



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 11:54 PM UTC

PDB ID : 8Z11 / pdb_00008z11
EMDB ID : EMD-39717
Title : Cryo-EM structure of haptophyte photosystem I
Authors : He, F.Y.; Zhao, L.S.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2024-04-10
Resolution : 2.74 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:

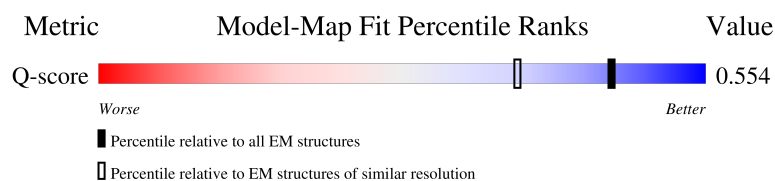
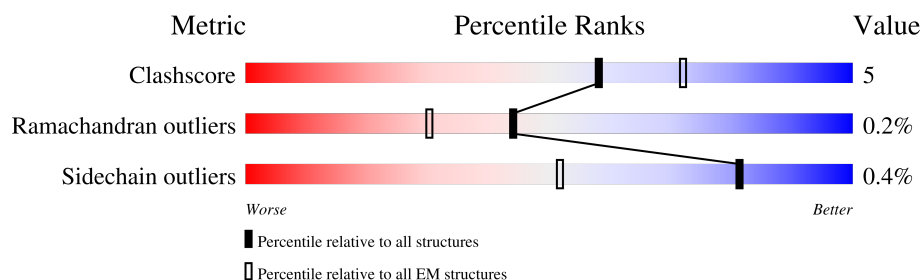
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.74 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	10492 (2.24 - 3.24)

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 $\leq 5\%$. 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	209	 78% 7% 14%
2	B	209	 56% 16% 24%
3	C	205	 76% 11% 14%
4	D	245	 62% 10% 27%

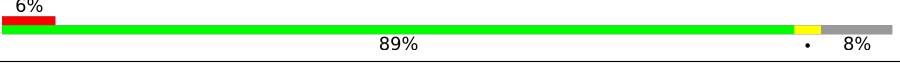
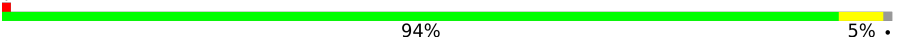
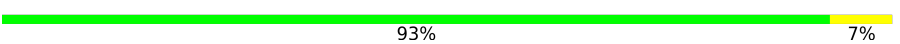
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Mol	Chain	Length	Quality of chain
5	E	206	
6	F	240	
7	G	198	
8	H	198	
9	I	194	
10	J	200	
11	K	202	
12	L	229	
13	M	217	
13	P	217	
13	W	217	
14	N	224	
15	O	206	
15	R	206	
15	T	206	
16	Q	187	
17	S	235	
18	U	203	
19	V	122	
20	a	752	
21	b	734	
22	c	81	
23	d	142	
24	e	124	
25	f	184	

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Mol	Chain	Length	Quality of chain
26	i	36	
27	j	40	
28	k	92	
29	l	145	
30	m	30	
31	r	133	

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
32	CLA	A	301	X	-	-	-
32	CLA	A	302	X	-	-	-
32	CLA	A	303	X	-	-	-
32	CLA	A	304	X	-	-	-
32	CLA	A	305	X	-	-	-
32	CLA	A	306	X	-	-	-
32	CLA	A	307	X	-	-	-
32	CLA	A	308	X	-	-	-
32	CLA	A	309	X	-	-	-
32	CLA	A	311	X	-	-	-
32	CLA	B	301	X	-	-	-
32	CLA	B	302	X	-	-	-
32	CLA	B	303	X	-	-	-
32	CLA	B	304	X	-	-	-
32	CLA	B	305	X	-	-	-
32	CLA	B	306	X	-	-	-
32	CLA	B	309	X	-	-	-
32	CLA	C	301	X	-	-	-
32	CLA	C	302	X	-	-	-
32	CLA	C	304	X	-	-	-
32	CLA	C	305	X	-	-	-
32	CLA	C	306	X	-	-	-
32	CLA	C	307	X	-	-	-
32	CLA	C	308	X	-	-	-
32	CLA	C	309	X	-	-	-
32	CLA	D	304	X	-	-	-
32	CLA	D	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	D	306	X	-	-	-
32	CLA	D	307	X	-	-	-
32	CLA	D	308	X	-	-	-
32	CLA	D	309	X	-	-	-
32	CLA	D	310	X	-	-	-
32	CLA	D	311	X	-	-	-
32	CLA	D	312	X	-	-	-
32	CLA	D	313	X	-	-	-
32	CLA	D	314	X	-	-	-
32	CLA	D	315	X	-	-	-
32	CLA	E	303	X	-	-	-
32	CLA	E	304	X	-	-	-
32	CLA	E	305	X	-	-	-
32	CLA	E	306	X	-	-	-
32	CLA	E	307	X	-	-	-
32	CLA	E	308	X	-	-	-
32	CLA	E	309	X	-	-	-
32	CLA	E	310	X	-	-	-
32	CLA	E	311	X	-	-	-
32	CLA	E	312	X	-	-	-
32	CLA	E	314	X	-	-	-
32	CLA	E	315	X	-	-	-
32	CLA	F	301	X	-	-	-
32	CLA	F	303	X	-	-	-
32	CLA	F	304	X	-	-	-
32	CLA	F	305	X	-	-	-
32	CLA	F	306	X	-	-	-
32	CLA	F	307	X	-	-	-
32	CLA	F	308	X	-	-	-
32	CLA	F	309	X	-	-	-
32	CLA	F	311	X	-	-	-
32	CLA	F	322	X	-	-	-
32	CLA	G	301	X	-	-	-
32	CLA	G	303	X	-	-	-
32	CLA	G	304	X	-	-	-
32	CLA	G	305	X	-	-	-
32	CLA	G	306	X	-	-	-
32	CLA	G	307	X	-	-	-
32	CLA	G	308	X	-	-	-
32	CLA	H	301	X	-	-	-
32	CLA	H	302	X	-	-	-
32	CLA	H	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	H	305	X	-	-	-
32	CLA	H	306	X	-	-	-
32	CLA	H	307	X	-	-	-
32	CLA	H	308	X	-	-	-
32	CLA	H	309	X	-	-	-
32	CLA	H	310	X	-	-	-
32	CLA	I	301	X	-	-	-
32	CLA	I	302	X	-	-	-
32	CLA	I	303	X	-	-	-
32	CLA	I	304	X	-	-	-
32	CLA	I	305	X	-	-	-
32	CLA	I	306	X	-	-	-
32	CLA	I	307	X	-	-	-
32	CLA	I	308	X	-	-	-
32	CLA	I	317	X	-	-	-
32	CLA	J	301	X	-	-	-
32	CLA	J	302	X	-	-	-
32	CLA	J	304	X	-	-	-
32	CLA	J	305	X	-	-	-
32	CLA	J	306	X	-	-	-
32	CLA	J	307	X	-	-	-
32	CLA	J	308	X	-	-	-
32	CLA	J	309	X	-	-	-
32	CLA	J	311	X	-	-	-
32	CLA	J	312	X	-	-	-
32	CLA	K	301	X	-	-	-
32	CLA	K	304	X	-	-	-
32	CLA	K	306	X	-	-	-
32	CLA	K	307	X	-	-	-
32	CLA	K	308	X	-	-	-
32	CLA	K	310	X	-	-	-
32	CLA	L	301	X	-	-	-
32	CLA	L	304	X	-	-	-
32	CLA	L	307	X	-	-	-
32	CLA	L	308	X	-	-	-
32	CLA	L	309	X	-	-	-
32	CLA	L	310	X	-	-	-
32	CLA	L	311	X	-	-	-
32	CLA	L	312	X	-	-	-
32	CLA	L	314	X	-	-	-
32	CLA	M	305	X	-	-	-
32	CLA	M	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	M	308	X	-	-	-
32	CLA	M	309	X	-	-	-
32	CLA	M	310	X	-	-	-
32	CLA	M	311	X	-	-	-
32	CLA	M	312	X	-	-	-
32	CLA	N	305	X	-	-	-
32	CLA	N	309	X	-	-	-
32	CLA	N	310	X	-	-	-
32	CLA	N	311	X	-	-	-
32	CLA	N	312	X	-	-	-
32	CLA	N	313	X	-	-	-
32	CLA	O	301	X	-	-	-
32	CLA	O	304	X	-	-	-
32	CLA	O	305	X	-	-	-
32	CLA	O	306	X	-	-	-
32	CLA	O	307	X	-	-	-
32	CLA	O	308	X	-	-	-
32	CLA	O	309	X	-	-	-
32	CLA	P	304	X	-	-	-
32	CLA	P	305	X	-	-	-
32	CLA	P	307	X	-	-	-
32	CLA	P	308	X	-	-	-
32	CLA	P	309	X	-	-	-
32	CLA	P	310	X	-	-	-
32	CLA	P	311	X	-	-	-
32	CLA	Q	301	X	-	-	-
32	CLA	Q	303	X	-	-	-
32	CLA	Q	304	X	-	-	-
32	CLA	Q	305	X	-	-	-
32	CLA	Q	306	X	-	-	-
32	CLA	Q	307	X	-	-	-
32	CLA	Q	308	X	-	-	-
32	CLA	Q	309	X	-	-	-
32	CLA	Q	310	X	-	-	-
32	CLA	R	301	X	-	-	-
32	CLA	R	304	X	-	-	-
32	CLA	R	306	X	-	-	-
32	CLA	R	307	X	-	-	-
32	CLA	R	308	X	-	-	-
32	CLA	R	309	X	-	-	-
32	CLA	R	310	X	-	-	-
32	CLA	S	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	S	304	X	-	-	-
32	CLA	S	305	X	-	-	-
32	CLA	S	307	X	-	-	-
32	CLA	S	308	X	-	-	-
32	CLA	S	309	X	-	-	-
32	CLA	S	310	X	-	-	-
32	CLA	S	311	X	-	-	-
32	CLA	S	313	X	-	-	-
32	CLA	T	302	X	-	-	-
32	CLA	T	305	X	-	-	-
32	CLA	T	306	X	-	-	-
32	CLA	T	307	X	-	-	-
32	CLA	T	308	X	-	-	-
32	CLA	T	309	X	-	-	-
32	CLA	T	310	X	-	-	-
32	CLA	U	301	X	-	-	-
32	CLA	U	302	X	-	-	-
32	CLA	U	303	X	-	-	-
32	CLA	U	305	X	-	-	-
32	CLA	U	306	X	-	-	-
32	CLA	U	307	X	-	-	-
32	CLA	V	201	X	-	-	-
32	CLA	V	203	X	-	-	-
32	CLA	V	204	X	-	-	-
32	CLA	W	306	X	-	-	-
32	CLA	W	307	X	-	-	-
32	CLA	W	309	X	-	-	-
32	CLA	W	310	X	-	-	-
32	CLA	W	311	X	-	-	-
32	CLA	W	312	X	-	-	-
32	CLA	W	313	X	-	-	-
32	CLA	a	801	X	-	-	-
32	CLA	a	802	X	-	-	-
32	CLA	a	803	X	-	-	-
32	CLA	a	804	X	-	-	-
32	CLA	a	805	X	-	-	-
32	CLA	a	806	X	-	-	-
32	CLA	a	807	X	-	-	-
32	CLA	a	808	X	-	-	-
32	CLA	a	809	X	-	-	-
32	CLA	a	810	X	-	-	-
32	CLA	a	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	a	812	X	-	-	-
32	CLA	a	813	X	-	-	-
32	CLA	a	814	X	-	-	-
32	CLA	a	815	X	-	-	-
32	CLA	a	816	X	-	-	-
32	CLA	a	817	X	-	-	-
32	CLA	a	818	X	-	-	-
32	CLA	a	819	X	-	-	-
32	CLA	a	820	X	-	-	-
32	CLA	a	821	X	-	-	-
32	CLA	a	822	X	-	-	-
32	CLA	a	823	X	-	-	-
32	CLA	a	824	X	-	-	-
32	CLA	a	825	X	-	-	-
32	CLA	a	826	X	-	-	-
32	CLA	a	827	X	-	-	-
32	CLA	a	828	X	-	-	-
32	CLA	a	829	X	-	-	-
32	CLA	a	830	X	-	-	-
32	CLA	a	831	X	-	-	-
32	CLA	a	832	X	-	-	-
32	CLA	a	833	X	-	-	-
32	CLA	a	834	X	-	-	-
32	CLA	a	835	X	-	-	-
32	CLA	a	836	X	-	-	-
32	CLA	a	837	X	-	-	-
32	CLA	a	838	X	-	-	-
32	CLA	a	839	X	-	-	-
32	CLA	a	840	X	-	-	-
32	CLA	a	841	X	-	-	-
32	CLA	a	842	X	-	-	-
32	CLA	a	852	X	-	-	-
32	CLA	a	853	X	-	-	-
32	CLA	b	801	X	-	-	-
32	CLA	b	802	X	-	-	-
32	CLA	b	803	X	-	-	-
32	CLA	b	804	X	-	-	-
32	CLA	b	805	X	-	-	-
32	CLA	b	806	X	-	-	-
32	CLA	b	807	X	-	-	-
32	CLA	b	808	X	-	-	-
32	CLA	b	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	b	810	X	-	-	-
32	CLA	b	811	X	-	-	-
32	CLA	b	812	X	-	-	-
32	CLA	b	813	X	-	-	-
32	CLA	b	814	X	-	-	-
32	CLA	b	815	X	-	-	-
32	CLA	b	816	X	-	-	-
32	CLA	b	817	X	-	-	-
32	CLA	b	818	X	-	-	-
32	CLA	b	819	X	-	-	-
32	CLA	b	820	X	-	-	-
32	CLA	b	821	X	-	-	-
32	CLA	b	822	X	-	-	-
32	CLA	b	823	X	-	-	-
32	CLA	b	824	X	-	-	-
32	CLA	b	825	X	-	-	-
32	CLA	b	826	X	-	-	-
32	CLA	b	827	X	-	-	-
32	CLA	b	828	X	-	-	-
32	CLA	b	829	X	-	-	-
32	CLA	b	830	X	-	-	-
32	CLA	b	831	X	-	-	-
32	CLA	b	832	X	-	-	-
32	CLA	b	833	X	-	-	-
32	CLA	b	834	X	-	-	-
32	CLA	b	835	X	-	-	-
32	CLA	b	836	X	-	-	-
32	CLA	b	837	X	-	-	-
32	CLA	b	838	X	-	-	-
32	CLA	b	839	X	-	-	-
32	CLA	b	840	X	-	-	-
32	CLA	f	201	X	-	-	-
32	CLA	f	203	X	-	-	-
32	CLA	f	204	X	-	-	-
32	CLA	j	101	X	-	-	-
32	CLA	k	201	X	-	-	-
32	CLA	k	202	X	-	-	-
32	CLA	k	203	X	-	-	-
32	CLA	l	202	X	-	-	-
32	CLA	l	203	X	-	-	-
32	CLA	l	204	X	-	-	-
32	CLA	r	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CLA	r	202	X	-	-	-
34	DD6	J	317	X	-	-	-
34	DD6	K	315	X	-	-	-
34	DD6	O	313	X	-	-	-
34	DD6	S	321	X	-	-	-
37	A86	O	312	X	-	-	-

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 73546 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 iFCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	180	Total	C	N	O	S	0	0
			1403	910	230	254	9		

- Molecule 2 is a protein called iFCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	158	Total	C	N	O	S	0	0
			1194	770	197	219	8		

- Molecule 3 is a protein called iFCPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	177	Total	C	N	O	S	0	0
			1346	872	223	244	7		

- Molecule 4 is a protein called iFCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	178	Total	C	N	O	S	1	0
			1392	910	220	254	8		

- Molecule 5 is a protein called iFCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	176	Total	C	N	O	S	0	0
			1316	854	212	240	10		

- Molecule 6 is a protein called iFCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	210	Total	C	N	O	S	0	0
			1573	1006	266	290	11		

- Molecule 7 is a protein called iFCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	167	Total	C	N	O	S	0	0
			1235	794	204	227	10		

- Molecule 8 is a protein called iFCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	S	0	0
			1266	808	212	233	13		

- Molecule 9 is a protein called iFCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	154	Total	C	N	O	S	0	0
			1190	770	198	213	9		

- Molecule 10 is a protein called iFCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1253	803	212	227	11		

- Molecule 11 is a protein called iFCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	166	Total	C	N	O	S	0	0
			1280	837	217	219	7		

- Molecule 12 is a protein called iFCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	198	Total	C	N	O	S	0	0
			1479	960	246	266	7		

- Molecule 13 is a protein called iFCPI-15/14/16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	193	Total	C	N	O	S	0	0
			1465	949	247	263	6		
13	P	193	Total	C	N	O	S	0	0
			1465	949	247	263	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	193	Total	C	N	O	S	0	0
			1465	949	247	263	6		

- Molecule 14 is a protein called iFCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	194	Total	C	N	O	S	0	0
			1451	941	247	255	8		

- Molecule 15 is a protein called iFCPI-20/19/21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	175	Total	C	N	O	S	0	0
			1299	842	215	237	5		
15	R	175	Total	C	N	O	S	0	0
			1299	842	215	237	5		
15	T	175	Total	C	N	O	S	0	0
			1299	842	215	237	5		

- Molecule 16 is a protein called iFCPI-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	157	Total	C	N	O	S	0	0
			1210	775	205	221	9		

- Molecule 17 is a protein called iFCPI-22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	205	Total	C	N	O	S	0	0
			1597	1046	264	279	8		

- Molecule 18 is a protein called iFCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	142	Total	C	N	O	S	0	0
			1084	698	180	199	7		

- Molecule 19 is a protein called L-iFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	47	Total	C	N	O	S	0	0
			357	229	60	66	2		

- Molecule 20 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	741	Total	C	N	O	S	0	0
			5826	3810	991	995	30		

- Molecule 21 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	732	Total	C	N	O	S	0	0
			5818	3832	981	984	21		

- Molecule 22 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	80	Total	C	N	O	S	0	0
			596	364	105	116	11		

- Molecule 23 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	137	Total	C	N	O	S	0	0
			1080	698	181	198	3		

- Molecule 24 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	65	Total	C	N	O	S	0	0
			504	320	87	94	3		

- Molecule 25 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	161	Total	C	N	O	S	0	0
			1243	804	211	224	4		

- Molecule 26 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	i	33	Total	C	N	O	S	0	0
			258	179	34	44	1		

- Molecule 27 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	40	Total	C	N	O	S	0	0
			316	210	47	57	2		

- Molecule 28 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	70	Total	C	N	O	S	0	0
			503	327	80	90	6		

- Molecule 29 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	143	Total	C	N	O	S	0	0
			1081	710	173	196	2		

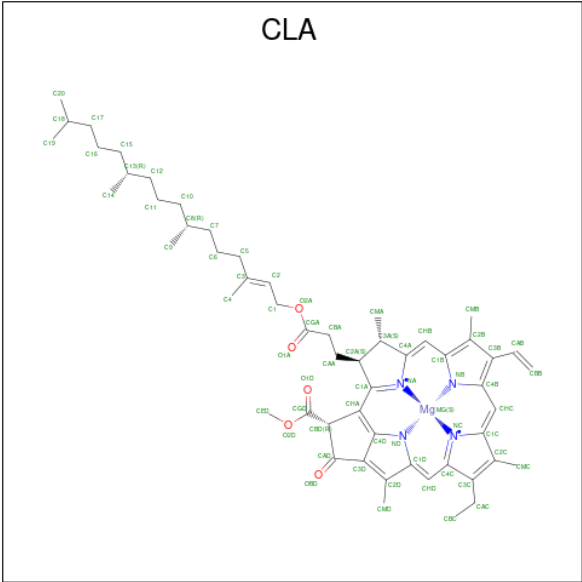
- Molecule 30 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	m	30	Total	C	N	O	S	0	0
			219	145	35	37	2		

- Molecule 31 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	r	91	Total	C	N	O	S	0	0
			682	441	111	129	1		

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
32	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	C	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	C	1	Total 43	C 35	Mg 1	N 4	O 3	0
32	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	D	1	Total 58	C 48	Mg 1	N 4	O 5	0
32	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	D	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	D	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	D	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
32	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
32	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
32	F	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
32	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
32	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
32	G	1	Total 40	C 32	Mg 1	N 4	O 3	0
32	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
32	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
32	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	I	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	I	1	Total 56	C 46	Mg 1	N 4	O 5	0
32	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	J	1	Total 52	C 42	Mg 1	N 4	O 5	0
32	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
32	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	K	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
32	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
32	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
32	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	M	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	M	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	M	1	Total 57	C 47	Mg 1	N 4	O 5	0
32	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	M	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	N	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	O	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	P	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	Q	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	Q	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	Q	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
32	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
32	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
32	S	1	Total 63	C 53	Mg 1	N 4	O 5	0
32	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
32	S	1	Total 44	C 34	Mg 1	N 4	O 5	0
32	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	S	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	T	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	U	1	Total 40	C 32	Mg 1	N 4	O 3	0
32	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	V	1	Total 58	C 48	Mg 1	N 4	O 5	0
32	V	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	W	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 63	C 53	Mg 1	N 4	O 5	0
32	a	1	Total 63	C 53	Mg 1	N 4	O 5	0
32	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	b	1	Total 55	C 45	Mg 1	N 4	O 5	0

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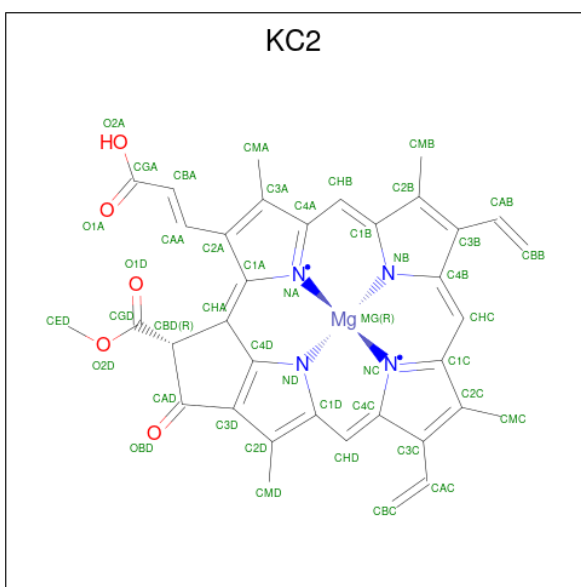
Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
32	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
32	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
32	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
32	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
32	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
32	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	l	1	Total 45	C 35	Mg 1	N 4	O 5	0
32	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
32	r	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 33 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	E	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	O	1	Total 45	C 35	Mg 1	N 4	O 5	0

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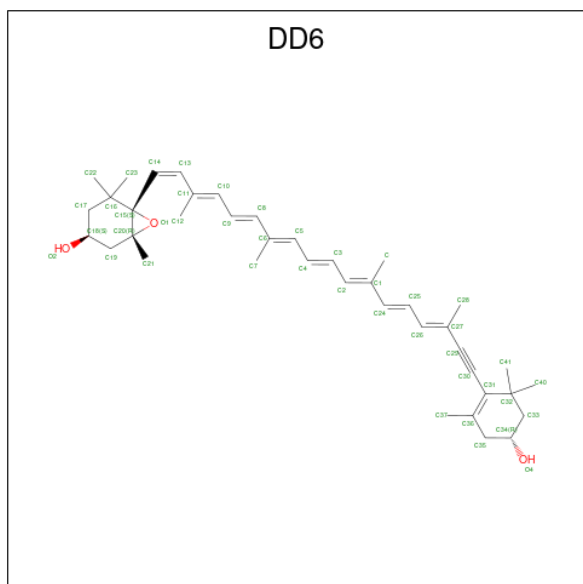
Mol	Chain	Residues	Atoms					AltConf
33	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	Q	1	Total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

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Mol	Chain	Residues	Atoms					AltConf
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
33	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 34 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: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O		0
			43	40	3		
34	A	1	Total	C	O		0
			43	40	3		
34	A	1	Total	C	O		0
			43	40	3		
34	A	1	Total	C	O		0
			43	40	3		

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Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total 43	C 40	O 3	0
34	C	1	Total 43	C 40	O 3	0
34	D	1	Total 43	C 40	O 3	0
34	D	1	Total 43	C 40	O 3	0
34	D	1	Total 43	C 40	O 3	0
34	D	1	Total 43	C 40	O 3	0
34	D	1	Total 43	C 40	O 3	0
34	E	1	Total 43	C 40	O 3	0
34	E	1	Total 43	C 40	O 3	0
34	E	1	Total 43	C 40	O 3	0
34	E	1	Total 43	C 40	O 3	0
34	F	1	Total 43	C 40	O 3	0
34	F	1	Total 43	C 40	O 3	0
34	F	1	Total 43	C 40	O 3	0
34	G	1	Total 43	C 40	O 3	0
34	H	1	Total 43	C 40	O 3	0
34	H	1	Total 43	C 40	O 3	0
34	H	1	Total 43	C 40	O 3	0
34	I	1	Total 43	C 40	O 3	0
34	I	1	Total 43	C 40	O 3	0
34	I	1	Total 43	C 40	O 3	0

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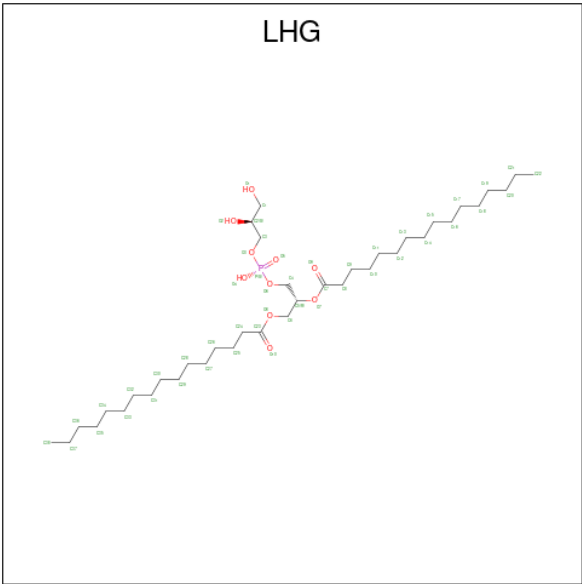
Mol	Chain	Residues	Atoms			AltConf
34	I	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	L	1	Total 43	C 40	O 3	0
34	M	1	Total 43	C 40	O 3	0
34	N	1	Total 43	C 40	O 3	0
34	N	1	Total 43	C 40	O 3	0
34	N	1	Total 43	C 40	O 3	0
34	O	1	Total 43	C 40	O 3	0
34	P	1	Total 43	C 40	O 3	0
34	Q	1	Total 43	C 40	O 3	0
34	Q	1	Total 43	C 40	O 3	0
34	Q	1	Total 43	C 40	O 3	0
34	Q	1	Total 43	C 40	O 3	0
34	R	1	Total 43	C 40	O 3	0
34	S	1	Total 43	C 40	O 3	0
34	T	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
34	U	1	Total	C	O	0
			43	40	3	
34	V	1	Total	C	O	0
			43	40	3	
34	W	1	Total	C	O	0
			43	40	3	
34	j	1	Total	C	O	0
			43	40	3	
34	k	1	Total	C	O	0
			43	40	3	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



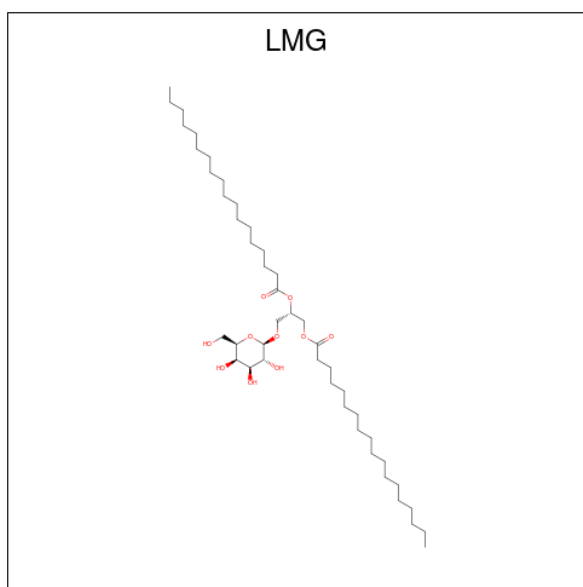
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			40	29	10	1	
35	B	1	Total	C	O	P	0
			31	20	10	1	
35	D	1	Total	C	O	P	0
			48	37	10	1	
35	E	1	Total	C	O	P	0
			46	35	10	1	
35	E	1	Total	C	O	P	0
			46	35	10	1	
35	F	1	Total	C	O	P	0
			41	30	10	1	

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Mol	Chain	Residues	Atoms				AltConf
35	F	1	Total	C	O	P	0
			40	29	10	1	
35	I	1	Total	C	O	P	0
			46	35	10	1	
35	I	1	Total	C	O	P	0
			37	26	10	1	
35	M	1	Total	C	O	P	0
			46	35	10	1	
35	P	1	Total	C	O	P	0
			46	35	10	1	
35	W	1	Total	C	O	P	0
			46	35	10	1	
35	a	1	Total	C	O	P	0
			48	37	10	1	
35	a	1	Total	C	O	P	0
			30	19	10	1	
35	a	1	Total	C	O	P	0
			38	27	10	1	
35	f	1	Total	C	O	P	0
			47	36	10	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



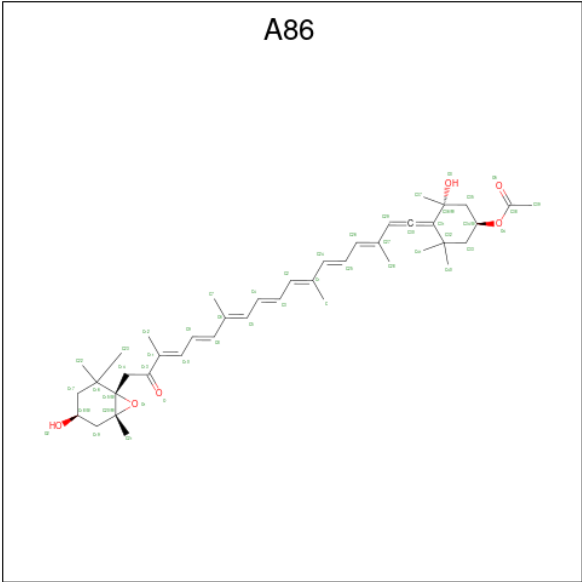
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			36	26	10	

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Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			40	30	10	
36	D	1	Total	C	O	0
			30	20	10	
36	D	1	Total	C	O	0
			36	26	10	
36	D	1	Total	C	O	0
			40	30	10	
36	D	1	Total	C	O	0
			35	25	10	
36	E	1	Total	C	O	0
			40	30	10	
36	E	1	Total	C	O	0
			31	21	10	
36	E	1	Total	C	O	0
			40	30	10	
36	F	1	Total	C	O	0
			40	30	10	
36	F	1	Total	C	O	0
			33	23	10	
36	L	1	Total	C	O	0
			37	27	10	
36	M	1	Total	C	O	0
			40	30	10	
36	N	1	Total	C	O	0
			40	30	10	
36	P	1	Total	C	O	0
			45	35	10	
36	S	1	Total	C	O	0
			33	23	10	
36	T	1	Total	C	O	0
			37	27	10	
36	W	1	Total	C	O	0
			39	29	10	
36	j	1	Total	C	O	0
			38	28	10	
36	l	1	Total	C	O	0
			49	39	10	

- Molecule 37 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: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			48	42	6	
37	C	1	Total	C	O	0
			48	42	6	
37	D	1	Total	C	O	0
			48	42	6	
37	D	1	Total	C	O	0
			48	42	6	
37	F	1	Total	C	O	0
			48	42	6	
37	F	1	Total	C	O	0
			48	42	6	
37	F	1	Total	C	O	0
			48	42	6	
37	G	1	Total	C	O	0
			48	42	6	
37	G	1	Total	C	O	0
			48	42	6	
37	H	1	Total	C	O	0
			48	42	6	
37	J	1	Total	C	O	0
			48	42	6	
37	K	1	Total	C	O	0
			48	42	6	
37	K	1	Total	C	O	0
			48	42	6	
37	K	1	Total	C	O	0
			48	42	6	

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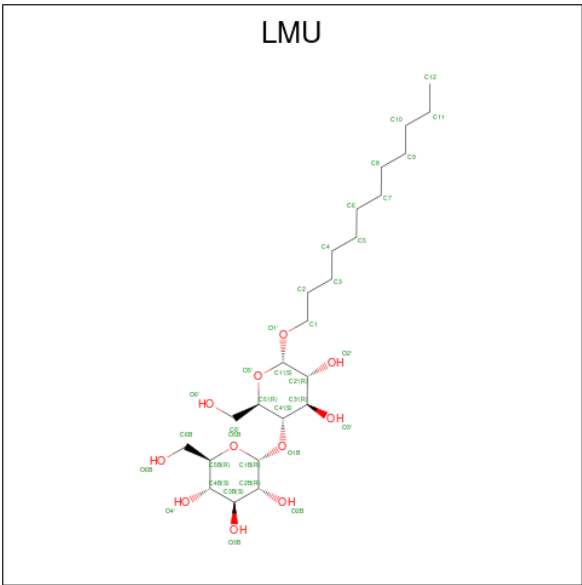
Mol	Chain	Residues	Atoms			AltConf
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0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

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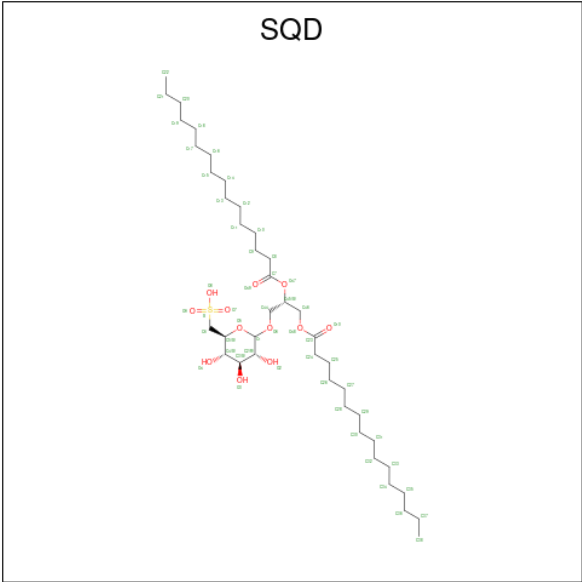
Mol	Chain	Residues	Atoms			AltConf
37	Q	1	Total	C	O	0
			48	42	6	
37	R	1	Total	C	O	0
			48	42	6	
37	R	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	T	1	Total	C	O	0
			48	42	6	
37	T	1	Total	C	O	0
			48	42	6	
37	T	1	Total	C	O	0
			48	42	6	
37	U	1	Total	C	O	0
			48	42	6	
37	W	1	Total	C	O	0
			48	42	6	
37	W	1	Total	C	O	0
			48	42	6	
37	W	1	Total	C	O	0
			48	42	6	
37	W	1	Total	C	O	0
			48	42	6	
37	r	1	Total	C	O	0
			48	42	6	

- Molecule 38 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



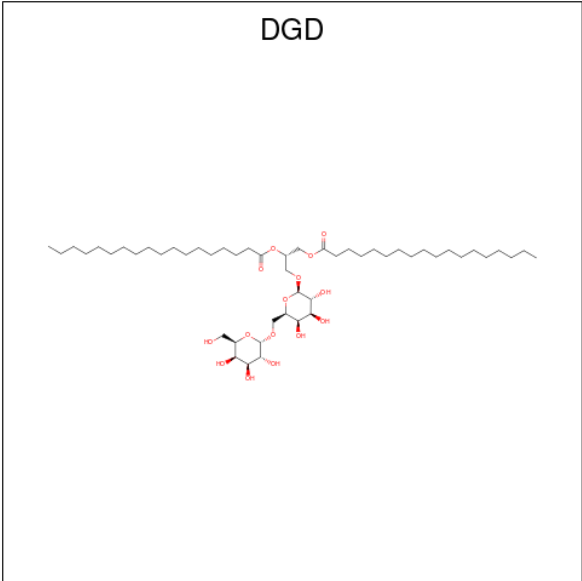
Mol	Chain	Residues	Atoms			AltConf
38	D	1	Total	C	O	0
			35	24	11	
38	I	1	Total	C	O	0
			35	24	11	
38	J	1	Total	C	O	0
			35	24	11	
38	V	1	Total	C	O	0
			34	23	11	
38	j	1	Total	C	O	0
			34	23	11	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
39	H	1	Total	C	O	S	0
			43	30	12	1	
39	k	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



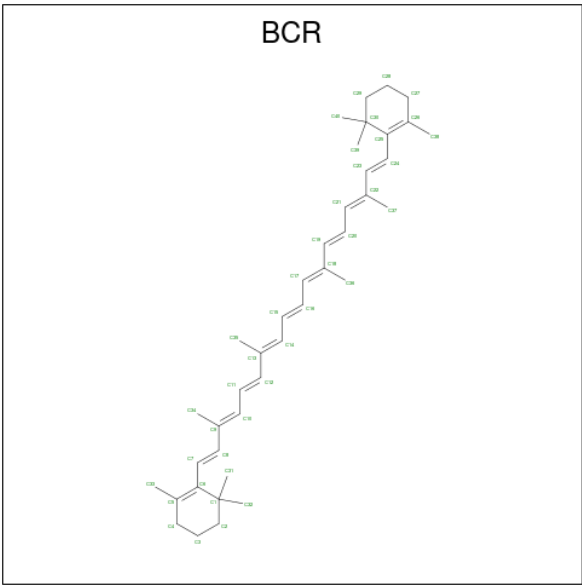
Mol	Chain	Residues	Atoms			AltConf
40	Q	1	Total	C	O	0
			56	41	15	

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Mol	Chain	Residues	Atoms			AltConf
40	b	1	Total	C	O	0
			56	41	15	

- Molecule 41 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



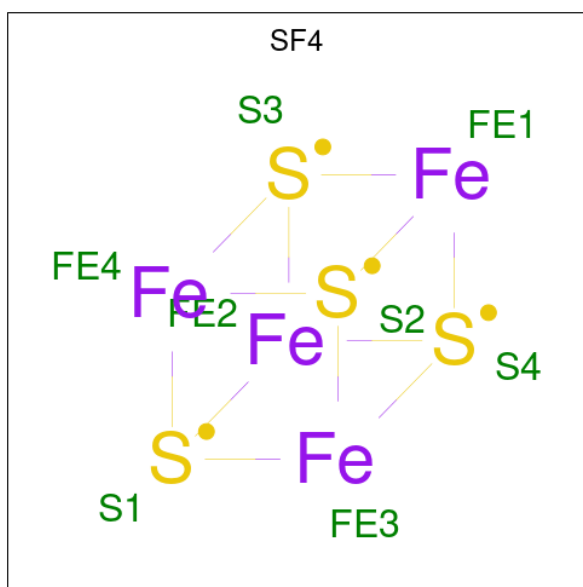
Mol	Chain	Residues	Atoms		AltConf
41	U	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
41	b	1	Total C 40 40	0
41	f	1	Total C 40 40	0
41	i	1	Total C 40 40	0
41	j	1	Total C 40 40	0
41	k	1	Total C 40 40	0
41	l	1	Total C 40 40	0
41	l	1	Total C 40 40	0
41	m	1	Total C 40 40	0
41	r	1	Total C 40 40	0
41	r	1	Total C 40 40	0

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



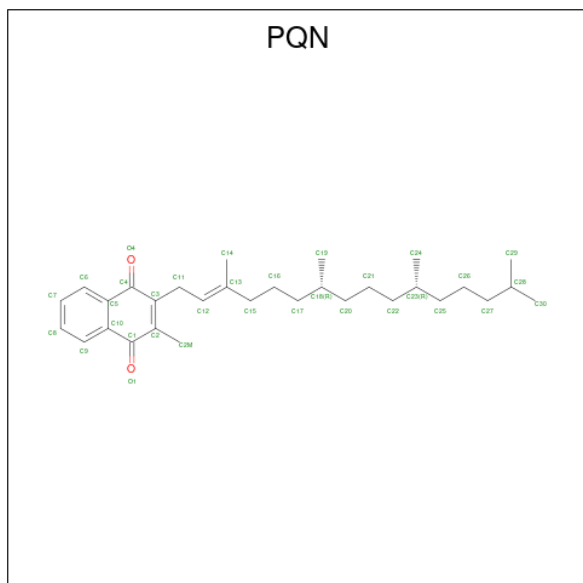
Mol	Chain	Residues	Atoms	AltConf
42	a	1	Total Fe S 8 4 4	0

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

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



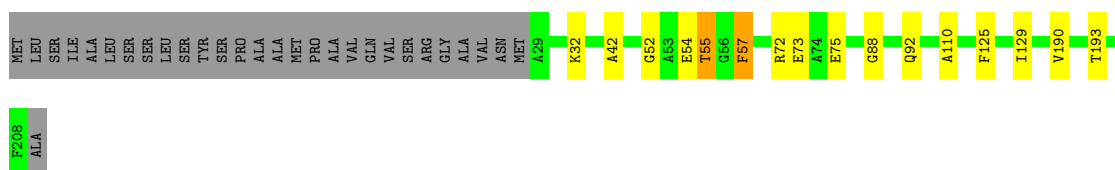
Mol	Chain	Residues	Atoms			AltConf
43	a	1	Total	C	O	0
			33	31	2	
43	b	1	Total	C	O	0
			33	31	2	

3 Residue-property plots

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.

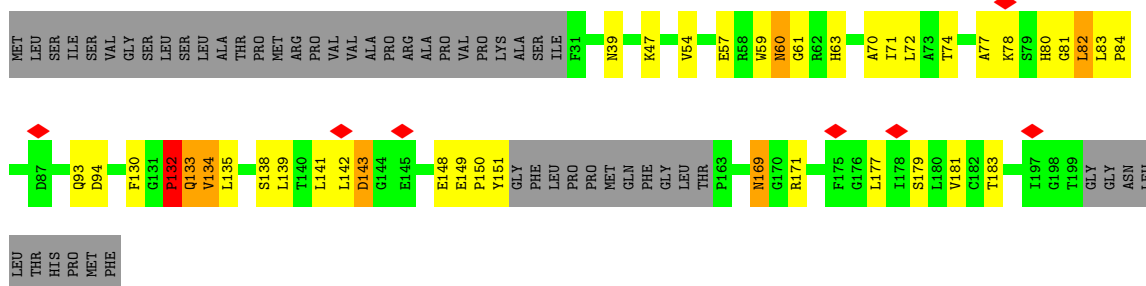
• Molecule 1: iFCPI-7

Chain A: 



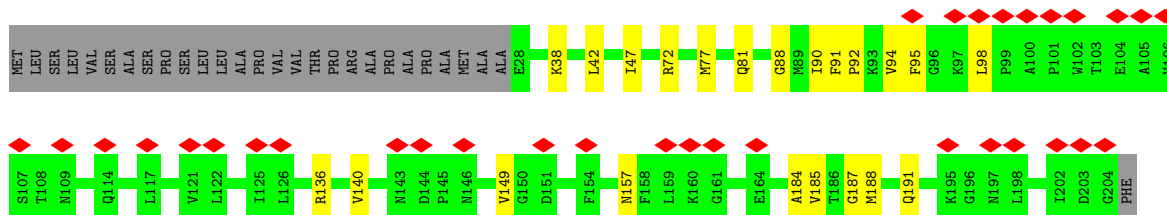
• Molecule 2: iFCPI-1

Chain B: 



• Molecule 3: iFCPI-11

Chain C: 



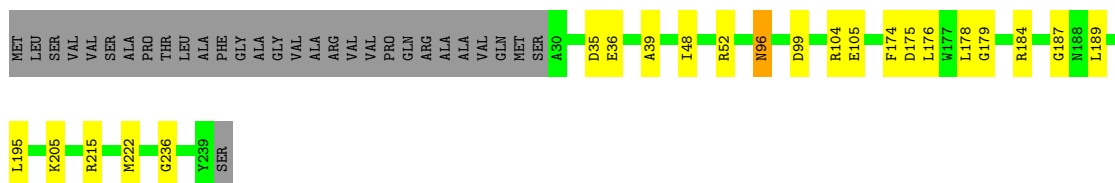
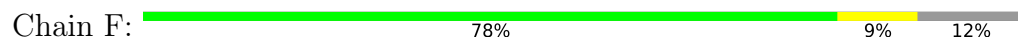
• Molecule 4: iFCPI-6

Chain D: 

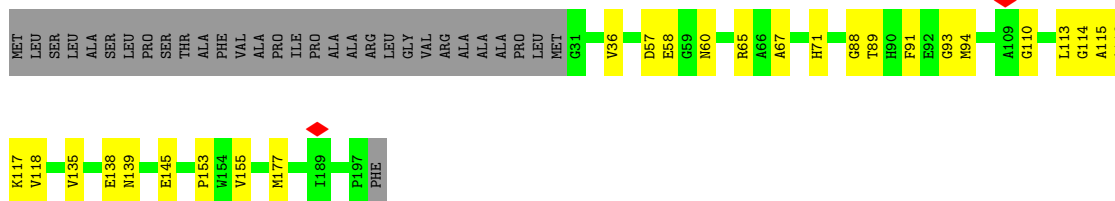
- Molecule 5: iFCPI-5



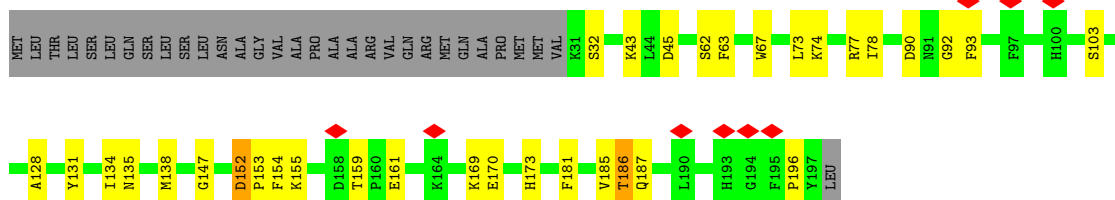
- Molecule 6: iFCPI-8



- Molecule 7: iFCPI-13



- Molecule 8: iFCPI-10



- Molecule 9: iFCPI-3

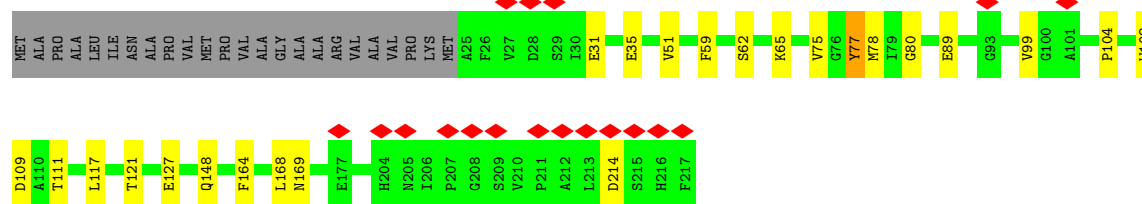
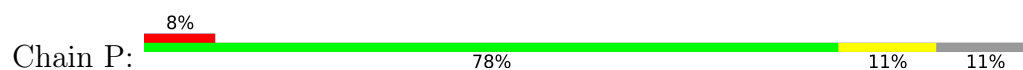
- Molecule 10: iFCPI-9

- Molecule 11: iFCPI-4

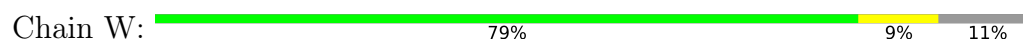
- Molecule 12: iFCPI-12

- Molecule 13: iFCPI-15/14/16

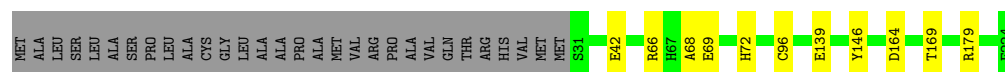
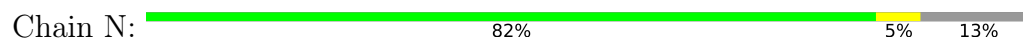
- Molecule 13: iFCPI-15/14/16



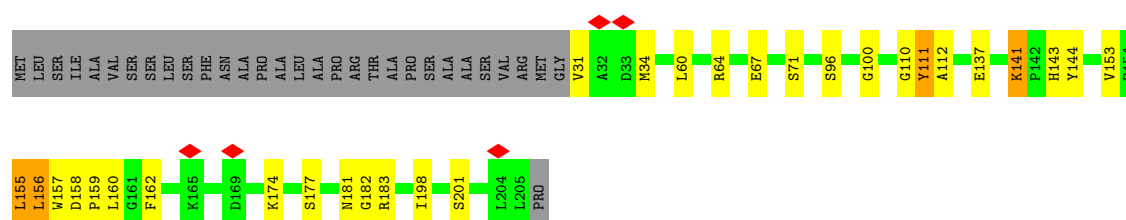
- Molecule 13: iFCPI-15/14/16



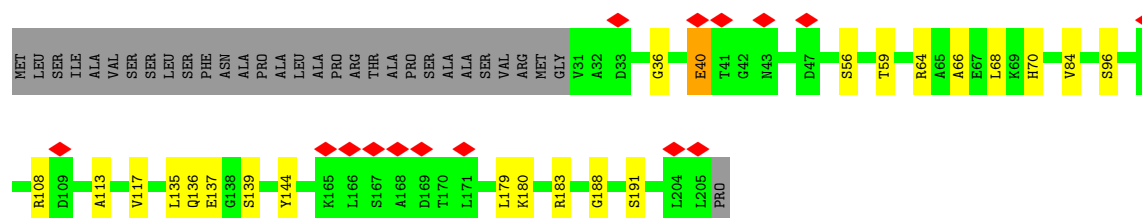
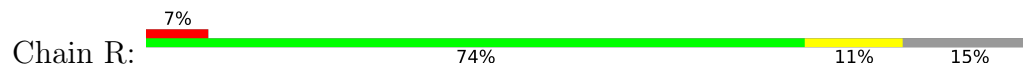
- Molecule 14: iFCPI-17



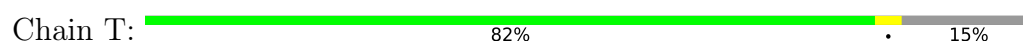
- Molecule 15: iFCPI-20/19/21

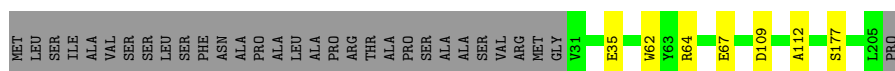


- Molecule 15: iFCPI-20/19/21



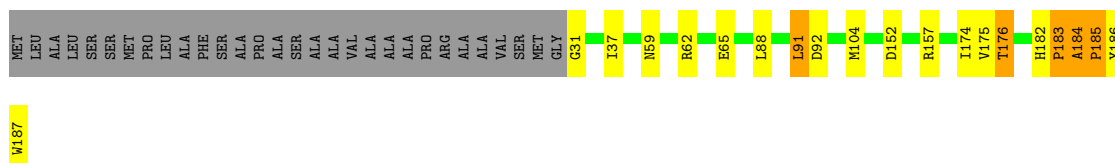
- Molecule 15: iFCPI-20/19/21





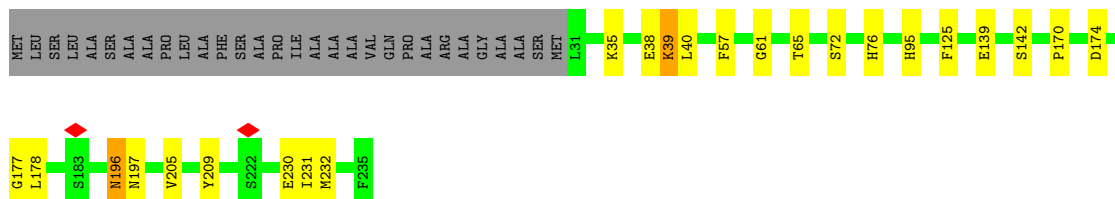
- Molecule 16: iFCPI-18

Chain Q: 73% 8% 16%



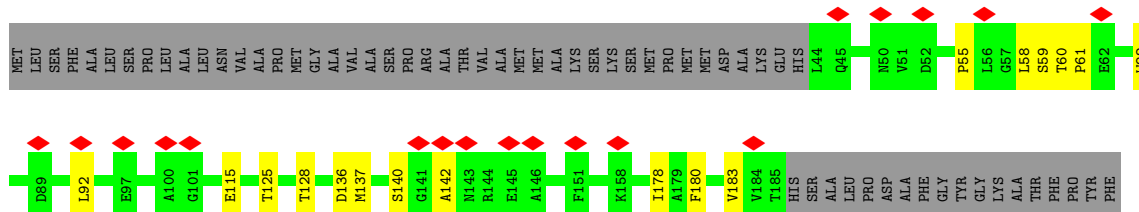
- Molecule 17: iFCPI-22

Chain S: 77% 9% 13%



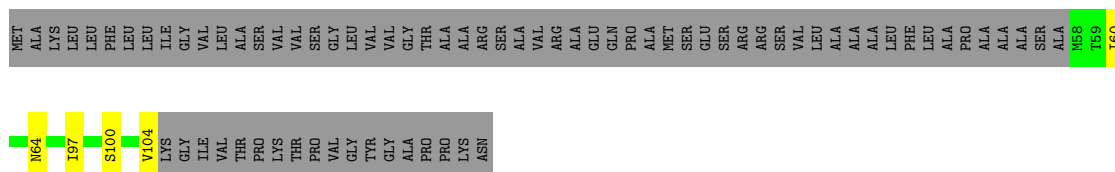
- Molecule 18: iFCPI-2

Chain U: 9% 62% 8% 30%



- Molecule 19: L-iFP

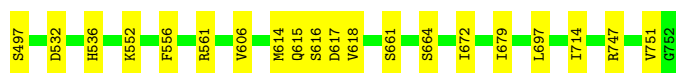
Chain V: 34% 61% 5%



- Molecule 20: Photosystem I P700 chlorophyll a apoprotein A1

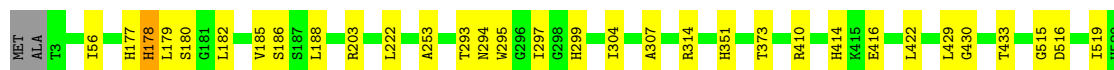
Chain a: 92% 6% 2%





- Molecule 21: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 92% 7%



- Molecule 22: Photosystem I iron-sulfur center

Chain c: 89% 10%



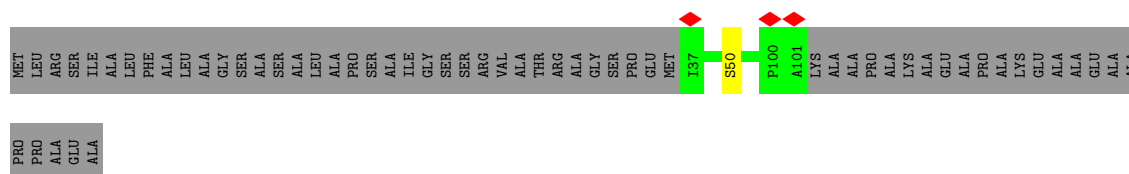
- Molecule 23: Photosystem I reaction center subunit II

Chain d: 89% 8%



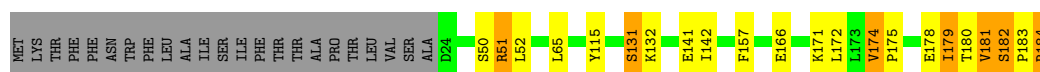
- Molecule 24: PsaE

Chain e: 52% 48%



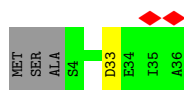
- Molecule 25: Photosystem I reaction center subunit III

Chain f: 76% 8% 12%



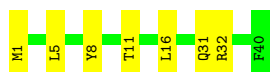
- Molecule 26: Photosystem I reaction center subunit VIII

Chain i: 6% 89% 8%



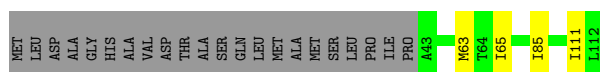
- Molecule 27: Photosystem I reaction center subunit IX

Chain j: 82% 18%



- Molecule 28: PsaK

Chain k: 72% . 24%



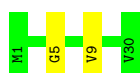
- Molecule 29: Photosystem I reaction center subunit XI

Chain l: 94% 5% .



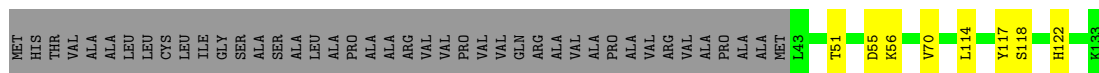
- Molecule 30: Photosystem I reaction center subunit XII

Chain m: 93% 7%



- Molecule 31: PsaR

Chain r: 62% 6% 32%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.577	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.065	Depositor
Map value standard deviation	0.129	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	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, LMG, KC2, PQN, SQD, DGD, LMU, CLA, LHG, SF4, BCR, DD6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	8/1443 (0.6%)	0.60	2/1956 (0.1%)
2	B	0.60	2/1224 (0.2%)	0.75	4/1661 (0.2%)
3	C	0.43	0/1377	0.50	0/1864
4	D	0.59	2/1432 (0.1%)	0.53	3/1939 (0.2%)
5	E	0.60	2/1350 (0.1%)	0.56	3/1839 (0.2%)
6	F	0.46	0/1616	0.50	2/2193 (0.1%)
7	G	0.42	0/1265	0.59	4/1722 (0.2%)
8	H	0.47	1/1297 (0.1%)	0.59	2/1751 (0.1%)
9	I	0.54	1/1219 (0.1%)	0.47	0/1646
10	J	0.34	0/1282	0.46	0/1729
11	K	0.60	4/1321 (0.3%)	0.57	2/1792 (0.1%)
12	L	0.58	0/1519	0.66	2/2057 (0.1%)
13	M	0.37	0/1505	0.51	1/2041 (0.0%)
13	P	0.49	1/1505 (0.1%)	0.52	1/2041 (0.0%)
13	W	0.51	1/1505 (0.1%)	0.56	1/2041 (0.0%)
14	N	0.21	0/1491	0.45	0/2023
15	O	0.51	3/1333 (0.2%)	0.60	3/1815 (0.2%)
15	R	0.28	0/1333	0.46	0/1815
15	T	0.23	0/1333	0.43	0/1815
16	Q	0.53	4/1244 (0.3%)	0.61	8/1690 (0.5%)
17	S	0.60	6/1650 (0.4%)	0.53	1/2234 (0.0%)
18	U	0.33	0/1107	0.53	1/1494 (0.1%)
19	V	0.26	0/369	0.49	0/503
20	a	0.37	6/6019 (0.1%)	0.38	2/8193 (0.0%)
21	b	0.48	11/6029 (0.2%)	0.42	3/8226 (0.0%)
22	c	0.43	0/606	0.41	0/822
23	d	0.36	0/1105	0.46	0/1492
24	e	0.25	0/515	0.44	0/699
25	f	0.89	7/1273 (0.5%)	0.66	4/1723 (0.2%)
26	i	0.20	0/265	0.38	0/363
27	j	0.19	0/323	0.34	0/439
28	k	0.22	0/512	0.46	0/693

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	l	0.19	0/1109	0.36	0/1510
30	m	0.19	0/220	0.33	0/298
31	r	0.18	0/700	0.37	0/957
All	All	0.47	59/49396 (0.1%)	0.50	49/67076 (0.1%)

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	177	HIS	C-O	-8.09	1.14	1.24
21	b	180	SER	CA-C	-7.74	1.42	1.52
20	a	423	TYR	CA-C	-7.54	1.43	1.52
5	E	162	ASP	CA-C	-7.53	1.42	1.52
8	H	32	SER	CA-C	-7.52	1.43	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	77	TYR	N-CA-C	-9.22	100.67	112.93
4	D	153	MET	N-CA-C	-8.49	103.36	114.31
2	B	133	GLN	N-CA-C	-8.40	99.00	110.68
7	G	93	GLY	N-CA-C	8.26	122.44	110.80
13	M	134	LYS	N-CA-C	8.21	123.64	112.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1403	0	1381	14	0
2	B	1194	0	1157	35	0
3	C	1346	0	1366	16	0
4	D	1392	0	1340	20	0
5	E	1316	0	1319	11	0
6	F	1573	0	1548	22	0
7	G	1235	0	1231	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1266	0	1241	27	0
9	I	1190	0	1194	14	0
10	J	1253	0	1243	8	0
11	K	1280	0	1275	29	0
12	L	1479	0	1476	51	0
13	M	1465	0	1469	18	0
13	P	1465	0	1469	20	0
13	W	1465	0	1469	24	0
14	N	1451	0	1475	8	0
15	O	1299	0	1315	23	0
15	R	1299	0	1315	16	0
15	T	1299	0	1315	5	0
16	Q	1210	0	1167	16	0
17	S	1597	0	1552	22	0
18	U	1084	0	1081	14	0
19	V	357	0	352	5	0
20	a	5826	0	5714	35	0
21	b	5818	0	5647	41	0
22	c	596	0	578	9	0
23	d	1080	0	1095	7	0
24	e	504	0	493	1	0
25	f	1243	0	1252	22	0
26	i	258	0	268	1	0
27	j	316	0	328	5	0
28	k	503	0	523	3	0
29	l	1081	0	1091	6	0
30	m	219	0	243	1	0
31	r	682	0	665	7	0
32	A	583	0	573	7	0
32	B	321	0	242	0	0
32	C	402	0	351	3	0
32	D	679	0	640	6	0
32	E	644	0	573	0	0
32	F	527	0	456	4	0
32	G	350	0	291	0	0
32	H	418	0	321	5	0
32	I	506	0	480	3	0
32	J	500	0	410	4	0
32	K	301	0	259	4	0
32	L	422	0	333	10	0
32	M	381	0	343	5	0
32	N	316	0	274	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	O	367	0	326	4	0
32	P	357	0	307	3	0
32	Q	481	0	423	1	0
32	R	336	0	269	1	0
32	S	446	0	366	1	0
32	T	360	0	305	2	0
32	U	265	0	193	3	0
32	V	163	0	143	0	0
32	W	410	0	403	14	0
32	a	2658	0	2697	23	0
32	b	2403	0	2432	17	0
32	f	152	0	127	0	0
32	j	45	0	33	1	0
32	k	165	0	147	7	0
32	l	175	0	177	0	0
32	r	105	0	92	0	0
33	A	45	0	0	2	0
33	C	45	0	0	0	0
33	E	45	0	0	0	0
33	F	90	0	0	2	0
33	G	90	0	0	1	0
33	H	45	0	0	0	0
33	I	90	0	0	4	0
33	J	90	0	0	0	0
33	K	180	0	0	3	0
33	L	225	0	0	0	0
33	M	270	0	0	1	0
33	N	315	0	0	2	0
33	O	135	0	0	1	0
33	P	225	0	0	2	0
33	Q	90	0	0	0	0
33	R	180	0	0	1	0
33	S	180	0	0	5	0
33	T	135	0	0	0	0
33	U	45	0	0	0	0
33	W	270	0	0	1	0
34	A	172	0	0	2	0
34	B	43	0	0	0	0
34	C	43	0	0	0	0
34	D	215	0	0	2	0
34	E	172	0	0	0	0
34	F	129	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	G	43	0	0	0	0
34	H	129	0	0	0	0
34	I	172	0	0	2	0
34	J	172	0	0	1	0
34	K	86	0	0	0	0
34	L	43	0	0	1	0
34	M	43	0	0	3	0
34	N	129	0	0	0	0
34	O	43	0	0	0	0
34	P	43	0	0	0	0
34	Q	172	0	0	0	0
34	R	43	0	0	0	0
34	S	43	0	0	2	0
34	T	43	0	0	0	0
34	U	43	0	0	1	0
34	V	43	0	0	0	0
34	W	43	0	0	1	0
34	j	43	0	0	0	0
34	k	43	0	0	1	0
35	A	40	0	50	0	0
35	B	31	0	32	2	0
35	D	48	0	69	0	0
35	E	92	0	130	0	0
35	F	81	0	102	2	0
35	I	83	0	109	0	0
35	M	46	0	65	0	0
35	P	46	0	65	1	0
35	W	46	0	65	0	0
35	a	116	0	145	7	0
35	f	47	0	67	1	0
36	A	76	0	92	1	0
36	D	141	0	162	1	0
36	E	111	0	132	0	0
36	F	73	0	86	18	0
36	L	37	0	44	0	0
36	M	40	0	48	9	0
36	N	40	0	49	5	0
36	P	45	0	59	7	0
36	S	33	0	34	8	0
36	T	37	0	44	2	0
36	W	39	0	46	11	0
36	j	38	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	l	49	0	69	5	0
37	C	96	0	0	0	0
37	D	96	0	0	1	0
37	F	144	0	0	2	0
37	G	96	0	0	0	0
37	H	48	0	0	1	0
37	J	48	0	0	0	0
37	K	144	0	0	0	0
37	L	192	0	0	4	0
37	M	288	0	0	6	0
37	N	192	0	0	0	0
37	O	96	0	0	0	0
37	P	192	0	0	1	0
37	Q	96	0	0	2	0
37	R	96	0	0	2	0
37	S	336	0	0	2	0
37	T	144	0	0	1	0
37	U	48	0	0	0	0
37	W	192	0	0	2	0
37	r	48	0	0	0	0
38	D	35	0	46	2	0
38	I	35	0	46	3	0
38	J	35	0	46	3	0
38	V	34	0	41	3	0
38	j	34	0	41	0	0
39	H	43	0	50	16	0
39	k	36	0	36	6	0
40	Q	56	0	70	3	0
40	b	56	0	70	0	0
41	U	40	0	56	1	0
41	a	200	0	280	2	0
41	b	200	0	280	6	0
41	f	40	0	56	0	0
41	i	40	0	56	0	0
41	j	40	0	56	0	0
41	k	40	0	56	1	0
41	l	80	0	112	1	0
41	m	40	0	56	0	0
41	r	80	0	112	0	0
42	a	8	0	0	0	0
42	c	16	0	0	1	0
43	a	33	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	b	33	0	46	0	0
All	All	73546	0	65101	651	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 5.

The worst 5 of 651 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)
20:a:497:SER:OG	35:a:851:LHG:C4	1.80	1.27
20:a:497:SER:OG	35:a:851:LHG:HC41	1.10	1.25
33:I:309:KC2:O1A	36:I:201:LMG:O3	1.52	1.20
34:A:313:DD6:C28	36:N:301:LMG:H322	1.77	1.14
37:S:315:A86:C39	36:S:322:LMG:H291	1.79	1.11

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	178/209 (85%)	175 (98%)	3 (2%)	0	100	100
2	B	154/209 (74%)	144 (94%)	8 (5%)	2 (1%)	9	16
3	C	175/205 (85%)	168 (96%)	6 (3%)	1 (1%)	21	36
4	D	177/245 (72%)	173 (98%)	4 (2%)	0	100	100
5	E	174/206 (84%)	161 (92%)	13 (8%)	0	100	100
6	F	208/240 (87%)	200 (96%)	8 (4%)	0	100	100
7	G	165/198 (83%)	158 (96%)	7 (4%)	0	100	100
8	H	165/198 (83%)	158 (96%)	6 (4%)	1 (1%)	21	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	152/194 (78%)	146 (96%)	5 (3%)	1 (1%)	18	32
10	J	169/200 (84%)	166 (98%)	3 (2%)	0	100	100
11	K	164/202 (81%)	157 (96%)	6 (4%)	1 (1%)	21	36
12	L	196/229 (86%)	190 (97%)	5 (3%)	1 (0%)	24	40
13	M	191/217 (88%)	183 (96%)	7 (4%)	1 (0%)	24	40
13	P	191/217 (88%)	183 (96%)	8 (4%)	0	100	100
13	W	191/217 (88%)	181 (95%)	9 (5%)	1 (0%)	24	40
14	N	192/224 (86%)	184 (96%)	8 (4%)	0	100	100
15	O	173/206 (84%)	160 (92%)	12 (7%)	1 (1%)	21	36
15	R	173/206 (84%)	167 (96%)	6 (4%)	0	100	100
15	T	173/206 (84%)	162 (94%)	11 (6%)	0	100	100
16	Q	155/187 (83%)	152 (98%)	2 (1%)	1 (1%)	21	36
17	S	203/235 (86%)	192 (95%)	10 (5%)	1 (0%)	24	40
18	U	140/203 (69%)	133 (95%)	7 (5%)	0	100	100
19	V	45/122 (37%)	43 (96%)	2 (4%)	0	100	100
20	a	739/752 (98%)	711 (96%)	28 (4%)	0	100	100
21	b	730/734 (100%)	708 (97%)	22 (3%)	0	100	100
22	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
23	d	135/142 (95%)	129 (96%)	6 (4%)	0	100	100
24	e	63/124 (51%)	57 (90%)	6 (10%)	0	100	100
25	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
26	i	31/36 (86%)	31 (100%)	0	0	100	100
27	j	38/40 (95%)	38 (100%)	0	0	100	100
28	k	68/92 (74%)	68 (100%)	0	0	100	100
29	l	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
30	m	28/30 (93%)	28 (100%)	0	0	100	100
31	r	89/133 (67%)	89 (100%)	0	0	100	100
All	All	6203/7268 (85%)	5960 (96%)	231 (4%)	12 (0%)	44	62

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	GLY

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Mol	Chain	Res	Type
9	I	136	PRO
11	K	44	GLY
13	M	136	HIS
15	O	156	LEU

5.3.2 Protein sidechains ⓘ

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	148/170 (87%)	148 (100%)	0	100	100
2	B	117/159 (74%)	114 (97%)	3 (3%)	40	62
3	C	143/164 (87%)	143 (100%)	0	100	100
4	D	143/186 (77%)	141 (99%)	2 (1%)	59	74
5	E	137/157 (87%)	137 (100%)	0	100	100
6	F	161/183 (88%)	161 (100%)	0	100	100
7	G	126/148 (85%)	126 (100%)	0	100	100
8	H	133/158 (84%)	132 (99%)	1 (1%)	73	83
9	I	125/156 (80%)	124 (99%)	1 (1%)	73	83
10	J	122/143 (85%)	122 (100%)	0	100	100
11	K	129/153 (84%)	128 (99%)	1 (1%)	73	83
12	L	151/176 (86%)	148 (98%)	3 (2%)	48	67
13	M	148/164 (90%)	147 (99%)	1 (1%)	76	85
13	P	148/164 (90%)	148 (100%)	0	100	100
13	W	148/164 (90%)	147 (99%)	1 (1%)	76	85
14	N	150/172 (87%)	150 (100%)	0	100	100
15	O	133/156 (85%)	133 (100%)	0	100	100
15	R	133/156 (85%)	132 (99%)	1 (1%)	73	83
15	T	133/156 (85%)	133 (100%)	0	100	100
16	Q	124/142 (87%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	S	160/177 (90%)	159 (99%)	1 (1%)	78	87
18	U	110/156 (70%)	110 (100%)	0	100	100
19	V	41/94 (44%)	41 (100%)	0	100	100
20	a	607/616 (98%)	607 (100%)	0	100	100
21	b	590/591 (100%)	589 (100%)	1 (0%)	87	94
22	c	68/69 (99%)	68 (100%)	0	100	100
23	d	116/121 (96%)	116 (100%)	0	100	100
24	e	53/88 (60%)	53 (100%)	0	100	100
25	f	127/147 (86%)	124 (98%)	3 (2%)	43	63
26	i	30/32 (94%)	30 (100%)	0	100	100
27	j	36/36 (100%)	36 (100%)	0	100	100
28	k	53/70 (76%)	53 (100%)	0	100	100
29	l	117/118 (99%)	117 (100%)	0	100	100
30	m	22/22 (100%)	22 (100%)	0	100	100
31	r	71/99 (72%)	70 (99%)	1 (1%)	59	74
All	All	4953/5663 (88%)	4933 (100%)	20 (0%)	81	90

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	W	27	VAL
25	f	182	SER
31	r	122	HIS
25	f	184	ARG
9	I	136	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
17	S	90	GLN
21	b	275	HIS
18	U	133	GLN
25	f	140	ASN
20	a	193	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

517 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	DD6	J	316	-	40,45,45	0.19	0	51,67,67	0.69	1 (1%)
32	CLA	L	310	-	44,48,73	2.18	9 (20%)	51,82,113	2.00	7 (13%)
32	CLA	C	302	-	45,49,73	2.21	10 (22%)	54,84,113	1.68	7 (12%)
32	CLA	a	820	-	69,73,73	1.71	9 (13%)	82,113,113	1.40	6 (7%)
32	CLA	P	304	-	49,53,73	2.07	9 (18%)	58,89,113	1.56	9 (15%)
32	CLA	a	826	-	69,73,73	1.66	9 (13%)	82,113,113	1.24	5 (6%)
33	KC2	Q	317	32	49,53,53	1.80	4 (8%)	60,89,89	1.13	5 (8%)
41	BCR	U	310	-	41,41,41	0.15	0	56,56,56	0.40	0
32	CLA	r	201	-	64,68,73	1.83	9 (14%)	76,107,113	1.46	10 (13%)
32	CLA	a	804	-	62,66,73	1.77	9 (14%)	73,104,113	1.39	7 (9%)
33	KC2	M	307	-	49,53,53	1.85	4 (8%)	60,89,89	1.04	5 (8%)
33	KC2	W	303	13	49,53,53	1.83	4 (8%)	60,89,89	1.06	4 (6%)
32	CLA	M	311	13	49,53,73	2.07	9 (18%)	58,89,113	1.64	7 (12%)
33	KC2	H	303	-	49,53,53	1.85	4 (8%)	60,89,89	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A86	K	311	-	47,50,50	0.58	1 (2%)	51,76,76	0.83	2 (3%)
32	CLA	b	813	-	49,53,73	2.01	9 (18%)	58,89,113	1.50	7 (12%)
32	CLA	b	820	-	68,72,73	1.74	9 (13%)	80,111,113	1.36	6 (7%)
34	DD6	I	312	-	40,45,45	0.20	0	51,67,67	0.64	1 (1%)
33	KC2	R	311	15	49,53,53	1.83	4 (8%)	60,89,89	1.04	4 (6%)
32	CLA	b	816	-	66,70,73	1.72	9 (13%)	78,109,113	1.29	7 (8%)
32	CLA	T	309	-	49,53,73	2.05	9 (18%)	58,89,113	1.53	6 (10%)
32	CLA	l	203	35	69,73,73	1.73	9 (13%)	82,113,113	1.23	6 (7%)
32	CLA	W	311	13	69,73,73	1.68	9 (13%)	82,113,113	1.26	6 (7%)
32	CLA	b	802	-	69,73,73	1.67	9 (13%)	82,113,113	1.35	7 (8%)
34	DD6	N	319	-	40,45,45	0.16	0	51,67,67	1.06	3 (5%)
32	CLA	b	818	-	69,73,73	1.72	9 (13%)	82,113,113	1.32	7 (8%)
37	A86	F	317	-	47,50,50	0.53	1 (2%)	51,76,76	0.60	2 (3%)
32	CLA	M	310	13	66,70,73	1.69	9 (13%)	78,109,113	1.29	6 (7%)
32	CLA	L	311	-	44,48,73	2.22	9 (20%)	51,82,113	2.10	10 (19%)
32	CLA	b	839	-	69,73,73	1.67	9 (13%)	82,113,113	1.22	5 (6%)
32	CLA	H	306	-	54,58,73	1.95	9 (16%)	64,95,113	1.48	6 (9%)
32	CLA	b	817	-	59,63,73	1.82	9 (15%)	70,101,113	1.40	7 (10%)
34	DD6	R	314	-	40,45,45	0.18	0	51,67,67	0.82	1 (1%)
35	LHG	I	318	32	36,36,48	1.05	2 (5%)	39,42,54	1.31	4 (10%)
32	CLA	k	203	-	59,63,73	1.83	9 (15%)	70,101,113	1.45	8 (11%)
32	CLA	a	815	-	54,58,73	1.88	9 (16%)	64,95,113	1.43	7 (10%)
32	CLA	a	817	-	65,69,73	1.72	9 (13%)	77,108,113	1.34	7 (9%)
37	A86	D	323	-	47,50,50	0.37	0	51,76,76	0.91	3 (5%)
37	A86	N	317	-	47,50,50	0.59	1 (2%)	51,76,76	0.83	2 (3%)
32	CLA	P	305	13	64,68,73	1.76	9 (14%)	76,107,113	1.34	7 (9%)
32	CLA	b	833	-	66,70,73	1.74	9 (13%)	78,109,113	1.40	6 (7%)
32	CLA	I	303	9	59,63,73	1.88	9 (15%)	70,101,113	1.53	8 (11%)
32	CLA	A	311	-	49,53,73	2.03	9 (18%)	58,89,113	1.58	6 (10%)
33	KC2	P	301	-	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
34	DD6	L	319	-	40,45,45	0.21	0	51,67,67	1.20	4 (7%)
32	CLA	R	310	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	6 (8%)
32	CLA	G	304	-	59,63,73	1.84	9 (15%)	70,101,113	1.40	7 (10%)
32	CLA	S	313	17	49,53,73	2.05	9 (18%)	58,89,113	1.56	6 (10%)
36	LMG	j	104	-	38,38,55	1.10	4 (10%)	46,46,63	1.49	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	KC2	L	303	-	49,53,53	1.82	4 (8%)	60,89,89	1.09	5 (8%)
32	CLA	M	306	13	66,70,73	1.76	9 (13%)	78,109,113	1.35	6 (7%)
32	CLA	a	831	-	64,68,73	1.77	9 (14%)	76,107,113	1.36	7 (9%)
33	KC2	L	305	12	49,53,53	1.84	4 (8%)	60,89,89	1.09	5 (8%)
32	CLA	A	308	-	59,63,73	1.82	9 (15%)	70,101,113	1.35	5 (7%)
32	CLA	F	301	-	44,48,73	2.17	9 (20%)	51,82,113	1.84	7 (13%)
33	KC2	R	305	15	49,53,53	1.85	4 (8%)	60,89,89	1.07	3 (5%)
34	DD6	E	317	-	40,45,45	0.19	0	51,67,67	0.85	3 (5%)
33	KC2	K	302	11	49,53,53	1.82	4 (8%)	60,89,89	1.09	4 (6%)
38	LMU	I	315	-	36,36,36	0.35	0	47,47,47	1.19	5 (10%)
34	DD6	J	314	-	40,45,45	0.23	0	51,67,67	0.64	1 (1%)
32	CLA	L	304	-	49,53,73	1.99	9 (18%)	58,89,113	1.49	8 (13%)
32	CLA	b	837	-	69,73,73	1.72	9 (13%)	82,113,113	1.42	6 (7%)
37	A86	S	319	-	47,50,50	0.38	0	51,76,76	0.85	2 (3%)
34	DD6	I	313	-	40,45,45	0.19	0	51,67,67	0.72	2 (3%)
32	CLA	b	824	-	62,66,73	1.78	9 (14%)	73,104,113	1.34	6 (8%)
32	CLA	Q	304	-	54,58,73	1.92	9 (16%)	64,95,113	1.47	8 (12%)
32	CLA	W	306	-	59,63,73	1.85	9 (15%)	70,101,113	1.42	6 (8%)
34	DD6	H	311	-	40,45,45	0.22	0	51,67,67	0.87	3 (5%)
36	LMG	D	321	-	40,40,55	0.81	0	48,48,63	1.30	6 (12%)
32	CLA	C	301	3	49,53,73	2.03	9 (18%)	58,89,113	1.48	6 (10%)
43	PQN	a	848	-	34,34,34	0.40	0	43,45,45	1.01	1 (2%)
32	CLA	a	829	-	64,68,73	1.80	9 (14%)	76,107,113	1.39	7 (9%)
33	KC2	M	303	13	49,53,53	1.84	4 (8%)	60,89,89	1.02	4 (6%)
32	CLA	a	812	-	59,63,73	1.90	10 (16%)	70,101,113	1.56	10 (14%)
32	CLA	E	306	5	64,68,73	1.81	9 (14%)	76,107,113	1.37	6 (7%)
32	CLA	G	305	-	49,53,73	2.00	9 (18%)	58,89,113	1.48	8 (13%)
34	DD6	F	314	-	40,45,45	0.22	0	51,67,67	0.71	1 (1%)
34	DD6	j	103	-	40,45,45	0.18	0	51,67,67	0.87	1 (1%)
32	CLA	N	313	-	64,68,73	1.77	9 (14%)	76,107,113	1.40	7 (9%)
34	DD6	A	313	-	40,45,45	0.16	0	51,67,67	0.79	2 (3%)
32	CLA	A	307	1	64,68,73	1.80	9 (14%)	76,107,113	1.40	7 (9%)
32	CLA	D	310	4	69,73,73	1.71	9 (13%)	82,113,113	1.43	11 (13%)
32	CLA	S	309	-	64,68,73	1.74	9 (14%)	76,107,113	1.36	8 (10%)
32	CLA	a	819	20	69,73,73	1.68	9 (13%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	b	831	-	64,68,73	1.72	9 (14%)	76,107,113	1.27	6 (7%)
32	CLA	T	307	-	54,58,73	1.94	9 (16%)	64,95,113	1.45	6 (9%)
32	CLA	a	840	-	69,73,73	1.70	9 (13%)	82,113,113	1.35	7 (8%)
33	KC2	Q	302	-	49,53,53	1.82	4 (8%)	60,89,89	1.06	4 (6%)
32	CLA	W	310	-	64,68,73	1.77	9 (14%)	76,107,113	1.34	7 (9%)
40	DGD	b	846	-	57,57,67	0.88	2 (3%)	71,71,81	1.32	6 (8%)
33	KC2	R	303	-	49,53,53	1.86	4 (8%)	60,89,89	1.07	3 (5%)
32	CLA	Q	303	16	64,68,73	1.83	9 (14%)	76,107,113	1.55	9 (11%)
35	LHG	E	301	-	45,45,48	0.66	1 (2%)	48,51,54	1.12	2 (4%)
37	A86	G	310	-	47,50,50	0.38	0	51,76,76	1.11	2 (3%)
32	CLA	E	310	5	49,53,73	2.01	9 (18%)	58,89,113	1.47	6 (10%)
32	CLA	a	832	-	64,68,73	1.76	9 (14%)	76,107,113	1.39	5 (6%)
32	CLA	E	303	5	49,53,73	1.99	9 (18%)	58,89,113	1.51	5 (8%)
32	CLA	k	202	-	59,63,73	1.85	9 (15%)	70,101,113	1.36	5 (7%)
33	KC2	L	306	12	49,53,53	1.84	4 (8%)	60,89,89	1.05	5 (8%)
32	CLA	a	813	-	49,53,73	2.07	9 (18%)	58,89,113	1.65	7 (12%)
36	LMG	D	325	-	35,35,55	1.06	2 (5%)	43,43,63	1.50	7 (16%)
32	CLA	H	309	-	49,53,73	2.09	9 (18%)	58,89,113	1.55	7 (12%)
32	CLA	a	835	-	69,73,73	1.68	9 (13%)	82,113,113	1.29	7 (8%)
32	CLA	Q	309	-	49,53,73	2.00	9 (18%)	58,89,113	1.53	5 (8%)
32	CLA	a	807	-	69,73,73	1.73	9 (13%)	82,113,113	1.41	8 (9%)
34	DD6	Q	314	-	40,45,45	0.17	0	51,67,67	0.63	1 (1%)
36	LMG	F	319	33	40,40,55	1.01	2 (5%)	48,48,63	1.09	2 (4%)
32	CLA	W	309	13	69,73,73	1.70	9 (13%)	82,113,113	1.28	6 (7%)
32	CLA	T	305	-	49,53,73	2.08	9 (18%)	58,89,113	1.55	8 (13%)
32	CLA	T	306	15	64,68,73	1.75	9 (14%)	76,107,113	1.27	5 (6%)
37	A86	F	313	-	47,50,50	0.43	1 (2%)	51,76,76	0.91	3 (5%)
32	CLA	b	836	-	69,73,73	1.70	9 (13%)	82,113,113	1.35	7 (8%)
32	CLA	E	311	5	49,53,73	2.05	9 (18%)	58,89,113	1.61	7 (12%)
41	BCR	a	854	-	41,41,41	0.15	0	56,56,56	0.43	0
34	DD6	Q	312	-	40,45,45	0.18	0	51,67,67	0.76	1 (1%)
33	KC2	N	304	14	49,53,53	1.80	4 (8%)	60,89,89	1.11	5 (8%)
32	CLA	O	309	-	66,70,73	1.74	9 (13%)	78,109,113	1.35	6 (7%)
32	CLA	a	828	-	62,66,73	1.76	9 (14%)	73,104,113	1.43	9 (12%)
34	DD6	G	312	-	40,45,45	0.24	0	51,67,67	0.81	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	J	306	-	59,63,73	1.80	9 (15%)	70,101,113	1.43	7 (10%)
33	KC2	A	310	1	49,53,53	1.85	4 (8%)	60,89,89	1.06	4 (6%)
32	CLA	a	842	-	59,63,73	1.83	9 (15%)	70,101,113	1.36	6 (8%)
37	A86	R	312	-	47,50,50	0.57	1 (2%)	51,76,76	0.81	1 (1%)
32	CLA	f	203	25	49,53,73	2.02	9 (18%)	58,89,113	1.54	6 (10%)
36	LMG	E	320	-	31,31,55	1.13	2 (6%)	39,39,63	1.56	7 (17%)
32	CLA	K	306	-	64,68,73	1.75	9 (14%)	76,107,113	1.44	10 (13%)
36	LMG	E	322	-	40,40,55	1.09	2 (5%)	48,48,63	1.34	3 (6%)
32	CLA	A	301	1	49,53,73	2.00	9 (18%)	58,89,113	1.48	7 (12%)
32	CLA	D	304	4	64,68,73	1.77	9 (14%)	76,107,113	1.36	8 (10%)
32	CLA	F	308	6	50,54,73	2.06	9 (18%)	59,90,113	1.50	6 (10%)
32	CLA	I	308	-	59,63,73	1.88	9 (15%)	70,101,113	1.48	6 (8%)
32	CLA	O	308	-	49,53,73	2.06	9 (18%)	58,89,113	1.57	7 (12%)
32	CLA	U	302	18	49,53,73	2.06	9 (18%)	58,89,113	1.52	8 (13%)
42	SF4	c	101	22	0,12,12	-	-	-	-	-
37	A86	P	319	-	47,50,50	0.50	1 (2%)	51,76,76	0.73	2 (3%)
41	BCR	j	102	-	41,41,41	0.16	0	56,56,56	0.50	0
32	CLA	E	312	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	6 (7%)
32	CLA	b	819	-	69,73,73	1.67	9 (13%)	82,113,113	1.25	8 (9%)
32	CLA	K	307	-	45,49,73	2.20	10 (22%)	54,84,113	1.56	8 (14%)
32	CLA	F	304	-	59,63,73	1.86	9 (15%)	70,101,113	1.45	8 (11%)
41	BCR	b	844	-	41,41,41	0.13	0	56,56,56	0.49	0
34	DD6	k	205	-	40,45,45	0.19	0	51,67,67	0.79	3 (5%)
32	CLA	D	307	4	65,69,73	1.76	9 (13%)	77,108,113	1.48	9 (11%)
32	CLA	a	825	-	69,73,73	1.66	9 (13%)	82,113,113	1.21	6 (7%)
32	CLA	b	827	-	54,58,73	1.94	9 (16%)	64,95,113	1.42	6 (9%)
32	CLA	a	833	-	69,73,73	1.68	9 (13%)	82,113,113	1.31	7 (8%)
32	CLA	C	304	3	47,51,73	2.15	9 (19%)	55,86,113	1.74	9 (16%)
33	KC2	T	303	-	49,53,53	1.84	4 (8%)	60,89,89	1.08	5 (8%)
32	CLA	E	304	-	64,68,73	1.81	9 (14%)	76,107,113	1.41	6 (7%)
32	CLA	P	310	-	45,49,73	2.22	10 (22%)	54,84,113	1.68	7 (12%)
32	CLA	T	308	15	64,68,73	1.79	9 (14%)	76,107,113	1.48	12 (15%)
37	A86	K	312	-	47,50,50	0.49	1 (2%)	51,76,76	0.79	1 (1%)
41	BCR	f	202	-	41,41,41	0.10	0	56,56,56	0.39	0
37	A86	H	314	-	47,50,50	0.40	0	51,76,76	1.08	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	J	302	-	49,53,73	2.03	9 (18%)	58,89,113	1.52	5 (8%)
32	CLA	G	306	7	60,64,73	1.86	9 (15%)	71,102,113	1.53	9 (12%)
32	CLA	E	307	5	59,63,73	1.80	9 (15%)	70,101,113	1.37	6 (8%)
34	DD6	F	315	-	40,45,45	0.18	0	51,67,67	0.88	2 (3%)
32	CLA	B	303	-	49,53,73	2.04	9 (18%)	58,89,113	1.46	6 (10%)
37	A86	S	318	-	47,50,50	0.44	1 (2%)	51,76,76	0.95	2 (3%)
32	CLA	I	317	35	69,73,73	1.68	9 (13%)	82,113,113	1.30	6 (7%)
32	CLA	Q	306	16	66,70,73	1.75	9 (13%)	78,109,113	1.38	9 (11%)
33	KC2	P	303	13	49,53,53	1.85	4 (8%)	60,89,89	1.05	4 (6%)
34	DD6	B	307	-	40,45,45	0.20	0	51,67,67	0.71	2 (3%)
41	BCR	b	845	-	41,41,41	0.16	0	56,56,56	0.30	0
32	CLA	a	810	-	66,70,73	1.71	9 (13%)	78,109,113	1.32	8 (10%)
33	KC2	J	303	-	49,53,53	1.82	4 (8%)	60,89,89	1.08	4 (6%)
32	CLA	S	308	-	48,52,73	2.11	10 (20%)	56,87,113	1.88	9 (16%)
32	CLA	a	805	-	69,73,73	1.84	12 (17%)	82,113,113	1.44	12 (14%)
32	CLA	V	201	-	62,66,73	1.80	9 (14%)	73,104,113	1.35	6 (8%)
34	DD6	E	318	-	40,45,45	0.17	0	51,67,67	0.72	2 (3%)
33	KC2	K	303	11	49,53,53	1.85	4 (8%)	60,89,89	1.06	5 (8%)
32	CLA	b	829	-	59,63,73	1.83	9 (15%)	70,101,113	1.42	6 (8%)
37	A86	O	312	-	47,50,50	0.47	1 (2%)	51,76,76	0.94	3 (5%)
32	CLA	C	305	-	64,68,73	1.87	9 (14%)	76,107,113	1.47	8 (10%)
38	LMU	j	105	-	35,35,36	0.27	0	46,46,47	1.12	4 (8%)
33	KC2	G	309	7	49,53,53	1.83	4 (8%)	60,89,89	1.10	5 (8%)
32	CLA	E	305	5	59,63,73	1.84	9 (15%)	70,101,113	1.39	6 (8%)
32	CLA	b	822	-	69,73,73	1.64	9 (13%)	82,113,113	1.31	7 (8%)
32	CLA	b	811	-	54,58,73	1.90	9 (16%)	64,95,113	1.46	7 (10%)
32	CLA	Q	310	-	50,54,73	2.05	9 (18%)	59,90,113	1.56	8 (13%)
32	CLA	J	304	10	59,63,73	1.89	10 (16%)	70,101,113	1.53	10 (14%)
32	CLA	A	302	35	64,68,73	1.76	9 (14%)	76,107,113	1.27	5 (6%)
36	LMG	W	320	33,37	39,39,55	1.06	2 (5%)	47,47,63	1.15	3 (6%)
37	A86	N	316	-	47,50,50	0.55	1 (2%)	51,76,76	1.23	3 (5%)
32	CLA	P	309	-	65,69,73	1.75	9 (13%)	77,108,113	1.35	8 (10%)
32	CLA	T	302	15	49,53,73	2.08	9 (18%)	58,89,113	1.55	7 (12%)
34	DD6	I	310	-	40,45,45	0.15	0	51,67,67	0.90	4 (7%)
32	CLA	R	301	-	49,53,73	2.08	9 (18%)	58,89,113	1.64	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LMG	A	317	-	36,36,55	1.07	2 (5%)	44,44,63	1.33	5 (11%)
38	LMU	J	318	-	36,36,36	0.69	0	47,47,47	1.01	1 (2%)
32	CLA	T	310	-	59,63,73	1.86	9 (15%)	70,101,113	1.47	7 (10%)
34	DD6	P	315	-	40,45,45	0.25	0	51,67,67	0.91	3 (5%)
37	A86	C	311	-	47,50,50	0.65	1 (2%)	51,76,76	1.00	2 (3%)
32	CLA	H	308	8	45,49,73	2.26	10 (22%)	54,84,113	1.75	8 (14%)
32	CLA	S	311	-	54,58,73	1.96	9 (16%)	64,95,113	1.54	8 (12%)
32	CLA	P	307	13	49,53,73	2.04	9 (18%)	58,89,113	1.56	6 (10%)
37	A86	M	322	-	47,50,50	0.42	1 (2%)	51,76,76	0.68	1 (1%)
32	CLA	a	802	-	67,71,73	1.71	9 (13%)	79,110,113	1.35	10 (12%)
32	CLA	J	308	-	49,53,73	2.09	9 (18%)	58,89,113	1.62	7 (12%)
33	KC2	O	303	15	49,53,53	1.82	4 (8%)	60,89,89	1.03	4 (6%)
32	CLA	a	814	-	69,73,73	1.65	9 (13%)	82,113,113	1.44	9 (10%)
32	CLA	R	306	15	49,53,73	2.04	9 (18%)	58,89,113	1.58	6 (10%)
32	CLA	S	310	17	49,53,73	2.02	9 (18%)	58,89,113	1.52	6 (10%)
41	BCR	a	844	-	41,41,41	0.15	0	56,56,56	0.41	0
32	CLA	D	306	4	64,68,73	1.74	9 (14%)	76,107,113	1.38	8 (10%)
37	A86	M	315	-	47,50,50	0.35	0	51,76,76	1.11	3 (5%)
32	CLA	M	308	13	61,65,73	1.84	9 (14%)	72,103,113	1.45	11 (15%)
32	CLA	O	301	15	49,53,73	2.09	9 (18%)	58,89,113	1.58	7 (12%)
32	CLA	O	306	-	49,53,73	2.03	9 (18%)	58,89,113	1.52	7 (12%)
32	CLA	b	815	-	69,73,73	1.65	9 (13%)	82,113,113	1.31	8 (9%)
32	CLA	J	307	10	59,63,73	1.87	10 (16%)	70,101,113	1.59	8 (11%)
32	CLA	b	803	-	69,73,73	1.66	9 (13%)	82,113,113	1.24	5 (6%)
32	CLA	a	827	-	69,73,73	1.69	9 (13%)	82,113,113	1.37	8 (9%)
32	CLA	a	821	-	59,63,73	1.83	9 (15%)	70,101,113	1.38	6 (8%)
32	CLA	b	840	-	65,69,73	1.74	9 (13%)	77,108,113	1.27	6 (7%)
32	CLA	a	811	-	59,63,73	1.84	9 (15%)	70,101,113	1.42	8 (11%)
32	CLA	A	304	-	69,73,73	1.69	9 (13%)	82,113,113	1.33	8 (9%)
37	A86	D	322	-	47,50,50	0.46	1 (2%)	51,76,76	0.89	2 (3%)
37	A86	S	316	-	47,50,50	0.61	1 (2%)	51,76,76	1.12	3 (5%)
35	LHG	M	319	-	45,45,48	0.65	0	48,51,54	1.20	4 (8%)
32	CLA	b	808	-	69,73,73	1.67	9 (13%)	82,113,113	1.25	7 (8%)
32	CLA	b	834	-	64,68,73	1.77	9 (14%)	76,107,113	1.36	6 (7%)
35	LHG	a	851	-	37,37,48	1.01	2 (5%)	40,43,54	1.28	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	SF4	c	102	-	0,12,12	-	-	-		
32	CLA	H	301	8	49,53,73	2.09	9 (18%)	58,89,113	1.65	8 (13%)
32	CLA	L	308	-	49,53,73	2.04	9 (18%)	58,89,113	1.52	6 (10%)
32	CLA	N	309	14	54,58,73	1.99	9 (16%)	64,95,113	1.57	9 (14%)
34	DD6	Q	313	-	40,45,45	0.20	0	51,67,67	0.63	1 (1%)
34	DD6	V	202	-	40,45,45	0.19	0	51,67,67	0.93	3 (5%)
37	A86	R	313	-	47,50,50	0.56	1 (2%)	51,76,76	0.94	2 (3%)
32	CLA	U	307	-	49,53,73	2.08	9 (18%)	58,89,113	1.60	7 (12%)
32	CLA	C	306	-	69,73,73	1.77	9 (13%)	82,113,113	1.38	7 (8%)
33	KC2	T	311	15	49,53,53	1.83	4 (8%)	60,89,89	1.09	5 (8%)
42	SF4	a	847	-	0,12,12	-	-	-		
37	A86	L	317	-	47,50,50	0.50	1 (2%)	51,76,76	1.12	3 (5%)
32	CLA	b	806	-	69,73,73	1.72	9 (13%)	82,113,113	1.30	7 (8%)
33	KC2	M	321	15	49,53,53	1.83	4 (8%)	60,89,89	1.10	4 (6%)
36	LMG	T	301	-	37,37,55	0.93	1 (2%)	45,45,63	1.27	5 (11%)
37	A86	W	316	36	47,50,50	0.61	1 (2%)	51,76,76	0.75	1 (1%)
37	A86	W	315	-	47,50,50	0.56	1 (2%)	51,76,76	1.04	2 (3%)
37	A86	U	308	-	47,50,50	0.63	1 (2%)	51,76,76	1.08	3 (5%)
33	KC2	P	306	-	49,53,53	1.85	4 (8%)	60,89,89	1.04	4 (6%)
32	CLA	L	309	-	49,53,73	2.07	9 (18%)	58,89,113	1.54	7 (12%)
41	BCR	l	205	-	41,41,41	0.11	0	56,56,56	0.34	0
41	BCR	l	206	-	41,41,41	0.21	0	56,56,56	0.92	3 (5%)
32	CLA	a	822	-	66,70,73	1.71	9 (13%)	78,109,113	1.32	7 (8%)
32	CLA	B	304	-	50,54,73	2.08	9 (18%)	59,90,113	1.60	8 (13%)
32	CLA	A	305	1	65,69,73	1.77	9 (13%)	77,108,113	1.36	6 (7%)
32	CLA	G	307	-	44,48,73	2.18	9 (20%)	51,82,113	2.00	8 (15%)
37	A86	Q	311	-	47,50,50	0.45	0	51,76,76	0.93	2 (3%)
32	CLA	F	305	-	53,57,73	1.99	9 (16%)	63,94,113	1.58	8 (12%)
32	CLA	F	306	-	59,63,73	1.87	9 (15%)	70,101,113	1.40	7 (10%)
36	LMG	E	302	-	40,40,55	1.10	3 (7%)	48,48,63	1.52	8 (16%)
41	BCR	r	203	-	41,41,41	0.14	0	56,56,56	0.43	0
32	CLA	D	312	4	59,63,73	1.86	9 (15%)	70,101,113	1.42	7 (10%)
32	CLA	Q	307	16	66,70,73	1.73	9 (13%)	78,109,113	1.30	6 (7%)
33	KC2	P	302	13	49,53,53	1.86	4 (8%)	60,89,89	1.10	5 (8%)
33	KC2	N	314	14	49,53,53	1.85	4 (8%)	60,89,89	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	KC2	F	302	6	49,53,53	1.85	4 (8%)	60,89,89	1.08	4 (6%)
36	LMG	P	318	-	45,45,55	0.97	2 (4%)	53,53,63	1.17	4 (7%)
34	DD6	A	312	-	40,45,45	0.21	0	51,67,67	0.88	3 (5%)
33	KC2	M	313	13,36	49,53,53	1.83	4 (8%)	60,89,89	1.06	5 (8%)
33	KC2	G	302	-	49,53,53	1.83	4 (8%)	60,89,89	1.05	4 (6%)
32	CLA	a	830	-	69,73,73	1.74	9 (13%)	82,113,113	1.34	8 (9%)
37	A86	r	204	-	47,50,50	0.43	1 (2%)	51,76,76	0.95	2 (3%)
34	DD6	E	319	-	40,45,45	0.19	0	51,67,67	0.76	3 (5%)
32	CLA	a	816	-	49,53,73	2.00	9 (18%)	58,89,113	1.52	6 (10%)
32	CLA	B	305	-	49,53,73	2.09	9 (18%)	58,89,113	1.64	7 (12%)
32	CLA	G	303	7	59,63,73	1.84	9 (15%)	70,101,113	1.53	10 (14%)
32	CLA	K	301	-	49,53,73	2.05	9 (18%)	58,89,113	1.51	7 (12%)
33	KC2	C	303	-	49,53,53	1.85	4 (8%)	60,89,89	1.05	4 (6%)
32	CLA	R	304	-	49,53,73	2.04	9 (18%)	58,89,113	1.56	7 (12%)
33	KC2	J	310	10	49,53,53	1.85	4 (8%)	60,89,89	1.05	4 (6%)
34	DD6	J	315	-	40,45,45	0.18	0	51,67,67	0.86	3 (5%)
32	CLA	a	836	-	59,63,73	1.85	9 (15%)	70,101,113	1.38	6 (8%)
37	A86	M	301	-	47,50,50	0.45	1 (2%)	51,76,76	0.64	1 (1%)
32	CLA	N	305	-	54,58,73	1.98	9 (16%)	64,95,113	1.51	7 (10%)
33	KC2	N	308	14	49,53,53	1.82	4 (8%)	60,89,89	1.00	4 (6%)
34	DD6	D	319	-	40,45,45	0.19	0	51,67,67	0.86	3 (5%)
32	CLA	a	818	-	64,68,73	1.78	9 (14%)	76,107,113	1.58	9 (11%)
34	DD6	S	321	-	40,45,45	0.44	0	51,67,67	1.72	7 (13%)
32	CLA	a	852	-	69,73,73	1.72	9 (13%)	82,113,113	1.20	8 (9%)
33	KC2	L	313	-	49,53,53	1.84	4 (8%)	60,89,89	1.03	3 (5%)
32	CLA	b	801	-	64,68,73	1.78	9 (14%)	76,107,113	1.46	7 (9%)
33	KC2	K	309	-	49,53,53	1.84	4 (8%)	60,89,89	1.07	4 (6%)
32	CLA	a	803	-	67,71,73	1.70	9 (13%)	79,110,113	1.39	6 (7%)
32	CLA	F	311	-	49,53,73	2.04	9 (18%)	58,89,113	1.57	6 (10%)
32	CLA	L	314	-	49,53,73	2.06	9 (18%)	58,89,113	1.50	6 (10%)
43	PQN	b	847	-	34,34,34	0.44	0	43,45,45	0.69	1 (2%)
32	CLA	b	821	-	59,63,73	1.82	9 (15%)	70,101,113	1.47	7 (10%)
32	CLA	k	201	-	59,63,73	1.83	9 (15%)	70,101,113	1.39	6 (8%)
32	CLA	C	309	-	47,51,73	2.09	9 (19%)	55,86,113	1.51	6 (10%)
37	A86	M	317	-	47,50,50	0.72	1 (2%)	51,76,76	0.55	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	K	308	-	69,73,73	1.73	9 (13%)	82,113,113	1.32	7 (8%)
32	CLA	R	308	15	64,68,73	1.74	9 (14%)	76,107,113	1.39	9 (11%)
37	A86	G	311	-	47,50,50	0.55	1 (2%)	51,76,76	0.79	2 (3%)
32	CLA	D	308	4	59,63,73	1.87	9 (15%)	70,101,113	1.49	7 (10%)
41	BCR	i	101	-	41,41,41	0.20	0	56,56,56	0.54	0
36	LMG	l	201	33	49,49,55	0.90	2 (4%)	57,57,63	1.48	12 (21%)
32	CLA	V	204	-	54,58,73	1.93	9 (16%)	64,95,113	1.43	5 (7%)
38	LMU	D	324	-	36,36,36	0.39	0	47,47,47	0.85	0
32	CLA	b	826	-	53,57,73	2.00	9 (16%)	61,93,113	1.58	8 (13%)
34	DD6	F	316	-	40,45,45	0.22	0	51,67,67	1.42	4 (7%)
32	CLA	f	204	-	51,55,73	2.00	9 (17%)	60,91,113	1.49	7 (11%)
38	LMU	V	205	-	35,35,36	0.48	0	46,46,47	1.18	3 (6%)
34	DD6	O	313	-	40,45,45	0.18	0	51,67,67	1.03	2 (3%)
32	CLA	E	308	-	69,73,73	1.69	9 (13%)	82,113,113	1.26	6 (7%)
32	CLA	B	301	-	44,48,73	2.17	9 (20%)	51,82,113	1.87	7 (13%)
35	LHG	A	316	-	39,39,48	0.71	2 (5%)	42,45,54	1.19	2 (4%)
37	A86	M	314	-	47,50,50	0.60	1 (2%)	51,76,76	0.81	2 (3%)
32	CLA	a	824	-	65,69,73	1.71	9 (13%)	77,108,113	1.32	7 (9%)
33	KC2	N	303	14	49,53,53	1.83	4 (8%)	60,89,89	1.11	5 (8%)
32	CLA	b	823	-	69,73,73	1.66	9 (13%)	82,113,113	1.31	7 (8%)
34	DD6	U	309	-	40,45,45	0.19	0	51,67,67	0.89	2 (3%)
32	CLA	N	312	-	45,49,73	2.18	10 (22%)	54,84,113	1.59	7 (12%)
33	KC2	W	301	15	49,53,53	1.82	4 (8%)	60,89,89	1.07	4 (6%)
33	KC2	S	302	17	49,53,53	1.85	4 (8%)	60,89,89	1.08	5 (8%)
41	BCR	b	843	-	41,41,41	0.11	0	56,56,56	0.56	0
41	BCR	r	205	-	41,41,41	0.14	0	56,56,56	0.37	0
32	CLA	a	839	-	59,63,73	1.83	9 (15%)	70,101,113	1.46	8 (11%)
37	A86	W	302	-	47,50,50	0.44	1 (2%)	51,76,76	0.65	1 (1%)
32	CLA	S	307	-	56,60,73	1.93	9 (16%)	65,97,113	1.77	12 (18%)
32	CLA	F	322	-	64,68,73	1.81	9 (14%)	76,107,113	1.42	7 (9%)
33	KC2	W	308	-	49,53,53	1.81	4 (8%)	60,89,89	1.08	4 (6%)
34	DD6	N	321	-	40,45,45	0.16	0	51,67,67	0.94	1 (1%)
32	CLA	D	305	-	62,66,73	1.78	9 (14%)	73,104,113	1.41	7 (9%)
32	CLA	D	313	-	62,66,73	1.79	9 (14%)	73,104,113	1.36	6 (8%)
32	CLA	I	304	9	49,53,73	2.05	9 (18%)	58,89,113	1.54	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	r	202	-	49,53,73	2.03	9 (18%)	58,89,113	1.52	5 (8%)
32	CLA	A	306	-	69,73,73	1.70	9 (13%)	82,113,113	1.25	7 (8%)
37	A86	J	313	-	47,50,50	0.47	1 (2%)	51,76,76	1.70	5 (9%)
32	CLA	a	823	-	69,73,73	1.69	9 (13%)	82,113,113	1.31	7 (8%)
32	CLA	P	308	-	49,53,73	2.02	9 (18%)	58,89,113	1.48	6 (10%)
36	LMG	L	320	-	37,37,55	0.82	1 (2%)	45,45,63	1.25	5 (11%)
32	CLA	a	808	20	54,58,73	1.95	9 (16%)	64,95,113	1.47	7 (10%)
39	SQD	H	315	-	41,43,54	1.25	3 (7%)	51,54,65	1.35	5 (9%)
32	CLA	L	301	-	49,53,73	2.05	9 (18%)	58,89,113	1.52	7 (12%)
37	A86	O	311	-	47,50,50	0.32	0	51,76,76	0.89	2 (3%)
33	KC2	O	302	-	49,53,53	1.84	4 (8%)	60,89,89	1.07	4 (6%)
32	CLA	H	305	8	49,53,73	2.04	9 (18%)	58,89,113	1.62	7 (12%)
32	CLA	F	303	6	66,70,73	1.73	9 (13%)	78,109,113	1.31	6 (7%)
37	A86	T	315	-	47,50,50	0.53	1 (2%)	51,76,76	0.53	1 (1%)
32	CLA	F	307	6	64,68,73	1.76	9 (14%)	76,107,113	1.35	7 (9%)
33	KC2	W	304	13	49,53,53	1.83	4 (8%)	60,89,89	1.08	5 (8%)
32	CLA	O	307	15	64,68,73	1.78	9 (14%)	76,107,113	1.38	8 (10%)
32	CLA	W	307	13	49,53,73	2.03	9 (18%)	58,89,113	1.50	8 (13%)
32	CLA	C	307	3	64,68,73	1.78	9 (14%)	76,107,113	1.45	9 (11%)
32	CLA	J	312	-	62,66,73	1.84	9 (14%)	73,104,113	1.34	7 (9%)
32	CLA	a	837	20	59,63,73	1.88	9 (15%)	70,101,113	1.49	8 (11%)
32	CLA	I	302	9	59,63,73	1.82	9 (15%)	70,101,113	1.41	6 (8%)
34	DD6	A	315	-	40,45,45	0.19	0	51,67,67	0.82	3 (5%)
32	CLA	D	314	4	56,60,73	1.85	10 (17%)	65,97,113	1.40	10 (15%)
32	CLA	P	311	-	64,68,73	1.76	9 (14%)	76,107,113	1.32	8 (10%)
32	CLA	J	309	-	49,53,73	2.03	9 (18%)	58,89,113	1.51	6 (10%)
32	CLA	Q	308	-	49,53,73	2.07	9 (18%)	58,89,113	1.54	7 (12%)
37	A86	S	315	-	47,50,50	0.54	1 (2%)	51,76,76	1.21	3 (5%)
37	A86	T	312	-	47,50,50	0.78	1 (2%)	51,76,76	1.01	3 (5%)
33	KC2	E	313	-	49,53,53	1.83	4 (8%)	60,89,89	1.06	4 (6%)
32	CLA	K	304	11	49,53,73	2.05	9 (18%)	58,89,113	1.56	7 (12%)
32	CLA	O	305	15	69,73,73	1.66	9 (13%)	82,113,113	1.31	7 (8%)
34	DD6	H	313	-	40,45,45	0.22	0	51,67,67	0.82	3 (5%)
33	KC2	F	310	36,6	49,53,53	1.81	4 (8%)	60,89,89	1.06	4 (6%)
32	CLA	U	301	-	44,48,73	2.17	9 (20%)	51,82,113	1.72	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	KC2	O	310	15	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
35	LHG	D	320	-	47,47,48	0.64	2 (4%)	50,53,54	1.20	3 (6%)
32	CLA	E	315	-	50,54,73	2.01	9 (18%)	59,90,113	1.51	7 (11%)
32	CLA	b	814	-	49,53,73	1.99	9 (18%)	58,89,113	1.49	7 (12%)
32	CLA	f	201	-	64,68,73	1.75	9 (14%)	76,107,113	1.26	6 (7%)
36	LMG	D	302	-	30,30,55	1.19	3 (10%)	38,38,63	1.40	5 (13%)
34	DD6	C	310	-	40,45,45	0.18	0	51,67,67	0.67	1 (1%)
37	A86	S	320	-	47,50,50	0.46	1 (2%)	51,76,76	0.59	0
37	A86	T	313	-	47,50,50	0.76	1 (2%)	51,76,76	0.93	2 (3%)
36	LMG	F	320	-	33,33,55	1.12	3 (9%)	41,41,63	1.28	5 (12%)
32	CLA	W	312	13	64,68,73	1.76	9 (14%)	76,107,113	1.34	7 (9%)
32	CLA	S	301	-	49,53,73	2.09	9 (18%)	58,89,113	1.66	8 (13%)
36	LMG	M	320	33	40,40,55	1.08	2 (5%)	48,48,63	1.11	4 (8%)
32	CLA	j	101	27	49,53,73	2.02	9 (18%)	58,89,113	1.48	6 (10%)
37	A86	L	316	-	47,50,50	0.43	1 (2%)	51,76,76	1.32	2 (3%)
33	KC2	W	314	13,36	49,53,53	1.84	4 (8%)	60,89,89	1.05	4 (6%)
34	DD6	J	317	-	40,45,45	0.17	0	51,67,67	0.89	3 (5%)
32	CLA	l	204	-	69,73,73	1.75	9 (13%)	82,113,113	1.39	10 (12%)
32	CLA	B	309	-	59,63,73	1.82	9 (15%)	70,101,113	1.31	6 (8%)
35	LHG	W	319	32	45,45,48	0.73	2 (4%)	48,51,54	1.18	4 (8%)
37	A86	K	314	-	47,50,50	0.56	1 (2%)	51,76,76	1.06	4 (7%)
33	KC2	N	306	14	49,53,53	1.81	4 (8%)	60,89,89	1.07	5 (8%)
35	LHG	f	205	-	46,46,48	0.60	0	49,52,54	1.13	2 (4%)
35	LHG	B	308	-	30,30,48	1.12	2 (6%)	33,36,54	1.22	4 (12%)
32	CLA	Q	301	33	64,68,73	1.80	9 (14%)	76,107,113	1.38	6 (7%)
35	LHG	I	314	-	45,45,48	0.65	1 (2%)	48,51,54	1.21	2 (4%)
34	DD6	I	311	-	40,45,45	0.16	0	51,67,67	0.73	2 (3%)
35	LHG	P	317	-	45,45,48	0.63	0	48,51,54	1.19	4 (8%)
32	CLA	A	309	1	69,73,73	1.70	9 (13%)	82,113,113	1.31	7 (8%)
32	CLA	L	312	-	64,68,73	1.75	9 (14%)	76,107,113	1.30	7 (9%)
41	BCR	b	841	-	41,41,41	0.12	0	56,56,56	0.42	0
41	BCR	m	101	-	41,41,41	0.12	0	56,56,56	0.43	0
32	CLA	F	309	-	59,63,73	1.83	9 (15%)	70,101,113	1.38	5 (7%)
32	CLA	W	313	-	64,68,73	1.81	9 (14%)	76,107,113	1.42	7 (9%)
33	KC2	I	316	-	49,53,53	1.83	4 (8%)	60,89,89	1.05	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	G	308	-	58,62,73	1.88	9 (15%)	68,99,113	1.43	6 (8%)
37	A86	L	315	-	47,50,50	0.51	1 (2%)	51,76,76	1.04	3 (5%)
32	CLA	U	303	18	49,53,73	2.04	9 (18%)	58,89,113	1.62	8 (13%)
37	A86	M	318	-	47,50,50	0.42	1 (2%)	51,76,76	0.81	4 (7%)
32	CLA	D	311	4	69,73,73	1.69	9 (13%)	82,113,113	1.29	7 (8%)
41	BCR	a	845	-	41,41,41	0.14	0	56,56,56	0.38	0
32	CLA	I	301	-	69,73,73	1.69	9 (13%)	82,113,113	1.29	6 (7%)
32	CLA	b	810	21	64,68,73	1.72	9 (14%)	76,107,113	1.24	6 (7%)
32	CLA	l	202	-	49,53,73	2.01	9 (18%)	58,89,113	1.54	6 (10%)
32	CLA	K	310	-	49,53,73	2.08	9 (18%)	58,89,113	1.62	7 (12%)
37	A86	N	315	-	47,50,50	0.53	1 (2%)	51,76,76	0.84	1 (1%)
32	CLA	M	312	-	64,68,73	1.77	9 (14%)	76,107,113	1.38	7 (9%)
33	KC2	I	309	36,9	49,53,53	1.82	4 (8%)	60,89,89	1.10	4 (6%)
35	LHG	a	850	32	29,29,48	0.84	0	32,35,54	1.27	3 (9%)
32	CLA	R	309	15	45,49,73	2.23	10 (22%)	54,84,113	1.71	6 (11%)
41	BCR	a	846	-	41,41,41	0.14	0	56,56,56	0.39	0
41	BCR	k	204	-	41,41,41	0.13	0	56,56,56	0.39	0
32	CLA	H	304	-	49,53,73	2.09	9 (18%)	58,89,113	1.70	8 (13%)
34	DD6	D	301	-	40,45,45	0.19	0	51,67,67	0.69	1 (1%)
34	DD6	N	318	-	40,45,45	0.18	0	51,67,67	0.81	2 (3%)
37	A86	S	317	-	47,50,50	0.48	1 (2%)	51,76,76	1.25	2 (3%)
32	CLA	H	307	-	64,68,73	1.80	9 (14%)	76,107,113	1.39	7 (9%)
32	CLA	L	307	-	61,65,73	1.82	9 (14%)	72,103,113	1.39	7 (9%)
34	DD6	H	312	-	40,45,45	0.19	0	51,67,67	0.79	2 (3%)
32	CLA	b	812	-	69,73,73	1.67	9 (13%)	82,113,113	1.30	6 (7%)
35	LHG	F	321	-	39,39,48	0.70	2 (5%)	42,45,54	1.18	2 (4%)
32	CLA	J	311	-	49,53,73	2.03	9 (18%)	58,89,113	1.60	7 (12%)
32	CLA	b	830	-	65,69,73	1.77	9 (13%)	77,108,113	1.52	10 (12%)
34	DD6	D	316	-	40,45,45	0.19	0	51,67,67	0.89	3 (5%)
37	A86	Q	316	-	47,50,50	0.56	1 (2%)	51,76,76	0.49	0
33	KC2	N	302	14	49,53,53	1.85	4 (8%)	60,89,89	1.03	3 (5%)
33	KC2	M	302	13	49,53,53	1.82	4 (8%)	60,89,89	1.06	4 (6%)
34	DD6	M	316	-	40,45,45	0.19	0	51,67,67	0.80	1 (1%)
32	CLA	D	309	-	49,53,73	2.05	9 (18%)	58,89,113	1.54	6 (10%)
32	CLA	A	303	1	66,70,73	1.73	9 (13%)	78,109,113	1.35	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	KC2	T	304	15	49,53,53	1.82	4 (8%)	60,89,89	1.09	5 (8%)
32	CLA	a	801	-	69,73,73	1.67	10 (14%)	82,113,113	1.24	9 (10%)
32	CLA	J	301	10	49,53,73	2.03	9 (18%)	58,89,113	1.45	6 (10%)
34	DD6	E	316	-	40,45,45	0.19	0	51,67,67	0.87	3 (5%)
35	LHG	a	849	-	47,47,48	0.64	1 (2%)	50,53,54	1.18	3 (6%)
36	LMG	S	322	33	33,33,55	1.11	2 (6%)	41,41,63	1.25	3 (7%)
32	CLA	I	305	-	60,64,73	1.86	9 (15%)	71,102,113	1.48	7 (9%)
34	DD6	T	314	-	40,45,45	0.19	0	51,67,67	0.78	3 (5%)
32	CLA	J	305	10	56,60,73	1.90	9 (16%)	65,97,113	1.41	7 (10%)
32	CLA	b	809	-	49,53,73	2.02	9 (18%)	58,89,113	1.51	7 (12%)
32	CLA	V	203	19	59,63,73	1.83	9 (15%)	70,101,113	1.37	6 (8%)
33	KC2	L	302	12	49,53,53	1.85	4 (8%)	60,89,89	1.08	5 (8%)
33	KC2	M	304	13	49,53,53	1.86	4 (8%)	60,89,89	1.06	4 (6%)
32	CLA	b	807	-	64,68,73	1.82	9 (14%)	76,107,113	1.50	7 (9%)
33	KC2	S	306	17	49,53,53	1.81	4 (8%)	60,89,89	1.04	3 (5%)
34	DD6	K	313	-	40,45,45	0.18	0	51,67,67	0.57	1 (1%)
32	CLA	M	309	-	49,53,73	2.01	9 (18%)	58,89,113	1.52	6 (10%)
40	DGD	Q	318	-	57,57,67	0.93	2 (3%)	71,71,81	1.15	6 (8%)
32	CLA	S	304	-	46,50,73	2.07	9 (19%)	53,85,113	1.52	7 (13%)
32	CLA	R	307	-	49,53,73	2.02	9 (18%)	58,89,113	1.52	6 (10%)
33	KC2	P	312	13	49,53,53	1.85	4 (8%)	60,89,89	1.06	4 (6%)
37	A86	N	320	-	47,50,50	0.60	1 (2%)	51,76,76	0.58	1 (1%)
32	CLA	O	304	-	49,53,73	2.08	9 (18%)	58,89,113	1.64	8 (13%)
32	CLA	E	309	5	62,66,73	1.77	9 (14%)	73,104,113	1.41	7 (9%)
34	DD6	W	317	-	40,45,45	0.19	0	51,67,67	0.64	2 (3%)
34	DD6	D	317	-	40,45,45	0.17	0	51,67,67	0.94	2 (3%)
32	CLA	b	804	-	69,73,73	1.71	9 (13%)	82,113,113	1.41	9 (10%)
33	KC2	S	312	36,17	49,53,53	1.73	4 (8%)	60,89,89	1.14	4 (6%)
32	CLA	H	302	-	45,49,73	2.27	10 (22%)	54,84,113	1.73	7 (12%)
32	CLA	N	311	14	64,68,73	1.75	9 (14%)	76,107,113	1.30	7 (9%)
32	CLA	b	838	-	69,73,73	1.77	9 (13%)	82,113,113	1.42	7 (8%)
32	CLA	a	834	-	69,73,73	1.68	9 (13%)	82,113,113	1.28	6 (7%)
36	LMG	A	318	-	40,40,55	0.94	2 (5%)	48,48,63	1.28	6 (12%)
41	BCR	b	842	-	41,41,41	0.22	0	56,56,56	0.57	1 (1%)
35	LHG	E	321	-	45,45,48	0.92	2 (4%)	48,51,54	1.17	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	E	314	-	54,58,73	1.94	9 (16%)	64,95,113	1.47	7 (10%)
37	A86	F	312	-	47,50,50	0.56	1 (2%)	51,76,76	1.23	3 (5%)
41	BCR	a	843	-	41,41,41	0.15	0	56,56,56	0.42	0
34	DD6	A	314	-	40,45,45	0.18	0	51,67,67	0.68	1 (1%)
32	CLA	N	310	-	59,63,73	1.89	10 (16%)	70,101,113	1.50	7 (10%)
33	KC2	N	307	-	49,53,53	1.84	4 (8%)	60,89,89	1.04	4 (6%)
37	A86	P	314	-	47,50,50	0.42	1 (2%)	51,76,76	1.09	3 (5%)
32	CLA	C	308	3	49,53,73	2.09	9 (18%)	58,89,113	1.67	8 (13%)
32	CLA	a	806	-	64,68,73	1.75	9 (14%)	76,107,113	1.32	9 (11%)
32	CLA	U	306	-	49,53,73	2.07	9 (18%)	58,89,113	1.53	6 (10%)
32	CLA	a	841	-	69,73,73	1.67	9 (13%)	82,113,113	1.29	7 (8%)
32	CLA	b	835	-	64,68,73	1.74	9 (14%)	76,107,113	1.39	9 (11%)
37	A86	P	313	-	47,50,50	0.55	1 (2%)	51,76,76	1.17	2 (3%)
32	CLA	D	315	-	49,53,73	2.00	9 (18%)	58,89,113	1.59	6 (10%)
37	A86	S	314	-	47,50,50	0.31	0	51,76,76	1.65	6 (11%)
32	CLA	B	306	-	49,53,73	2.05	9 (18%)	58,89,113	1.54	7 (12%)
39	SQD	k	206	-	34,36,54	1.40	4 (11%)	44,47,65	1.46	7 (15%)
32	CLA	S	305	-	67,71,73	1.73	9 (13%)	79,110,113	1.29	5 (6%)
33	KC2	U	304	-	49,53,53	1.82	4 (8%)	60,89,89	1.10	4 (6%)
37	A86	W	318	-	47,50,50	0.37	0	51,76,76	1.36	4 (7%)
33	KC2	R	302	15	49,53,53	1.86	4 (8%)	60,89,89	1.11	4 (6%)
34	DD6	K	315	-	40,45,45	0.18	0	51,67,67	1.09	3 (5%)
32	CLA	I	306	9	69,73,73	1.70	9 (13%)	82,113,113	1.34	6 (7%)
36	LMG	N	301	-	40,40,55	1.07	2 (5%)	48,48,63	1.17	4 (8%)
37	A86	L	318	-	47,50,50	0.65	1 (2%)	51,76,76	0.99	2 (3%)
32	CLA	b	828	-	65,69,73	1.78	9 (13%)	77,108,113	1.41	7 (9%)
32	CLA	H	310	-	50,54,73	2.05	9 (18%)	59,90,113	1.48	6 (10%)
32	CLA	a	838	-	69,73,73	1.68	9 (13%)	82,113,113	1.36	8 (9%)
32	CLA	a	853	-	69,73,73	1.69	9 (13%)	82,113,113	1.34	9 (10%)
34	DD6	D	318	-	40,45,45	0.19	0	51,67,67	0.63	0
32	CLA	b	825	-	64,68,73	1.73	10 (15%)	76,107,113	1.34	5 (6%)
33	KC2	W	305	13	49,53,53	1.81	4 (8%)	60,89,89	1.10	3 (5%)
32	CLA	G	301	-	49,53,73	2.08	9 (18%)	58,89,113	1.52	6 (10%)
32	CLA	Q	305	-	55,59,73	1.89	9 (16%)	64,96,113	1.46	6 (9%)
32	CLA	b	832	-	69,73,73	1.73	9 (13%)	82,113,113	1.34	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	U	305	18	49,53,73	2.09	9 (18%)	58,89,113	1.65	9 (15%)
32	CLA	B	302	-	49,53,73	1.99	9 (18%)	58,89,113	1.48	8 (13%)
32	CLA	I	307	-	49,53,73	2.05	9 (18%)	58,89,113	1.60	7 (12%)
37	A86	C	312	-	47,50,50	0.40	1 (2%)	51,76,76	1.12	2 (3%)
32	CLA	a	809	-	64,68,73	1.75	9 (14%)	76,107,113	1.38	6 (7%)
37	A86	P	316	-	47,50,50	0.44	0	51,76,76	1.62	5 (9%)
36	LMG	D	303	-	36,36,55	1.04	2 (5%)	44,44,63	1.48	8 (18%)
35	LHG	F	318	-	40,40,48	0.71	1 (2%)	43,46,54	1.14	3 (6%)
32	CLA	b	805	-	69,73,73	1.66	9 (13%)	82,113,113	1.21	9 (10%)
33	KC2	K	305	-	49,53,53	1.82	4 (8%)	60,89,89	1.11	4 (6%)
33	KC2	S	303	17	49,53,53	1.81	4 (8%)	60,89,89	1.08	4 (6%)
34	DD6	Q	315	-	40,45,45	0.18	0	51,67,67	0.82	3 (5%)
32	CLA	M	305	-	54,58,73	1.90	9 (16%)	64,95,113	1.44	10 (15%)

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
34	DD6	J	316	-	-	0/26/80/80	0/3/3/3
32	CLA	L	310	-	1/1/9/20	4/10/82/115	-
32	CLA	C	302	-	1/1/10/20	0/10/86/115	-
32	CLA	a	820	-	1/1/15/20	9/39/115/115	-
32	CLA	P	304	-	1/1/11/20	6/15/91/115	-
32	CLA	a	826	-	1/1/15/20	14/39/115/115	-
33	KC2	Q	317	32	-	8/15/71/71	-
41	BCR	U	310	-	-	3/29/63/63	0/2/2/2
32	CLA	r	201	-	1/1/14/20	7/33/109/115	-
32	CLA	a	804	-	1/1/13/20	4/31/107/115	-
33	KC2	M	307	-	-	4/15/71/71	-
33	KC2	W	303	13	-	6/15/71/71	-
32	CLA	M	311	13	1/1/11/20	7/15/91/115	-
33	KC2	H	303	-	-	8/15/71/71	-
37	A86	K	311	-	-	8/34/90/90	0/3/3/3
32	CLA	b	813	-	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	820	-	1/1/14/20	6/38/114/115	-
34	DD6	I	312	-	-	0/26/80/80	0/3/3/3
33	KC2	R	311	15	-	5/15/71/71	-
32	CLA	b	816	-	1/1/14/20	8/36/112/115	-
32	CLA	T	309	-	1/1/11/20	4/15/91/115	-
32	CLA	l	203	35	1/1/15/20	16/39/115/115	-
32	CLA	W	311	13	1/1/15/20	12/39/115/115	-
32	CLA	b	802	-	1/1/15/20	3/39/115/115	-
34	DD6	N	319	-	-	1/26/80/80	0/3/3/3
32	CLA	b	818	-	1/1/15/20	8/39/115/115	-
37	A86	F	317	-	-	8/34/90/90	0/3/3/3
32	CLA	M	310	13	1/1/14/20	4/36/112/115	-
32	CLA	L	311	-	1/1/9/20	2/10/82/115	-
32	CLA	b	839	-	1/1/15/20	12/39/115/115	-
32	CLA	H	306	-	1/1/12/20	2/21/97/115	-
32	CLA	b	817	-	1/1/13/20	9/27/103/115	-
34	DD6	R	314	-	-	0/26/80/80	0/3/3/3
35	LHG	I	318	32	-	16/41/41/53	-
32	CLA	k	203	-	1/1/13/20	8/27/103/115	-
32	CLA	a	815	-	1/1/12/20	0/21/97/115	-
32	CLA	a	817	-	1/1/14/20	8/35/111/115	-
37	A86	D	323	-	-	10/34/90/90	0/3/3/3
37	A86	N	317	-	-	7/34/90/90	0/3/3/3
32	CLA	P	305	13	1/1/14/20	13/33/109/115	-
32	CLA	b	833	-	1/1/14/20	11/36/112/115	-
32	CLA	I	303	9	1/1/13/20	5/27/103/115	-
32	CLA	A	311	-	1/1/11/20	6/15/91/115	-
33	KC2	P	301	-	-	8/15/71/71	-
34	DD6	L	319	-	-	2/26/80/80	0/3/3/3
32	CLA	R	310	-	1/1/13/20	5/27/103/115	-
32	CLA	G	304	-	1/1/13/20	4/27/103/115	-
32	CLA	S	313	17	1/1/11/20	6/15/91/115	-
36	LMG	j	104	-	-	21/33/53/70	0/1/1/1
33	KC2	L	303	-	-	4/15/71/71	-
32	CLA	M	306	13	1/1/14/20	3/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	a	831	-	1/1/14/20	4/33/109/115	-
33	KC2	L	305	12	-	10/15/71/71	-
32	CLA	A	308	-	1/1/13/20	3/27/103/115	-
32	CLA	F	301	-	1/1/9/20	2/10/82/115	-
33	KC2	R	305	15	-	7/15/71/71	-
34	DD6	E	317	-	-	0/26/80/80	0/3/3/3
33	KC2	K	302	11	-	6/15/71/71	-
38	LMU	I	315	-	-	6/21/61/61	0/2/2/2
34	DD6	J	314	-	-	1/26/80/80	0/3/3/3
32	CLA	L	304	-	1/1/11/20	2/15/91/115	-
32	CLA	b	837	-	1/1/15/20	11/39/115/115	-
37	A86	S	319	-	-	4/34/90/90	0/3/3/3
34	DD6	I	313	-	-	0/26/80/80	0/3/3/3
32	CLA	b	824	-	1/1/13/20	7/31/107/115	-
32	CLA	Q	304	-	1/1/12/20	3/21/97/115	-
32	CLA	W	306	-	1/1/13/20	6/27/103/115	-
34	DD6	H	311	-	-	0/26/80/80	0/3/3/3
36	LMG	D	321	-	-	15/35/55/70	0/1/1/1
32	CLA	C	301	3	1/1/11/20	3/15/91/115	-
43	PQN	a	848	-	-	8/23/43/43	0/2/2/2
32	CLA	a	829	-	1/1/14/20	7/33/109/115	-
33	KC2	M	303	13	-	4/15/71/71	-
32	CLA	a	812	-	1/1/13/20	6/27/103/115	-
32	CLA	E	306	5	1/1/14/20	6/33/109/115	-
32	CLA	G	305	-	1/1/11/20	5/15/91/115	-
34	DD6	F	314	-	-	1/26/80/80	0/3/3/3
34	DD6	j	103	-	-	2/26/80/80	0/3/3/3
32	CLA	N	313	-	1/1/14/20	7/33/109/115	-
34	DD6	A	313	-	-	2/26/80/80	0/3/3/3
32	CLA	A	307	1	1/1/14/20	2/33/109/115	-
32	CLA	D	310	4	1/1/15/20	6/39/115/115	-
32	CLA	S	309	-	1/1/14/20	13/33/109/115	-
32	CLA	a	819	20	1/1/15/20	12/39/115/115	-
32	CLA	b	831	-	1/1/14/20	11/33/109/115	-
32	CLA	T	307	-	1/1/12/20	3/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	a	840	-	1/1/15/20	6/39/115/115	-
33	KC2	Q	302	-	-	8/15/71/71	-
32	CLA	W	310	-	1/1/14/20	12/33/109/115	-
40	DGD	b	846	-	-	21/45/85/95	0/2/2/2
33	KC2	R	303	-	-	5/15/71/71	-
32	CLA	Q	303	16	1/1/14/20	6/33/109/115	-
35	LHG	E	301	-	-	18/50/50/53	-
37	A86	G	310	-	-	10/34/90/90	0/3/3/3
32	CLA	E	310	5	1/1/11/20	6/15/91/115	-
32	CLA	a	832	-	1/1/14/20	4/33/109/115	-
32	CLA	E	303	5	1/1/11/20	3/15/91/115	-
32	CLA	k	202	-	1/1/13/20	10/27/103/115	-
33	KC2	L	306	12	-	4/15/71/71	-
32	CLA	a	813	-	1/1/11/20	5/15/91/115	-
36	LMG	D	325	-	-	9/30/50/70	0/1/1/1
32	CLA	H	309	-	1/1/11/20	6/15/91/115	-
32	CLA	a	835	-	1/1/15/20	8/39/115/115	-
32	CLA	Q	309	-	1/1/11/20	3/15/91/115	-
32	CLA	a	807	-	1/1/15/20	10/39/115/115	-
34	DD6	Q	314	-	-	0/26/80/80	0/3/3/3
36	LMG	F	319	33	-	16/35/55/70	0/1/1/1
32	CLA	W	309	13	1/1/15/20	6/39/115/115	-
32	CLA	T	305	-	1/1/11/20	10/15/91/115	-
32	CLA	T	306	15	1/1/14/20	4/33/109/115	-
37	A86	F	313	-	-	5/34/90/90	0/3/3/3
32	CLA	b	836	-	1/1/15/20	8/39/115/115	-
32	CLA	E	311	5	1/1/11/20	1/15/91/115	-
41	BCR	a	854	-	-	2/29/63/63	0/2/2/2
34	DD6	Q	312	-	-	1/26/80/80	0/3/3/3
33	KC2	N	304	14	-	9/15/71/71	-
32	CLA	O	309	-	1/1/14/20	6/36/112/115	-
32	CLA	a	828	-	1/1/13/20	7/31/107/115	-
34	DD6	G	312	-	-	1/26/80/80	0/3/3/3
32	CLA	J	306	-	1/1/13/20	6/27/103/115	-
33	KC2	A	310	1	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	a	842	-	1/1/13/20	7/27/103/115	-
37	A86	R	312	-	-	3/34/90/90	0/3/3/3
32	CLA	f	203	25	1/1/11/20	2/15/91/115	-
36	LMG	E	320	-	-	13/26/46/70	0/1/1/1
32	CLA	K	306	-	1/1/14/20	8/33/109/115	-
36	LMG	E	322	-	-	12/35/55/70	0/1/1/1
32	CLA	A	301	1	1/1/11/20	5/15/91/115	-
32	CLA	D	304	4	1/1/14/20	9/33/109/115	-
32	CLA	F	308	6	1/1/11/20	2/17/93/115	-
32	CLA	I	308	-	1/1/13/20	7/27/103/115	-
32	CLA	O	308	-	1/1/11/20	4/15/91/115	-
32	CLA	U	302	18	1/1/11/20	4/15/91/115	-
42	SF4	c	101	22	-	-	0/6/5/5
37	A86	P	319	-	-	4/34/90/90	0/3/3/3
41	BCR	j	102	-	-	5/29/63/63	0/2/2/2
32	CLA	E	312	-	1/1/14/20	6/33/109/115	-
32	CLA	b	819	-	1/1/15/20	4/39/115/115	-
32	CLA	K	307	-	1/1/10/20	2/10/86/115	-
32	CLA	F	304	-	1/1/13/20	3/27/103/115	-
41	BCR	b	844	-	-	3/29/63/63	0/2/2/2
34	DD6	k	205	-	-	0/26/80/80	0/3/3/3
32	CLA	D	307	4	1/1/14/20	6/35/111/115	-
32	CLA	a	825	-	1/1/15/20	2/39/115/115	-
32	CLA	b	827	-	1/1/12/20	4/21/97/115	-
32	CLA	a	833	-	1/1/15/20	2/39/115/115	-
32	CLA	C	304	3	1/1/10/20	4/13/89/115	-
33	KC2	T	303	-	-	6/15/71/71	-
32	CLA	E	304	-	1/1/14/20	4/33/109/115	-
32	CLA	P	310	-	1/1/10/20	2/10/86/115	-
32	CLA	T	308	15	1/1/14/20	7/33/109/115	-
37	A86	K	312	-	-	7/34/90/90	0/3/3/3
41	BCR	f	202	-	-	2/29/63/63	0/2/2/2
37	A86	H	314	-	-	5/34/90/90	0/3/3/3
32	CLA	J	302	-	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	G	306	7	1/1/13/20	9/29/105/115	-
32	CLA	E	307	5	1/1/13/20	8/27/103/115	-
34	DD6	F	315	-	-	3/26/80/80	0/3/3/3
32	CLA	B	303	-	1/1/11/20	2/15/91/115	-
37	A86	S	318	-	-	4/34/90/90	0/3/3/3
32	CLA	I	317	35	1/1/15/20	3/39/115/115	-
32	CLA	Q	306	16	1/1/14/20	13/36/112/115	-
33	KC2	P	303	13	-	2/15/71/71	-
34	DD6	B	307	-	-	2/26/80/80	0/3/3/3
41	BCR	b	845	-	-	2/29/63/63	0/2/2/2
32	CLA	a	810	-	1/1/14/20	14/36/112/115	-
33	KC2	J	303	-	-	8/15/71/71	-
32	CLA	S	308	-	1/1/11/20	4/15/91/115	-
32	CLA	a	805	-	1/1/15/20	13/39/115/115	-
32	CLA	V	201	-	1/1/13/20	6/31/107/115	-
34	DD6	E	318	-	-	1/26/80/80	0/3/3/3
33	KC2	K	303	11	-	8/15/71/71	-
32	CLA	b	829	-	1/1/13/20	7/27/103/115	-
37	A86	O	312	-	1/1/14/25	3/34/90/90	0/3/3/3
32	CLA	C	305	-	1/1/14/20	8/33/109/115	-
38	LMU	j	105	-	-	12/20/60/61	0/2/2/2
33	KC2	G	309	7	-	8/15/71/71	-
32	CLA	E	305	5	1/1/13/20	1/27/103/115	-
32	CLA	b	822	-	1/1/15/20	7/39/115/115	-
32	CLA	b	811	-	1/1/12/20	5/21/97/115	-
32	CLA	Q	310	-	1/1/11/20	4/17/93/115	-
32	CLA	J	304	10	1/1/13/20	5/27/103/115	-
32	CLA	A	302	35	1/1/14/20	4/33/109/115	-
36	LMG	W	320	33,37	-	13/34/54/70	0/1/1/1
37	A86	N	316	-	-	10/34/90/90	0/3/3/3
32	CLA	P	309	-	1/1/14/20	5/35/111/115	-
32	CLA	T	302	15	1/1/11/20	5/15/91/115	-
34	DD6	I	310	-	-	1/26/80/80	0/3/3/3
32	CLA	R	301	-	1/1/11/20	4/15/91/115	-
36	LMG	A	317	-	-	15/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LMU	J	318	-	-	5/21/61/61	0/2/2/2
32	CLA	T	310	-	1/1/13/20	2/27/103/115	-
34	DD6	P	315	-	-	0/26/80/80	0/3/3/3
37	A86	C	311	-	-	5/34/90/90	0/3/3/3
32	CLA	H	308	8	1/1/10/20	0/10/86/115	-
32	CLA	S	311	-	1/1/12/20	3/21/97/115	-
32	CLA	P	307	13	1/1/11/20	0/15/91/115	-
37	A86	M	322	-	-	3/34/90/90	0/3/3/3
32	CLA	a	802	-	1/1/14/20	8/37/113/115	-
32	CLA	J	308	-	1/1/11/20	6/15/91/115	-
33	KC2	O	303	15	-	6/15/71/71	-
32	CLA	a	814	-	1/1/15/20	9/39/115/115	-
32	CLA	R	306	15	1/1/11/20	3/15/91/115	-
32	CLA	S	310	17	1/1/11/20	6/15/91/115	-
41	BCR	a	844	-	-	1/29/63/63	0/2/2/2
32	CLA	D	306	4	1/1/14/20	7/33/109/115	-
37	A86	M	315	-	-	4/34/90/90	0/3/3/3
32	CLA	M	308	13	1/1/13/20	9/30/106/115	-
32	CLA	O	301	15	1/1/11/20	5/15/91/115	-
32	CLA	O	306	-	1/1/11/20	4/15/91/115	-
32	CLA	b	815	-	1/1/15/20	5/39/115/115	-
32	CLA	J	307	10	1/1/13/20	4/27/103/115	-
32	CLA	b	803	-	1/1/15/20	9/39/115/115	-
32	CLA	a	827	-	1/1/15/20	9/39/115/115	-
32	CLA	a	821	-	1/1/13/20	5/27/103/115	-
32	CLA	b	840	-	1/1/14/20	9/35/111/115	-
32	CLA	a	811	-	1/1/13/20	4/27/103/115	-
32	CLA	A	304	-	1/1/15/20	11/39/115/115	-
37	A86	D	322	-	-	3/34/90/90	0/3/3/3
37	A86	S	316	-	-	2/34/90/90	0/3/3/3
35	LHG	M	319	-	-	18/50/50/53	-
32	CLA	b	808	-	1/1/15/20	7/39/115/115	-
32	CLA	b	834	-	1/1/14/20	4/33/109/115	-
35	LHG	a	851	-	-	7/42/42/53	-
42	SF4	c	102	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	H	301	8	1/1/11/20	7/15/91/115	-
32	CLA	L	308	-	1/1/11/20	4/15/91/115	-
32	CLA	N	309	14	1/1/12/20	4/21/97/115	-
34	DD6	Q	313	-	-	0/26/80/80	0/3/3/3
34	DD6	V	202	-	-	4/26/80/80	0/3/3/3
37	A86	R	313	-	-	4/34/90/90	0/3/3/3
32	CLA	U	307	-	1/1/11/20	4/15/91/115	-
32	CLA	C	306	-	1/1/15/20	11/39/115/115	-
33	KC2	T	311	15	-	7/15/71/71	-
42	SF4	a	847	-	-	-	0/6/5/5
37	A86	L	317	-	-	10/34/90/90	0/3/3/3
32	CLA	b	806	-	1/1/15/20	9/39/115/115	-
33	KC2	M	321	15	-	5/15/71/71	-
36	LMG	T	301	-	-	13/32/52/70	0/1/1/1
37	A86	W	316	36	-	4/34/90/90	0/3/3/3
37	A86	W	315	-	-	7/34/90/90	0/3/3/3
37	A86	U	308	-	-	2/34/90/90	1/3/3/3
33	KC2	P	306	-	-	6/15/71/71	-
32	CLA	L	309	-	1/1/11/20	5/15/91/115	-
41	BCR	l	205	-	-	4/29/63/63	0/2/2/2
41	BCR	l	206	-	-	5/29/63/63	0/2/2/2
32	CLA	a	822	-	1/1/14/20	9/36/112/115	-
32	CLA	B	304	-	1/1/11/20	5/17/93/115	-
32	CLA	A	305	1	1/1/14/20	6/35/111/115	-
32	CLA	G	307	-	1/1/9/20	2/10/82/115	-
37	A86	Q	311	-	-	7/34/90/90	0/3/3/3
32	CLA	F	305	-	1/1/12/20	1/19/95/115	-
32	CLA	F	306	-	1/1/13/20	5/27/103/115	-
36	LMG	E	302	-	-	19/35/55/70	0/1/1/1
41	BCR	r	203	-	-	4/29/63/63	0/2/2/2
32	CLA	D	312	4	1/1/13/20	6/27/103/115	-
32	CLA	Q	307	16	1/1/14/20	6/36/112/115	-
33	KC2	P	302	13	-	8/15/71/71	-
33	KC2	N	314	14	-	5/15/71/71	-
33	KC2	F	302	6	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	P	318	-	-	20/40/60/70	0/1/1/1
34	DD6	A	312	-	-	0/26/80/80	0/3/3/3
33	KC2	M	313	13,36	-	6/15/71/71	-
33	KC2	G	302	-	-	8/15/71/71	-
32	CLA	a	830	-	1/1/15/20	9/39/115/115	-
37	A86	r	204	-	-	7/34/90/90	0/3/3/3
34	DD6	E	319	-	-	0/26/80/80	0/3/3/3
32	CLA	a	816	-	1/1/11/20	6/15/91/115	-
32	CLA	B	305	-	1/1/11/20	4/15/91/115	-
32	CLA	G	303	7	1/1/13/20	10/27/103/115	-
32	CLA	K	301	-	1/1/11/20	2/15/91/115	-
33	KC2	C	303	-	-	10/15/71/71	-
32	CLA	R	304	-	1/1/11/20	3/15/91/115	-
33	KC2	J	310	10	-	8/15/71/71	-
34	DD6	J	315	-	-	1/26/80/80	0/3/3/3
32	CLA	a	836	-	1/1/13/20	10/27/103/115	-
37	A86	M	301	-	-	4/34/90/90	0/3/3/3
32	CLA	N	305	-	1/1/12/20	5/21/97/115	-
34	DD6	S	321	-	1/1/12/24	5/26/80/80	0/3/3/3
33	KC2	N	308	14	-	5/15/71/71	-
32	CLA	a	818	-	1/1/14/20	9/33/109/115	-
34	DD6	D	319	-	-	2/26/80/80	0/3/3/3
32	CLA	a	852	-	1/1/15/20	11/39/115/115	-
33	KC2	L	313	-	-	8/15/71/71	-
32	CLA	b	801	-	1/1/14/20	4/33/109/115	-
33	KC2	K	309	-	-	8/15/71/71	-
32	CLA	a	803	-	1/1/14/20	8/37/113/115	-
32	CLA	F	311	-	1/1/11/20	0/15/91/115	-
32	CLA	L	314	-	1/1/11/20	7/15/91/115	-
43	PQN	b	847	-	-	1/23/43/43	0/2/2/2
32	CLA	b	821	-	1/1/13/20	2/27/103/115	-
32	CLA	k	201	-	1/1/13/20	10/27/103/115	-
32	CLA	C	309	-	1/1/10/20	3/13/89/115	-
37	A86	M	317	-	-	7/34/90/90	1/3/3/3
32	CLA	K	308	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	R	308	15	1/1/14/20	3/33/109/115	-
37	A86	G	311	-	-	4/34/90/90	1/3/3/3
32	CLA	D	308	4	1/1/13/20	4/27/103/115	-
41	BCR	i	101	-	-	1/29/63/63	0/2/2/2
36	LMG	l	201	33	-	24/44/64/70	0/1/1/1
32	CLA	V	204	-	1/1/12/20	2/21/97/115	-
38	LMU	D	324	-	-	12/21/61/61	0/2/2/2
32	CLA	b	826	-	1/1/11/20	3/20/96/115	-
34	DD6	F	316	-	-	3/26/80/80	0/3/3/3
32	CLA	f	204	-	1/1/11/20	1/18/94/115	-
38	LMU	V	205	-	-	6/20/60/61	0/2/2/2
34	DD6	O	313	-	1/1/12/24	0/26/80/80	0/3/3/3
32	CLA	E	308	-	1/1/15/20	10/39/115/115	-
32	CLA	B	301	-	1/1/9/20	2/10/82/115	-
35	LHG	A	316	-	-	21/44/44/53	-
37	A86	M	314	-	-	4/34/90/90	1/3/3/3
32	CLA	a	824	-	1/1/14/20	7/35/111/115	-
33	KC2	N	303	14	-	7/15/71/71	-
32	CLA	b	823	-	1/1/15/20	10/39/115/115	-
34	DD6	U	309	-	-	0/26/80/80	0/3/3/3
32	CLA	N	312	-	1/1/10/20	4/10/86/115	-
33	KC2	W	301	15	-	6/15/71/71	-
33	KC2	S	302	17	-	4/15/71/71	-
41	BCR	b	843	-	-	0/29/63/63	0/2/2/2
41	BCR	r	205	-	-	2/29/63/63	0/2/2/2
32	CLA	a	839	-	1/1/13/20	4/27/103/115	-
37	A86	W	302	-	-	1/34/90/90	0/3/3/3
32	CLA	S	307	-	1/1/12/20	2/24/100/115	-
32	CLA	F	322	-	1/1/14/20	8/33/109/115	-
33	KC2	W	308	-	-	5/15/71/71	-
34	DD6	N	321	-	-	2/26/80/80	0/3/3/3
32	CLA	D	305	-	1/1/13/20	8/31/107/115	-
32	CLA	D	313	-	1/1/13/20	9/31/107/115	-
32	CLA	I	304	9	1/1/11/20	5/15/91/115	-
32	CLA	r	202	-	1/1/11/20	0/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	A	306	-	1/1/15/20	9/39/115/115	-
37	A86	J	313	-	-	8/34/90/90	0/3/3/3
32	CLA	a	823	-	1/1/15/20	5/39/115/115	-
32	CLA	P	308	-	1/1/11/20	2/15/91/115	-
36	LMG	L	320	-	-	13/32/52/70	0/1/1/1
32	CLA	a	808	20	1/1/12/20	3/21/97/115	-
39	SQD	H	315	-	-	23/38/58/69	0/1/1/1
32	CLA	L	301	-	1/1/11/20	5/15/91/115	-
37	A86	O	311	-	-	4/34/90/90	0/3/3/3
33	KC2	O	302	-	-	8/15/71/71	-
32	CLA	H	305	8	1/1/11/20	5/15/91/115	-
32	CLA	F	303	6	1/1/14/20	10/36/112/115	-
37	A86	T	315	-	-	2/34/90/90	0/3/3/3
32	CLA	F	307	6	1/1/14/20	3/33/109/115	-
33	KC2	W	304	13	-	7/15/71/71	-
32	CLA	O	307	15	1/1/14/20	7/33/109/115	-
32	CLA	W	307	13	1/1/11/20	6/15/91/115	-
32	CLA	C	307	3	1/1/14/20	9/33/109/115	-
32	CLA	J	312	-	1/1/13/20	12/31/107/115	-
32	CLA	a	837	20	1/1/13/20	7/27/103/115	-
32	CLA	I	302	9	1/1/13/20	7/27/103/115	-
34	DD6	A	315	-	-	2/26/80/80	0/3/3/3
32	CLA	D	314	4	1/1/12/20	6/24/100/115	-
32	CLA	P	311	-	1/1/14/20	11/33/109/115	-
32	CLA	J	309	-	1/1/11/20	2/15/91/115	-
32	CLA	Q	308	-	1/1/11/20	4/15/91/115	-
37	A86	S	315	-	-	3/34/90/90	1/3/3/3
37	A86	T	312	-	-	4/34/90/90	0/3/3/3
33	KC2	E	313	-	-	8/15/71/71	-
32	CLA	K	304	11	1/1/11/20	5/15/91/115	-
32	CLA	O	305	15	1/1/15/20	8/39/115/115	-
34	DD6	H	313	-	-	2/26/80/80	0/3/3/3
33	KC2	F	310	36,6	-	7/15/71/71	-
32	CLA	U	301	-	1/1/9/20	2/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	KC2	O	310	15	-	6/15/71/71	-
35	LHG	D	320	-	-	22/52/52/53	-
32	CLA	E	315	-	1/1/11/20	5/17/93/115	-
32	CLA	b	814	-	1/1/11/20	7/15/91/115	-
32	CLA	f	201	-	1/1/14/20	2/33/109/115	-
36	LMG	D	302	-	-	8/25/45/70	0/1/1/1
34	DD6	C	310	-	-	0/26/80/80	0/3/3/3
37	A86	S	320	-	-	6/34/90/90	0/3/3/3
37	A86	T	313	-	-	9/34/90/90	0/3/3/3
36	LMG	F	320	-	-	7/28/48/70	0/1/1/1
32	CLA	W	312	13	1/1/14/20	9/33/109/115	-
32	CLA	S	301	-	1/1/11/20	3/15/91/115	-
36	LMG	M	320	33	-	9/35/55/70	0/1/1/1
32	CLA	j	101	27	1/1/11/20	4/15/91/115	-
37	A86	L	316	-	-	8/34/90/90	0/3/3/3
33	KC2	W	314	13,36	-	6/15/71/71	-
34	DD6	J	317	-	1/1/12/24	0/26/80/80	0/3/3/3
32	CLA	l	204	-	1/1/15/20	15/39/115/115	-
32	CLA	B	309	-	1/1/13/20	5/27/103/115	-
35	LHG	W	319	32	-	17/50/50/53	-
37	A86	K	314	-	-	4/34/90/90	0/3/3/3
33	KC2	N	306	14	-	4/15/71/71	-
35	LHG	f	205	-	-	24/51/51/53	-
35	LHG	B	308	-	-	18/35/35/53	-
32	CLA	Q	301	33	1/1/14/20	6/33/109/115	-
35	LHG	I	314	-	-	22/50/50/53	-
34	DD6	I	311	-	-	0/26/80/80	0/3/3/3
35	LHG	P	317	-	-	19/50/50/53	-
32	CLA	A	309	1	1/1/15/20	10/39/115/115	-
32	CLA	L	312	-	1/1/14/20	7/33/109/115	-
41	BCR	b	841	-	-	0/29/63/63	0/2/2/2
41	BCR	m	101	-	-	1/29/63/63	0/2/2/2
32	CLA	F	309	-	1/1/13/20	5/27/103/115	-
32	CLA	W	313	-	1/1/14/20	2/33/109/115	-
33	KC2	I	316	-	-	9/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	G	308	-	1/1/12/20	6/26/102/115	-
37	A86	L	315	-	-	4/34/90/90	0/3/3/3
32	CLA	U	303	18	1/1/11/20	3/15/91/115	-
37	A86	M	318	-	-	3/34/90/90	0/3/3/3
32	CLA	D	311	4	1/1/15/20	5/39/115/115	-
41	BCR	a	845	-	-	4/29/63/63	0/2/2/2
32	CLA	I	301	-	1/1/15/20	9/39/115/115	-
32	CLA	b	810	21	1/1/14/20	5/33/109/115	-
32	CLA	l	202	-	1/1/11/20	4/15/91/115	-
32	CLA	K	310	-	1/1/11/20	3/15/91/115	-
37	A86	N	315	-	-	2/34/90/90	0/3/3/3
32	CLA	M	312	-	1/1/14/20	9/33/109/115	-
33	KC2	I	309	36,9	-	6/15/71/71	-
35	LHG	a	850	32	-	13/34/34/53	-
32	CLA	R	309	15	1/1/10/20	2/10/86/115	-
41	BCR	a	846	-	-	2/29/63/63	0/2/2/2
41	BCR	k	204	-	-	3/29/63/63	0/2/2/2
32	CLA	H	304	-	1/1/11/20	7/15/91/115	-
34	DD6	D	301	-	-	2/26/80/80	0/3/3/3
34	DD6	N	318	-	-	2/26/80/80	0/3/3/3
37	A86	S	317	-	-	6/34/90/90	0/3/3/3
32	CLA	H	307	-	1/1/14/20	10/33/109/115	-
32	CLA	L	307	-	1/1/13/20	2/30/106/115	-
34	DD6	H	312	-	-	2/26/80/80	0/3/3/3
32	CLA	b	812	-	1/1/15/20	10/39/115/115	-
35	LHG	F	321	-	-	15/44/44/53	-
32	CLA	J	311	-	1/1/11/20	2/15/91/115	-
32	CLA	b	830	-	1/1/14/20	7/35/111/115	-
34	DD6	D	316	-	-	1/26/80/80	0/3/3/3
37	A86	Q	316	-	-	5/34/90/90	0/3/3/3
33	KC2	N	302	14	-	4/15/71/71	-
33	KC2	M	302	13	-	6/15/71/71	-
34	DD6	M	316	-	-	1/26/80/80	0/3/3/3
32	CLA	D	309	-	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	A	303	1	1/1/14/20	10/36/112/115	-
33	KC2	T	304	15	-	3/15/71/71	-
32	CLA	a	801	-	1/1/15/20	5/39/115/115	-
32	CLA	J	301	10	1/1/11/20	3/15/91/115	-
34	DD6	E	316	-	-	0/26/80/80	0/3/3/3
35	LHG	a	849	-	-	22/52/52/53	-
36	LMG	S	322	33	-	12/28/48/70	0/1/1/1
32	CLA	I	305	-	1/1/13/20	6/29/105/115	-
34	DD6	T	314	-	-	1/26/80/80	0/3/3/3
32	CLA	J	305	10	1/1/12/20	3/24/100/115	-
32	CLA	b	809	-	1/1/11/20	4/15/91/115	-
32	CLA	V	203	19	1/1/13/20	2/27/103/115	-
33	KC2	L	302	12	-	4/15/71/71	-
33	KC2	M	304	13	-	6/15/71/71	-
32	CLA	b	807	-	1/1/14/20	10/33/109/115	-
33	KC2	S	306	17	-	6/15/71/71	-
34	DD6	K	313	-	-	0/26/80/80	0/3/3/3
32	CLA	M	309	-	1/1/11/20	6/15/91/115	-
40	DGD	Q	318	-	-	27/45/85/95	0/2/2/2
32	CLA	S	304	-	1/1/10/20	2/12/88/115	-
32	CLA	R	307	-	1/1/11/20	2/15/91/115	-
33	KC2	P	312	13	-	6/15/71/71	-
37	A86	N	320	-	-	0/34/90/90	0/3/3/3
32	CLA	O	304	-	1/1/11/20	2/15/91/115	-
32	CLA	E	309	5	1/1/13/20	8/31/107/115	-
34	DD6	W	317	-	-	1/26/80/80	0/3/3/3
34	DD6	D	317	-	-	0/26/80/80	0/3/3/3
32	CLA	b	804	-	1/1/15/20	17/39/115/115	-
33	KC2	S	312	36,17	-	4/15/71/71	-
32	CLA	H	302	-	1/1/10/20	5/10/86/115	-
32	CLA	N	311	14	1/1/14/20	6/33/109/115	-
32	CLA	b	838	-	1/1/15/20	9/39/115/115	-
32	CLA	a	834	-	1/1/15/20	7/39/115/115	-
36	LMG	A	318	-	-	9/35/55/70	0/1/1/1
41	BCR	b	842	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	E	321	-	-	17/50/50/53	-
32	CLA	E	314	-	1/1/12/20	0/21/97/115	-
37	A86	F	312	-	-	2/34/90/90	0/3/3/3
41	BCR	a	843	-	-	3/29/63/63	0/2/2/2
34	DD6	A	314	-	-	1/26/80/80	0/3/3/3
32	CLA	N	310	-	1/1/13/20	6/27/103/115	-
33	KC2	N	307	-	-	4/15/71/71	-
37	A86	P	314	-	-	4/34/90/90	0/3/3/3
32	CLA	C	308	3	1/1/11/20	3/15/91/115	-
32	CLA	a	806	-	1/1/14/20	6/33/109/115	-
32	CLA	U	306	-	1/1/11/20	7/15/91/115	-
32	CLA	a	841	-	1/1/15/20	9/39/115/115	-
32	CLA	b	835	-	1/1/14/20	7/33/109/115	-
37	A86	P	313	-	-	7/34/90/90	1/3/3/3
32	CLA	D	315	-	1/1/11/20	4/15/91/115	-
37	A86	S	314	-	-	6/34/90/90	0/3/3/3
32	CLA	B	306	-	1/1/11/20	4/15/91/115	-
39	SQD	k	206	-	-	13/31/51/69	0/1/1/1
32	CLA	S	305	-	1/1/14/20	5/37/113/115	-
33	KC2	U	304	-	-	6/15/71/71	-
37	A86	W	318	-	-	6/34/90/90	0/3/3/3
33	KC2	R	302	15	-	6/15/71/71	-
34	DD6	K	315	-	1/1/12/24	1/26/80/80	0/3/3/3
32	CLA	I	306	9	1/1/15/20	7/39/115/115	-
36	LMG	N	301	-	-	19/35/55/70	0/1/1/1
37	A86	L	318	-	-	3/34/90/90	0/3/3/3
32	CLA	b	828	-	1/1/14/20	6/35/111/115	-
32	CLA	H	310	-	1/1/11/20	3/17/93/115	-
32	CLA	a	838	-	1/1/15/20	4/39/115/115	-
32	CLA	a	853	-	1/1/15/20	7/39/115/115	-
34	DD6	D	318	-	-	2/26/80/80	0/3/3/3
32	CLA	b	825	-	1/1/14/20	6/33/109/115	-
33	KC2	W	305	13	-	4/15/71/71	-
32	CLA	G	301	-	1/1/11/20	6/15/91/115	-
32	CLA	Q	305	-	1/1/12/20	5/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	832	-	1/1/15/20	9/39/115/115	-
32	CLA	U	305	18	1/1/11/20	5/15/91/115	-
32	CLA	B	302	-	1/1/11/20	4/15/91/115	-
32	CLA	I	307	-	1/1/11/20	4/15/91/115	-
37	A86	C	312	-	-	6/34/90/90	0/3/3/3
32	CLA	a	809	-	1/1/14/20	7/33/109/115	-
37	A86	P	316	-	-	7/34/90/90	0/3/3/3
36	LMG	D	303	-	-	17/31/51/70	0/1/1/1
35	LHG	F	318	-	-	15/45/45/53	-
32	CLA	b	805	-	1/1/15/20	6/39/115/115	-
33	KC2	K	305	-	-	4/15/71/71	-
33	KC2	S	303	17	-	8/15/71/71	-
34	DD6	Q	315	-	-	2/26/80/80	0/3/3/3
32	CLA	M	305	-	1/1/12/20	3/21/97/115	-

The worst 5 of 2902 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	S	312	KC2	MG-ND	-10.20	1.85	2.05
33	K	303	KC2	MG-ND	-10.20	1.85	2.05
33	N	308	KC2	MG-ND	-10.20	1.85	2.05
33	W	305	KC2	MG-ND	-10.13	1.85	2.05
33	P	303	KC2	MG-ND	-10.08	1.85	2.05

The worst 5 of 2680 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	S	307	CLA	C4A-NA-C1A	-8.43	102.83	106.68
32	a	818	CLA	C4A-NA-C1A	-8.16	102.95	106.68
32	S	308	CLA	C1C-NC-C4C	-8.02	103.02	106.68
32	L	311	CLA	C3A-C2A-C1A	-7.92	98.20	106.30
32	b	837	CLA	C4A-NA-C1A	-7.73	103.15	106.68

5 of 285 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	301	CLA	ND
32	A	302	CLA	ND
32	A	303	CLA	ND

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Mol	Chain	Res	Type	Atom
32	A	304	CLA	ND
32	A	305	CLA	ND

5 of 3093 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	304	CLA	C1A-C2A-CAA-CBA
32	A	304	CLA	C3A-C2A-CAA-CBA
32	A	305	CLA	C2B-C3B-CAB-CBB
32	A	305	CLA	C4B-C3B-CAB-CBB
32	A	311	CLA	C1A-C2A-CAA-CBA

5 of 6 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	M	314	A86	C31-C32-C33-C34-C35-C36
37	M	317	A86	C31-C32-C33-C34-C35-C36
37	S	315	A86	C31-C32-C33-C34-C35-C36
37	U	308	A86	C31-C32-C33-C34-C35-C36
37	G	311	A86	C31-C32-C33-C34-C35-C36

163 monomers are involved in 261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	L	310	CLA	5	0
32	a	820	CLA	1	0
41	U	310	BCR	1	0
32	M	311	CLA	3	0
34	I	312	DD6	1	0
33	R	311	KC2	1	0
32	b	816	CLA	1	0
32	W	311	CLA	1	0
32	M	310	CLA	1	0
32	L	311	CLA	3	0
32	H	306	CLA	1	0
32	b	817	CLA	2	0
32	k	203	CLA	6	0
32	a	817	CLA	1	0
32	b	833	CLA	4	0
32	I	303	CLA	1	0
34	L	319	DD6	1	0
36	j	104	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	I	315	LMU	3	0
32	W	306	CLA	1	0
34	A	313	DD6	2	0
32	A	307	CLA	1	0
32	b	831	CLA	1	0
32	T	307	CLA	1	0
32	W	310	CLA	5	0
32	Q	303	CLA	1	0
32	a	832	CLA	2	0
36	D	325	LMG	1	0
32	H	309	CLA	1	0
32	a	807	CLA	1	0
36	F	319	LMG	5	0
32	W	309	CLA	1	0
37	F	313	A86	1	0
32	a	828	CLA	3	0
33	A	310	KC2	2	0
37	R	312	A86	1	0
32	K	306	CLA	1	0
32	A	301	CLA	3	0
32	D	304	CLA	1	0
42	c	101	SF4	1	0
32	F	304	CLA	2	0
34	k	205	DD6	1	0
32	D	307	CLA	1	0
32	b	827	CLA	1	0
32	a	833	CLA	1	0
37	H	314	A86	1	0
41	b	845	BCR	3	0
32	a	810	CLA	1	0
32	a	805	CLA	1	0
33	K	303	KC2	1	0
32	C	305	CLA	2	0
33	G	309	KC2	1	0
32	b	822	CLA	1	0
32	b	811	CLA	1	0
36	W	320	LMG	11	0
32	T	302	CLA	1	0
36	A	317	LMG	1	0
38	J	318	LMU	3	0
32	P	307	CLA	1	0
32	a	802	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	a	814	CLA	1	0
37	M	315	A86	1	0
32	a	821	CLA	1	0
37	D	322	A86	1	0
32	b	834	CLA	1	0
35	a	851	LHG	7	0
32	H	301	CLA	1	0
37	R	313	A86	1	0
36	T	301	LMG	2	0
37	W	316	A86	1	0
32	L	309	CLA	2	0
41	l	206	BCR	1	0
32	a	822	CLA	1	0
33	N	314	KC2	1	0
33	F	302	KC2	1	0
36	P	318	LMG	7	0
33	M	313	KC2	1	0
32	K	301	CLA	2	0
32	a	836	CLA	1	0
37	M	301	A86	1	0
34	S	321	DD6	2	0
32	a	852	CLA	1	0
33	K	309	KC2	2	0
32	a	803	CLA	1	0
32	k	201	CLA	1	0
37	M	317	A86	3	0
32	R	308	CLA	1	0
32	D	308	CLA	1	0
36	l	201	LMG	5	0
38	D	324	LMU	2	0
32	b	826	CLA	2	0
38	V	205	LMU	3	0
32	a	824	CLA	1	0
33	N	303	KC2	1	0
34	U	309	DD6	1	0
32	N	312	CLA	4	0
41	b	843	BCR	2	0
37	W	302	A86	1	0
32	a	823	CLA	2	0
39	H	315	SQD	16	0
33	O	302	KC2	1	0
32	H	305	CLA	2	0

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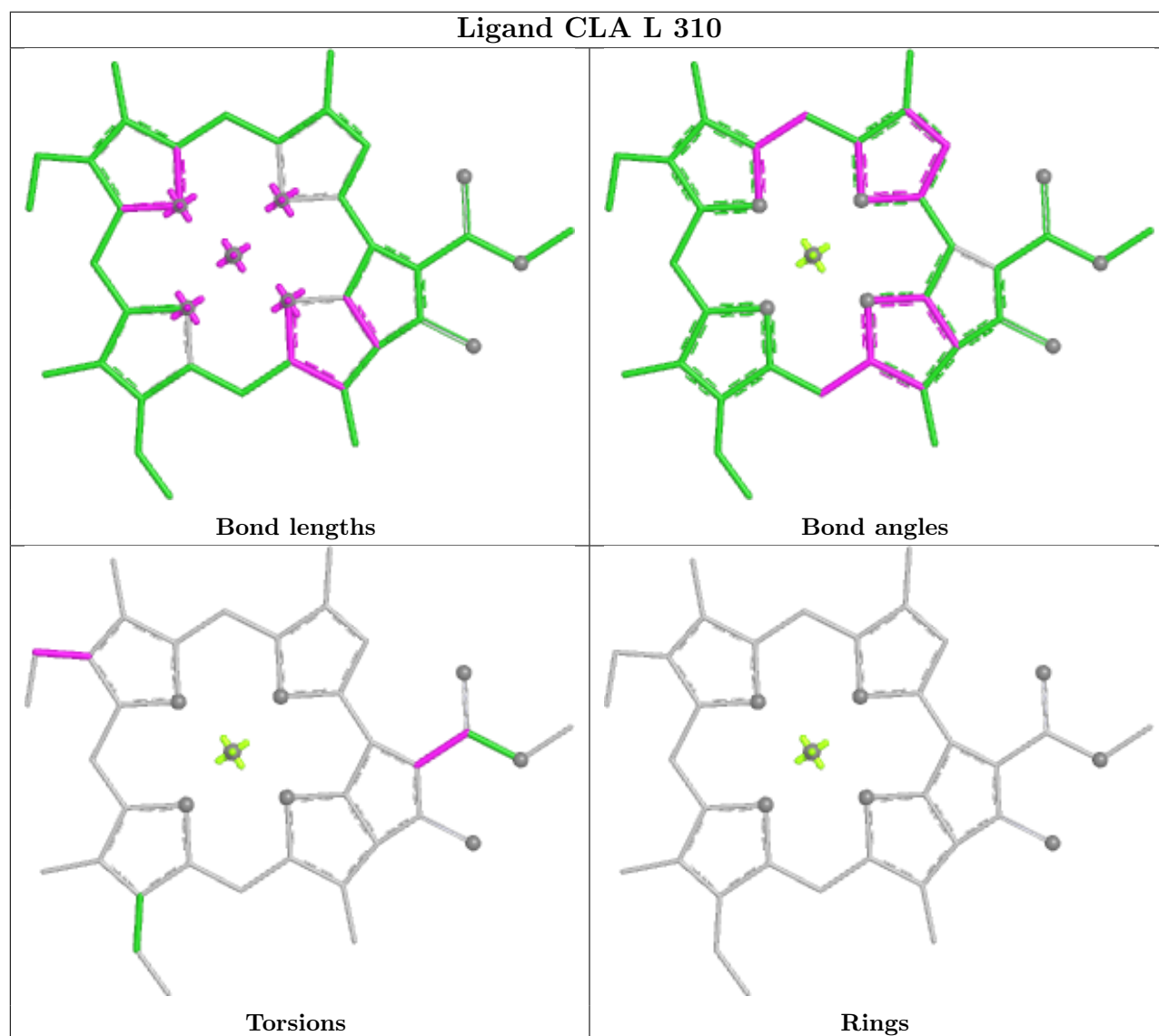
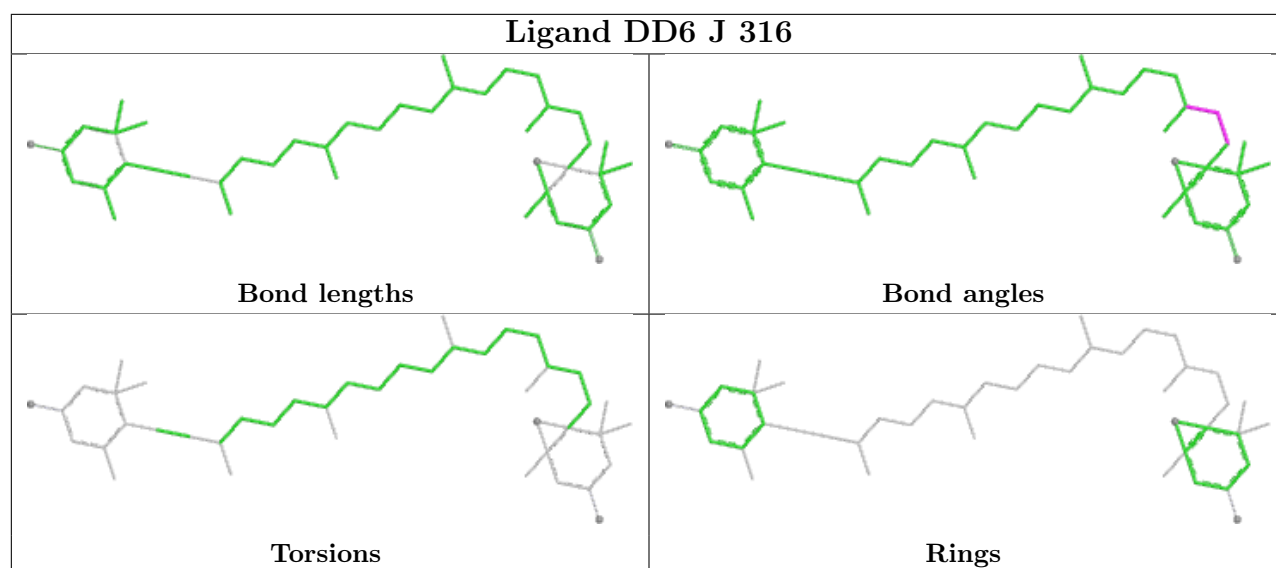
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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32	J	312	CLA	4	0
32	D	314	CLA	1	0
32	P	311	CLA	2	0
37	S	315	A86	2	0
32	K	304	CLA	1	0
33	F	310	KC2	1	0
32	b	814	CLA	1	0
37	T	313	A86	1	0
36	F	320	LMG	13	0
32	W	312	CLA	7	0
36	M	320	LMG	9	0
32	j	101	CLA	1	0
37	L	316	A86	1	0
33	W	314	KC2	1	0
34	J	317	DD6	1	0
35	f	205	LHG	1	0
35	B	308	LHG	2	0
34	I	311	DD6	1	0
35	P	317	LHG	1	0
32	A	309	CLA	2	0
41	b	841	BCR	1	0
37	L	315	A86	3	0
37	M	318	A86	1	0
32	I	301	CLA	2	0
33	I	309	KC2	4	0
41	a	846	BCR	1	0
41	k	204	BCR	1	0
35	F	321	LHG	1	0
32	b	830	CLA	1	0
34	D	316	DD6	1	0
37	Q	316	A86	2	0
34	M	316	DD6	3	0
32	A	303	CLA	1	0
36	S	322	LMG	8	0
32	b	807	CLA	1	0
32	M	309	CLA	1	0
40	Q	318	DGD	3	0
33	P	312	KC2	2	0
32	O	304	CLA	4	0
34	W	317	DD6	1	0
33	S	312	KC2	5	0

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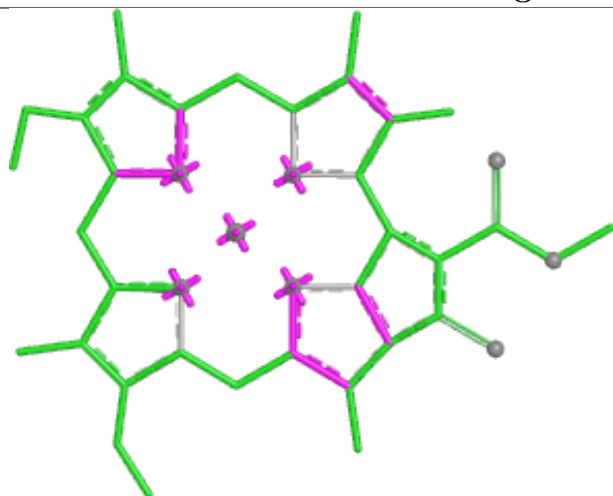
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	N	311	CLA	1	0
32	a	834	CLA	1	0
36	A	318	LMG	1	0
37	F	312	A86	1	0
41	a	843	BCR	1	0
32	N	310	CLA	1	0
32	C	308	CLA	1	0
32	U	306	CLA	1	0
32	b	835	CLA	1	0
32	D	315	CLA	2	0
39	k	206	SQD	6	0
32	S	305	CLA	1	0
36	N	301	LMG	5	0
32	b	828	CLA	1	0
32	a	838	CLA	1	0
34	D	318	DD6	1	0
32	U	305	CLA	2	0
37	P	316	A86	1	0
35	F	318	LHG	1	0

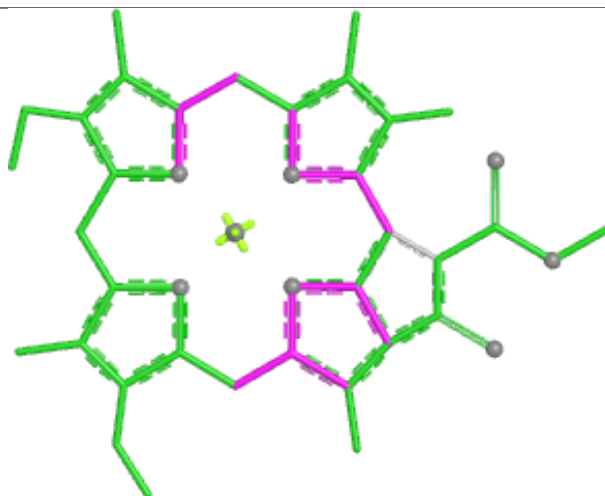
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



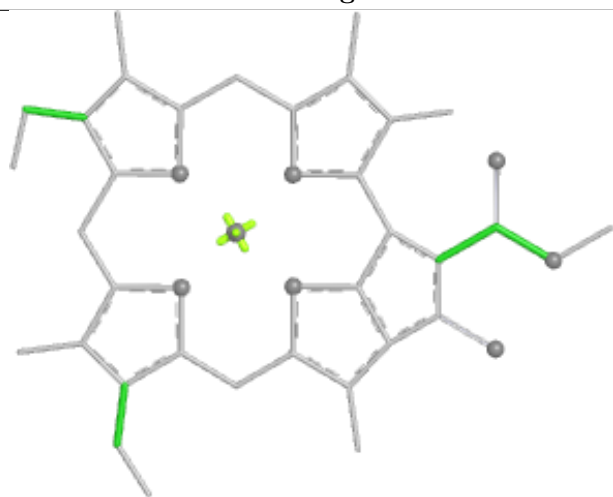
Ligand CLA C 302



Bond lengths



Bond angles

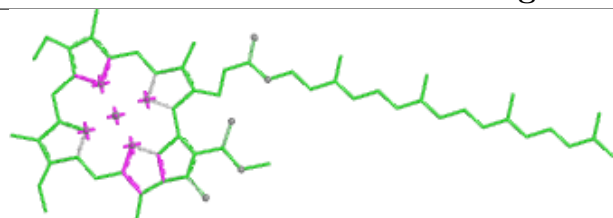


Torsions

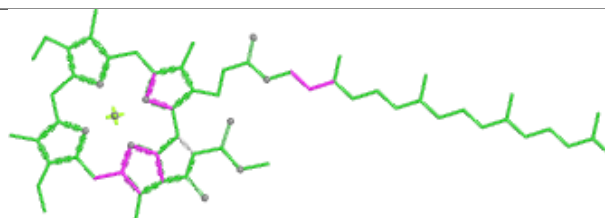


Rings

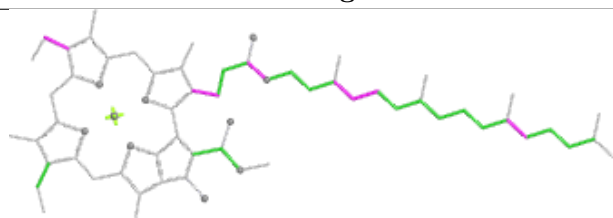
Ligand CLA a 820



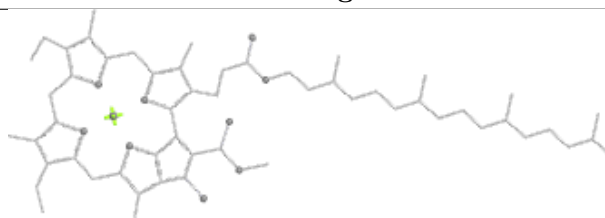
Bond lengths



Bond angles

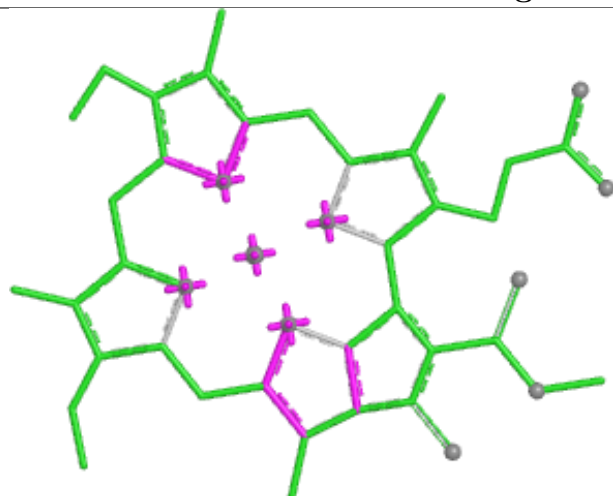


Torsions

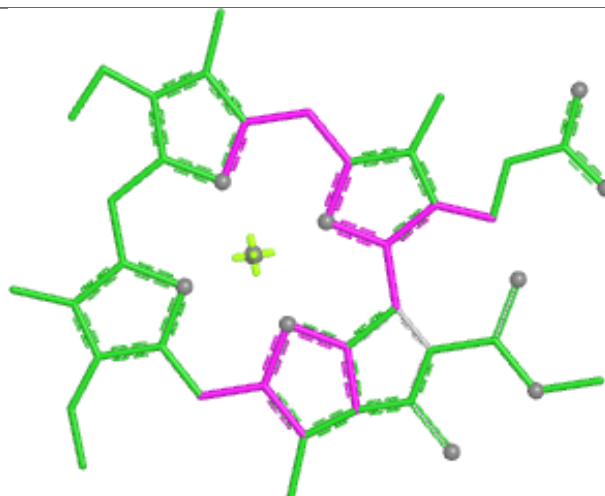


Rings

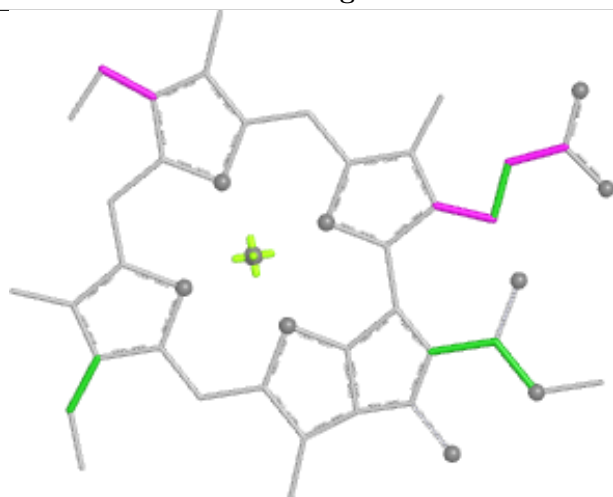
Ligand CLA P 304



Bond lengths



Bond angles

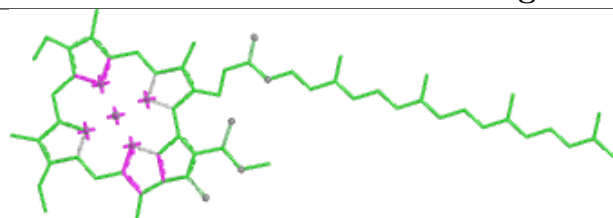


Torsions

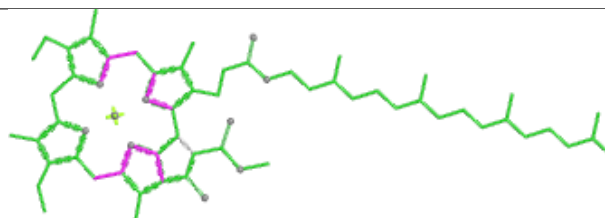


Rings

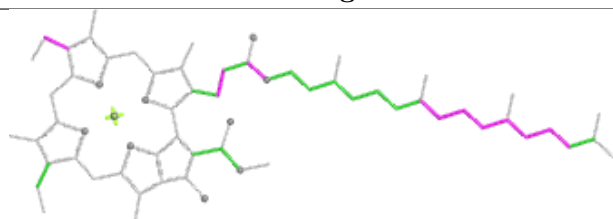
Ligand CLA a 826



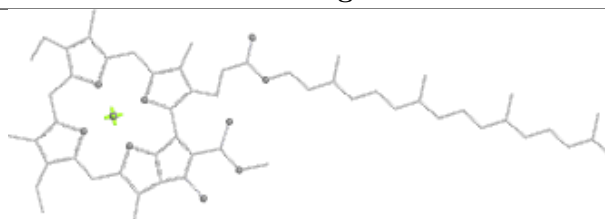
Bond lengths



Bond angles

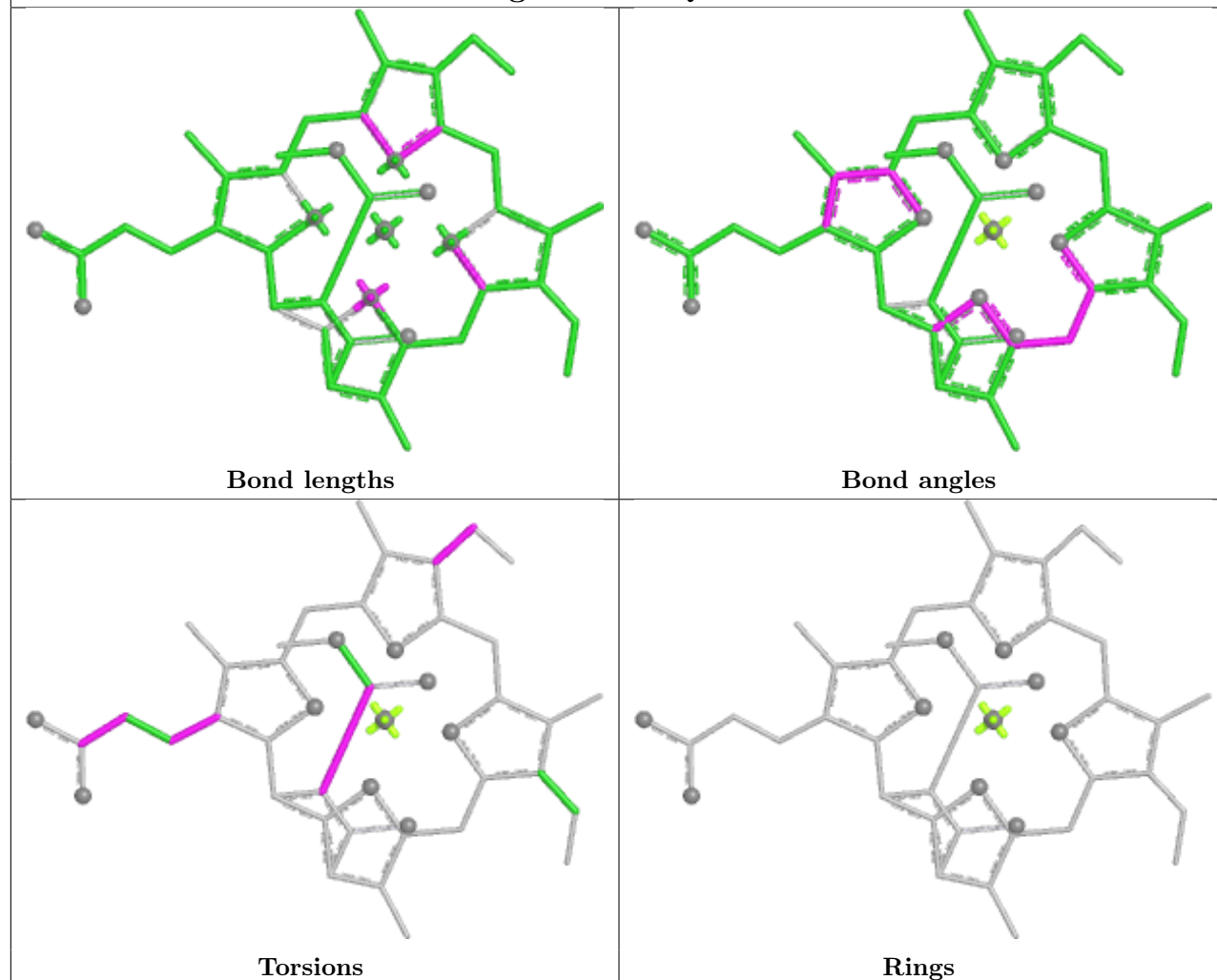


Torsions

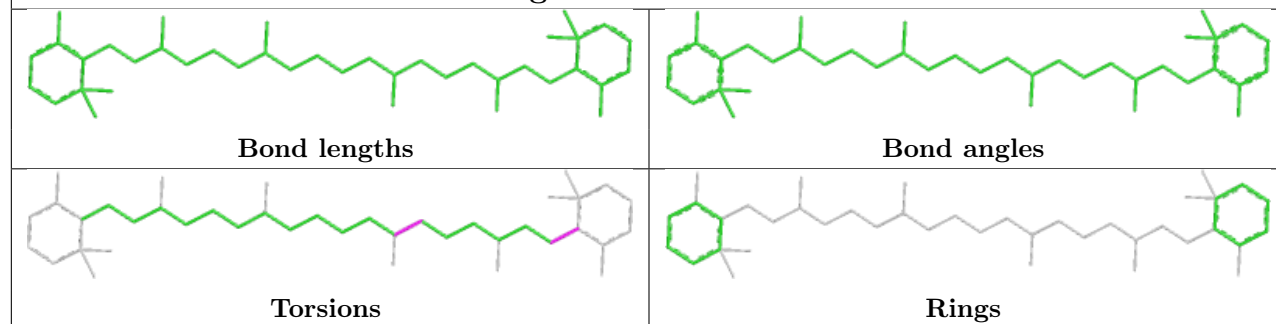


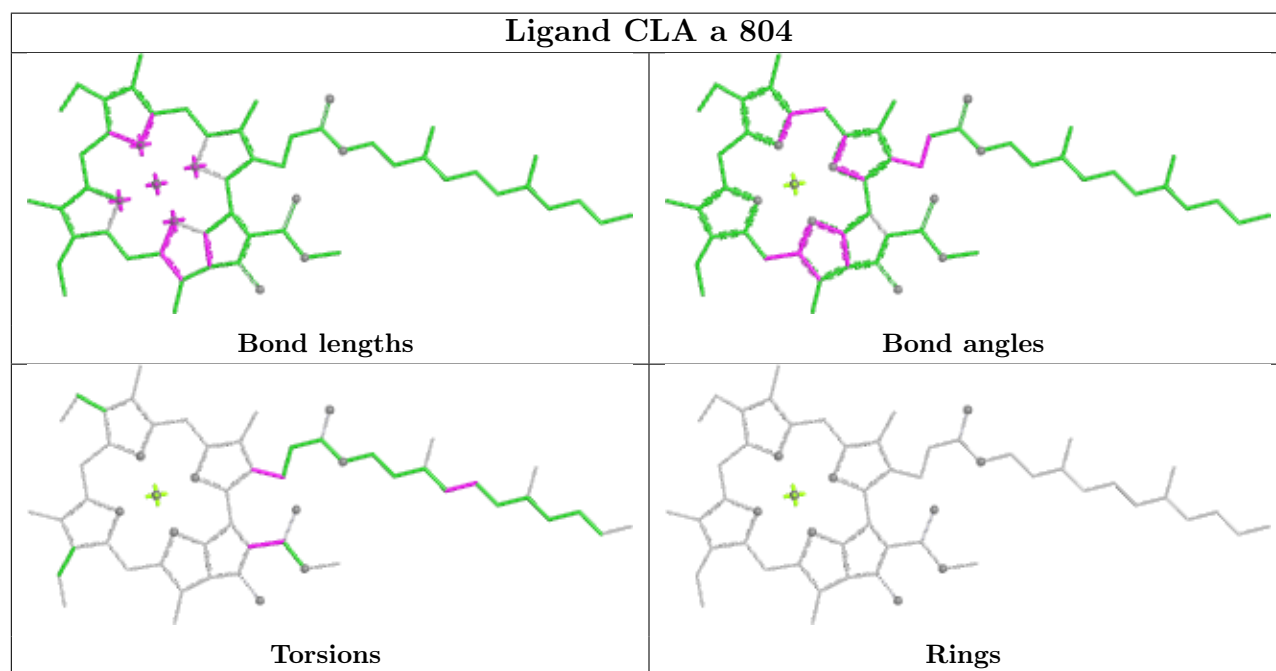
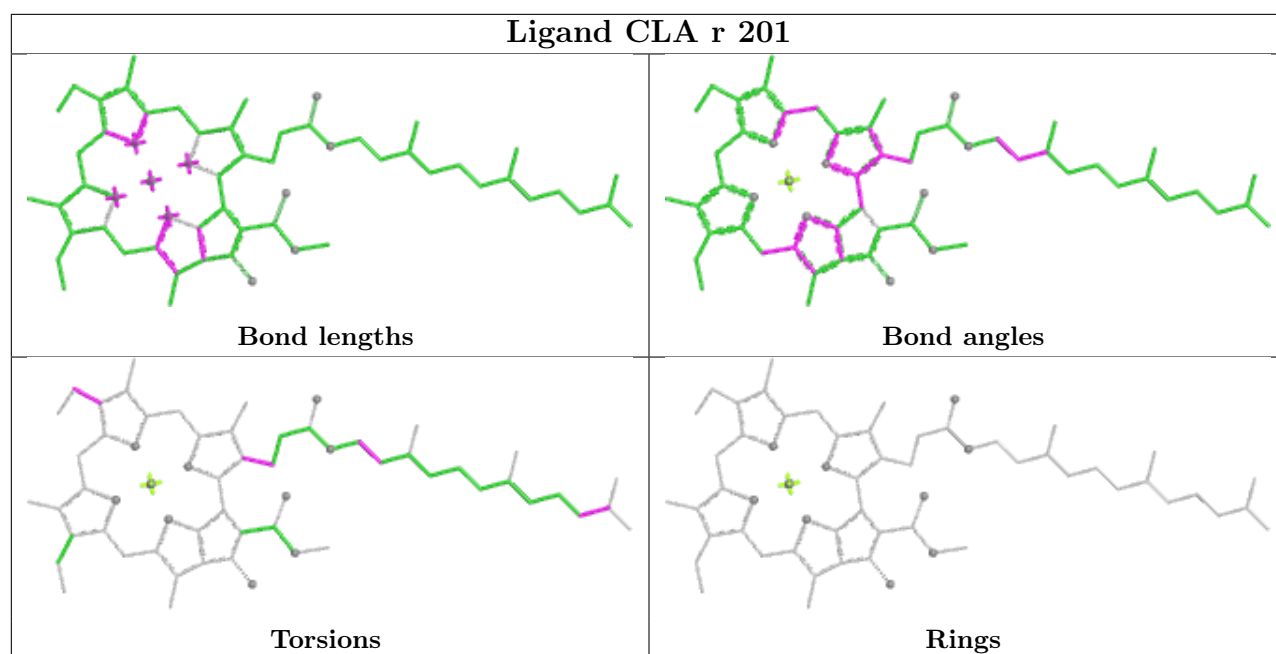
Rings

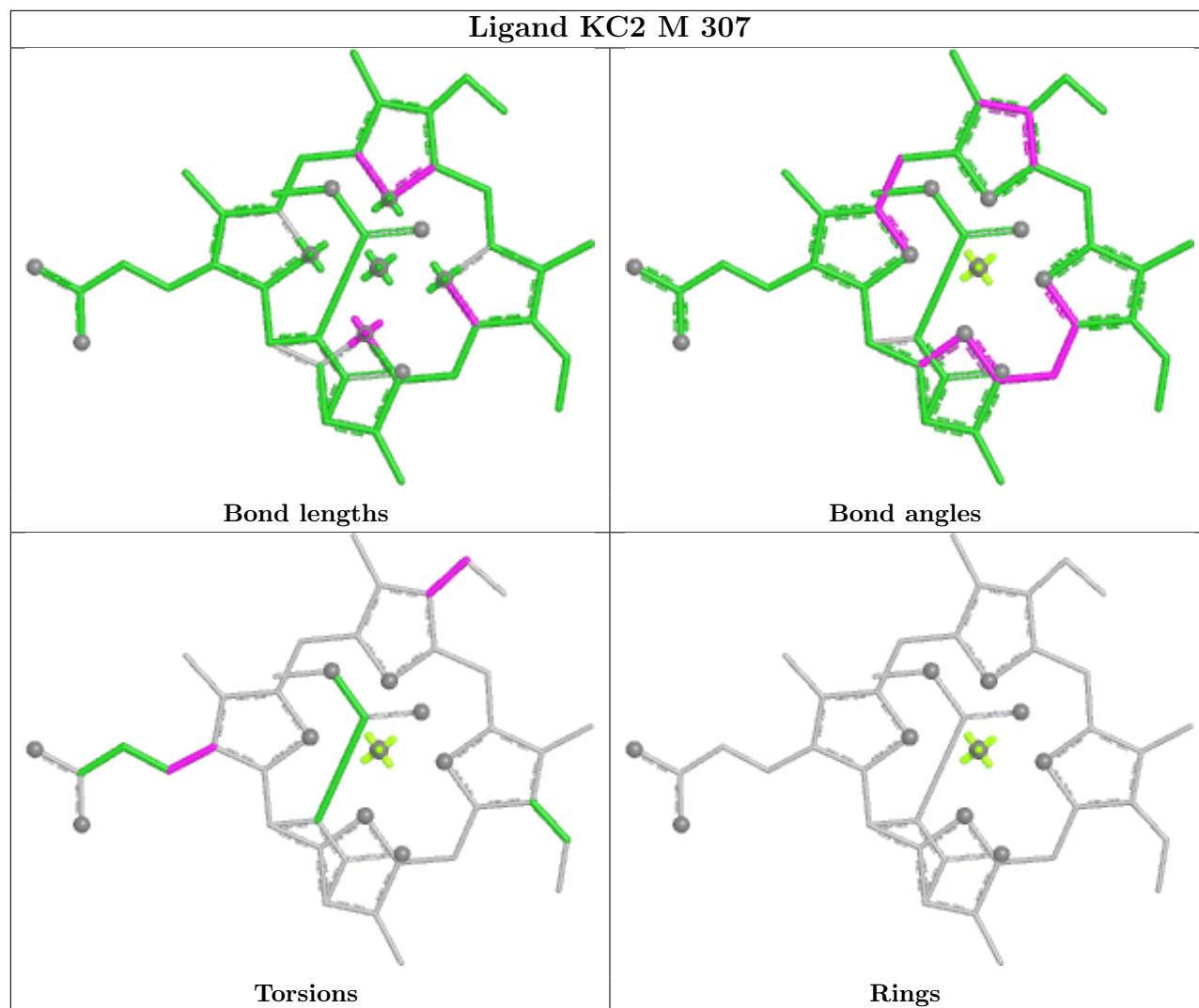
Ligand KC2 Q 317

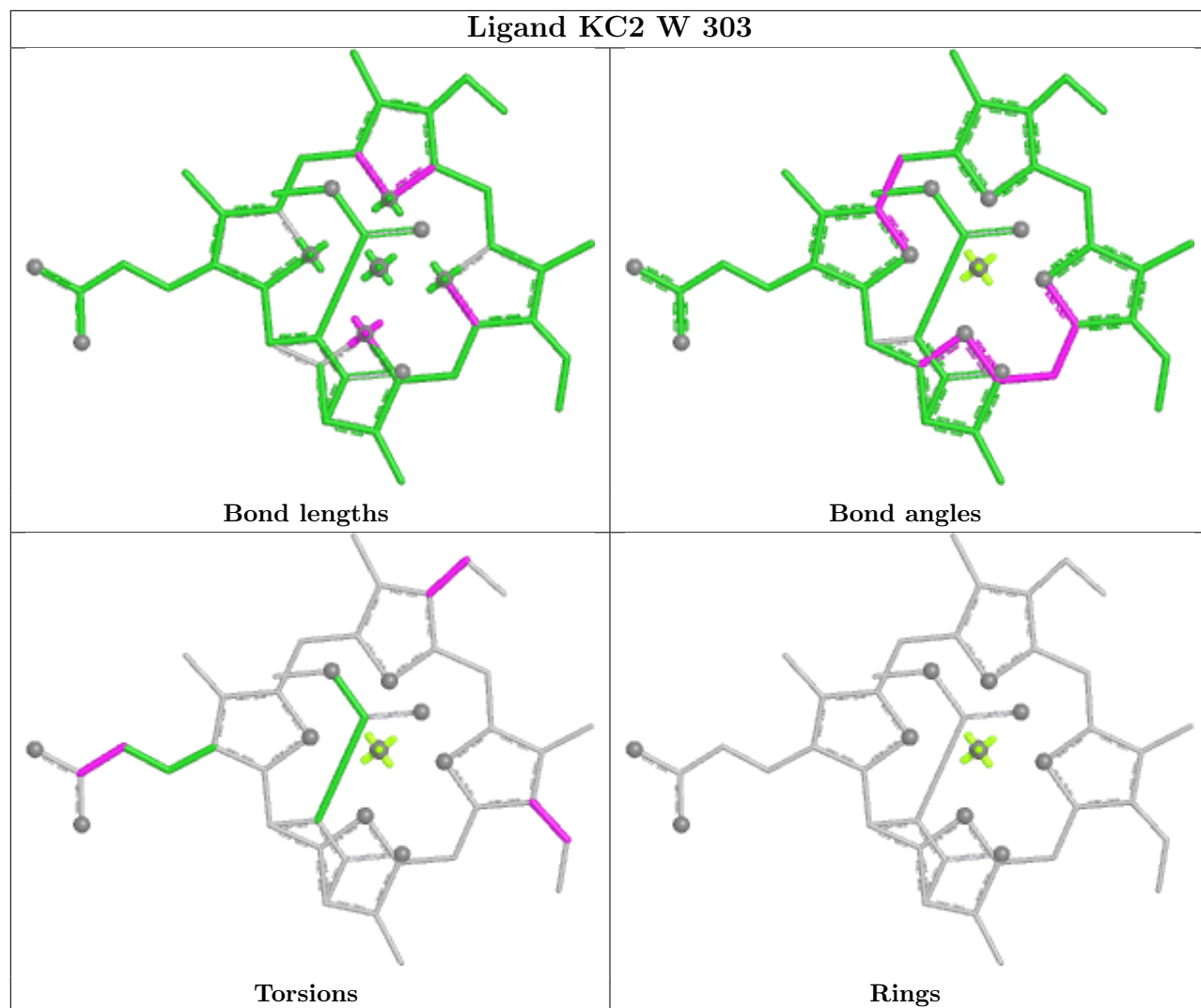


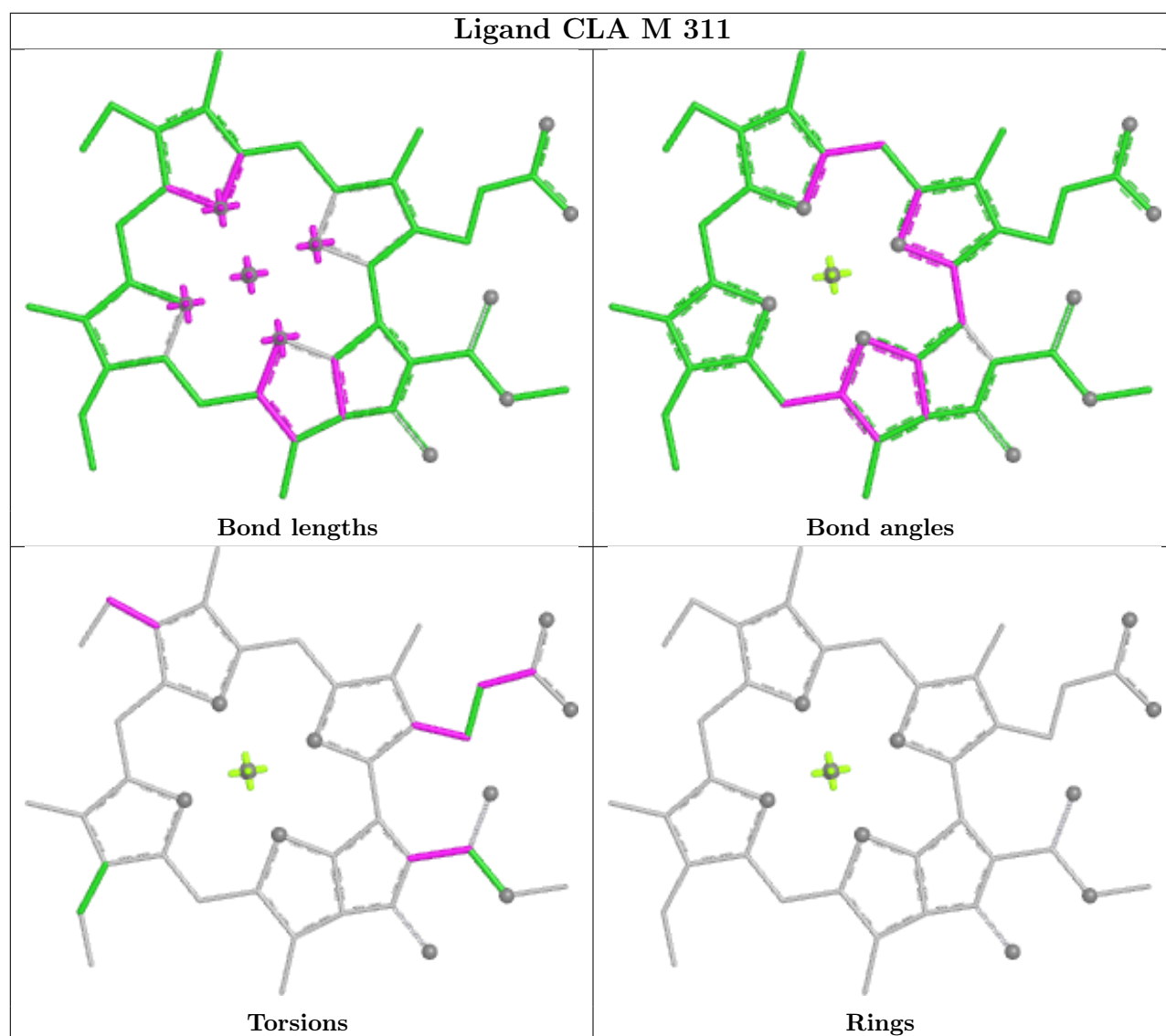
Ligand BCR U 310



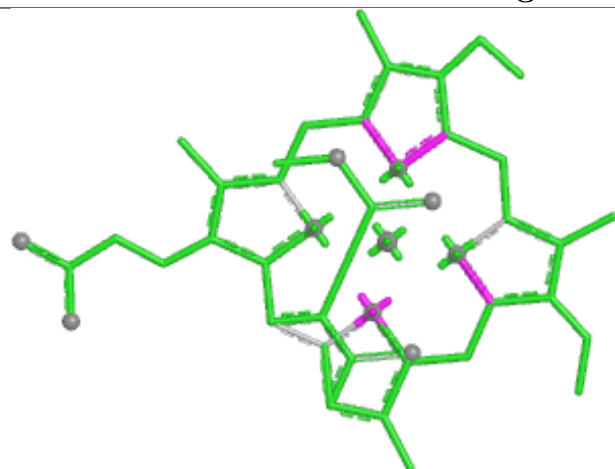




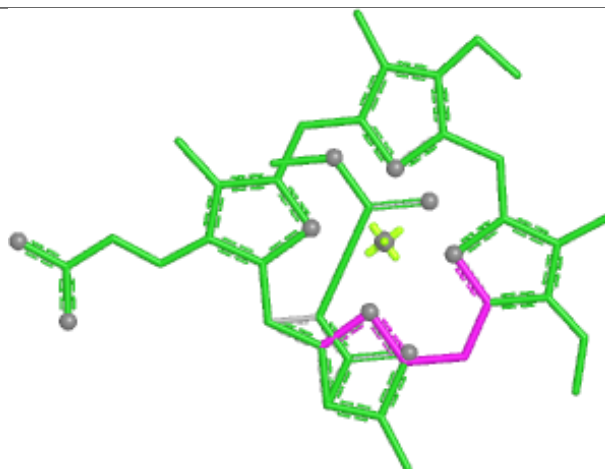




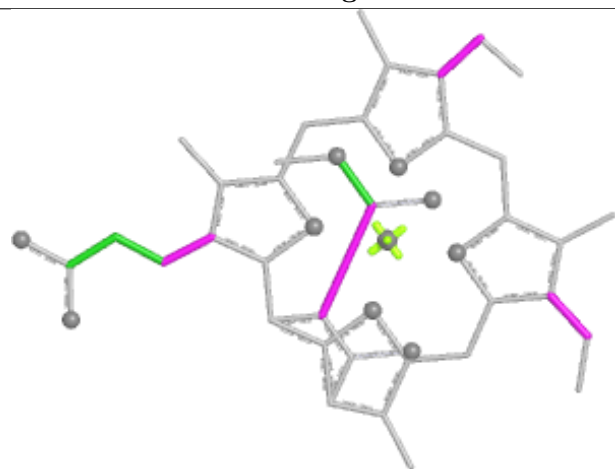
Ligand KC2 H 303



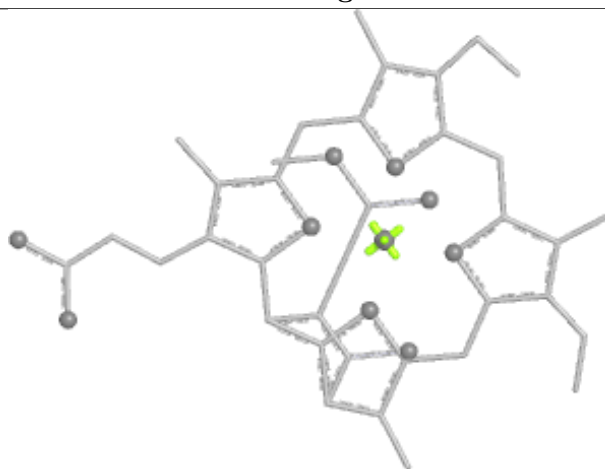
Bond lengths



Bond angles

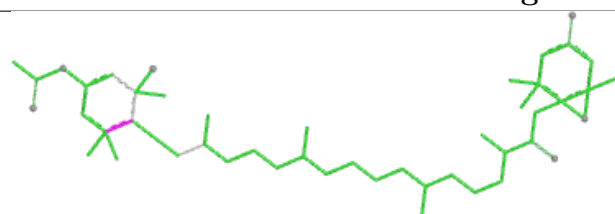


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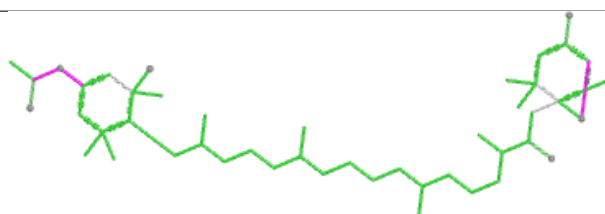


Rings

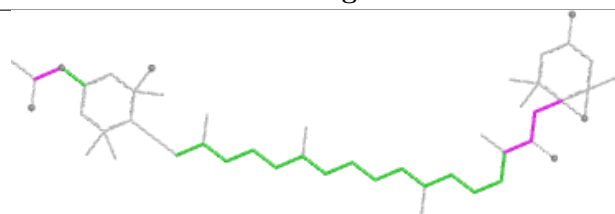
Ligand A86 K 311



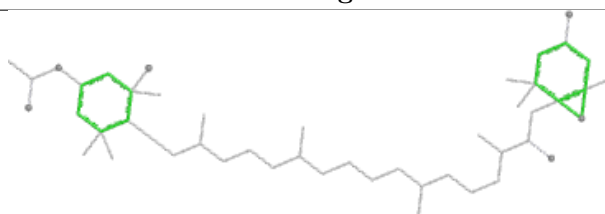
Bond lengths



Bond angles

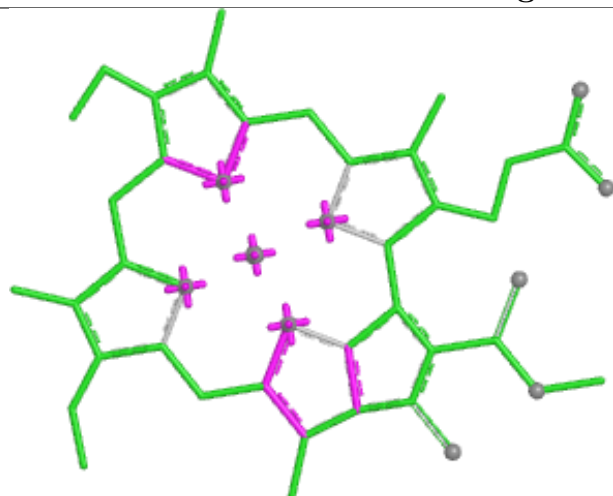


Torsions

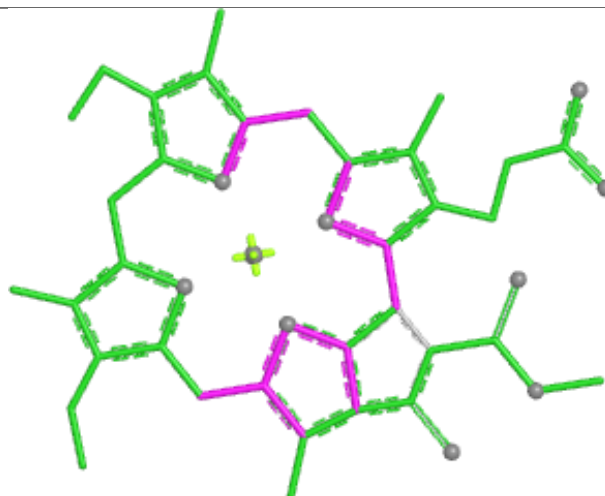


Rings

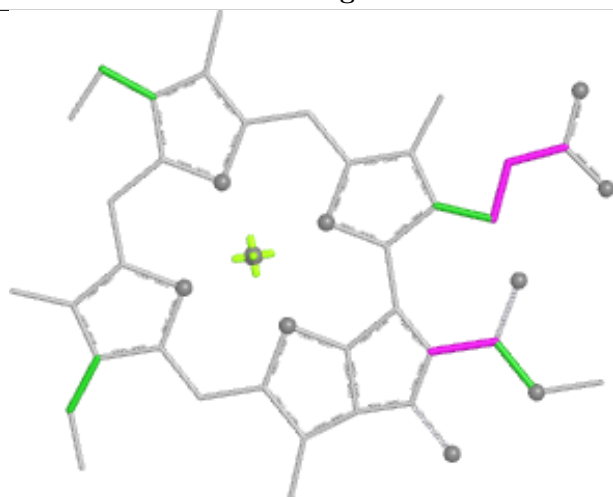
Ligand CLA b 813



Bond lengths



Bond angles

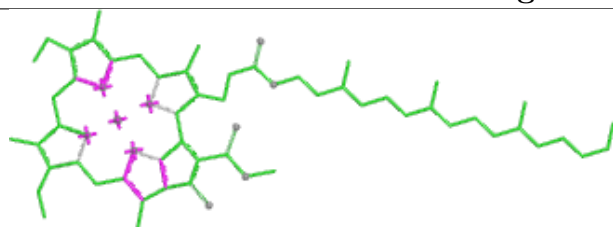


Torsions

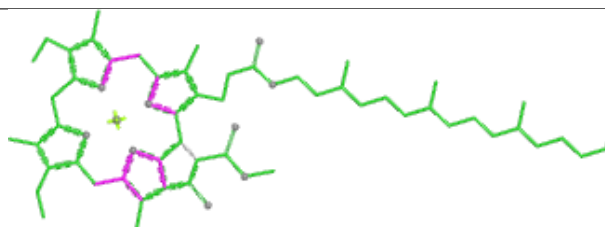


Rings

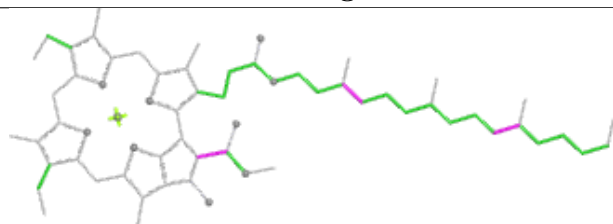
Ligand CLA b 820



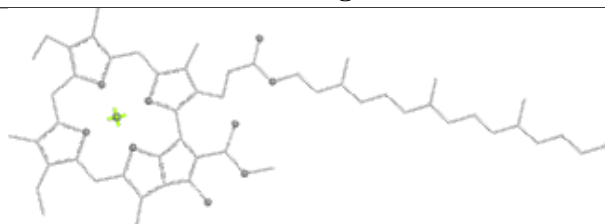
Bond lengths



Bond angles

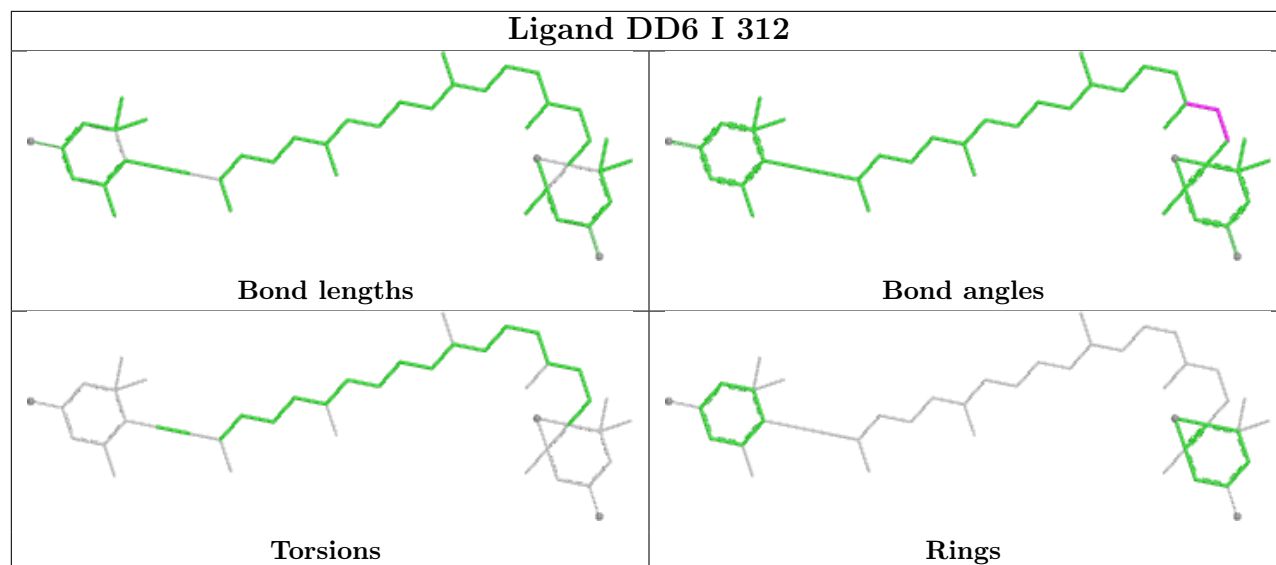


Torsions

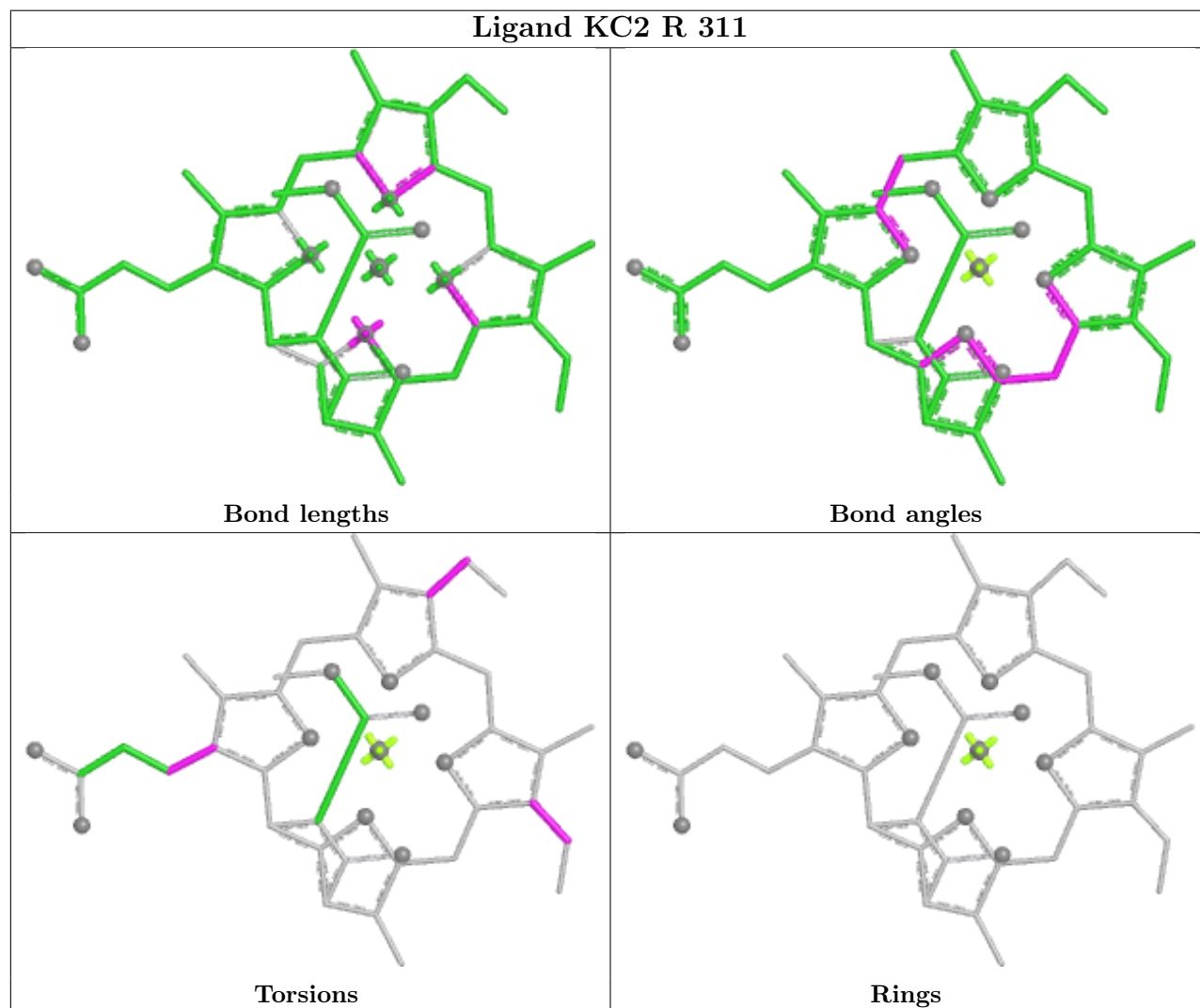


Rings

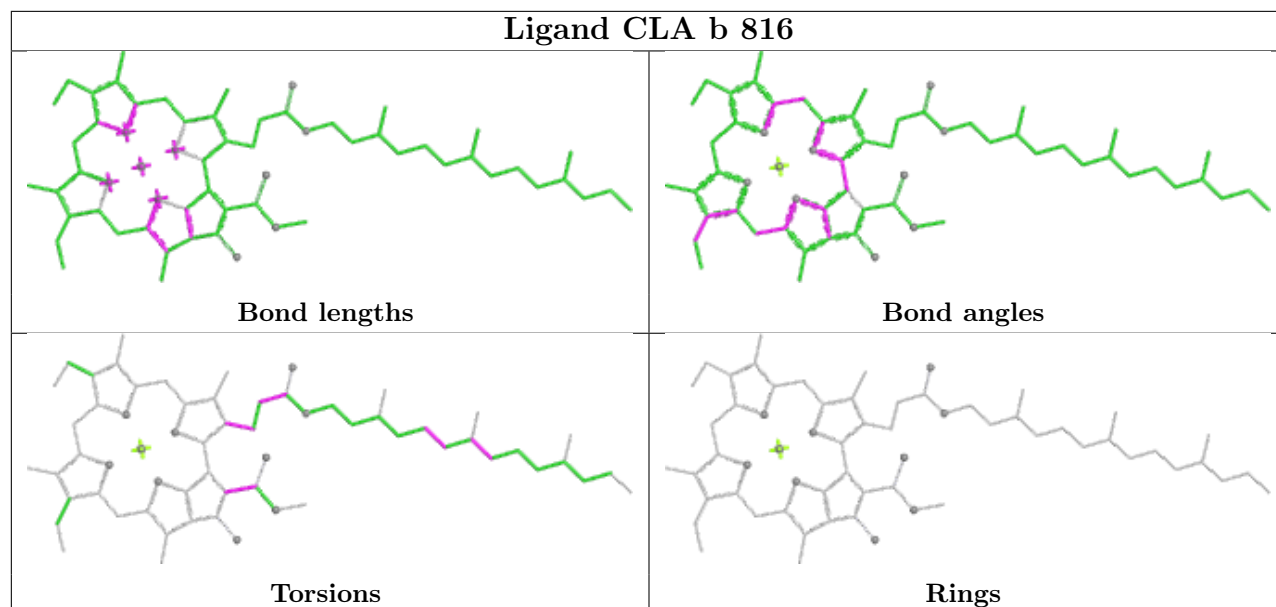
Ligand DD6 I 312



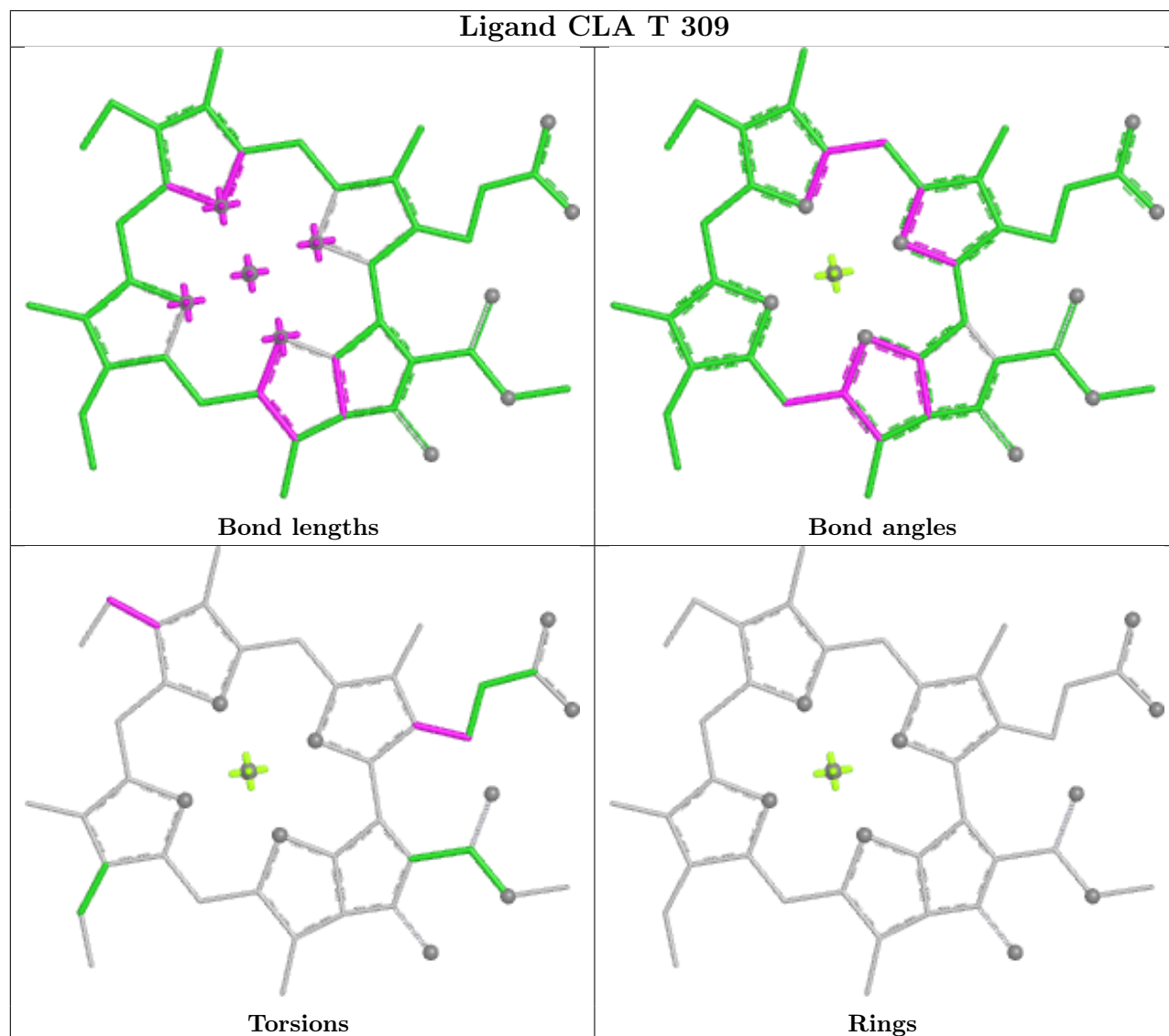
Ligand KC2 R 311

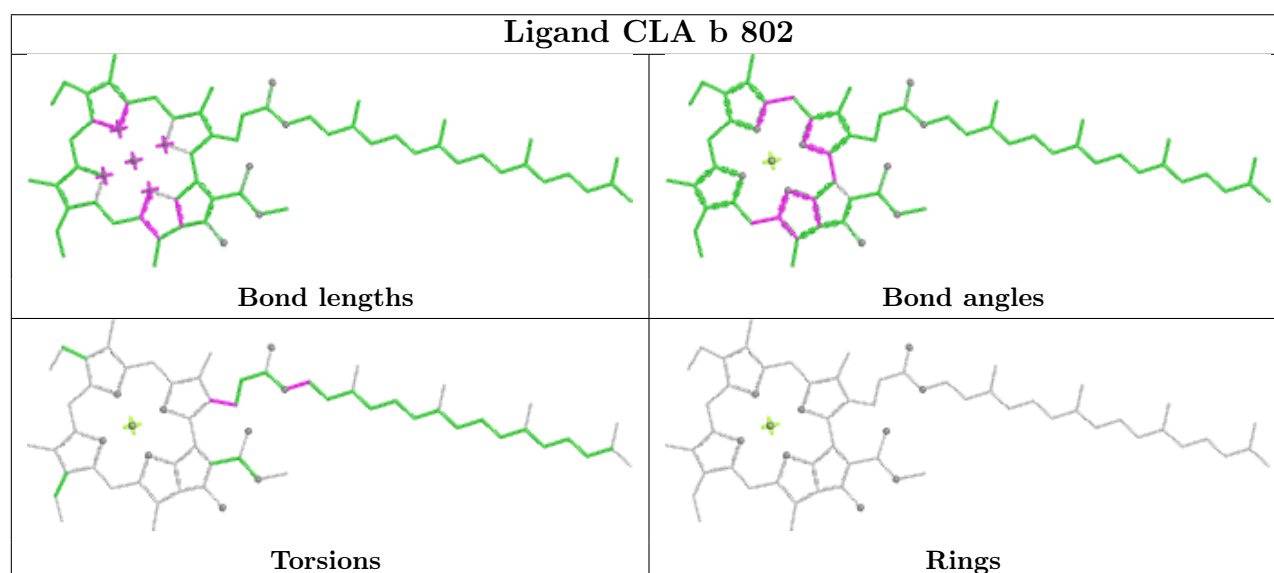
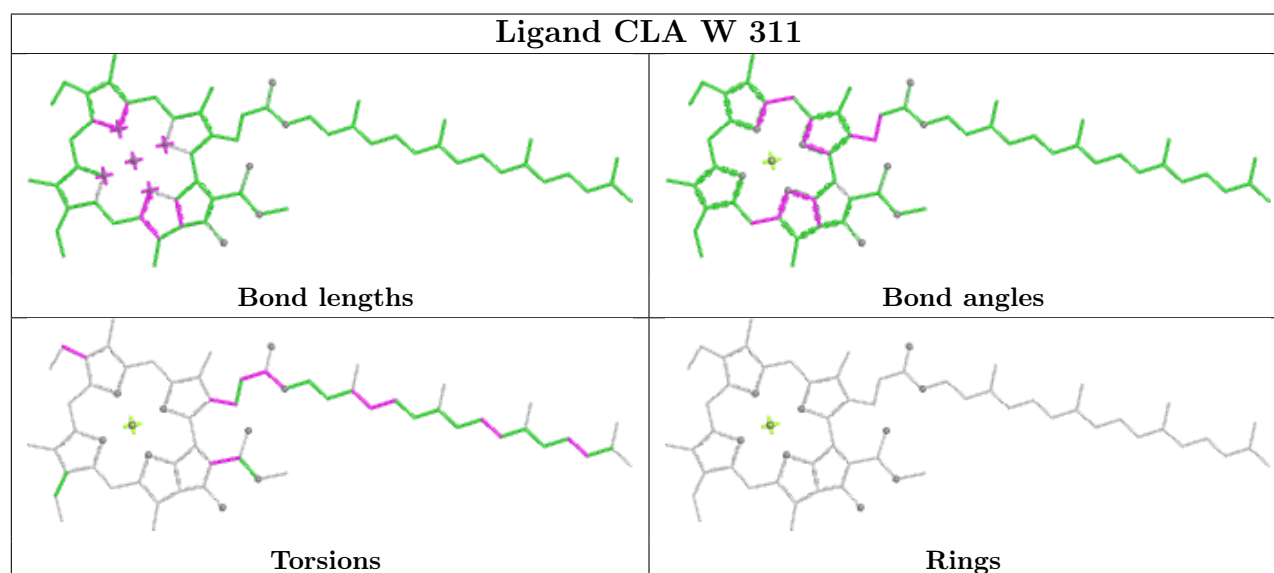
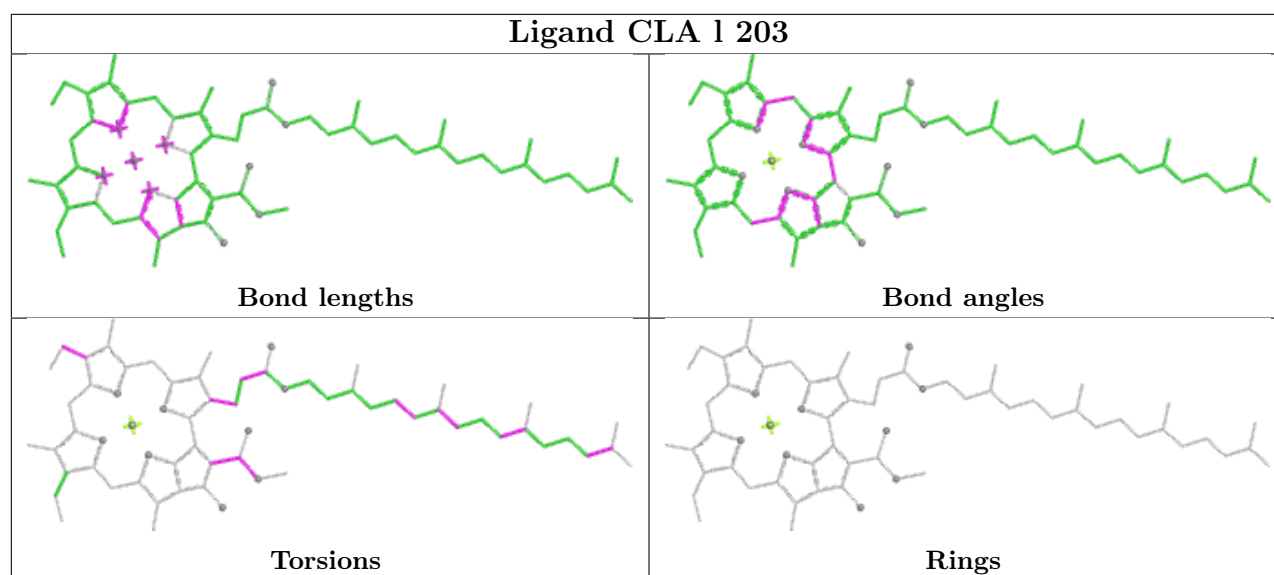


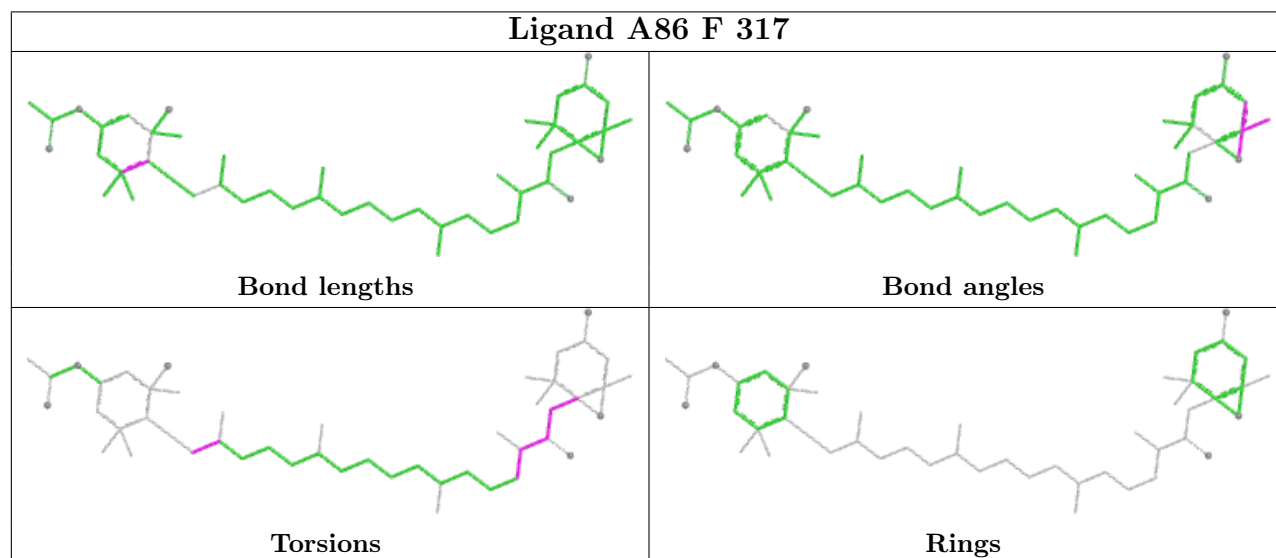
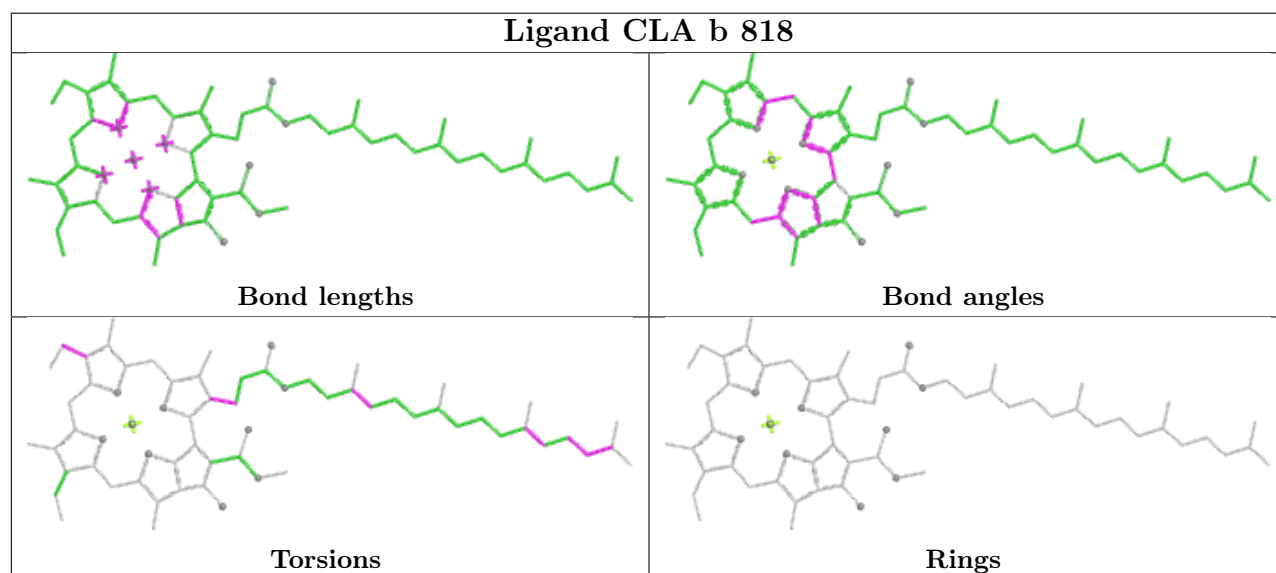
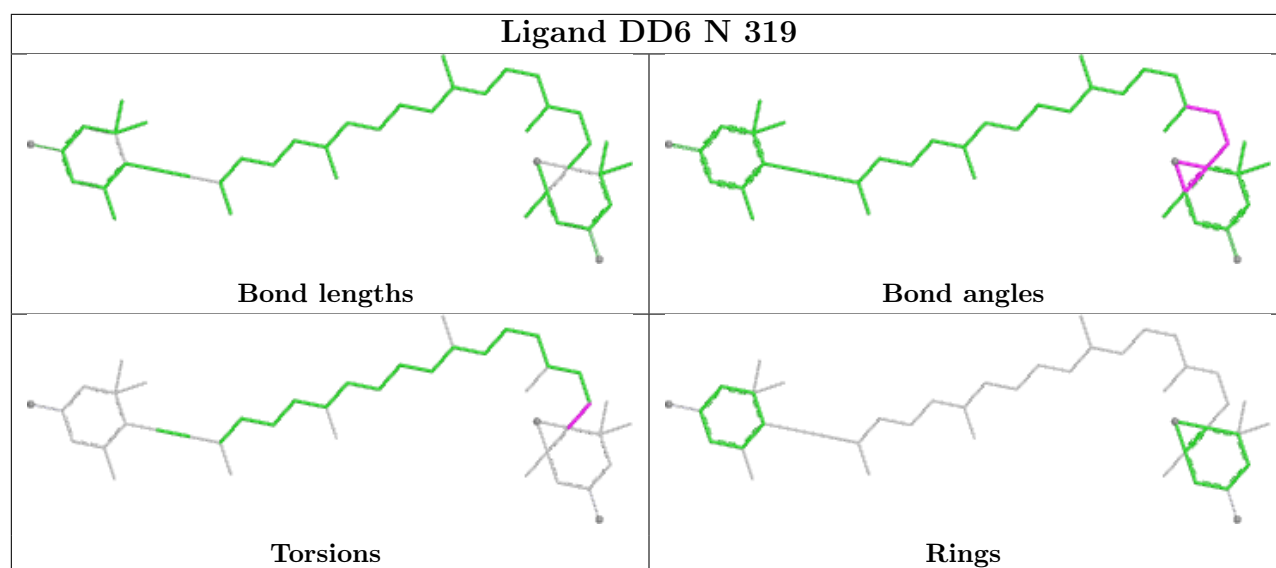
Ligand CLA b 816

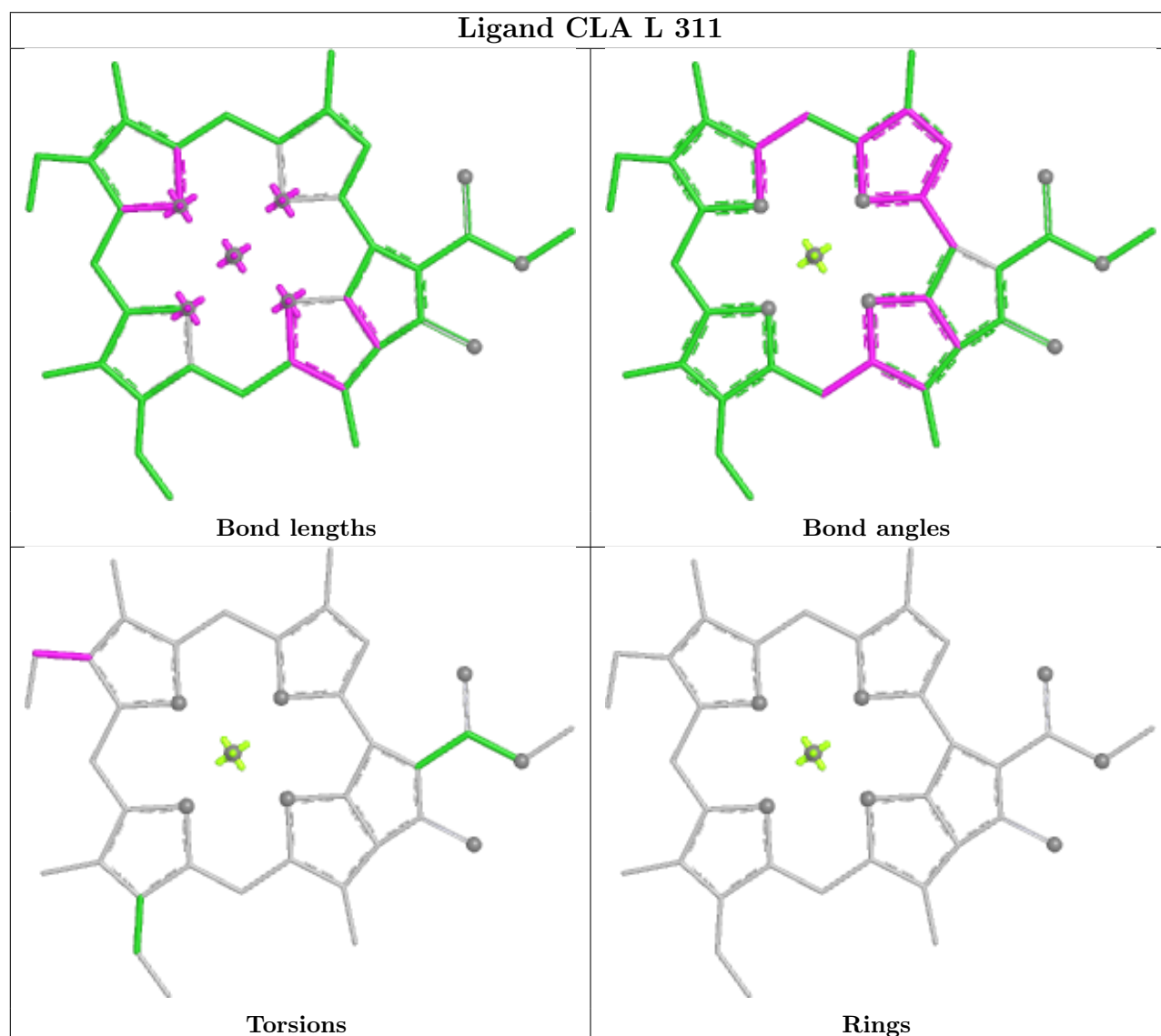
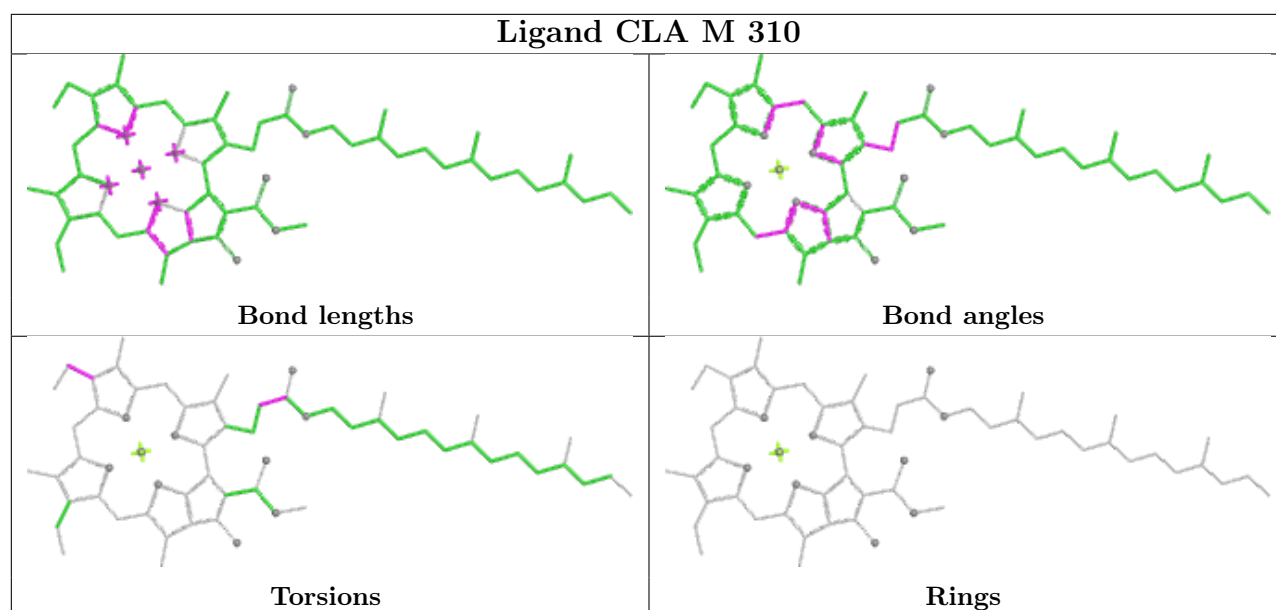


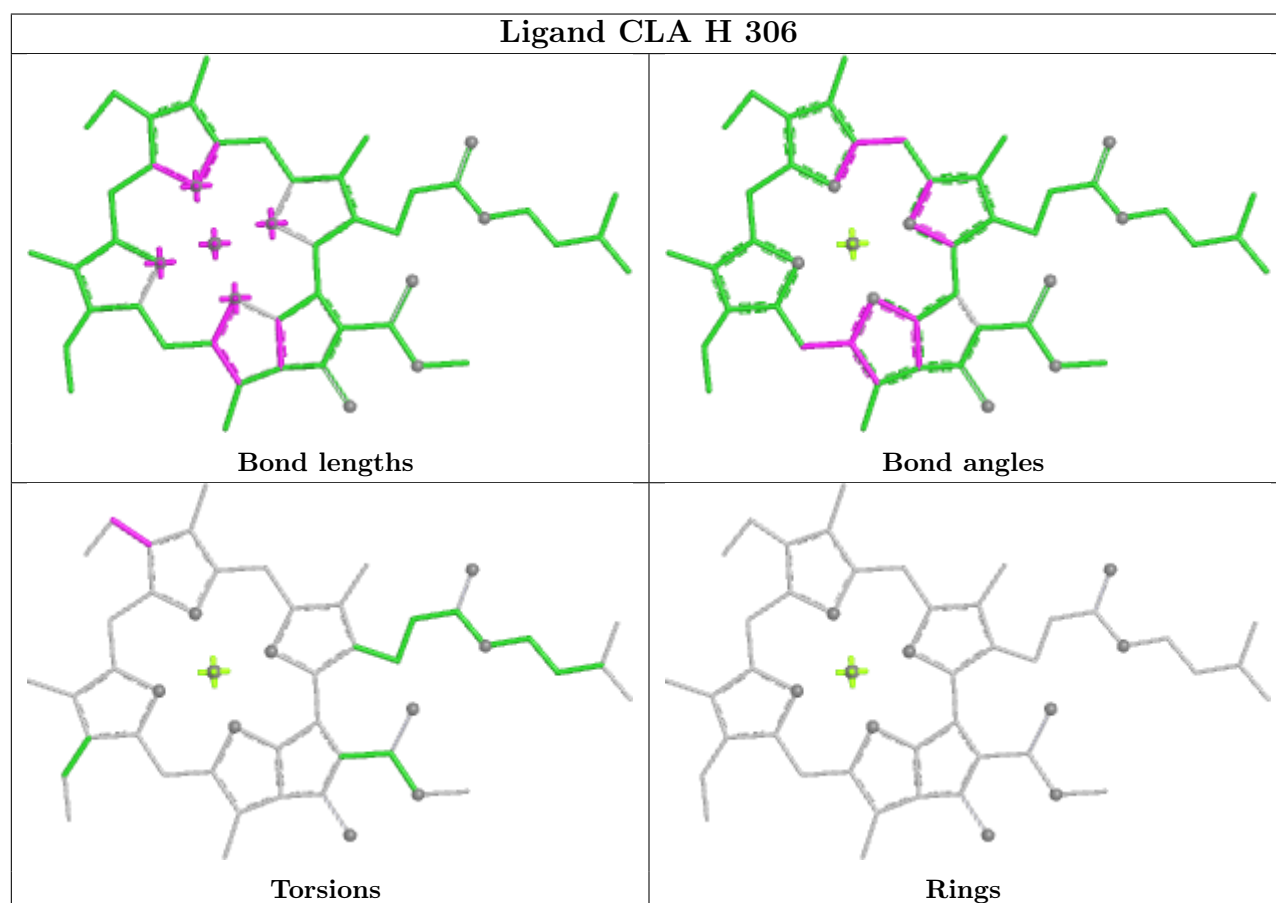
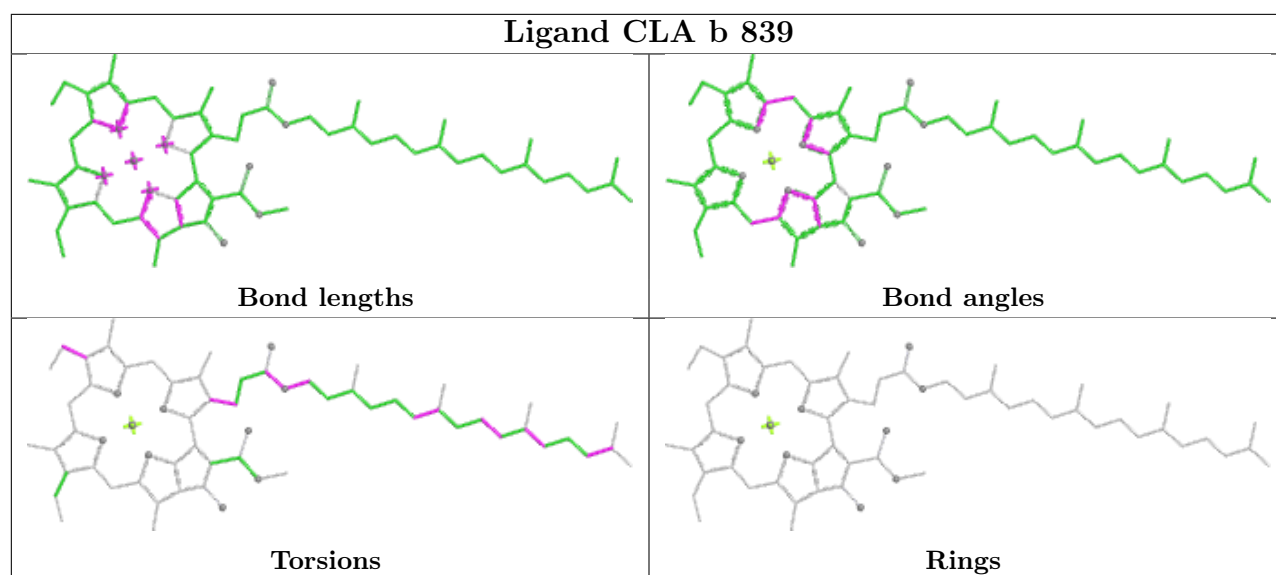
Ligand CLA T 309

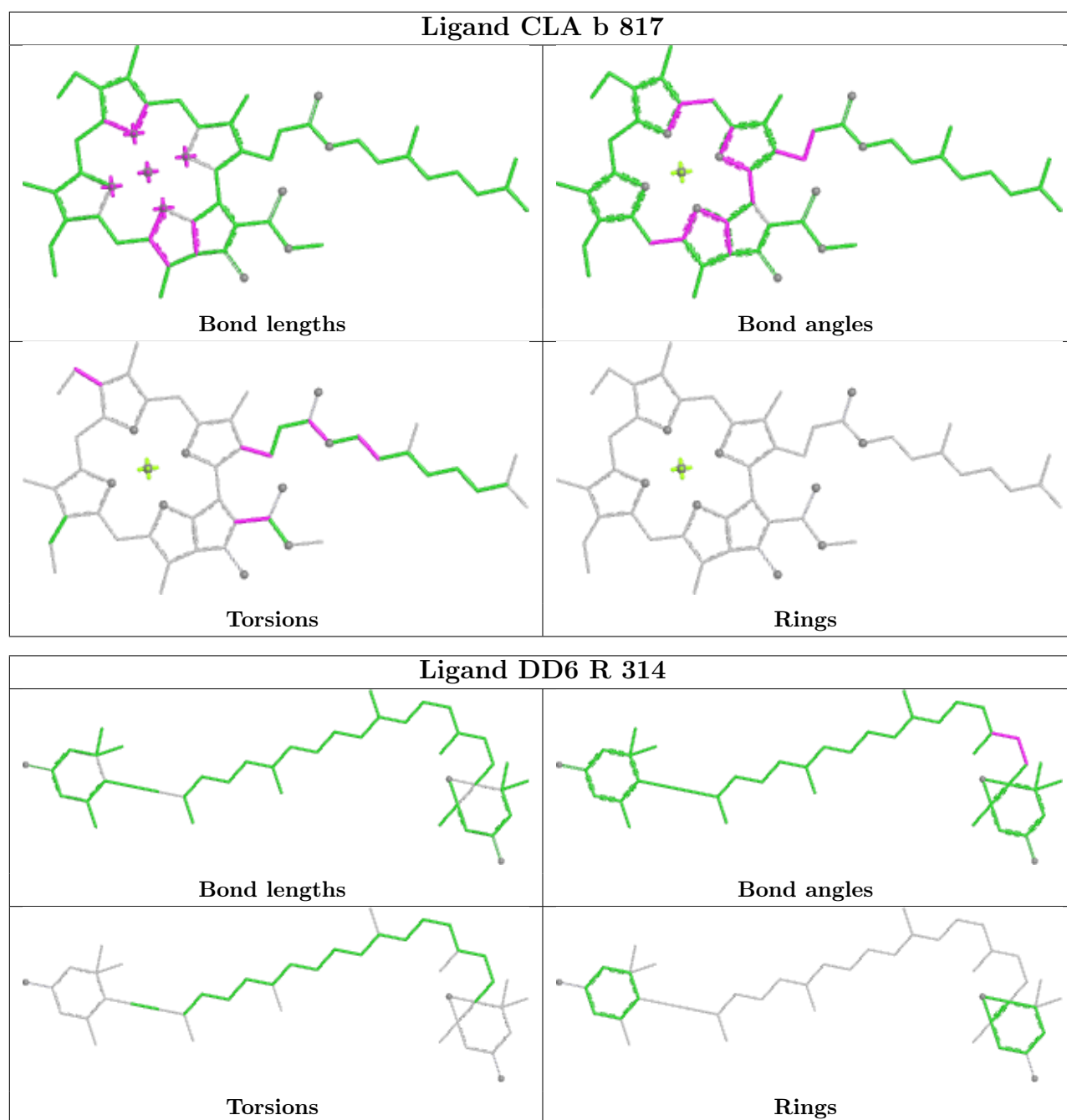




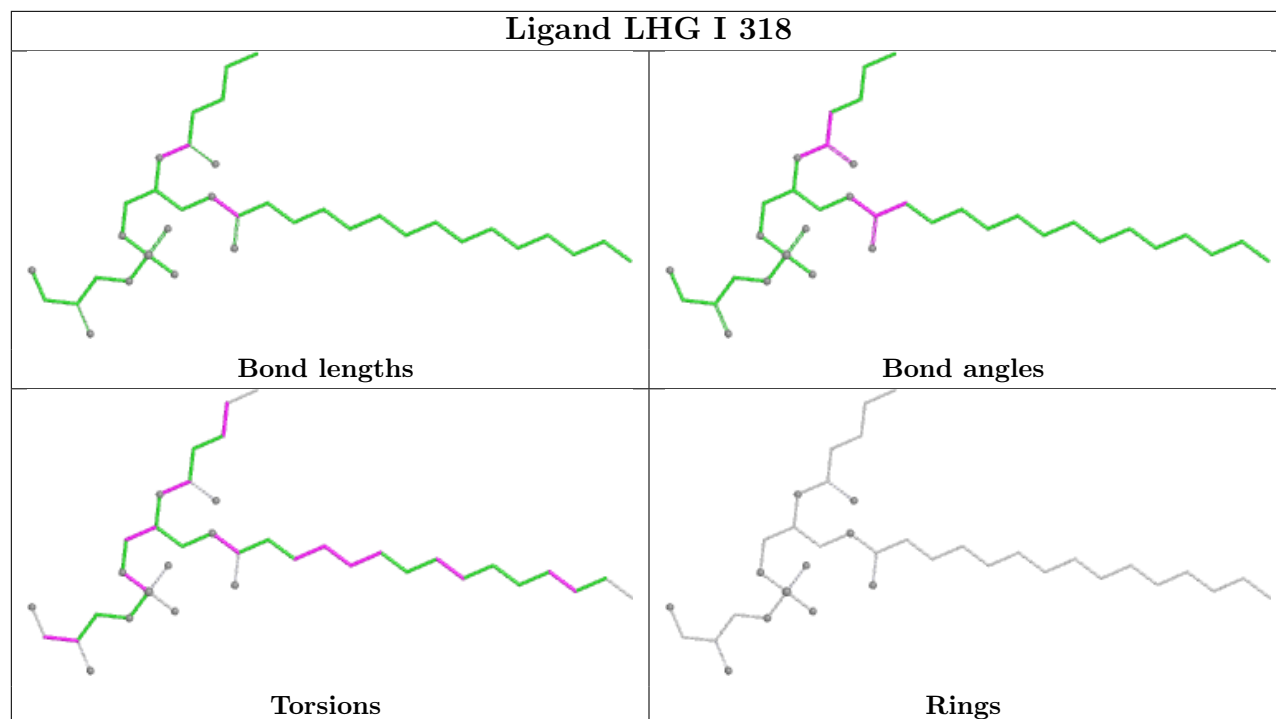




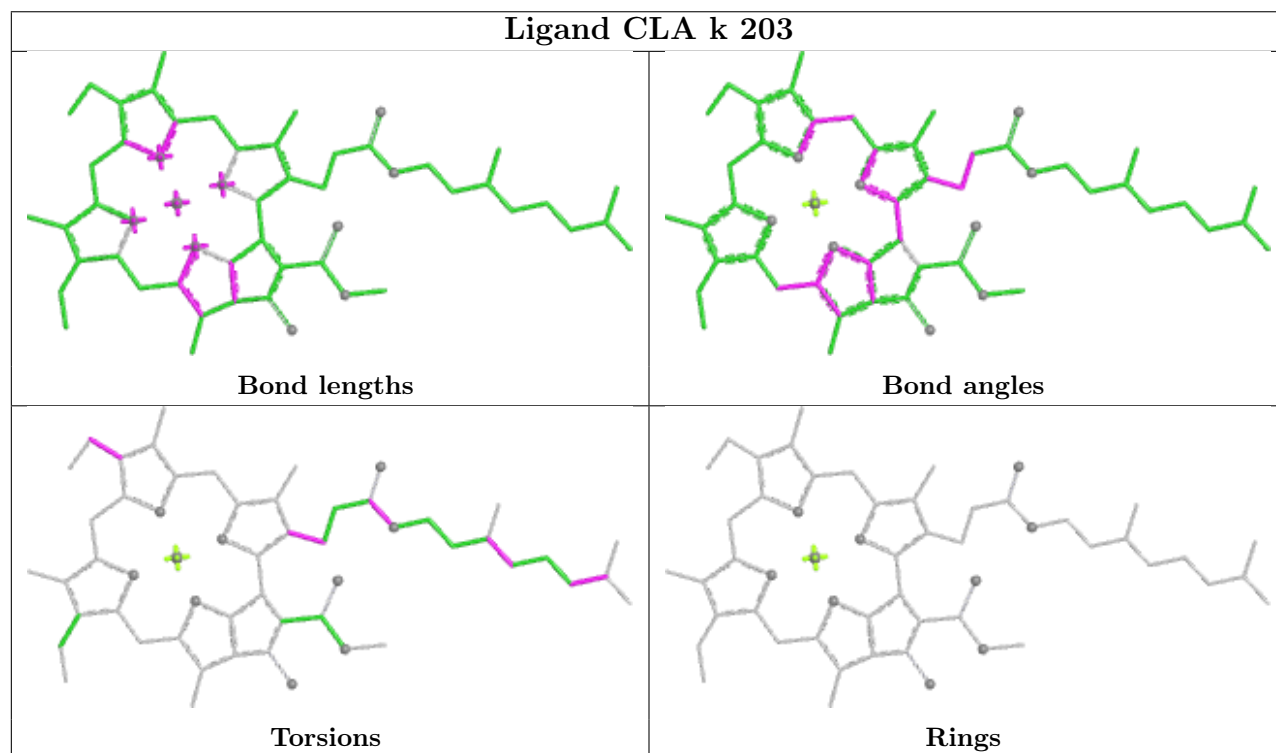




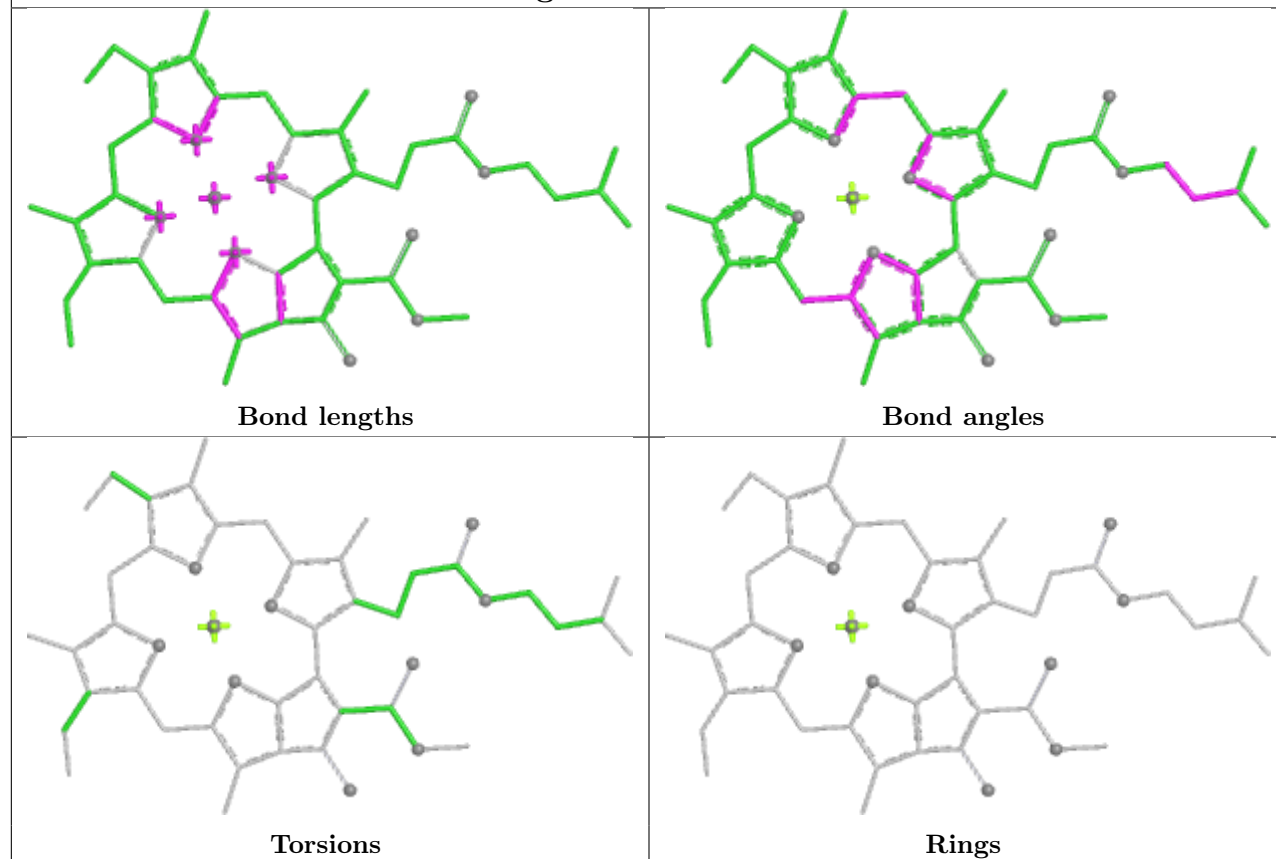
Ligand LHG I 318



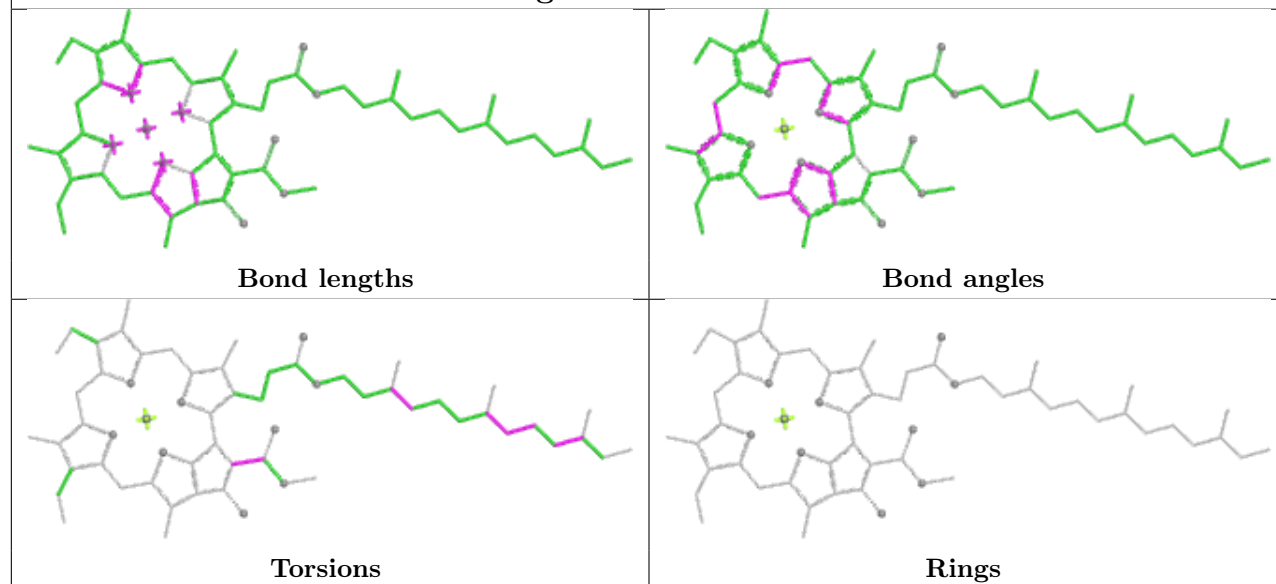
Ligand CLA k 203

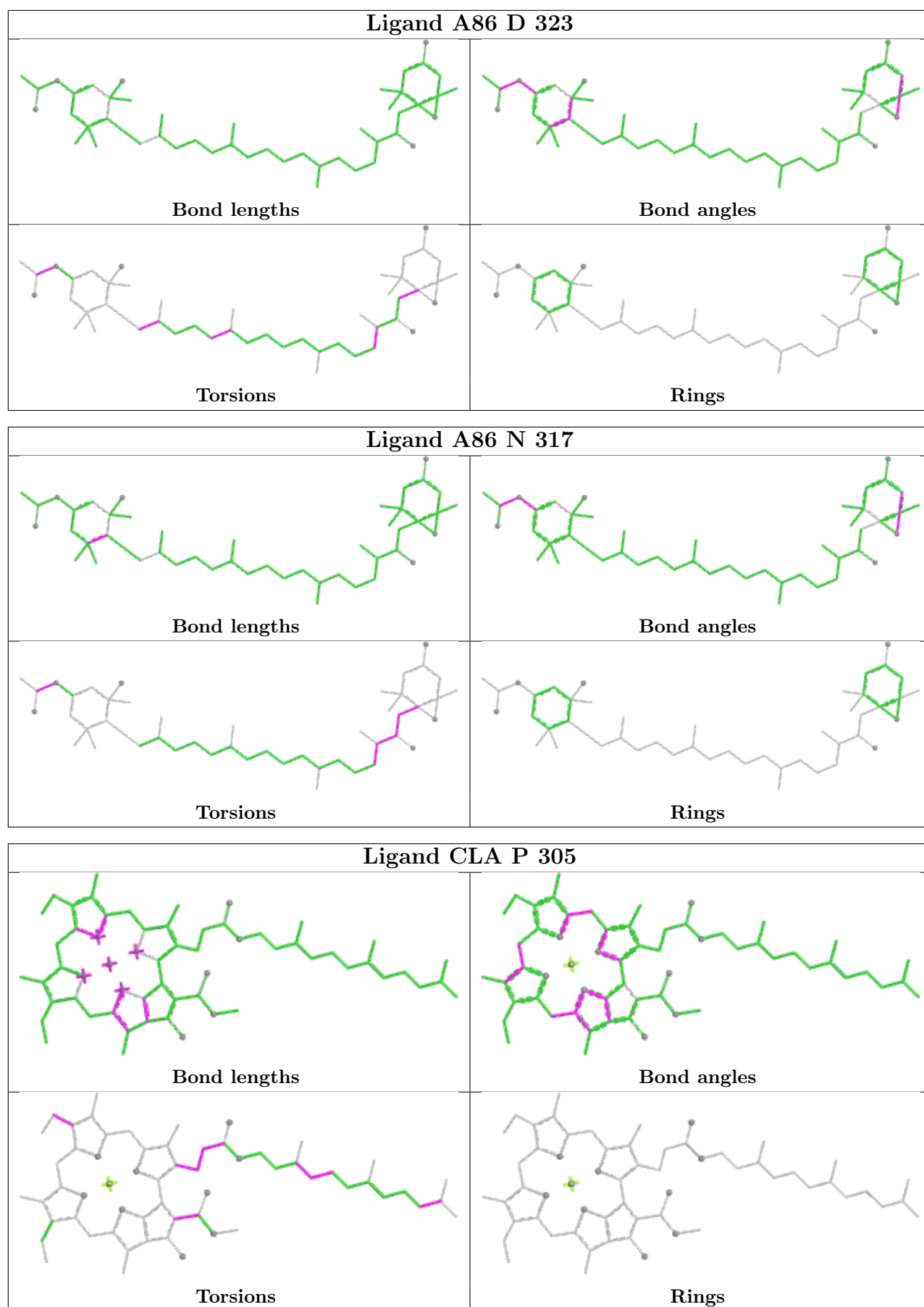


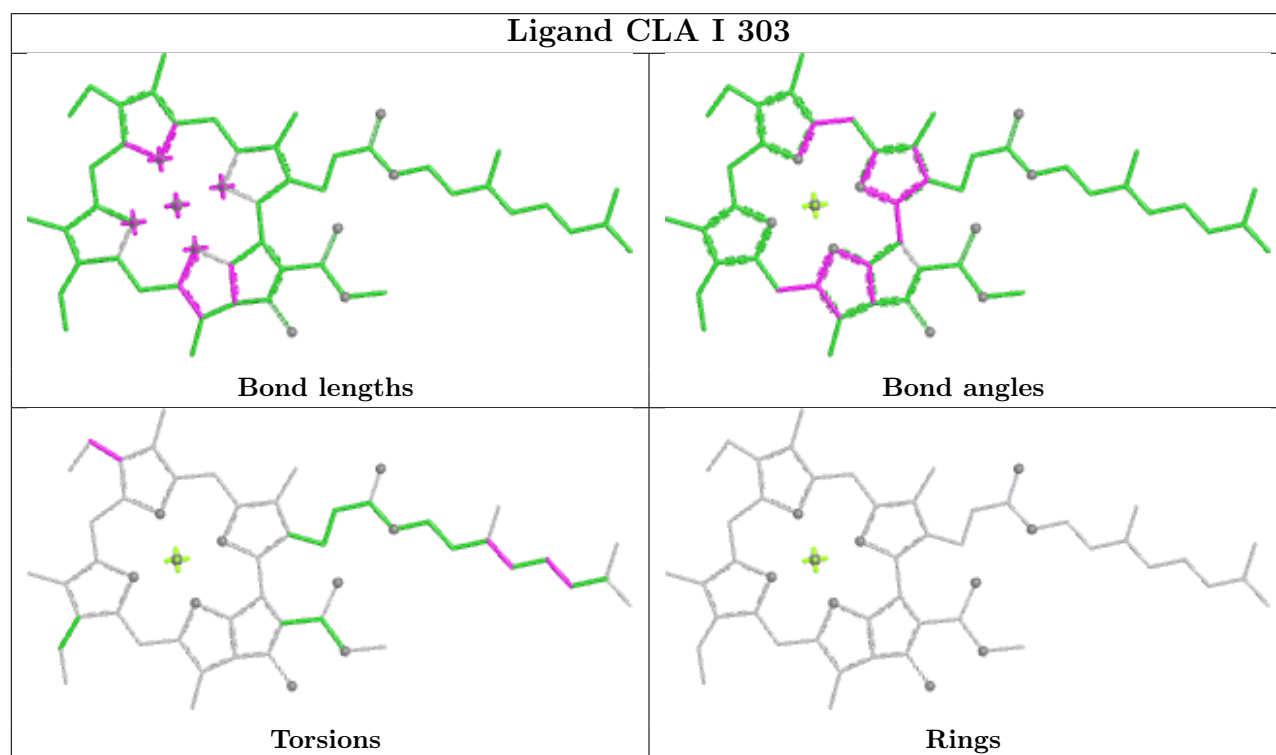
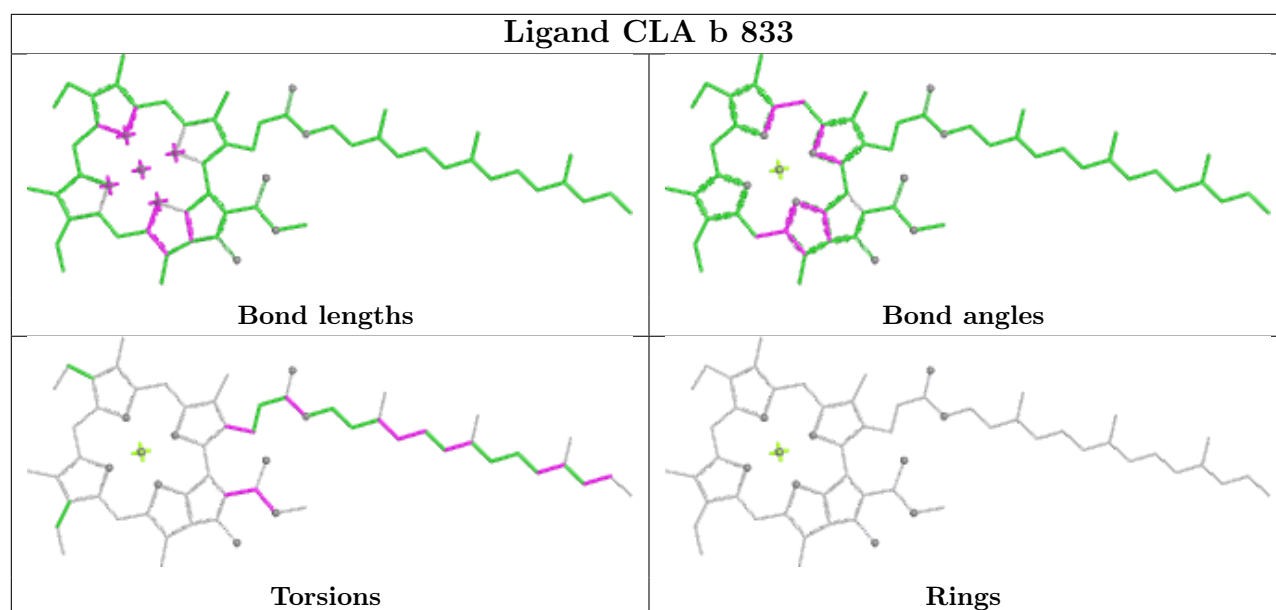
Ligand CLA a 815



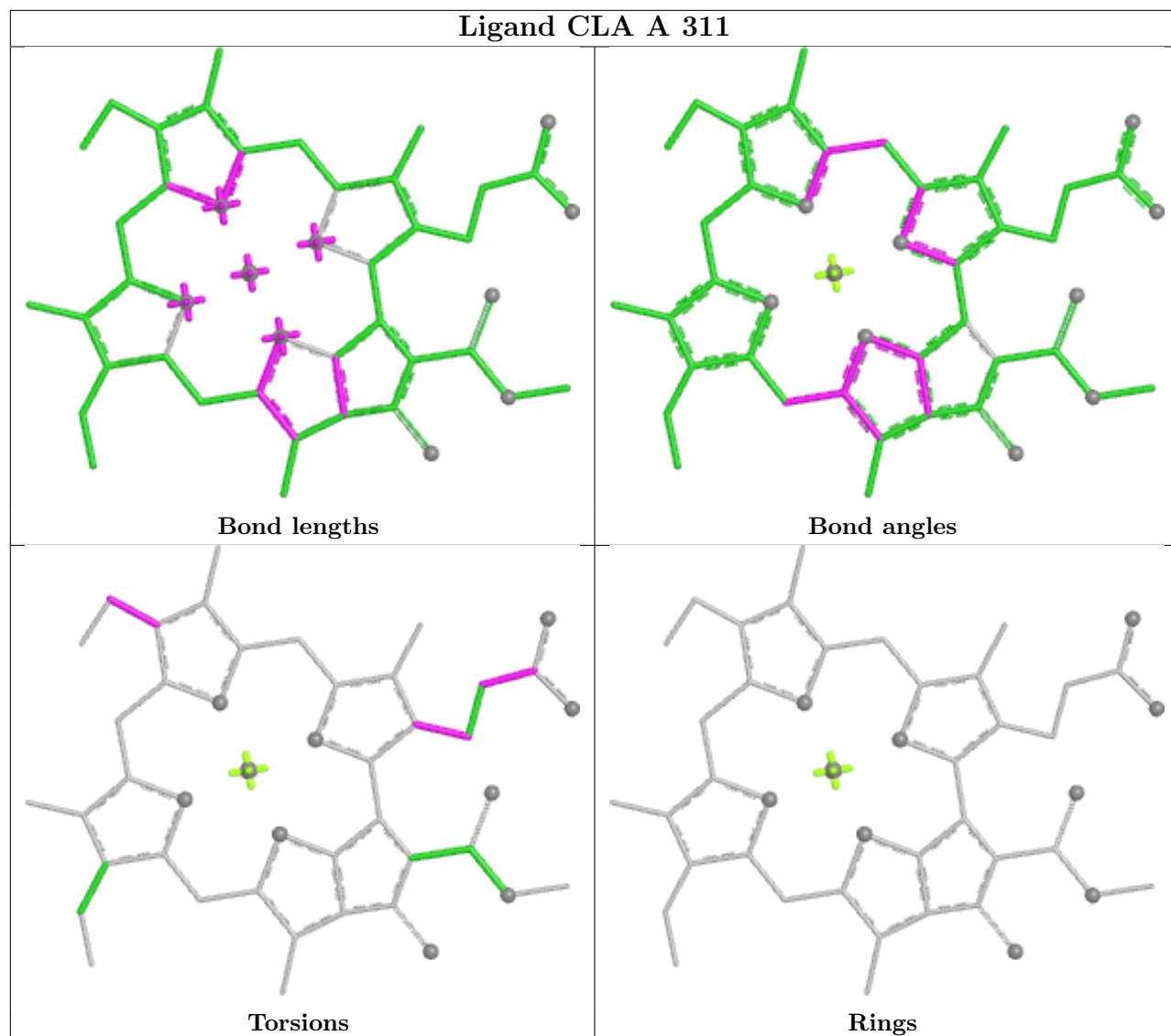
Ligand CLA a 817



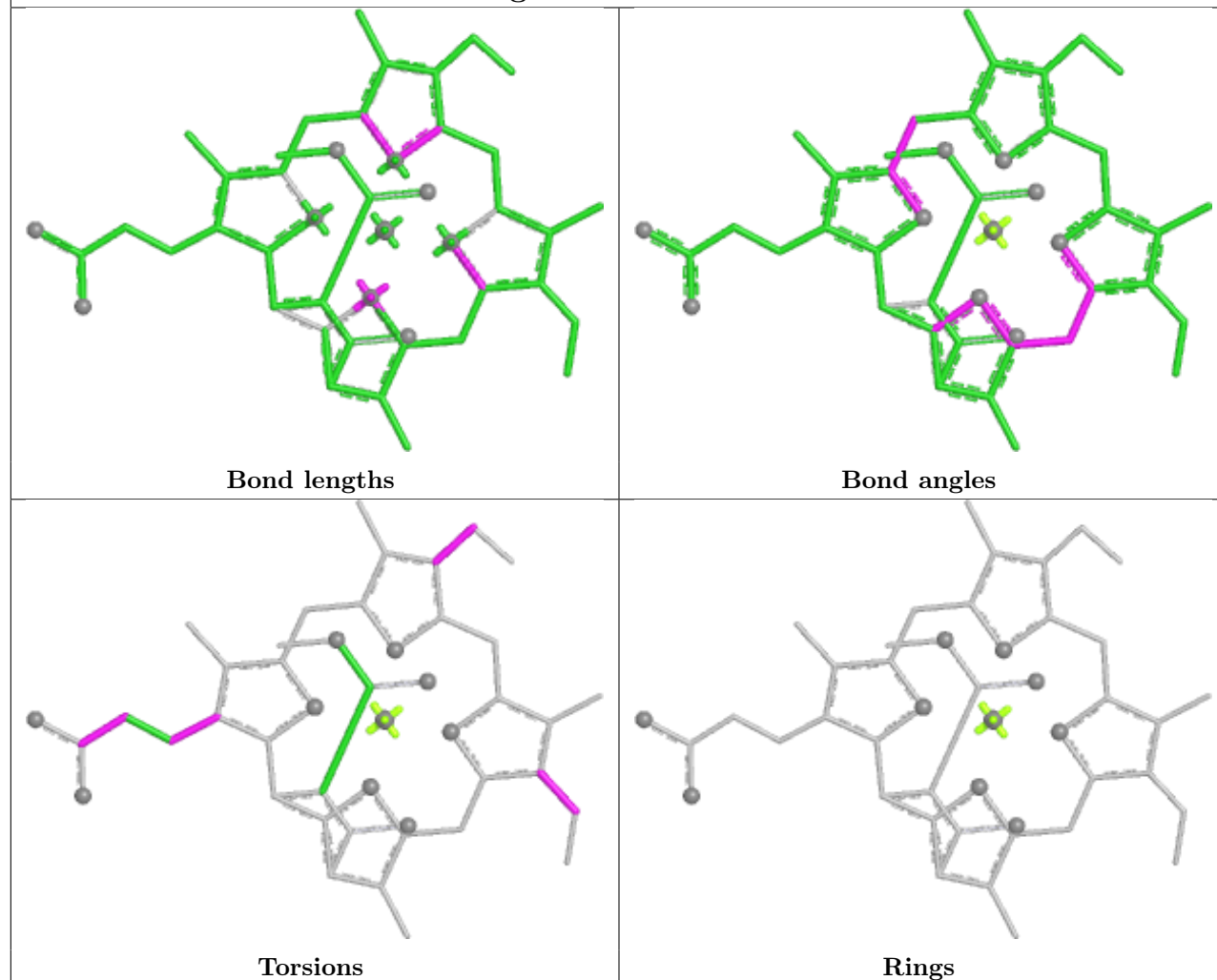




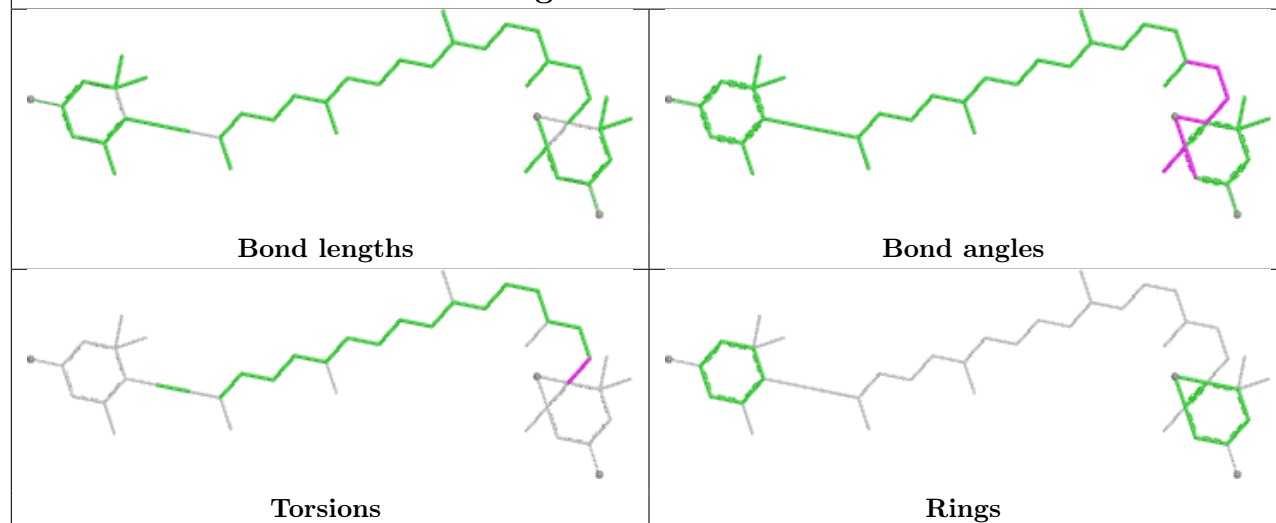
Ligand CLA A 311



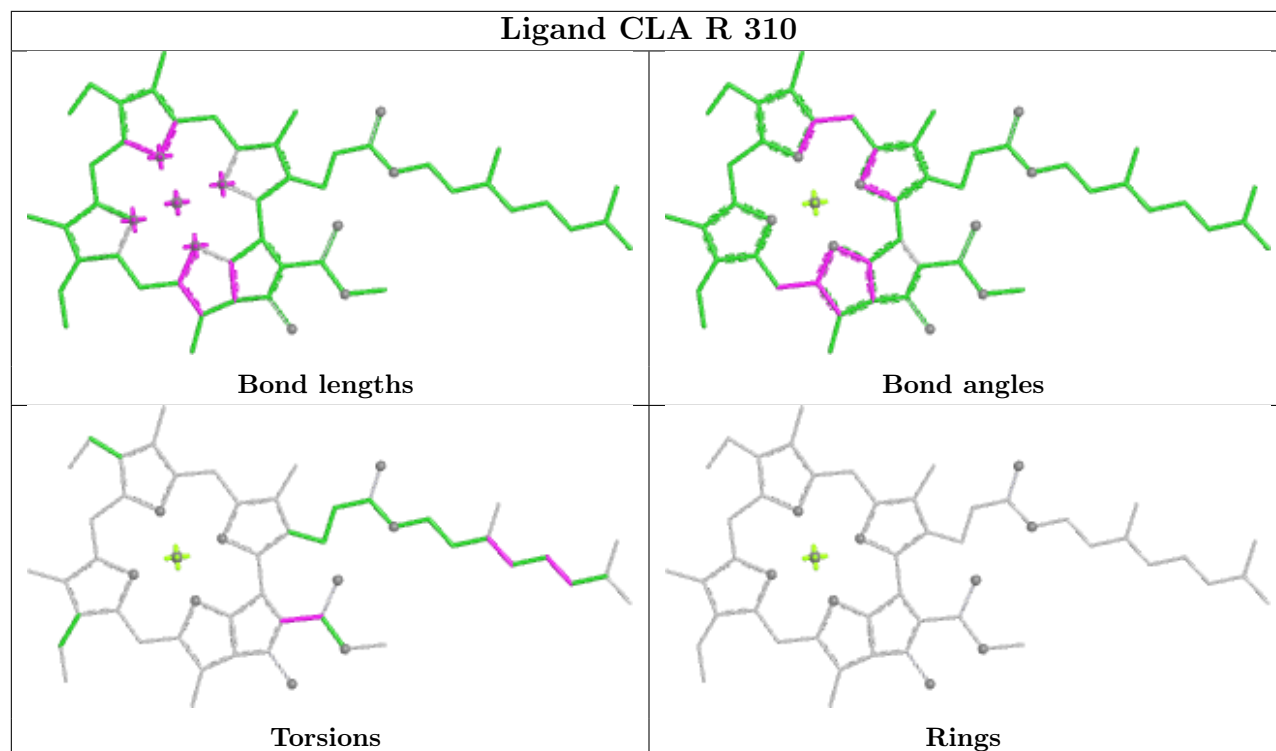
Ligand KC2 P 301



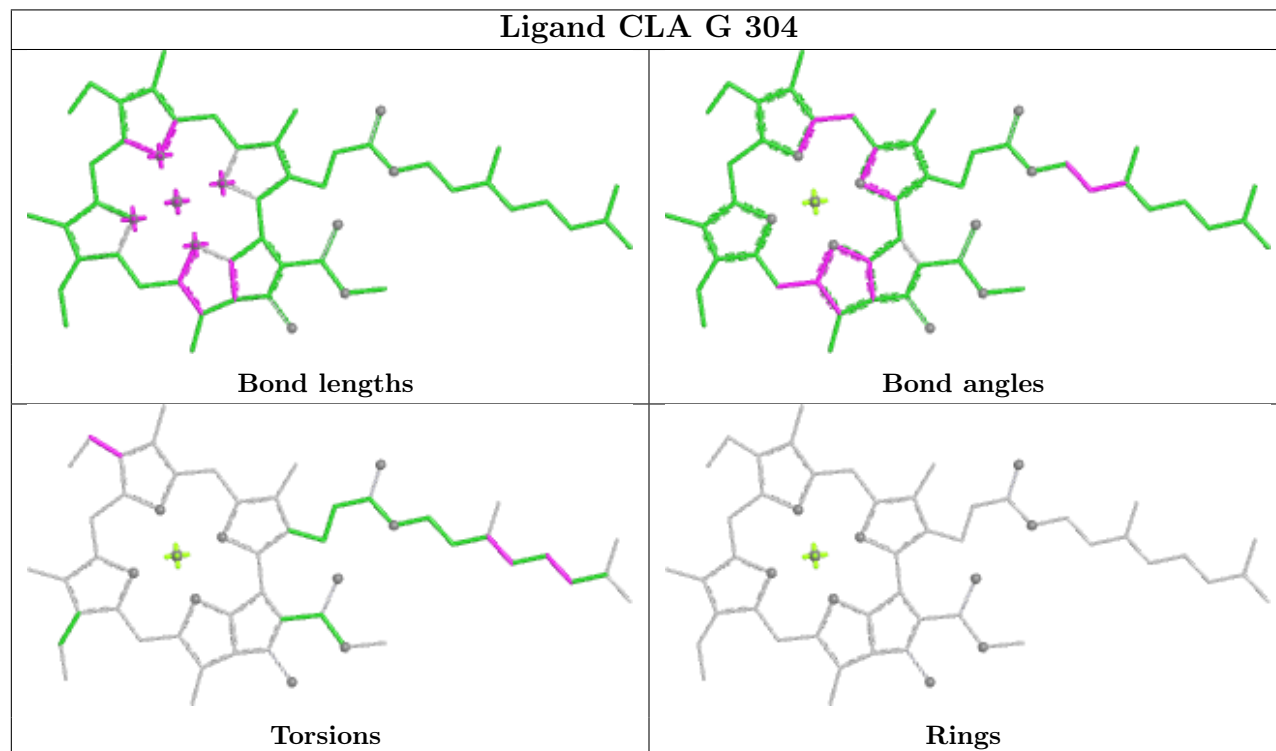
Ligand DD6 L 319



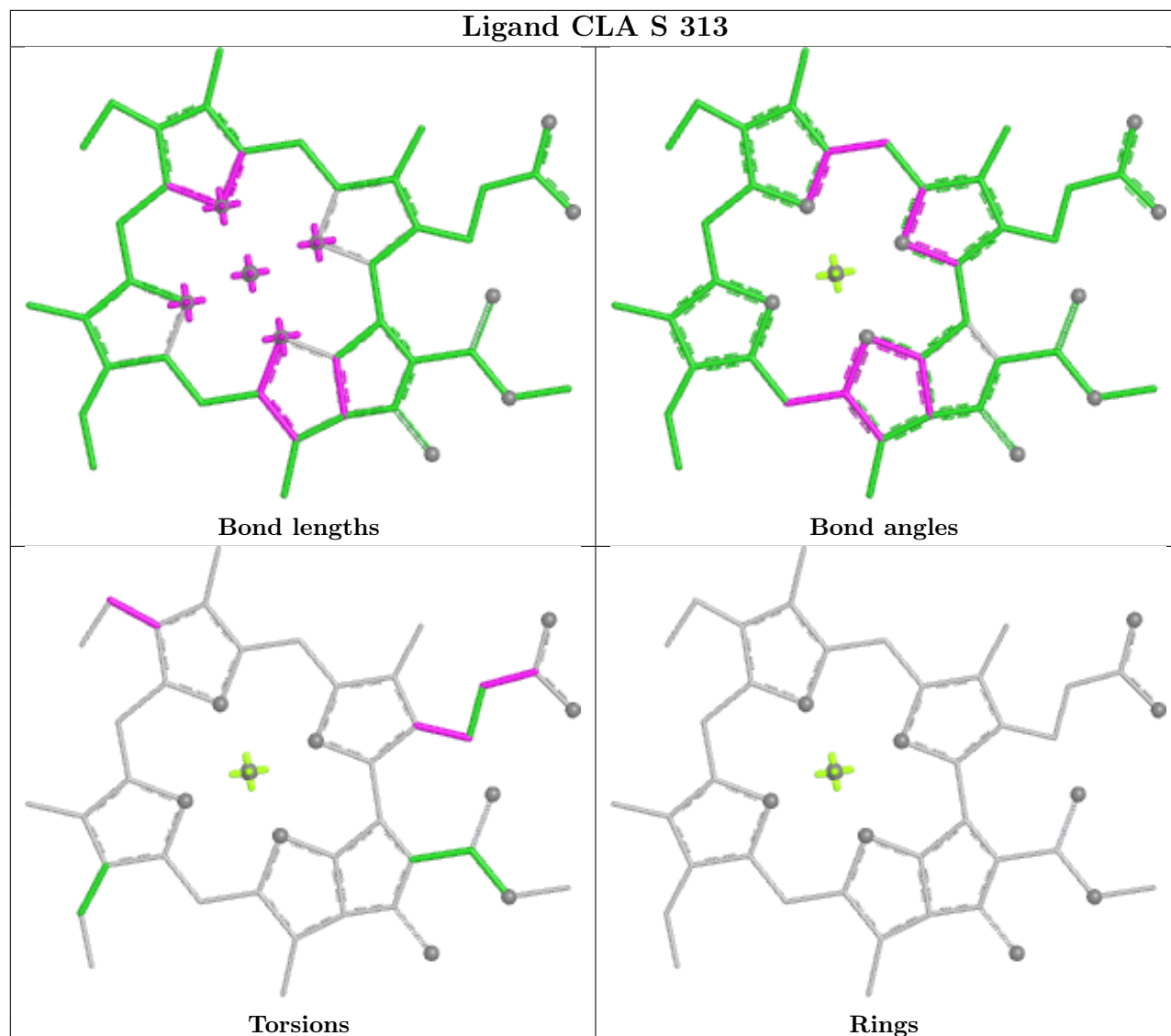
Ligand CLA R 310



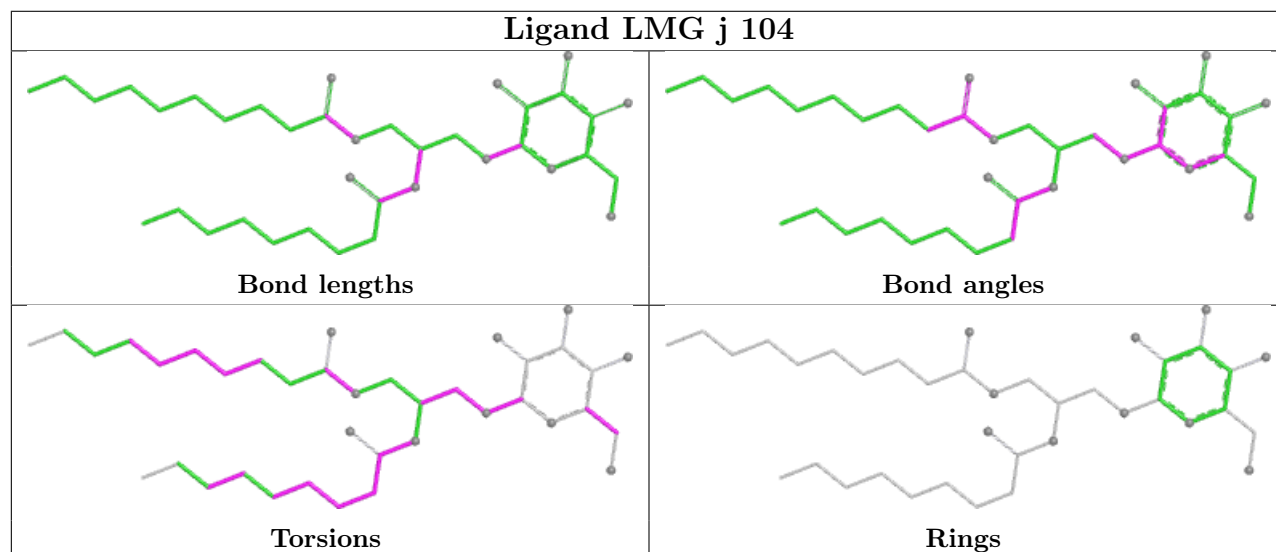
Ligand CLA G 304



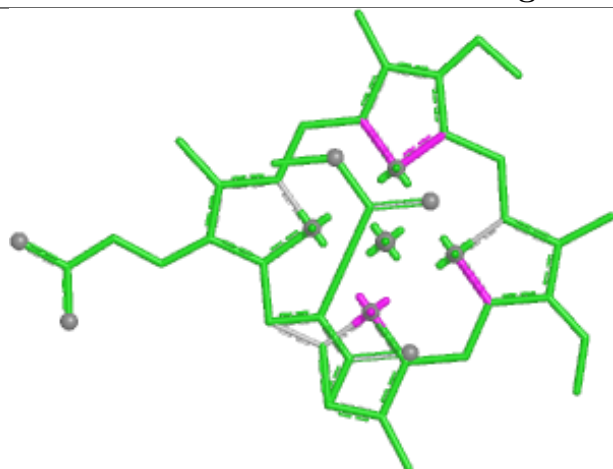
Ligand CLA S 313



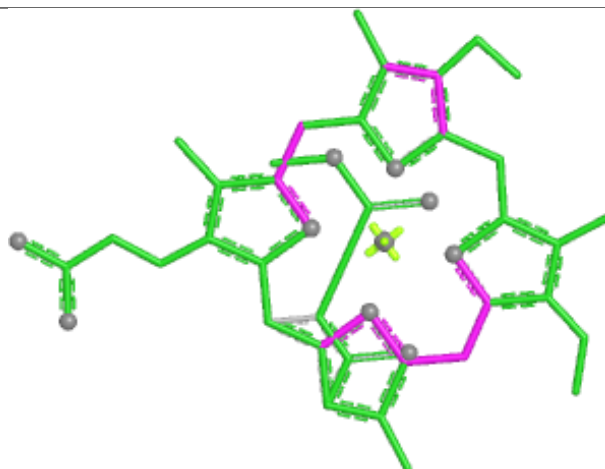
Ligand LMG j 104



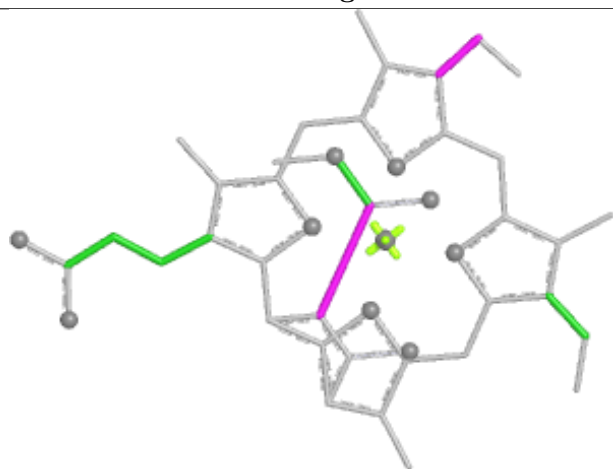
Ligand KC2 L 303



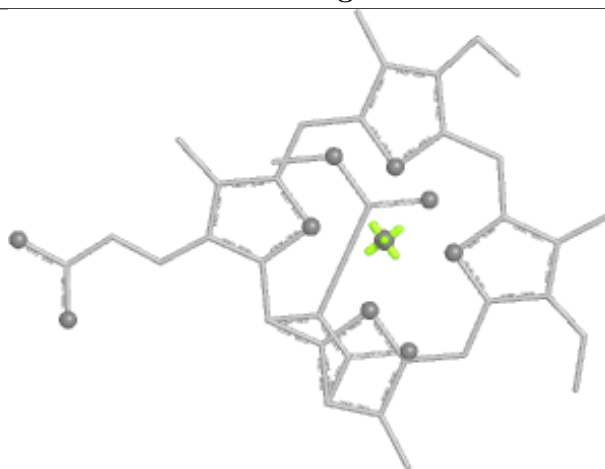
Bond lengths



Bond angles

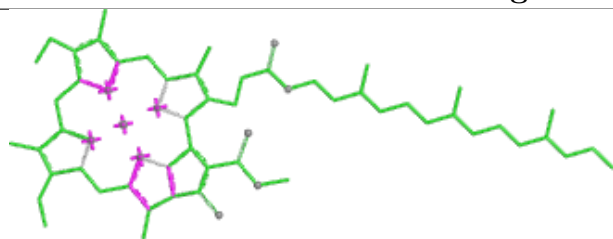


Torsions

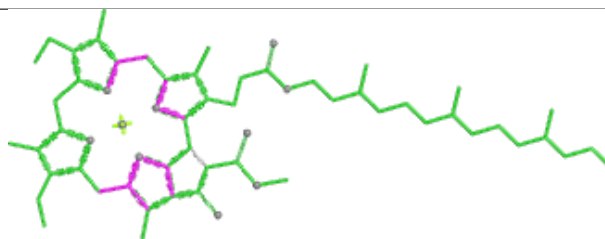


Rings

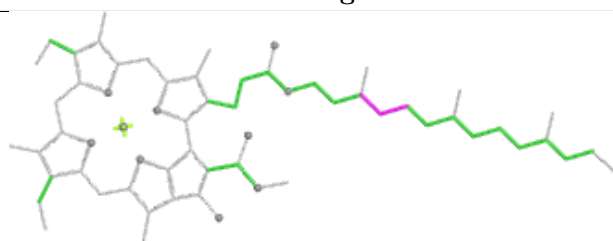
Ligand CLA M 306



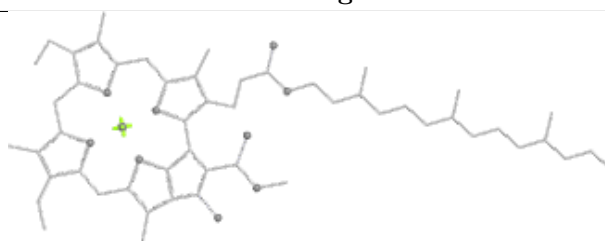
Bond lengths



Bond angles

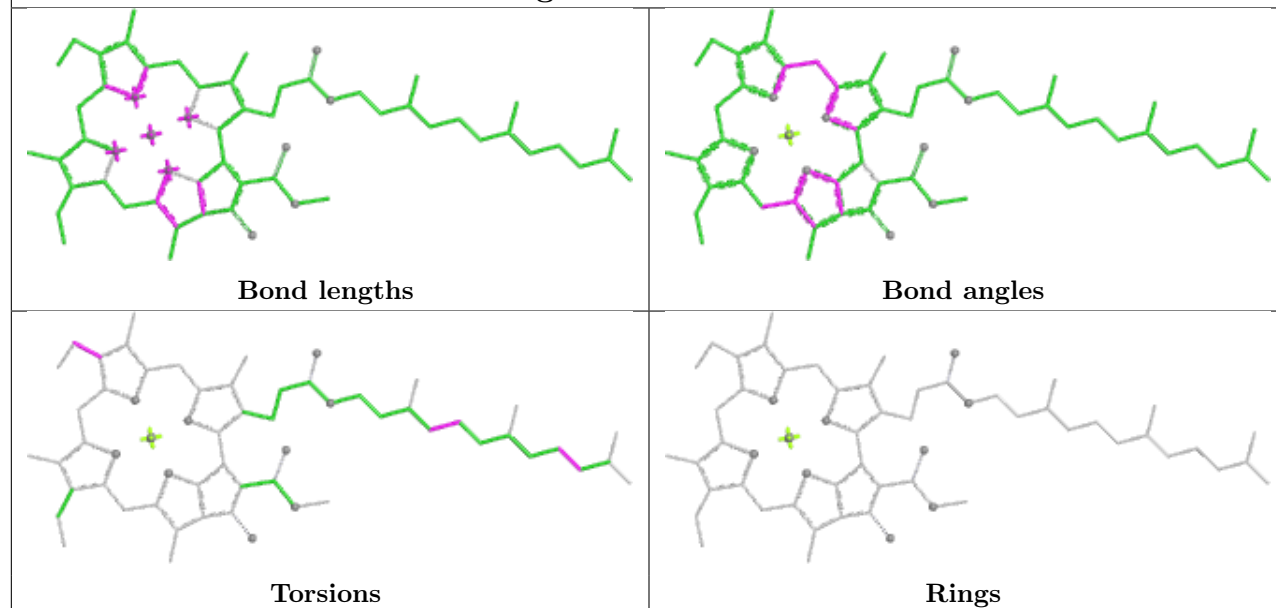


Torsions

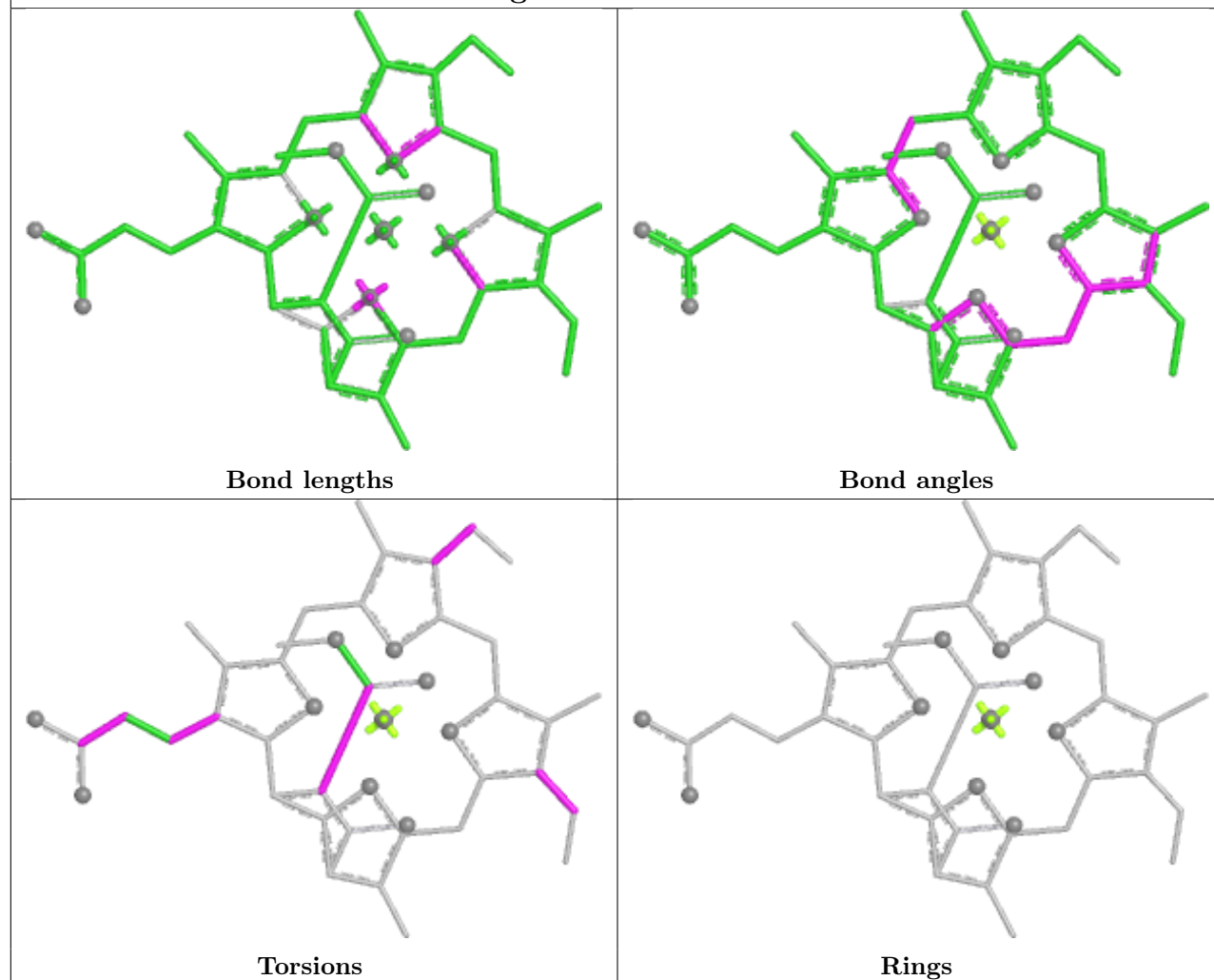


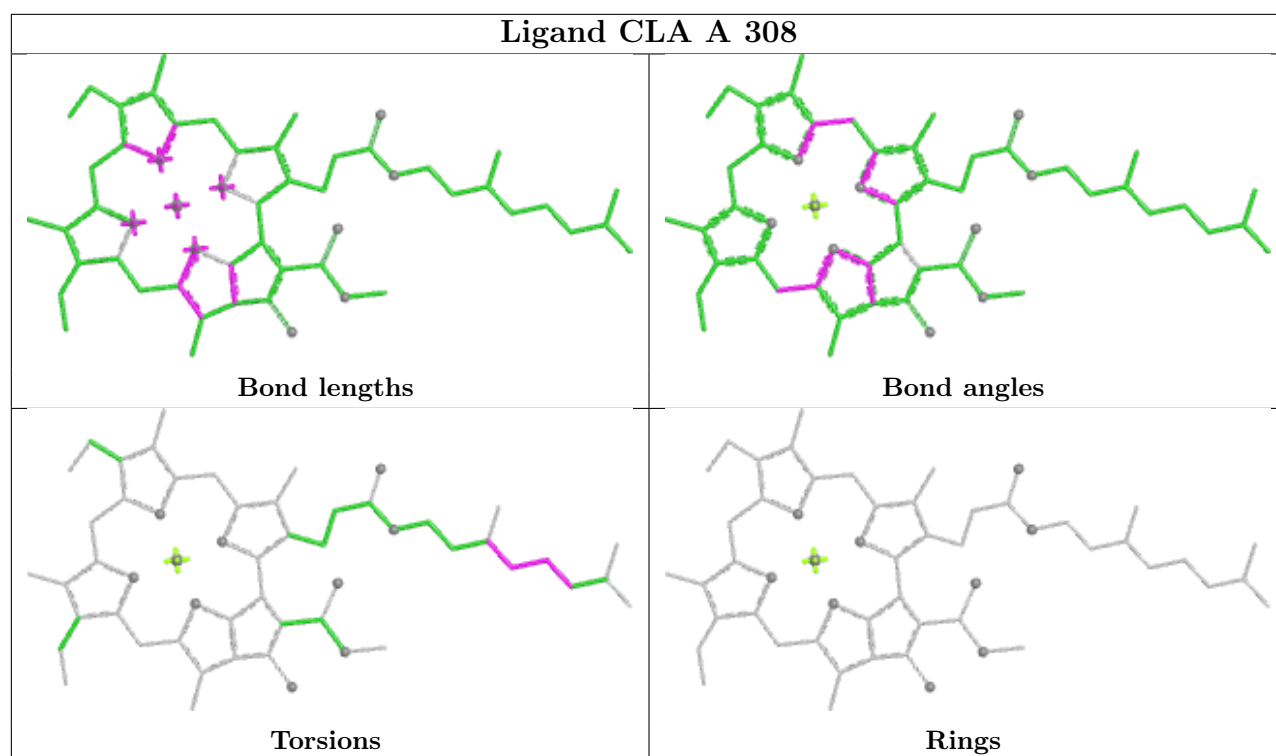
Rings

Ligand CLA a 831

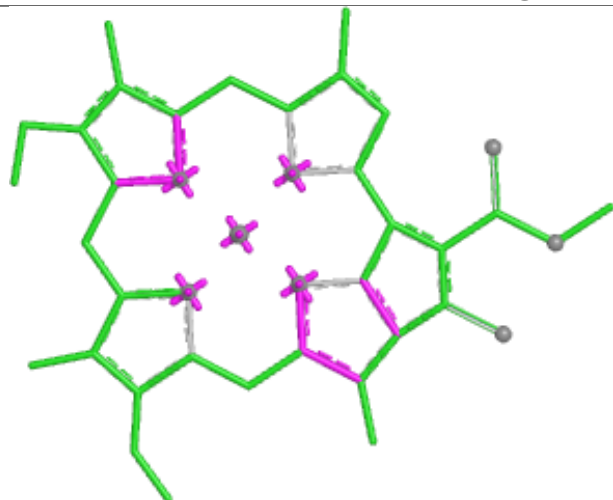


Ligand KC2 L 305

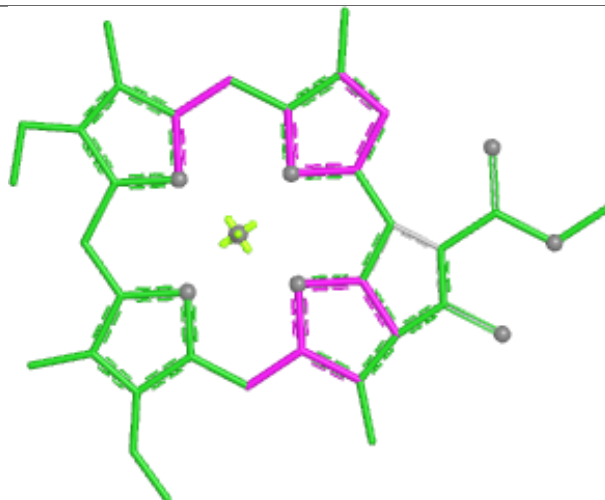




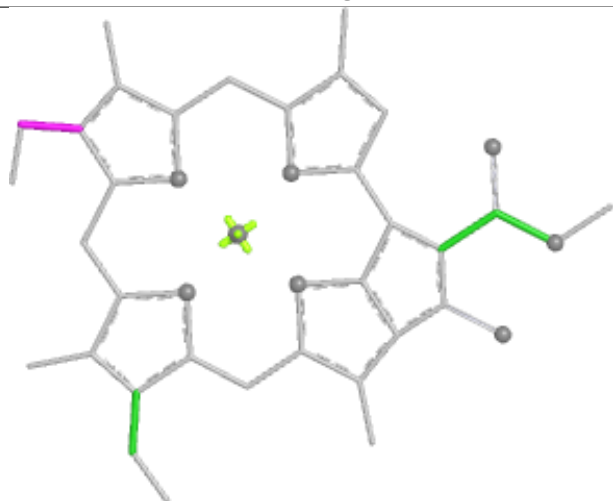
Ligand CLA F 301



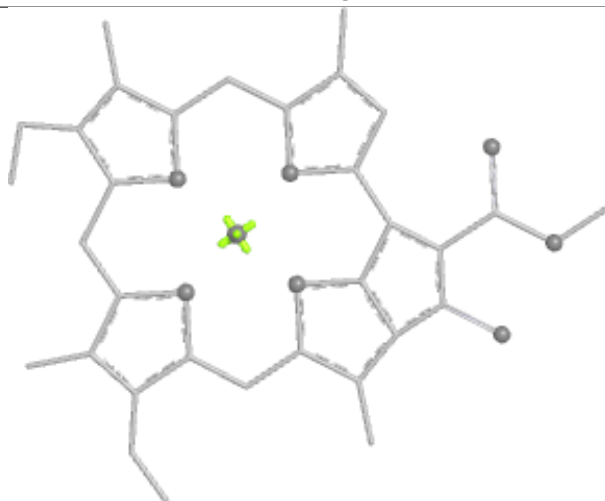
Bond lengths



Bond angles

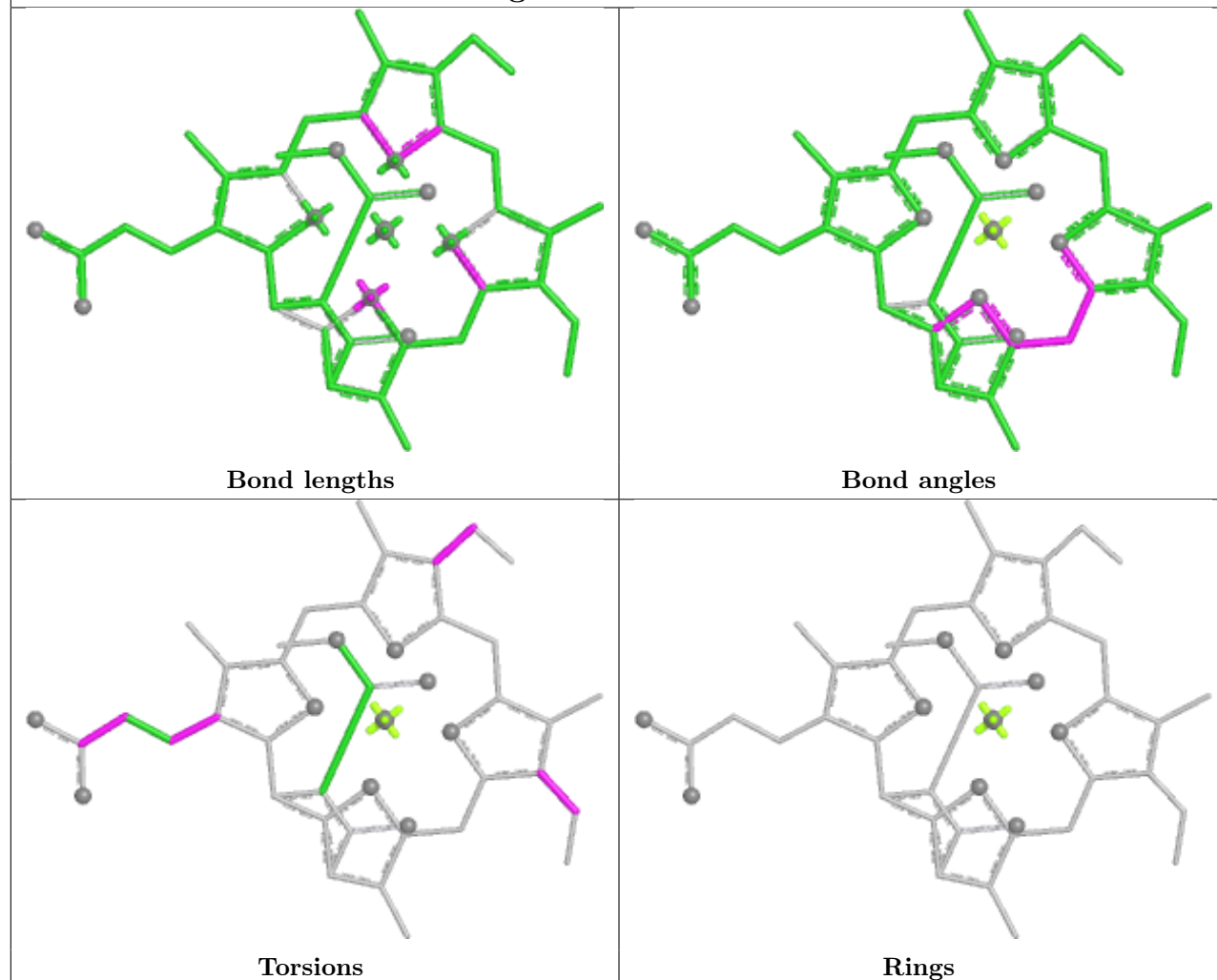


Torsions

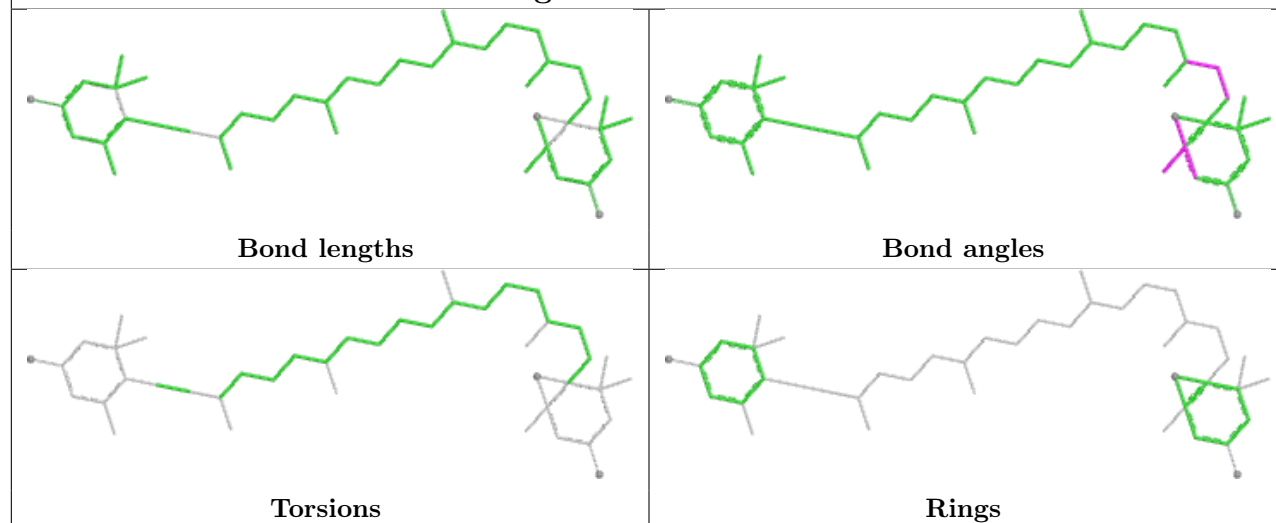


Rings

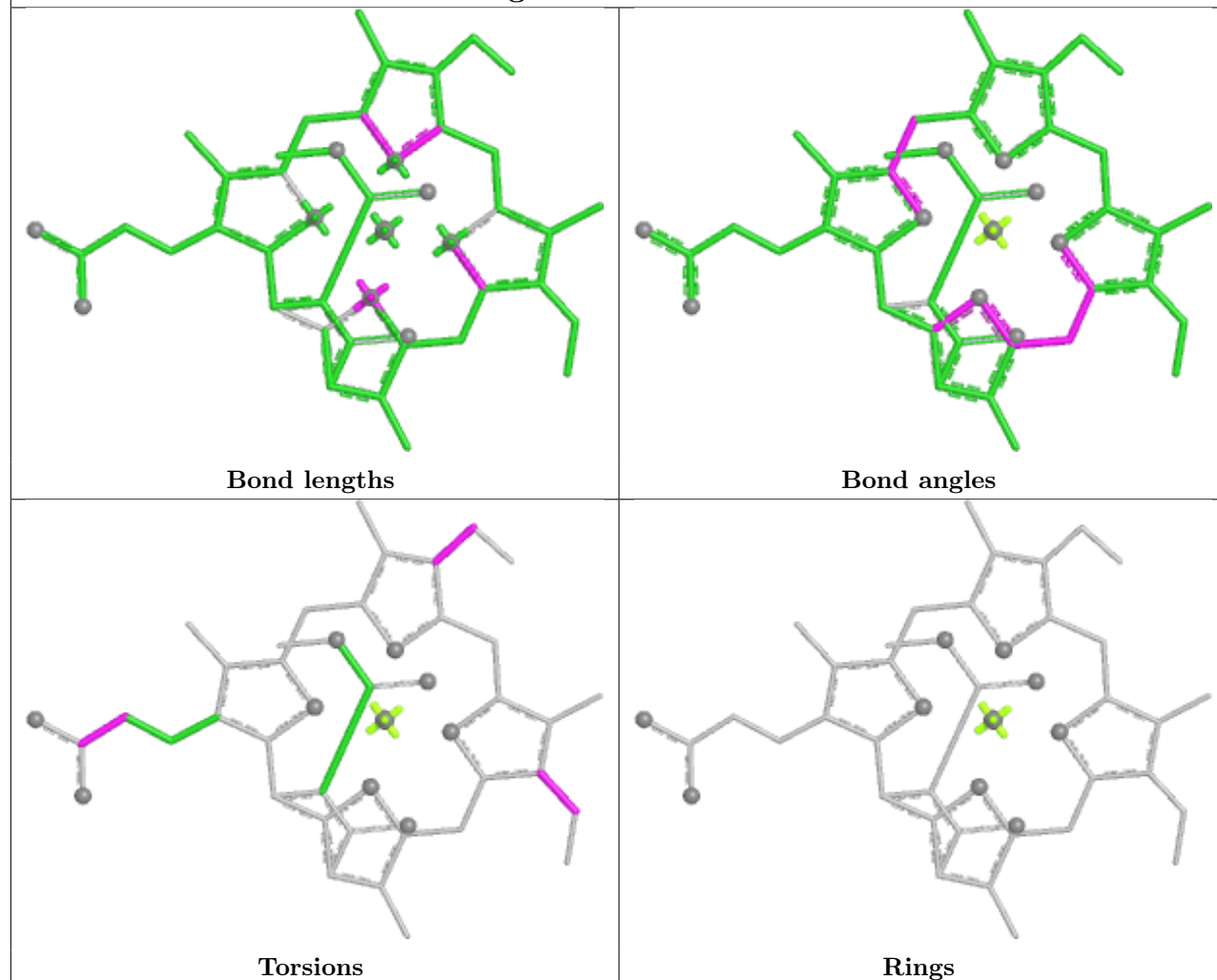
Ligand KC2 R 305



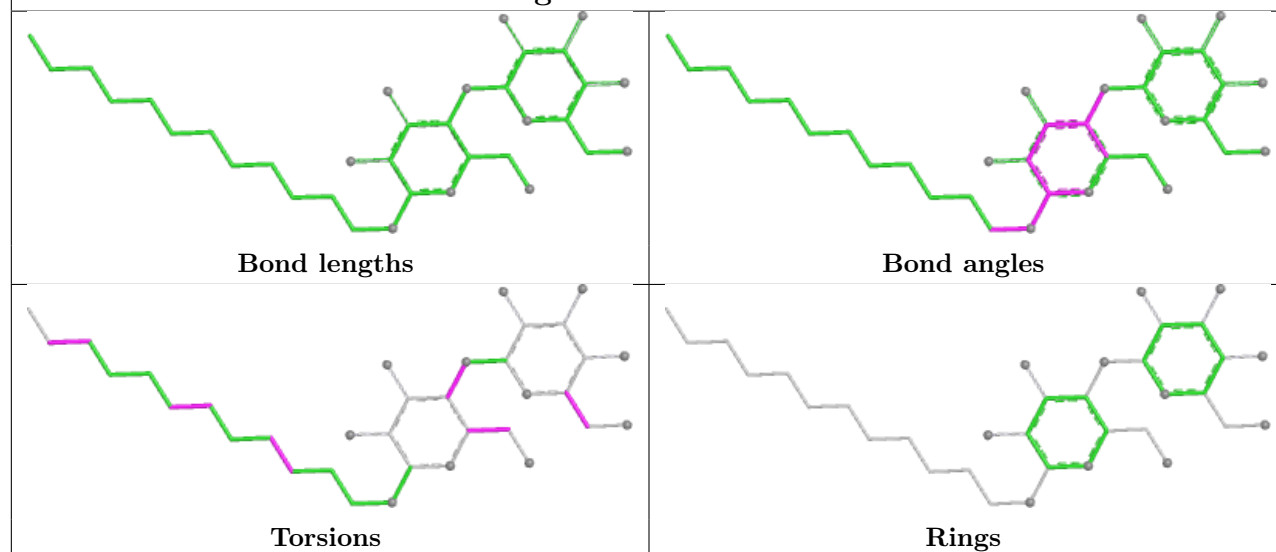
Ligand DD6 E 317



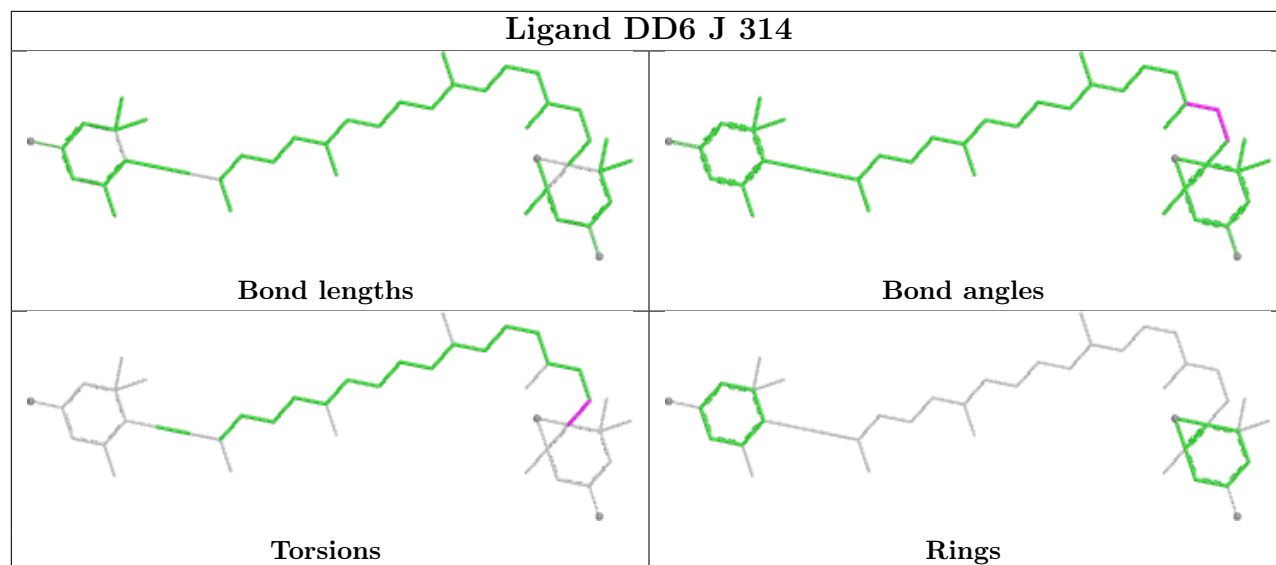
Ligand KC2 K 302



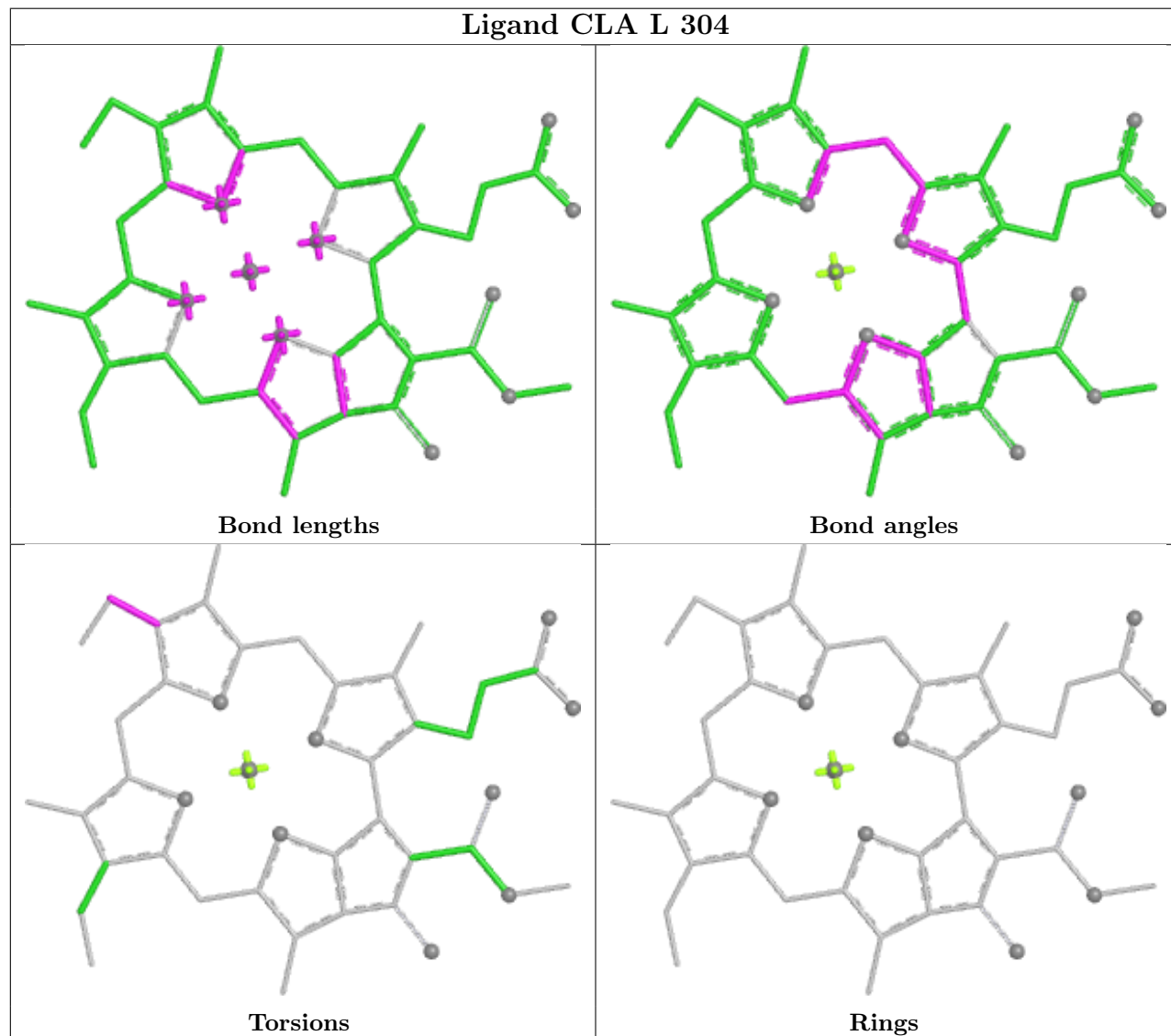
Ligand LMU I 315

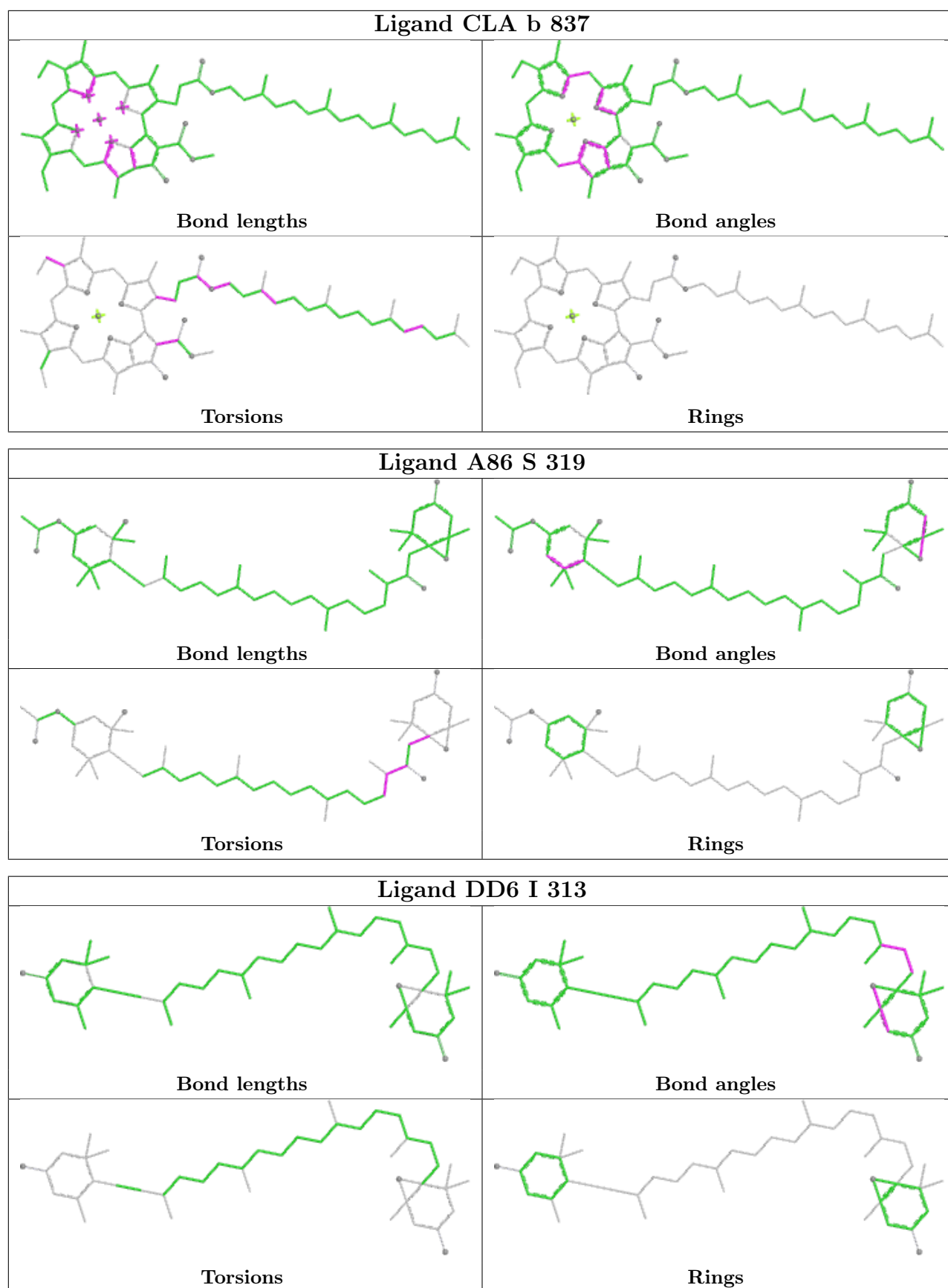


Ligand DD6 J 314

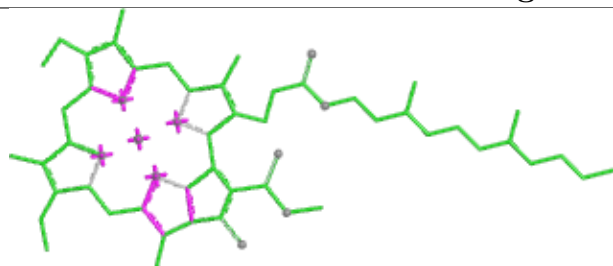


Ligand CLA L 304

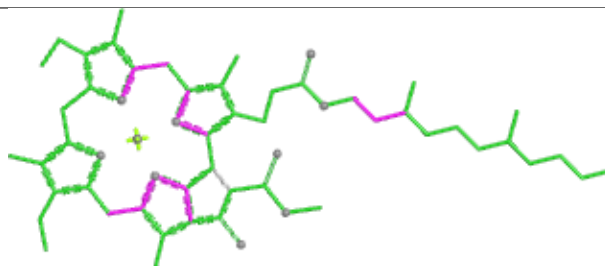




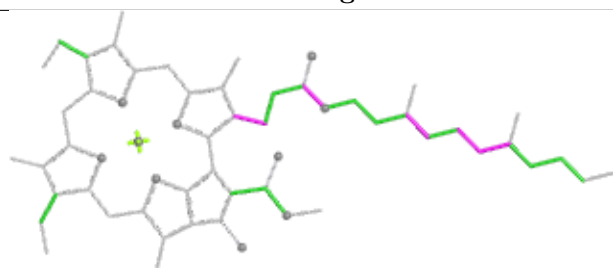
Ligand CLA b 824



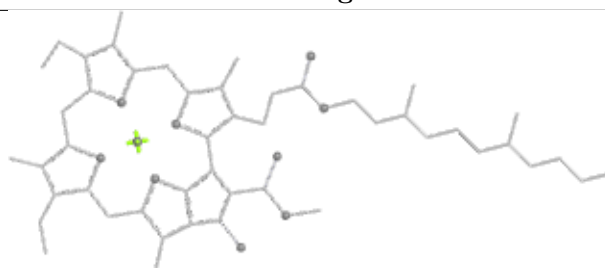
Bond lengths



Bond angles

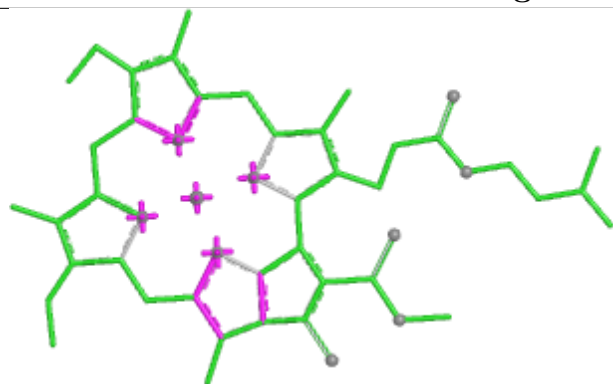


Torsions

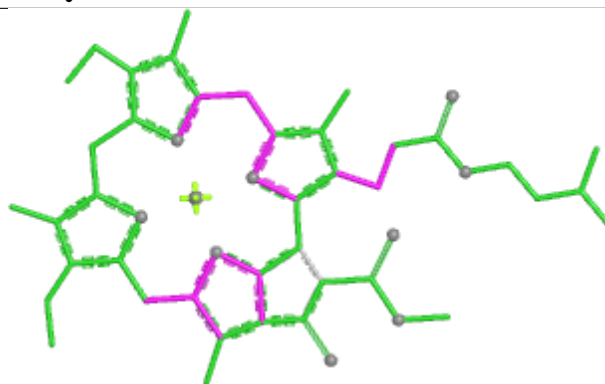


Rings

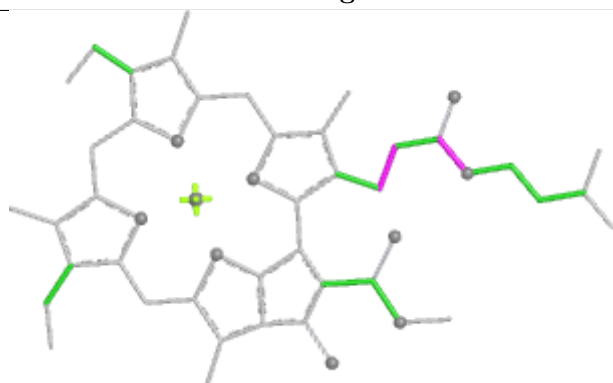
Ligand CLA Q 304



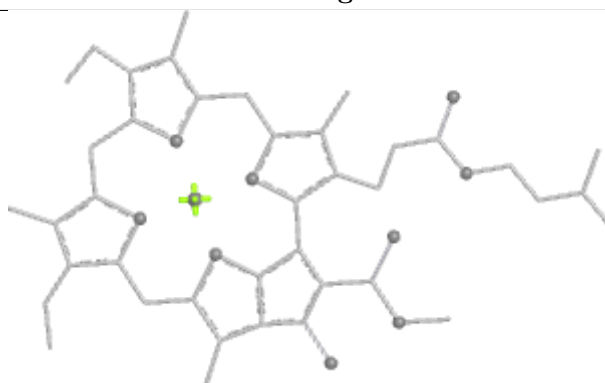
Bond lengths



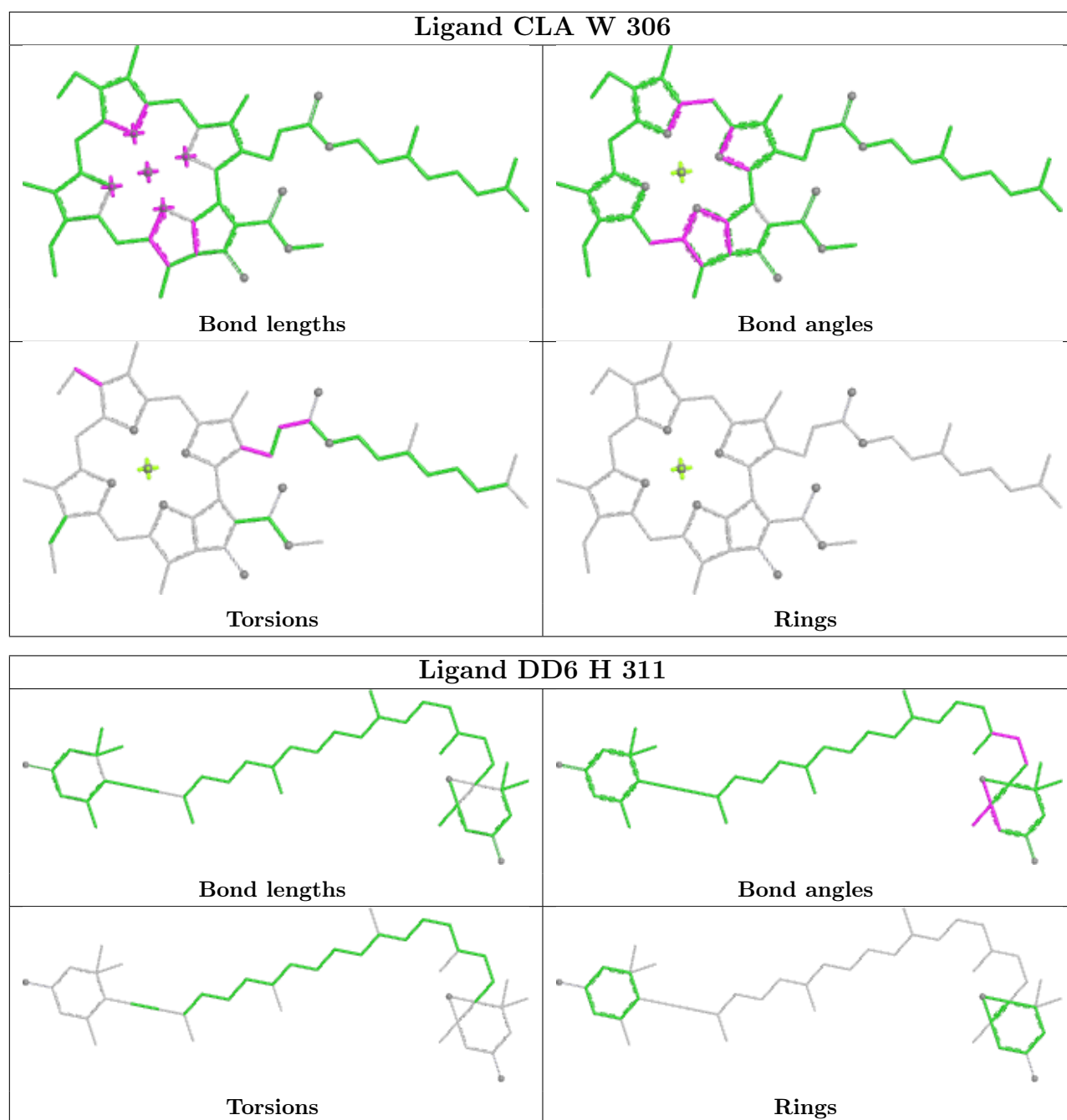
Bond angles

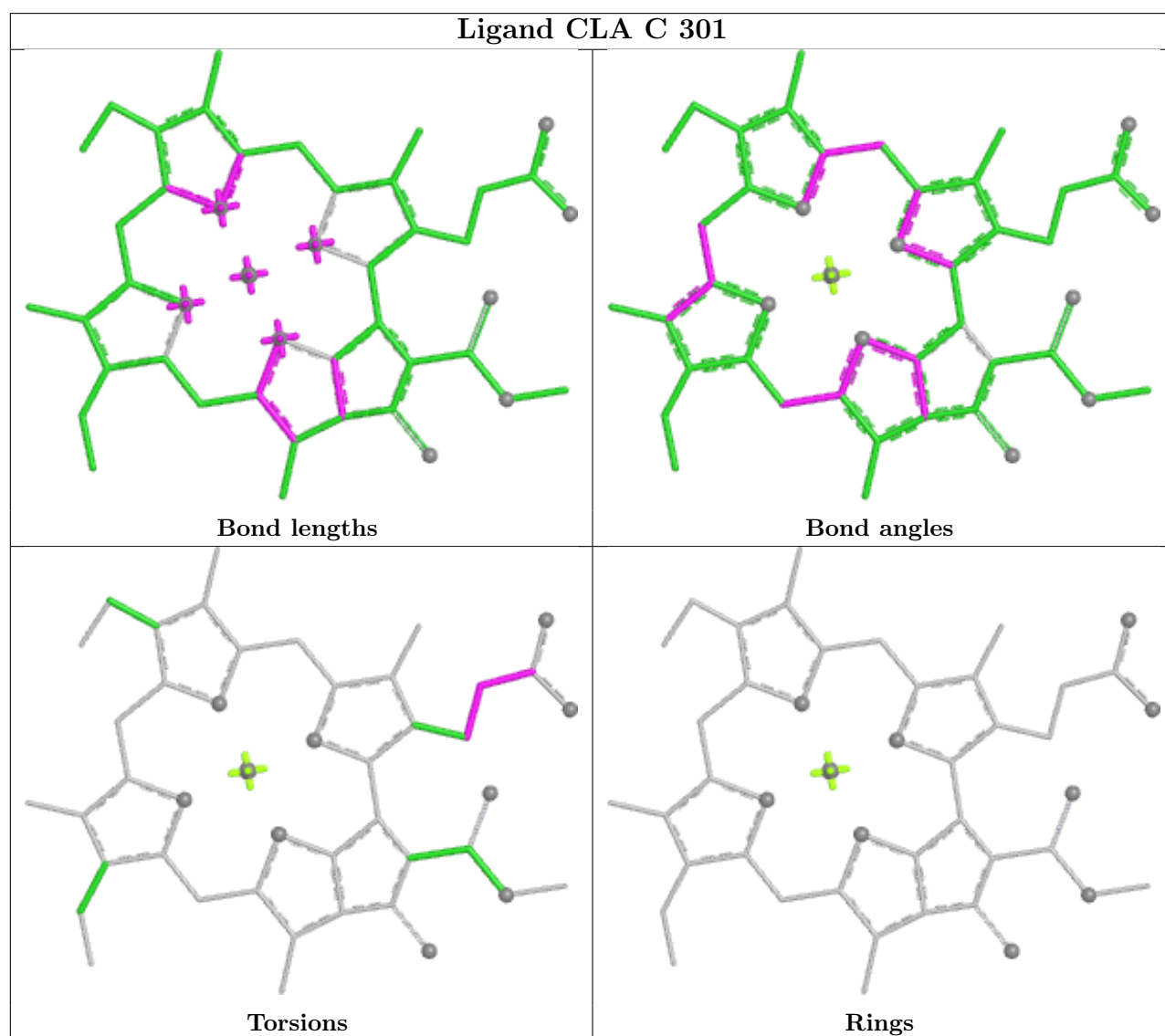
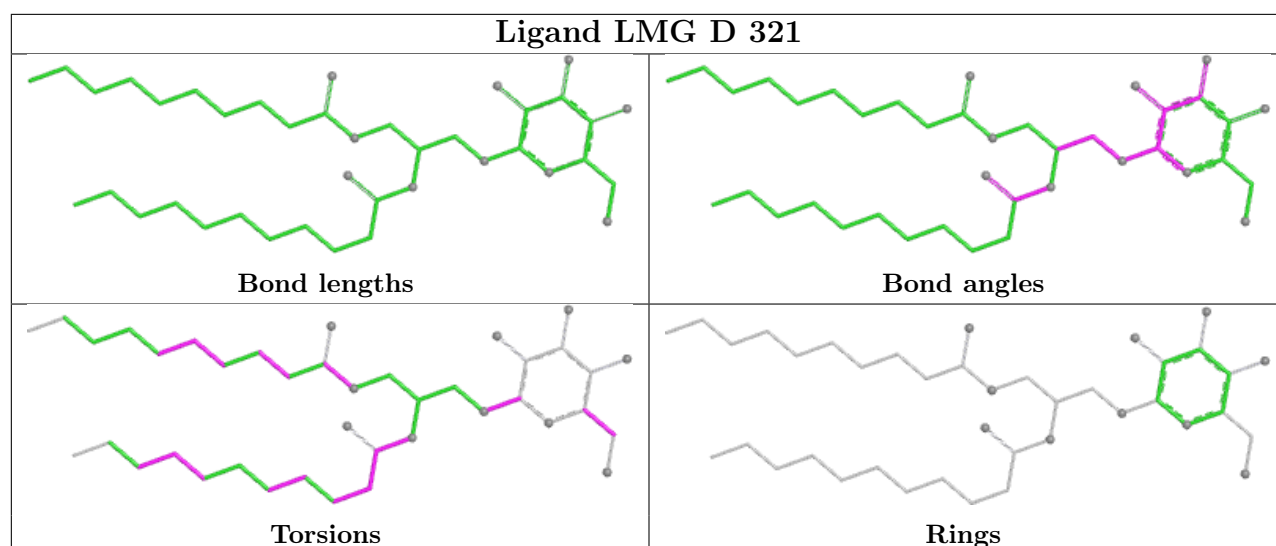


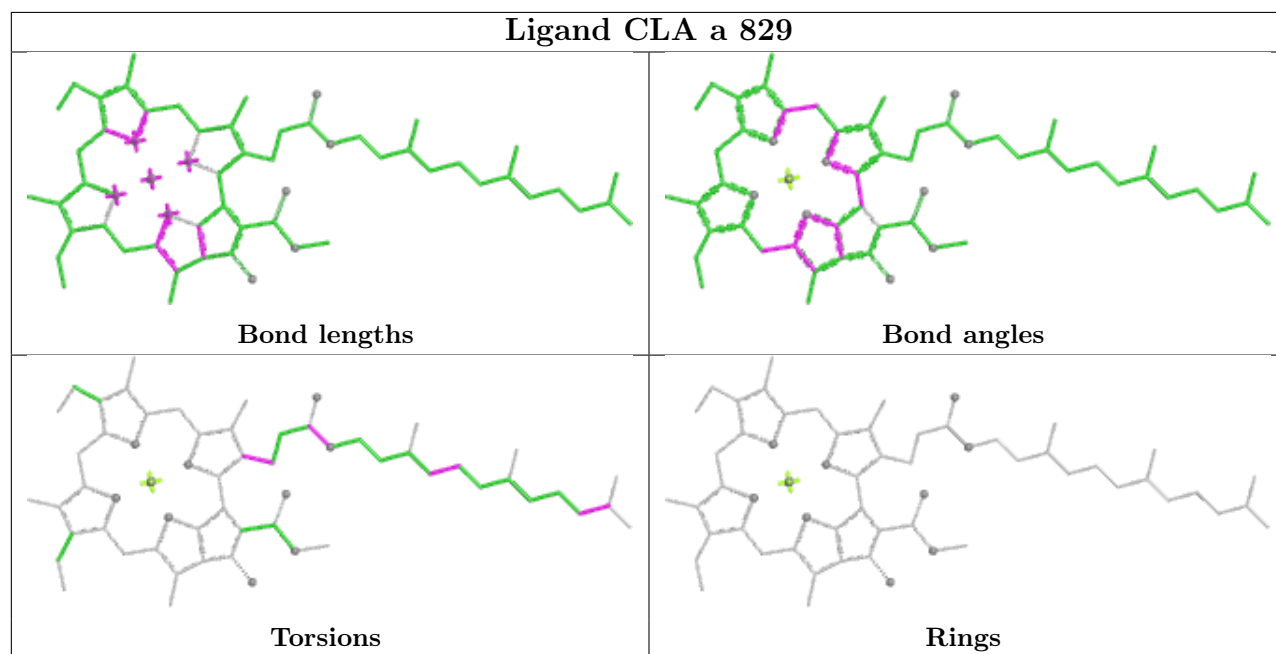
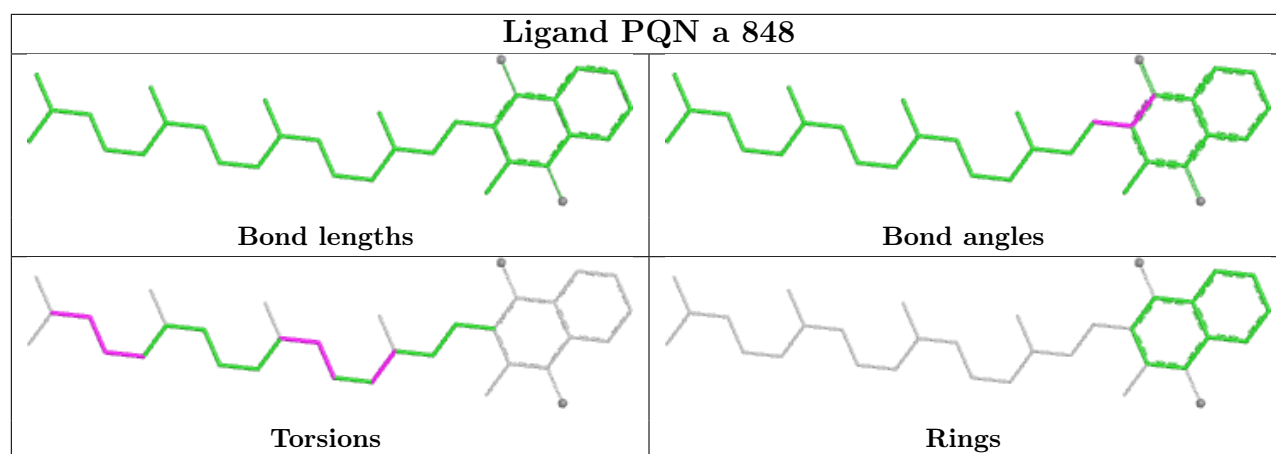
Torsions

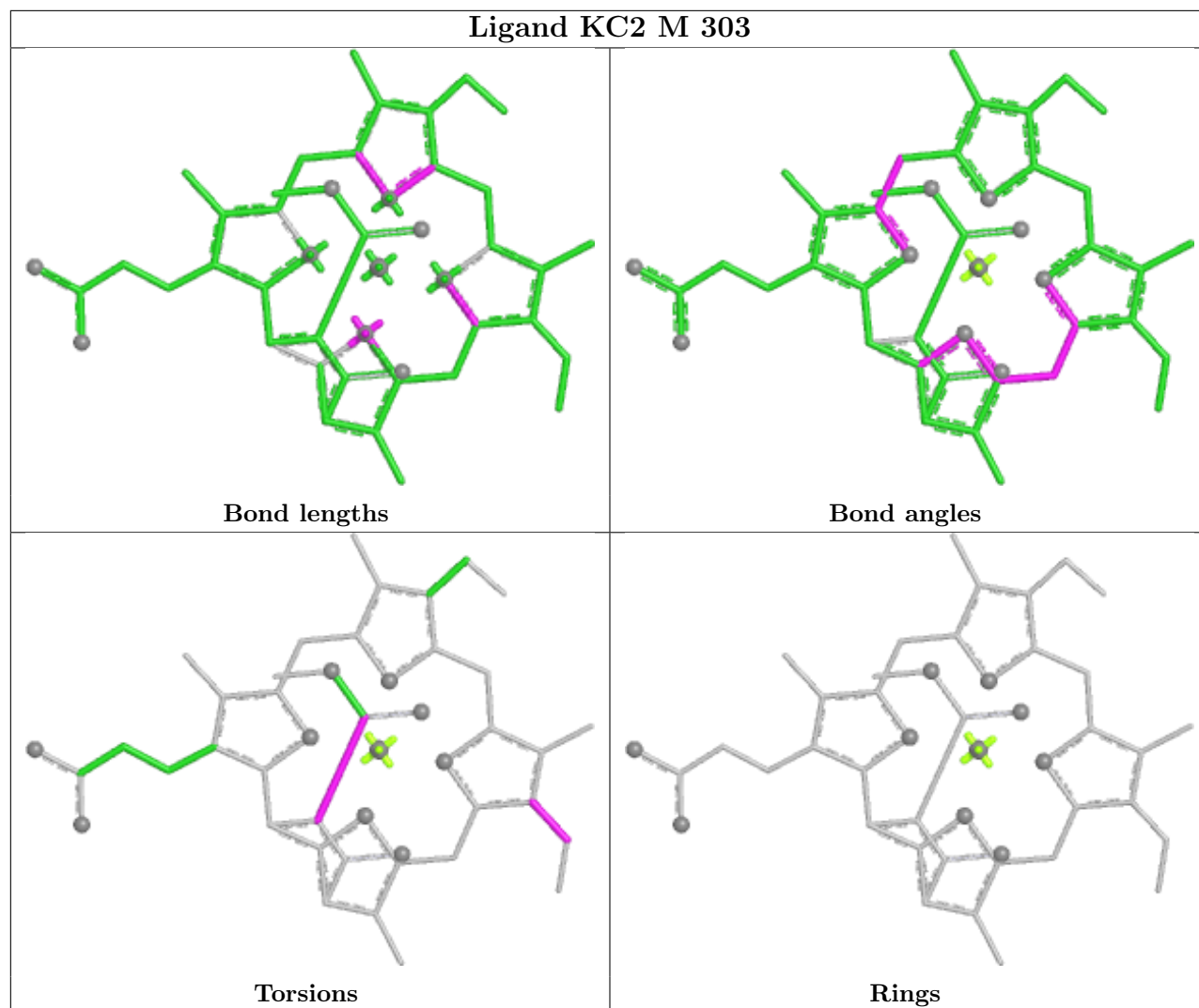


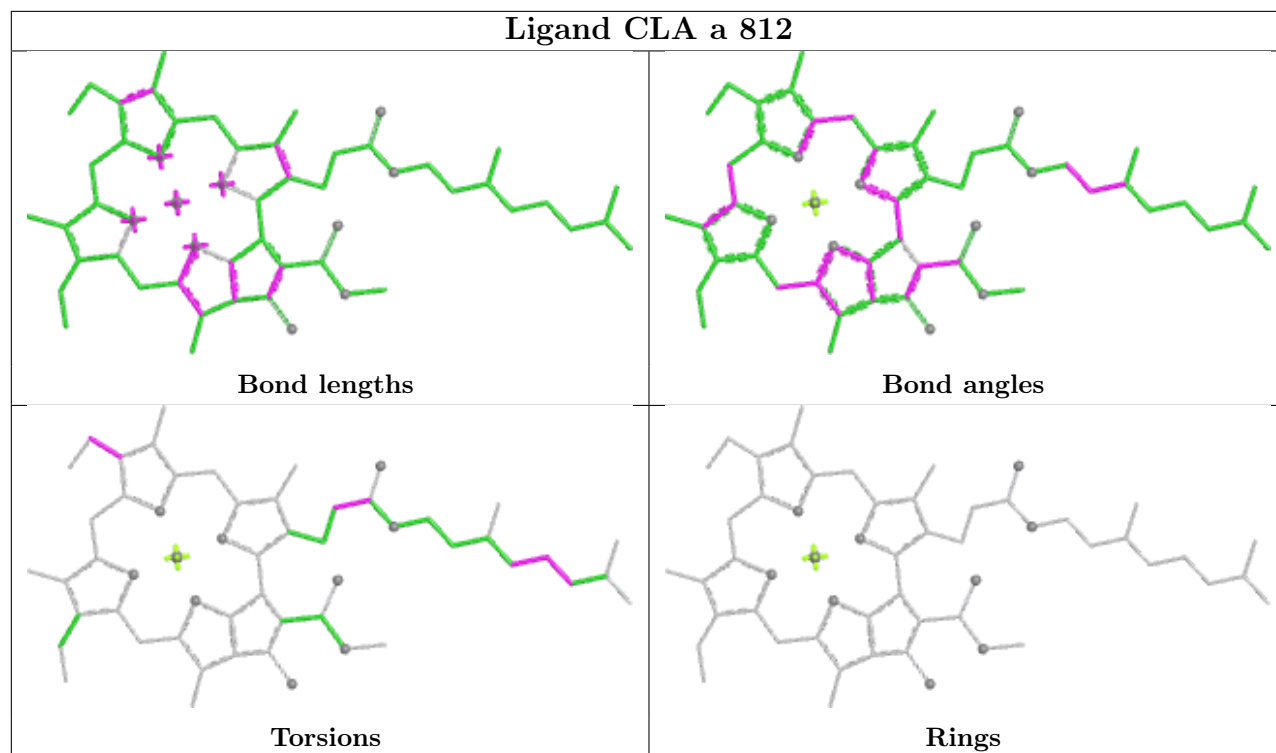
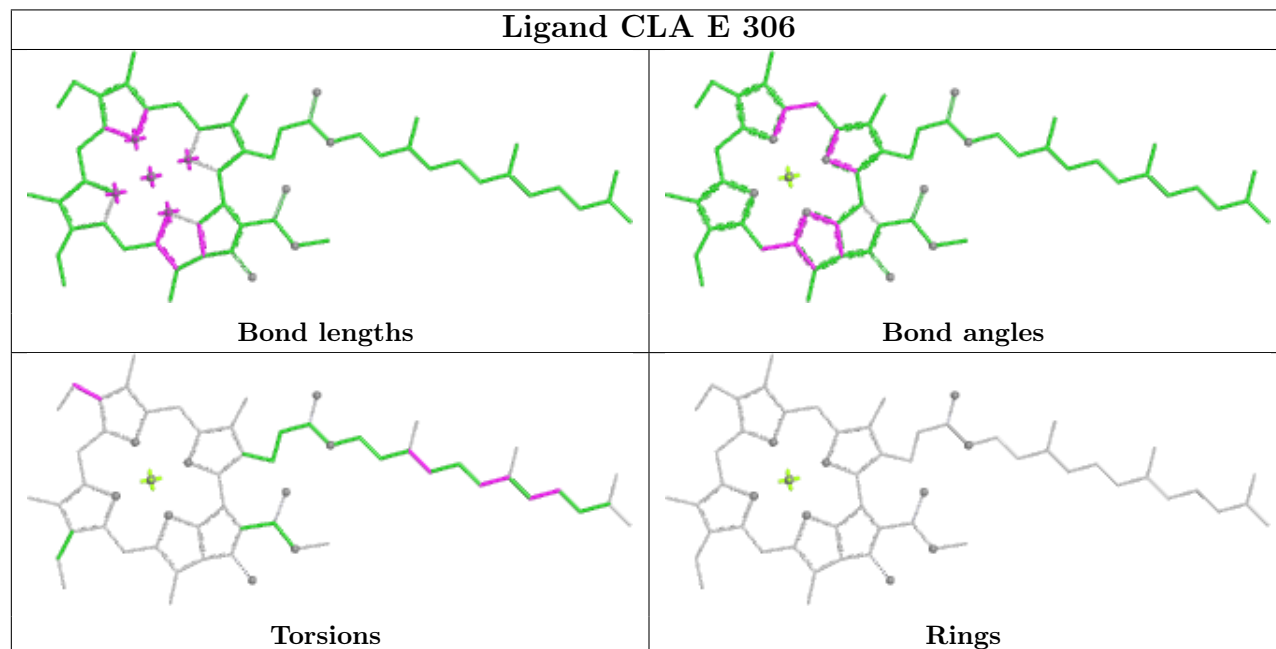
Rings

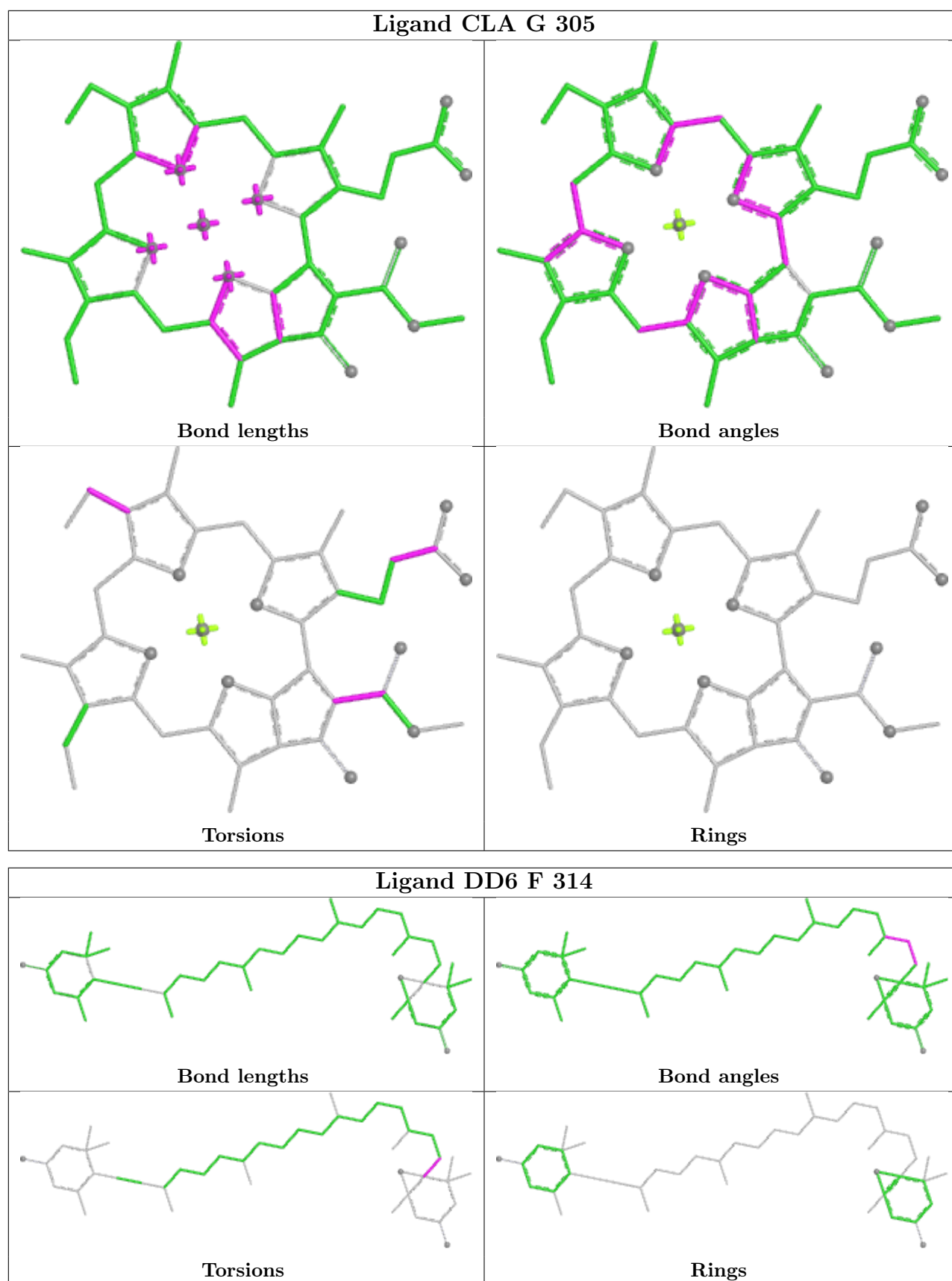


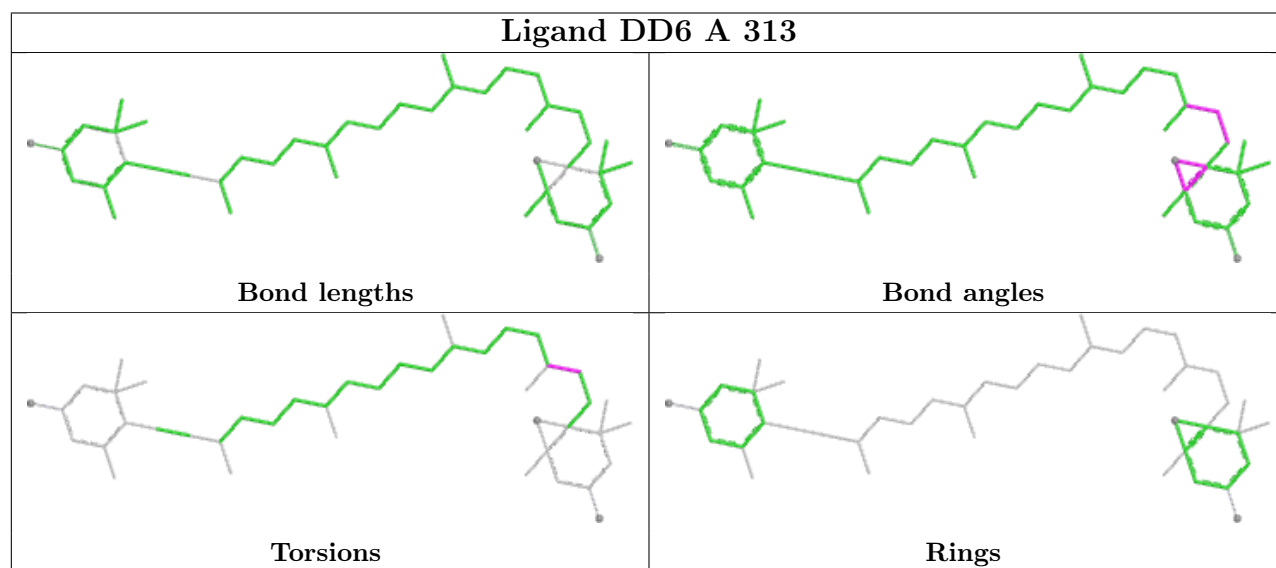
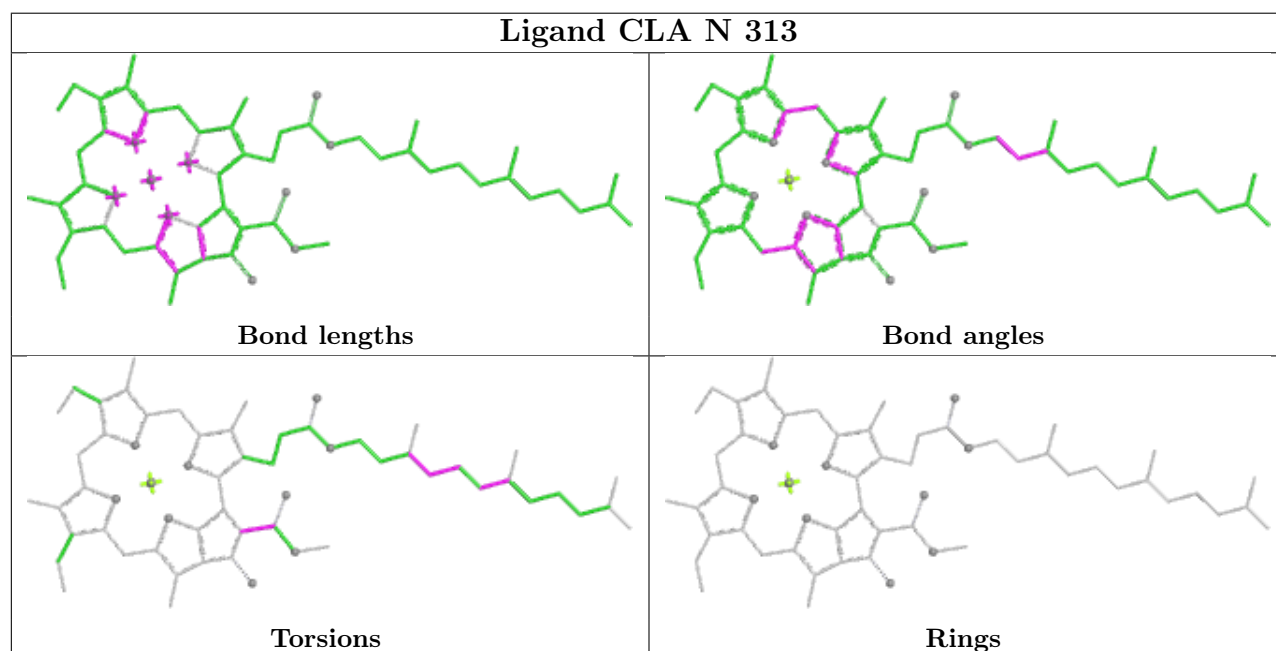
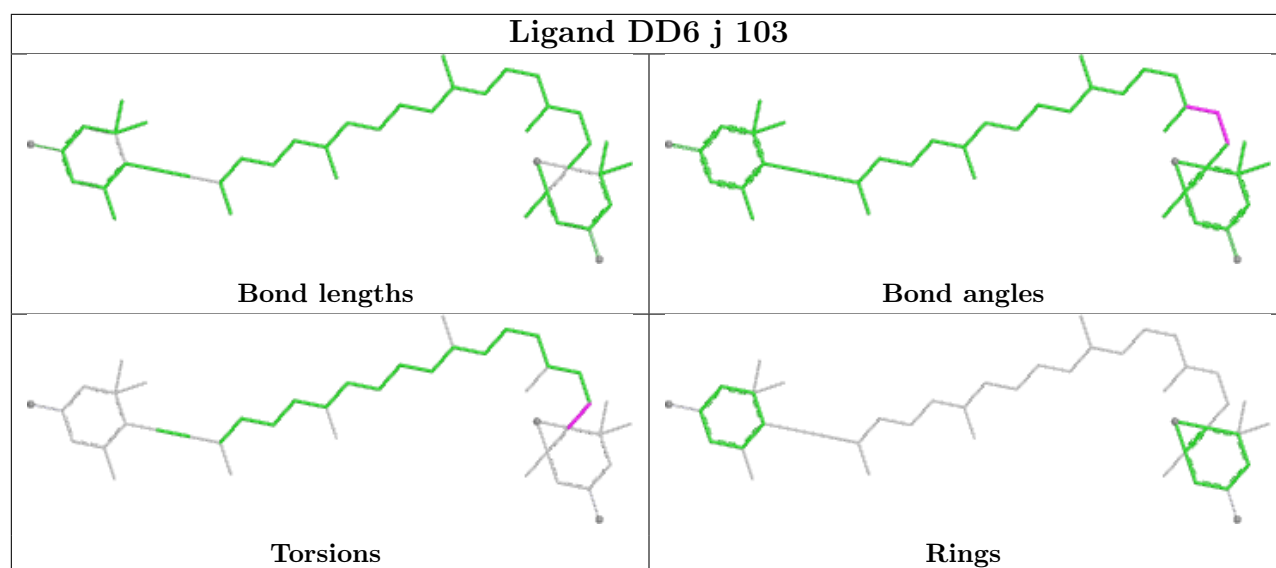


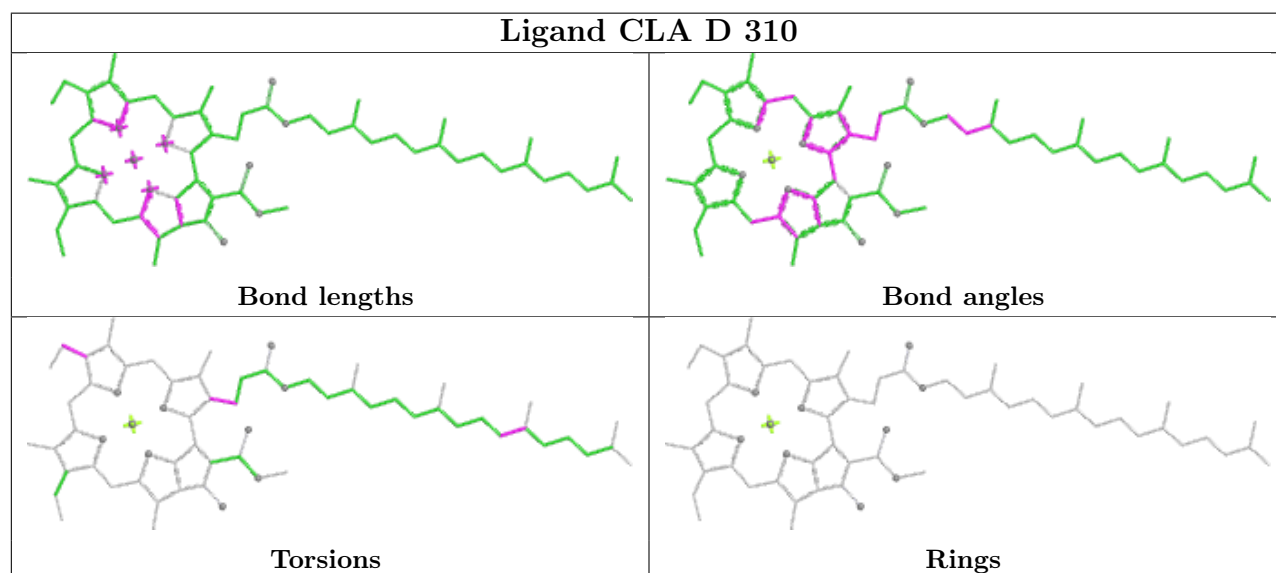
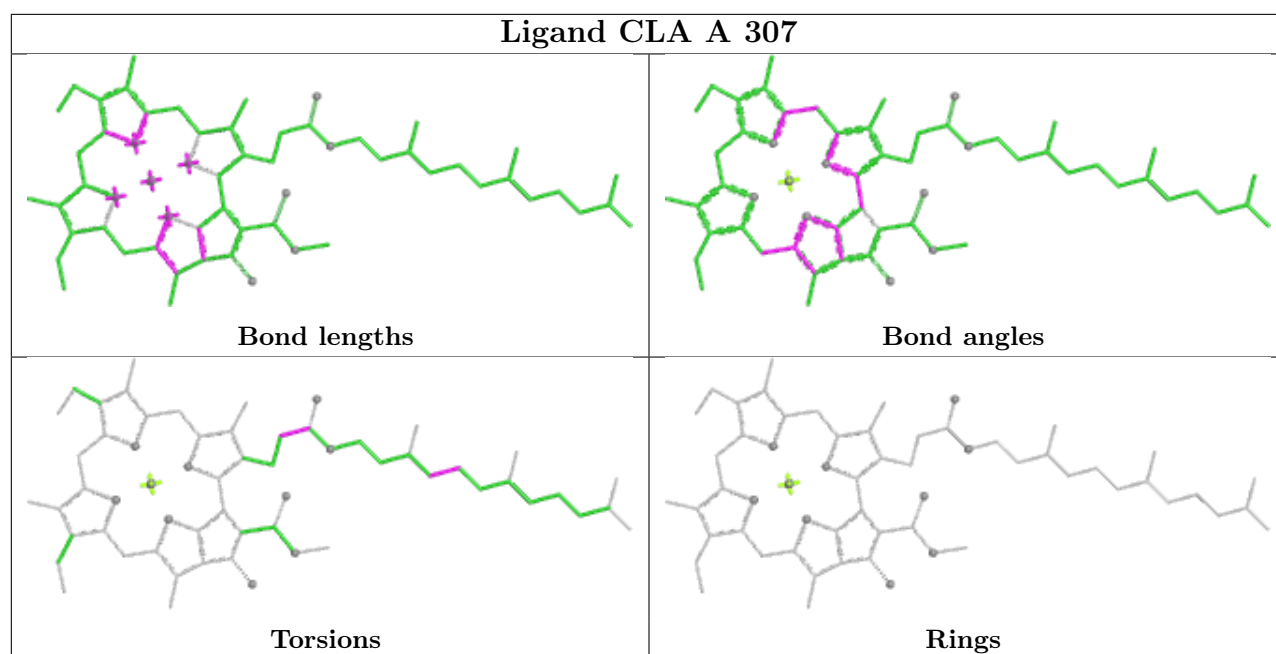


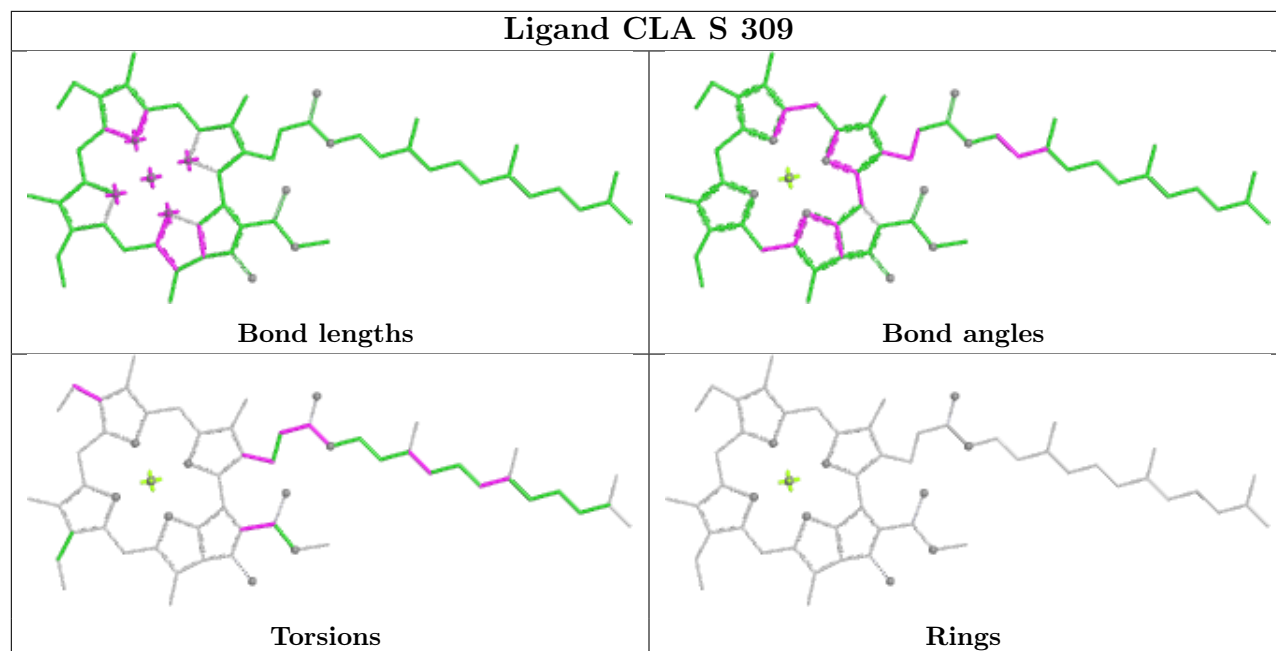
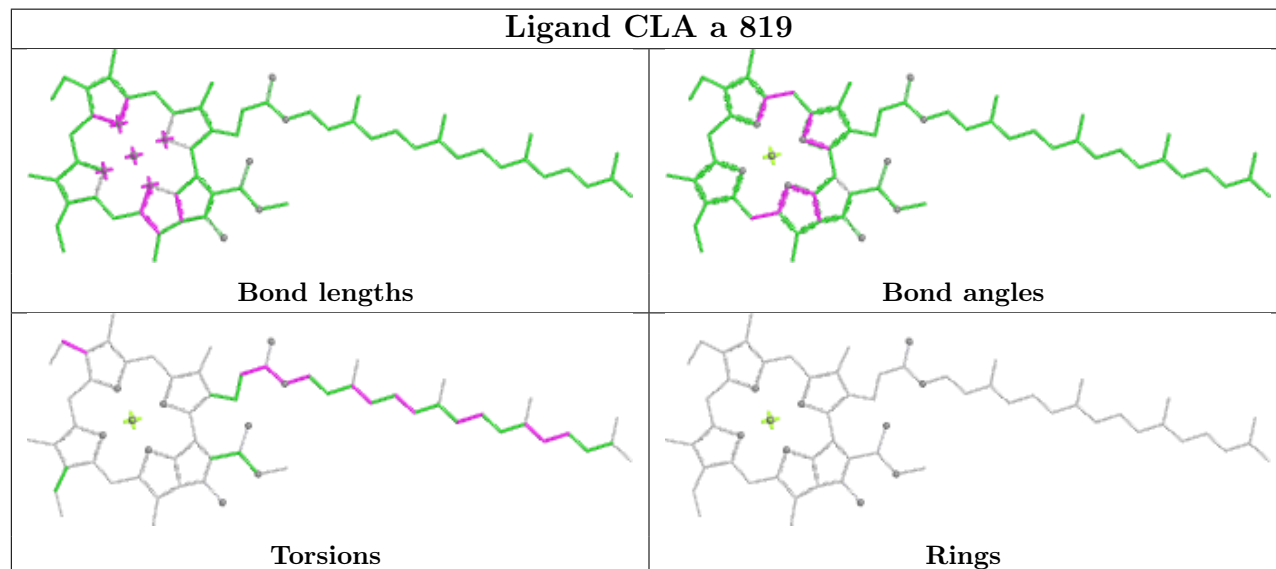


Ligand CLA a 812**Ligand CLA E 306**

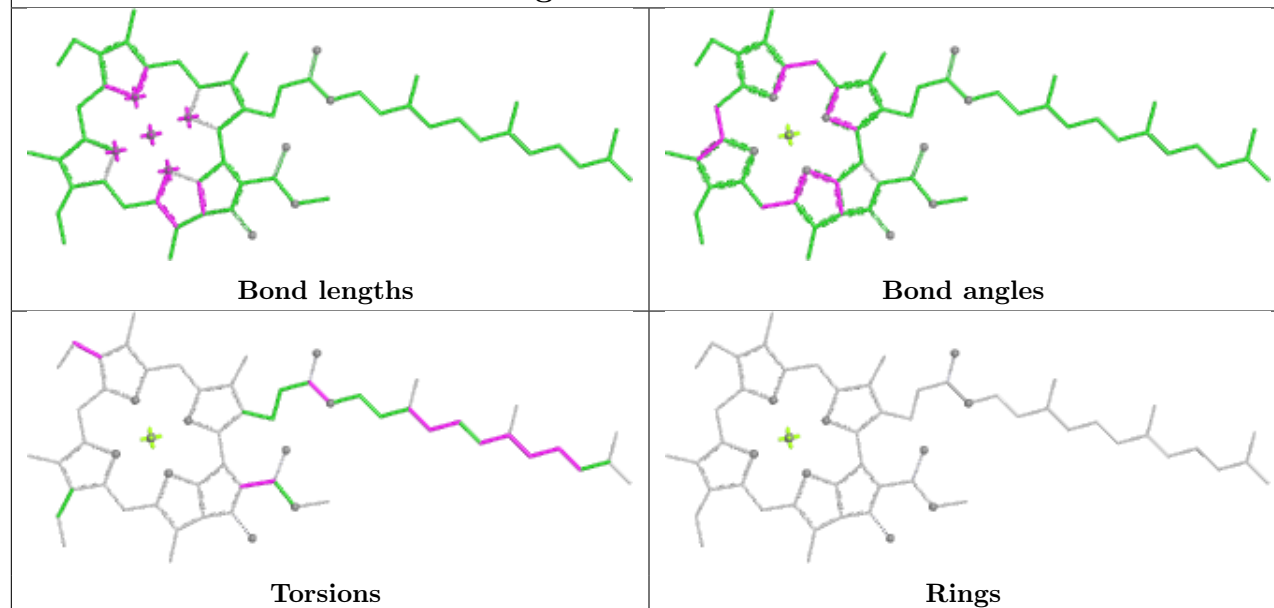




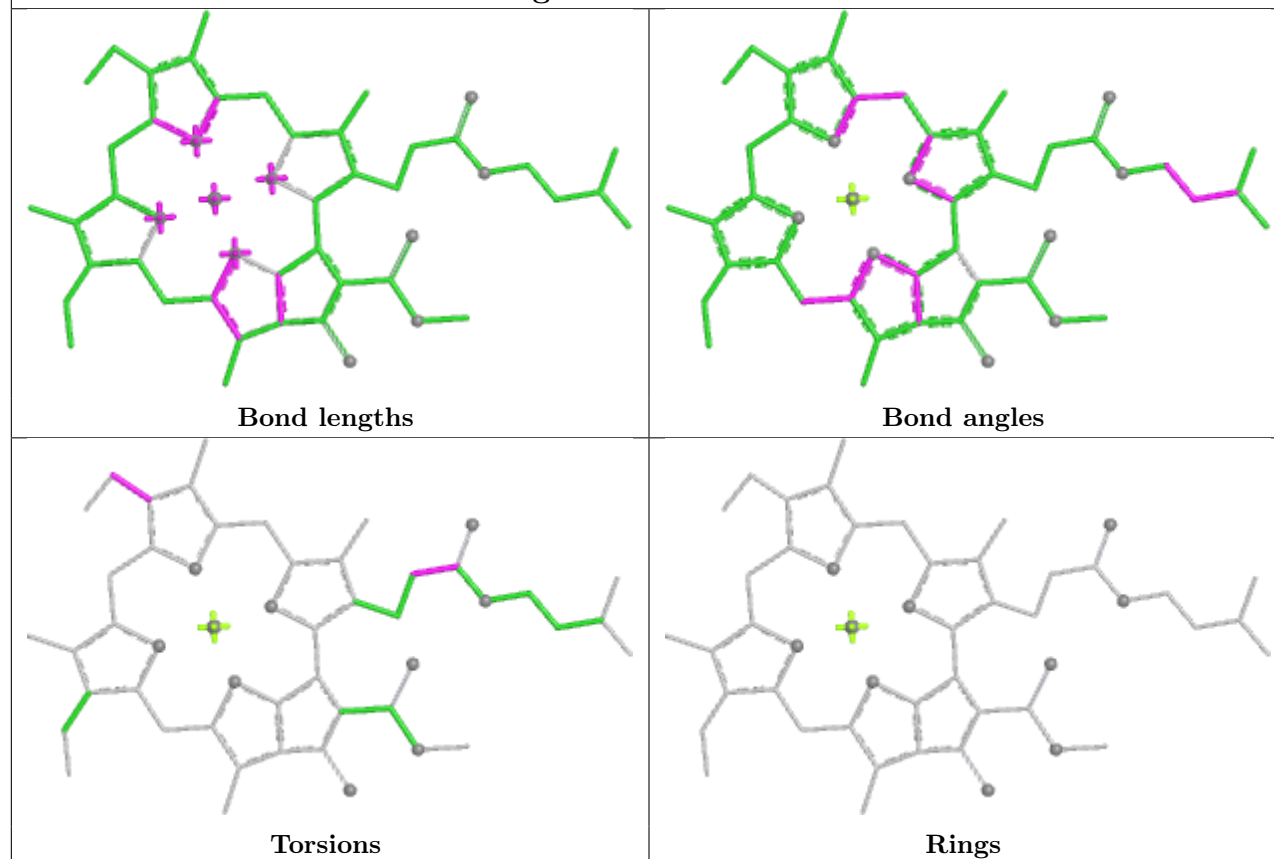


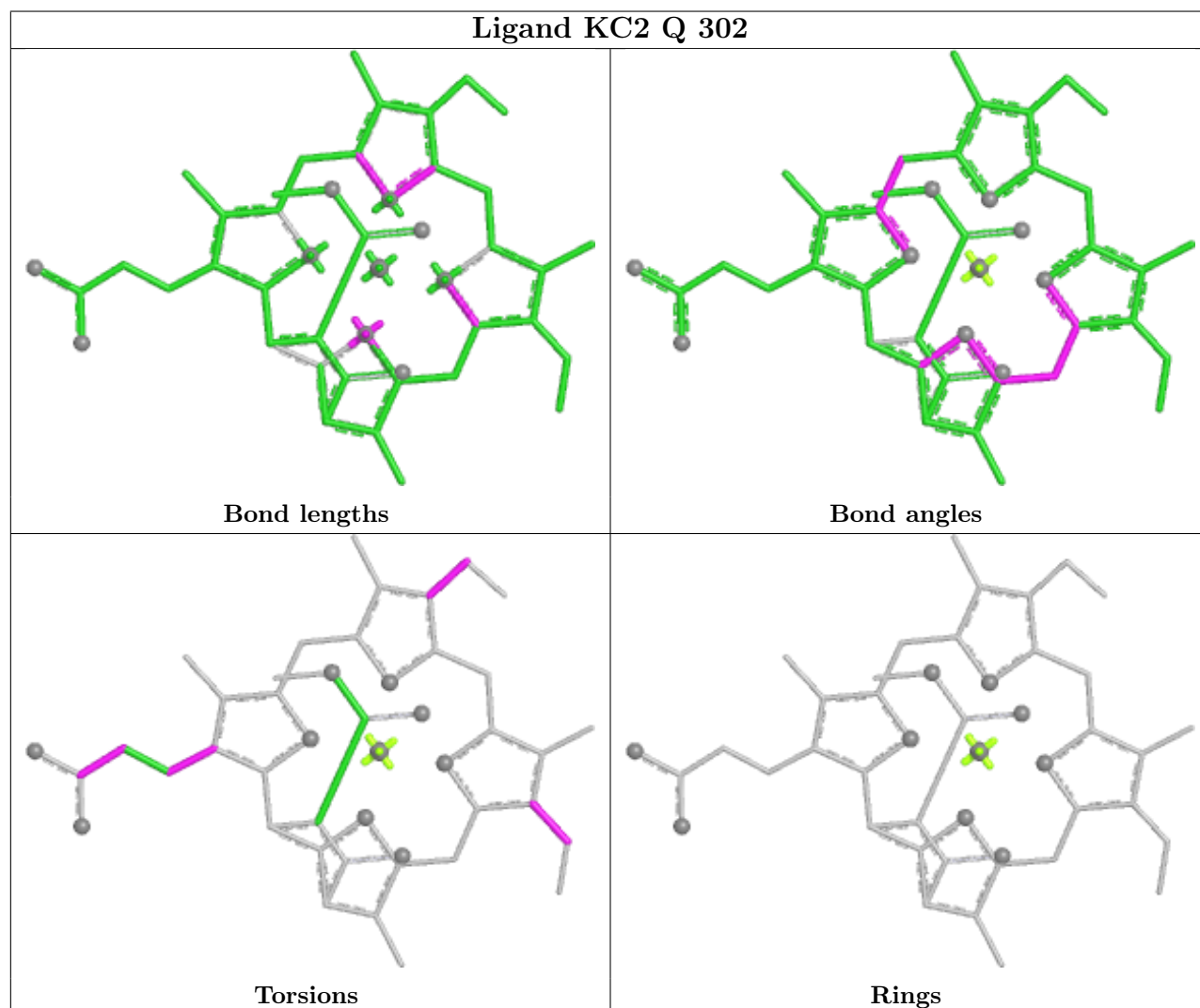
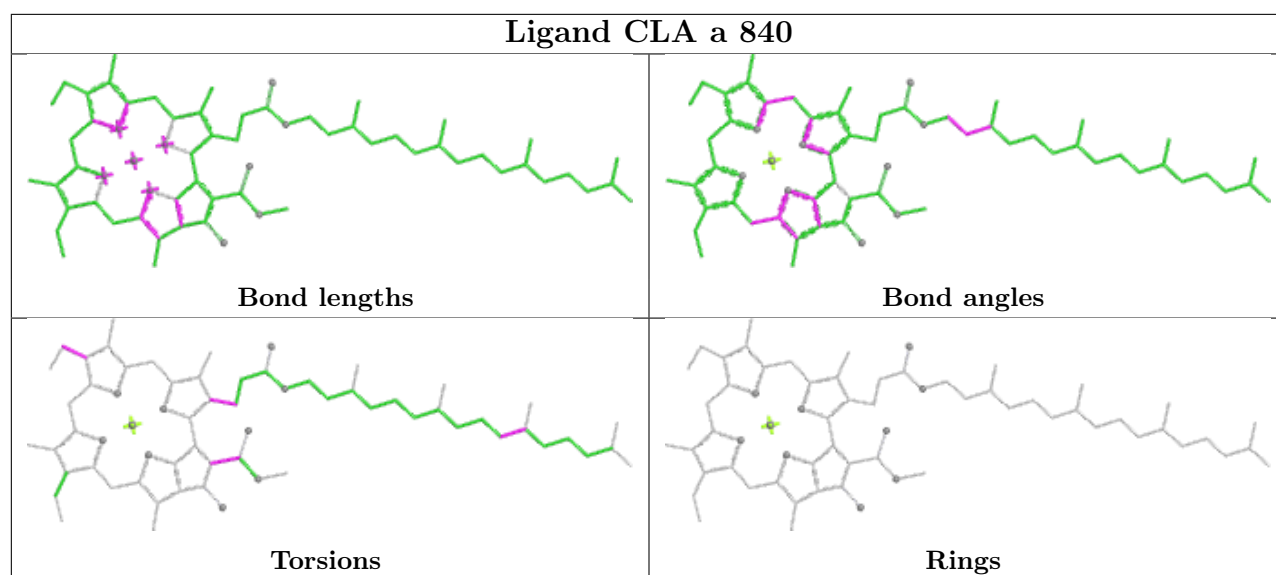
Ligand CLA S 309**Ligand CLA a 819**

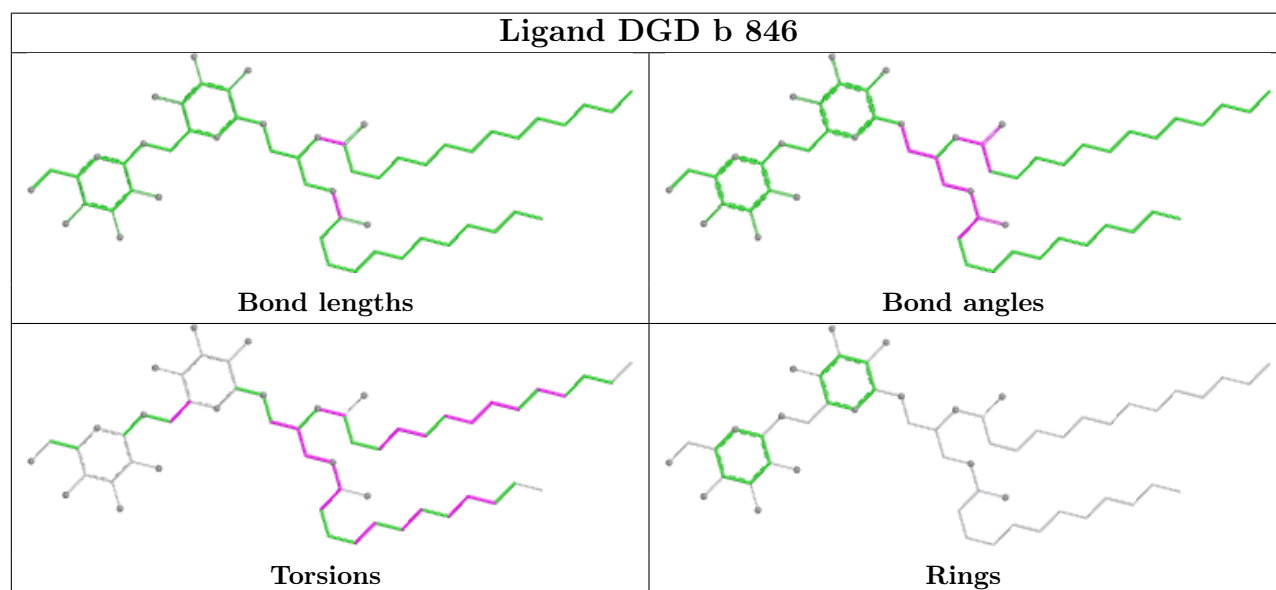
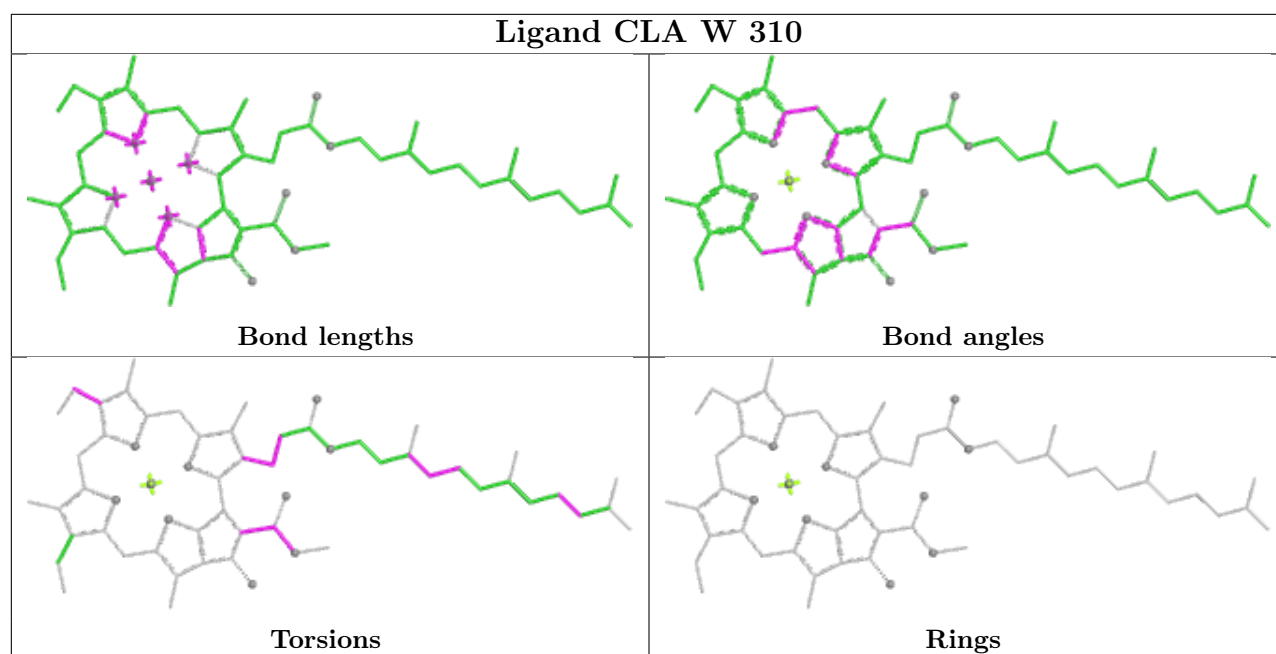
Ligand CLA b 831



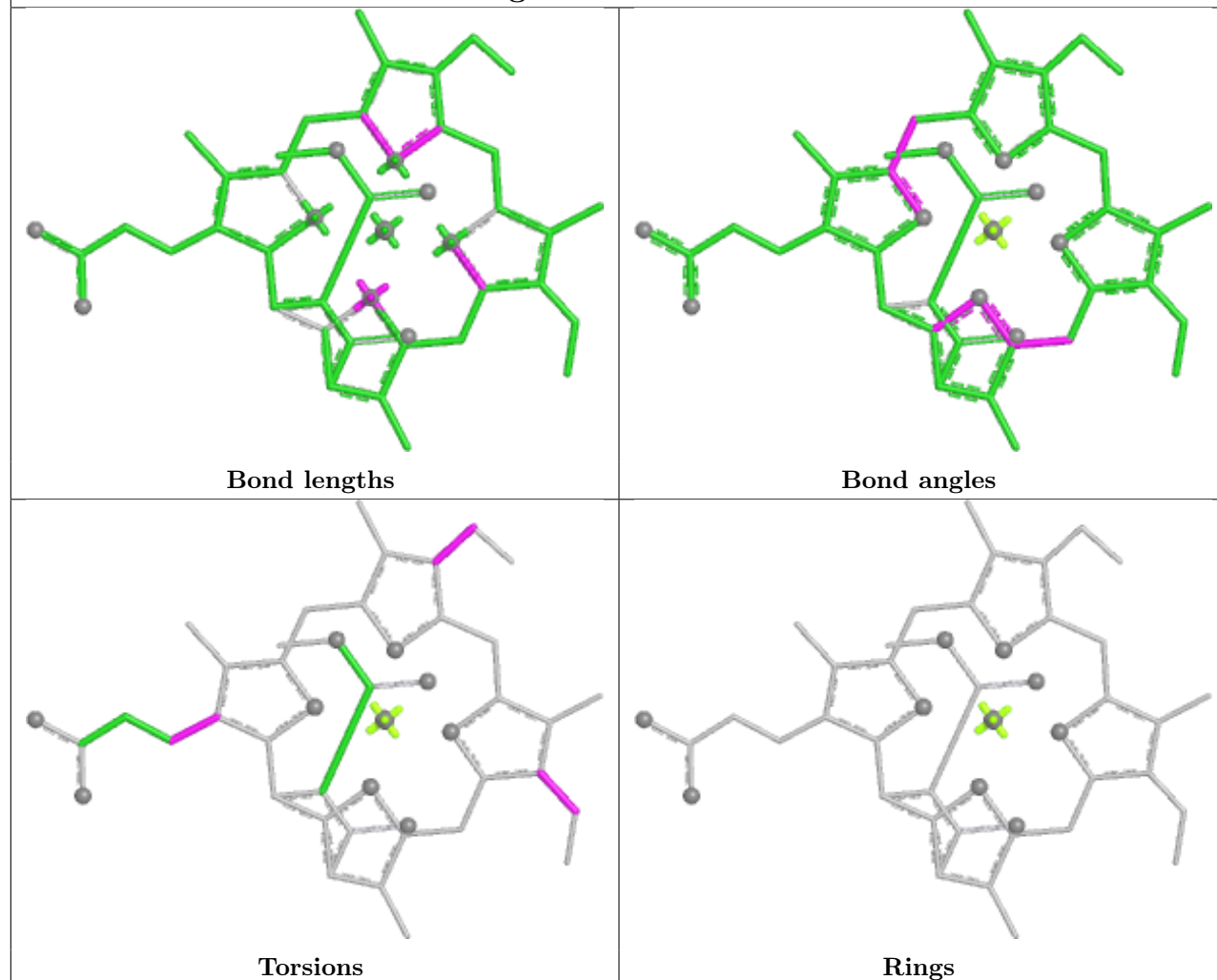
Ligand CLA T 307



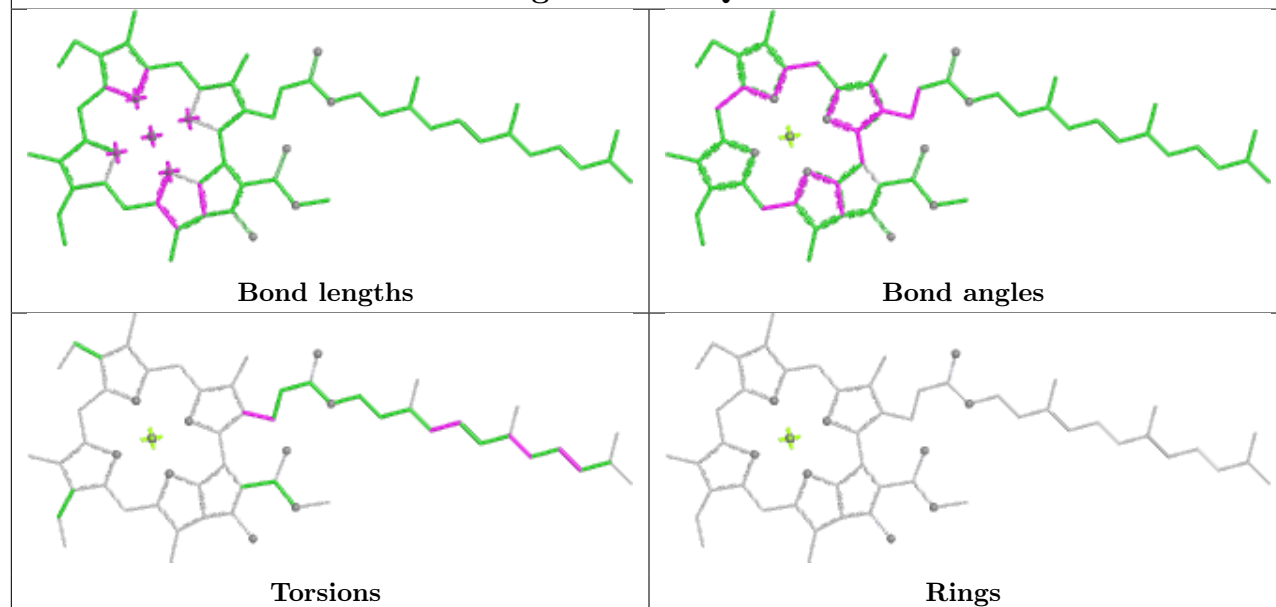


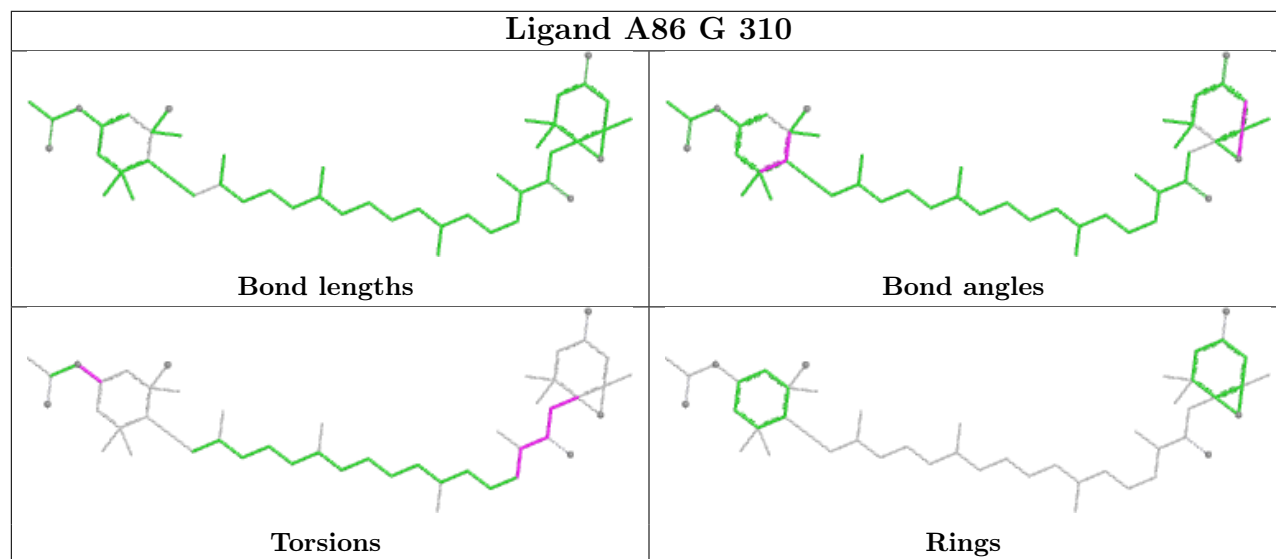
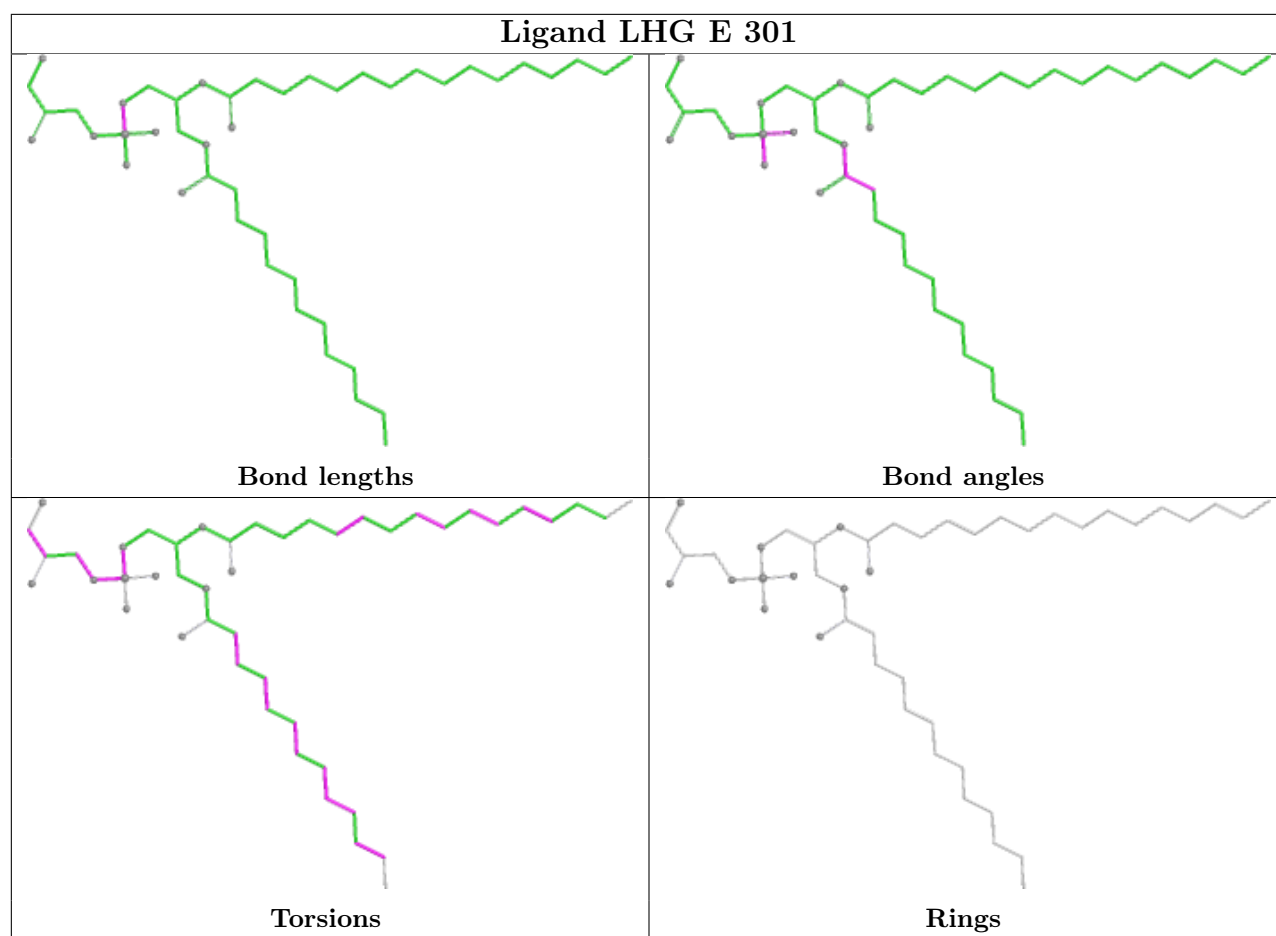


Ligand KC2 R 303

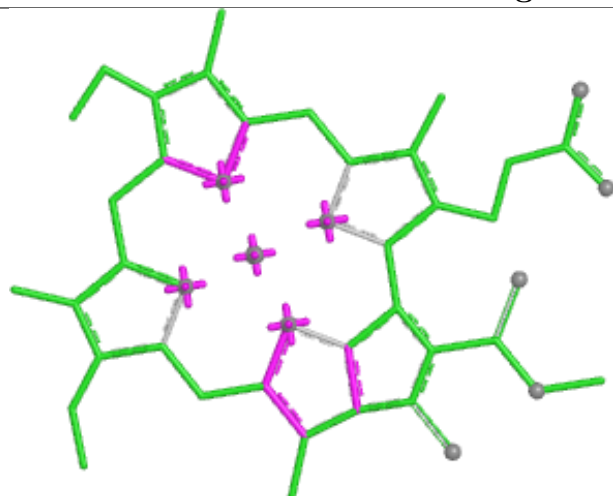


Ligand CLA Q 303

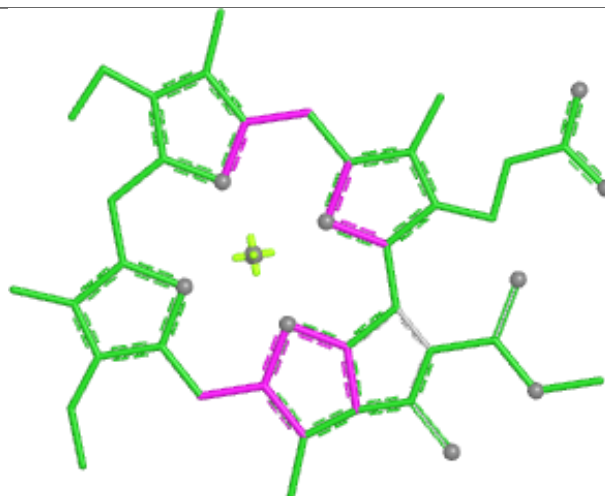




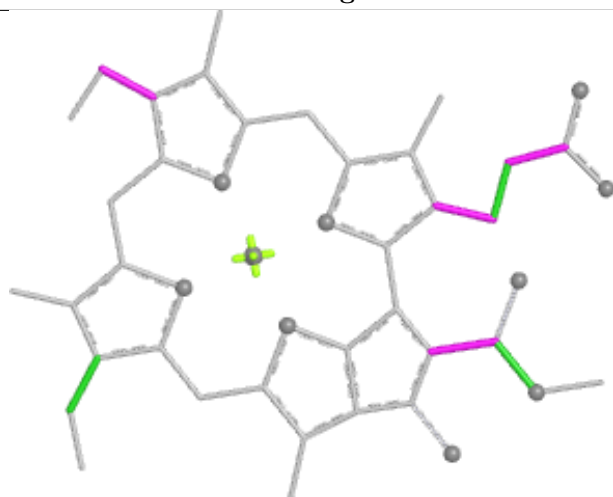
Ligand CLA E 310



Bond lengths



Bond angles

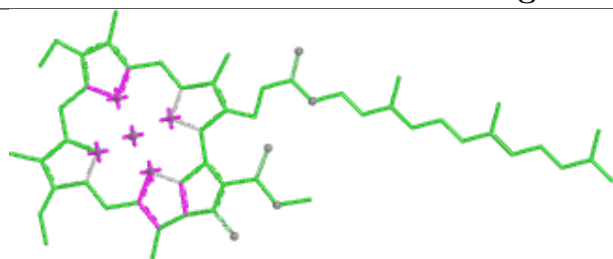


Torsions

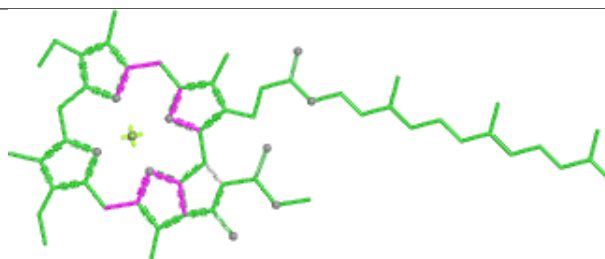


Rings

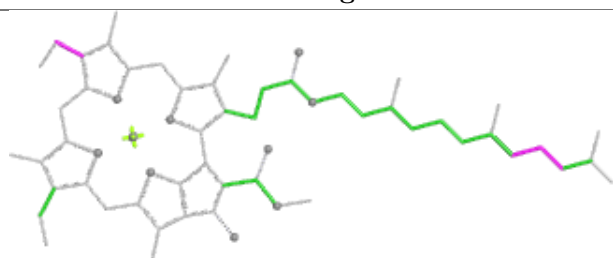
Ligand CLA a 832



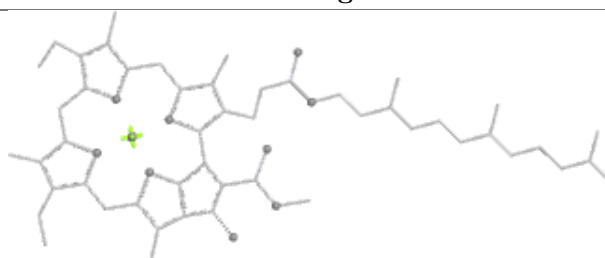
Bond lengths



Bond angles

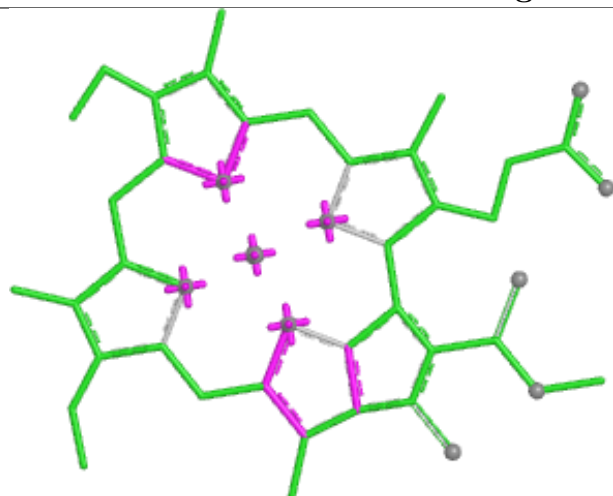


Torsions

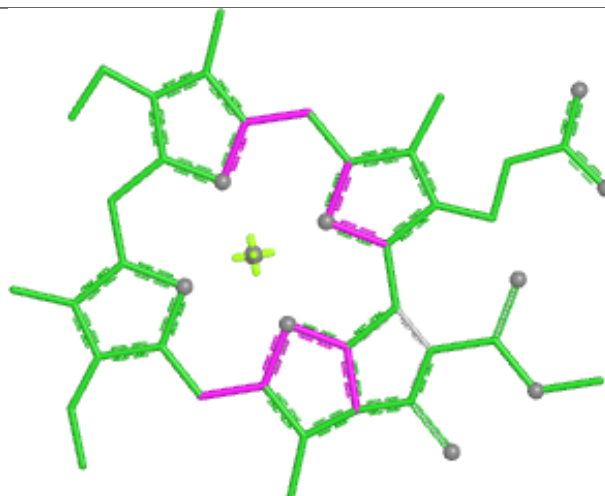


Rings

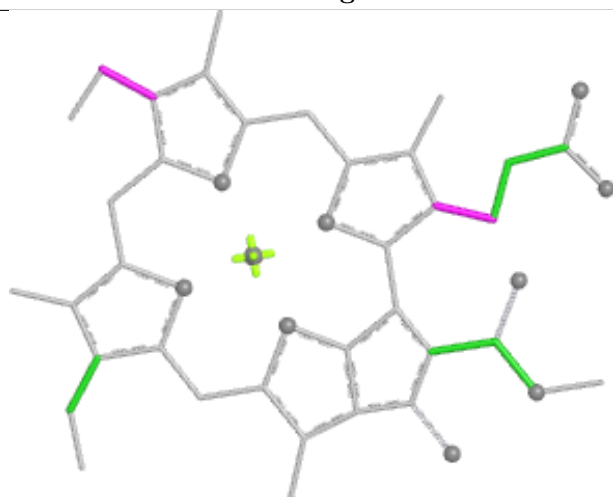
Ligand CLA E 303



Bond lengths



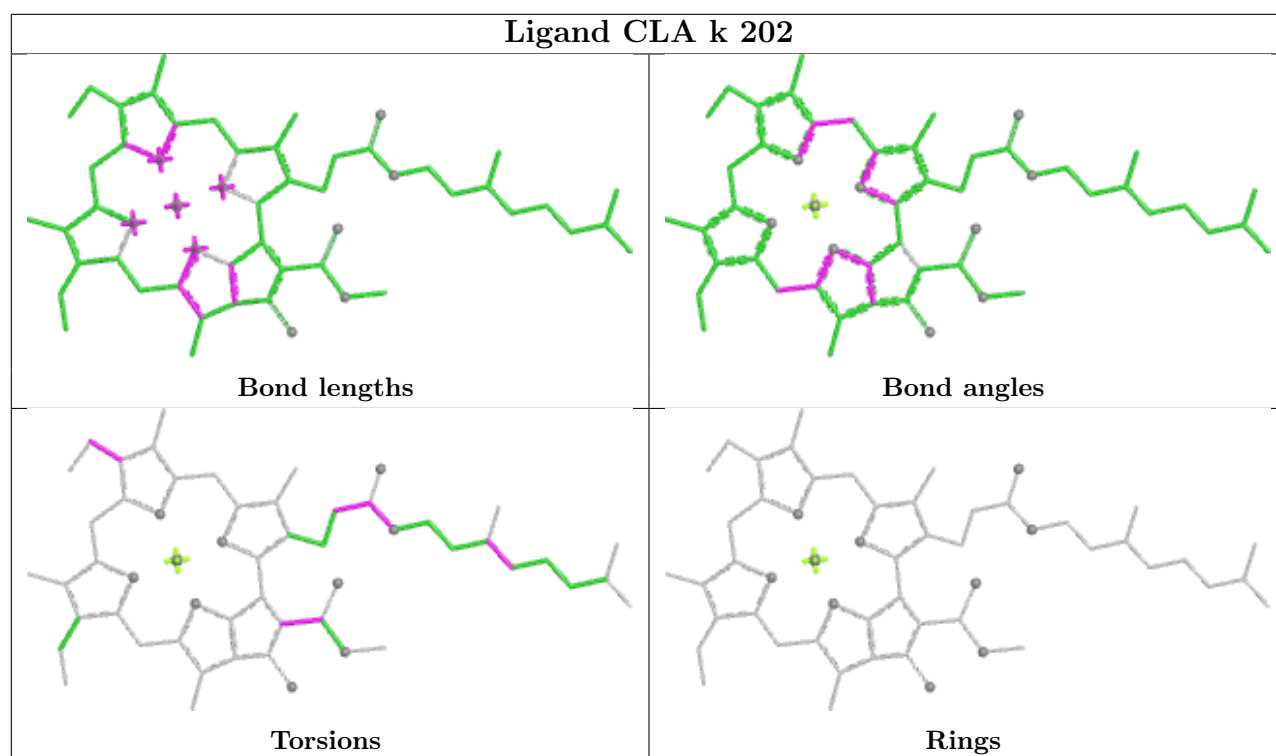
Bond angles



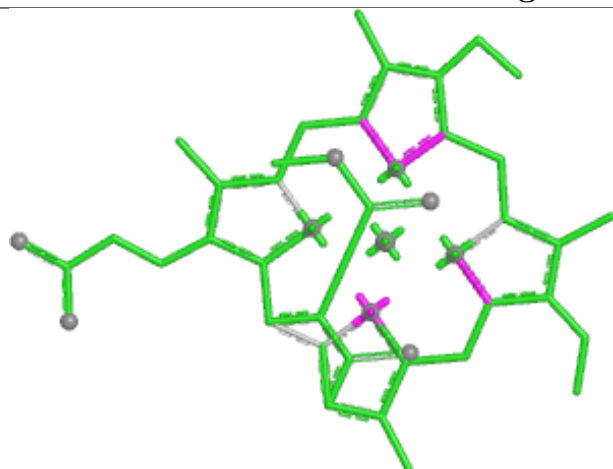
Torsions



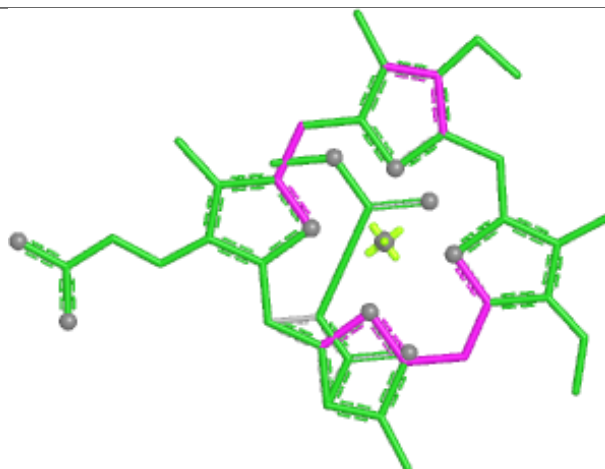
Rings



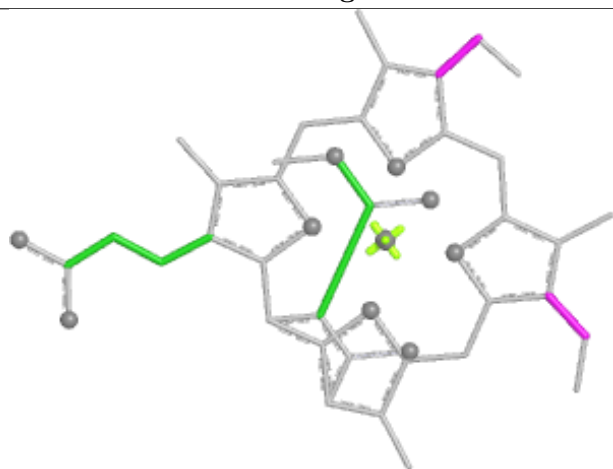
Ligand KC2 L 306



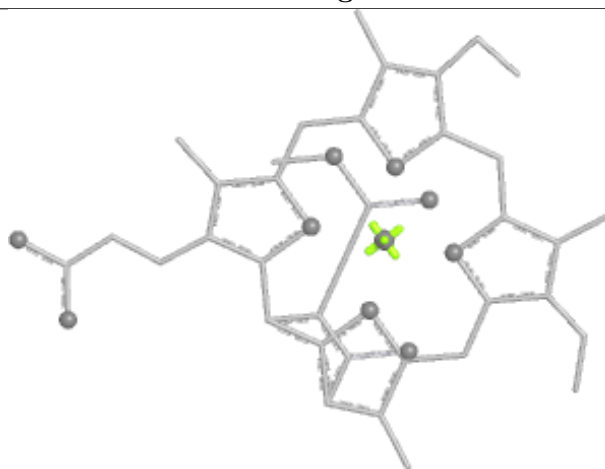
Bond lengths



Bond angles

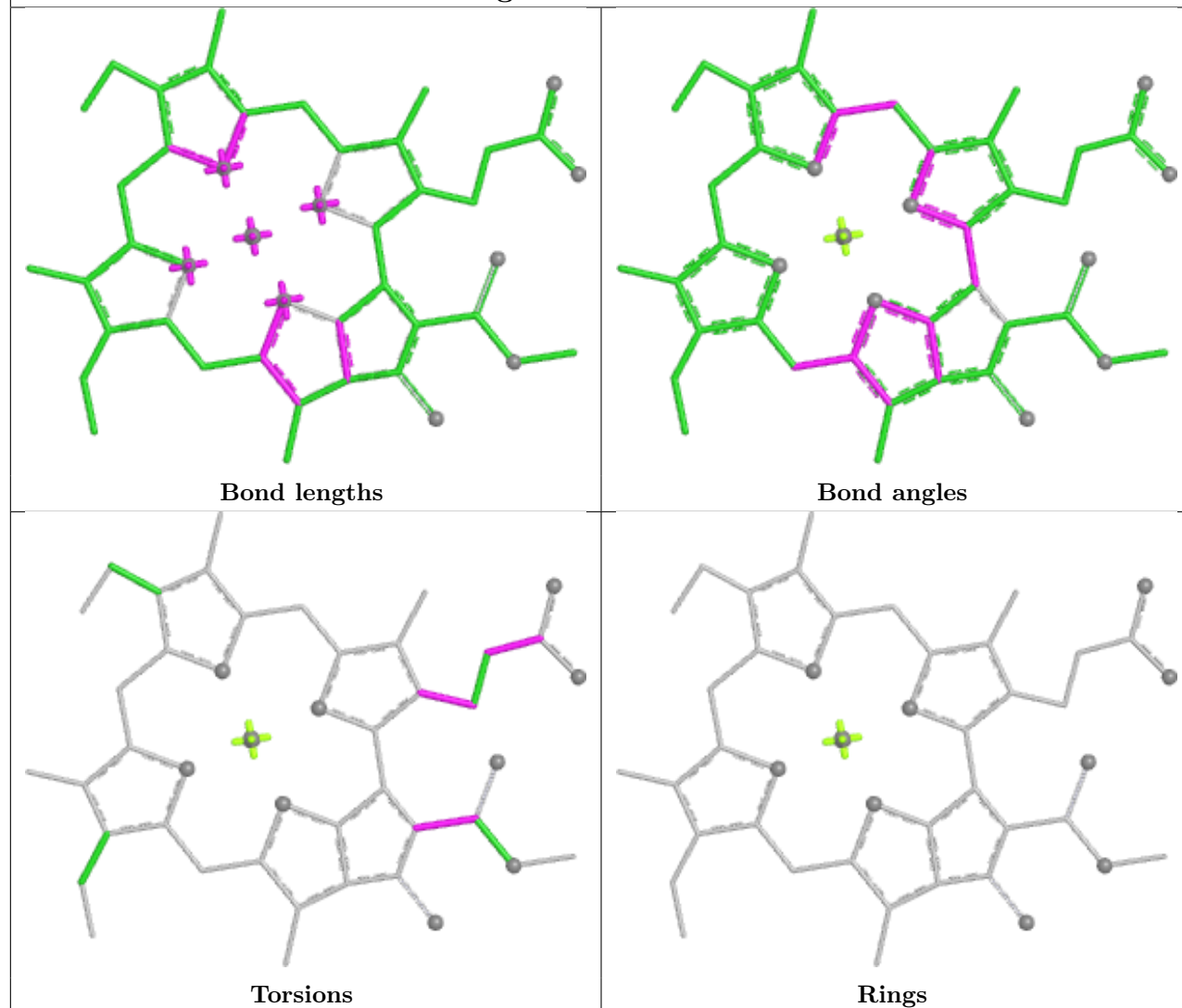


Torsions

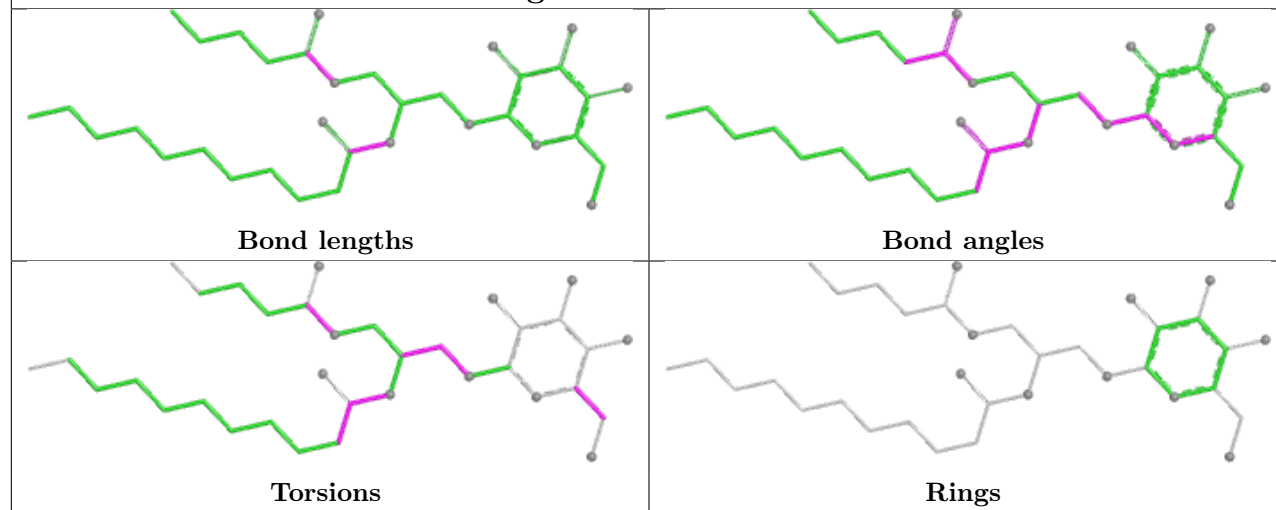


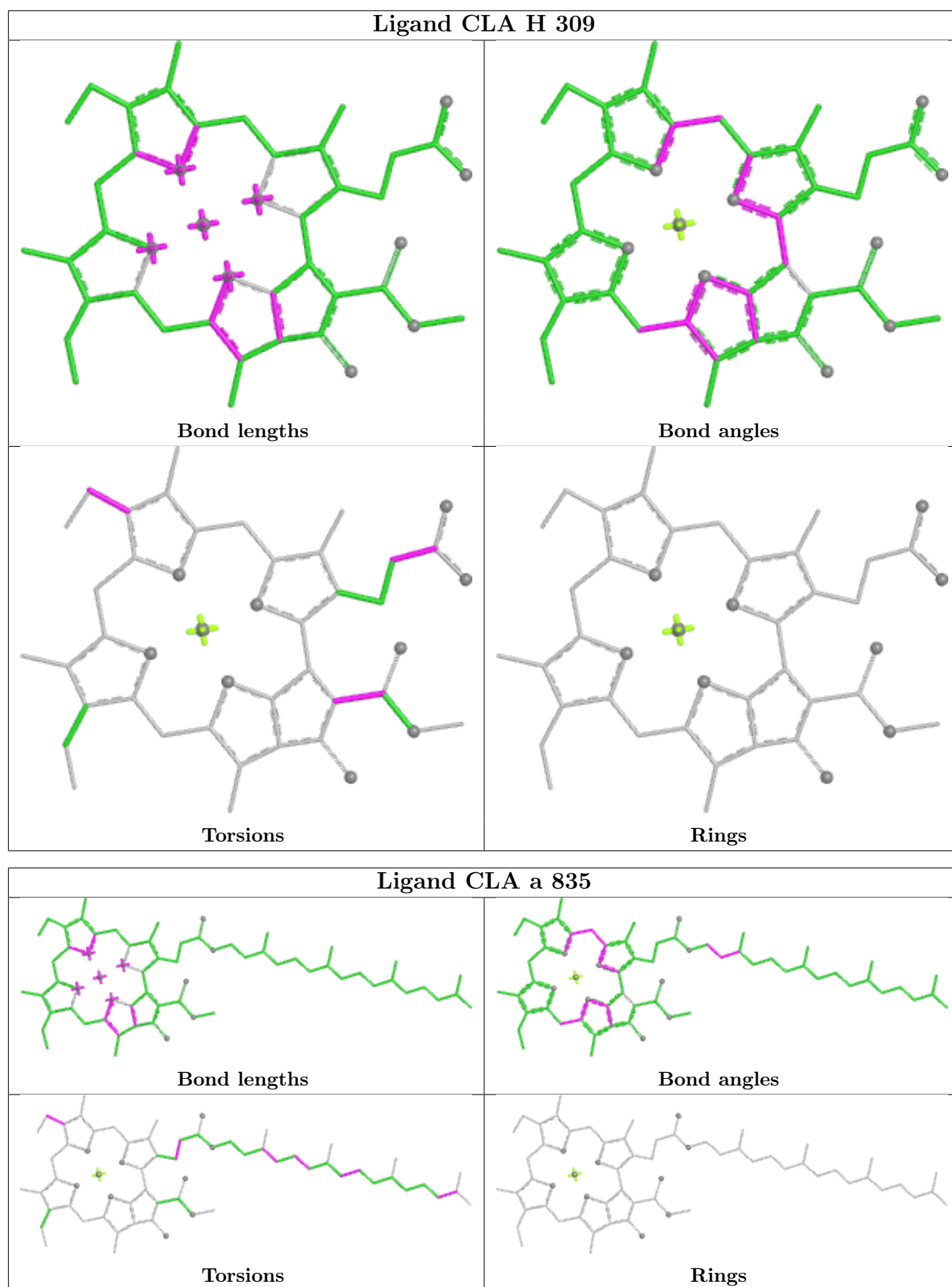
Rings

Ligand CLA a 813

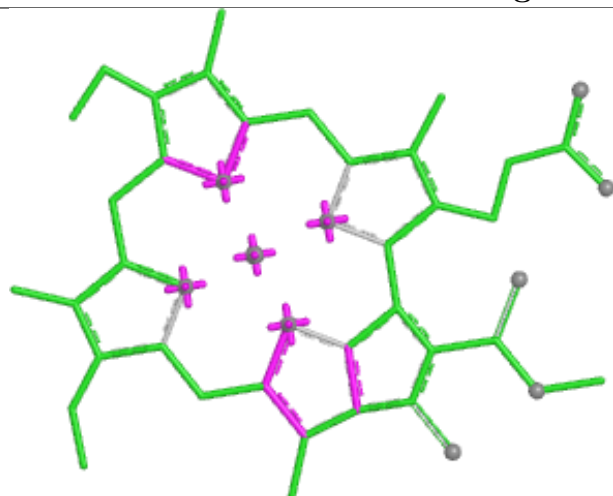


Ligand LMG D 325

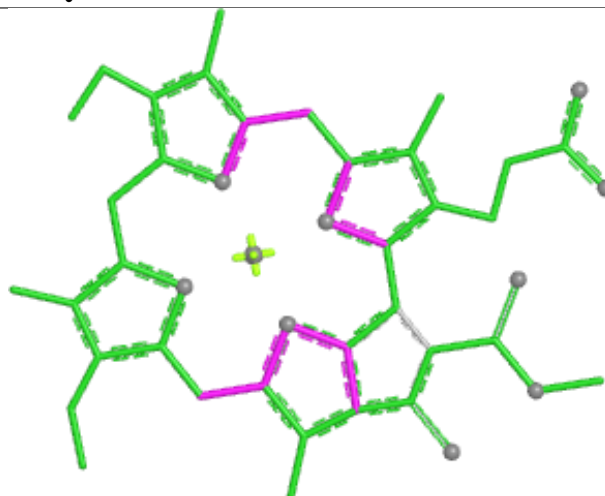




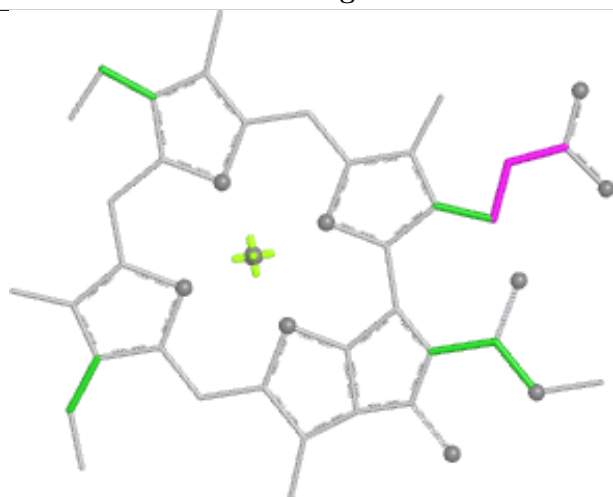
Ligand CLA Q 309



Bond lengths



Bond angles

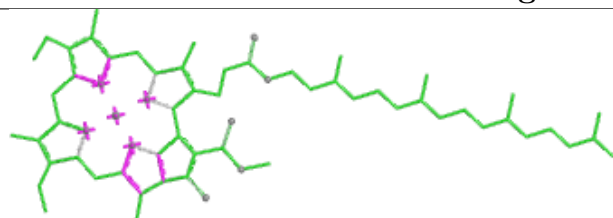


Torsions

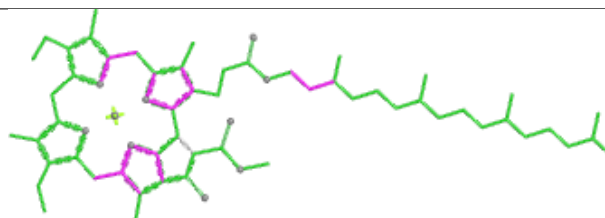


Rings

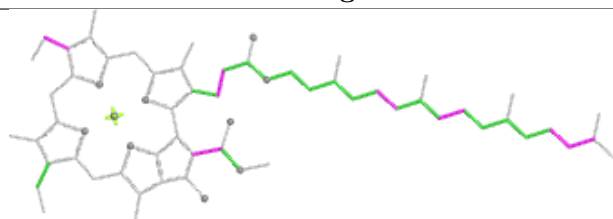
Ligand CLA a 807



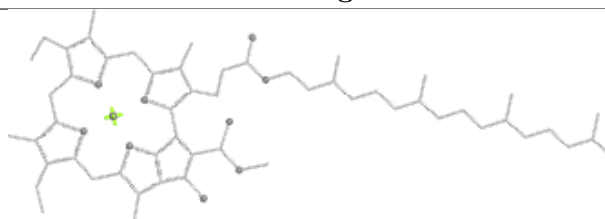
Bond lengths



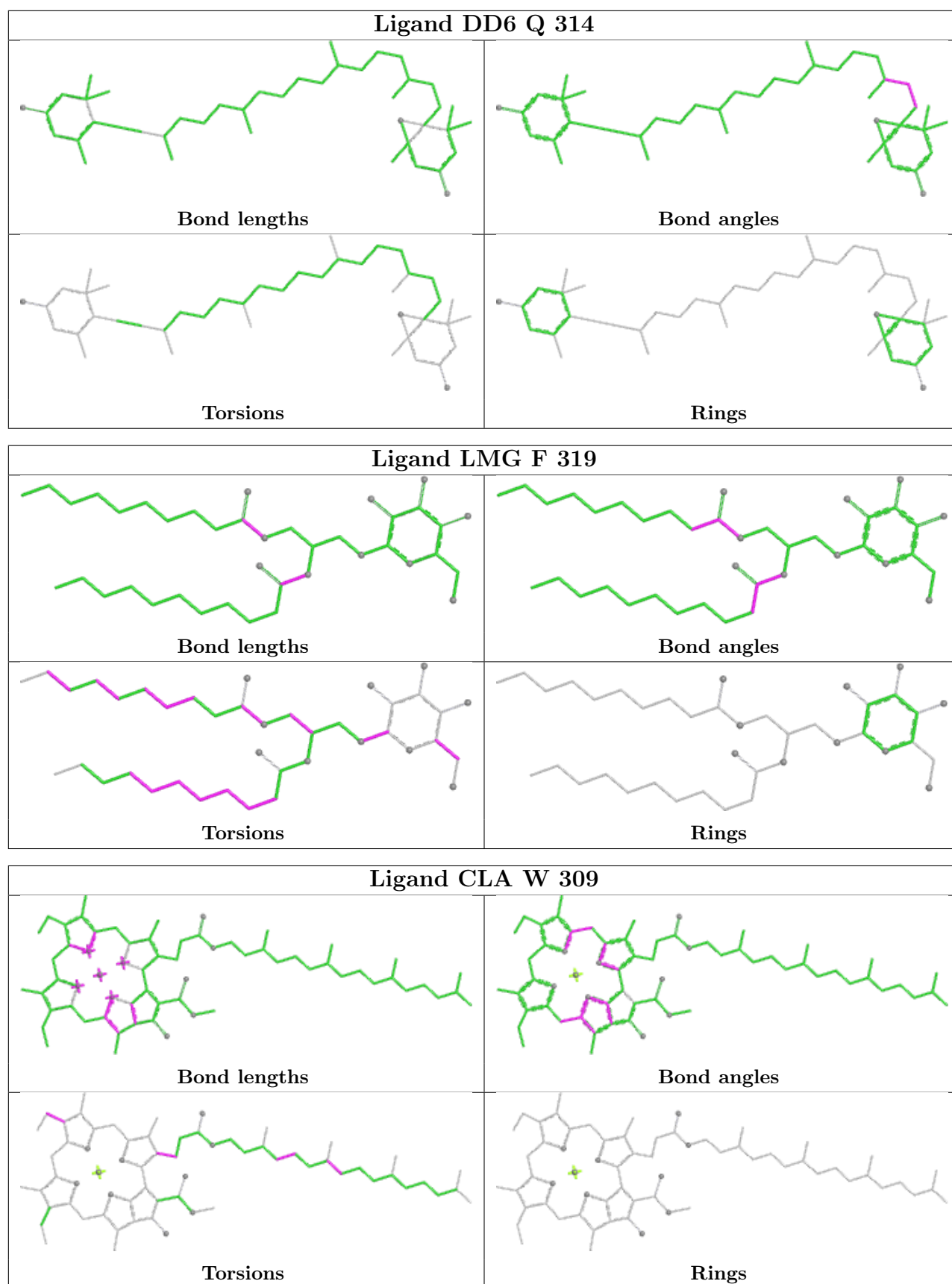
Bond angles



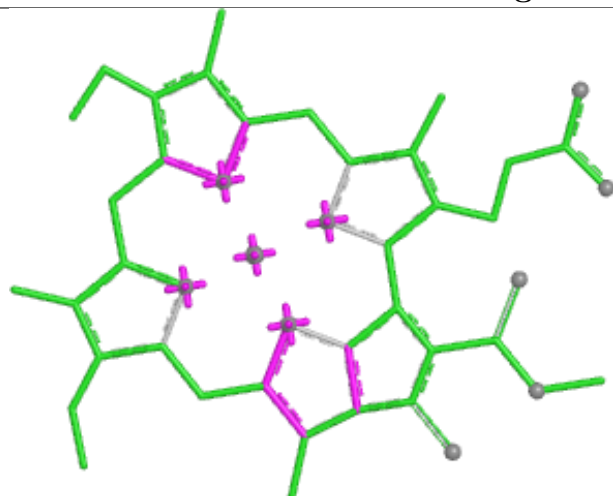
Torsions



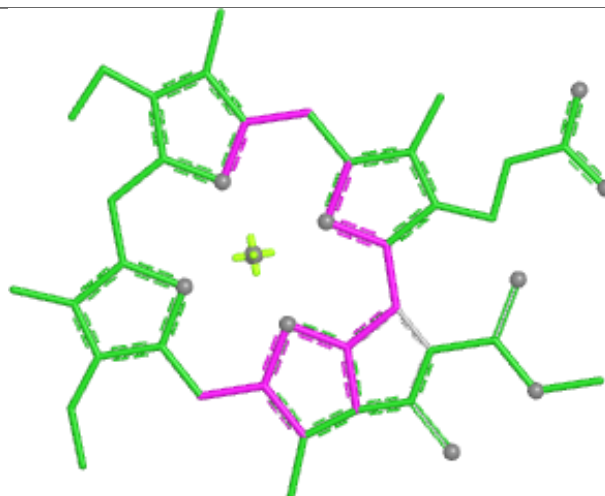
Rings



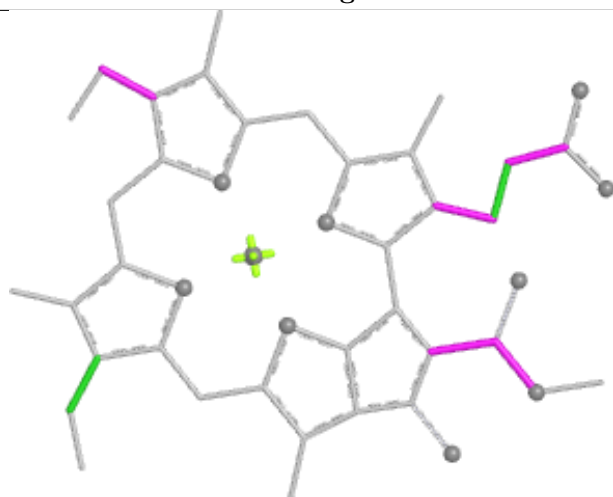
Ligand CLA T 305



Bond lengths



Bond angles

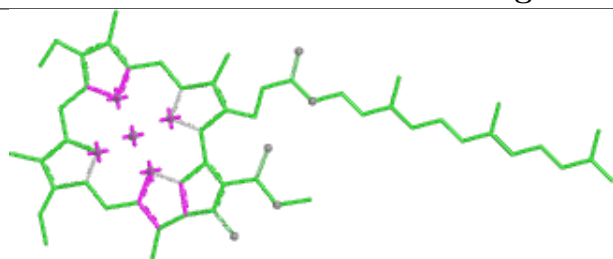


Torsions

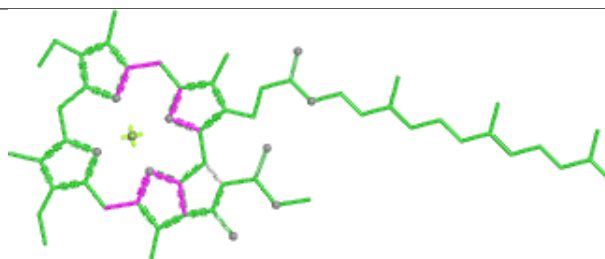


Rings

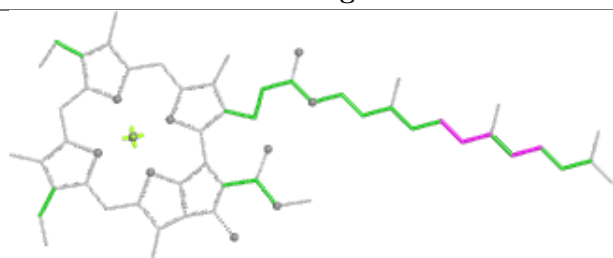
Ligand CLA T 306



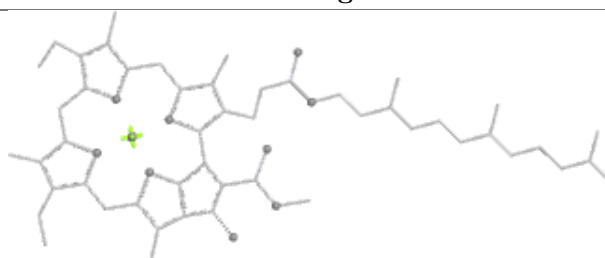
Bond lengths



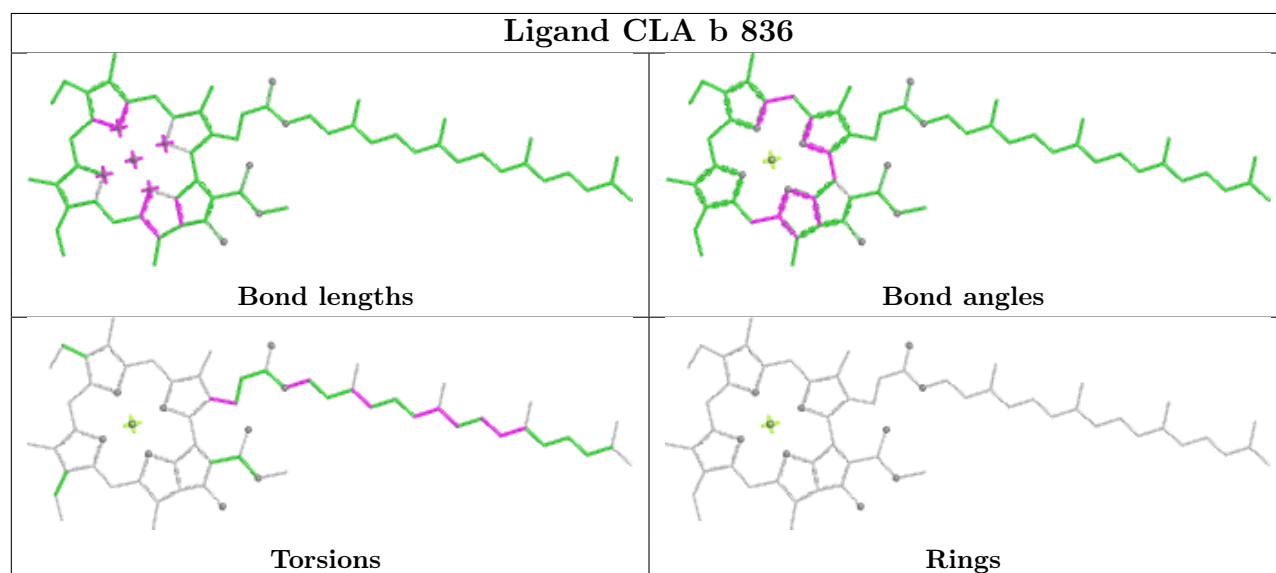
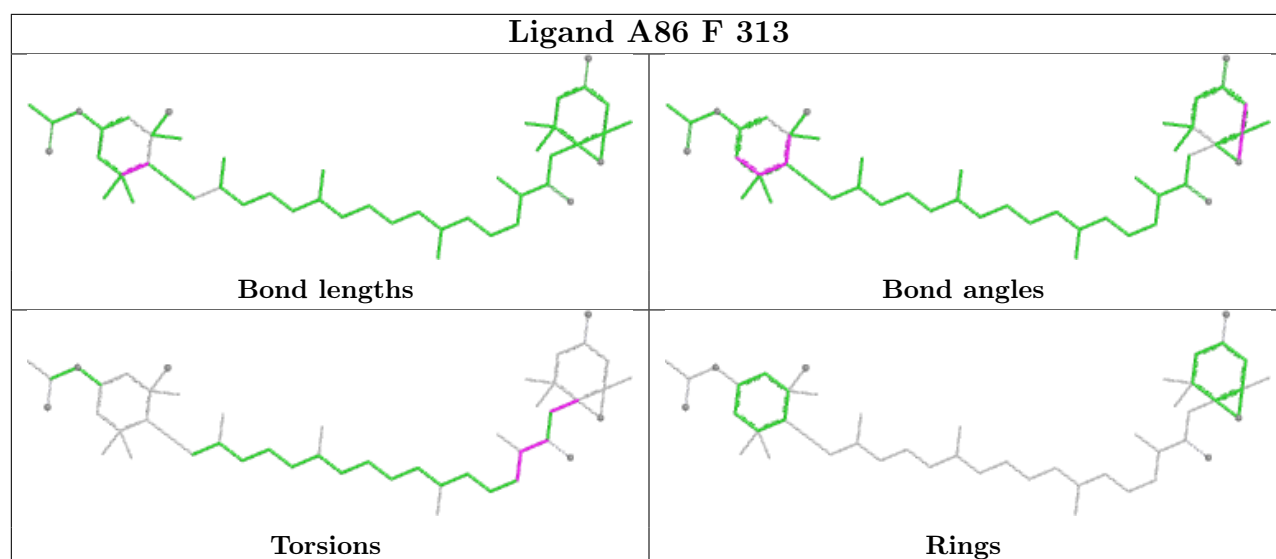
Bond angles



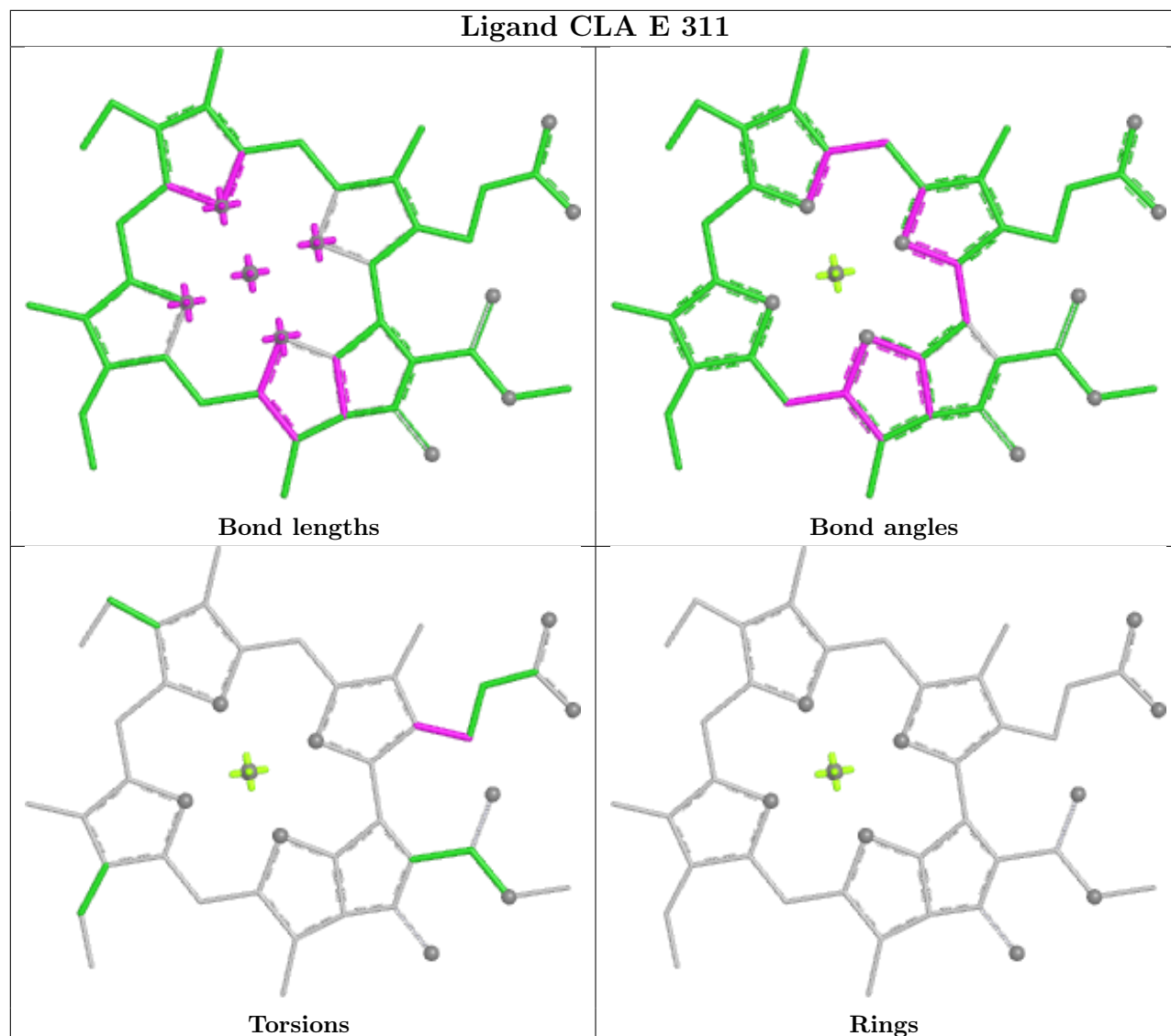
Torsions



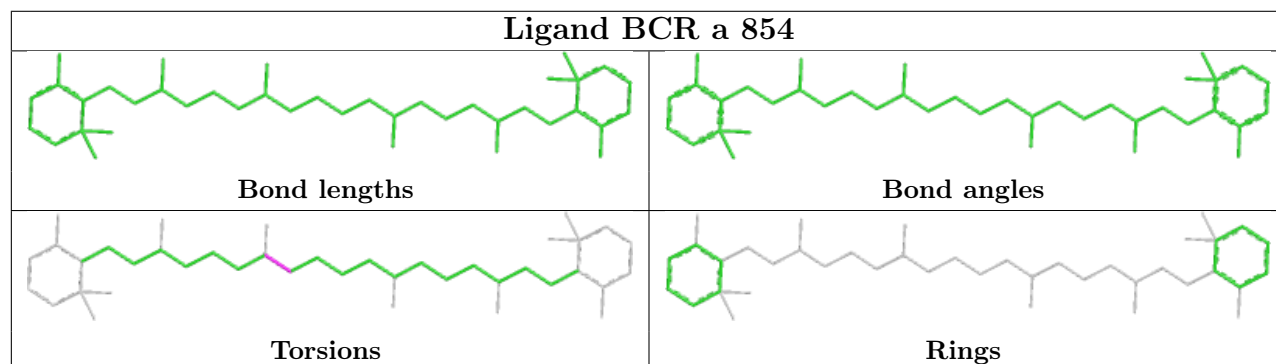
Rings

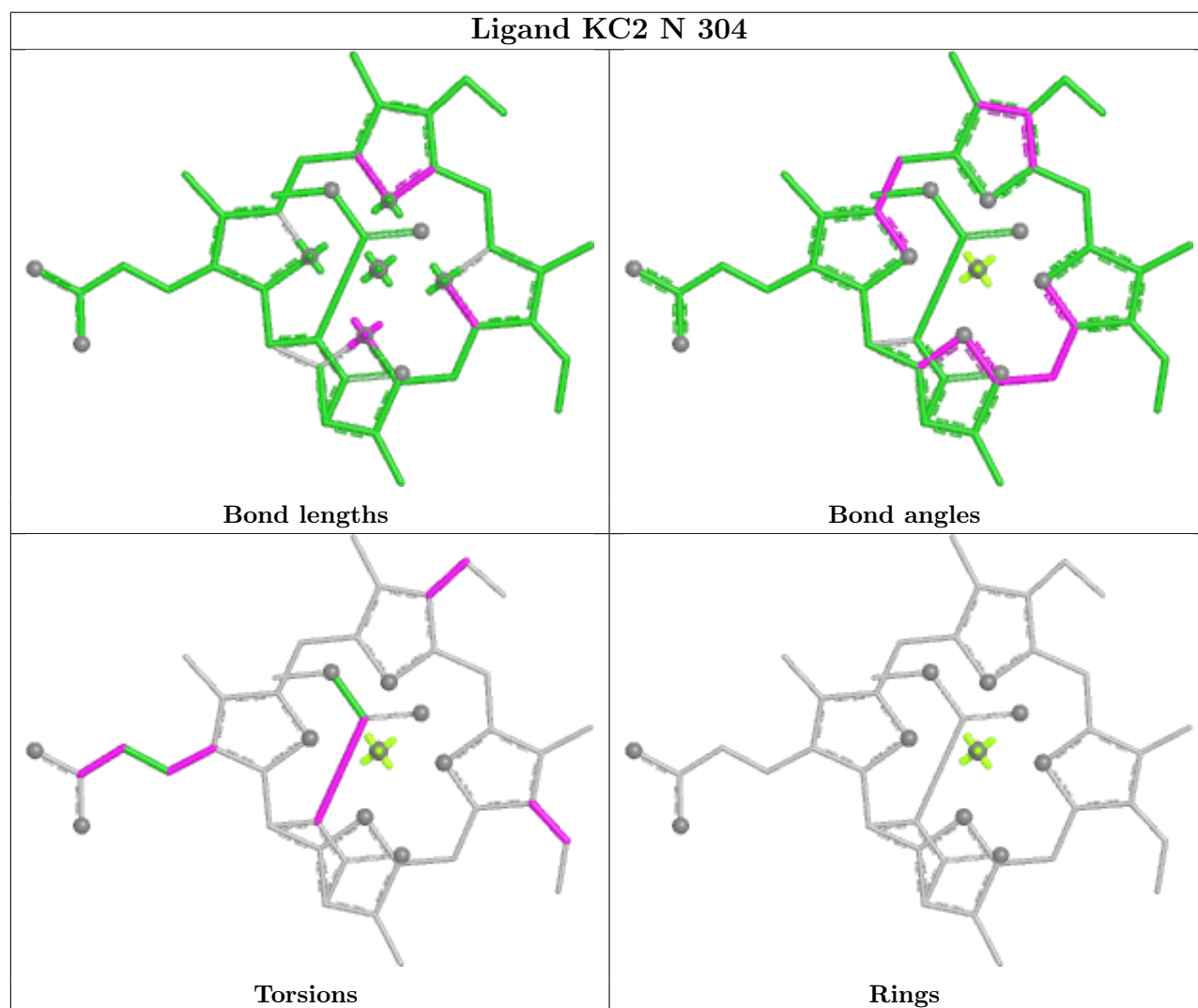
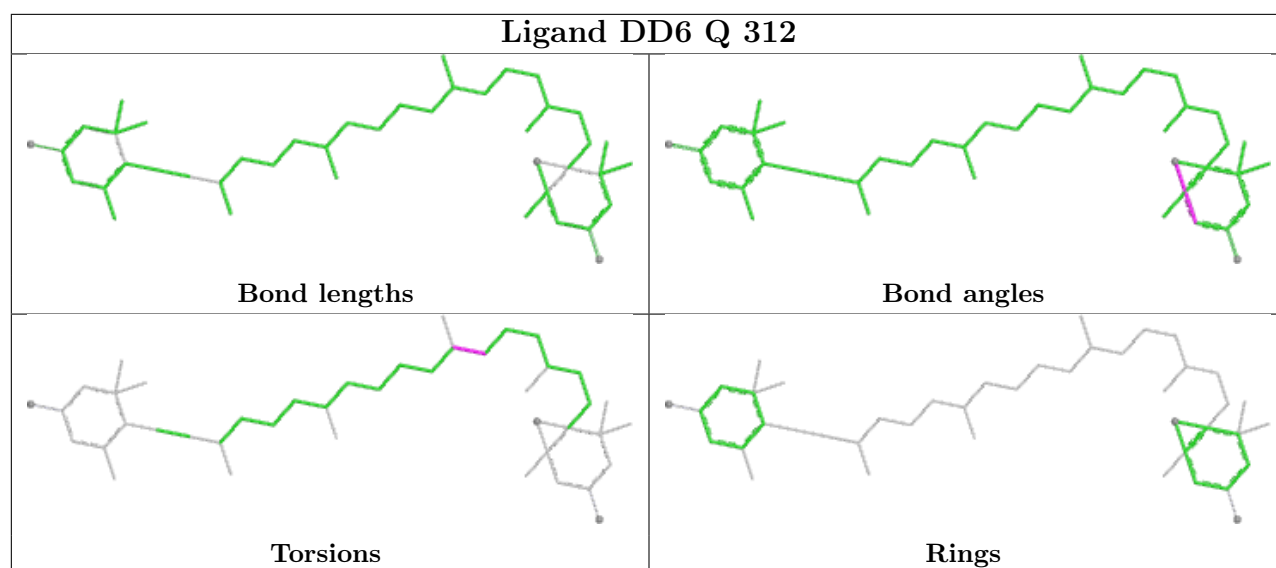


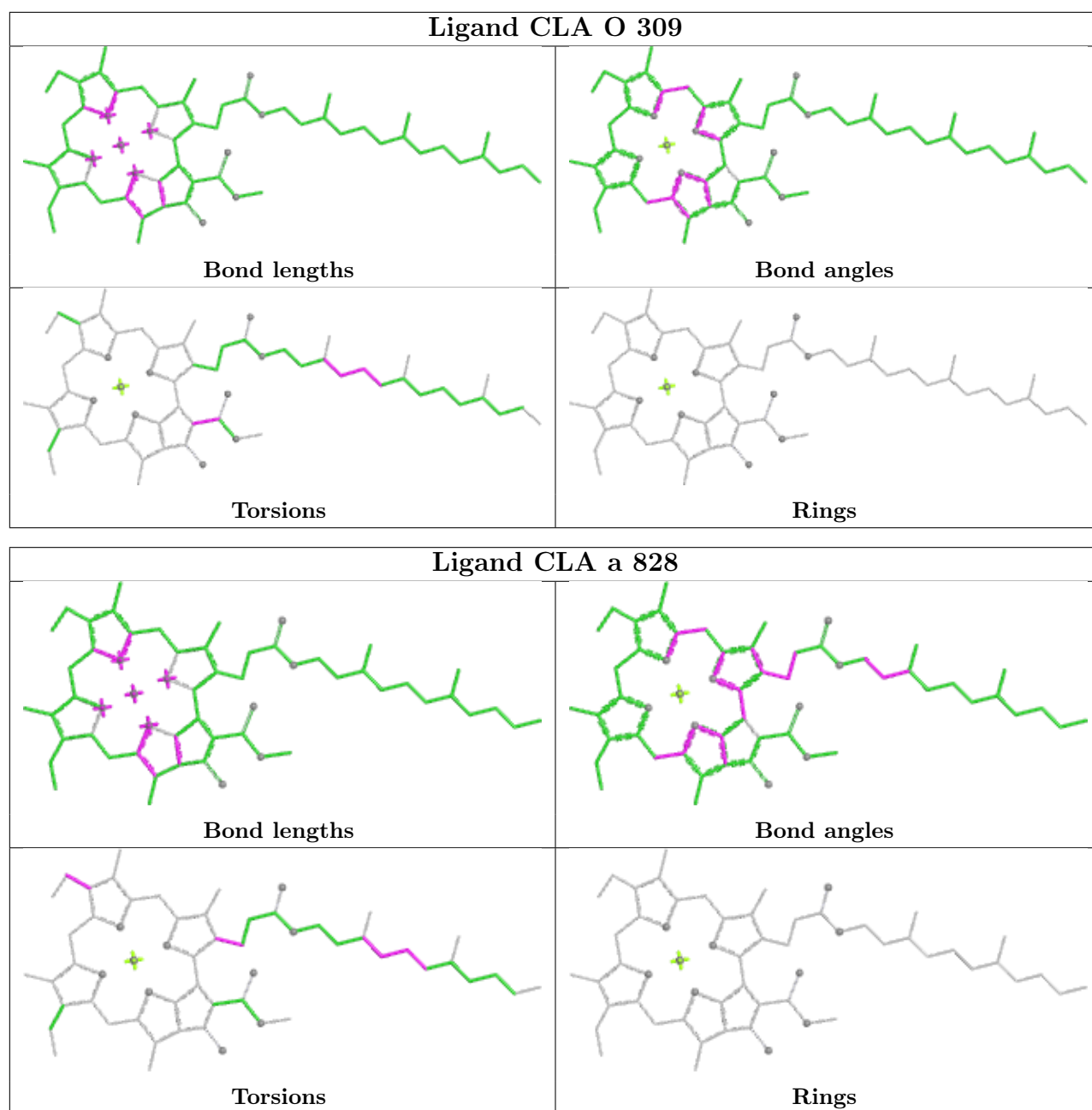
Ligand CLA E 311

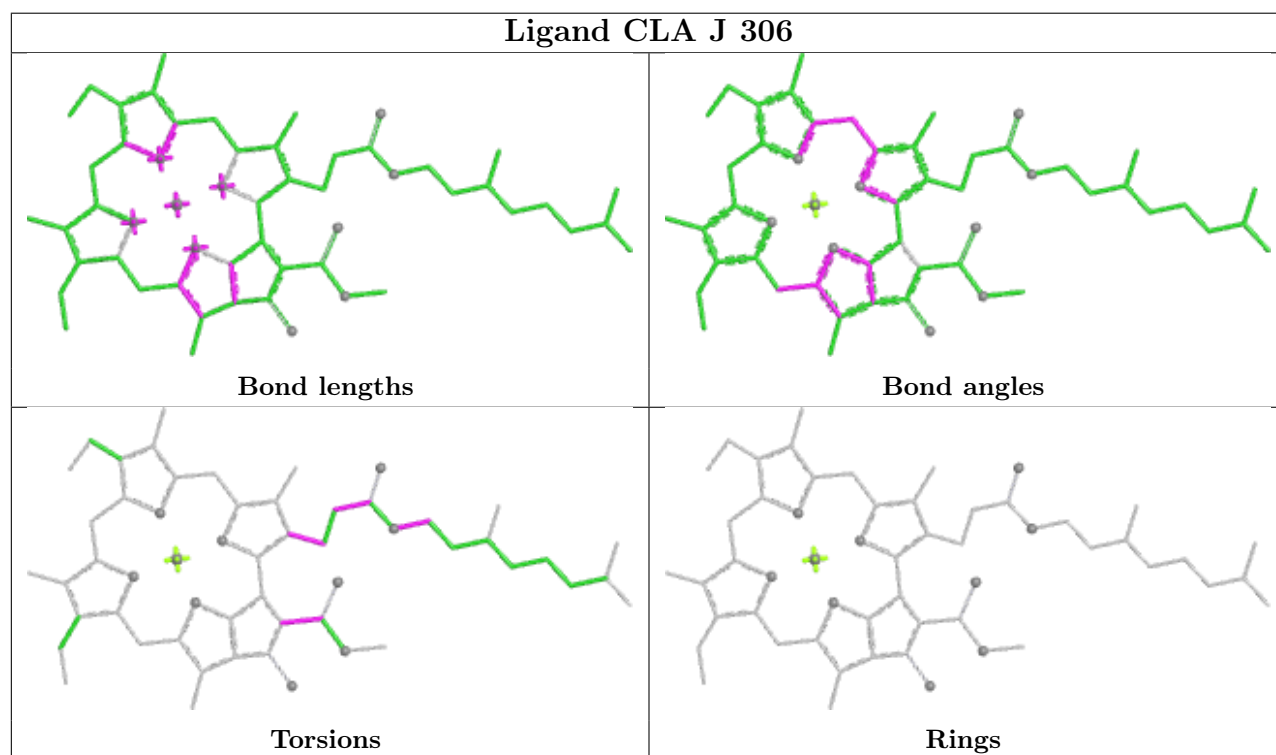
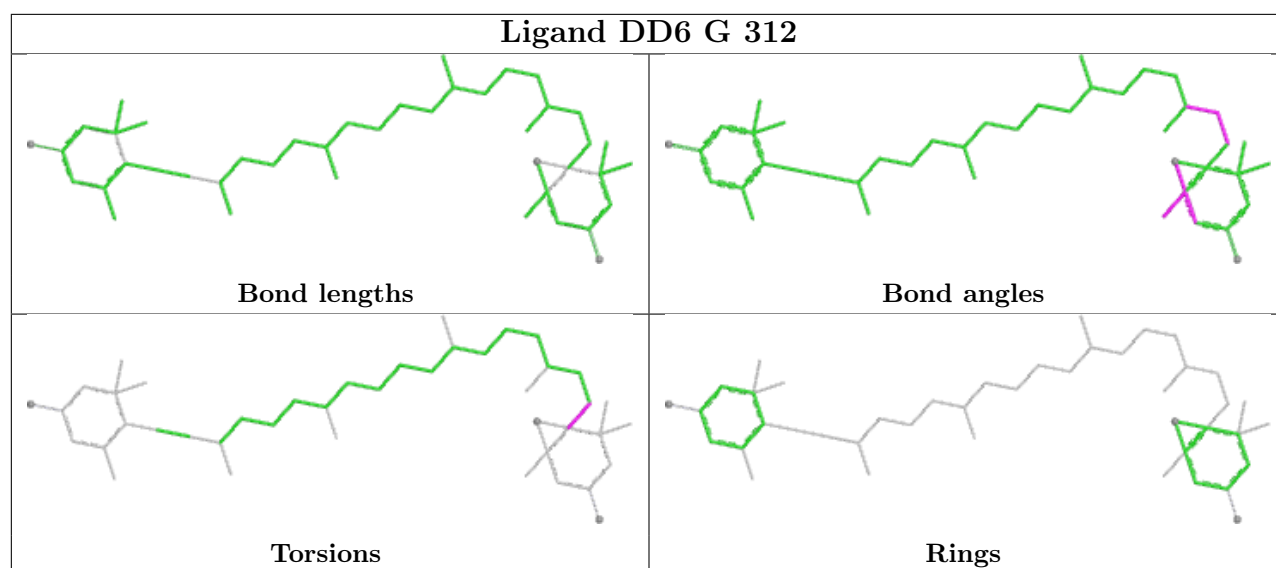


Ligand BCR a 854

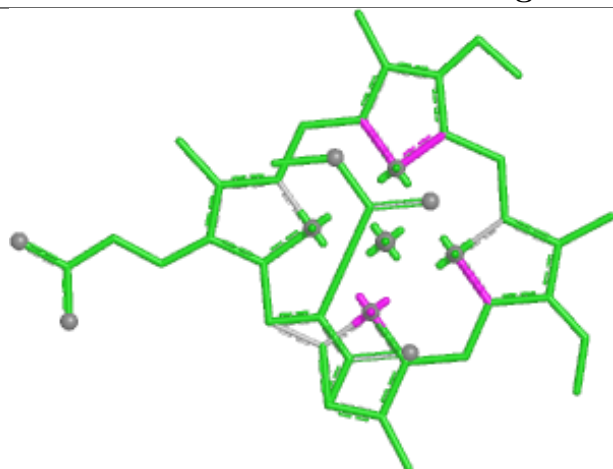




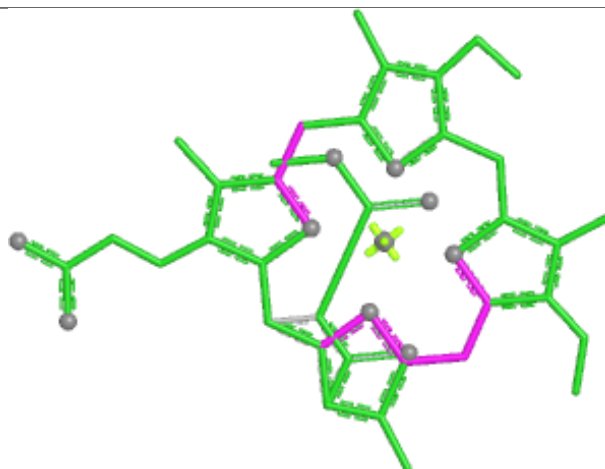




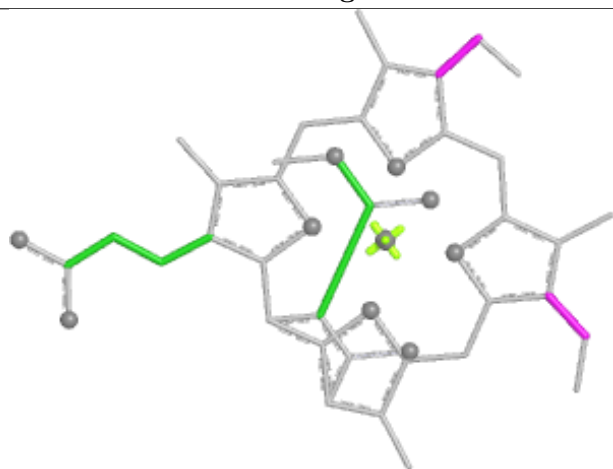
Ligand KC2 A 310



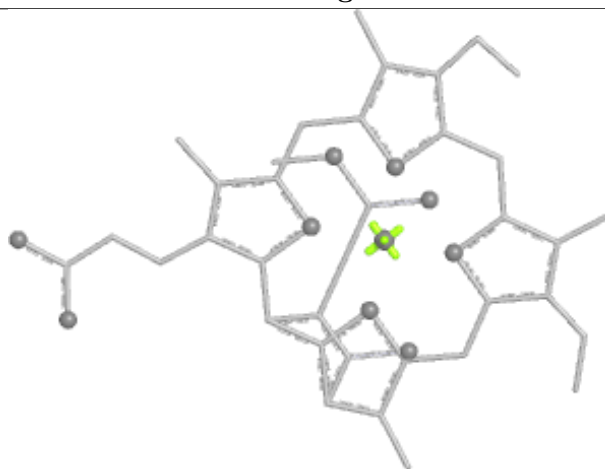
Bond lengths



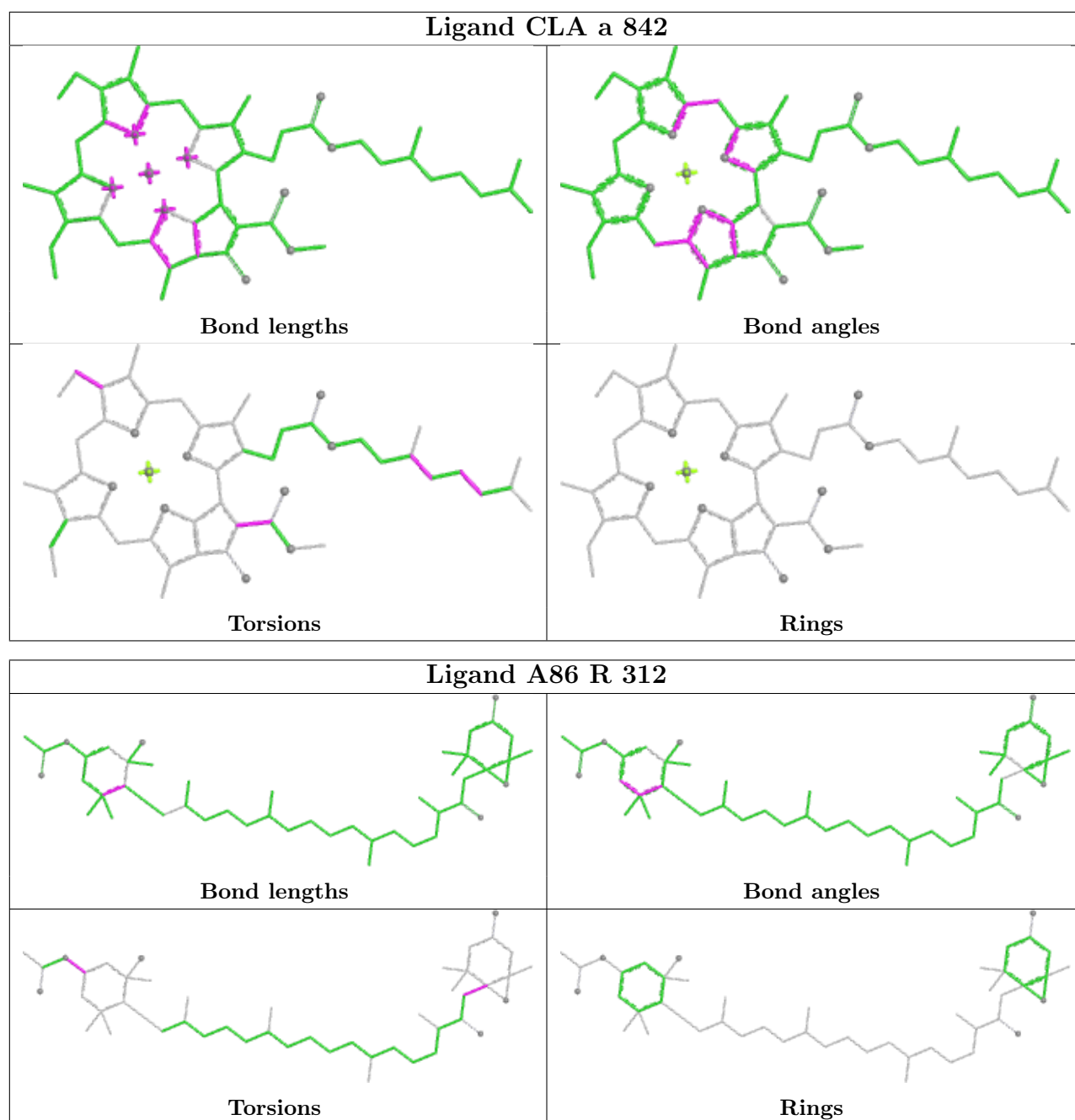
Bond angles



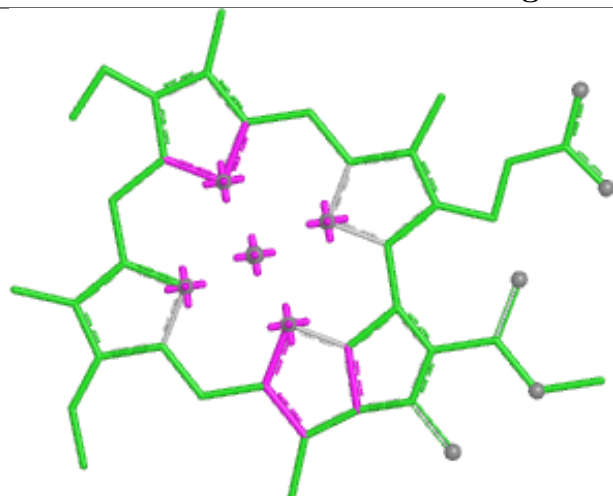
Torsions



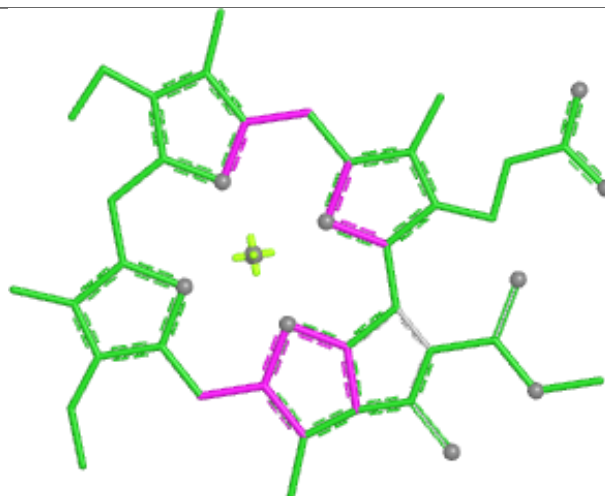
Rings



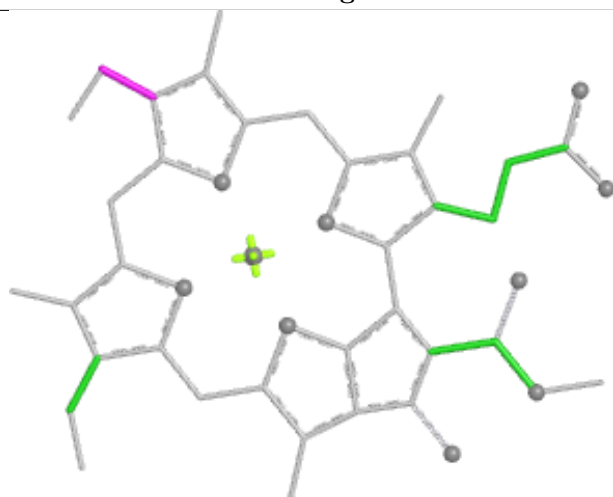
Ligand CLA f 203



Bond lengths



Bond angles

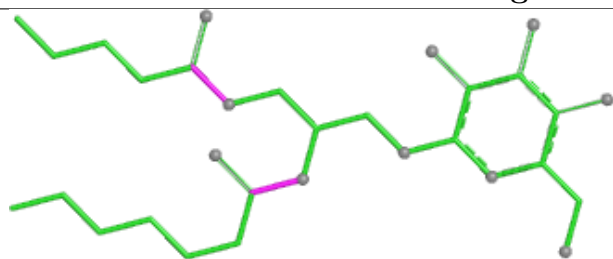


Torsions

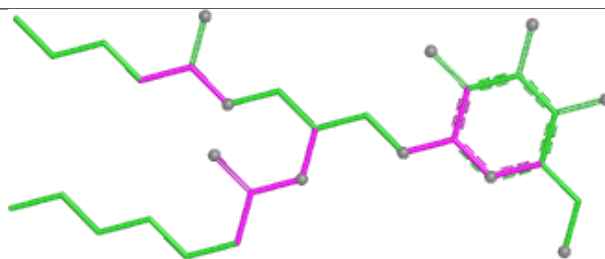


Rings

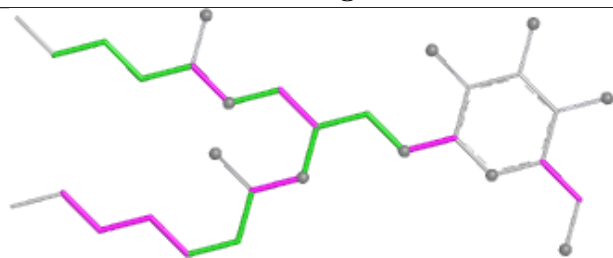
Ligand LMG E 320



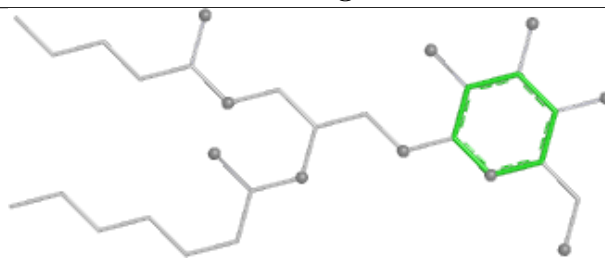
Bond lengths



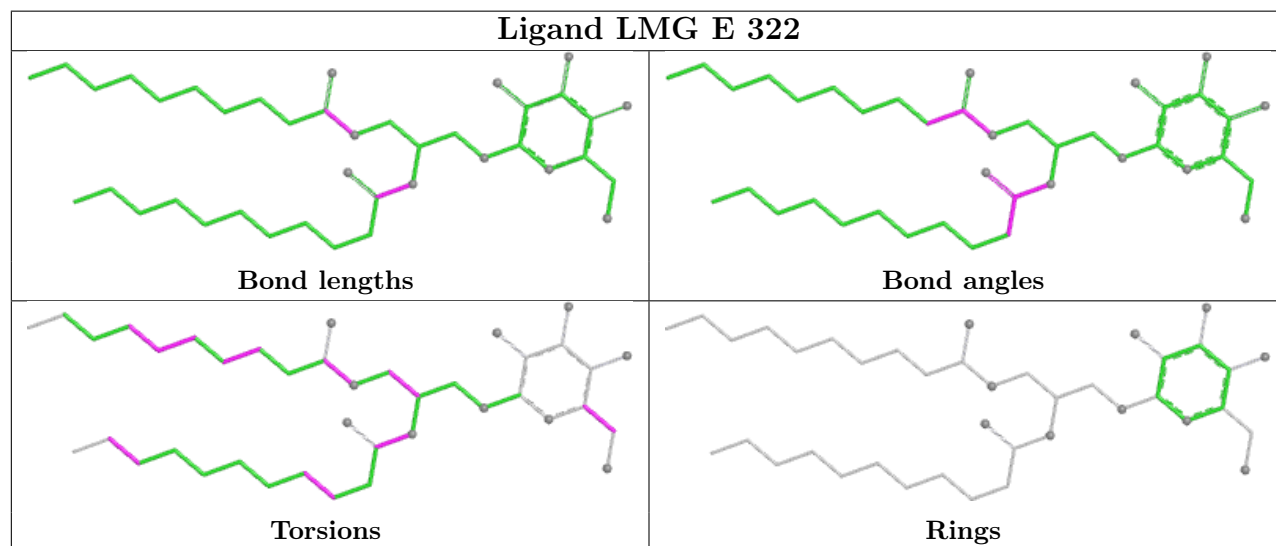
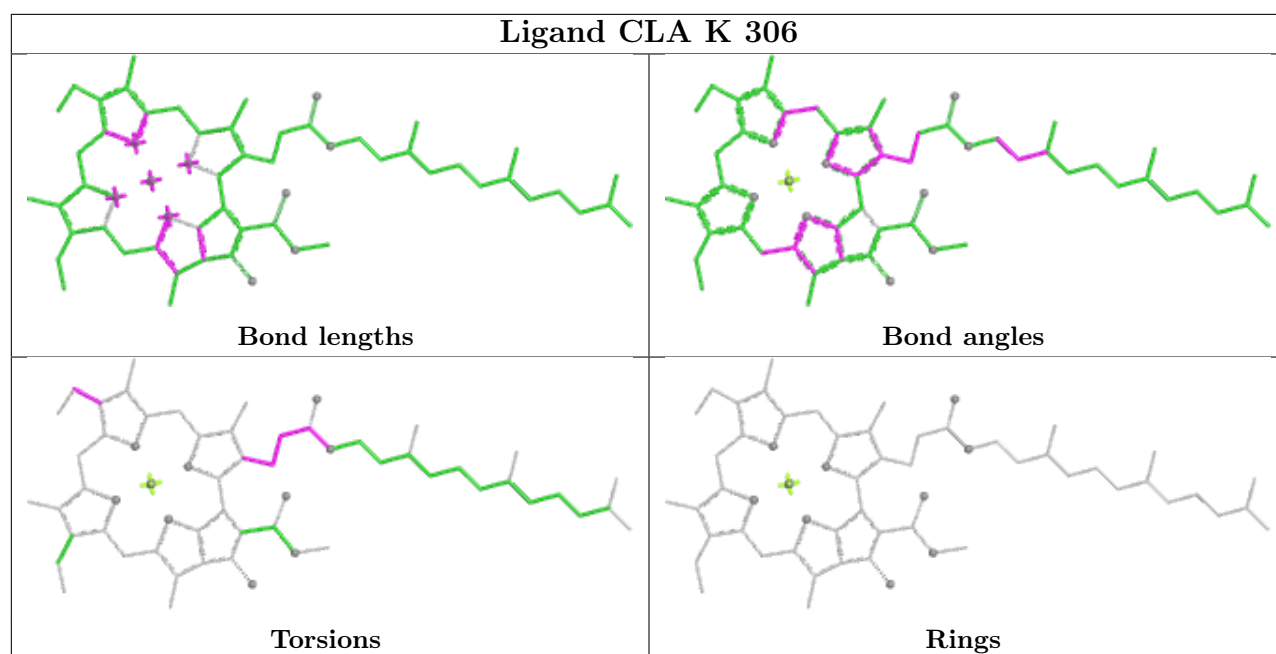
Bond angles



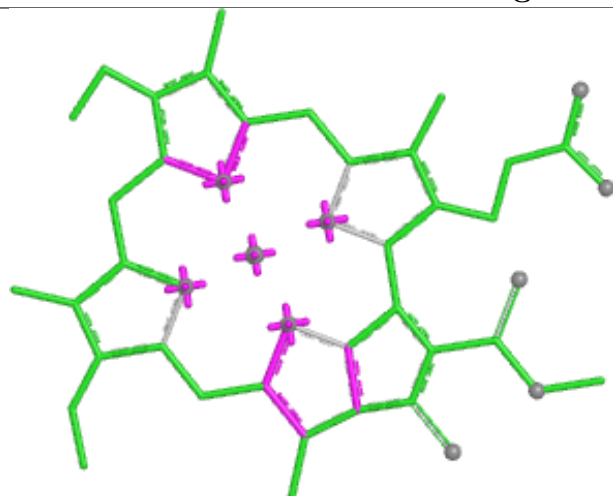
Torsions



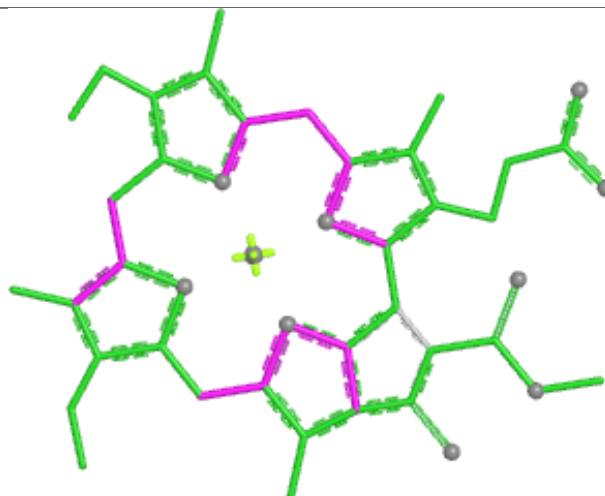
Rings



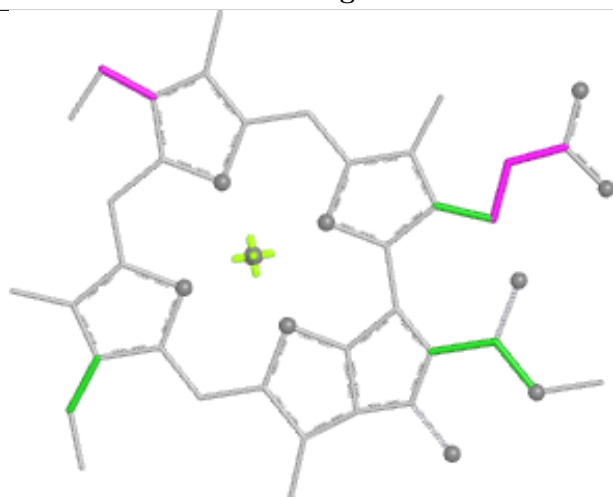
Ligand CLA A 301



Bond lengths



Bond angles

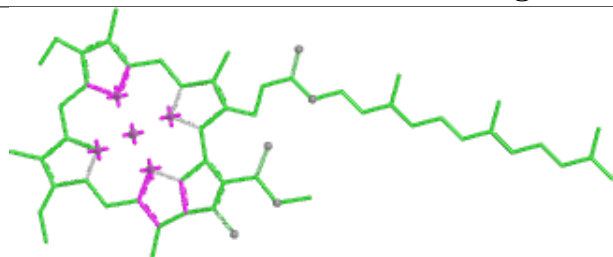


Torsions

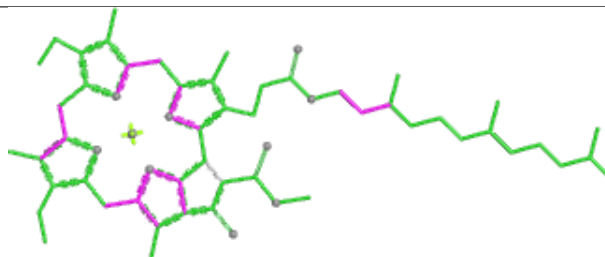


Rings

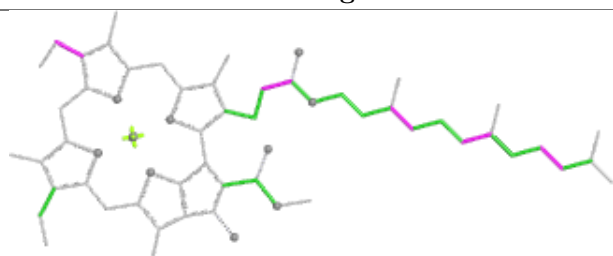
Ligand CLA D 304



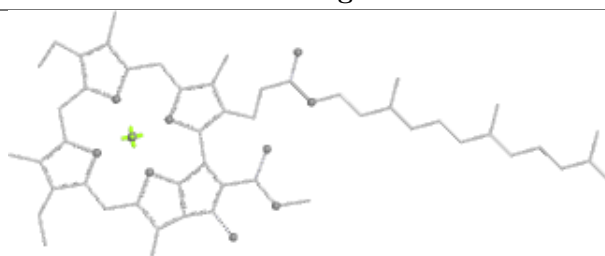
Bond lengths



Bond angles

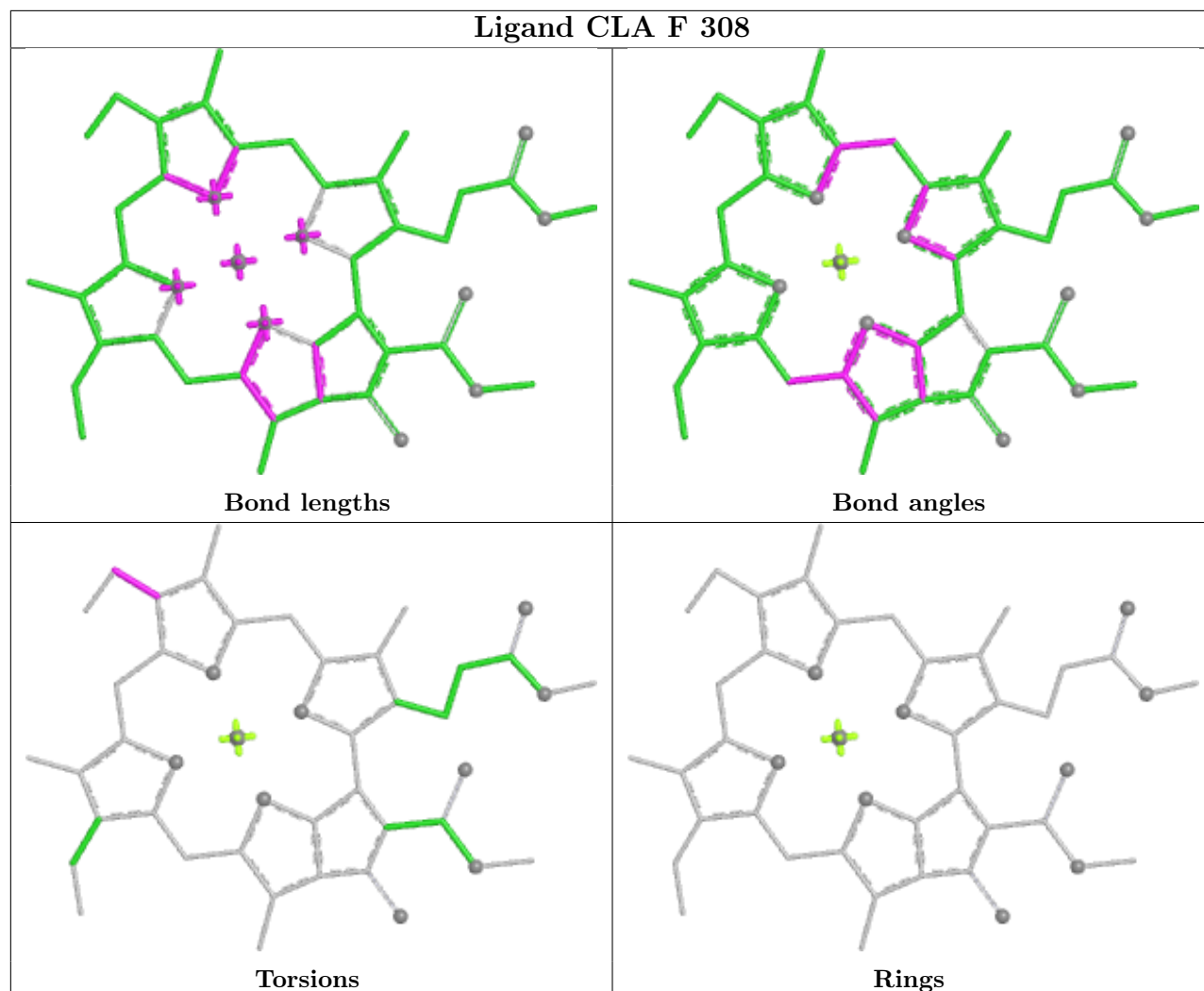


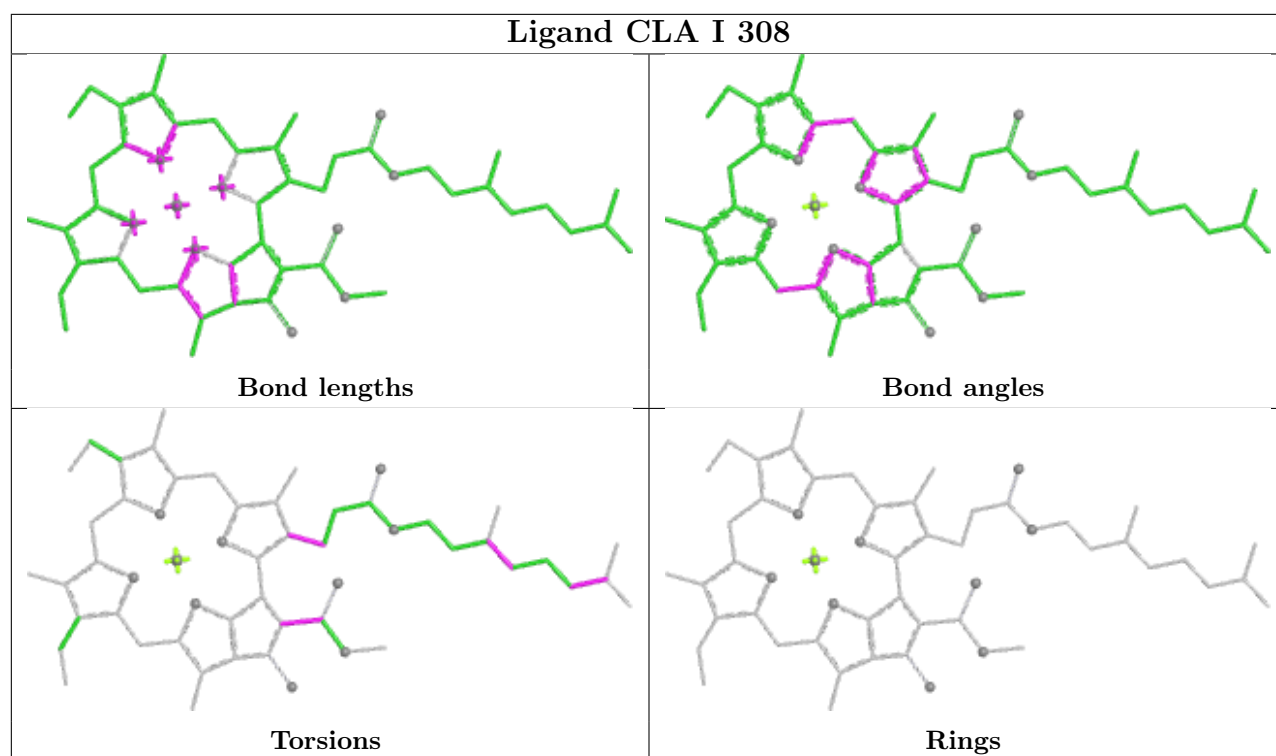
Torsions



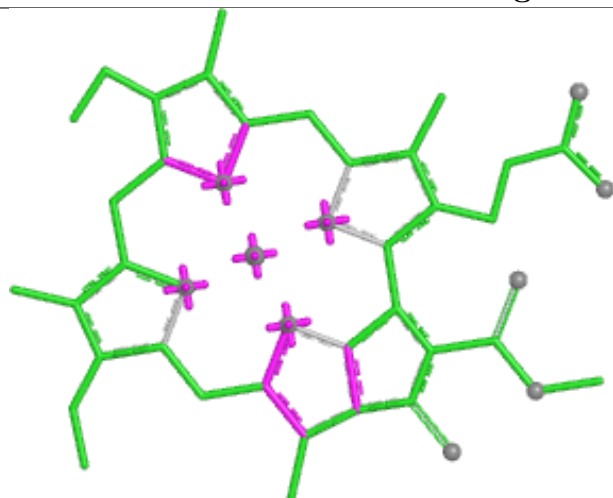
Rings

Ligand CLA F 308

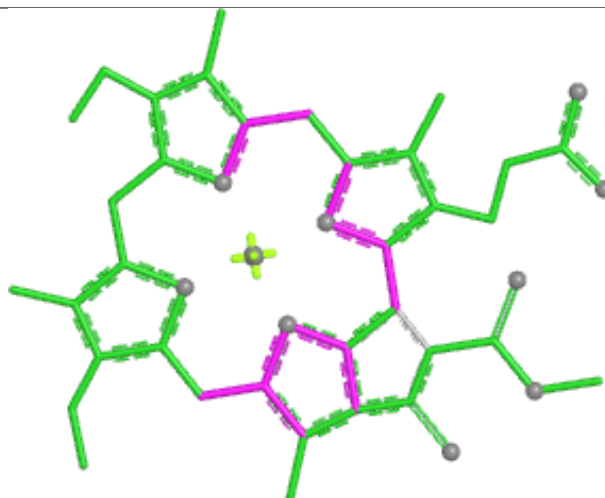




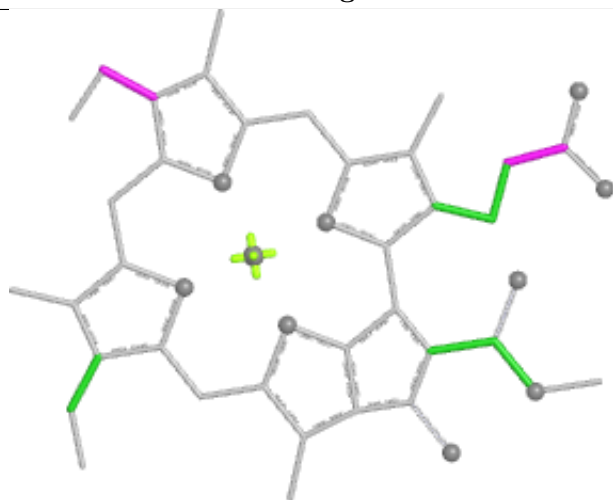
Ligand CLA O 308



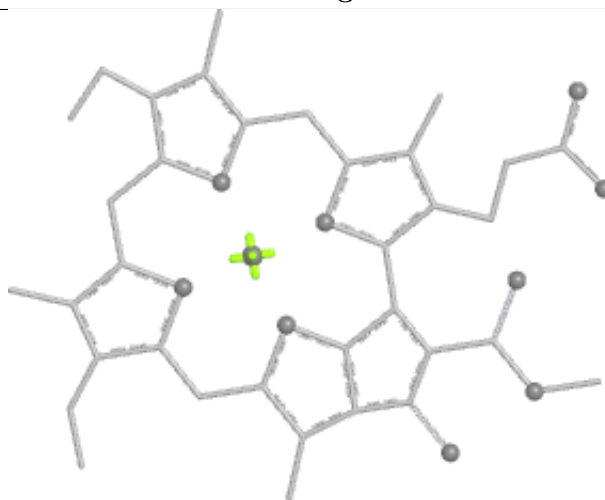
Bond lengths



Bond angles

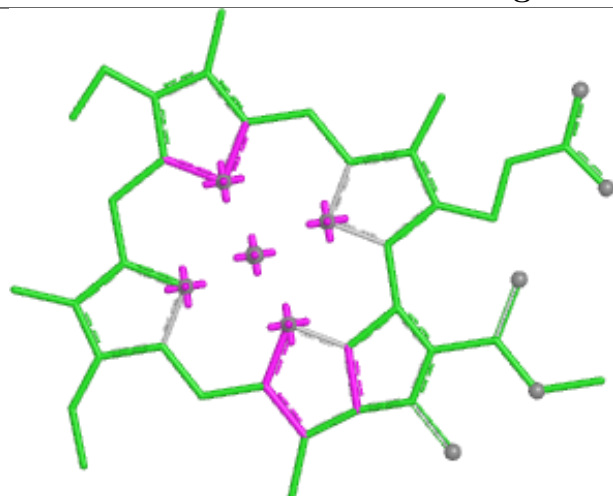


Torsions

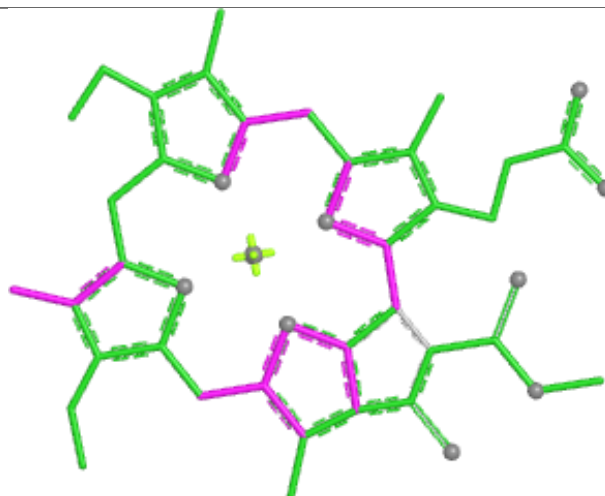


Rings

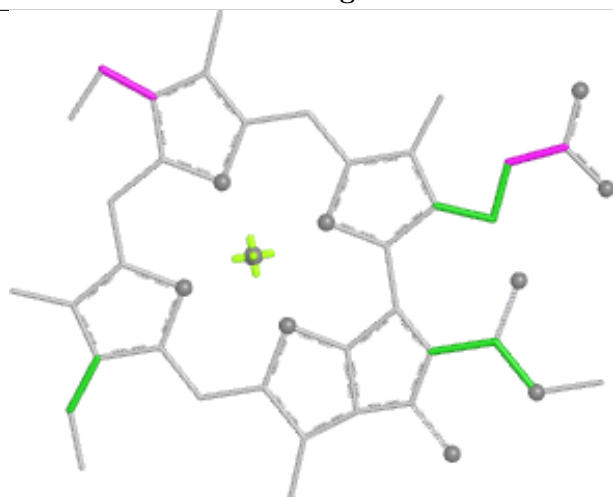
Ligand CLA U 302



Bond lengths



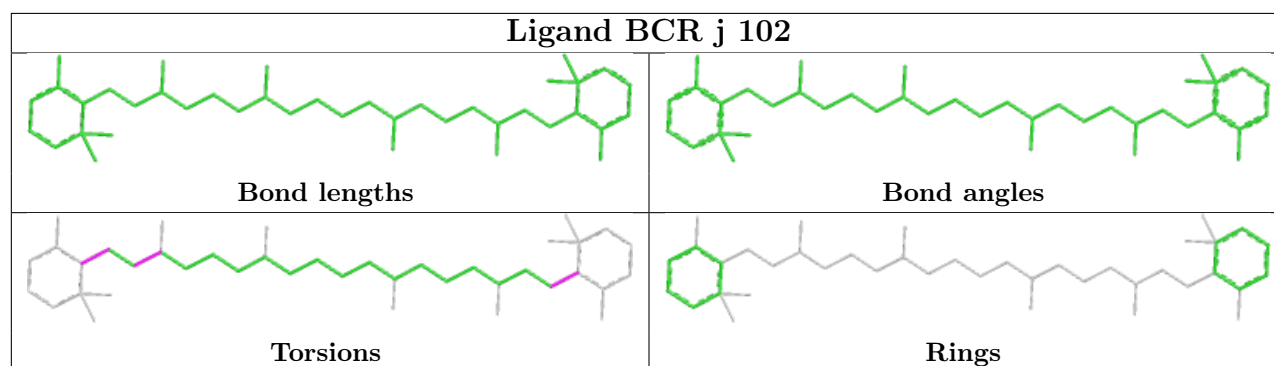
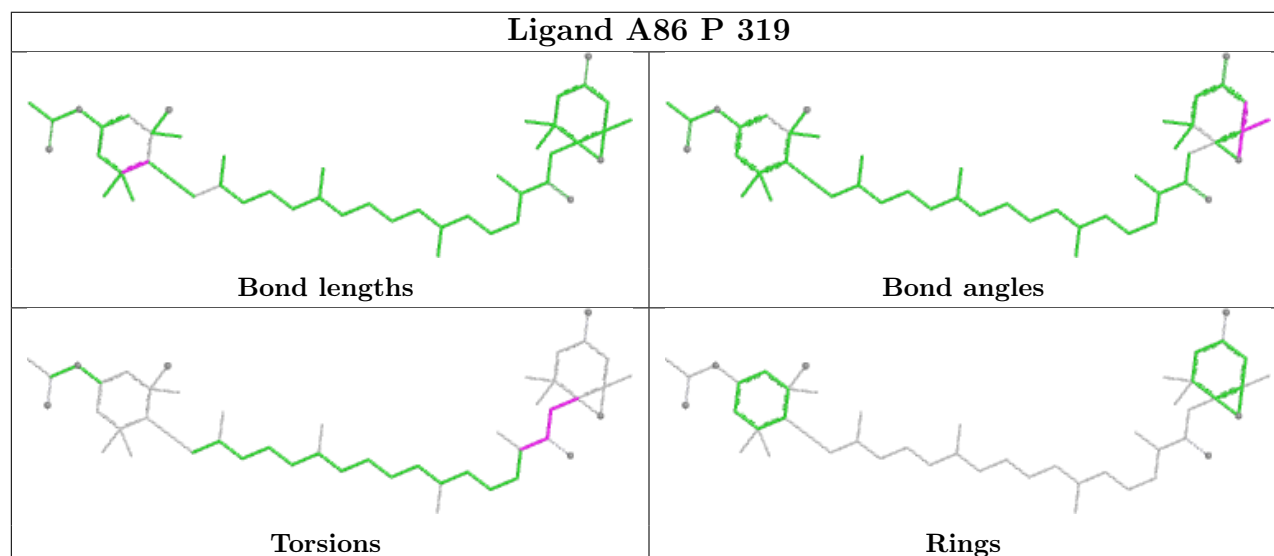
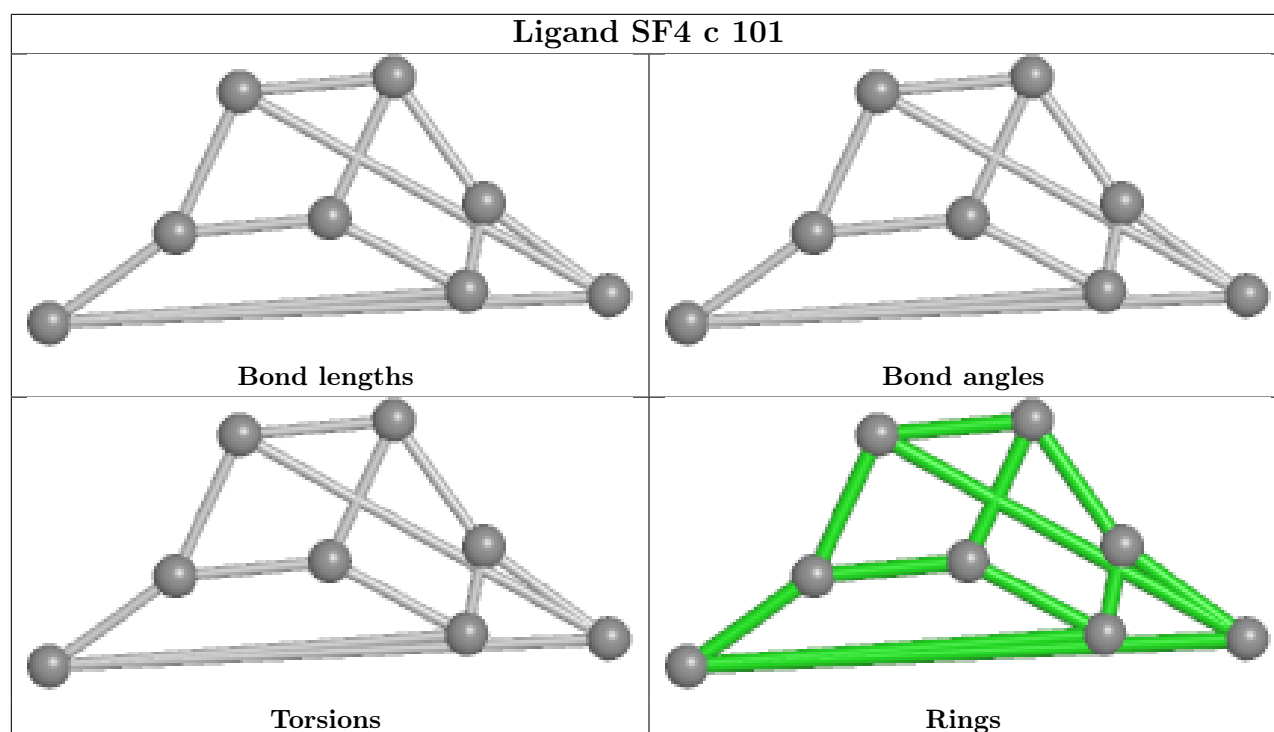
Bond angles

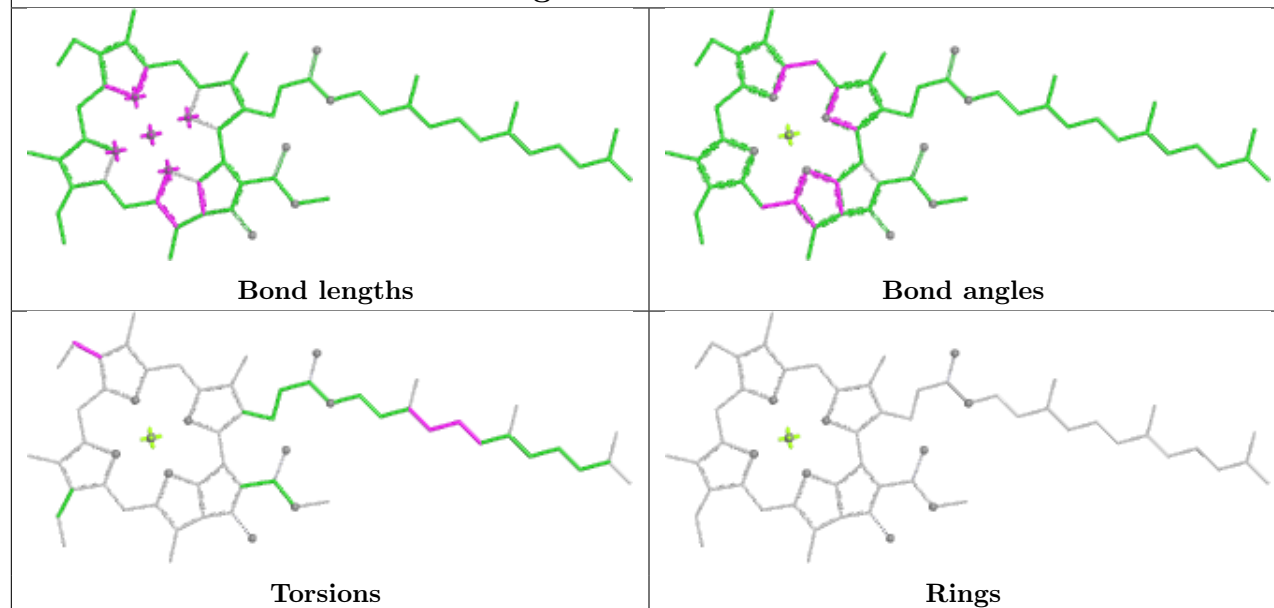
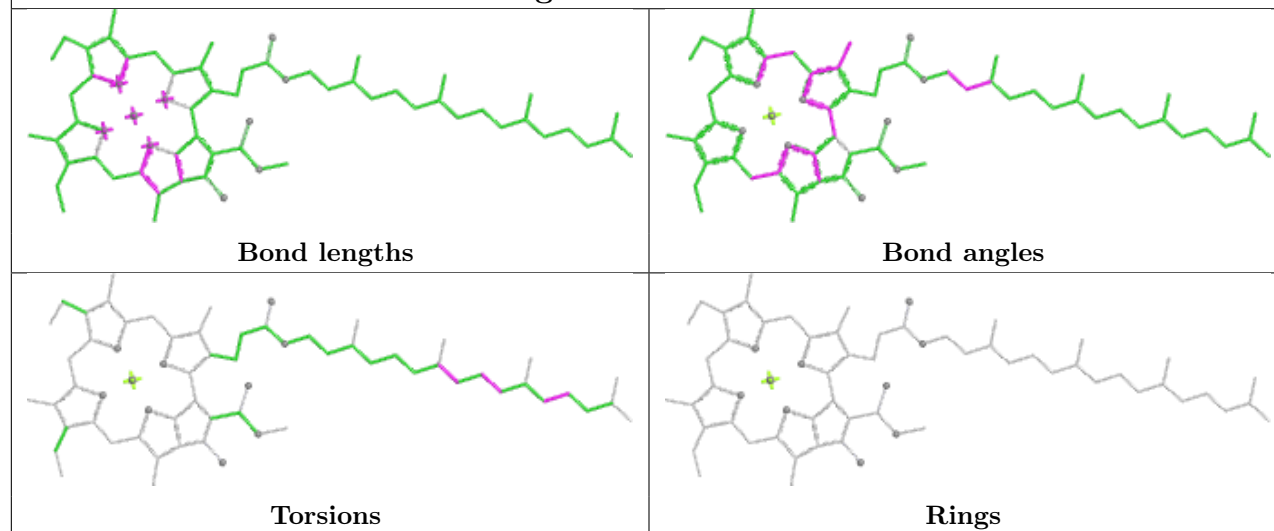


Torsions

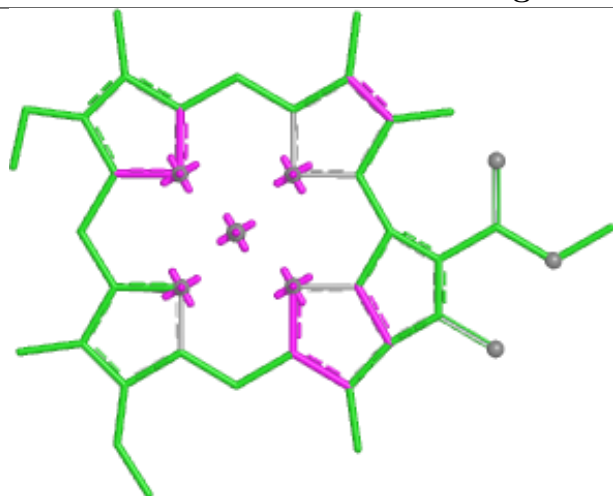


Rings

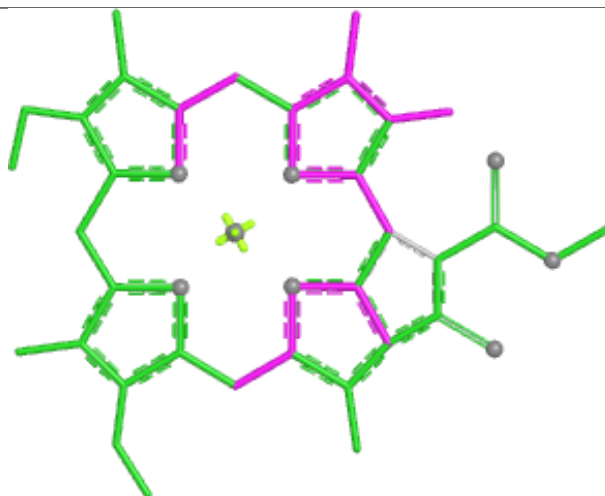


Ligand CLA E 312**Ligand CLA b 819**

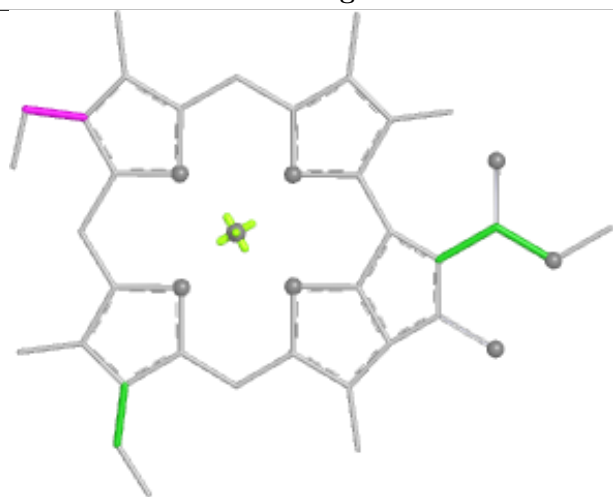
Ligand CLA K 307



Bond lengths



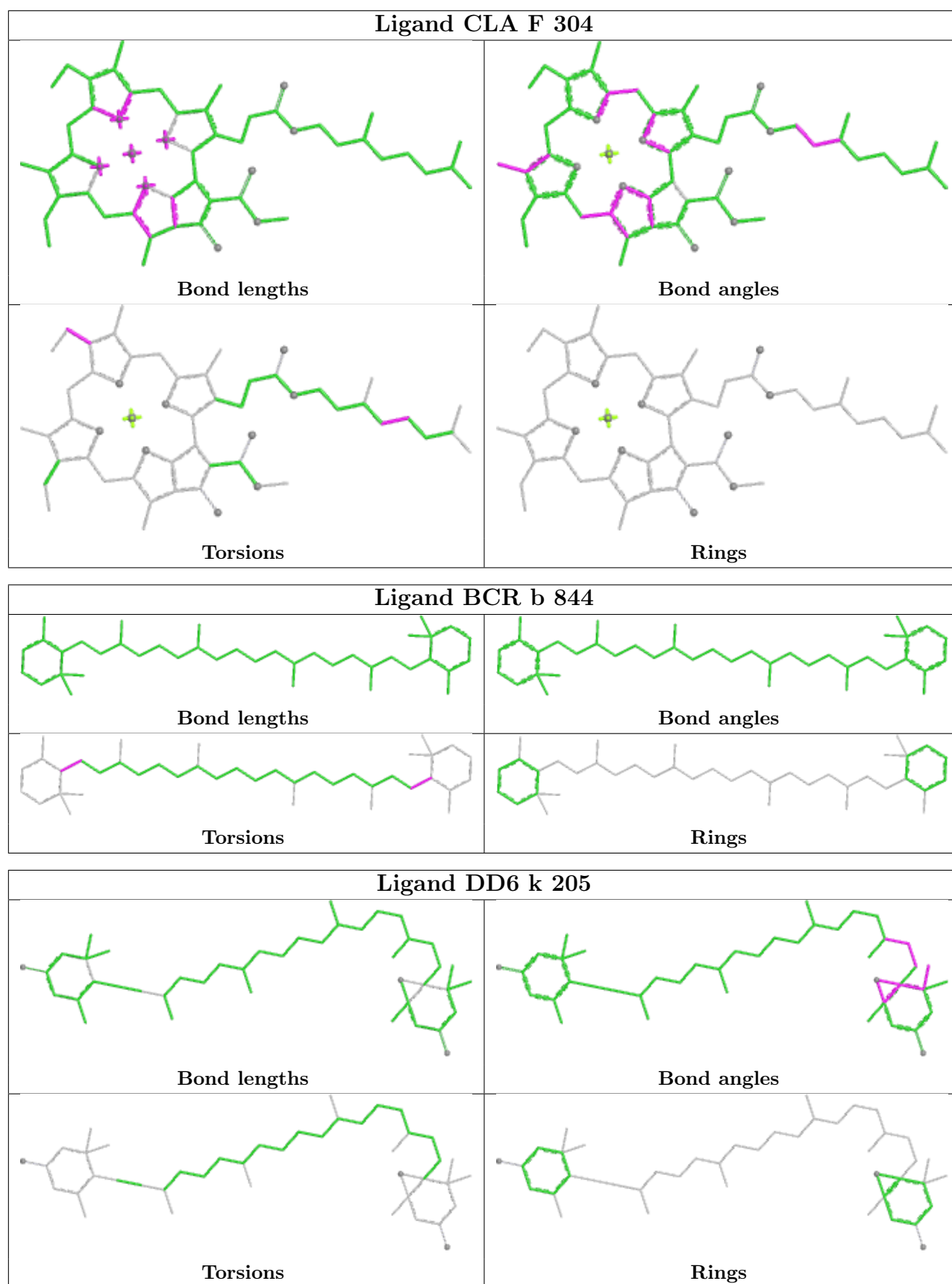
Bond angles

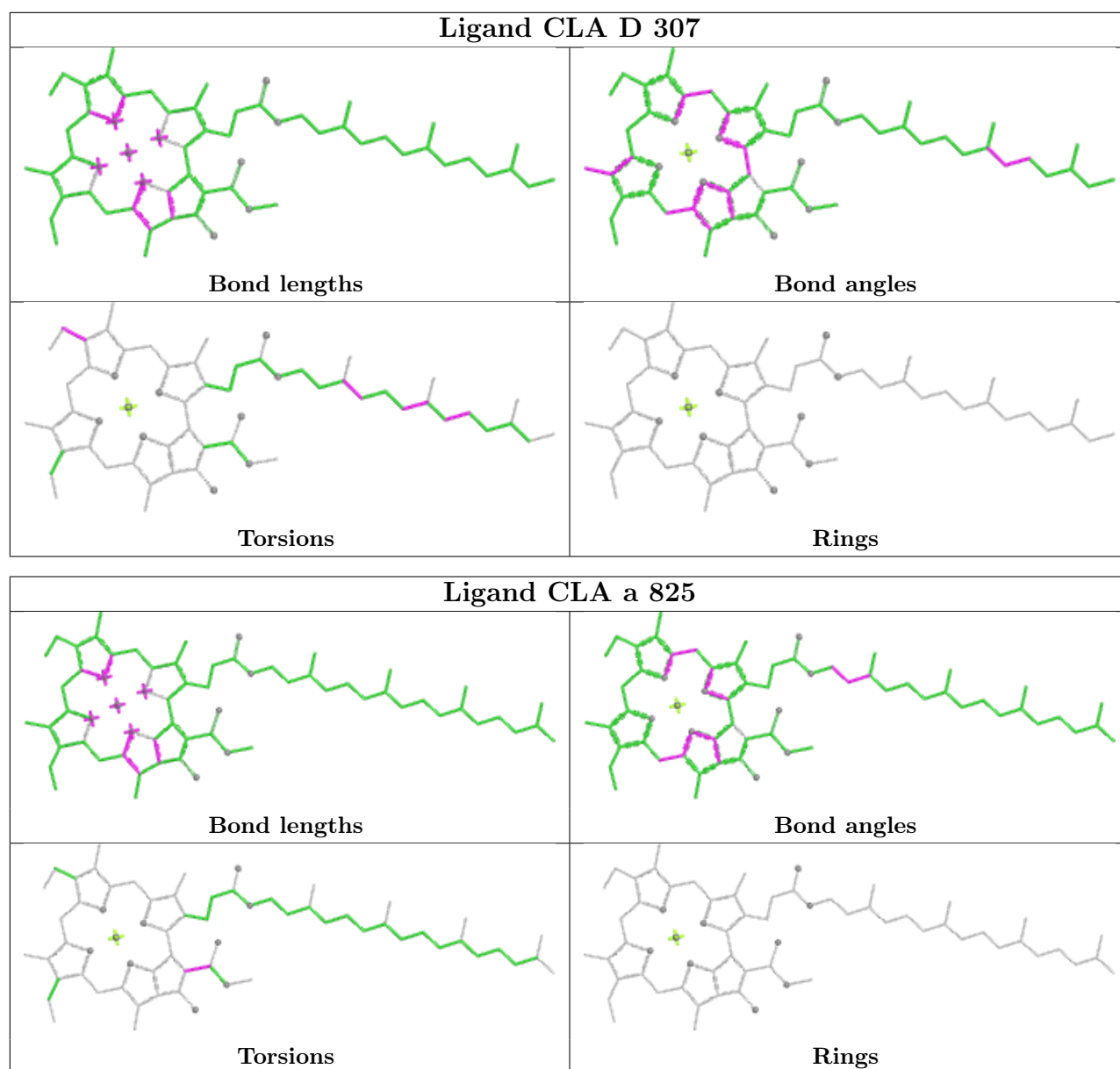


Torsions

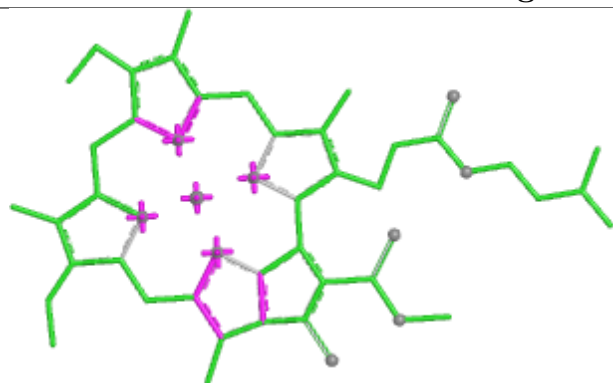


Rings

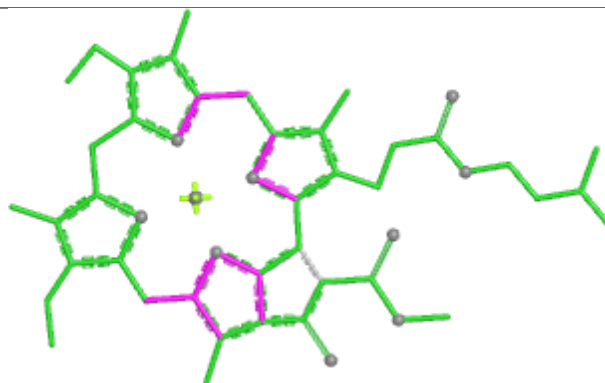




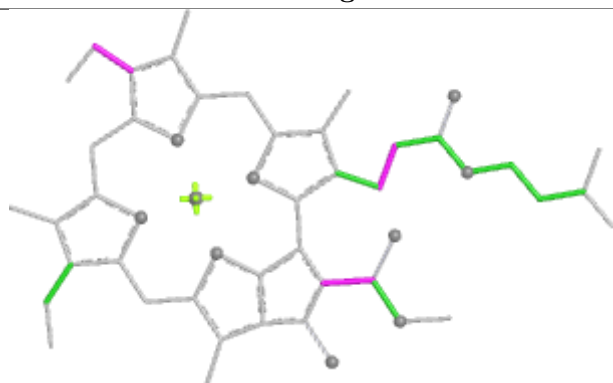
Ligand CLA b 827



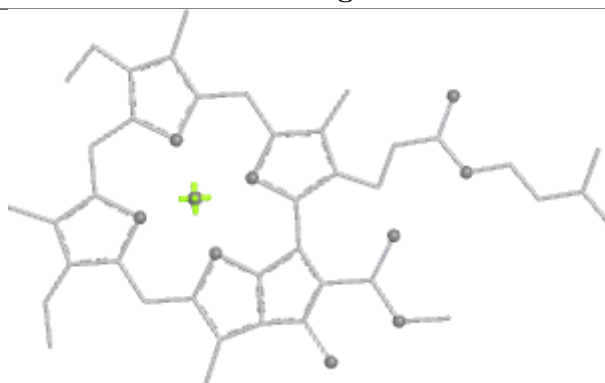
Bond lengths



Bond angles

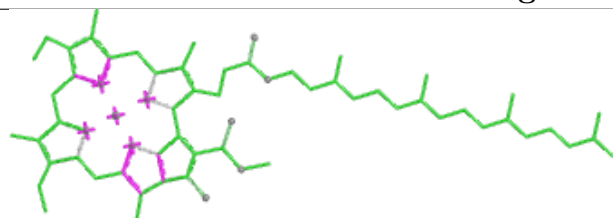


Torsions

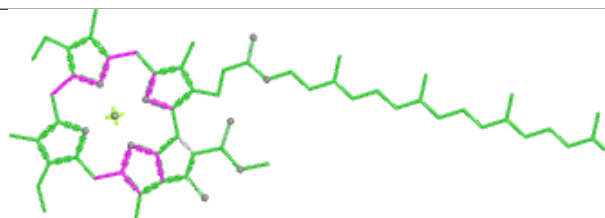


Rings

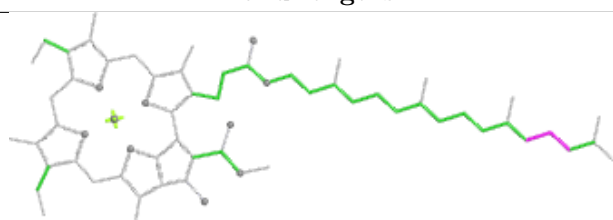
Ligand CLA a 833



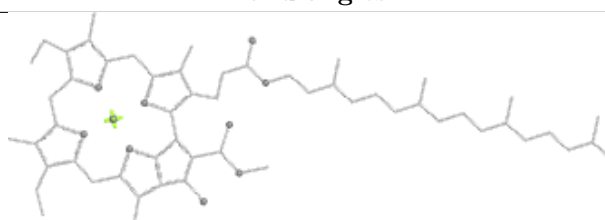
Bond lengths



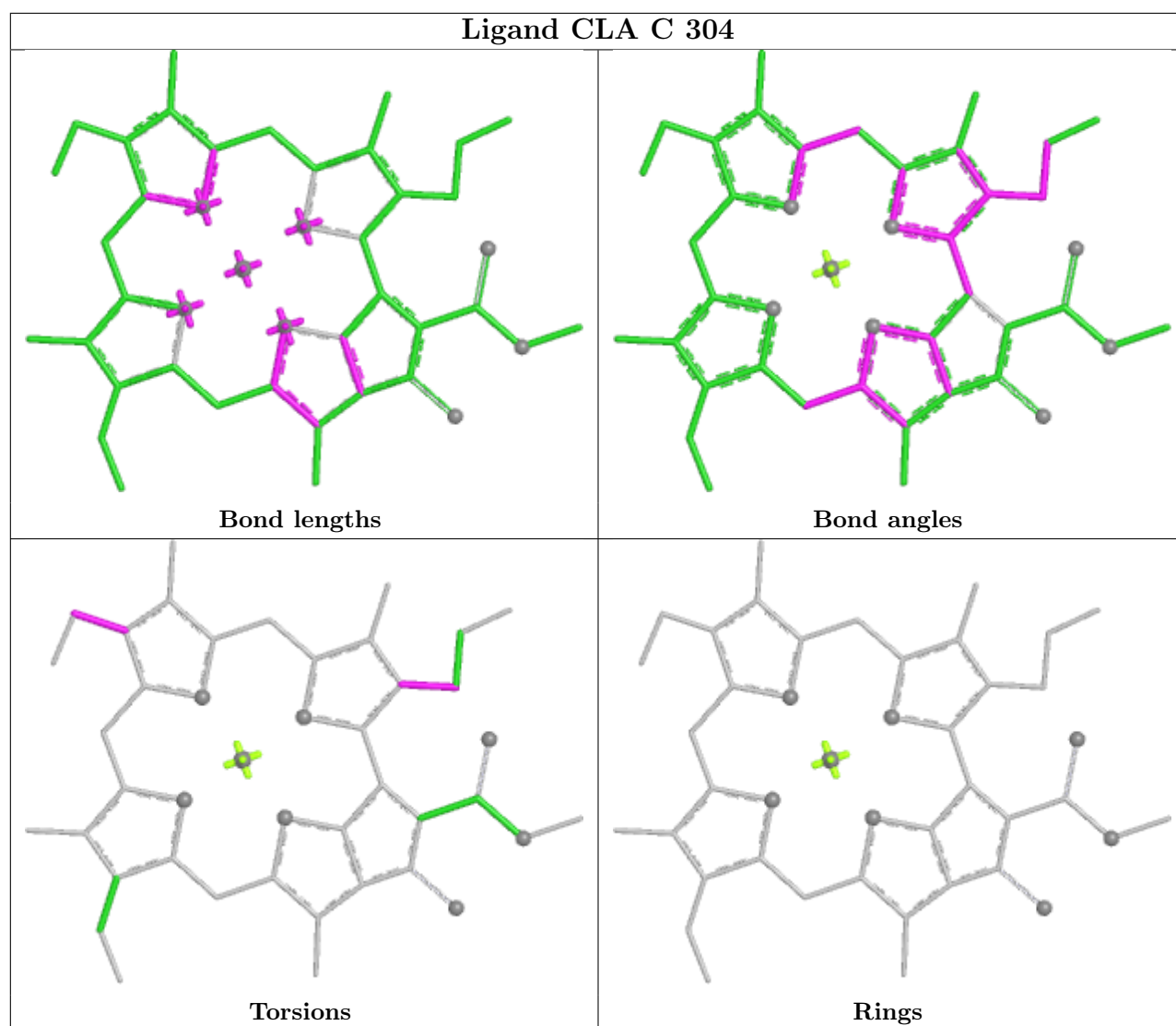
Bond angles



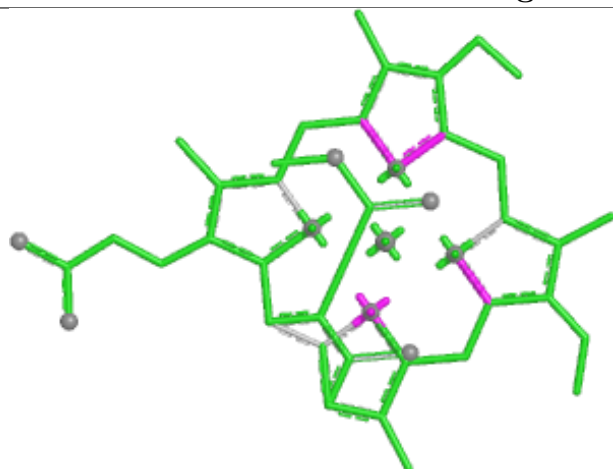
Torsions



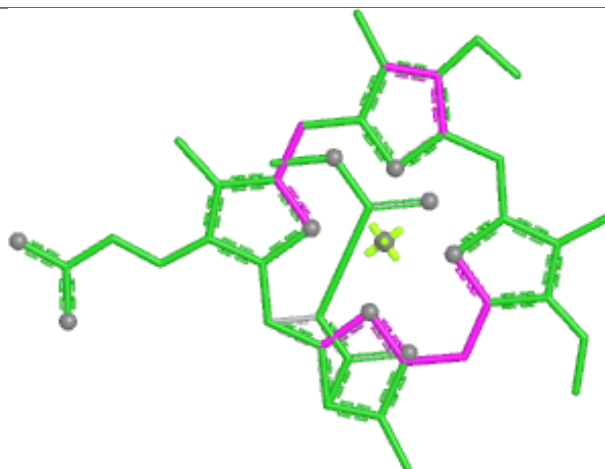
Rings



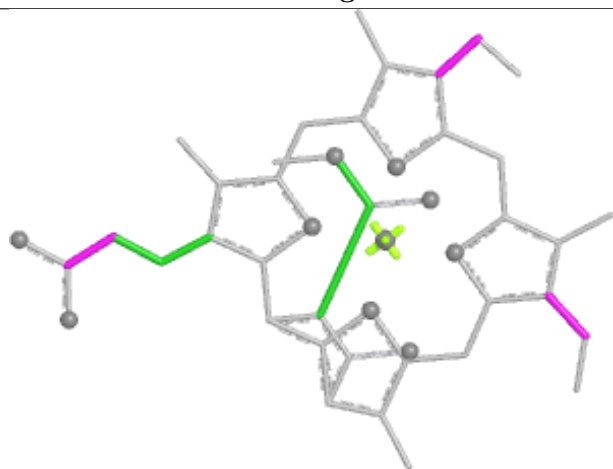
Ligand KC2 T 303



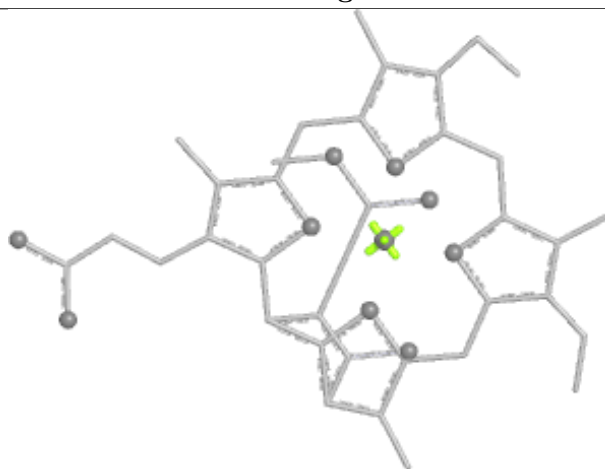
Bond lengths



Bond angles

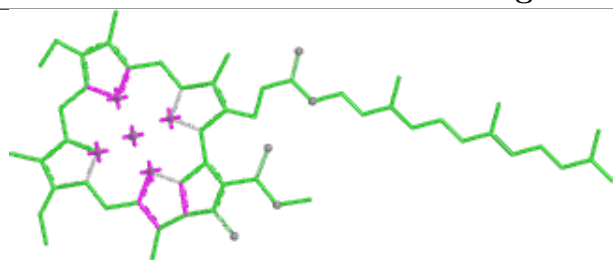


Torsions

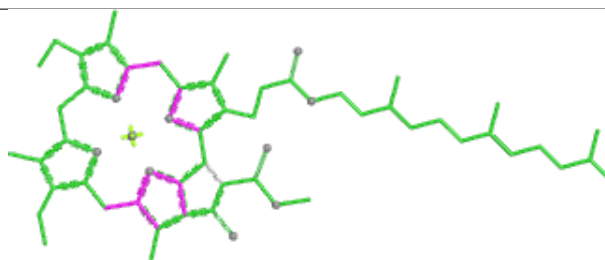


Rings

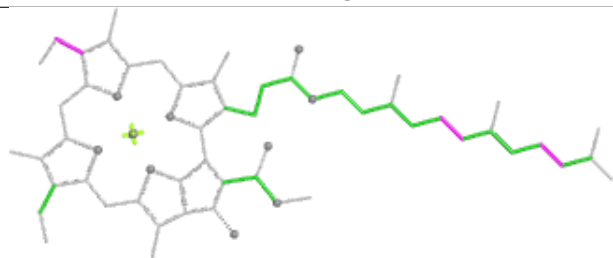
Ligand CLA E 304



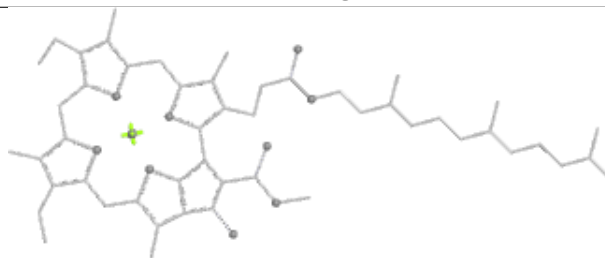
Bond lengths



Bond angles

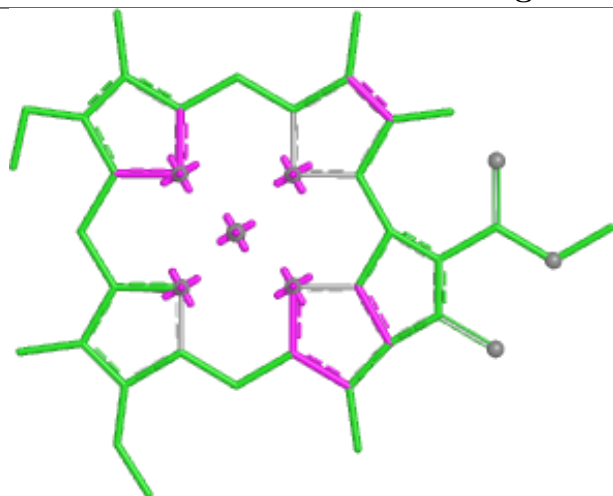


Torsions

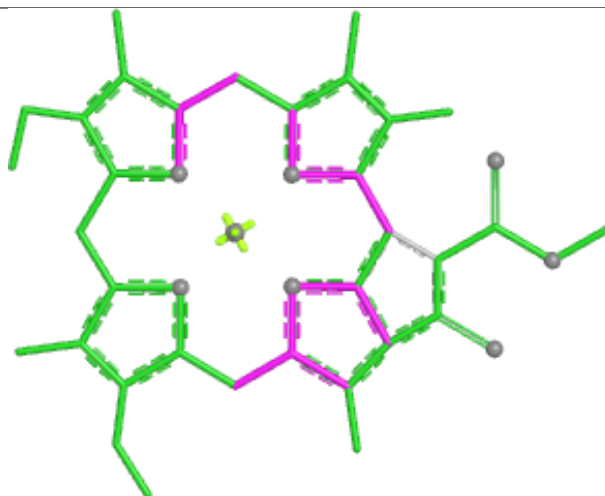


Rings

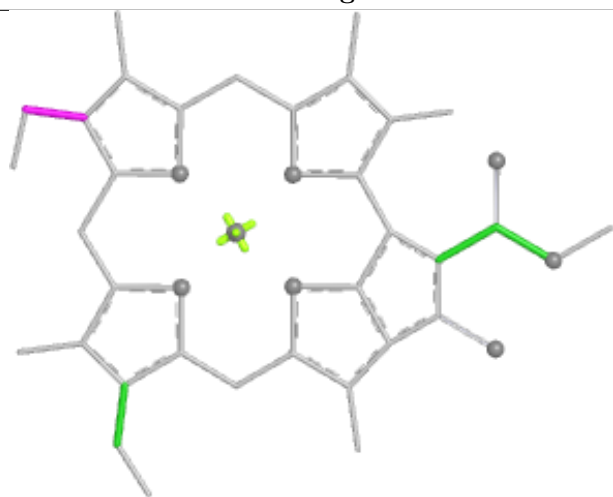
Ligand CLA P 310



Bond lengths



Bond angles

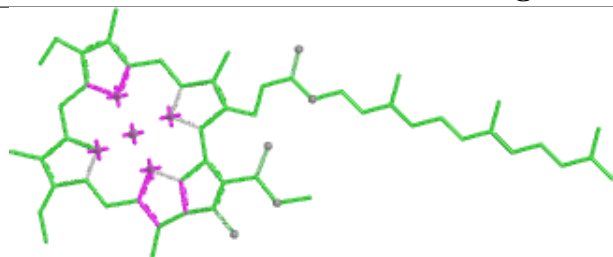


Torsions

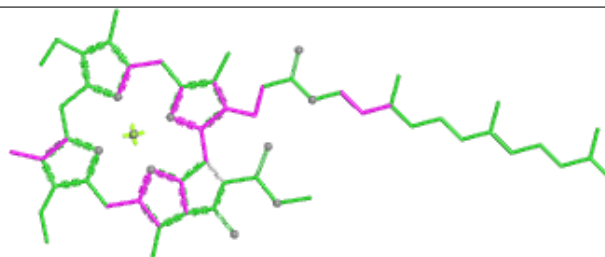


Rings

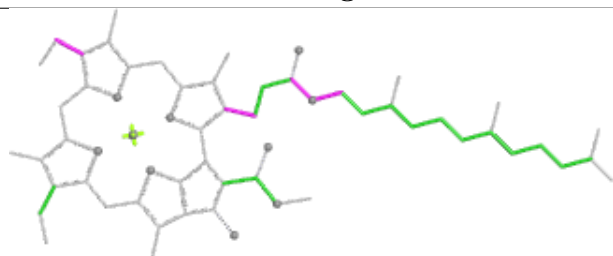
Ligand CLA T 308



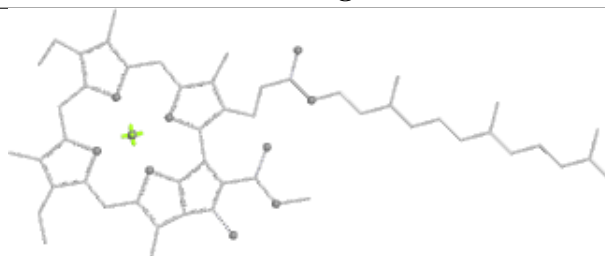
Bond lengths



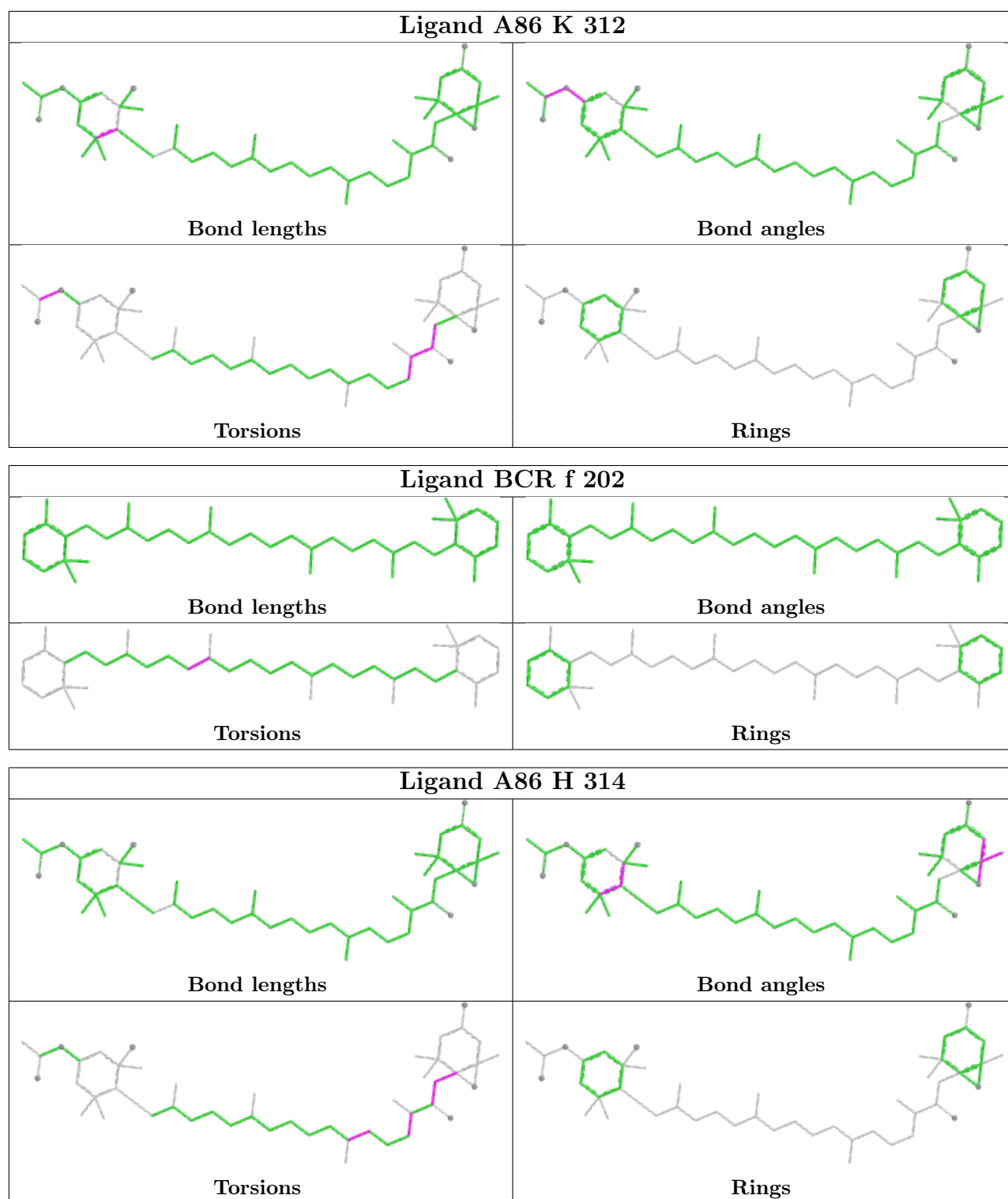
Bond angles



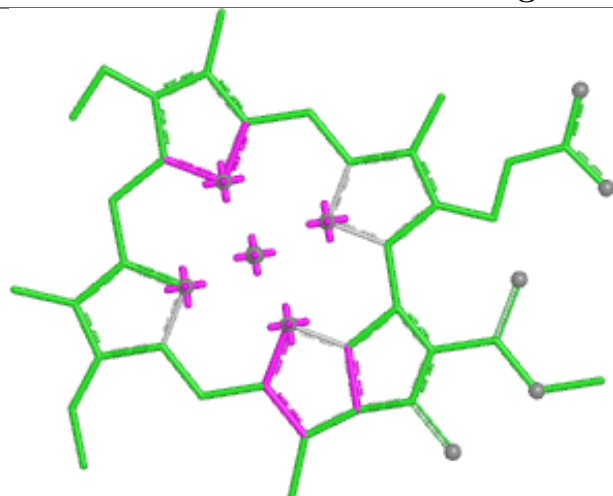
Torsions



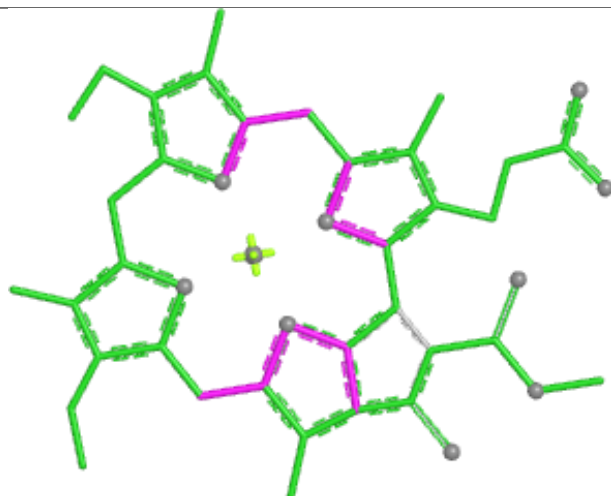
Rings



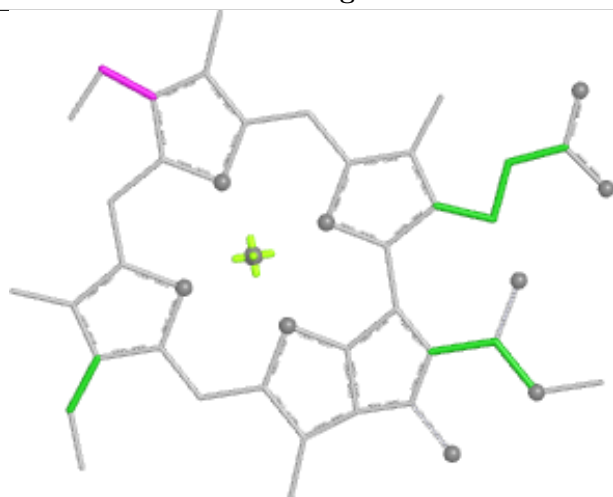
Ligand CLA J 302



Bond lengths



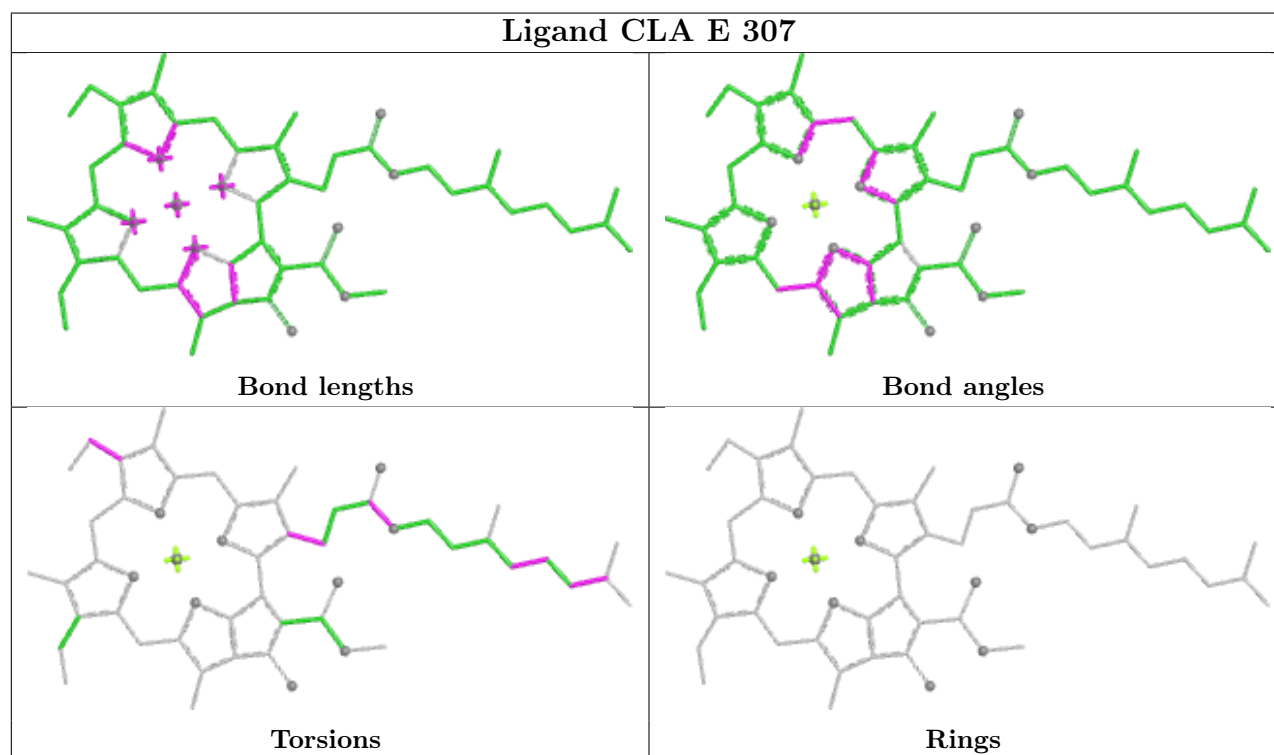
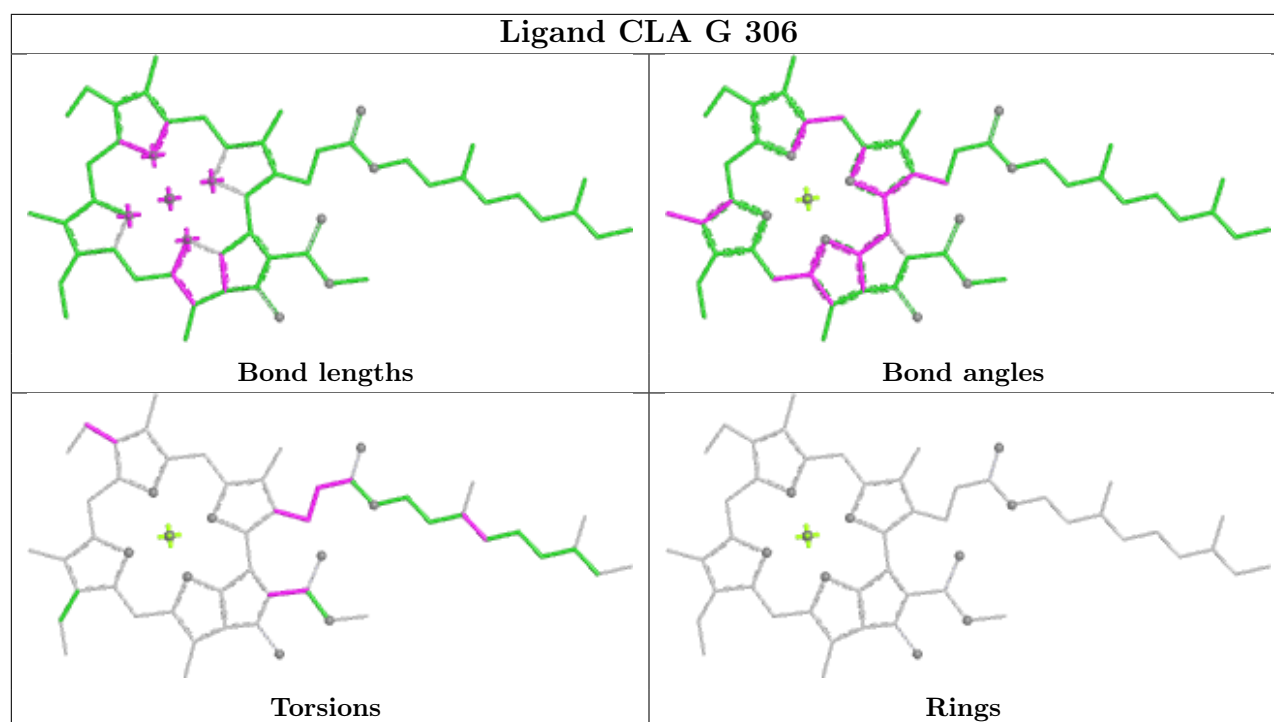
Bond angles

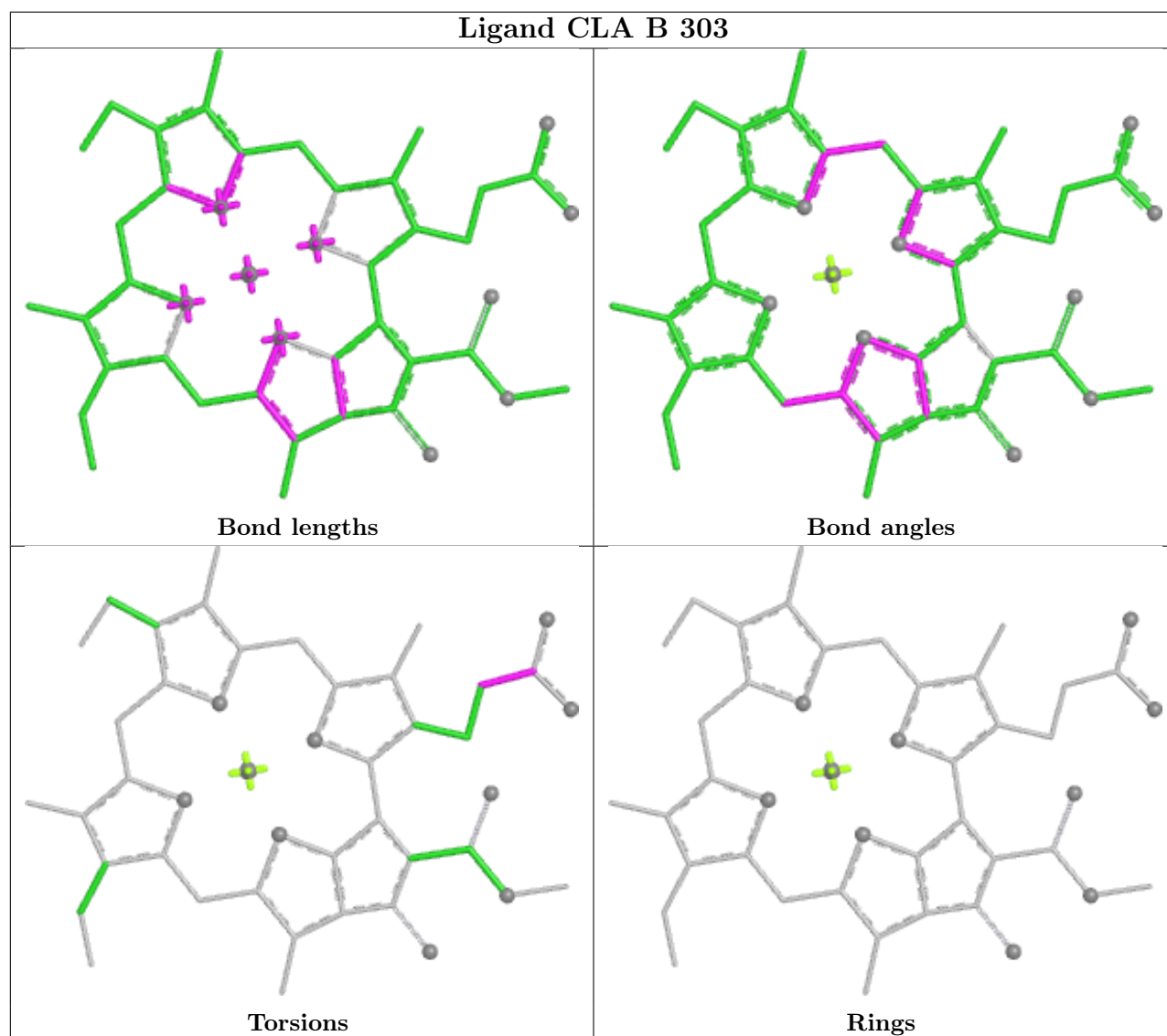
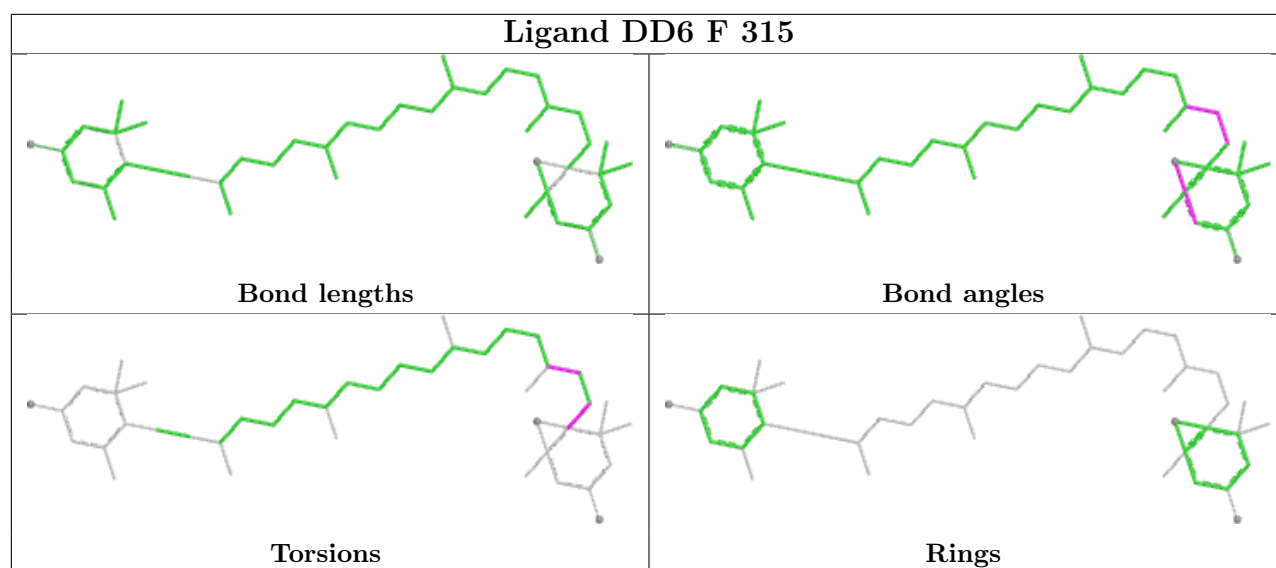


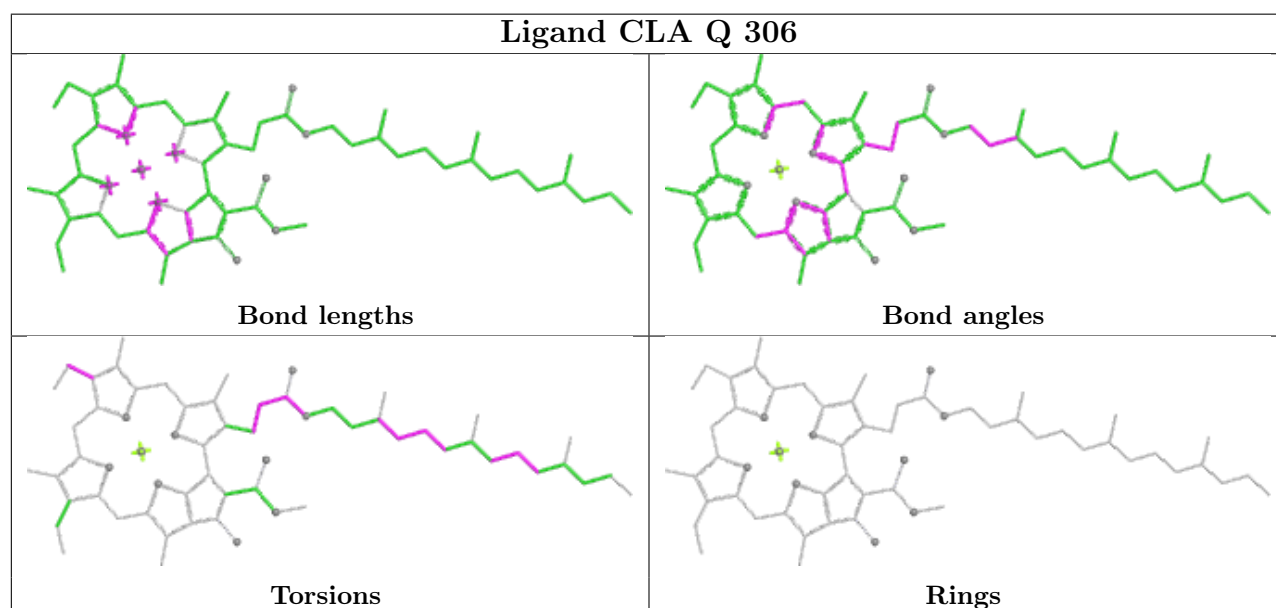
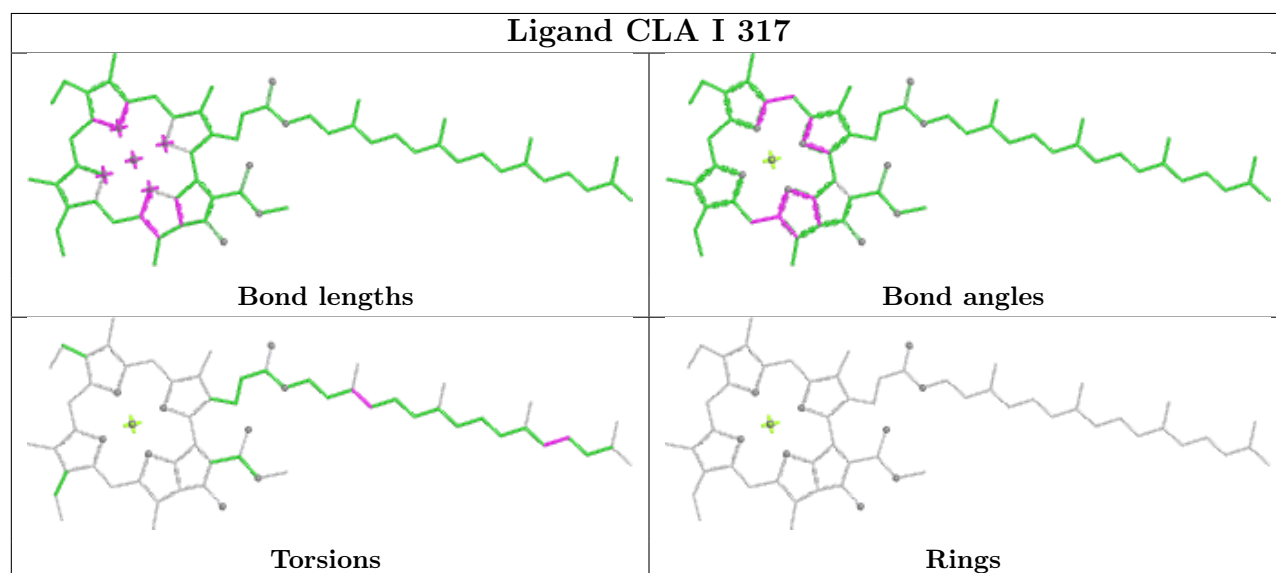
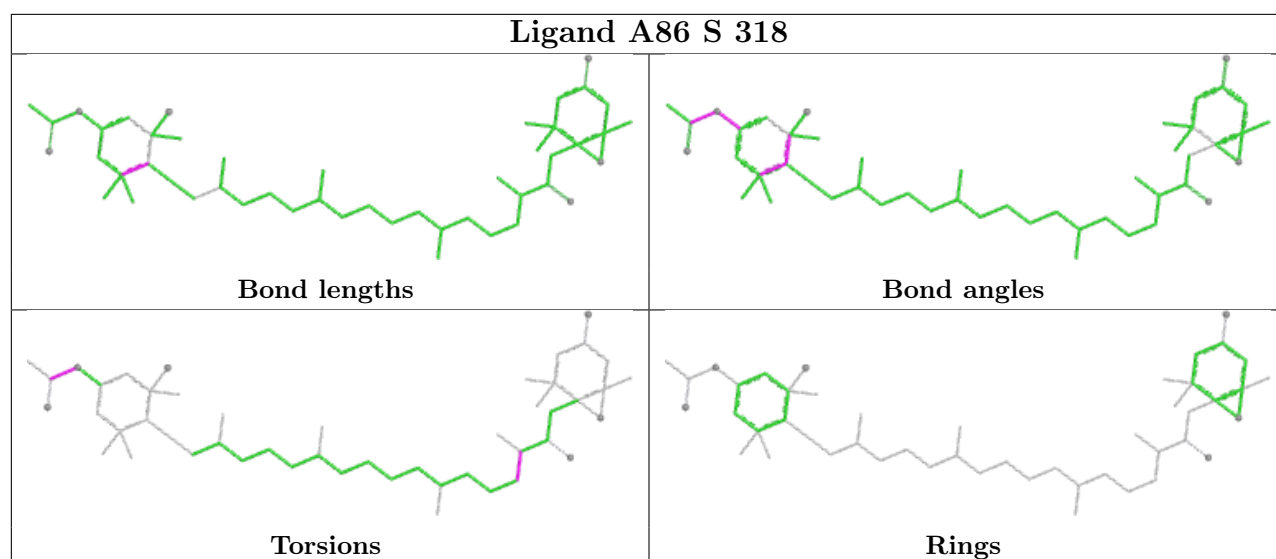
Torsions



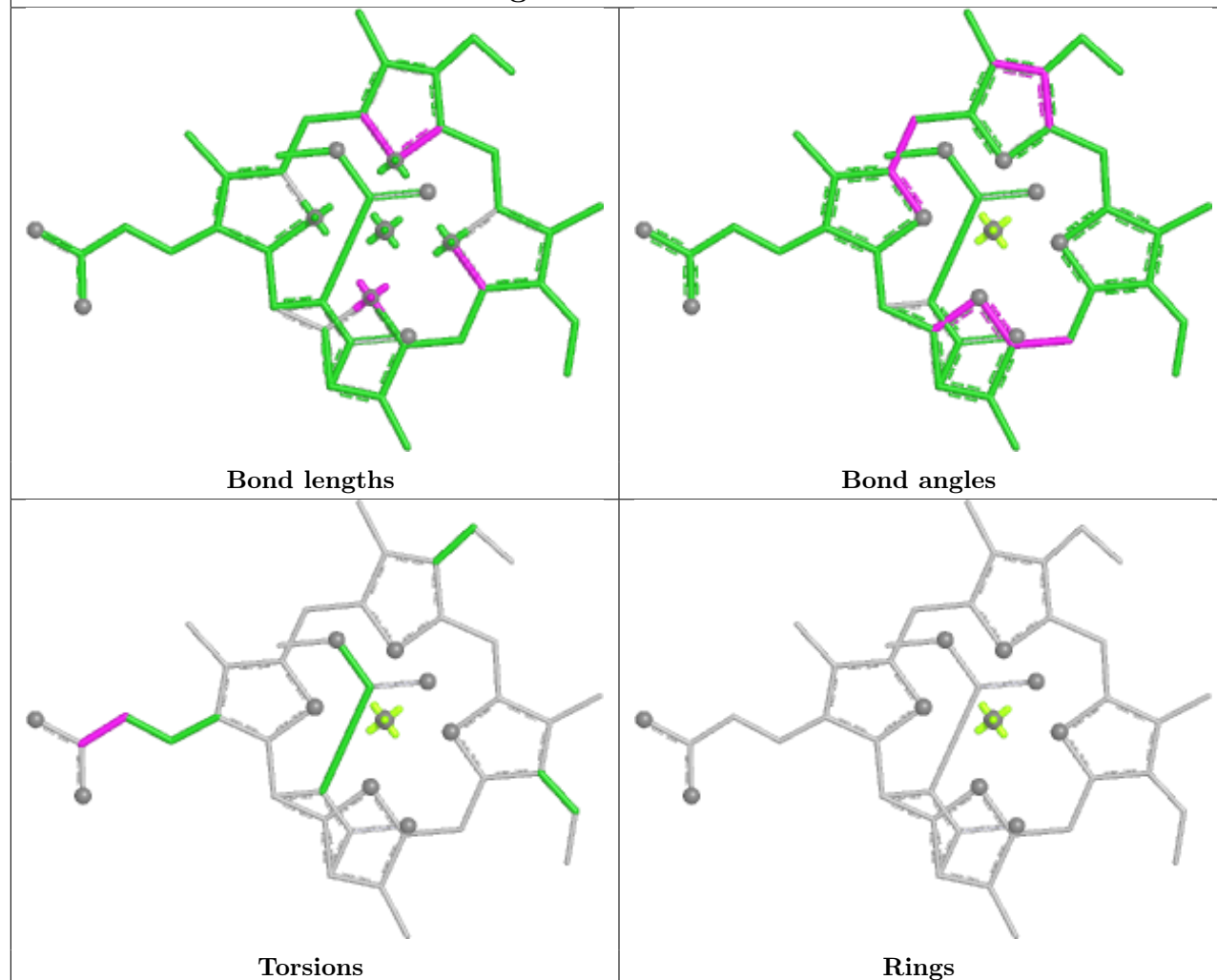
Rings



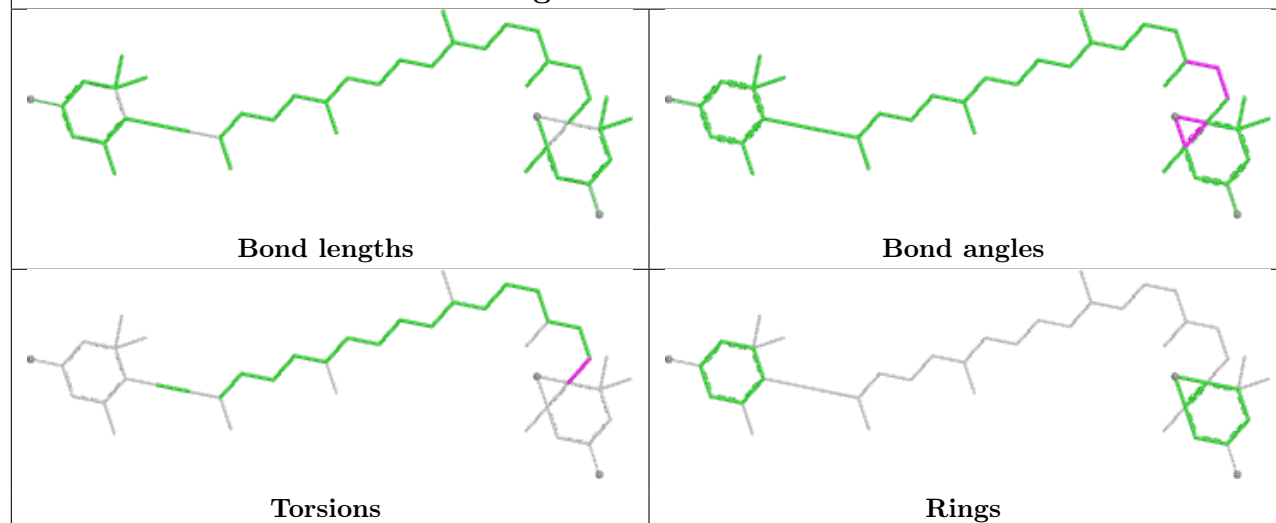


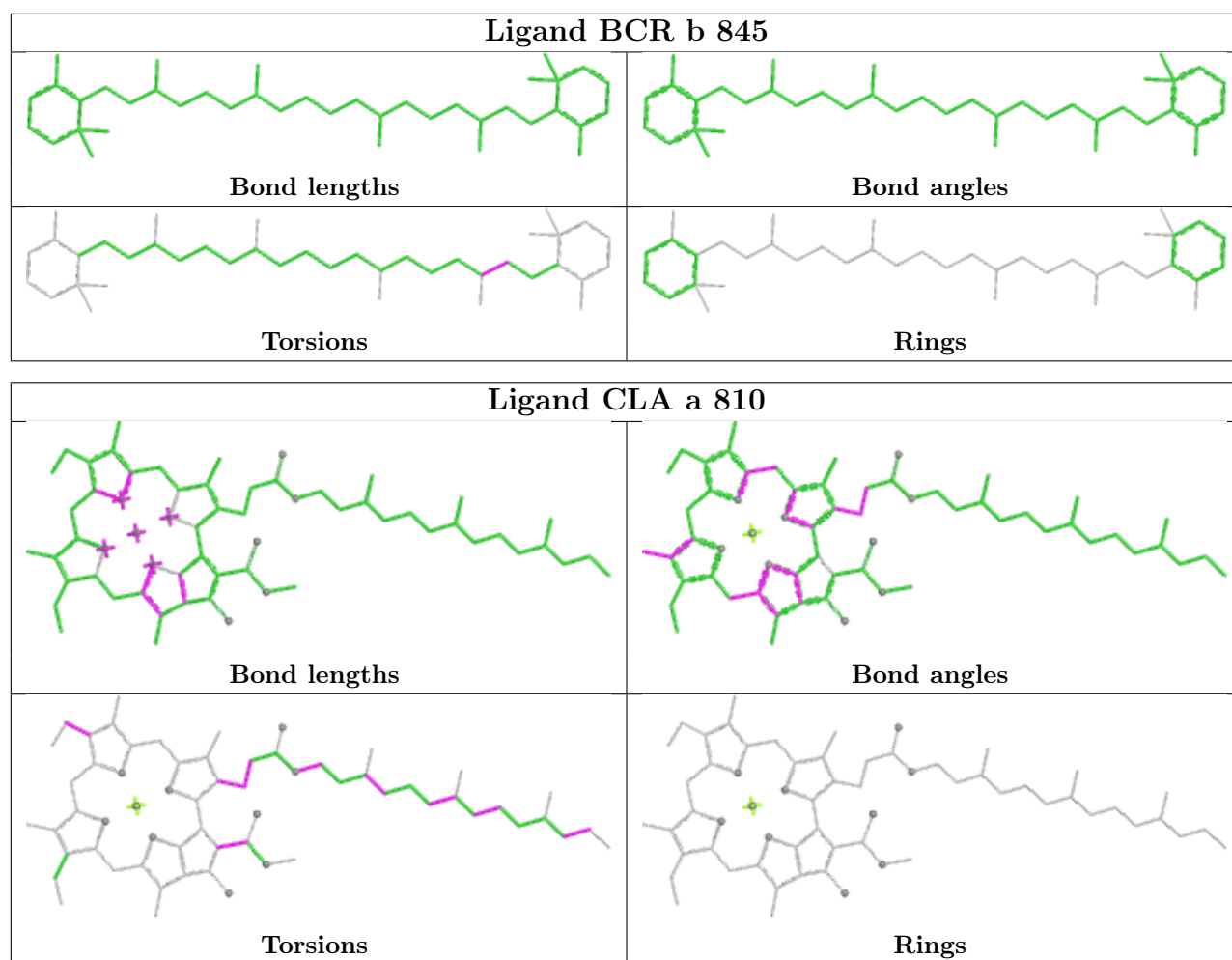


Ligand KC2 P 303

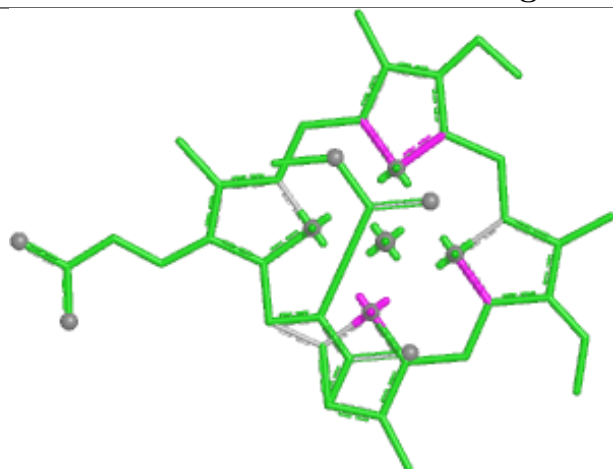


Ligand DD6 B 307

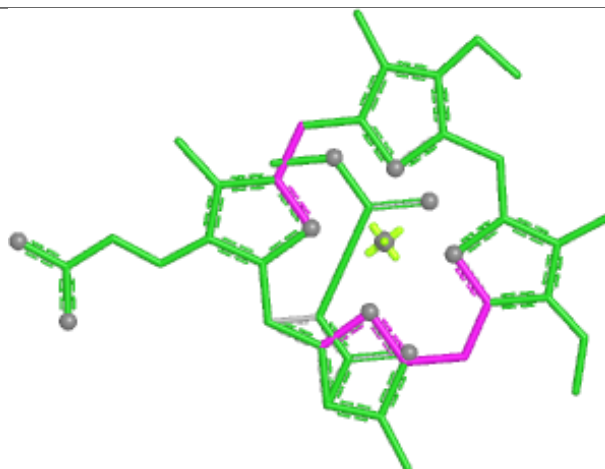




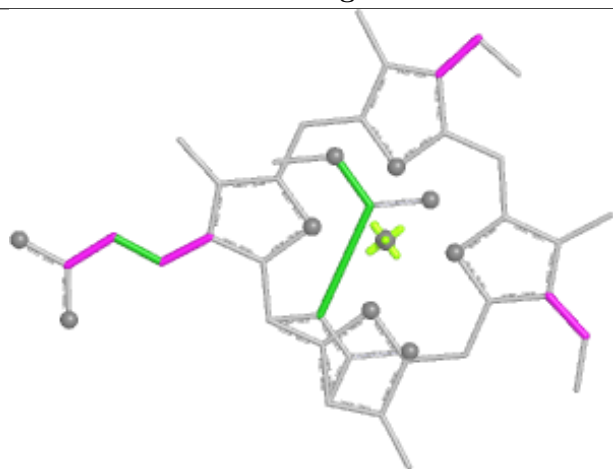
Ligand KC2 J 303



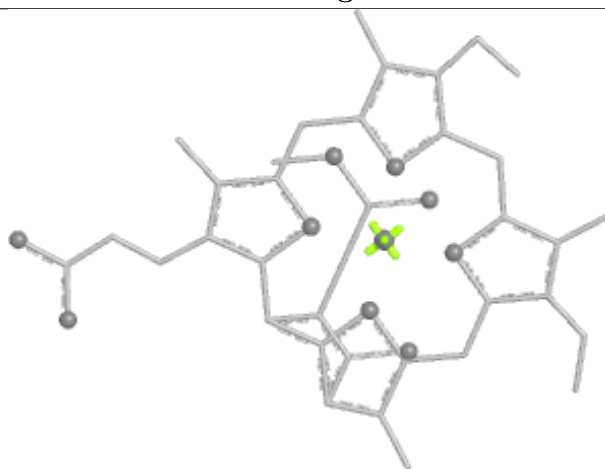
Bond lengths



Bond angles

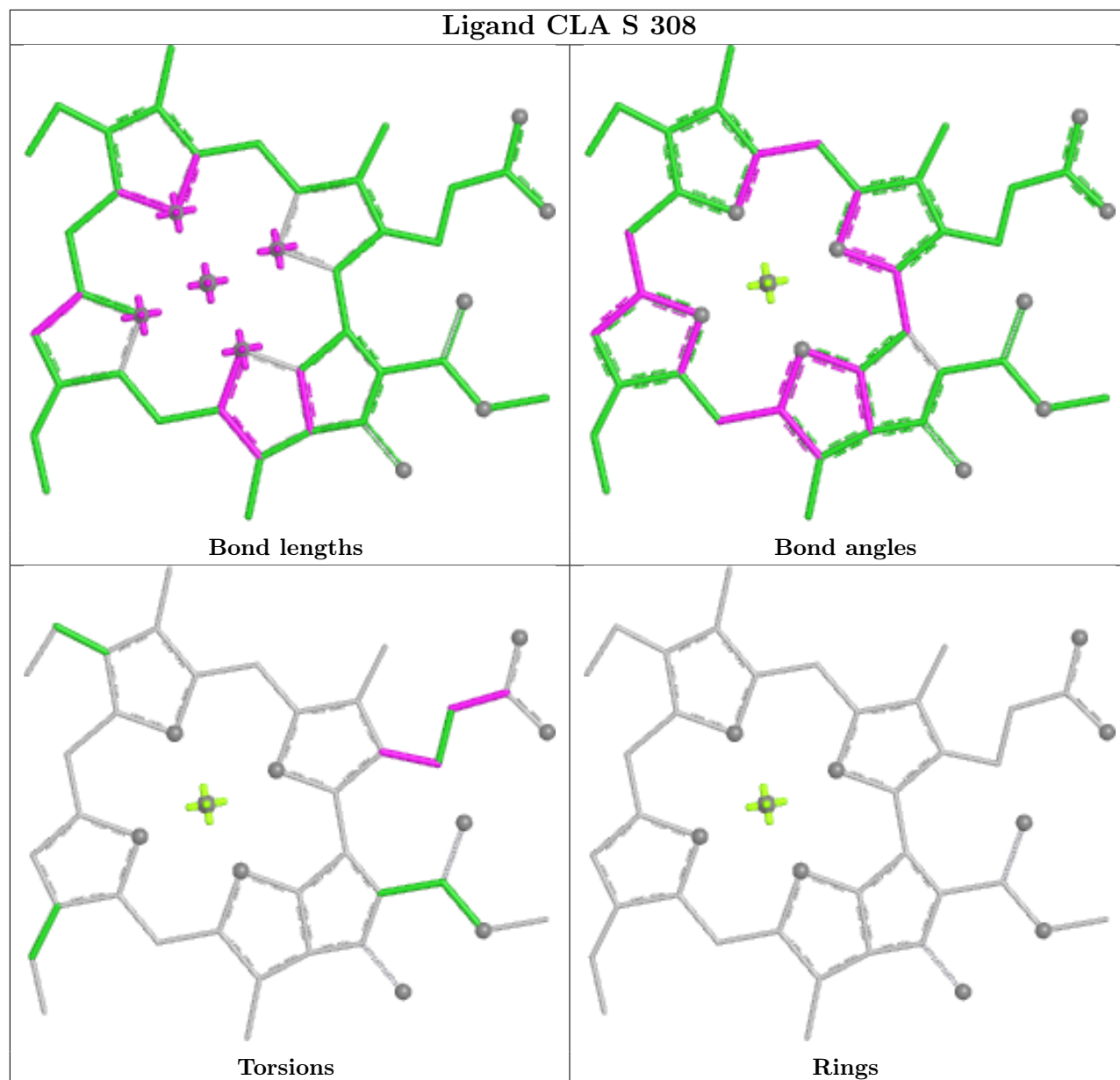


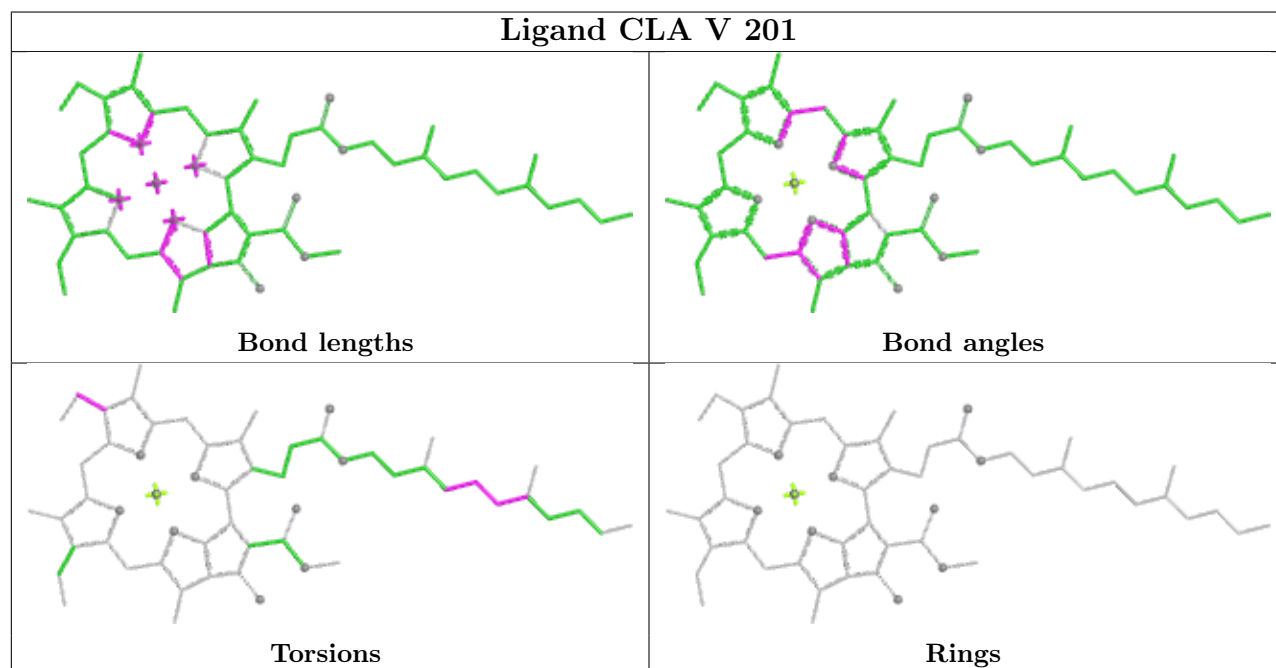
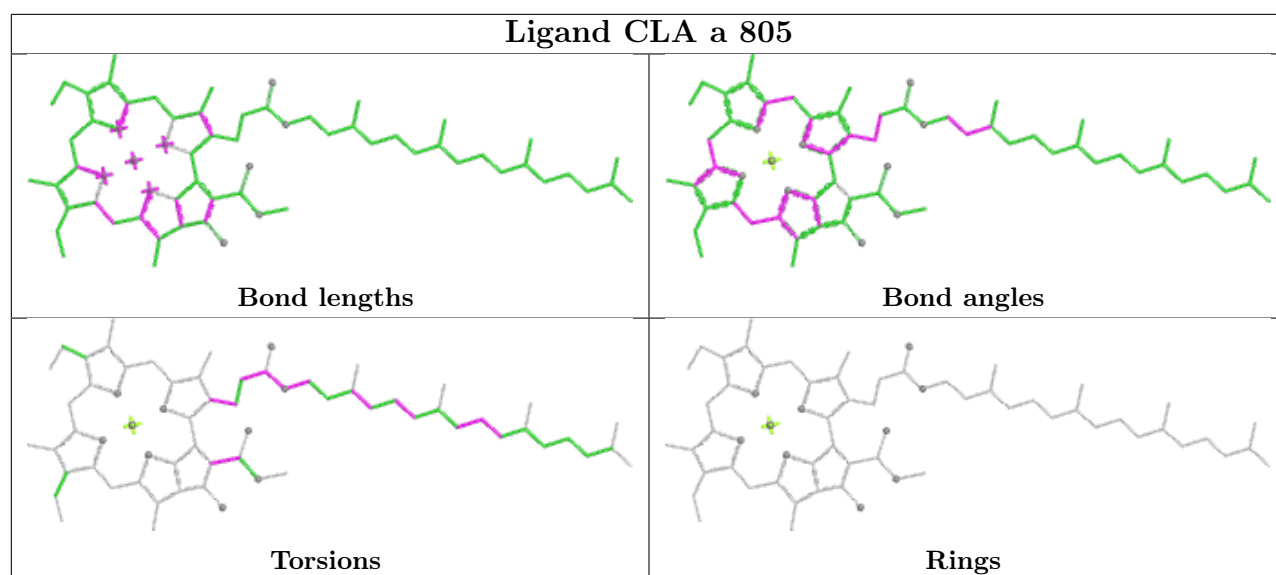
Torsions



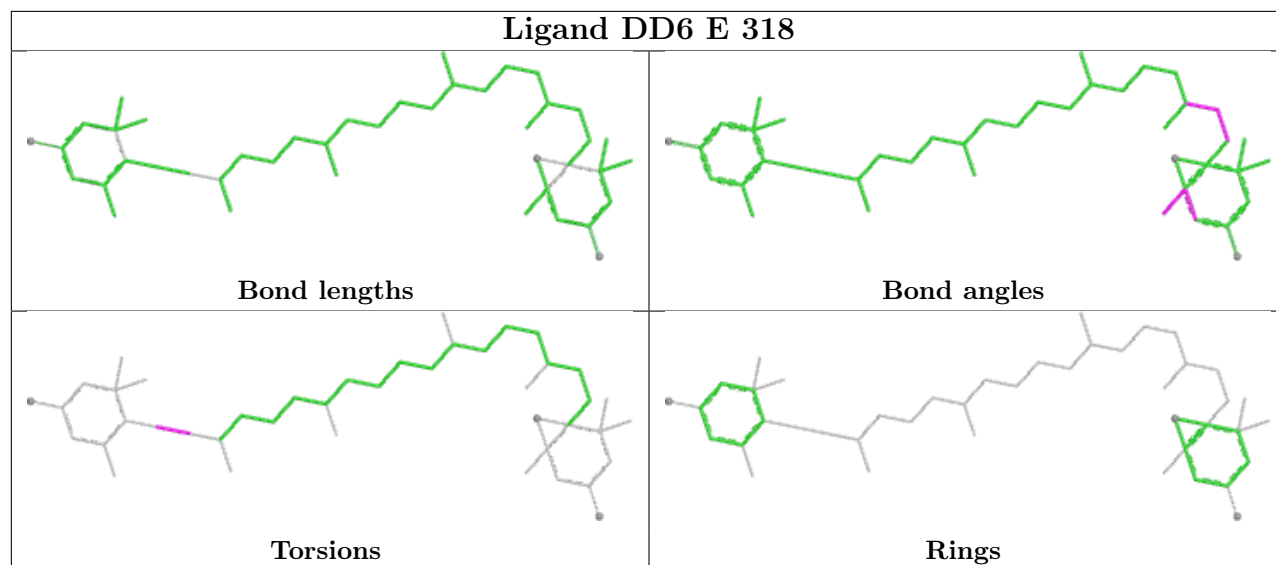
Rings

Ligand CLA S 308

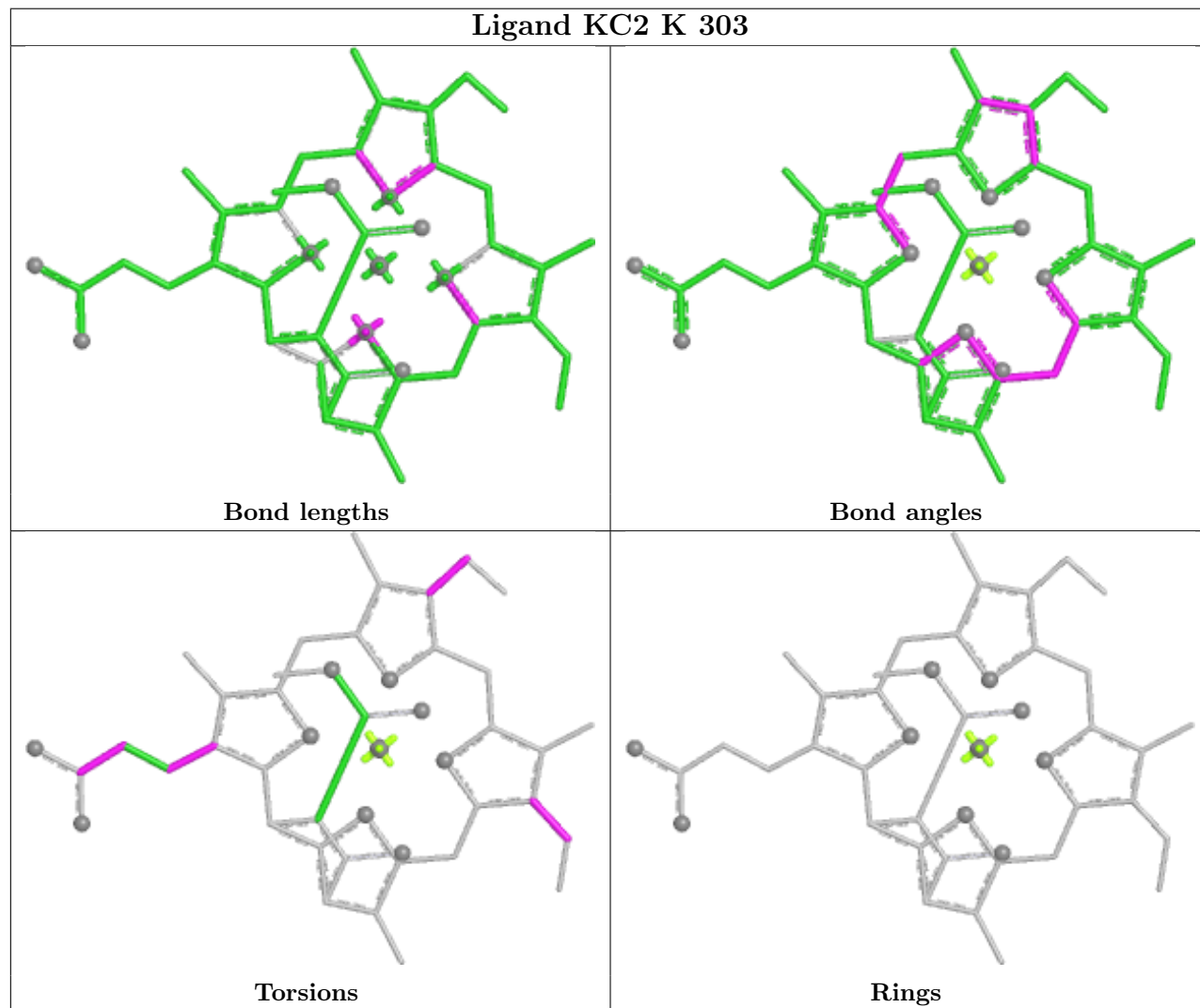


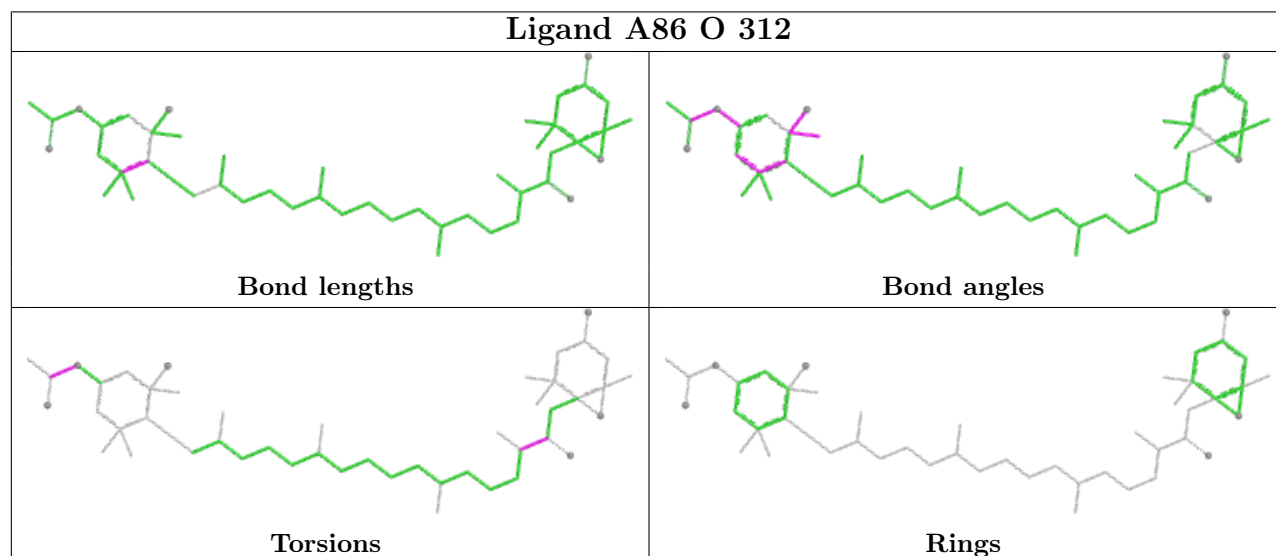
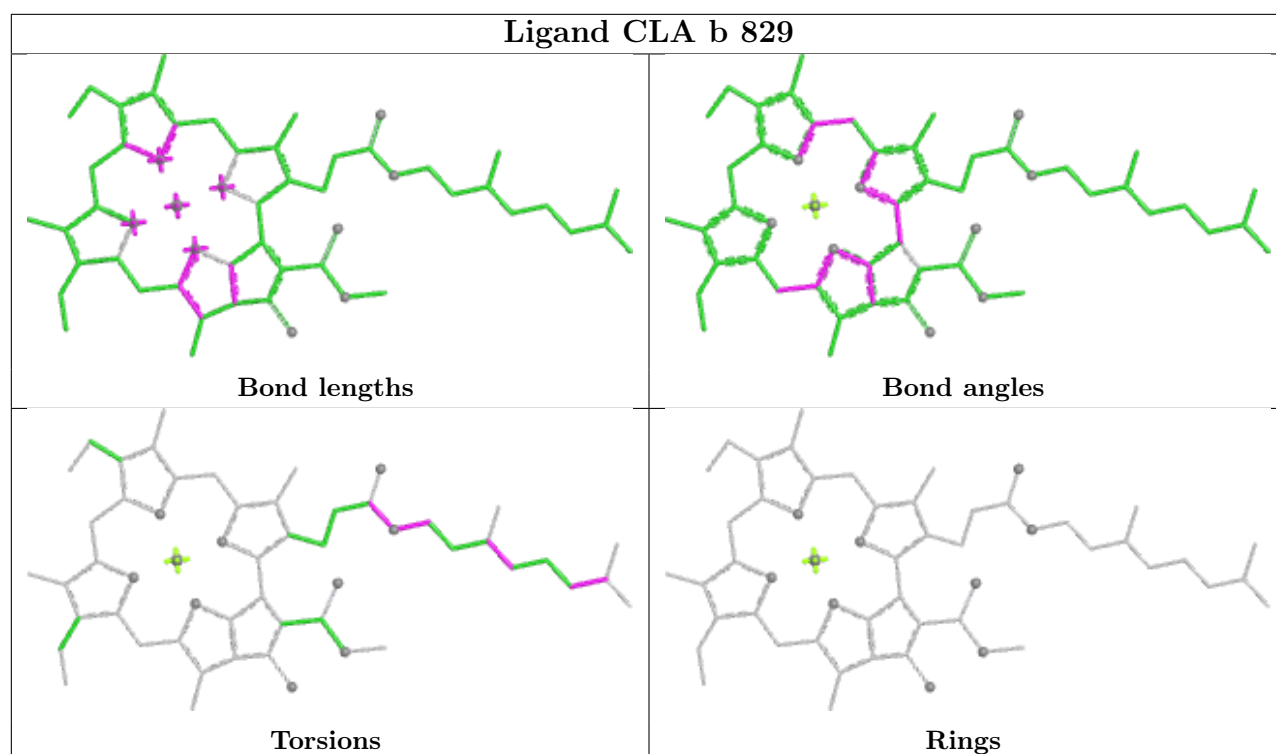


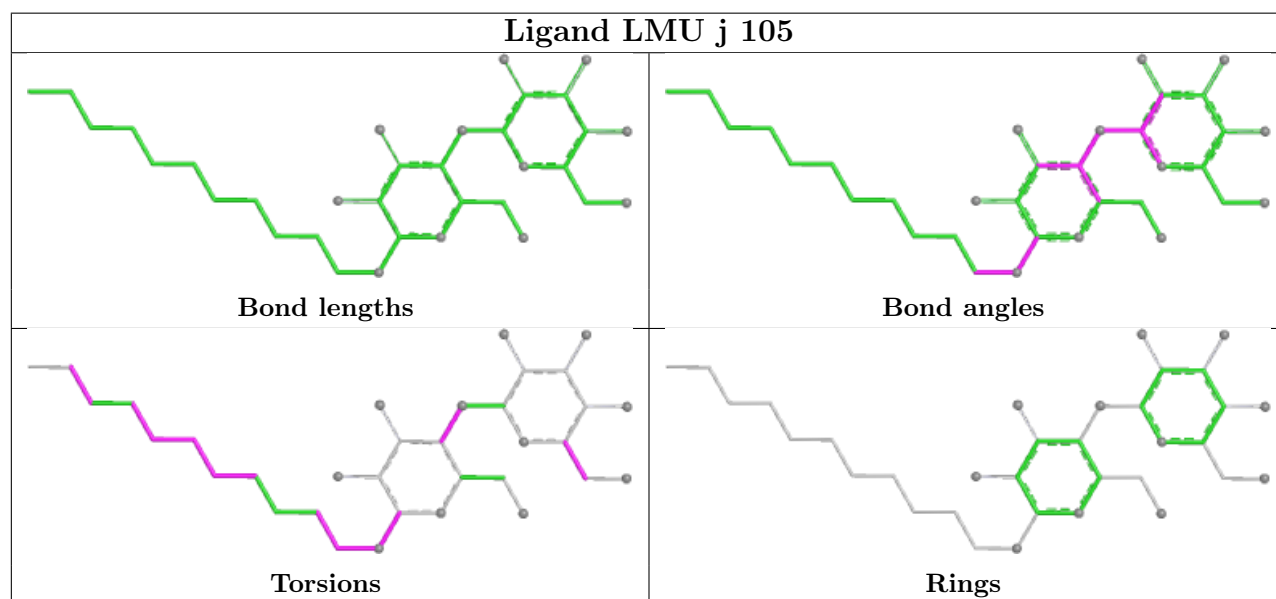
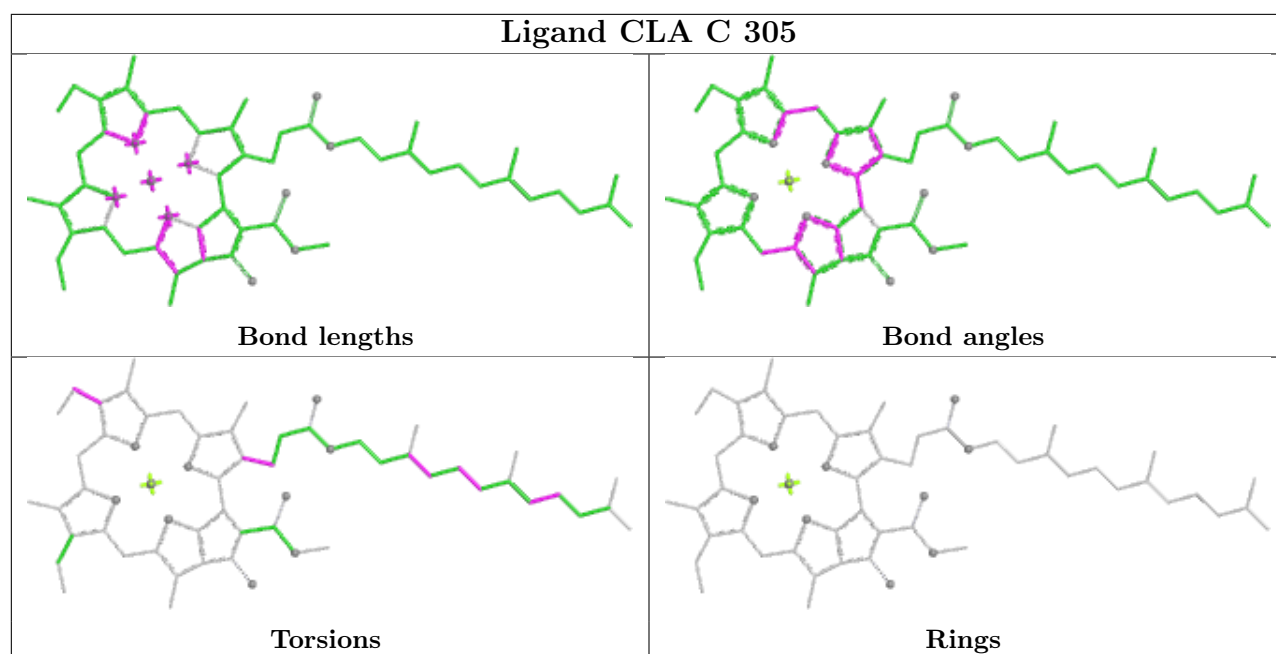
Ligand DD6 E 318



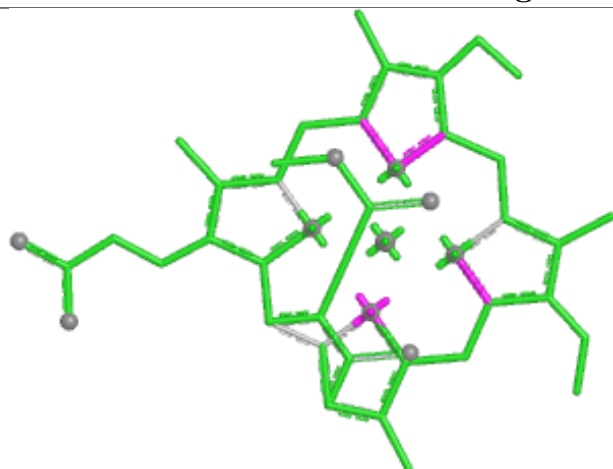
Ligand KC2 K 303



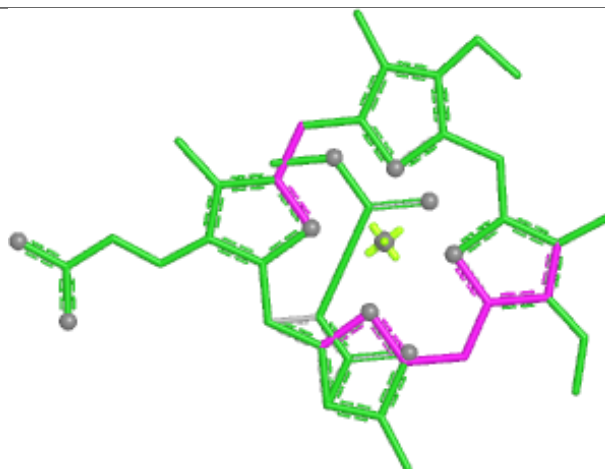




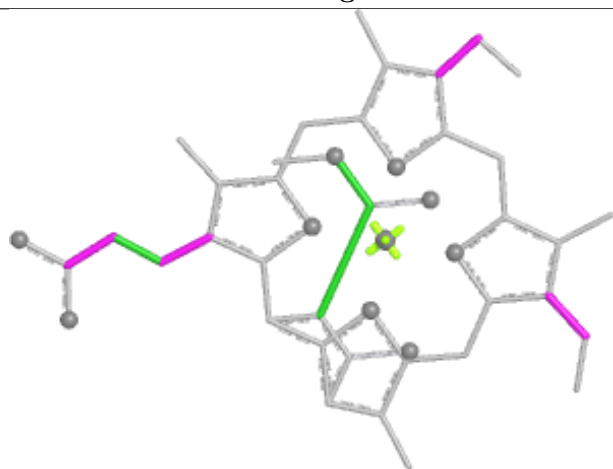
Ligand KC2 G 309



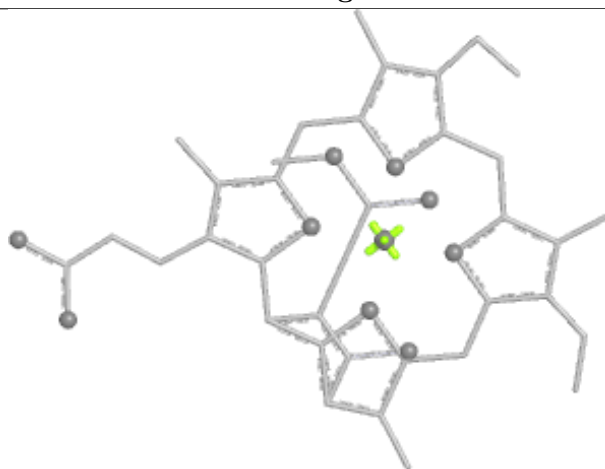
Bond lengths



Bond angles

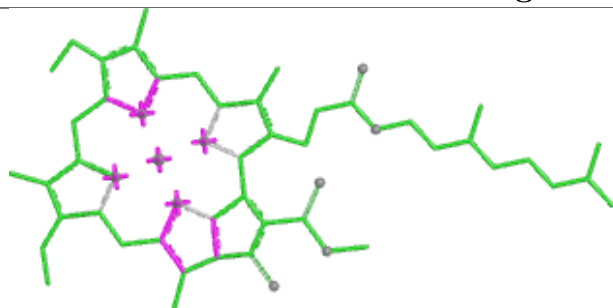


Torsions

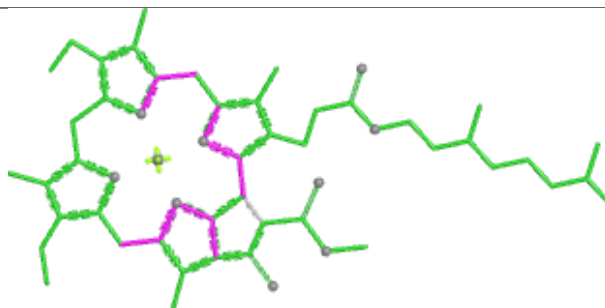


Rings

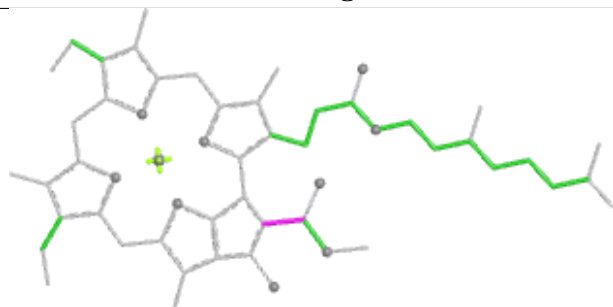
Ligand CLA E 305



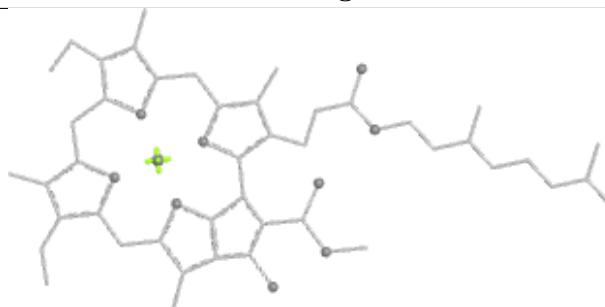
Bond lengths



Bond angles

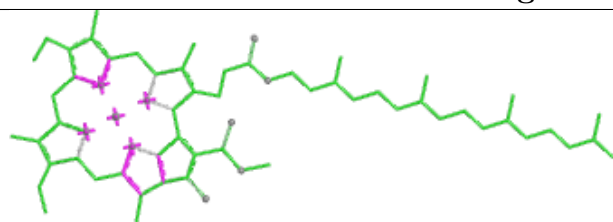


Torsions

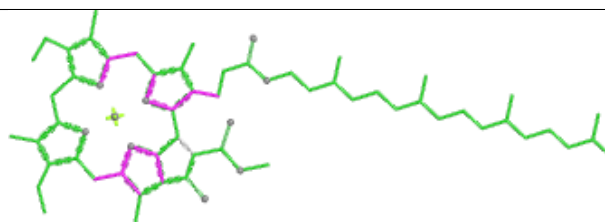


Rings

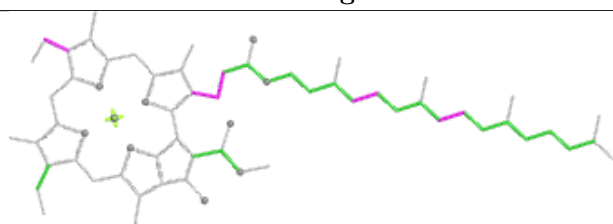
Ligand CLA b 822



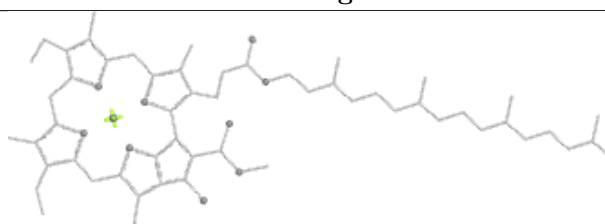
Bond lengths



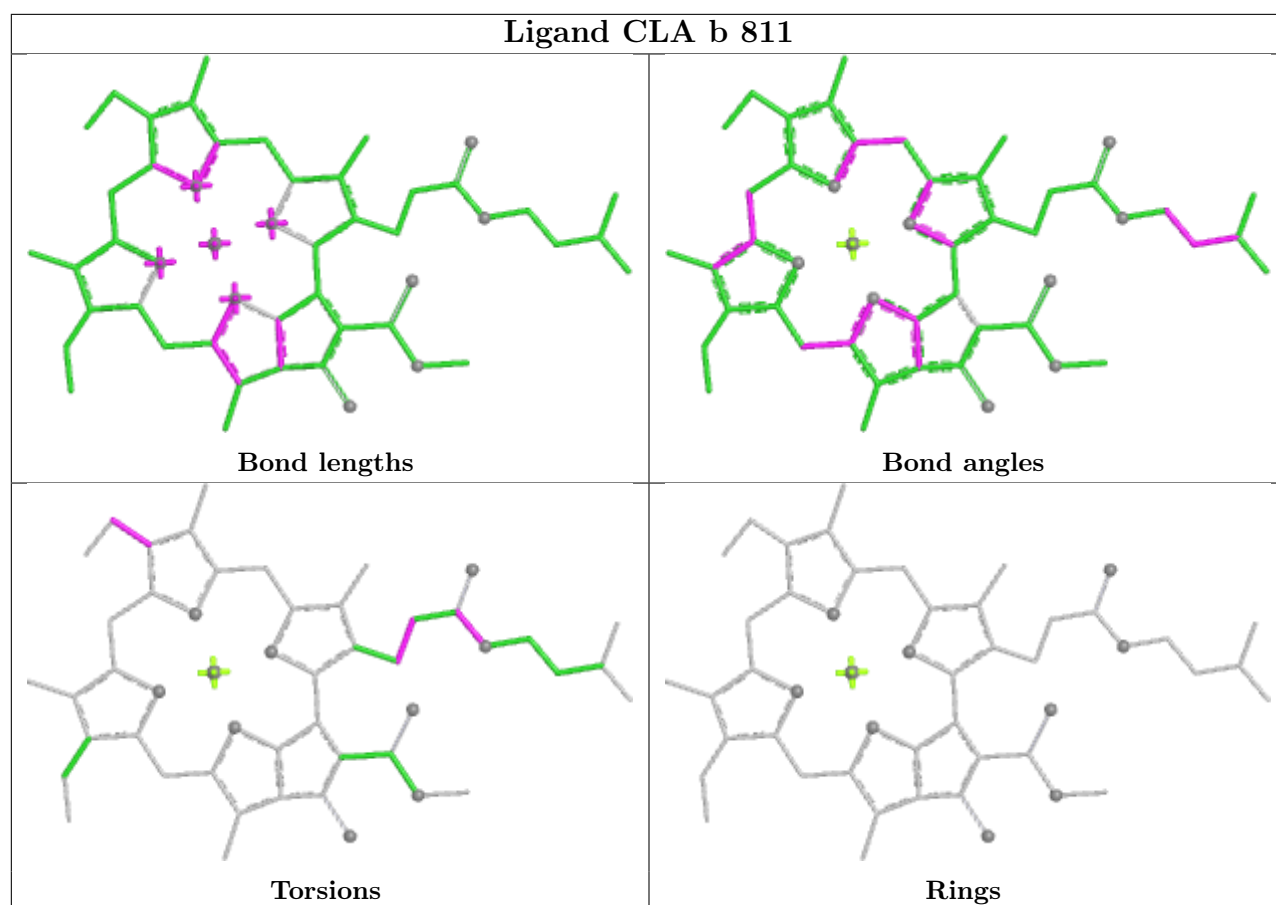
Bond angles

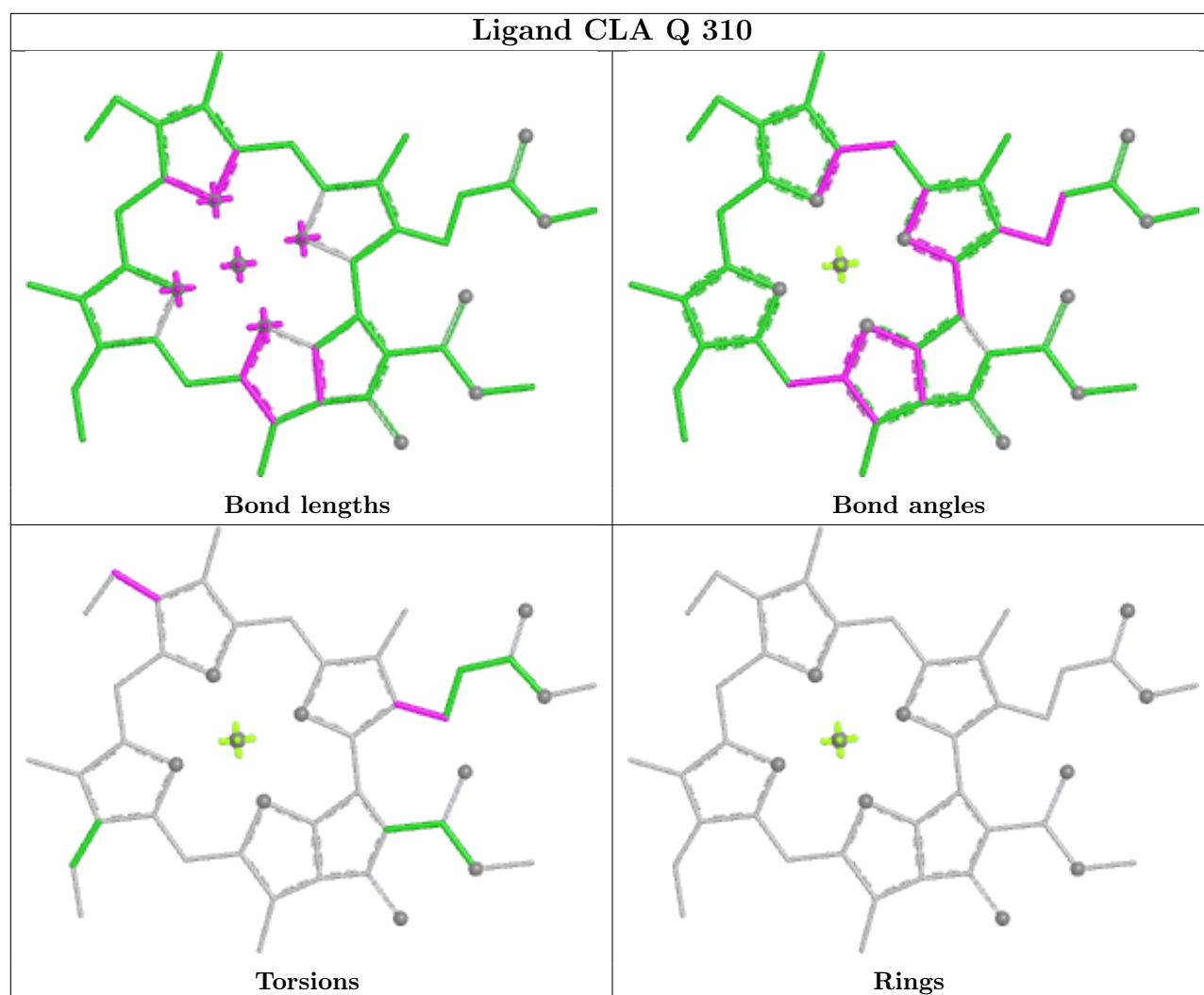


Torsions

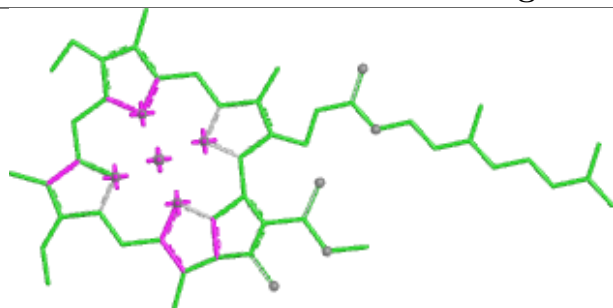


Rings

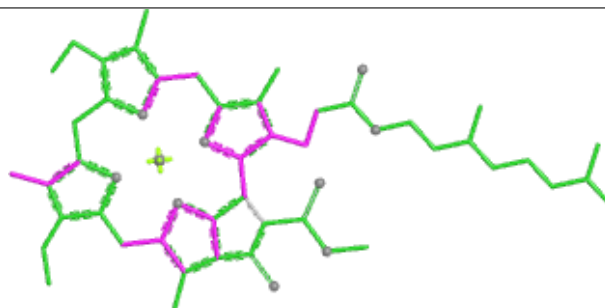




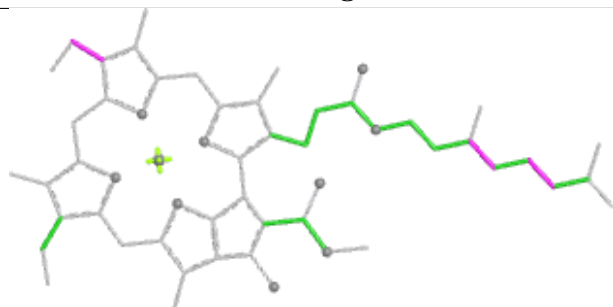
Ligand CLA J 304



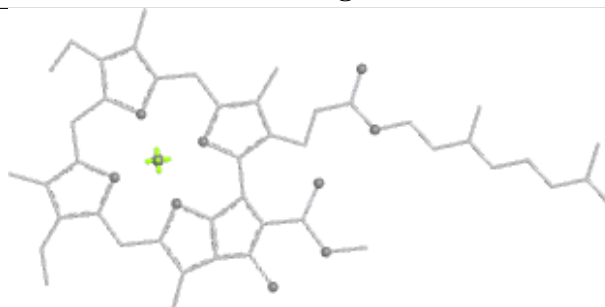
Bond lengths



Bond angles

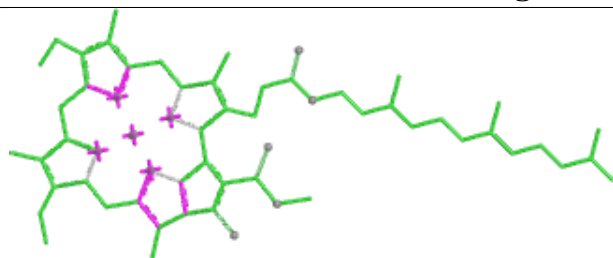


Torsions

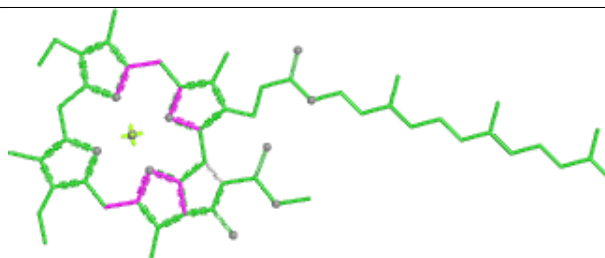


Rings

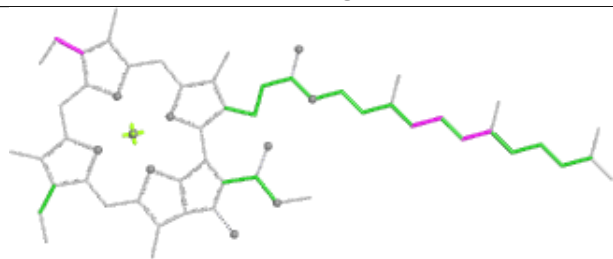
Ligand CLA A 302



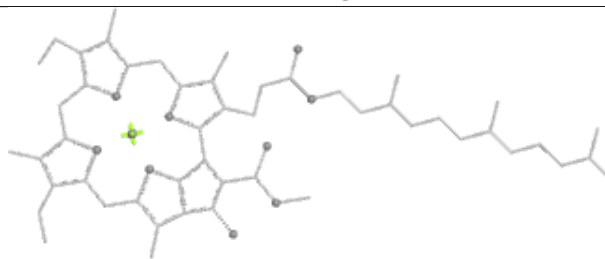
Bond lengths



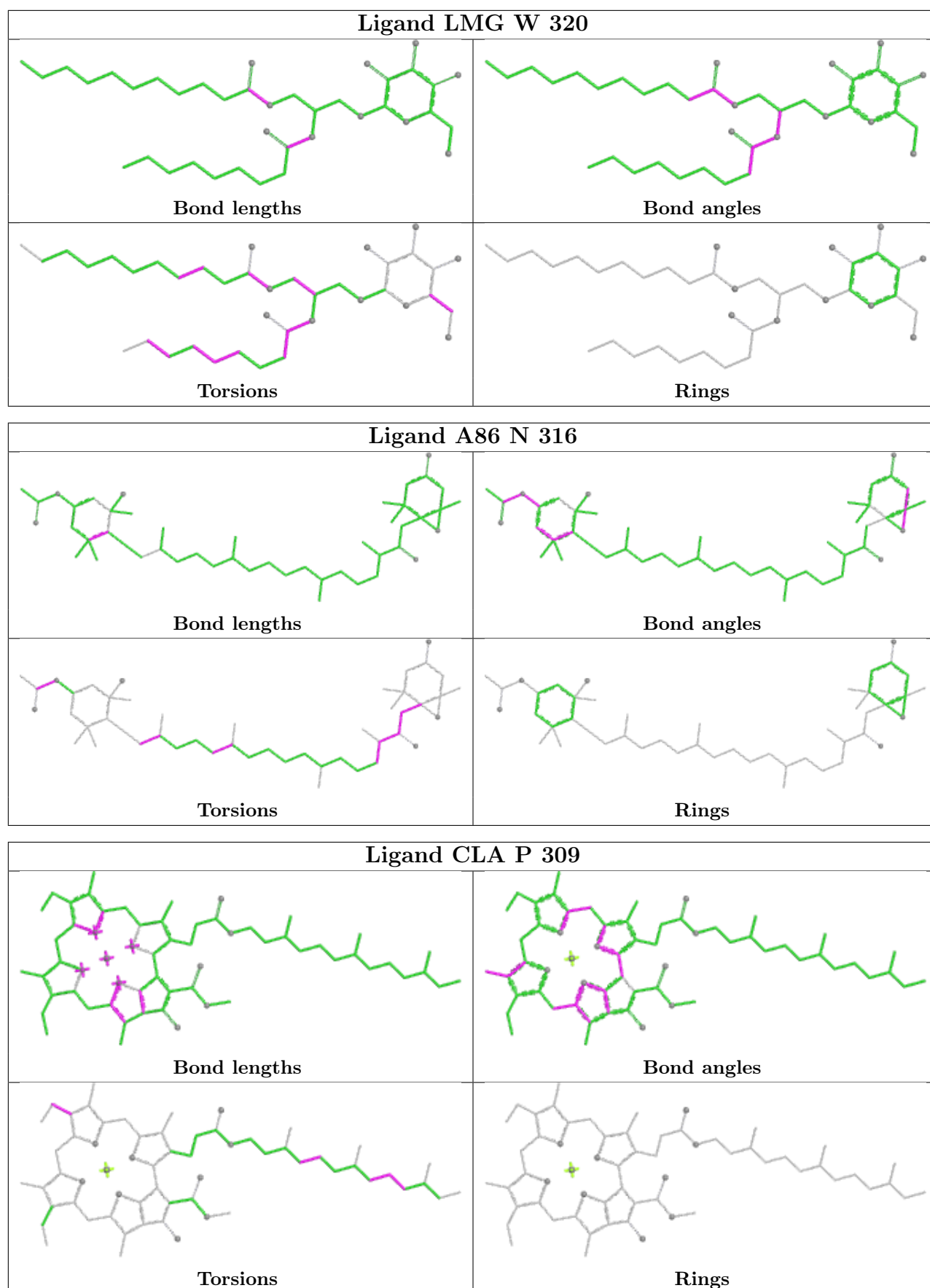
Bond angles



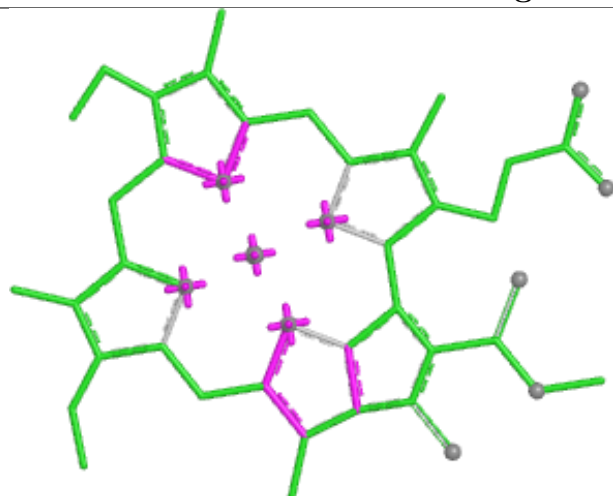
Torsions



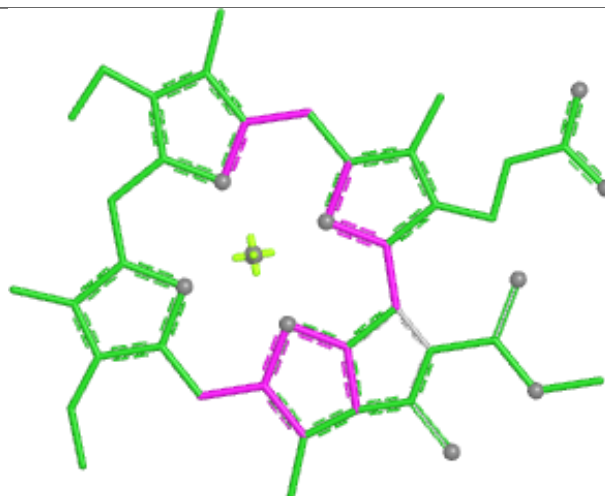
Rings



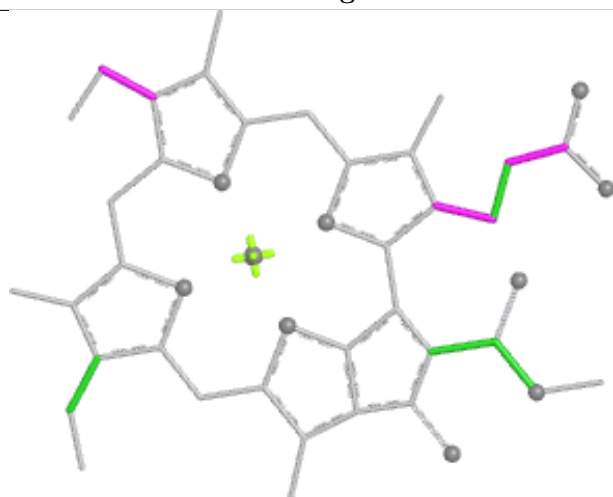
Ligand CLA T 302



Bond lengths



Bond angles

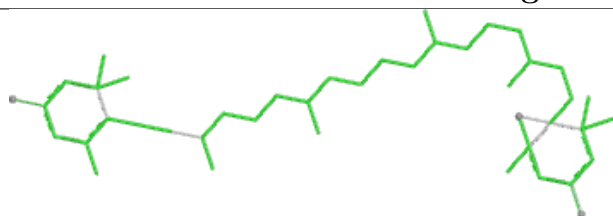


Torsions

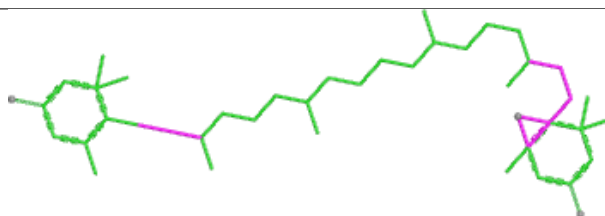


Rings

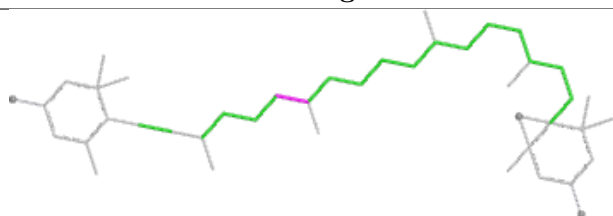
Ligand DD6 I 310



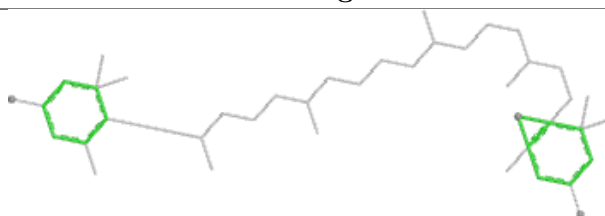
Bond lengths



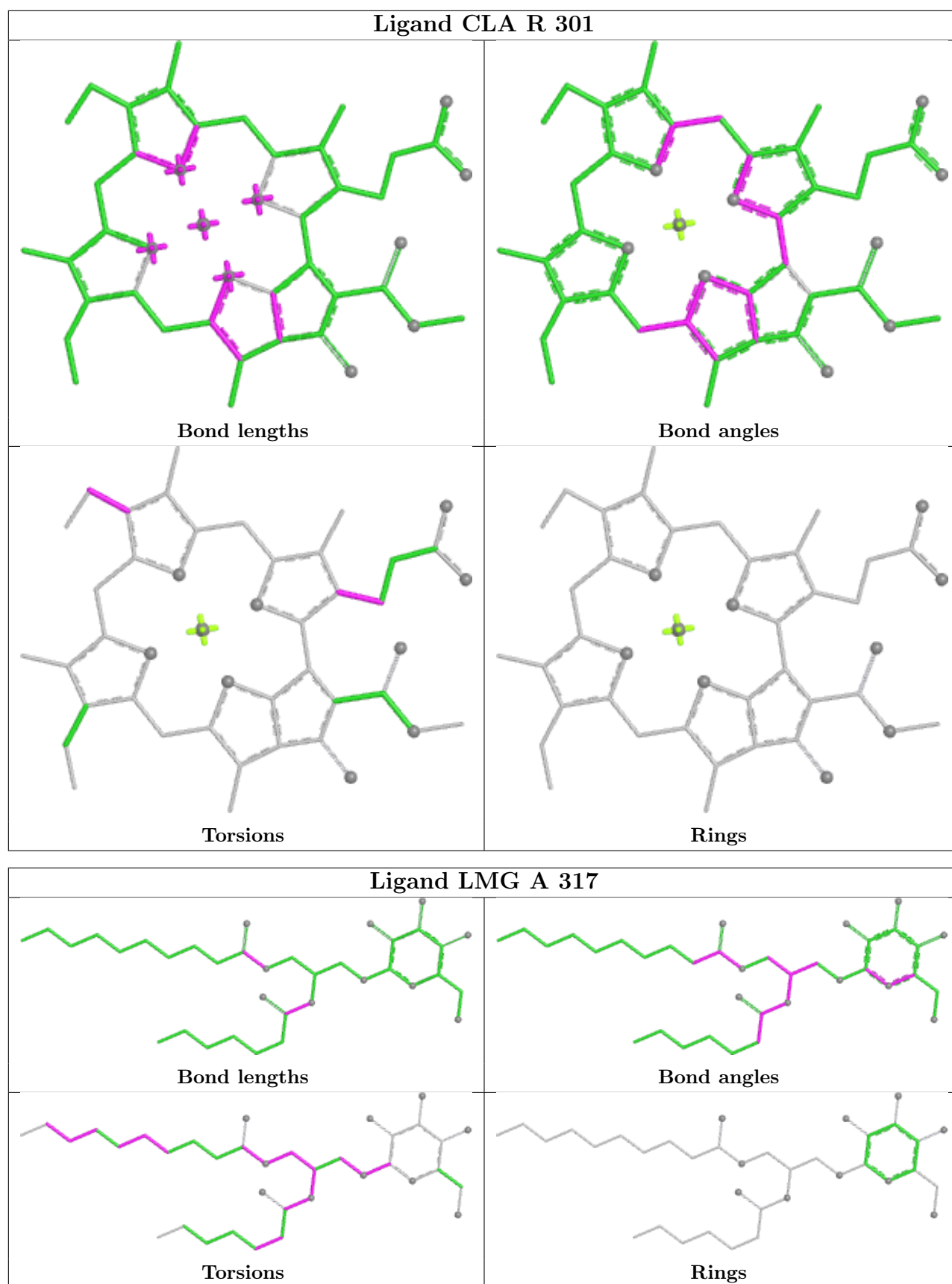
Bond angles

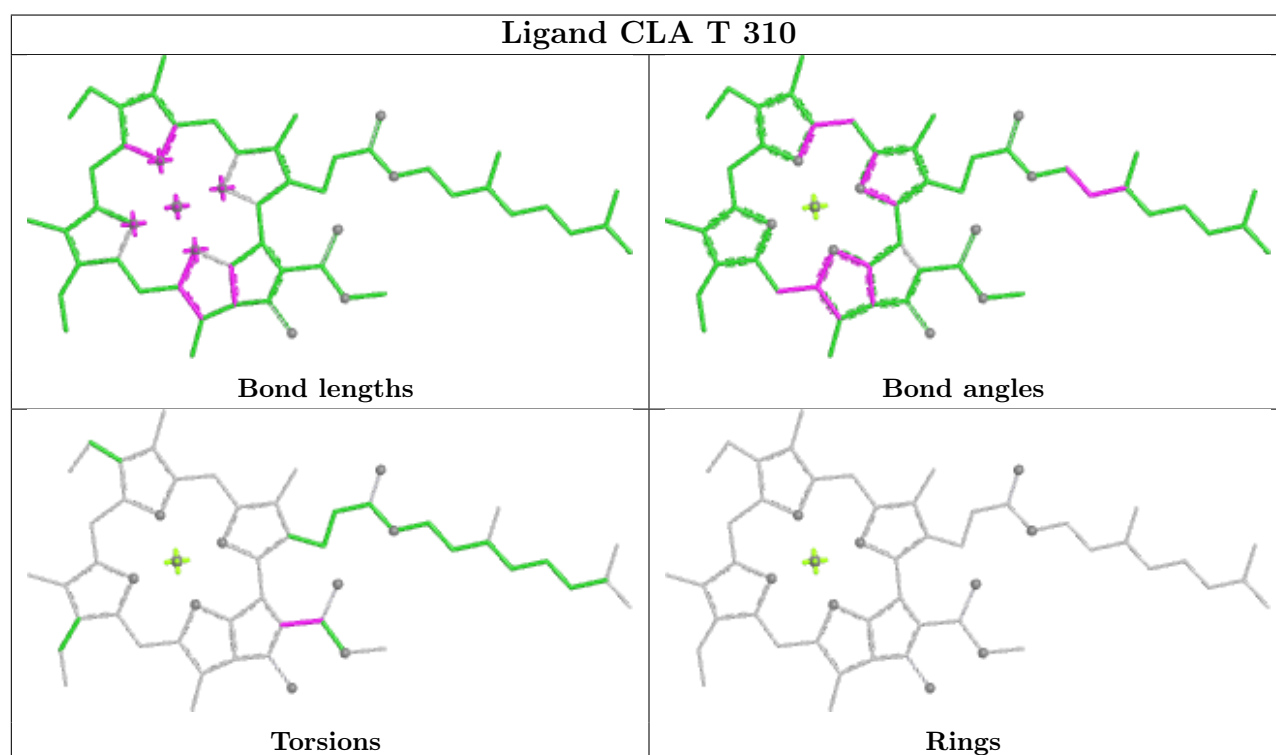
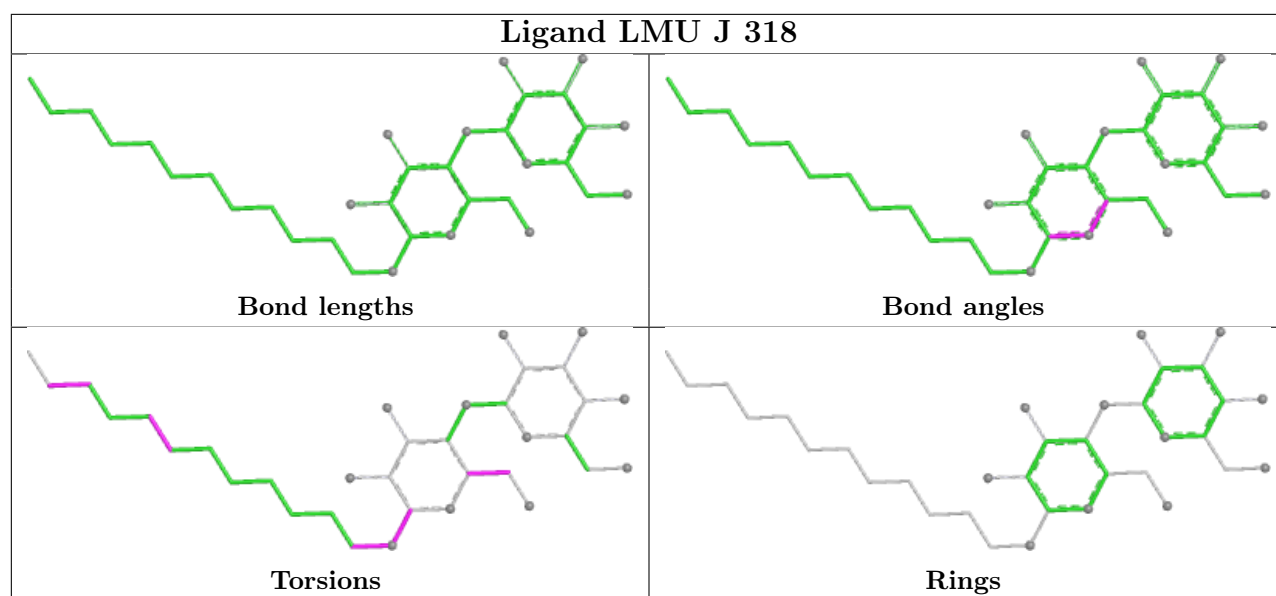


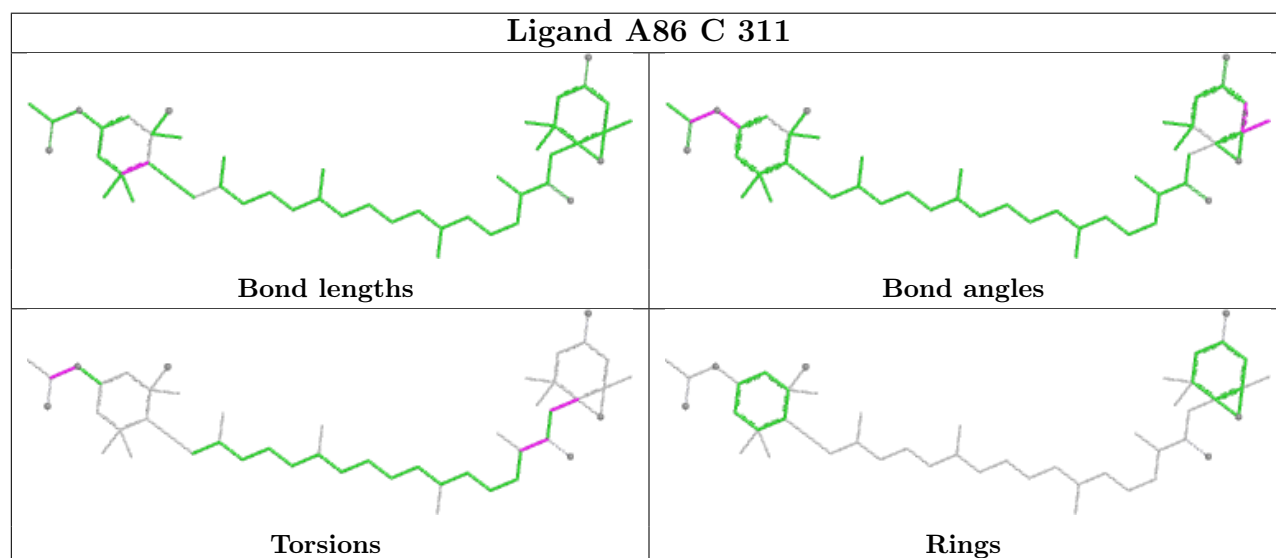
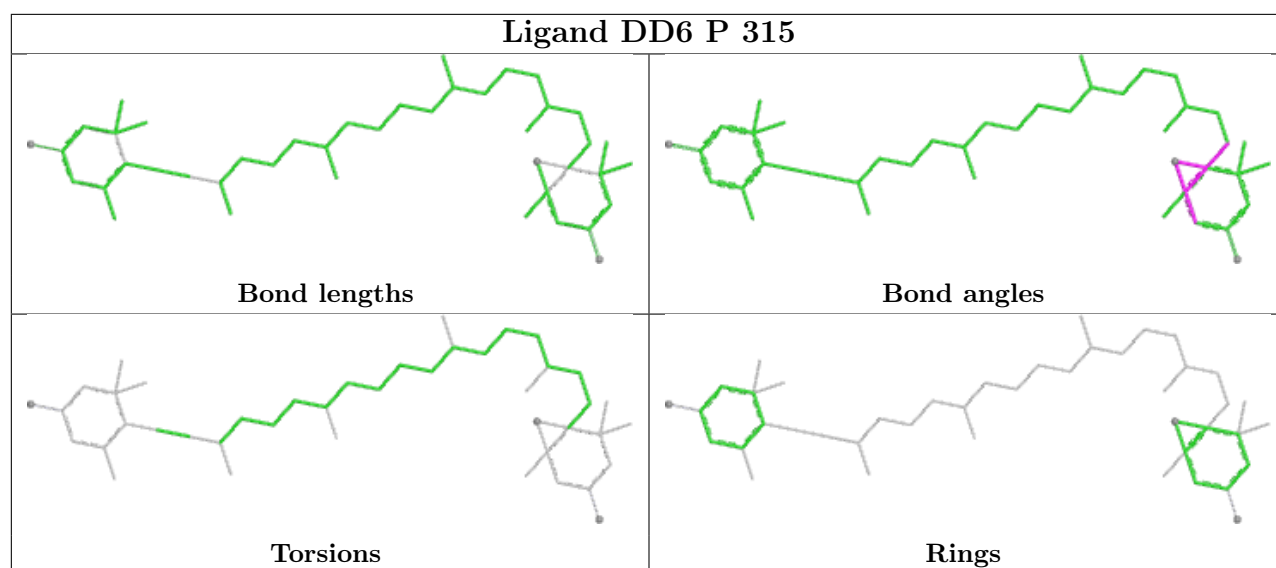
Torsions

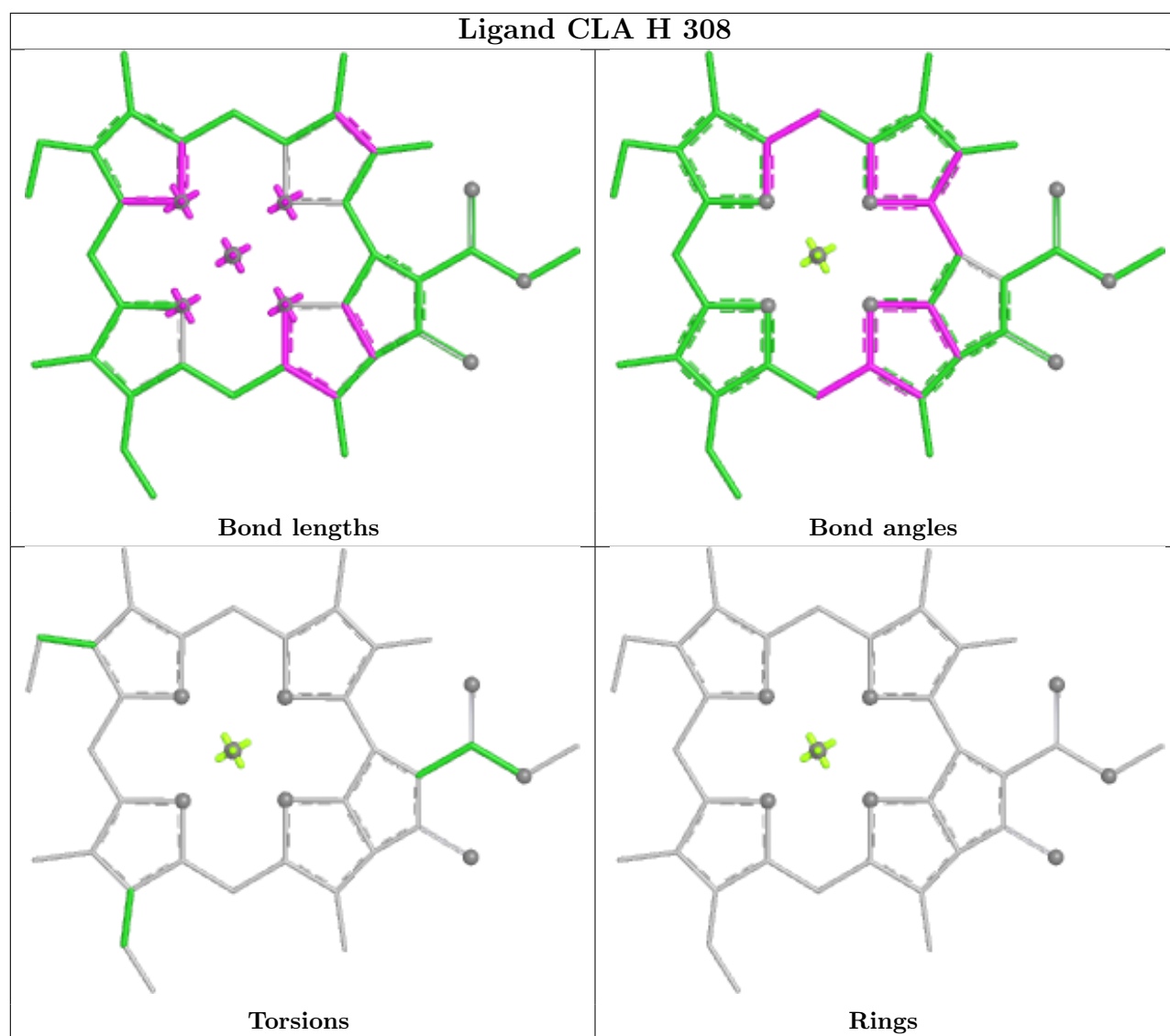


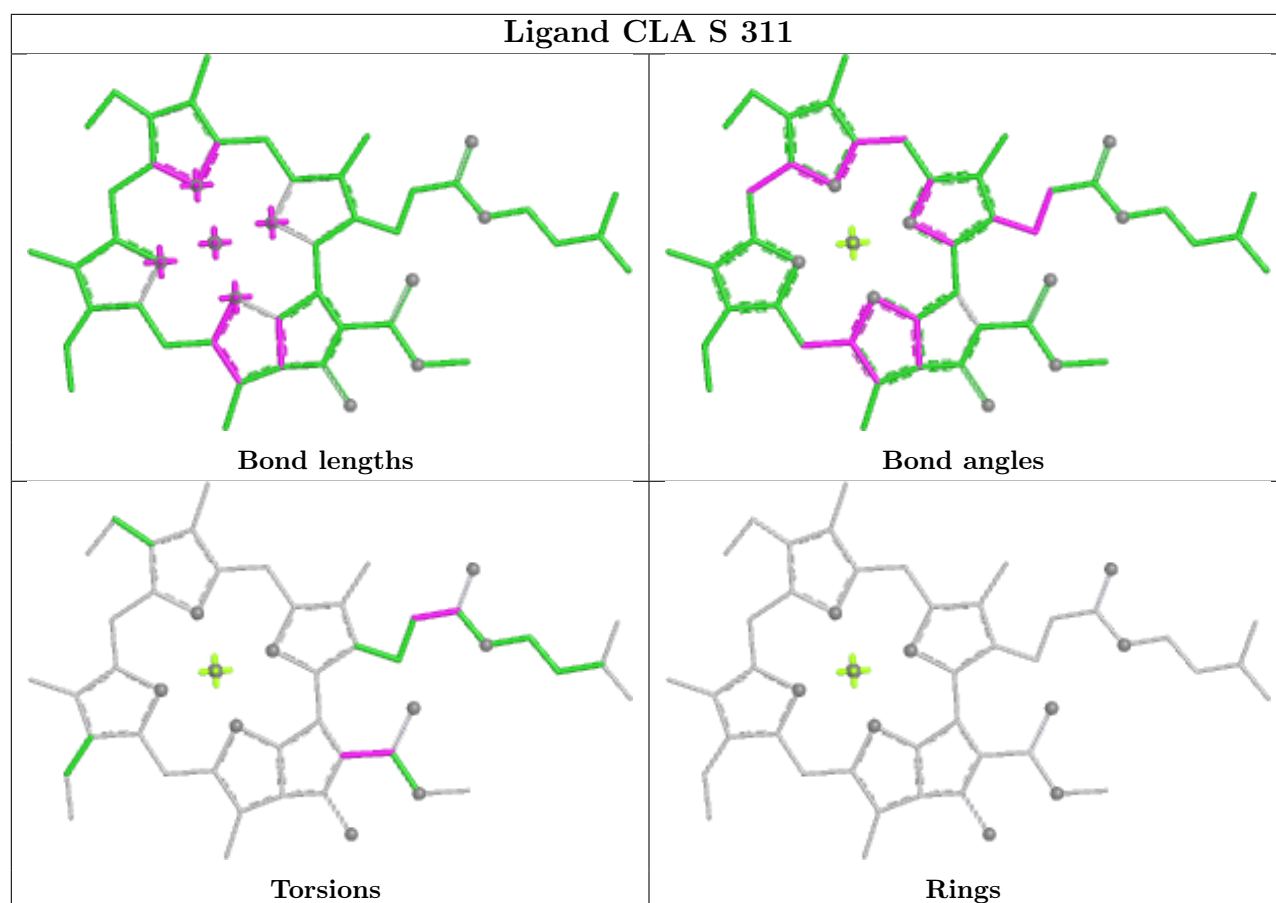
Rings



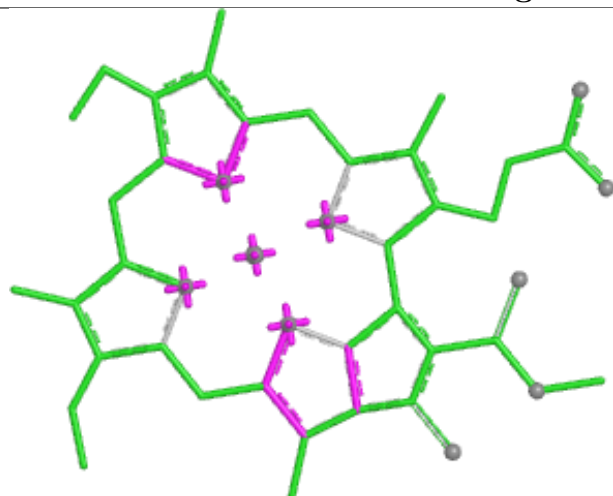




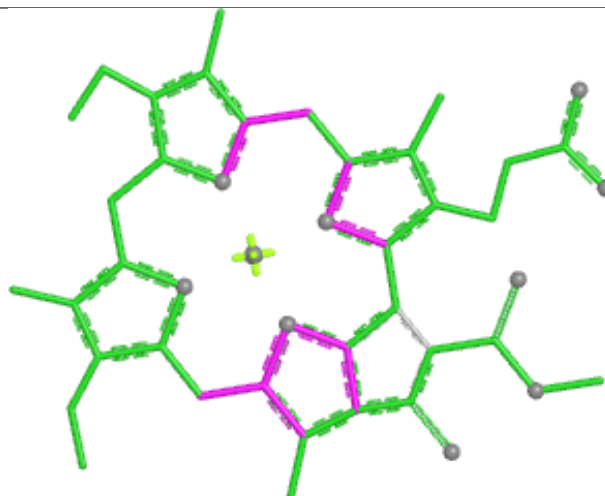




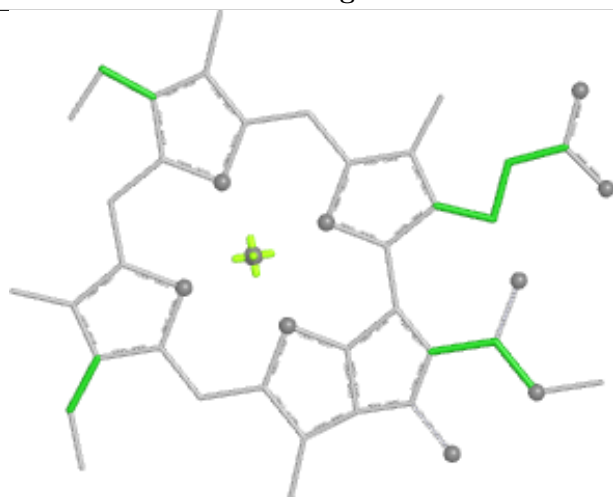
Ligand CLA P 307



Bond lengths



Bond angles

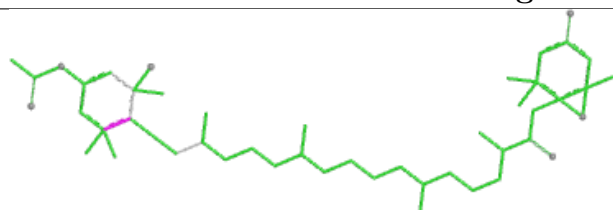


Torsions

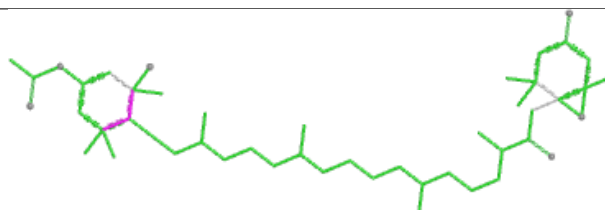


Rings

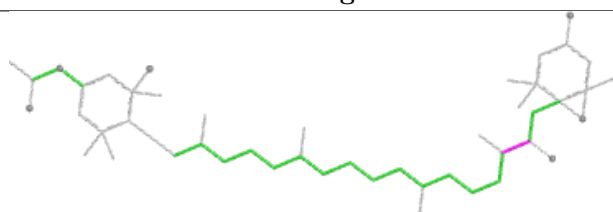
Ligand A86 M 322



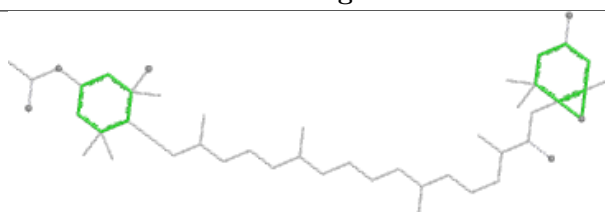
Bond lengths



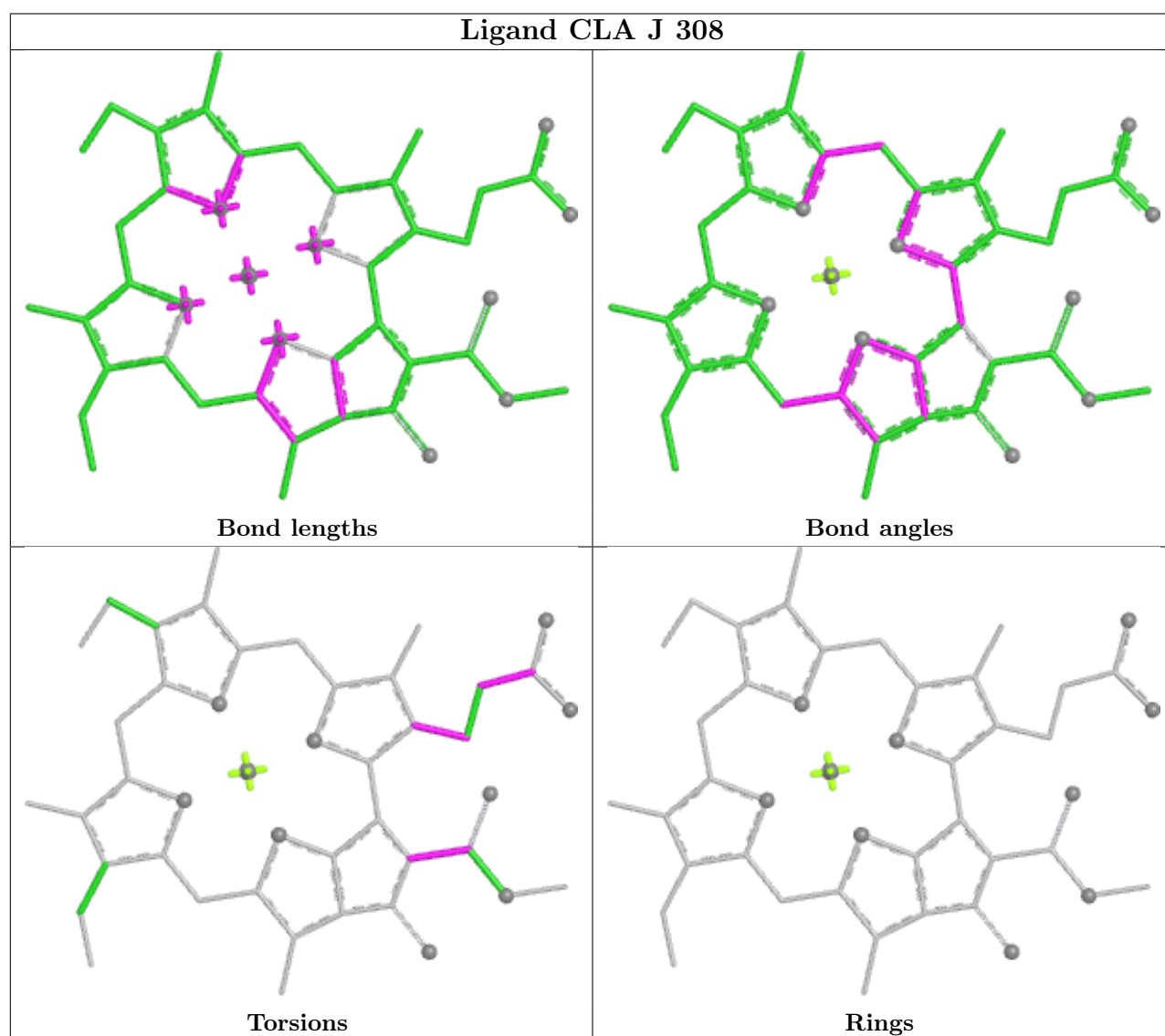
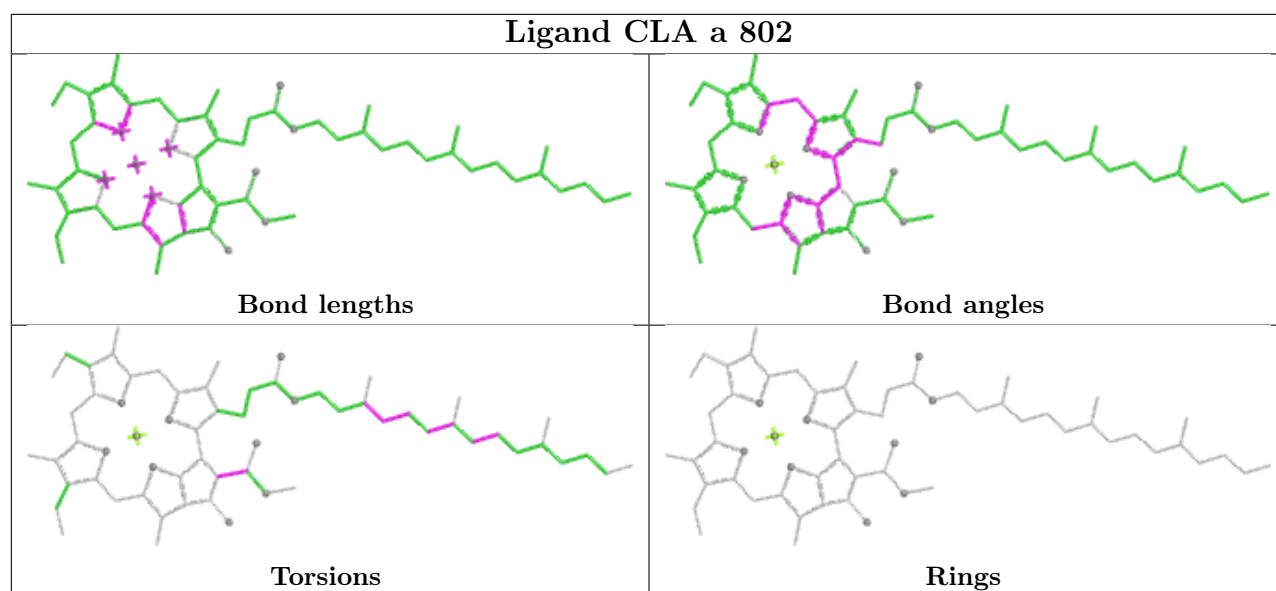
Bond angles



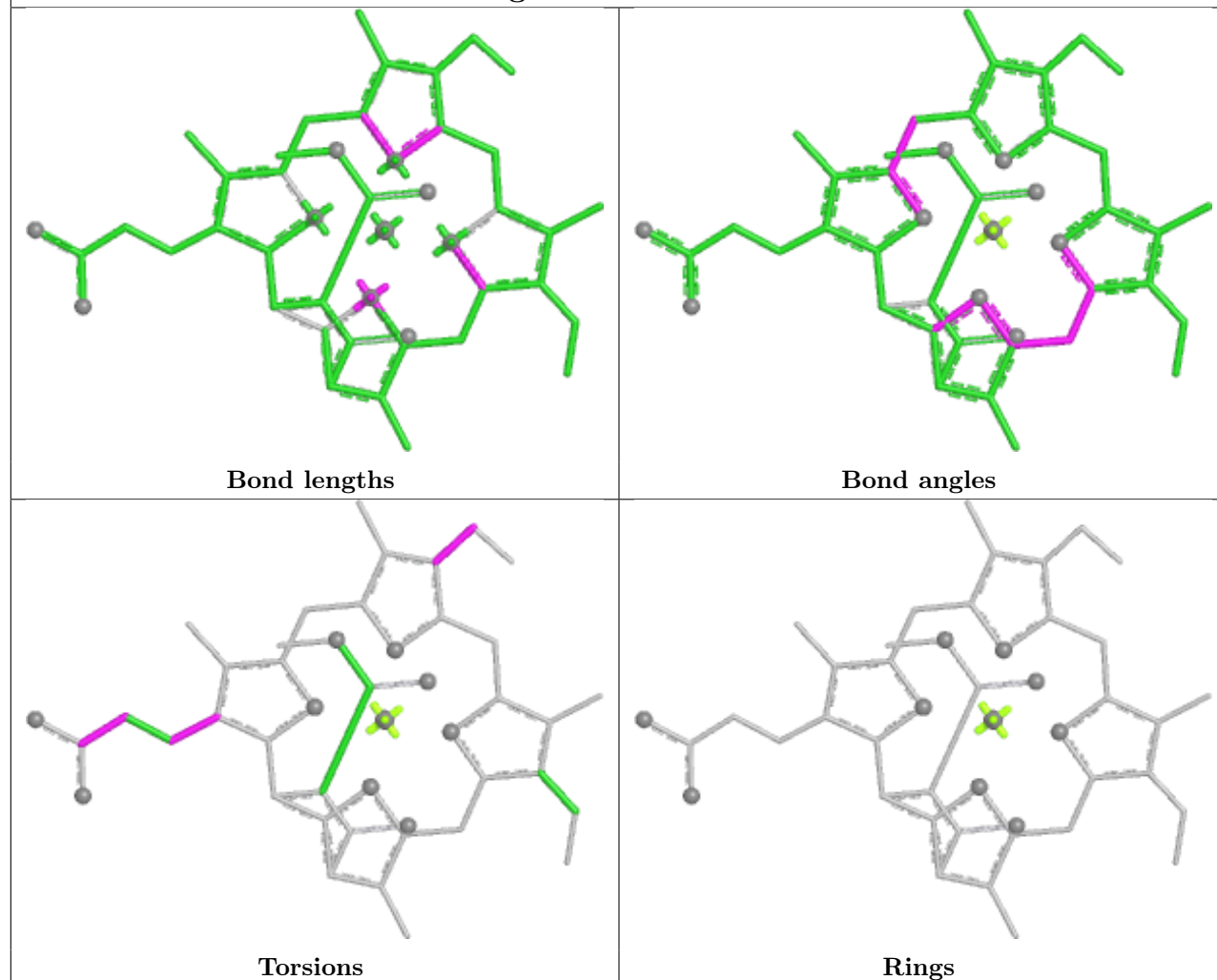
Torsions



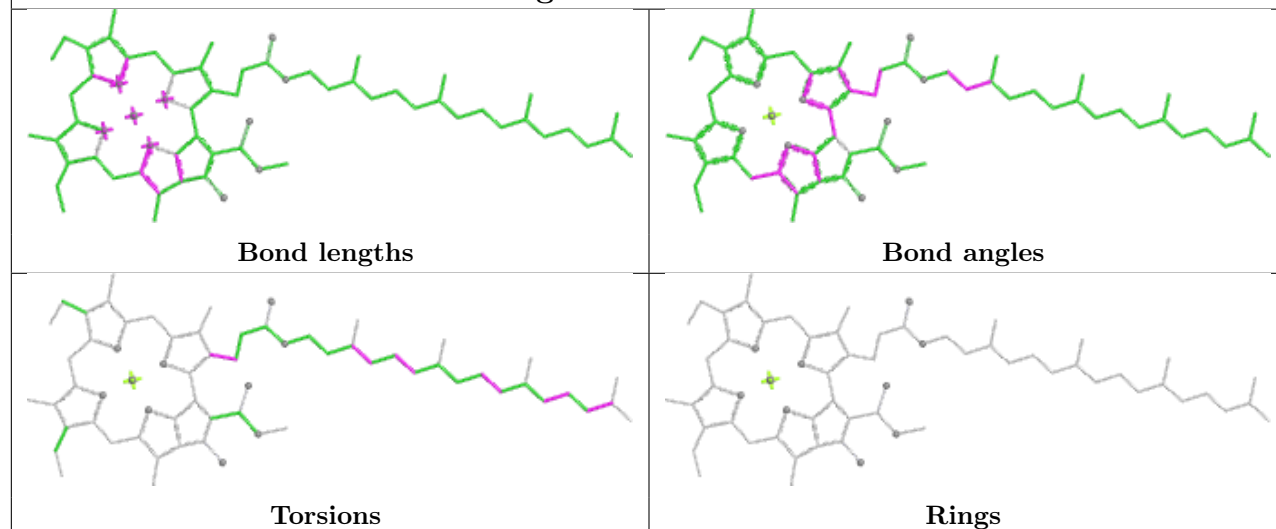
Rings



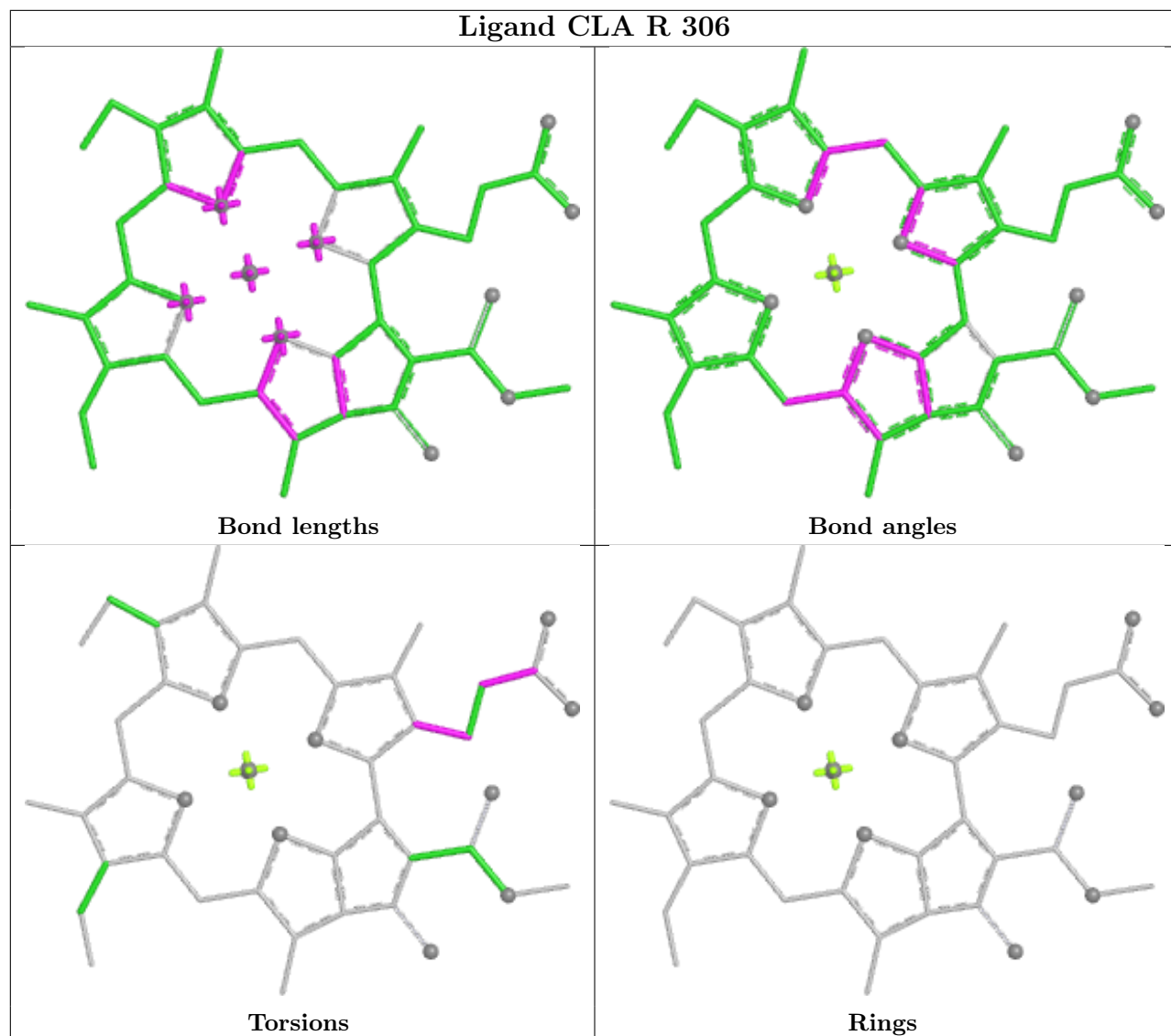
Ligand KC2 O 303



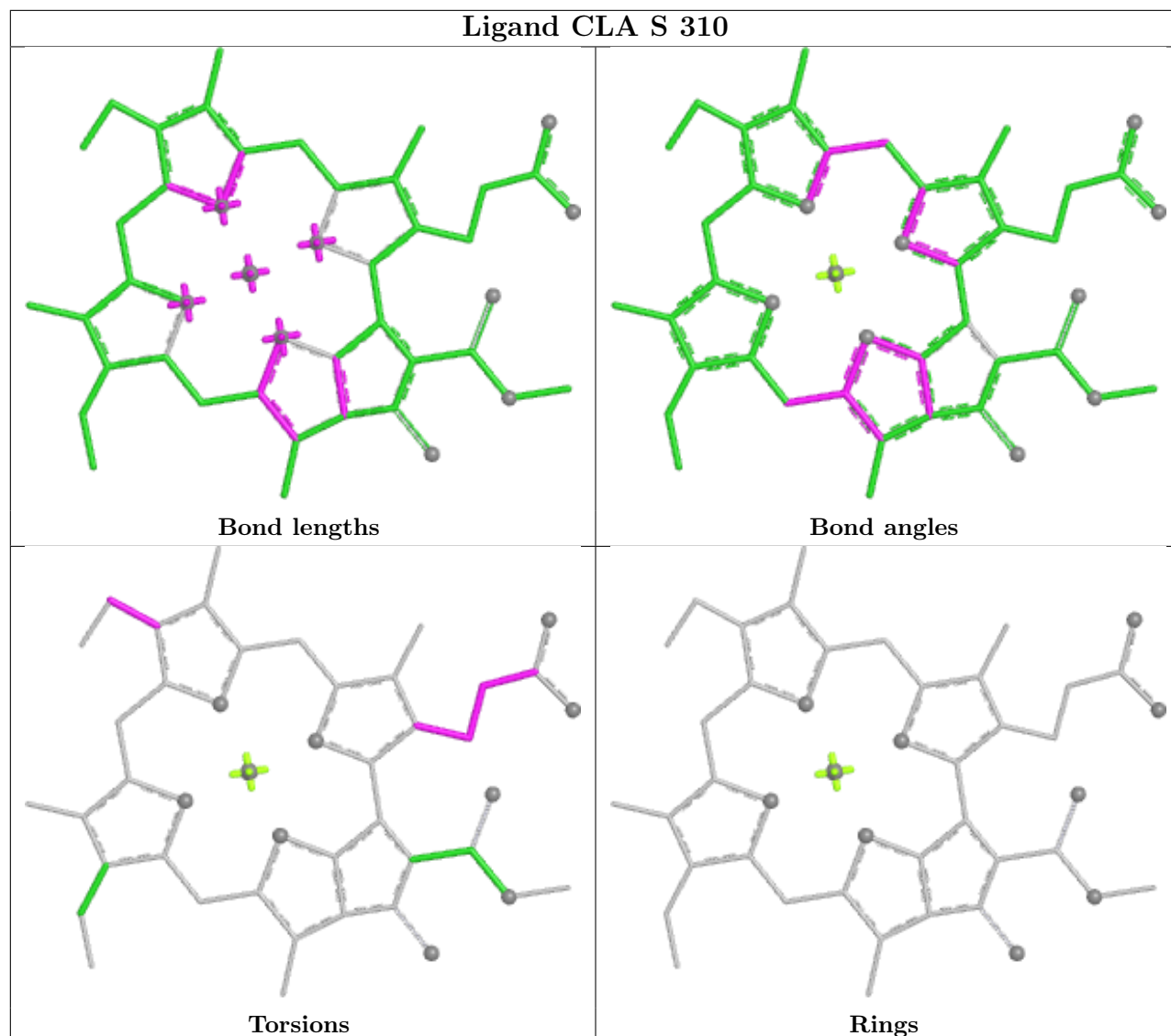
Ligand CLA a 814



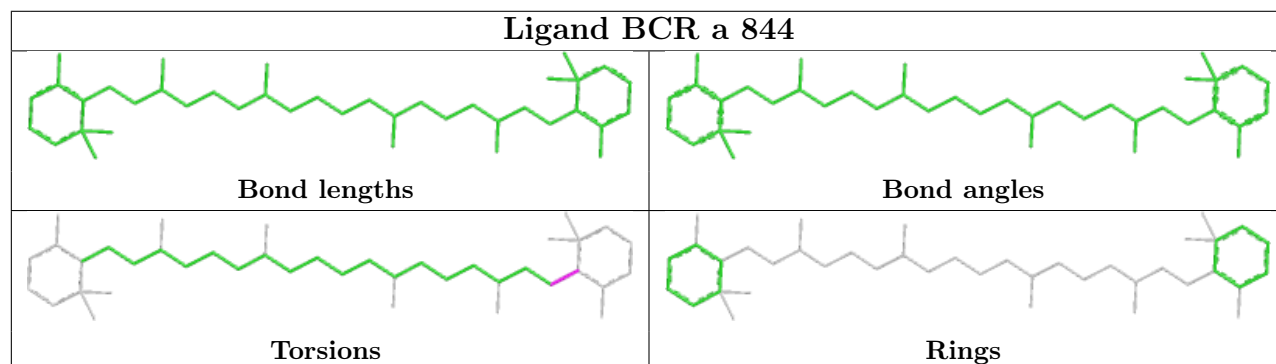
Ligand CLA R 306

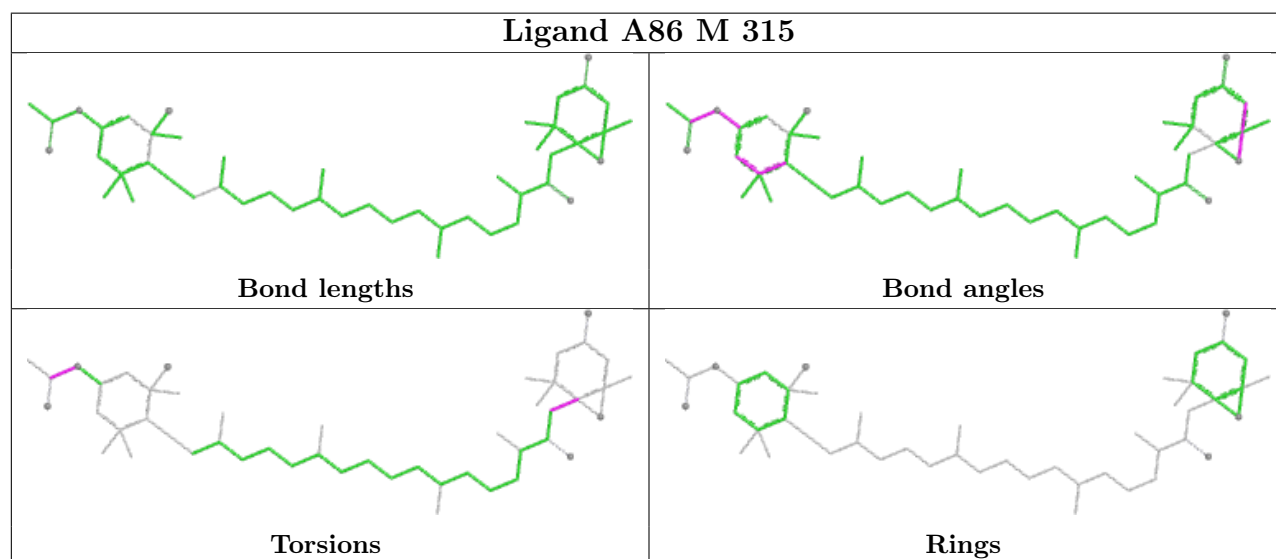
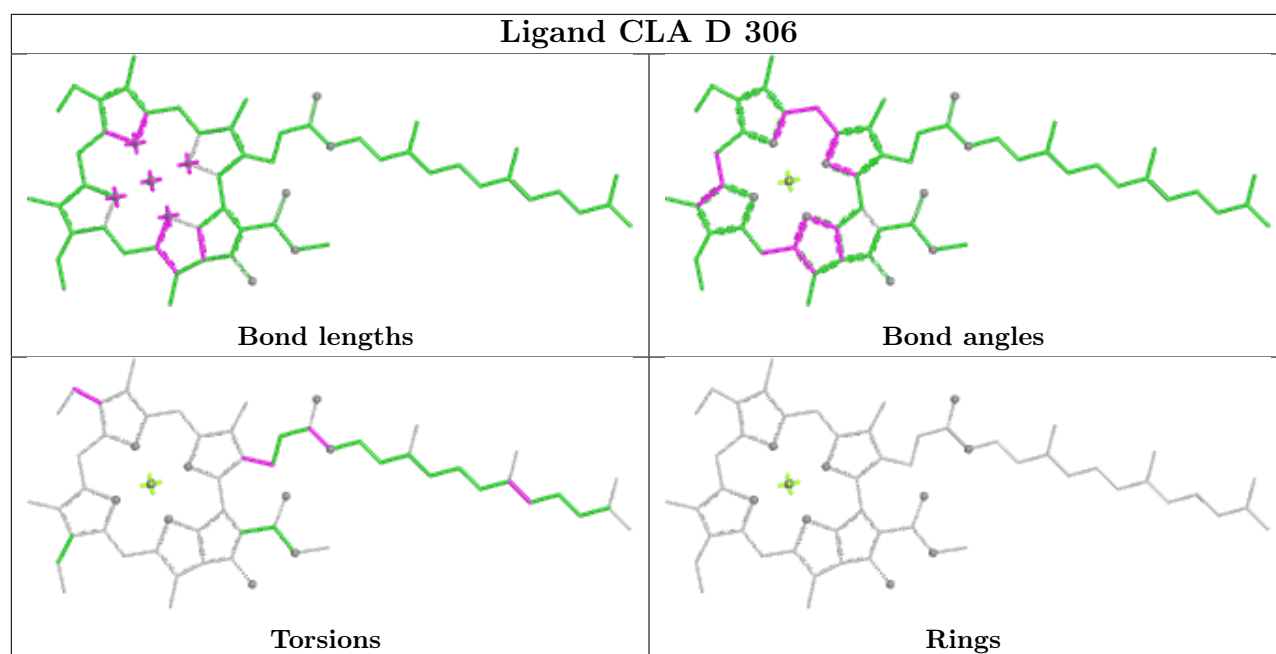


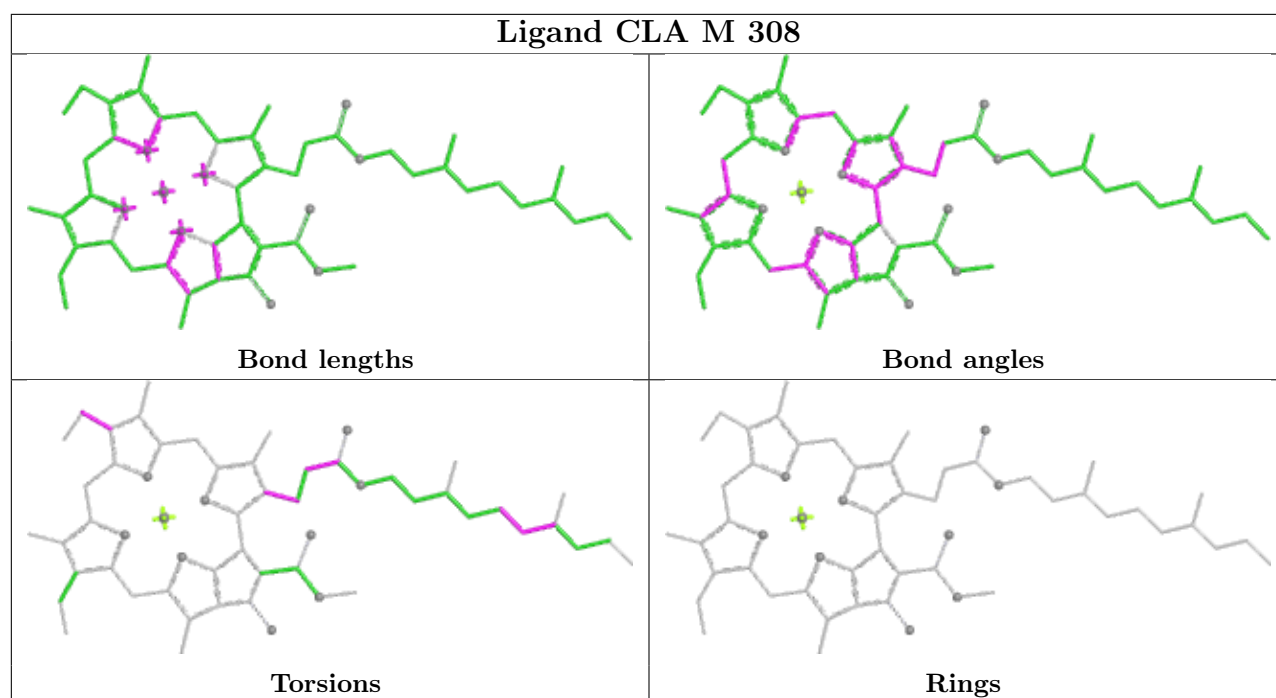
Ligand CLA S 310



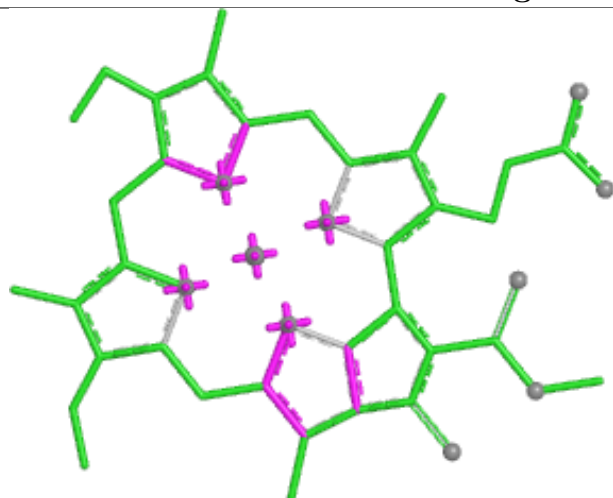
Ligand BCR a 844



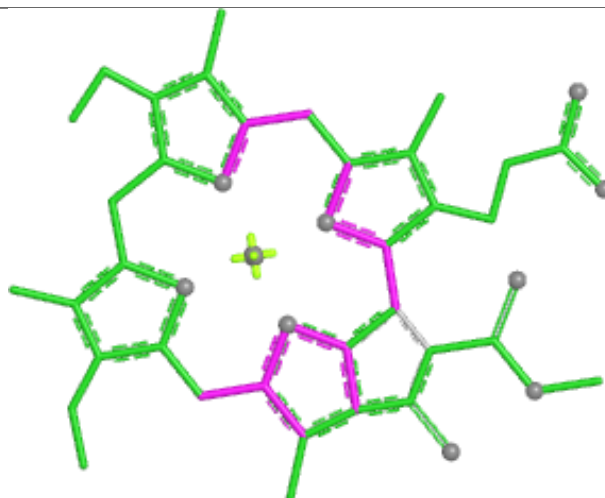




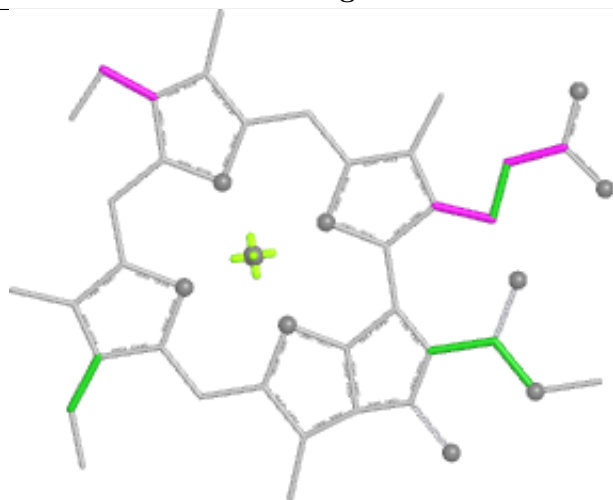
Ligand CLA O 301



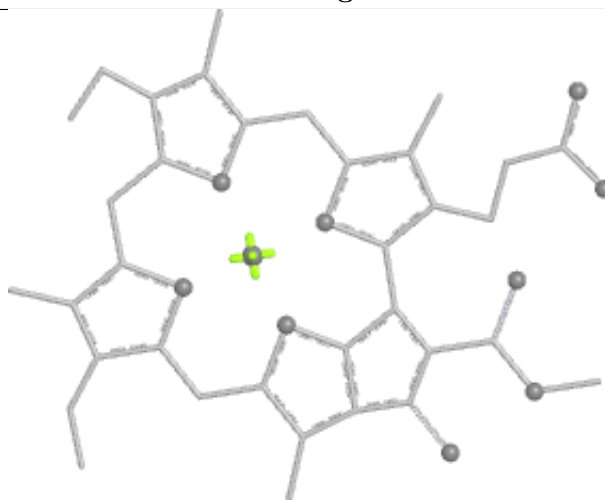
Bond lengths



Bond angles

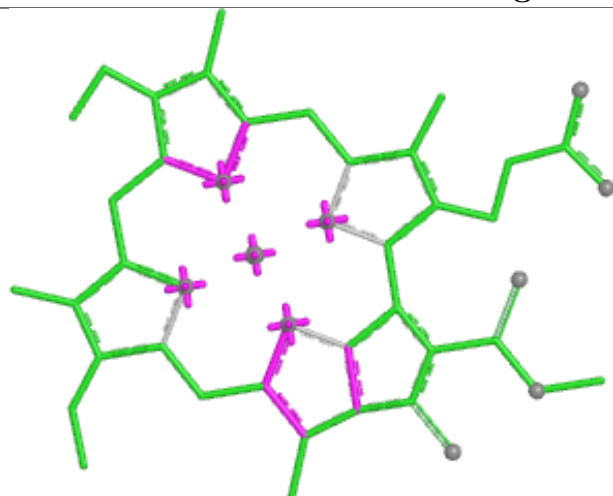


Torsions

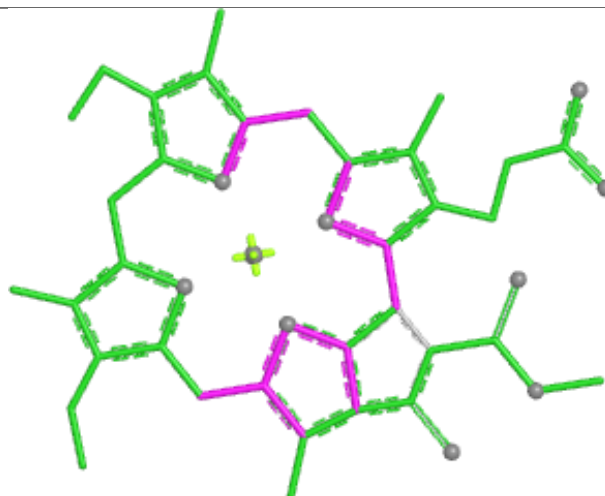


Rings

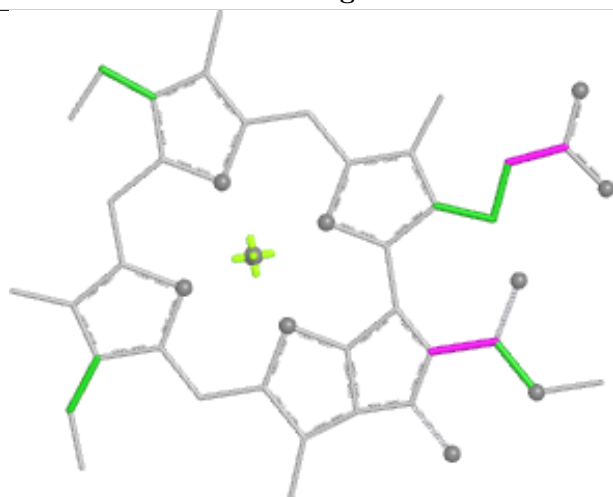
Ligand CLA O 306



Bond lengths



Bond angles

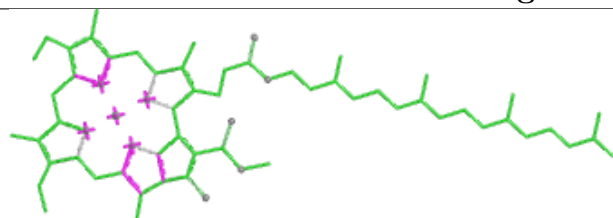


Torsions

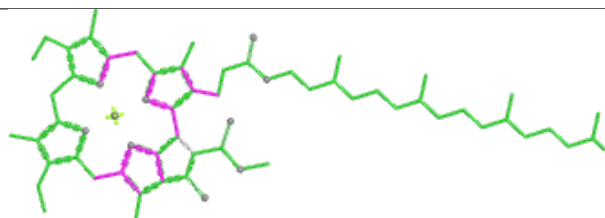


Rings

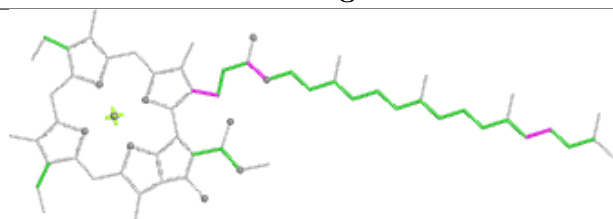
Ligand CLA b 815



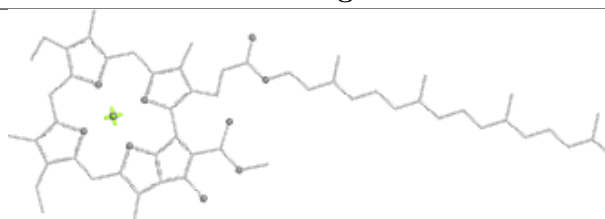
Bond lengths



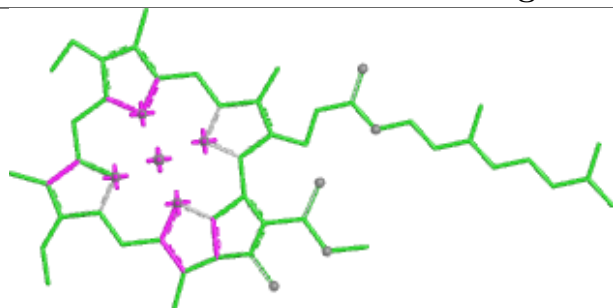
Bond angles



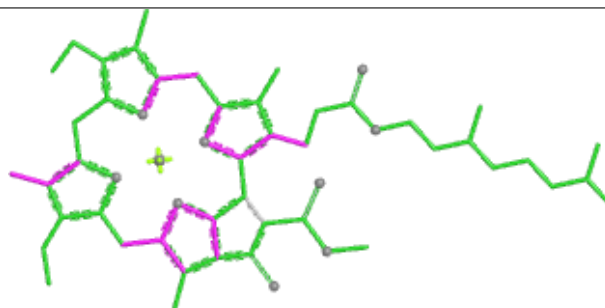
Torsions



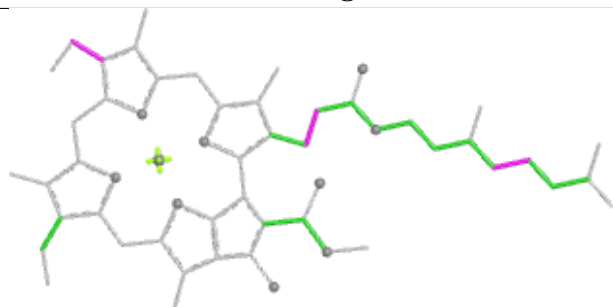
Rings

Ligand CLA J 307

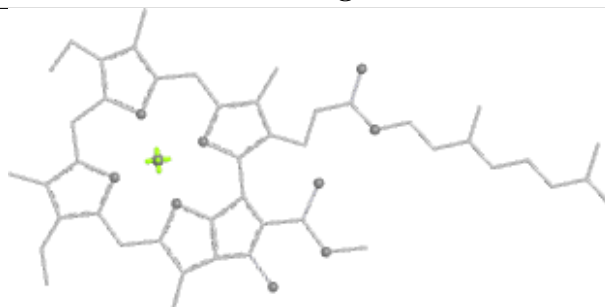
Bond lengths



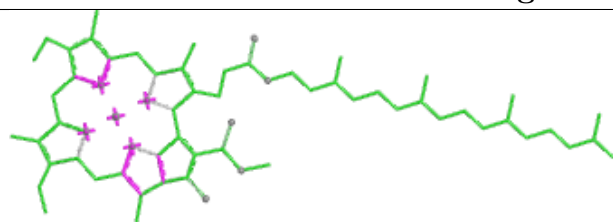
Bond angles



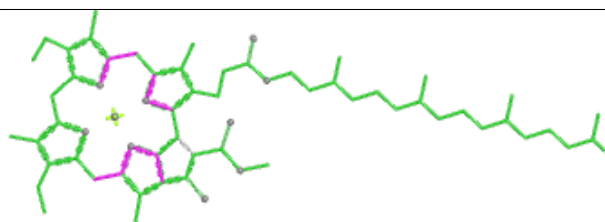
Torsions



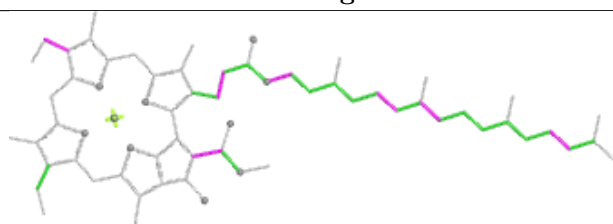
Rings

Ligand CLA b 803

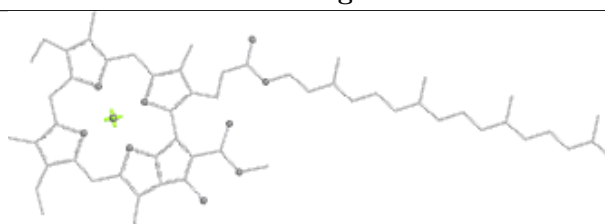
Bond lengths



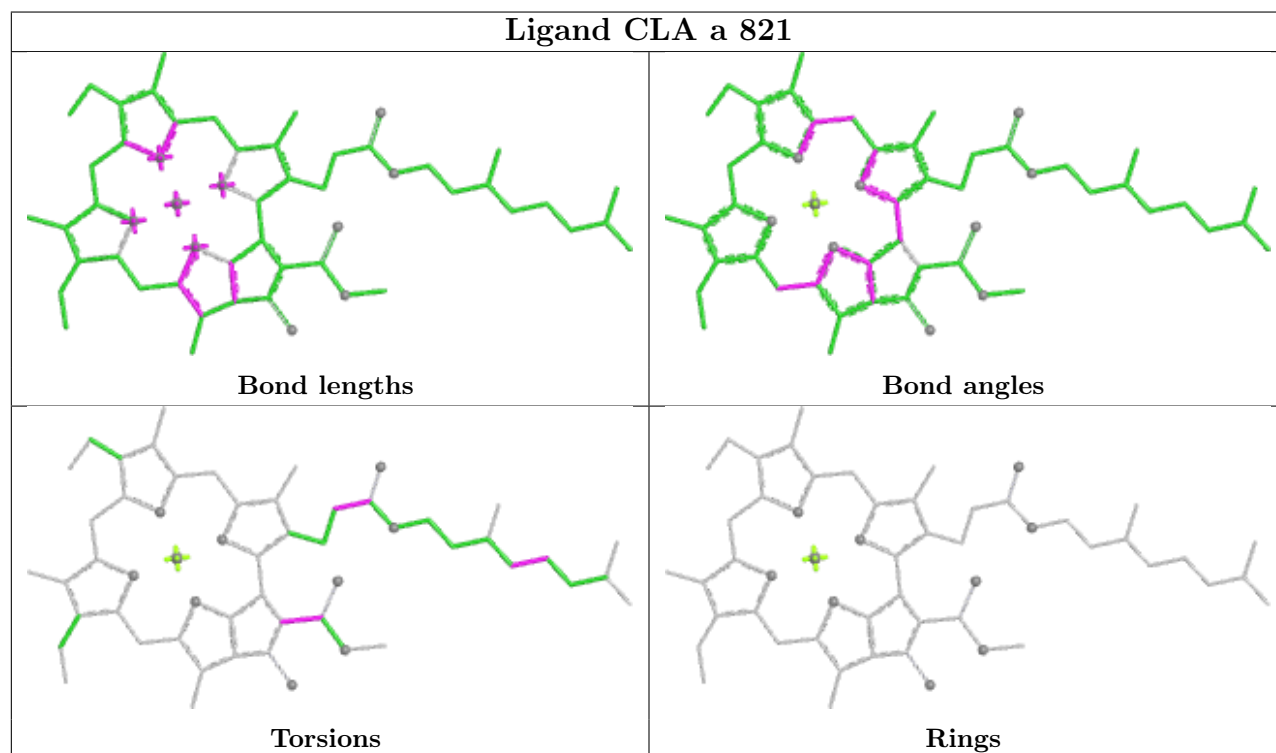
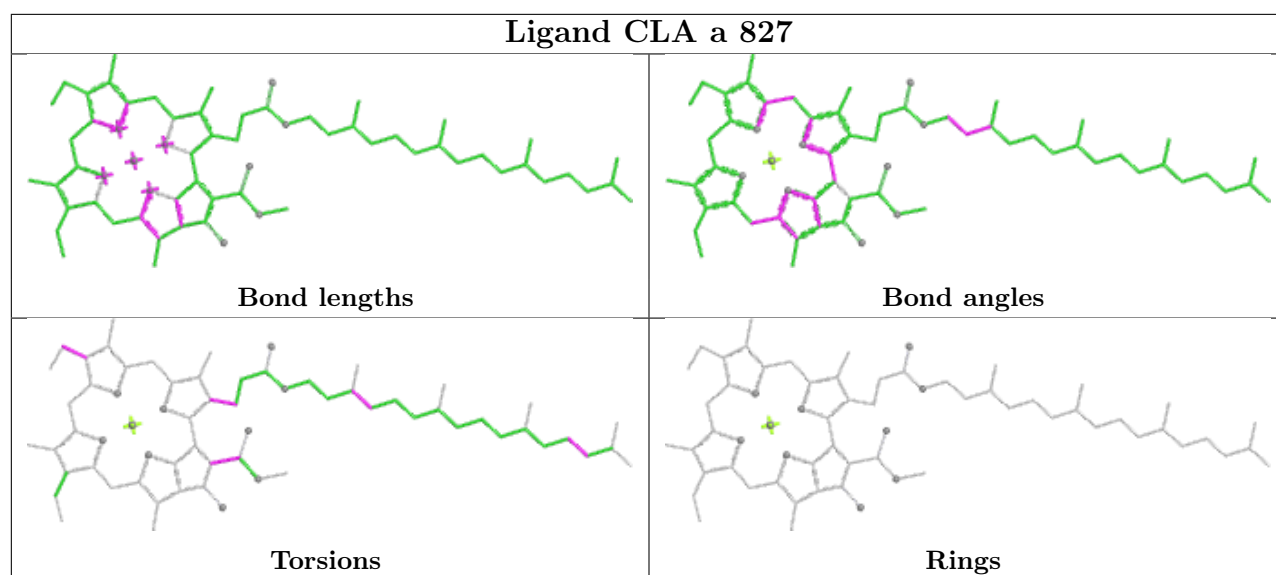
Bond angles

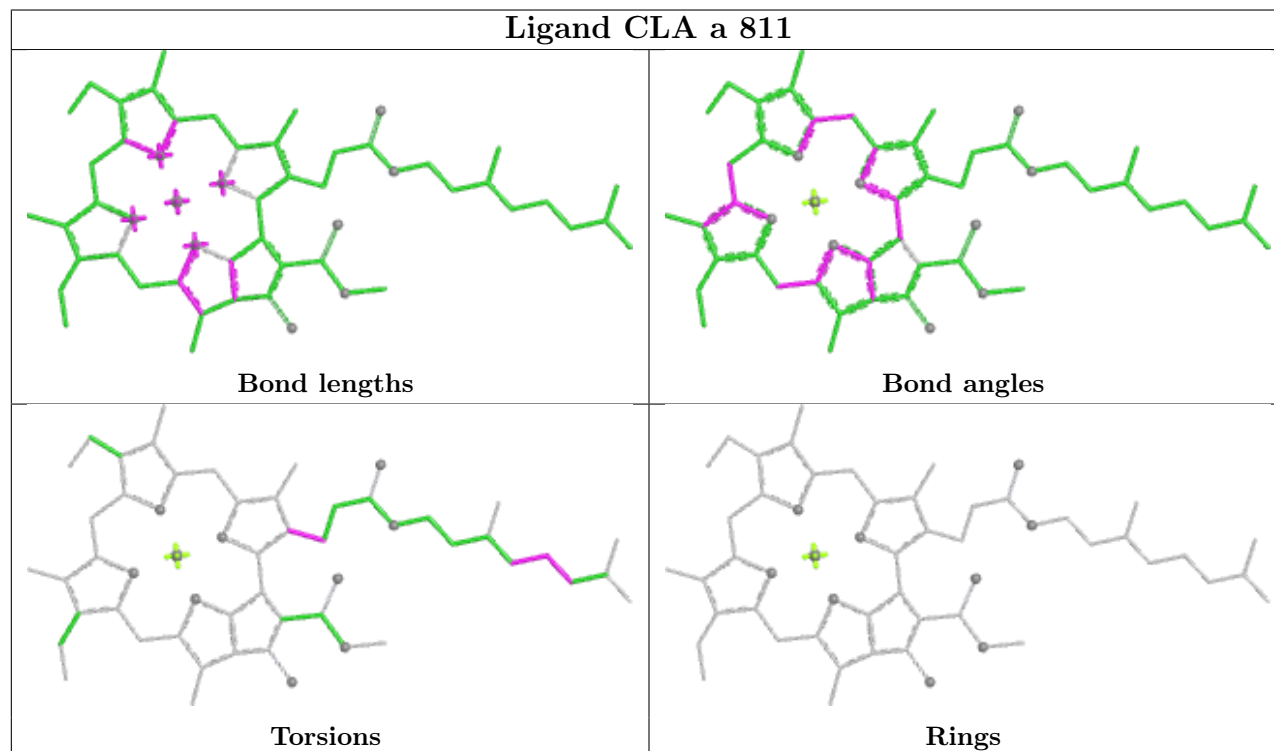
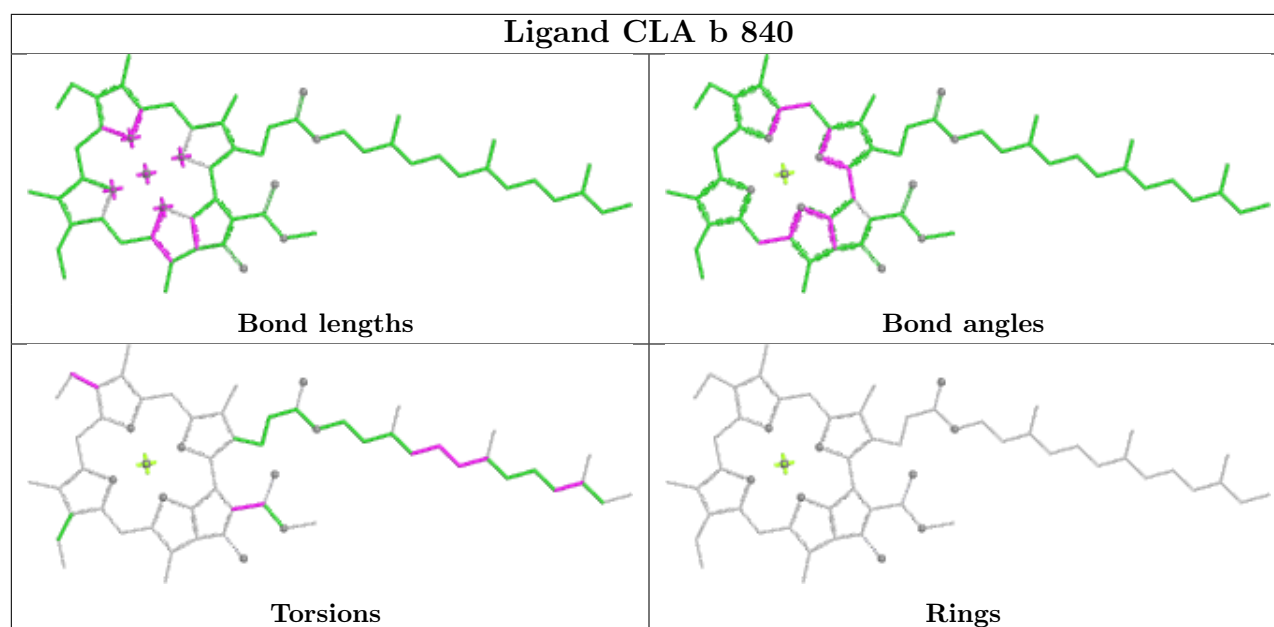


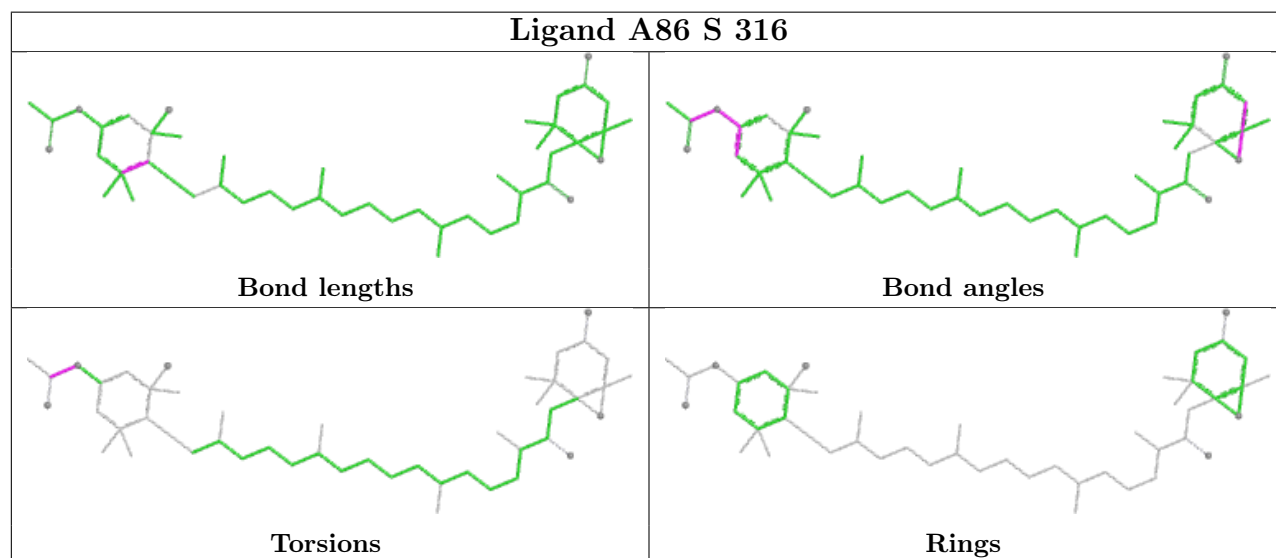
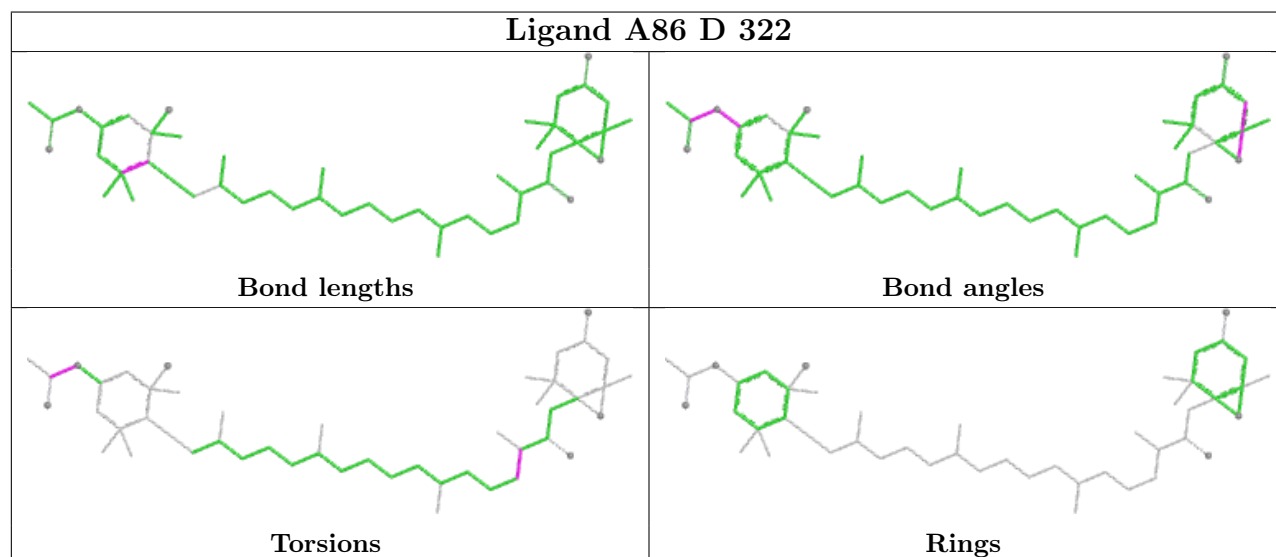
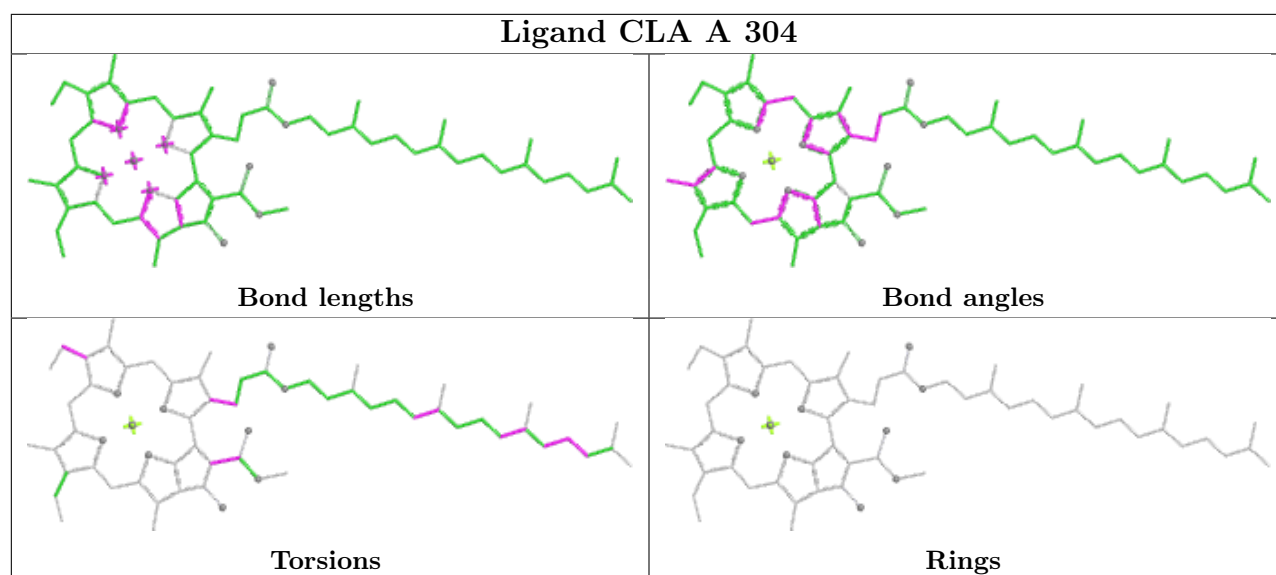
Torsions

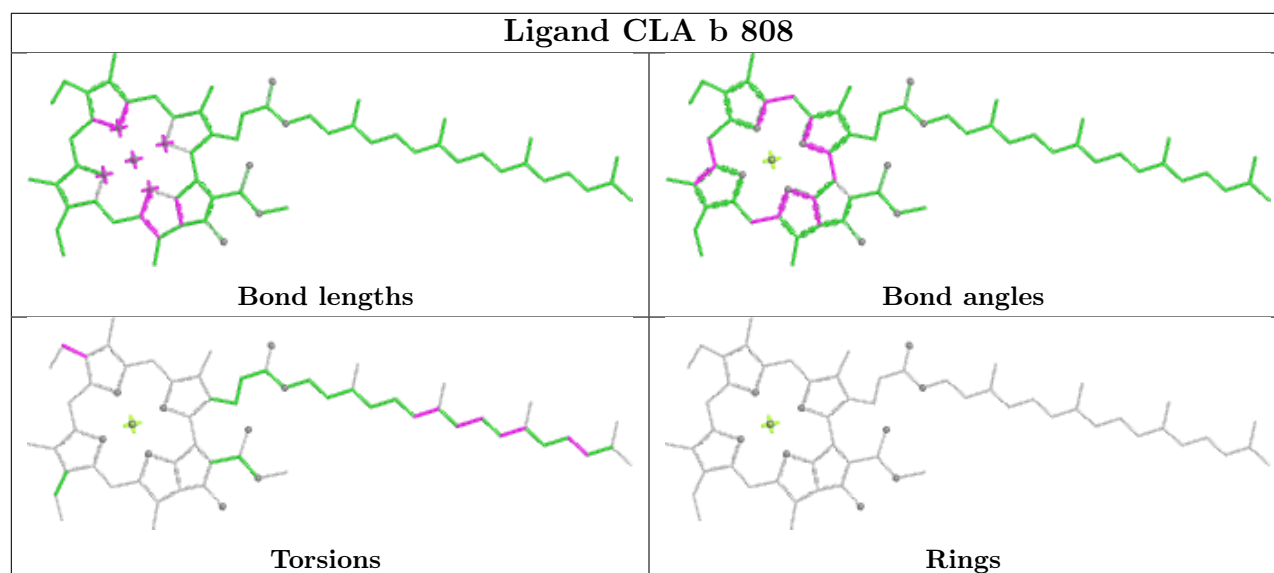
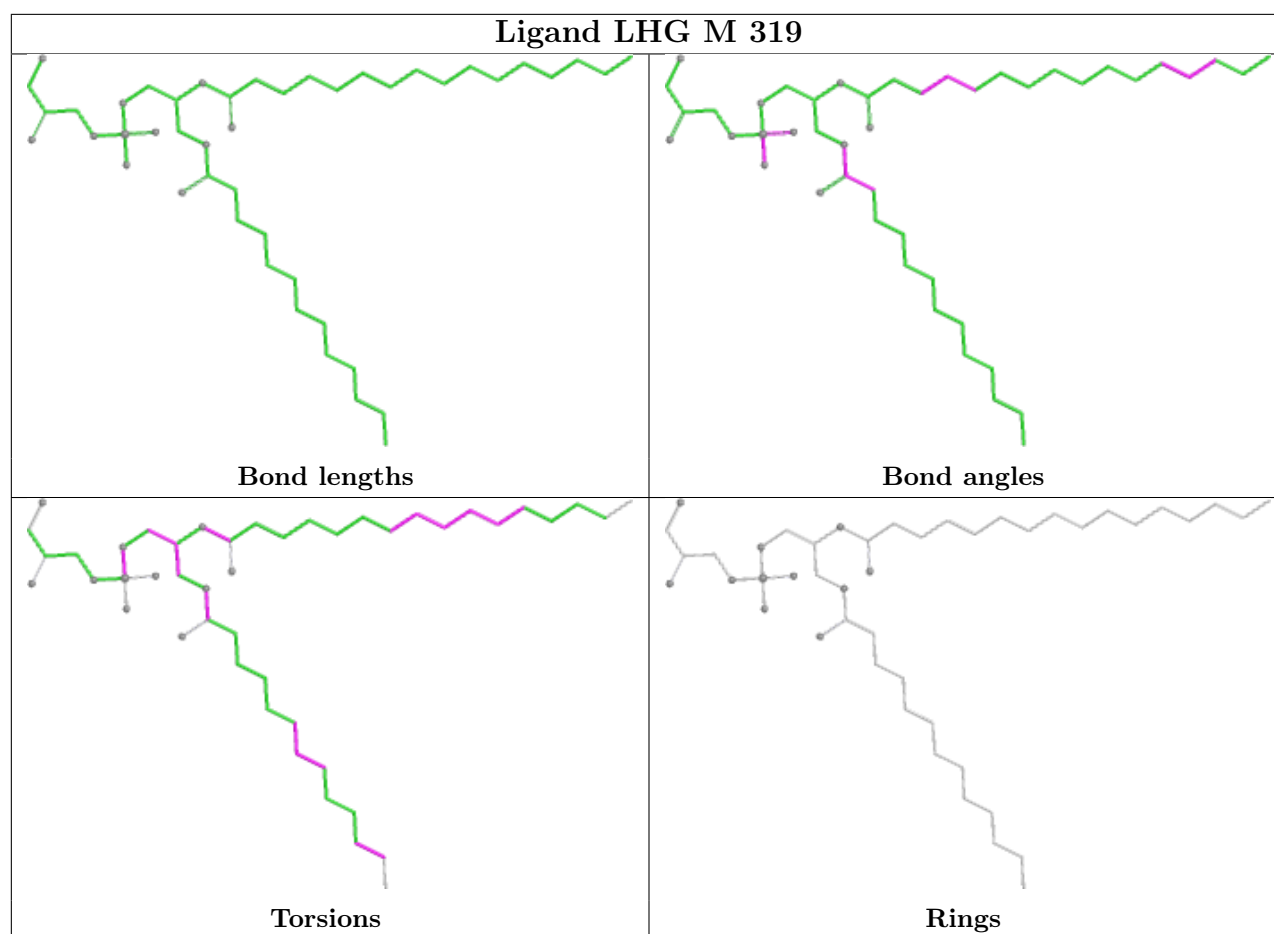


Rings

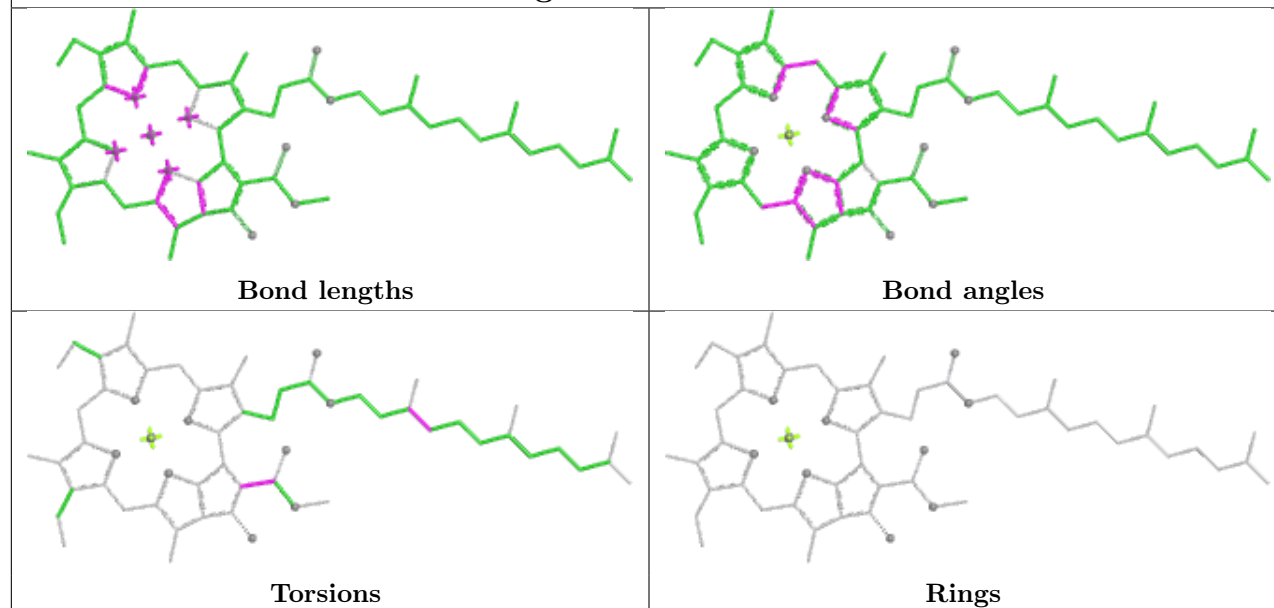




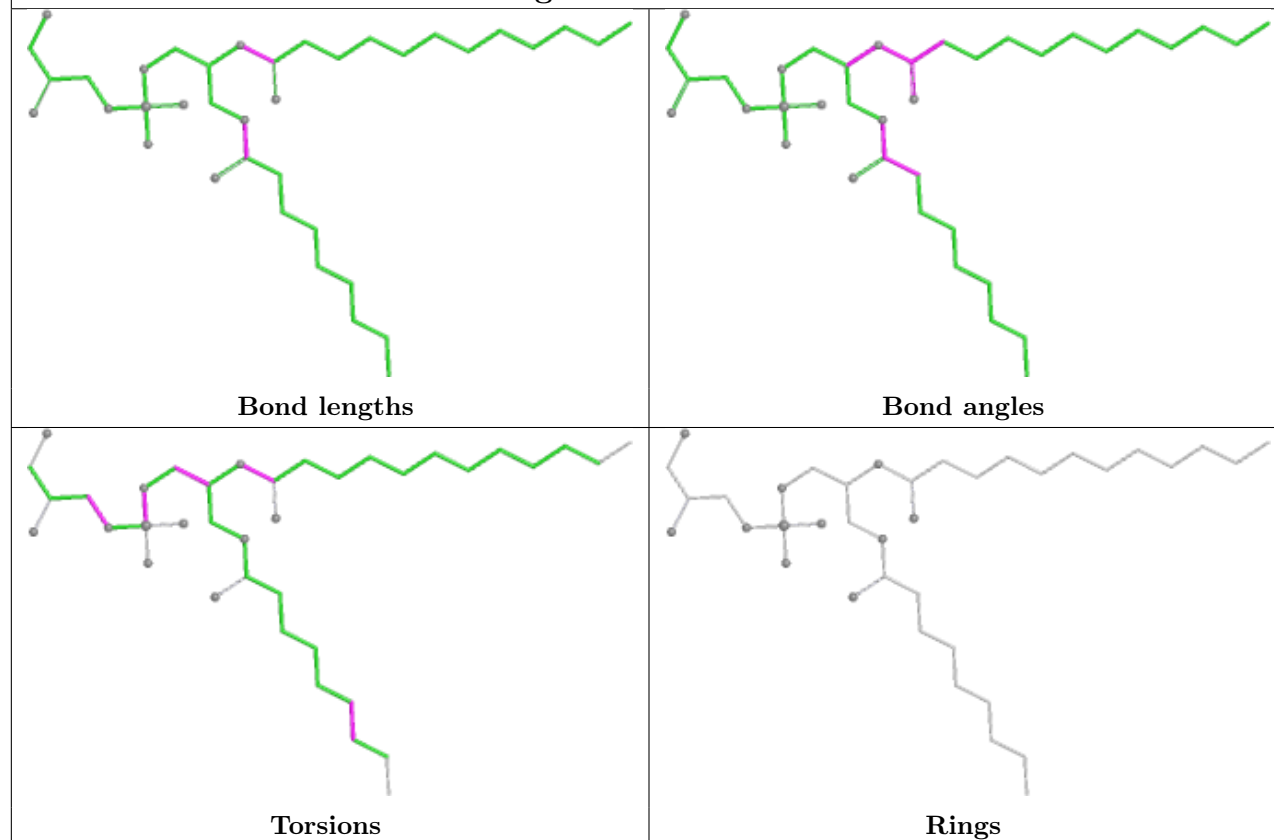


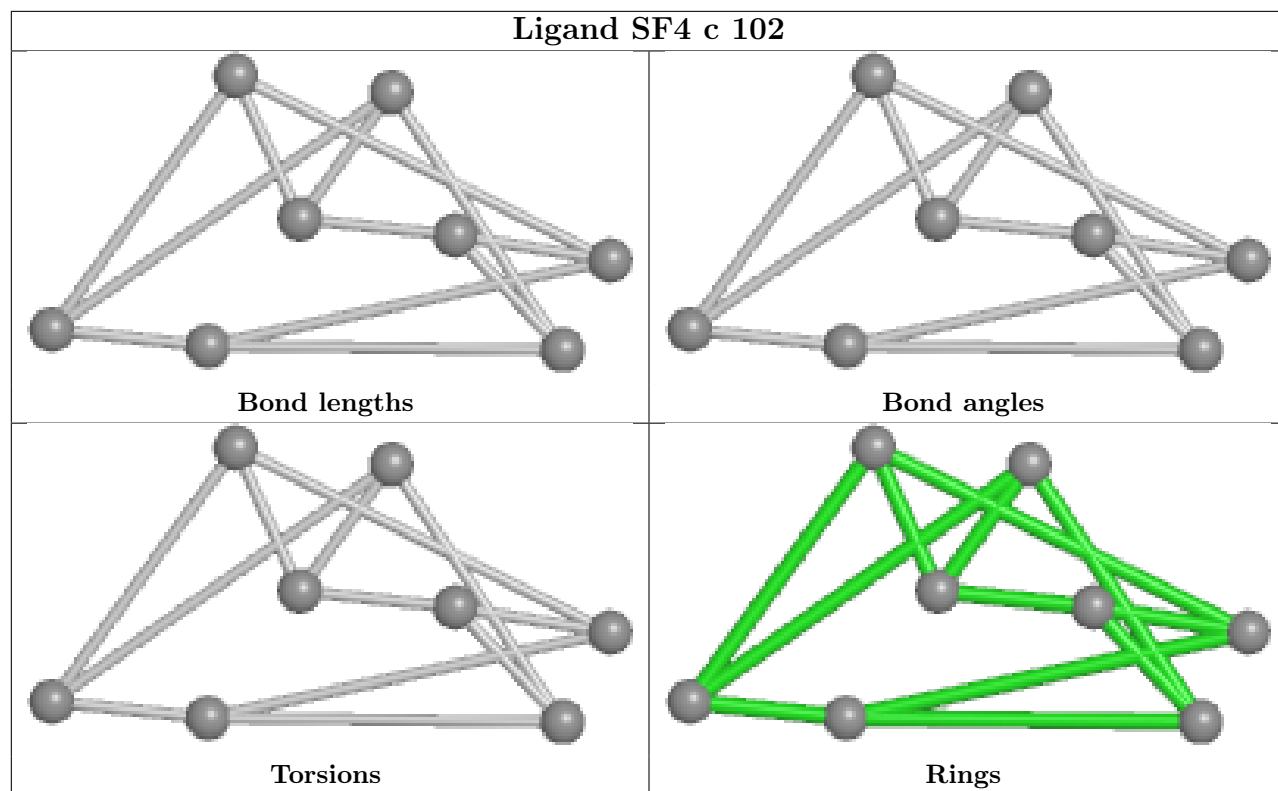


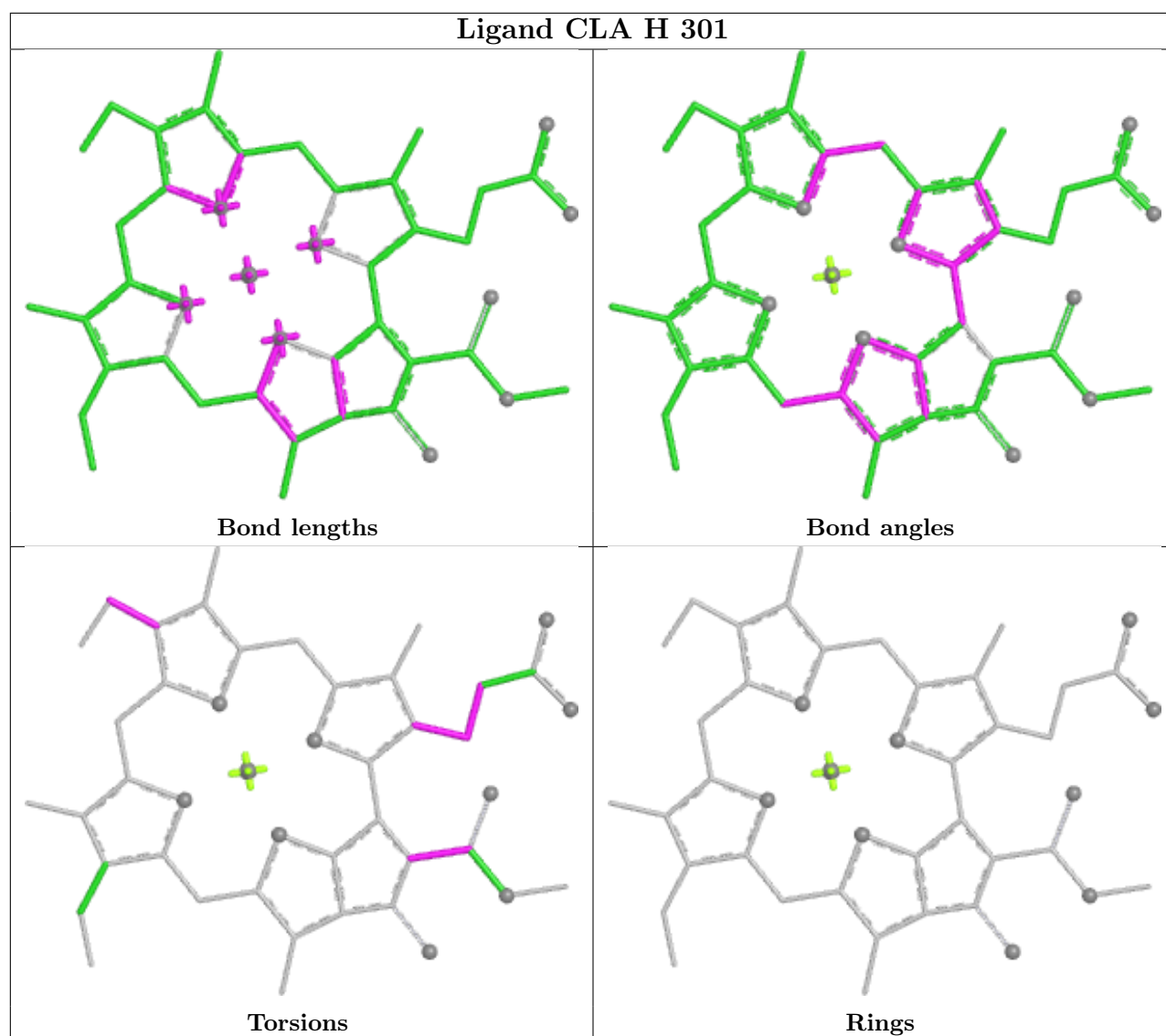
Ligand CLA b 834



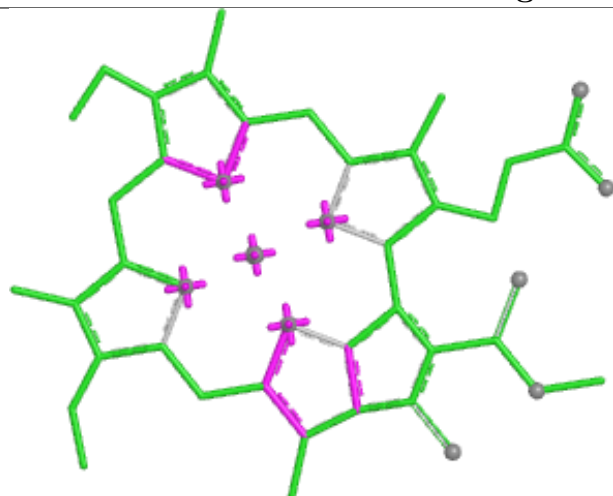
Ligand LHG a 851



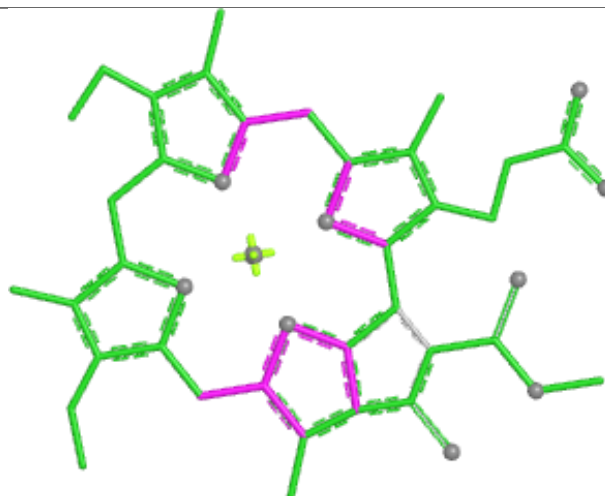




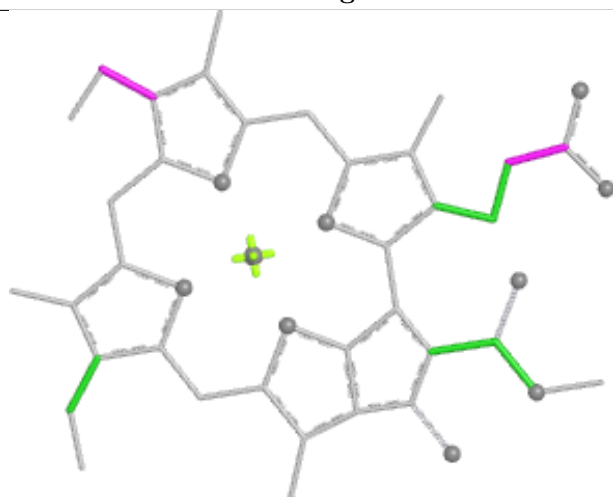
Ligand CLA L 308



Bond lengths



Bond angles

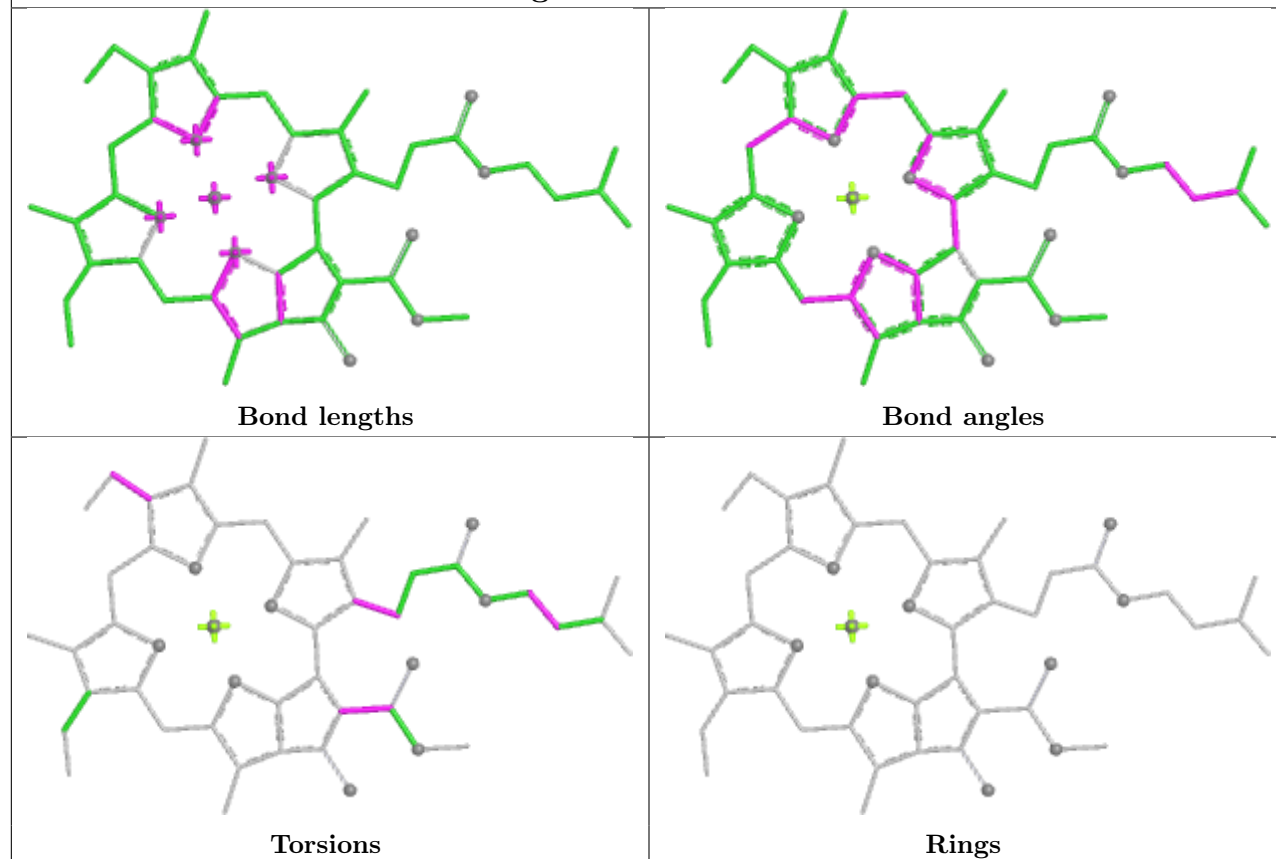


Torsions

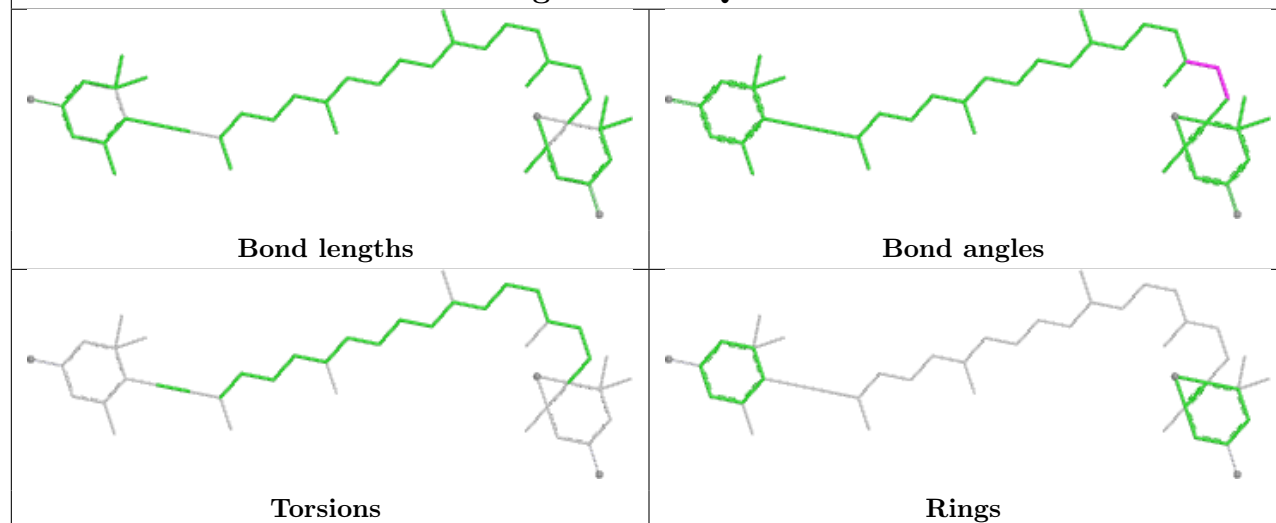


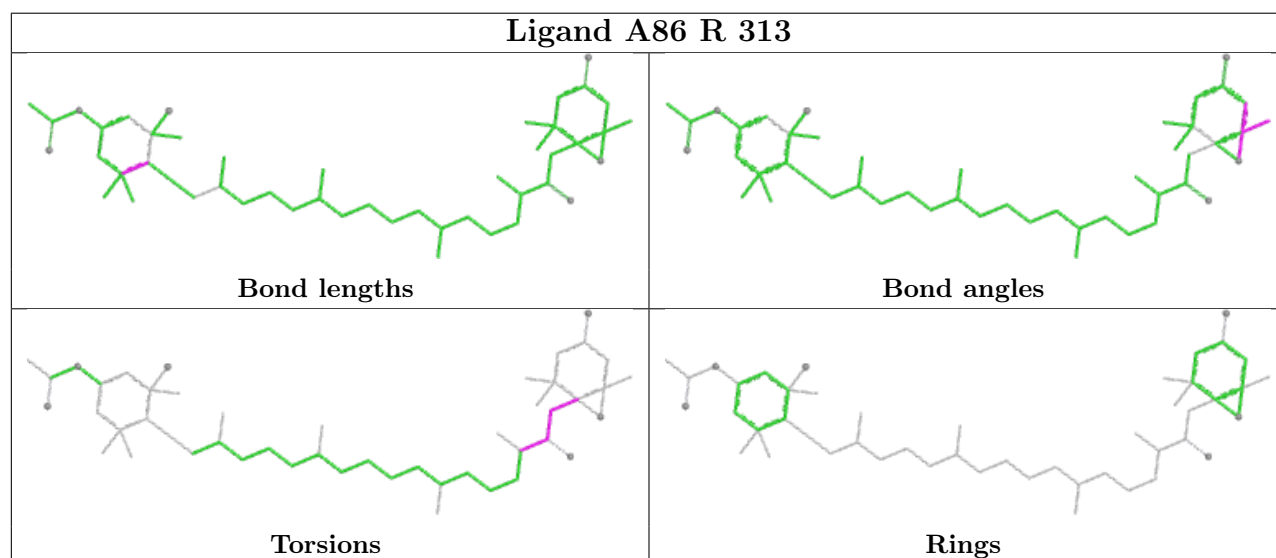
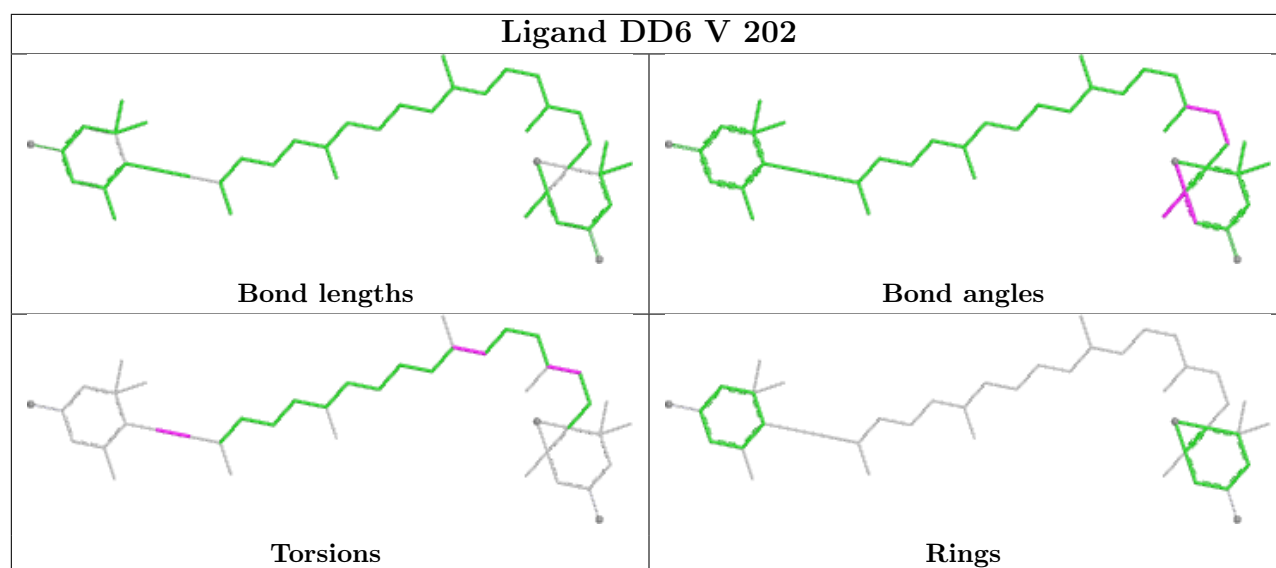
Rings

Ligand CLA N 309

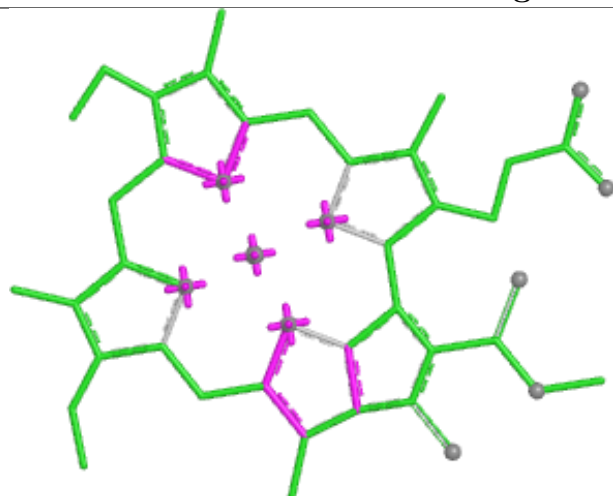


Ligand DD6 Q 313

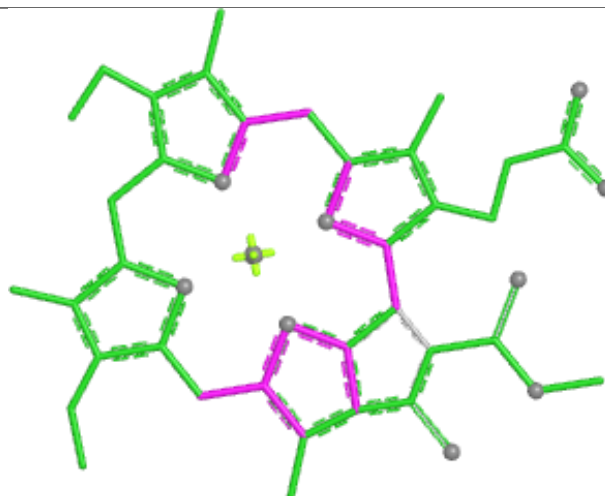




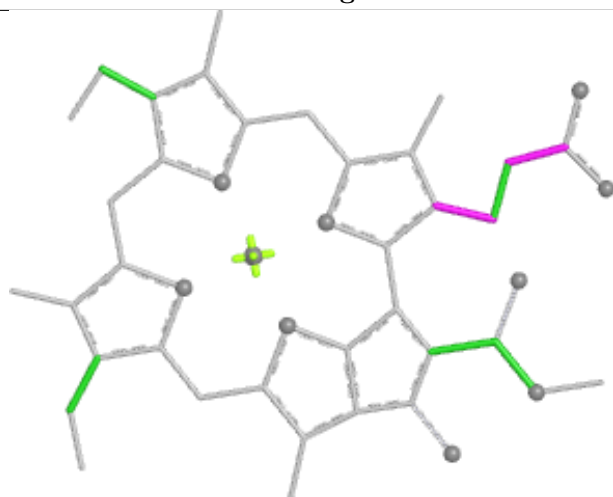
Ligand CLA U 307



Bond lengths



Bond angles

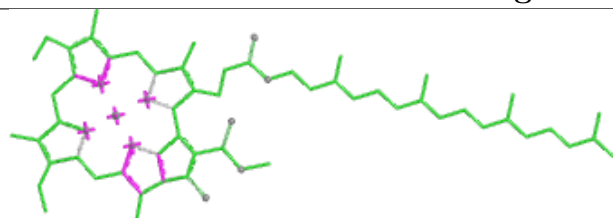


Torsions

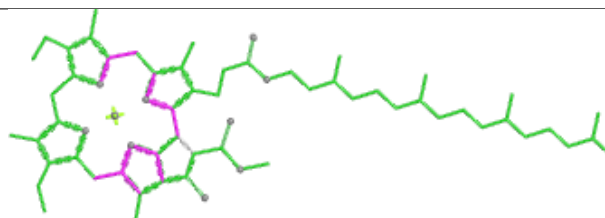


Rings

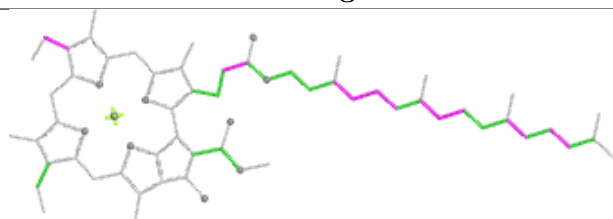
Ligand CLA C 306



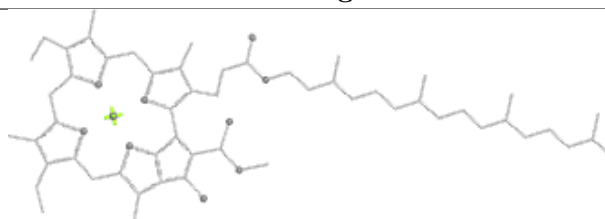
Bond lengths



Bond angles

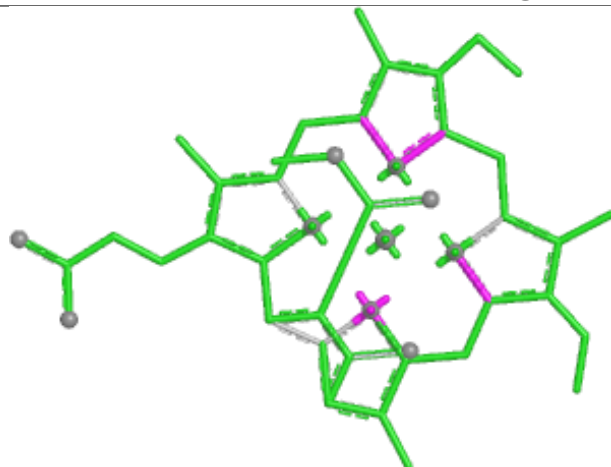


Torsions

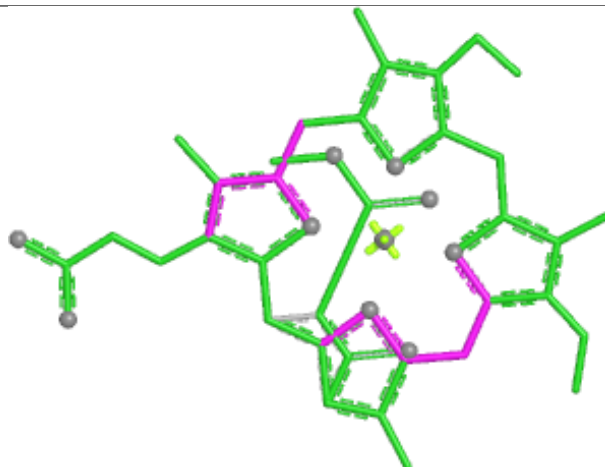


Rings

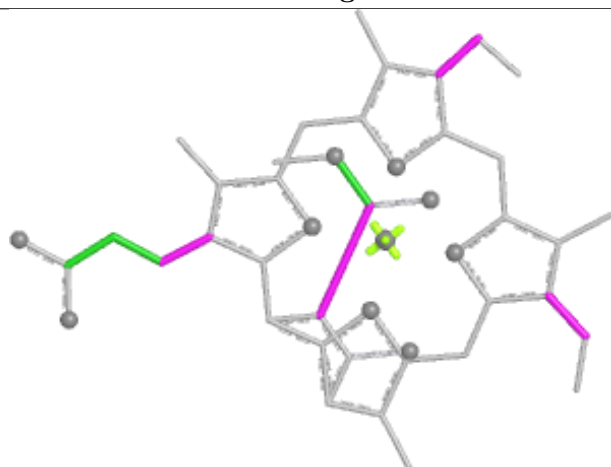
Ligand KC2 T 311



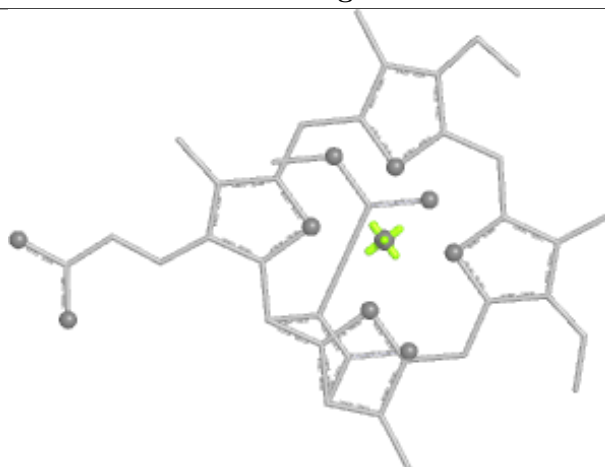
Bond lengths



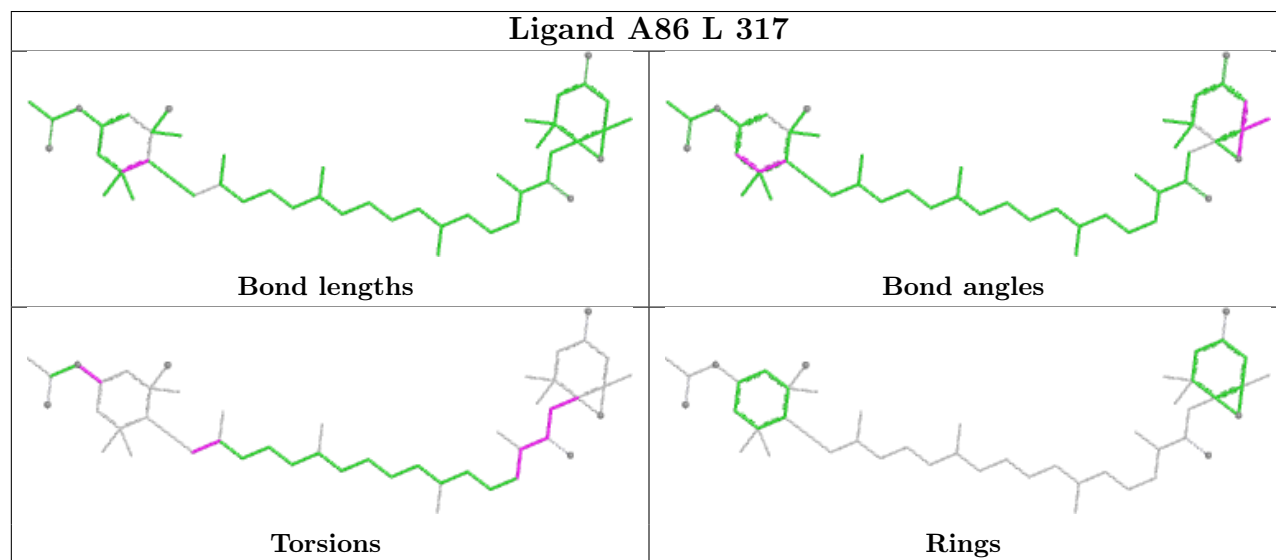
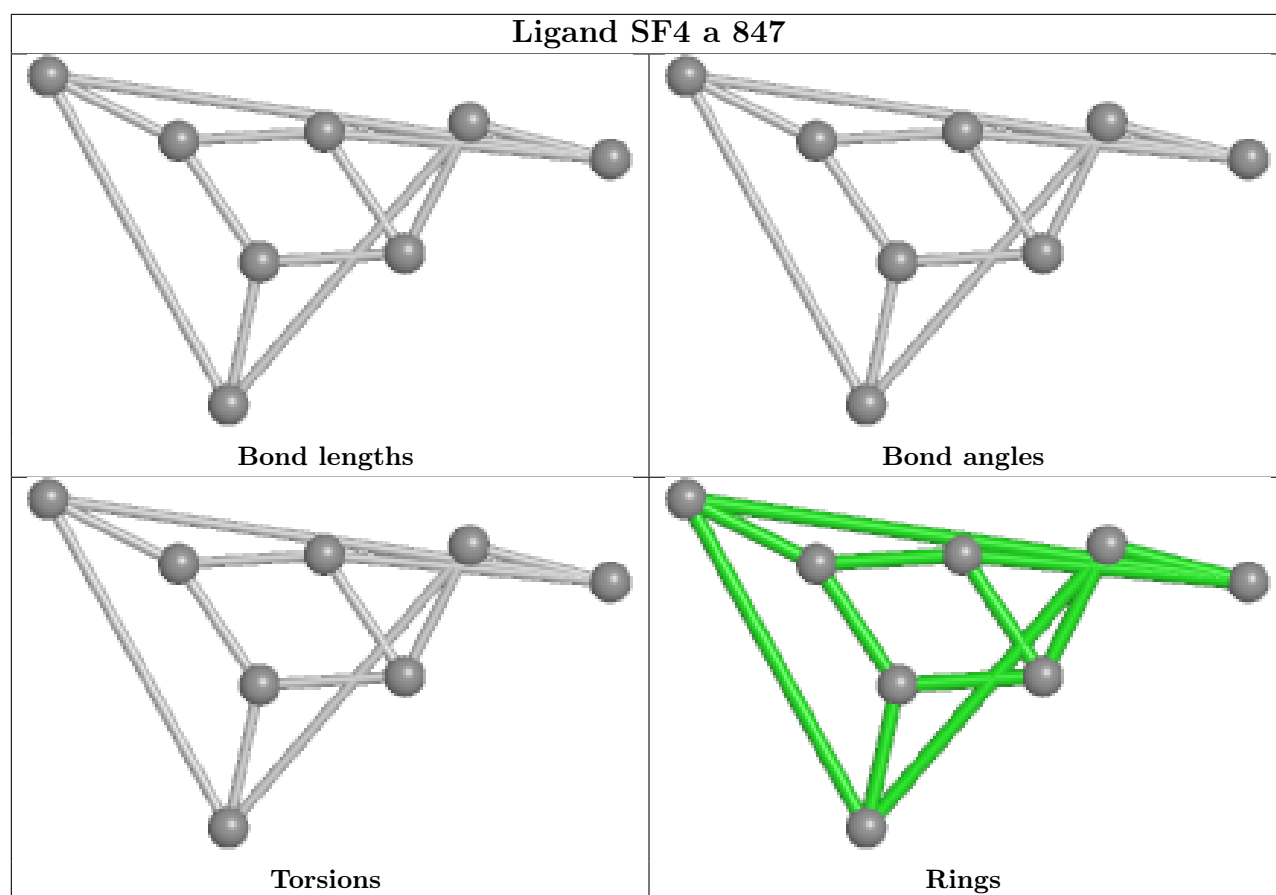
Bond angles

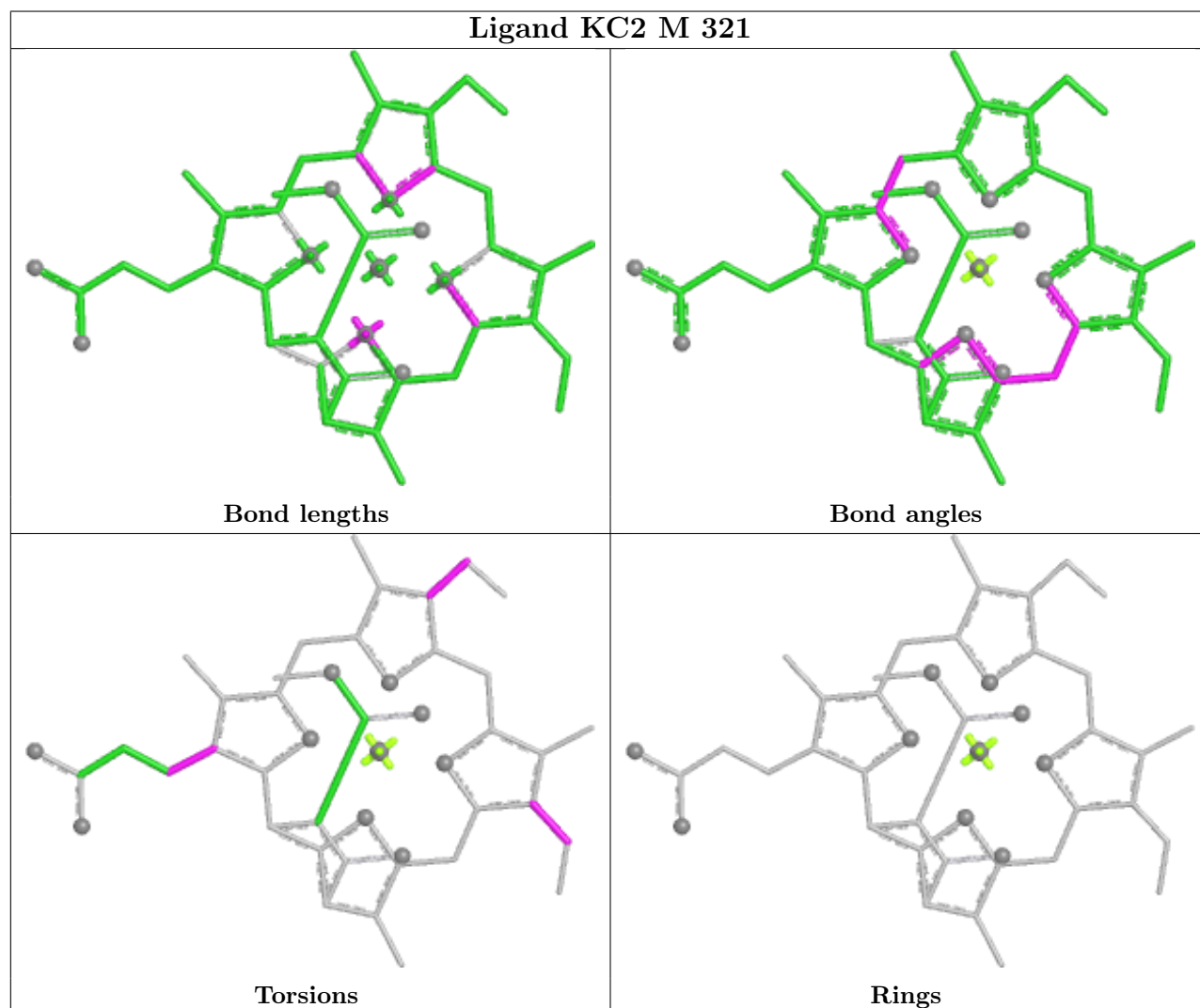
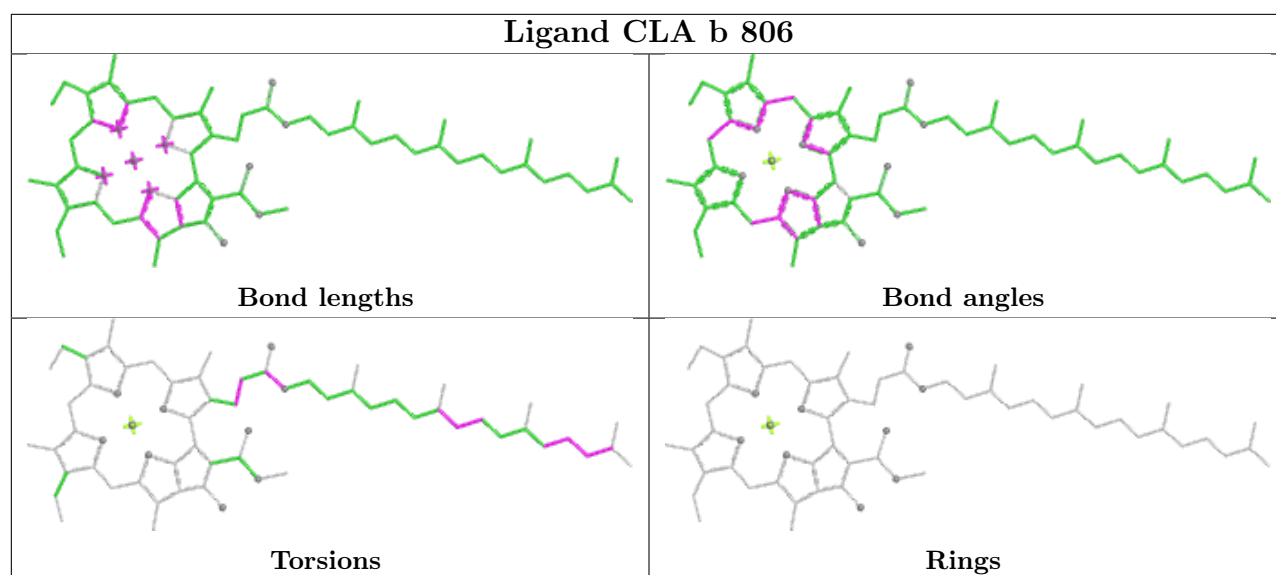


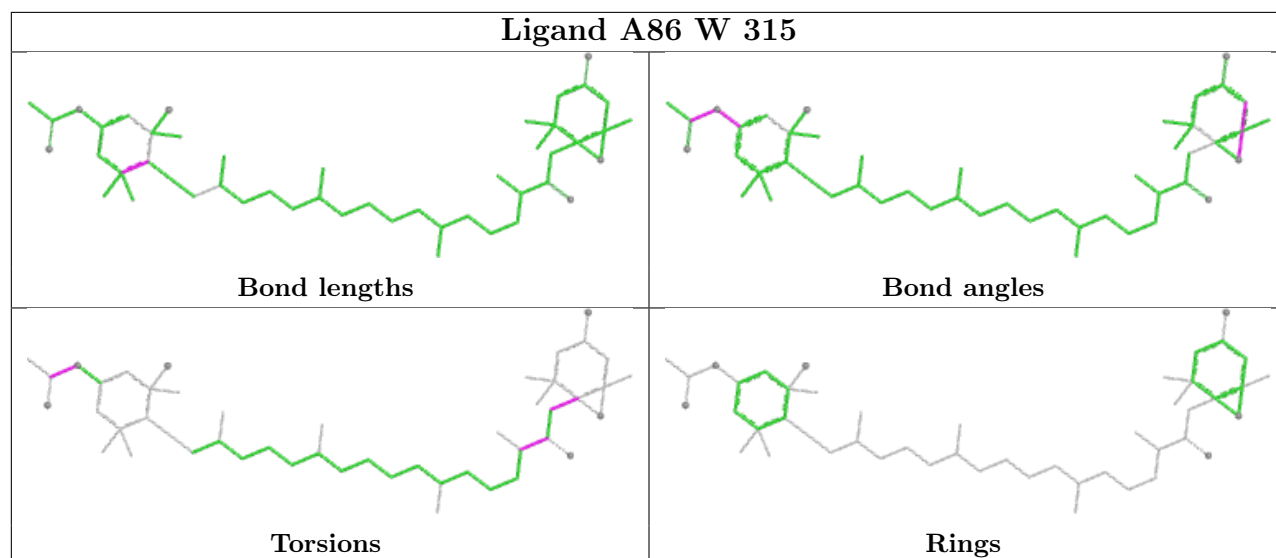
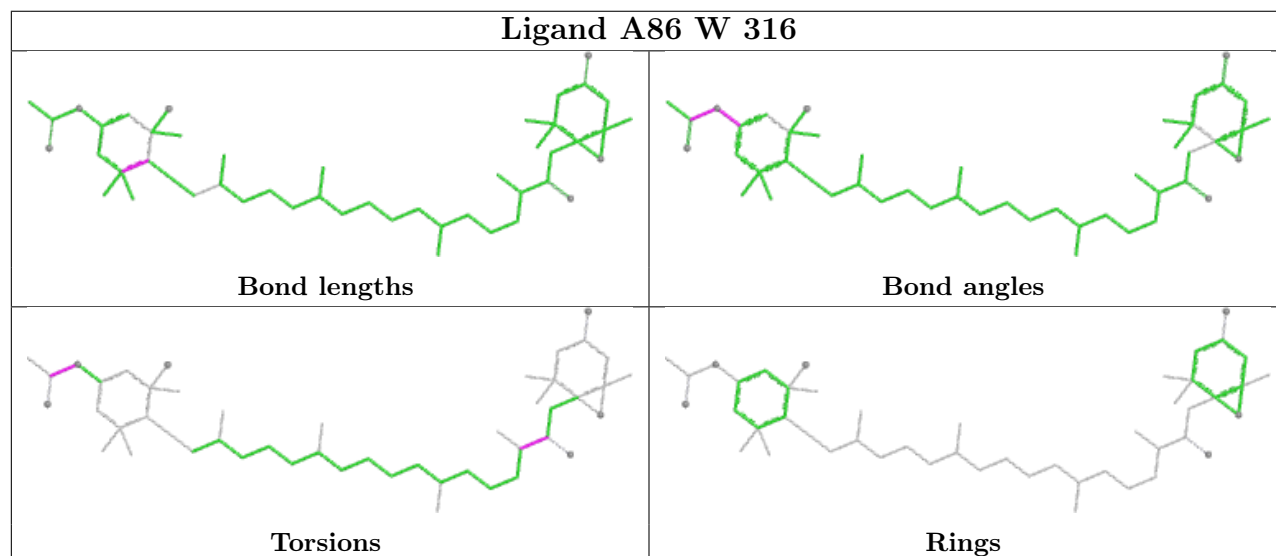
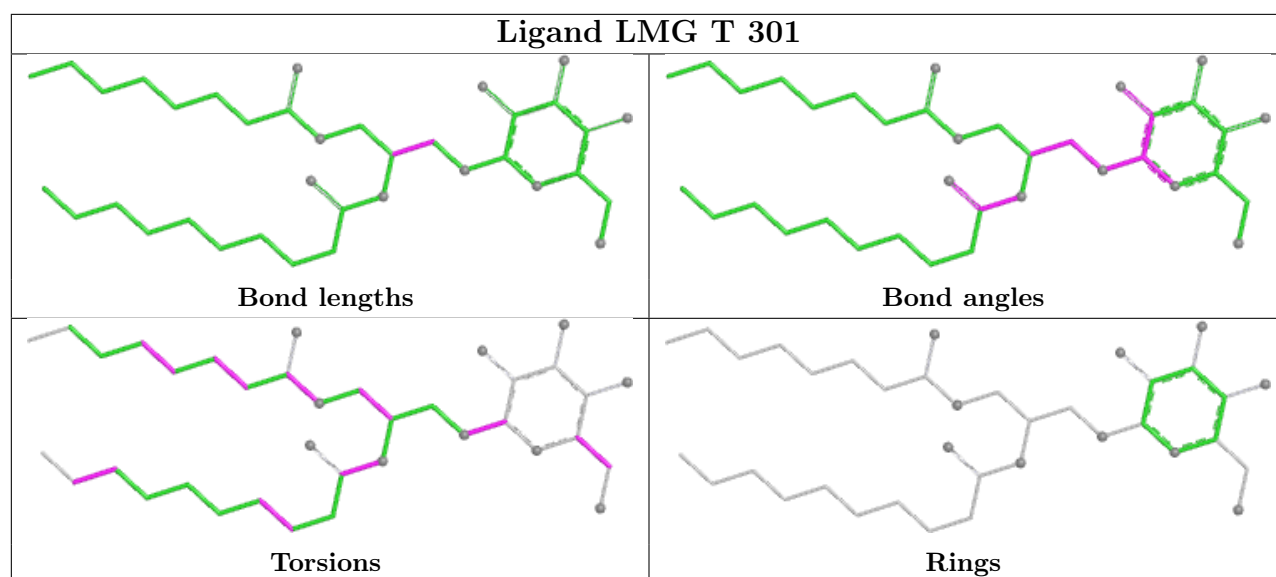
Torsions

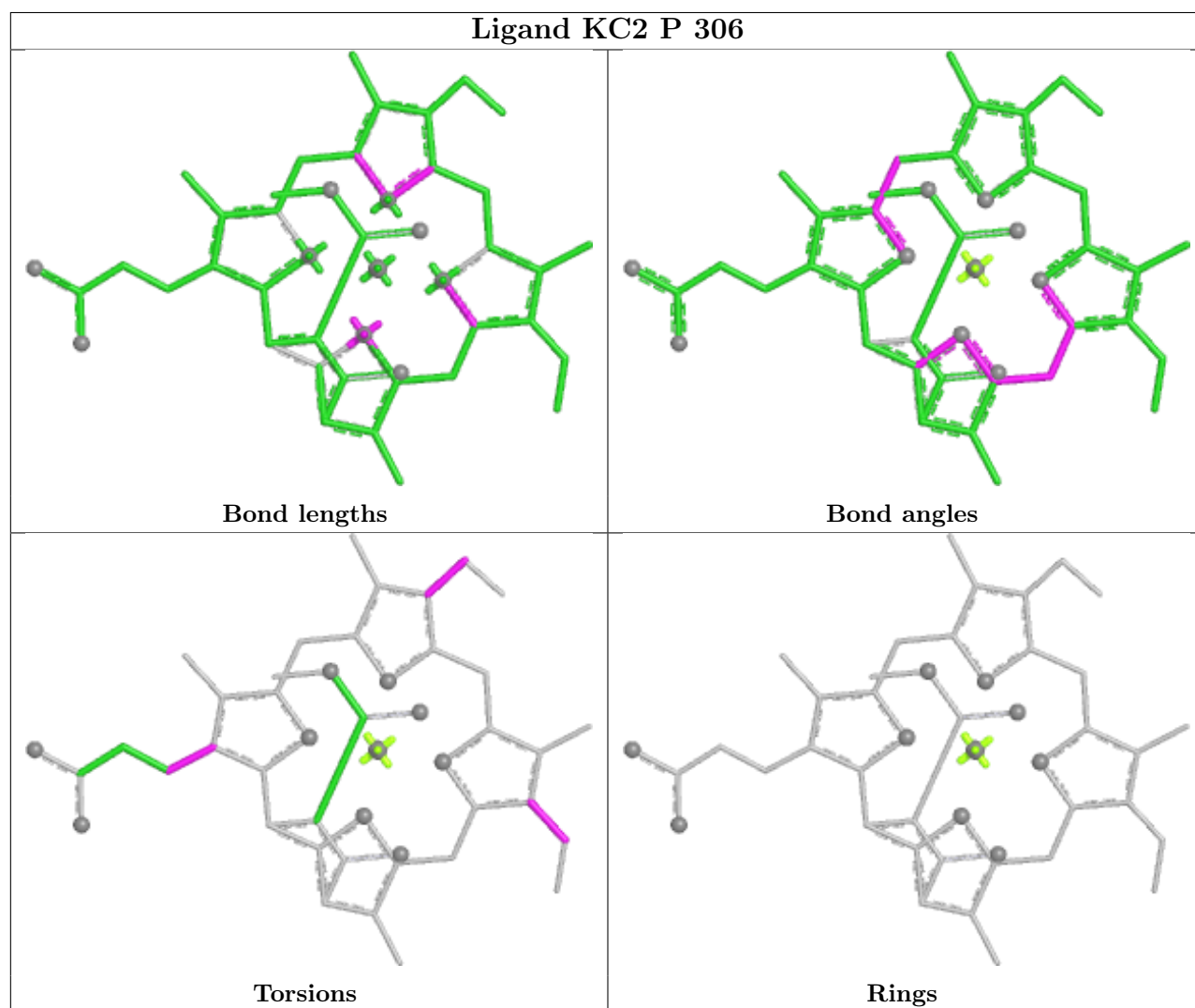
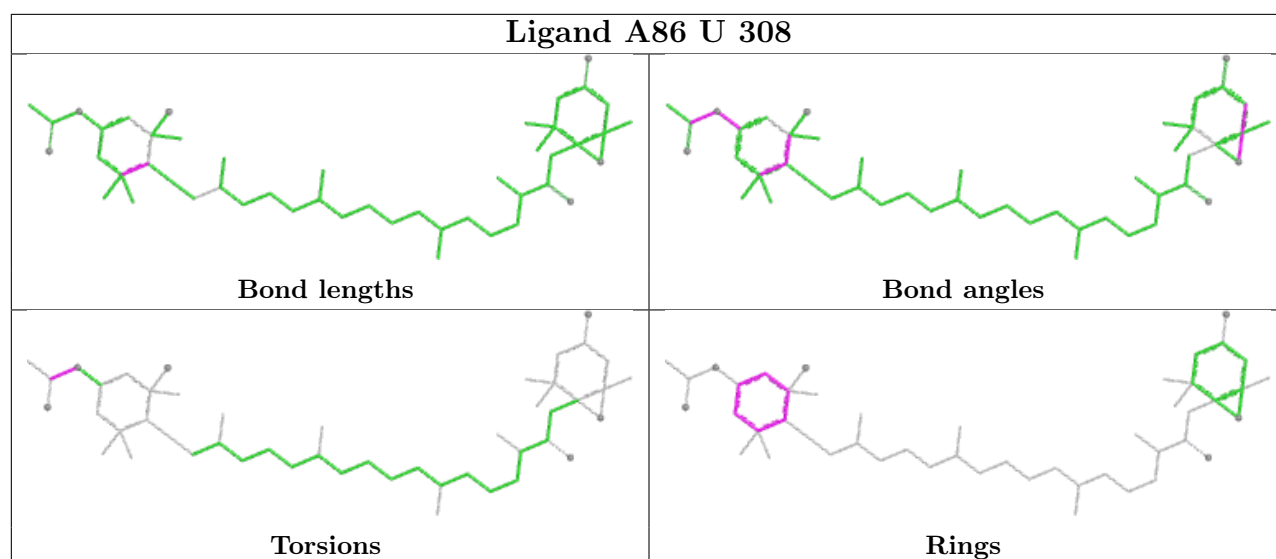


Rings

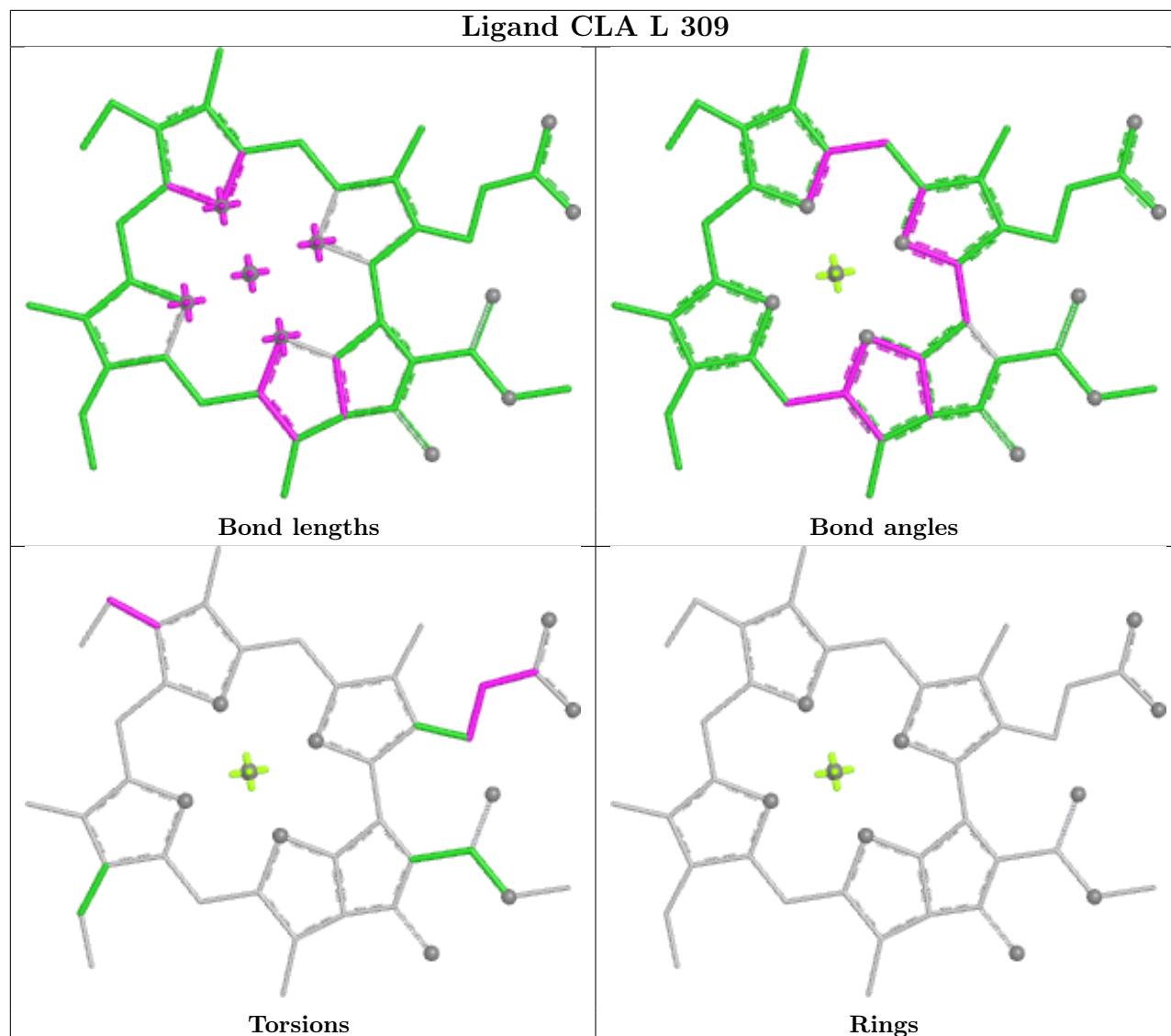




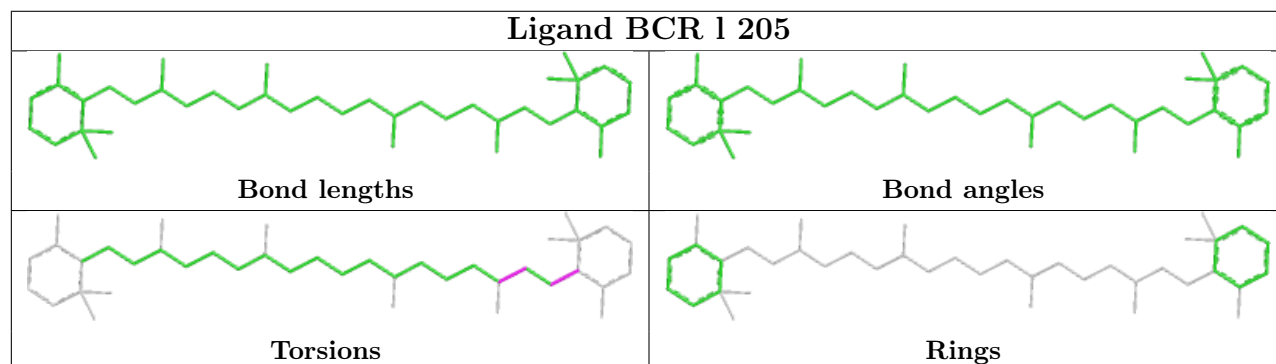


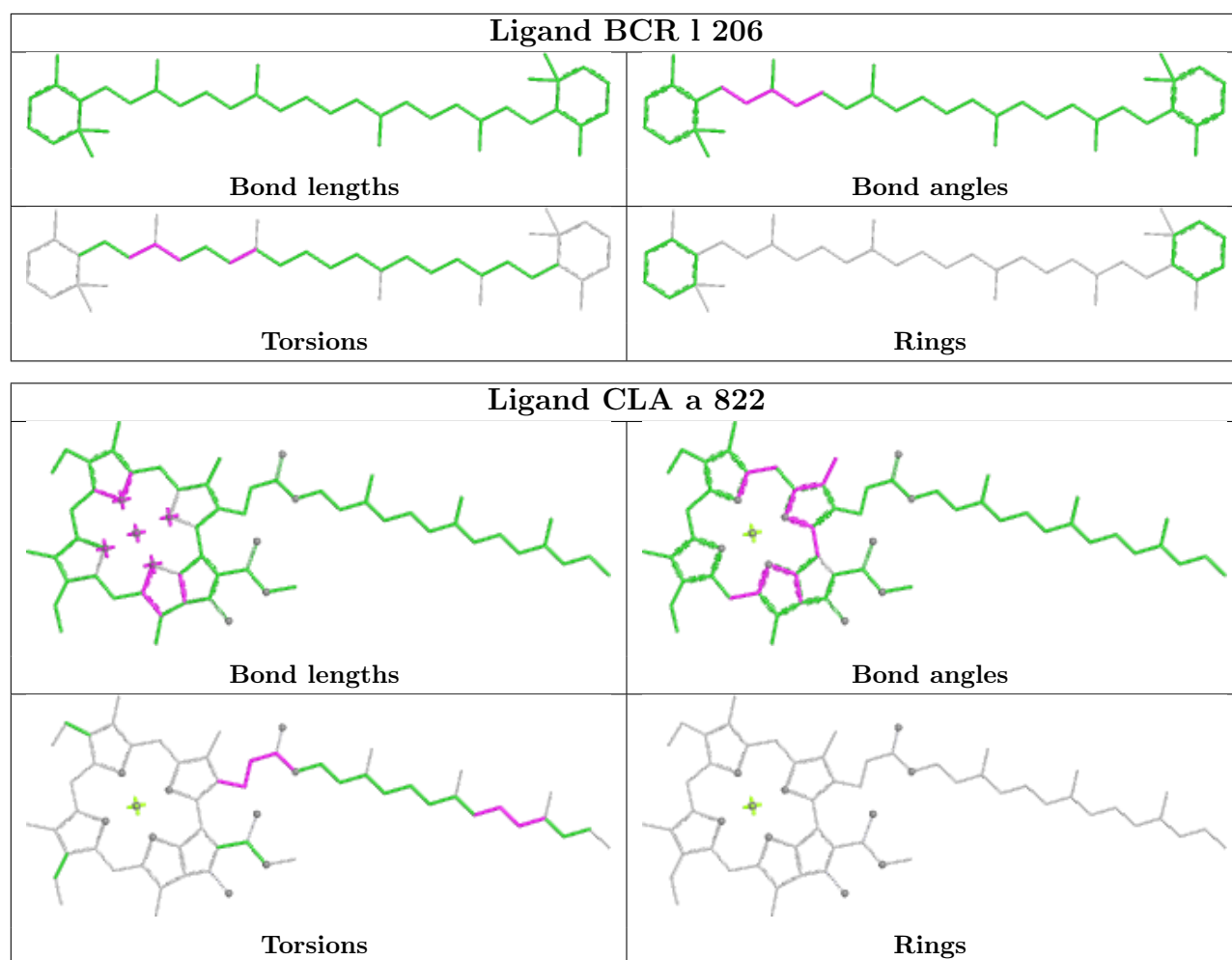


Ligand CLA L 309

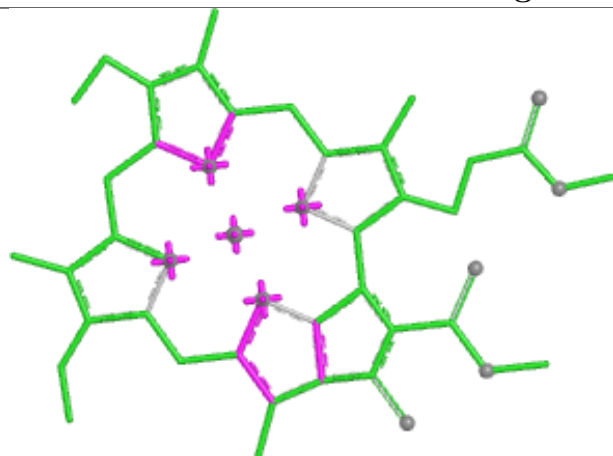


Ligand BCR 1 205

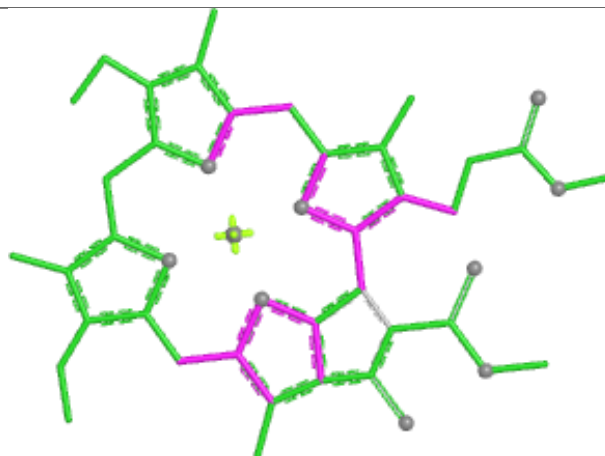




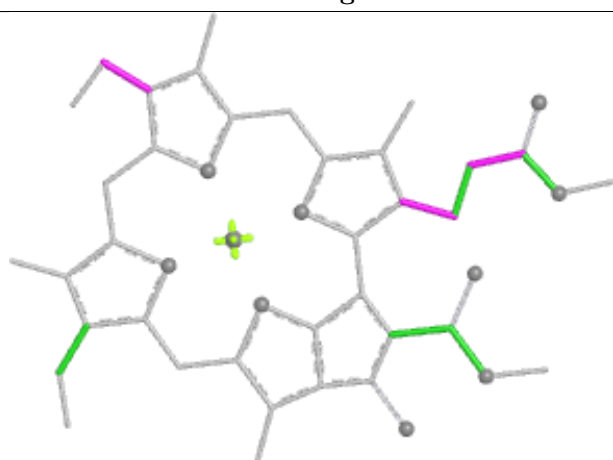
Ligand CLA B 304



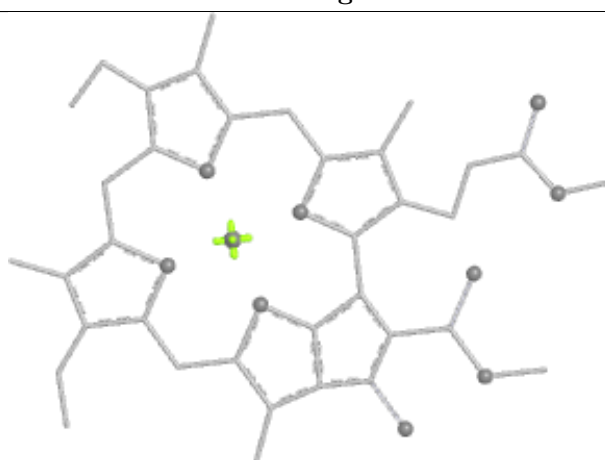
Bond lengths



Bond angles

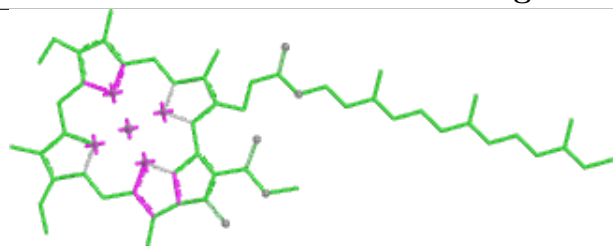


Torsions

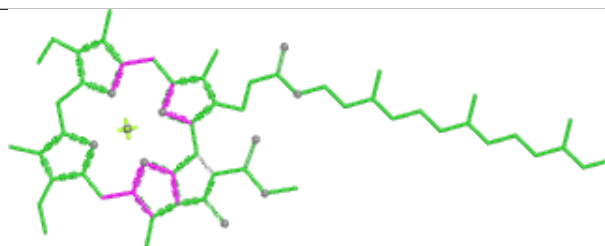


Rings

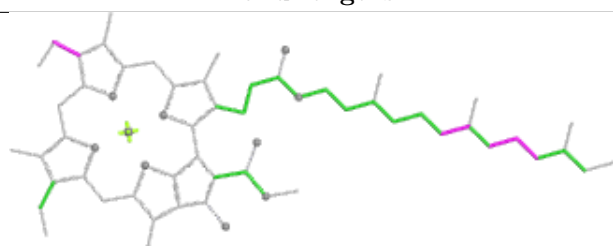
Ligand CLA A 305



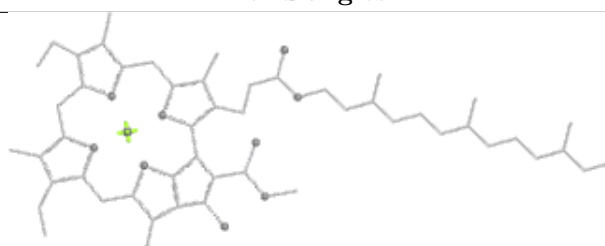
Bond lengths



Bond angles

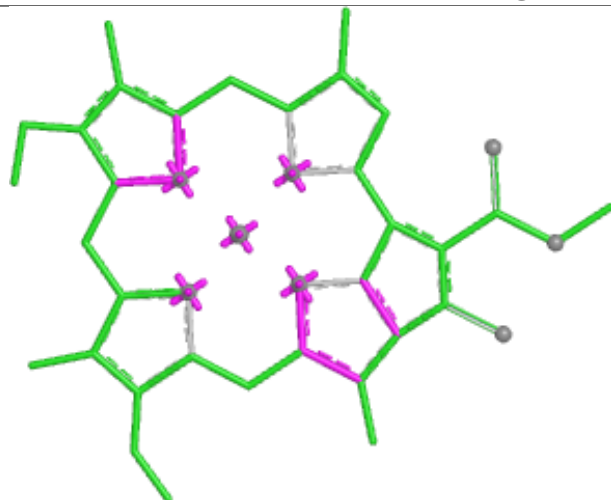


Torsions

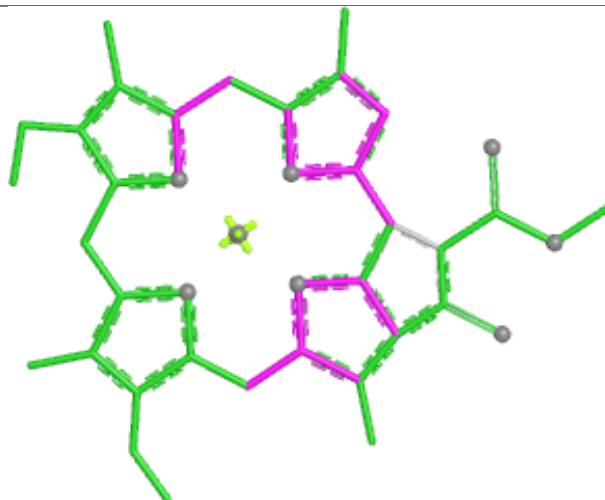


Rings

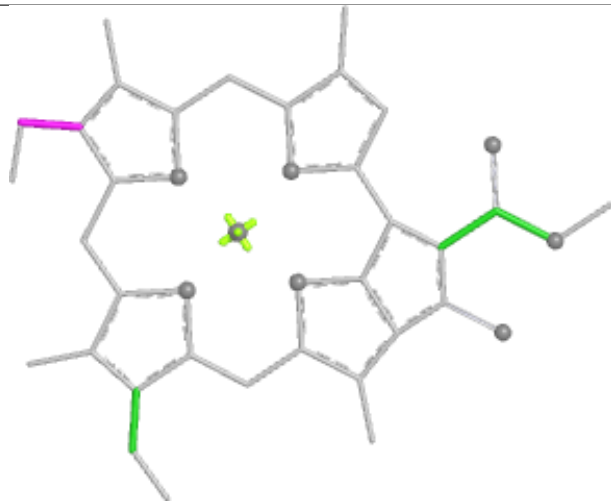
Ligand CLA G 307



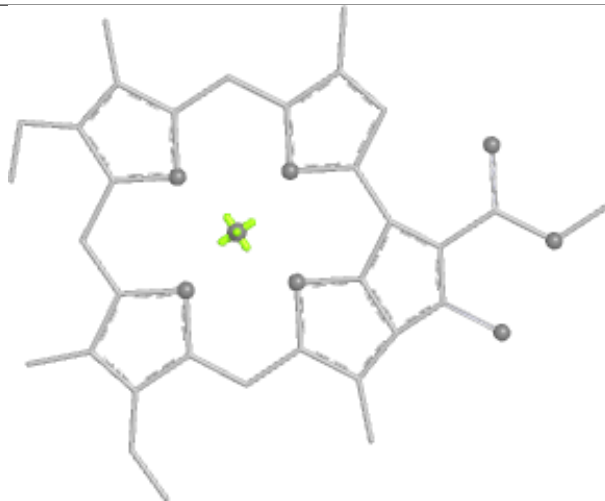
Bond lengths



Bond angles



Torsions



Rings

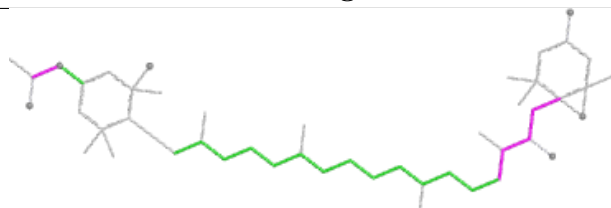
Ligand A86 Q 311



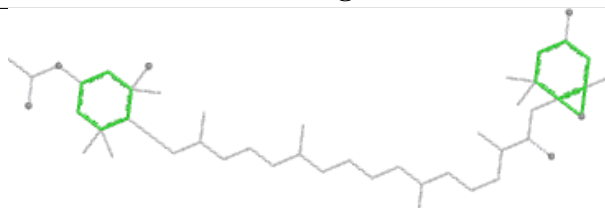
Bond lengths



Bond angles

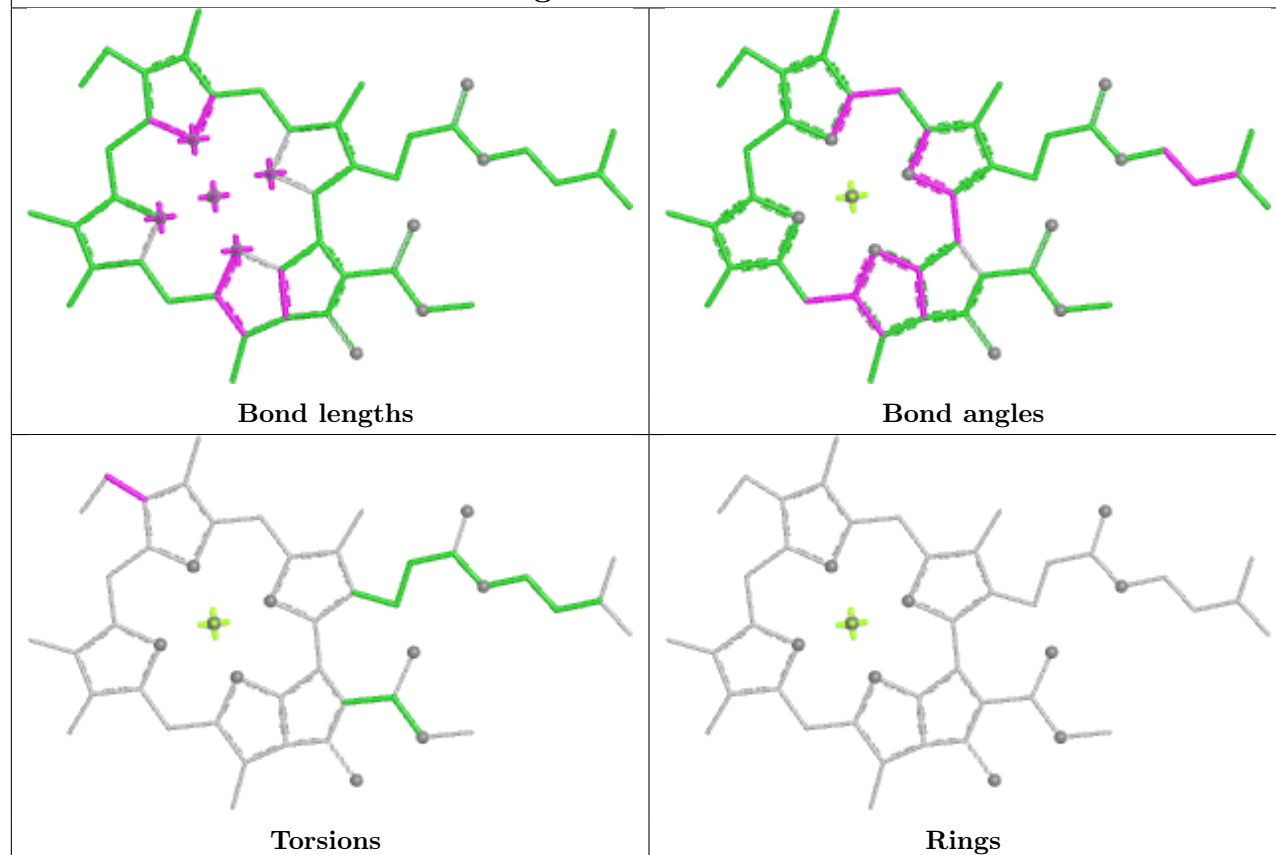


Torsions

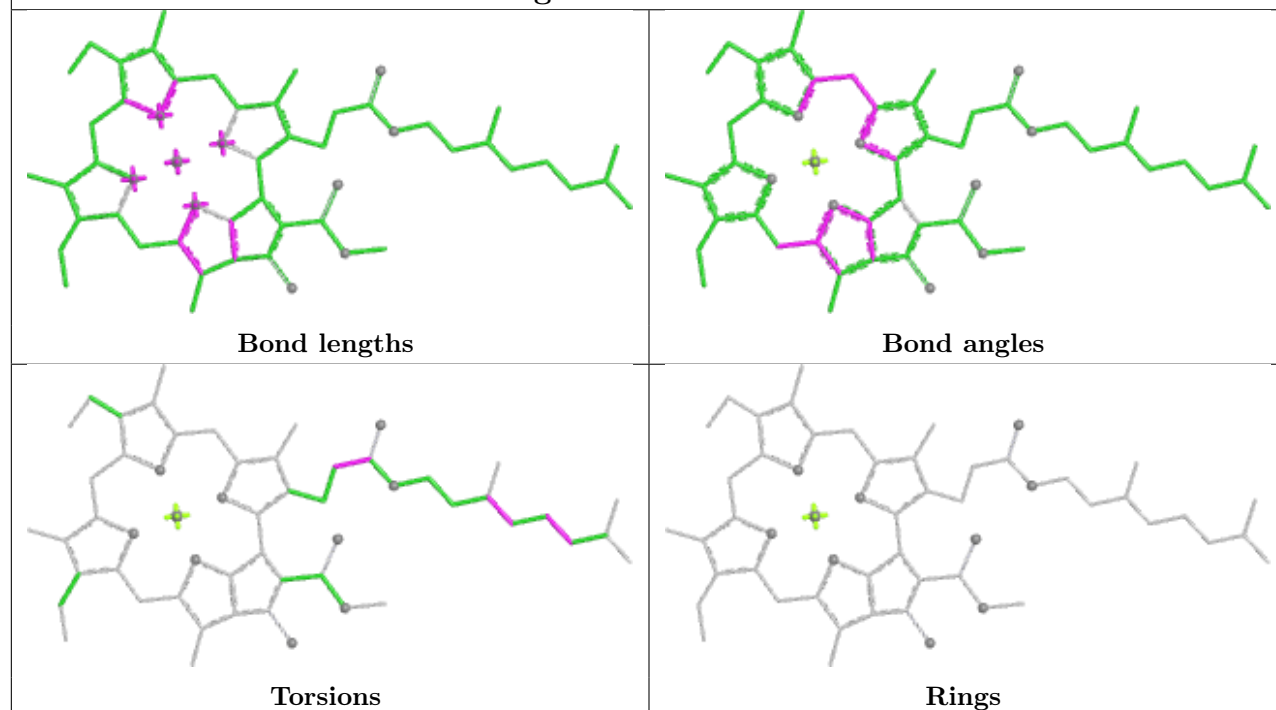


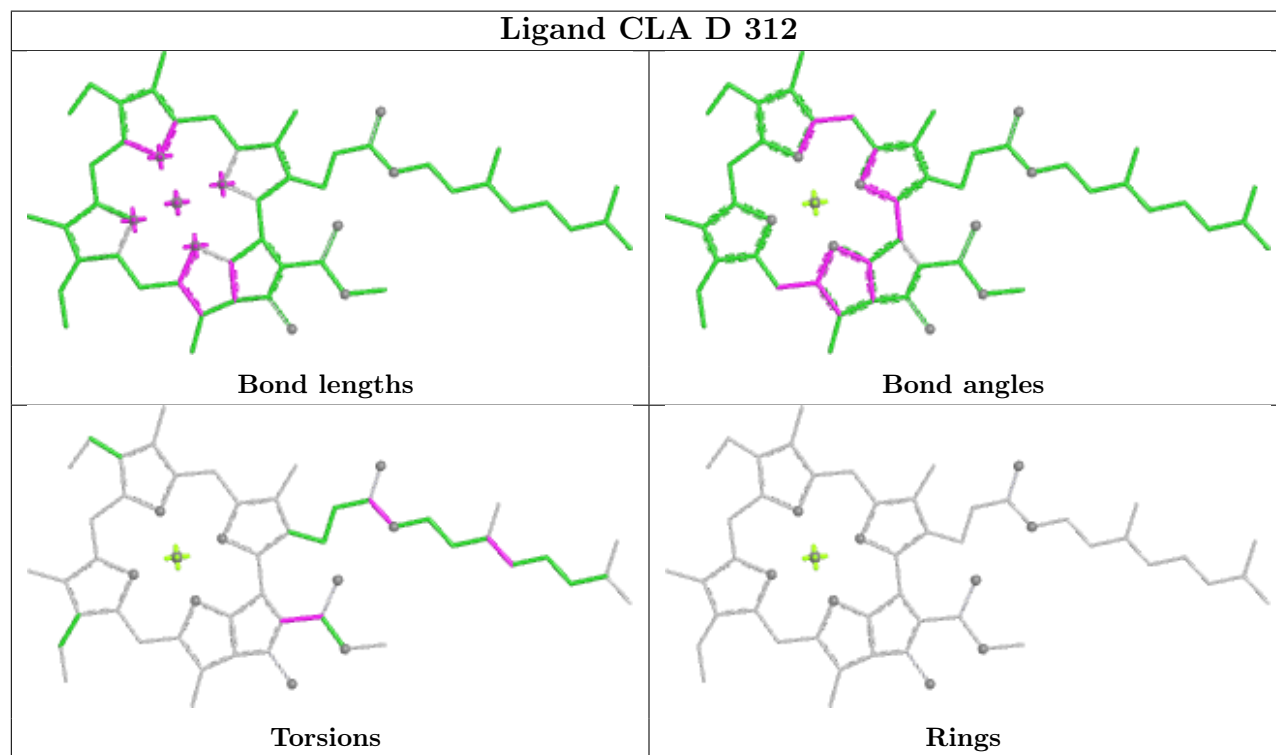
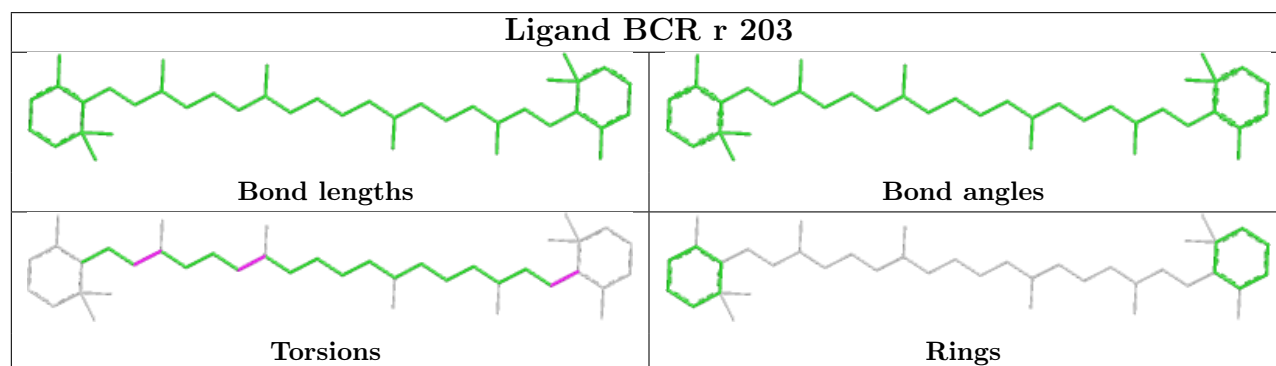
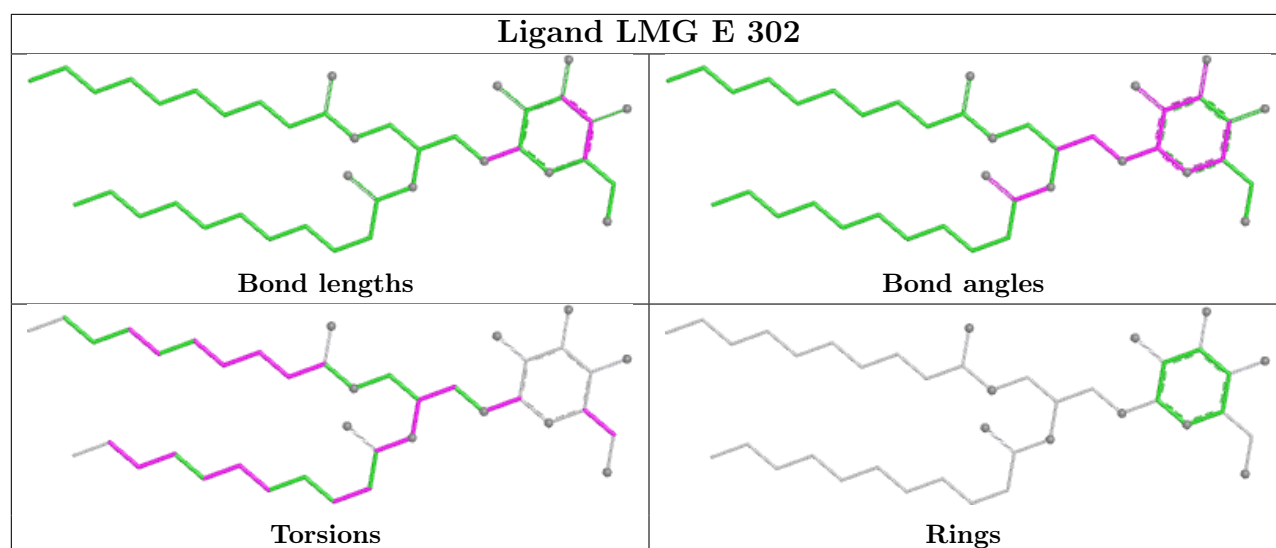
Rings

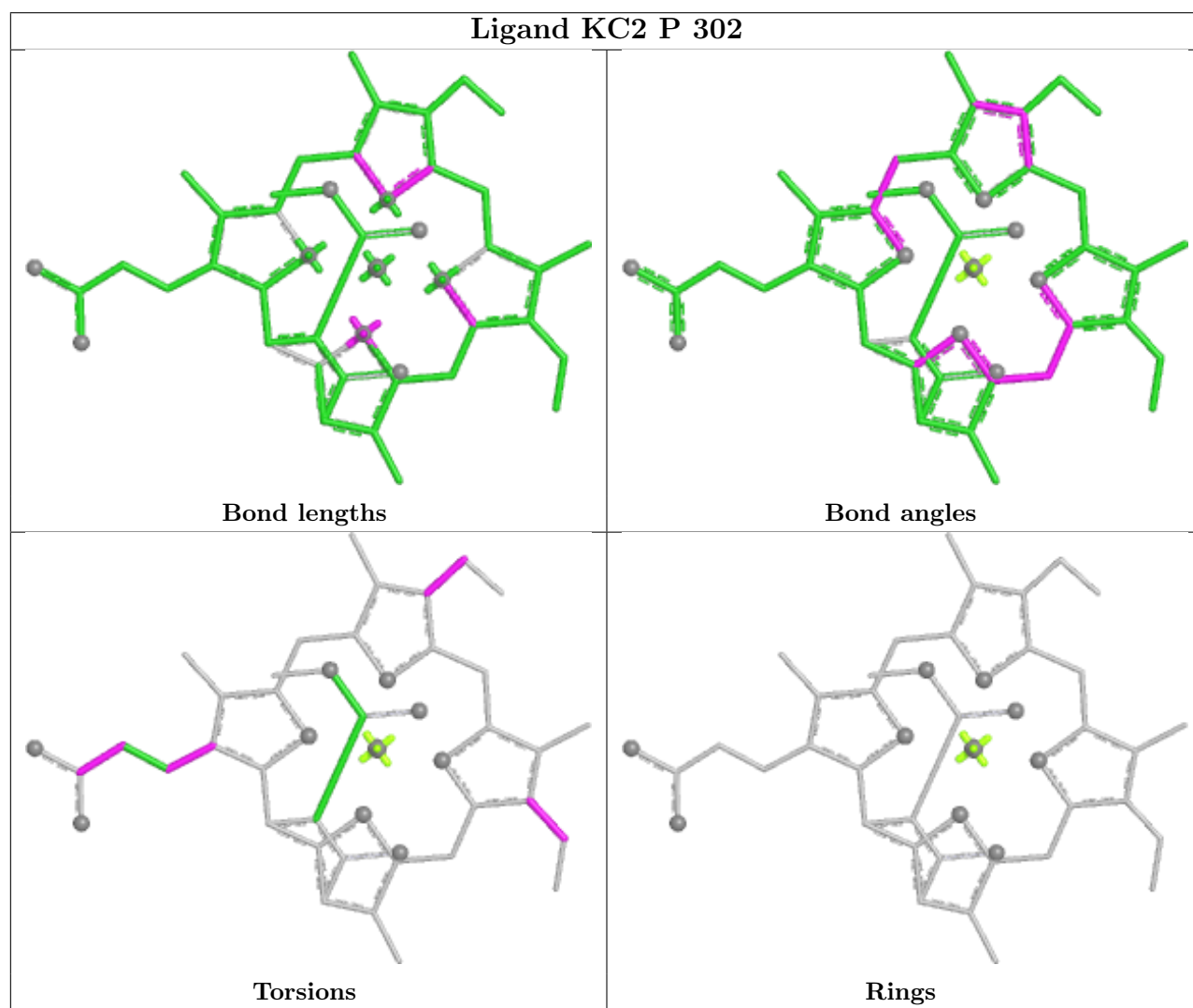
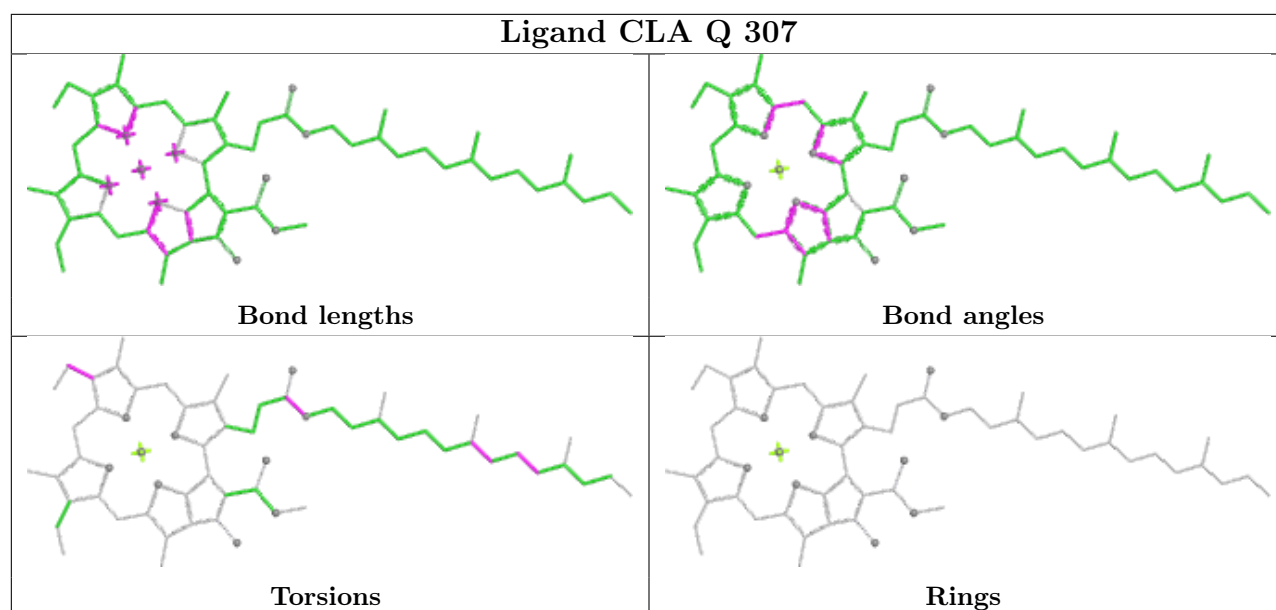
Ligand CLA F 305



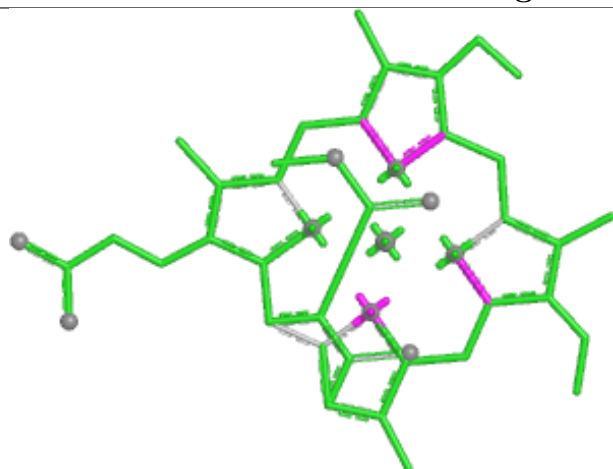
Ligand CLA F 306



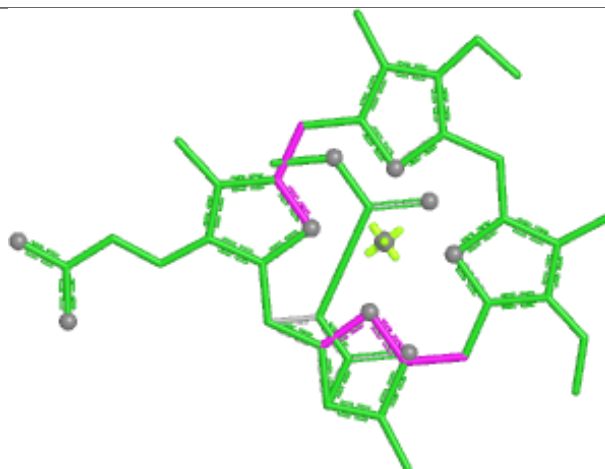




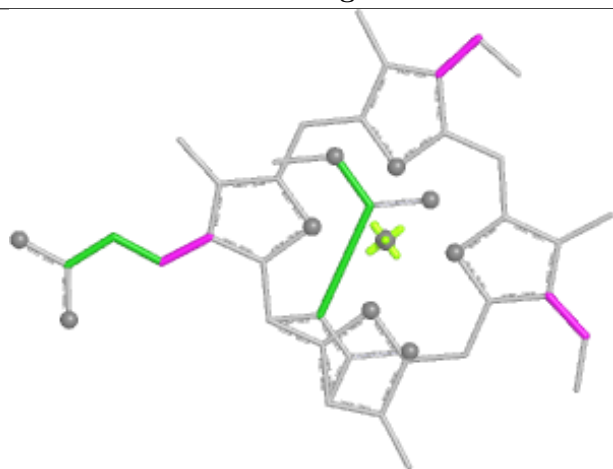
Ligand KC2 N 314



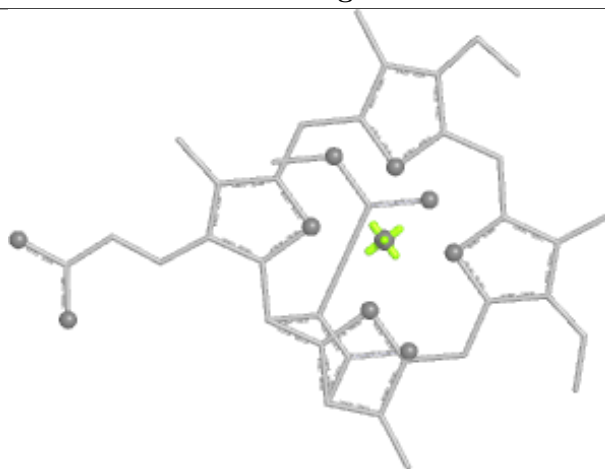
Bond lengths



Bond angles

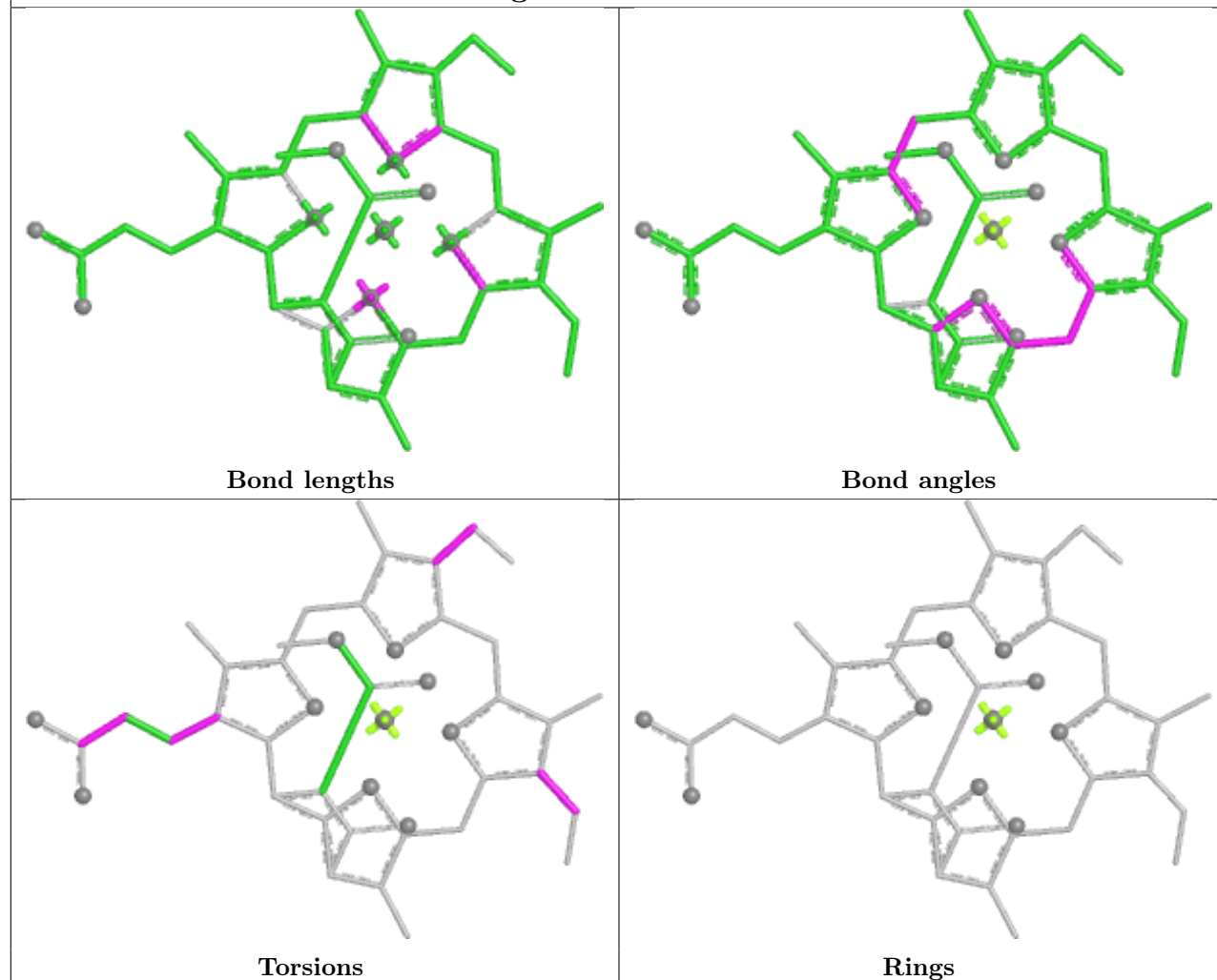


Torsions

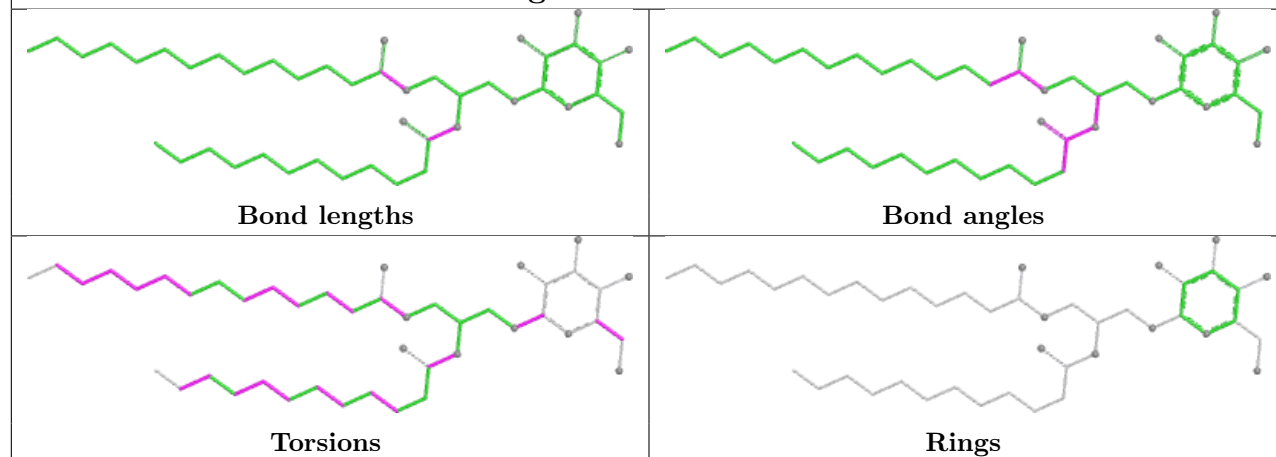


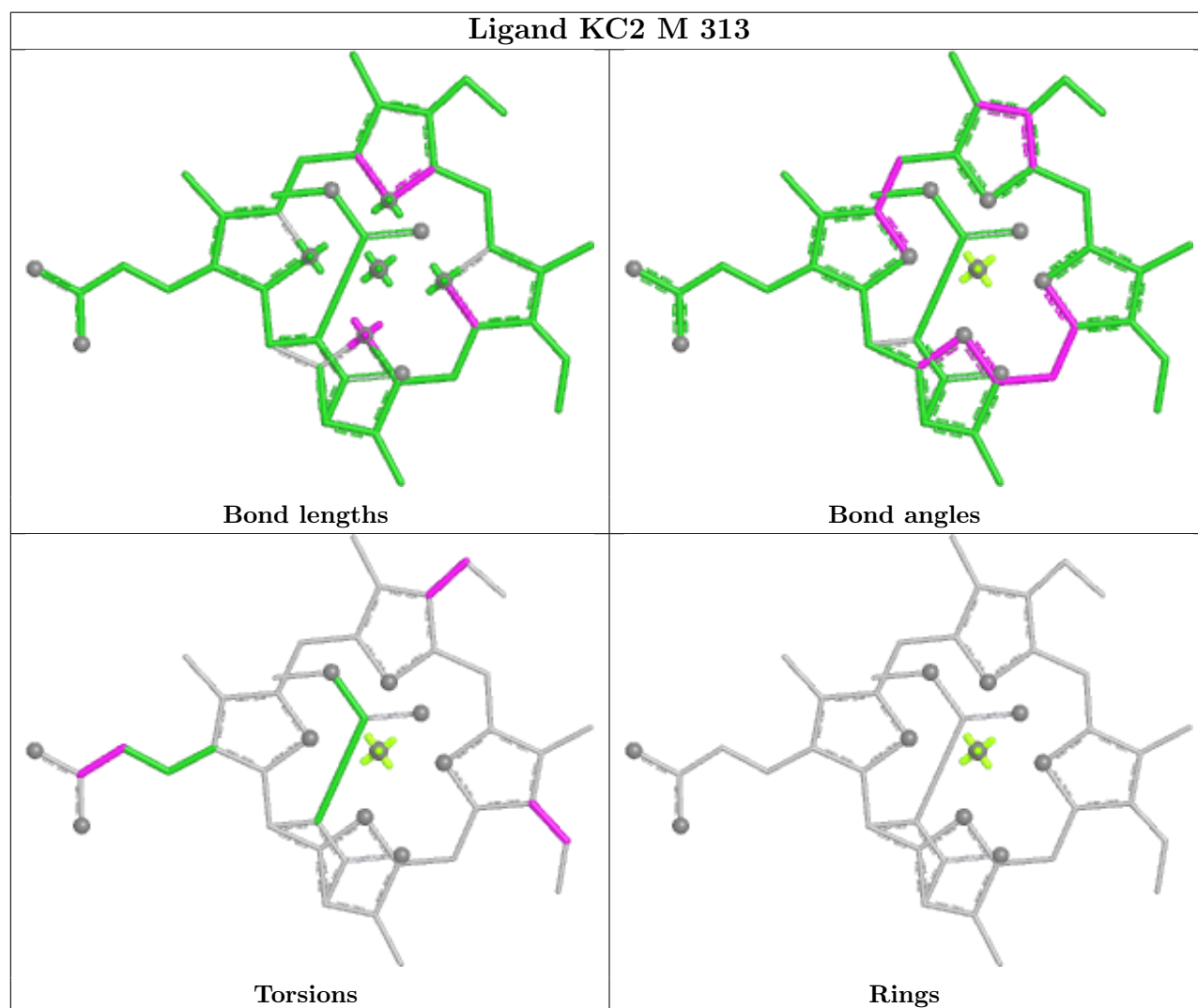
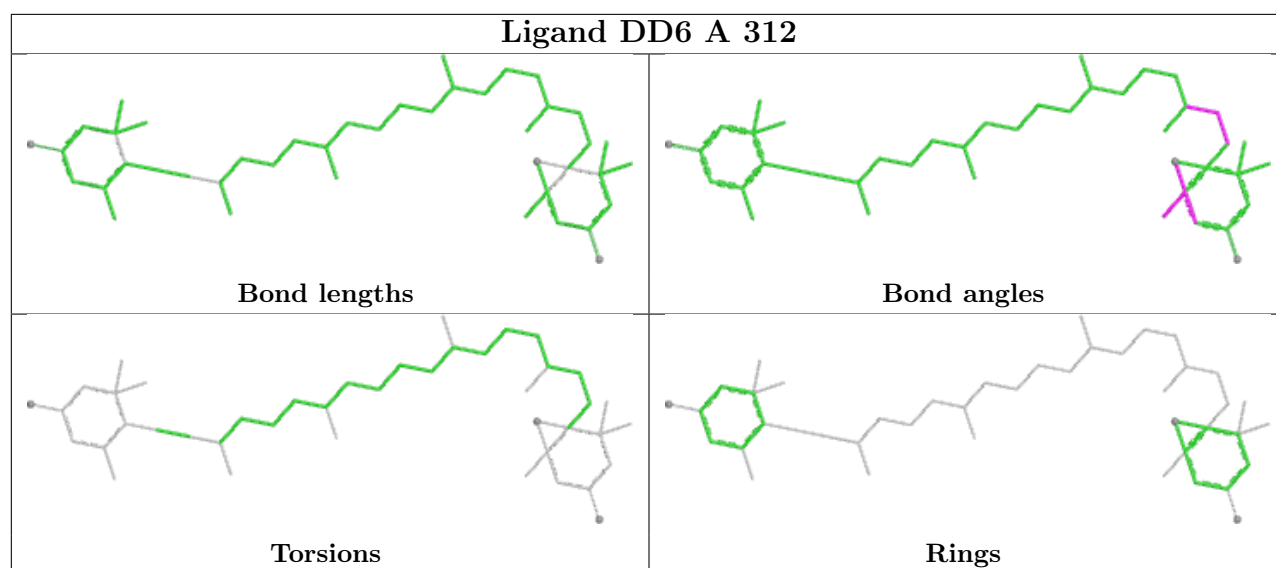
Rings

Ligand KC2 F 302

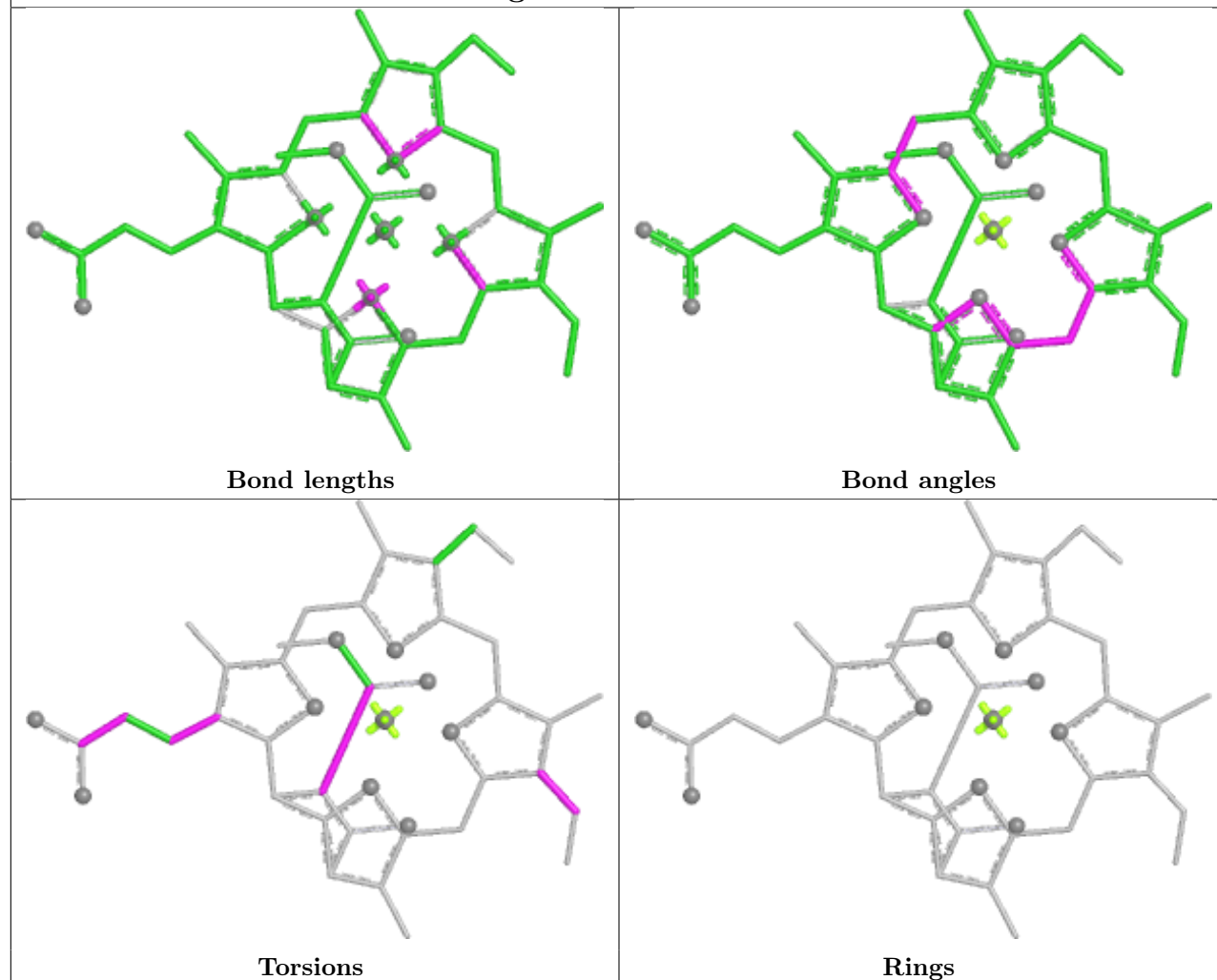


Ligand LMG P 318

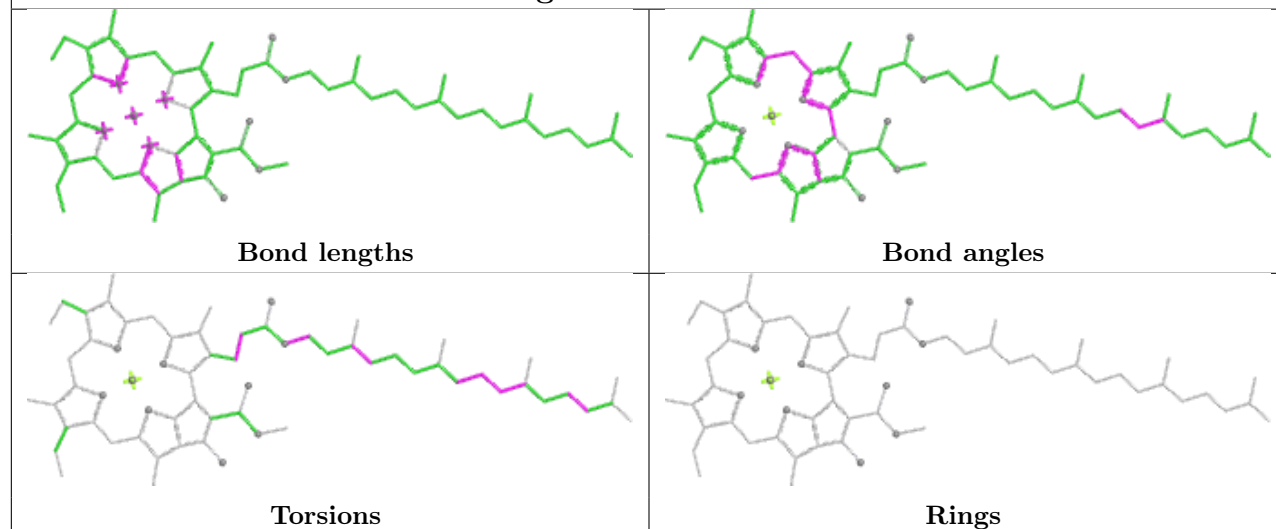


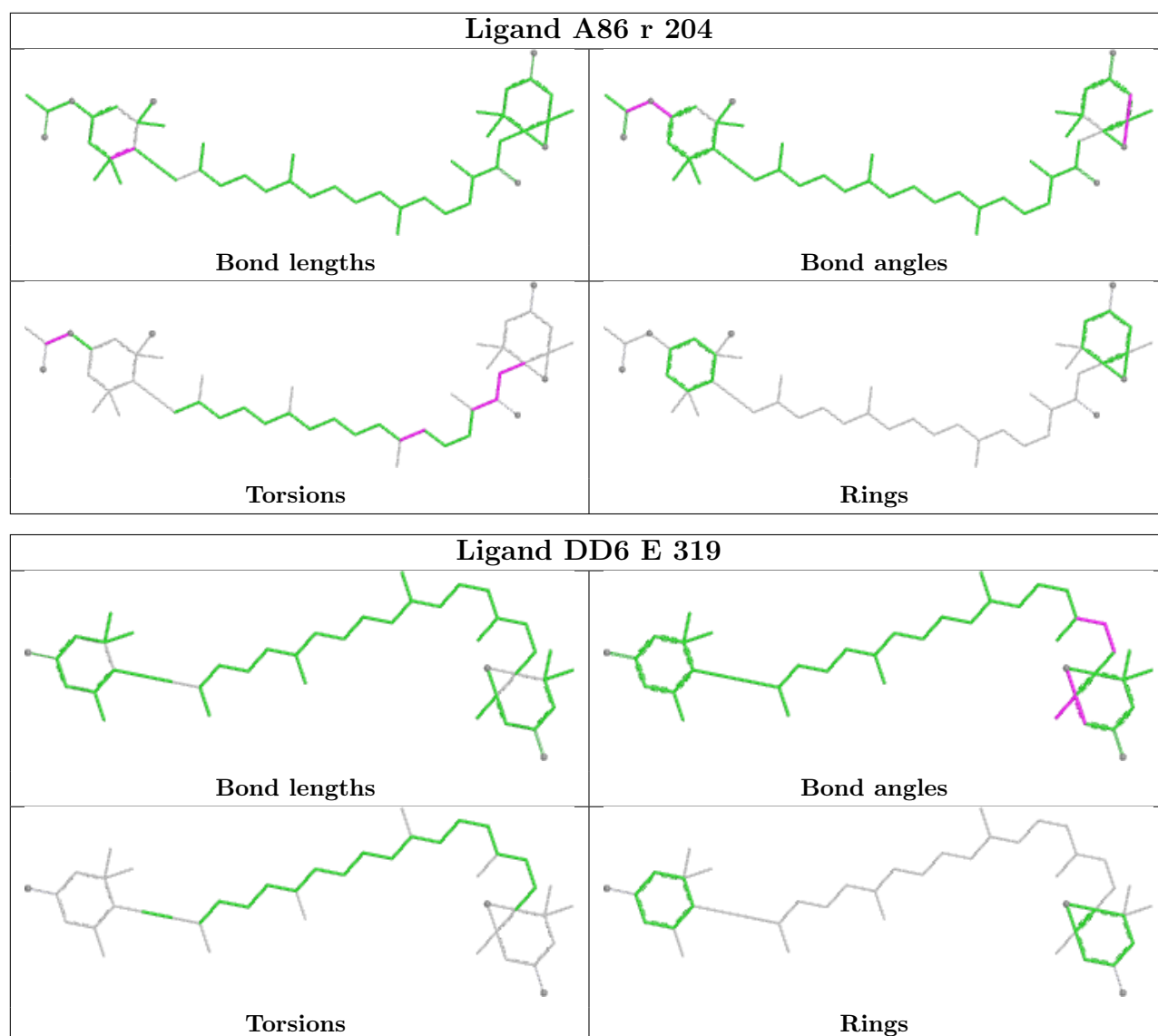


Ligand KC2 G 302

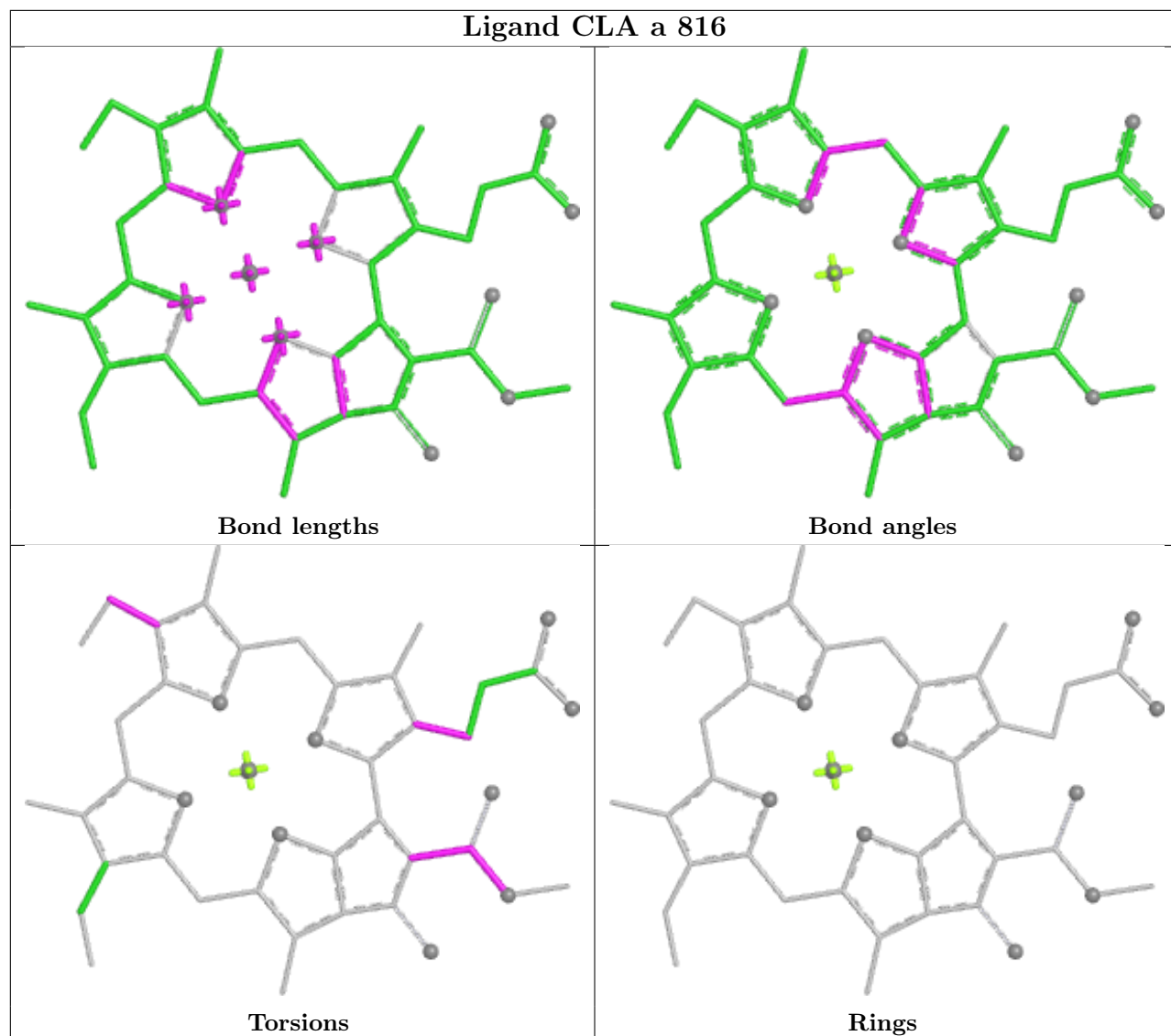


Ligand CLA a 830

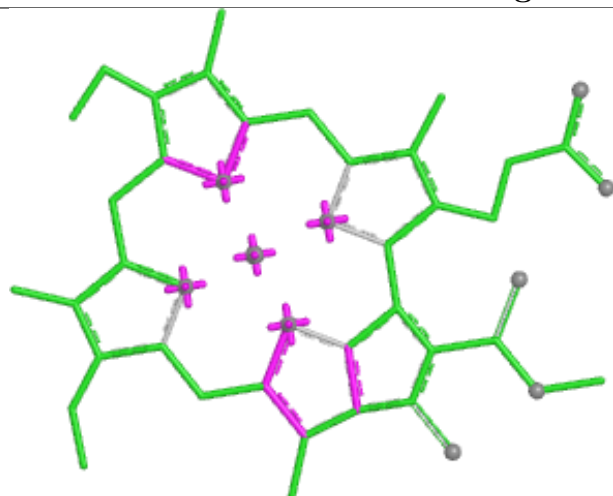




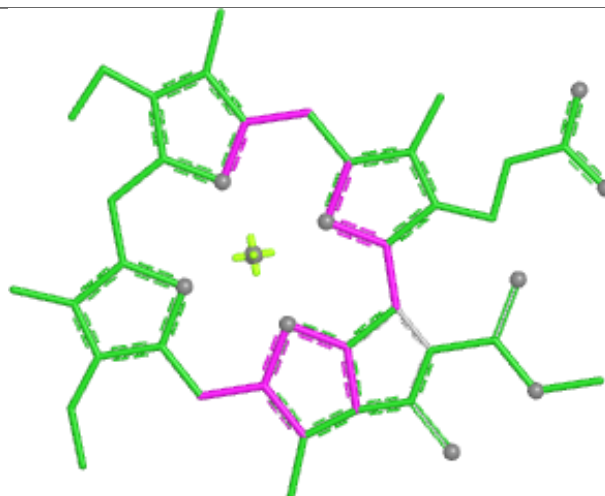
Ligand CLA a 816



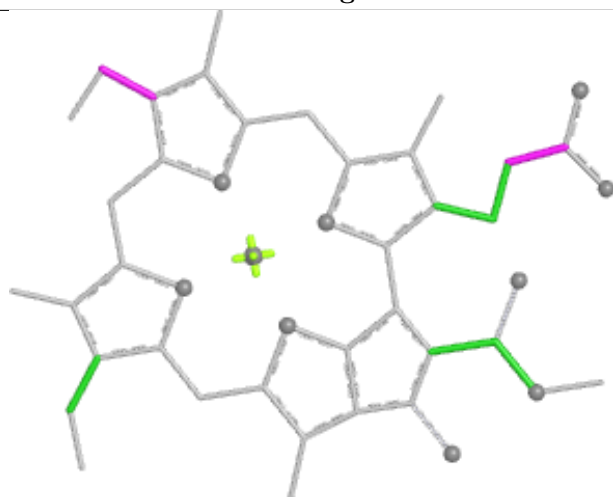
Ligand CLA B 305



Bond lengths



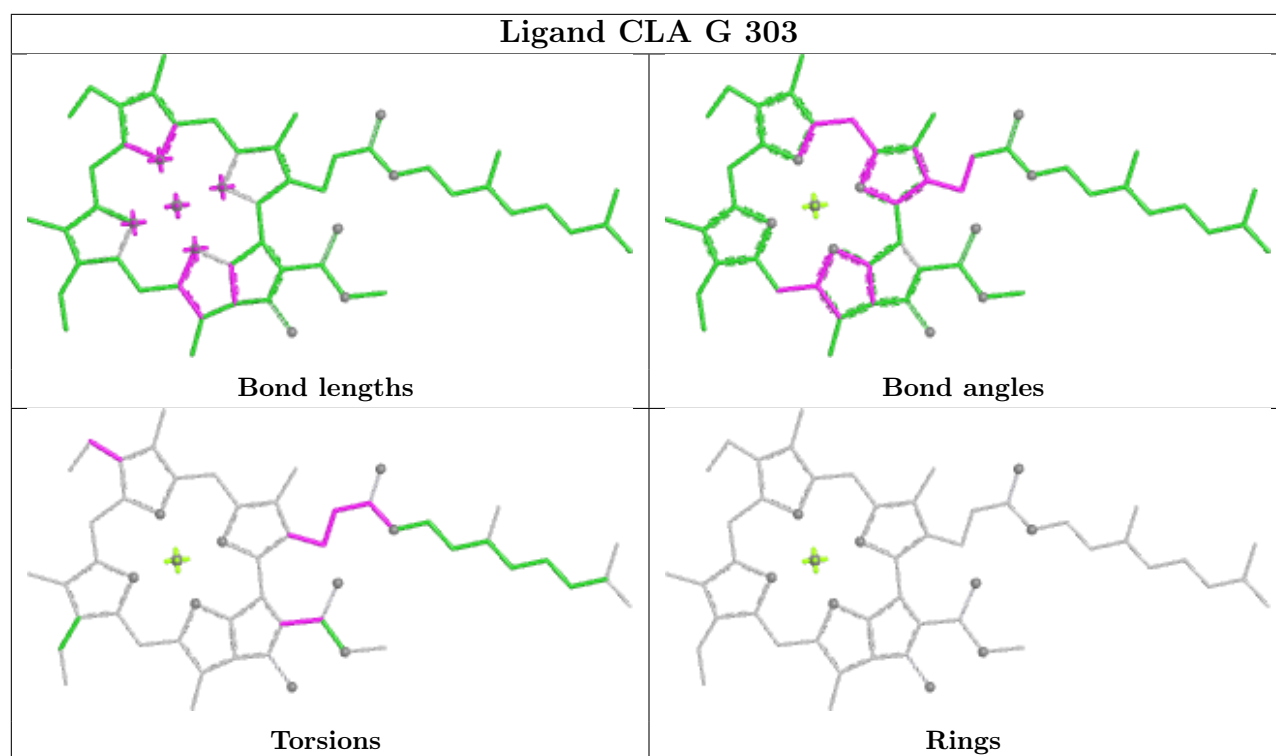
Bond angles



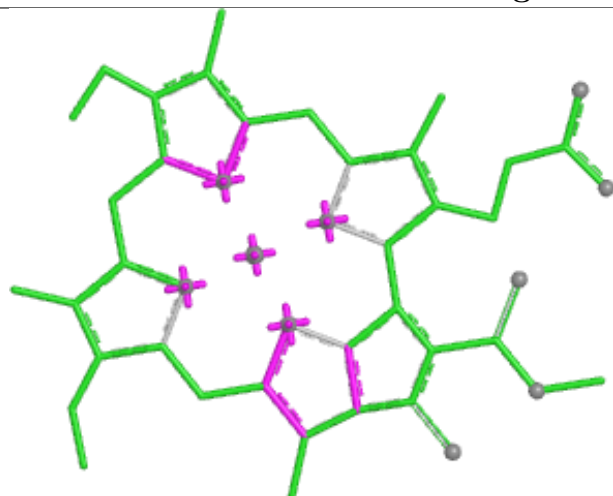
Torsions



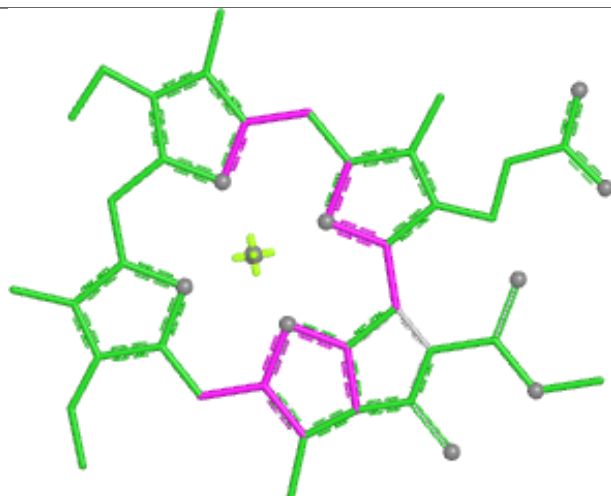
Rings



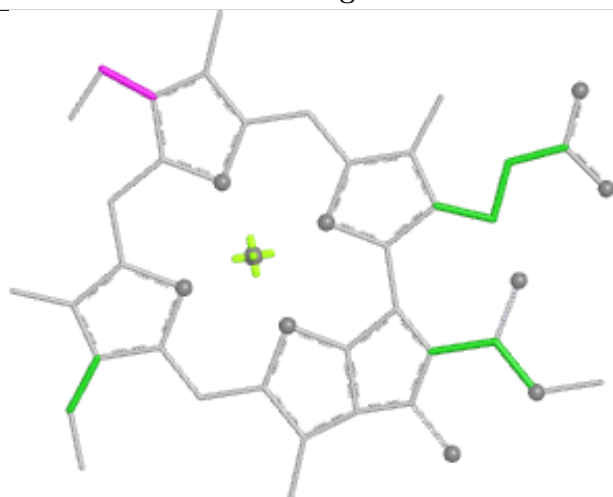
Ligand CLA K 301



Bond lengths



Bond angles

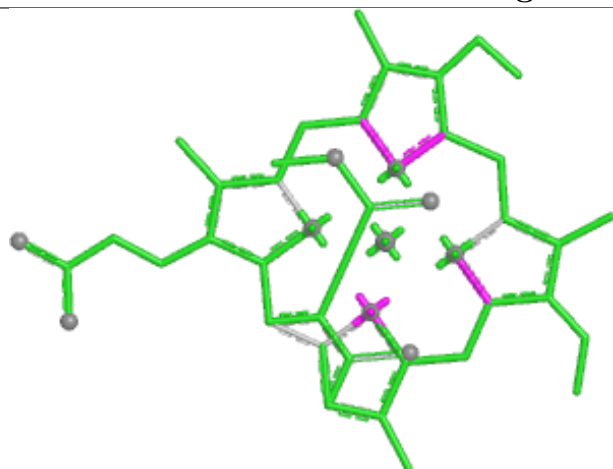


Torsions

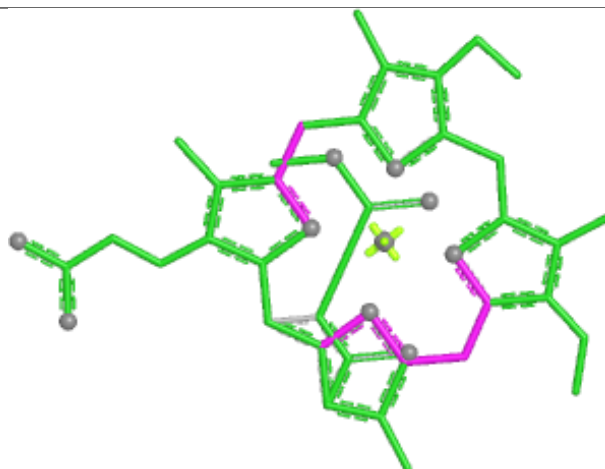


Rings

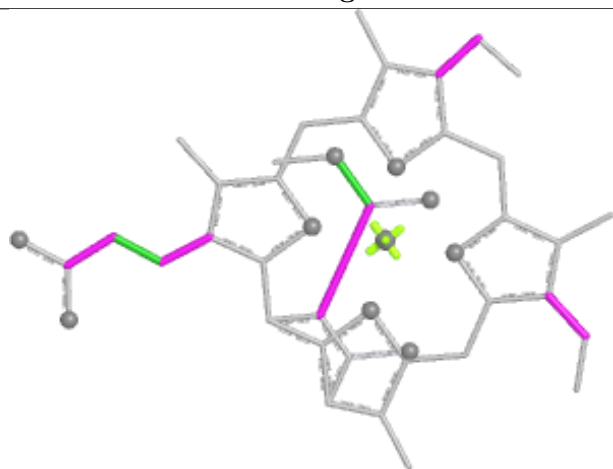
Ligand KC2 C 303



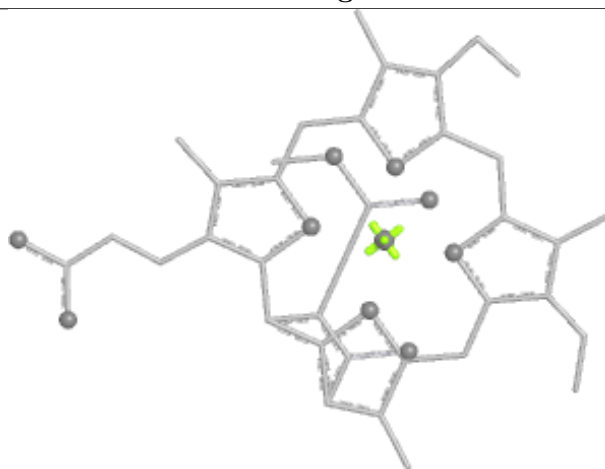
Bond lengths



Bond angles

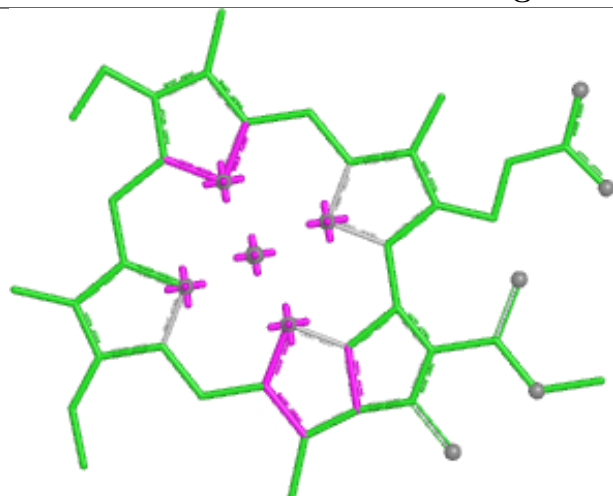


Torsions

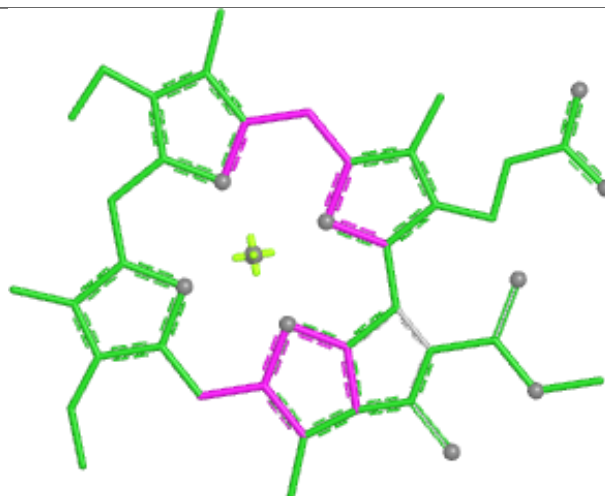


Rings

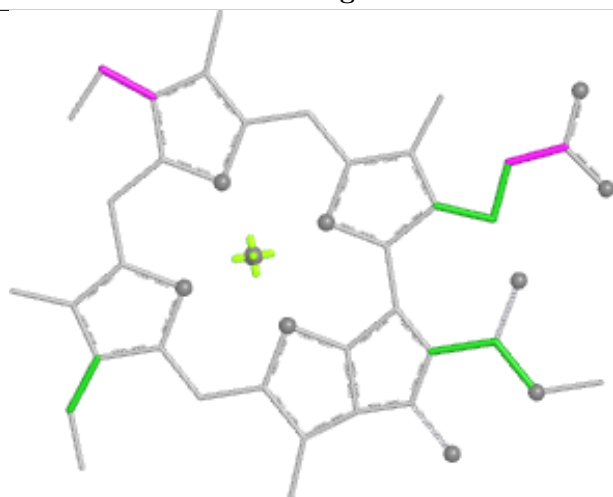
Ligand CLA R 304



Bond lengths



Bond angles

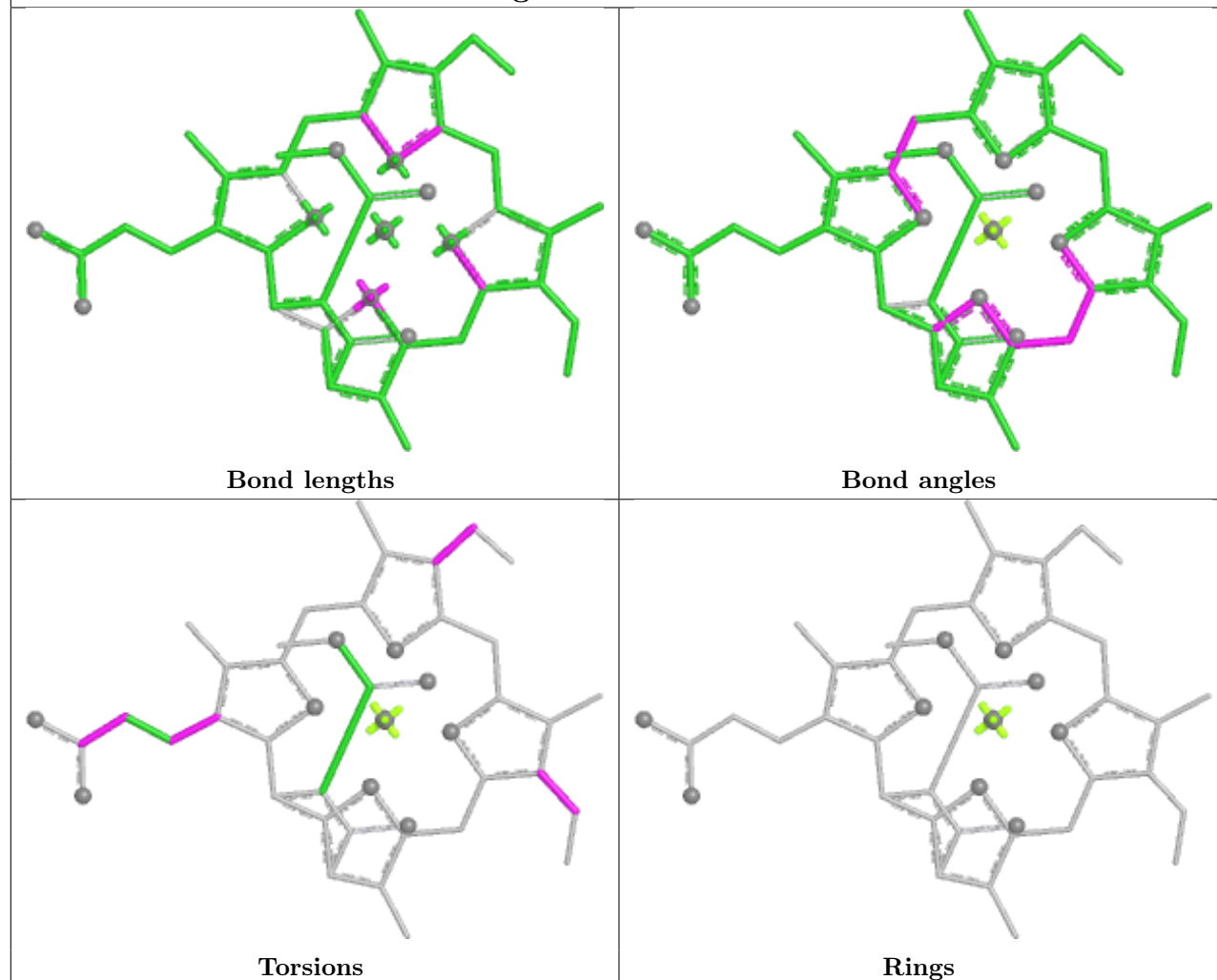


Torsions

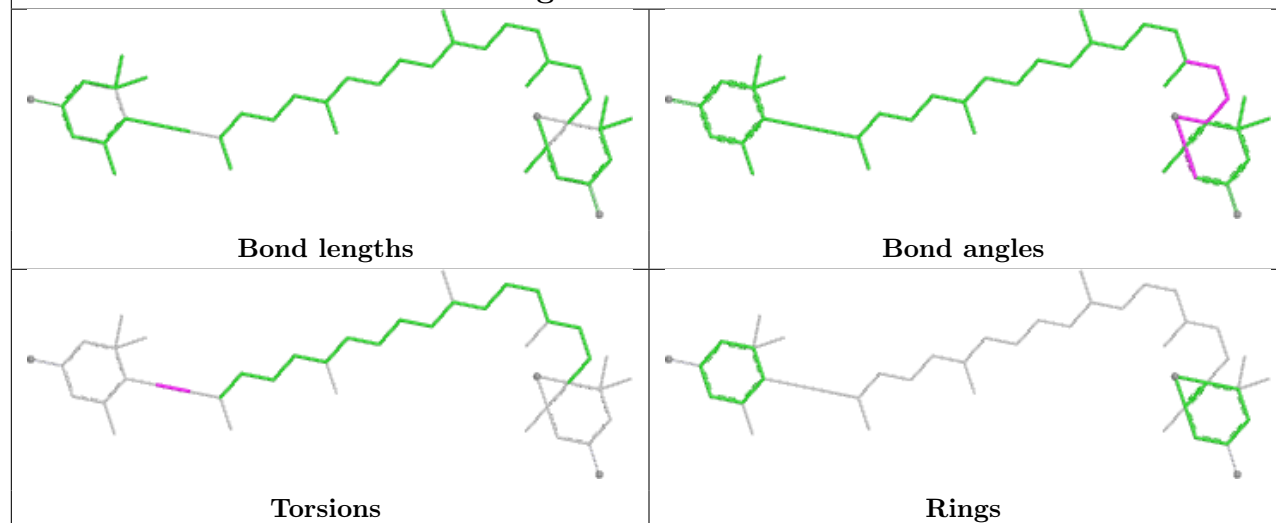


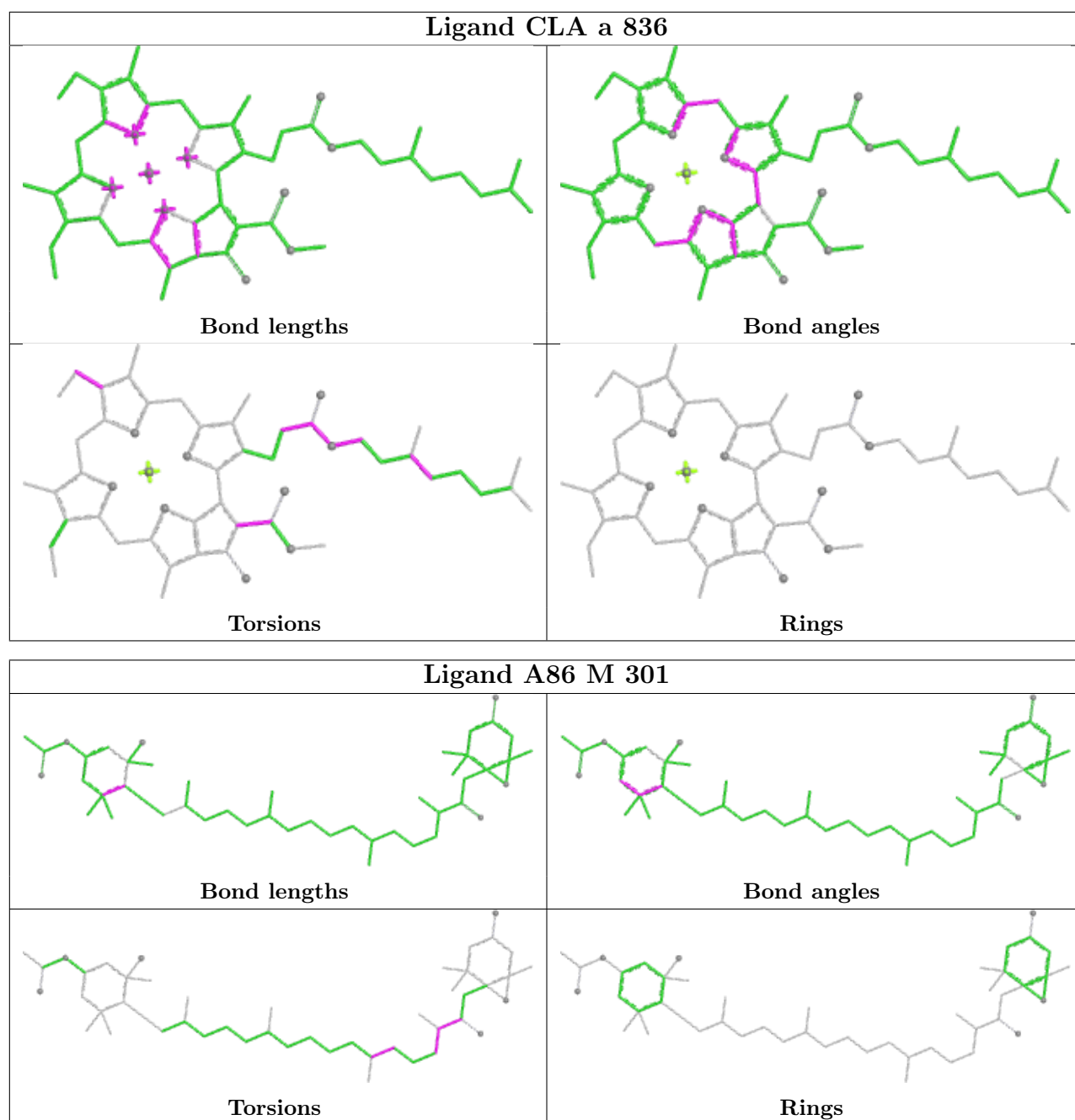
Rings

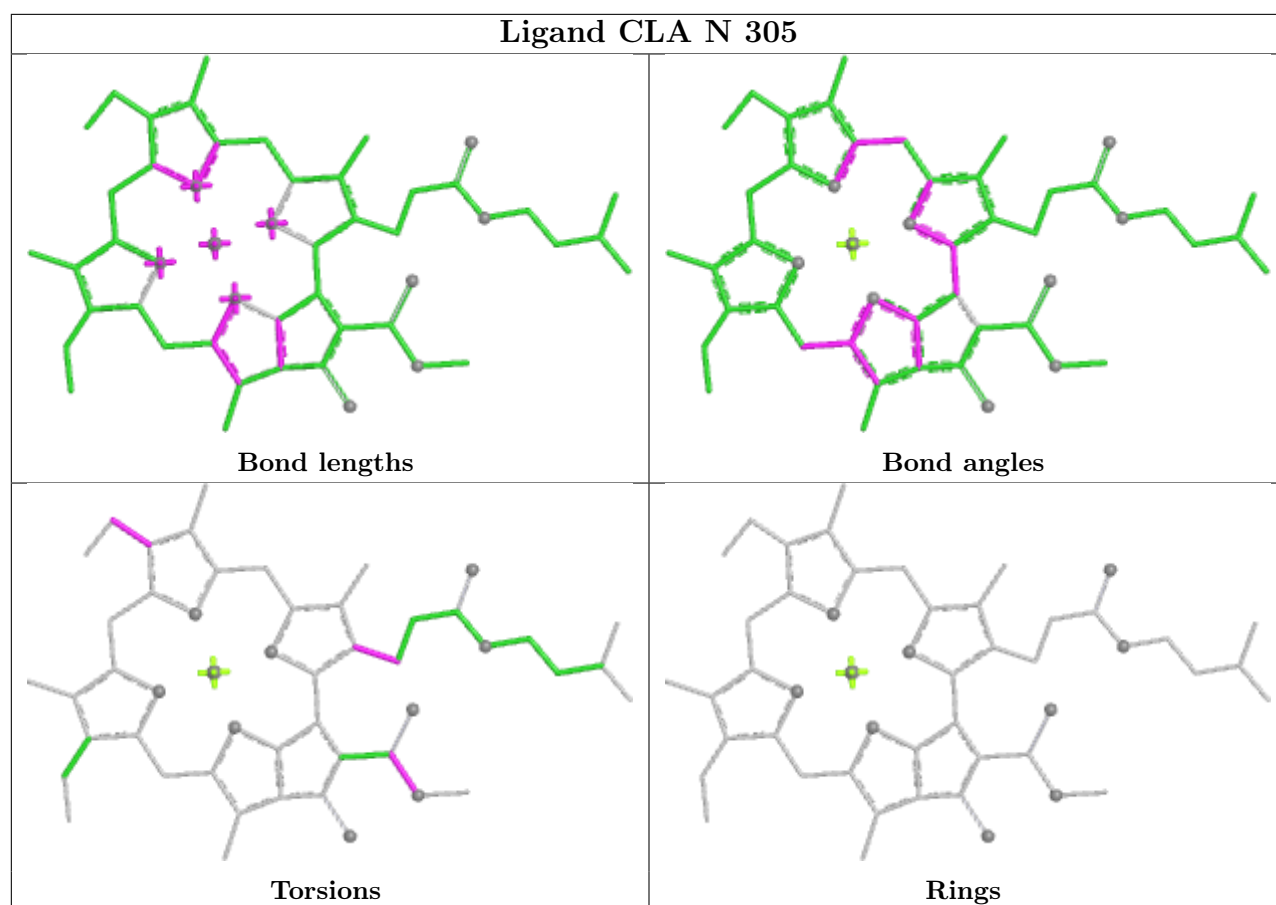
Ligand KC2 J 310



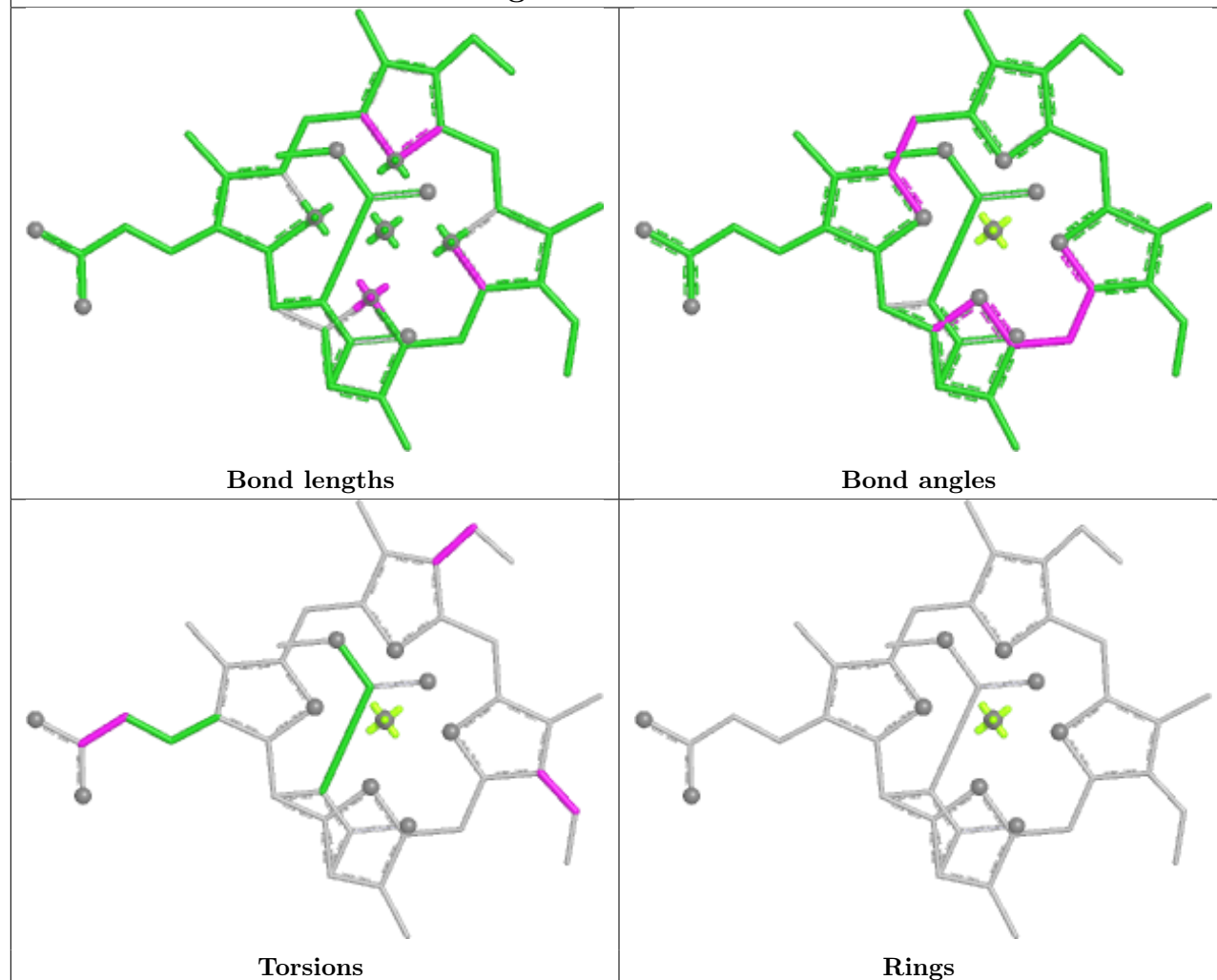
Ligand DD6 J 315



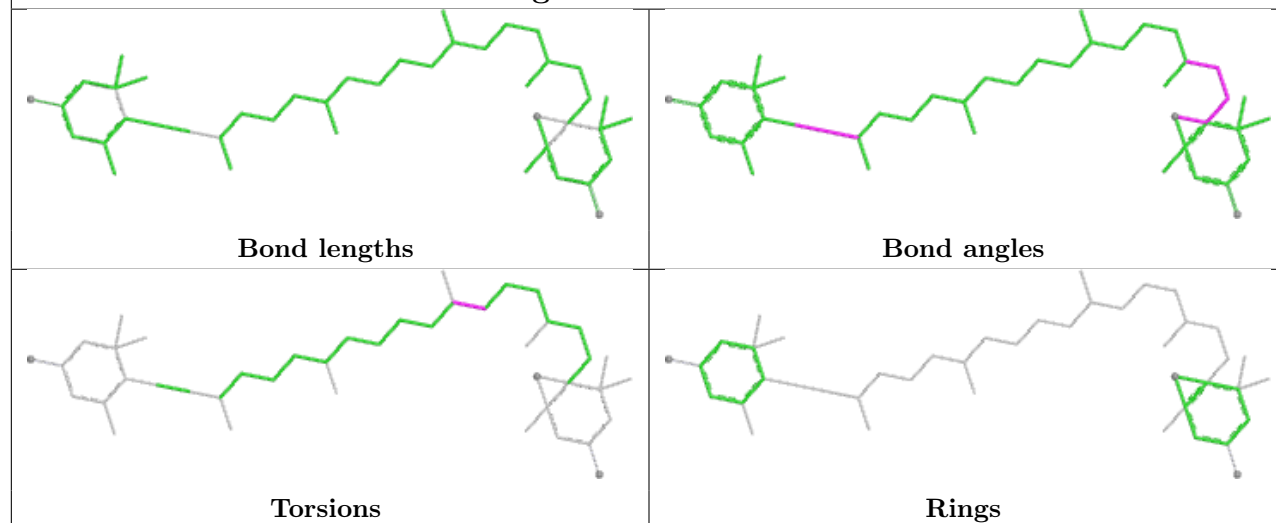


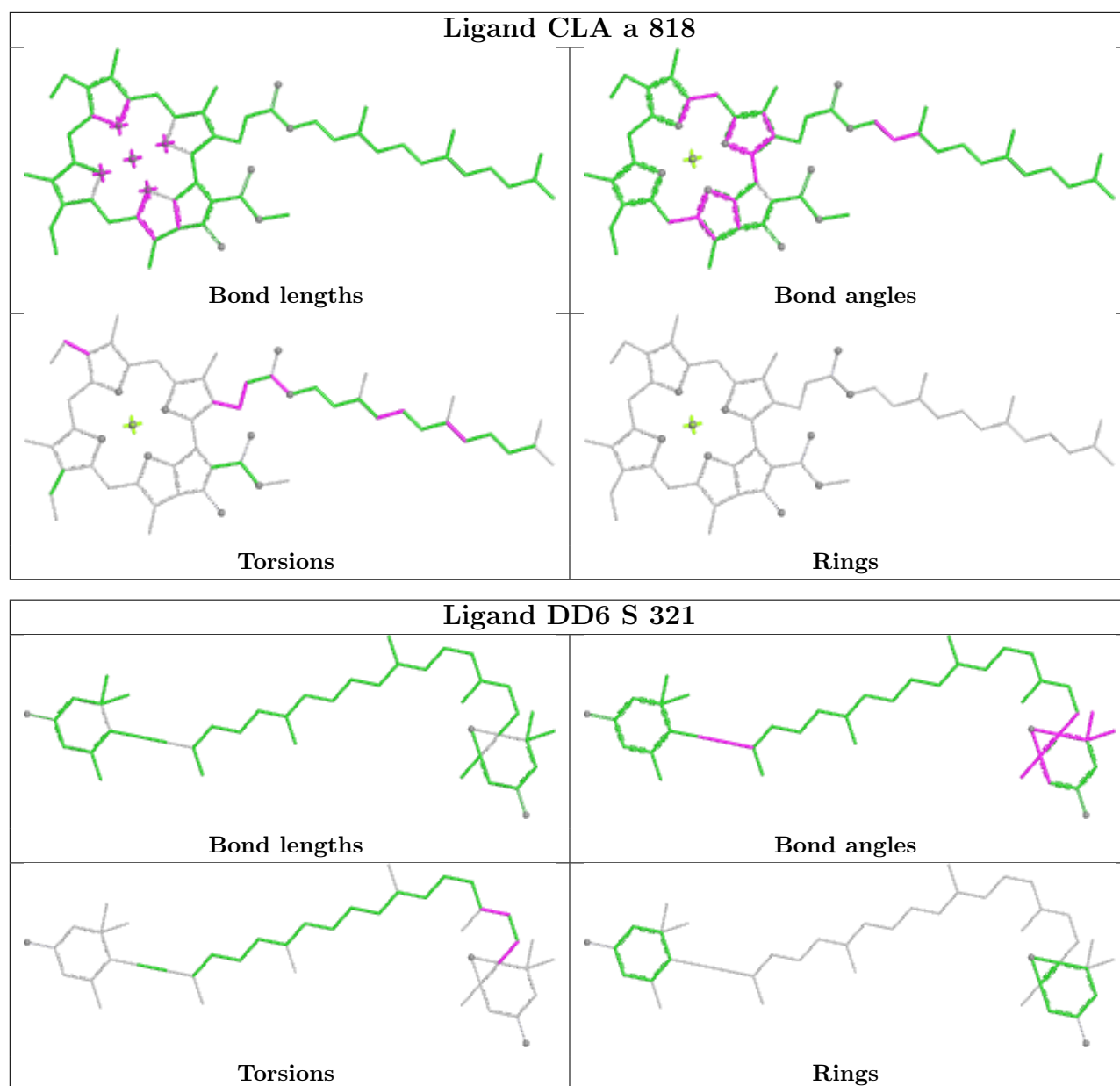


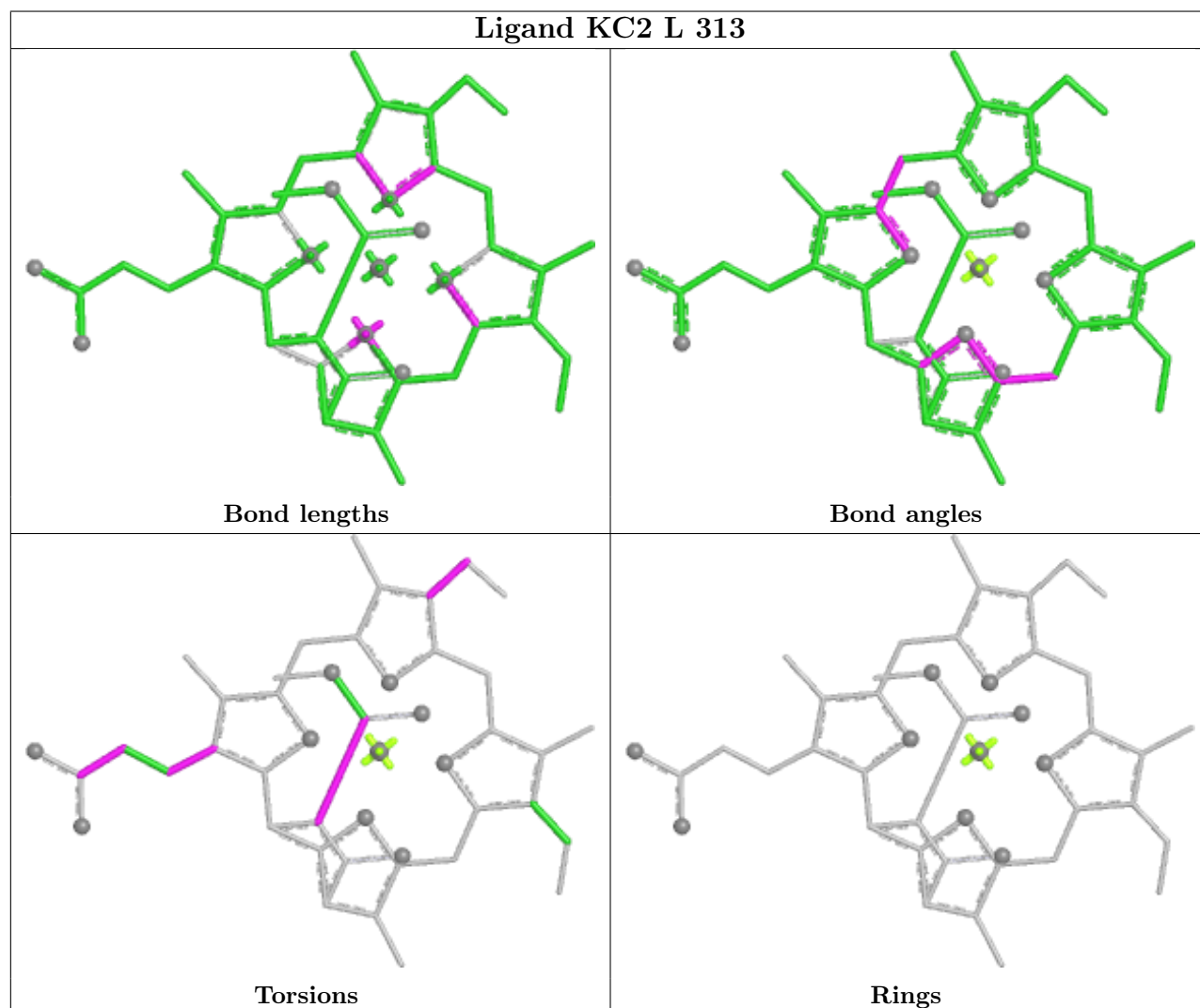
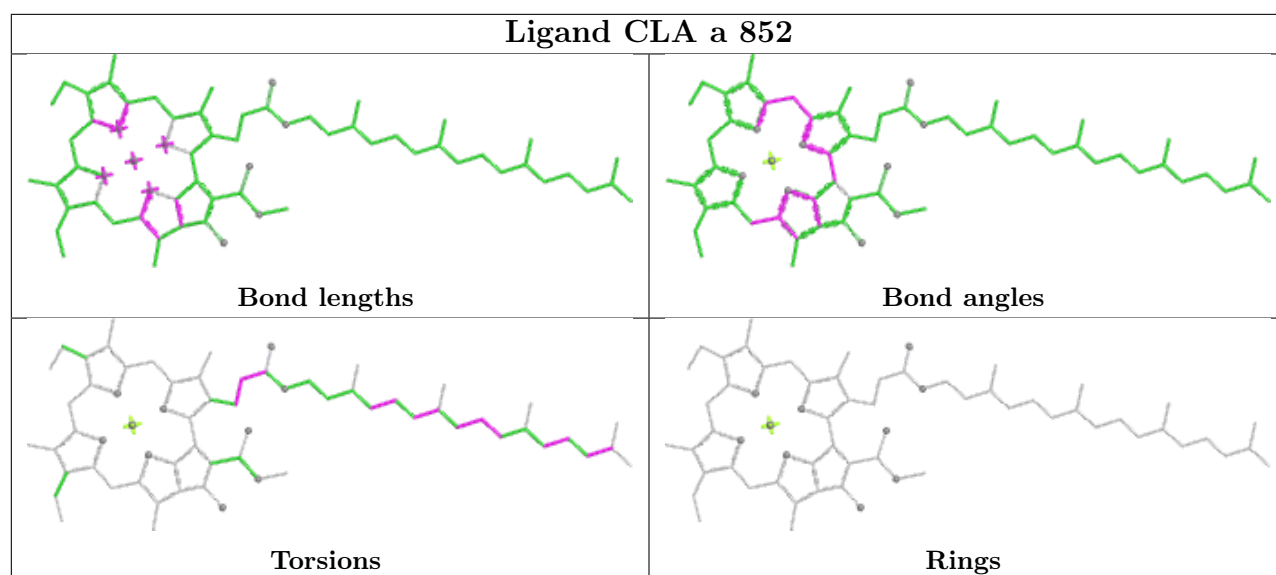
Ligand KC2 N 308

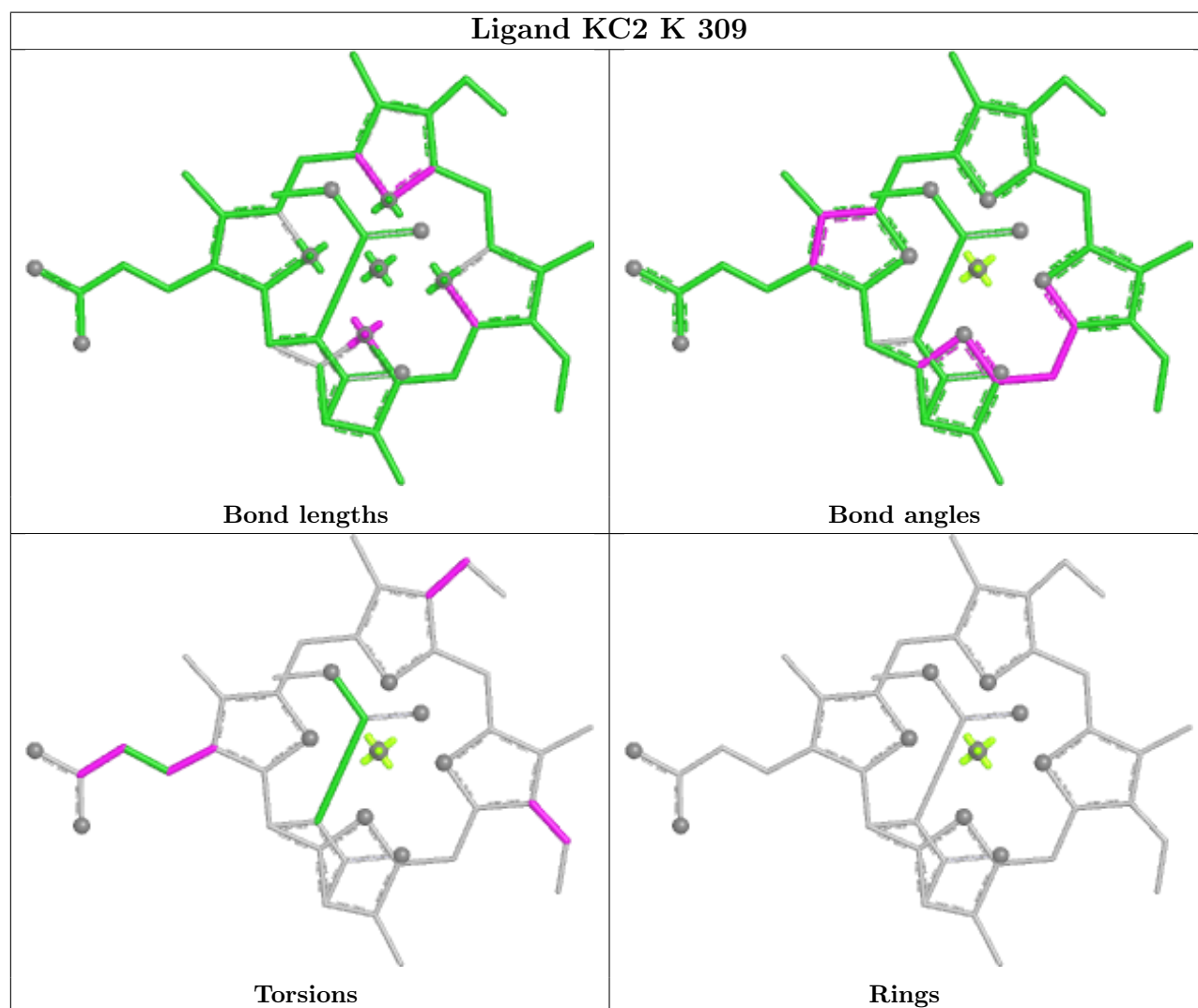
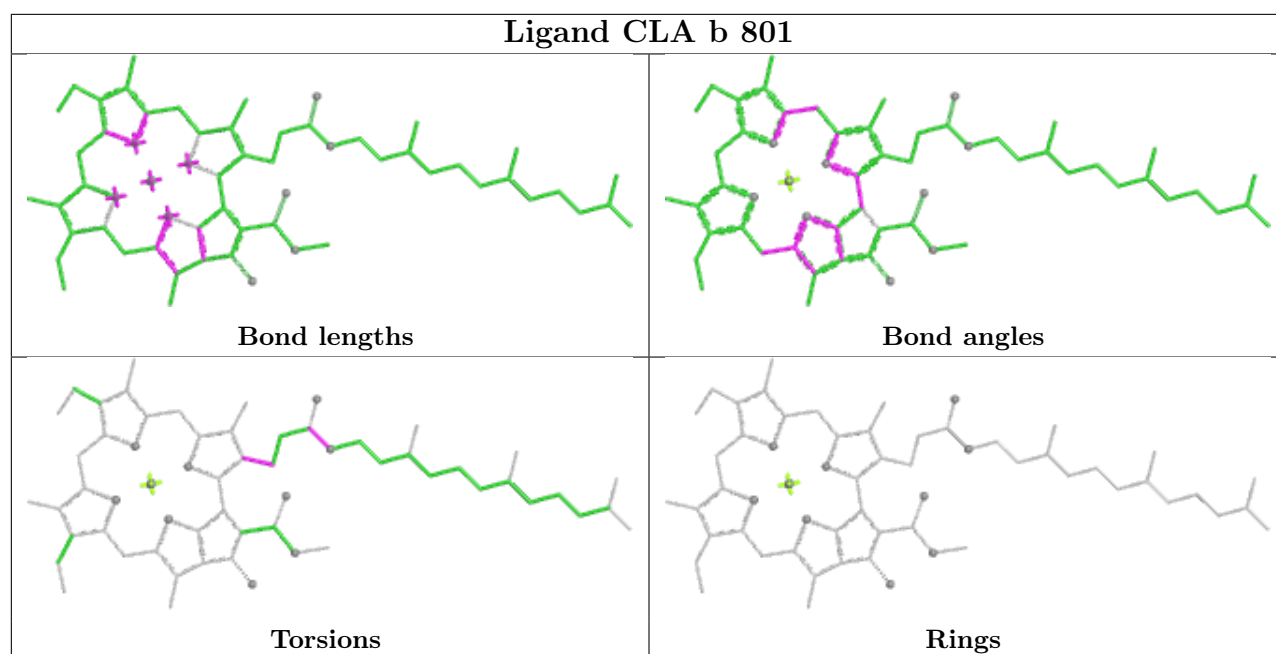


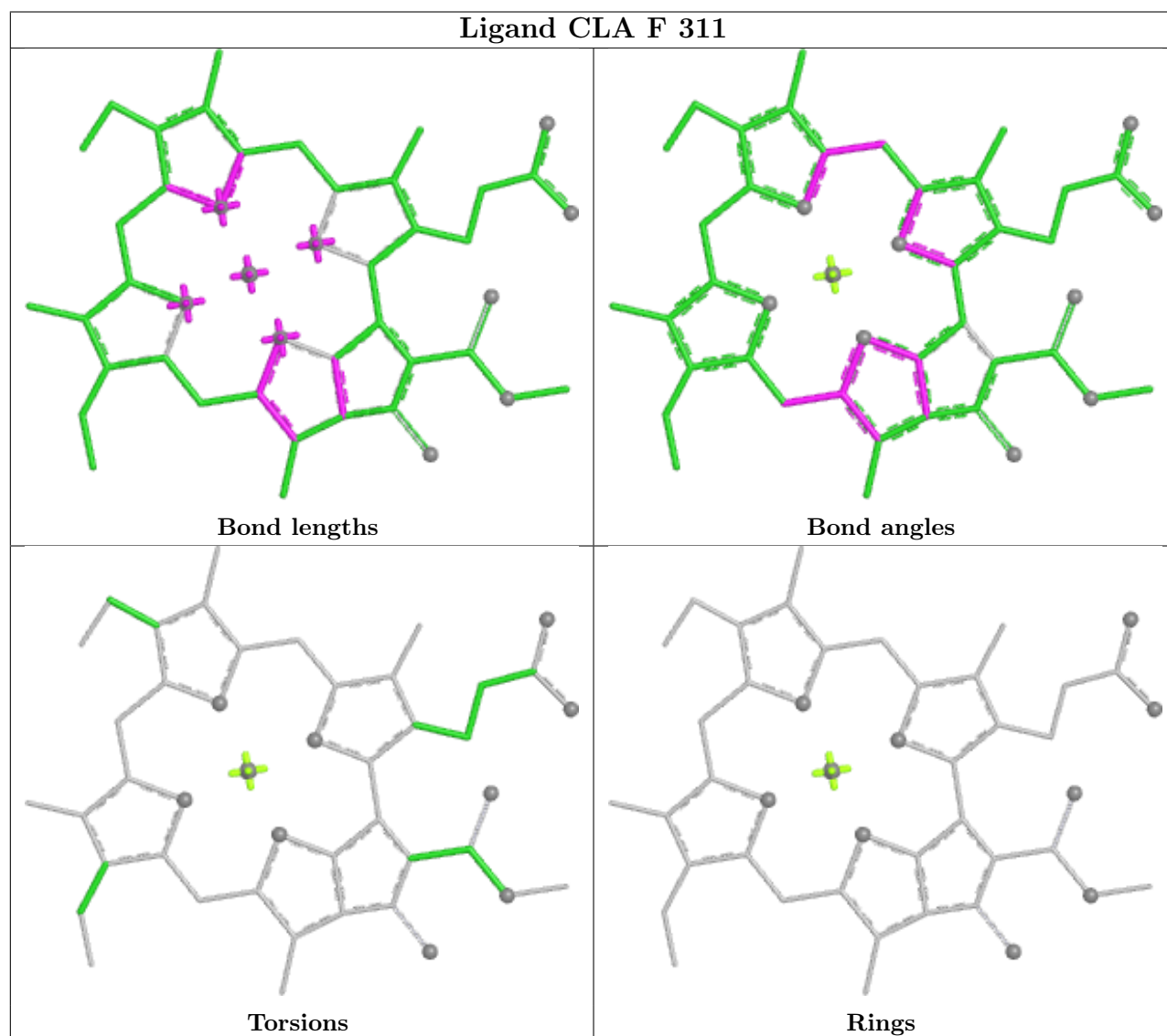
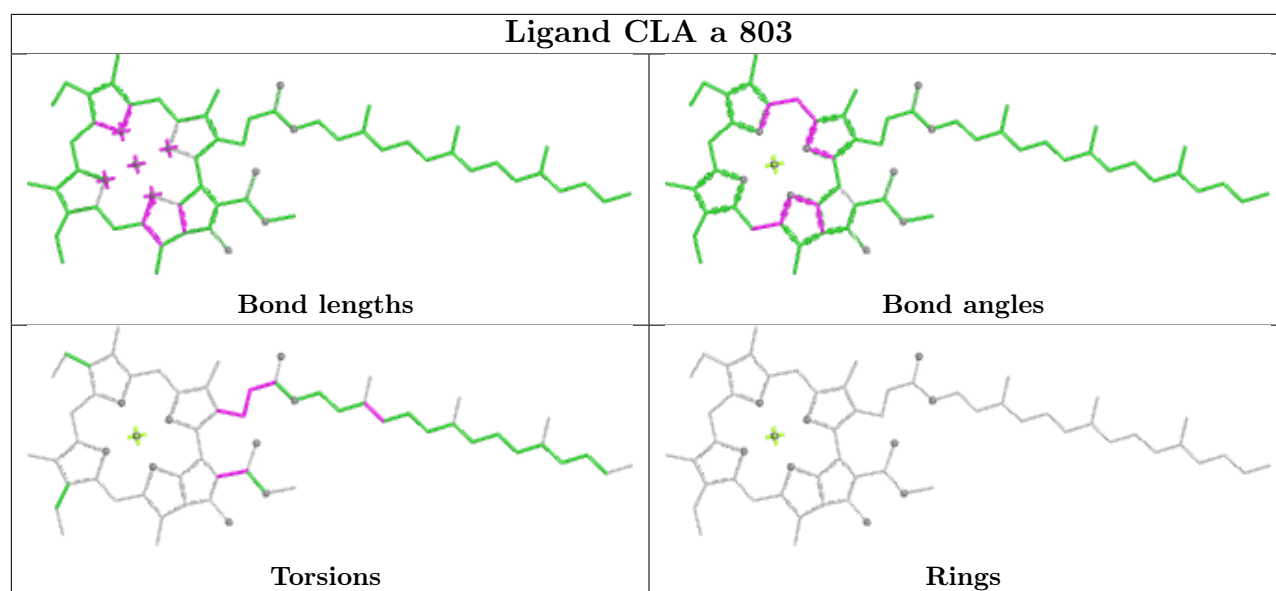
Ligand DD6 D 319



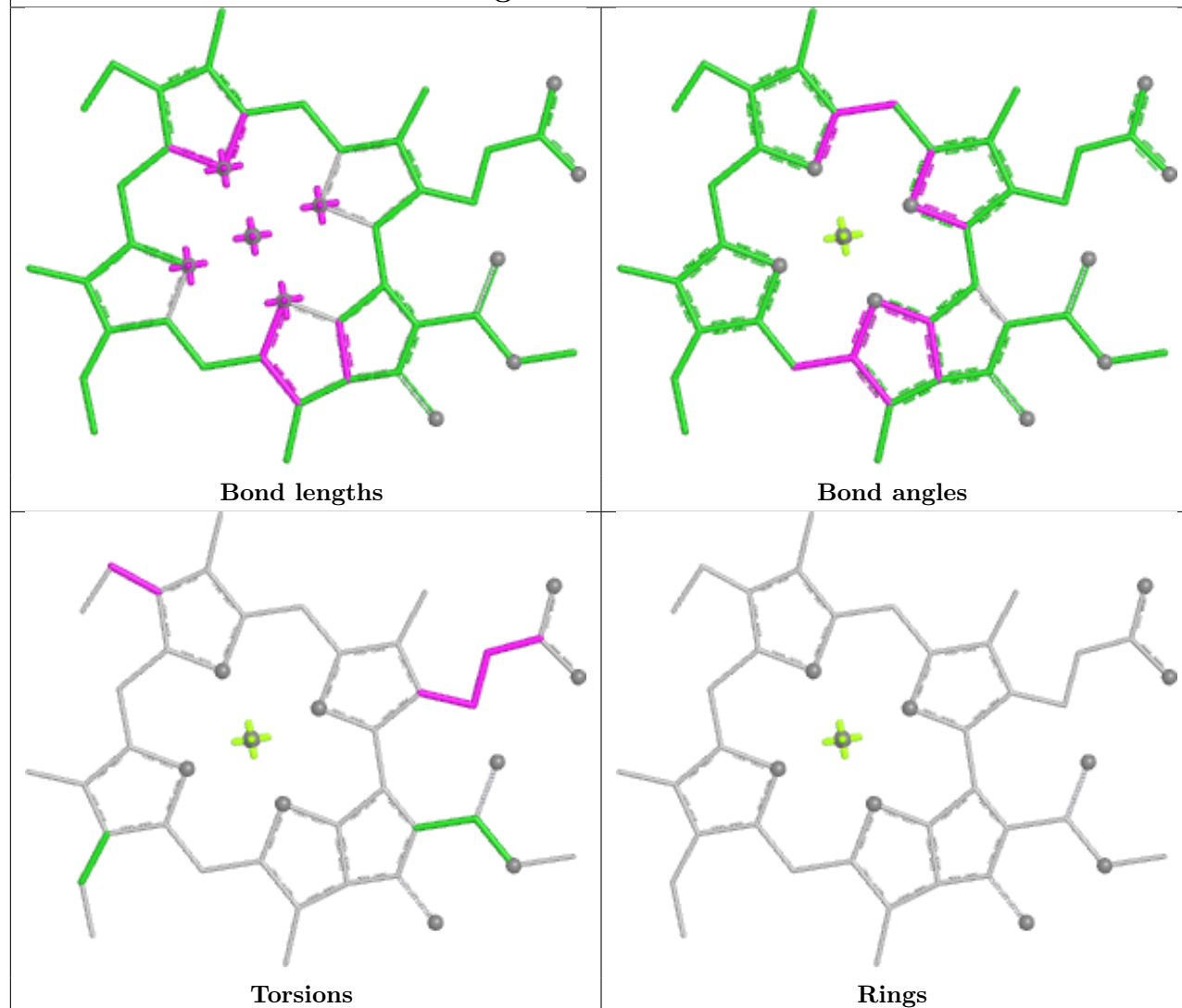




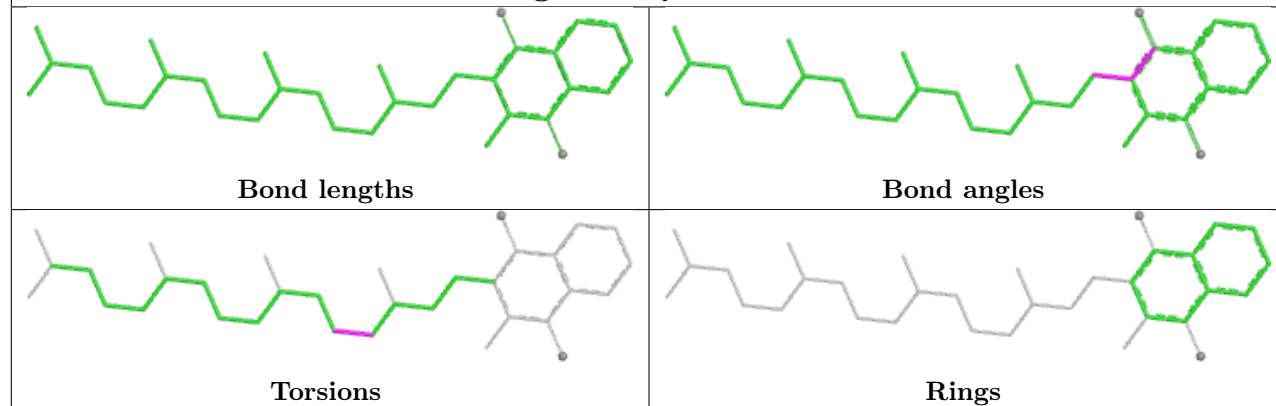




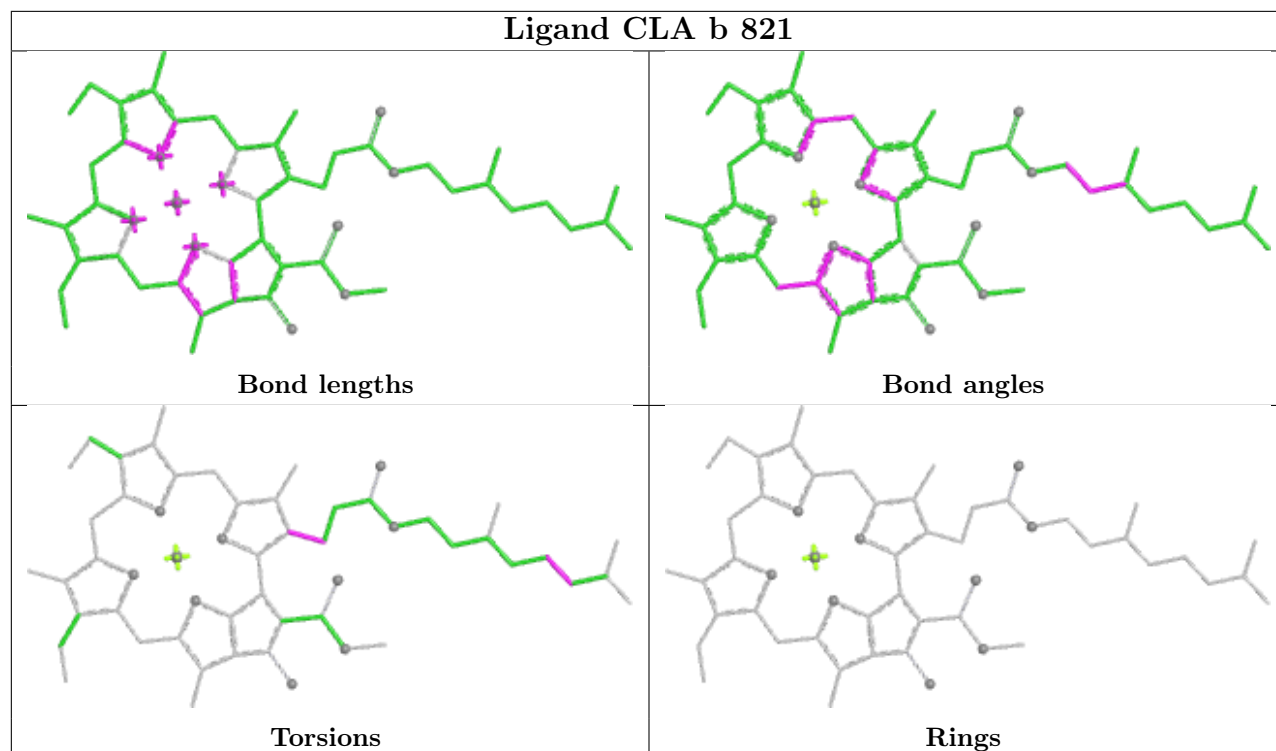
Ligand CLA L 314



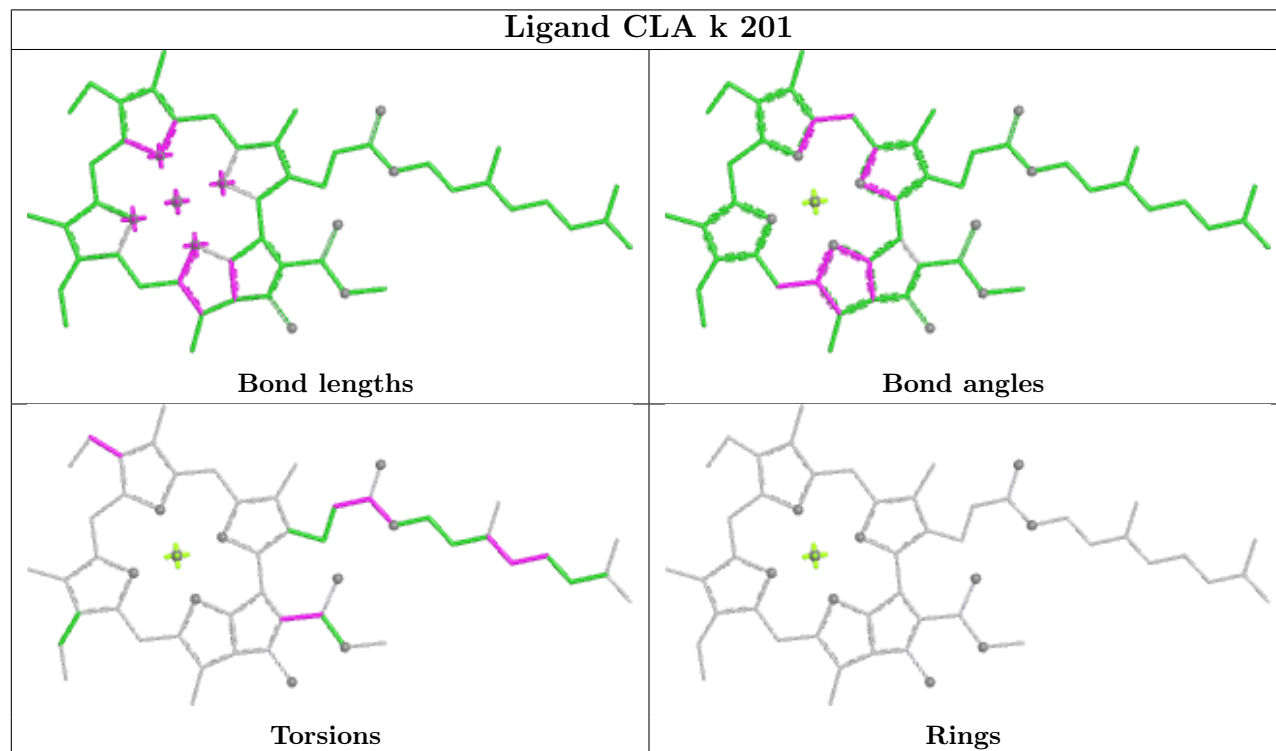
Ligand PQN b 847

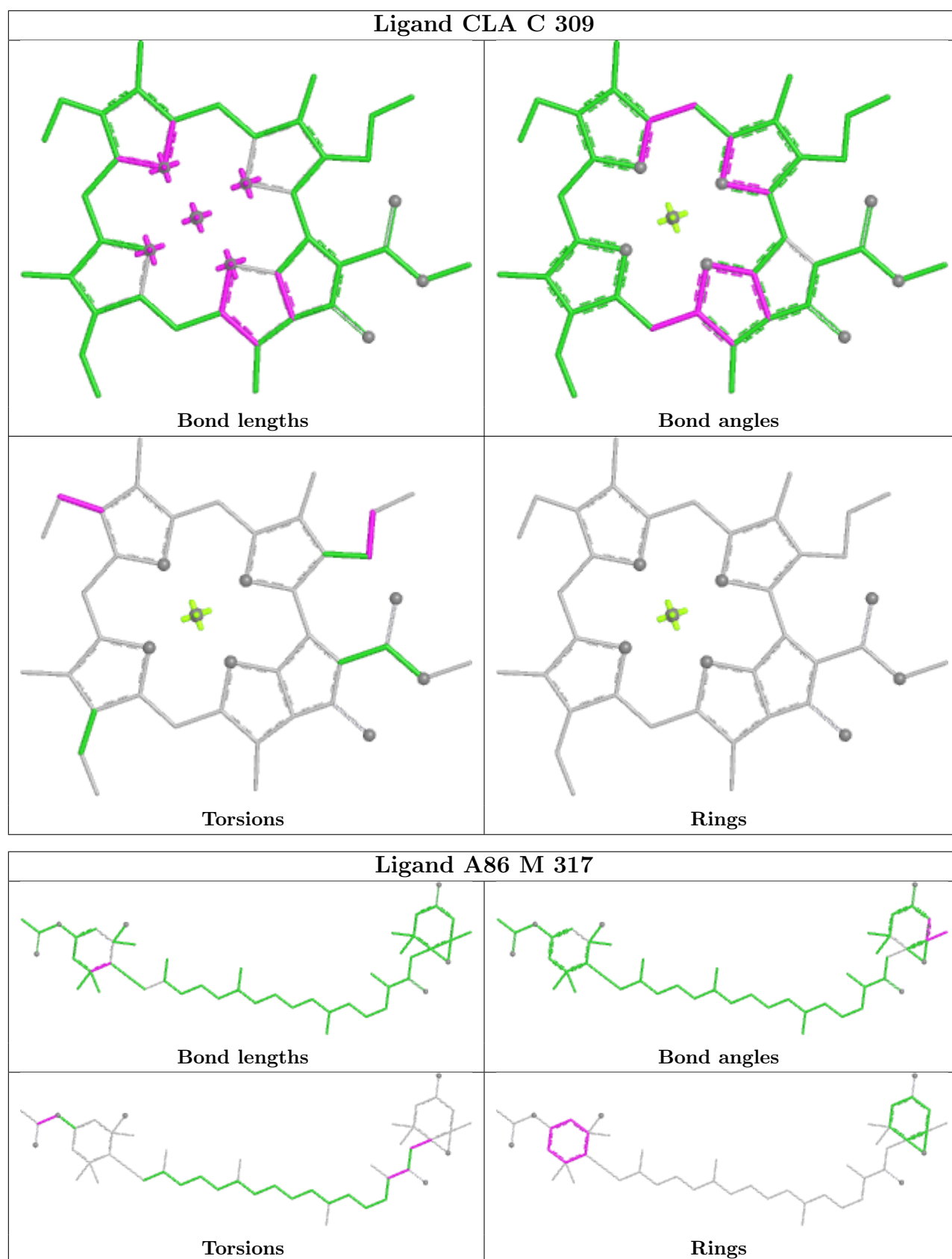


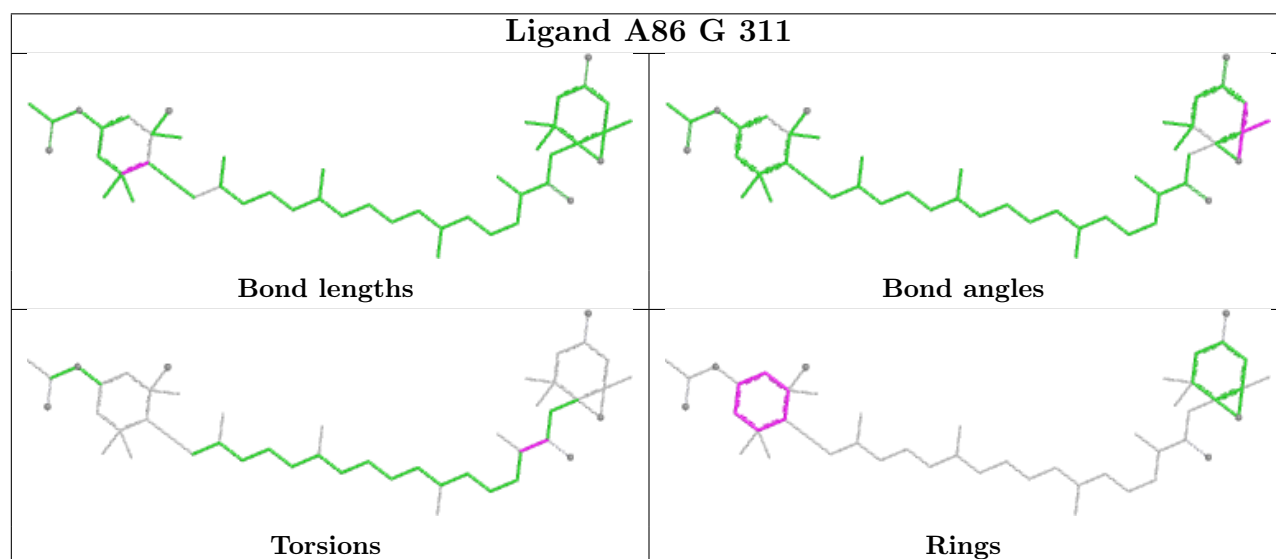
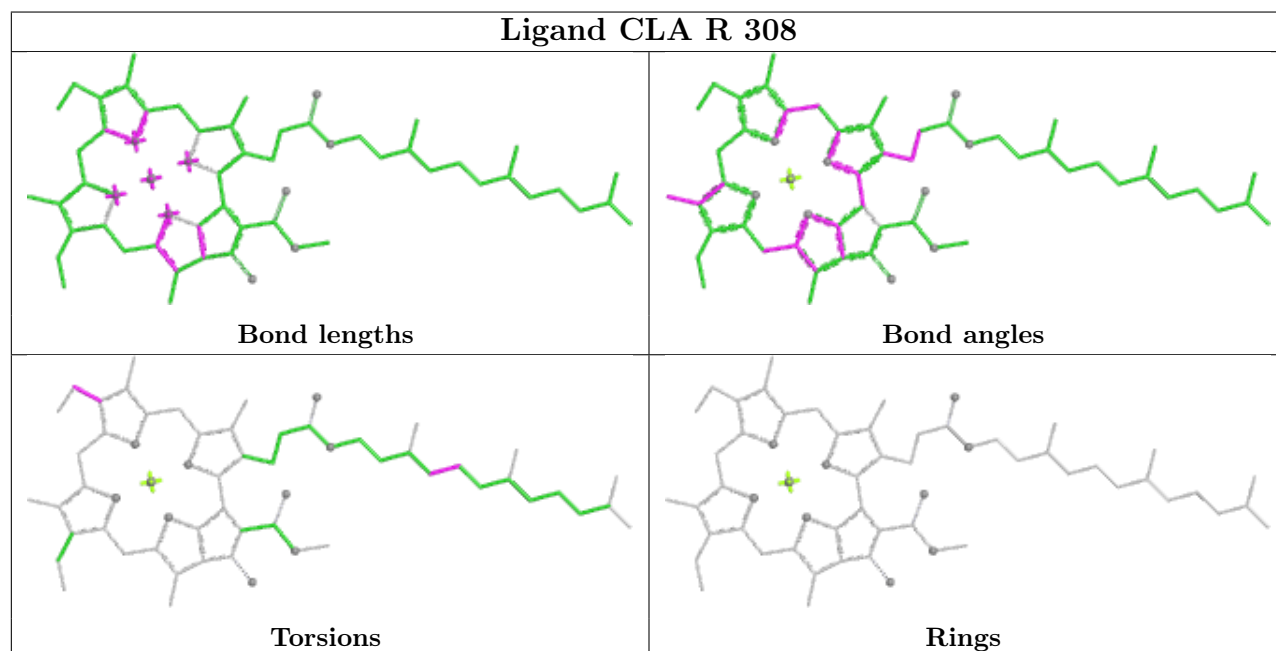
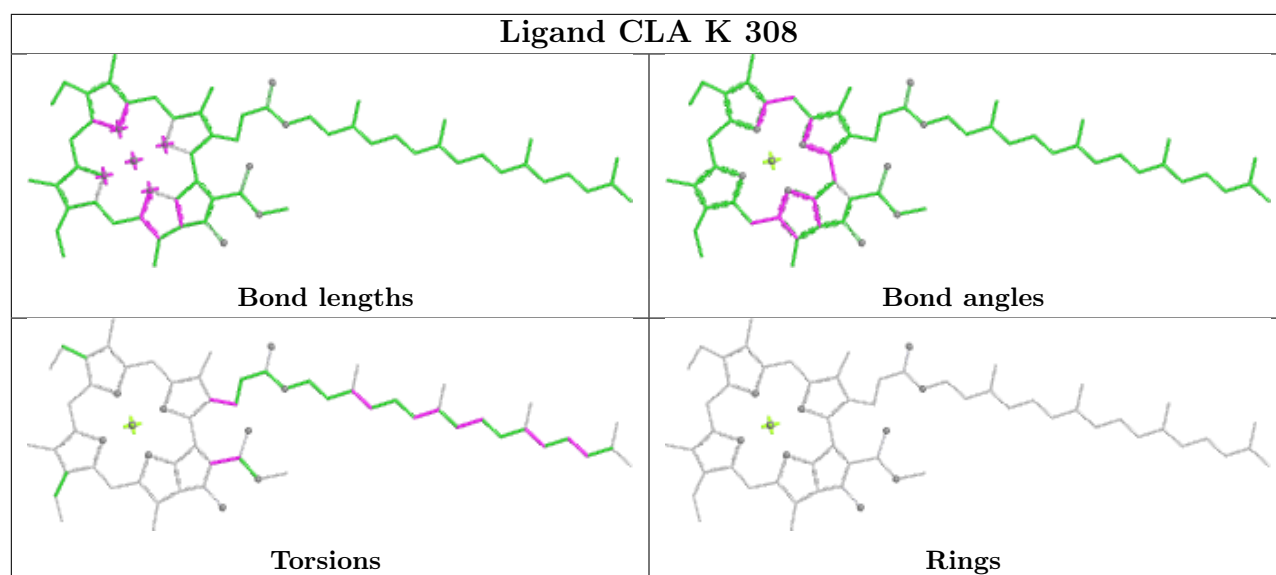
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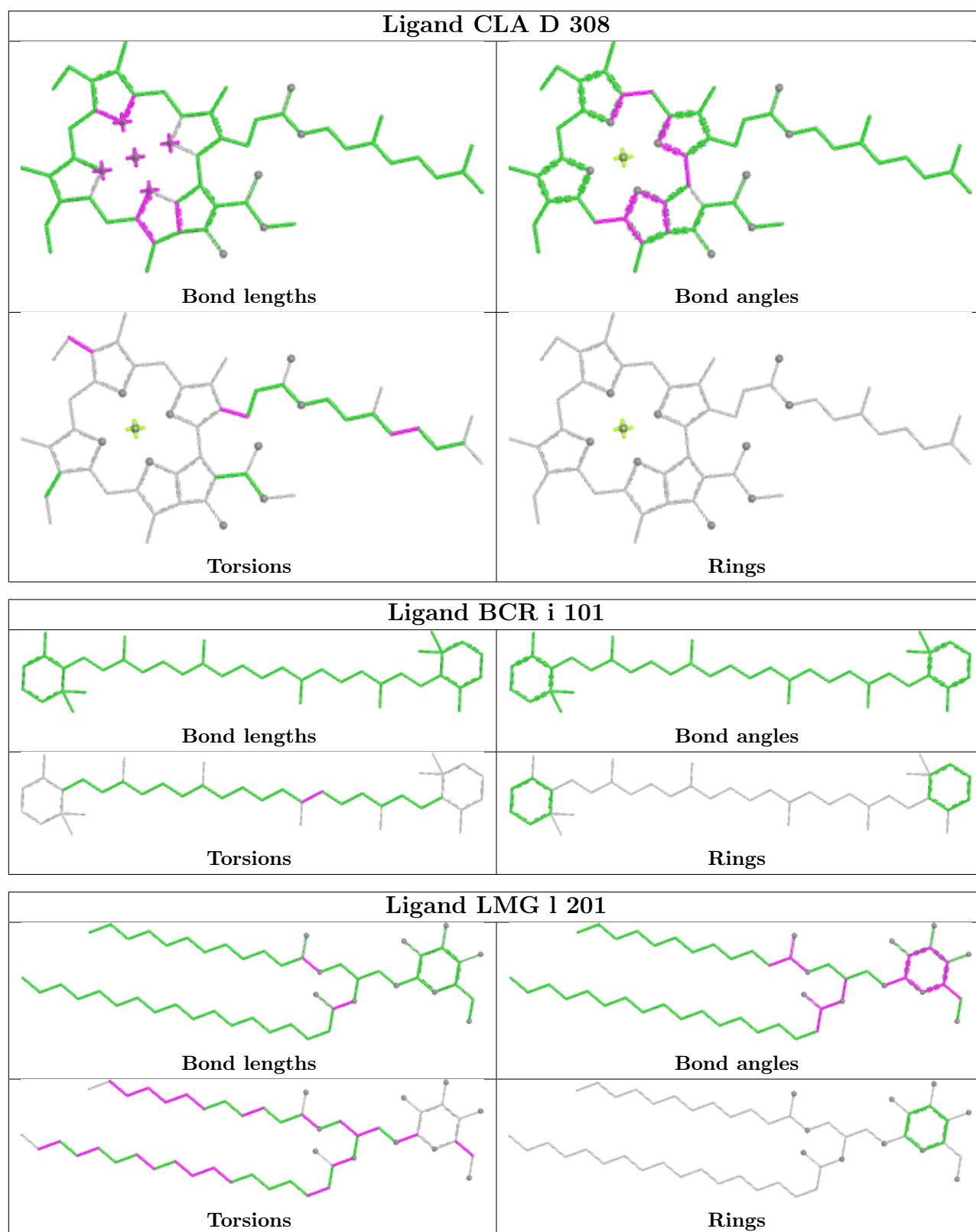


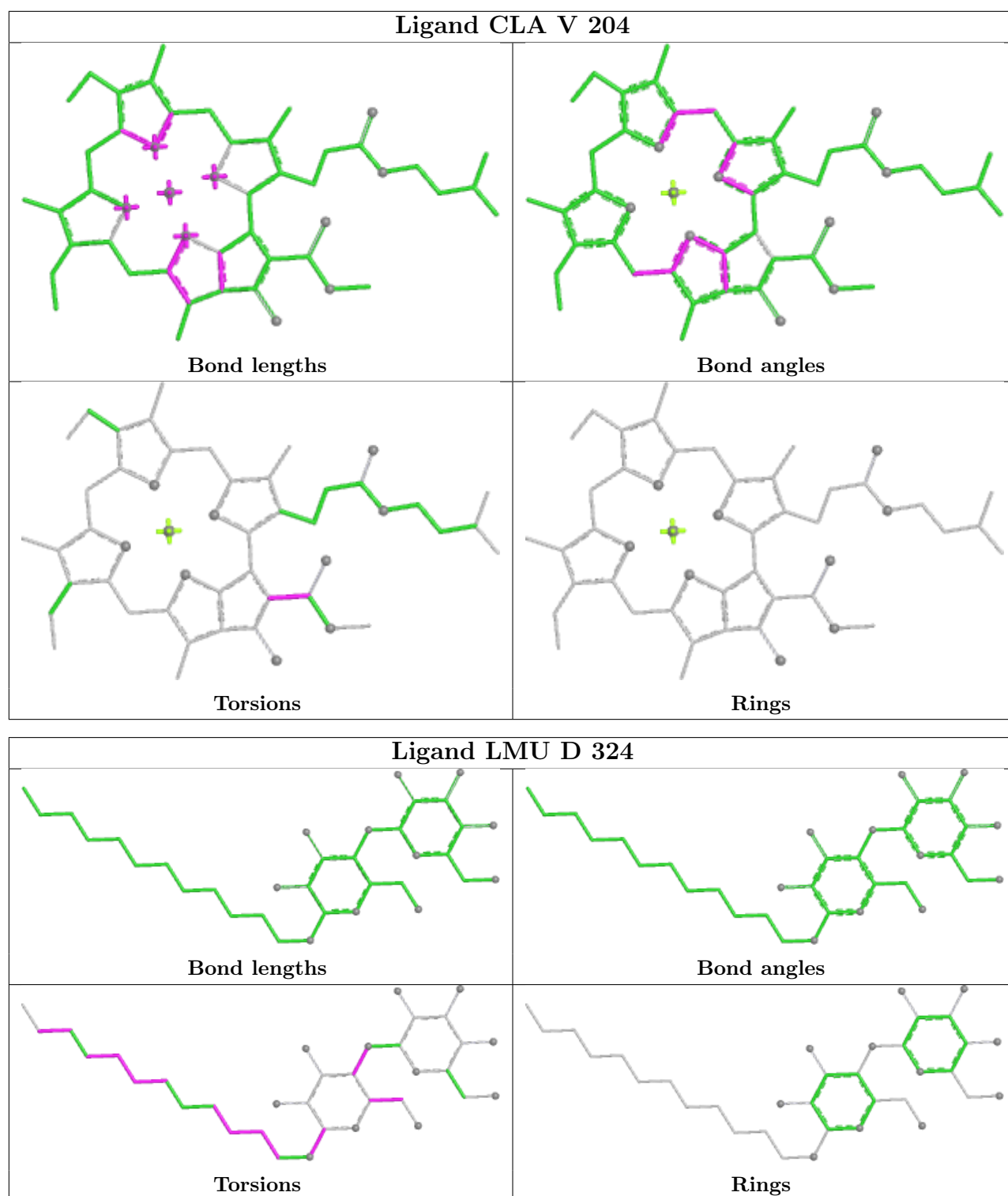
Ligand CLA k 201



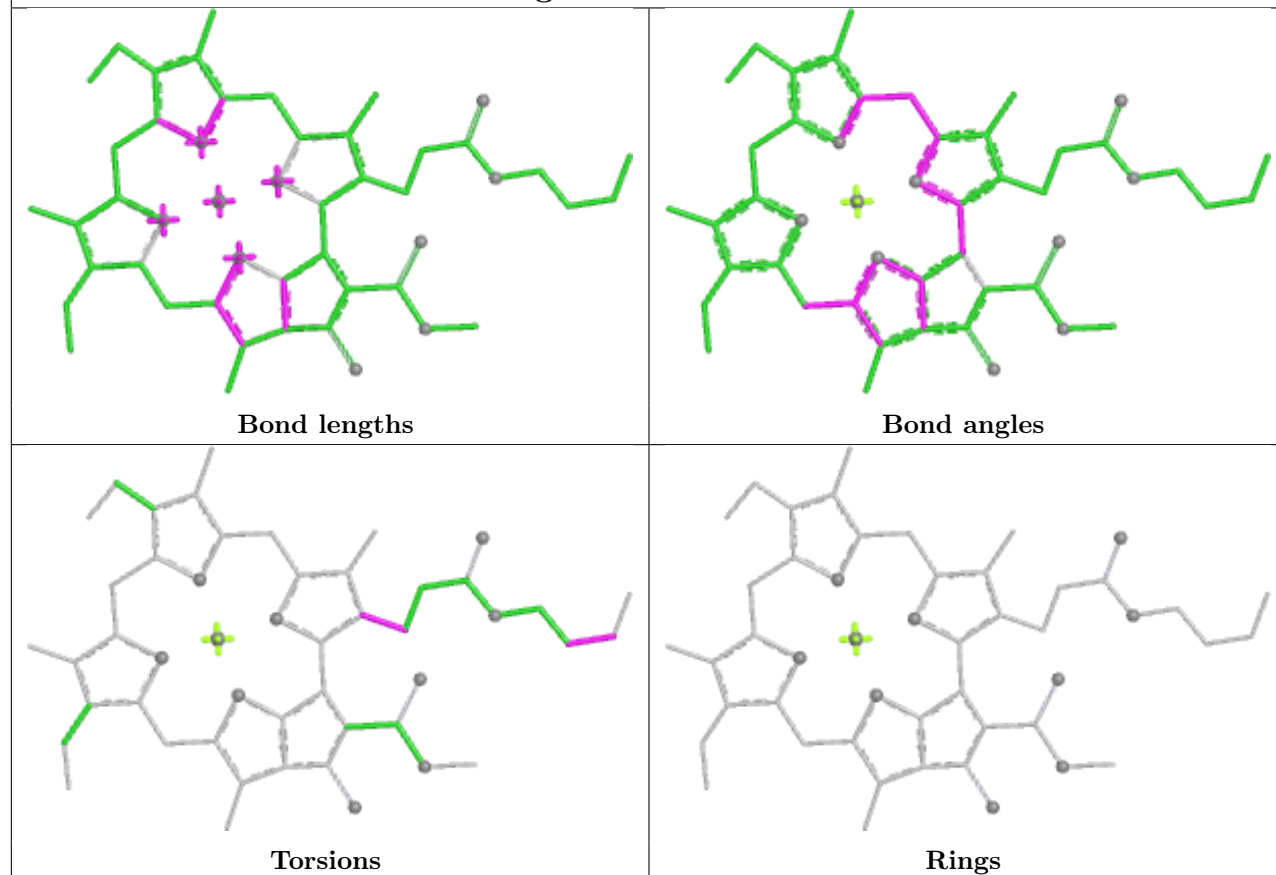




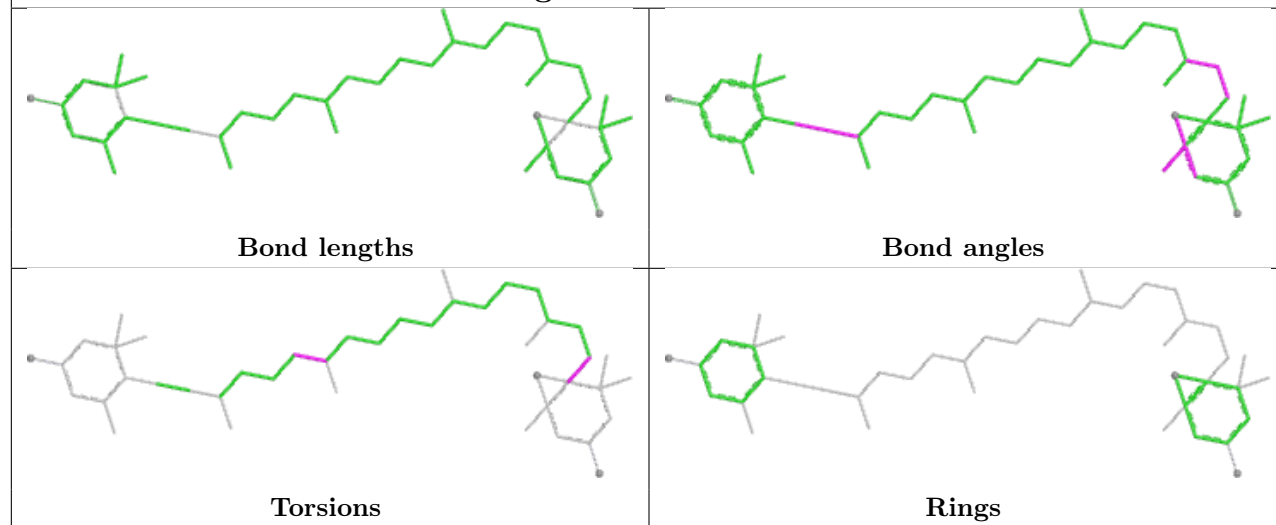




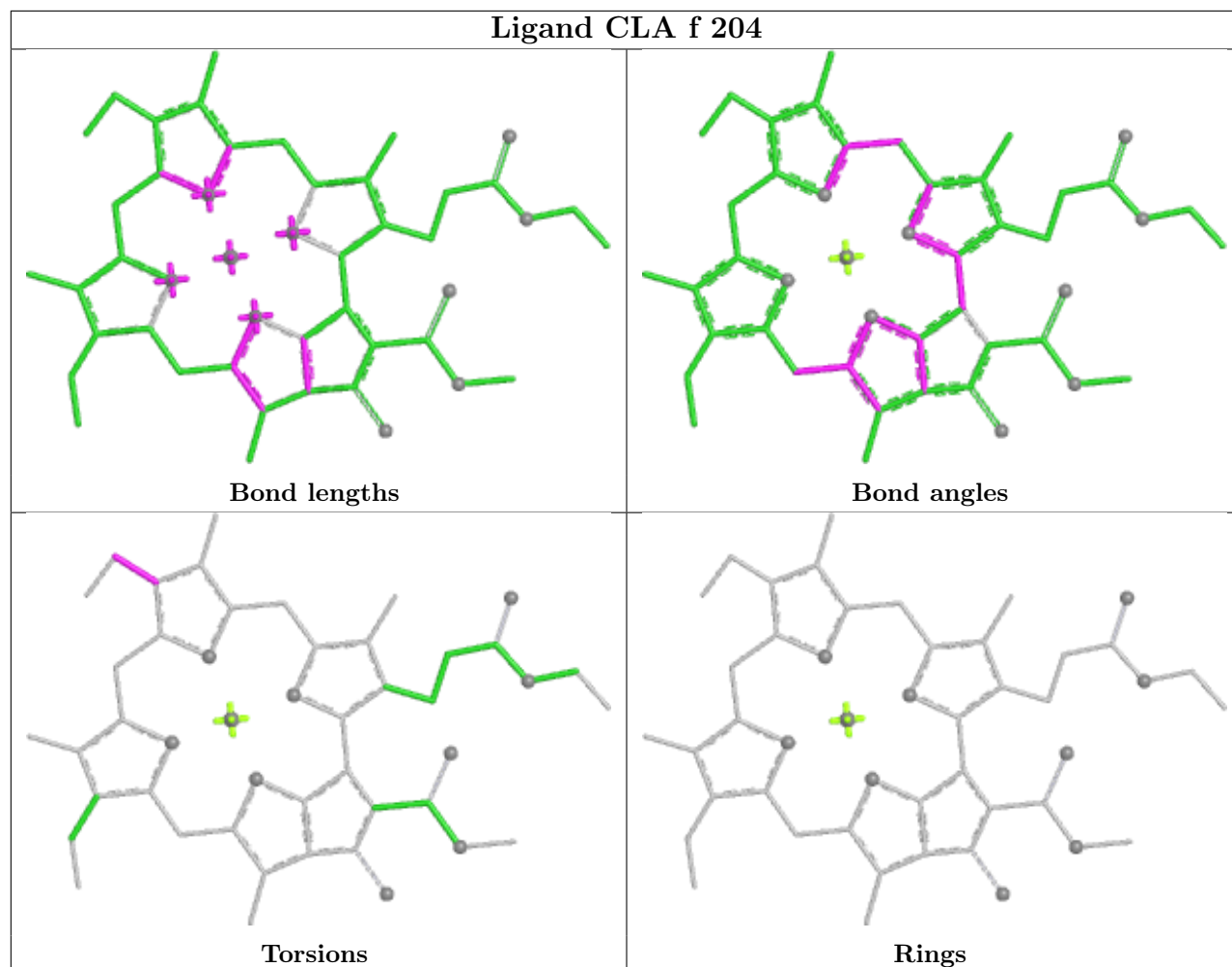
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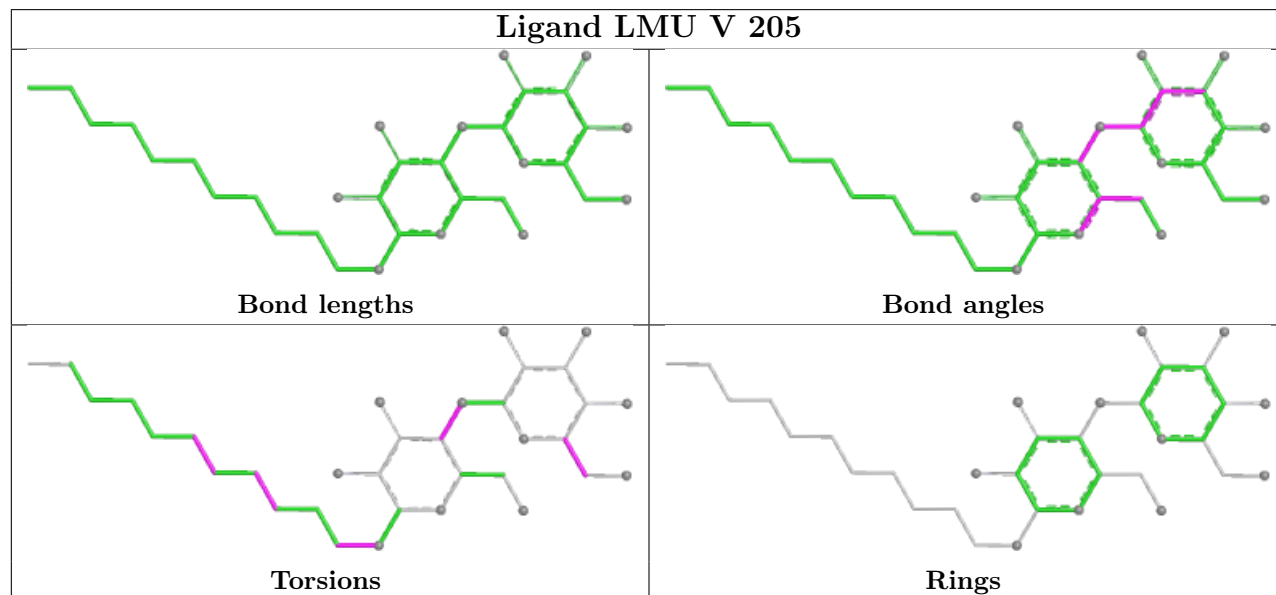
Ligand DD6 F 316

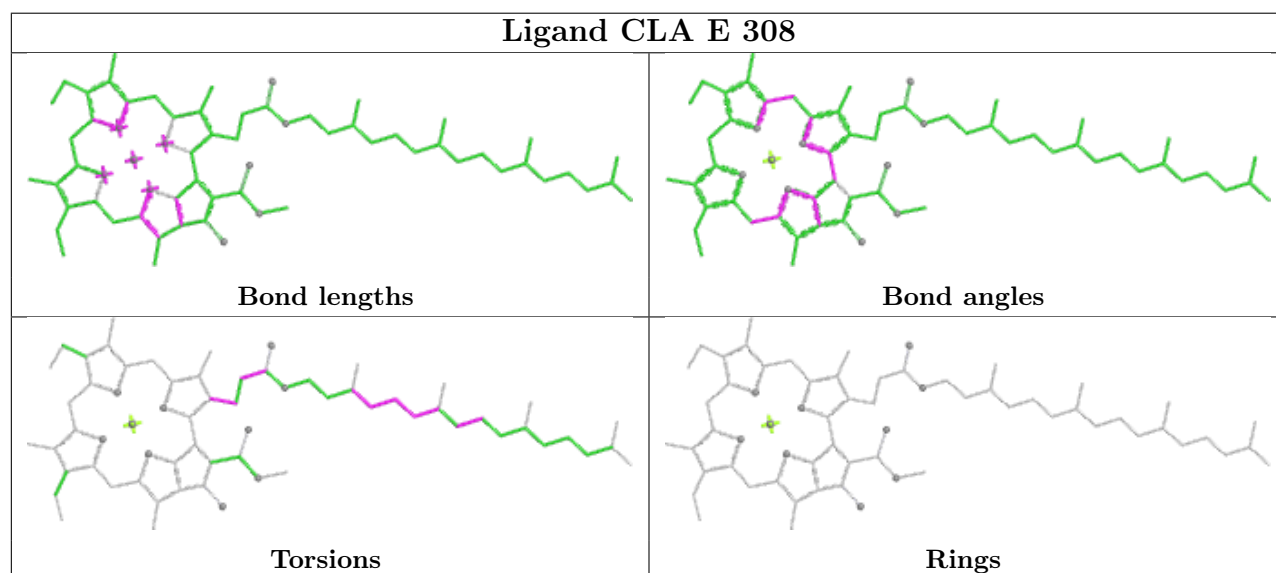
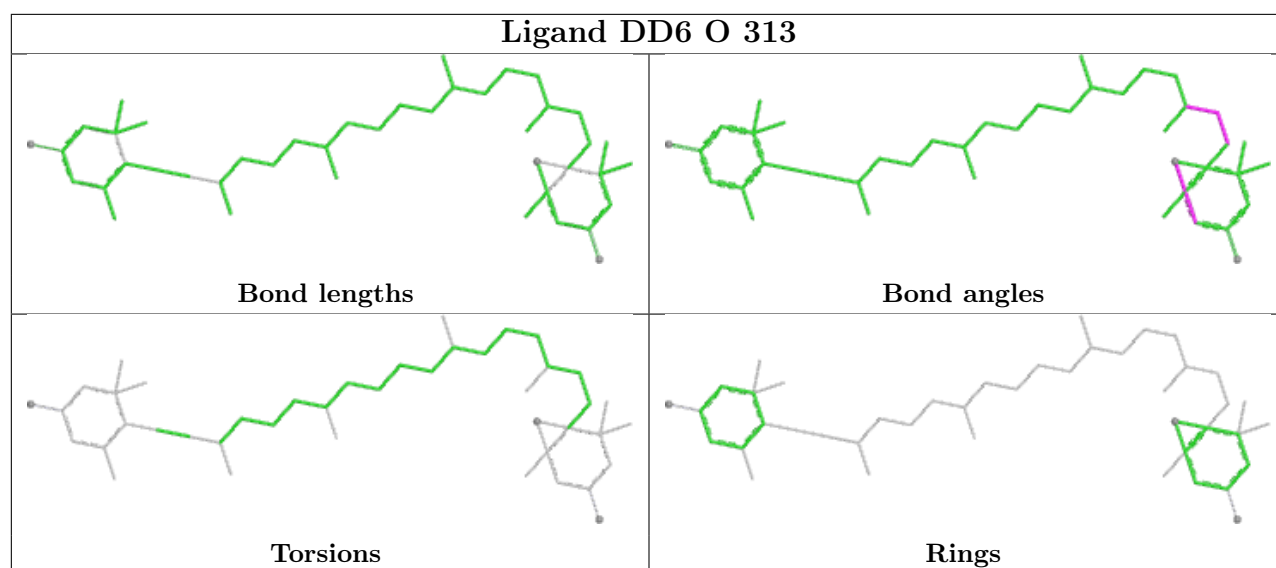


Ligand CLA f 204

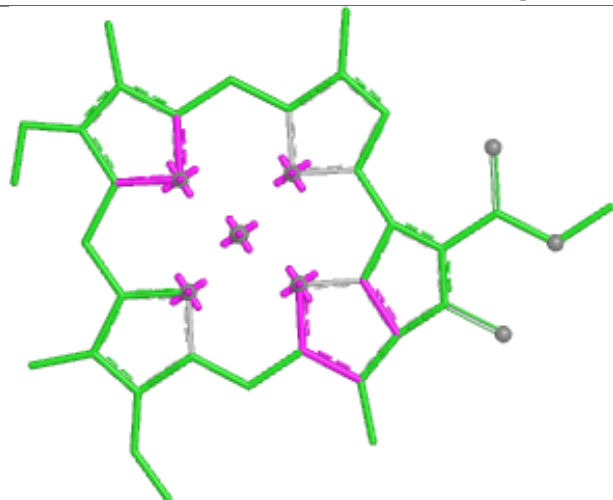


Ligand LMU V 205

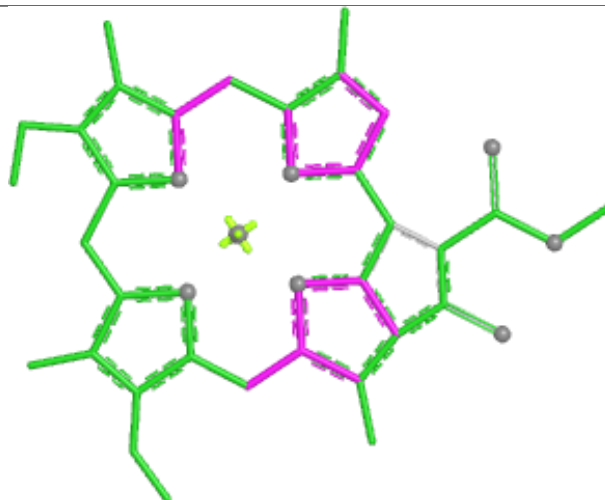




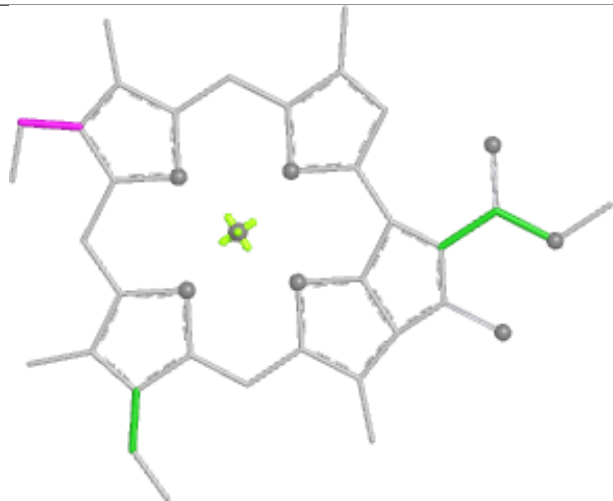
Ligand CLA B 301



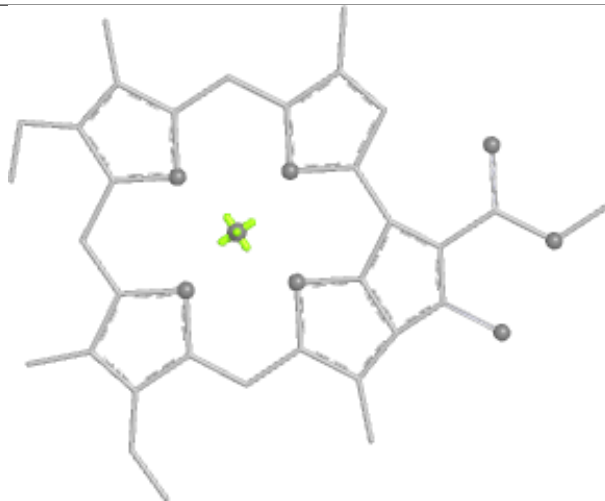
Bond lengths



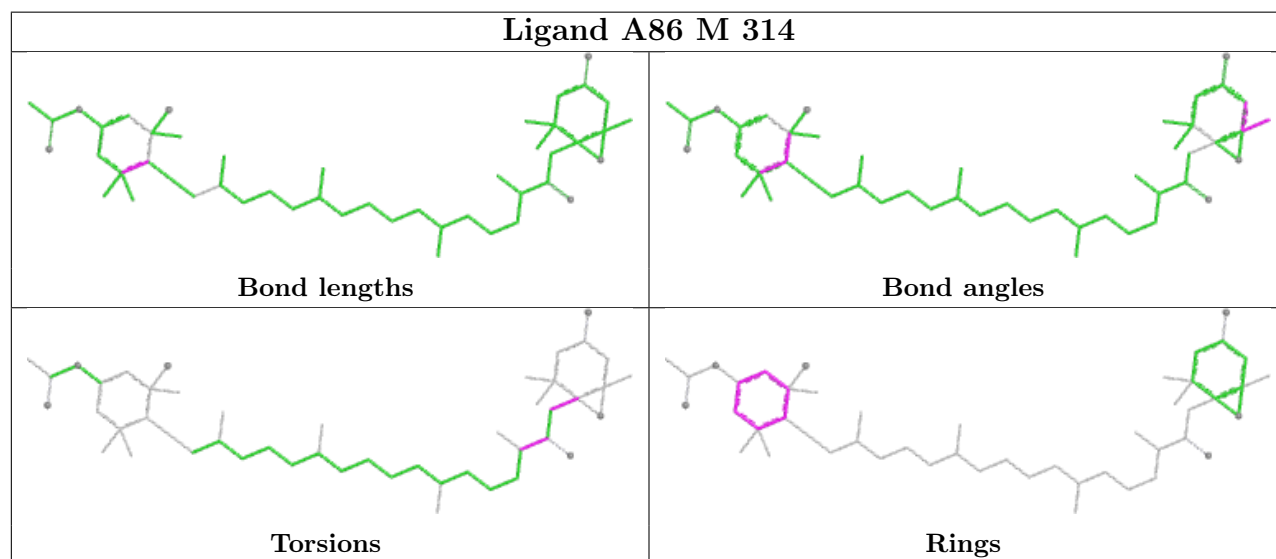
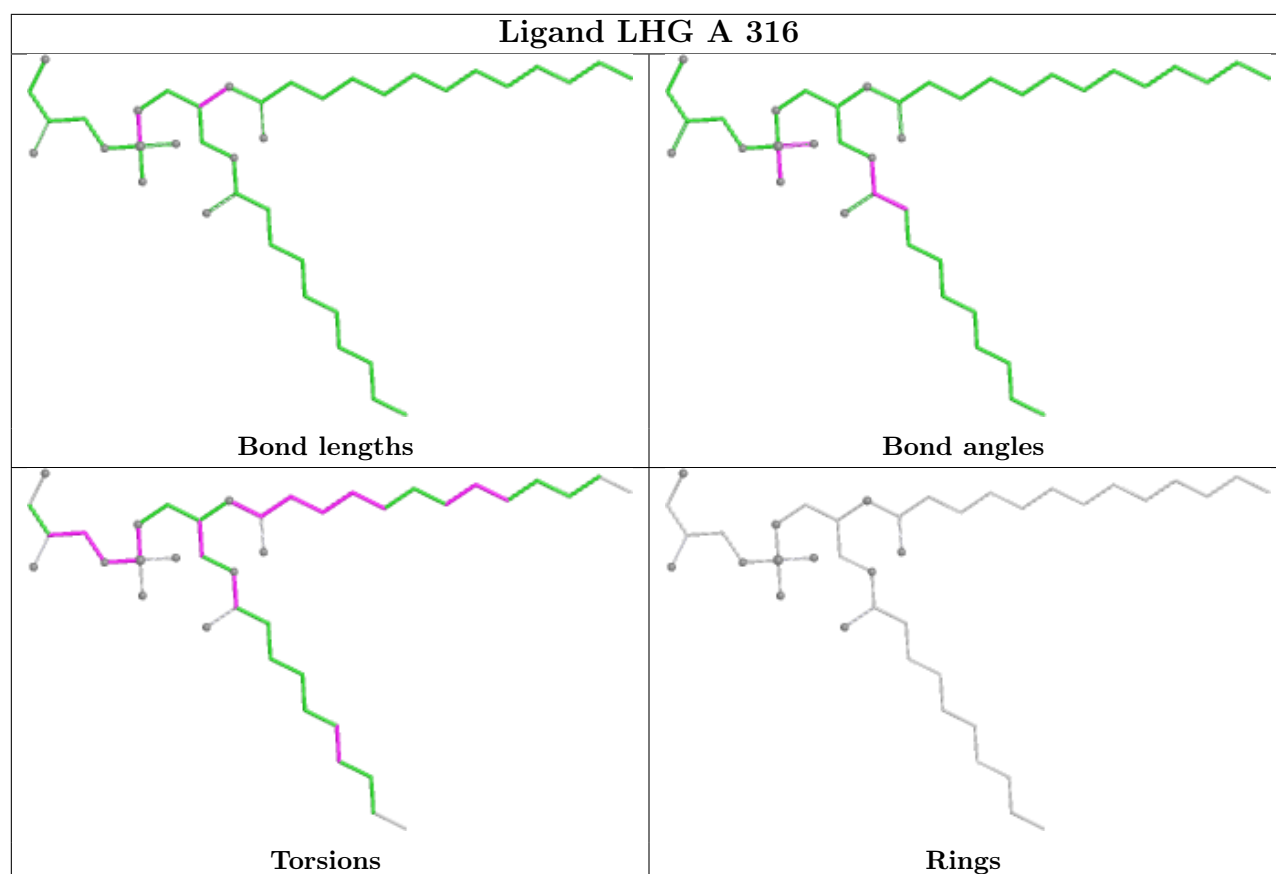
Bond angles

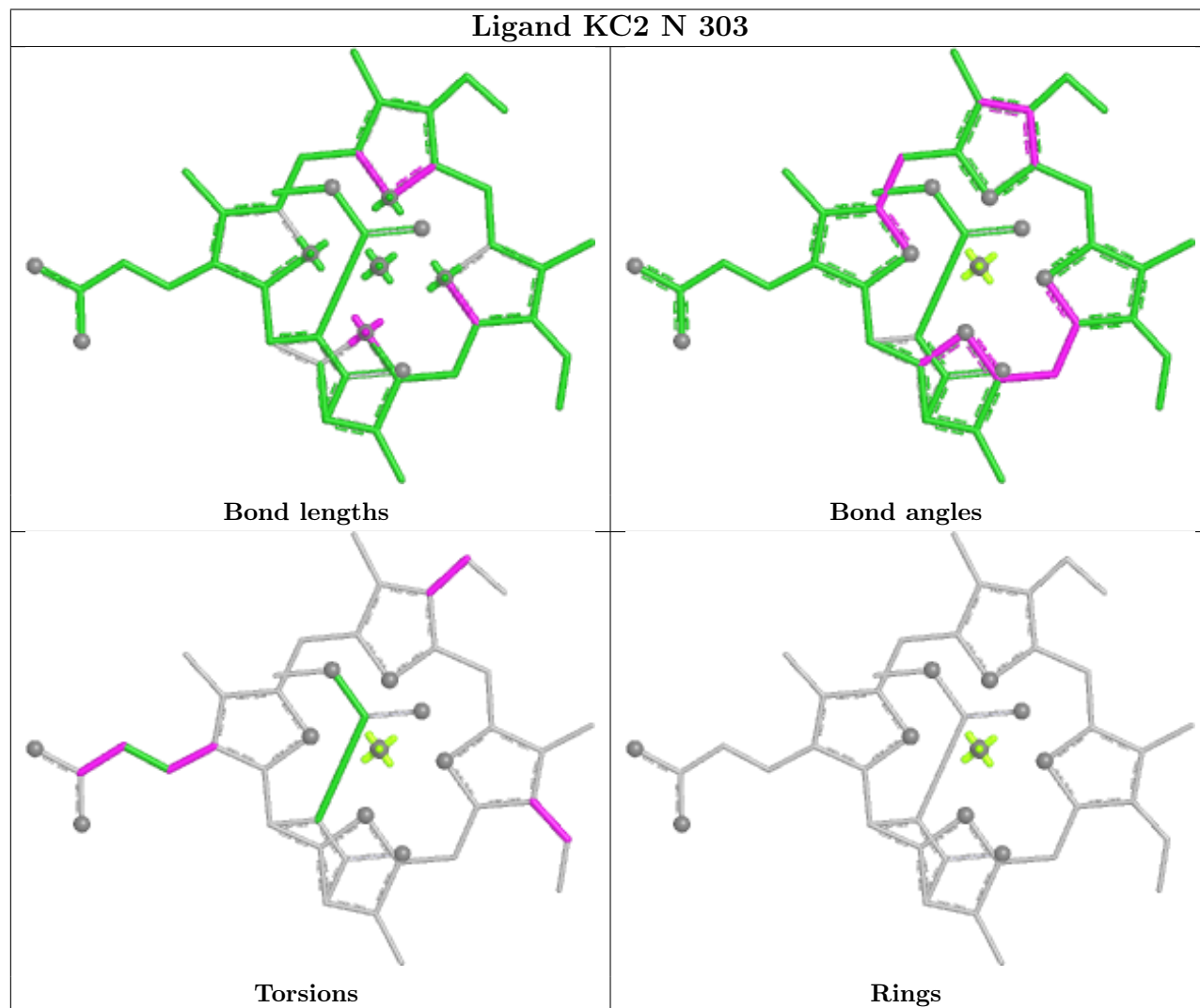
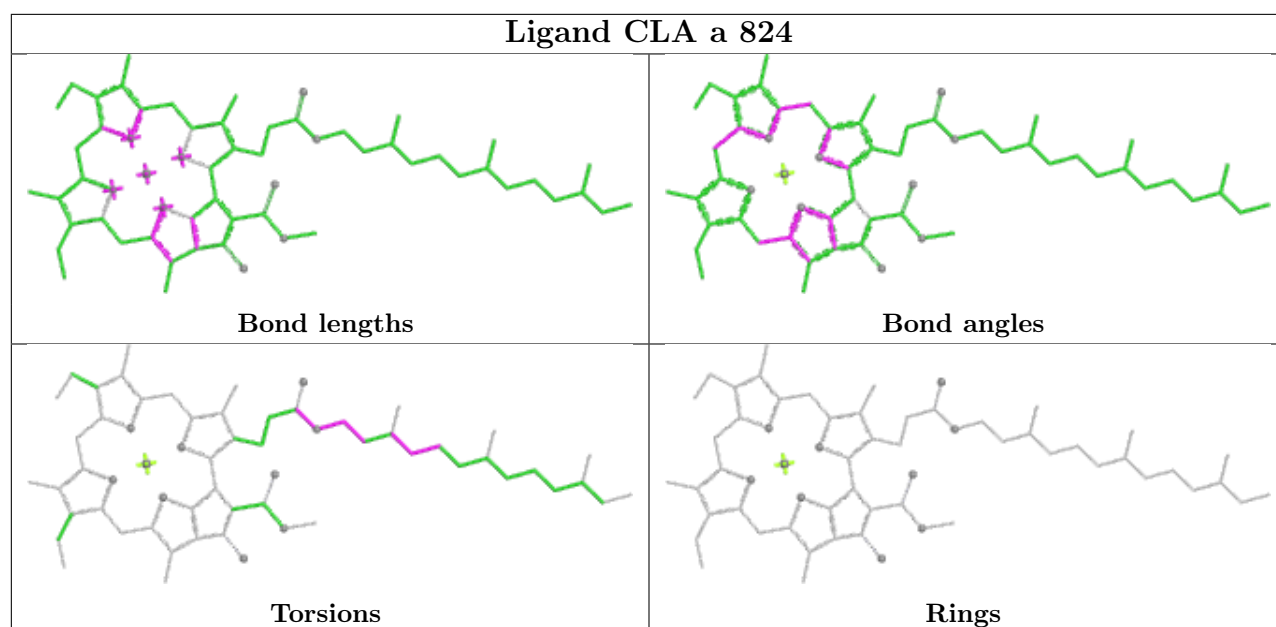


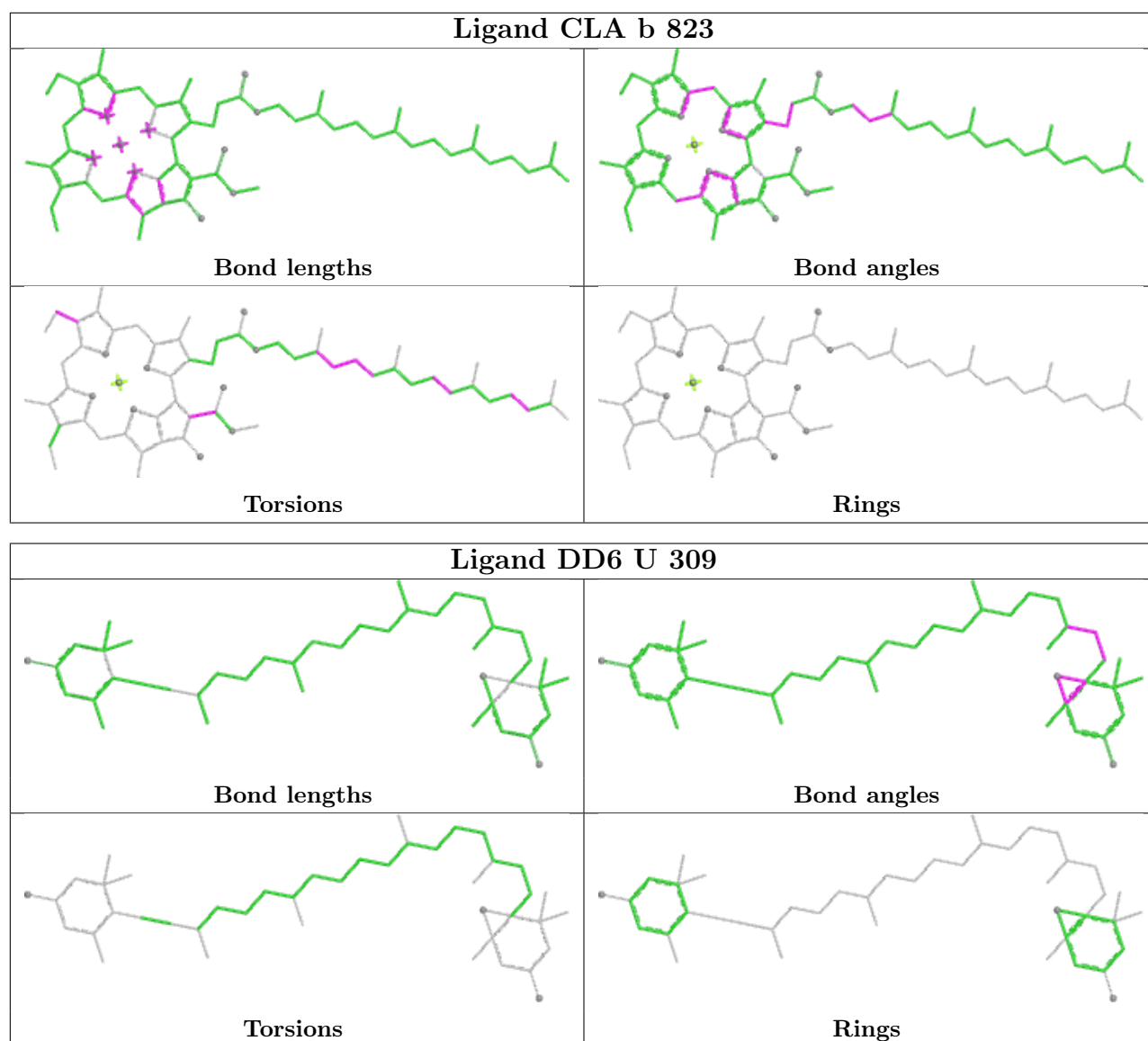
Torsions



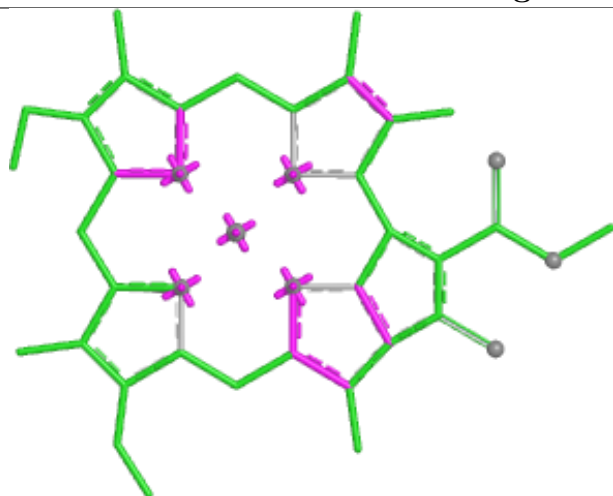
Rings



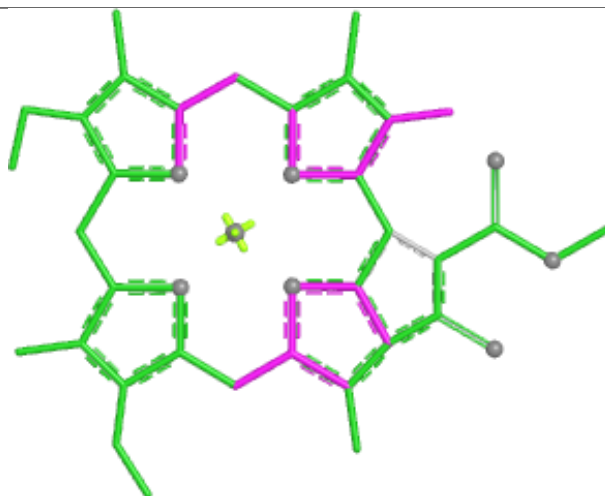




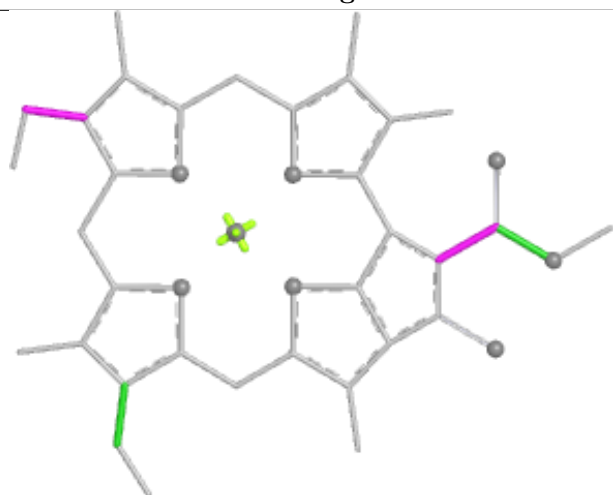
Ligand CLA N 312



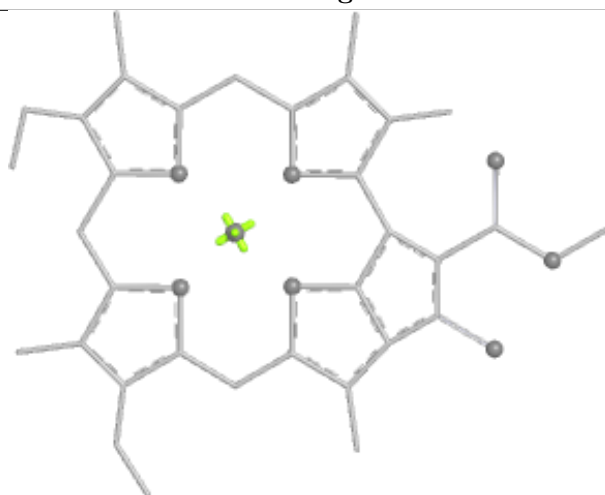
Bond lengths



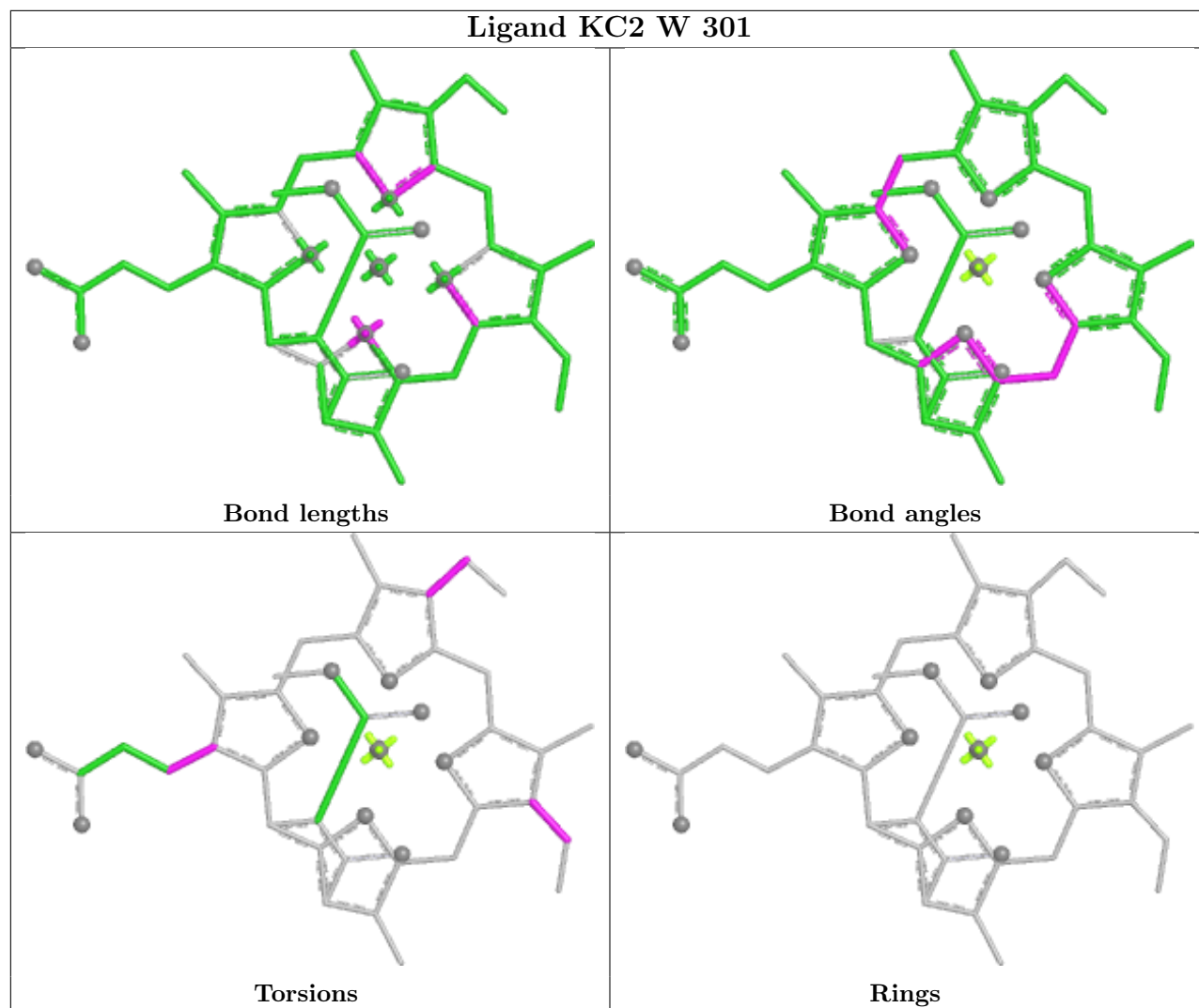
Bond angles



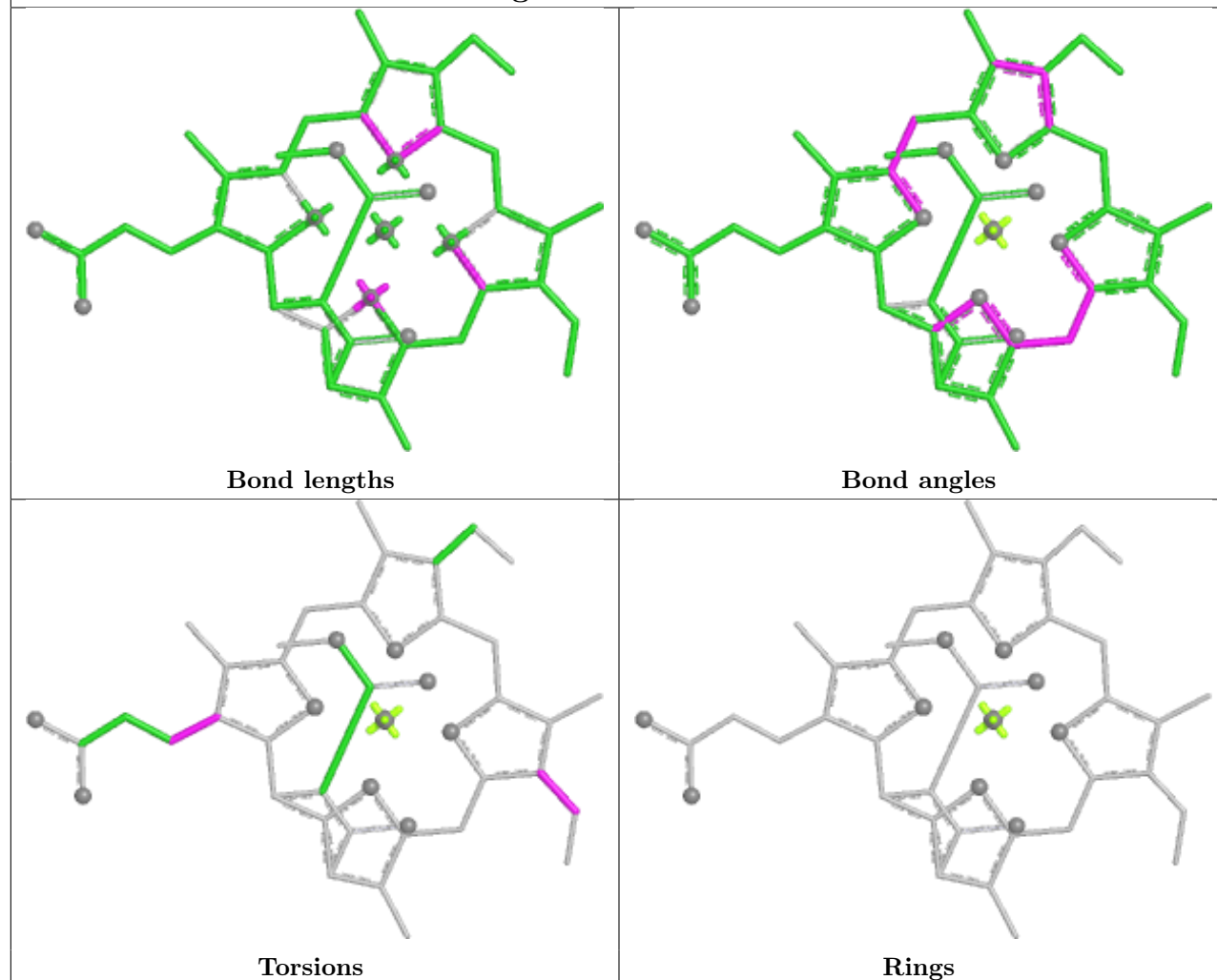
Torsions



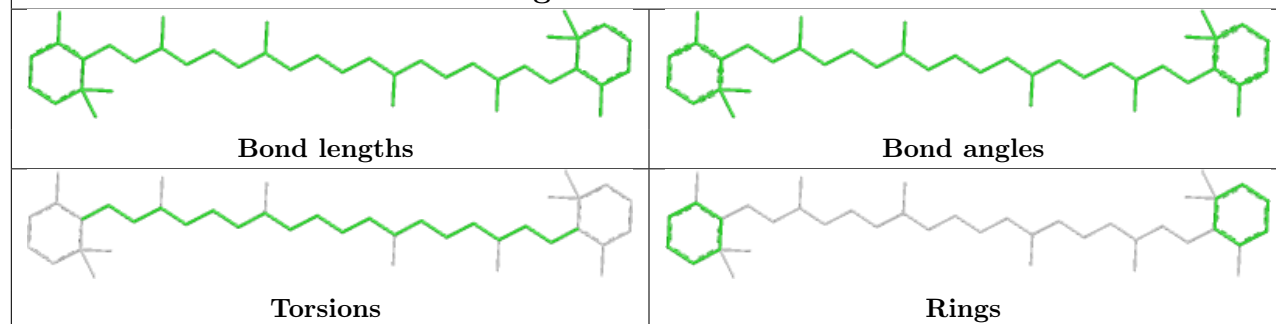
Rings

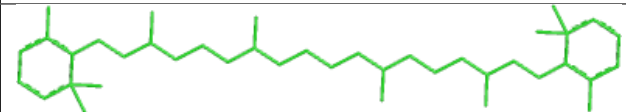
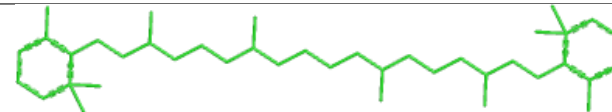
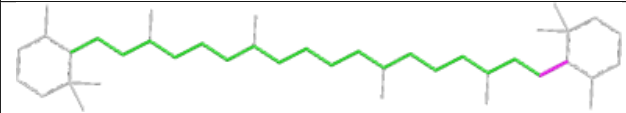
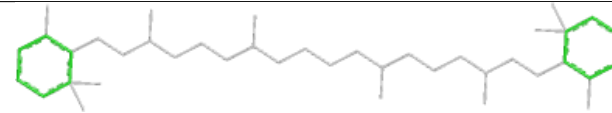


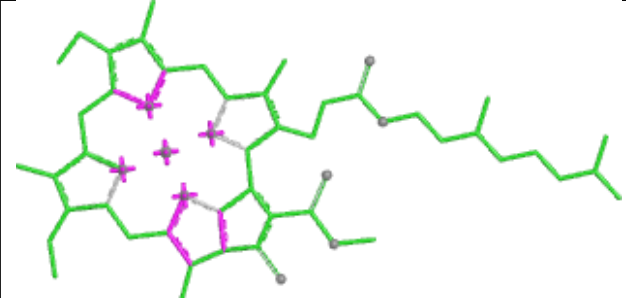
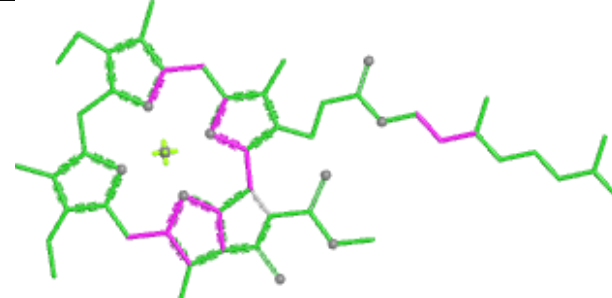
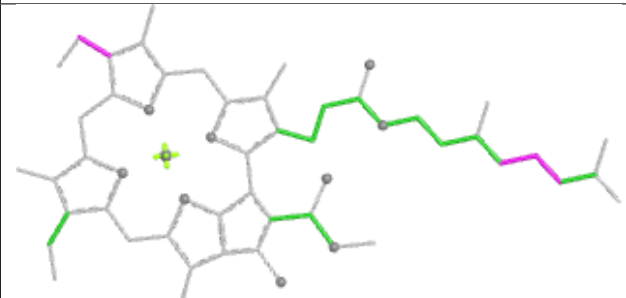
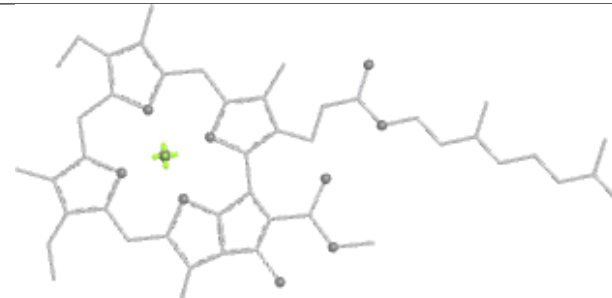
Ligand KC2 S 302

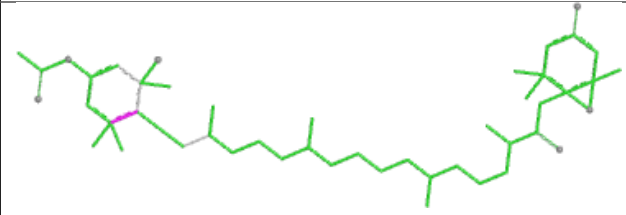
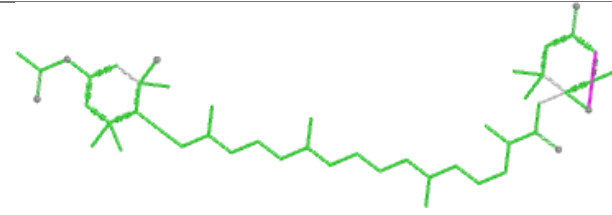
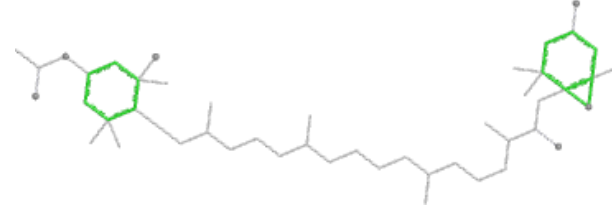


Ligand BCR b 843

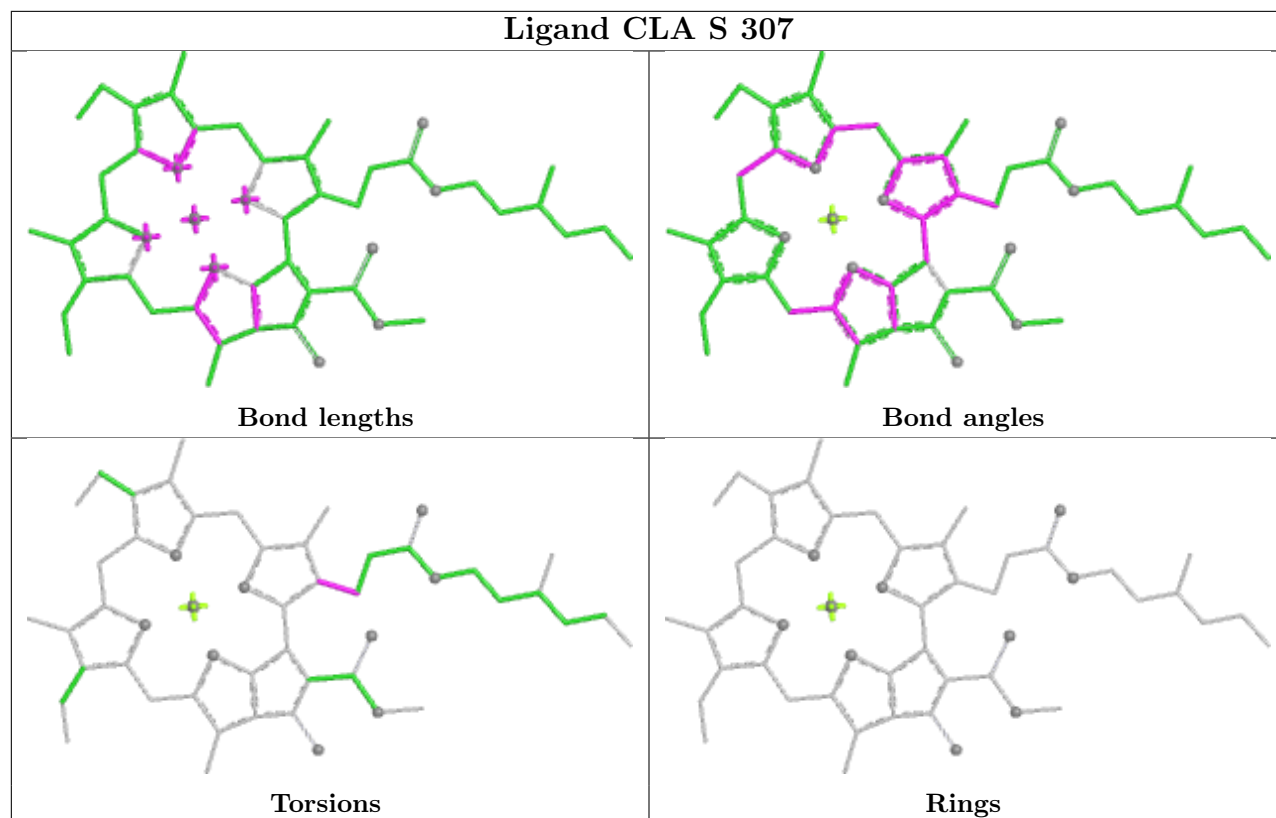


Ligand BCR r 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

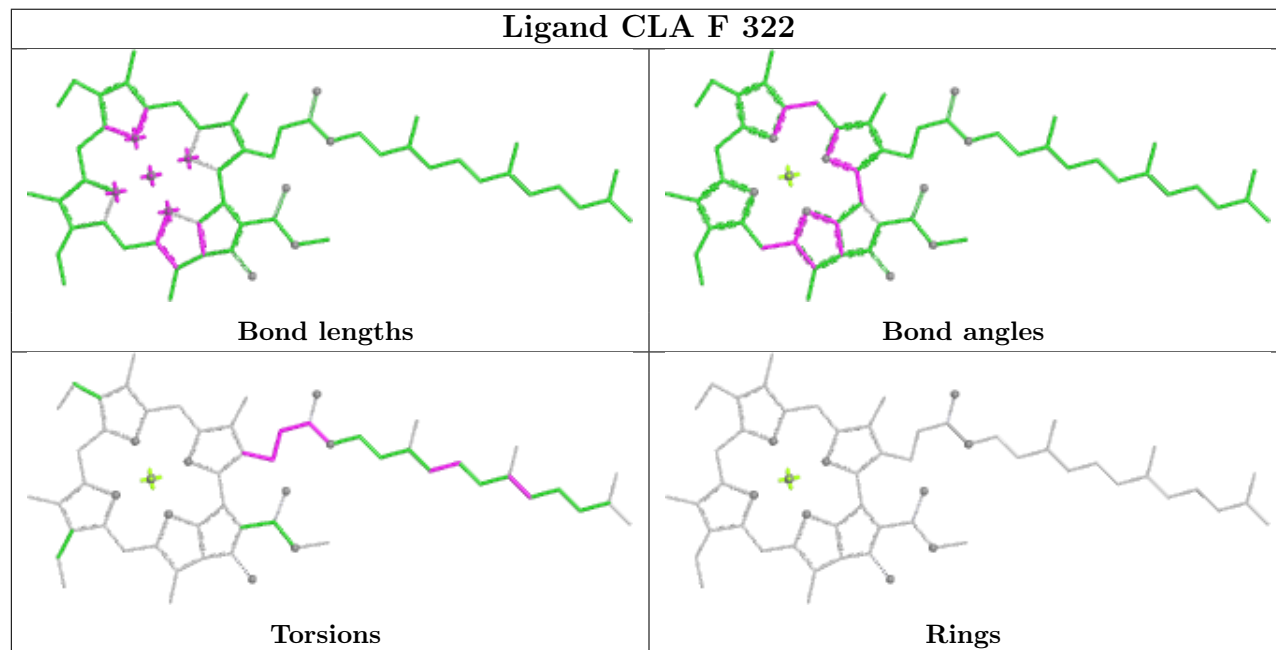
Ligand CLA a 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

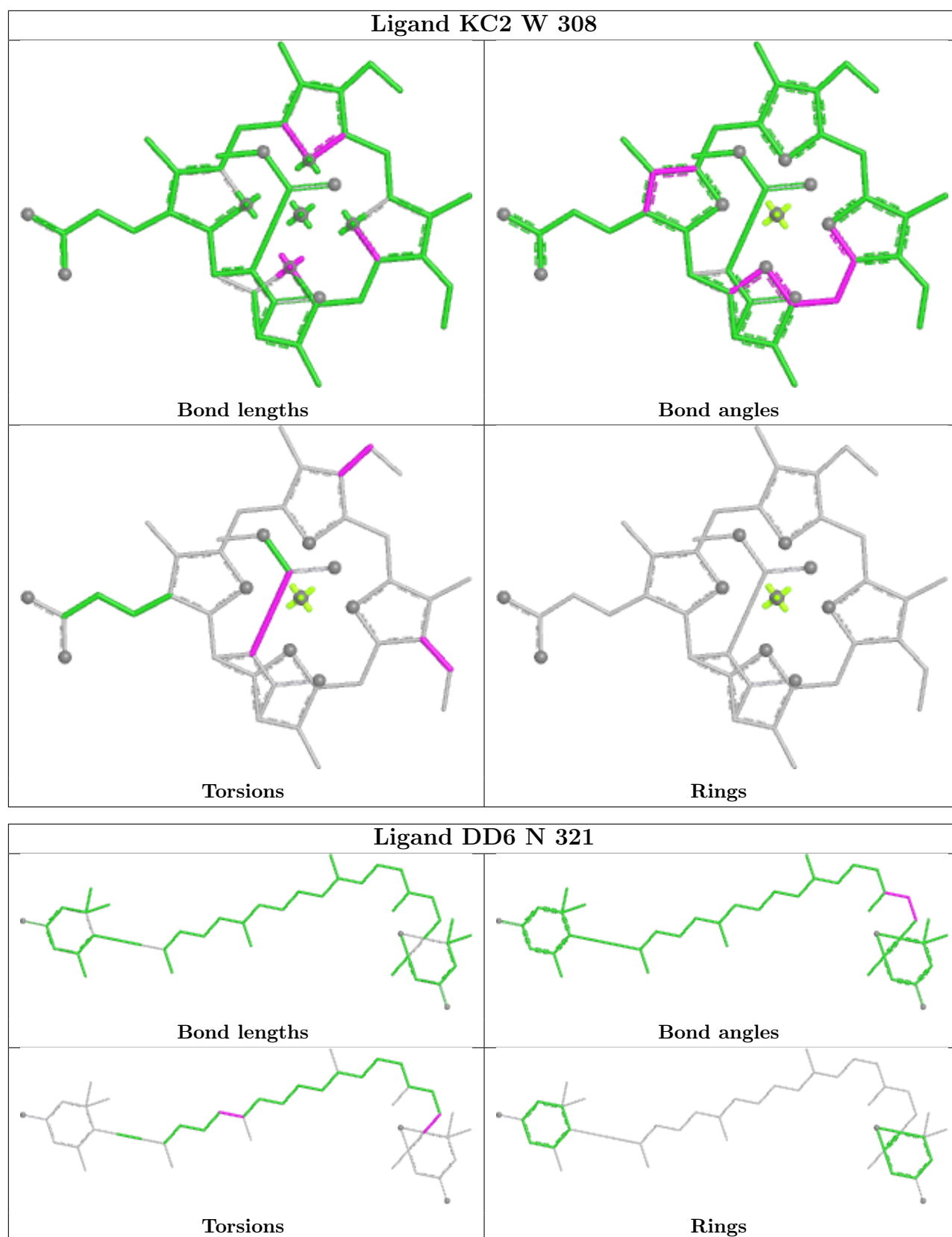
Ligand A86 W 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

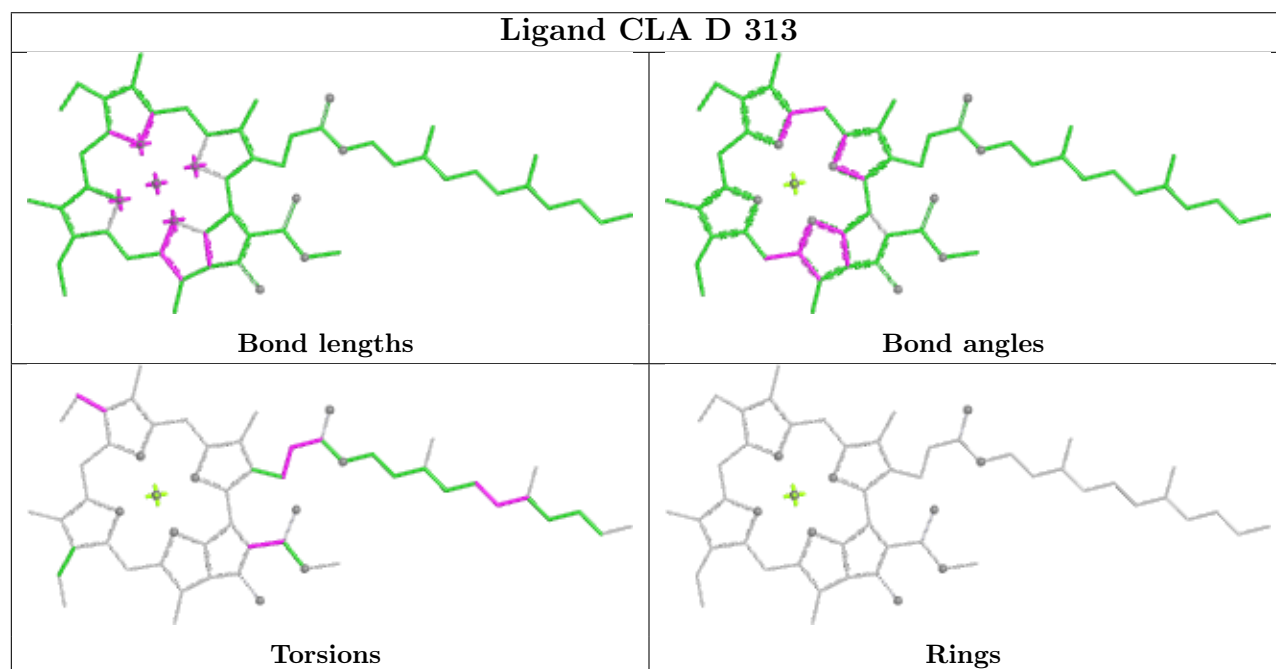
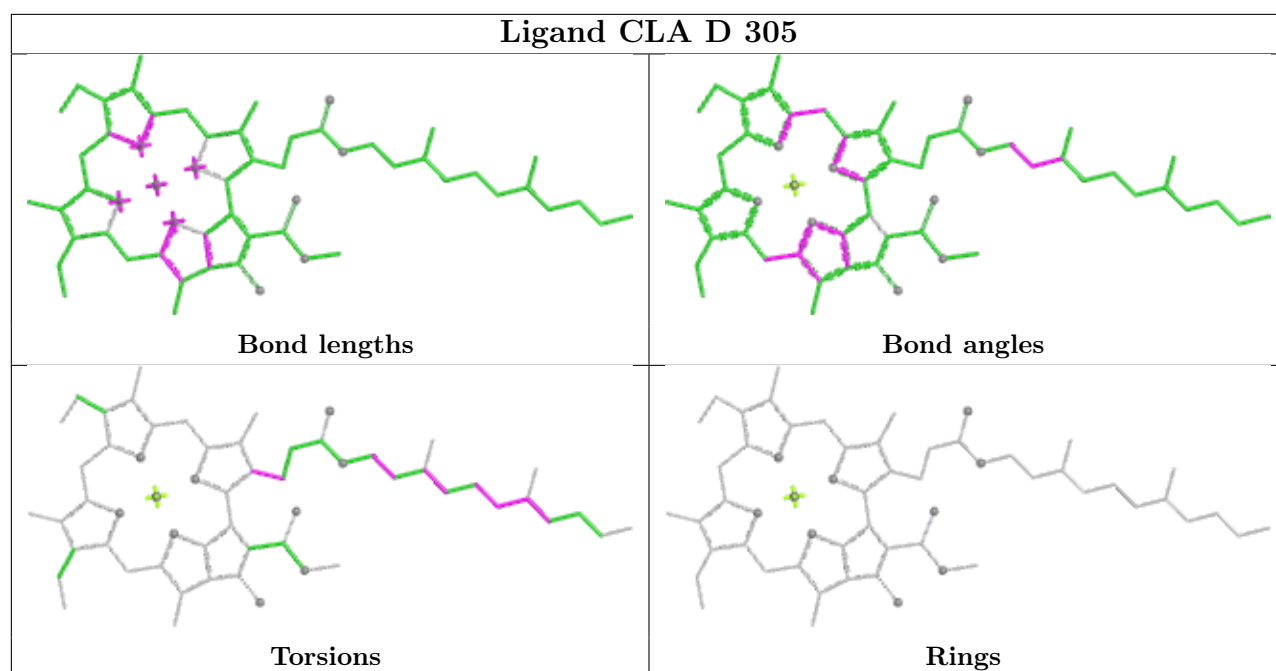
Ligand CLA S 307



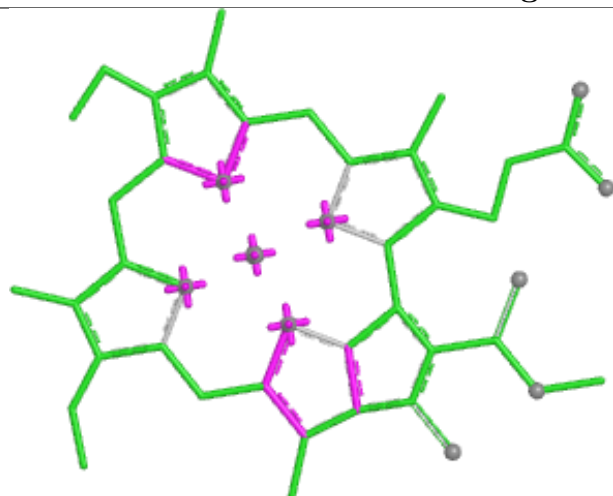
Ligand CLA F 322



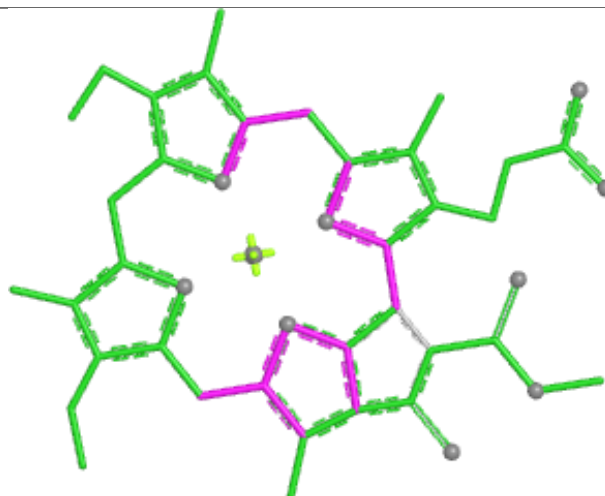




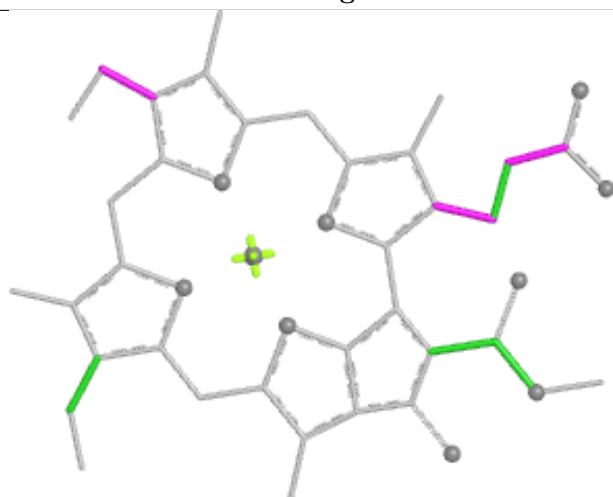
Ligand CLA I 304



Bond lengths



Bond angles

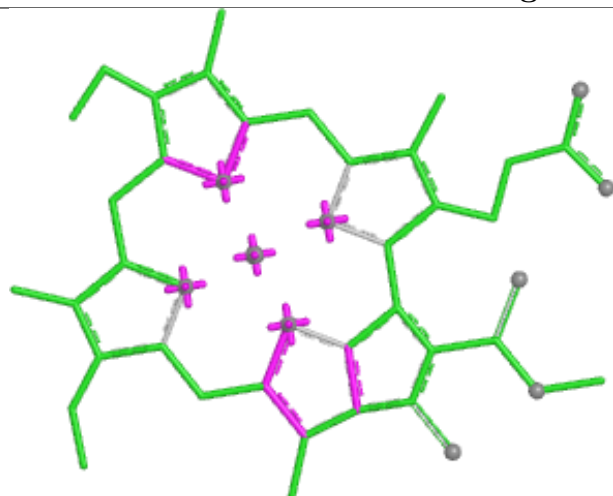


Torsions

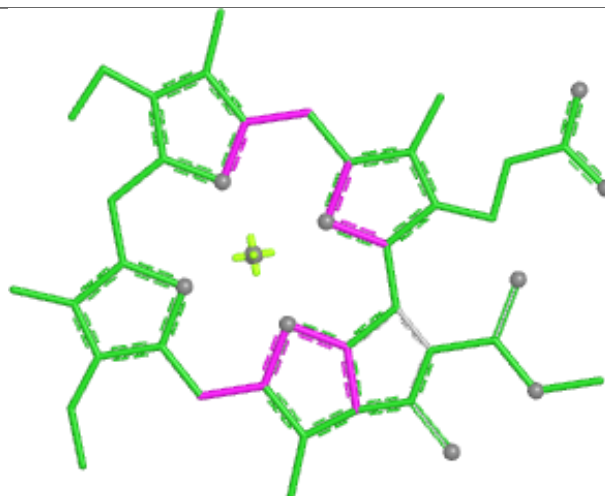


Rings

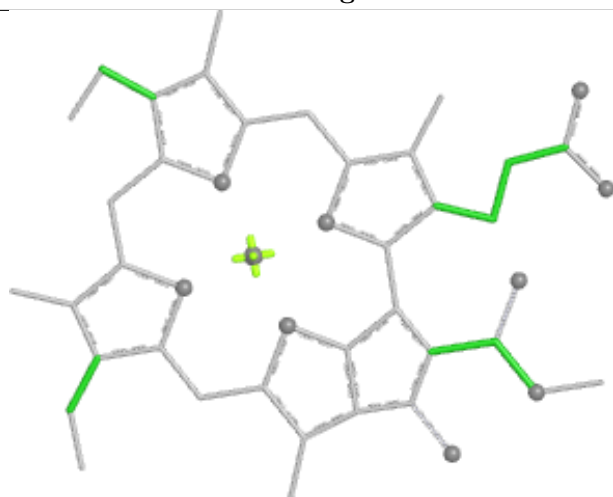
Ligand CLA r 202



Bond lengths



Bond angles

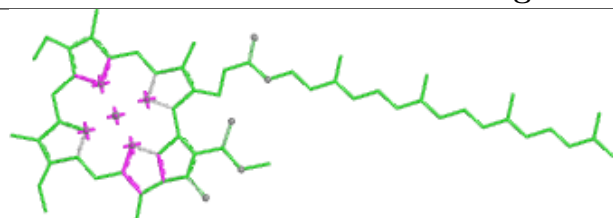


Torsions

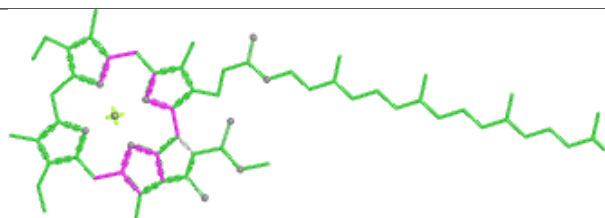


Rings

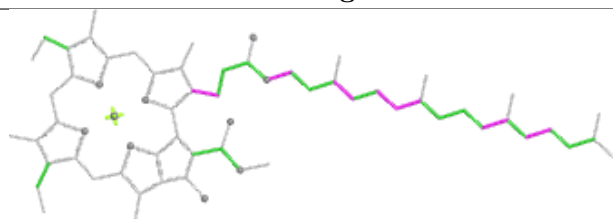
Ligand CLA A 306



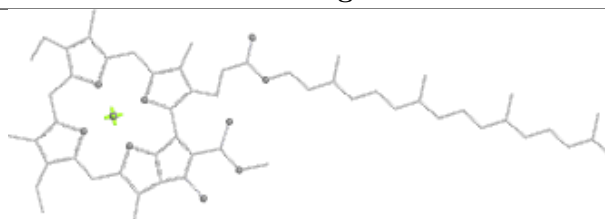
Bond lengths



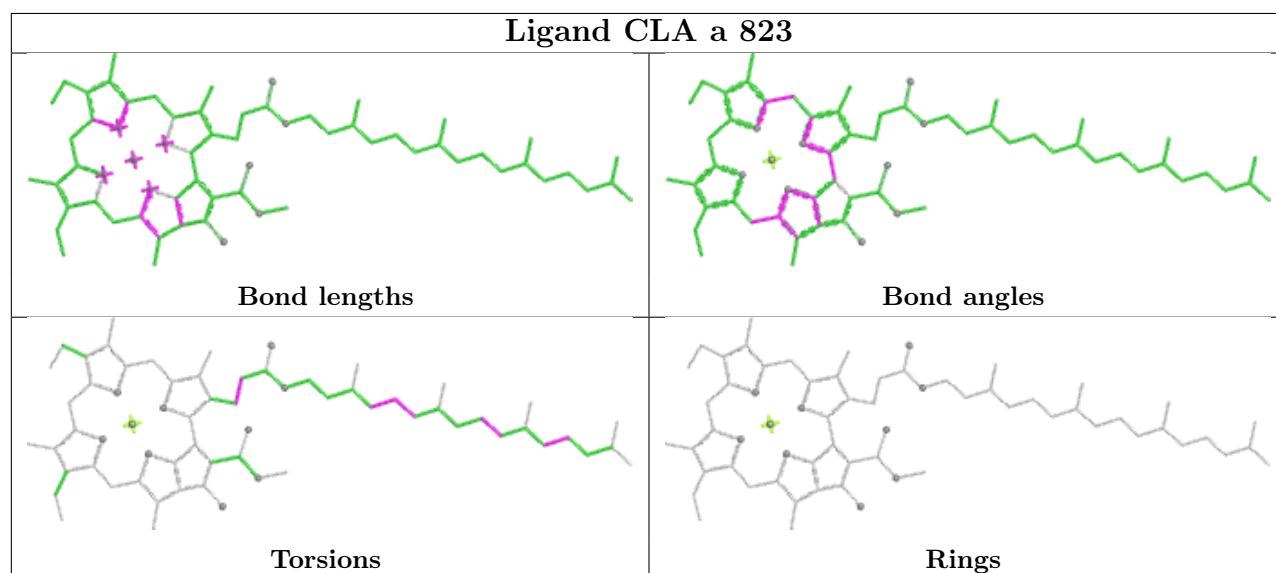
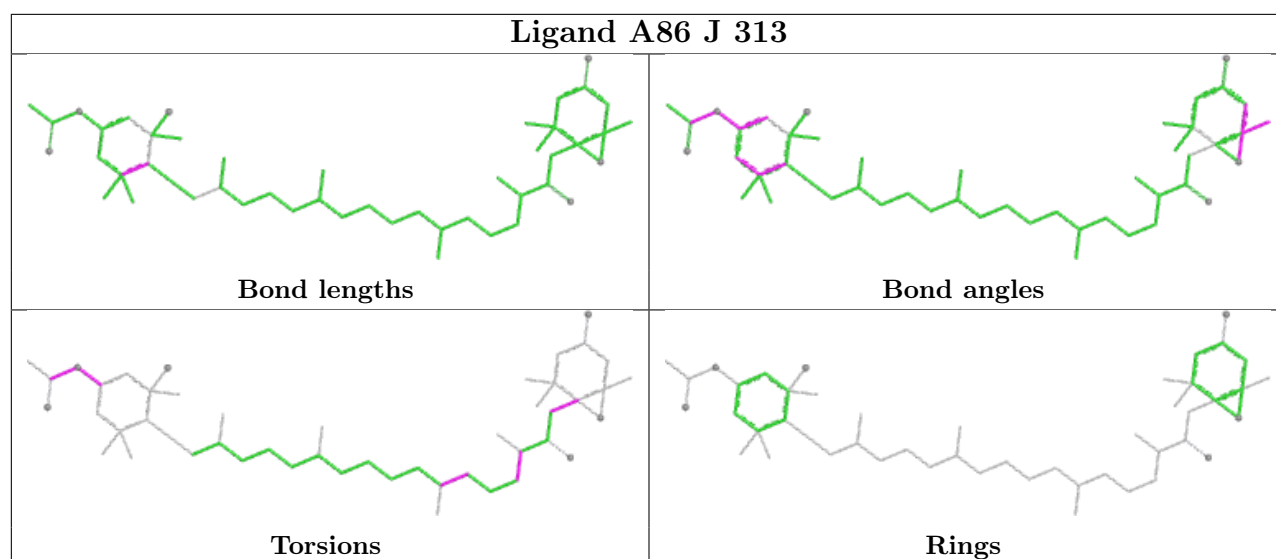
Bond angles



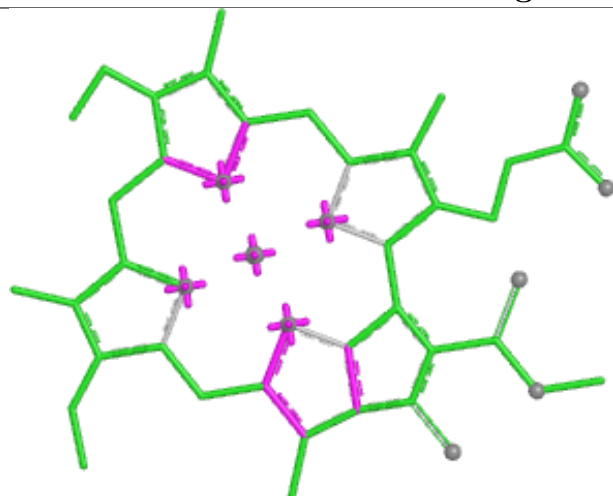
Torsions



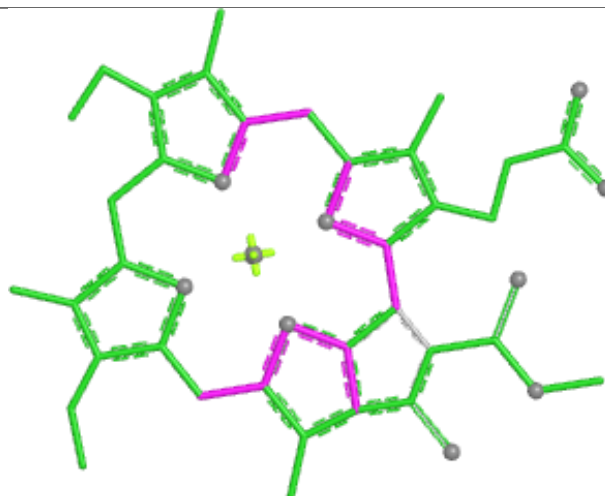
Rings



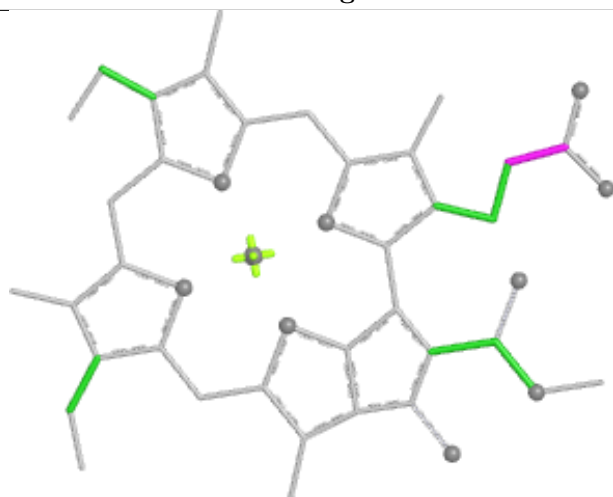
Ligand CLA P 308



Bond lengths



Bond angles

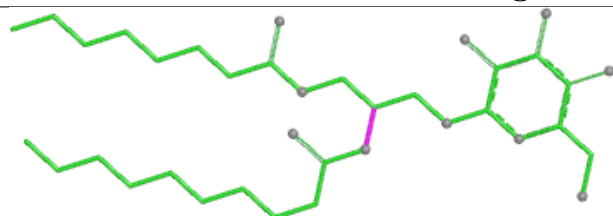


Torsions

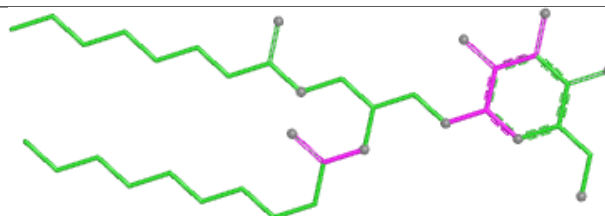


Rings

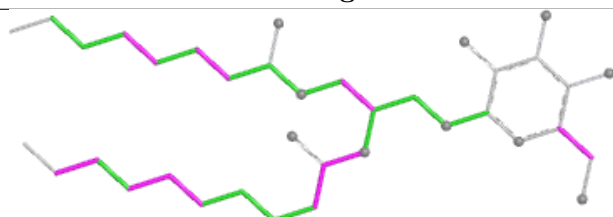
Ligand LMG L 320



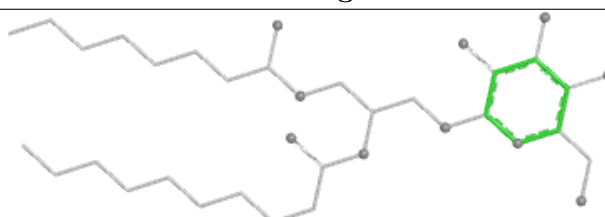
Bond lengths



Bond angles

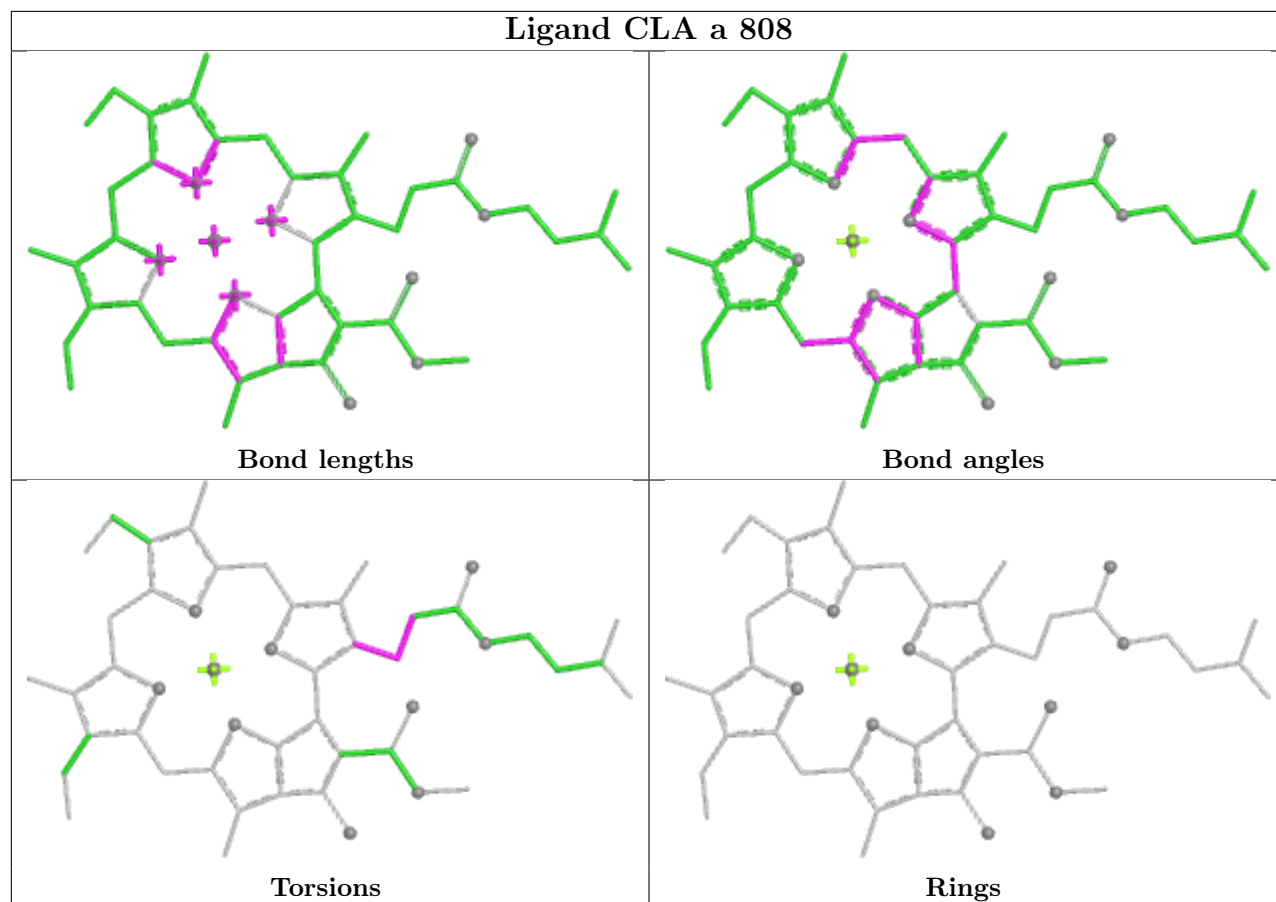


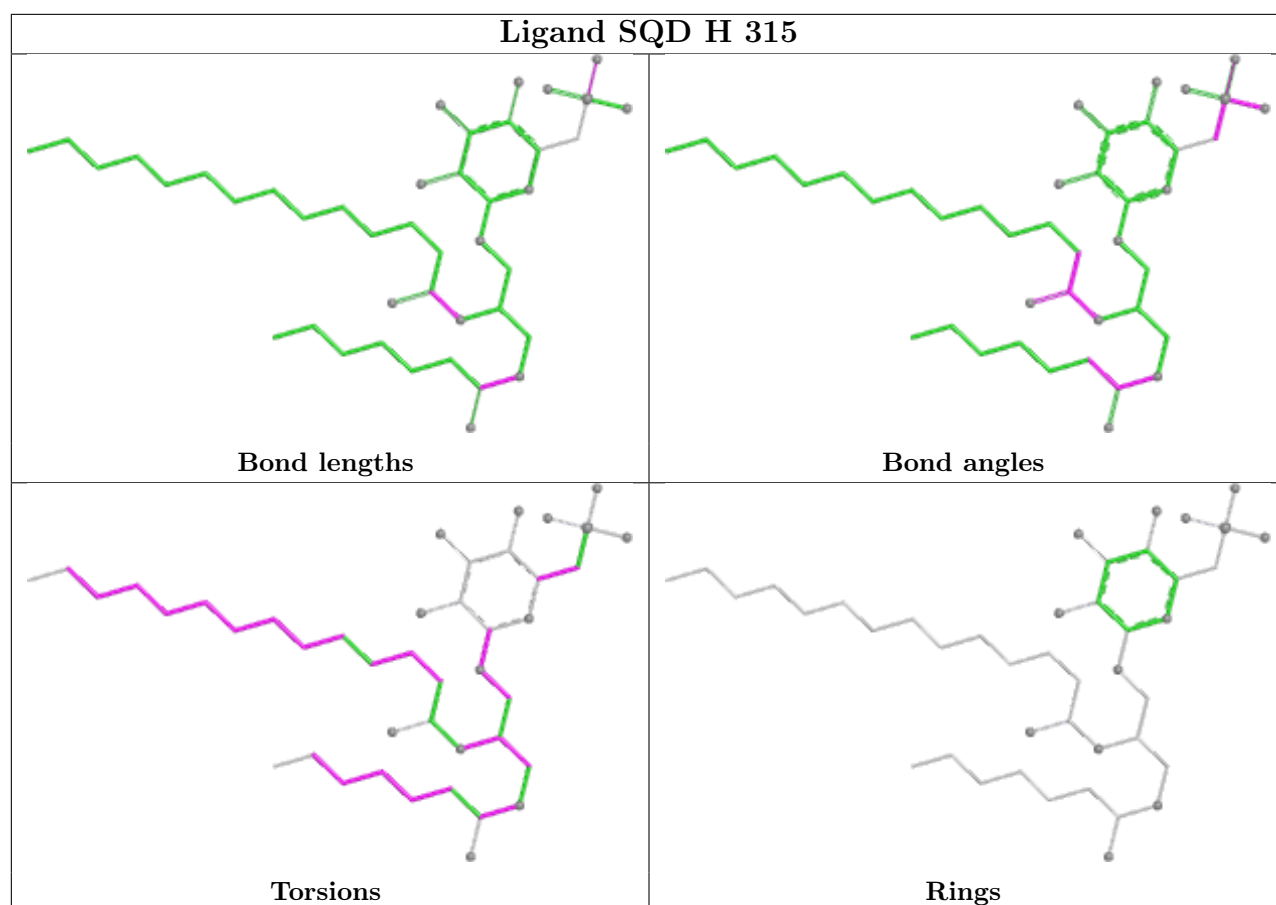
Torsions



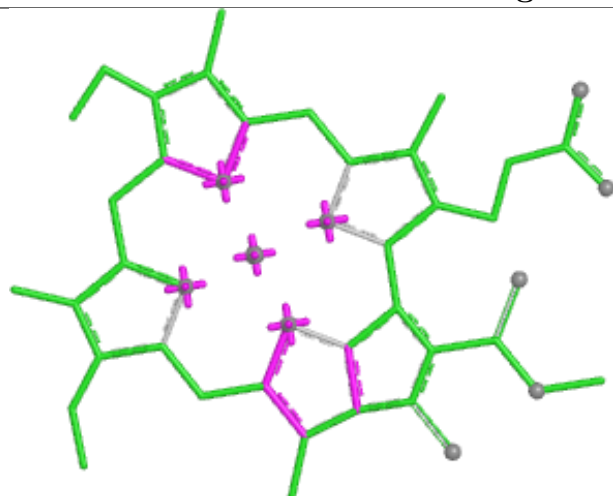
Rings

Ligand CLA a 808

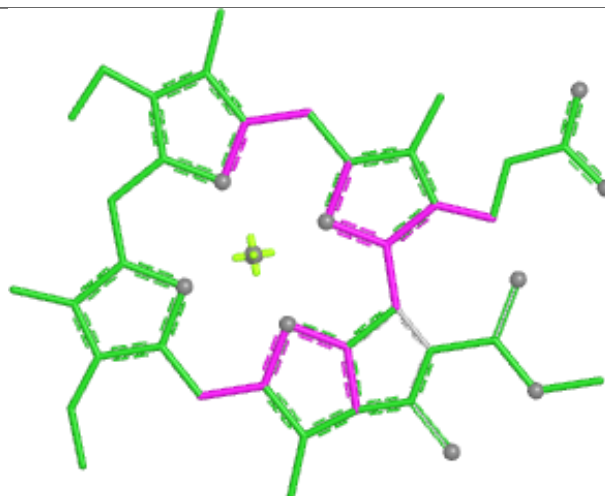




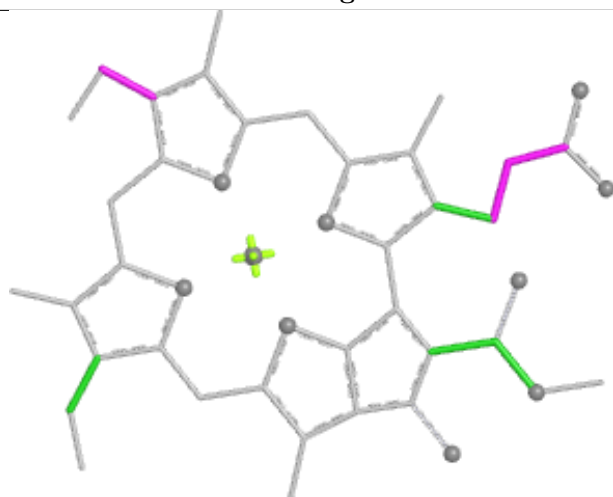
Ligand CLA L 301



Bond lengths



Bond angles

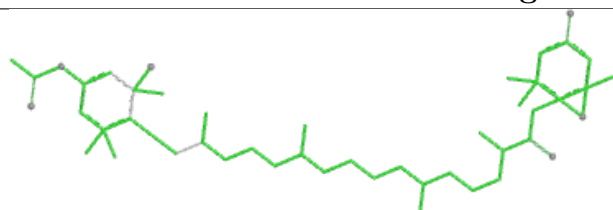


Torsions

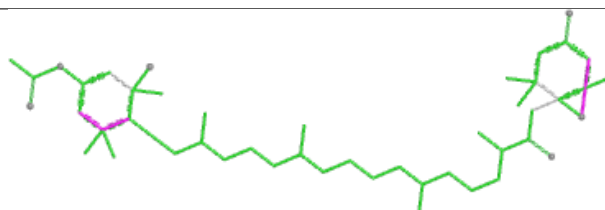


Rings

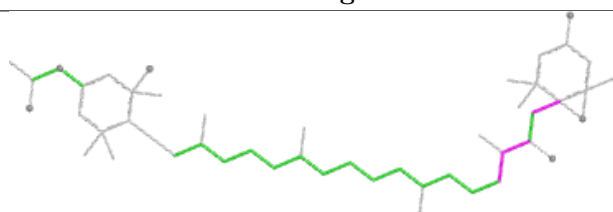
Ligand A86 O 311



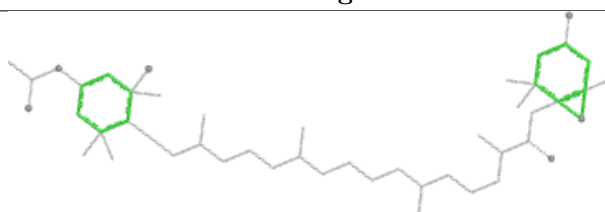
Bond lengths



Bond angles

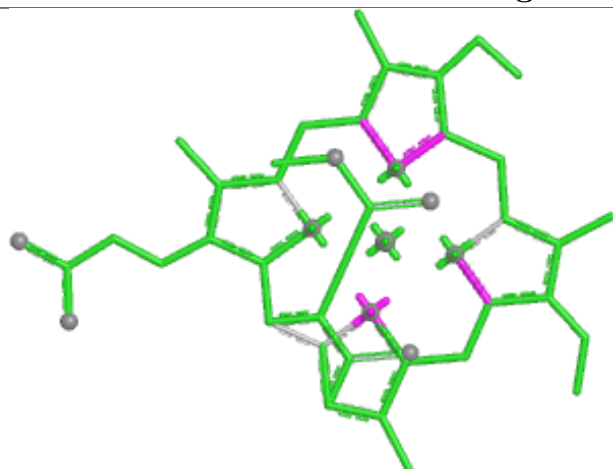


Torsions

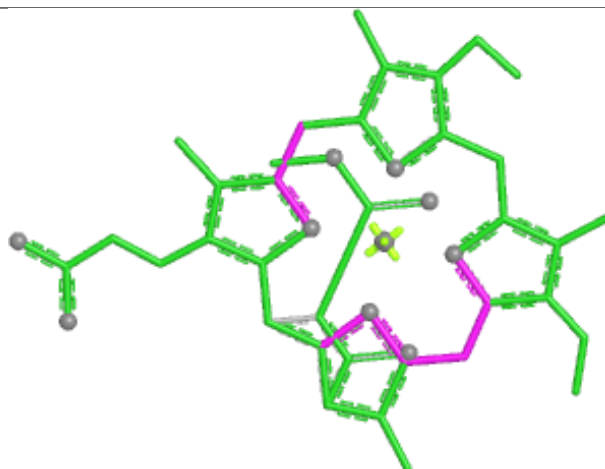


Rings

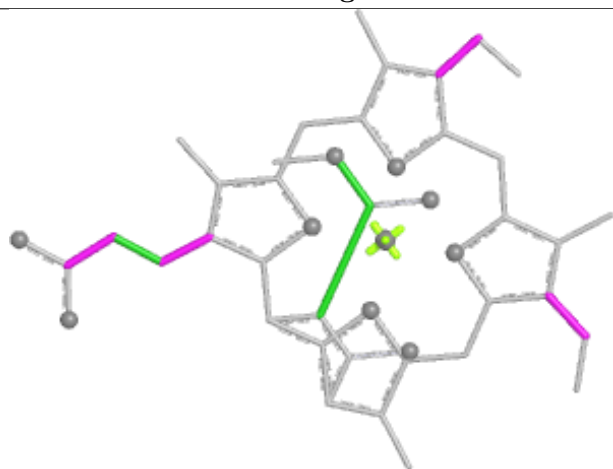
Ligand KC2 O 302



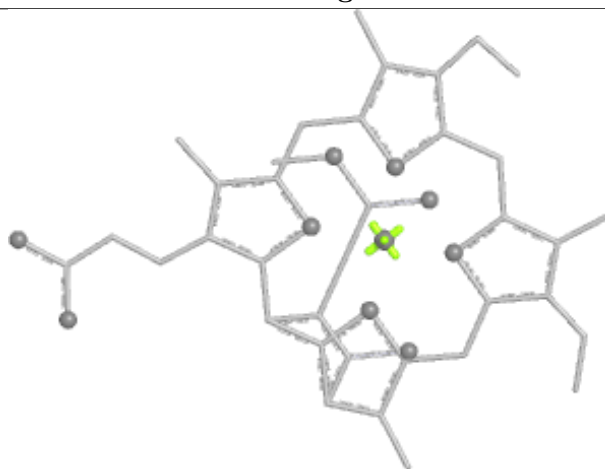
Bond lengths



Bond angles

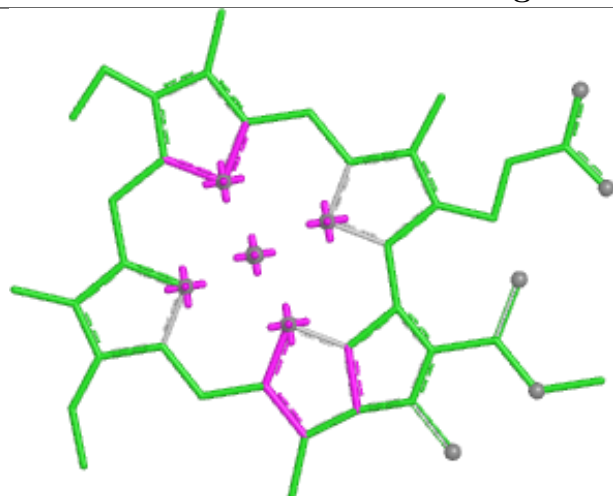


Torsions

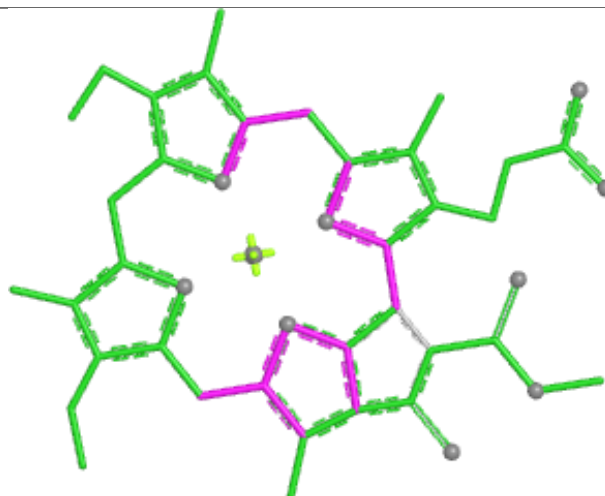


Rings

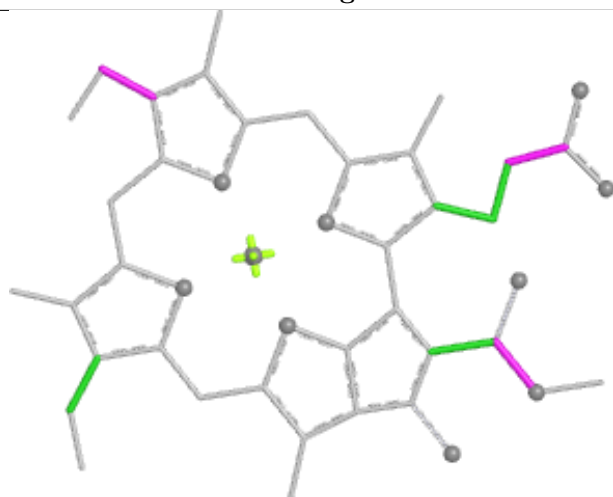
Ligand CLA H 305



Bond lengths



Bond angles

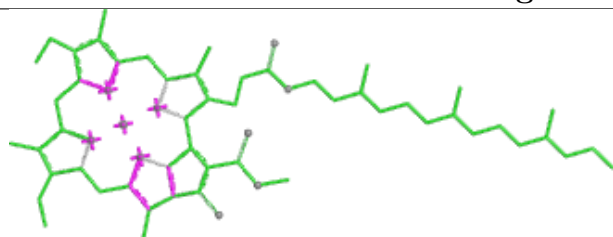


Torsions

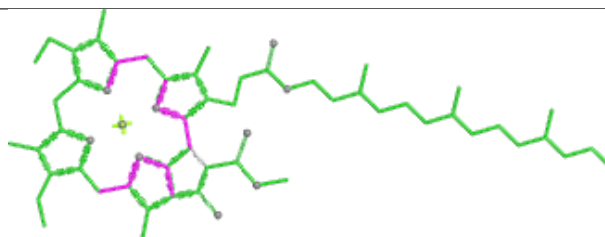


Rings

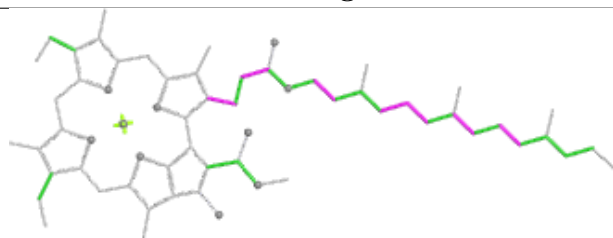
Ligand CLA F 303



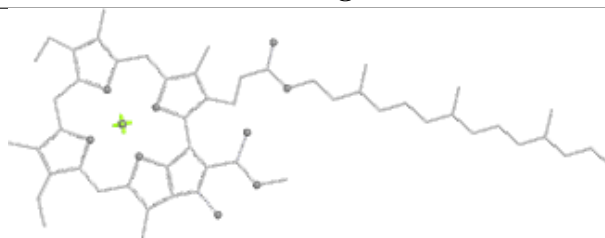
Bond lengths



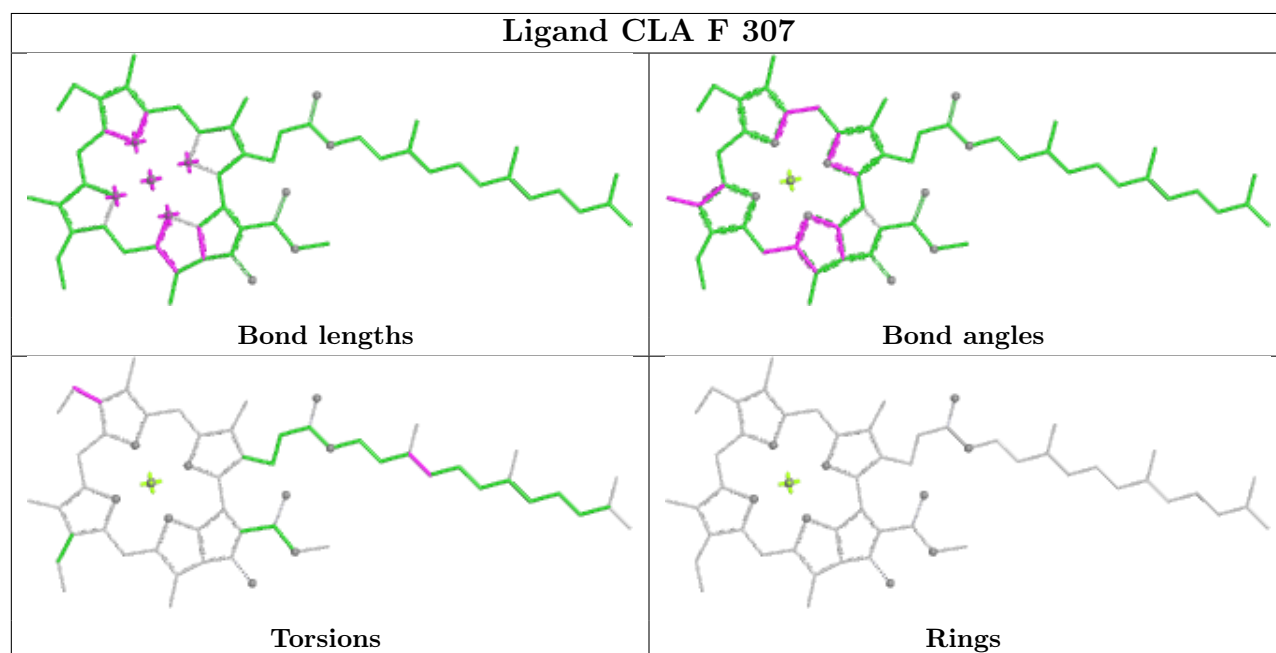
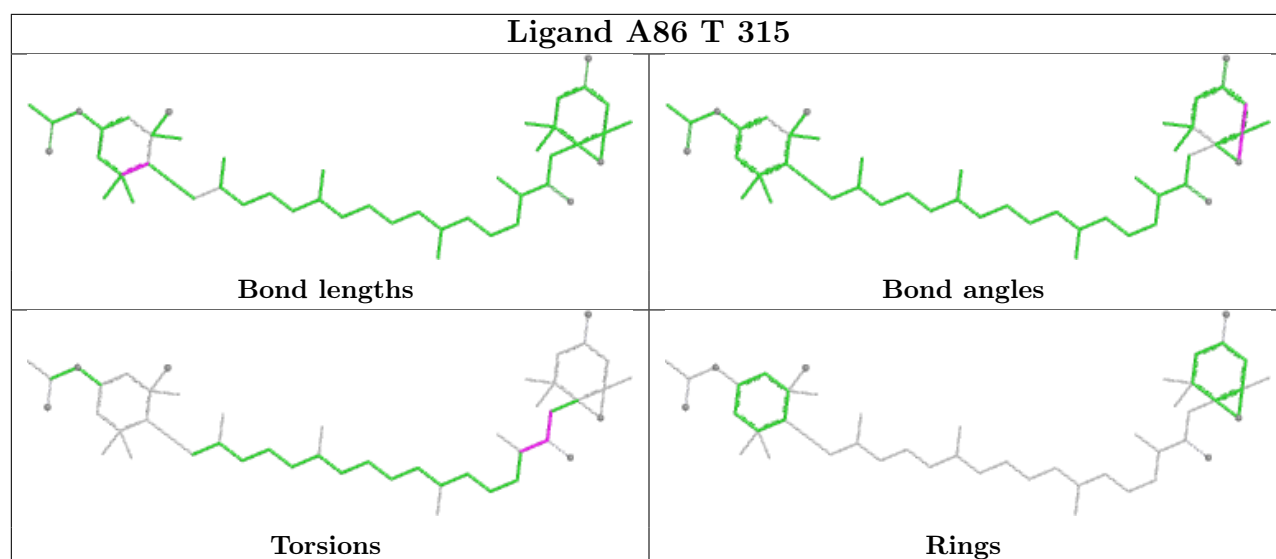
Bond angles

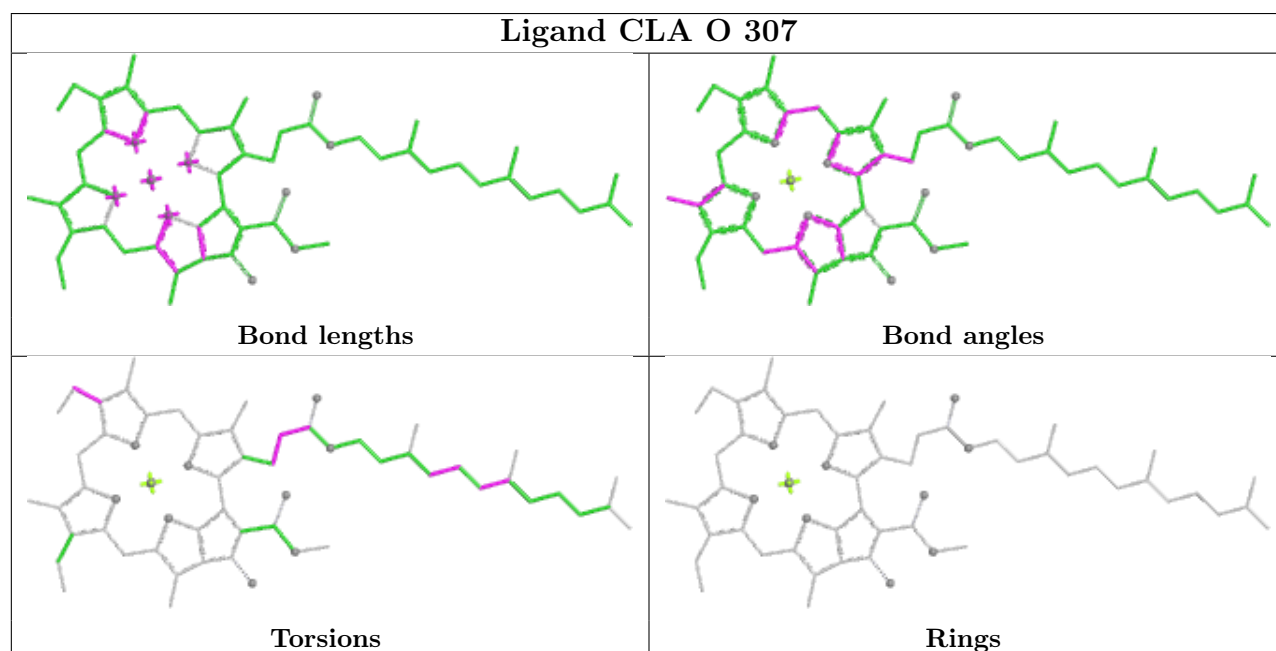
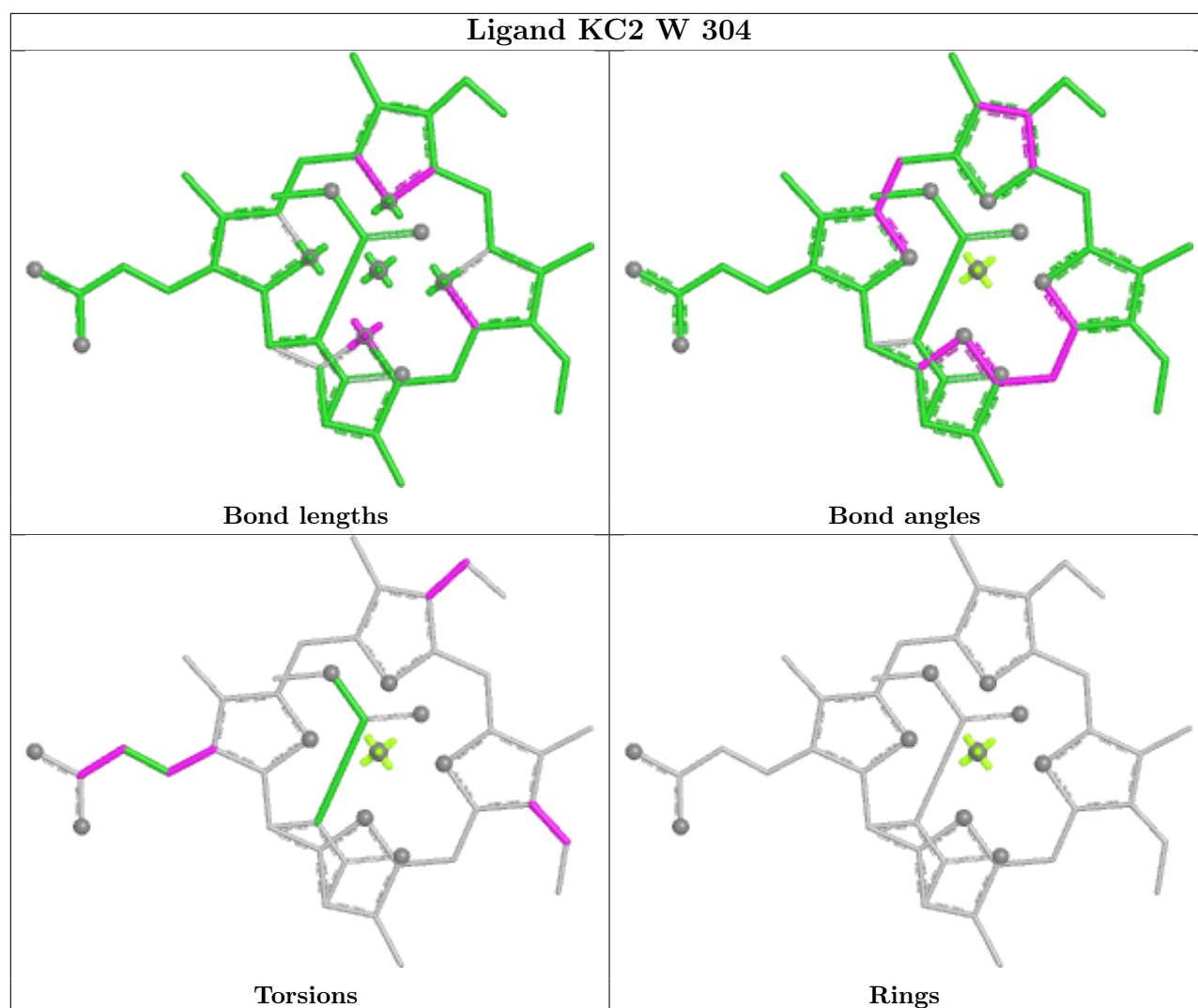


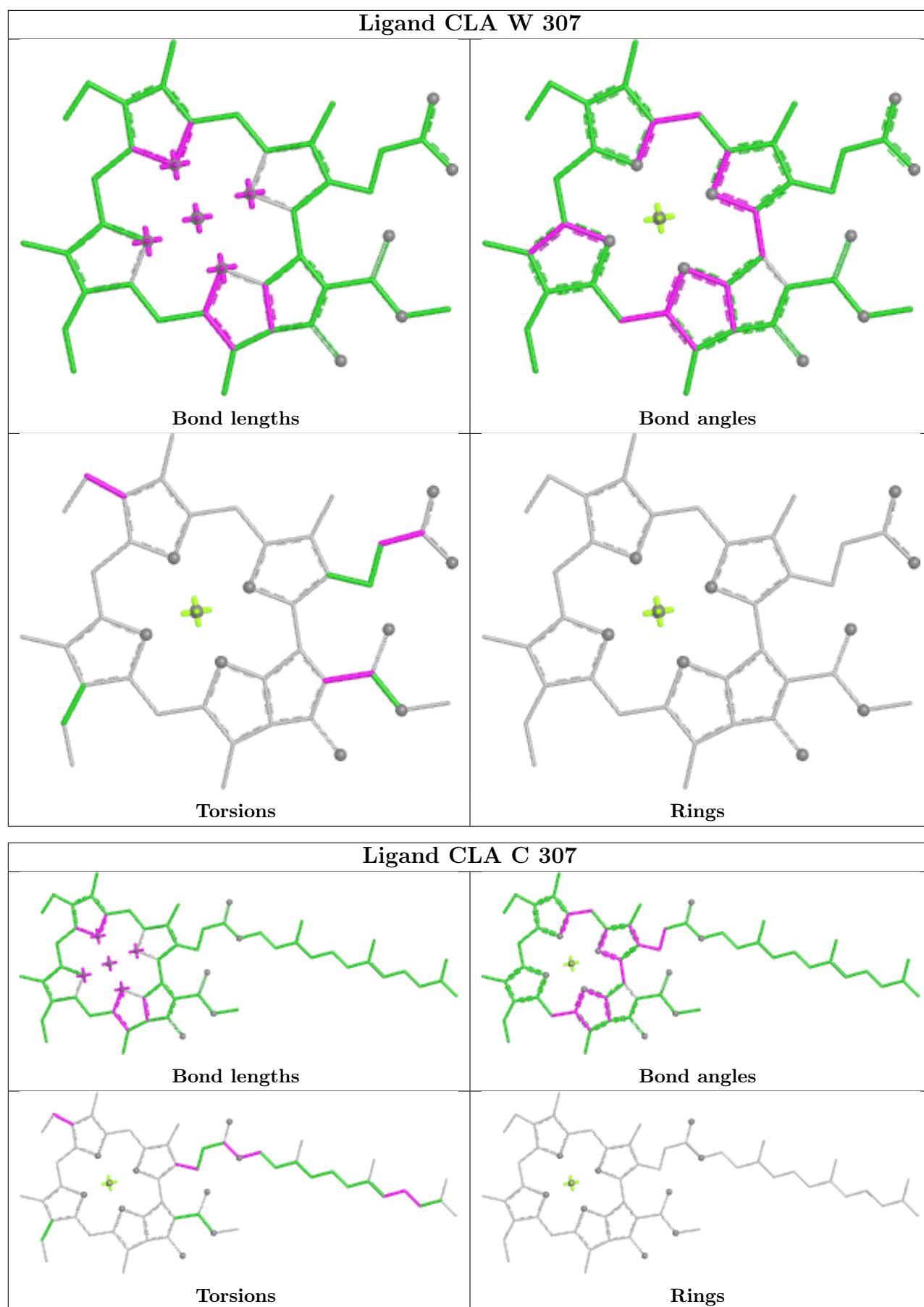
Torsions



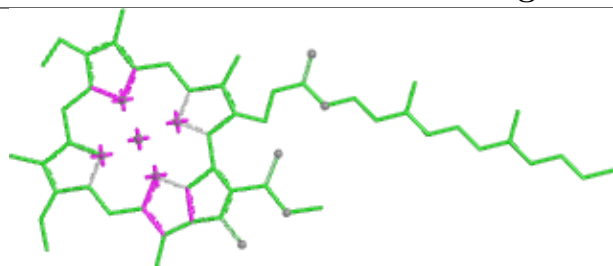
Rings



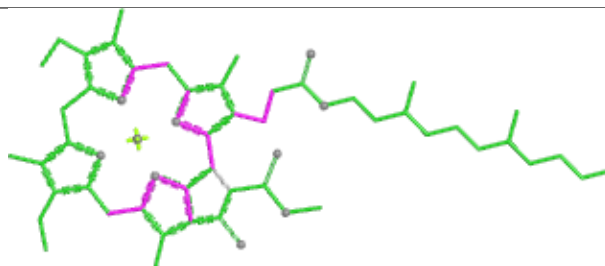




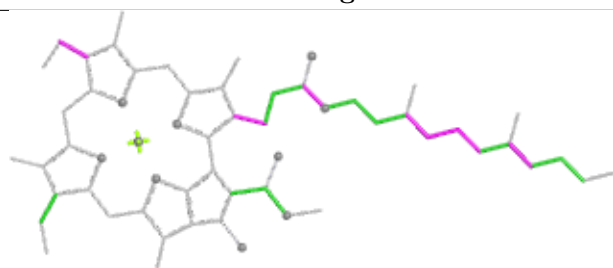
Ligand CLA J 312



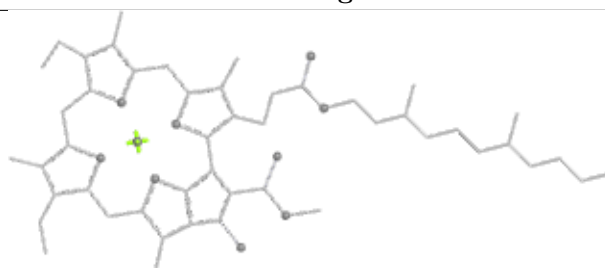
Bond lengths



Bond angles

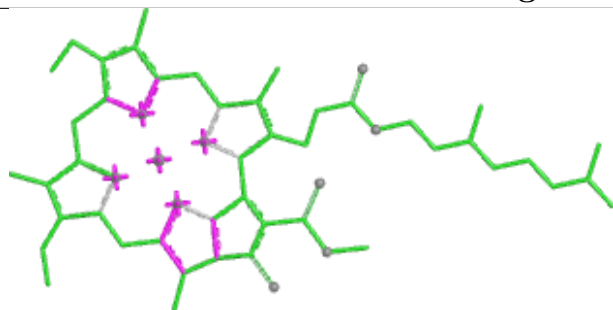


Torsions

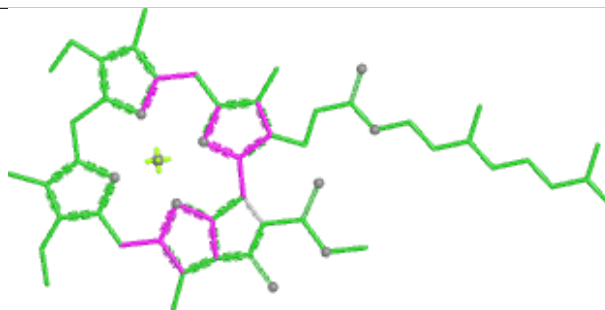


Rings

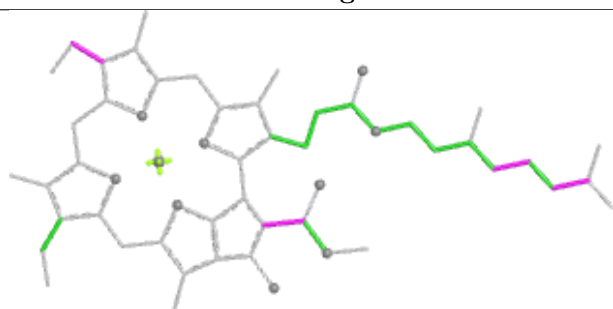
Ligand CLA a 837



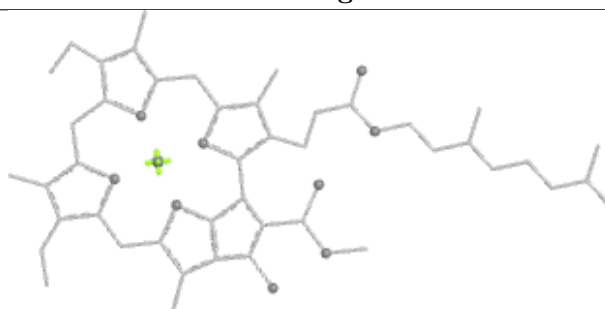
Bond lengths



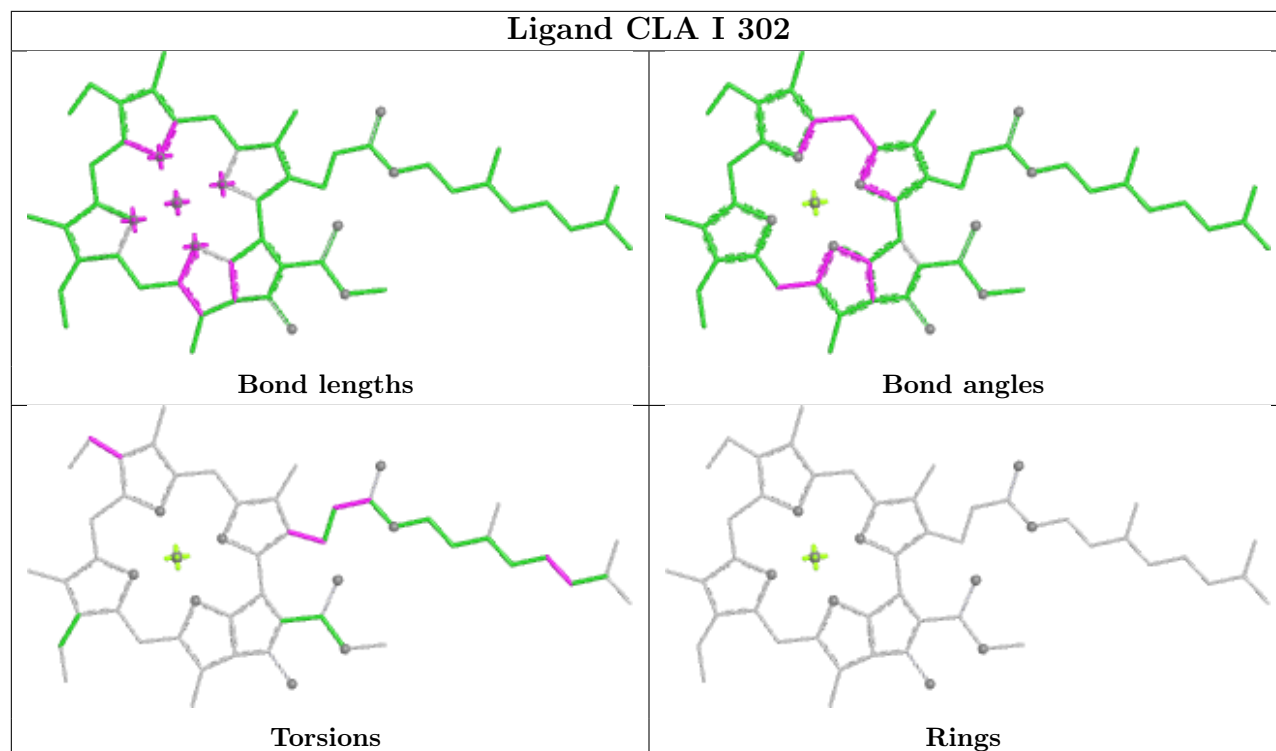
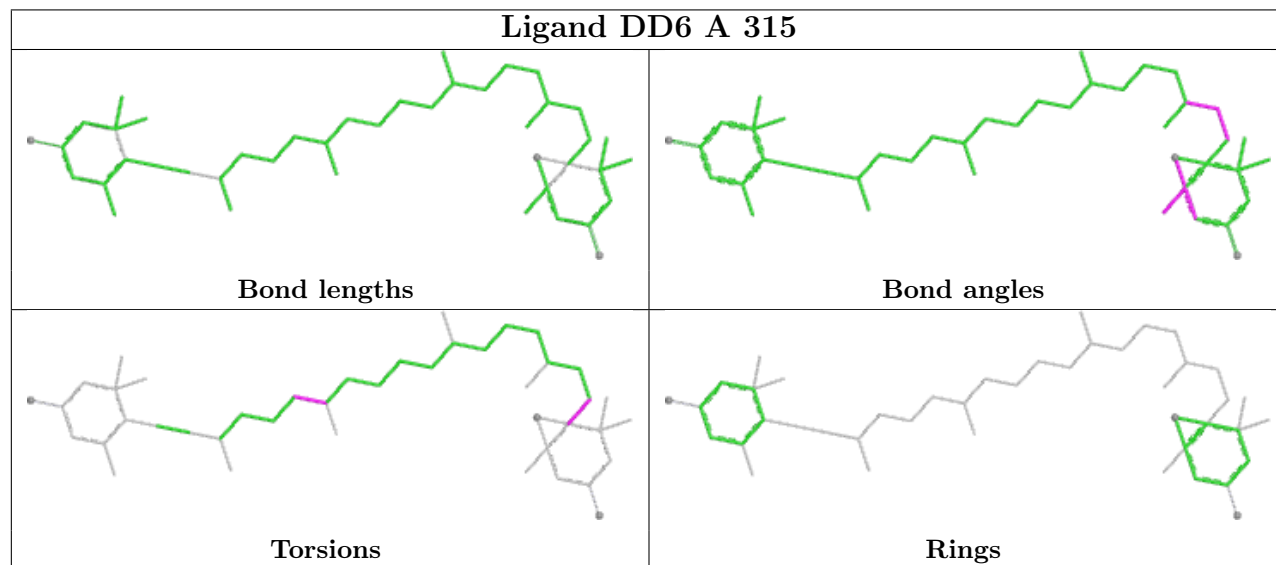
Bond angles

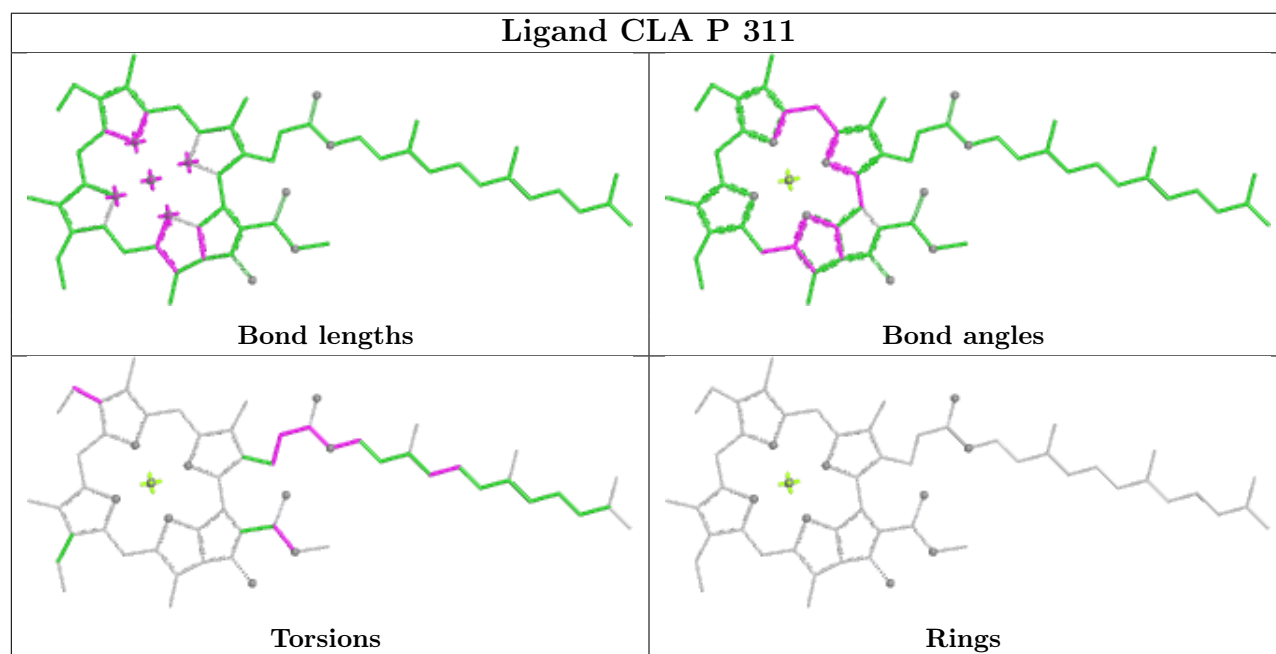
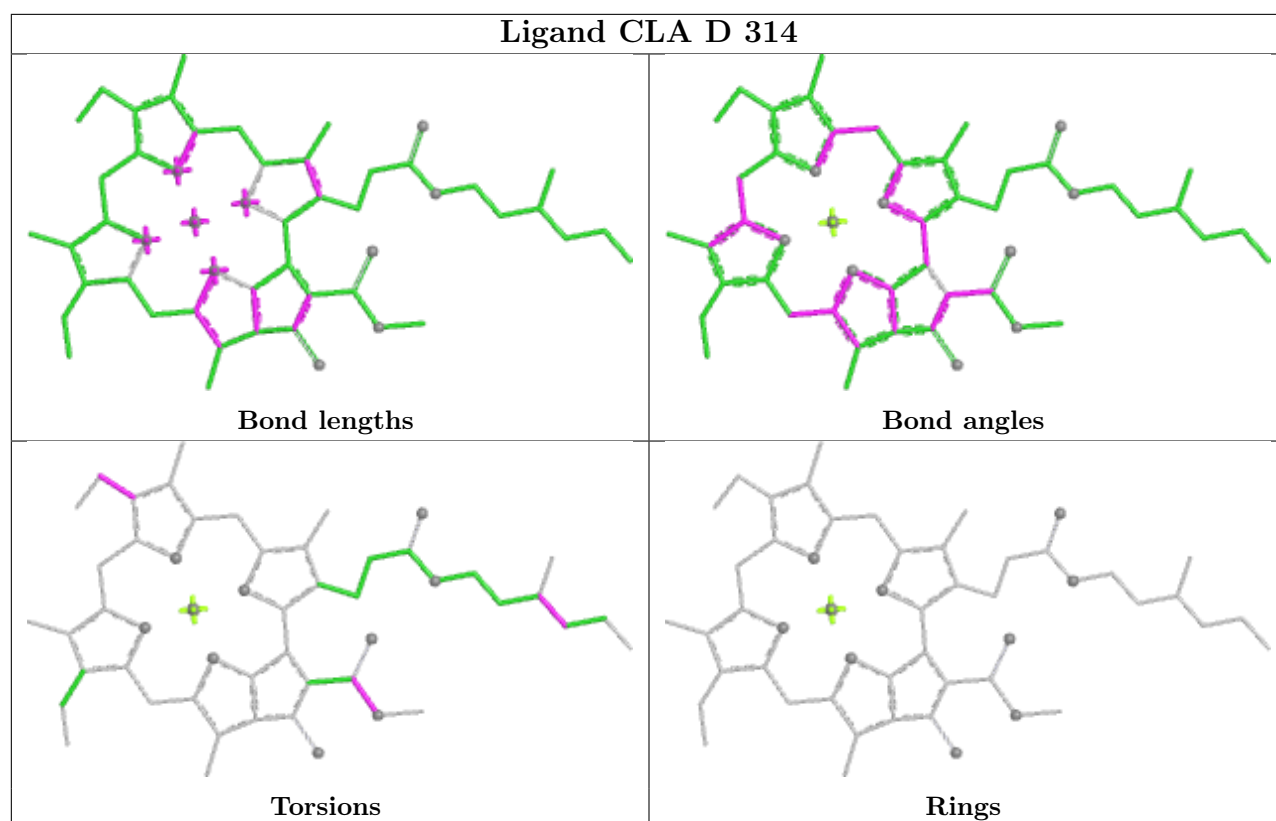


Torsions

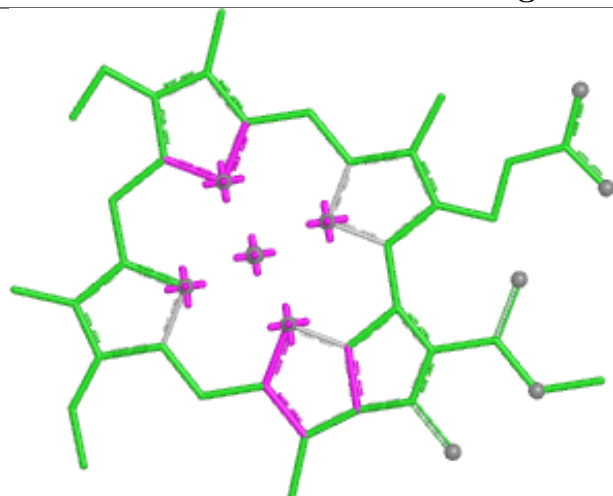


Rings

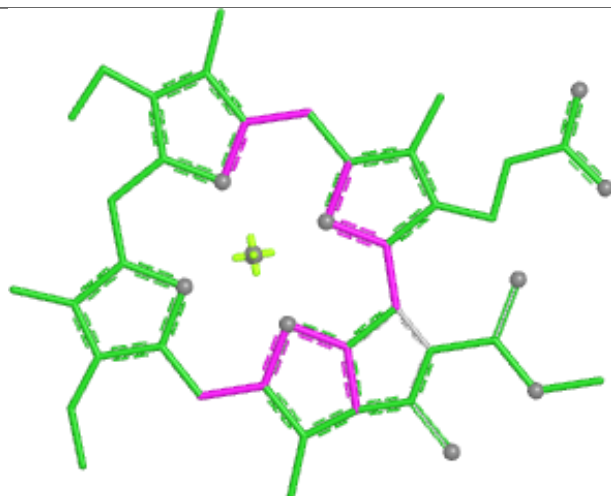
Ligand CLA I 302**Ligand DD6 A 315**



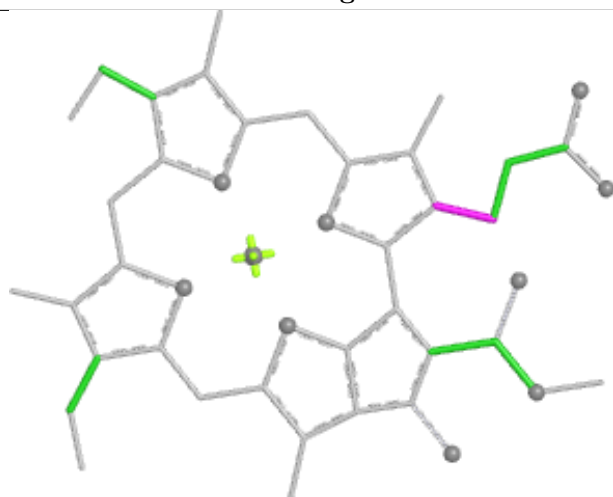
Ligand CLA J 309



Bond lengths



Bond angles

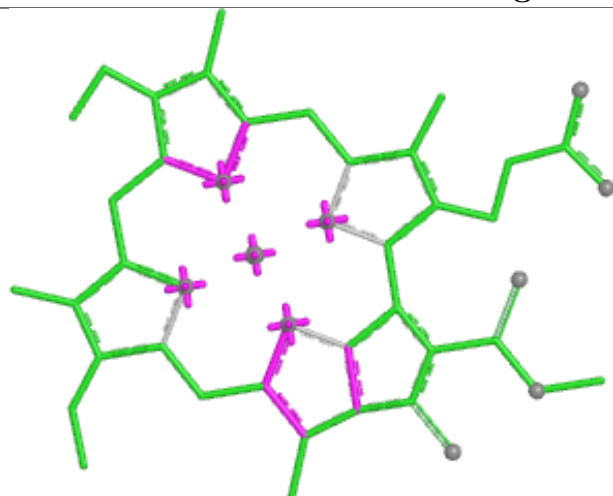


Torsions

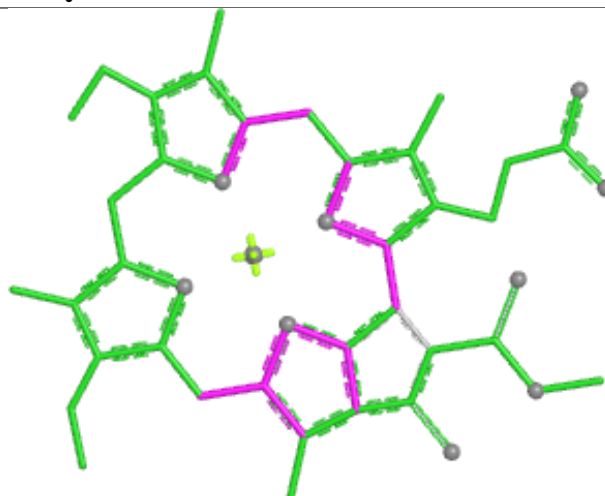


Rings

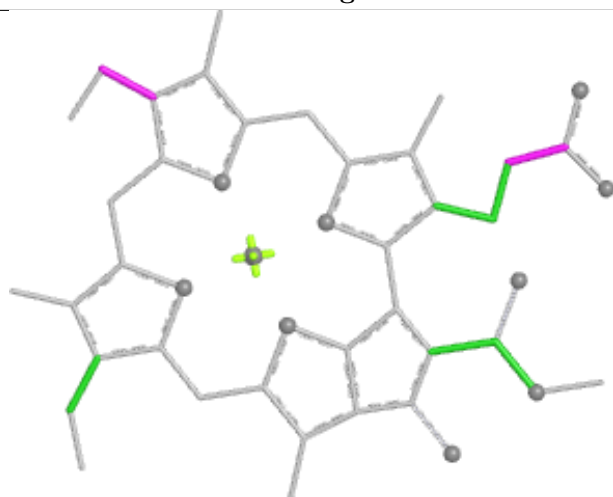
Ligand CLA Q 308



Bond lengths



Bond angles

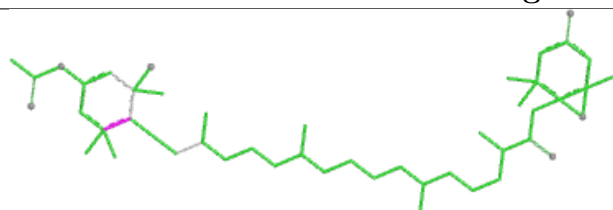


Torsions

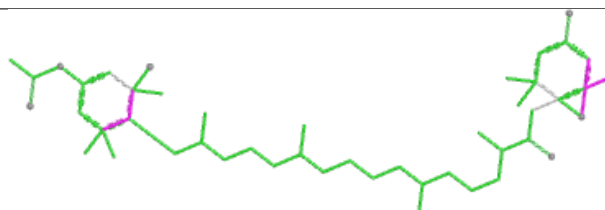


Rings

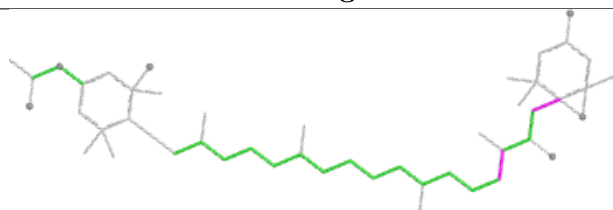
Ligand A86 S 315



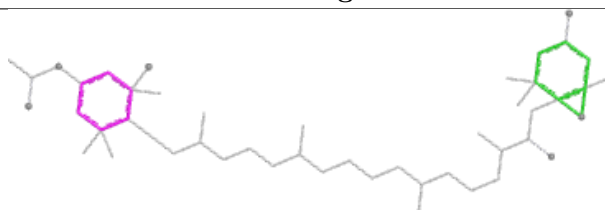
Bond lengths



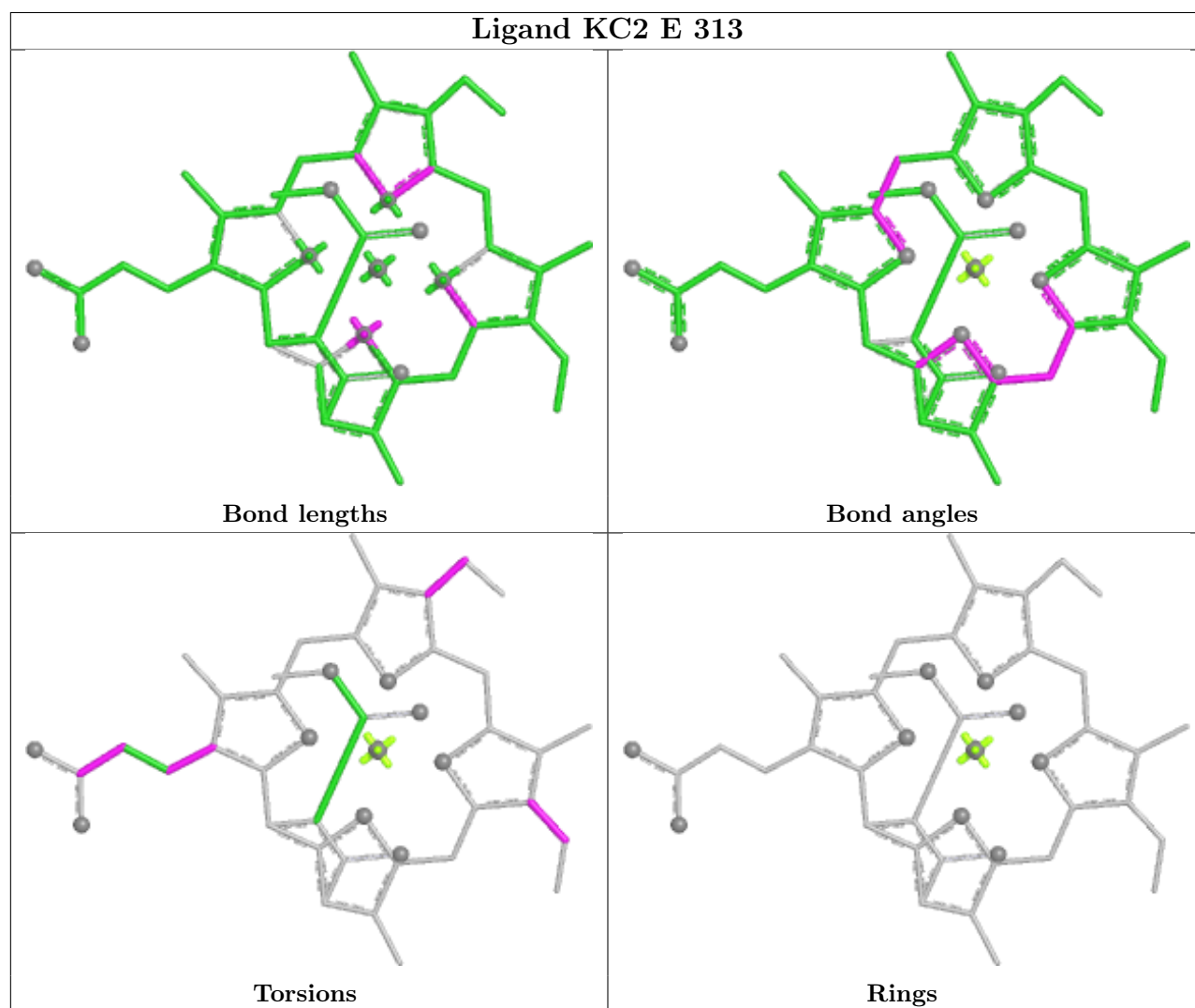
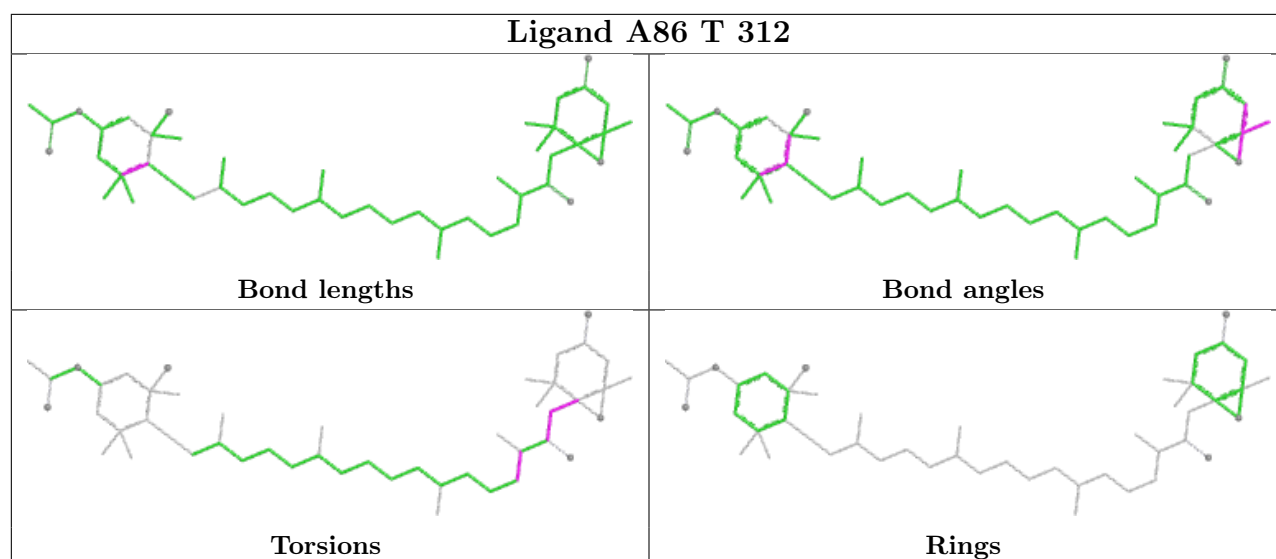
Bond angles



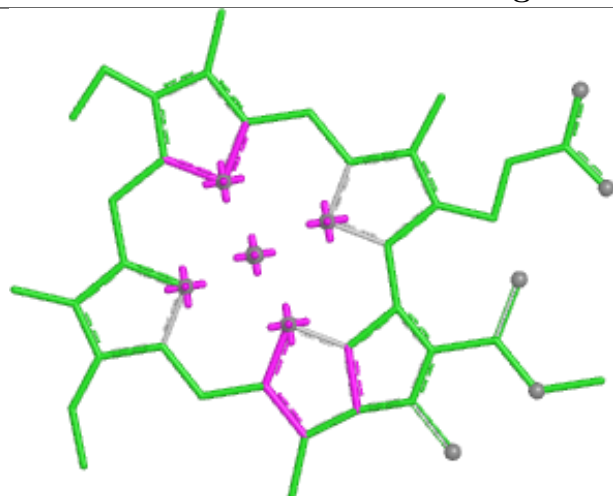
Torsions



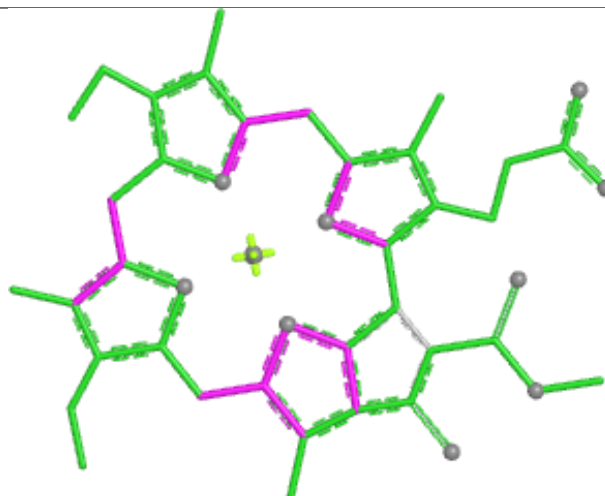
Rings



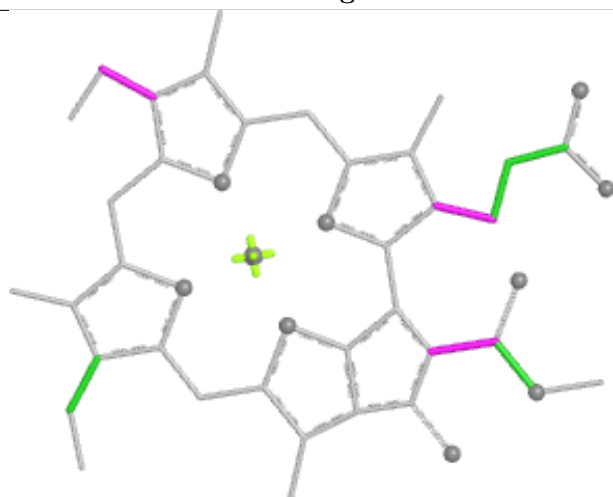
Ligand CLA K 304



Bond lengths



Bond angles

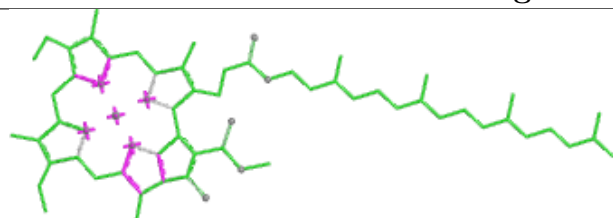


Torsions

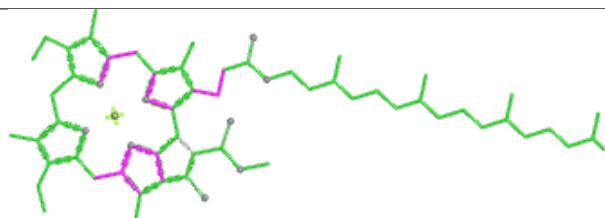


Rings

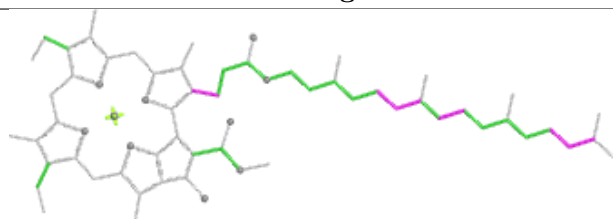
Ligand CLA O 305



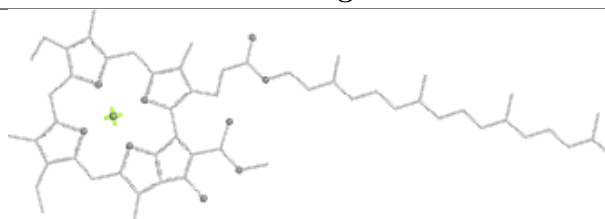
Bond lengths



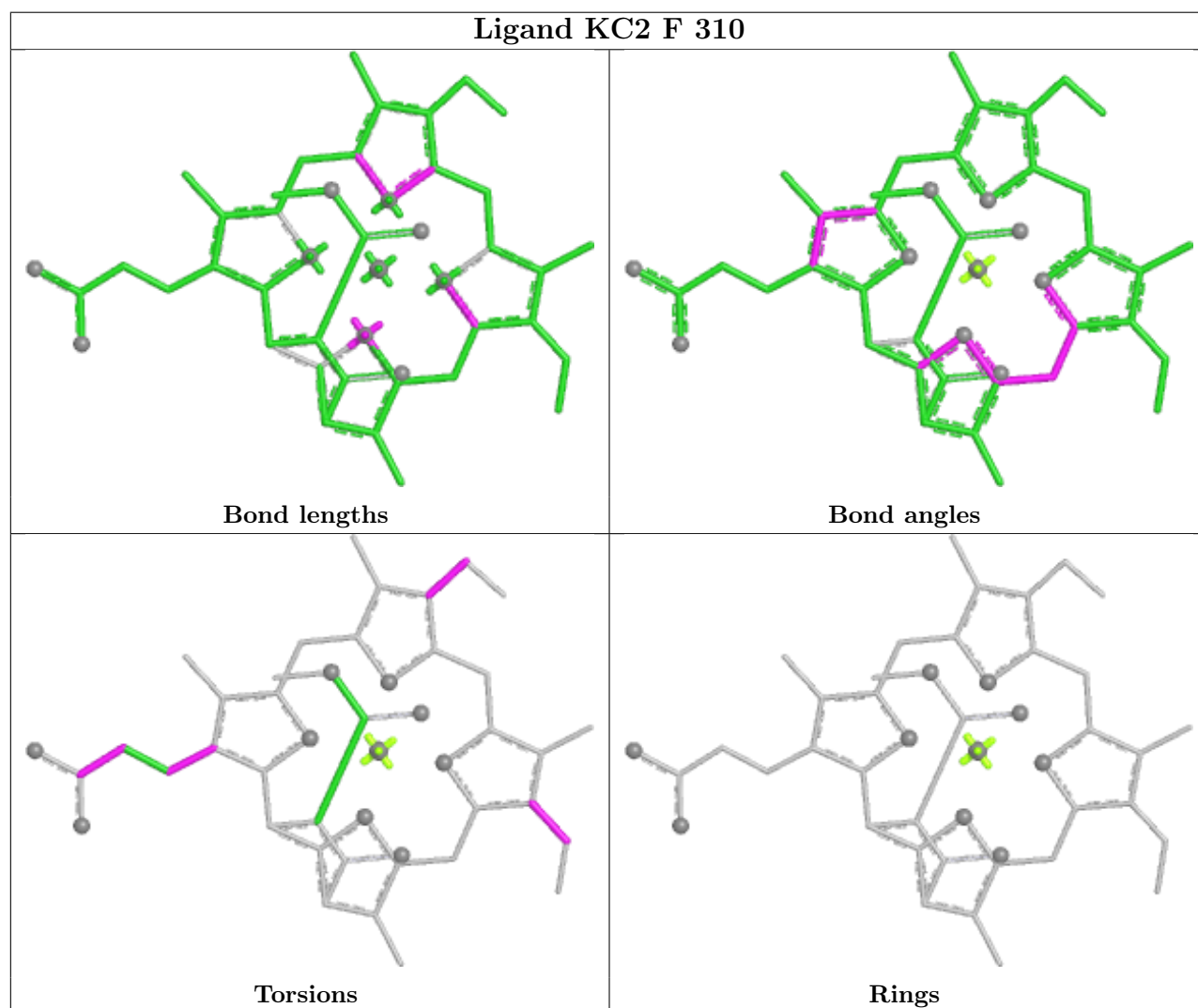
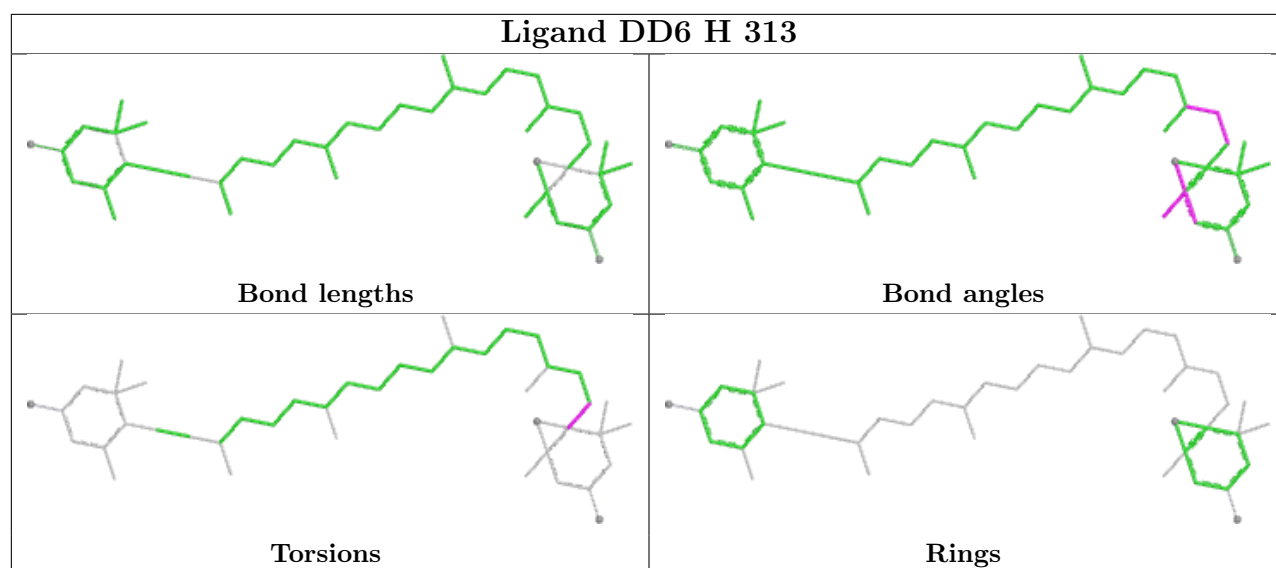
Bond angles



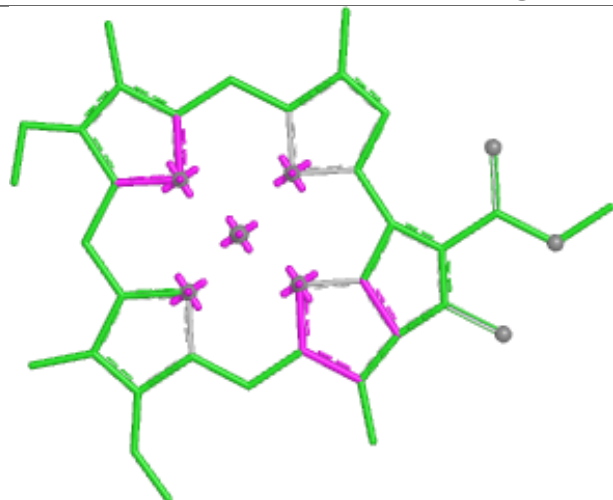
Torsions



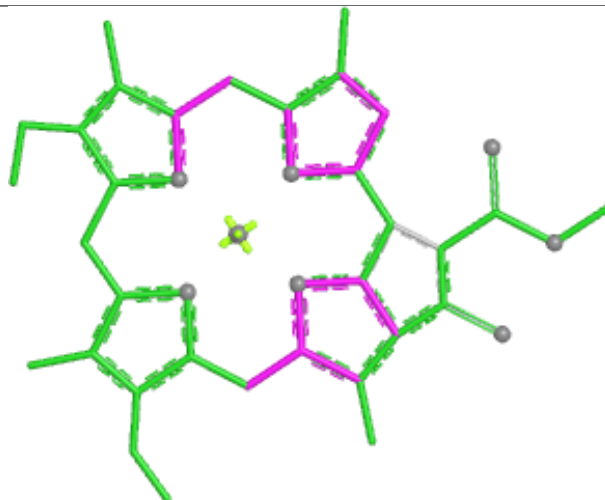
Rings



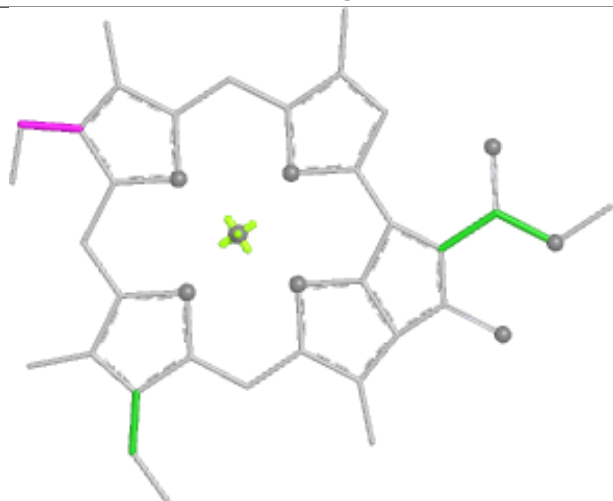
Ligand CLA U 301



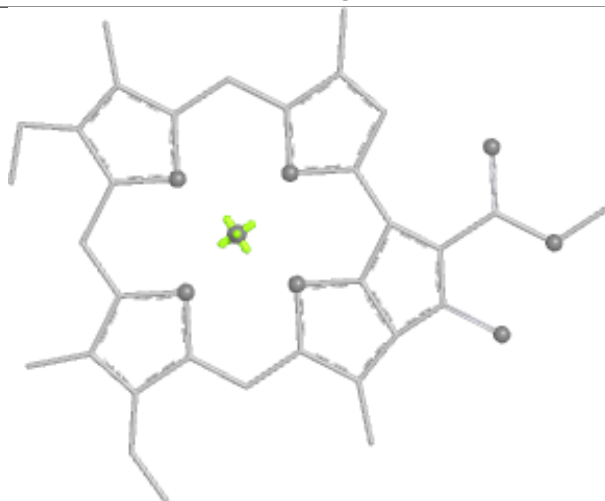
Bond lengths



Bond angles

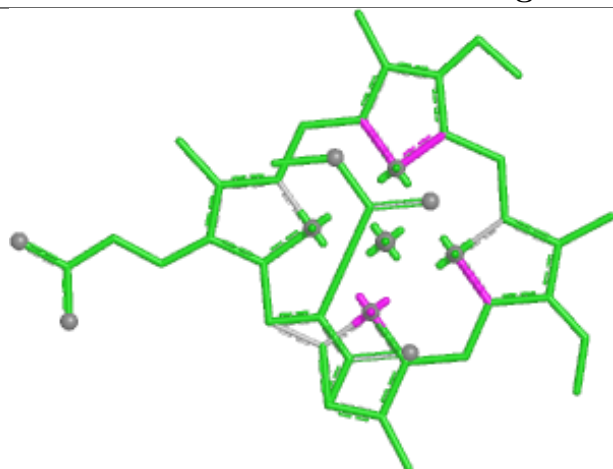


Torsions

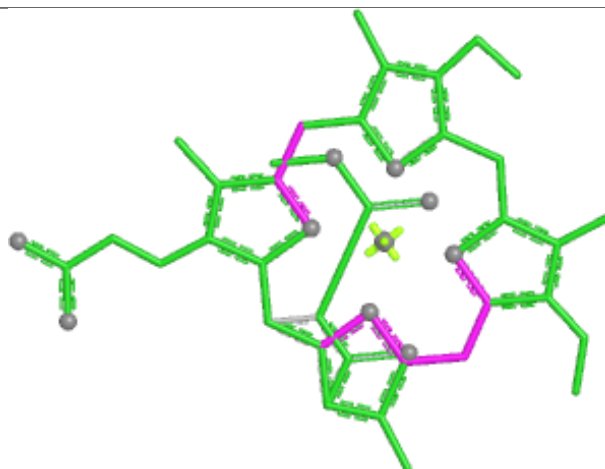


Rings

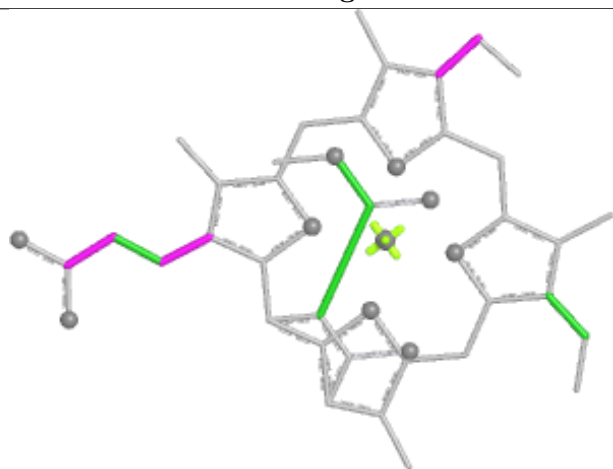
Ligand KC2 O 310



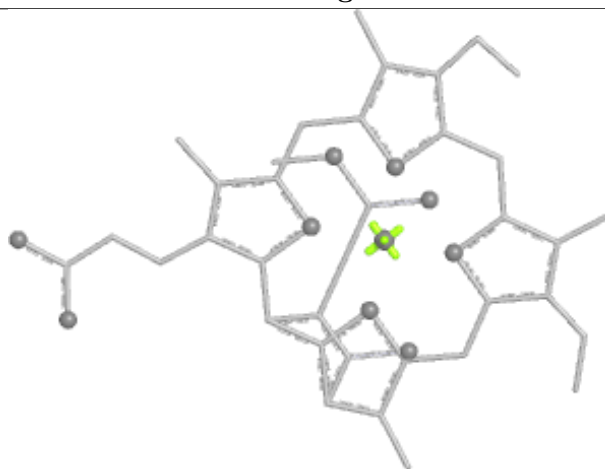
Bond lengths



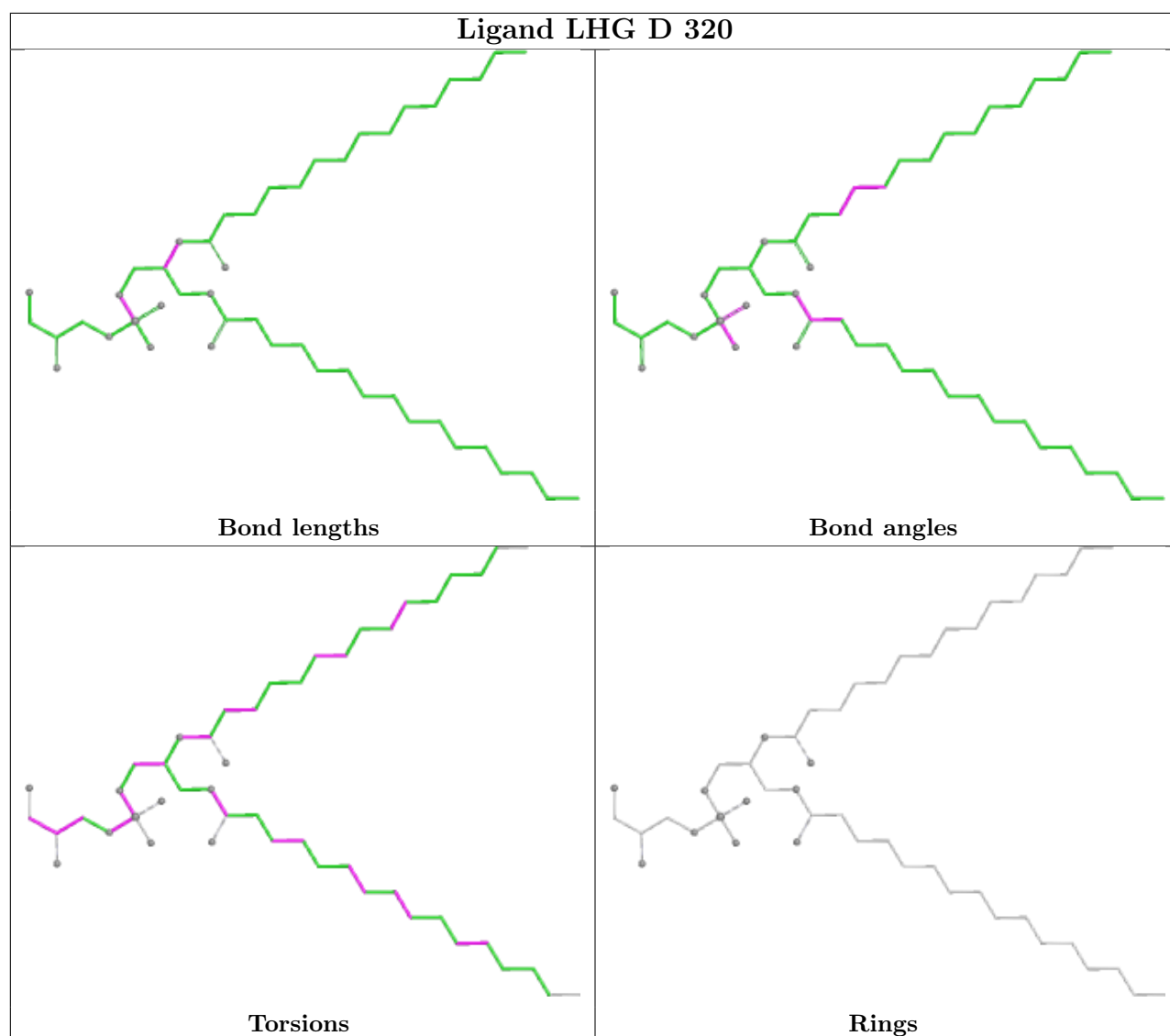
Bond angles



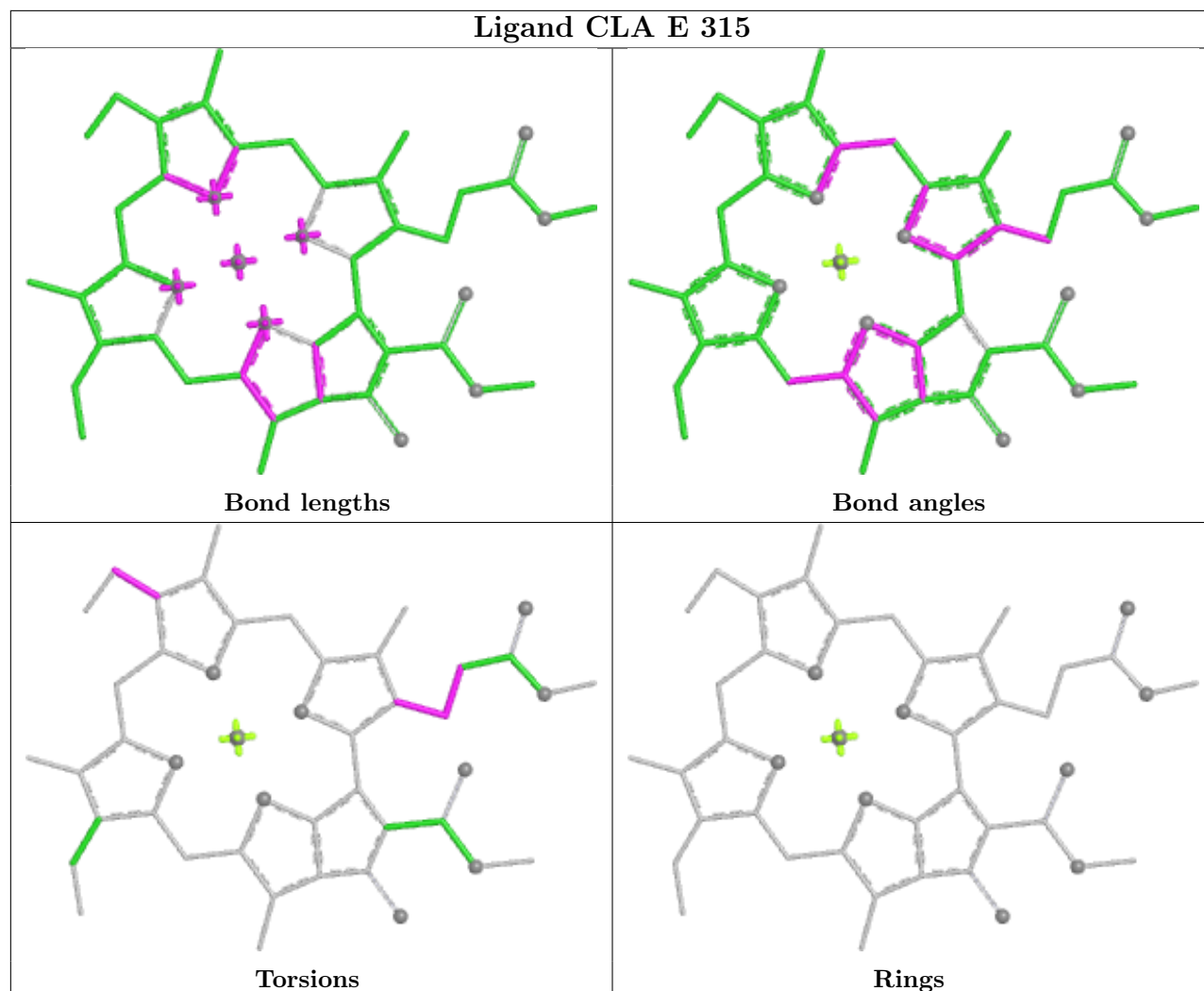
Torsions



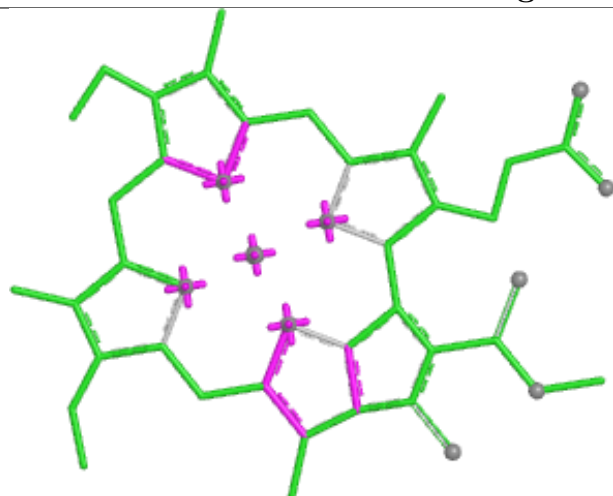
Rings



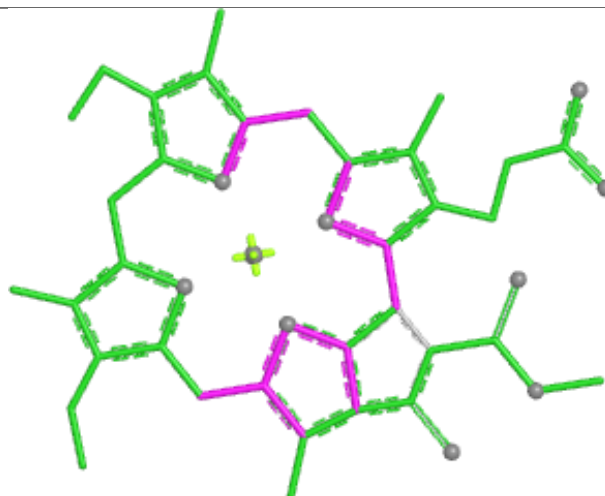
Ligand CLA E 315



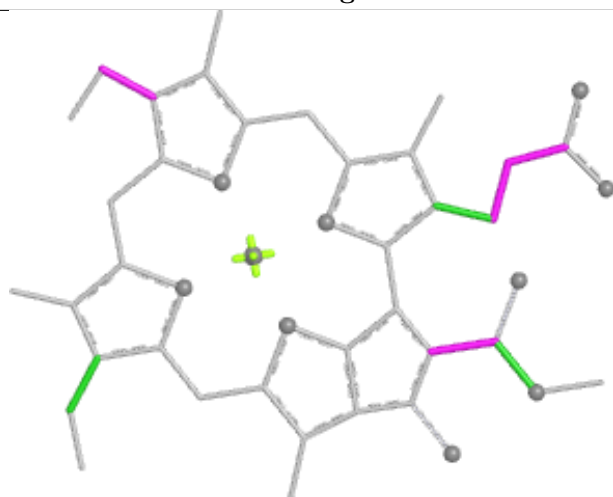
Ligand CLA b 814



Bond lengths



Bond angles

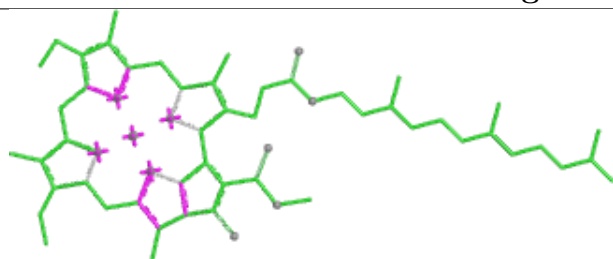


Torsions

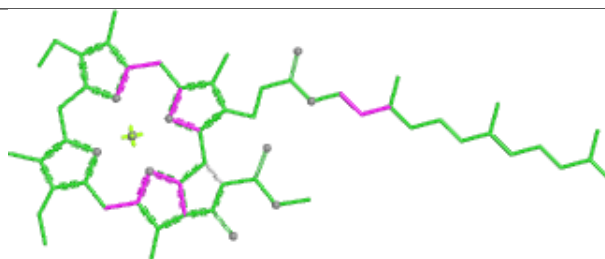


Rings

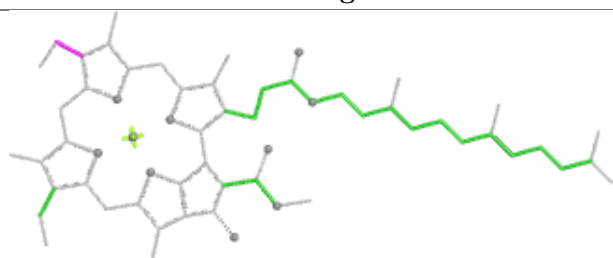
Ligand CLA f 201



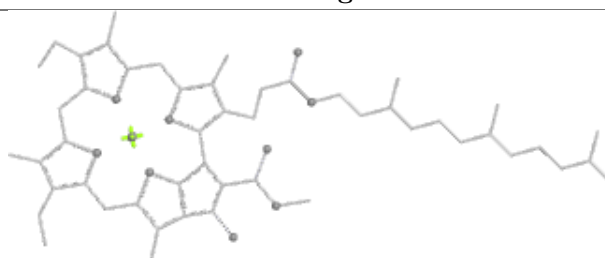
Bond lengths



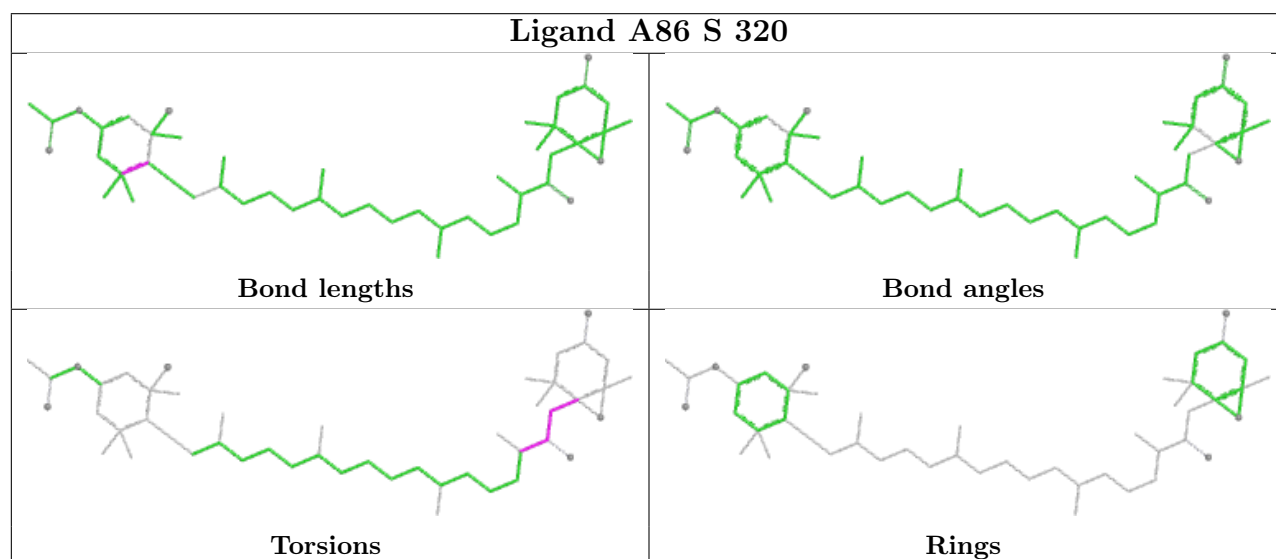
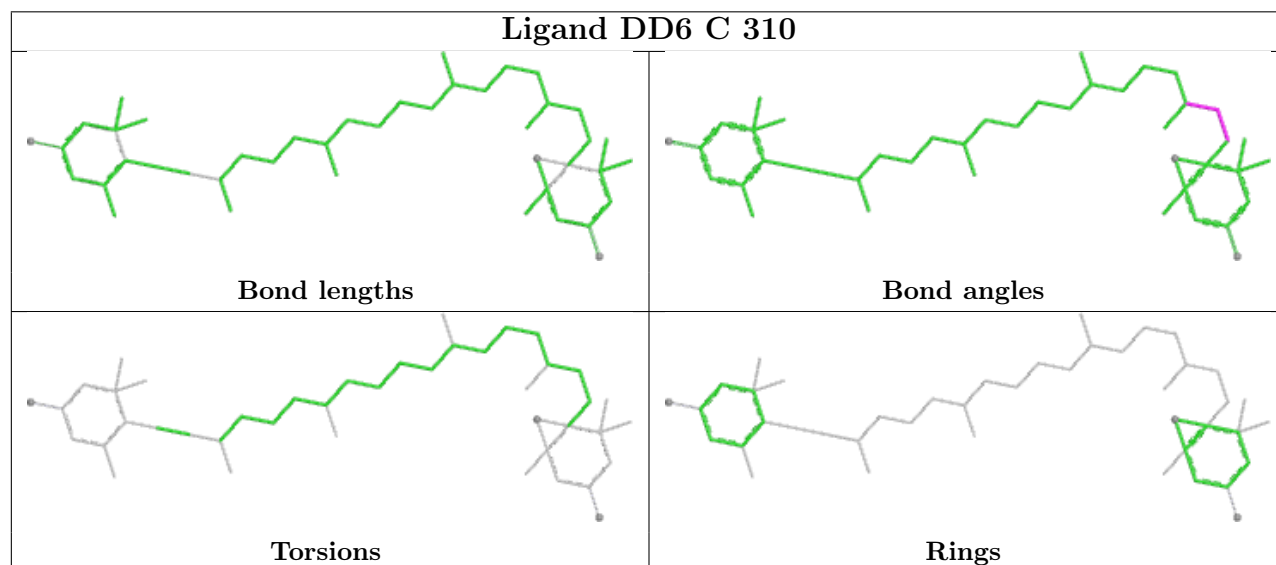
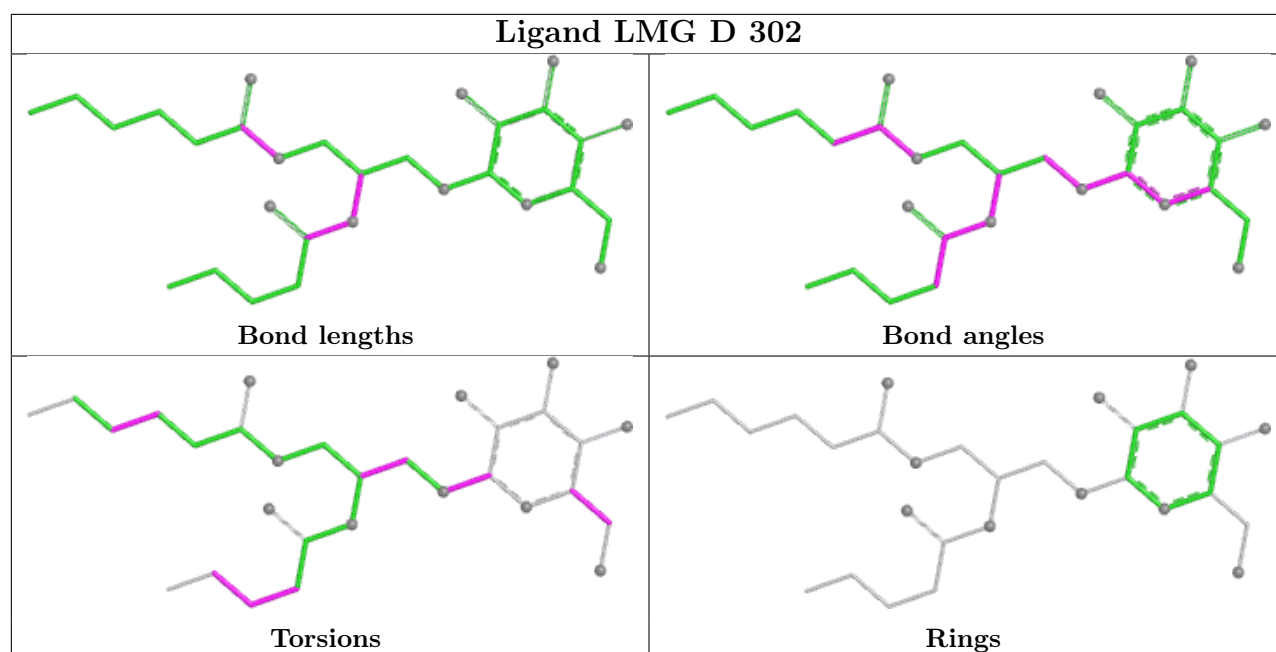
Bond angles

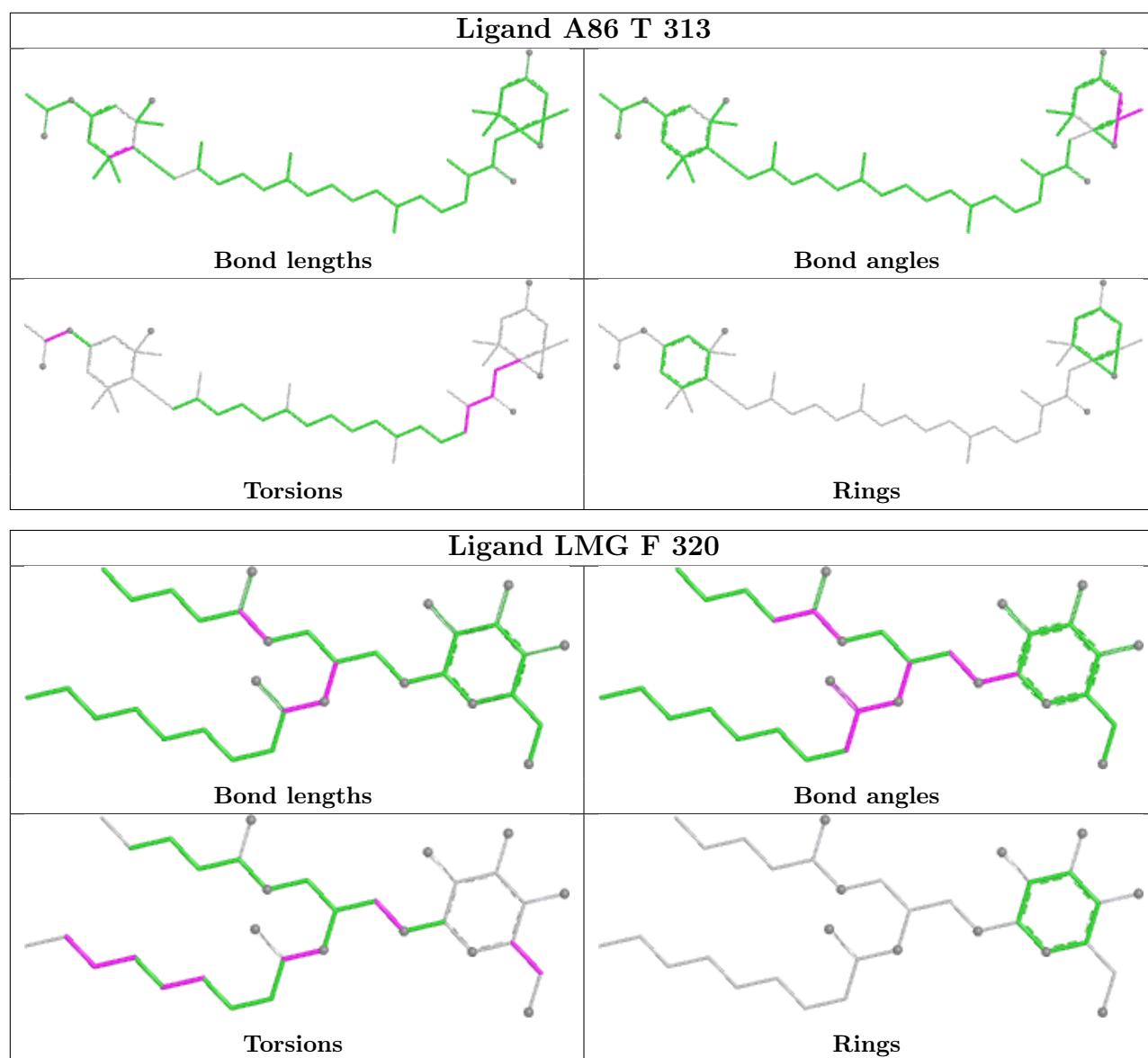


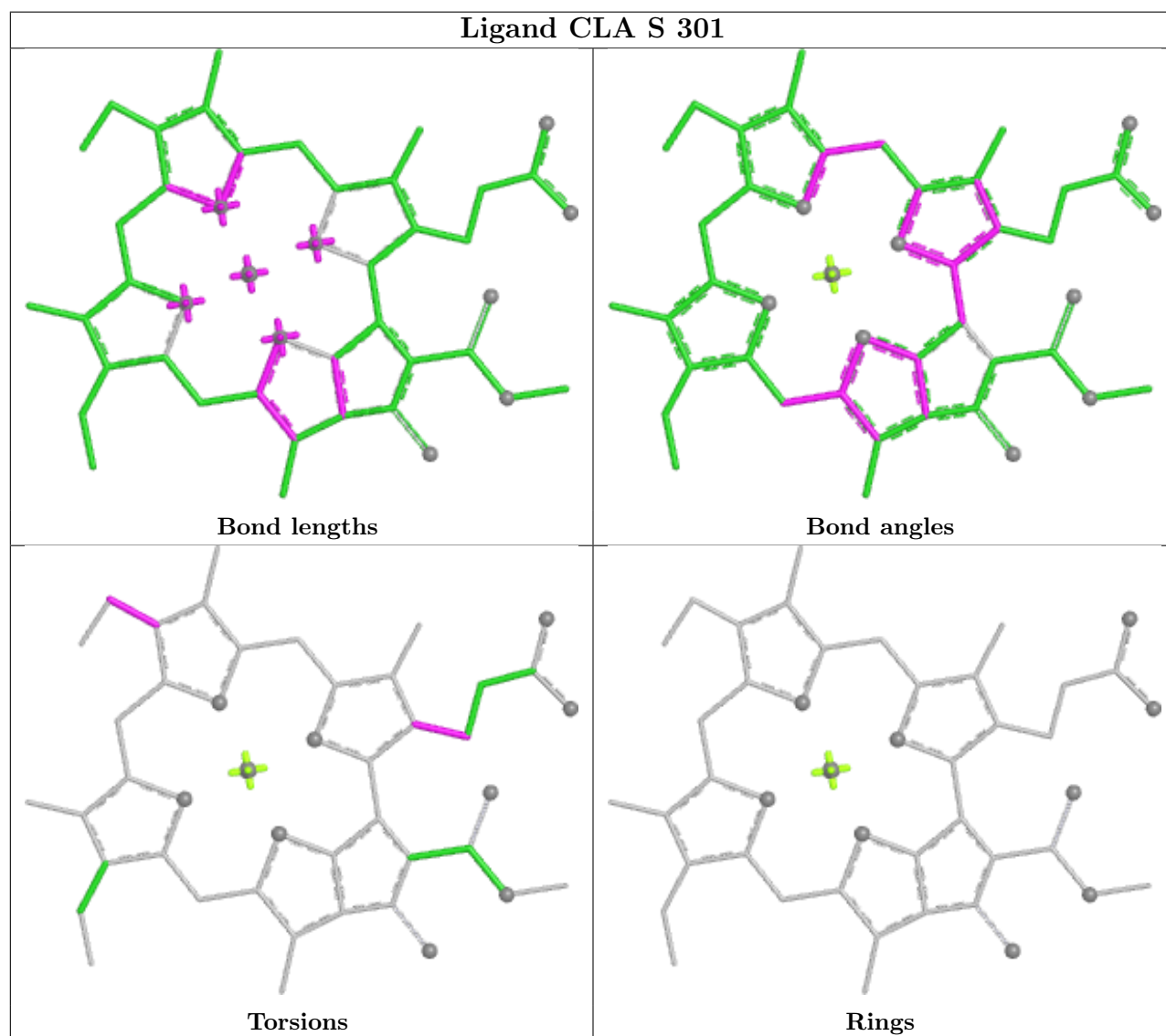
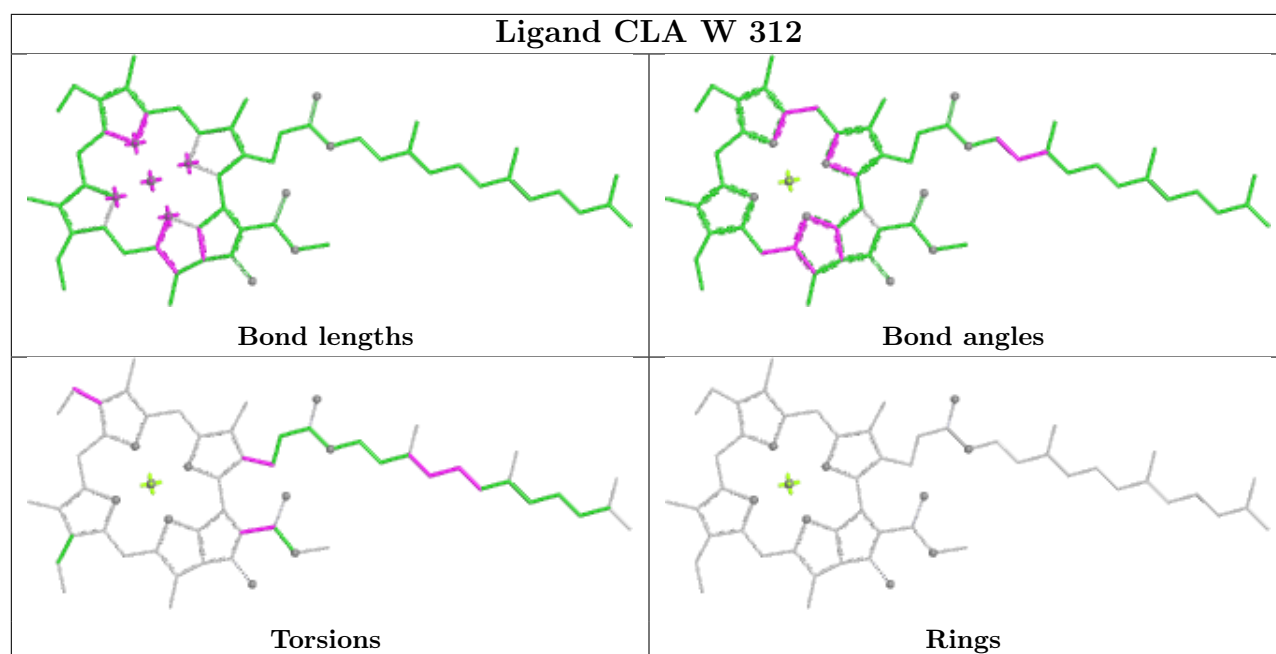
Torsions

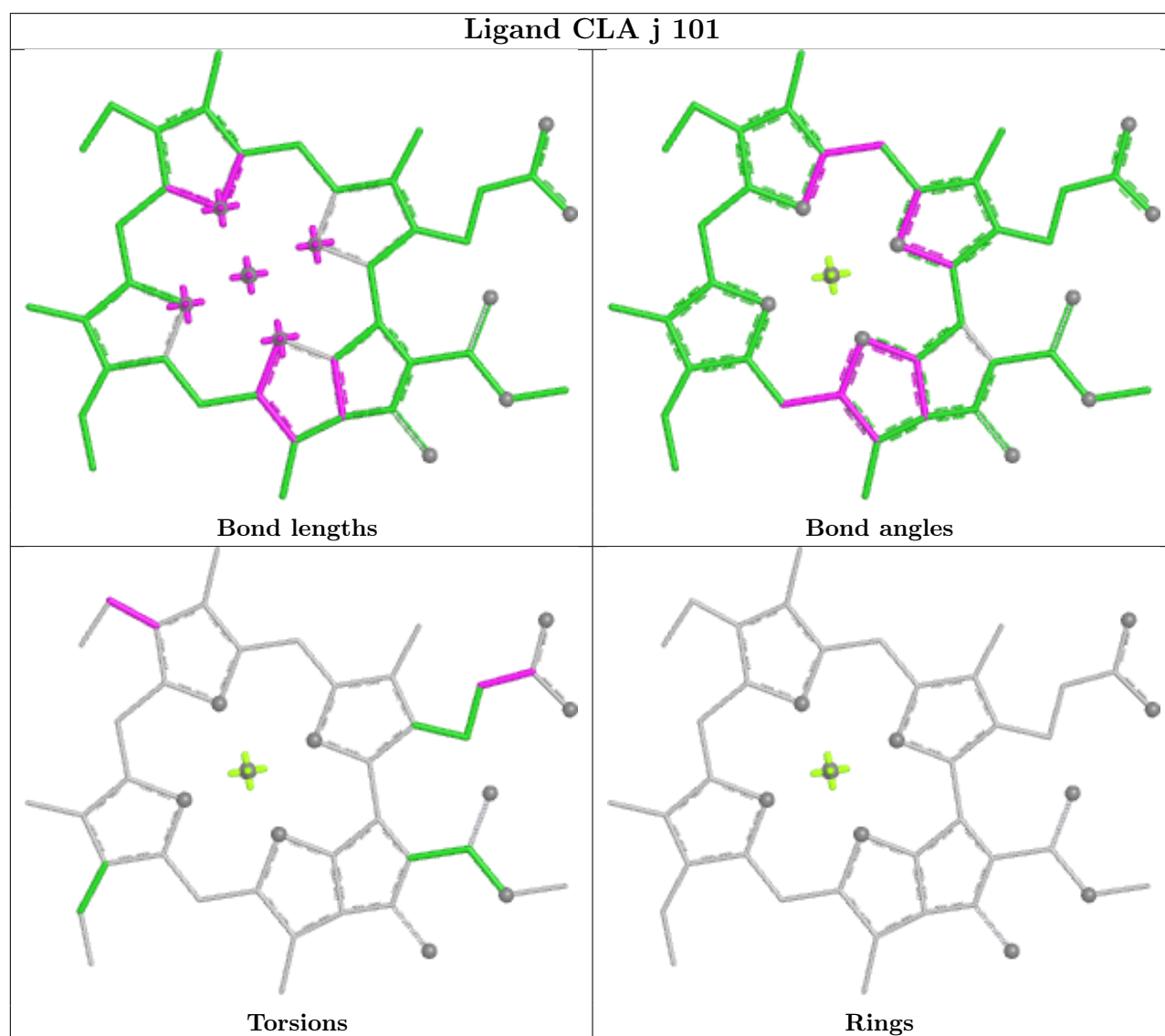
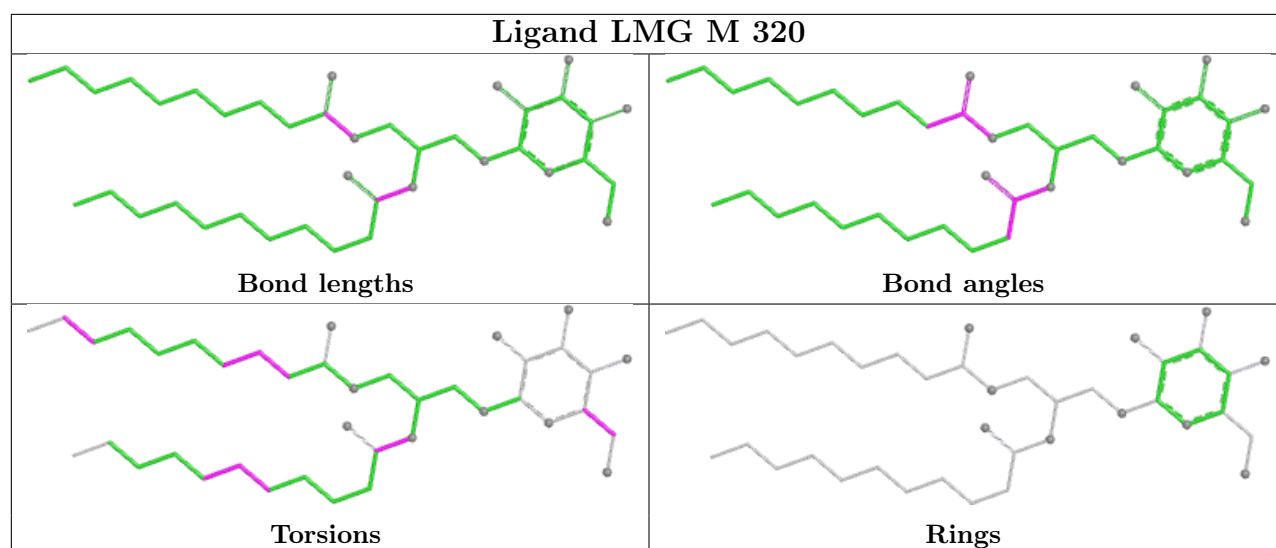


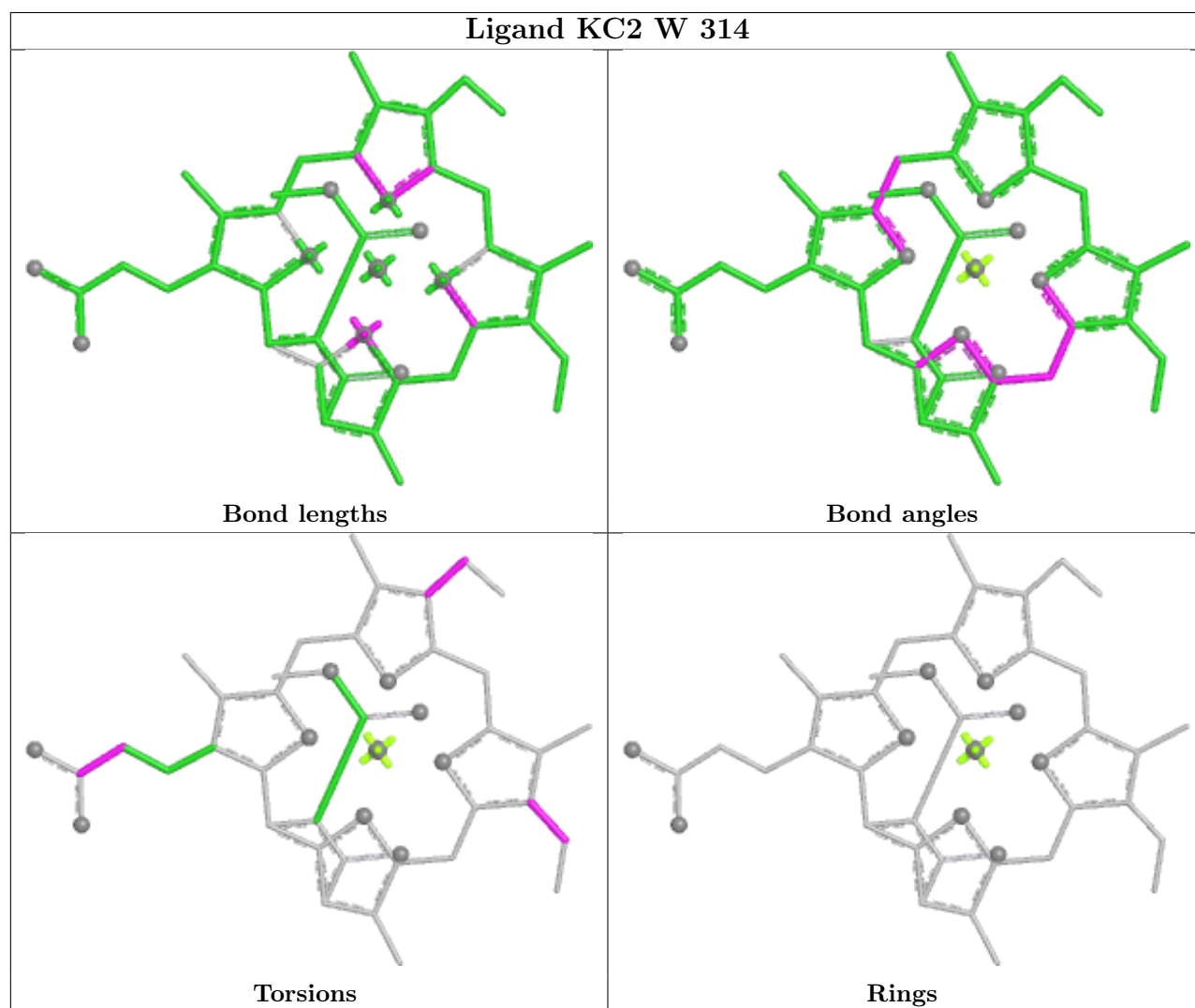
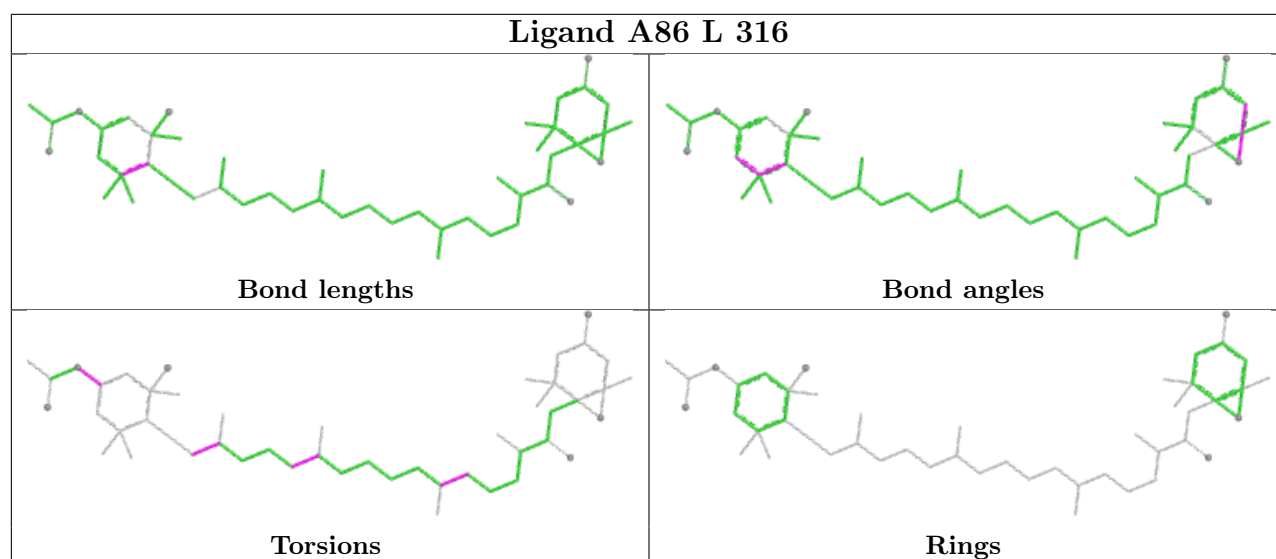
Rings

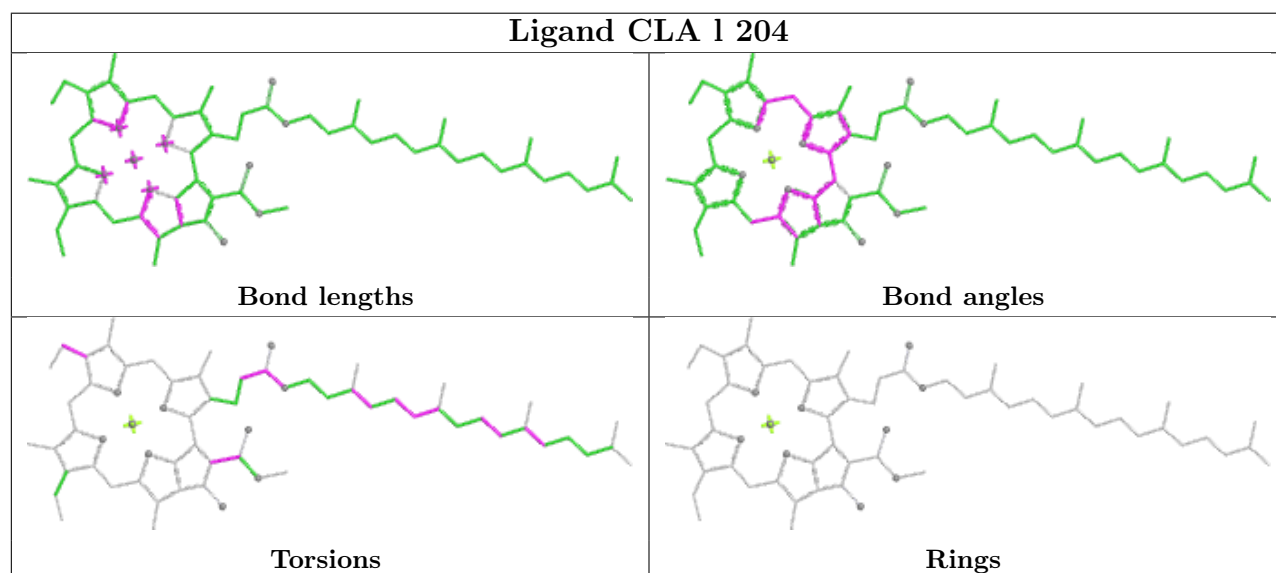
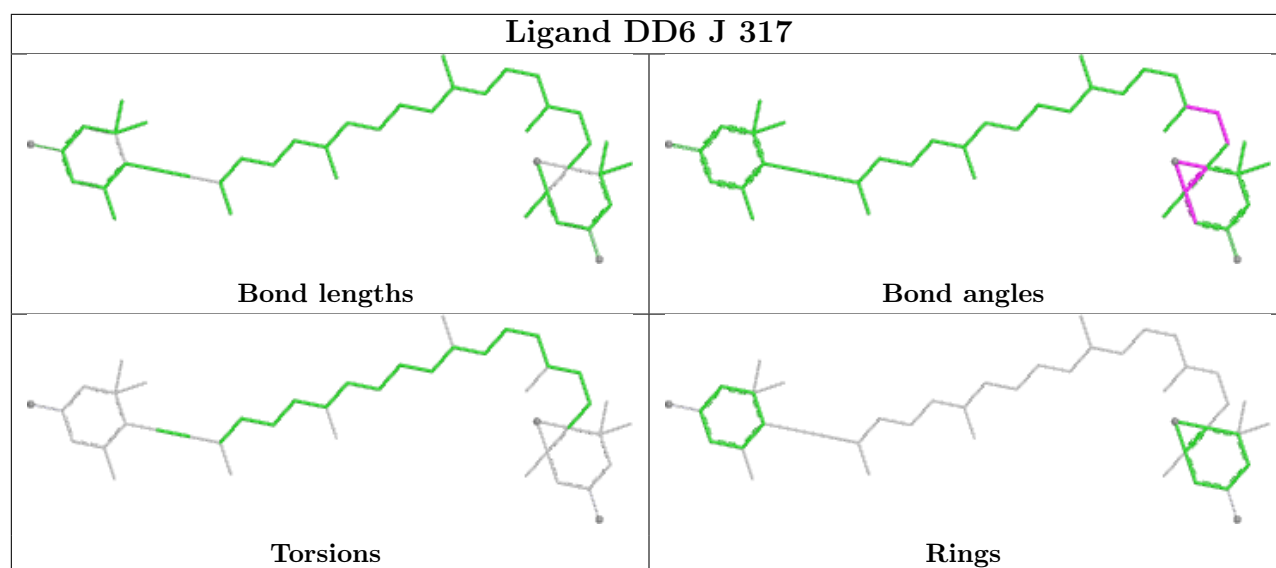


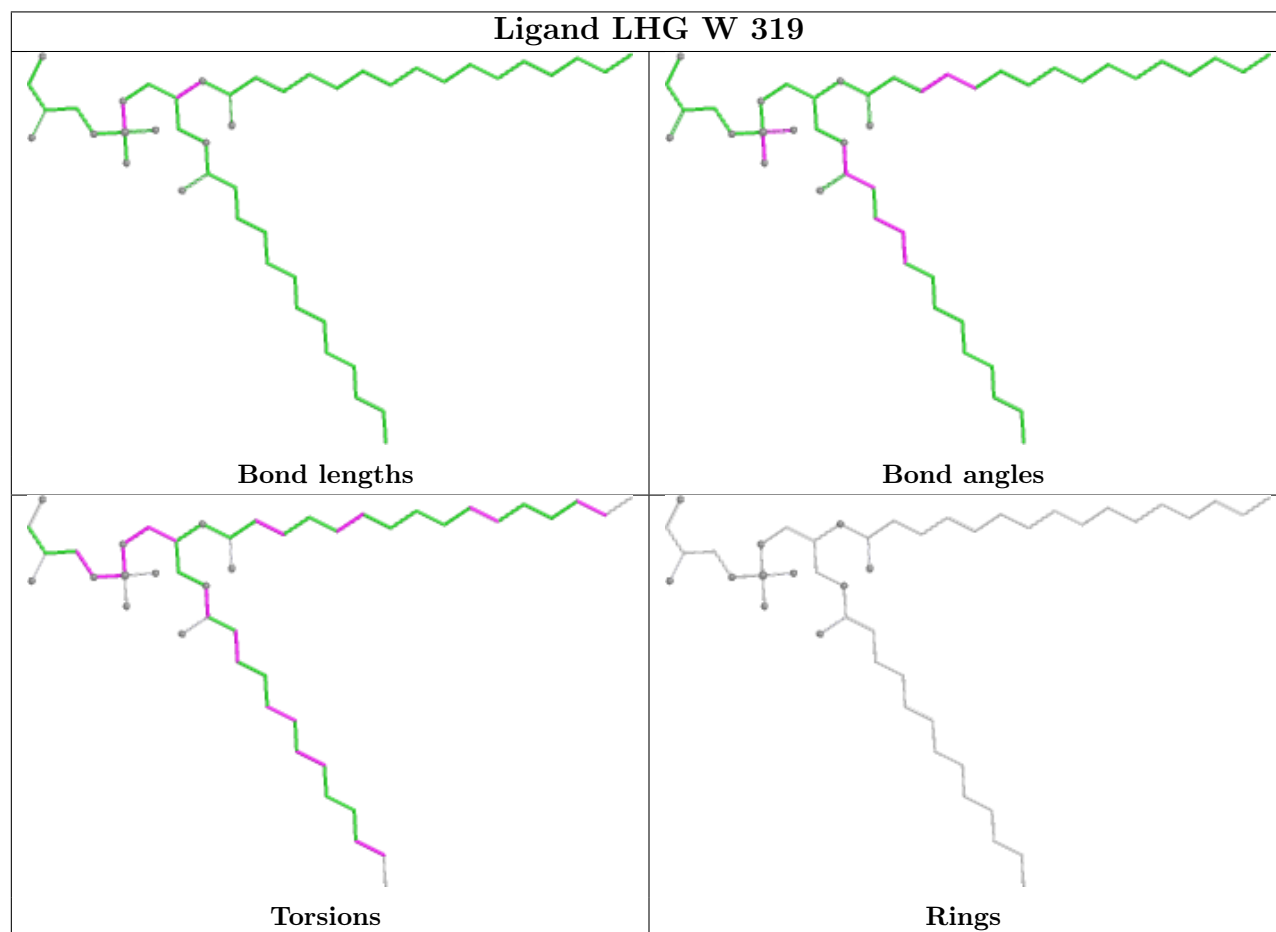
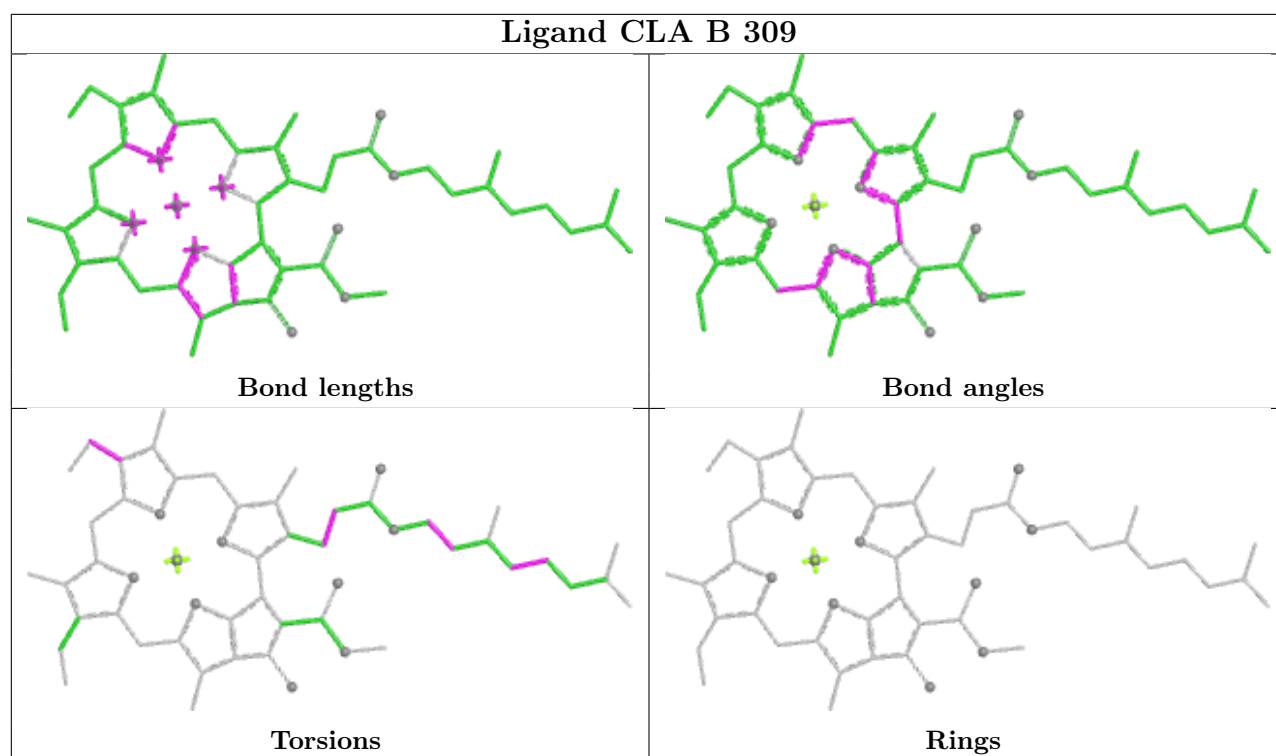


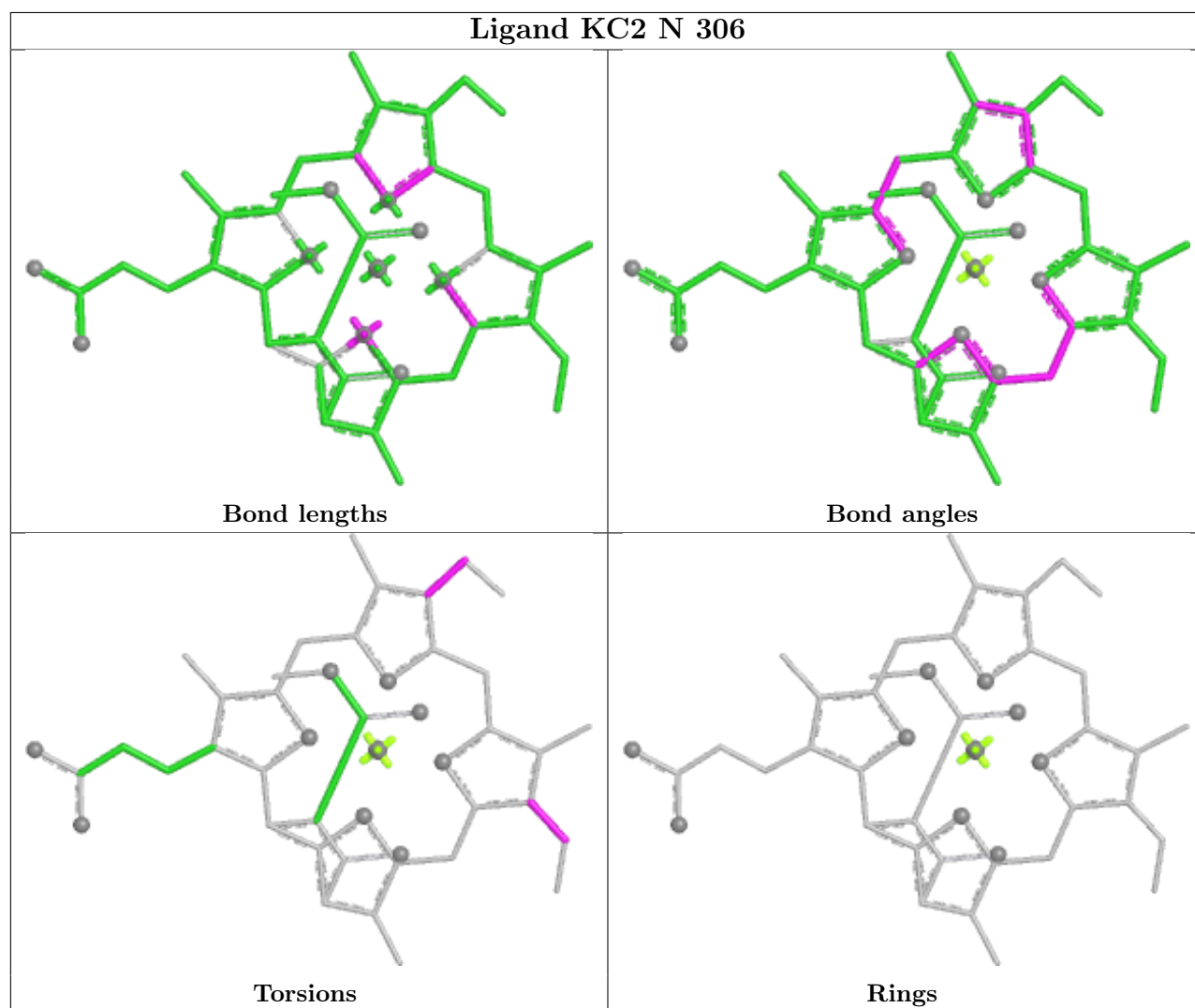
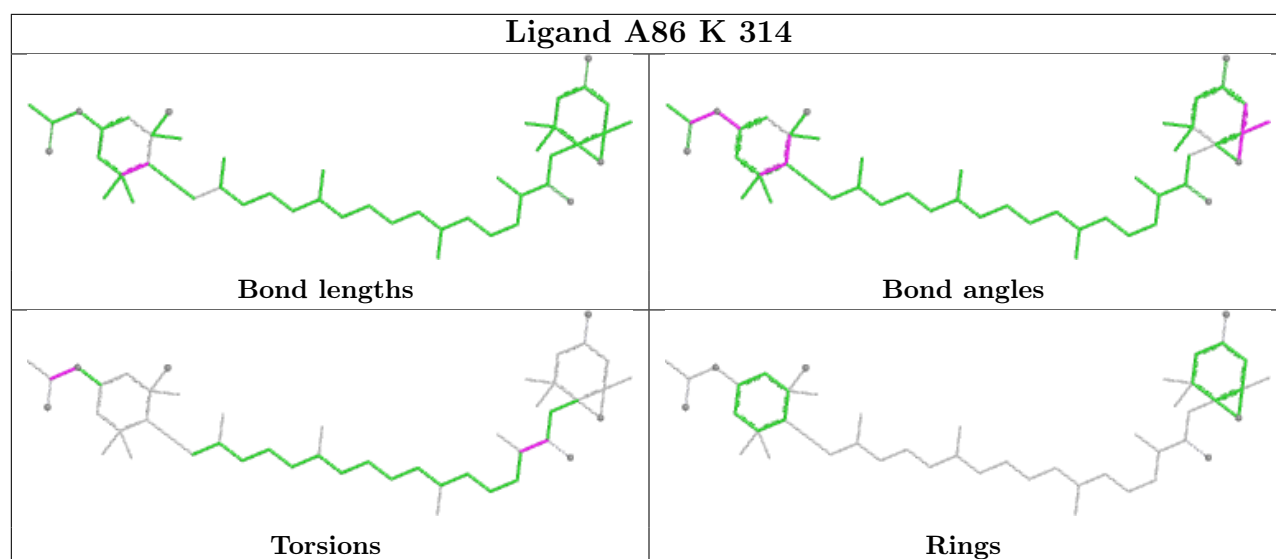


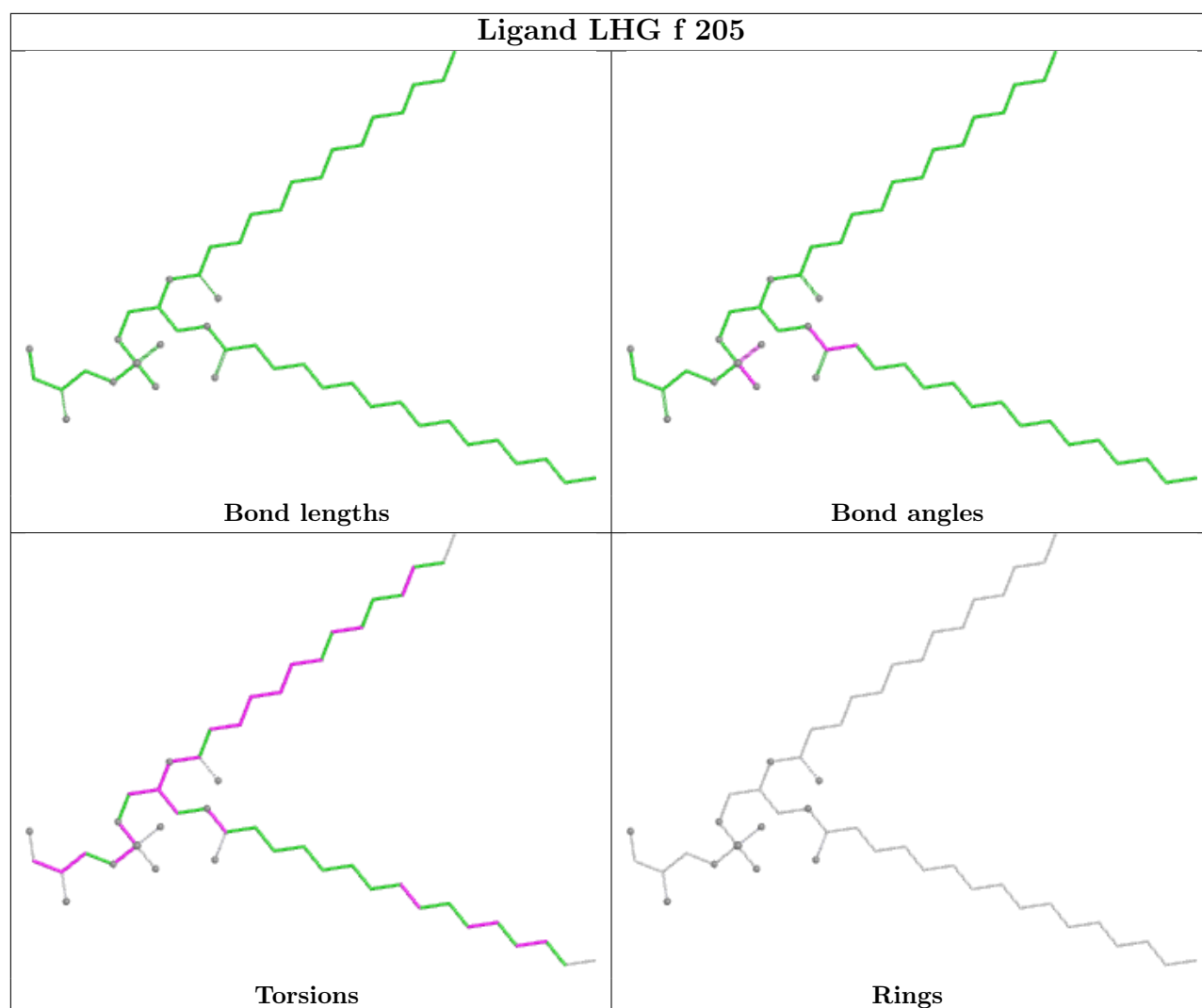


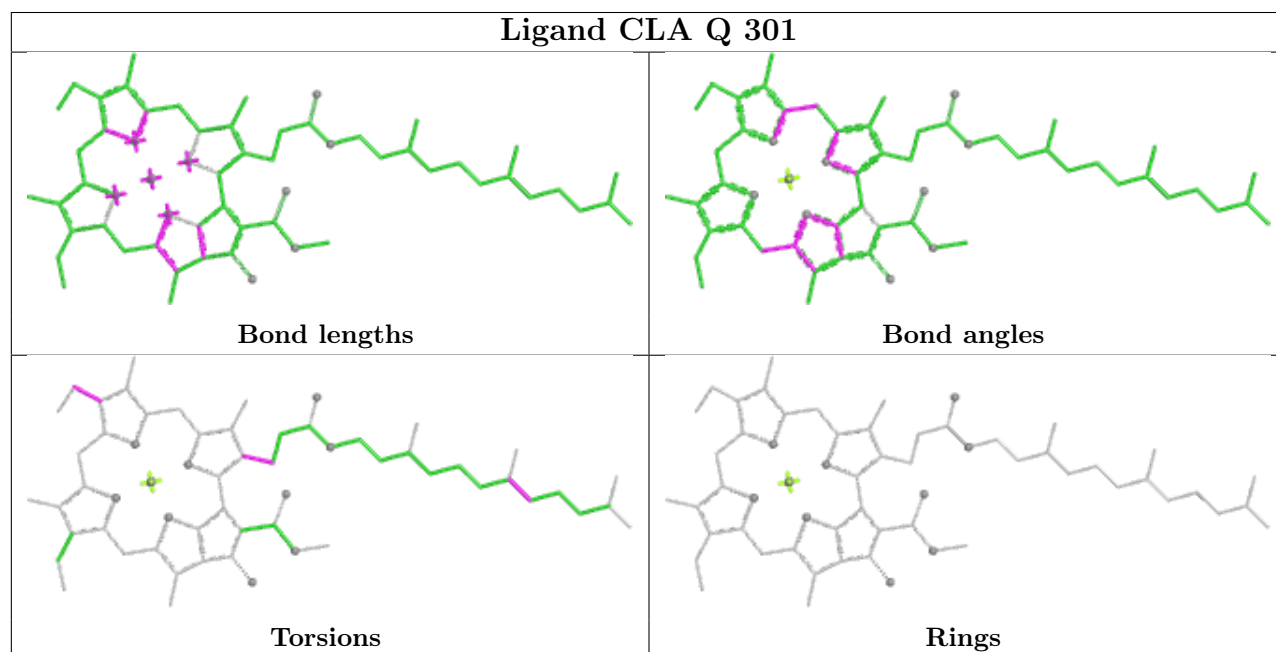
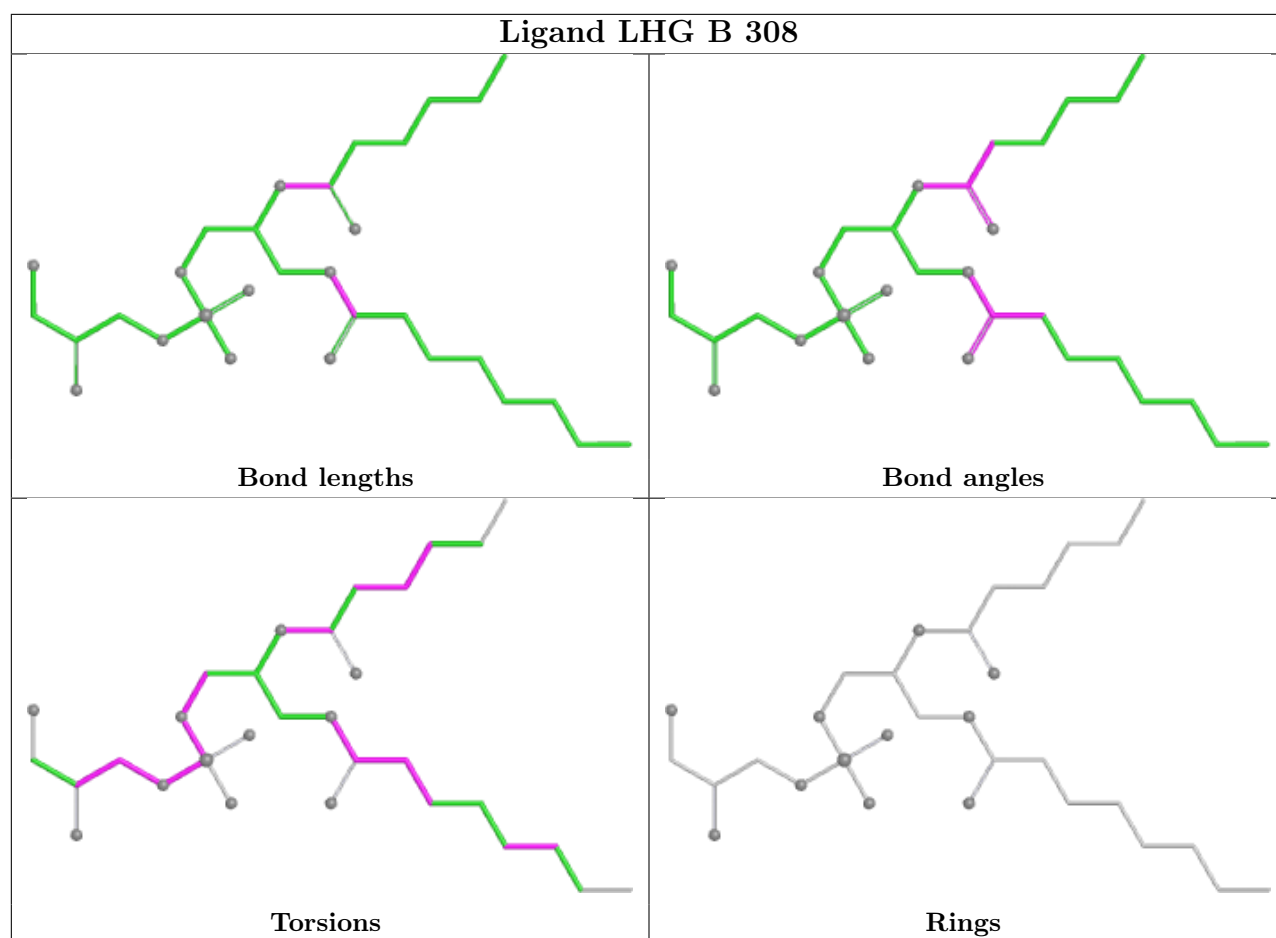


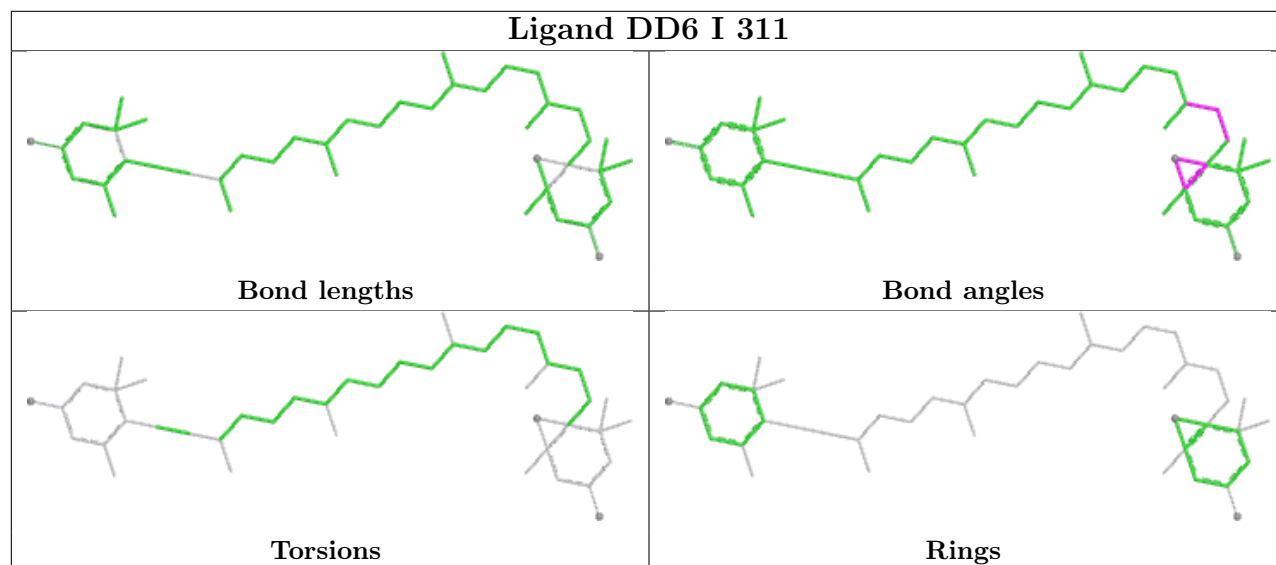
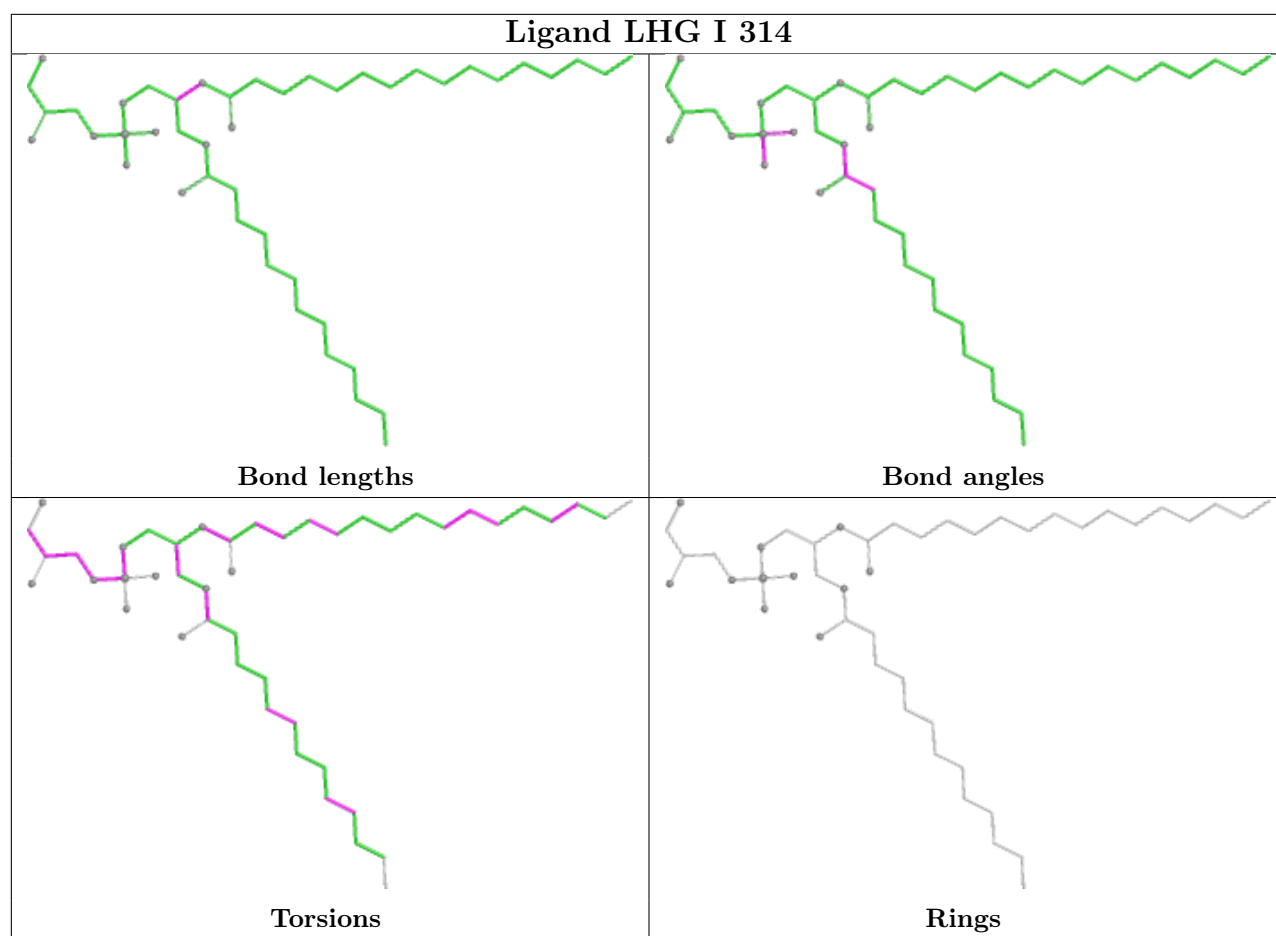


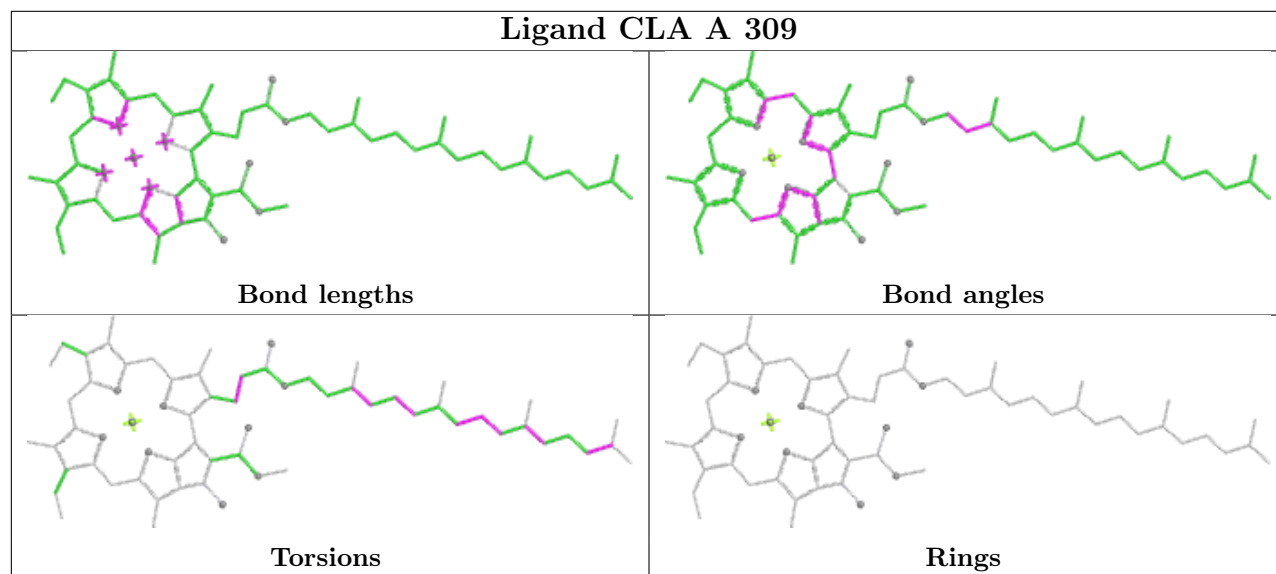
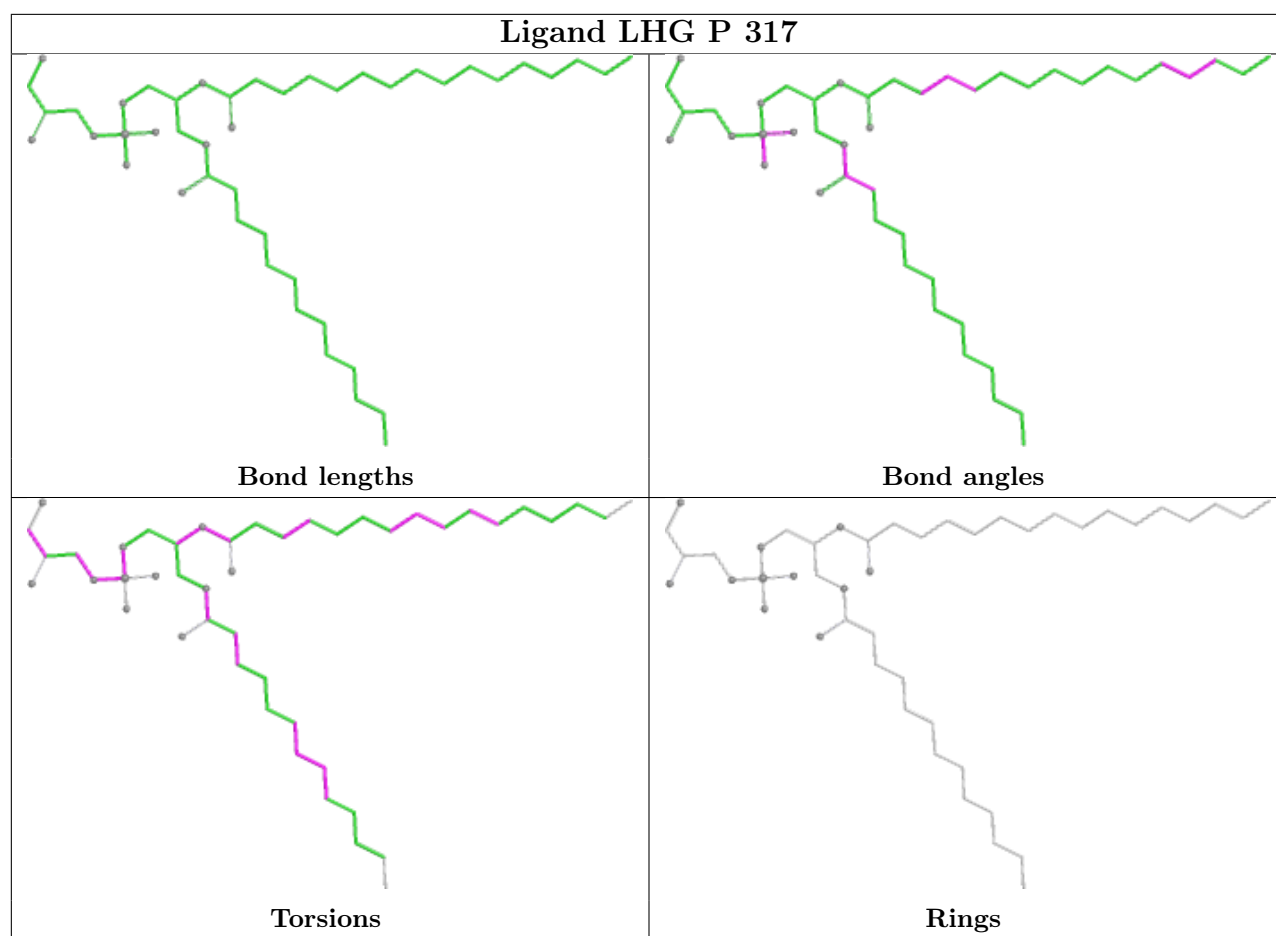


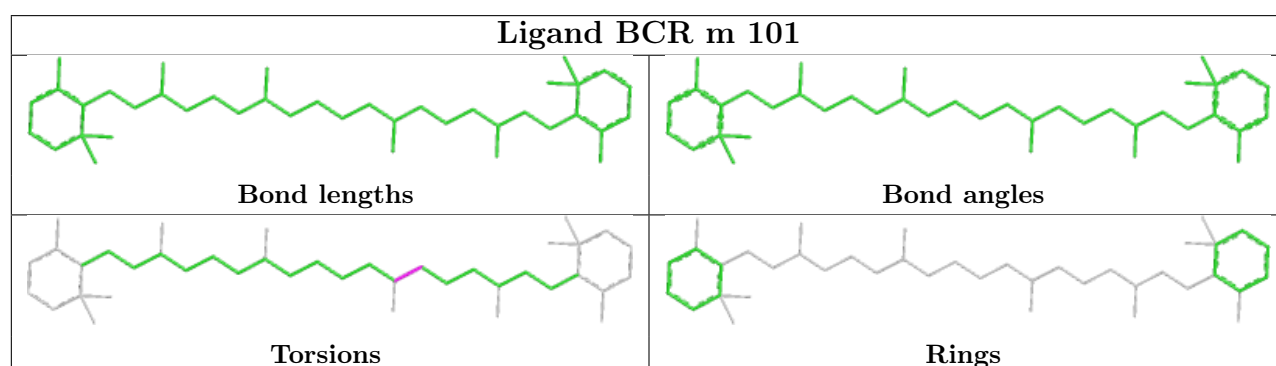
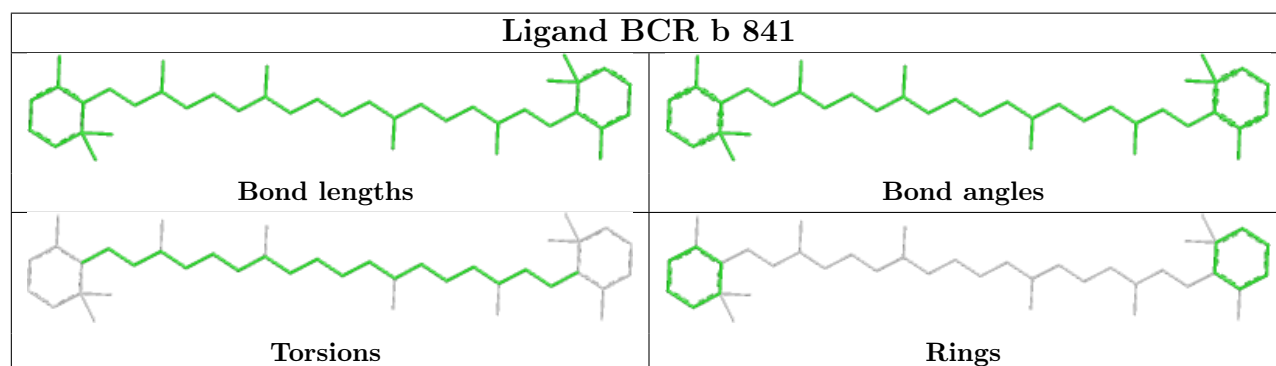
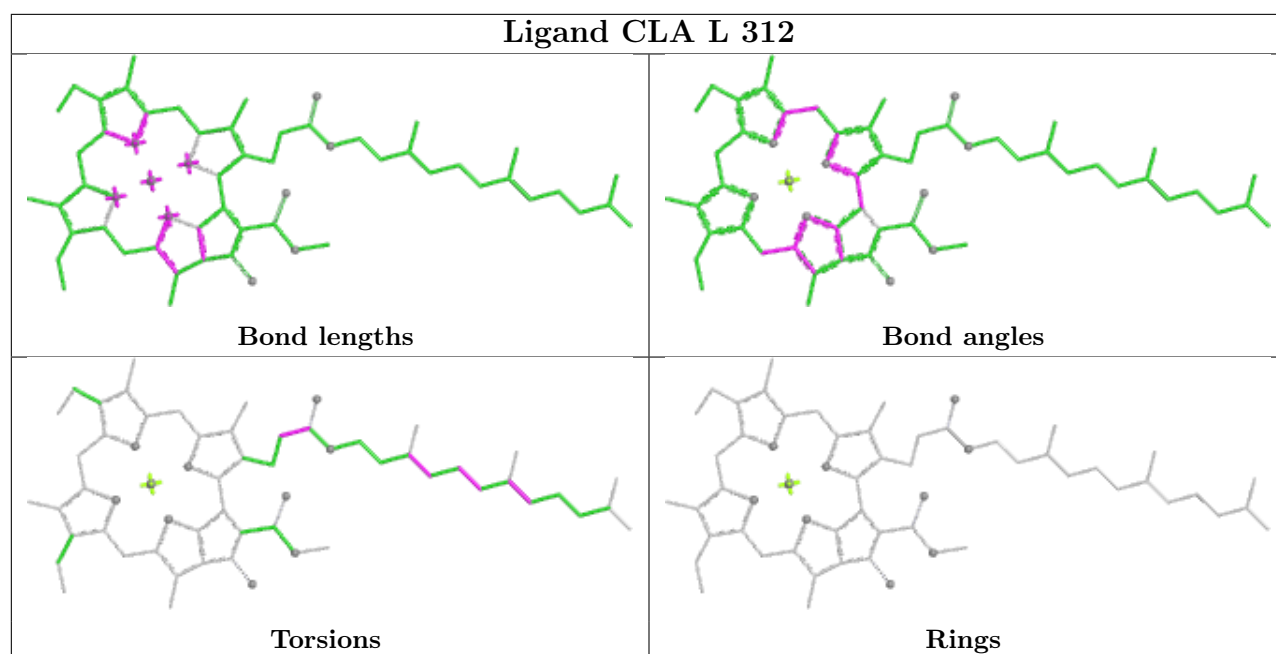




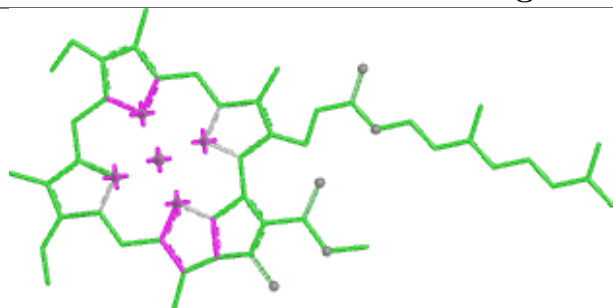




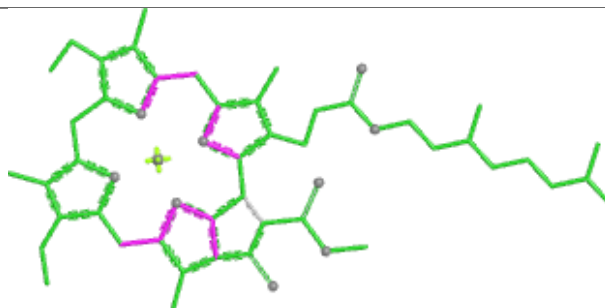




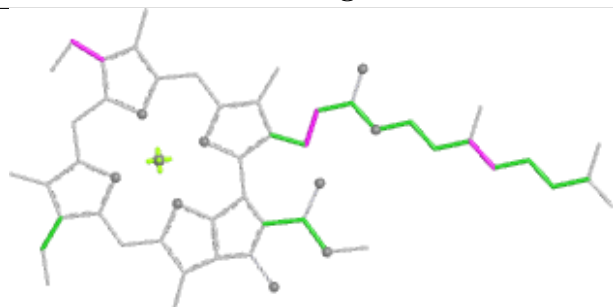
Ligand CLA F 309



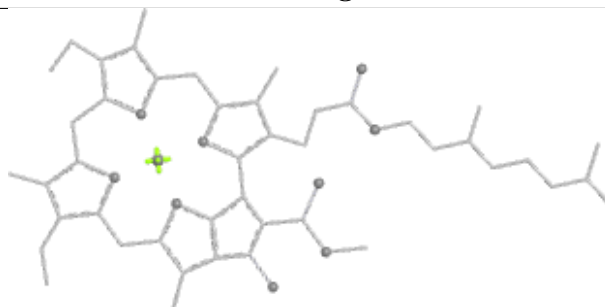
Bond lengths



Bond angles

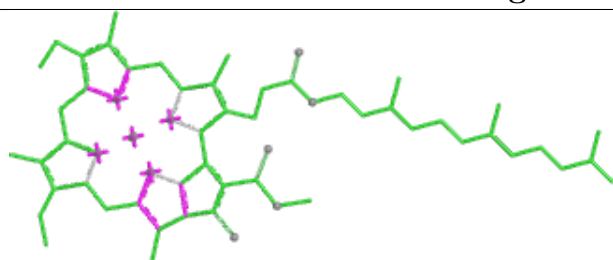


Torsions

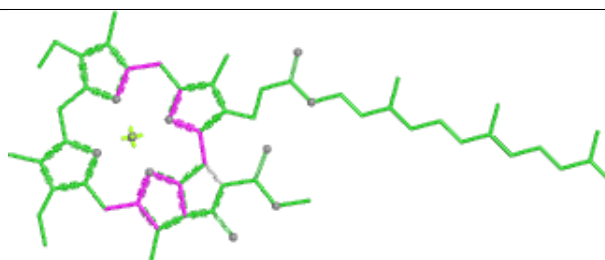


Rings

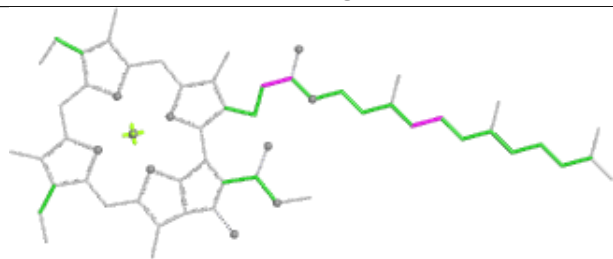
Ligand CLA W 313



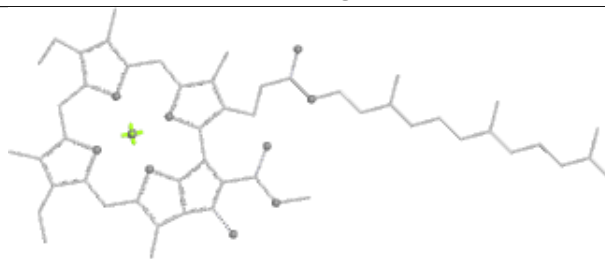
Bond lengths



Bond angles

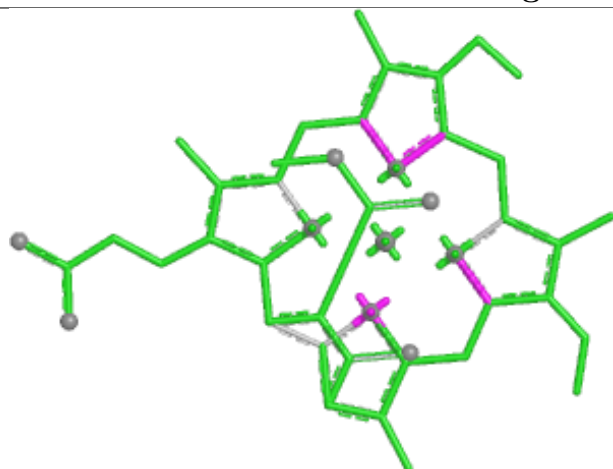


Torsions

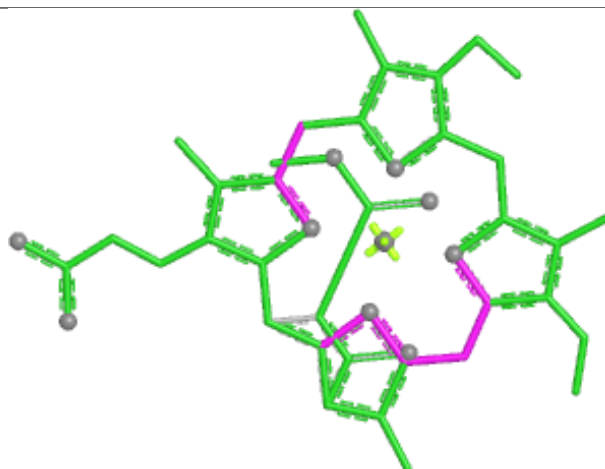


Rings

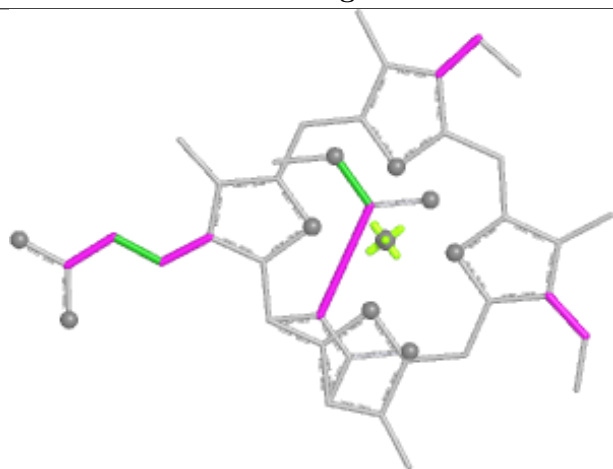
Ligand KC2 I 316



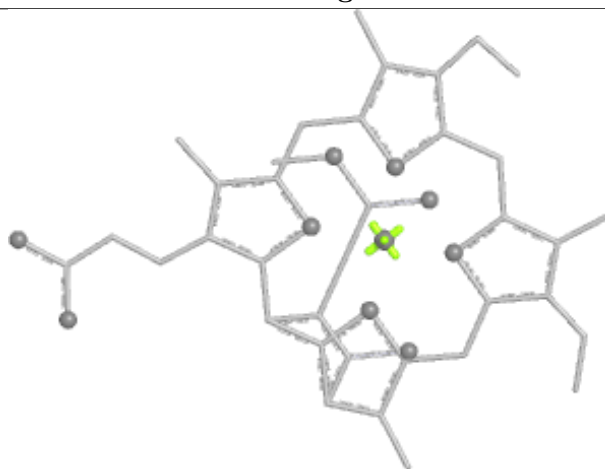
Bond lengths



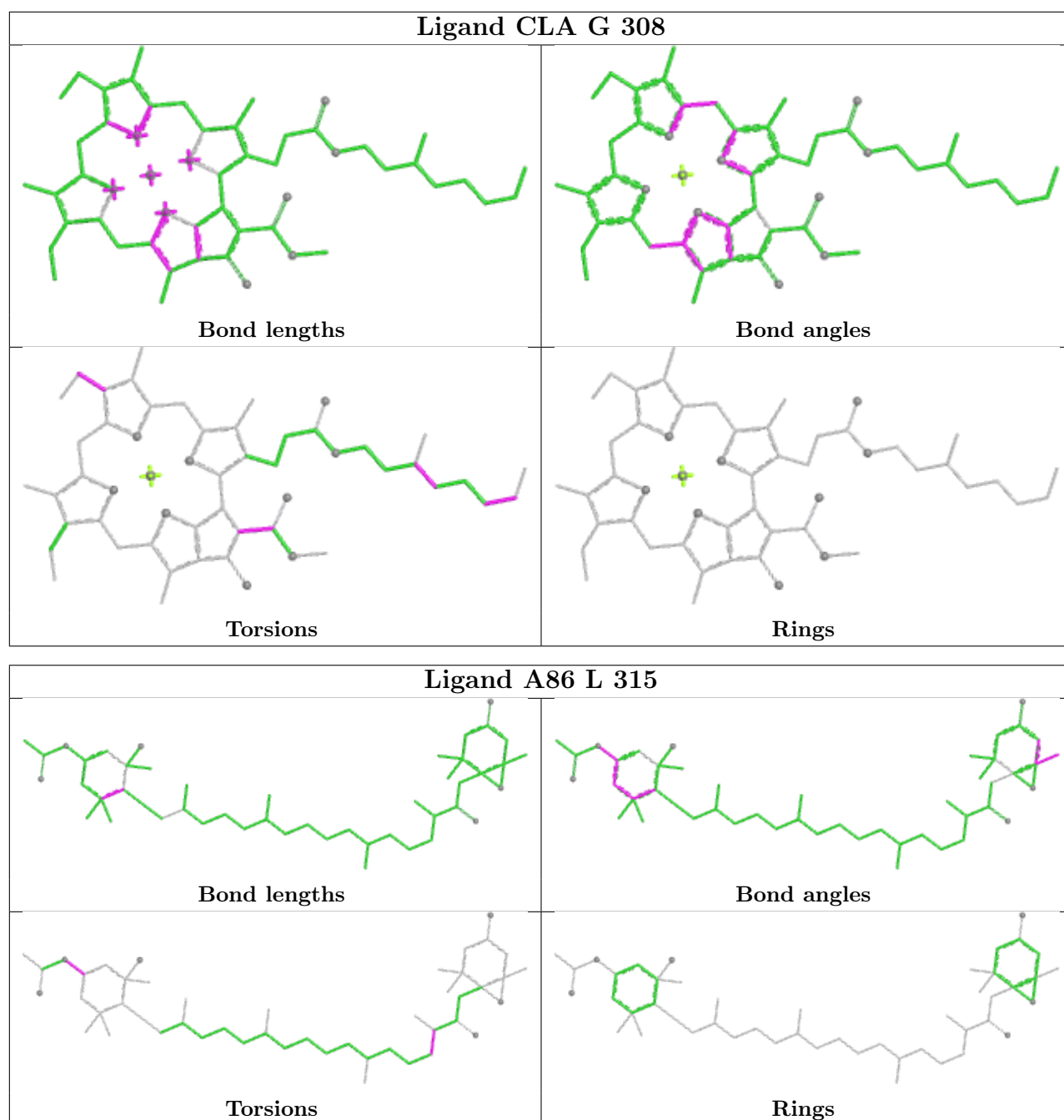
Bond angles



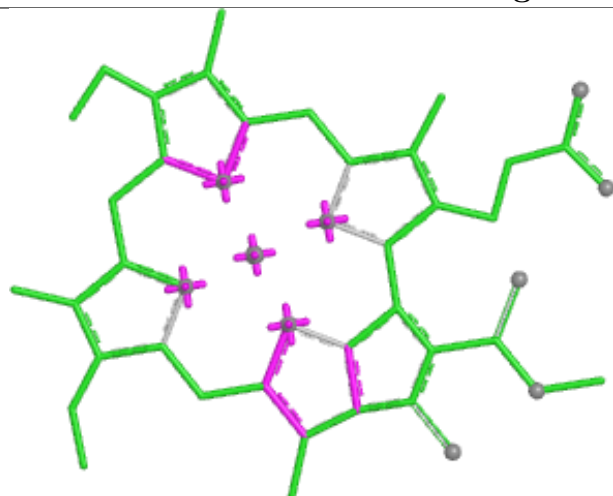
Torsions



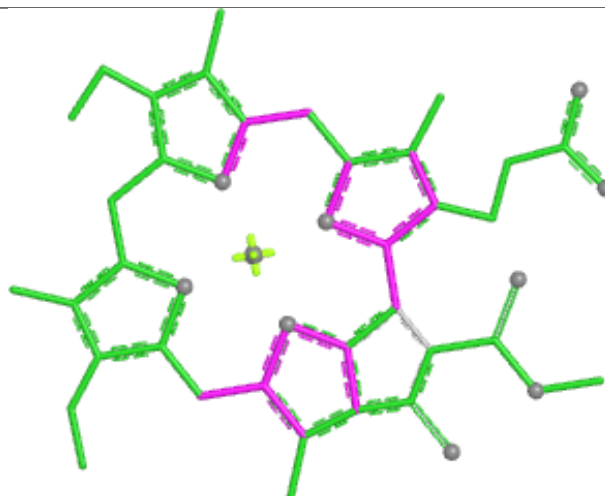
Rings



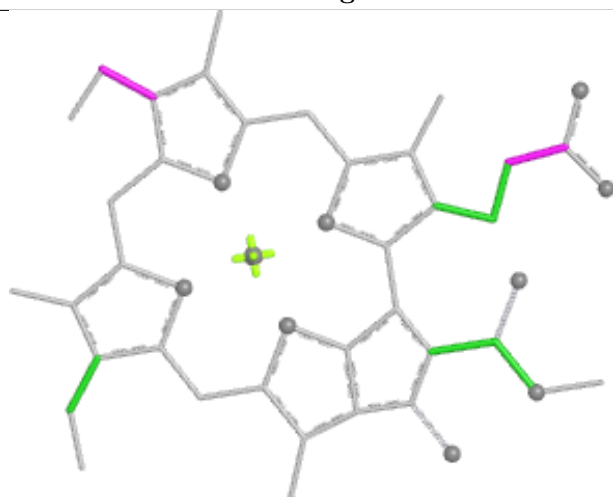
Ligand CLA U 303



Bond lengths



Bond angles

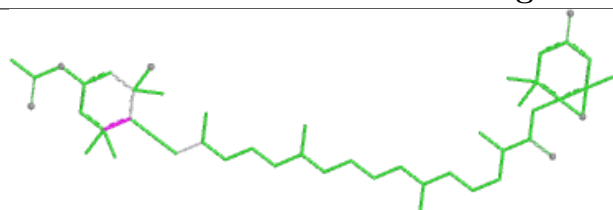


Torsions

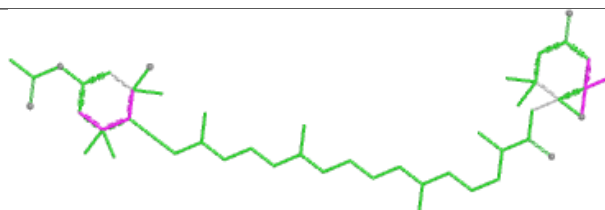


Rings

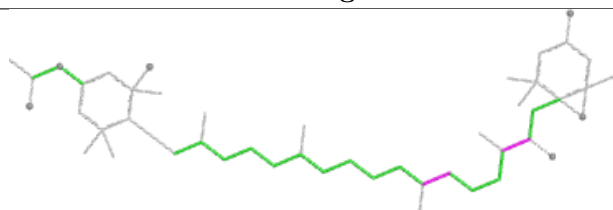
Ligand A86 M 318



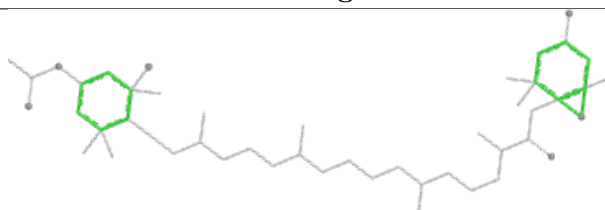
Bond lengths



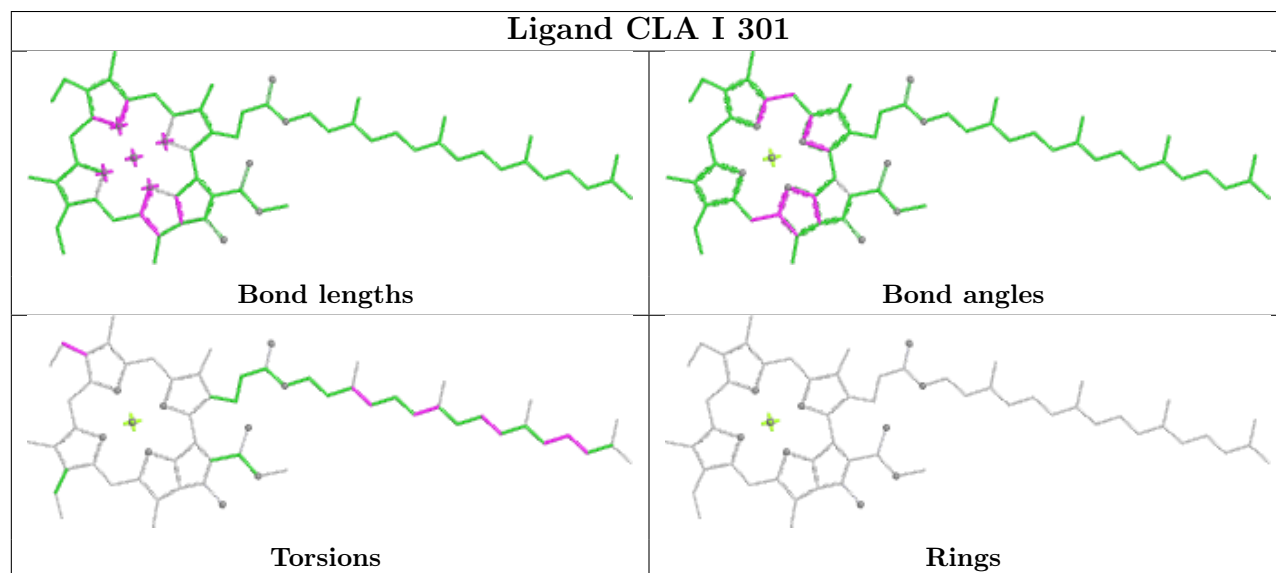
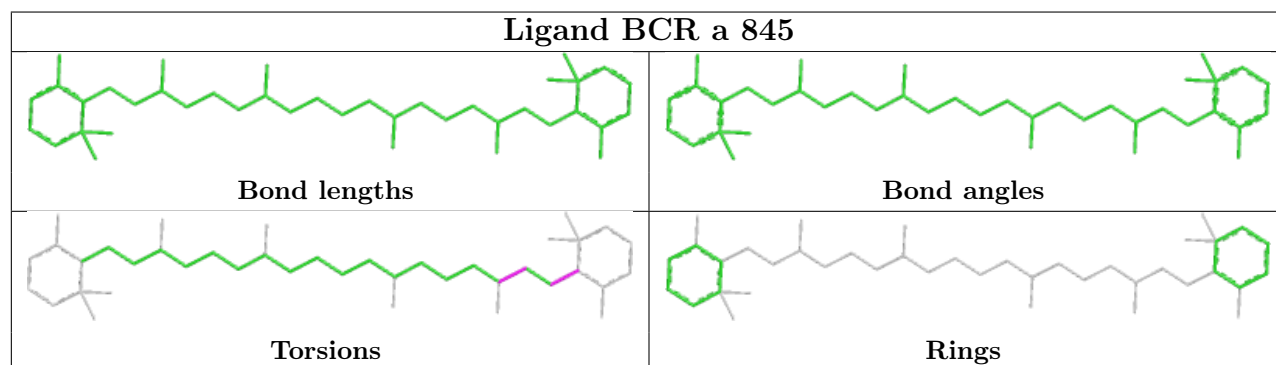
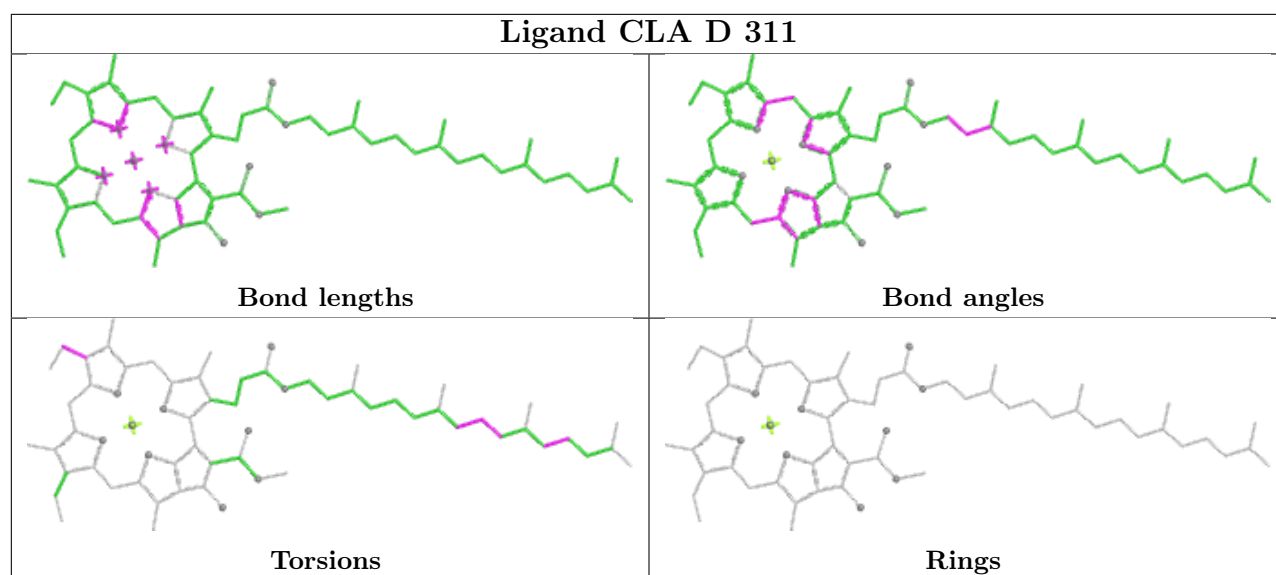
Bond angles



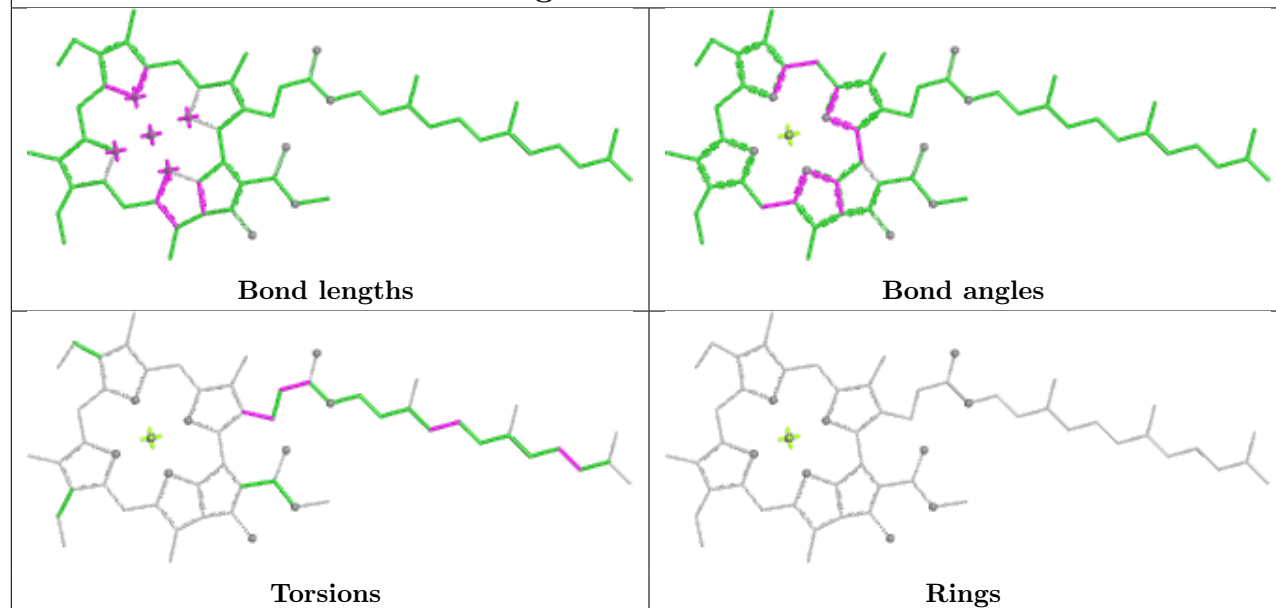
Torsions



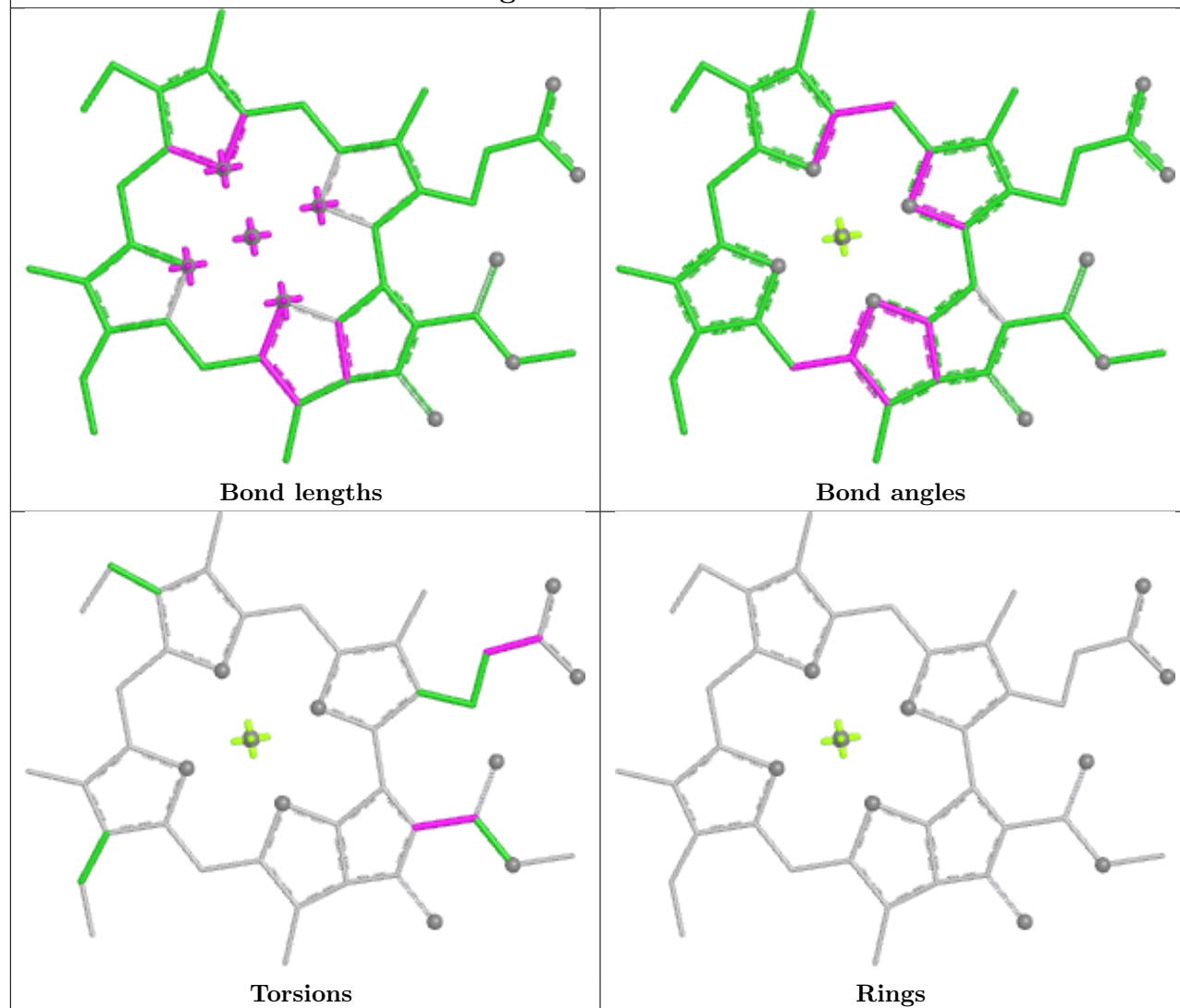
Rings



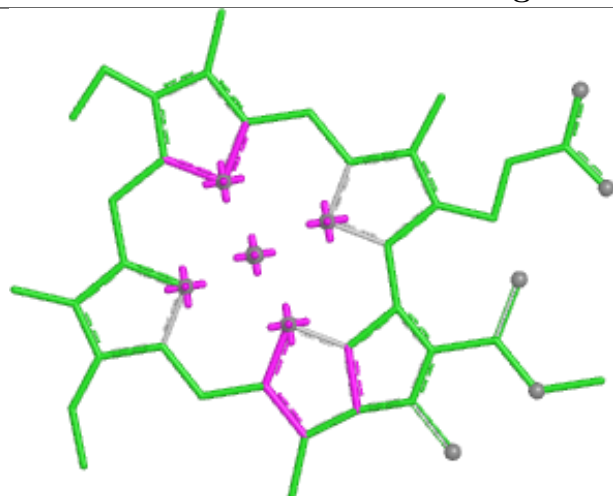
Ligand CLA b 810



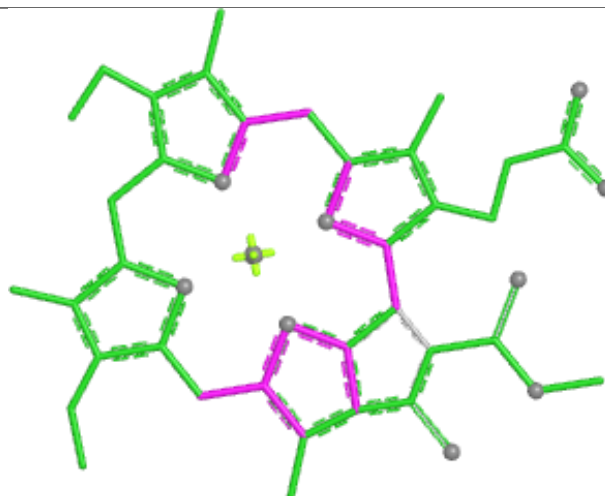
Ligand CLA l 202



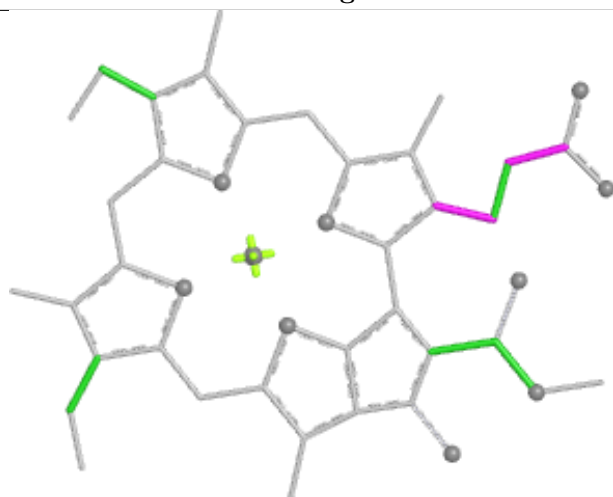
Ligand CLA K 310



Bond lengths



Bond angles

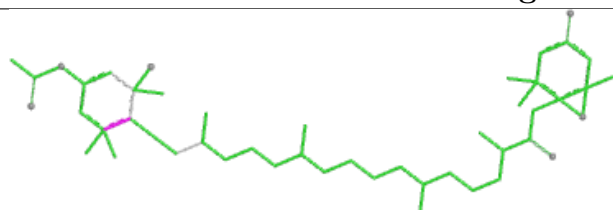


Torsions

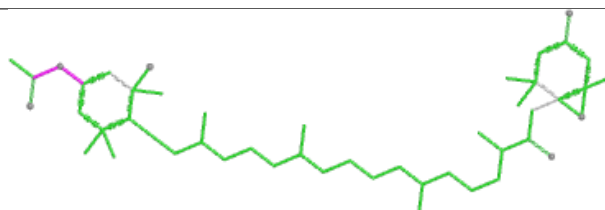


Rings

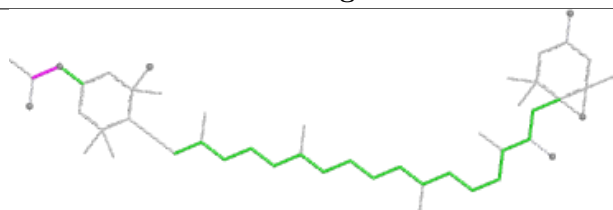
Ligand A86 N 315



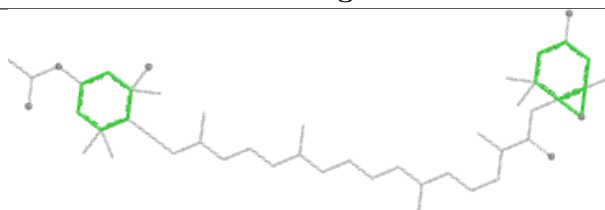
Bond lengths



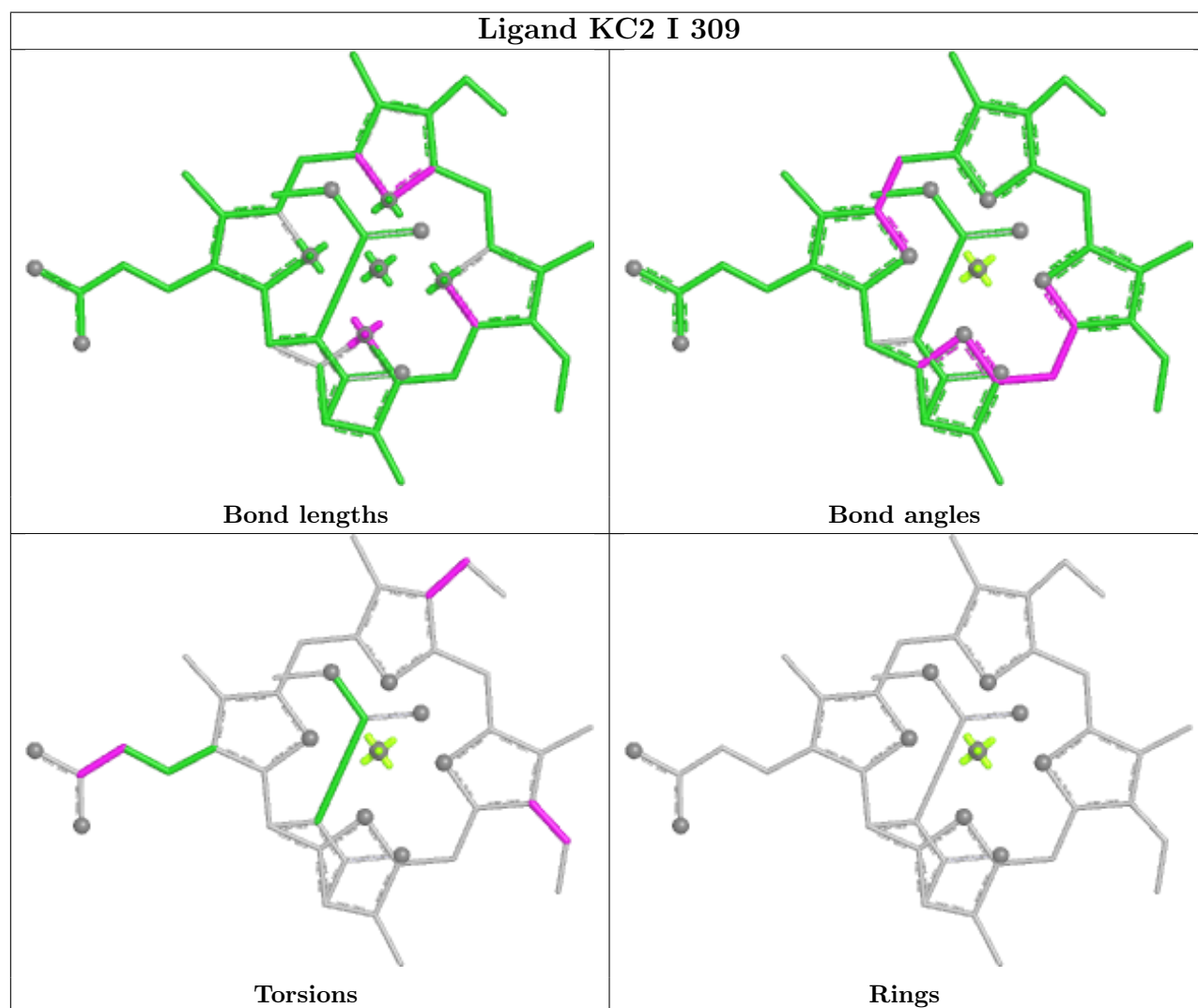
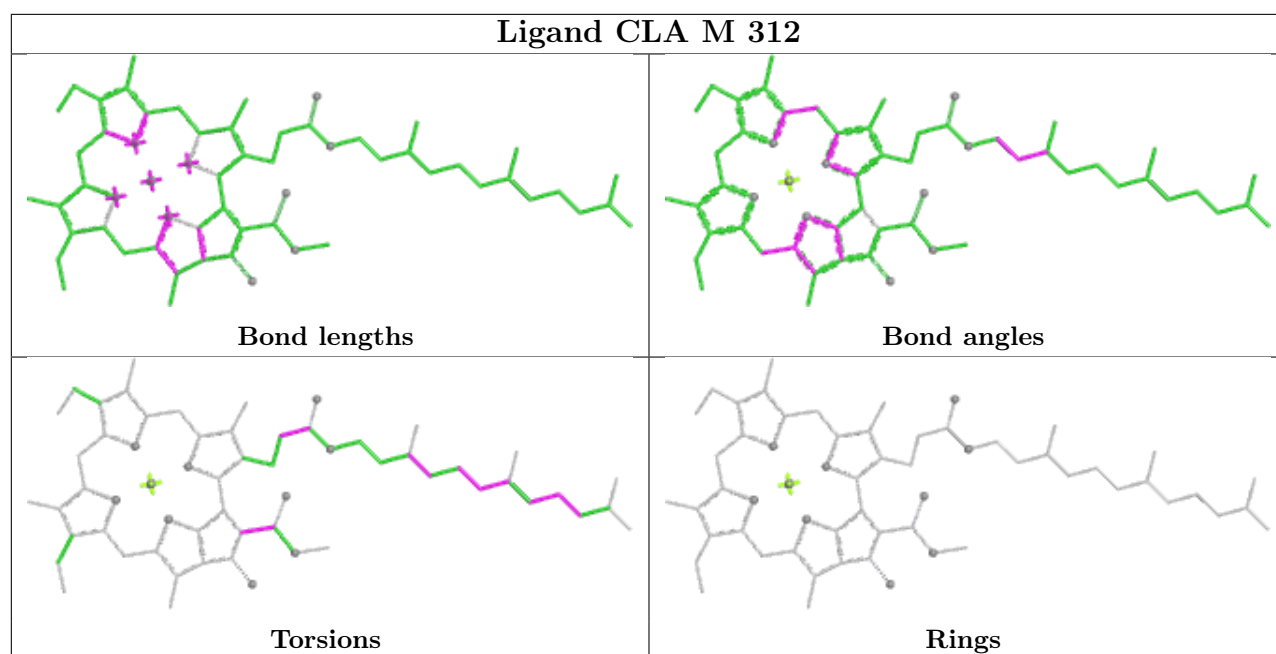
Bond angles

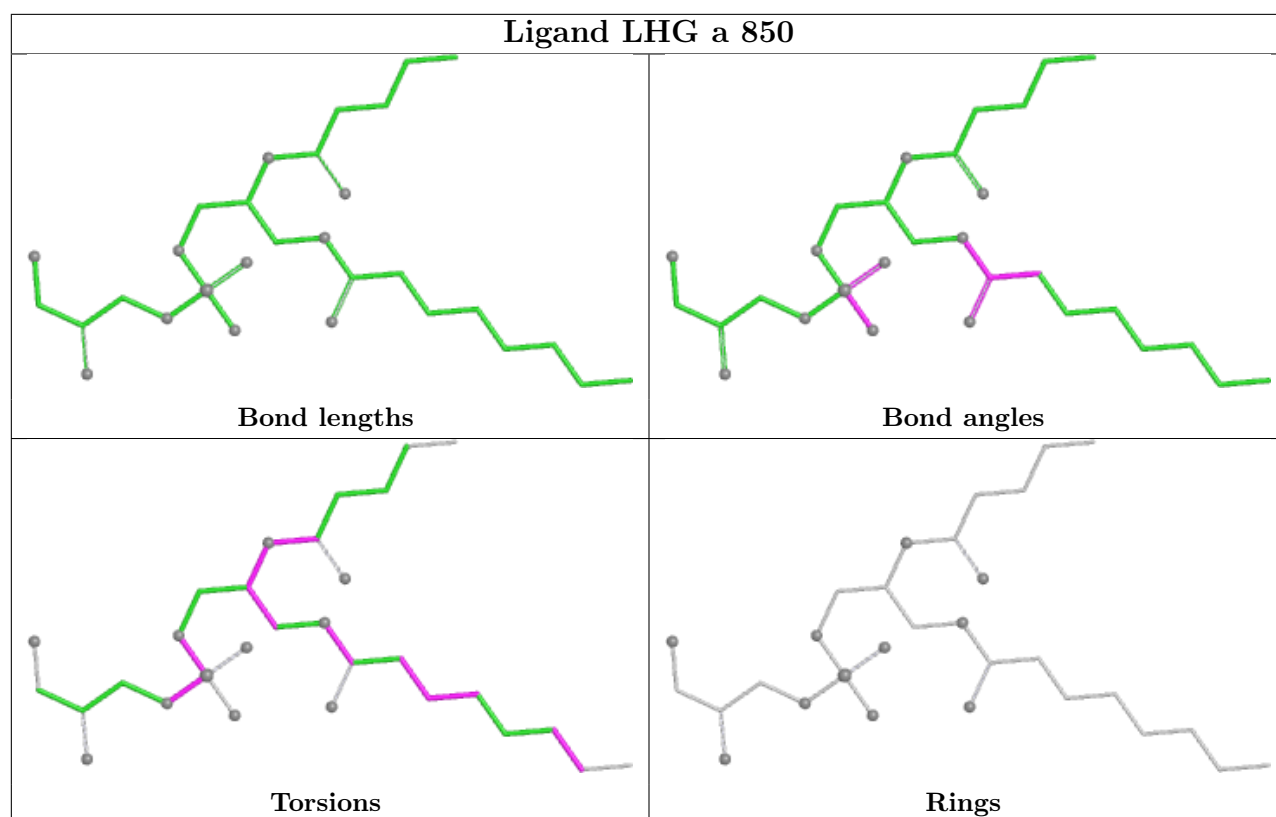


Torsions

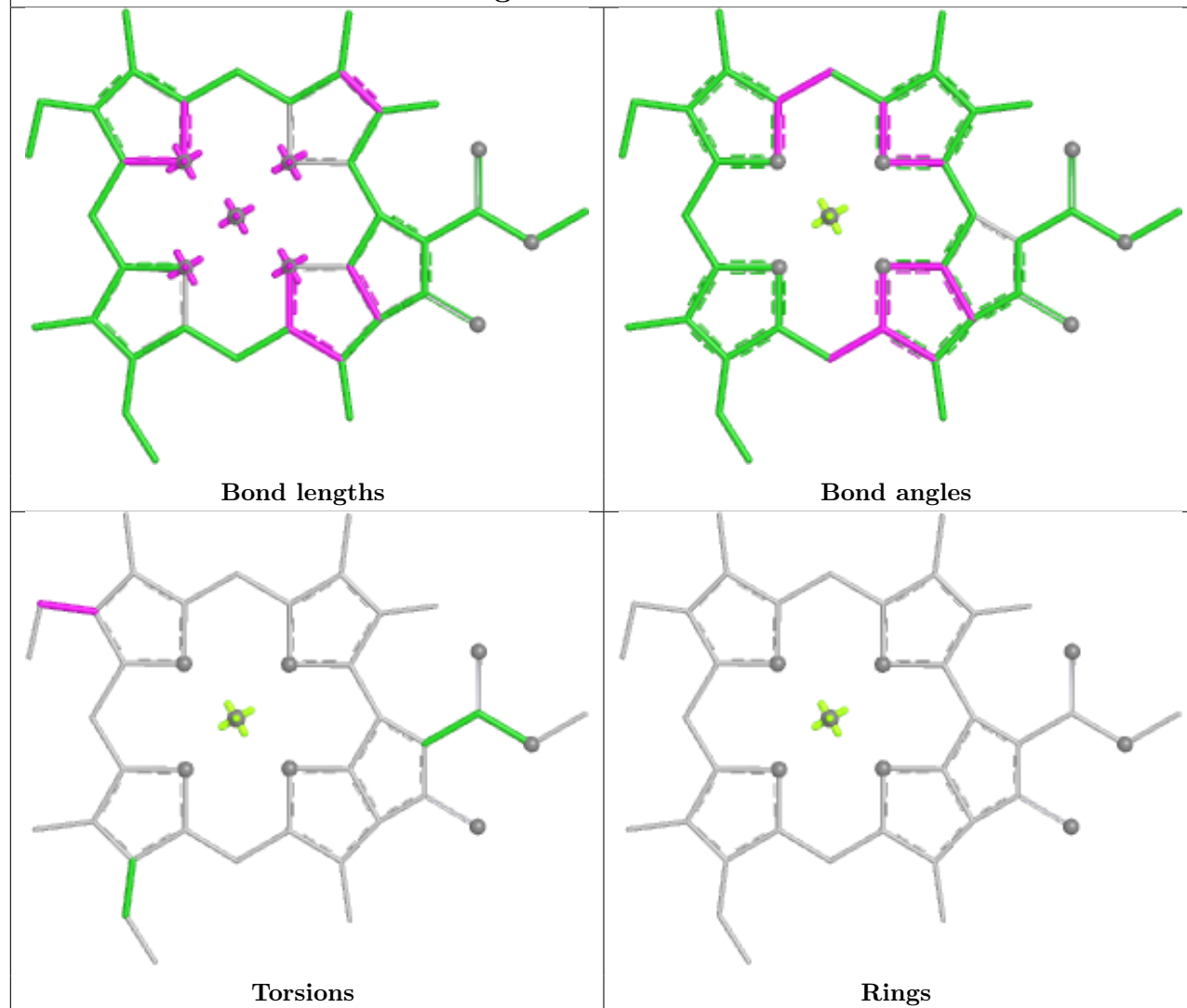


Rings

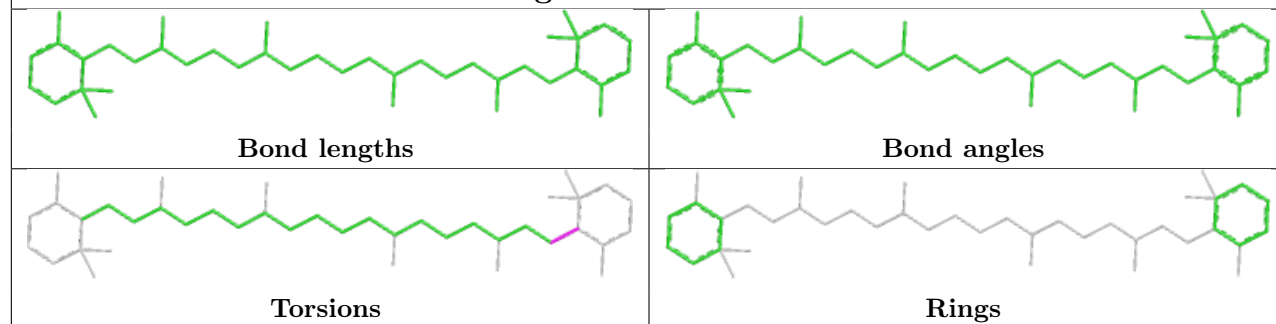


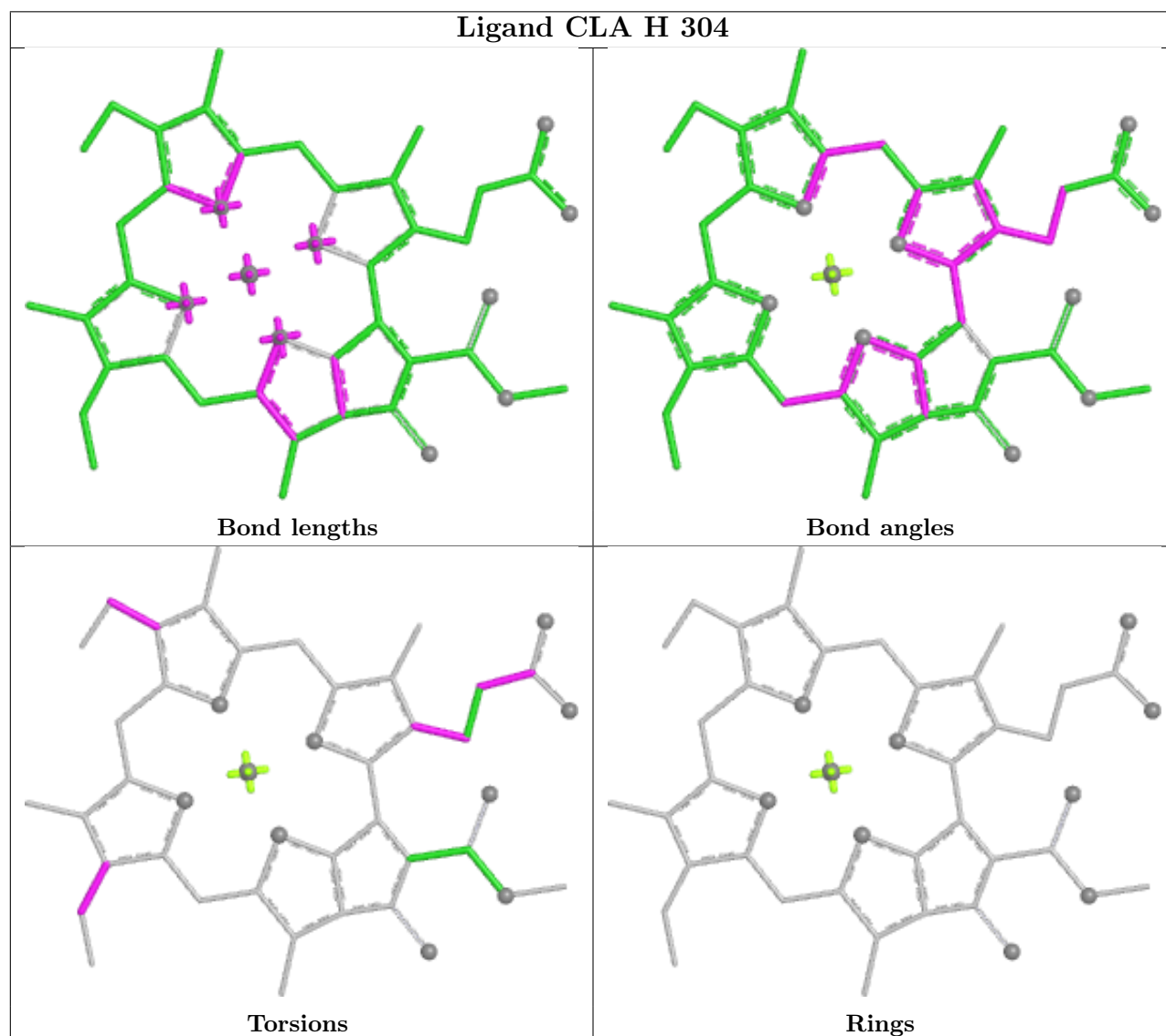
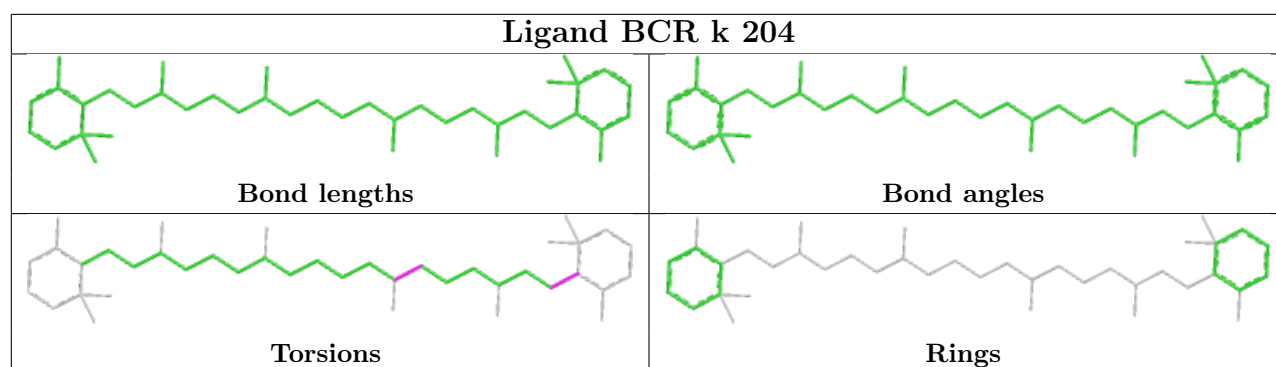


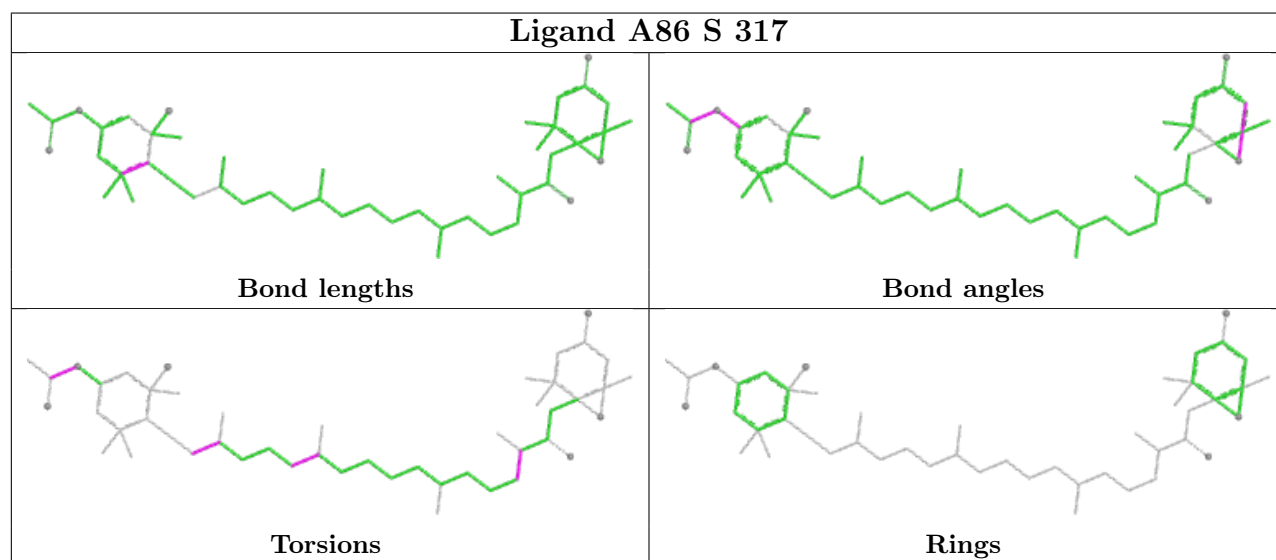
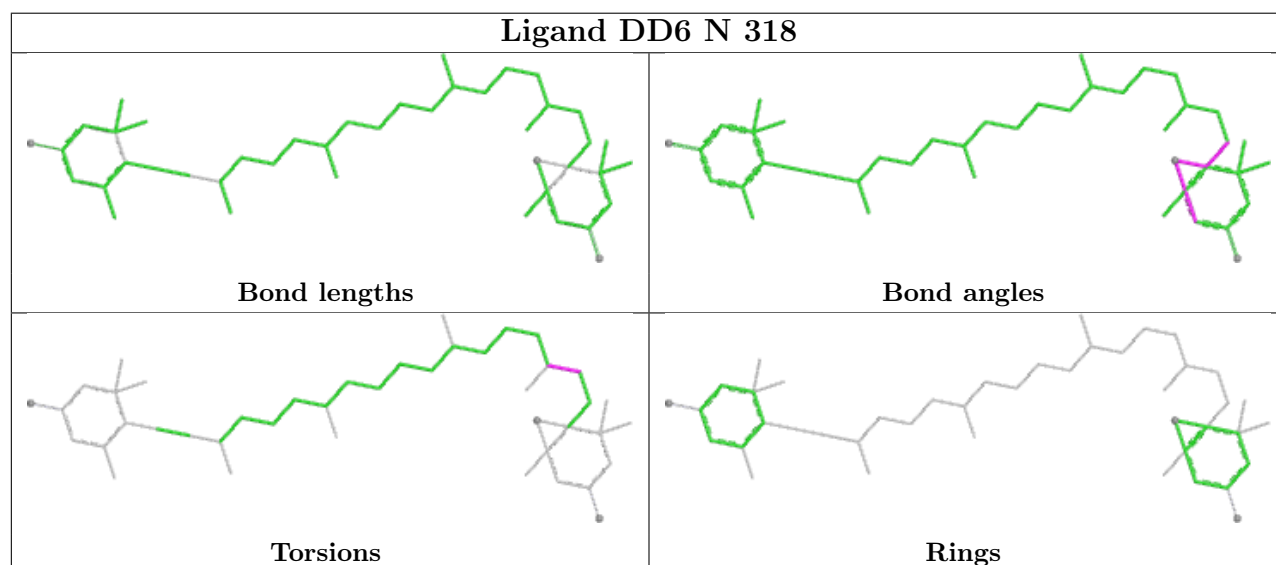
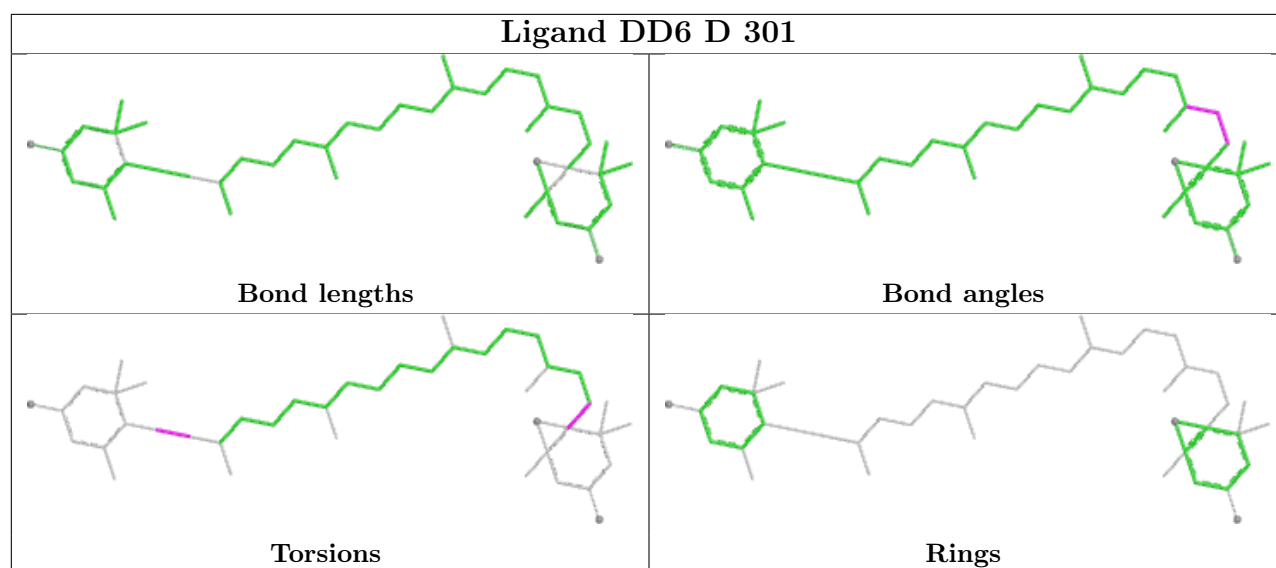
Ligand CLA R 309

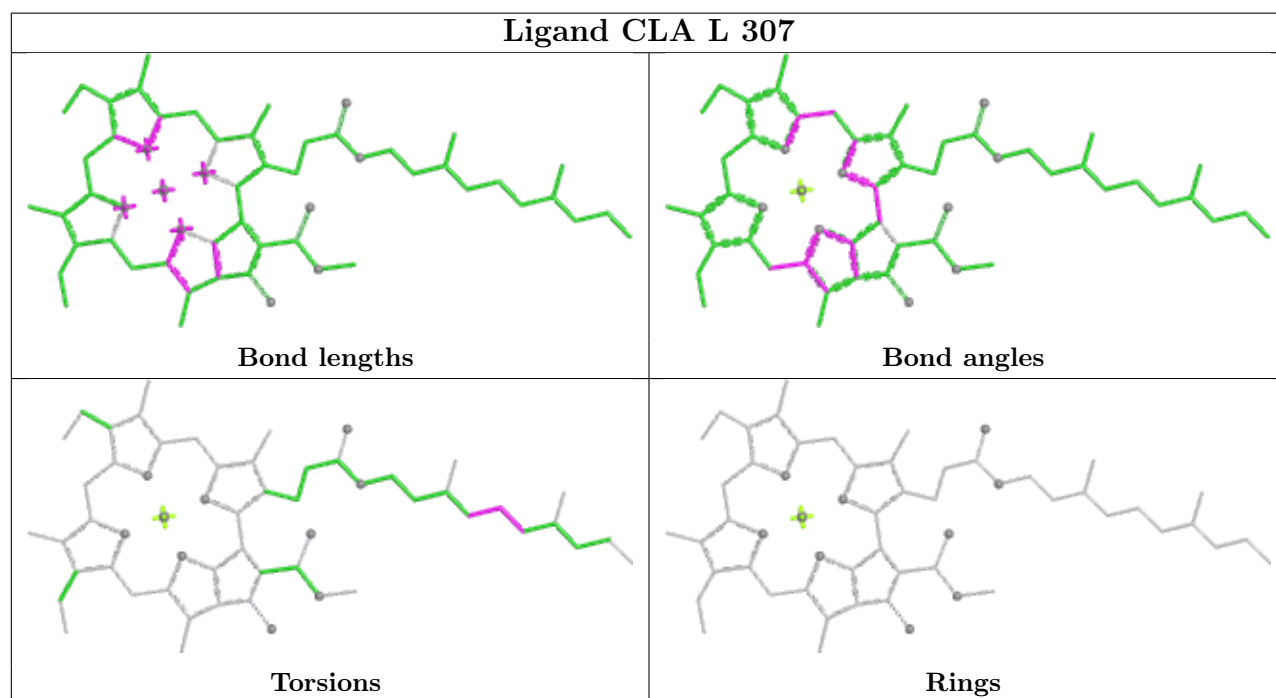
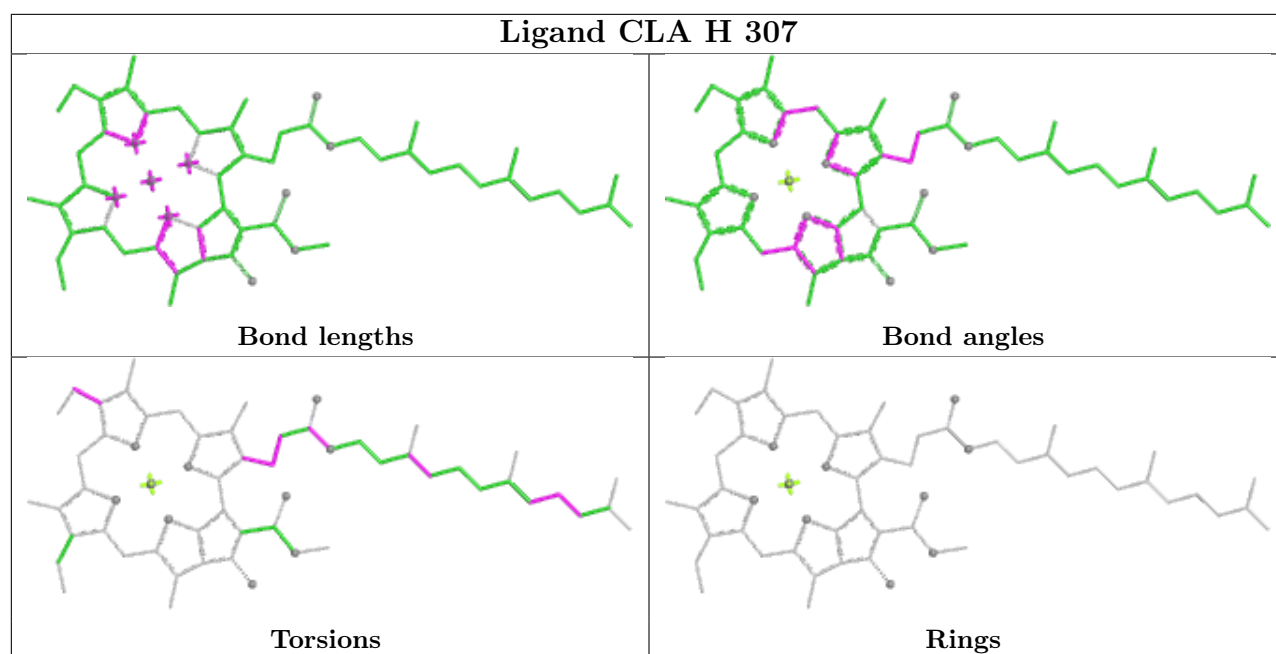


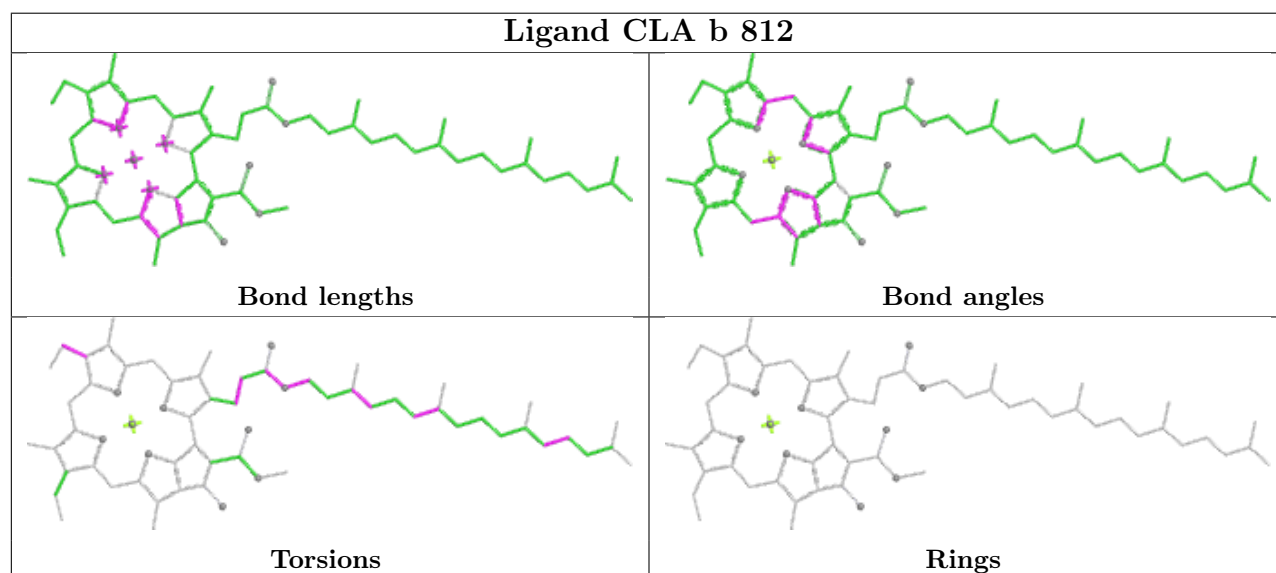
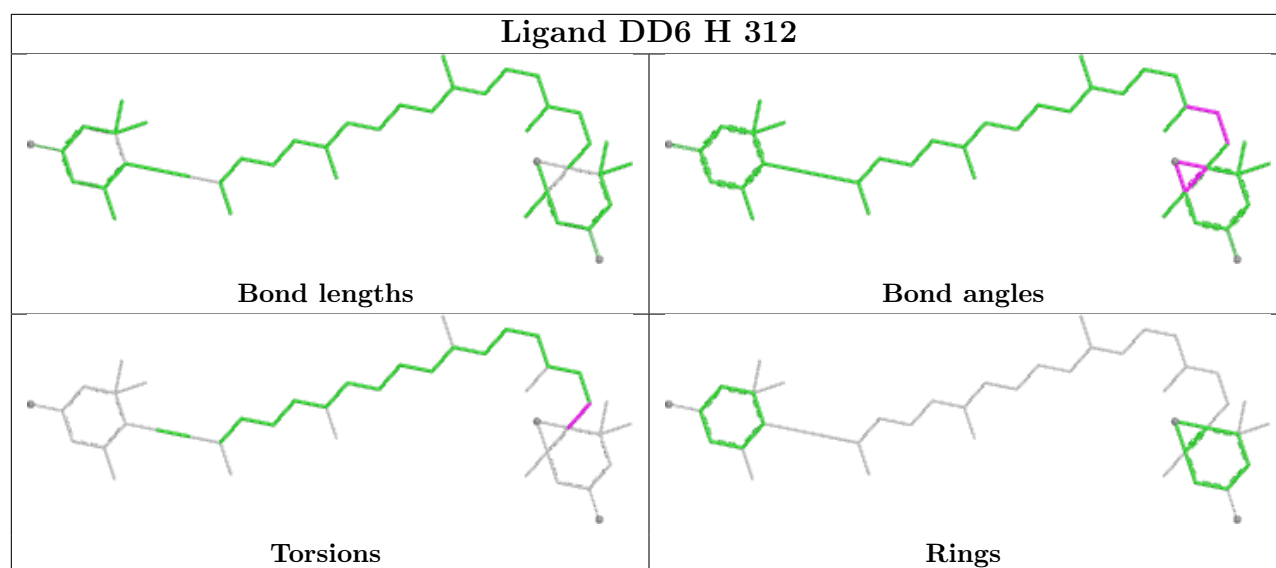
Ligand BCR a 846

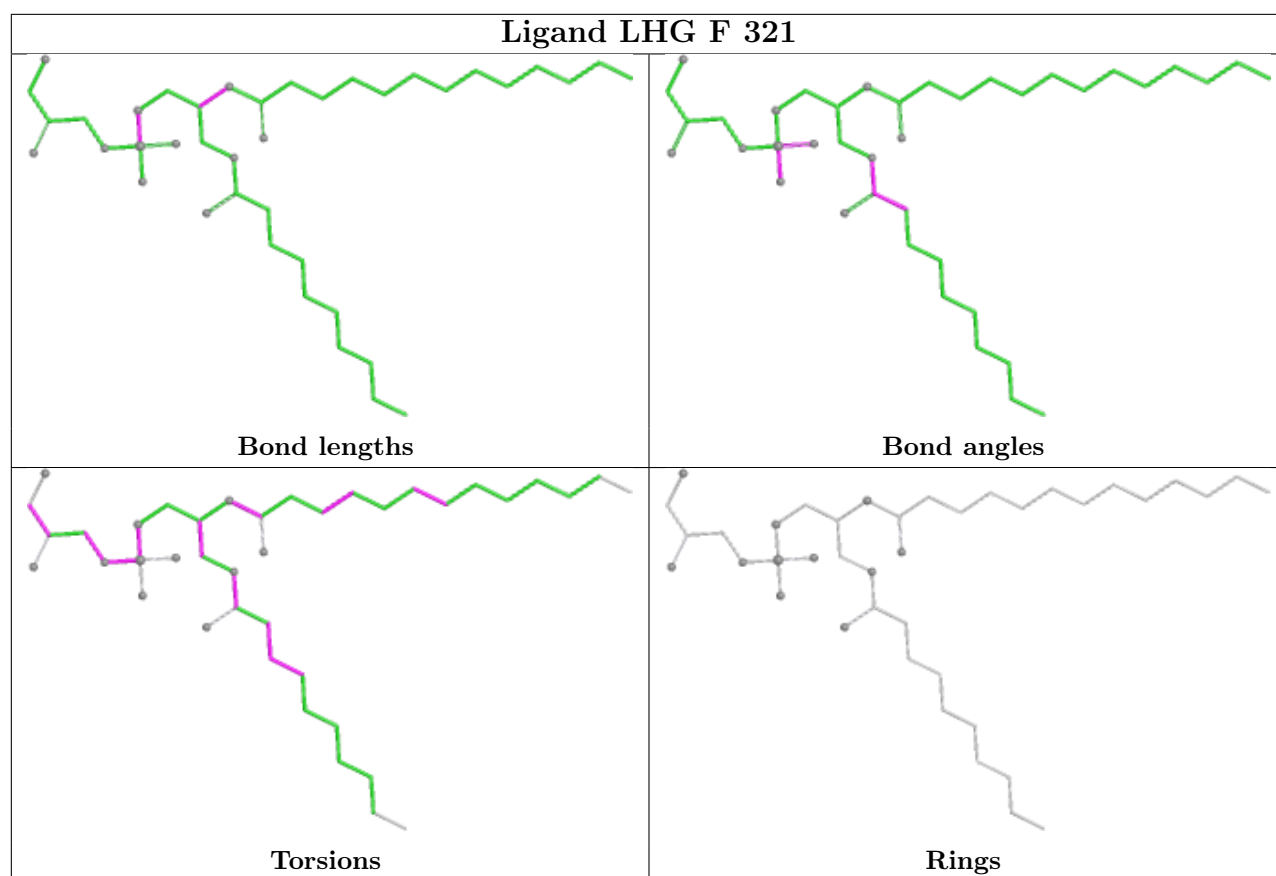




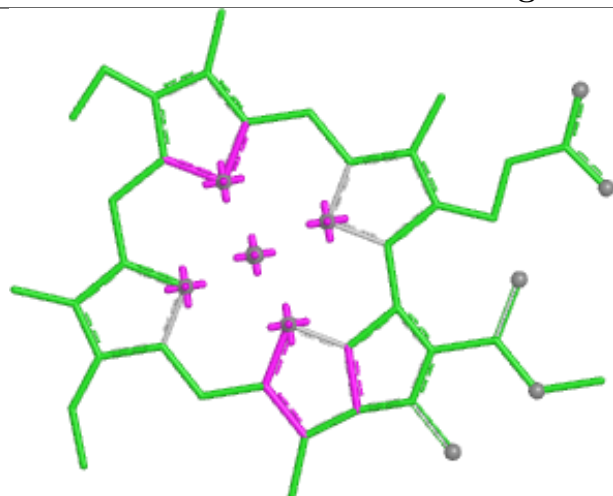




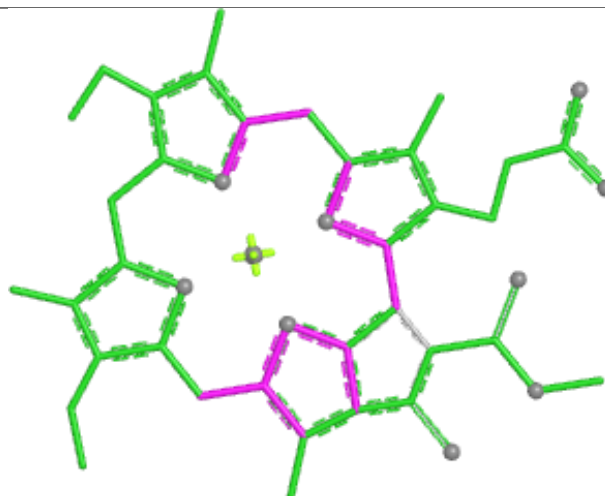




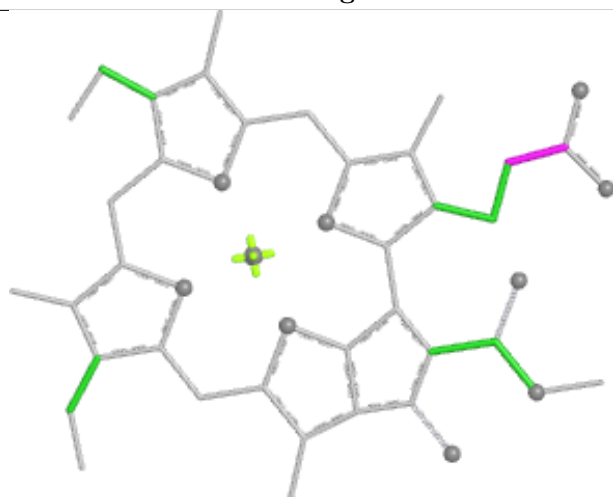
Ligand CLA J 311



Bond lengths



Bond angles

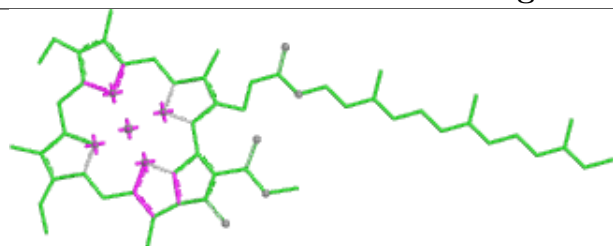


Torsions

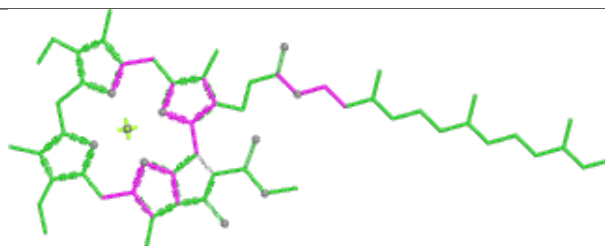


Rings

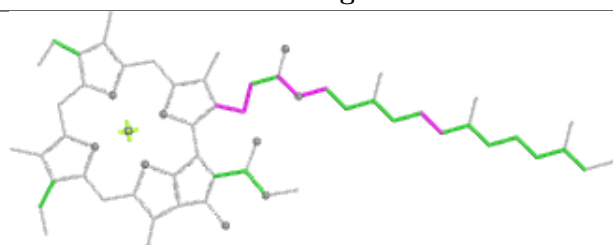
Ligand CLA b 830



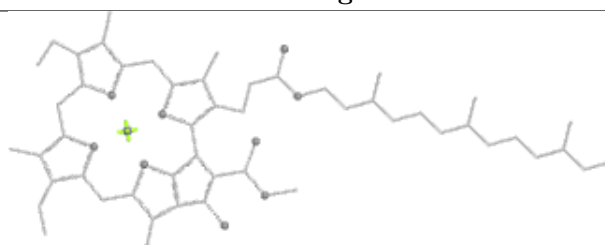
Bond lengths



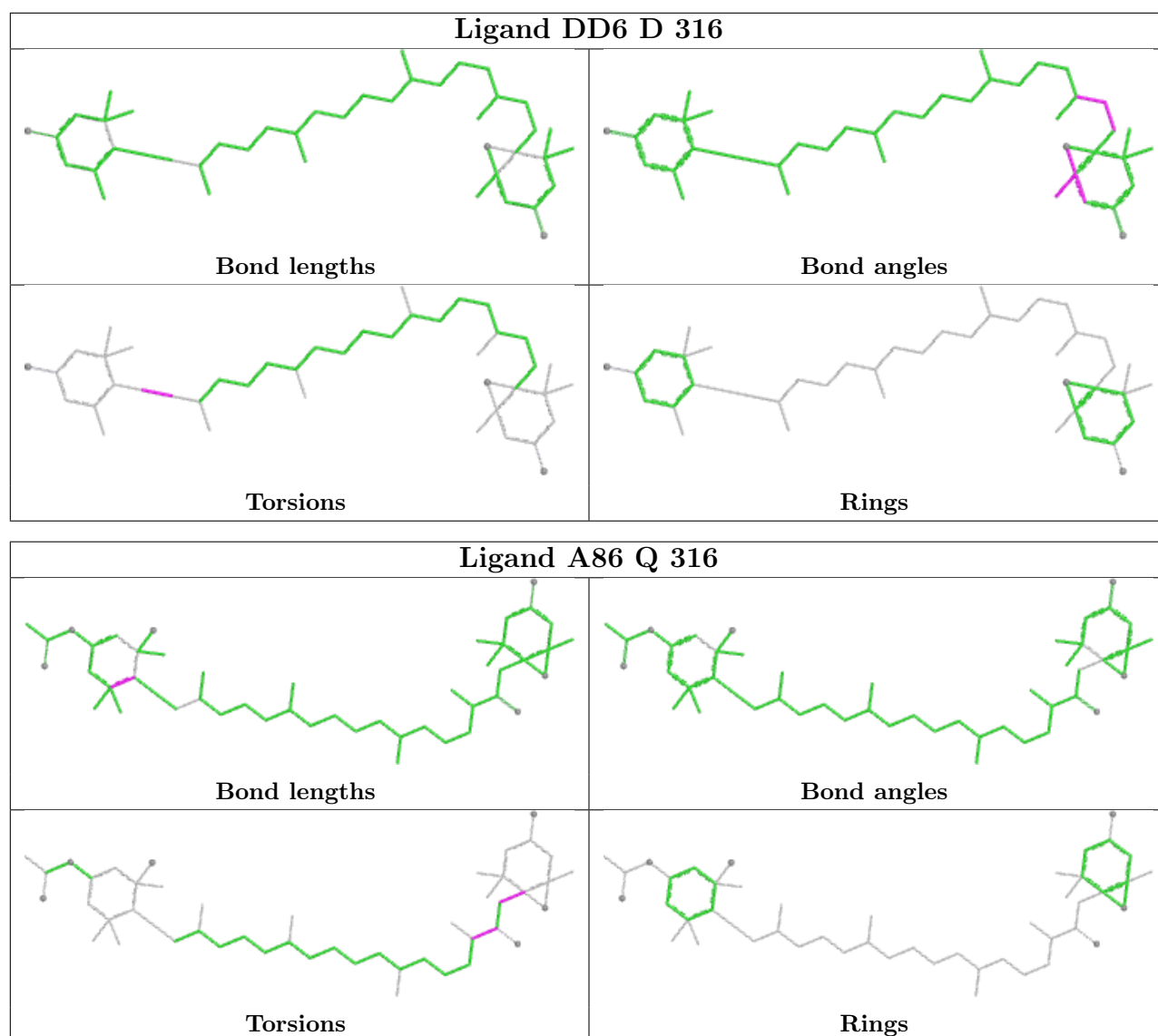
Bond angles



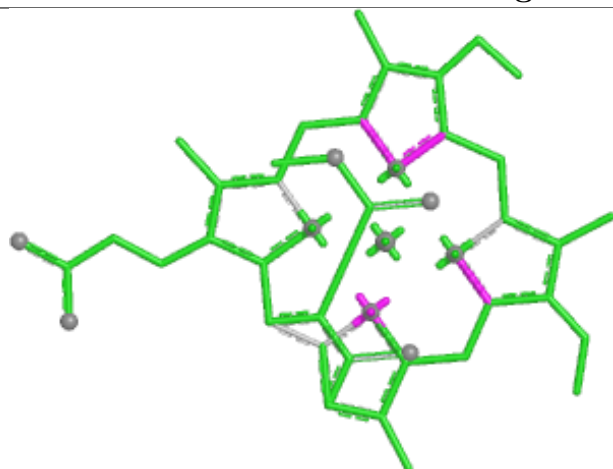
Torsions



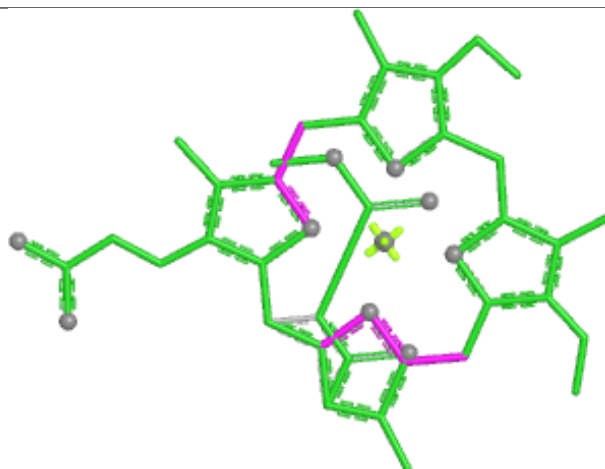
Rings



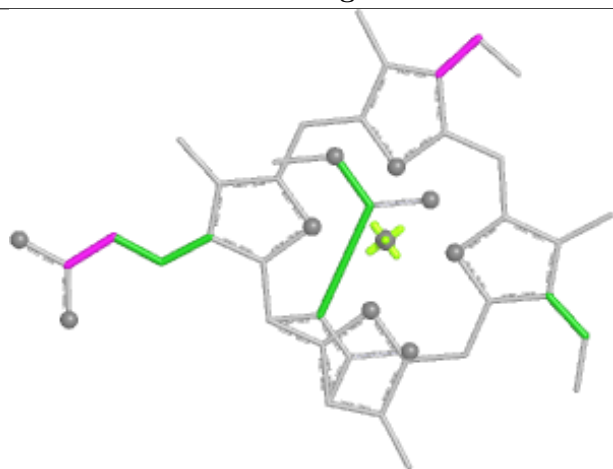
Ligand KC2 N 302



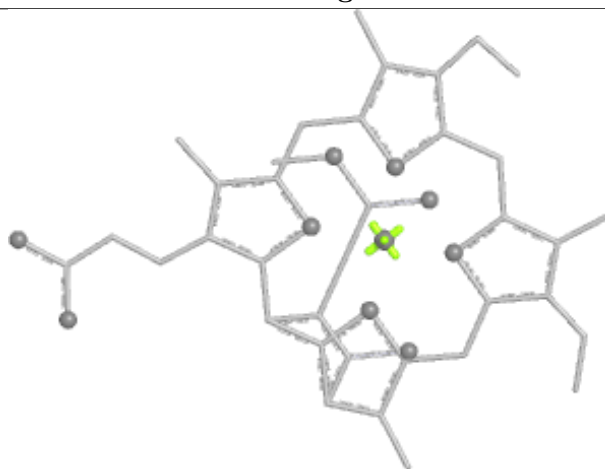
Bond lengths



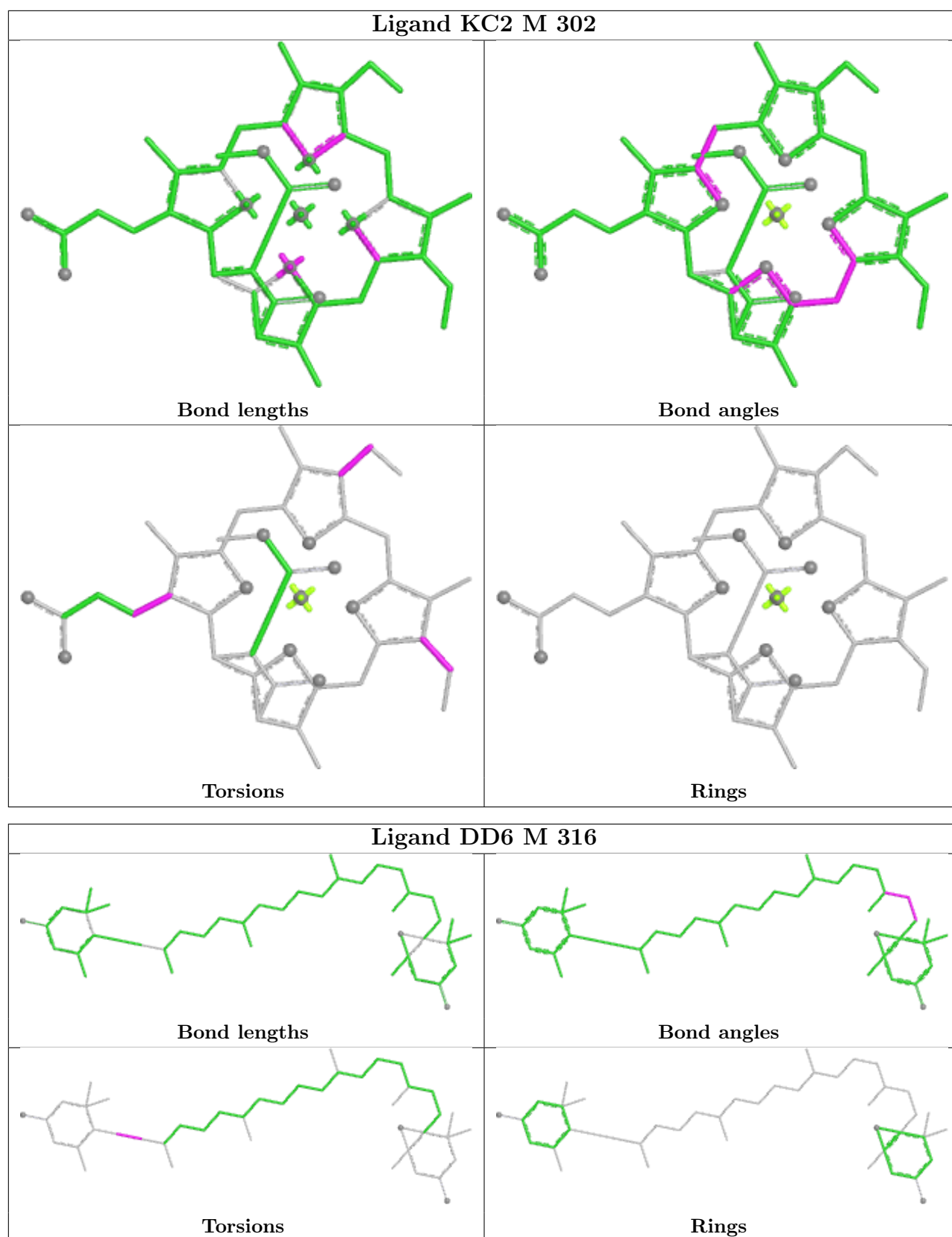
Bond angles



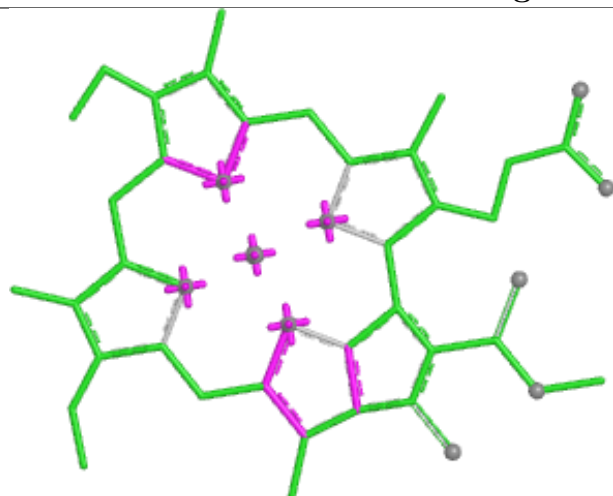
Torsions



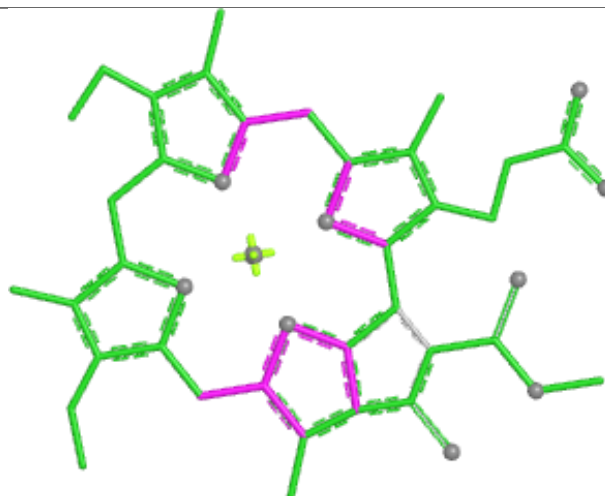
Rings



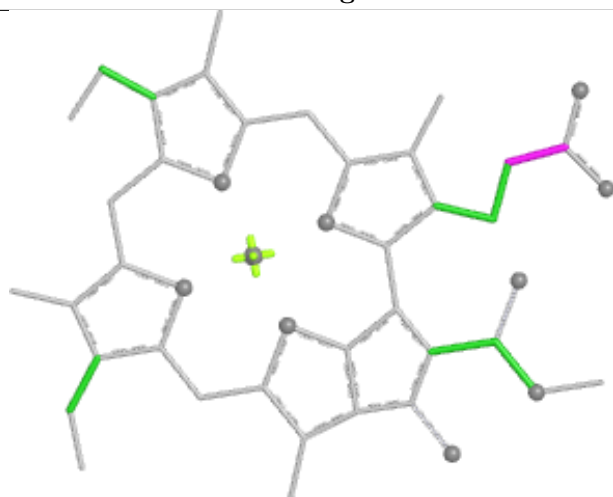
Ligand CLA D 309



Bond lengths



Bond angles

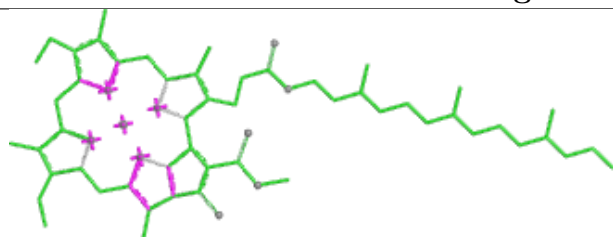


Torsions

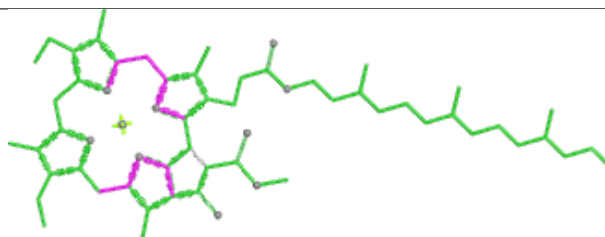


Rings

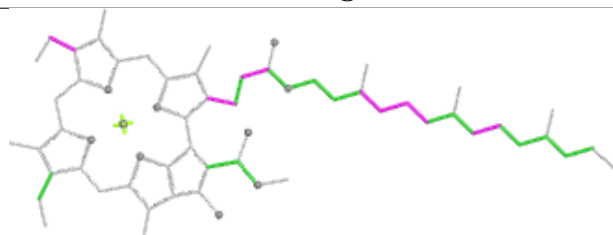
Ligand CLA A 303



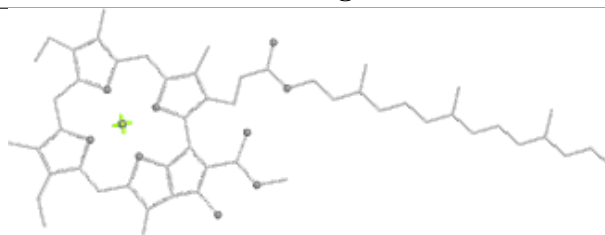
Bond lengths



Bond angles

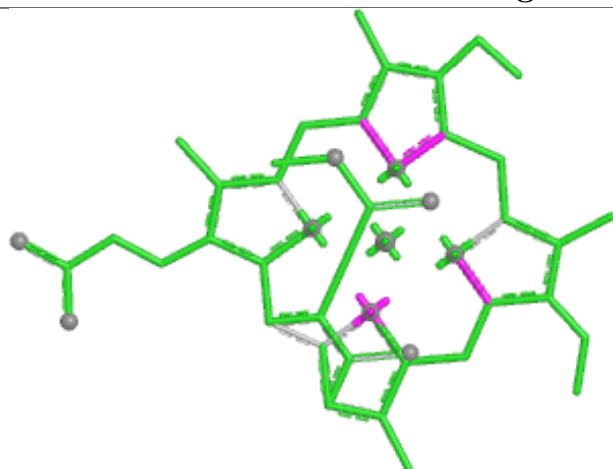


Torsions

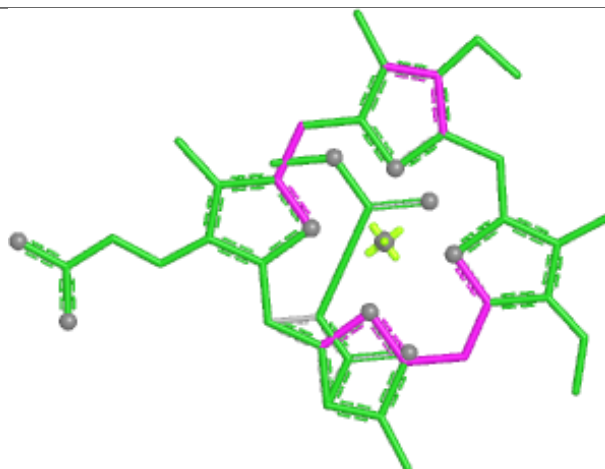


Rings

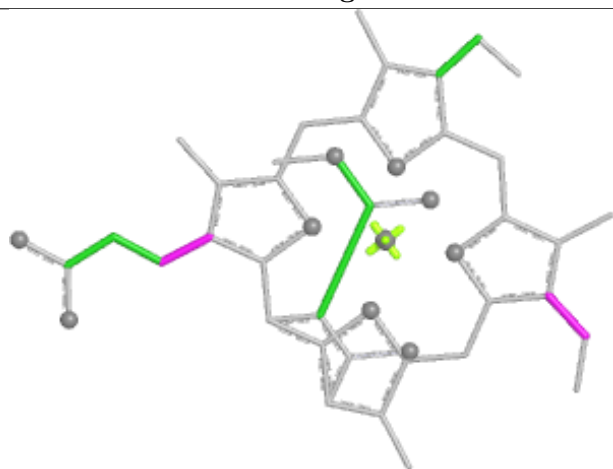
Ligand KC2 T 304



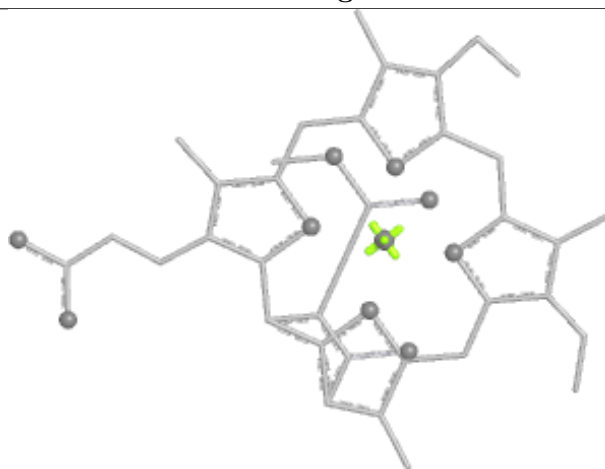
Bond lengths



Bond angles

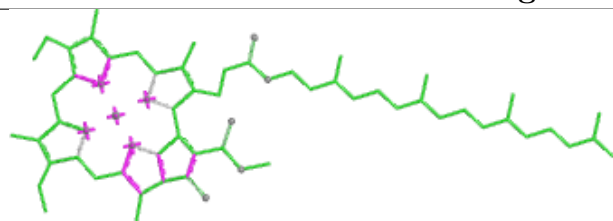


Torsions

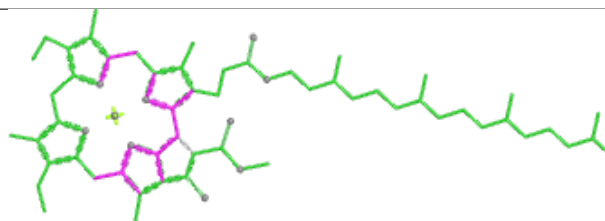


Rings

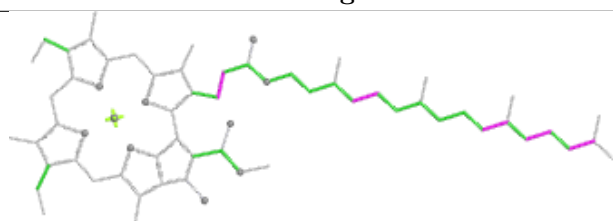
Ligand CLA a 801



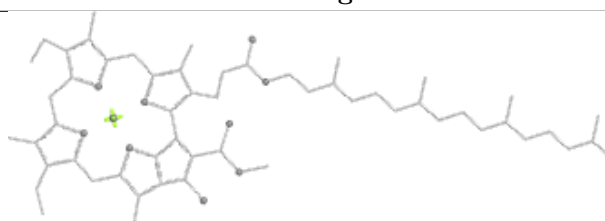
Bond lengths



Bond angles

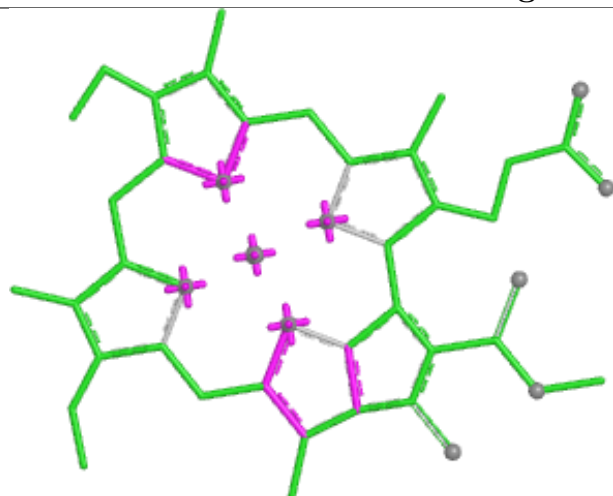


Torsions

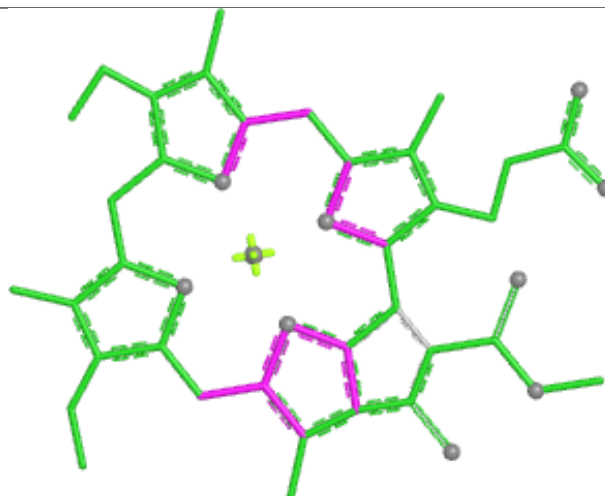


Rings

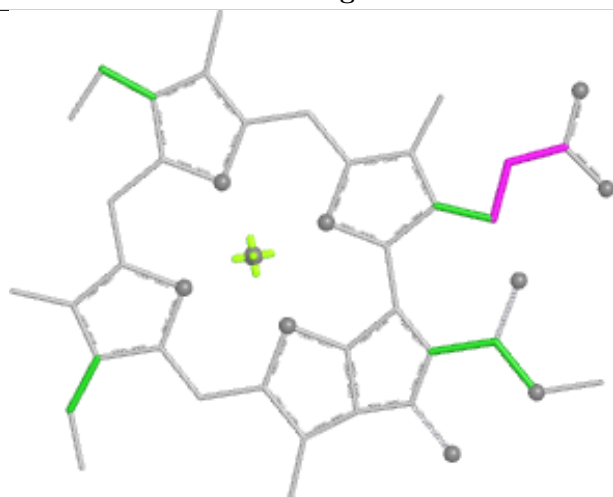
Ligand CLA J 301



Bond lengths



Bond angles

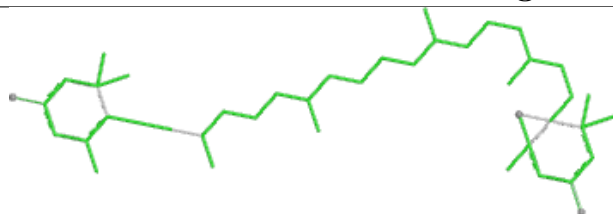


Torsions

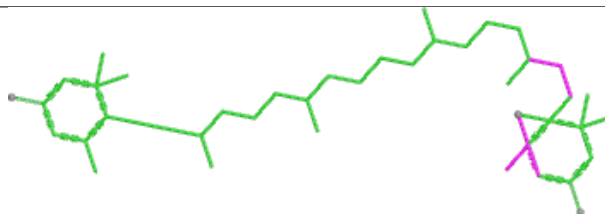


Rings

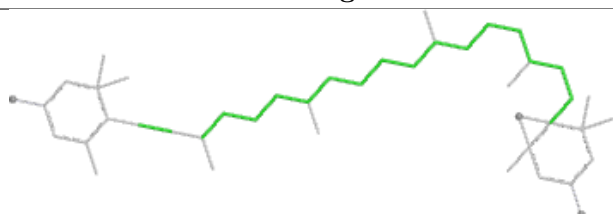
Ligand DD6 E 316



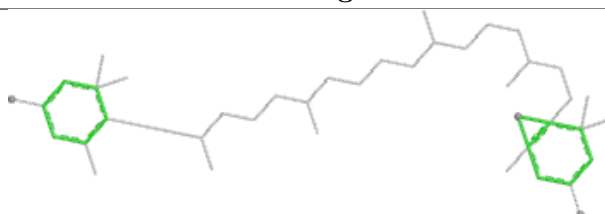
Bond lengths



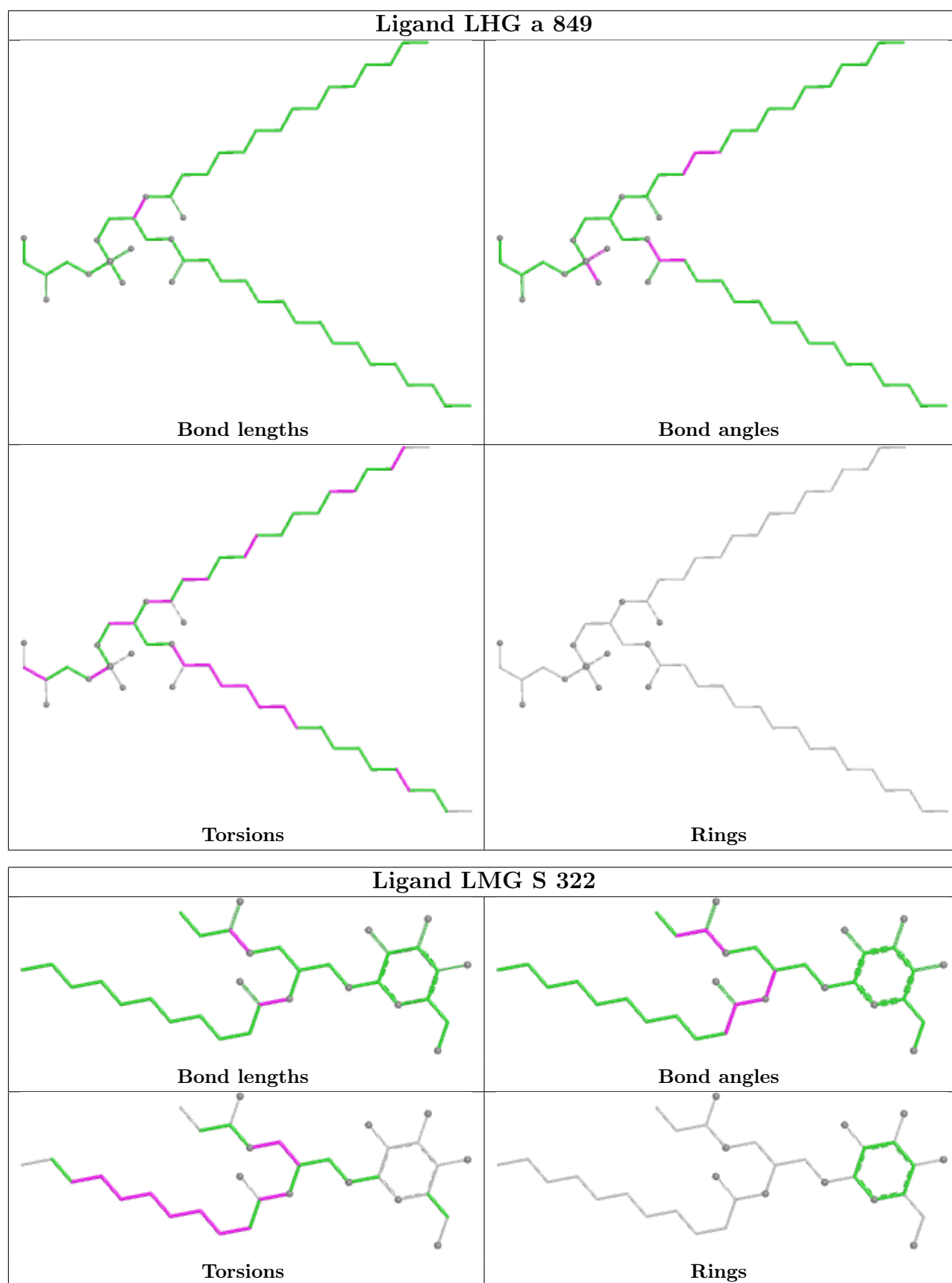
Bond angles

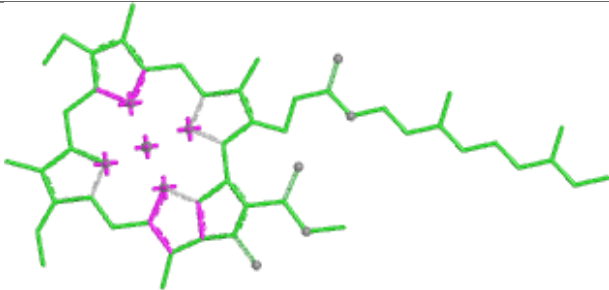
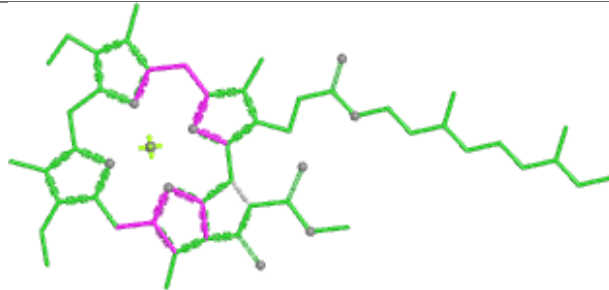
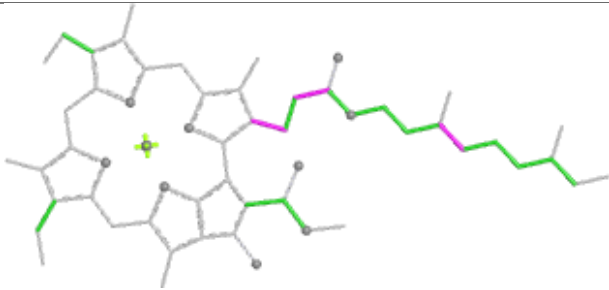
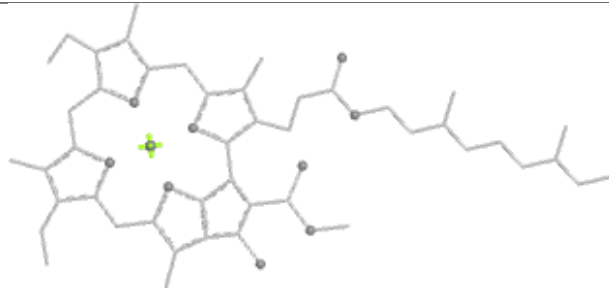


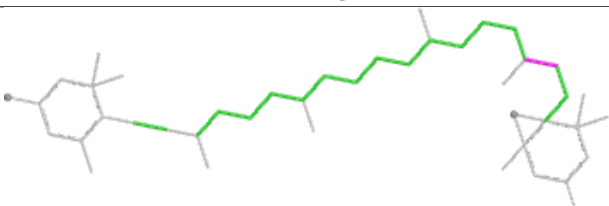
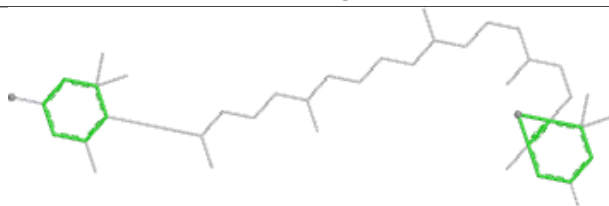
Torsions

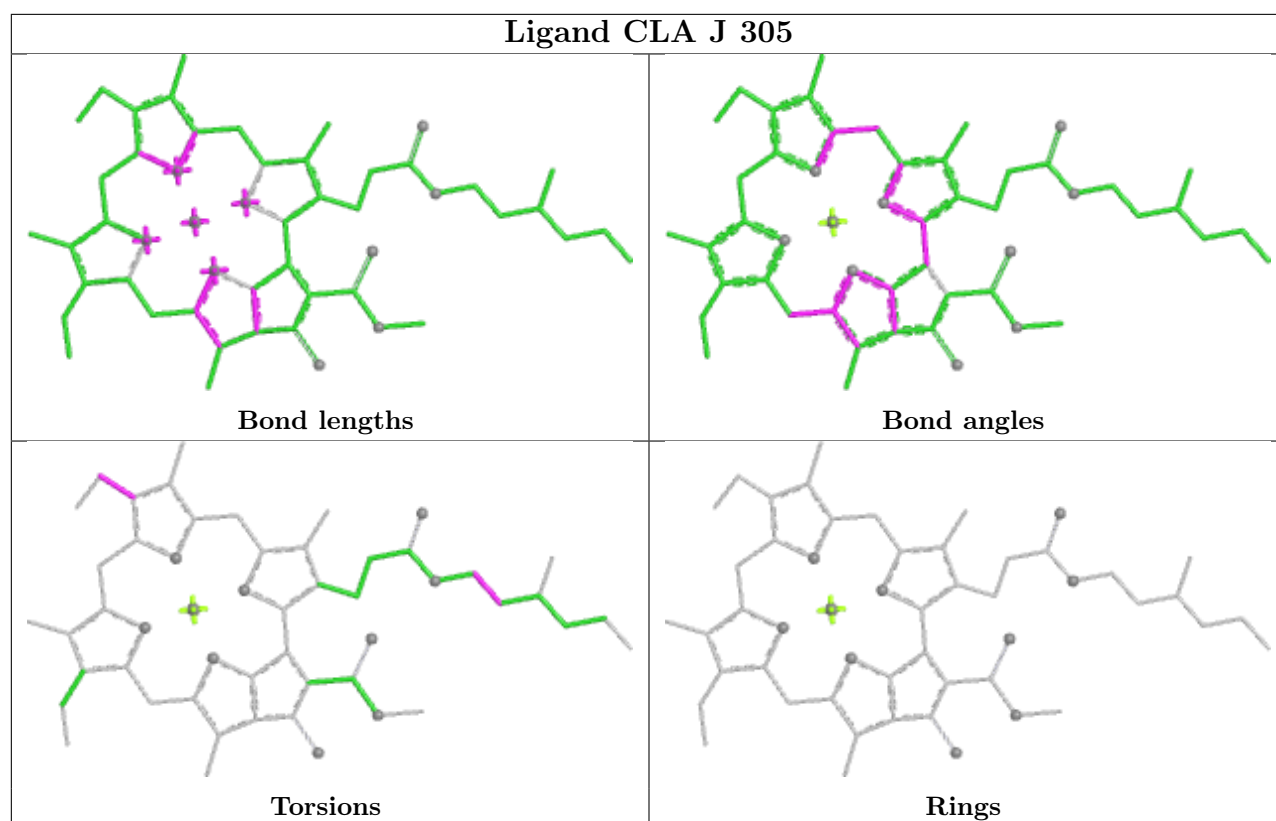


Rings

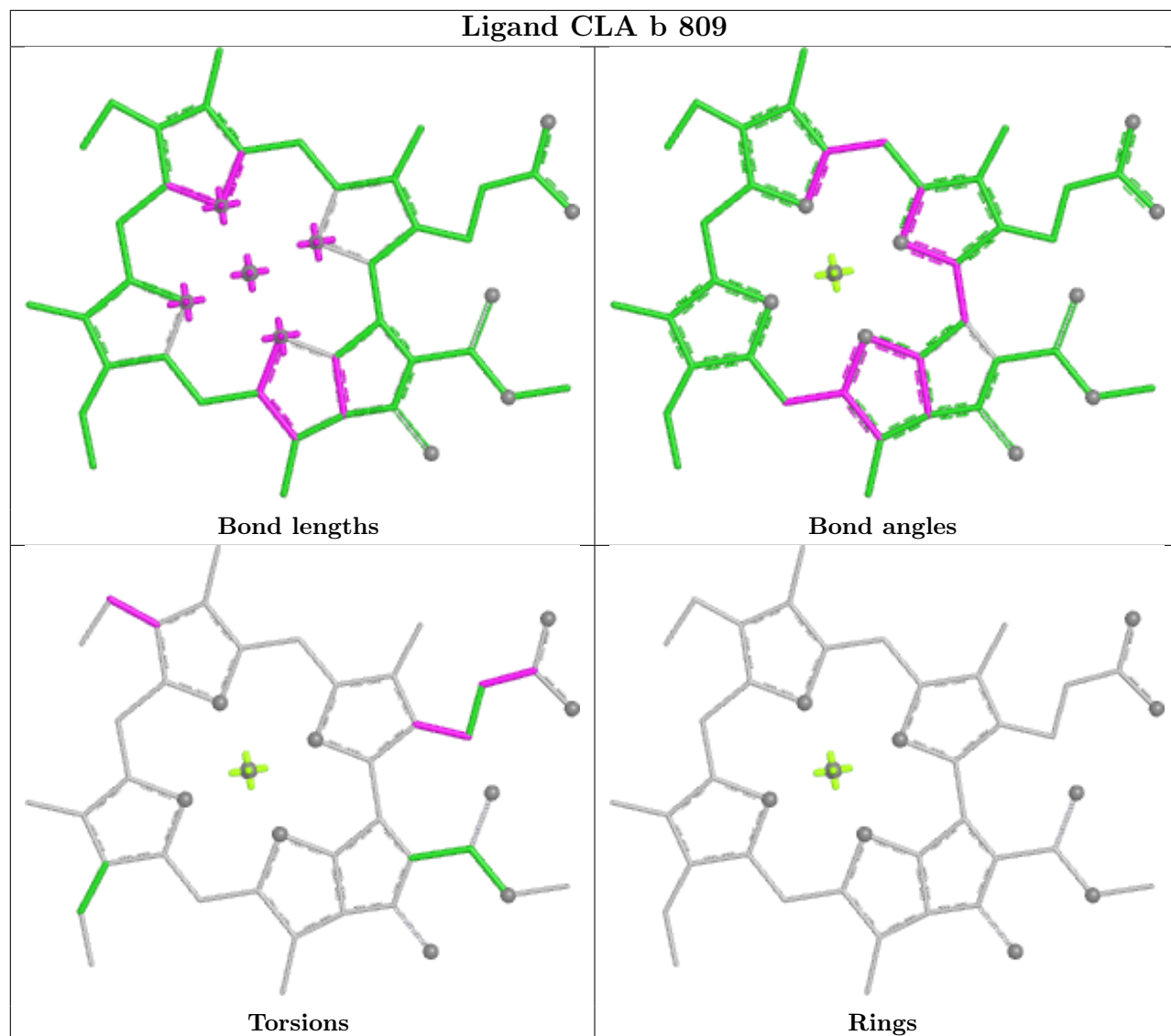


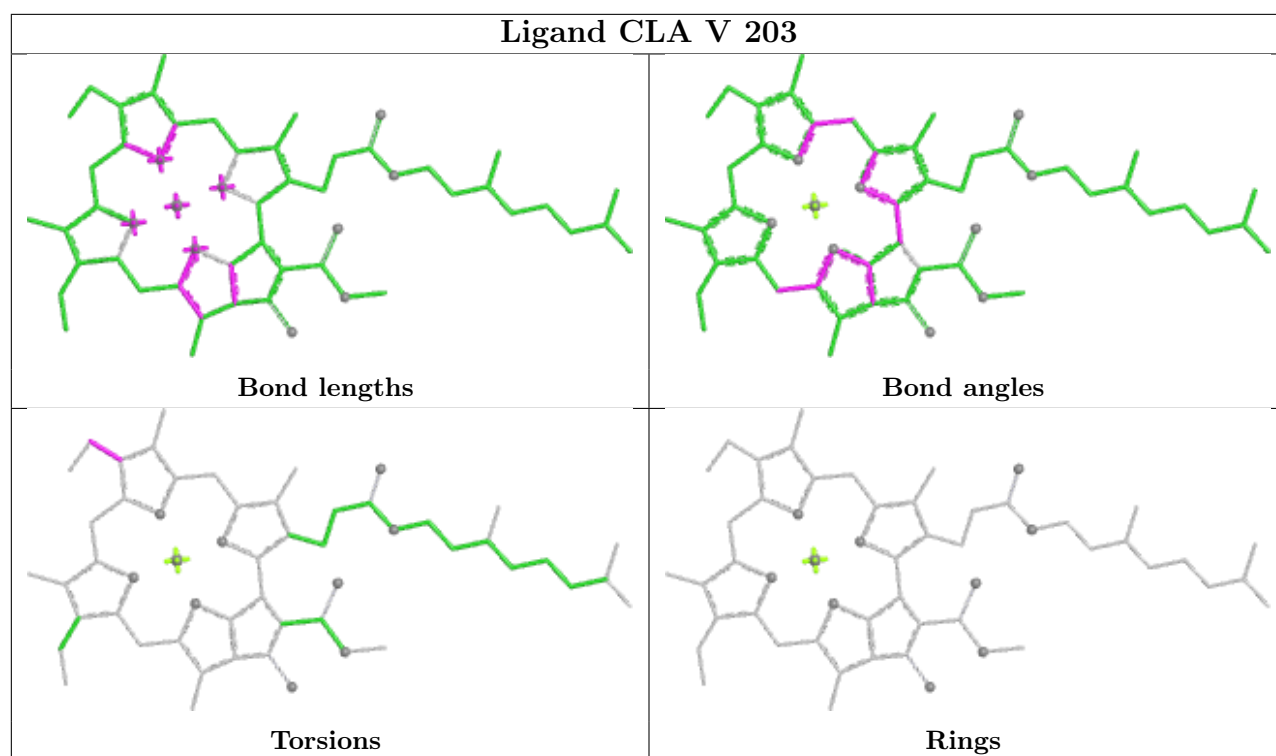
Ligand CLA I 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 T 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

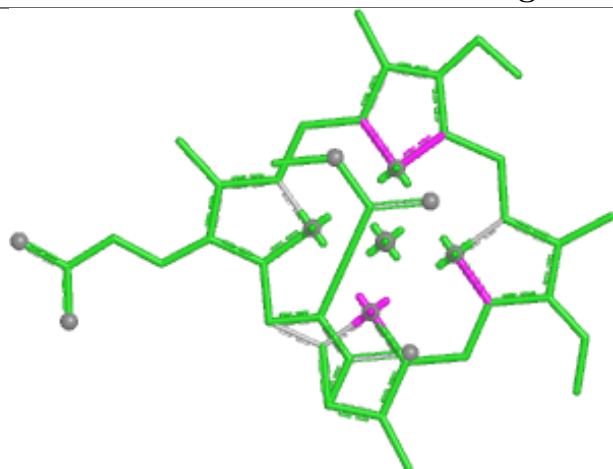


Ligand CLA b 809

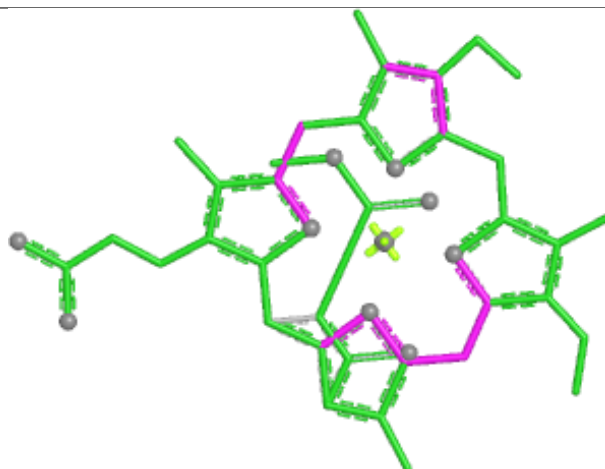




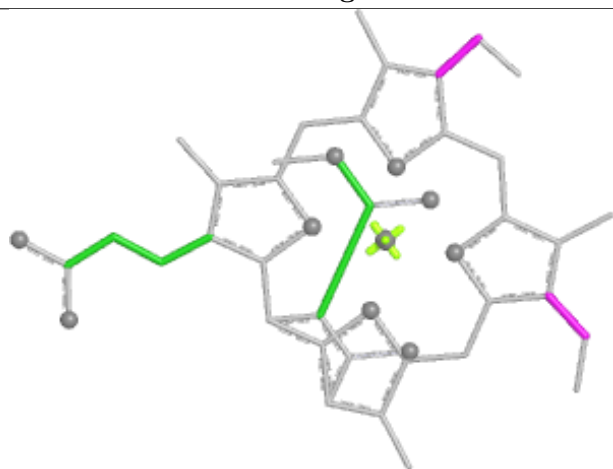
Ligand KC2 L 302



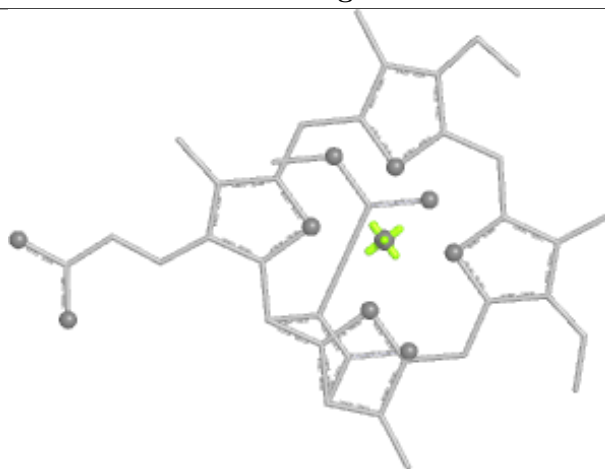
Bond lengths



Bond angles

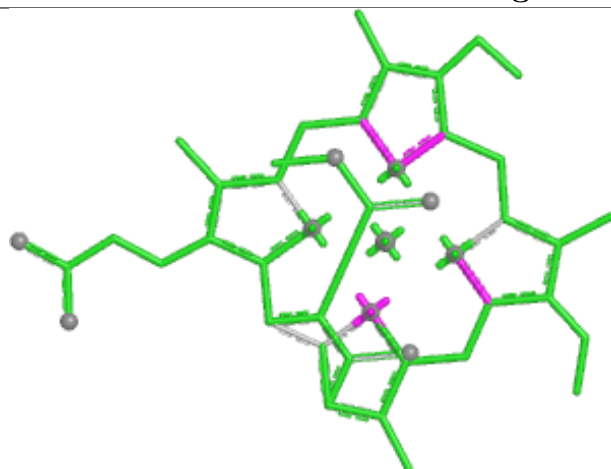


Torsions

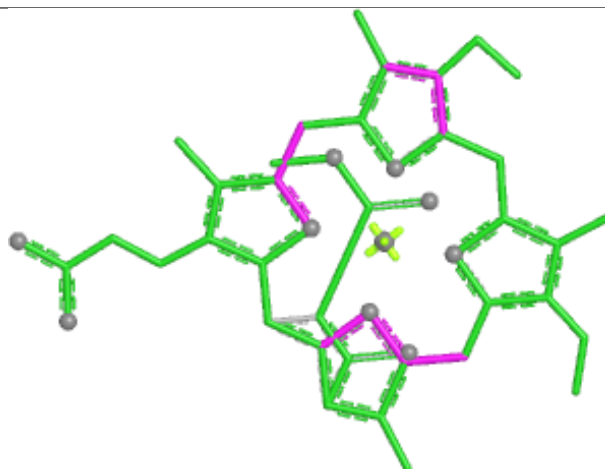


Rings

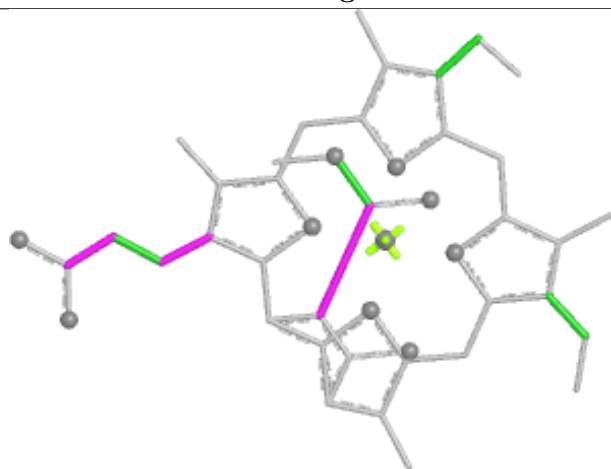
Ligand KC2 M 304



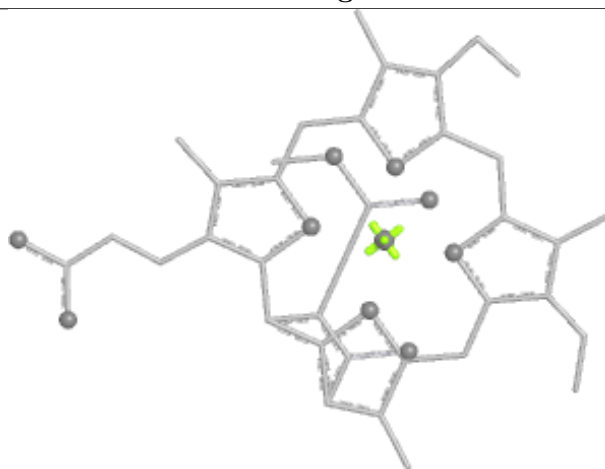
Bond lengths



Bond angles

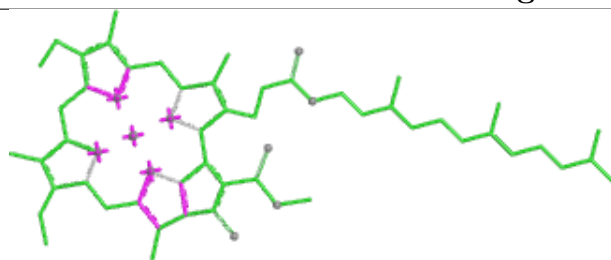


Torsions

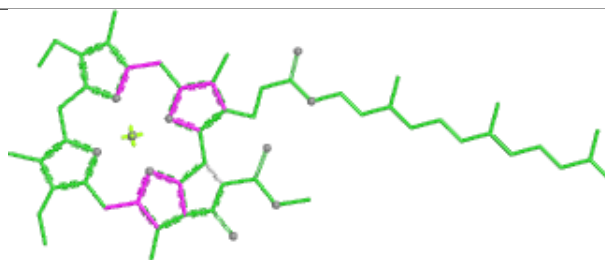


Rings

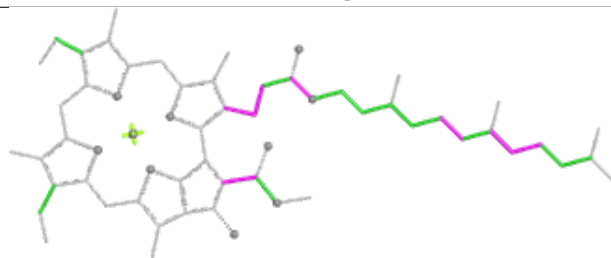
Ligand CLA b 807



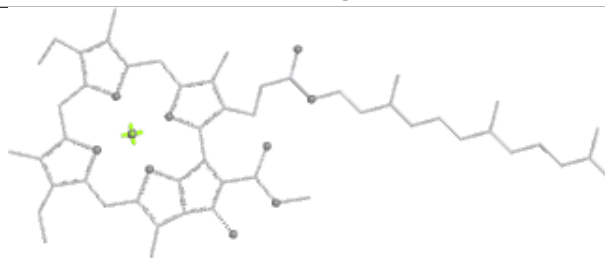
Bond lengths



Bond angles

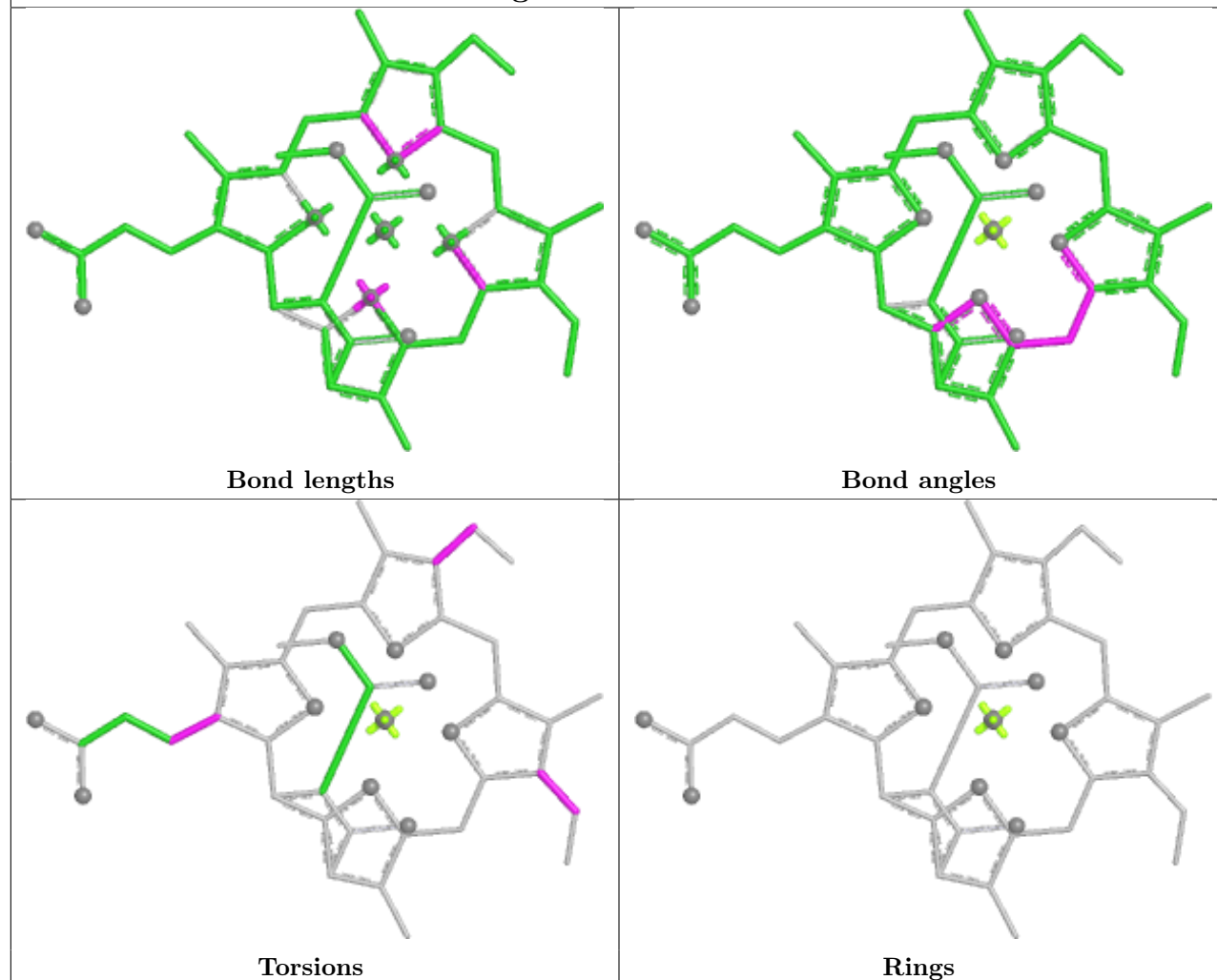


Torsions

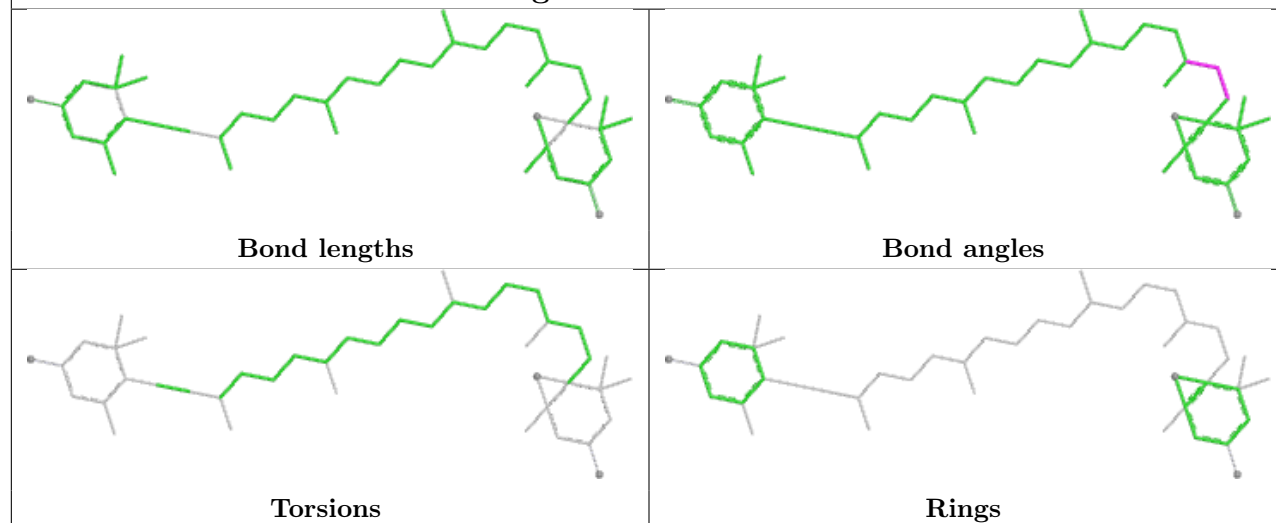


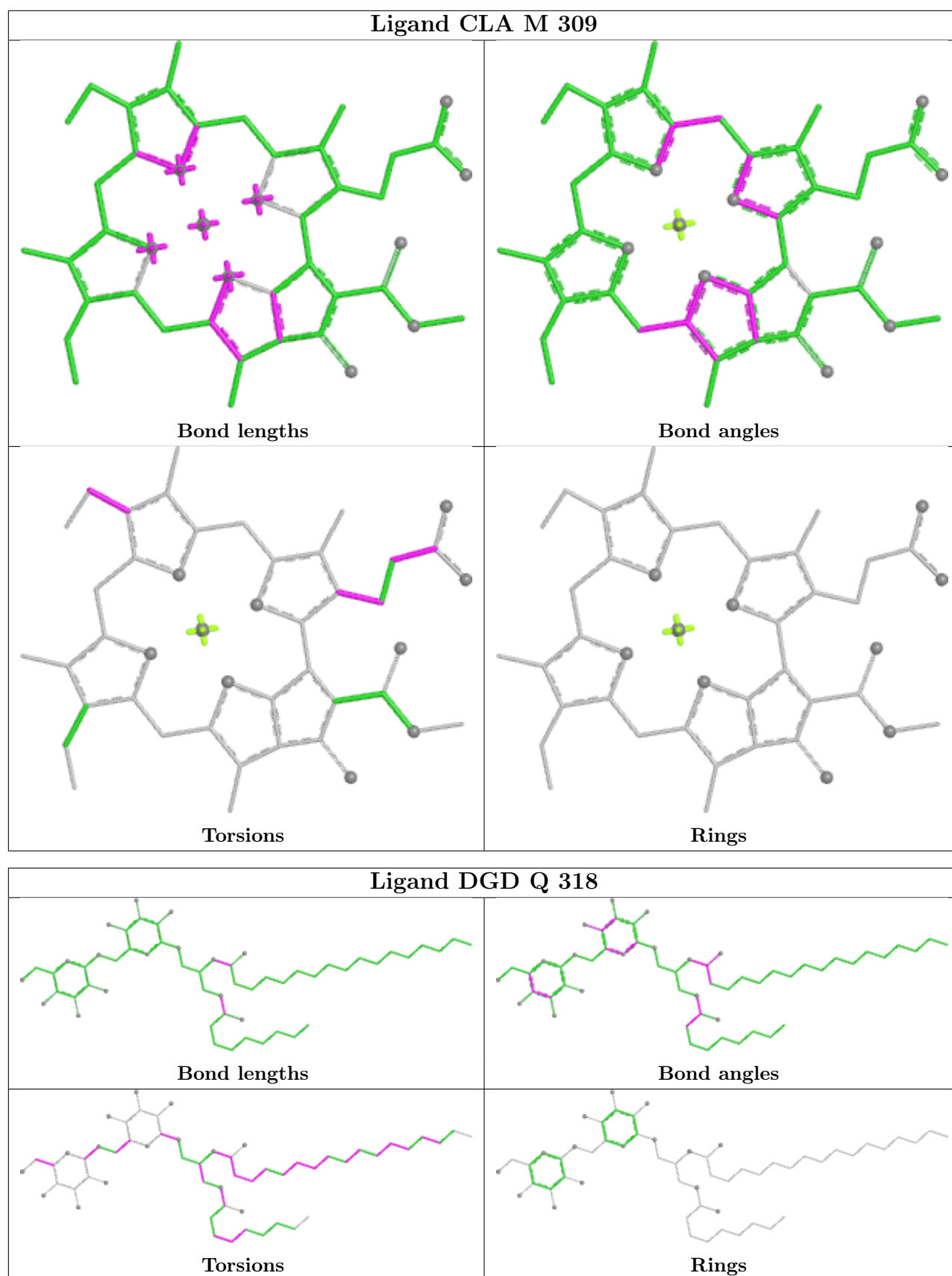
Rings

Ligand KC2 S 306

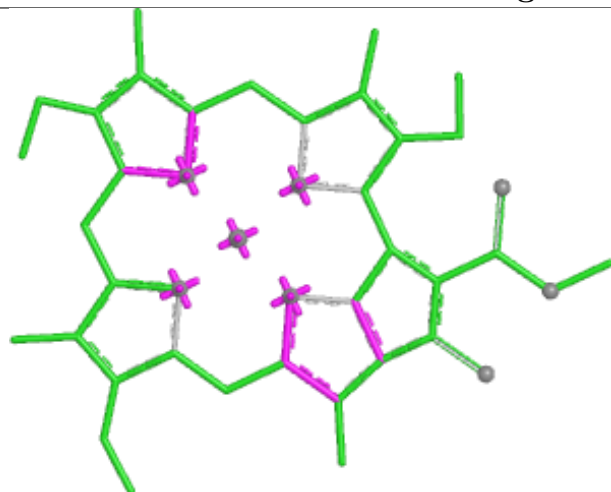


Ligand DD6 K 313

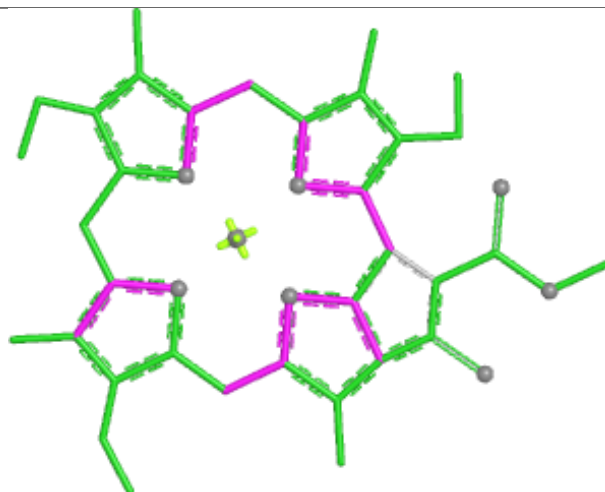




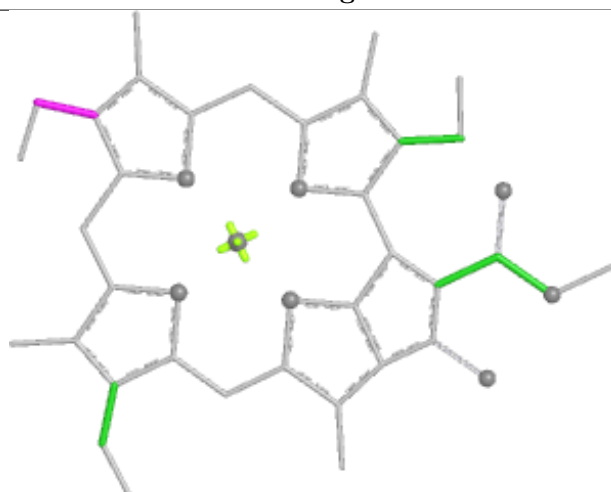
Ligand CLA S 304



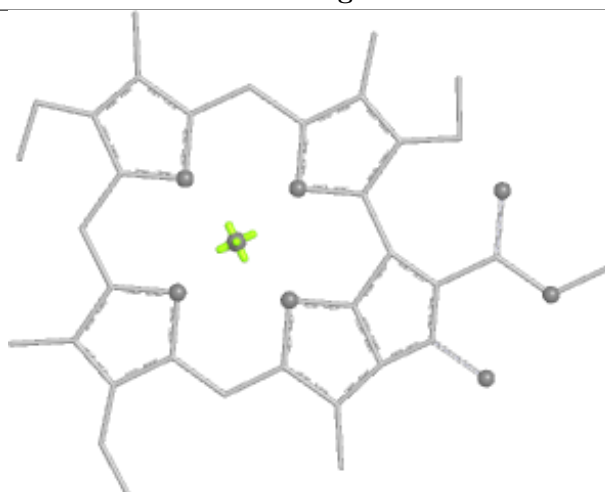
Bond lengths



Bond angles

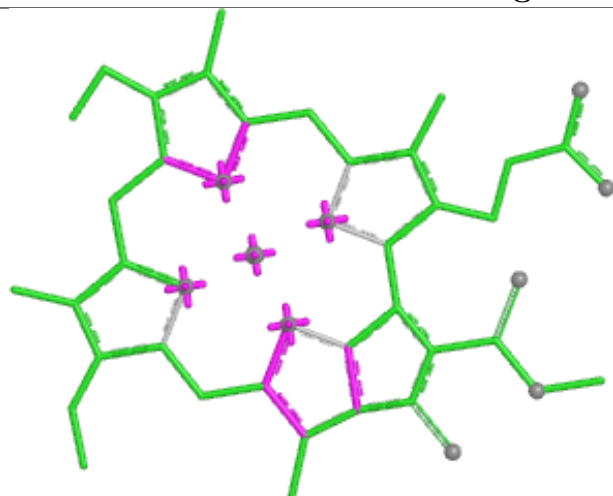


Torsions

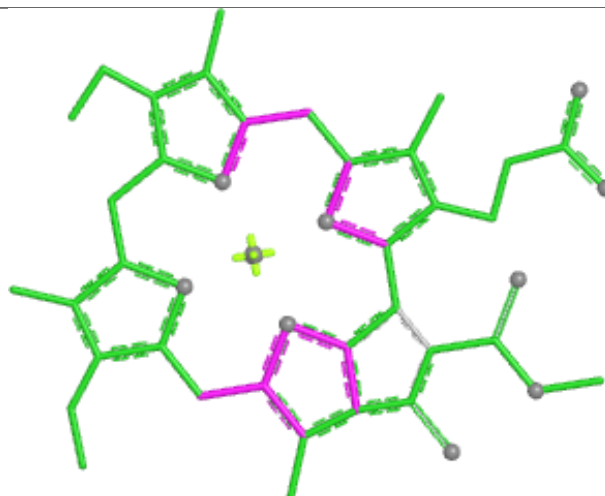


Rings

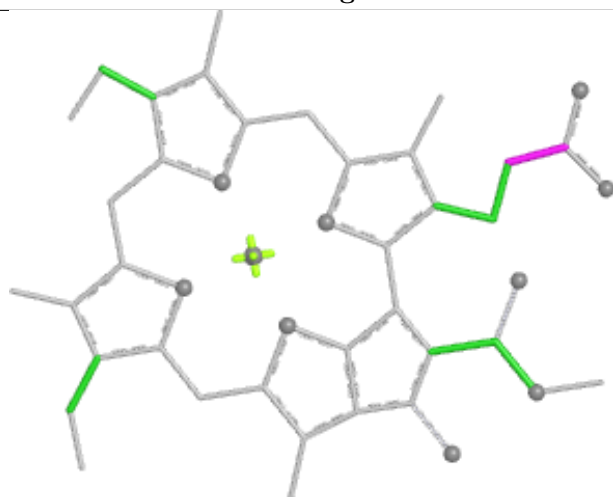
Ligand CLA R 307



Bond lengths



Bond angles

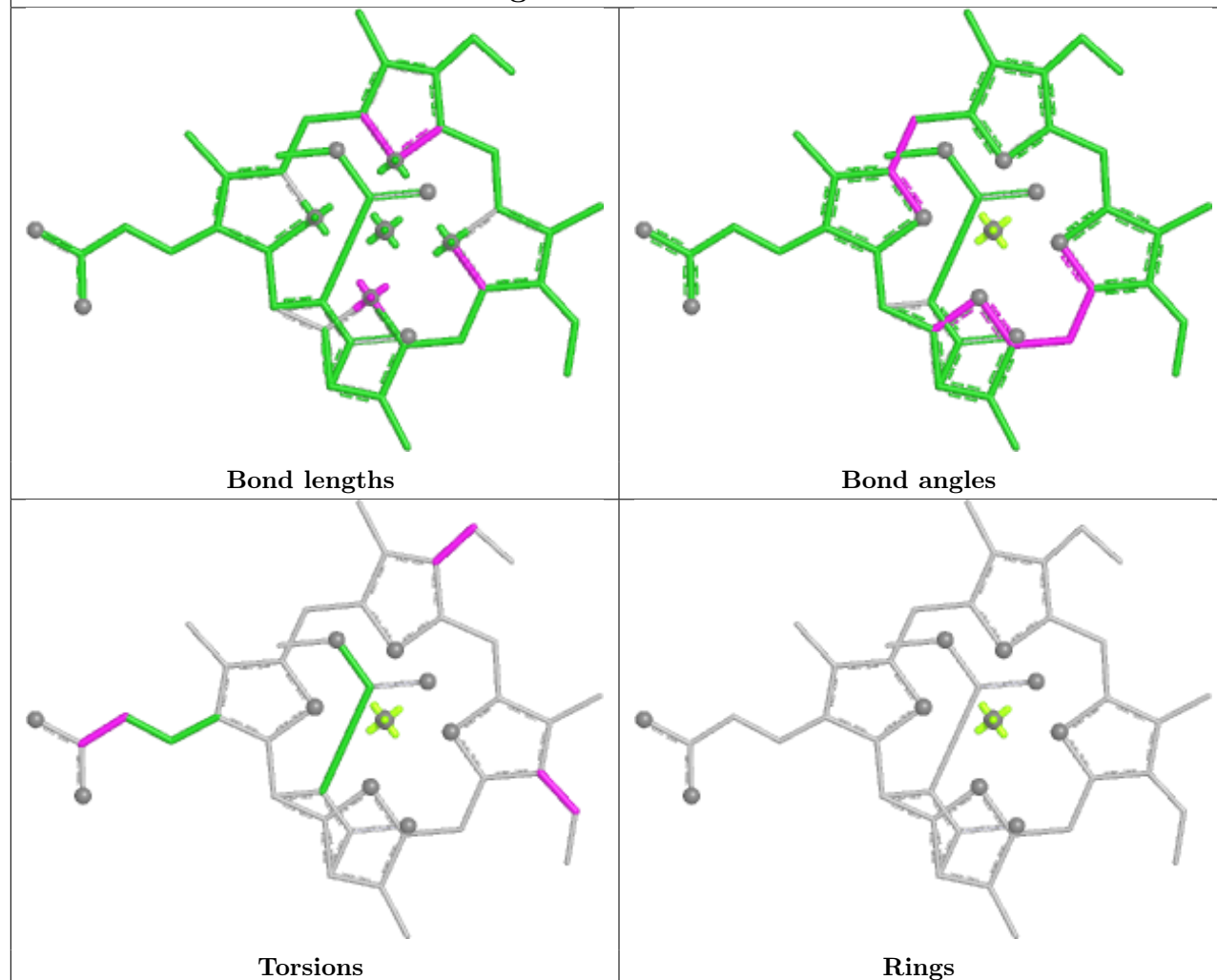


Torsions

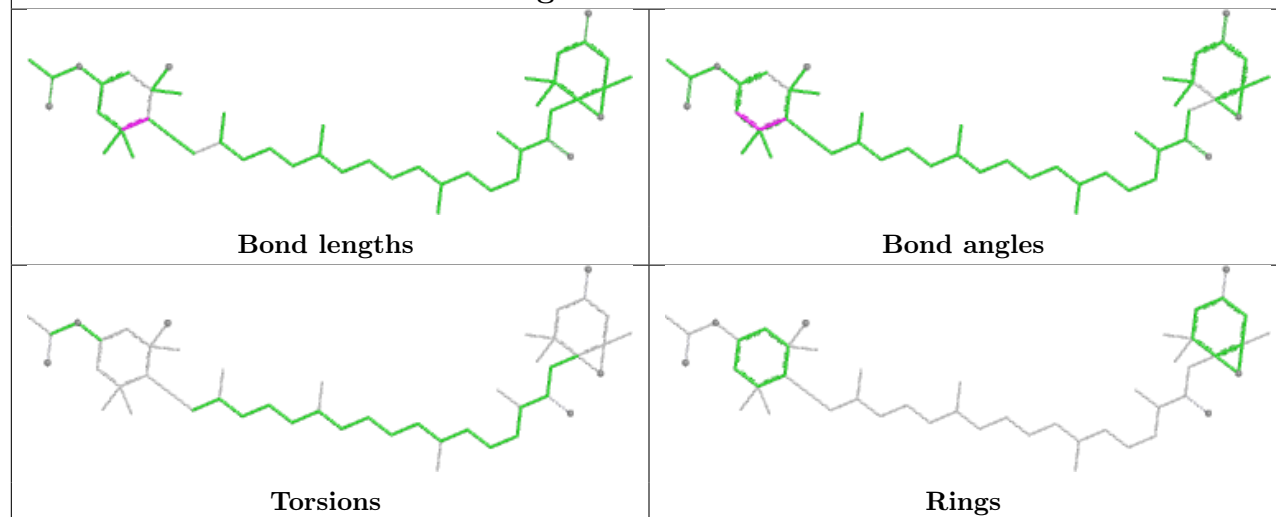


Rings

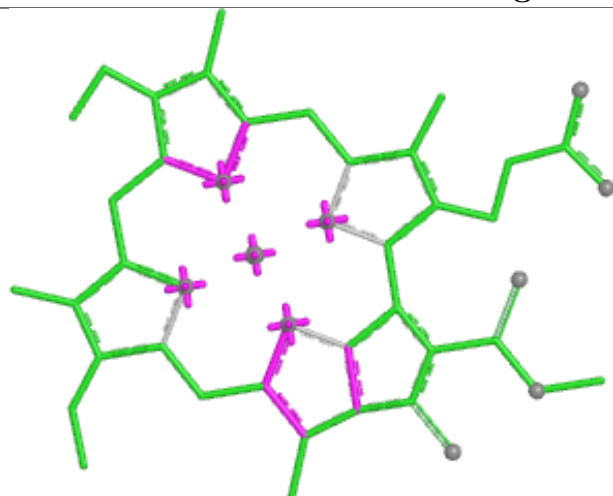
Ligand KC2 P 312



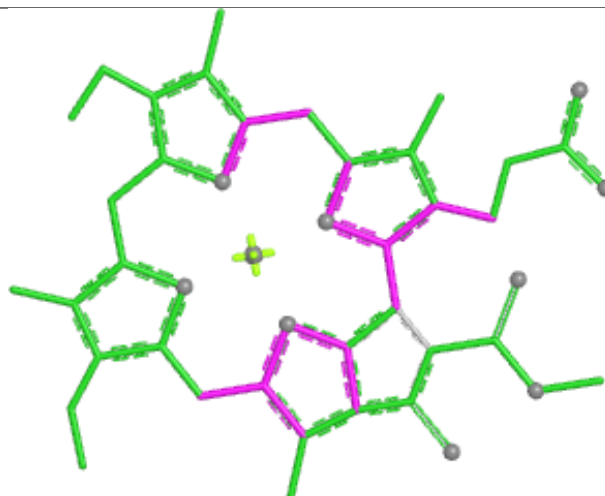
Ligand A86 N 320



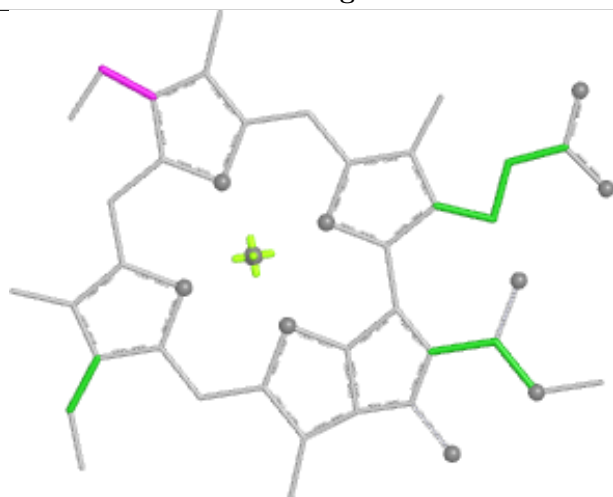
Ligand CLA O 304



Bond lengths



Bond angles

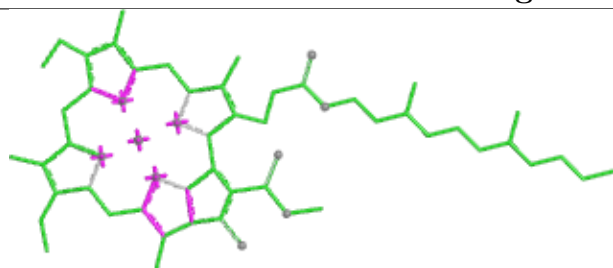


Torsions

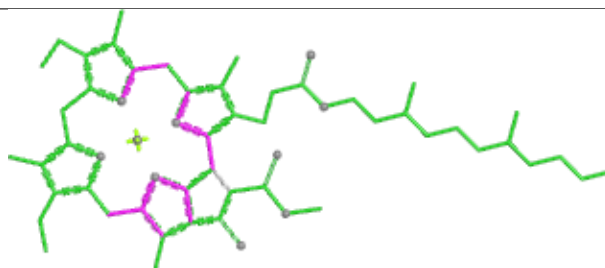


Rings

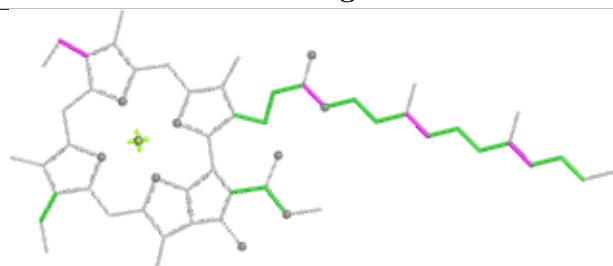
Ligand CLA E 309



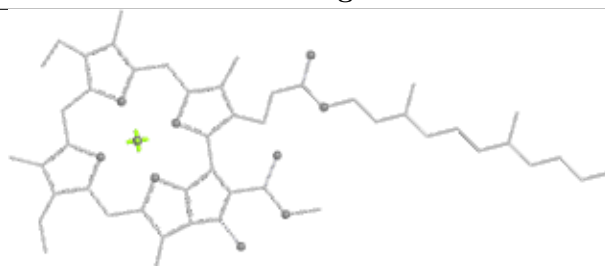
Bond lengths



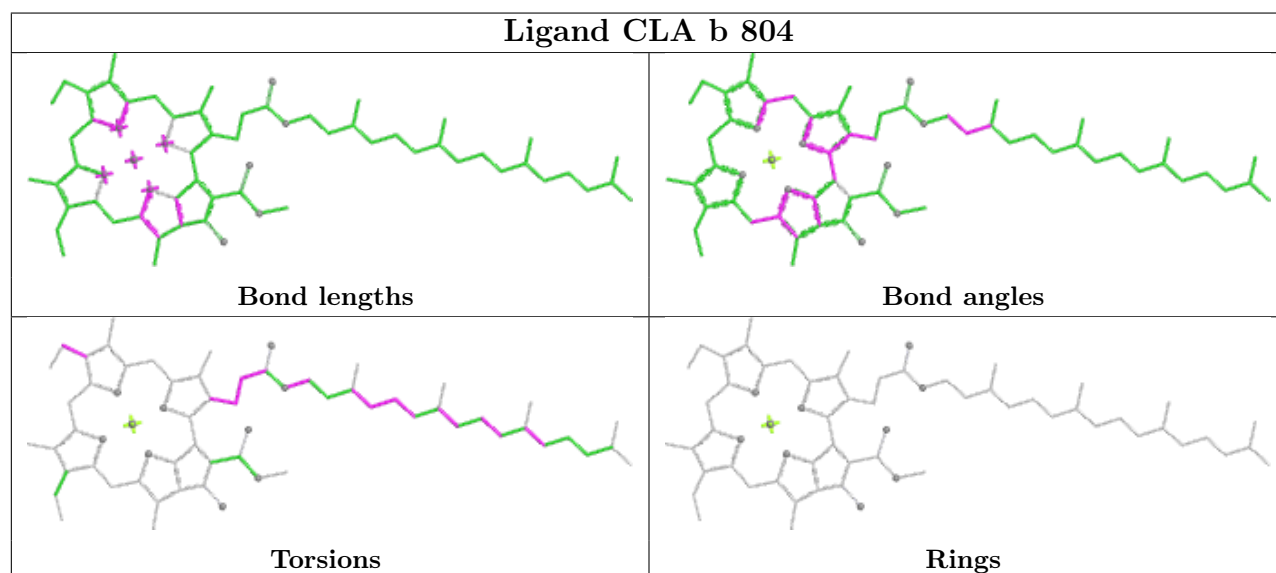
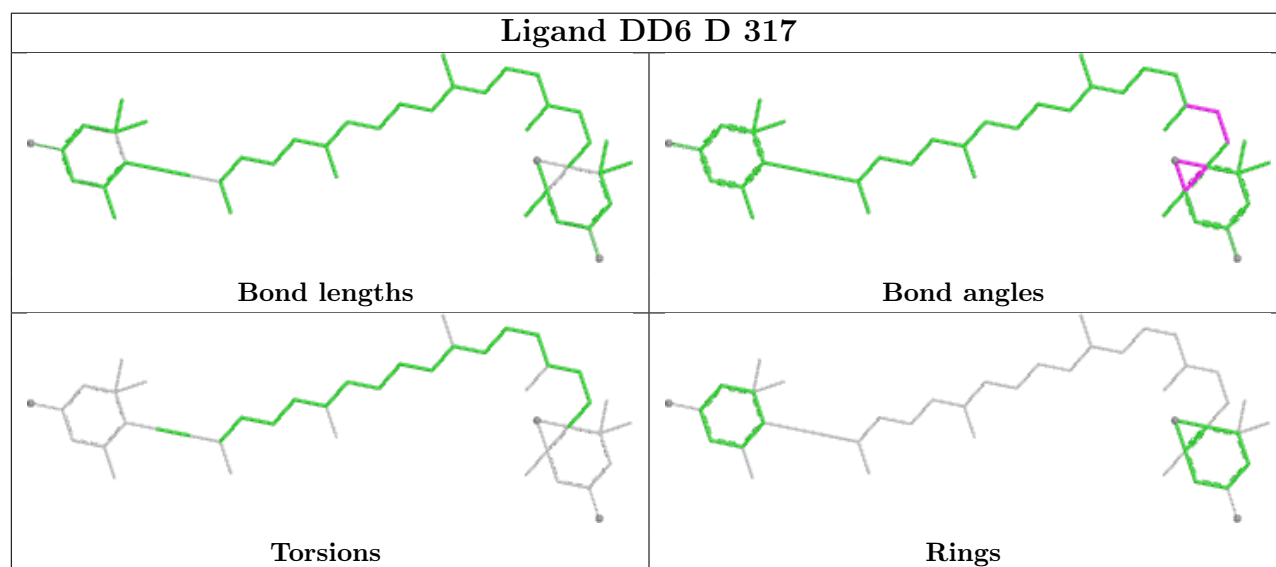
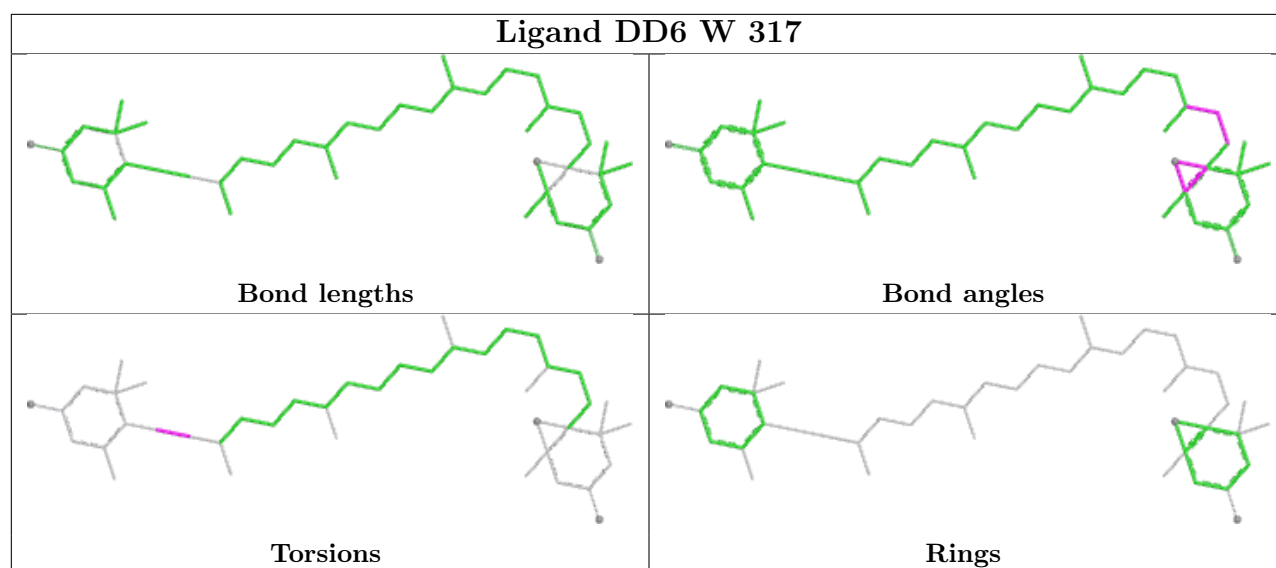
Bond angles



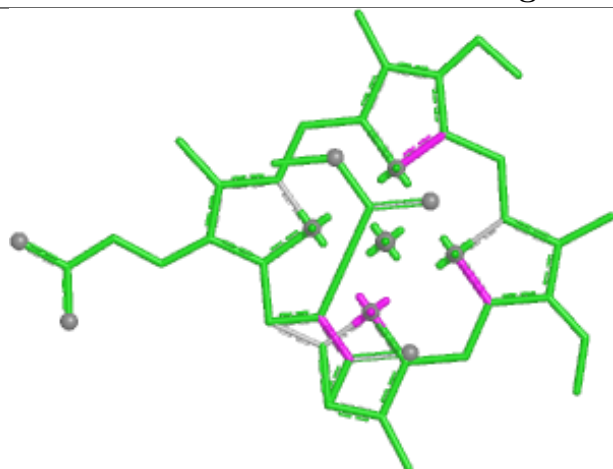
Torsions



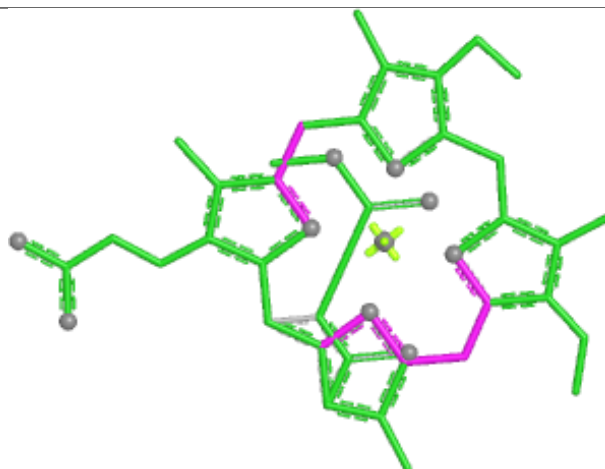
Rings



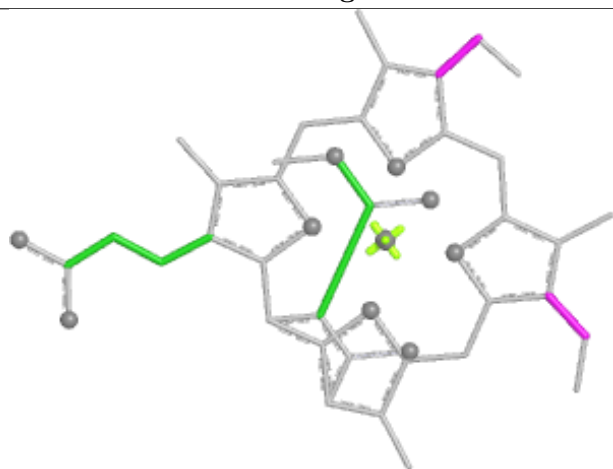
Ligand KC2 S 312



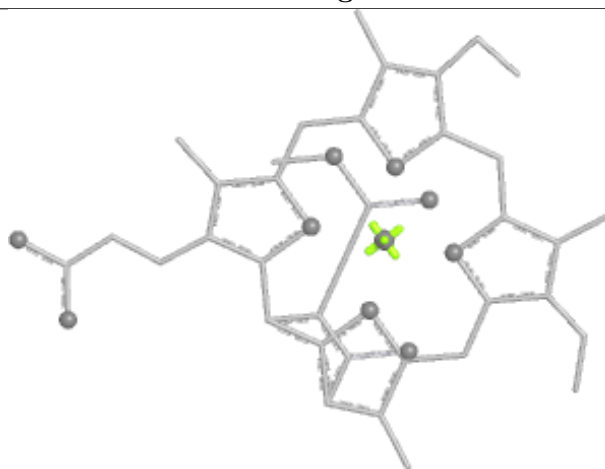
Bond lengths



Bond angles

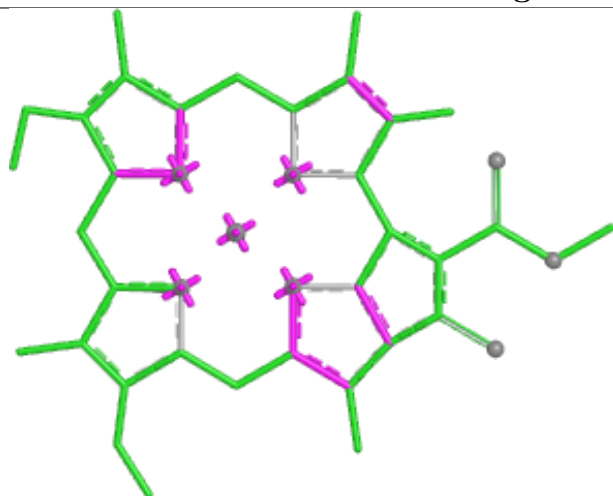


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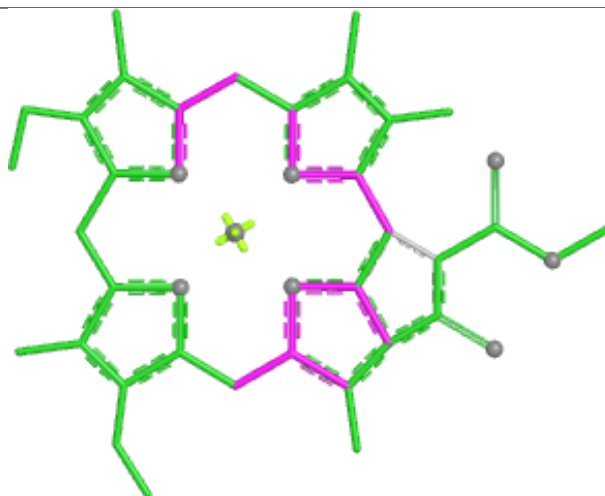


Rings

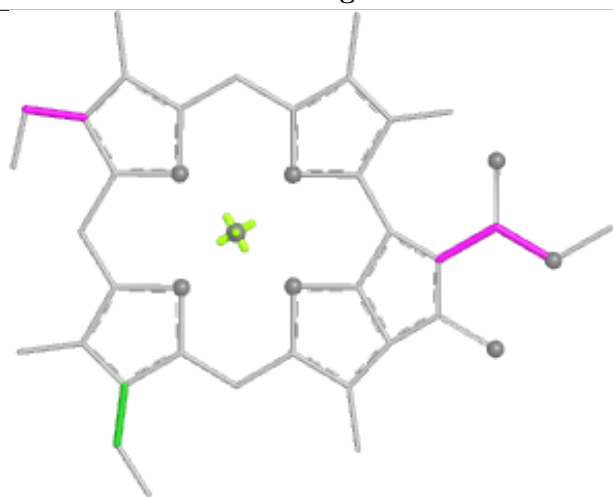
Ligand CLA H 302



Bond lengths



Bond angles

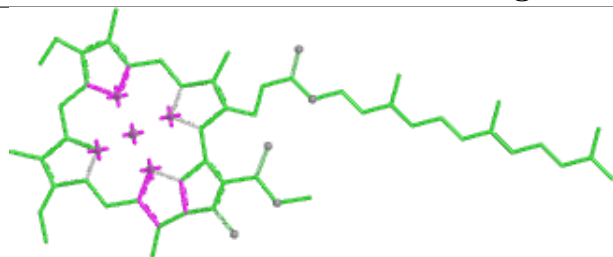


Torsions

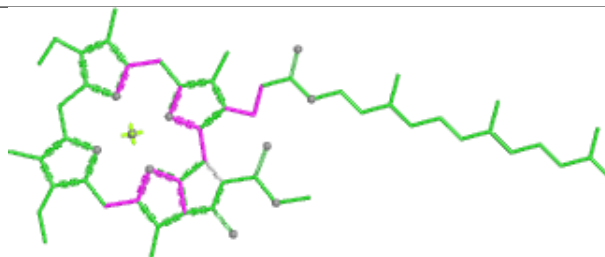


Rings

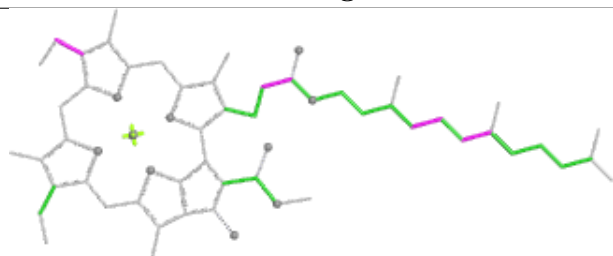
Ligand CLA N 311



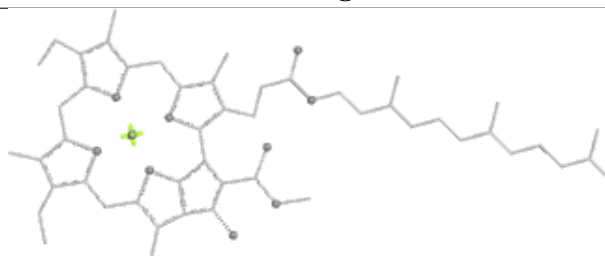
Bond lengths



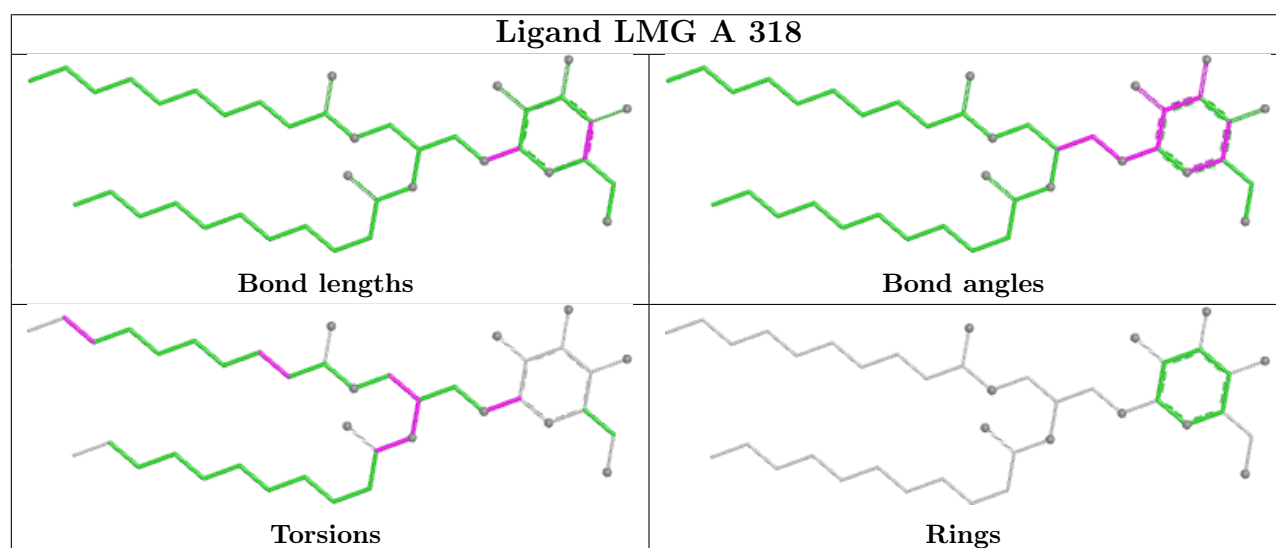
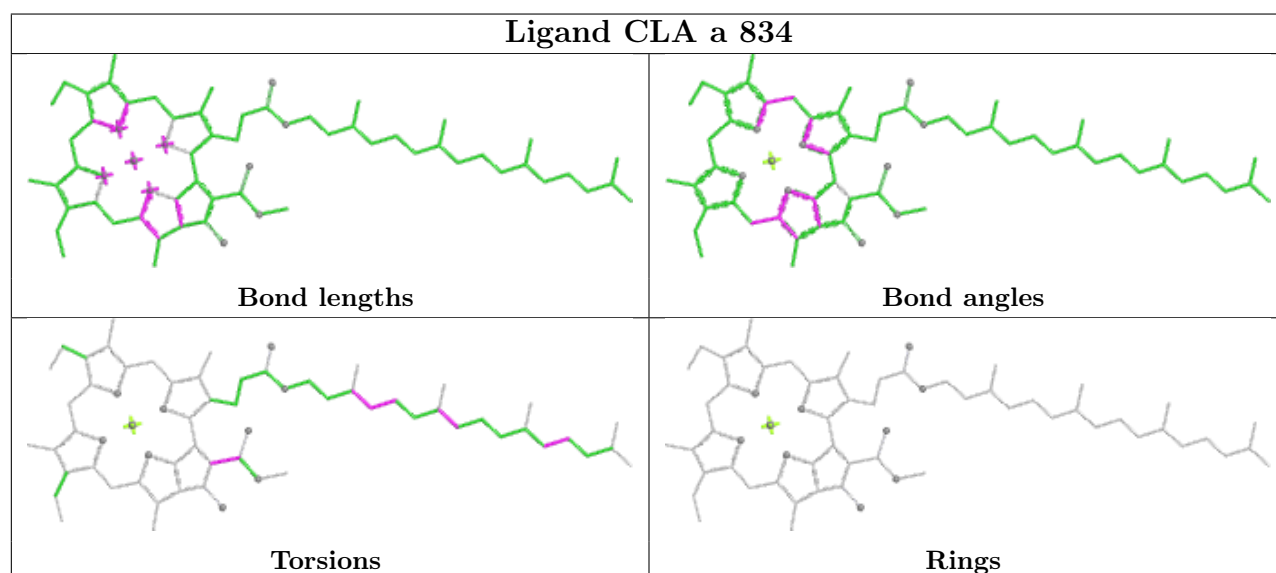
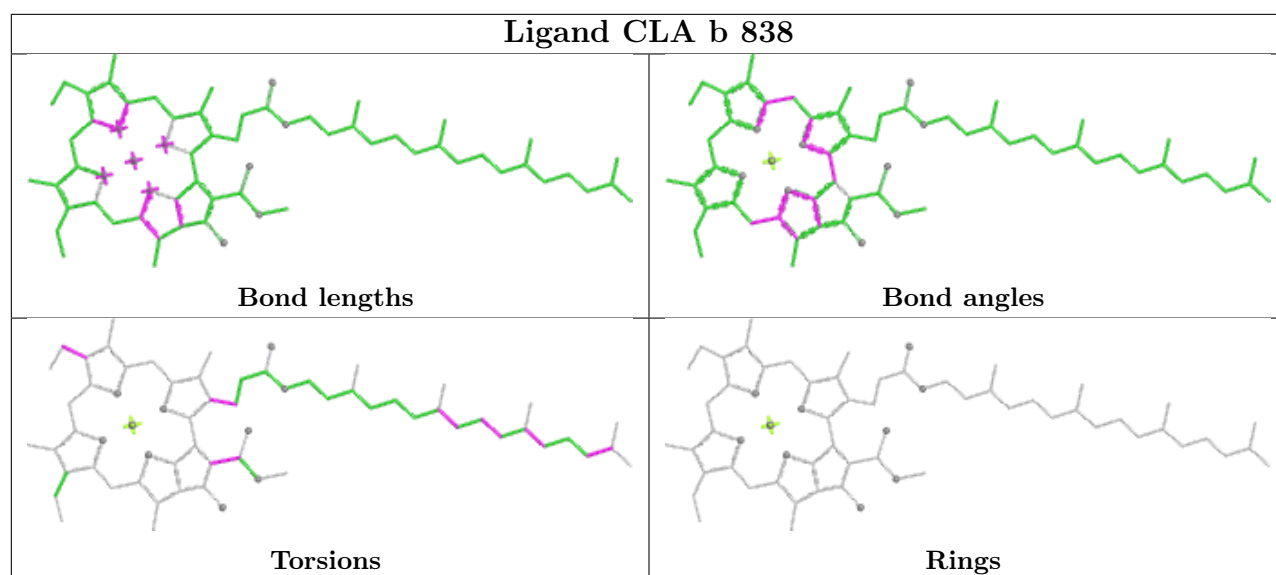
Bond angles

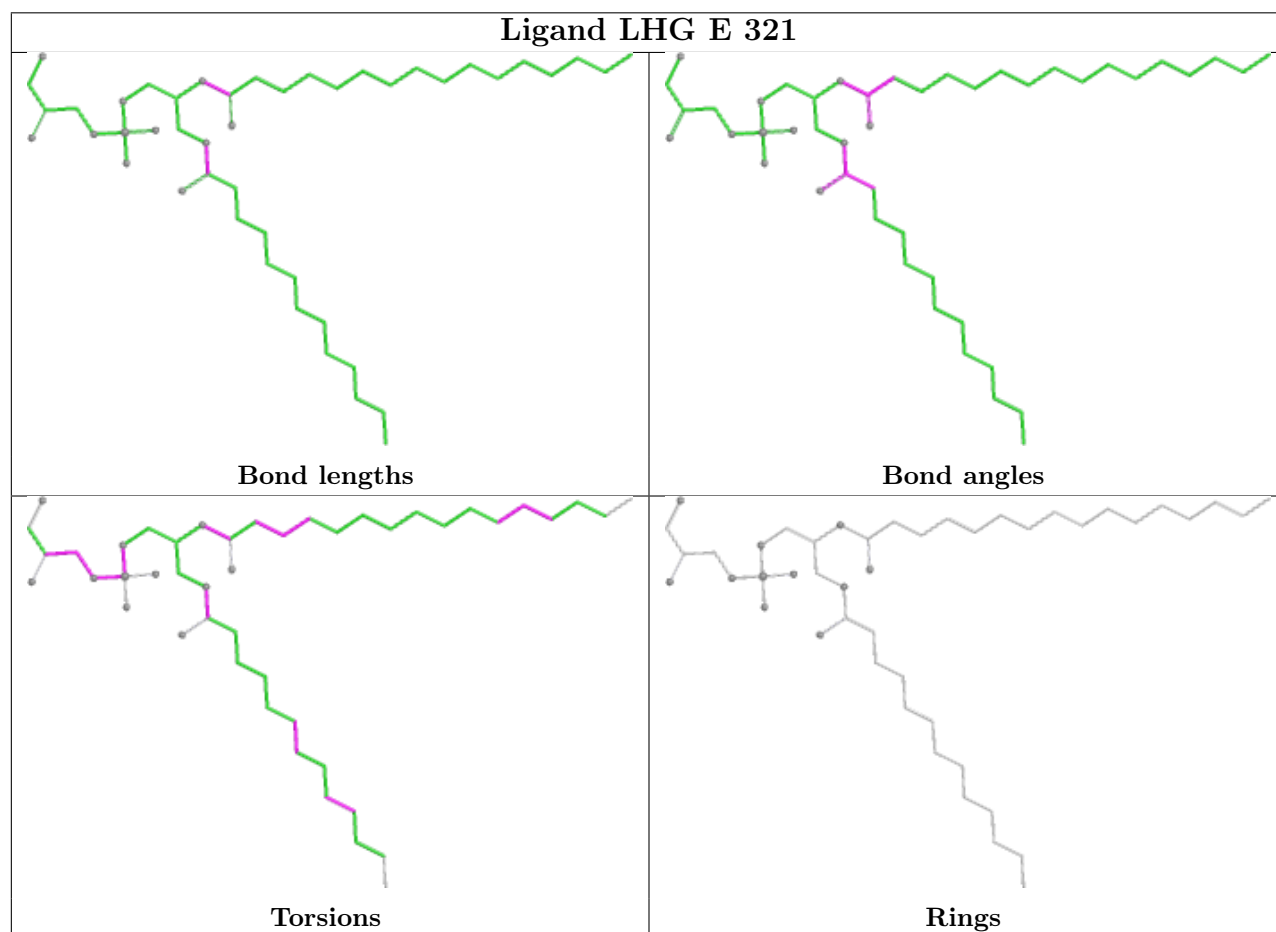
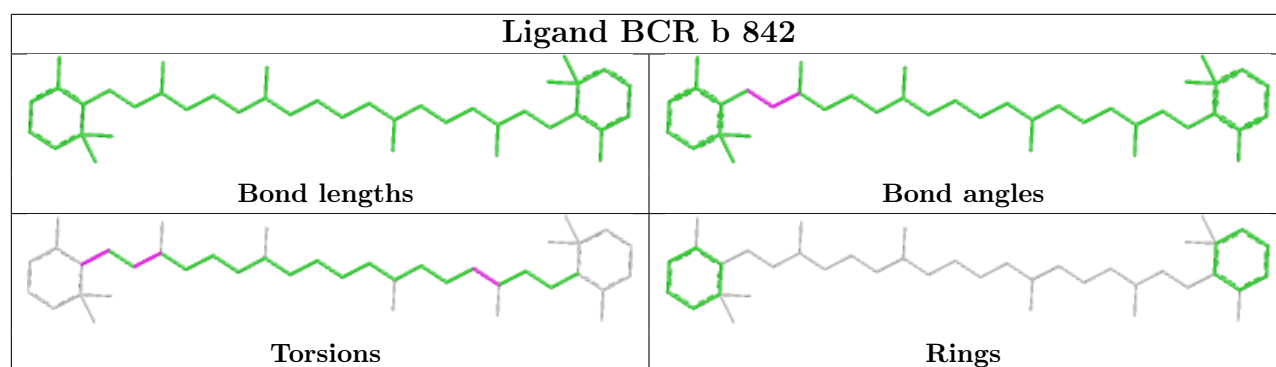


Torsions

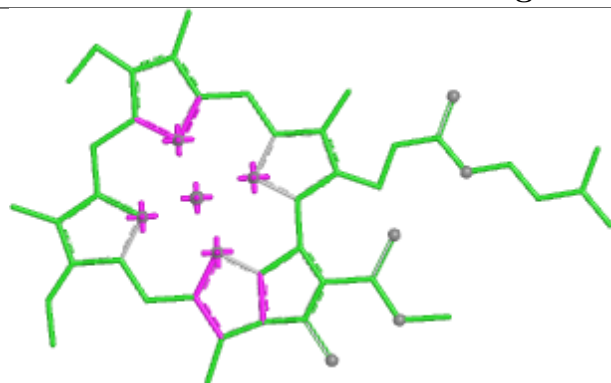


Rings

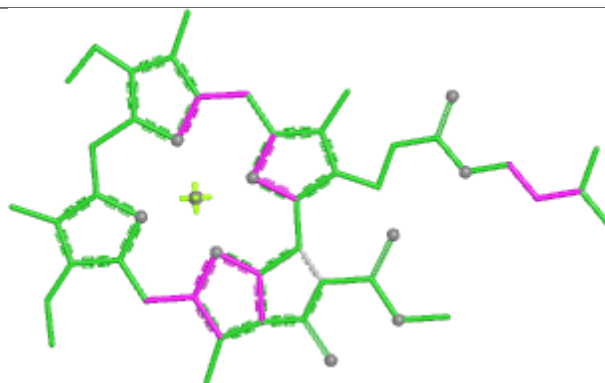




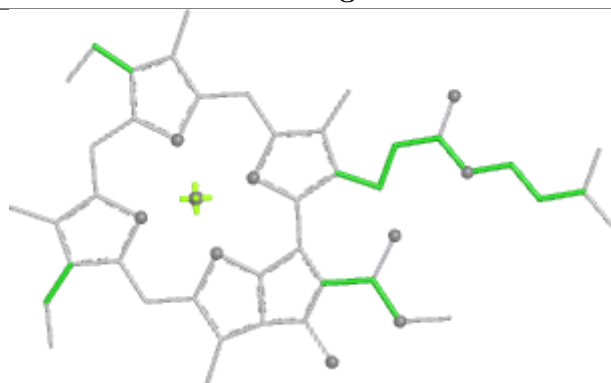
Ligand CLA E 314



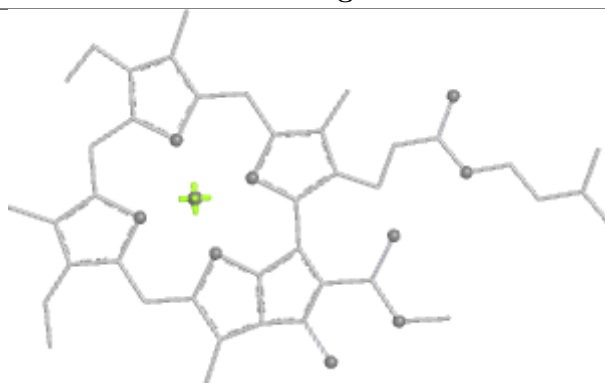
Bond lengths



Bond angles

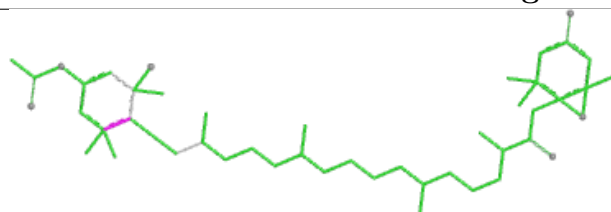


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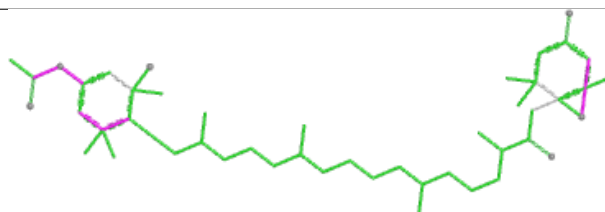


Rings

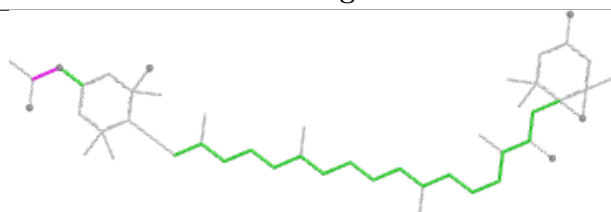
Ligand A86 F 312



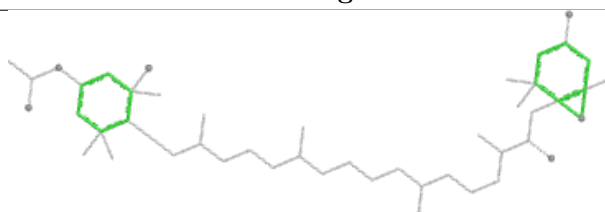
Bond lengths



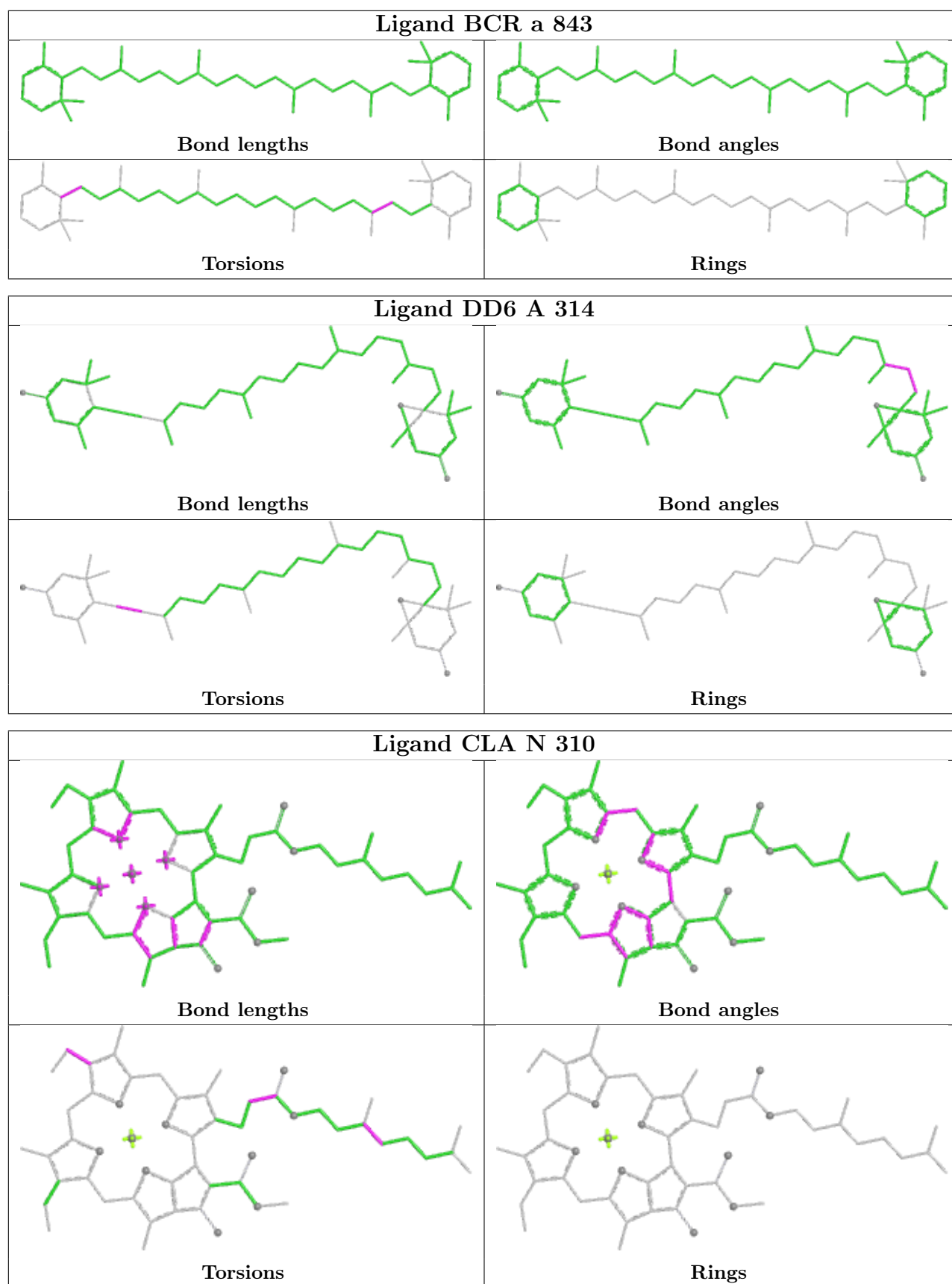
Bond angles



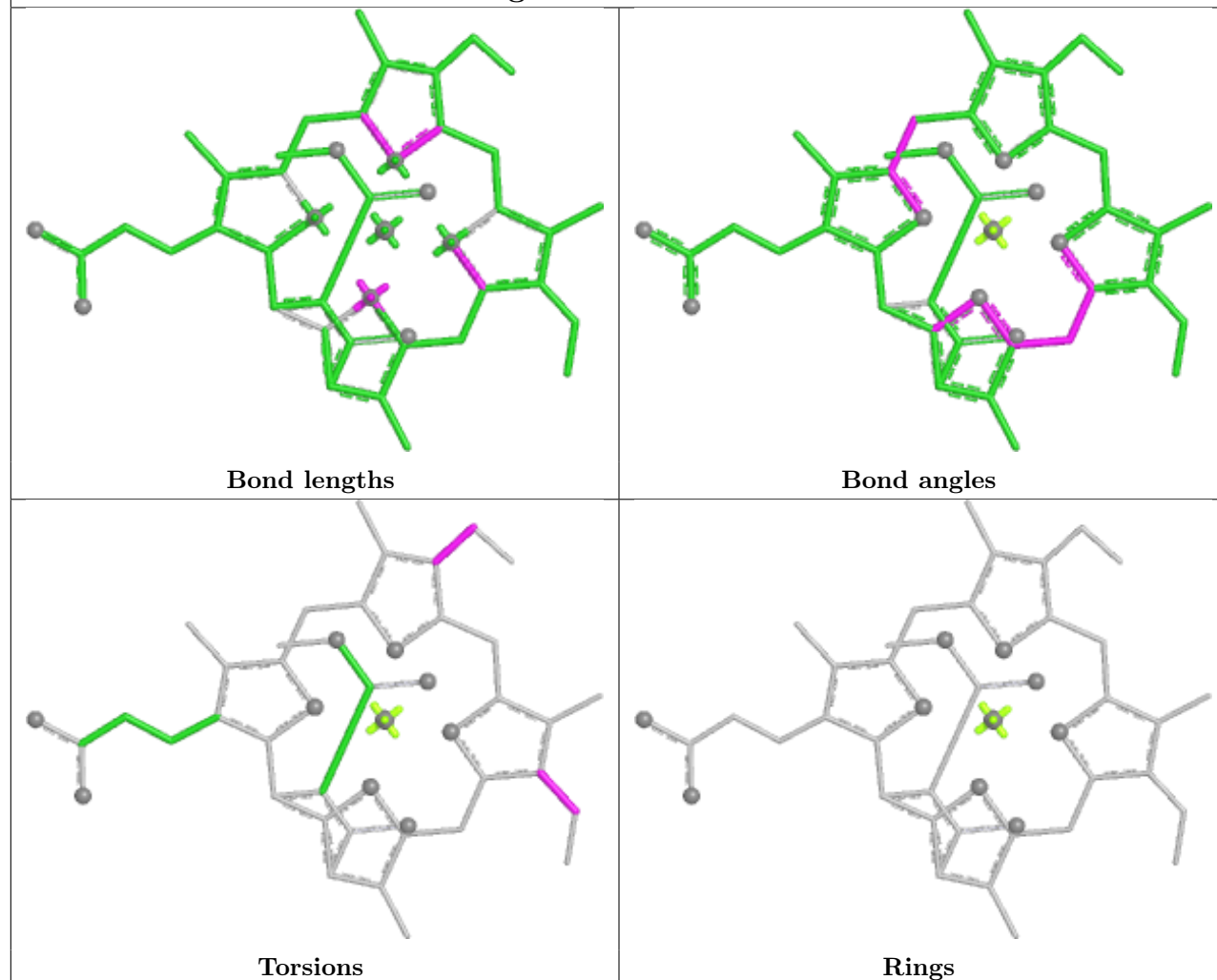
Torsions



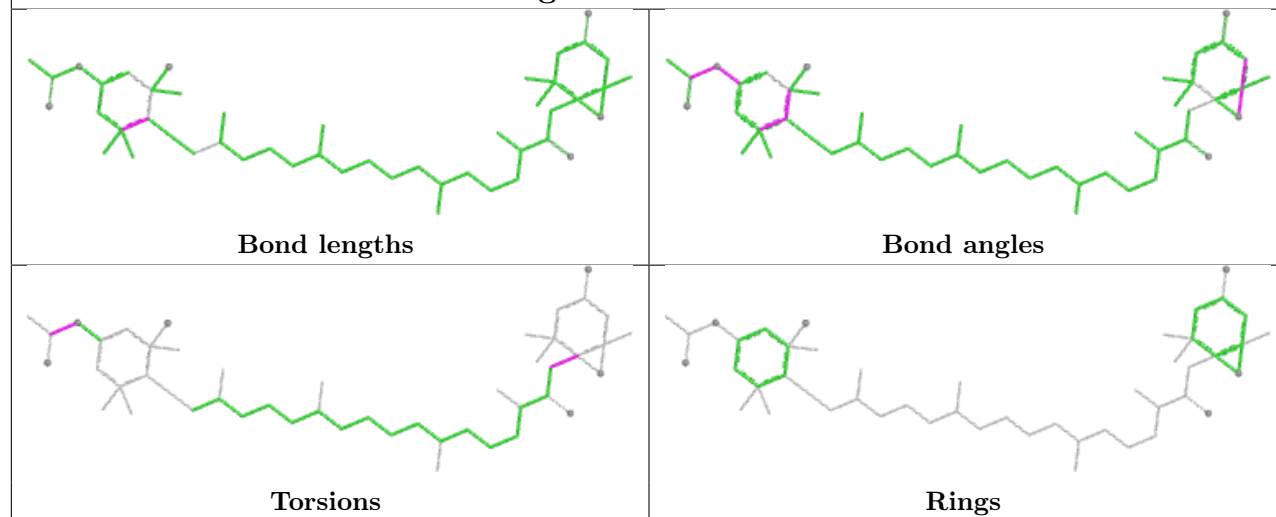
Rings



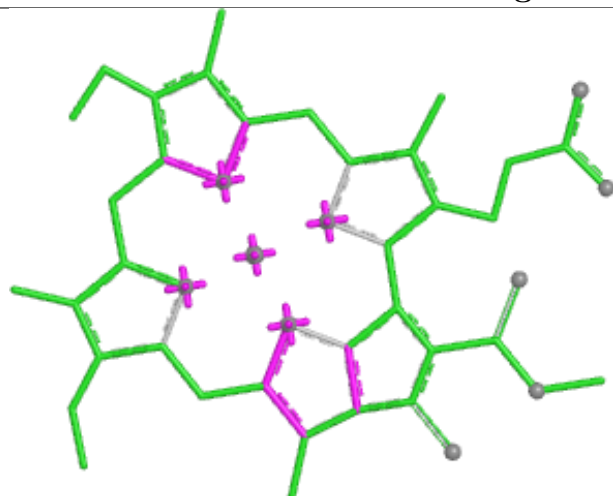
Ligand KC2 N 307



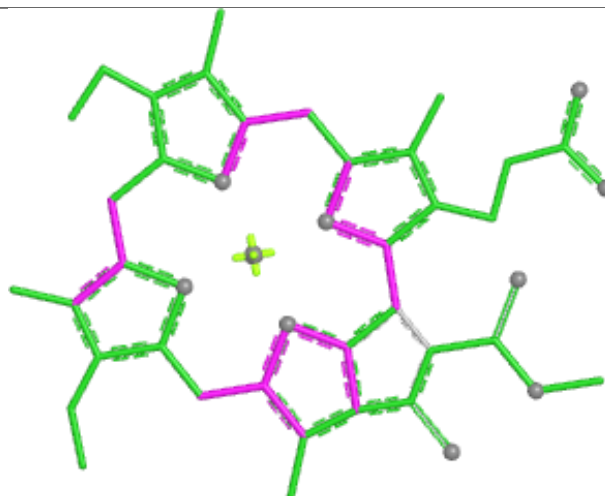
Ligand A86 P 314



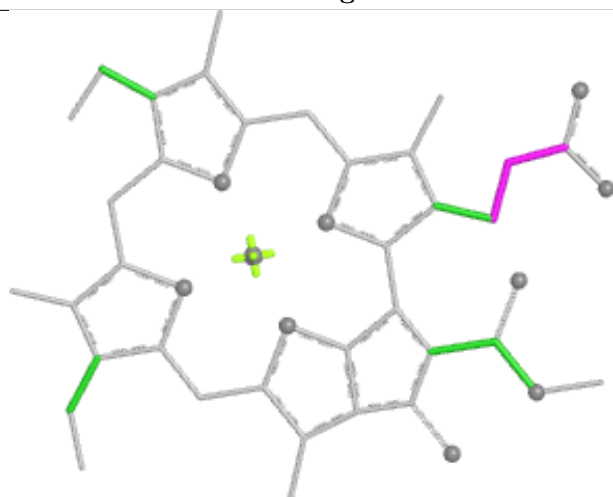
Ligand CLA C 308



Bond lengths



Bond angles

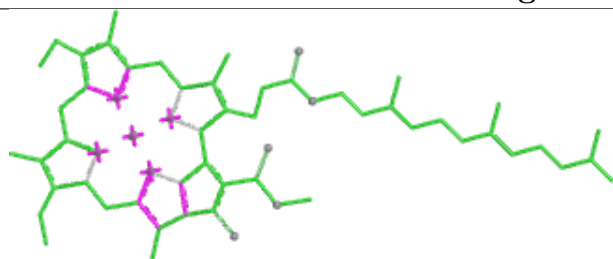


Torsions

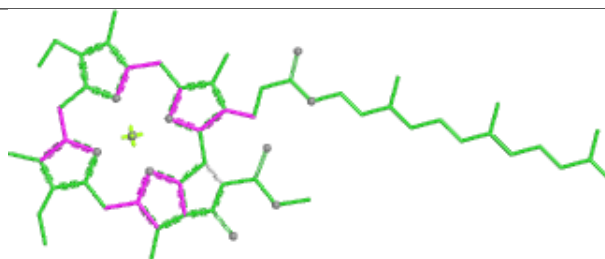


Rings

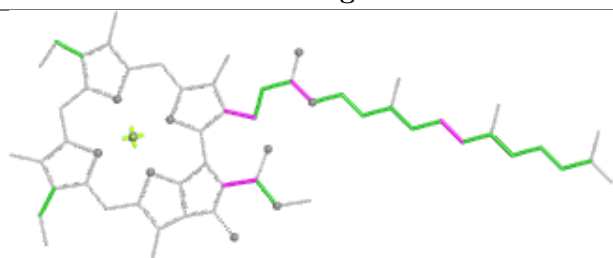
Ligand CLA a 806



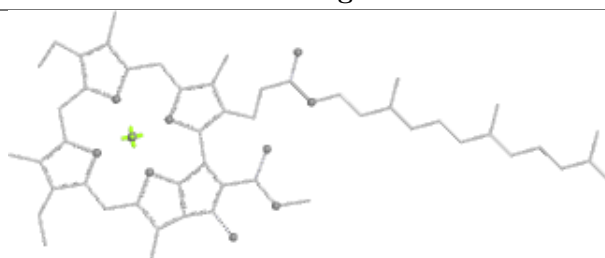
Bond lengths



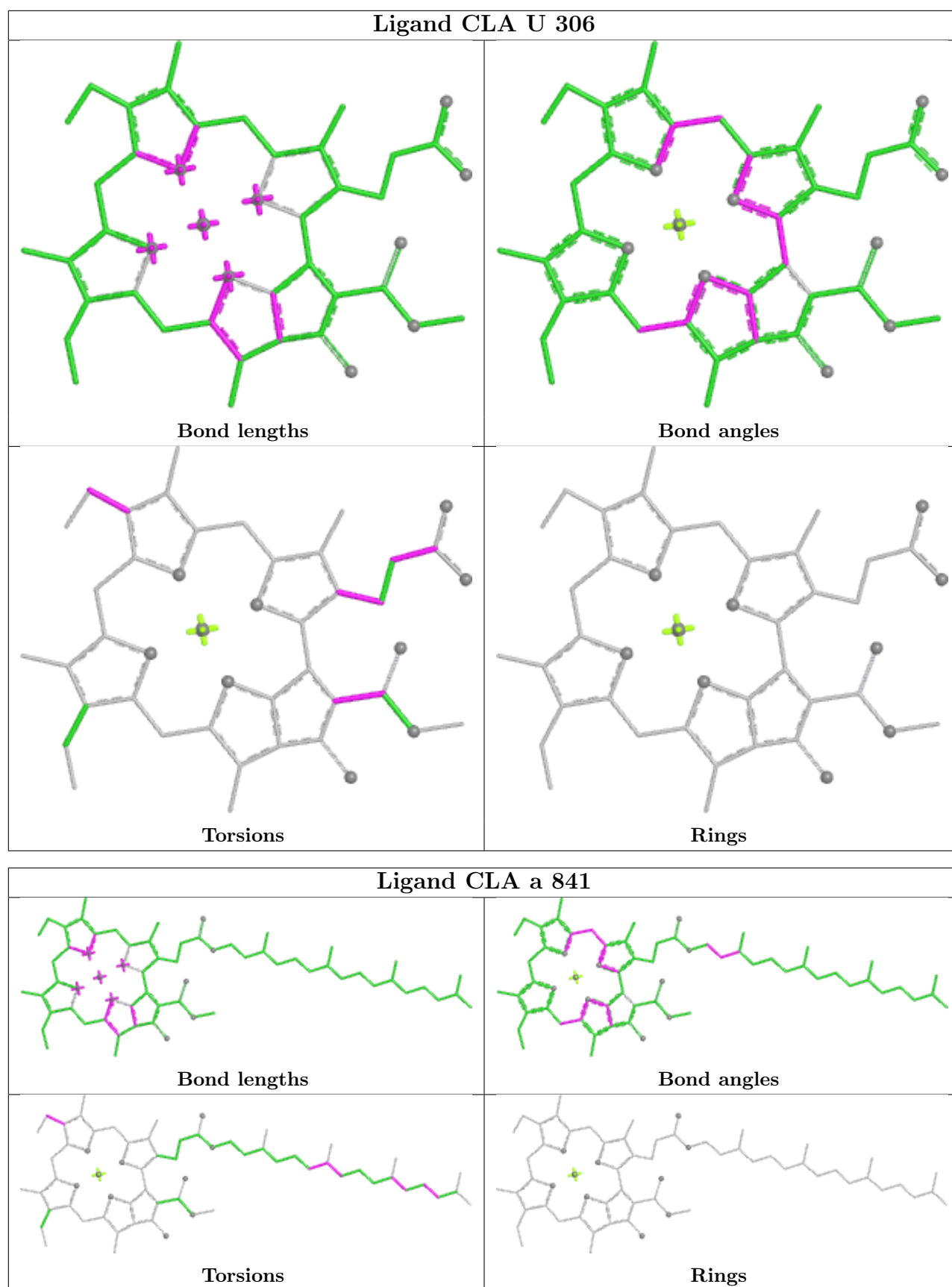
Bond angles

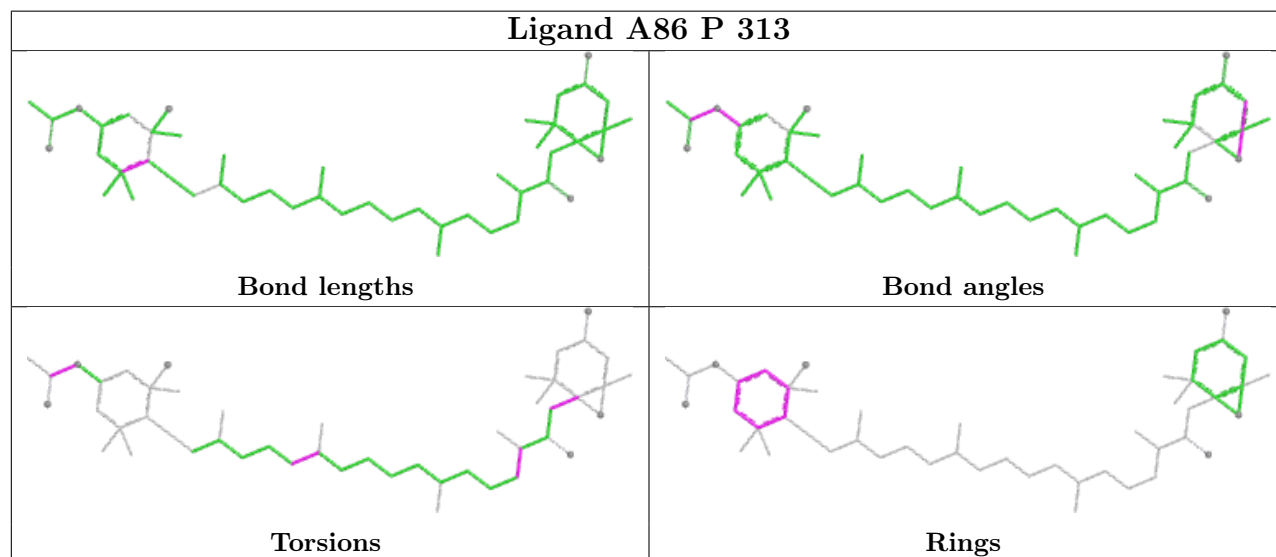
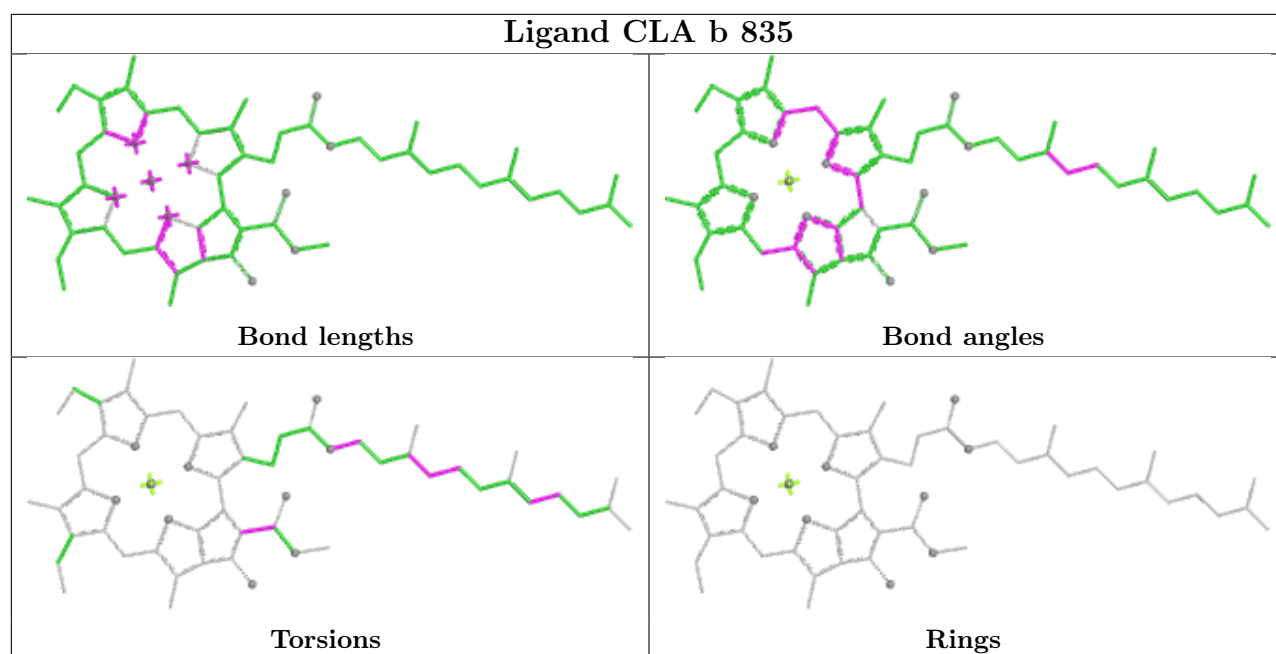


Torsions

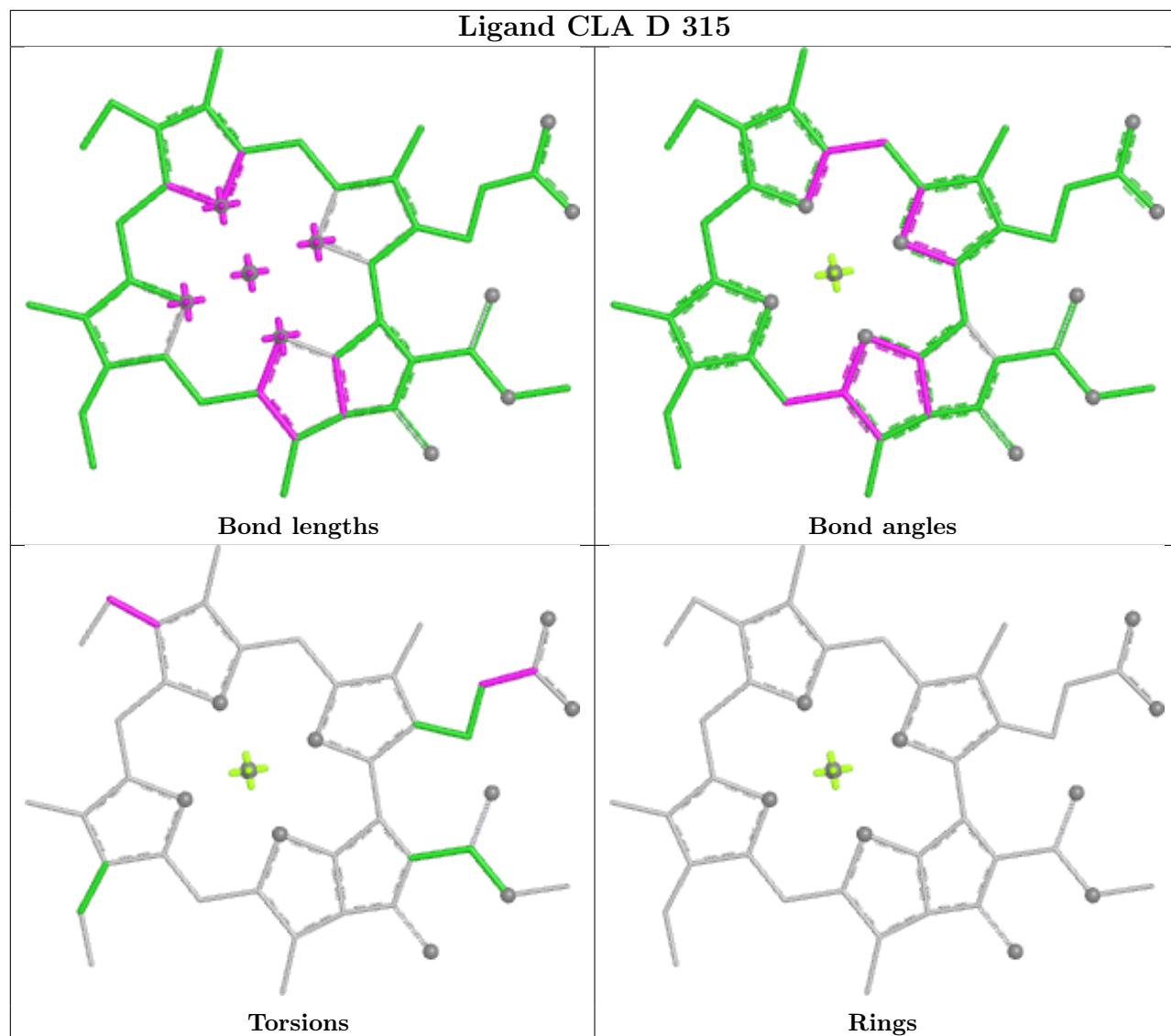


Rings

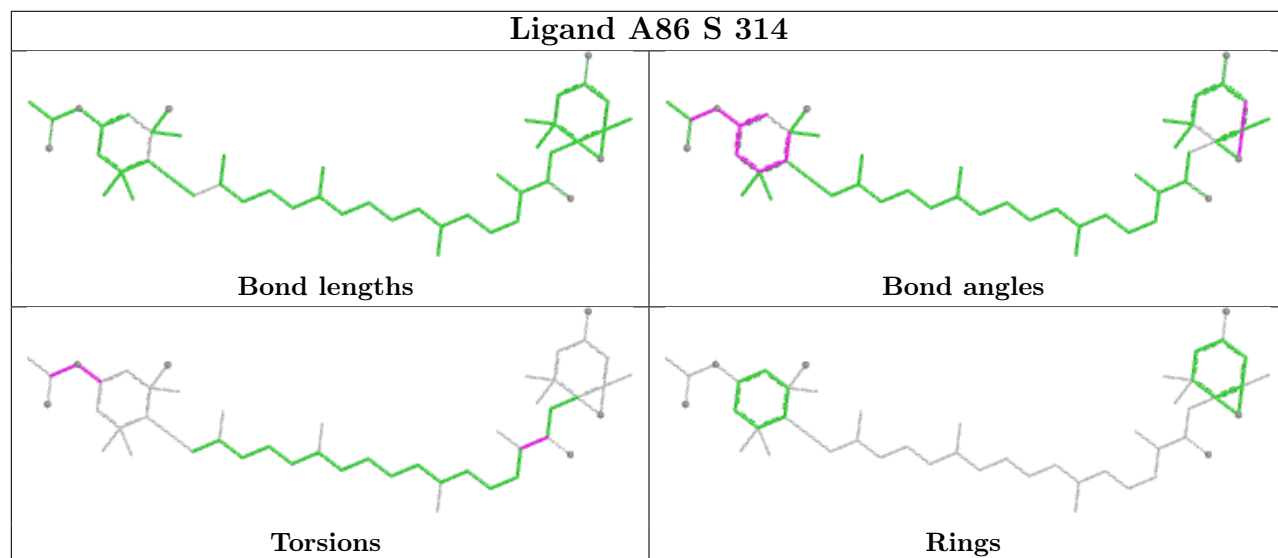




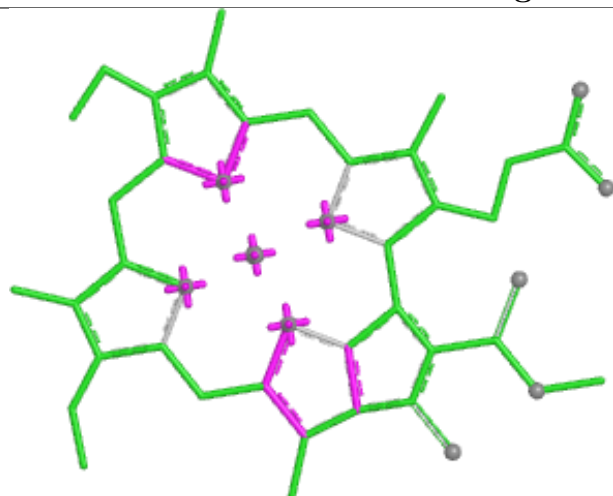
Ligand CLA D 315



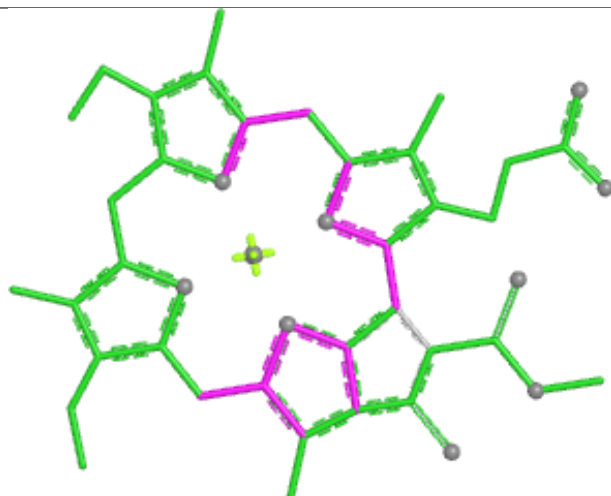
Ligand A86 S 314



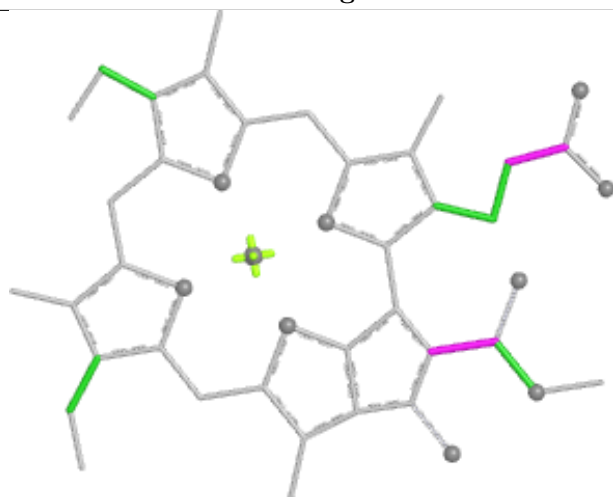
Ligand CLA B 306



Bond lengths



Bond angles

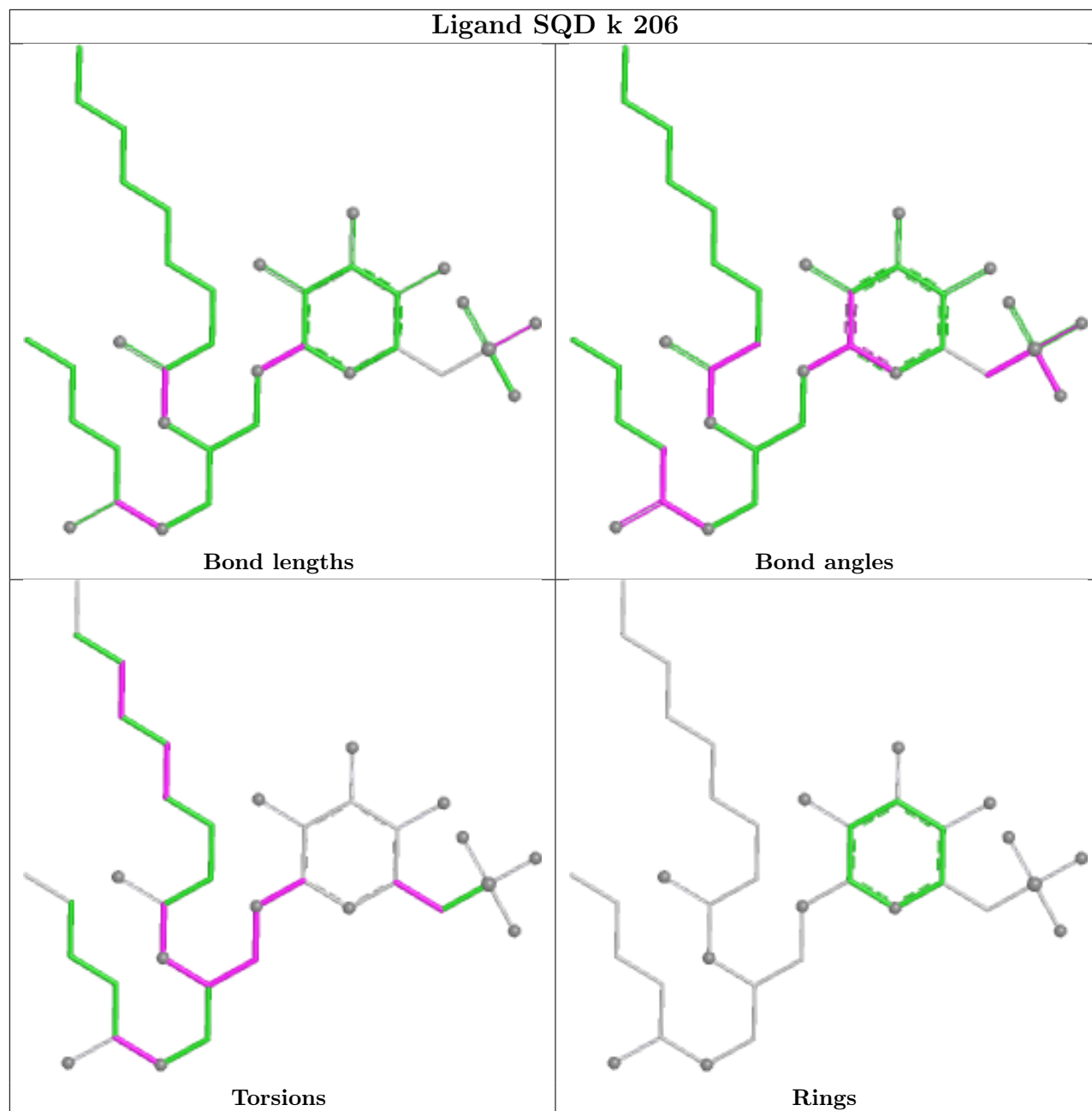


Torsions

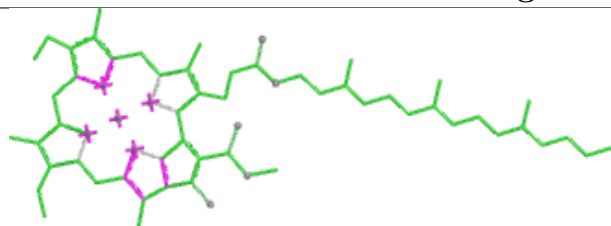


Rings

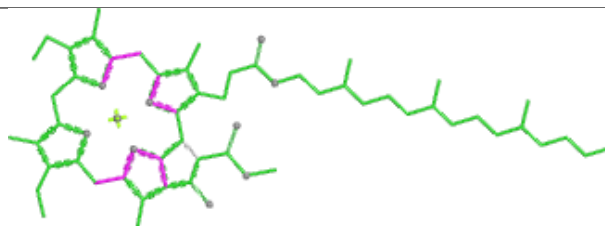
Ligand SQD k 206



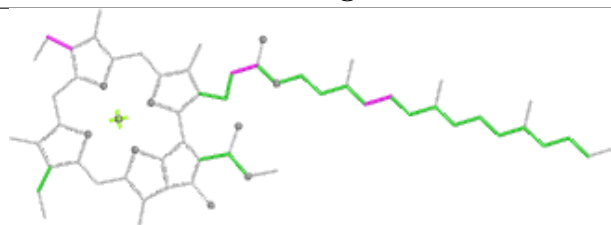
Ligand CLA S 305



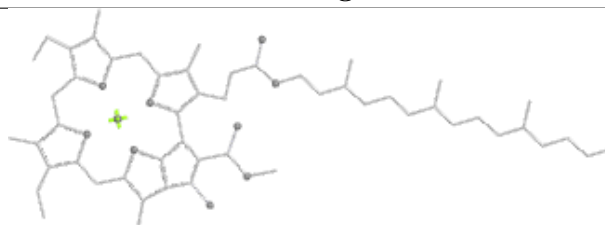
Bond lengths



Bond angles

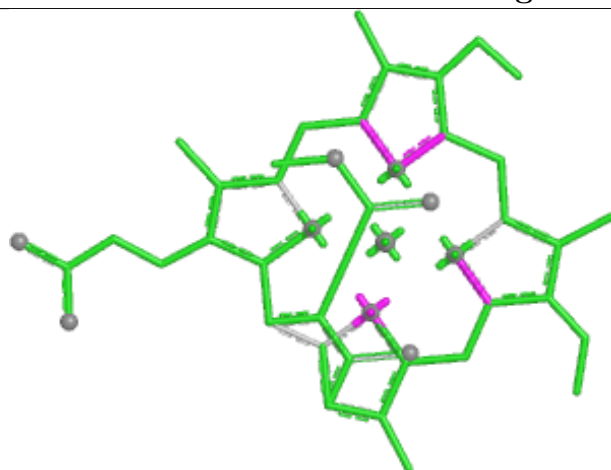


Torsions

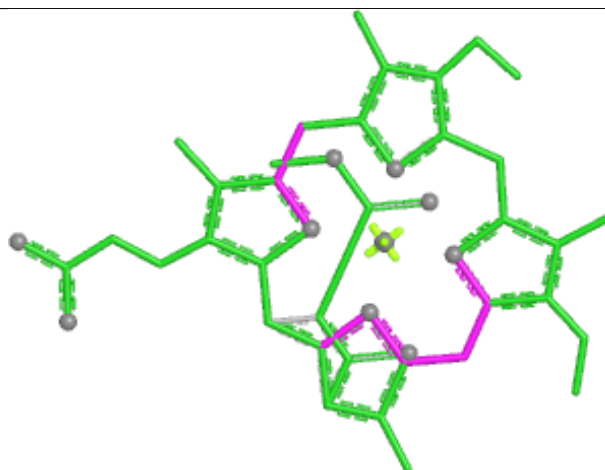


Rings

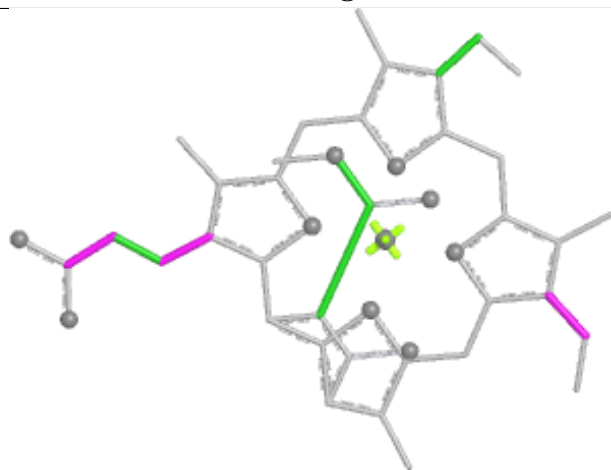
Ligand KC2 U 304



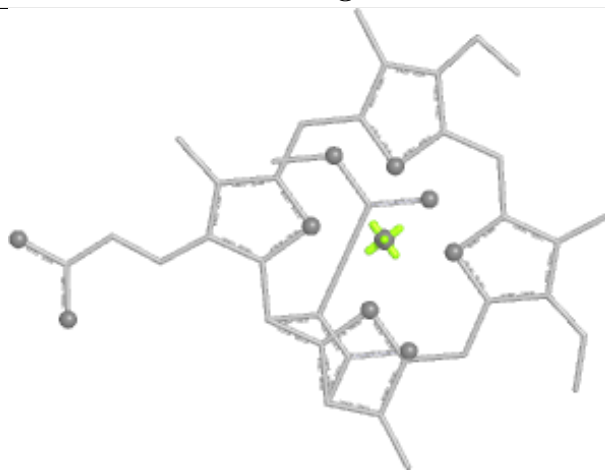
Bond lengths



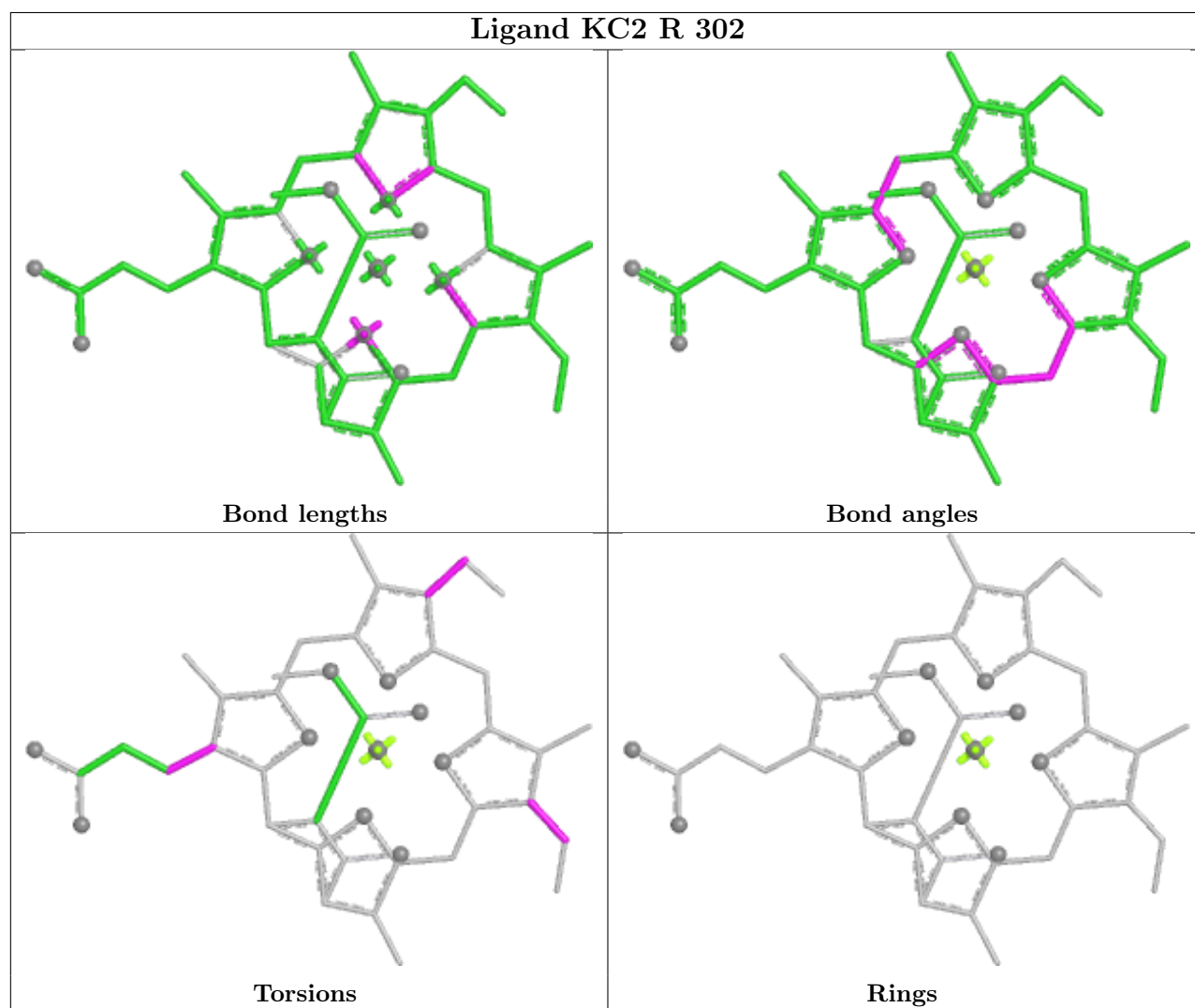
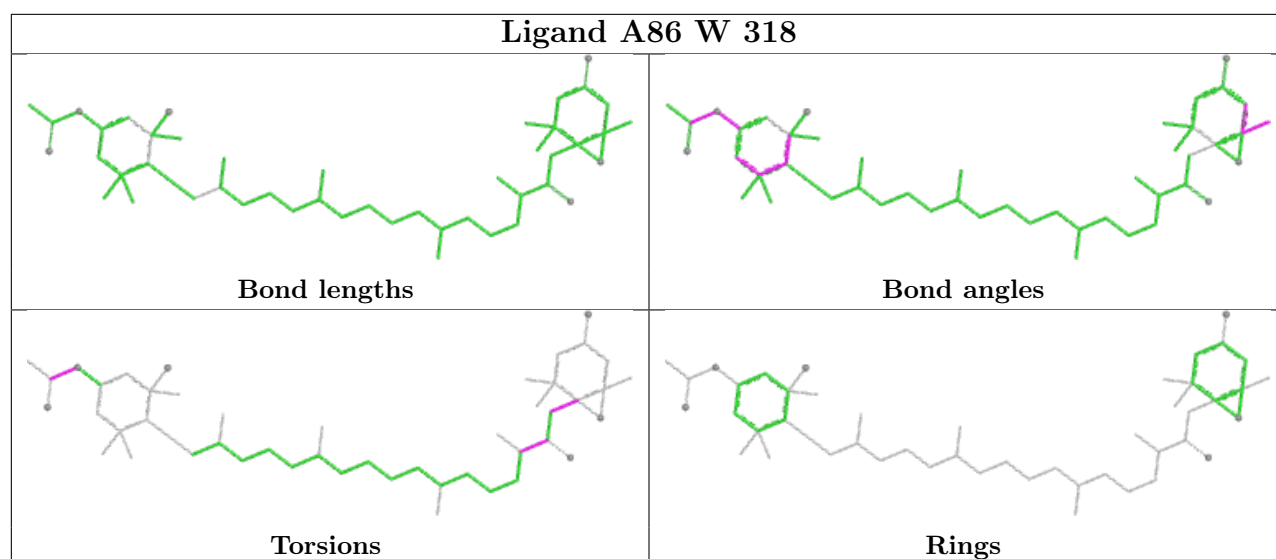
Bond angles

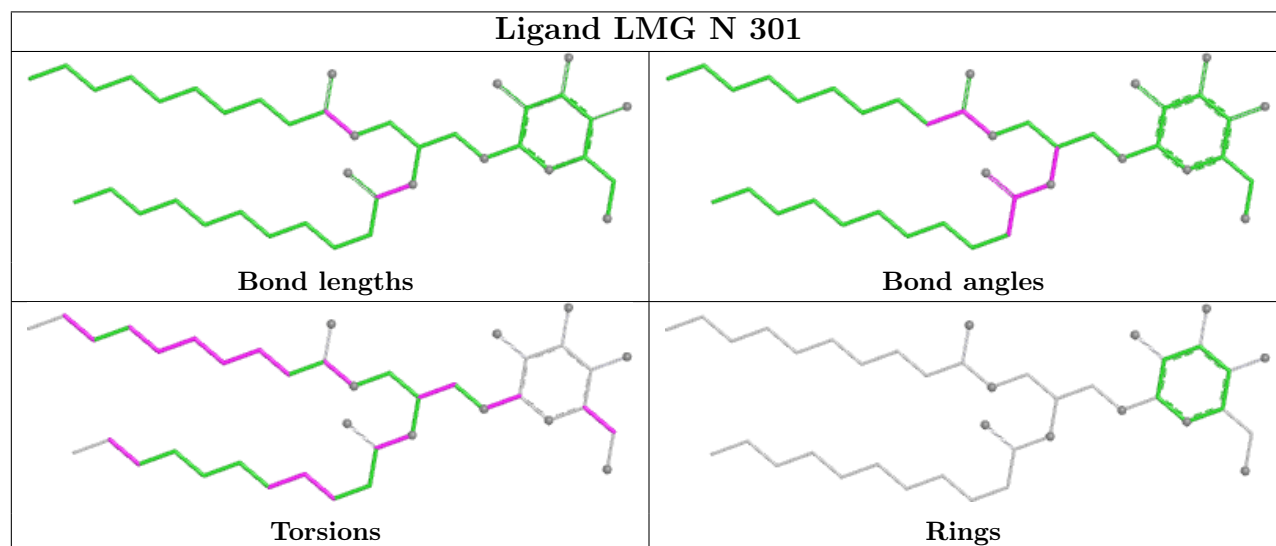
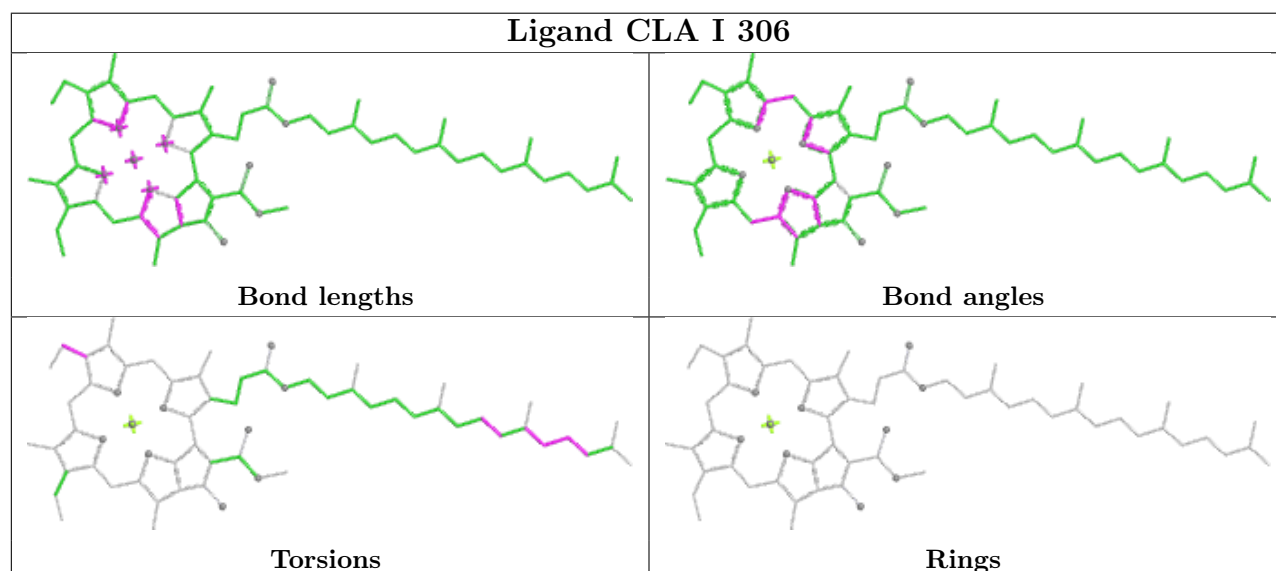
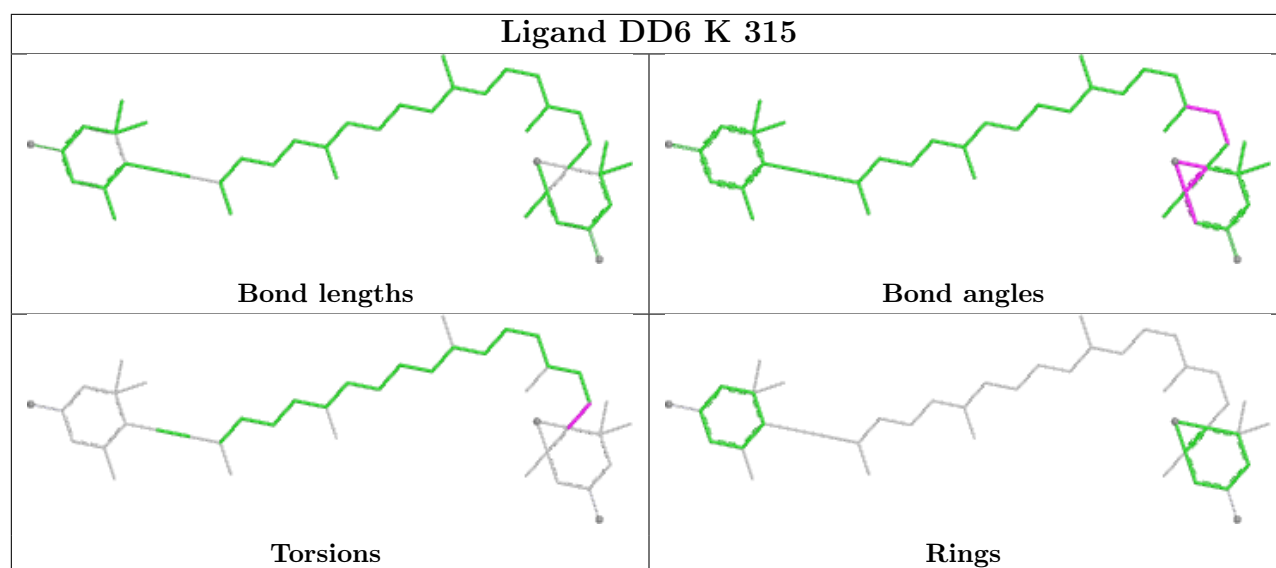


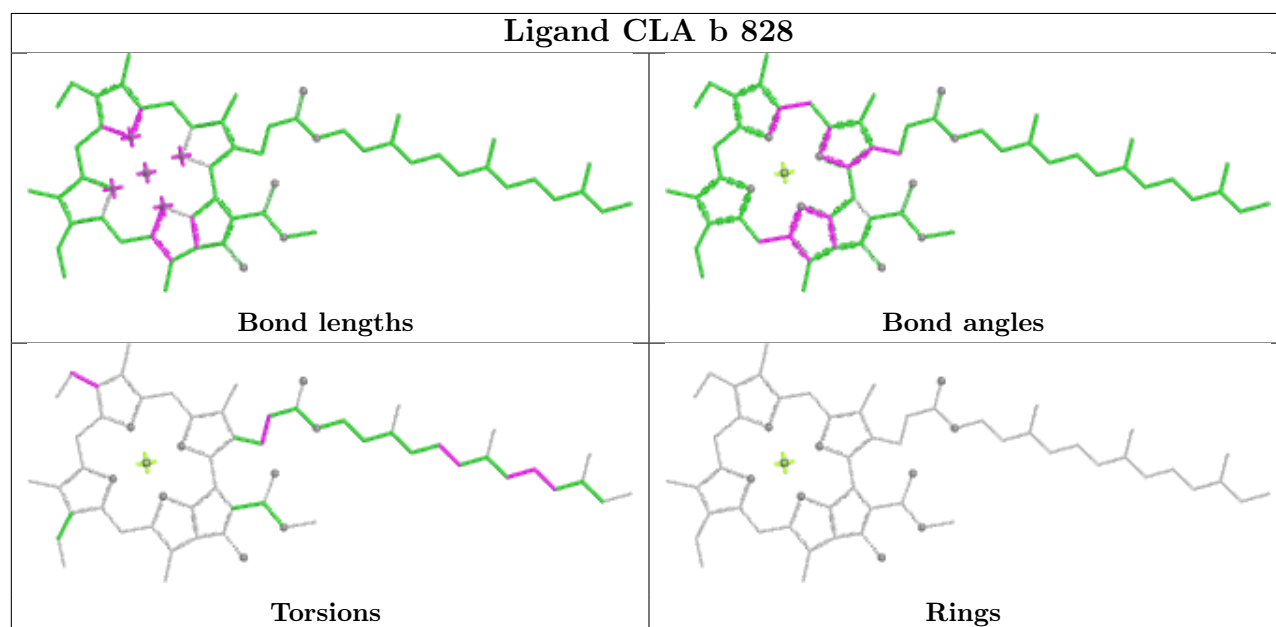
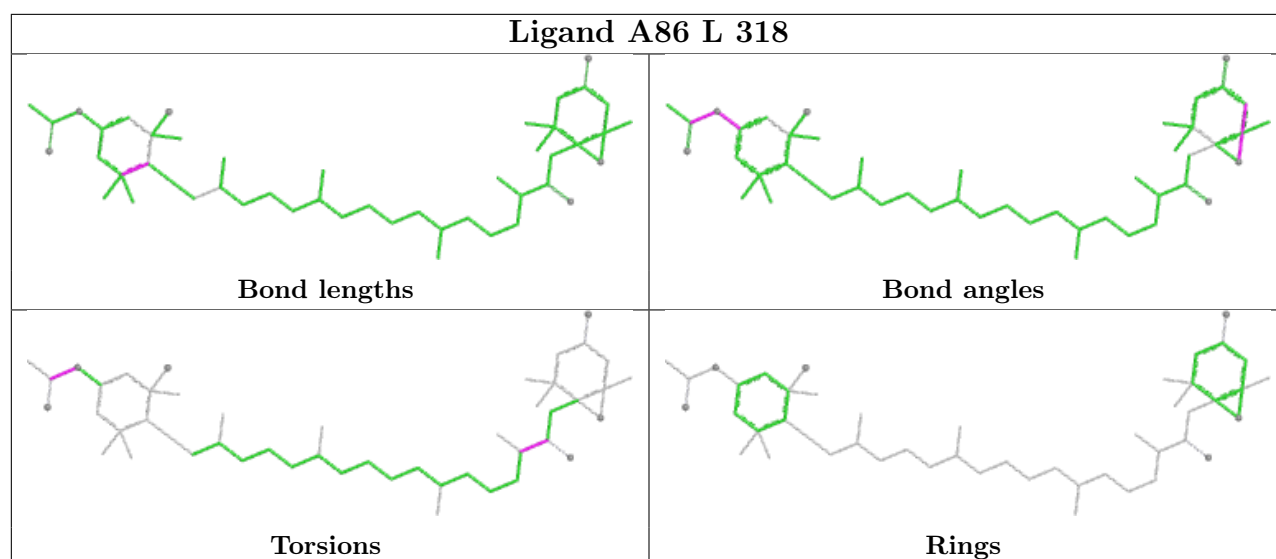
Torsions



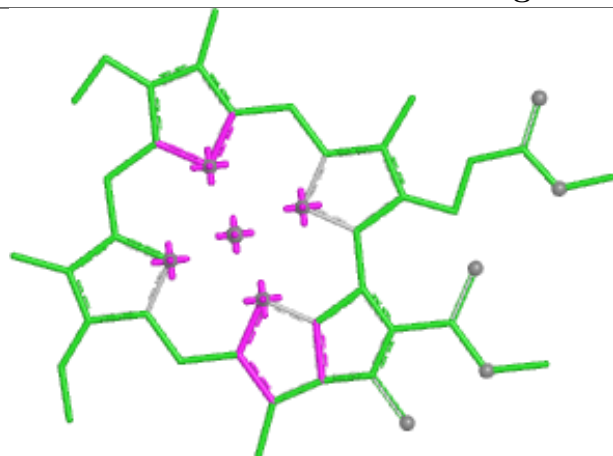
Rings



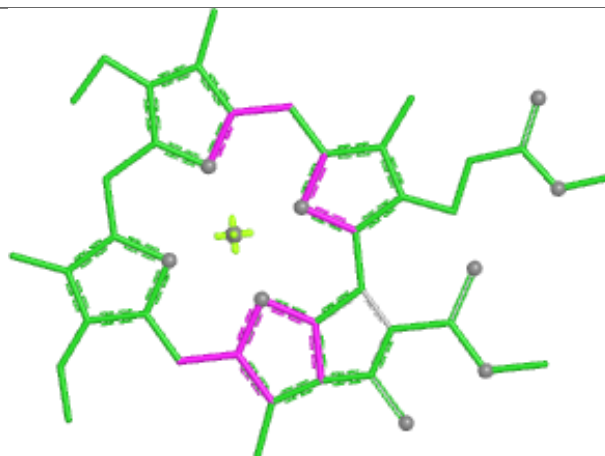




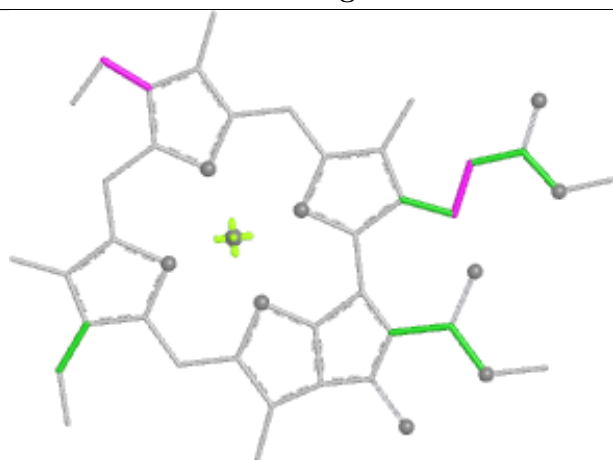
Ligand CLA H 310



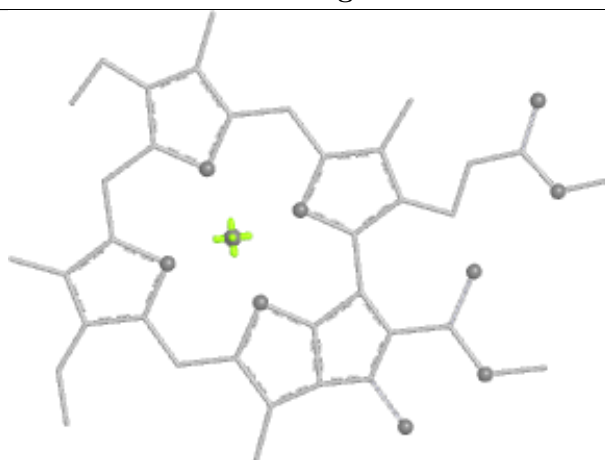
Bond lengths



Bond angles

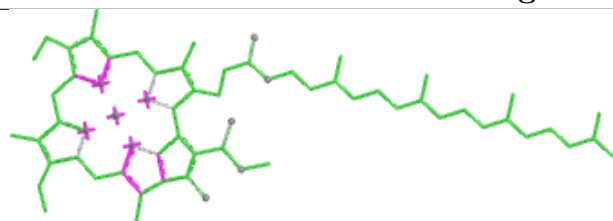


Torsions

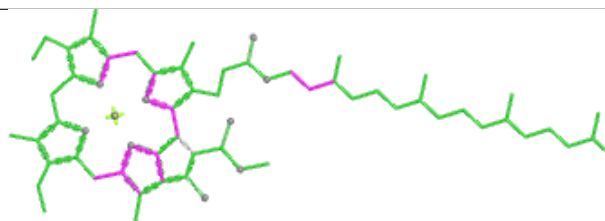


Rings

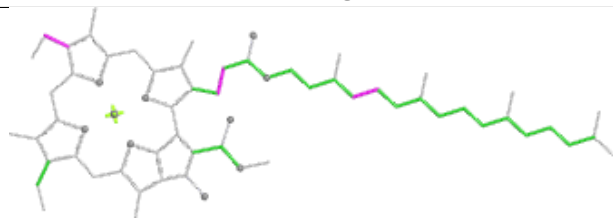
Ligand CLA a 838



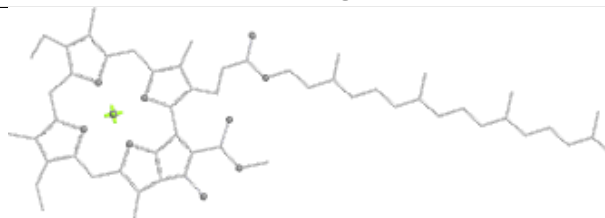
Bond lengths



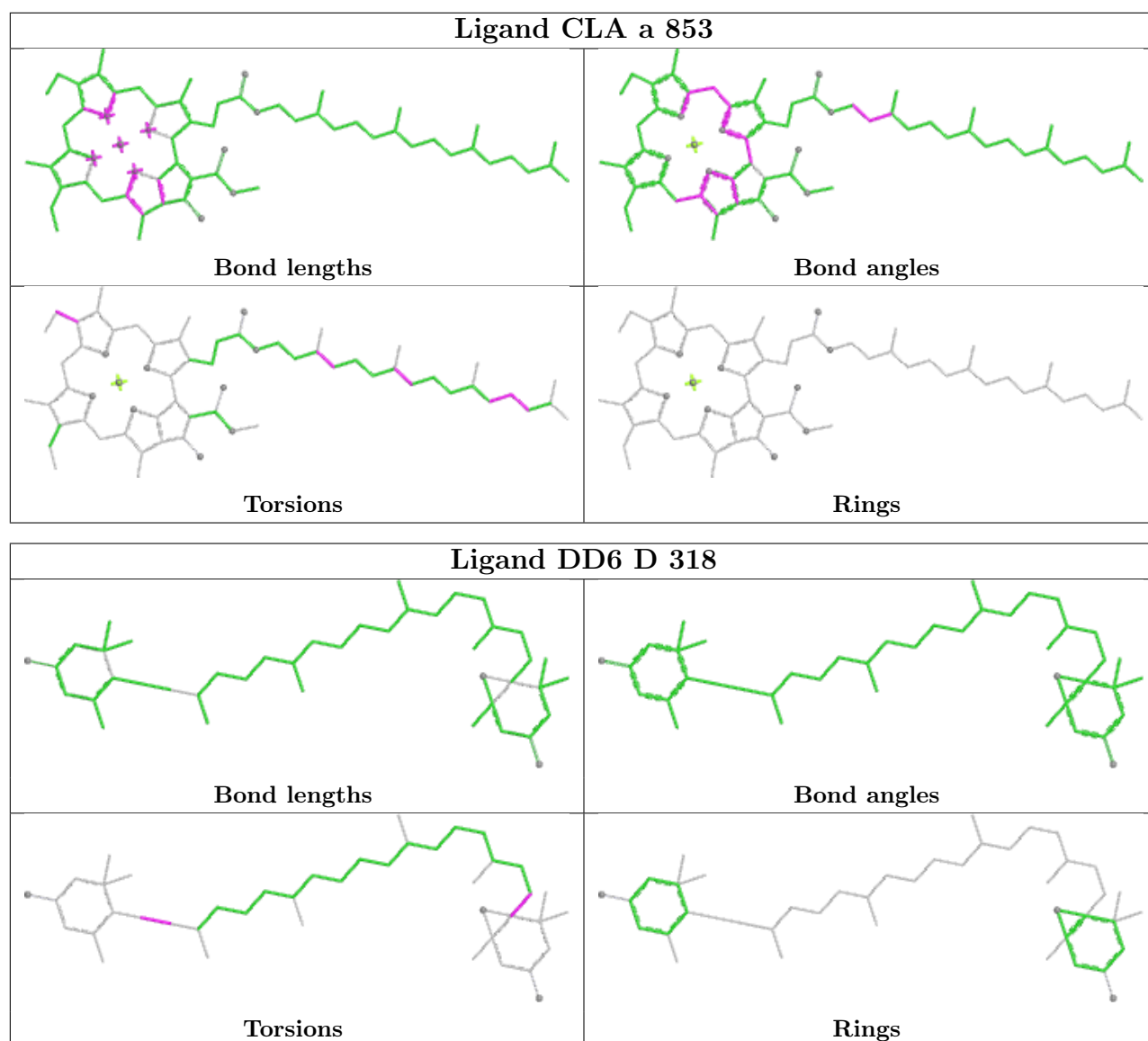
Bond angles



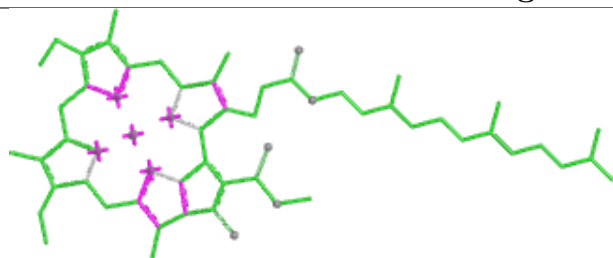
Torsions



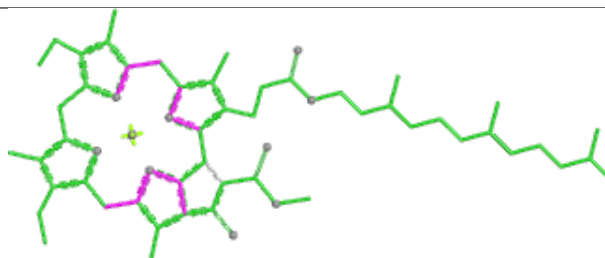
Rings



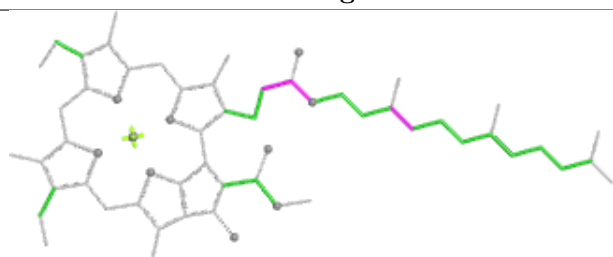
Ligand CLA b 825



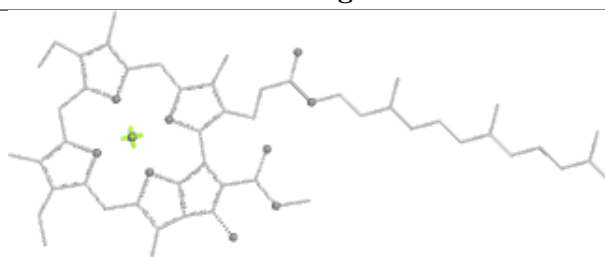
Bond lengths



Bond angles

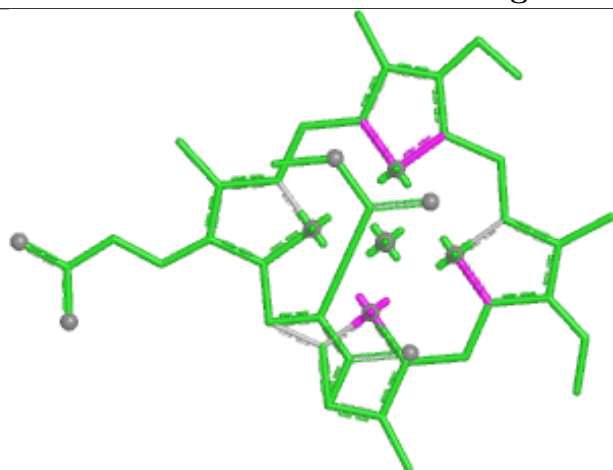


Torsions

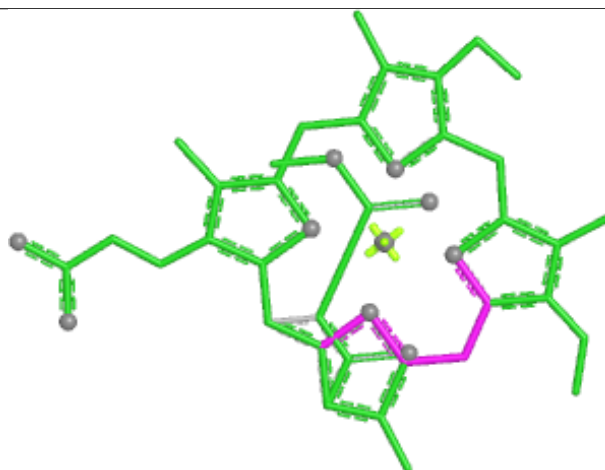


Rings

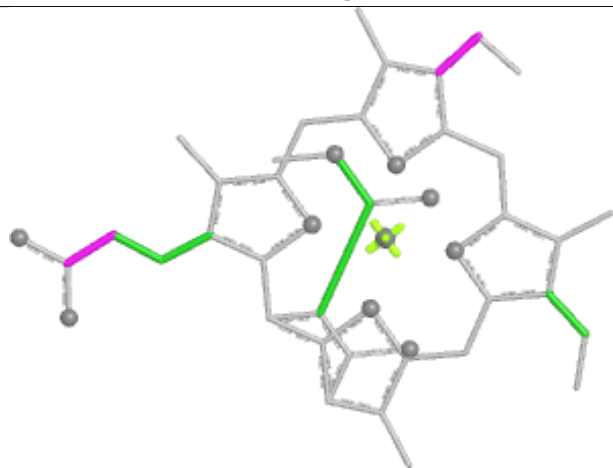
Ligand KC2 W 305



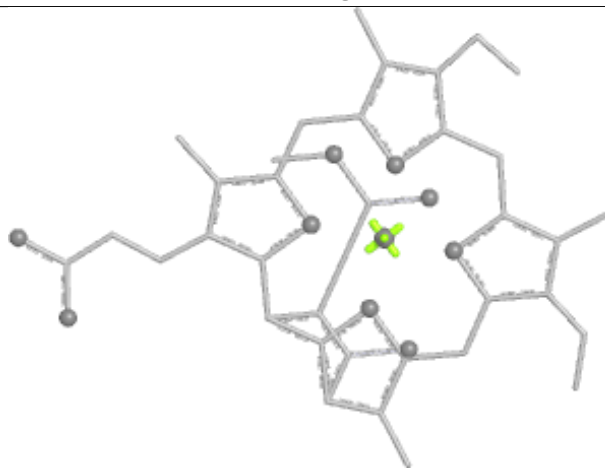
Bond lengths



Bond angles

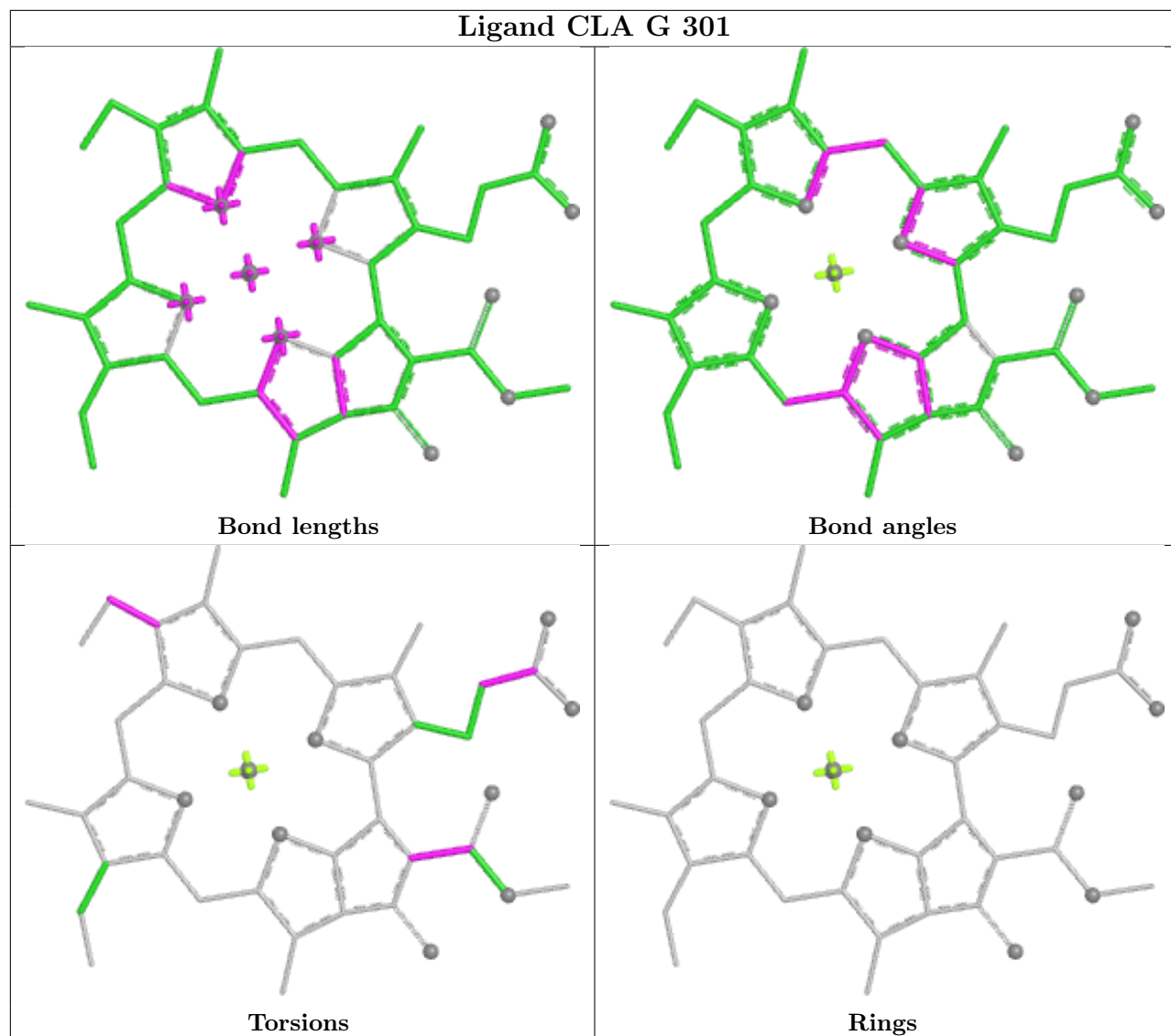


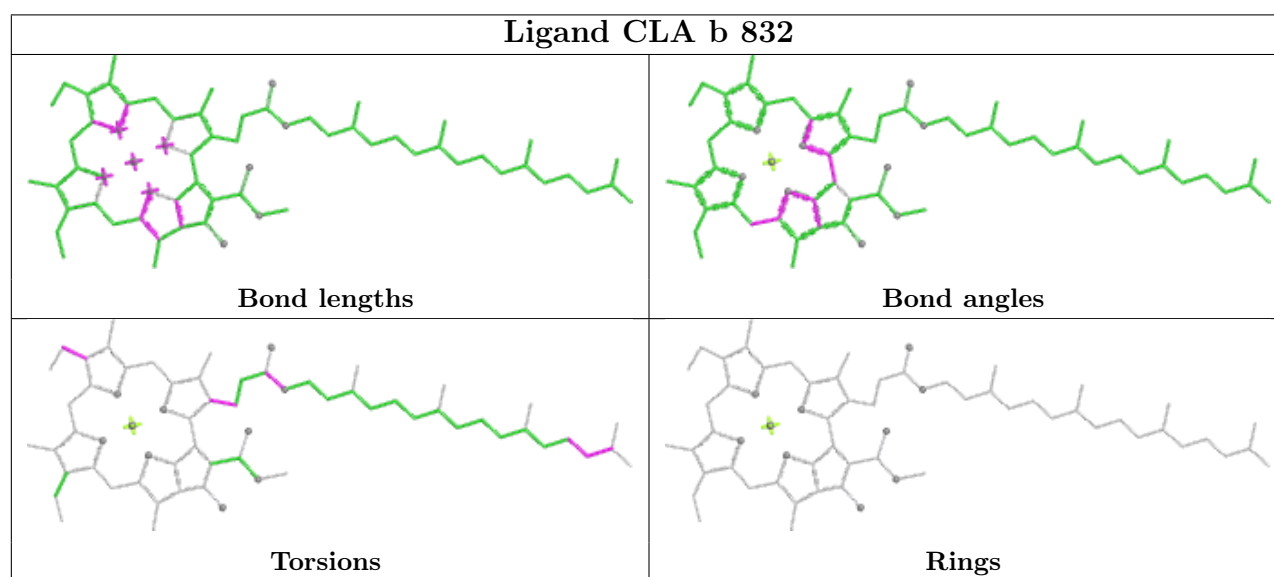
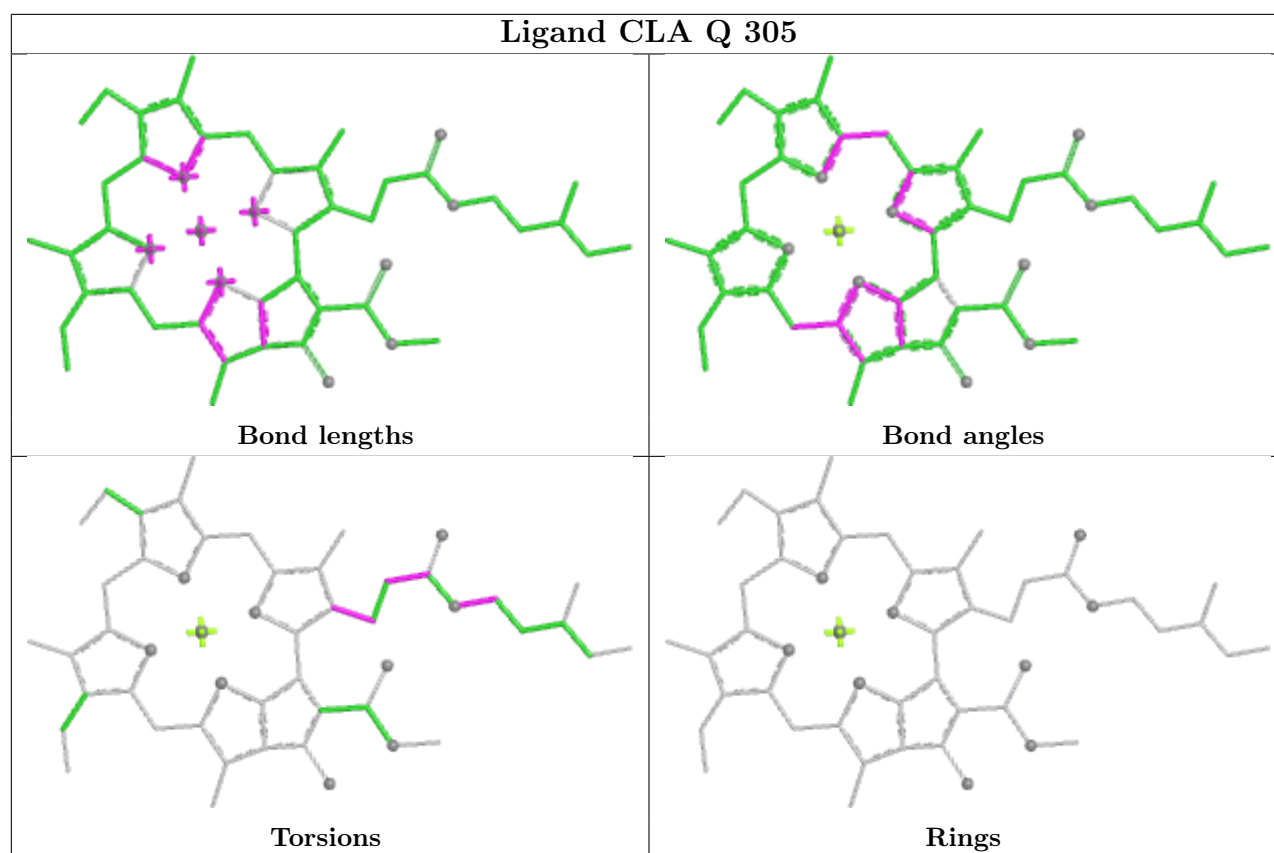
Torsions



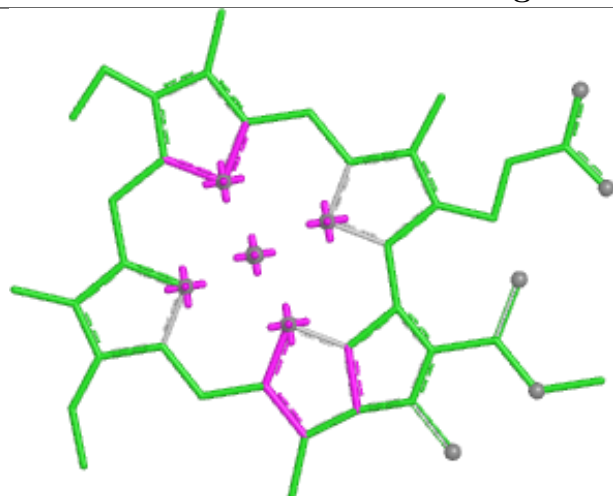
Rings

Ligand CLA G 301

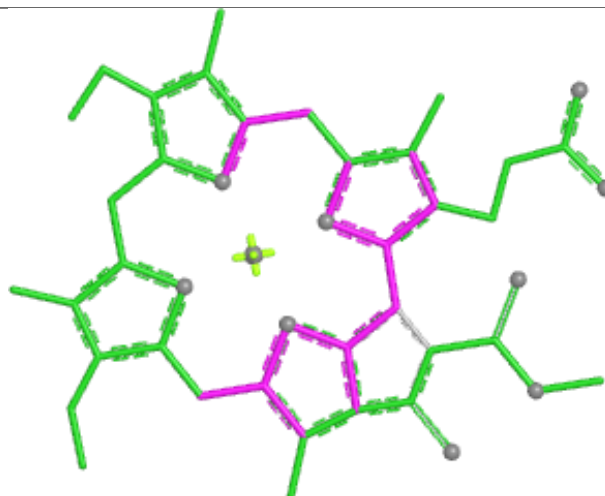




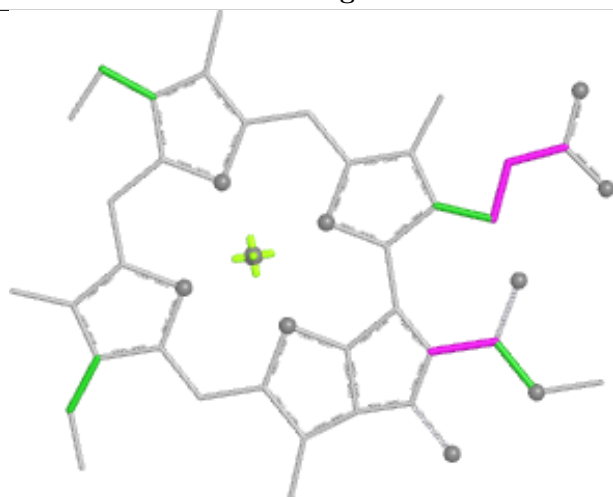
Ligand CLA U 305



Bond lengths



Bond angles

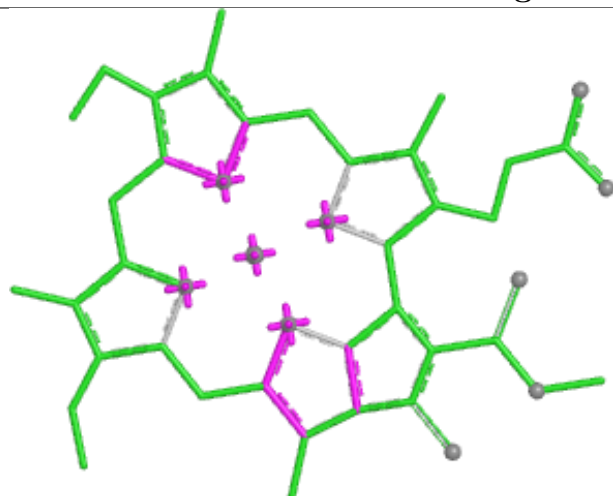


Torsions

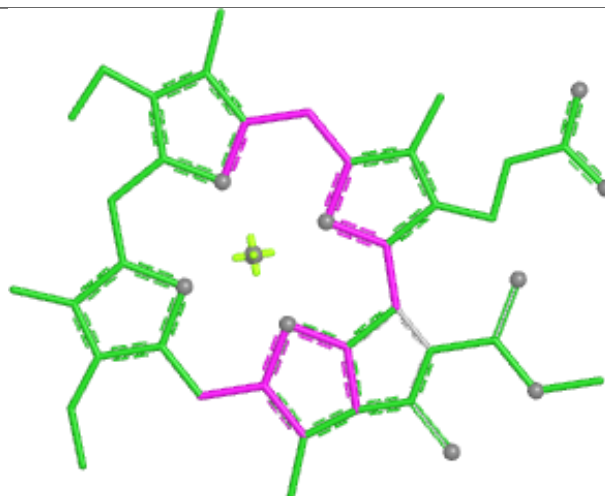


Rings

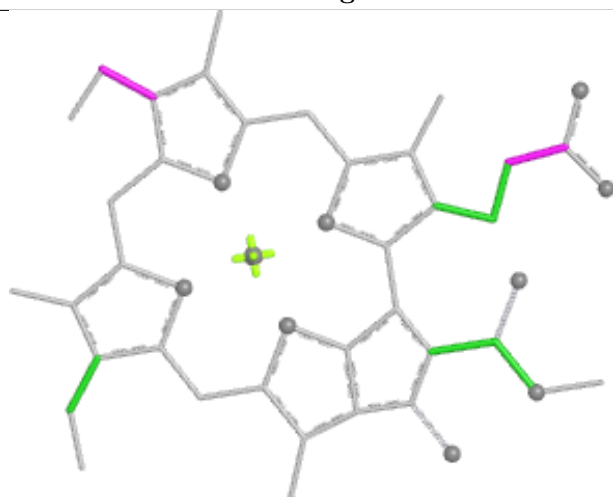
Ligand CLA B 302



Bond lengths



Bond angles

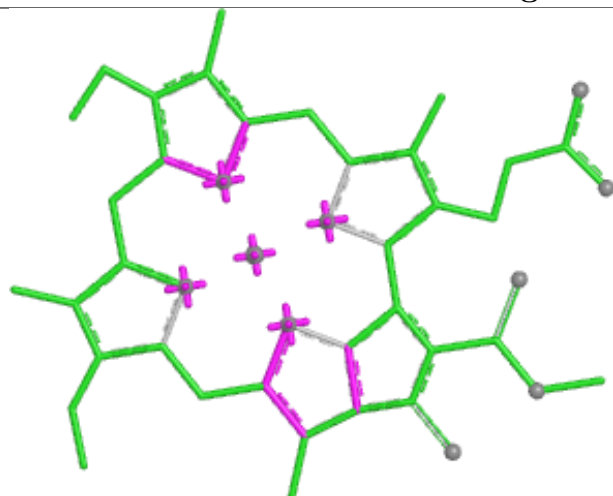


Torsions

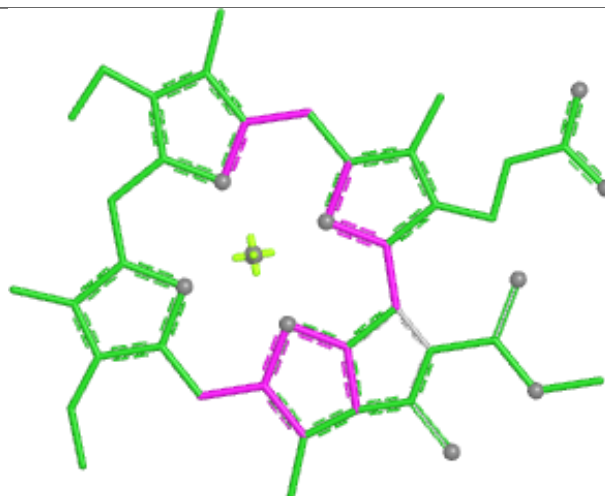


Rings

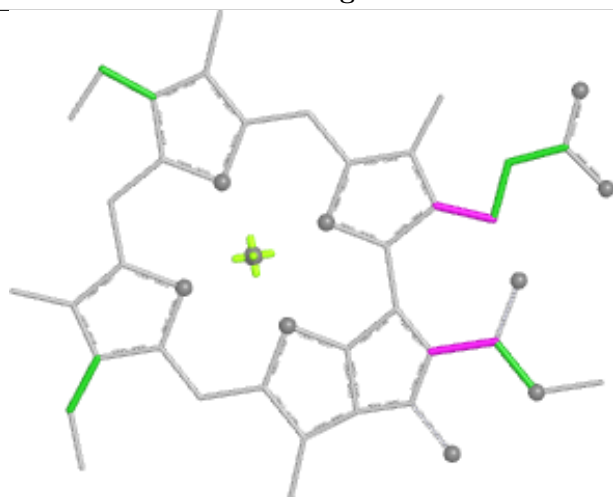
Ligand CLA I 307



Bond lengths



Bond angles

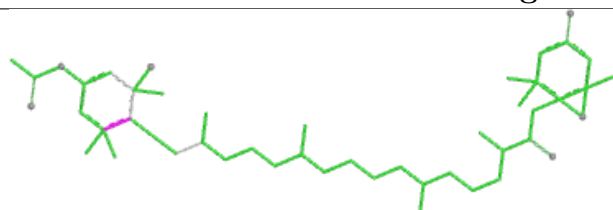


Torsions

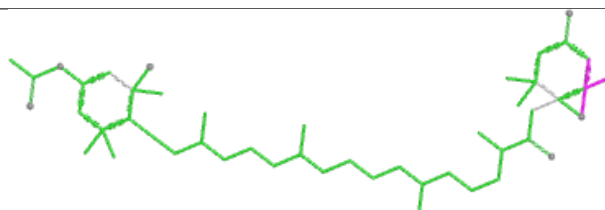


Rings

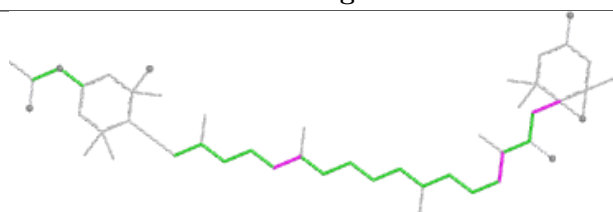
Ligand A86 C 312



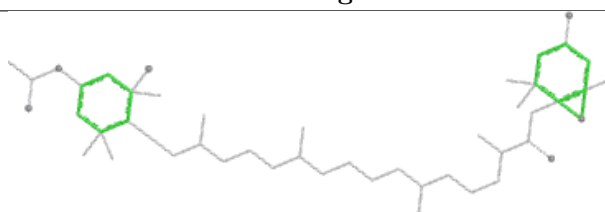
Bond lengths



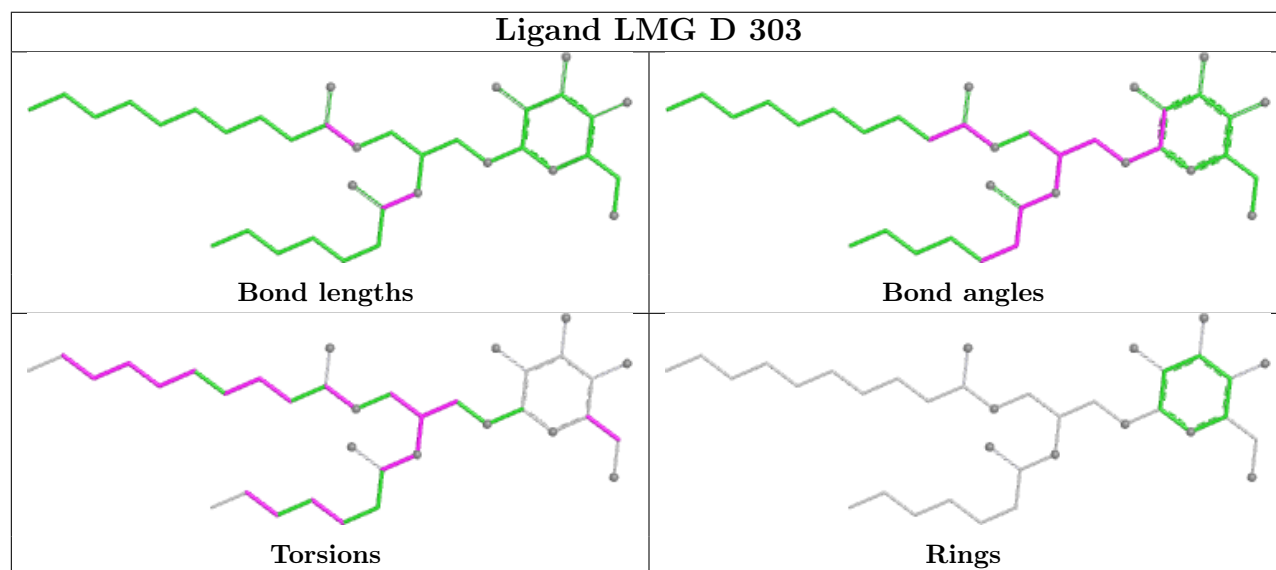
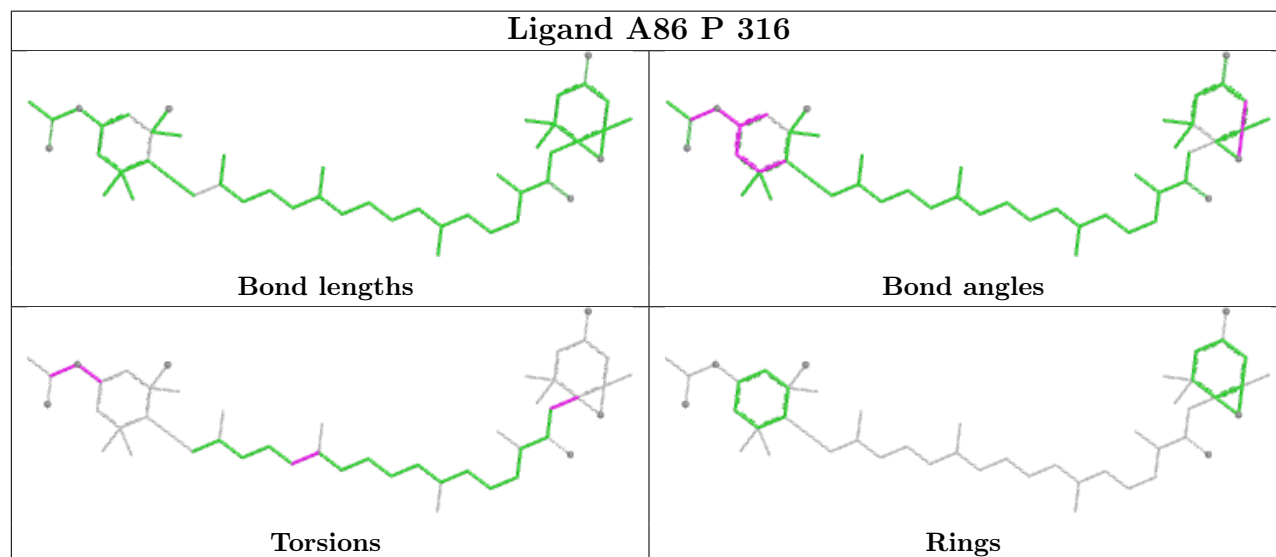
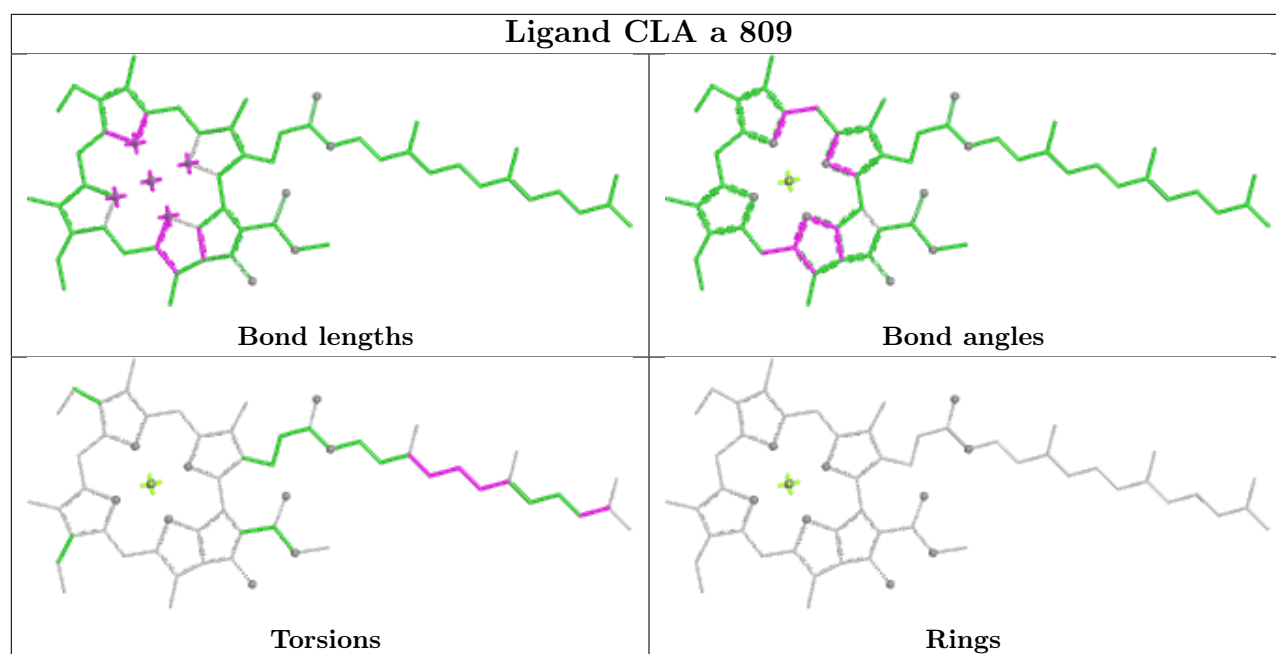
Bond angles

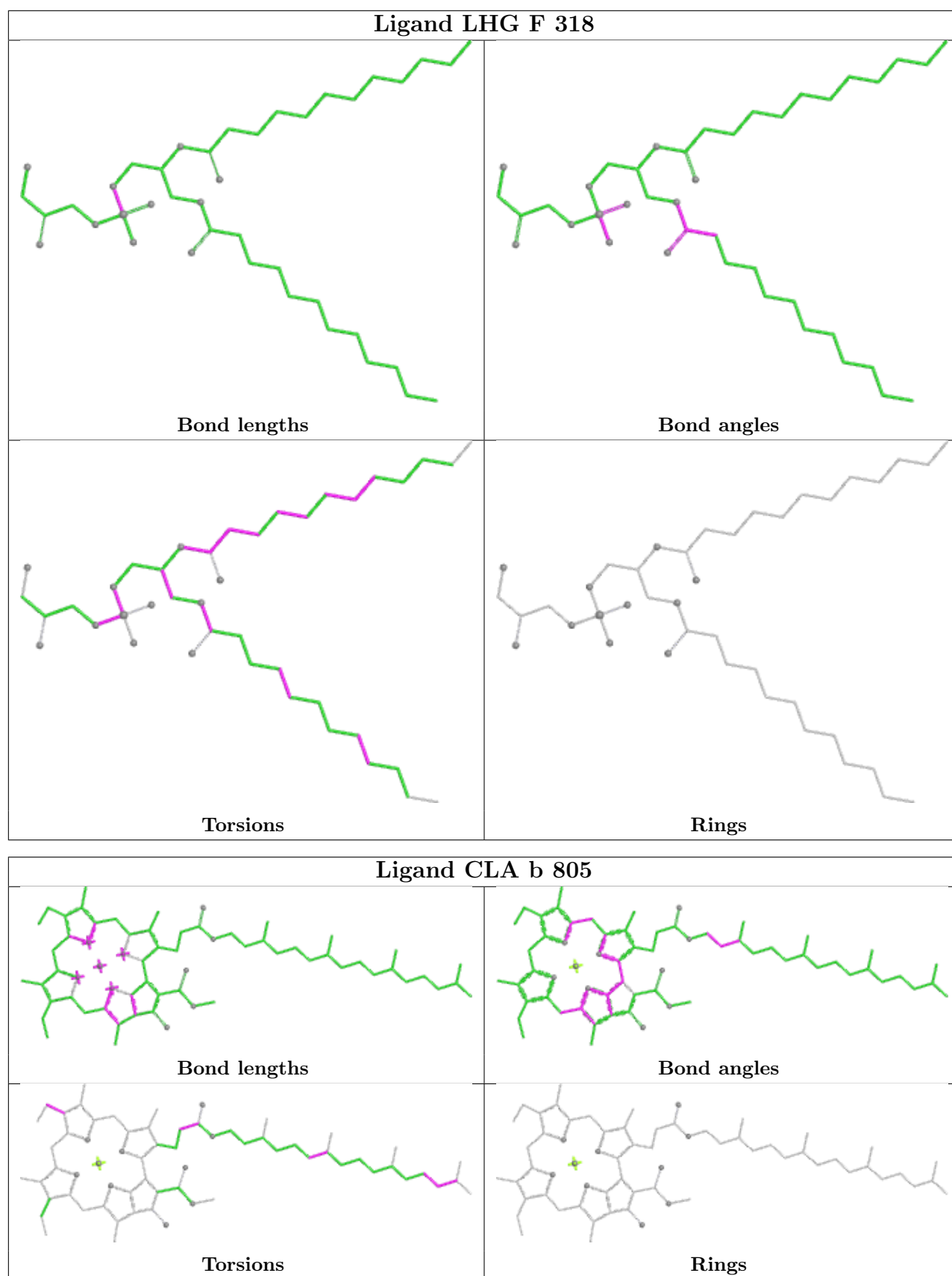


Torsions

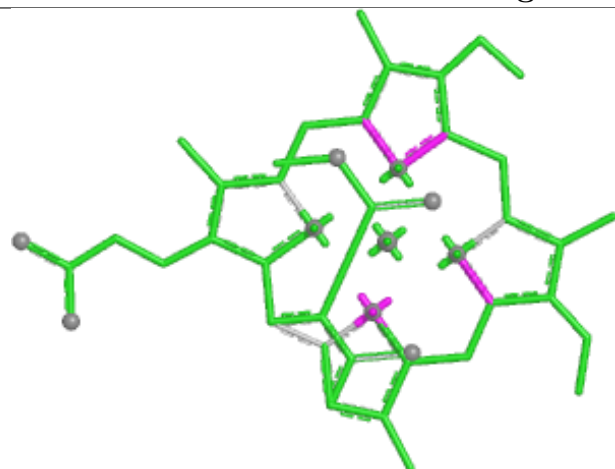


Rings

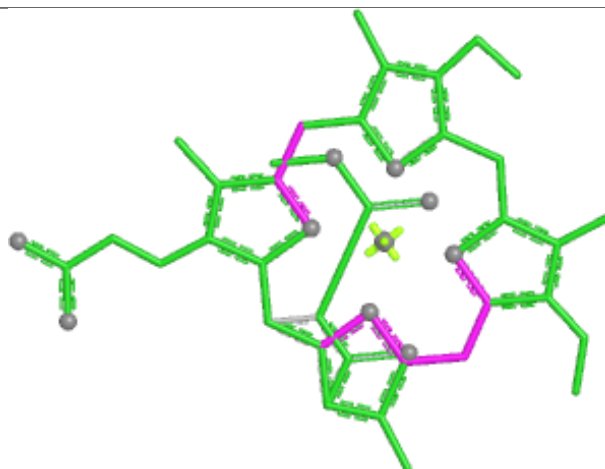




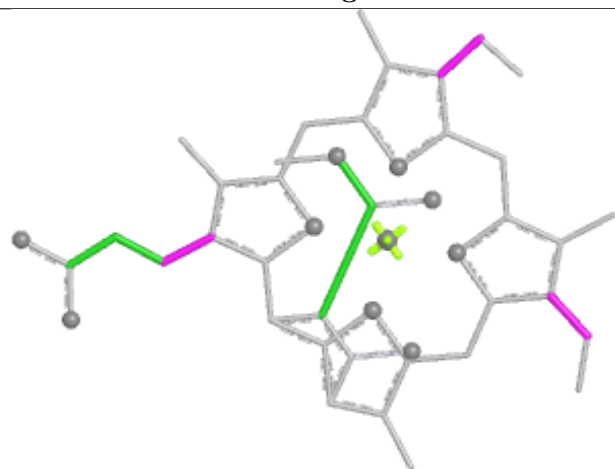
Ligand KC2 K 305



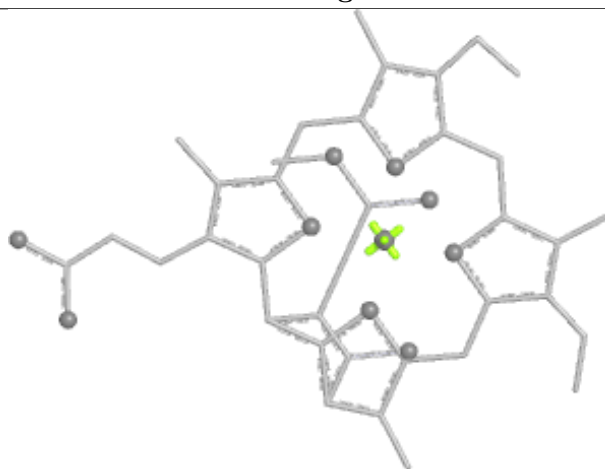
Bond lengths



Bond angles

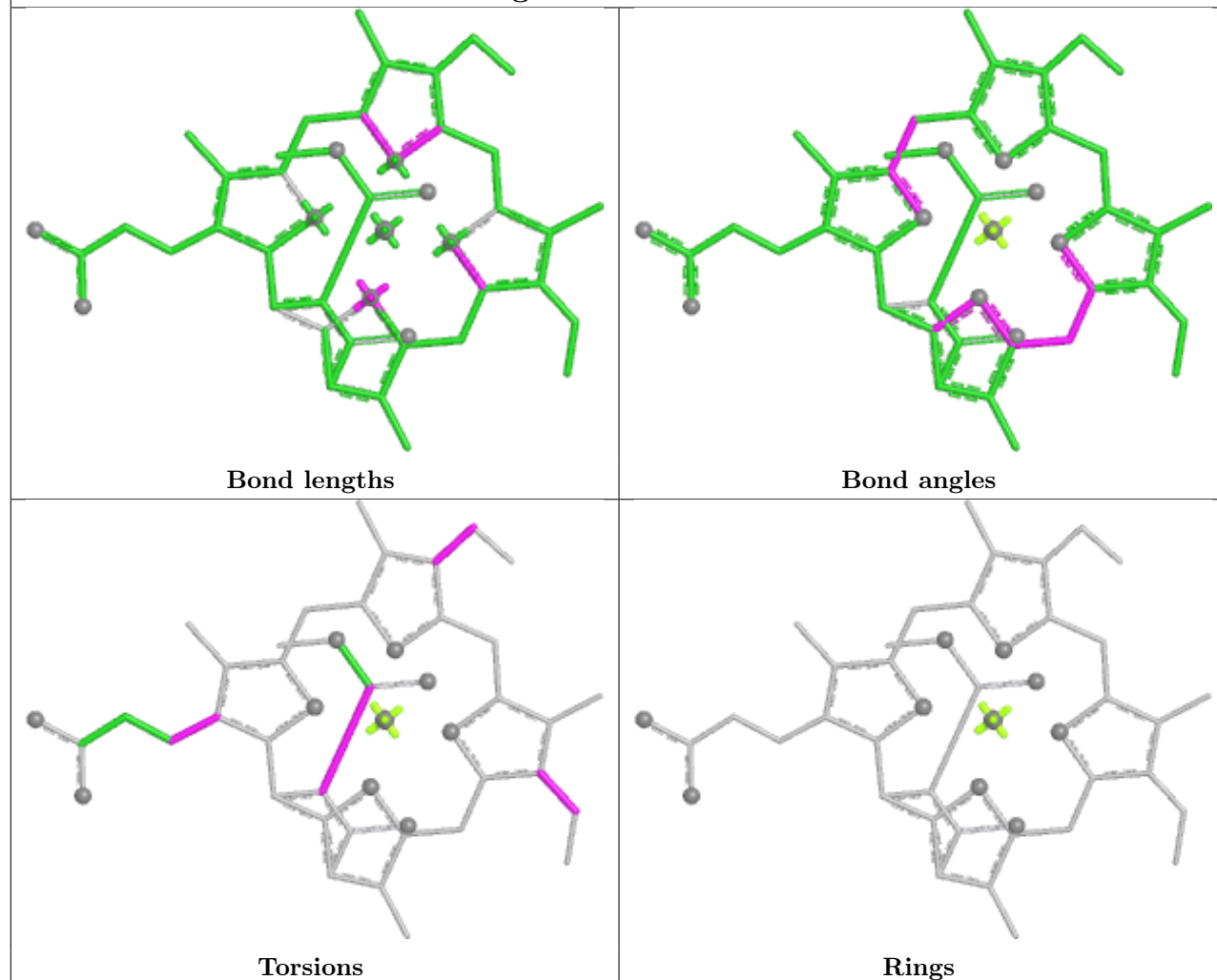


Torsions

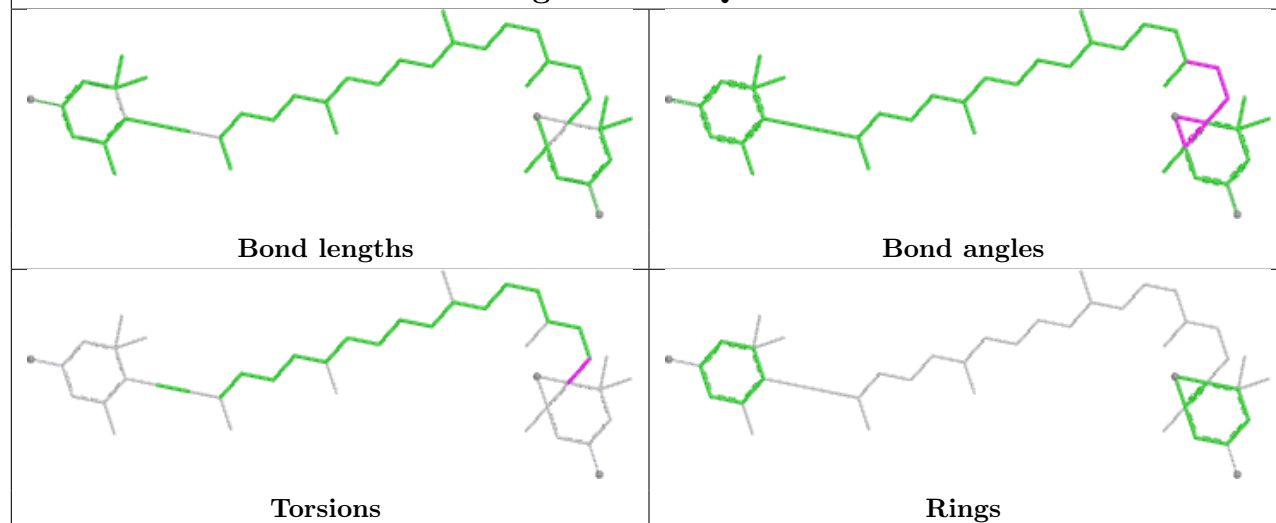


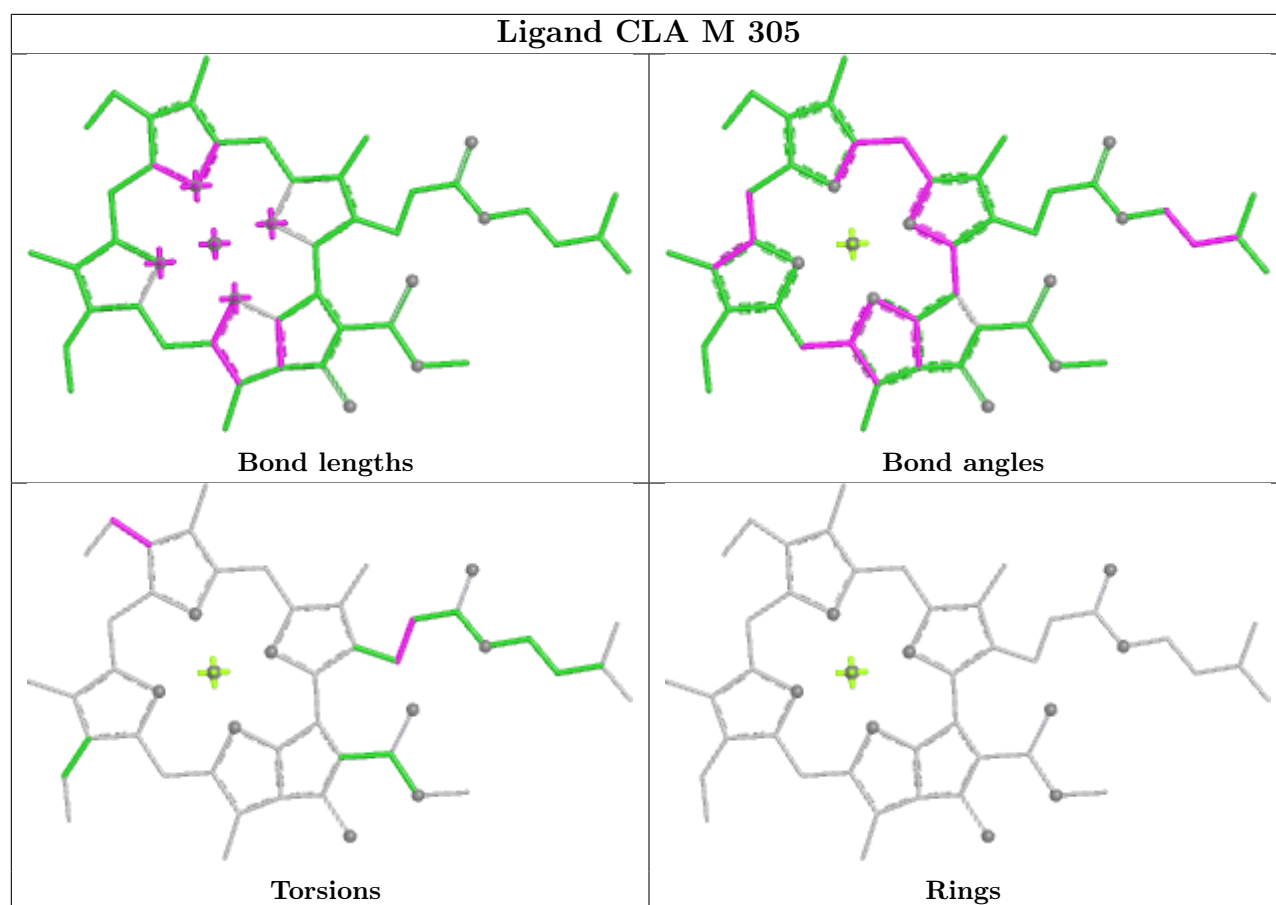
Rings

Ligand KC2 S 303



Ligand DD6 Q 315





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.

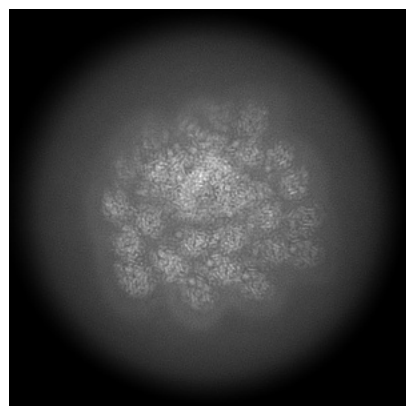
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39717. These allow visual inspection of the internal detail of the map and identification of artifacts.

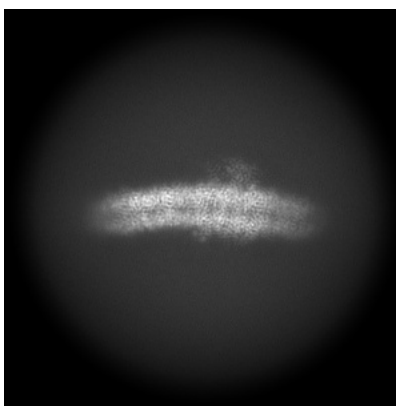
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

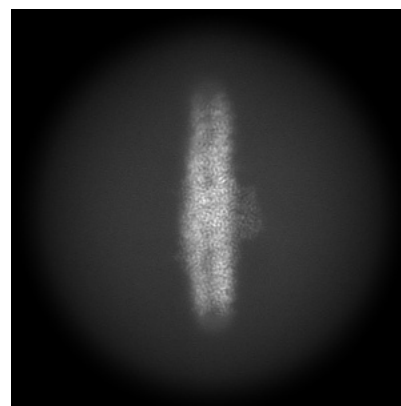
6.1.1 Primary map



X

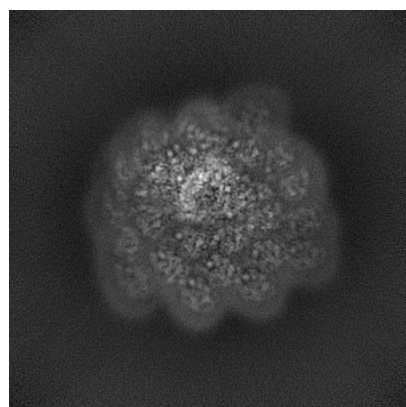


Y

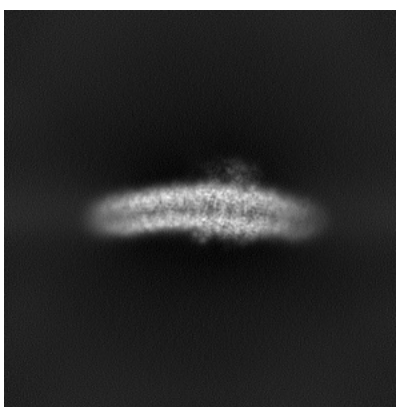


Z

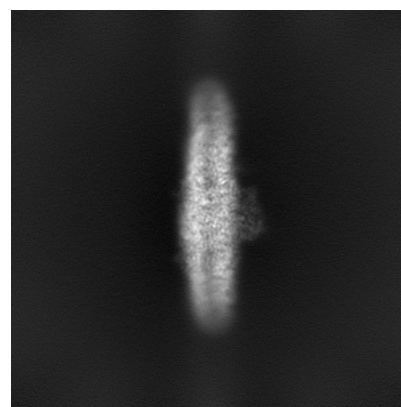
6.1.2 Raw map



X



Y

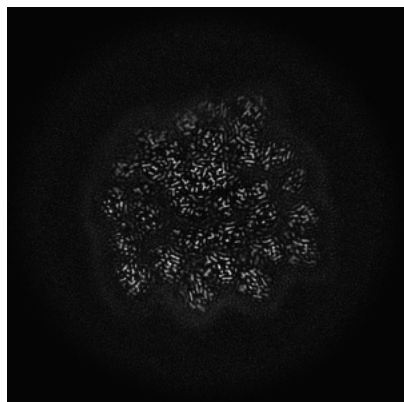


Z

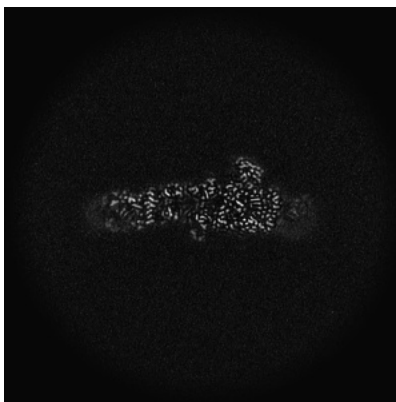
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

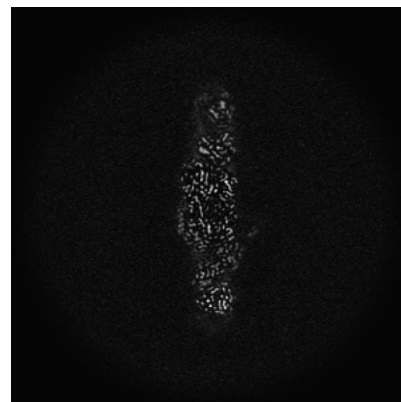
6.2.1 Primary map



X Index: 200

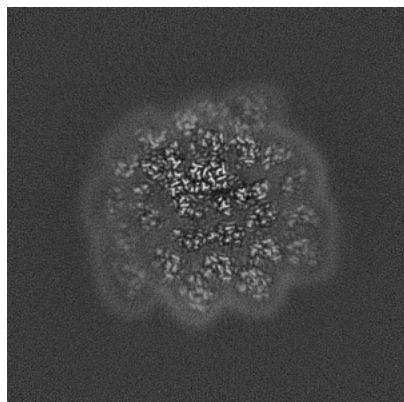


Y Index: 200

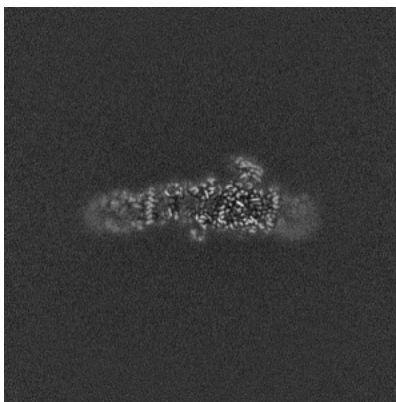


Z Index: 200

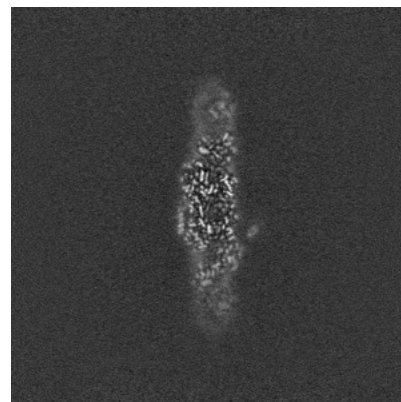
6.2.2 Raw map



X Index: 200



Y Index: 200

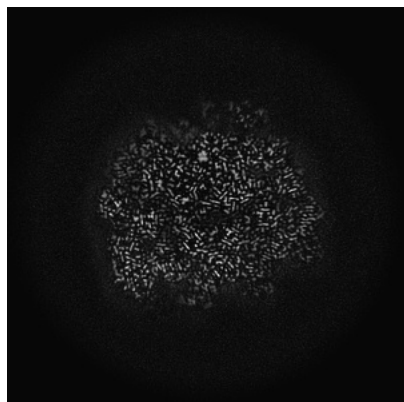


Z Index: 200

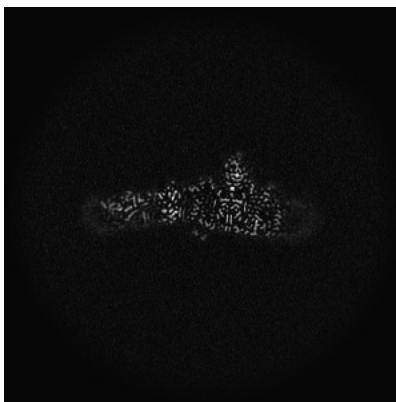
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

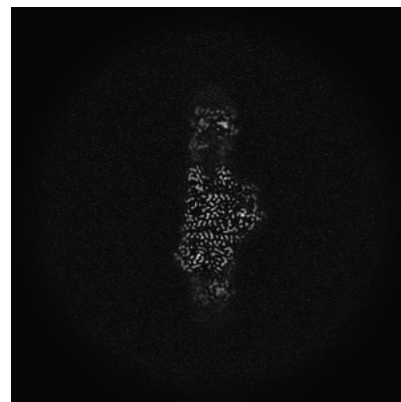
6.3.1 Primary map



X Index: 210

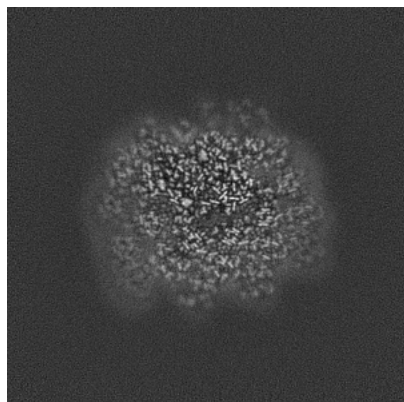


Y Index: 191

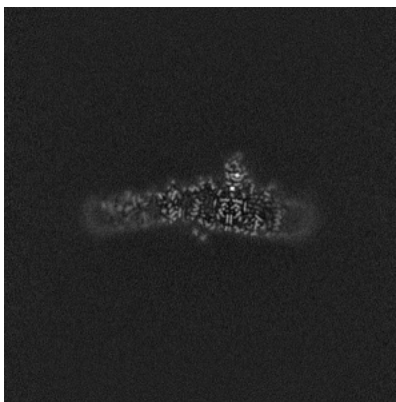


Z Index: 232

6.3.2 Raw map



X Index: 211



Y Index: 191

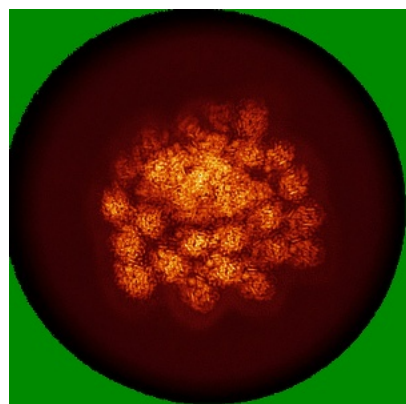


Z Index: 232

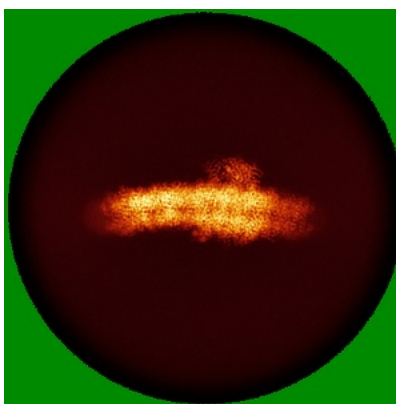
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

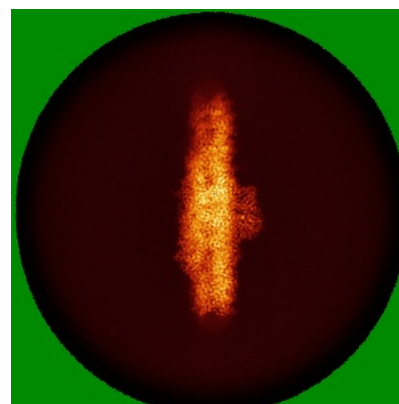
6.4.1 Primary map



X

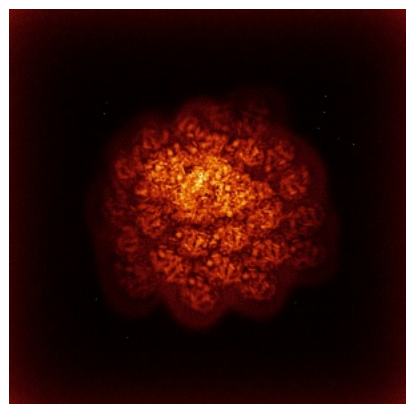


Y

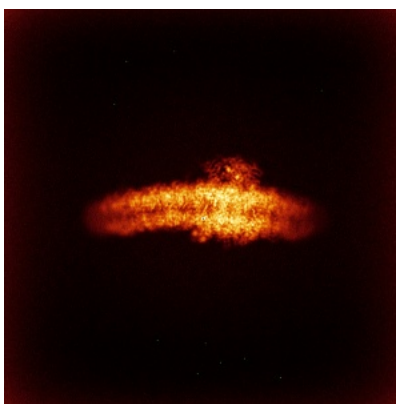


Z

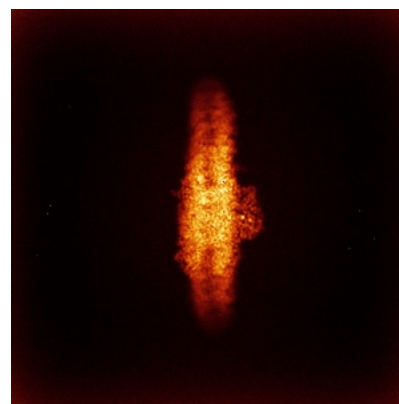
6.4.2 Raw map



X



Y

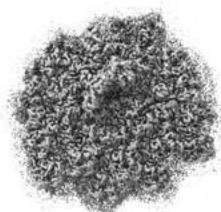


Z

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



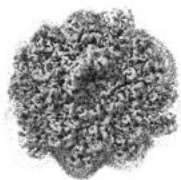
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

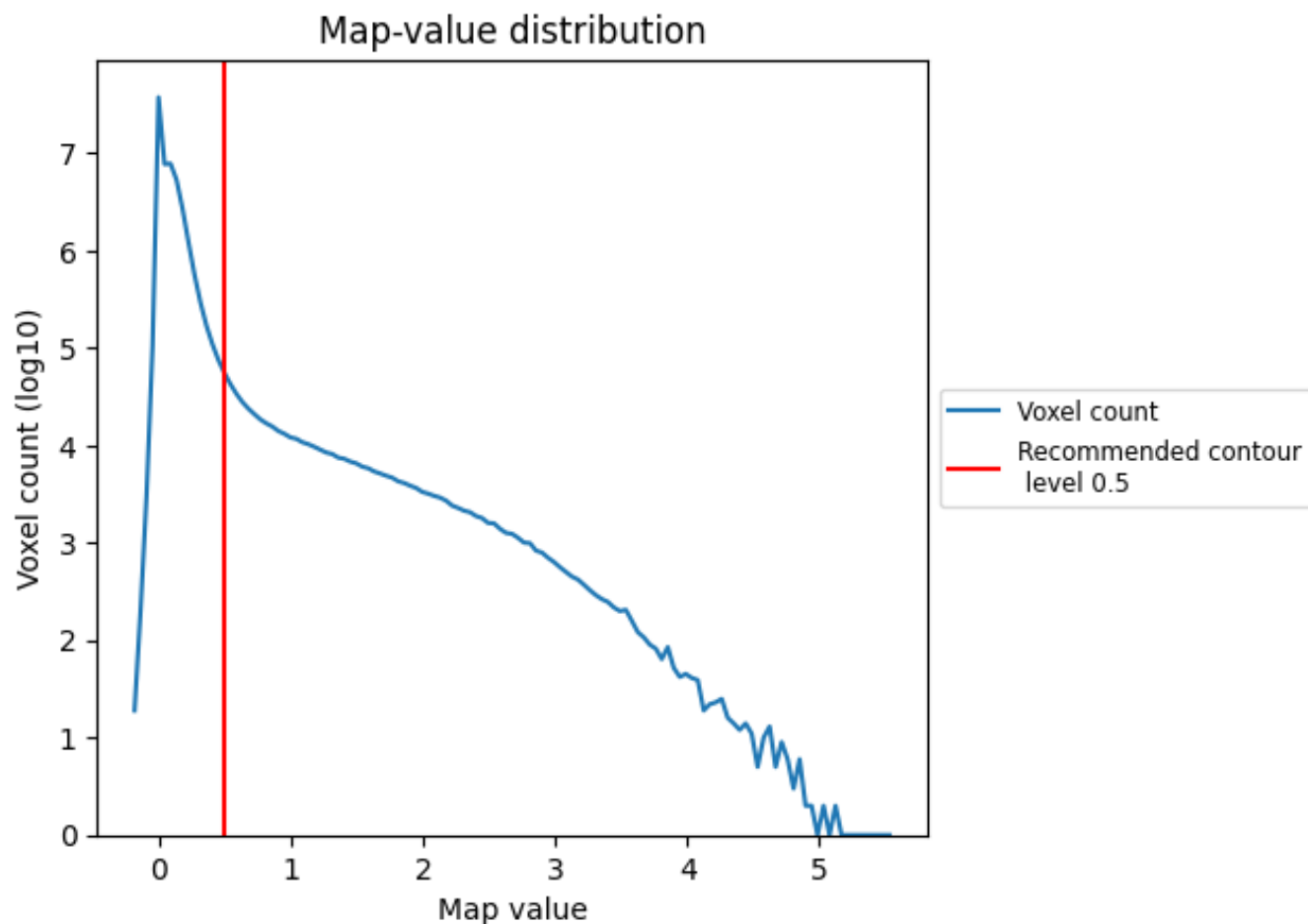
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

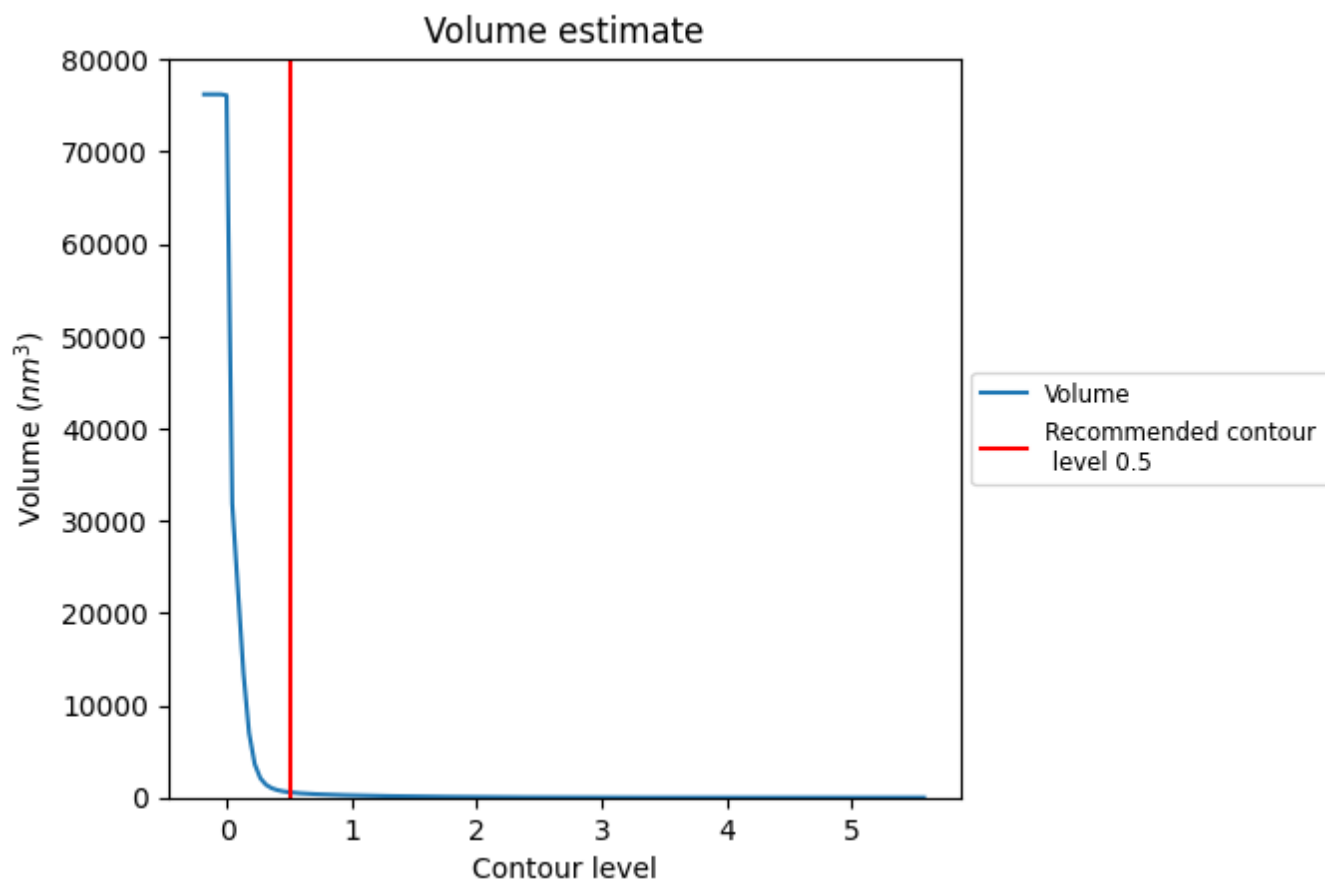
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

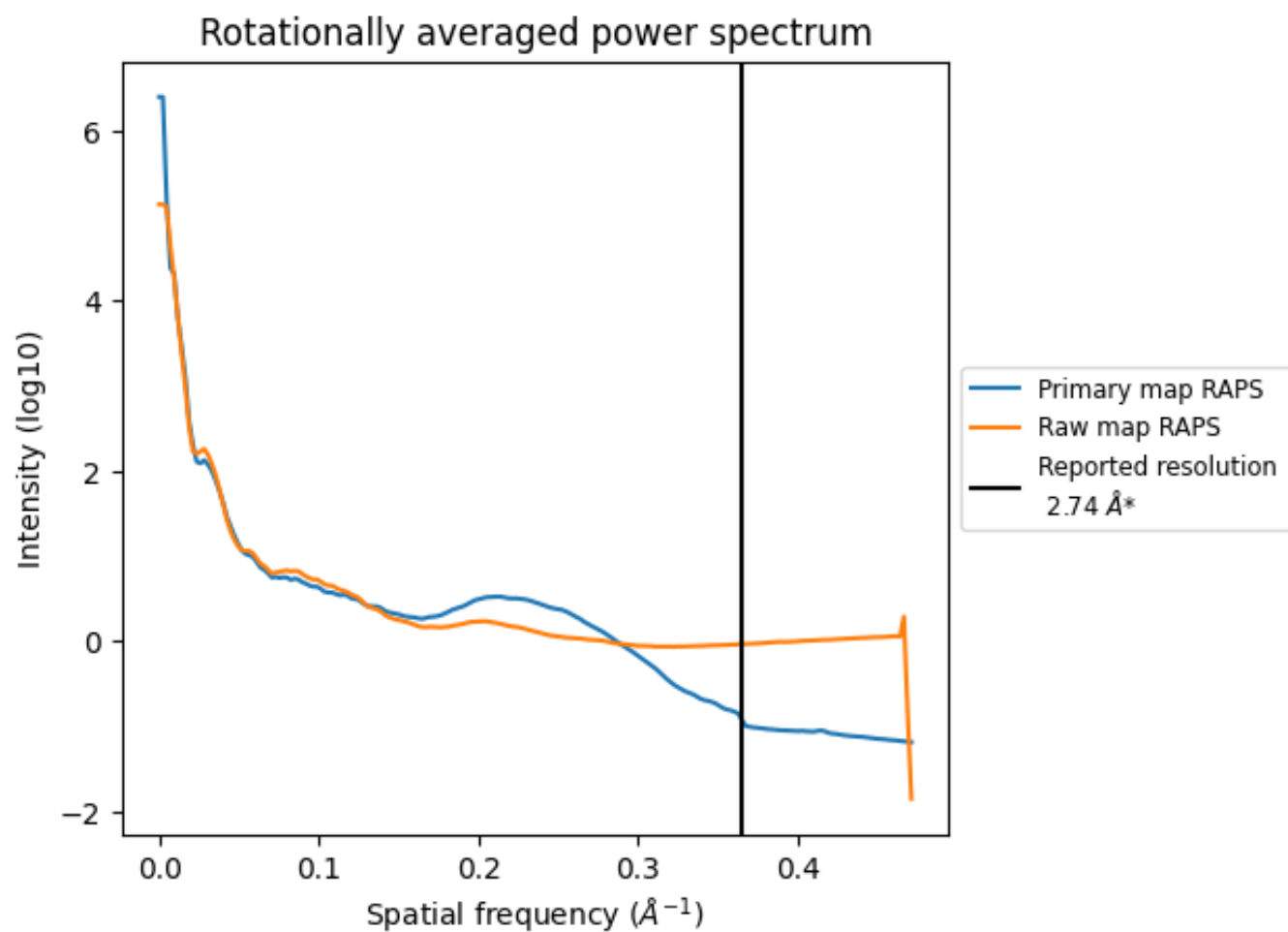
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 575 nm³; this corresponds to an approximate mass of 519 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 ⓘ

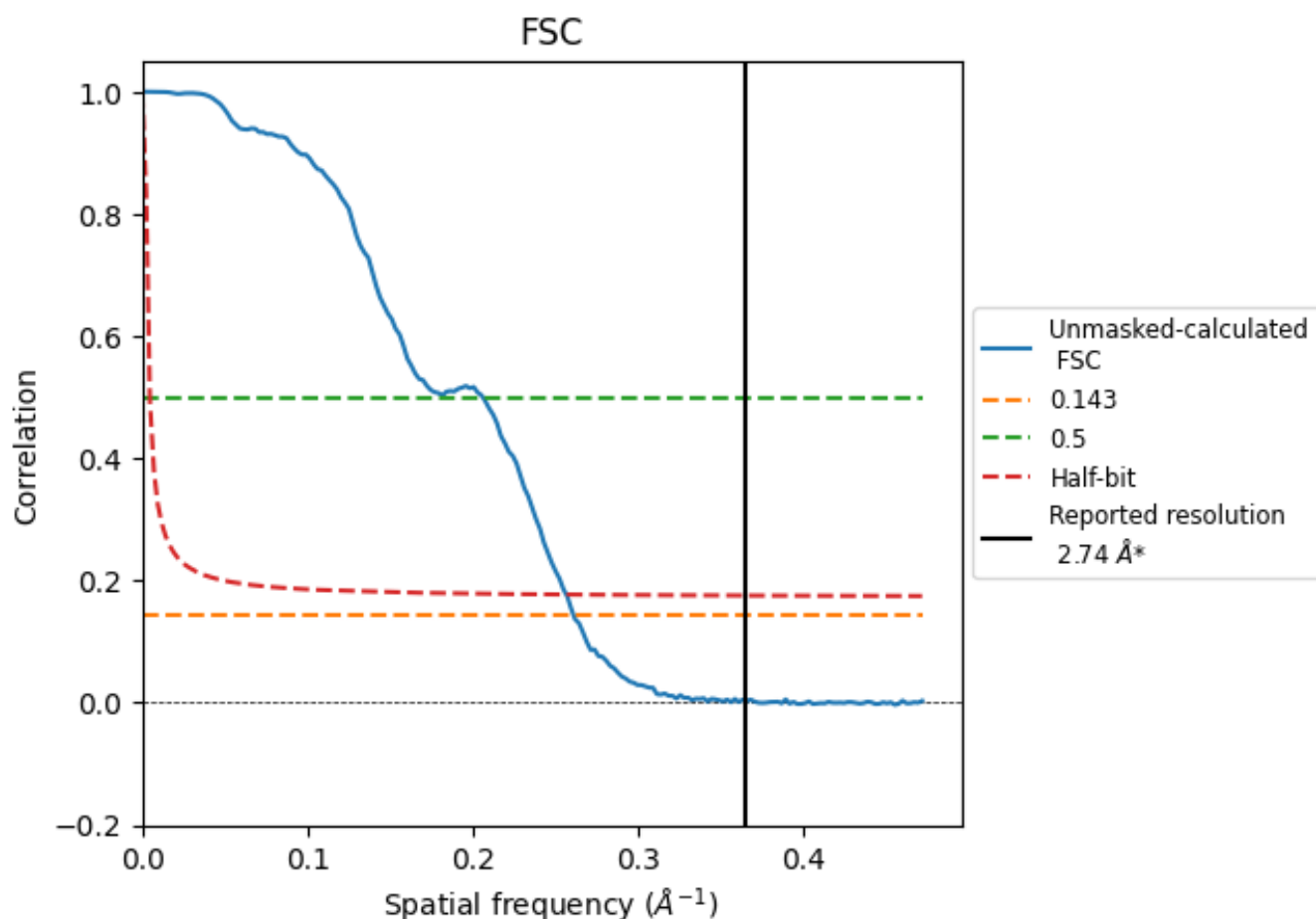


*Reported resolution corresponds to spatial frequency of 0.365 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

8.2 Resolution estimates [i](#)

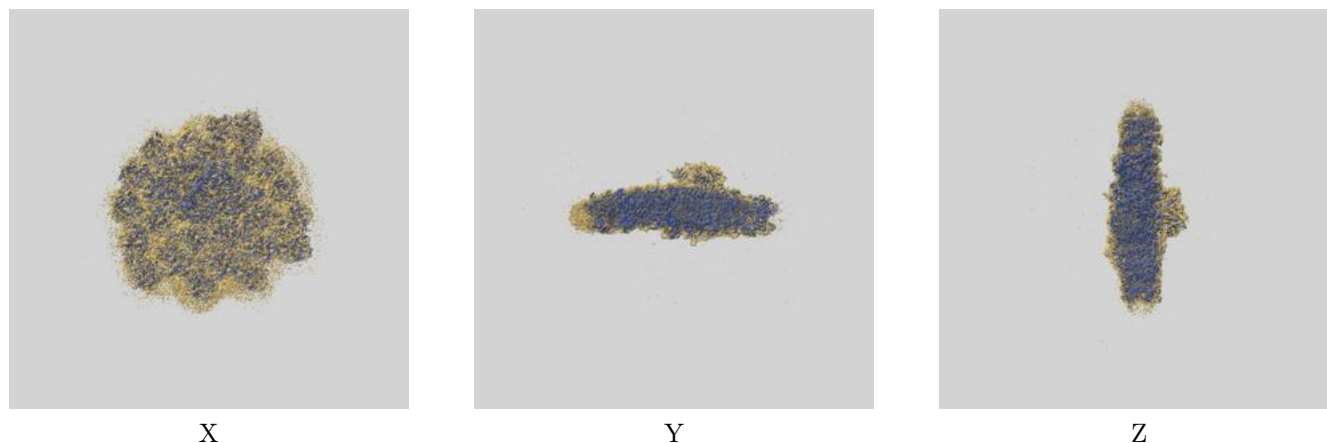
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.85	3.90

*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 3.83 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

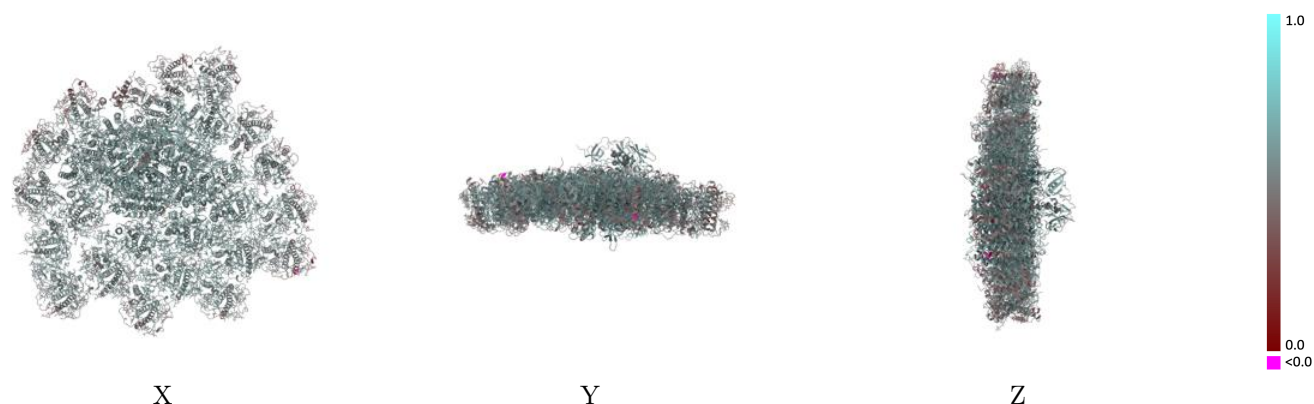
This section contains information regarding the fit between EMDB map EMD-39717 and PDB model 8Z11. Per-residue inclusion information can be found in [section 3](#) on [page 48](#).

9.1 Map-model overlay [i](#)



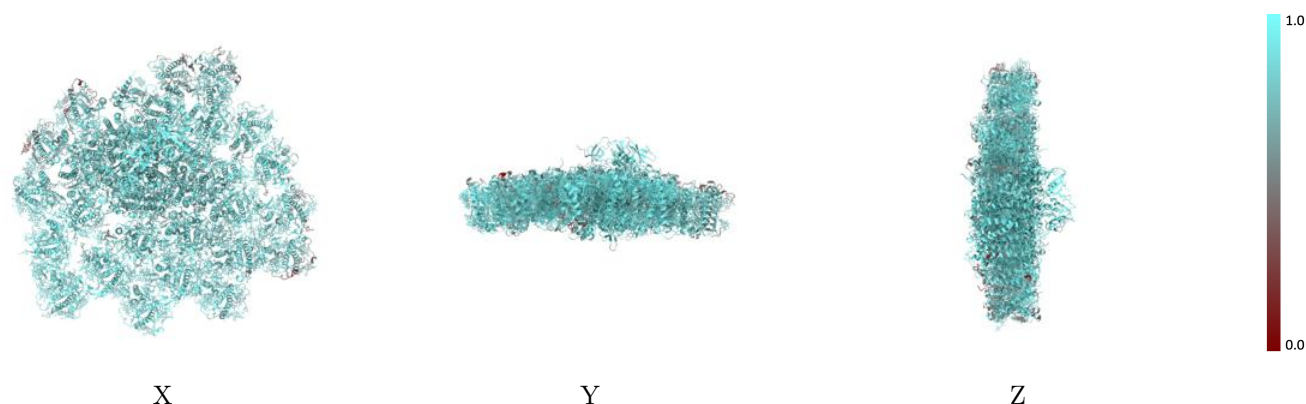
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



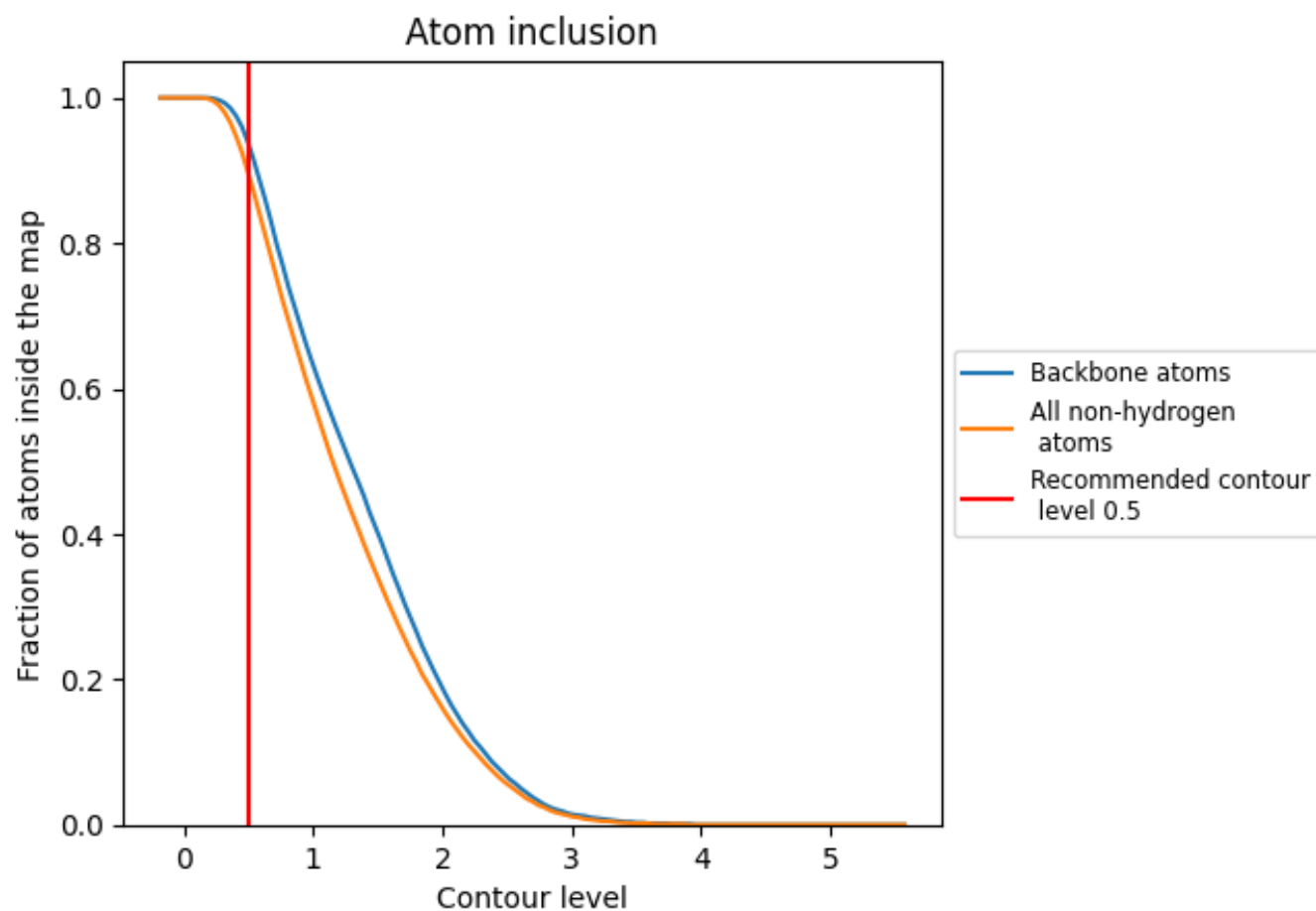
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.5540
A	 0.9310	 0.5850
B	 0.8270	 0.4560
C	 0.7020	 0.4480
D	 0.9360	 0.5930
E	 0.9290	 0.5770
F	 0.9270	 0.5630
G	 0.8590	 0.5040
H	 0.7340	 0.4810
I	 0.9360	 0.5770
J	 0.8740	 0.5120
K	 0.8540	 0.4960
L	 0.7800	 0.5020
M	 0.8860	 0.5630
N	 0.9480	 0.5340
O	 0.8590	 0.5240
P	 0.7880	 0.5110
Q	 0.9360	 0.5540
R	 0.7400	 0.4820
S	 0.8870	 0.5170
T	 0.8950	 0.5000
U	 0.7030	 0.4630
V	 0.9140	 0.5920
W	 0.9540	 0.5780
a	 0.9600	 0.6160
b	 0.9620	 0.6110
c	 0.9680	 0.5860
d	 0.9330	 0.5640
e	 0.8630	 0.5660
f	 0.9020	 0.5840
i	 0.9090	 0.5680
j	 0.9090	 0.5940
k	 0.9480	 0.5680
l	 0.9540	 0.5790
m	 0.9100	 0.5640
r	 0.8910	 0.5630

