.33	0/996	0.46	0/1364
18	v	0.33	0/996	0.46	0/1364
19	W	0.46	0/310	0.85	3/421 (0.7%)
19	w	0.42	0/310	0.85	3/421 (0.7%)
20	X	0.35	0/233	0.45	0/315
20	x	0.35	0/233	0.45	0/315
21	Y	0.49	0/216	0.72	0/297
21	y	0.50	0/216	0.72	0/297
22	Z	0.40	0/419	0.45	0/578
22	z	0.40	0/419	0.45	0/578
23	0	0.27	0/1312	0.48	0/1792
23	5	0.27	0/1312	0.49	0/1792
24	2	0.24	0/1258	0.44	0/1714
24	7	0.24	0/1258	0.44	0/1714
25	1	0.31	0/1242	0.47	0/1697
25	6	0.31	0/1242	0.47	0/1697
26	P	0.33	0/1287	0.69	1/1778 (0.1%)
26	p	0.33	0/1287	0.69	1/1778 (0.1%)
28	3	0.39	0/1003	0.65	0/1373
28	8	0.39	0/1003	0.65	0/1373
All	All	0.29	4/55476 (0.0%)	0.46	18/75682 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	j	34	SER	N-CA	5.75	1.54	1.46
9	J	34	SER	N-CA	5.72	1.54	1.46
9	j	33	TYR	CA-C	5.59	1.60	1.52
9	J	33	TYR	CA-C	5.57	1.60	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	33	TYR	N-CA-C	6.89	122.03	112.45
9	j	33	TYR	N-CA-C	6.87	122.00	112.45
9	J	34	SER	N-CA-C	6.75	122.07	107.49
9	j	34	SER	N-CA-C	6.75	122.07	107.49
19	w	97	GLY	N-CA-C	-6.11	102.47	111.03

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	2530	0	2400	56	0
1	a	2530	0	2400	53	0
2	B	3748	0	3581	61	0
2	b	3748	0	3581	64	0
3	C	3437	0	3297	74	0
3	c	3437	0	3297	74	0
4	D	2667	0	2551	61	0
4	d	2667	0	2551	57	0
5	E	602	0	576	10	0
5	e	602	0	576	10	0
6	F	242	0	237	12	0
6	f	242	0	237	12	0
7	H	499	0	521	17	0
7	h	499	0	521	16	0
8	I	266	0	264	11	0
8	i	266	0	264	11	0
9	J	247	0	256	7	0
9	j	247	0	256	5	0
10	K	294	0	295	10	0
10	k	294	0	295	10	0
11	L	294	0	281	7	0
11	l	294	0	281	7	0
12	M	295	0	292	6	0
12	m	295	0	292	6	0
13	N	150	0	33	1	0
13	n	150	0	33	1	0
14	O	1824	0	1775	54	0
14	o	1824	0	1775	54	0
15	Q	1050	0	988	67	0
15	q	1050	0	988	65	0
16	T	234	0	241	4	0
16	t	234	0	241	4	0
17	U	678	0	663	16	0
17	u	678	0	663	17	0
18	V	979	0	942	27	0
18	v	979	0	942	28	0
19	W	338	0	254	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	w	338	0	254	18	0
20	X	233	0	254	17	0
20	x	233	0	254	19	0
21	Y	216	0	210	12	0
21	y	216	0	210	11	0
22	Z	413	0	402	22	0
22	z	413	0	402	24	0
23	0	1280	0	1242	42	0
23	5	1280	0	1242	43	0
24	2	1222	0	1142	64	0
24	7	1222	0	1142	63	0
25	1	1209	0	1150	43	0
25	6	1209	0	1150	40	0
26	P	1265	0	946	18	0
26	p	1265	0	946	16	0
27	4	765	0	161	3	0
27	9	765	0	161	2	0
28	3	992	0	778	20	0
28	8	992	0	778	19	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	1	0	0	0	0
30	a	1	0	0	0	0
31	0	528	0	439	21	0
31	1	580	0	441	14	0
31	2	525	0	395	22	0
31	3	416	0	257	8	0
31	4	372	0	234	0	0
31	5	528	0	439	21	0
31	6	580	0	441	15	0
31	7	525	0	395	22	0
31	8	416	0	257	7	0
31	9	372	0	234	0	0
31	A	174	0	170	4	0
31	B	959	0	994	39	0
31	C	792	0	822	19	0
31	D	186	0	190	4	0
31	P	341	0	213	10	0
31	W	45	0	33	1	0
31	Z	51	0	41	6	0
31	a	174	0	170	3	0
31	b	959	0	994	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	792	0	822	20	0
31	d	186	0	190	4	0
31	p	341	0	213	10	0
31	w	45	0	33	1	0
31	z	51	0	41	6	0
32	A	128	0	148	4	0
32	a	128	0	148	3	0
33	A	40	0	56	3	0
33	B	120	0	168	13	0
33	C	120	0	168	6	0
33	D	40	0	56	2	0
33	H	40	0	56	2	0
33	K	40	0	56	2	0
33	a	40	0	56	3	0
33	b	120	0	168	12	0
33	c	120	0	168	8	0
33	d	40	0	56	1	0
33	h	40	0	56	2	0
33	k	40	0	56	2	0
34	0	48	0	63	5	0
34	5	48	0	63	5	0
34	A	108	0	156	6	0
34	B	94	0	122	3	0
34	a	54	0	78	0	0
34	b	40	0	44	1	0
35	A	32	0	39	3	0
35	D	55	0	80	3	0
35	a	32	0	39	3	0
35	d	55	0	80	4	0
36	A	69	0	81	4	0
36	B	49	0	74	4	0
36	D	110	0	141	9	0
36	H	42	0	54	6	0
36	a	69	0	81	4	0
36	b	49	0	74	4	0
36	d	110	0	141	9	0
36	h	42	0	54	5	0
37	0	48	0	69	1	0
37	5	48	0	69	1	0
37	B	28	0	26	1	0
37	C	51	0	72	4	0
37	D	123	0	156	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	J	50	0	73	3	0
37	M	91	0	122	2	0
37	W	48	0	66	2	0
37	Y	46	0	62	3	0
37	b	28	0	26	1	0
37	c	51	0	72	4	0
37	d	123	0	156	3	0
37	j	50	0	73	2	0
37	m	91	0	122	2	0
37	w	48	0	66	2	0
37	y	46	0	62	4	0
38	C	1	0	0	0	0
38	c	1	0	0	0	0
39	C	179	0	232	10	0
39	H	62	0	82	4	0
39	c	179	0	232	10	0
39	h	62	0	82	4	0
40	D	4	0	1	0	0
40	d	4	0	1	0	0
41	F	43	0	30	3	0
41	V	43	0	30	6	0
41	f	43	0	30	3	0
41	v	43	0	30	6	0
42	0	144	0	0	1	0
42	1	48	0	0	1	0
42	2	96	0	0	0	0
42	3	96	0	0	0	0
42	4	144	0	0	0	0
42	5	144	0	0	1	0
42	6	48	0	0	1	0
42	7	96	0	0	0	0
42	8	96	0	0	0	0
42	9	144	0	0	0	0
42	P	48	0	0	0	0
42	p	48	0	0	0	0
43	0	42	0	0	0	0
43	5	42	0	0	0	0
44	1	86	0	0	3	0
44	2	86	0	0	24	0
44	3	43	0	0	1	0
44	6	86	0	0	3	0
44	7	86	0	0	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	8	43	0	0	1	0
44	P	43	0	0	7	0
44	p	43	0	0	7	0
All	All	71446	0	64844	1569	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 12.

The worst 5 of 1569 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)
24:7:65:MET:HG2	44:7:304:DD6:C3	1.71	1.19
24:2:65:MET:HG2	44:2:304:DD6:C3	1.71	1.19
31:B:514:CLA:H43	33:B:517:BCR:H383	1.19	1.14
31:b:515:CLA:H43	33:b:518:BCR:H383	1.19	1.13
31:p:604:CLA:C2B	44:p:611:DD6:C37	2.31	1.09

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	331/333 (99%)	316 (96%)	15 (4%)	0	100	100
1	a	331/333 (99%)	316 (96%)	15 (4%)	0	100	100
2	B	479/481 (100%)	456 (95%)	22 (5%)	1 (0%)	43	65
2	b	479/481 (100%)	456 (95%)	22 (5%)	1 (0%)	43	65
3	C	448/450 (100%)	435 (97%)	12 (3%)	1 (0%)	43	65
3	c	448/450 (100%)	435 (97%)	12 (3%)	1 (0%)	43	65
4	D	338/340 (99%)	325 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	338/340 (99%)	325 (96%)	13 (4%)	0	100	100
5	E	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
5	e	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
6	F	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	7
6	f	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	3	7
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
9	J	32/34 (94%)	32 (100%)	0	0	100	100
9	j	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	k	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	39/41 (95%)	39 (100%)	0	0	100	100
12	m	39/41 (95%)	39 (100%)	0	0	100	100
14	O	246/248 (99%)	223 (91%)	21 (8%)	2 (1%)	16	36
14	o	246/248 (99%)	223 (91%)	21 (8%)	2 (1%)	16	36
15	Q	143/145 (99%)	113 (79%)	17 (12%)	13 (9%)	0	1
15	q	143/145 (99%)	113 (79%)	17 (12%)	13 (9%)	0	1
16	T	27/29 (93%)	27 (100%)	0	0	100	100
16	t	27/29 (93%)	27 (100%)	0	0	100	100
17	U	90/92 (98%)	82 (91%)	8 (9%)	0	100	100
17	u	90/92 (98%)	82 (91%)	8 (9%)	0	100	100
18	V	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	18	40
18	v	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	18	40
19	W	42/50 (84%)	36 (86%)	2 (5%)	4 (10%)	0	1
19	w	42/50 (84%)	36 (86%)	2 (5%)	4 (10%)	0	1
20	X	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	8
20	x	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Y	31/33 (94%)	26 (84%)	5 (16%)	0	100	100
21	y	31/33 (94%)	26 (84%)	5 (16%)	0	100	100
22	Z	57/59 (97%)	44 (77%)	11 (19%)	2 (4%)	3	7
22	z	57/59 (97%)	44 (77%)	11 (19%)	2 (4%)	3	7
23	0	167/169 (99%)	143 (86%)	24 (14%)	0	100	100
23	5	167/169 (99%)	143 (86%)	24 (14%)	0	100	100
24	2	162/164 (99%)	143 (88%)	19 (12%)	0	100	100
24	7	162/164 (99%)	143 (88%)	19 (12%)	0	100	100
25	1	162/164 (99%)	135 (83%)	26 (16%)	1 (1%)	21	45
25	6	162/164 (99%)	135 (83%)	26 (16%)	1 (1%)	21	45
26	P	212/214 (99%)	172 (81%)	38 (18%)	2 (1%)	14	34
26	p	212/214 (99%)	173 (82%)	37 (18%)	2 (1%)	14	34
28	3	161/163 (99%)	140 (87%)	20 (12%)	1 (1%)	21	45
28	8	161/163 (99%)	140 (87%)	20 (12%)	1 (1%)	21	45
All	All	7200/7316 (98%)	6589 (92%)	551 (8%)	60 (1%)	18	36

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	460	ASP
6	F	43	ILE
14	O	268	GLU
15	Q	70	ILE
15	Q	84	THR

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	250/272 (92%)	242 (97%)	8 (3%)	34	59
1	a	250/272 (92%)	243 (97%)	7 (3%)	38	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	370/384 (96%)	360 (97%)	10 (3%)	39 64
2	b	370/384 (96%)	360 (97%)	10 (3%)	39 64
3	C	337/355 (95%)	334 (99%)	3 (1%)	70 82
3	c	337/355 (95%)	334 (99%)	3 (1%)	70 82
4	D	265/272 (97%)	264 (100%)	1 (0%)	84 92
4	d	265/272 (97%)	264 (100%)	1 (0%)	84 92
5	E	65/69 (94%)	64 (98%)	1 (2%)	57 75
5	e	65/69 (94%)	64 (98%)	1 (2%)	57 75
6	F	22/25 (88%)	19 (86%)	3 (14%)	3 10
6	f	22/25 (88%)	19 (86%)	3 (14%)	3 10
7	H	52/54 (96%)	49 (94%)	3 (6%)	18 40
7	h	52/54 (96%)	49 (94%)	3 (6%)	18 40
8	I	30/33 (91%)	27 (90%)	3 (10%)	7 19
8	i	30/33 (91%)	27 (90%)	3 (10%)	7 19
9	J	26/26 (100%)	26 (100%)	0	100 100
9	j	26/26 (100%)	26 (100%)	0	100 100
10	K	30/32 (94%)	29 (97%)	1 (3%)	33 58
10	k	30/32 (94%)	29 (97%)	1 (3%)	33 58
11	L	31/33 (94%)	31 (100%)	0	100 100
11	l	31/33 (94%)	31 (100%)	0	100 100
12	M	26/30 (87%)	24 (92%)	2 (8%)	12 28
12	m	26/30 (87%)	24 (92%)	2 (8%)	12 28
14	O	185/201 (92%)	176 (95%)	9 (5%)	22 47
14	o	185/201 (92%)	176 (95%)	9 (5%)	22 47
15	Q	99/116 (85%)	89 (90%)	10 (10%)	7 19
15	q	99/116 (85%)	89 (90%)	10 (10%)	7 19
16	T	24/26 (92%)	24 (100%)	0	100 100
16	t	24/26 (92%)	24 (100%)	0	100 100
17	U	70/77 (91%)	65 (93%)	5 (7%)	13 31
17	u	70/77 (91%)	65 (93%)	5 (7%)	13 31
18	V	101/114 (89%)	99 (98%)	2 (2%)	48 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	v	101/114 (89%)	99 (98%)	2 (2%)	48 70
19	W	25/34 (74%)	24 (96%)	1 (4%)	28 53
19	w	25/34 (74%)	24 (96%)	1 (4%)	28 53
20	X	25/26 (96%)	24 (96%)	1 (4%)	28 53
20	x	25/26 (96%)	24 (96%)	1 (4%)	28 53
21	Y	18/26 (69%)	16 (89%)	2 (11%)	6 16
21	y	18/26 (69%)	16 (89%)	2 (11%)	6 16
22	Z	39/48 (81%)	32 (82%)	7 (18%)	2 4
22	z	39/48 (81%)	32 (82%)	7 (18%)	2 4
23	0	129/136 (95%)	129 (100%)	0	100 100
23	5	129/136 (95%)	129 (100%)	0	100 100
24	2	110/131 (84%)	109 (99%)	1 (1%)	70 82
24	7	110/131 (84%)	109 (99%)	1 (1%)	70 82
25	1	107/129 (83%)	105 (98%)	2 (2%)	50 71
25	6	107/129 (83%)	105 (98%)	2 (2%)	50 71
26	P	70/166 (42%)	70 (100%)	0	100 100
26	p	70/166 (42%)	70 (100%)	0	100 100
28	3	54/128 (42%)	54 (100%)	0	100 100
28	8	54/128 (42%)	54 (100%)	0	100 100
All	All	5120/5886 (87%)	4971 (97%)	149 (3%)	38 62

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	q	67	PHE
24	7	139	GLU
15	q	78	GLU
18	v	24	GLU
15	Q	78	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
7	h	69	ASN

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Mol	Chain	Res	Type
23	5	185	GLN
10	k	53	GLN
17	u	16	ASN
23	5	196	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 336 ligands modelled in this entry, 4 are monoatomic - leaving 332 for Mogul analysis.

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	$\#\|Z\| > 2$
31	CLA	7	309	24	63,67,73	1.21	9 (14%)	74,105,113	1.32	7 (9%)
37	LMG	y	101	-	46,46,55	0.75	1 (2%)	54,54,63	1.39	11 (20%)
39	DGD	C	518	-	56,56,67	0.95	3 (5%)	70,70,81	1.45	11 (15%)
31	CLA	8	309	-	43,48,73	1.40	9 (20%)	51,83,113	1.70	6 (11%)
31	CLA	9	213	-	37,43,73	1.67	10 (27%)	49,76,113	1.69	11 (22%)
32	PHO	a	406	-	58,69,69	2.09	10 (17%)	55,99,99	1.46	7 (12%)
31	CLA	B	505	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
31	CLA	4	205	-	38,43,73	1.61	11 (28%)	48,75,113	1.47	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	B	516	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
42	A86	1	202	-	47,50,50	1.48	6 (12%)	51,76,76	2.40	15 (29%)
31	CLA	6	212	-	45,49,73	1.40	7 (15%)	54,84,113	1.49	6 (11%)
36	LHG	d	407	-	44,47,48	0.56	1 (2%)	44,51,54	1.23	6 (13%)
34	SQD	B	522	-	52,54,54	0.94	2 (3%)	62,65,65	1.60	12 (19%)
42	A86	6	202	-	47,50,50	1.49	6 (12%)	51,76,76	2.40	15 (29%)
42	A86	4	203	-	47,50,50	1.82	6 (12%)	51,76,76	3.65	22 (43%)
44	DD6	2	303	-	40,45,45	1.57	2 (5%)	51,67,67	2.17	17 (33%)
31	CLA	2	305	-	45,49,73	1.40	8 (17%)	54,84,113	1.51	6 (11%)
35	PL9	D	406	-	55,55,55	1.32	5 (9%)	68,69,69	1.53	12 (17%)
31	CLA	C	502	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	6 (7%)
31	CLA	c	504	-	55,59,73	1.29	9 (16%)	64,96,113	1.46	7 (10%)
31	CLA	0	312	-	46,50,73	1.39	8 (17%)	53,85,113	1.44	4 (7%)
31	CLA	1	210	25	69,73,73	1.15	8 (11%)	82,113,113	1.33	8 (9%)
31	CLA	8	314	-	39,43,73	1.61	10 (25%)	50,76,113	1.52	7 (14%)
37	LMG	D	409	-	37,37,55	0.78	1 (2%)	45,45,63	1.33	7 (15%)
31	CLA	6	214	25	40,46,73	1.45	8 (20%)	52,80,113	1.52	7 (13%)
31	CLA	3	306	-	35,41,73	1.74	10 (28%)	47,72,113	1.66	8 (17%)
42	A86	9	203	-	47,50,50	1.82	6 (12%)	51,76,76	3.64	22 (43%)
37	LMG	5	315	-	48,48,55	0.77	1 (2%)	56,56,63	1.29	6 (10%)
44	DD6	6	203	-	40,45,45	1.57	2 (5%)	51,67,67	2.16	17 (33%)
31	CLA	B	514	-	64,68,73	1.20	9 (14%)	75,106,113	1.31	5 (6%)
31	CLA	6	216	25	40,46,73	1.45	7 (17%)	52,80,113	1.46	5 (9%)
31	CLA	4	207	-	40,46,73	1.44	8 (20%)	52,80,113	1.59	6 (11%)
31	CLA	c	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
31	CLA	a	404	-	53,57,73	1.29	9 (16%)	61,93,113	1.45	6 (9%)
31	CLA	1	206	25	49,53,73	1.35	7 (14%)	58,89,113	1.50	5 (8%)
42	A86	7	301	-	47,50,50	1.54	5 (10%)	51,76,76	2.59	18 (35%)
42	A86	P	610	-	47,50,50	1.60	7 (14%)	51,76,76	3.91	25 (49%)
31	CLA	3	311	28	43,48,73	1.44	8 (18%)	51,83,113	1.57	6 (11%)
31	CLA	W	202	19	49,53,73	1.35	10 (20%)	58,89,113	1.47	7 (12%)
33	BCR	k	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.25	5 (8%)
36	LHG	B	521	-	48,48,48	0.65	1 (2%)	51,54,54	1.31	6 (11%)
31	CLA	7	316	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
31	CLA	8	308	-	40,43,73	1.57	11 (27%)	46,73,113	2.00	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	LMG	J	101	-	50,50,55	0.79	1 (2%)	58,58,63	1.35	6 (10%)
31	CLA	3	314	-	39,43,73	1.61	11 (28%)	50,76,113	1.53	7 (14%)
31	CLA	C	510	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
31	CLA	9	212	-	40,44,73	1.59	10 (25%)	51,77,113	1.54	6 (11%)
31	CLA	B	511	-	68,72,73	1.18	9 (13%)	80,111,113	1.34	7 (8%)
31	CLA	1	208	-	51,55,73	1.34	9 (17%)	60,91,113	1.41	5 (8%)
31	CLA	9	211	-	37,42,73	1.65	10 (27%)	47,74,113	1.50	5 (10%)
31	CLA	5	313	23	40,46,73	1.46	7 (17%)	52,80,113	1.51	5 (9%)
31	CLA	9	207	-	40,46,73	1.44	8 (20%)	52,80,113	1.60	6 (11%)
31	CLA	z	101	-	55,59,73	1.32	8 (14%)	64,96,113	1.35	5 (7%)
31	CLA	b	517	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
31	CLA	4	206	-	39,45,73	1.50	9 (23%)	49,78,113	1.49	6 (12%)
31	CLA	9	205	-	38,43,73	1.62	12 (31%)	48,75,113	1.48	5 (10%)
36	LHG	a	412	-	25,25,48	0.82	1 (4%)	28,31,54	1.30	2 (7%)
43	ET4	0	302	-	41,43,43	1.72	10 (24%)	52,60,60	2.18	14 (26%)
37	LMG	w	201	-	48,48,55	0.77	1 (2%)	56,56,63	1.34	7 (12%)
33	BCR	b	518	-	41,41,41	1.21	2 (4%)	56,56,56	1.26	7 (12%)
42	A86	7	302	-	47,50,50	1.79	7 (14%)	51,76,76	2.85	17 (33%)
31	CLA	2	306	24	49,53,73	1.36	8 (16%)	58,89,113	1.44	4 (6%)
31	CLA	A	404	-	53,57,73	1.29	9 (16%)	61,93,113	1.45	6 (9%)
33	BCR	K	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	5 (8%)
37	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.05	4 (6%)
31	CLA	A	407	-	64,68,73	1.19	8 (12%)	76,107,113	1.34	9 (11%)
31	CLA	c	507	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
42	A86	3	301	-	47,50,50	1.77	9 (19%)	51,76,76	4.95	22 (43%)
31	CLA	p	604	-	43,48,73	1.40	9 (20%)	51,83,113	1.57	7 (13%)
31	CLA	C	512	3	69,73,73	1.15	9 (13%)	82,113,113	1.32	5 (6%)
44	DD6	1	203	-	40,45,45	1.58	2 (5%)	51,67,67	2.16	17 (33%)
43	ET4	5	302	-	41,43,43	1.72	10 (24%)	52,60,60	2.18	14 (26%)
31	CLA	c	511	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
31	CLA	8	305	-	44,49,73	1.40	10 (22%)	50,84,113	1.55	5 (10%)
31	CLA	1	211	25	59,63,73	1.27	9 (15%)	70,101,113	1.33	6 (8%)
31	CLA	b	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
31	CLA	2	315	24	40,46,73	1.47	9 (22%)	52,80,113	1.51	6 (11%)
37	LMG	D	408	-	46,46,55	0.77	1 (2%)	54,54,63	1.34	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	5	306	-	49,53,73	1.37	7 (14%)	58,89,113	1.42	4 (6%)
31	CLA	c	514	-	53,57,73	1.30	8 (15%)	61,93,113	1.44	6 (9%)
39	DGD	c	518	-	56,56,67	0.95	3 (5%)	70,70,81	1.44	11 (15%)
32	PHO	A	406	-	58,69,69	2.10	10 (17%)	55,99,99	1.46	7 (12%)
42	A86	0	303	-	47,50,50	1.53	7 (14%)	51,76,76	2.73	22 (43%)
31	CLA	p	607	-	38,44,73	1.61	10 (26%)	50,77,113	1.50	6 (12%)
31	CLA	0	314	23	40,46,73	1.46	8 (20%)	52,80,113	1.50	6 (11%)
36	LHG	D	411	-	33,33,48	0.74	2 (6%)	36,39,54	1.34	4 (11%)
31	CLA	7	311	-	47,51,73	1.38	8 (17%)	55,86,113	1.38	6 (10%)
33	BCR	C	515	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	8 (14%)
34	SQD	A	409	-	52,54,54	0.96	4 (7%)	62,65,65	1.43	8 (12%)
31	CLA	p	603	-	39,45,73	1.47	9 (23%)	51,79,113	1.66	7 (13%)
31	CLA	B	515	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	7 (8%)
31	CLA	7	313	24	40,46,73	1.46	7 (17%)	52,80,113	1.49	6 (11%)
31	CLA	6	205	-	45,49,73	1.40	8 (17%)	54,84,113	1.47	5 (9%)
31	CLA	8	307	-	46,50,73	1.37	10 (21%)	55,84,113	1.44	5 (9%)
31	CLA	p	606	-	39,45,73	1.50	10 (25%)	49,78,113	1.51	6 (12%)
31	CLA	0	304	-	45,49,73	1.41	8 (17%)	54,84,113	1.53	6 (11%)
31	CLA	b	515	-	64,68,73	1.20	9 (14%)	75,106,113	1.31	5 (6%)
41	HEM	v	201	18	50,50,50	1.29	5 (10%)	67,82,82	1.27	5 (7%)
39	DGD	c	520	-	63,63,67	0.85	2 (3%)	77,77,81	0.94	3 (3%)
31	CLA	2	307	-	51,55,73	1.33	8 (15%)	60,91,113	1.44	5 (8%)
31	CLA	A	403	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
31	CLA	C	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
36	LHG	b	522	-	48,48,48	0.65	1 (2%)	51,54,54	1.31	6 (11%)
31	CLA	7	310	24	59,63,73	1.25	8 (13%)	70,101,113	1.36	6 (8%)
42	A86	4	201	-	47,50,50	1.69	6 (12%)	51,76,76	3.96	23 (45%)
31	CLA	2	314	-	40,46,73	1.47	8 (20%)	52,80,113	1.50	6 (11%)
44	DD6	2	304	-	40,45,45	1.58	2 (5%)	51,67,67	2.45	15 (29%)
31	CLA	c	505	-	68,72,73	1.16	8 (11%)	80,111,113	1.29	4 (5%)
31	CLA	6	213	25	43,48,73	1.43	8 (18%)	51,83,113	1.45	5 (9%)
31	CLA	B	503	-	68,72,73	1.16	9 (13%)	80,111,113	1.28	5 (6%)
33	BCR	b	519	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	7 (12%)
31	CLA	2	308	-	48,52,73	1.48	9 (18%)	59,88,113	1.44	6 (10%)
33	BCR	c	515	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	4	209	-	45,49,73	1.38	9 (20%)	54,84,113	1.56	5 (9%)
39	DGD	C	519	-	63,63,67	0.92	3 (4%)	77,77,81	1.45	12 (15%)
31	CLA	3	305	-	44,49,73	1.41	10 (22%)	50,84,113	1.54	5 (10%)
31	CLA	6	206	25	49,53,73	1.35	8 (16%)	58,89,113	1.51	5 (8%)
44	DD6	7	303	-	40,45,45	1.58	2 (5%)	51,67,67	2.16	17 (33%)
39	DGD	C	520	-	63,63,67	0.85	2 (3%)	77,77,81	0.93	3 (3%)
31	CLA	P	605	-	39,45,73	1.46	10 (25%)	51,79,113	1.64	5 (9%)
31	CLA	c	508	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	4 (4%)
31	CLA	2	310	24	59,63,73	1.25	8 (13%)	70,101,113	1.37	6 (8%)
34	SQD	5	316	-	46,48,54	1.03	6 (13%)	56,59,65	1.39	8 (14%)
31	CLA	1	205	-	45,49,73	1.41	9 (20%)	54,84,113	1.46	5 (9%)
34	SQD	B	523	-	38,40,54	1.11	3 (7%)	48,51,65	1.70	11 (22%)
31	CLA	0	309	23	45,49,73	1.41	9 (20%)	54,84,113	1.50	6 (11%)
34	SQD	b	501	-	38,40,54	1.11	3 (7%)	48,51,65	1.70	11 (22%)
37	LMG	B	520	-	28,28,55	0.94	1 (3%)	36,36,63	1.35	7 (19%)
31	CLA	P	606	-	39,45,73	1.50	10 (25%)	49,78,113	1.51	6 (12%)
37	LMG	m	101	-	51,51,55	0.77	1 (1%)	59,59,63	1.41	9 (15%)
31	CLA	B	513	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	8 (9%)
31	CLA	6	201	-	48,52,73	1.48	9 (18%)	59,88,113	1.48	7 (11%)
34	SQD	a	409	-	52,54,54	0.96	4 (7%)	62,65,65	1.43	8 (12%)
42	A86	p	610	-	47,50,50	1.60	7 (14%)	51,76,76	3.91	24 (47%)
39	DGD	c	519	-	63,63,67	0.92	3 (4%)	77,77,81	1.45	12 (15%)
31	CLA	p	602	-	45,49,73	1.39	9 (20%)	54,84,113	1.60	9 (16%)
31	CLA	C	503	-	68,72,73	1.18	9 (13%)	80,111,113	1.31	6 (7%)
31	CLA	d	401	-	63,67,73	1.20	8 (12%)	74,105,113	1.37	7 (9%)
36	LHG	h	103	-	41,41,48	0.65	1 (2%)	44,47,54	1.16	3 (6%)
31	CLA	6	210	25	69,73,73	1.15	7 (10%)	82,113,113	1.34	8 (9%)
31	CLA	B	510	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
44	DD6	P	611	-	40,45,45	1.55	2 (5%)	51,67,67	1.87	14 (27%)
31	CLA	4	208	-	43,48,73	1.45	10 (23%)	51,83,113	1.61	8 (15%)
42	A86	4	202	-	47,50,50	1.85	7 (14%)	51,76,76	3.72	28 (54%)
31	CLA	C	514	-	53,57,73	1.30	8 (15%)	61,93,113	1.44	6 (9%)
31	CLA	B	504	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
31	CLA	6	208	-	51,55,73	1.33	8 (15%)	60,91,113	1.41	5 (8%)
31	CLA	8	313	-	41,47,73	1.43	10 (24%)	51,81,113	1.46	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	Z	101	-	55,59,73	1.31	8 (14%)	64,96,113	1.35	6 (9%)
44	DD6	8	303	-	40,45,45	1.61	3 (7%)	51,67,67	2.83	16 (31%)
31	CLA	C	511	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
31	CLA	B	506	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	6 (7%)
31	CLA	a	407	-	64,68,73	1.19	8 (12%)	76,107,113	1.35	9 (11%)
41	HEM	f	101	5,6	50,50,50	1.36	9 (18%)	67,82,82	1.03	1 (1%)
31	CLA	C	504	-	55,59,73	1.30	9 (16%)	64,96,113	1.46	7 (10%)
37	LMG	M	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.41	9 (15%)
31	CLA	2	312	24	39,44,73	1.55	9 (23%)	50,77,113	1.59	9 (18%)
31	CLA	P	607	-	38,44,73	1.61	10 (26%)	50,77,113	1.48	6 (12%)
40	BCT	d	402	30	3,3,3	1.12	0	2,3,3	4.14	2 (100%)
31	CLA	5	314	23	40,46,73	1.47	8 (20%)	52,80,113	1.49	6 (11%)
37	LMG	j	101	-	50,50,55	0.80	1 (2%)	58,58,63	1.34	6 (10%)
31	CLA	b	508	-	45,49,73	1.39	9 (20%)	54,84,113	1.51	7 (12%)
31	CLA	c	503	-	68,72,73	1.17	9 (13%)	80,111,113	1.31	6 (7%)
42	A86	5	317	-	47,50,50	1.54	5 (10%)	51,76,76	2.60	17 (33%)
31	CLA	D	404	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	5 (6%)
36	LHG	D	407	-	44,47,48	0.56	1 (2%)	44,51,54	1.23	6 (13%)
33	BCR	b	520	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	8 (14%)
31	CLA	b	509	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
31	CLA	p	605	-	39,45,73	1.46	10 (25%)	51,79,113	1.65	5 (9%)
31	CLA	4	210	-	40,46,73	1.44	9 (22%)	52,80,113	1.58	7 (13%)
37	LMG	m	102	-	40,40,55	0.86	1 (2%)	48,48,63	1.30	5 (10%)
31	CLA	P	609	-	42,47,73	1.44	9 (21%)	53,81,113	1.56	5 (9%)
31	CLA	c	510	-	69,73,73	1.14	8 (11%)	82,113,113	1.33	8 (9%)
31	CLA	5	307	-	65,69,73	1.20	7 (10%)	77,108,113	1.32	6 (7%)
41	HEM	F	101	5,6	50,50,50	1.35	8 (16%)	67,82,82	1.02	1 (1%)
31	CLA	1	215	-	40,46,73	1.45	8 (20%)	52,80,113	1.51	5 (9%)
31	CLA	9	206	-	39,45,73	1.48	9 (23%)	49,78,113	1.50	5 (10%)
31	CLA	3	308	-	40,43,73	1.57	11 (27%)	46,73,113	2.00	5 (10%)
31	CLA	0	310	23	59,63,73	1.26	9 (15%)	70,101,113	1.34	6 (8%)
31	CLA	C	513	-	68,72,73	1.16	9 (13%)	80,111,113	1.27	6 (7%)
31	CLA	0	311	-	49,53,73	1.38	9 (18%)	58,89,113	1.47	4 (6%)
33	BCR	c	517	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	8 (14%)
36	LHG	d	411	-	33,33,48	0.73	2 (6%)	36,39,54	1.34	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	PHO	a	405	-	58,69,69	2.14	10 (17%)	55,99,99	1.52	8 (14%)
33	BCR	a	408	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	6 (10%)
31	CLA	6	209	-	48,52,73	1.48	9 (18%)	59,88,113	1.45	6 (10%)
31	CLA	8	306	-	35,41,73	1.74	10 (28%)	47,72,113	1.65	8 (17%)
31	CLA	4	211	-	37,42,73	1.64	10 (27%)	47,74,113	1.50	5 (10%)
31	CLA	w	202	19	49,53,73	1.36	10 (20%)	58,89,113	1.46	7 (12%)
37	LMG	C	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.05	4 (6%)
31	CLA	B	512	-	45,49,73	1.37	7 (15%)	54,84,113	1.57	8 (14%)
31	CLA	2	309	24	63,67,73	1.21	9 (14%)	74,105,113	1.33	7 (9%)
31	CLA	5	304	-	45,49,73	1.40	8 (17%)	54,84,113	1.51	6 (11%)
39	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.42	10 (12%)
42	A86	5	301	-	47,50,50	1.61	5 (10%)	51,76,76	3.00	18 (35%)
31	CLA	p	601	26	39,44,73	1.51	8 (20%)	50,77,113	1.69	7 (14%)
39	DGD	h	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.42	10 (12%)
31	CLA	8	312	-	44,49,73	1.40	7 (15%)	50,84,113	1.42	4 (8%)
44	DD6	7	304	-	40,45,45	1.58	2 (5%)	51,67,67	2.45	15 (29%)
31	CLA	d	404	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
31	CLA	P	602	-	45,49,73	1.39	9 (20%)	54,84,113	1.60	9 (16%)
31	CLA	3	309	-	43,48,73	1.40	8 (18%)	51,83,113	1.69	6 (11%)
31	CLA	0	307	-	65,69,73	1.21	8 (12%)	77,108,113	1.33	6 (7%)
42	A86	9	201	-	47,50,50	1.68	6 (12%)	51,76,76	3.94	22 (43%)
31	CLA	1	212	-	45,49,73	1.41	7 (15%)	54,84,113	1.48	6 (11%)
31	CLA	7	308	-	48,52,73	1.48	9 (18%)	59,88,113	1.45	6 (10%)
35	PL9	a	410	-	32,32,55	1.09	4 (12%)	39,40,69	1.57	9 (23%)
31	CLA	2	313	24	40,46,73	1.47	7 (17%)	52,80,113	1.49	6 (11%)
31	CLA	0	313	23	40,46,73	1.46	8 (20%)	52,80,113	1.52	5 (9%)
31	CLA	B	509	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
31	CLA	6	215	-	40,46,73	1.45	8 (20%)	52,80,113	1.51	5 (9%)
37	LMG	M	102	-	40,40,55	0.86	1 (2%)	48,48,63	1.30	4 (8%)
31	CLA	P	608	-	41,46,73	1.55	10 (24%)	49,80,113	1.52	8 (16%)
44	DD6	3	303	-	40,45,45	1.61	3 (7%)	51,67,67	2.83	16 (31%)
42	A86	5	303	-	47,50,50	1.53	7 (14%)	51,76,76	2.74	22 (43%)
31	CLA	6	207	-	48,52,73	1.48	9 (18%)	59,88,113	1.41	6 (10%)
33	BCR	A	408	-	41,41,41	1.17	2 (4%)	56,56,56	1.17	6 (10%)
31	CLA	9	204	-	40,46,73	1.46	9 (22%)	52,80,113	1.52	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LHG	a	411	-	42,42,48	0.70	1 (2%)	45,48,54	1.29	5 (11%)
31	CLA	7	305	-	45,49,73	1.41	8 (17%)	54,84,113	1.51	6 (11%)
31	CLA	1	214	25	40,46,73	1.45	8 (20%)	52,80,113	1.53	7 (13%)
31	CLA	C	507	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
36	LHG	d	412	-	27,27,48	0.89	2 (7%)	30,32,54	1.77	4 (13%)
31	CLA	P	604	-	43,48,73	1.40	9 (20%)	51,83,113	1.58	7 (13%)
31	CLA	c	513	-	68,72,73	1.16	8 (11%)	80,111,113	1.26	6 (7%)
42	A86	0	301	-	47,50,50	1.61	5 (10%)	51,76,76	3.00	18 (35%)
31	CLA	2	316	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	6 (11%)
37	LMG	d	410	-	40,40,55	0.94	3 (7%)	48,48,63	1.36	6 (12%)
31	CLA	5	311	-	49,53,73	1.37	9 (18%)	58,89,113	1.47	4 (6%)
31	CLA	5	305	23	65,69,73	1.21	9 (13%)	77,108,113	1.33	6 (7%)
31	CLA	5	308	-	65,69,73	1.21	8 (12%)	77,108,113	1.33	6 (7%)
31	CLA	p	608	-	41,46,73	1.56	10 (24%)	49,80,113	1.54	8 (16%)
31	CLA	2	311	-	47,51,73	1.38	8 (17%)	55,86,113	1.38	6 (10%)
29	OEX	A	401	3,1	0,15,15	-	-	-		
31	CLA	b	505	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	6 (7%)
31	CLA	d	403	-	66,70,73	1.27	10 (15%)	80,109,113	1.34	8 (10%)
33	BCR	d	405	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	7 (12%)
31	CLA	b	502	-	47,51,73	1.37	8 (17%)	55,86,113	1.46	4 (7%)
31	CLA	9	209	-	45,49,73	1.37	9 (20%)	54,84,113	1.56	5 (9%)
35	PL9	A	410	-	32,32,55	1.09	4 (12%)	39,40,69	1.57	9 (23%)
33	BCR	H	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	6 (10%)
31	CLA	3	310	-	40,43,73	1.58	10 (25%)	48,75,113	1.61	5 (10%)
33	BCR	B	517	-	41,41,41	1.21	2 (4%)	56,56,56	1.26	7 (12%)
31	CLA	b	503	-	64,69,73	1.18	8 (12%)	73,106,113	1.26	5 (6%)
31	CLA	b	513	-	45,49,73	1.36	7 (15%)	54,84,113	1.57	8 (14%)
37	LMG	D	410	-	40,40,55	0.94	3 (7%)	48,48,63	1.36	6 (12%)
31	CLA	B	508	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
31	CLA	5	309	23	45,49,73	1.40	8 (17%)	54,84,113	1.50	6 (11%)
31	CLA	c	512	3	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
37	LMG	0	315	-	48,48,55	0.77	0	56,56,63	1.29	6 (10%)
36	LHG	H	103	-	41,41,48	0.66	1 (2%)	44,47,54	1.17	3 (6%)
42	A86	3	302	-	47,50,50	1.81	7 (14%)	51,76,76	3.04	24 (47%)
34	SQD	0	316	-	46,48,54	1.04	6 (13%)	56,59,65	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	C	505	-	68,72,73	1.16	8 (11%)	80,111,113	1.30	4 (5%)
31	CLA	1	213	25	43,48,73	1.43	8 (18%)	51,83,113	1.44	5 (9%)
36	LHG	A	412	-	42,42,48	0.70	1 (2%)	45,48,54	1.29	5 (11%)
31	CLA	6	211	25	59,63,73	1.26	9 (15%)	70,101,113	1.33	6 (8%)
33	BCR	B	518	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	7 (12%)
33	BCR	C	516	-	41,41,41	1.16	2 (4%)	56,56,56	1.30	8 (14%)
31	CLA	8	304	-	39,42,73	1.66	12 (30%)	49,74,113	1.62	7 (14%)
31	CLA	p	609	-	42,47,73	1.44	9 (21%)	53,81,113	1.56	7 (13%)
31	CLA	4	213	-	37,43,73	1.66	10 (27%)	49,76,113	1.69	10 (20%)
31	CLA	D	403	-	66,70,73	1.28	10 (15%)	80,109,113	1.34	8 (10%)
31	CLA	b	507	-	69,73,73	1.15	8 (11%)	82,113,113	1.33	6 (7%)
31	CLA	3	313	-	41,47,73	1.43	10 (24%)	51,81,113	1.47	4 (7%)
31	CLA	b	516	-	69,73,73	1.17	9 (13%)	82,113,113	1.32	6 (7%)
31	CLA	b	511	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
37	LMG	d	409	-	37,37,55	0.78	0	45,45,63	1.33	7 (15%)
31	CLA	1	209	-	48,52,73	1.49	9 (18%)	59,88,113	1.45	6 (10%)
31	CLA	c	502	-	69,73,73	1.14	8 (11%)	82,113,113	1.32	6 (7%)
42	A86	8	301	-	47,50,50	1.77	9 (19%)	51,76,76	4.95	22 (43%)
31	CLA	b	504	-	68,72,73	1.17	9 (13%)	80,111,113	1.28	6 (7%)
31	CLA	7	306	24	49,53,73	1.36	8 (16%)	58,89,113	1.44	4 (6%)
34	SQD	A	411	-	52,54,54	0.94	2 (3%)	62,65,65	1.60	12 (19%)
31	CLA	1	216	25	40,46,73	1.45	6 (15%)	52,80,113	1.47	5 (9%)
29	OEX	a	401	3,1	0,15,15	-	-	-		
31	CLA	3	312	-	44,49,73	1.40	8 (18%)	50,84,113	1.43	4 (8%)
31	CLA	1	207	-	48,52,73	1.49	9 (18%)	59,88,113	1.41	6 (10%)
36	LHG	D	412	-	27,27,48	0.89	2 (7%)	30,32,54	1.76	4 (13%)
42	A86	8	302	-	47,50,50	1.81	7 (14%)	51,76,76	3.03	24 (47%)
36	LHG	A	413	-	25,25,48	0.83	1 (4%)	28,31,54	1.31	2 (7%)
31	CLA	3	307	-	46,50,73	1.37	10 (21%)	55,84,113	1.42	5 (9%)
33	BCR	c	516	-	41,41,41	1.16	2 (4%)	56,56,56	1.31	8 (14%)
31	CLA	3	304	-	39,42,73	1.66	12 (30%)	49,74,113	1.63	7 (14%)
31	CLA	a	403	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	8 (9%)
31	CLA	9	210	-	40,46,73	1.44	9 (22%)	52,80,113	1.57	7 (13%)
31	CLA	1	201	-	48,52,73	1.48	9 (18%)	59,88,113	1.48	7 (11%)
44	DD6	6	204	-	40,45,45	1.72	3 (7%)	51,67,67	2.31	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	8	310	-	40,43,73	1.58	10 (25%)	48,75,113	1.61	5 (10%)
33	BCR	C	517	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)
35	PL9	d	406	-	55,55,55	1.32	5 (9%)	68,69,69	1.53	12 (17%)
31	CLA	8	311	28	43,48,73	1.43	8 (18%)	51,83,113	1.57	6 (11%)
41	HEM	V	201	18	50,50,50	1.29	5 (10%)	67,82,82	1.27	5 (7%)
33	BCR	D	405	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	7 (12%)
31	CLA	c	506	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	8 (9%)
31	CLA	4	204	-	40,46,73	1.46	9 (22%)	52,80,113	1.53	5 (9%)
37	LMG	b	521	-	28,28,55	0.95	1 (3%)	36,36,63	1.35	7 (19%)
31	CLA	7	307	-	51,55,73	1.33	9 (17%)	60,91,113	1.44	5 (8%)
31	CLA	7	312	24	39,44,73	1.56	10 (25%)	50,77,113	1.60	10 (20%)
31	CLA	0	305	23	65,69,73	1.21	9 (13%)	77,108,113	1.34	6 (7%)
44	DD6	p	611	-	40,45,45	1.54	2 (5%)	51,67,67	1.87	14 (27%)
31	CLA	D	401	-	63,67,73	1.20	8 (12%)	74,105,113	1.37	7 (9%)
42	A86	0	317	-	47,50,50	1.54	5 (10%)	51,76,76	2.60	17 (33%)
31	CLA	0	306	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	4 (6%)
31	CLA	5	310	23	59,63,73	1.26	9 (15%)	70,101,113	1.33	6 (8%)
33	BCR	B	519	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	8 (14%)
40	BCT	D	402	30	3,3,3	1.11	0	2,3,3	4.14	2 (100%)
42	A86	2	302	-	47,50,50	1.79	7 (14%)	51,76,76	2.85	17 (33%)
42	A86	9	202	-	47,50,50	1.85	7 (14%)	51,76,76	3.72	28 (54%)
31	CLA	B	507	-	45,49,73	1.40	9 (20%)	54,84,113	1.51	6 (11%)
33	BCR	h	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)
31	CLA	0	308	-	65,69,73	1.21	9 (13%)	77,108,113	1.32	6 (7%)
31	CLA	B	501	-	47,51,73	1.37	8 (17%)	55,86,113	1.45	4 (7%)
32	PHO	A	405	-	58,69,69	2.14	10 (17%)	55,99,99	1.53	8 (14%)
31	CLA	5	312	-	46,50,73	1.40	8 (17%)	53,85,113	1.44	4 (7%)
37	LMG	d	408	-	46,46,55	0.76	1 (2%)	54,54,63	1.34	7 (12%)
31	CLA	C	508	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	4 (4%)
31	CLA	B	502	-	64,69,73	1.18	9 (14%)	73,106,113	1.25	5 (6%)
31	CLA	7	314	-	40,46,73	1.47	8 (20%)	52,80,113	1.51	6 (11%)
31	CLA	P	603	-	39,45,73	1.48	9 (23%)	51,79,113	1.65	7 (13%)
31	CLA	b	512	-	68,72,73	1.18	9 (13%)	80,111,113	1.33	7 (8%)
31	CLA	P	601	26	39,44,73	1.51	8 (20%)	50,77,113	1.67	7 (14%)
31	CLA	9	208	-	43,48,73	1.45	10 (23%)	51,83,113	1.61	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	b	506	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
31	CLA	7	315	24	40,46,73	1.47	8 (20%)	52,80,113	1.51	6 (11%)
37	LMG	Y	101	-	46,46,55	0.75	1 (2%)	54,54,63	1.39	11 (20%)
37	LMG	W	201	-	48,48,55	0.76	1 (2%)	56,56,63	1.34	7 (12%)
31	CLA	C	506	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	8 (9%)
31	CLA	4	212	-	40,44,73	1.60	10 (25%)	51,77,113	1.53	6 (11%)
31	CLA	b	514	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	8 (9%)
44	DD6	1	204	-	40,45,45	1.71	3 (7%)	51,67,67	2.30	14 (27%)
42	A86	2	301	-	47,50,50	1.54	5 (10%)	51,76,76	2.59	18 (35%)

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
31	CLA	7	309	24	1/1/13/20	10/32/108/115	-
37	LMG	y	101	-	-	18/41/61/70	0/1/1/1
39	DGD	C	518	-	-	19/44/84/95	0/2/2/2
31	CLA	8	309	-	1/1/10/20	3/8/84/115	-
31	CLA	9	213	-	1/1/8/20	-	-
32	PHO	a	406	-	-	11/37/103/103	0/5/6/6
31	CLA	B	505	-	1/1/15/20	10/39/115/115	-
31	CLA	4	205	-	1/1/7/20	0/2/70/115	-
31	CLA	B	516	-	1/1/15/20	13/39/115/115	-
42	A86	1	202	-	-	7/34/90/90	0/3/3/3
31	CLA	6	212	-	1/1/10/20	2/10/86/115	-
36	LHG	d	407	-	-	22/47/51/53	-
34	SQD	B	522	-	-	18/49/69/69	0/1/1/1
42	A86	6	202	-	-	7/34/90/90	0/3/3/3
42	A86	4	203	-	-	6/34/90/90	0/3/3/3
44	DD6	2	303	-	-	2/26/80/80	0/3/3/3
31	CLA	2	305	-	1/1/10/20	4/10/86/115	-
35	PL9	D	406	-	-	8/53/73/73	0/1/1/1
31	CLA	C	502	-	1/1/15/20	12/39/115/115	-
31	CLA	c	504	-	1/1/12/20	4/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	0	312	-	1/1/10/20	6/12/88/115	-
31	CLA	1	210	25	1/1/15/20	16/39/115/115	-
31	CLA	8	314	-	1/1/8/20	-	-
37	LMG	D	409	-	-	13/32/52/70	0/1/1/1
31	CLA	6	214	25	1/1/9/20	0/4/80/115	-
31	CLA	3	306	-	1/1/7/20	-	-
42	A86	9	203	-	-	6/34/90/90	0/3/3/3
37	LMG	5	315	-	-	26/43/63/70	0/1/1/1
44	DD6	6	203	-	-	2/26/80/80	0/3/3/3
31	CLA	B	514	-	1/1/13/20	12/33/109/115	-
31	CLA	6	216	25	1/1/9/20	2/4/80/115	-
31	CLA	4	207	-	1/1/9/20	2/4/80/115	-
31	CLA	c	509	-	1/1/15/20	11/39/115/115	-
31	CLA	a	404	-	1/1/11/20	1/20/96/115	-
31	CLA	1	206	25	1/1/11/20	6/15/91/115	-
42	A86	7	301	-	-	8/34/90/90	0/3/3/3
42	A86	P	610	-	-	9/34/90/90	0/3/3/3
31	CLA	3	311	28	1/1/10/20	2/8/84/115	-
31	CLA	W	202	19	1/1/11/20	3/15/91/115	-
33	BCR	k	101	-	-	14/29/63/63	0/2/2/2
36	LHG	B	521	-	-	18/53/53/53	-
31	CLA	7	316	-	1/1/10/20	2/10/86/115	-
31	CLA	8	308	-	1/1/6/20	4/6/66/115	-
37	LMG	J	101	-	-	29/45/65/70	0/1/1/1
31	CLA	3	314	-	1/1/8/20	-	-
31	CLA	C	510	-	1/1/15/20	5/39/115/115	-
31	CLA	9	212	-	1/1/8/20	0/2/74/115	-
31	CLA	B	511	-	1/1/14/20	12/37/113/115	-
31	CLA	1	208	-	1/1/11/20	6/18/94/115	-
31	CLA	9	211	-	1/1/7/20	-	-
31	CLA	5	313	23	1/1/9/20	2/4/80/115	-
31	CLA	9	207	-	1/1/9/20	2/4/80/115	-
31	CLA	z	101	-	1/1/12/20	8/23/99/115	-
31	CLA	b	517	-	1/1/15/20	13/39/115/115	-
31	CLA	4	206	-	1/1/8/20	2/4/76/115	-
31	CLA	9	205	-	1/1/7/20	0/2/70/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	a	412	-	-	11/29/29/53	-
43	ET4	0	302	-	-	9/25/67/67	0/2/2/2
37	LMG	w	201	-	-	26/43/63/70	0/1/1/1
33	BCR	b	518	-	-	4/29/63/63	0/2/2/2
42	A86	7	302	-	-	8/34/90/90	0/3/3/3
31	CLA	2	306	24	1/1/11/20	3/15/91/115	-
31	CLA	A	404	-	1/1/11/20	1/20/96/115	-
33	BCR	K	101	-	-	14/29/63/63	0/2/2/2
37	LMG	c	521	-	-	26/46/66/70	0/1/1/1
31	CLA	A	407	-	1/1/14/20	4/33/109/115	-
31	CLA	c	507	-	1/1/11/20	4/15/91/115	-
42	A86	3	301	-	-	12/34/90/90	0/3/3/3
31	CLA	p	604	-	1/1/10/20	2/8/84/115	-
31	CLA	C	512	3	1/1/15/20	8/39/115/115	-
44	DD6	1	203	-	-	2/26/80/80	0/3/3/3
43	ET4	5	302	-	-	9/25/67/67	0/2/2/2
31	CLA	c	511	-	1/1/15/20	12/39/115/115	-
31	CLA	8	305	-	1/1/10/20	3/10/86/115	-
31	CLA	1	211	25	1/1/13/20	5/27/103/115	-
31	CLA	b	510	-	1/1/15/20	10/39/115/115	-
31	CLA	2	315	24	1/1/9/20	2/4/80/115	-
37	LMG	D	408	-	-	16/41/61/70	0/1/1/1
31	CLA	5	306	-	1/1/11/20	3/15/91/115	-
31	CLA	c	514	-	1/1/11/20	5/20/96/115	-
39	DGD	c	518	-	-	19/44/84/95	0/2/2/2
32	PHO	A	406	-	-	11/37/103/103	0/5/6/6
42	A86	0	303	-	-	5/34/90/90	0/3/3/3
31	CLA	p	607	-	1/1/8/20	0/2/74/115	-
31	CLA	0	314	23	1/1/9/20	0/4/80/115	-
36	LHG	D	411	-	-	26/38/38/53	-
31	CLA	7	311	-	1/1/10/20	5/13/89/115	-
33	BCR	C	515	-	-	0/29/63/63	0/2/2/2
34	SQD	A	409	-	-	14/49/69/69	0/1/1/1
31	CLA	p	603	-	1/1/9/20	0/2/78/115	-
31	CLA	B	515	-	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	7	313	24	1/1/9/20	2/4/80/115	-
31	CLA	6	205	-	1/1/10/20	2/10/86/115	-
31	CLA	8	307	-	1/1/9/20	2/11/83/115	-
31	CLA	p	606	-	1/1/8/20	2/4/76/115	-
31	CLA	0	304	-	1/1/10/20	4/10/86/115	-
31	CLA	b	515	-	1/1/13/20	12/33/109/115	-
41	HEM	v	201	18	-	6/14/54/54	-
39	DGD	c	520	-	-	8/51/91/95	0/2/2/2
31	CLA	2	307	-	1/1/11/20	3/18/94/115	-
31	CLA	A	403	-	1/1/15/20	10/39/115/115	-
31	CLA	C	509	-	1/1/15/20	11/39/115/115	-
36	LHG	b	522	-	-	18/53/53/53	-
31	CLA	7	310	24	1/1/13/20	10/27/103/115	-
42	A86	4	201	-	-	7/34/90/90	1/3/3/3
31	CLA	2	314	-	1/1/9/20	0/4/80/115	-
44	DD6	2	304	-	-	10/26/80/80	0/3/3/3
31	CLA	c	505	-	1/1/14/20	9/37/113/115	-
31	CLA	6	213	25	1/1/10/20	5/8/84/115	-
31	CLA	B	503	-	1/1/14/20	11/37/113/115	-
33	BCR	b	519	-	-	4/29/63/63	0/2/2/2
31	CLA	2	308	-	1/1/11/20	7/13/89/115	-
33	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	CLA	4	209	-	1/1/10/20	4/10/86/115	-
39	DGD	C	519	-	-	22/51/91/95	0/2/2/2
31	CLA	3	305	-	1/1/10/20	3/10/86/115	-
31	CLA	6	206	25	1/1/11/20	6/15/91/115	-
44	DD6	7	303	-	-	2/26/80/80	0/3/3/3
39	DGD	C	520	-	-	8/51/91/95	0/2/2/2
31	CLA	P	605	-	1/1/9/20	2/2/78/115	-
31	CLA	c	508	-	1/1/15/20	15/39/115/115	-
31	CLA	2	310	24	1/1/13/20	10/27/103/115	-
34	SQD	5	316	-	-	18/43/63/69	0/1/1/1
31	CLA	1	205	-	1/1/10/20	2/10/86/115	-
34	SQD	B	523	-	-	14/35/55/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	0	309	23	1/1/10/20	4/10/86/115	-
34	SQD	b	501	-	-	14/35/55/69	0/1/1/1
37	LMG	B	520	-	-	5/23/43/70	0/1/1/1
31	CLA	P	606	-	1/1/8/20	2/4/76/115	-
37	LMG	m	101	-	-	18/46/66/70	0/1/1/1
31	CLA	B	513	-	1/1/15/20	7/39/115/115	-
31	CLA	6	201	-	1/1/11/20	4/13/89/115	-
34	SQD	a	409	-	-	14/49/69/69	0/1/1/1
42	A86	p	610	-	-	9/34/90/90	0/3/3/3
39	DGD	c	519	-	-	22/51/91/95	0/2/2/2
31	CLA	p	602	-	1/1/10/20	2/10/86/115	-
31	CLA	C	503	-	1/1/14/20	14/37/113/115	-
31	CLA	d	401	-	1/1/13/20	2/32/108/115	-
36	LHG	h	103	-	-	10/46/46/53	-
31	CLA	6	210	25	1/1/15/20	16/39/115/115	-
31	CLA	B	510	-	1/1/15/20	8/39/115/115	-
44	DD6	P	611	-	-	5/26/80/80	0/3/3/3
31	CLA	4	208	-	1/1/10/20	2/8/84/115	-
42	A86	4	202	-	-	7/34/90/90	0/3/3/3
31	CLA	C	514	-	1/1/11/20	5/20/96/115	-
31	CLA	B	504	-	1/1/15/20	12/39/115/115	-
31	CLA	6	208	-	1/1/11/20	6/18/94/115	-
31	CLA	8	313	-	1/1/9/20	3/6/82/115	-
31	CLA	Z	101	-	1/1/12/20	8/23/99/115	-
44	DD6	8	303	-	-	2/26/80/80	0/3/3/3
31	CLA	C	511	-	1/1/15/20	12/39/115/115	-
31	CLA	B	506	-	1/1/15/20	6/39/115/115	-
31	CLA	a	407	-	1/1/14/20	4/33/109/115	-
41	HEM	f	101	5,6	-	4/14/54/54	-
31	CLA	C	504	-	1/1/12/20	4/23/99/115	-
37	LMG	M	101	-	-	18/46/66/70	0/1/1/1
31	CLA	2	312	24	1/1/9/20	0/2/78/115	-
31	CLA	P	607	-	1/1/8/20	0/2/74/115	-
31	CLA	5	314	23	1/1/9/20	0/4/80/115	-
37	LMG	j	101	-	-	29/45/65/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	508	-	1/1/10/20	2/10/86/115	-
31	CLA	c	503	-	1/1/14/20	14/37/113/115	-
42	A86	5	317	-	-	8/34/90/90	0/3/3/3
31	CLA	D	404	-	1/1/15/20	8/39/115/115	-
36	LHG	D	407	-	-	22/47/51/53	-
33	BCR	b	520	-	-	8/29/63/63	0/2/2/2
31	CLA	b	509	-	1/1/15/20	7/39/115/115	-
31	CLA	p	605	-	1/1/9/20	2/2/78/115	-
31	CLA	4	210	-	1/1/9/20	0/4/80/115	-
37	LMG	m	102	-	-	12/35/55/70	0/1/1/1
31	CLA	P	609	-	1/1/9/20	2/6/82/115	-
31	CLA	c	510	-	1/1/15/20	5/39/115/115	-
31	CLA	5	307	-	1/1/14/20	20/35/111/115	-
41	HEM	F	101	5,6	-	4/14/54/54	-
31	CLA	1	215	-	1/1/9/20	0/4/80/115	-
31	CLA	9	206	-	1/1/8/20	2/4/76/115	-
31	CLA	3	308	-	1/1/6/20	4/6/66/115	-
31	CLA	0	310	23	1/1/13/20	5/27/103/115	-
31	CLA	C	513	-	1/1/14/20	17/37/113/115	-
31	CLA	0	311	-	1/1/11/20	9/15/91/115	-
33	BCR	c	517	-	-	2/29/63/63	0/2/2/2
36	LHG	d	411	-	-	26/38/38/53	-
32	PHO	a	405	-	-	10/37/103/103	0/5/6/6
33	BCR	a	408	-	-	1/29/63/63	0/2/2/2
31	CLA	6	209	-	1/1/11/20	6/13/89/115	-
31	CLA	8	306	-	1/1/7/20	-	-
31	CLA	4	211	-	1/1/7/20	-	-
31	CLA	w	202	19	1/1/11/20	3/15/91/115	-
37	LMG	C	521	-	-	26/46/66/70	0/1/1/1
31	CLA	B	512	-	1/1/10/20	0/10/86/115	-
31	CLA	2	309	24	1/1/13/20	10/32/108/115	-
31	CLA	5	304	-	1/1/10/20	4/10/86/115	-
39	DGD	H	102	-	-	16/51/91/95	0/2/2/2
42	A86	5	301	-	-	9/34/90/90	0/3/3/3
31	CLA	p	601	26	1/1/9/20	2/2/78/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGD	h	102	-	-	16/51/91/95	0/2/2/2
31	CLA	8	312	-	1/1/10/20	4/10/86/115	-
44	DD6	7	304	-	-	10/26/80/80	0/3/3/3
31	CLA	d	404	-	1/1/15/20	8/39/115/115	-
31	CLA	P	602	-	1/1/10/20	2/10/86/115	-
31	CLA	3	309	-	1/1/10/20	3/8/84/115	-
31	CLA	0	307	-	1/1/14/20	20/35/111/115	-
42	A86	9	201	-	-	7/34/90/90	1/3/3/3
31	CLA	1	212	-	1/1/10/20	2/10/86/115	-
31	CLA	7	308	-	1/1/11/20	7/13/89/115	-
35	PL9	a	410	-	-	13/25/45/73	0/1/1/1
31	CLA	2	313	24	1/1/9/20	2/4/80/115	-
31	CLA	0	313	23	1/1/9/20	2/4/80/115	-
31	CLA	B	509	-	1/1/15/20	10/39/115/115	-
31	CLA	6	215	-	1/1/9/20	0/4/80/115	-
37	LMG	M	102	-	-	12/35/55/70	0/1/1/1
31	CLA	P	608	-	1/1/9/20	3/6/78/115	-
44	DD6	3	303	-	-	3/26/80/80	0/3/3/3
42	A86	5	303	-	-	5/34/90/90	0/3/3/3
31	CLA	6	207	-	1/1/11/20	5/13/89/115	-
33	BCR	A	408	-	-	1/29/63/63	0/2/2/2
31	CLA	9	204	-	1/1/9/20	2/4/80/115	-
36	LHG	a	411	-	-	13/47/47/53	-
31	CLA	7	305	-	1/1/10/20	4/10/86/115	-
31	CLA	1	214	25	1/1/9/20	0/4/80/115	-
31	CLA	C	507	-	1/1/11/20	4/15/91/115	-
36	LHG	d	412	-	-	17/29/29/53	-
31	CLA	P	604	-	1/1/10/20	2/8/84/115	-
31	CLA	c	513	-	1/1/14/20	17/37/113/115	-
42	A86	0	301	-	-	9/34/90/90	0/3/3/3
31	CLA	2	316	-	1/1/10/20	2/10/86/115	-
37	LMG	d	410	-	-	16/35/55/70	0/1/1/1
31	CLA	5	311	-	1/1/11/20	9/15/91/115	-
31	CLA	5	305	23	1/1/14/20	13/35/111/115	-
31	CLA	5	308	-	1/1/14/20	9/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	p	608	-	1/1/9/20	2/6/78/115	-
31	CLA	2	311	-	1/1/10/20	5/13/89/115	-
31	CLA	b	505	-	1/1/15/20	12/39/115/115	-
31	CLA	d	403	-	1/1/14/20	5/33/109/115	-
33	BCR	d	405	-	-	2/29/63/63	0/2/2/2
31	CLA	b	502	-	1/1/10/20	3/13/89/115	-
31	CLA	9	209	-	1/1/10/20	4/10/86/115	-
35	PL9	A	410	-	-	13/25/45/73	0/1/1/1
33	BCR	H	101	-	-	4/29/63/63	0/2/2/2
31	CLA	3	310	-	1/1/8/20	0/2/74/115	-
33	BCR	B	517	-	-	4/29/63/63	0/2/2/2
31	CLA	b	503	-	1/1/12/20	14/29/107/115	-
31	CLA	b	513	-	1/1/10/20	0/10/86/115	-
37	LMG	D	410	-	-	16/35/55/70	0/1/1/1
31	CLA	B	508	-	1/1/15/20	7/39/115/115	-
31	CLA	5	309	23	1/1/10/20	4/10/86/115	-
31	CLA	c	512	3	1/1/15/20	8/39/115/115	-
37	LMG	0	315	-	-	26/43/63/70	0/1/1/1
36	LHG	H	103	-	-	10/46/46/53	-
42	A86	3	302	-	-	6/34/90/90	0/3/3/3
34	SQD	0	316	-	-	18/43/63/69	0/1/1/1
31	CLA	C	505	-	1/1/14/20	9/37/113/115	-
31	CLA	1	213	25	1/1/10/20	5/8/84/115	-
36	LHG	A	412	-	-	13/47/47/53	-
31	CLA	6	211	25	1/1/13/20	5/27/103/115	-
33	BCR	B	518	-	-	4/29/63/63	0/2/2/2
33	BCR	C	516	-	-	4/29/63/63	0/2/2/2
31	CLA	8	304	-	1/1/8/20	-	-
31	CLA	p	609	-	1/1/9/20	2/6/82/115	-
31	CLA	4	213	-	1/1/8/20	-	-
31	CLA	D	403	-	1/1/14/20	5/33/109/115	-
31	CLA	b	507	-	1/1/15/20	5/39/115/115	-
31	CLA	3	313	-	1/1/9/20	3/6/82/115	-
31	CLA	b	516	-	1/1/15/20	6/39/115/115	-
31	CLA	b	511	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	d	409	-	-	13/32/52/70	0/1/1/1
31	CLA	1	209	-	1/1/11/20	6/13/89/115	-
31	CLA	c	502	-	1/1/15/20	12/39/115/115	-
42	A86	8	301	-	-	12/34/90/90	0/3/3/3
31	CLA	b	504	-	1/1/14/20	11/37/113/115	-
31	CLA	7	306	24	1/1/11/20	3/15/91/115	-
34	SQD	A	411	-	-	18/49/69/69	0/1/1/1
31	CLA	1	216	25	1/1/9/20	2/4/80/115	-
31	CLA	3	312	-	1/1/10/20	4/10/86/115	-
31	CLA	1	207	-	1/1/11/20	5/13/89/115	-
36	LHG	D	412	-	-	17/29/29/53	-
42	A86	8	302	-	-	6/34/90/90	0/3/3/3
36	LHG	A	413	-	-	11/29/29/53	-
31	CLA	3	307	-	1/1/9/20	2/11/83/115	-
33	BCR	c	516	-	-	4/29/63/63	0/2/2/2
31	CLA	3	304	-	1/1/8/20	-	-
31	CLA	a	403	-	1/1/15/20	10/39/115/115	-
31	CLA	9	210	-	1/1/9/20	0/4/80/115	-
31	CLA	1	201	-	1/1/11/20	4/13/89/115	-
44	DD6	6	204	-	-	5/26/80/80	0/3/3/3
31	CLA	8	310	-	1/1/8/20	0/2/74/115	-
33	BCR	C	517	-	-	2/29/63/63	0/2/2/2
35	PL9	d	406	-	-	8/53/73/73	0/1/1/1
31	CLA	8	311	28	1/1/10/20	2/8/84/115	-
41	HEM	V	201	18	-	6/14/54/54	-
33	BCR	D	405	-	-	2/29/63/63	0/2/2/2
31	CLA	c	506	-	1/1/15/20	17/39/115/115	-
31	CLA	4	204	-	1/1/9/20	2/4/80/115	-
37	LMG	b	521	-	-	5/23/43/70	0/1/1/1
31	CLA	7	307	-	1/1/11/20	3/18/94/115	-
31	CLA	7	312	24	1/1/9/20	0/2/78/115	-
31	CLA	0	305	23	1/1/14/20	13/35/111/115	-
44	DD6	p	611	-	-	5/26/80/80	0/3/3/3
31	CLA	D	401	-	1/1/13/20	2/32/108/115	-
42	A86	0	317	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	0	306	-	1/1/11/20	3/15/91/115	-
31	CLA	5	310	23	1/1/13/20	5/27/103/115	-
33	BCR	B	519	-	-	8/29/63/63	0/2/2/2
42	A86	2	302	-	-	8/34/90/90	0/3/3/3
42	A86	9	202	-	-	7/34/90/90	0/3/3/3
31	CLA	B	507	-	1/1/10/20	2/10/86/115	-
33	BCR	h	101	-	-	4/29/63/63	0/2/2/2
31	CLA	0	308	-	1/1/14/20	9/35/111/115	-
31	CLA	B	501	-	1/1/10/20	3/13/89/115	-
32	PHO	A	405	-	-	10/37/103/103	0/5/6/6
31	CLA	5	312	-	1/1/10/20	6/12/88/115	-
37	LMG	d	408	-	-	16/41/61/70	0/1/1/1
31	CLA	C	508	-	1/1/15/20	15/39/115/115	-
31	CLA	B	502	-	1/1/12/20	14/29/107/115	-
31	CLA	7	314	-	1/1/9/20	0/4/80/115	-
31	CLA	P	603	-	1/1/9/20	0/2/78/115	-
31	CLA	b	512	-	1/1/14/20	12/37/113/115	-
31	CLA	P	601	26	1/1/9/20	2/2/78/115	-
31	CLA	9	208	-	1/1/10/20	2/8/84/115	-
31	CLA	b	506	-	1/1/15/20	10/39/115/115	-
31	CLA	7	315	24	1/1/9/20	2/4/80/115	-
37	LMG	Y	101	-	-	18/41/61/70	0/1/1/1
37	LMG	W	201	-	-	26/43/63/70	0/1/1/1
31	CLA	C	506	-	1/1/15/20	17/39/115/115	-
31	CLA	4	212	-	1/1/8/20	0/2/74/115	-
31	CLA	b	514	-	1/1/15/20	7/39/115/115	-
44	DD6	1	204	-	-	5/26/80/80	0/3/3/3
42	A86	2	301	-	-	8/34/90/90	0/3/3/3

The worst 5 of 2228 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	406	PHO	C1B-C2B	9.26	1.49	1.39
32	a	406	PHO	C1B-C2B	9.25	1.49	1.39
32	A	405	PHO	C1B-C2B	9.23	1.49	1.39
32	a	405	PHO	C1B-C2B	9.23	1.49	1.39
44	6	204	DD6	C30-C31	-9.20	1.24	1.42

The worst 5 of 2549 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	3	301	A86	C40-C32-C31	-17.41	94.89	110.47
42	8	301	A86	C40-C32-C31	-17.36	94.94	110.47
42	8	301	A86	O1-C20-C19	-16.74	97.80	113.49
42	3	301	A86	O1-C20-C19	-16.71	97.83	113.49
42	9	202	A86	C20-O1-C15	14.55	67.28	61.03

5 of 206 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	403	CLA	ND
31	A	404	CLA	ND
31	A	407	CLA	ND
31	B	501	CLA	ND
31	B	502	CLA	ND

5 of 2419 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	B	501	CLA	CAD-CBD-CGD-O1D
31	B	501	CLA	CAD-CBD-CGD-O2D
31	B	516	CLA	C2B-C3B-CAB-CBB
31	B	516	CLA	C4B-C3B-CAB-CBB
31	C	502	CLA	CAD-CBD-CGD-O1D

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	4	201	A86	C31-C32-C33-C34-C35-C36
42	9	201	A86	C31-C32-C33-C34-C35-C36

217 monomers are involved in 516 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	309	CLA	6	0
37	y	101	LMG	4	0
39	C	518	DGD	1	0
32	a	406	PHO	1	0
31	B	505	CLA	4	0
31	B	516	CLA	5	0
42	1	202	A86	1	0
36	d	407	LHG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	B	522	SQD	2	0
42	6	202	A86	1	0
44	2	303	DD6	18	0
31	2	305	CLA	1	0
35	D	406	PL9	3	0
31	C	502	CLA	3	0
31	1	210	CLA	5	0
31	8	314	CLA	1	0
37	D	409	LMG	2	0
31	6	214	CLA	1	0
37	5	315	LMG	1	0
44	6	203	DD6	1	0
31	B	514	CLA	7	0
31	c	509	CLA	5	0
31	1	206	CLA	4	0
31	3	311	CLA	1	0
31	W	202	CLA	1	0
33	k	101	BCR	2	0
36	B	521	LHG	4	0
31	8	308	CLA	1	0
37	J	101	LMG	3	0
31	3	314	CLA	1	0
31	C	510	CLA	2	0
31	B	511	CLA	1	0
31	5	313	CLA	1	0
31	z	101	CLA	6	0
31	b	517	CLA	4	0
36	a	412	LHG	2	0
37	w	201	LMG	2	0
33	b	518	BCR	5	0
31	2	306	CLA	5	0
33	K	101	BCR	2	0
37	c	521	LMG	4	0
31	c	507	CLA	1	0
31	p	604	CLA	5	0
31	C	512	CLA	3	0
44	1	203	DD6	1	0
31	c	511	CLA	2	0
31	8	305	CLA	1	0
31	1	211	CLA	1	0
31	b	510	CLA	2	0
39	c	518	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	406	PHO	1	0
42	0	303	A86	1	0
31	p	607	CLA	1	0
31	0	314	CLA	3	0
36	D	411	LHG	2	0
33	C	515	BCR	1	0
34	A	409	SQD	3	0
31	p	603	CLA	2	0
31	B	515	CLA	2	0
31	0	304	CLA	3	0
31	b	515	CLA	8	0
41	v	201	HEM	6	0
39	c	520	DGD	6	0
31	2	307	CLA	3	0
31	A	403	CLA	4	0
31	C	509	CLA	5	0
36	b	522	LHG	4	0
31	7	310	CLA	7	0
44	2	304	DD6	6	0
31	c	505	CLA	2	0
31	B	503	CLA	2	0
33	b	519	BCR	2	0
33	c	515	BCR	2	0
39	C	519	DGD	5	0
31	3	305	CLA	1	0
31	6	206	CLA	4	0
44	7	303	DD6	18	0
39	C	520	DGD	7	0
31	c	508	CLA	1	0
31	2	310	CLA	6	0
34	5	316	SQD	5	0
34	B	523	SQD	1	0
34	b	501	SQD	1	0
37	B	520	LMG	1	0
37	m	101	LMG	1	0
31	B	513	CLA	2	0
31	6	201	CLA	2	0
39	c	519	DGD	5	0
31	p	602	CLA	2	0
31	d	401	CLA	1	0
36	h	103	LHG	5	0
31	6	210	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	510	CLA	3	0
44	P	611	DD6	7	0
31	B	504	CLA	7	0
31	8	313	CLA	1	0
31	Z	101	CLA	6	0
44	8	303	DD6	1	0
31	C	511	CLA	2	0
31	B	506	CLA	4	0
41	f	101	HEM	3	0
37	M	101	LMG	1	0
31	2	312	CLA	1	0
31	P	607	CLA	1	0
31	5	314	CLA	3	0
37	j	101	LMG	2	0
31	D	404	CLA	3	0
36	D	407	LHG	5	0
33	b	520	BCR	5	0
31	b	509	CLA	2	0
37	m	102	LMG	1	0
31	c	510	CLA	2	0
31	5	307	CLA	3	0
41	F	101	HEM	3	0
31	3	308	CLA	1	0
31	0	310	CLA	1	0
31	0	311	CLA	2	0
33	c	517	BCR	4	0
36	d	411	LHG	2	0
32	a	405	PHO	2	0
33	a	408	BCR	3	0
31	6	209	CLA	1	0
31	w	202	CLA	1	0
37	C	521	LMG	4	0
31	B	512	CLA	2	0
31	2	309	CLA	6	0
31	5	304	CLA	3	0
39	H	102	DGD	4	0
39	h	102	DGD	4	0
31	8	312	CLA	1	0
44	7	304	DD6	7	0
31	d	404	CLA	3	0
31	P	602	CLA	2	0
31	0	307	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	a	410	PL9	3	0
31	0	313	CLA	1	0
31	B	509	CLA	2	0
37	M	102	LMG	1	0
44	3	303	DD6	1	0
42	5	303	A86	1	0
33	A	408	BCR	3	0
36	a	411	LHG	2	0
31	7	305	CLA	1	0
31	1	214	CLA	1	0
31	C	507	CLA	1	0
36	d	412	LHG	2	0
31	P	604	CLA	5	0
37	d	410	LMG	2	0
31	5	311	CLA	2	0
31	5	305	CLA	3	0
31	5	308	CLA	6	0
31	b	505	CLA	7	0
33	d	405	BCR	1	0
31	b	502	CLA	1	0
35	A	410	PL9	3	0
33	H	101	BCR	2	0
31	3	310	CLA	1	0
33	B	517	BCR	7	0
31	b	503	CLA	1	0
31	b	513	CLA	1	0
37	D	410	LMG	2	0
31	B	508	CLA	3	0
31	c	512	CLA	3	0
37	0	315	LMG	1	0
36	H	103	LHG	6	0
34	0	316	SQD	5	0
31	C	505	CLA	2	0
36	A	412	LHG	2	0
31	6	211	CLA	2	0
33	B	518	BCR	2	0
33	C	516	BCR	1	0
31	b	507	CLA	3	0
31	3	313	CLA	1	0
31	b	516	CLA	2	0
31	b	511	CLA	3	0
37	d	409	LMG	3	0

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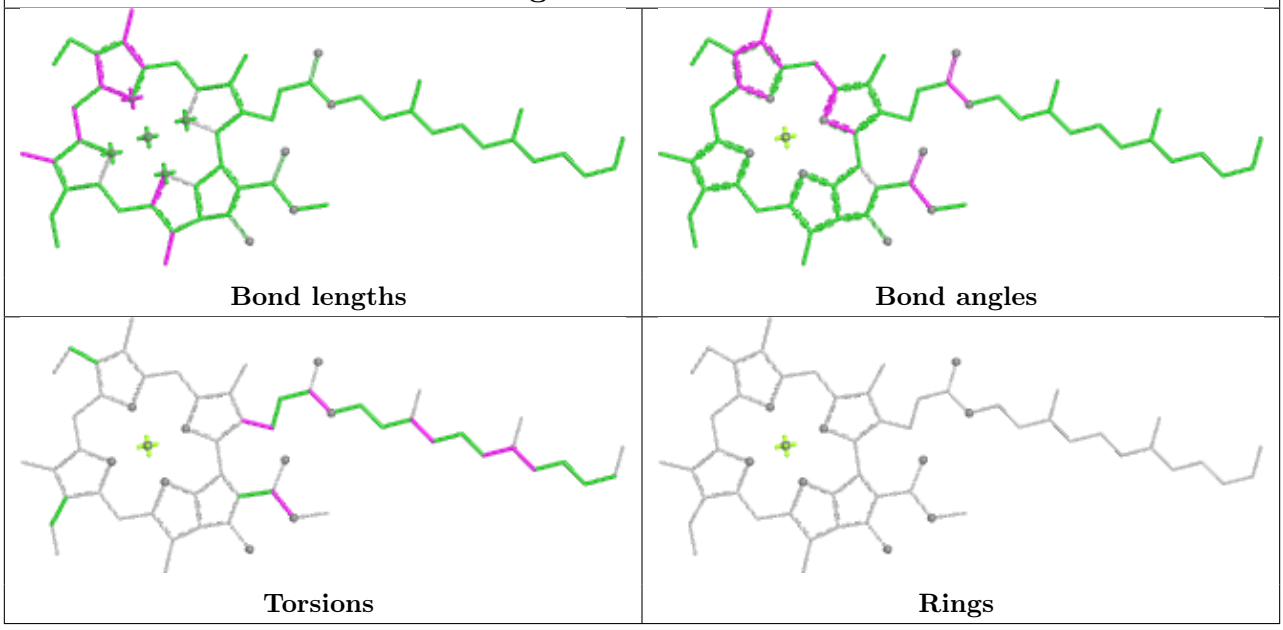
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	1	209	CLA	1	0
31	c	502	CLA	3	0
31	b	504	CLA	2	0
31	7	306	CLA	4	0
34	A	411	SQD	3	0
31	3	312	CLA	1	0
36	D	412	LHG	2	0
36	A	413	LHG	2	0
31	3	307	CLA	1	0
33	c	516	BCR	2	0
31	a	403	CLA	3	0
31	1	201	CLA	2	0
44	6	204	DD6	2	0
31	8	310	CLA	1	0
33	C	517	BCR	4	0
35	d	406	PL9	4	0
31	8	311	CLA	1	0
41	V	201	HEM	6	0
33	D	405	BCR	2	0
31	c	506	CLA	2	0
37	b	521	LMG	1	0
31	7	307	CLA	3	0
31	7	312	CLA	1	0
31	0	305	CLA	3	0
44	p	611	DD6	7	0
31	D	401	CLA	1	0
31	5	310	CLA	1	0
33	B	519	BCR	4	0
33	h	101	BCR	2	0
31	0	308	CLA	6	0
31	B	501	CLA	1	0
32	A	405	PHO	3	0
31	B	502	CLA	1	0
31	P	603	CLA	2	0
31	b	512	CLA	1	0
31	b	506	CLA	3	0
37	Y	101	LMG	3	0
37	W	201	LMG	2	0
31	C	506	CLA	2	0
31	b	514	CLA	1	0
44	1	204	DD6	2	0

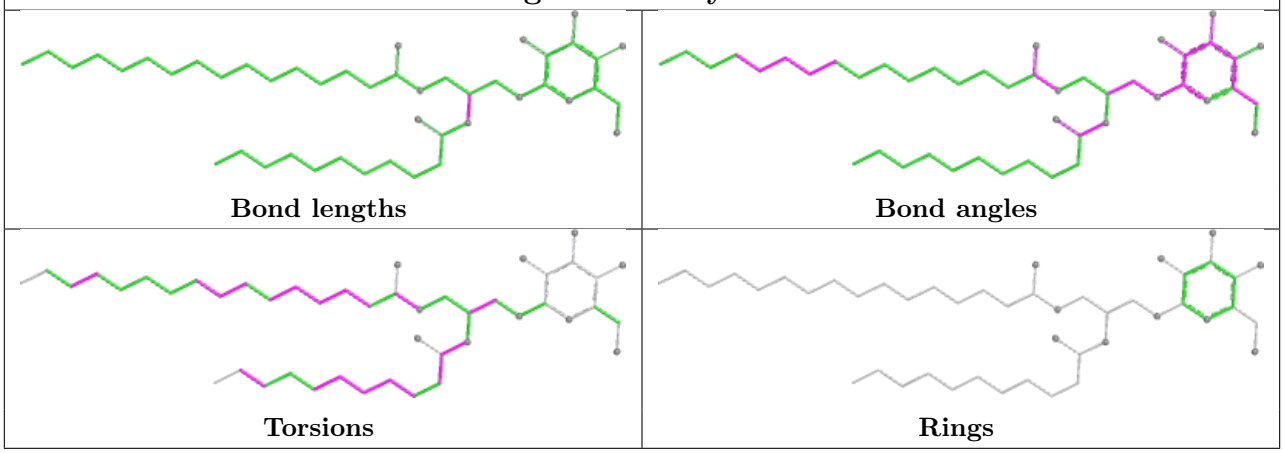
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

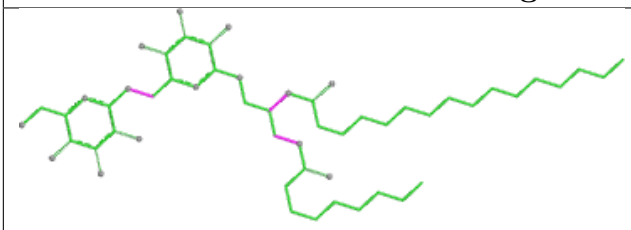
Ligand CLA 7 309



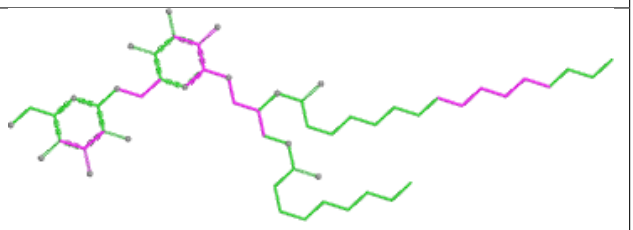
Ligand LMG y 101



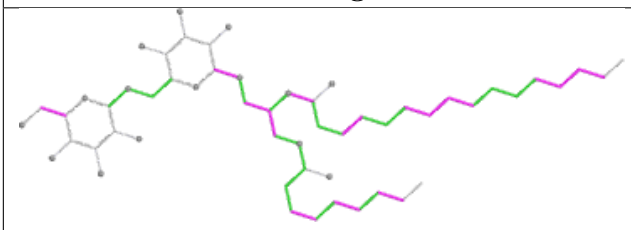
Ligand DGD C 518



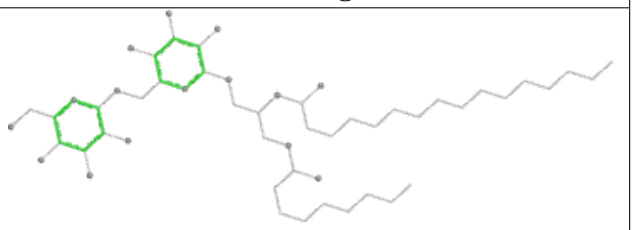
Bond lengths



Bond angles

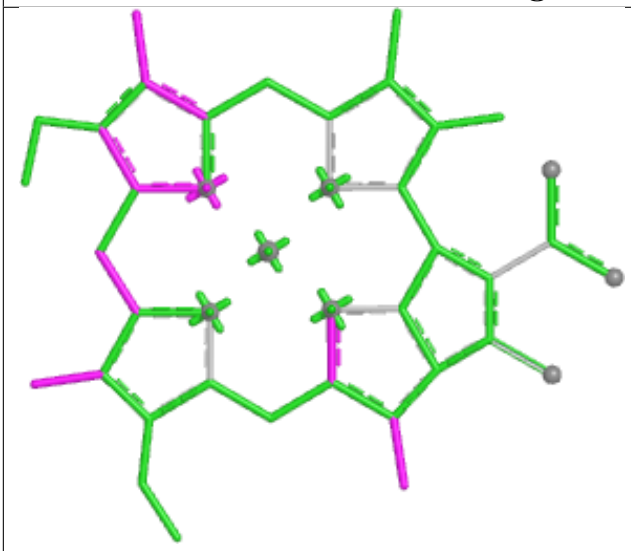


Torsions

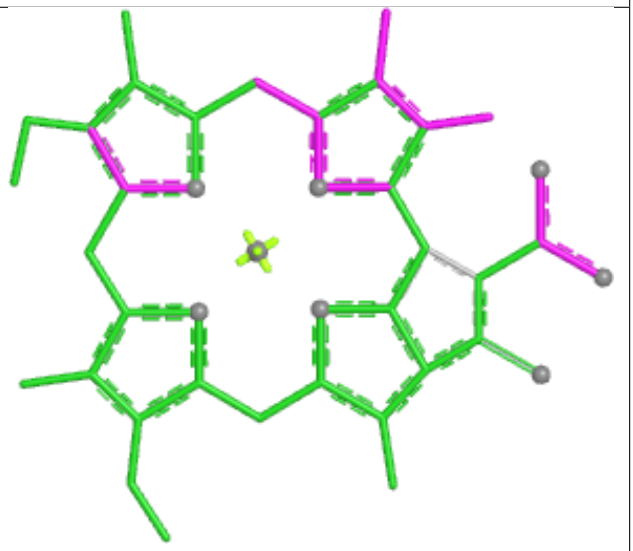


Rings

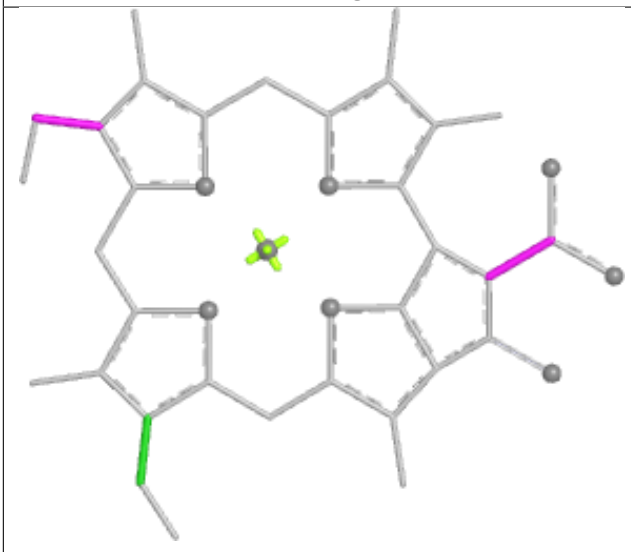
Ligand CLA 8 309



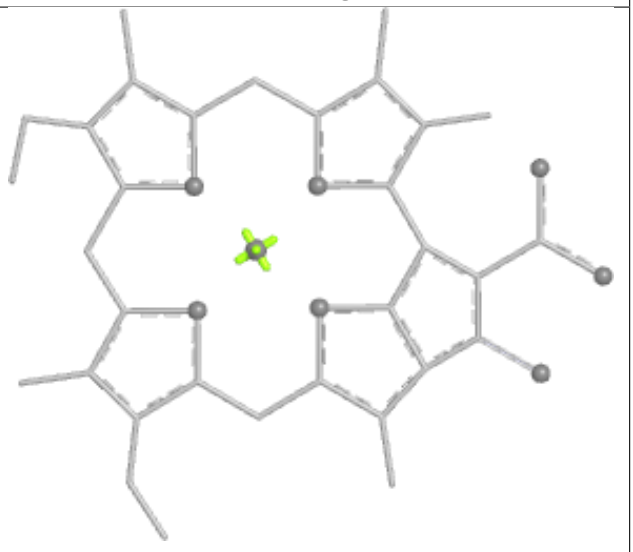
Bond lengths



Bond angles

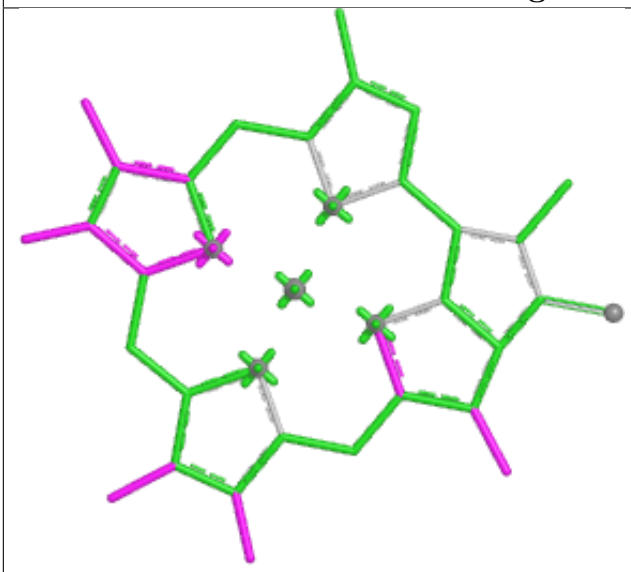


Torsions

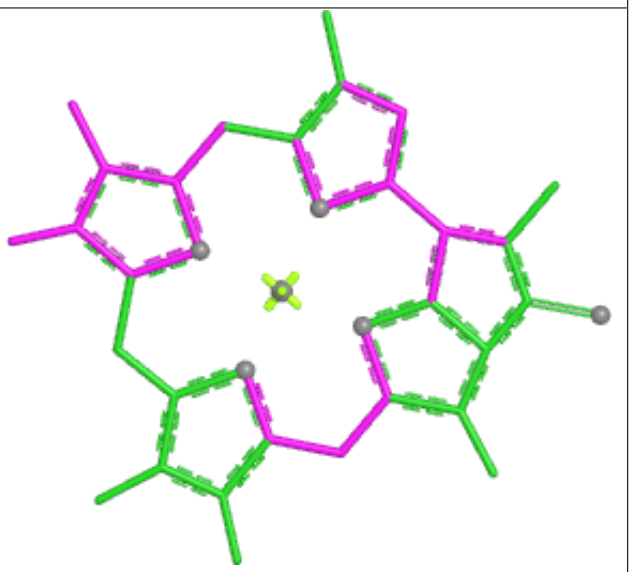


Rings

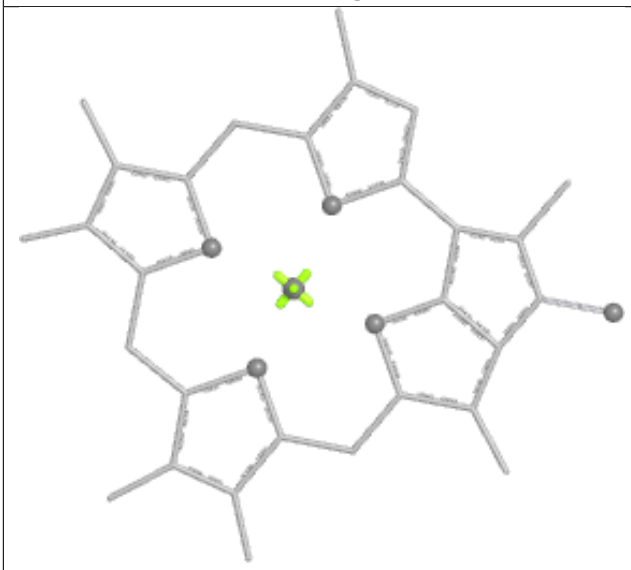
Ligand CLA 9 213



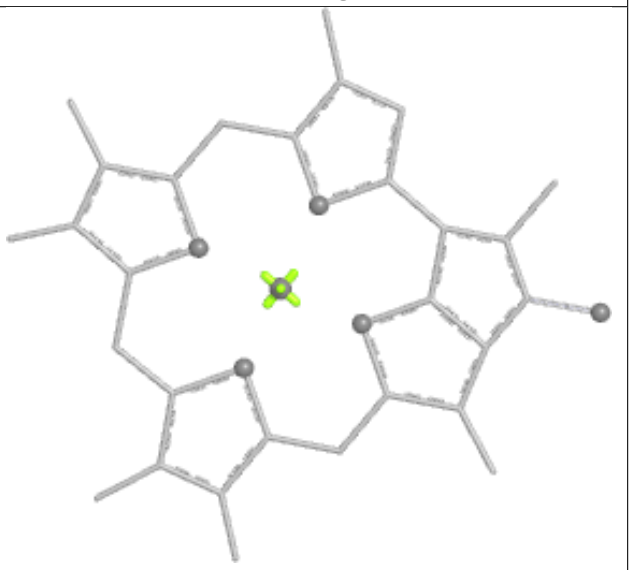
Bond lengths



Bond angles

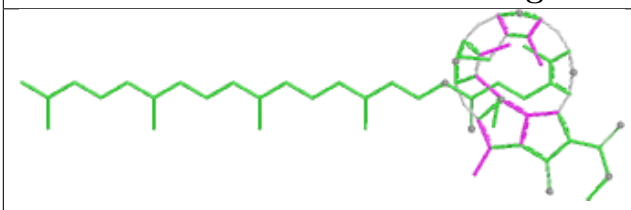


Torsions

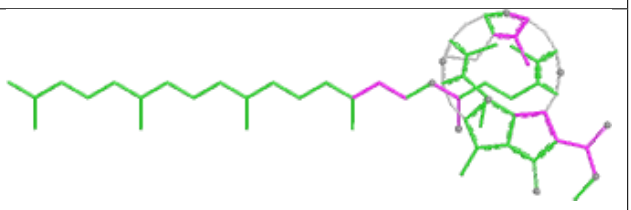


Rings

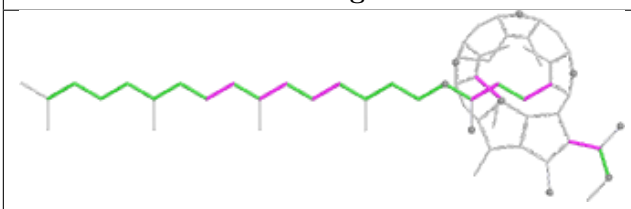
Ligand PHO a 406



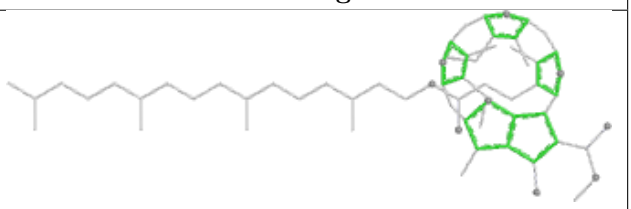
Bond lengths



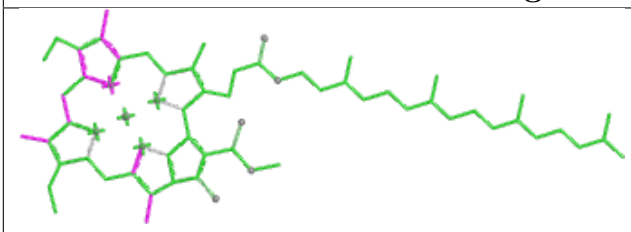
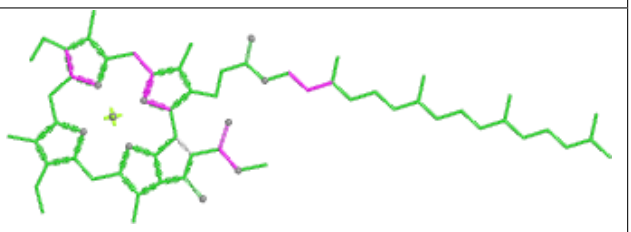
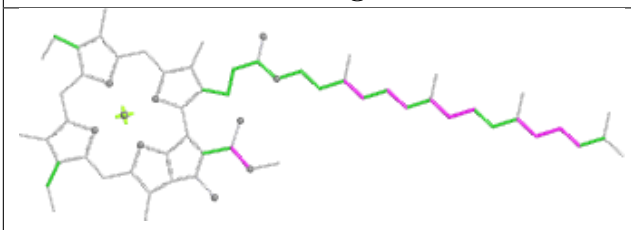
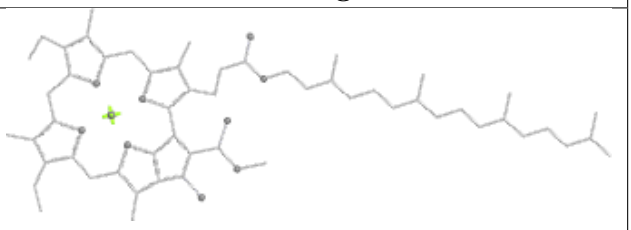
Bond angles



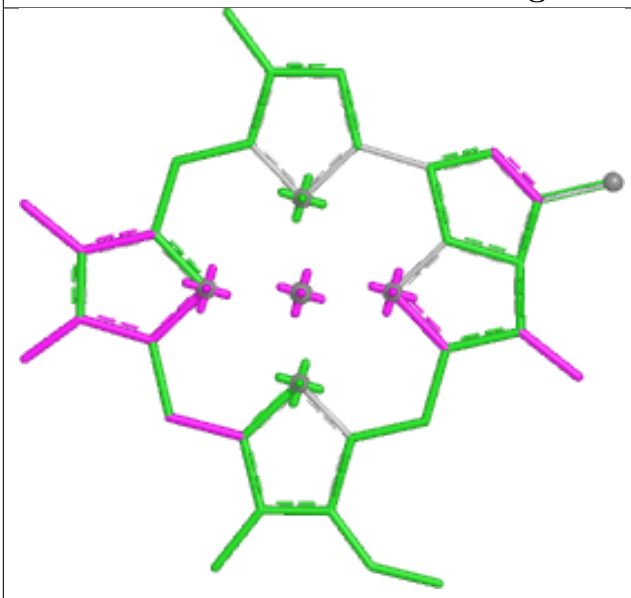
Torsions



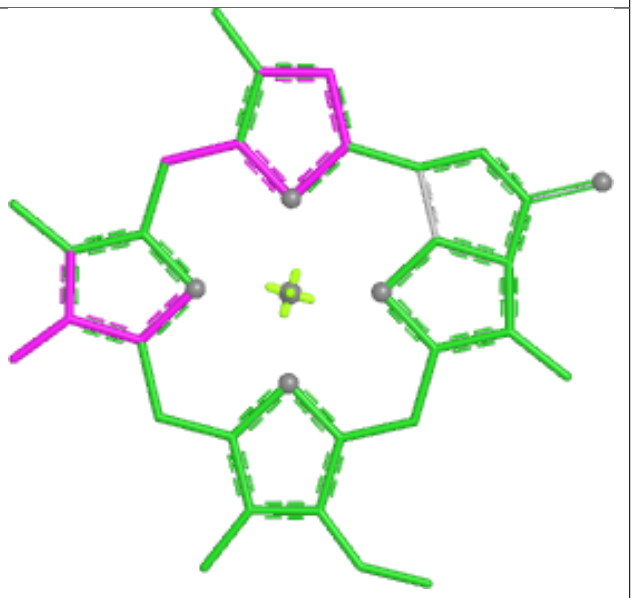
Rings

Ligand CLA B 505	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

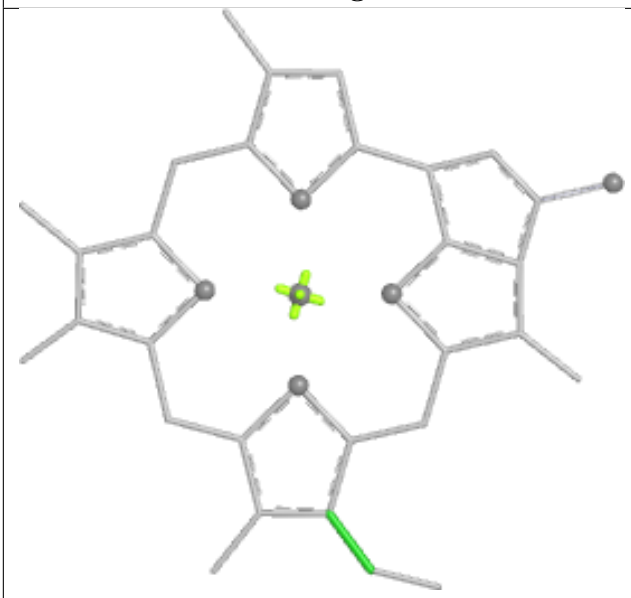
Ligand CLA 4 205



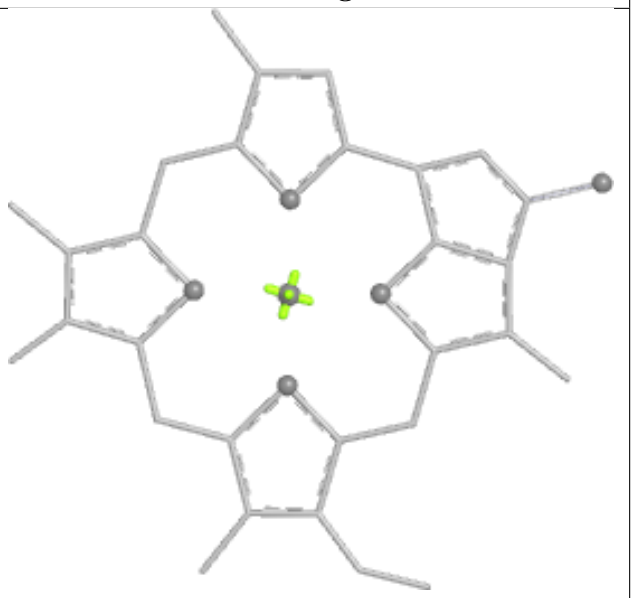
Bond lengths



Bond angles

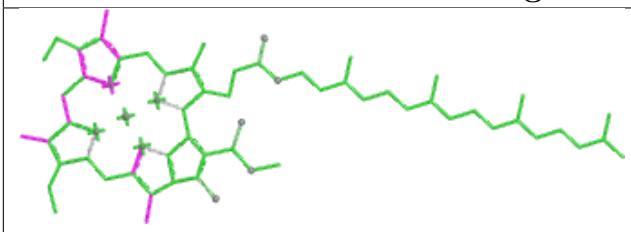


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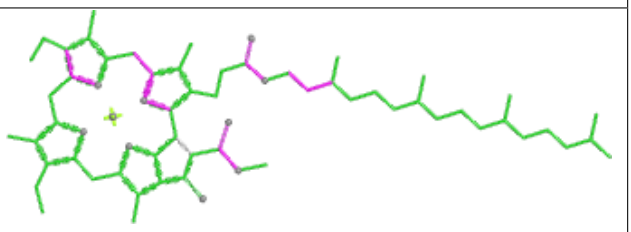


Rings

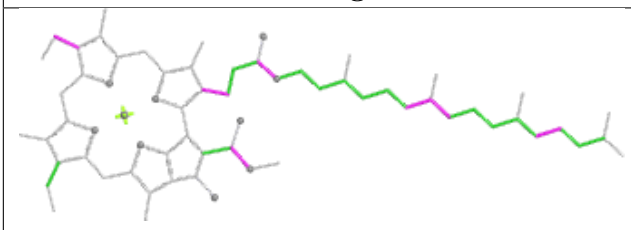
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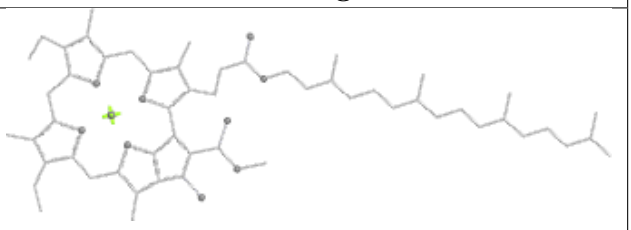
Bond lengths



Bond angles



Torsions

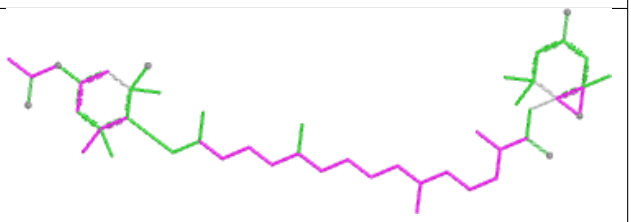


Rings

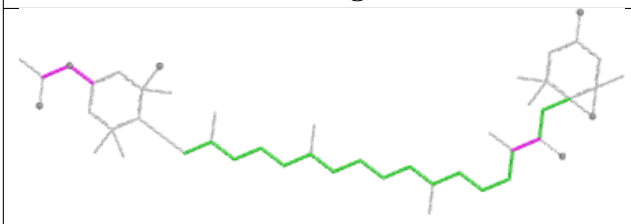
Ligand A86 1 202



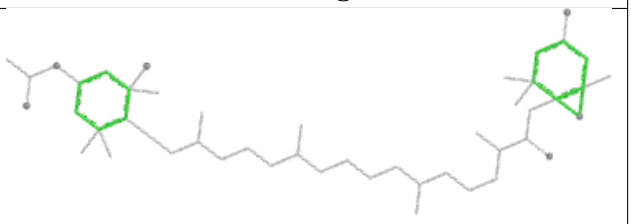
Bond lengths



Bond angles

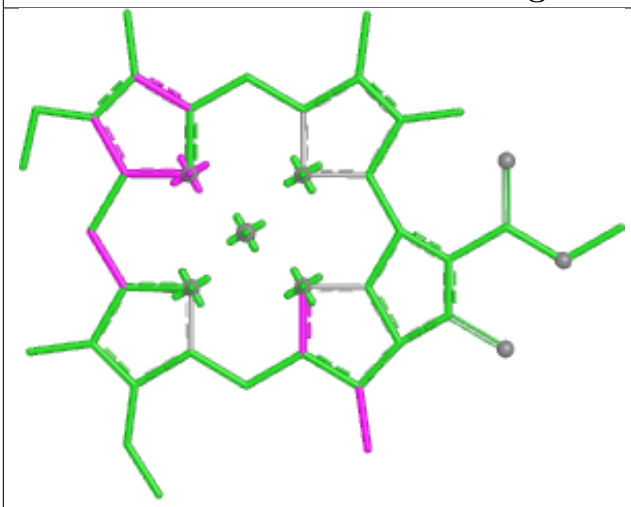


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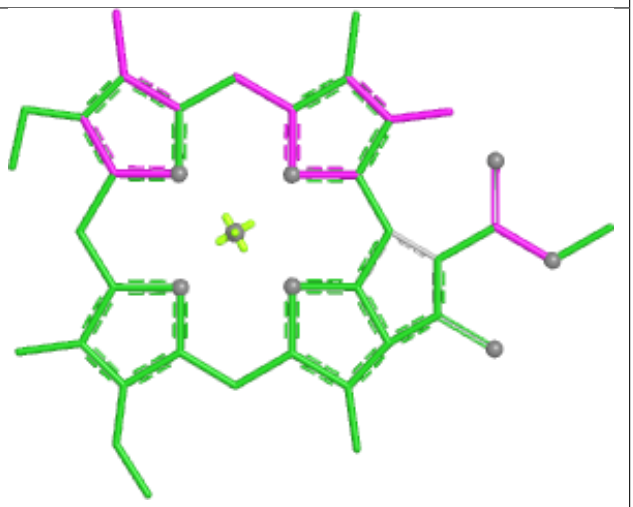


Rings

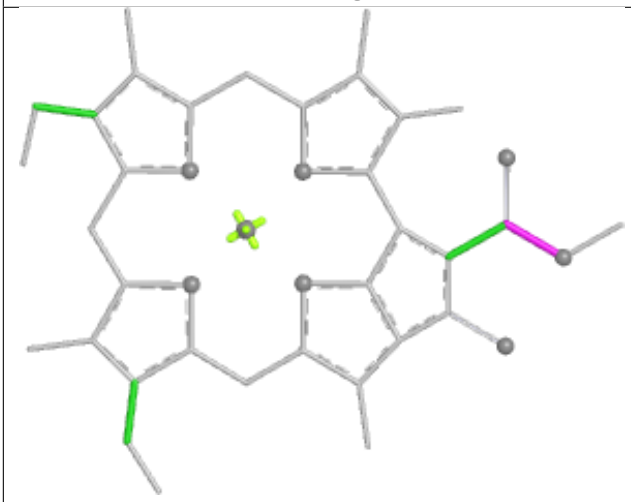
Ligand CLA 6 212



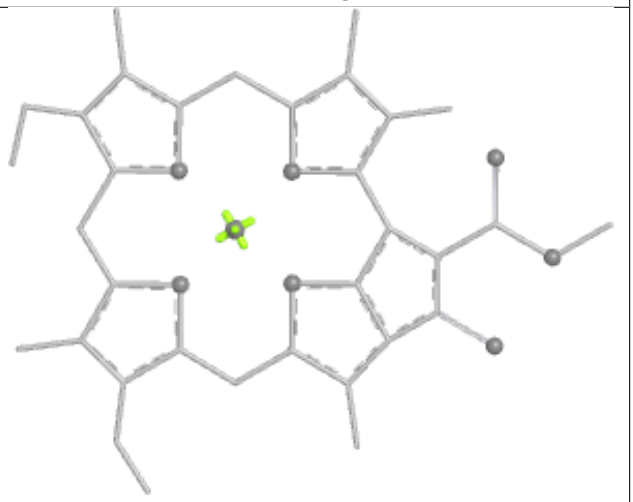
Bond lengths



Bond angles

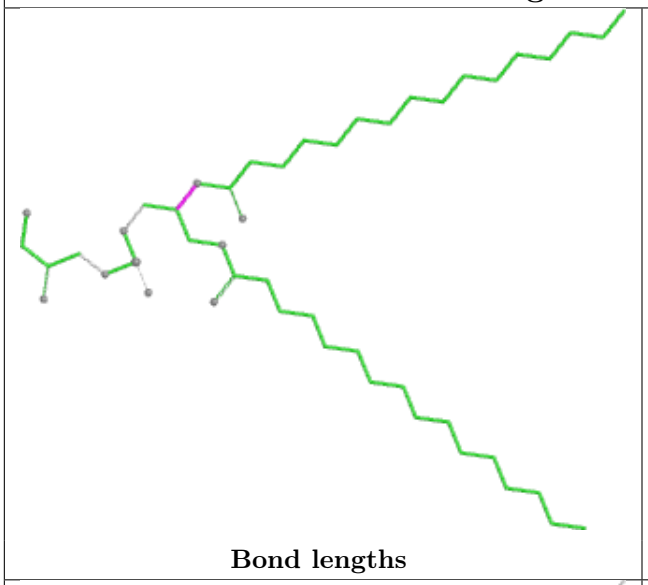


Torsions

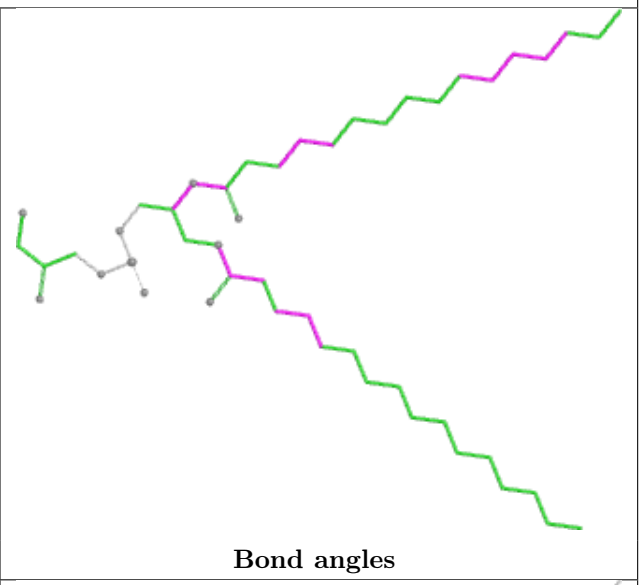


Rings

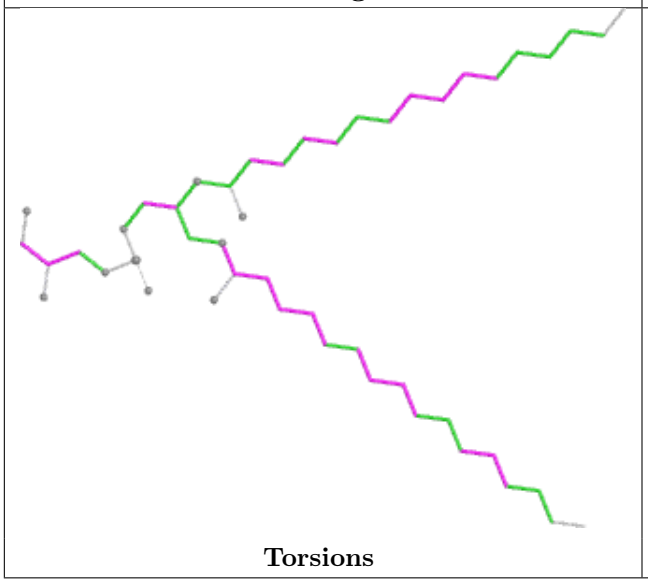
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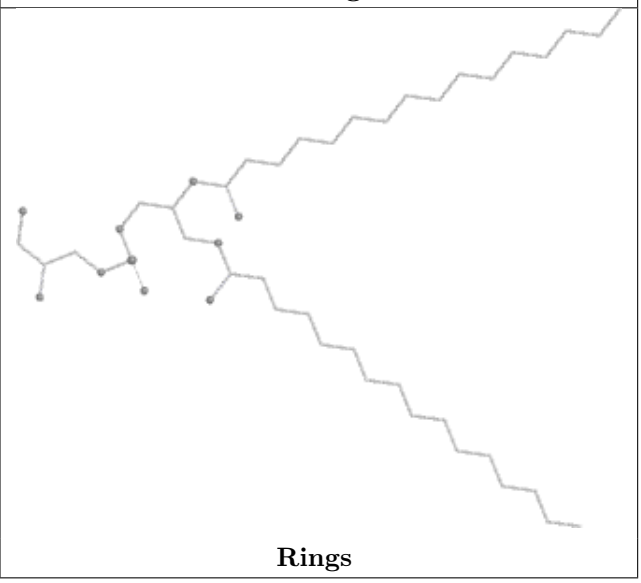
Bond lengths



Bond angles

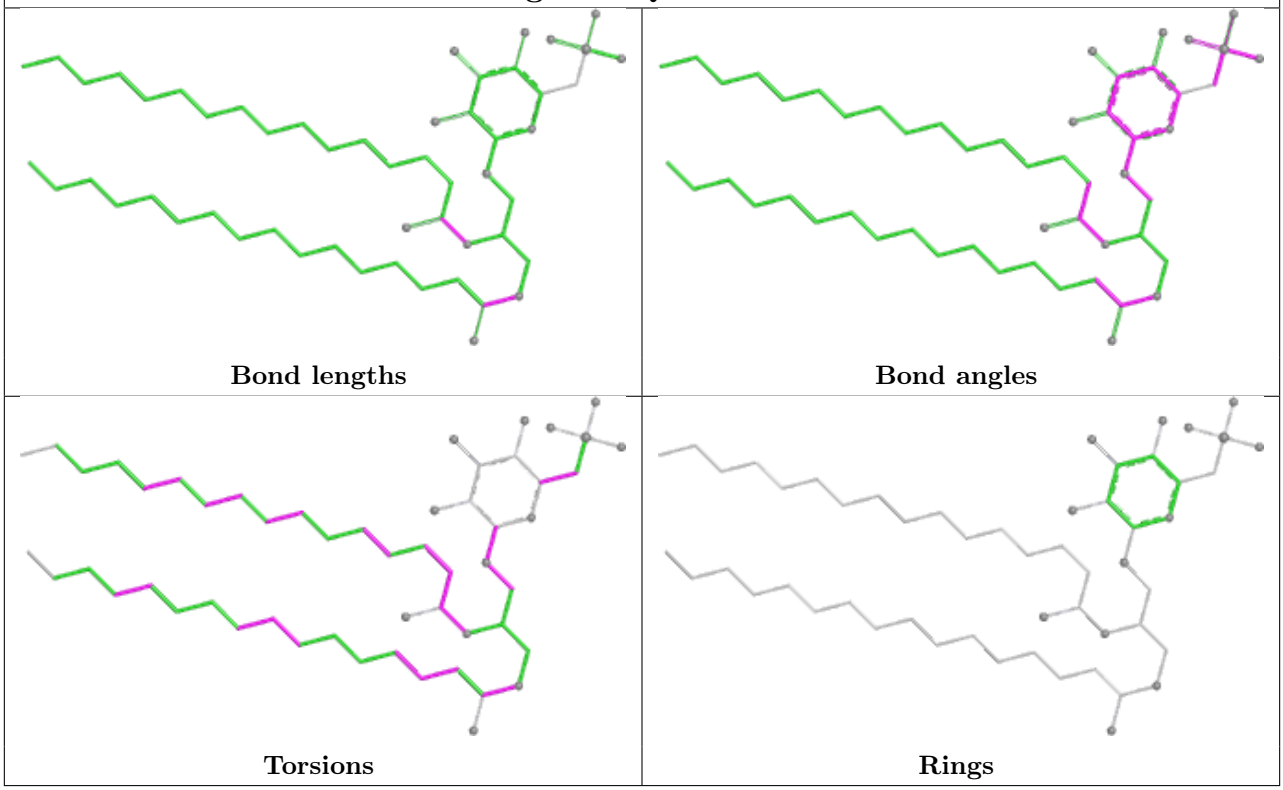


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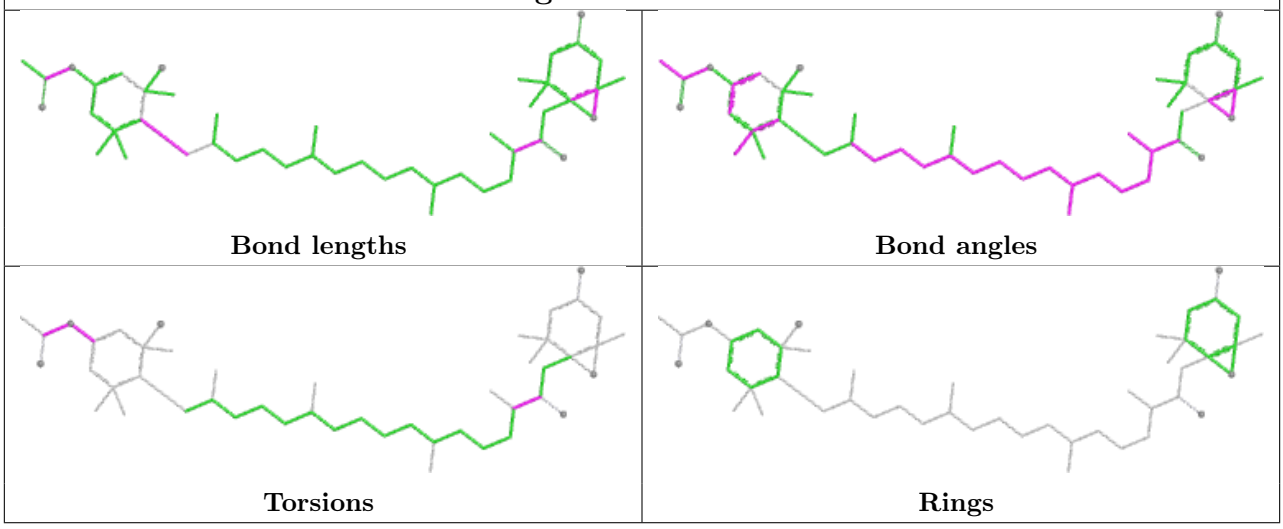


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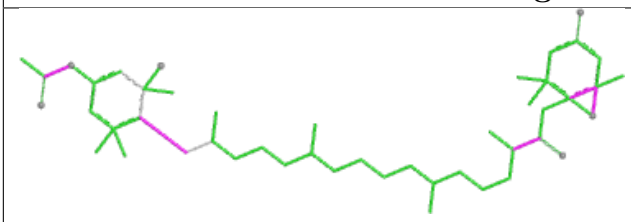
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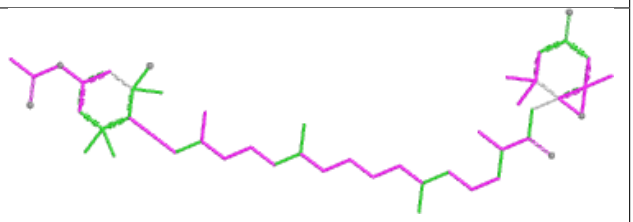
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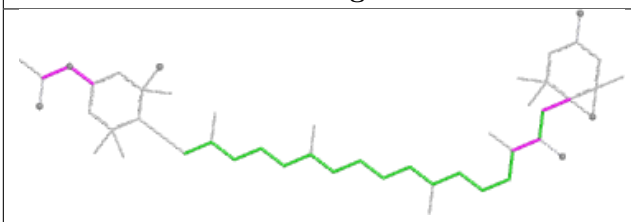
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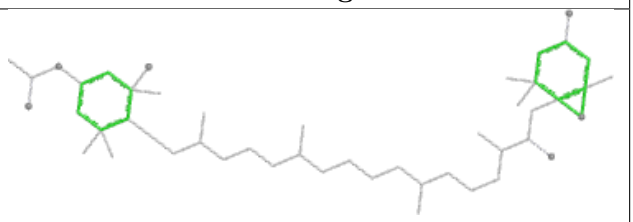
Bond lengths



Bond angles

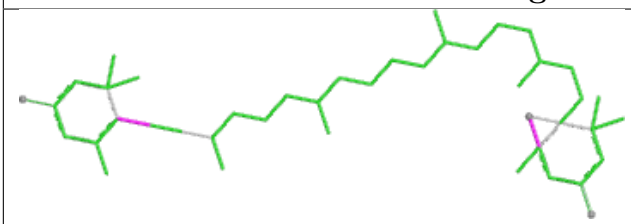


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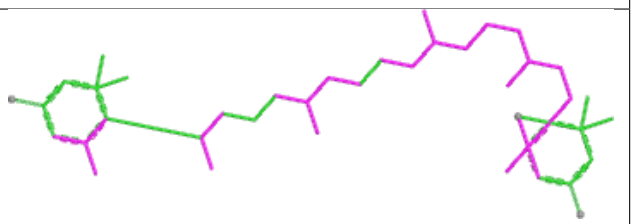


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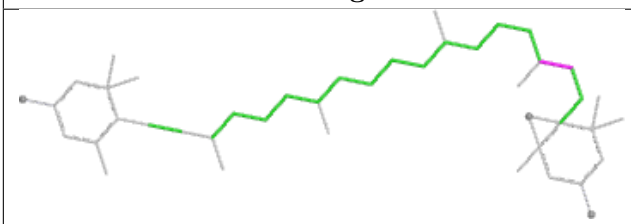
Ligand DD6 2 303



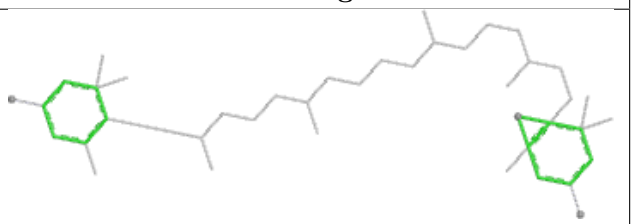
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Bond angles

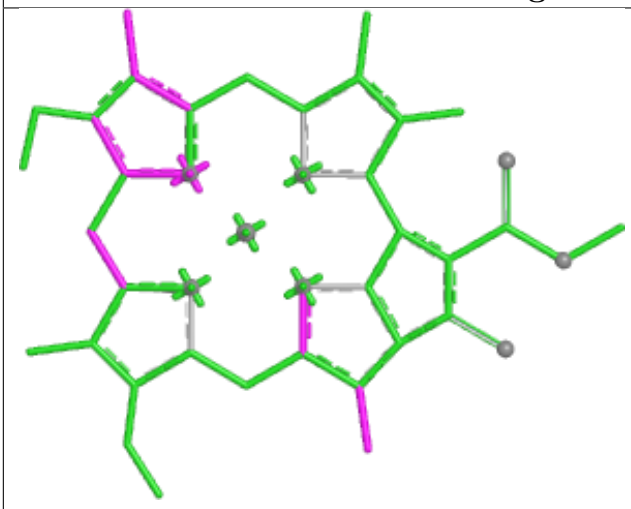


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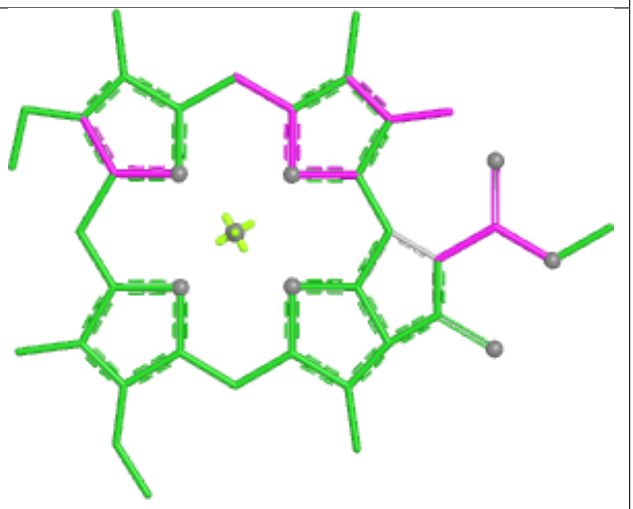


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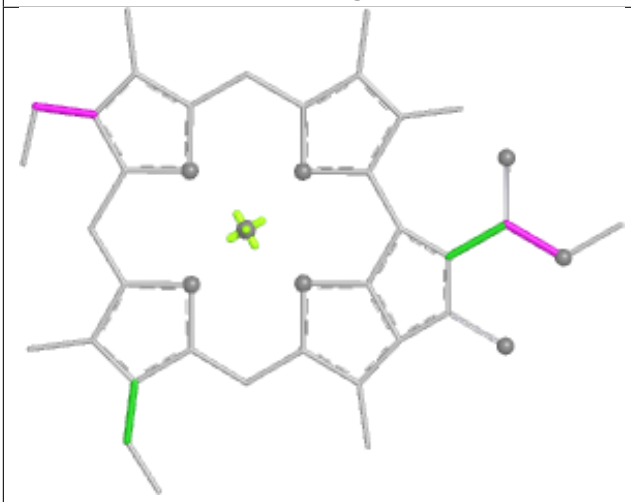
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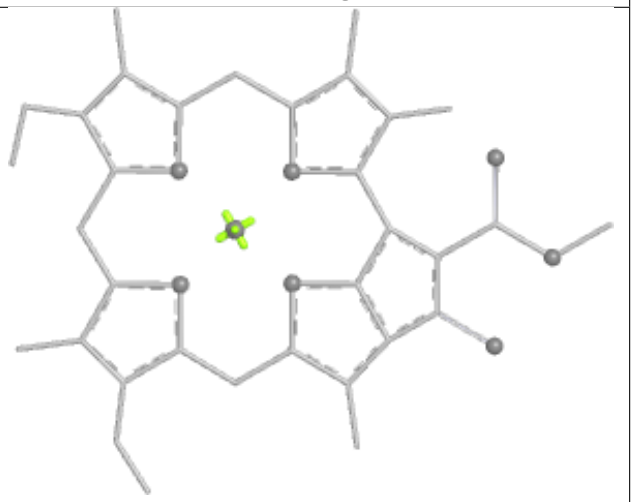
Bond lengths



Bond angles

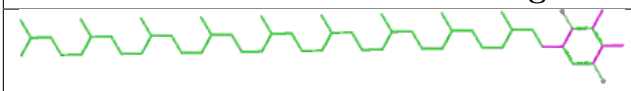


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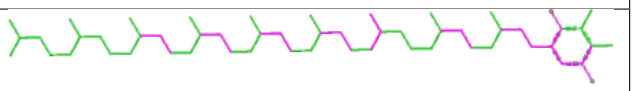


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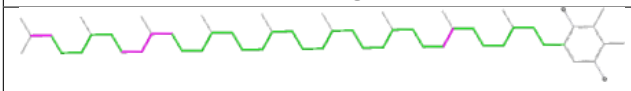
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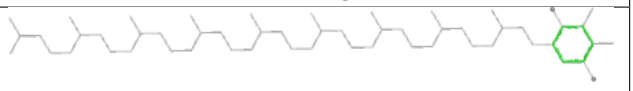
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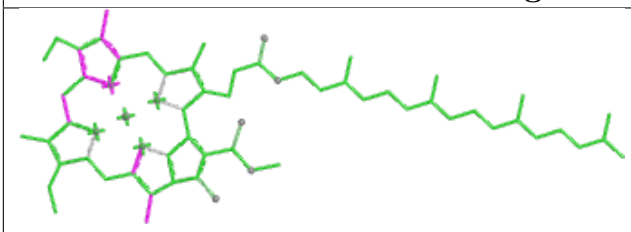


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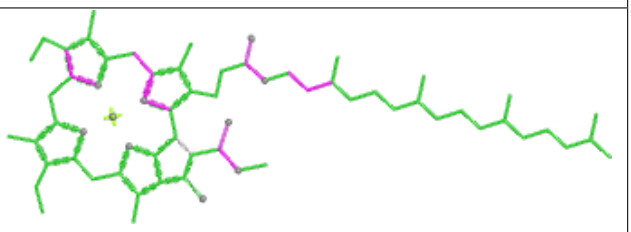


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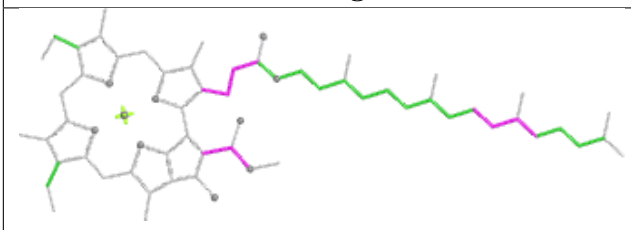
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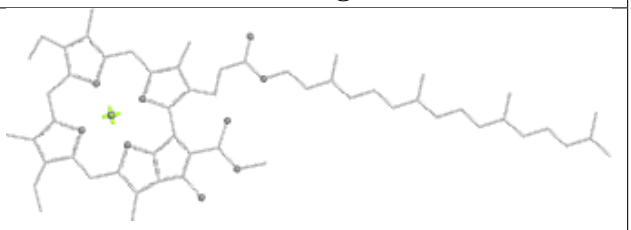
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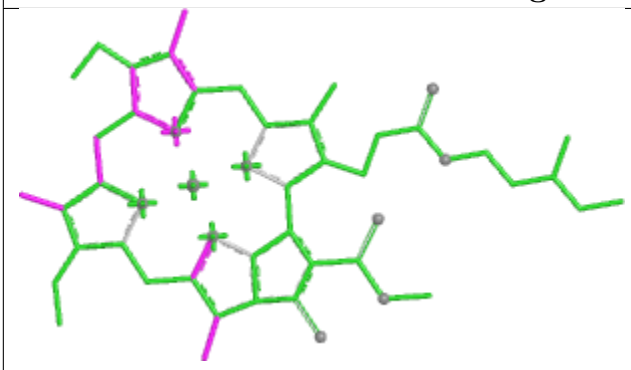


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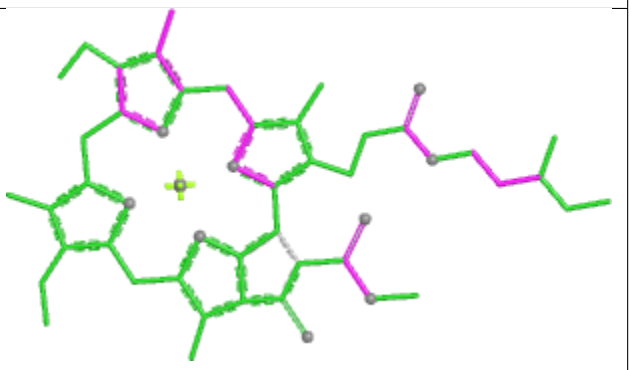


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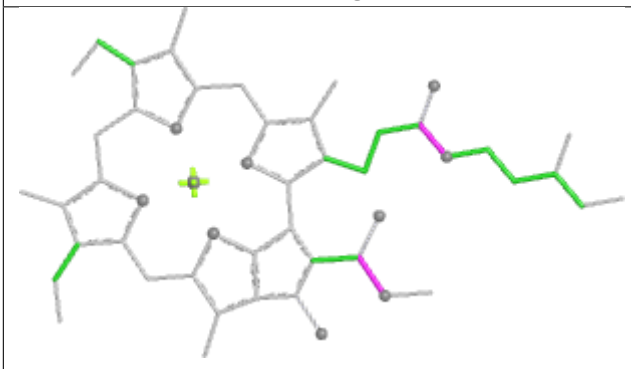
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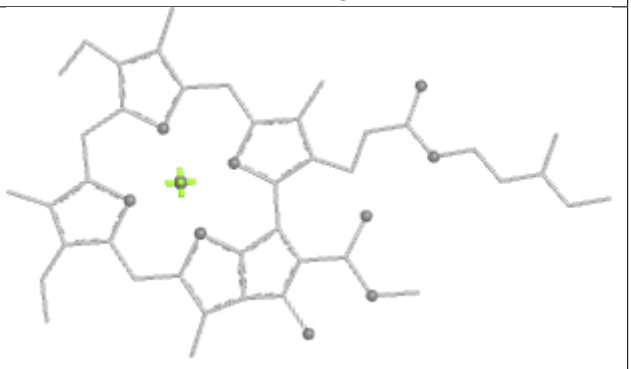
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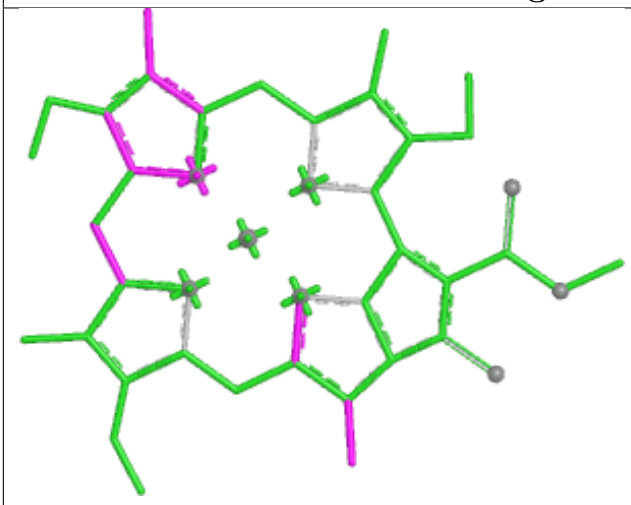


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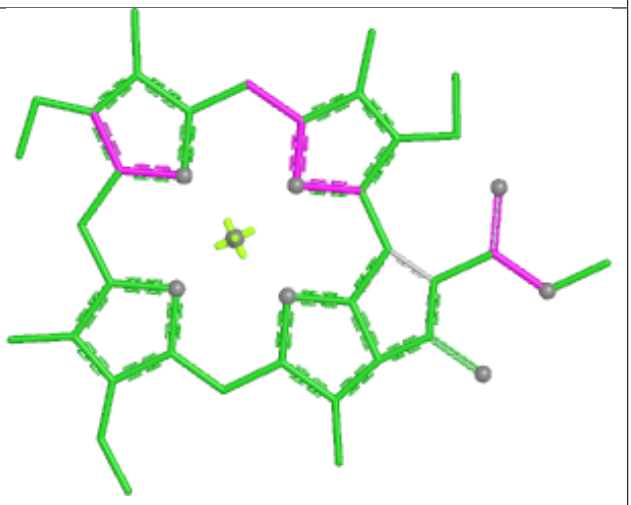


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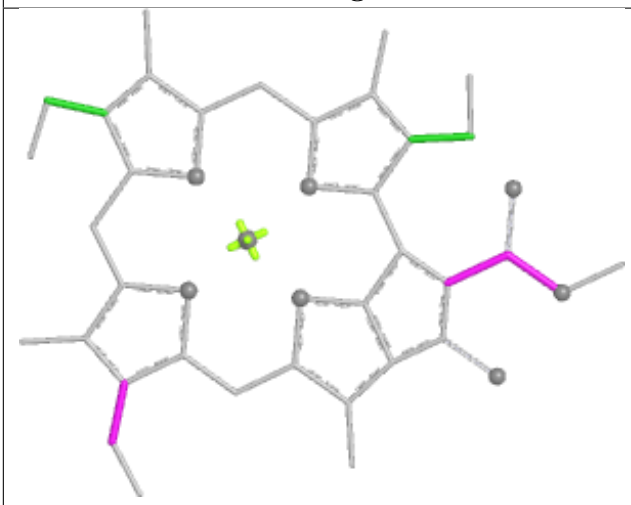
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Bond lengths



Bond angles

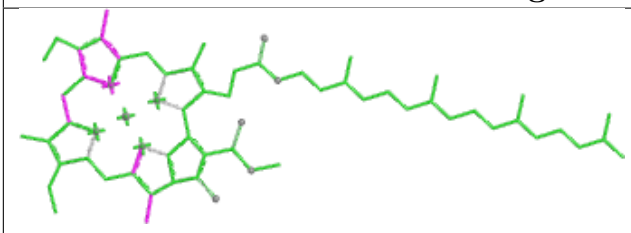


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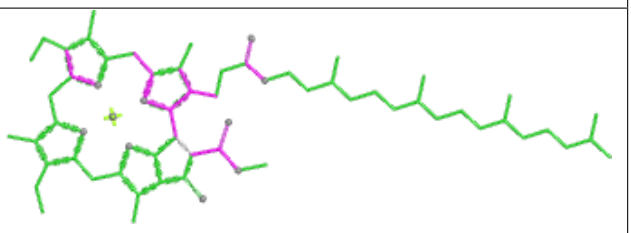


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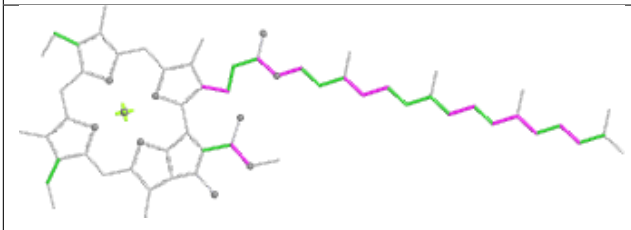
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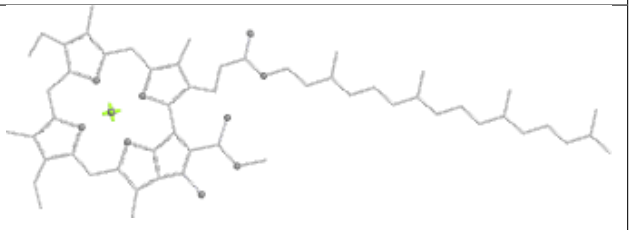
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Bond angles

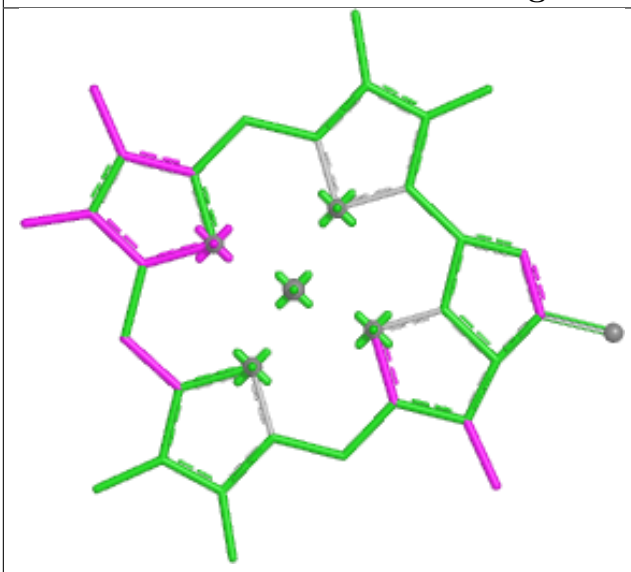


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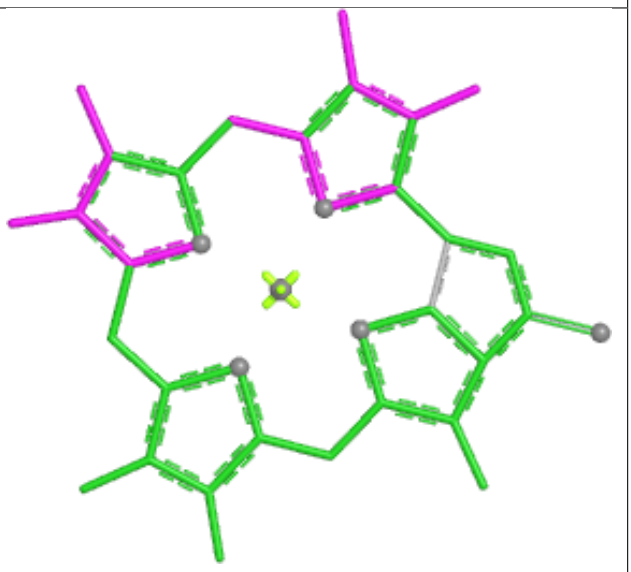


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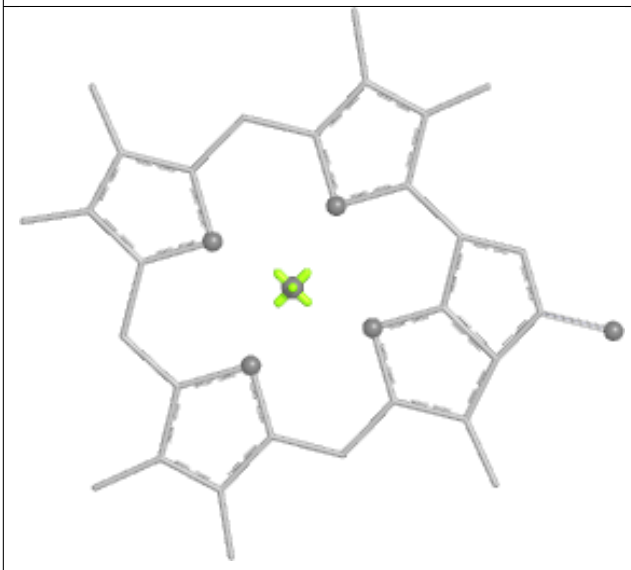
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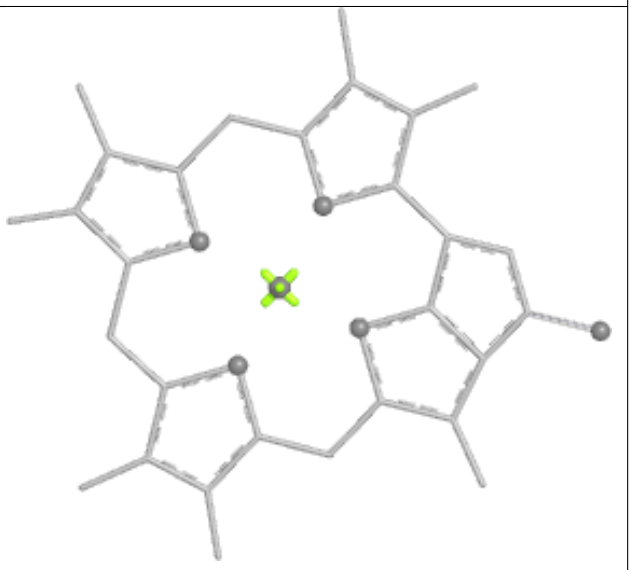
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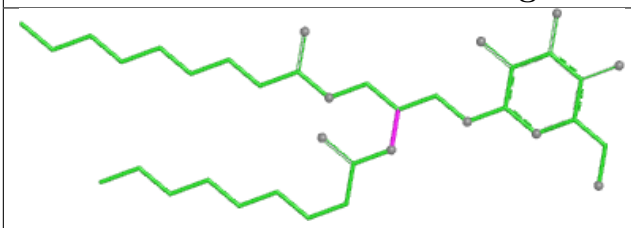
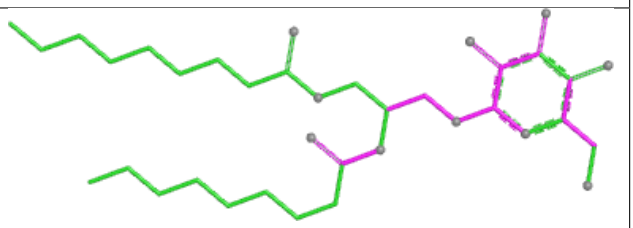
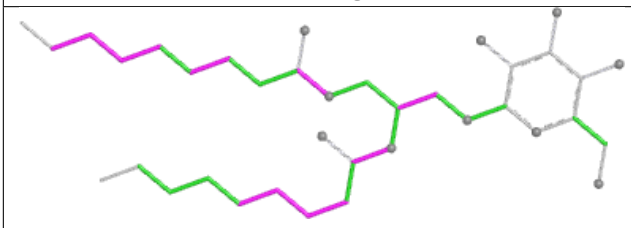
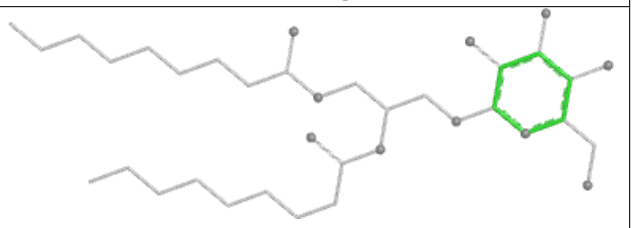
Bond angles



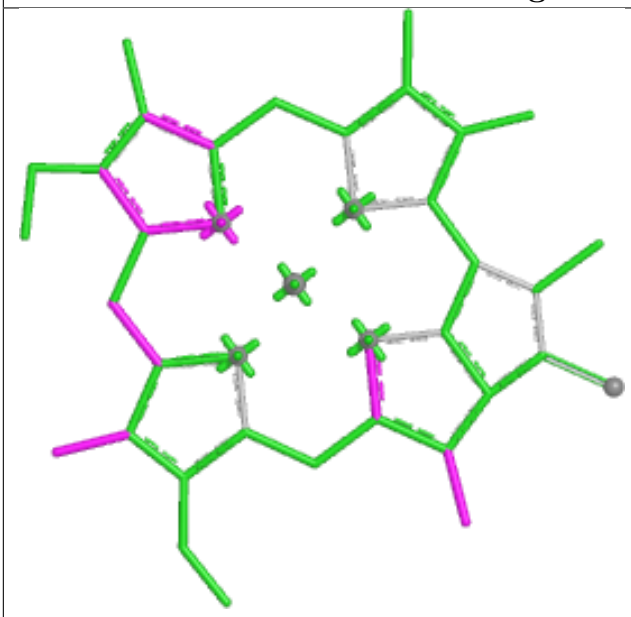
Torsions



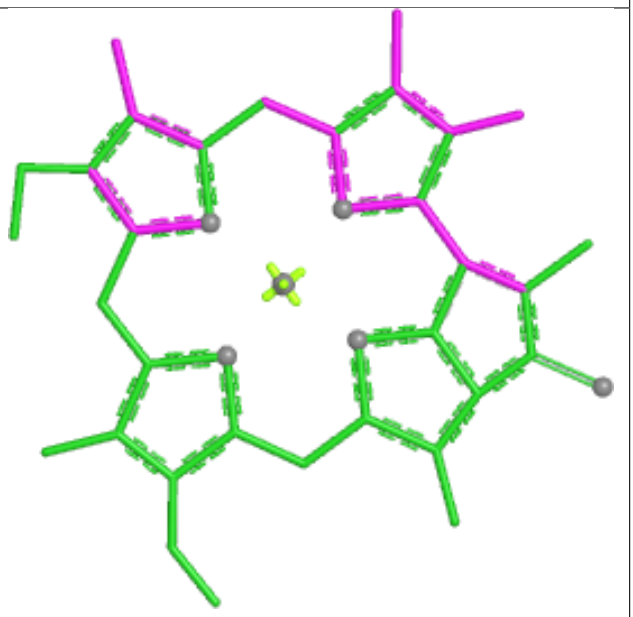
Rings

Ligand LMG D 409	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

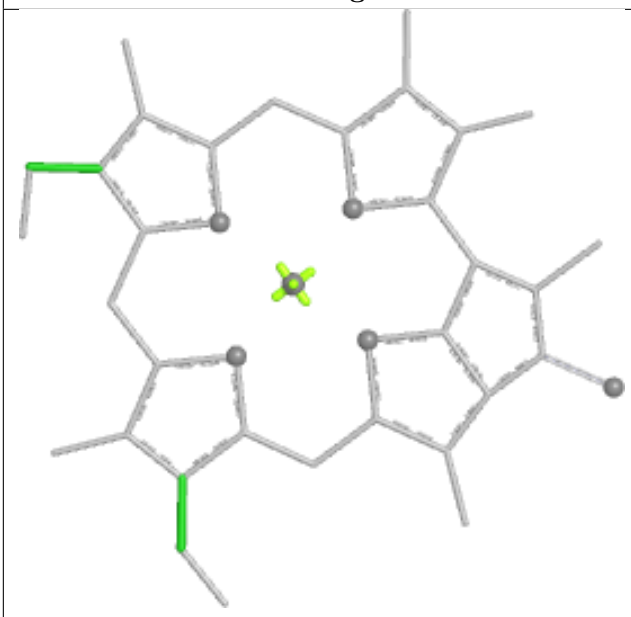
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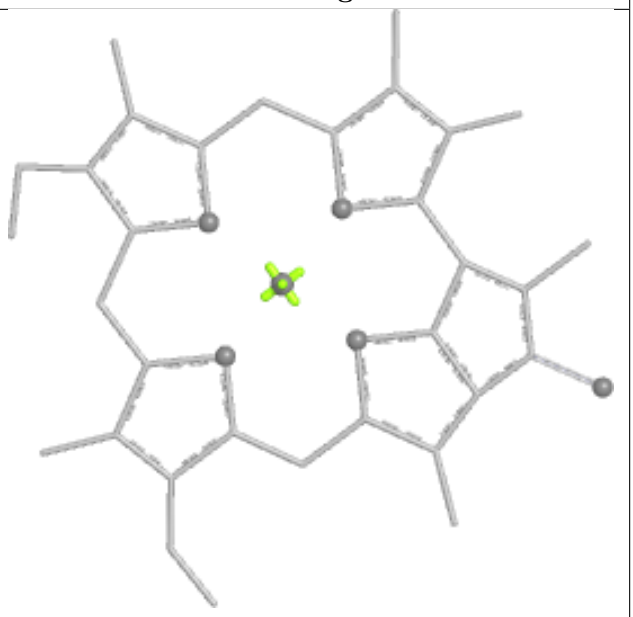
Bond lengths



Bond angles

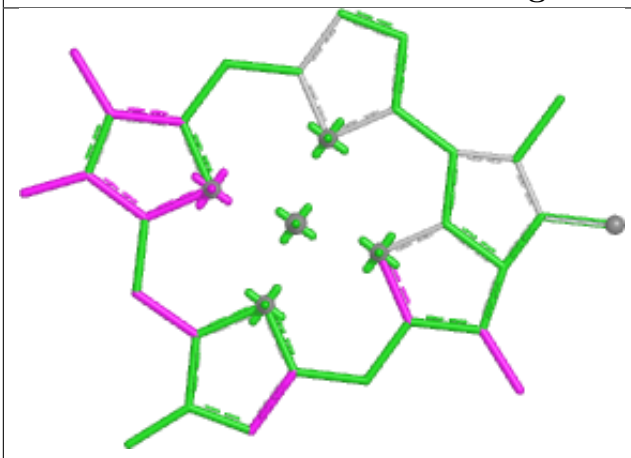


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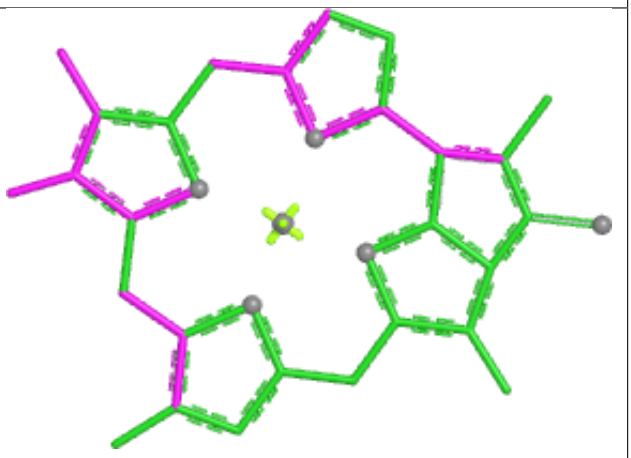


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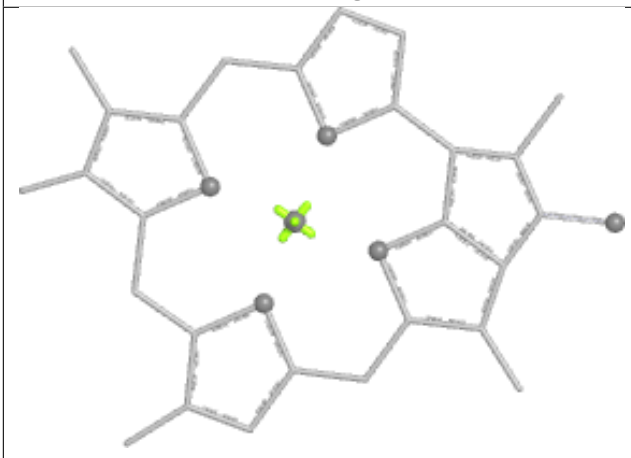
Ligand CLA 3 306



Bond lengths



Bond angles

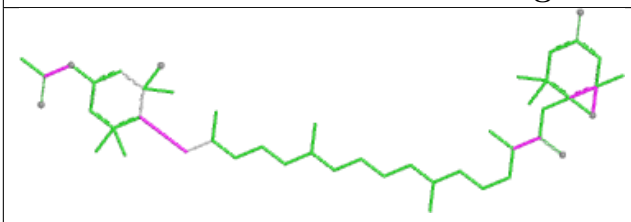


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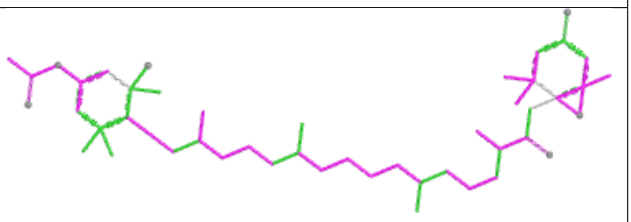


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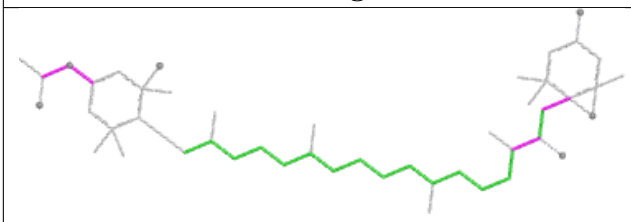
Ligand A86 9 203



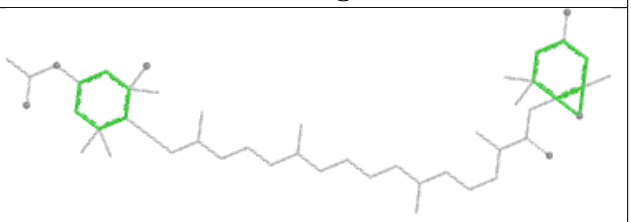
Bond lengths



Bond angles

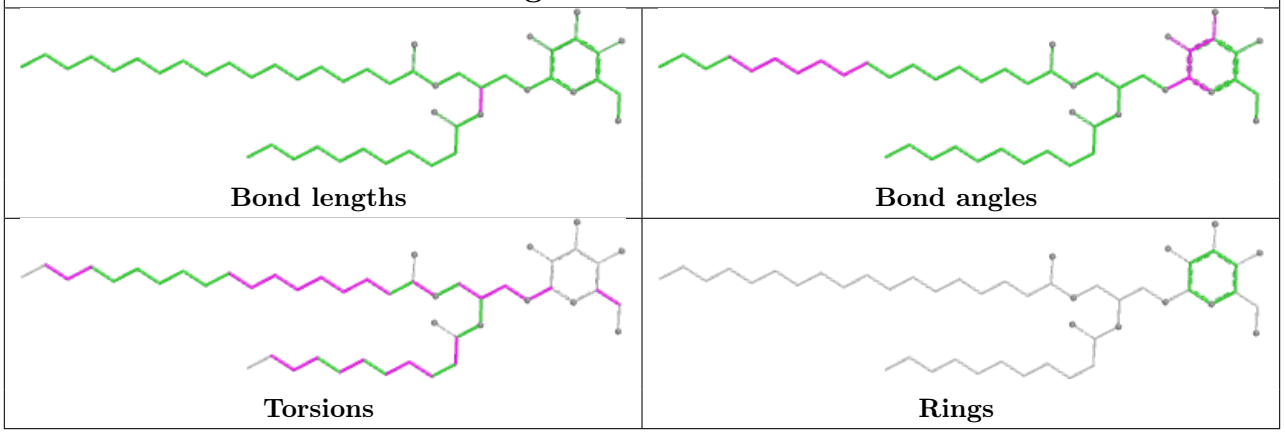


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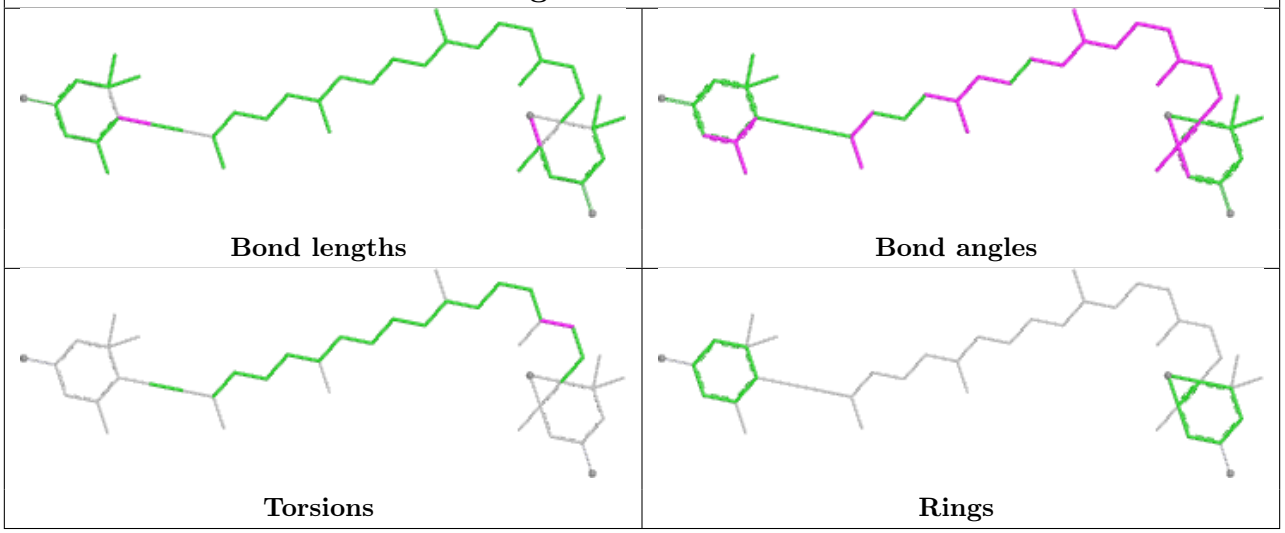


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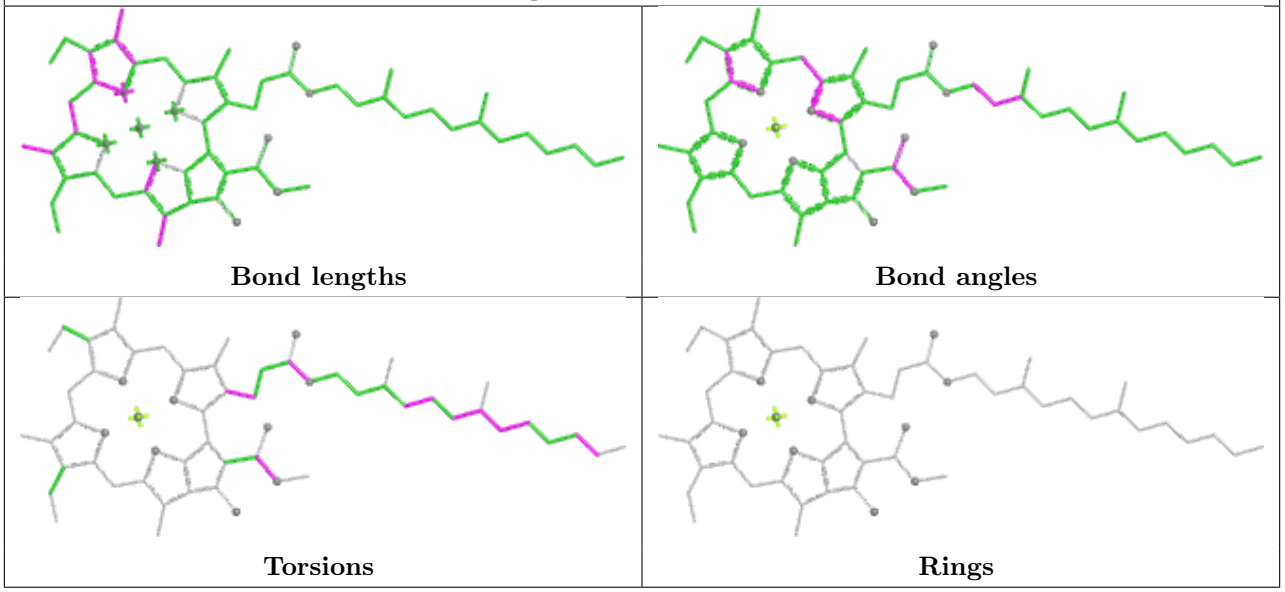
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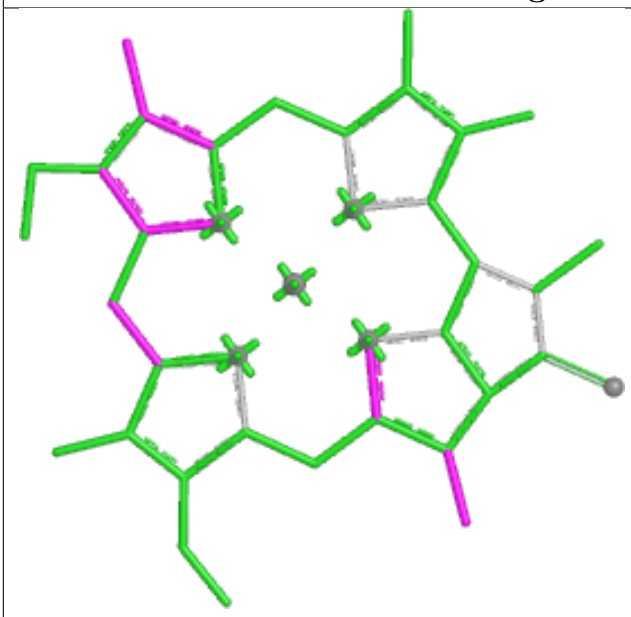
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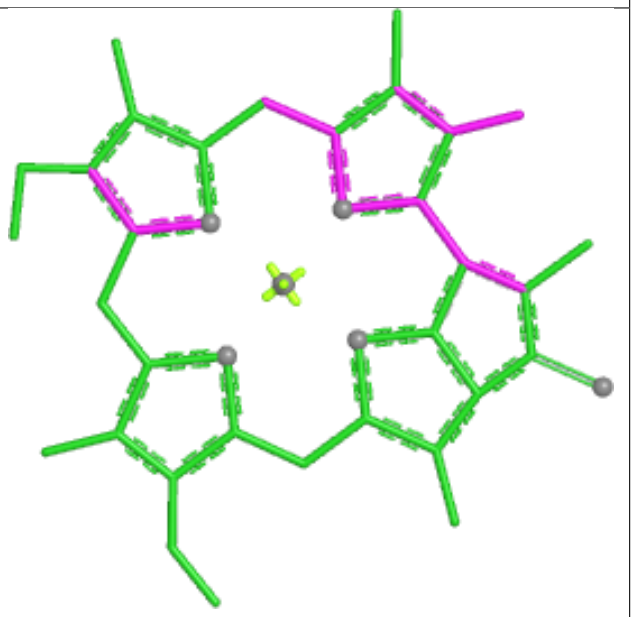
Ligand CLA B 514



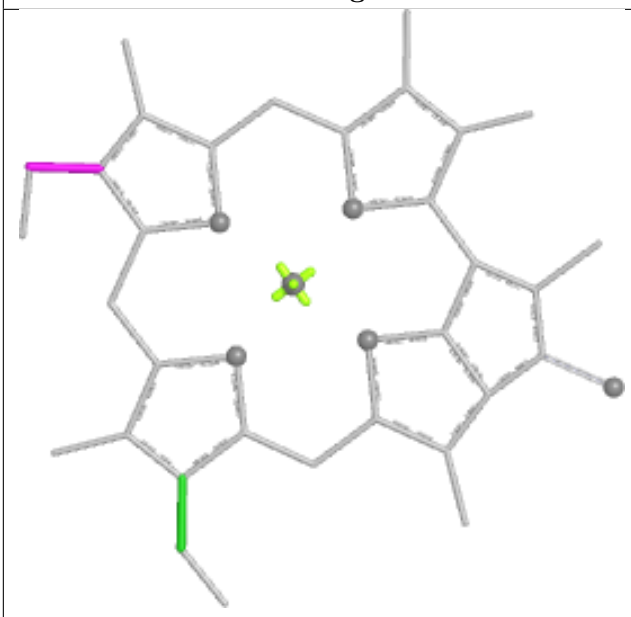
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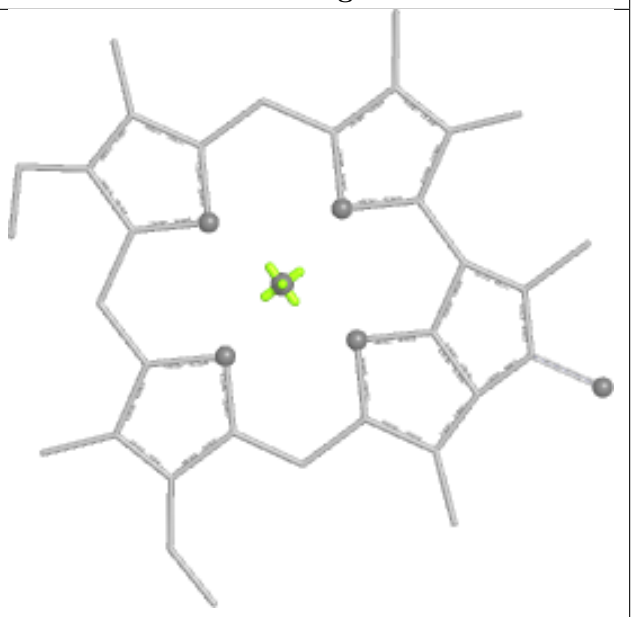
Bond lengths



Bond angles

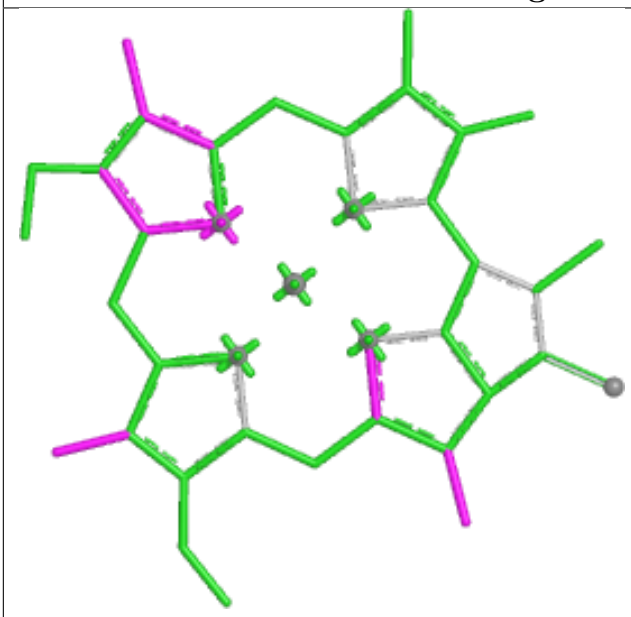


Torsions

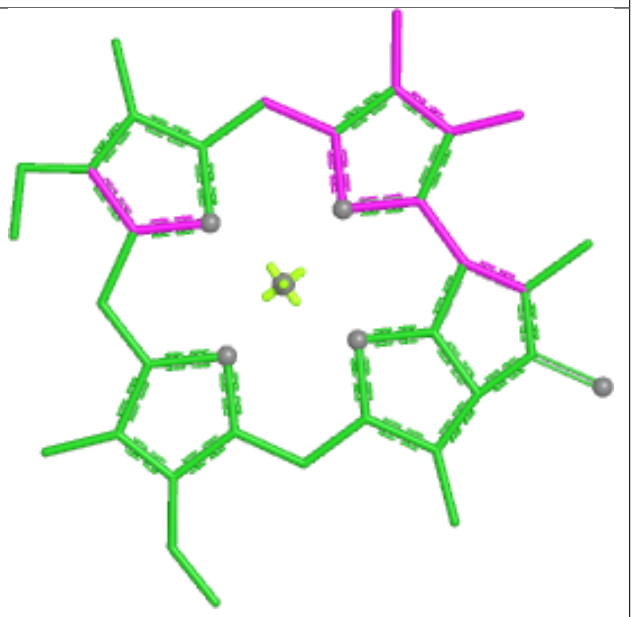


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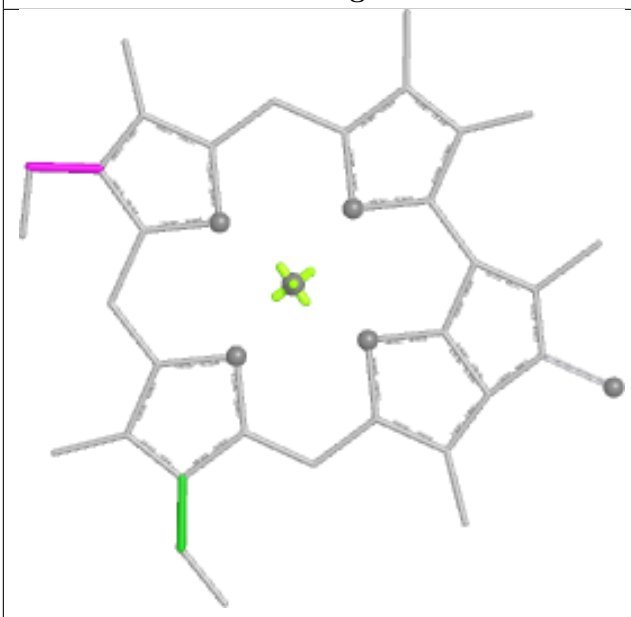
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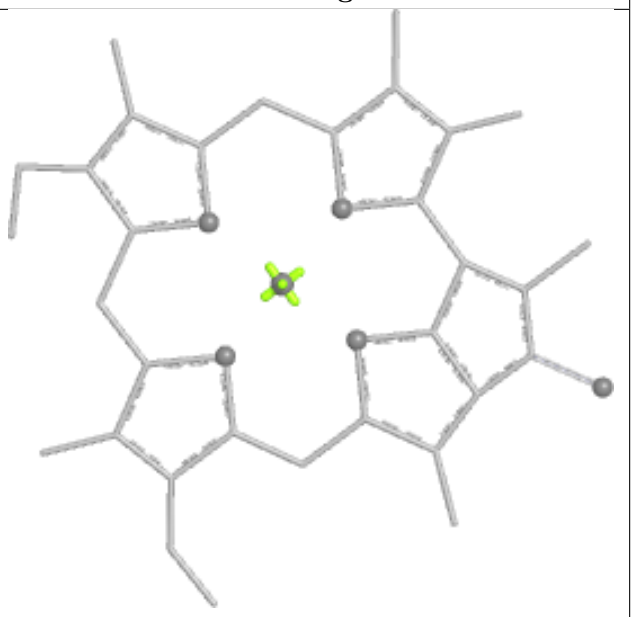
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Bond angles

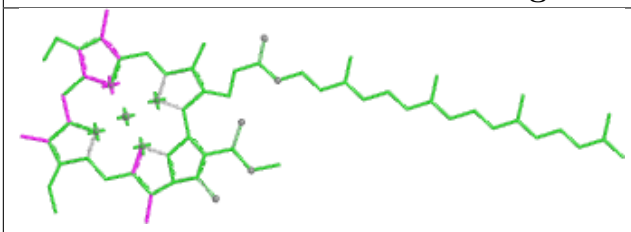


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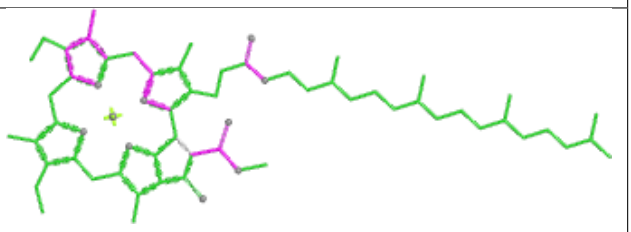


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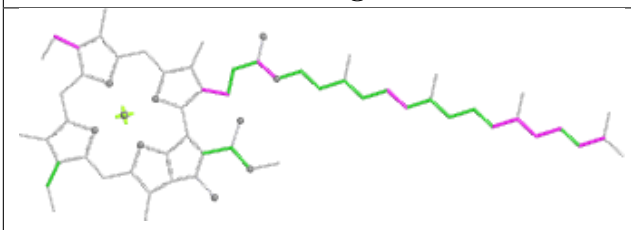
Ligand CLA c 509



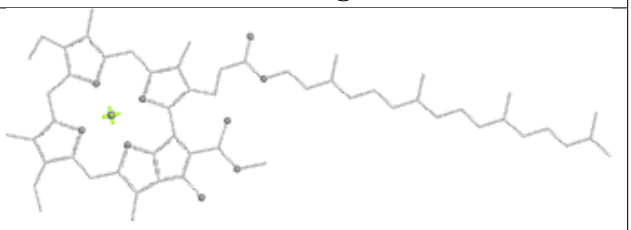
Bond lengths



Bond angles

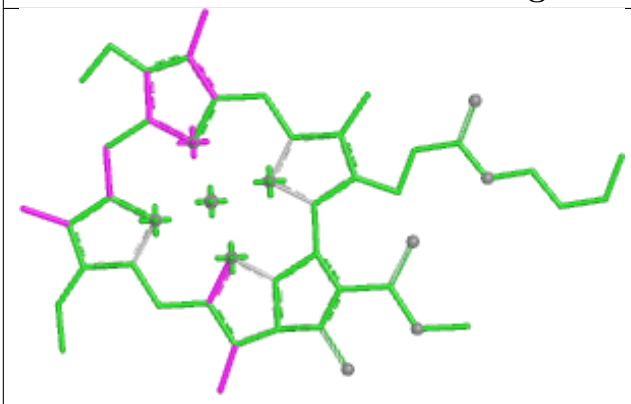


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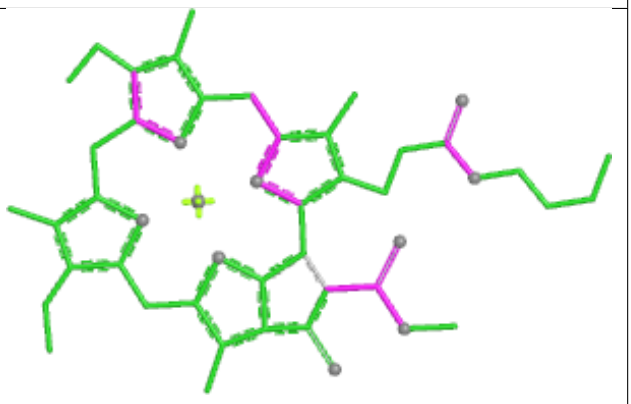


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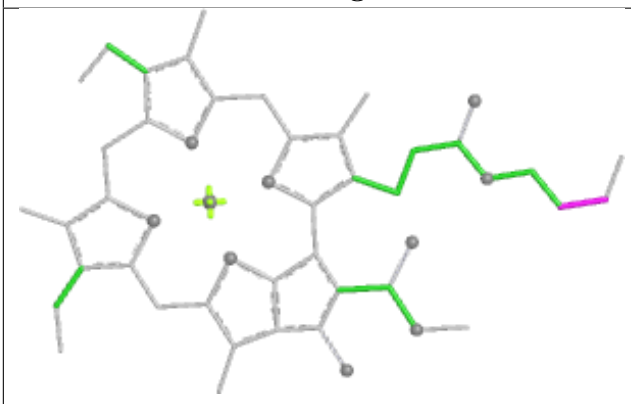
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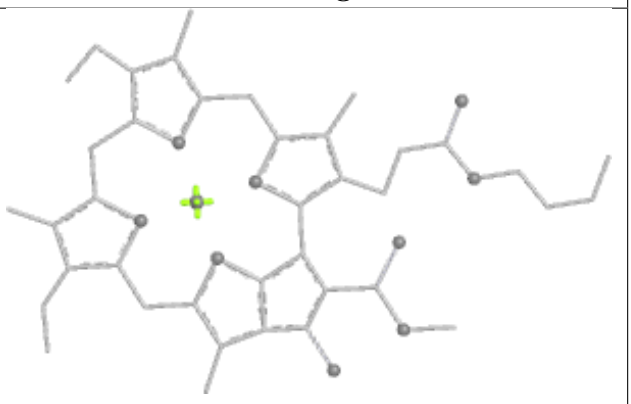
Bond lengths



Bond angles

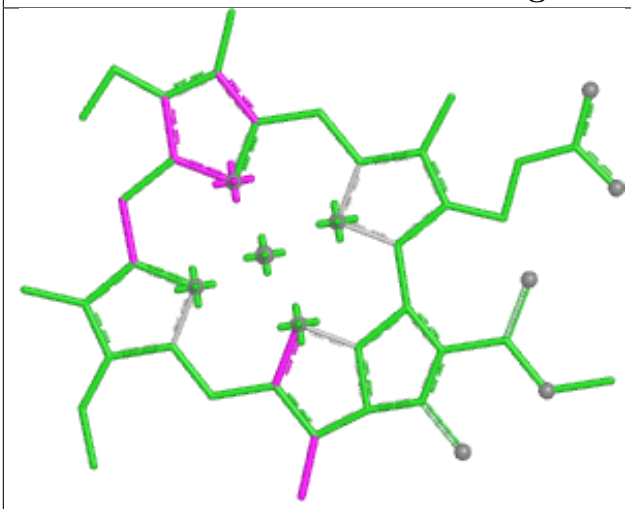


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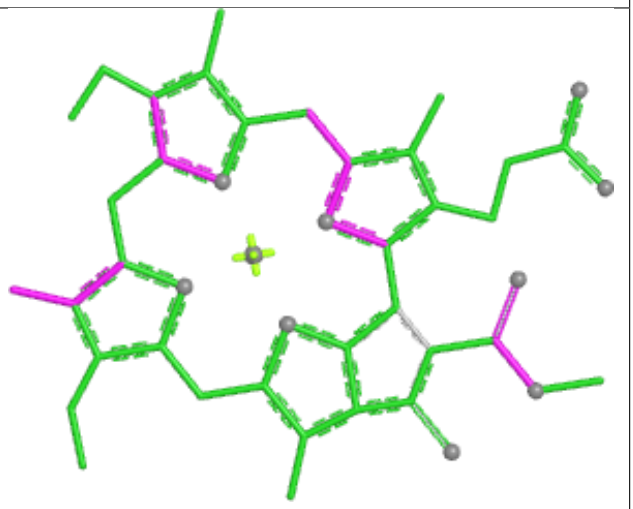


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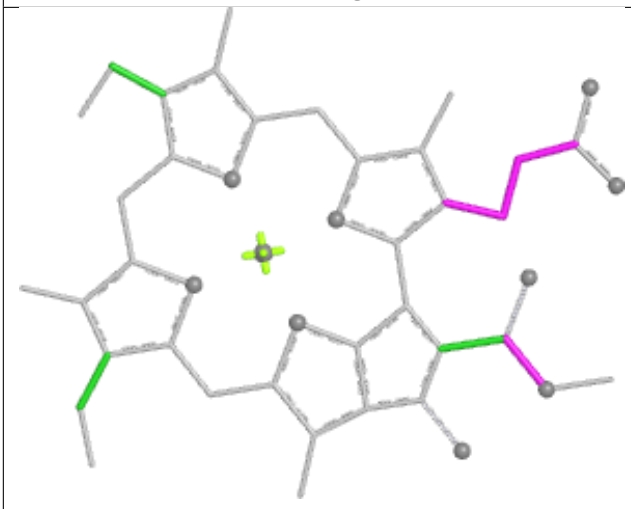
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Bond lengths



Bond angles

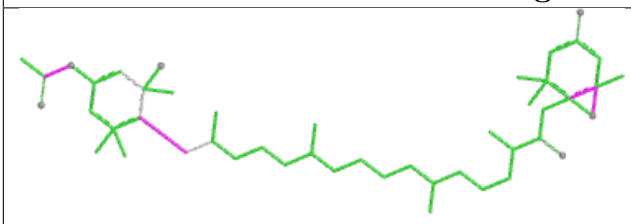


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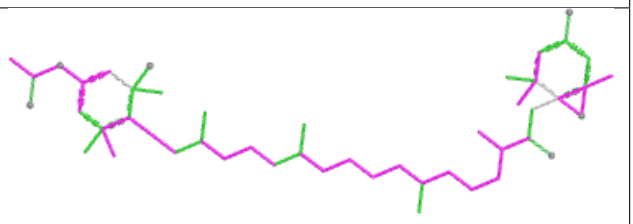


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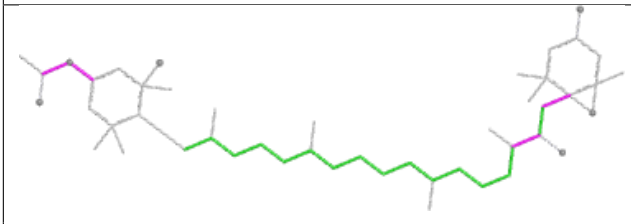
Ligand A86 7 301



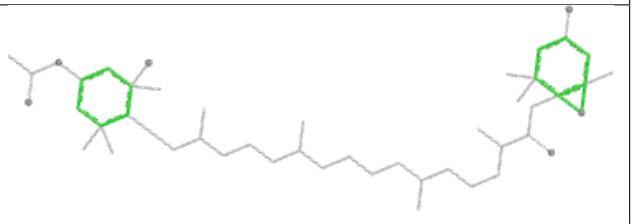
Bond lengths



Bond angles

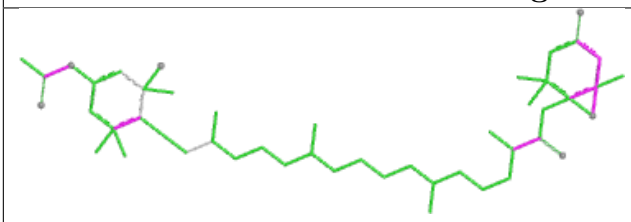


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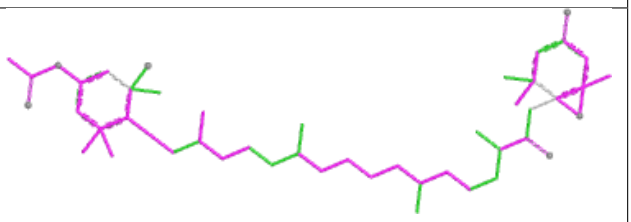


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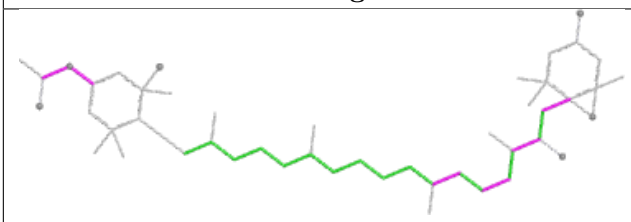
Ligand A86 P 610



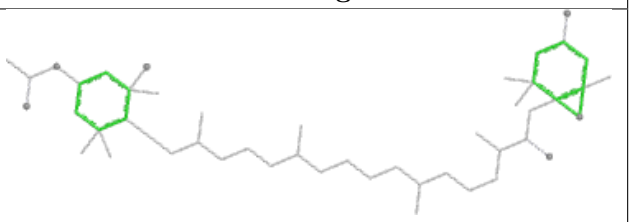
Bond lengths



Bond angles

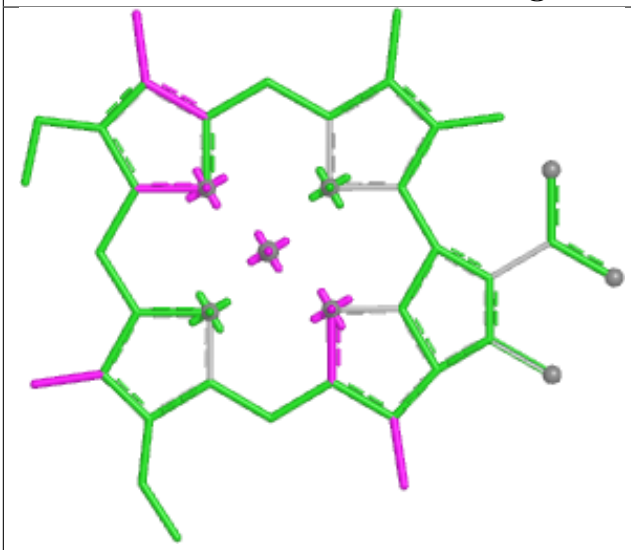


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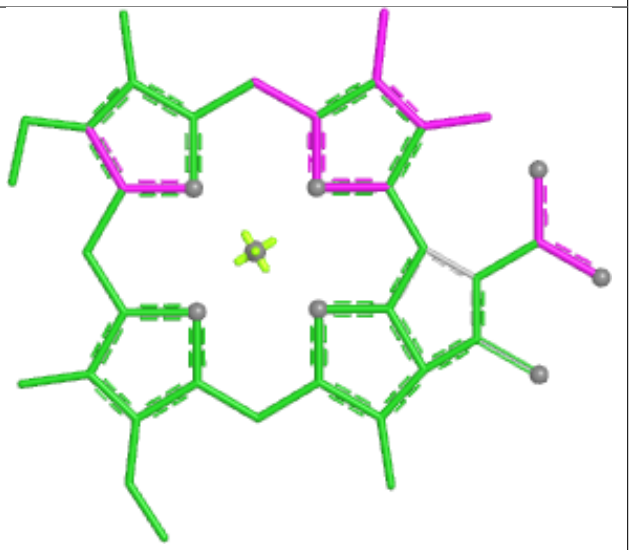


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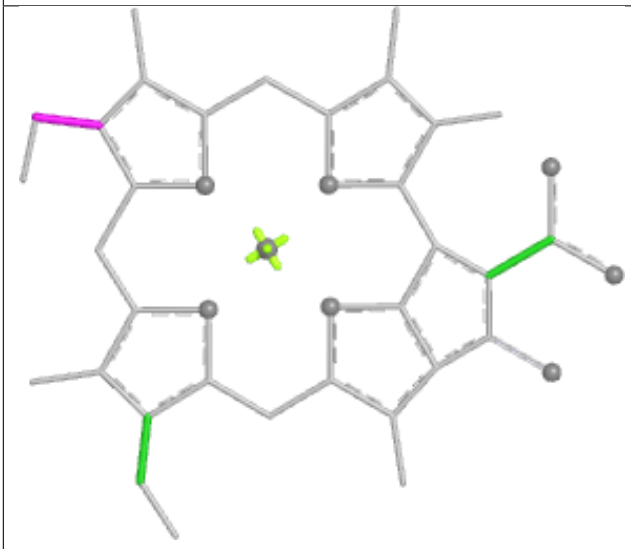
Ligand CLA 3 311



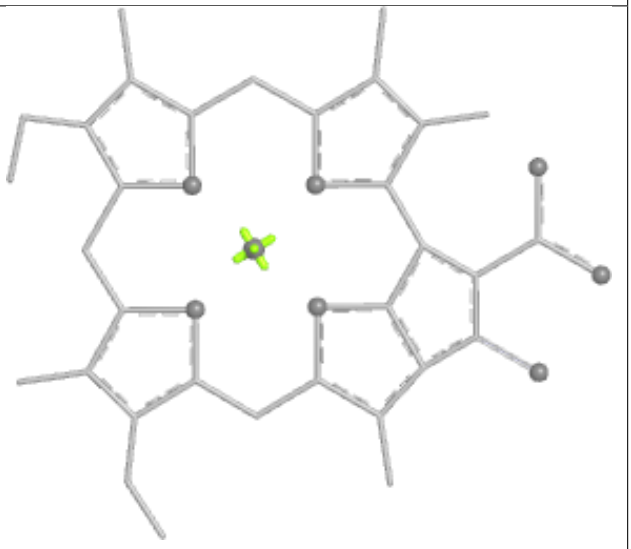
Bond lengths



Bond angles

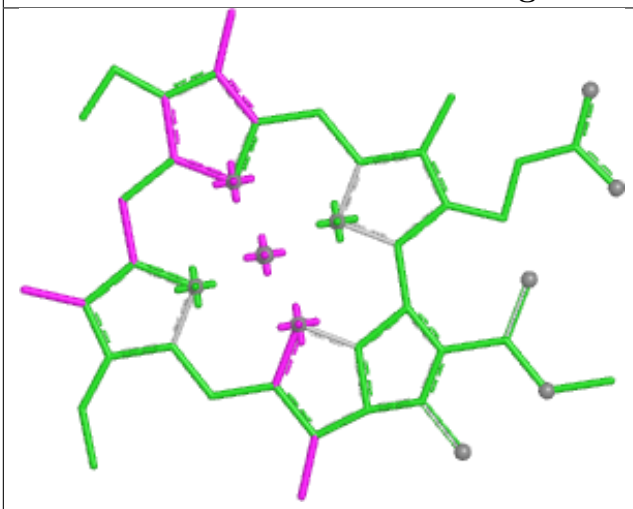


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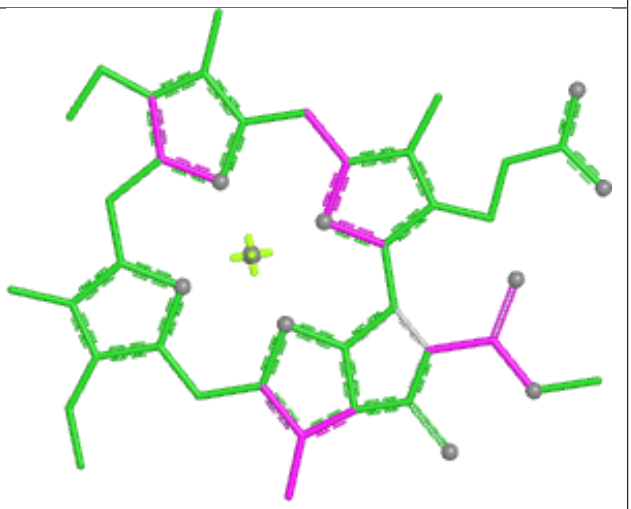


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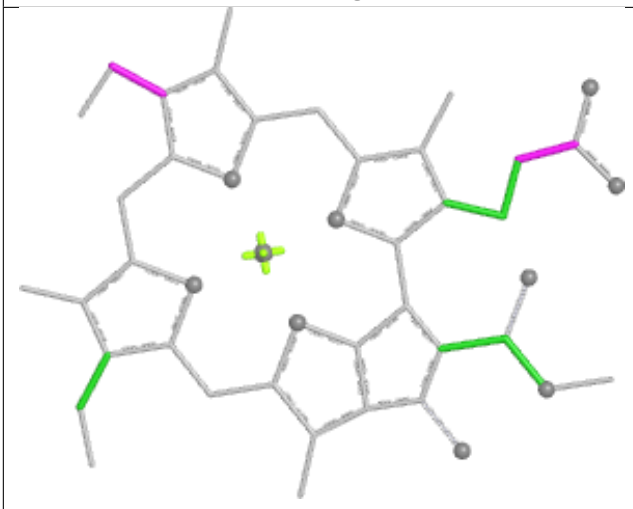
Ligand CLA W 202



Bond lengths



Bond angles

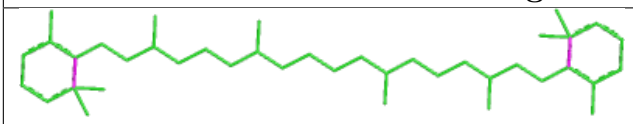


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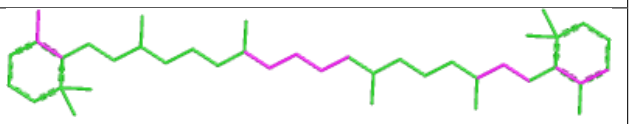


Rings

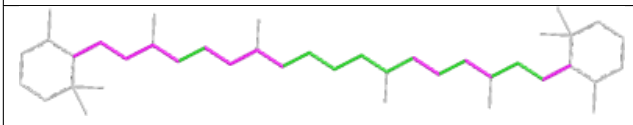
Ligand BCR k 101



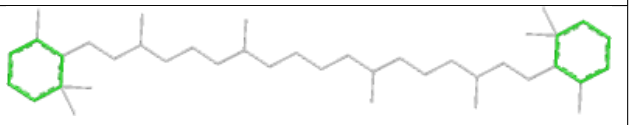
Bond lengths



Bond angles

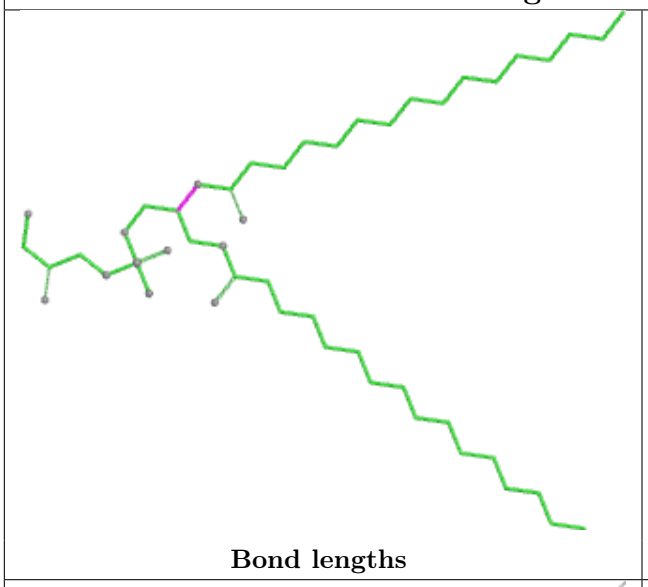


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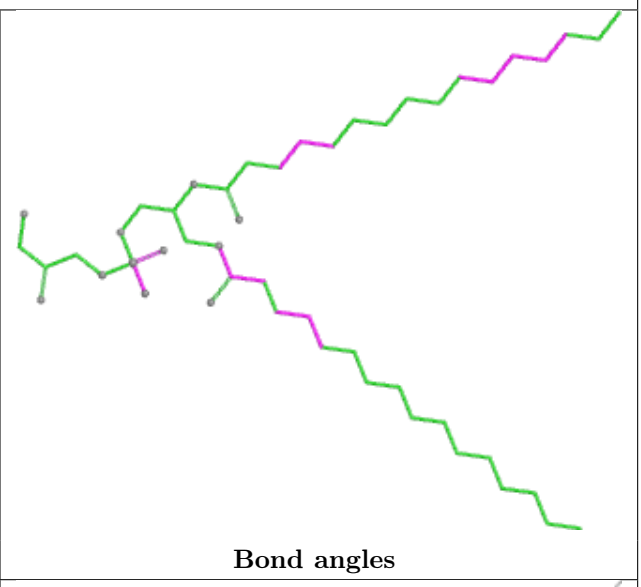


Rings

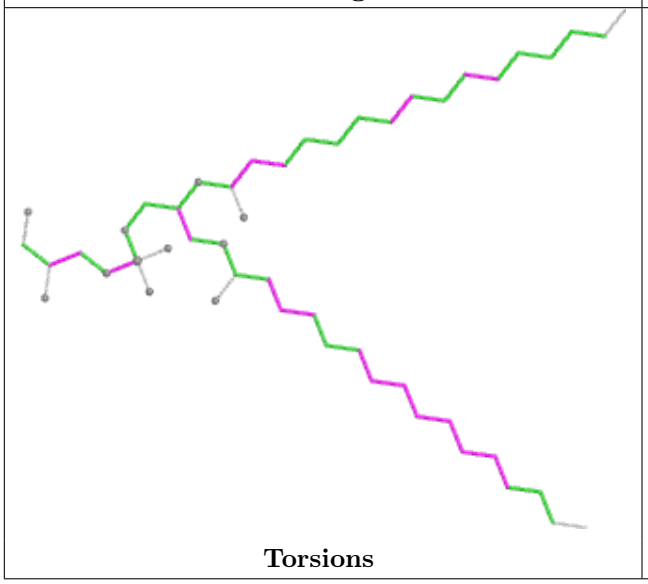
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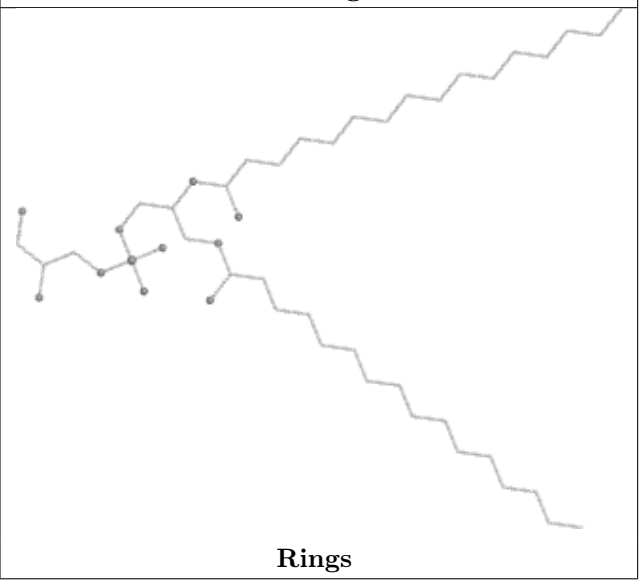
Bond lengths



Bond angles

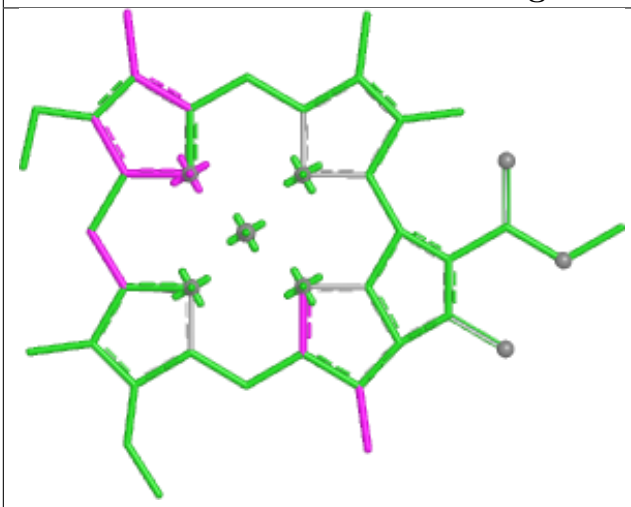


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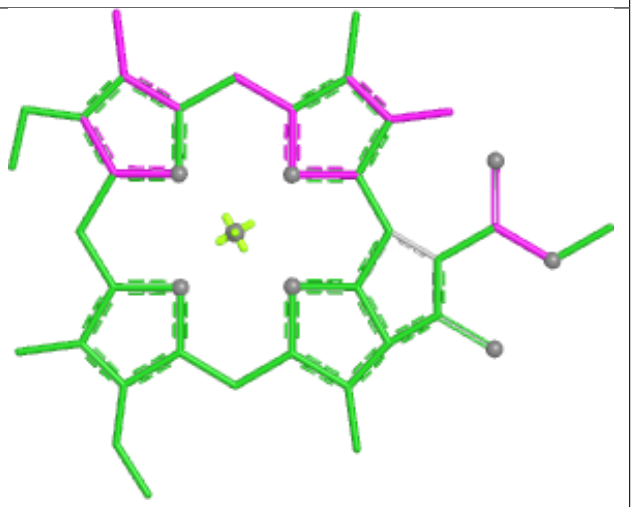


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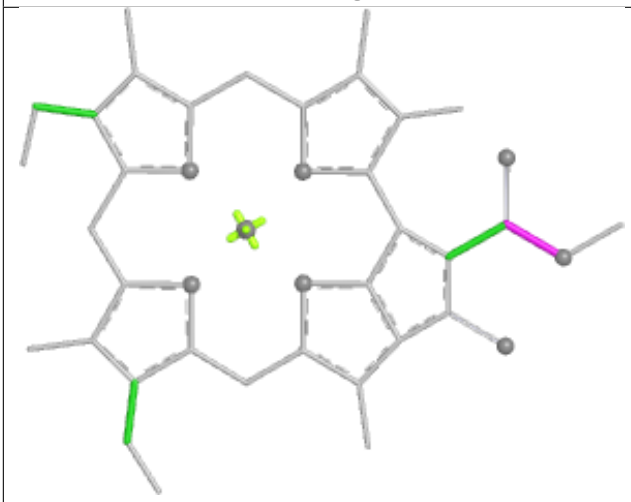
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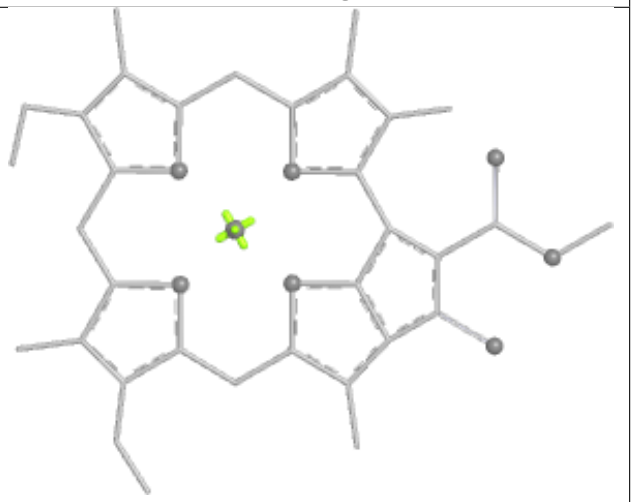
Bond lengths



Bond angles

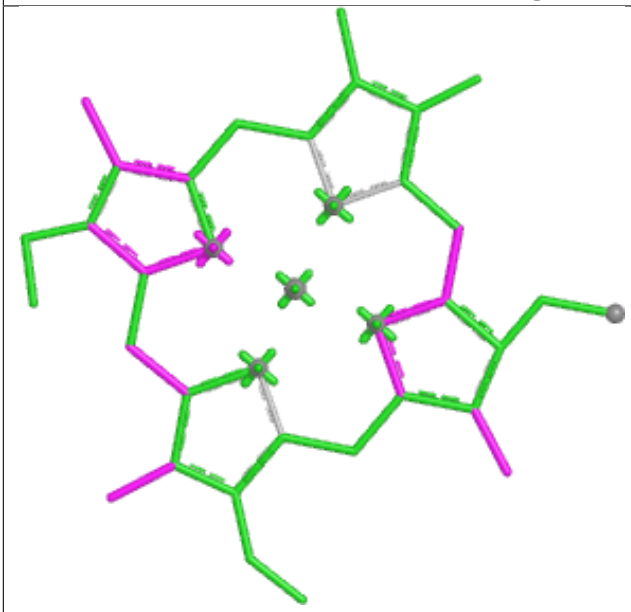


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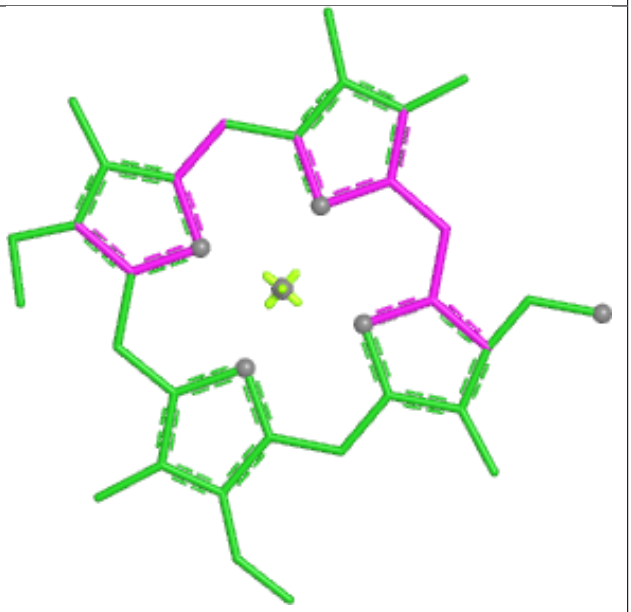


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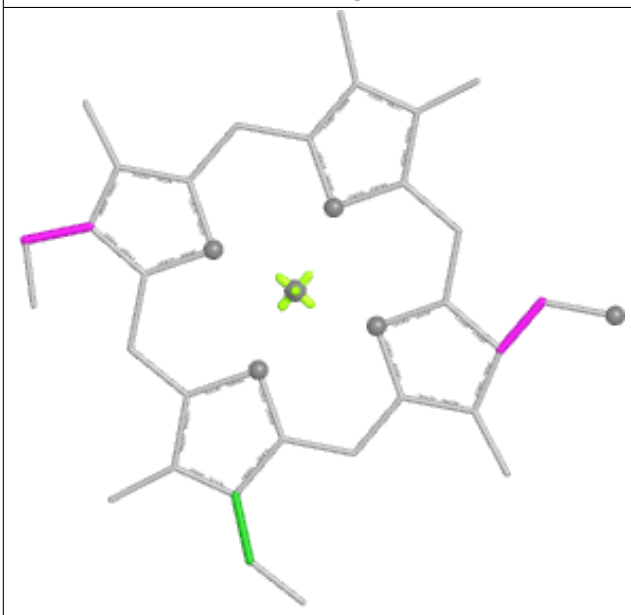
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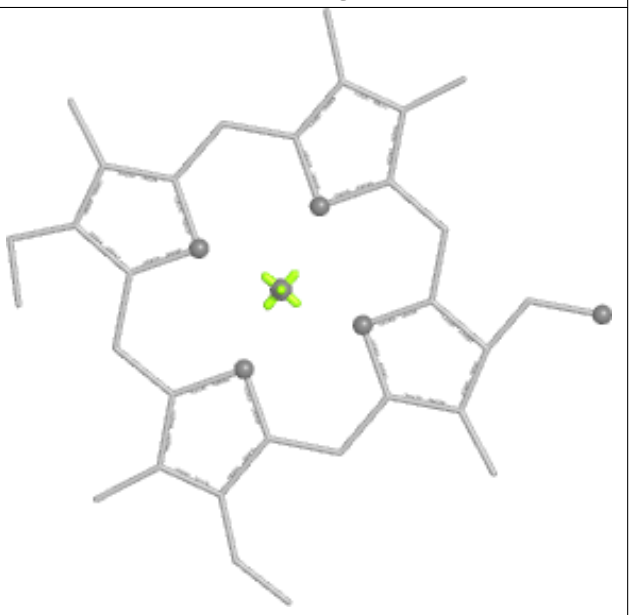
Bond lengths



Bond angles

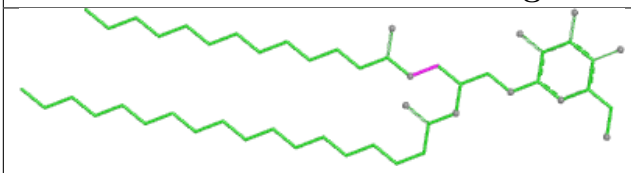


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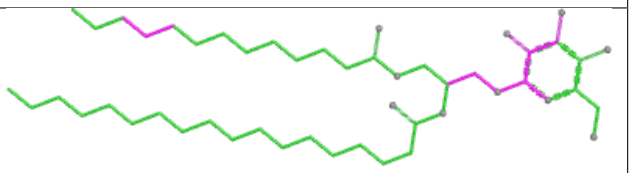


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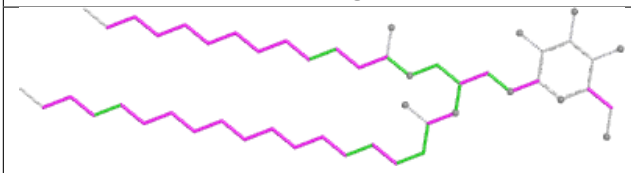
Ligand LMG J 101



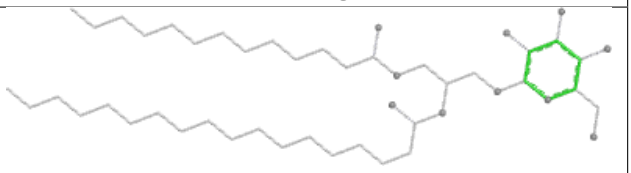
Bond lengths



Bond angles

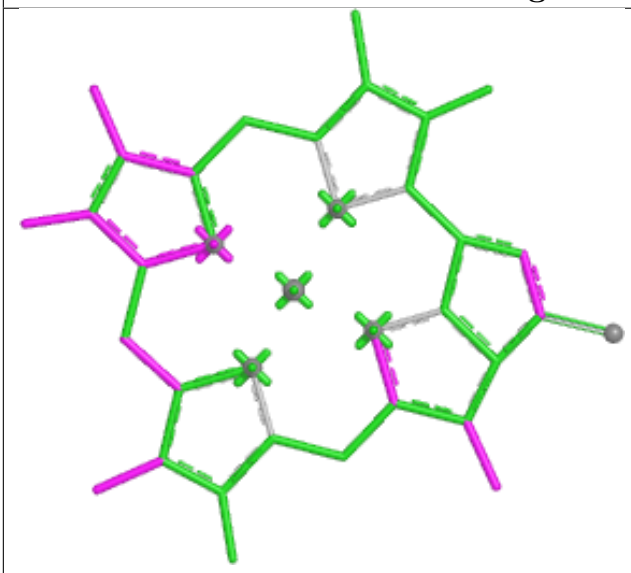


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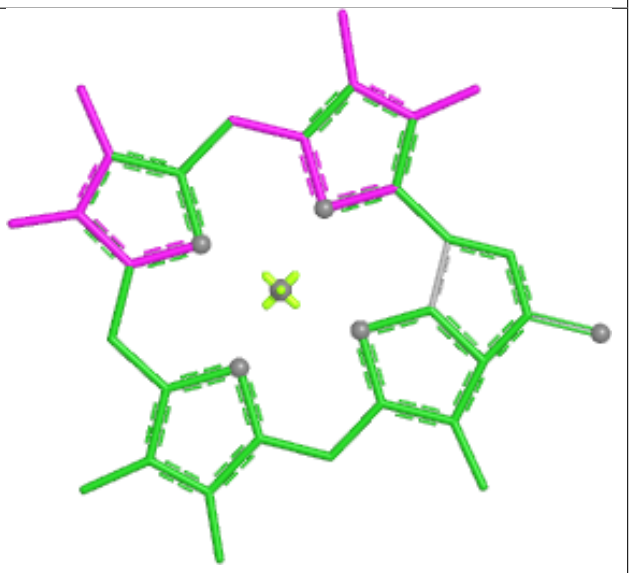


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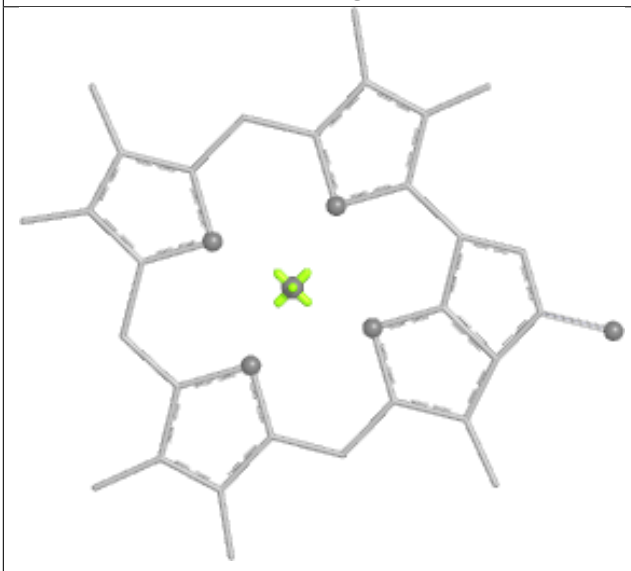
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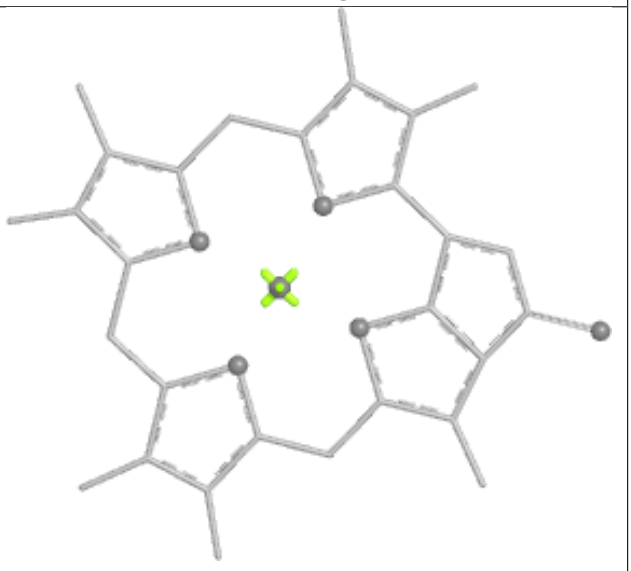
Bond lengths



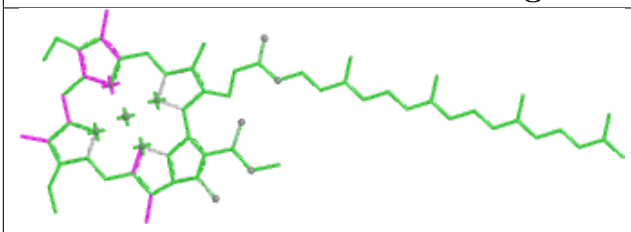
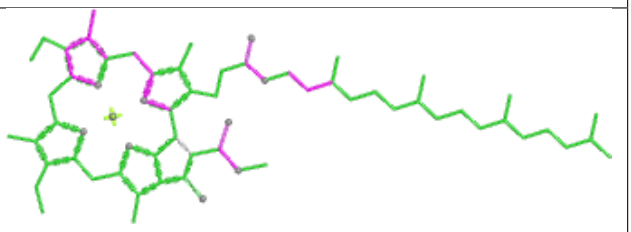
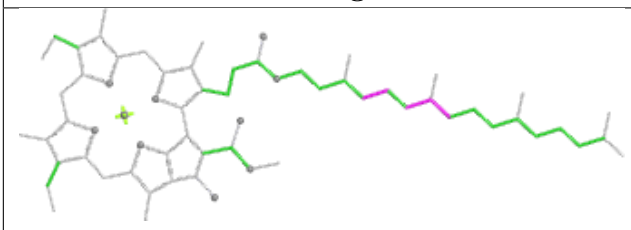
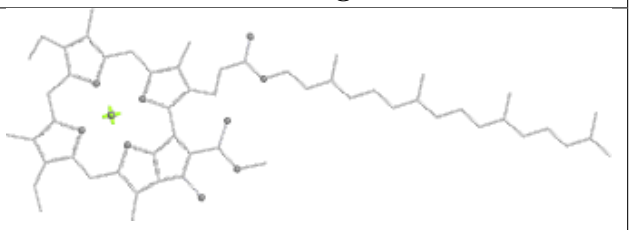
Bond angles



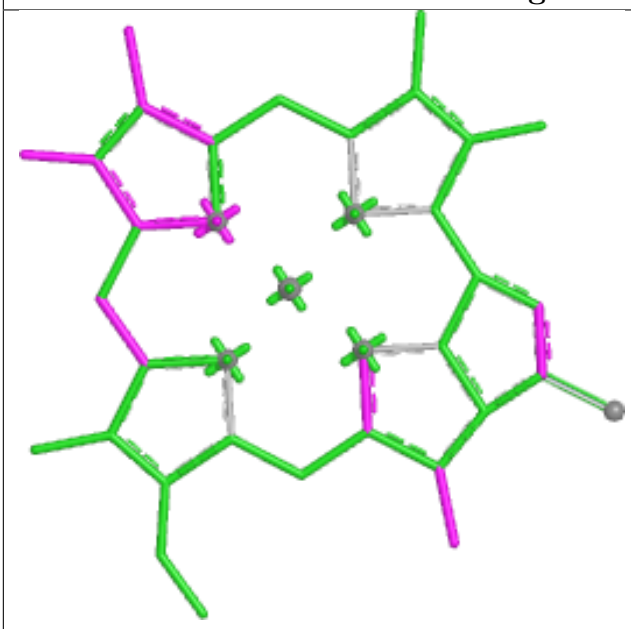
Torsions



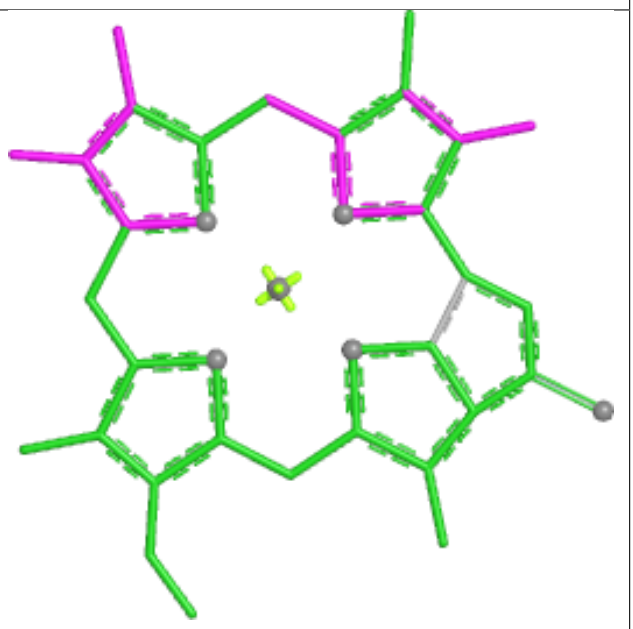
Rings

Ligand CLA C 510	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

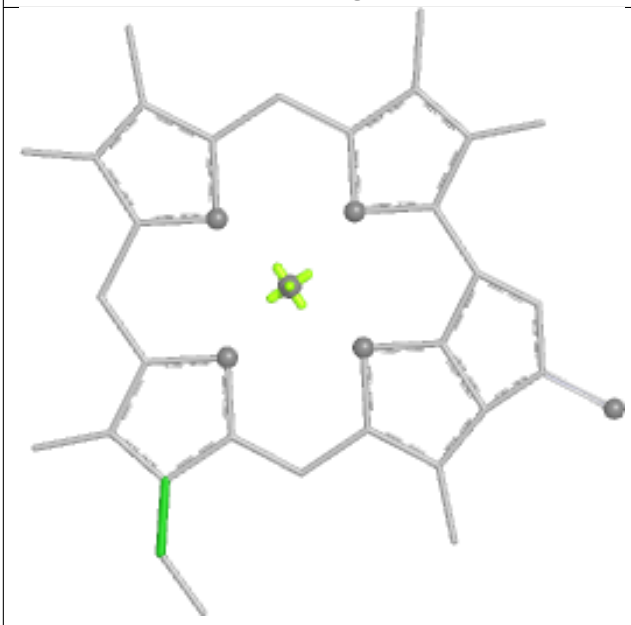
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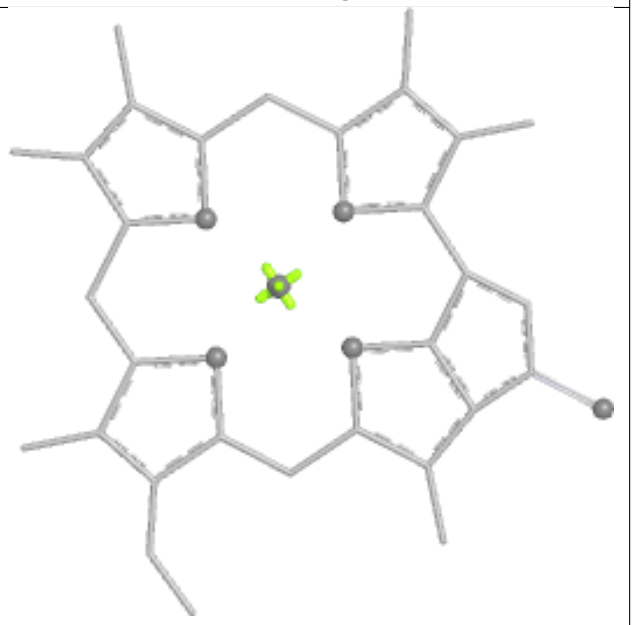
Bond lengths



Bond angles

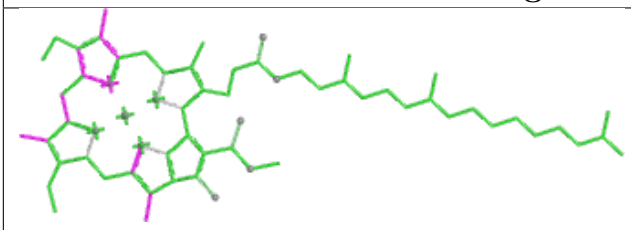


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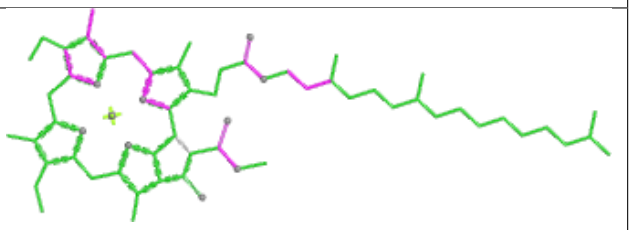


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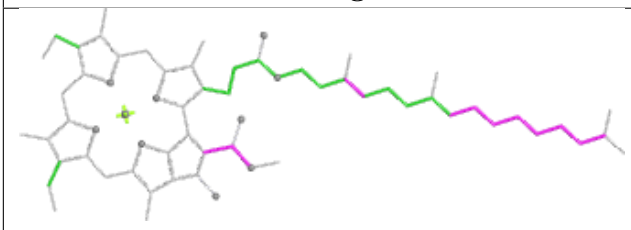
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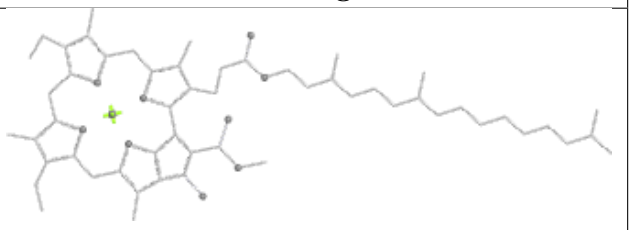
Bond lengths



Bond angles

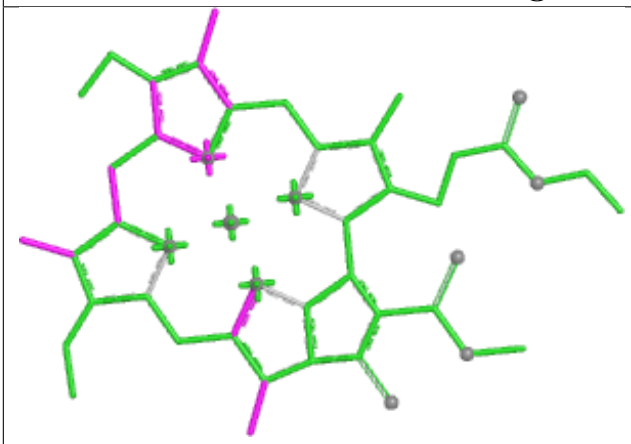


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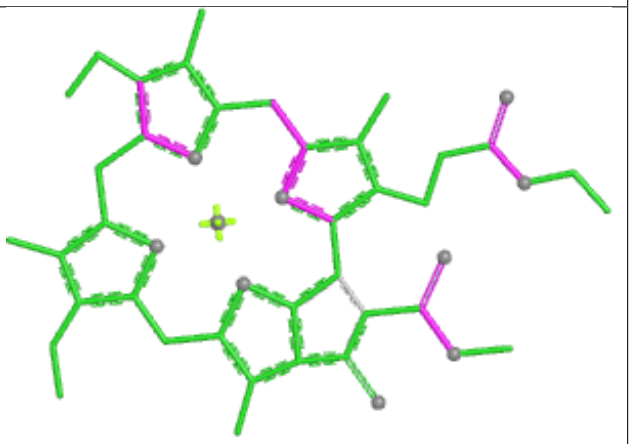


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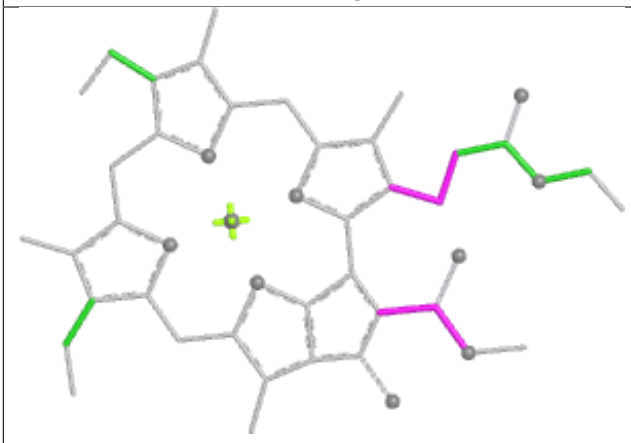
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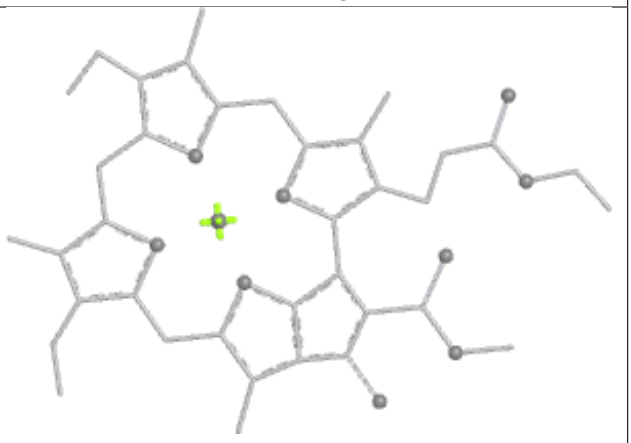
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Bond angles

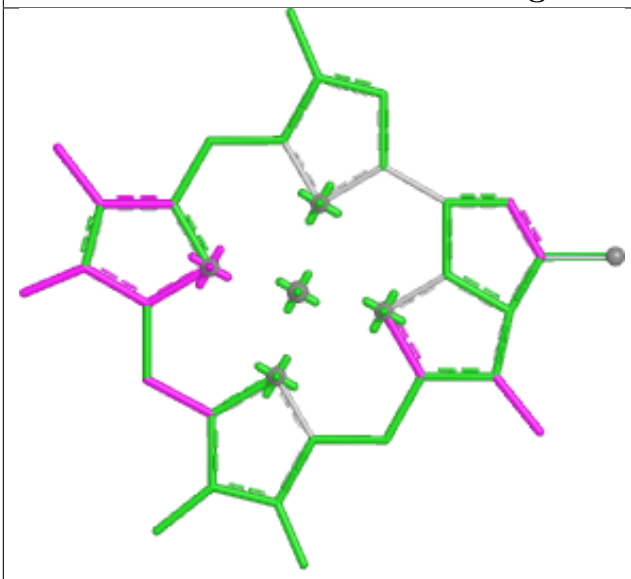


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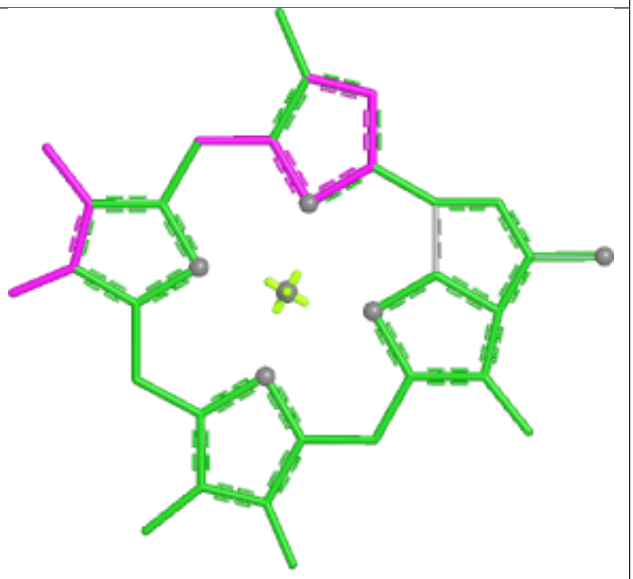


Rings

Ligand CLA 9 211



Bond lengths



Bond angles

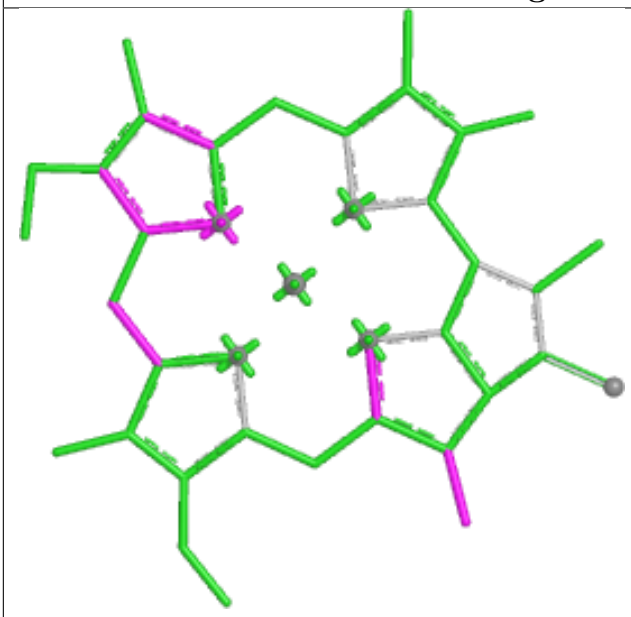


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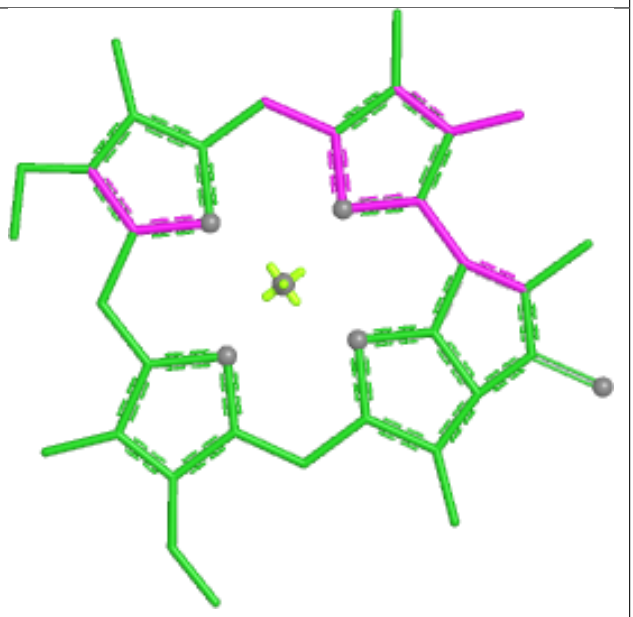


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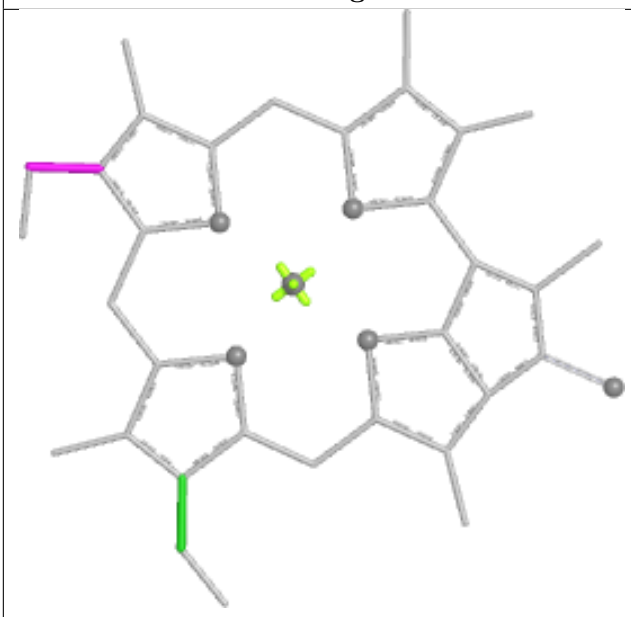
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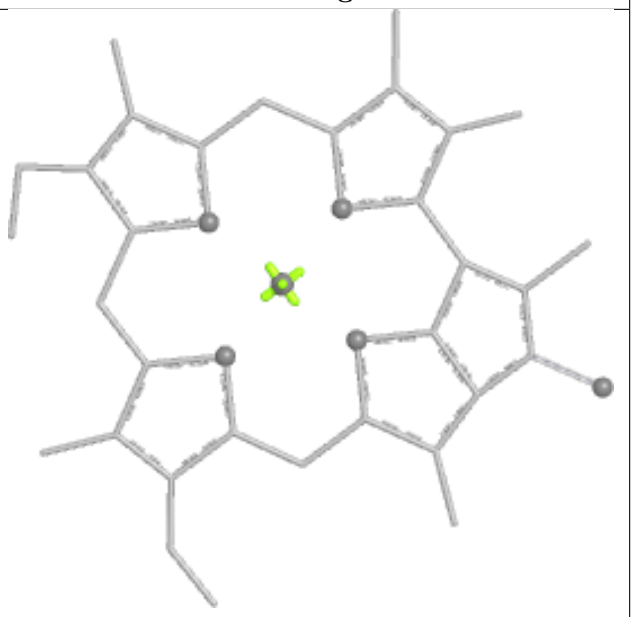
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Bond angles

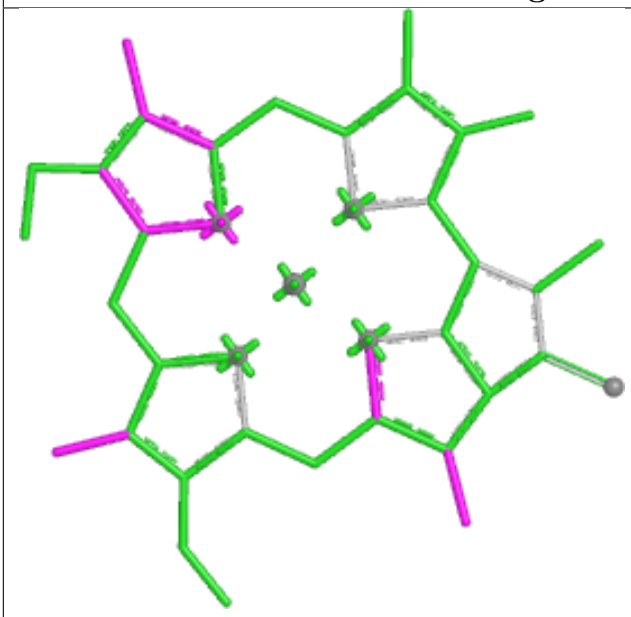


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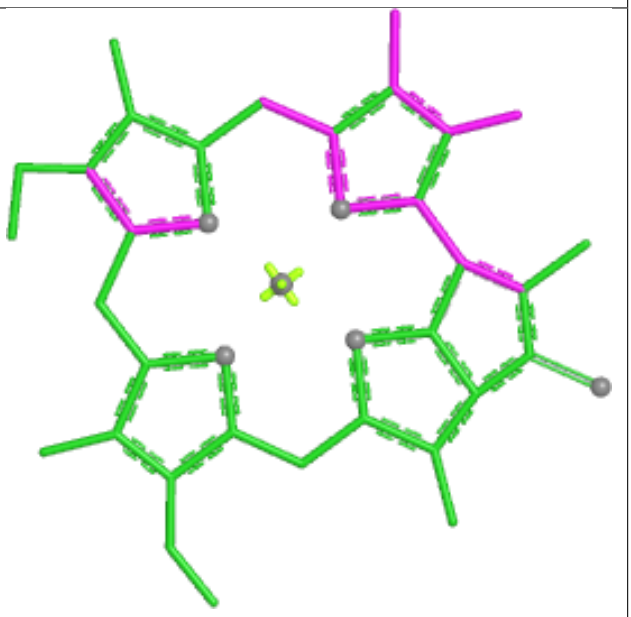


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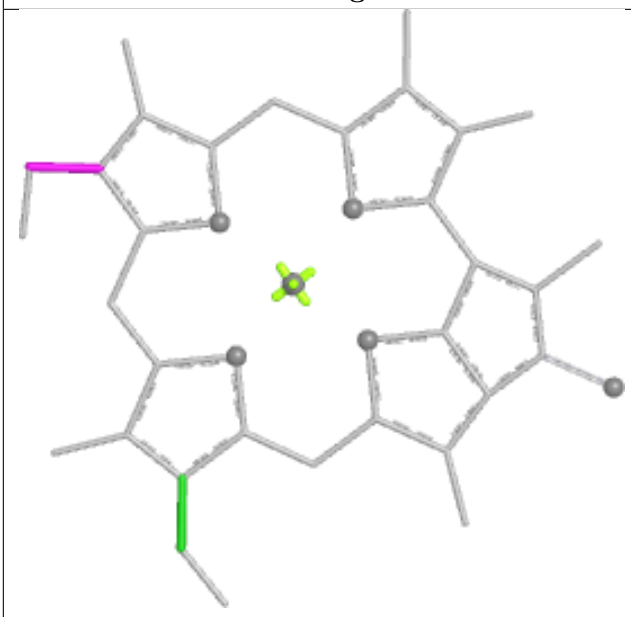
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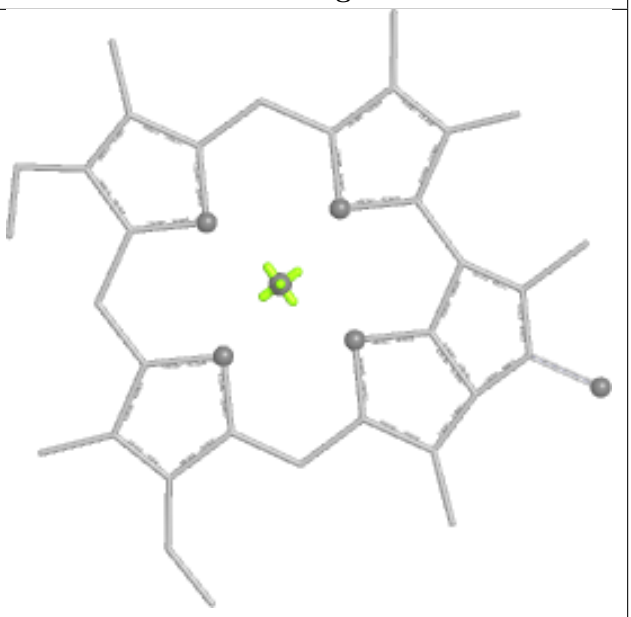
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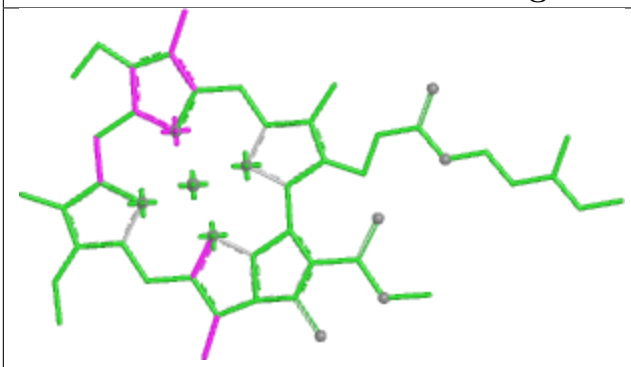


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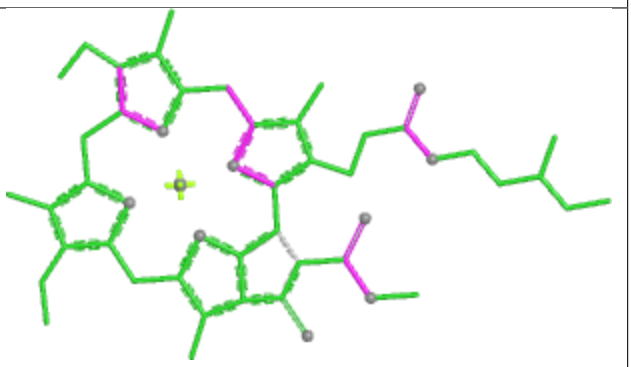


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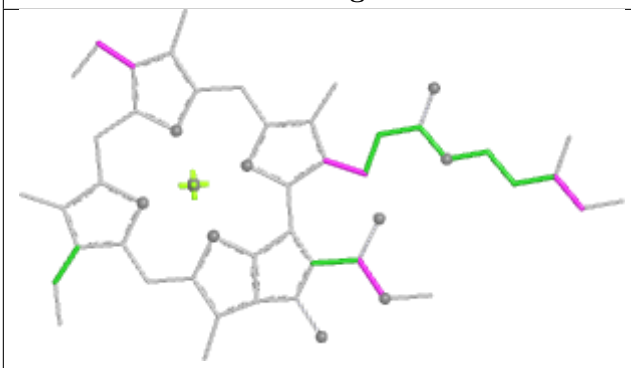
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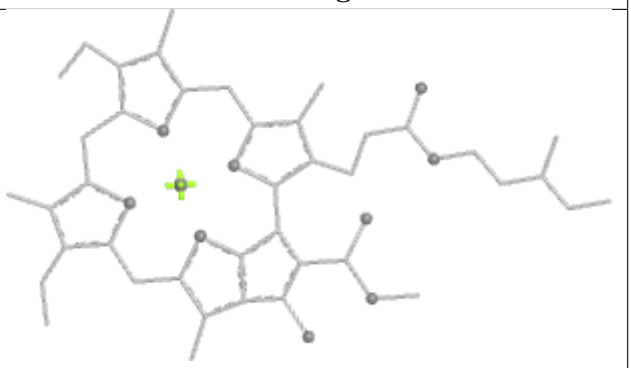
Bond lengths



Bond angles

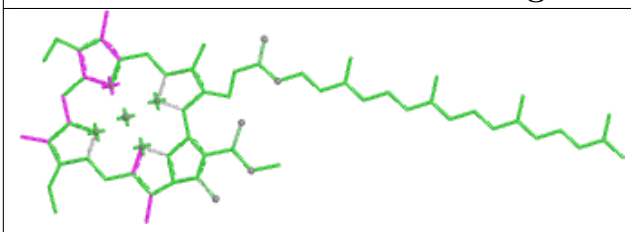


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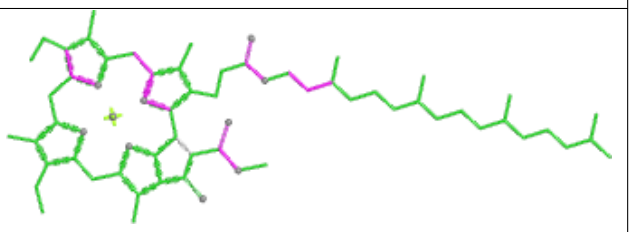


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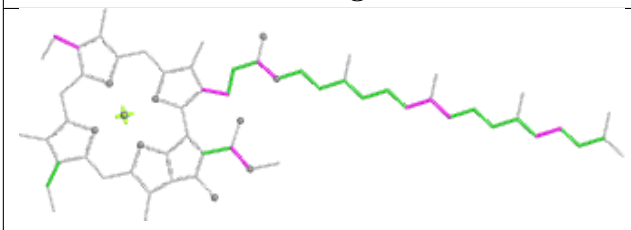
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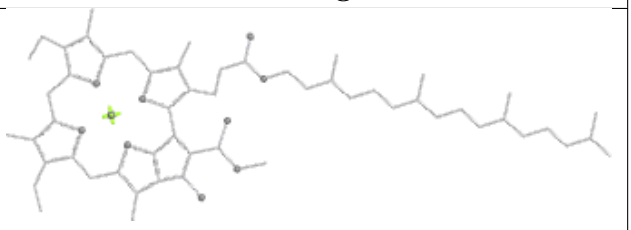
Bond lengths



Bond angles

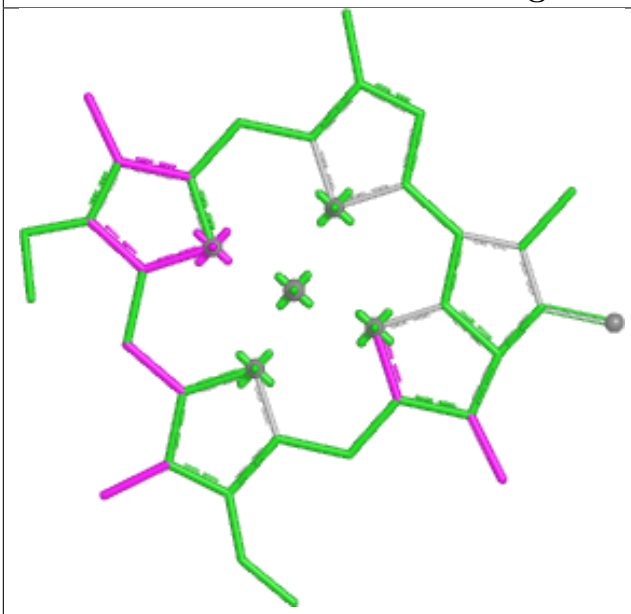


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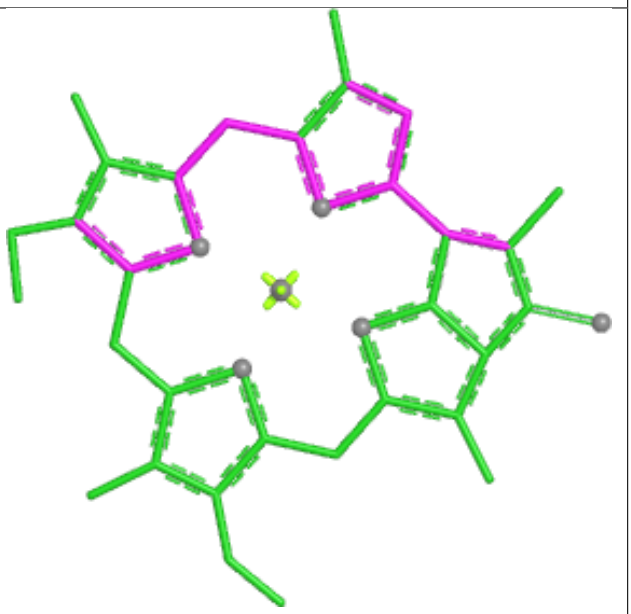


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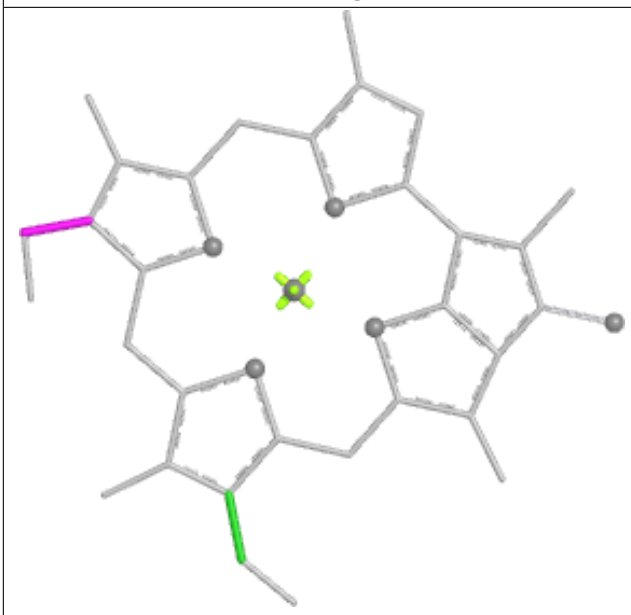
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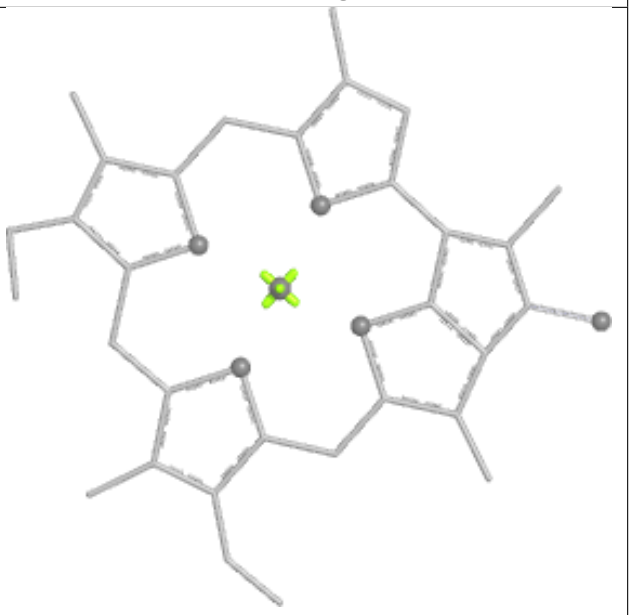
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Bond angles

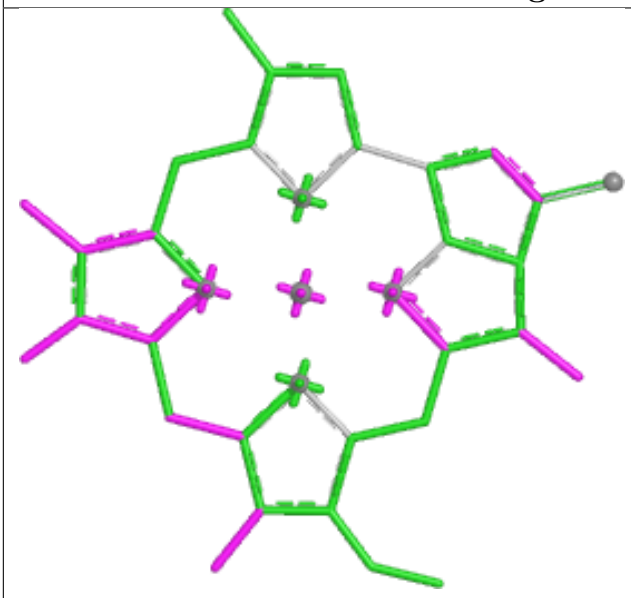


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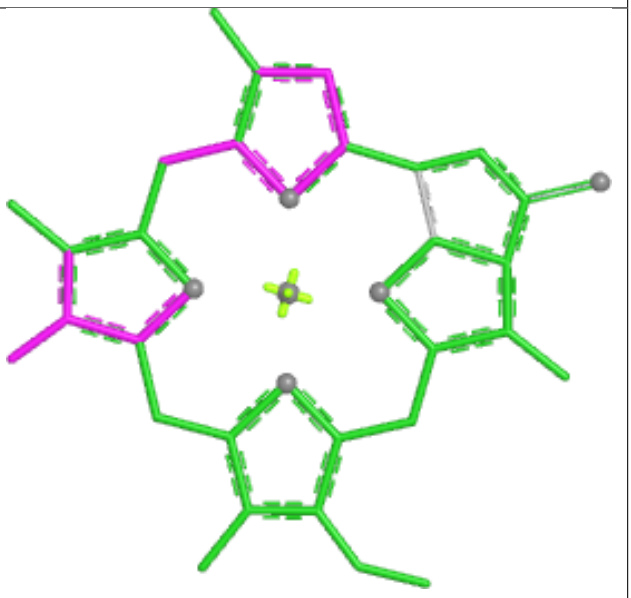


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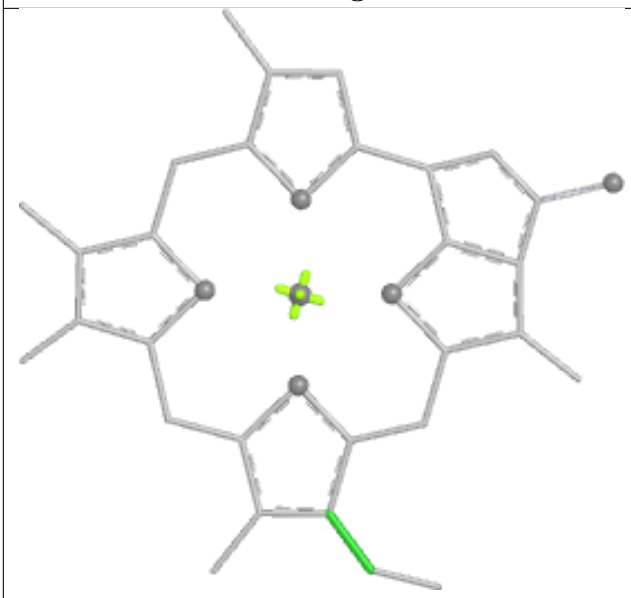
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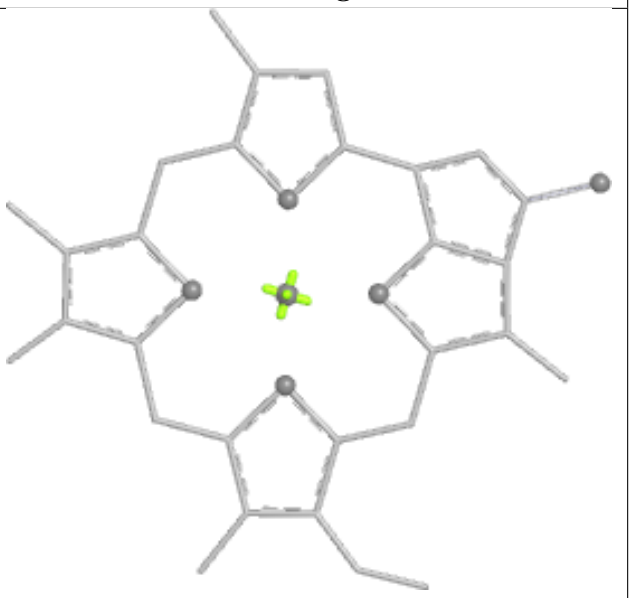
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Bond angles

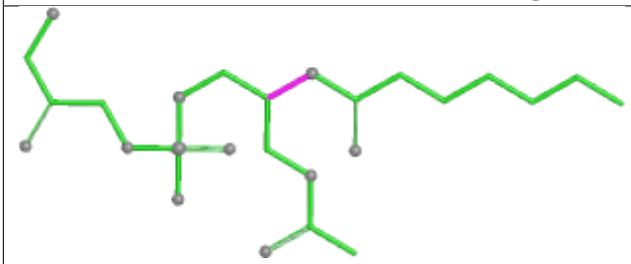


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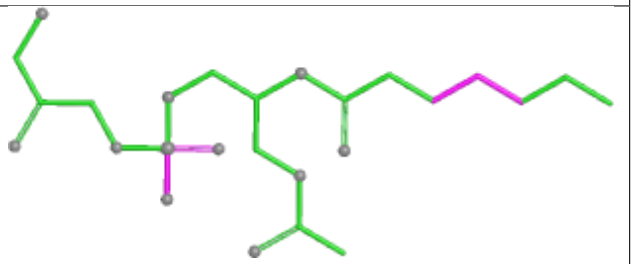


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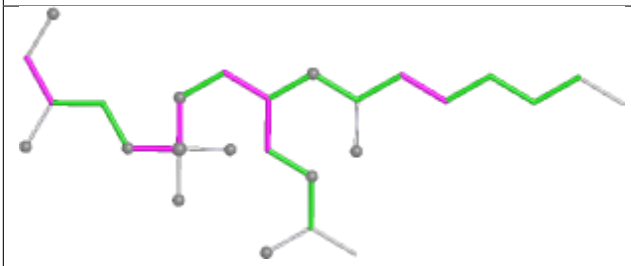
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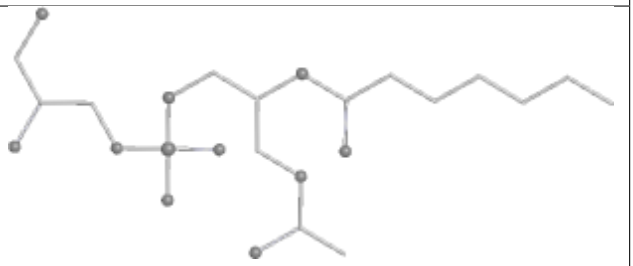
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Bond angles

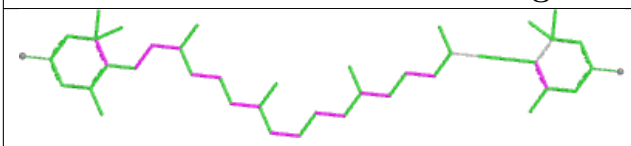


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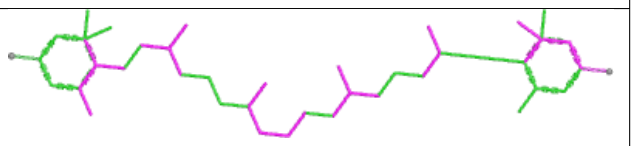


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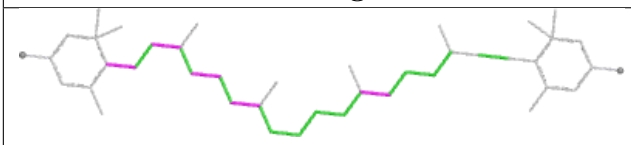
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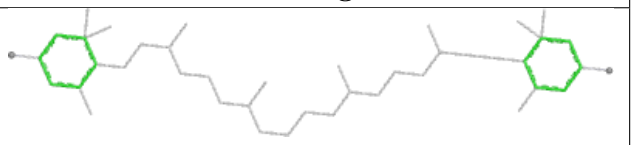
Bond lengths



Bond angles

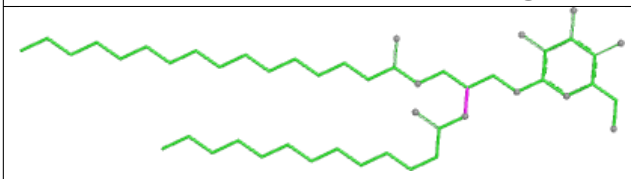


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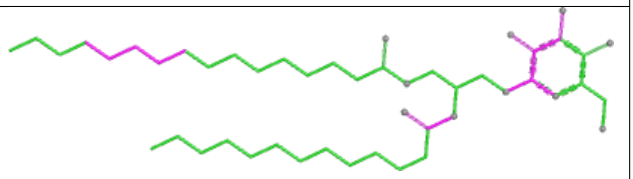


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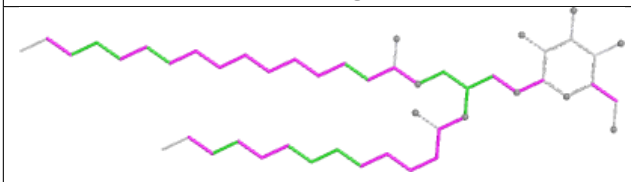
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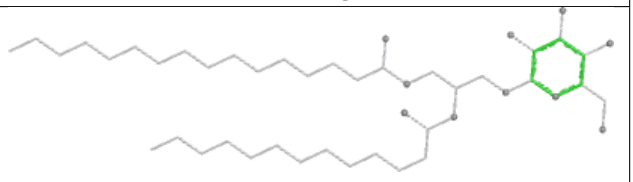
Bond lengths



Bond angles

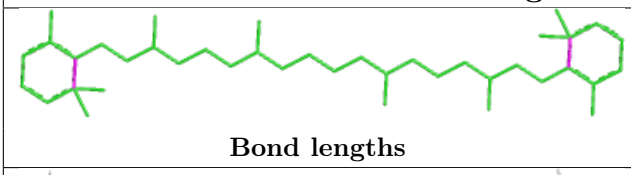


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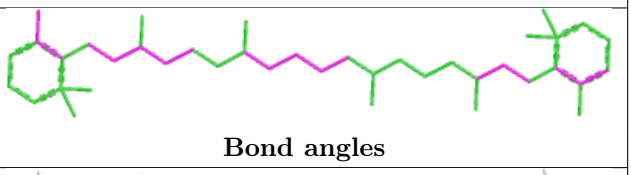


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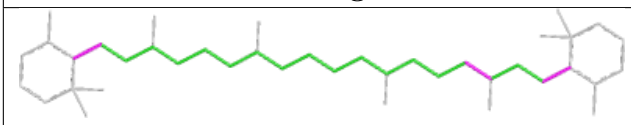
Ligand BCR b 518



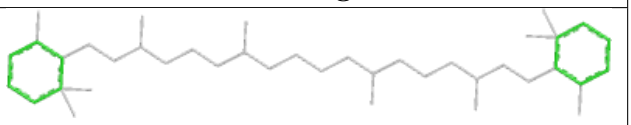
Bond lengths



Bond angles



Torsions

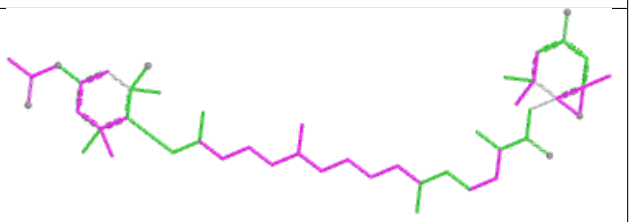


Rings

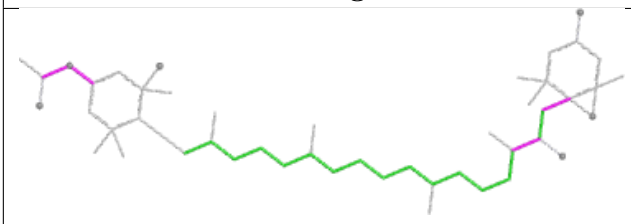
Ligand A86 7 302



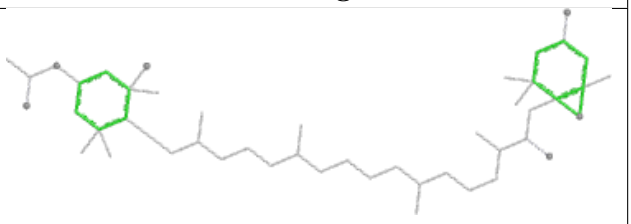
Bond lengths



Bond angles

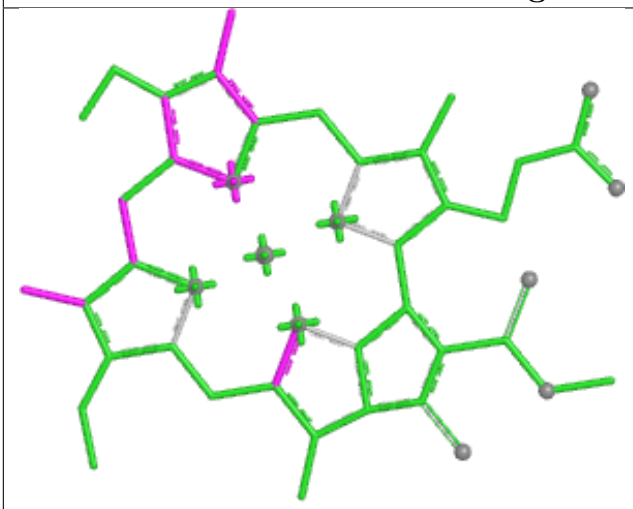


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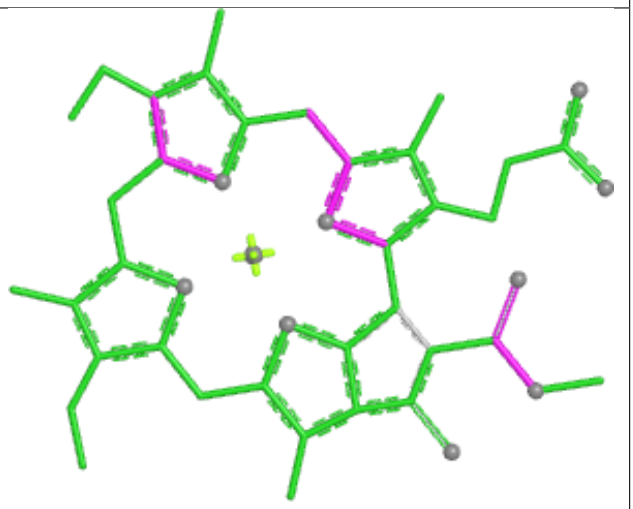


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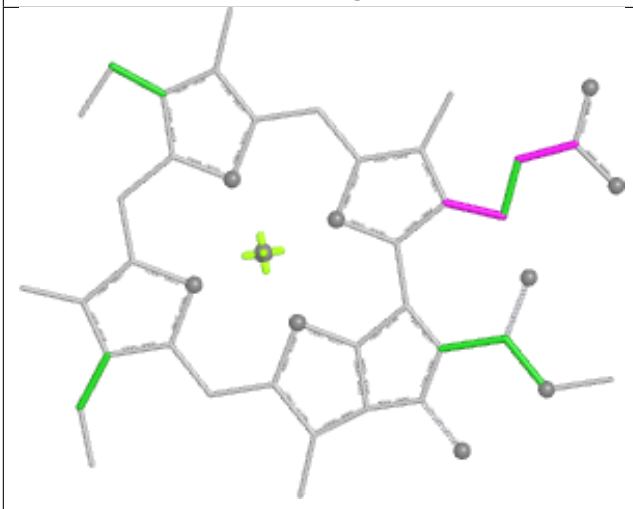
Ligand CLA 2 306



Bond lengths



Bond angles

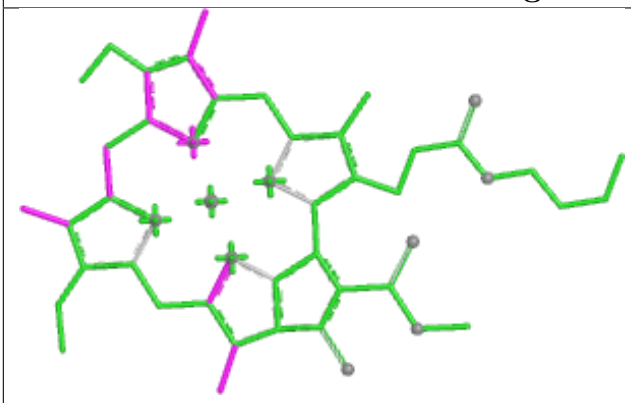


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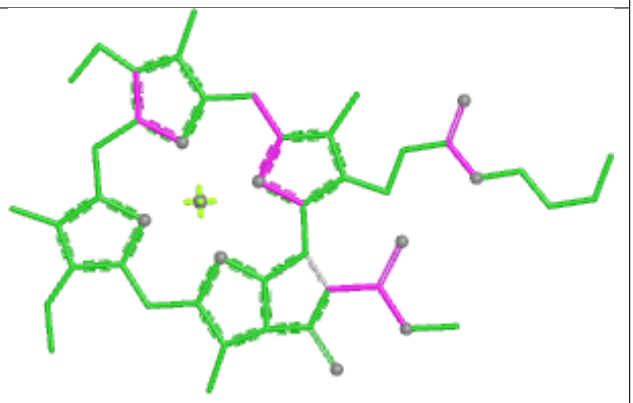


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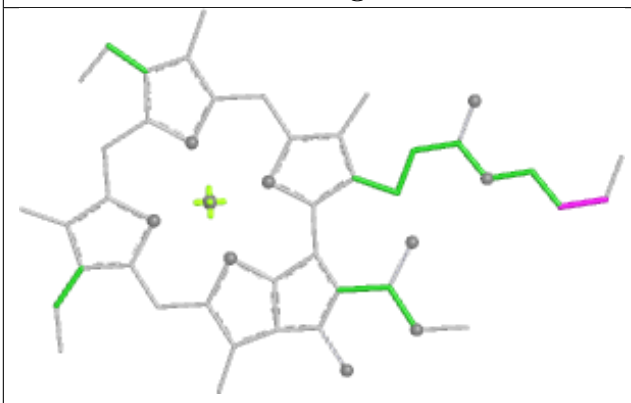
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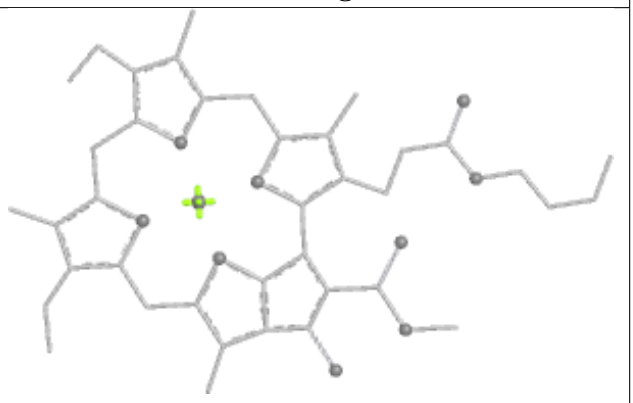
Bond lengths



Bond angles



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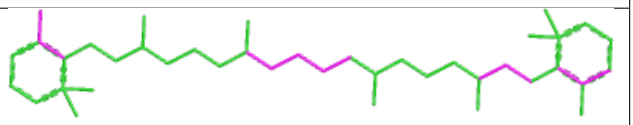


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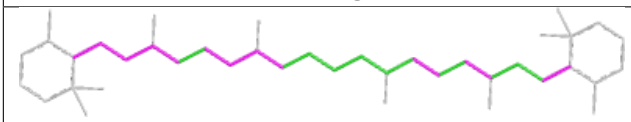
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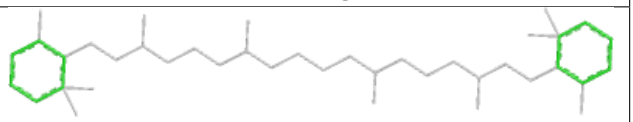
Bond lengths



Bond angles

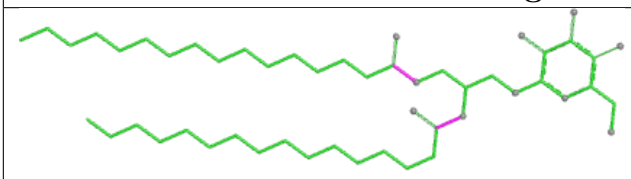


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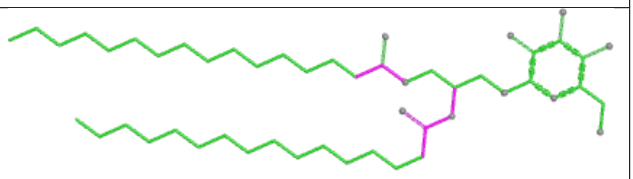


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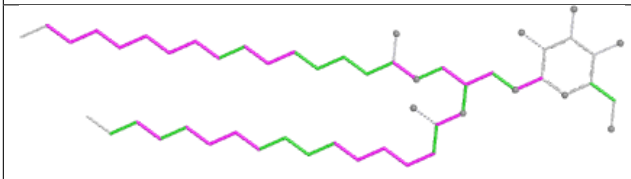
Ligand LMG c 521



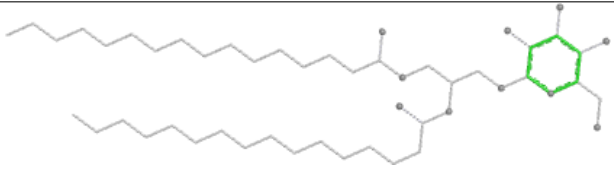
Bond lengths



Bond angles

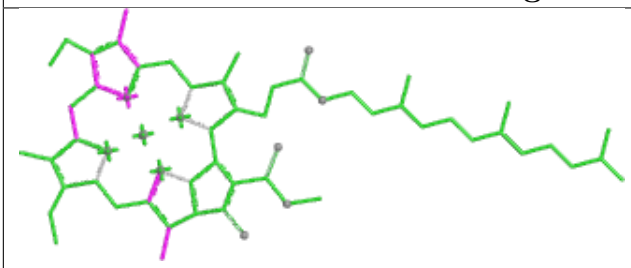


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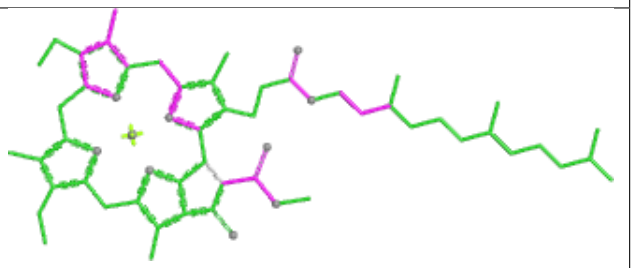


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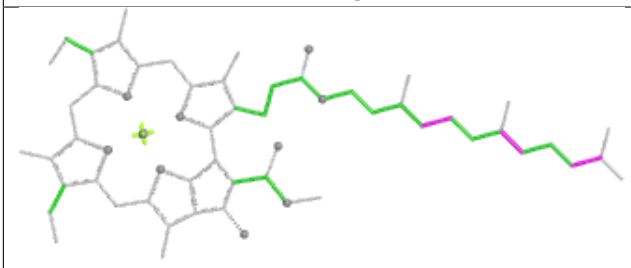
Ligand CLA A 407



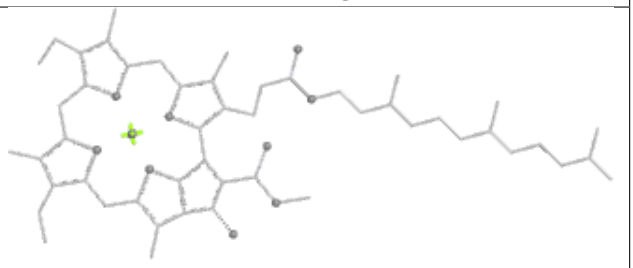
Bond lengths



Bond angles

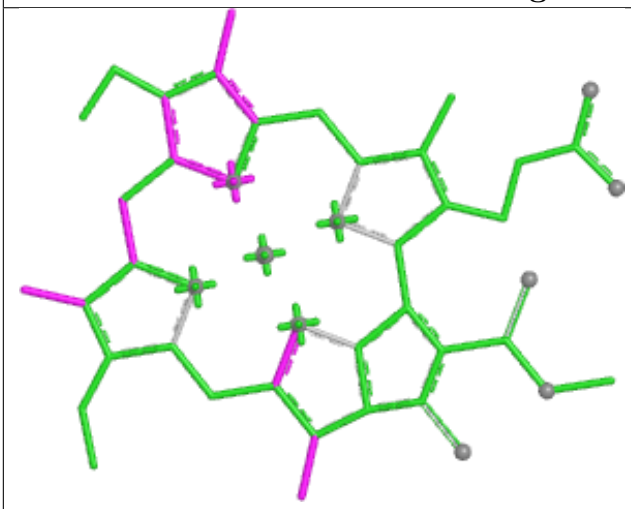


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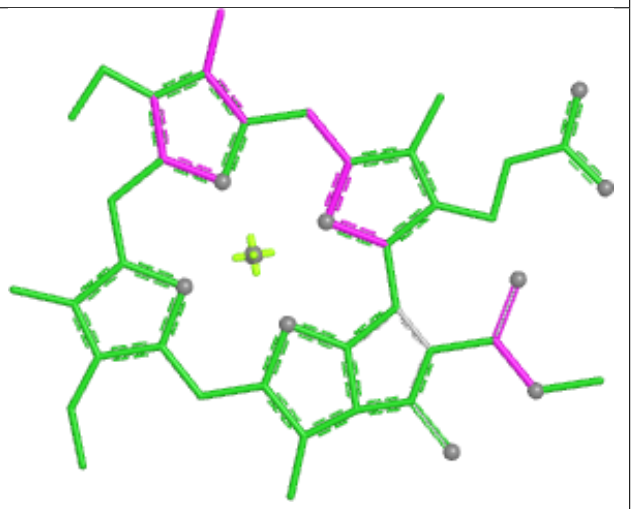


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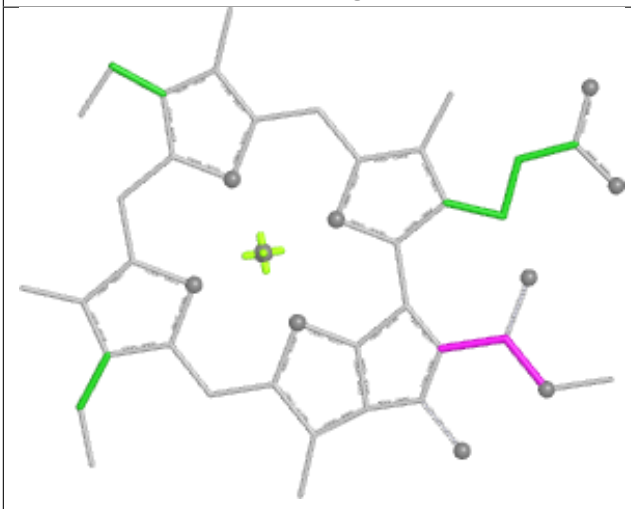
Ligand CLA c 507



Bond lengths



Bond angles

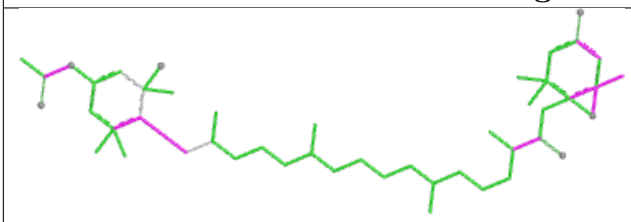


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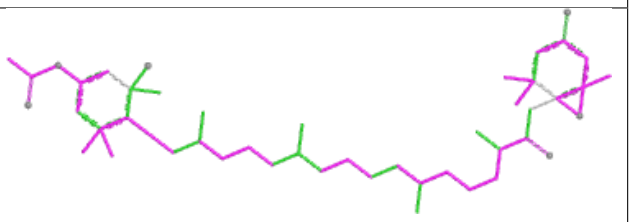


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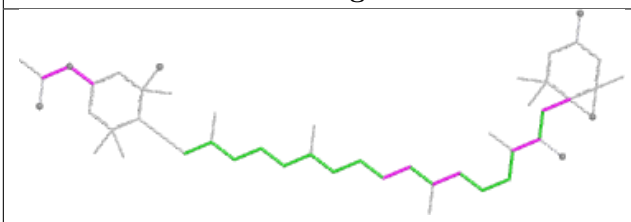
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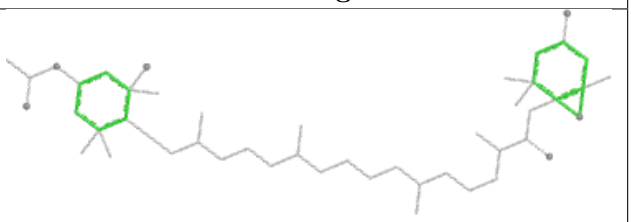
Bond lengths



Bond angles

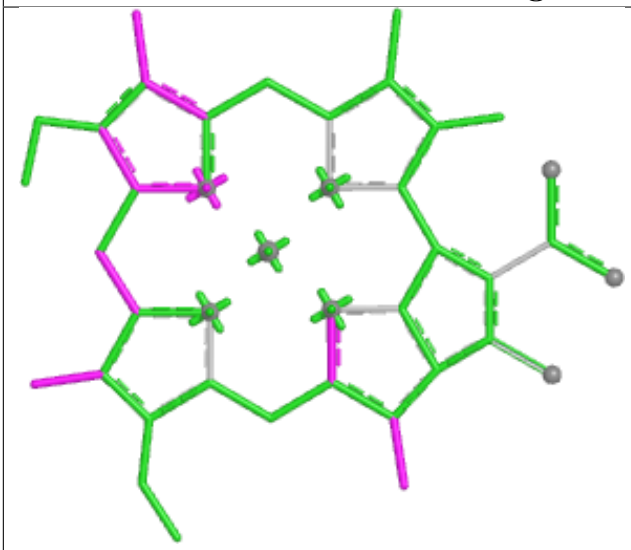


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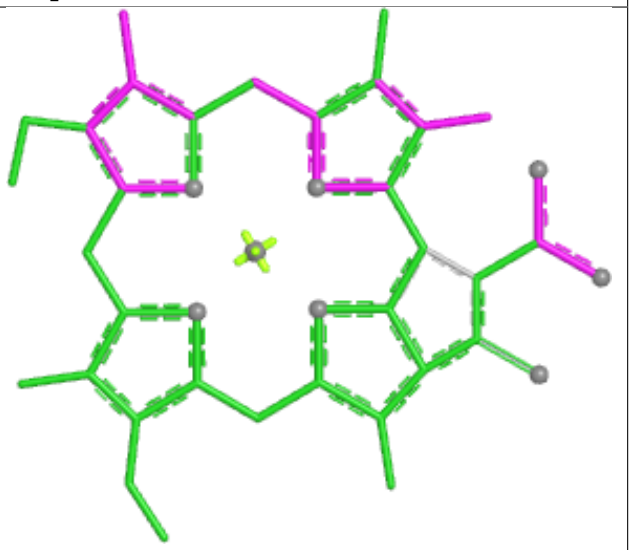


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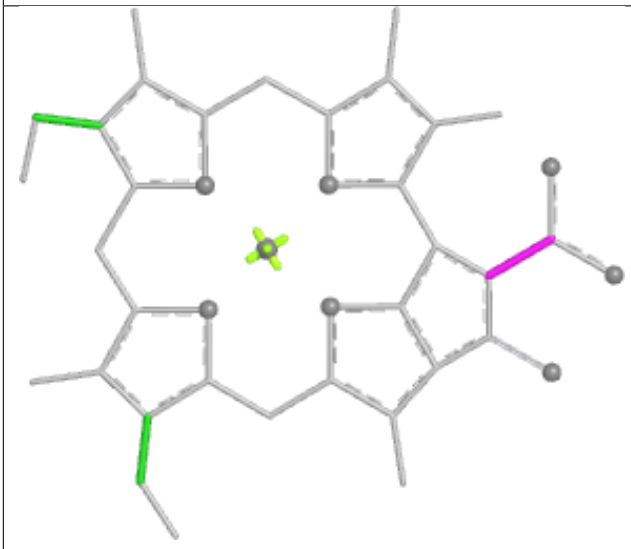
Ligand CLA p 604



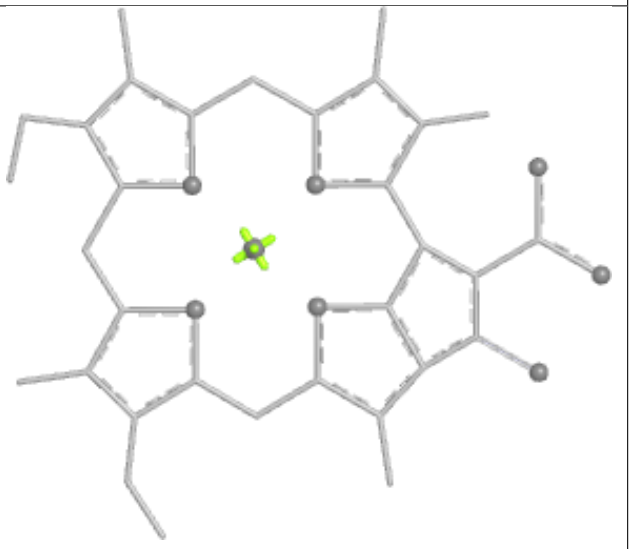
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Bond angles

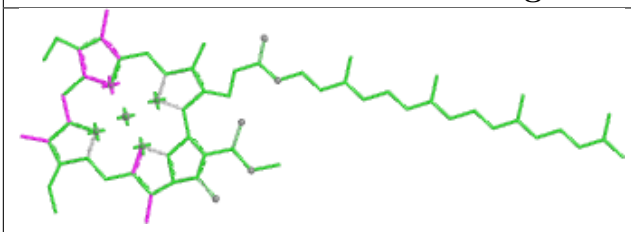


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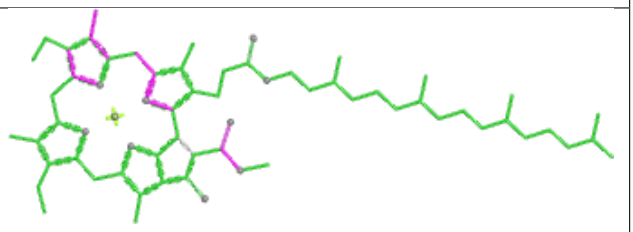


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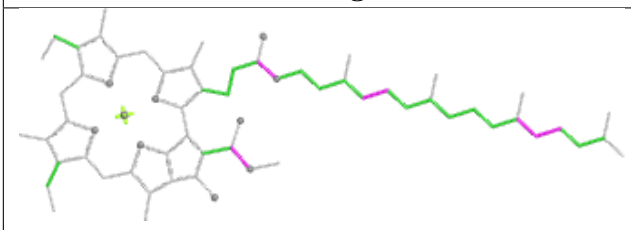
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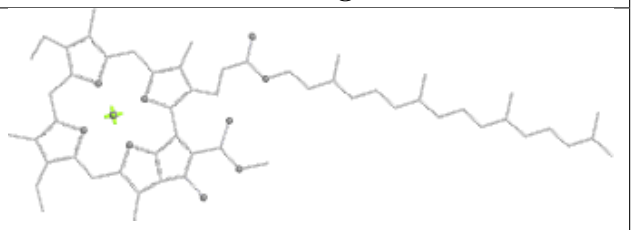
Bond lengths



Bond angles



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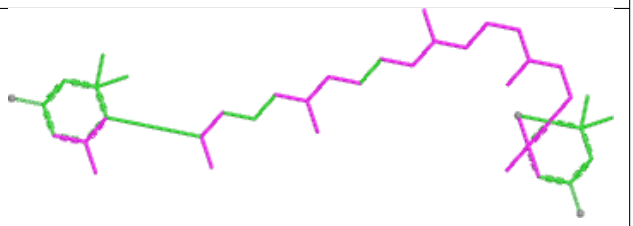


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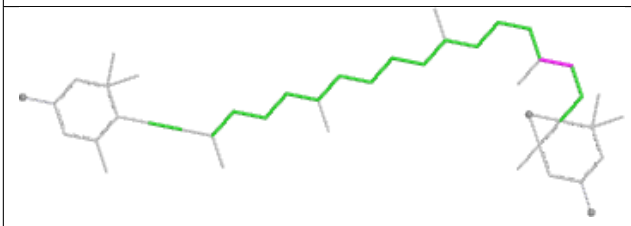
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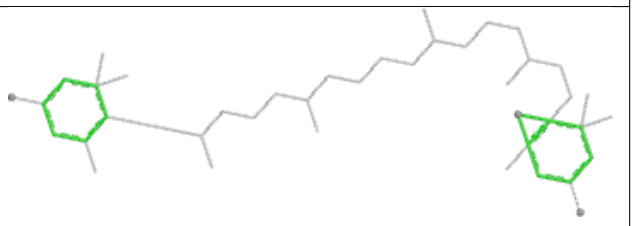
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Bond angles

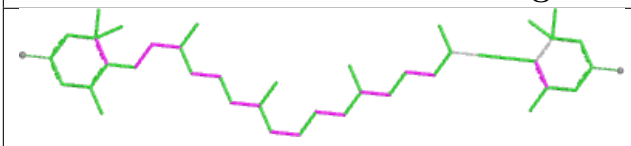


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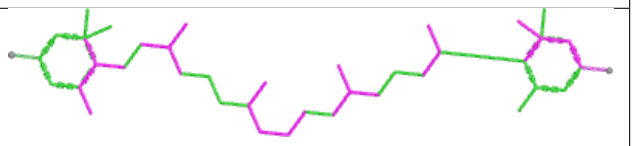


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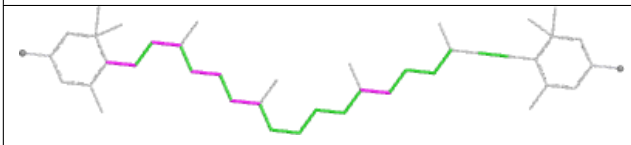
Ligand ET4 5 302



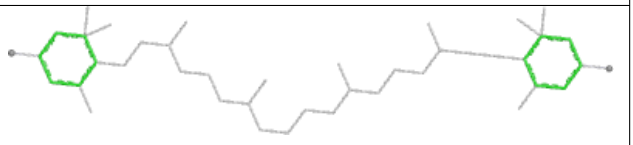
Bond lengths



Bond angles

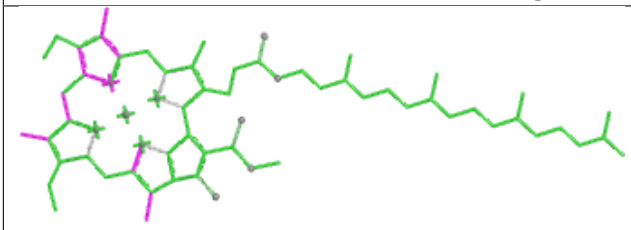


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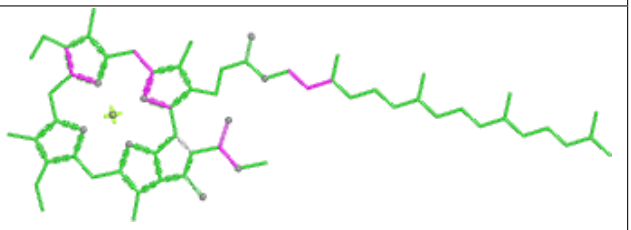


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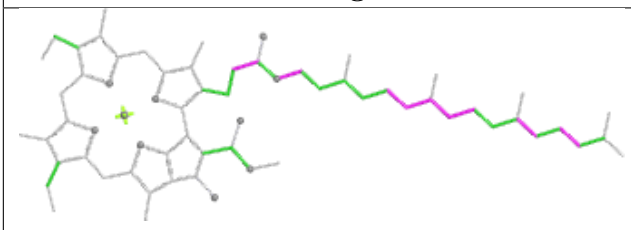
Ligand CLA c 511



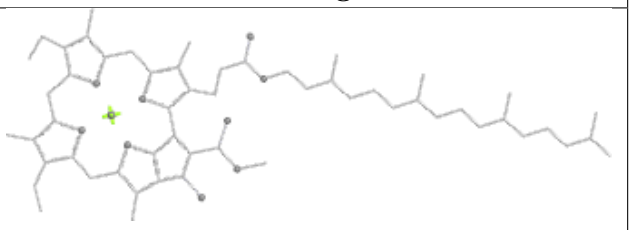
Bond lengths



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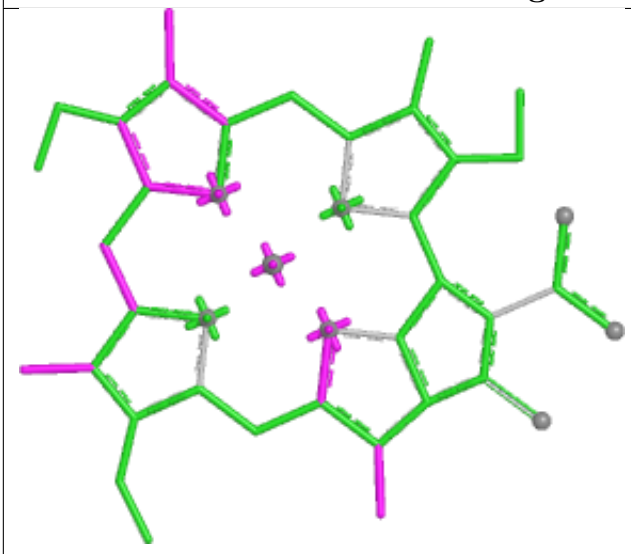


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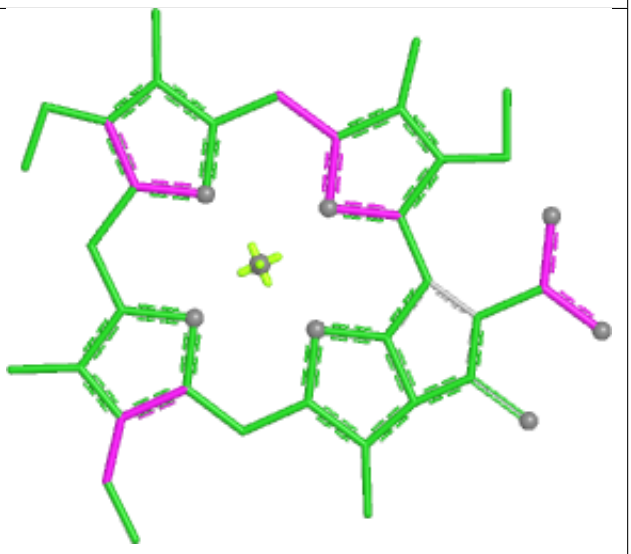


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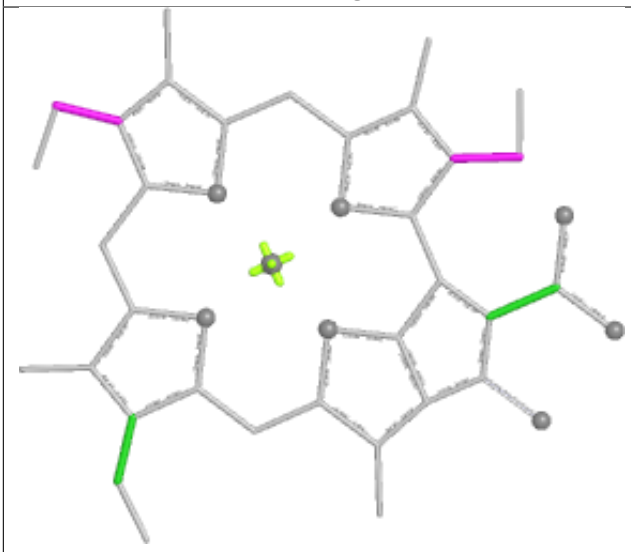
Ligand CLA 8 305



Bond lengths



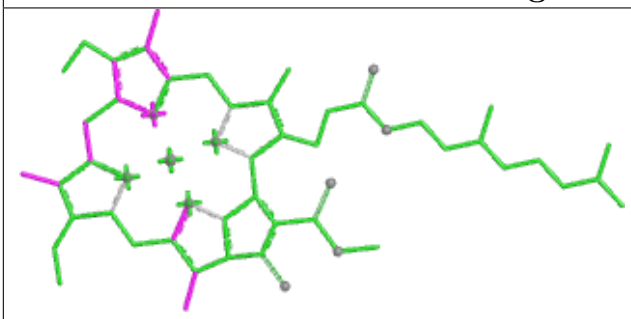
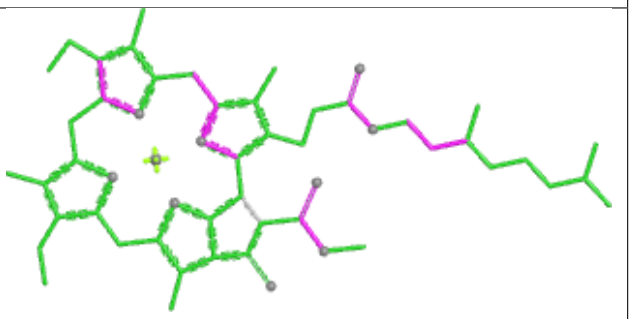
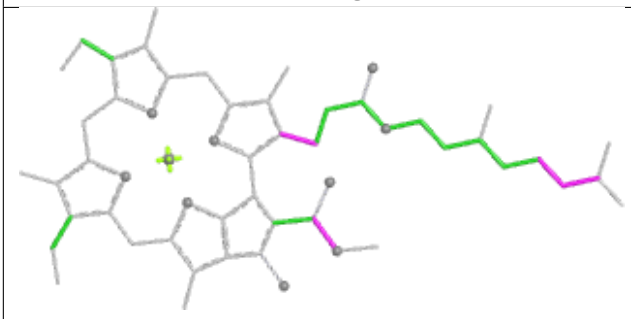
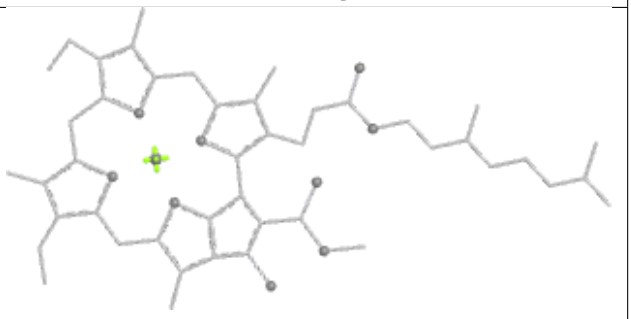
Bond angles

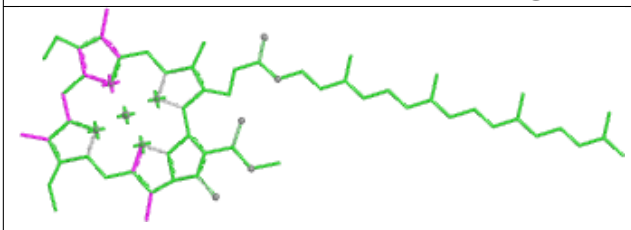
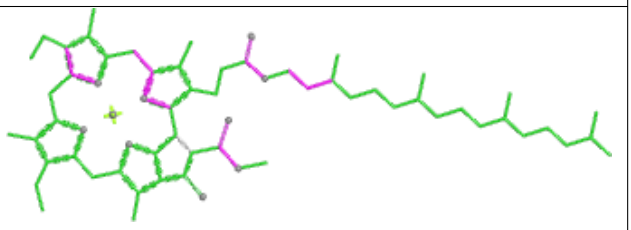
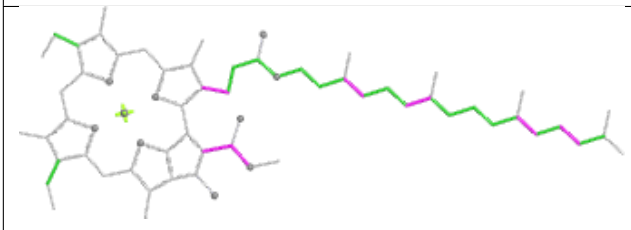
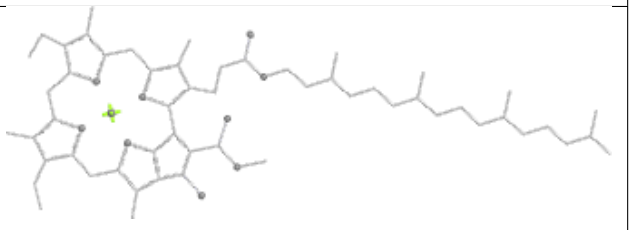


Torsions

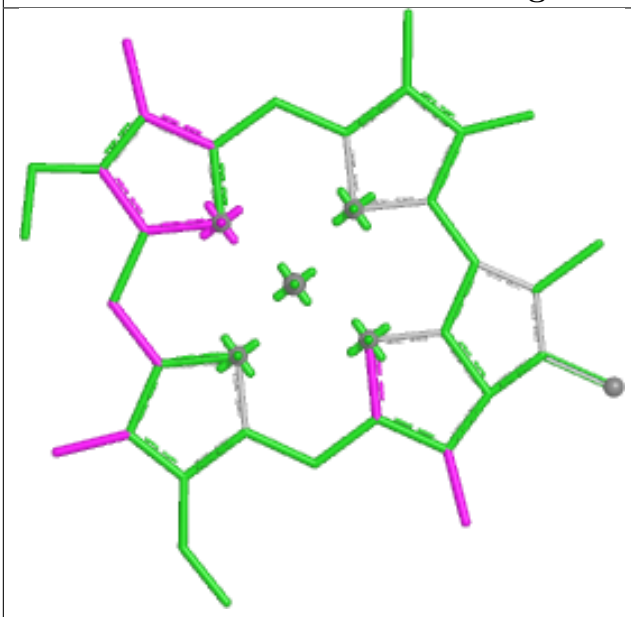


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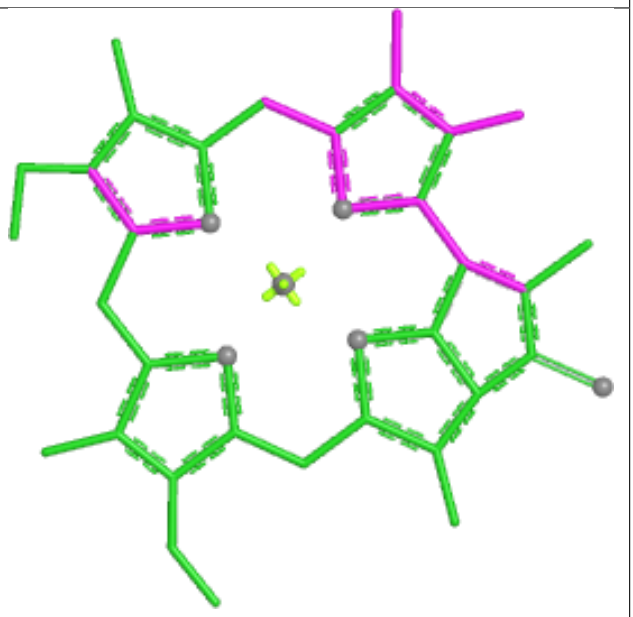
Ligand CLA 1 211	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

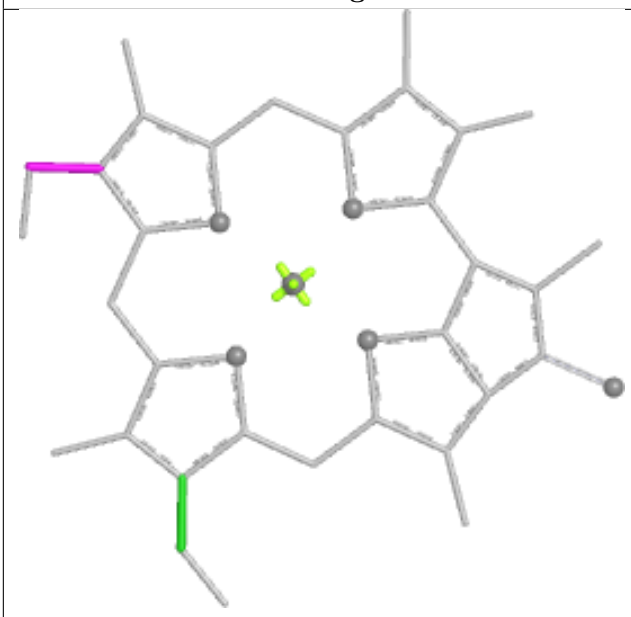
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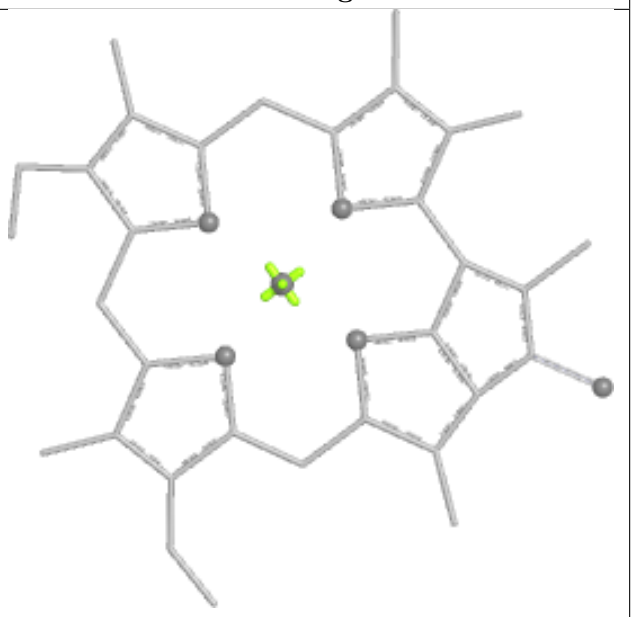
Bond lengths



Bond angles

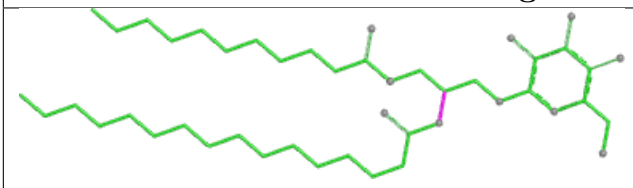


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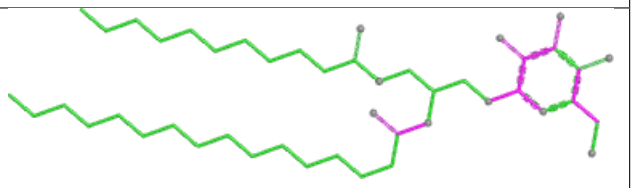


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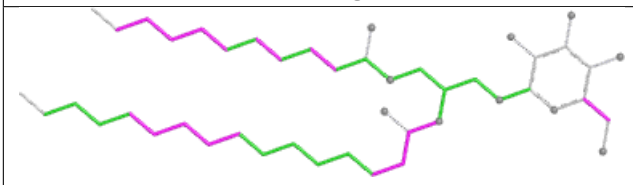
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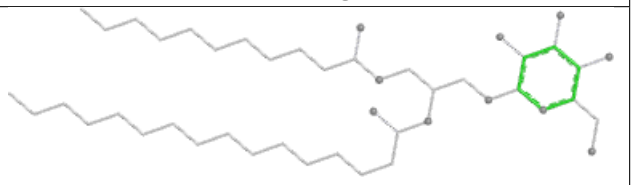
Bond lengths



Bond angles

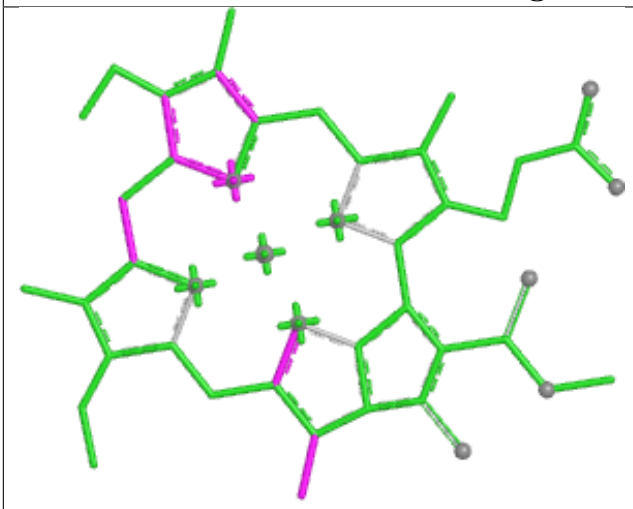


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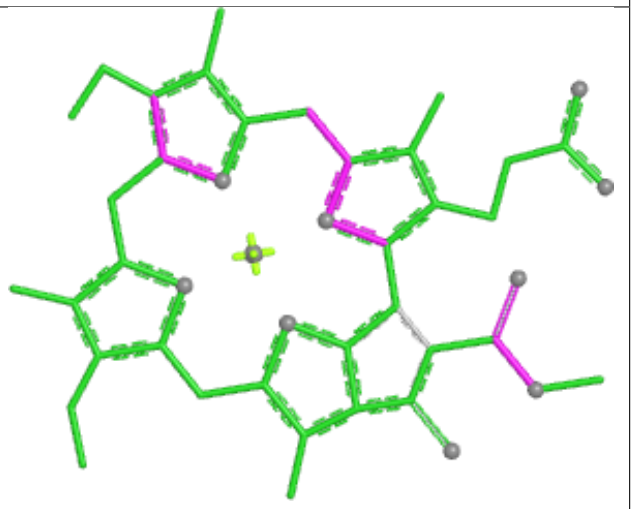


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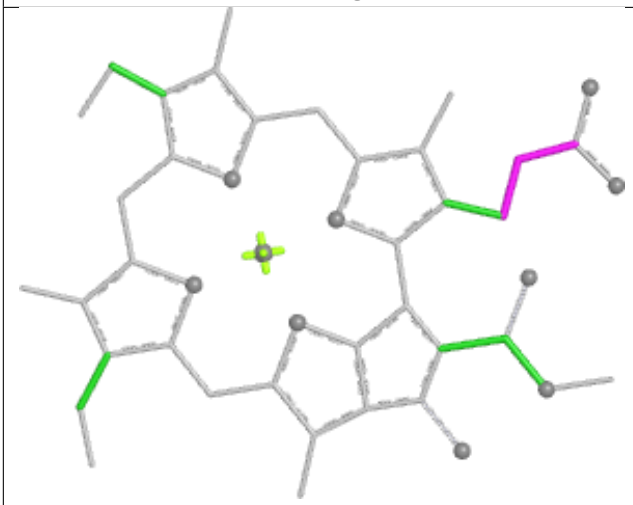
Ligand CLA 5 306



Bond lengths



Bond angles

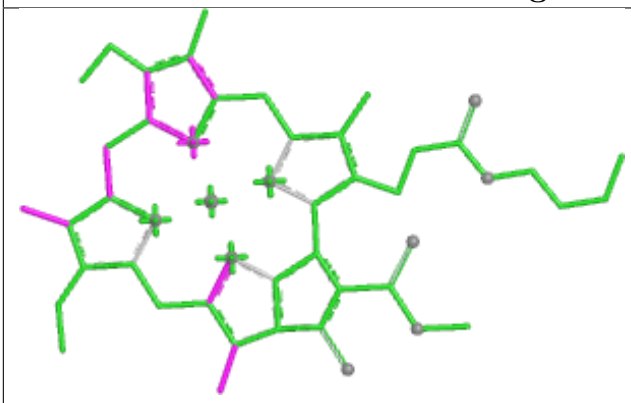


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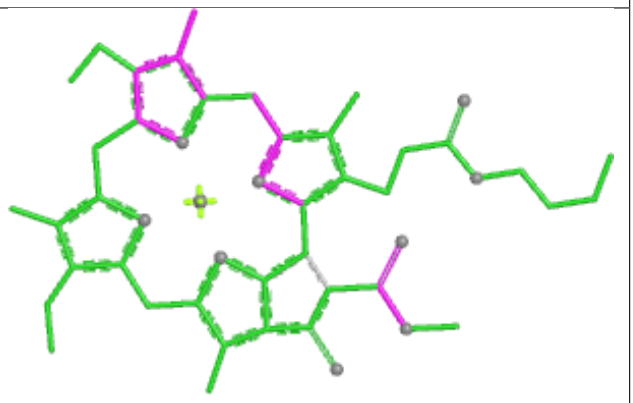


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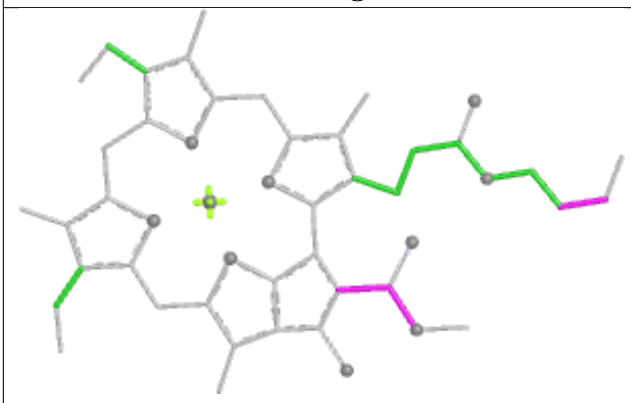
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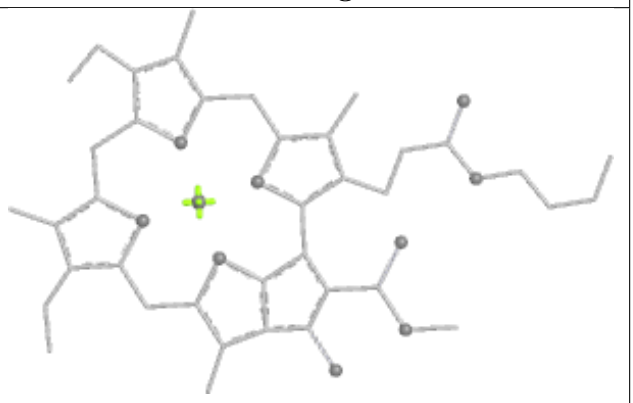
Bond lengths



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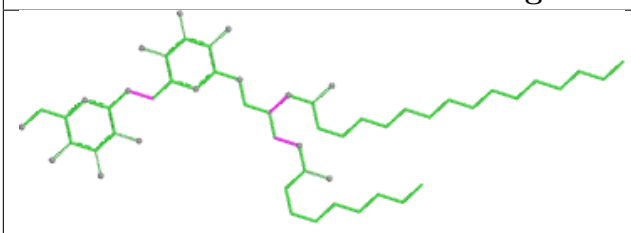


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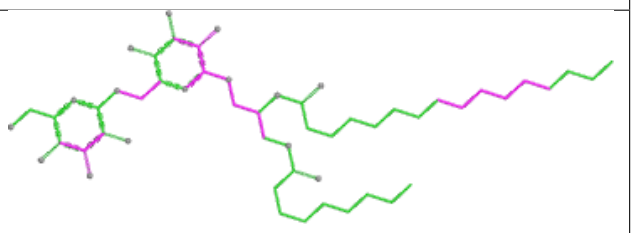


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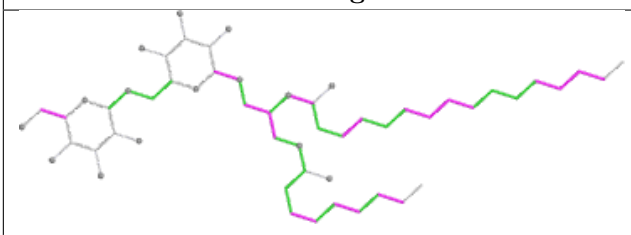
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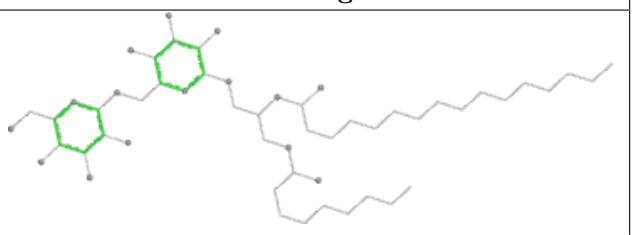
Bond lengths



Bond angles

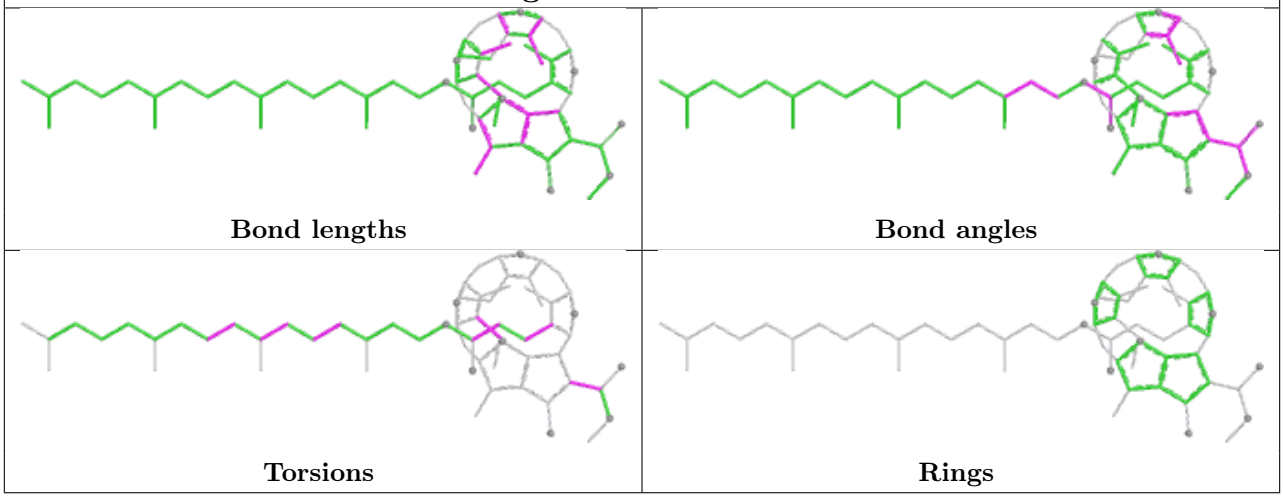


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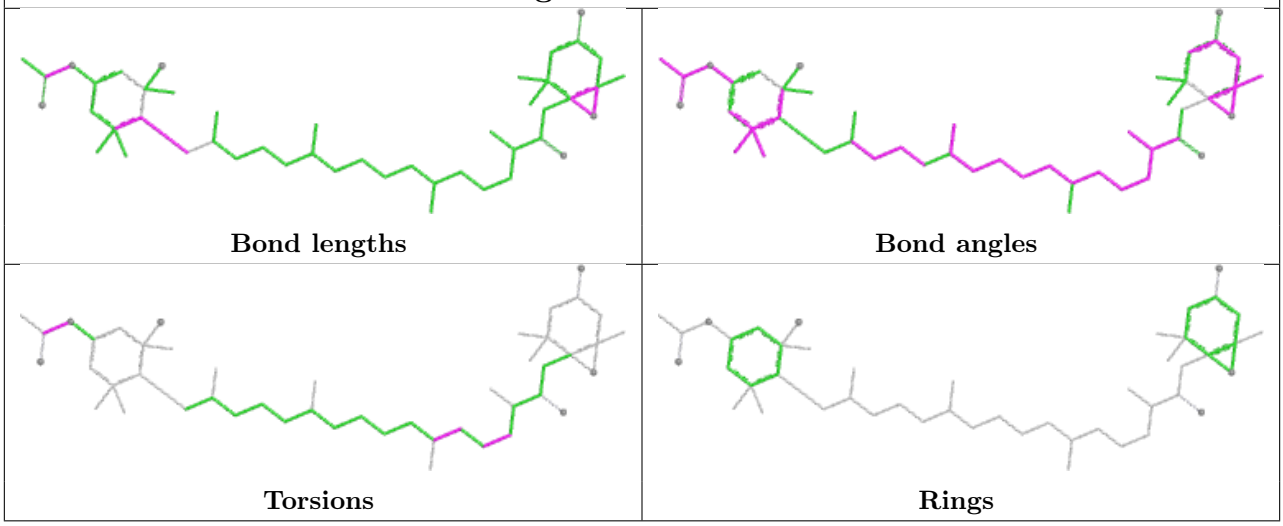


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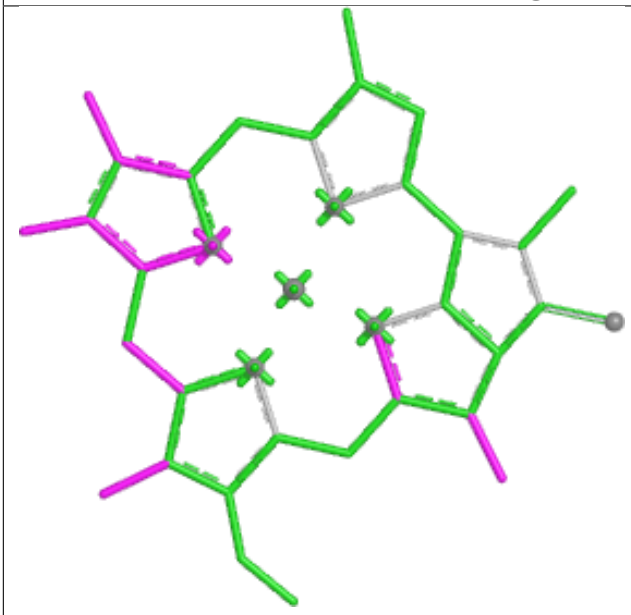
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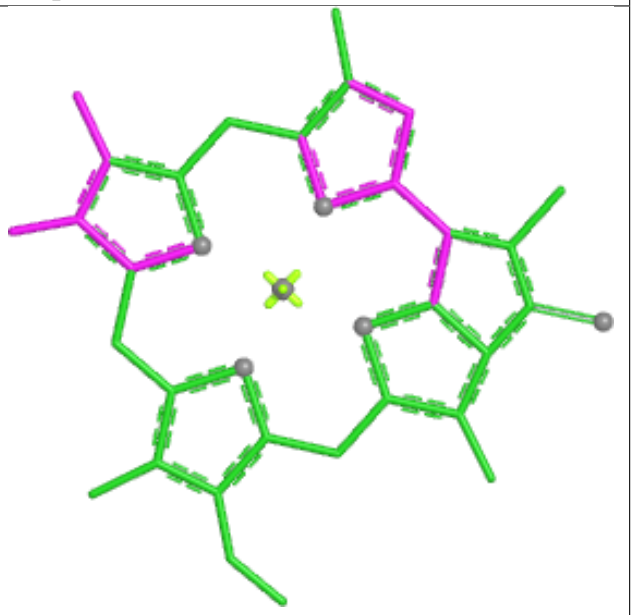
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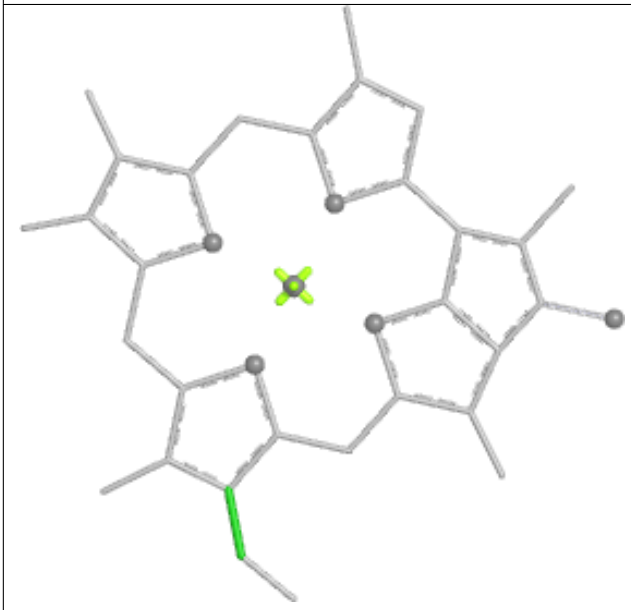
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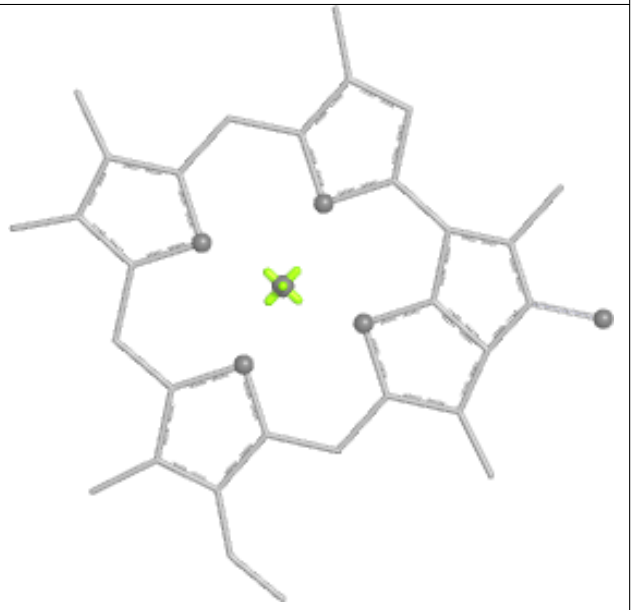
Bond lengths



Bond angles

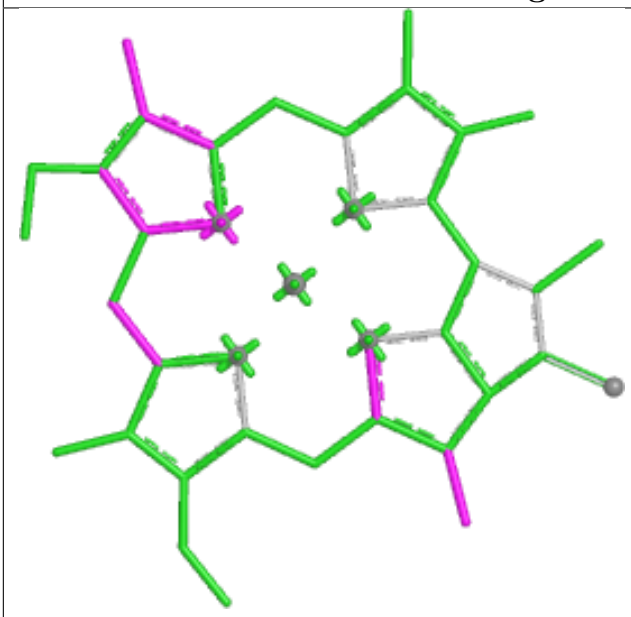


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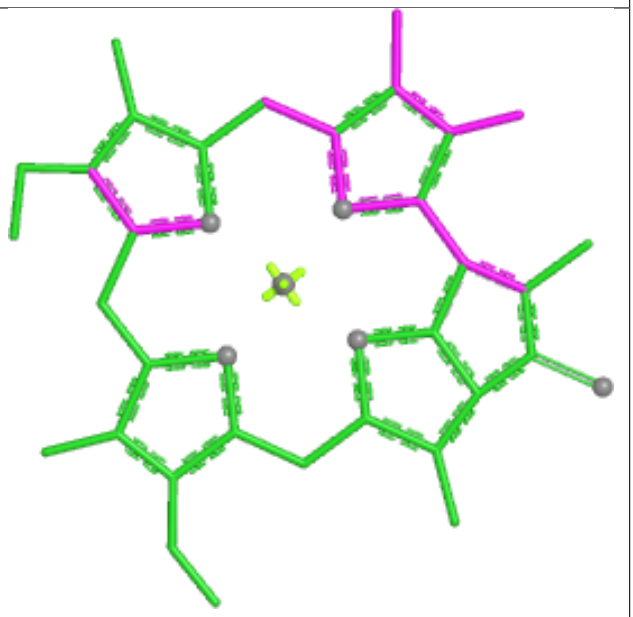


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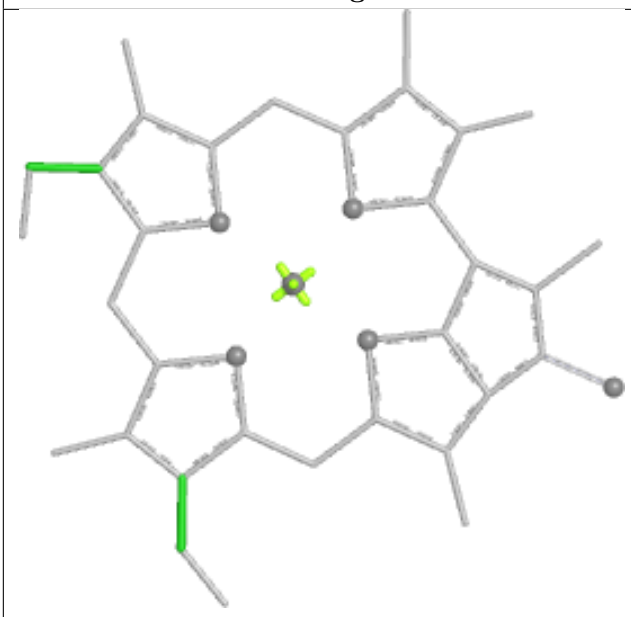
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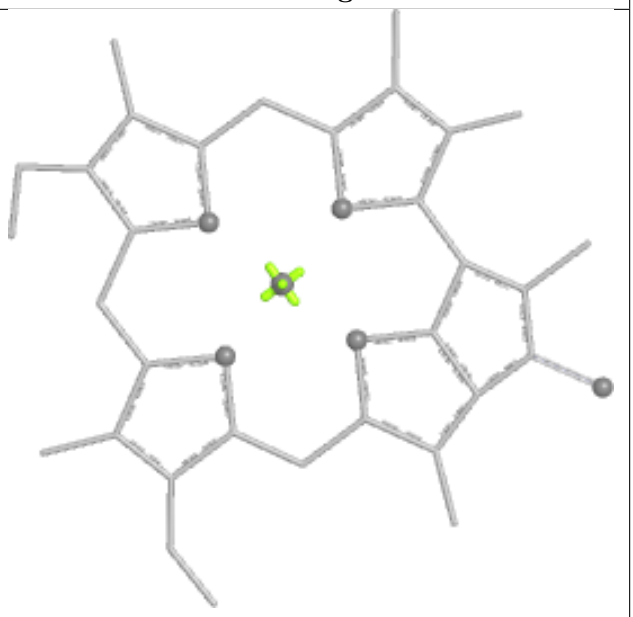
Bond lengths



Bond angles

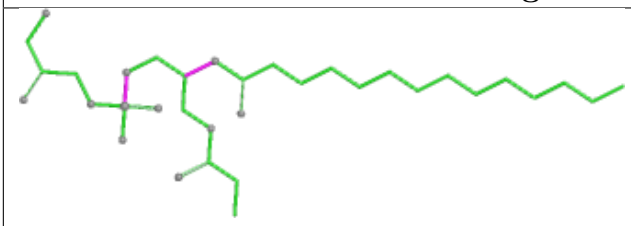


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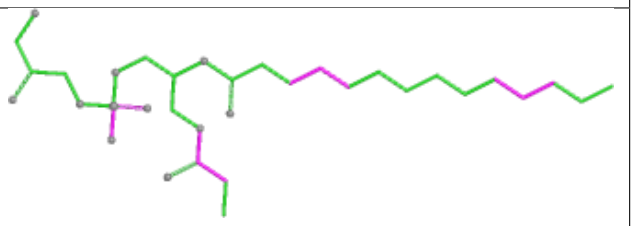


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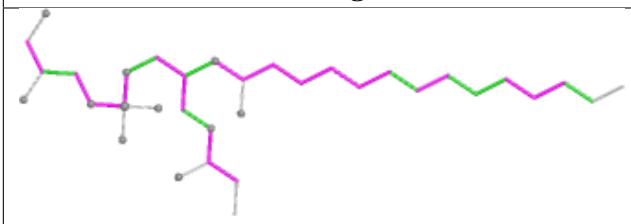
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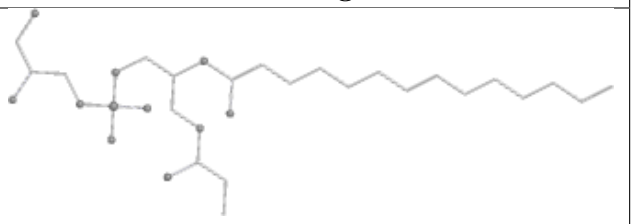
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Bond angles

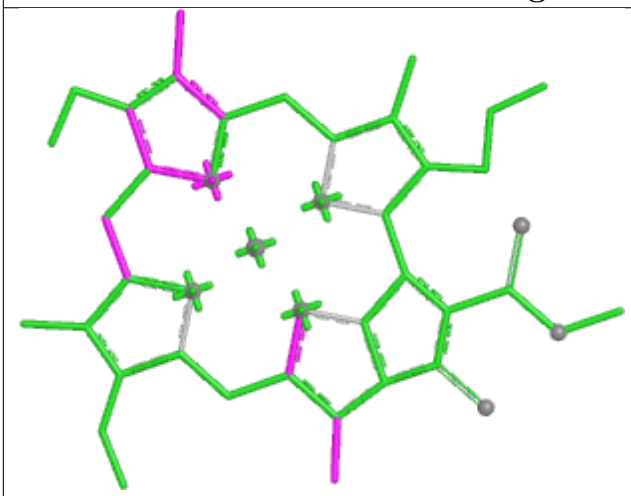


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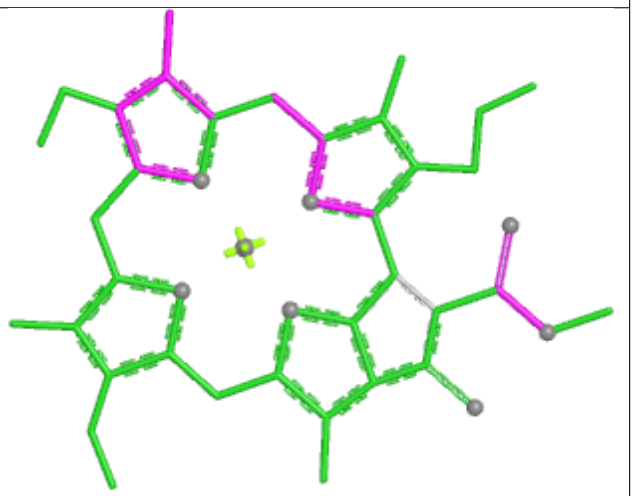


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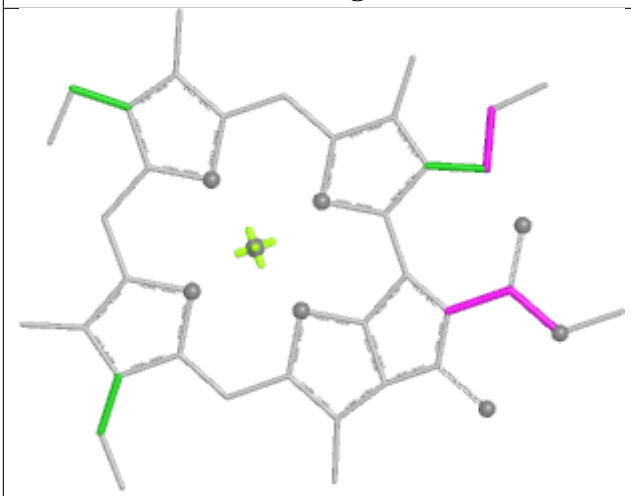
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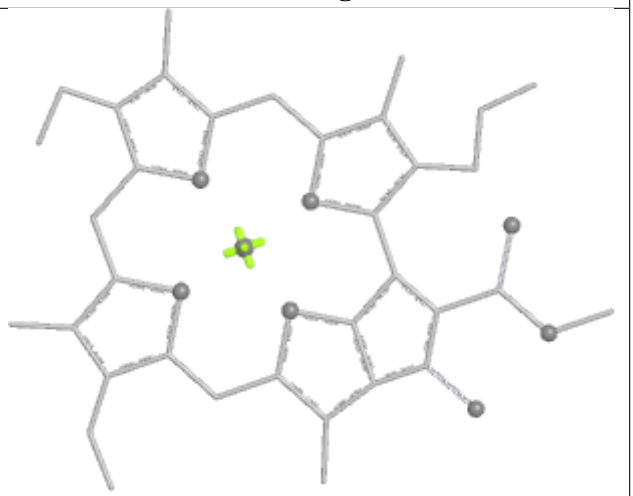
Bond lengths



Bond angles

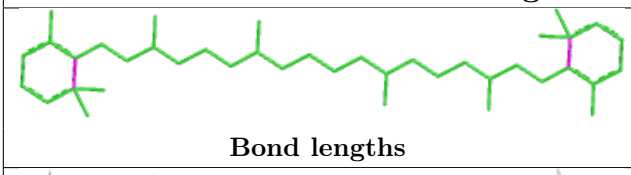


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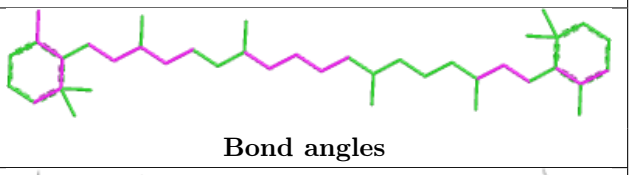


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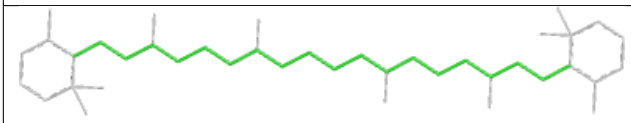
Ligand BCR C 515



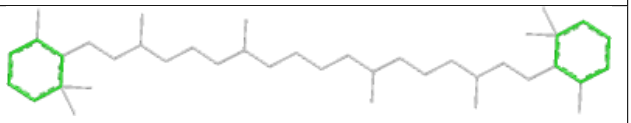
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Bond angles

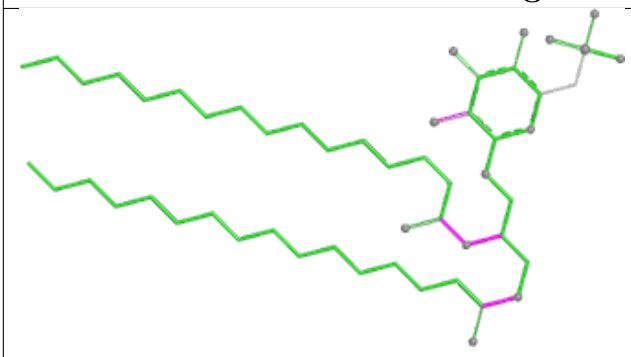


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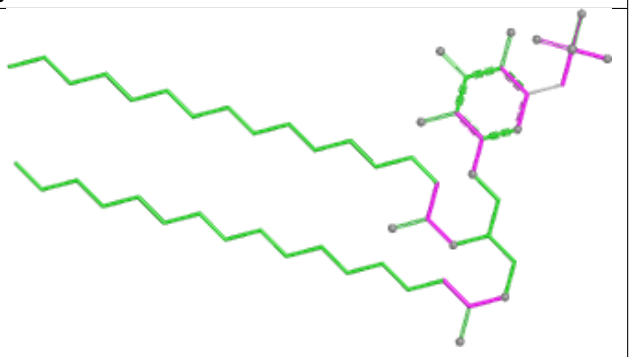


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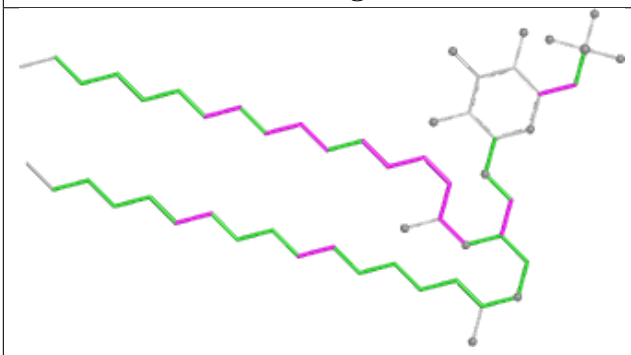
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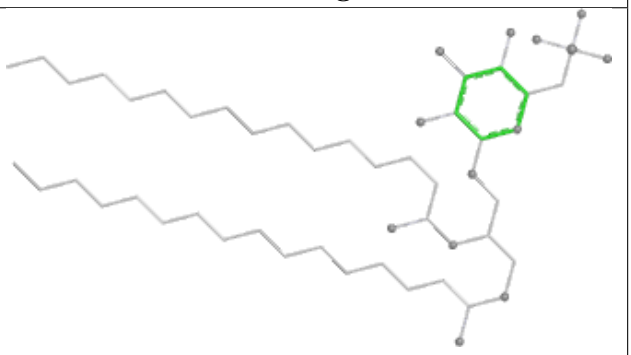
Bond lengths



Bond angles

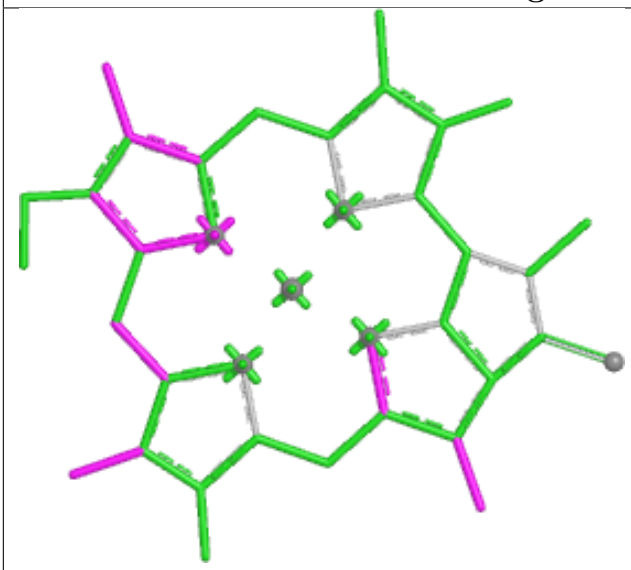


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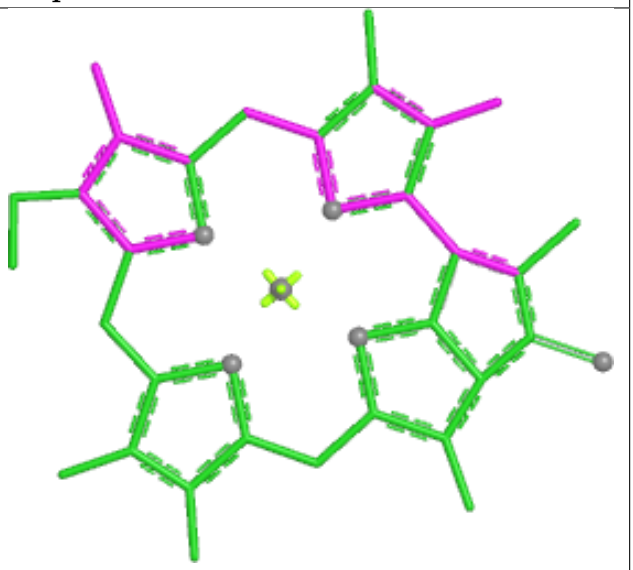


Rings

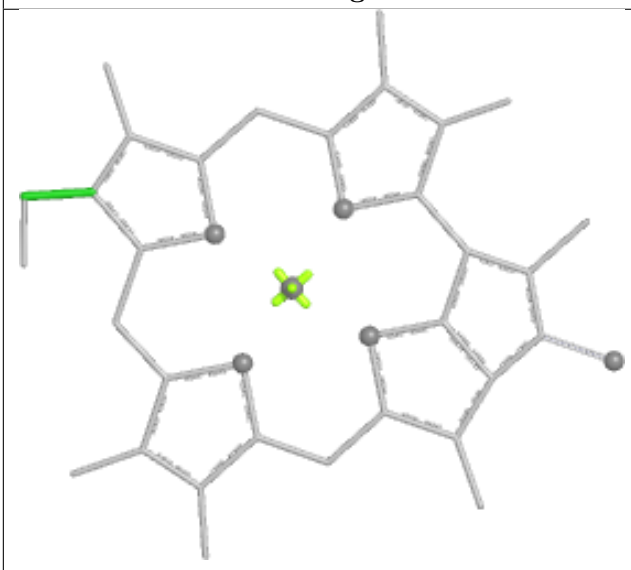
Ligand CLA p 603



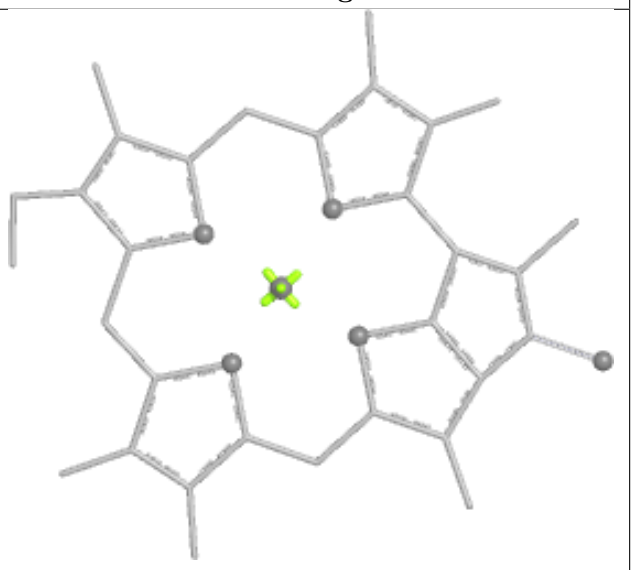
Bond lengths



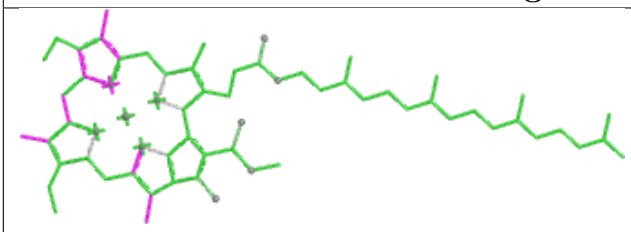
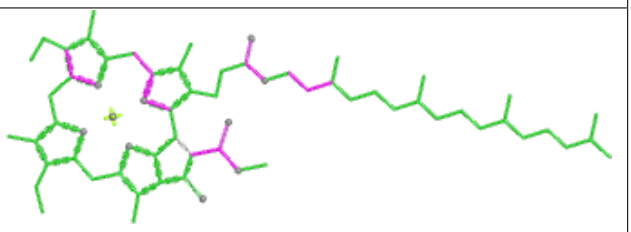
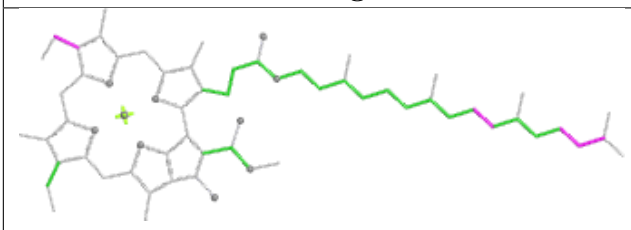
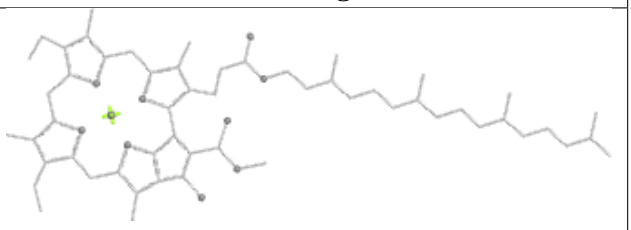
Bond angles



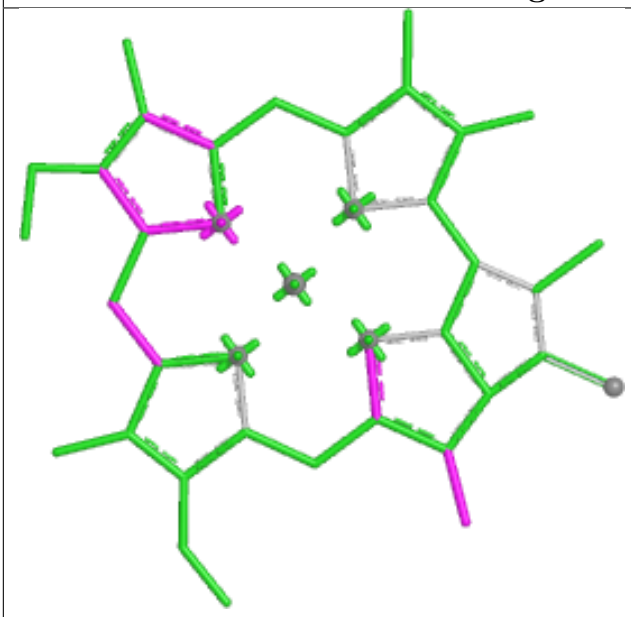
Torsions



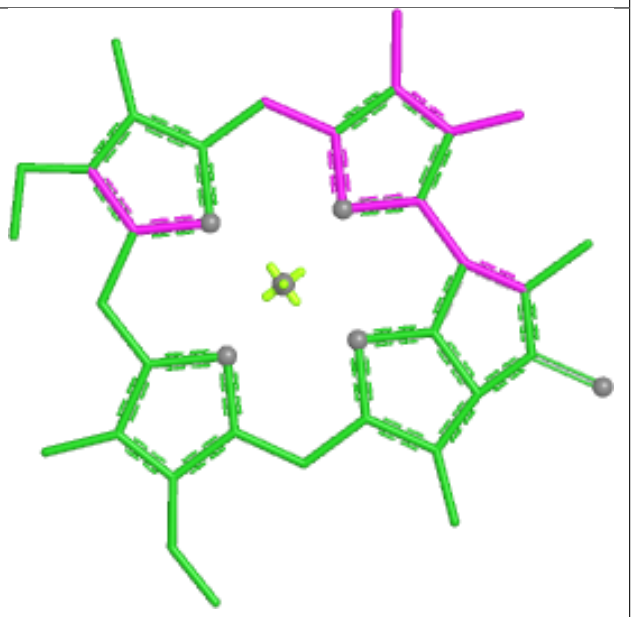
Rings

Ligand CLA B 515	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

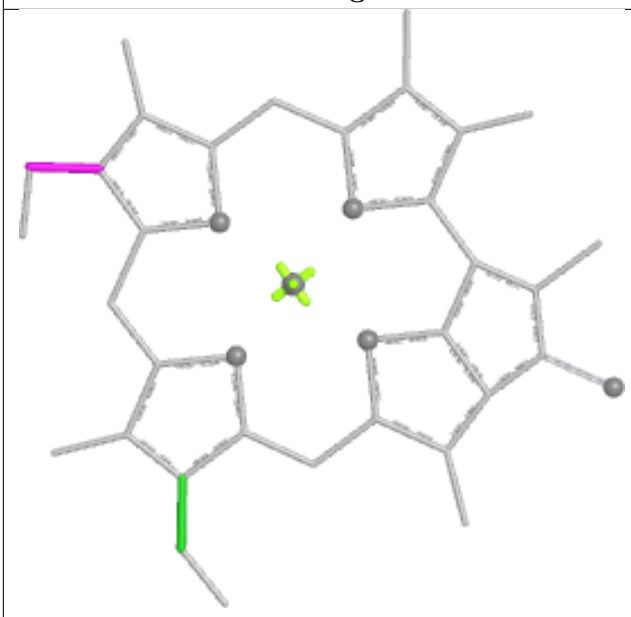
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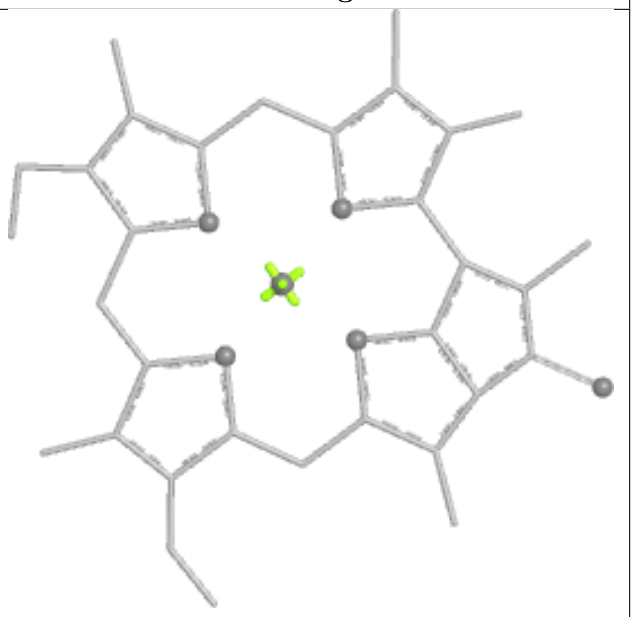
Bond lengths



Bond angles

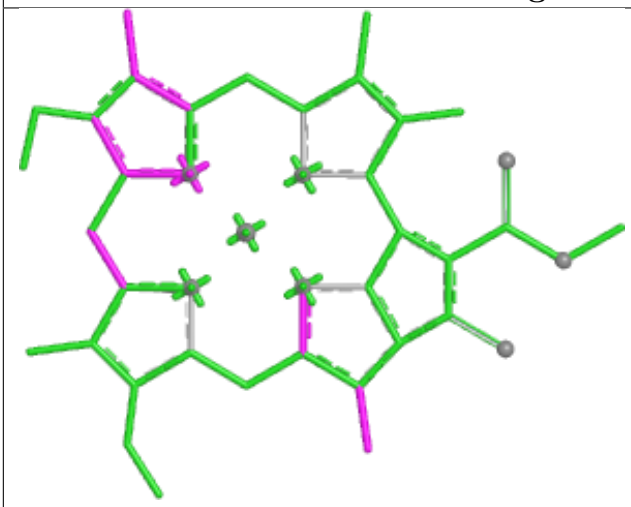


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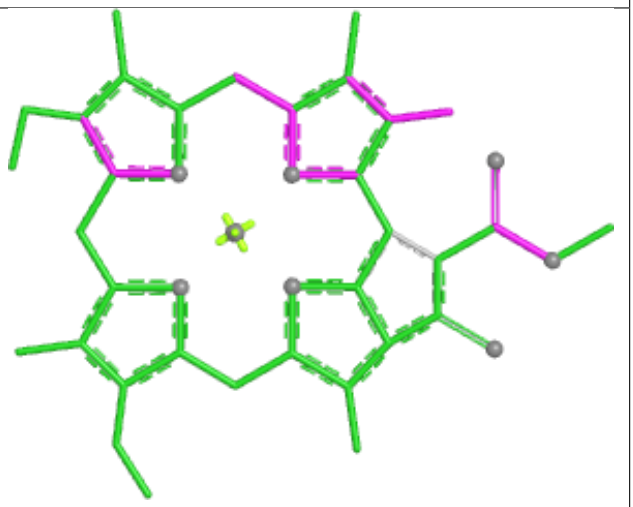


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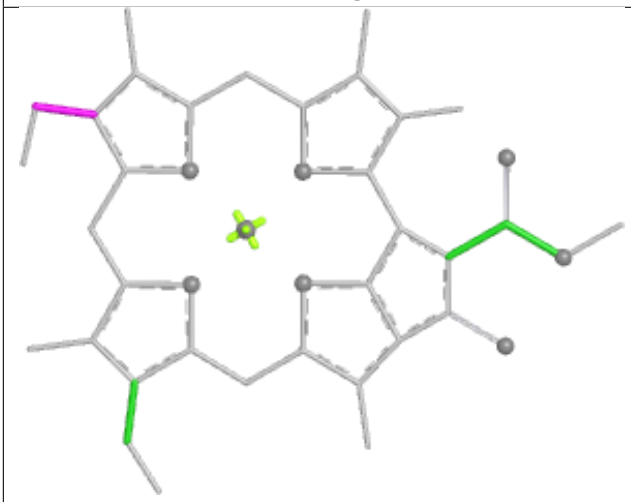
Ligand CLA 6 205



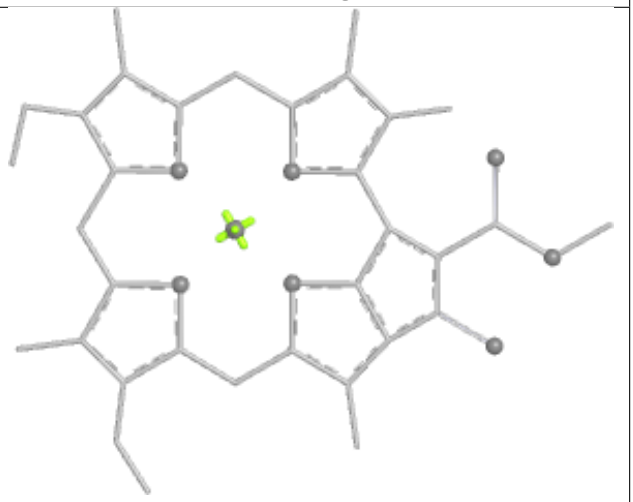
Bond lengths



Bond angles

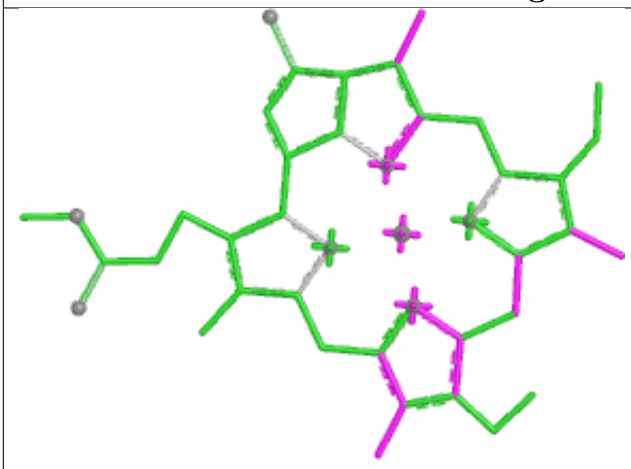


Torsions

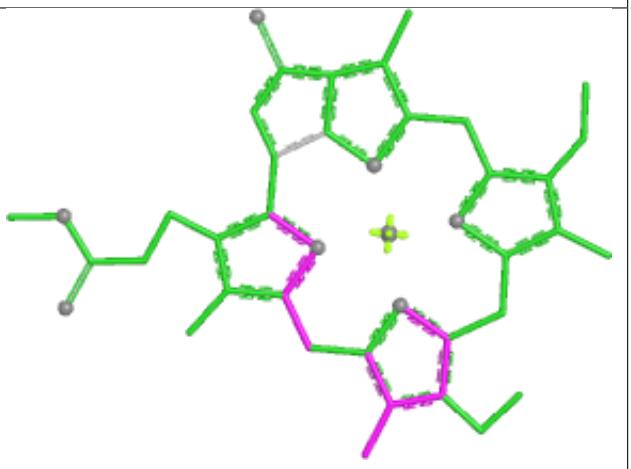


Rings

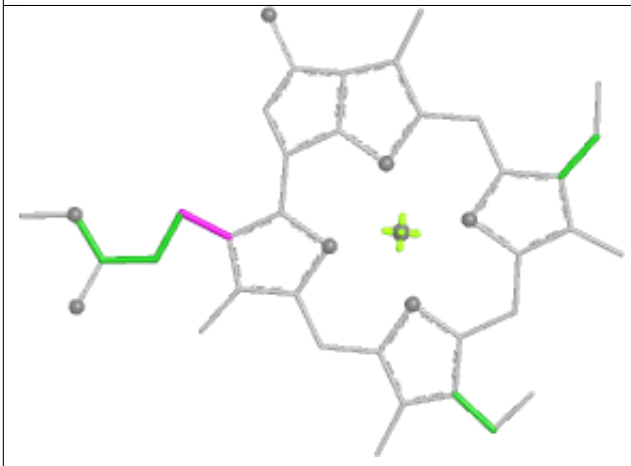
Ligand CLA 8 307



Bond lengths



Bond angles

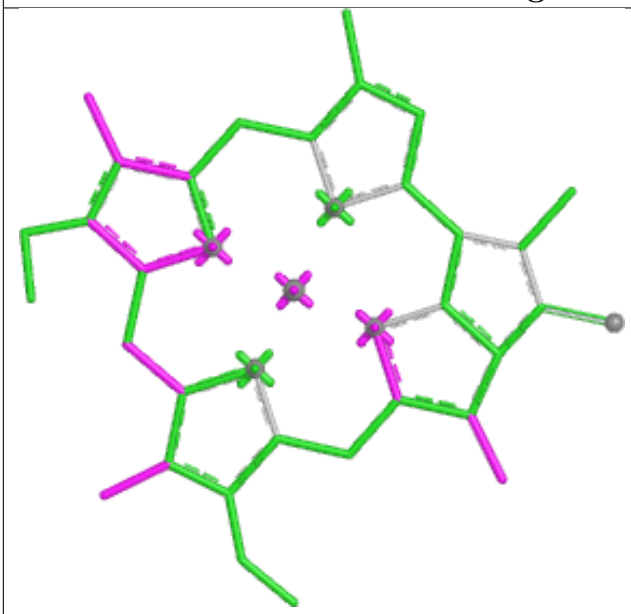


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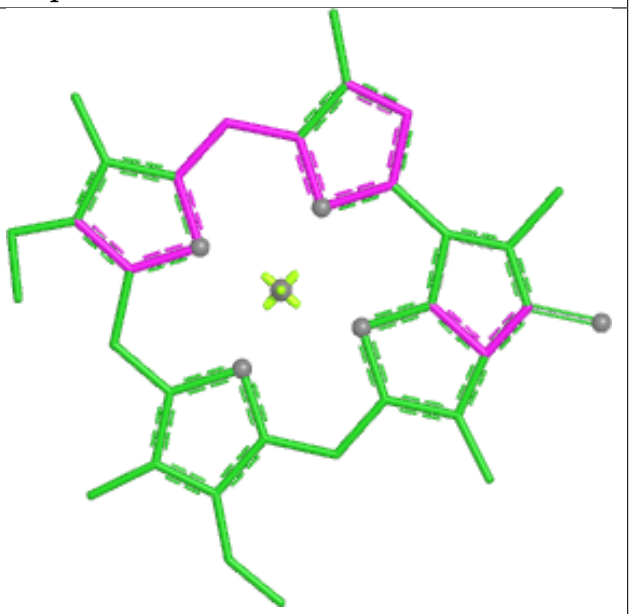


Rings

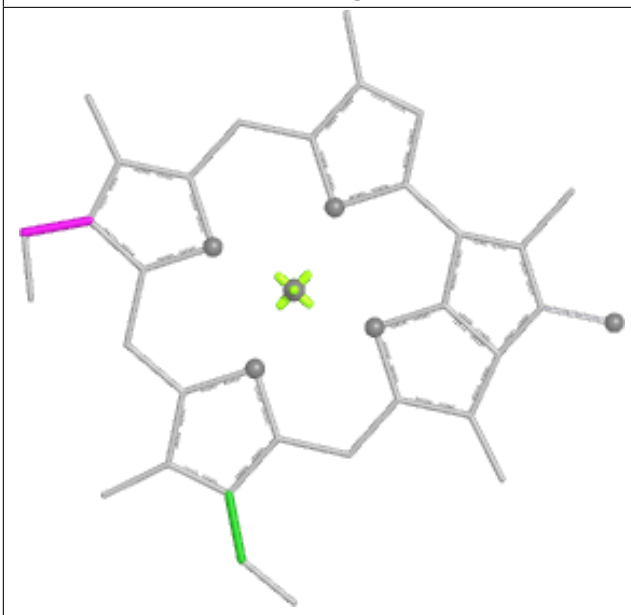
Ligand CLA p 606



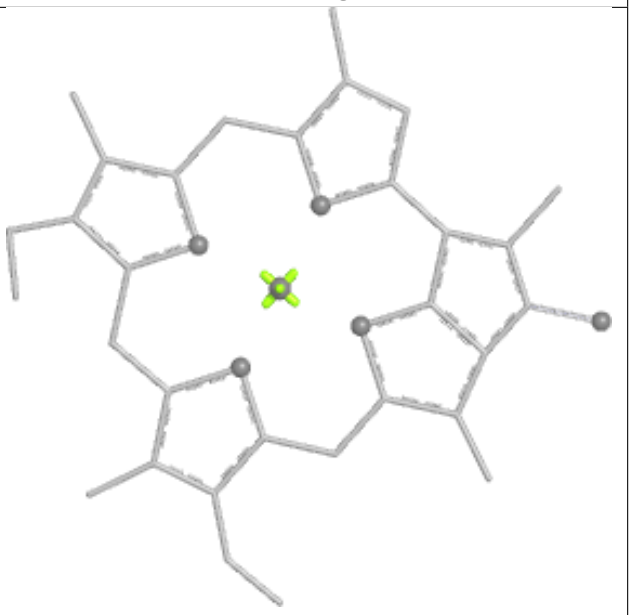
Bond lengths



Bond angles

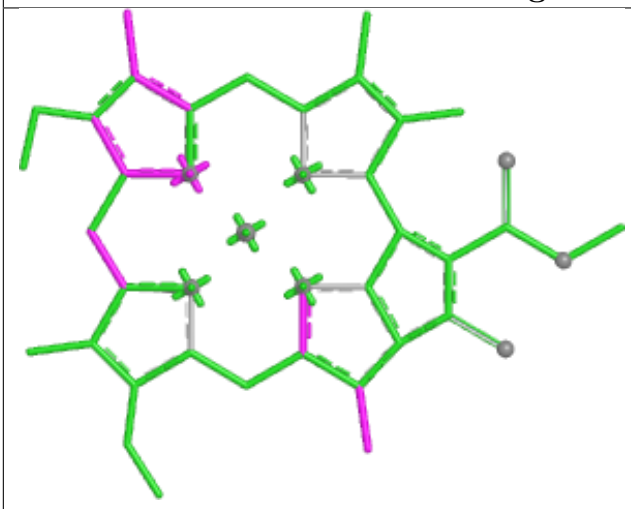


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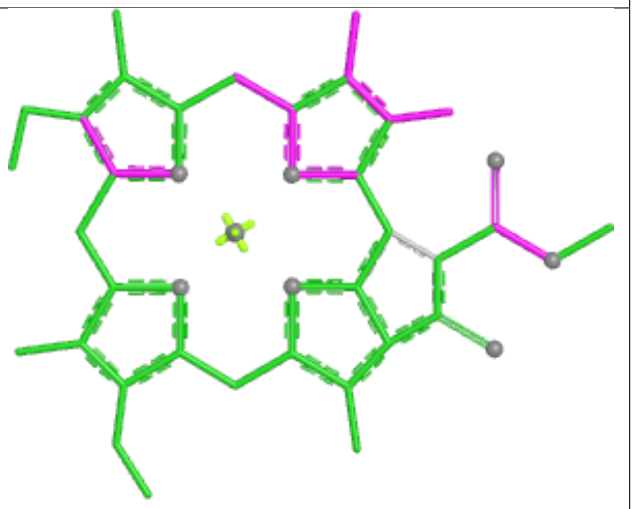


Rings

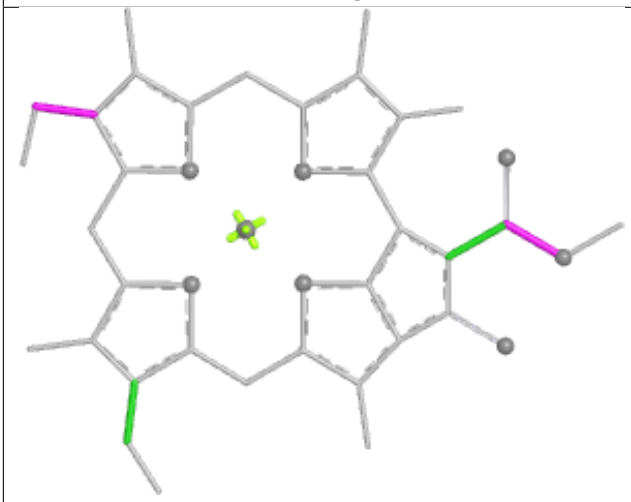
Ligand CLA 0 304



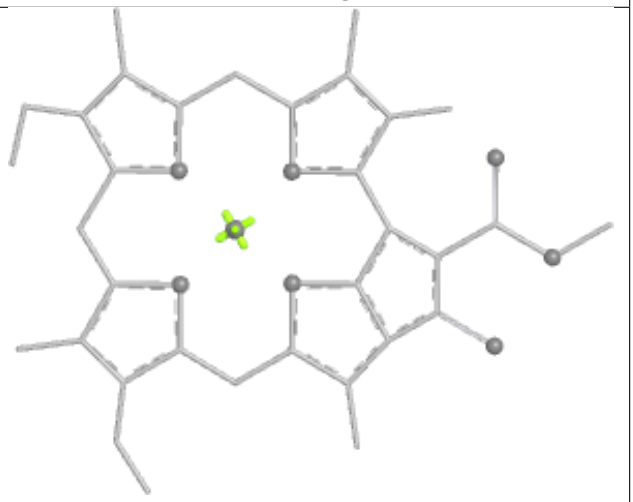
Bond lengths



Bond angles

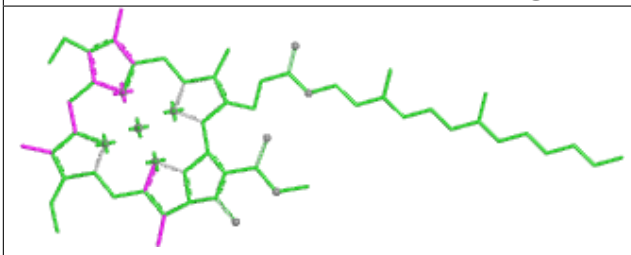


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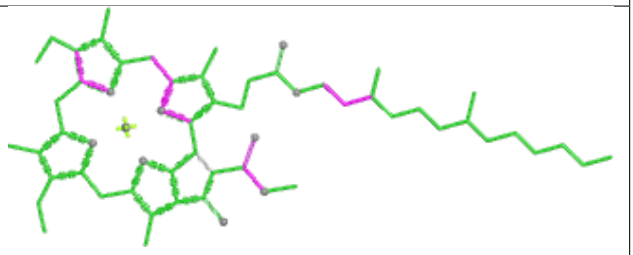


Rings

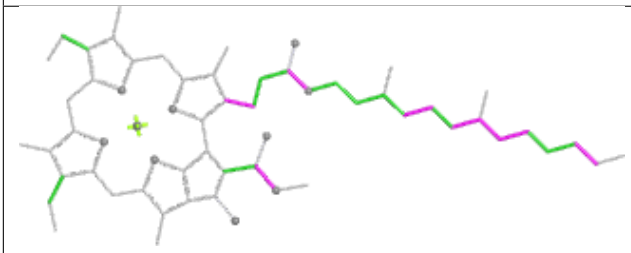
Ligand CLA b 515



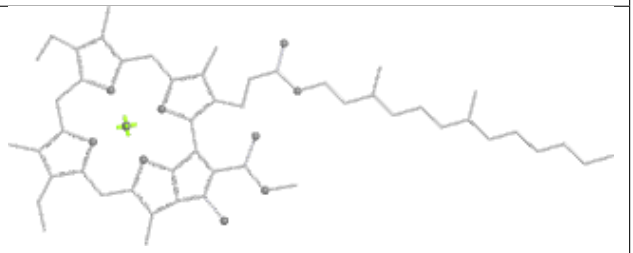
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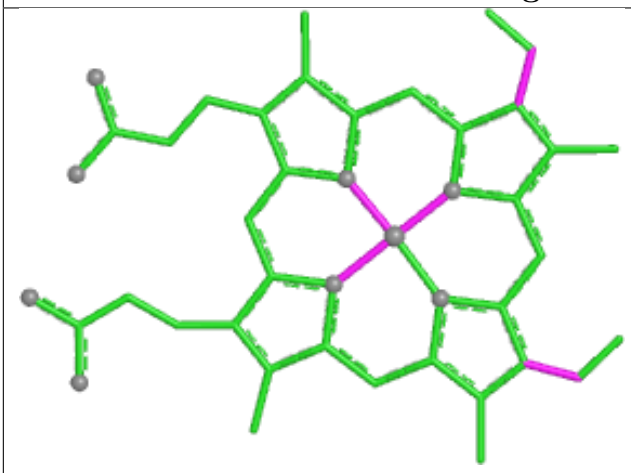
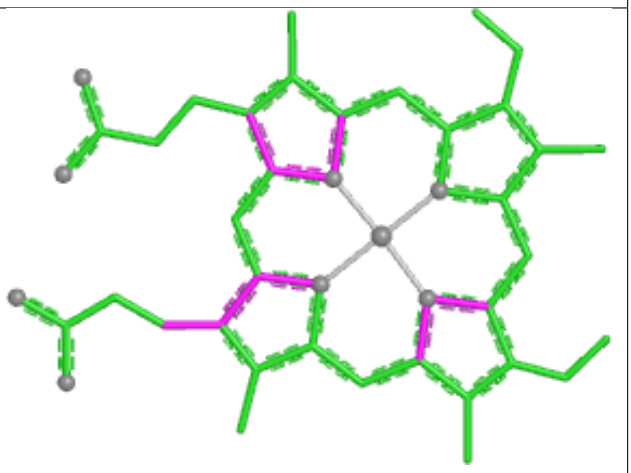
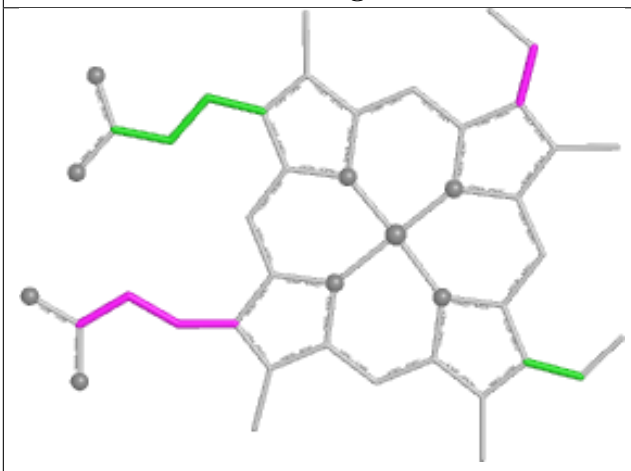
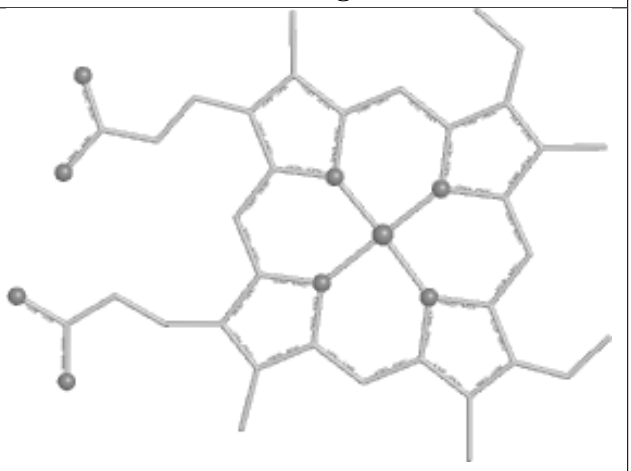
Bond angles

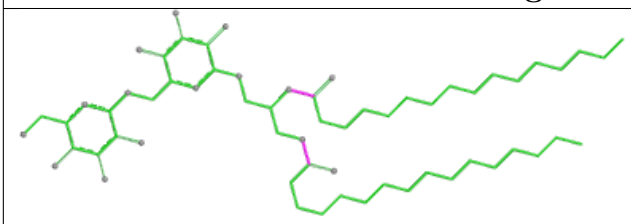
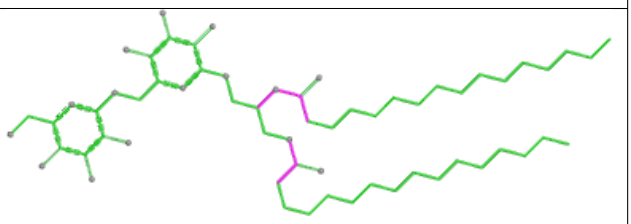
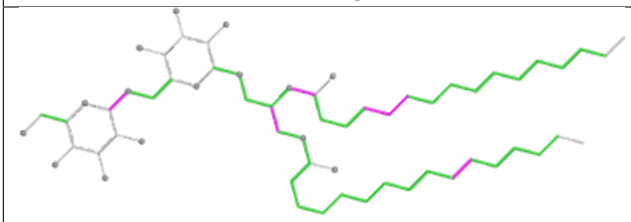
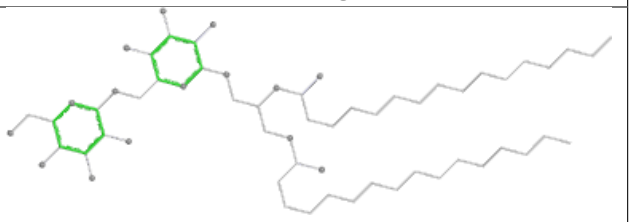


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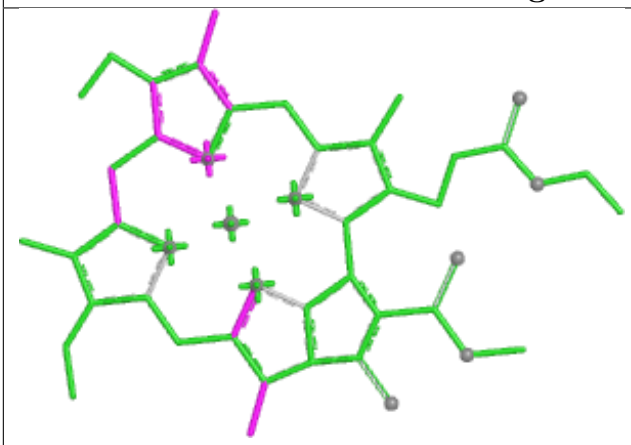


Rings

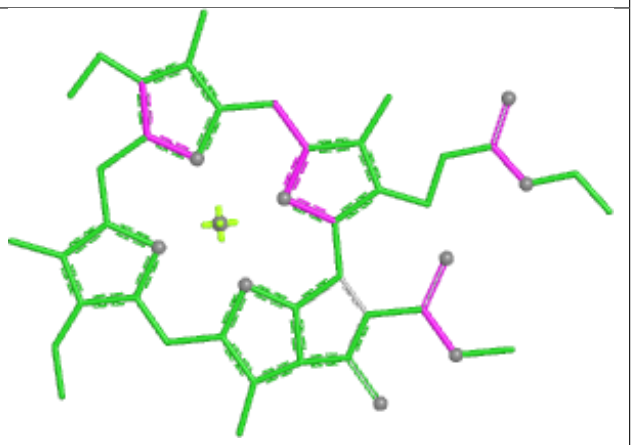
Ligand HEM v 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

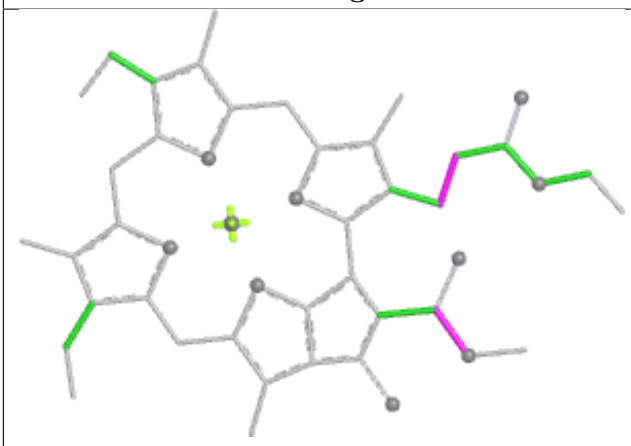
Ligand CLA 2 307



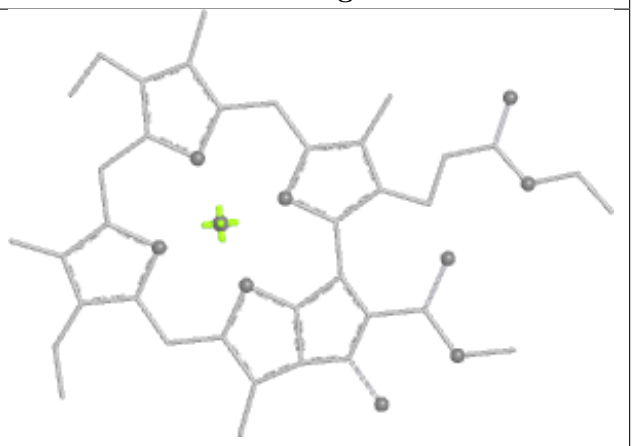
Bond lengths



Bond angles

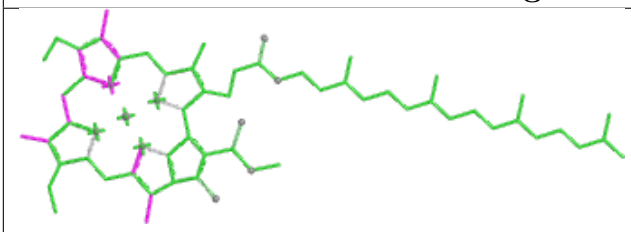


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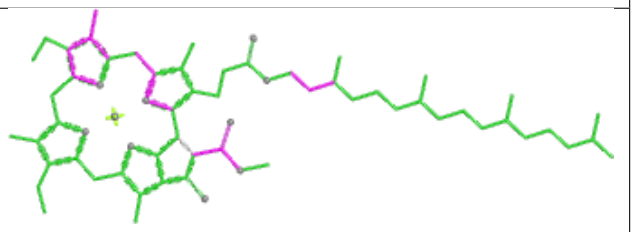


Rings

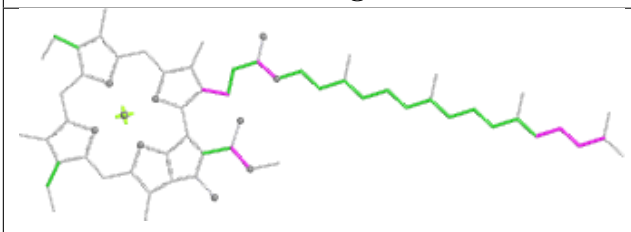
Ligand CLA A 403



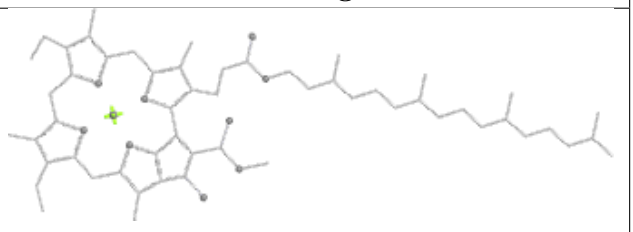
Bond lengths



Bond angles

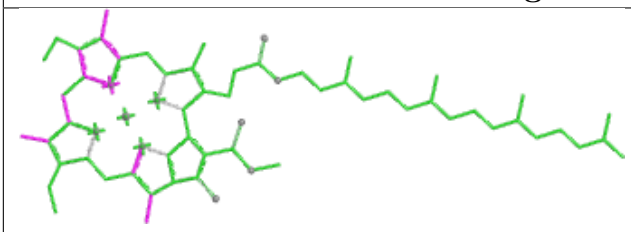


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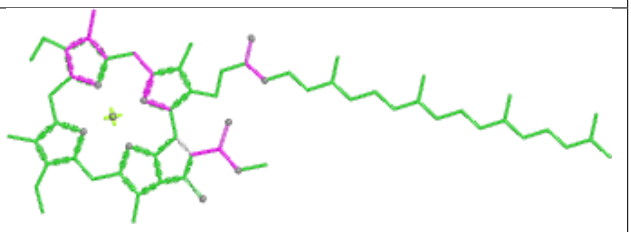


Rings

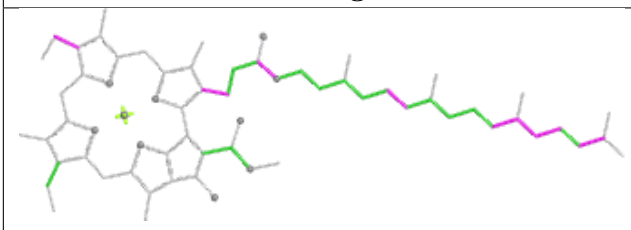
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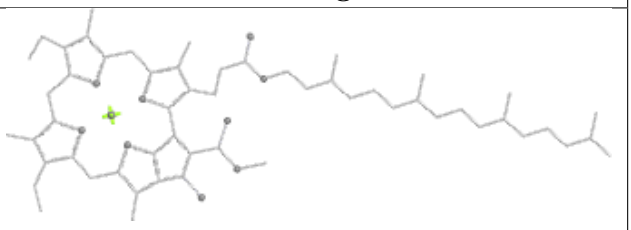
Bond lengths



Bond angles

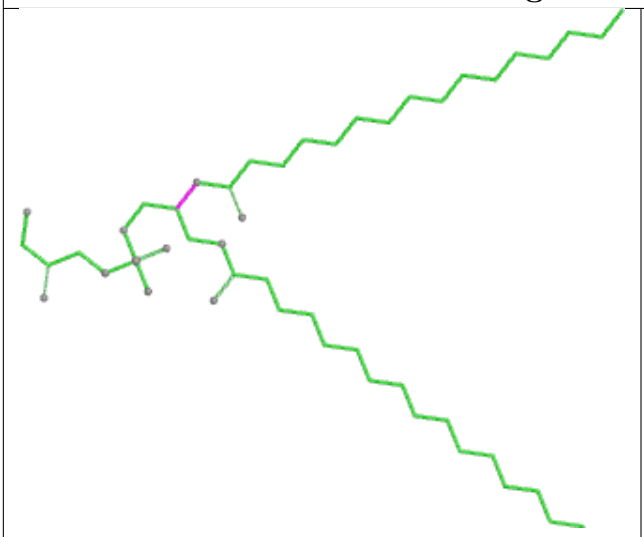


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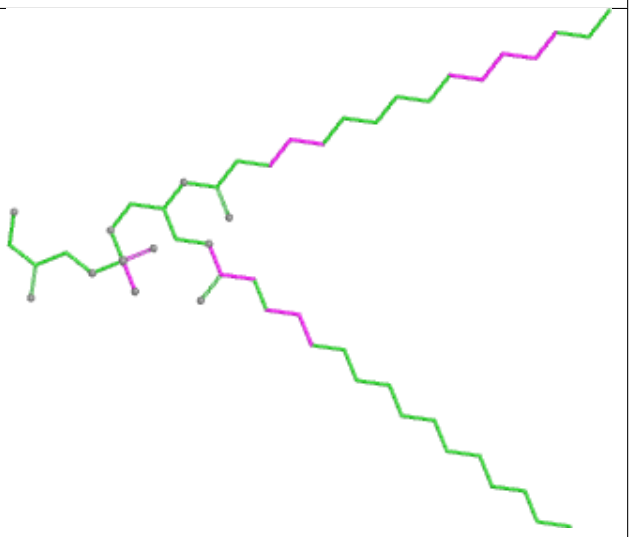


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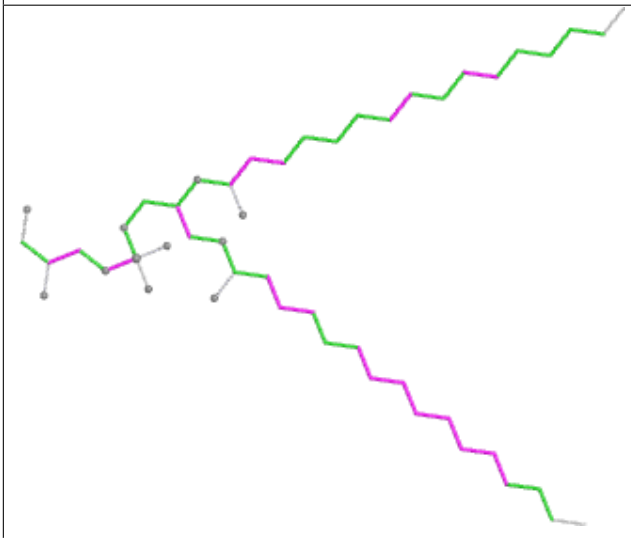
Ligand LHG b 522



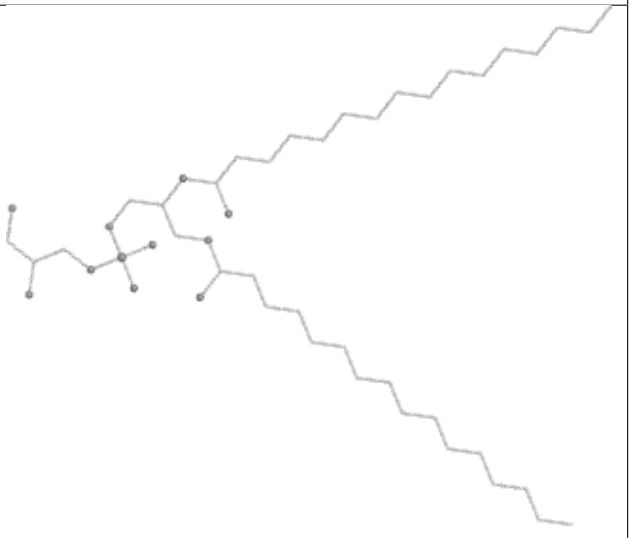
Bond lengths



Bond angles

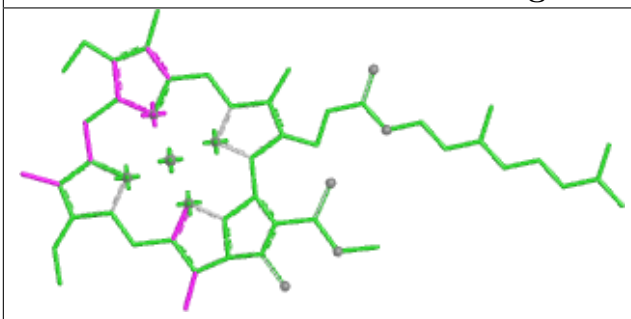


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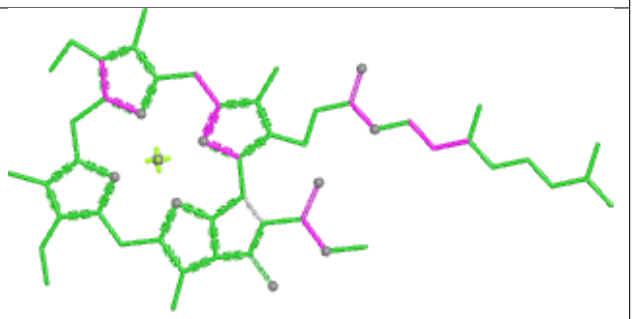


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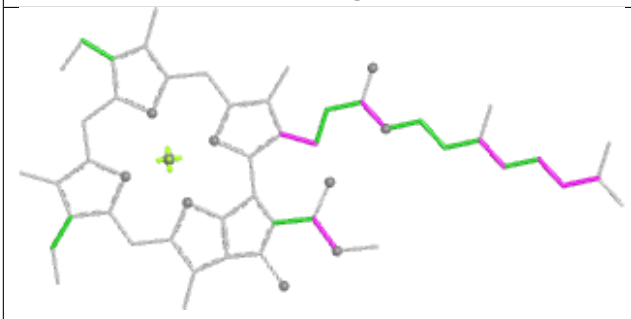
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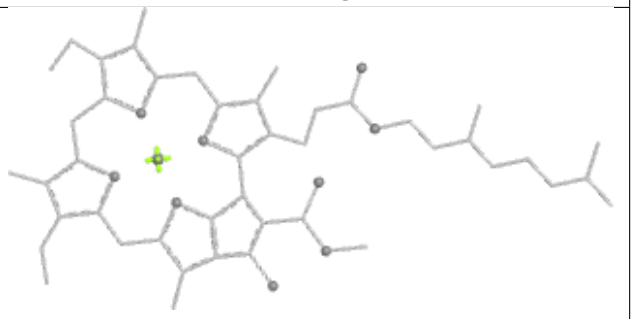
Bond lengths



Bond angles

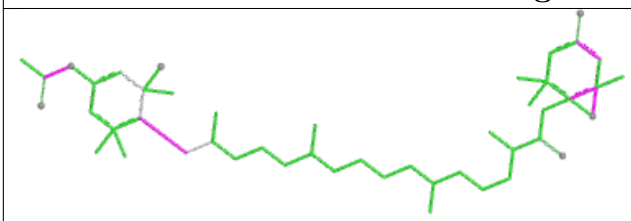


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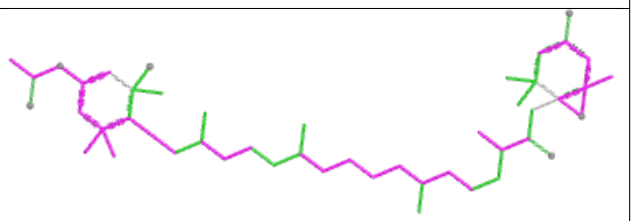


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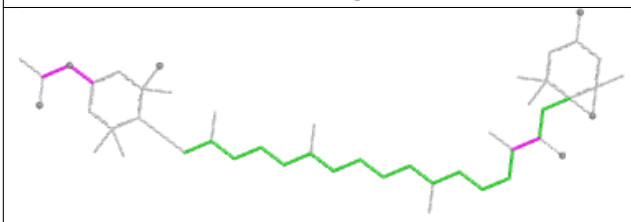
Ligand A86 4 201



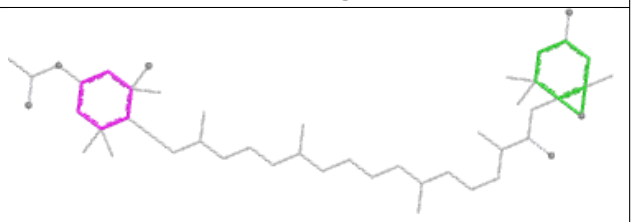
Bond lengths



Bond angles

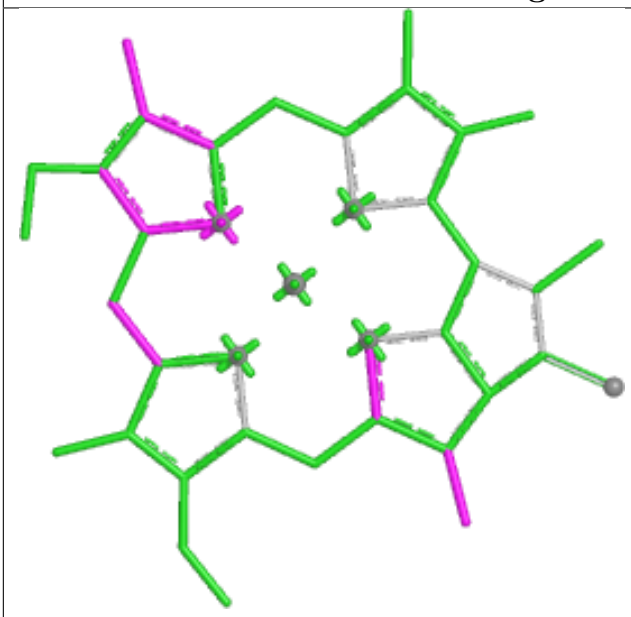


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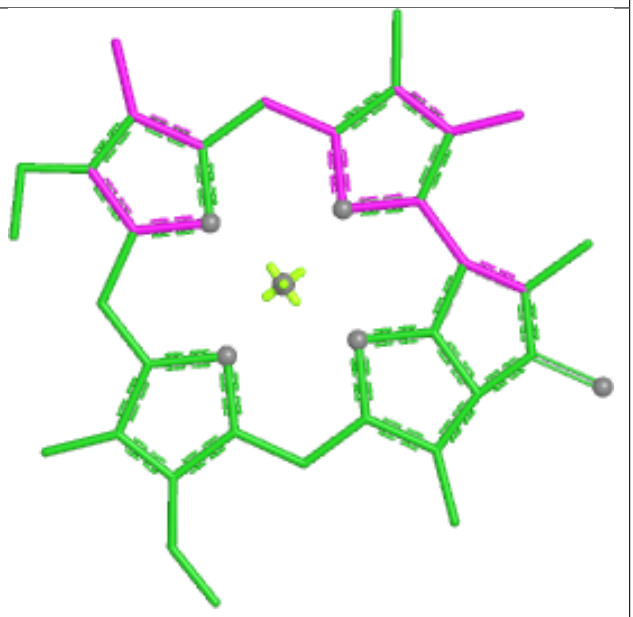


Rings

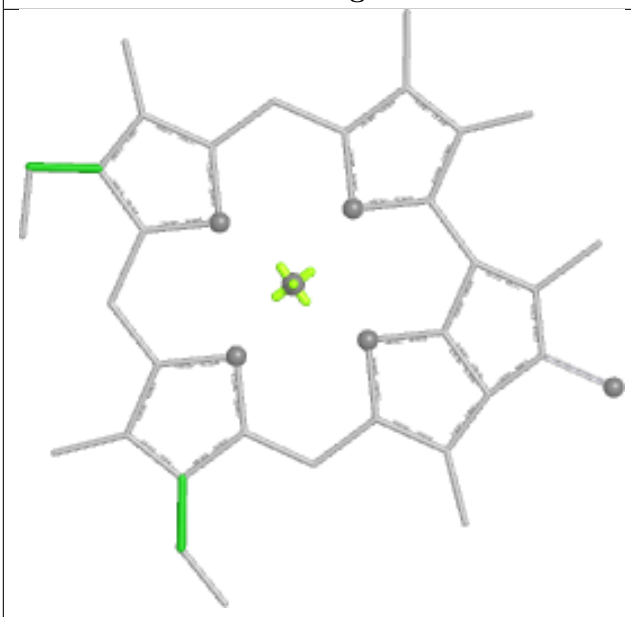
Ligand CLA 2 314



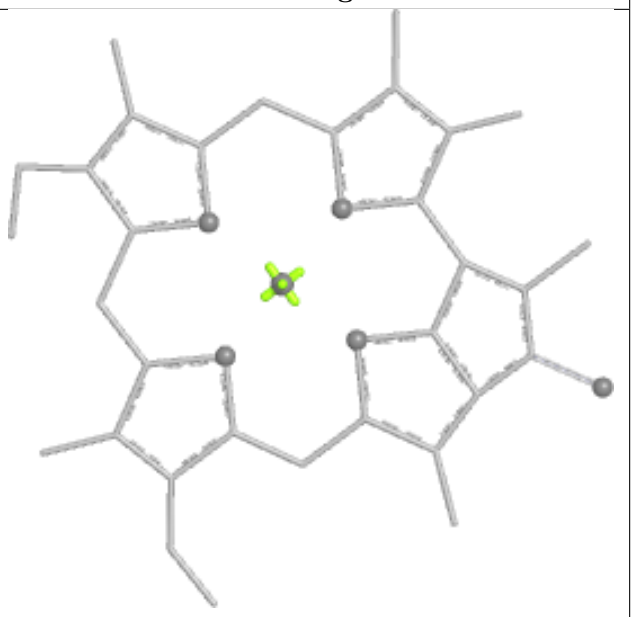
Bond lengths



Bond angles

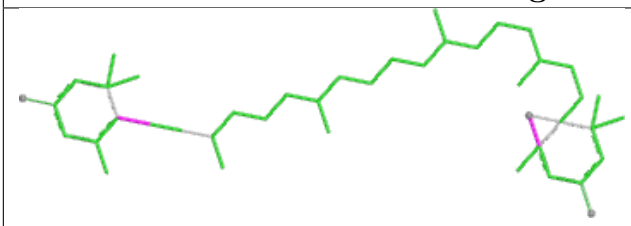


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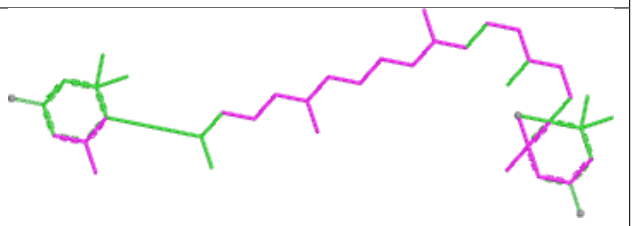


Rings

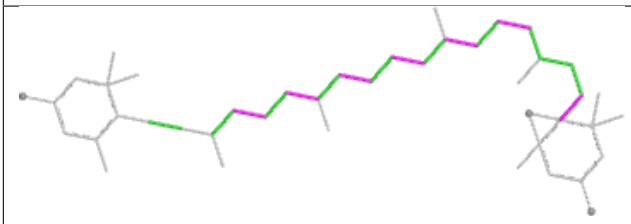
Ligand DD6 2 304



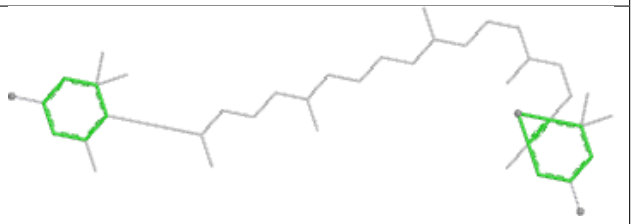
Bond lengths



Bond angles

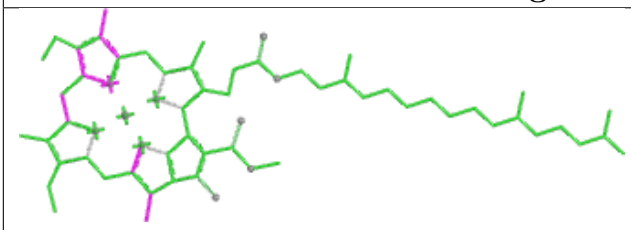


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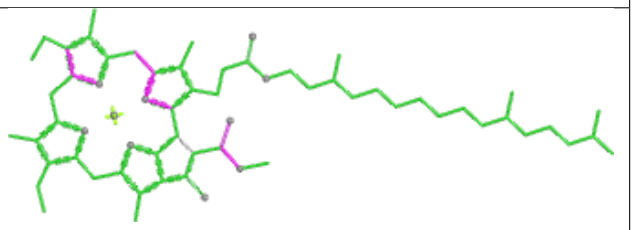


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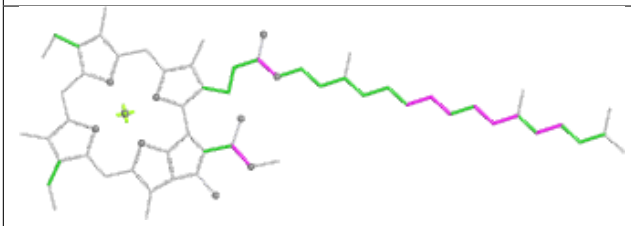
Ligand CLA c 505



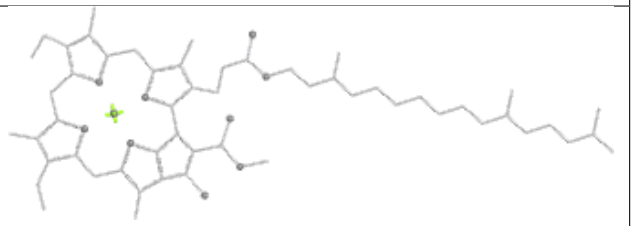
Bond lengths



Bond angles

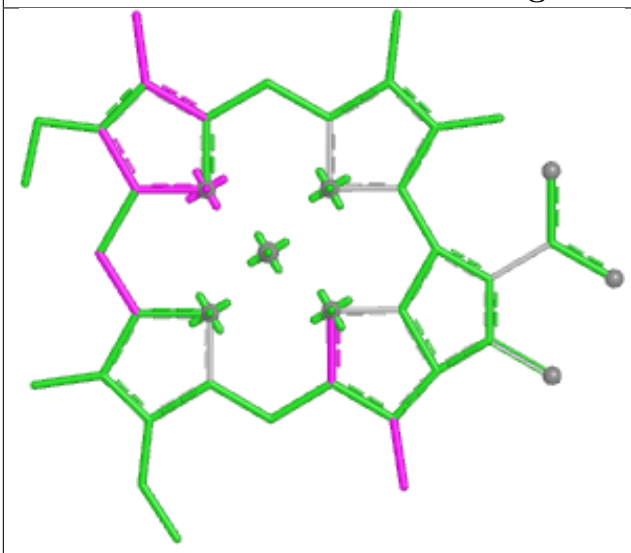


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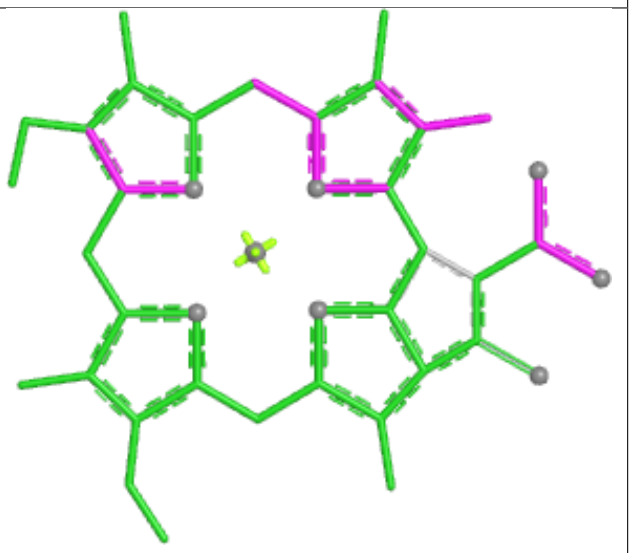


Rings

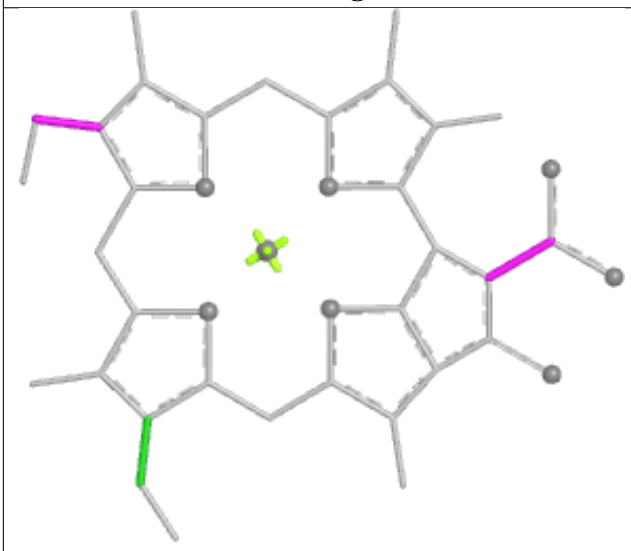
Ligand CLA 6 213



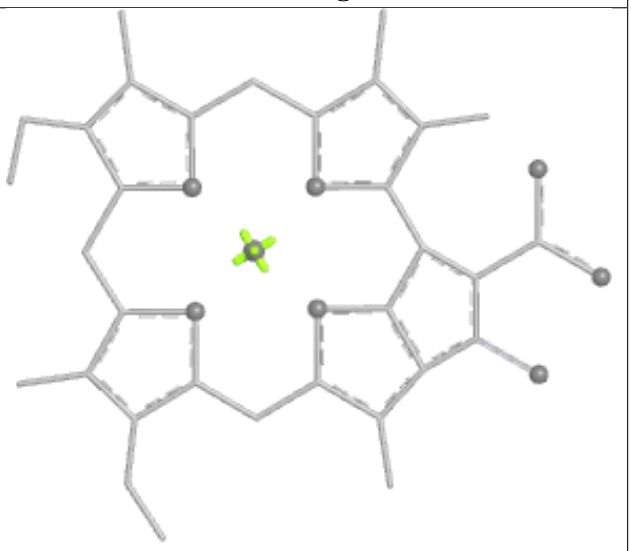
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Bond angles

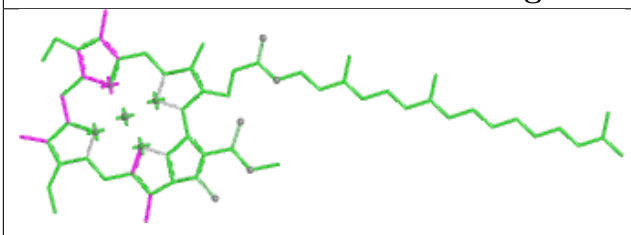


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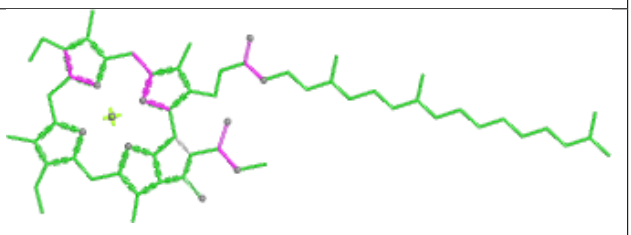


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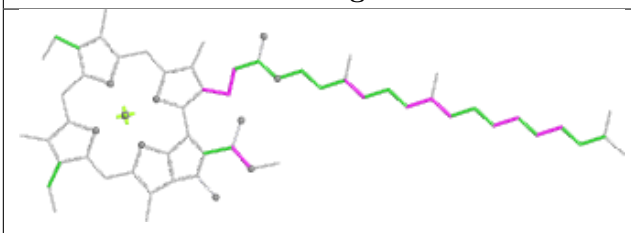
Ligand CLA B 503



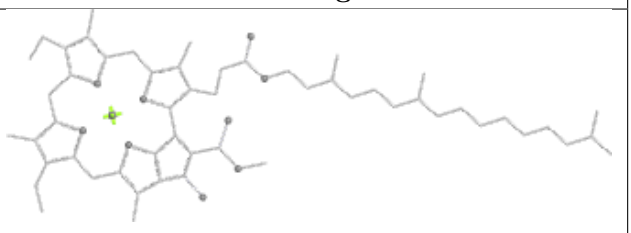
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Bond angles

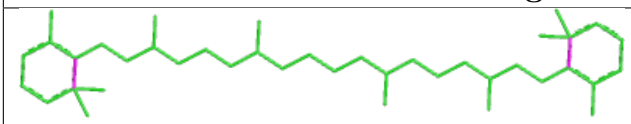


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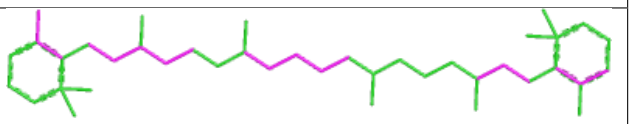


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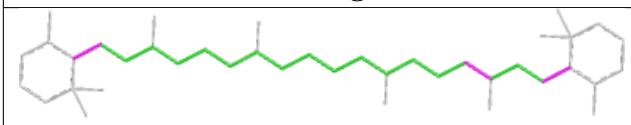
Ligand BCR b 519



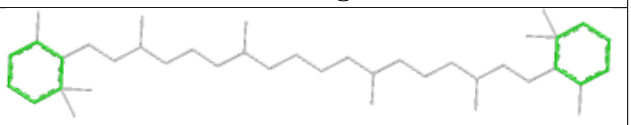
Bond lengths



Bond angles

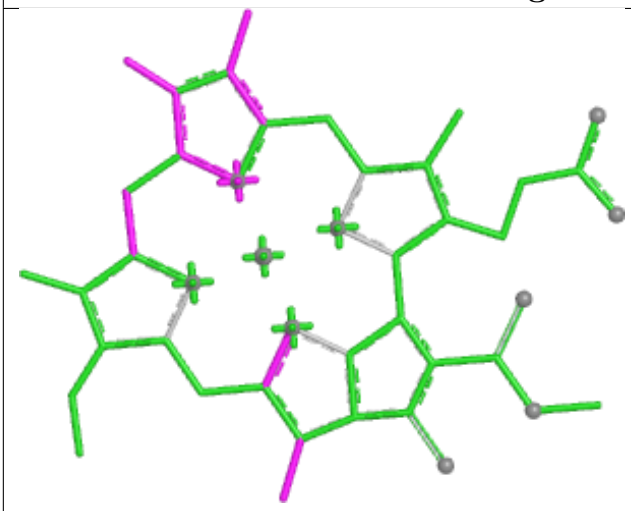


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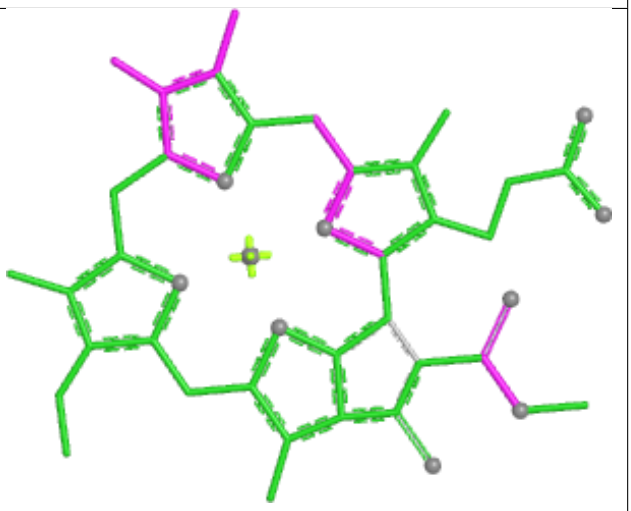


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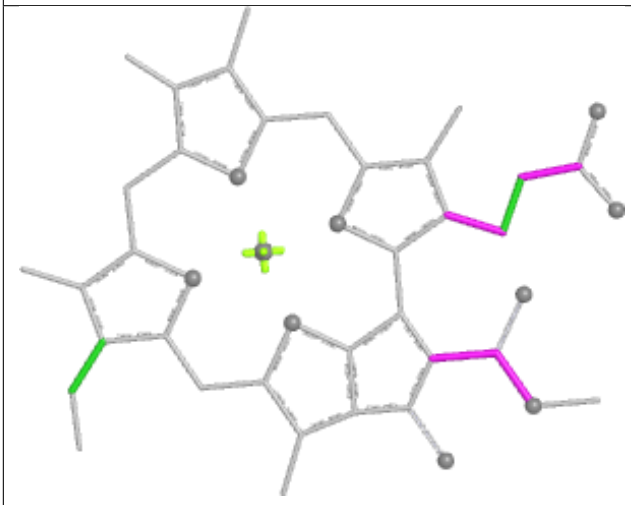
Ligand CLA 2 308



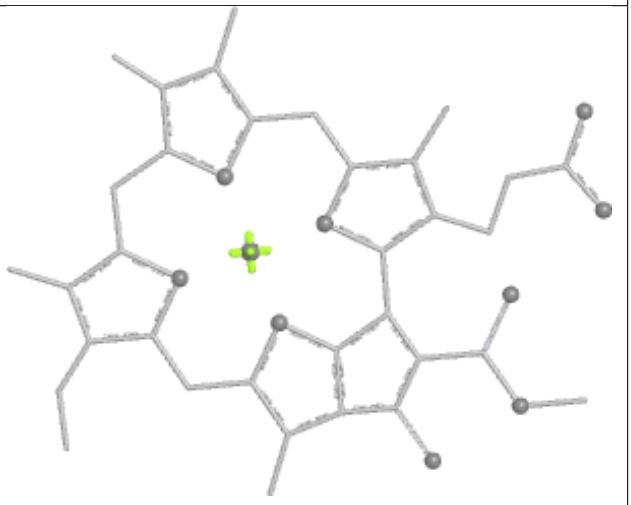
Bond lengths



Bond angles

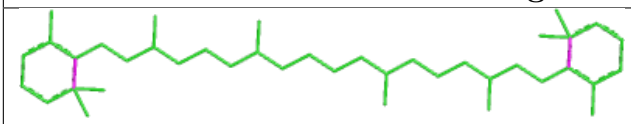


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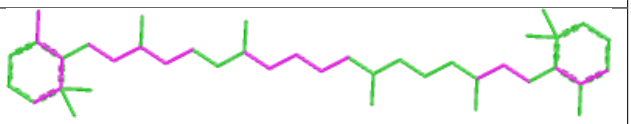


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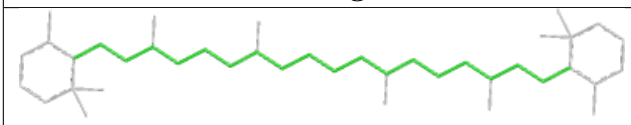
Ligand BCR c 515



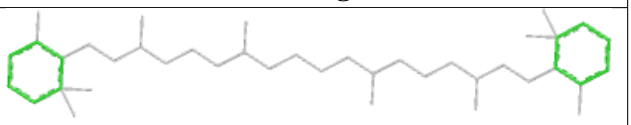
Bond lengths



Bond angles

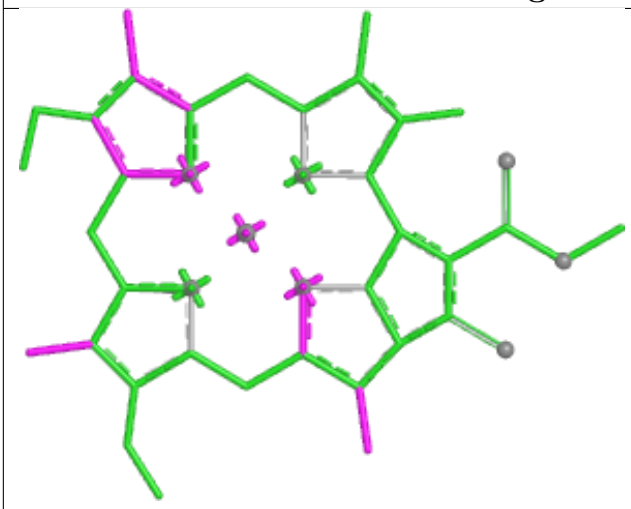


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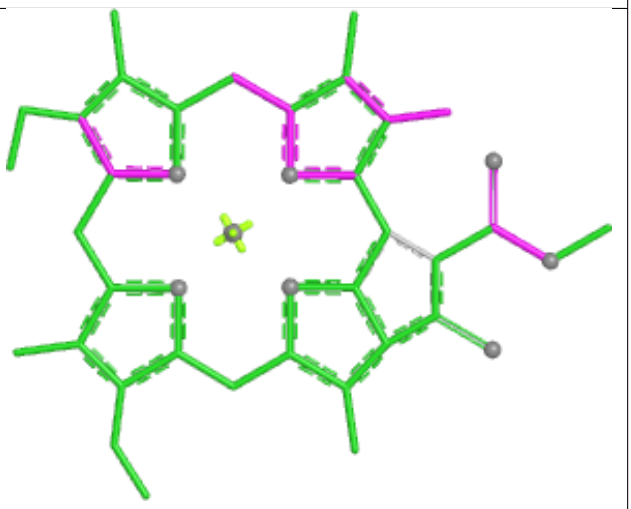


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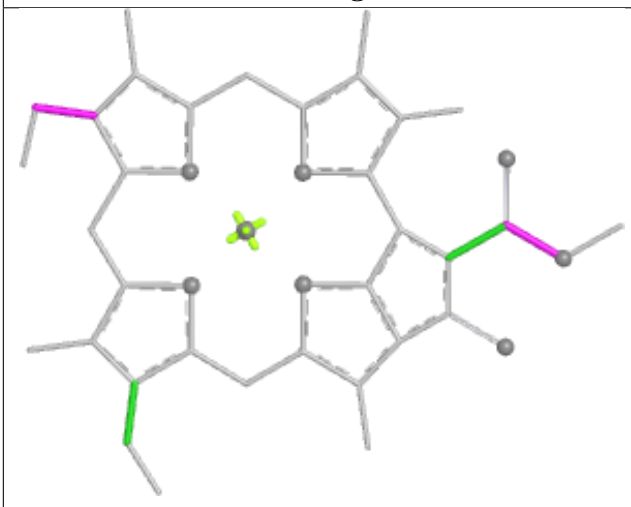
Ligand CLA 4 209



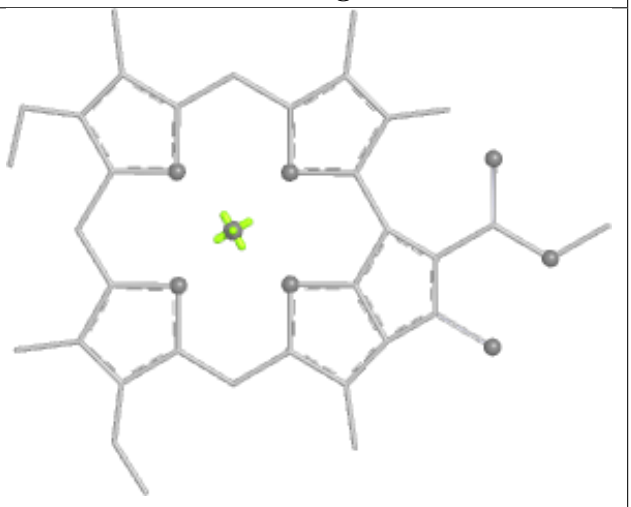
Bond lengths



Bond angles

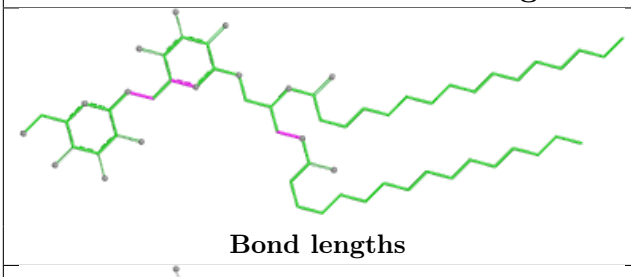


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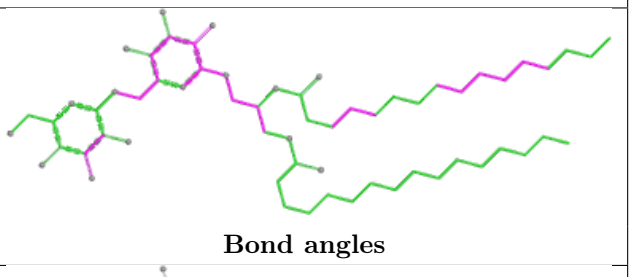


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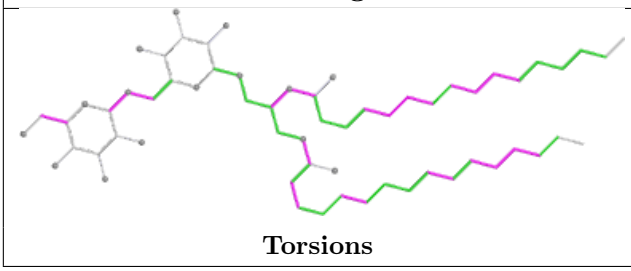
Ligand DGD C 519



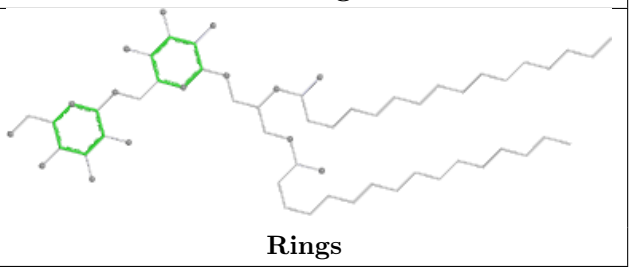
Bond lengths



Bond angles

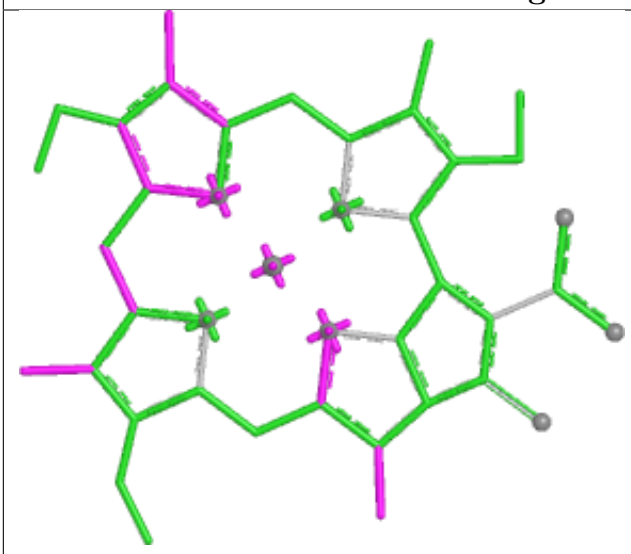


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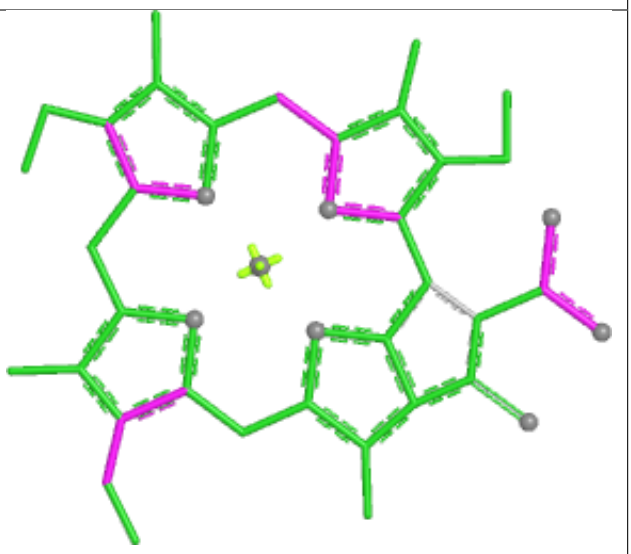


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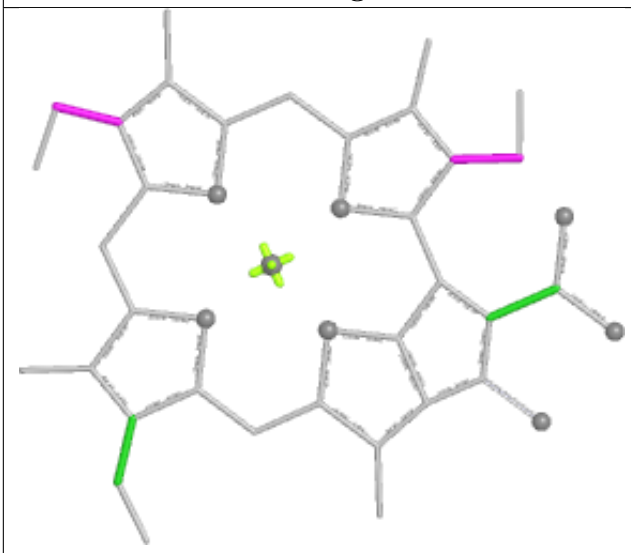
Ligand CLA 3 305



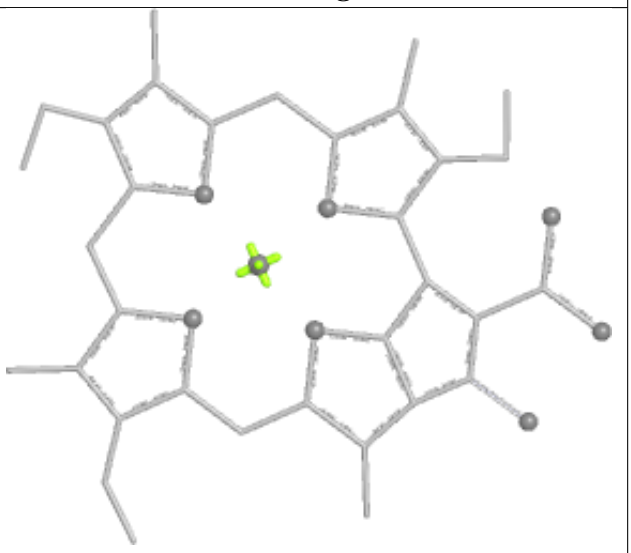
Bond lengths



Bond angles

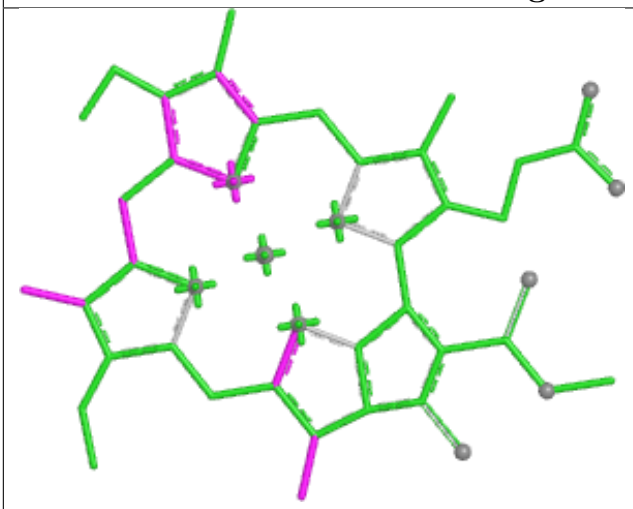


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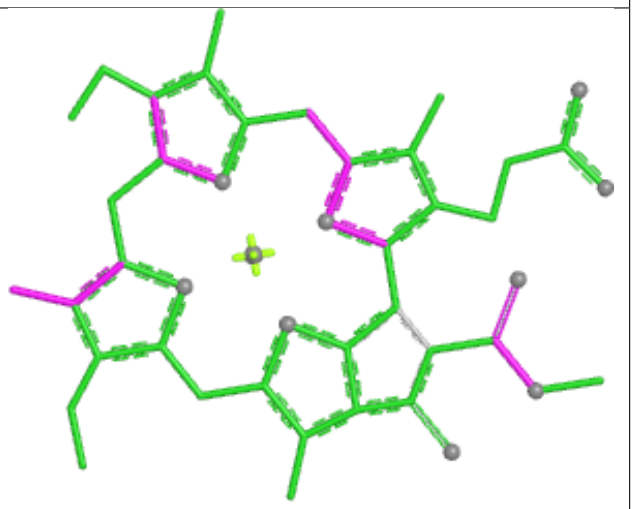


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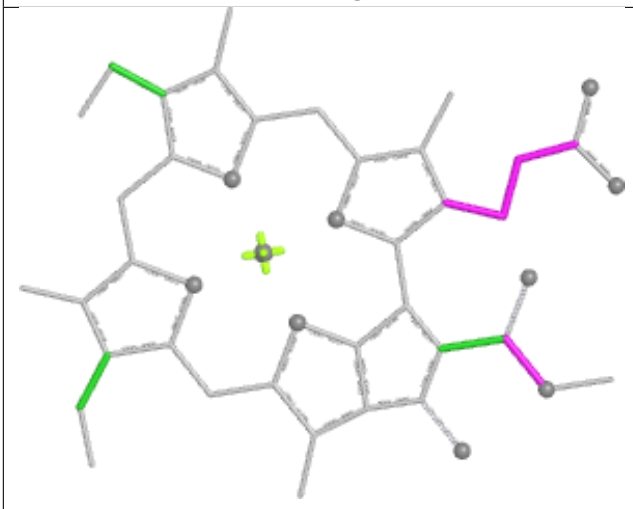
Ligand CLA 6 206



Bond lengths



Bond angles

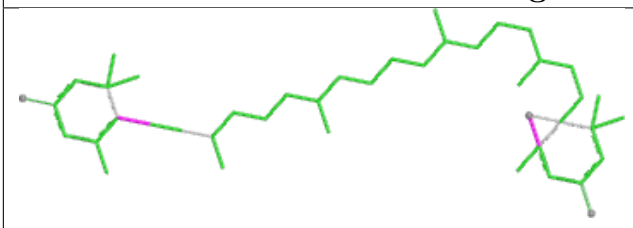


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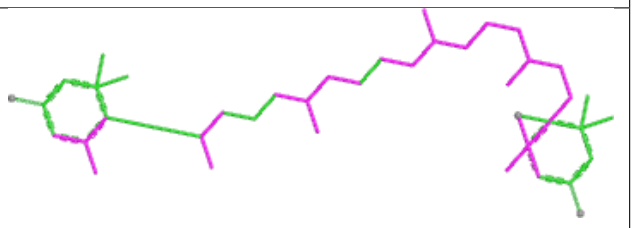


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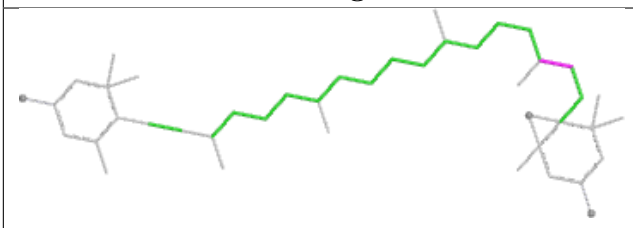
Ligand DD6 7 303



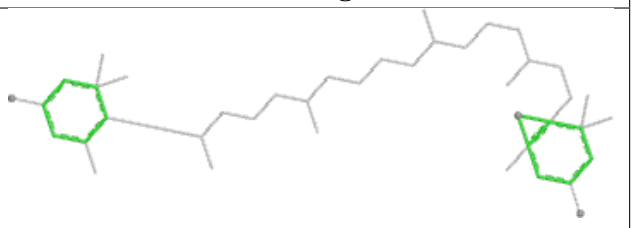
Bond lengths



Bond angles

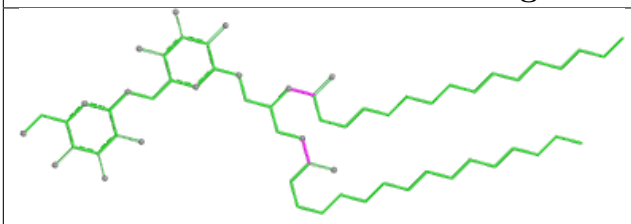


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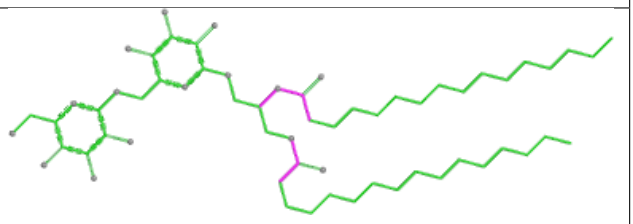


Rings

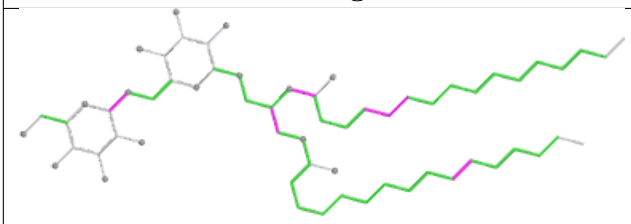
Ligand DGD C 520



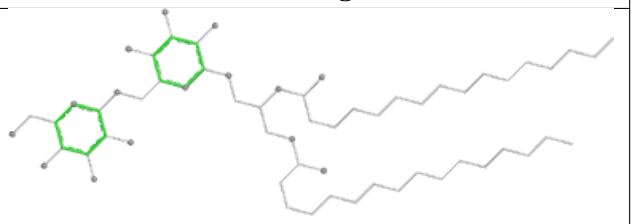
Bond lengths



Bond angles

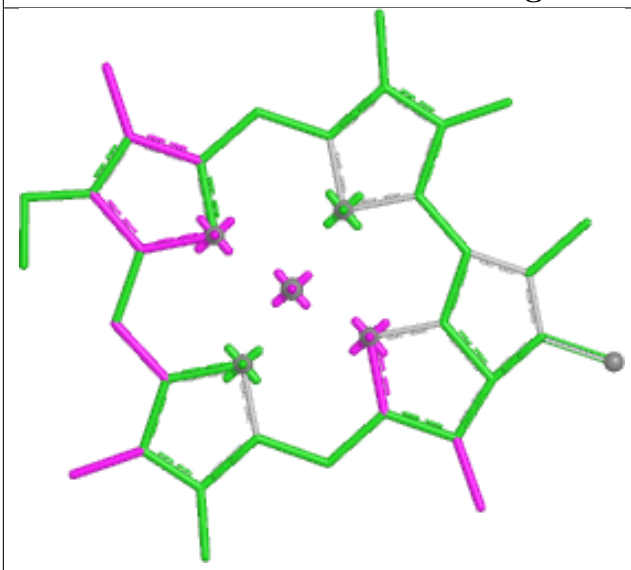


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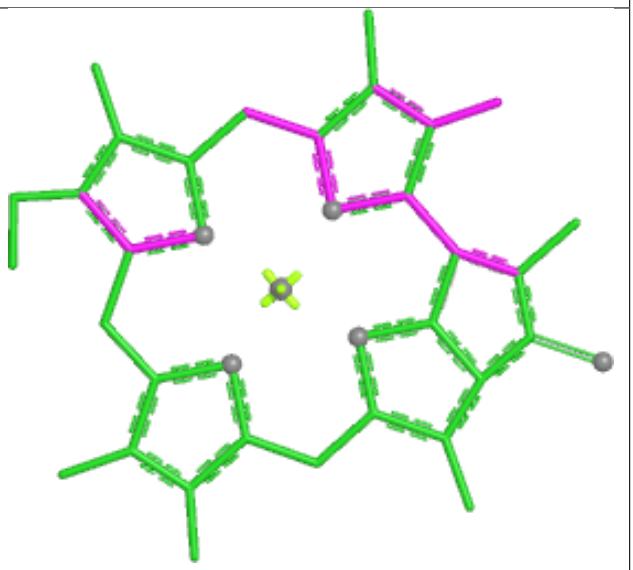


Rings

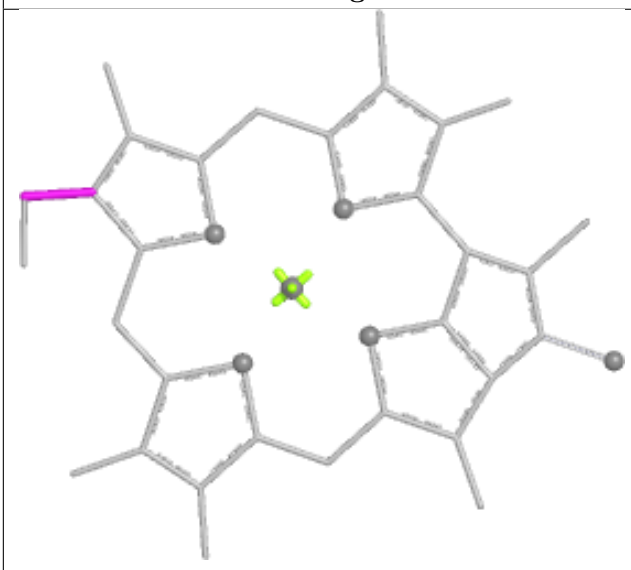
Ligand CLA P 605



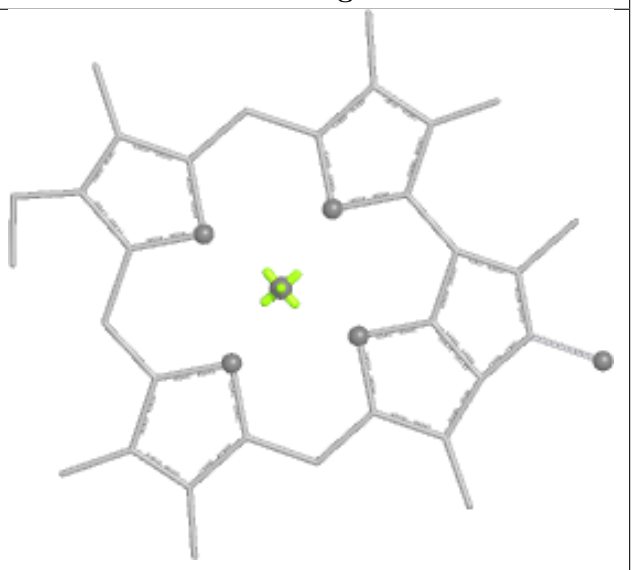
Bond lengths



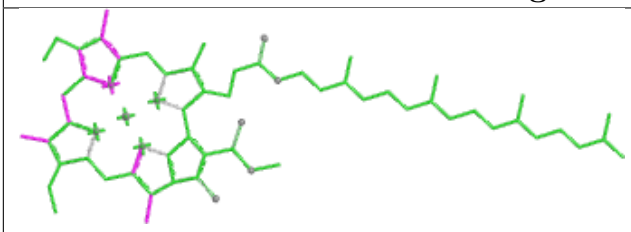
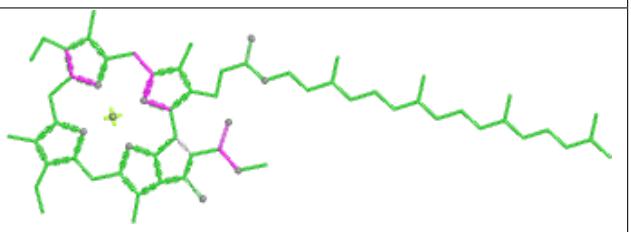
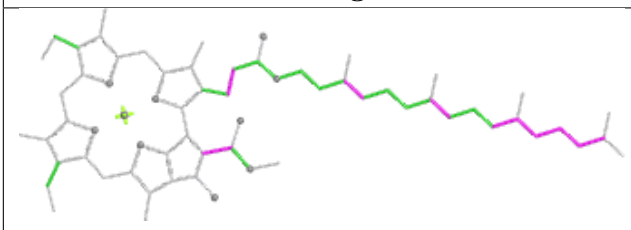
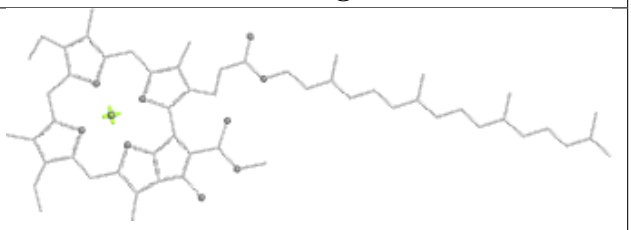
Bond angles

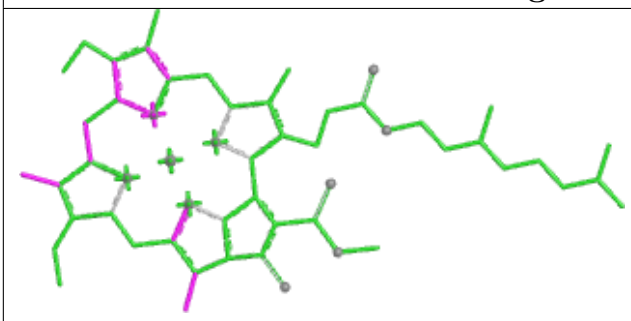
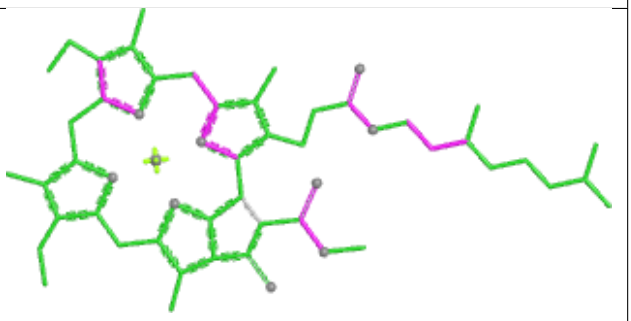
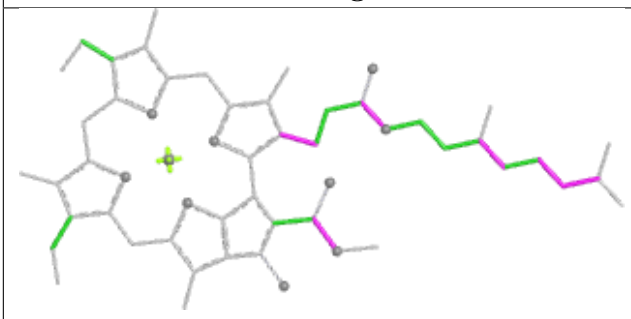
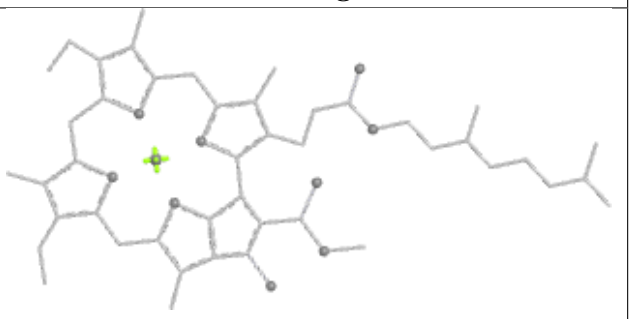


Torsions

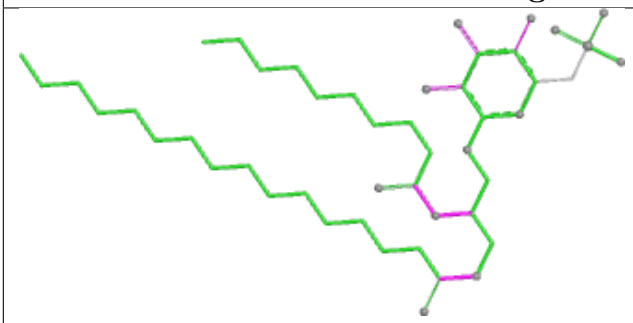


Rings

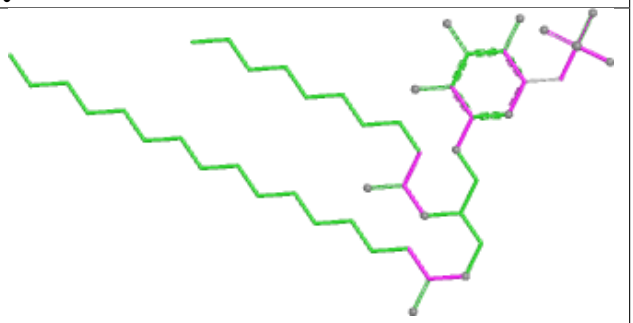
Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

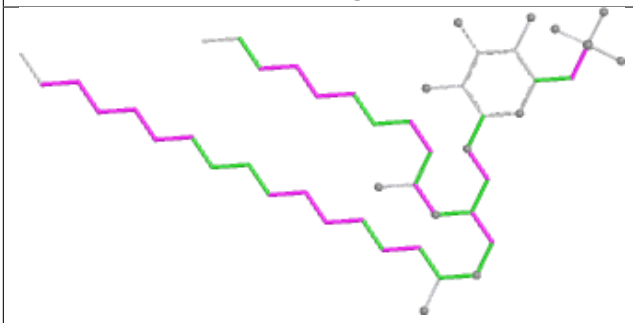
Ligand SQD 5 316



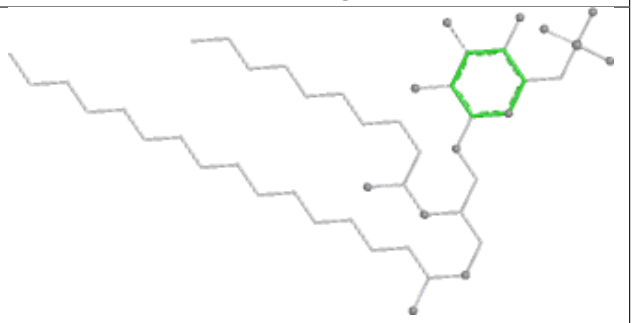
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Bond angles

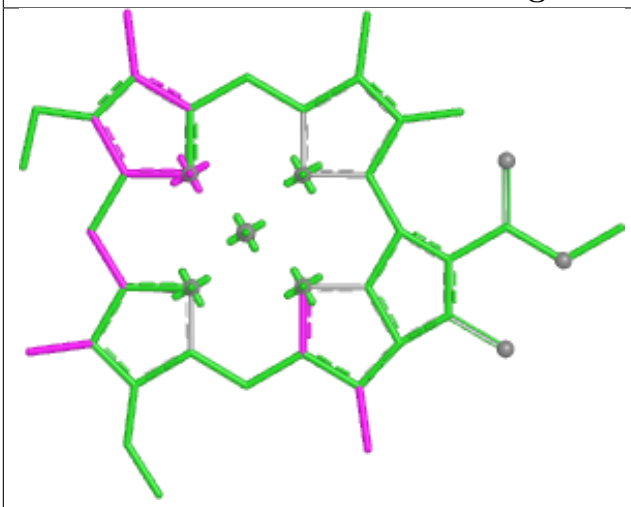


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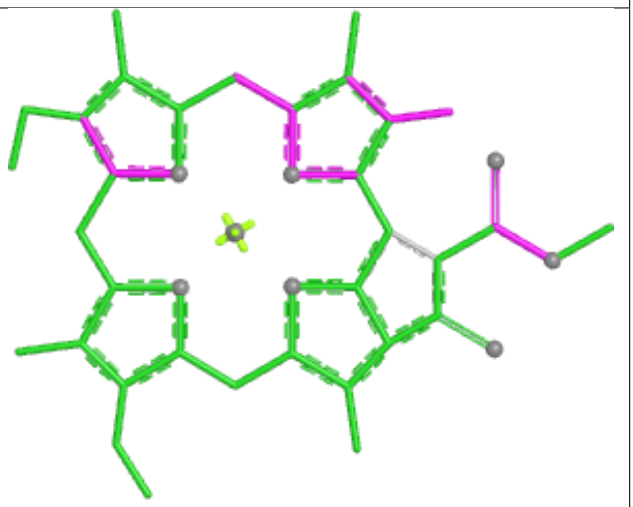


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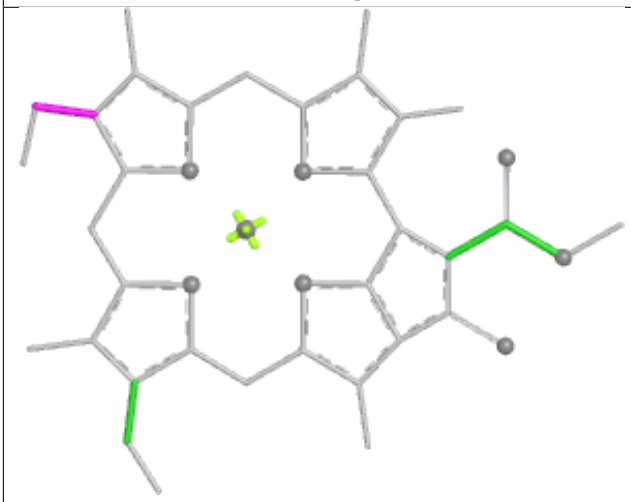
Ligand CLA 1 205



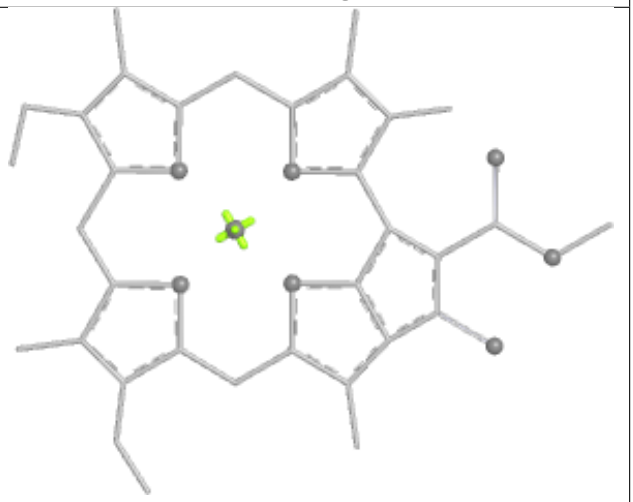
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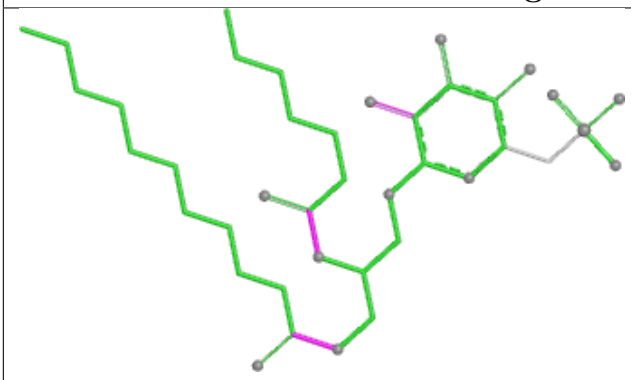


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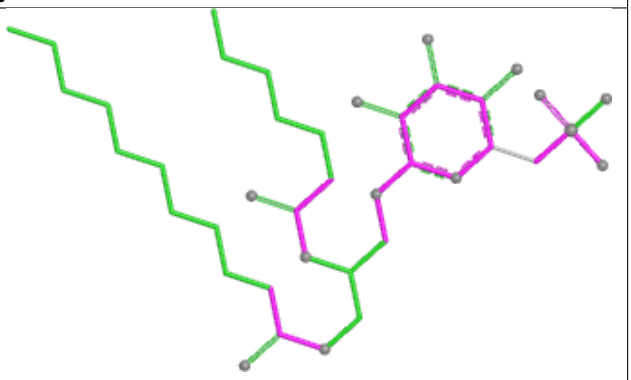


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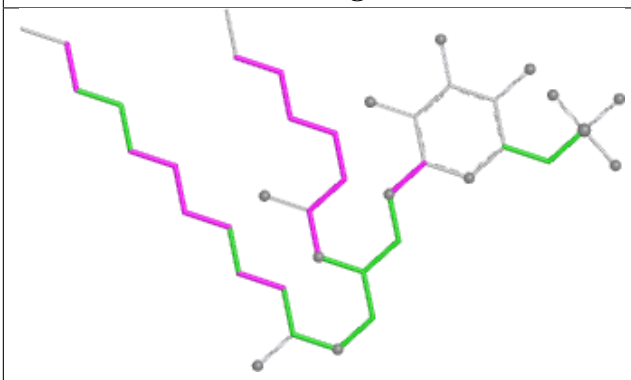
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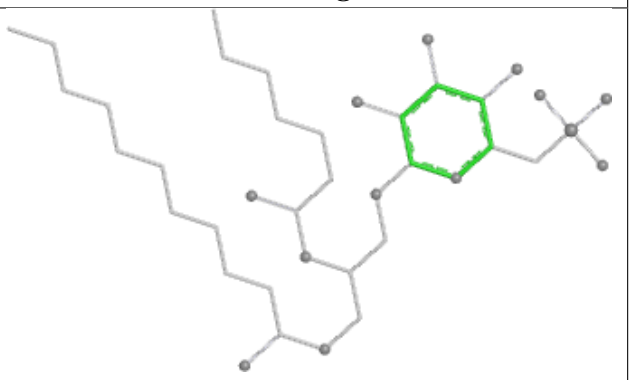
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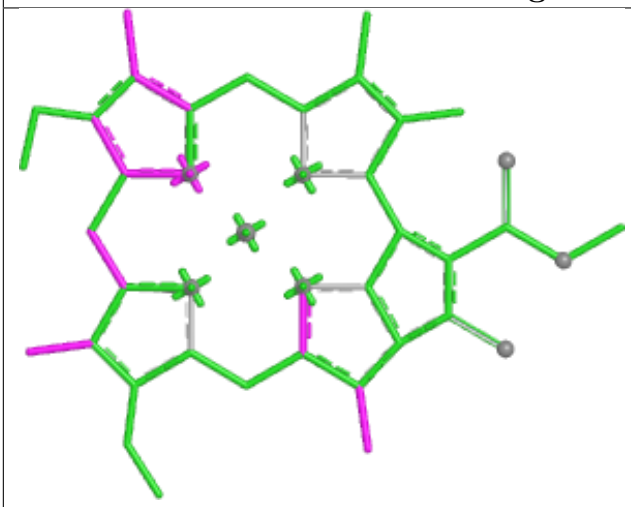


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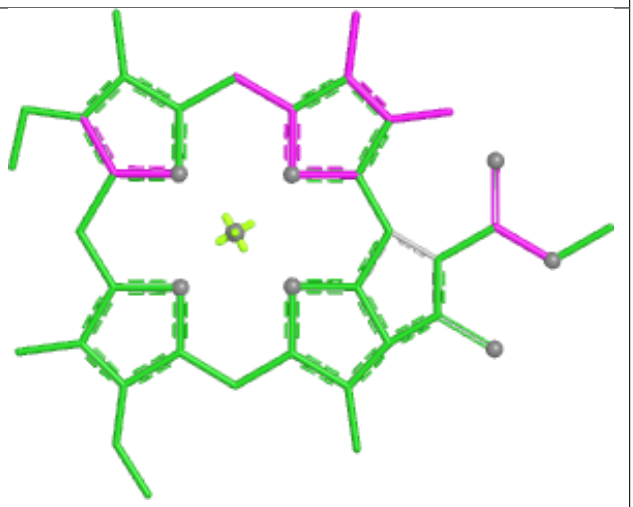


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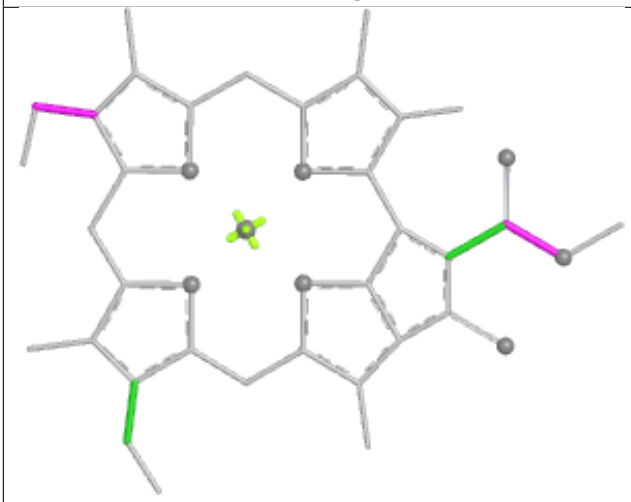
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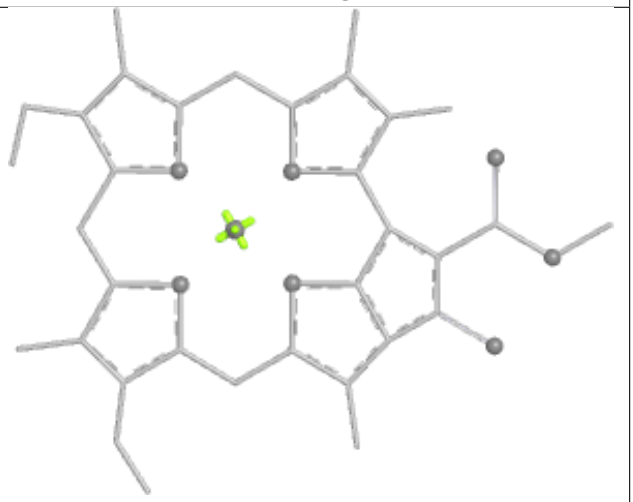
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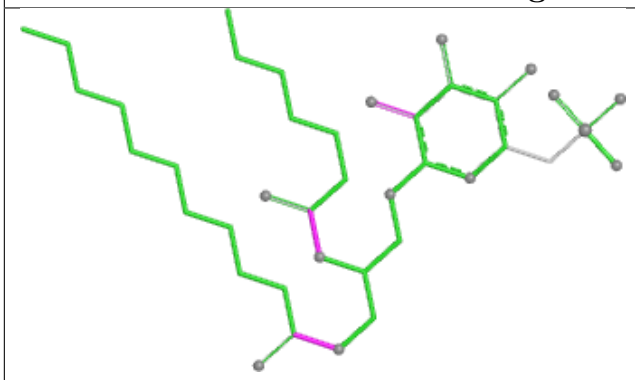


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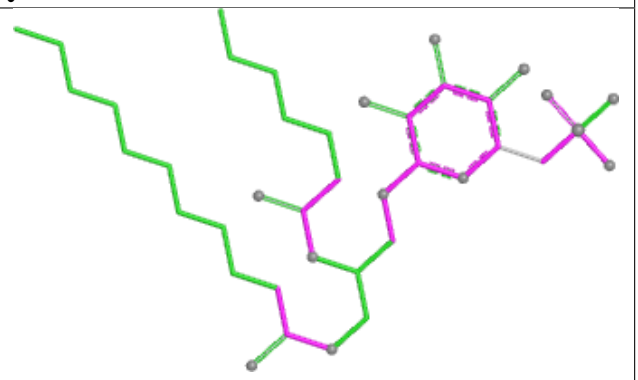


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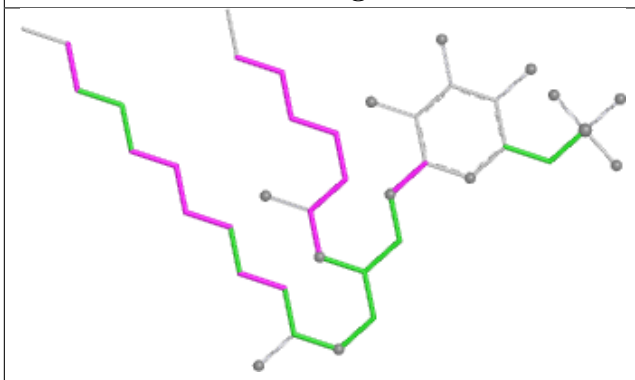
Ligand SQD b 501



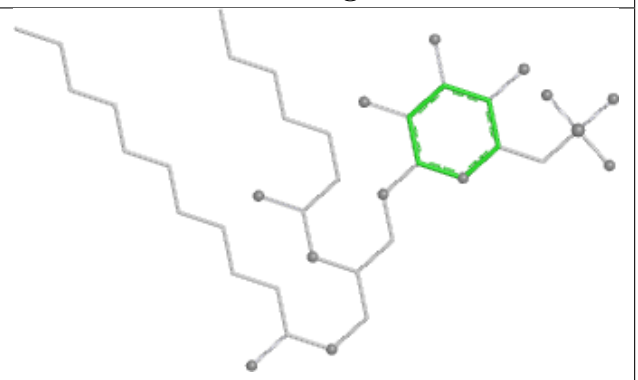
Bond lengths



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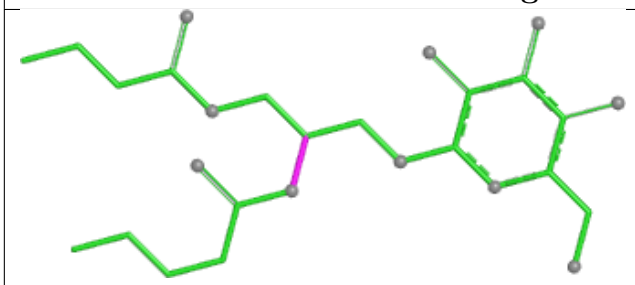


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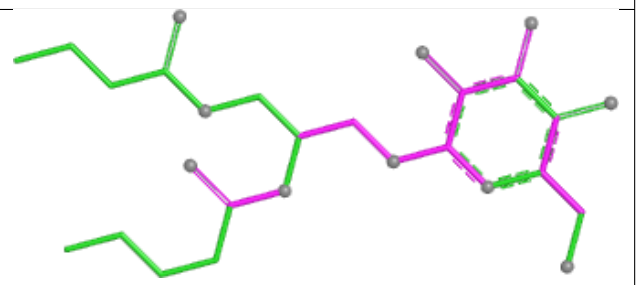


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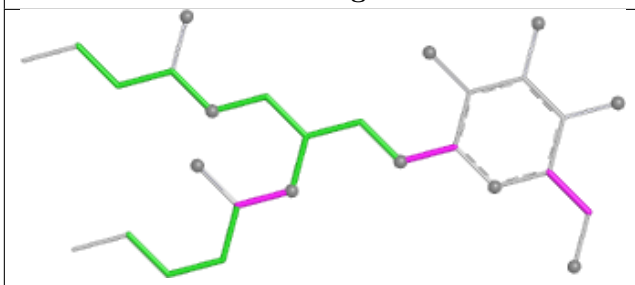
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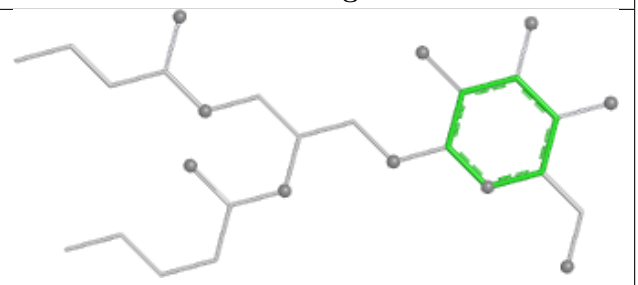
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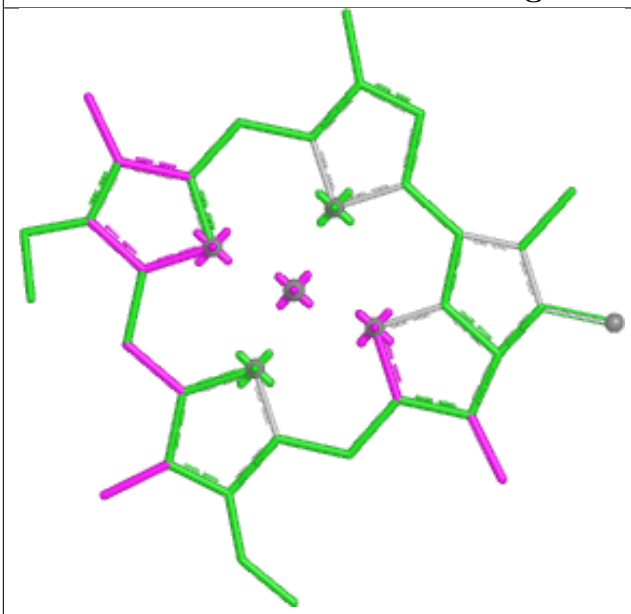


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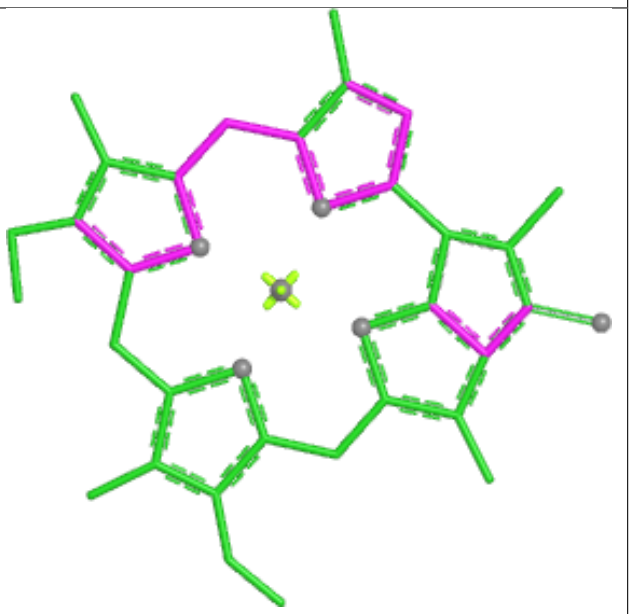


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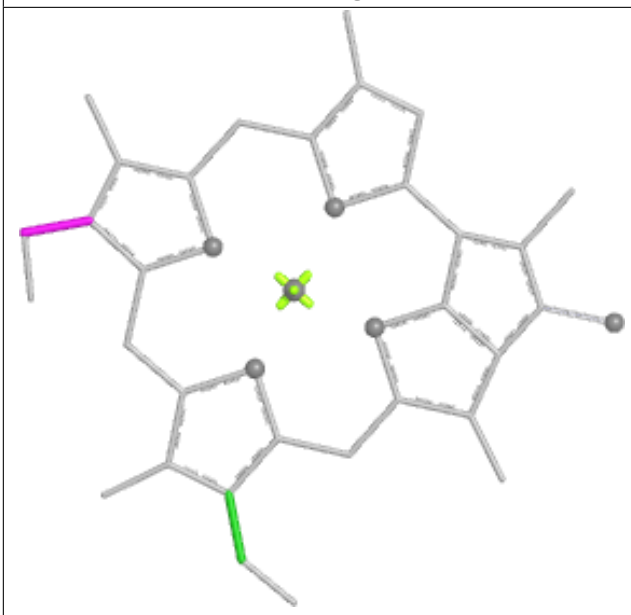
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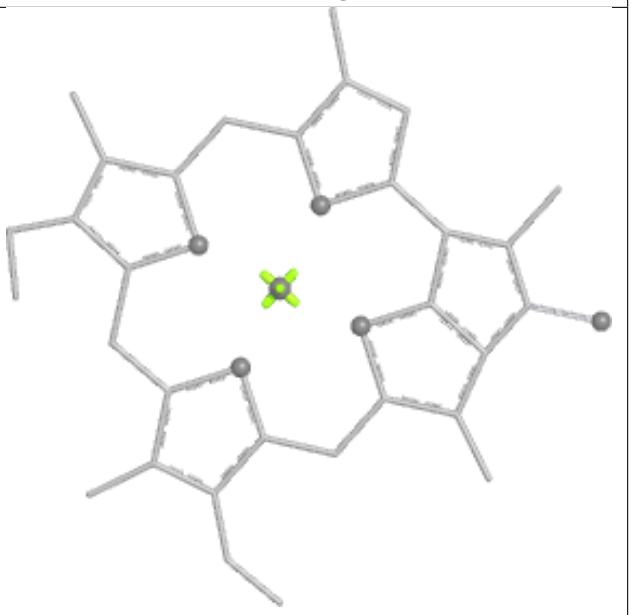
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Bond angles

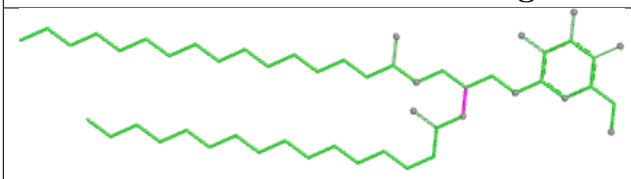


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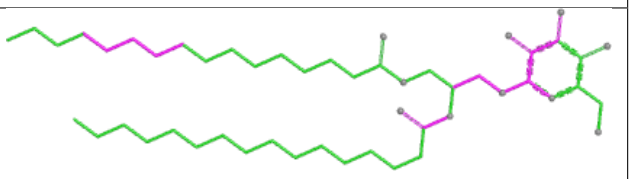


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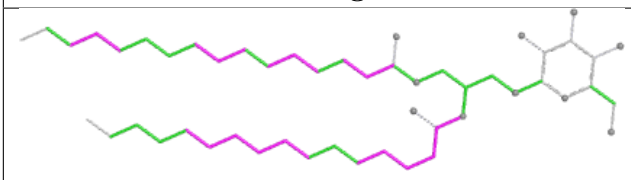
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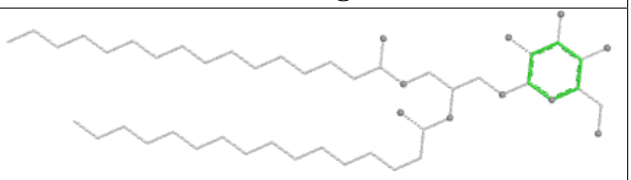
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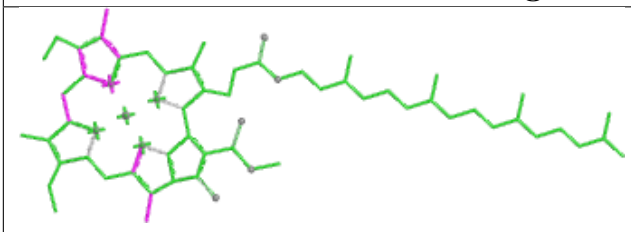


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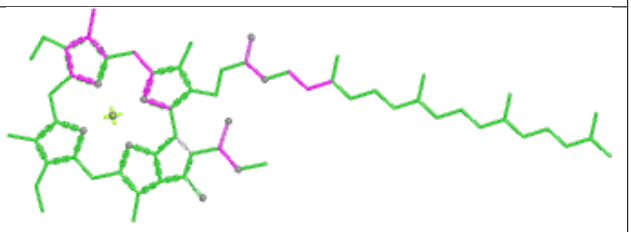


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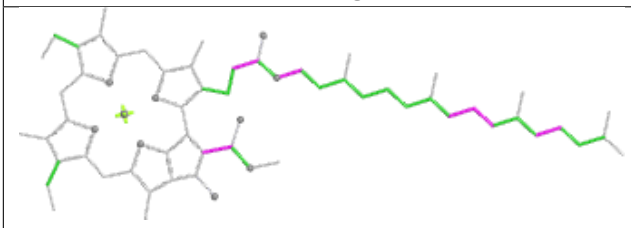
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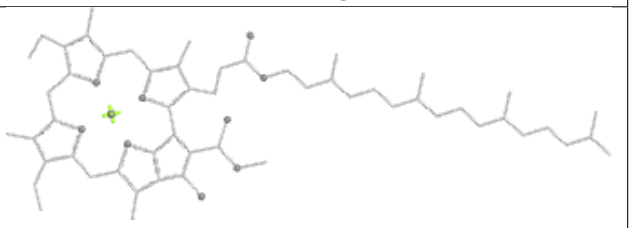
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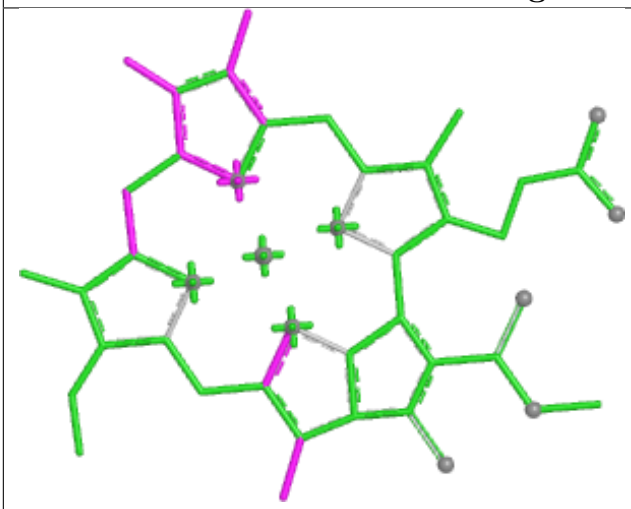


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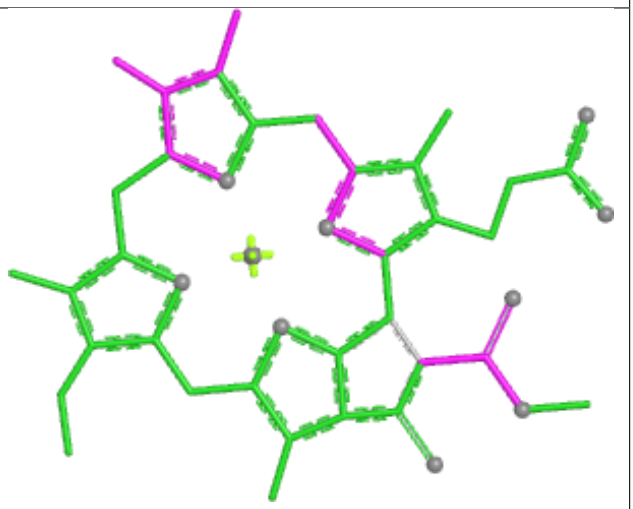


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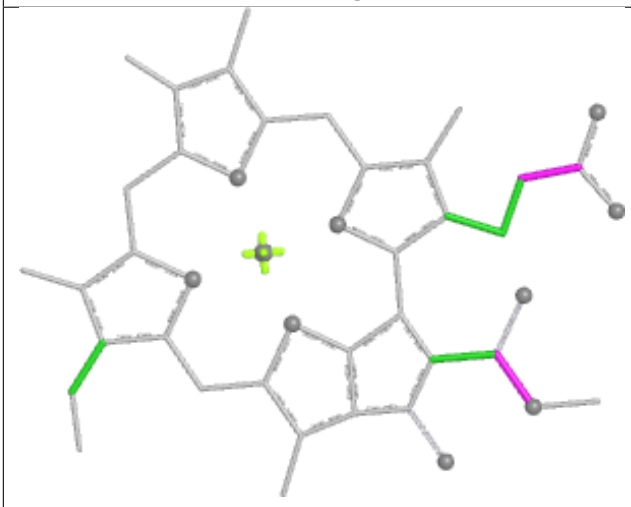
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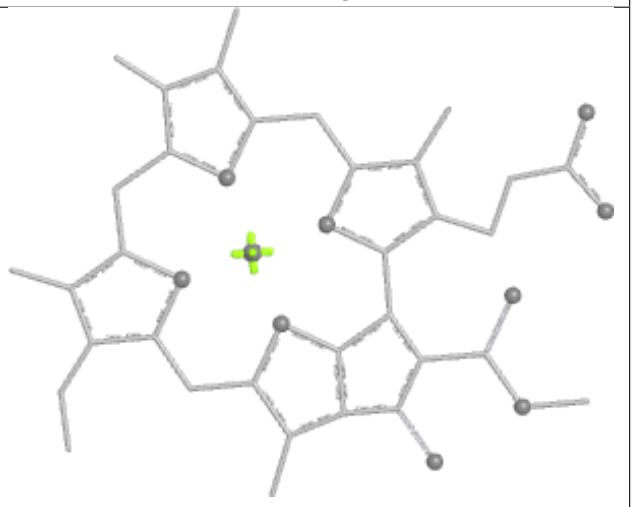
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Bond angles

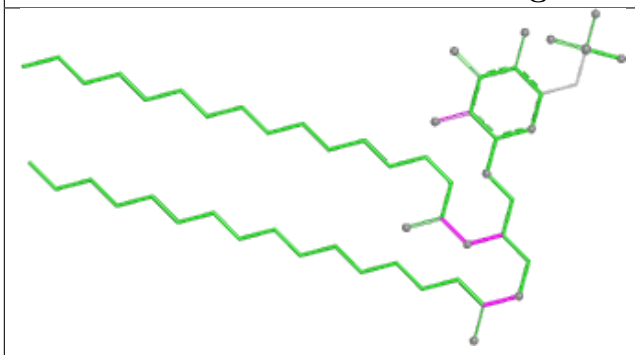


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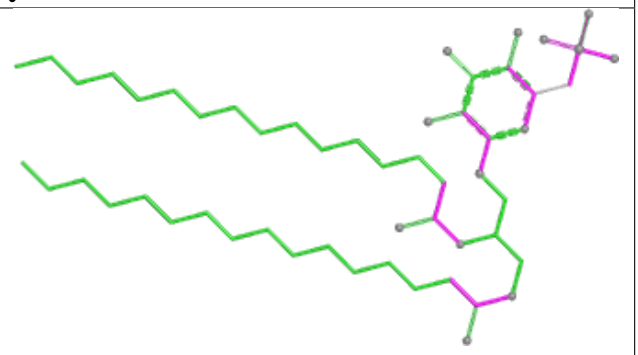


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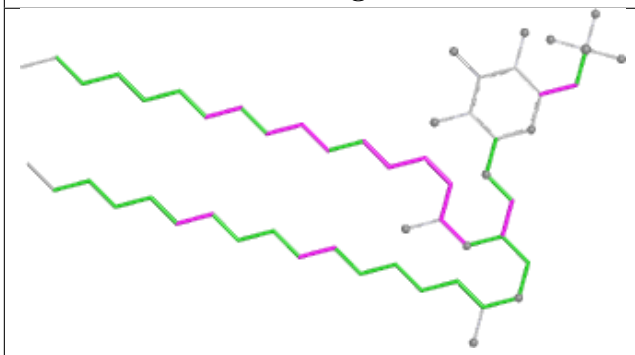
Ligand SQD a 409



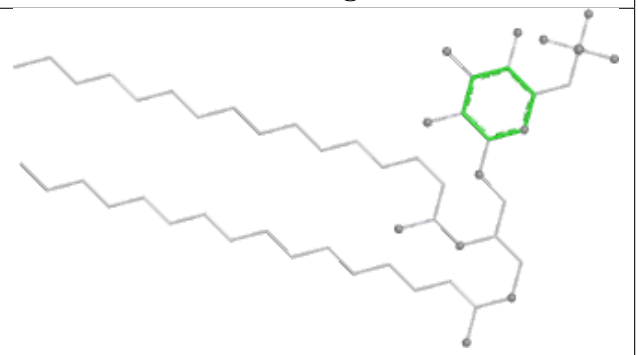
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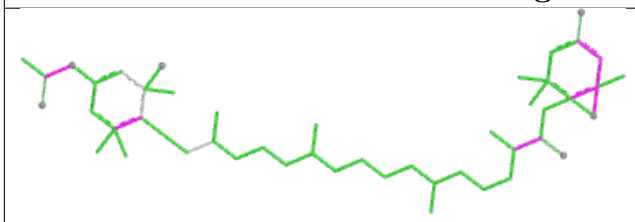


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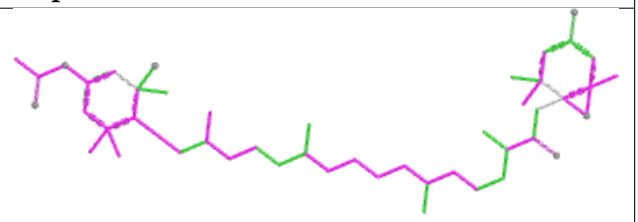


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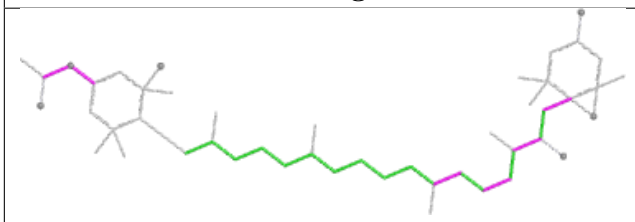
Ligand A86 p 610



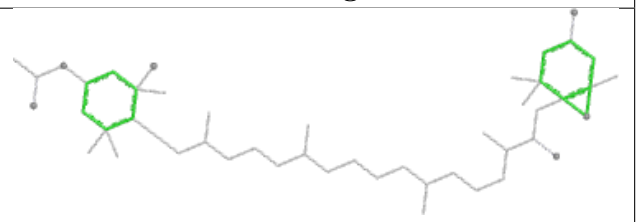
Bond lengths



Bond angles

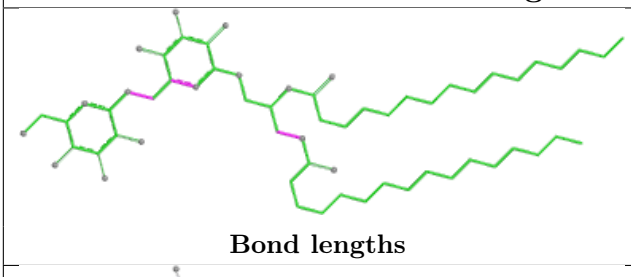


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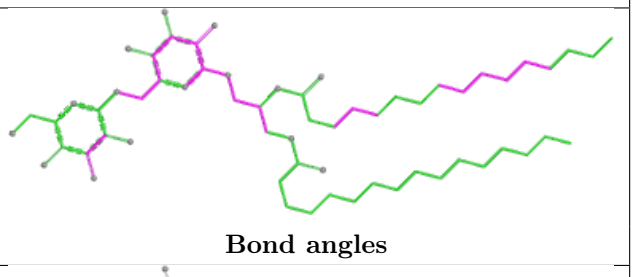


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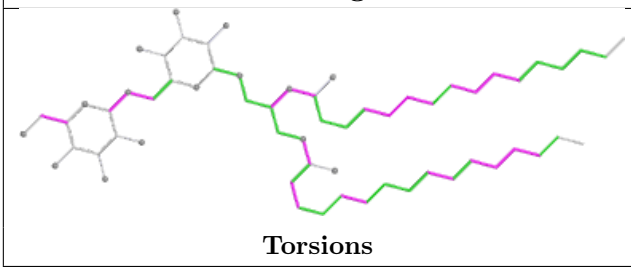
Ligand DGD c 519



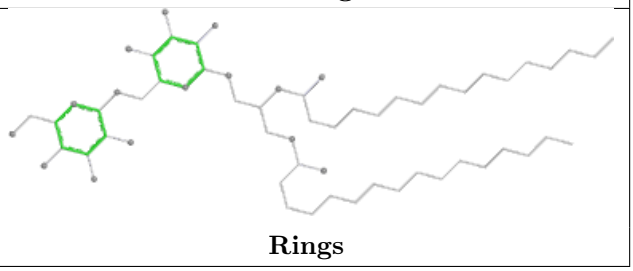
Bond lengths



Bond angles

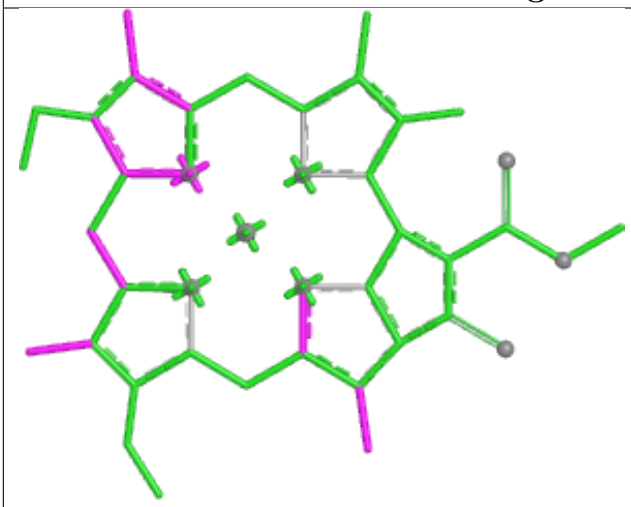


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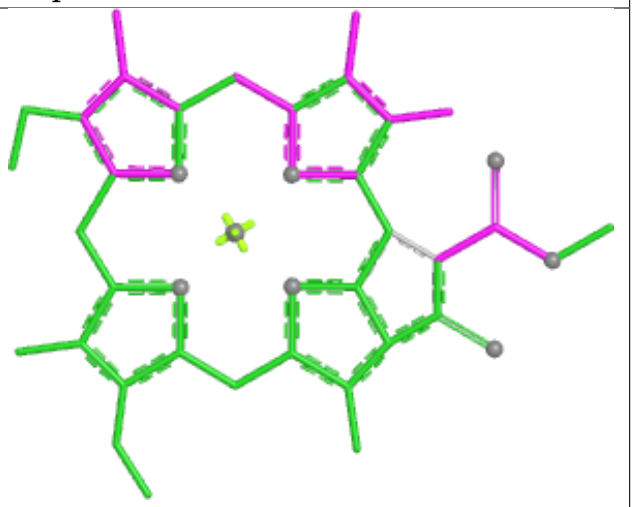


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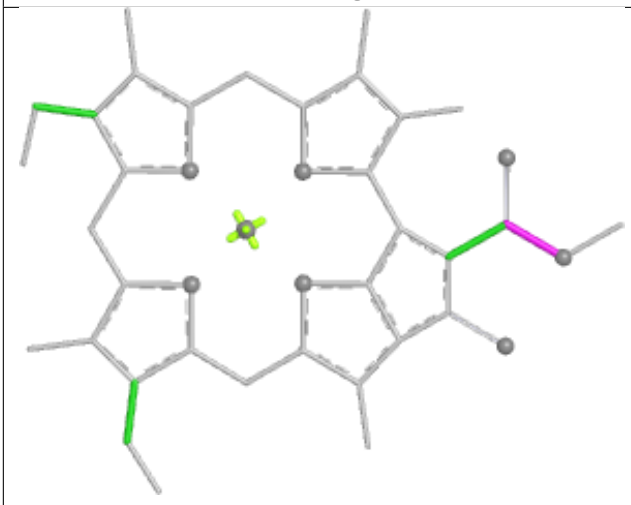
Ligand CLA p 602



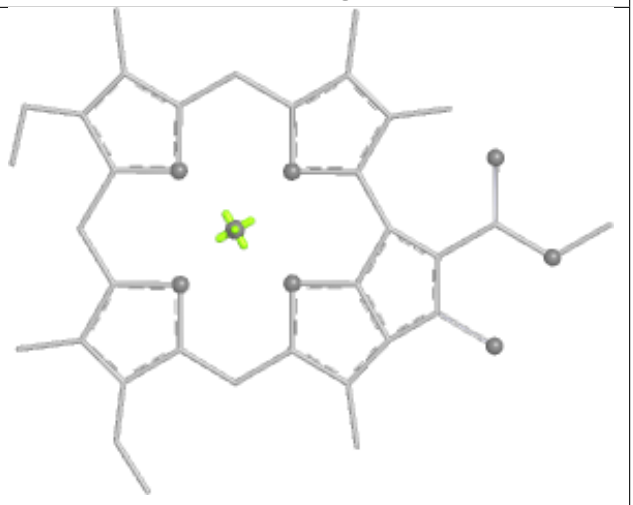
Bond lengths



Bond angles

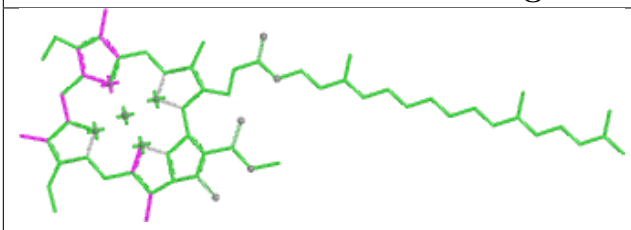


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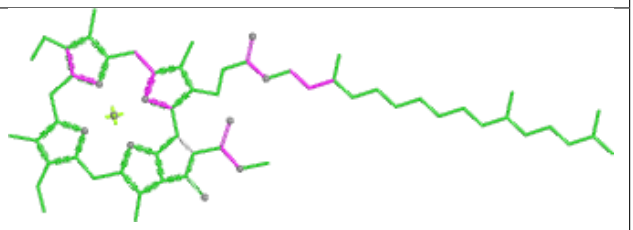


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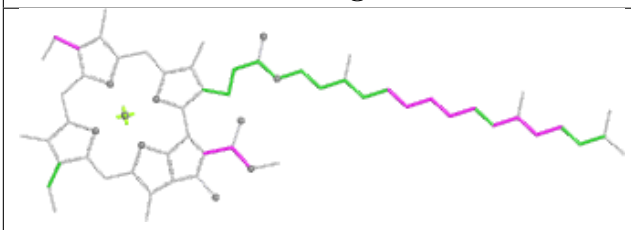
Ligand CLA C 503



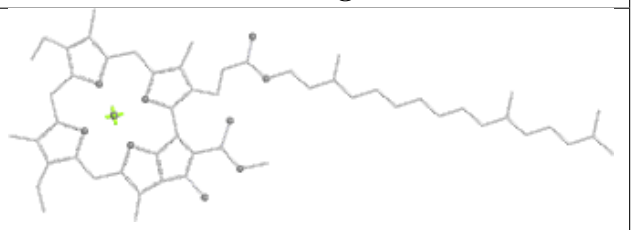
Bond lengths



Bond angles

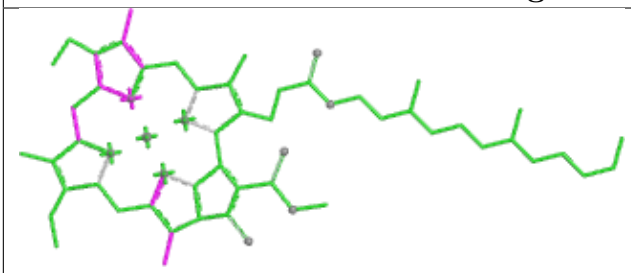


Torsions

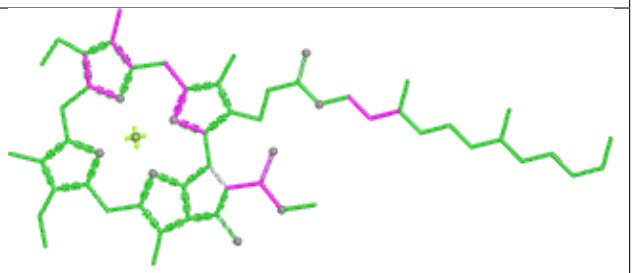


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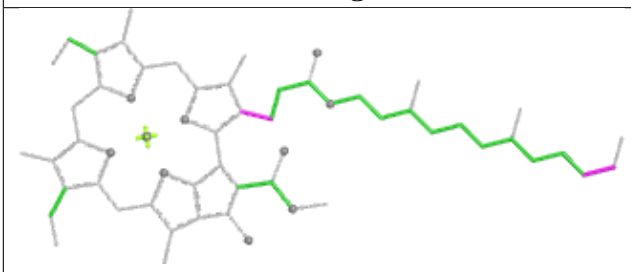
Ligand CLA d 401



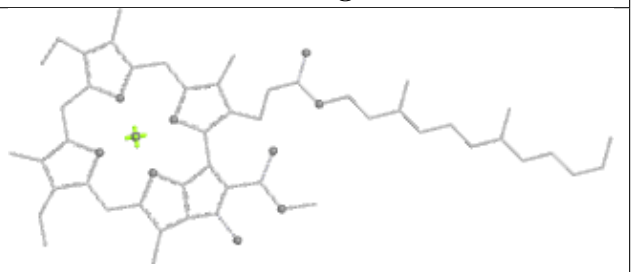
Bond lengths



Bond angles



Torsions

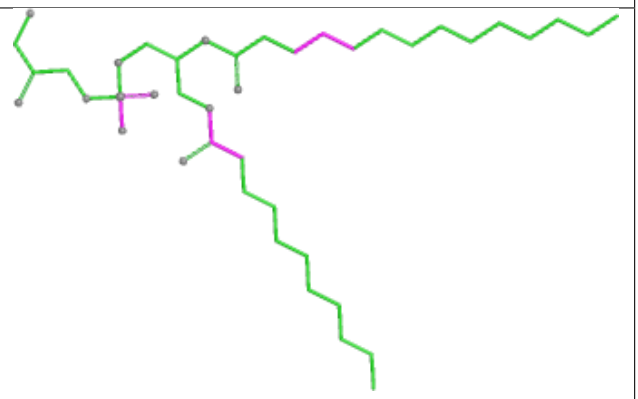


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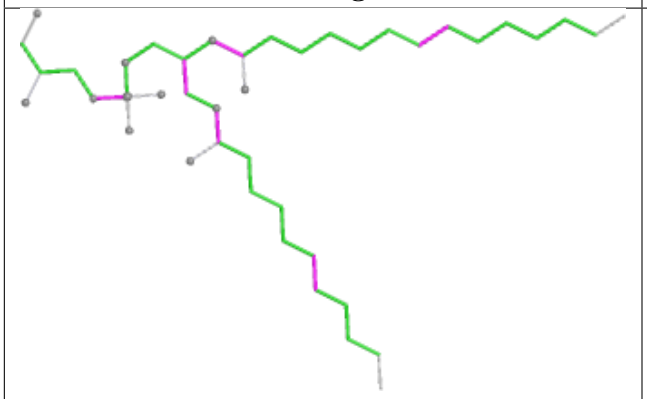
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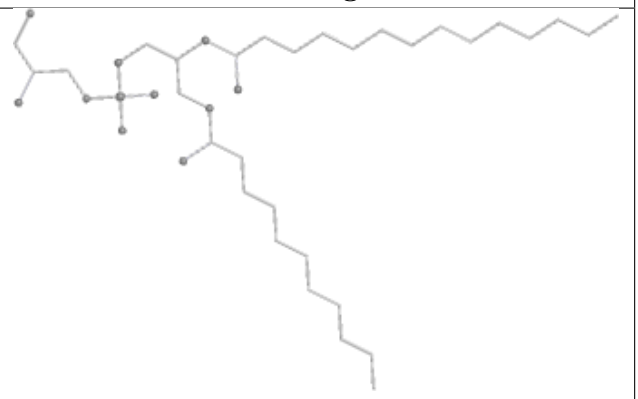
Bond lengths



Bond angles

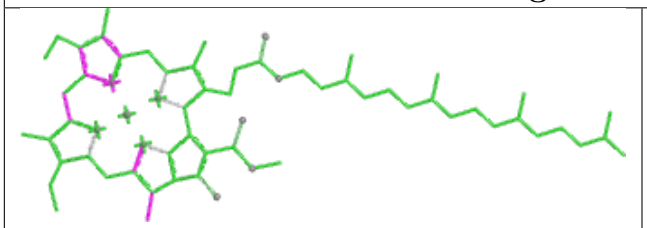


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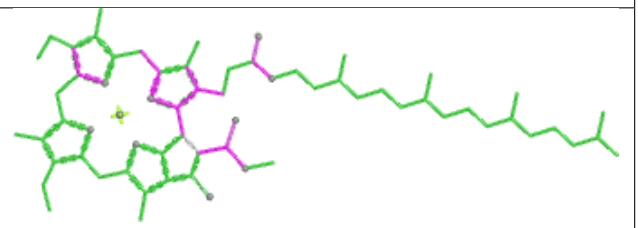


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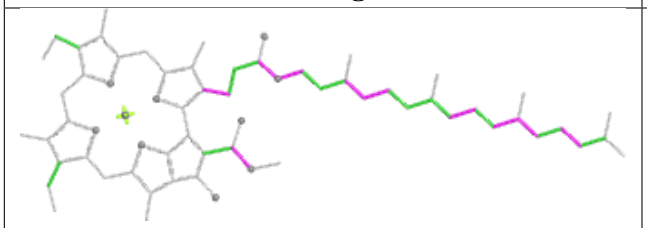
Ligand CLA 6 210



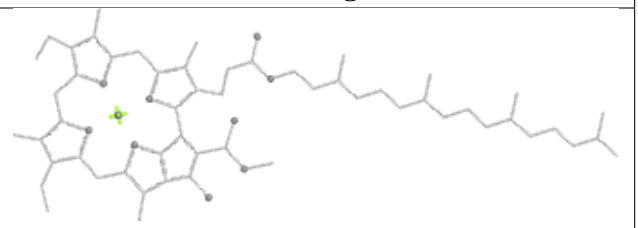
Bond lengths



Bond angles

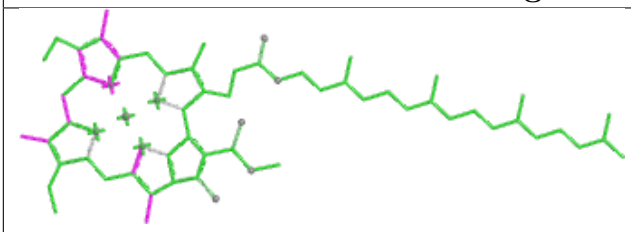


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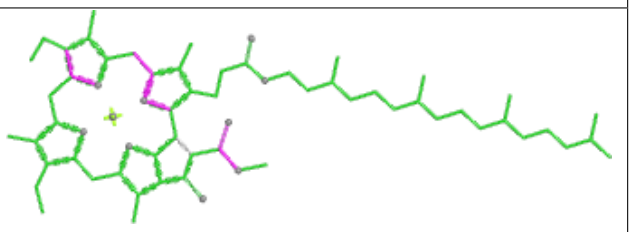


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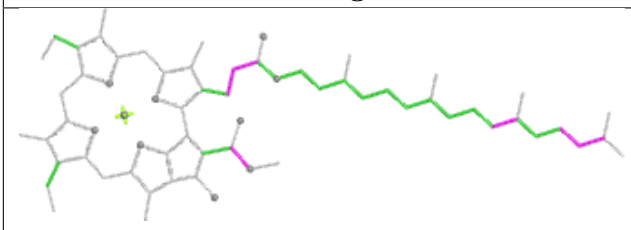
Ligand CLA B 510



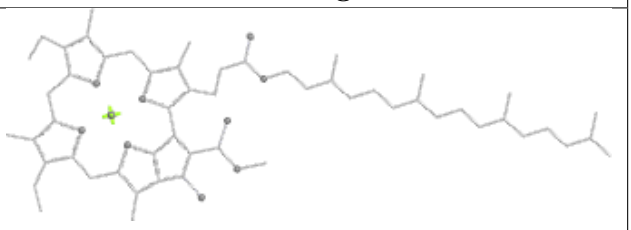
Bond lengths



Bond angles



Torsions

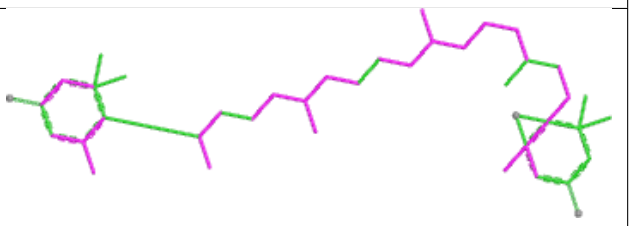


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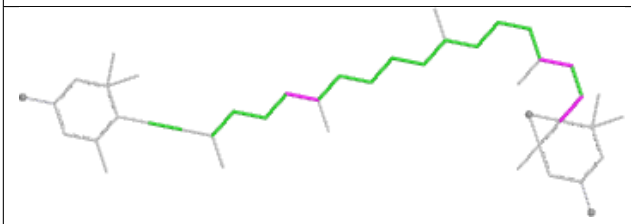
Ligand DD6 P 611



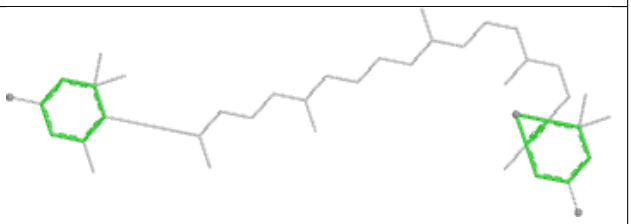
Bond lengths



Bond angles

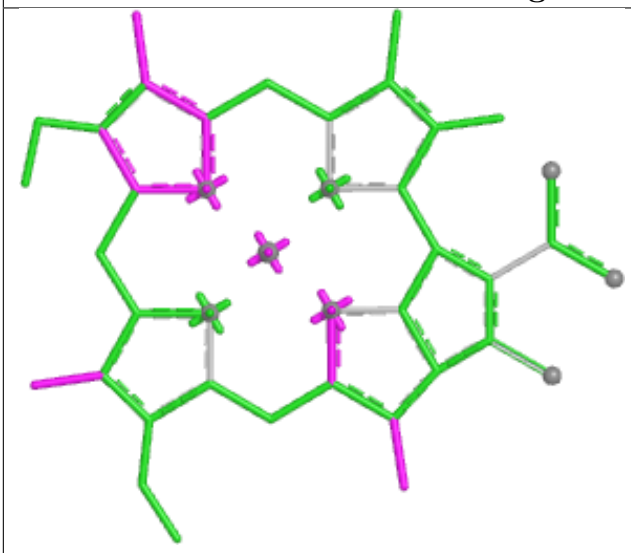


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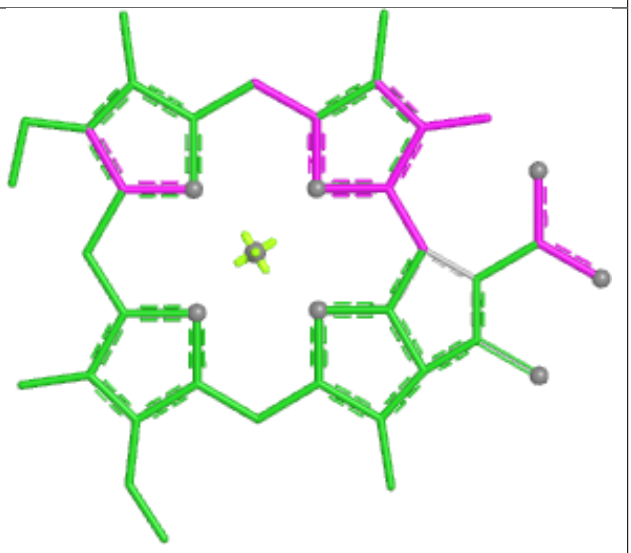


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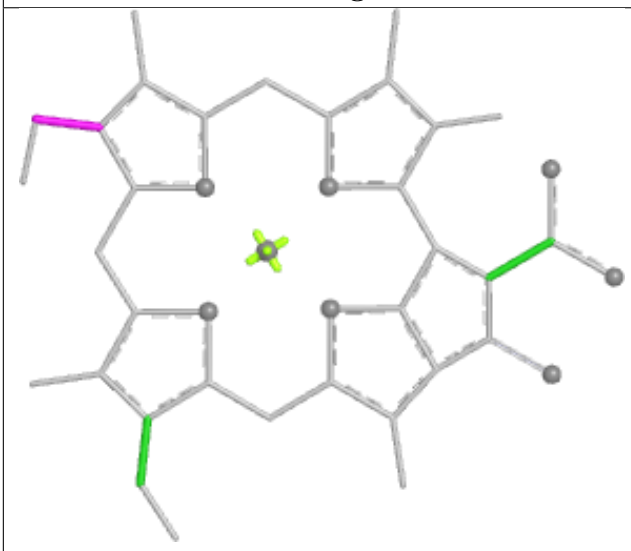
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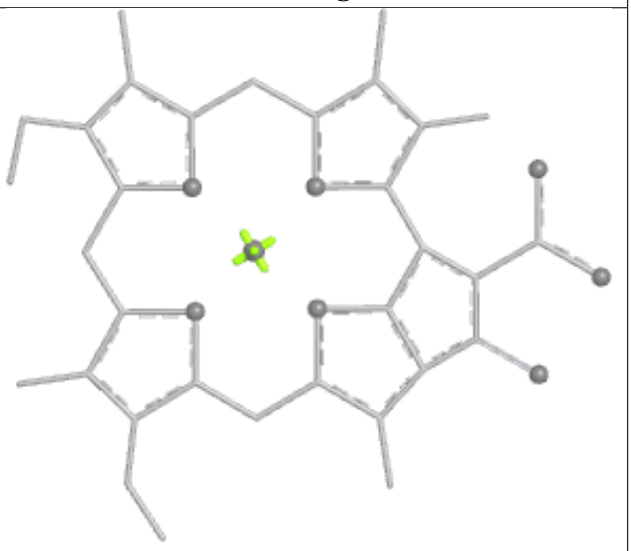
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Bond angles

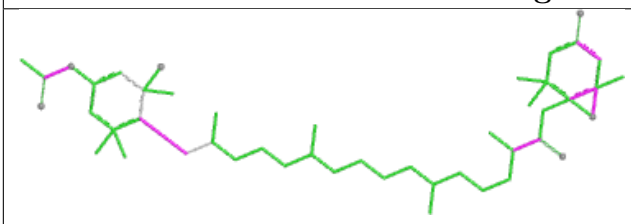


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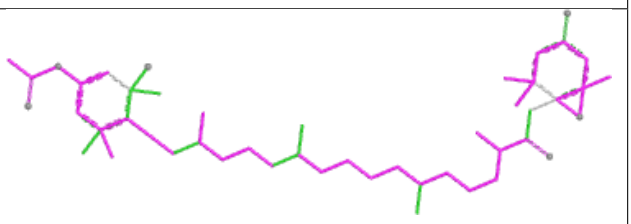


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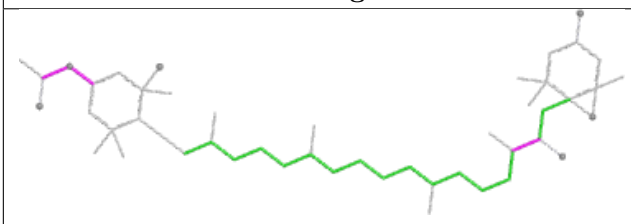
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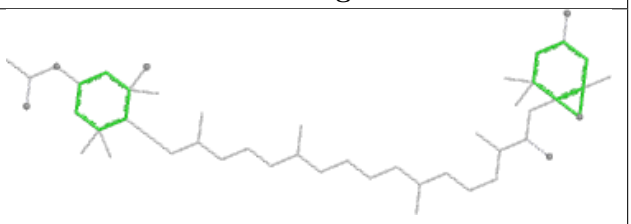
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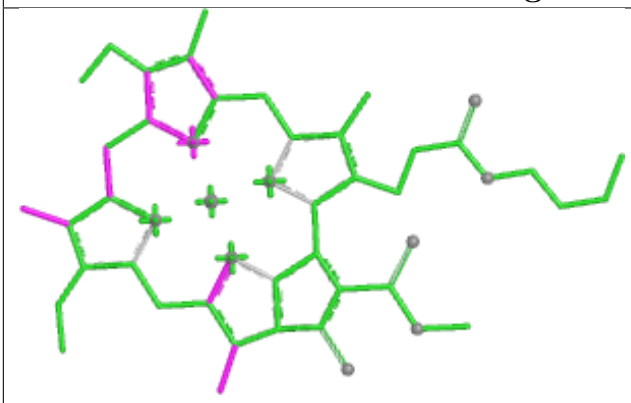


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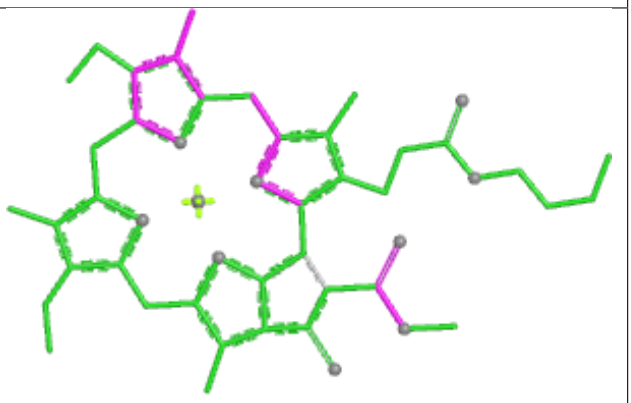


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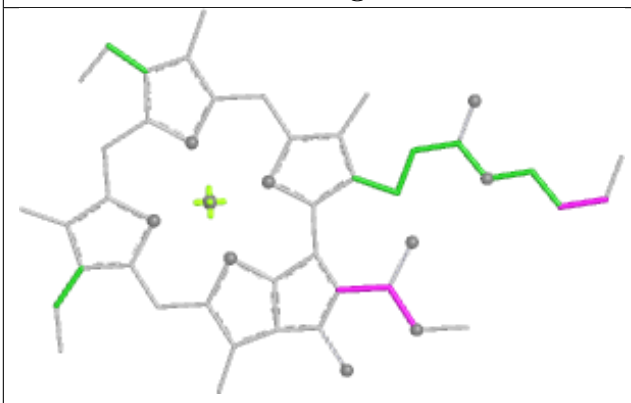
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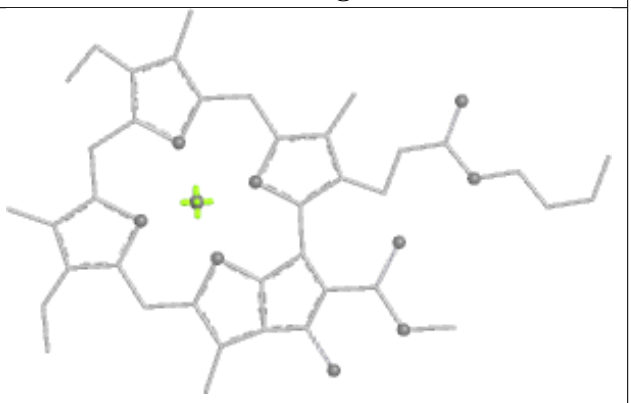
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Bond angles

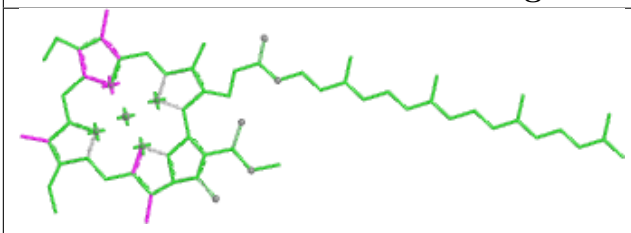


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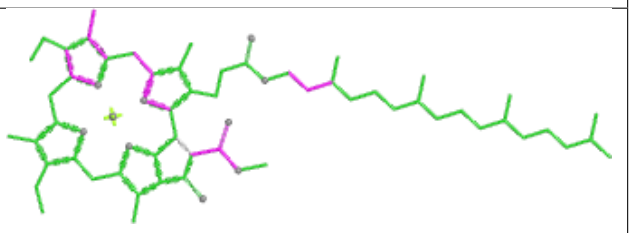


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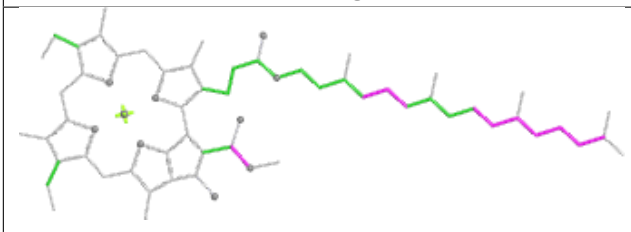
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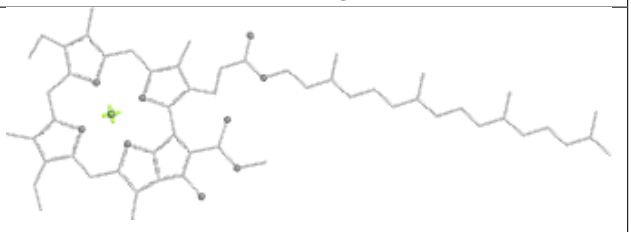
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Bond angles

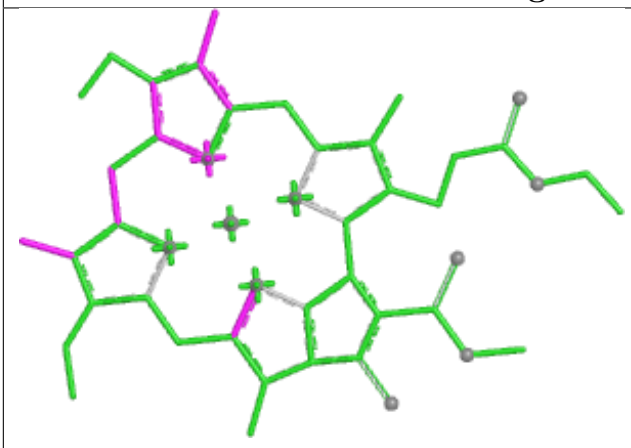


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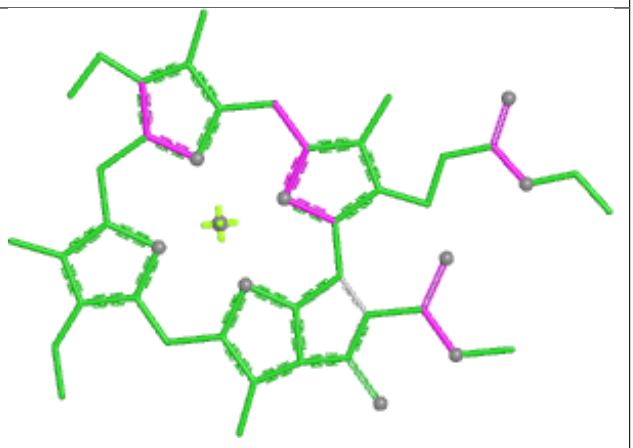


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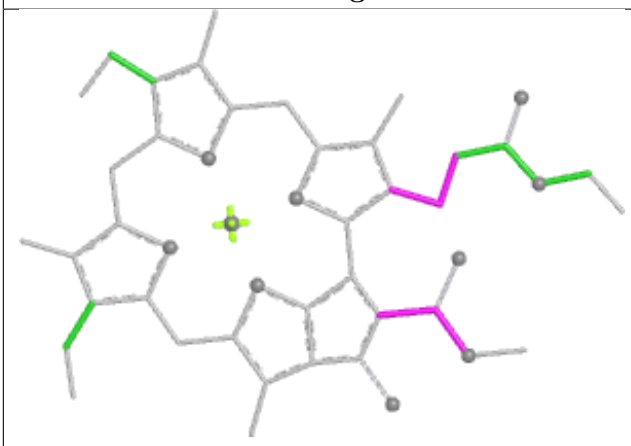
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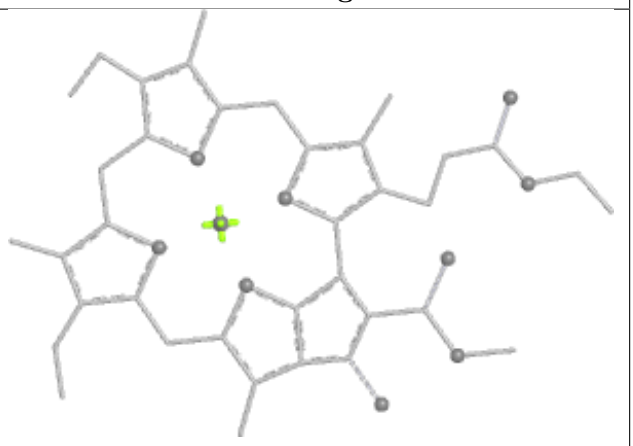
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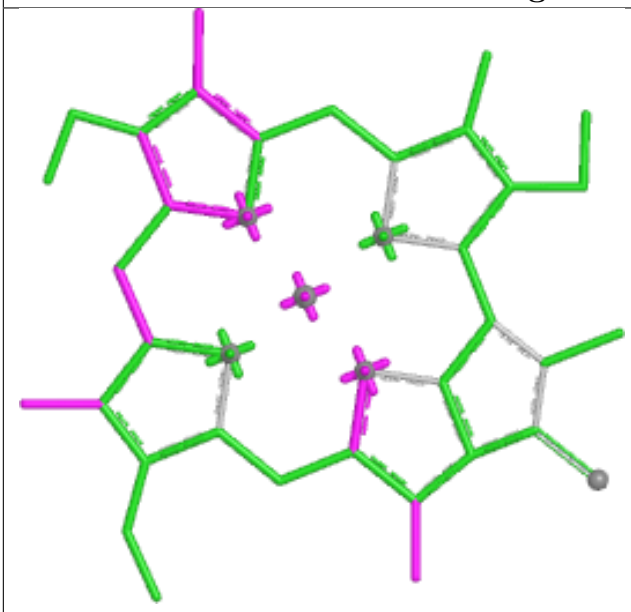


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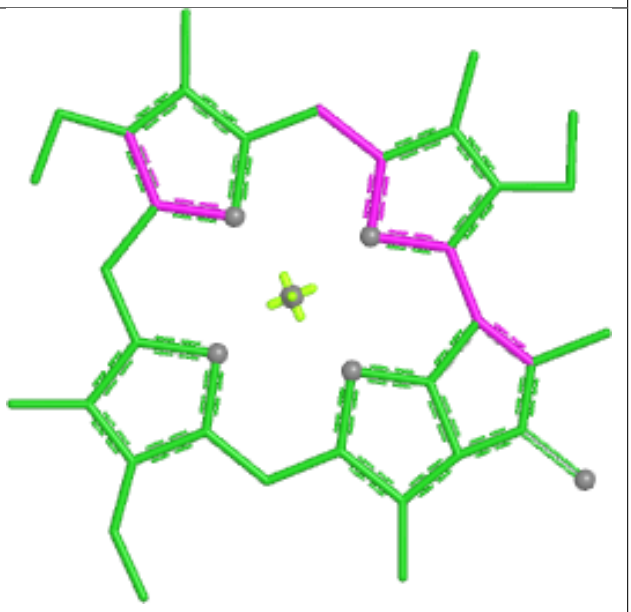


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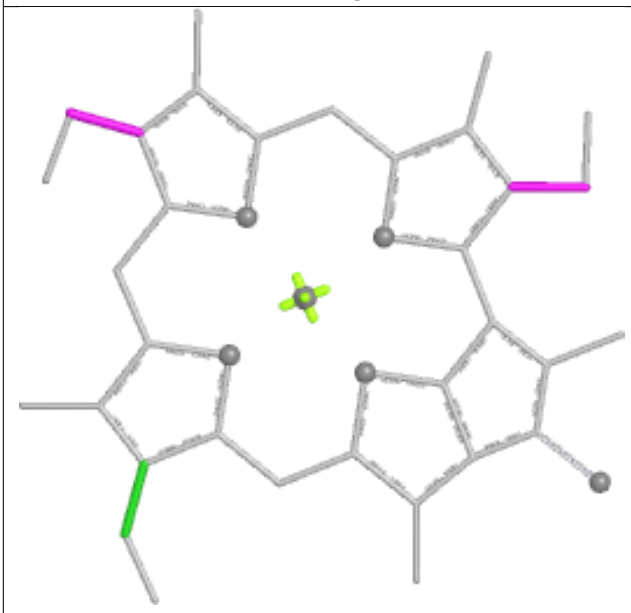
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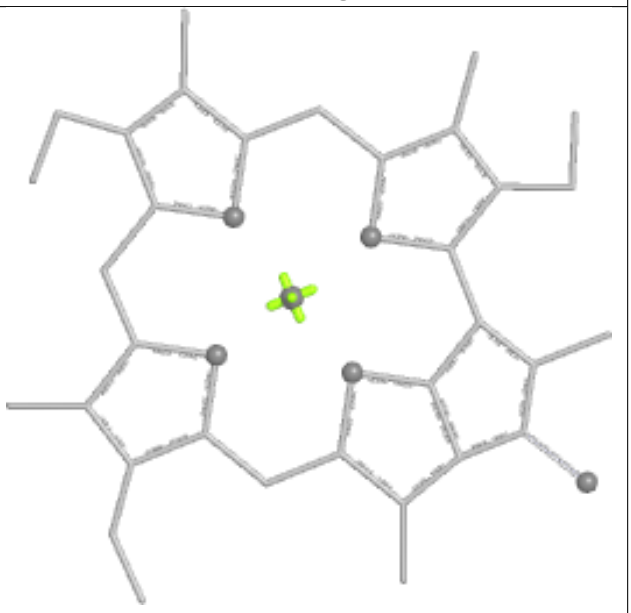
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Bond angles

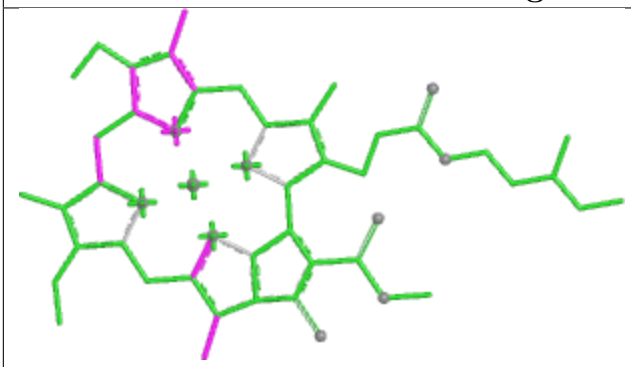


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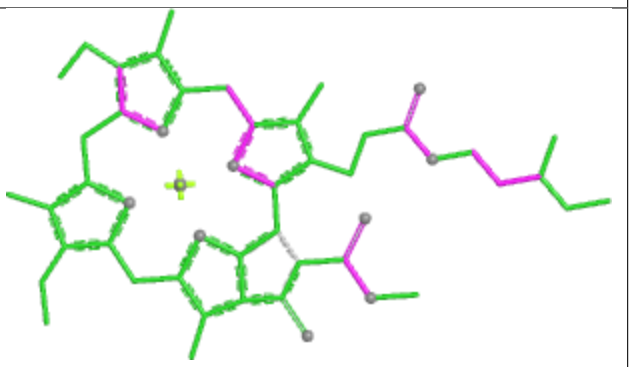


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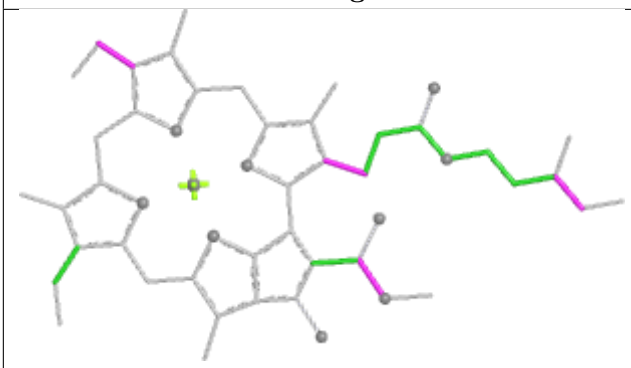
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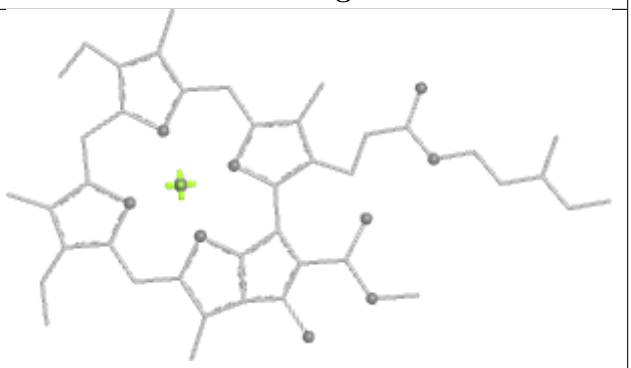
Bond lengths



Bond angles

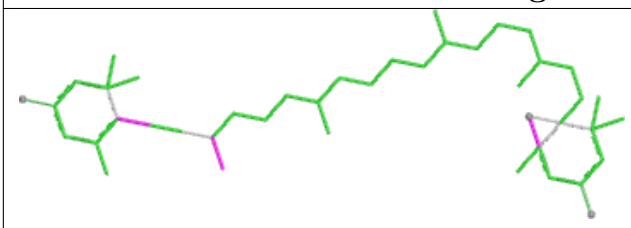


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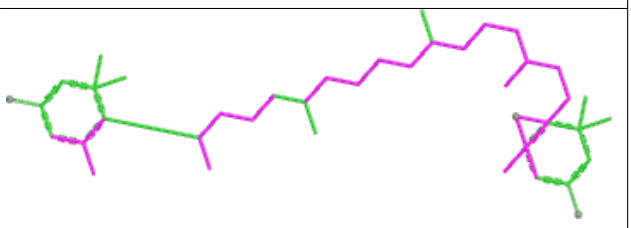


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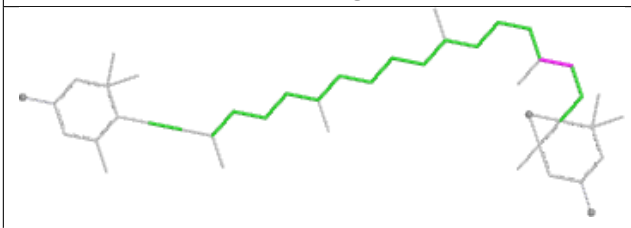
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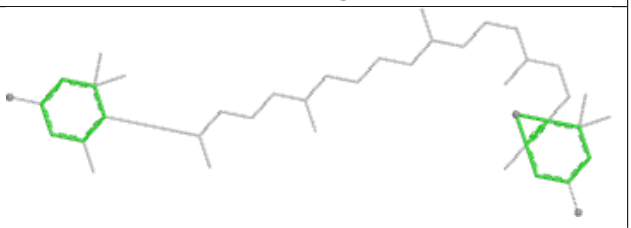
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Bond angles

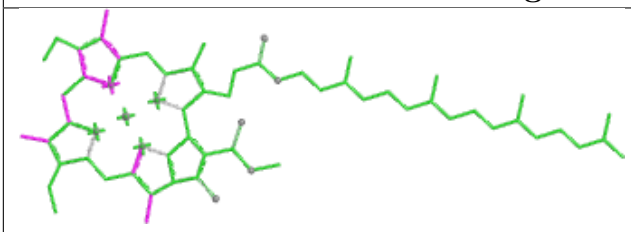


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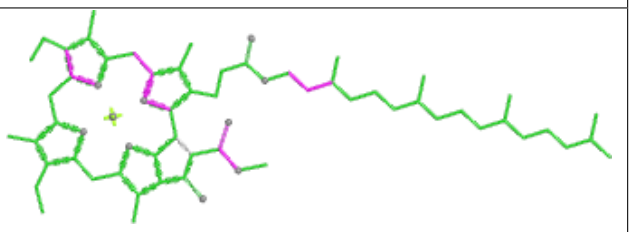


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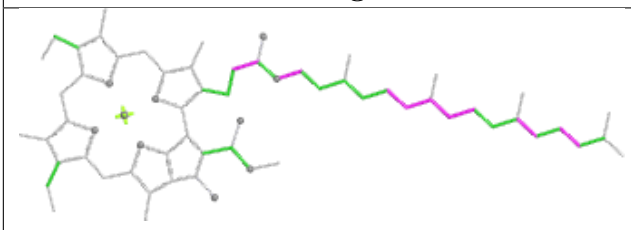
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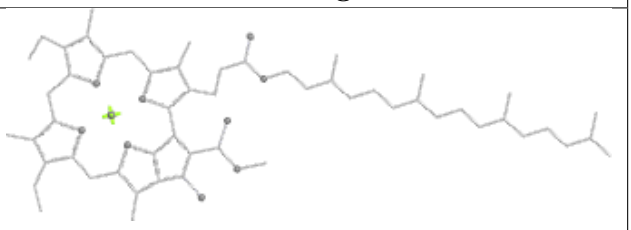
Bond lengths



Bond angles

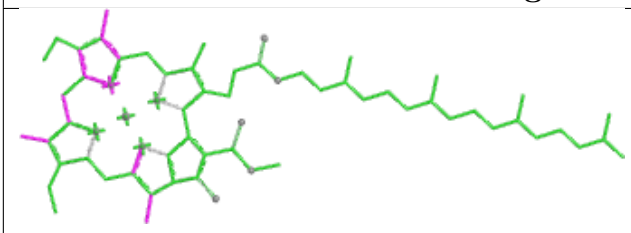


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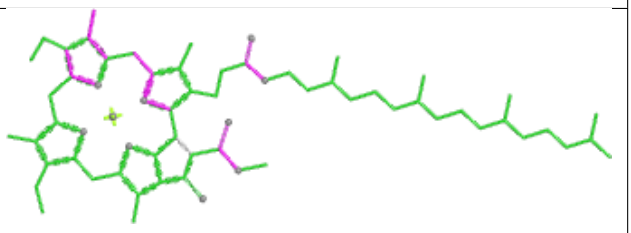


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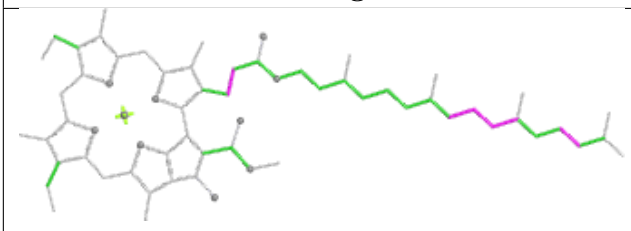
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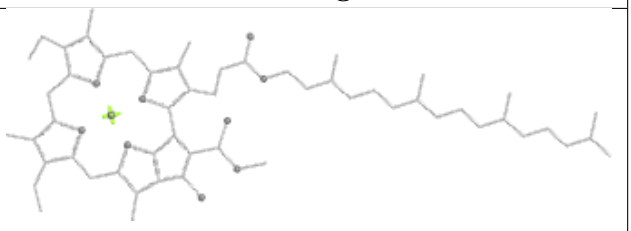
Bond lengths



Bond angles

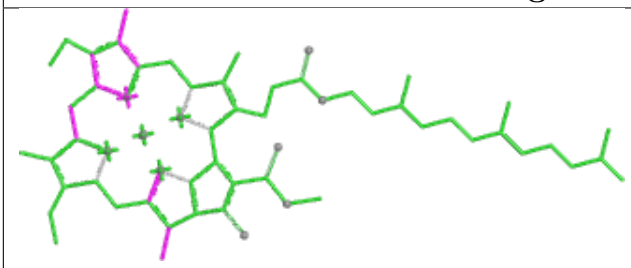


Torsions

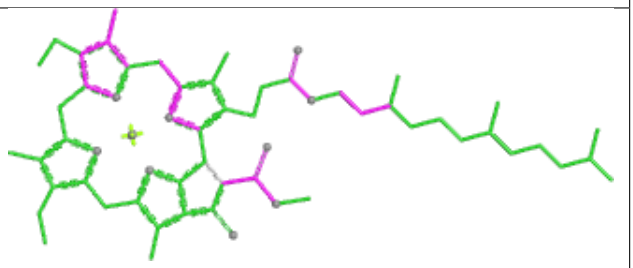


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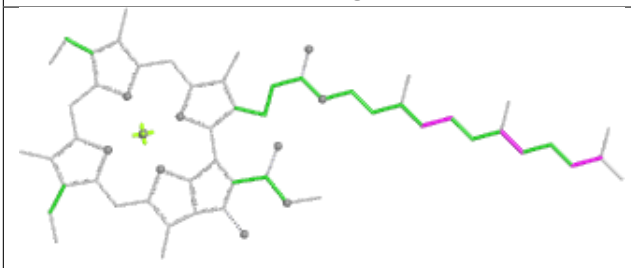
Ligand CLA a 407



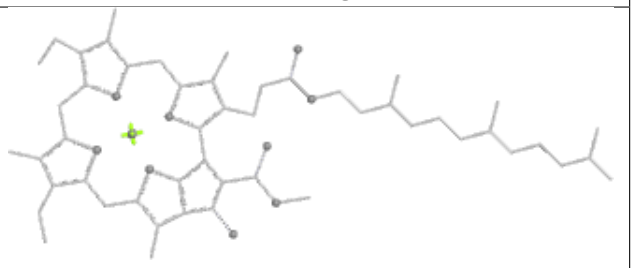
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Bond angles

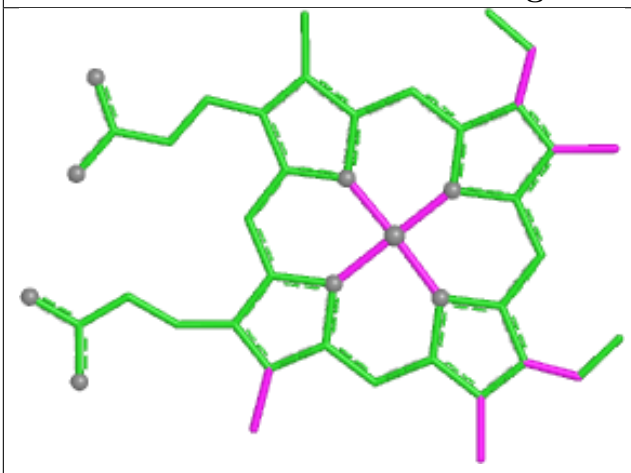


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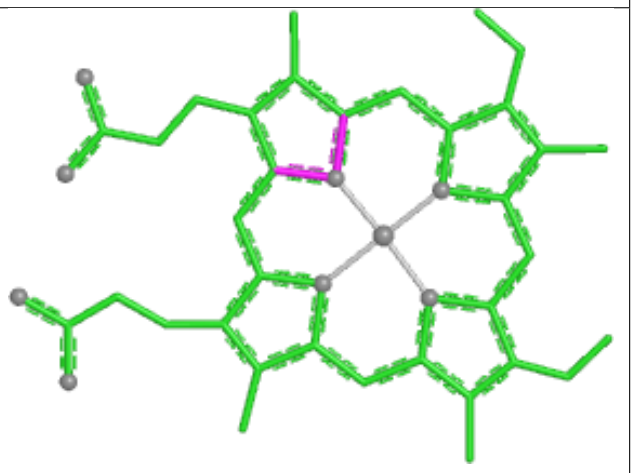


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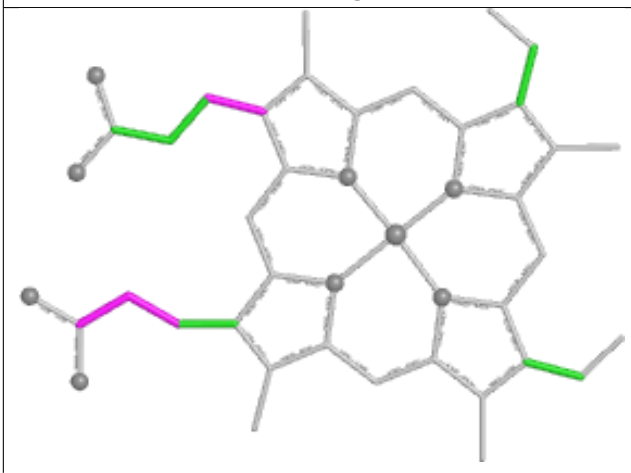
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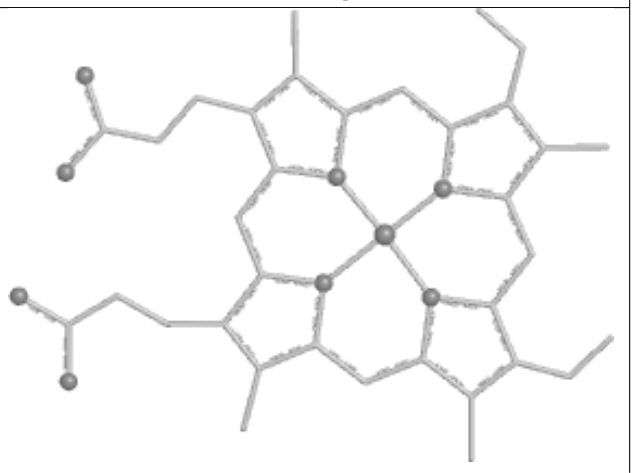
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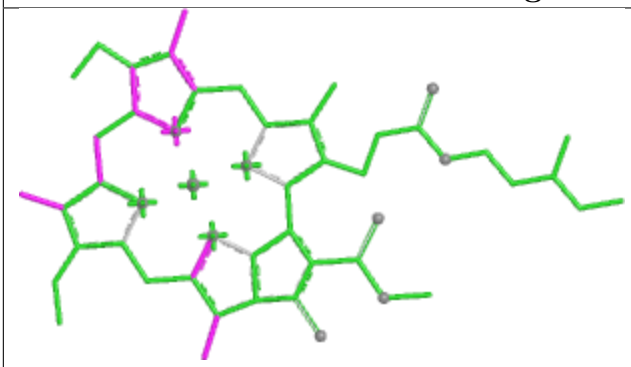


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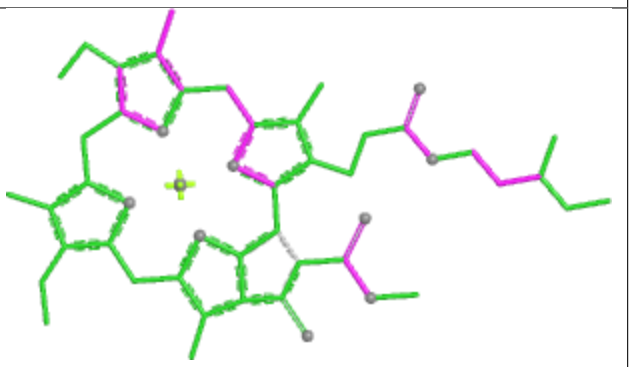


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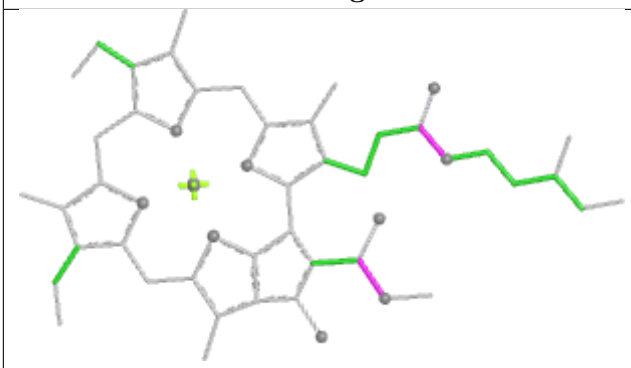
Ligand CLA C 504



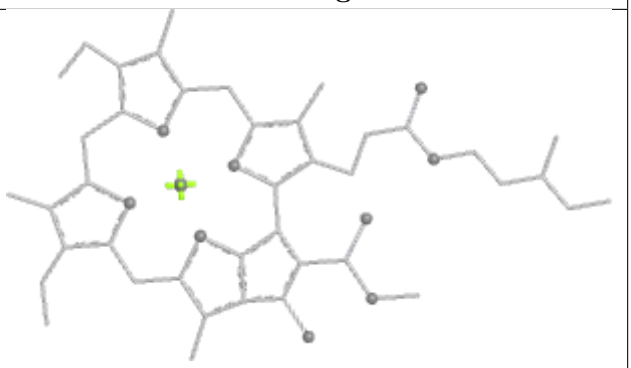
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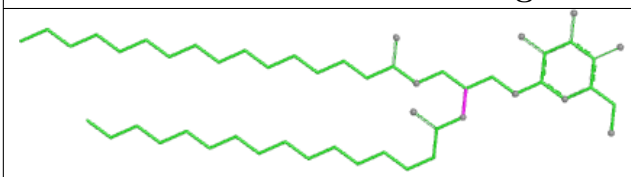


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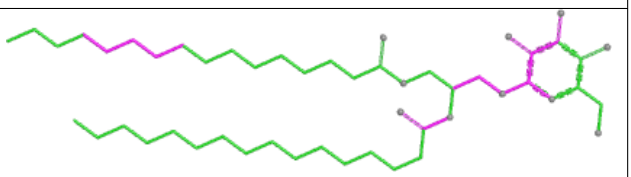


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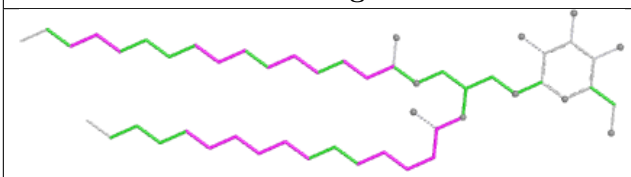
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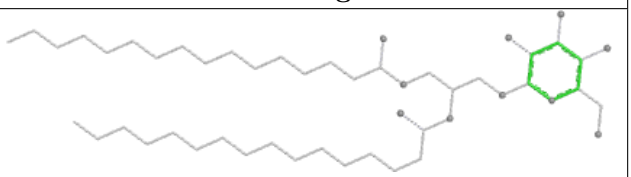
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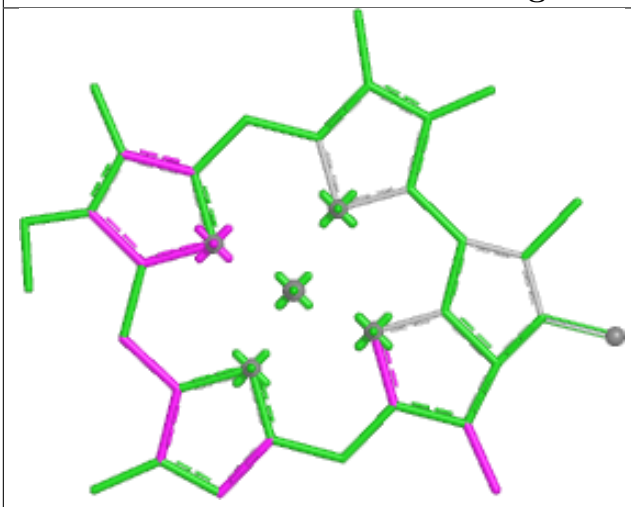


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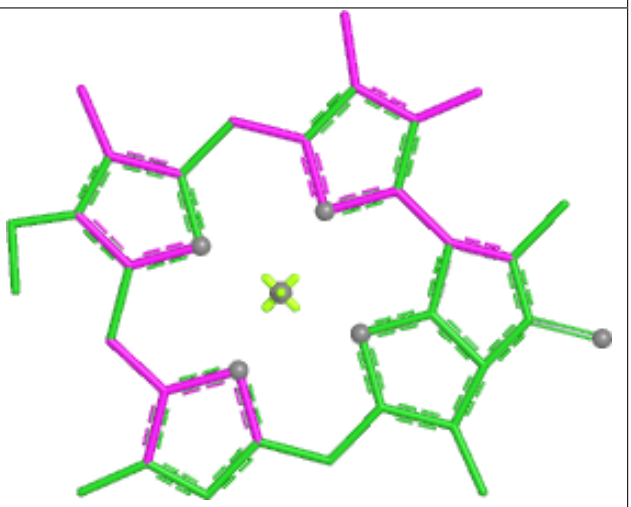


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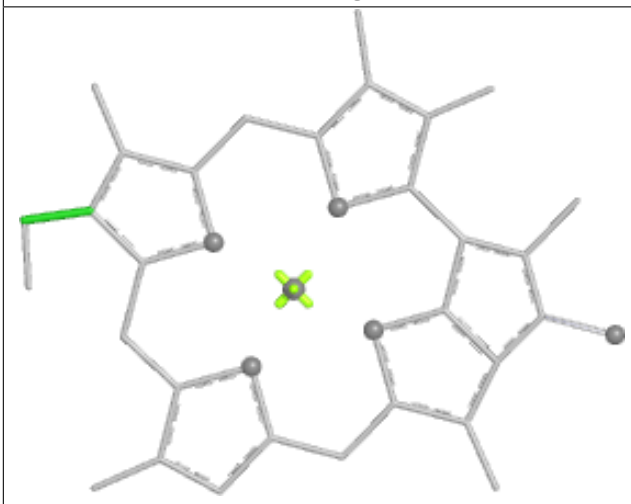
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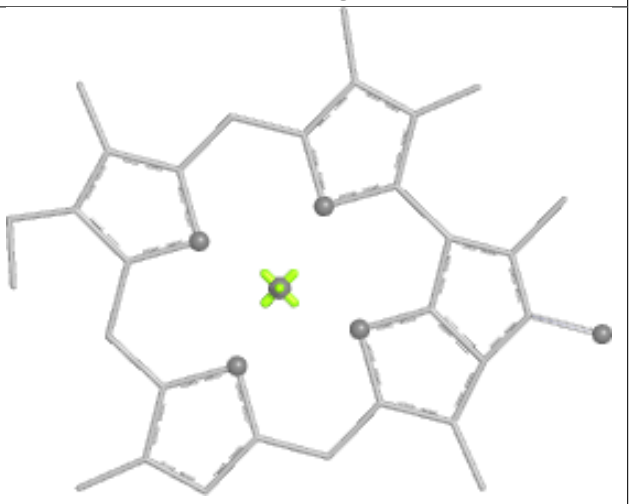
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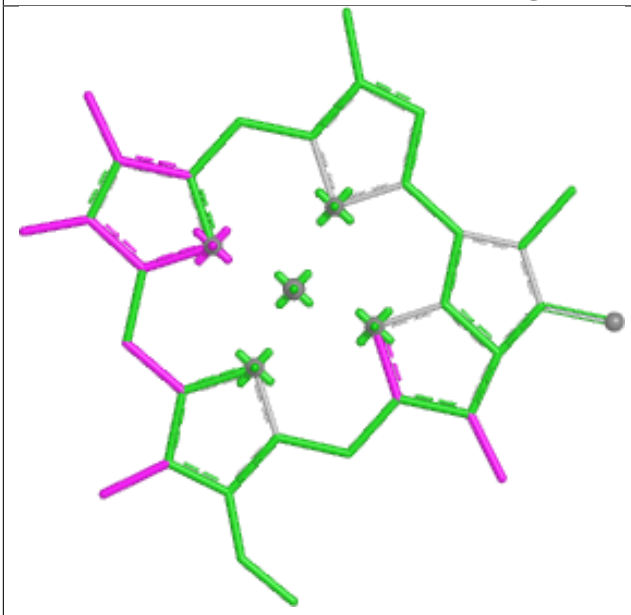


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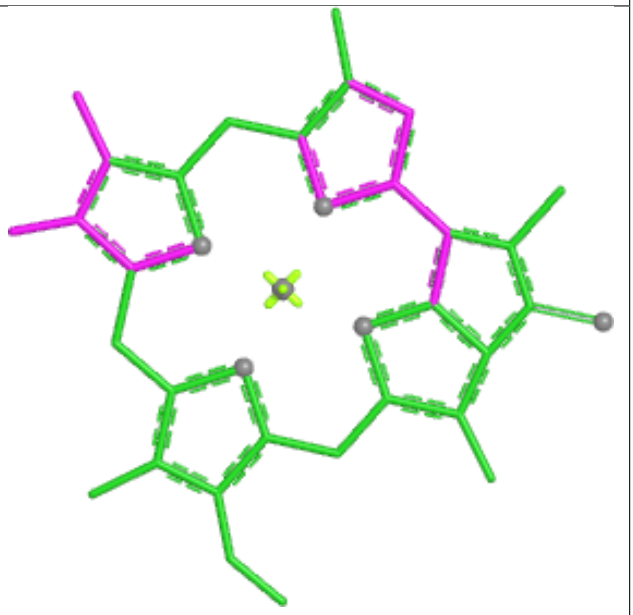


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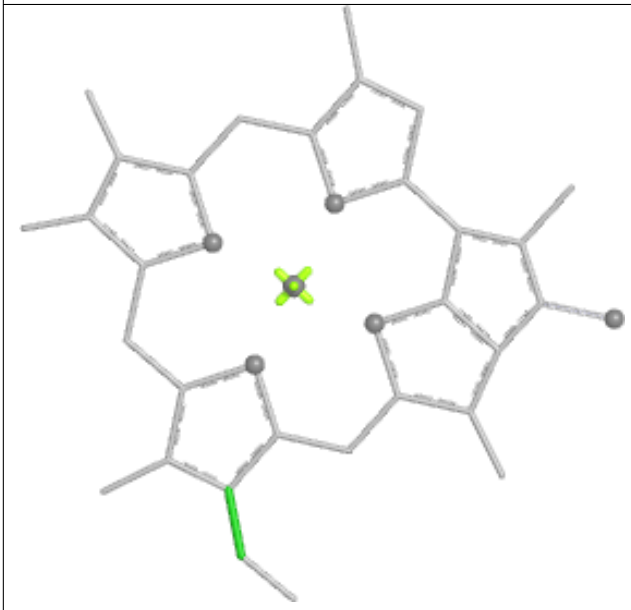
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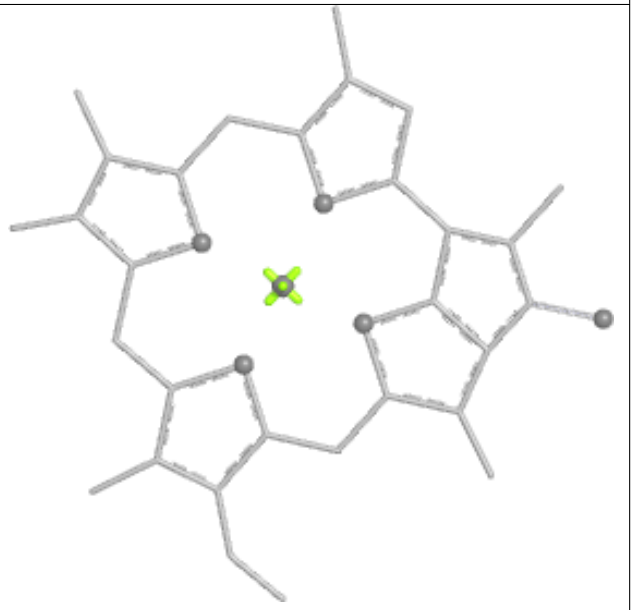
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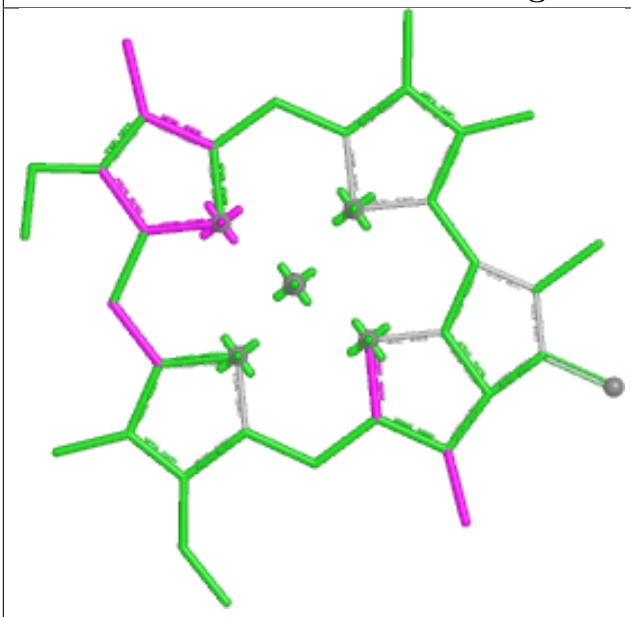


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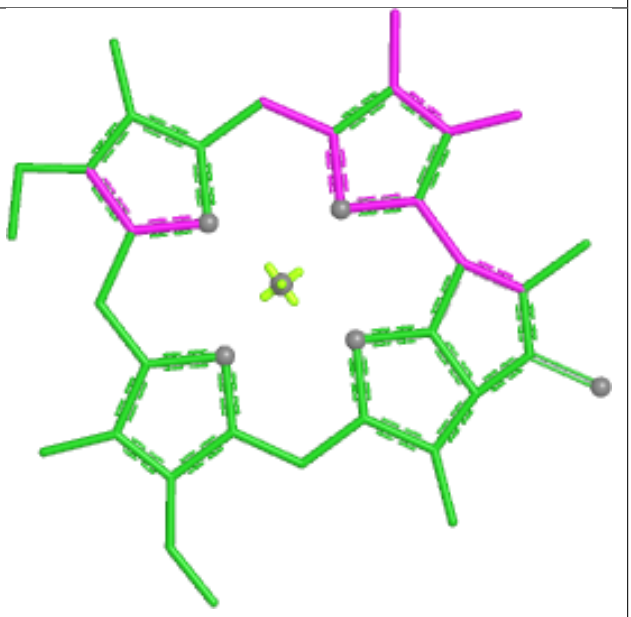


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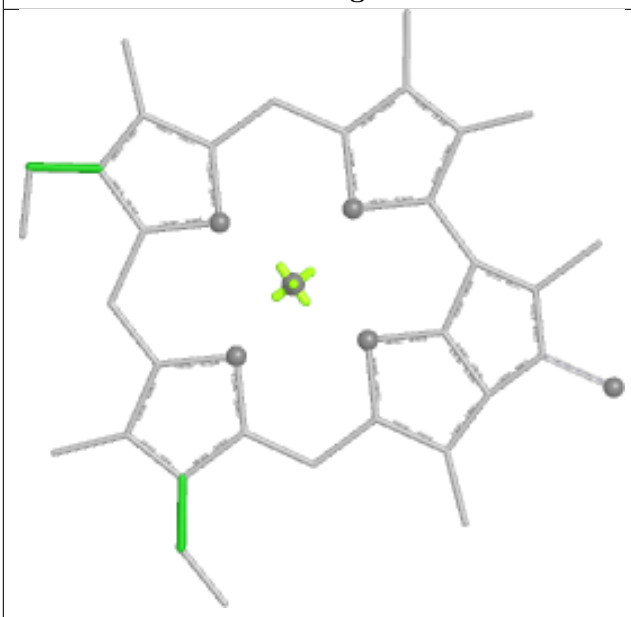
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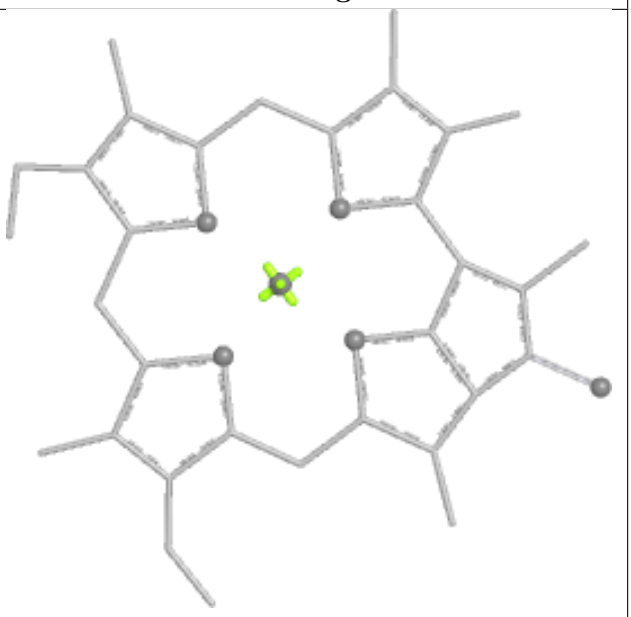
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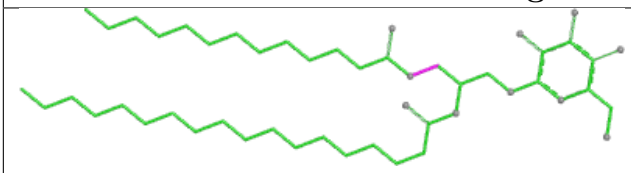


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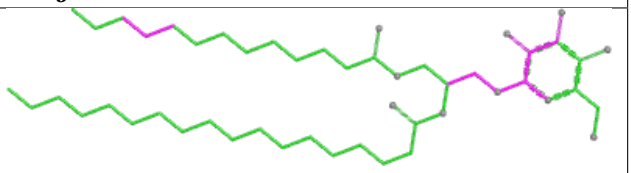


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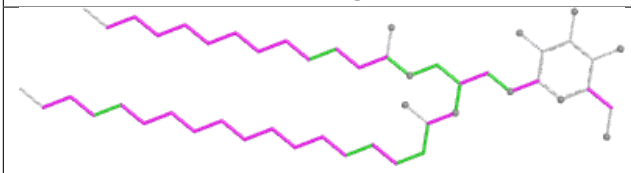
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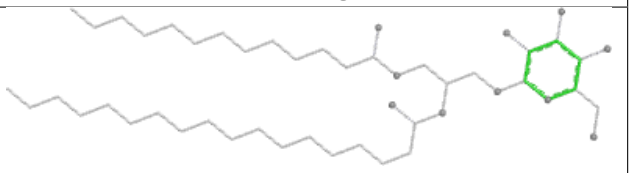
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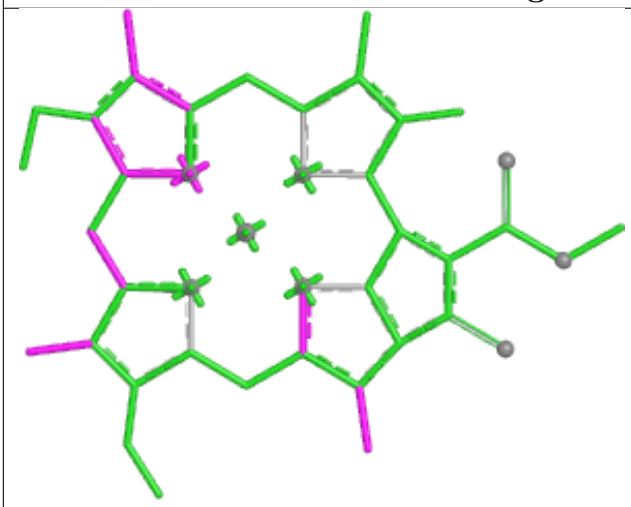


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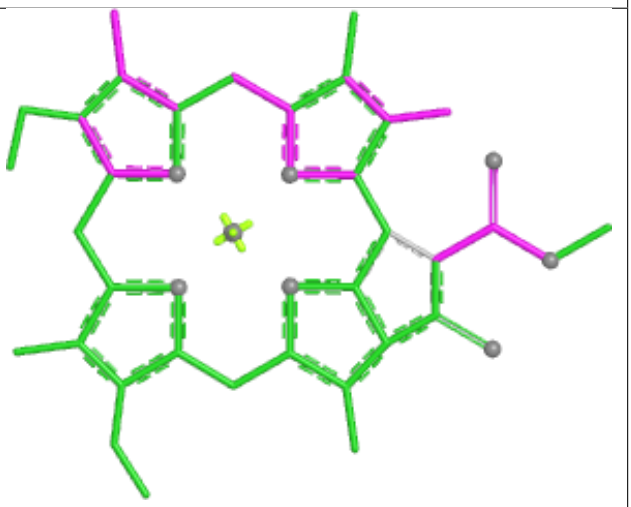


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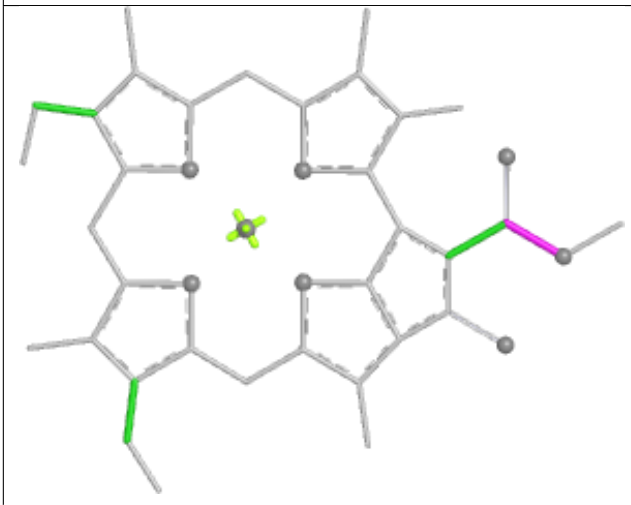
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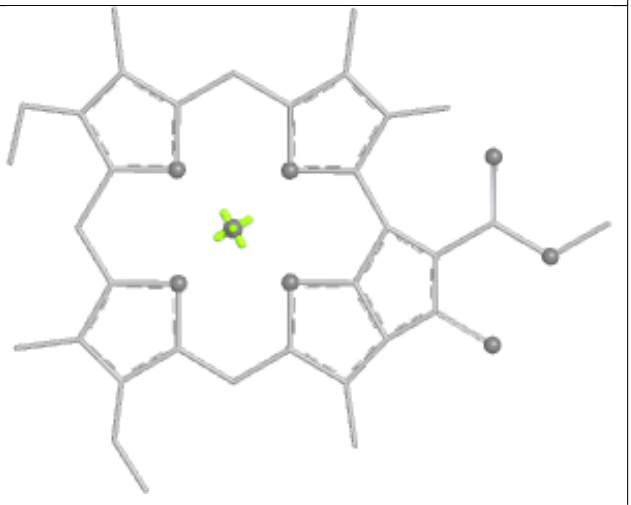
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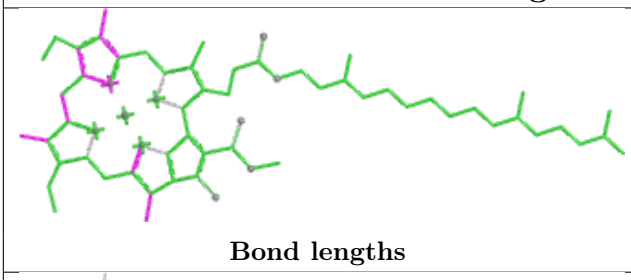


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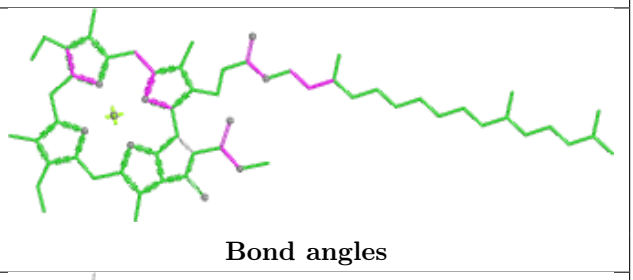


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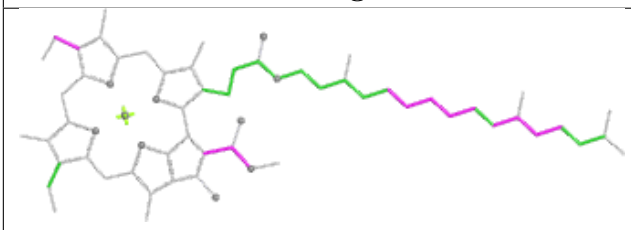
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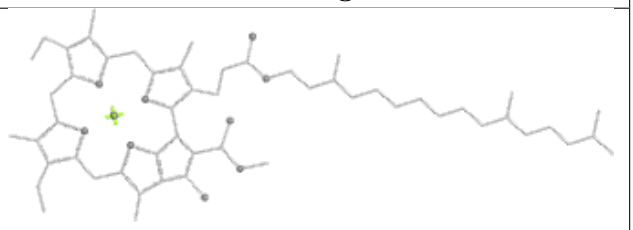
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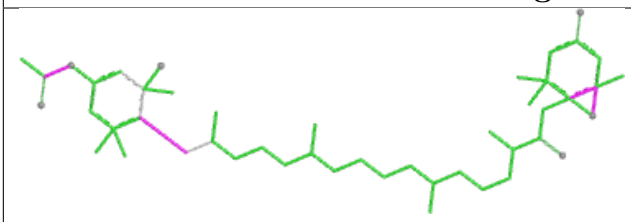


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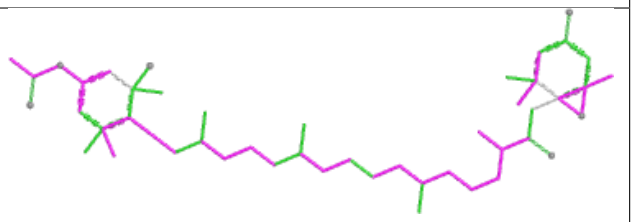


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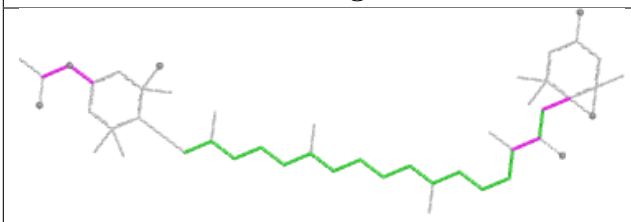
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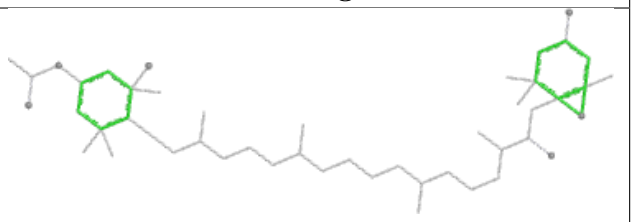
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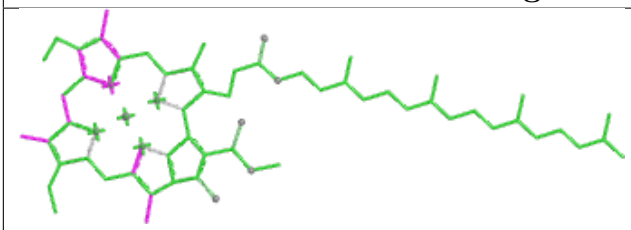


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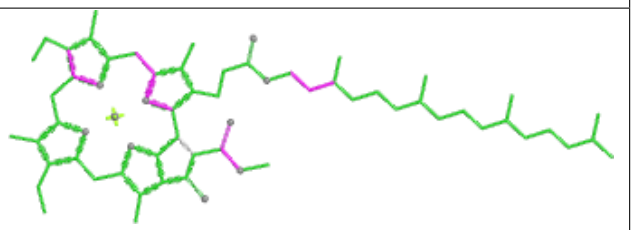


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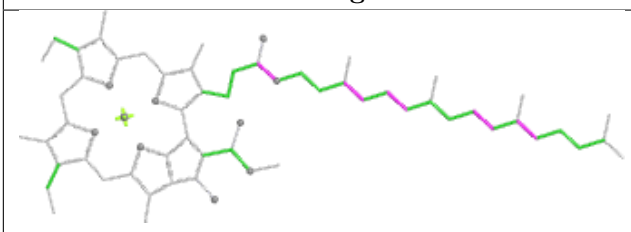
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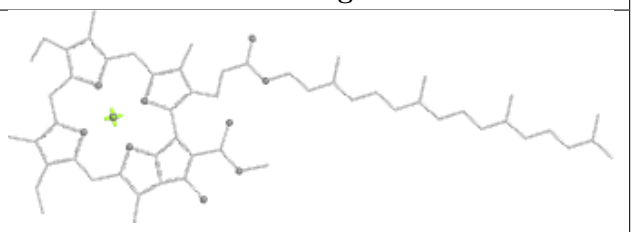
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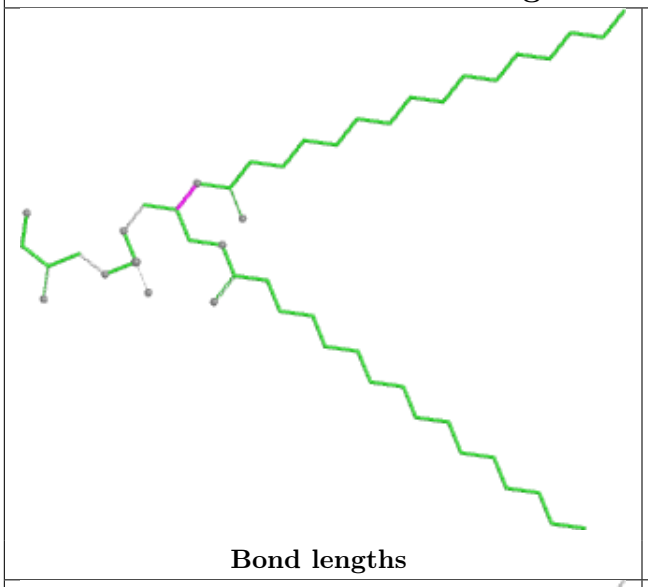


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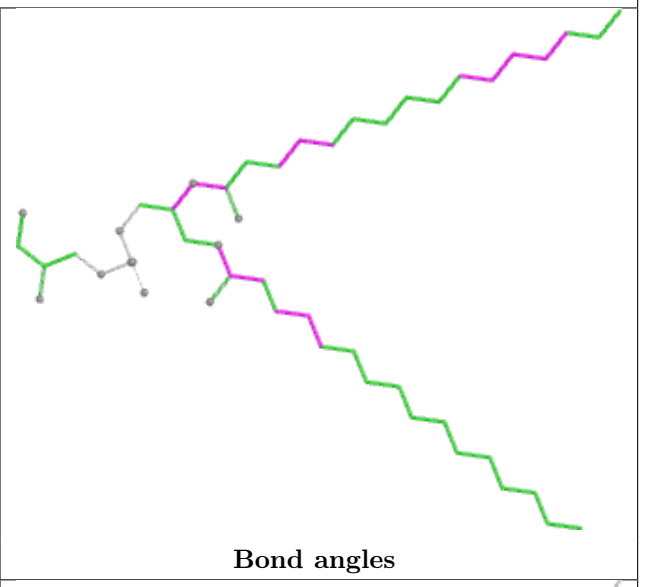


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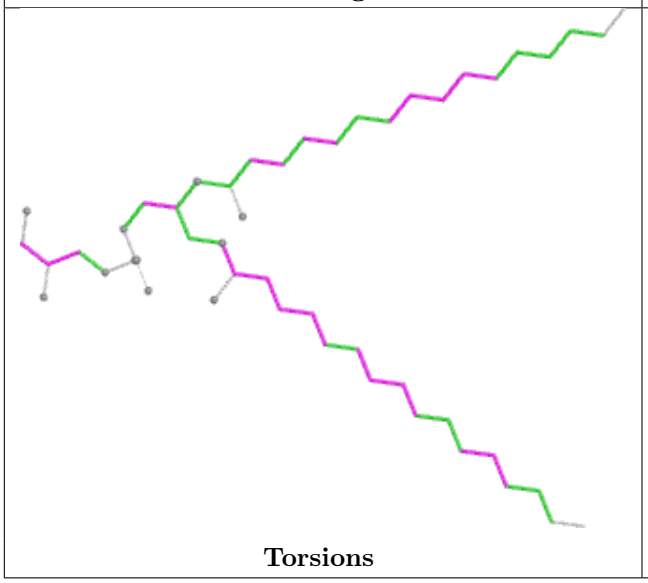
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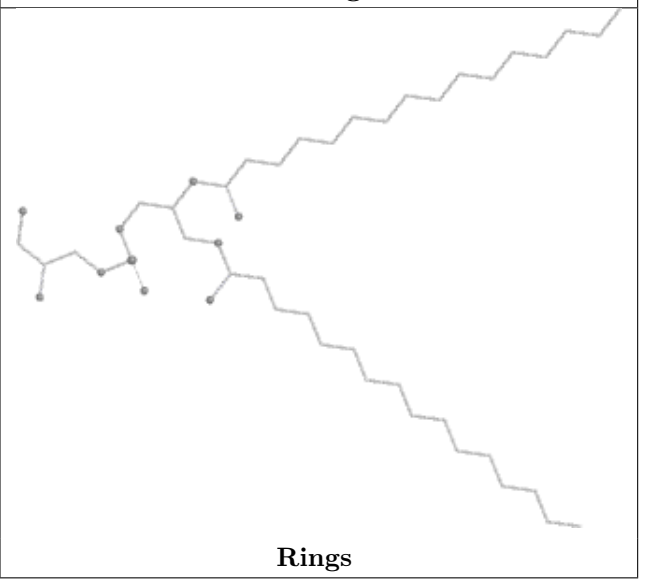
Bond lengths



Bond angles



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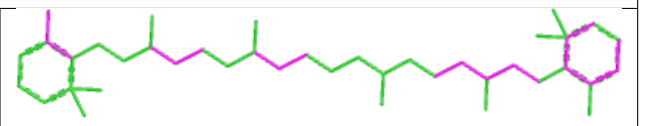


Rings

Ligand BCR b 520



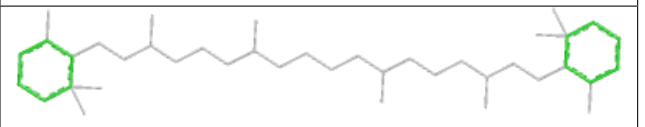
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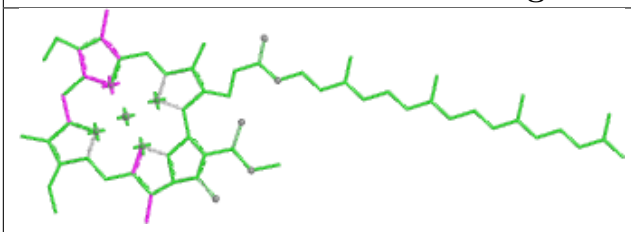
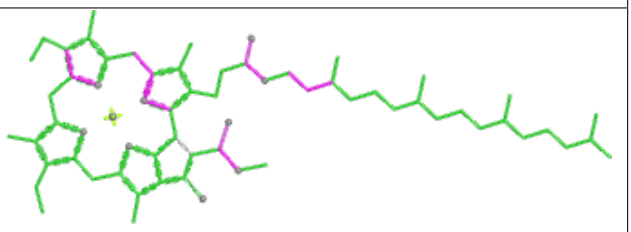
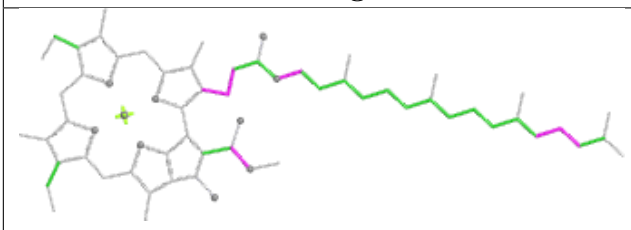
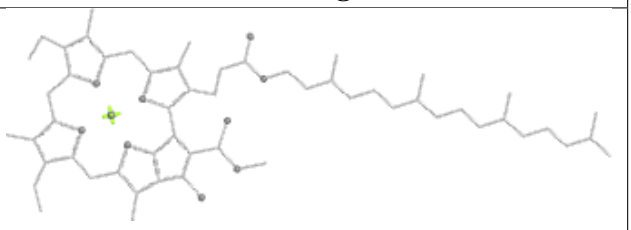
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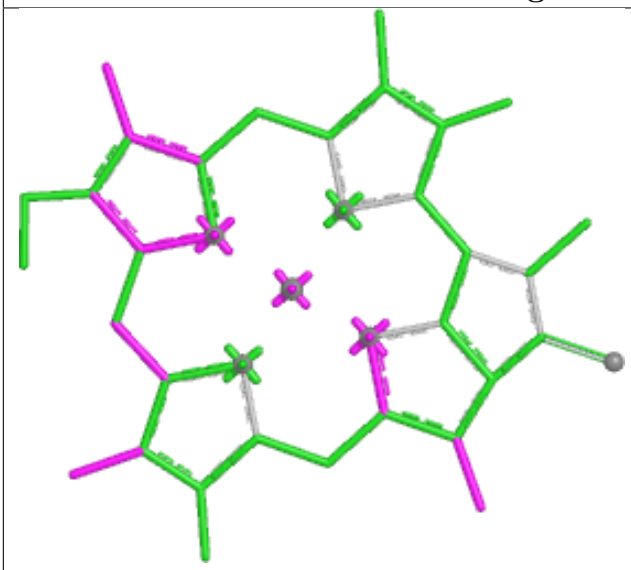
Torsions



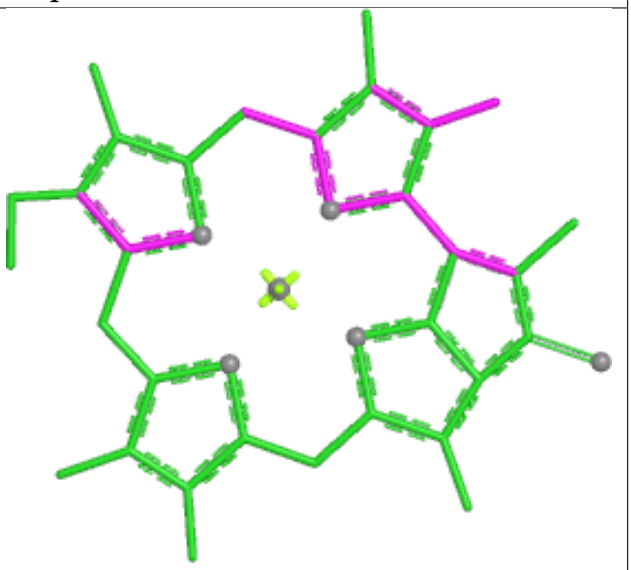
Rings

Ligand CLA b 509	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

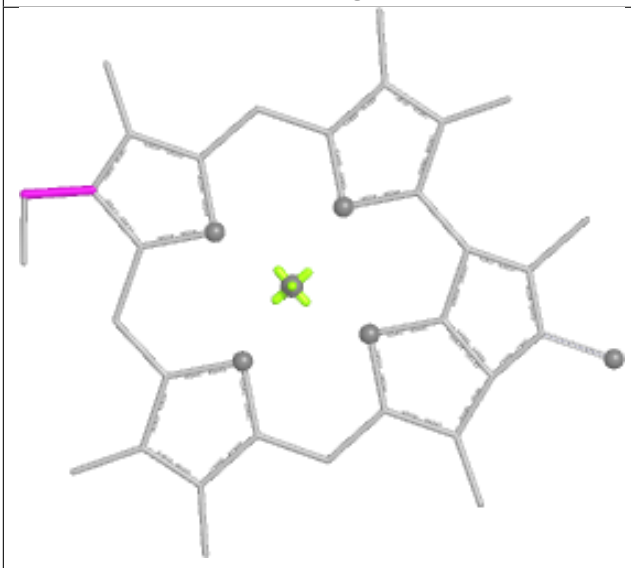
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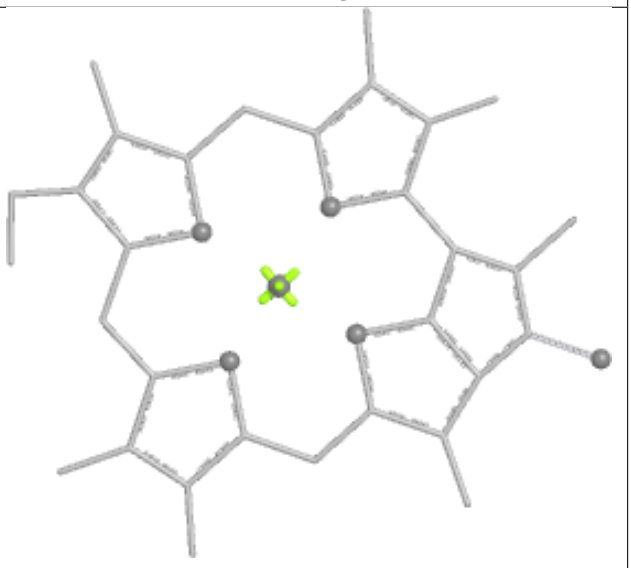
Bond lengths



Bond angles

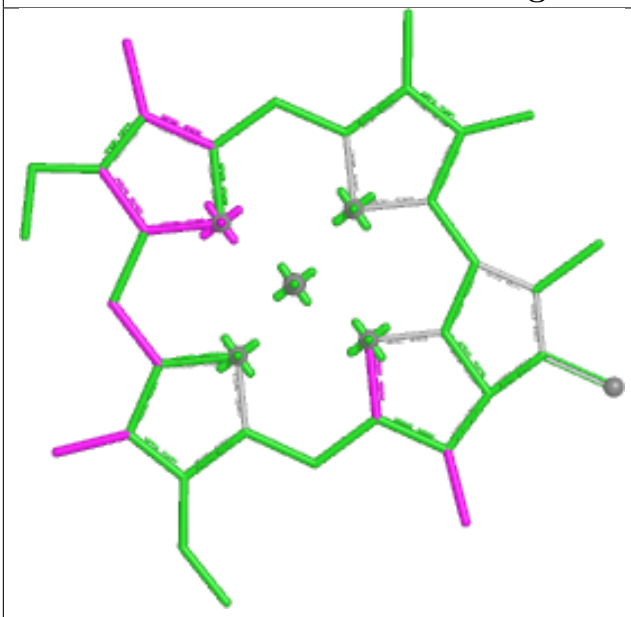


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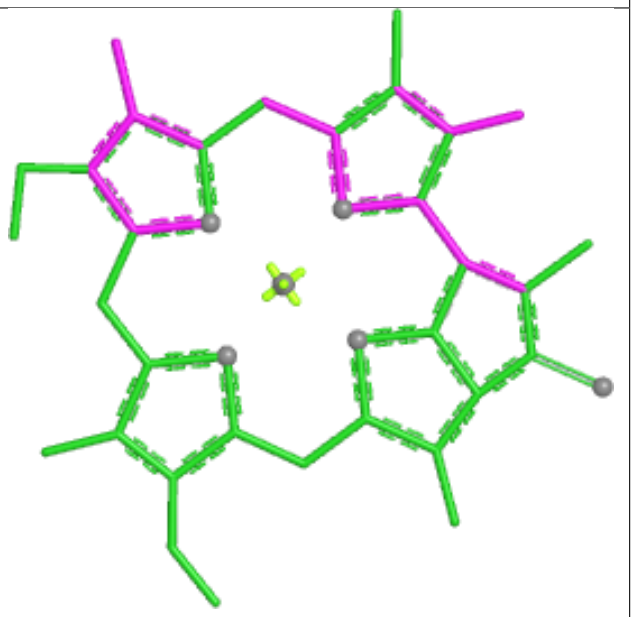


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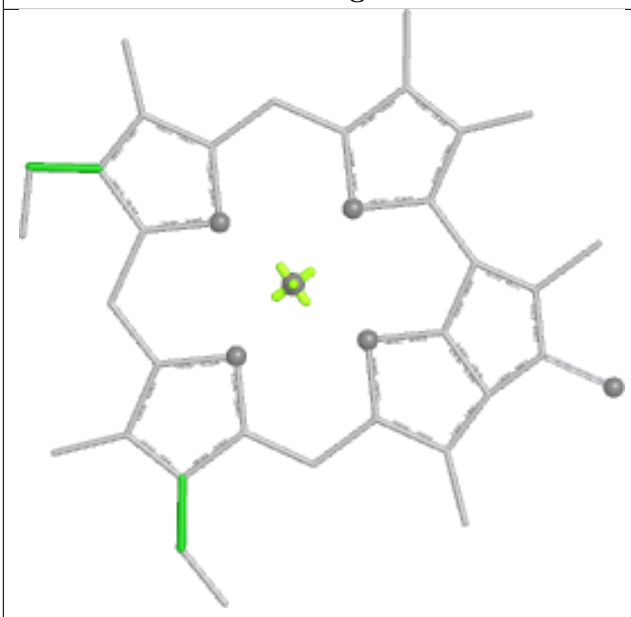
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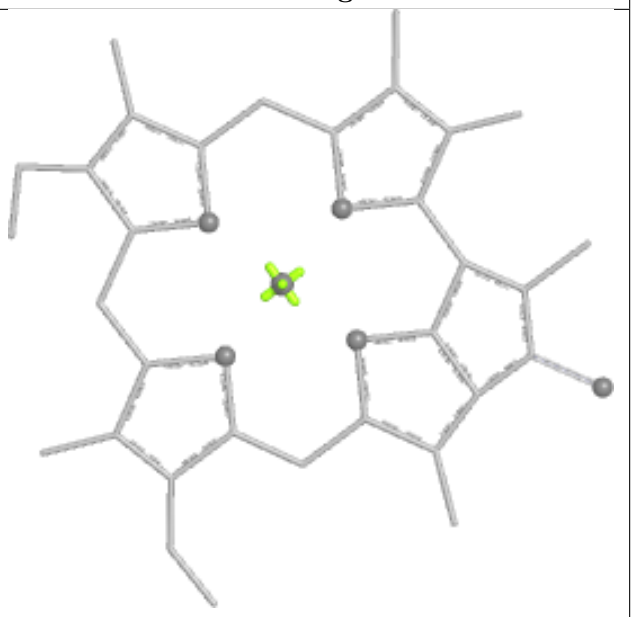
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Bond angles

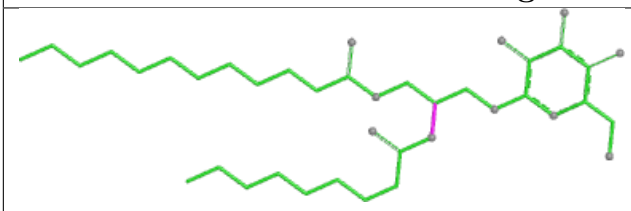


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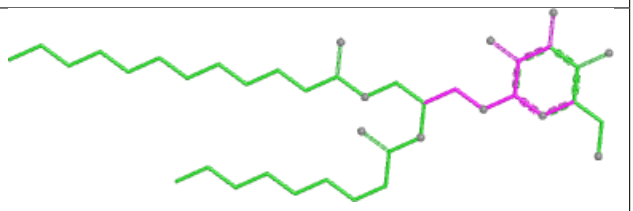


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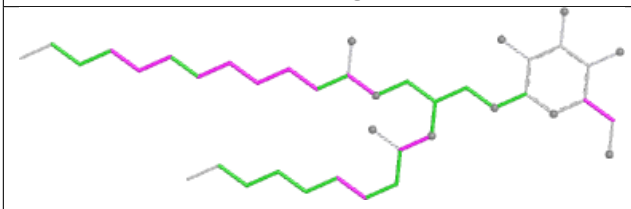
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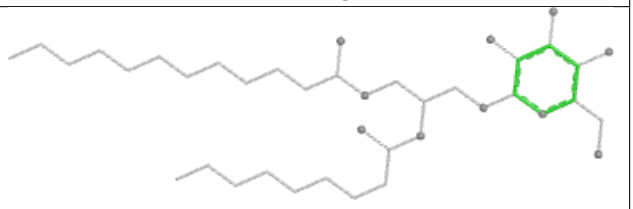
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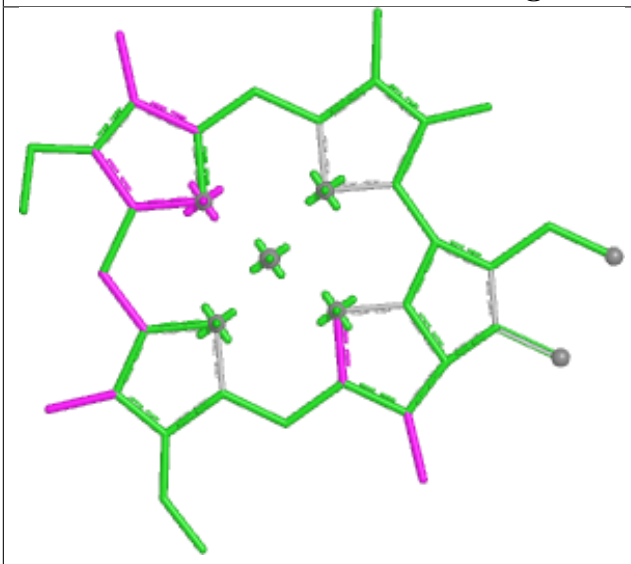


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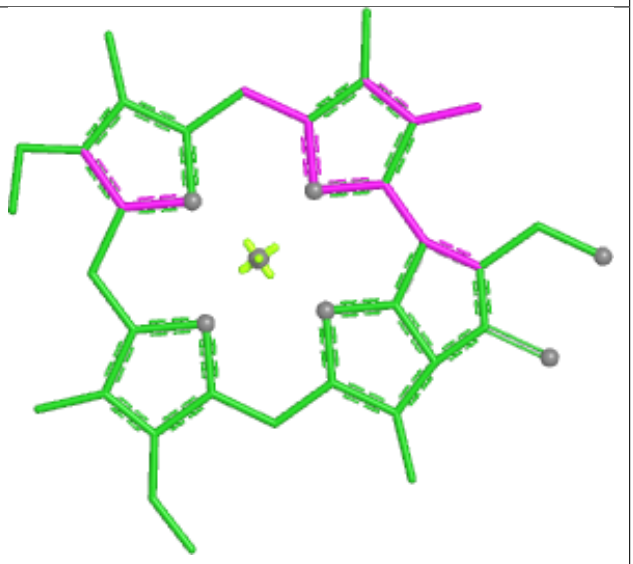


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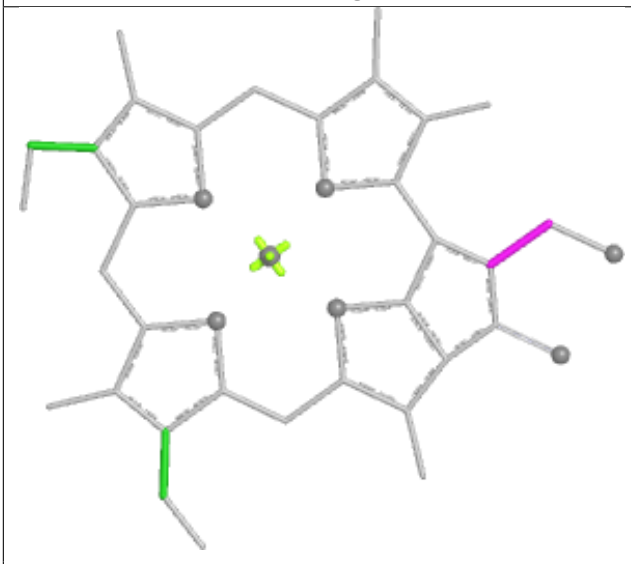
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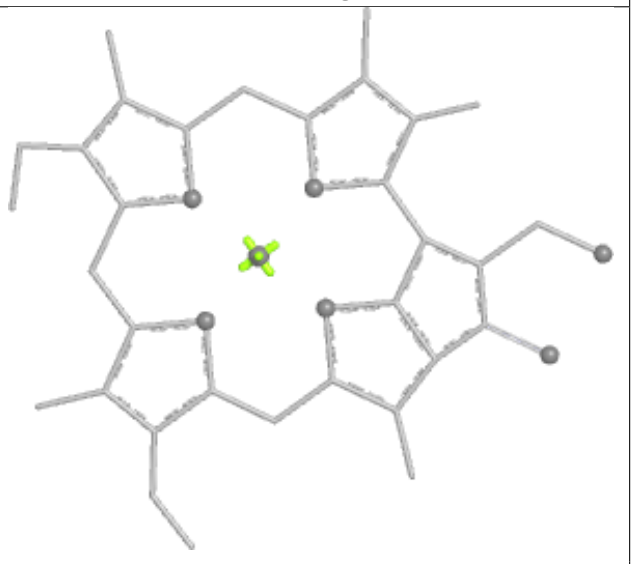
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Bond angles

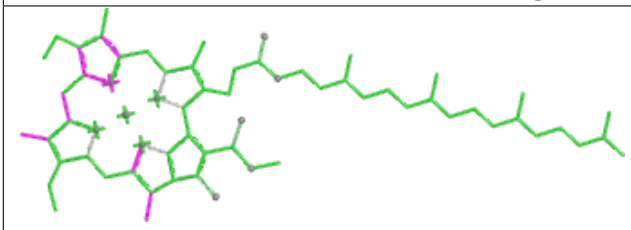


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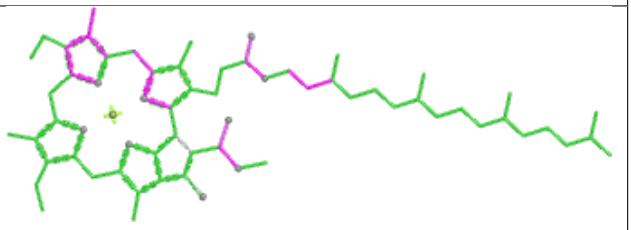


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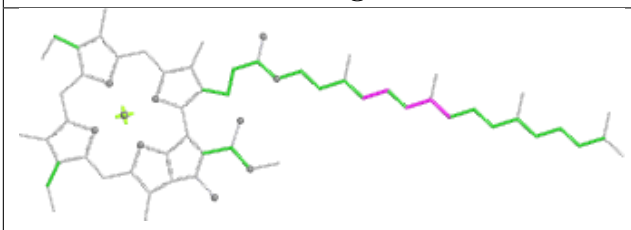
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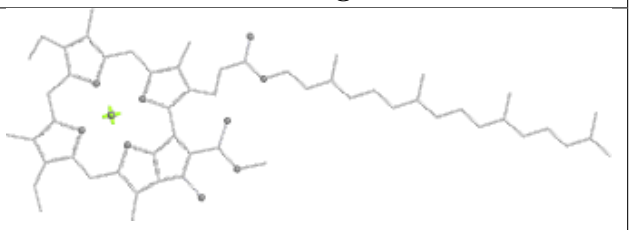
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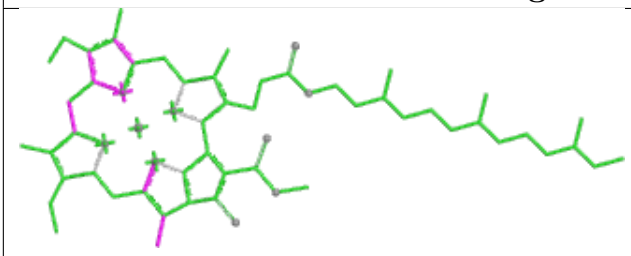


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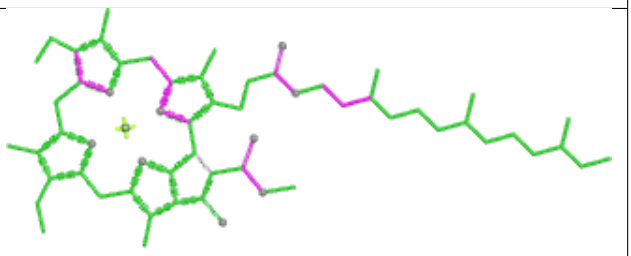


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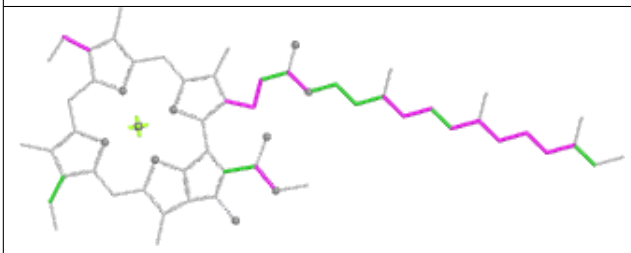
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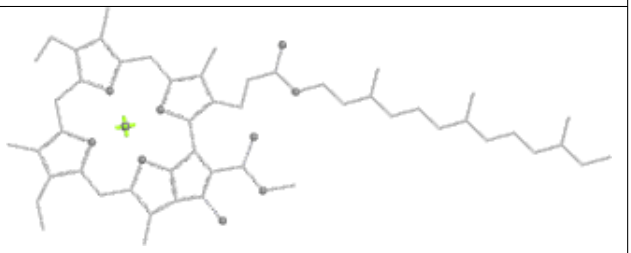
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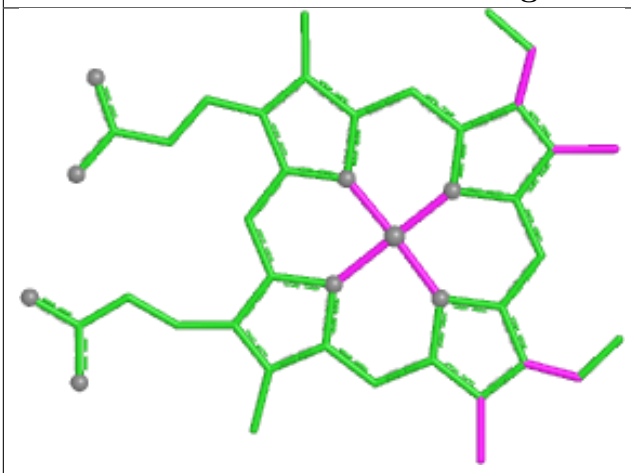


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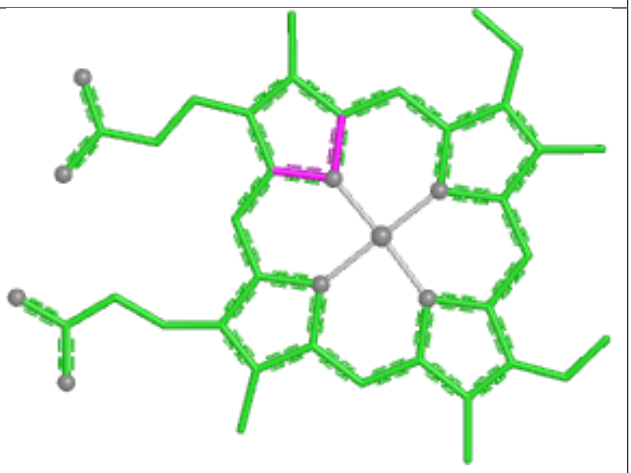


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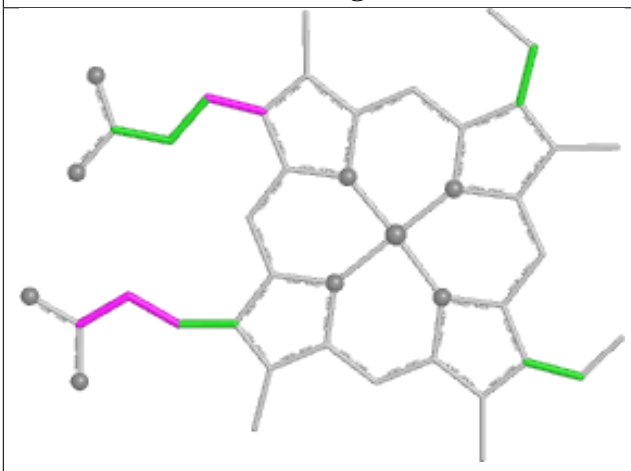
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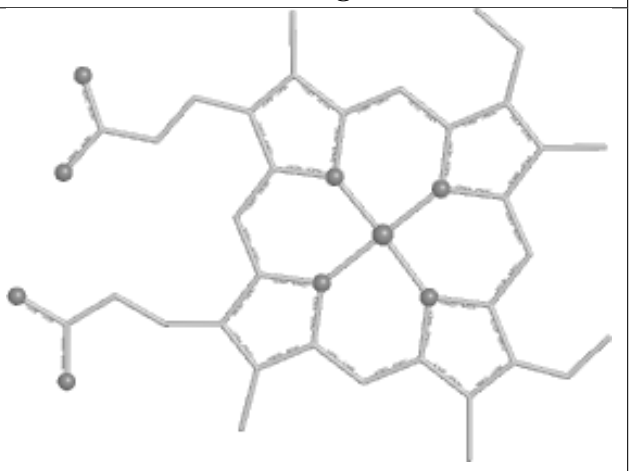
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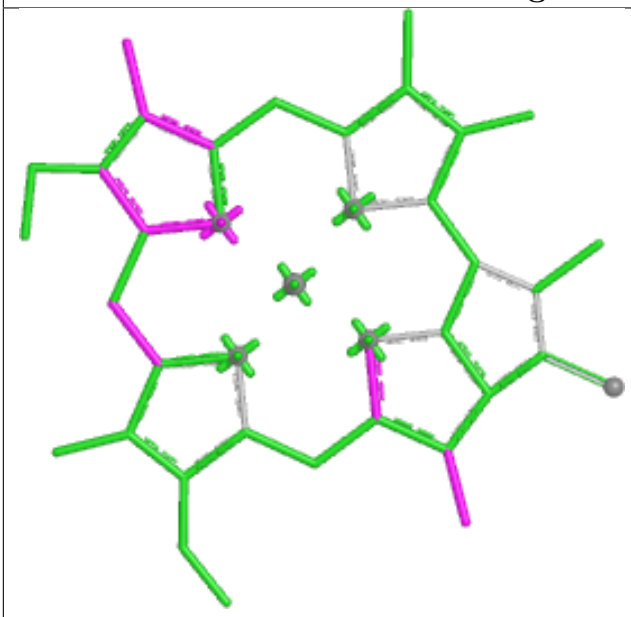


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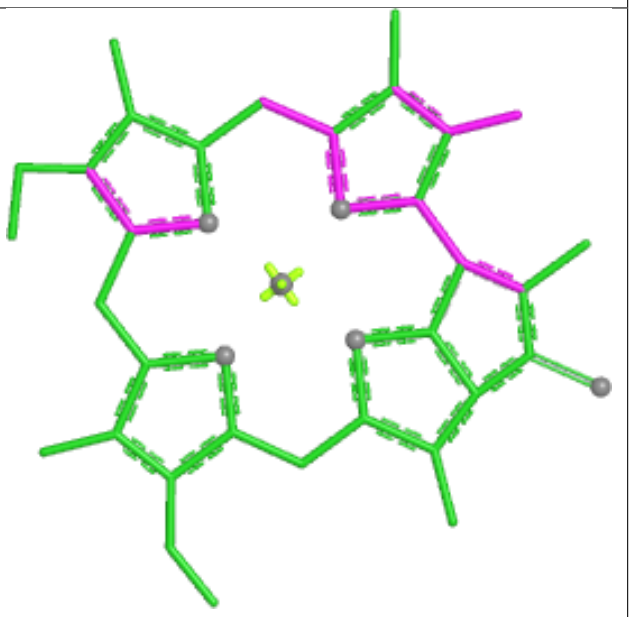


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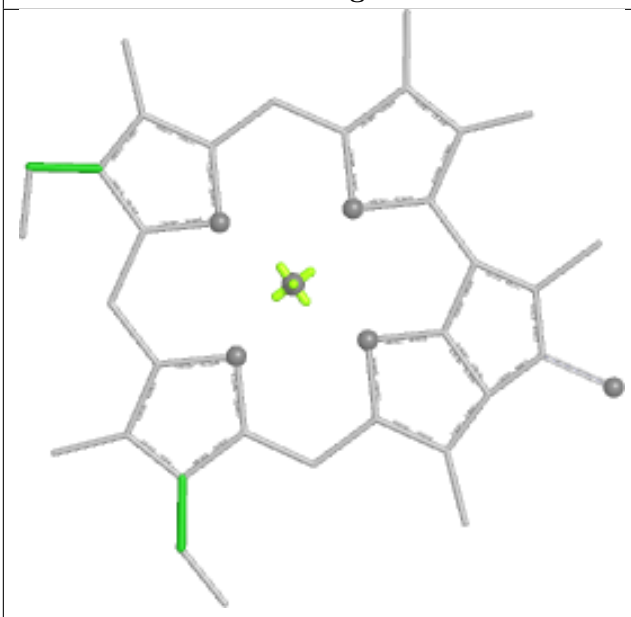
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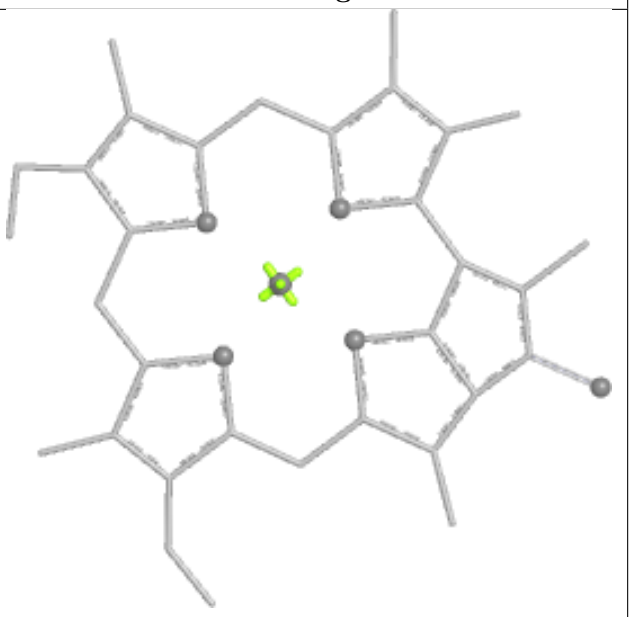
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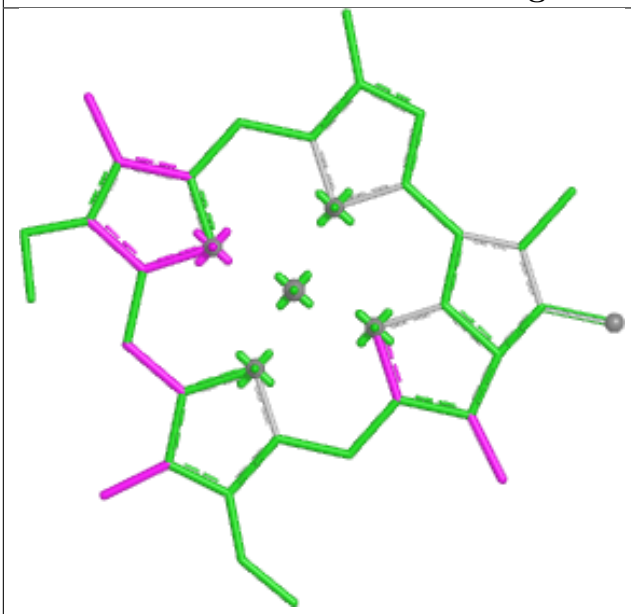


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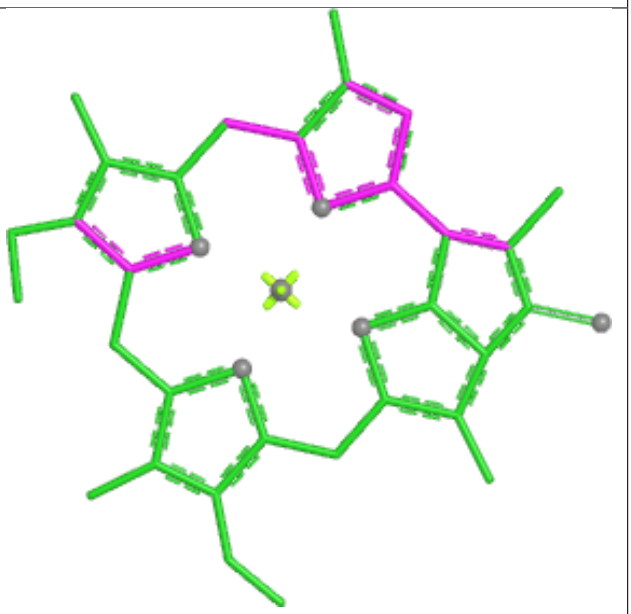


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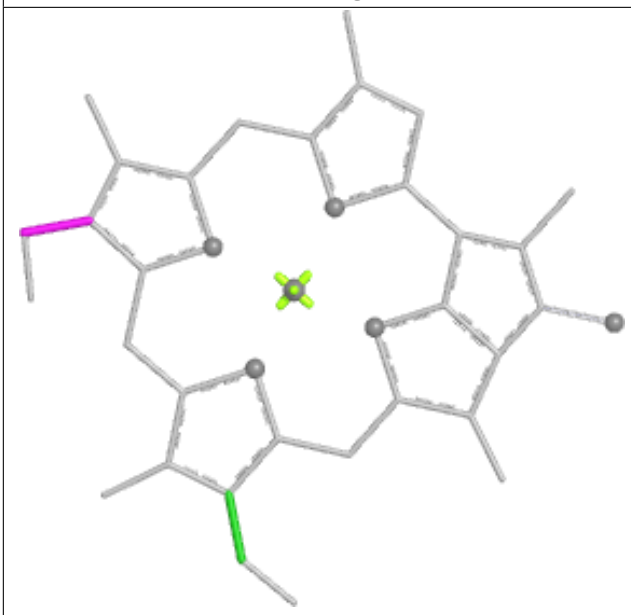
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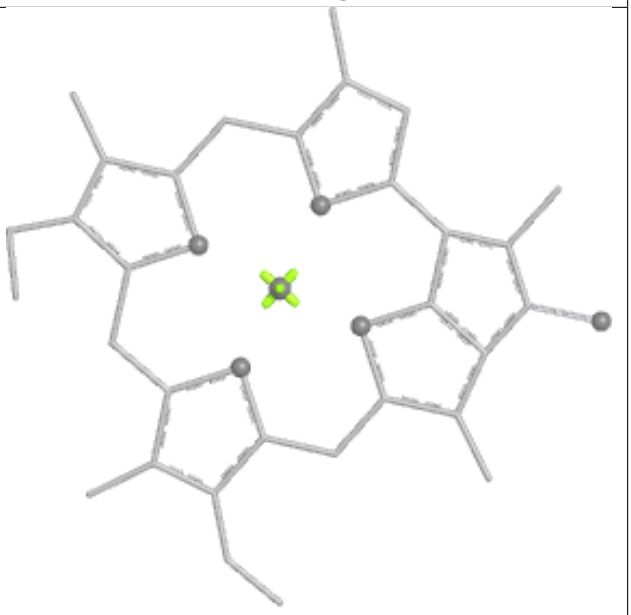
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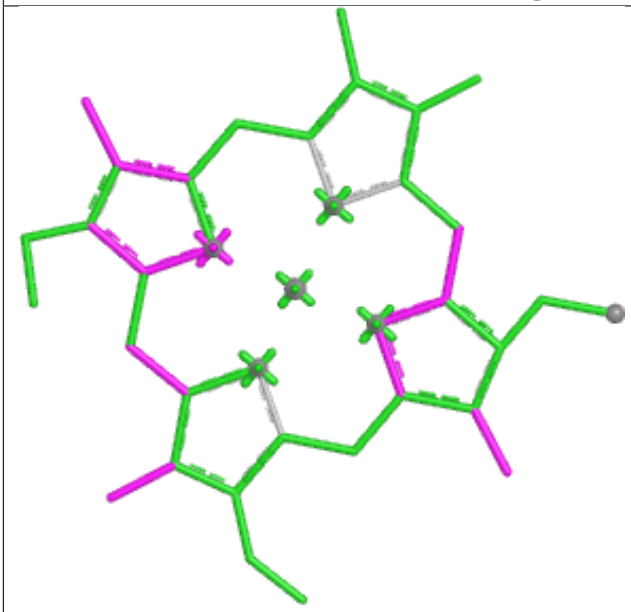


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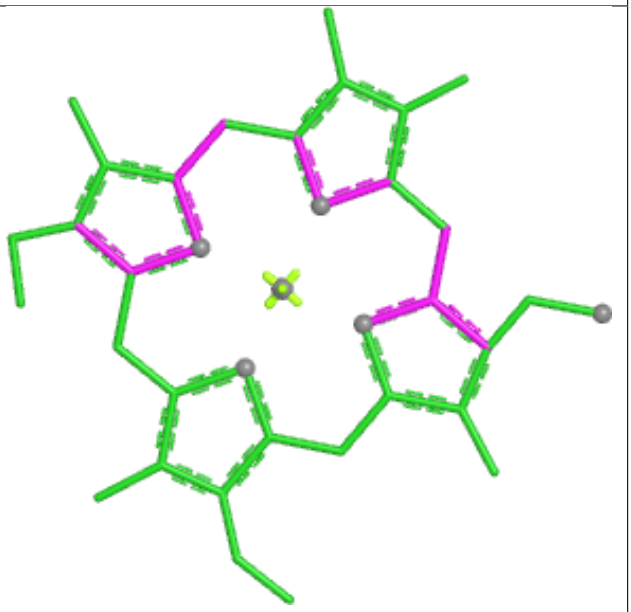


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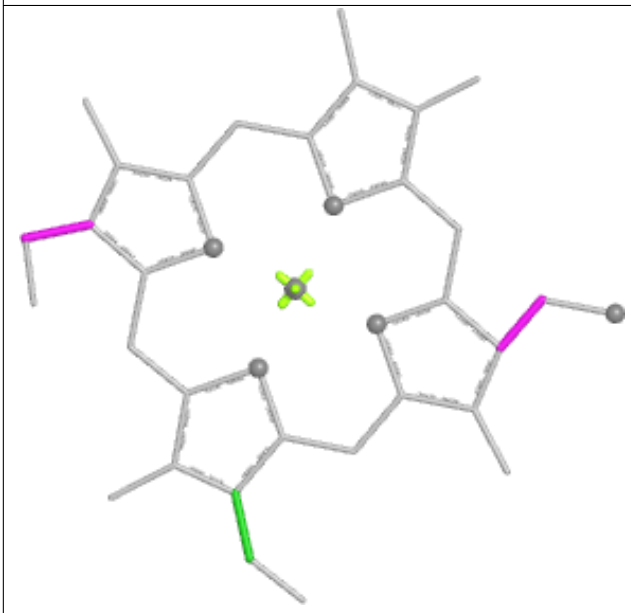
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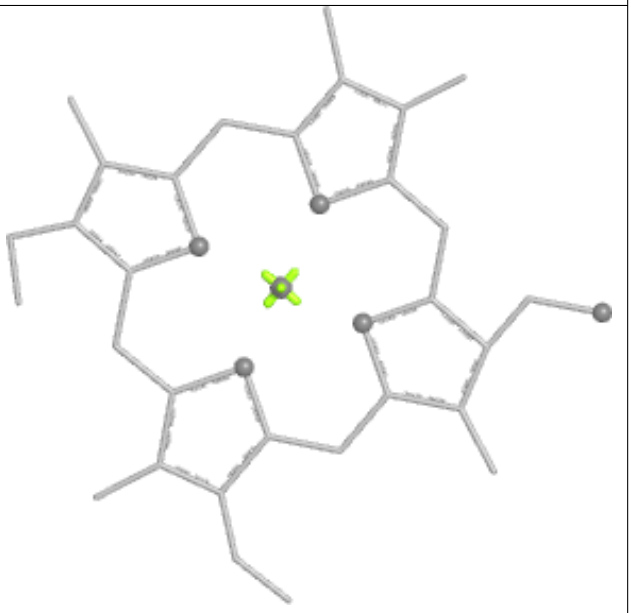
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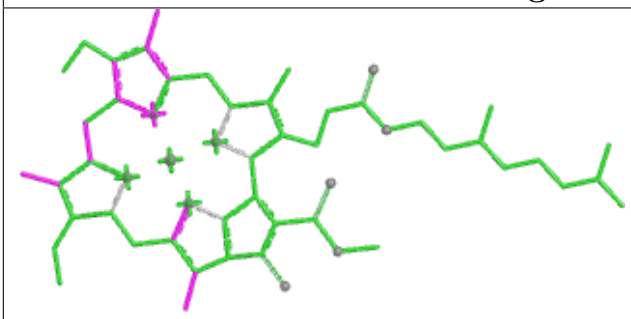


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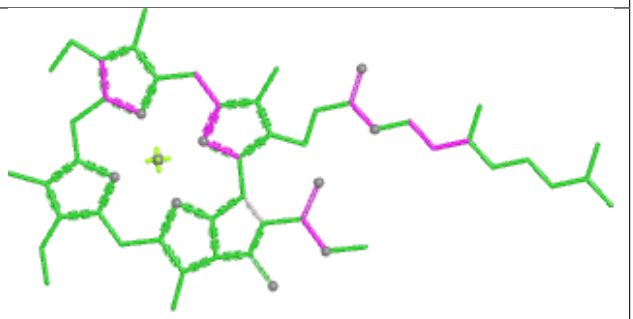


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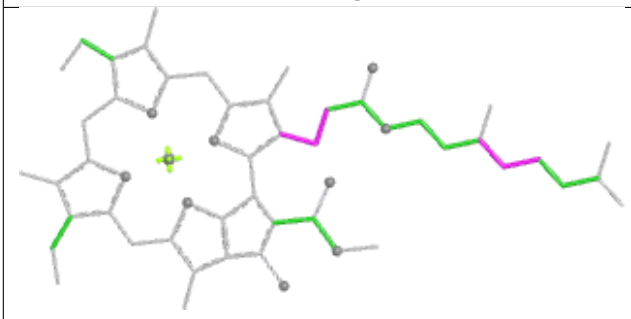
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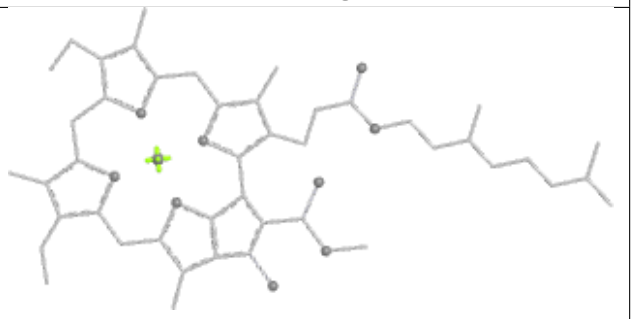
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Bond angles

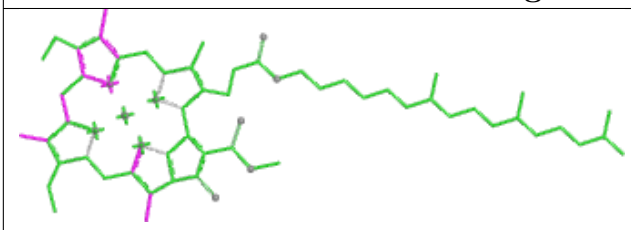


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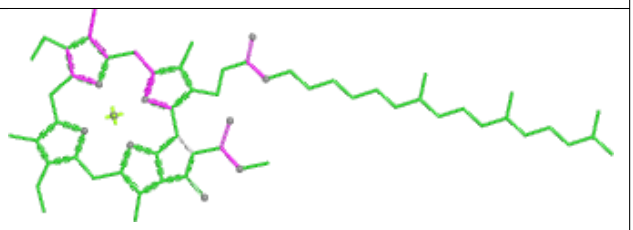


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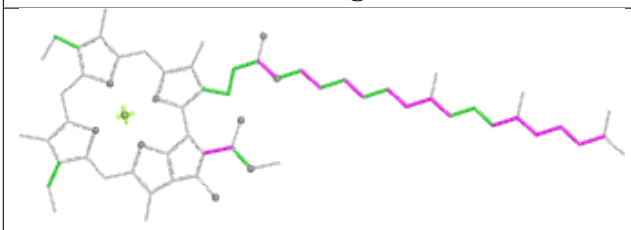
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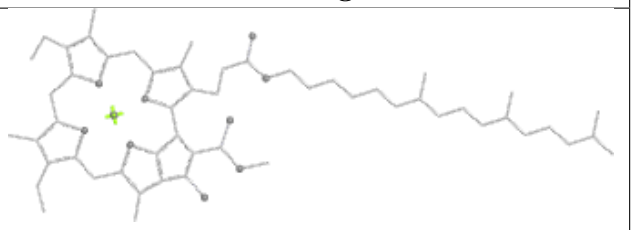
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Bond angles

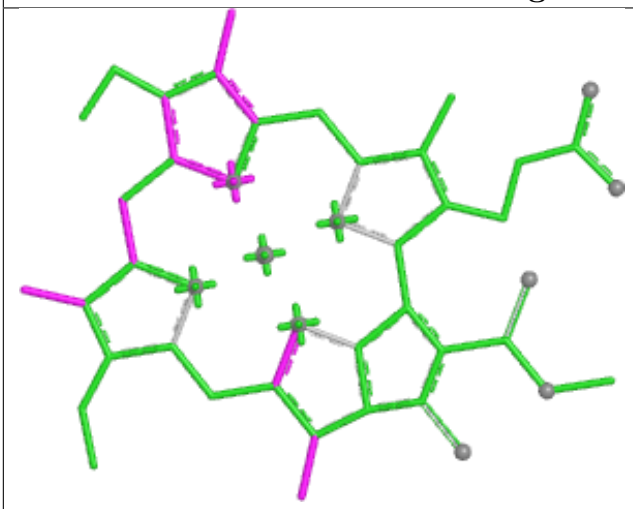


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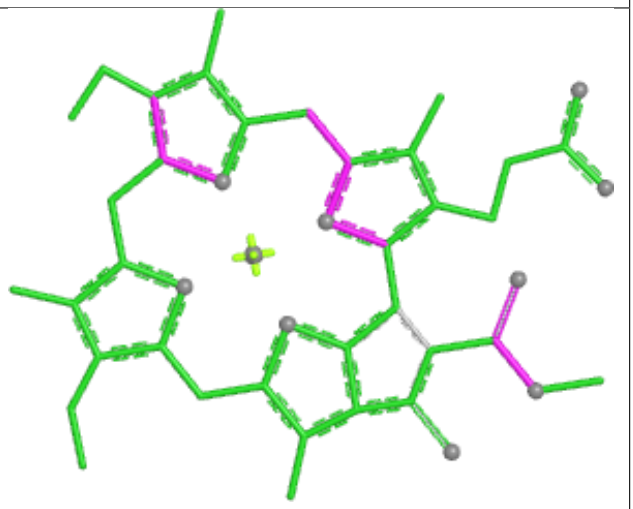


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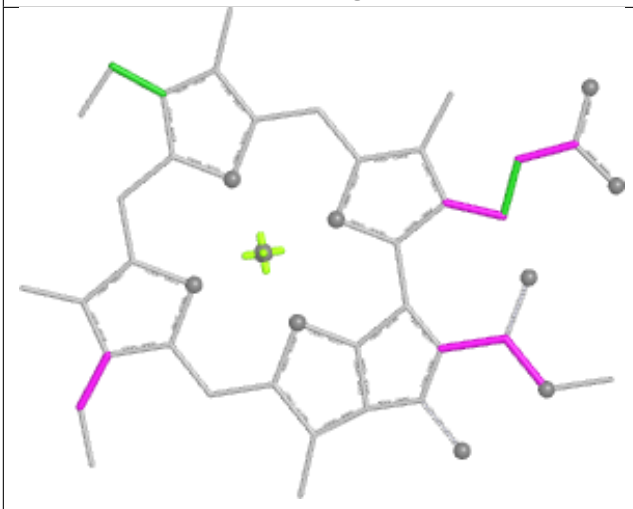
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Bond lengths



Bond angles

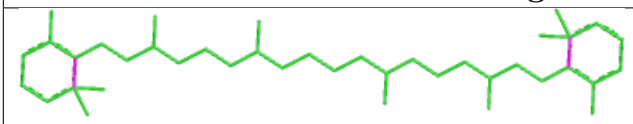


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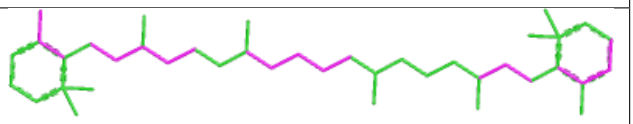


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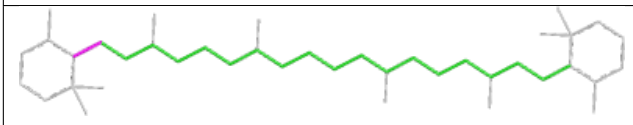
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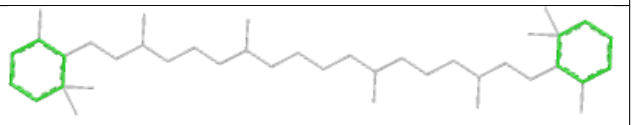
Bond lengths



Bond angles

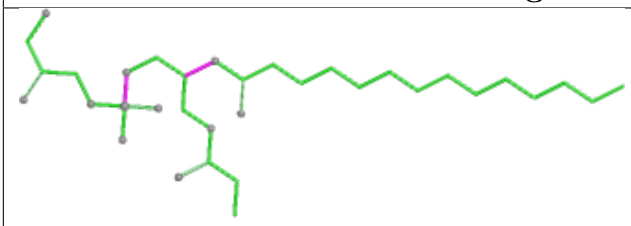


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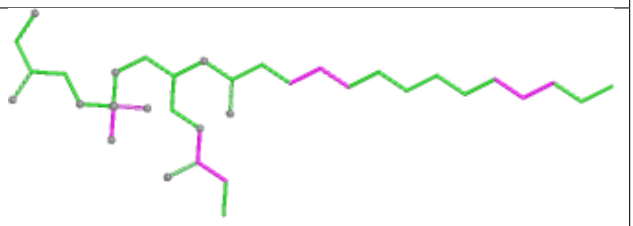


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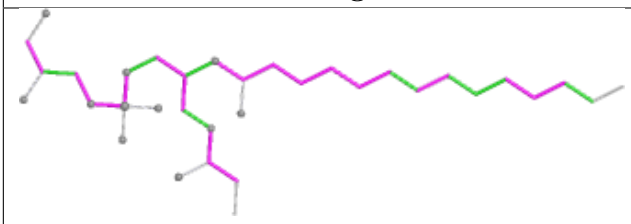
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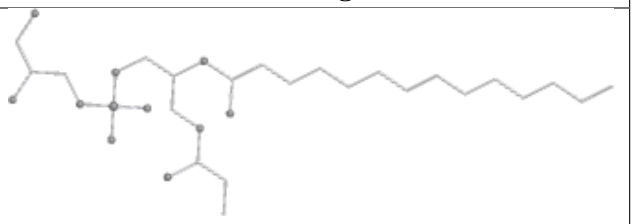
Bond lengths



Bond angles

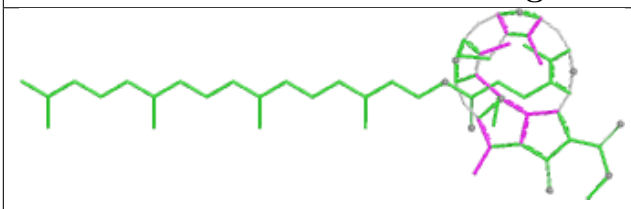


Torsions

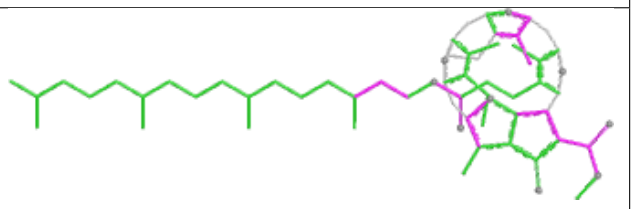


Rings

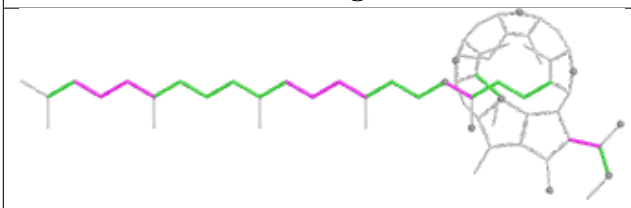
Ligand PHO a 405



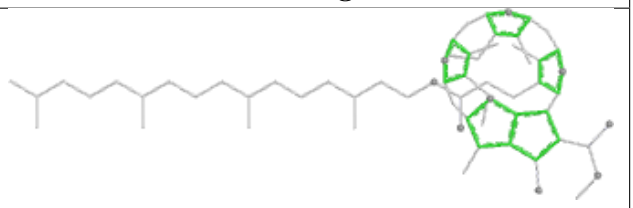
Bond lengths



Bond angles

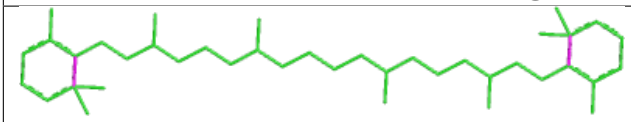


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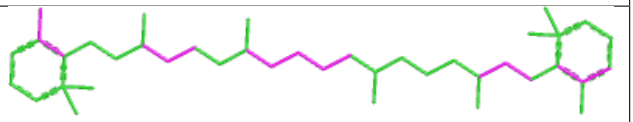


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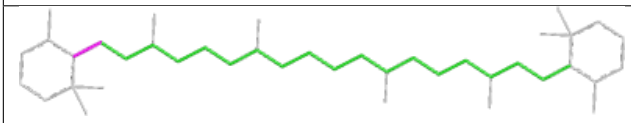
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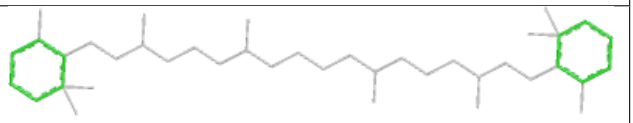
Bond lengths



Bond angles

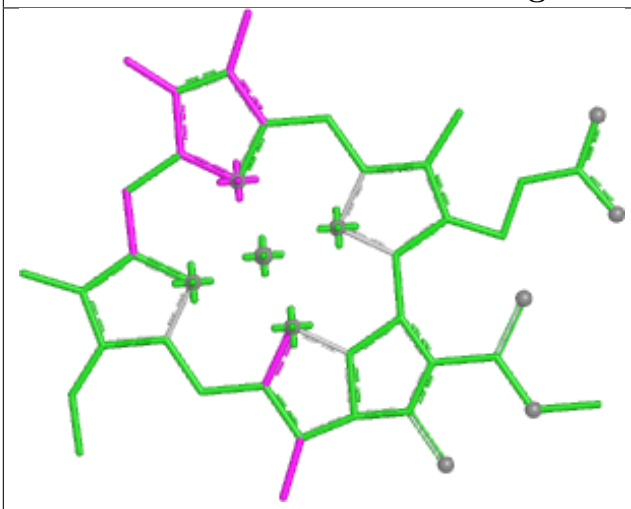


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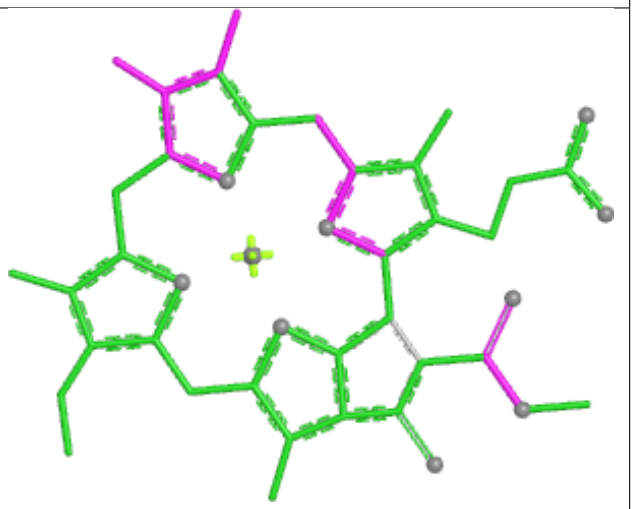


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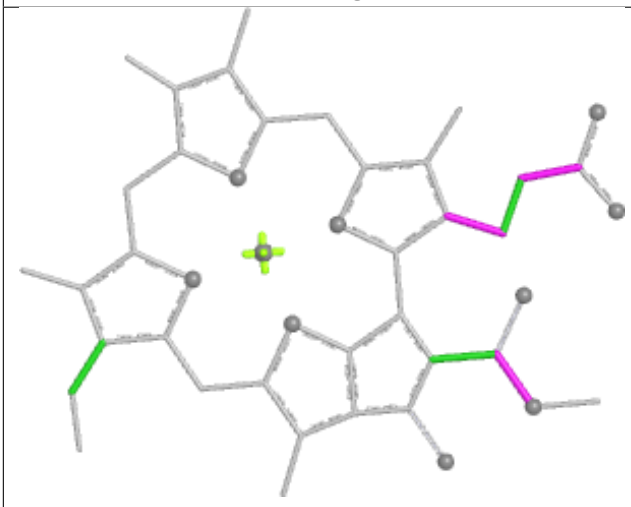
Ligand CLA 6 209



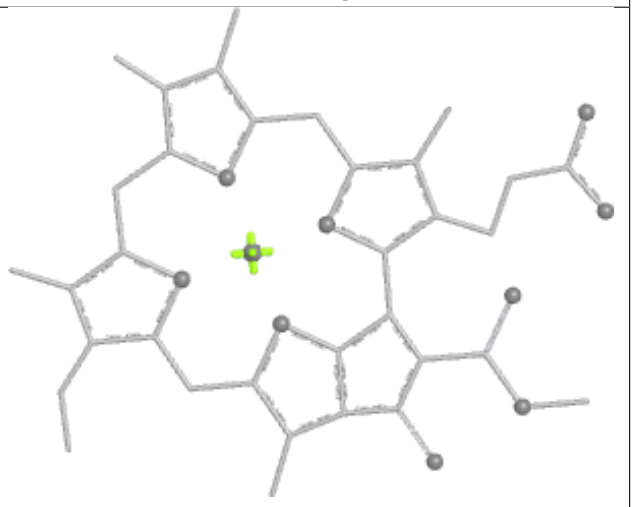
Bond lengths



Bond angles

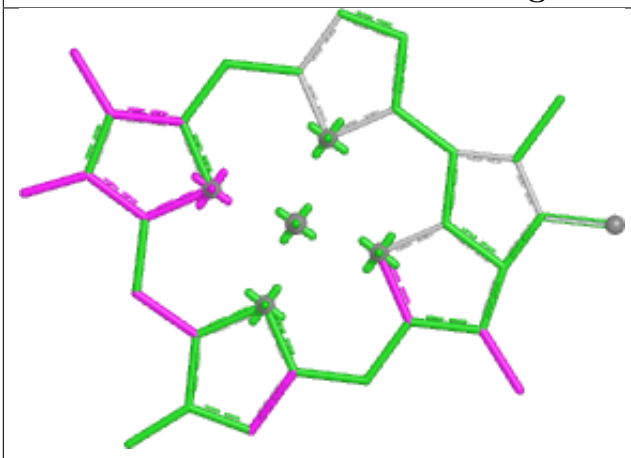


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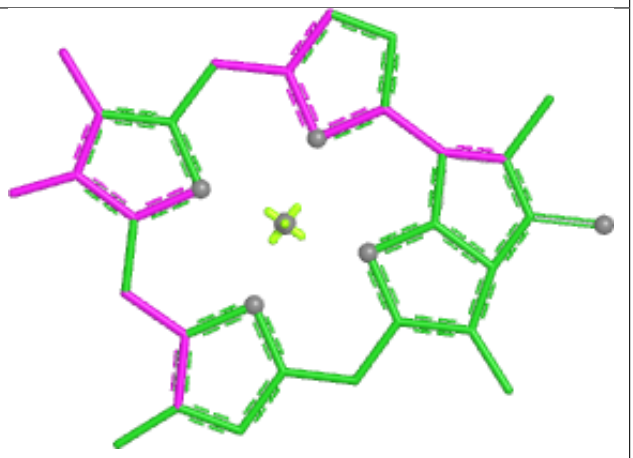


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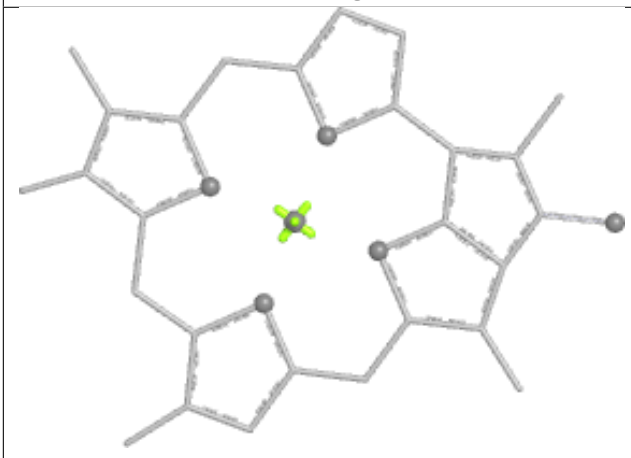
Ligand CLA 8 306



Bond lengths



Bond angles

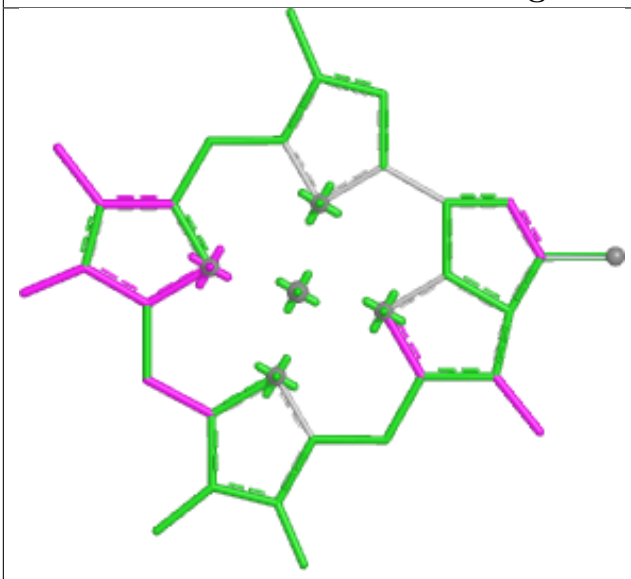


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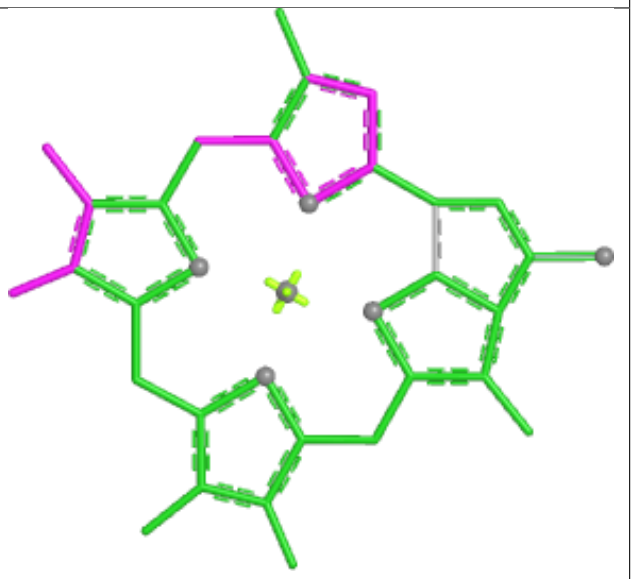


Rings

Ligand CLA 4 211



Bond lengths



Bond angles

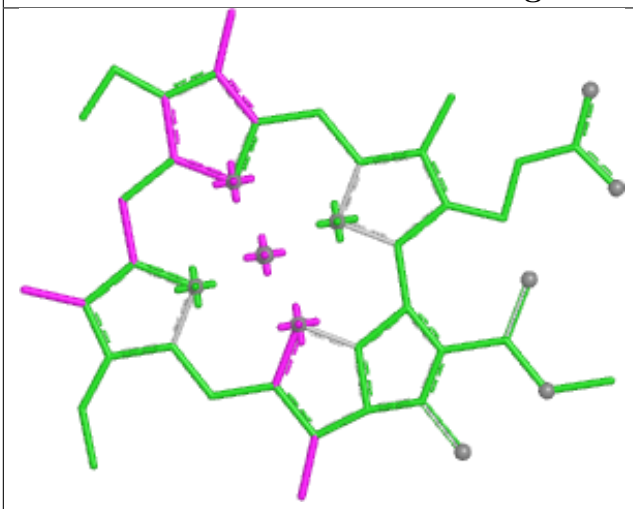


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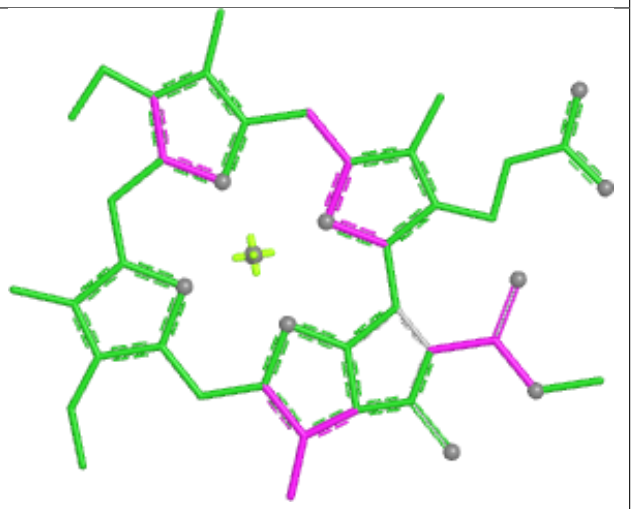


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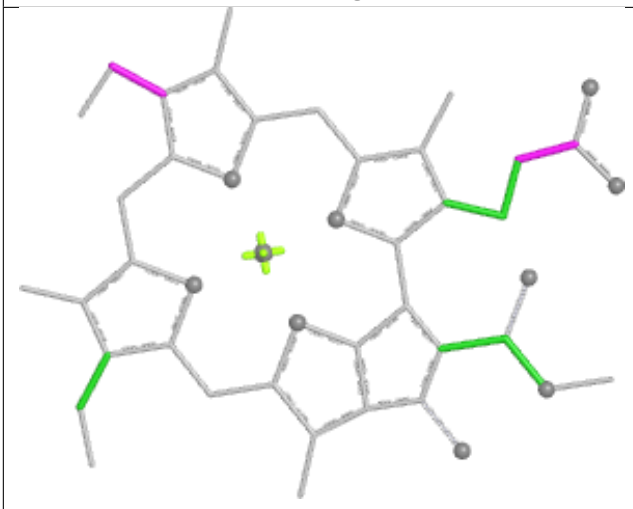
Ligand CLA w 202



Bond lengths



Bond angles

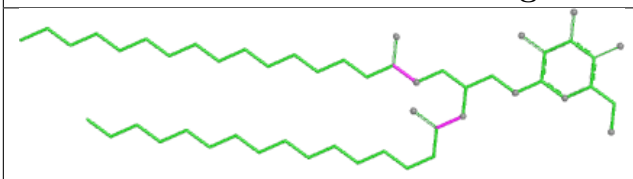


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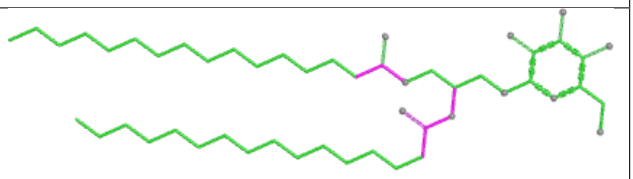


Rings

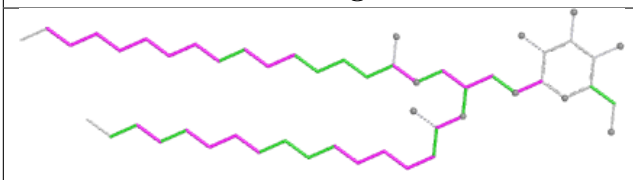
Ligand LMG C 521



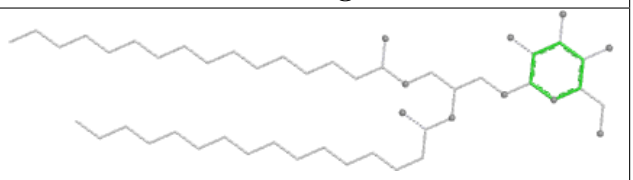
Bond lengths



Bond angles

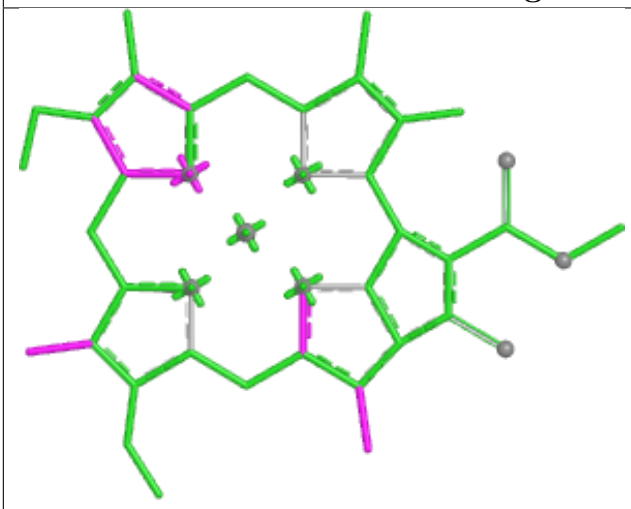


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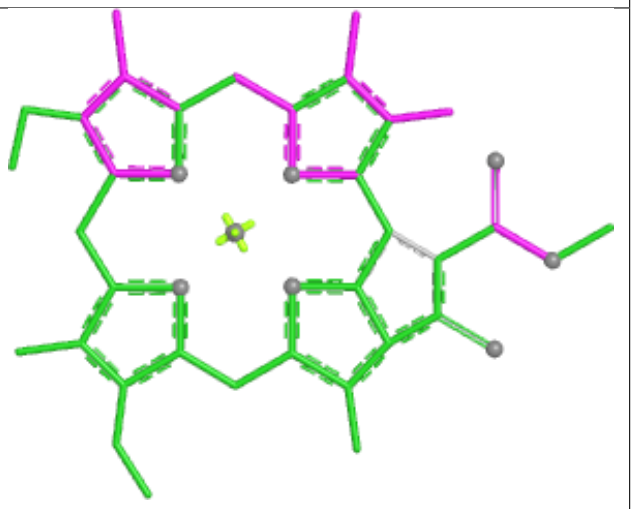


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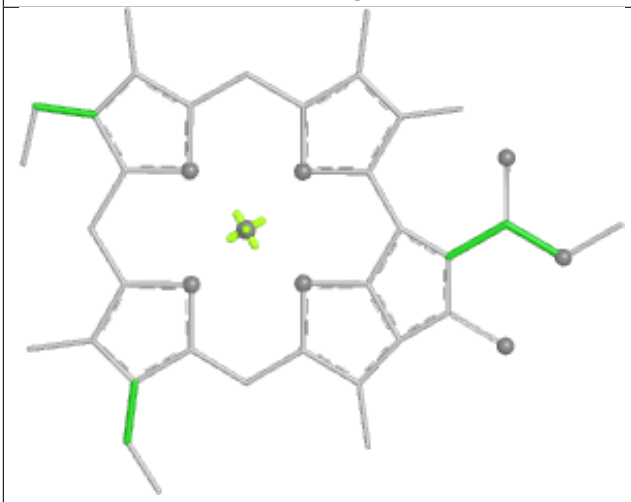
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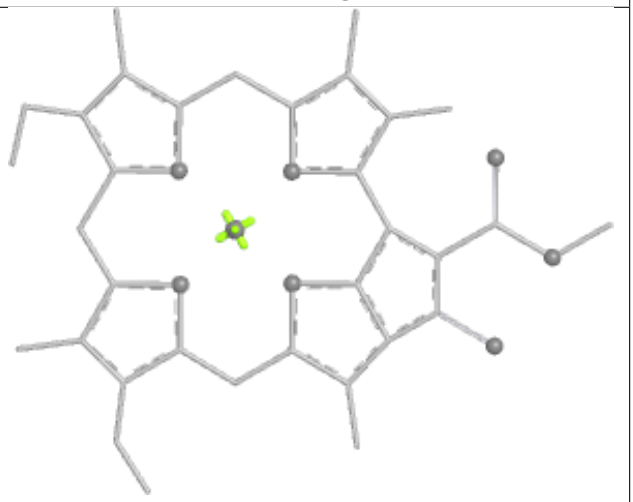
Bond lengths



Bond angles

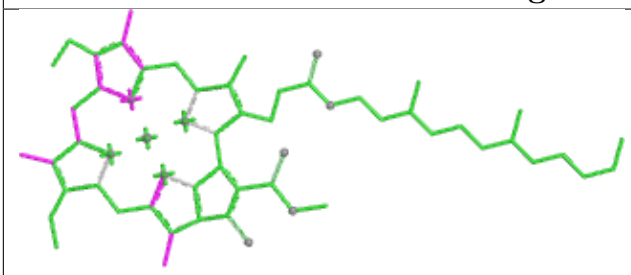


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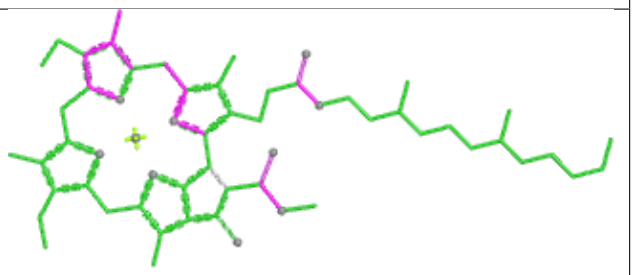


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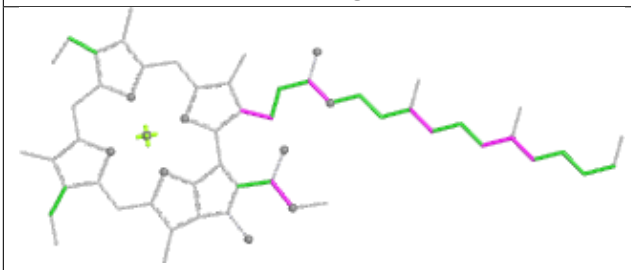
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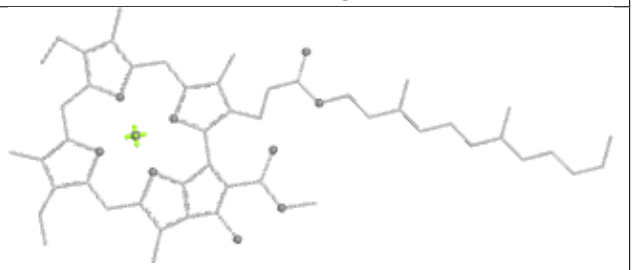
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Bond angles

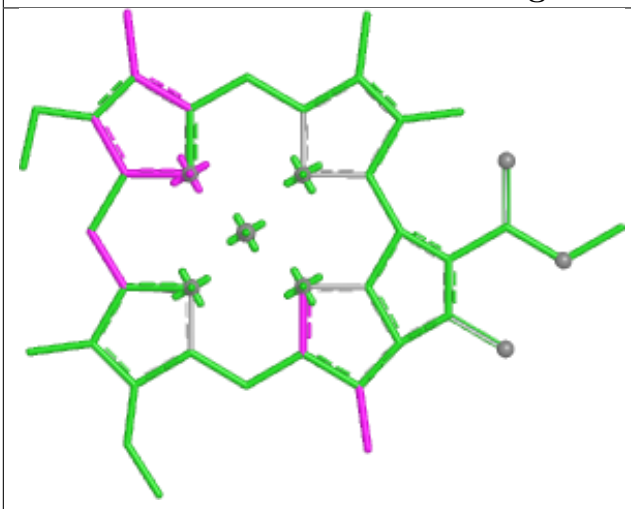


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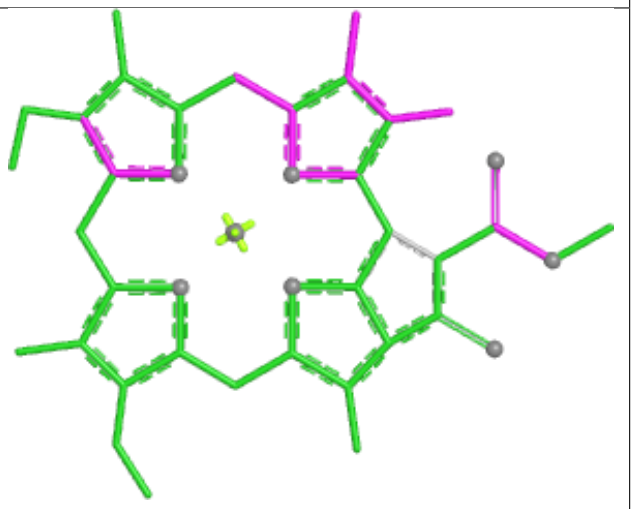


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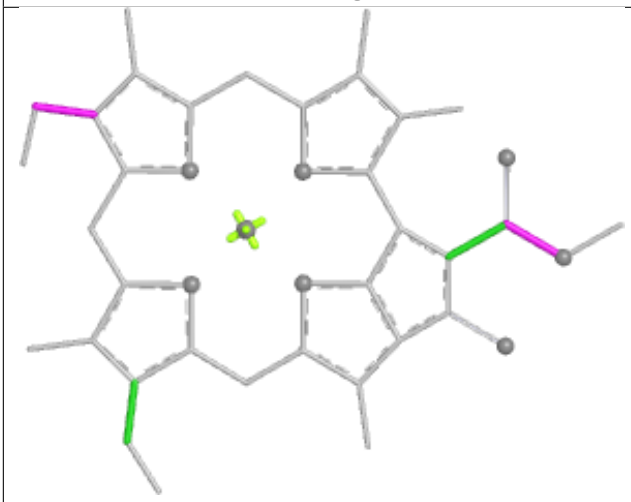
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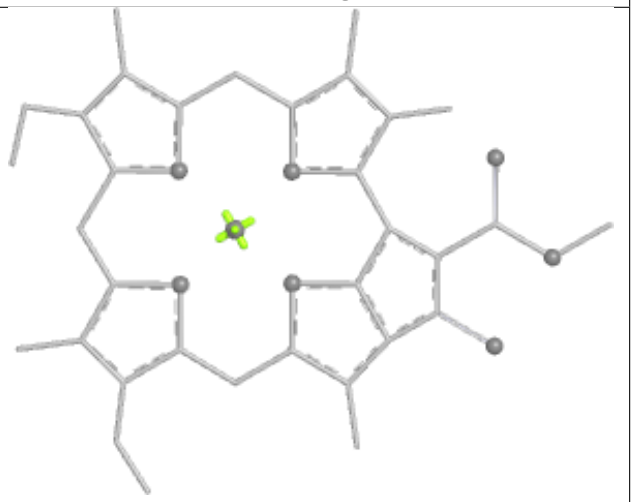
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Bond angles

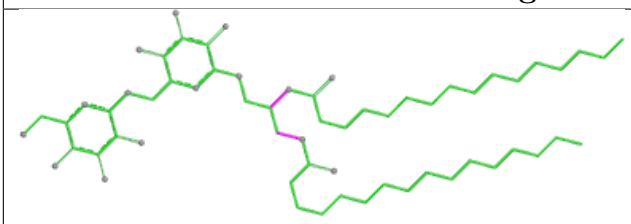


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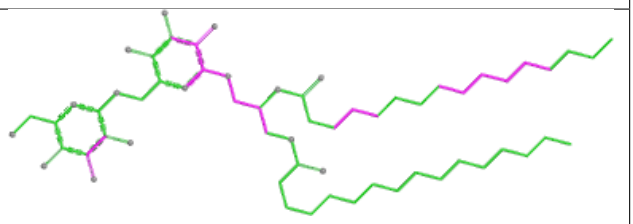


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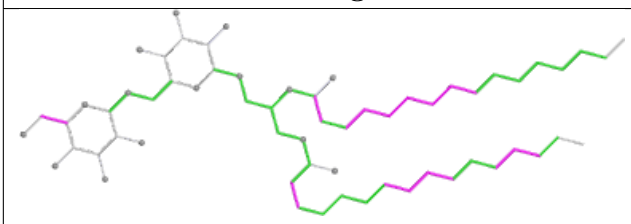
Ligand DGD H 102



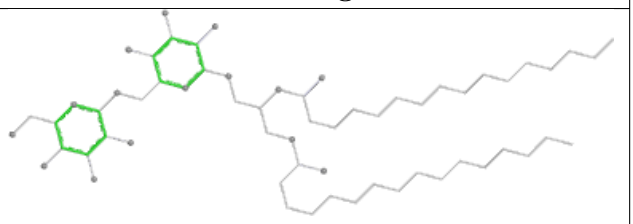
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Bond angles

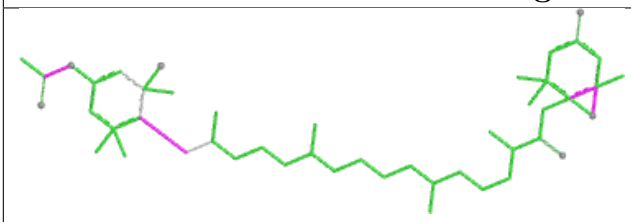


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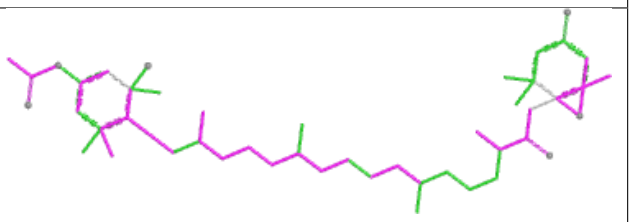


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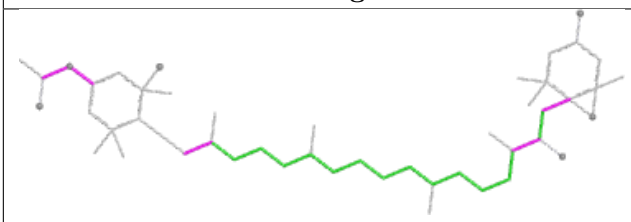
Ligand A86 5 301



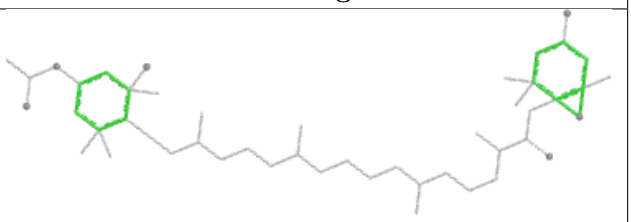
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Bond angles

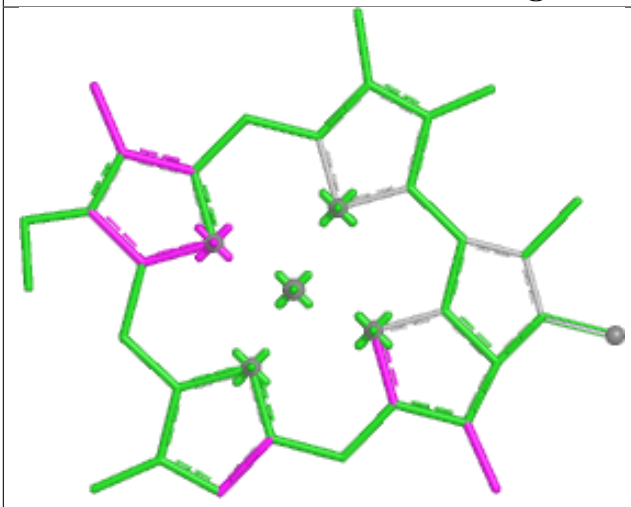


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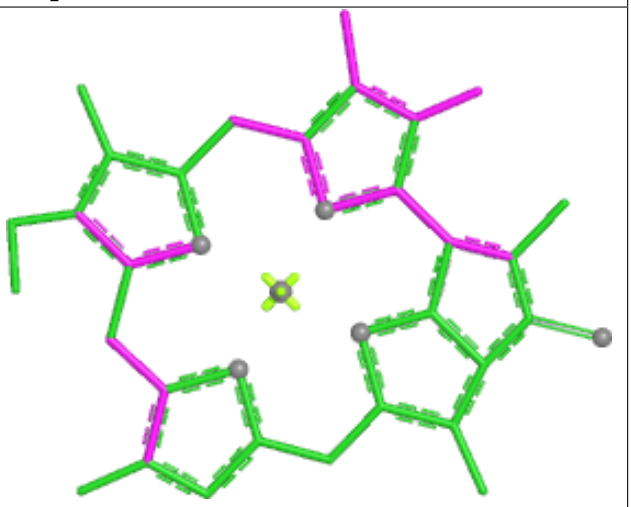


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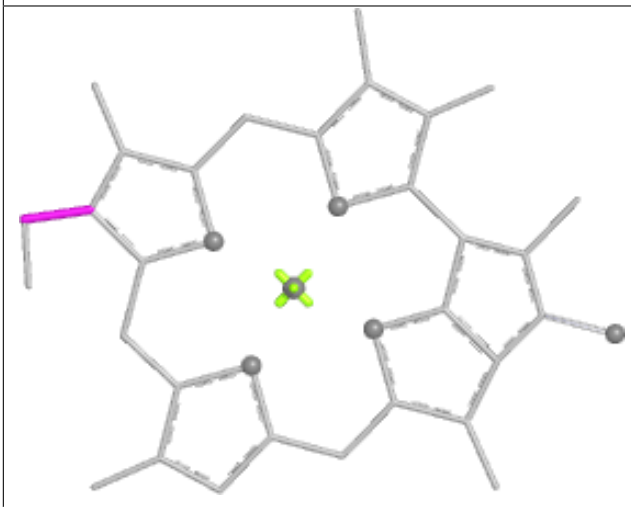
Ligand CLA p 601



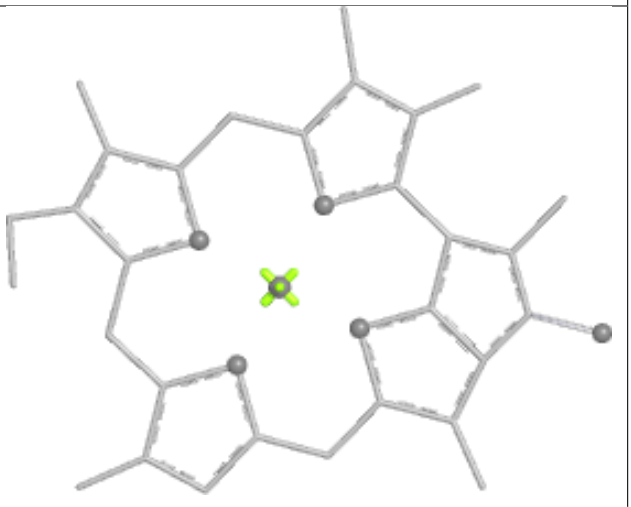
Bond lengths



Bond angles

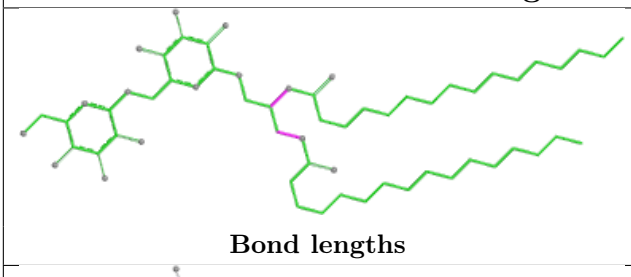


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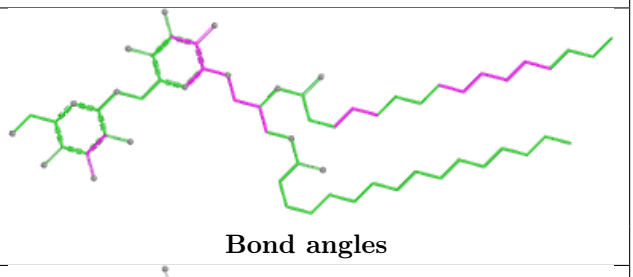


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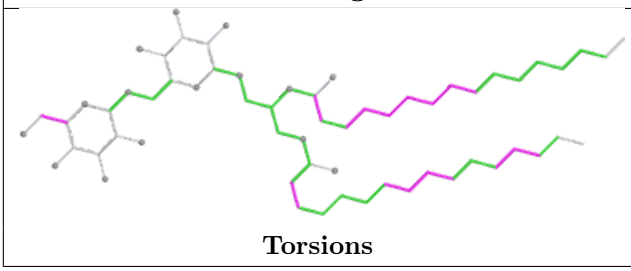
Ligand DGD h 102



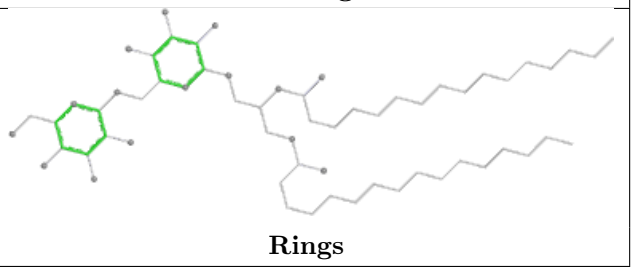
Bond lengths



Bond angles

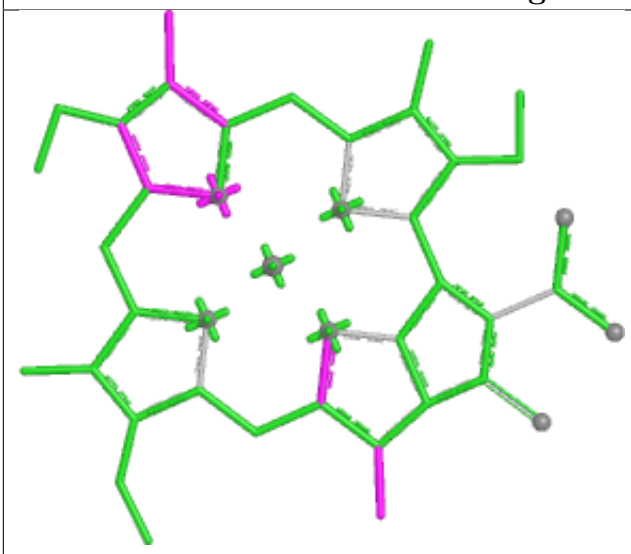


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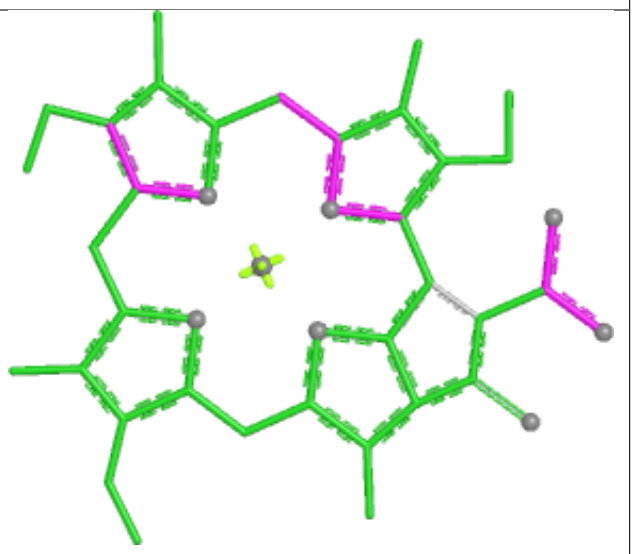


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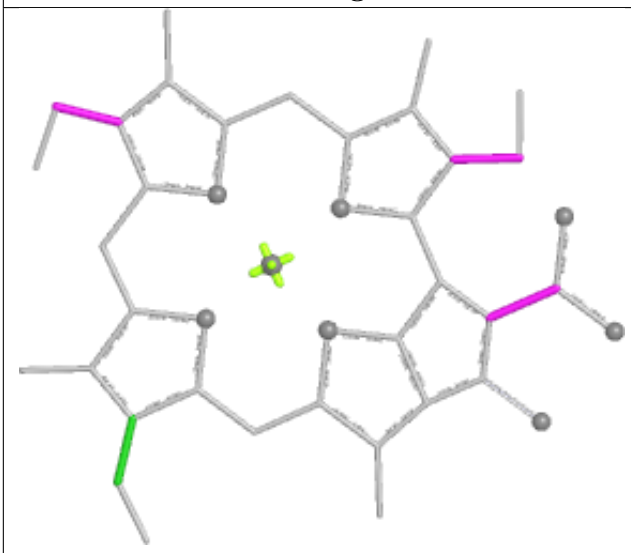
Ligand CLA 8 312



Bond lengths



Bond angles

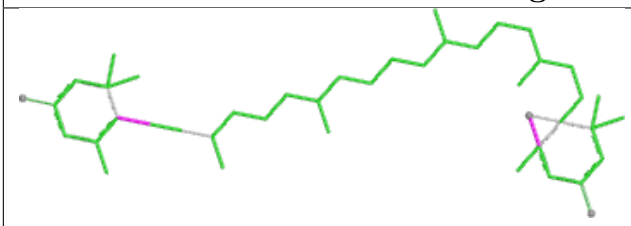


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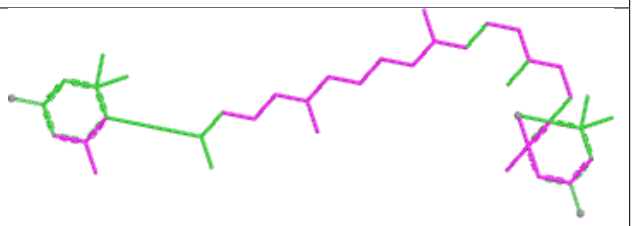


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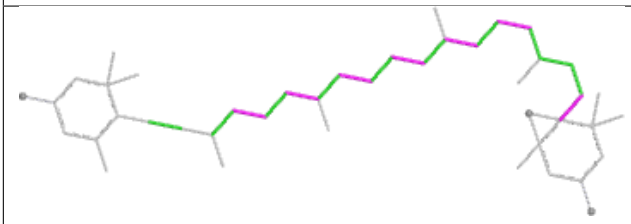
Ligand DD6 7 304



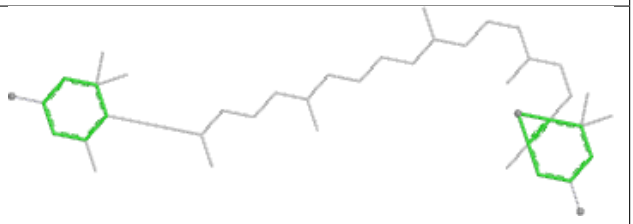
Bond lengths



Bond angles

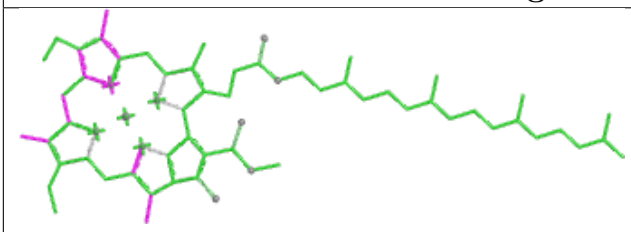


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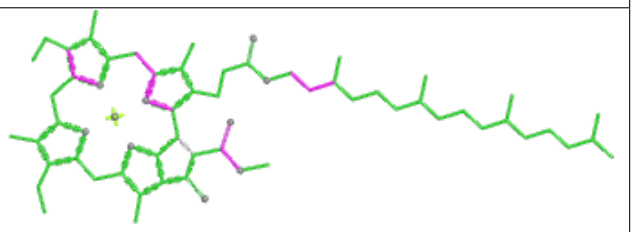


Rings

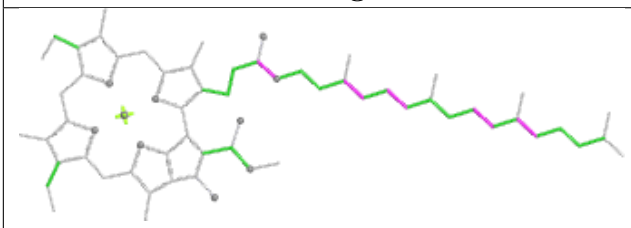
Ligand CLA d 404



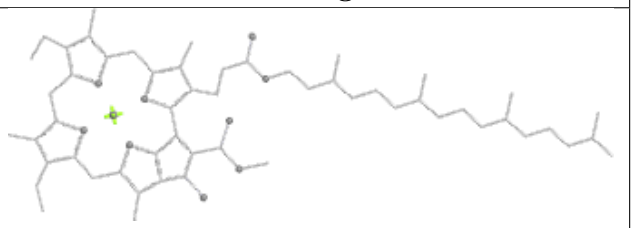
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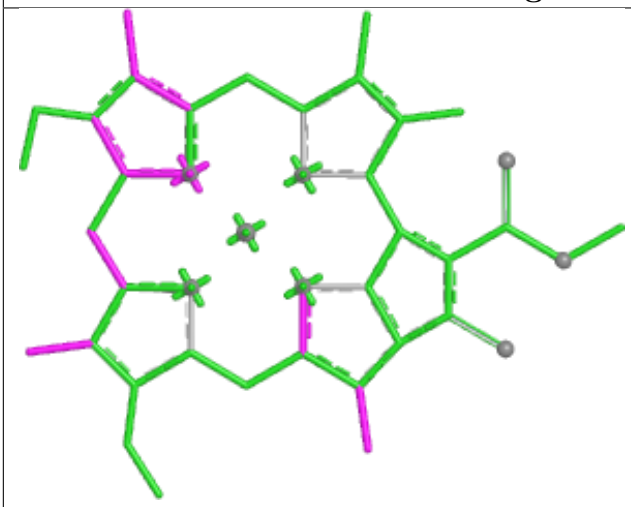


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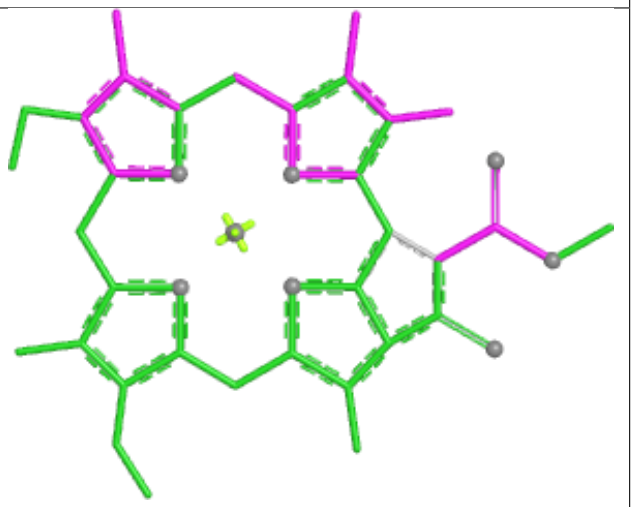


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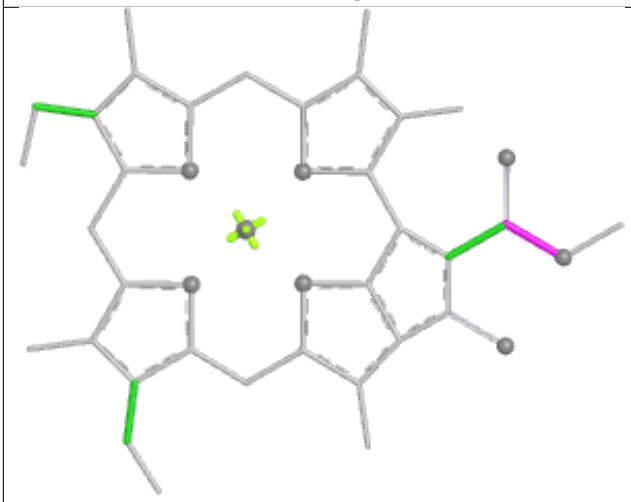
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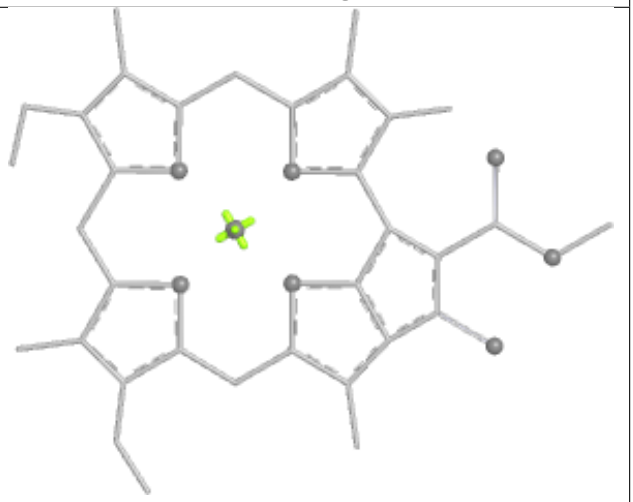
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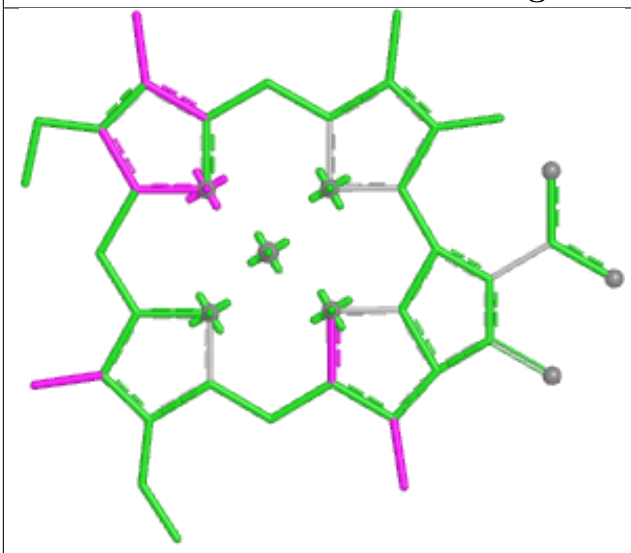


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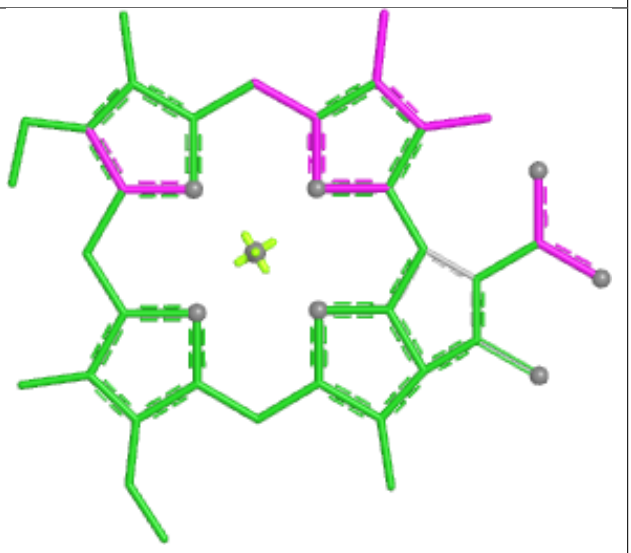


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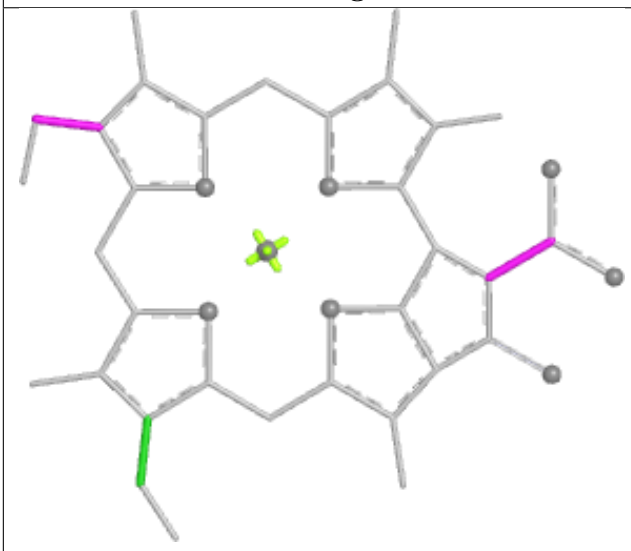
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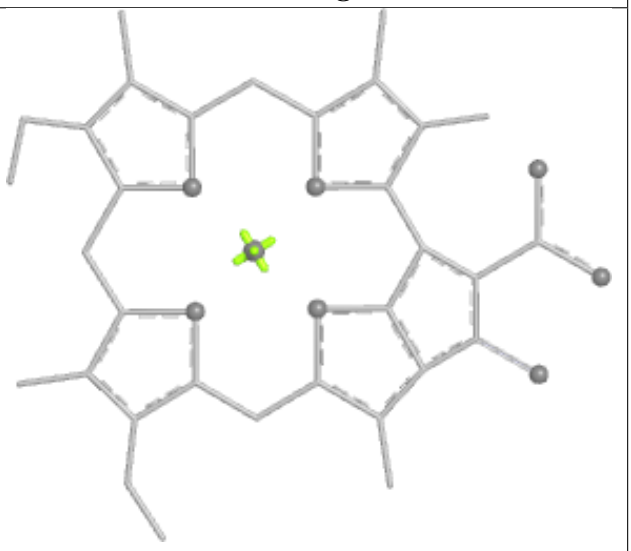
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Bond angles

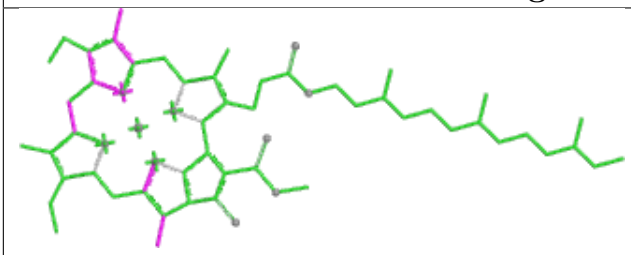


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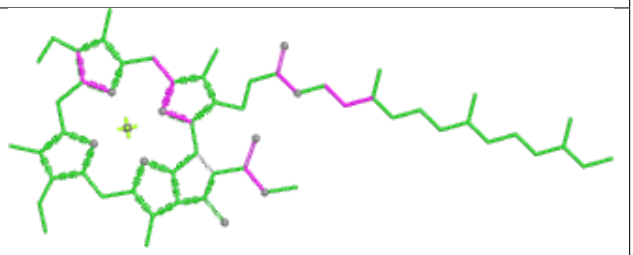


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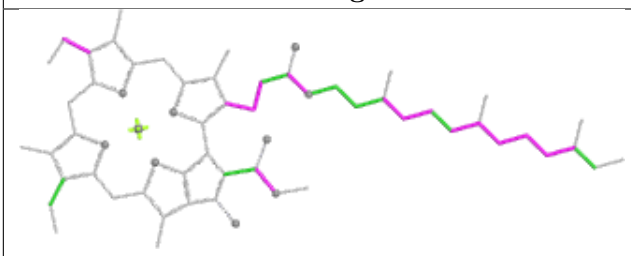
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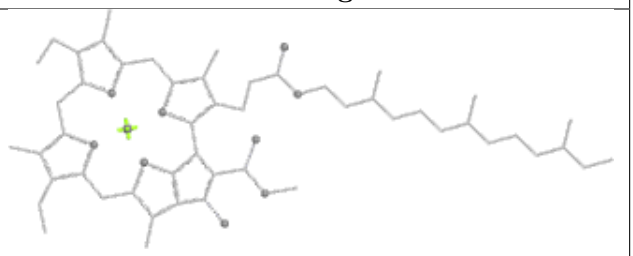
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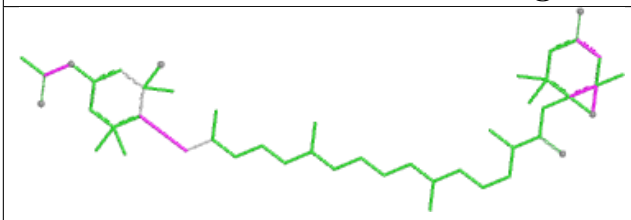


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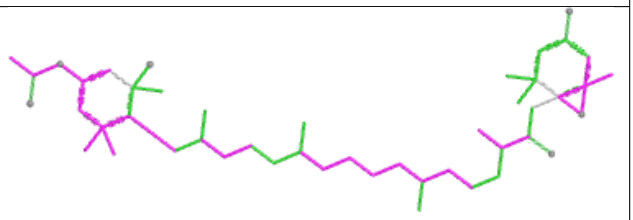


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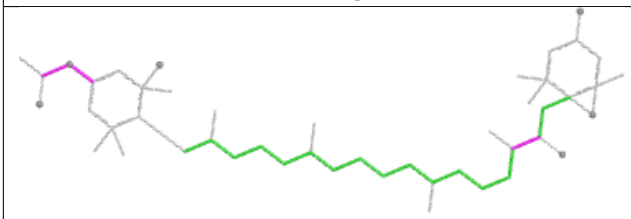
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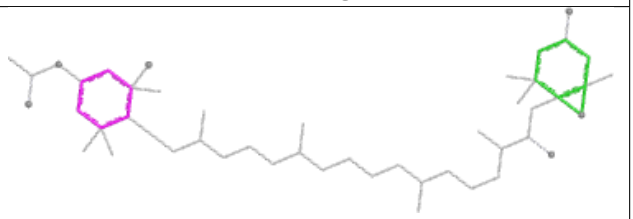
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Bond angles

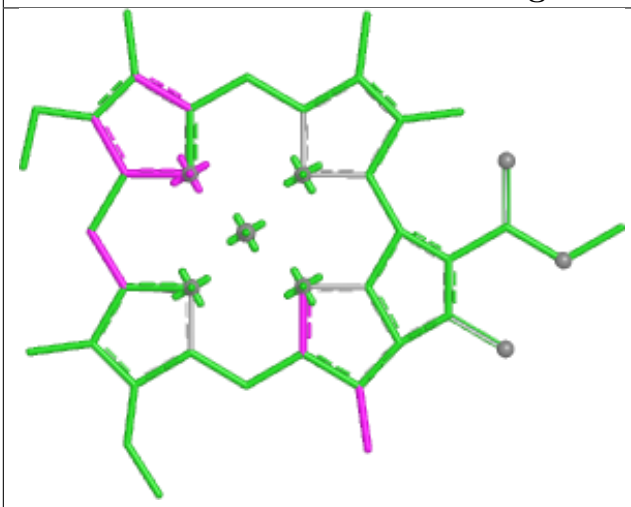


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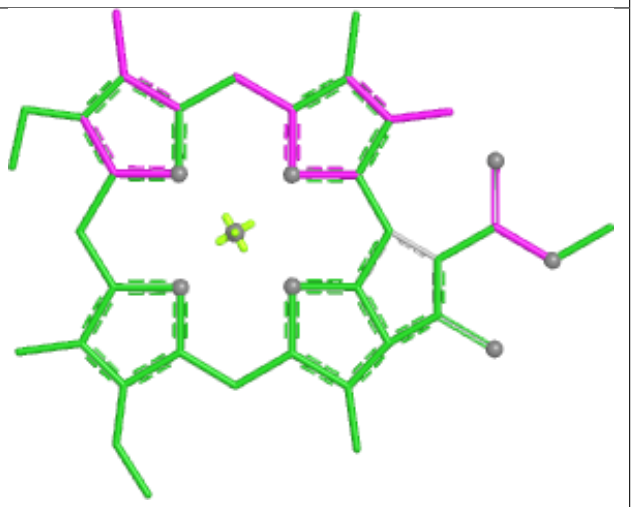


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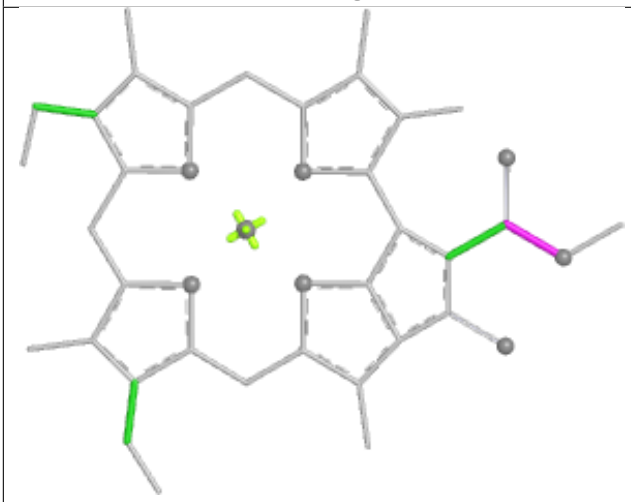
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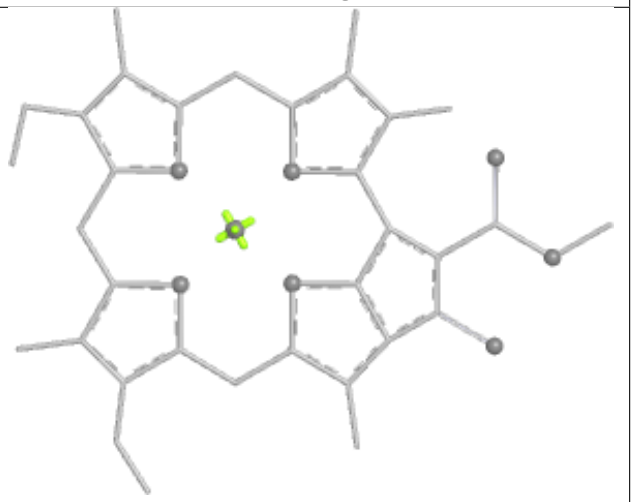
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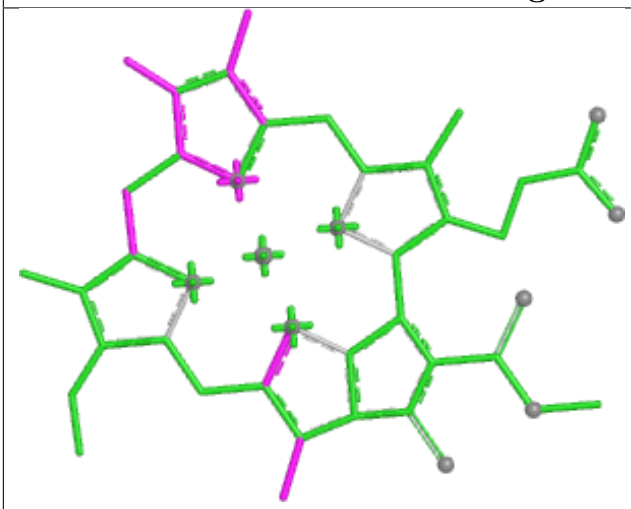


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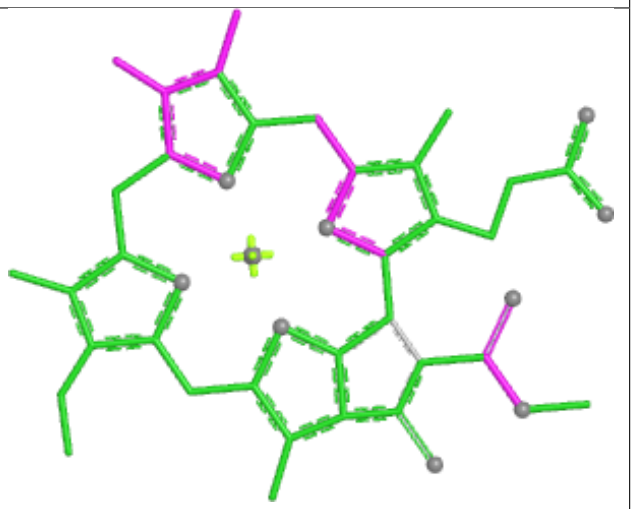


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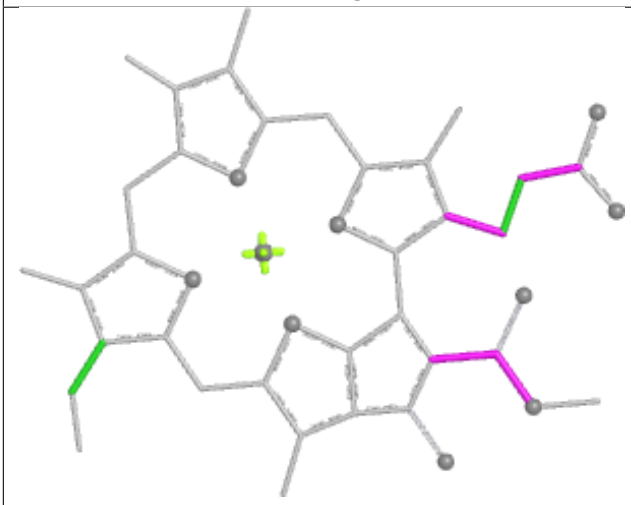
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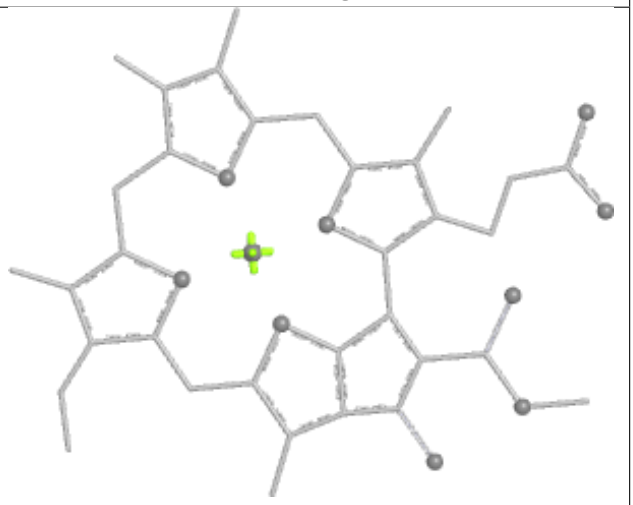
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Bond angles

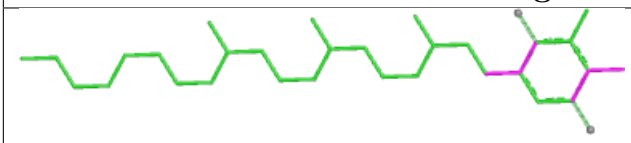


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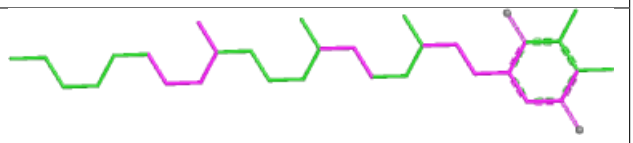


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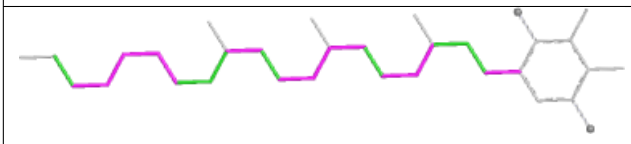
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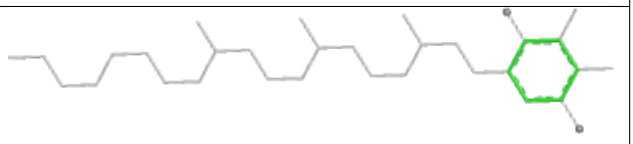
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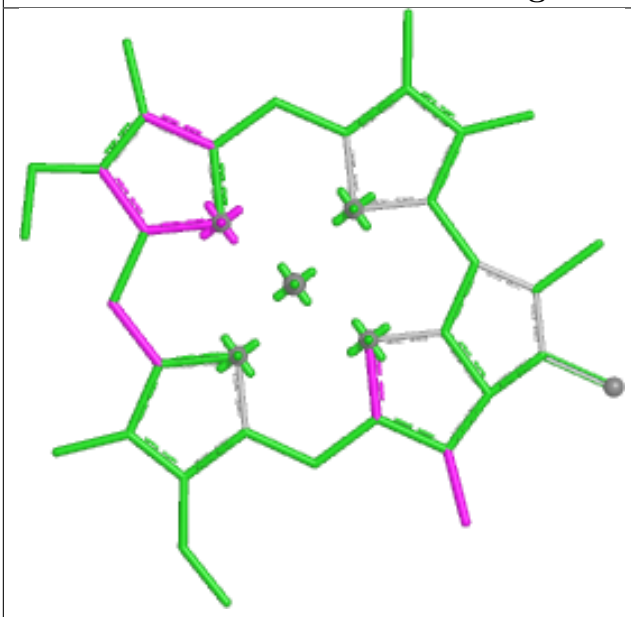


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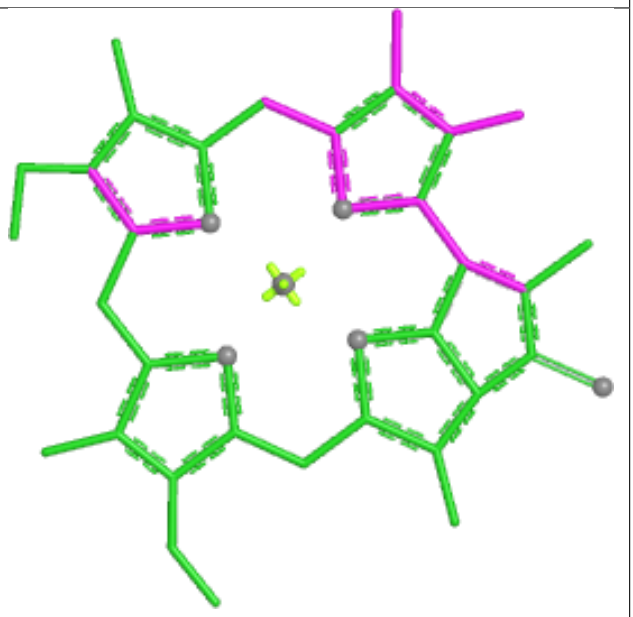


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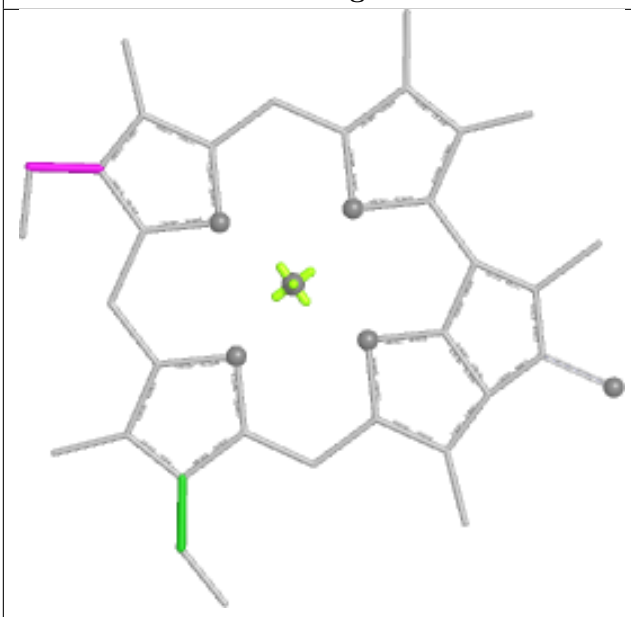
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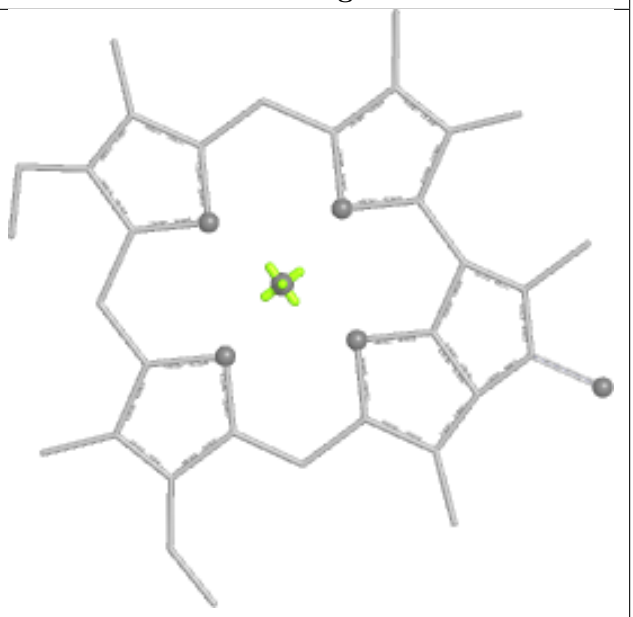
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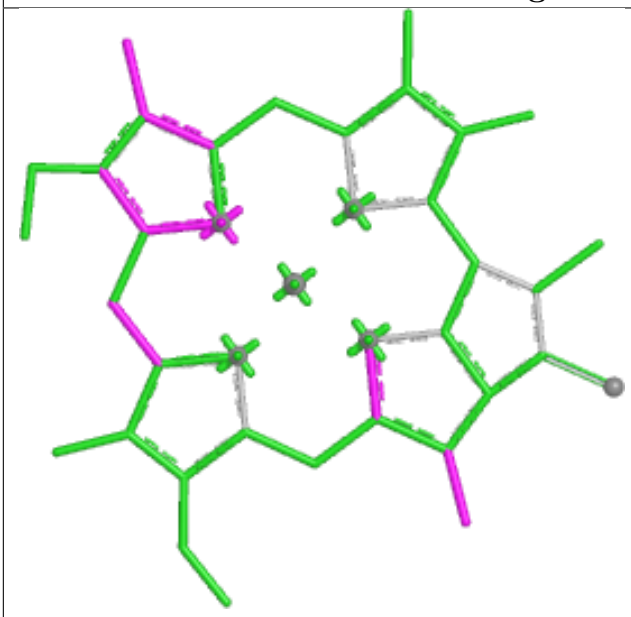


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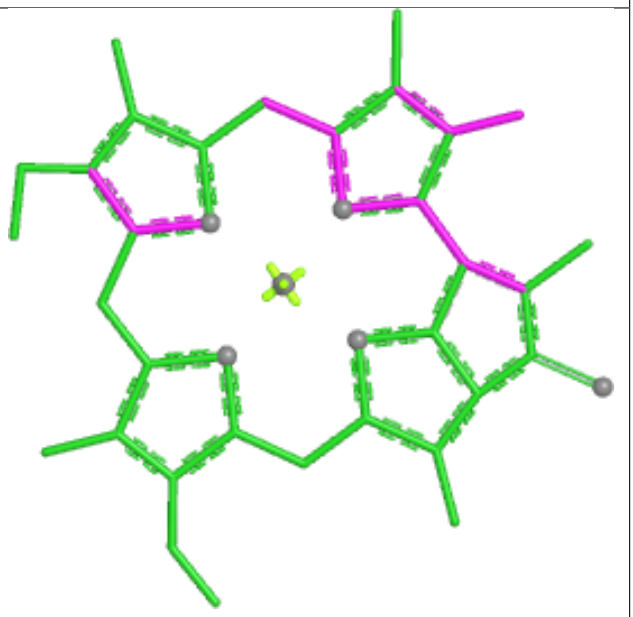


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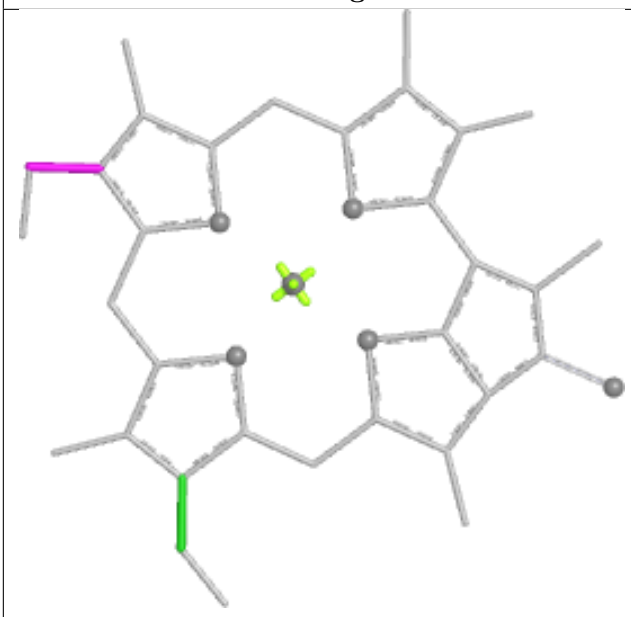
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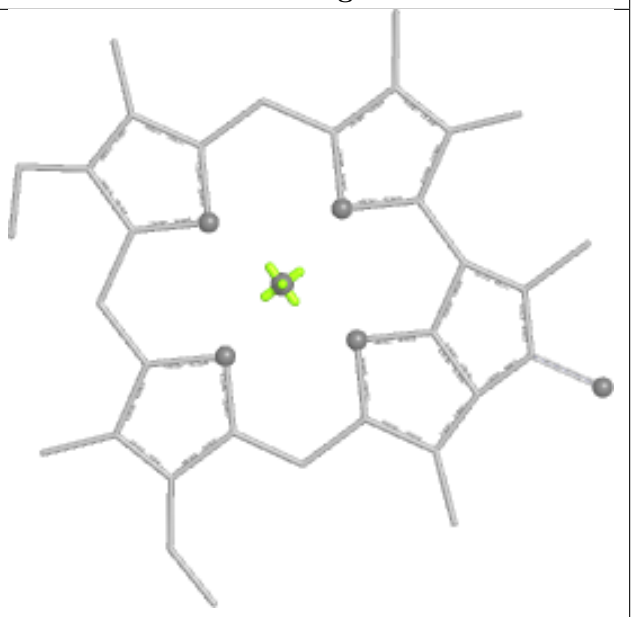
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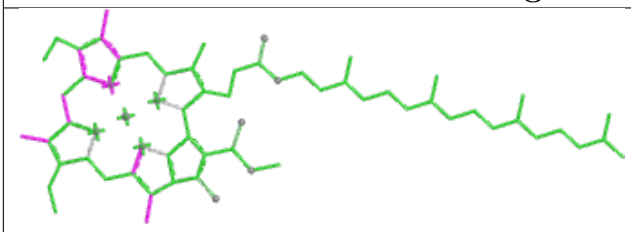
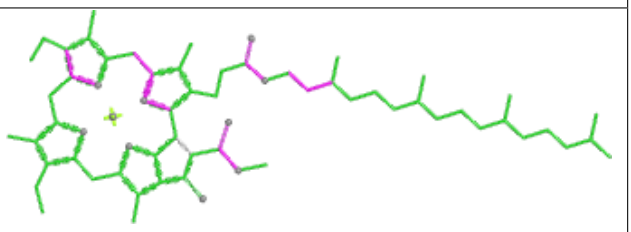
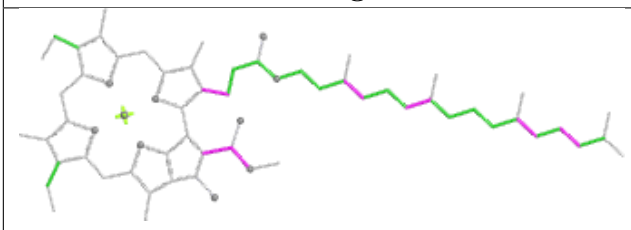
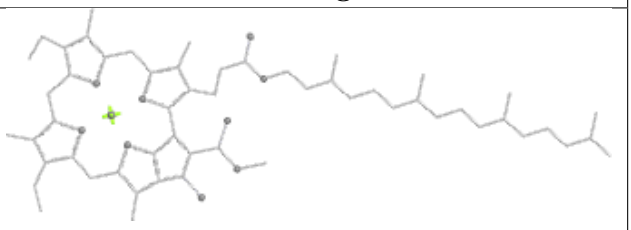
Bond angles



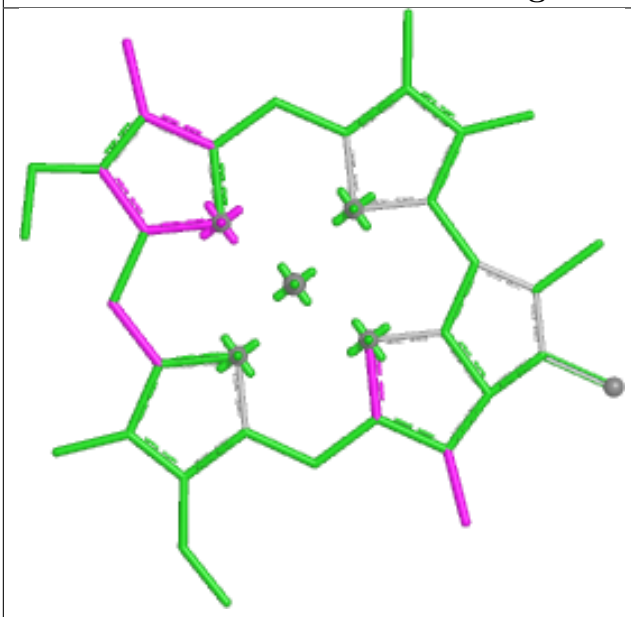
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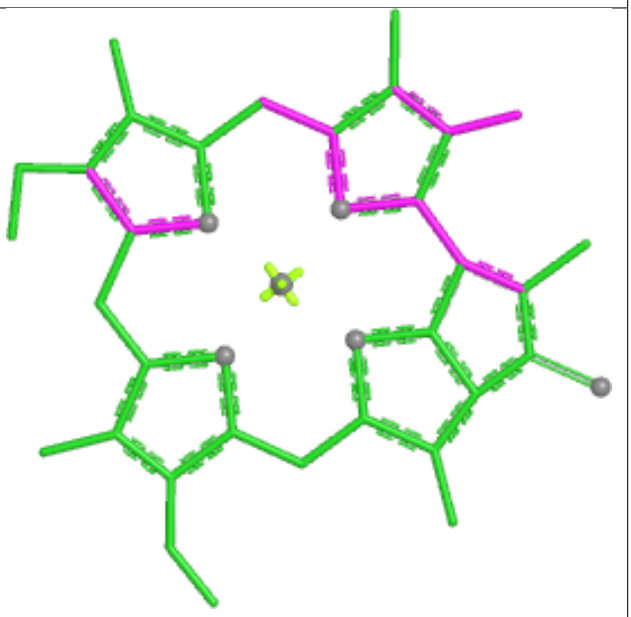
Rings

Ligand CLA B 509	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

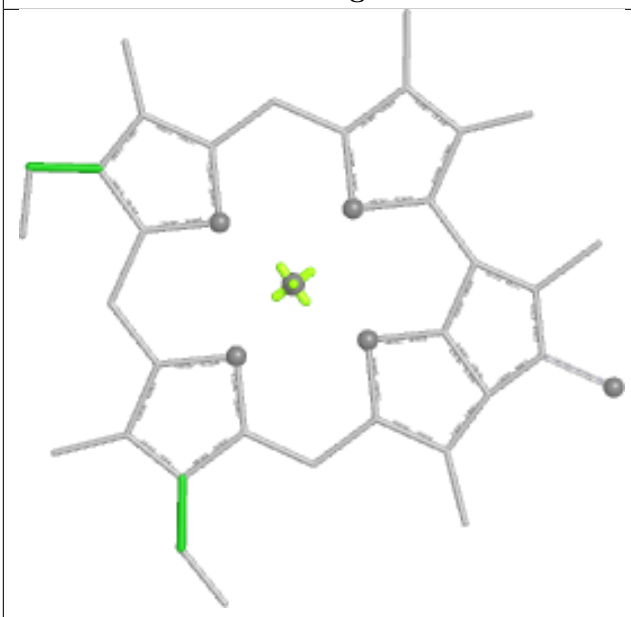
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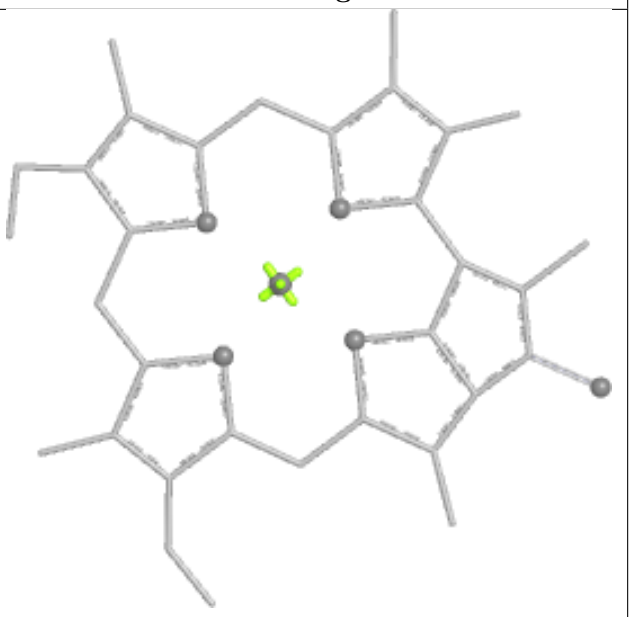
Bond lengths



Bond angles

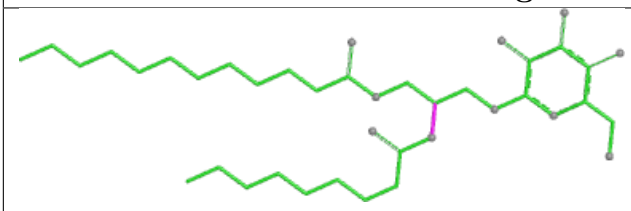


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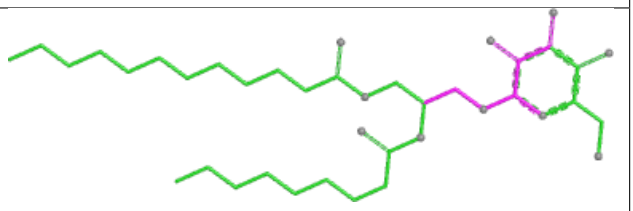


Rings

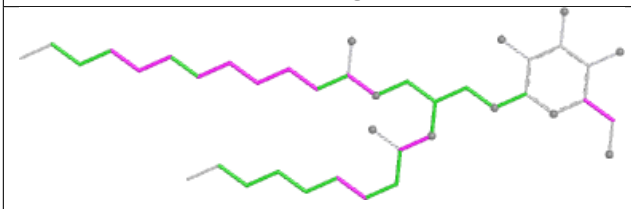
Ligand LMG M 102



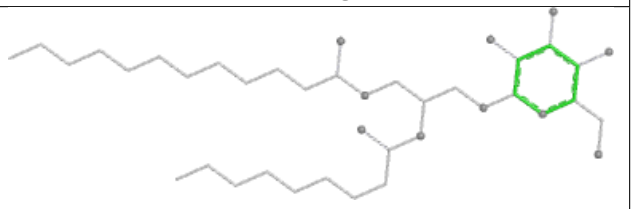
Bond lengths



Bond angles

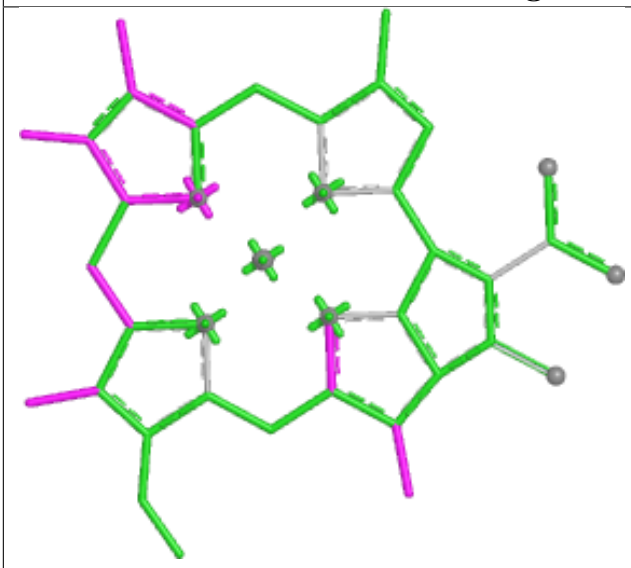


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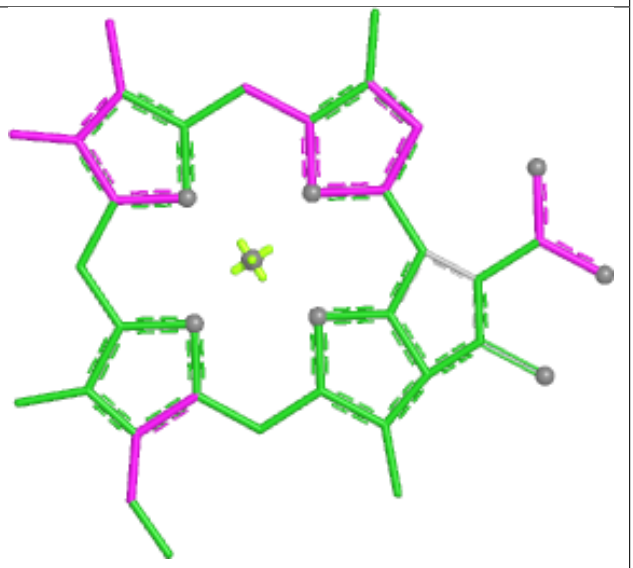


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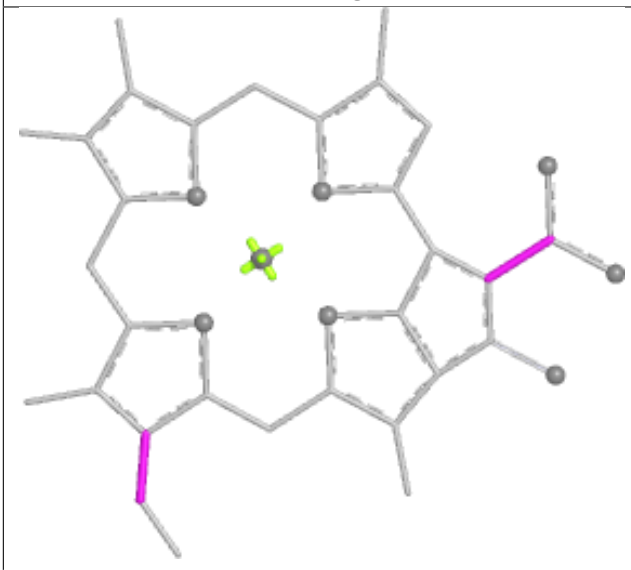
Ligand CLA P 608



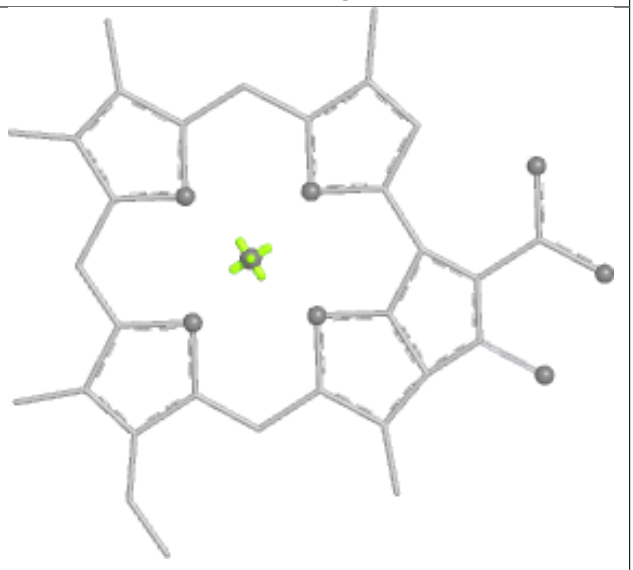
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Bond angles

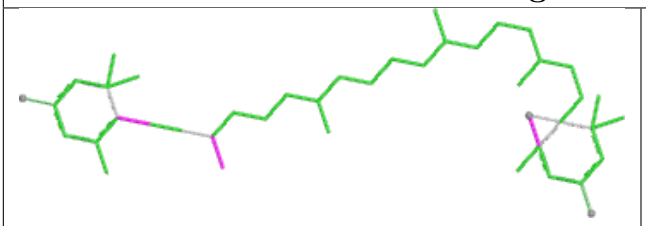


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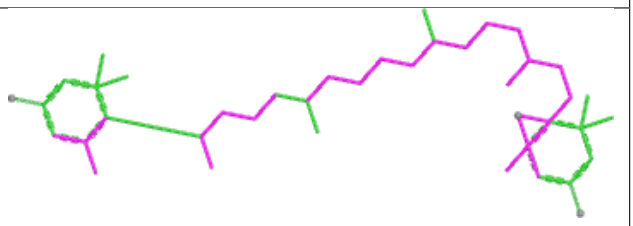


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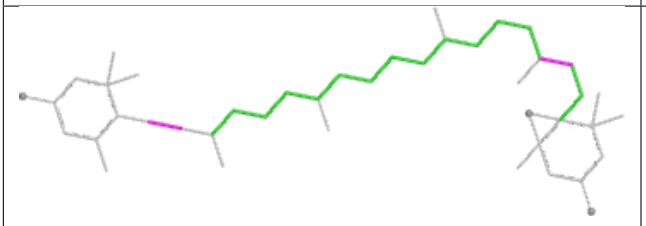
Ligand DD6 3 303



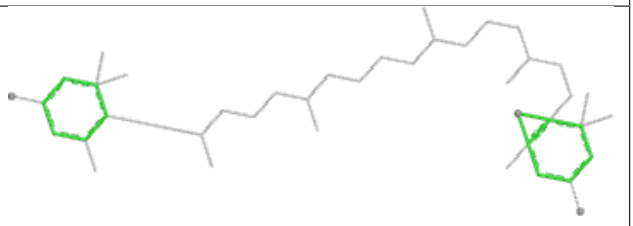
Bond lengths



Bond angles

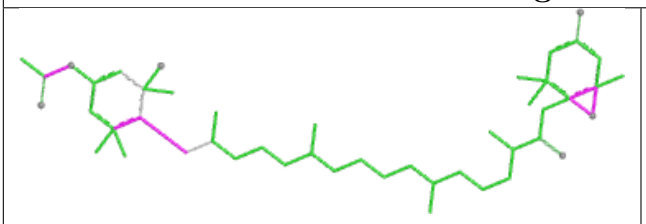


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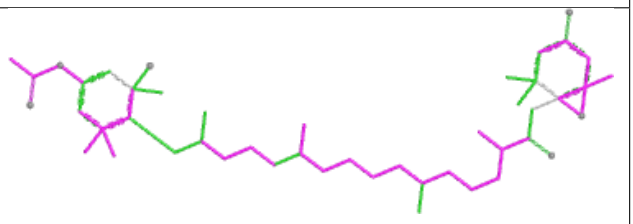


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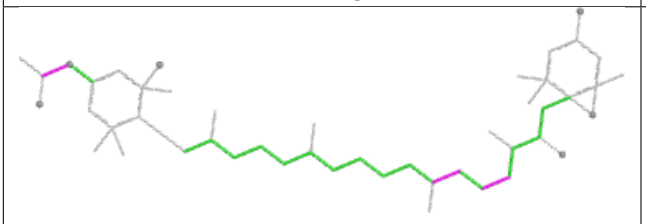
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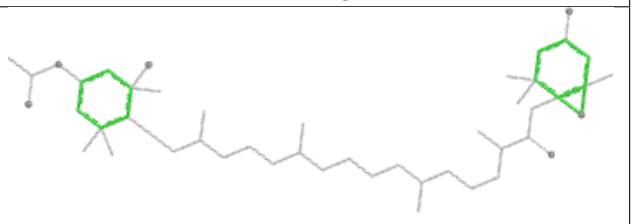
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Bond angles

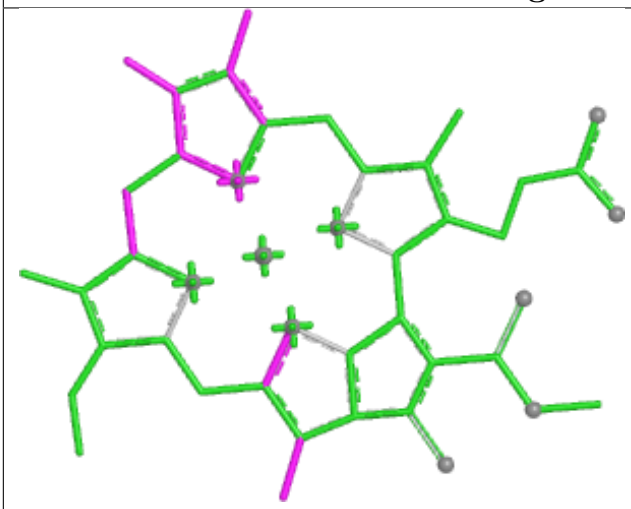


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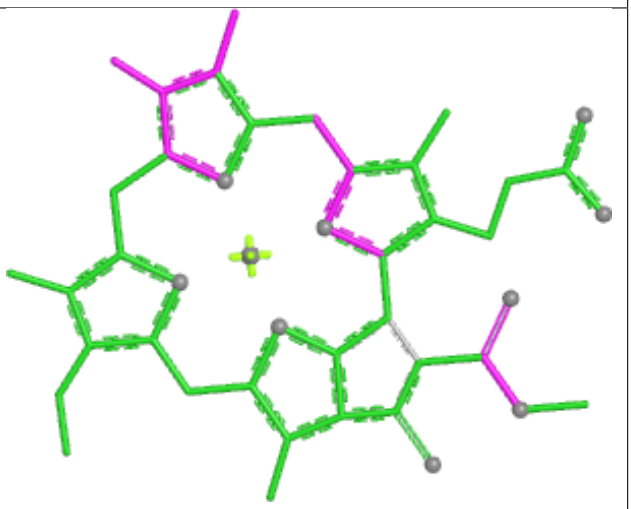


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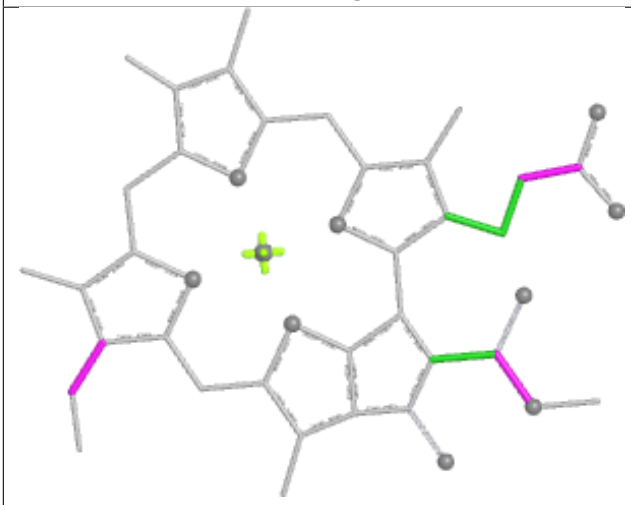
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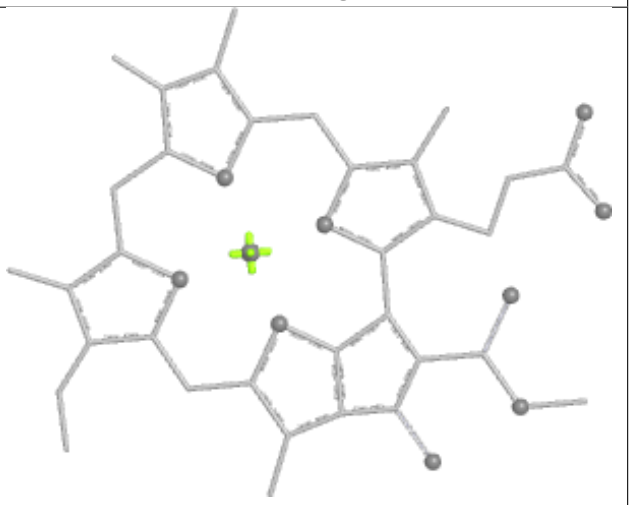
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Bond angles

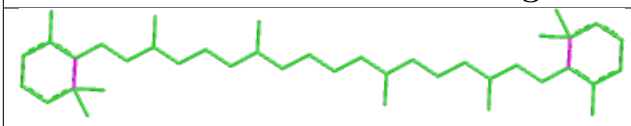


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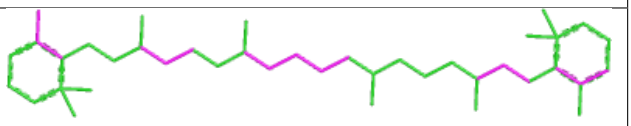


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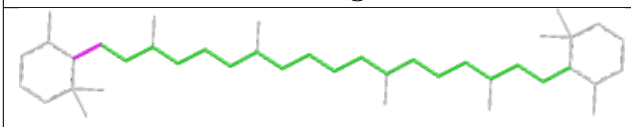
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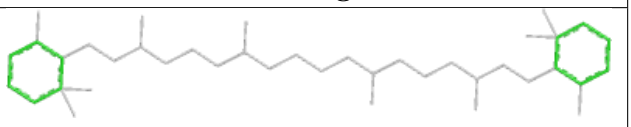
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Bond angles

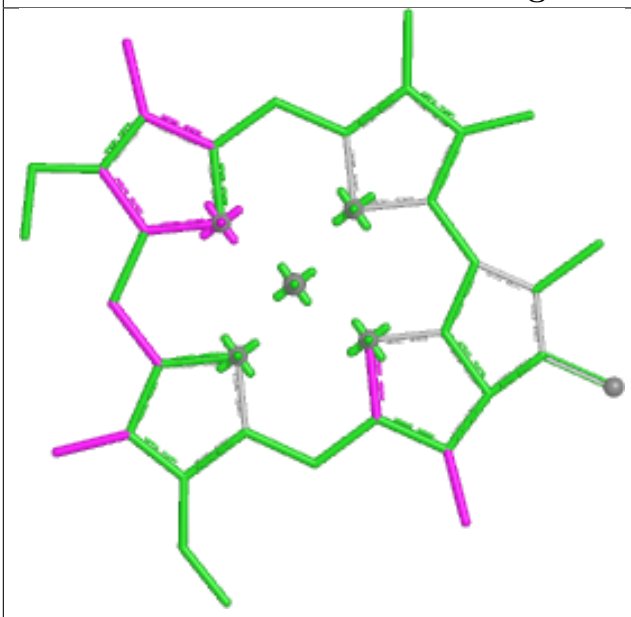


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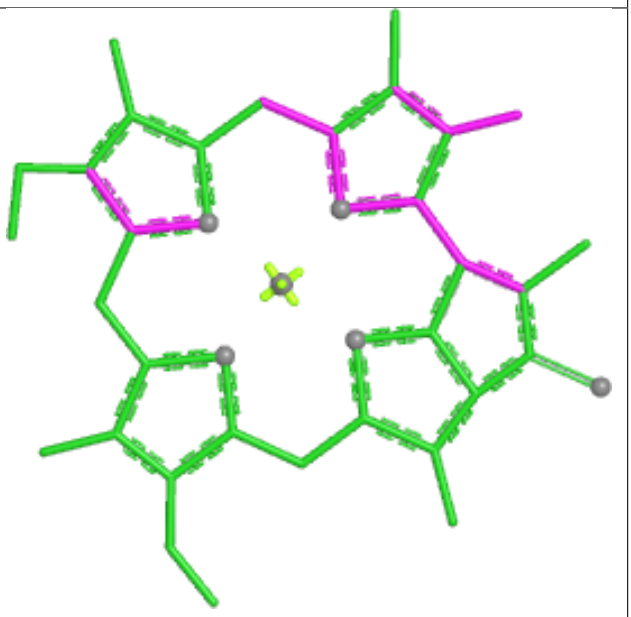


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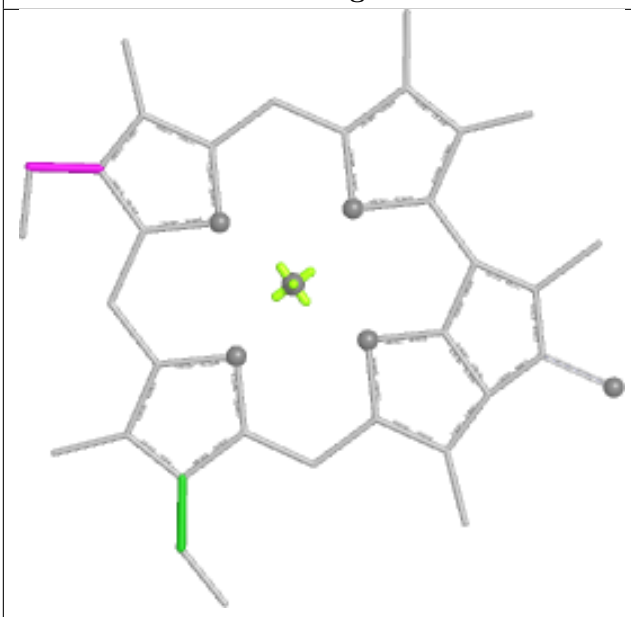
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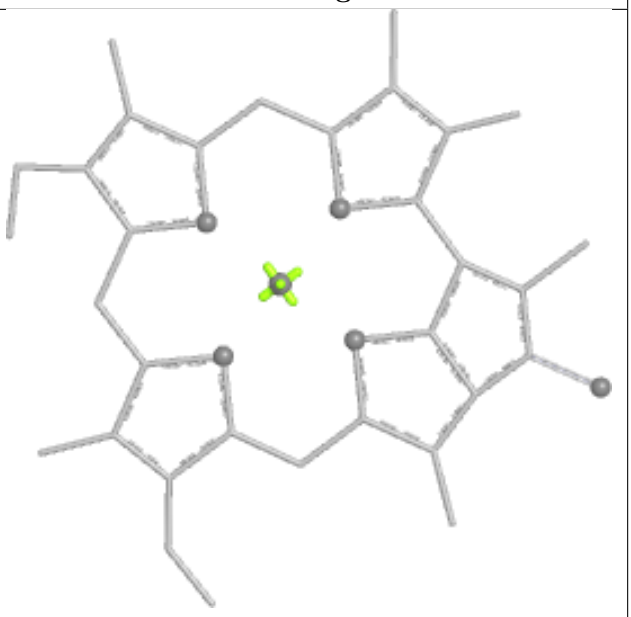
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Bond angles

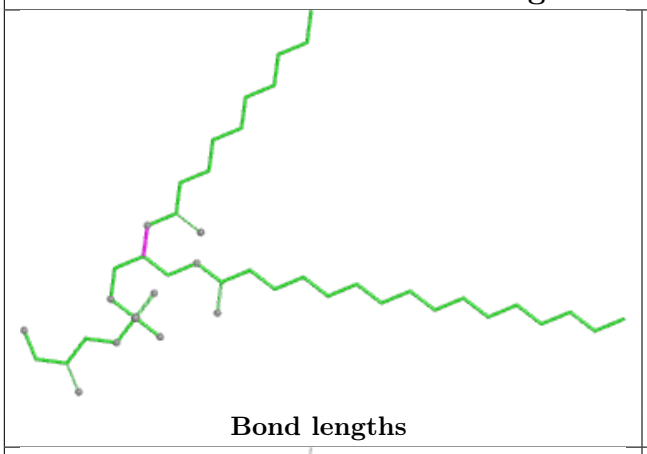


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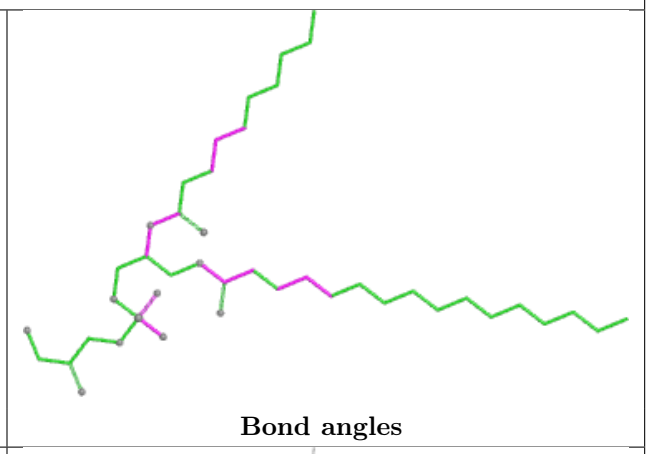


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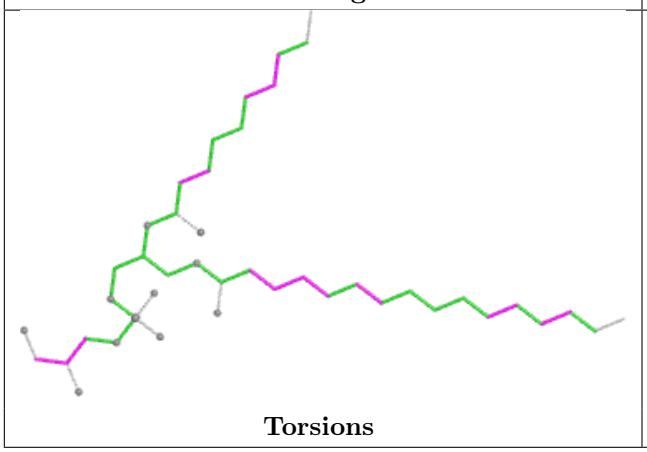
Ligand LHG a 411



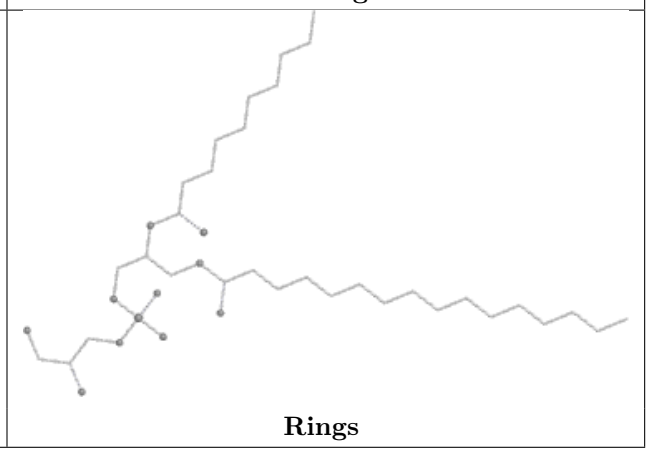
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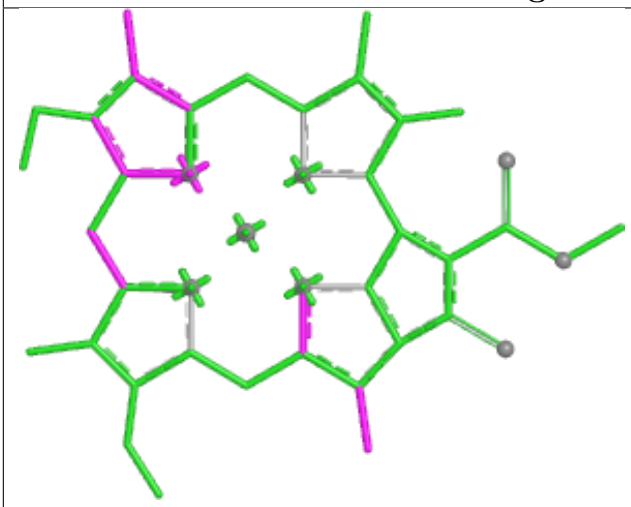


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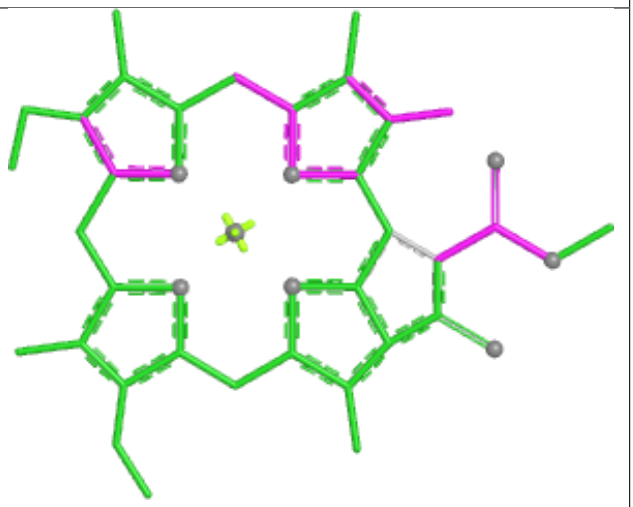


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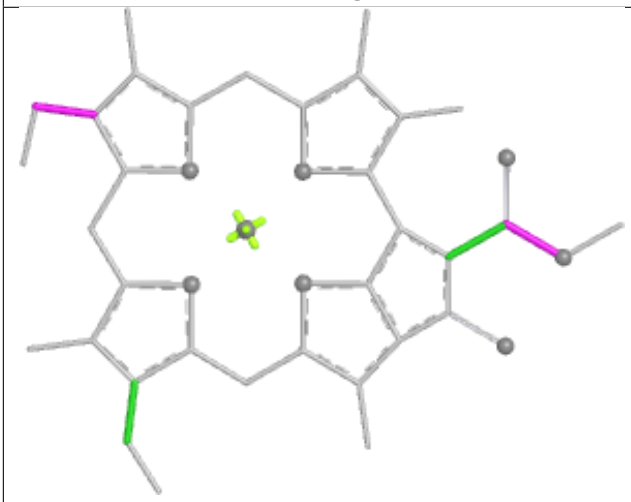
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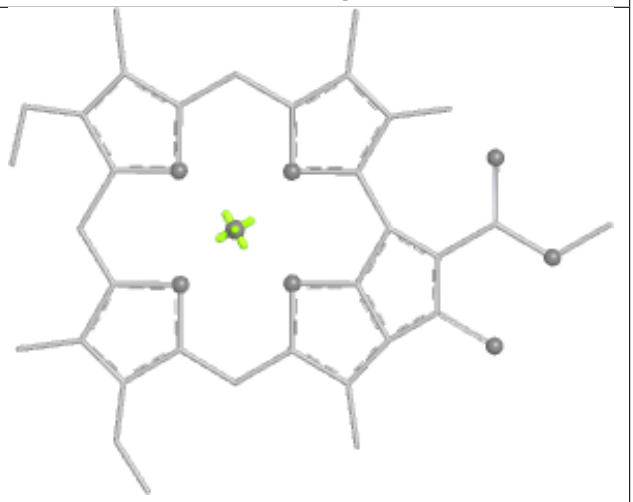
Bond lengths



Bond angles

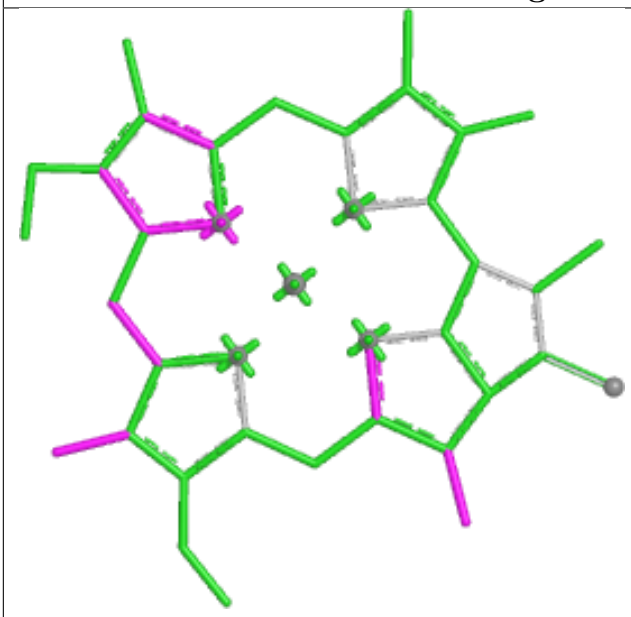


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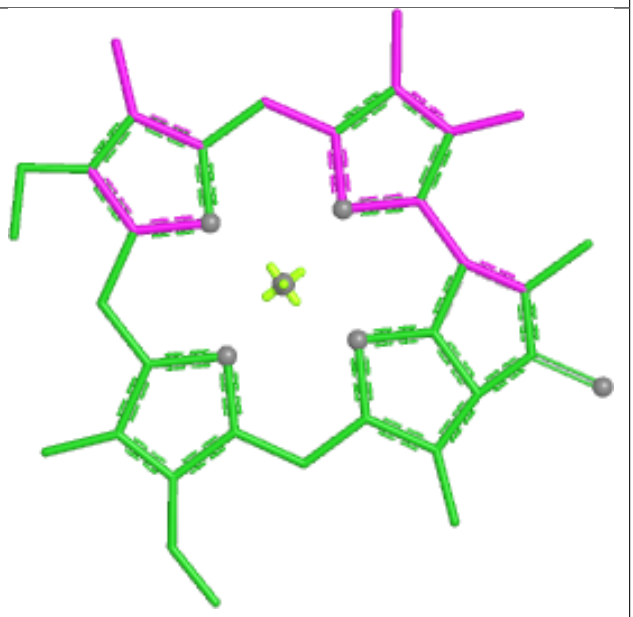


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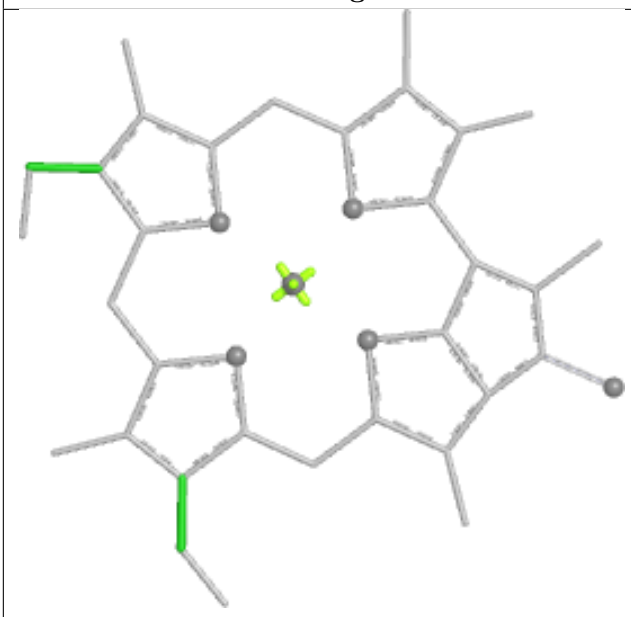
Ligand CLA 1 214



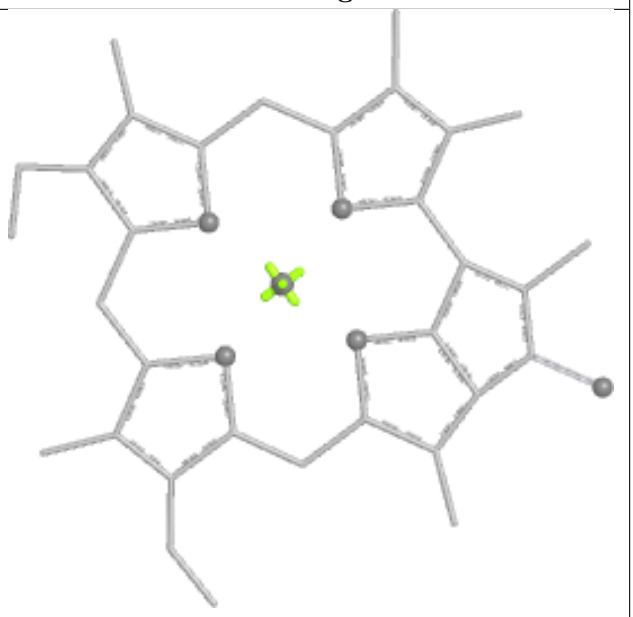
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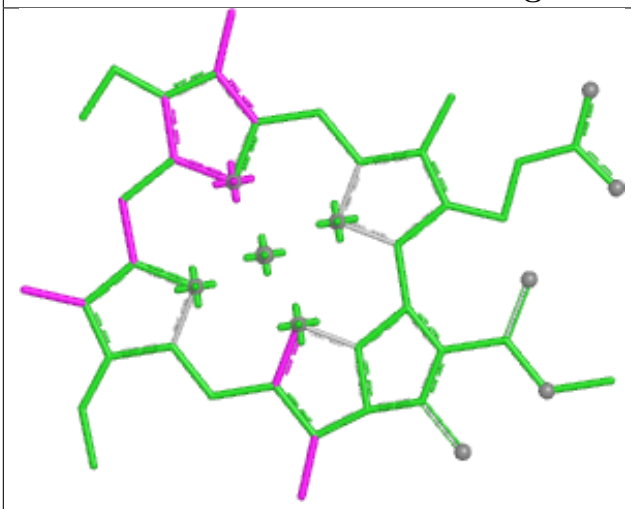


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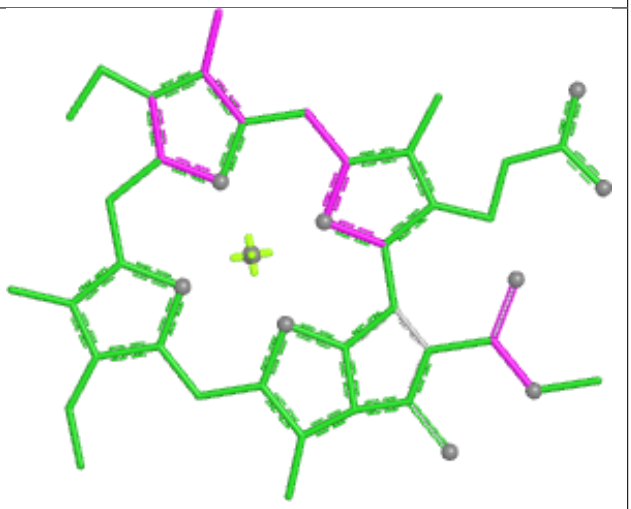


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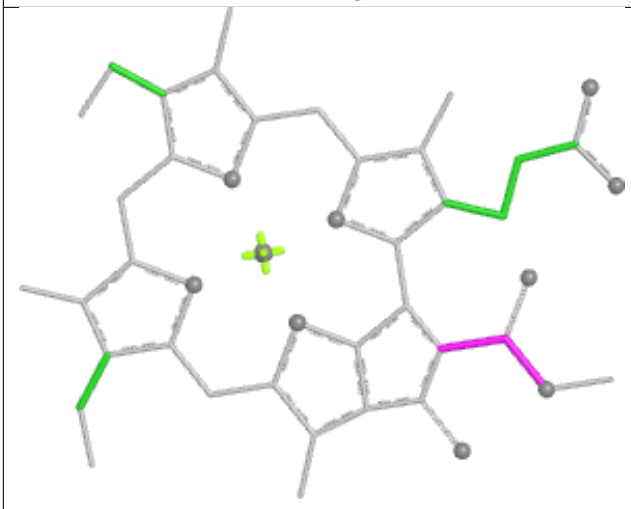
Ligand CLA C 507



Bond lengths



Bond angles

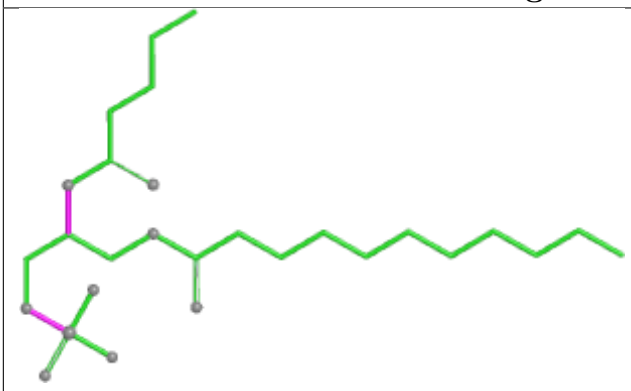


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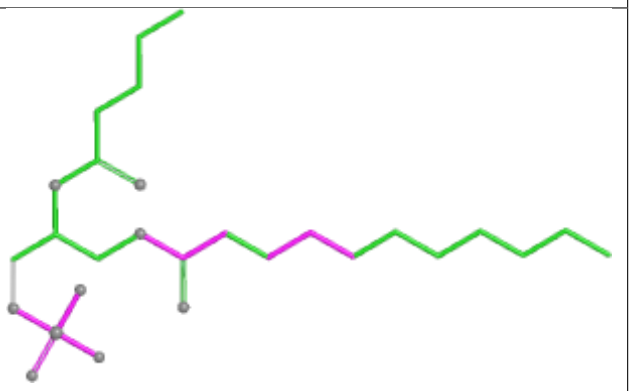


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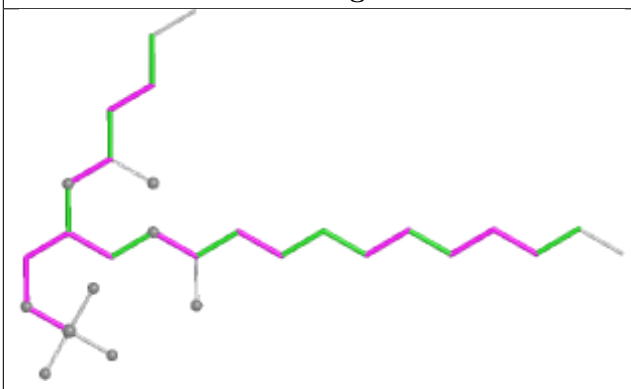
Ligand LHG d 412



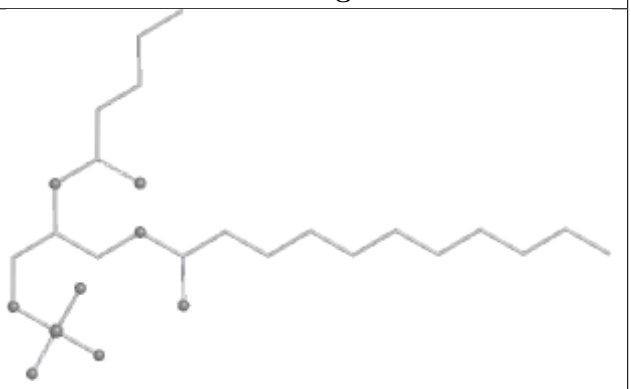
Bond lengths



Bond angles

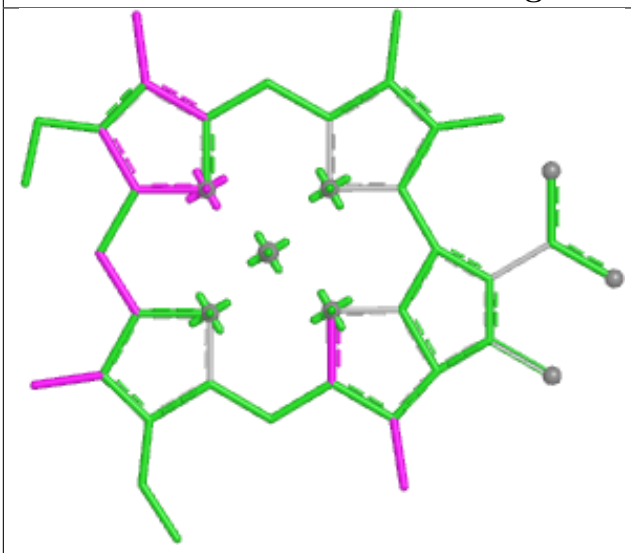


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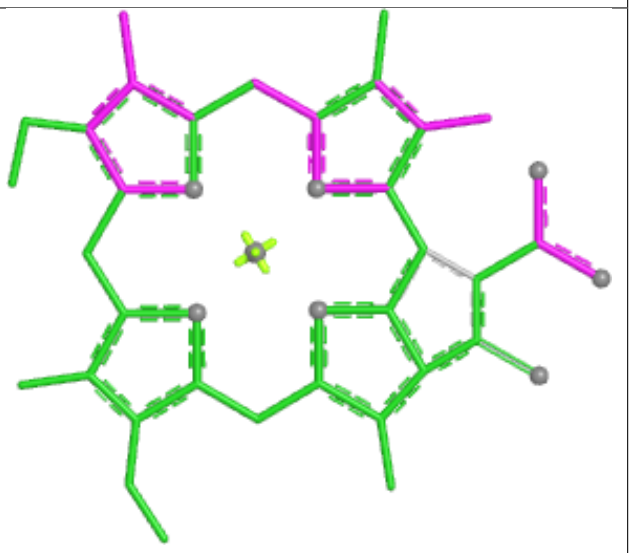


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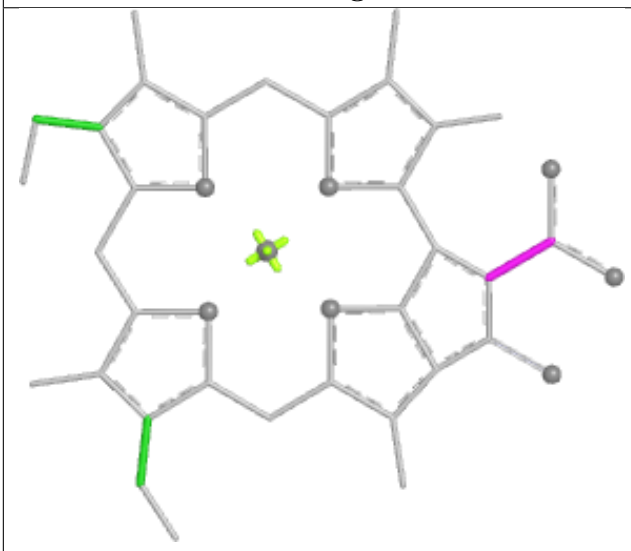
Ligand CLA P 604



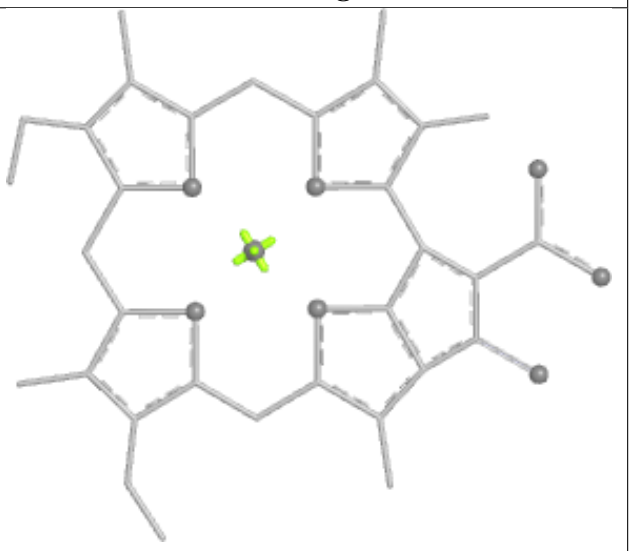
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Bond angles

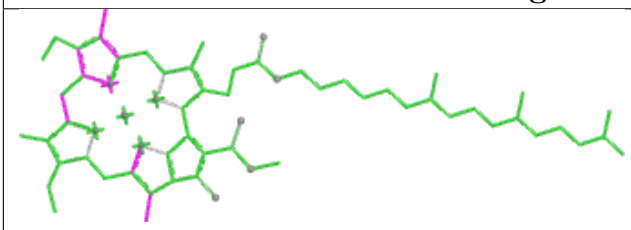


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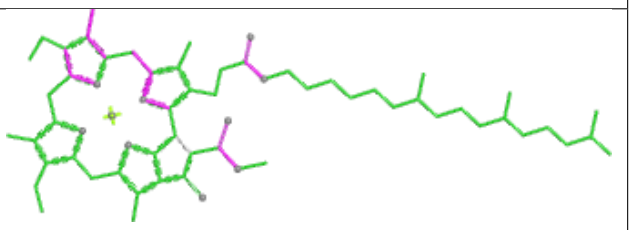


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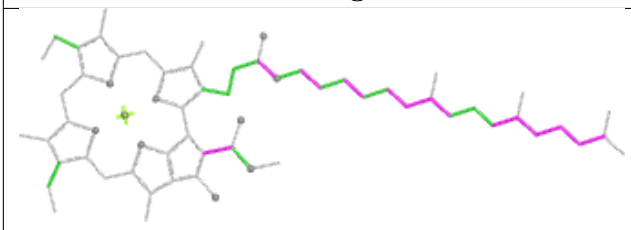
Ligand CLA c 513



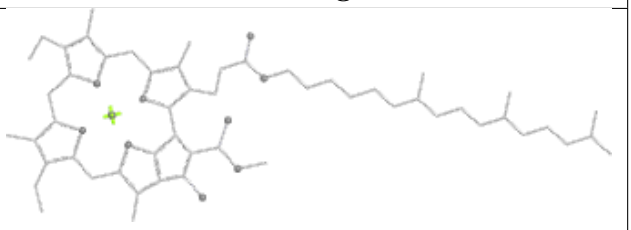
Bond lengths



Bond angles

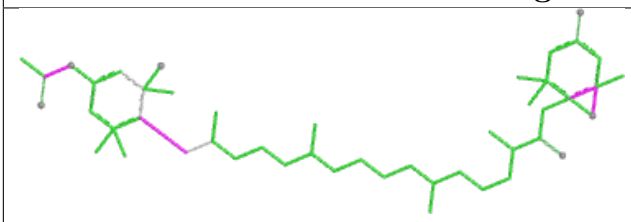


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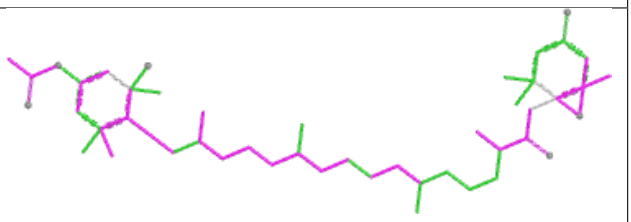


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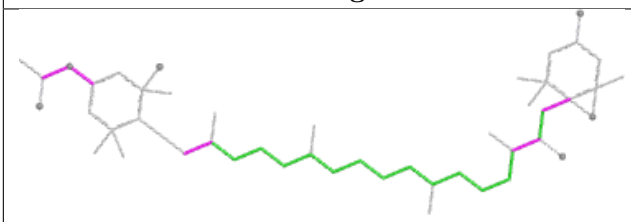
Ligand A86 0 301



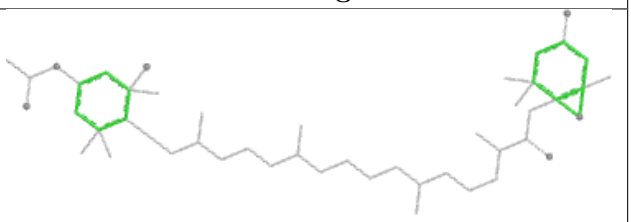
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Bond angles

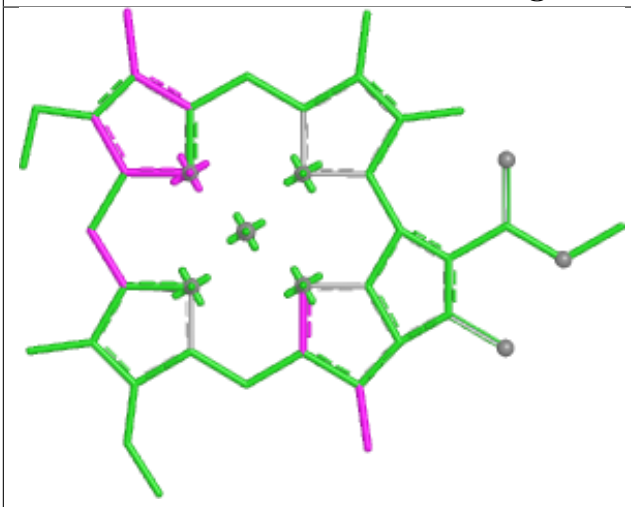


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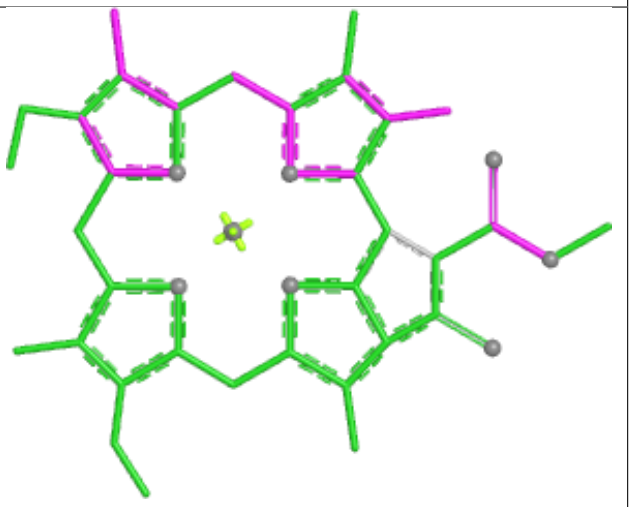


Rings

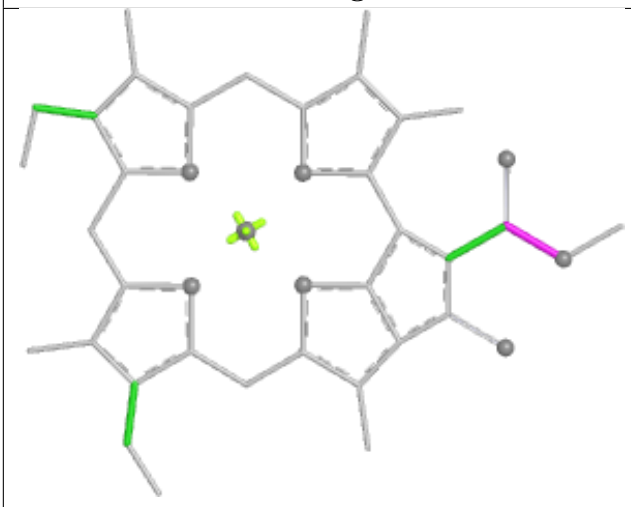
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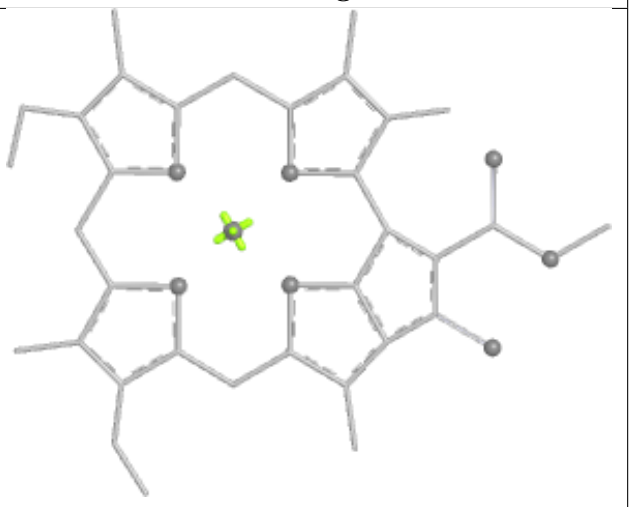
Bond lengths



Bond angles

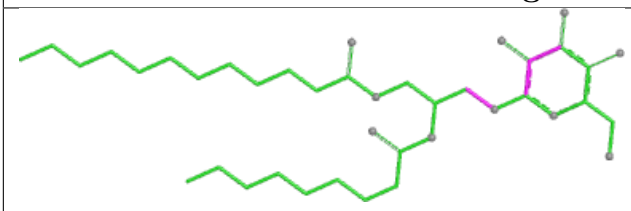


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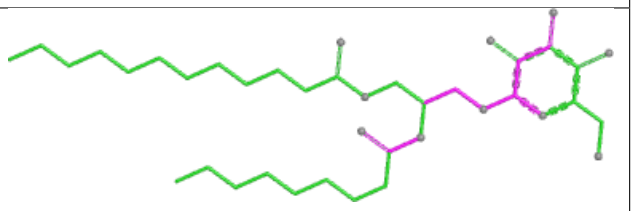


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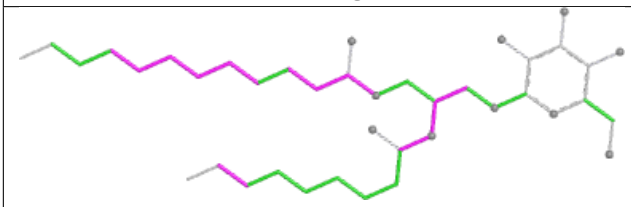
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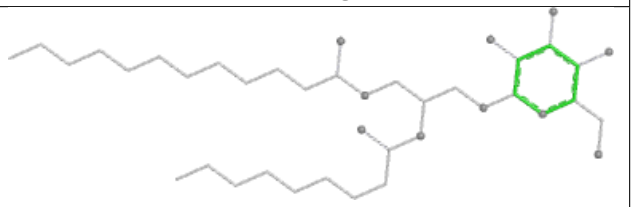
Bond lengths



Bond angles

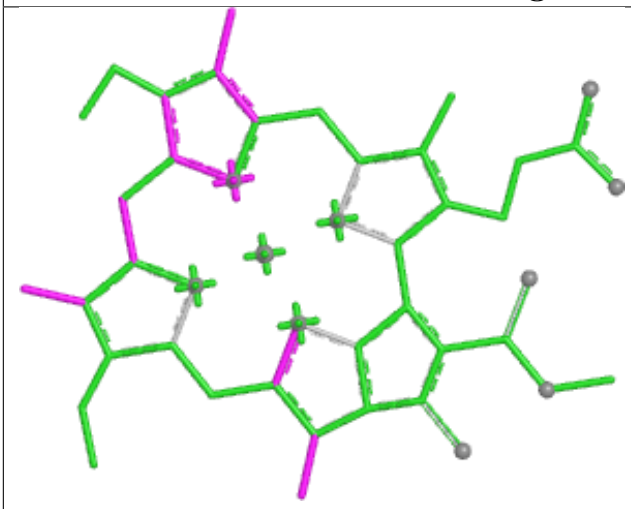


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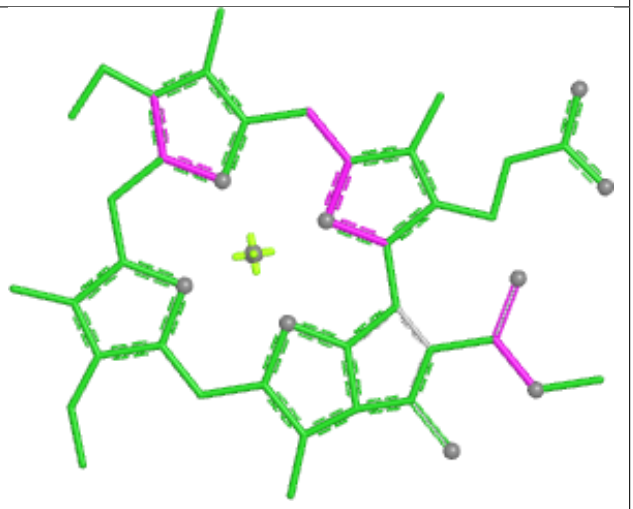


Rings

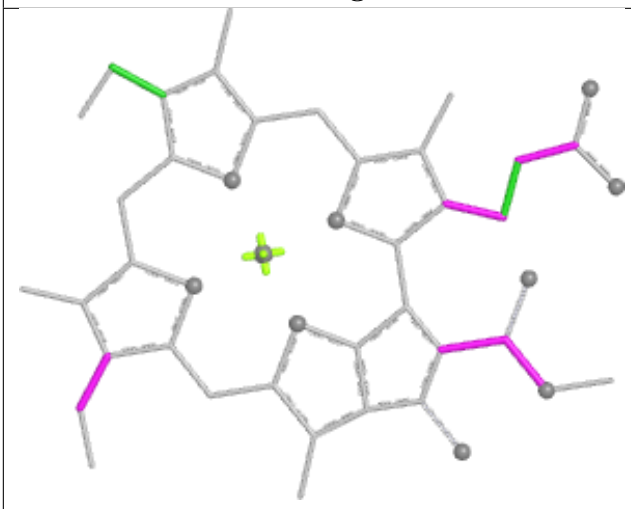
Ligand CLA 5 311



Bond lengths



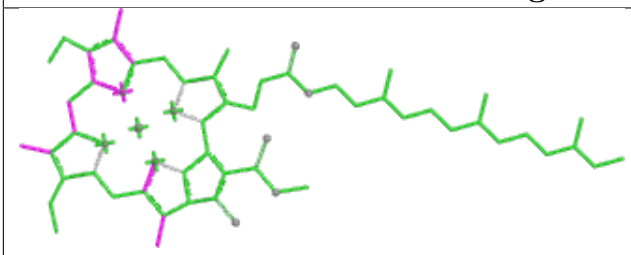
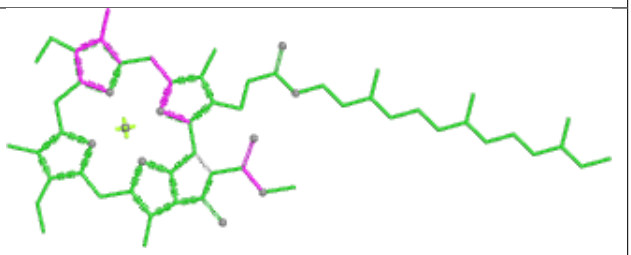
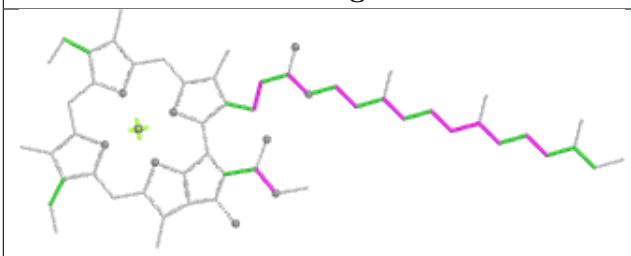
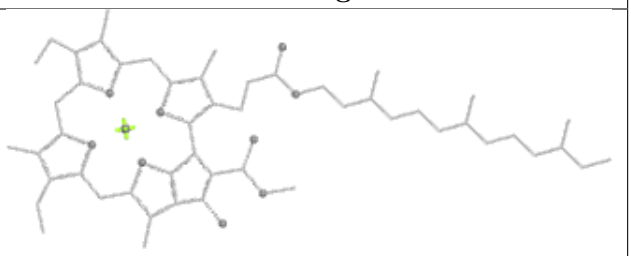
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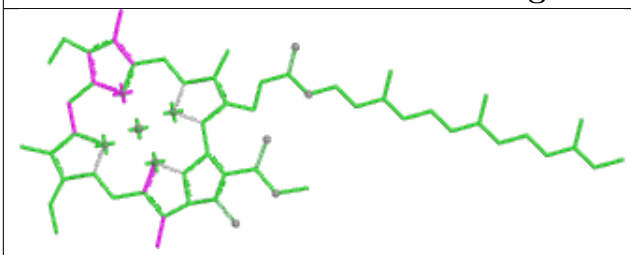
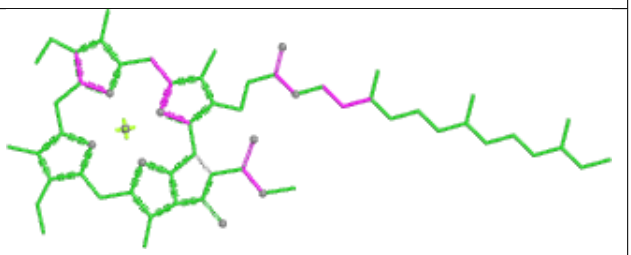
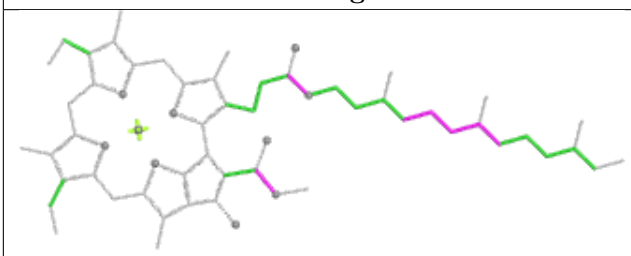
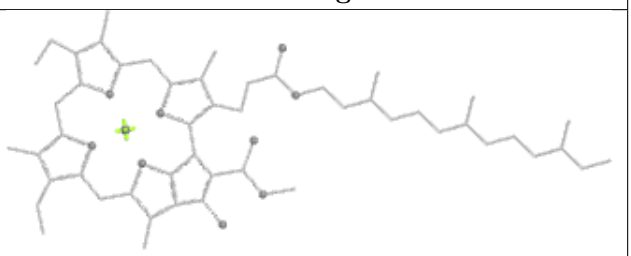


Torsions

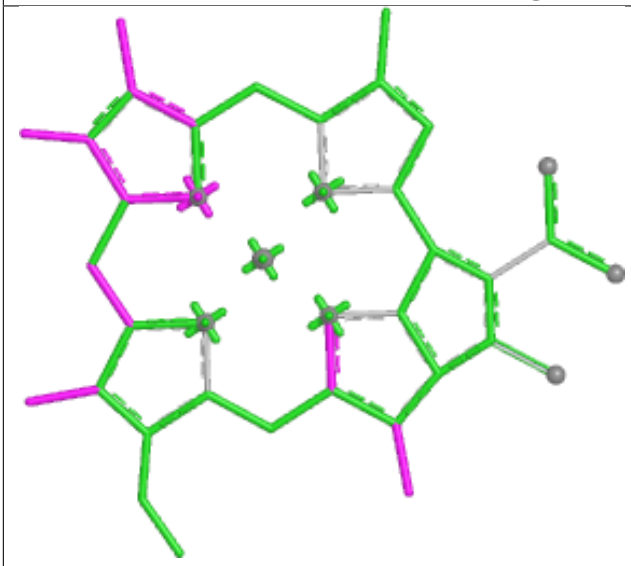


Rings

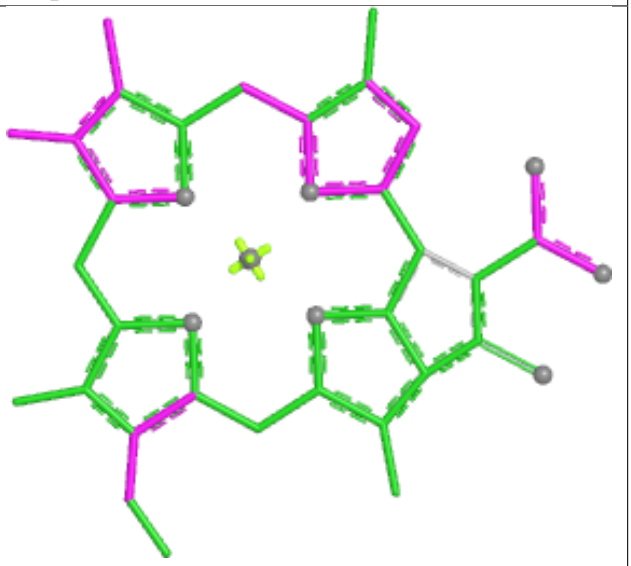
Ligand CLA 5 305	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 5 308	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

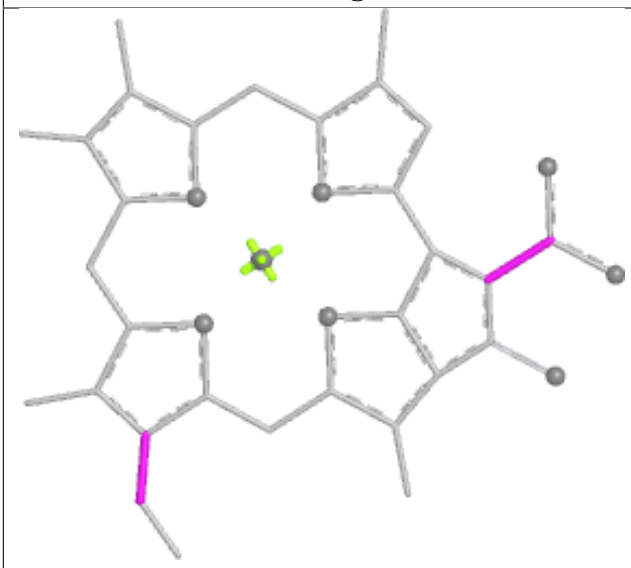
Ligand CLA p 608



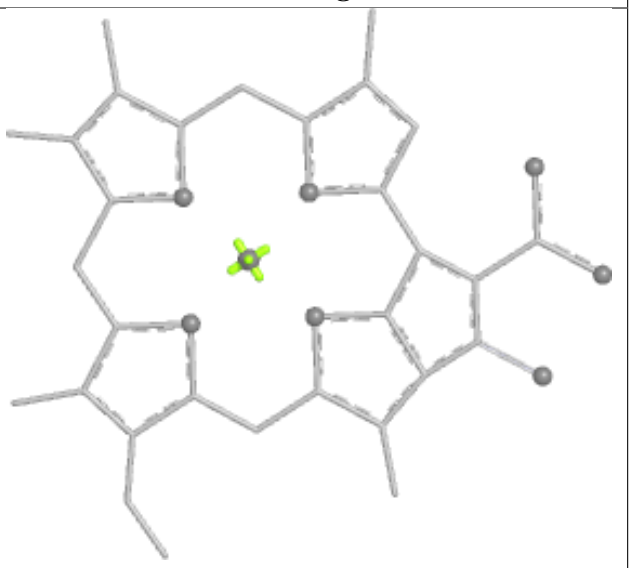
Bond lengths



Bond angles

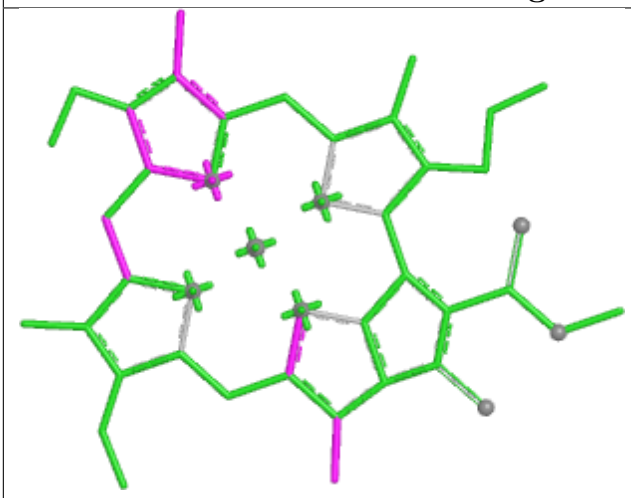


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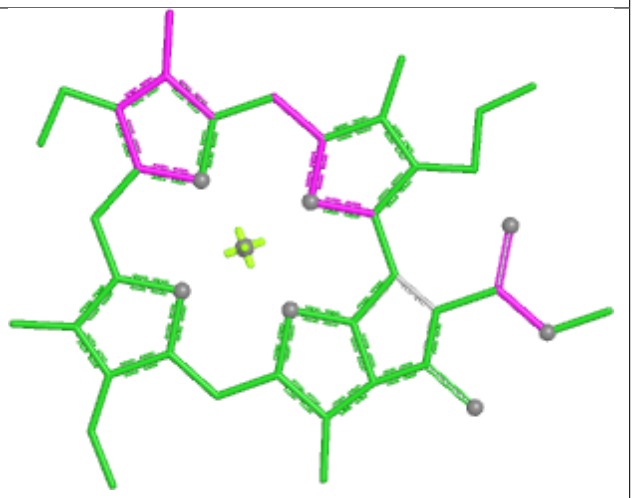


Rings

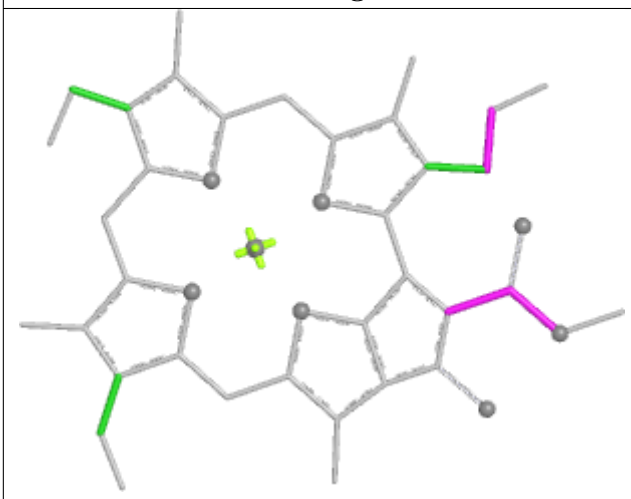
Ligand CLA 2 311



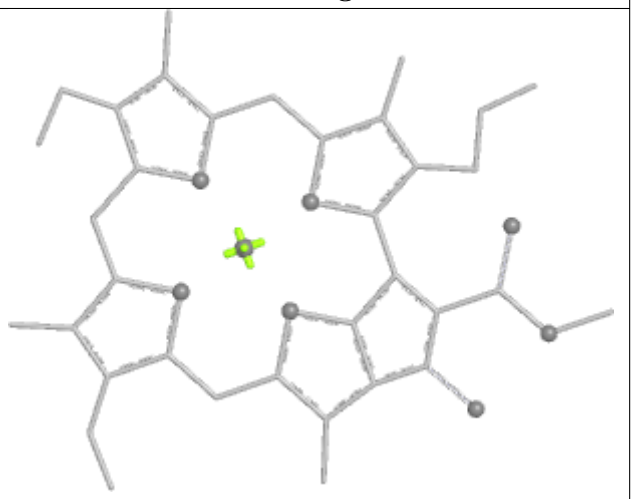
Bond lengths



Bond angles

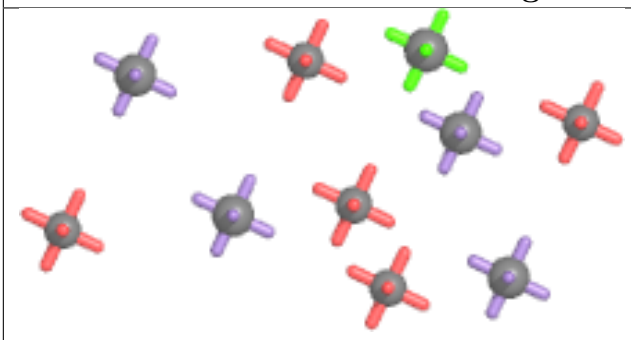


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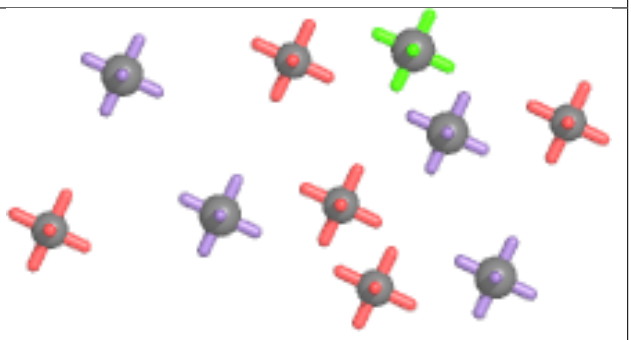


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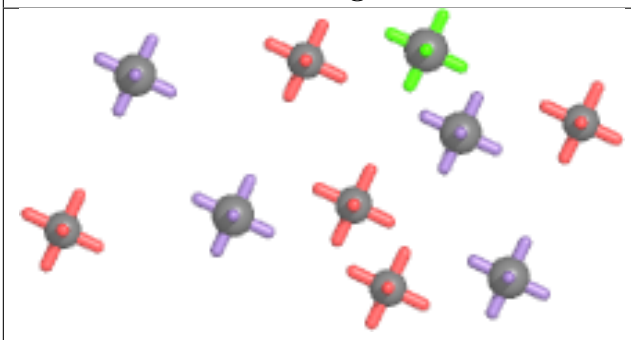
Ligand OEX A 401



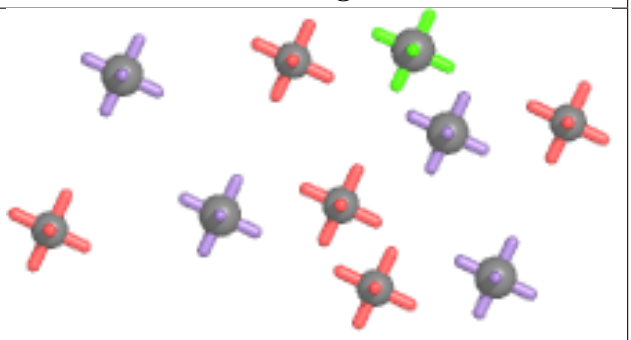
Bond lengths



Bond angles

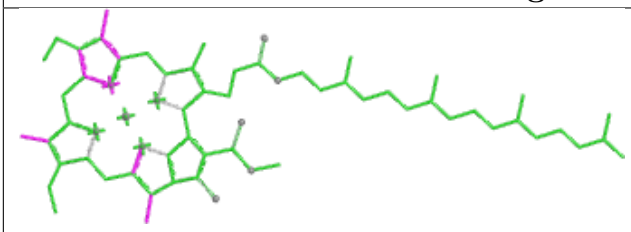


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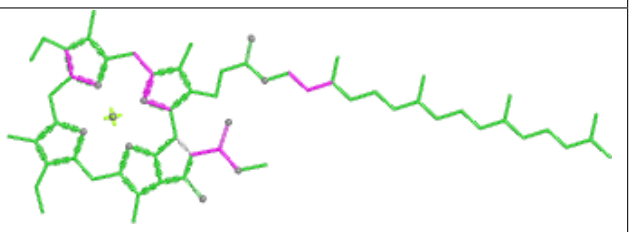


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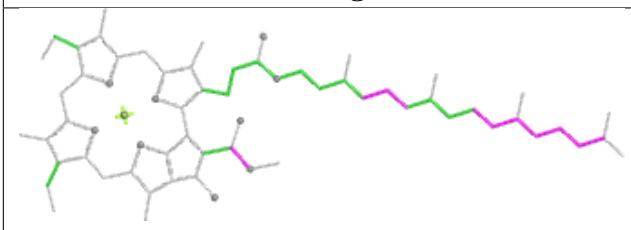
Ligand CLA b 505



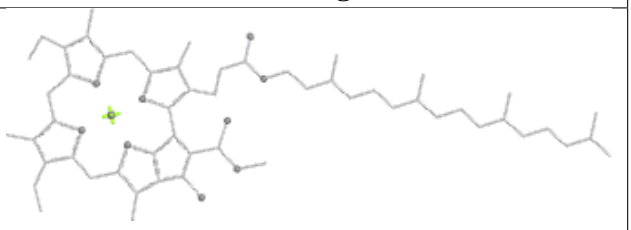
Bond lengths



Bond angles

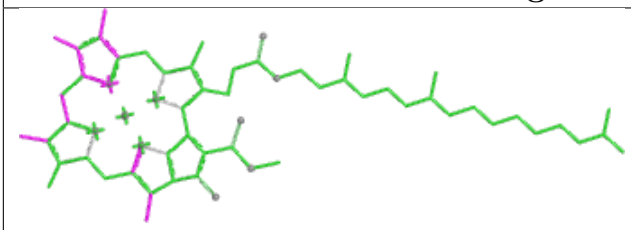


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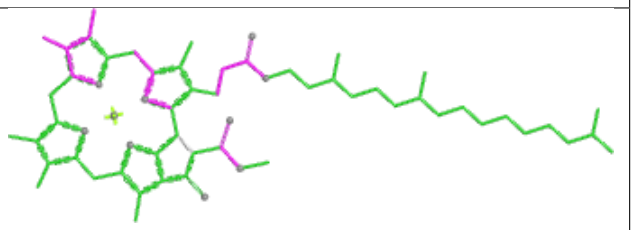


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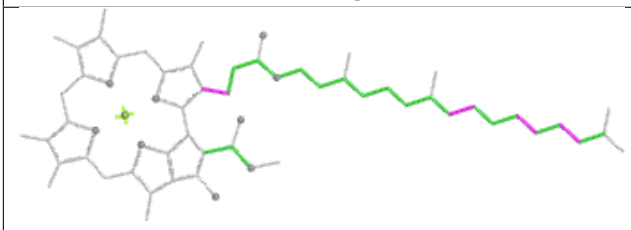
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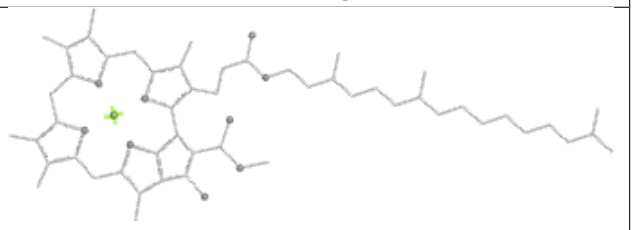
Bond lengths



Bond angles



Torsions

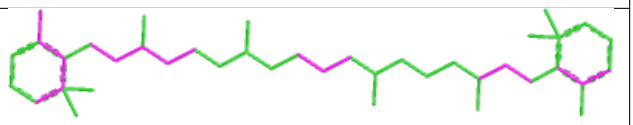


Rings

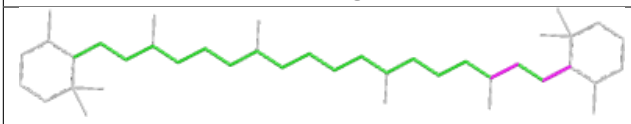
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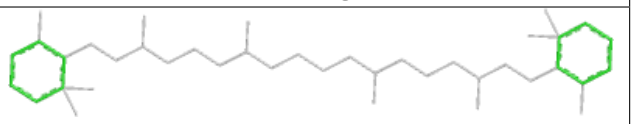
Bond lengths



Bond angles

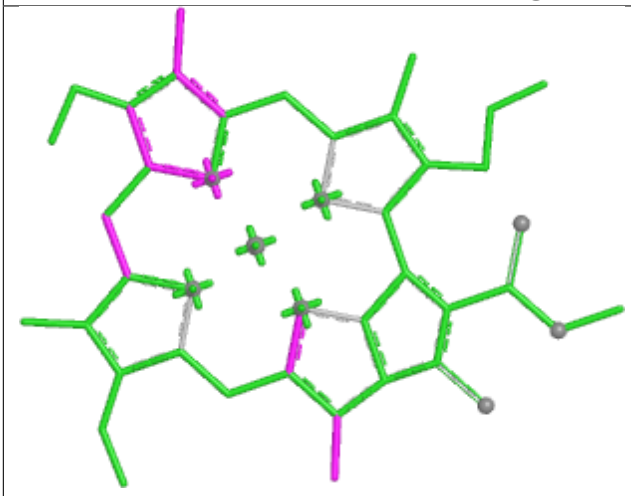


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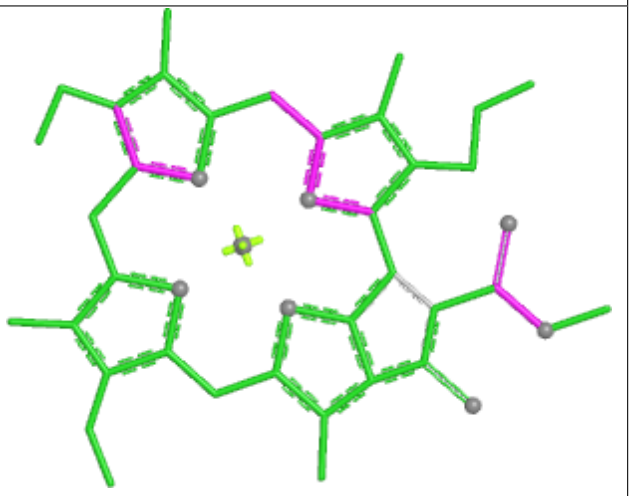


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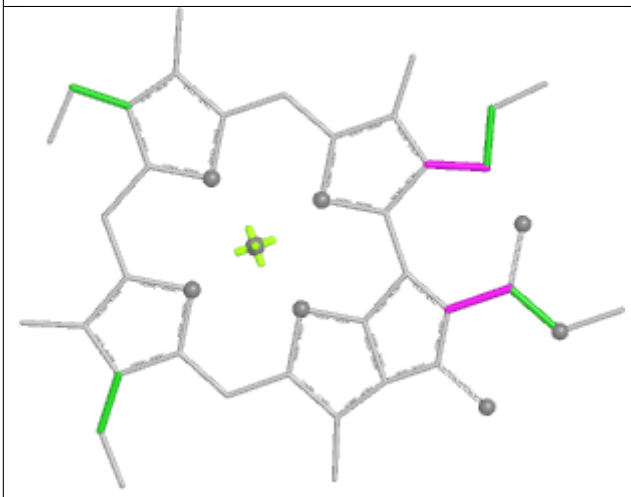
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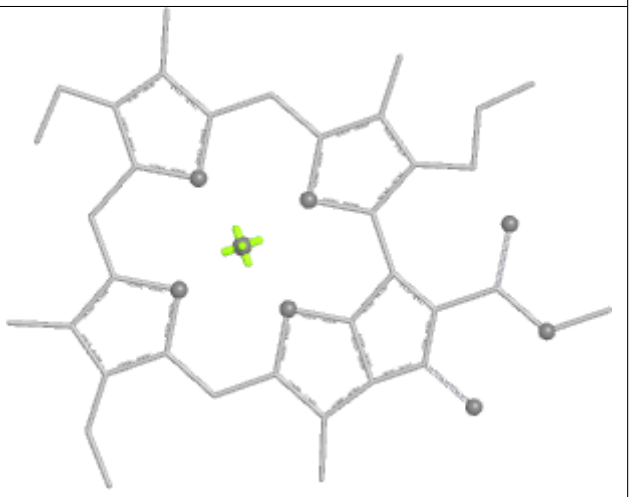
Bond lengths



Bond angles

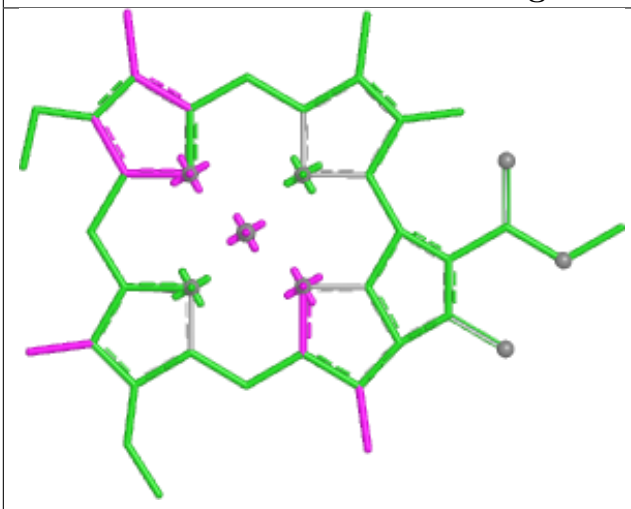


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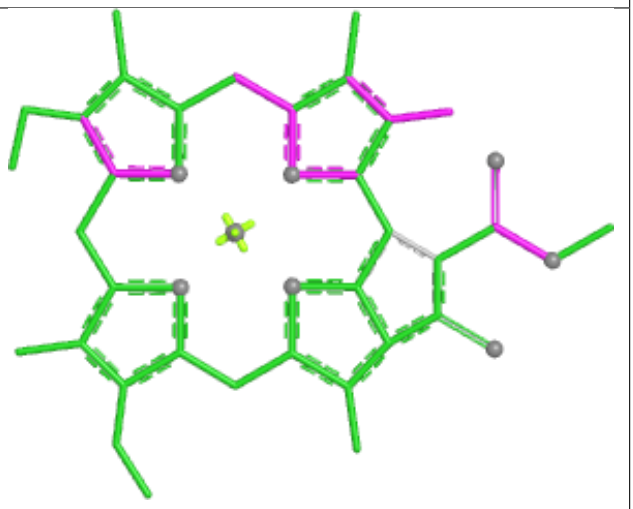


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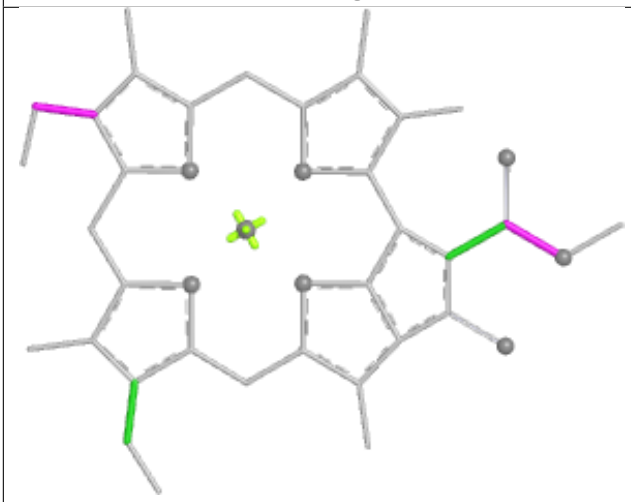
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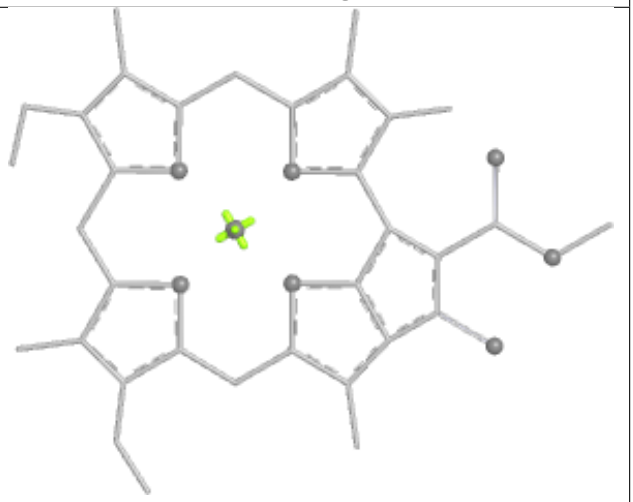
Bond lengths



Bond angles

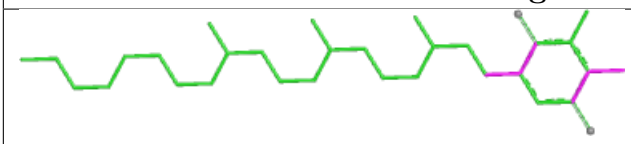


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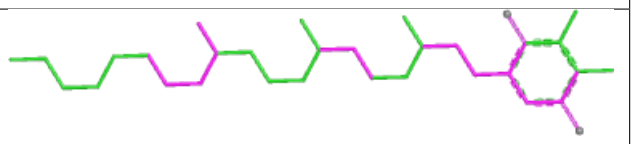


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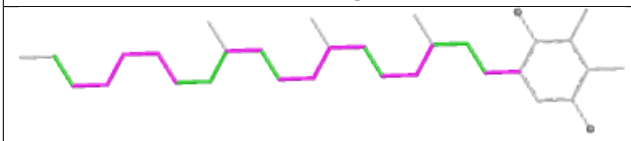
Ligand PL9 A 410



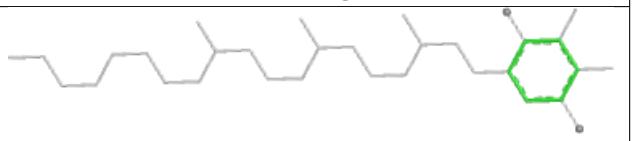
Bond lengths



Bond angles

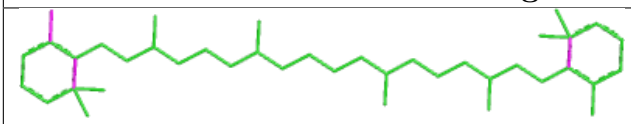


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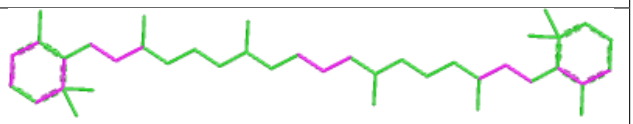


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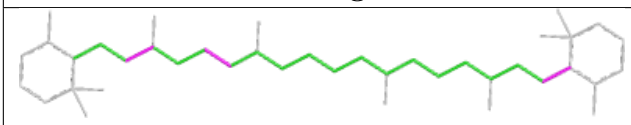
Ligand BCR H 101



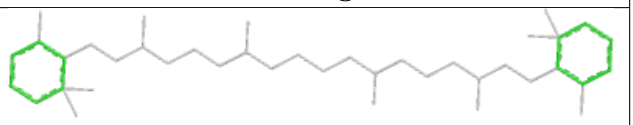
Bond lengths



Bond angles

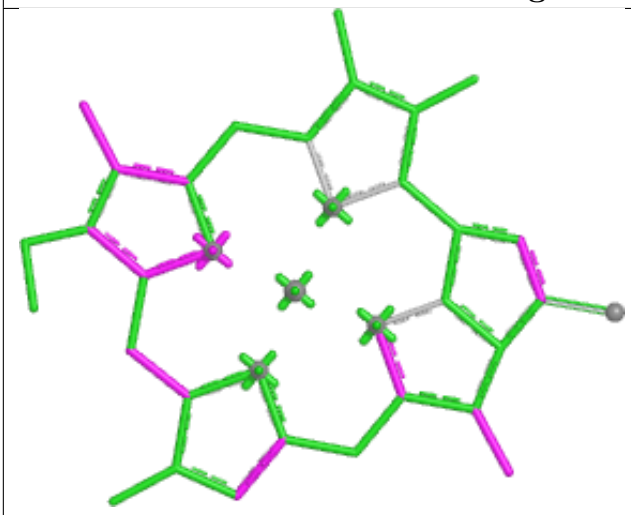


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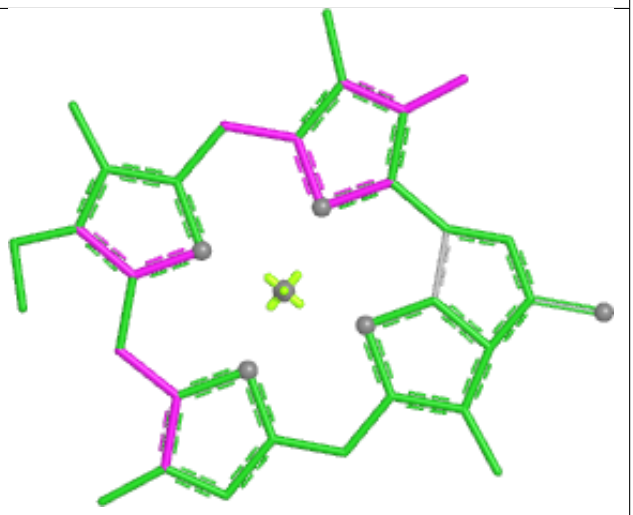


Rings

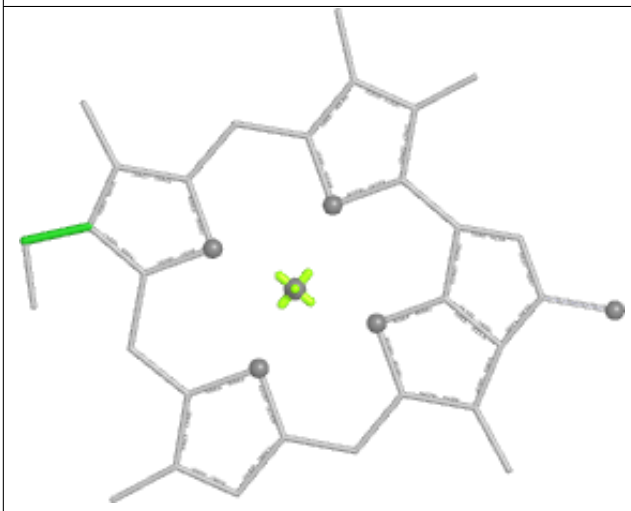
Ligand CLA 3 310



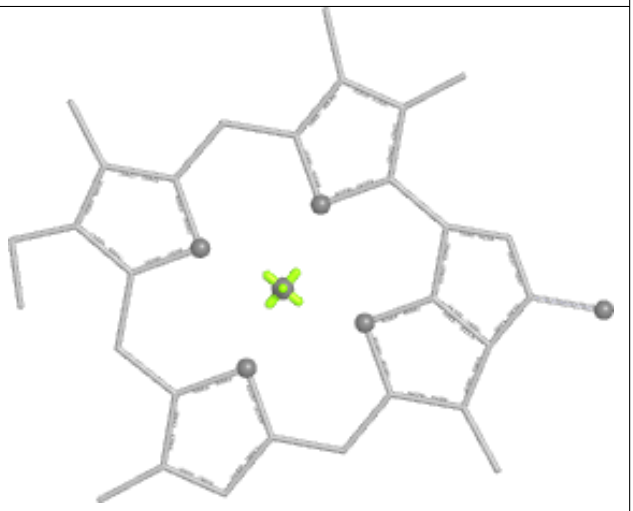
Bond lengths



Bond angles

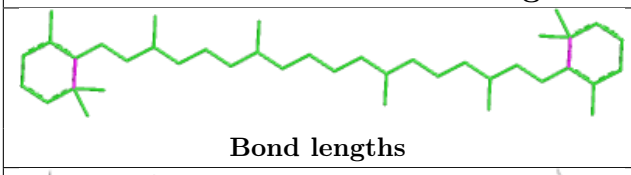


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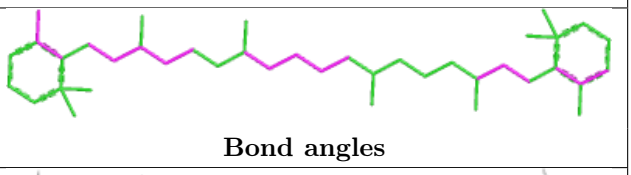


Rings

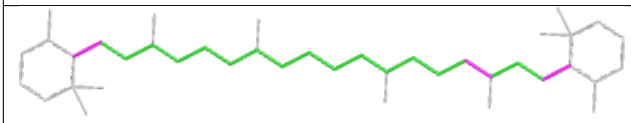
Ligand BCR B 517



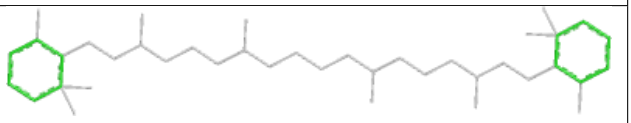
Bond lengths



Bond angles

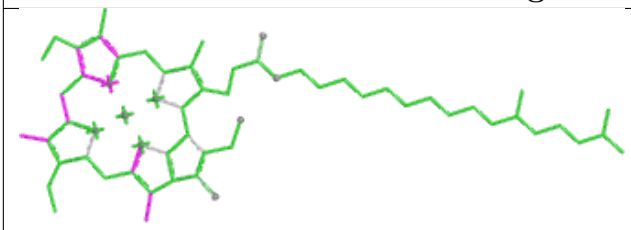


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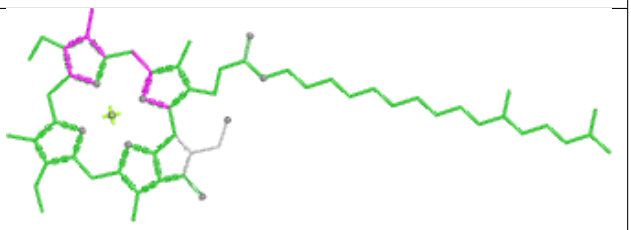


Rings

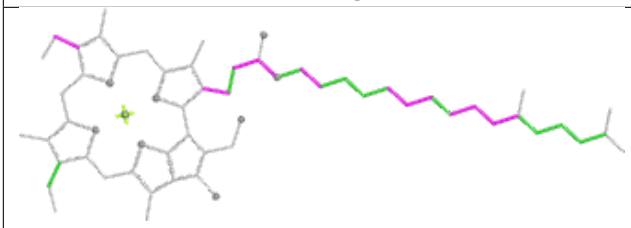
Ligand CLA b 503



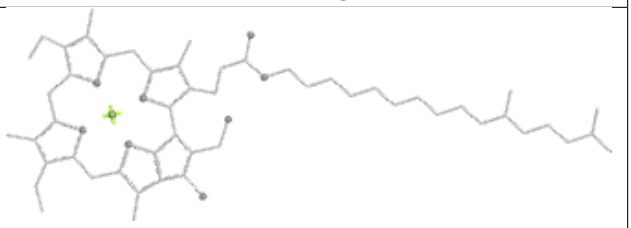
Bond lengths



Bond angles

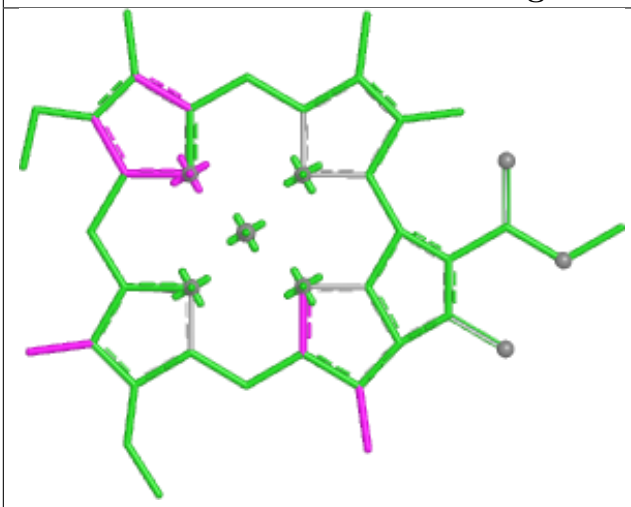


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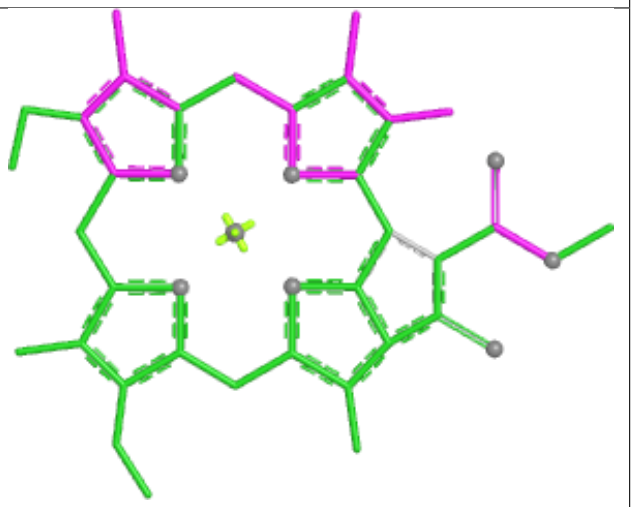


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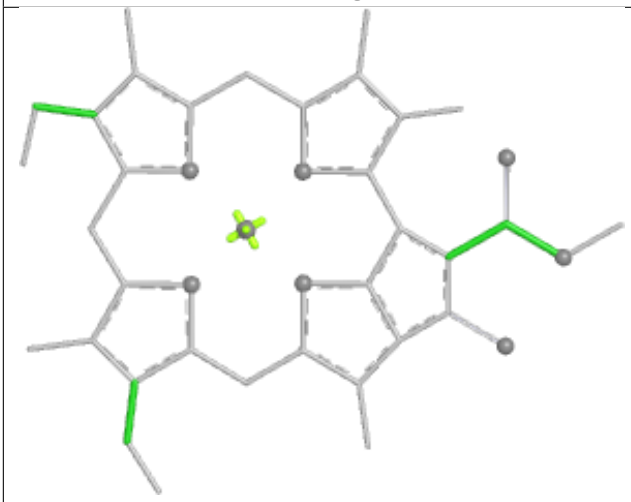
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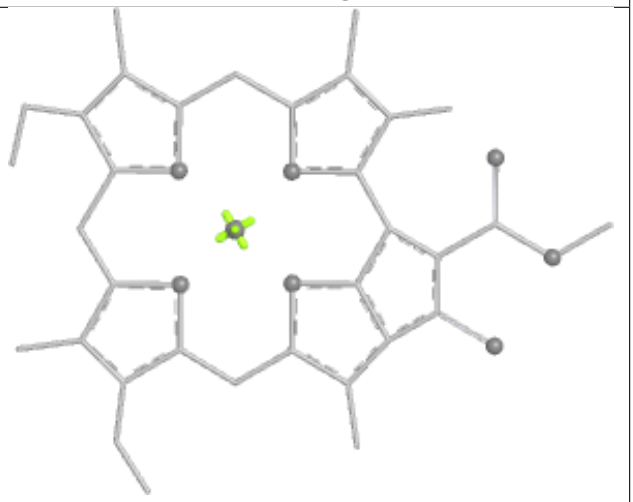
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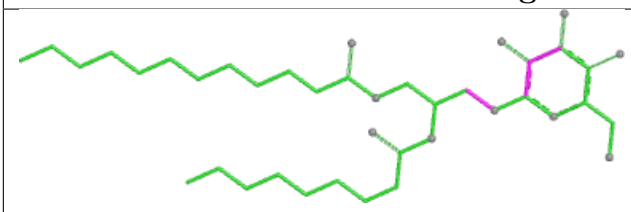


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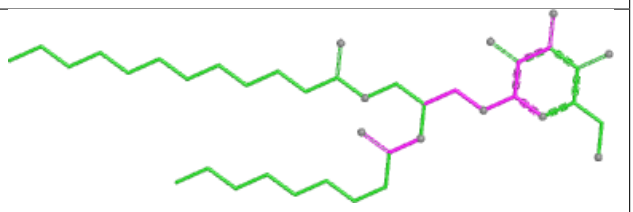


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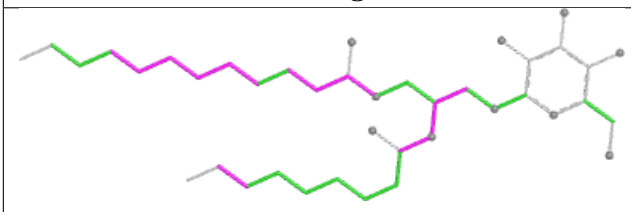
Ligand LMG D 410



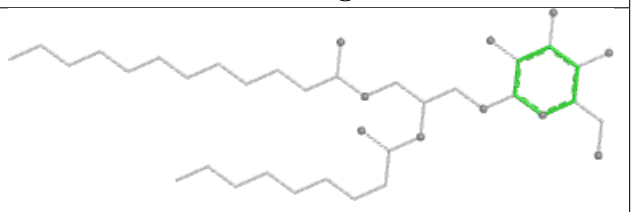
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Bond angles

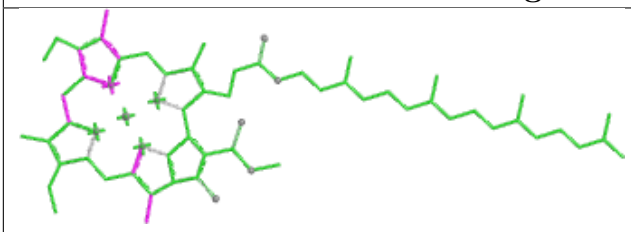


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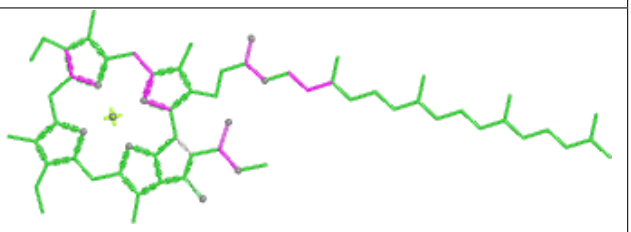


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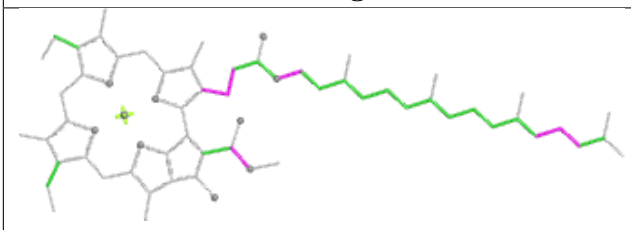
Ligand CLA B 508



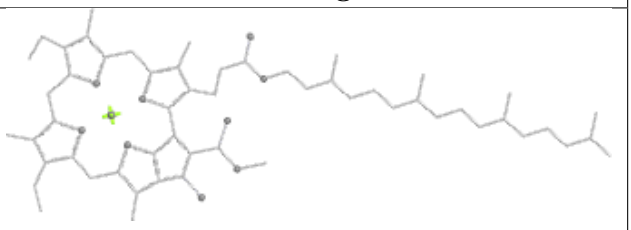
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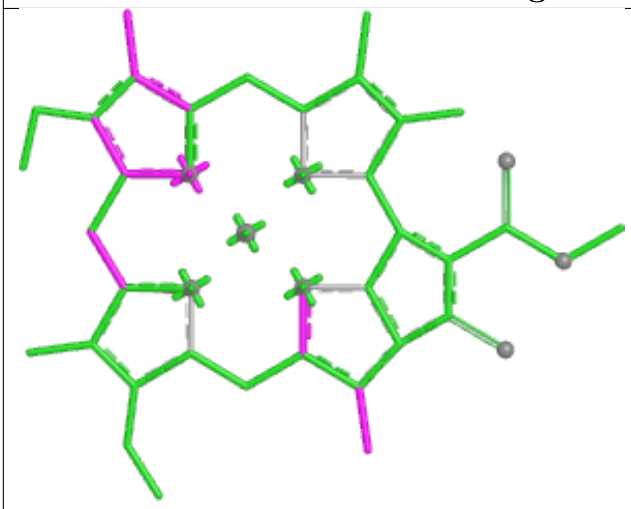


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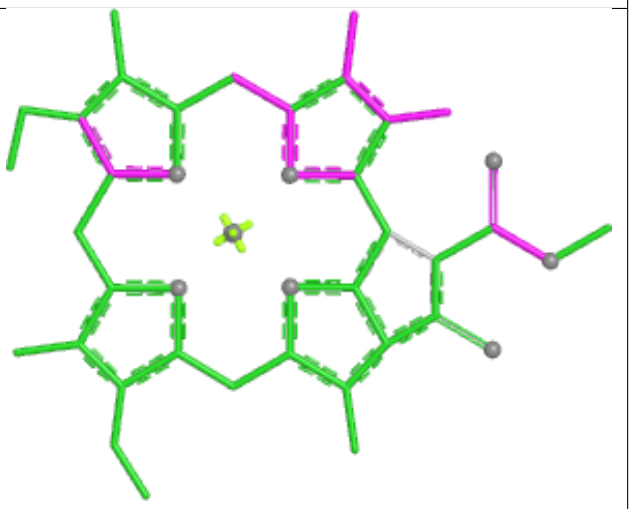


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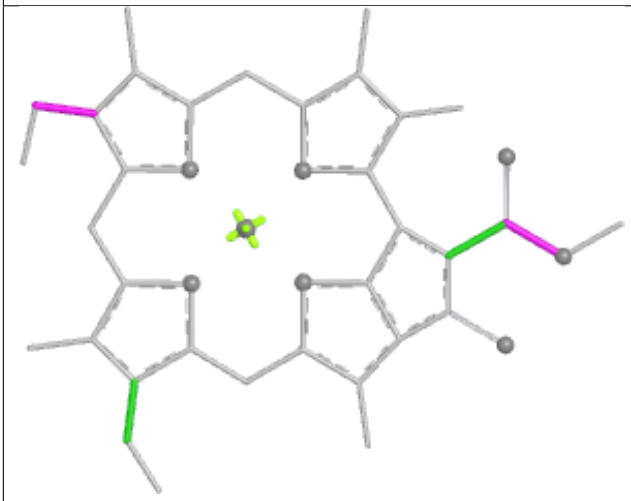
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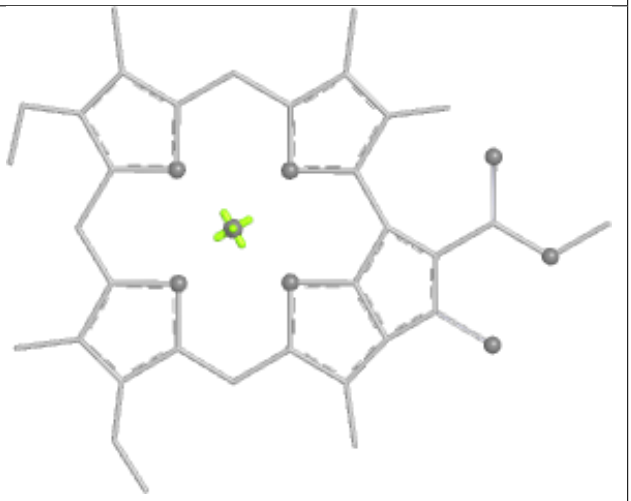
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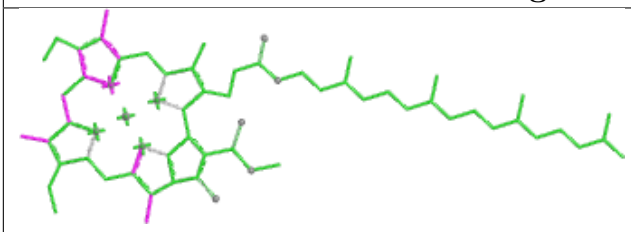


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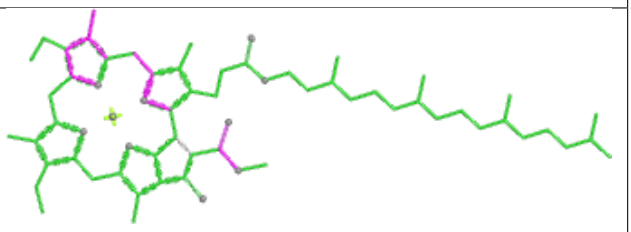


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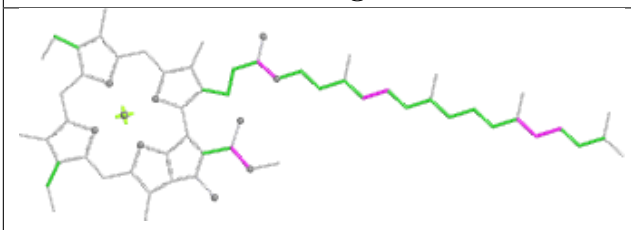
Ligand CLA c 512



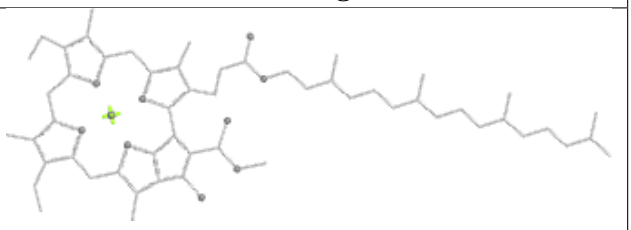
Bond lengths



Bond angles

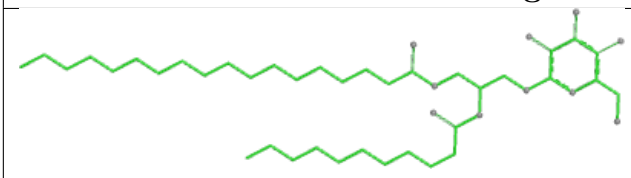


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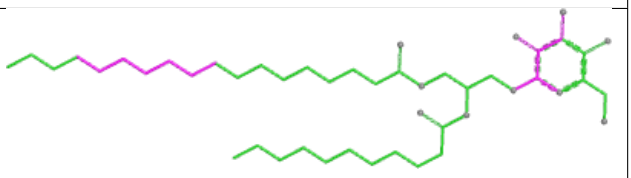


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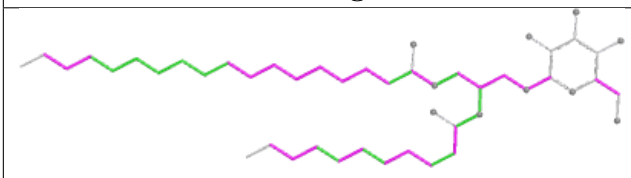
Ligand LMG 0 315



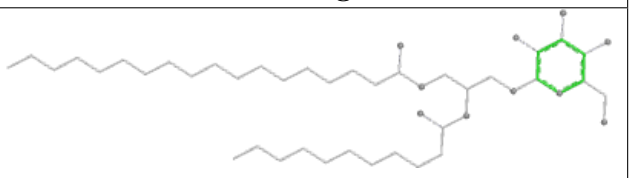
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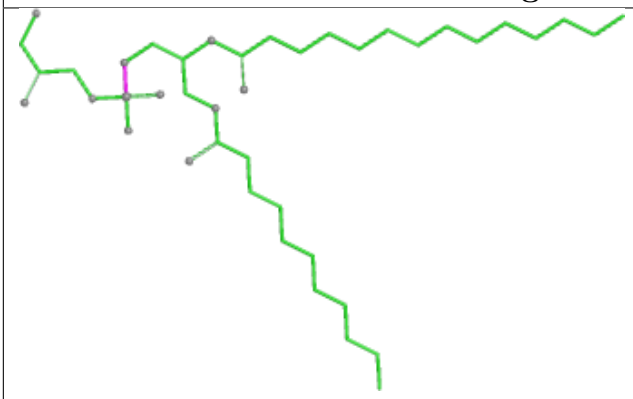


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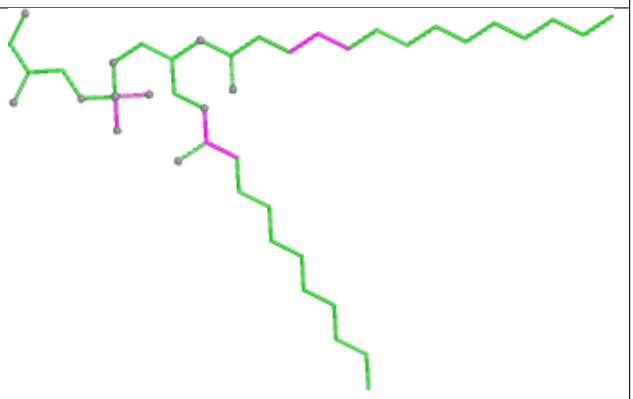


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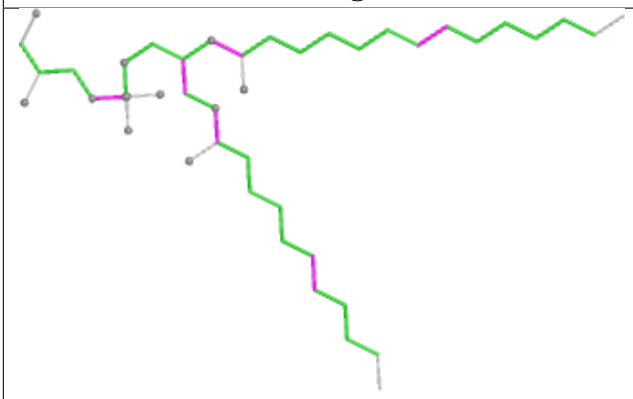
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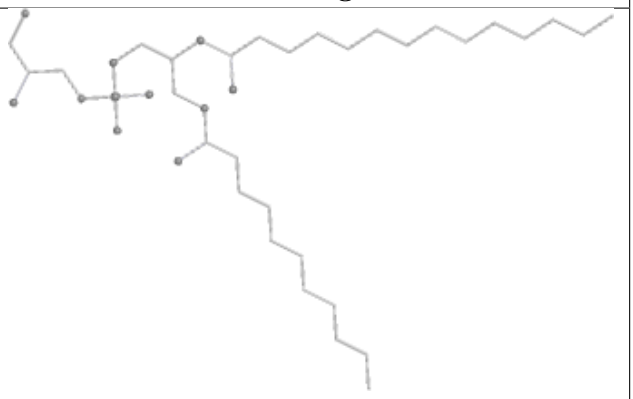
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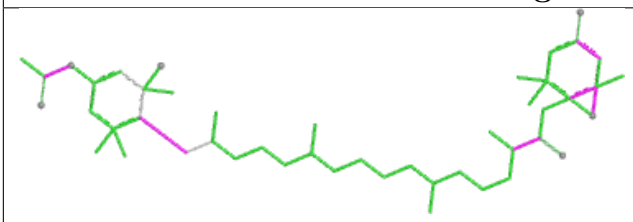


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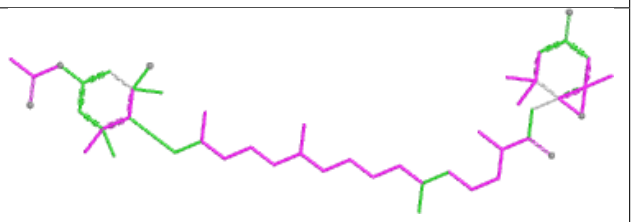


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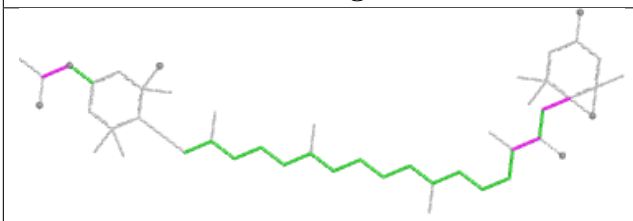
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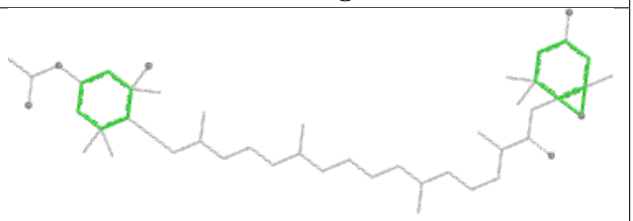
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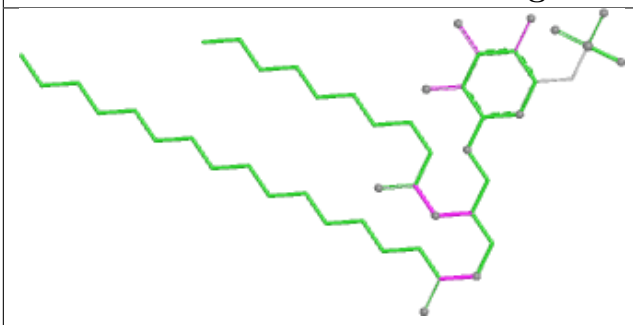


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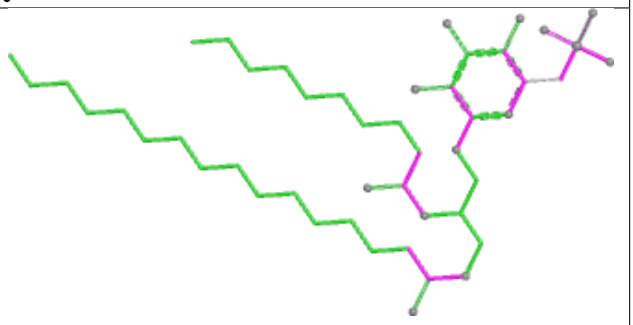


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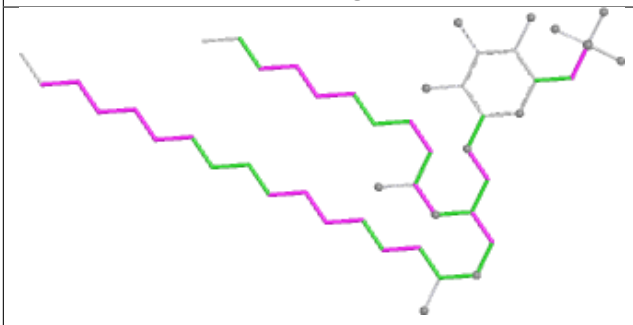
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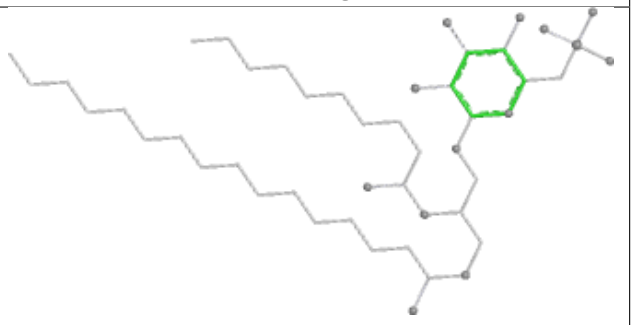
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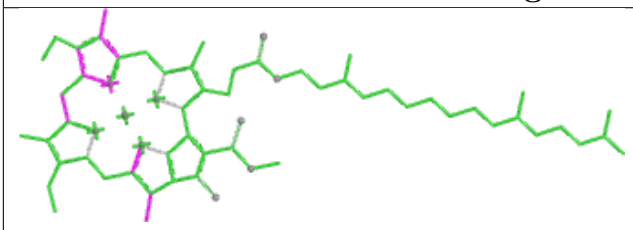


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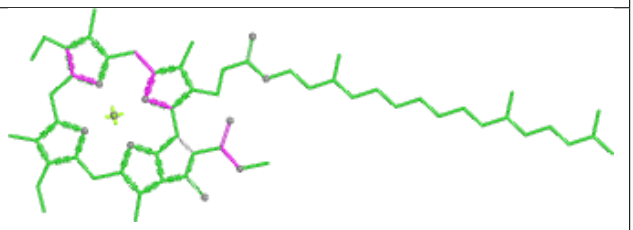


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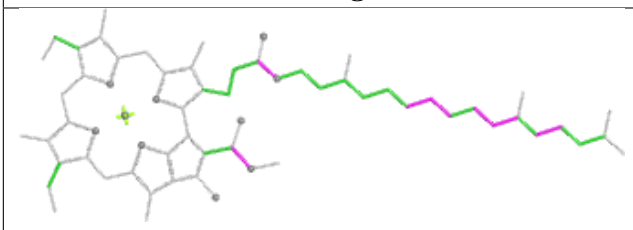
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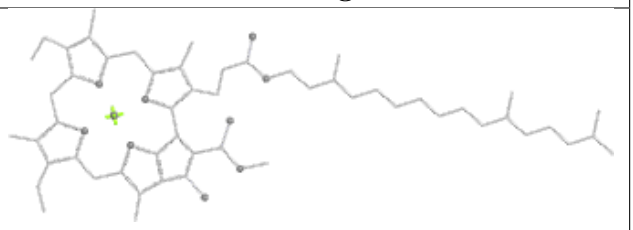
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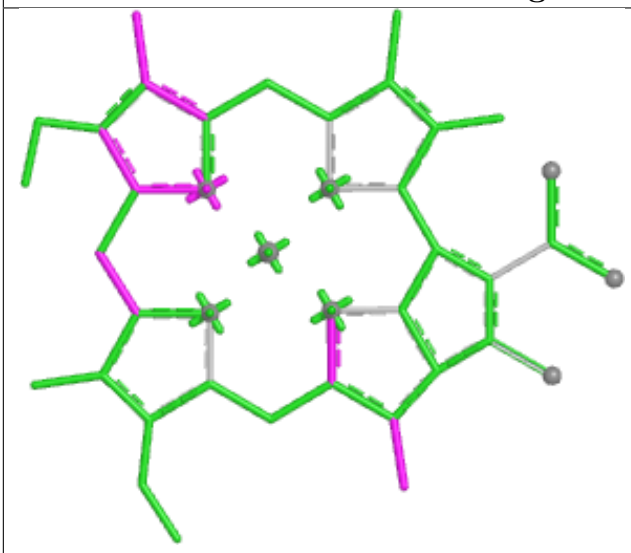


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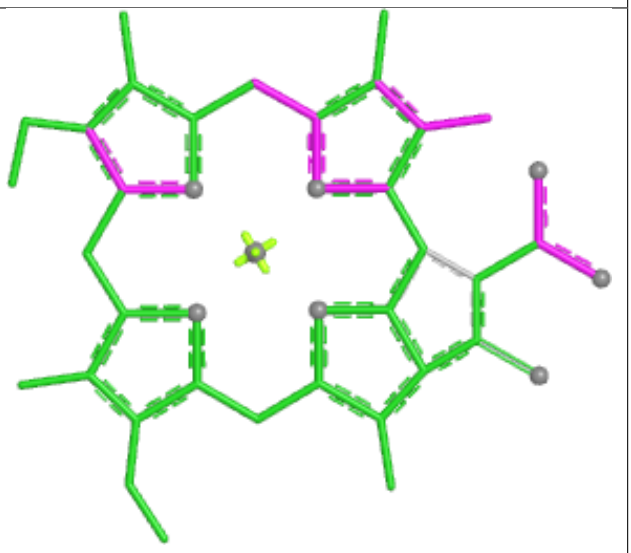


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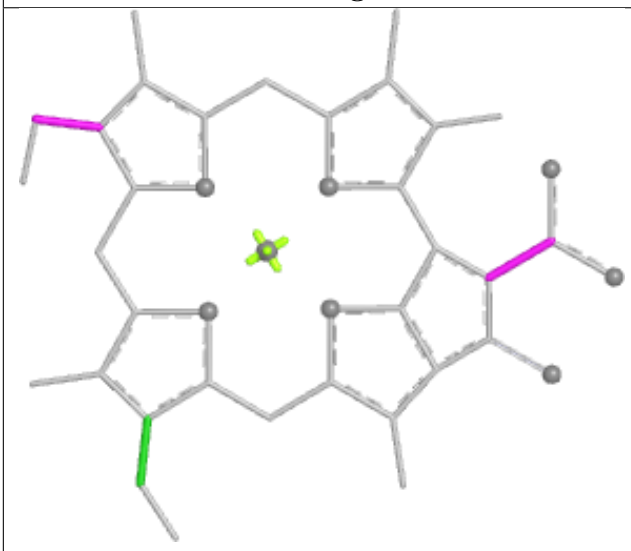
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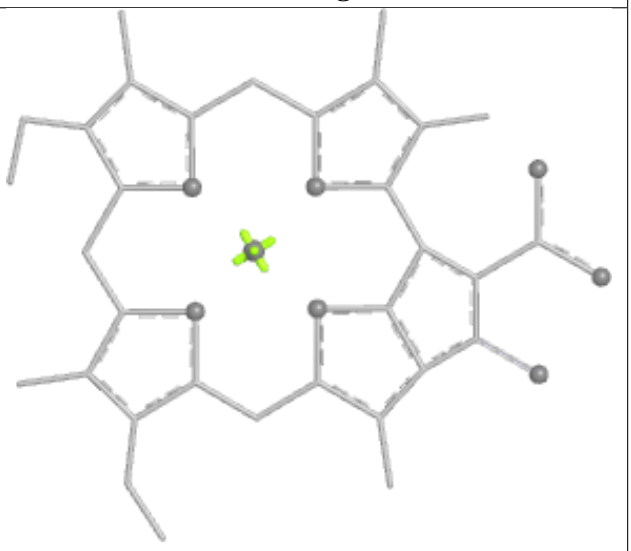
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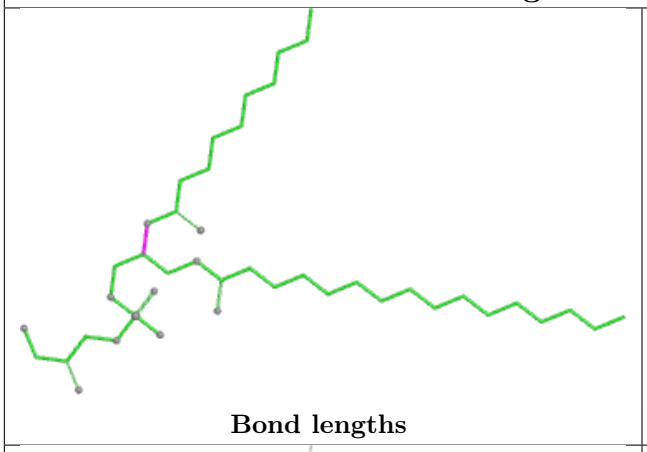


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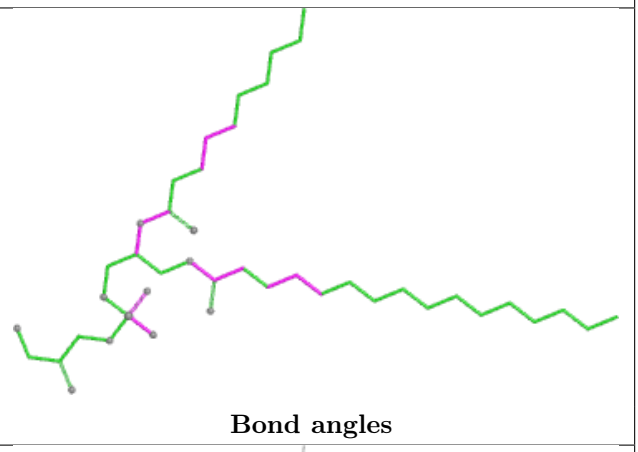


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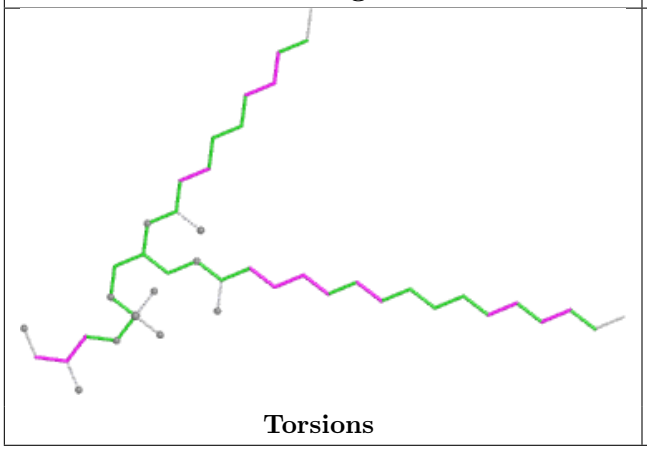
Ligand LHG A 412



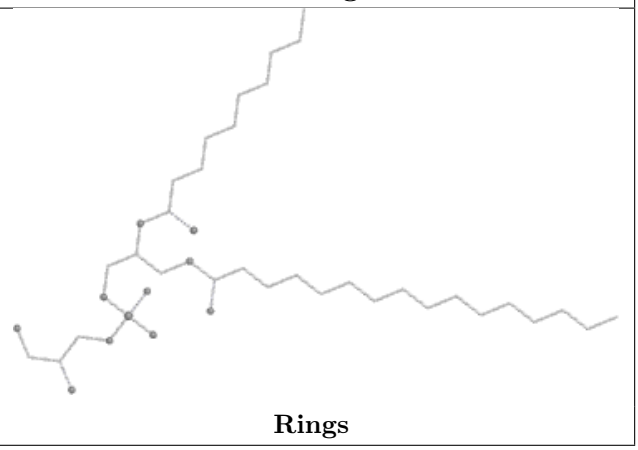
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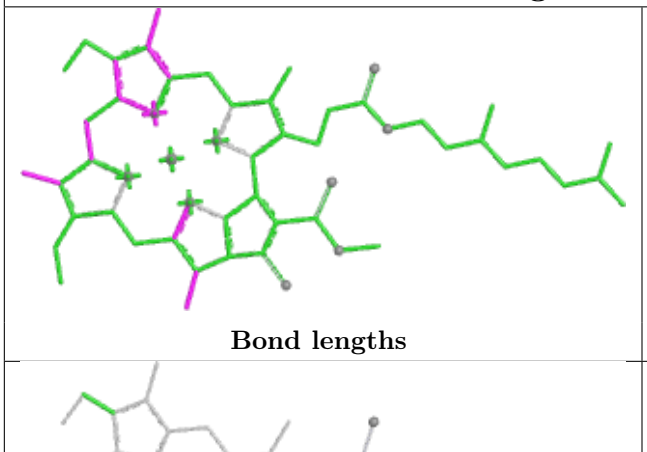


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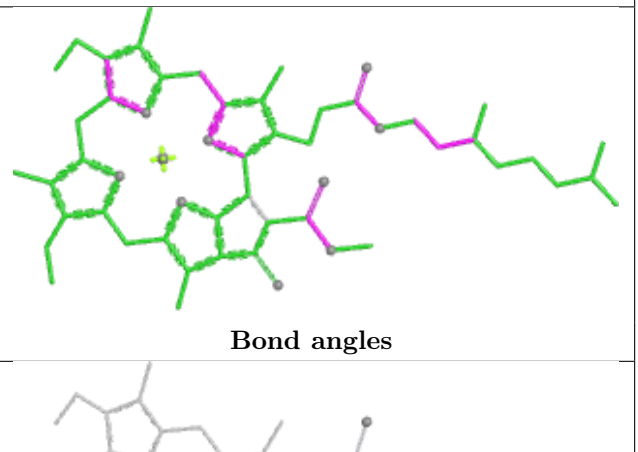


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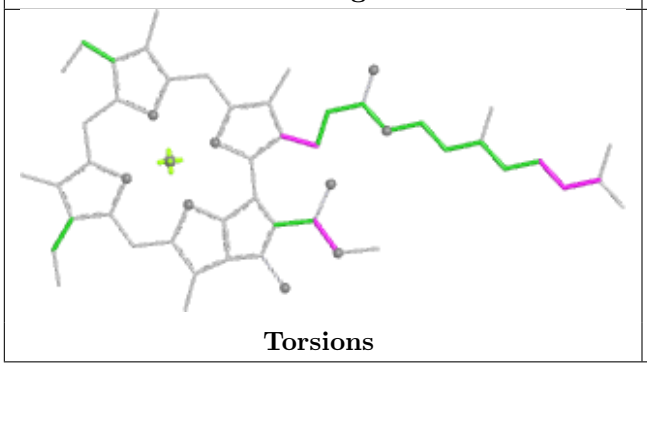
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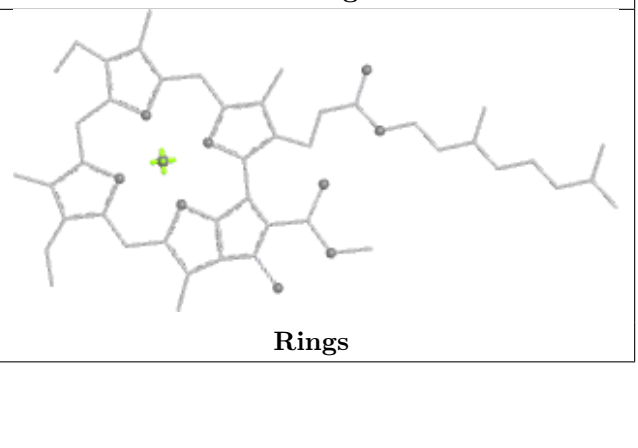
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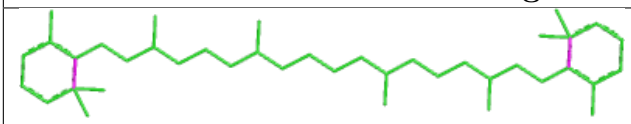
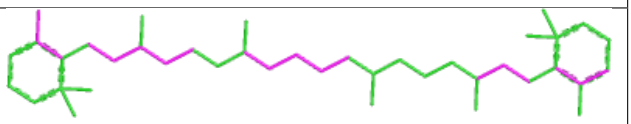
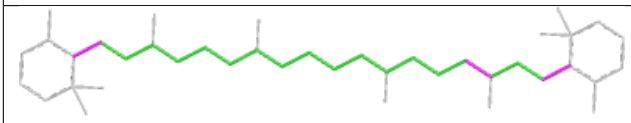
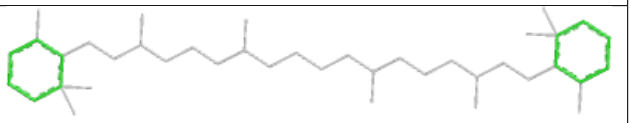
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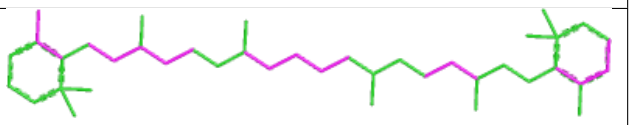
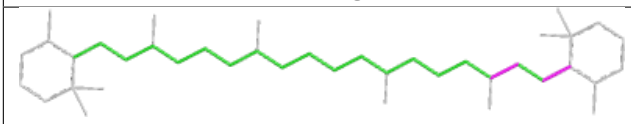
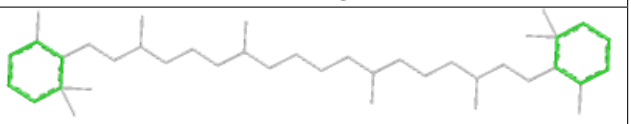


Torsions

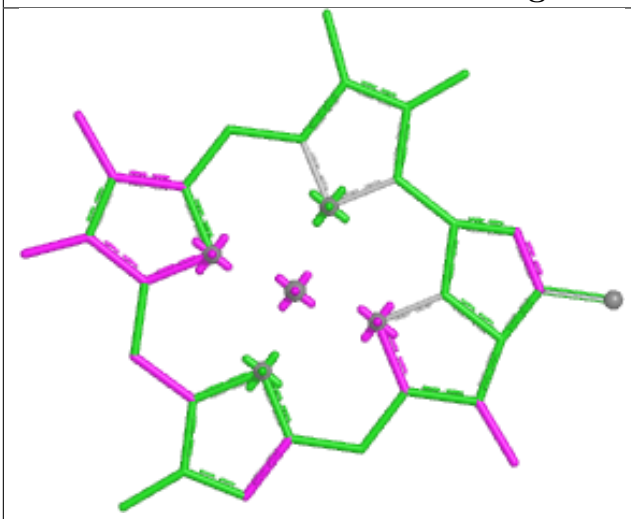


Rings

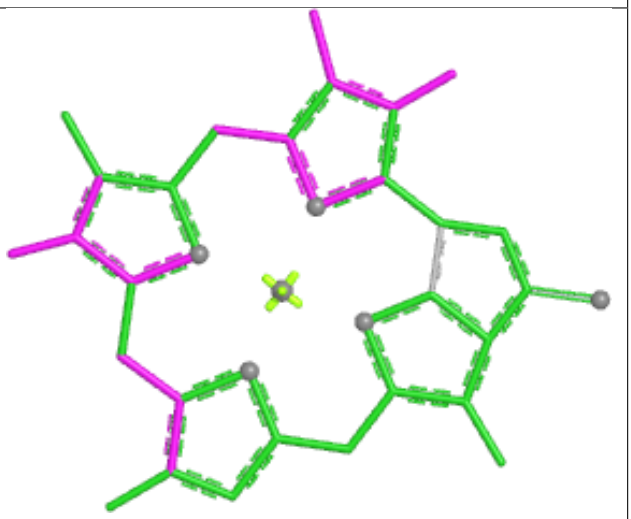
Ligand BCR B 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 304



Bond lengths



Bond angles

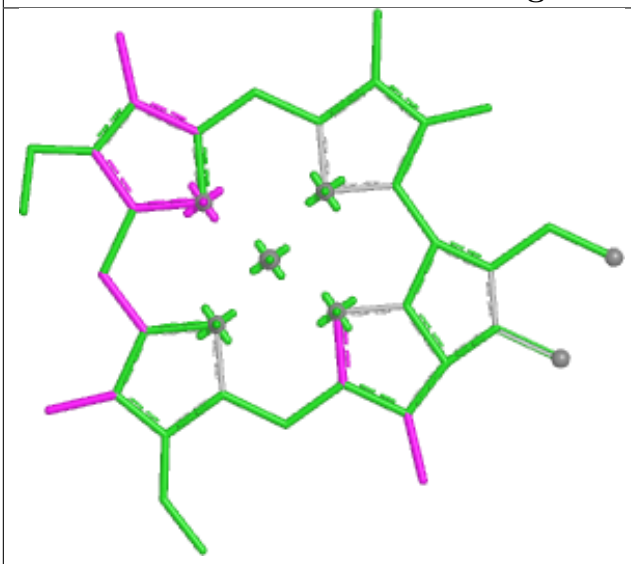


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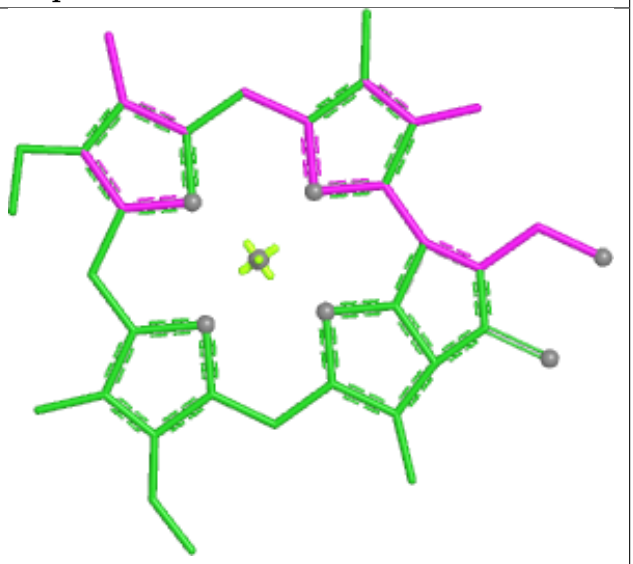


Rings

Ligand CLA p 609



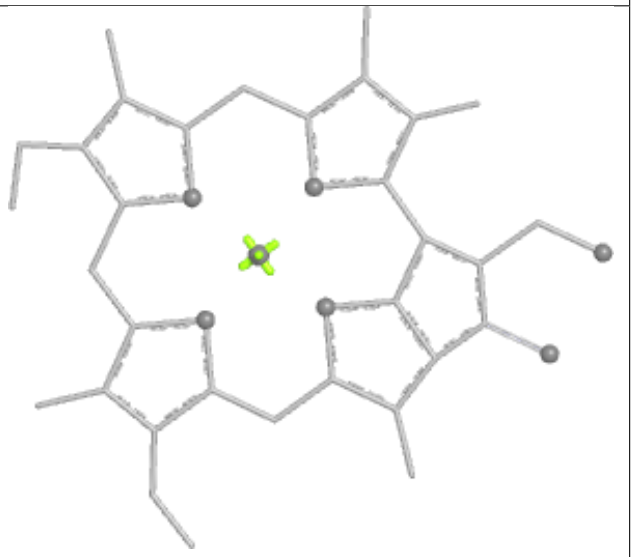
Bond lengths



Bond angles

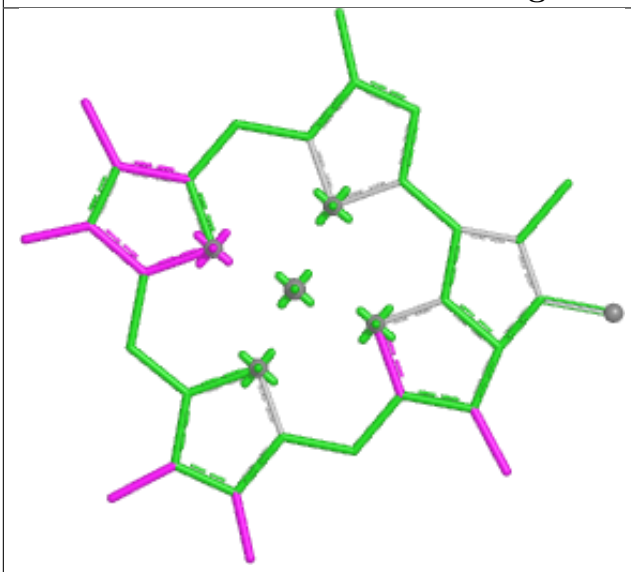


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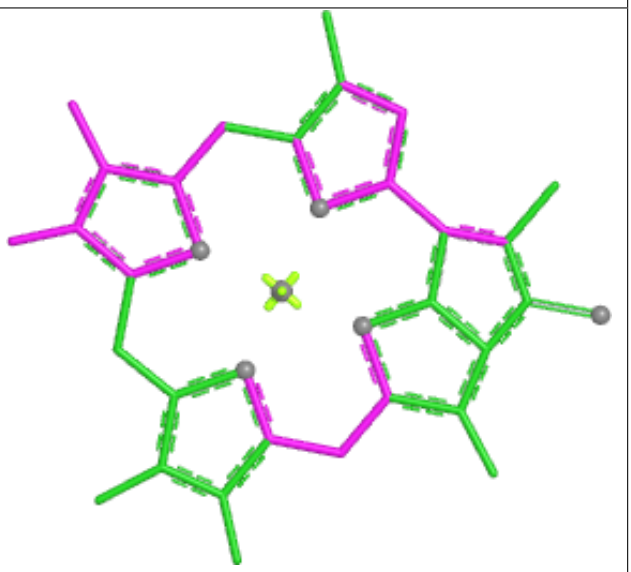


Rings

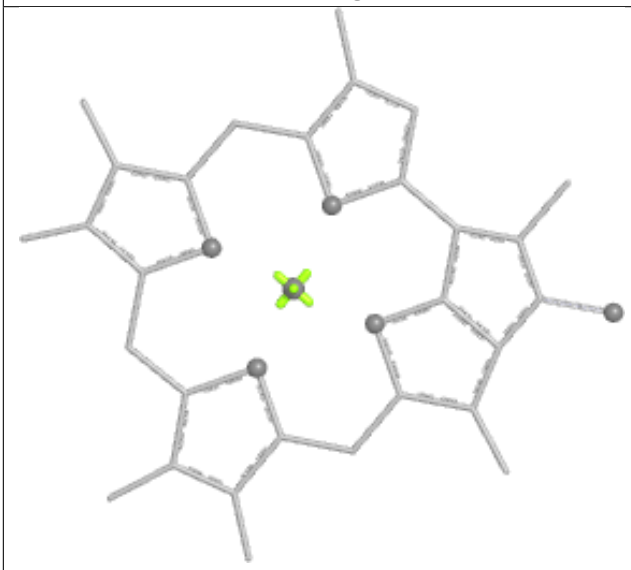
Ligand CLA 4 213



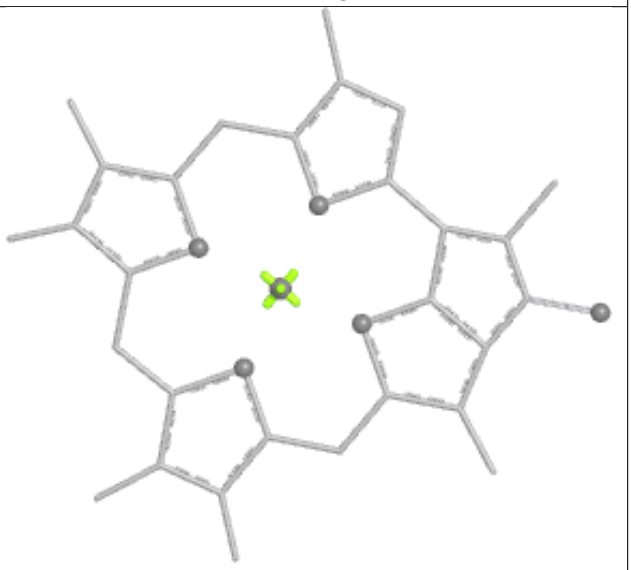
Bond lengths



Bond angles

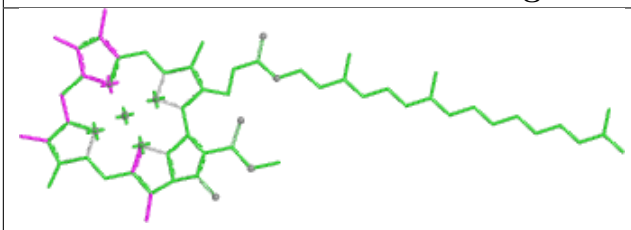


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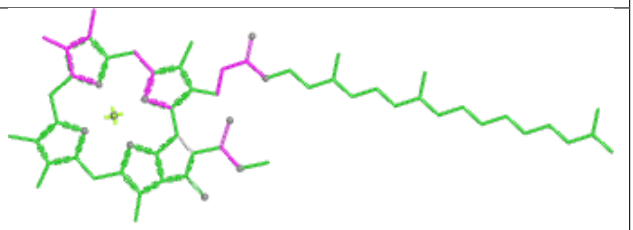


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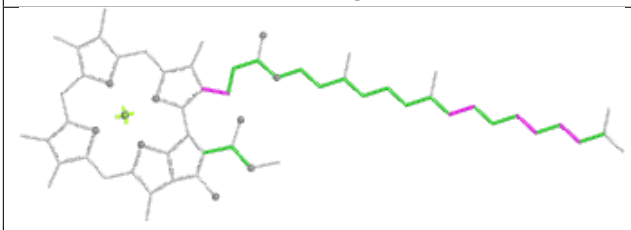
Ligand CLA D 403



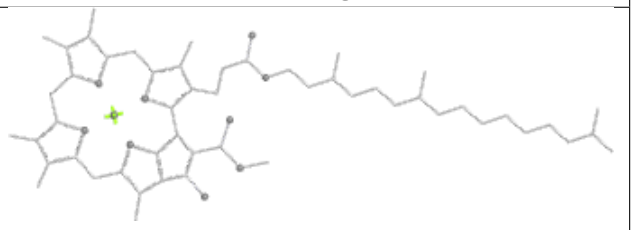
Bond lengths



Bond angles

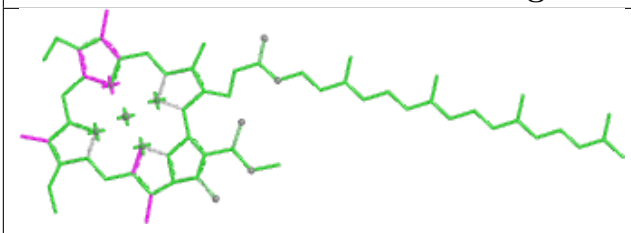


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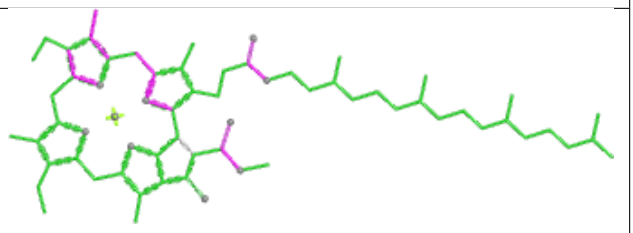


Rings

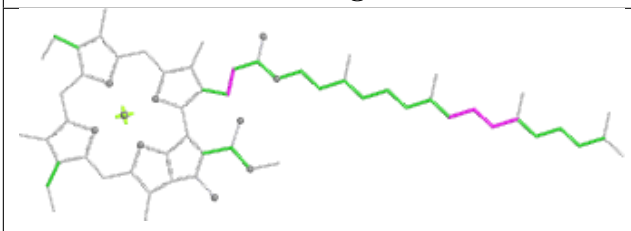
Ligand CLA b 507



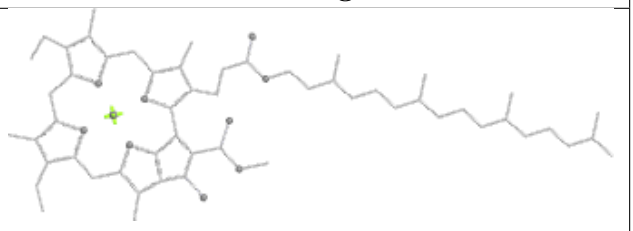
Bond lengths



Bond angles

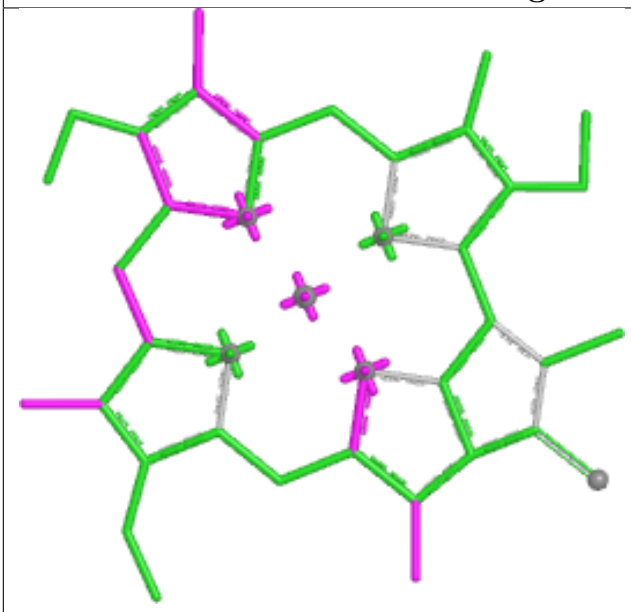


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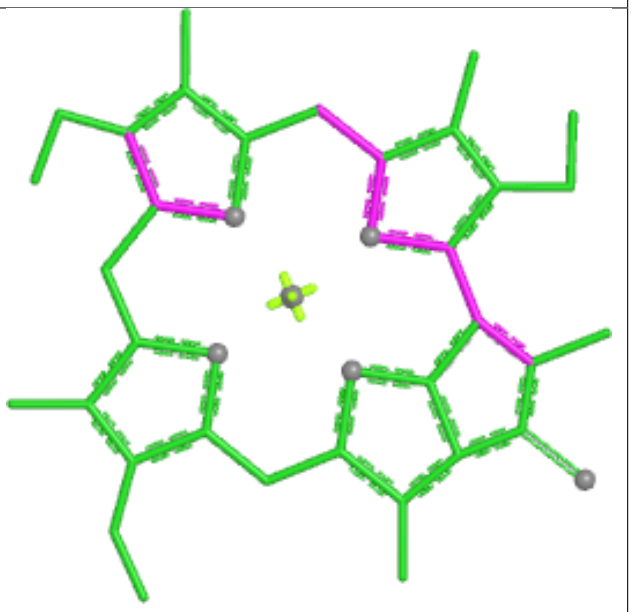


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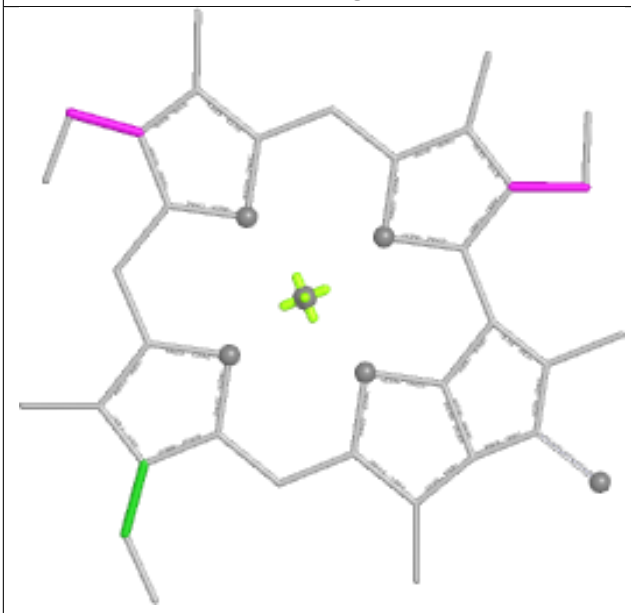
Ligand CLA 3 313



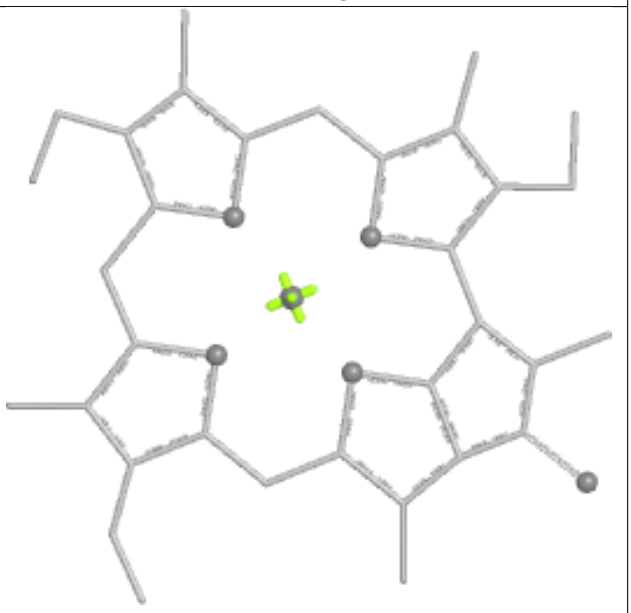
Bond lengths



Bond angles

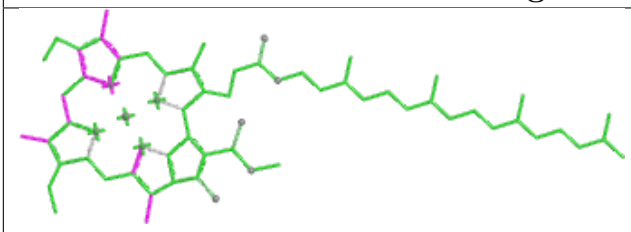


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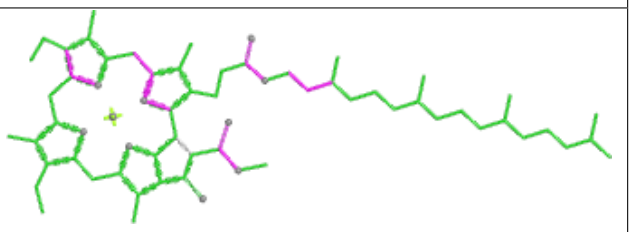


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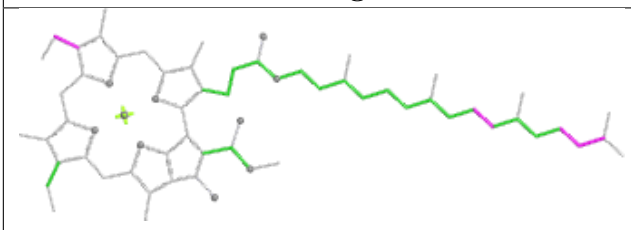
Ligand CLA b 516



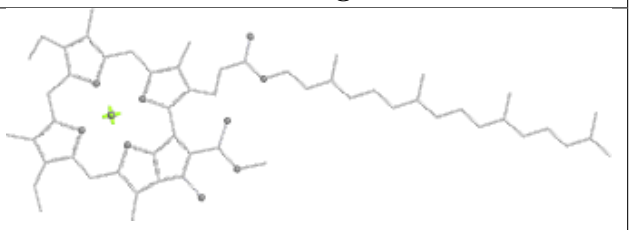
Bond lengths



Bond angles

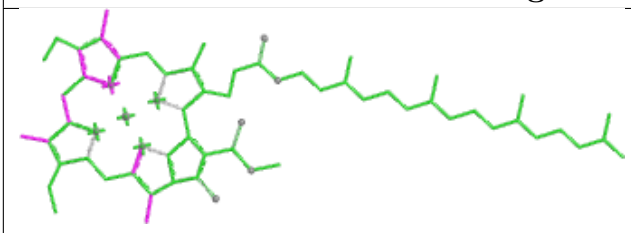


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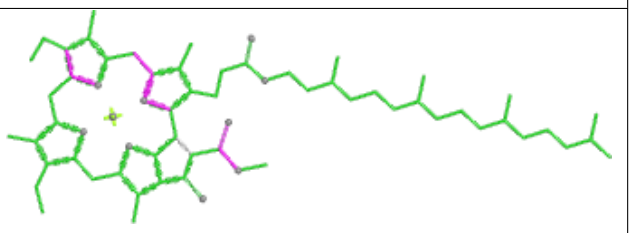


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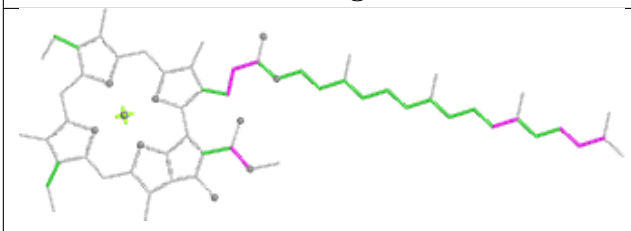
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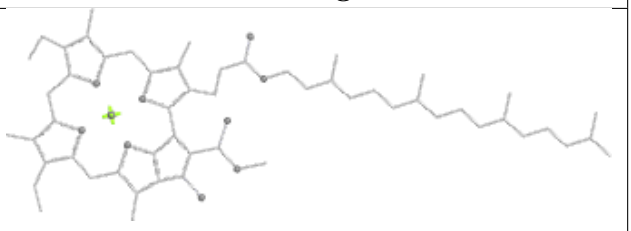
Bond lengths



Bond angles

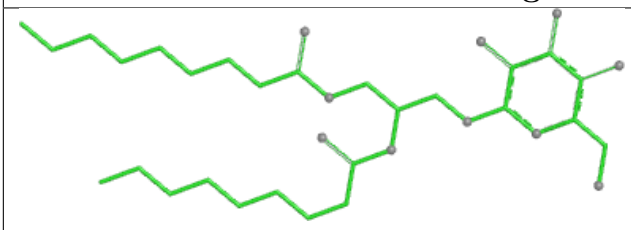


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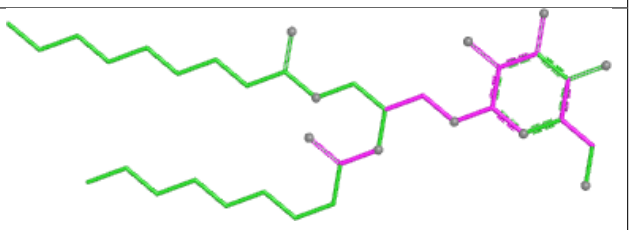


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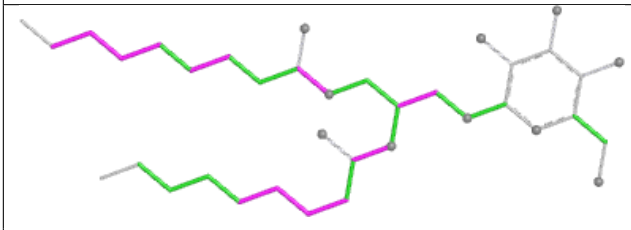
Ligand LMG d 409



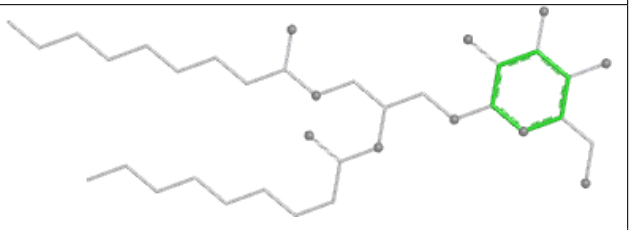
Bond lengths



Bond angles

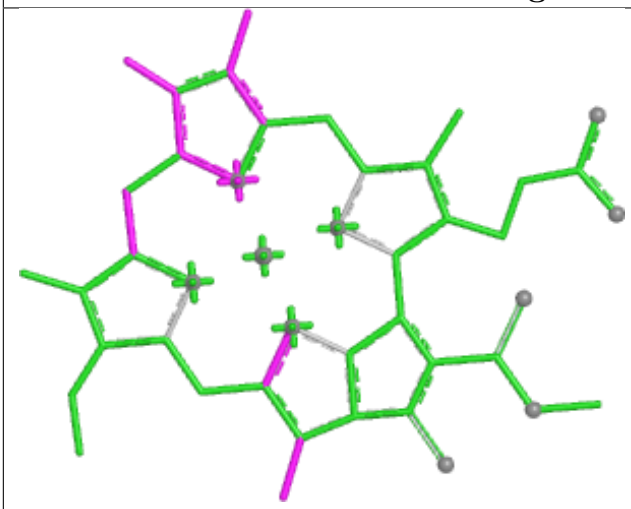


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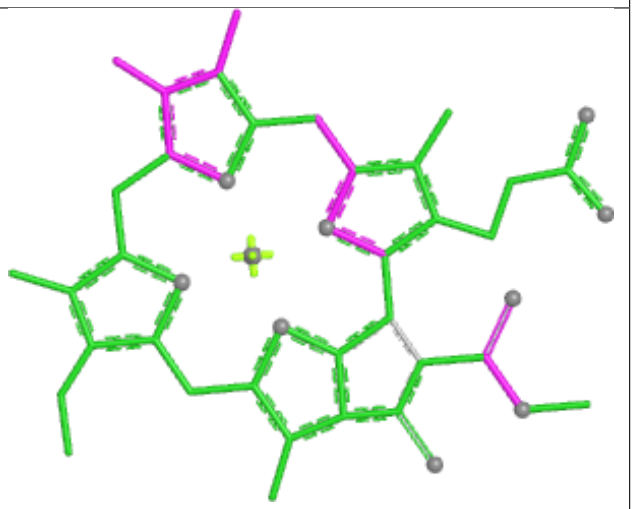


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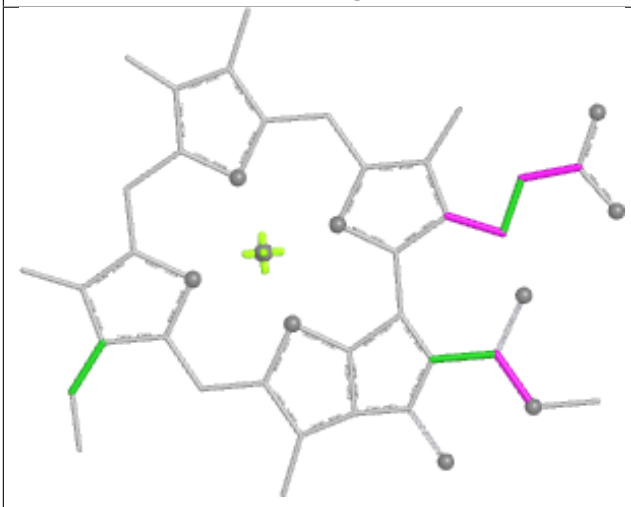
Ligand CLA 1 209



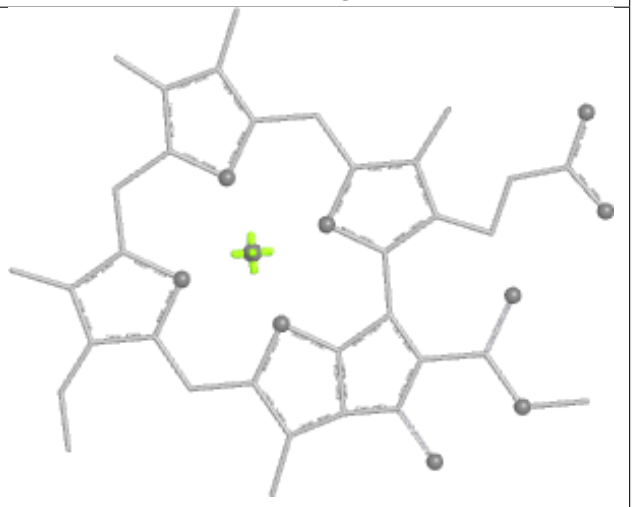
Bond lengths



Bond angles

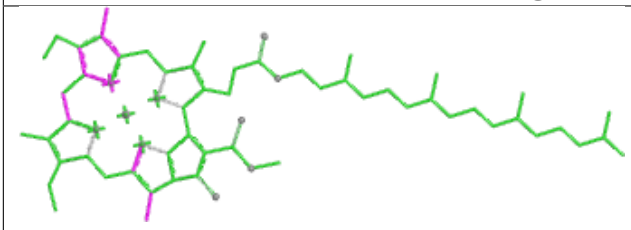


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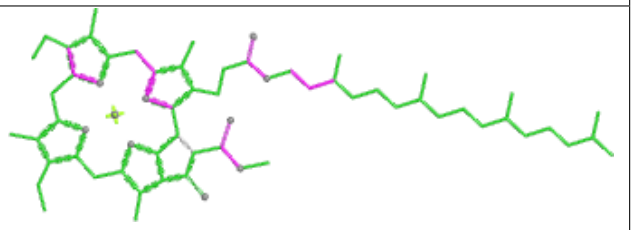


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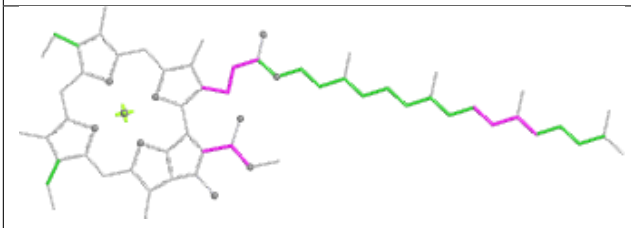
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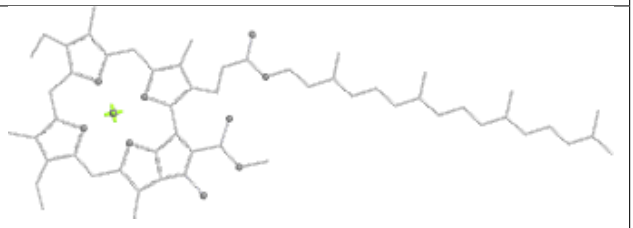
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Bond angles

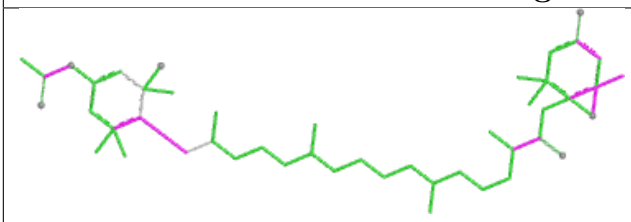


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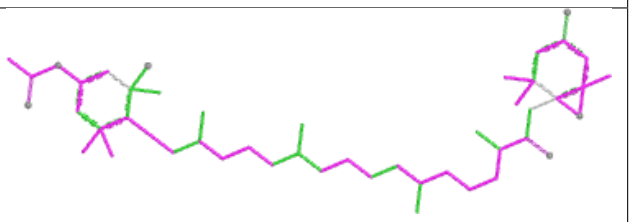


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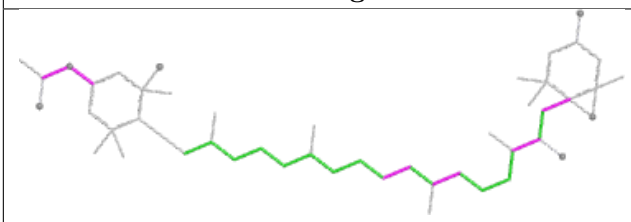
Ligand A86 8 301



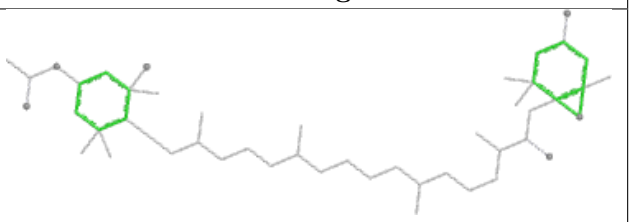
Bond lengths



Bond angles

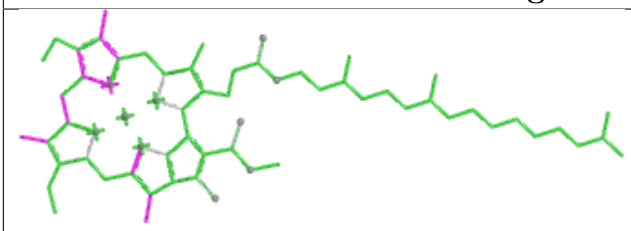


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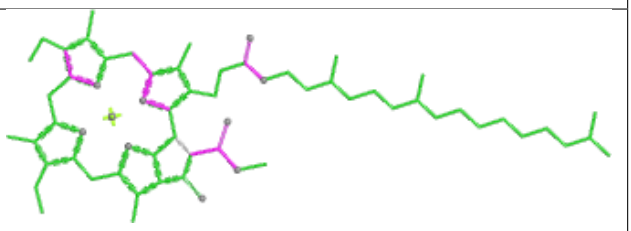


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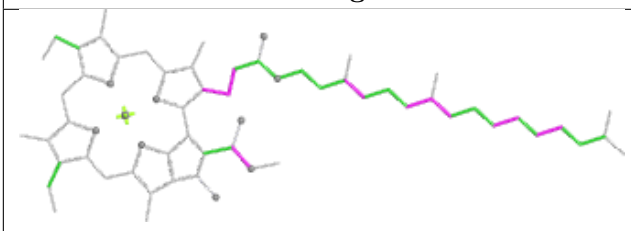
Ligand CLA b 504



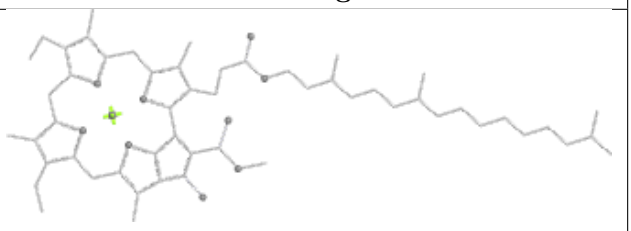
Bond lengths



Bond angles

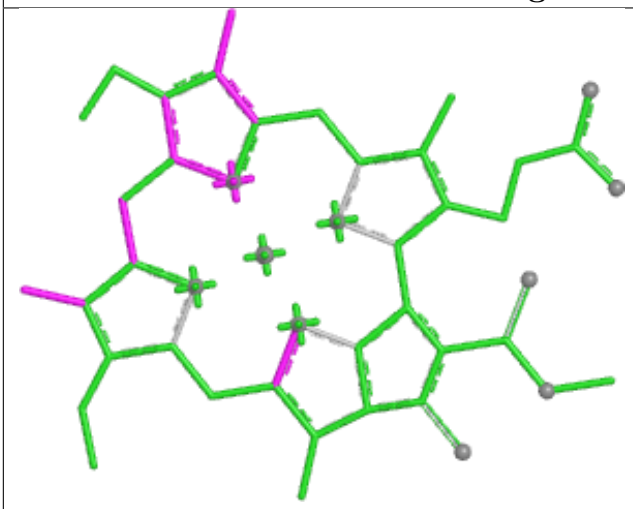


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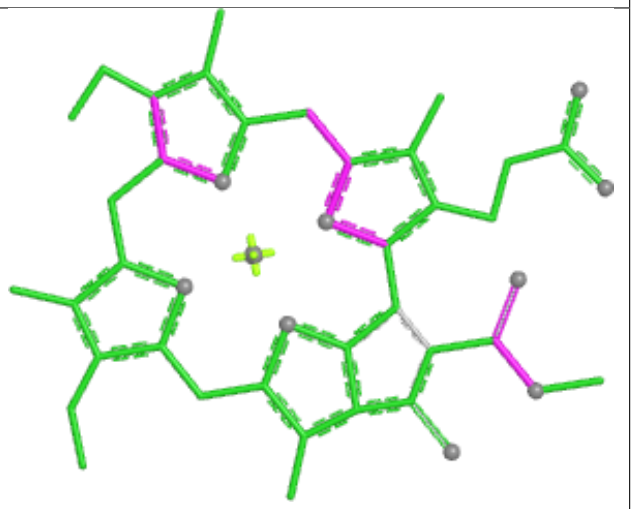


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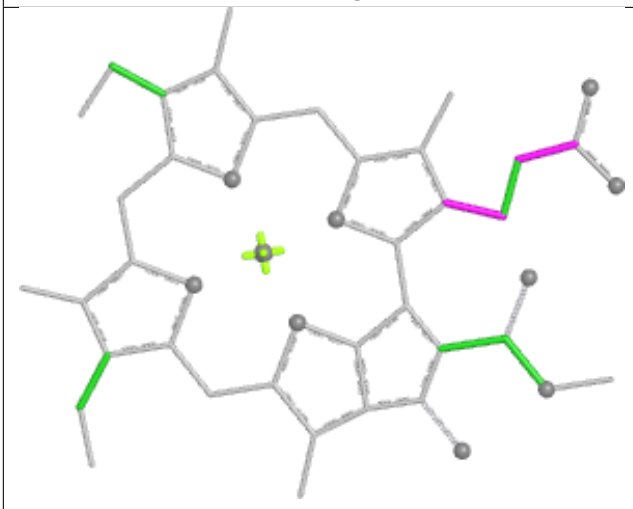
Ligand CLA 7 306



Bond lengths



Bond angles

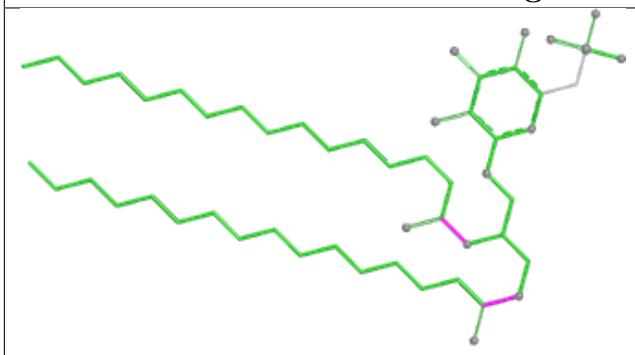


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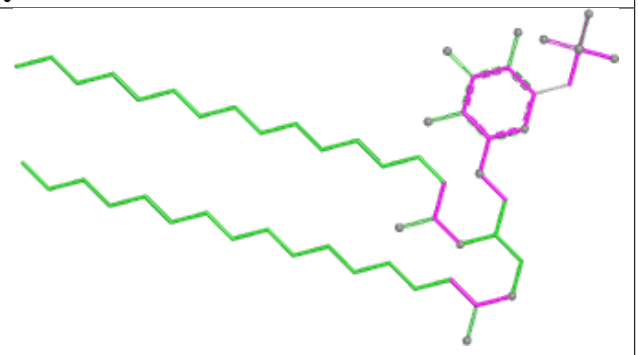


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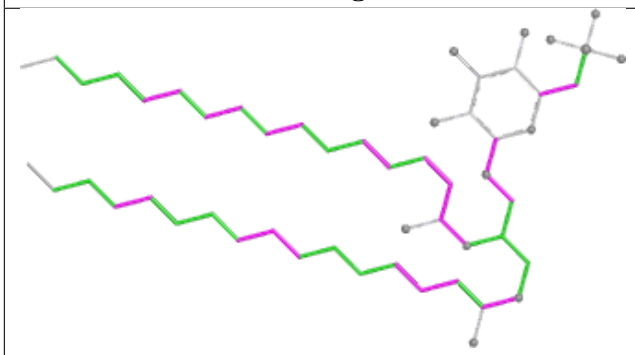
Ligand SQD A 411



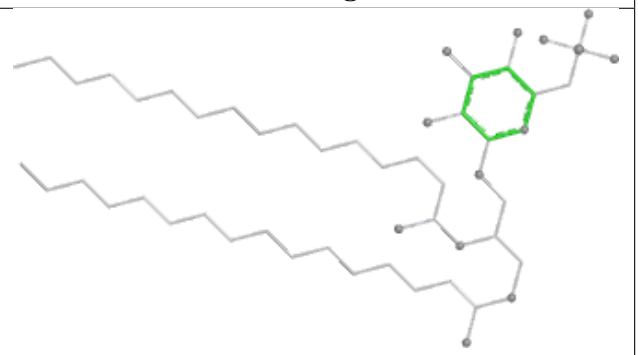
Bond lengths



Bond angles

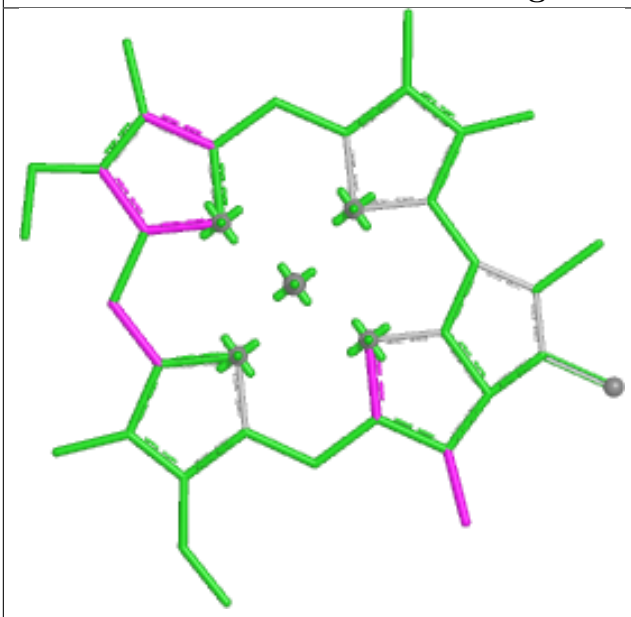


Torsions

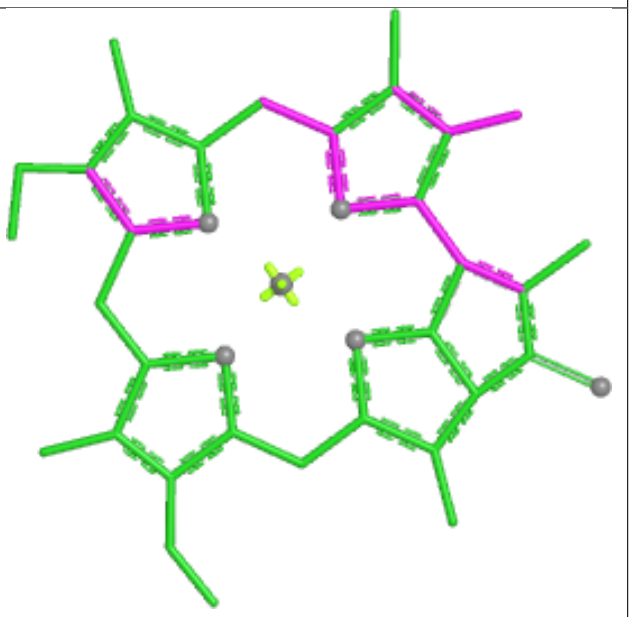


Rings

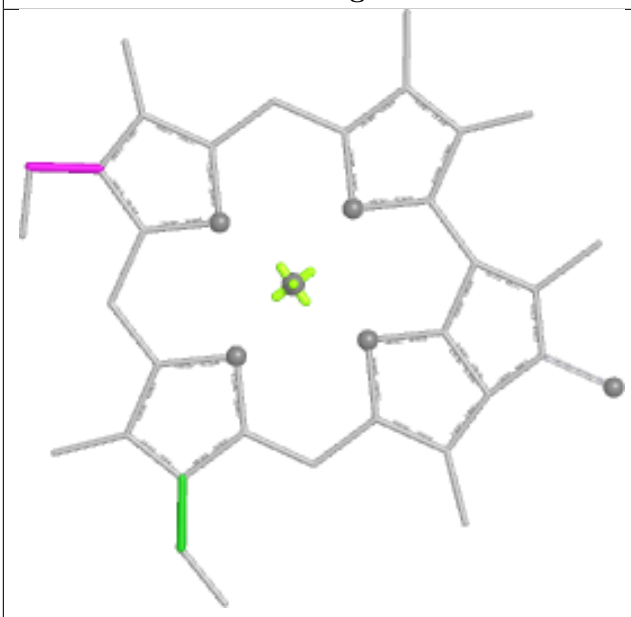
Ligand CLA 1 216



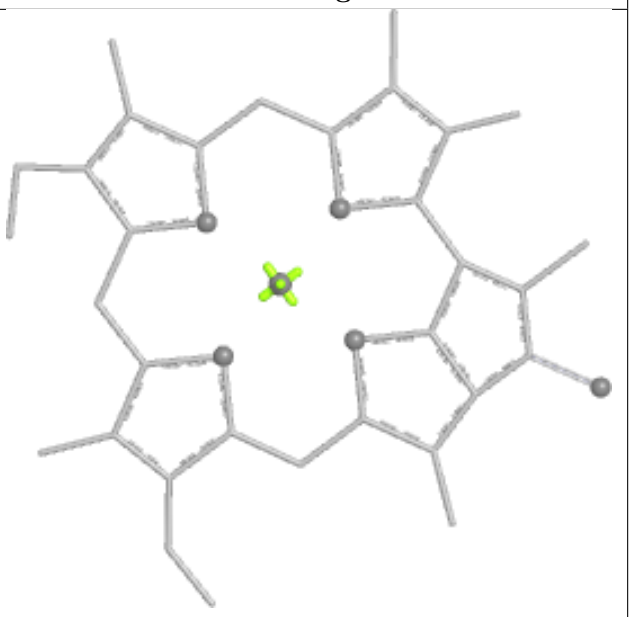
Bond lengths



Bond angles

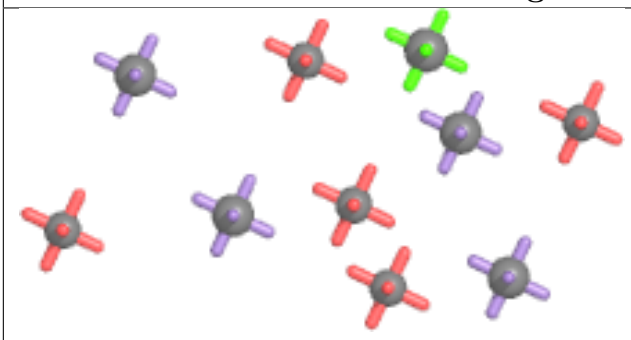


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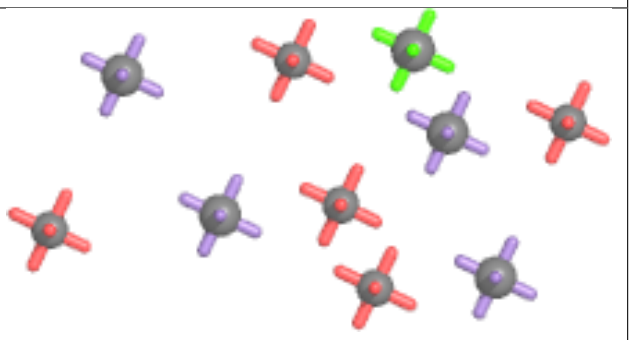


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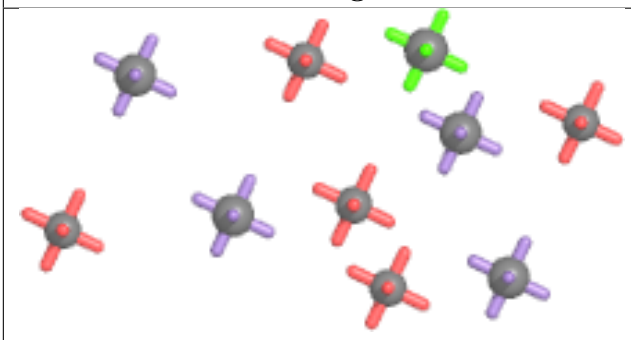
Ligand OEX a 401



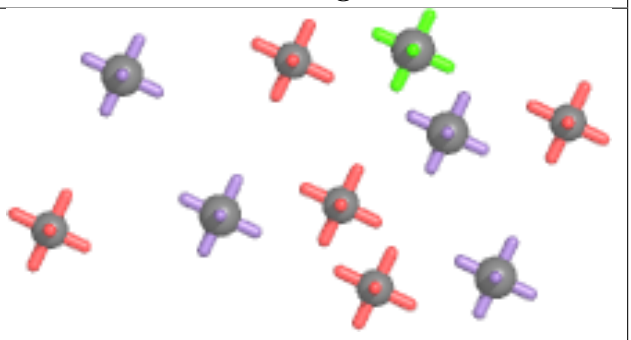
Bond lengths



Bond angles

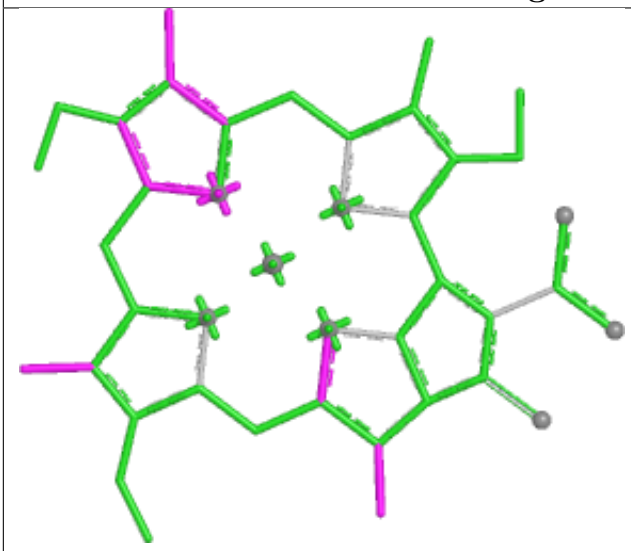


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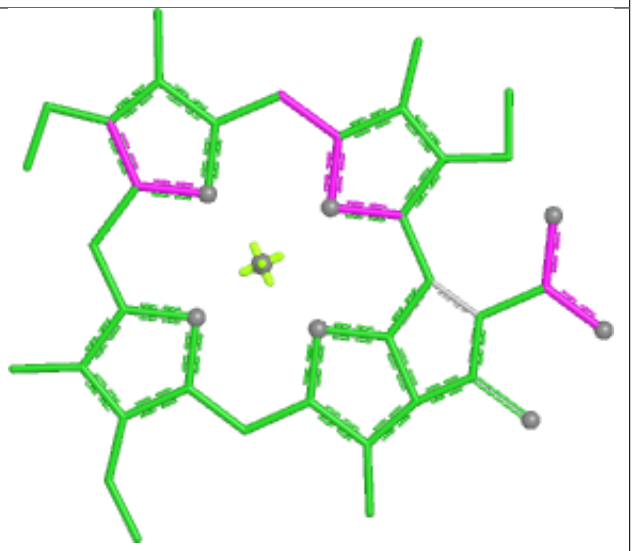


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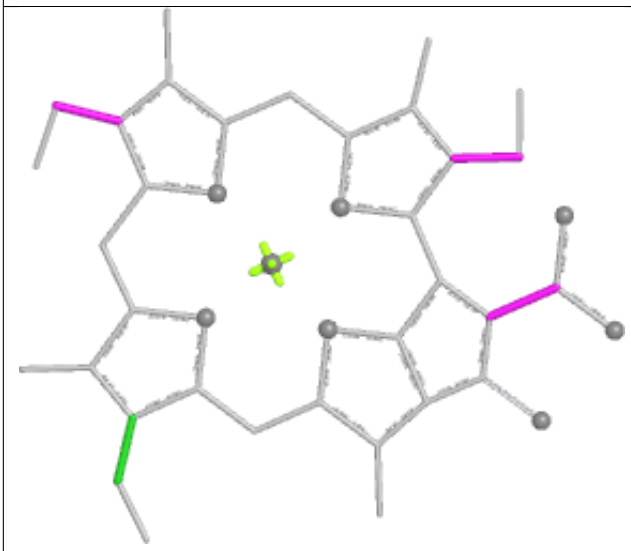
Ligand CLA 3 312



Bond lengths



Bond angles

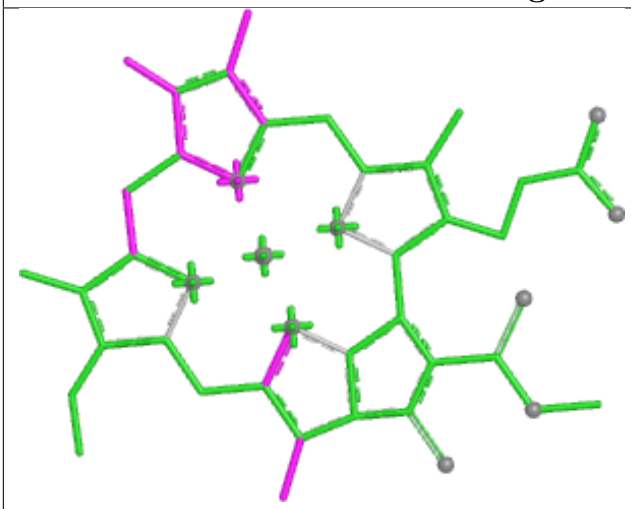


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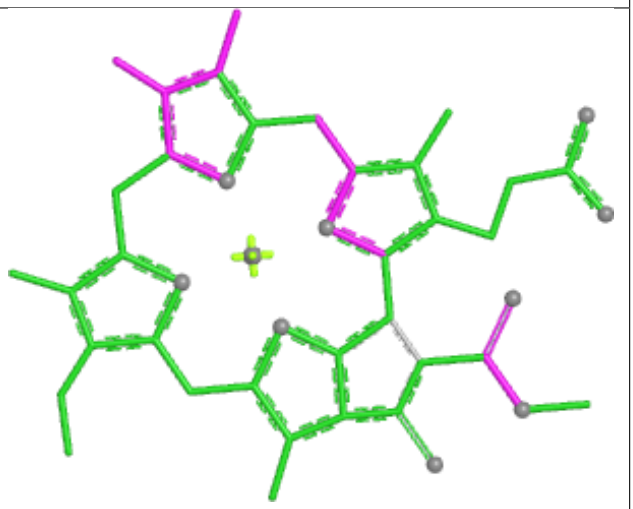


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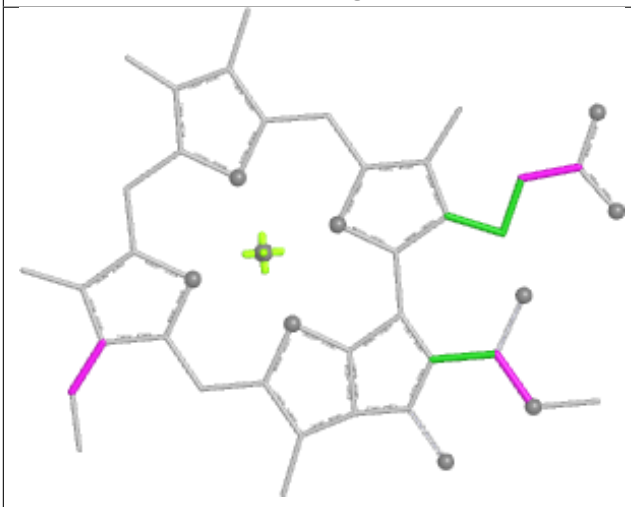
Ligand CLA 1 207



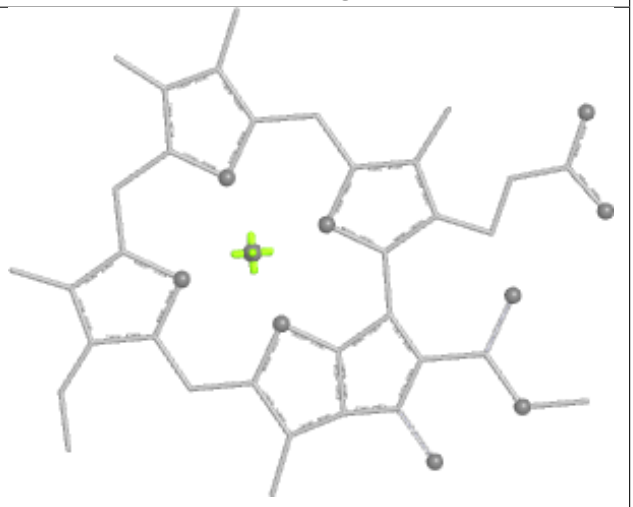
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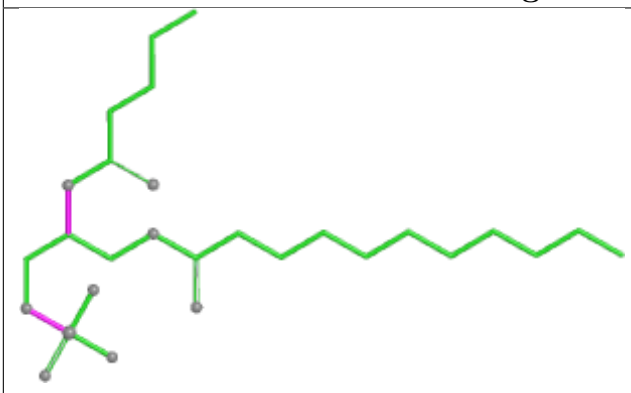


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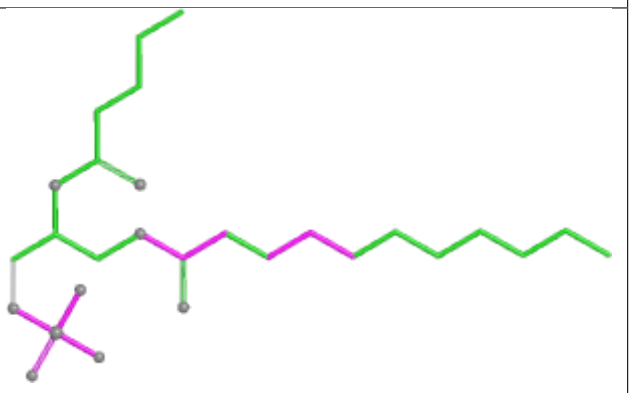


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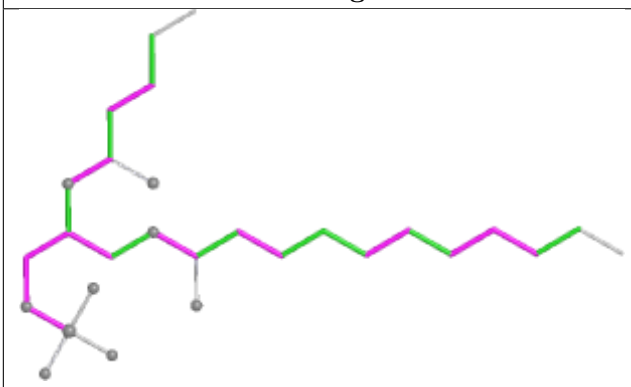
Ligand LHG D 412



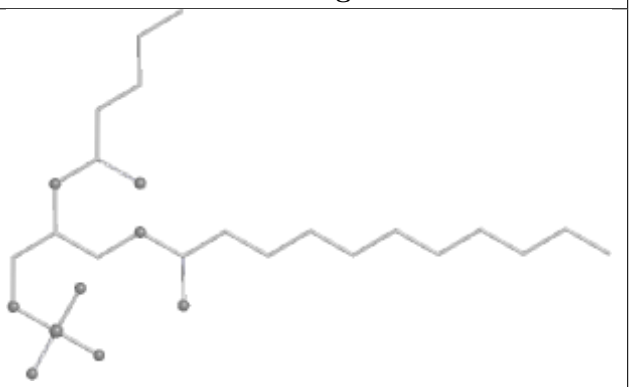
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Bond angles

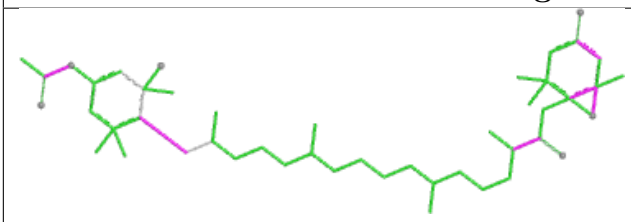


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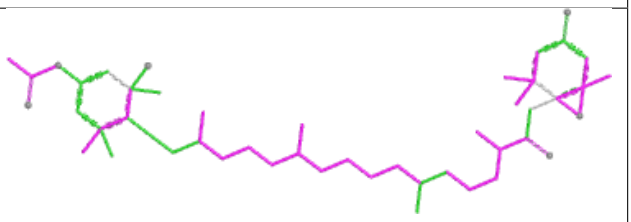


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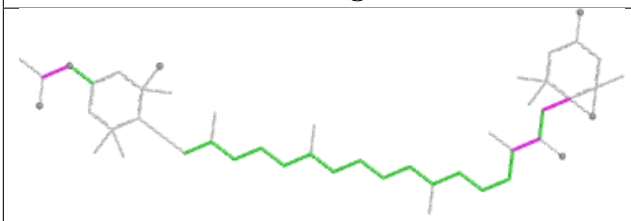
Ligand A86 8 302



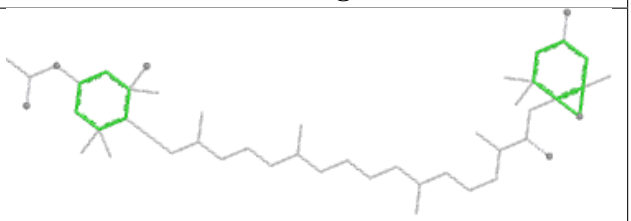
Bond lengths



Bond angles

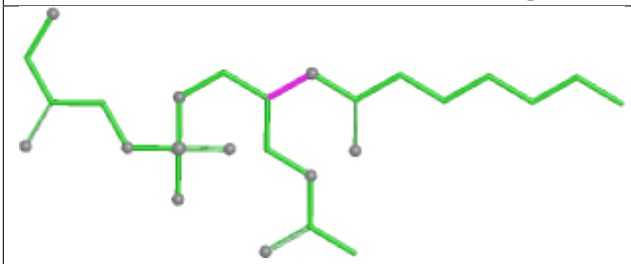


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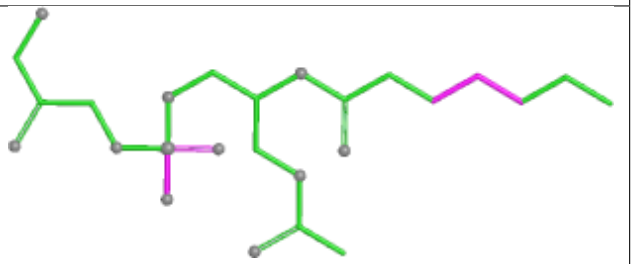


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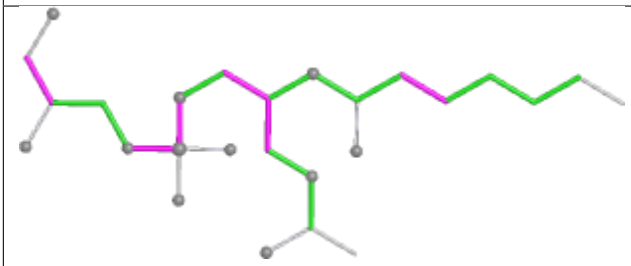
Ligand LHG A 413



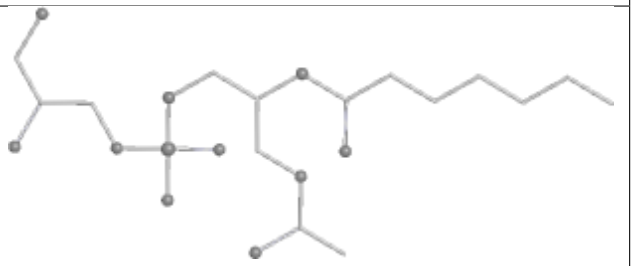
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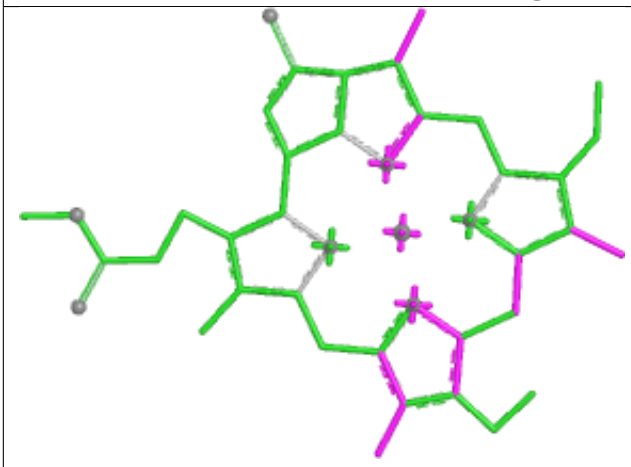


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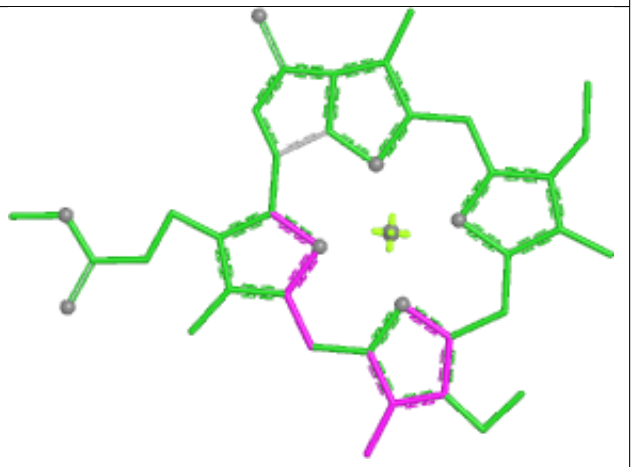


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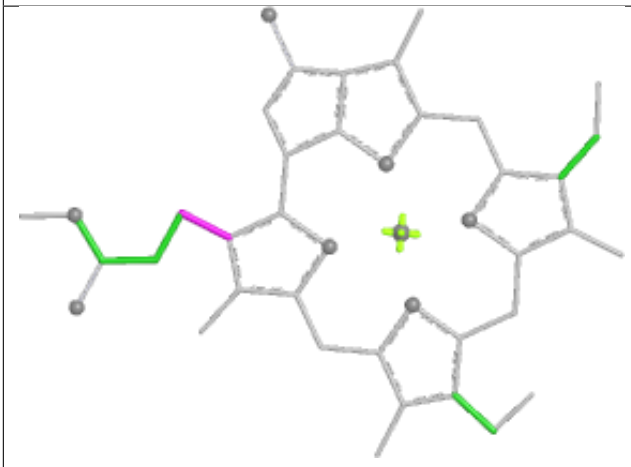
Ligand CLA 3 307



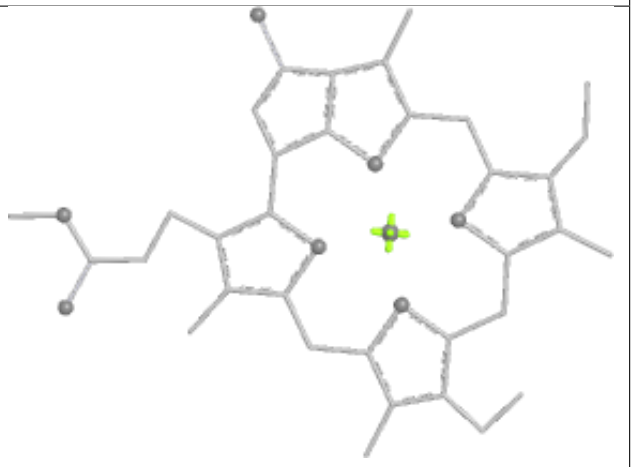
Bond lengths



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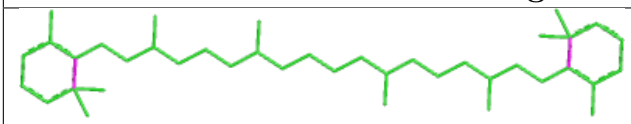


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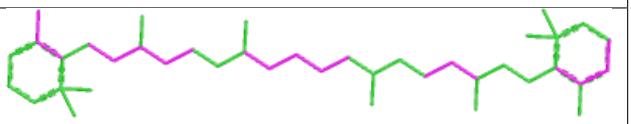


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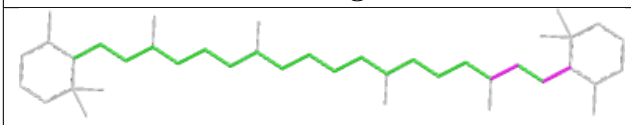
Ligand BCR c 516



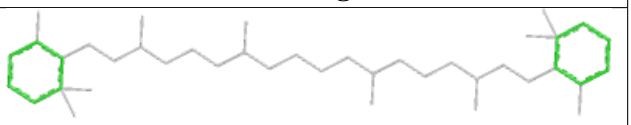
Bond lengths



Bond angles

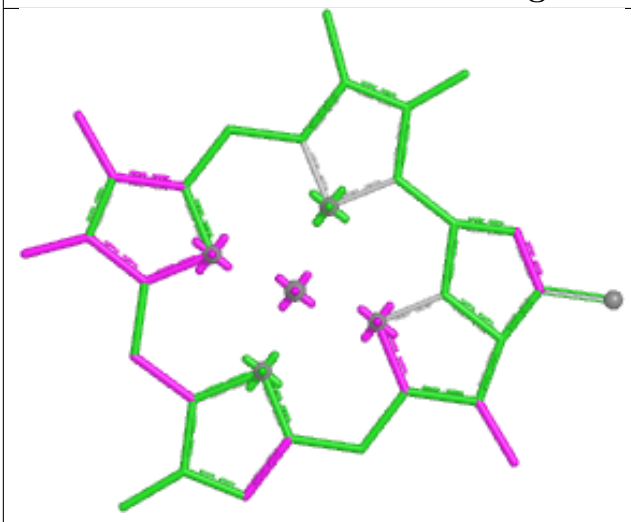


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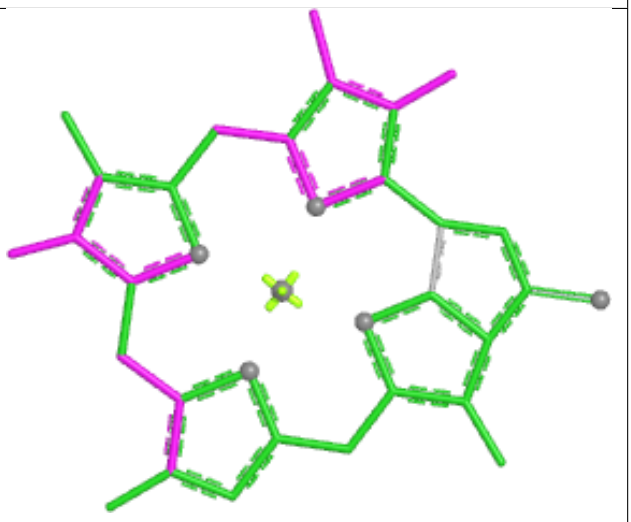


Rings

Ligand CLA 3 304



Bond lengths



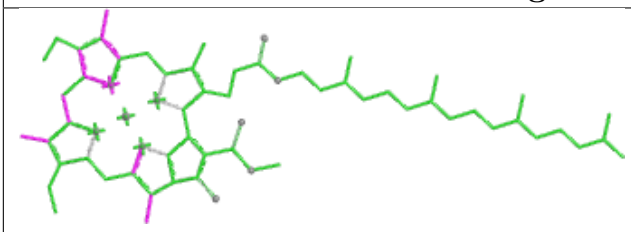
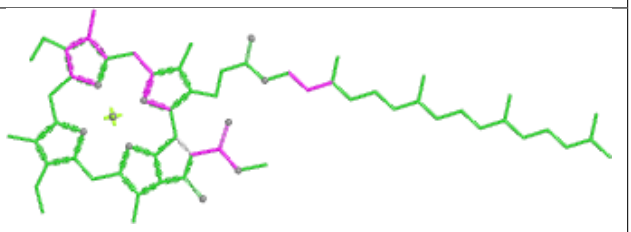
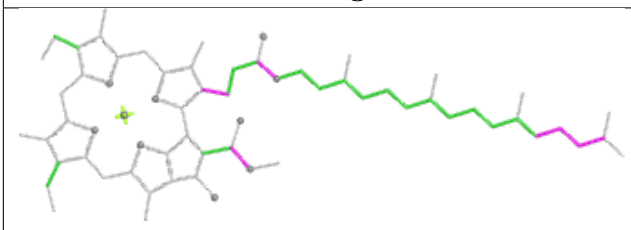
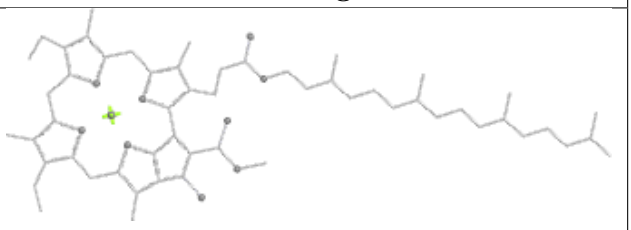
Bond angles



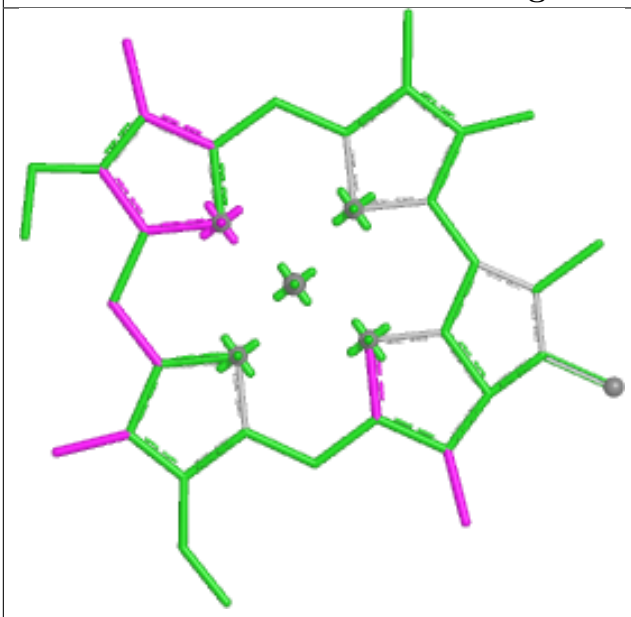
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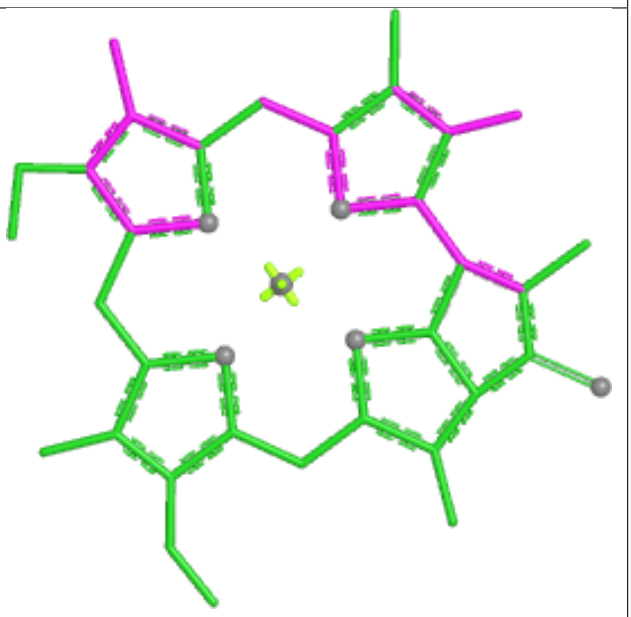
Rings

Ligand CLA a 403	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

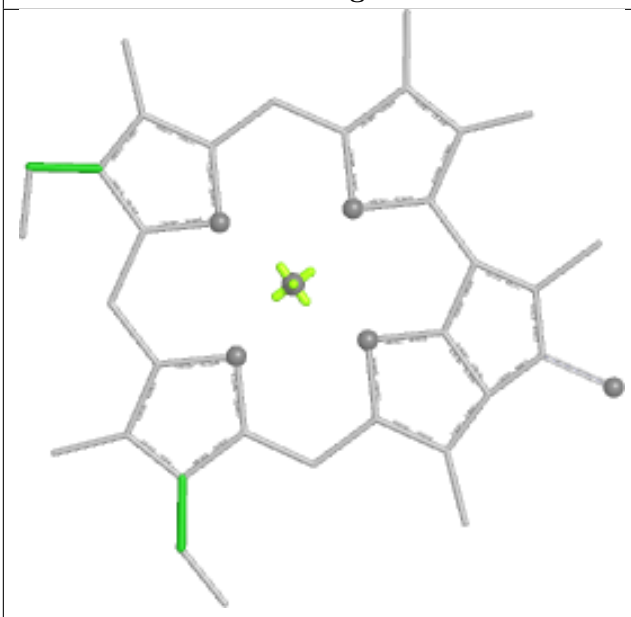
Ligand CLA 9 210



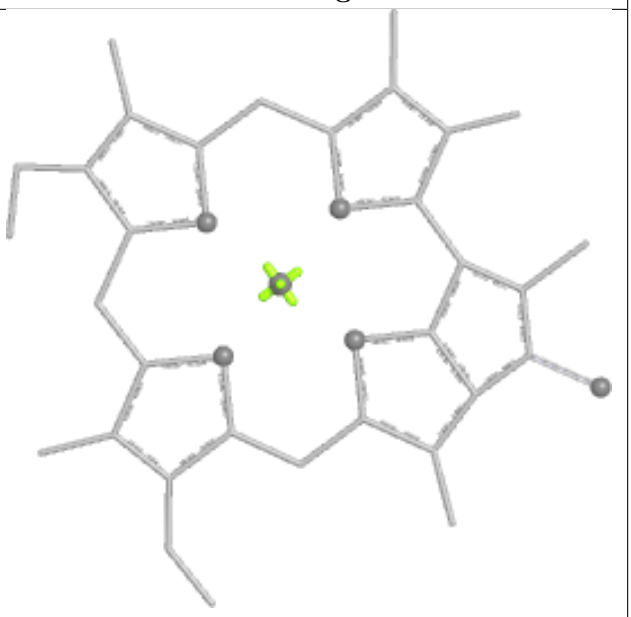
Bond lengths



Bond angles

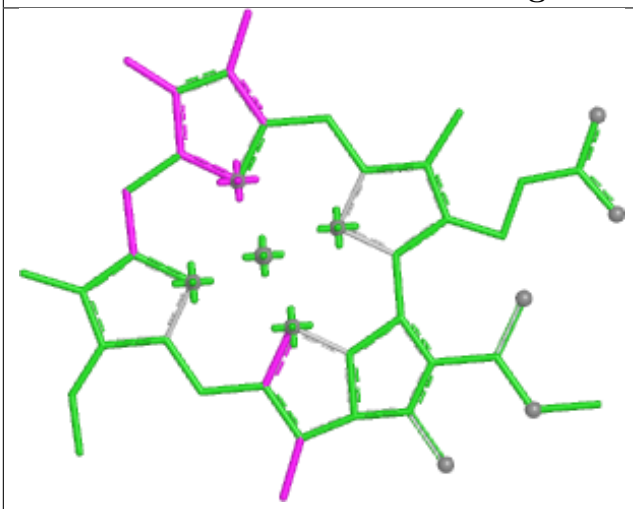


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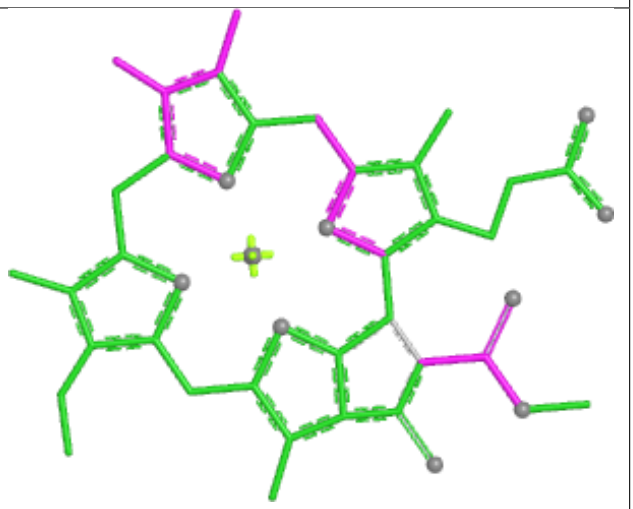


Rings

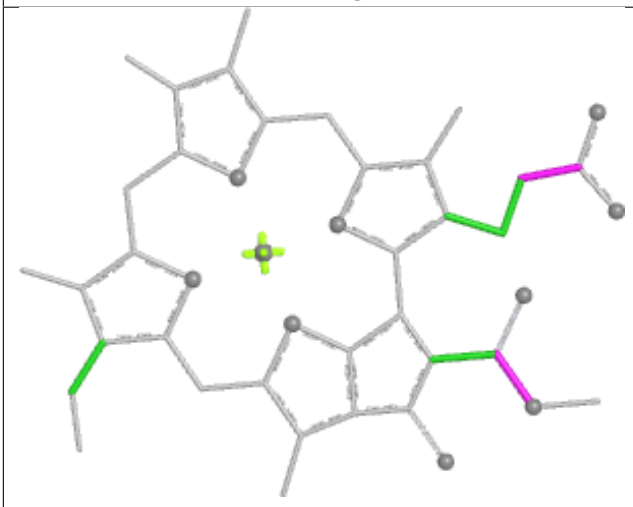
Ligand CLA 1 201



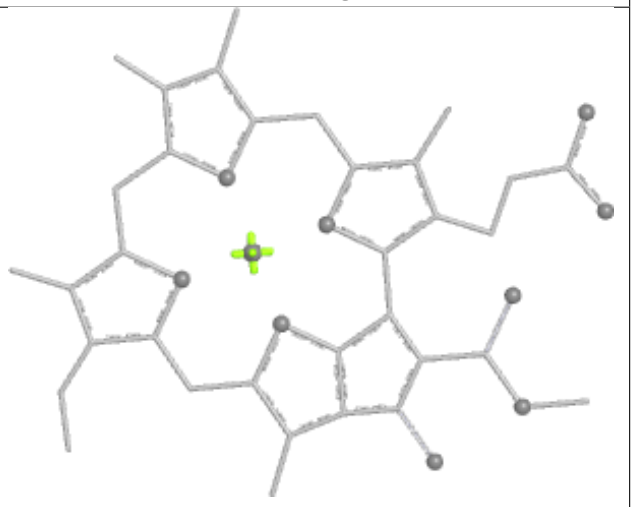
Bond lengths



Bond angles

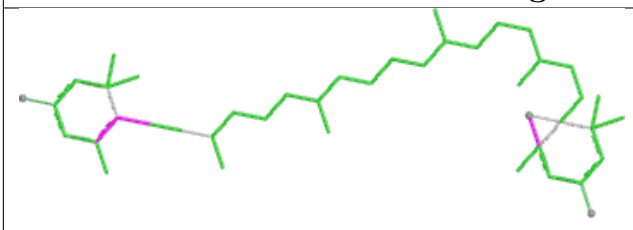


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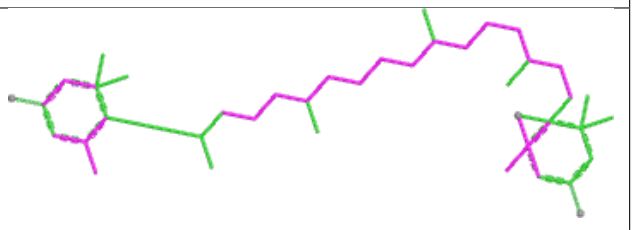


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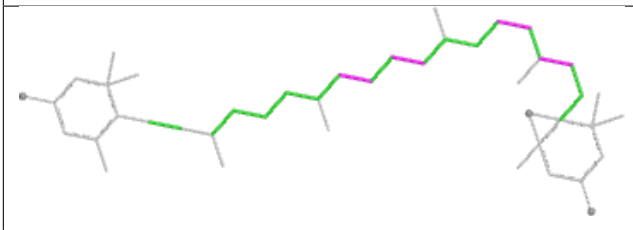
Ligand DD6 6 204



Bond lengths



Bond angles

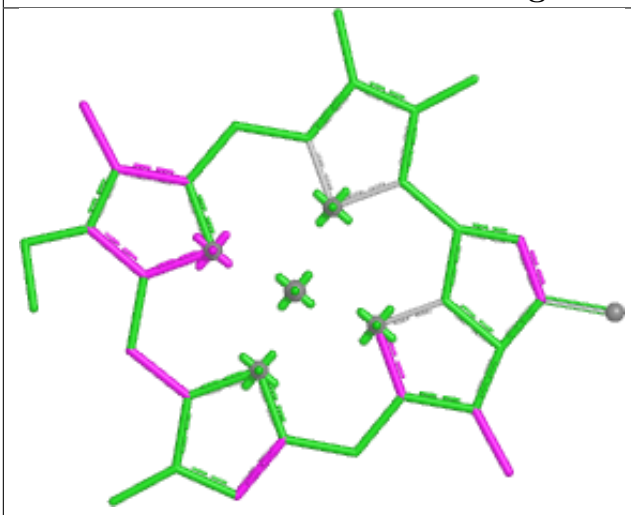


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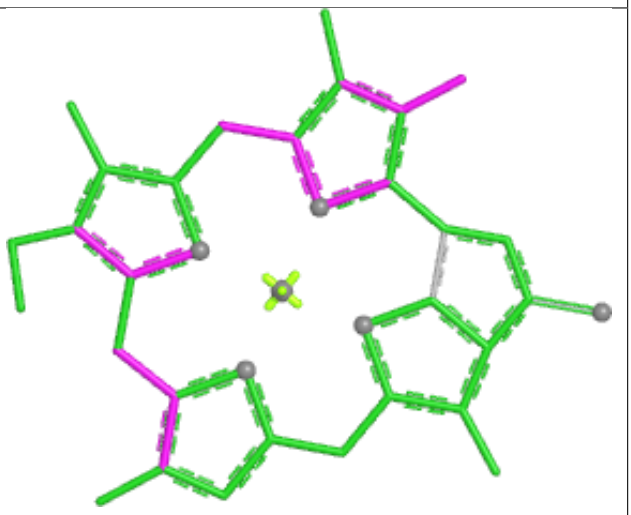


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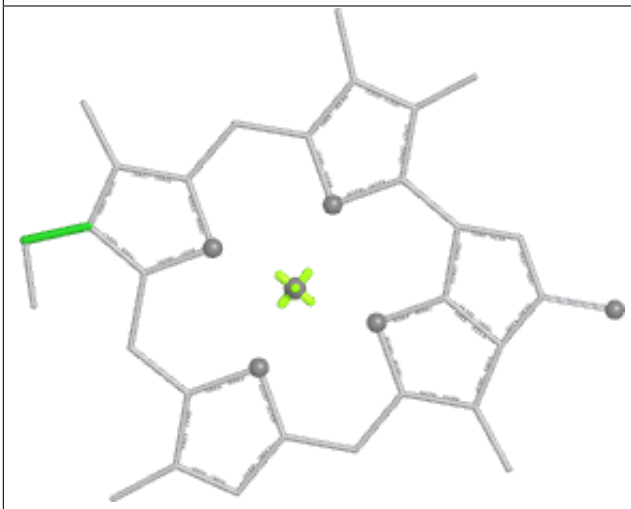
Ligand CLA 8 310



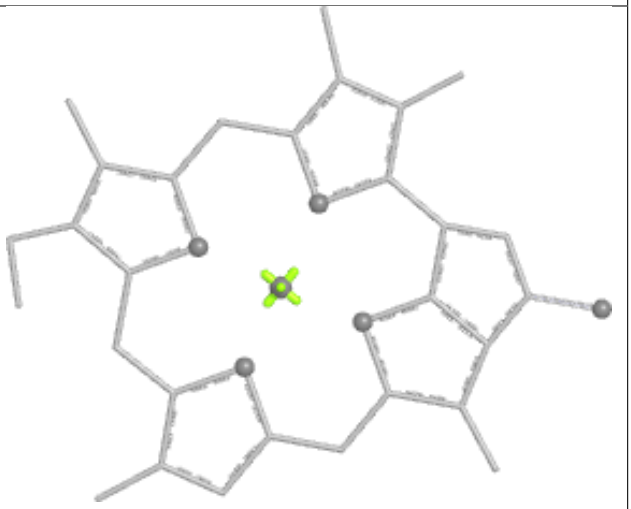
Bond lengths



Bond angles

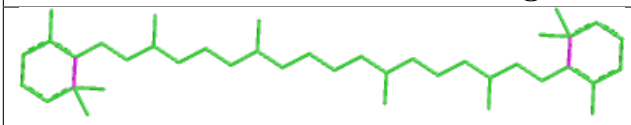


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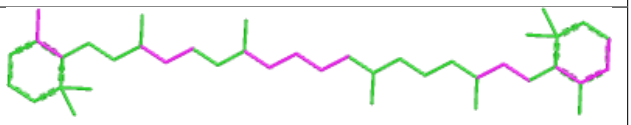


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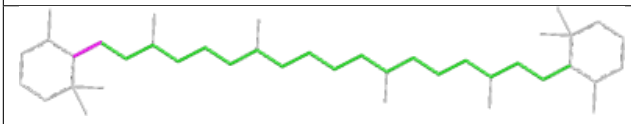
Ligand BCR C 517



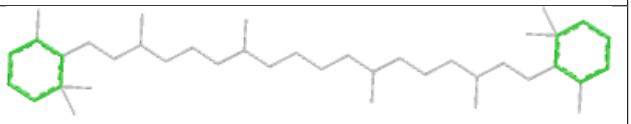
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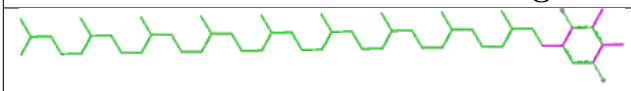
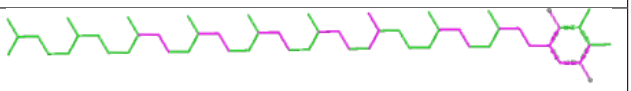
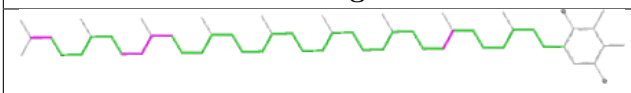
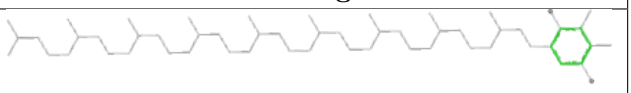
Bond angles

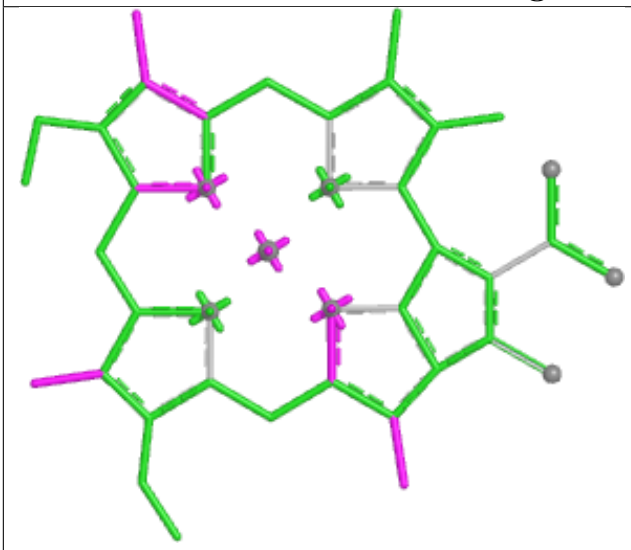
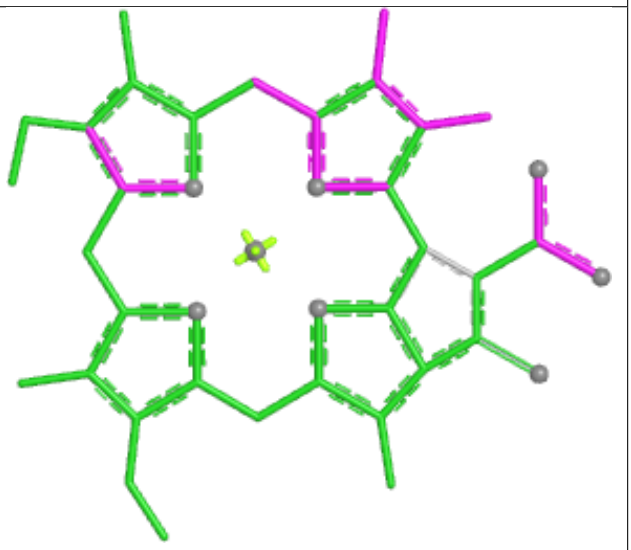
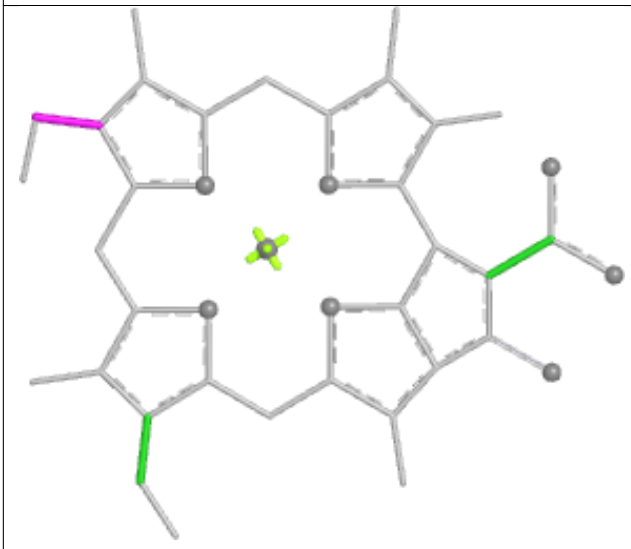
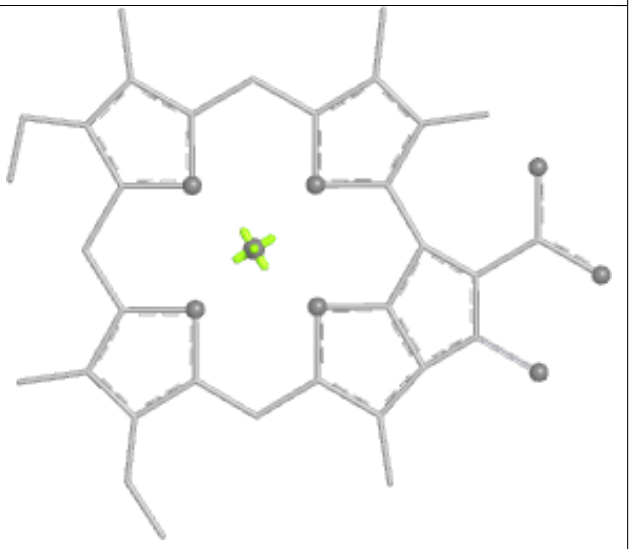


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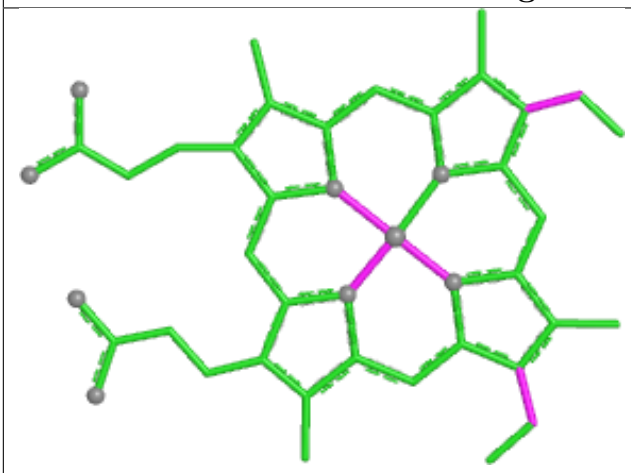


Rings

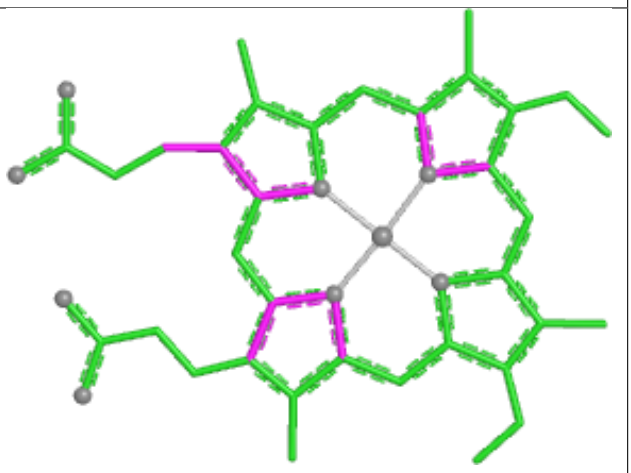
Ligand PL9 d 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

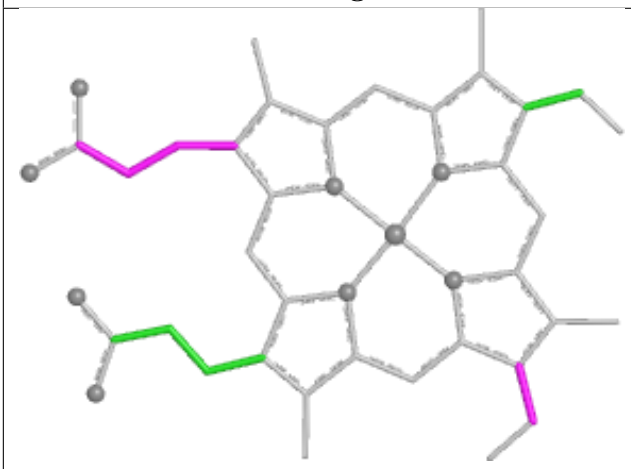
Ligand HEM V 201



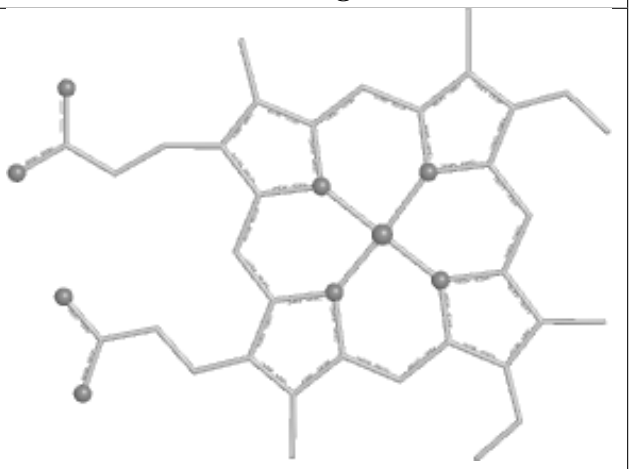
Bond lengths



Bond angles

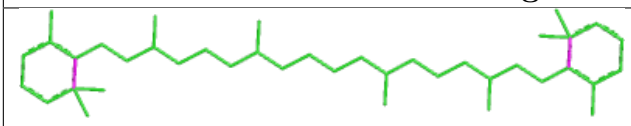


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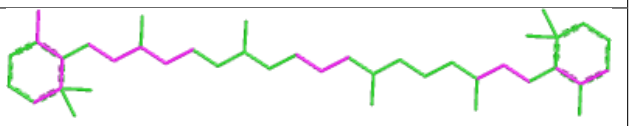


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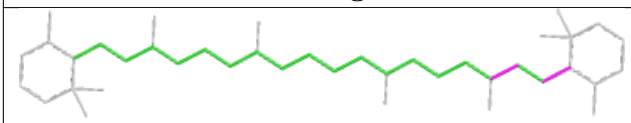
Ligand BCR D 405



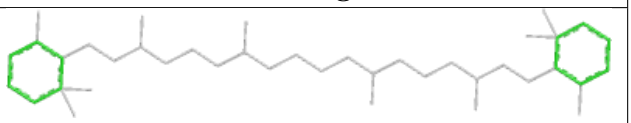
Bond lengths



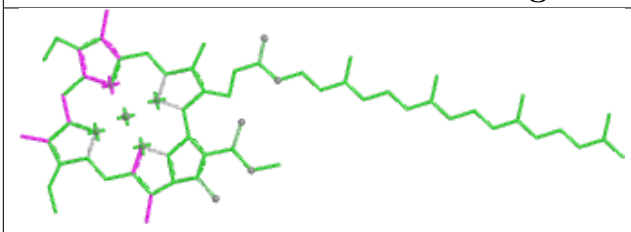
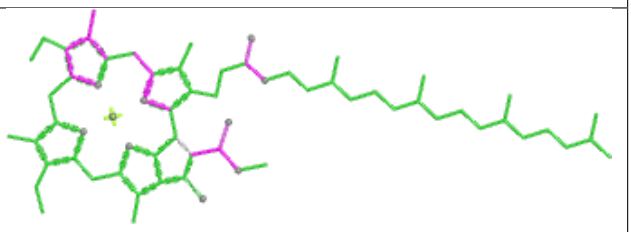
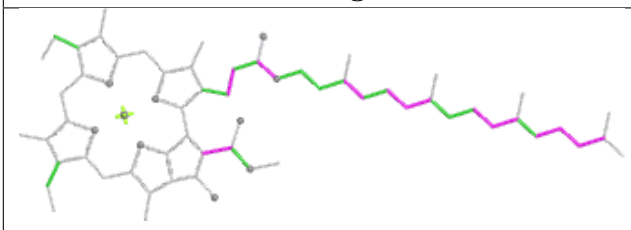
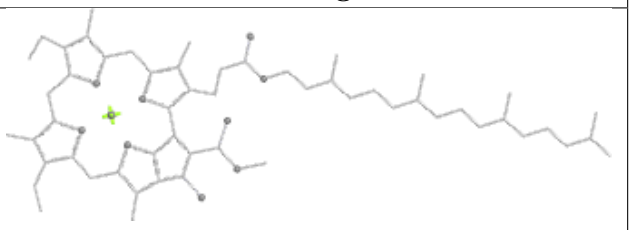
Bond angles



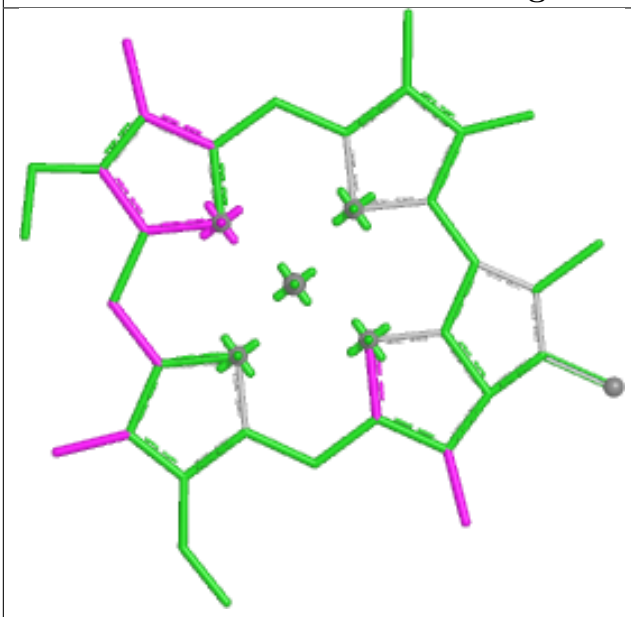
Torsions



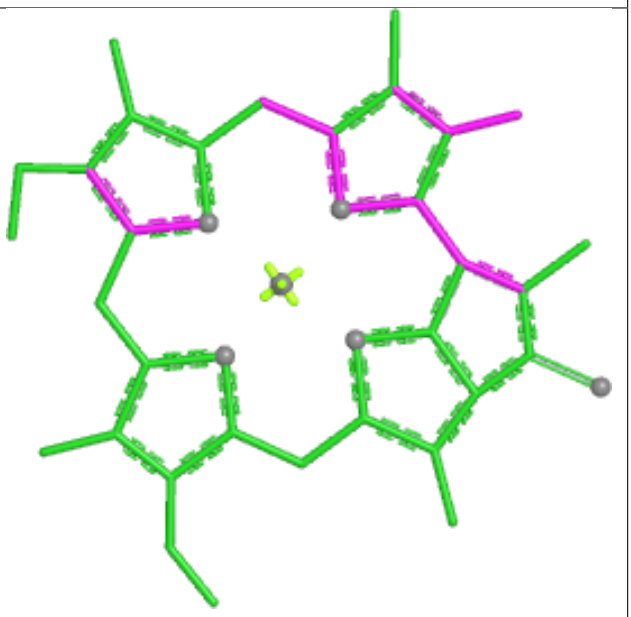
Rings

Ligand CLA c 506	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

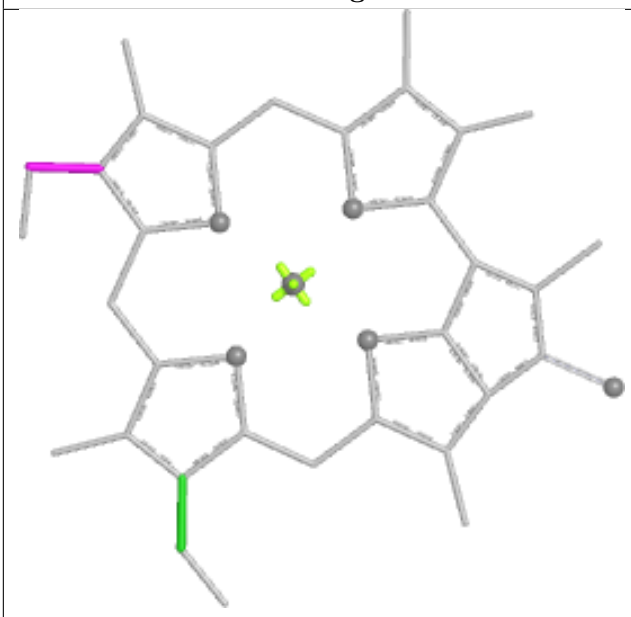
Ligand CLA 4 204



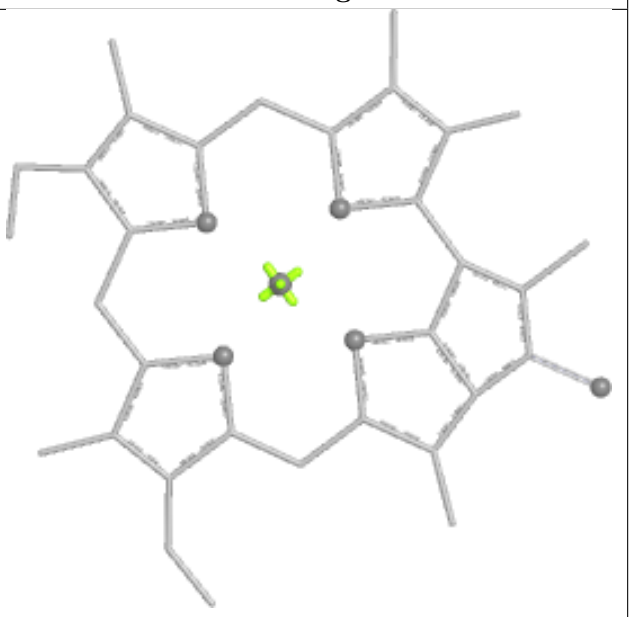
Bond lengths



Bond angles

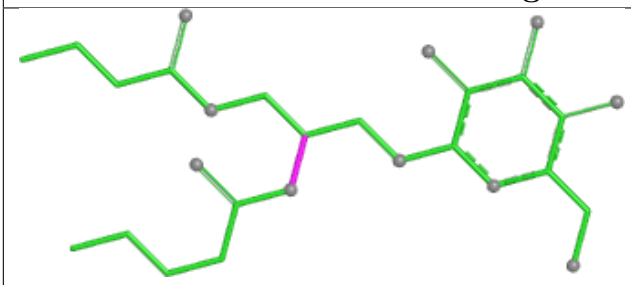


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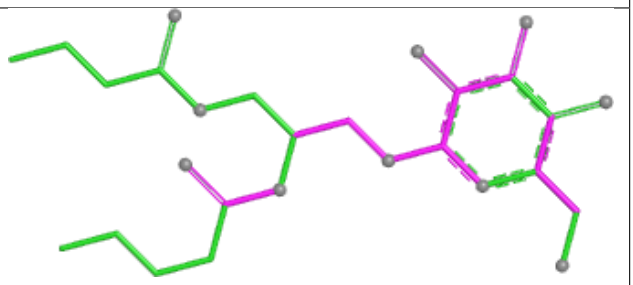


Rings

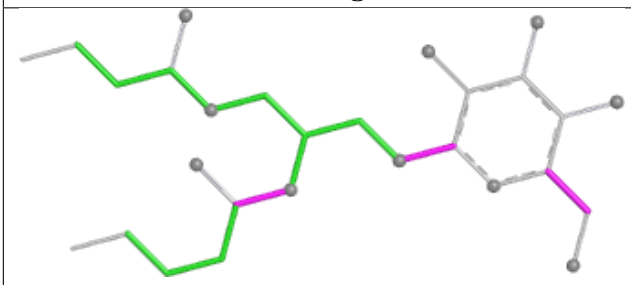
Ligand LMG b 521



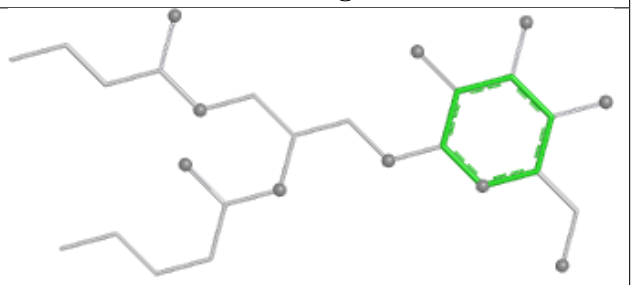
Bond lengths



Bond angles

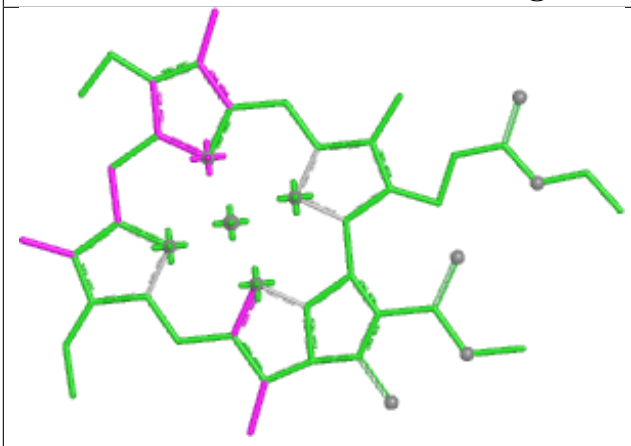


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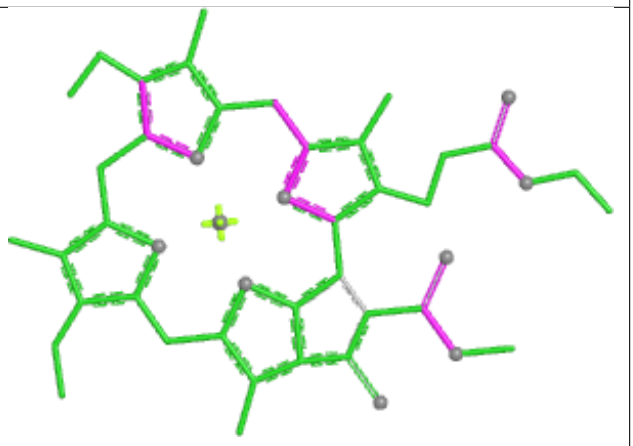


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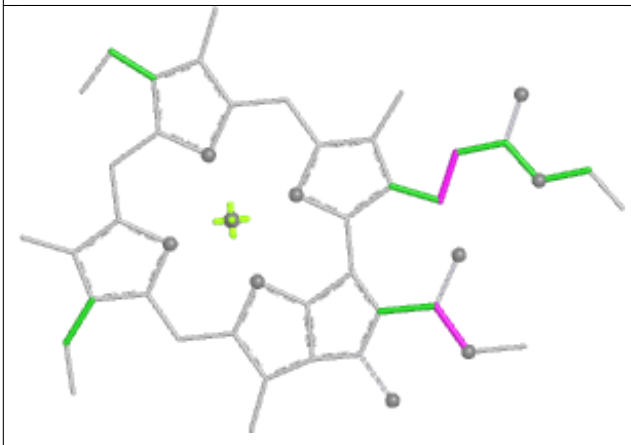
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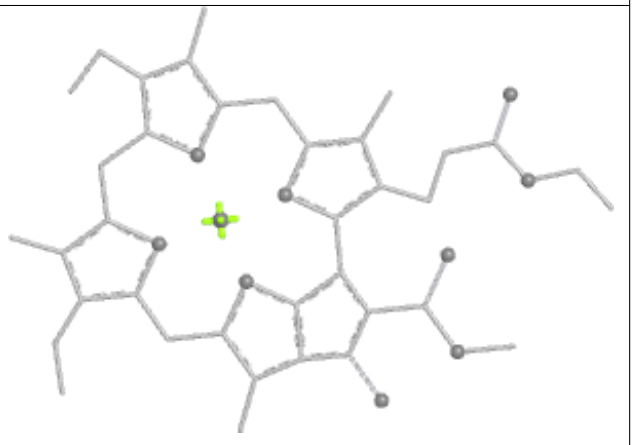
Bond lengths



Bond angles

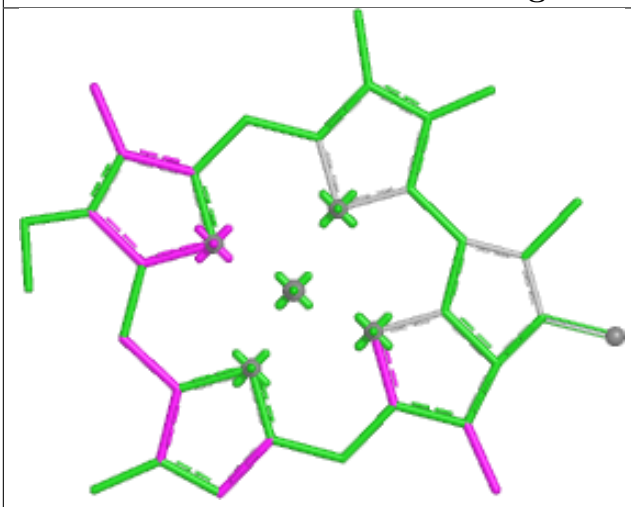


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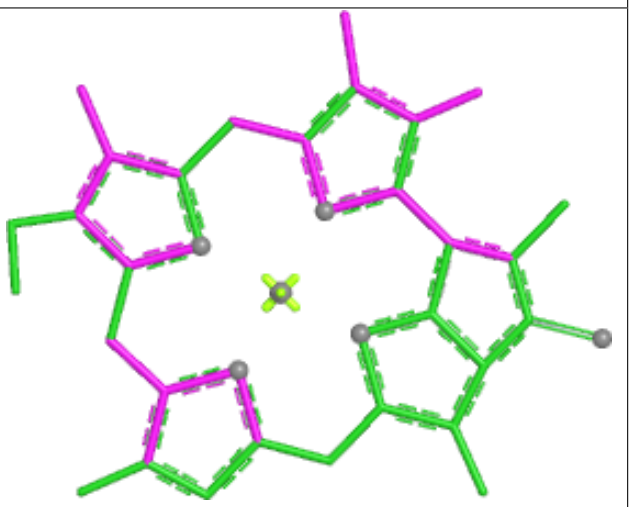


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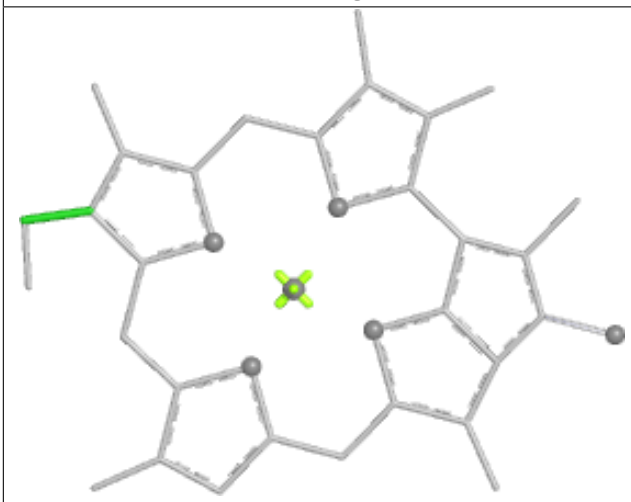
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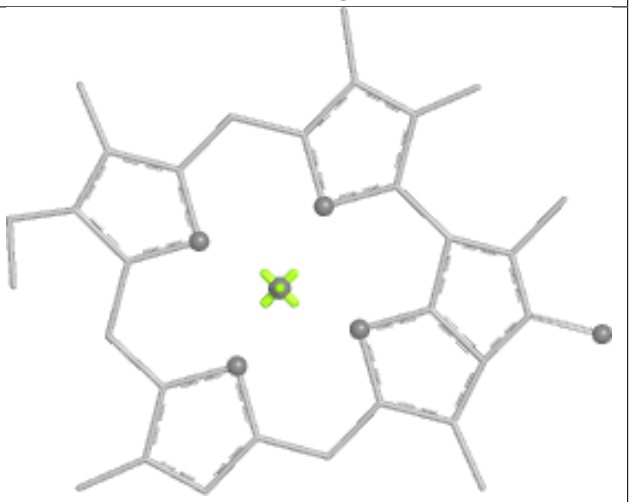
Bond lengths



Bond angles

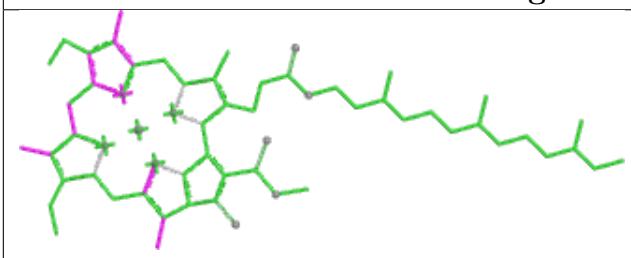


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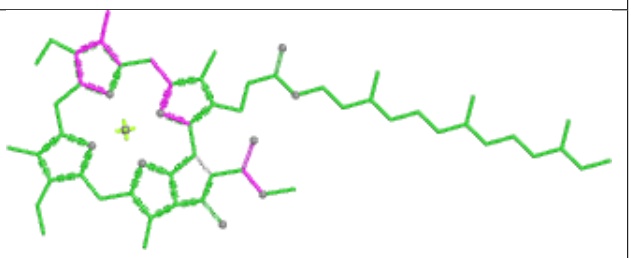


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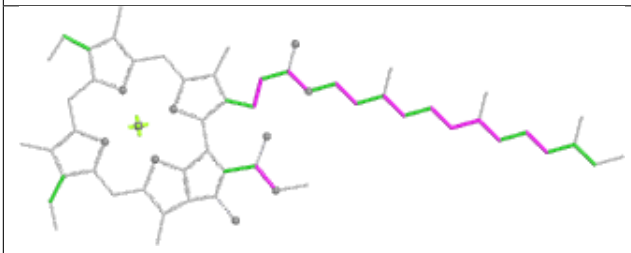
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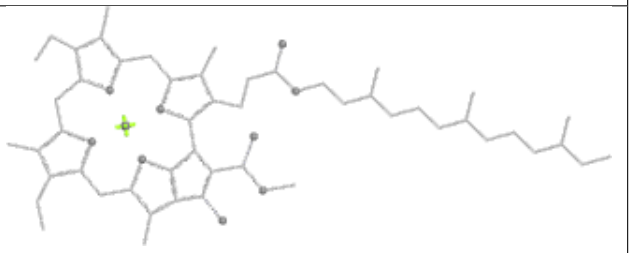
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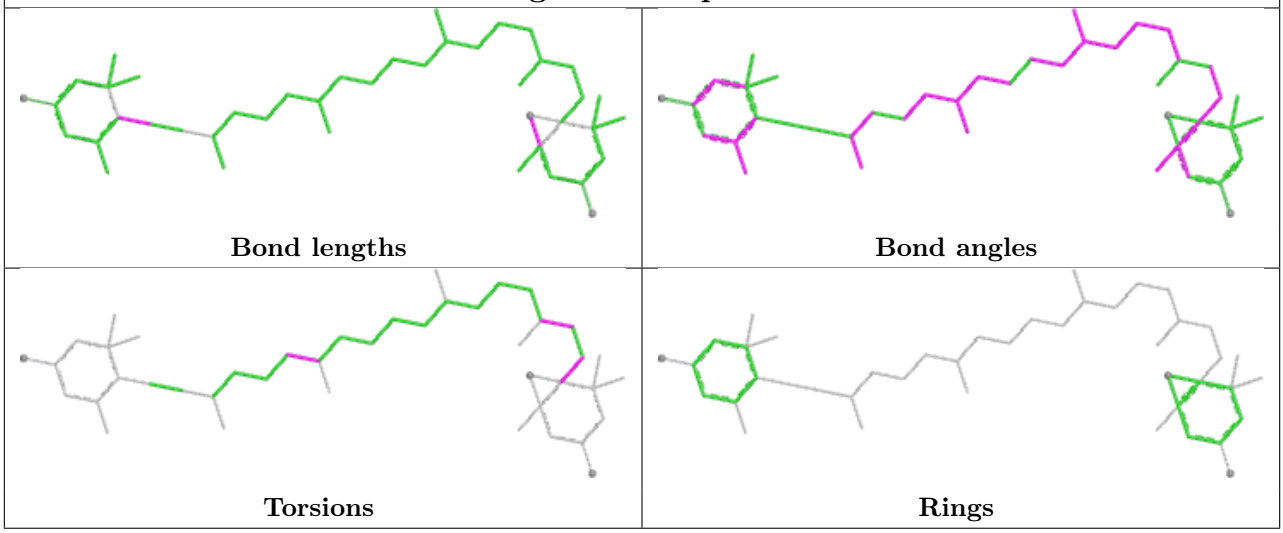


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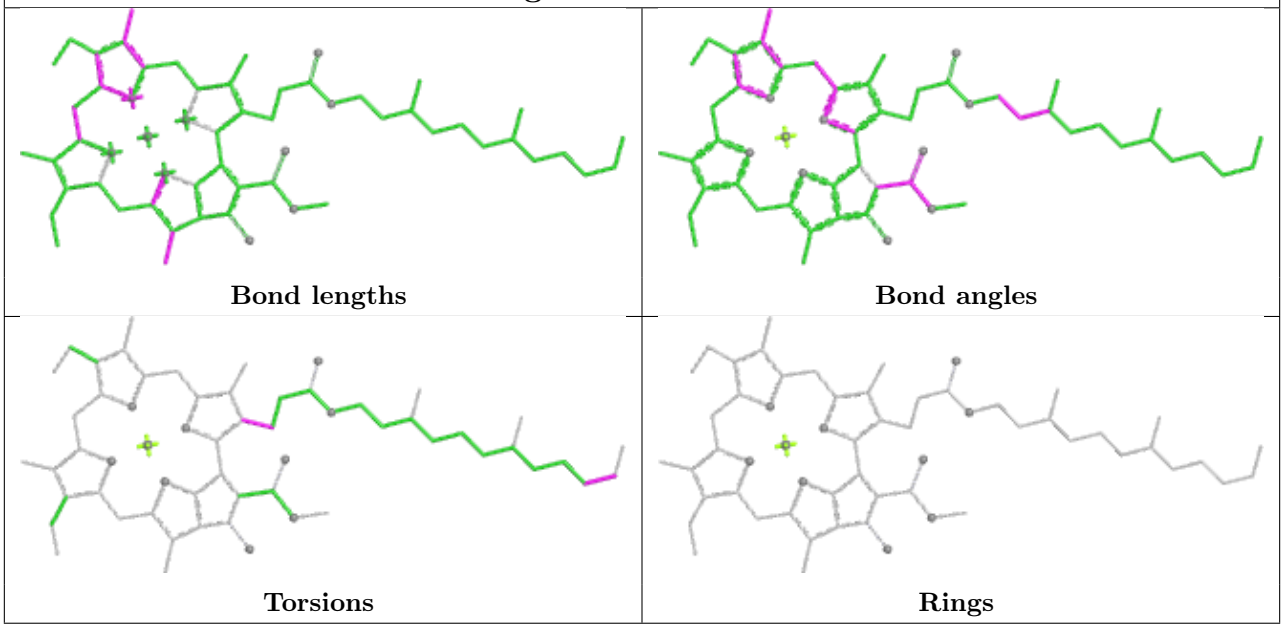


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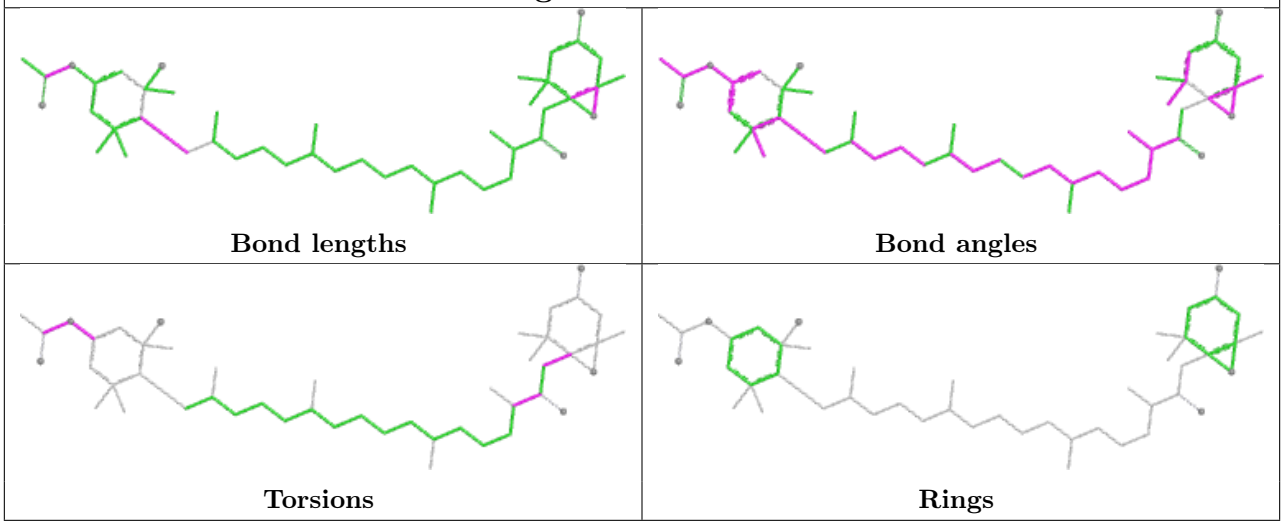
Ligand DD6 p 611



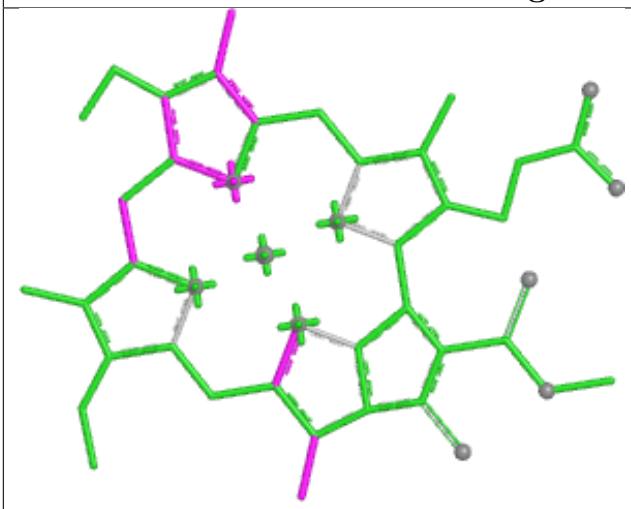
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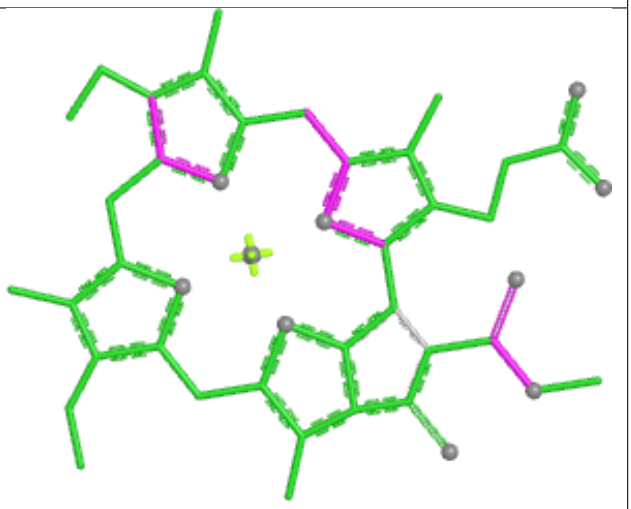
Ligand A86 0 317



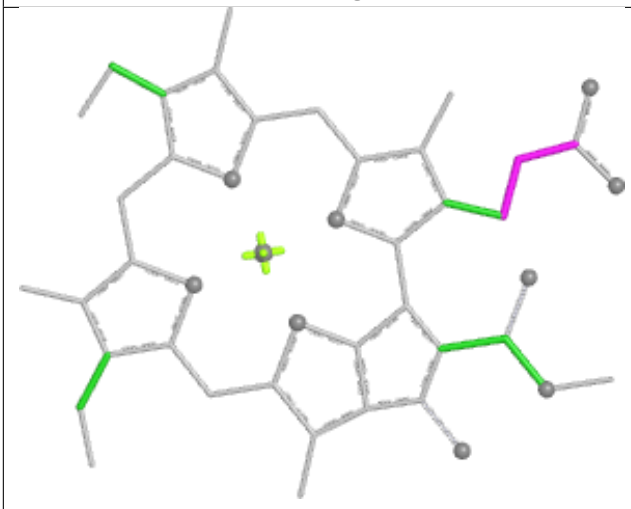
Ligand CLA 0 306



Bond lengths



Bond angles

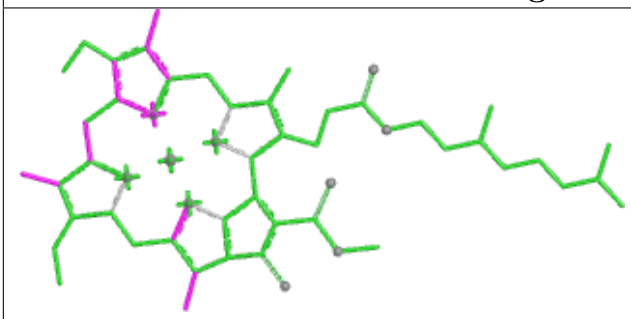


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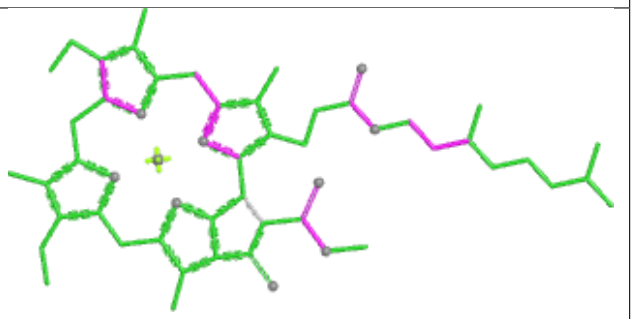


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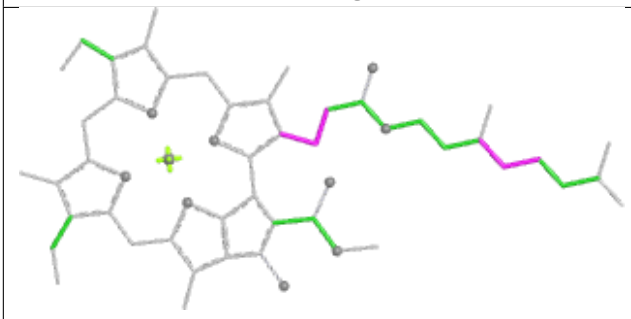
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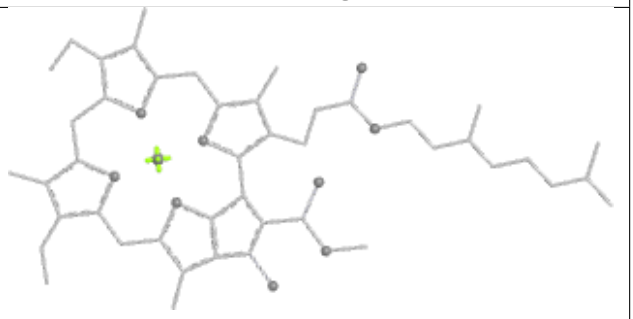
Bond lengths



Bond angles

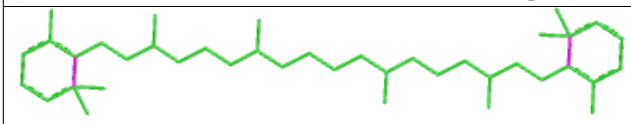


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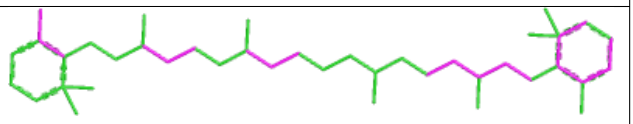


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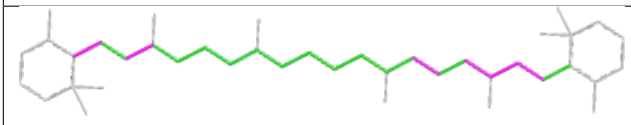
Ligand BCR B 519



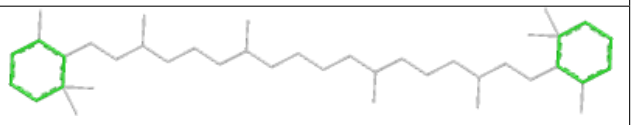
Bond lengths



Bond angles

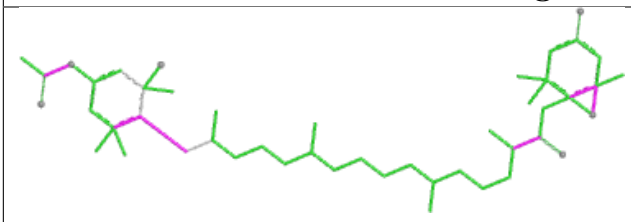


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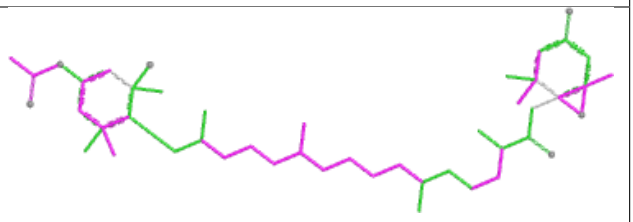


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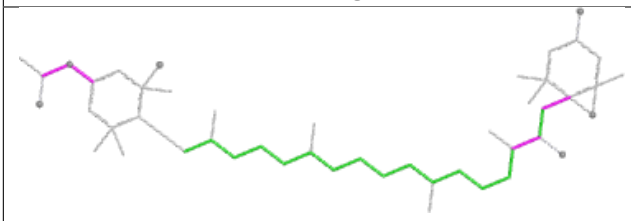
Ligand A86 2 302



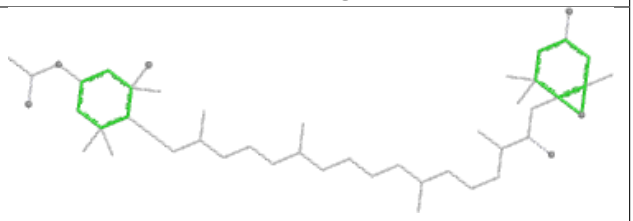
Bond lengths



Bond angles

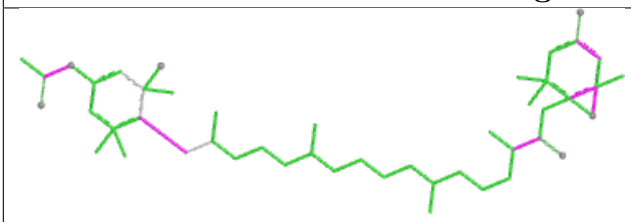


Torsions

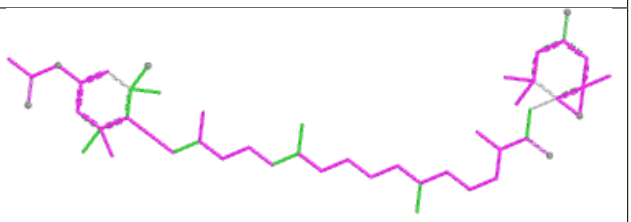


Rings

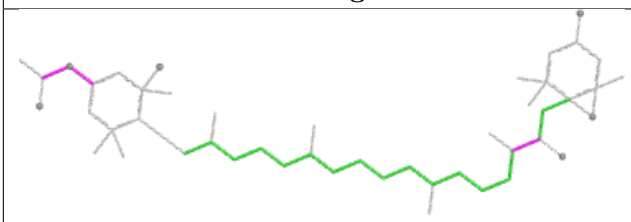
Ligand A86 9 202



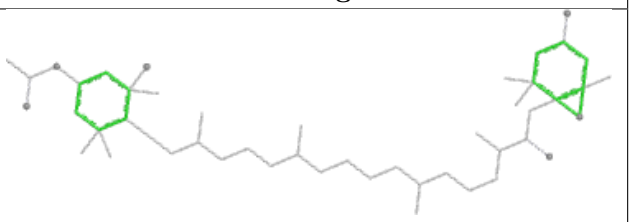
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Bond angles

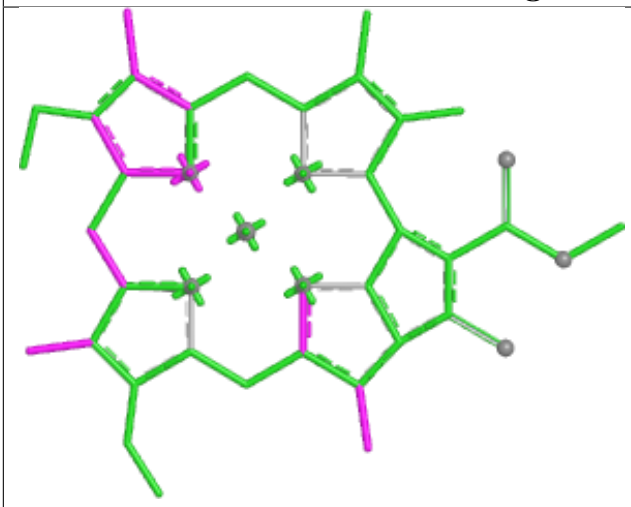


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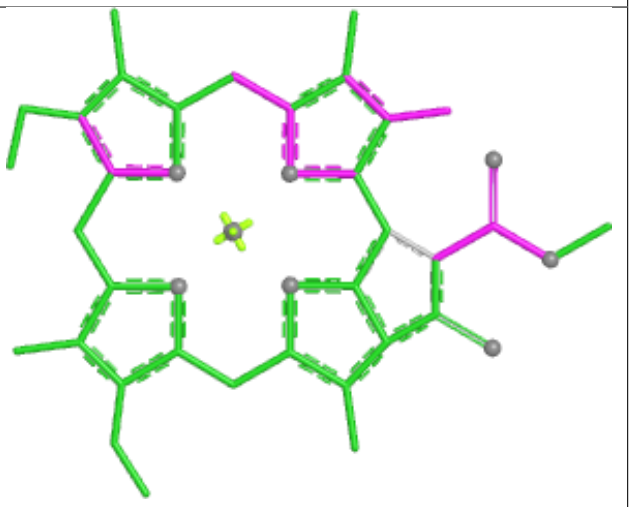


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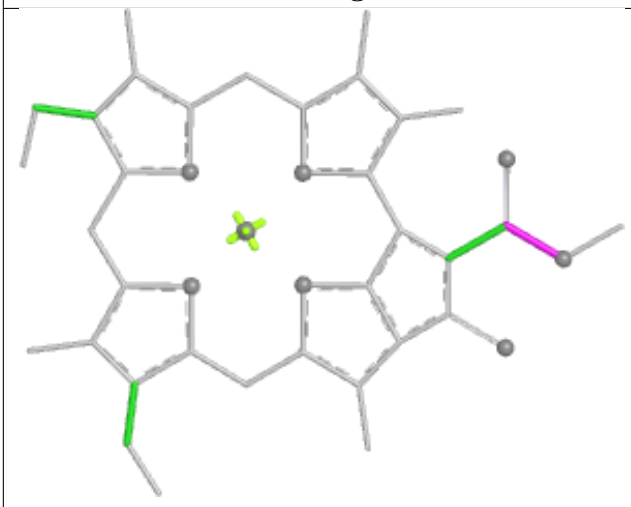
Ligand CLA B 507



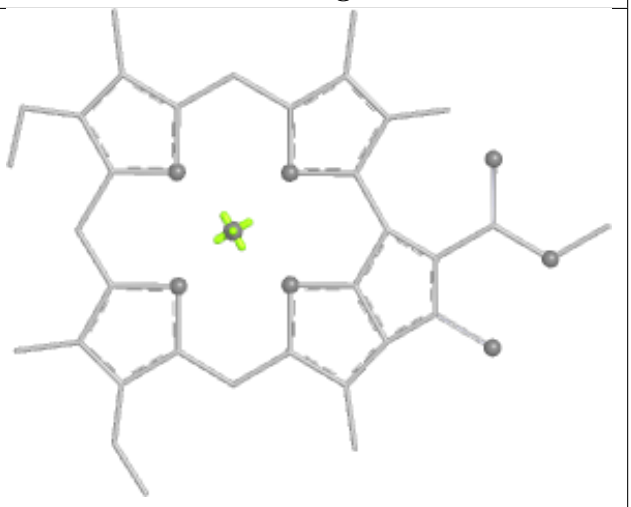
Bond lengths



Bond angles

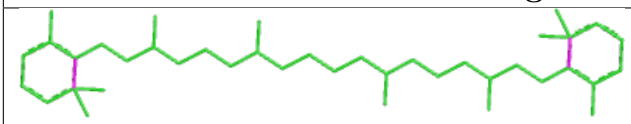


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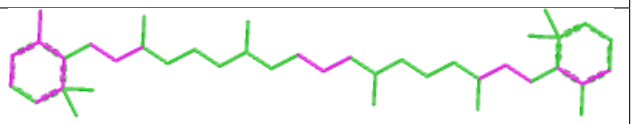


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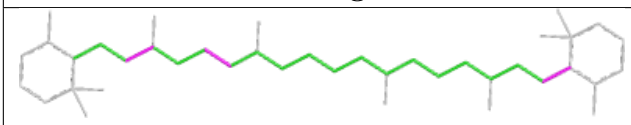
Ligand BCR h 101



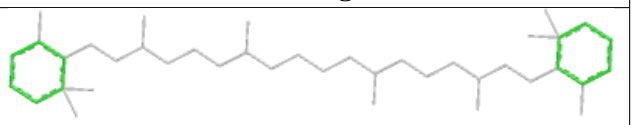
Bond lengths



Bond angles

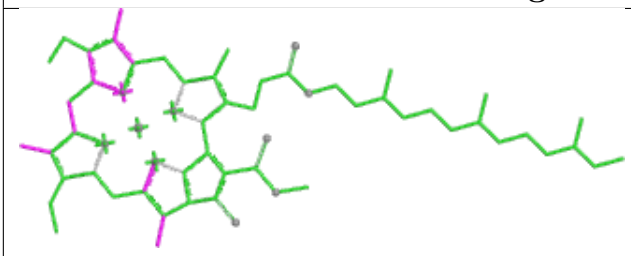


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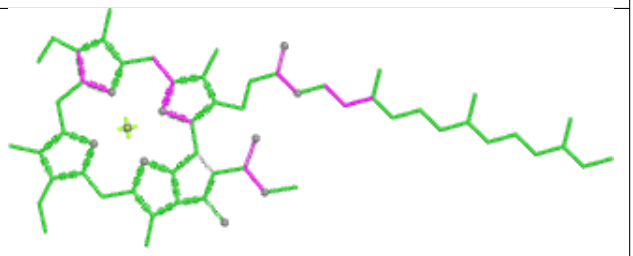


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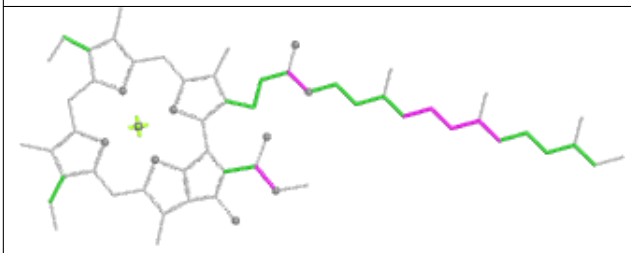
Ligand CLA 0 308



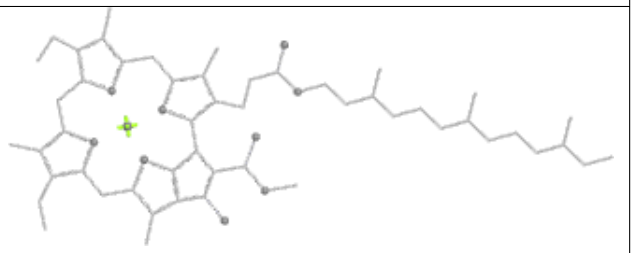
Bond lengths



Bond angles

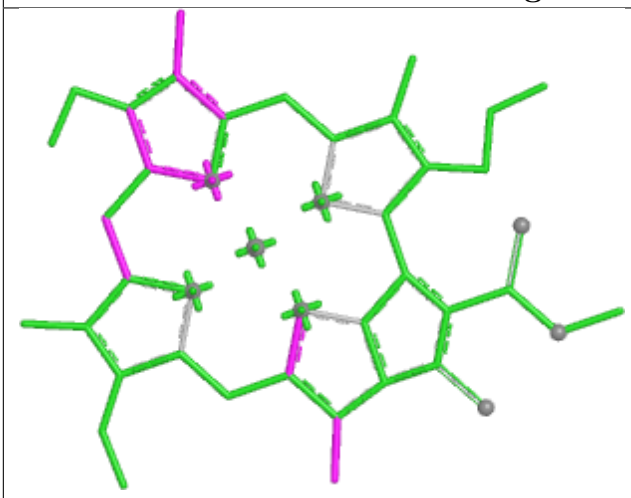


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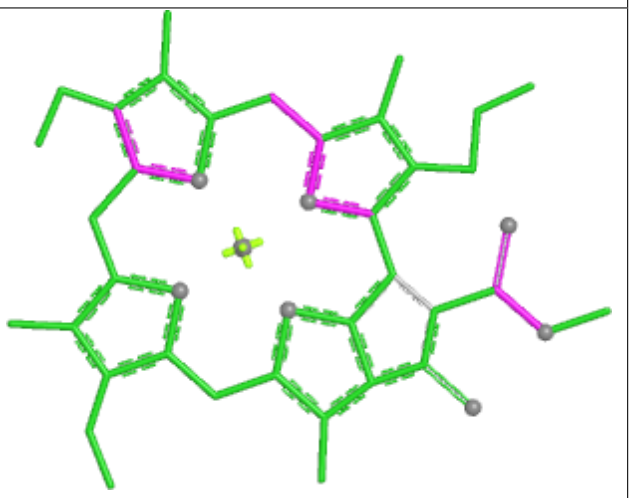


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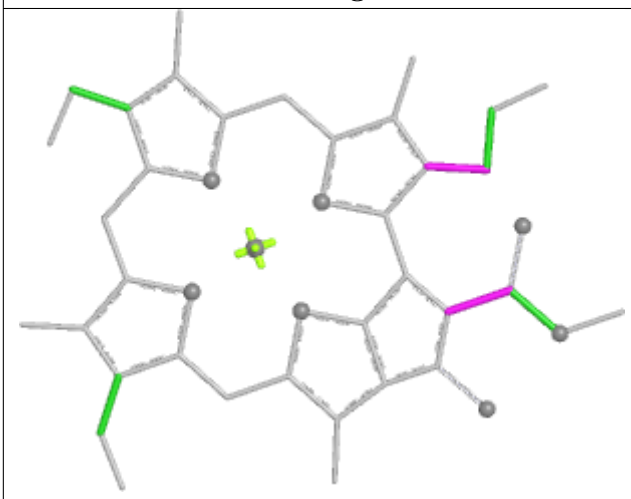
Ligand CLA B 501



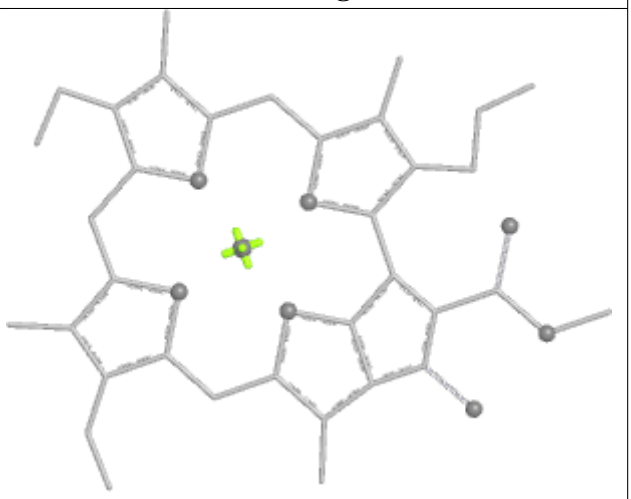
Bond lengths



Bond angles

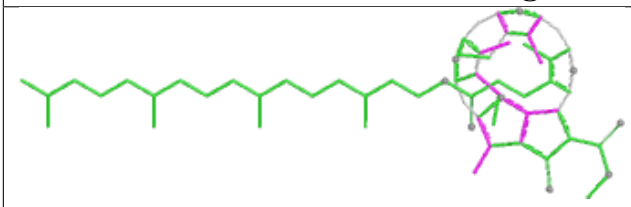


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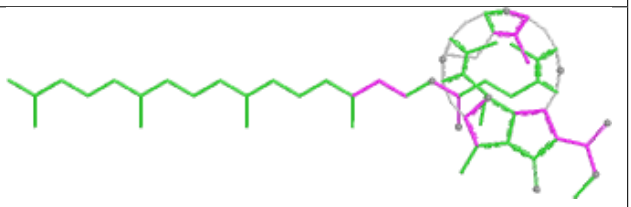


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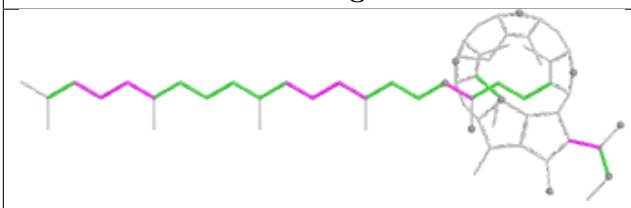
Ligand PHO A 405



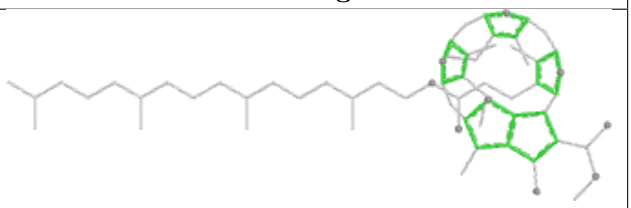
Bond lengths



Bond angles

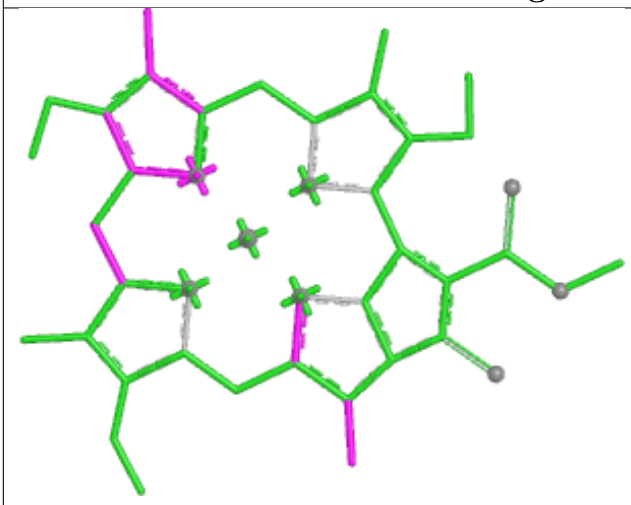


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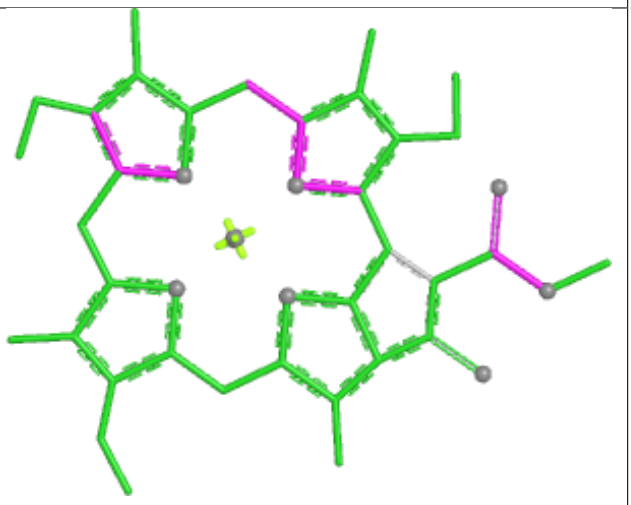


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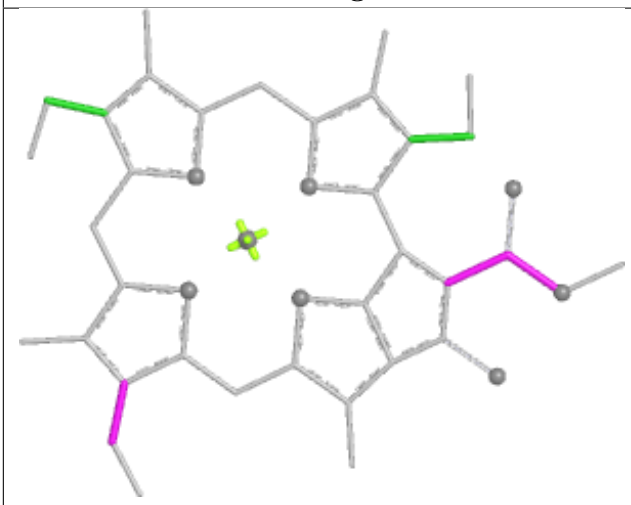
Ligand CLA 5 312



Bond lengths



Bond angles

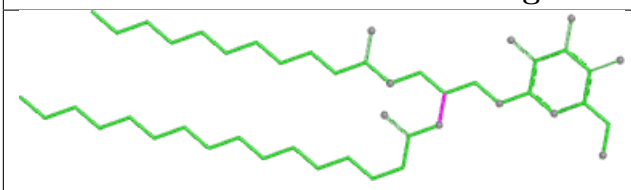


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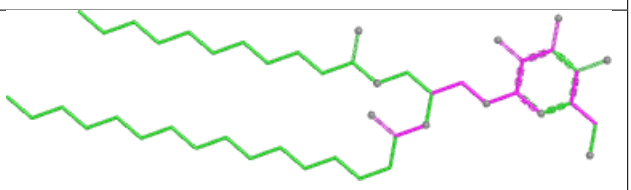


Rings

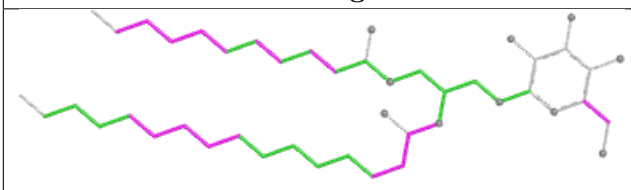
Ligand LMG d 408



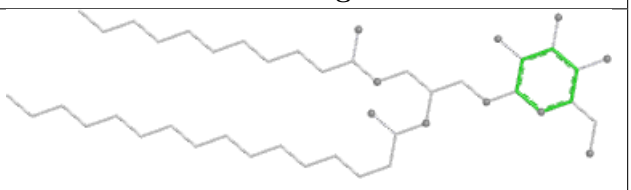
Bond lengths



Bond angles

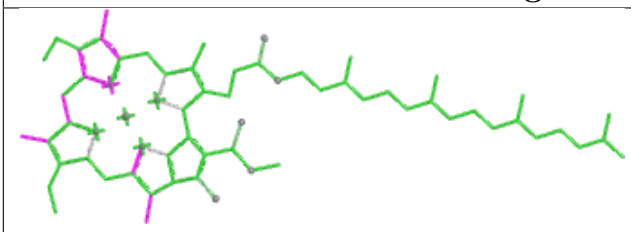


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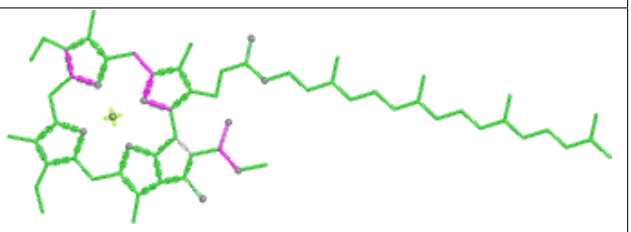


Rings

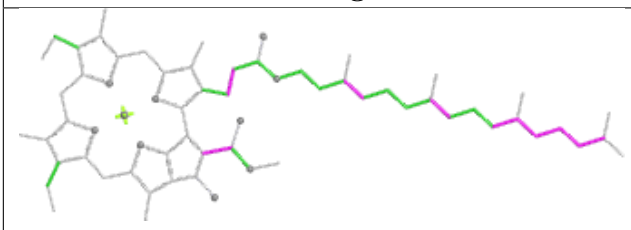
Ligand CLA C 508



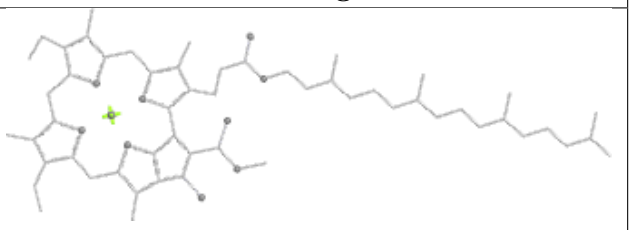
Bond lengths



Bond angles

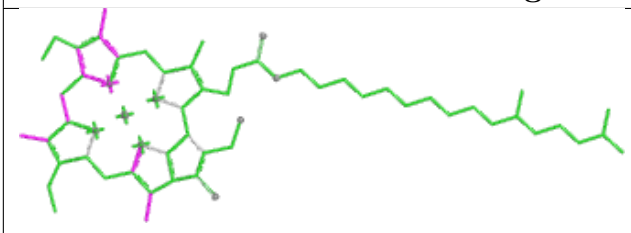


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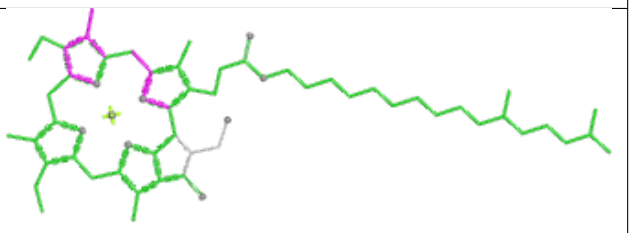


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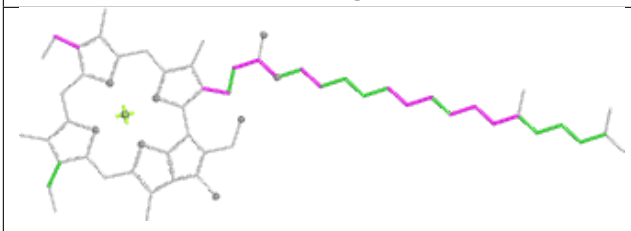
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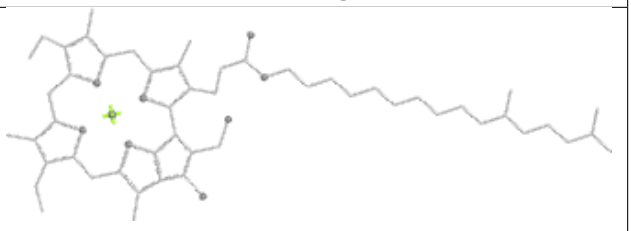
Bond lengths



Bond angles

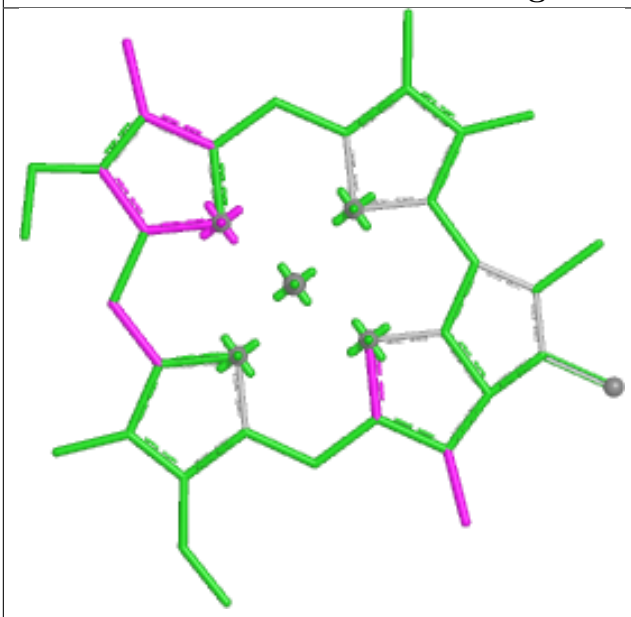


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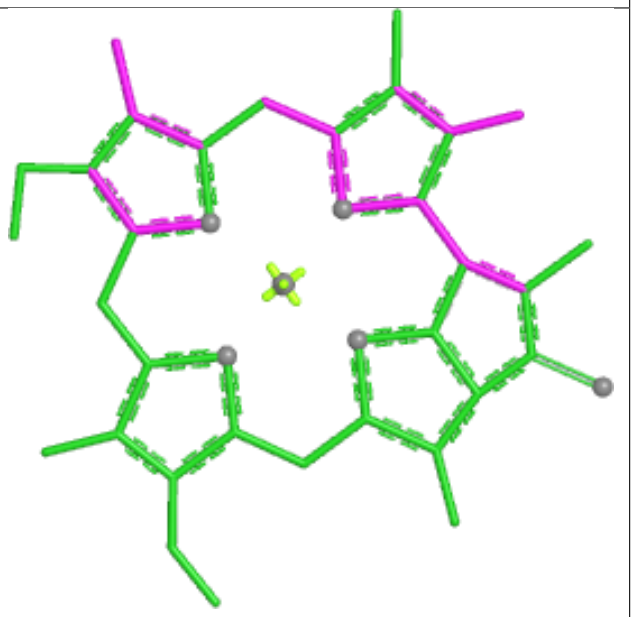


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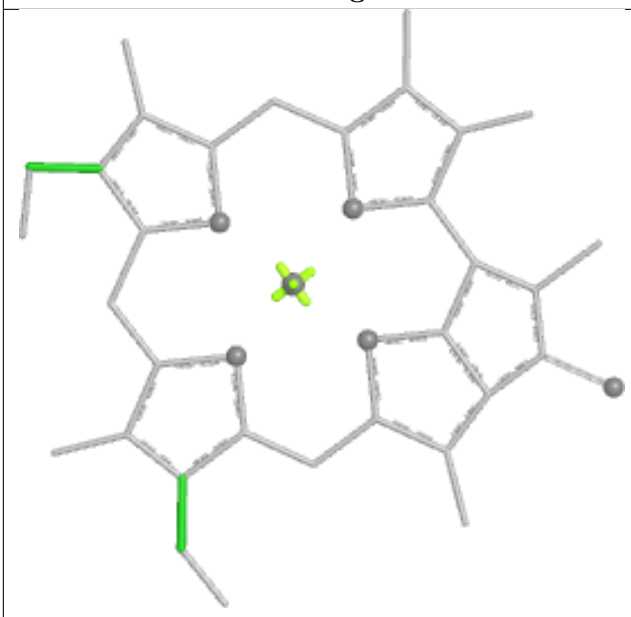
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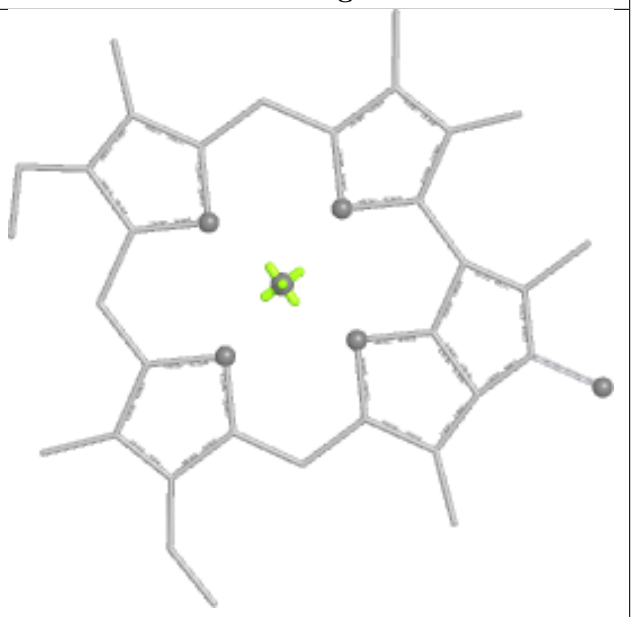
Bond lengths



Bond angles

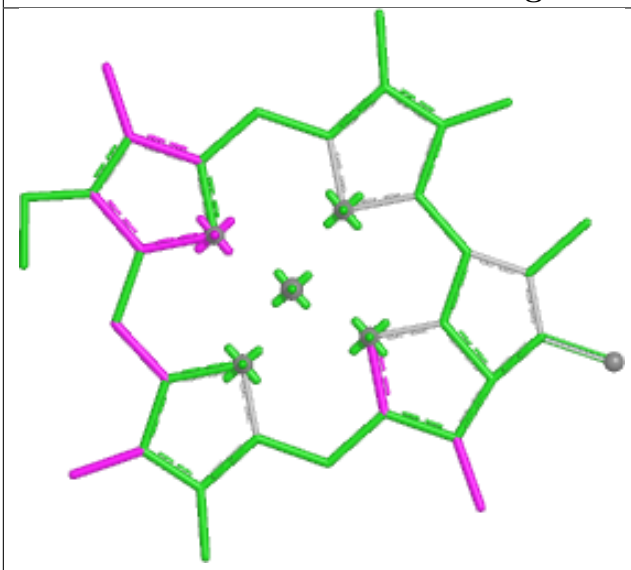


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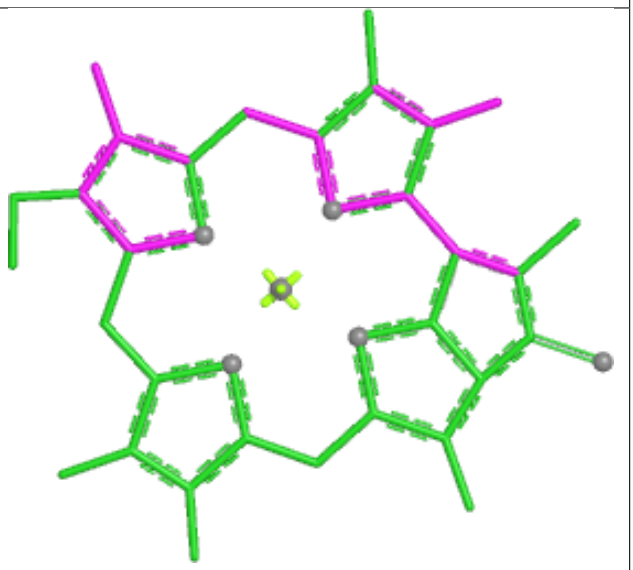


Rings

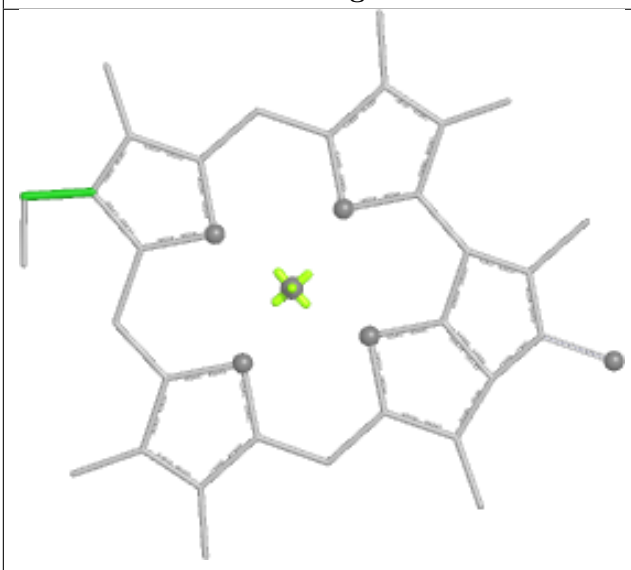
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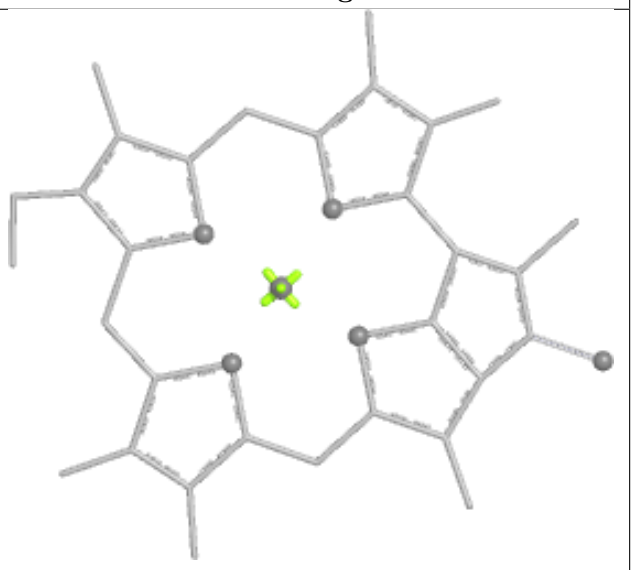
Bond lengths



Bond angles

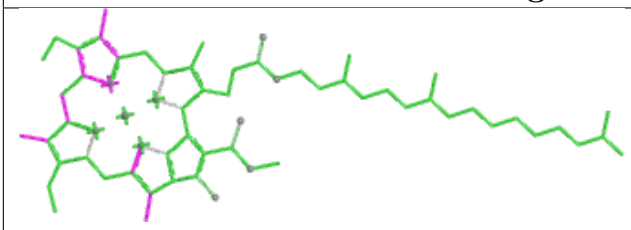


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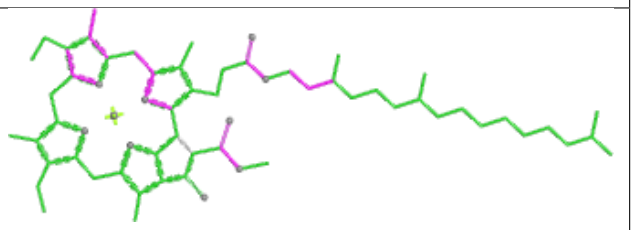


Rings

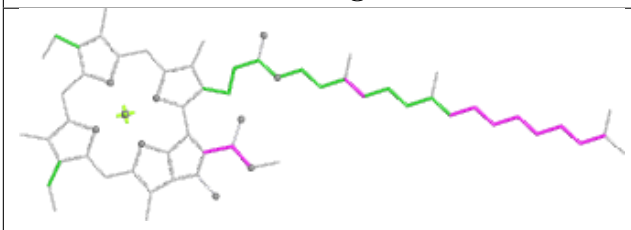
Ligand CLA b 512



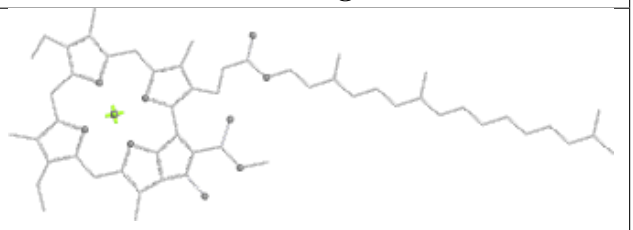
Bond lengths



Bond angles

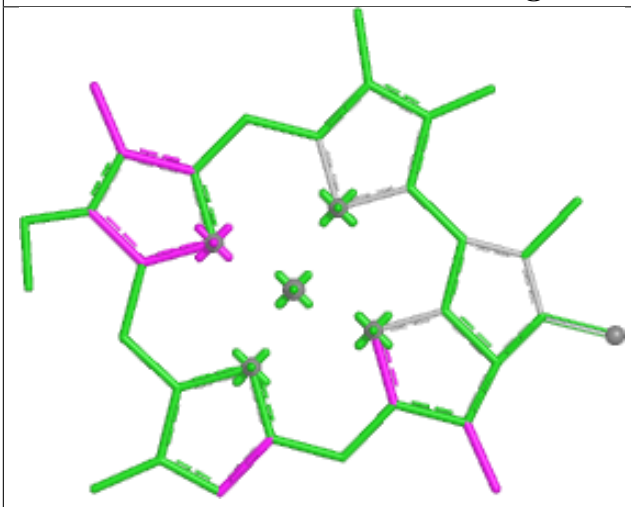


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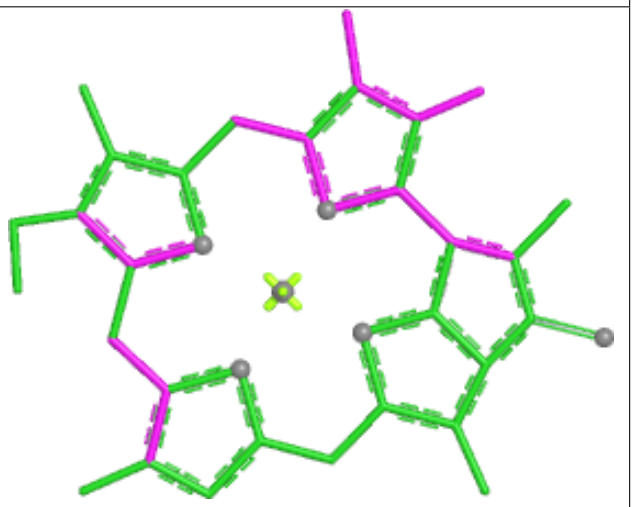


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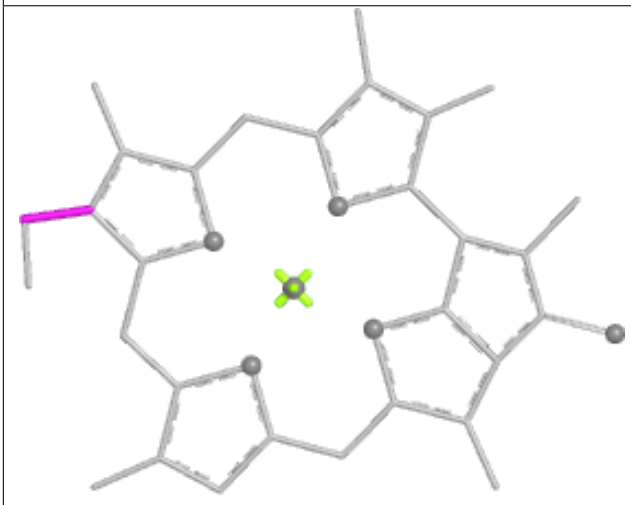
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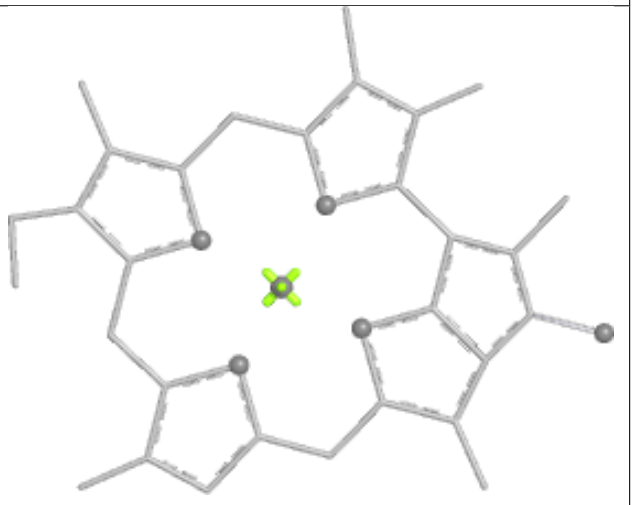
Bond lengths



Bond angles

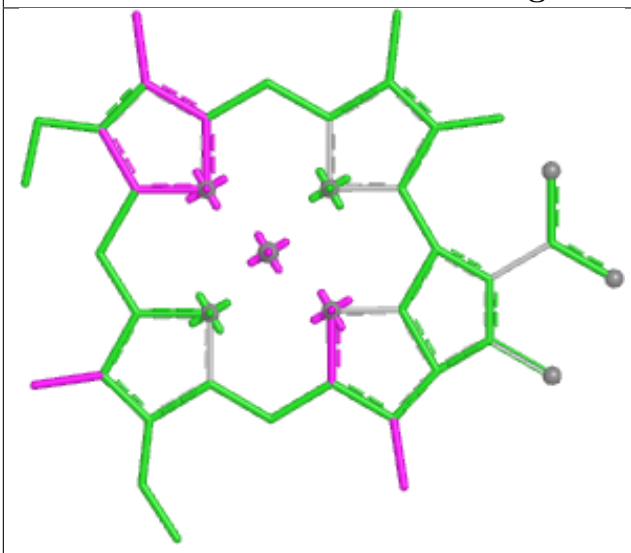


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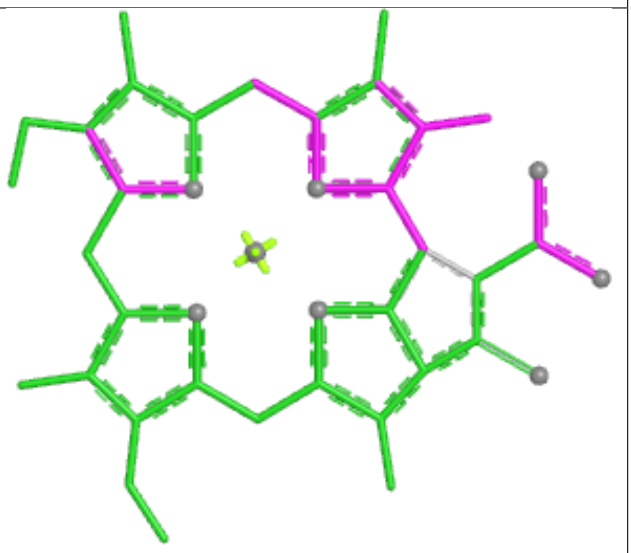


Rings

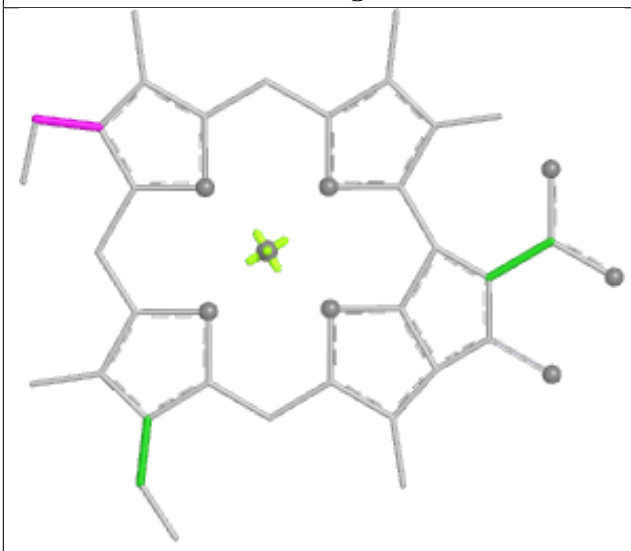
Ligand CLA 9 208



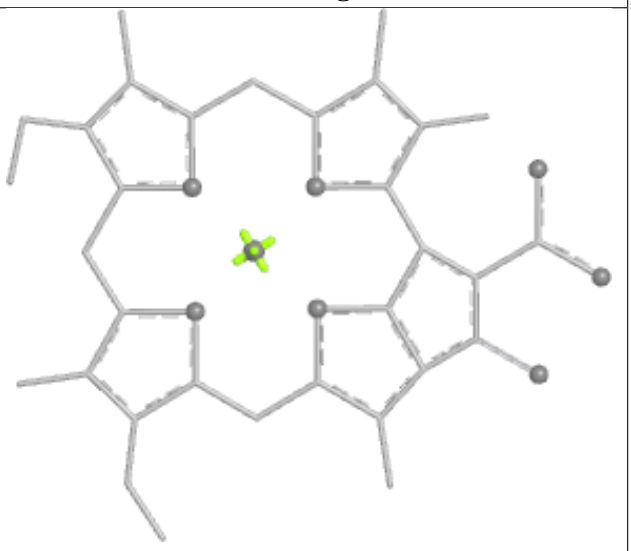
Bond lengths



Bond angles

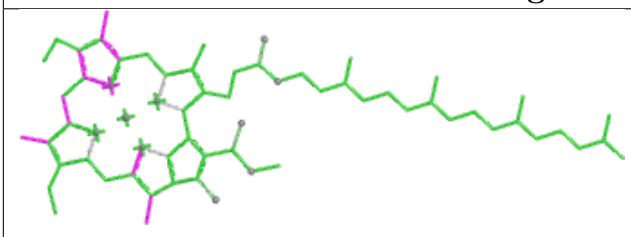


Torsions

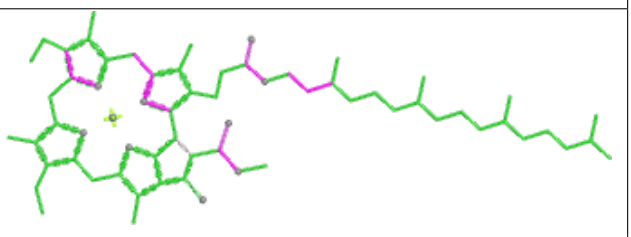


Rings

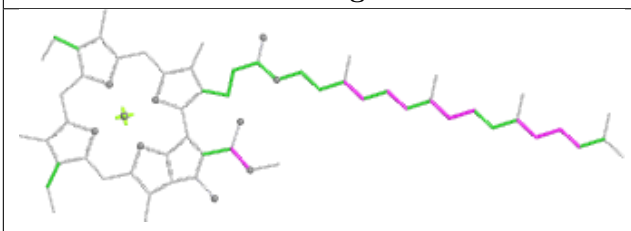
Ligand CLA b 506



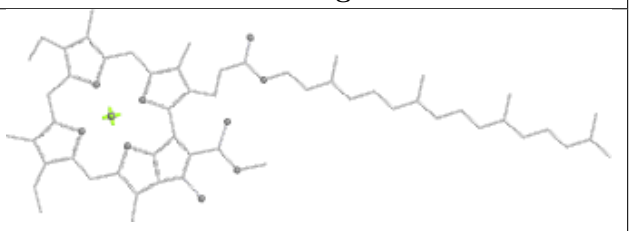
Bond lengths



Bond angles

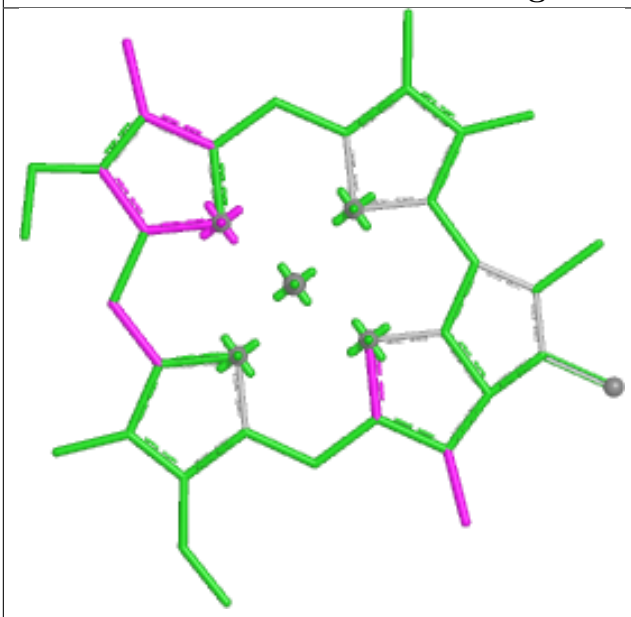


Torsions

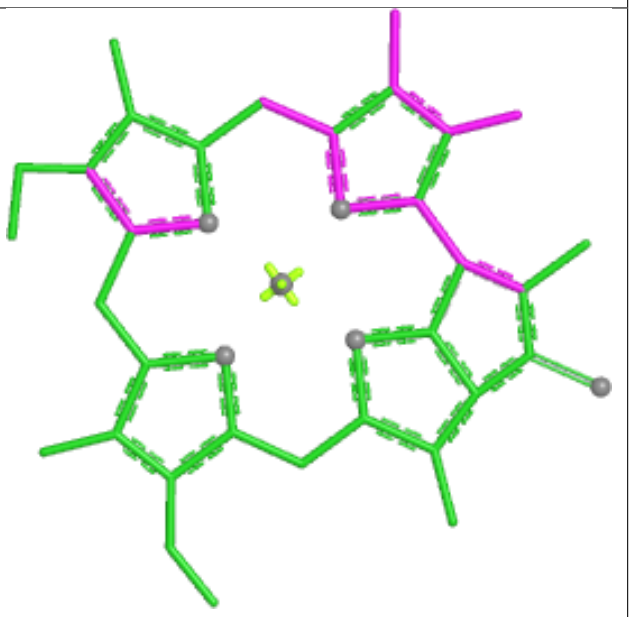


Rings

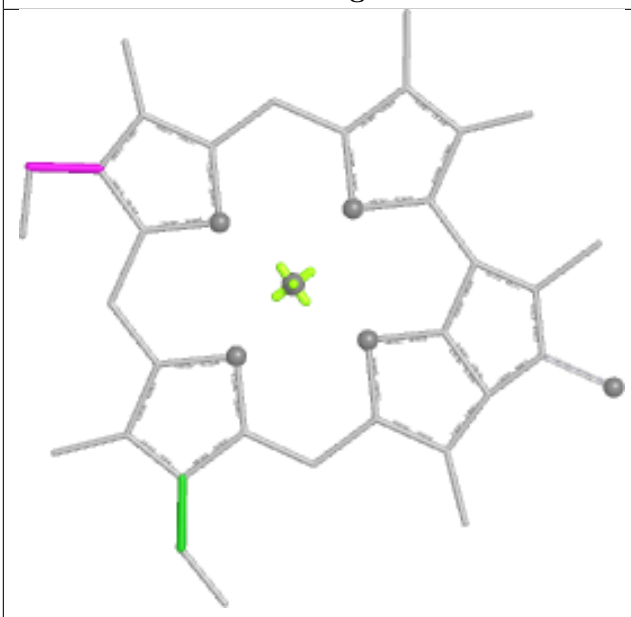
Ligand CLA 7 315



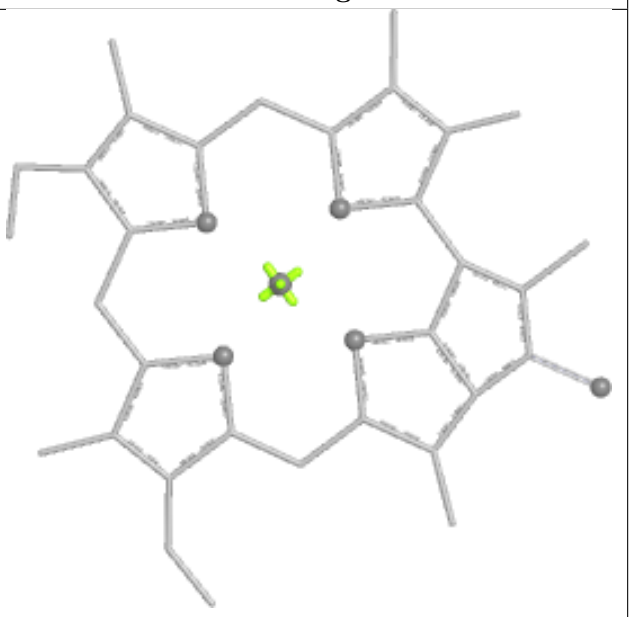
Bond lengths



Bond angles

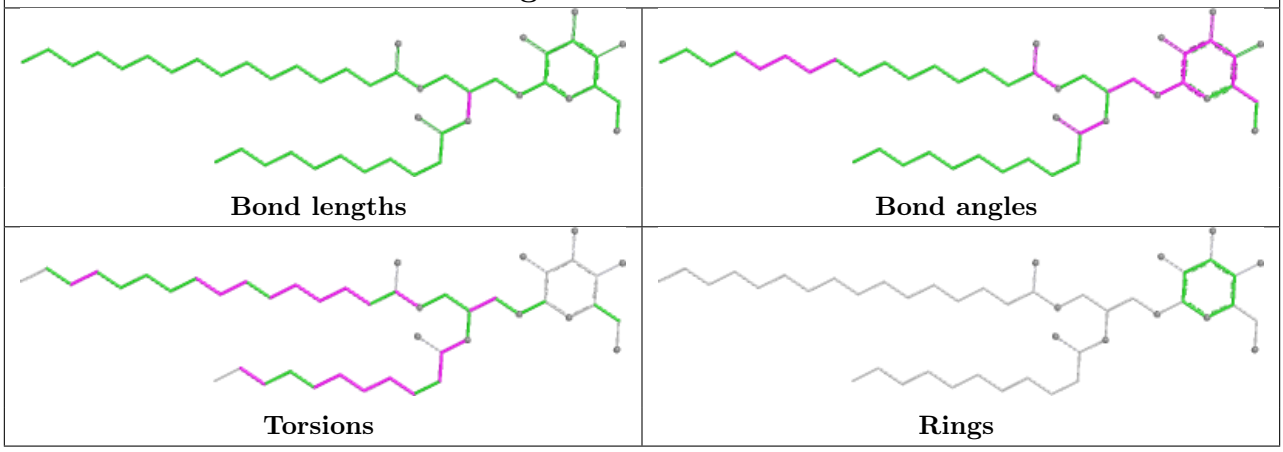


Torsions

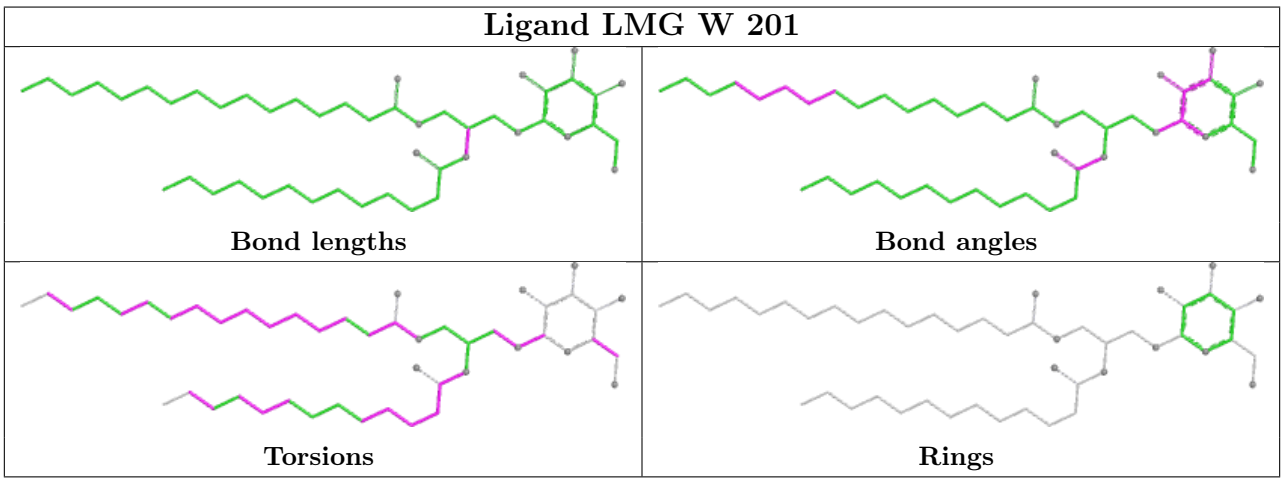


Rings

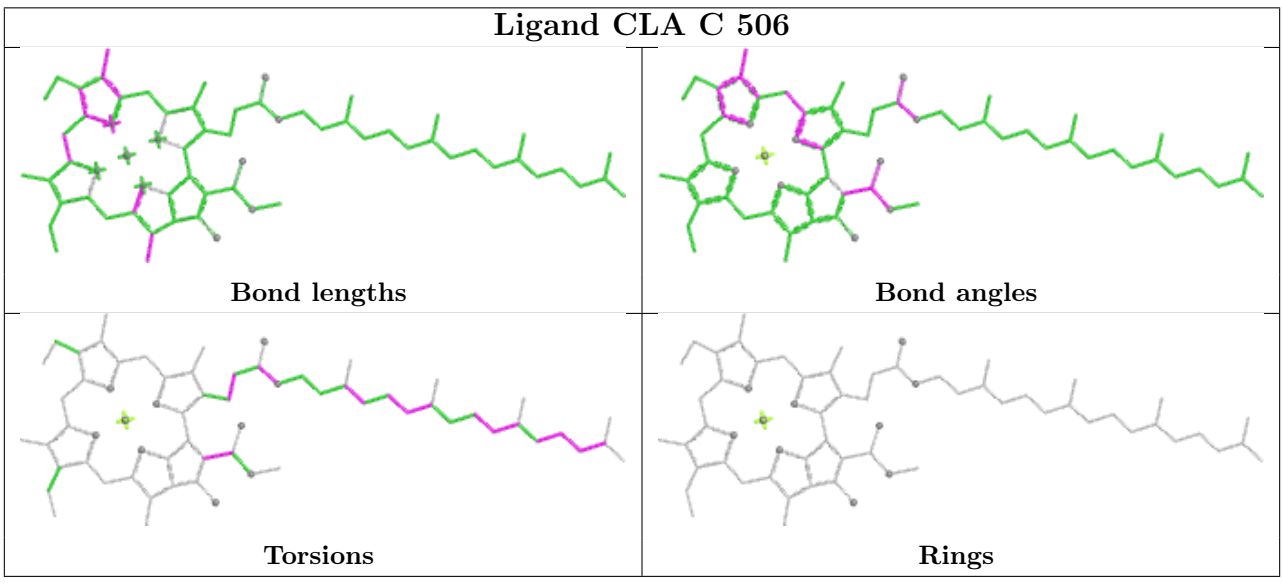
Ligand LMG Y 101



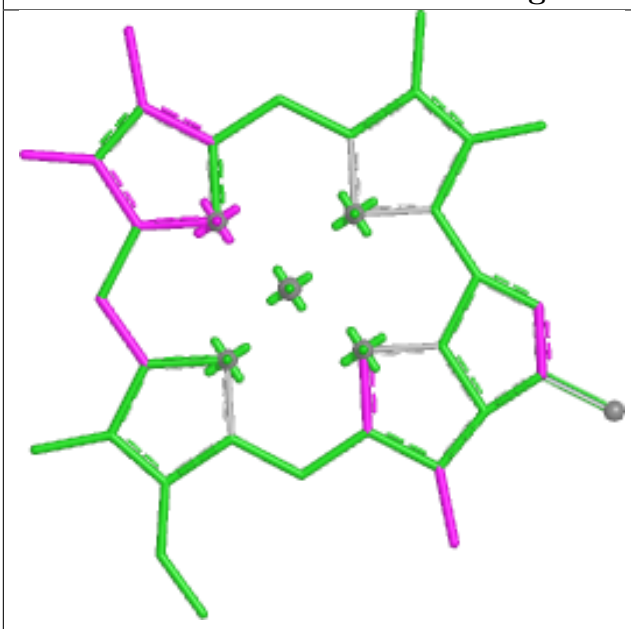
Ligand LMG W 201



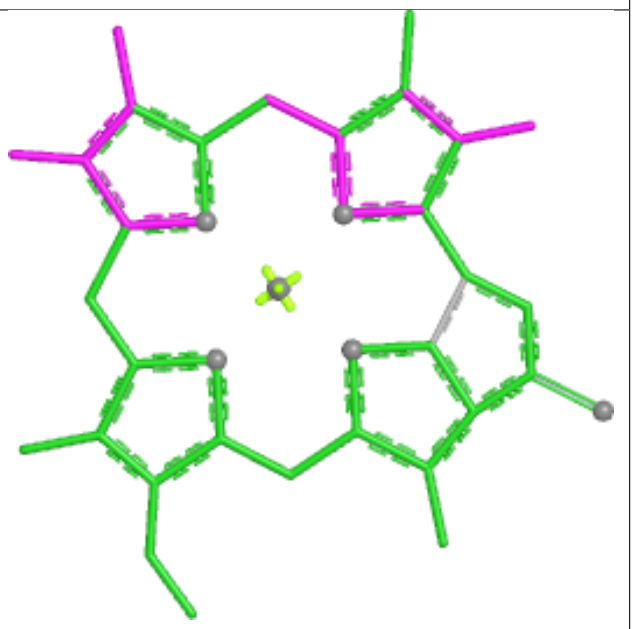
Ligand CLA C 506



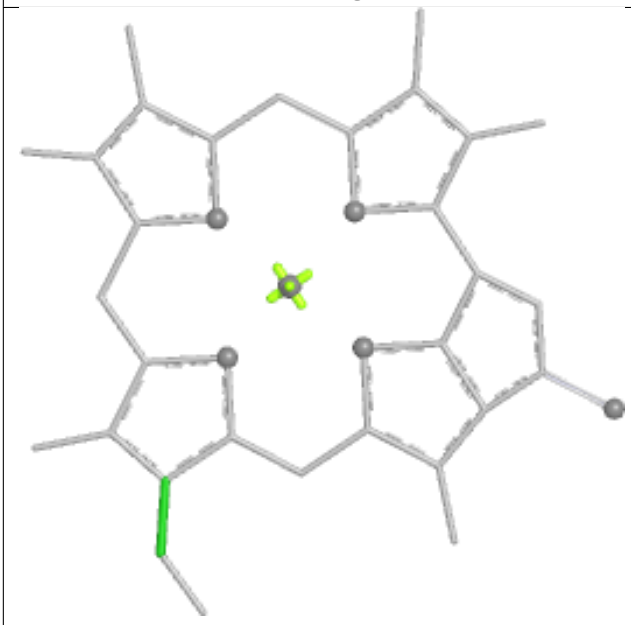
Ligand CLA 4 212



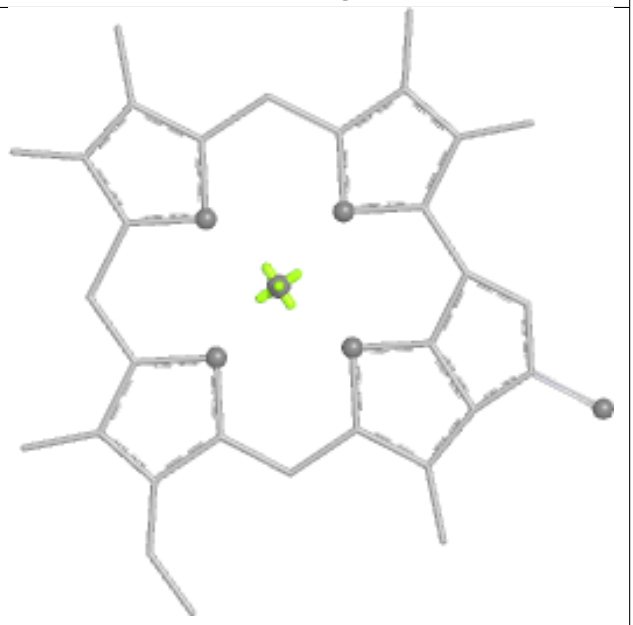
Bond lengths



Bond angles

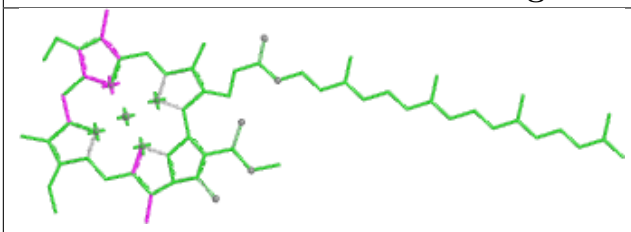


Torsions

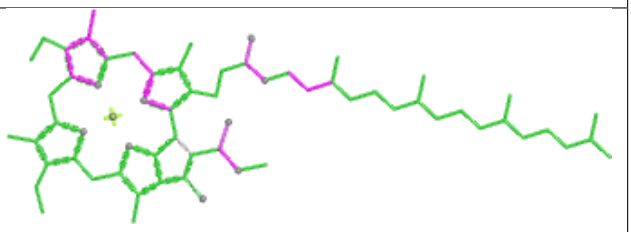


Rings

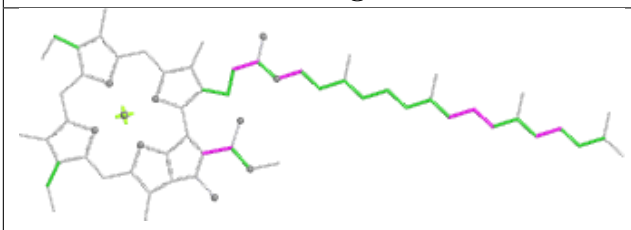
Ligand CLA b 514



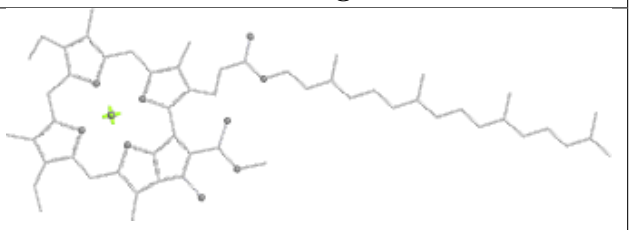
Bond lengths



Bond angles



Torsions

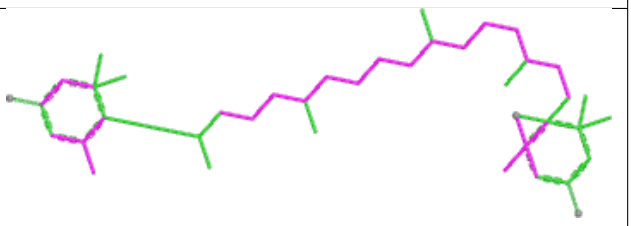


Rings

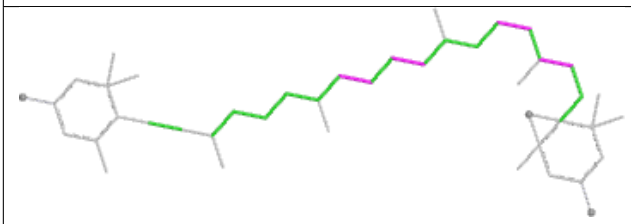
Ligand DD6 1 204



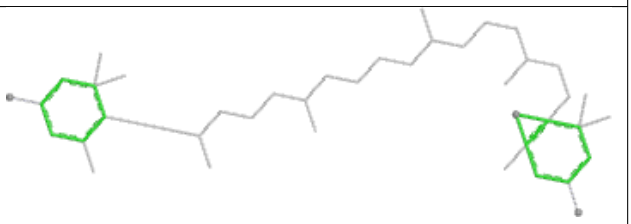
Bond lengths



Bond angles

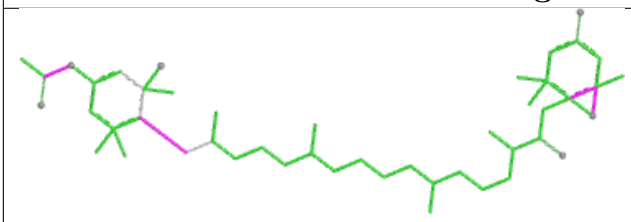


Torsions

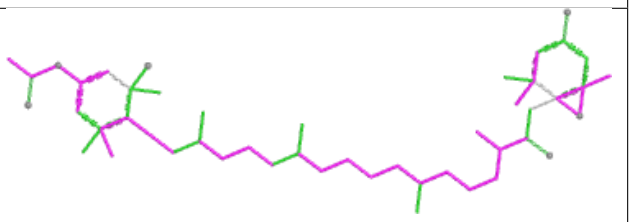


Rings

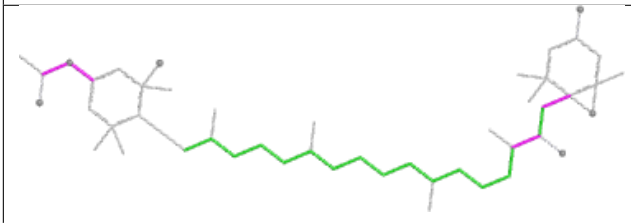
Ligand A86 2 301



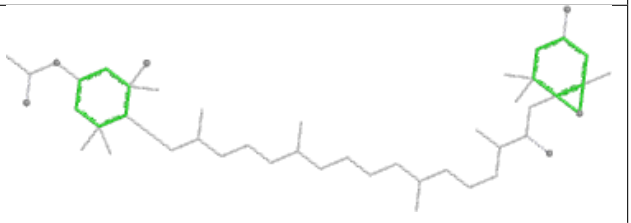
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

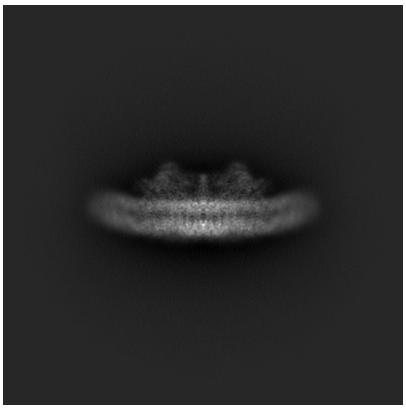
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35987. These allow visual inspection of the internal detail of the map and identification of artifacts.

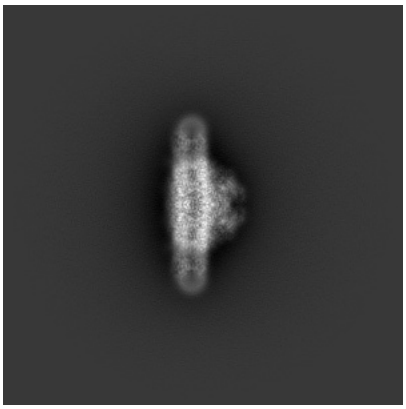
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

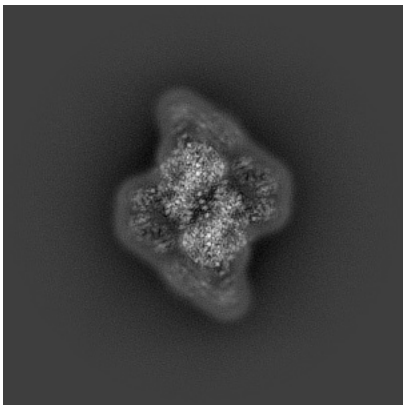
6.1.1 Primary map



X

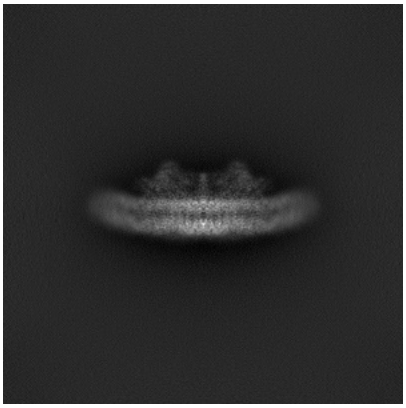


Y

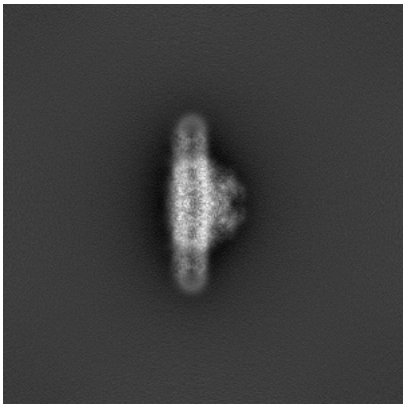


Z

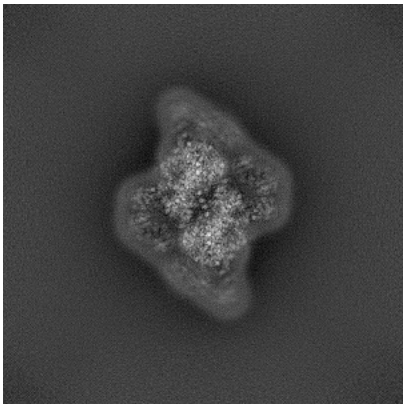
6.1.2 Raw map



X



Y

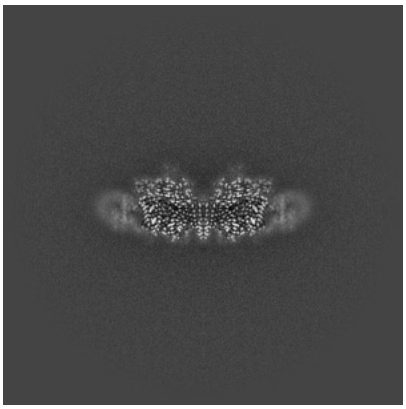


Z

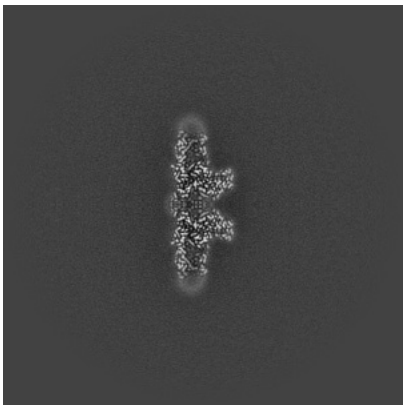
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

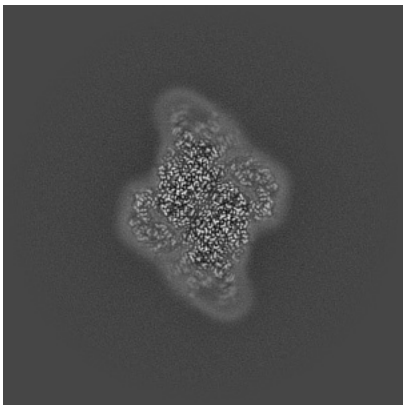
6.2.1 Primary map



X Index: 256

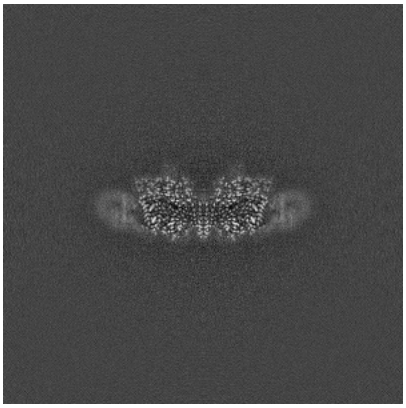


Y Index: 256

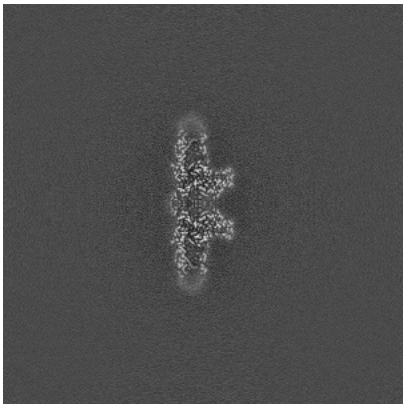


Z Index: 256

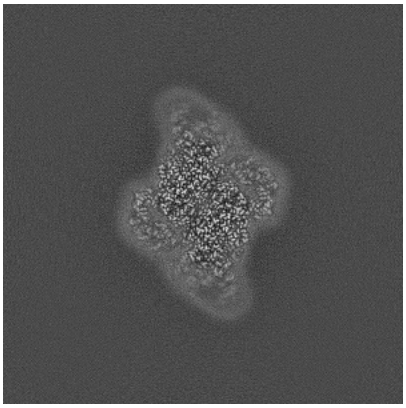
6.2.2 Raw map



X Index: 256



Y Index: 256

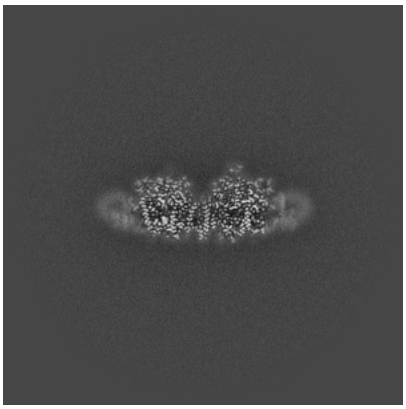


Z Index: 256

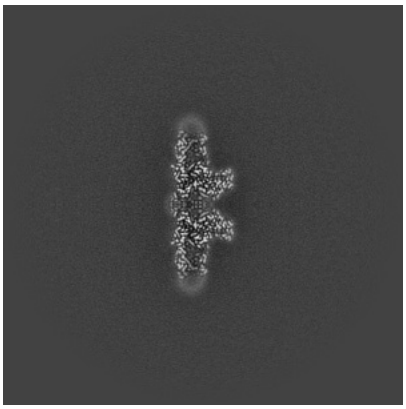
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

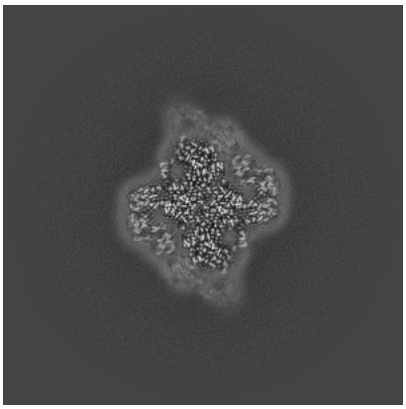
6.3.1 Primary map



X Index: 254

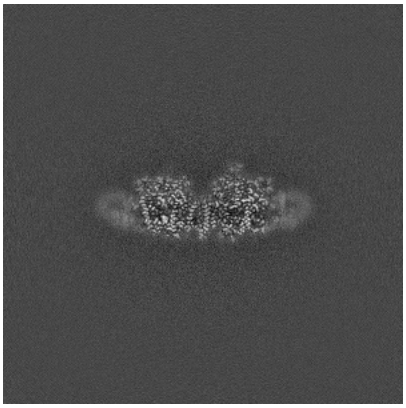


Y Index: 256

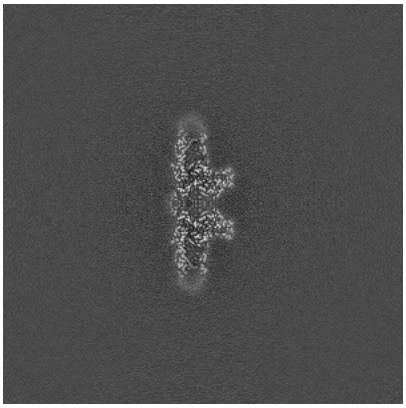


Z Index: 230

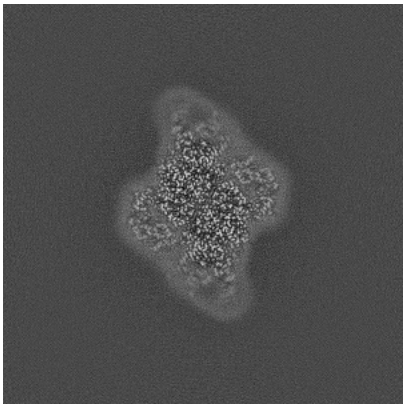
6.3.2 Raw map



X Index: 254



Y Index: 256

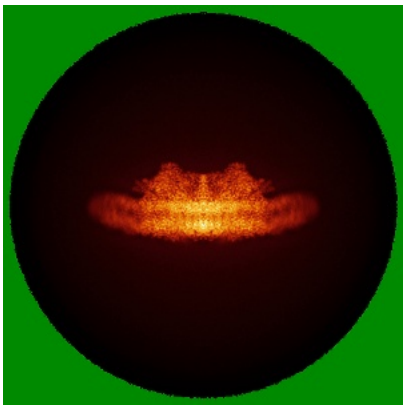


Z Index: 255

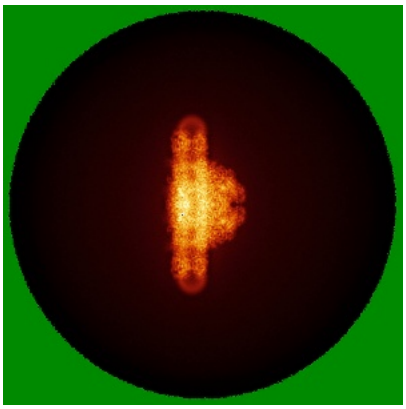
The images above show the largest variance slices of the map in three orthogonal directions.

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

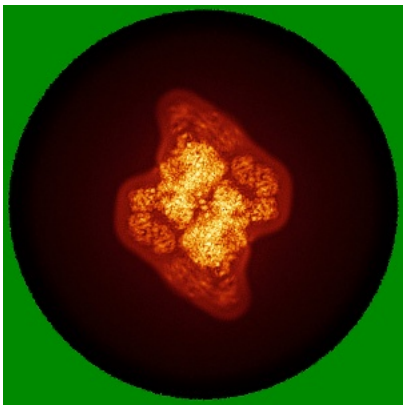
6.4.1 Primary map



X

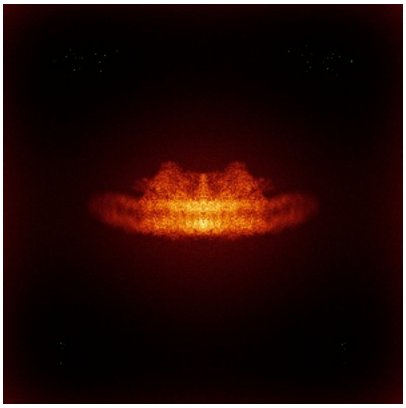


Y

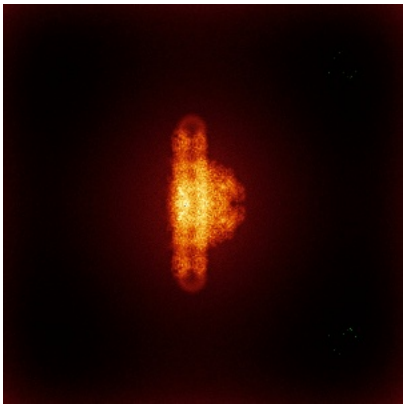


Z

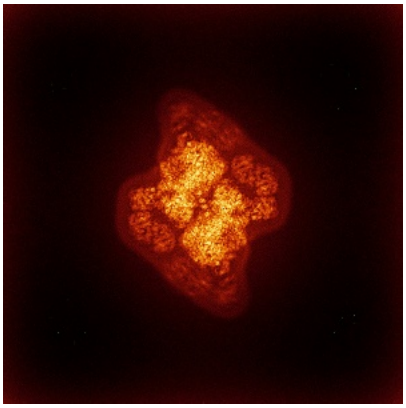
6.4.2 Raw map



X



Y

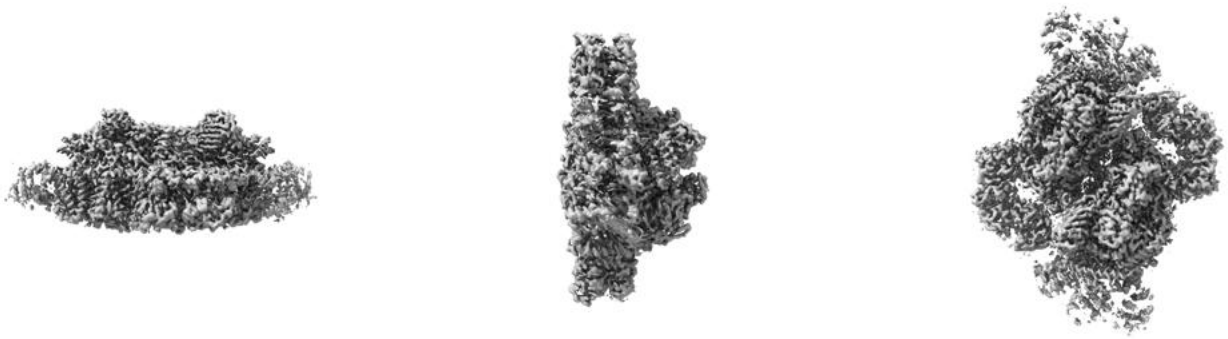


Z

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 0.158. 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.

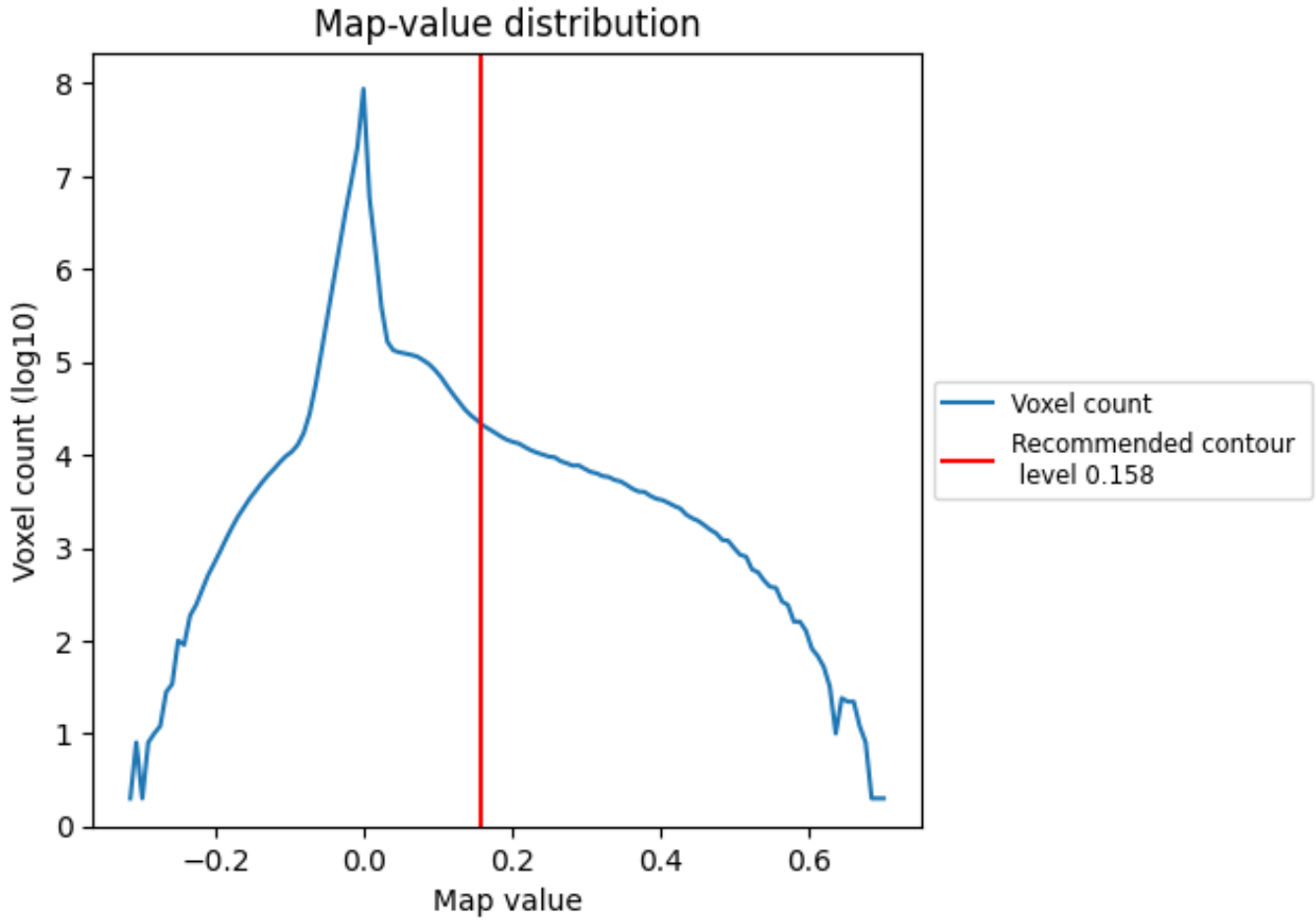
6.6 Mask visualisation (i)

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

7 Map analysis

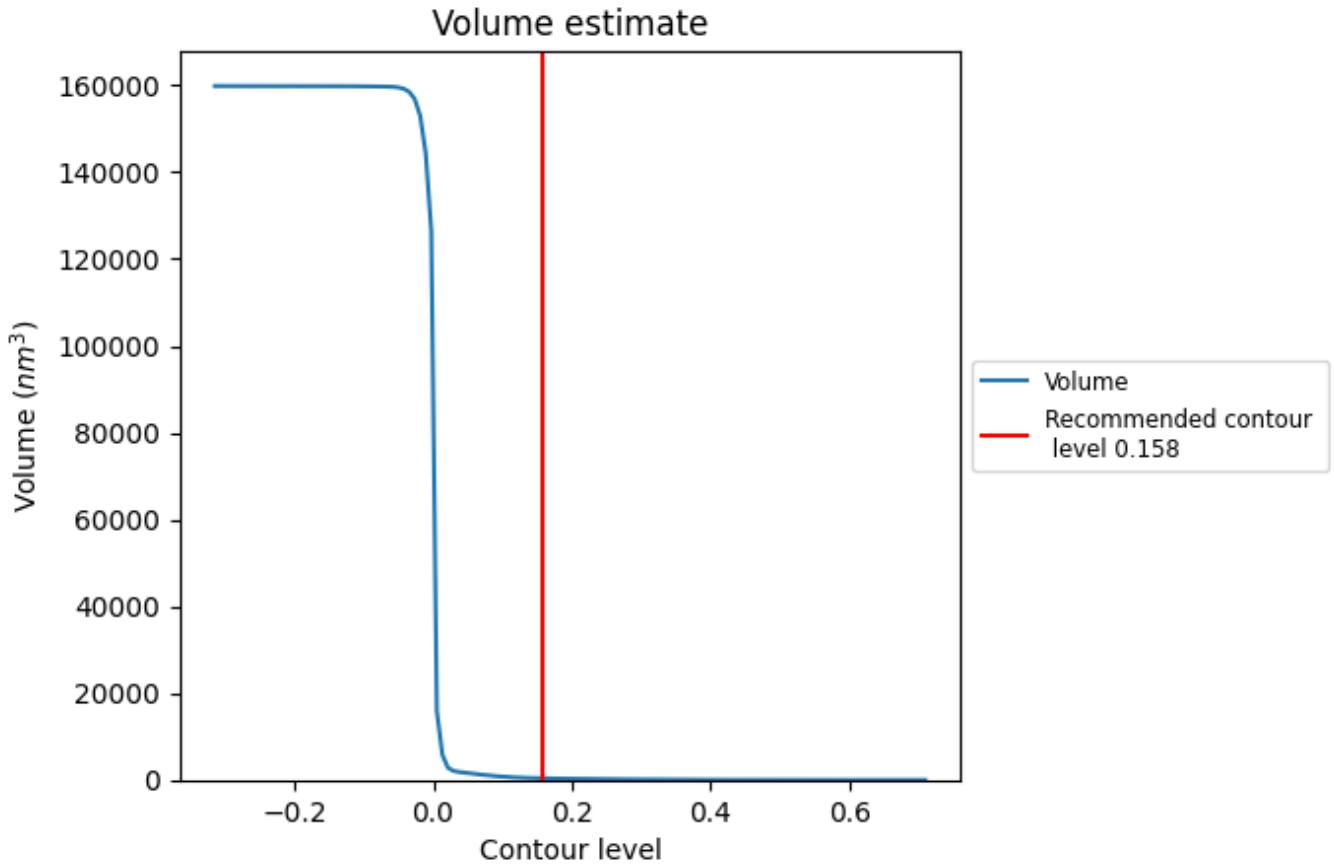
This section contains the results of statistical analysis of the map.

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.

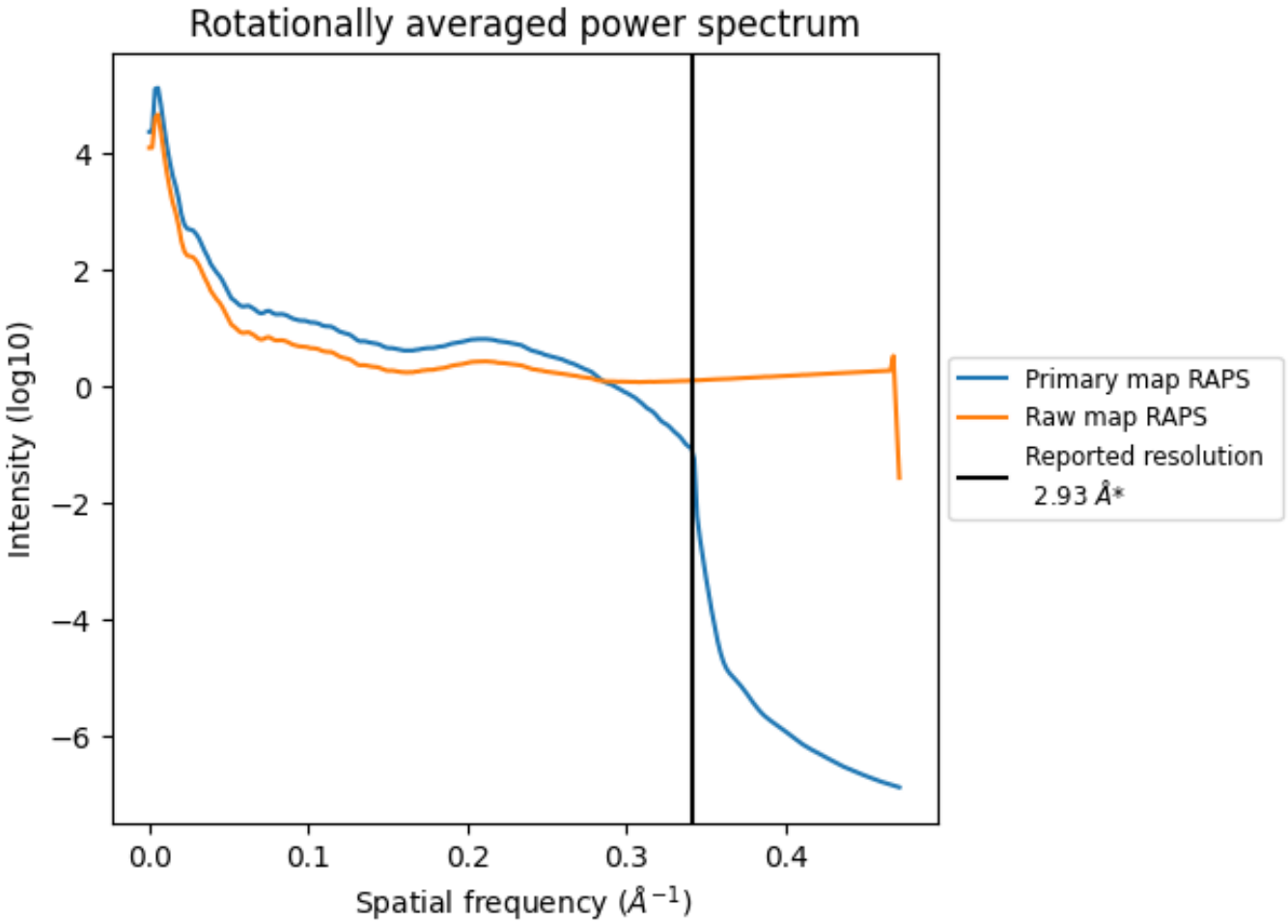
7.2 Volume estimate (i)



The volume at the recommended contour level is 376 nm^3; this corresponds to an approximate mass of 339 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)

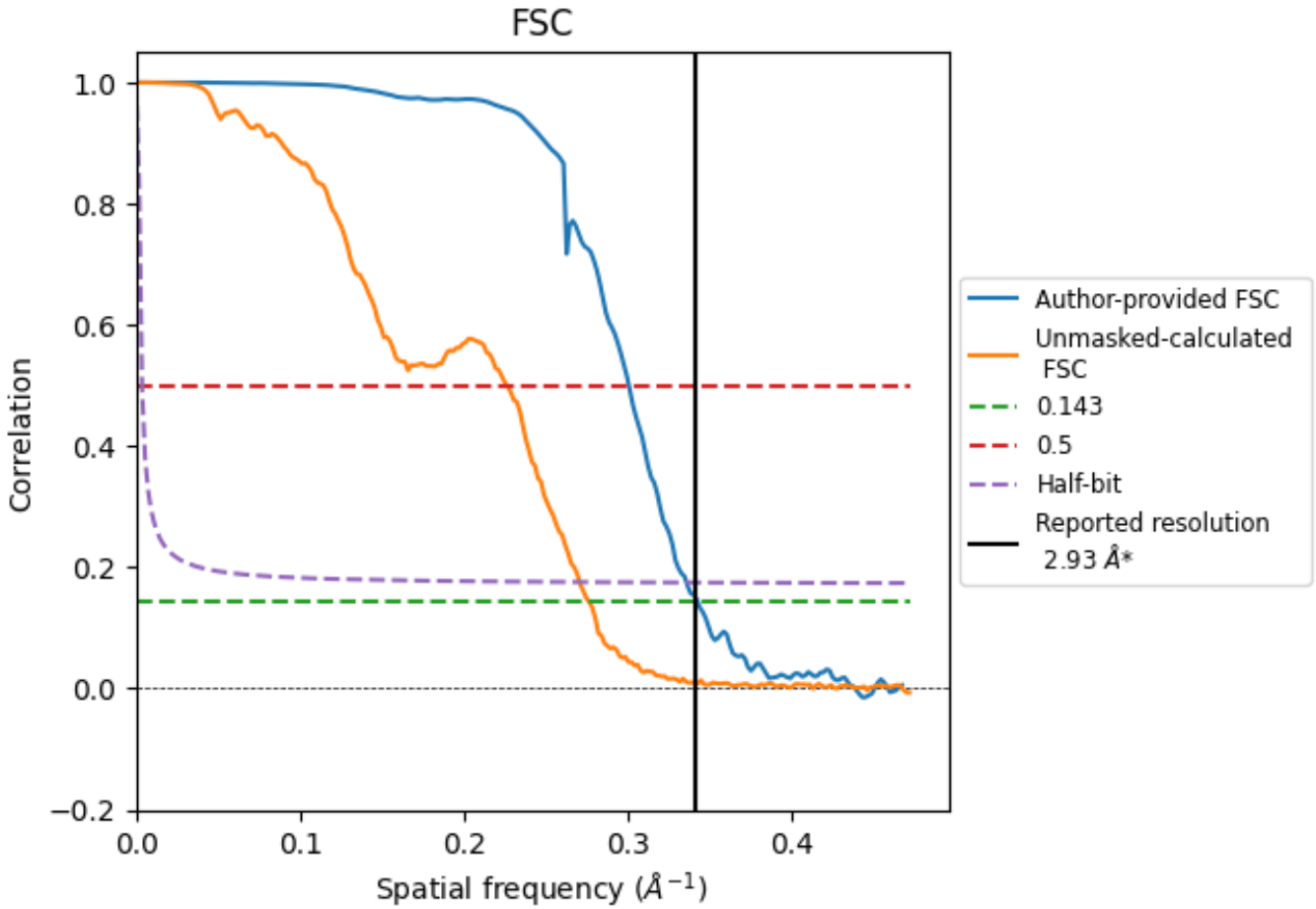


*Reported resolution corresponds to spatial frequency of 0.341 Å^{-1}

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 0.341 Å^{-1}

8.2 Resolution estimates (i)

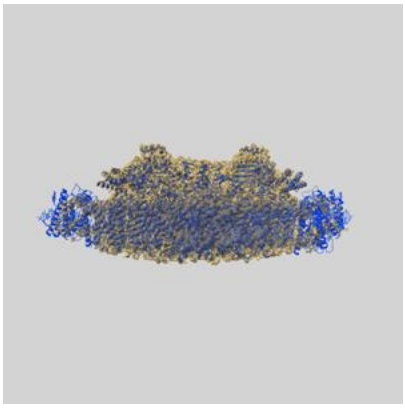
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.92	3.33	2.98
Unmasked-calculated*	3.62	4.42	3.70

*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 3.62 differs from the reported value 2.93 by more than 10 %

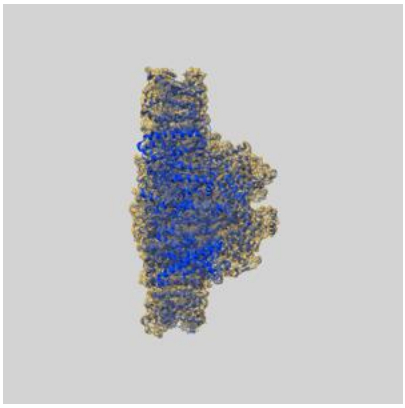
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35987 and PDB model 8J5K. Per-residue inclusion information can be found in section 3 on page 40.

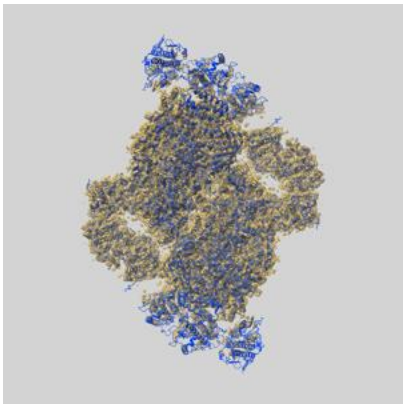
9.1 Map-model overlay



X



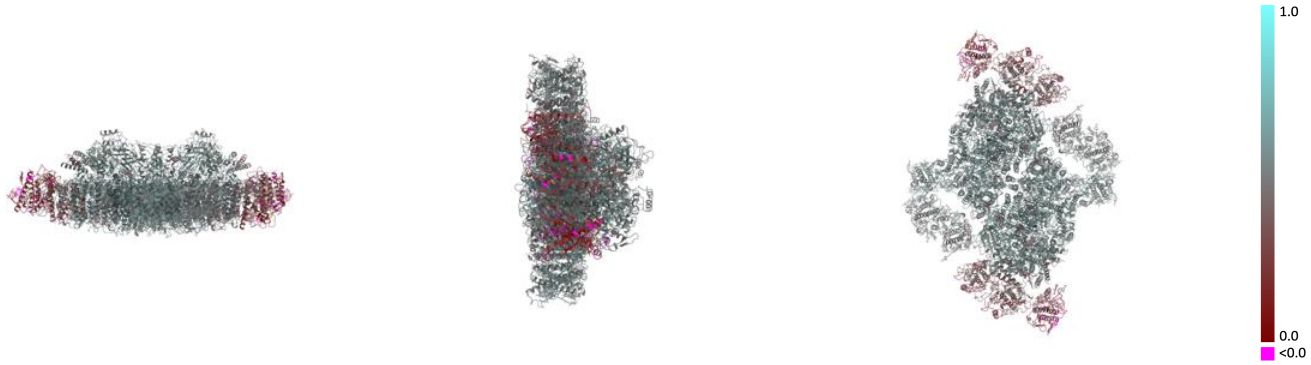
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.158 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.

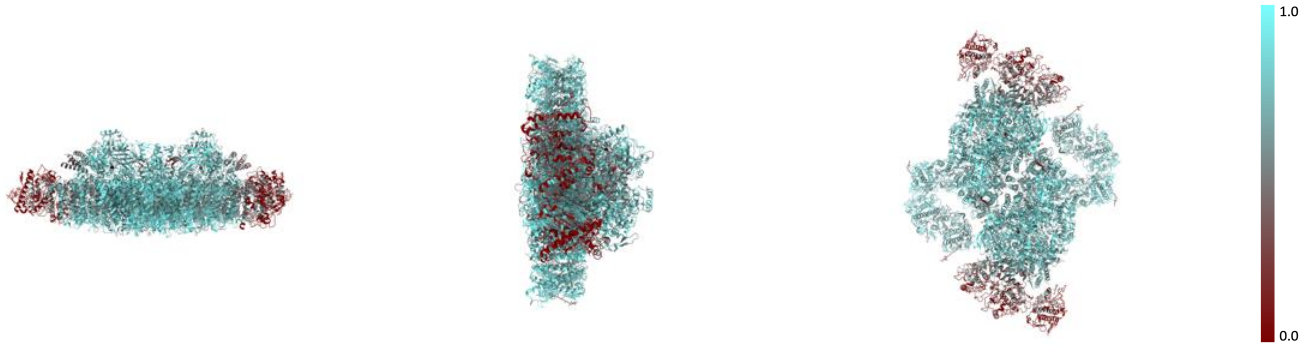
9.2 Q-score mapped to coordinate model



X Y Z

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.

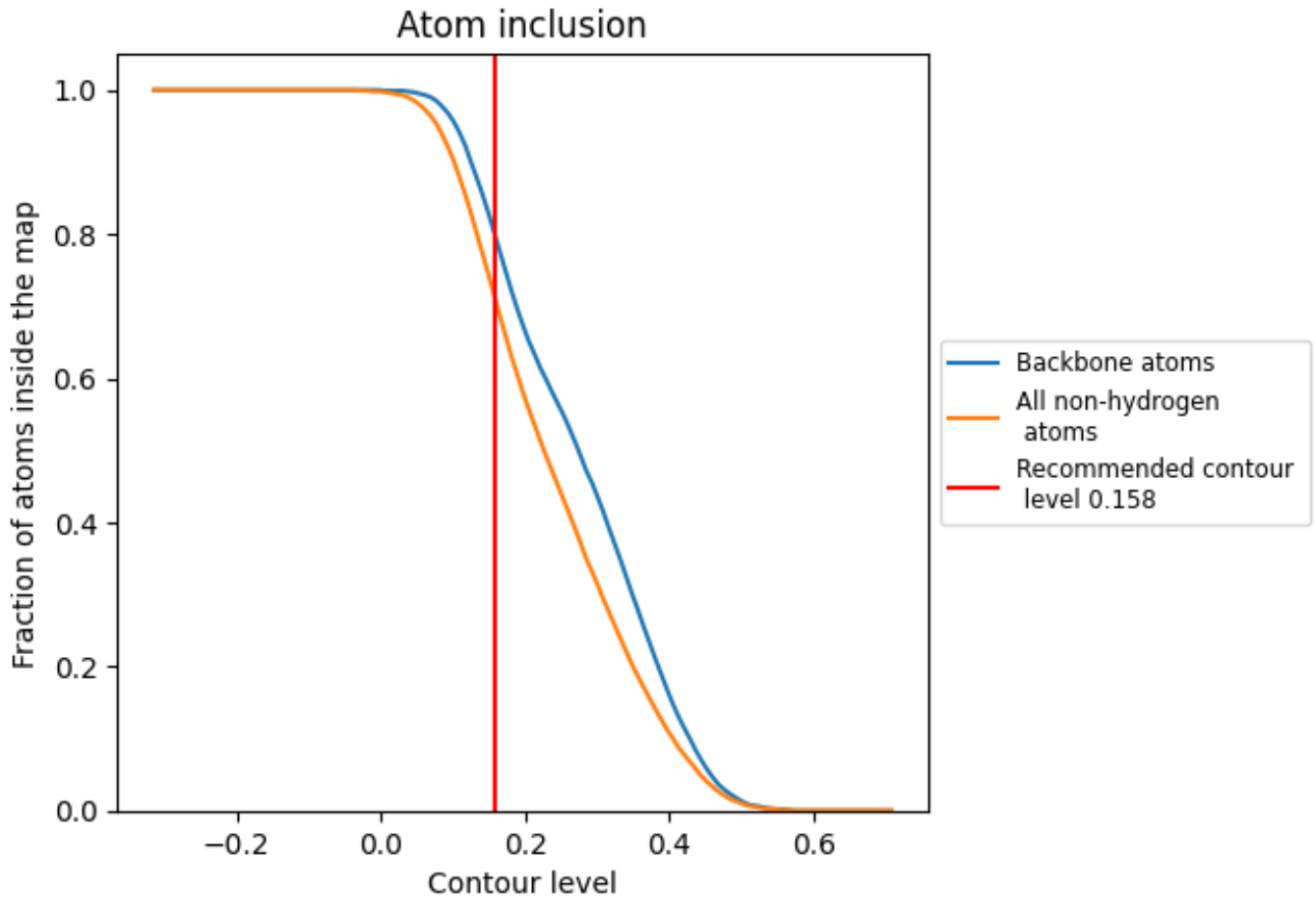
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.158).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7130	0.5040
0	0.7910	0.5330
1	0.7530	0.5000
2	0.6890	0.4730
3	0.2070	0.2790
4	0.1270	0.1640
5	0.7910	0.5340
6	0.7530	0.5000
7	0.6880	0.4740
8	0.2140	0.2820
9	0.1320	0.1850
A	0.8080	0.5670
B	0.8430	0.5670
C	0.8320	0.5600
D	0.8480	0.5720
E	0.7890	0.5110
F	0.8080	0.5150
H	0.8140	0.5580
I	0.8520	0.5500
J	0.6470	0.5260
K	0.7820	0.5170
L	0.8580	0.5820
M	0.7210	0.5590
N	0.7000	0.4400
O	0.7150	0.5260
P	0.2690	0.2840
Q	0.5210	0.4800
T	0.7490	0.5580
U	0.7670	0.5160
V	0.7710	0.5320
W	0.7160	0.4810
X	0.7790	0.5410
Y	0.6610	0.4860
Z	0.7290	0.4790
a	0.8200	0.5700



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Chain	Atom inclusion	Q-score
b	0.8480	0.5690
c	0.8310	0.5600
d	0.8460	0.5730
e	0.7840	0.5110
f	0.8080	0.5160
h	0.8090	0.5590
i	0.8440	0.5450
j	0.6400	0.5240
k	0.7820	0.5120
l	0.8510	0.5740
m	0.7260	0.5600
n	0.7130	0.4310
o	0.7190	0.5250
p	0.2710	0.2870
q	0.5150	0.4750
t	0.7530	0.5600
u	0.7590	0.5170
v	0.7800	0.5300
w	0.7180	0.4830
x	0.7880	0.5390
y	0.6580	0.4930
z	0.7310	0.4820