



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 02:08 AM UTC

PDB ID : 9KQP / pdb_00009kqp
EMDB ID : EMD-62511
Title : PSI-LHCI supercomplex binding with 10 Lhcas from *C. subellipsoidea*
Authors : Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.
Deposited on : 2024-11-26
Resolution : 1.92 Å (reported)
Based on initial model : 6zzx

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:

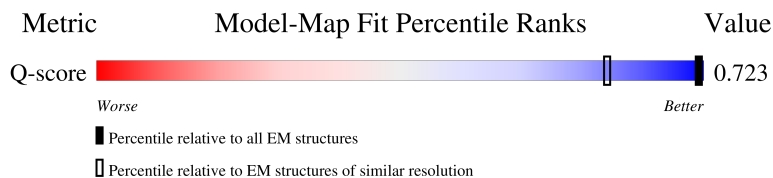
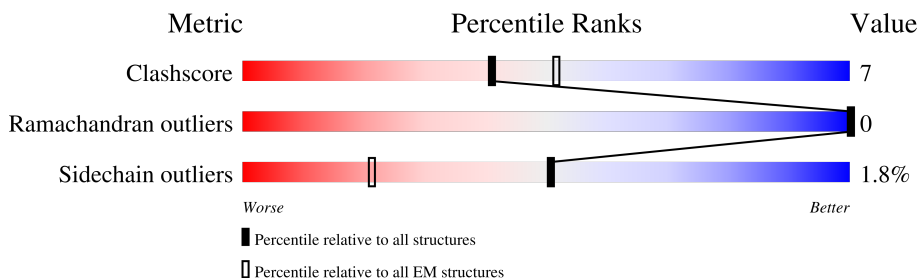
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 1.92 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.



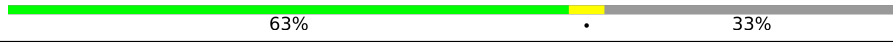
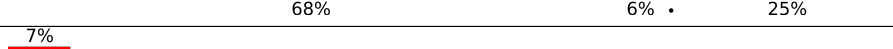
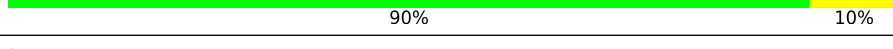
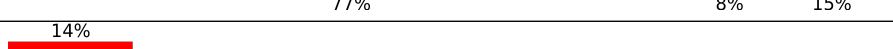
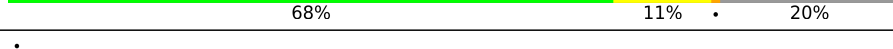
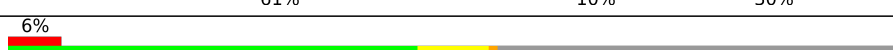
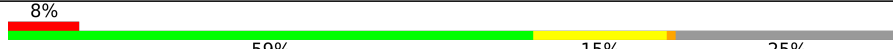
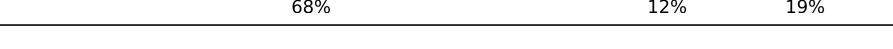
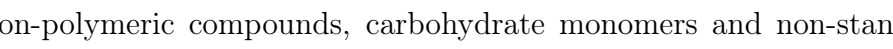
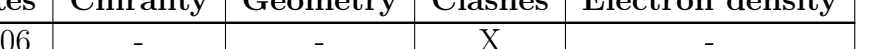
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1227 (1.42 - 2.42)

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	751	 91% 8% .
2	B	734	 93% 7%
3	C	81	 94% . .
4	D	192	 68% 7% 26%

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Mol	Chain	Length	Quality of chain
5	E	71	
6	F	245	
7	G	138	
8	H	133	
9	I	36	
10	J	41	
11	K	131	
12	M	31	
13	a	229	
13	b	229	
14	3	246	
15	7	259	
16	8	255	
17	9	230	
18	L	210	
19	O	142	
20	2	273	
21	4	246	
22	5	274	
23	6	272	

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
29	UNL	3	306	-	-	X	-
30	CL0	A	813	X	-	-	-
31	CLA	2	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	2	306	X	-	-	-
31	CLA	2	307	X	-	-	-
31	CLA	2	308	X	-	-	-
31	CLA	2	310	X	-	-	-
31	CLA	2	311	X	-	-	-
31	CLA	2	312	X	-	-	-
31	CLA	2	313	X	-	-	-
31	CLA	2	314	X	-	-	-
31	CLA	2	315	X	-	-	-
31	CLA	3	307	X	-	-	-
31	CLA	3	308	X	-	-	-
31	CLA	3	309	X	-	-	-
31	CLA	3	310	X	-	-	-
31	CLA	3	311	X	-	-	-
31	CLA	3	312	X	-	-	-
31	CLA	3	313	X	-	-	-
31	CLA	3	316	X	-	-	-
31	CLA	3	317	X	-	-	-
31	CLA	3	319	X	-	-	-
31	CLA	3	320	X	-	-	-
31	CLA	4	306	X	-	-	-
31	CLA	4	307	X	-	-	-
31	CLA	4	308	X	-	-	-
31	CLA	4	309	X	-	-	-
31	CLA	4	311	X	-	-	-
31	CLA	4	312	X	-	-	-
31	CLA	4	314	X	-	-	-
31	CLA	4	315	X	-	-	-
31	CLA	4	318	X	-	-	-
31	CLA	4	319	X	-	-	-
31	CLA	4	320	X	-	-	-
31	CLA	4	321	X	-	-	-
31	CLA	5	307	X	-	-	-
31	CLA	5	308	X	-	-	-
31	CLA	5	310	X	-	-	-
31	CLA	5	311	X	-	-	-
31	CLA	5	312	X	-	-	-
31	CLA	5	315	X	-	-	-
31	CLA	5	318	X	-	-	-
31	CLA	5	323	X	-	-	-
31	CLA	6	307	X	-	-	-
31	CLA	6	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	6	310	X	-	-	-
31	CLA	6	311	X	-	-	-
31	CLA	6	312	X	-	-	-
31	CLA	6	313	X	-	-	-
31	CLA	6	315	X	-	-	-
31	CLA	6	316	X	-	-	-
31	CLA	7	309	X	-	-	-
31	CLA	7	310	X	-	-	-
31	CLA	7	312	X	-	-	-
31	CLA	7	313	X	-	-	-
31	CLA	7	315	X	-	-	-
31	CLA	7	316	X	-	-	-
31	CLA	7	322	X	-	-	-
31	CLA	8	307	X	-	-	-
31	CLA	8	308	X	-	-	-
31	CLA	8	309	X	-	-	-
31	CLA	8	310	X	-	-	-
31	CLA	8	311	X	-	-	-
31	CLA	8	312	X	-	-	-
31	CLA	8	313	X	-	-	-
31	CLA	8	314	X	-	-	-
31	CLA	8	315	X	-	-	-
31	CLA	8	318	X	-	-	-
31	CLA	8	321	X	-	-	-
31	CLA	9	311	X	-	-	-
31	CLA	9	312	X	-	-	-
31	CLA	9	313	X	-	-	-
31	CLA	9	314	X	-	-	-
31	CLA	9	315	X	-	-	-
31	CLA	9	316	X	-	-	-
31	CLA	9	318	X	-	-	-
31	CLA	9	321	X	-	-	-
31	CLA	A	814	X	-	-	-
31	CLA	A	816	X	-	-	-
31	CLA	A	817	X	-	-	-
31	CLA	A	818	X	-	-	-
31	CLA	A	819	X	-	-	-
31	CLA	A	821	X	-	-	-
31	CLA	A	824	X	-	-	-
31	CLA	A	826	X	-	-	-
31	CLA	A	834	X	-	-	-
31	CLA	A	838	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	A	841	X	-	-	-
31	CLA	A	849	X	-	-	-
31	CLA	A	850	X	-	-	-
31	CLA	A	851	X	-	-	-
31	CLA	A	854	X	-	-	-
31	CLA	A	856	X	-	-	-
31	CLA	A	857	X	-	-	-
31	CLA	B	811	X	-	-	-
31	CLA	B	812	X	-	-	-
31	CLA	B	814	X	-	-	-
31	CLA	B	815	X	-	-	-
31	CLA	B	817	X	-	-	-
31	CLA	B	818	X	-	-	-
31	CLA	B	819	X	-	-	-
31	CLA	B	822	X	-	-	-
31	CLA	B	823	X	-	-	-
31	CLA	B	827	X	-	-	-
31	CLA	B	828	X	-	-	-
31	CLA	B	832	X	-	-	-
31	CLA	B	833	X	-	-	-
31	CLA	B	834	X	-	-	-
31	CLA	B	835	X	-	-	-
31	CLA	B	840	X	-	-	-
31	CLA	B	842	X	-	-	-
31	CLA	B	843	X	-	-	-
31	CLA	B	844	X	-	-	-
31	CLA	B	848	X	-	-	-
31	CLA	B	849	X	-	-	-
31	CLA	F	301	X	-	-	-
31	CLA	F	305	X	-	-	-
31	CLA	F	306	X	-	-	-
31	CLA	G	204	X	-	-	-
31	CLA	G	205	X	-	-	-
31	CLA	G	206	X	-	-	-
31	CLA	H	901	X	-	-	-
31	CLA	H	902	X	-	-	-
31	CLA	J	105	X	-	-	-
31	CLA	K	205	X	-	-	-
31	CLA	L	307	X	-	-	-
31	CLA	O	202	X	-	-	-
31	CLA	O	203	X	-	-	-
31	CLA	O	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	a	309	X	-	-	-
31	CLA	a	310	X	-	-	-
31	CLA	a	311	X	-	-	-
31	CLA	a	312	X	-	-	-
31	CLA	a	313	X	-	-	-
31	CLA	a	314	X	-	-	-
31	CLA	a	315	X	-	-	-
31	CLA	a	319	X	-	-	-
31	CLA	a	322	X	-	-	-
31	CLA	b	302	X	-	-	-
31	CLA	b	303	X	-	-	-
31	CLA	b	304	X	-	-	-
31	CLA	b	305	X	-	-	-
31	CLA	b	307	X	-	-	-
31	CLA	b	310	X	-	-	-
31	CLA	b	311	X	-	-	-
31	CLA	b	313	X	-	-	-
32	CHL	3	315	X	-	-	-
32	CHL	4	310	X	-	-	-
32	CHL	4	313	X	-	-	-
32	CHL	4	317	X	-	-	-
32	CHL	5	316	X	-	-	-
32	CHL	5	317	X	-	-	-
32	CHL	5	319	X	-	-	-
32	CHL	5	322	X	-	-	-
32	CHL	6	309	X	-	-	-
32	CHL	6	317	X	-	-	-
32	CHL	6	318	X	-	-	-
32	CHL	6	319	X	-	-	-
32	CHL	6	320	X	-	-	-
32	CHL	6	321	X	-	-	-
32	CHL	7	317	X	-	-	-
32	CHL	7	318	X	-	-	-
32	CHL	7	319	X	-	-	-
32	CHL	7	320	X	-	-	-
32	CHL	7	324	X	-	-	-
32	CHL	8	316	X	-	-	-
32	CHL	8	319	X	-	-	-
32	CHL	9	320	X	-	-	-
32	CHL	9	322	X	-	-	-
32	CHL	A	831	X	-	-	-
32	CHL	A	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	CHL	A	840	X	-	-	-
32	CHL	K	201	X	-	-	-
32	CHL	a	317	X	-	-	-
32	CHL	a	318	X	-	-	-
32	CHL	a	320	X	-	-	-
32	CHL	b	309	X	-	-	-
36	LUT	4	302	-	X	-	-
36	LUT	5	304	-	X	-	-
36	LUT	6	303	-	X	-	-
36	LUT	8	303	-	X	-	-
36	LUT	9	302	-	X	-	-
36	LUT	9	305	-	X	-	-
36	LUT	F	304	-	X	-	-
36	LUT	J	103	-	X	-	-
36	LUT	L	304	-	X	-	-
36	LUT	a	305	-	X	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 52991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5814	3800	992	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5808	3812	985	998	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			596	365	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1110	711	193	203	3		

- Molecule 5 is a protein called Photosystem I reaction centre subunit IV/PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	60	Total	C	N	O	S	0	0
			490	316	83	90	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1264	805	223	234	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	103	Total	C	N	O	S	0	0
			767	488	132	146	1		

- Molecule 8 is a protein called Photosystem I reaction centre subunit VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	S	0	0
			706	449	120	137			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			248	171	34	41	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	39	Total	C	N	O	S	0	0
			319	220	46	52	1		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			560	356	96	107	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			237	160	35	41	1		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	195	Total	C	N	O	S	0	0
			1458	944	245	267	2		
13	b	126	Total	C	N	O	S	0	0
			952	606	168	176	2		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	203	Total	C	N	O	S	0	0
			1580	1036	255	286	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	214	Total	C	N	O	S	0	0
			1633	1059	276	296	2		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	222	Total	C	N	O	S	0	0
			1701	1112	276	310	3		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	9	184	Total	C	N	O	S	0	0
			1414	915	238	258	3		

- Molecule 18 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	148	Total	C	N	O	S	0	0
			1102	723	183	194	2		

- Molecule 19 is a protein called Photosystem I PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	78	Total	C	N	O	0	0
			605	403	98	104		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic/Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	204	Total	C	N	O	S	0	0
			1606	1046	270	286	4		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4	193	Total	C	N	O	S	0	0
			1506	984	246	273	3		

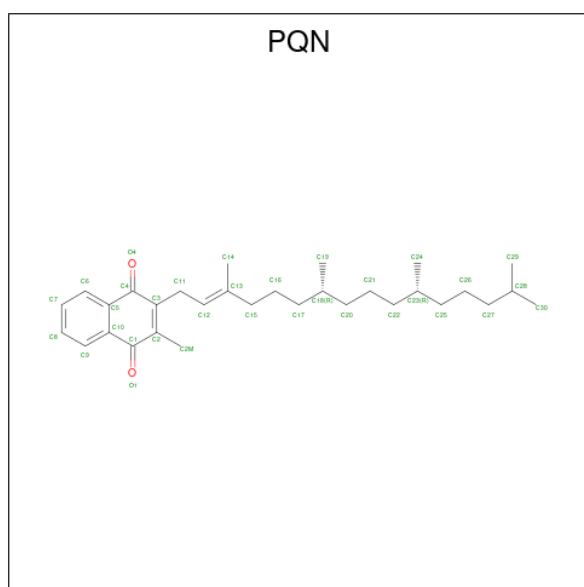
- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	5	229	Total	C	N	O	S	0	0
			1766	1152	303	307	4		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

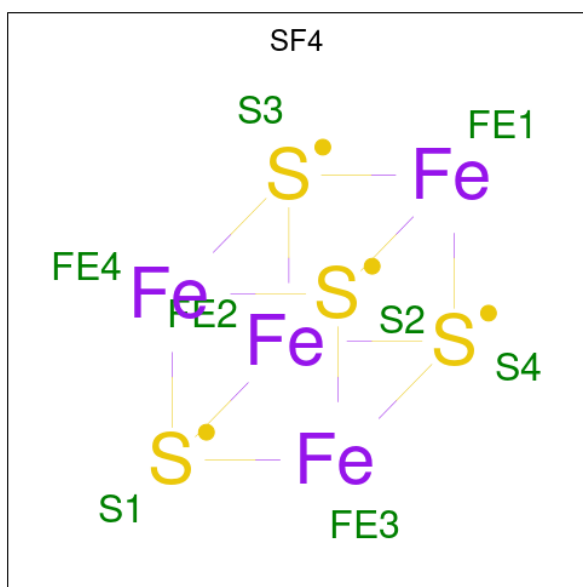
Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	219	Total	C	N	O	S	0	0
			1658	1088	276	287	7		

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



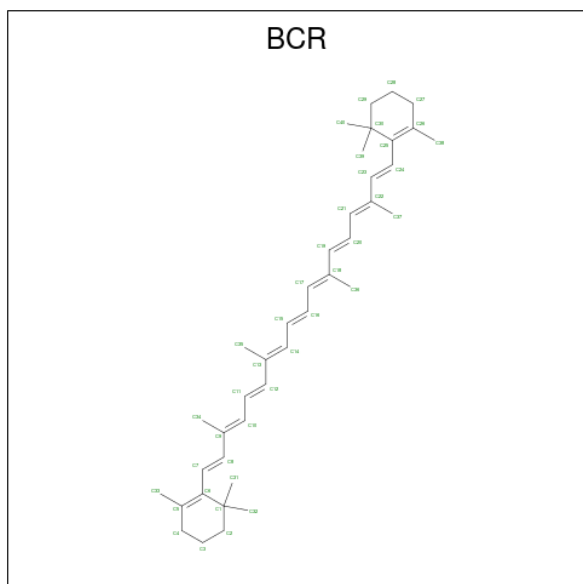
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			33	31	2	
24	B	1	Total	C	O	0
			33	31	2	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



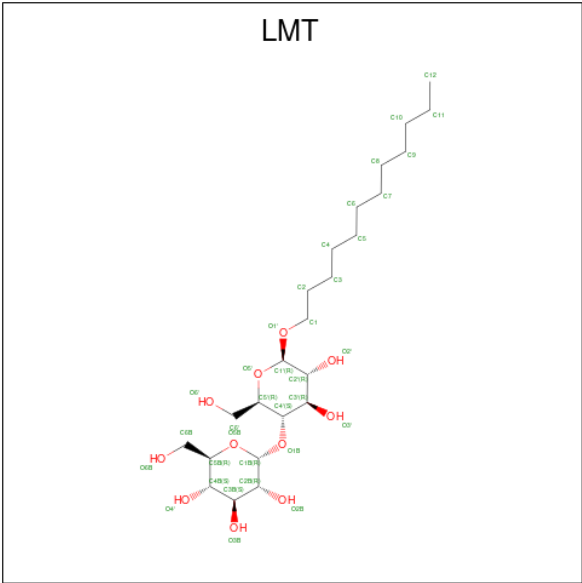
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	I	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	M	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	7	1	Total C 40 40	0
26	8	1	Total C 40 40	0

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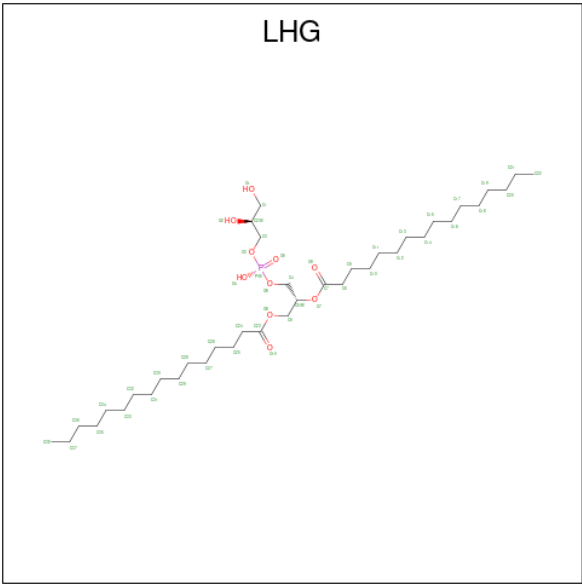
Mol	Chain	Residues	Atoms		AltConf
26	L	1	Total	C	0
			40	40	
26	L	1	Total	C	0
			40	40	
26	L	1	Total	C	0
			40	40	
26	O	1	Total	C	0
			40	40	
26	2	1	Total	C	0
			40	40	
26	5	1	Total	C	0
			40	40	
26	6	1	Total	C	0
			40	40	

- Molecule 27 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			35	24	11	
27	9	1	Total	C	O	0
			35	24	11	
27	5	1	Total	C	O	0
			35	24	11	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

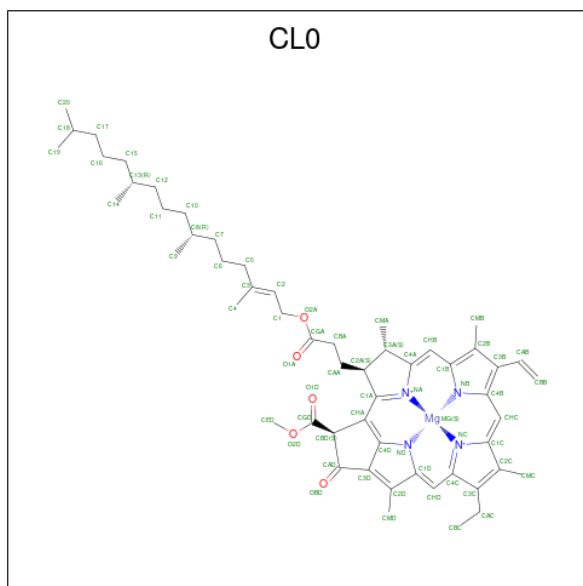


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	A	1	42	31	10	1	0
28	A	1	42	31	10	1	0
28	A	1	49	38	10	1	0
28	B	1	32	21	10	1	0
28	a	1	49	38	10	1	0
28	7	1	49	38	10	1	0
28	7	1	37	26	10	1	0
28	8	1	49	38	10	1	0
28	5	1	35	24	10	1	0
28	6	1	27	16	10	1	0
28	6	1	32	21	10	1	0

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

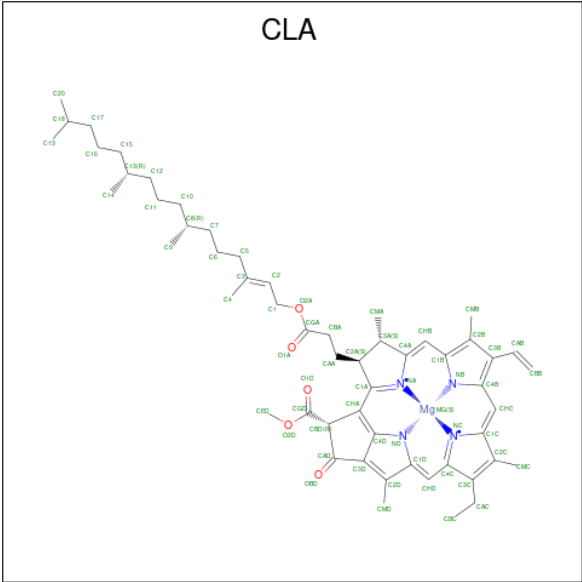
Mol	Chain	Residues	Atoms		AltConf
29	A	2	Total	C	0
			20	20	
29	B	2	Total	C	0
			24	24	
29	a	2	Total	C	0
			27	27	
29	3	1	Total	C	0
			11	11	
29	7	1	Total	C	0
			8	8	
29	8	1	Total	C	0
			18	18	
29	9	6	Total	C	0
			81	81	
29	2	1	Total	C	0
			11	11	
29	4	1	Total	C	0
			13	13	

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	7	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
31	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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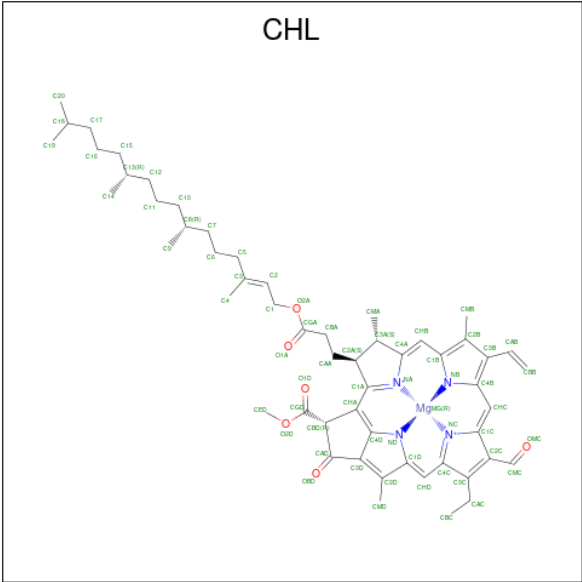
Mol	Chain	Residues	Atoms					AltConf
31	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 32 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



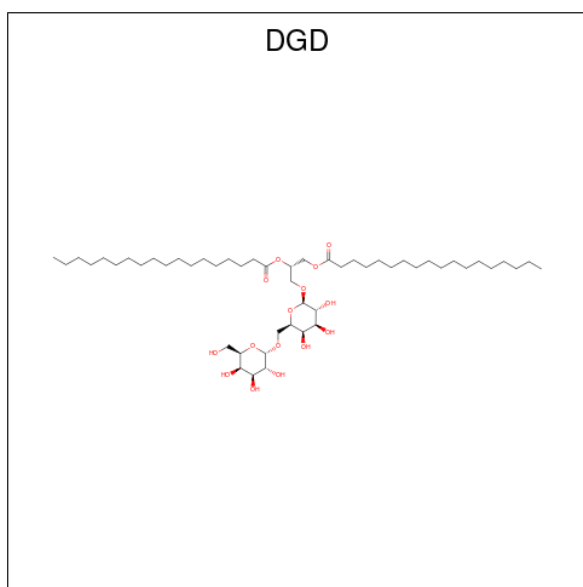
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
32	A	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	K	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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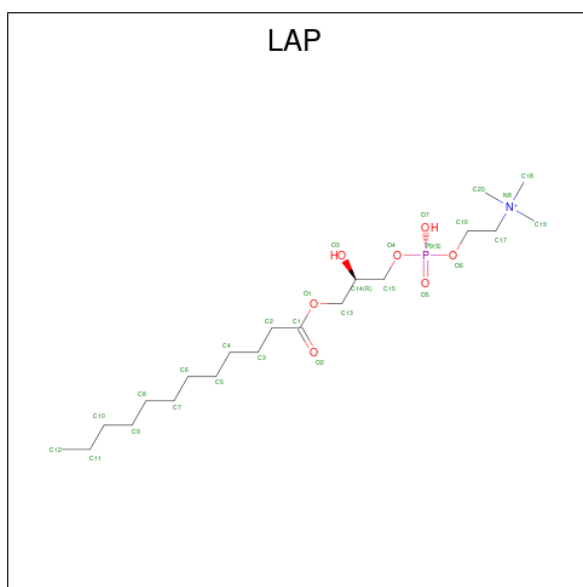
Mol	Chain	Residues	Atoms					AltConf
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



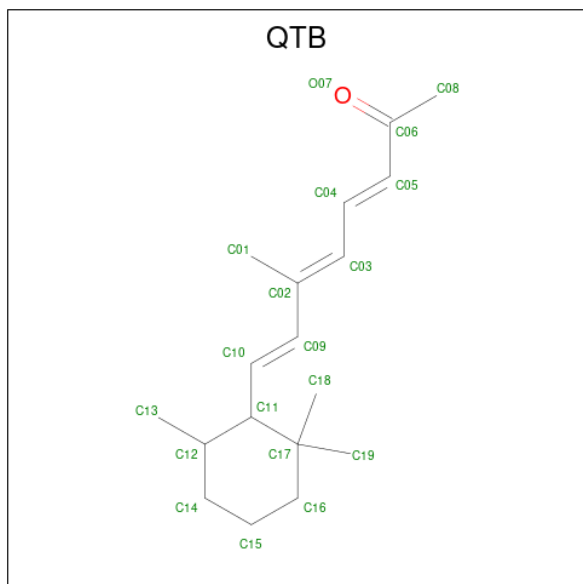
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			61	46	15	
33	7	1	Total	C	O	0
			52	37	15	

- Molecule 34 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (CCD ID: LAP) (formula: C₂₀H₄₃NO₇P) (labeled as "Ligand of Interest" by depositor).



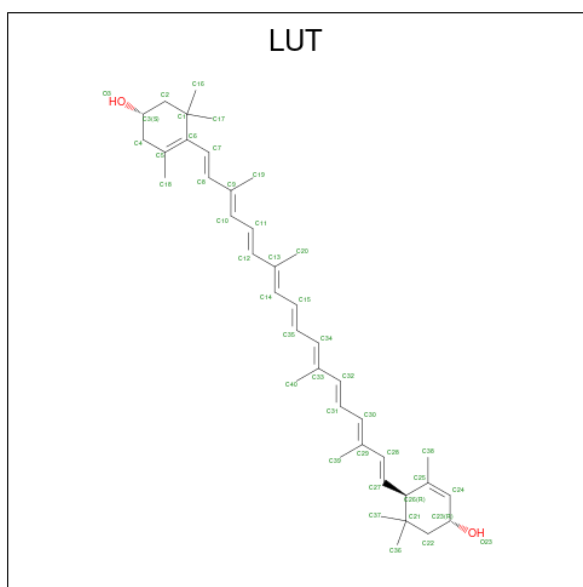
Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 35 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: C₁₈H₂₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	F	1	Total	C	O	0
			19	18	1	
35	a	1	Total	C	O	0
			19	18	1	
35	7	1	Total	C	O	0
			19	18	1	
35	9	1	Total	C	O	0
			19	18	1	

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



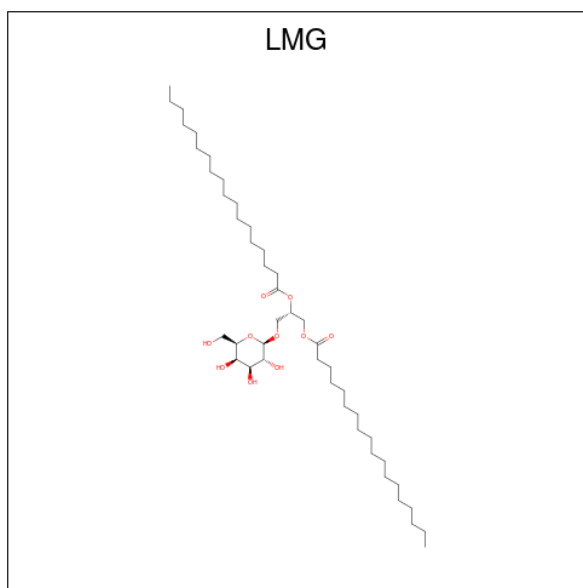
Mol	Chain	Residues	Atoms			AltConf
36	F	1	Total 42	C 40	O 2	0
36	J	1	Total 42	C 40	O 2	0
36	a	1	Total 42	C 40	O 2	0
36	a	1	Total 42	C 40	O 2	0
36	3	1	Total 42	C 40	O 2	0
36	3	1	Total 42	C 40	O 2	0
36	7	1	Total 42	C 40	O 2	0
36	8	1	Total 42	C 40	O 2	0
36	8	1	Total 42	C 40	O 2	0
36	9	1	Total 42	C 40	O 2	0
36	9	1	Total 42	C 40	O 2	0
36	9	1	Total 42	C 40	O 2	0
36	L	1	Total 42	C 40	O 2	0
36	b	1	Total 42	C 40	O 2	0

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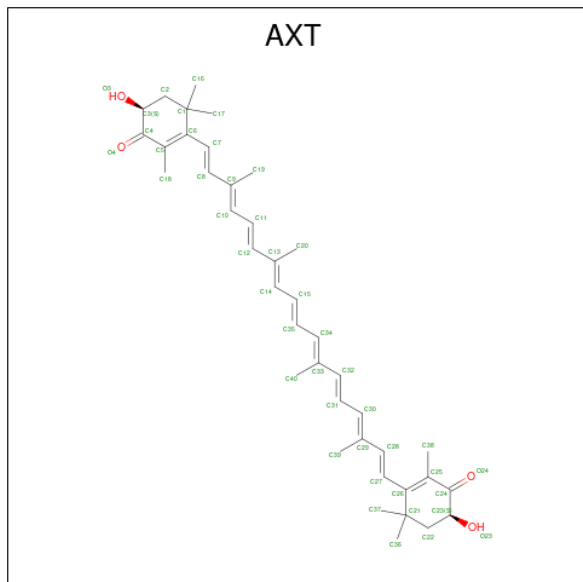
Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



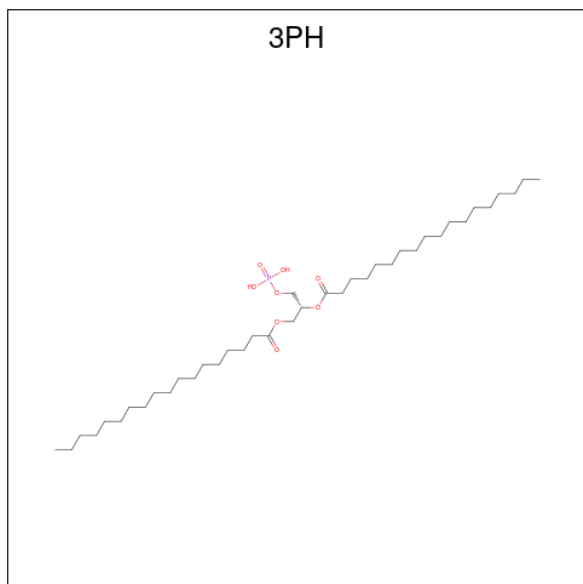
Mol	Chain	Residues	Atoms			AltConf
37	G	1	Total	C	O	0
			44	34	10	
37	J	1	Total	C	O	0
			49	39	10	
37	J	1	Total	C	O	0
			29	19	10	
37	a	1	Total	C	O	0
			42	32	10	

- Molecule 38 is ASTAXANTHIN (CCD ID: AXT) (formula: $C_{40}H_{52}O_4$) (labeled as "Ligand of Interest" by depositor).



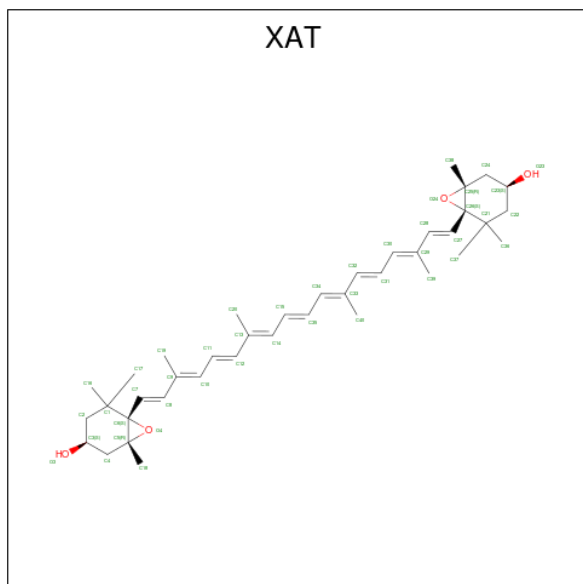
Mol	Chain	Residues	Atoms			AltConf
38	a	1	Total	C	O	0
			43	40	3	

- Molecule 39 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



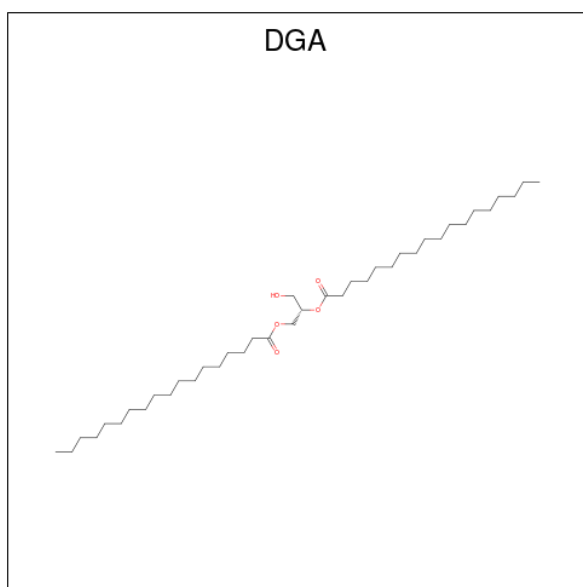
Mol	Chain	Residues	Atoms				AltConf
39	7	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 40 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



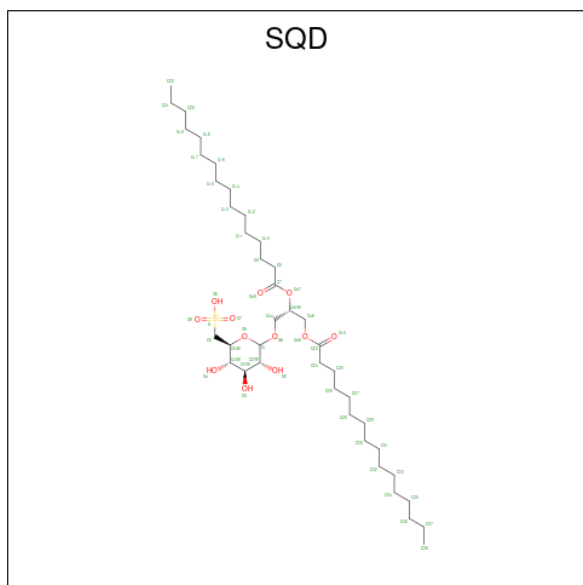
Mol	Chain	Residues	Atoms			AltConf
40	7	1	Total	C	O	0
			44	40	4	

- Molecule 41 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



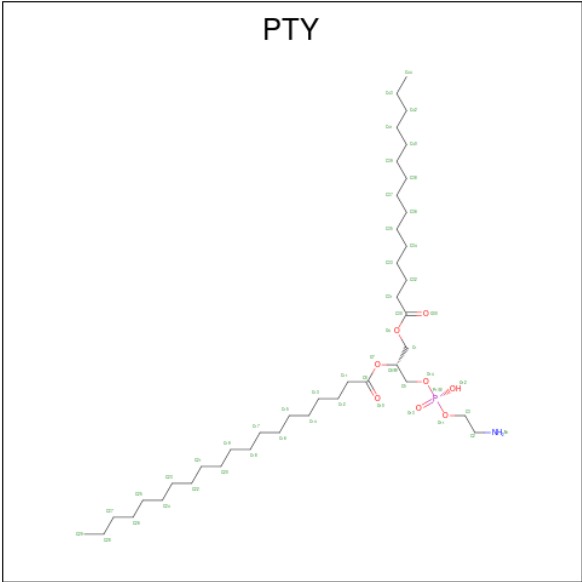
Mol	Chain	Residues	Atoms			AltConf
41	8	1	Total	C	O	0
			28	23	5	

- Molecule 42 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
42	4	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 43 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
43	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	297	Total	O	0
			297	297	
44	B	311	Total	O	0
			311	311	
44	C	60	Total	O	0
			60	60	
44	D	53	Total	O	0
			53	53	
44	E	28	Total	O	0
			28	28	
44	F	57	Total	O	0
			57	57	
44	G	18	Total	O	0
			18	18	
44	H	6	Total	O	0
			6	6	
44	I	6	Total	O	0
			6	6	
44	J	16	Total	O	0
			16	16	
44	K	2	Total	O	0
			2	2	

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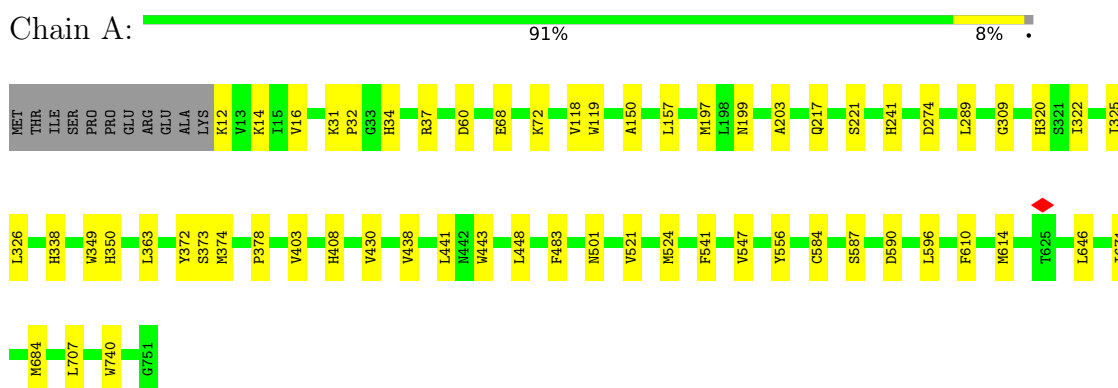
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Mol	Chain	Residues	Atoms		AltConf
44	M	5	Total 5	O 5	0
44	a	34	Total 34	O 34	0
44	3	32	Total 32	O 32	0
44	7	39	Total 39	O 39	0
44	8	37	Total 37	O 37	0
44	9	21	Total 21	O 21	0
44	L	17	Total 17	O 17	0
44	O	4	Total 4	O 4	0
44	2	3	Total 3	O 3	0
44	4	1	Total 1	O 1	0
44	5	11	Total 11	O 11	0
44	6	2	Total 2	O 2	0

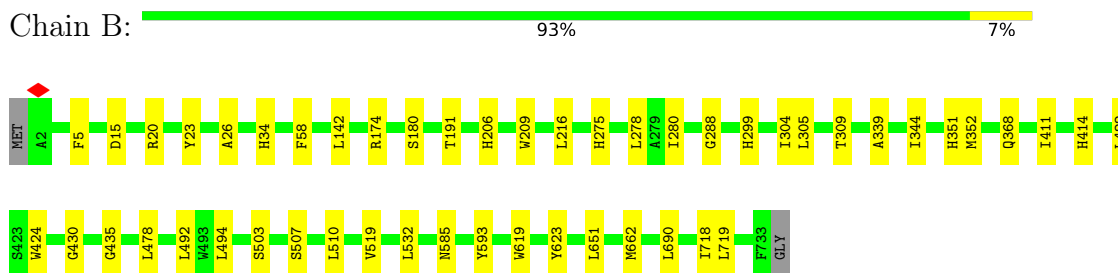
3 Residue-property plots

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.

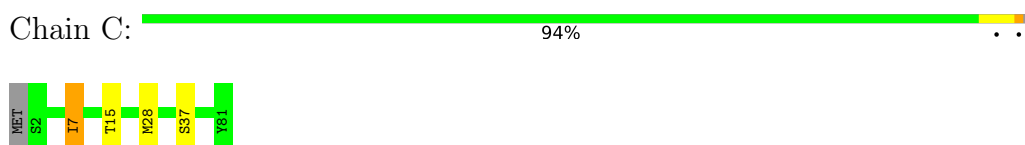
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

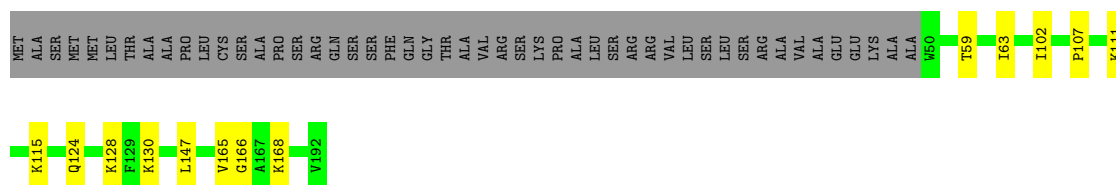


- Molecule 3: Photosystem I iron-sulfur center

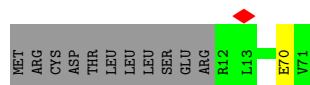
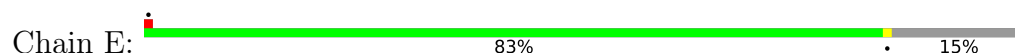


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

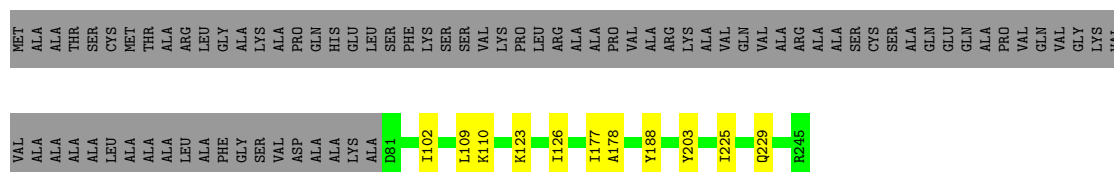




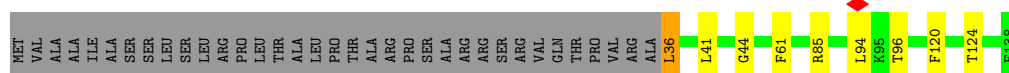
- Molecule 5: Photosystem I reaction centre subunit IV/PsaE



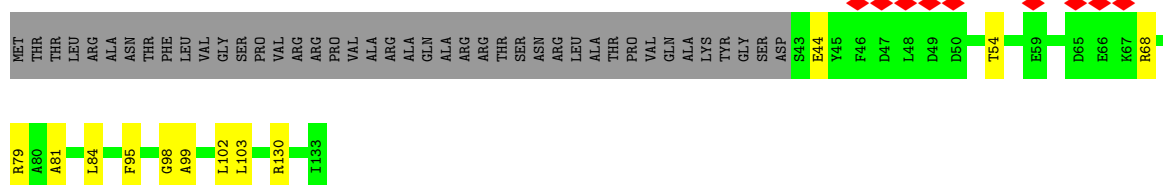
- Molecule 6: Photosystem I reaction center subunit III



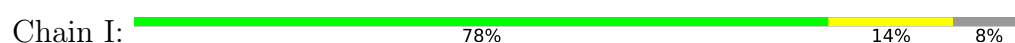
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction centre subunit VI



- Molecule 9: Photosystem I reaction center subunit VIII



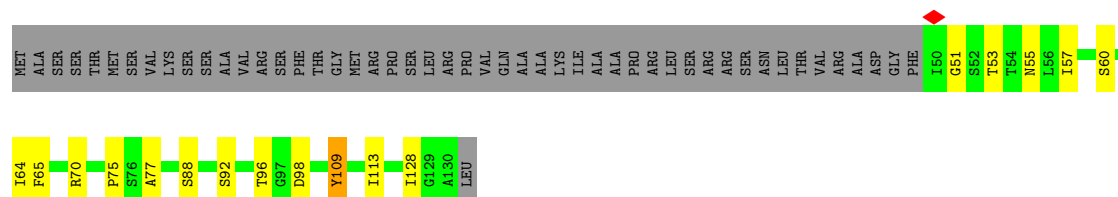
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  78% 17% 5%



• Molecule 11: PSI-K

Chain K:  49% 12% 38%



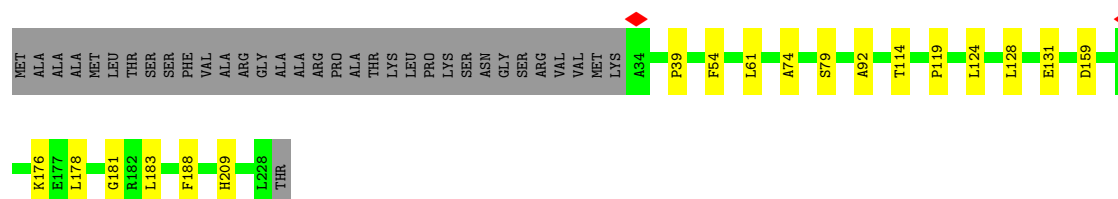
• Molecule 12: Photosystem I reaction center subunit XII

Chain M:  90% 10%

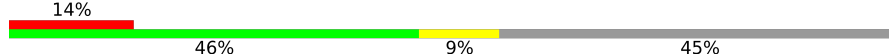


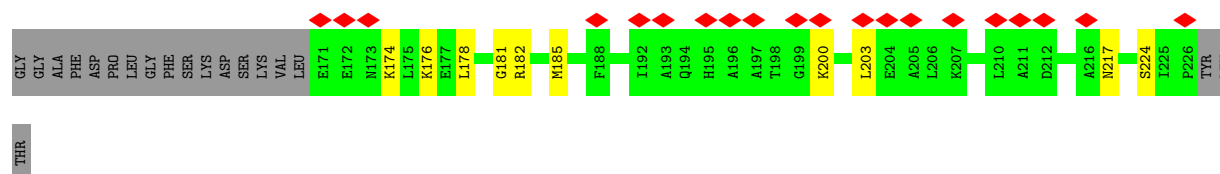
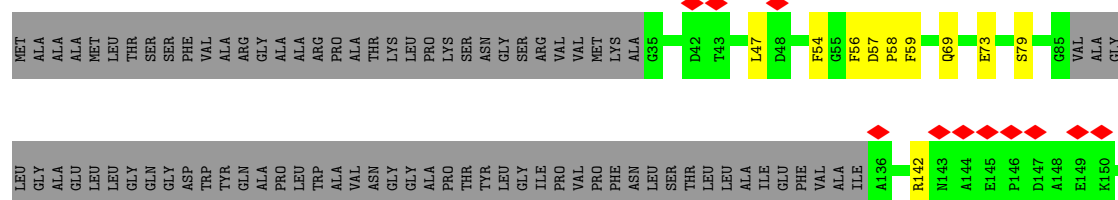
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain a:  77% 8% 15%

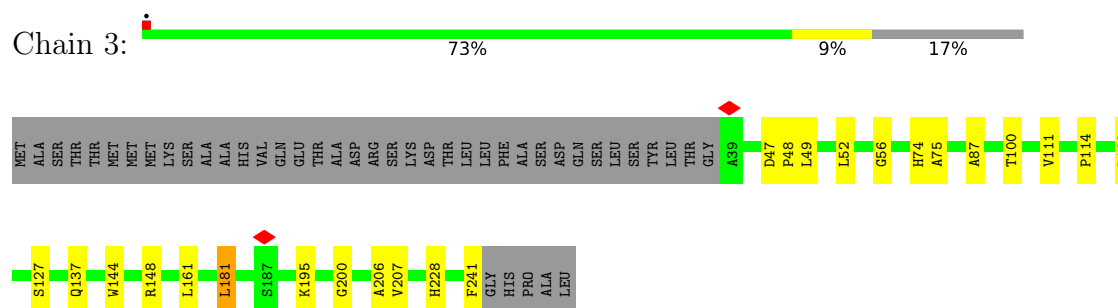


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

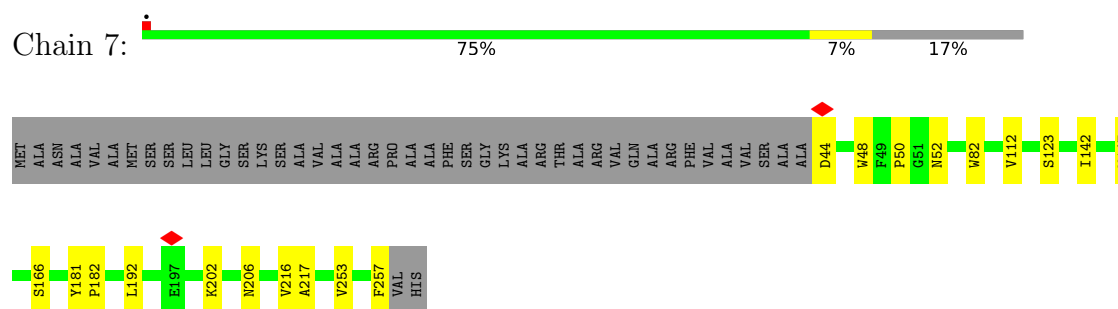
Chain b:  14% 46% 9% 45%



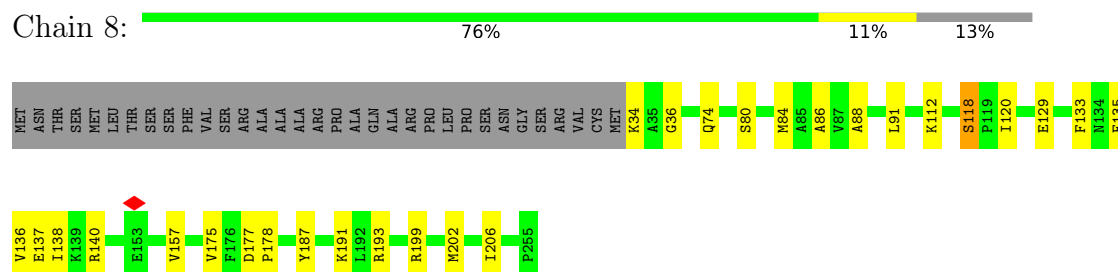
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



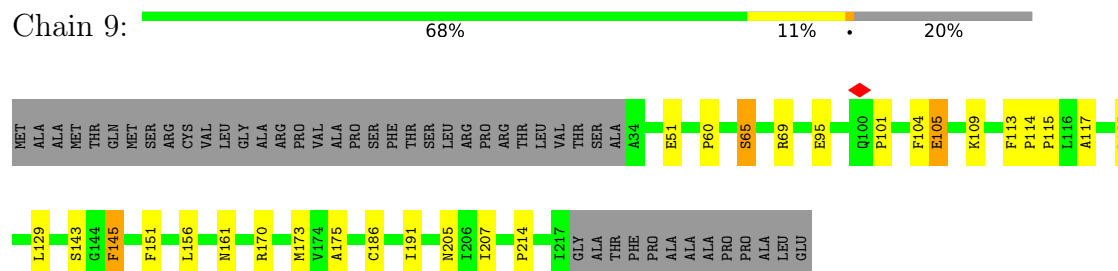
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



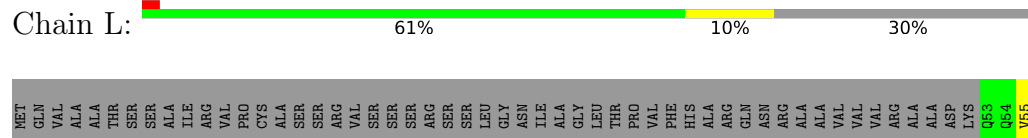
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



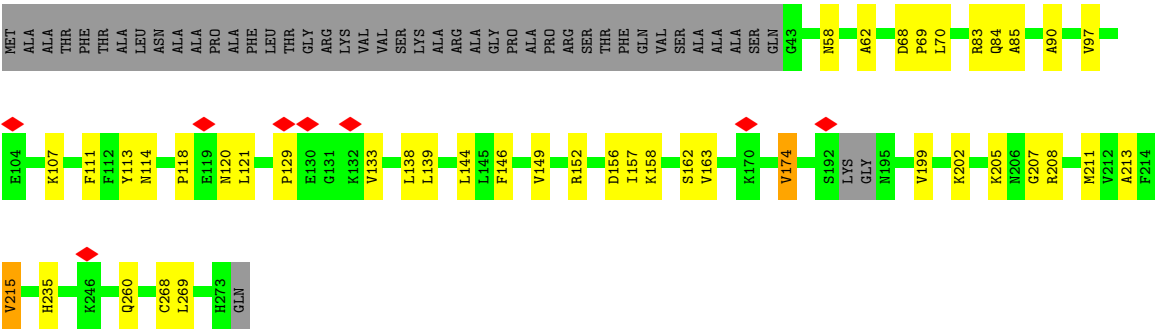
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



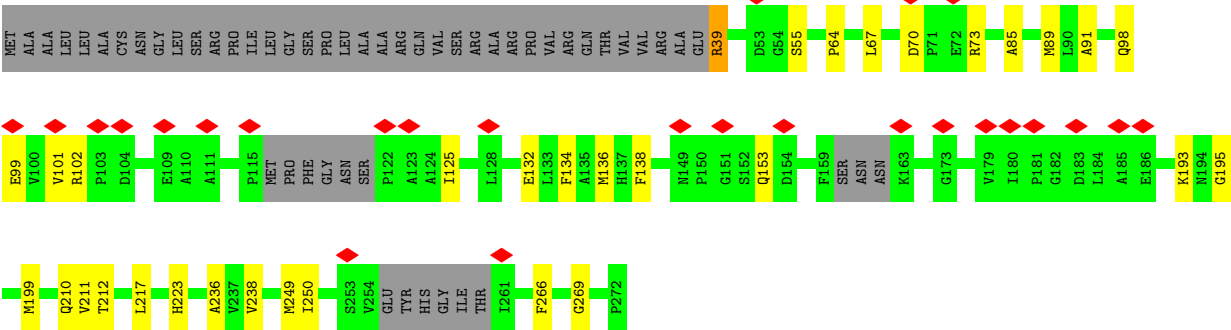
- Molecule 18: PSI subunit V







• Molecule 23: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224674	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.393	Depositor
Minimum map value	-0.655	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.085	Depositor
Map size ($\text{\AA}$)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, XAT, DGD, LAP, SF4, QTB, CHL, LHG, 3PH, SQD, PTY, BCR, AXT, PQN, LMG, LUT, CL0, LMT, UNL, DGA

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	0.24	0/6012	0.45	0/8202
2	B	0.23	0/6017	0.45	0/8218
3	C	0.30	0/606	0.58	0/822
4	D	0.18	0/1136	0.37	0/1537
5	E	0.19	0/502	0.38	0/686
6	F	0.20	0/1288	0.38	0/1737
7	G	0.18	0/783	0.39	0/1063
8	H	0.18	0/722	0.42	0/972
9	I	0.28	0/254	0.51	0/347
10	J	0.20	0/330	0.41	0/452
11	K	0.18	0/568	0.42	0/773
12	M	0.21	0/240	0.34	0/325
13	a	0.20	0/1501	0.41	0/2045
13	b	0.13	0/977	0.29	0/1322
14	3	0.26	0/1629	0.47	0/2217
15	7	0.20	0/1684	0.38	0/2298
16	8	0.21	0/1752	0.39	0/2379
17	9	0.20	0/1451	0.41	0/1964
18	L	0.19	0/1129	0.42	0/1542
19	O	0.16	0/619	0.39	0/839
20	2	0.22	0/1654	0.54	1/2254 (0.0%)
21	4	0.18	0/1553	0.37	0/2113
22	5	0.21	0/1820	0.46	1/2477 (0.0%)
23	6	0.21	0/1709	0.38	0/2328
All	All	0.22	0/35936	0.43	2/48912 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
23	6	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	66	PRO	CA-N-CD	-8.66	99.87	112.00
22	5	129	PRO	N-CD-CG	-7.27	92.30	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	6	39	ARG	Sidechain

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	5814	0	5649	45	0
2	B	5808	0	5584	38	0
3	C	596	0	573	3	0
4	D	1110	0	1131	9	0
5	E	490	0	482	0	0
6	F	1264	0	1300	9	0
7	G	767	0	749	6	0
8	H	706	0	687	12	0
9	I	248	0	269	4	0
10	J	319	0	326	7	0
11	K	560	0	583	9	0
12	M	237	0	260	2	0
13	a	1458	0	1423	17	0
13	b	952	0	917	15	0
14	3	1580	0	1546	25	0
15	7	1633	0	1579	16	0
16	8	1701	0	1683	18	0
17	9	1414	0	1405	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1102	0	1129	14	0
19	O	605	0	616	7	0
20	2	1606	0	1578	34	0
21	4	1506	0	1468	25	0
22	5	1766	0	1746	34	0
23	6	1658	0	1657	28	0
24	A	33	0	46	1	0
24	B	33	0	46	2	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	2	40	0	56	3	0
26	3	120	0	168	7	0
26	5	40	0	56	2	0
26	6	40	0	56	2	0
26	7	40	0	56	6	0
26	8	40	0	56	4	0
26	A	160	0	224	11	0
26	B	200	0	280	16	0
26	F	40	0	56	1	0
26	G	80	0	112	1	0
26	I	40	0	56	1	0
26	J	40	0	56	1	0
26	K	80	0	112	7	0
26	L	120	0	168	6	0
26	M	40	0	56	3	0
26	O	40	0	56	2	0
27	5	35	0	44	0	0
27	9	35	0	44	0	0
27	A	70	0	89	4	0
28	5	35	0	40	1	0
28	6	59	0	58	3	0
28	7	86	0	118	8	0
28	8	49	0	74	0	0
28	A	133	0	188	7	0
28	B	32	0	34	1	0
28	a	49	0	74	9	0
29	2	11	0	0	0	0
29	3	11	0	0	4	0
29	4	13	0	0	1	0
29	7	8	0	0	0	0
29	8	18	0	0	0	0
29	9	81	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	20	0	0	0	0
29	B	24	0	0	0	0
29	a	27	0	0	0	0
30	A	65	0	72	3	0
31	2	574	0	442	16	0
31	3	736	0	697	19	0
31	4	685	0	550	25	0
31	5	678	0	588	21	0
31	6	545	0	436	15	0
31	7	523	0	445	11	0
31	8	692	0	606	19	0
31	9	524	0	452	4	0
31	A	2450	0	2472	93	0
31	B	2382	0	2381	63	0
31	F	161	0	144	4	0
31	G	141	0	105	8	0
31	H	138	0	99	10	0
31	J	42	0	31	1	0
31	K	142	0	105	1	0
31	L	150	0	125	6	0
31	O	134	0	98	0	0
31	a	601	0	547	18	0
31	b	520	0	389	7	0
32	3	56	0	46	1	0
32	4	141	0	92	13	0
32	5	197	0	136	15	0
32	6	296	0	217	18	0
32	7	297	0	272	25	0
32	8	111	0	99	9	0
32	9	95	0	62	5	0
32	A	180	0	165	10	0
32	K	47	0	31	1	0
32	a	157	0	120	13	0
32	b	47	0	30	1	0
33	7	52	0	65	0	0
33	B	61	0	83	4	0
34	B	29	0	42	4	0
35	7	19	0	0	0	0
35	9	19	0	0	0	0
35	F	19	0	0	0	0
35	a	19	0	0	0	0
36	2	42	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	3	84	0	111	10	0
36	4	84	0	111	11	0
36	5	84	0	111	9	0
36	6	84	0	111	5	0
36	7	42	0	56	3	0
36	8	84	0	112	7	0
36	9	126	0	165	8	0
36	F	42	0	55	2	0
36	J	42	0	54	3	0
36	L	42	0	55	1	0
36	a	84	0	109	10	0
36	b	42	0	56	5	0
37	G	44	0	58	4	0
37	J	78	0	99	4	0
37	a	42	0	54	2	0
38	a	43	0	52	1	0
39	7	33	0	39	1	0
40	7	44	0	56	0	0
41	8	28	0	38	2	0
42	4	35	0	34	1	0
43	5	31	0	35	1	0
44	2	3	0	0	0	0
44	3	32	0	0	0	0
44	4	1	0	0	0	0
44	5	11	0	0	0	0
44	6	2	0	0	0	0
44	7	39	0	0	0	0
44	8	37	0	0	0	0
44	9	21	0	0	0	0
44	A	297	0	0	1	0
44	B	311	0	0	2	0
44	C	60	0	0	0	0
44	D	53	0	0	0	0
44	E	28	0	0	0	0
44	F	57	0	0	0	0
44	G	18	0	0	0	0
44	H	6	0	0	1	0
44	I	6	0	0	0	0
44	J	16	0	0	0	0
44	K	2	0	0	0	0
44	L	17	0	0	0	0
44	M	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	O	4	0	0	0	0
44	a	34	0	0	0	0
All	All	52991	0	50690	710	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 7.

The worst 5 of 710 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)
31:H:902:CLA:HAA1	20:2:153:LEU:HD23	1.31	1.06
14:3:241:PHE:CD2	29:3:306:UNL:C2	2.39	1.05
31:A:829:CLA:HBA2	28:7:302:LHG:H242	1.39	1.02
31:H:902:CLA:O1A	20:2:153:LEU:HD21	1.61	0.99
20:2:243:ALA:O	20:2:247:ILE:HG13	1.64	0.96

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	738/751 (98%)	721 (98%)	17 (2%)	0	100	100
2	B	730/734 (100%)	719 (98%)	11 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	141/192 (73%)	138 (98%)	3 (2%)	0	100	100
5	E	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
6	F	163/245 (66%)	160 (98%)	3 (2%)	0	100	100
7	G	101/138 (73%)	99 (98%)	2 (2%)	0	100	100
8	H	89/133 (67%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	31/36 (86%)	31 (100%)	0	0	100	100
10	J	37/41 (90%)	37 (100%)	0	0	100	100
11	K	79/131 (60%)	79 (100%)	0	0	100	100
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	a	193/229 (84%)	191 (99%)	2 (1%)	0	100	100
13	b	120/229 (52%)	119 (99%)	1 (1%)	0	100	100
14	3	201/246 (82%)	194 (96%)	7 (4%)	0	100	100
15	7	212/259 (82%)	209 (99%)	3 (1%)	0	100	100
16	8	220/255 (86%)	215 (98%)	5 (2%)	0	100	100
17	9	182/230 (79%)	179 (98%)	3 (2%)	0	100	100
18	L	142/210 (68%)	139 (98%)	3 (2%)	0	100	100
19	O	72/142 (51%)	71 (99%)	1 (1%)	0	100	100
20	2	198/273 (72%)	184 (93%)	14 (7%)	0	100	100
21	4	187/246 (76%)	180 (96%)	7 (4%)	0	100	100
22	5	225/274 (82%)	216 (96%)	9 (4%)	0	100	100
23	6	211/272 (78%)	206 (98%)	5 (2%)	0	100	100
All	All	4437/5449 (81%)	4336 (98%)	101 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	603/613 (98%)	597 (99%)	6 (1%)	68	64
2	B	592/593 (100%)	588 (99%)	4 (1%)	76	73
3	C	68/69 (99%)	66 (97%)	2 (3%)	37	21
4	D	118/156 (76%)	117 (99%)	1 (1%)	73	71
5	E	56/67 (84%)	55 (98%)	1 (2%)	51	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	131/183 (72%)	131 (100%)	0	100	100
7	G	78/106 (74%)	75 (96%)	3 (4%)	29	14
8	H	71/105 (68%)	71 (100%)	0	100	100
9	I	26/28 (93%)	26 (100%)	0	100	100
10	J	35/37 (95%)	35 (100%)	0	100	100
11	K	59/100 (59%)	55 (93%)	4 (7%)	14	4
12	M	26/26 (100%)	25 (96%)	1 (4%)	29	14
13	a	141/166 (85%)	141 (100%)	0	100	100
13	b	92/166 (55%)	90 (98%)	2 (2%)	45	32
14	3	162/197 (82%)	160 (99%)	2 (1%)	63	57
15	7	166/195 (85%)	163 (98%)	3 (2%)	51	39
16	8	175/202 (87%)	171 (98%)	4 (2%)	44	30
17	9	143/177 (81%)	136 (95%)	7 (5%)	22	8
18	L	115/161 (71%)	112 (97%)	3 (3%)	40	24
19	O	65/110 (59%)	60 (92%)	5 (8%)	12	3
20	2	166/225 (74%)	161 (97%)	5 (3%)	36	20
21	4	155/195 (80%)	152 (98%)	3 (2%)	50	37
22	5	178/208 (86%)	172 (97%)	6 (3%)	32	16
23	6	170/212 (80%)	168 (99%)	2 (1%)	63	57
All	All	3591/4297 (84%)	3527 (98%)	64 (2%)	51	39

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	5	133	VAL
22	5	163	VAL
15	7	44	ASP
14	3	181	LEU
22	5	174	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
20	2	227	ASN

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Mol	Chain	Res	Type
23	6	210	GLN
21	4	82	GLN
22	5	125	ASN
11	K	55	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 17 are unknown - leaving 337 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	CHL	7	317	15	51,65,74	3.67	22 (43%)	47,103,114	2.93	17 (36%)
32	CHL	6	309	23	60,74,74	3.09	21 (35%)	58,114,114	2.58	16 (27%)
31	CLA	A	842	1	69,73,73	2.81	23 (33%)	82,113,113	2.28	25 (30%)
31	CLA	a	316	13	49,53,73	3.22	20 (40%)	58,89,113	2.46	24 (41%)
31	CLA	4	311	28	50,54,73	6.46	22 (44%)	59,90,113	2.45	22 (37%)
31	CLA	b	307	-	50,54,73	5.48	22 (44%)	59,90,113	2.62	24 (40%)
32	CHL	7	318	44	60,74,74	3.10	22 (36%)	58,114,114	2.87	18 (31%)
32	CHL	a	317	13	55,69,74	3.28	22 (40%)	52,108,114	2.71	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	9	317	-	51,55,73	3.32	22 (43%)	60,91,113	2.52	20 (33%)
31	CLA	9	319	17	50,54,73	5.00	20 (40%)	59,90,113	2.56	25 (42%)
31	CLA	7	310	15	48,52,73	3.28	22 (45%)	57,88,113	2.60	24 (42%)
31	CLA	B	818	2	59,63,73	2.43	19 (32%)	70,101,113	2.38	27 (38%)
31	CLA	O	203	44	59,63,73	2.73	21 (35%)	70,101,113	2.37	28 (40%)
37	LMG	a	301	-	42,42,55	0.83	0	50,50,63	1.26	4 (8%)
32	CHL	5	316	44	50,64,74	4.00	20 (40%)	46,102,114	3.13	18 (39%)
32	CHL	4	310	-	41,55,74	4.38	22 (53%)	35,91,114	2.87	12 (34%)
28	LHG	5	305	31	34,34,48	0.33	0	37,40,54	0.40	0
31	CLA	A	829	-	54,58,73	2.53	16 (29%)	64,95,113	2.98	27 (42%)
31	CLA	a	310	13	49,53,73	3.21	22 (44%)	58,89,113	2.59	23 (39%)
31	CLA	B	823	2	59,63,73	2.67	22 (37%)	70,101,113	2.40	26 (37%)
31	CLA	4	319	-	46,50,73	4.14	21 (45%)	53,85,113	2.55	22 (41%)
32	CHL	4	317	-	40,54,74	3.93	20 (50%)	34,90,114	3.04	12 (35%)
32	CHL	6	318	44	40,54,74	4.65	22 (55%)	34,90,114	3.25	14 (41%)
42	SQD	4	304	-	33,35,54	1.81	7 (21%)	43,46,65	1.45	6 (13%)
31	CLA	7	313	15	47,52,73	3.08	22 (46%)	55,88,113	2.44	20 (36%)
31	CLA	2	305	20	49,53,73	4.11	21 (42%)	58,89,113	2.56	23 (39%)
31	CLA	F	301	44	69,73,73	2.47	22 (31%)	82,113,113	2.28	29 (35%)
31	CLA	6	306	23	50,54,73	3.17	24 (48%)	59,90,113	2.54	19 (32%)
26	BCR	B	802	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	5 (8%)
31	CLA	A	850	1	55,59,73	2.80	24 (43%)	64,96,113	2.52	27 (42%)
31	CLA	F	306	44	54,58,73	2.77	20 (37%)	64,95,113	2.46	26 (40%)
31	CLA	5	311	22	50,54,73	2.75	20 (40%)	59,90,113	2.54	26 (44%)
26	BCR	6	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	6 (10%)
31	CLA	B	822	2	69,73,73	2.63	22 (31%)	82,113,113	2.15	24 (29%)
27	LMT	A	808	-	36,36,36	1.18	5 (13%)	47,47,47	1.00	2 (4%)
31	CLA	5	308	22	50,54,73	3.74	21 (42%)	59,90,113	2.53	25 (42%)
28	LHG	6	301	31	26,26,48	0.79	0	29,32,54	1.26	2 (6%)
31	CLA	b	310	-	50,54,73	2.79	19 (38%)	59,90,113	2.41	22 (37%)
32	CHL	6	321	23	37,51,74	3.85	19 (51%)	30,86,114	3.24	13 (43%)
31	CLA	3	309	14	69,73,73	2.31	20 (28%)	82,113,113	2.23	26 (31%)
26	BCR	3	301	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	6 (10%)
31	CLA	B	828	44	64,68,73	2.46	21 (32%)	76,107,113	2.24	26 (34%)
27	LMT	A	807	-	36,36,36	1.18	5 (13%)	47,47,47	1.07	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	G	205	7	50,54,73	2.88	22 (44%)	59,90,113	2.52	22 (37%)
31	CLA	8	311	16	59,63,73	2.85	23 (38%)	70,101,113	2.41	27 (38%)
25	SF4	C	101	3	0,12,12	-	-	-		
31	CLA	B	842	2	65,69,73	2.73	21 (32%)	77,108,113	2.27	27 (35%)
26	BCR	B	804	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
27	LMT	9	306	-	36,36,36	1.24	5 (13%)	47,47,47	0.96	2 (4%)
31	CLA	9	315	17	58,62,73	2.69	21 (36%)	68,99,113	2.46	29 (42%)
31	CLA	B	847	2	69,73,73	2.78	22 (31%)	82,113,113	2.24	22 (26%)
31	CLA	B	848	28	69,73,73	2.28	22 (31%)	82,113,113	2.19	22 (26%)
31	CLA	A	815	-	69,73,73	2.62	21 (30%)	82,113,113	2.17	25 (30%)
31	CLA	3	314	14	56,60,73	2.98	18 (32%)	65,97,113	2.36	26 (40%)
31	CLA	A	837	1	69,73,73	2.49	21 (30%)	82,113,113	2.18	23 (28%)
41	DGA	8	305	-	27,27,43	0.25	0	29,29,45	0.17	0
31	CLA	8	315	16	56,60,73	2.83	22 (39%)	65,97,113	2.38	27 (41%)
31	CLA	K	206	11	50,54,73	3.34	19 (38%)	59,90,113	2.49	22 (37%)
31	CLA	b	308	13	50,54,73	3.59	21 (42%)	59,90,113	2.40	23 (38%)
31	CLA	4	318	21	49,53,73	3.72	21 (42%)	58,89,113	2.48	23 (39%)
28	LHG	7	307	31	36,36,48	0.78	2 (5%)	39,42,54	1.27	4 (10%)
31	CLA	2	314	20	50,54,73	4.79	21 (42%)	59,90,113	2.45	24 (40%)
31	CLA	4	315	44	49,53,73	5.08	21 (42%)	58,89,113	2.44	22 (37%)
33	DGD	B	808	-	62,62,67	1.02	2 (3%)	76,76,81	1.28	4 (5%)
31	CLA	B	843	44	49,53,73	2.88	19 (38%)	58,89,113	2.56	25 (43%)
36	LUT	6	303	-	42,43,43	4.54	19 (45%)	51,60,60	6.04	35 (68%)
32	CHL	7	319	15	41,55,74	4.06	22 (53%)	35,91,114	3.91	13 (37%)
31	CLA	A	844	1	54,58,73	3.10	21 (38%)	64,95,113	2.46	24 (37%)
32	CHL	8	319	44	39,53,74	3.74	18 (46%)	32,88,114	3.61	12 (37%)
35	QTB	F	303	-	19,19,19	1.12	3 (15%)	23,26,26	1.22	3 (13%)
31	CLA	b	305	13	50,54,73	3.17	22 (44%)	59,90,113	2.42	25 (42%)
31	CLA	9	311	17	59,63,73	4.98	21 (35%)	70,101,113	2.30	29 (41%)
31	CLA	A	820	1	59,63,73	2.99	23 (38%)	70,101,113	2.43	25 (35%)
28	LHG	A	810	31	41,41,48	0.72	1 (2%)	44,47,54	1.17	4 (9%)
31	CLA	H	902	44	50,54,73	3.74	20 (40%)	59,90,113	2.48	23 (38%)
26	BCR	A	803	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	3 (5%)
32	CHL	4	313	21	42,56,74	3.67	20 (47%)	36,92,114	2.94	14 (38%)
31	CLA	5	309	22	51,55,73	3.82	21 (41%)	60,91,113	2.49	23 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B	814	2	69,73,73	3.06	23 (33%)	82,113,113	2.21	25 (30%)
31	CLA	B	821	2	62,66,73	2.66	20 (32%)	73,104,113	2.27	23 (31%)
35	QTB	7	303	-	19,19,19	1.06	2 (10%)	23,26,26	1.41	4 (17%)
31	CLA	3	316	44	54,58,73	2.59	21 (38%)	64,95,113	2.37	24 (37%)
31	CLA	L	306	44	49,53,73	2.74	22 (44%)	58,89,113	2.50	23 (39%)
31	CLA	A	854	28	50,54,73	2.84	20 (40%)	59,90,113	2.59	24 (40%)
31	CLA	8	317	44	54,58,73	2.82	21 (38%)	64,95,113	2.53	26 (40%)
31	CLA	a	315	28	59,63,73	2.54	21 (35%)	70,101,113	2.45	23 (32%)
32	CHL	3	315	44	50,64,74	3.28	20 (40%)	46,102,114	3.17	16 (34%)
36	LUT	9	302	-	42,43,43	4.51	20 (47%)	51,60,60	5.90	35 (68%)
32	CHL	7	324	16	60,74,74	3.00	20 (33%)	58,114,114	2.61	18 (31%)
26	BCR	J	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.23	3 (5%)
26	BCR	A	804	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
31	CLA	B	840	2	69,73,73	2.47	23 (33%)	82,113,113	2.19	23 (28%)
30	CL0	A	813	1	58,73,73	2.83	18 (31%)	60,113,113	2.62	14 (23%)
31	CLA	A	821	1	69,73,73	2.54	20 (28%)	82,113,113	2.28	28 (34%)
31	CLA	7	311	15	69,73,73	2.44	20 (28%)	82,113,113	2.20	26 (31%)
32	CHL	b	309	13	41,55,74	3.79	22 (53%)	35,91,114	3.11	15 (42%)
31	CLA	B	839	2	64,68,73	2.55	23 (35%)	76,107,113	2.23	27 (35%)
31	CLA	a	314	44	54,58,73	3.85	21 (38%)	64,95,113	2.48	25 (39%)
31	CLA	A	818	1	69,73,73	2.24	22 (31%)	82,113,113	2.22	26 (31%)
26	BCR	B	805	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	7 (12%)
31	CLA	8	310	16	69,73,73	2.53	22 (31%)	82,113,113	2.27	23 (28%)
31	CLA	B	815	2	69,73,73	2.29	22 (31%)	82,113,113	2.21	25 (30%)
31	CLA	B	849	2	54,58,73	3.06	23 (42%)	64,95,113	2.39	25 (39%)
31	CLA	A	846	1	69,73,73	2.59	20 (28%)	82,113,113	2.25	26 (31%)
40	XAT	7	306	-	41,47,47	1.28	5 (12%)	54,74,74	1.45	8 (14%)
32	CHL	a	320	44	42,56,74	3.75	22 (52%)	36,92,114	3.39	15 (41%)
32	CHL	6	317	23	41,55,74	3.70	21 (51%)	35,91,114	3.05	15 (42%)
31	CLA	8	318	16	54,58,73	2.51	21 (38%)	64,95,113	2.41	26 (40%)
31	CLA	A	819	1	69,73,73	2.30	20 (28%)	82,113,113	2.29	28 (34%)
25	SF4	C	102	3	0,12,12	-	-	-	-	-
31	CLA	L	307	36	49,53,73	3.86	19 (38%)	58,89,113	2.51	23 (39%)
31	CLA	5	321	22	50,54,73	3.33	19 (38%)	59,90,113	2.56	23 (38%)
31	CLA	B	835	2	61,65,73	3.03	22 (36%)	72,103,113	2.36	24 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B	826	2	54,58,73	2.81	22 (40%)	64,95,113	2.57	25 (39%)
31	CLA	9	312	17	50,54,73	2.86	19 (38%)	59,90,113	2.51	22 (37%)
31	CLA	5	314	22	49,53,73	3.32	22 (44%)	58,89,113	2.55	22 (37%)
31	CLA	H	903	18	50,54,73	3.02	19 (38%)	59,90,113	2.44	21 (35%)
31	CLA	3	308	14	50,54,73	3.61	21 (42%)	59,90,113	2.57	23 (38%)
31	CLA	A	830	1	64,68,73	2.88	22 (34%)	76,107,113	2.35	27 (35%)
26	BCR	2	302	-	41,41,41	1.11	3 (7%)	56,56,56	1.30	7 (12%)
31	CLA	B	844	2	69,73,73	2.41	22 (31%)	82,113,113	2.19	24 (29%)
32	CHL	8	316	44	60,74,74	3.23	22 (36%)	58,114,114	2.71	18 (31%)
31	CLA	2	308	20	50,54,73	3.01	21 (42%)	59,90,113	2.57	26 (44%)
31	CLA	8	321	16	50,54,73	3.17	21 (42%)	59,90,113	2.53	22 (37%)
31	CLA	b	313	13	64,68,73	3.40	21 (32%)	76,107,113	2.20	24 (31%)
31	CLA	B	817	2	69,73,73	2.46	21 (30%)	82,113,113	2.30	25 (30%)
31	CLA	6	315	28	50,54,73	5.68	23 (46%)	59,90,113	2.51	22 (37%)
36	LUT	3	304	-	42,43,43	4.58	20 (47%)	51,60,60	5.76	34 (66%)
37	LMG	J	104	-	29,29,55	1.02	2 (6%)	37,37,63	1.20	3 (8%)
26	BCR	B	803	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	2 (3%)
26	BCR	M	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	4 (7%)
32	CHL	A	831	1	52,66,74	3.36	21 (40%)	48,104,114	3.17	16 (33%)
31	CLA	G	206	44	49,53,73	3.44	21 (42%)	58,89,113	2.41	21 (36%)
31	CLA	3	317	44	55,59,73	3.07	19 (34%)	64,96,113	2.53	26 (40%)
37	LMG	G	202	-	44,44,55	0.86	1 (2%)	52,52,63	1.30	5 (9%)
26	BCR	L	302	-	41,41,41	1.05	2 (4%)	56,56,56	1.16	6 (10%)
31	CLA	7	322	15	50,54,73	3.18	21 (42%)	59,90,113	2.46	21 (35%)
36	LUT	a	303	-	42,43,43	4.60	19 (45%)	51,60,60	5.69	35 (68%)
31	CLA	8	320	16	69,73,73	2.55	21 (30%)	82,113,113	2.18	29 (35%)
31	CLA	O	202	19	41,46,73	3.28	21 (51%)	47,80,113	2.56	21 (44%)
31	CLA	B	845	2	54,58,73	2.76	21 (38%)	64,95,113	2.53	26 (40%)
31	CLA	B	820	2	69,73,73	3.03	23 (33%)	82,113,113	2.20	26 (31%)
31	CLA	4	312	21	51,55,73	2.89	21 (41%)	60,91,113	2.48	23 (38%)
31	CLA	A	834	44	69,73,73	2.41	21 (30%)	82,113,113	2.13	26 (31%)
31	CLA	a	311	44	64,68,73	2.67	21 (32%)	76,107,113	2.36	28 (36%)
31	CLA	5	323	22	60,64,73	2.99	18 (30%)	71,102,113	2.43	26 (36%)
31	CLA	6	314	23	51,55,73	4.14	20 (39%)	60,91,113	2.53	24 (40%)
31	CLA	6	311	23	59,63,73	4.03	21 (35%)	70,101,113	2.39	26 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	I	801	-	41,41,41	1.06	3 (7%)	56,56,56	1.20	5 (8%)
31	CLA	6	322	23	50,54,73	3.08	21 (42%)	59,90,113	2.43	24 (40%)
31	CLA	A	832	1	69,73,73	2.29	18 (26%)	82,113,113	2.12	25 (30%)
26	BCR	L	303	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	6 (10%)
32	CHL	7	320	44	55,69,74	3.87	21 (38%)	52,108,114	2.82	16 (30%)
34	LAP	B	851	-	28,28,28	0.34	0	33,35,35	0.38	0
31	CLA	6	307	23	54,58,73	3.89	21 (38%)	64,95,113	2.40	26 (40%)
31	CLA	b	302	13	50,54,73	2.96	20 (40%)	59,90,113	2.55	24 (40%)
31	CLA	A	845	1	60,64,73	2.58	21 (35%)	71,102,113	2.35	24 (33%)
31	CLA	A	826	1	69,73,73	2.52	21 (30%)	82,113,113	2.19	26 (31%)
32	CHL	5	322	22	41,55,74	4.35	22 (53%)	35,91,114	3.05	14 (40%)
25	SF4	A	802	1,2	0,12,12	-	-	-	-	-
33	DGD	7	308	-	53,53,67	1.05	3 (5%)	67,67,81	1.54	12 (17%)
32	CHL	5	317	44	41,55,74	3.70	20 (48%)	35,91,114	2.98	14 (40%)
31	CLA	A	853	1	69,73,73	2.67	22 (31%)	82,113,113	2.21	27 (32%)
31	CLA	A	851	1	69,73,73	2.76	22 (31%)	82,113,113	2.19	23 (28%)
26	BCR	8	301	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
31	CLA	H	901	8	50,54,73	2.76	21 (42%)	59,90,113	2.43	24 (40%)
31	CLA	b	311	13	50,54,73	3.85	22 (44%)	59,90,113	2.49	23 (38%)
31	CLA	B	838	2	50,54,73	2.98	23 (46%)	59,90,113	2.42	22 (37%)
31	CLA	a	309	13	64,68,73	4.59	22 (34%)	76,107,113	2.33	27 (35%)
31	CLA	3	313	-	64,68,73	2.75	18 (28%)	76,107,113	2.37	27 (35%)
26	BCR	3	303	-	41,41,41	1.09	3 (7%)	56,56,56	1.27	5 (8%)
38	AXT	a	304	-	44,44,45	0.70	1 (2%)	54,62,64	0.88	1 (1%)
31	CLA	L	305	18	64,68,73	2.53	22 (34%)	76,107,113	2.25	24 (31%)
31	CLA	2	315	44	50,54,73	3.22	22 (44%)	59,90,113	2.54	23 (38%)
31	CLA	3	307	14	69,73,73	3.11	23 (33%)	82,113,113	2.20	28 (34%)
31	CLA	A	836	1	64,68,73	2.56	21 (32%)	76,107,113	2.31	24 (31%)
31	CLA	B	812	-	69,73,73	2.29	22 (31%)	82,113,113	2.23	26 (31%)
31	CLA	2	306	20	64,68,73	3.43	21 (32%)	76,107,113	2.23	27 (35%)
31	CLA	O	204	-	45,49,73	3.02	20 (44%)	54,84,113	2.57	24 (44%)
31	CLA	A	833	1	51,55,73	3.40	22 (43%)	60,91,113	2.64	24 (40%)
31	CLA	8	312	44	54,58,73	2.84	20 (37%)	64,95,113	2.43	24 (37%)
31	CLA	5	313	28	50,54,73	3.52	22 (44%)	59,90,113	2.58	20 (33%)
31	CLA	9	313	17	49,53,73	4.50	22 (44%)	58,89,113	2.59	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CHL	5	319	-	41,55,74	3.73	22 (53%)	35,91,114	3.20	13 (37%)
36	LUT	5	303	-	42,43,43	4.54	19 (45%)	51,60,60	5.90	35 (68%)
36	LUT	5	304	-	42,43,43	4.57	19 (45%)	51,60,60	5.68	34 (66%)
32	CHL	A	840	1	60,74,74	3.18	21 (35%)	58,114,114	2.49	16 (27%)
31	CLA	5	310	22	69,73,73	2.64	20 (28%)	82,113,113	2.27	28 (34%)
31	CLA	A	848	1	61,65,73	2.76	21 (34%)	72,103,113	2.23	24 (33%)
31	CLA	6	312	23	69,73,73	3.12	22 (31%)	82,113,113	2.20	25 (30%)
37	LMG	J	101	-	49,49,55	0.82	2 (4%)	57,57,63	1.24	2 (3%)
31	CLA	B	819	2	69,73,73	2.52	23 (33%)	82,113,113	2.31	29 (35%)
31	CLA	B	846	44	69,73,73	2.40	20 (28%)	82,113,113	2.15	25 (30%)
31	CLA	3	311	14	69,73,73	2.76	24 (34%)	82,113,113	2.20	27 (32%)
31	CLA	6	310	23	51,55,73	4.58	21 (41%)	60,91,113	2.51	25 (41%)
24	PQN	B	801	-	34,34,34	0.53	0	43,45,45	0.78	1 (2%)
36	LUT	8	303	-	42,43,43	4.51	20 (47%)	51,60,60	5.90	35 (68%)
31	CLA	7	312	15	66,70,73	2.65	22 (33%)	78,109,113	2.21	26 (33%)
31	CLA	4	320	21	49,53,73	3.33	22 (44%)	58,89,113	2.47	21 (36%)
36	LUT	8	302	-	42,43,43	4.49	19 (45%)	51,60,60	5.74	32 (62%)
31	CLA	B	830	2	64,68,73	2.63	21 (32%)	76,107,113	2.23	28 (36%)
36	LUT	J	103	-	42,43,43	4.62	20 (47%)	51,60,60	5.80	33 (64%)
31	CLA	8	309	16	54,58,73	3.08	21 (38%)	64,95,113	2.56	28 (43%)
32	CHL	9	320	44	42,56,74	3.84	22 (52%)	36,92,114	3.03	16 (44%)
32	CHL	6	320	-	41,55,74	3.82	22 (53%)	35,91,114	3.12	16 (45%)
36	LUT	7	305	-	42,43,43	4.59	20 (47%)	51,60,60	5.86	32 (62%)
31	CLA	b	306	-	50,54,73	4.60	21 (42%)	59,90,113	2.46	22 (37%)
31	CLA	3	312	44	69,73,73	2.68	20 (28%)	82,113,113	2.20	27 (32%)
35	QTB	9	304	-	19,19,19	1.05	2 (10%)	23,26,26	1.30	2 (8%)
31	CLA	a	322	13	50,54,73	3.18	20 (40%)	59,90,113	2.39	22 (37%)
31	CLA	2	310	20	49,53,73	6.62	21 (42%)	58,89,113	2.54	23 (39%)
36	LUT	6	304	-	42,43,43	4.55	19 (45%)	51,60,60	5.56	33 (64%)
28	LHG	A	811	-	48,48,48	0.75	1 (2%)	51,54,54	1.28	5 (9%)
28	LHG	a	306	31	48,48,48	0.63	1 (2%)	51,54,54	1.25	5 (9%)
31	CLA	a	321	44	54,58,73	2.90	18 (33%)	64,95,113	2.48	28 (43%)
26	BCR	K	202	-	41,41,41	1.09	3 (7%)	56,56,56	1.27	8 (14%)
28	LHG	A	809	-	41,41,48	0.73	2 (4%)	44,47,54	1.31	6 (13%)
31	CLA	4	321	21	54,58,73	3.72	21 (38%)	64,95,113	2.47	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	2	311	20	49,53,73	4.95	22 (44%)	58,89,113	2.47	21 (36%)
31	CLA	5	320	22	50,54,73	5.58	24 (48%)	59,90,113	2.49	24 (40%)
31	CLA	4	316	-	51,55,73	3.29	22 (43%)	60,91,113	2.64	19 (31%)
31	CLA	A	855	1	69,73,73	2.73	21 (30%)	82,113,113	2.25	27 (32%)
31	CLA	B	825	2	64,68,73	2.69	22 (34%)	76,107,113	2.33	26 (34%)
26	BCR	L	301	-	41,41,41	0.99	1 (2%)	56,56,56	1.23	5 (8%)
36	LUT	4	303	-	42,43,43	4.58	19 (45%)	51,60,60	5.69	32 (62%)
26	BCR	A	806	-	41,41,41	1.02	2 (4%)	56,56,56	1.12	4 (7%)
31	CLA	5	307	22	59,63,73	3.79	22 (37%)	70,101,113	2.32	28 (40%)
31	CLA	5	315	22	69,73,73	4.21	21 (30%)	82,113,113	4.09	27 (32%)
26	BCR	F	302	-	41,41,41	1.00	2 (4%)	56,56,56	1.03	2 (3%)
32	CHL	a	318	44	42,56,74	4.38	22 (52%)	36,92,114	3.22	15 (41%)
24	PQN	A	801	-	34,34,34	0.36	0	43,45,45	0.63	1 (2%)
31	CLA	2	304	20	50,54,73	3.18	22 (44%)	59,90,113	2.44	21 (35%)
36	LUT	F	304	-	42,43,43	4.46	20 (47%)	51,60,60	6.13	35 (68%)
31	CLA	B	850	2	66,70,73	2.58	22 (33%)	78,109,113	2.17	23 (29%)
26	BCR	3	302	-	41,41,41	1.08	3 (7%)	56,56,56	1.19	5 (8%)
31	CLA	B	832	44	69,73,73	2.36	21 (30%)	82,113,113	2.39	31 (37%)
26	BCR	G	203	-	41,41,41	1.10	3 (7%)	56,56,56	1.19	5 (8%)
31	CLA	7	314	44	58,62,73	2.74	20 (34%)	69,100,113	2.39	27 (39%)
31	CLA	8	314	44	56,60,73	2.72	20 (35%)	65,97,113	2.44	27 (41%)
31	CLA	B	836	2	69,73,73	2.51	22 (31%)	82,113,113	2.14	27 (32%)
26	BCR	K	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	6 (10%)
31	CLA	7	309	15	64,68,73	2.30	21 (32%)	76,107,113	2.25	25 (32%)
31	CLA	2	309	-	50,54,73	2.67	20 (40%)	59,90,113	2.40	22 (37%)
31	CLA	8	307	16	50,54,73	3.00	22 (44%)	59,90,113	2.59	23 (38%)
36	LUT	9	305	-	42,43,43	4.64	19 (45%)	51,60,60	6.12	33 (64%)
31	CLA	B	841	2	59,63,73	2.66	21 (35%)	70,101,113	2.38	26 (37%)
26	BCR	7	304	-	41,41,41	1.05	2 (4%)	56,56,56	1.22	6 (10%)
31	CLA	3	318	14	55,59,73	3.46	20 (36%)	64,96,113	2.47	26 (40%)
28	LHG	6	305	31	31,31,48	0.76	1 (3%)	34,37,54	1.33	4 (11%)
31	CLA	6	316	23	54,58,73	4.62	22 (40%)	64,95,113	2.48	26 (40%)
31	CLA	4	307	21	60,64,73	2.70	21 (35%)	71,102,113	2.29	27 (38%)
31	CLA	a	312	13	69,73,73	3.08	21 (30%)	82,113,113	2.26	25 (30%)
31	CLA	A	843	1	69,73,73	2.81	22 (31%)	82,113,113	2.18	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	A	823	1	59,63,73	3.00	21 (35%)	70,101,113	2.27	22 (31%)
31	CLA	6	313	23	50,54,73	2.95	22 (44%)	59,90,113	2.63	24 (40%)
36	LUT	b	301	-	42,43,43	4.60	19 (45%)	51,60,60	5.95	35 (68%)
28	LHG	B	807	31	31,31,48	0.83	2 (6%)	34,37,54	1.30	4 (11%)
31	CLA	K	204	44	54,58,73	3.39	21 (38%)	64,95,113	2.45	22 (34%)
31	CLA	A	841	1	69,73,73	2.48	21 (30%)	82,113,113	2.35	31 (37%)
31	CLA	3	310	14	64,68,73	3.05	22 (34%)	76,107,113	2.31	26 (34%)
31	CLA	4	308	21	64,68,73	2.39	21 (32%)	76,107,113	2.35	28 (36%)
27	LMT	5	301	-	36,36,36	1.19	5 (13%)	47,47,47	0.97	2 (4%)
31	CLA	A	814	44	69,73,73	2.68	23 (33%)	82,113,113	2.20	25 (30%)
32	CHL	K	201	11	41,55,74	4.03	19 (46%)	35,91,114	2.95	10 (28%)
31	CLA	7	316	15	50,54,73	3.26	19 (38%)	59,90,113	2.54	24 (40%)
31	CLA	b	303	-	50,54,73	4.09	22 (44%)	59,90,113	2.57	22 (37%)
31	CLA	b	304	13	50,54,73	4.03	22 (44%)	59,90,113	2.43	23 (38%)
31	CLA	A	827	1	59,63,73	2.82	21 (35%)	70,101,113	2.34	23 (32%)
31	CLA	5	312	44	54,58,73	2.78	21 (38%)	64,95,113	2.51	26 (40%)
31	CLA	B	827	2	64,68,73	2.41	18 (28%)	76,107,113	2.28	26 (34%)
31	CLA	F	305	6	50,54,73	2.87	22 (44%)	59,90,113	2.64	24 (40%)
31	CLA	b	312	13	50,54,73	5.14	21 (42%)	59,90,113	2.46	24 (40%)
28	LHG	7	302	-	48,48,48	0.60	0	51,54,54	1.28	5 (9%)
31	CLA	B	833	44	59,63,73	2.39	21 (35%)	70,101,113	2.27	20 (28%)
31	CLA	B	811	2	69,73,73	2.55	21 (30%)	82,113,113	2.28	25 (30%)
31	CLA	4	305	-	56,60,73	2.34	19 (33%)	65,97,113	4.32	34 (52%)
31	CLA	2	313	20	50,54,73	3.34	20 (40%)	59,90,113	2.39	21 (35%)
31	CLA	7	321	44	51,55,73	3.16	21 (41%)	60,91,113	2.55	24 (40%)
31	CLA	4	309	21	64,68,73	2.52	22 (34%)	76,107,113	2.33	30 (39%)
31	CLA	J	105	10	46,50,73	3.13	20 (43%)	53,85,113	2.70	22 (41%)
31	CLA	a	319	13	69,73,73	2.48	19 (27%)	82,113,113	2.27	24 (29%)
35	QTB	a	302	-	19,19,19	1.07	2 (10%)	23,26,26	1.55	4 (17%)
31	CLA	A	847	1	69,73,73	2.58	21 (30%)	82,113,113	2.27	25 (30%)
31	CLA	9	318	44	69,73,73	2.87	19 (27%)	82,113,113	2.18	25 (30%)
31	CLA	A	835	1	59,63,73	2.84	23 (38%)	70,101,113	2.34	21 (30%)
39	3PH	7	301	-	32,32,47	0.76	1 (3%)	35,37,52	0.74	1 (2%)
31	CLA	B	834	2	69,73,73	2.85	21 (30%)	82,113,113	2.22	26 (31%)
26	BCR	A	805	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	A	856	44	69,73,73	2.39	22 (31%)	82,113,113	2.20	27 (32%)
31	CLA	A	849	1	50,54,73	3.41	21 (42%)	59,90,113	2.45	24 (40%)
31	CLA	B	816	2	65,69,73	3.01	20 (30%)	77,108,113	2.37	25 (32%)
31	CLA	A	838	44	69,73,73	2.63	22 (31%)	82,113,113	2.35	25 (30%)
26	BCR	O	201	-	41,41,41	1.08	3 (7%)	56,56,56	1.28	6 (10%)
31	CLA	2	307	20	61,65,73	2.87	21 (34%)	72,103,113	2.37	26 (36%)
31	CLA	4	314	-	49,53,73	4.19	21 (42%)	58,89,113	2.62	24 (41%)
31	CLA	4	306	21	49,53,73	3.24	22 (44%)	58,89,113	2.46	24 (41%)
26	BCR	5	302	-	41,41,41	1.14	2 (4%)	56,56,56	1.29	7 (12%)
31	CLA	7	315	28	59,63,73	3.77	22 (37%)	69,100,113	2.36	24 (34%)
26	BCR	B	806	-	41,41,41	1.05	2 (4%)	56,56,56	1.07	5 (8%)
31	CLA	A	852	1	55,59,73	3.29	22 (40%)	64,96,113	2.55	26 (40%)
31	CLA	9	314	17	64,68,73	3.48	21 (32%)	76,107,113	2.32	26 (34%)
31	CLA	3	320	14	49,53,73	3.54	22 (44%)	58,89,113	2.57	21 (36%)
31	CLA	B	829	2	59,63,73	2.53	19 (32%)	70,101,113	2.52	25 (35%)
31	CLA	A	816	1	69,73,73	2.47	20 (28%)	82,113,113	2.19	25 (30%)
31	CLA	8	308	16	69,73,73	2.61	24 (34%)	82,113,113	2.22	28 (34%)
31	CLA	5	318	22	69,73,73	5.33	23 (33%)	82,113,113	2.17	25 (30%)
32	CHL	6	319	-	41,55,74	4.11	22 (53%)	35,91,114	3.22	14 (40%)
31	CLA	6	308	44	51,55,73	3.09	22 (43%)	60,91,113	2.52	24 (40%)
31	CLA	A	828	1	69,73,73	2.52	22 (31%)	82,113,113	2.25	26 (31%)
36	LUT	a	305	-	42,43,43	4.70	20 (47%)	51,60,60	5.95	30 (58%)
31	CLA	3	319	14	65,69,73	2.79	22 (33%)	77,108,113	2.32	27 (35%)
31	CLA	B	824	2	61,65,73	3.08	22 (36%)	72,103,113	2.37	27 (37%)
31	CLA	A	825	1	58,62,73	2.75	24 (41%)	68,99,113	2.46	26 (38%)
32	CHL	9	322	44	41,55,74	4.48	21 (51%)	35,91,114	3.35	14 (40%)
43	PTY	5	306	-	30,30,49	0.54	0	33,35,54	0.82	1 (3%)
31	CLA	A	822	1	59,63,73	2.64	23 (38%)	70,101,113	2.44	28 (40%)
31	CLA	K	205	11	50,54,73	3.17	21 (42%)	59,90,113	2.51	25 (42%)
26	BCR	G	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	4 (7%)
36	LUT	2	301	-	42,43,43	4.49	19 (45%)	51,60,60	5.94	35 (68%)
31	CLA	B	837	2	59,63,73	2.93	21 (35%)	70,101,113	2.26	25 (35%)
31	CLA	A	817	31,1	59,63,73	2.75	21 (35%)	70,101,113	2.38	24 (34%)
31	CLA	9	321	17	60,64,73	2.57	21 (35%)	71,102,113	2.34	29 (40%)
31	CLA	9	316	17	54,58,73	2.96	21 (38%)	64,95,113	2.45	23 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LUT	4	302	-	42,43,43	4.62	19 (45%)	51,60,60	5.99	36 (70%)
31	CLA	A	824	31,1	66,70,73	2.70	20 (30%)	78,109,113	2.24	28 (35%)
28	LHG	8	304	31	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
32	CHL	A	839	44	50,64,74	3.47	23 (46%)	46,102,114	3.50	15 (32%)
36	LUT	9	303	-	42,43,43	4.49	19 (45%)	51,60,60	5.71	31 (60%)
31	CLA	a	313	13	64,68,73	2.67	23 (35%)	76,107,113	2.31	25 (32%)
31	CLA	G	204	7	54,58,73	3.11	21 (38%)	64,95,113	2.42	24 (37%)
31	CLA	B	831	2	54,58,73	2.65	22 (40%)	64,95,113	2.43	28 (43%)
31	CLA	B	813	2	69,73,73	2.71	24 (34%)	82,113,113	2.31	25 (30%)
31	CLA	2	312	20	50,54,73	3.60	21 (42%)	59,90,113	2.53	23 (38%)
31	CLA	A	857	44	69,73,73	2.22	20 (28%)	82,113,113	2.31	29 (35%)
36	LUT	L	304	31	42,43,43	4.61	20 (47%)	51,60,60	5.99	35 (68%)
31	CLA	8	313	28	50,54,73	3.47	21 (42%)	59,90,113	2.53	22 (37%)
36	LUT	3	305	-	42,43,43	4.45	19 (45%)	51,60,60	5.93	34 (66%)

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
32	CHL	7	317	15	3/3/18/26	7/29/127/137	-
32	CHL	6	309	23	3/3/20/26	16/39/137/137	-
31	CLA	A	842	1	-	5/39/115/115	-
31	CLA	4	311	28	1/1/11/20	7/17/93/115	-
31	CLA	a	316	13	-	9/15/91/115	-
31	CLA	b	307	-	1/1/11/20	6/17/93/115	-
32	CHL	7	318	44	3/3/20/26	25/39/137/137	-
32	CHL	a	317	13	2/2/19/26	13/33/131/137	-
31	CLA	9	317	-	-	8/18/94/115	-
31	CLA	9	319	17	-	9/17/93/115	-
31	CLA	7	310	15	1/1/11/20	4/13/89/115	-
31	CLA	B	818	2	1/1/13/20	4/27/103/115	-
31	CLA	O	203	44	1/1/13/20	14/27/103/115	-
37	LMG	a	301	-	-	21/37/57/70	0/1/1/1
32	CHL	5	316	44	3/3/18/26	11/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CHL	4	310	-	2/2/16/26	3/17/115/137	-
28	LHG	5	305	31	-	25/39/39/53	-
31	CLA	A	829	-	-	4/21/97/115	-
31	CLA	a	310	13	1/1/11/20	6/15/91/115	-
31	CLA	B	823	2	1/1/13/20	9/27/103/115	-
31	CLA	4	319	-	1/1/10/20	6/12/88/115	-
32	CHL	4	317	-	3/3/16/26	11/15/113/137	-
32	CHL	6	318	44	3/3/16/26	10/15/113/137	-
42	SQD	4	304	-	-	12/30/50/69	0/1/1/1
31	CLA	7	313	15	1/1/11/20	3/13/89/115	-
31	CLA	2	305	20	1/1/11/20	7/15/91/115	-
31	CLA	F	301	44	1/1/15/20	7/39/115/115	-
31	CLA	6	306	23	-	5/17/93/115	-
31	CLA	A	850	1	1/1/12/20	6/23/99/115	-
31	CLA	F	306	44	1/1/12/20	4/21/97/115	-
26	BCR	B	802	-	-	3/29/63/63	0/2/2/2
31	CLA	5	311	22	1/1/11/20	5/17/93/115	-
26	BCR	6	302	-	-	15/29/63/63	0/2/2/2
31	CLA	B	822	2	1/1/15/20	16/39/115/115	-
27	LMT	A	808	-	-	6/21/61/61	0/2/2/2
31	CLA	5	308	22	1/1/11/20	5/17/93/115	-
31	CLA	b	310	-	1/1/11/20	4/17/93/115	-
32	CHL	6	321	23	3/3/15/26	8/12/110/137	-
28	LHG	6	301	31	-	15/31/31/53	-
31	CLA	3	309	14	1/1/15/20	16/39/115/115	-
26	BCR	3	301	-	-	9/29/63/63	0/2/2/2
31	CLA	B	828	44	1/1/14/20	4/33/109/115	-
27	LMT	A	807	-	-	6/21/61/61	0/2/2/2
31	CLA	G	205	7	1/1/11/20	5/17/93/115	-
31	CLA	8	311	16	1/1/13/20	11/27/103/115	-
25	SF4	C	101	3	-	-	0/6/5/5
31	CLA	B	842	2	1/1/14/20	10/35/111/115	-
26	BCR	B	804	-	-	4/29/63/63	0/2/2/2
27	LMT	9	306	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	9	315	17	1/1/12/20	9/26/102/115	-
31	CLA	B	847	2	-	11/39/115/115	-
31	CLA	B	848	28	1/1/15/20	7/39/115/115	-
31	CLA	A	815	-	-	4/39/115/115	-
31	CLA	3	314	14	-	9/24/100/115	-
31	CLA	A	837	1	-	16/39/115/115	-
41	DGA	8	305	-	-	16/29/29/45	-
31	CLA	8	315	16	1/1/12/20	6/24/100/115	-
31	CLA	K	206	11	-	4/17/93/115	-
31	CLA	b	308	13	-	4/17/93/115	-
31	CLA	4	318	21	1/1/11/20	7/15/91/115	-
28	LHG	7	307	31	-	20/41/41/53	-
31	CLA	2	314	20	1/1/11/20	2/17/93/115	-
31	CLA	4	315	44	1/1/11/20	4/15/91/115	-
33	DGD	B	808	-	-	21/50/90/95	0/2/2/2
31	CLA	B	843	44	1/1/11/20	4/15/91/115	-
36	LUT	6	303	-	-	19/29/67/67	0/2/2/2
32	CHL	7	319	15	3/3/16/26	3/17/115/137	-
31	CLA	A	844	1	-	4/21/97/115	-
32	CHL	8	319	44	3/3/15/26	3/14/112/137	-
35	QTB	F	303	-	-	8/11/28/28	1/1/1/1
31	CLA	b	305	13	1/1/11/20	6/17/93/115	-
31	CLA	9	311	17	1/1/13/20	6/27/103/115	-
31	CLA	A	820	1	-	5/27/103/115	-
28	LHG	A	810	31	-	17/46/46/53	-
31	CLA	H	902	44	1/1/11/20	2/17/93/115	-
26	BCR	A	803	-	-	4/29/63/63	0/2/2/2
32	CHL	4	313	21	2/2/16/26	5/18/116/137	-
31	CLA	5	309	22	-	6/18/94/115	-
31	CLA	B	814	2	1/1/15/20	15/39/115/115	-
31	CLA	B	821	2	-	4/31/107/115	-
35	QTB	7	303	-	-	10/11/28/28	1/1/1/1
31	CLA	3	316	44	1/1/12/20	4/21/97/115	-
31	CLA	L	306	44	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	854	28	1/1/11/20	5/17/93/115	-
31	CLA	8	317	44	-	2/21/97/115	-
31	CLA	a	315	28	1/1/13/20	6/27/103/115	-
32	CHL	3	315	44	2/2/18/26	7/27/125/137	-
36	LUT	9	302	-	-	17/29/67/67	0/2/2/2
32	CHL	7	324	16	2/2/20/26	11/39/137/137	-
26	BCR	J	102	-	-	4/29/63/63	0/2/2/2
26	BCR	A	804	-	-	7/29/63/63	0/2/2/2
31	CLA	B	840	2	1/1/15/20	12/39/115/115	-
30	CL0	A	813	1	1/1/20/25	9/37/135/135	-
31	CLA	A	821	1	1/1/15/20	14/39/115/115	-
31	CLA	7	311	15	-	12/39/115/115	-
32	CHL	b	309	13	2/2/16/26	6/17/115/137	-
31	CLA	B	839	2	-	8/33/109/115	-
31	CLA	a	314	44	1/1/12/20	6/21/97/115	-
31	CLA	A	818	1	1/1/15/20	9/39/115/115	-
26	BCR	B	805	-	-	7/29/63/63	0/2/2/2
31	CLA	8	310	16	1/1/15/20	10/39/115/115	-
31	CLA	B	815	2	1/1/15/20	16/39/115/115	-
31	CLA	B	849	2	1/1/12/20	2/21/97/115	-
31	CLA	A	846	1	-	7/39/115/115	-
40	XAT	7	306	-	-	4/31/93/93	0/4/4/4
32	CHL	a	320	44	3/3/16/26	8/18/116/137	-
32	CHL	6	317	23	2/2/16/26	4/17/115/137	-
31	CLA	8	318	16	1/1/12/20	2/21/97/115	-
31	CLA	A	819	1	1/1/15/20	12/39/115/115	-
25	SF4	C	102	3	-	-	0/6/5/5
31	CLA	L	307	36	1/1/11/20	9/15/91/115	-
31	CLA	5	321	22	-	5/17/93/115	-
31	CLA	B	835	2	1/1/13/20	5/30/106/115	-
31	CLA	B	826	2	-	6/21/97/115	-
31	CLA	9	312	17	1/1/11/20	2/17/93/115	-
31	CLA	5	314	22	-	7/15/91/115	-
31	CLA	H	903	18	-	4/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	3	308	14	1/1/11/20	5/17/93/115	-
31	CLA	A	830	1	-	10/33/109/115	-
26	BCR	2	302	-	-	7/29/63/63	0/2/2/2
31	CLA	B	844	2	1/1/15/20	9/39/115/115	-
32	CHL	8	316	44	3/3/20/26	15/39/137/137	-
31	CLA	2	308	20	1/1/11/20	4/17/93/115	-
31	CLA	8	321	16	1/1/11/20	2/17/93/115	-
31	CLA	b	313	13	1/1/14/20	10/33/109/115	-
31	CLA	B	817	2	1/1/15/20	12/39/115/115	-
31	CLA	6	315	28	1/1/11/20	2/17/93/115	-
36	LUT	3	304	-	-	13/29/67/67	0/2/2/2
37	LMG	J	104	-	-	10/24/44/70	0/1/1/1
26	BCR	B	803	-	-	9/29/63/63	0/2/2/2
26	BCR	M	101	-	-	7/29/63/63	0/2/2/2
32	CHL	A	831	1	2/2/18/26	12/30/128/137	-
31	CLA	G	206	44	1/1/11/20	2/15/91/115	-
31	CLA	3	317	44	1/1/12/20	7/23/99/115	-
37	LMG	G	202	-	-	23/39/59/70	0/1/1/1
26	BCR	L	302	-	-	5/29/63/63	0/2/2/2
31	CLA	7	322	15	1/1/11/20	6/17/93/115	-
36	LUT	a	303	-	-	14/29/67/67	0/2/2/2
31	CLA	8	320	16	-	10/39/115/115	-
31	CLA	O	202	19	1/1/9/20	3/6/78/115	-
31	CLA	B	845	2	-	3/21/97/115	-
31	CLA	B	820	2	-	11/39/115/115	-
31	CLA	4	312	21	1/1/11/20	9/18/94/115	-
31	CLA	A	834	44	1/1/15/20	7/39/115/115	-
31	CLA	a	311	44	1/1/14/20	9/33/109/115	-
31	CLA	5	323	22	1/1/13/20	9/29/105/115	-
31	CLA	6	314	23	-	6/18/94/115	-
31	CLA	6	311	23	1/1/13/20	10/27/103/115	-
26	BCR	I	801	-	-	6/29/63/63	0/2/2/2
31	CLA	6	322	23	-	6/17/93/115	-
31	CLA	A	832	1	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	L	303	-	-	7/29/63/63	0/2/2/2
32	CHL	7	320	44	3/3/19/26	15/33/131/137	-
34	LAP	B	851	-	-	16/30/30/30	-
31	CLA	6	307	23	1/1/12/20	6/21/97/115	-
31	CLA	b	302	13	1/1/11/20	6/17/93/115	-
31	CLA	A	845	1	-	7/29/105/115	-
31	CLA	A	826	1	1/1/15/20	11/39/115/115	-
32	CHL	5	322	22	3/3/16/26	6/17/115/137	-
25	SF4	A	802	1,2	-	-	0/6/5/5
33	DGD	7	308	-	-	14/41/81/95	0/2/2/2
32	CHL	5	317	44	2/2/16/26	8/17/115/137	-
31	CLA	A	853	1	-	11/39/115/115	-
31	CLA	A	851	1	1/1/15/20	5/39/115/115	-
26	BCR	8	301	-	-	6/29/63/63	0/2/2/2
31	CLA	H	901	8	1/1/11/20	9/17/93/115	-
31	CLA	b	311	13	1/1/11/20	7/17/93/115	-
31	CLA	B	838	2	-	3/17/93/115	-
31	CLA	a	309	13	1/1/14/20	3/33/109/115	-
31	CLA	3	313	-	1/1/14/20	10/33/109/115	-
26	BCR	3	303	-	-	8/29/63/63	0/2/2/2
38	AXT	a	304	-	-	2/29/71/75	0/2/2/2
31	CLA	L	305	18	-	8/33/109/115	-
31	CLA	2	315	44	1/1/11/20	7/17/93/115	-
31	CLA	3	307	14	1/1/15/20	9/39/115/115	-
31	CLA	B	812	-	1/1/15/20	9/39/115/115	-
31	CLA	A	836	1	-	8/33/109/115	-
31	CLA	2	306	20	1/1/14/20	10/33/109/115	-
31	CLA	O	204	-	1/1/10/20	4/10/86/115	-
31	CLA	A	833	1	-	10/18/94/115	-
31	CLA	8	312	44	1/1/12/20	4/21/97/115	-
31	CLA	5	313	28	-	5/17/93/115	-
31	CLA	9	313	17	1/1/11/20	4/15/91/115	-
32	CHL	5	319	-	2/2/16/26	2/17/115/137	-
36	LUT	5	303	-	-	13/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LUT	5	304	-	-	16/29/67/67	0/2/2/2
32	CHL	A	840	1	2/2/20/26	9/39/137/137	-
31	CLA	5	310	22	1/1/15/20	6/39/115/115	-
31	CLA	A	848	1	-	12/30/106/115	-
31	CLA	6	312	23	1/1/15/20	10/39/115/115	-
37	LMG	J	101	-	-	20/44/64/70	0/1/1/1
31	CLA	B	819	2	1/1/15/20	7/39/115/115	-
31	CLA	B	846	44	-	10/39/115/115	-
31	CLA	3	311	14	1/1/15/20	11/39/115/115	-
31	CLA	6	310	23	1/1/11/20	4/18/94/115	-
24	PQN	B	801	-	-	4/23/43/43	0/2/2/2
36	LUT	8	303	-	-	14/29/67/67	0/2/2/2
31	CLA	7	312	15	1/1/14/20	8/36/112/115	-
31	CLA	4	320	21	1/1/11/20	8/15/91/115	-
36	LUT	8	302	-	-	16/29/67/67	0/2/2/2
31	CLA	B	830	2	-	5/33/109/115	-
36	LUT	J	103	-	-	16/29/67/67	0/2/2/2
31	CLA	8	309	16	1/1/12/20	6/21/97/115	-
32	CHL	9	320	44	3/3/16/26	6/18/116/137	-
32	CHL	6	320	-	3/3/16/26	7/17/115/137	-
36	LUT	7	305	-	-	14/29/67/67	0/2/2/2
31	CLA	b	306	-	-	7/17/93/115	-
31	CLA	3	312	44	1/1/15/20	8/39/115/115	-
35	QTB	9	304	-	-	6/11/28/28	0/1/1/1
31	CLA	a	322	13	1/1/11/20	5/17/93/115	-
31	CLA	2	310	20	1/1/11/20	5/15/91/115	-
36	LUT	6	304	-	-	16/29/67/67	0/2/2/2
28	LHG	A	811	-	-	17/53/53/53	-
28	LHG	a	306	31	-	18/53/53/53	-
31	CLA	a	321	44	-	5/21/97/115	-
26	BCR	K	202	-	-	9/29/63/63	0/2/2/2
28	LHG	A	809	-	-	20/46/46/53	-
31	CLA	4	321	21	1/1/12/20	9/21/97/115	-
31	CLA	2	311	20	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	5	320	22	-	3/17/93/115	-
31	CLA	4	316	-	-	5/18/94/115	-
31	CLA	A	855	1	-	15/39/115/115	-
31	CLA	B	825	2	-	8/33/109/115	-
26	BCR	L	301	-	-	7/29/63/63	0/2/2/2
36	LUT	4	303	-	-	16/29/67/67	0/2/2/2
26	BCR	A	806	-	-	7/29/63/63	0/2/2/2
31	CLA	5	307	22	1/1/13/20	4/27/103/115	-
31	CLA	5	315	22	1/1/15/20	9/39/115/115	-
26	BCR	F	302	-	-	5/29/63/63	0/2/2/2
32	CHL	a	318	44	2/2/16/26	6/18/116/137	-
24	PQN	A	801	-	-	2/23/43/43	0/2/2/2
31	CLA	2	304	20	-	9/17/93/115	-
36	LUT	F	304	-	-	17/29/67/67	0/2/2/2
31	CLA	B	850	2	-	8/36/112/115	-
26	BCR	3	302	-	-	8/29/63/63	0/2/2/2
31	CLA	B	832	44	1/1/15/20	9/39/115/115	-
26	BCR	G	203	-	-	11/29/63/63	0/2/2/2
31	CLA	7	314	44	-	7/25/101/115	-
31	CLA	8	314	44	1/1/12/20	5/24/100/115	-
31	CLA	B	836	2	-	5/39/115/115	-
31	CLA	7	309	15	1/1/14/20	3/33/109/115	-
26	BCR	K	203	-	-	5/29/63/63	0/2/2/2
31	CLA	2	309	-	-	4/17/93/115	-
31	CLA	8	307	16	1/1/11/20	2/17/93/115	-
36	LUT	9	305	-	-	18/29/67/67	0/2/2/2
31	CLA	B	841	2	-	10/27/103/115	-
26	BCR	7	304	-	-	6/29/63/63	0/2/2/2
31	CLA	3	318	14	-	9/23/99/115	-
28	LHG	6	305	31	-	8/36/36/53	-
31	CLA	6	316	23	1/1/12/20	3/21/97/115	-
31	CLA	4	307	21	1/1/13/20	9/29/105/115	-
31	CLA	a	312	13	1/1/15/20	10/39/115/115	-
31	CLA	A	843	1	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	823	1	-	7/27/103/115	-
31	CLA	6	313	23	1/1/11/20	5/17/93/115	-
36	LUT	b	301	-	-	14/29/67/67	0/2/2/2
28	LHG	B	807	31	-	7/36/36/53	-
31	CLA	K	204	44	-	4/21/97/115	-
31	CLA	A	841	1	1/1/15/20	13/39/115/115	-
31	CLA	3	310	14	1/1/14/20	10/33/109/115	-
31	CLA	4	308	21	1/1/14/20	6/33/109/115	-
27	LMT	5	301	-	-	9/21/61/61	0/2/2/2
31	CLA	A	814	44	1/1/15/20	8/39/115/115	-
32	CHL	K	201	11	3/3/16/26	6/17/115/137	-
31	CLA	7	316	15	1/1/11/20	4/17/93/115	-
31	CLA	b	303	-	1/1/11/20	3/17/93/115	-
31	CLA	b	304	13	1/1/11/20	5/17/93/115	-
31	CLA	5	312	44	1/1/12/20	8/21/97/115	-
31	CLA	A	827	1	-	8/27/103/115	-
31	CLA	B	827	2	1/1/14/20	9/33/109/115	-
31	CLA	F	305	6	1/1/11/20	5/17/93/115	-
31	CLA	b	312	13	-	4/17/93/115	-
28	LHG	7	302	-	-	31/53/53/53	-
31	CLA	B	833	44	1/1/13/20	7/27/103/115	-
31	CLA	B	811	2	1/1/15/20	5/39/115/115	-
31	CLA	4	305	-	-	7/24/100/115	-
31	CLA	2	313	20	1/1/11/20	6/17/93/115	-
31	CLA	7	321	44	-	6/18/94/115	-
31	CLA	4	309	21	1/1/14/20	11/33/109/115	-
31	CLA	J	105	10	1/1/10/20	5/12/88/115	-
31	CLA	a	319	13	1/1/15/20	12/39/115/115	-
35	QTB	a	302	-	-	5/11/28/28	0/1/1/1
31	CLA	9	318	44	1/1/15/20	10/39/115/115	-
31	CLA	A	847	1	-	7/39/115/115	-
31	CLA	A	835	1	-	5/27/103/115	-
39	3PH	7	301	-	-	15/34/34/49	-
31	CLA	B	834	2	1/1/15/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	A	805	-	-	8/29/63/63	0/2/2/2
31	CLA	A	856	44	1/1/15/20	7/39/115/115	-
31	CLA	A	849	1	1/1/11/20	6/17/93/115	-
31	CLA	B	816	2	-	4/35/111/115	-
31	CLA	A	838	44	1/1/15/20	10/39/115/115	-
26	BCR	O	201	-	-	2/29/63/63	0/2/2/2
31	CLA	2	307	20	1/1/13/20	7/30/106/115	-
31	CLA	4	314	-	1/1/11/20	6/15/91/115	-
31	CLA	4	306	21	1/1/11/20	4/15/91/115	-
26	BCR	5	302	-	-	13/29/63/63	0/2/2/2
31	CLA	7	315	28	1/1/12/20	8/27/103/115	-
31	CLA	9	314	17	1/1/14/20	9/33/109/115	-
26	BCR	B	806	-	-	6/29/63/63	0/2/2/2
31	CLA	A	852	1	-	1/23/99/115	-
31	CLA	3	320	14	1/1/11/20	4/15/91/115	-
31	CLA	8	308	16	1/1/15/20	13/39/115/115	-
31	CLA	A	816	1	1/1/15/20	5/39/115/115	-
31	CLA	B	829	2	-	5/27/103/115	-
31	CLA	5	318	22	1/1/15/20	10/39/115/115	-
32	CHL	6	319	-	1/1/16/26	3/17/115/137	-
31	CLA	6	308	44	1/1/11/20	5/18/94/115	-
31	CLA	A	828	1	-	7/39/115/115	-
36	LUT	a	305	-	-	23/29/67/67	0/2/2/2
31	CLA	3	319	14	1/1/14/20	6/35/111/115	-
31	CLA	B	824	2	-	10/30/106/115	-
31	CLA	A	825	1	-	2/26/102/115	-
32	CHL	9	322	44	3/3/16/26	5/17/115/137	-
43	PTY	5	306	-	-	16/34/34/53	-
31	CLA	A	822	1	-	9/27/103/115	-
31	CLA	K	205	11	1/1/11/20	2/17/93/115	-
26	BCR	G	201	-	-	8/29/63/63	0/2/2/2
36	LUT	2	301	-	-	13/29/67/67	0/2/2/2
31	CLA	B	837	2	-	6/27/103/115	-
31	CLA	A	817	31,1	1/1/13/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	9	321	17	1/1/13/20	13/29/105/115	-
31	CLA	9	316	17	1/1/12/20	4/21/97/115	-
36	LUT	4	302	-	-	16/29/67/67	0/2/2/2
31	CLA	A	824	31,1	1/1/14/20	8/36/112/115	-
28	LHG	8	304	31	-	15/53/53/53	-
32	CHL	A	839	44	2/2/18/26	6/27/125/137	-
36	LUT	9	303	-	-	16/29/67/67	0/2/2/2
31	CLA	a	313	13	1/1/14/20	7/33/109/115	-
31	CLA	G	204	7	1/1/12/20	5/21/97/115	-
31	CLA	B	831	2	-	4/21/97/115	-
31	CLA	B	813	2	-	7/39/115/115	-
31	CLA	2	312	20	1/1/11/20	5/17/93/115	-
31	CLA	A	857	44	1/1/15/20	14/39/115/115	-
36	LUT	L	304	31	-	15/29/67/67	0/2/2/2
31	CLA	8	313	28	1/1/11/20	7/17/93/115	-
36	LUT	3	305	-	-	13/29/67/67	0/2/2/2

The worst 5 of 5823 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	310	CLA	MG-NA	30.68	2.79	2.06
31	b	307	CLA	MG-NA	29.70	2.76	2.06
31	6	315	CLA	MG-NA	29.56	2.76	2.06
31	5	318	CLA	MG-ND	-28.84	1.48	2.05
31	9	319	CLA	MG-NA	28.29	2.73	2.06

The worst 5 of 6859 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	315	CLA	C4-C3-C5	-19.27	81.78	115.23
31	5	315	CLA	C4-C3-C2	-17.63	78.34	123.63
36	7	305	LUT	C15-C14-C13	-17.40	102.87	127.28
31	5	315	CLA	C5-C3-C2	17.27	159.93	121.17
36	2	301	LUT	C15-C14-C13	-16.41	104.26	127.28

5 of 223 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	A	813	CL0	NC
31	A	814	CLA	ND
31	A	816	CLA	ND
31	A	817	CLA	ND
31	A	818	CLA	ND

5 of 2747 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	804	BCR	C7-C8-C9-C10
26	A	804	BCR	C7-C8-C9-C34
26	A	804	BCR	C20-C21-C22-C23
26	A	805	BCR	C20-C21-C22-C37
26	A	806	BCR	C21-C22-C23-C24

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	F	303	QTB	C11-C12-C14-C15-C16-C17
35	7	303	QTB	C11-C12-C14-C15-C16-C17

268 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	7	317	CHL	6	0
32	6	309	CHL	7	0
31	a	316	CLA	1	0
31	4	311	CLA	1	0
32	7	318	CHL	9	0
32	a	317	CHL	6	0
31	B	818	CLA	2	0
37	a	301	LMG	2	0
32	5	316	CHL	6	0
32	4	310	CHL	7	0
28	5	305	LHG	1	0
31	A	829	CLA	10	0
31	a	310	CLA	1	0
31	B	823	CLA	1	0
31	4	319	CLA	1	0
32	4	317	CHL	7	0
32	6	318	CHL	5	0
42	4	304	SQD	1	0
31	7	313	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	F	301	CLA	3	0
31	6	306	CLA	5	0
26	B	802	BCR	4	0
31	A	850	CLA	2	0
31	F	306	CLA	1	0
31	5	311	CLA	2	0
26	6	302	BCR	2	0
31	B	822	CLA	3	0
31	5	308	CLA	1	0
28	6	301	LHG	2	0
32	6	321	CHL	2	0
31	3	309	CLA	6	0
26	3	301	BCR	1	0
27	A	807	LMT	4	0
31	G	205	CLA	1	0
31	8	311	CLA	4	0
31	B	842	CLA	4	0
26	B	804	BCR	4	0
31	9	315	CLA	1	0
31	B	847	CLA	2	0
31	B	848	CLA	2	0
31	A	815	CLA	3	0
31	3	314	CLA	1	0
31	A	837	CLA	4	0
41	8	305	DGA	2	0
31	8	315	CLA	1	0
31	K	206	CLA	1	0
31	b	308	CLA	1	0
31	4	318	CLA	5	0
28	7	307	LHG	4	0
31	2	314	CLA	3	0
31	4	315	CLA	2	0
33	B	808	DGD	4	0
31	B	843	CLA	2	0
36	6	303	LUT	2	0
32	7	319	CHL	3	0
32	8	319	CHL	1	0
31	b	305	CLA	1	0
31	A	820	CLA	2	0
28	A	810	LHG	2	0
31	H	902	CLA	6	0
26	A	803	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	4	313	CHL	3	0
31	5	309	CLA	1	0
31	B	814	CLA	3	0
31	A	854	CLA	1	0
31	8	317	CLA	1	0
31	a	315	CLA	3	0
32	3	315	CHL	1	0
36	9	302	LUT	1	0
32	7	324	CHL	3	0
26	J	102	BCR	1	0
26	A	804	BCR	2	0
31	B	840	CLA	2	0
30	A	813	CL0	3	0
31	A	821	CLA	3	0
31	7	311	CLA	3	0
32	b	309	CHL	1	0
31	B	839	CLA	2	0
31	a	314	CLA	2	0
31	A	818	CLA	3	0
26	B	805	BCR	5	0
31	8	310	CLA	3	0
31	B	815	CLA	1	0
31	A	846	CLA	3	0
32	a	320	CHL	3	0
32	6	317	CHL	3	0
31	A	819	CLA	3	0
31	B	835	CLA	2	0
31	B	826	CLA	1	0
31	H	903	CLA	2	0
31	3	308	CLA	2	0
31	A	830	CLA	2	0
26	2	302	BCR	3	0
31	B	844	CLA	2	0
32	8	316	CHL	8	0
31	2	308	CLA	1	0
31	8	321	CLA	2	0
31	b	313	CLA	3	0
31	B	817	CLA	2	0
31	6	315	CLA	1	0
36	3	304	LUT	3	0
26	B	803	BCR	1	0
26	M	101	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	831	CHL	2	0
31	G	206	CLA	6	0
37	G	202	LMG	4	0
26	L	302	BCR	2	0
31	7	322	CLA	1	0
36	a	303	LUT	4	0
31	8	320	CLA	1	0
31	B	845	CLA	4	0
31	B	820	CLA	3	0
31	4	312	CLA	1	0
31	A	834	CLA	6	0
31	a	311	CLA	1	0
31	5	323	CLA	3	0
31	6	314	CLA	2	0
31	6	311	CLA	1	0
26	I	801	BCR	1	0
31	6	322	CLA	3	0
31	A	832	CLA	2	0
26	L	303	BCR	3	0
32	7	320	CHL	6	0
34	B	851	LAP	4	0
31	6	307	CLA	2	0
31	b	302	CLA	1	0
31	A	845	CLA	4	0
31	A	826	CLA	3	0
32	5	322	CHL	4	0
32	5	317	CHL	4	0
31	A	853	CLA	4	0
31	A	851	CLA	3	0
26	8	301	BCR	4	0
31	H	901	CLA	2	0
31	b	311	CLA	1	0
31	B	838	CLA	1	0
31	a	309	CLA	3	0
31	3	313	CLA	2	0
26	3	303	BCR	2	0
38	a	304	AXT	1	0
31	L	305	CLA	6	0
31	2	315	CLA	1	0
31	A	836	CLA	3	0
31	B	812	CLA	2	0
31	2	306	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	833	CLA	3	0
31	5	313	CLA	1	0
31	9	313	CLA	1	0
32	5	319	CHL	4	0
36	5	303	LUT	3	0
36	5	304	LUT	6	0
32	A	840	CHL	5	0
31	5	310	CLA	4	0
31	A	848	CLA	1	0
31	6	312	CLA	1	0
37	J	101	LMG	4	0
31	B	819	CLA	2	0
31	B	846	CLA	3	0
31	3	311	CLA	2	0
24	B	801	PQN	2	0
36	8	303	LUT	2	0
36	8	302	LUT	5	0
36	J	103	LUT	3	0
31	8	309	CLA	1	0
32	9	320	CHL	3	0
32	6	320	CHL	1	0
36	7	305	LUT	3	0
31	2	310	CLA	1	0
36	6	304	LUT	3	0
28	A	811	LHG	3	0
28	a	306	LHG	9	0
31	a	321	CLA	1	0
26	K	202	BCR	4	0
28	A	809	LHG	2	0
31	4	321	CLA	1	0
31	2	311	CLA	1	0
31	5	320	CLA	1	0
31	4	316	CLA	4	0
31	A	855	CLA	3	0
31	B	825	CLA	4	0
26	L	301	BCR	1	0
36	4	303	LUT	4	0
26	A	806	BCR	4	0
31	5	307	CLA	2	0
31	5	315	CLA	1	0
26	F	302	BCR	1	0
32	a	318	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	801	PQN	1	0
31	2	304	CLA	4	0
36	F	304	LUT	2	0
31	B	850	CLA	4	0
26	3	302	BCR	4	0
31	B	832	CLA	2	0
31	8	314	CLA	1	0
31	B	836	CLA	1	0
26	K	203	BCR	3	0
31	7	309	CLA	1	0
31	8	307	CLA	1	0
36	9	305	LUT	1	0
31	B	841	CLA	3	0
26	7	304	BCR	6	0
31	3	318	CLA	1	0
28	6	305	LHG	1	0
31	6	316	CLA	1	0
31	a	312	CLA	2	0
31	A	843	CLA	2	0
31	A	823	CLA	4	0
31	6	313	CLA	1	0
36	b	301	LUT	5	0
28	B	807	LHG	1	0
31	A	841	CLA	5	0
31	3	310	CLA	1	0
31	4	308	CLA	1	0
31	A	814	CLA	5	0
32	K	201	CHL	1	0
31	A	827	CLA	2	0
28	7	302	LHG	4	0
31	B	833	CLA	1	0
31	B	811	CLA	1	0
31	4	305	CLA	5	0
31	2	313	CLA	2	0
31	7	321	CLA	1	0
31	J	105	CLA	1	0
31	a	319	CLA	3	0
31	A	835	CLA	3	0
39	7	301	3PH	1	0
31	B	834	CLA	3	0
26	A	805	BCR	2	0
31	A	856	CLA	3	0

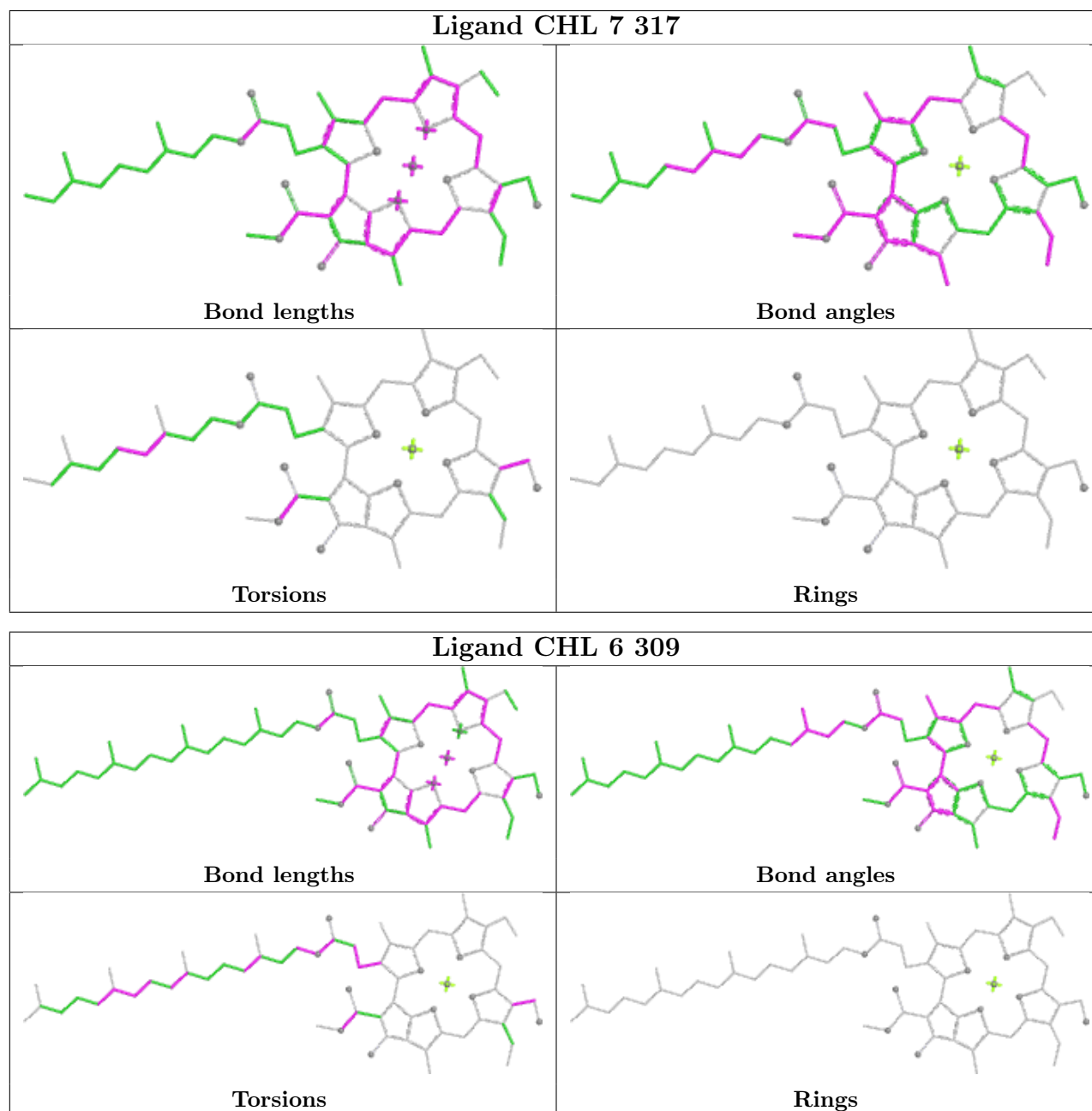
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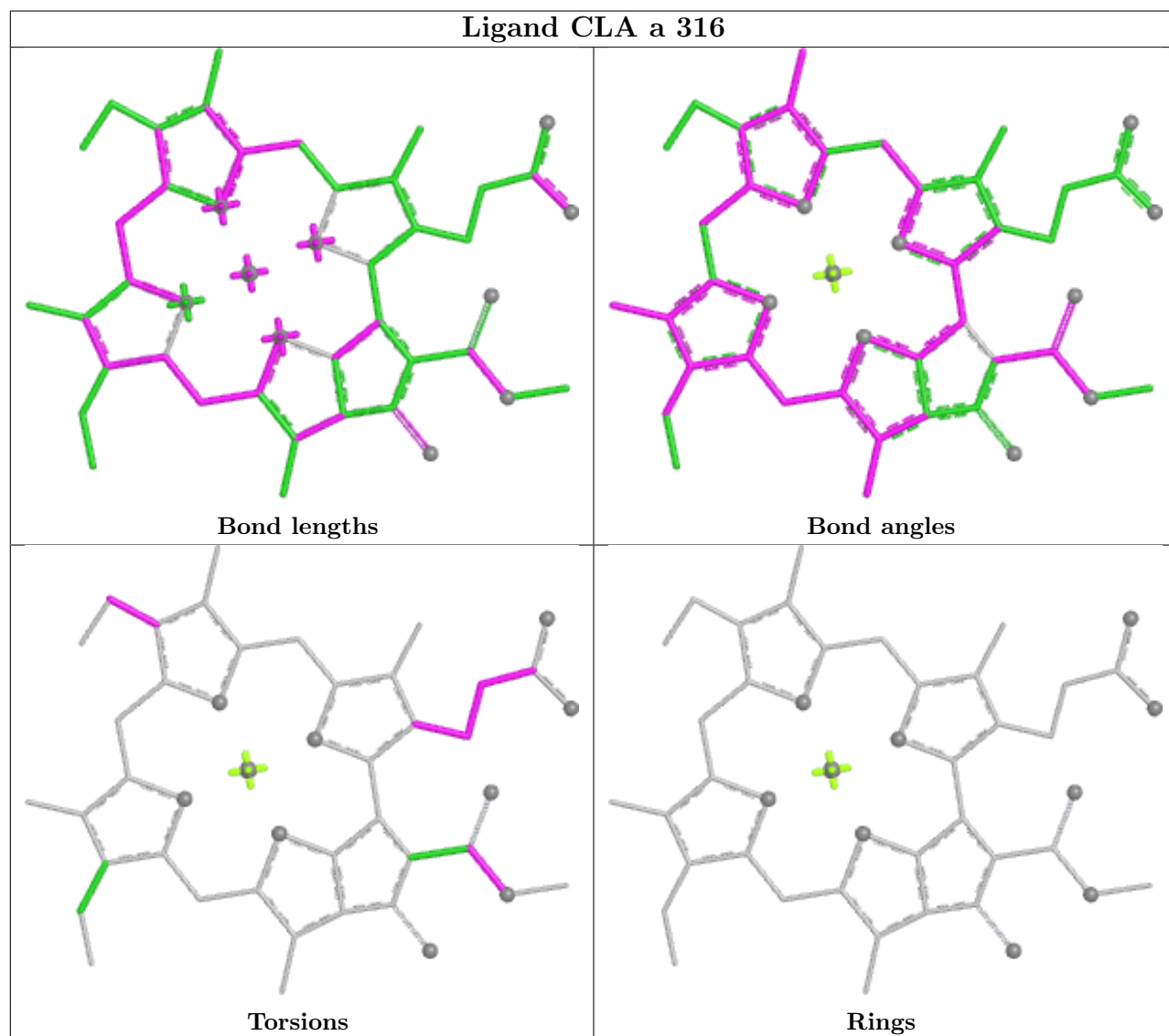
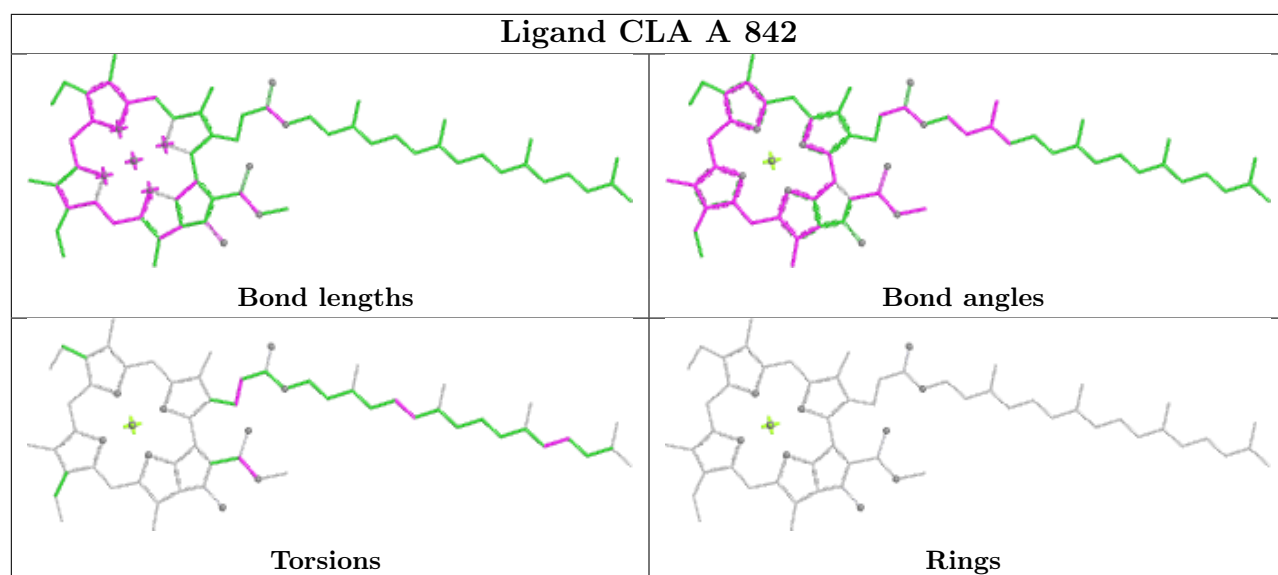
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	849	CLA	1	0
31	B	816	CLA	2	0
31	A	838	CLA	1	0
26	O	201	BCR	2	0
31	4	314	CLA	5	0
26	5	302	BCR	2	0
31	7	315	CLA	4	0
26	B	806	BCR	2	0
31	A	852	CLA	1	0
31	9	314	CLA	2	0
31	3	320	CLA	2	0
31	A	816	CLA	2	0
31	8	308	CLA	3	0
31	5	318	CLA	5	0
32	6	319	CHL	2	0
31	6	308	CLA	1	0
31	A	828	CLA	2	0
36	a	305	LUT	6	0
31	3	319	CLA	4	0
31	A	825	CLA	4	0
32	9	322	CHL	3	0
43	5	306	PTY	1	0
31	A	822	CLA	2	0
26	G	201	BCR	1	0
36	2	301	LUT	4	0
31	B	837	CLA	4	0
36	4	302	LUT	7	0
31	A	824	CLA	1	0
32	A	839	CHL	4	0
36	9	303	LUT	6	0
31	a	313	CLA	1	0
31	G	204	CLA	1	0
31	B	831	CLA	2	0
31	B	813	CLA	4	0
31	2	312	CLA	1	0
31	A	857	CLA	3	0
36	L	304	LUT	1	0
31	8	313	CLA	1	0
36	3	305	LUT	7	0

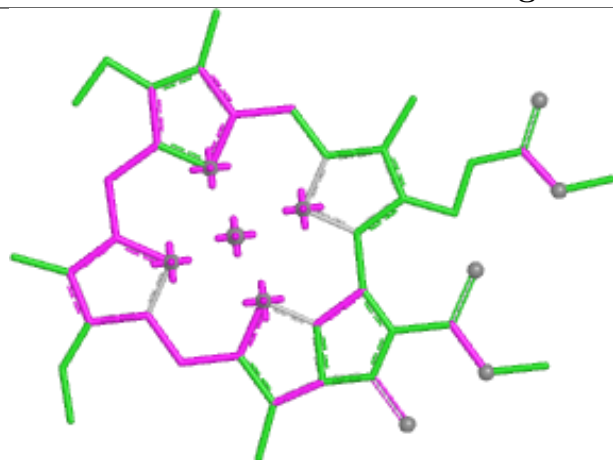
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

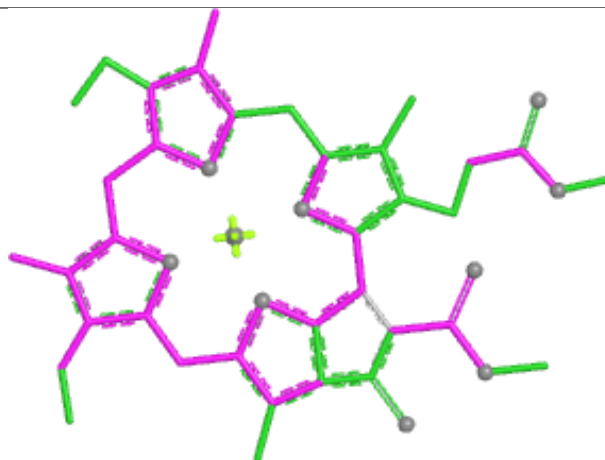




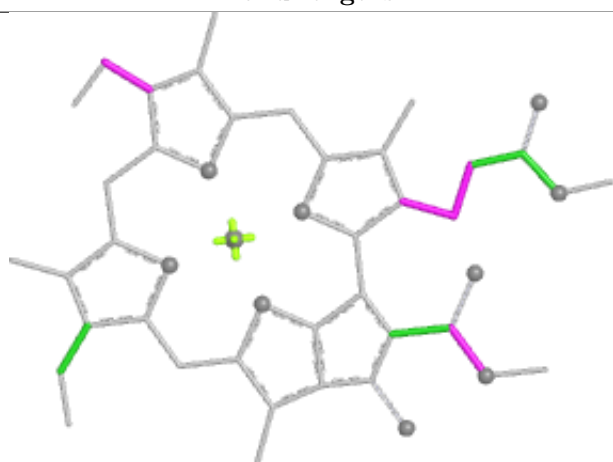
Ligand CLA 4 311



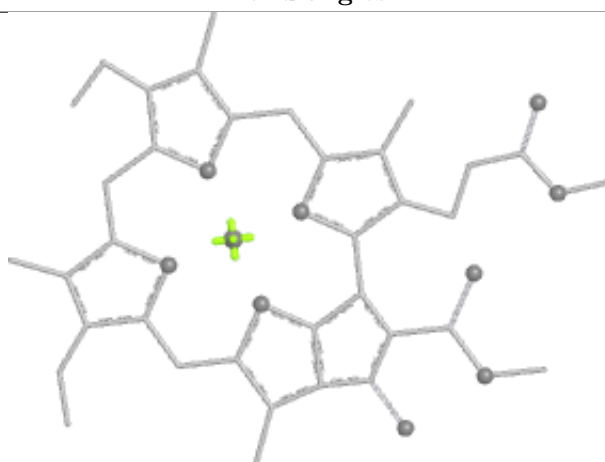
Bond lengths



Bond angles

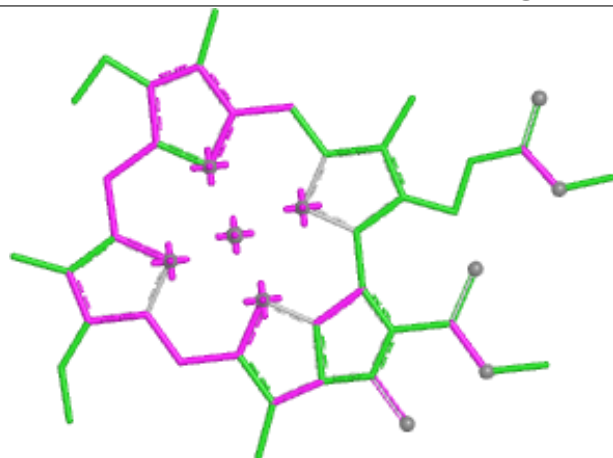


Torsions

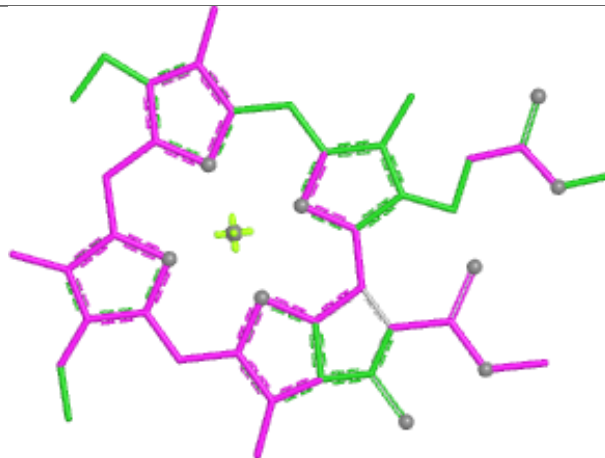


Rings

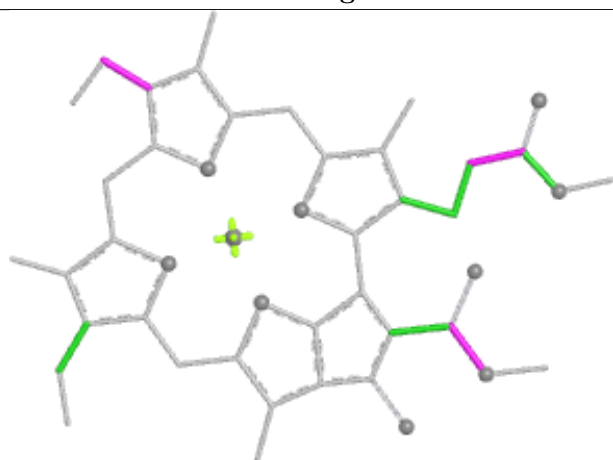
Ligand CLA b 307



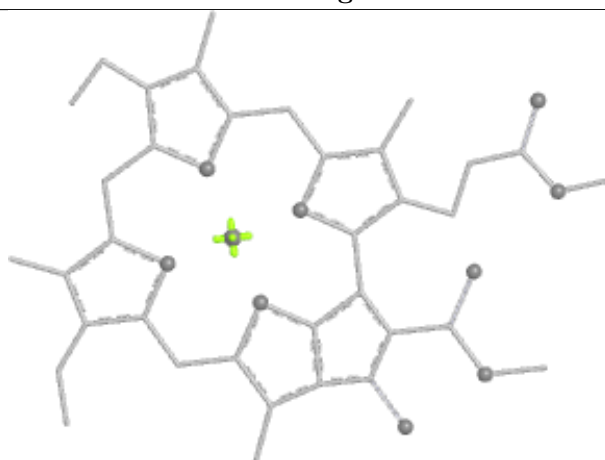
Bond lengths



Bond angles

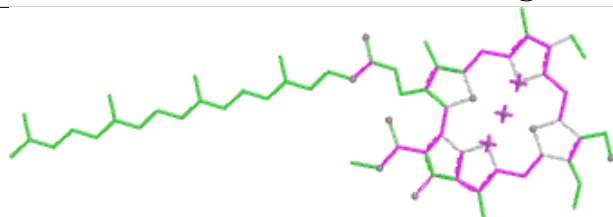


Torsions

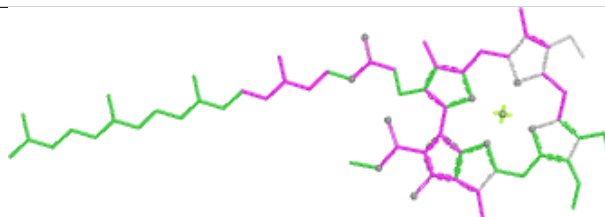


Rings

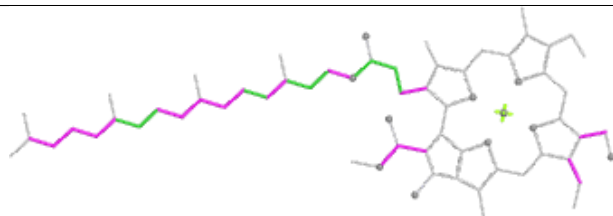
Ligand CHL 7 318



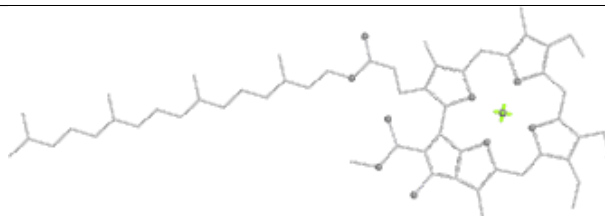
Bond lengths



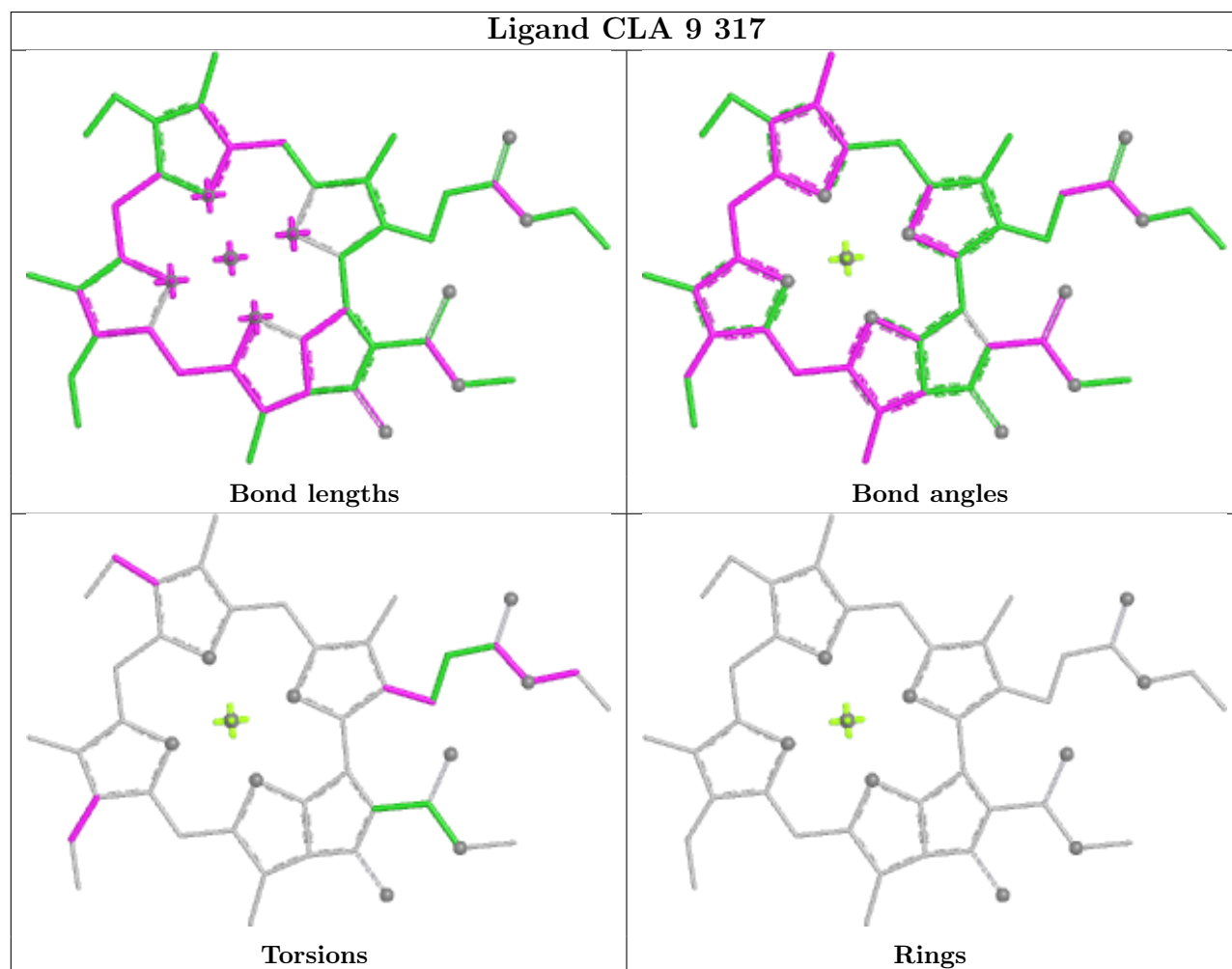
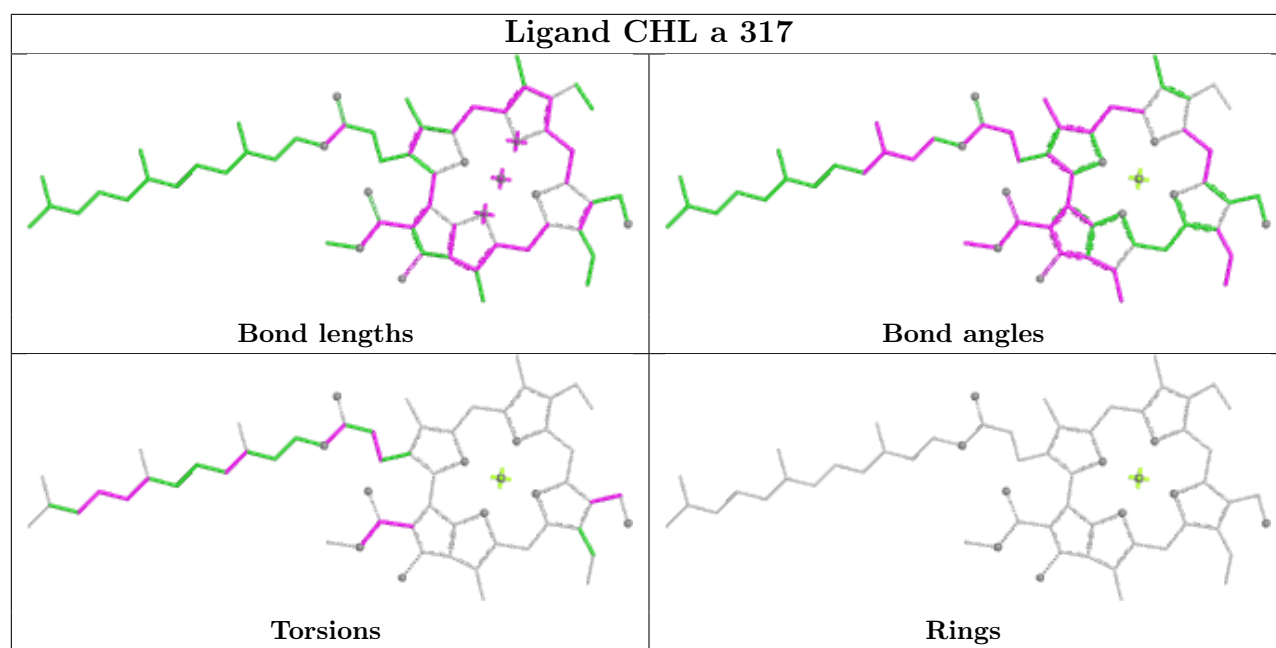
Bond angles



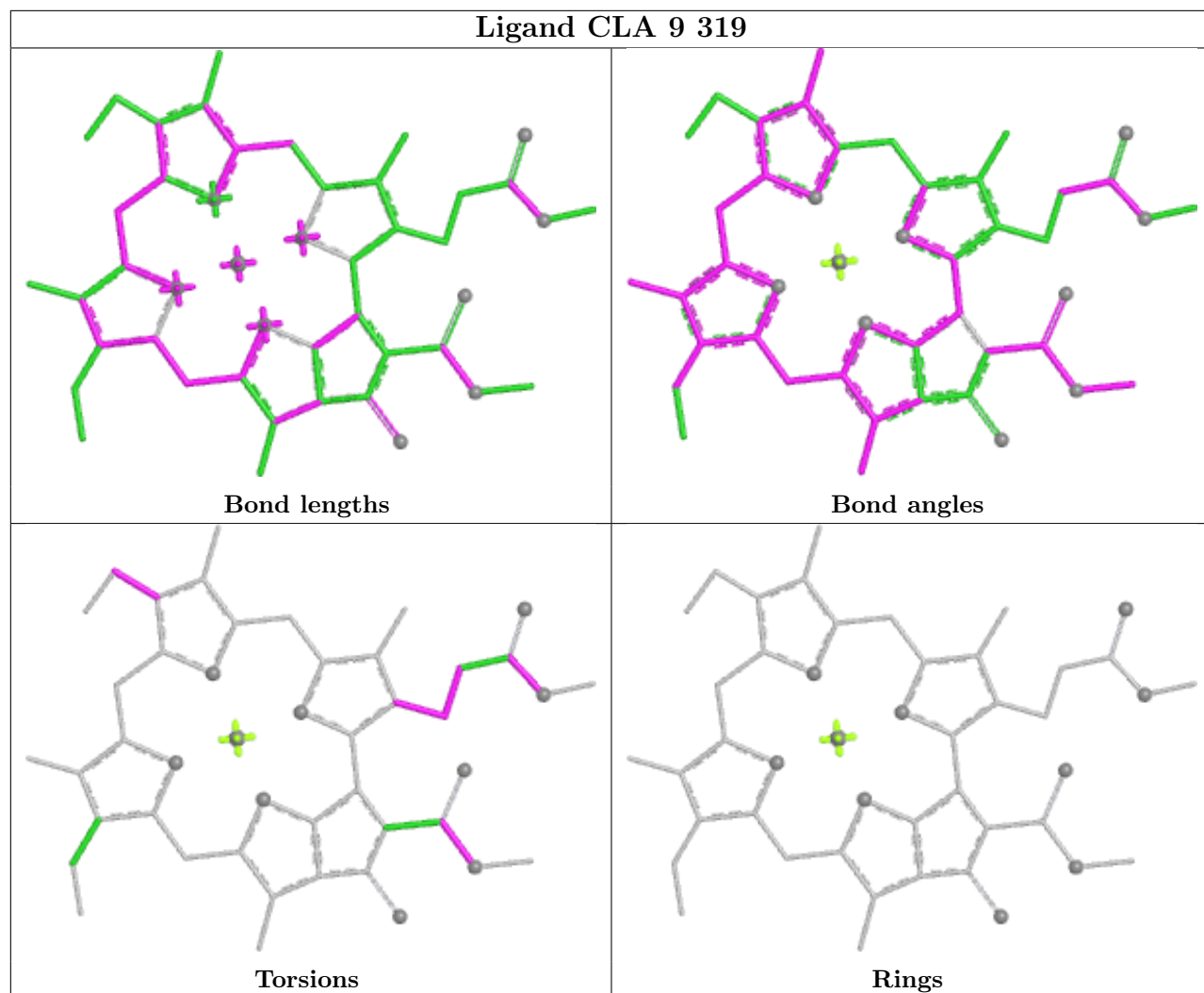
Torsions



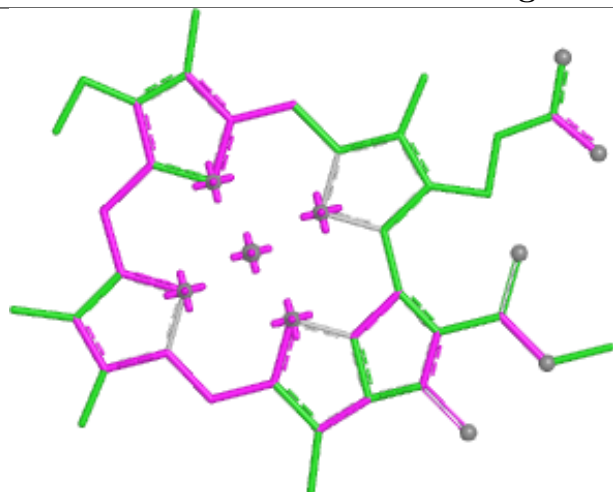
Rings



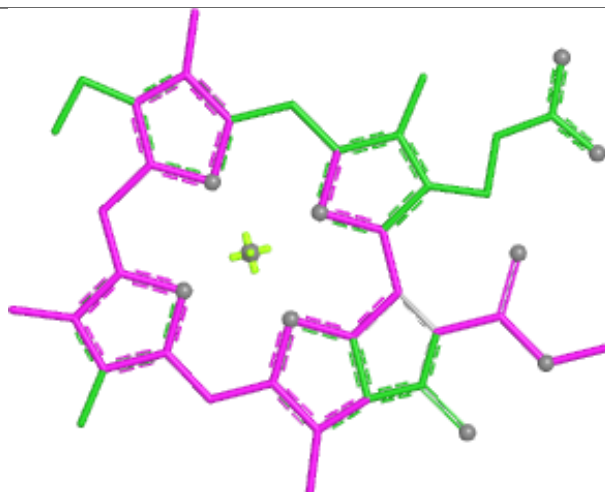
Ligand CLA 9 319



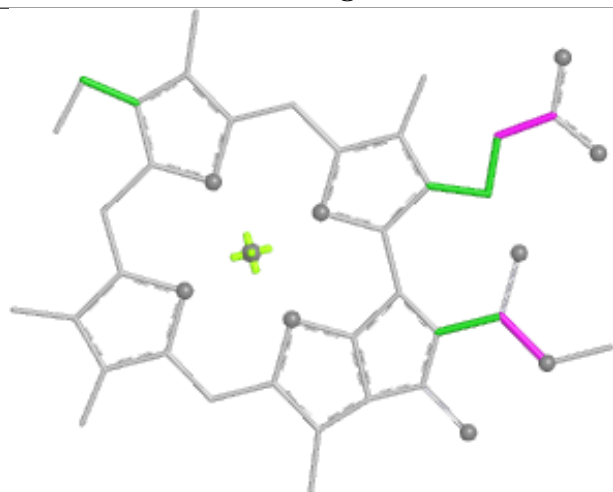
Ligand CLA 7 310



Bond lengths



Bond angles

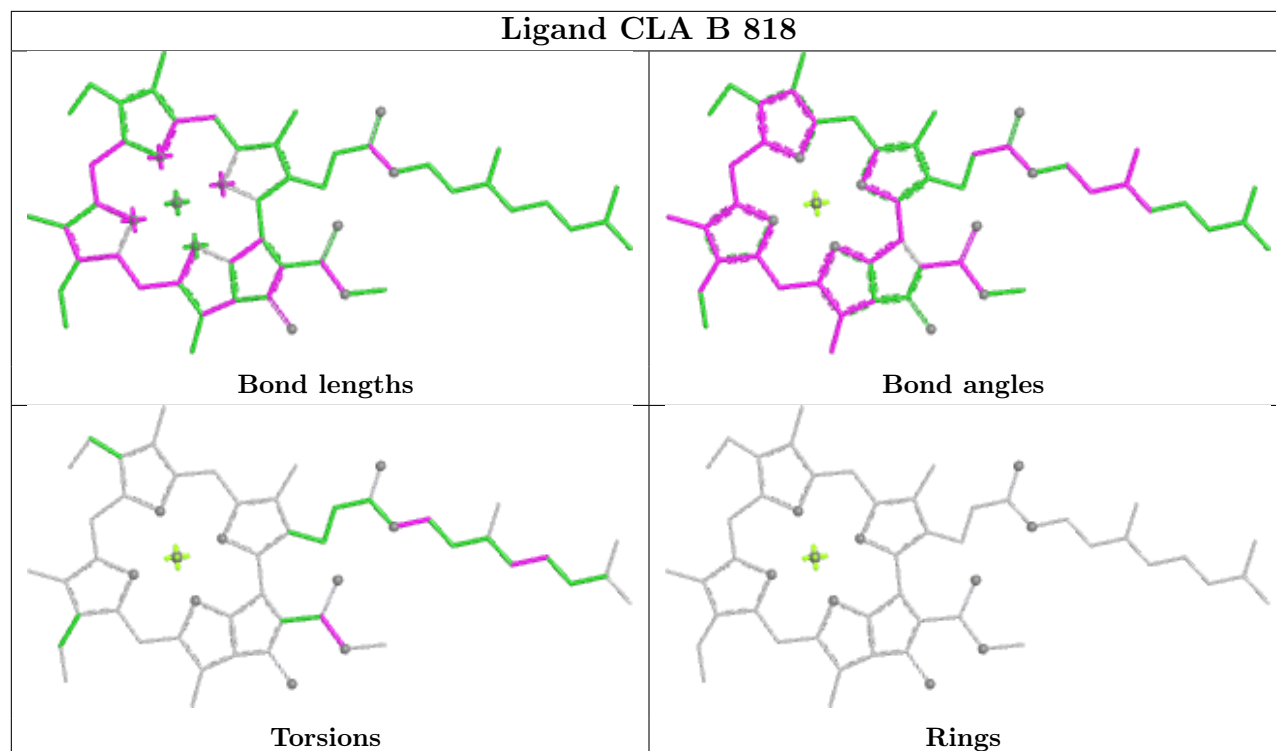


Torsions

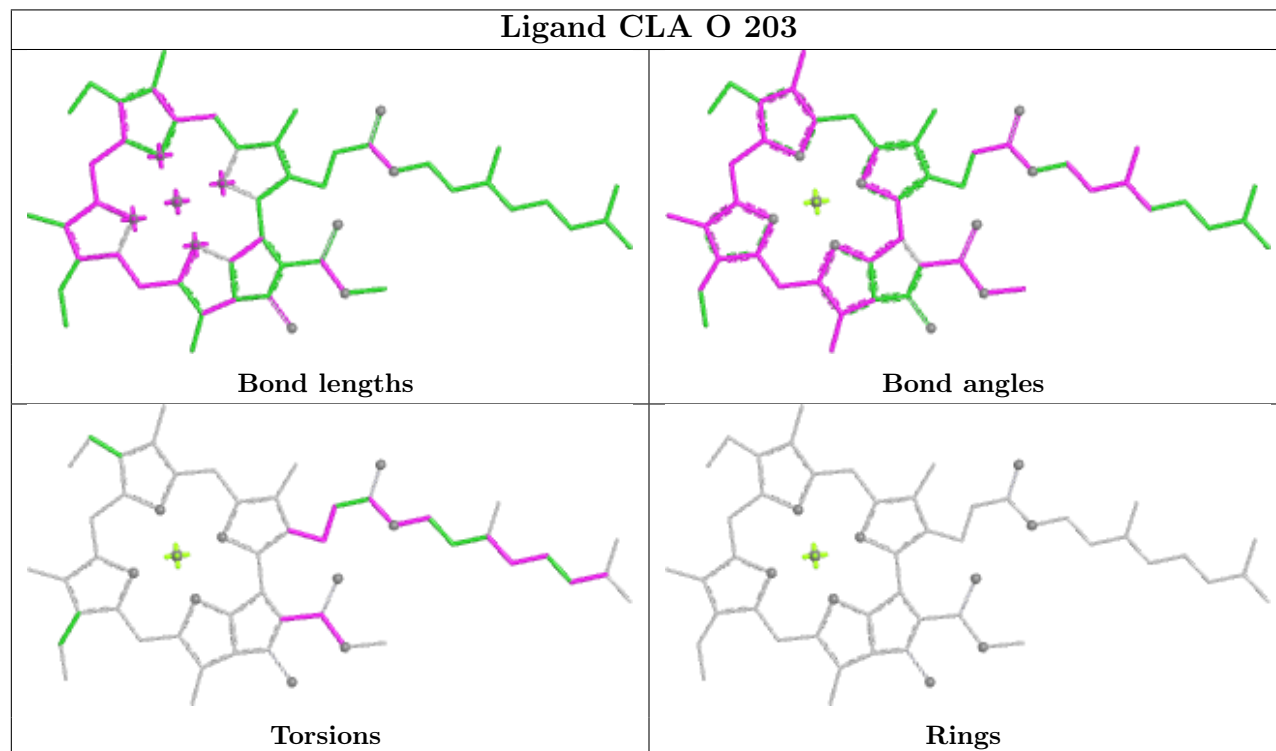


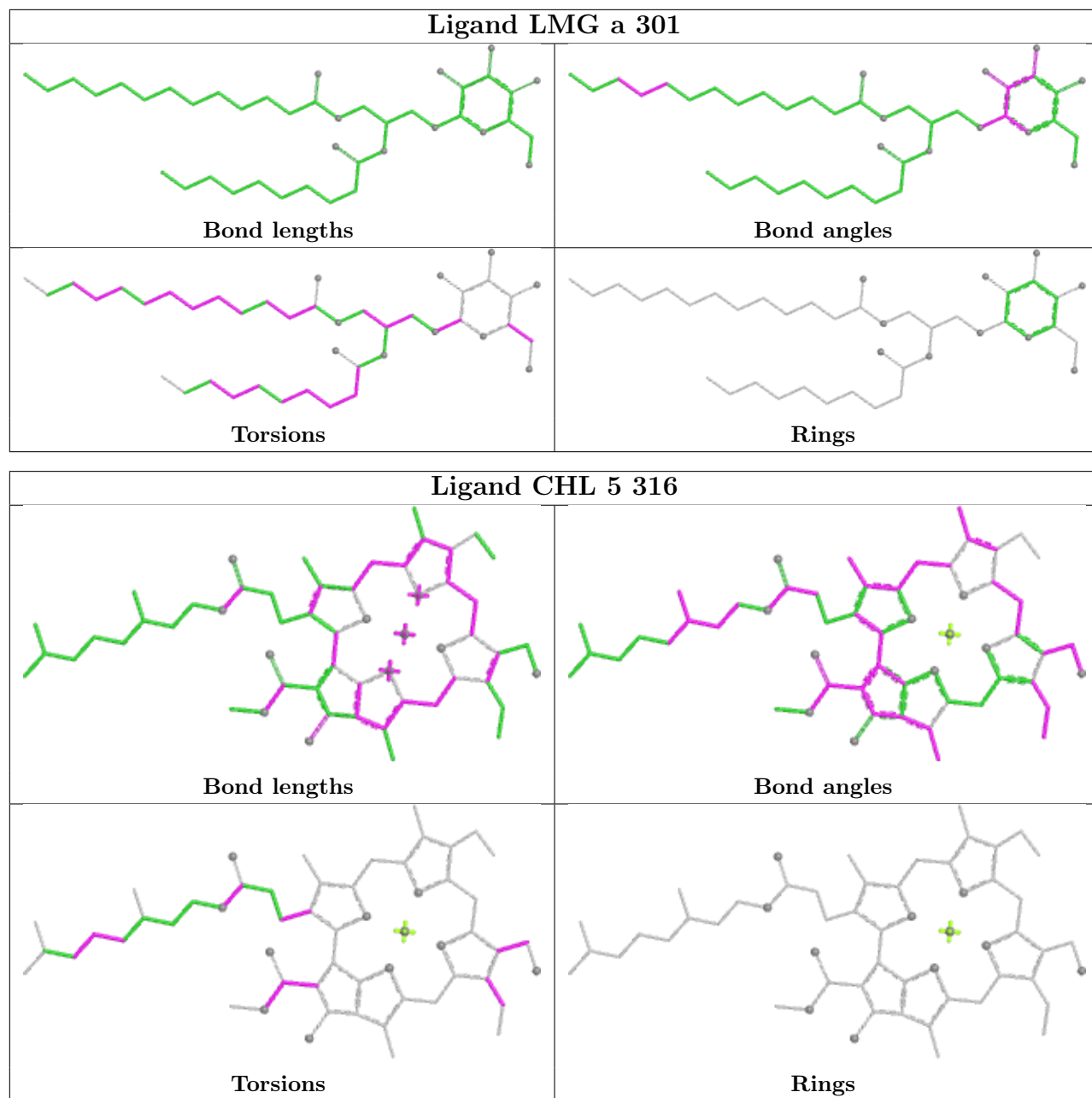
Rings

Ligand CLA B 818

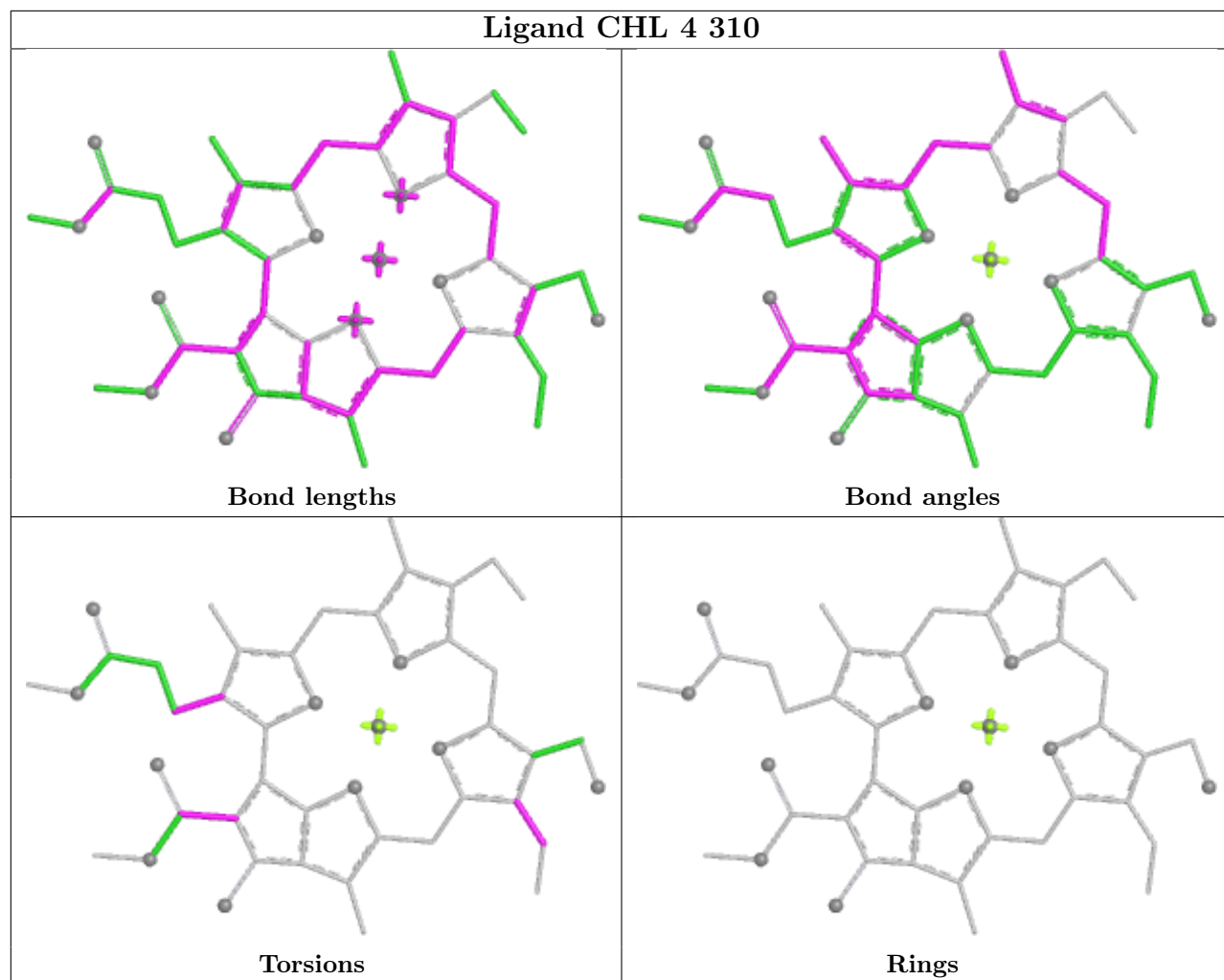


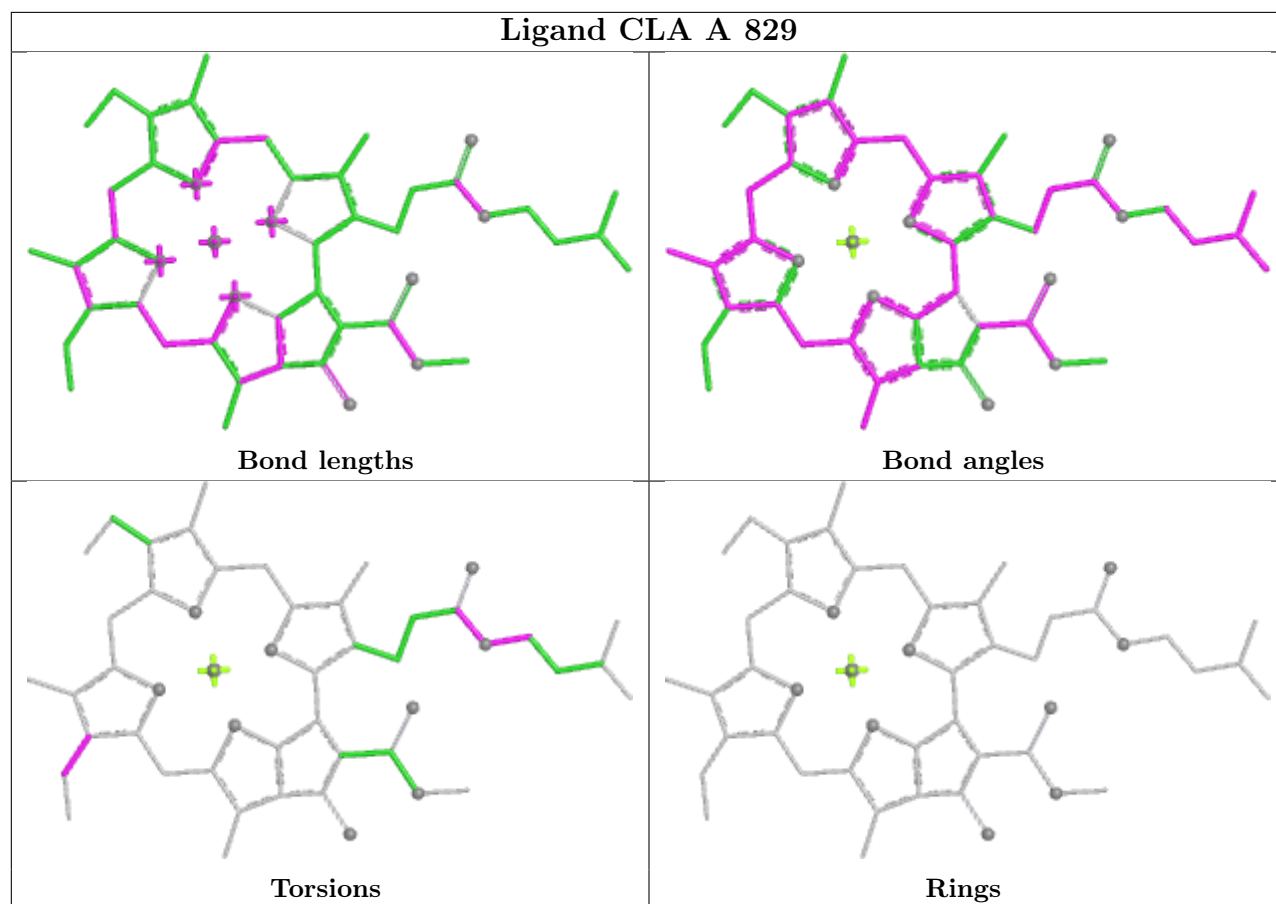
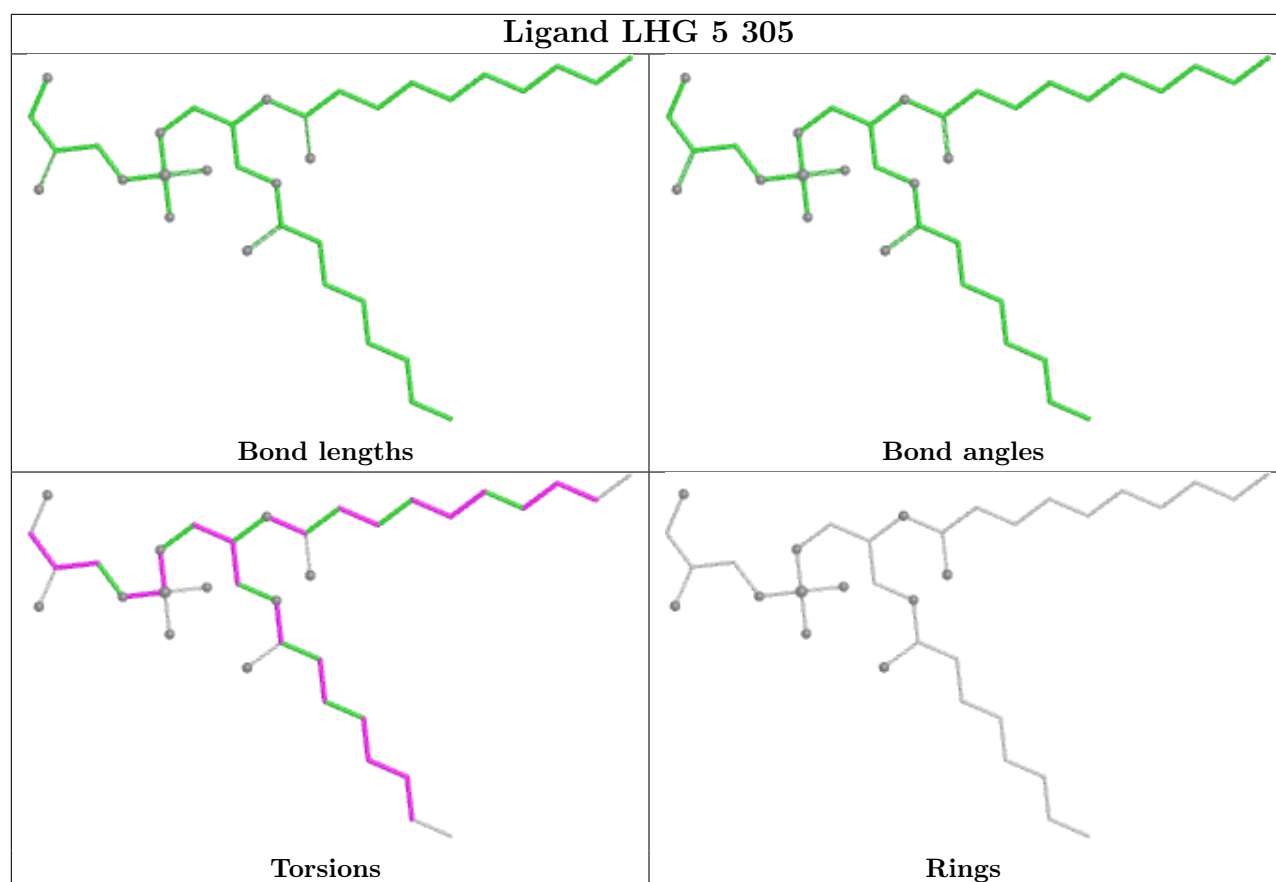
Ligand CLA O 203



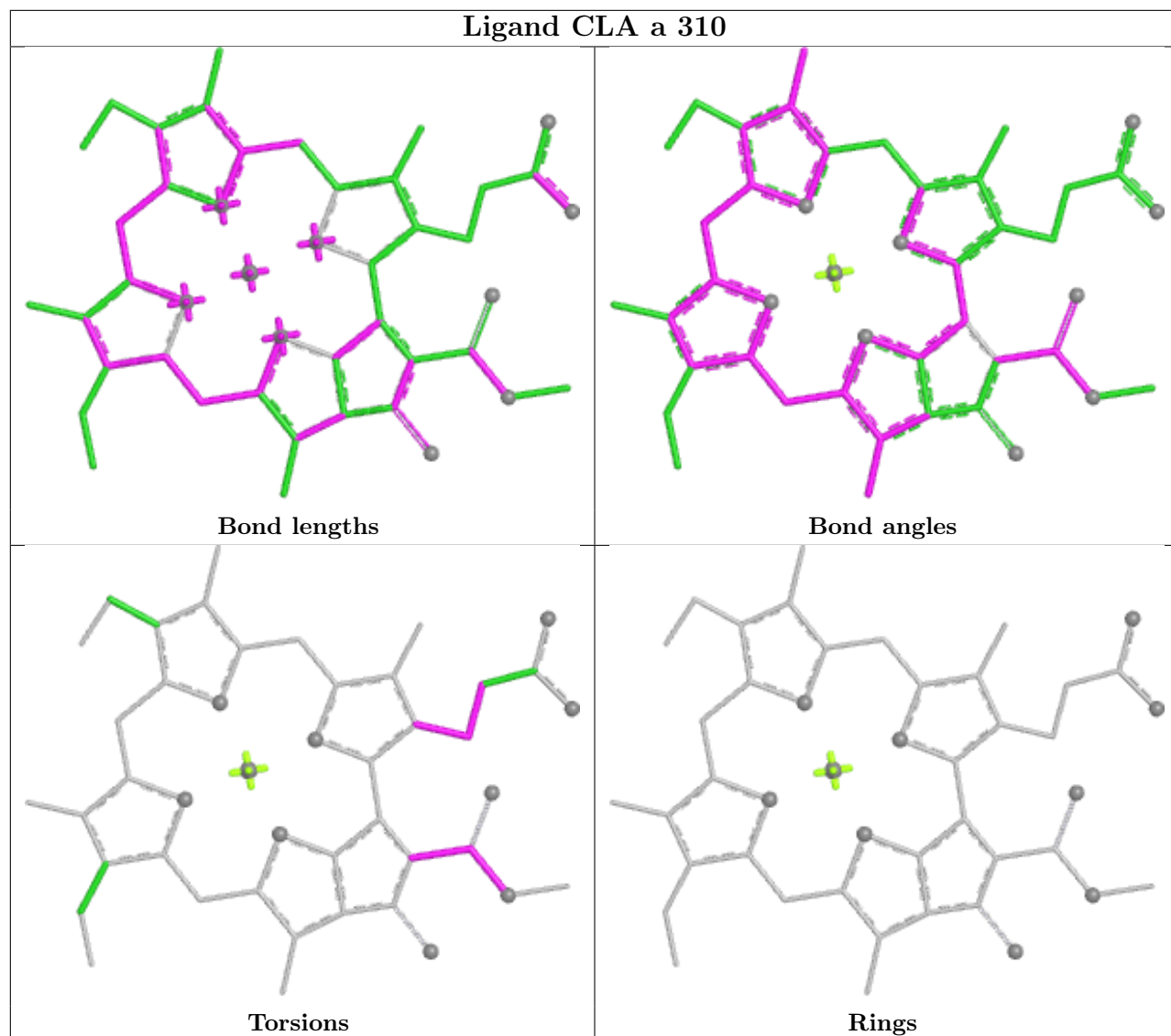


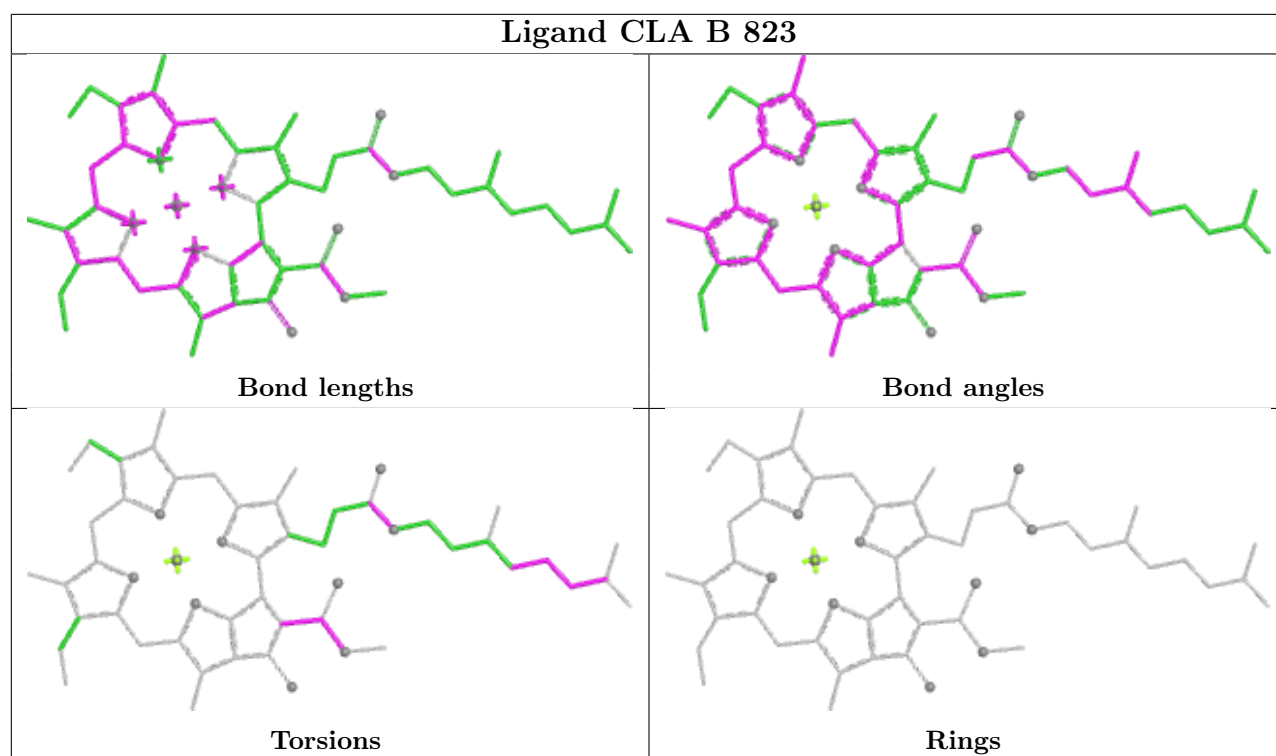
Ligand CHL 4 310



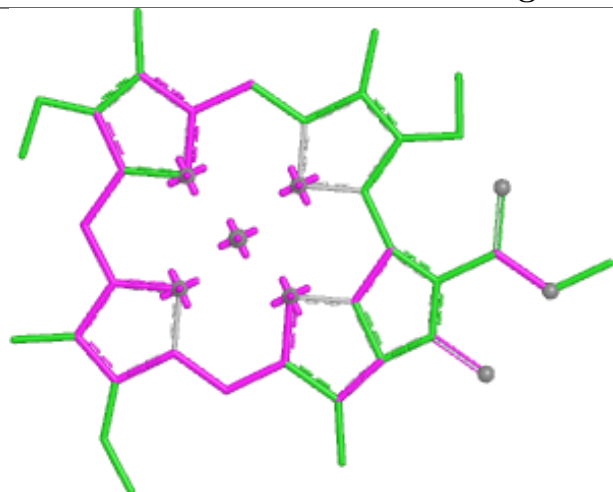


Ligand CLA a 310





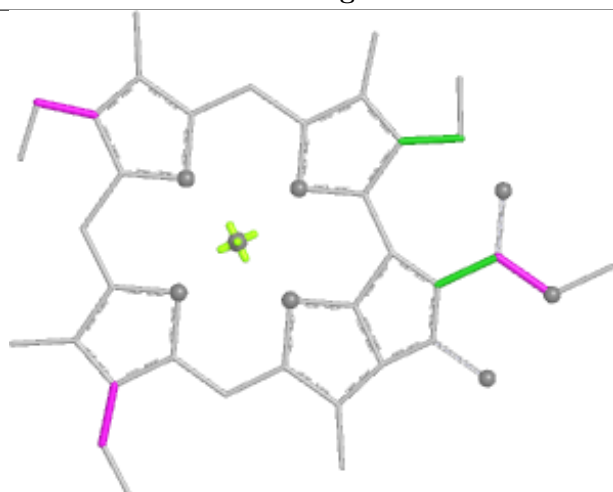
Ligand CLA 4 319



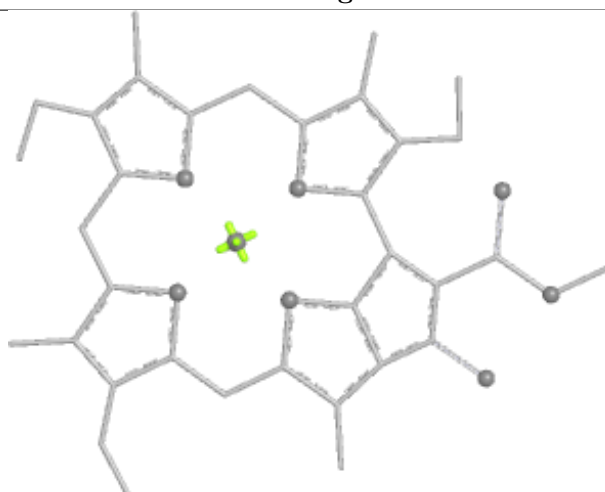
Bond lengths



Bond angles

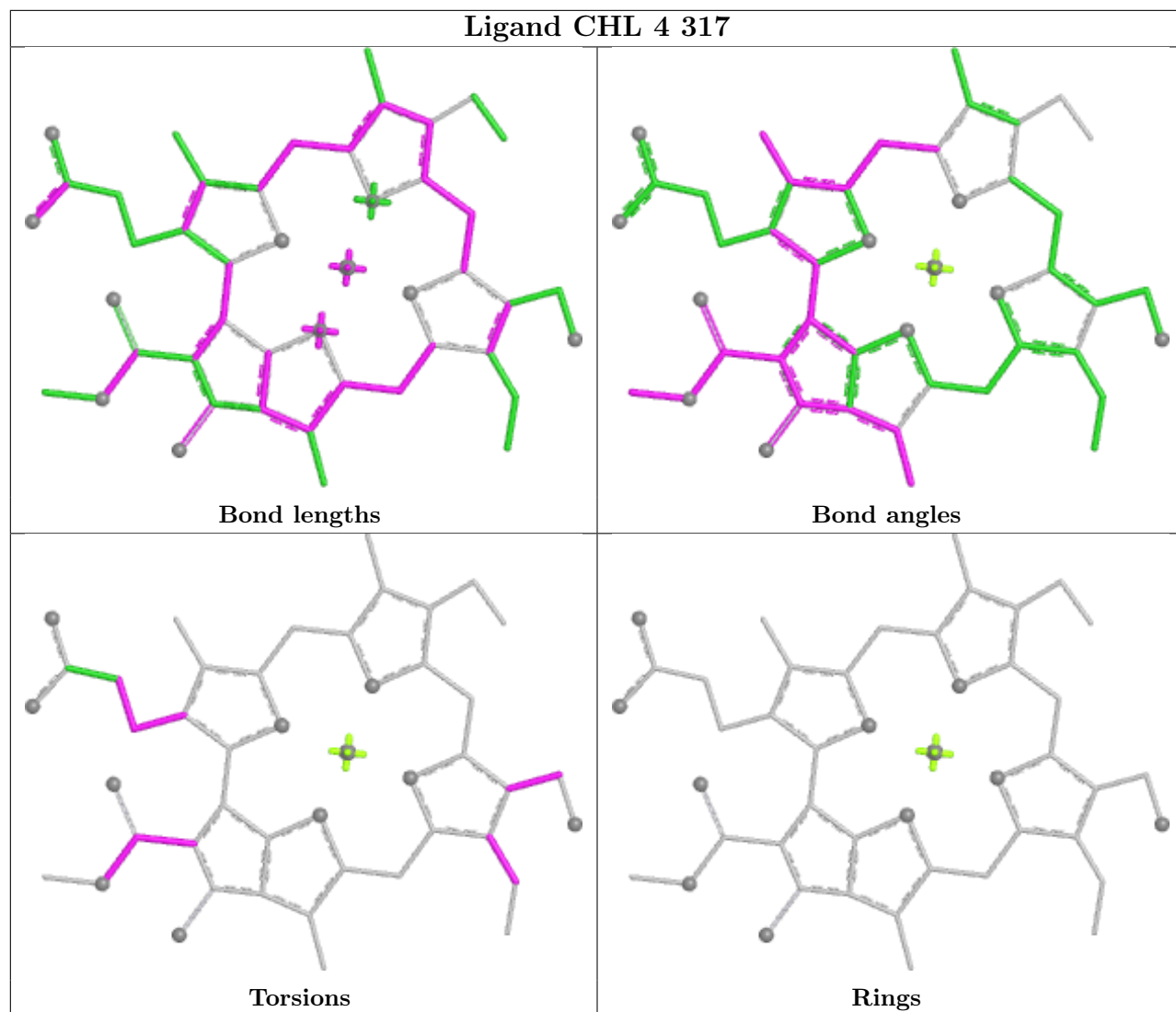


Torsions

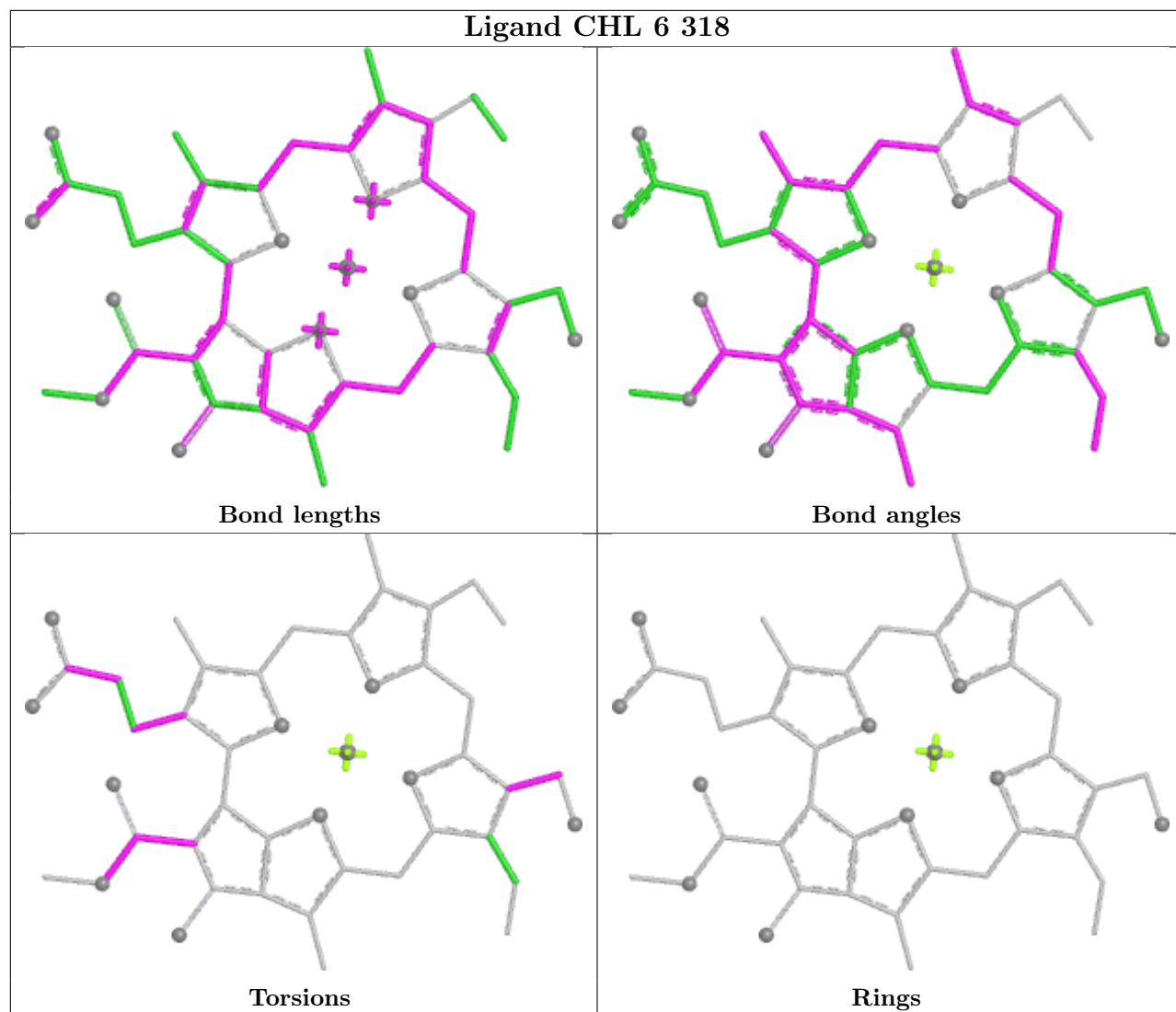


Rings

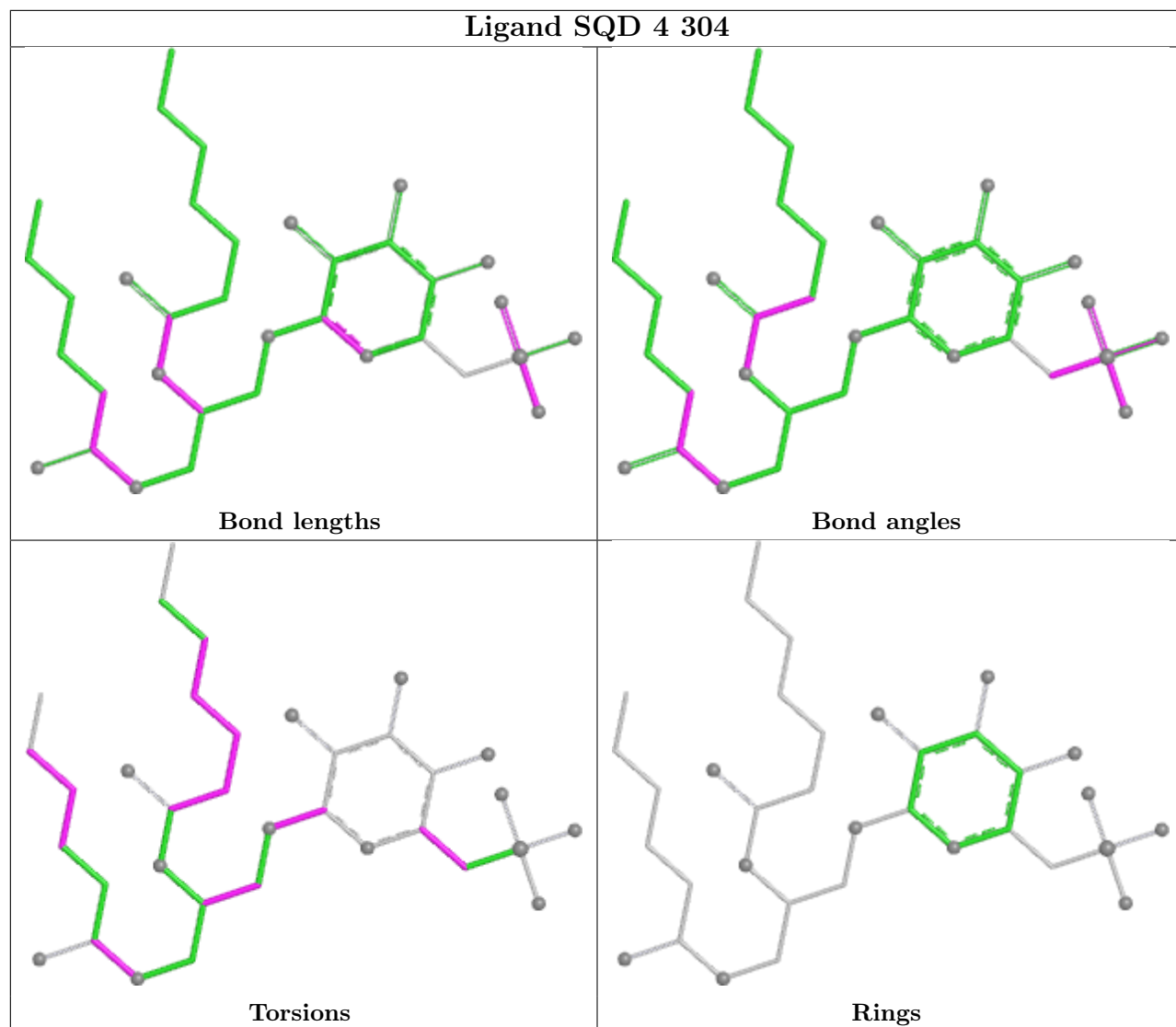
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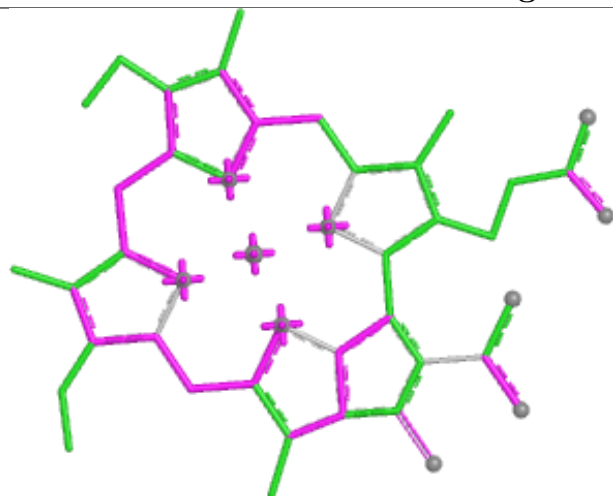
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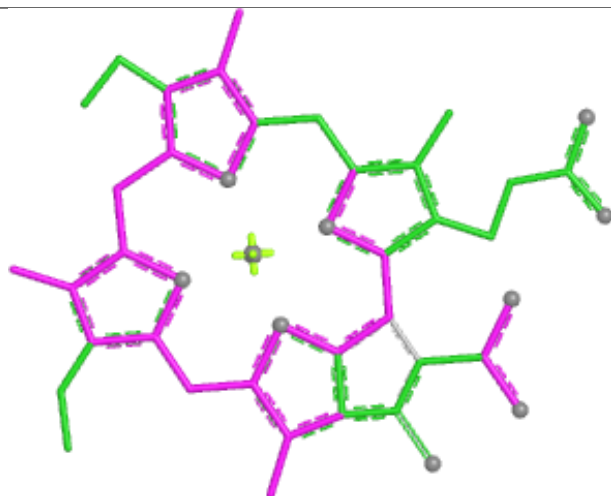
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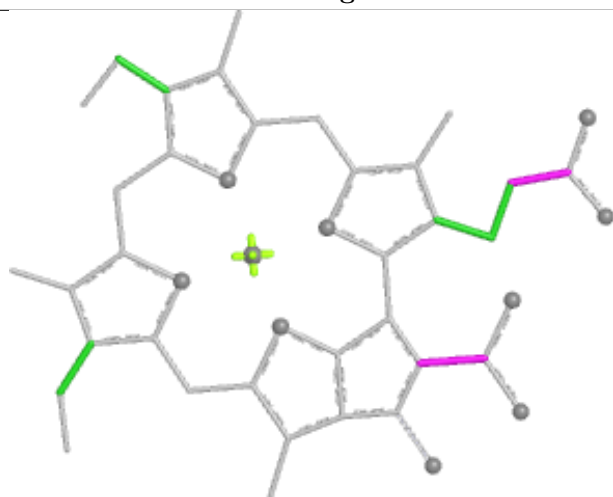
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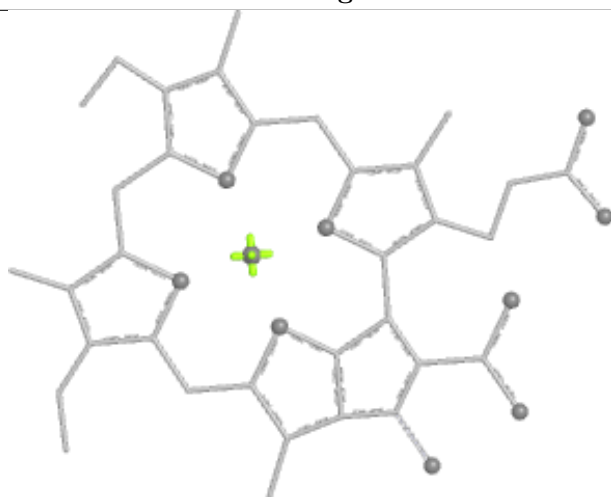
Bond lengths



Bond angles

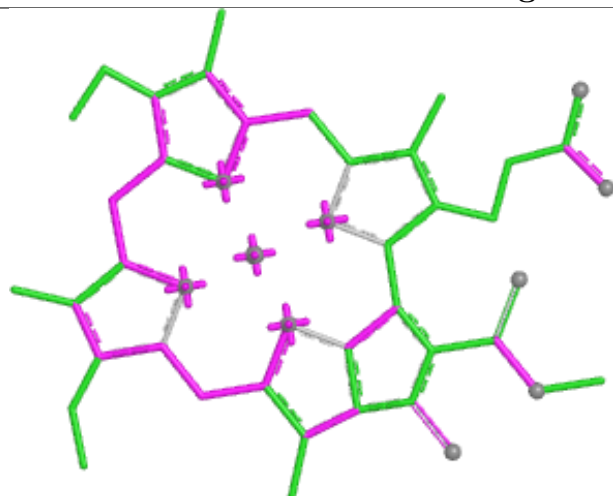


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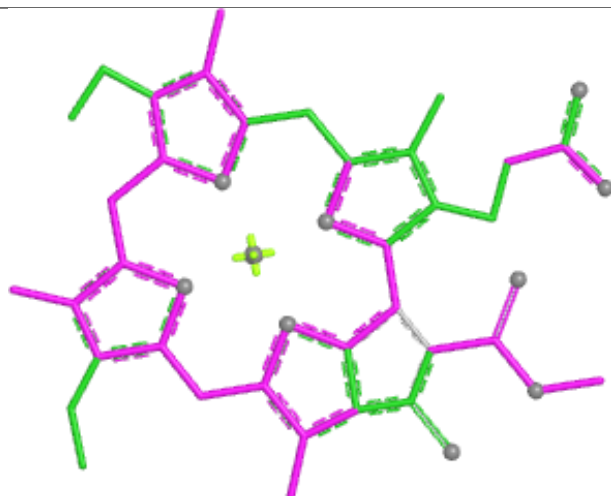


Rings

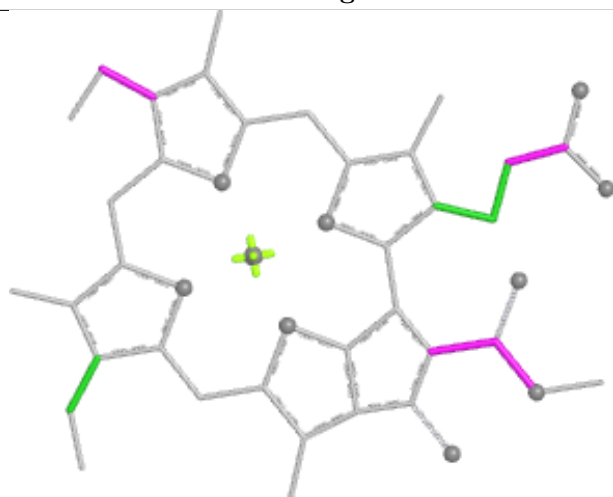
Ligand CLA 2 305



Bond lengths



Bond angles

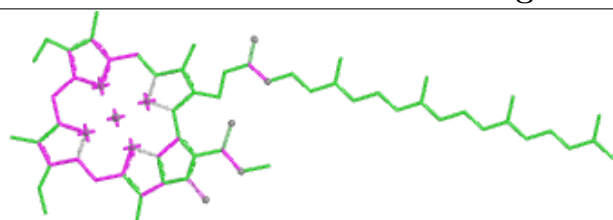


Torsions

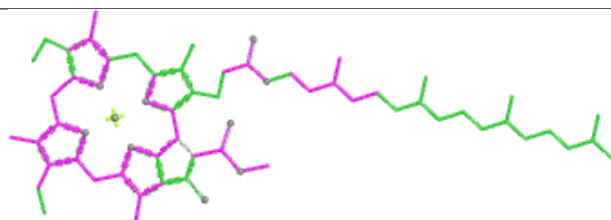


Rings

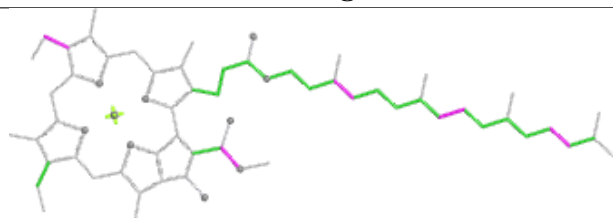
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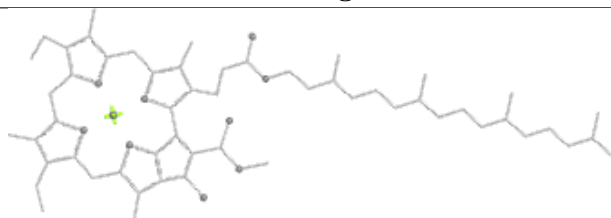
Bond lengths



Bond angles

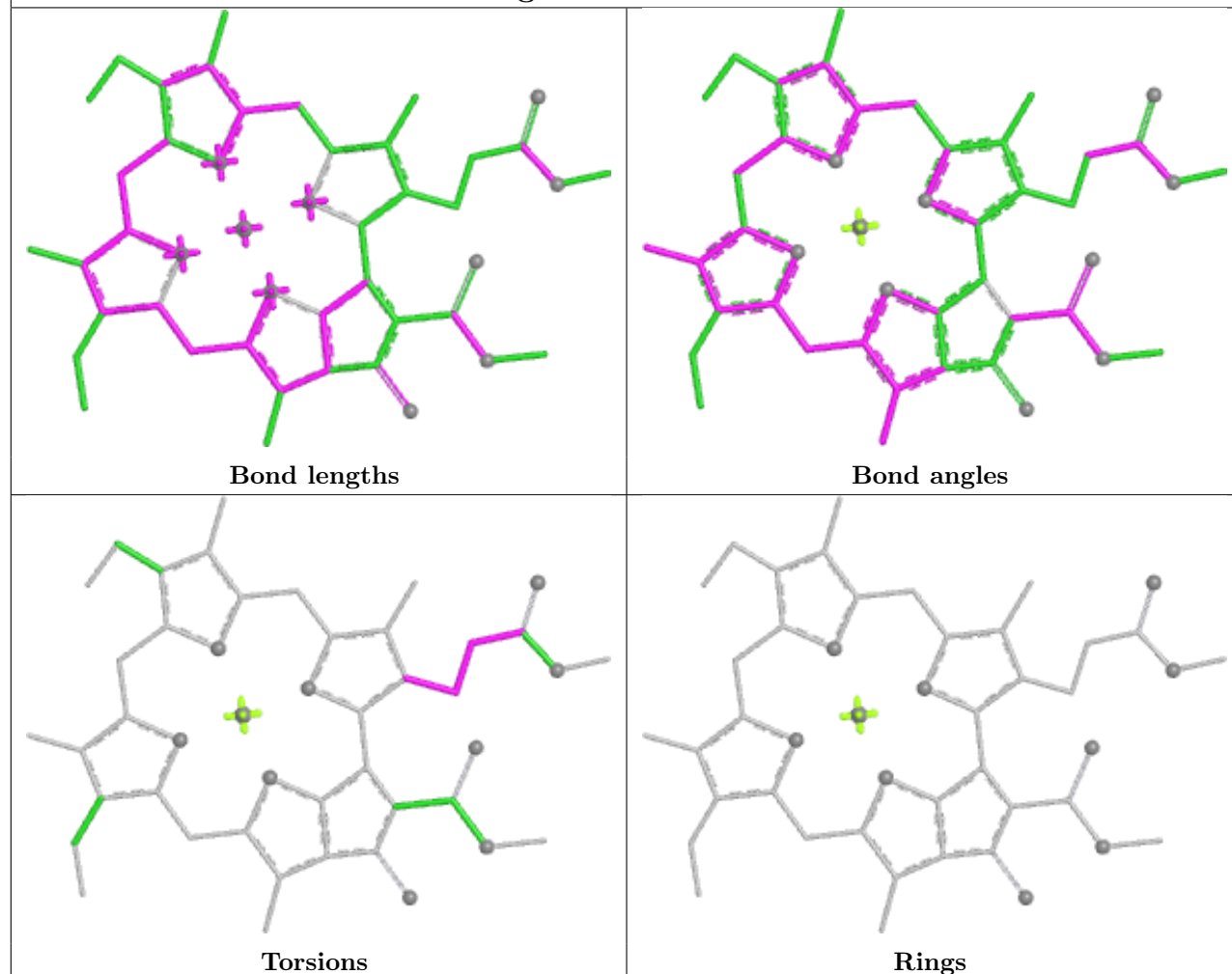


Torsions

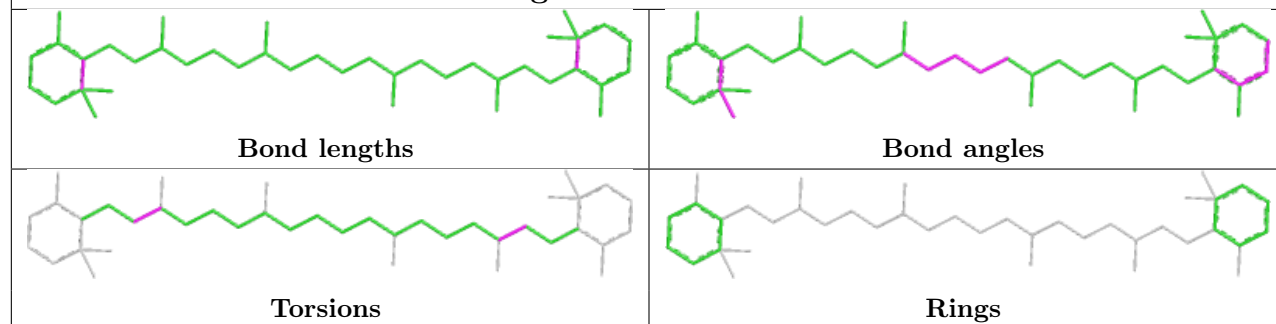


Rings

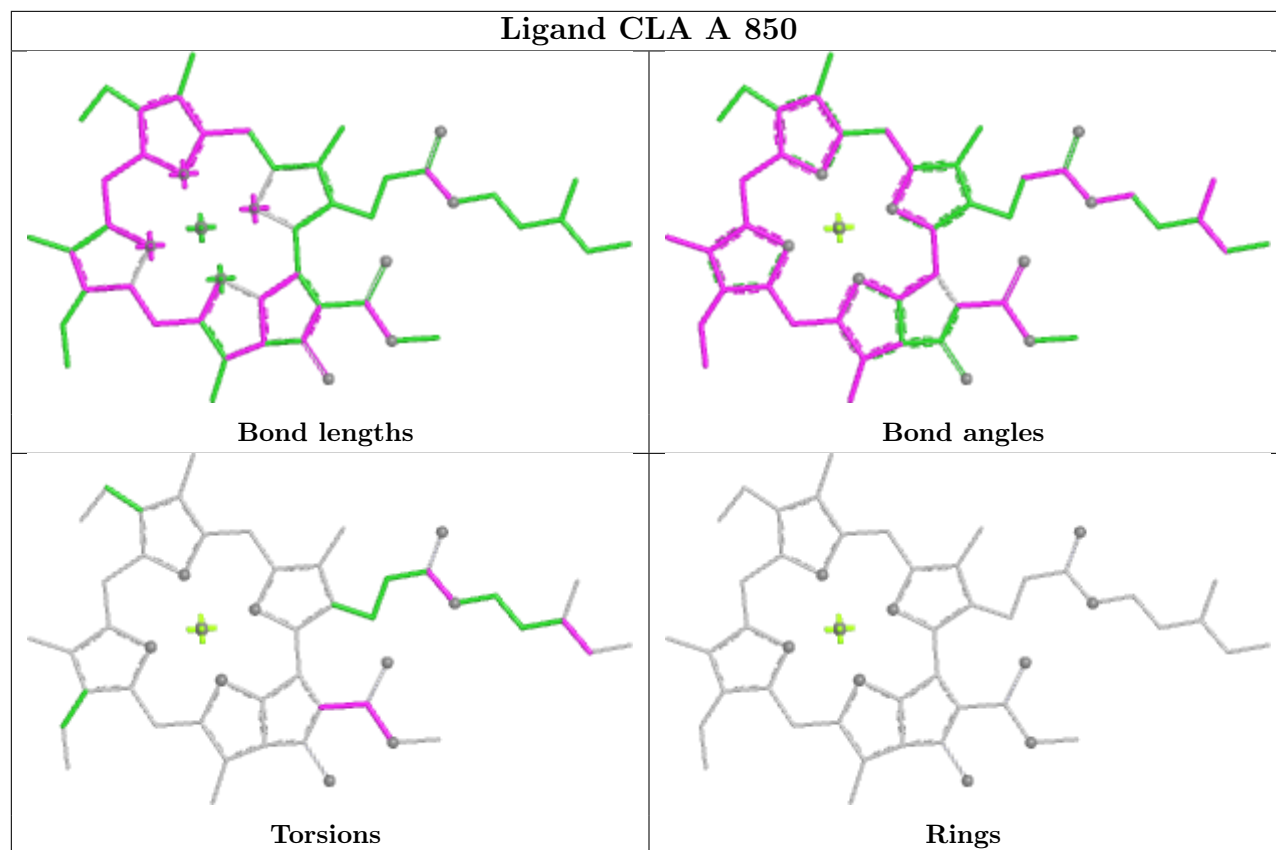
Ligand CLA 6 306



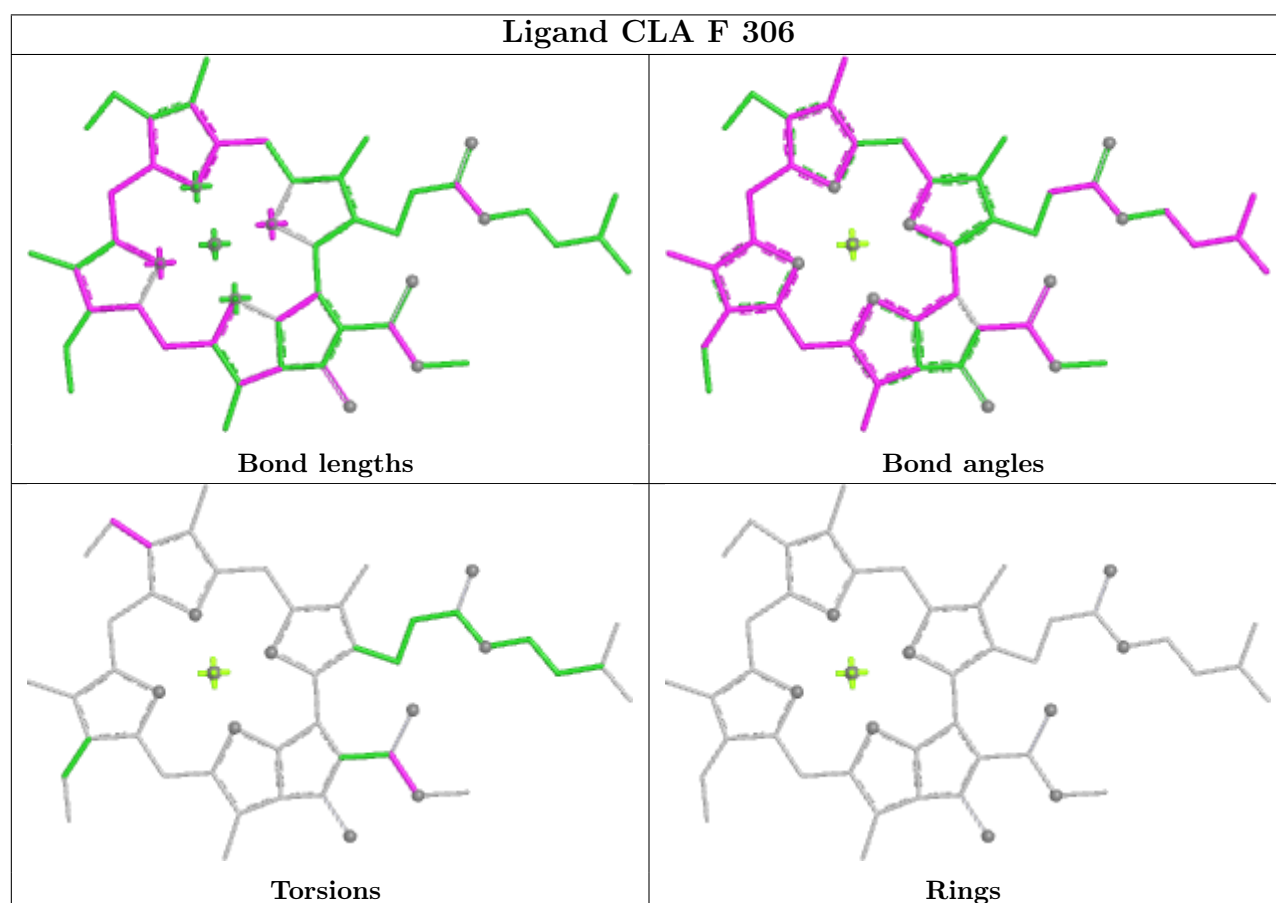
Ligand BCR B 802



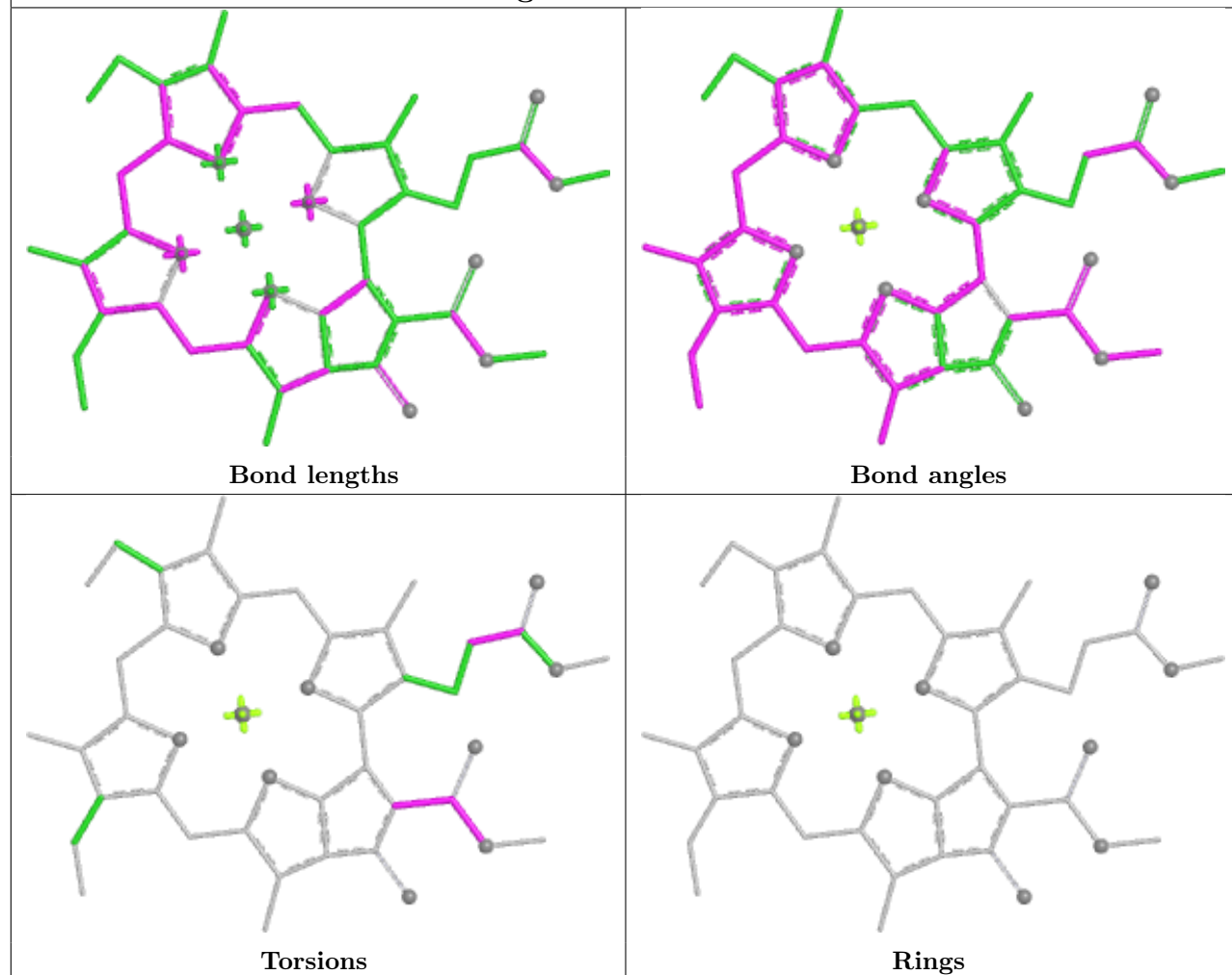
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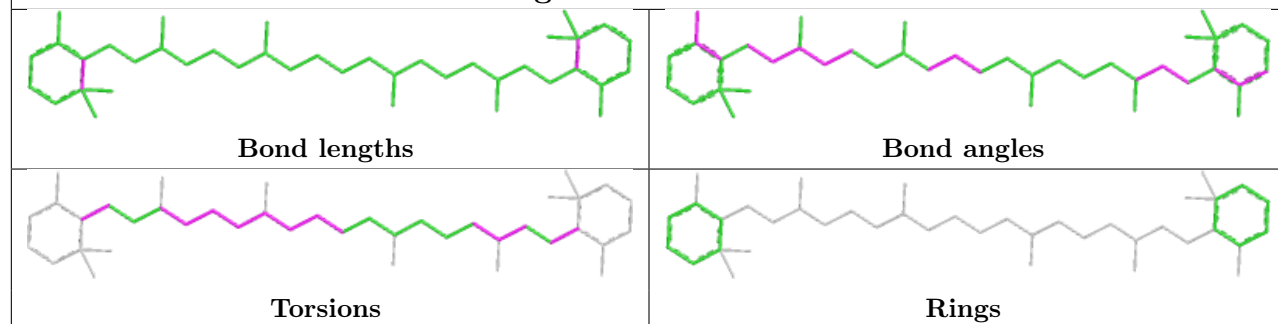
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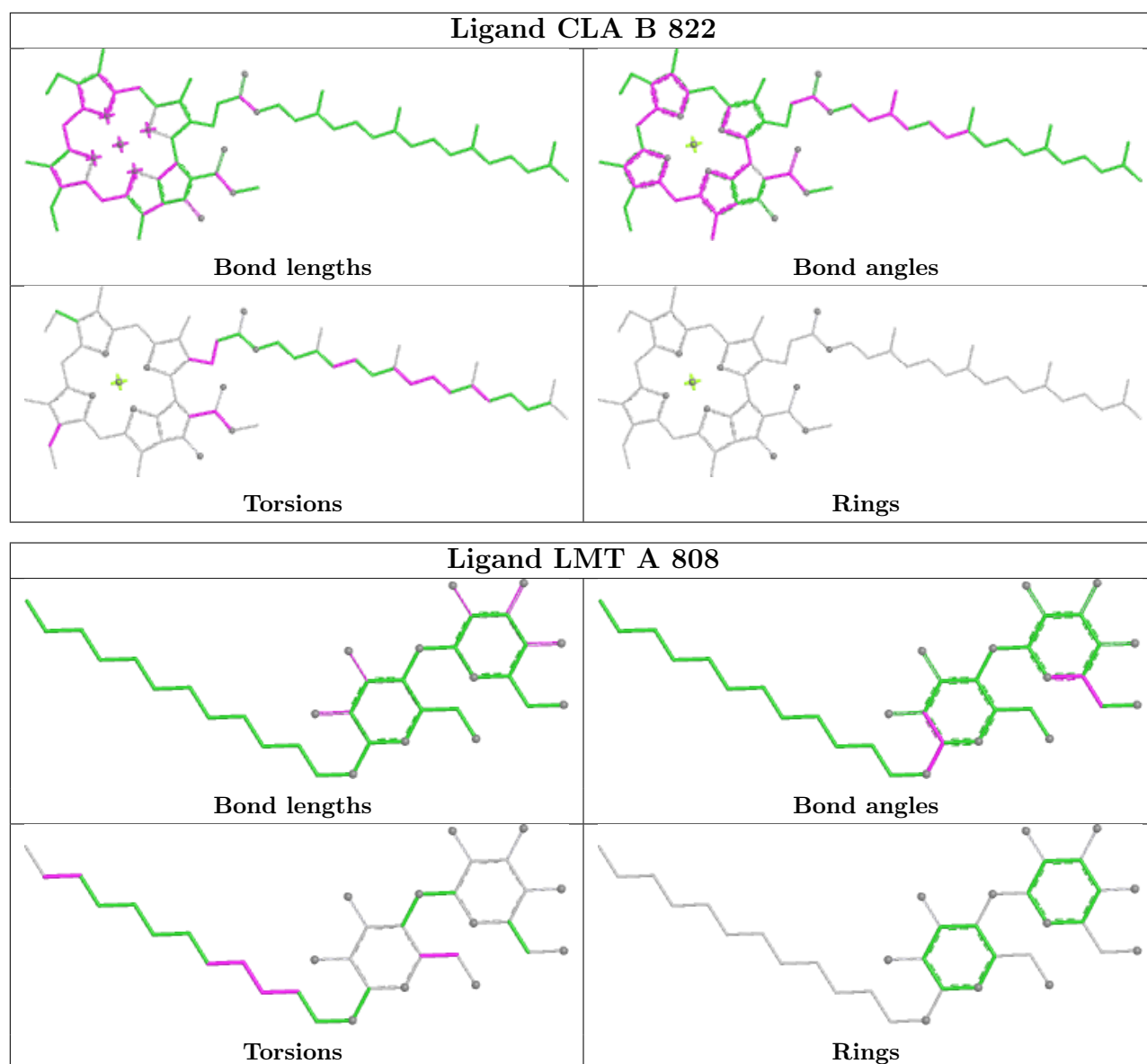


Ligand CLA 5 311

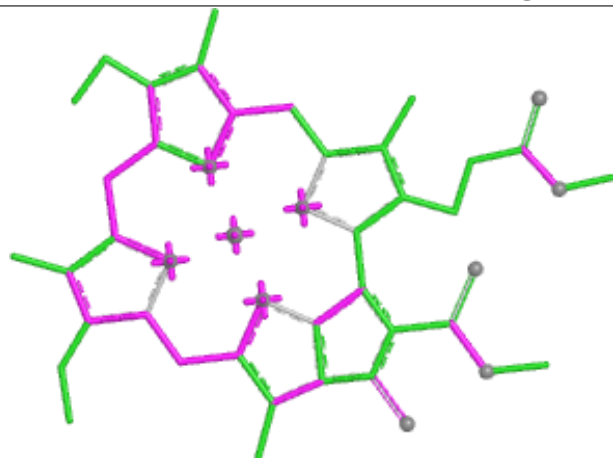


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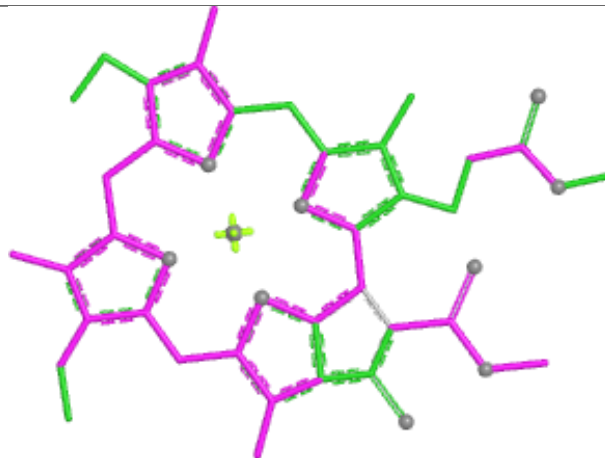




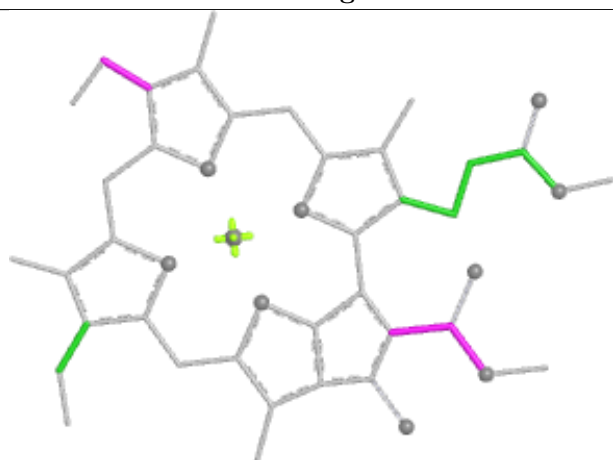
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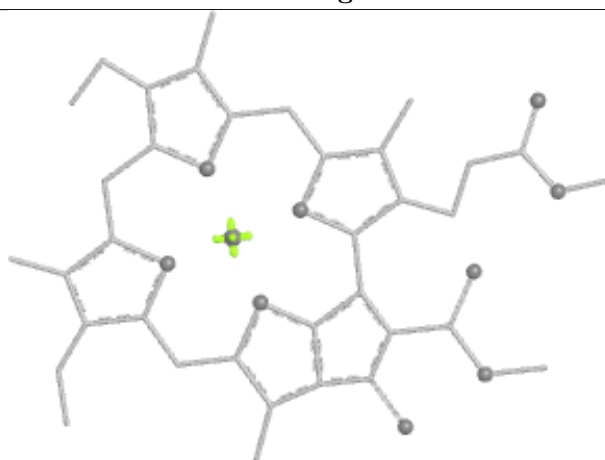
Bond lengths



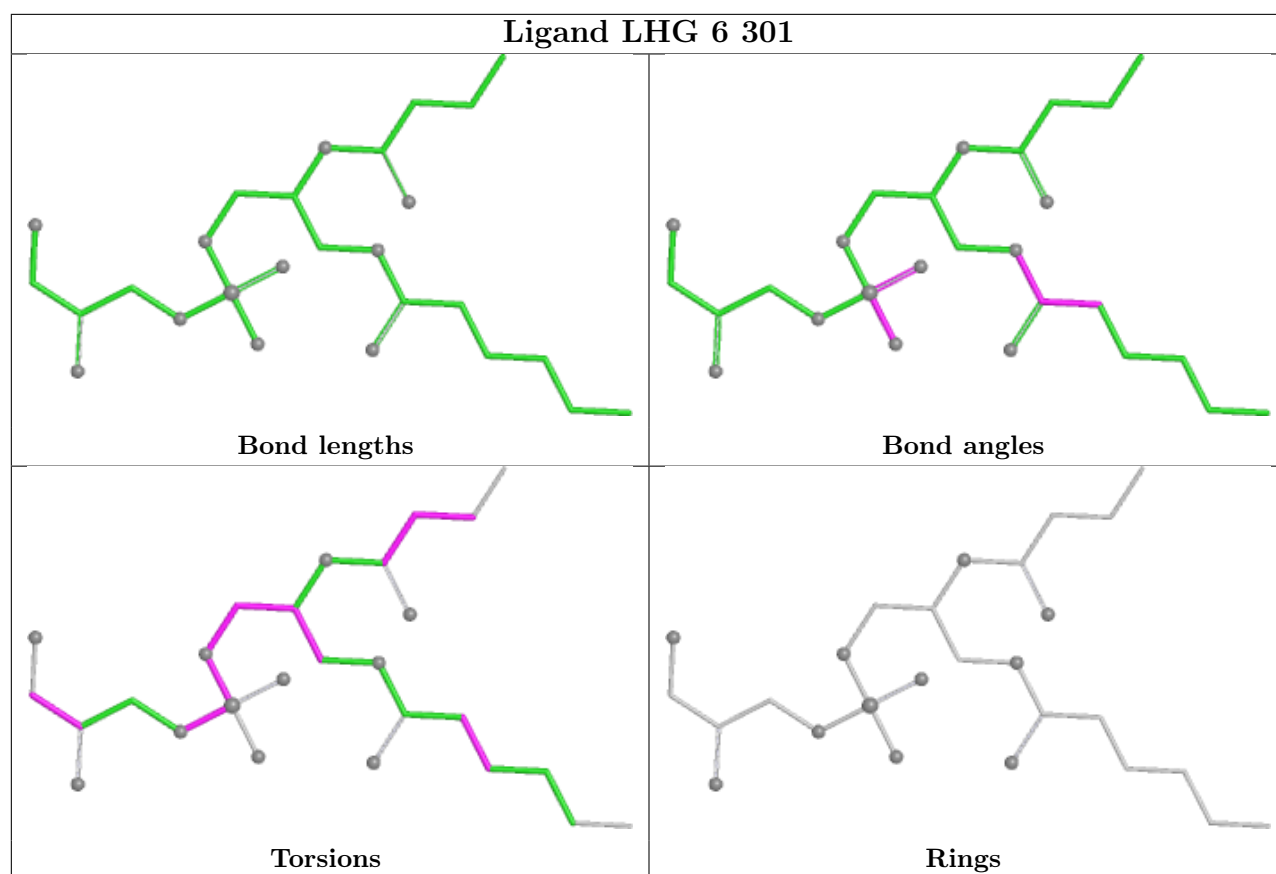
Bond angles



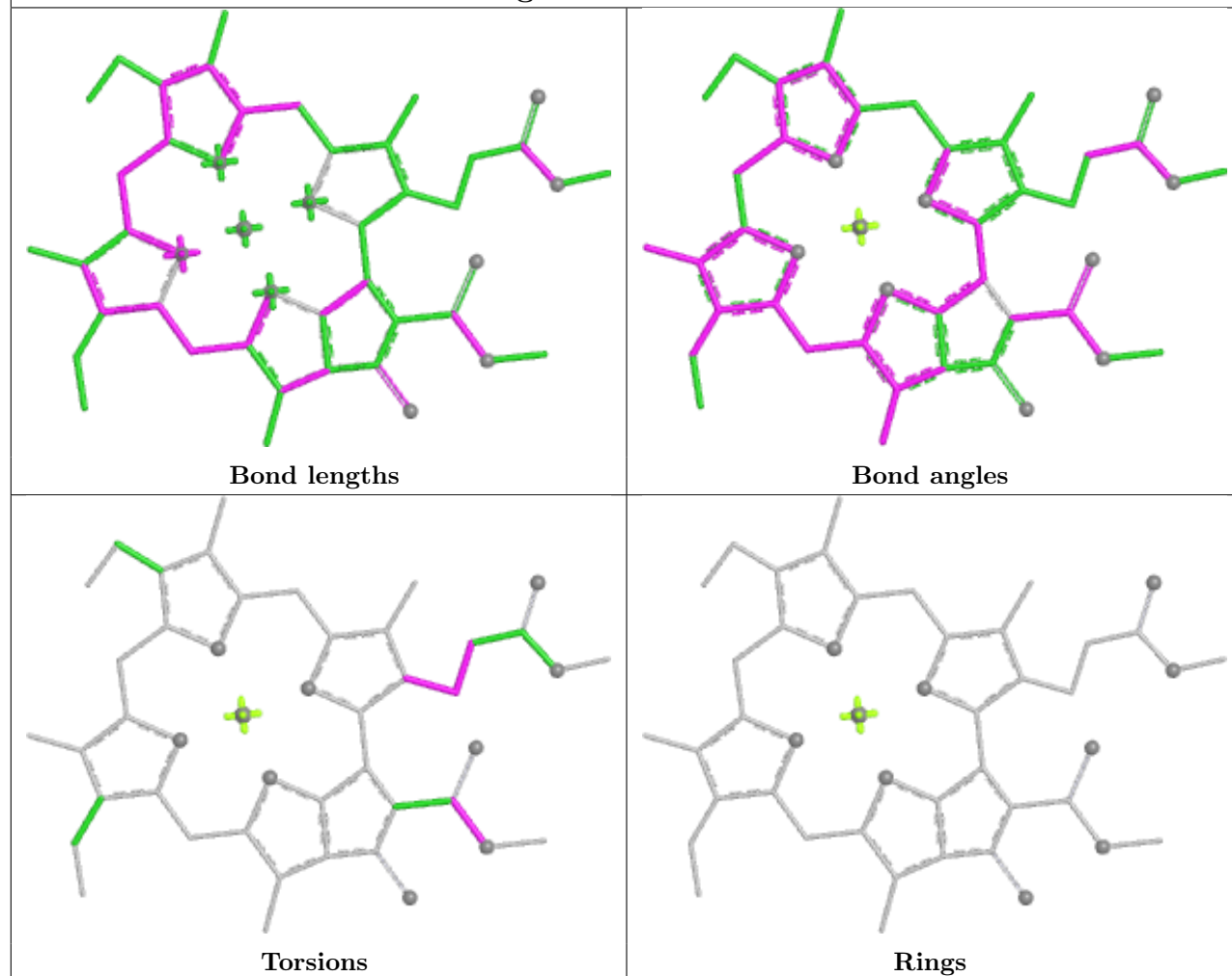
Torsions



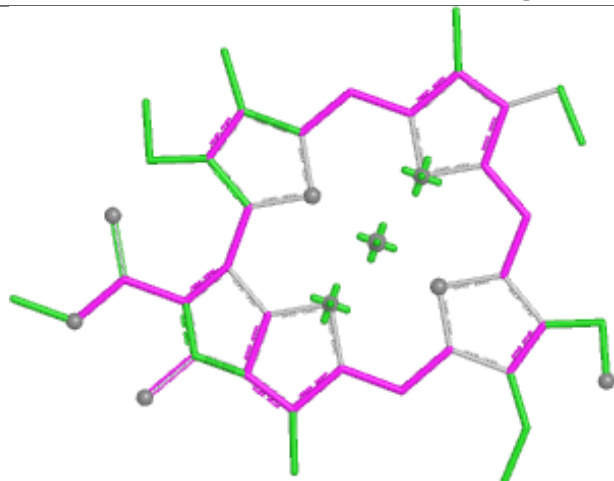
Rings



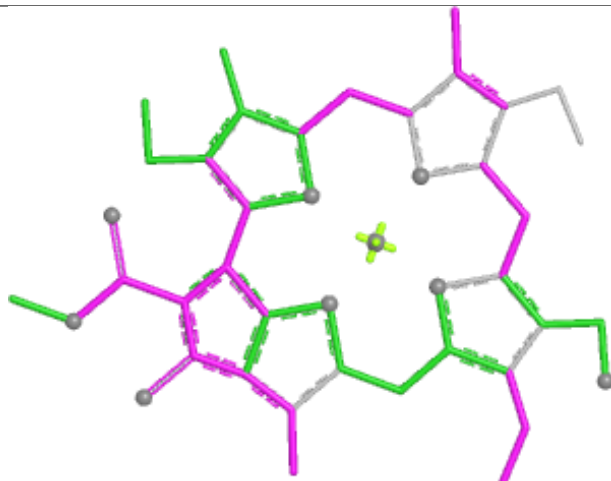
Ligand CLA b 310



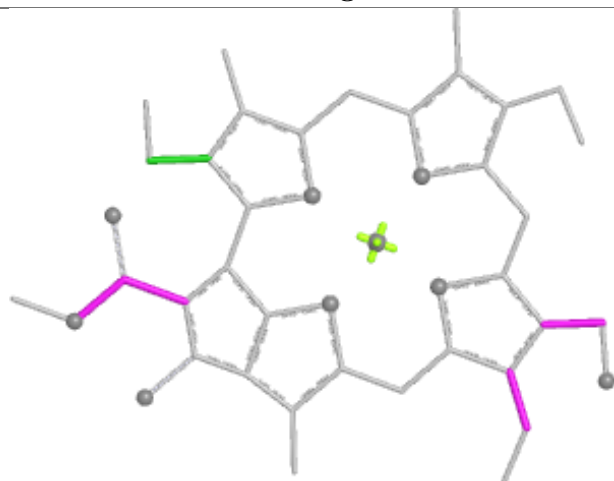
Ligand CHL 6 321



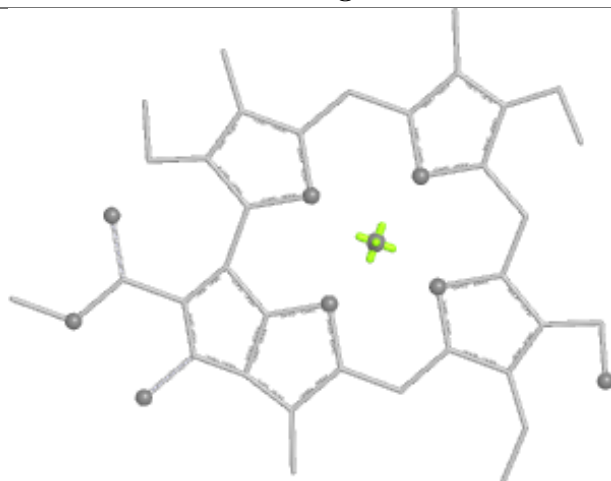
Bond lengths



Bond angles

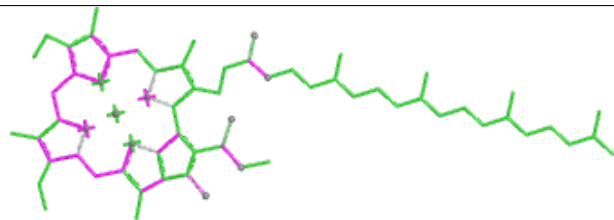


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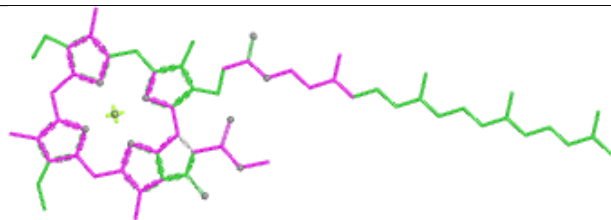


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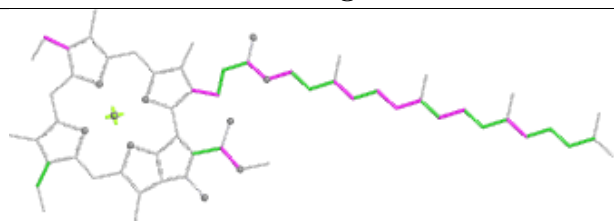
Ligand CLA 3 309



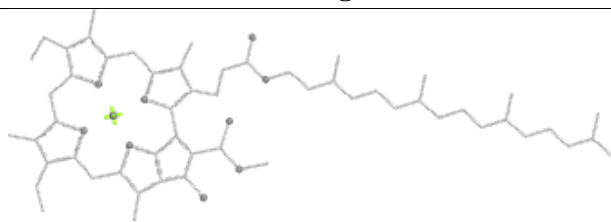
Bond lengths



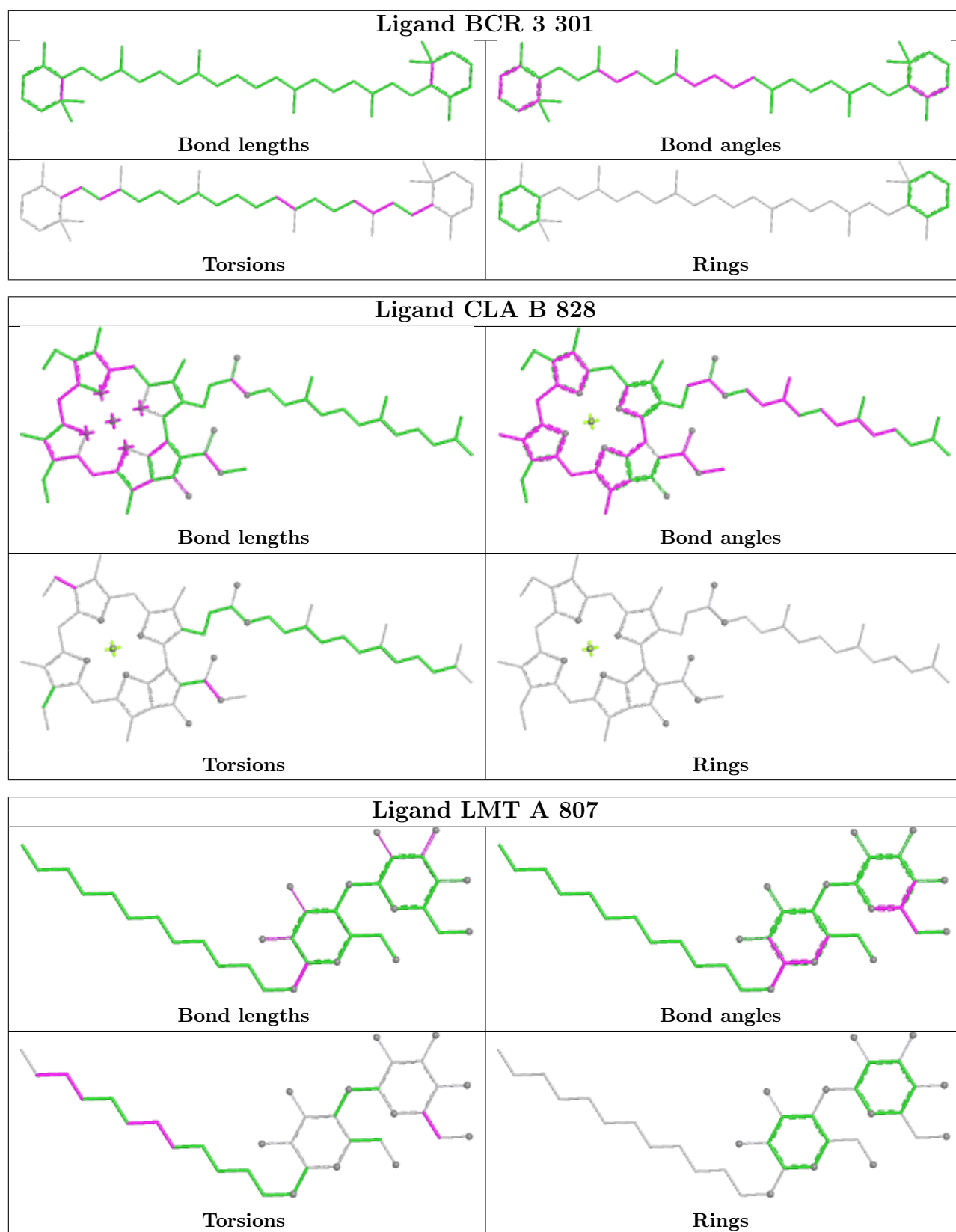
Bond angles

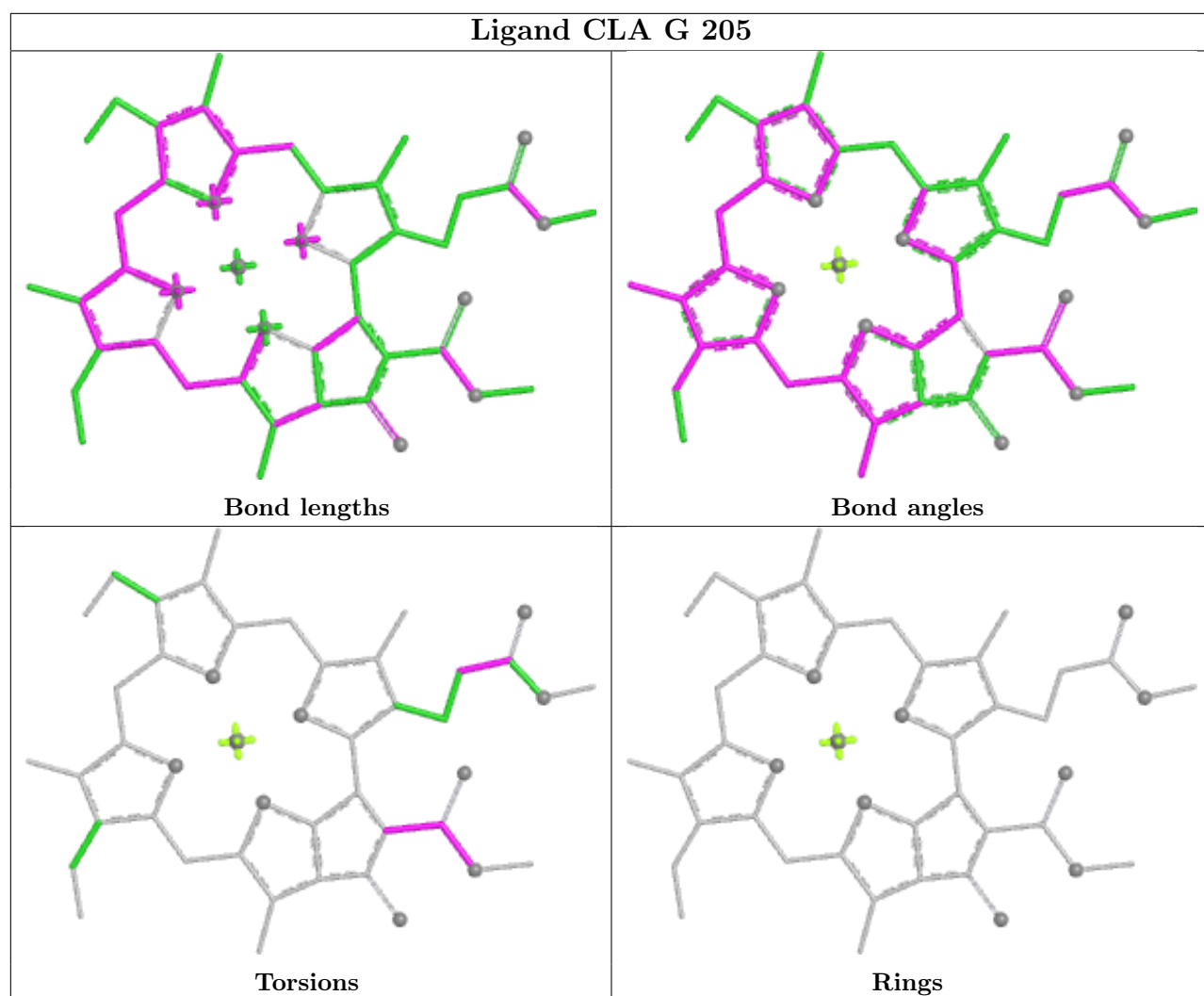


Torsions

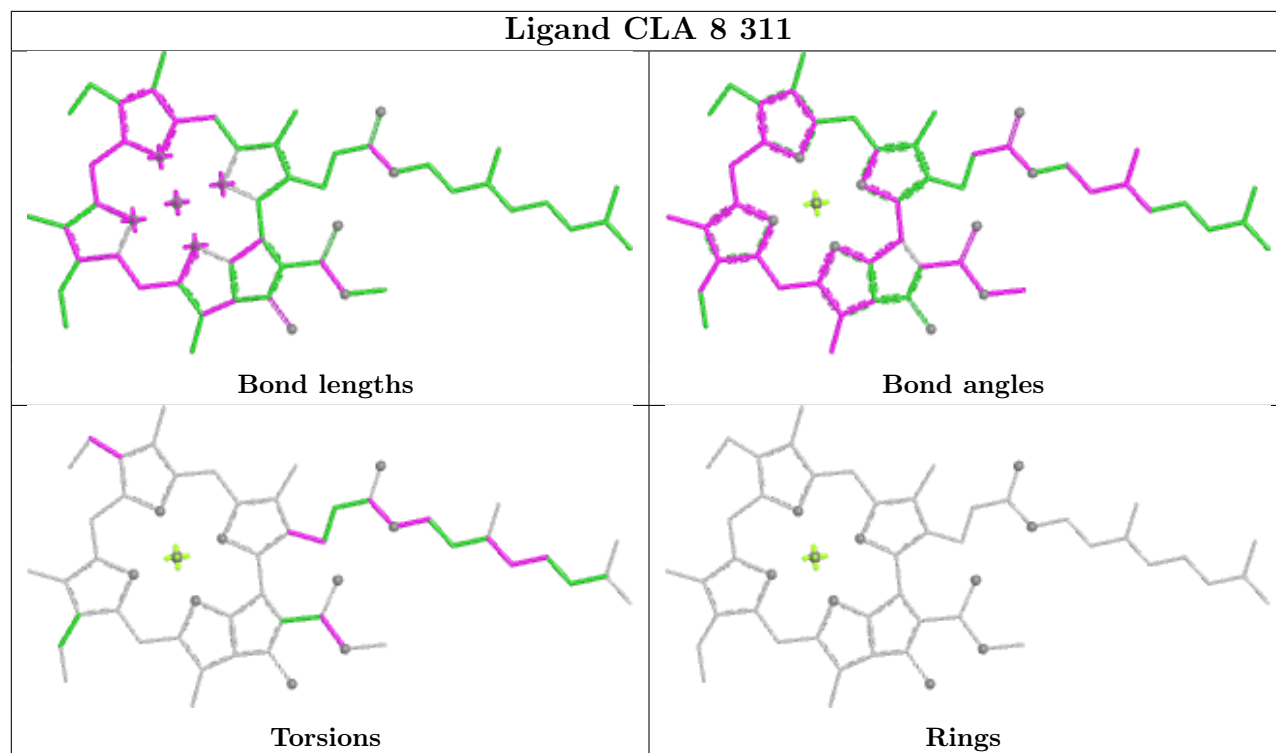


Rings

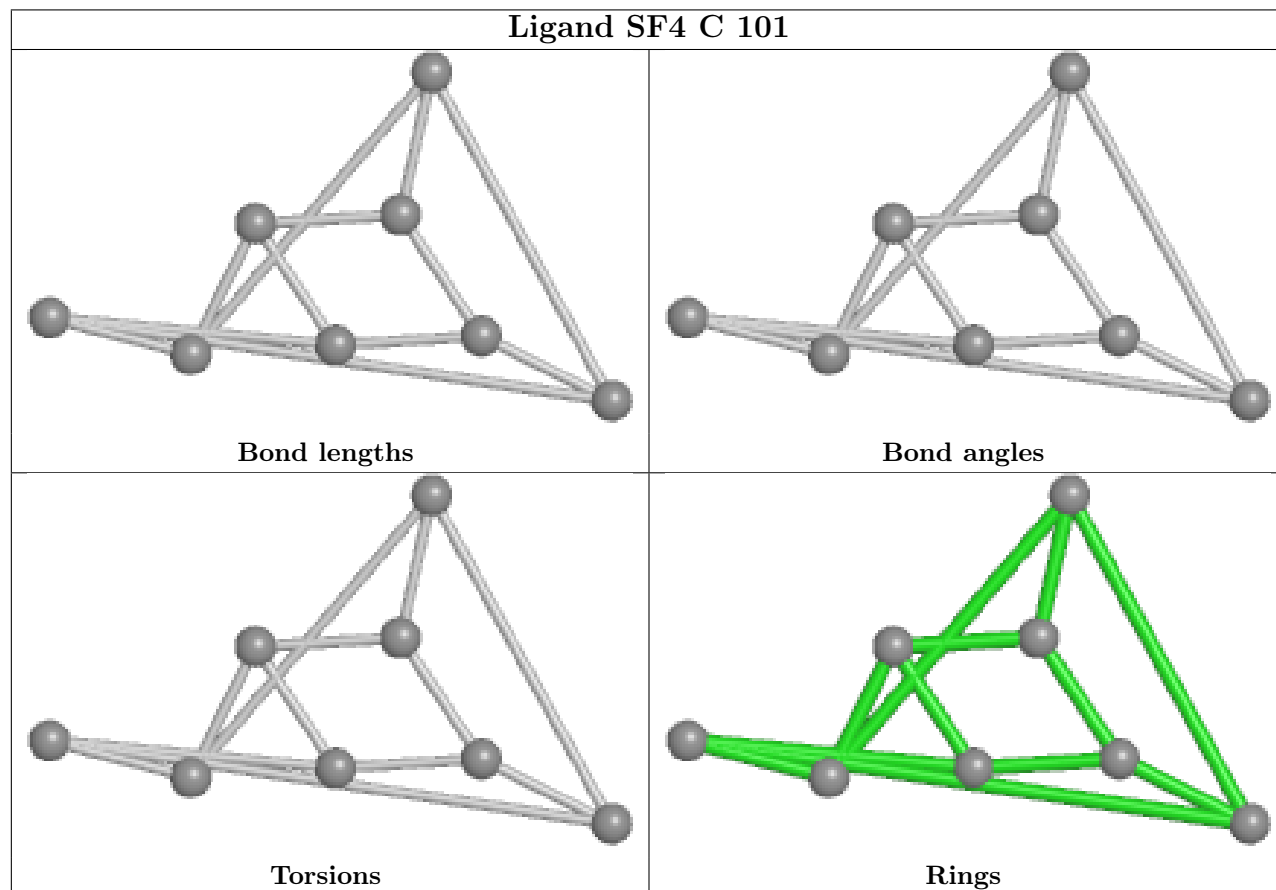


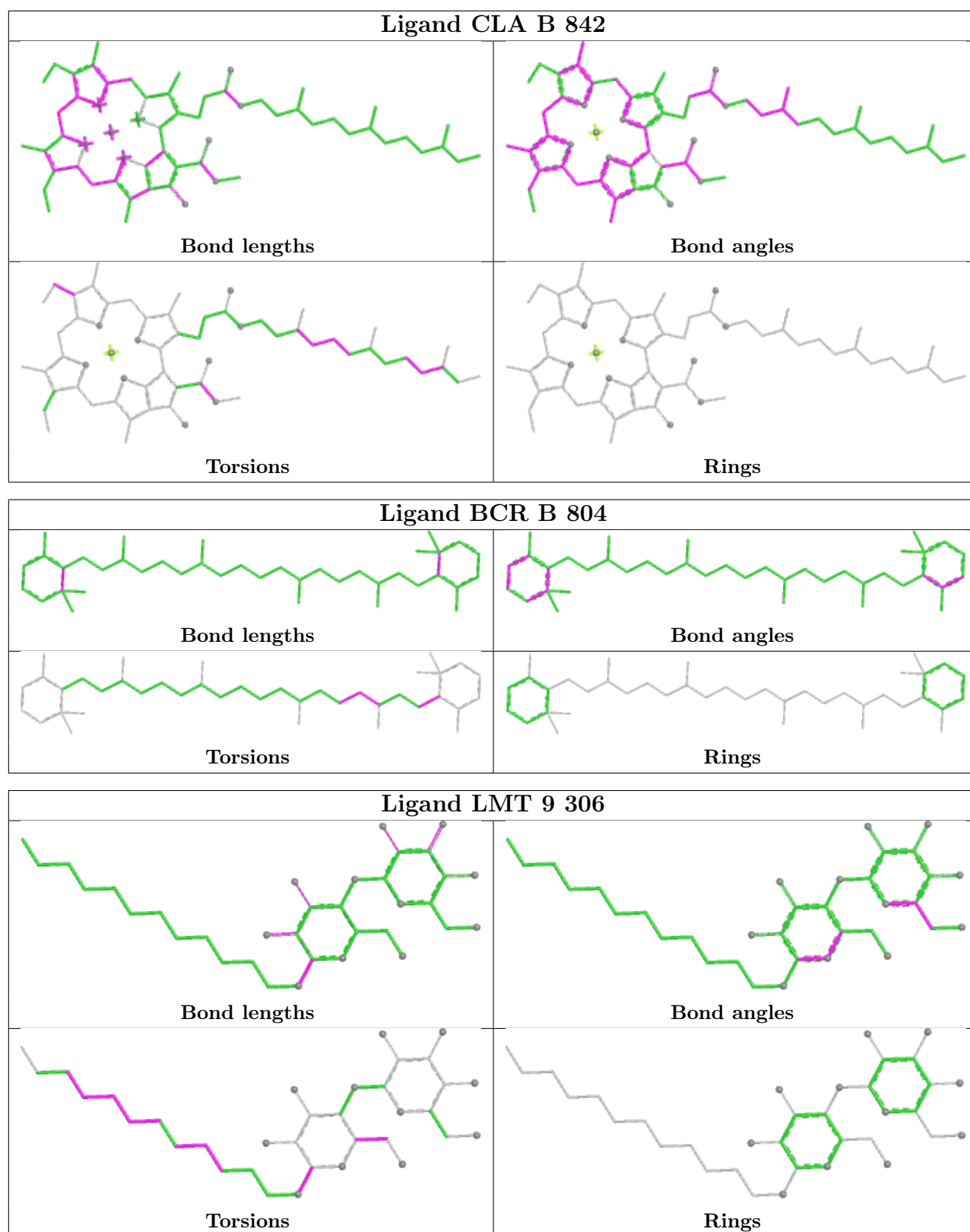


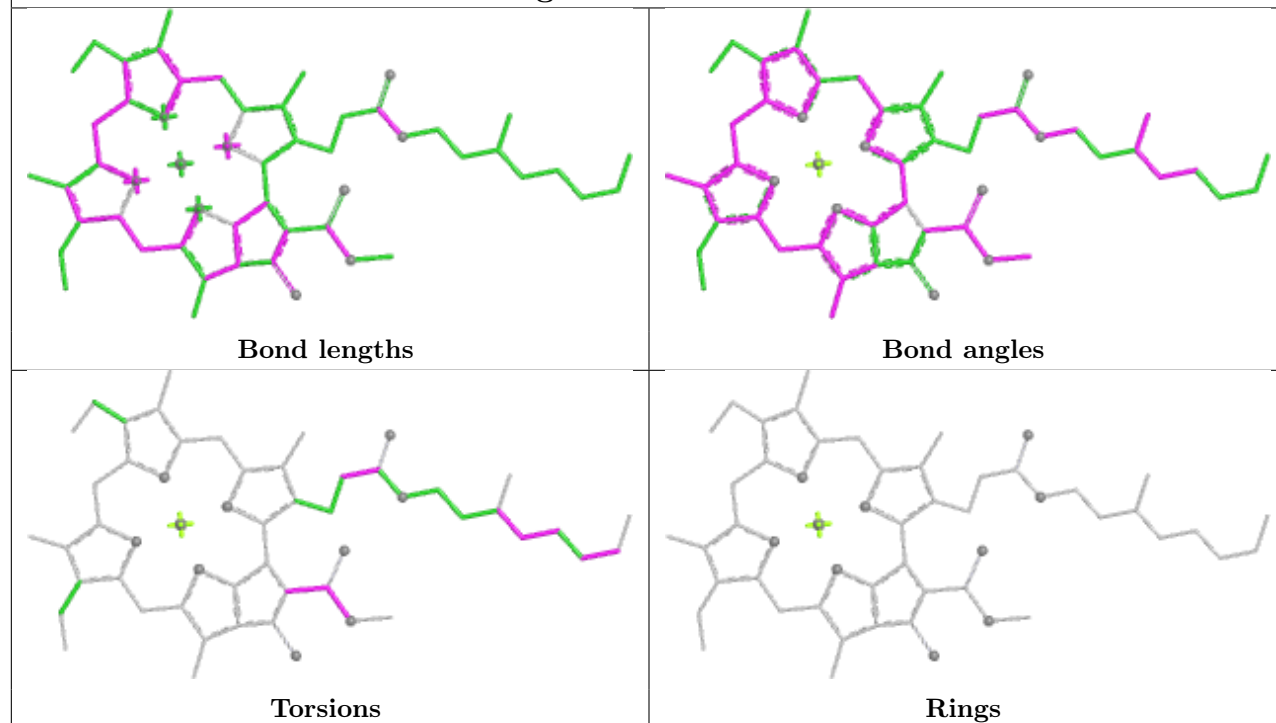
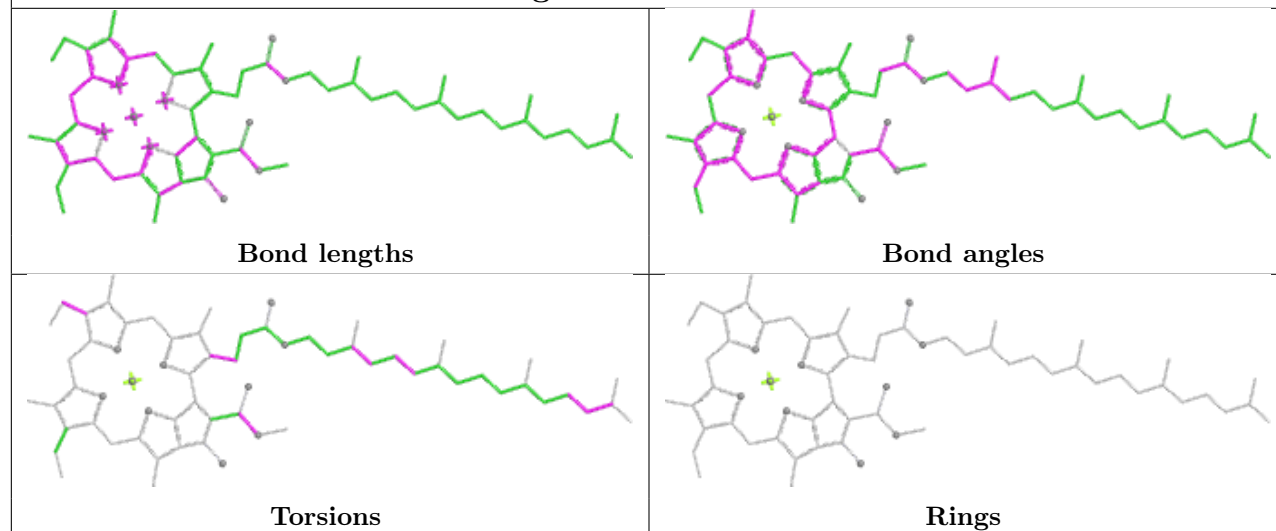
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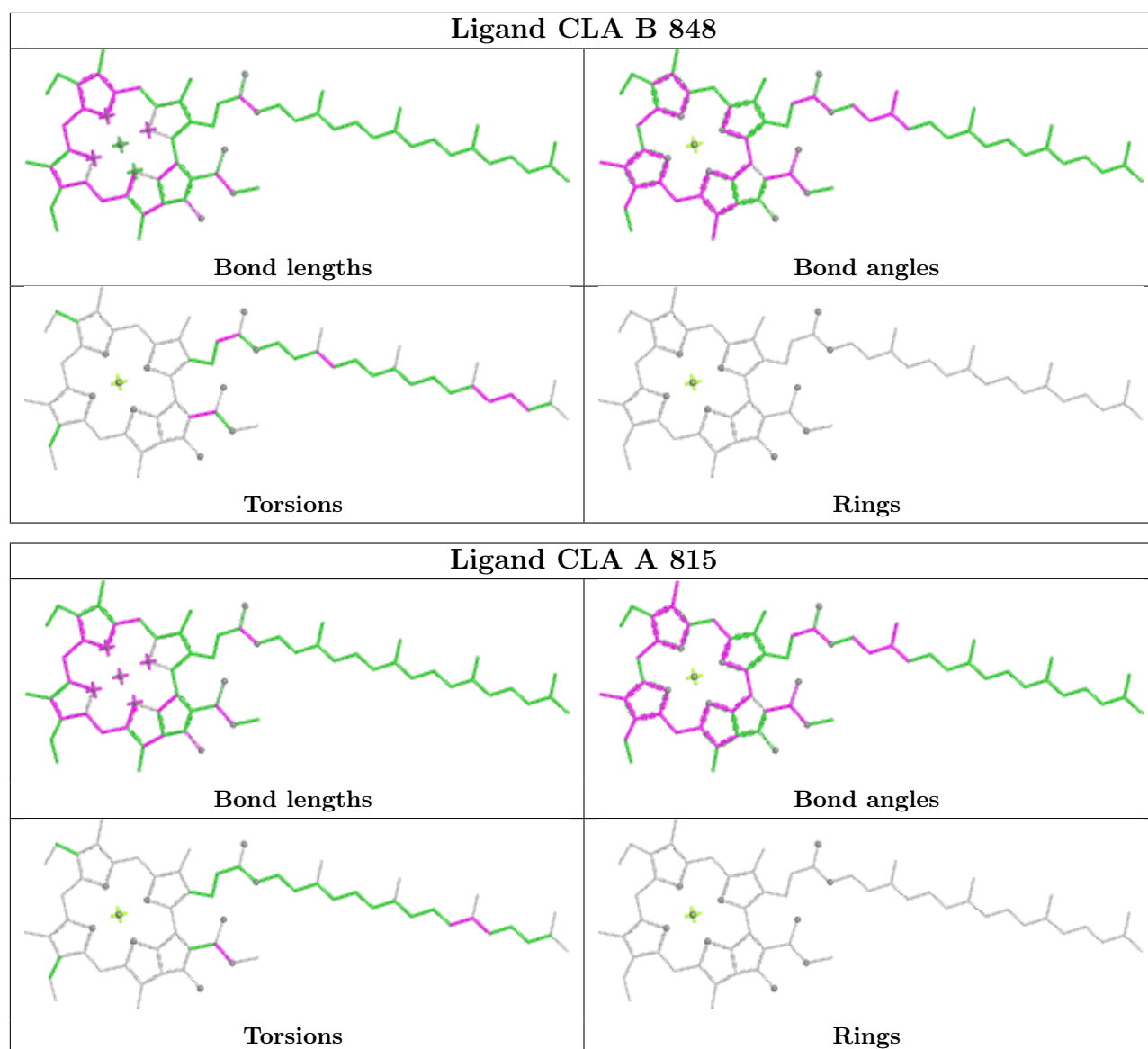


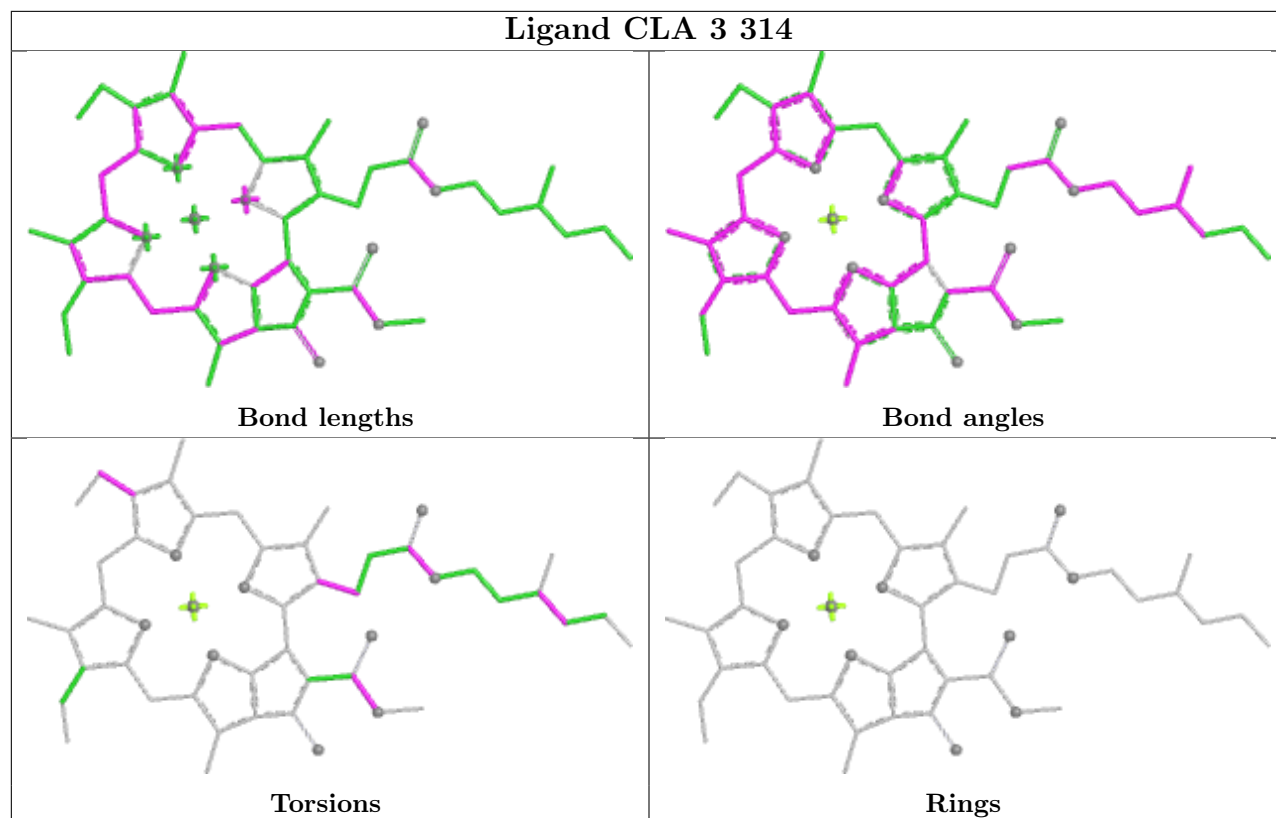
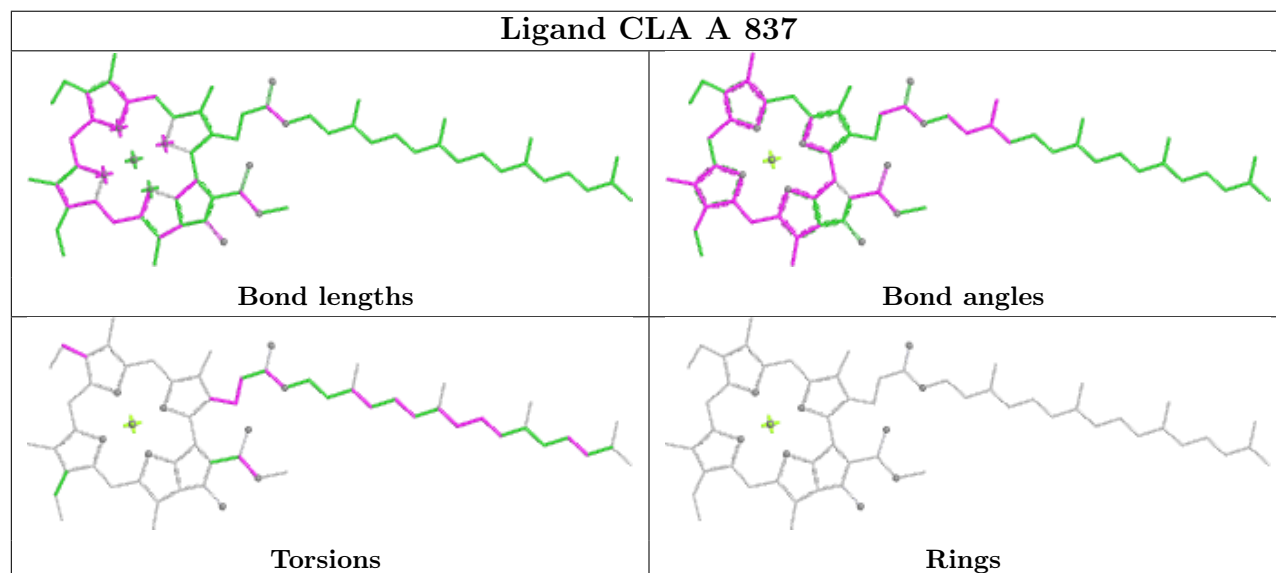
Ligand SF4 C 101

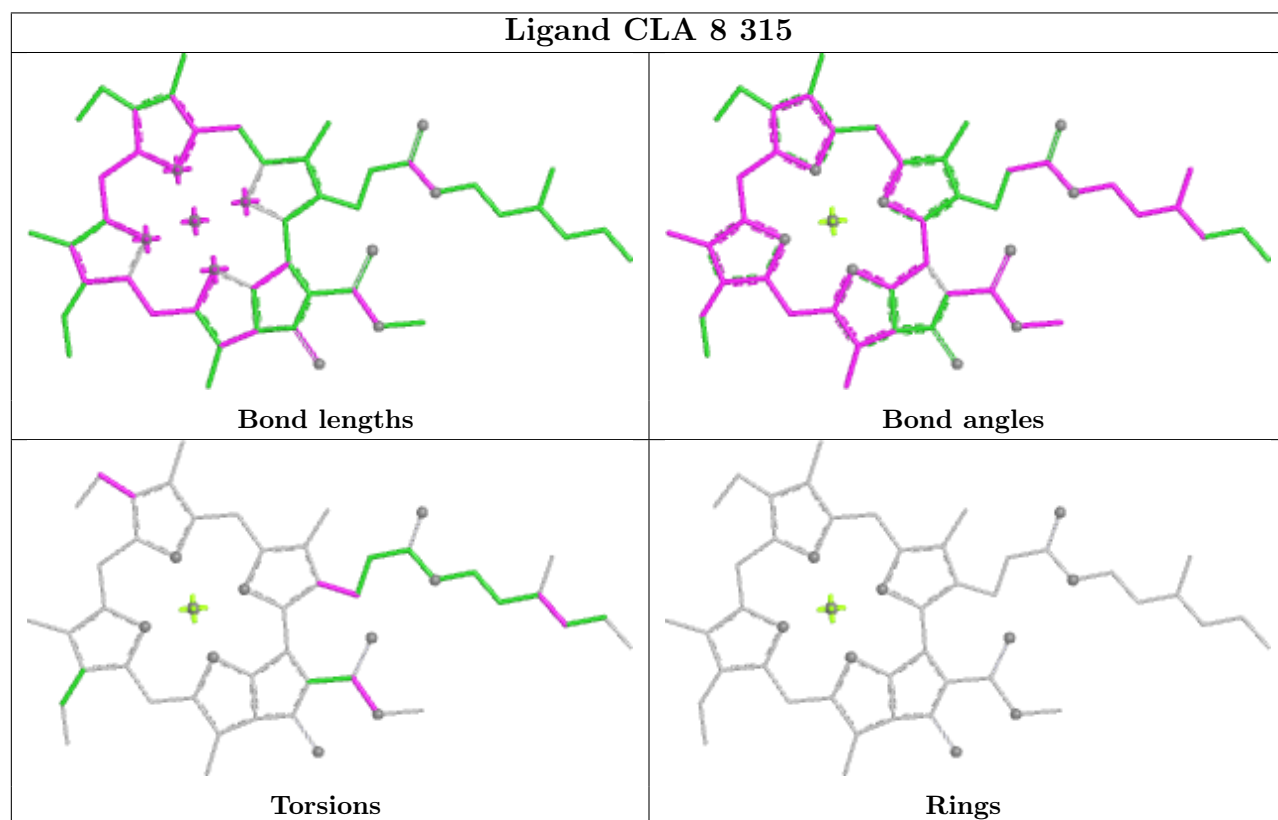
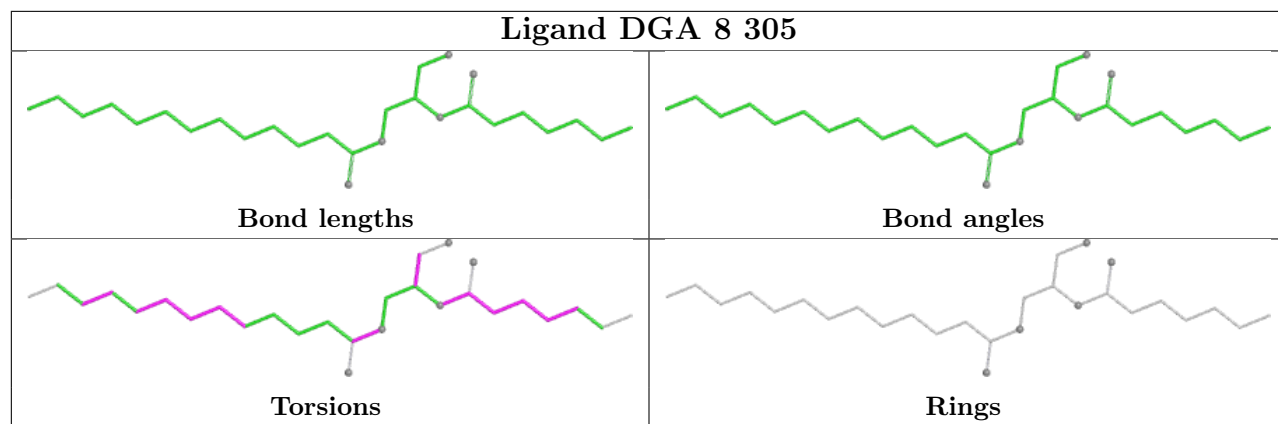




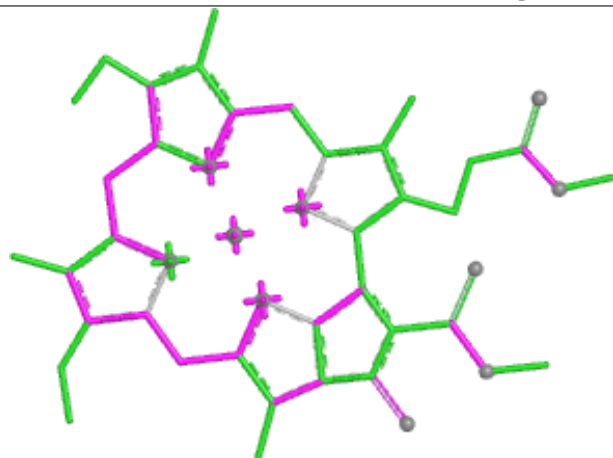
Ligand CLA 9 315**Ligand CLA B 847**



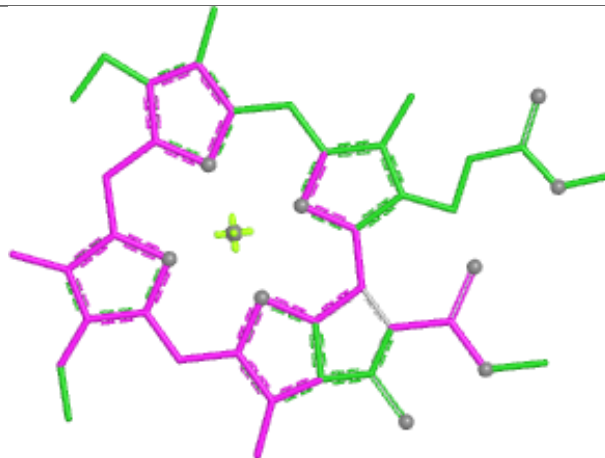
Ligand CLA 3 314**Ligand CLA A 837**



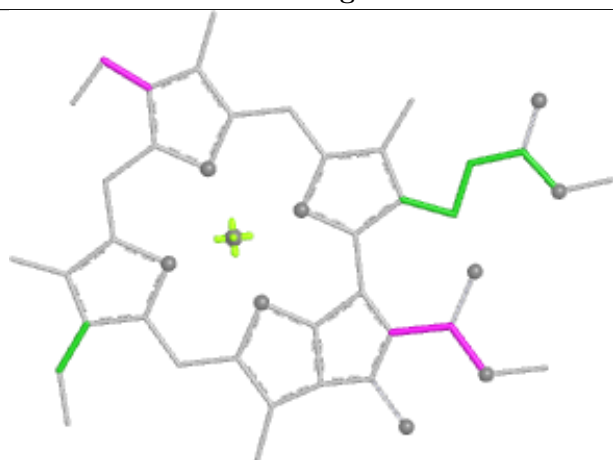
Ligand CLA K 206



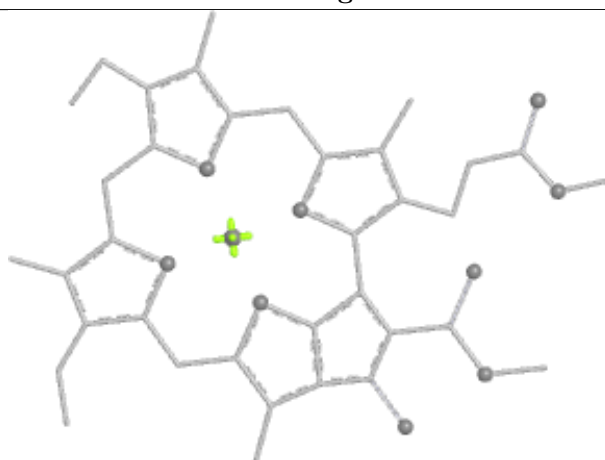
Bond lengths



Bond angles

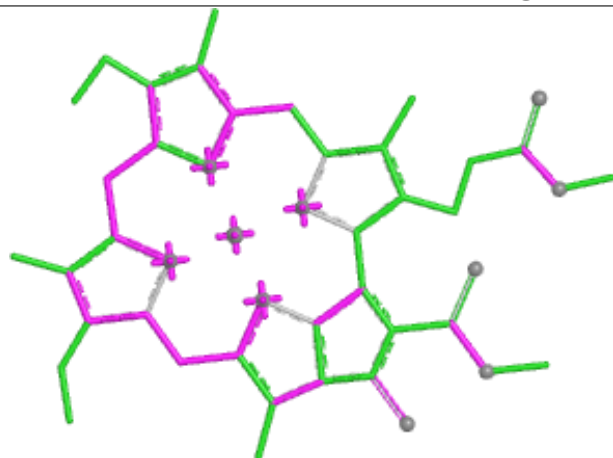


Torsions

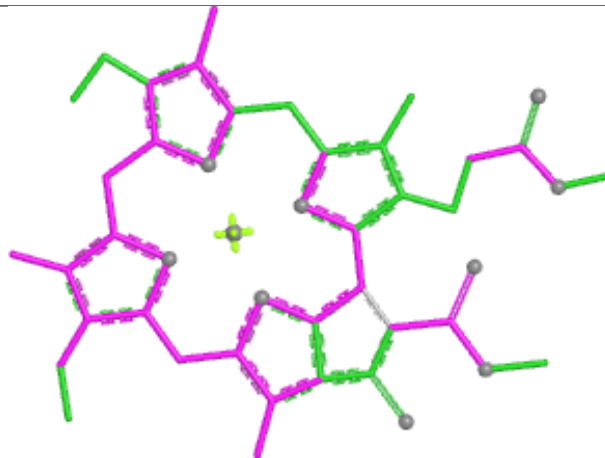


Rings

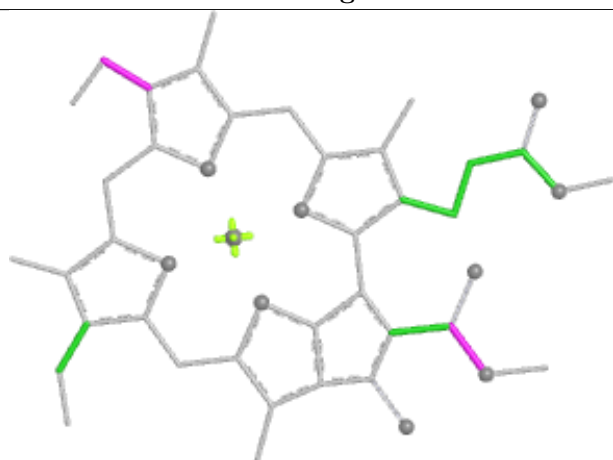
Ligand CLA b 308



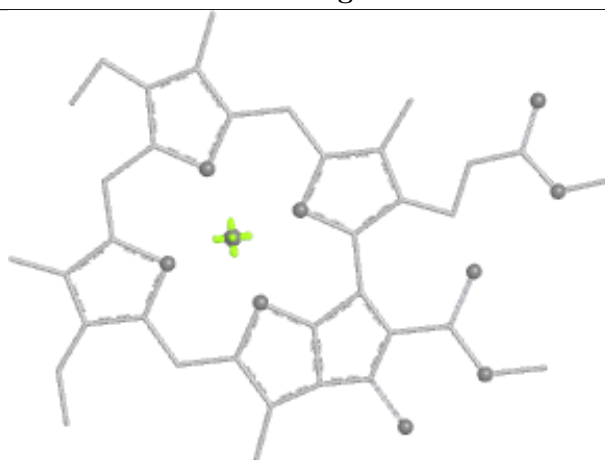
Bond lengths



Bond angles

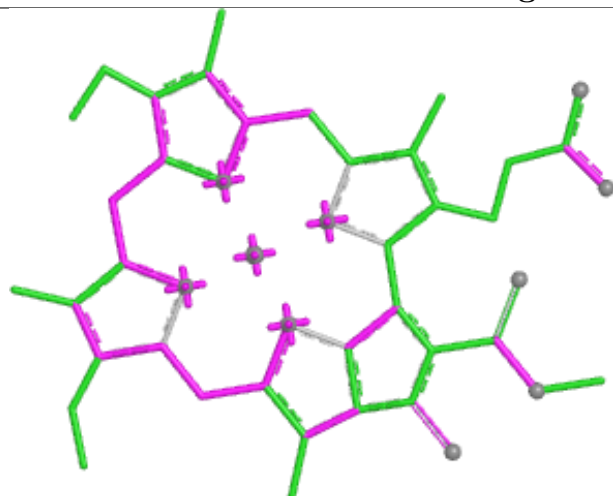


Torsions

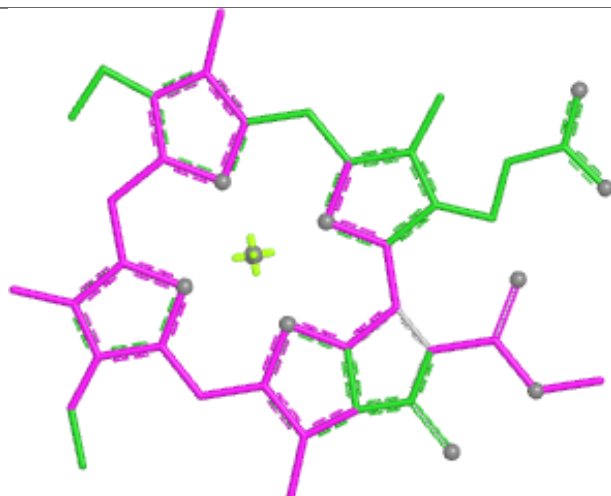


Rings

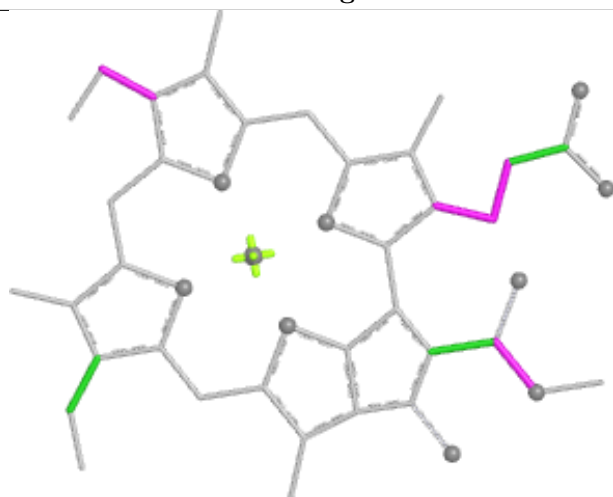
Ligand CLA 4 318



Bond lengths



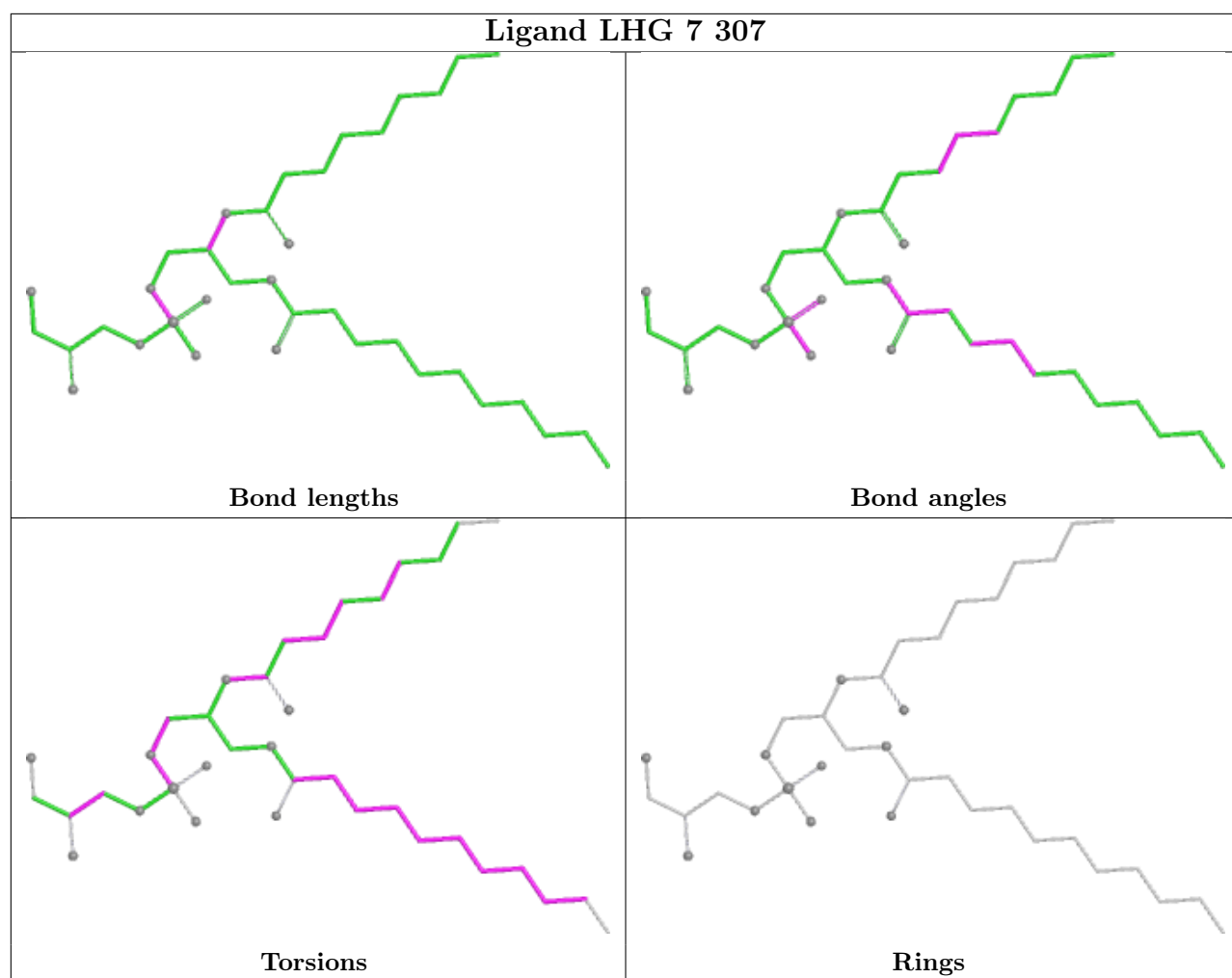
Bond angles



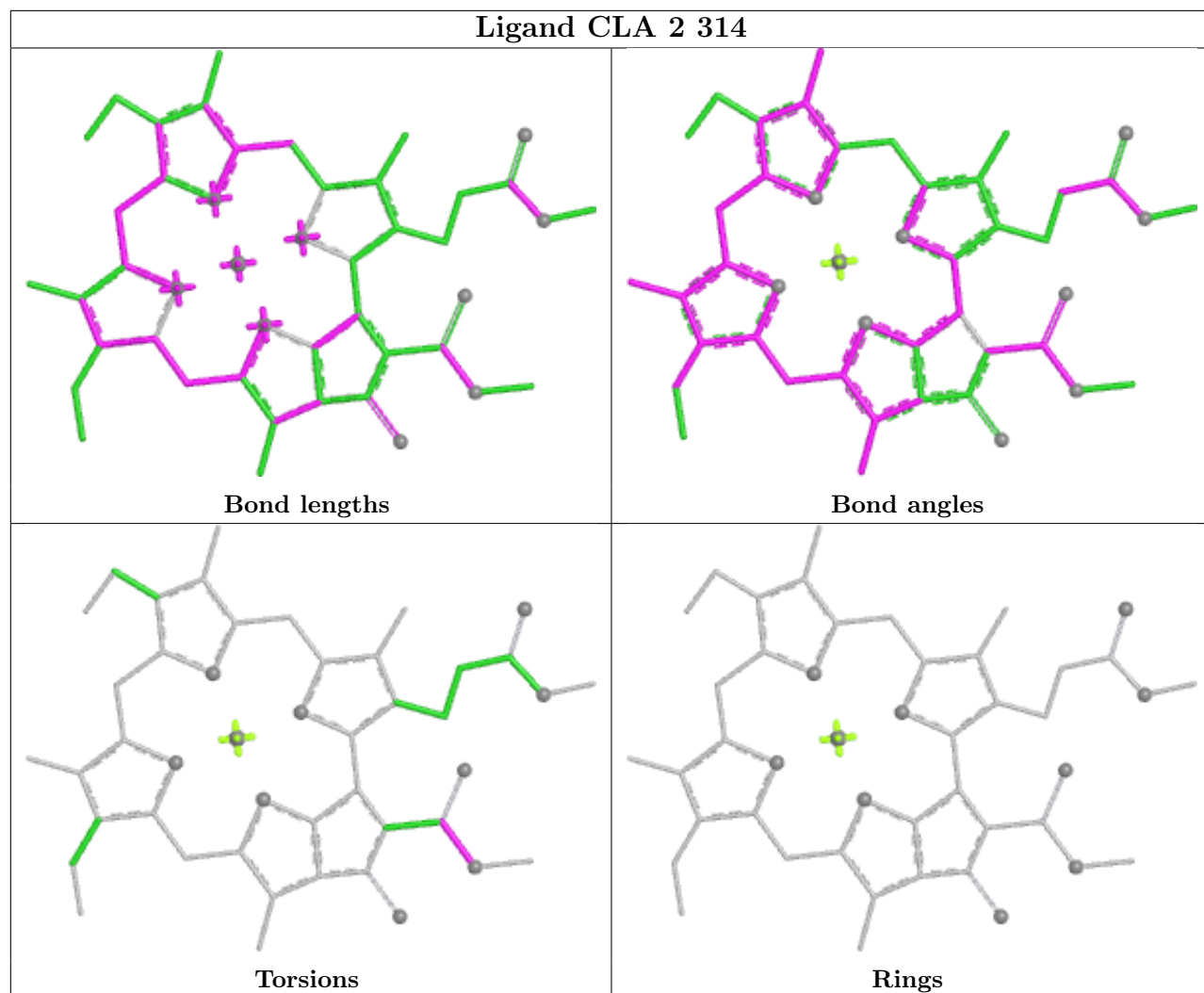
Torsions



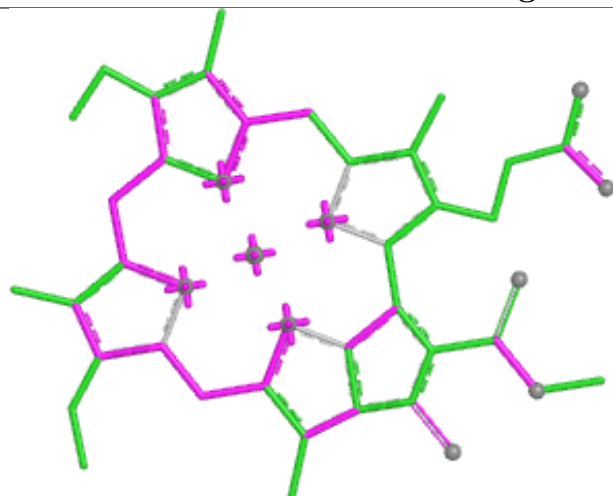
Rings



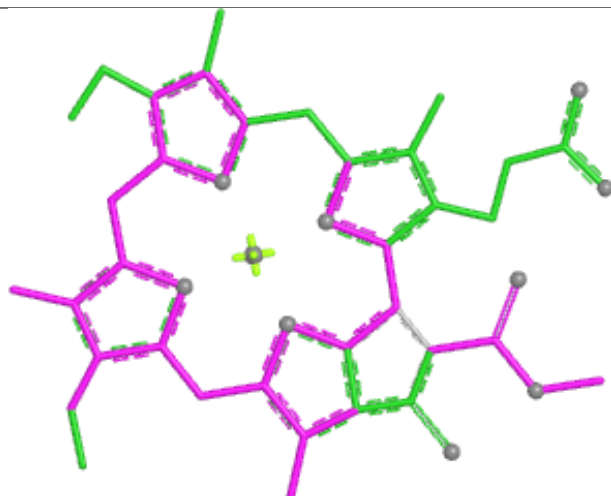
Ligand CLA 2 314



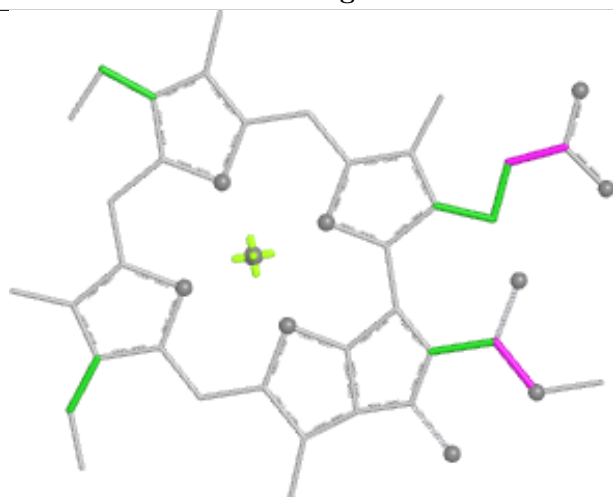
Ligand CLA 4 315



Bond lengths



Bond angles

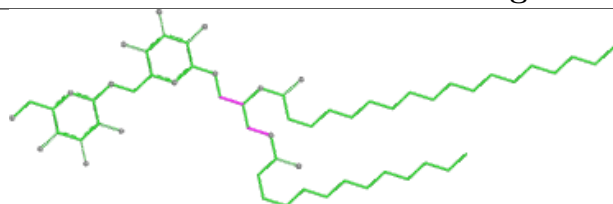


Torsions

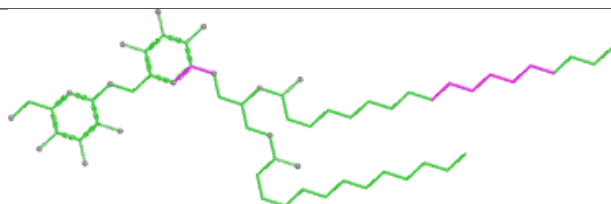


Rings

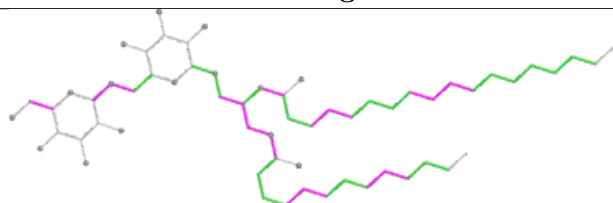
Ligand DGD B 808



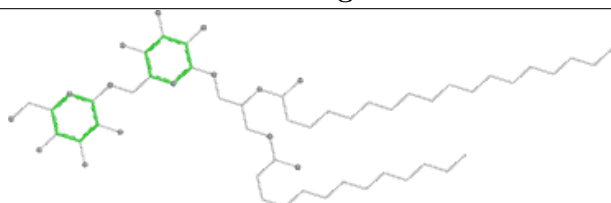
Bond lengths



Bond angles

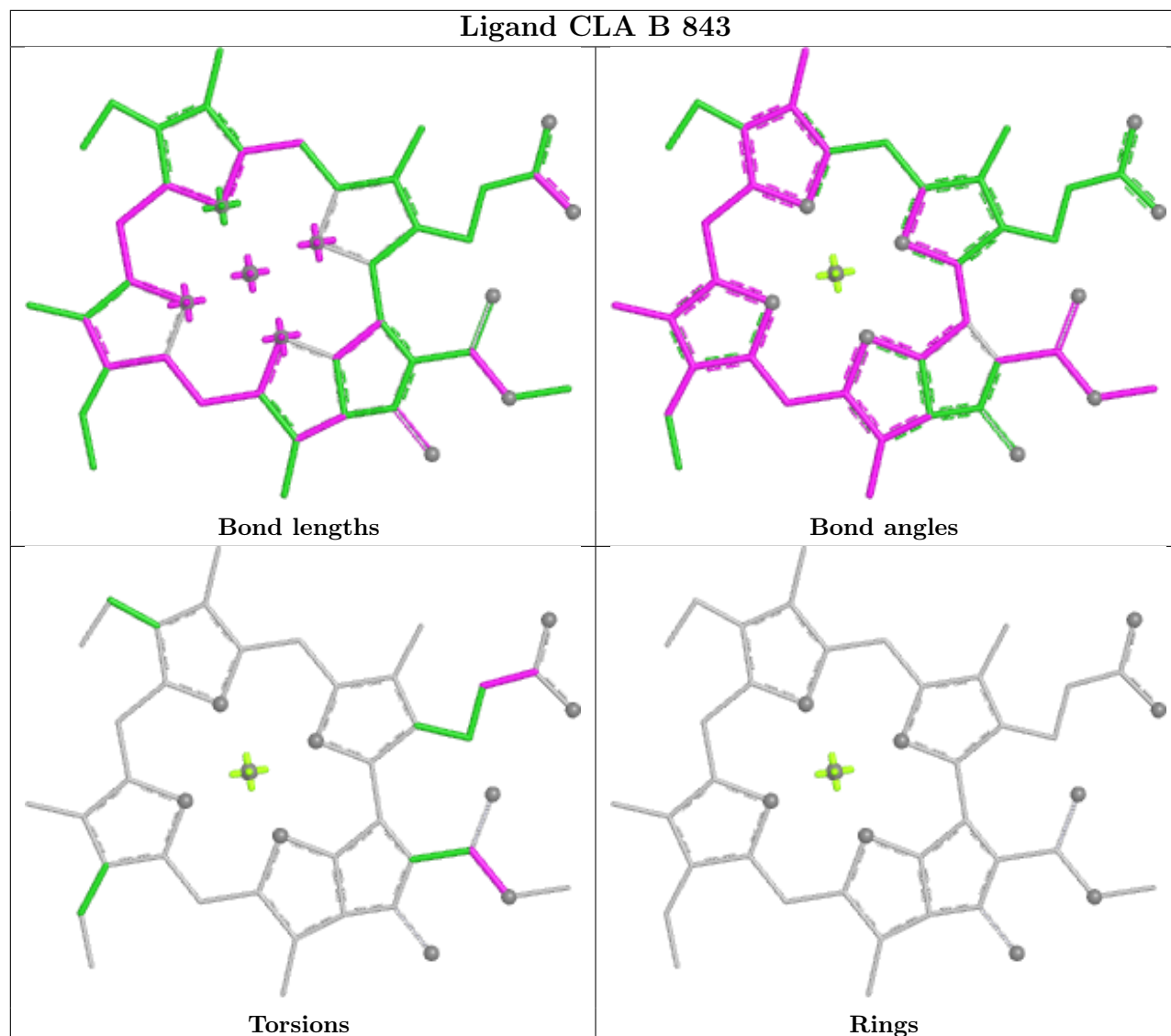


Torsions

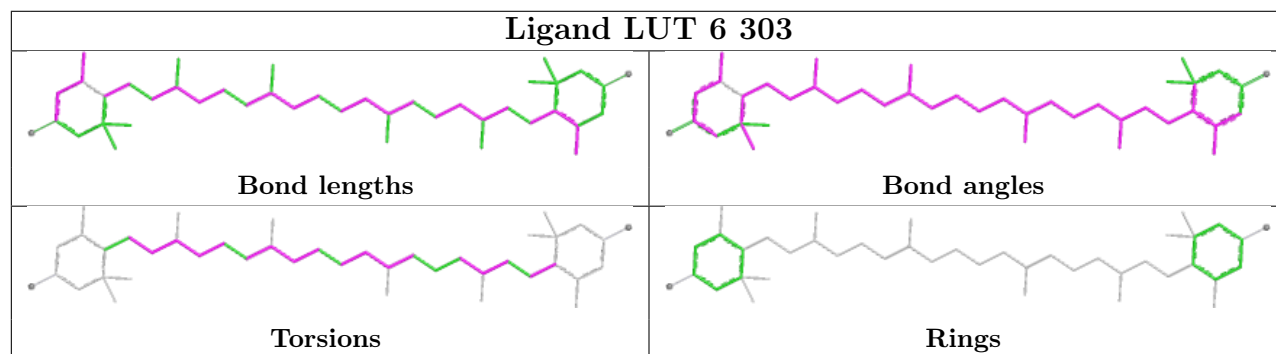


Rings

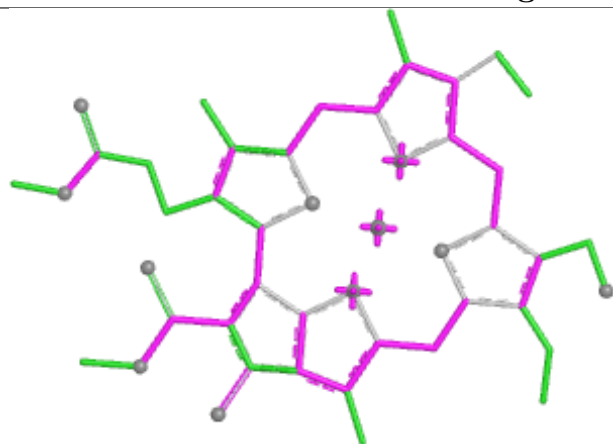
Ligand CLA B 843



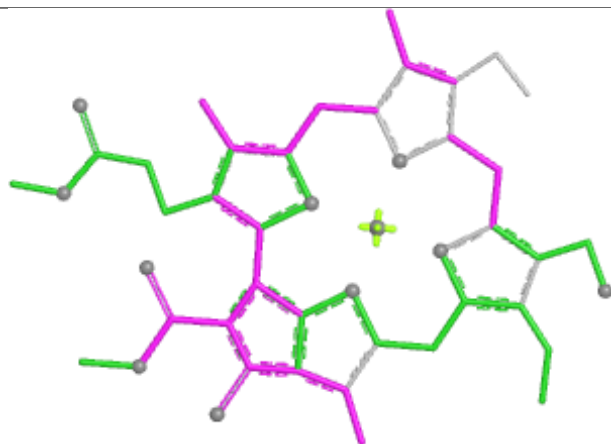
Ligand LUT 6 303



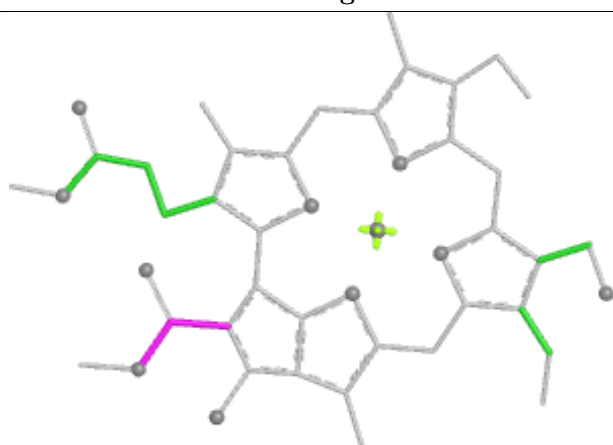
Ligand CHL 7 319



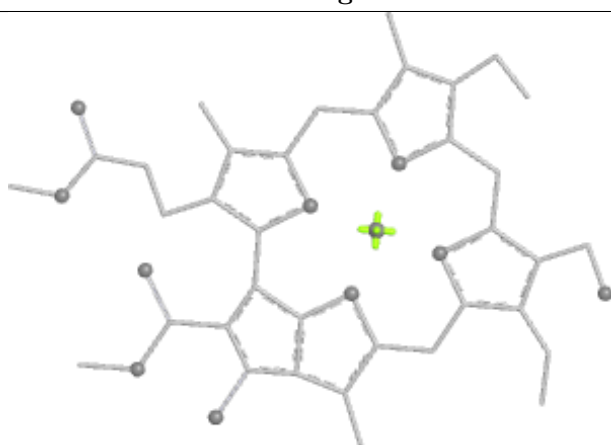
Bond lengths



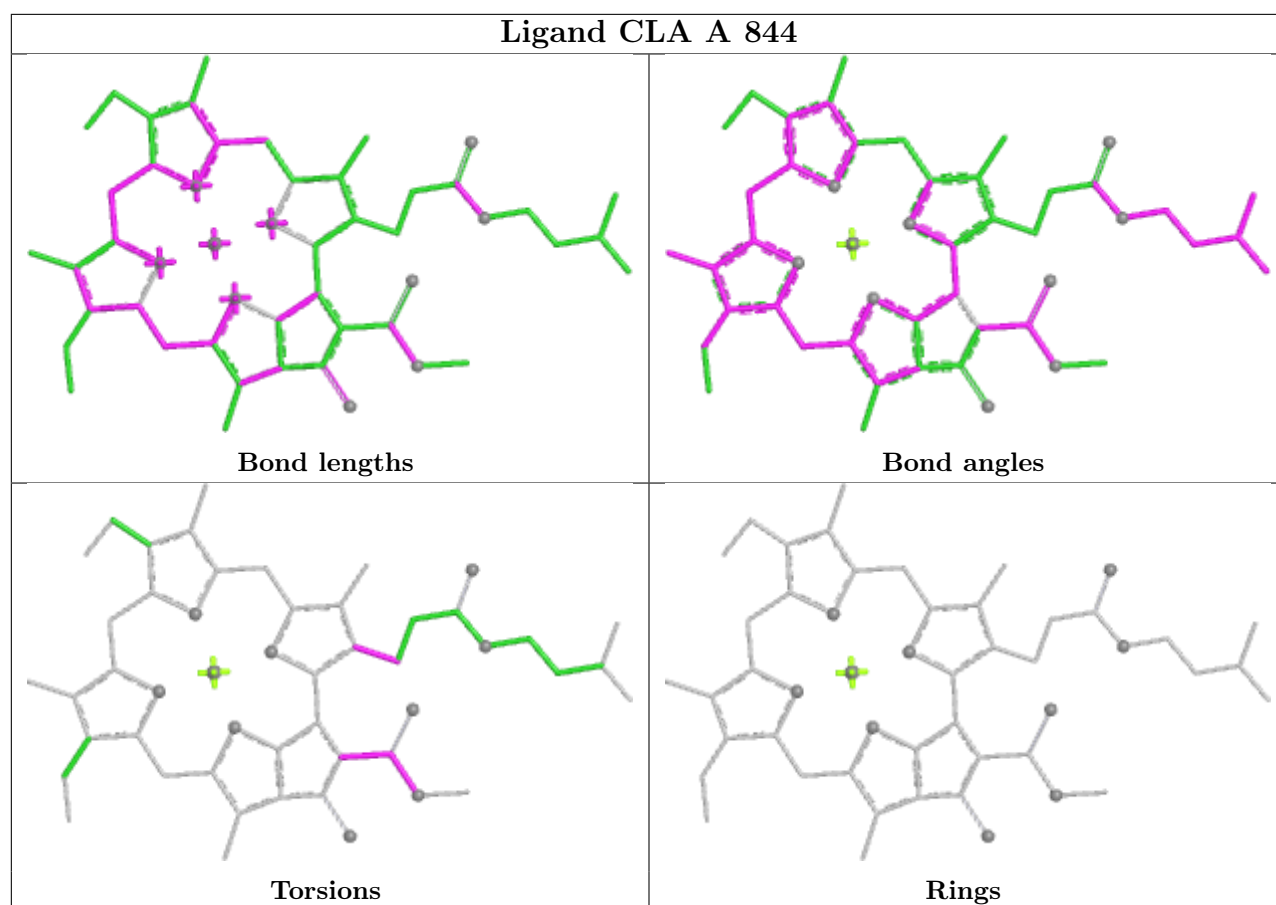
Bond angles



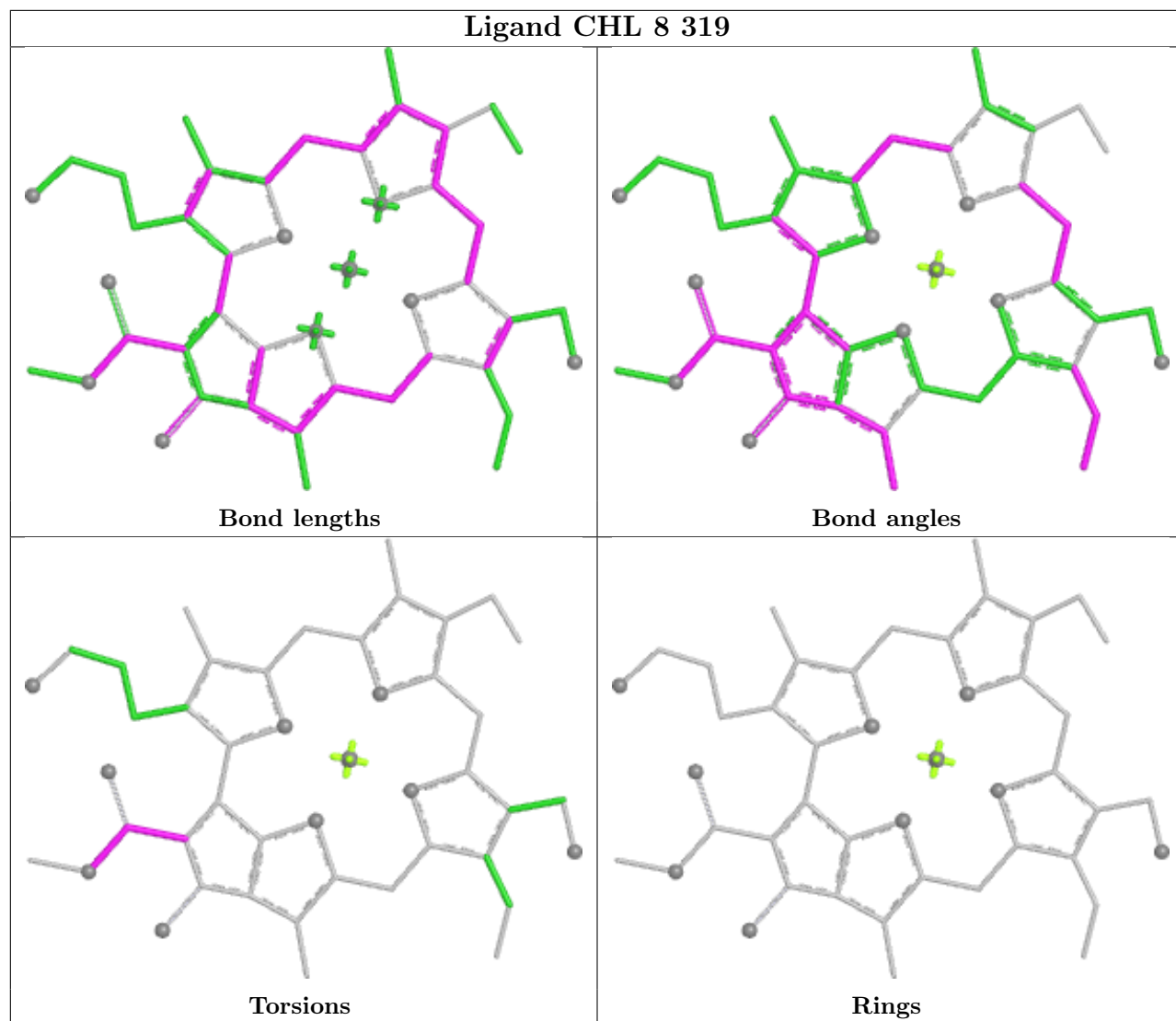
Torsions



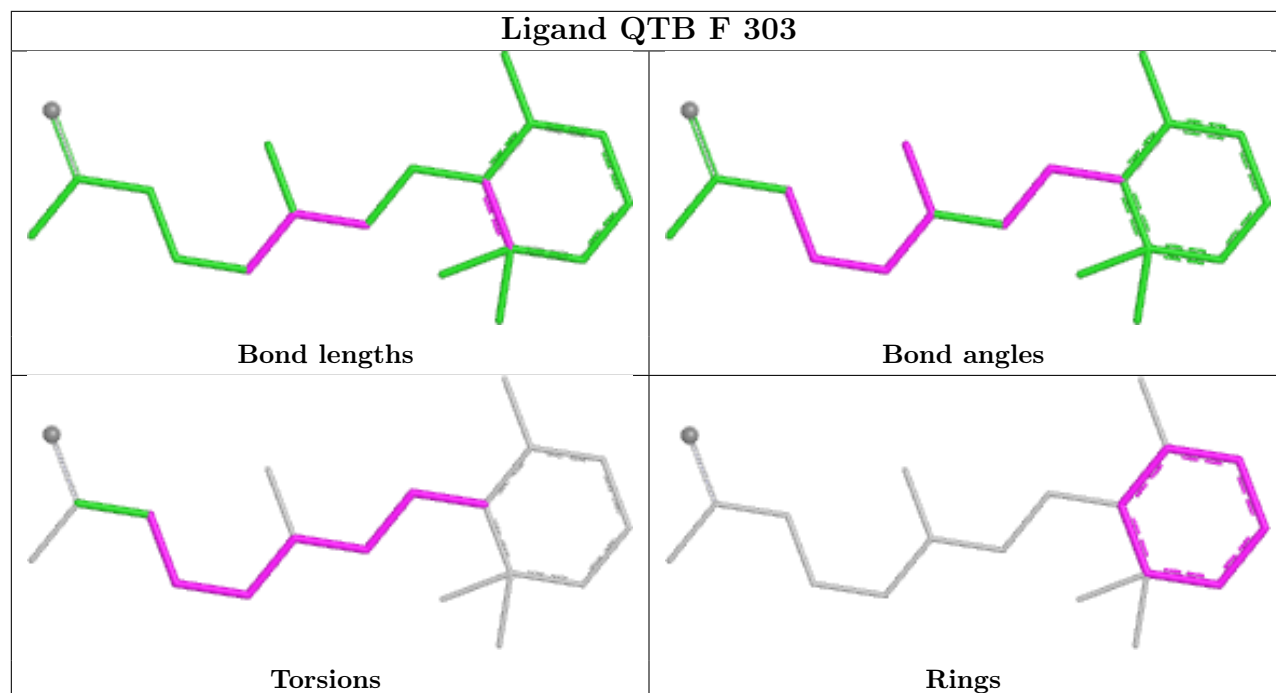
Rings



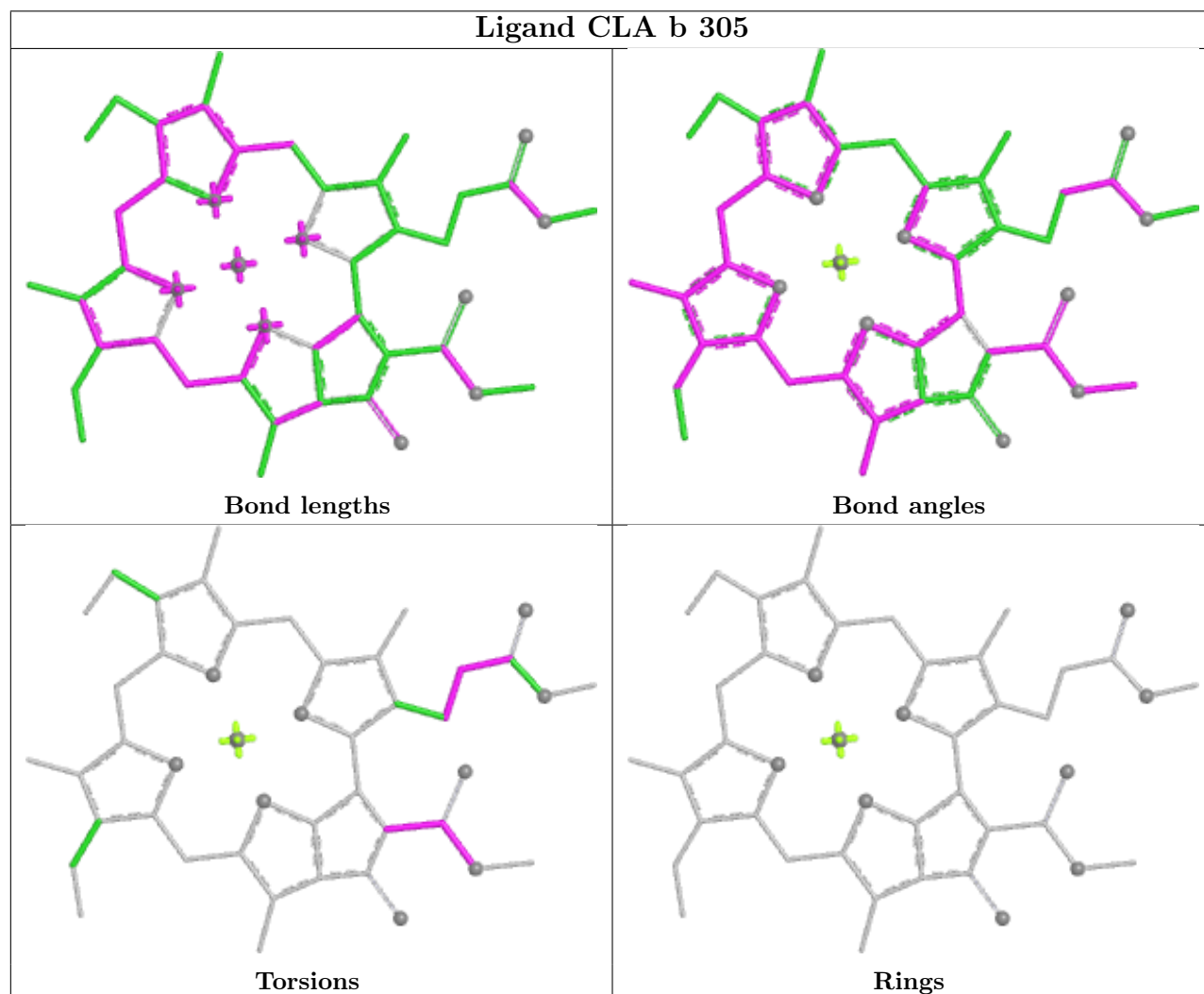
Ligand CHL 8 319



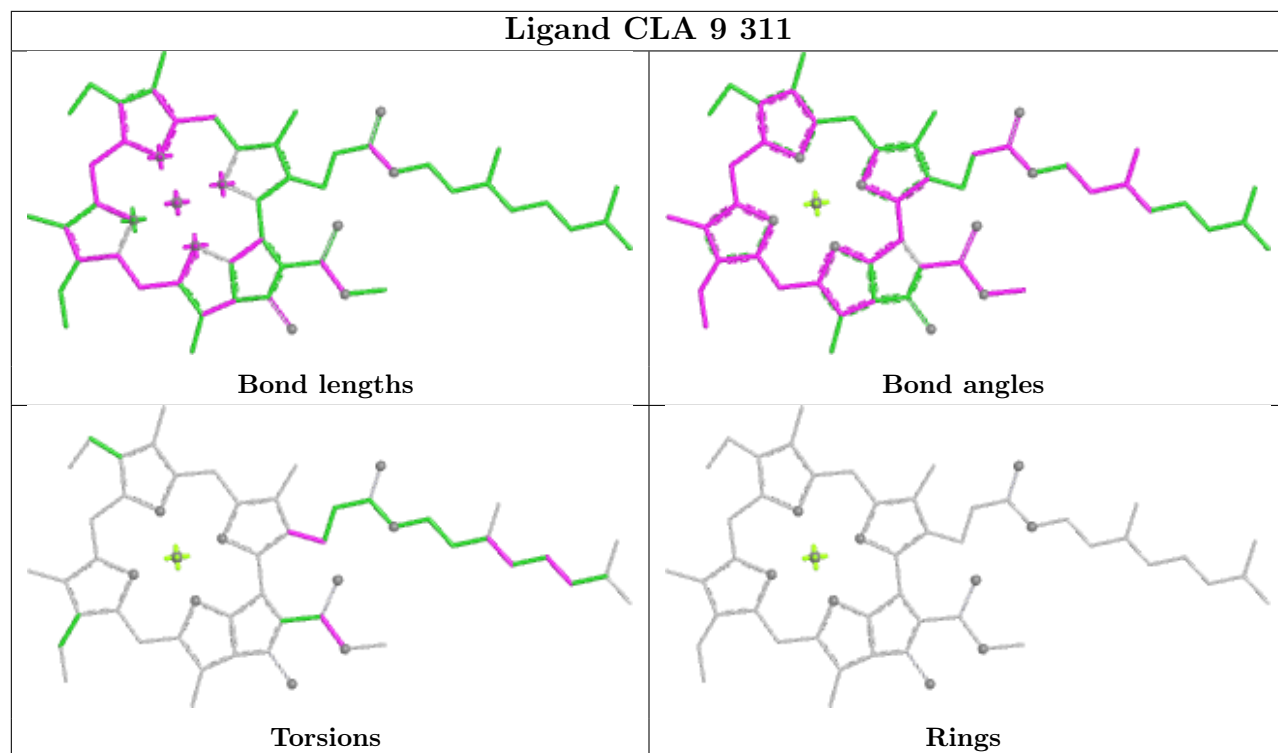
Ligand QTB F 303



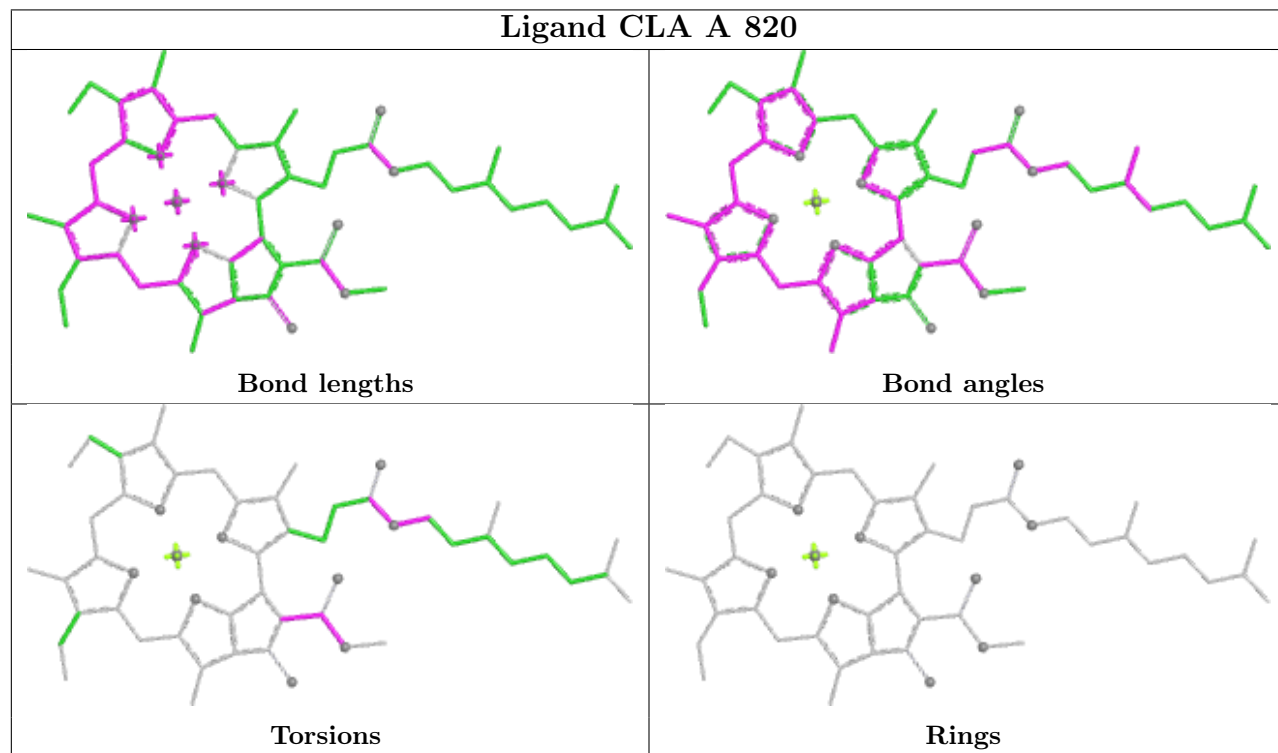
Ligand CLA b 305

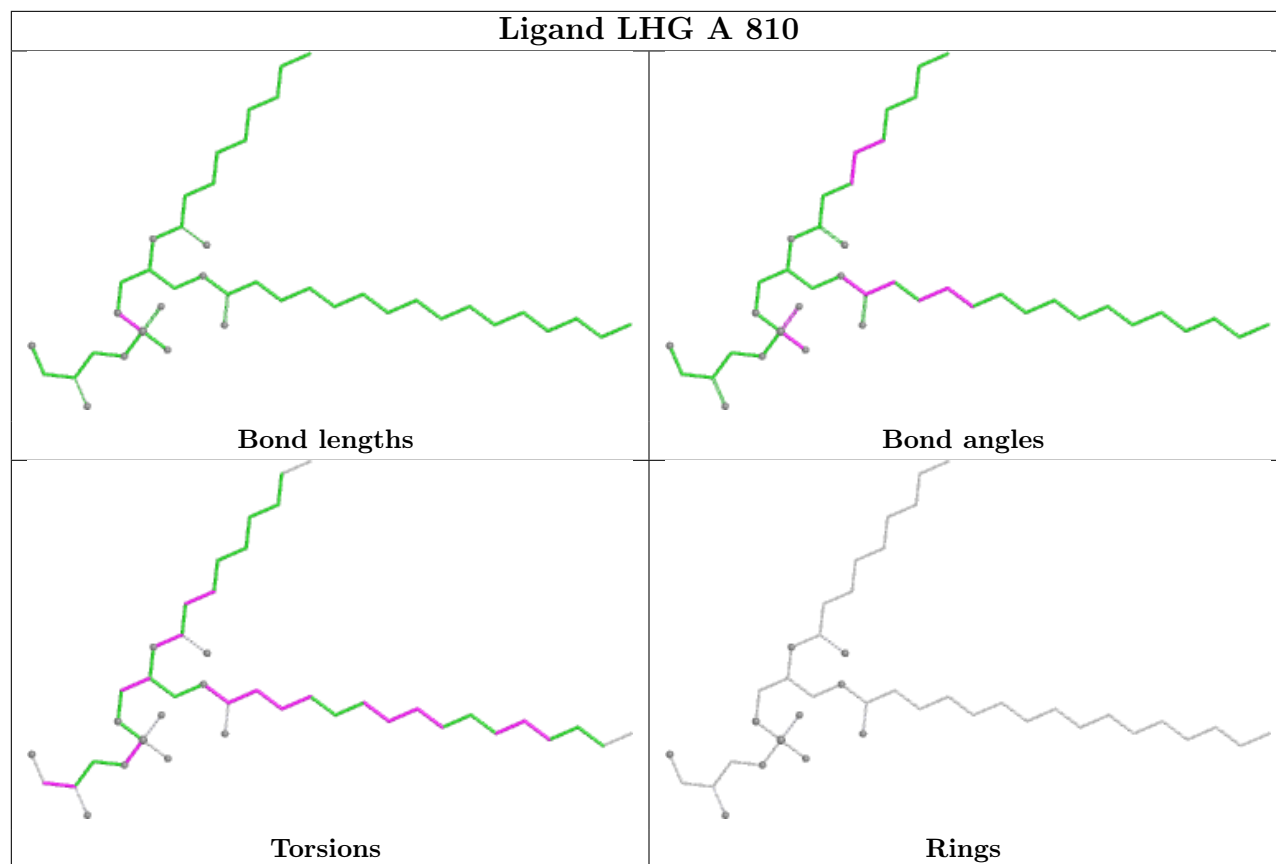


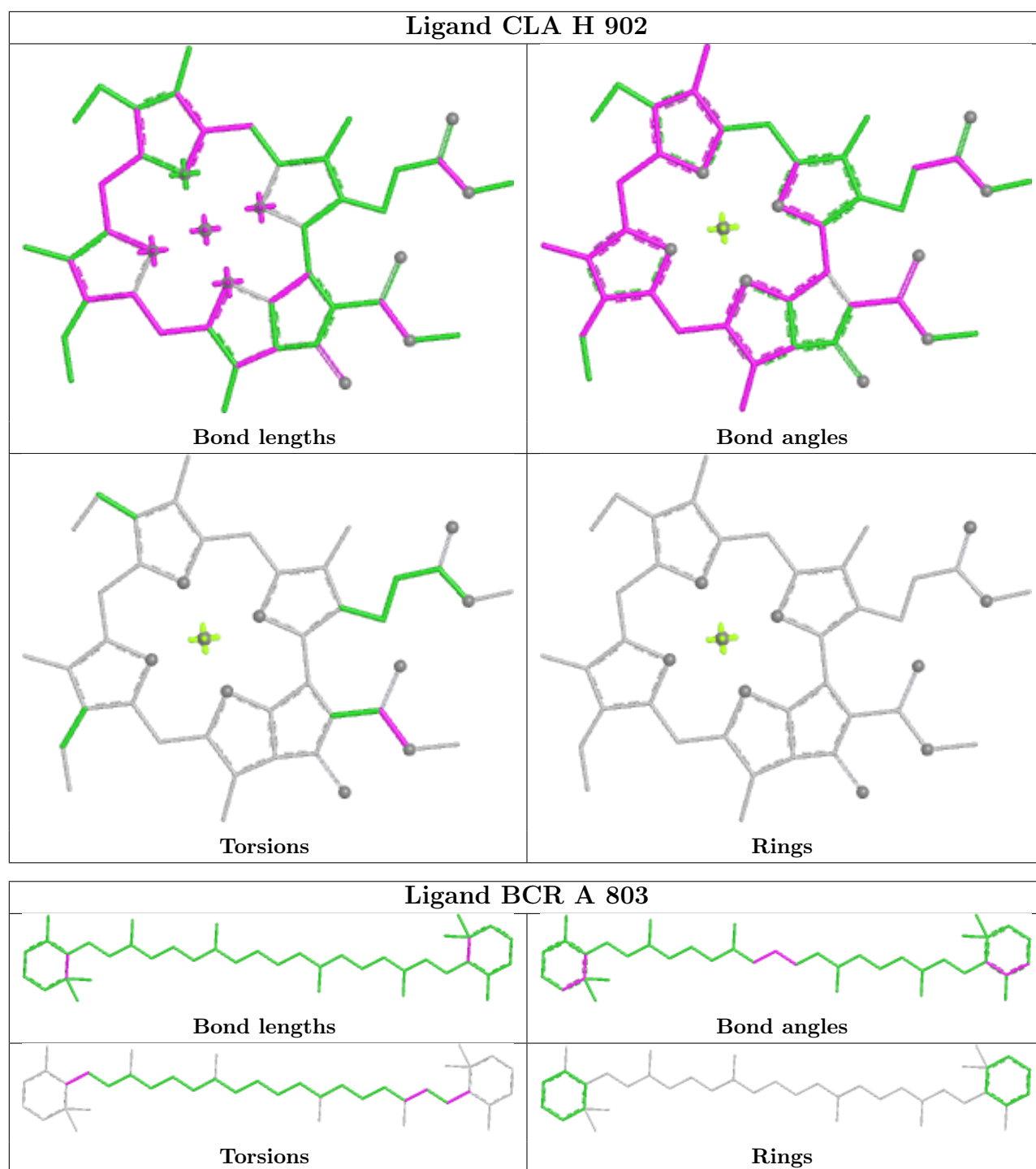
Ligand CLA 9 311



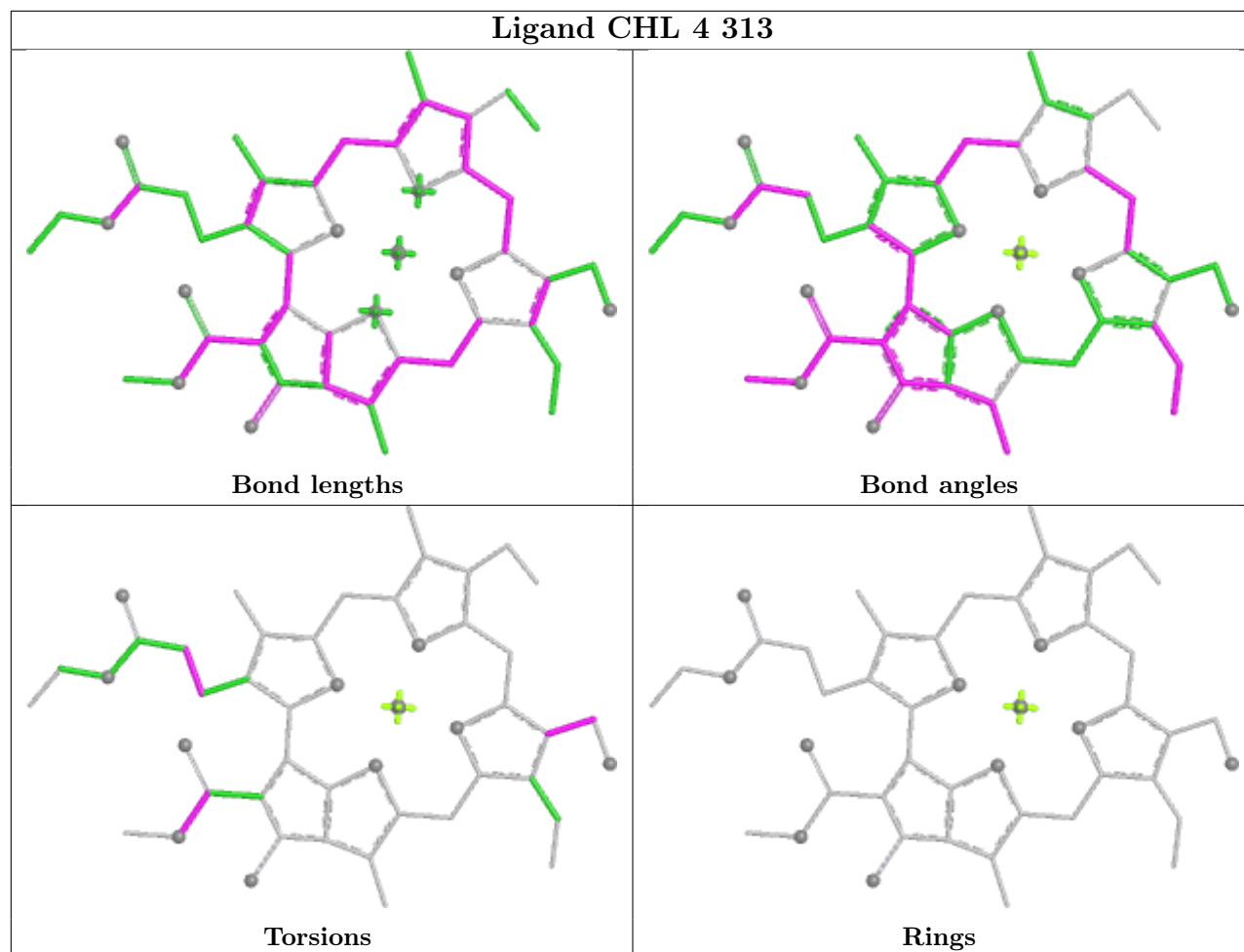
Ligand CLA A 820



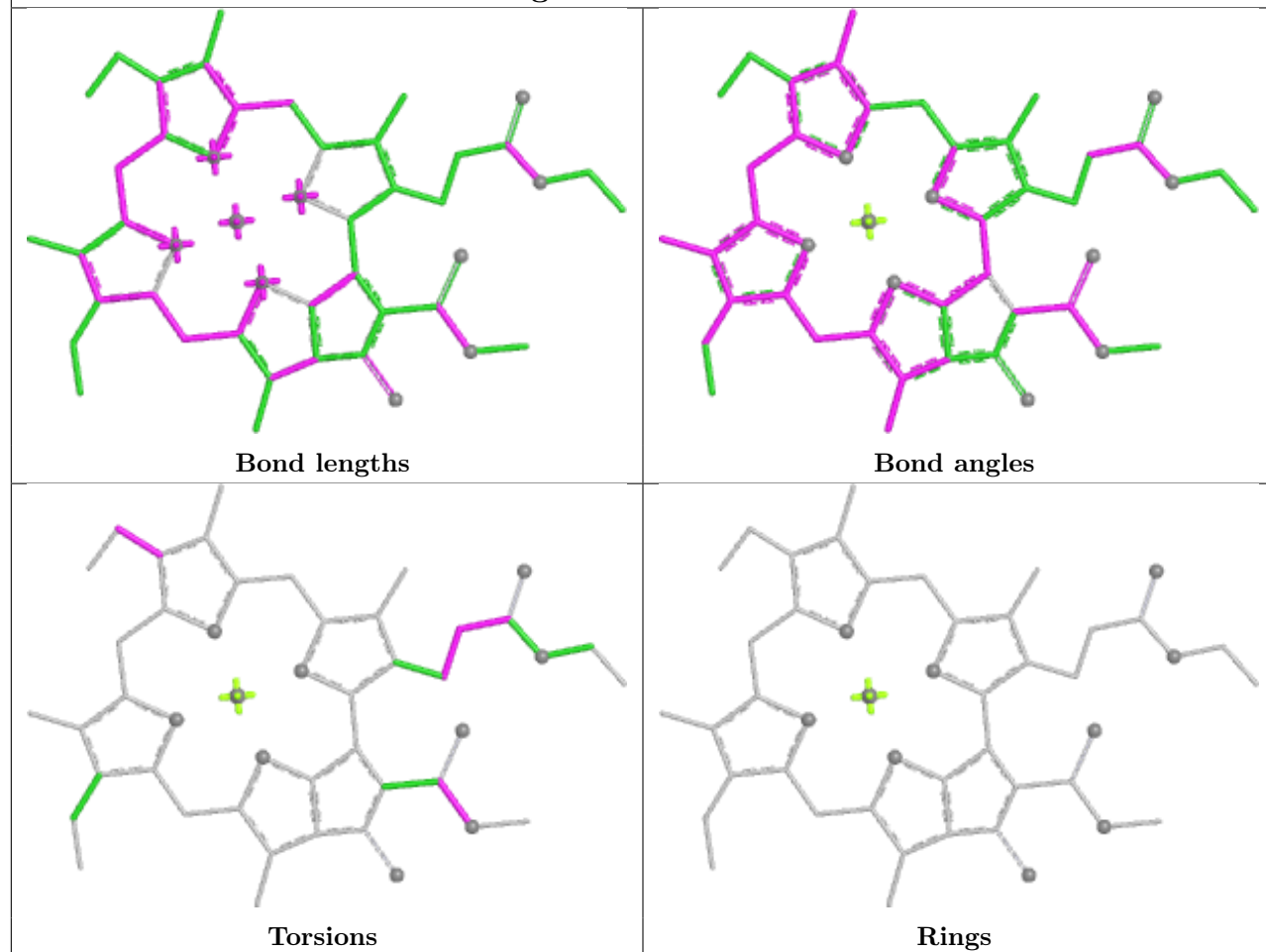




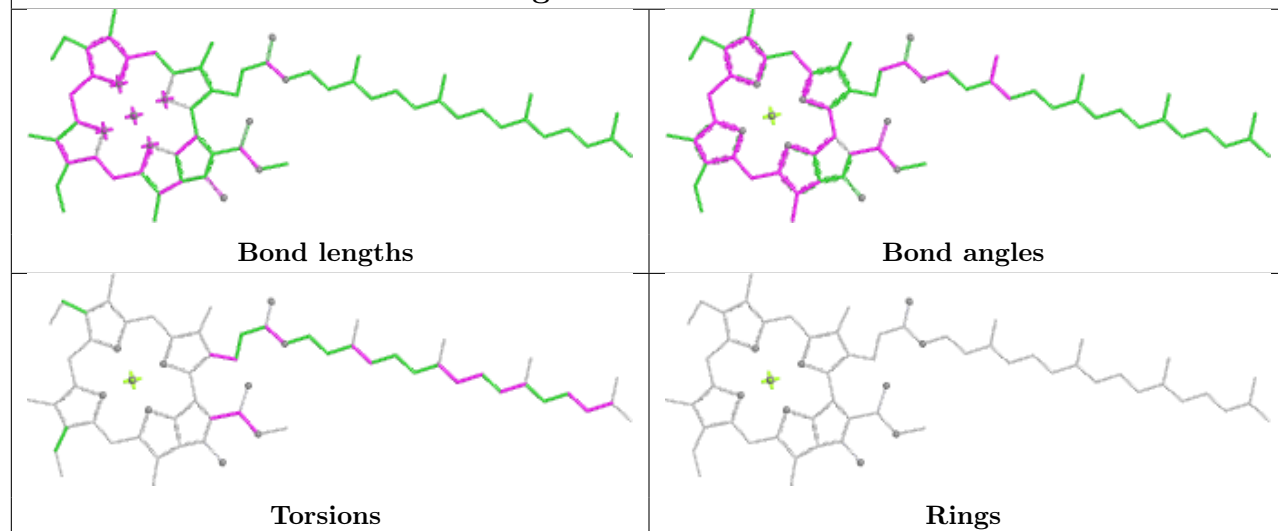
Ligand CHL 4 313



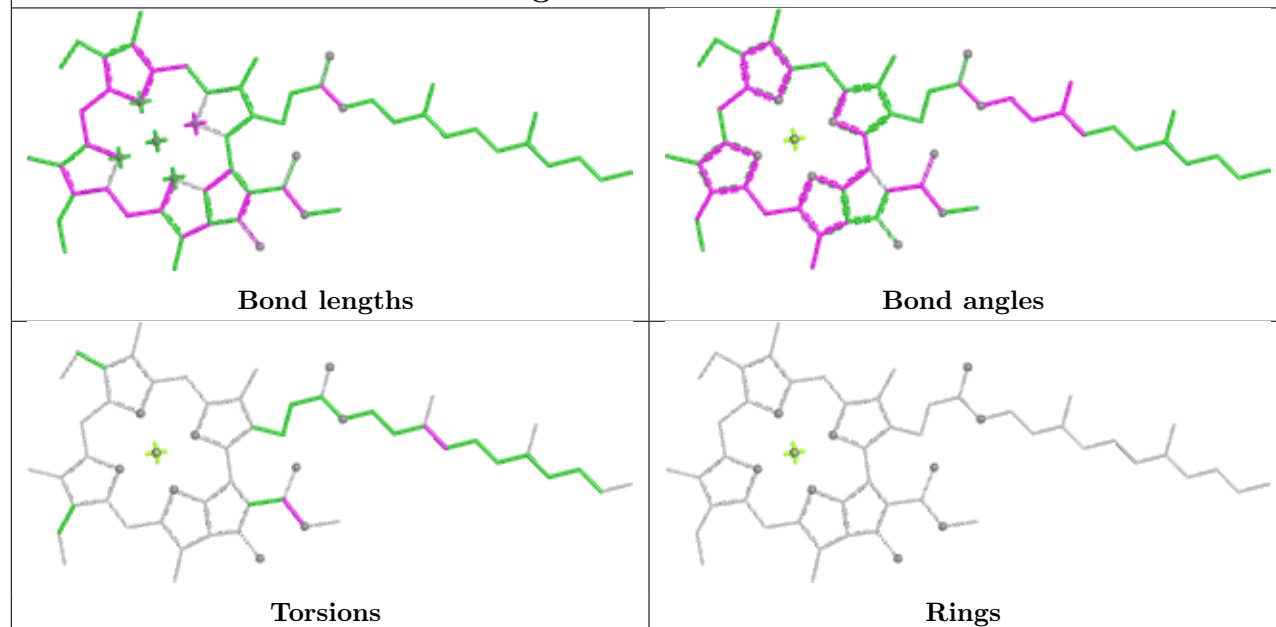
Ligand CLA 5 309



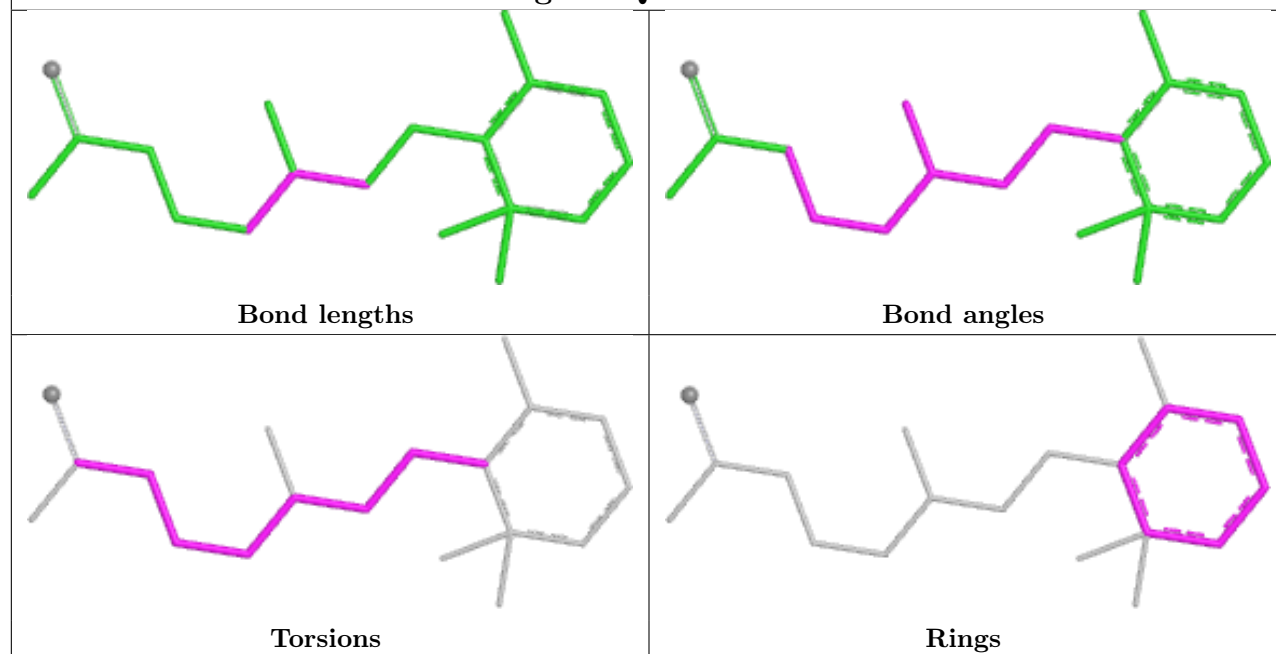
Ligand CLA B 814



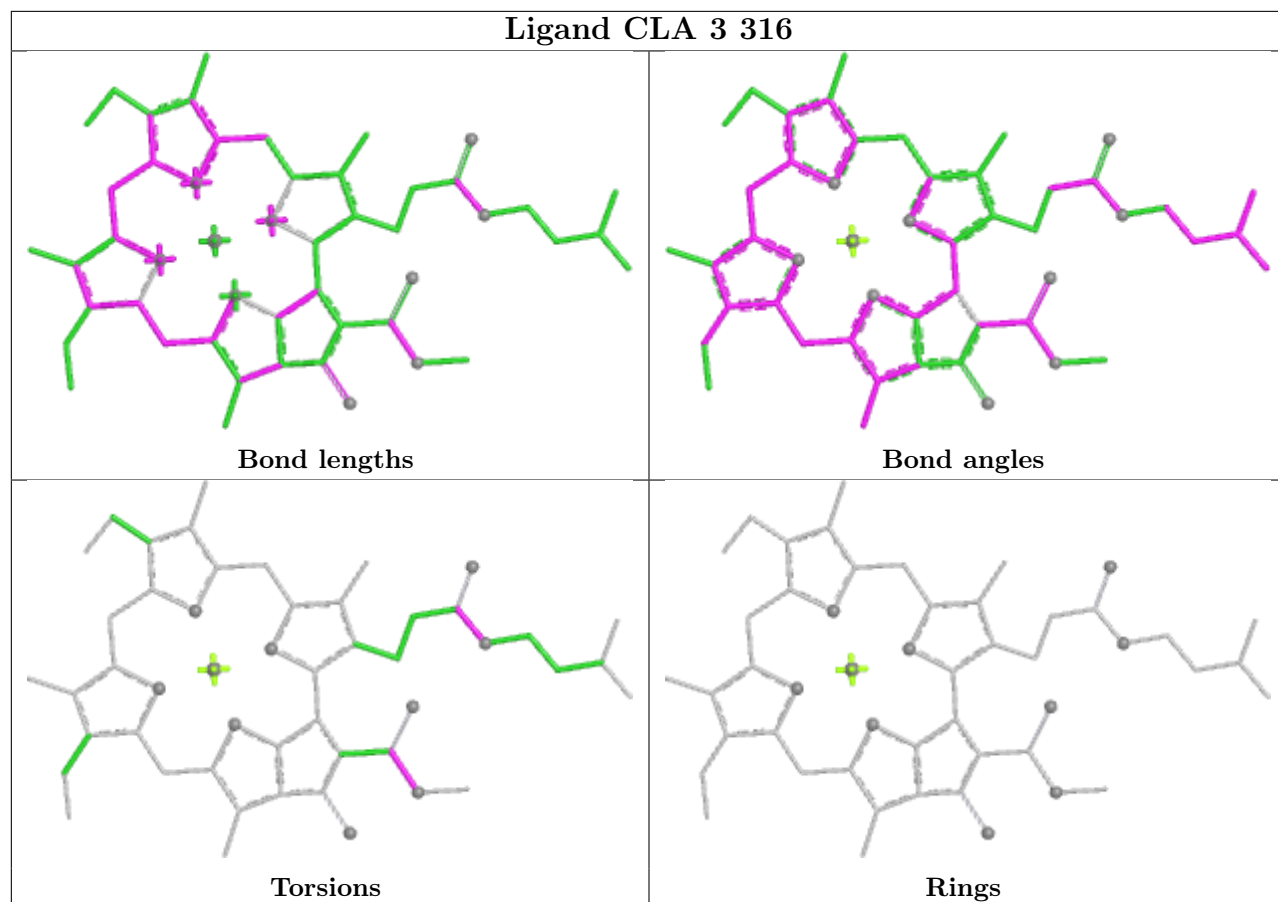
Ligand CLA B 821



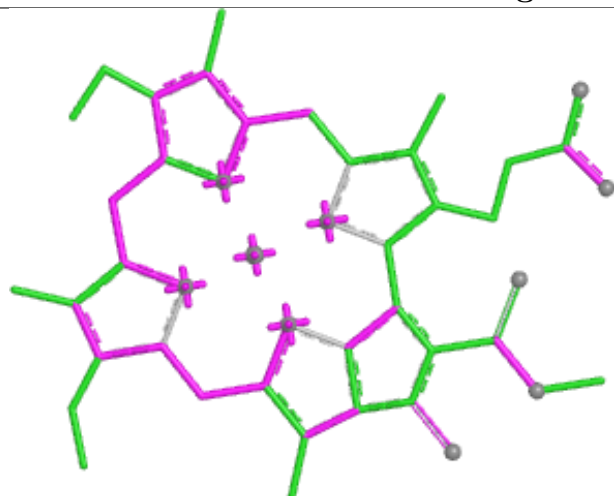
Ligand QTB 7 303



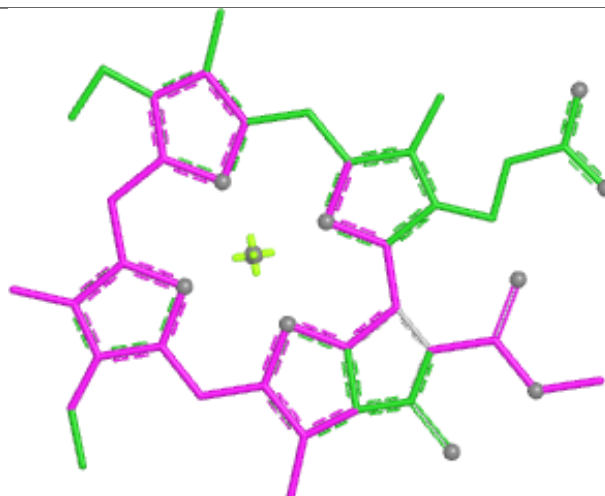
Ligand CLA 3 316



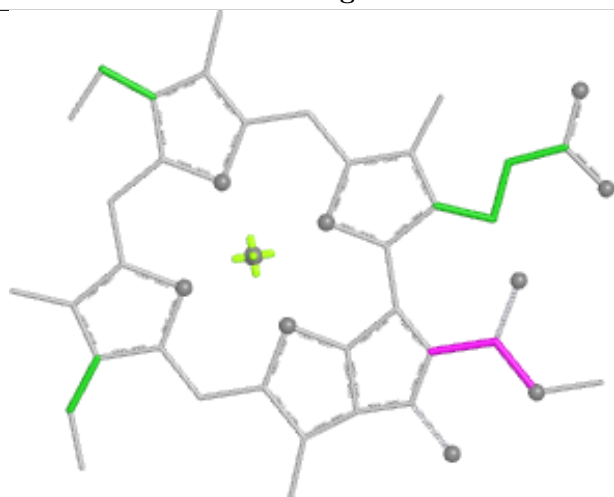
Ligand CLA L 306



Bond lengths



Bond angles

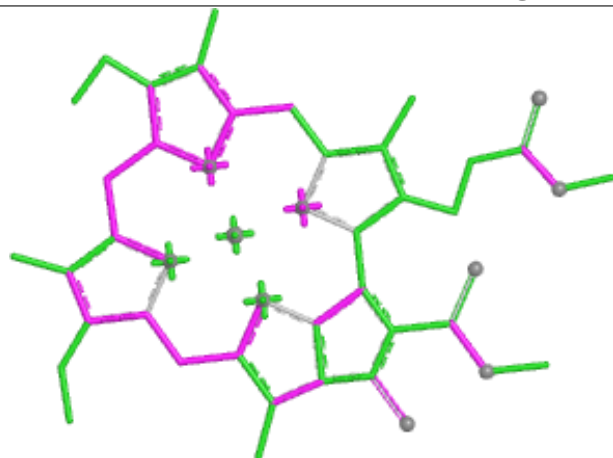


Torsions

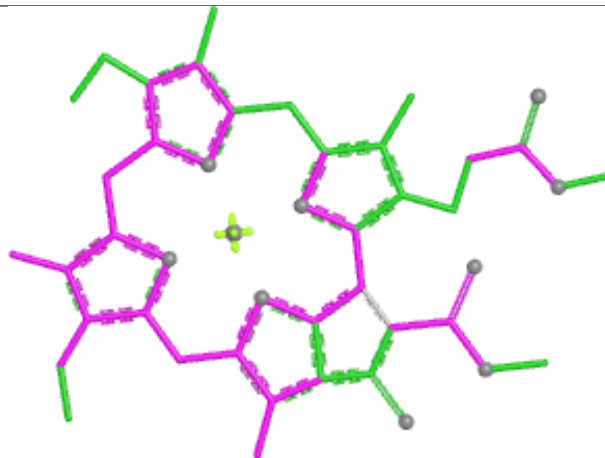


Rings

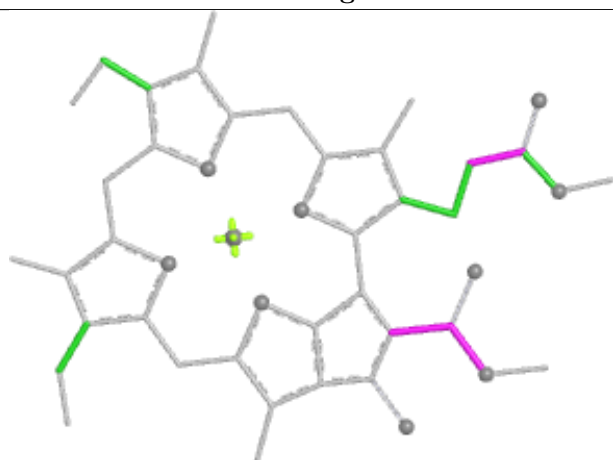
Ligand CLA A 854



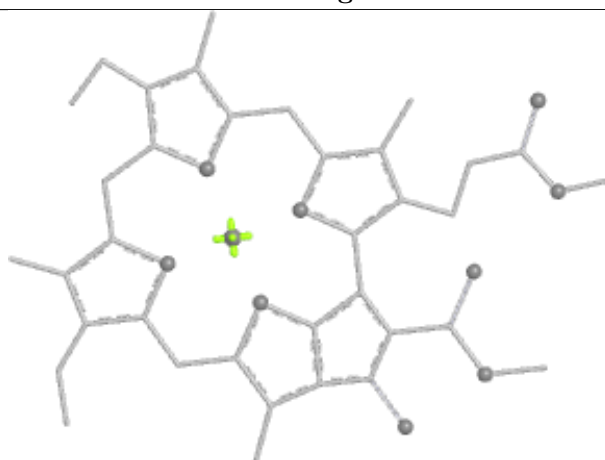
Bond lengths



Bond angles

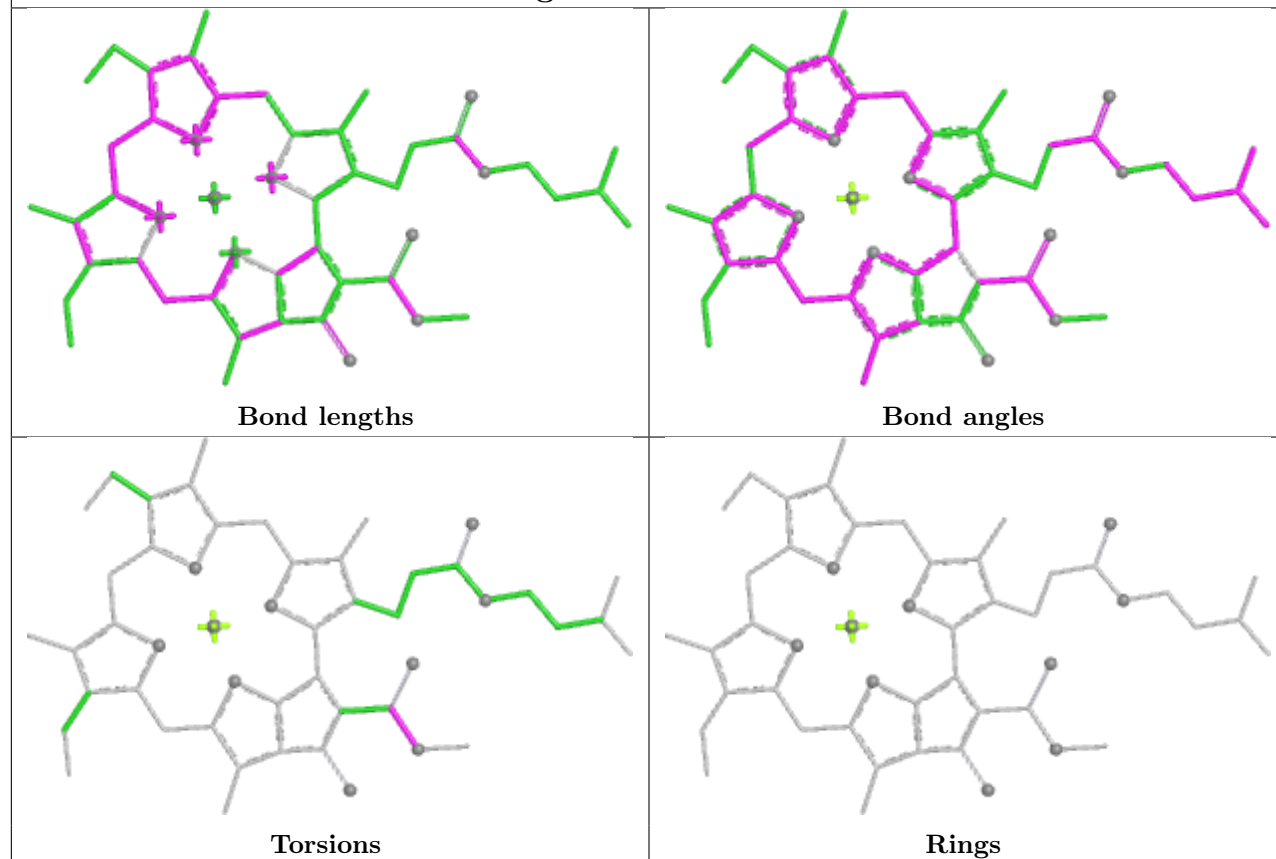


Torsions

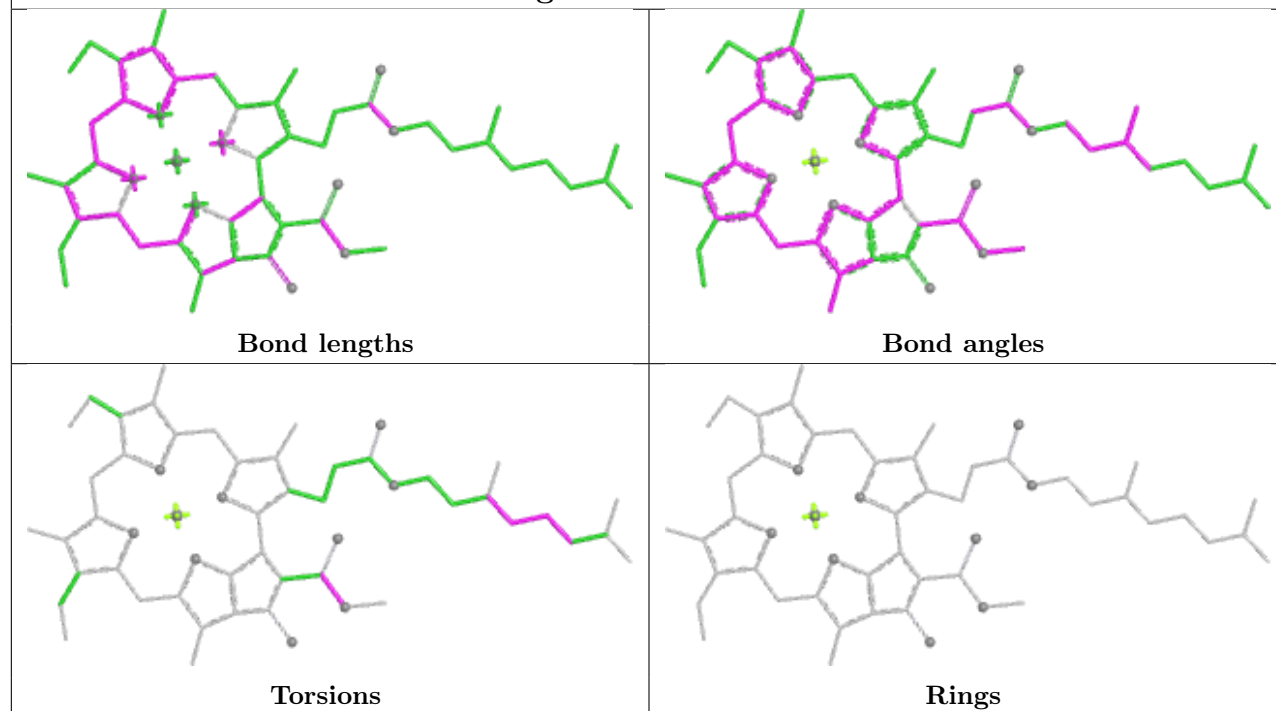


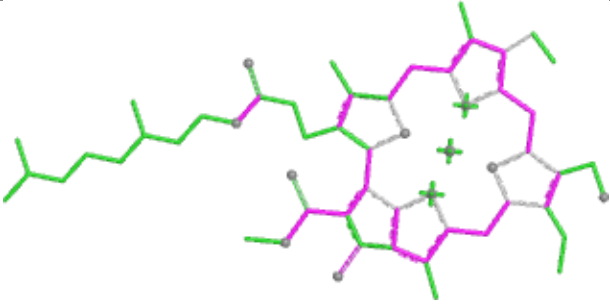
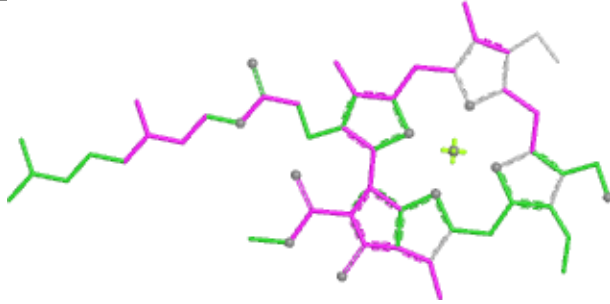
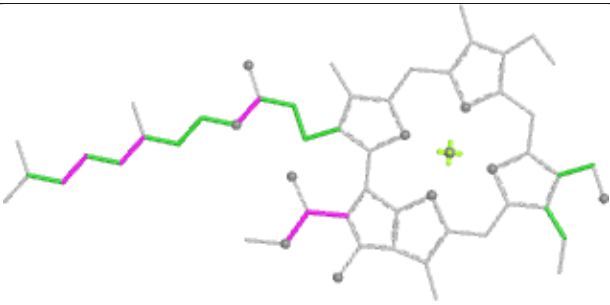
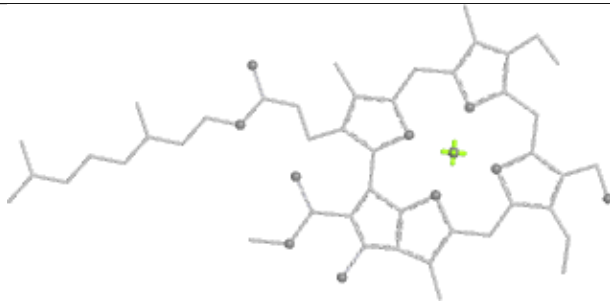
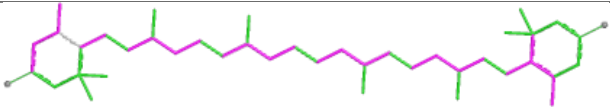
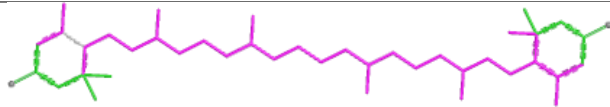
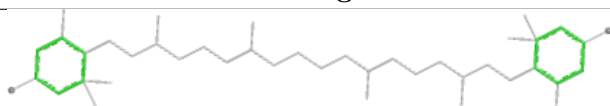
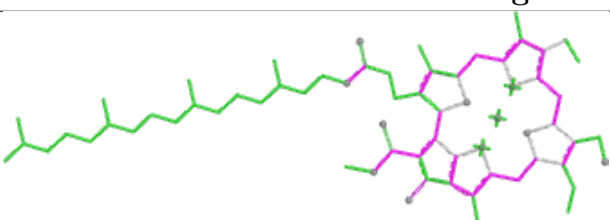
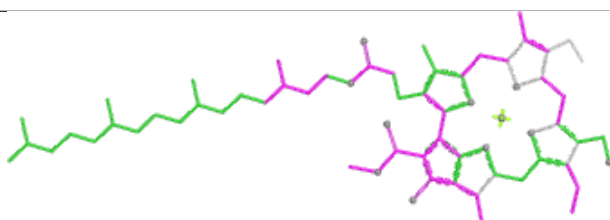
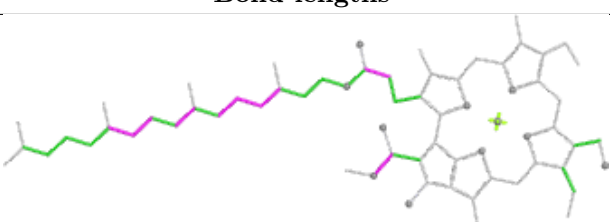
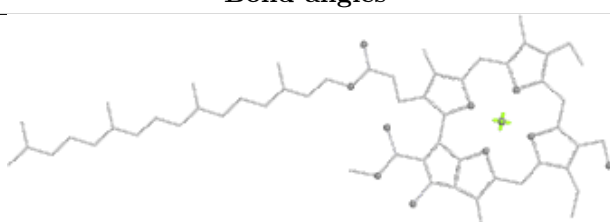
Rings

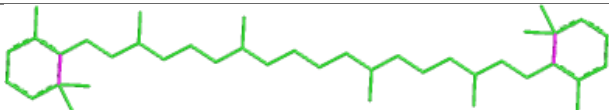
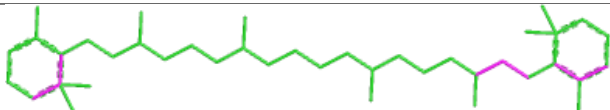
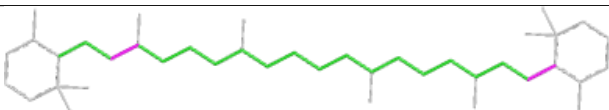
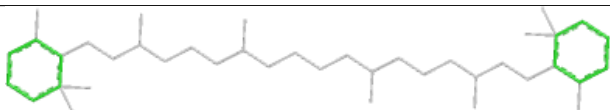
Ligand CLA 8 317

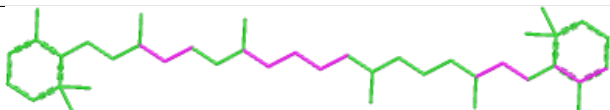
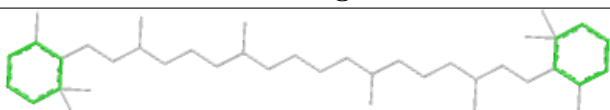


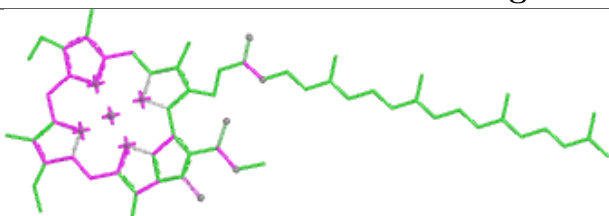
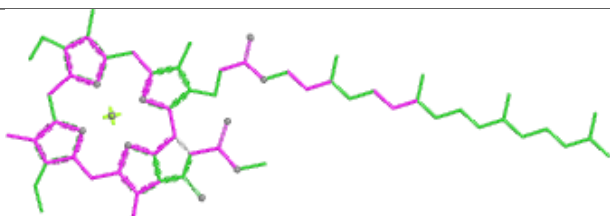
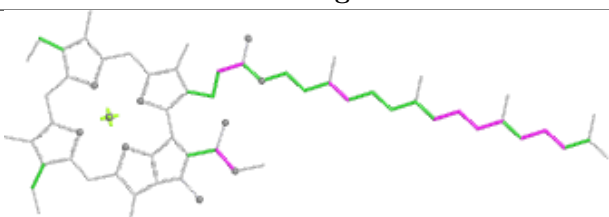
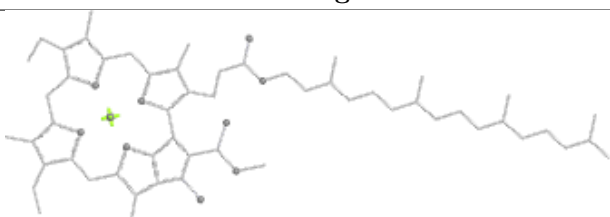
Ligand CLA a 315

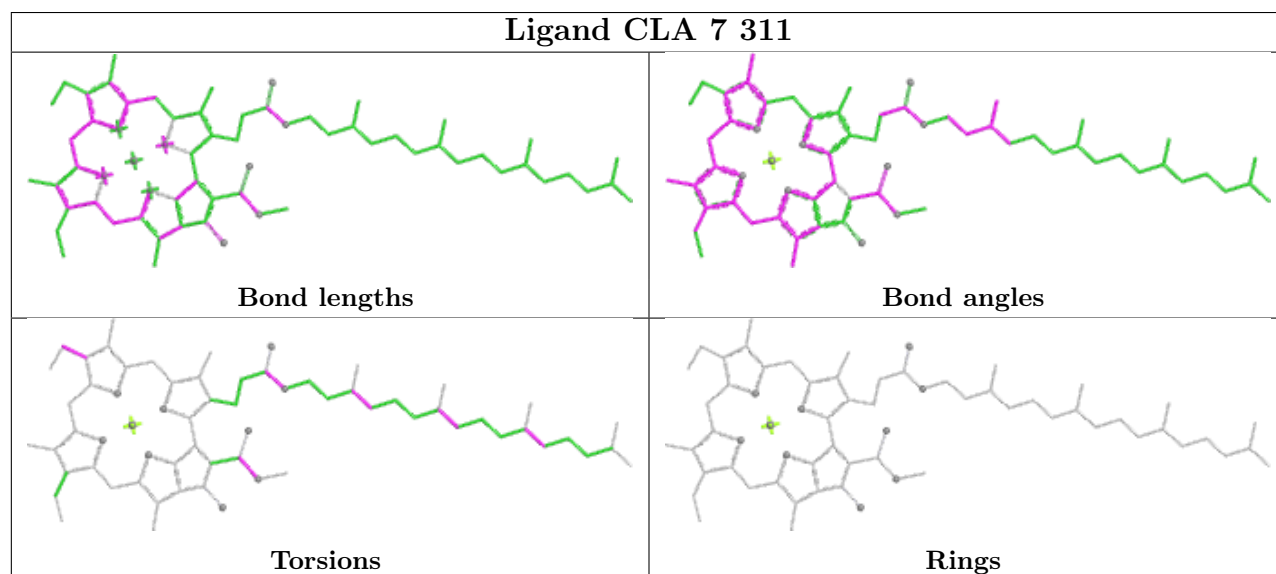
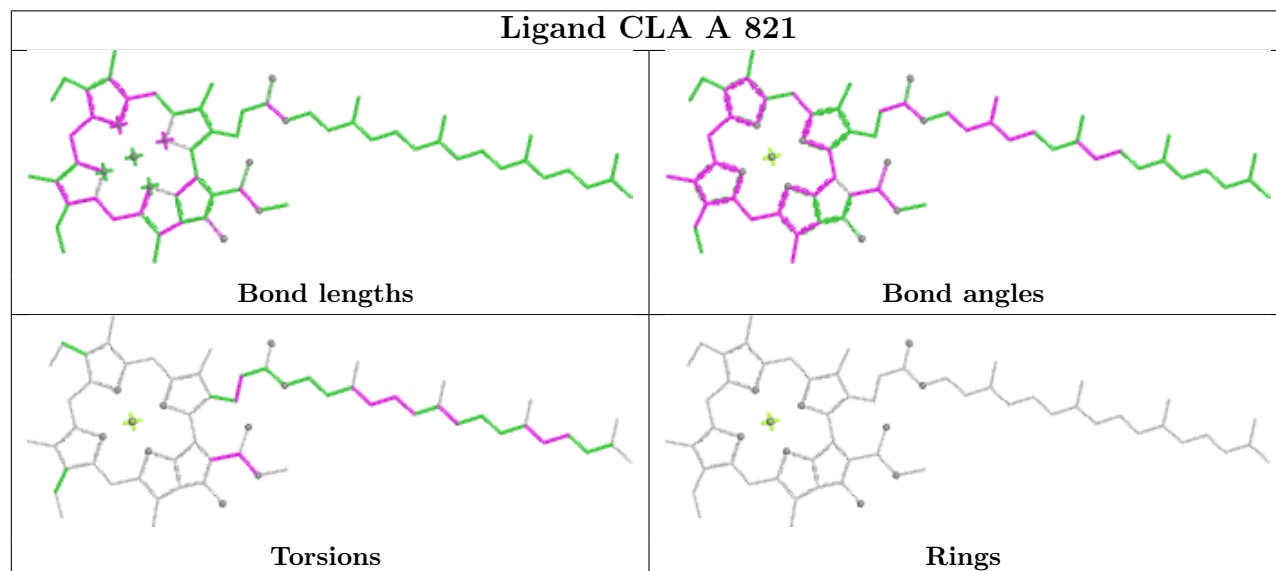
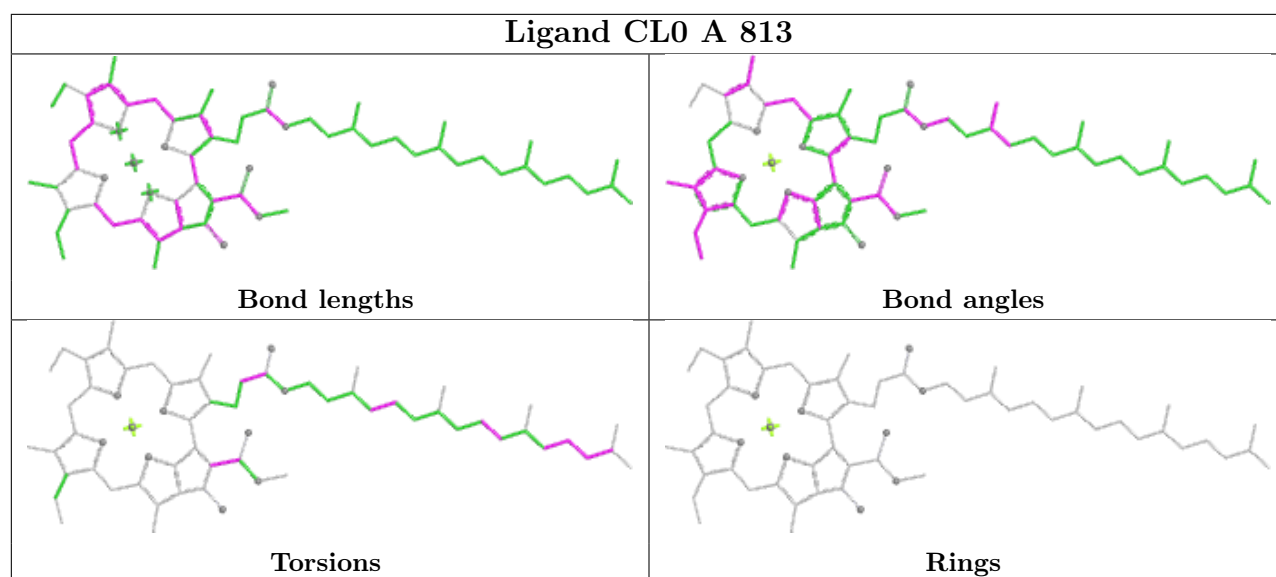


Ligand CHL 3 315	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT 9 302	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CHL 7 324	
	
Bond lengths	Bond angles
	
Torsions	Rings

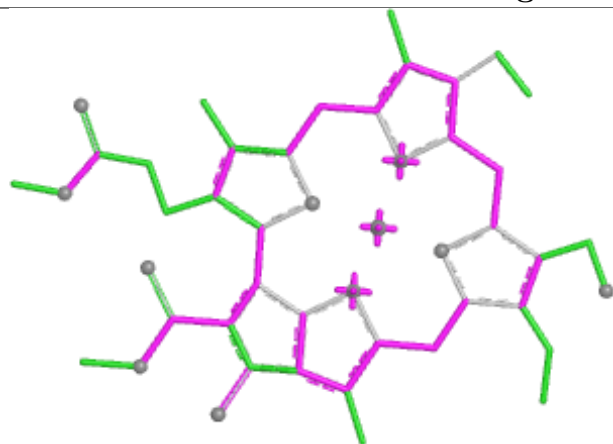
Ligand BCR J 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

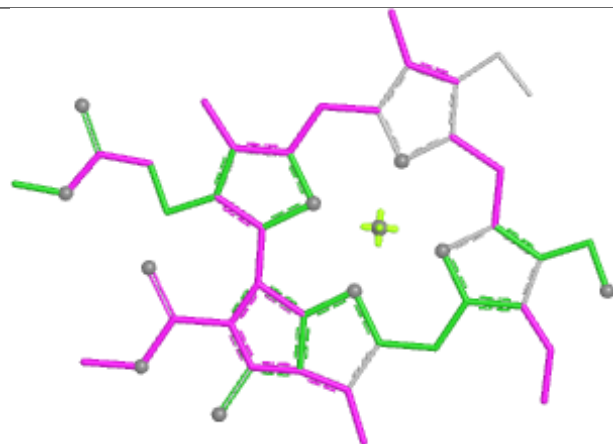
Ligand CLA B 840	
	
Bond lengths	Bond angles
	
Torsions	Rings



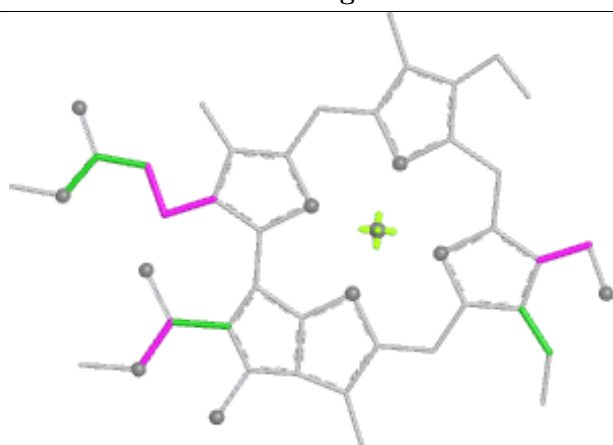
Ligand CHL b 309



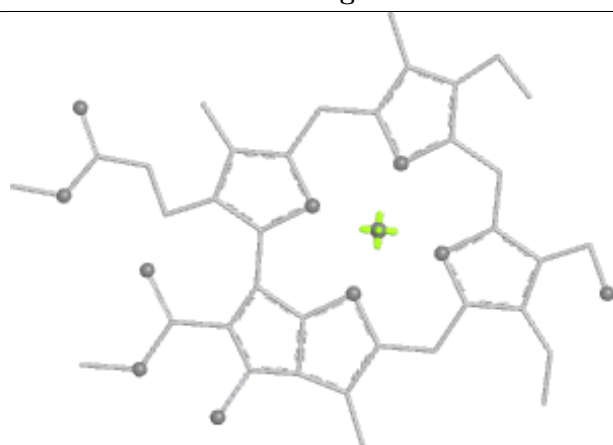
Bond lengths



Bond angles

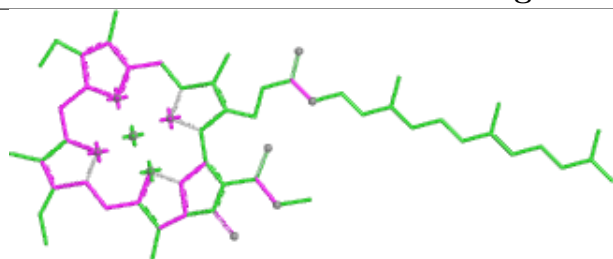


Torsions

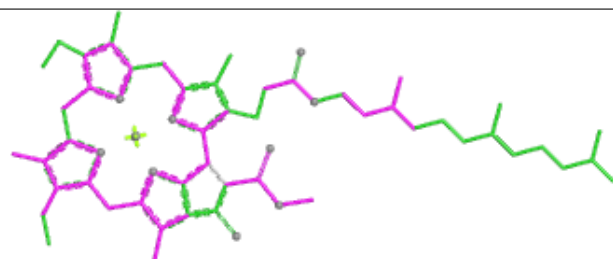


Rings

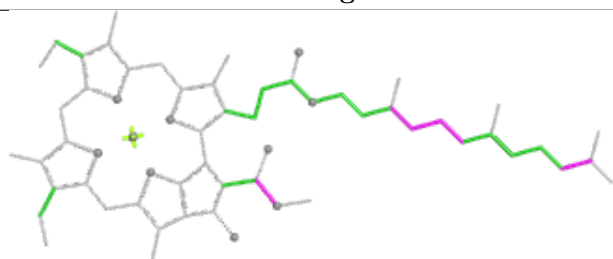
Ligand CLA B 839



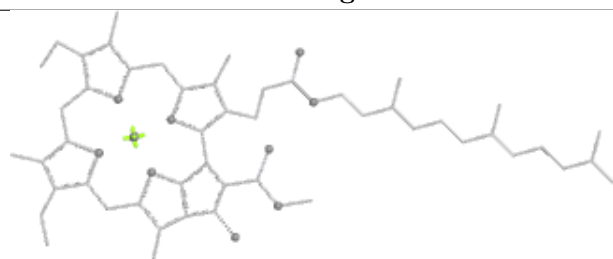
Bond lengths



Bond angles

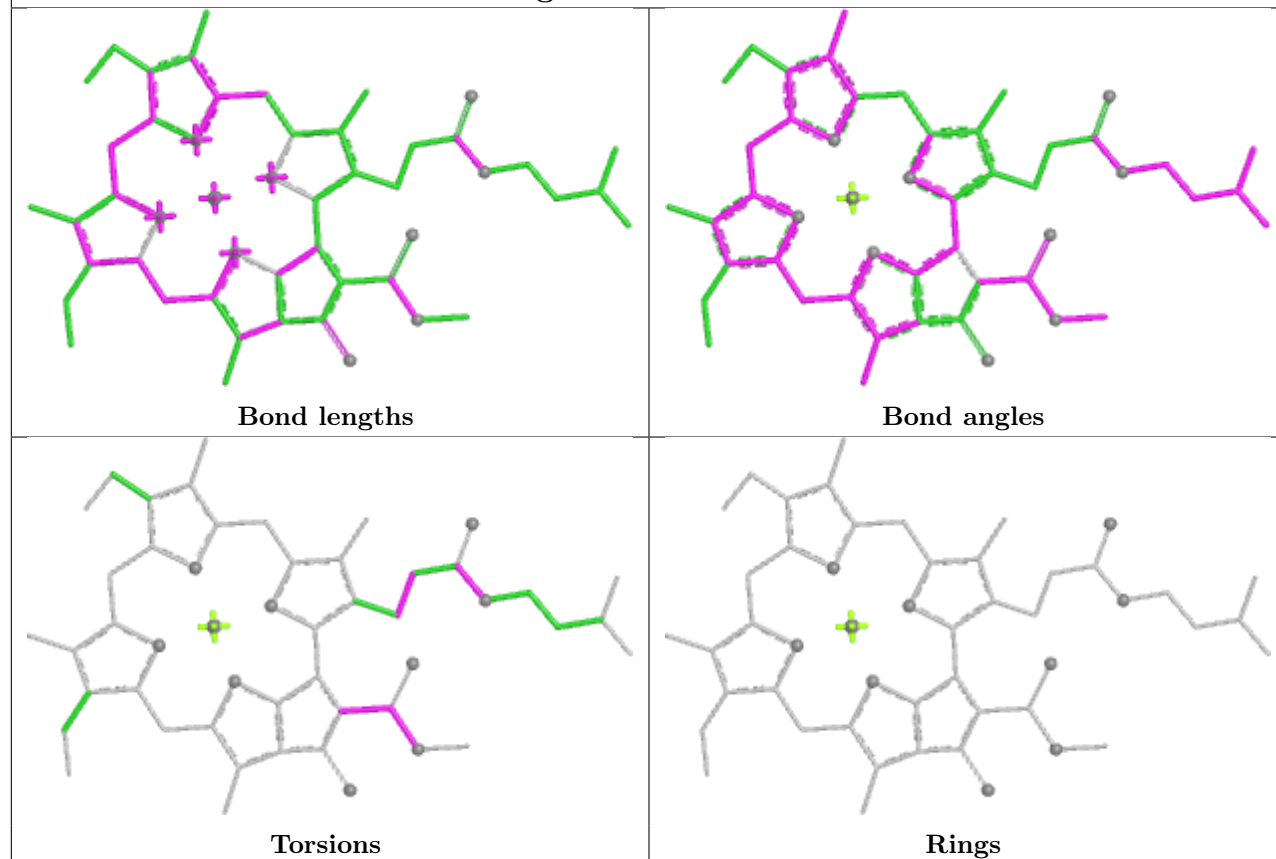


Torsions

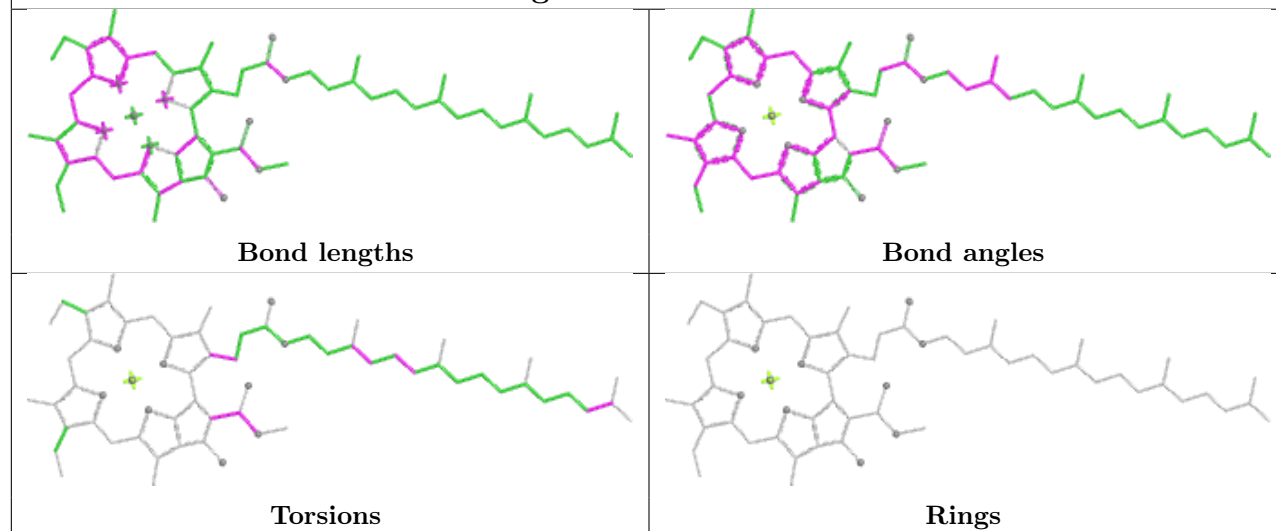


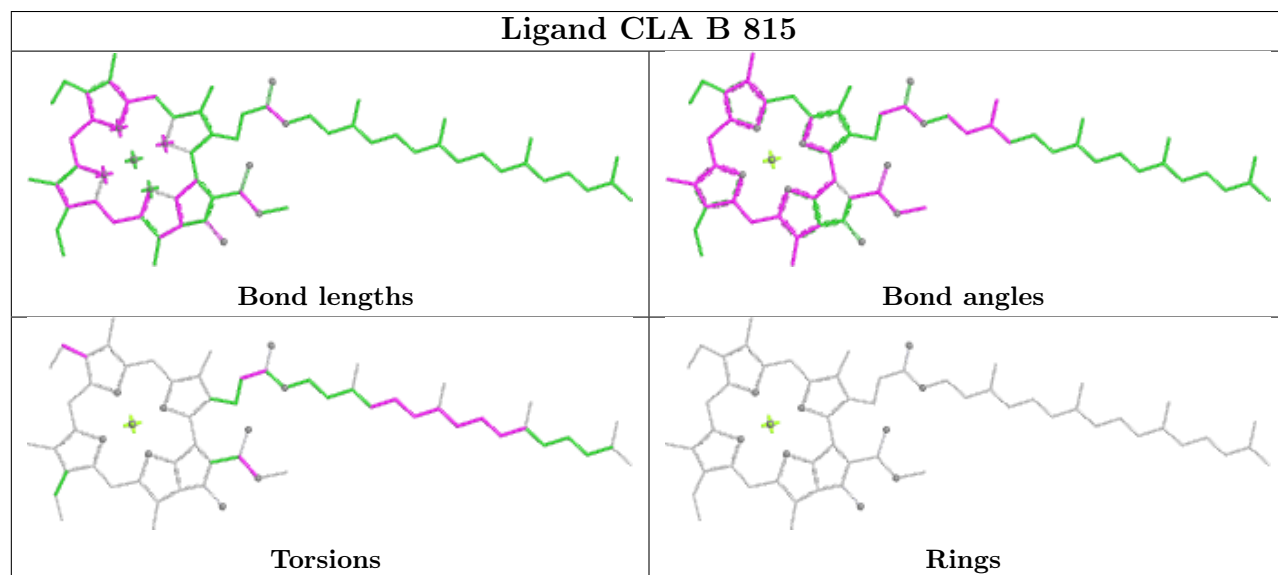
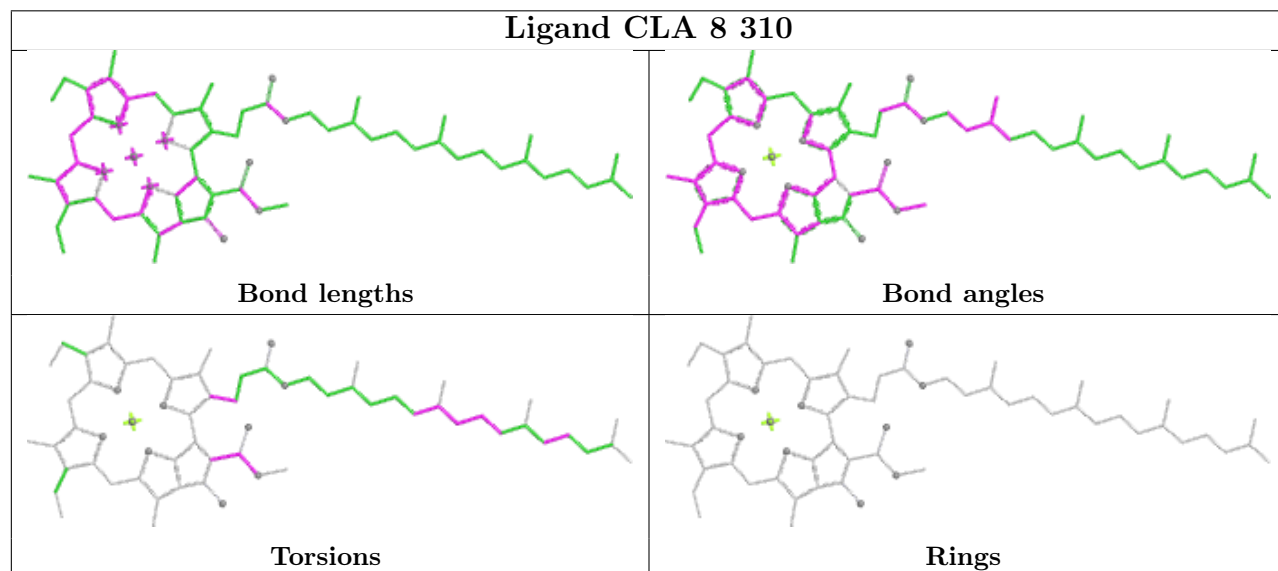
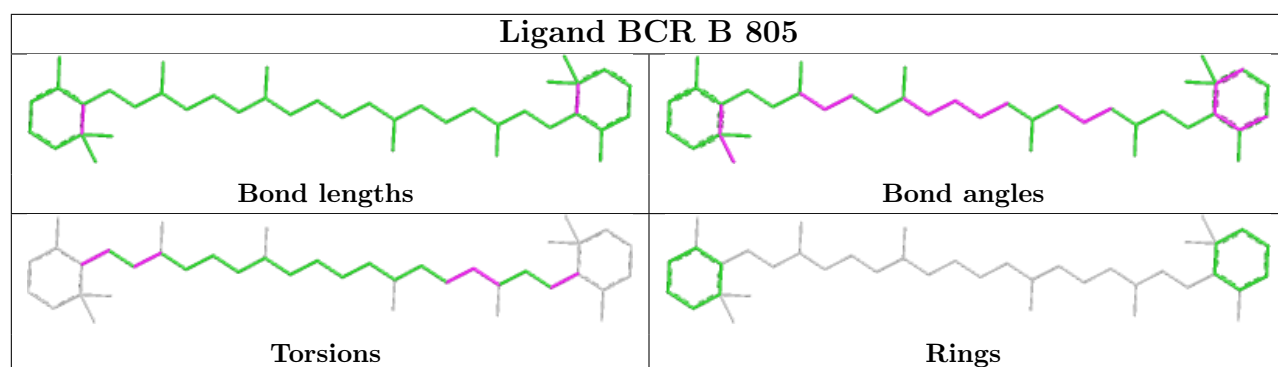
Rings

Ligand CLA a 314

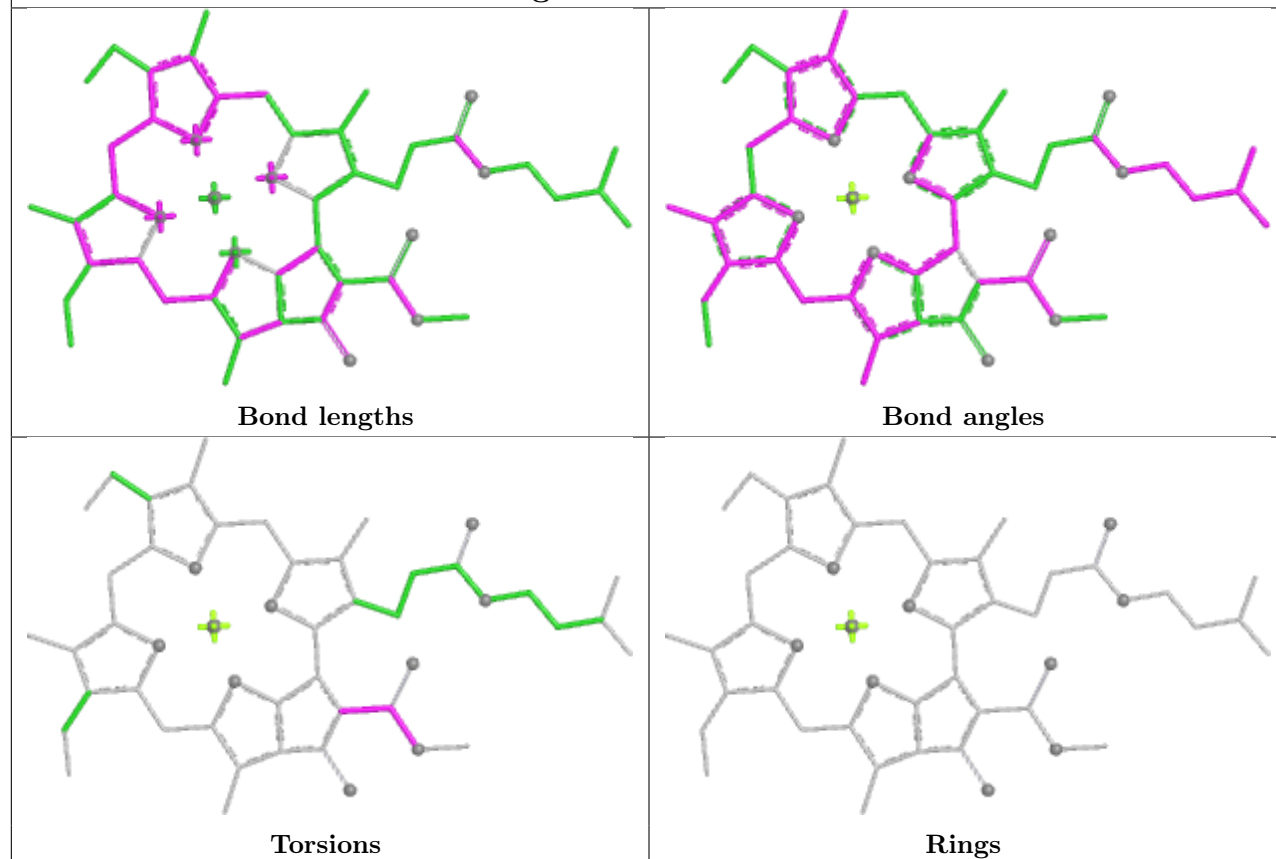


Ligand CLA A 818

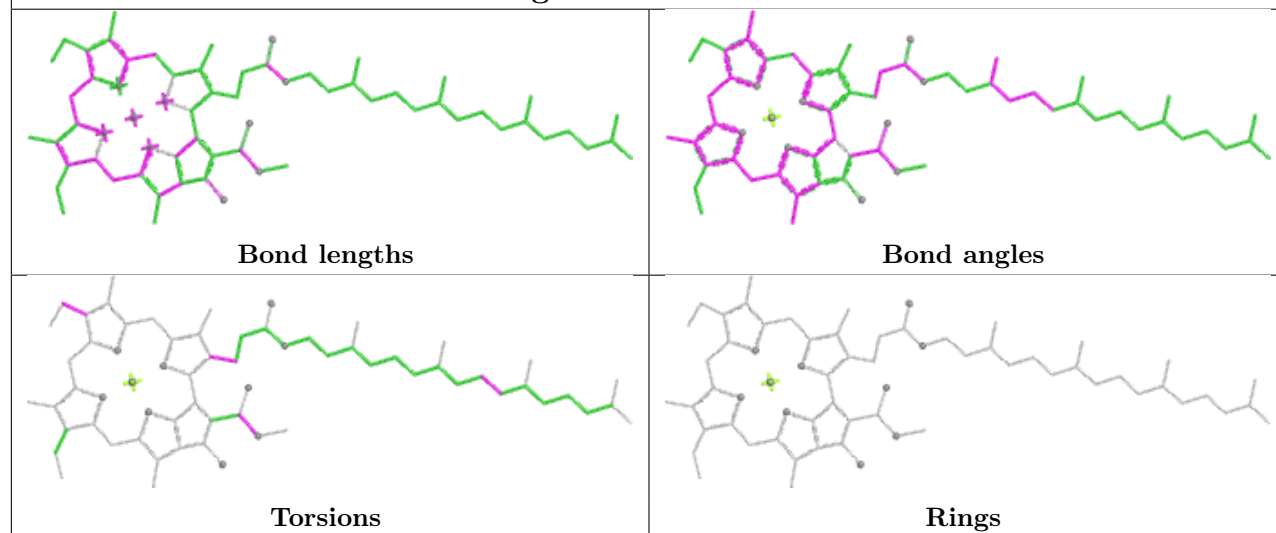


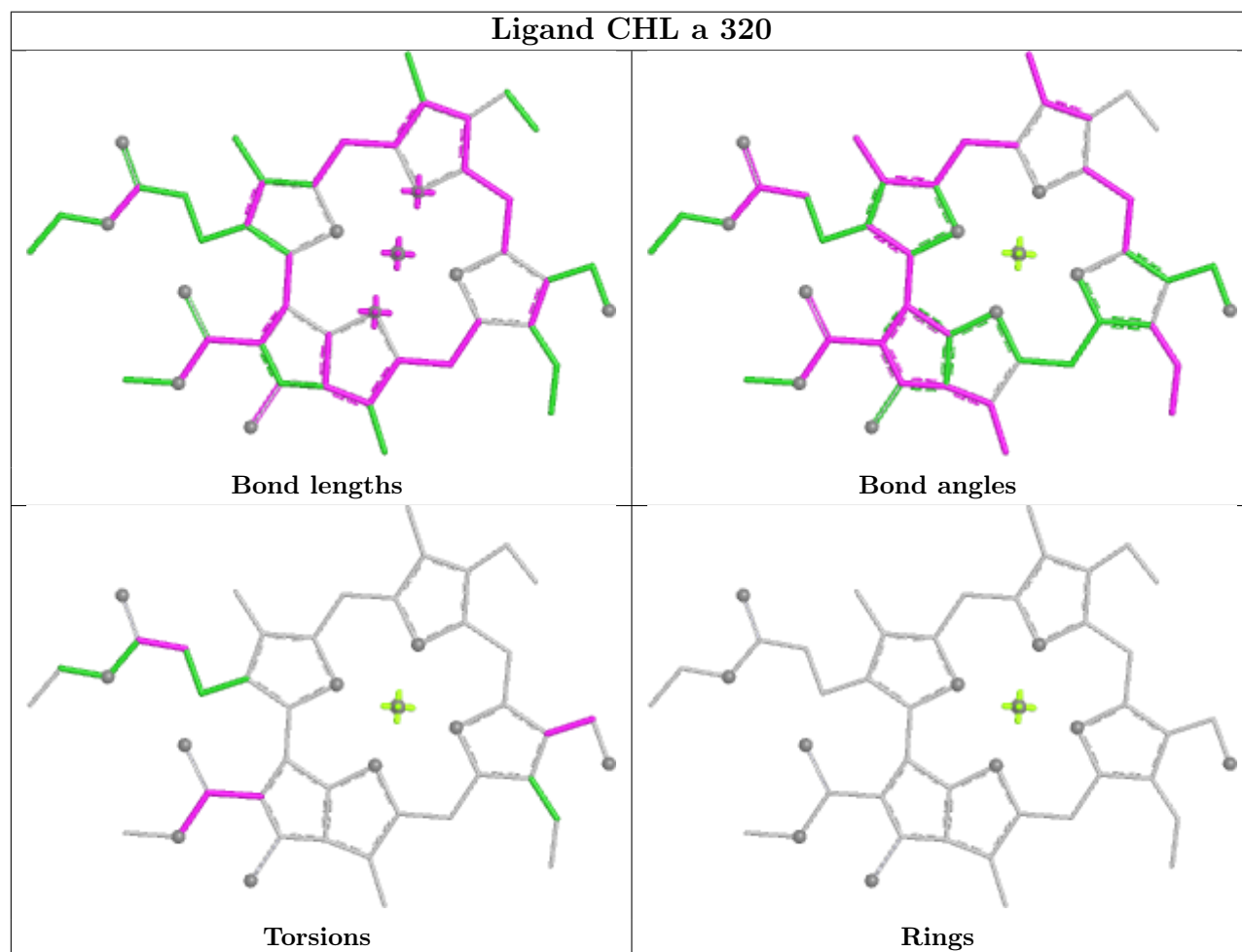
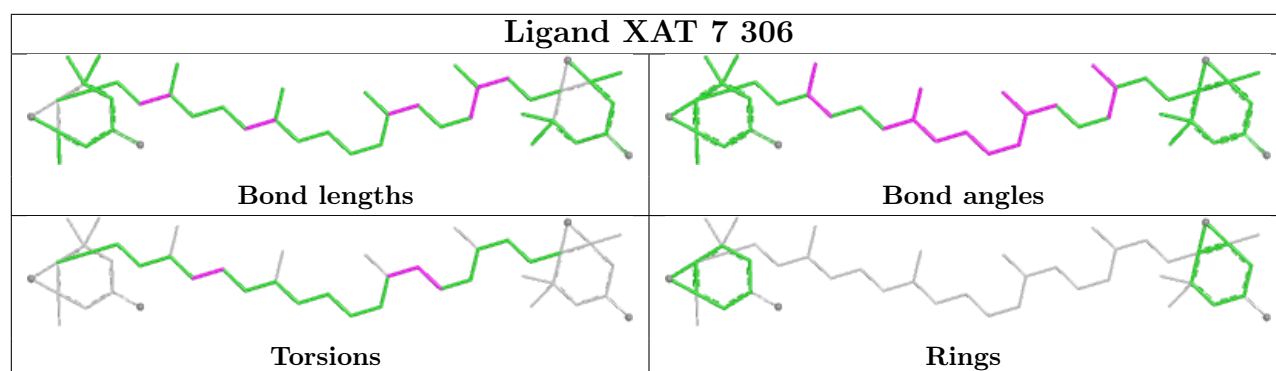


Ligand CLA B 849

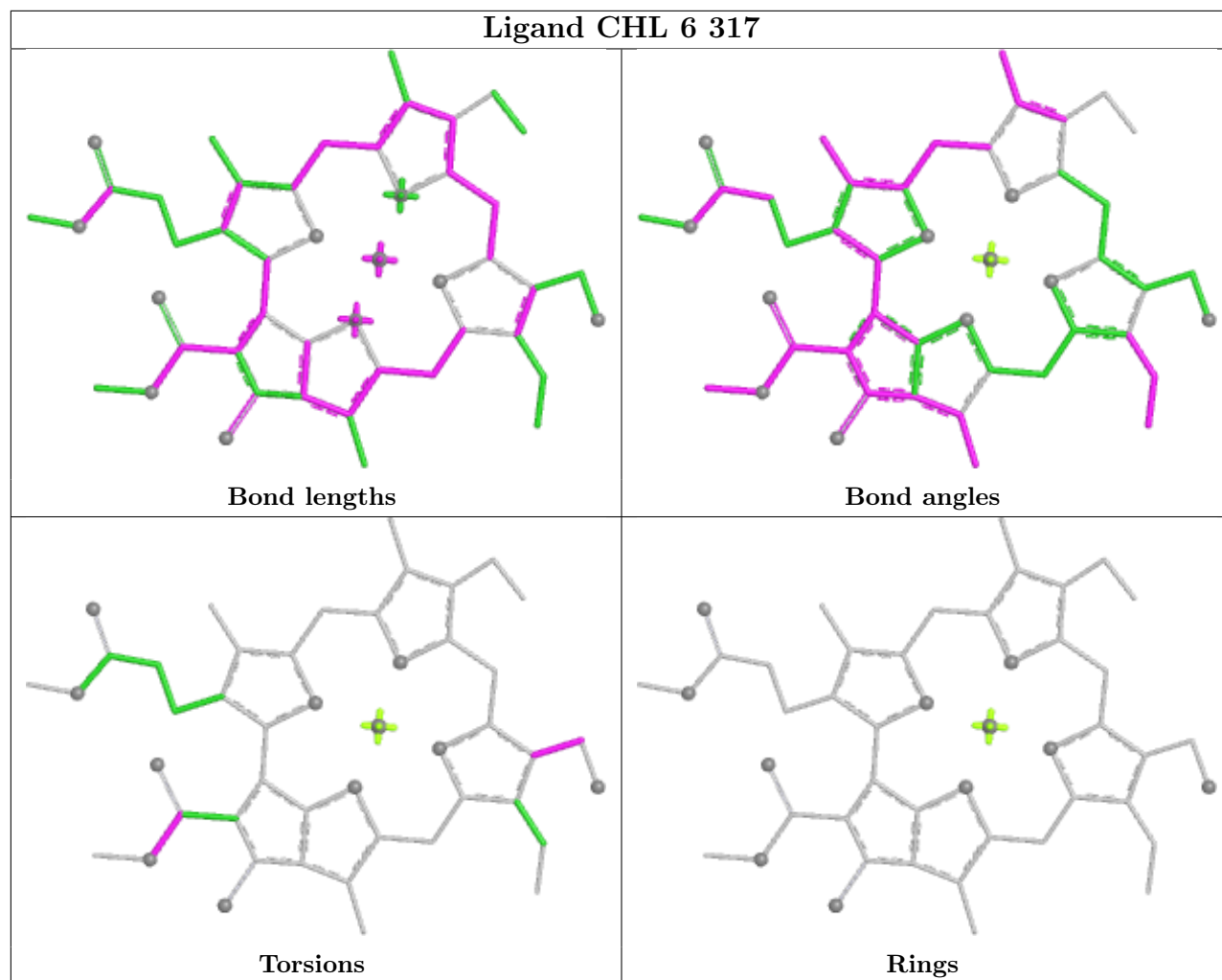


Ligand CLA A 846

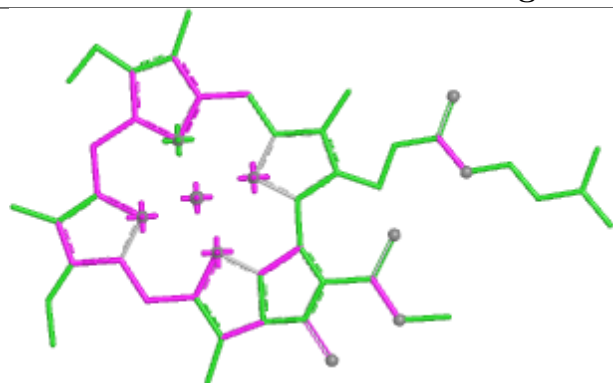




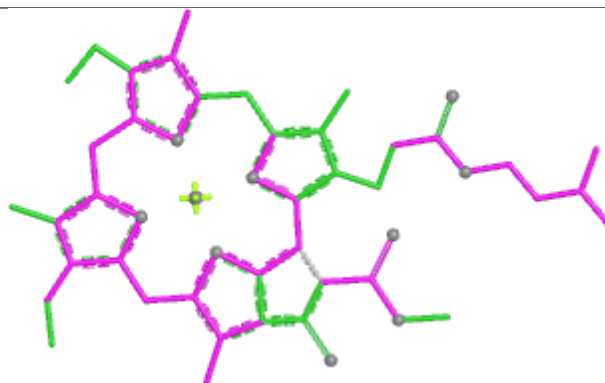
Ligand CHL 6 317



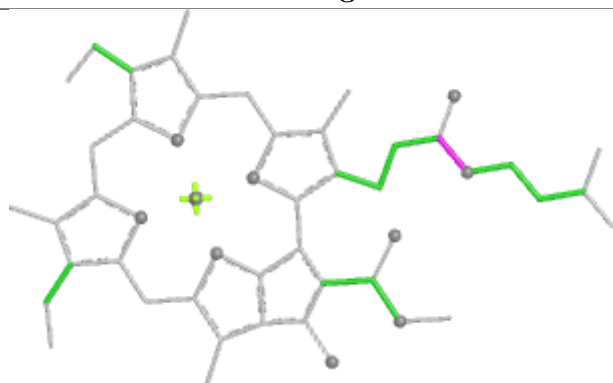
Ligand CLA 8 318



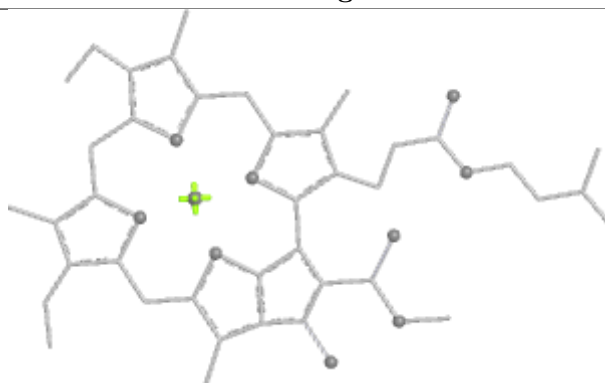
Bond lengths



Bond angles

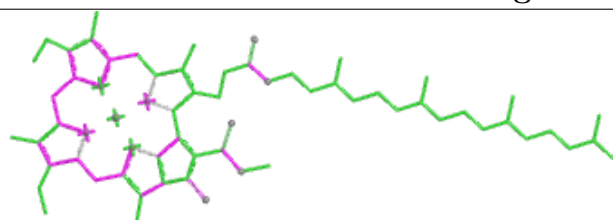


Torsions

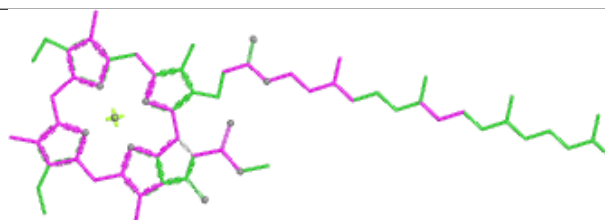


Rings

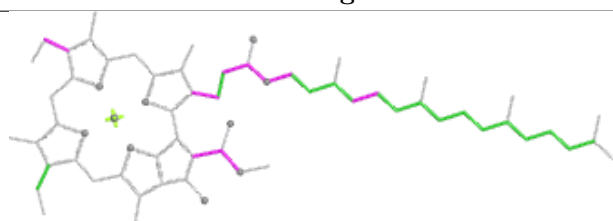
Ligand CLA A 819



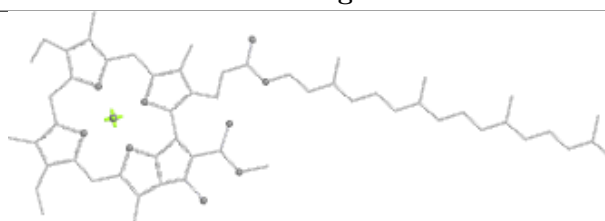
Bond lengths



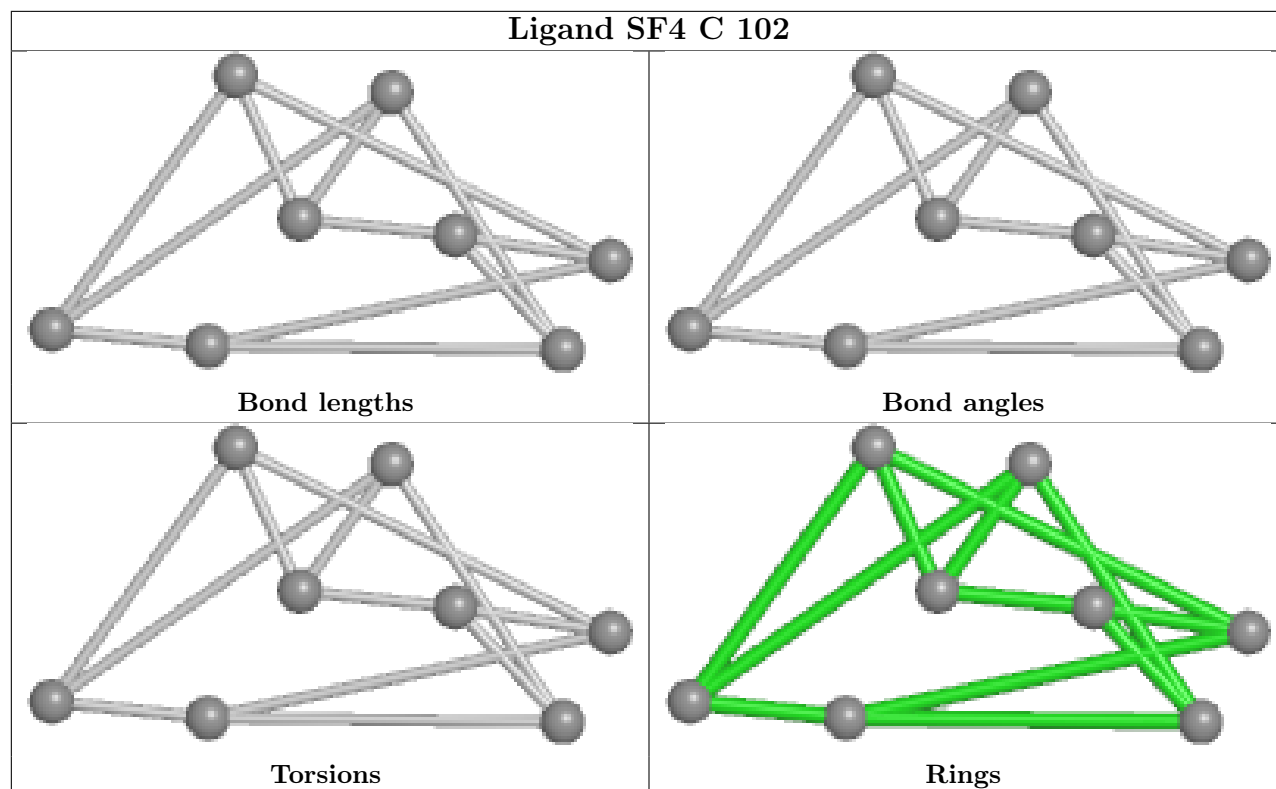
Bond angles



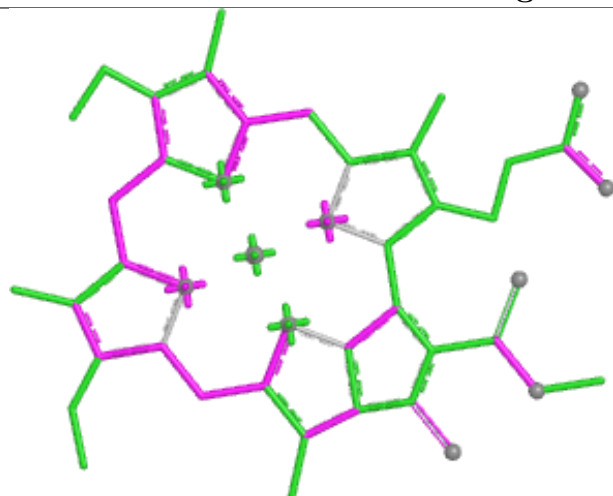
Torsions



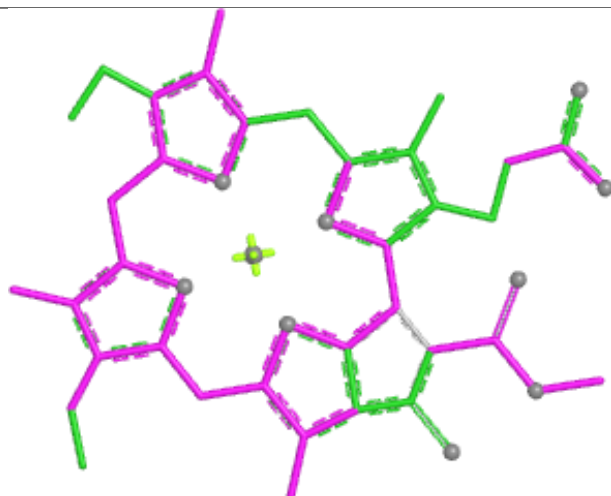
Rings



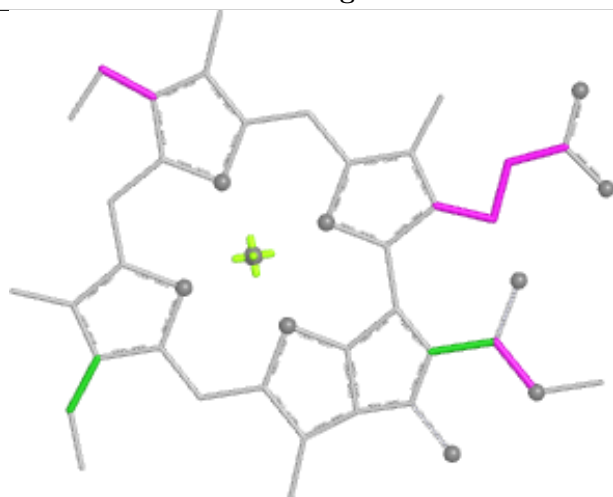
Ligand CLA L 307



Bond lengths



Bond angles

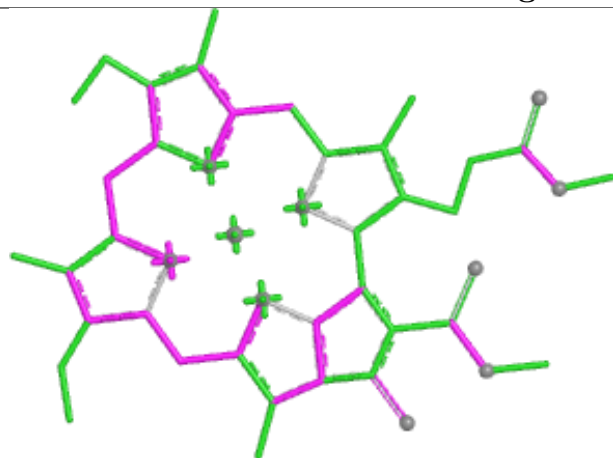


Torsions

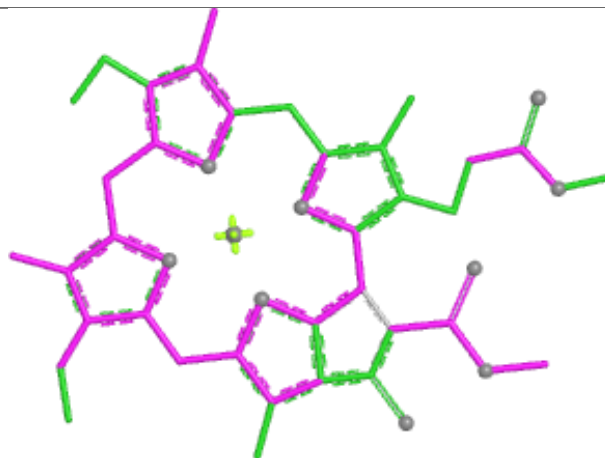


Rings

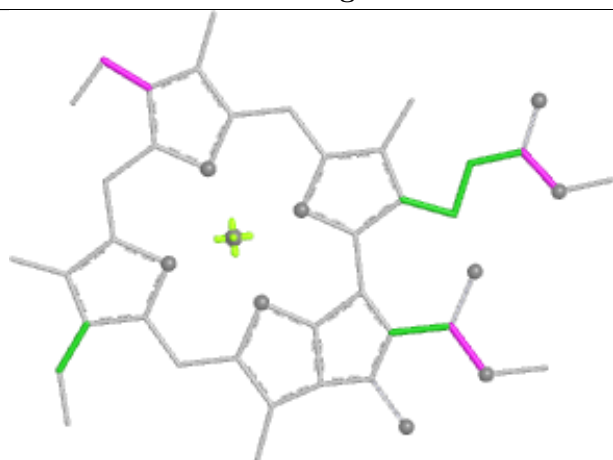
Ligand CLA 5 321



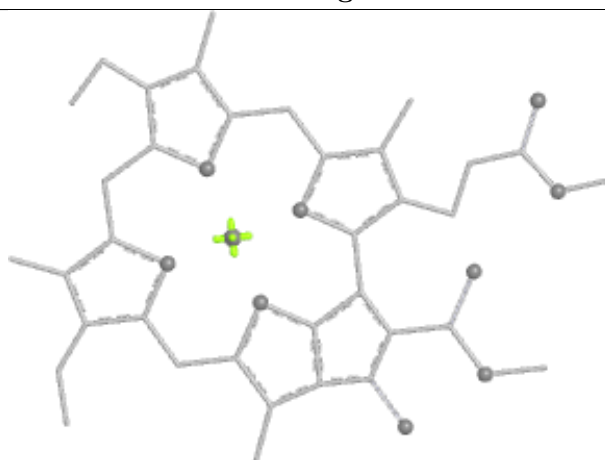
Bond lengths



Bond angles

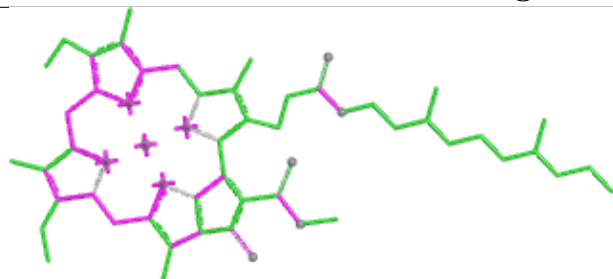


Torsions

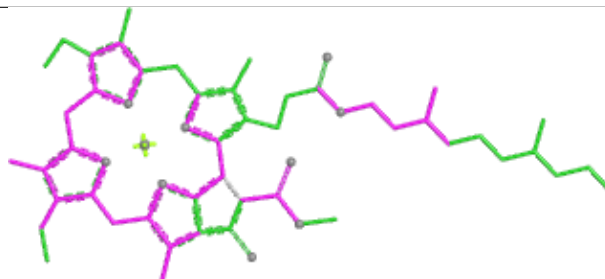


Rings

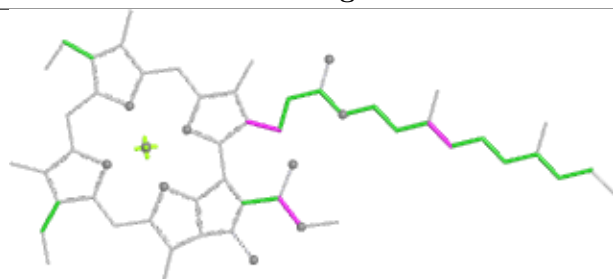
Ligand CLA B 835



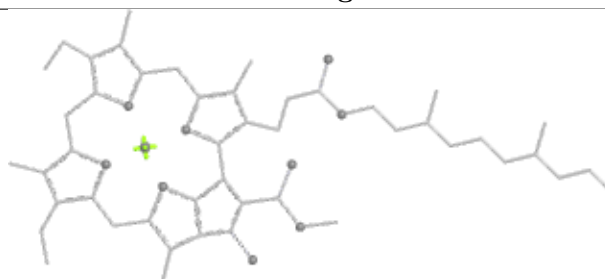
Bond lengths



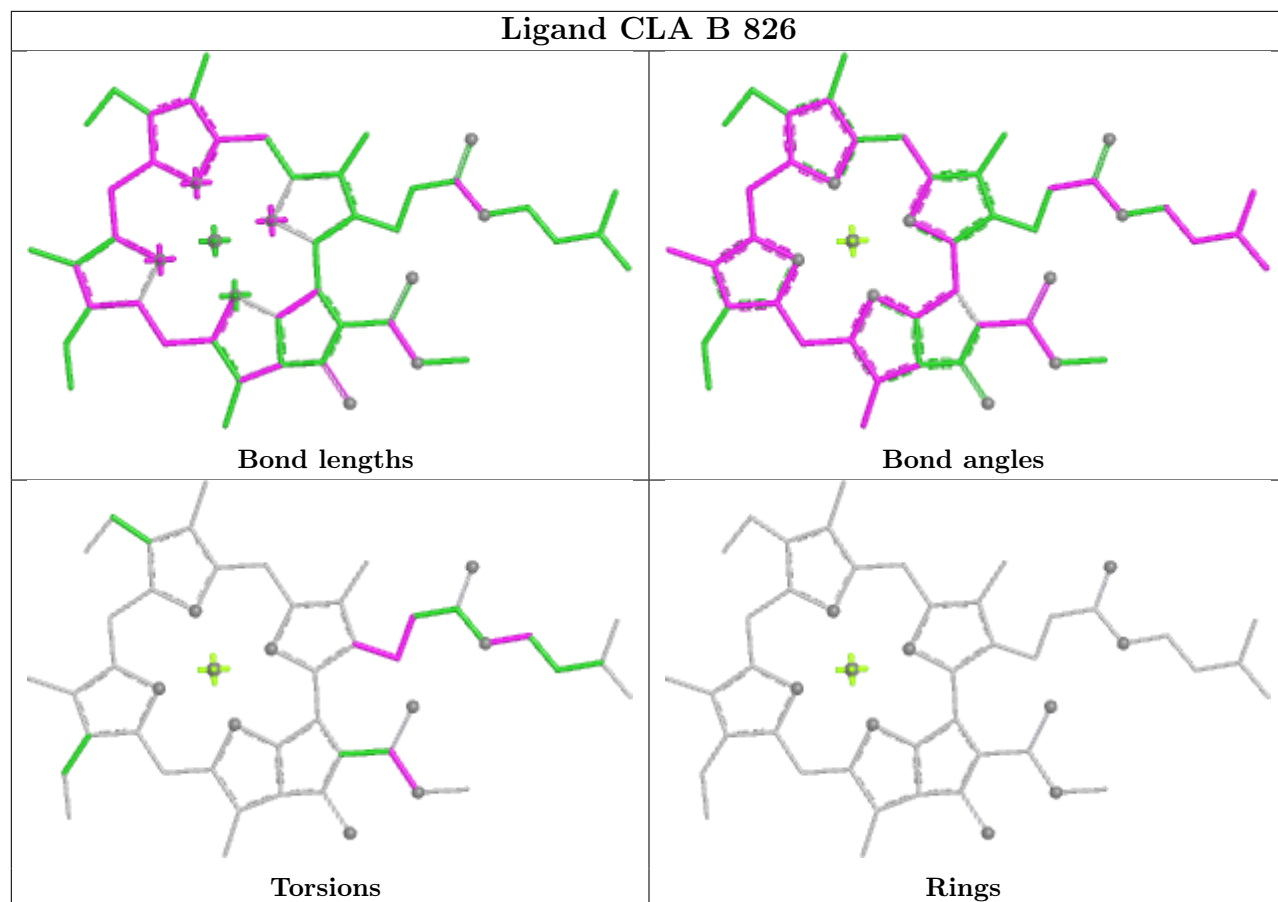
Bond angles



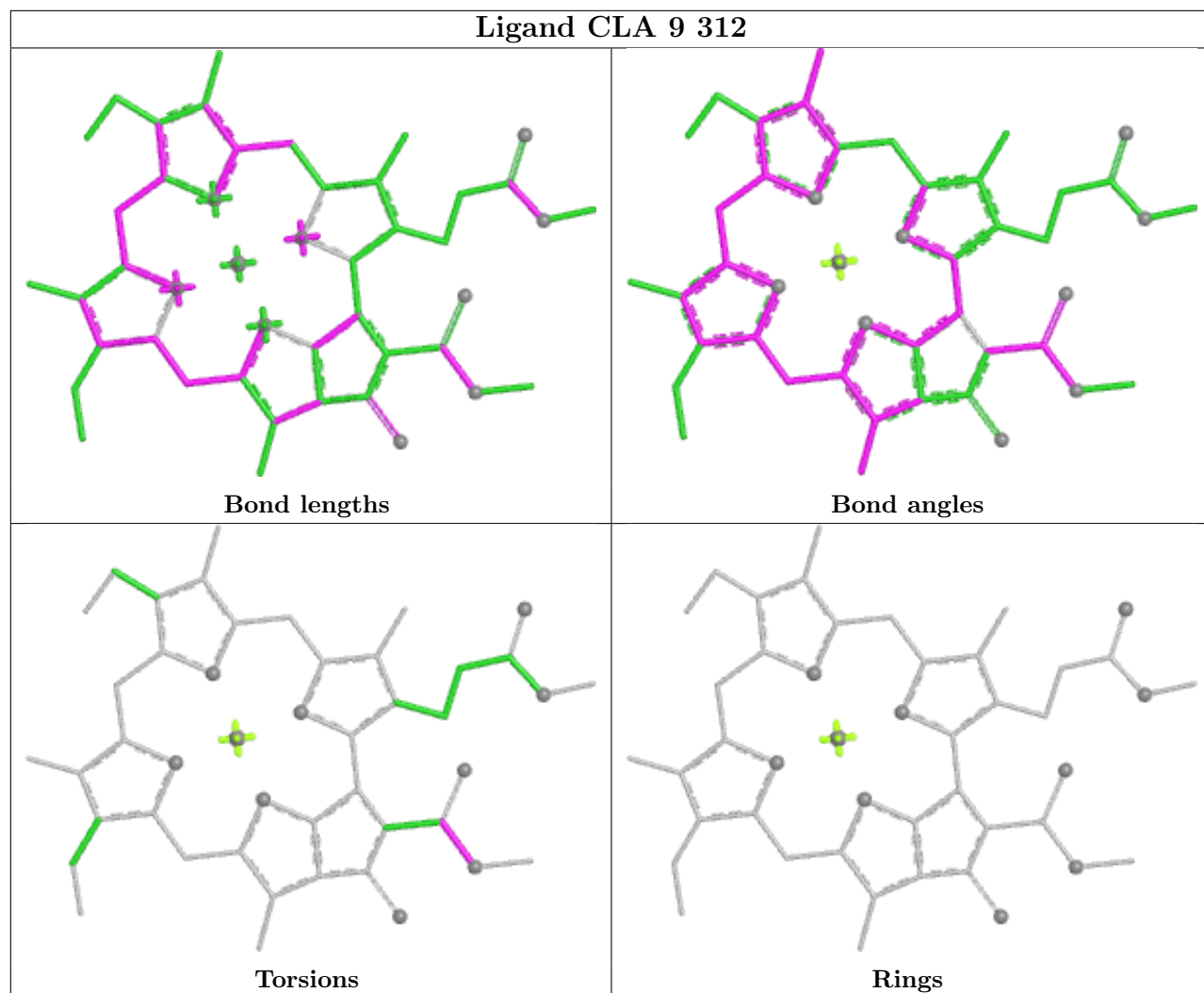
Torsions



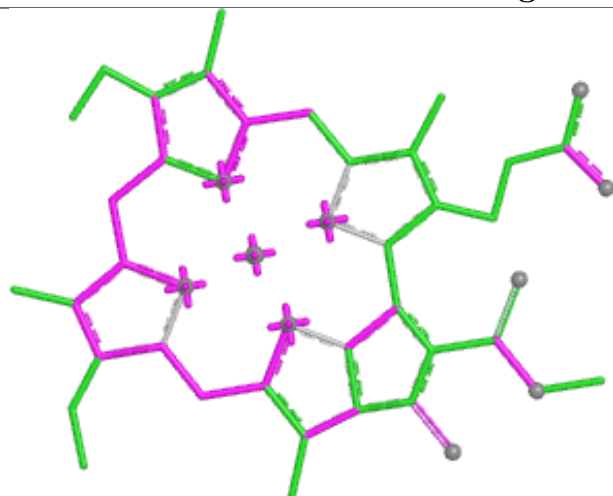
Rings



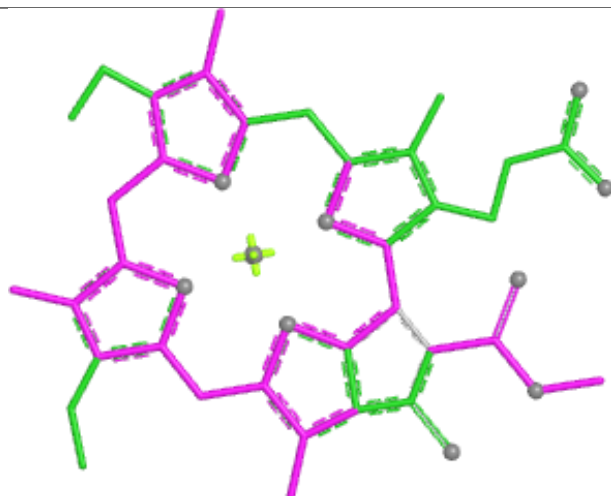
Ligand CLA 9 312



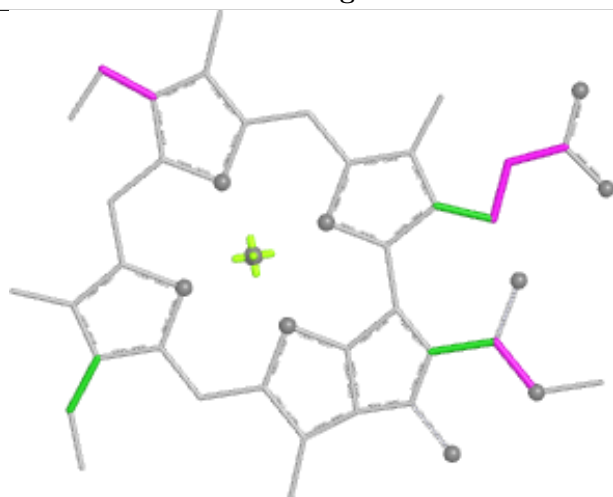
Ligand CLA 5 314



Bond lengths



Bond angles

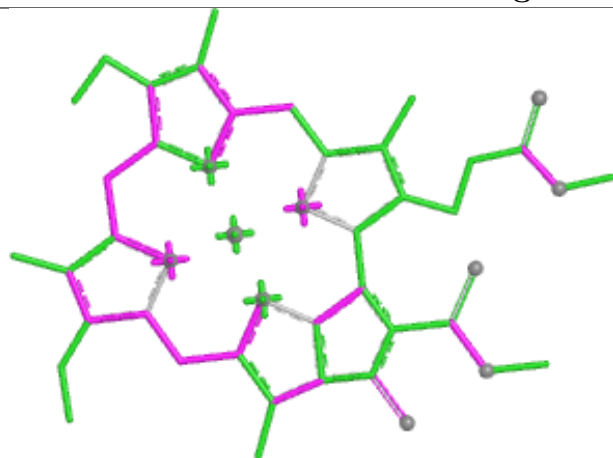


Torsions

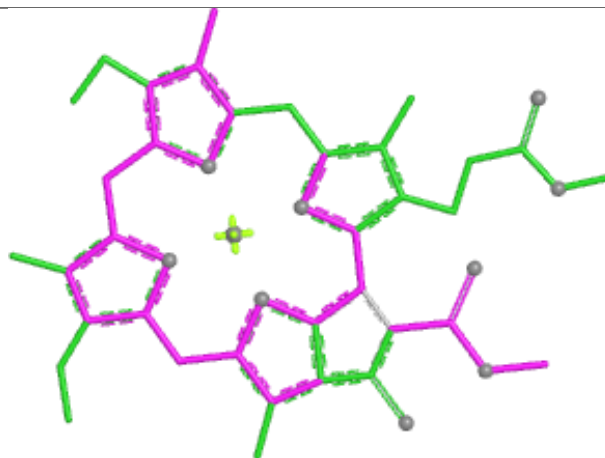


Rings

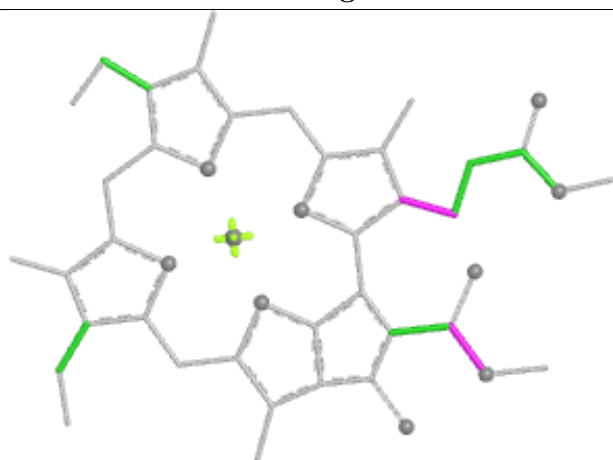
Ligand CLA H 903



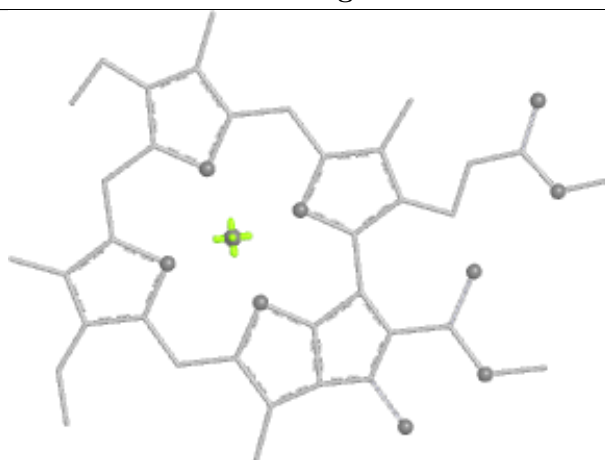
Bond lengths



Bond angles

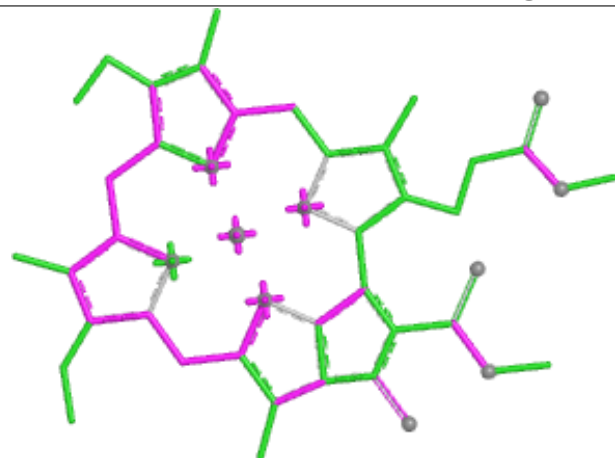


Torsions

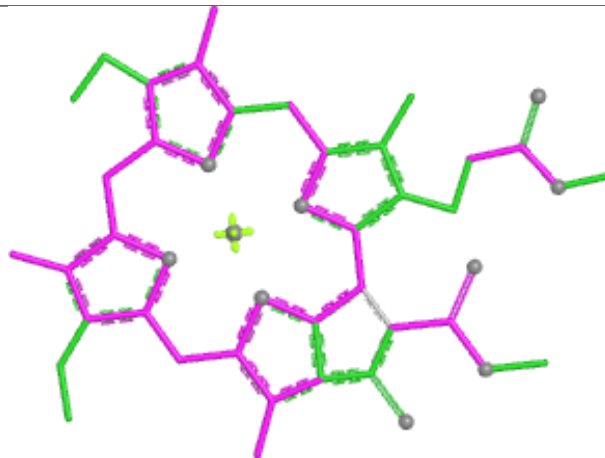


Rings

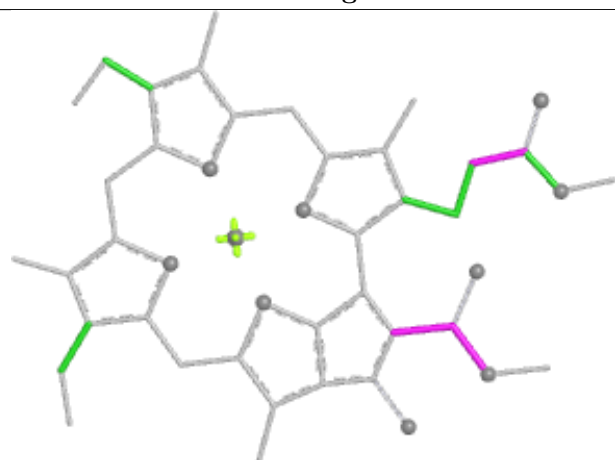
Ligand CLA 3 308



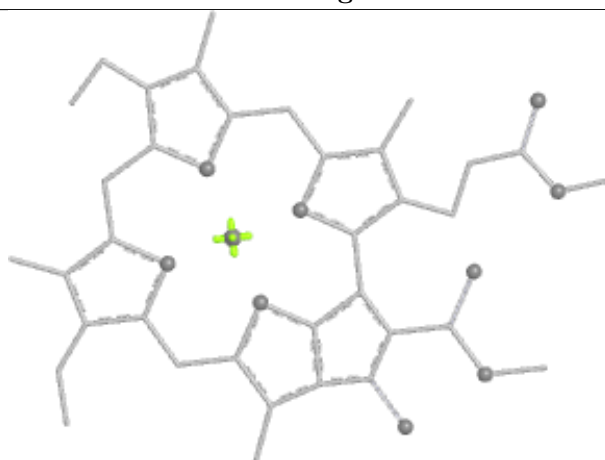
Bond lengths



Bond angles

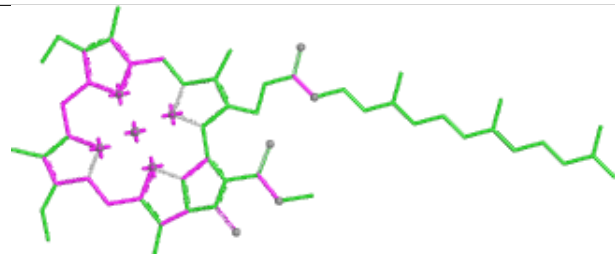


Torsions

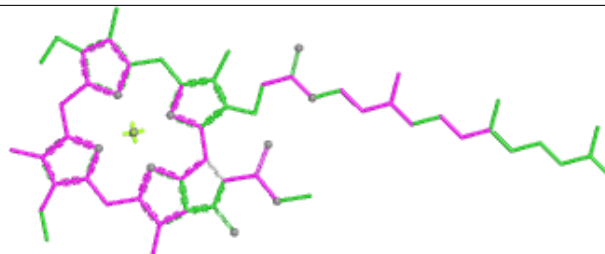


Rings

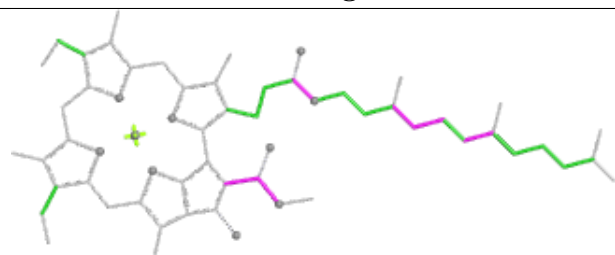
Ligand CLA A 830



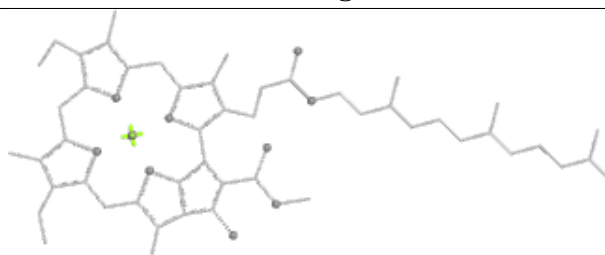
Bond lengths



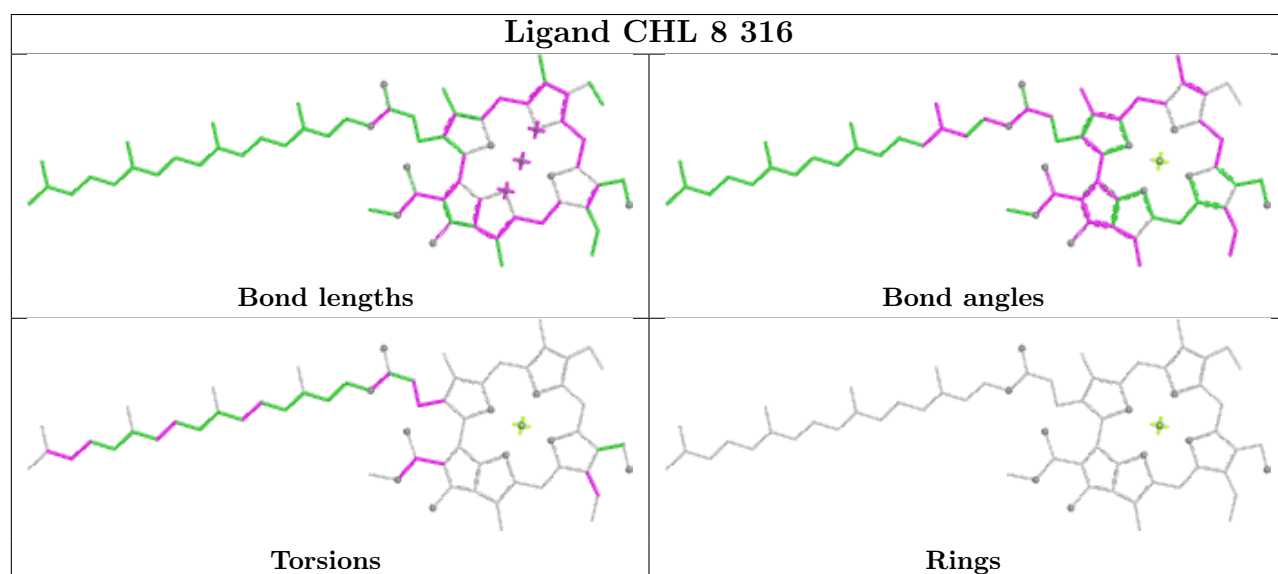
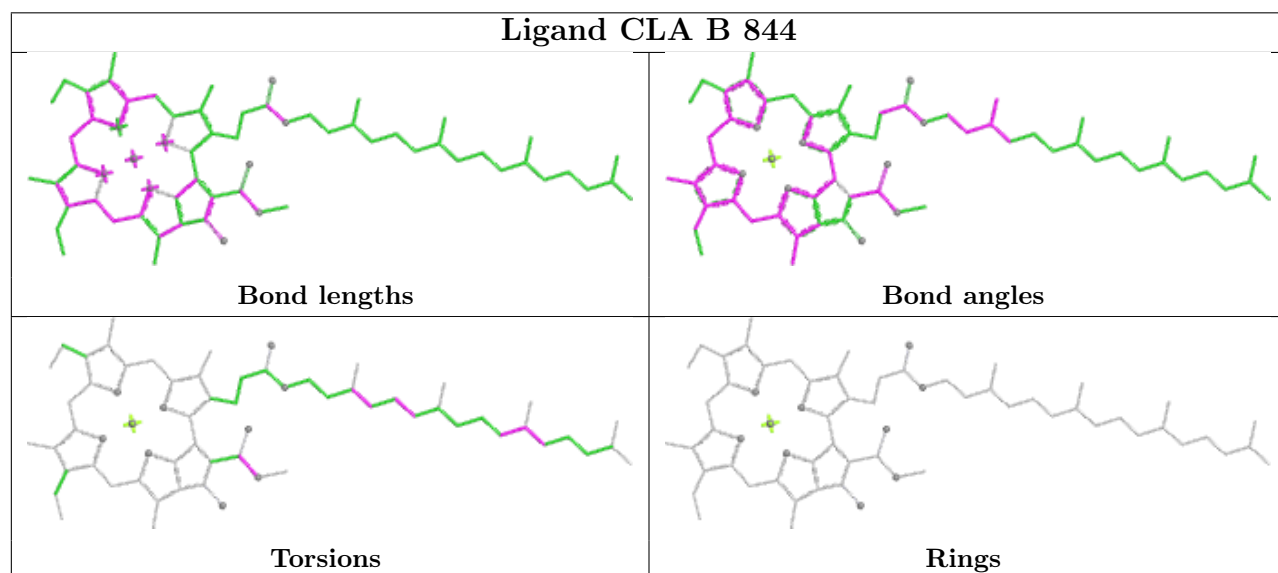
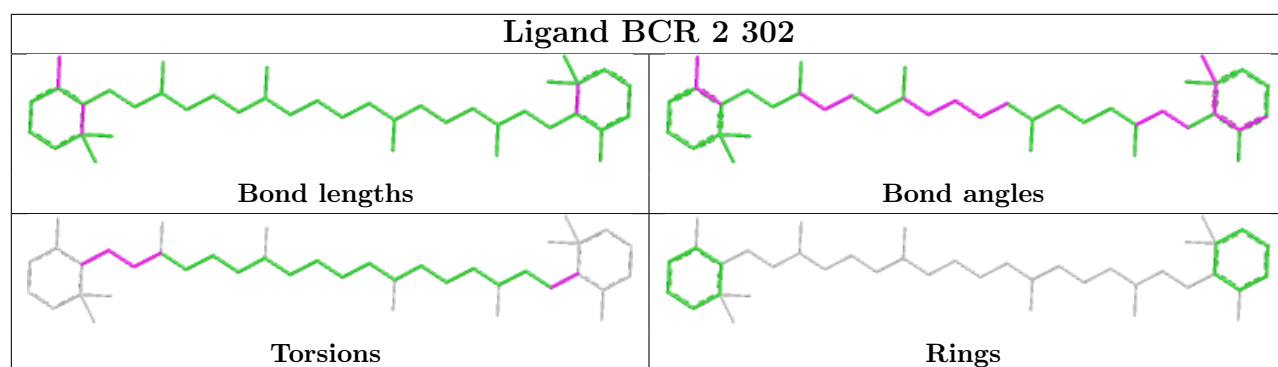
Bond angles



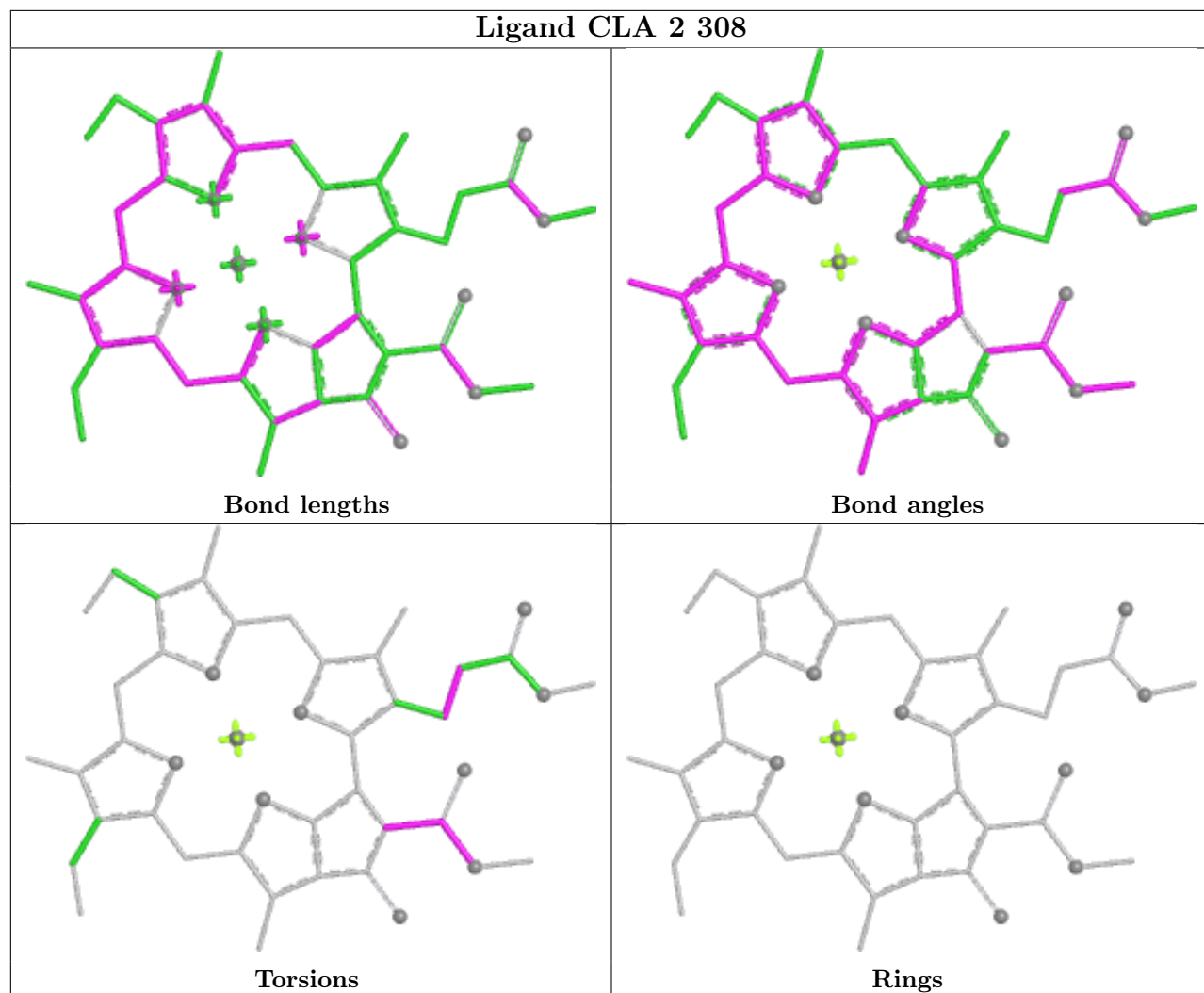
Torsions



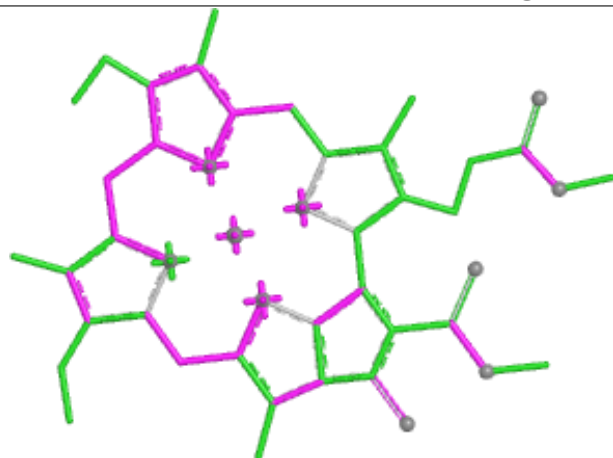
Rings



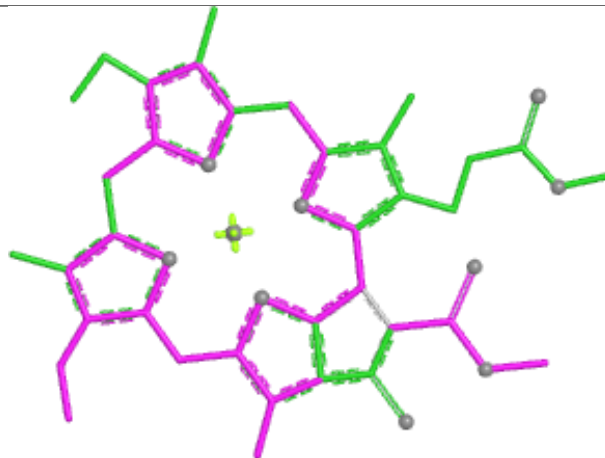
Ligand CLA 2 308



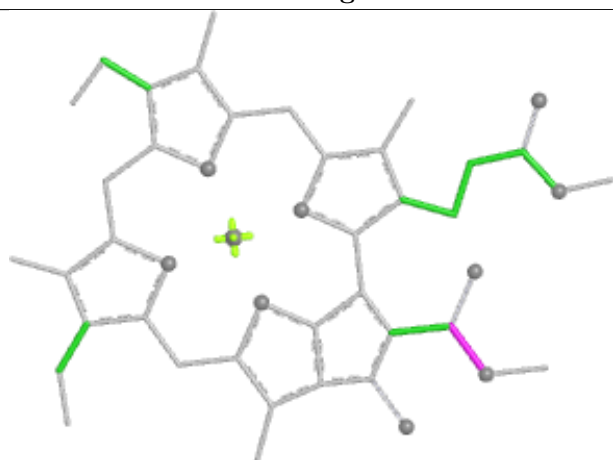
Ligand CLA 8 321



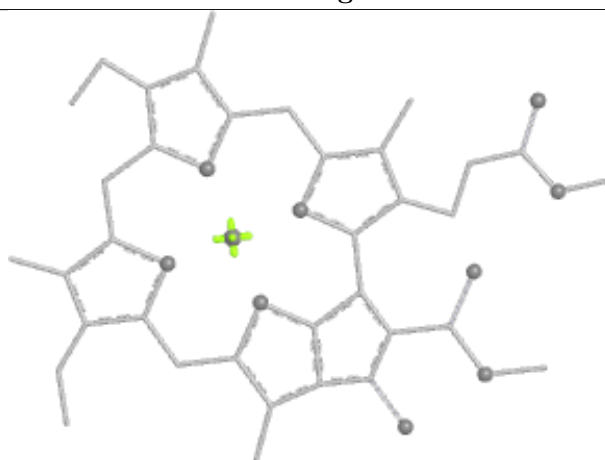
Bond lengths



Bond angles

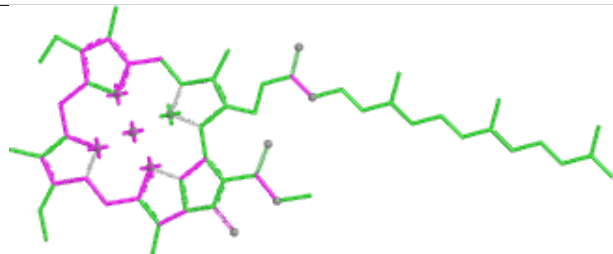


Torsions

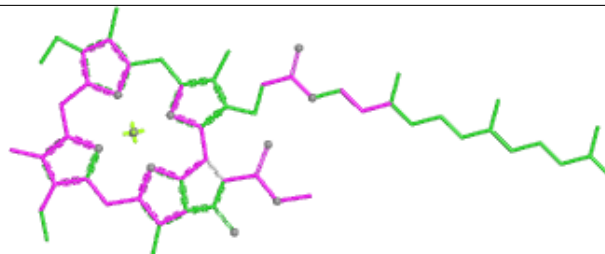


Rings

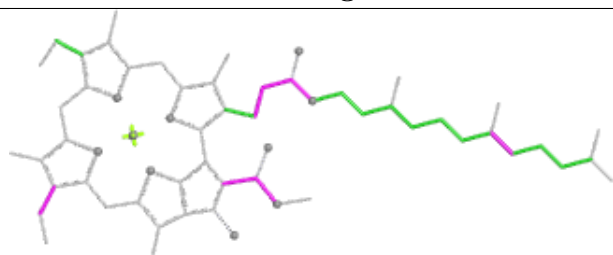
Ligand CLA b 313



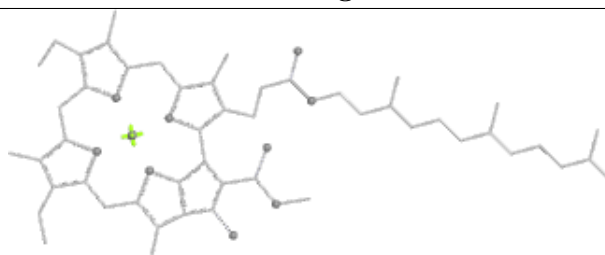
Bond lengths



Bond angles

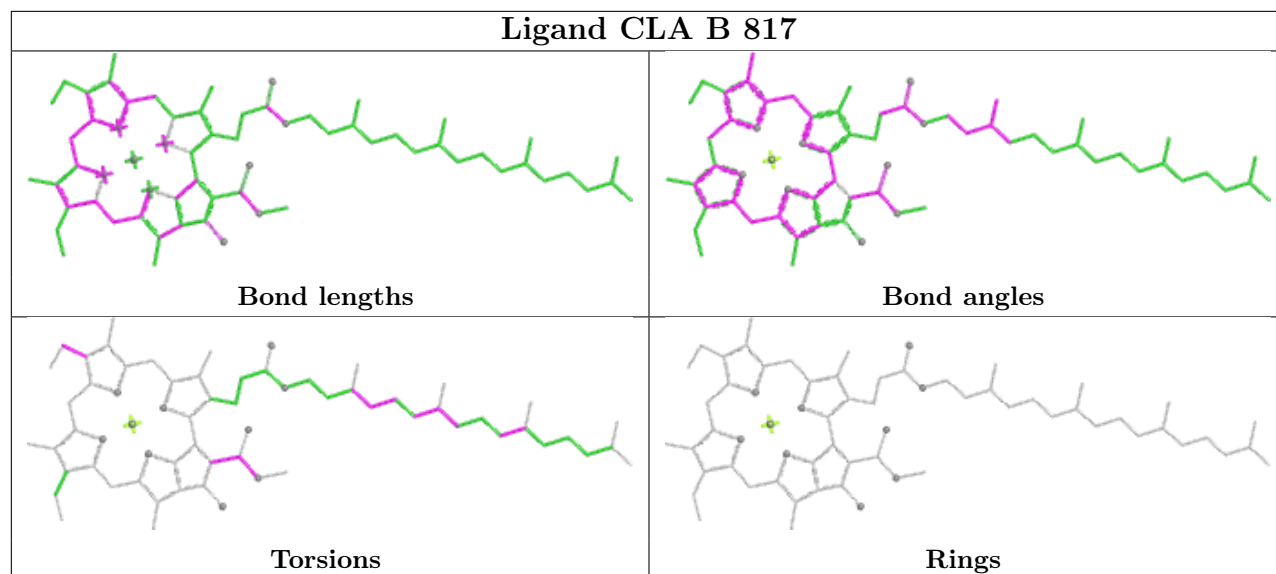


Torsions

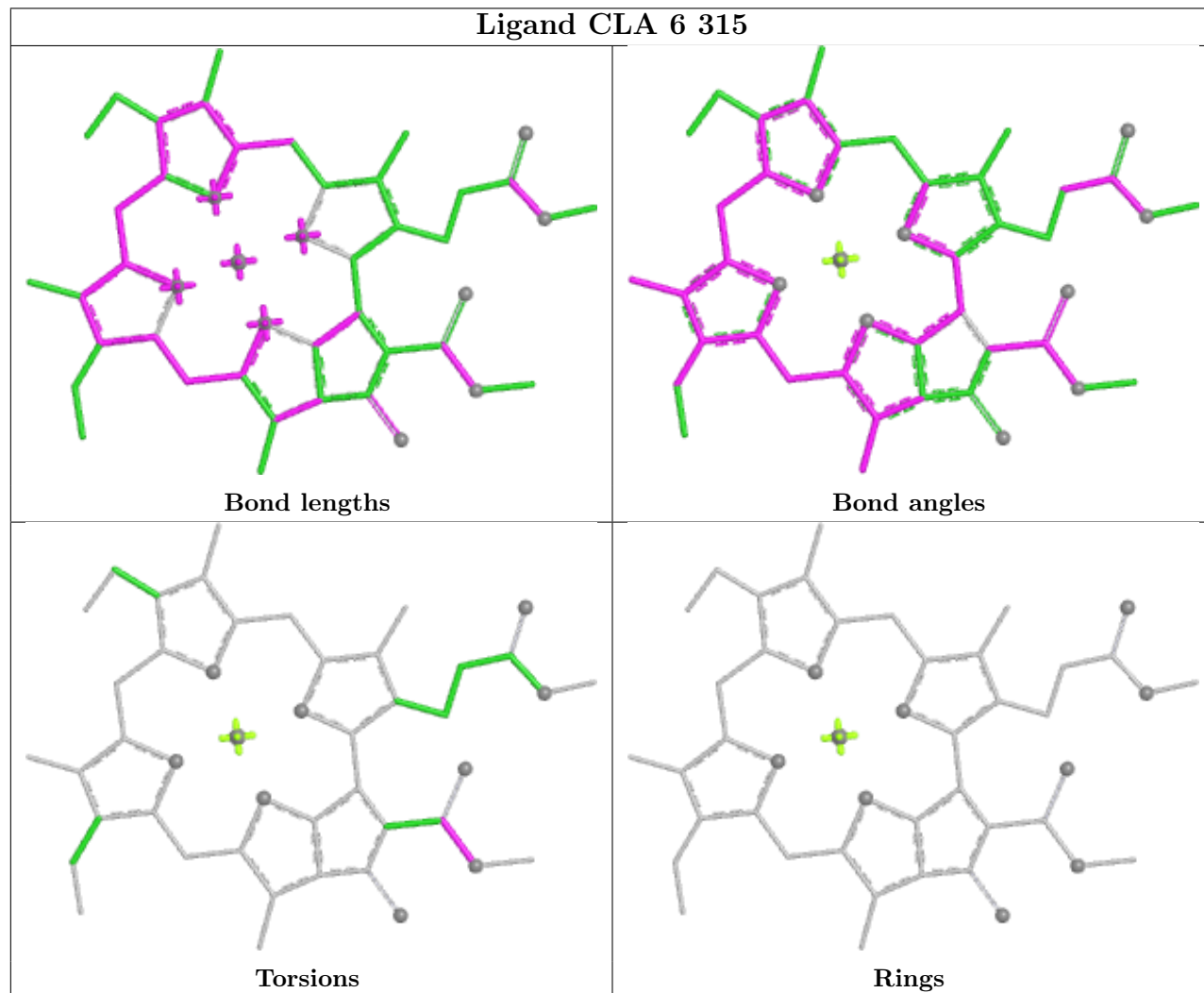


Rings

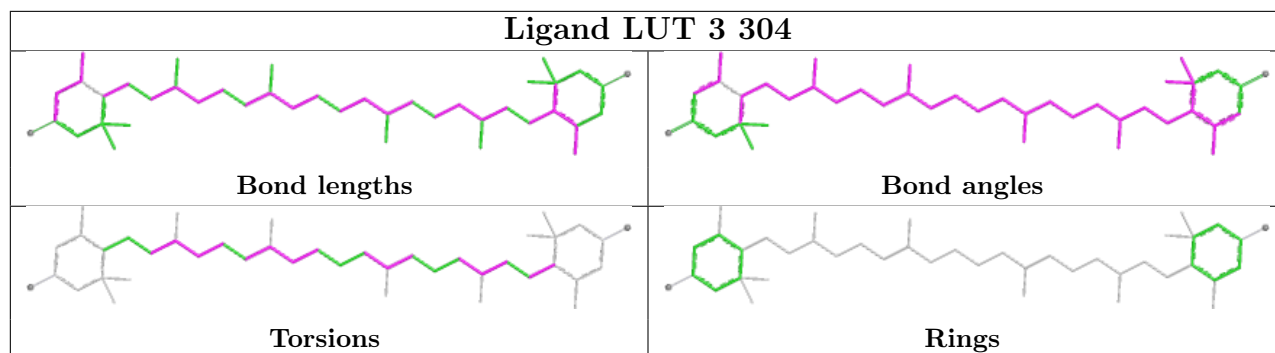
Ligand CLA B 817



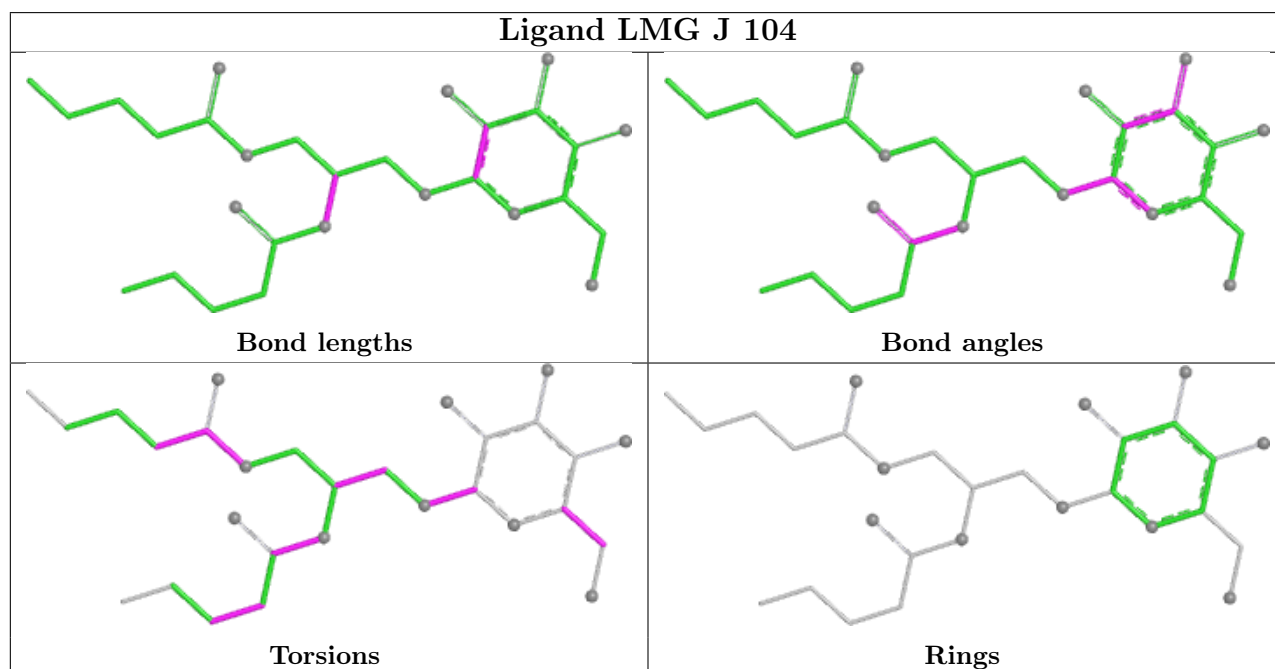
Ligand CLA 6 315



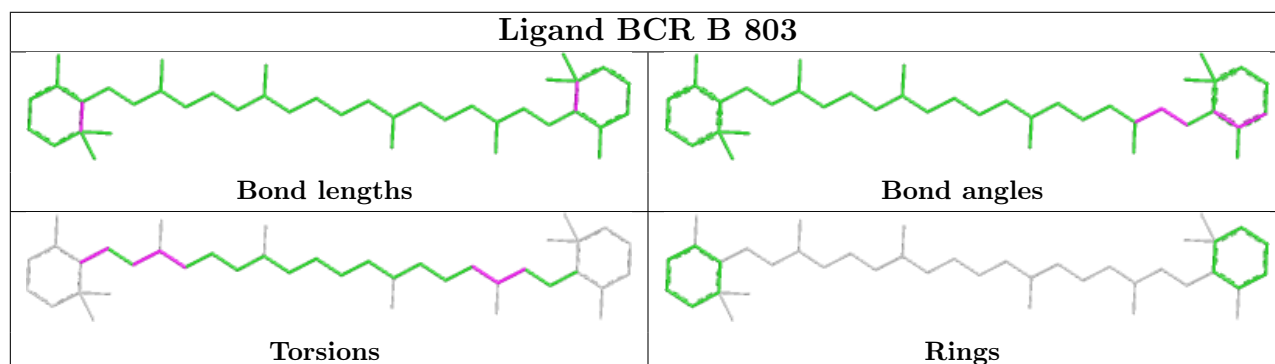
Ligand LUT 3 304



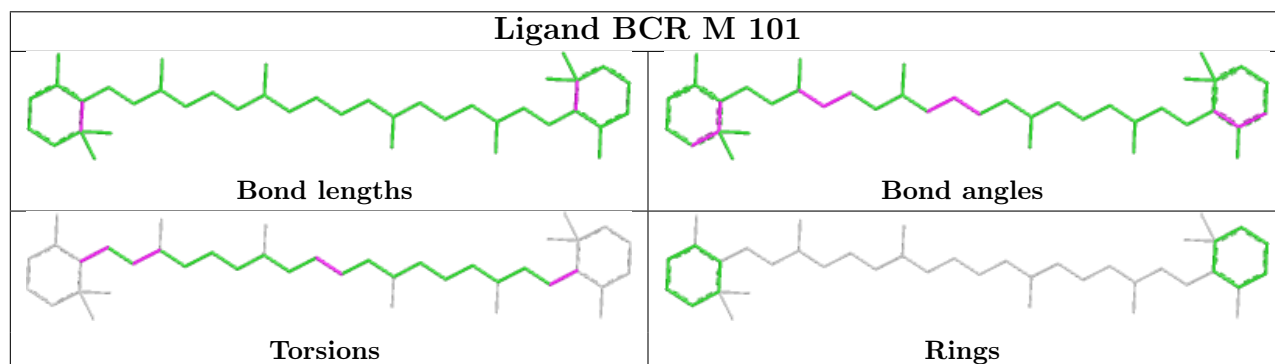
Ligand LMG J 104

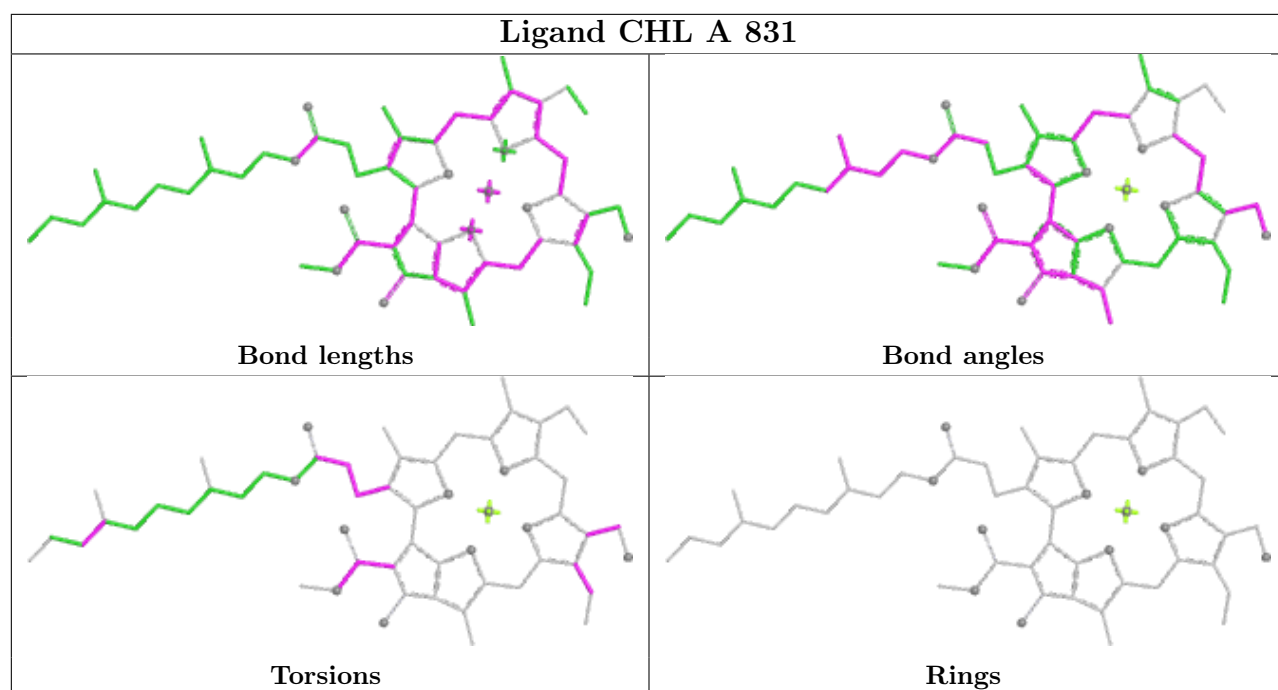


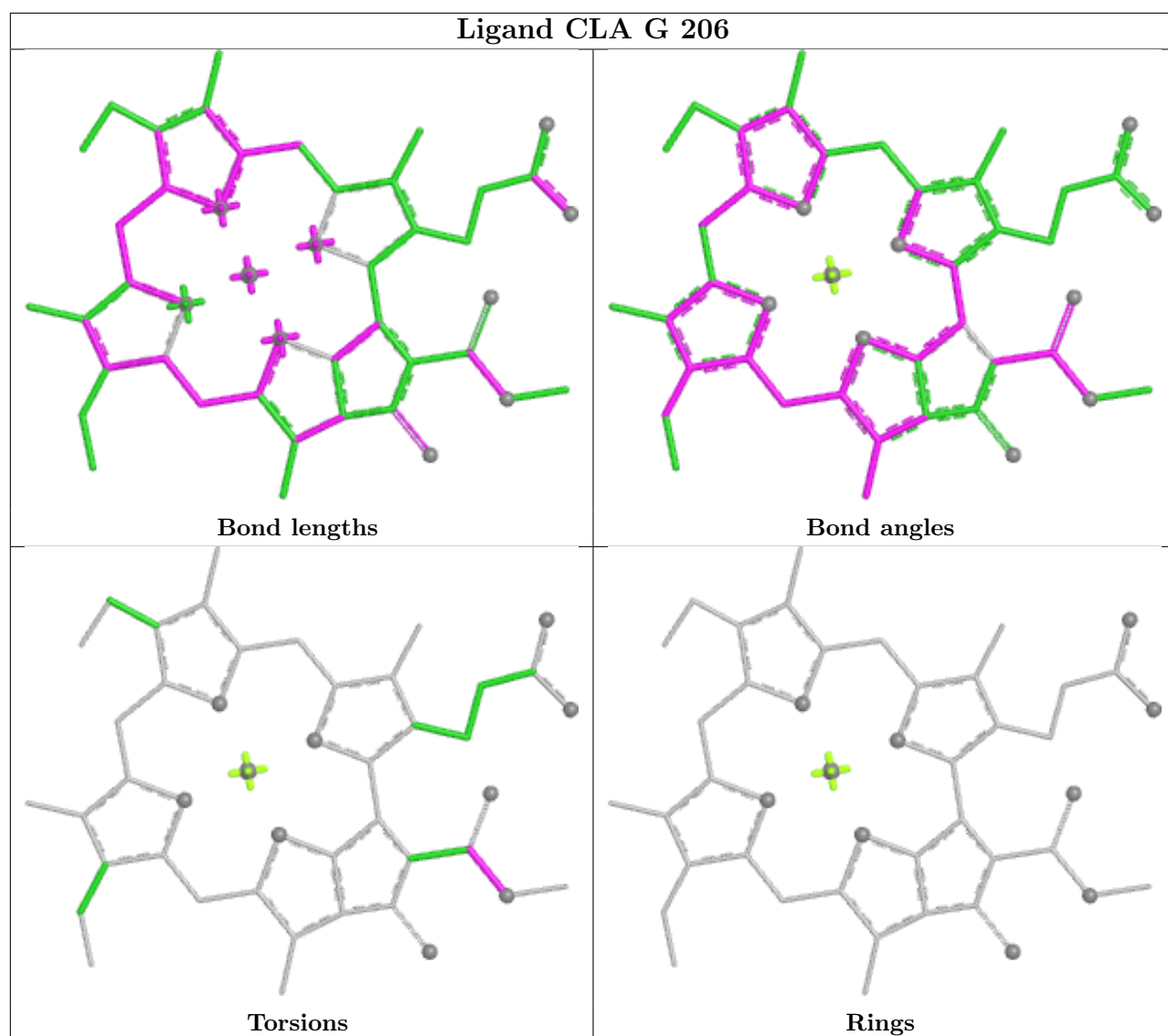
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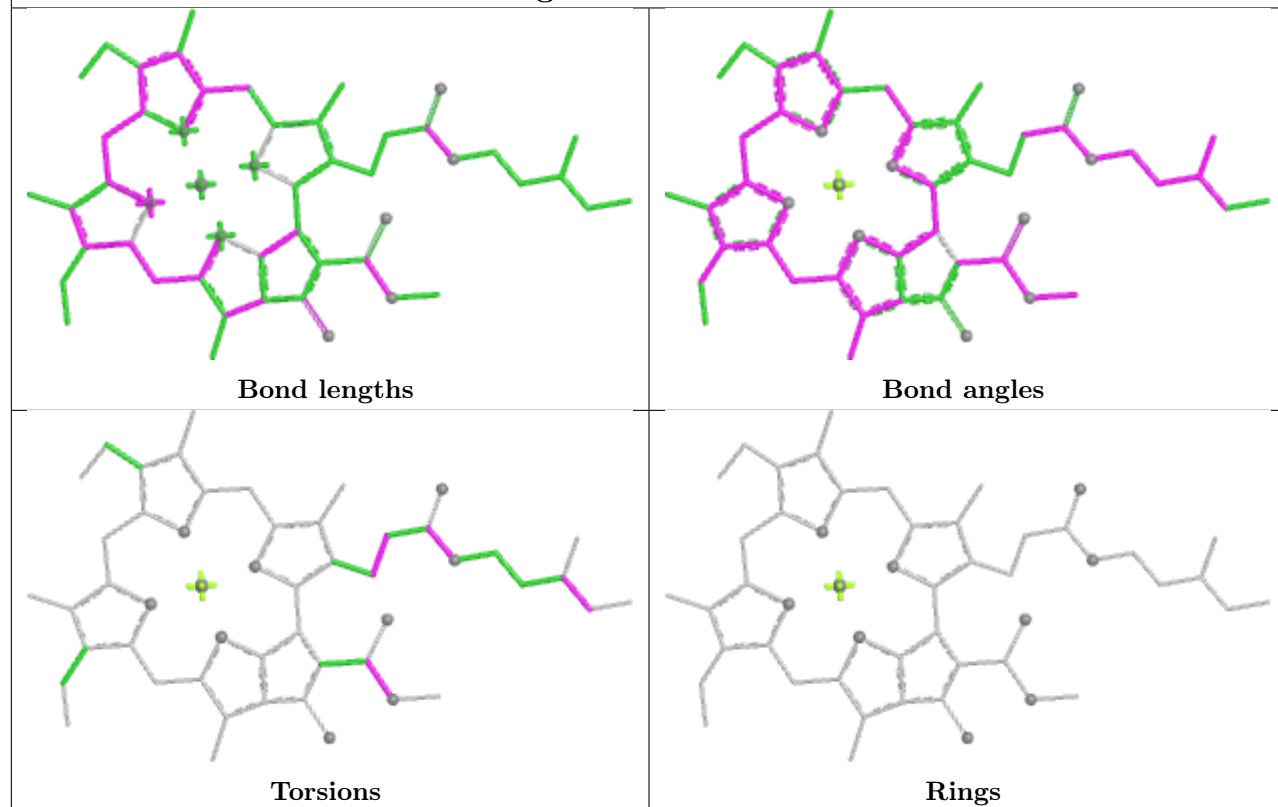
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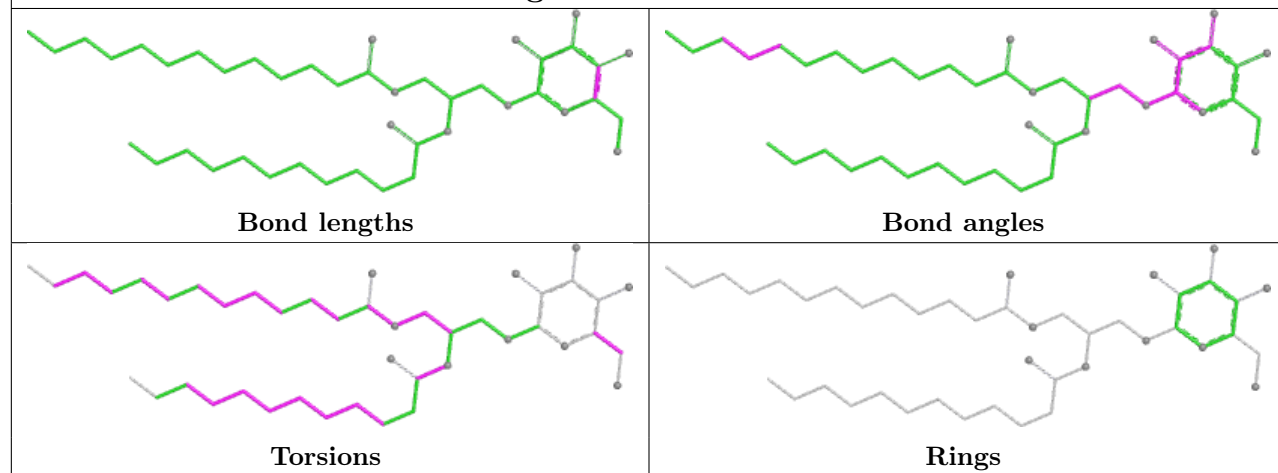




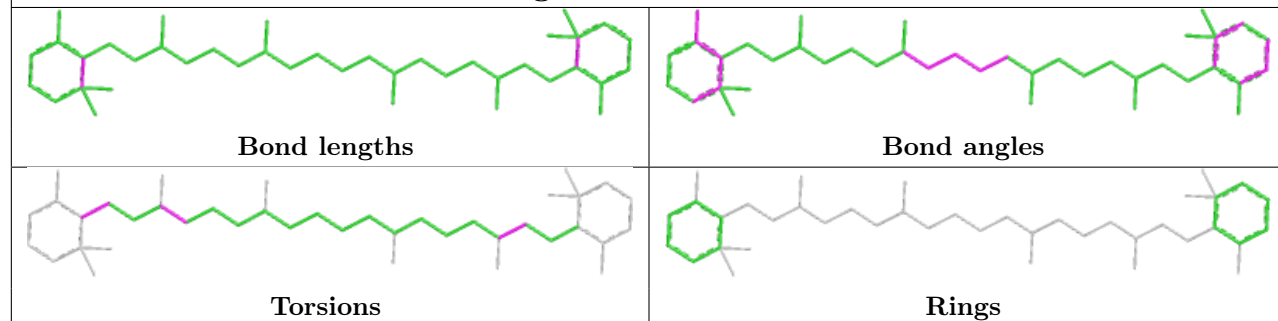
Ligand CLA 3 317



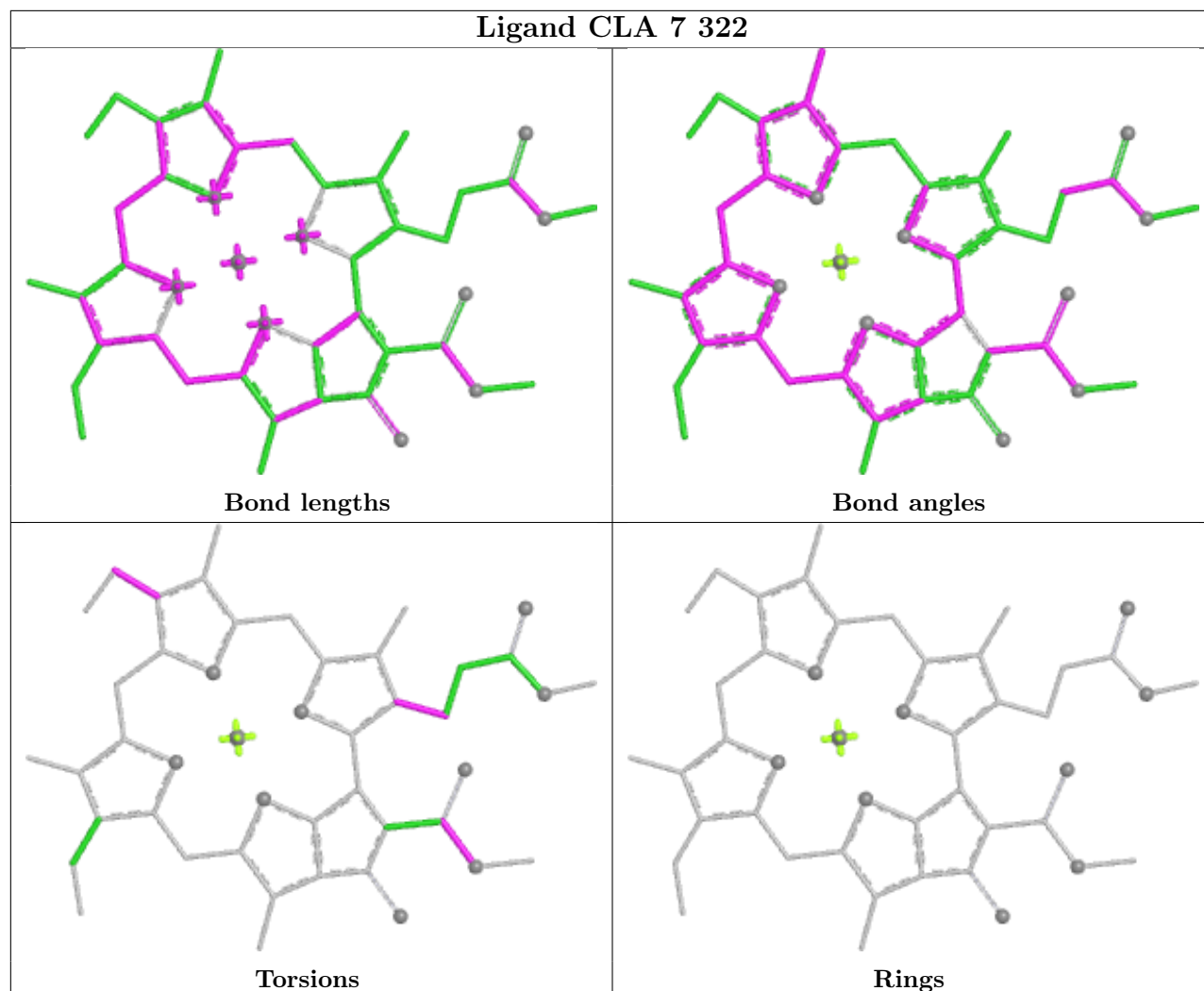
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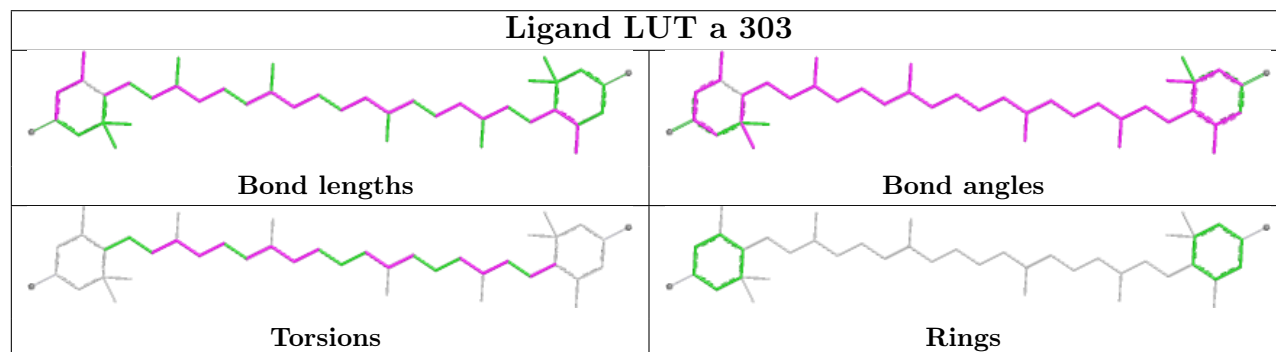
Ligand BCR L 302



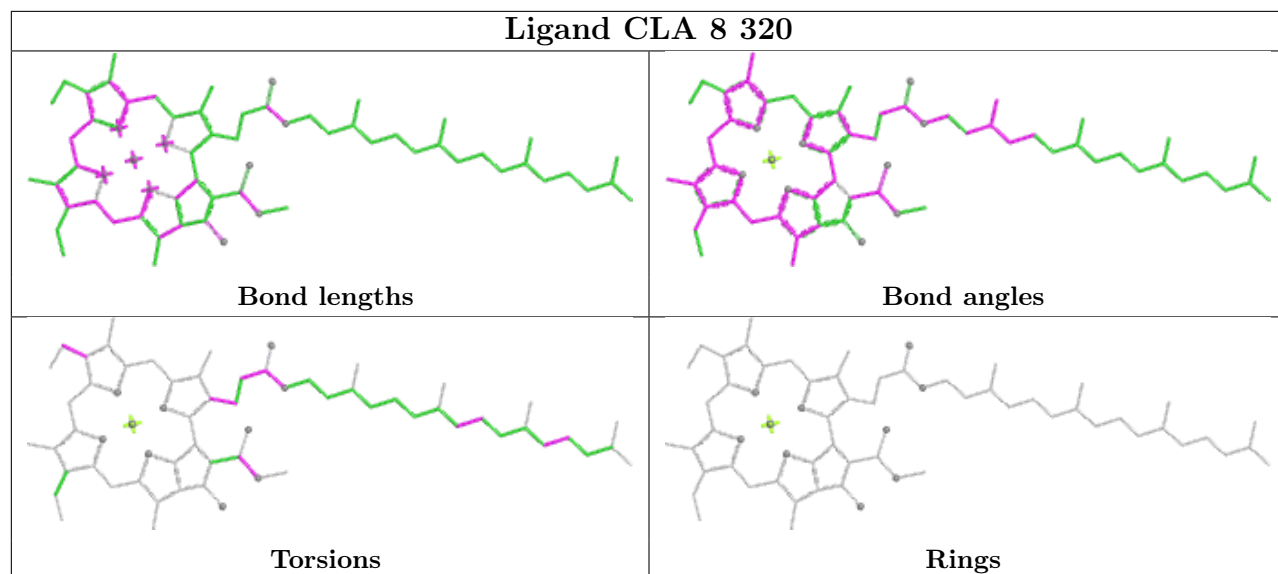
Ligand CLA 7 322



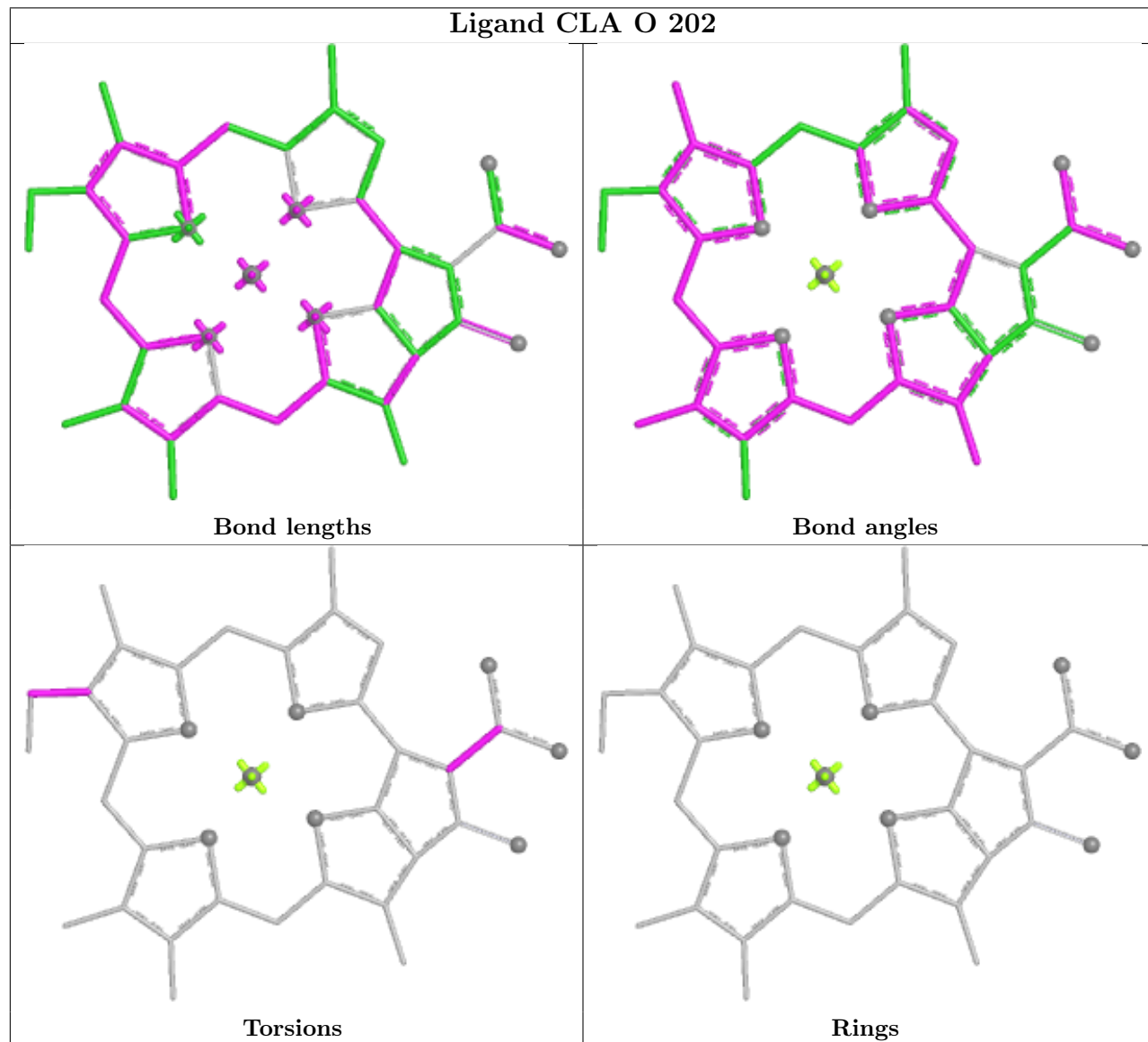
Ligand LUT a 303



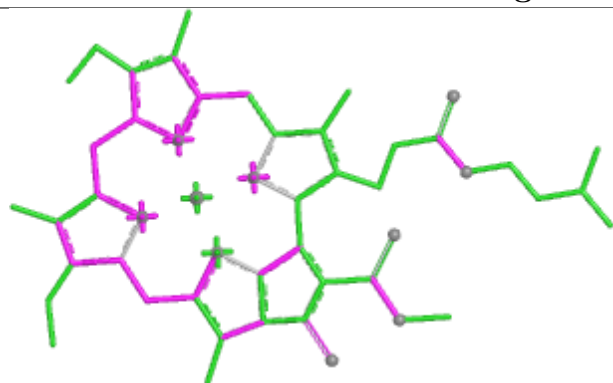
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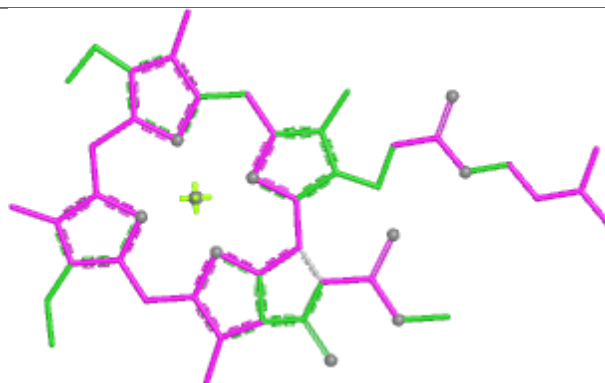
Ligand CLA O 202



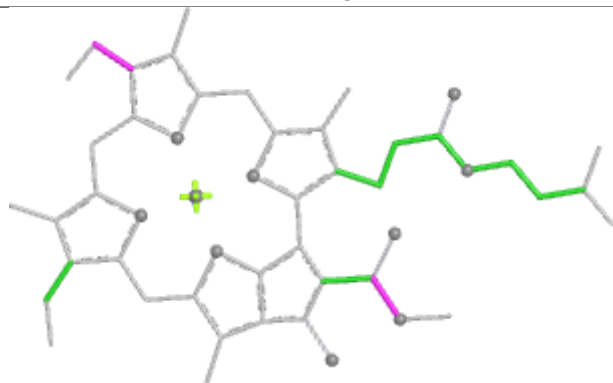
Ligand CLA B 845



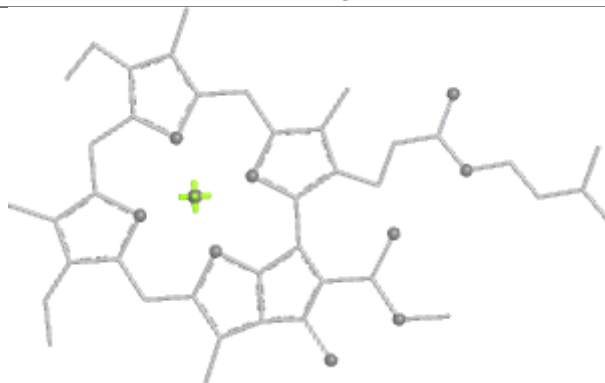
Bond lengths



Bond angles

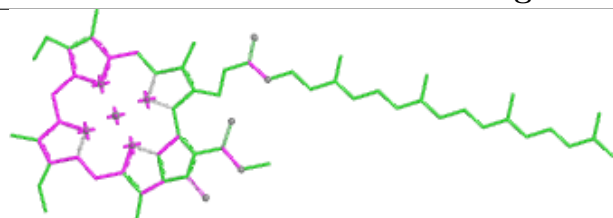


Torsions

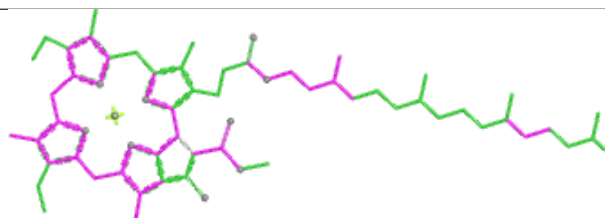


Rings

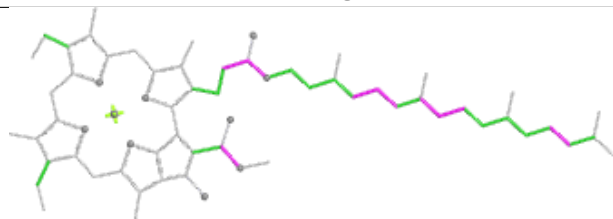
Ligand CLA B 820



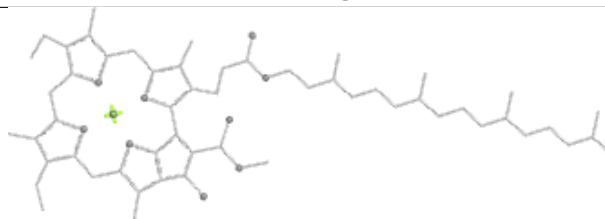
Bond lengths



Bond angles

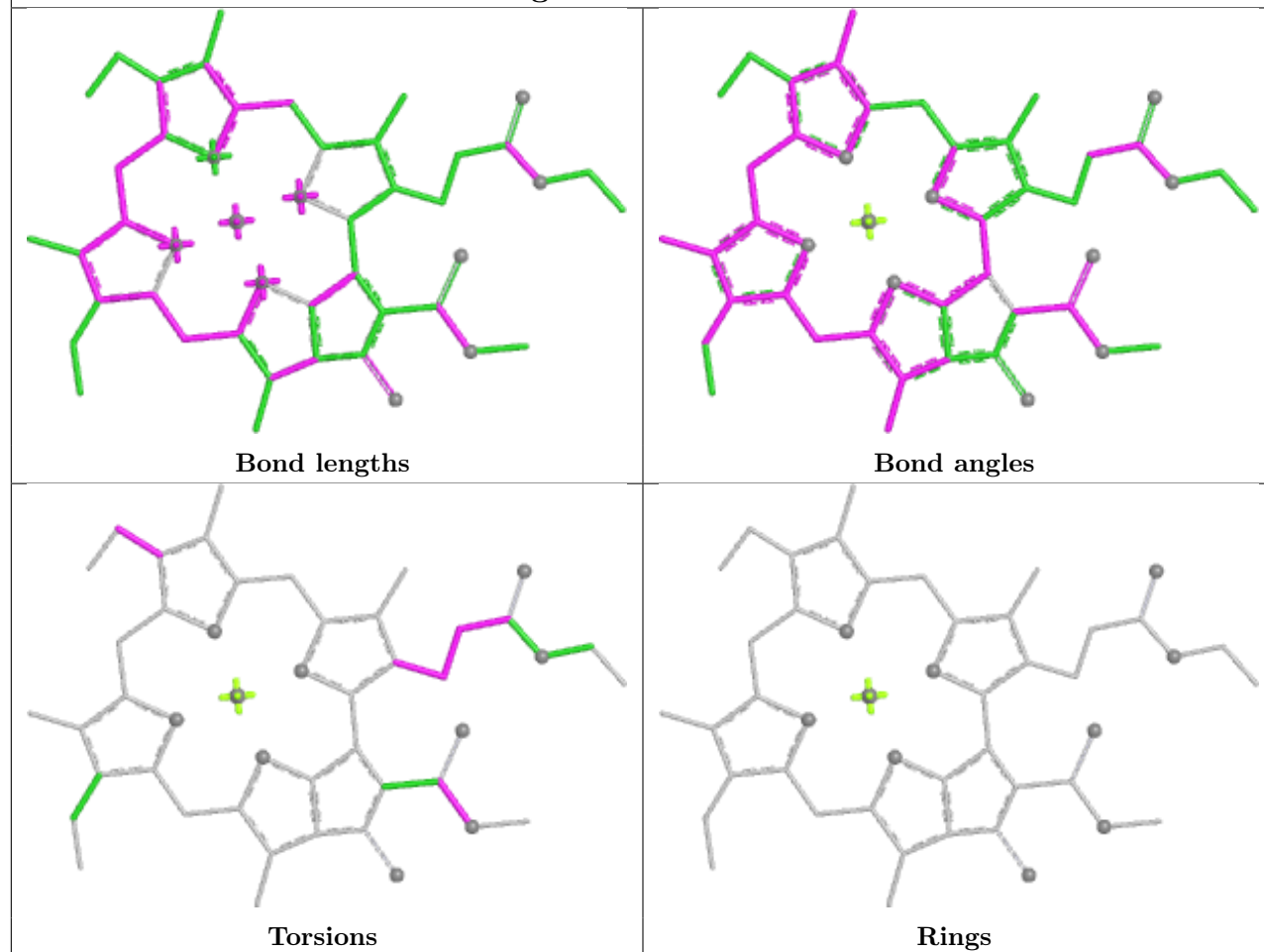


Torsions

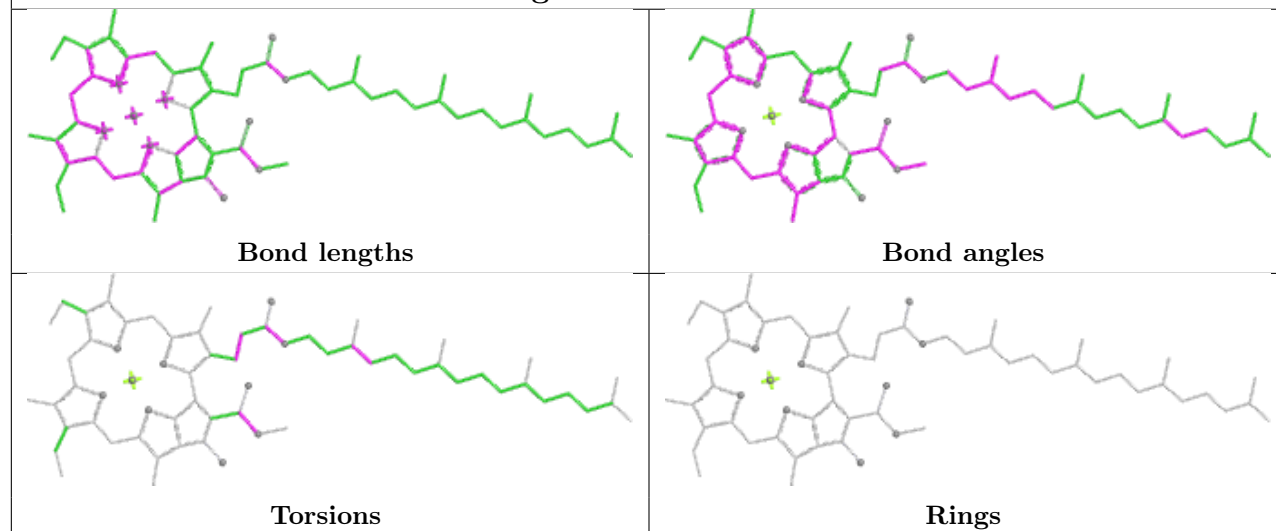


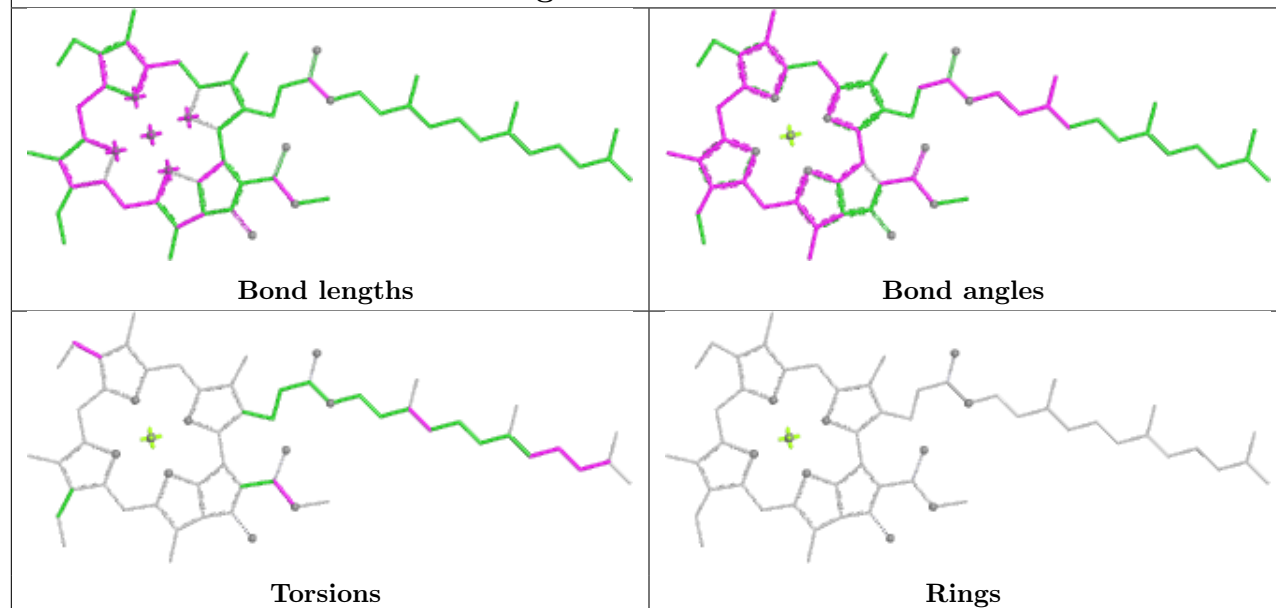
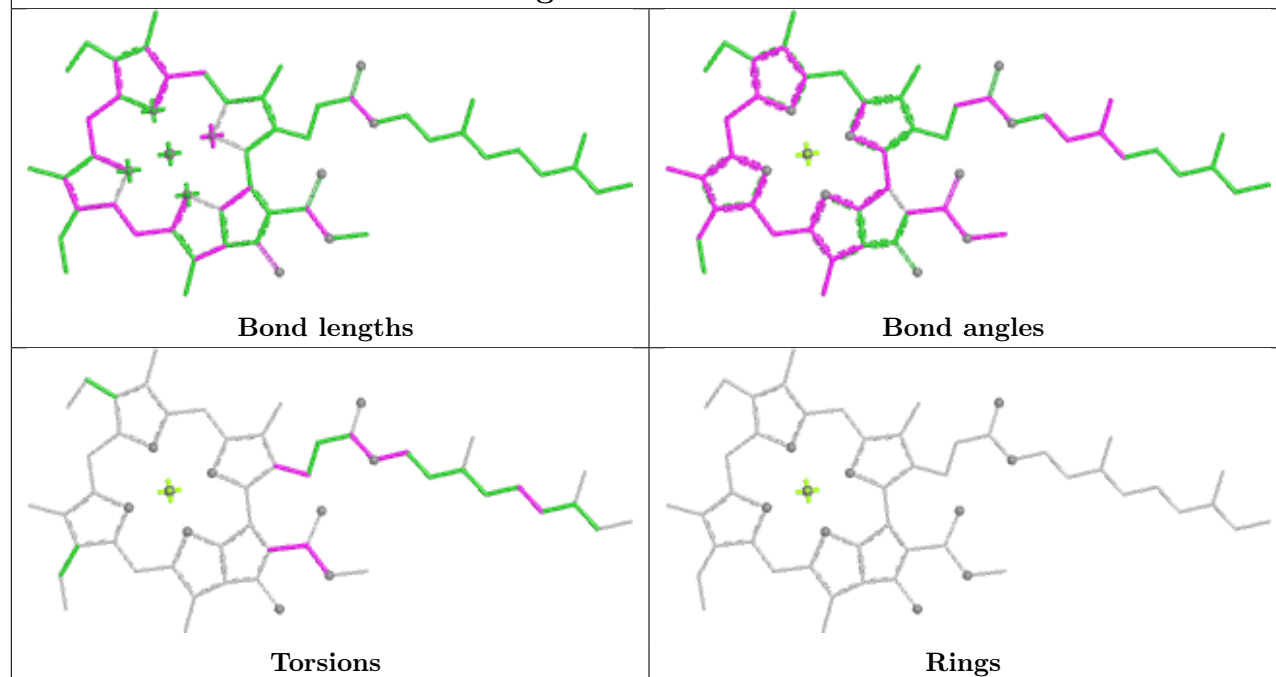
Rings

Ligand CLA 4 312

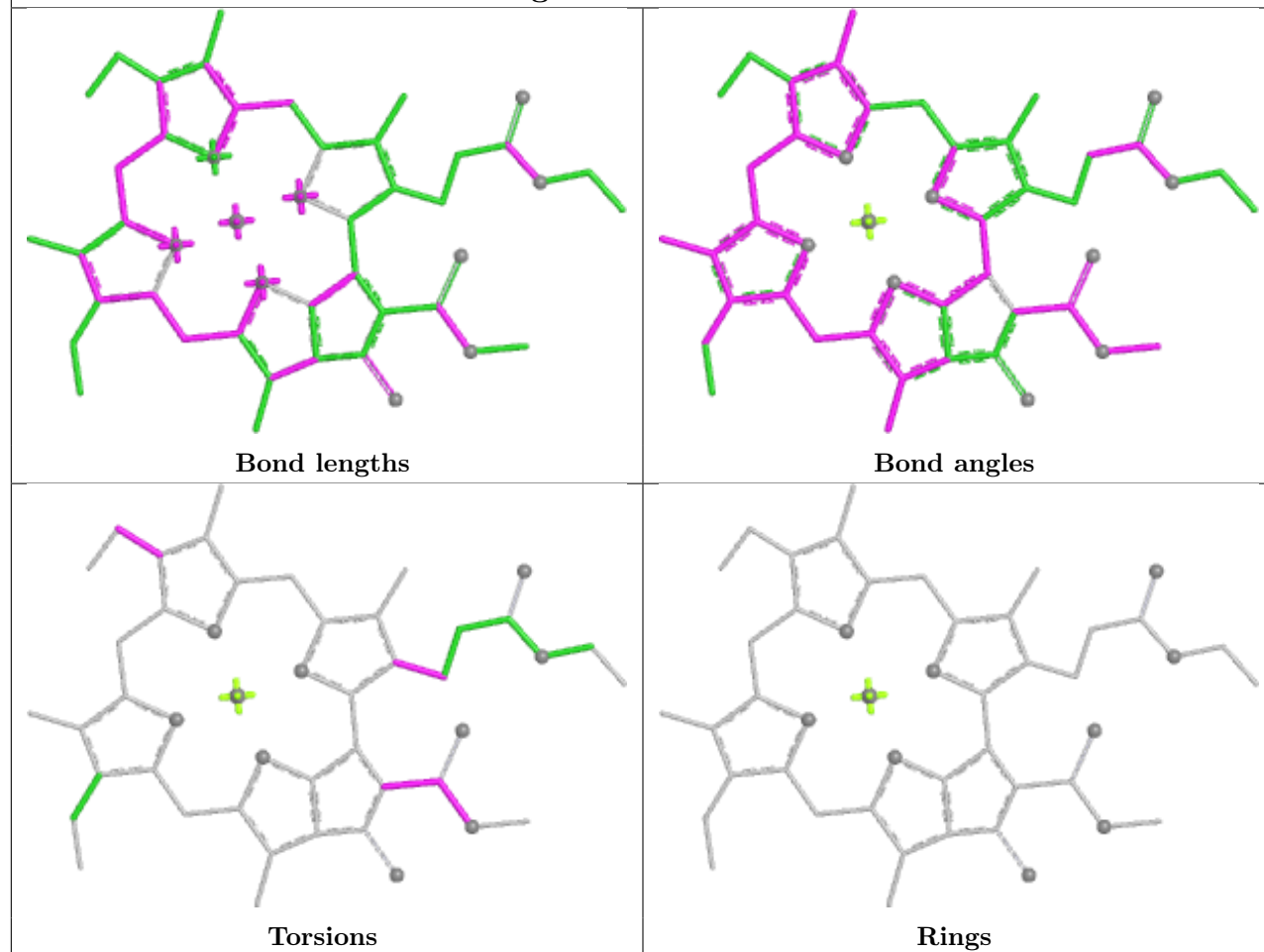


Ligand CLA A 834

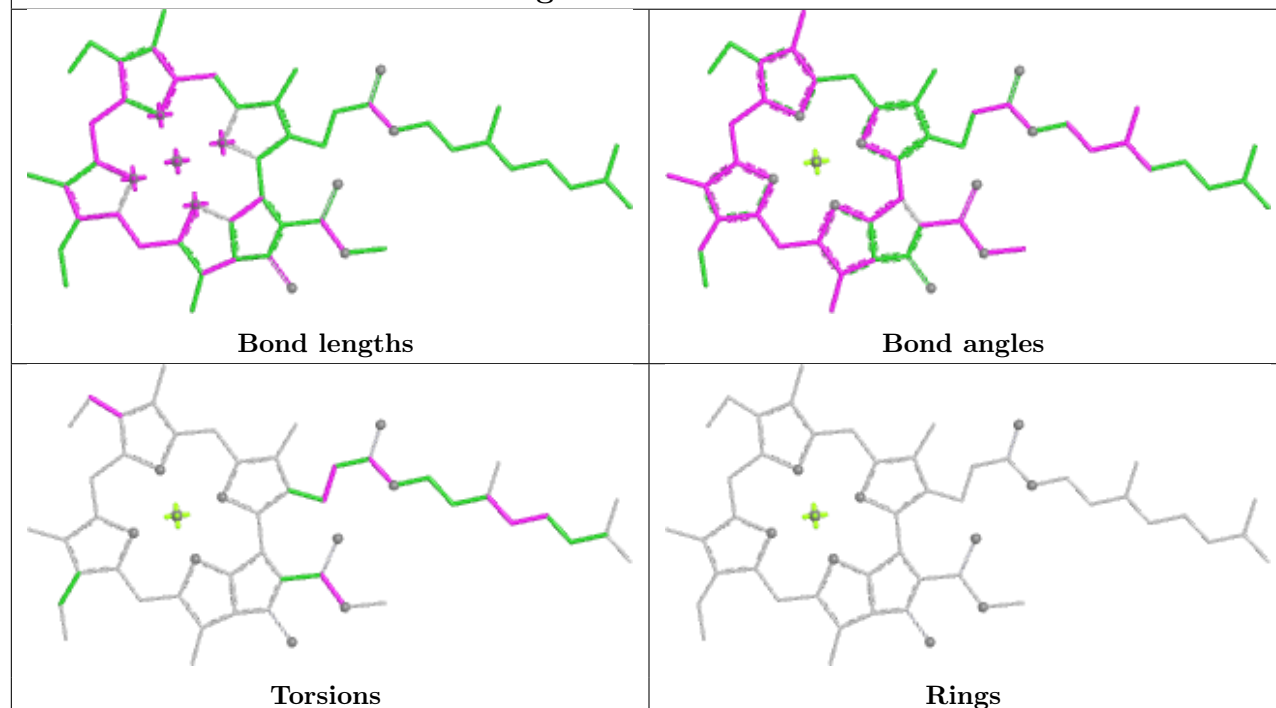


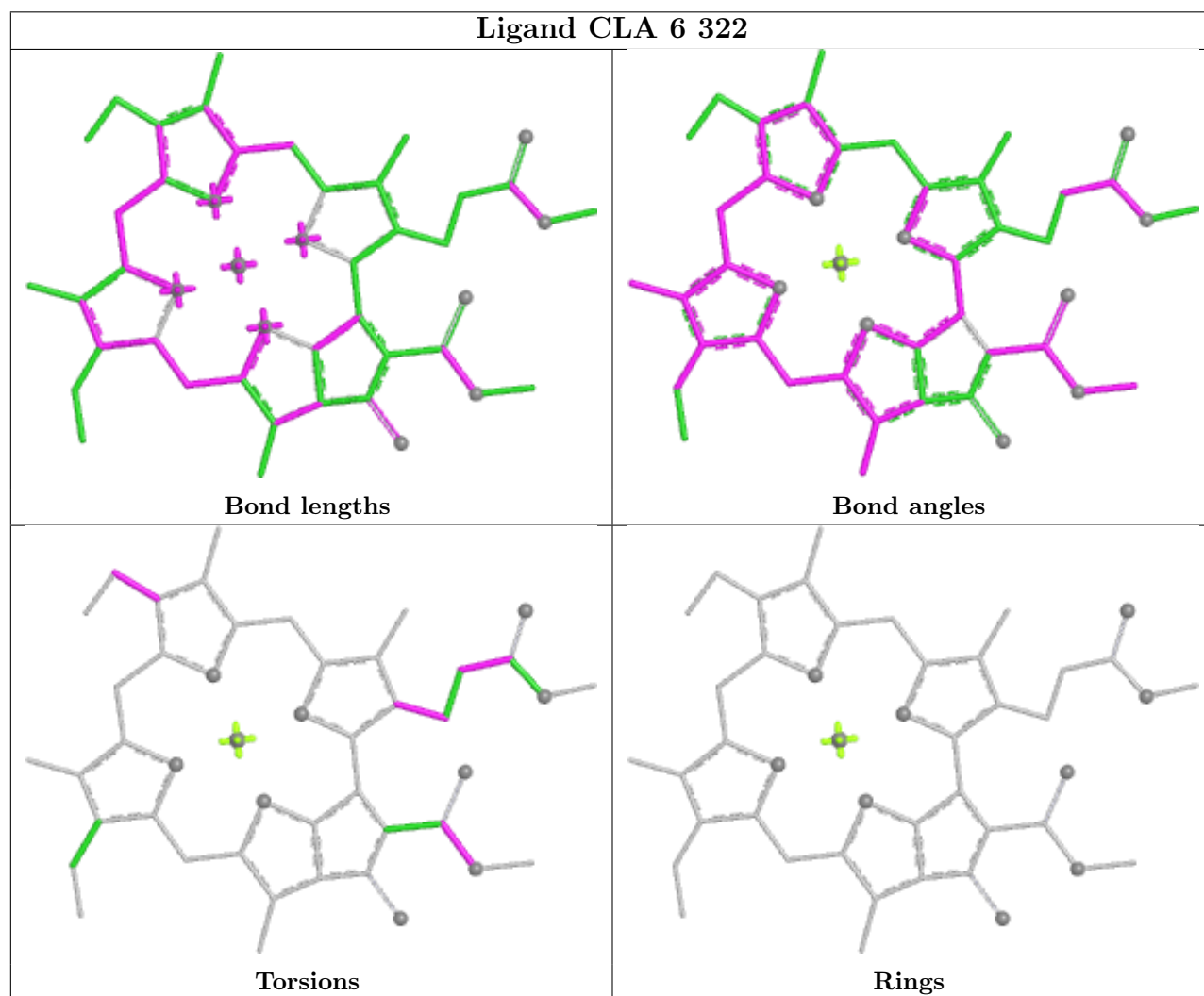
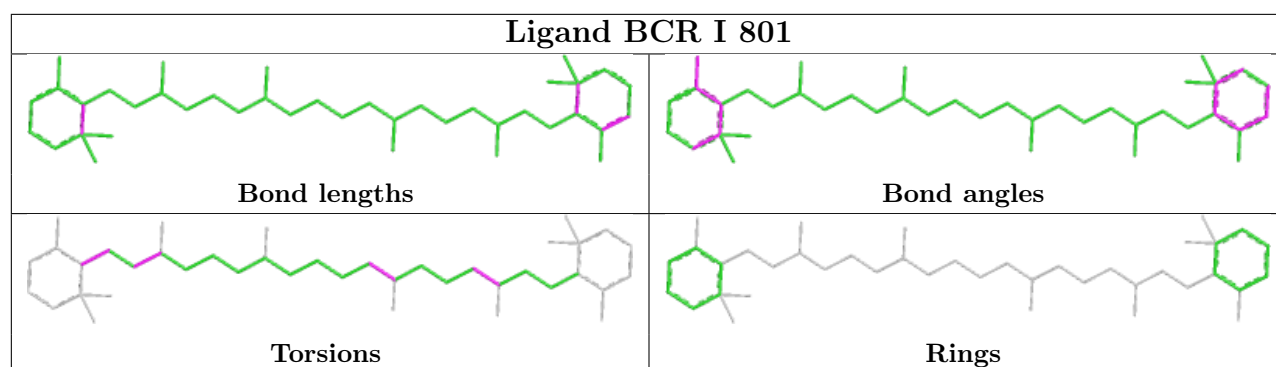
Ligand CLA a 311**Ligand CLA 5 323**

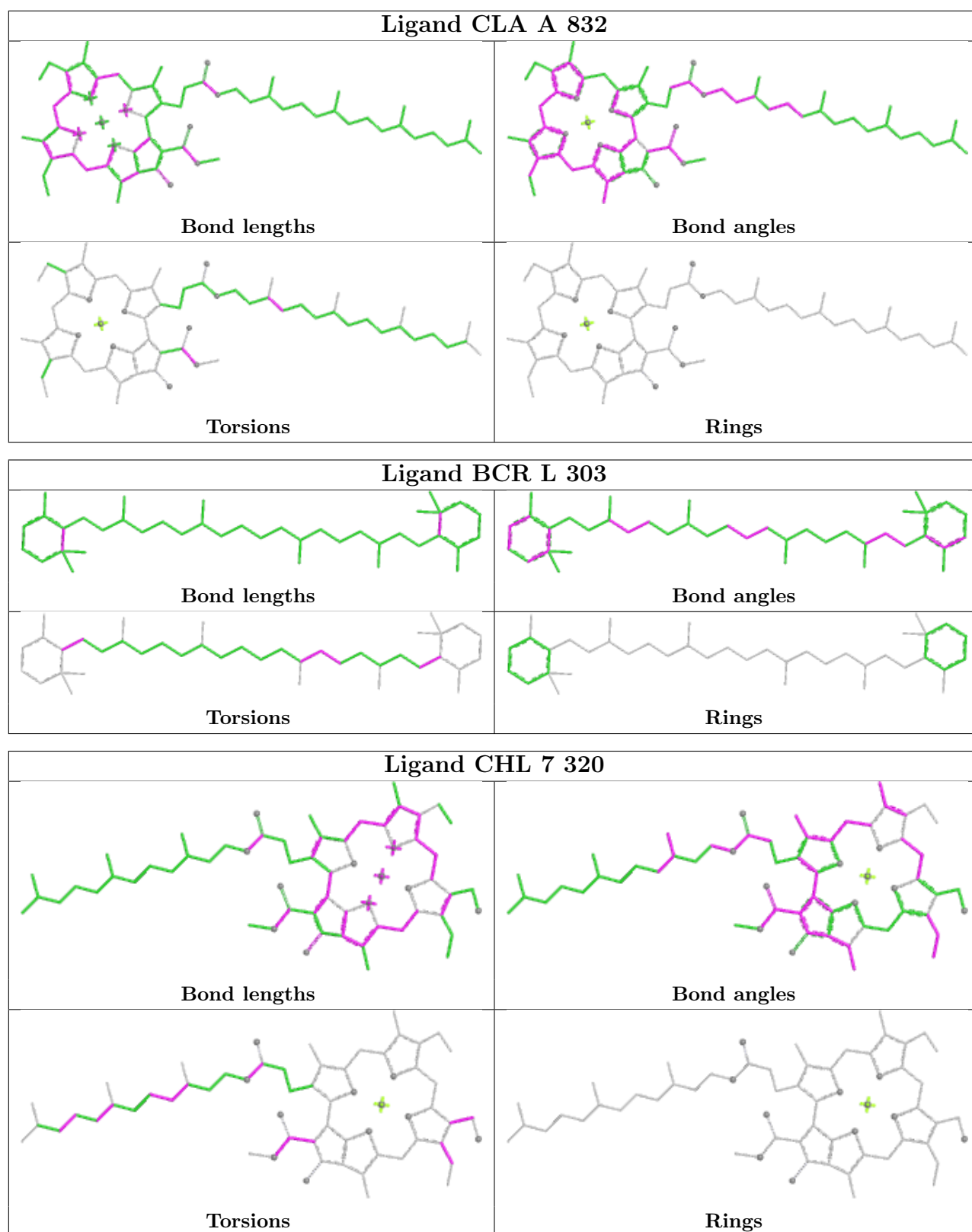
Ligand CLA 6 314

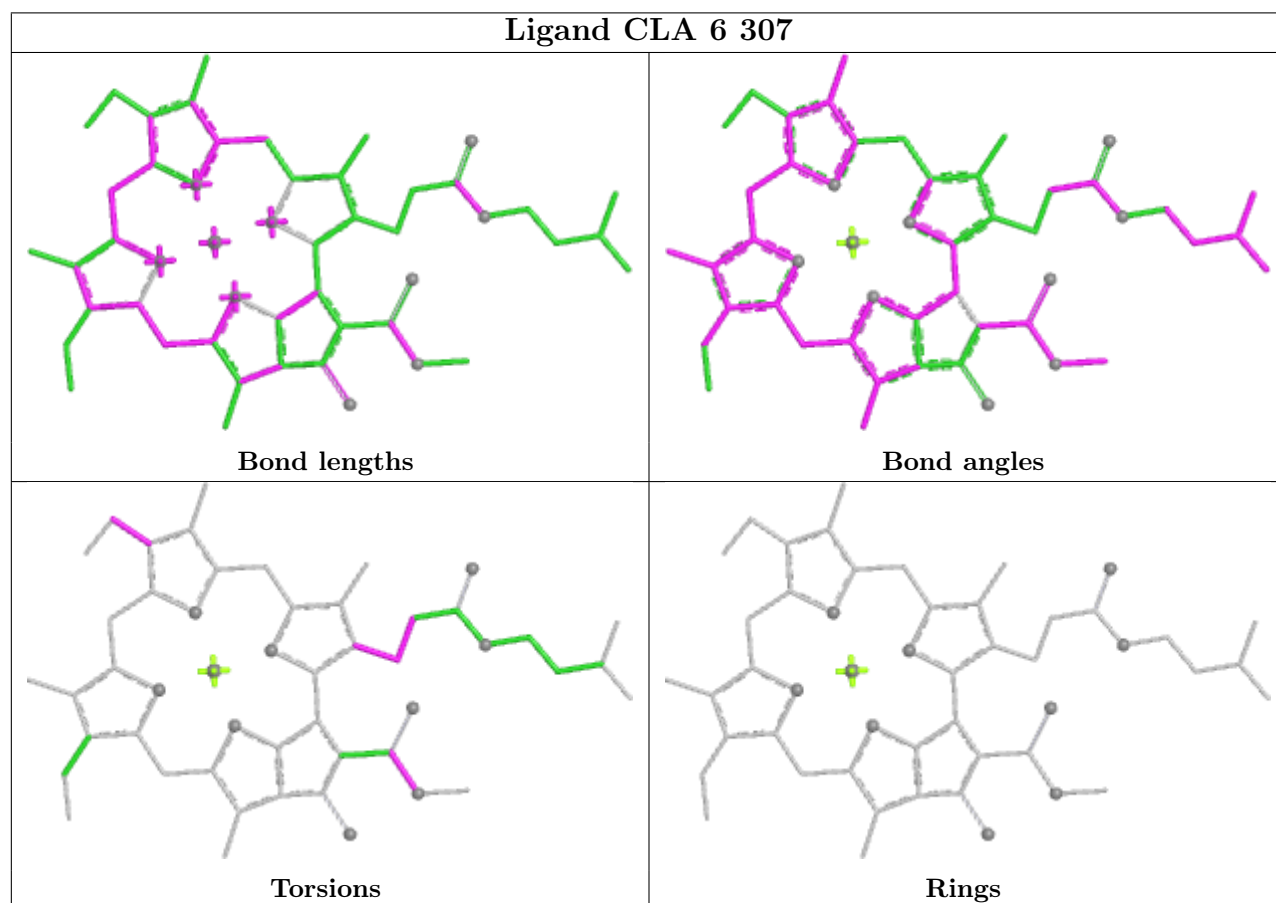
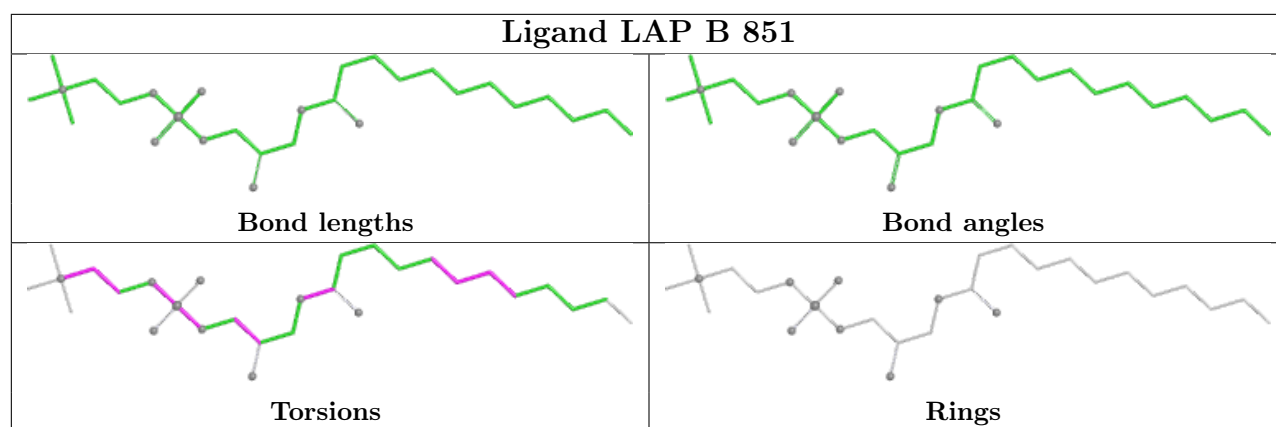


Ligand CLA 6 311

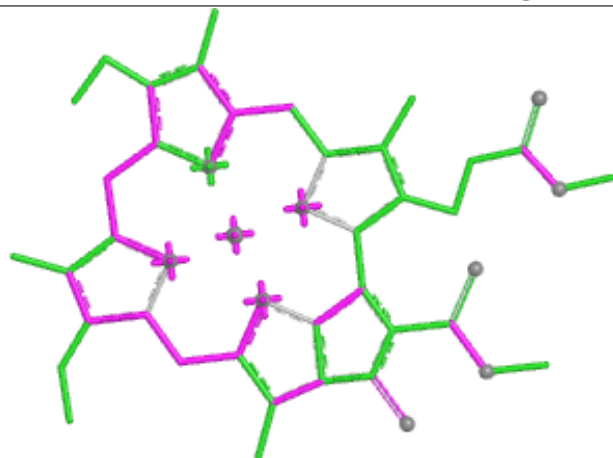




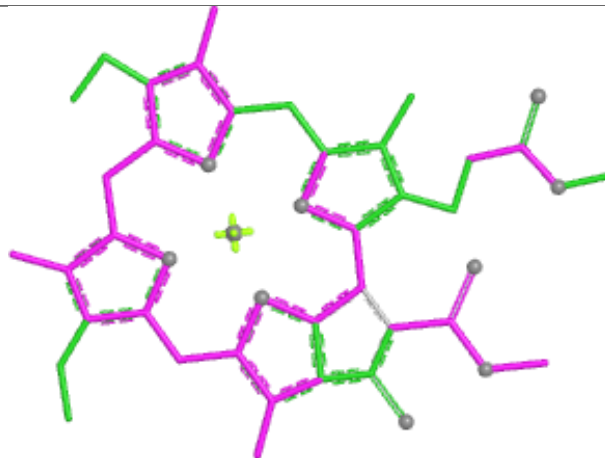




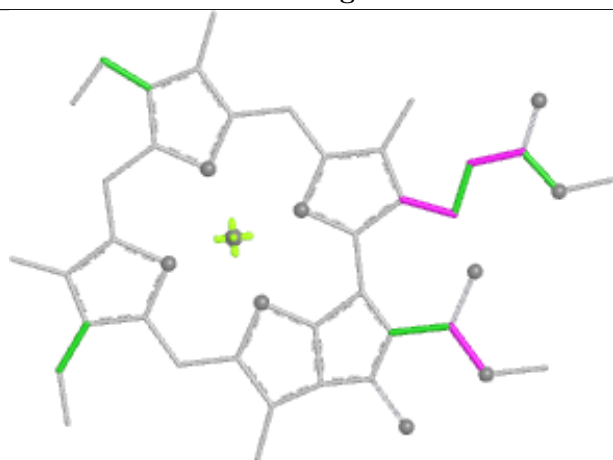
Ligand CLA b 302



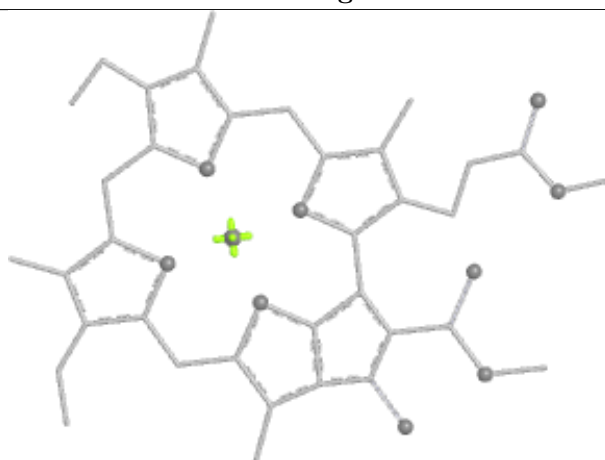
Bond lengths



Bond angles

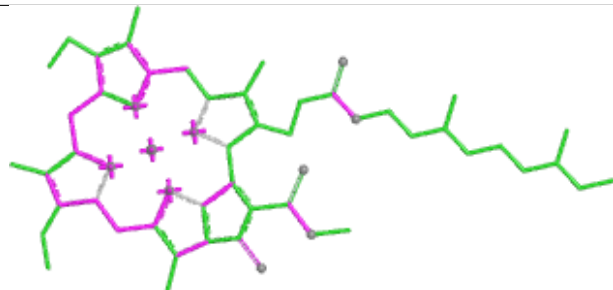


Torsions

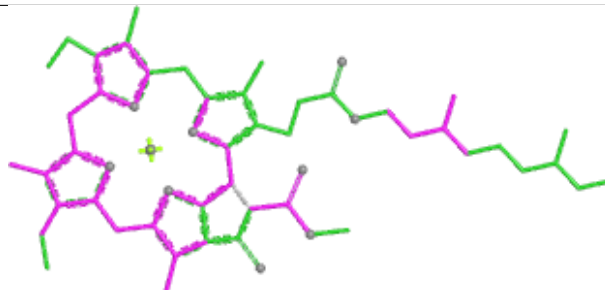


Rings

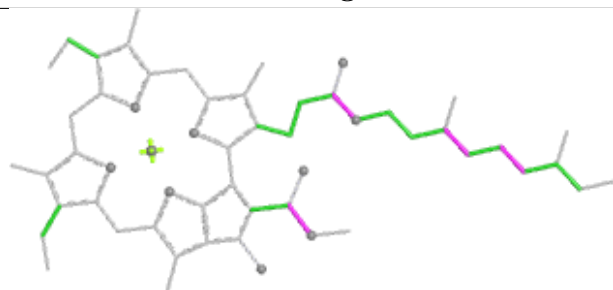
Ligand CLA A 845



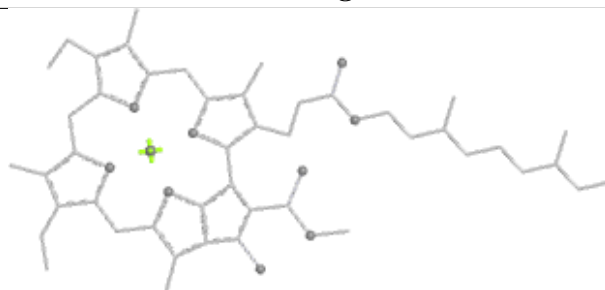
Bond lengths



Bond angles

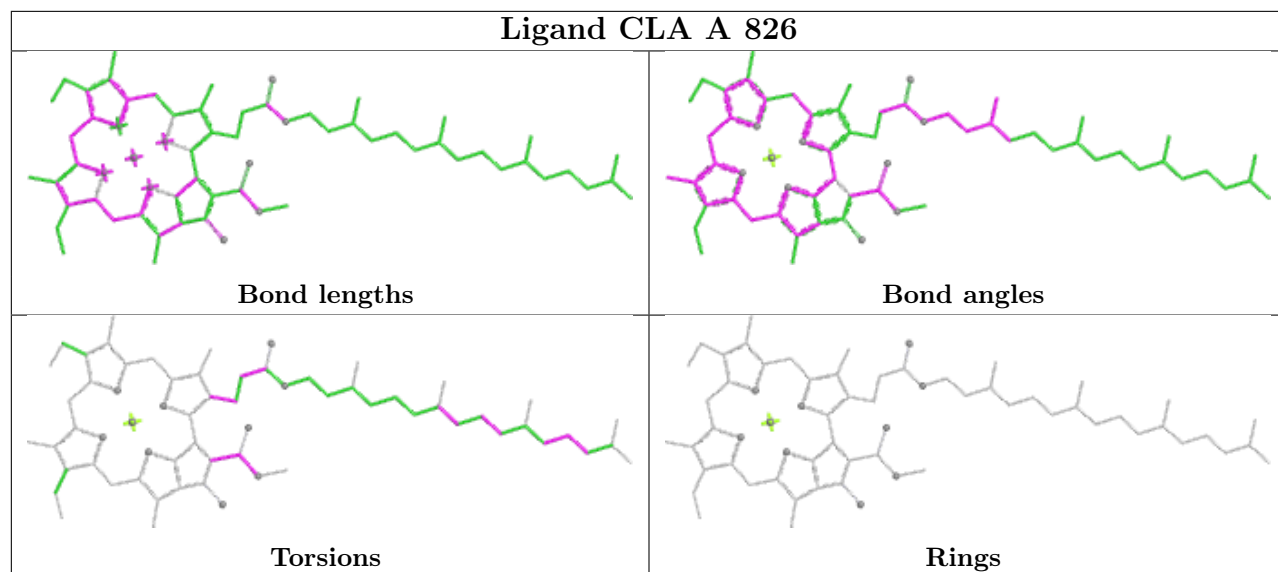


Torsions

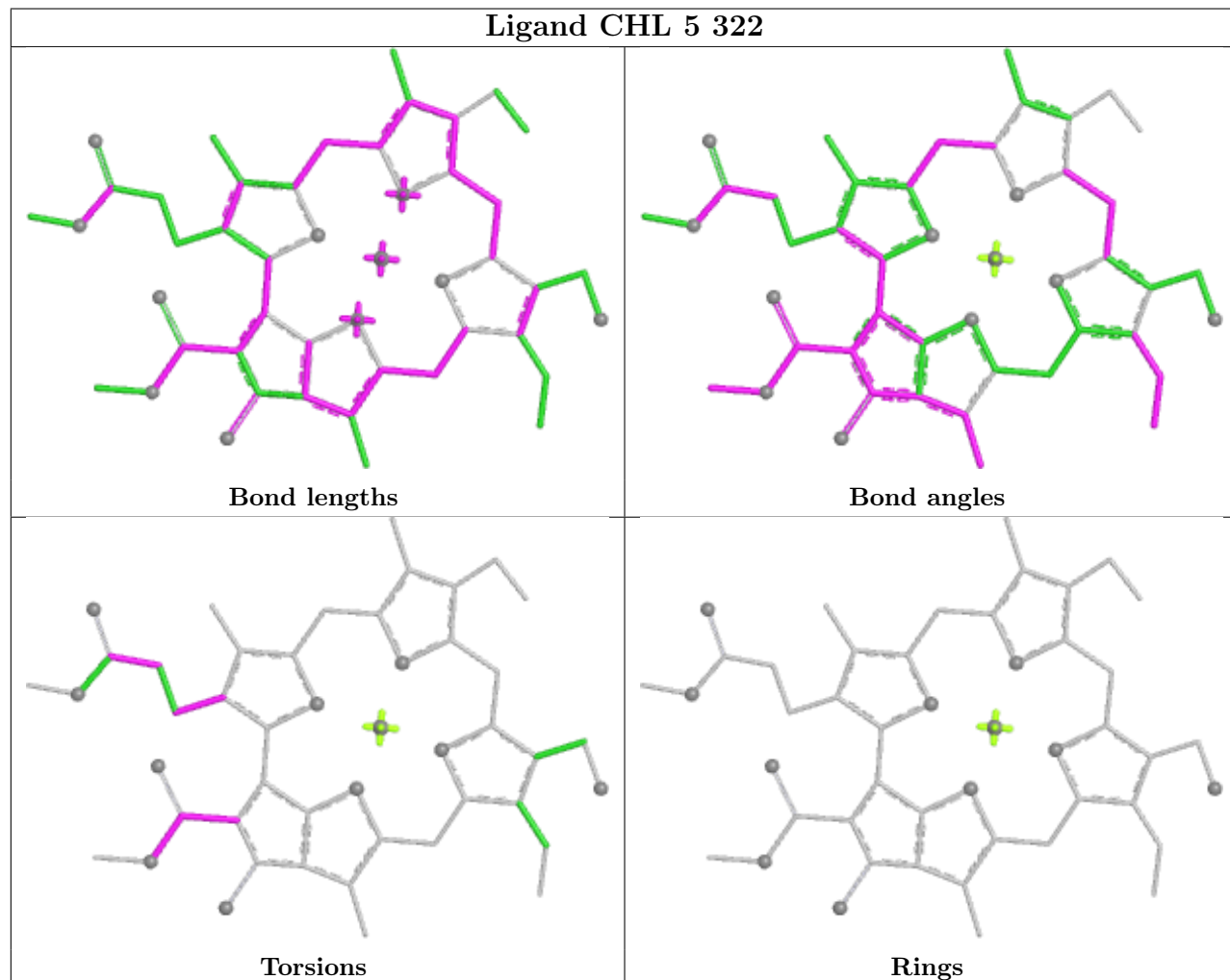


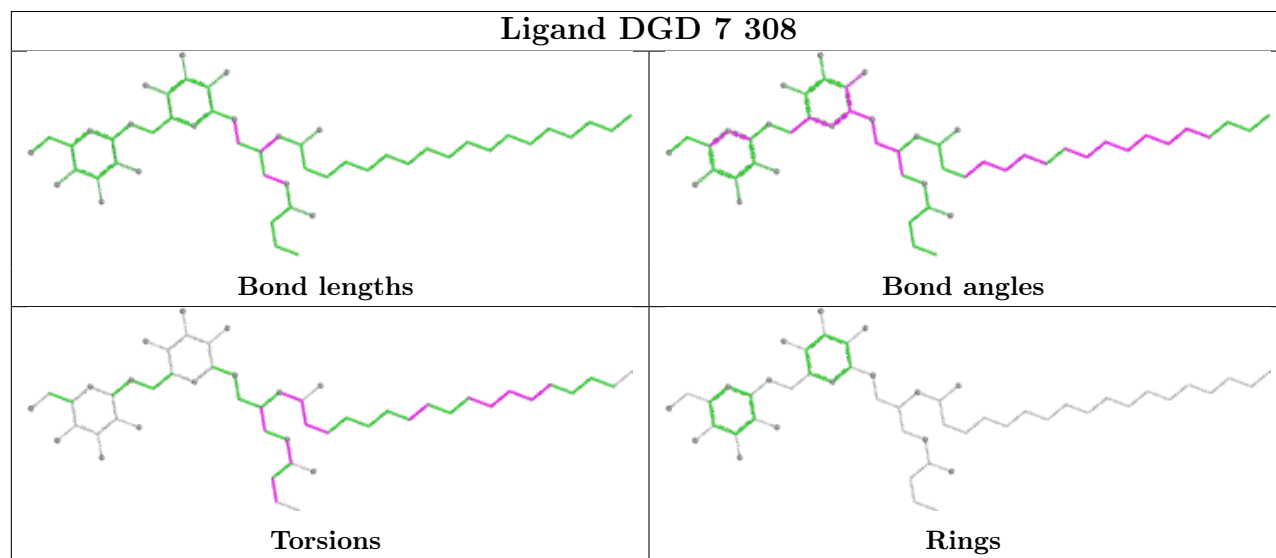
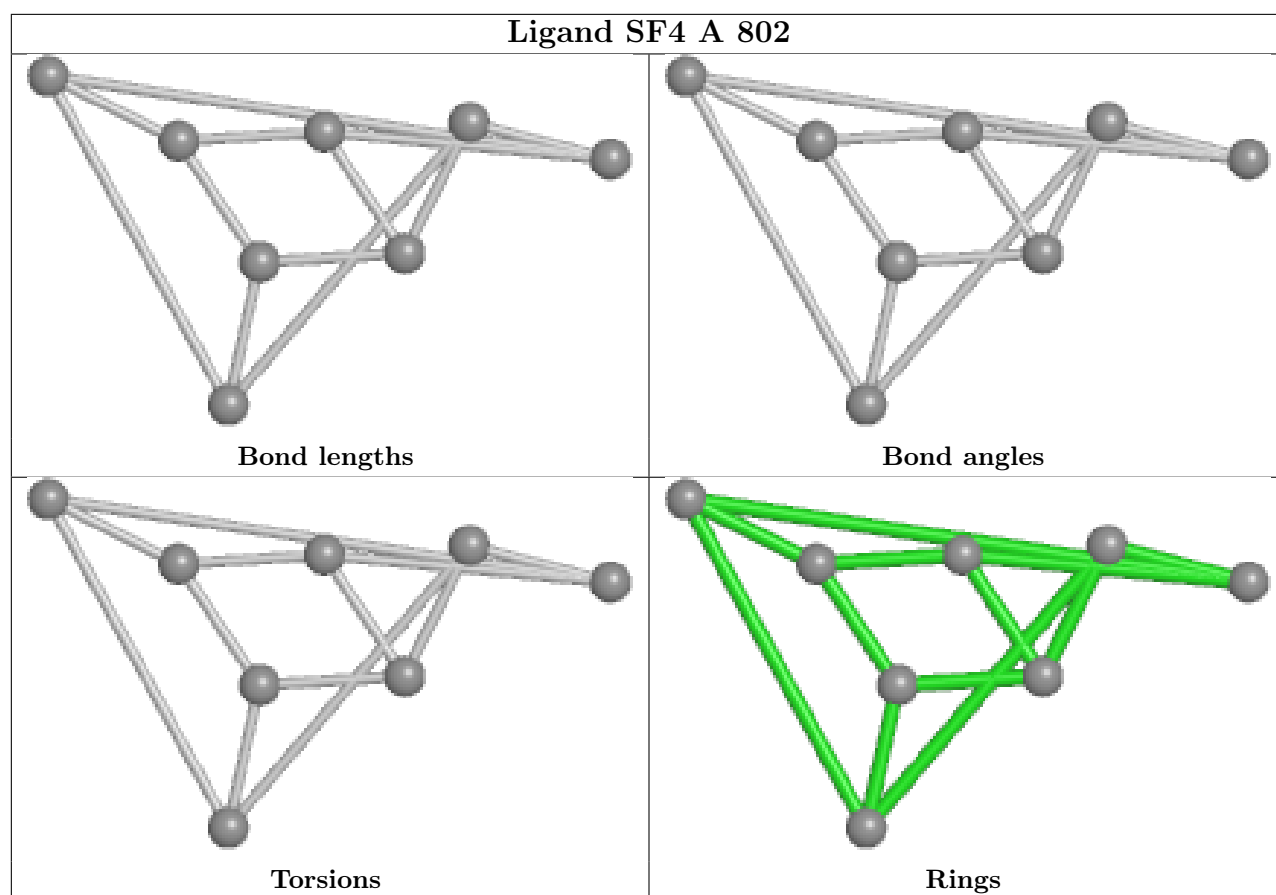
Rings

Ligand CLA A 826

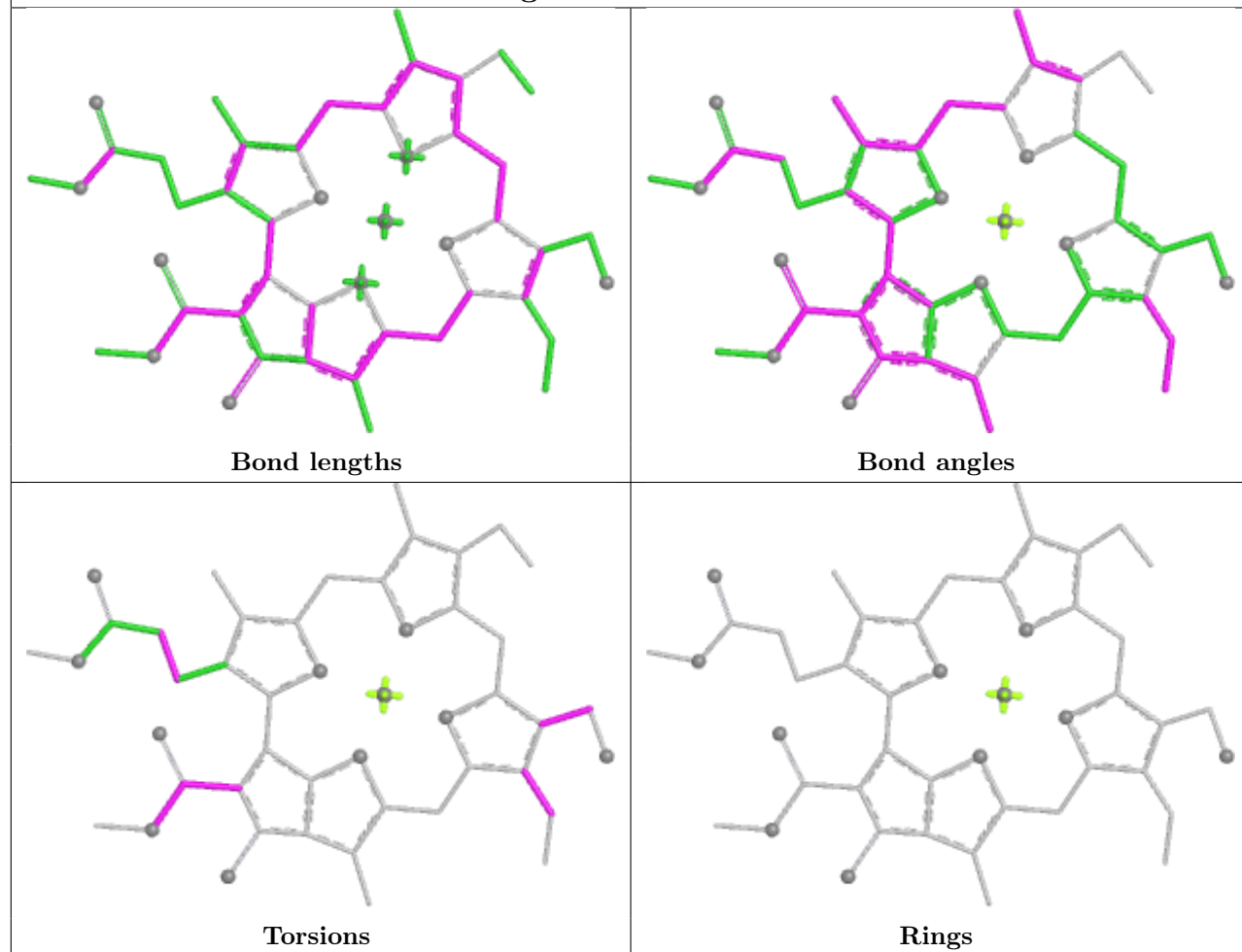


Ligand CHL 5 322

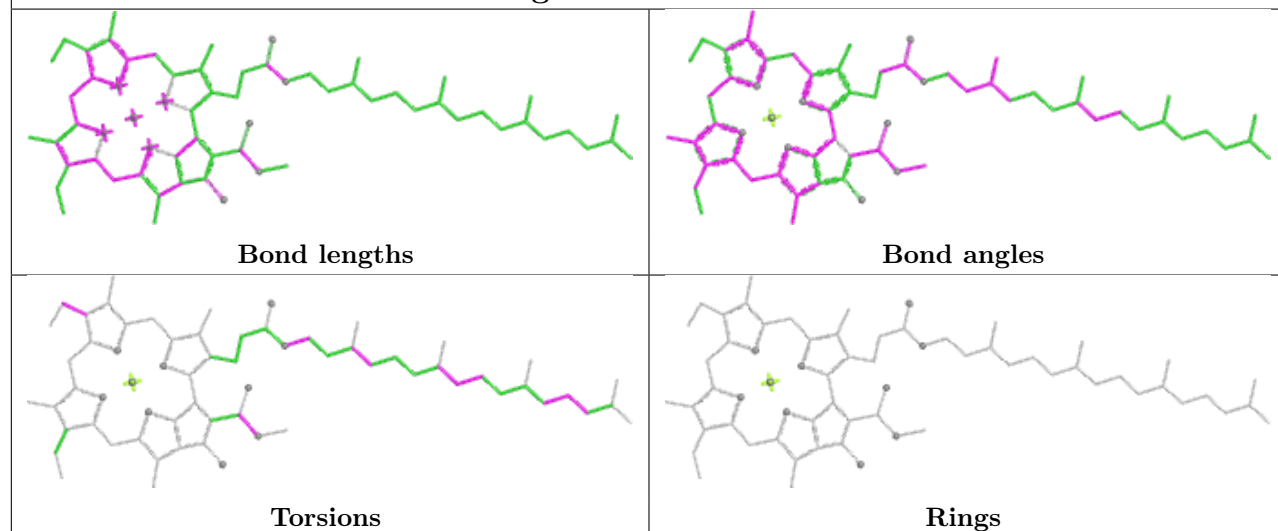


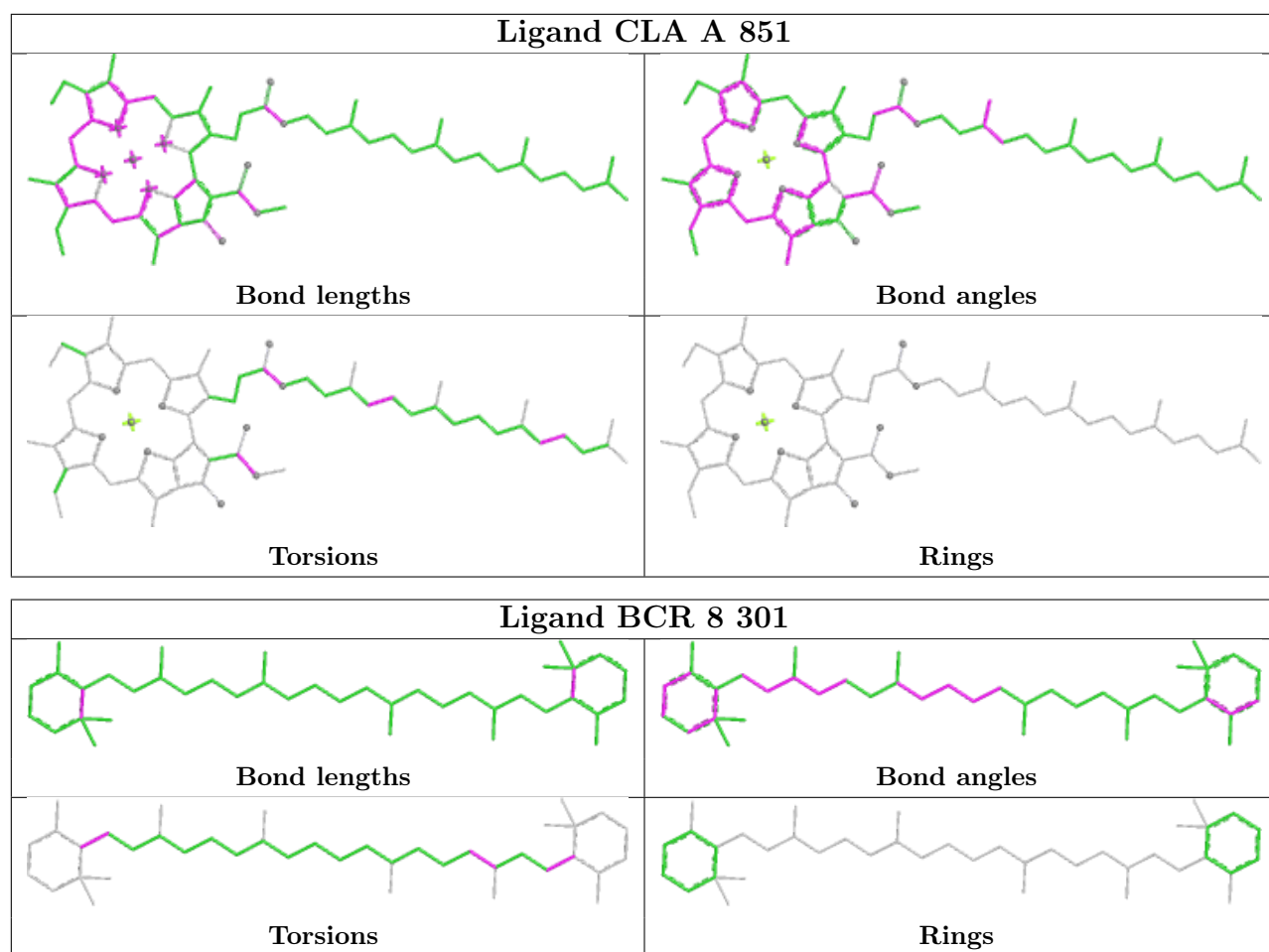


Ligand CHL 5 317

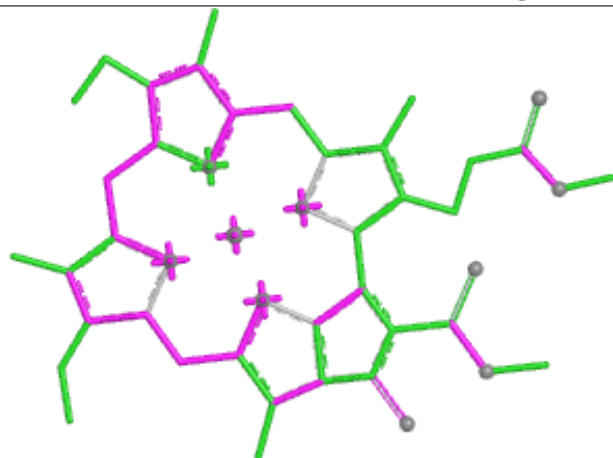


Ligand CLA A 853

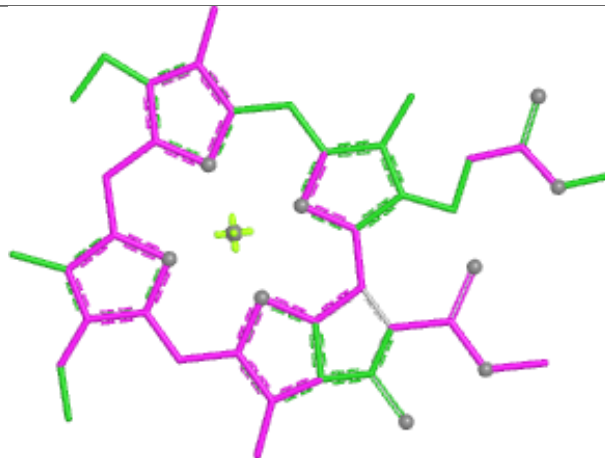




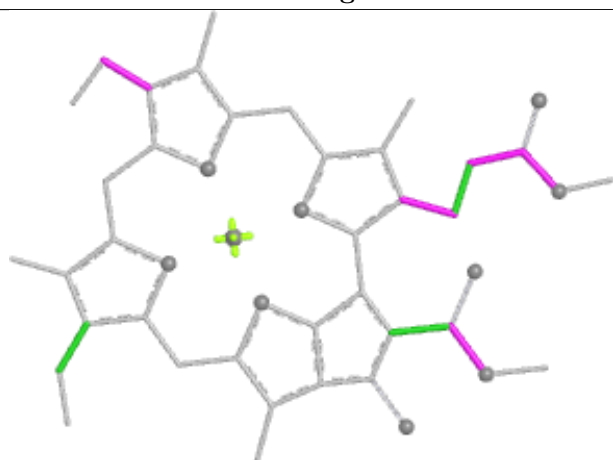
Ligand CLA H 901



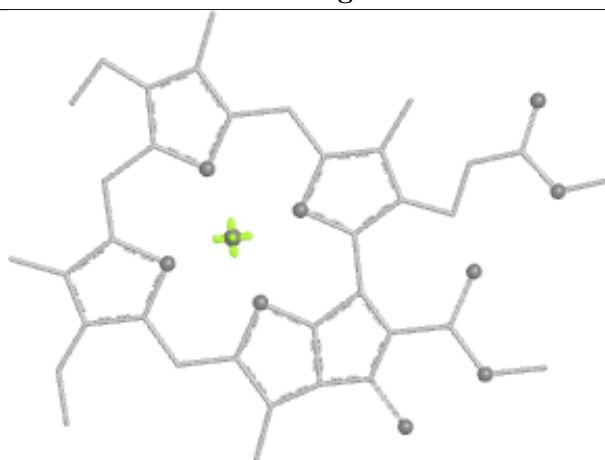
Bond lengths



Bond angles

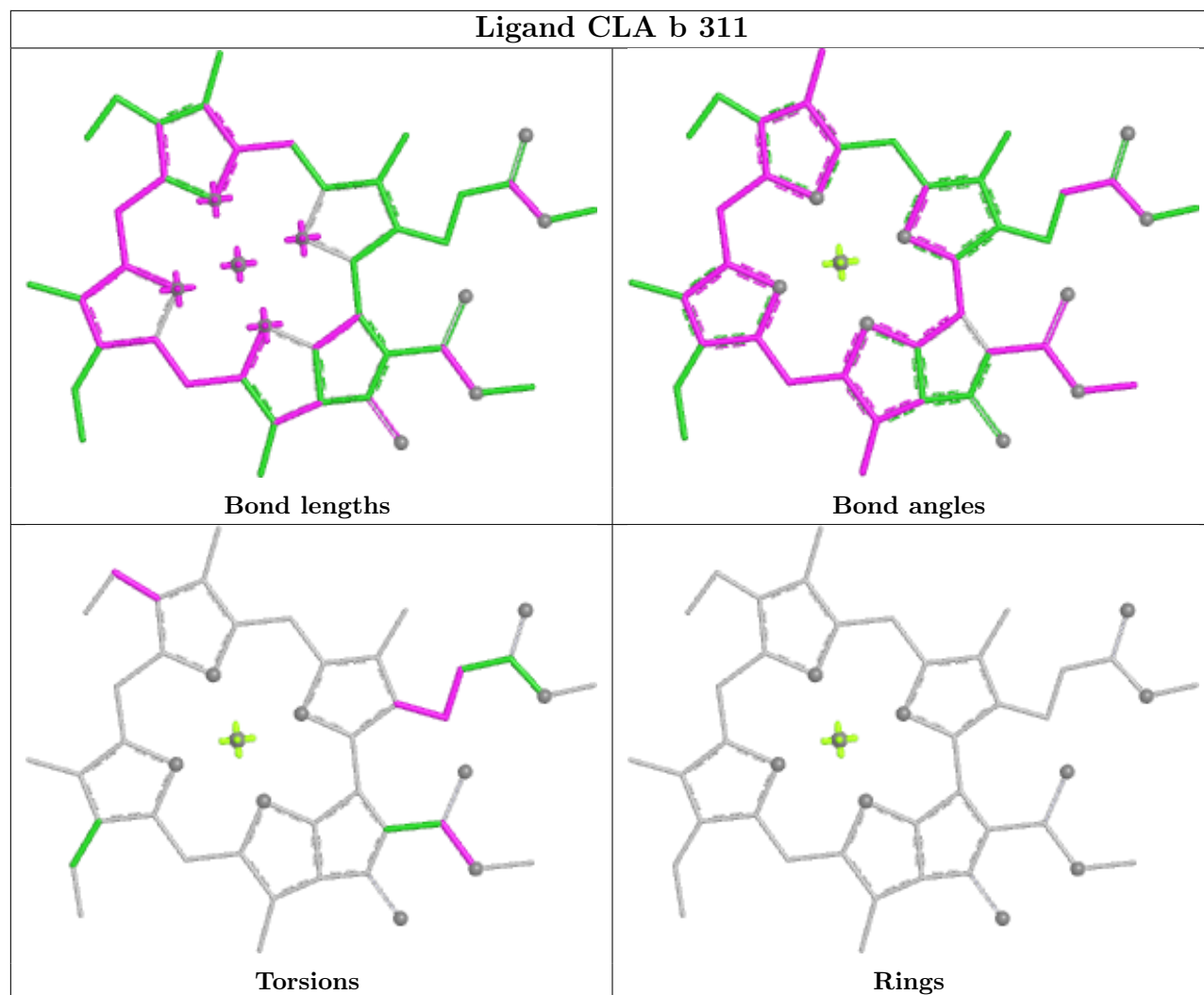


Torsions

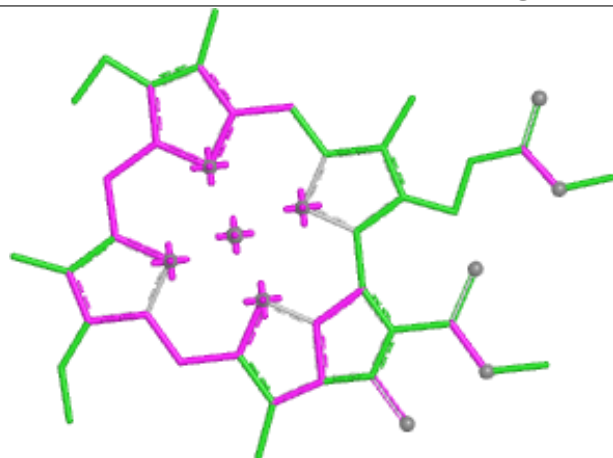


Rings

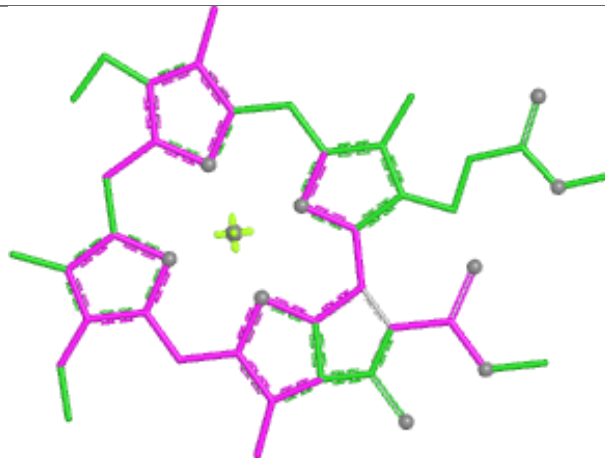
Ligand CLA b 311



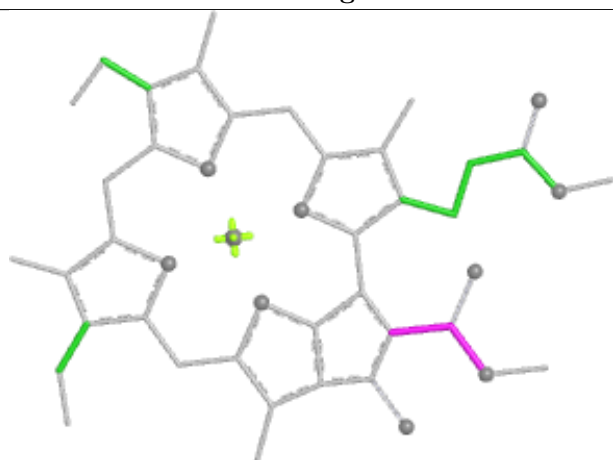
Ligand CLA B 838



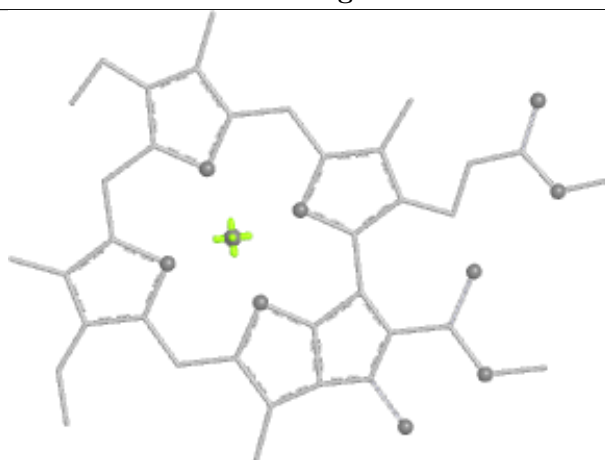
Bond lengths



Bond angles

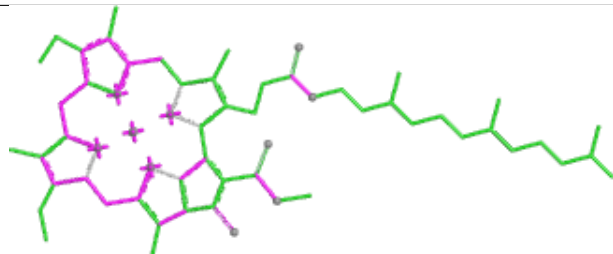


Torsions

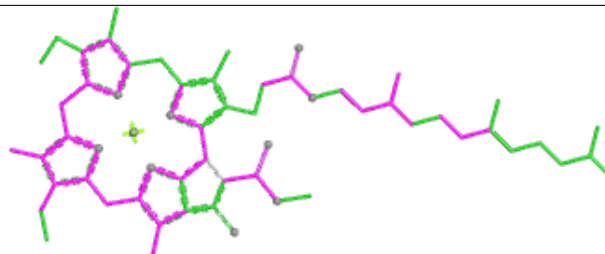


Rings

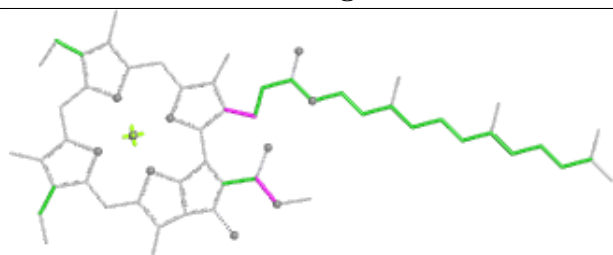
Ligand CLA a 309



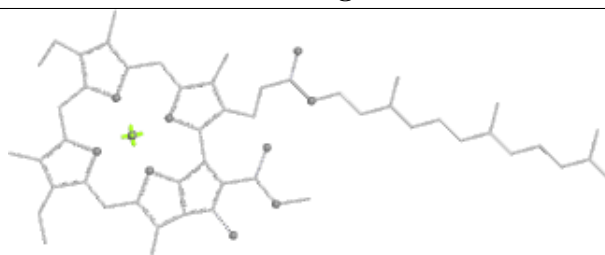
Bond lengths



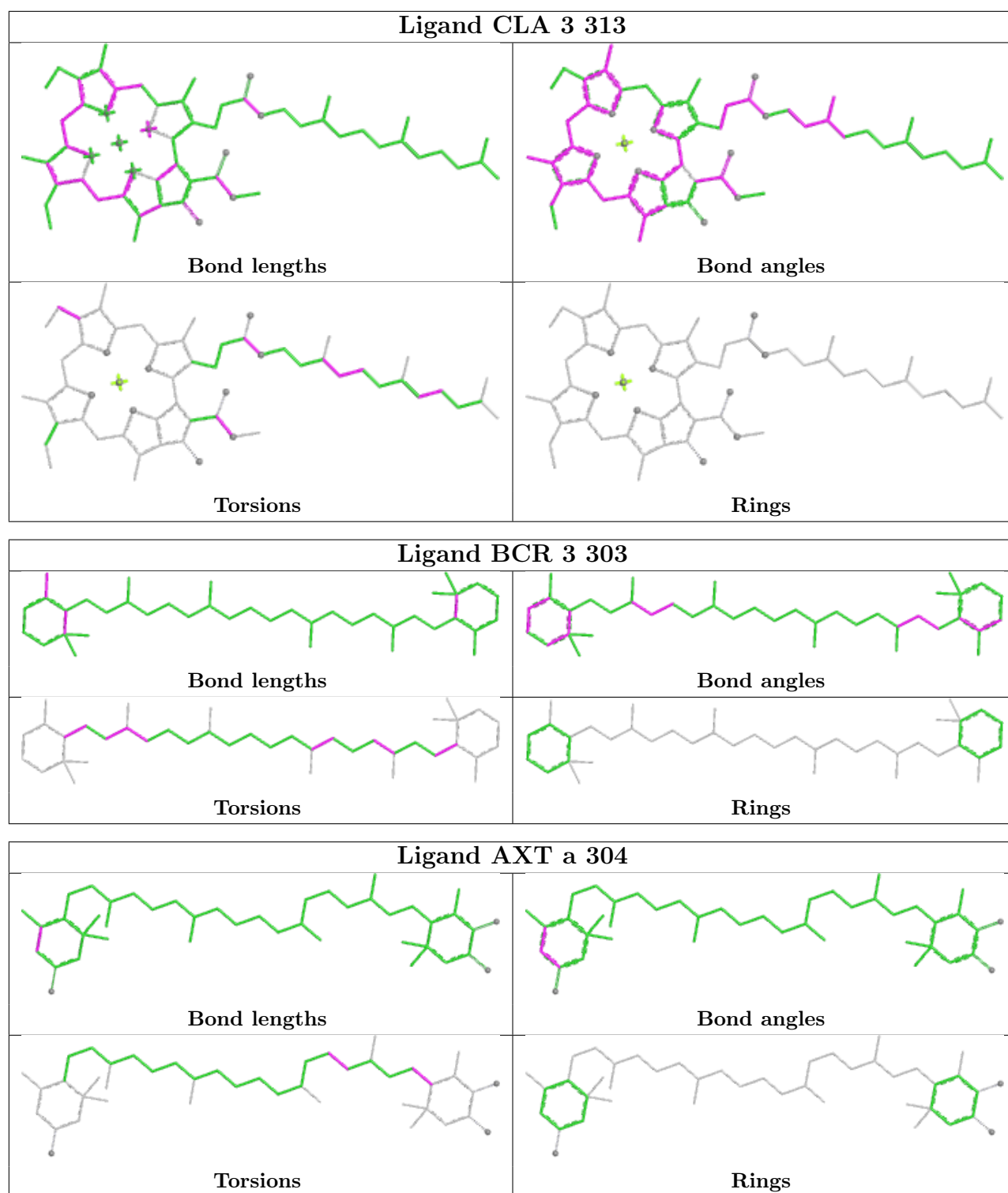
Bond angles



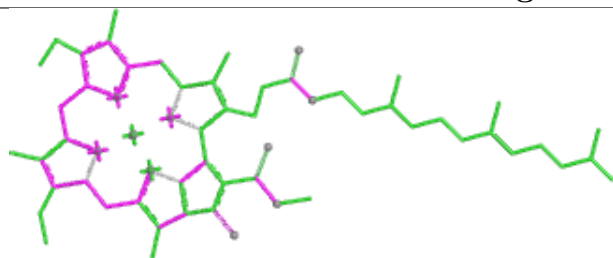
Torsions



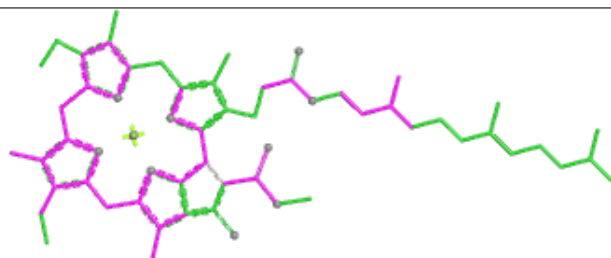
Rings



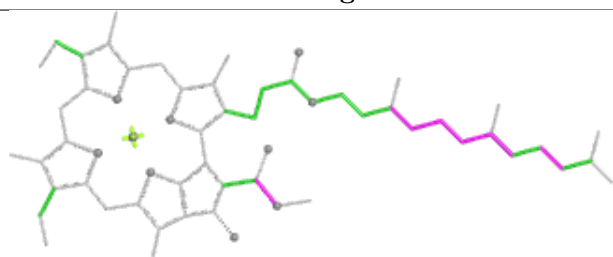
Ligand CLA L 305



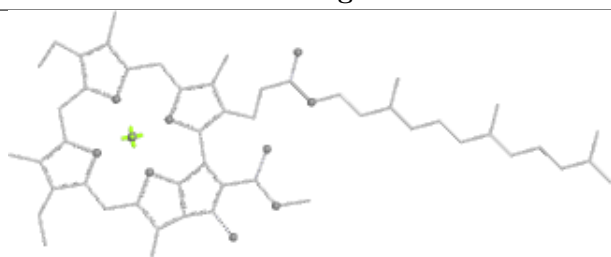
Bond lengths



Bond angles

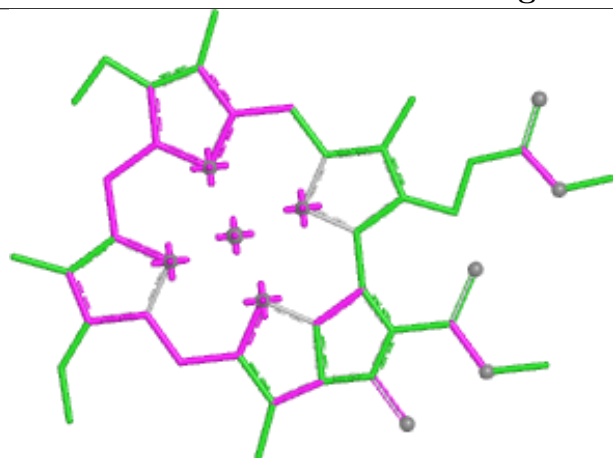


Torsions

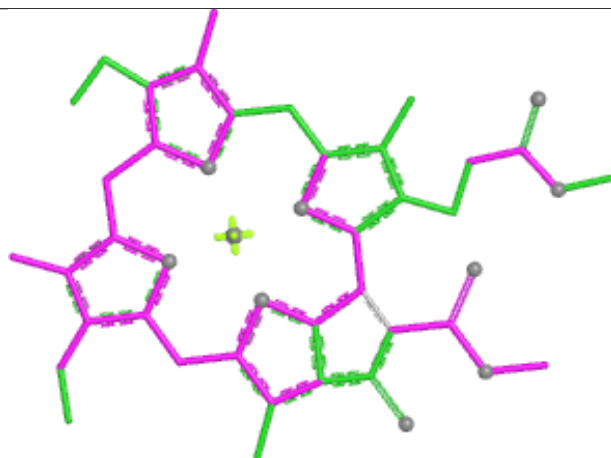


Rings

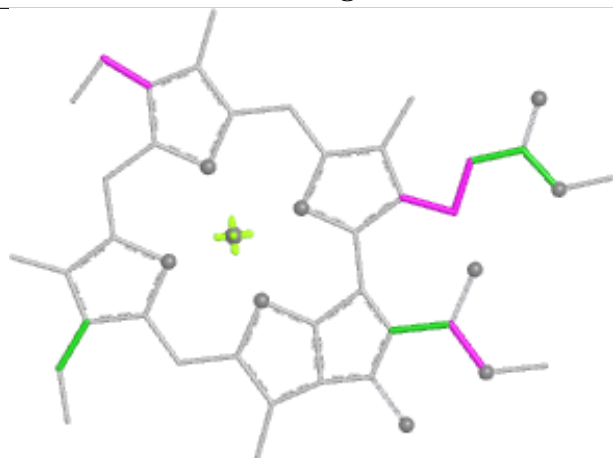
Ligand CLA 2 315



Bond lengths



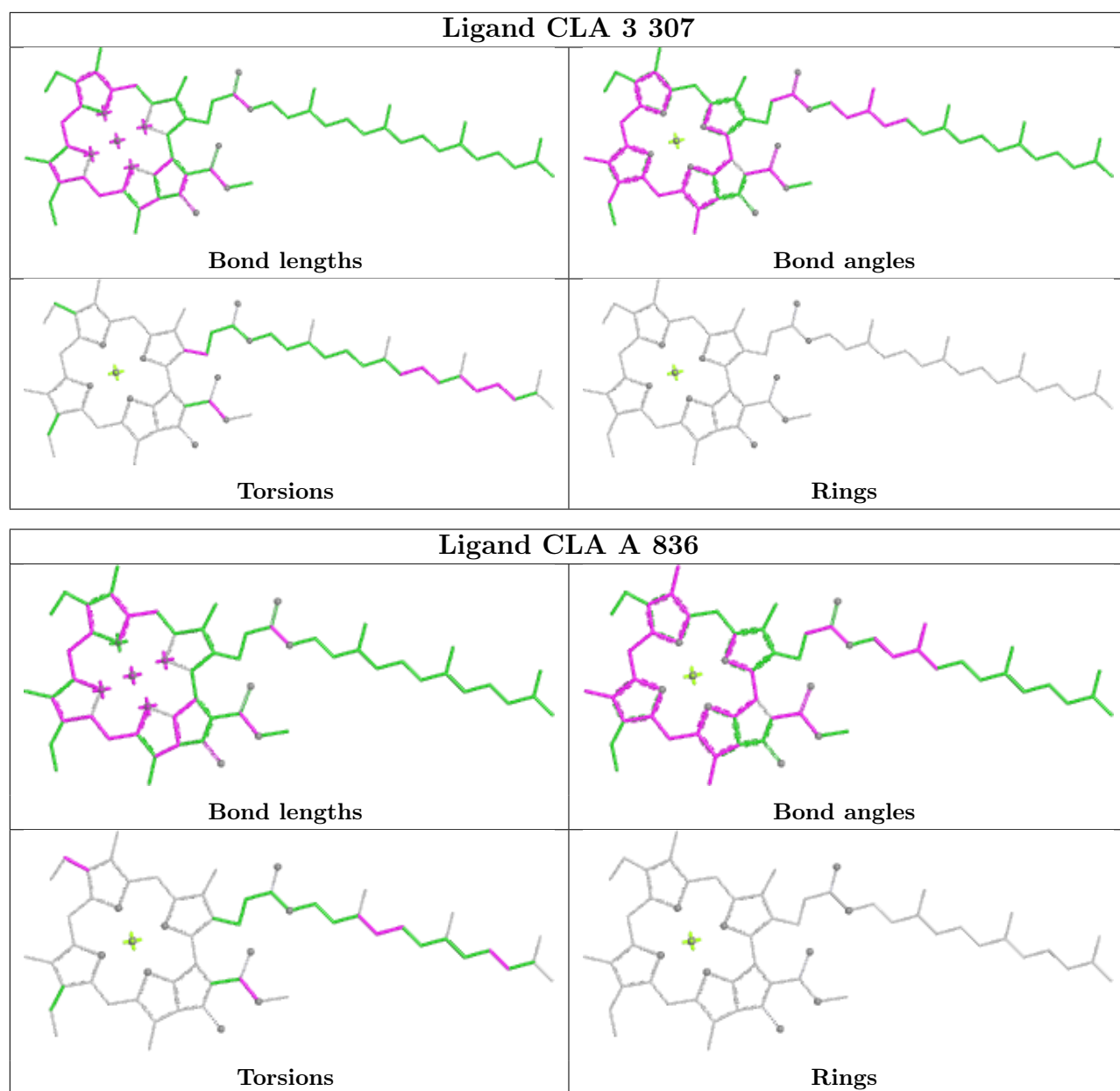
Bond angles

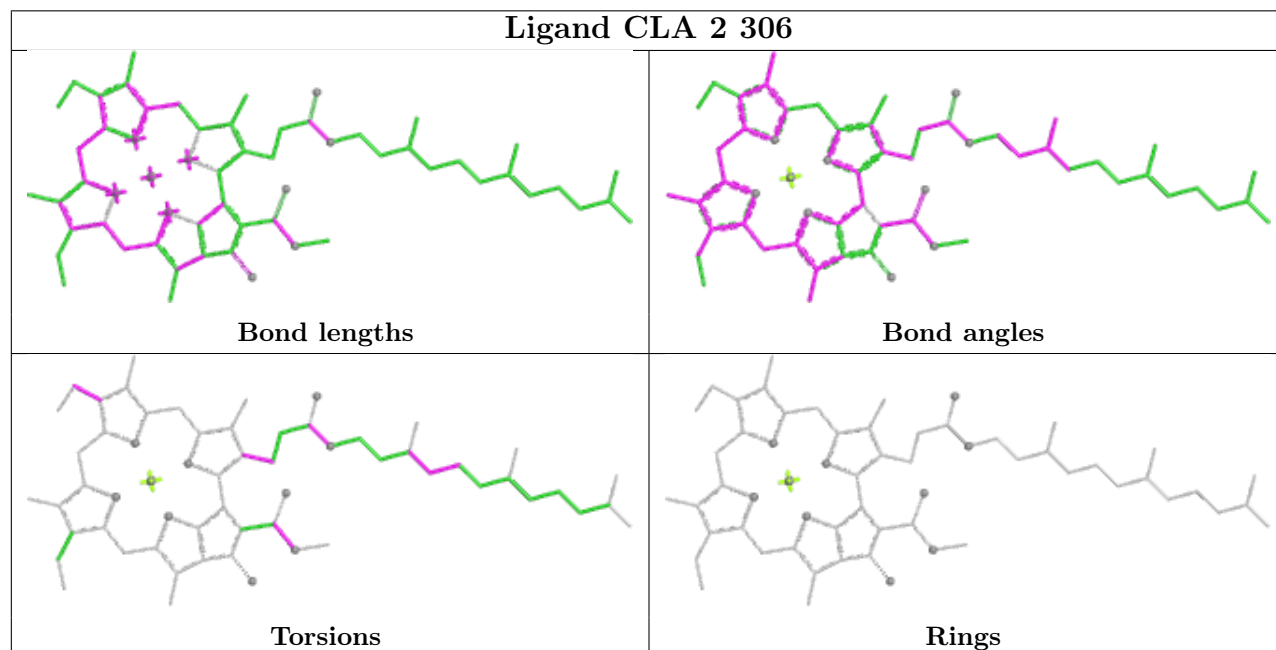
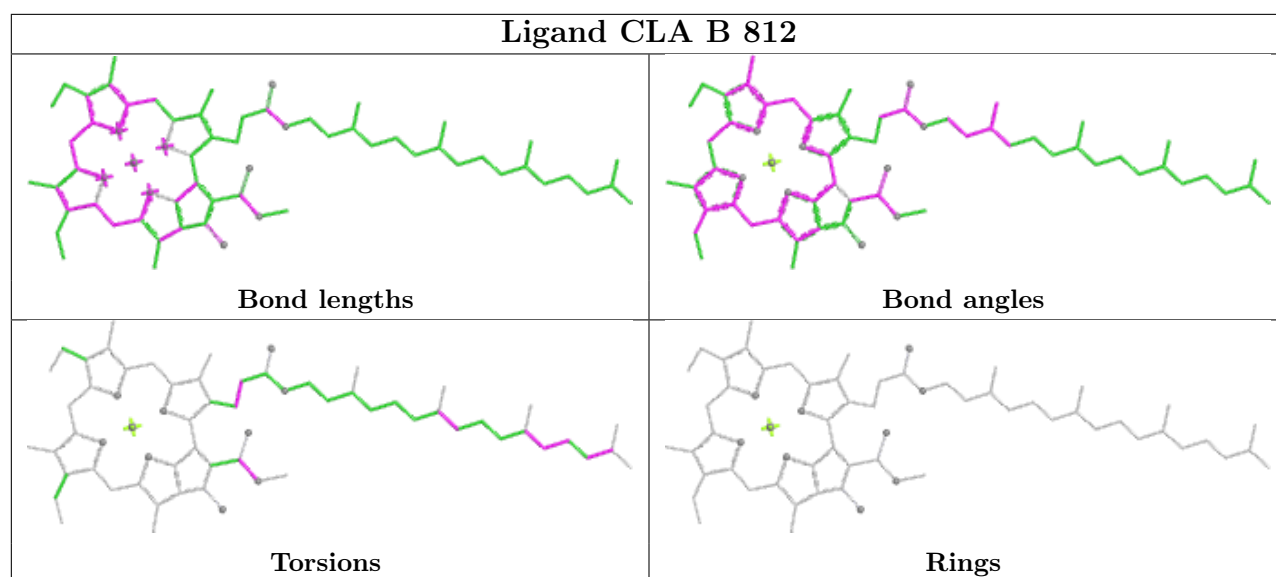


Torsions

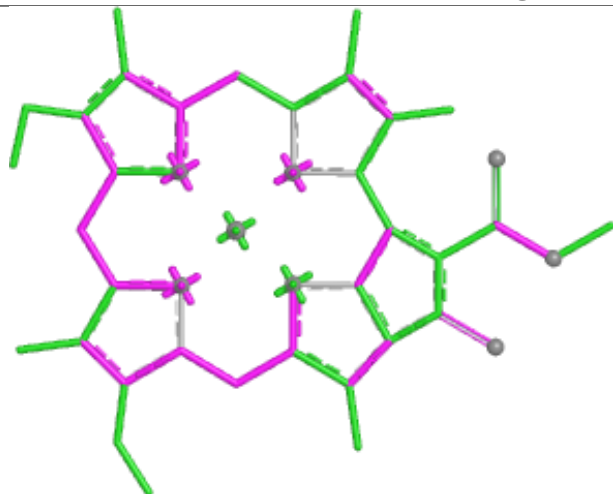


Rings

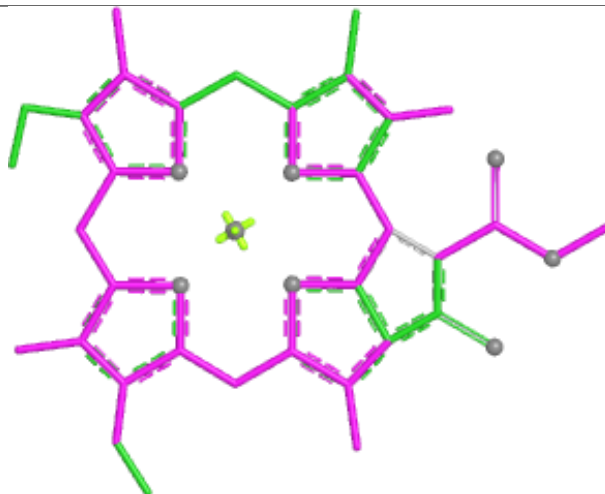




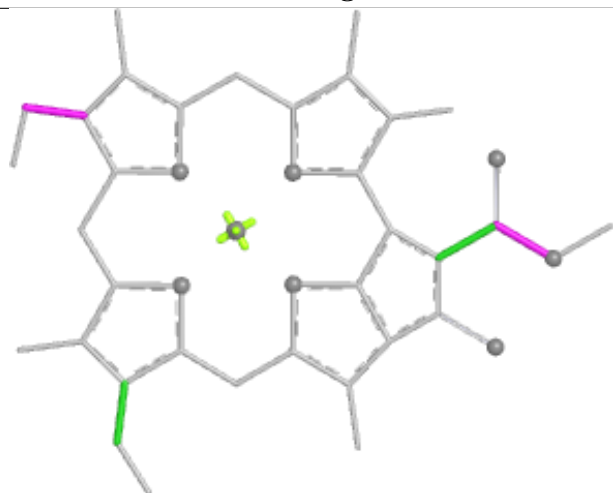
Ligand CLA O 204



Bond lengths



Bond angles

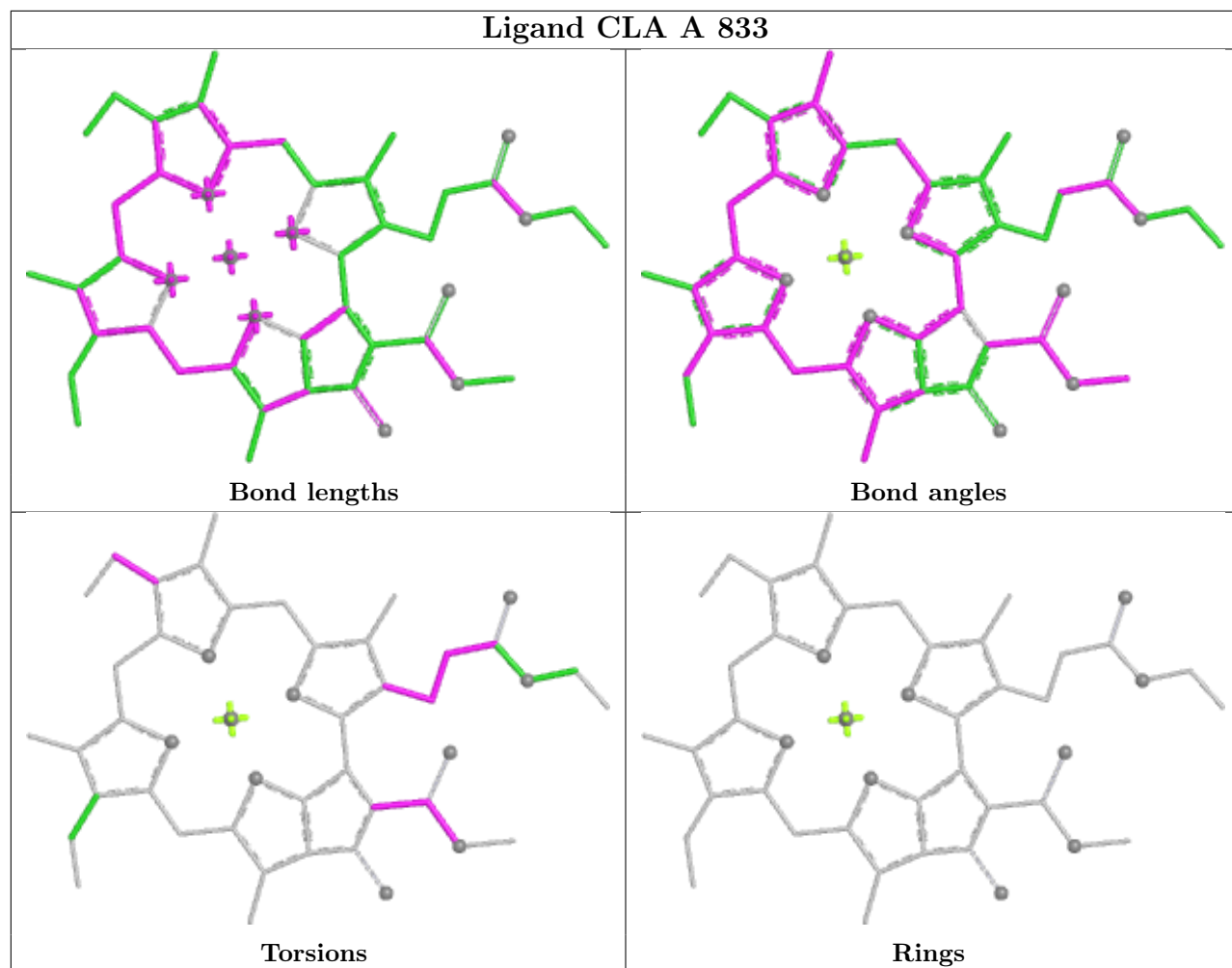


Torsions

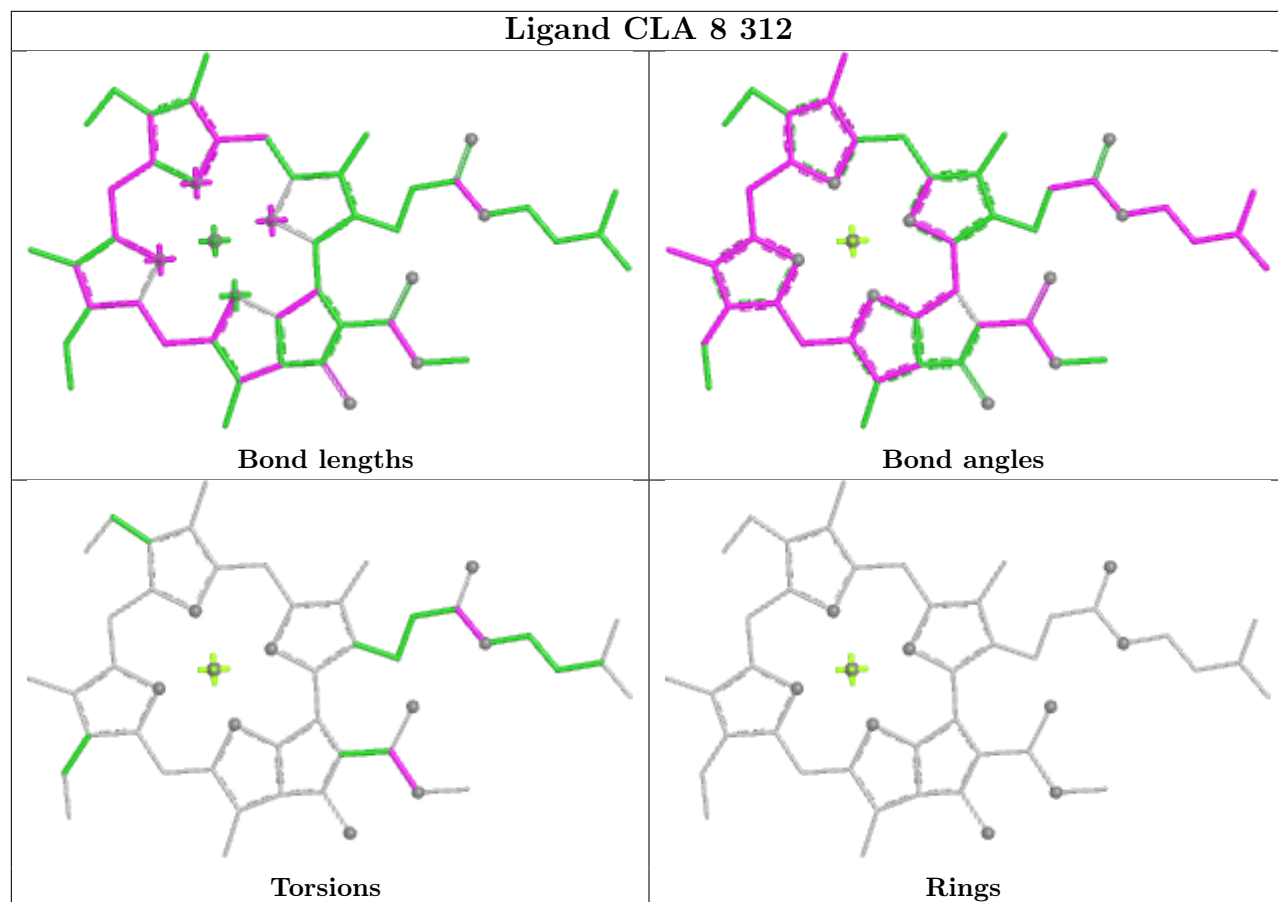


Rings

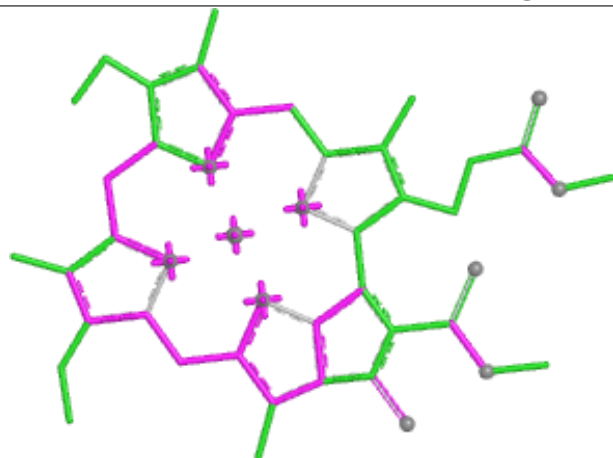
Ligand CLA A 833



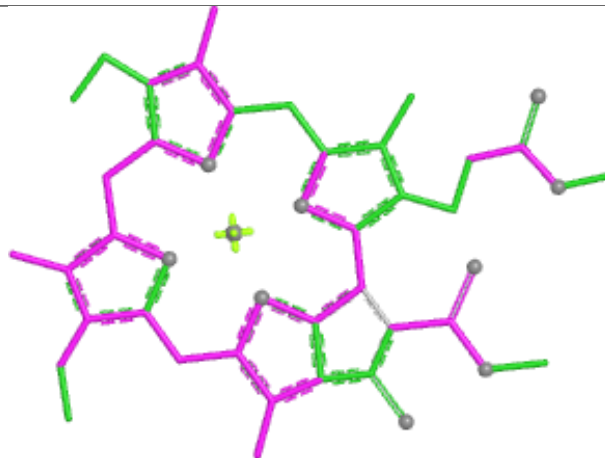
Ligand CLA 8 312



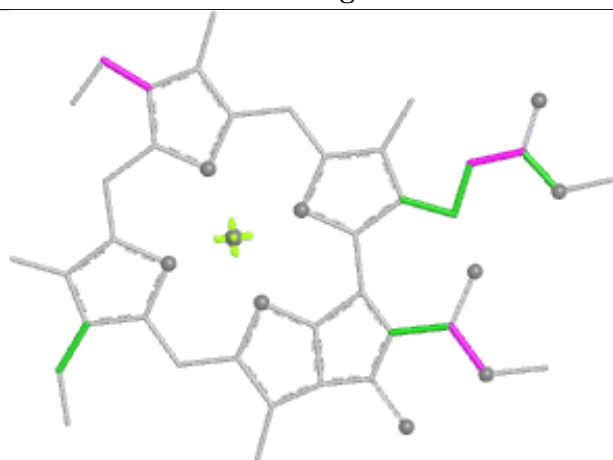
Ligand CLA 5 313



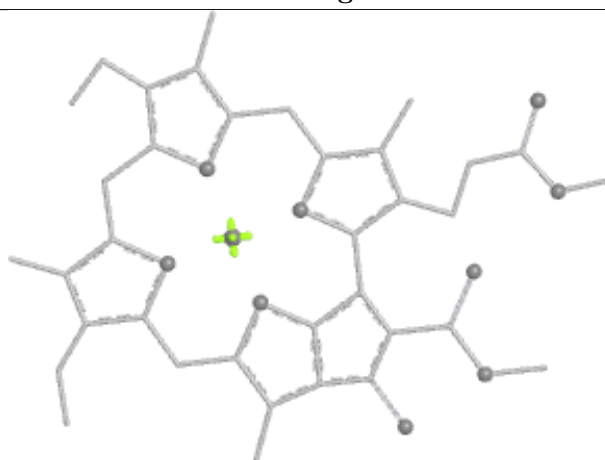
Bond lengths



Bond angles

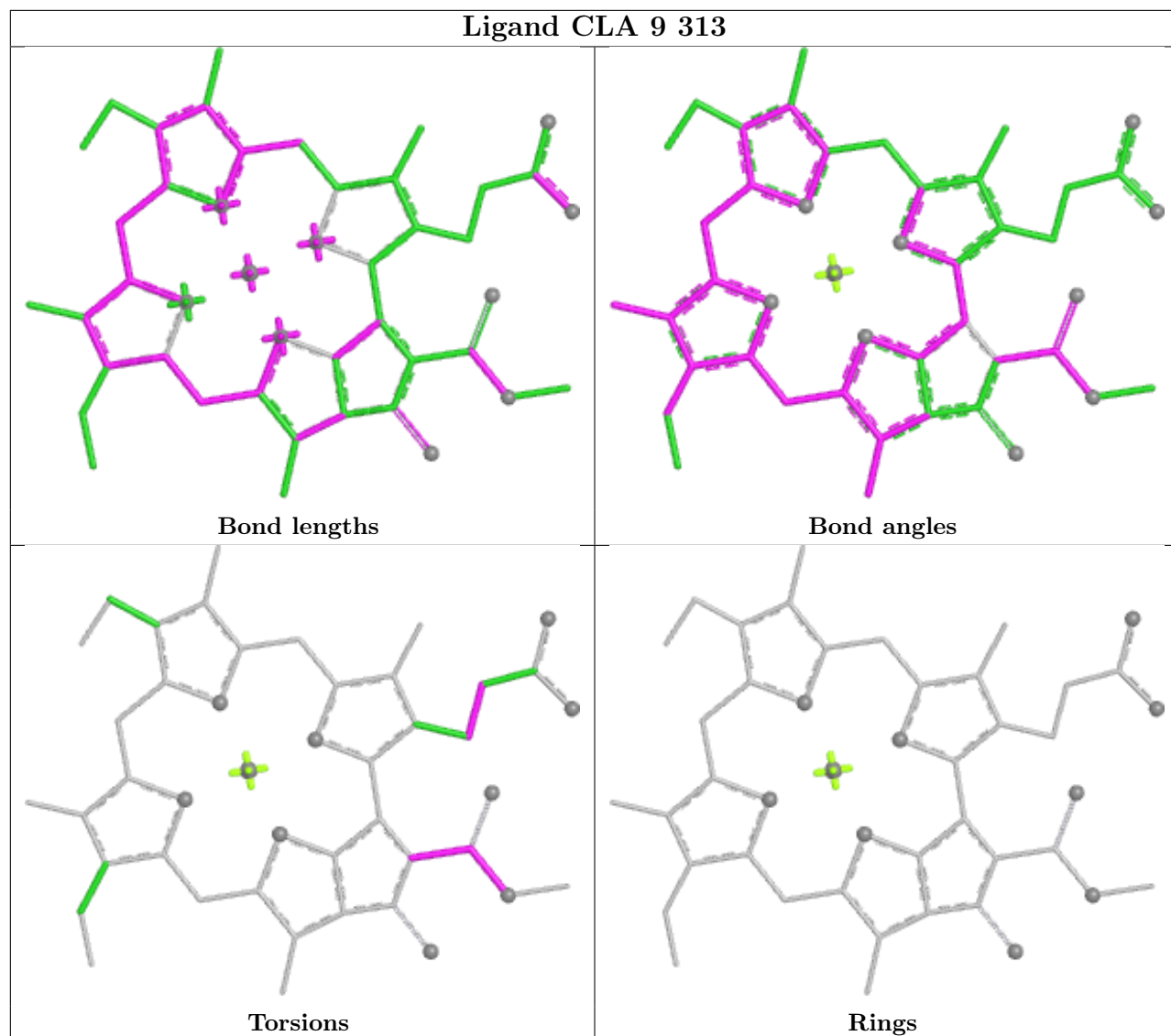


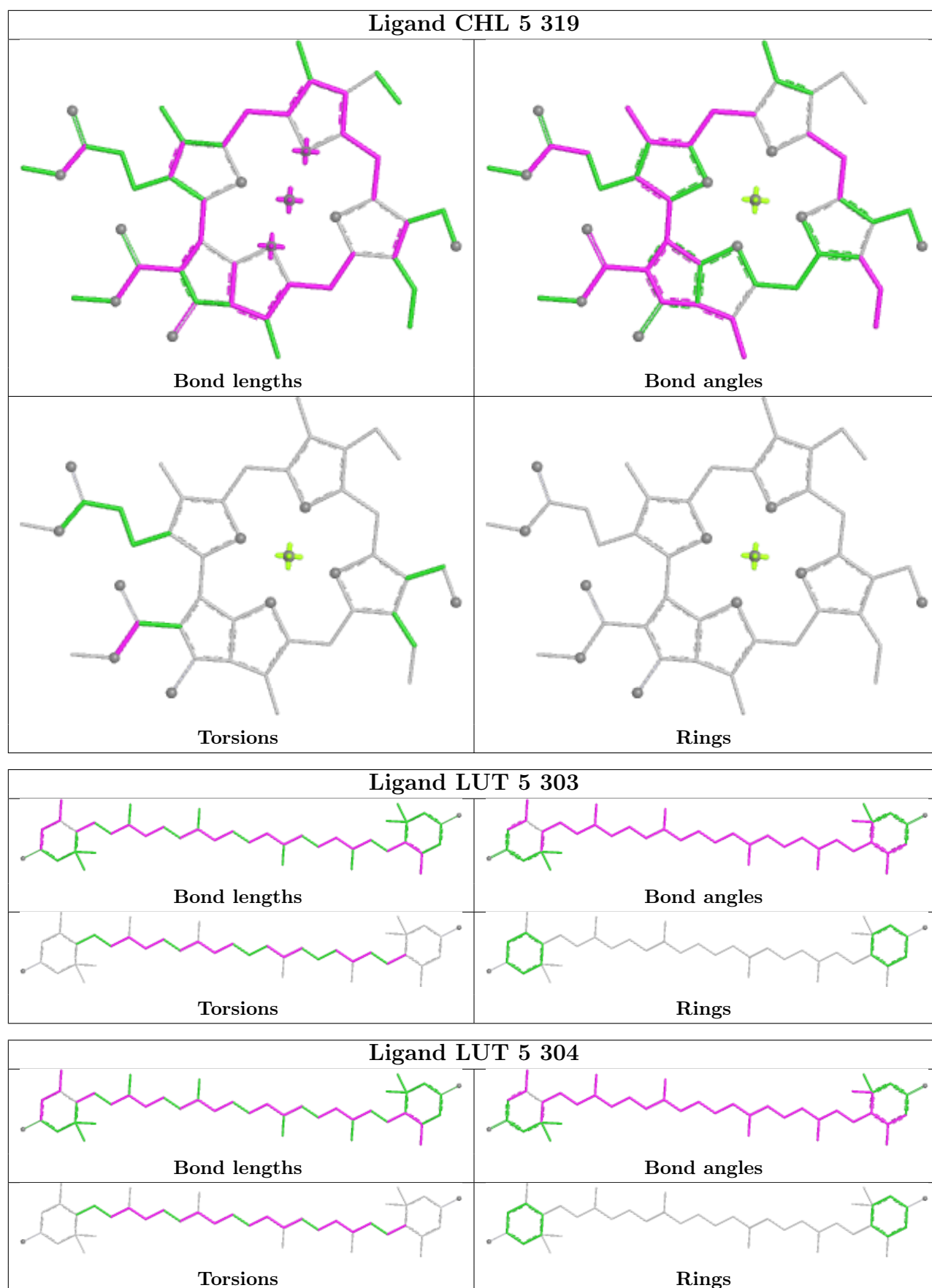
Torsions

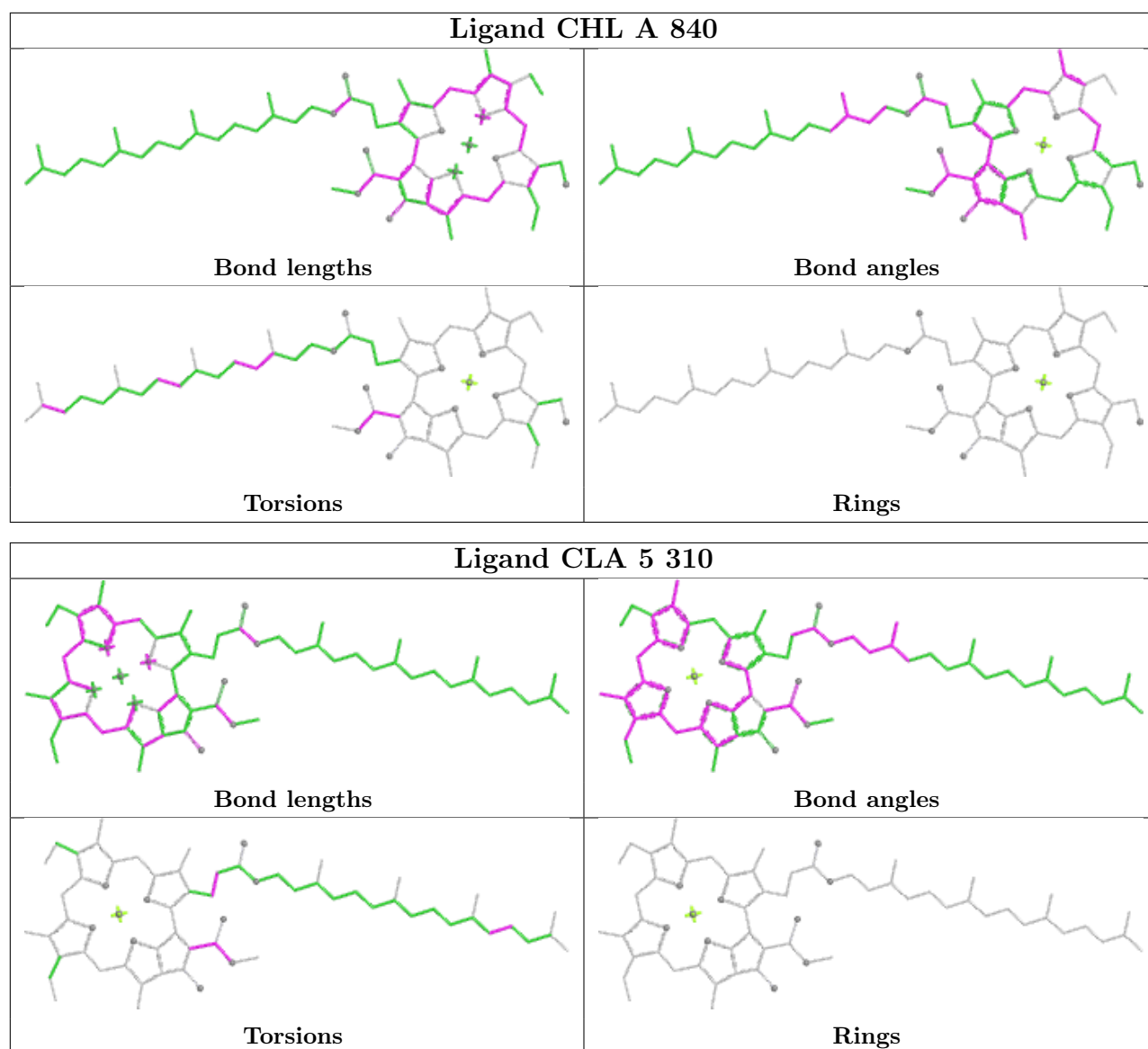


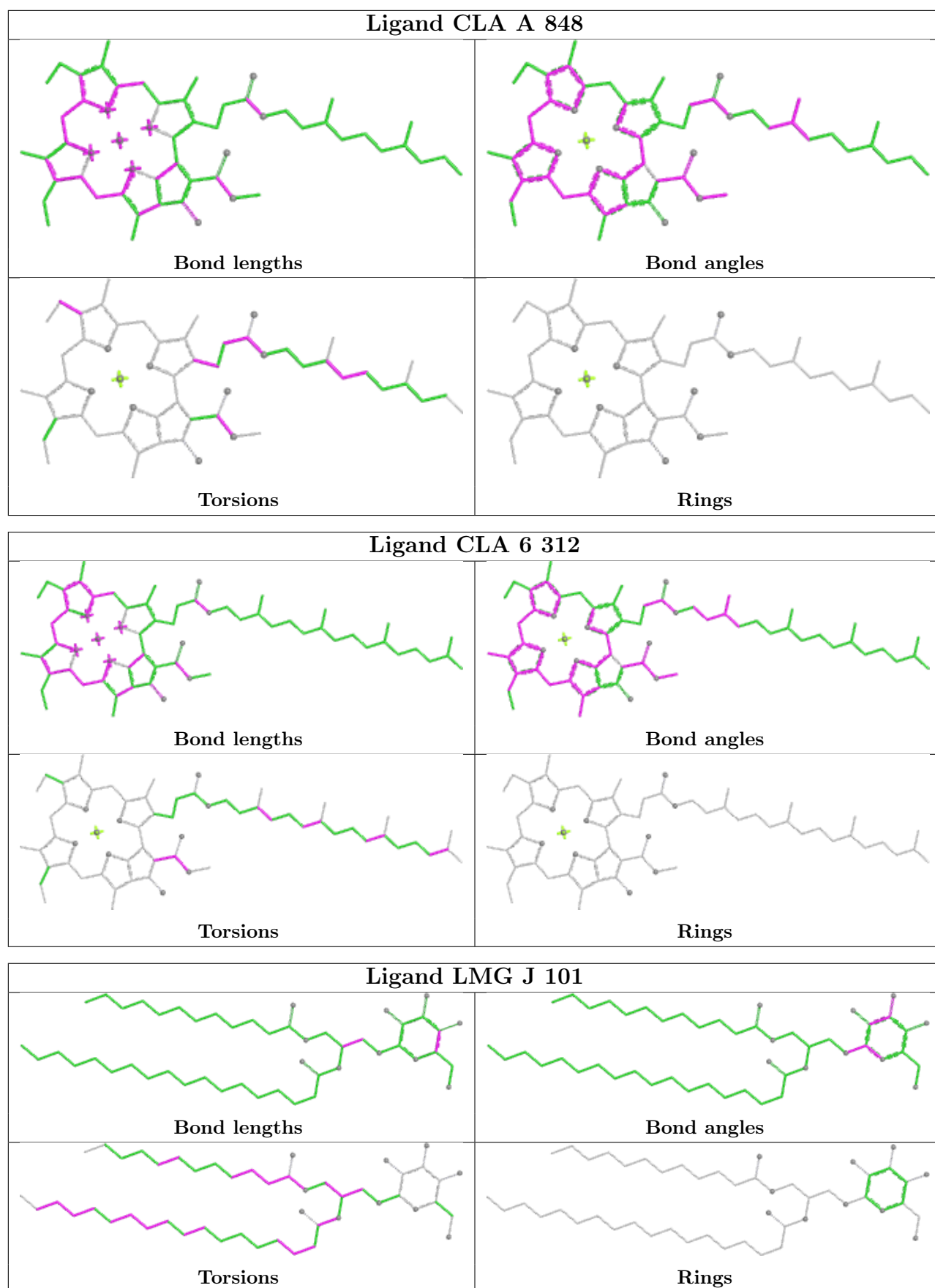
Rings

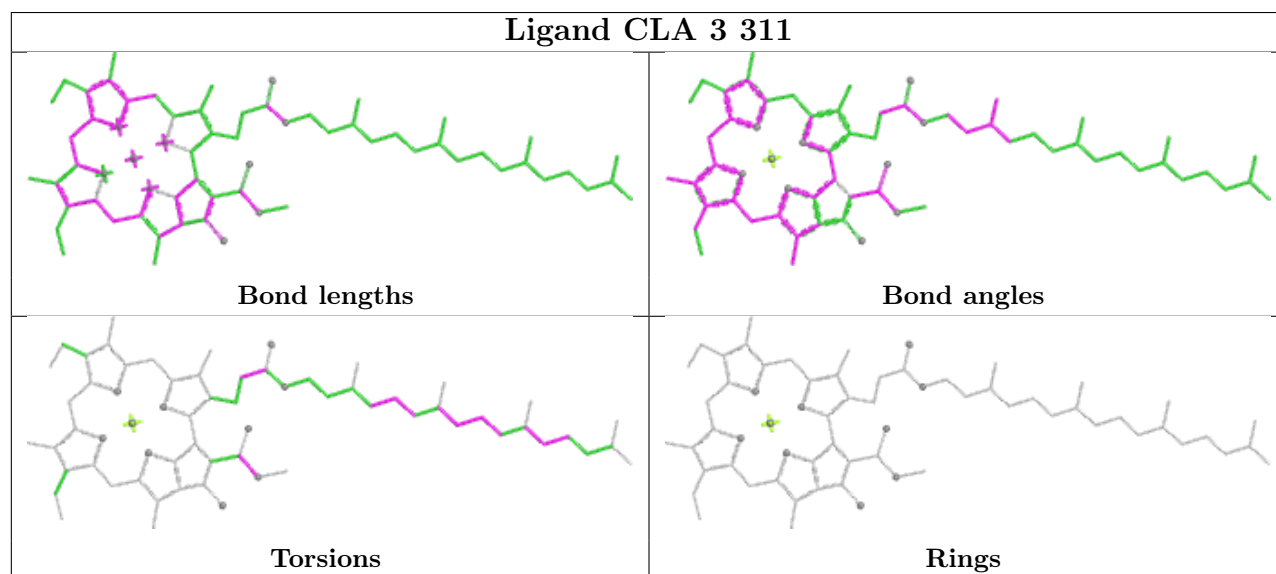
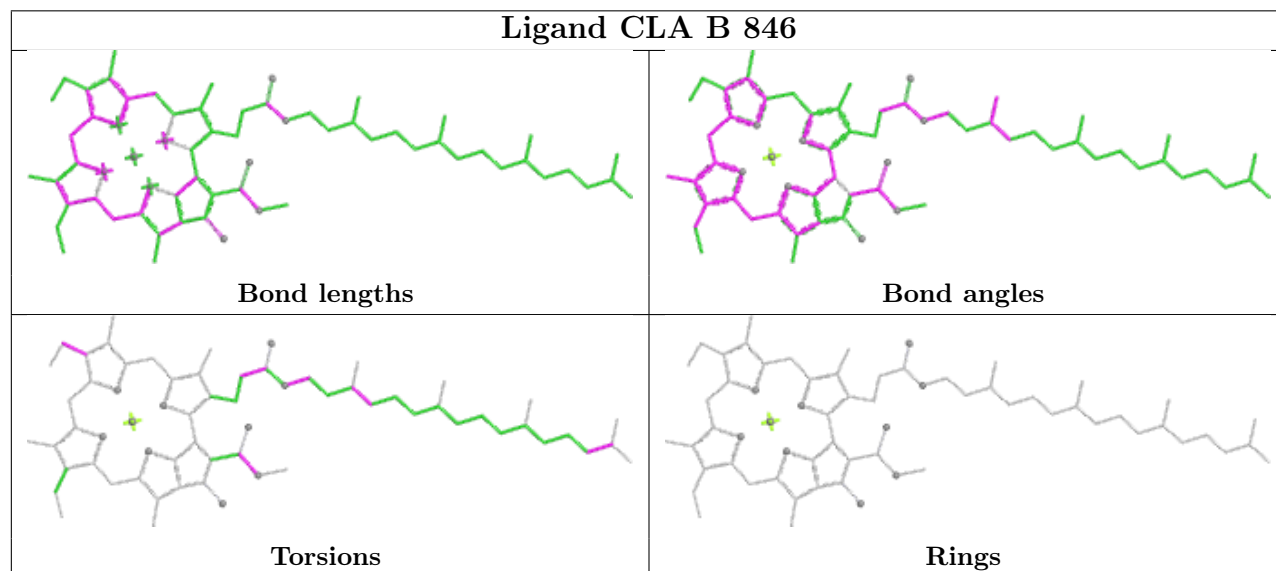
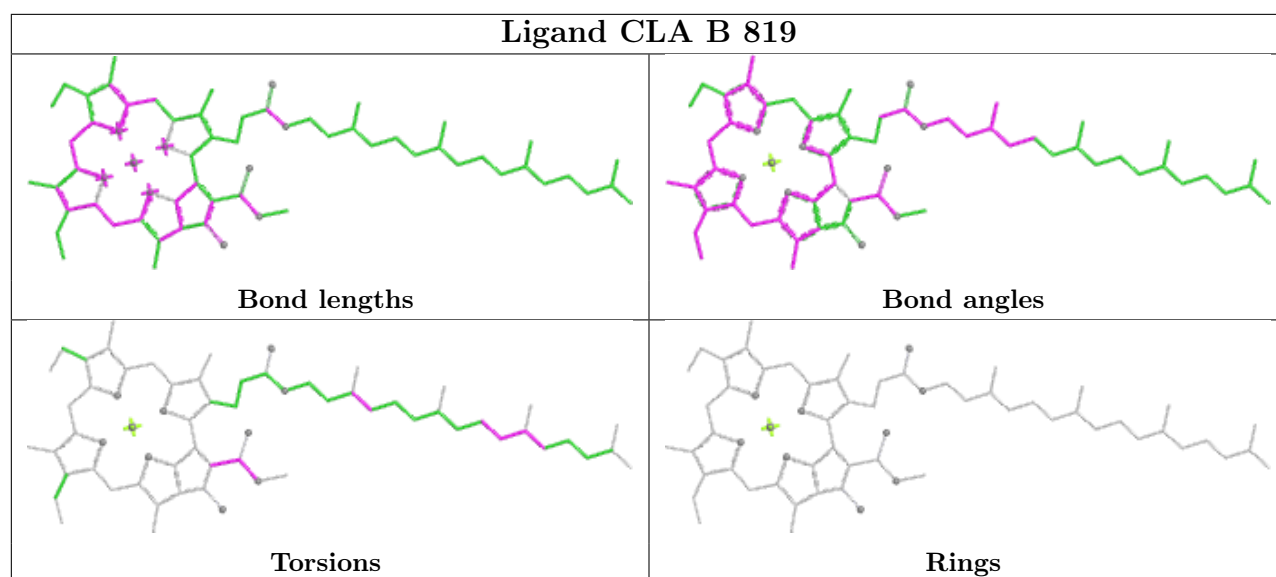
Ligand CLA 9 313



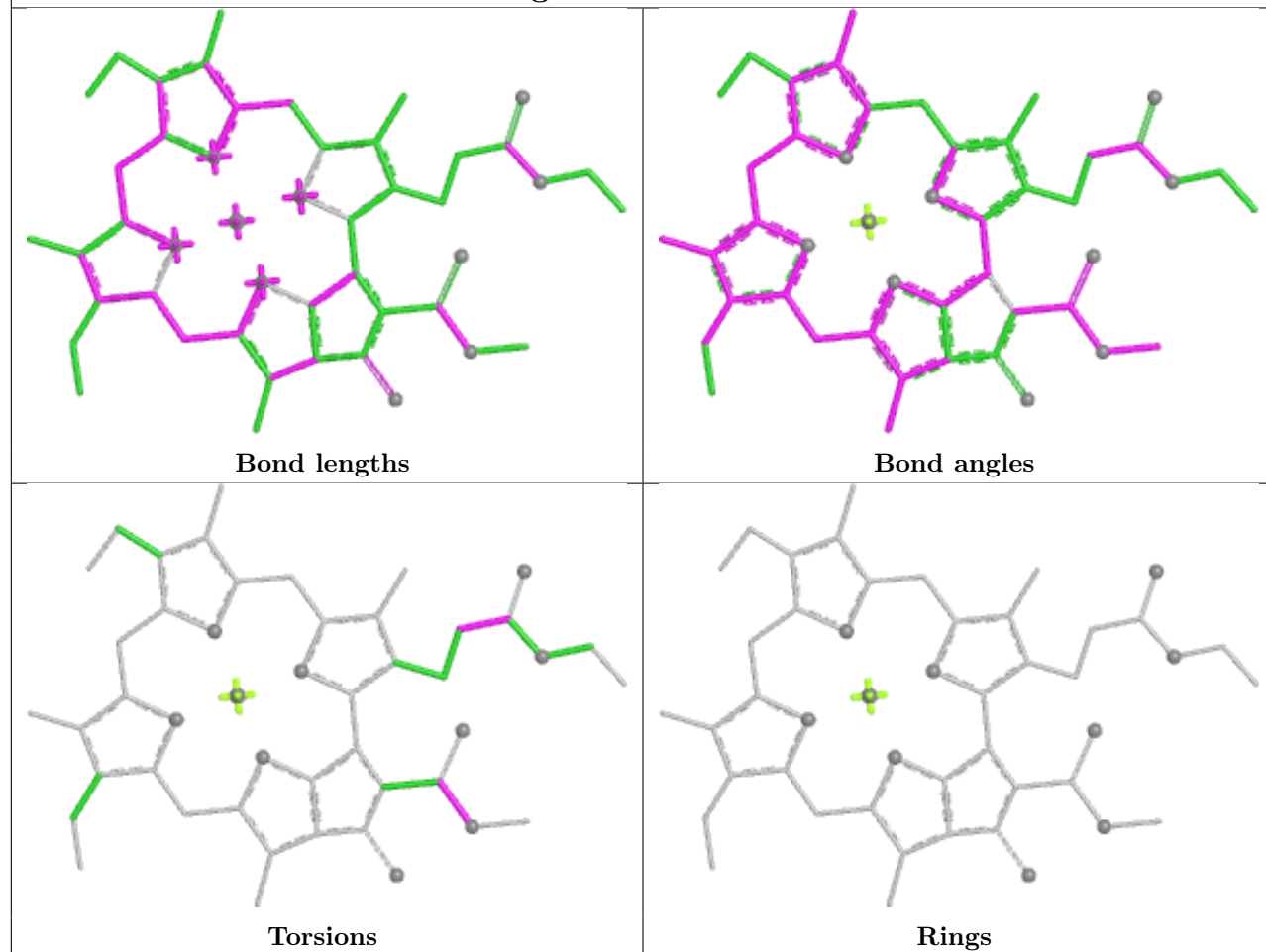




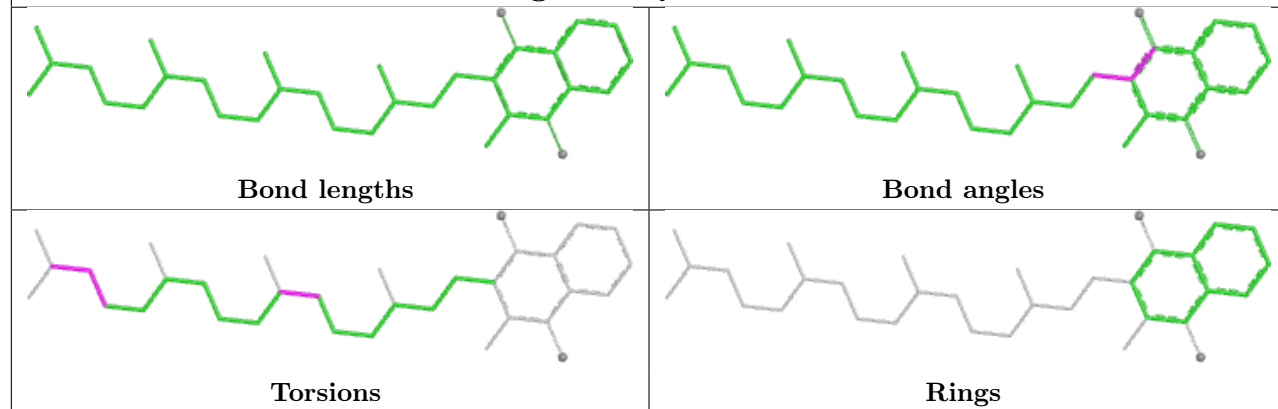


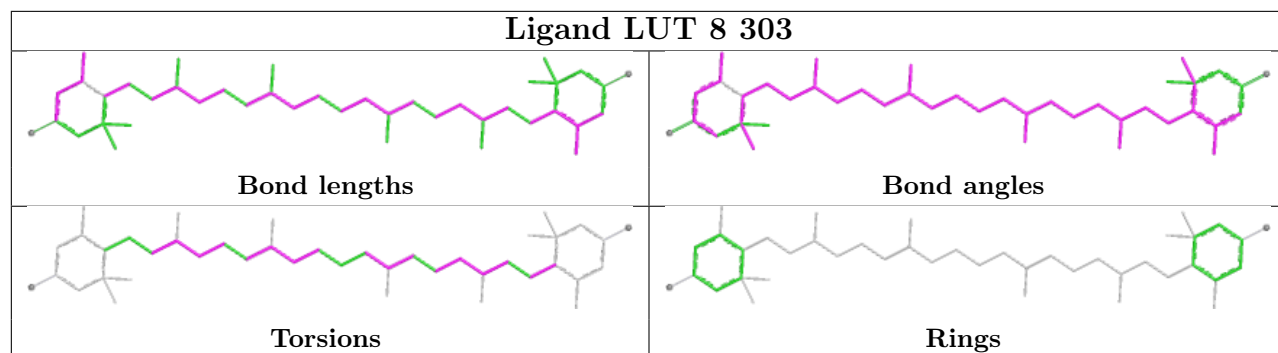
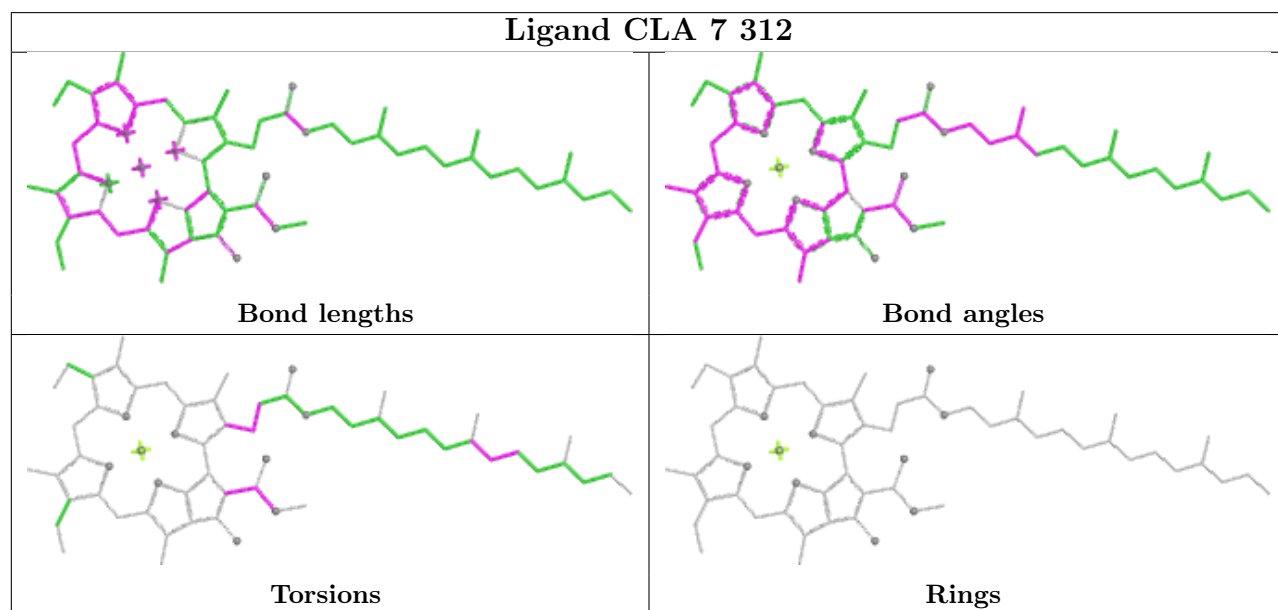


Ligand CLA 6 310

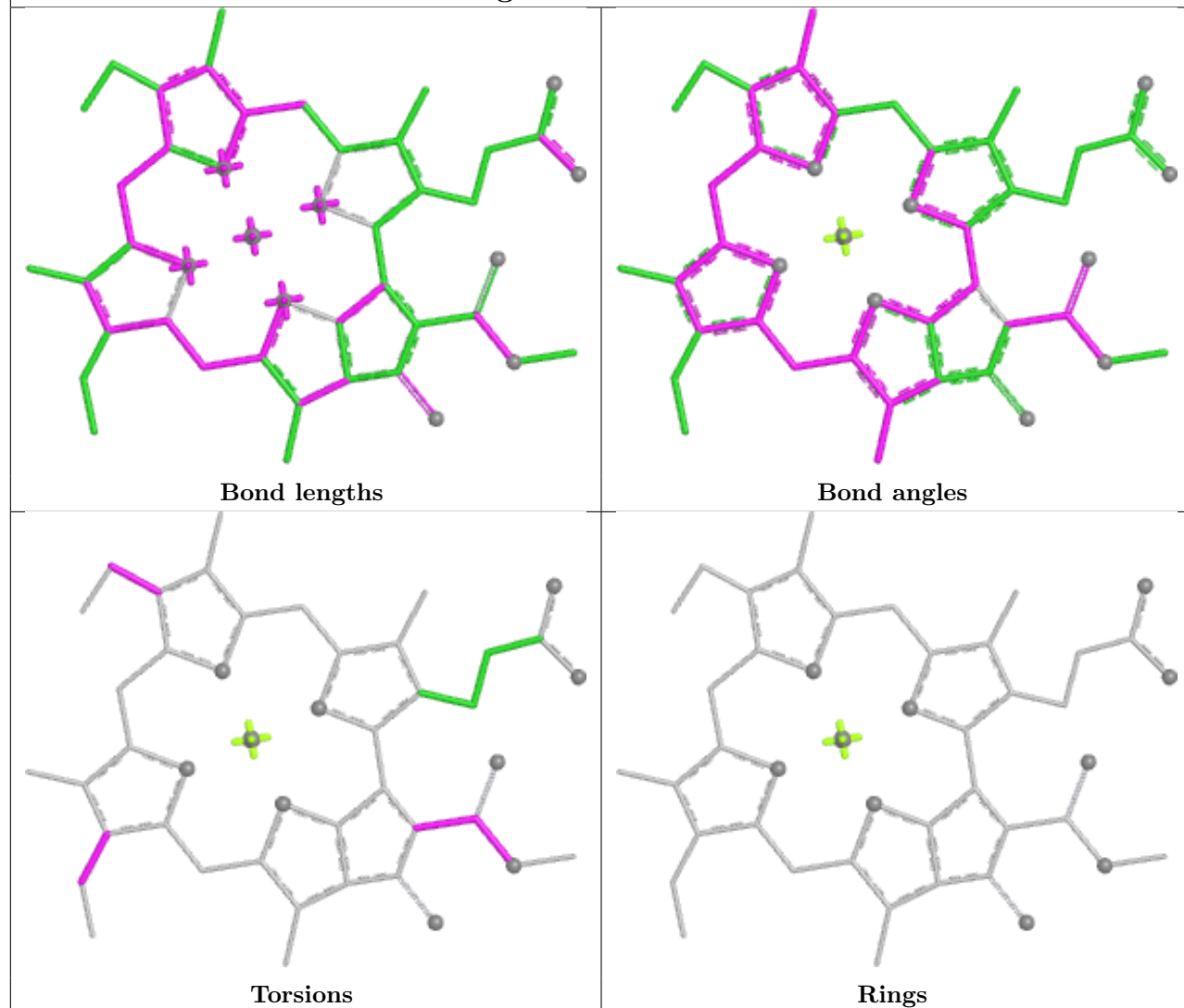


Ligand PQN B 801

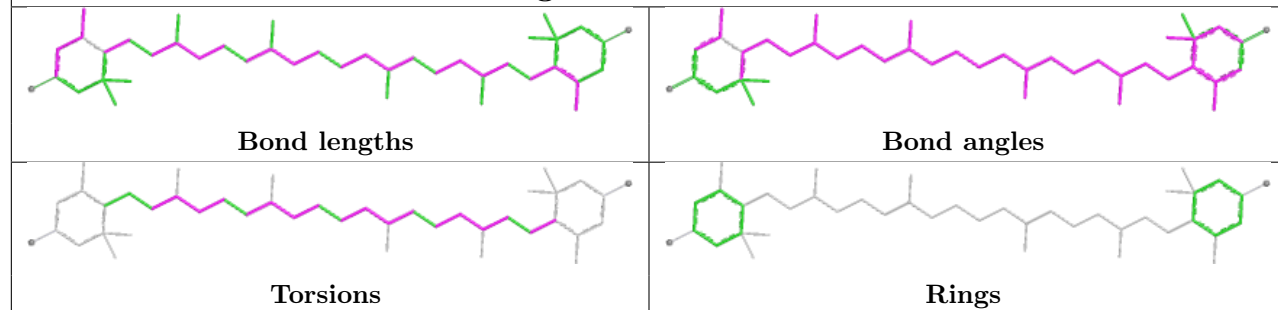


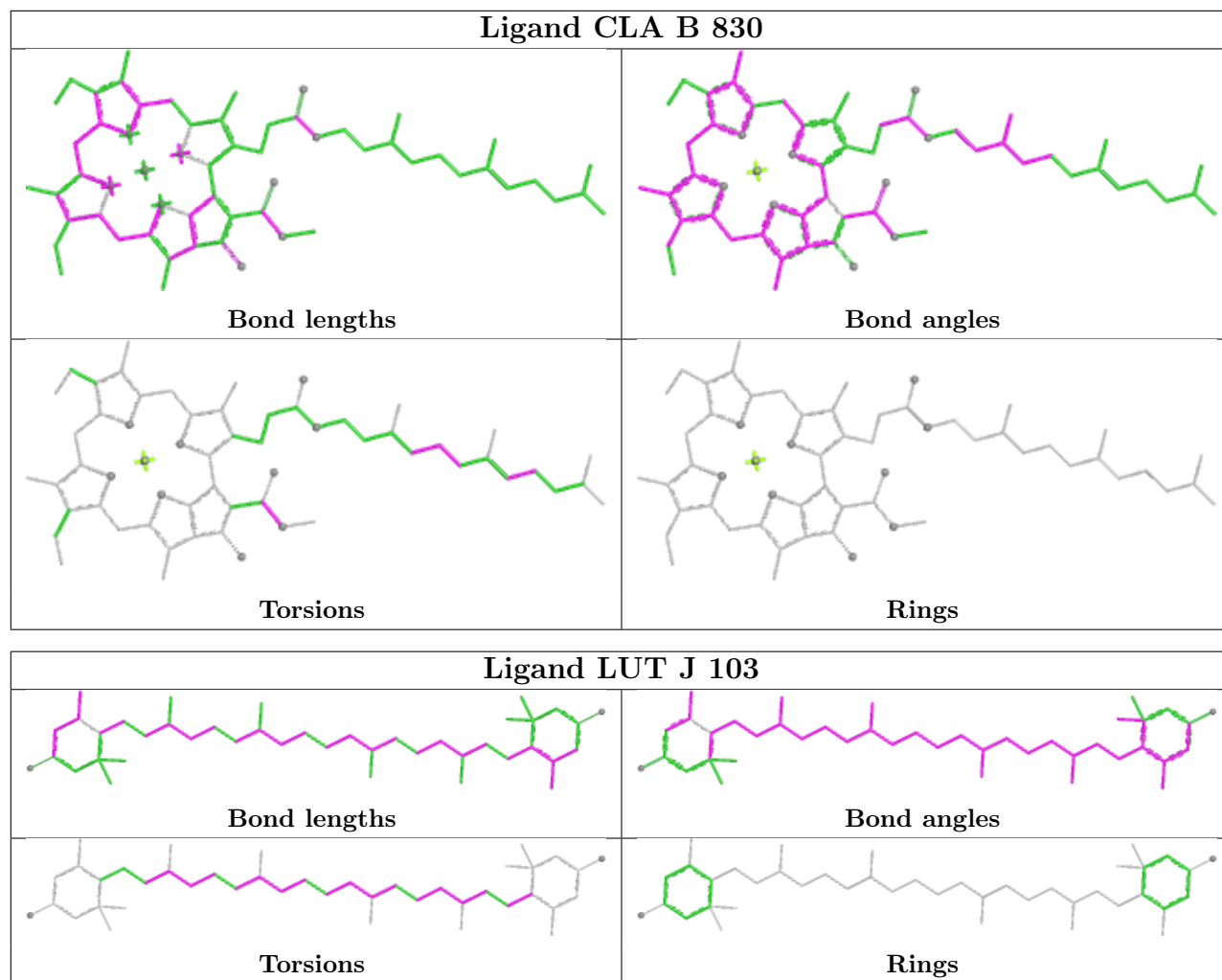
Ligand LUT 8 303**Ligand CLA 7 312**

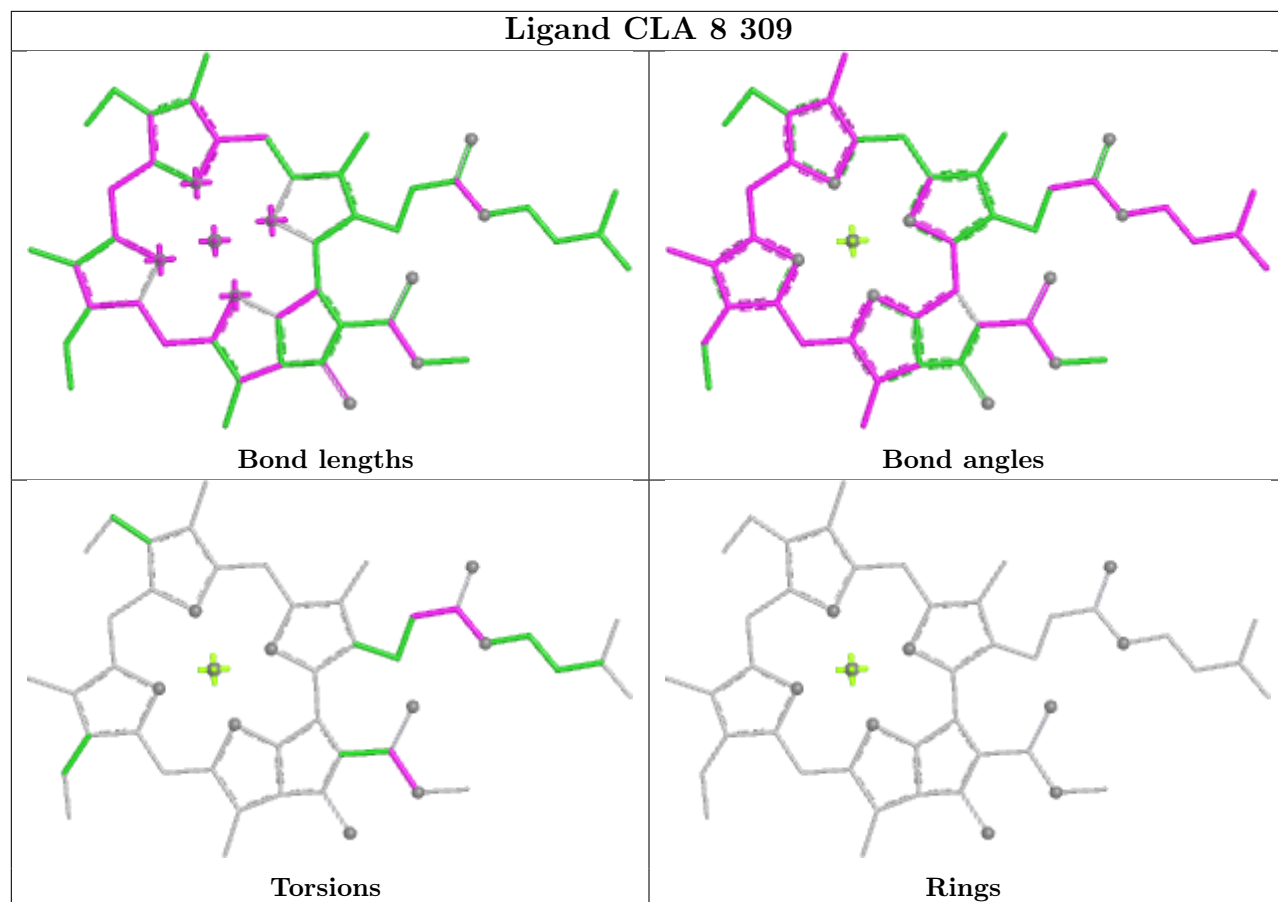
Ligand CLA 4 320



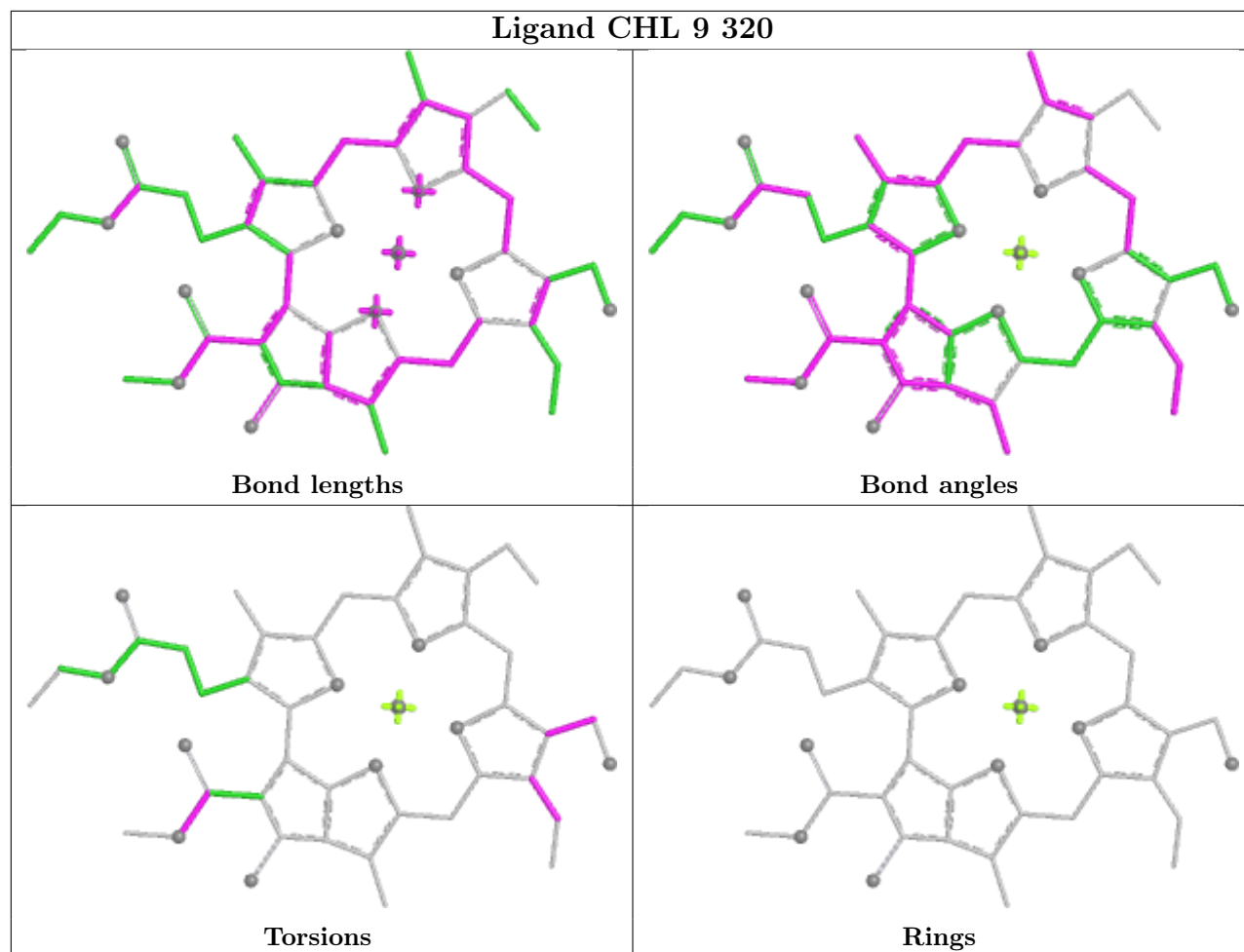
Ligand LUT 8 302



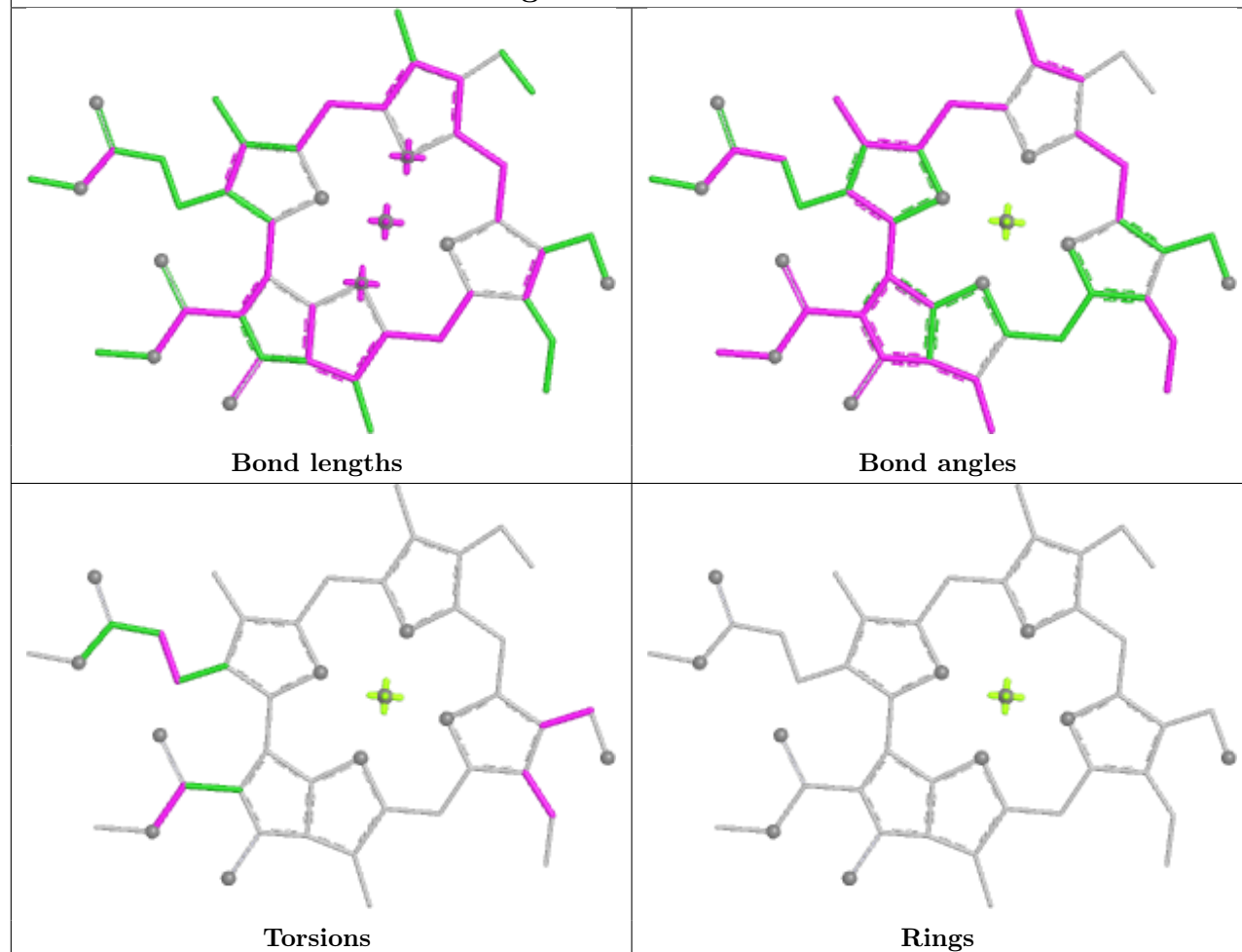




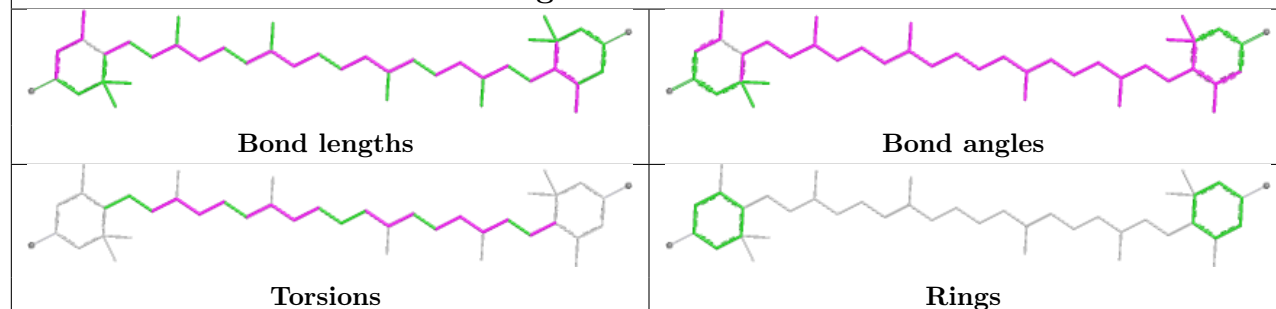
Ligand CHL 9 320



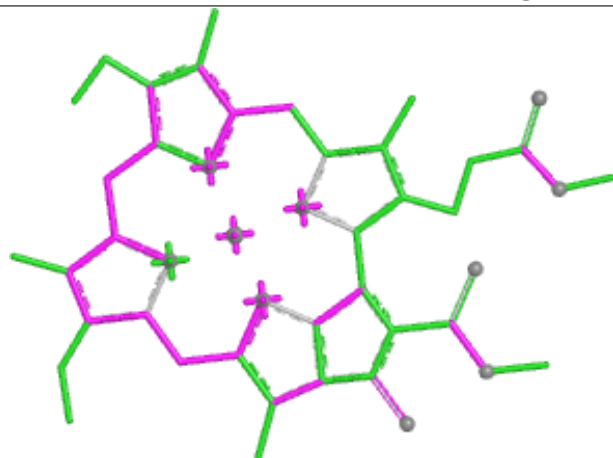
Ligand CHL 6 320



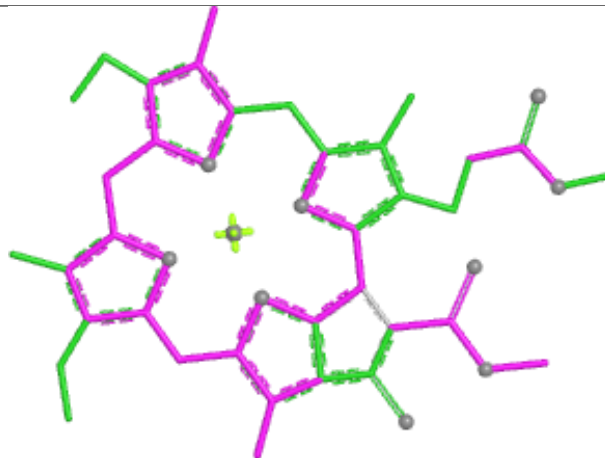
Ligand LUT 7 305



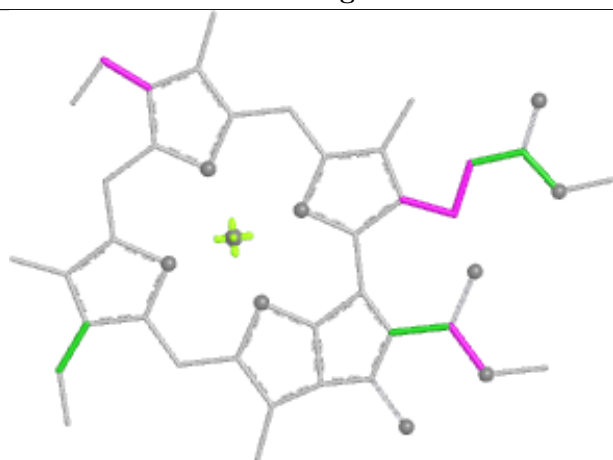
Ligand CLA b 306



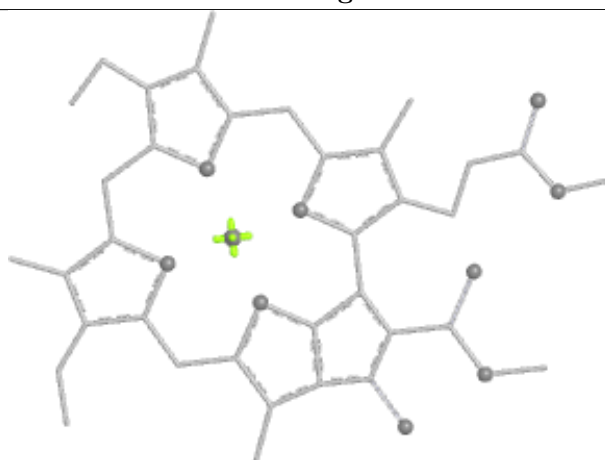
Bond lengths



Bond angles

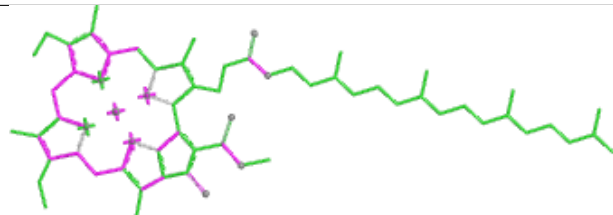


Torsions

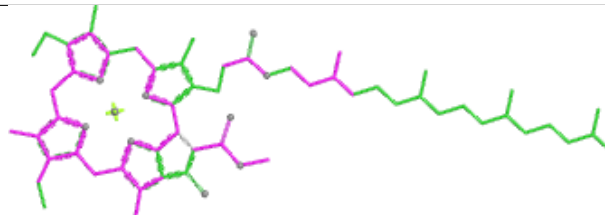


Rings

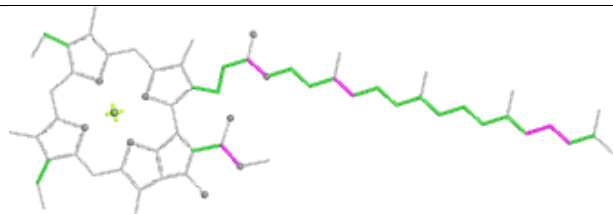
Ligand CLA 3 312



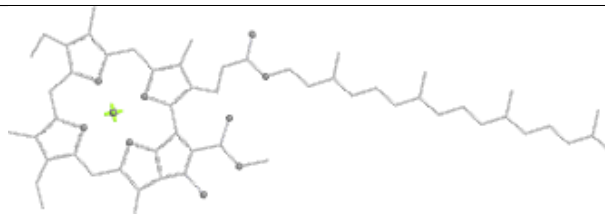
Bond lengths



Bond angles

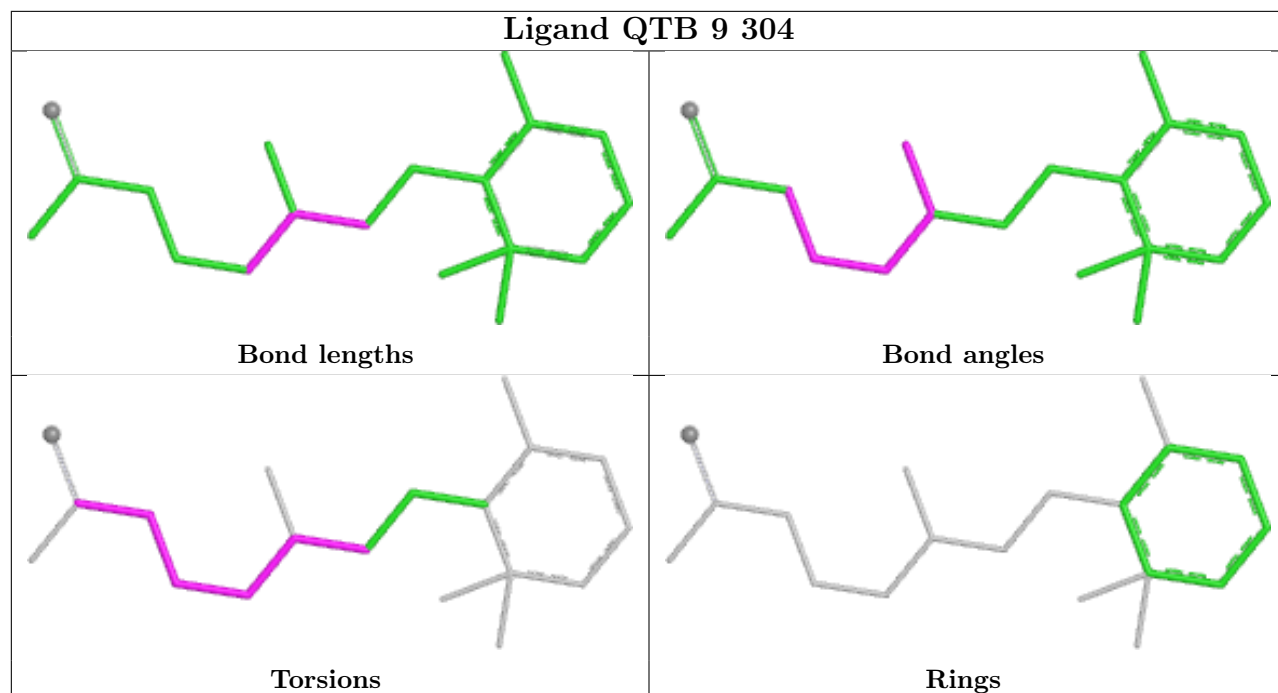


Torsions

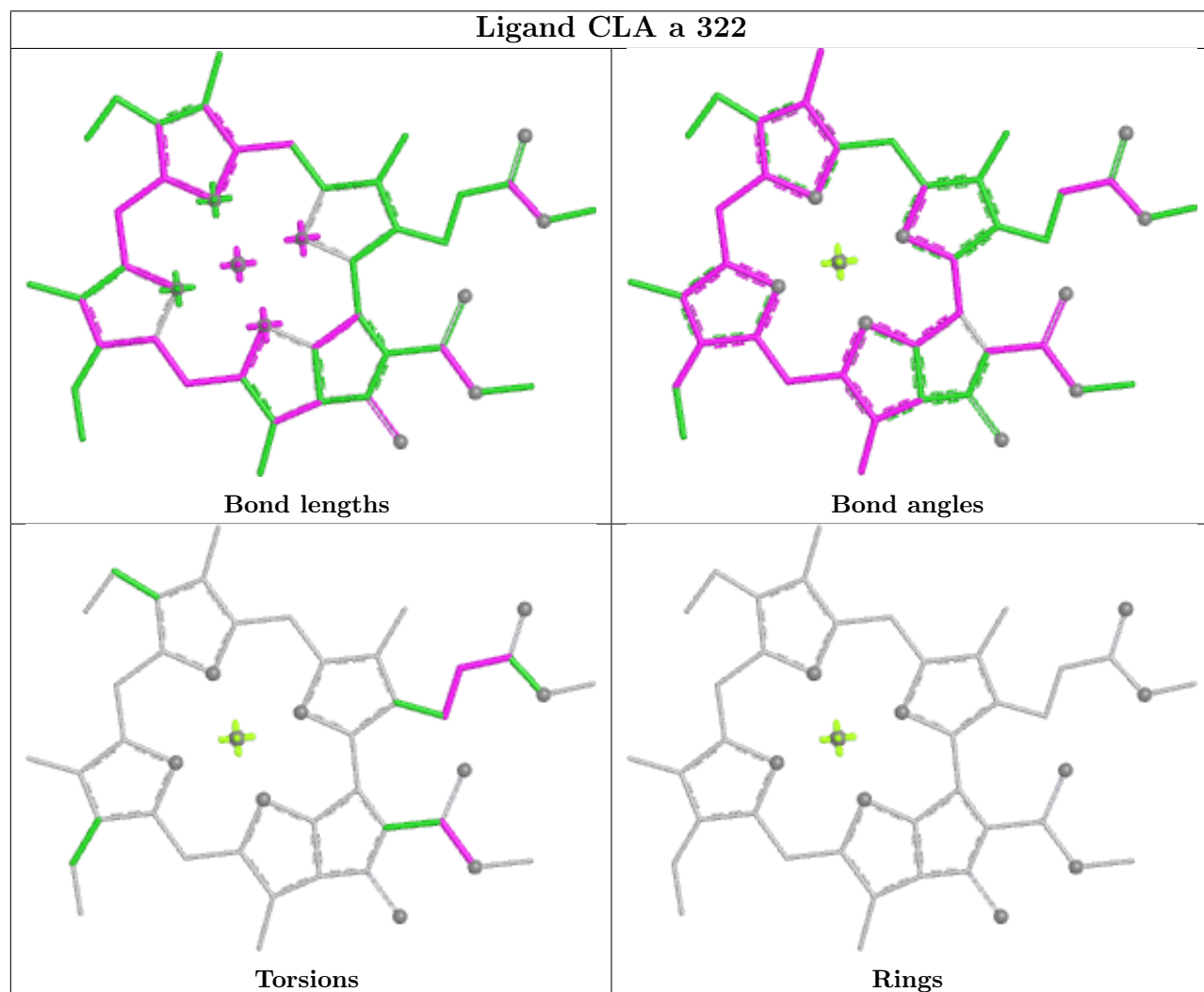


Rings

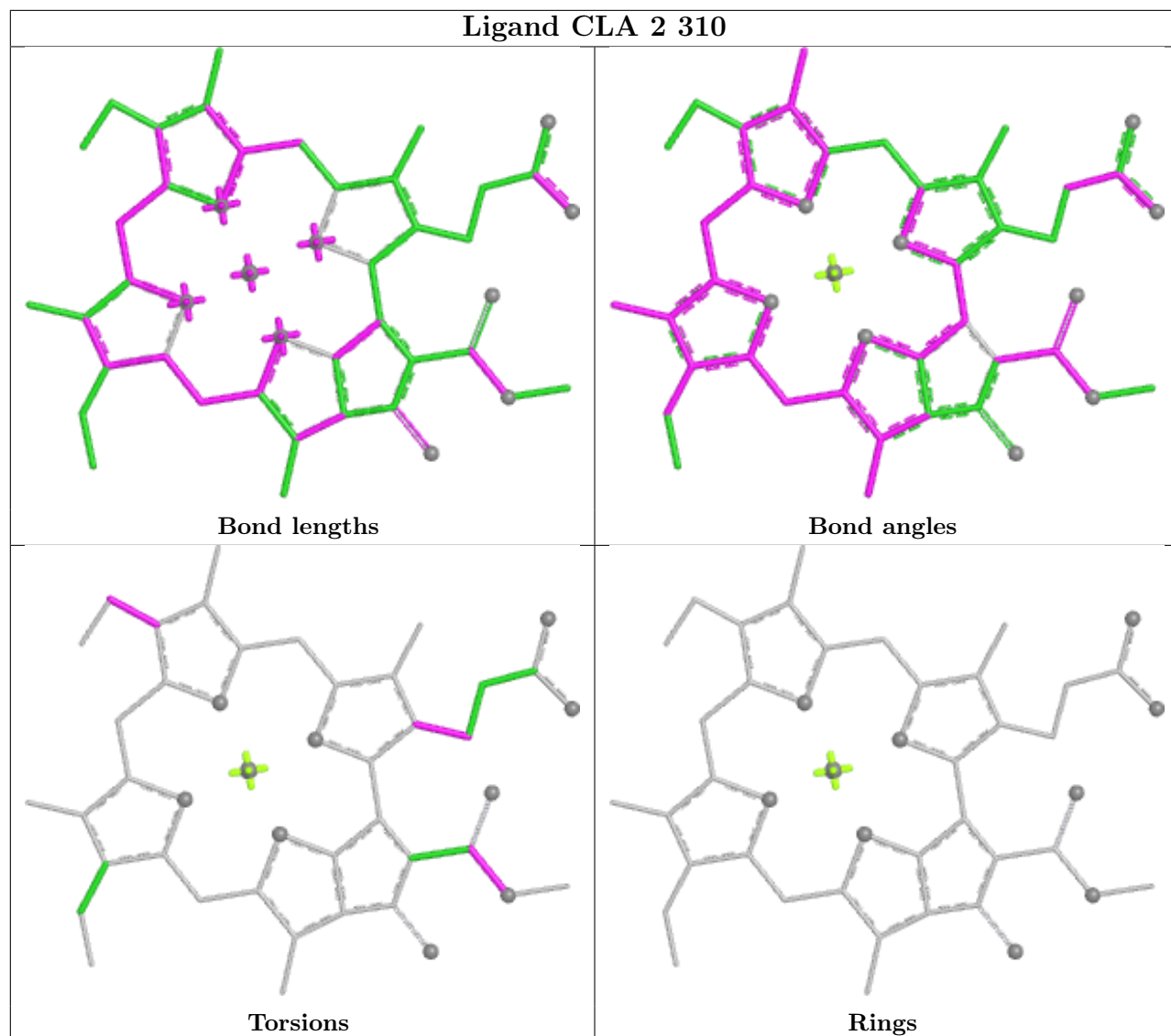
Ligand QTB 9 304



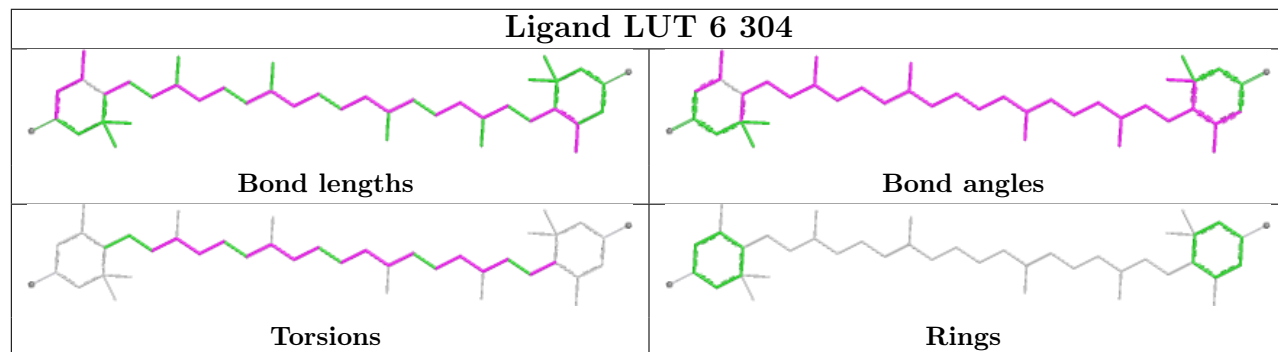
Ligand CLA a 322

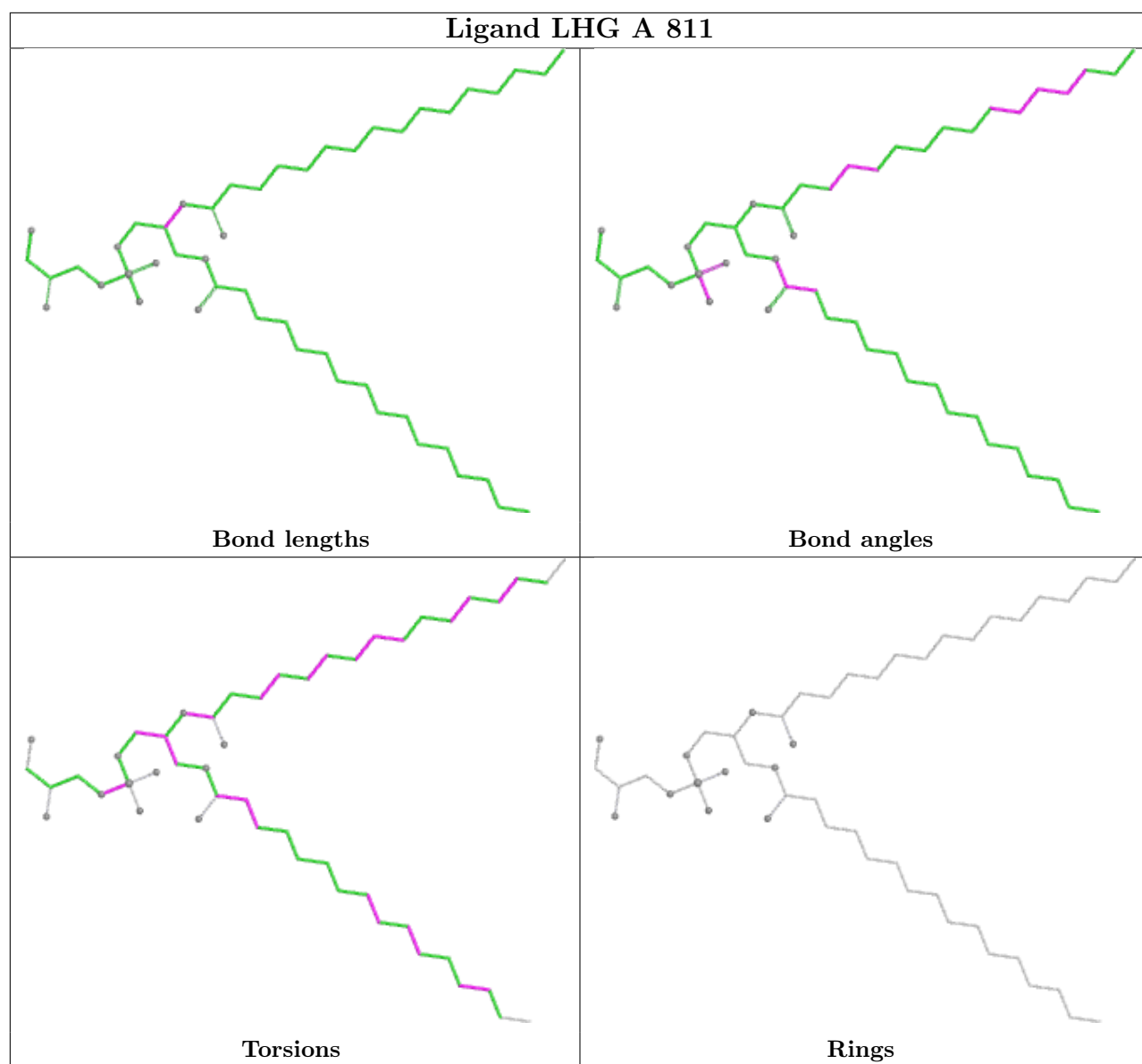


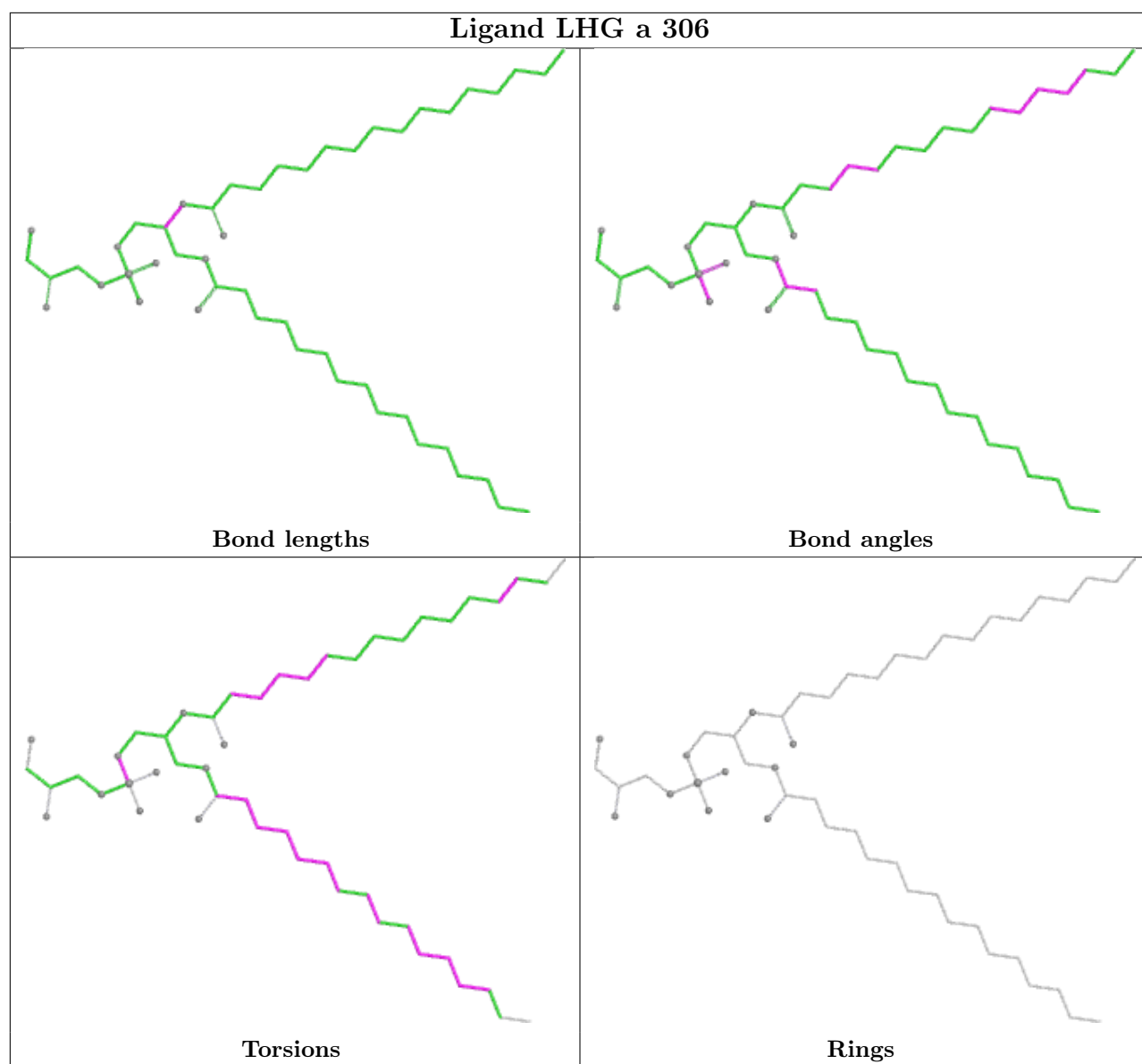
Ligand CLA 2 310

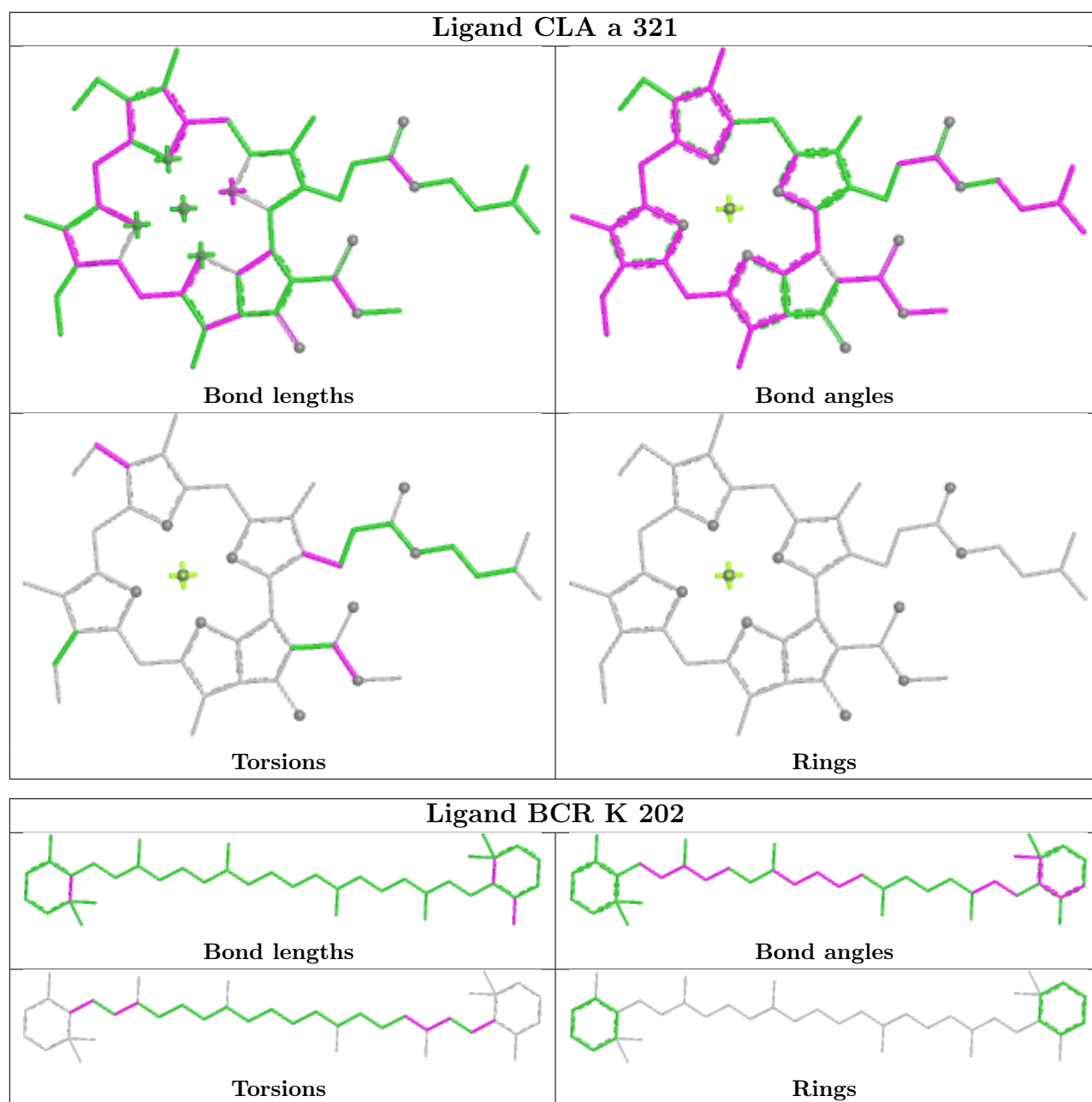


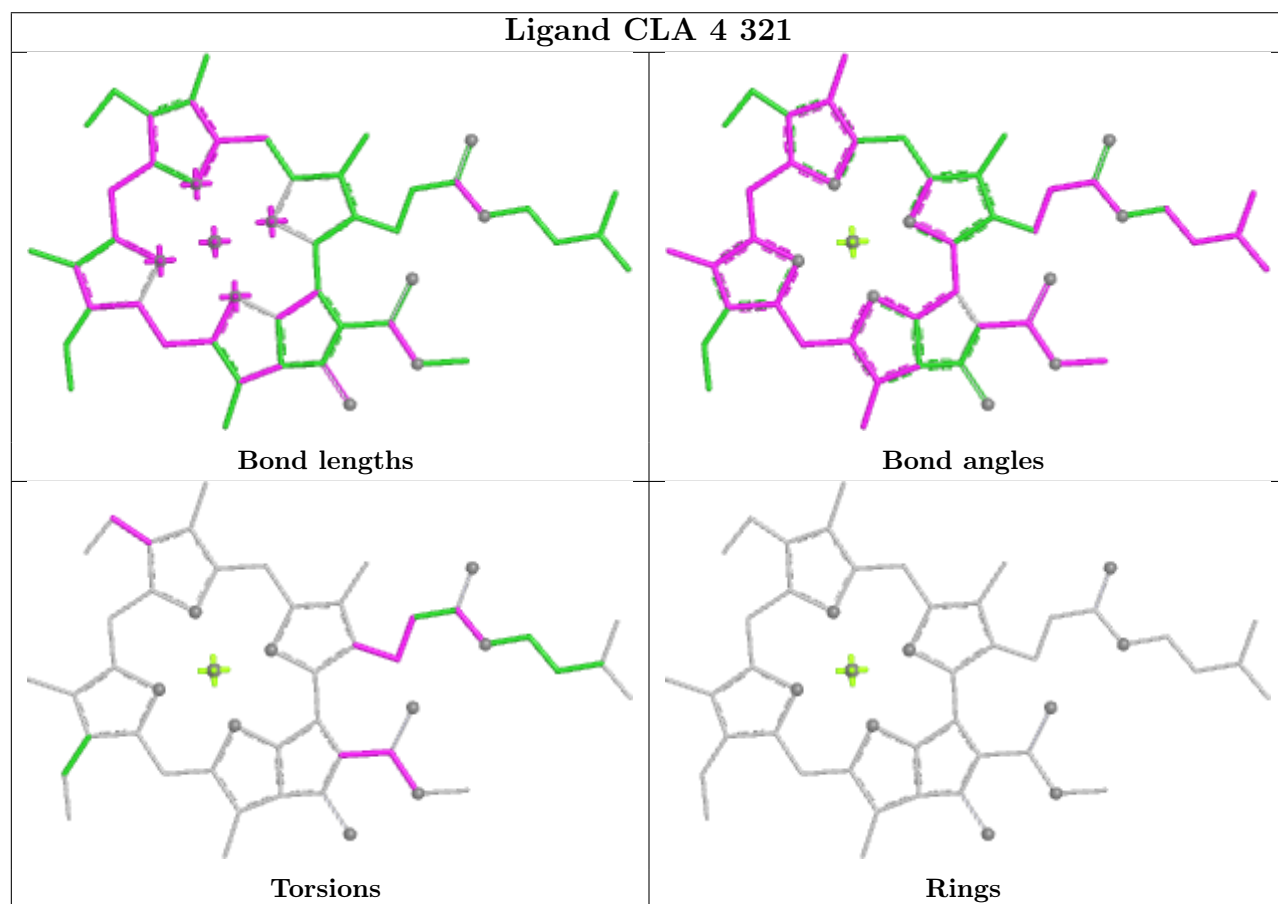
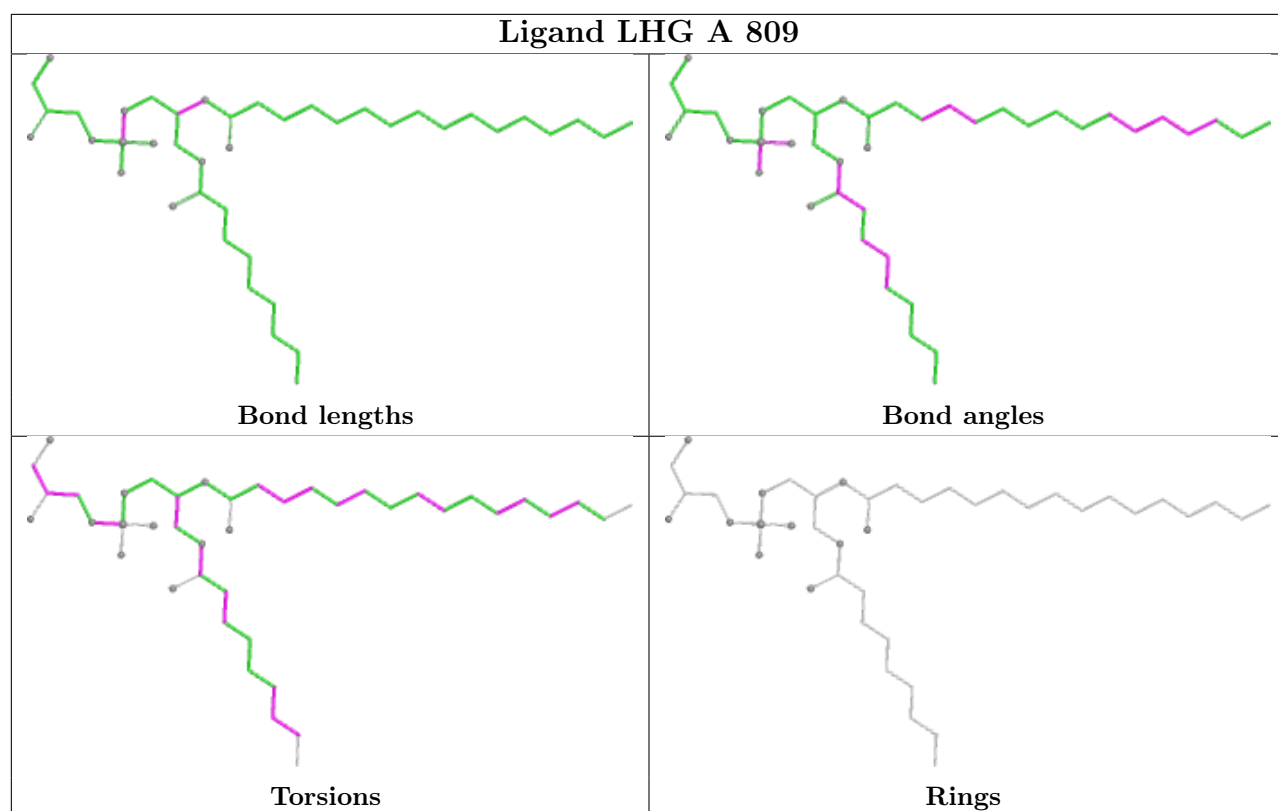
Ligand LUT 6 304



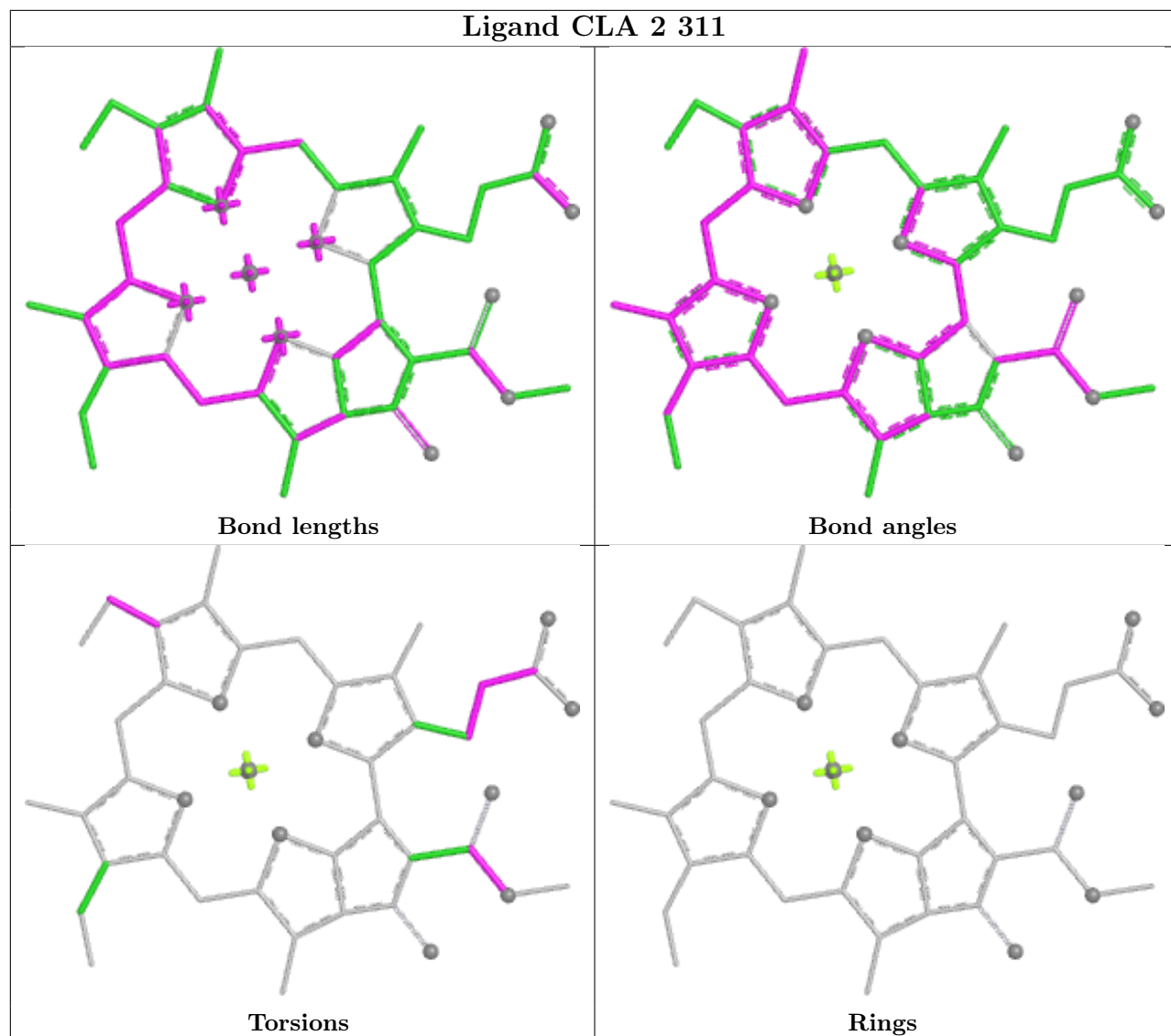




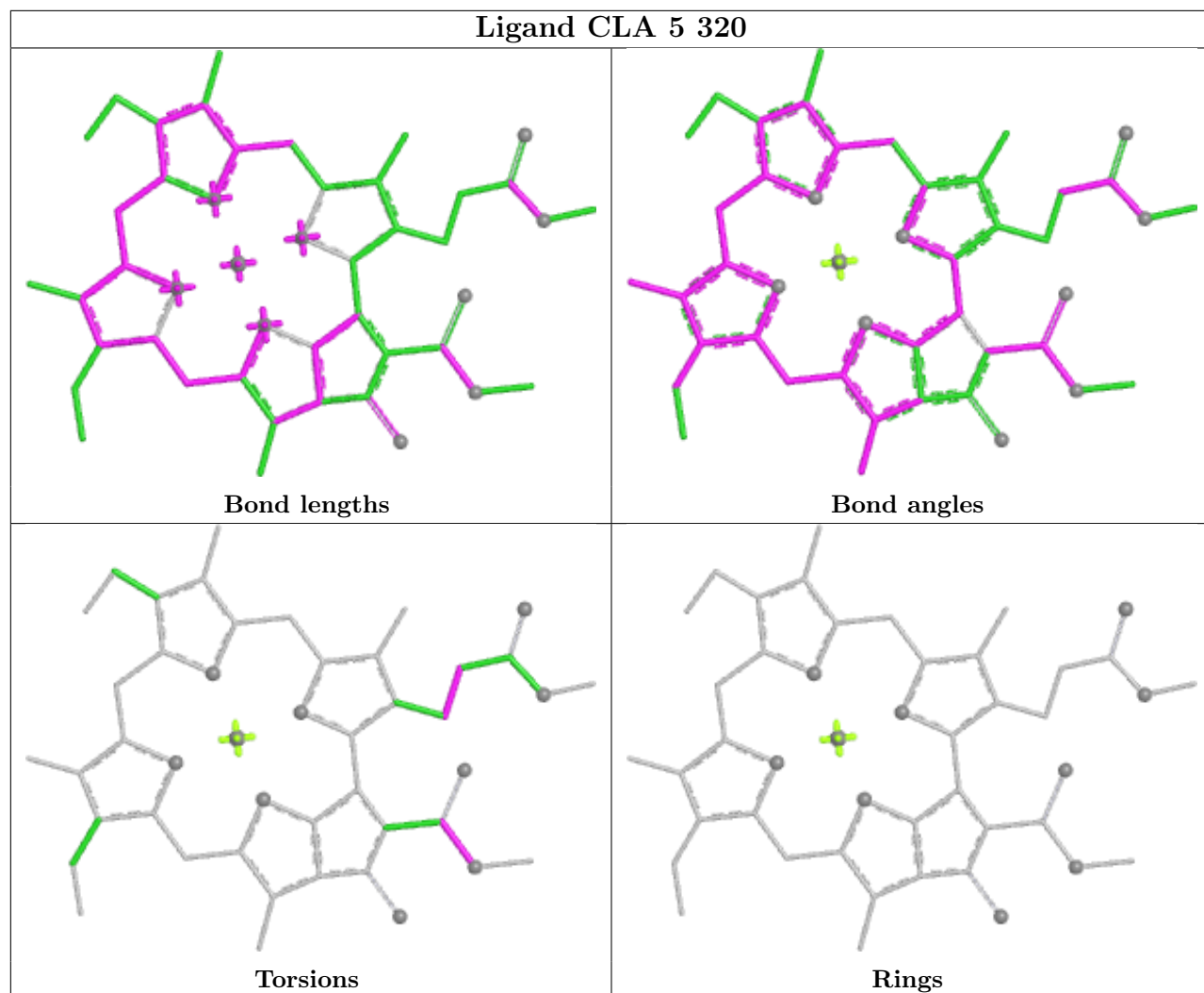




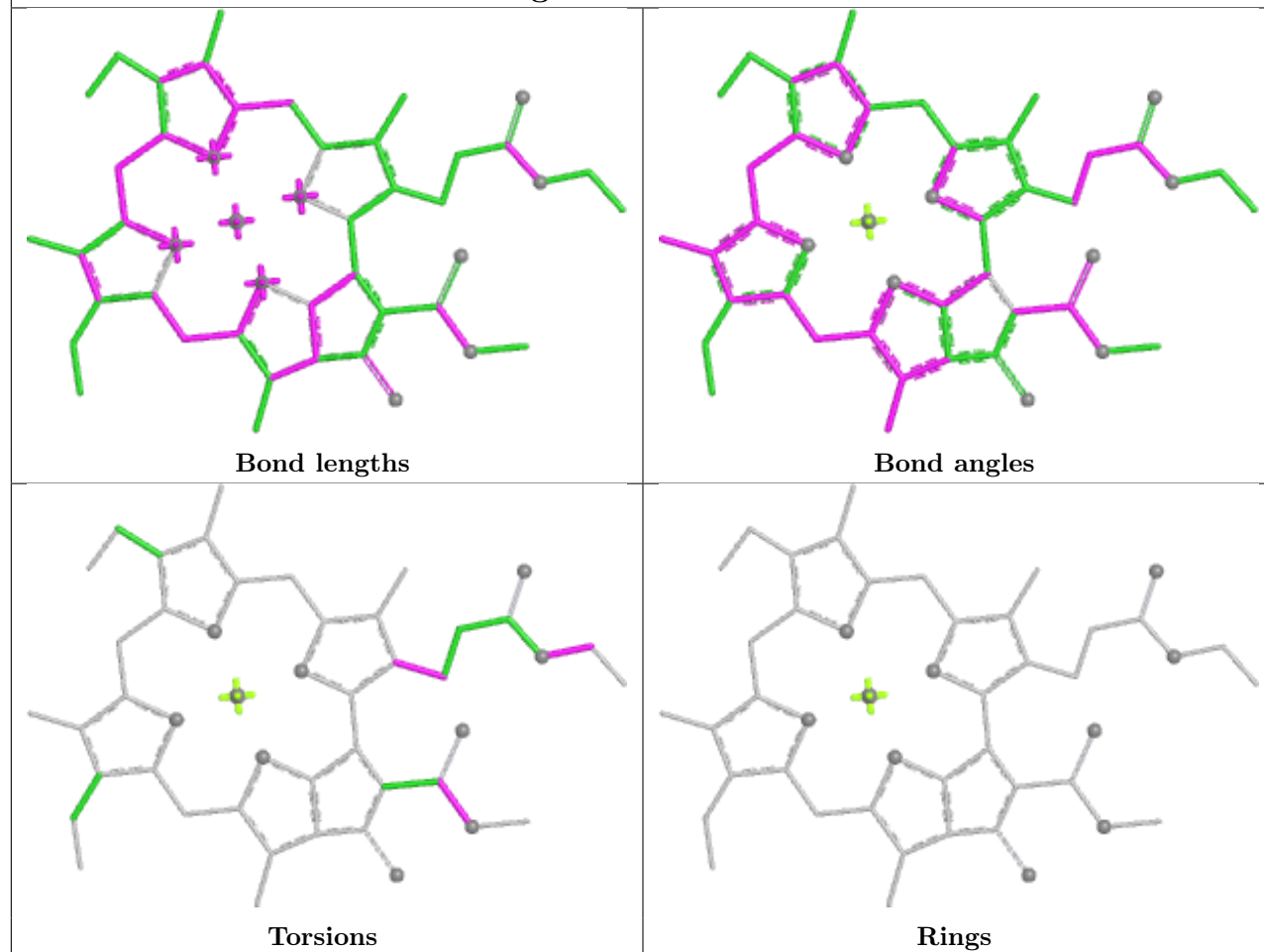
Ligand CLA 2 311



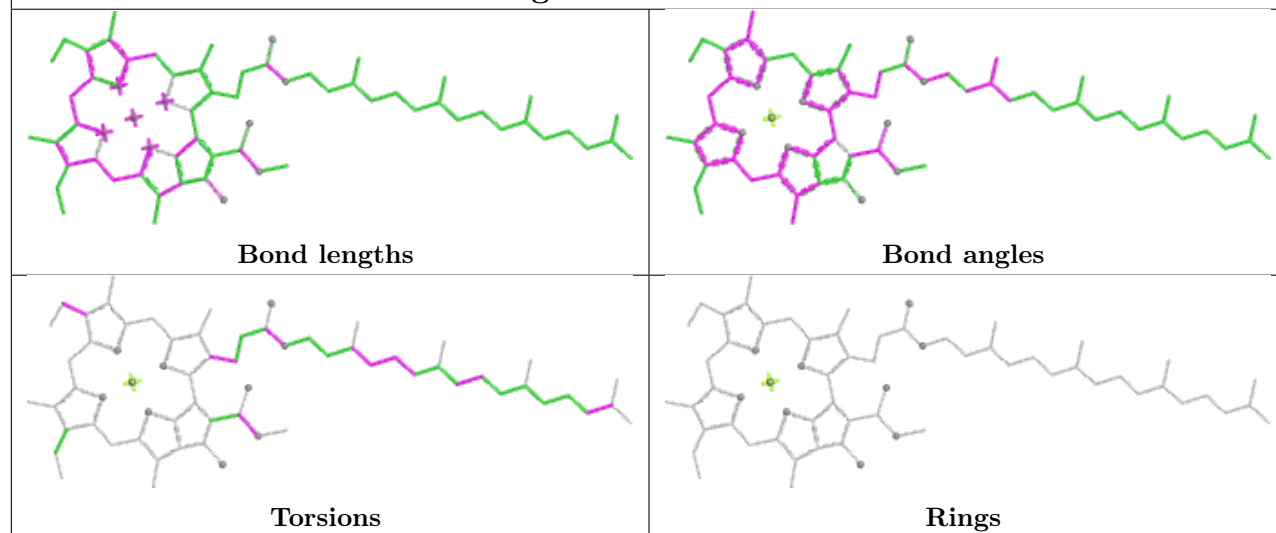
Ligand CLA 5 320

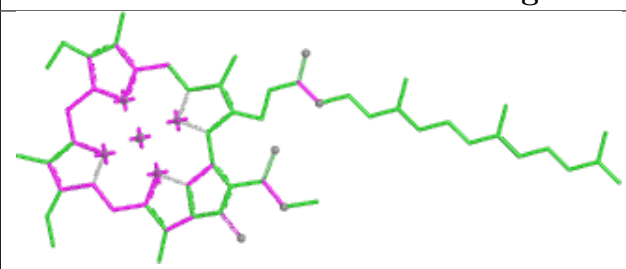
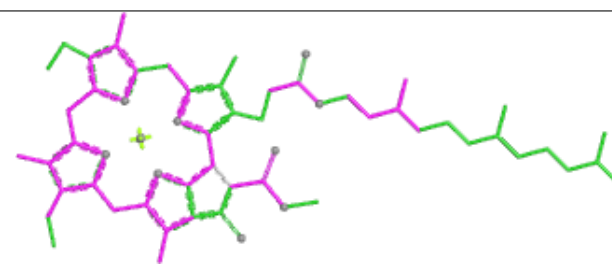
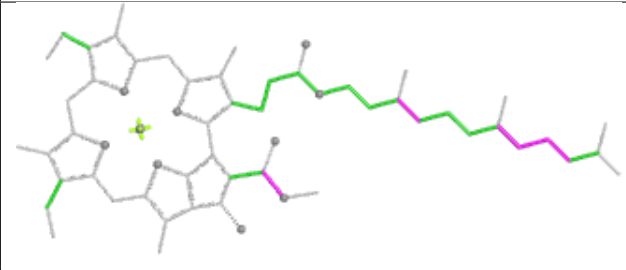
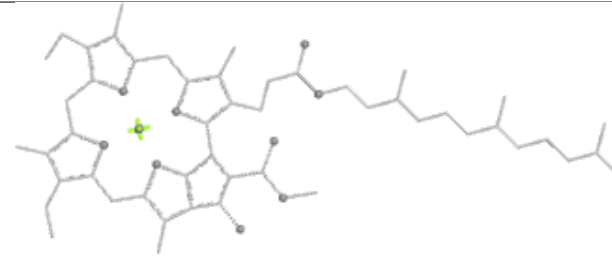


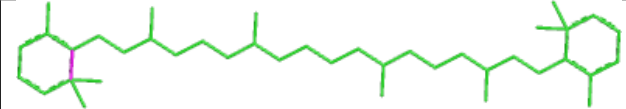
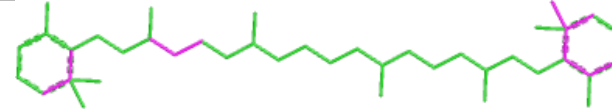
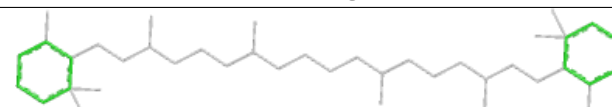
Ligand CLA 4 316

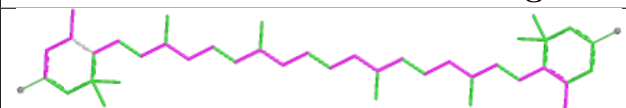
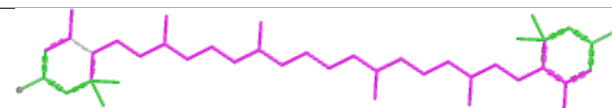
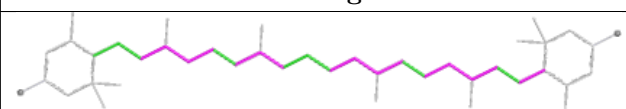
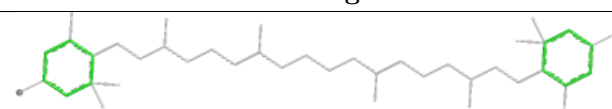


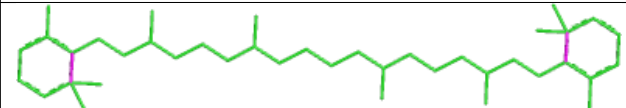
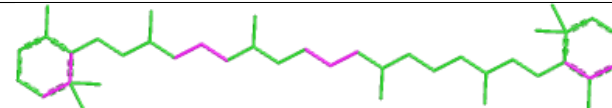
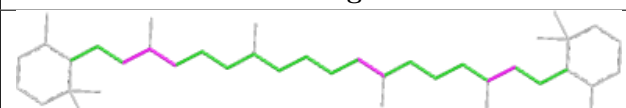
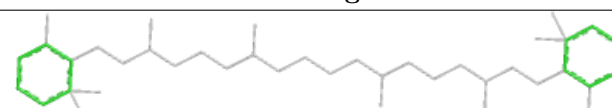
Ligand CLA A 855

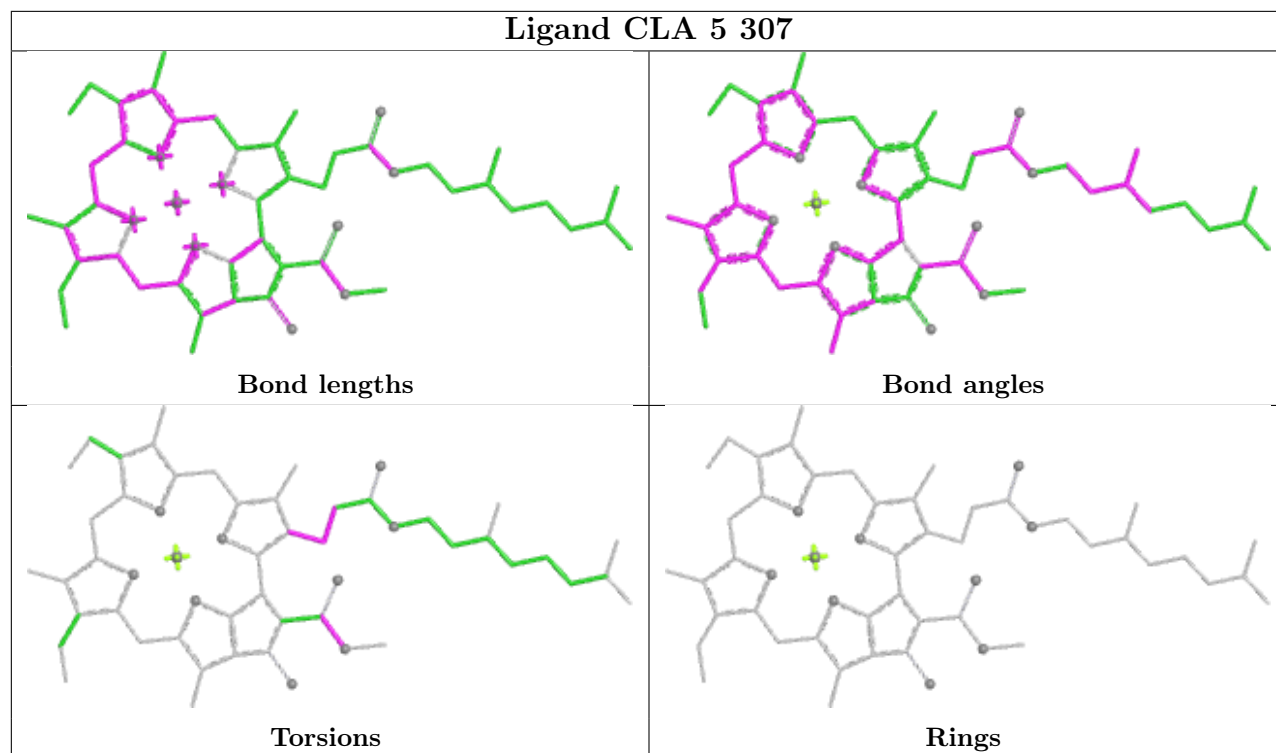
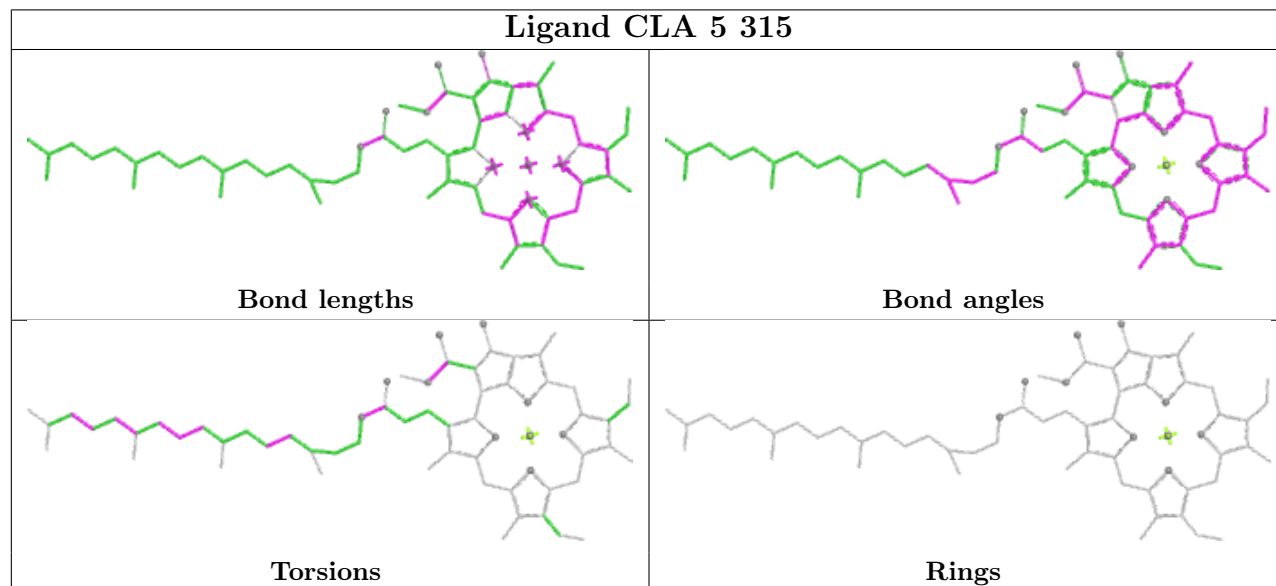
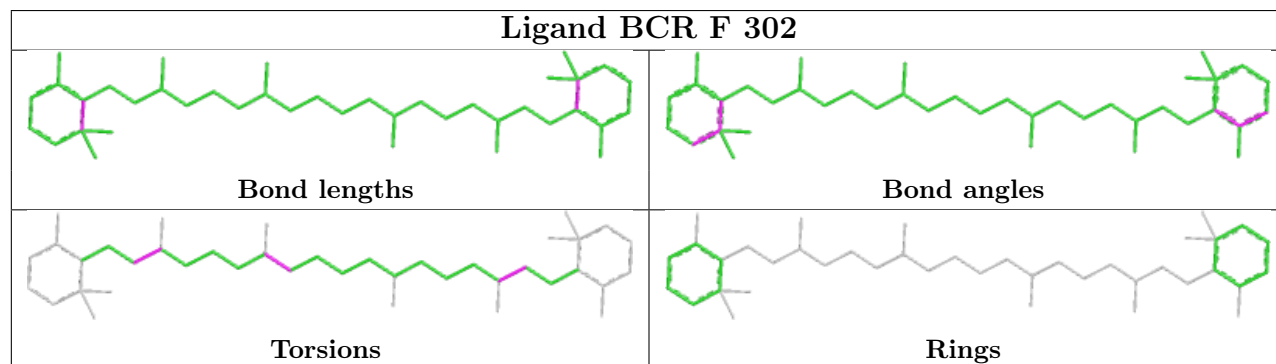


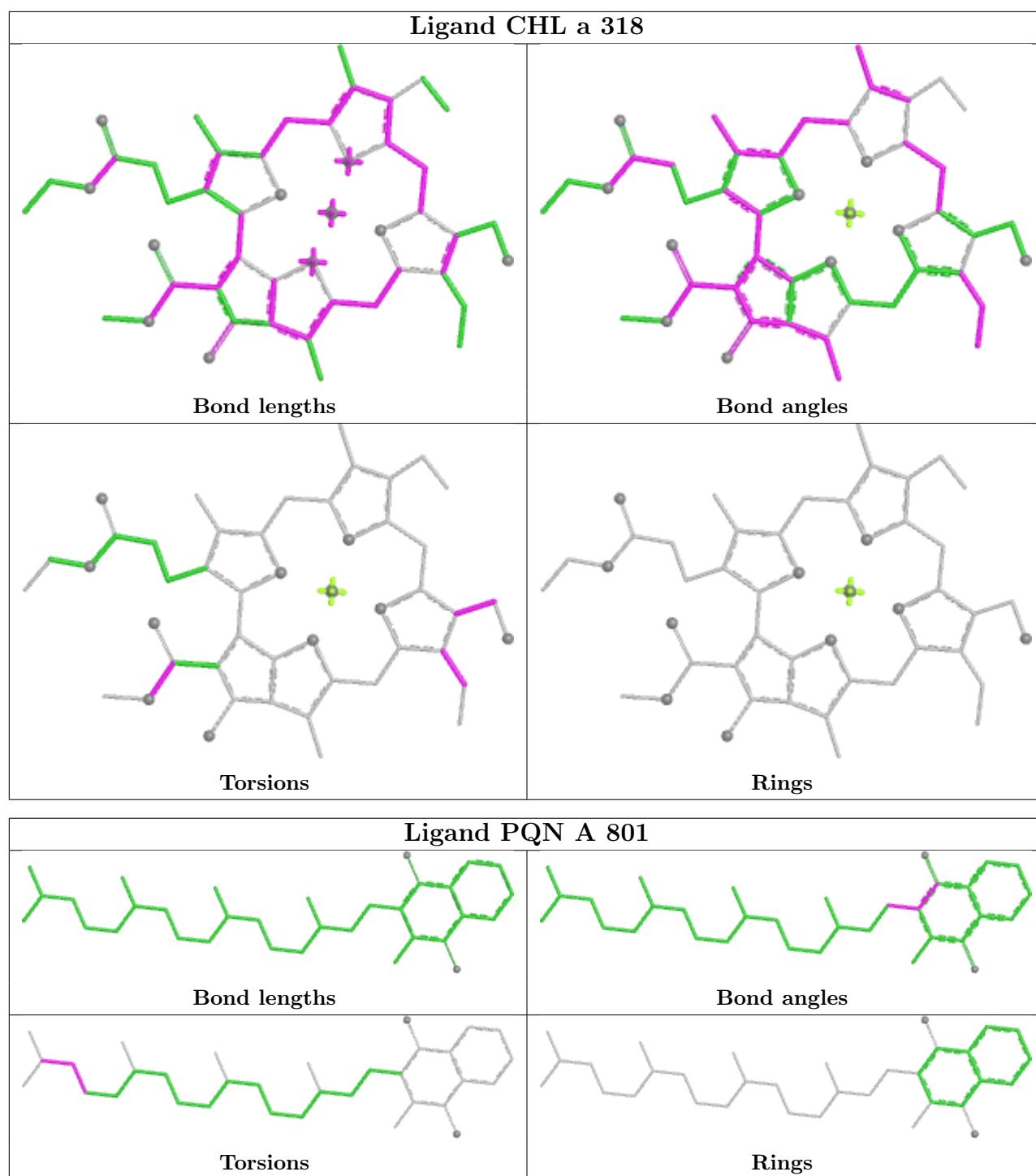
Ligand CLA B 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

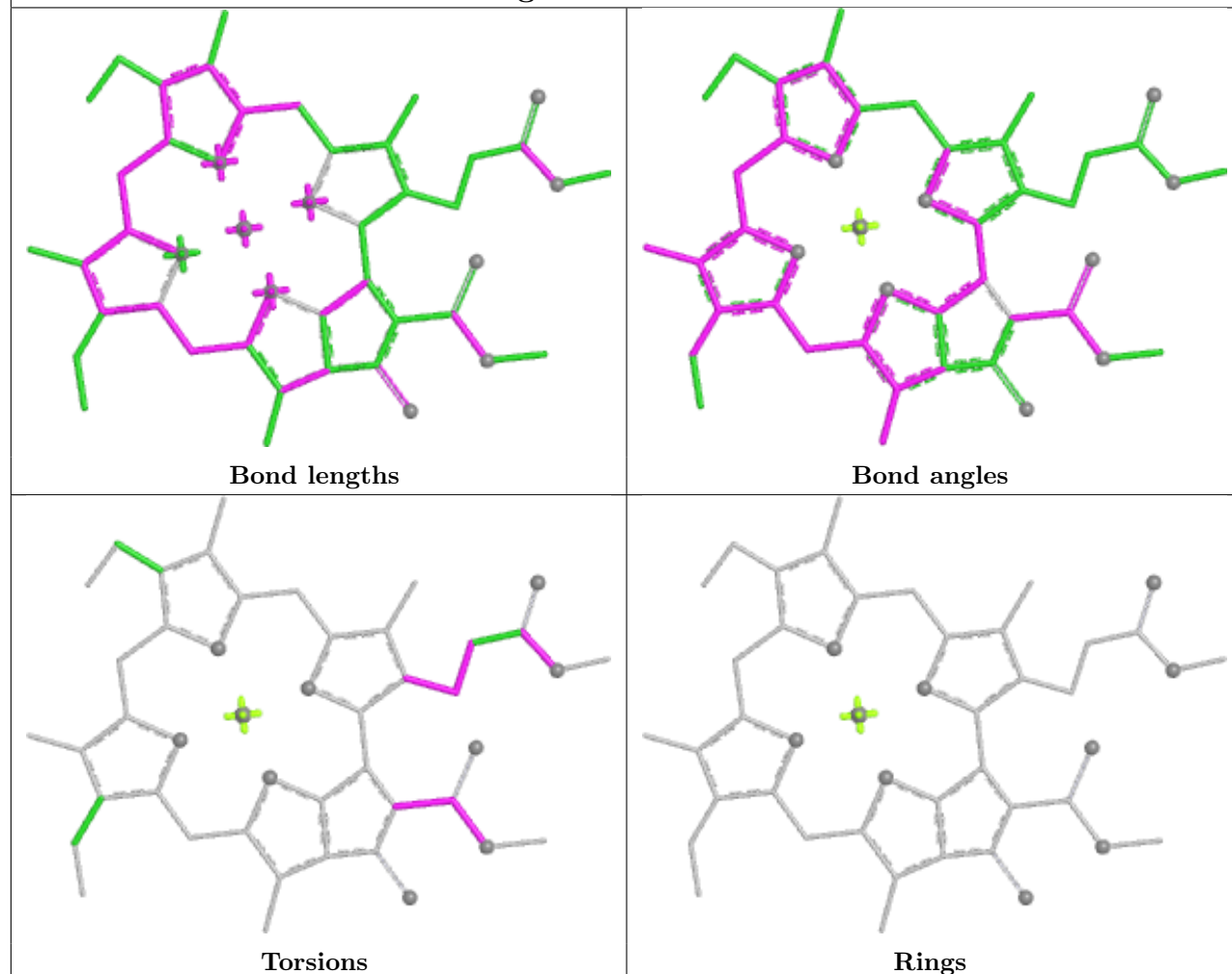
Ligand LUT 4 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

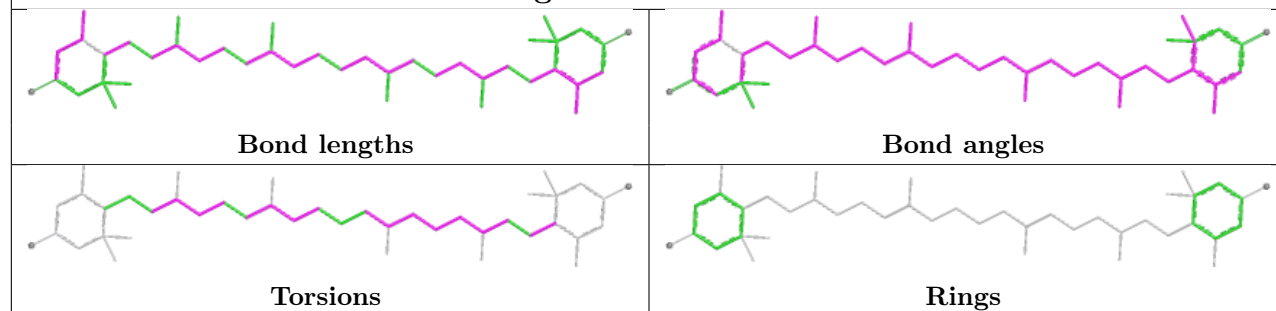
Ligand CLA 5 307**Ligand CLA 5 315****Ligand BCR F 302**

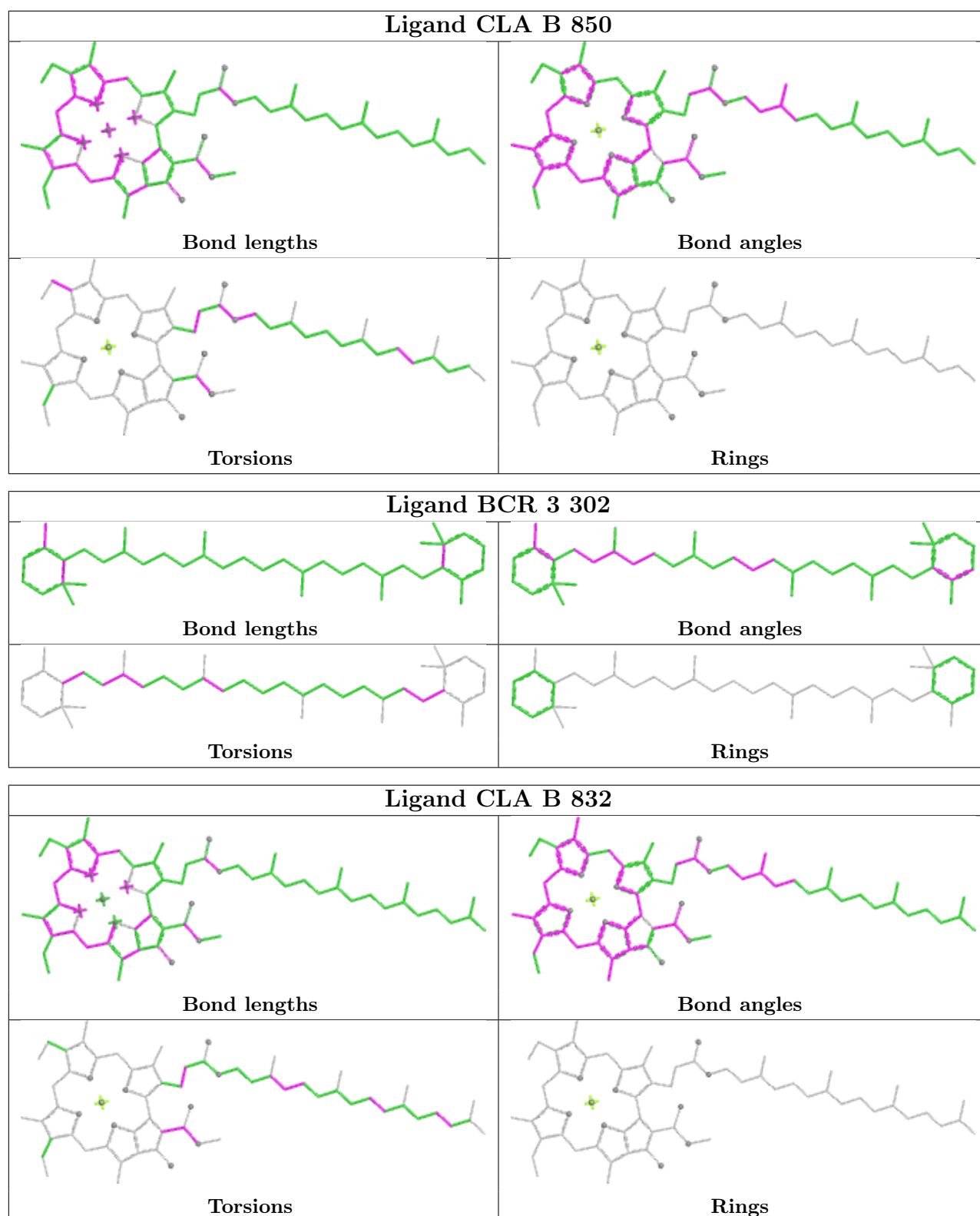


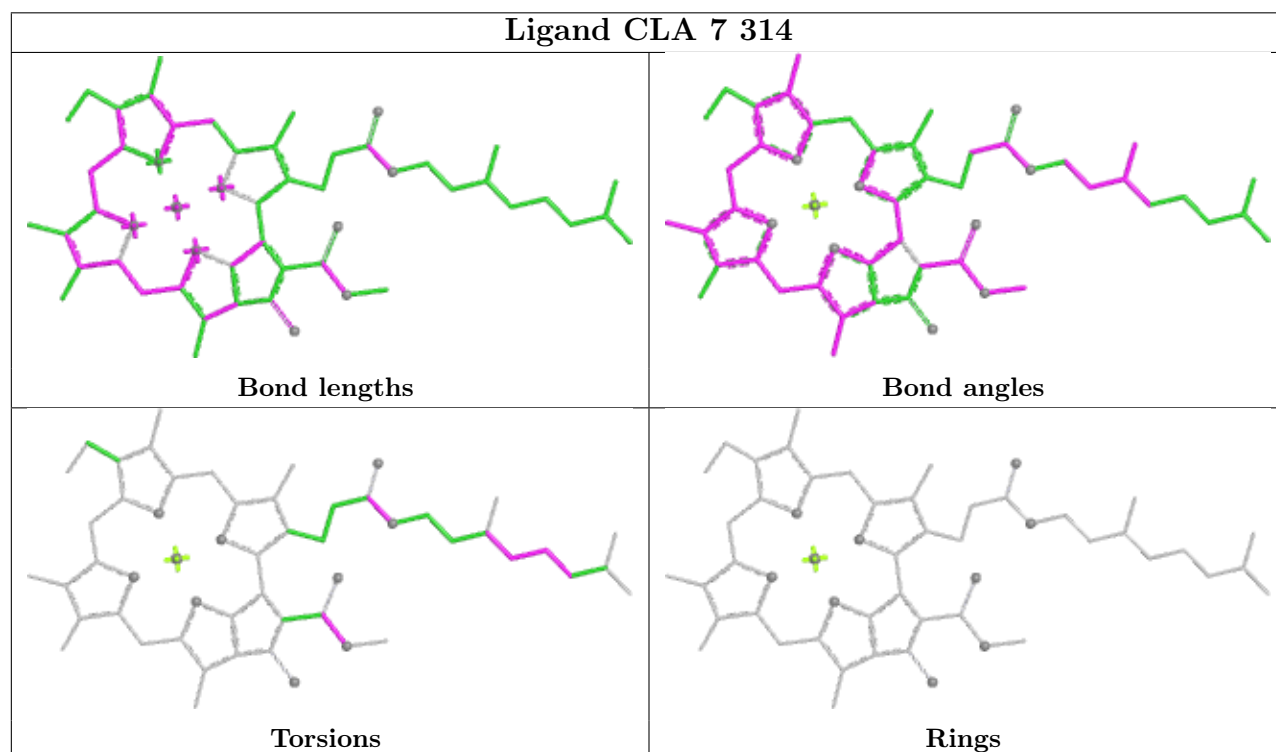
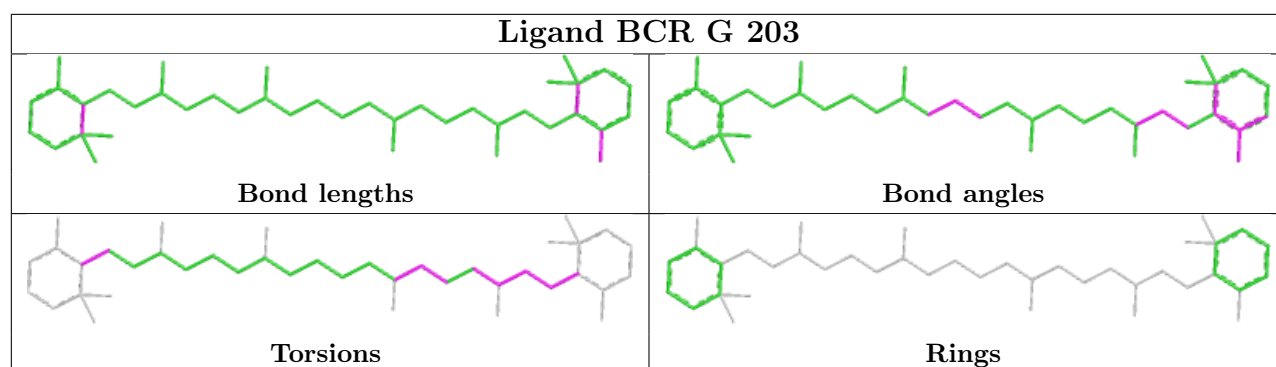
Ligand CLA 2 304

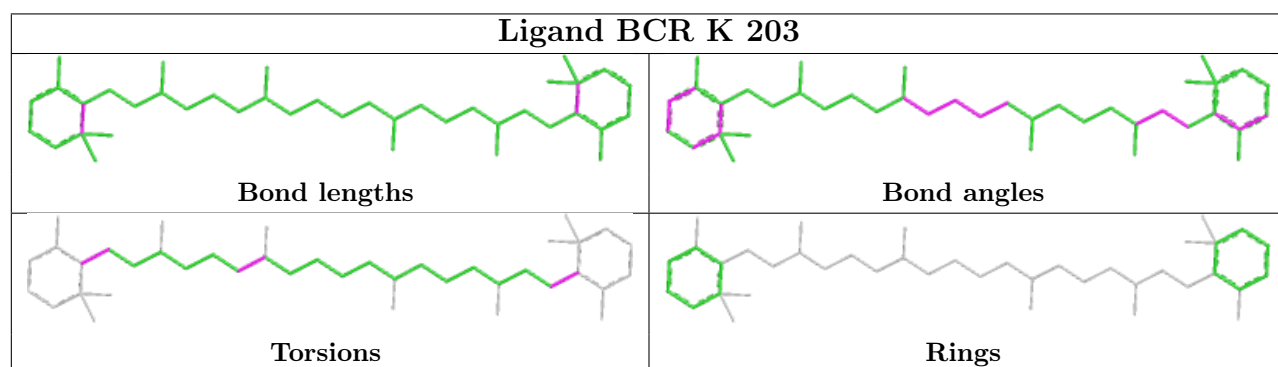
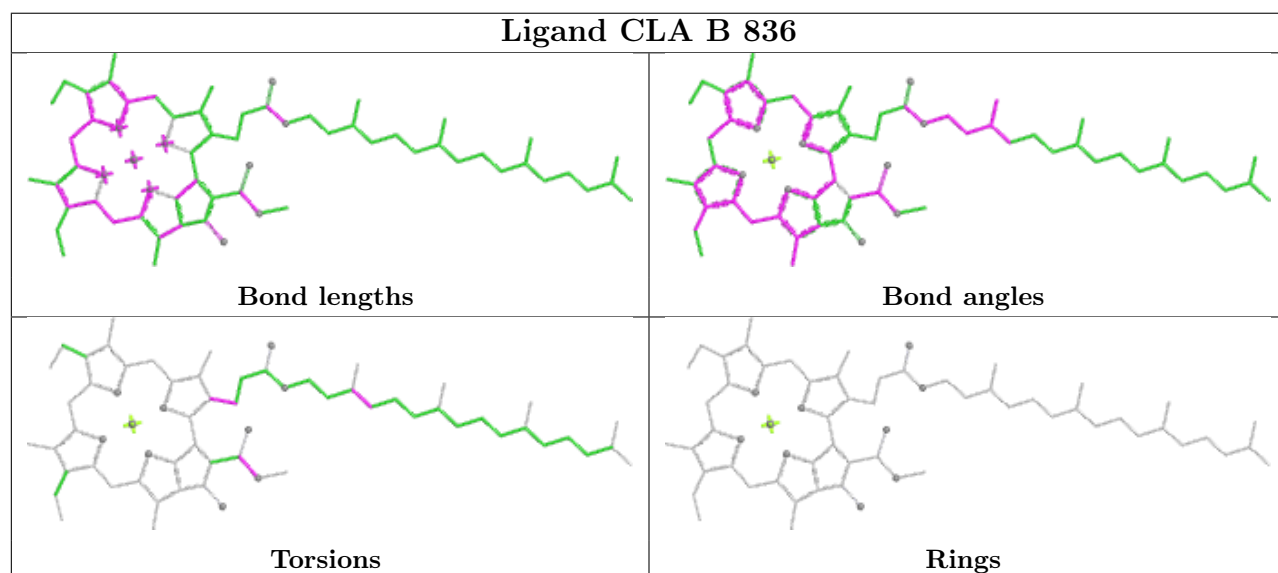
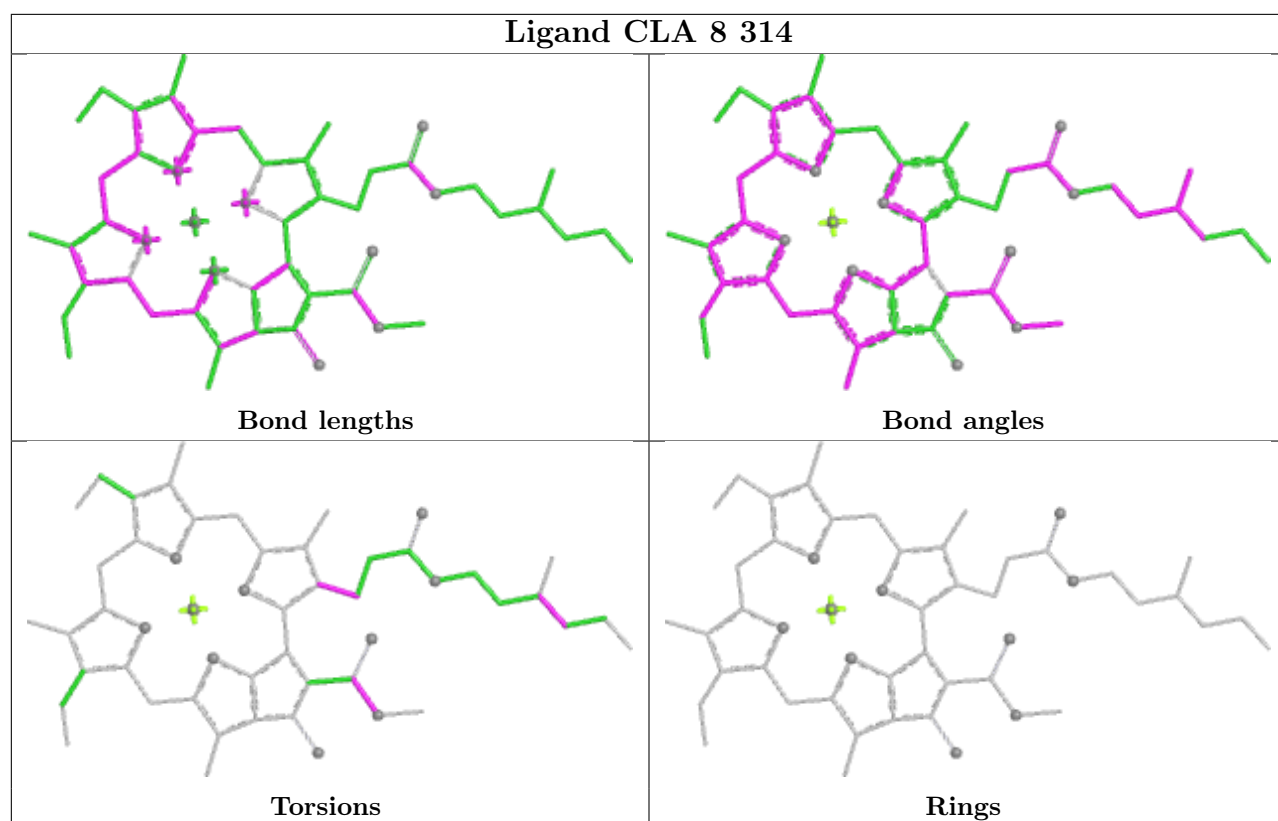


Ligand LUT F 304

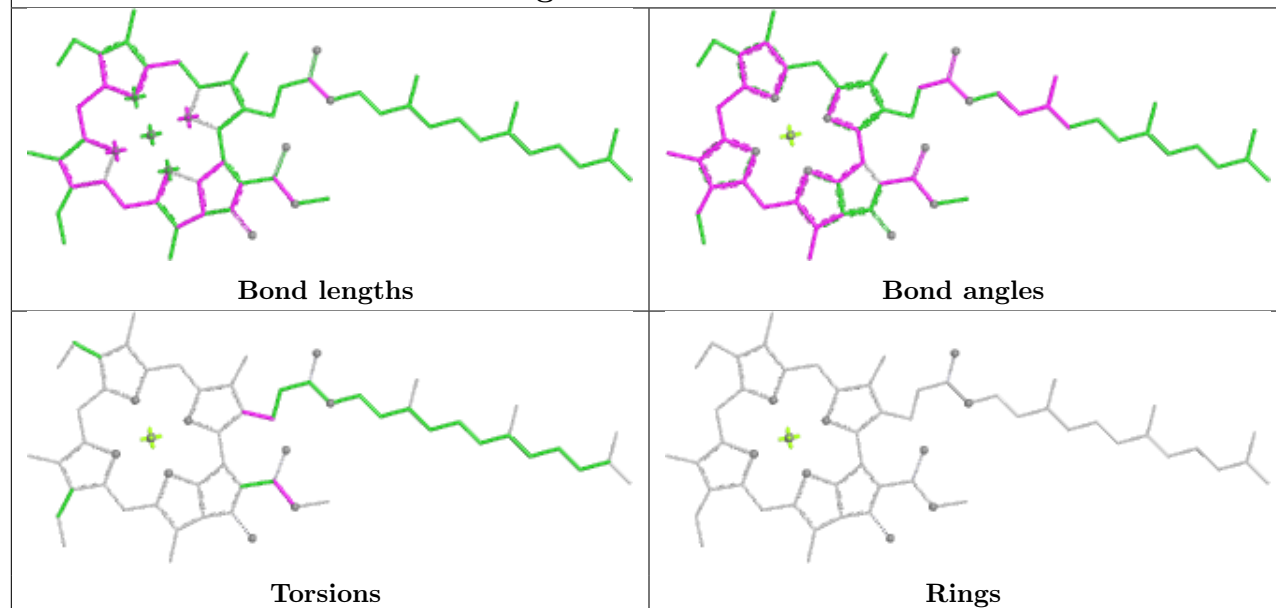




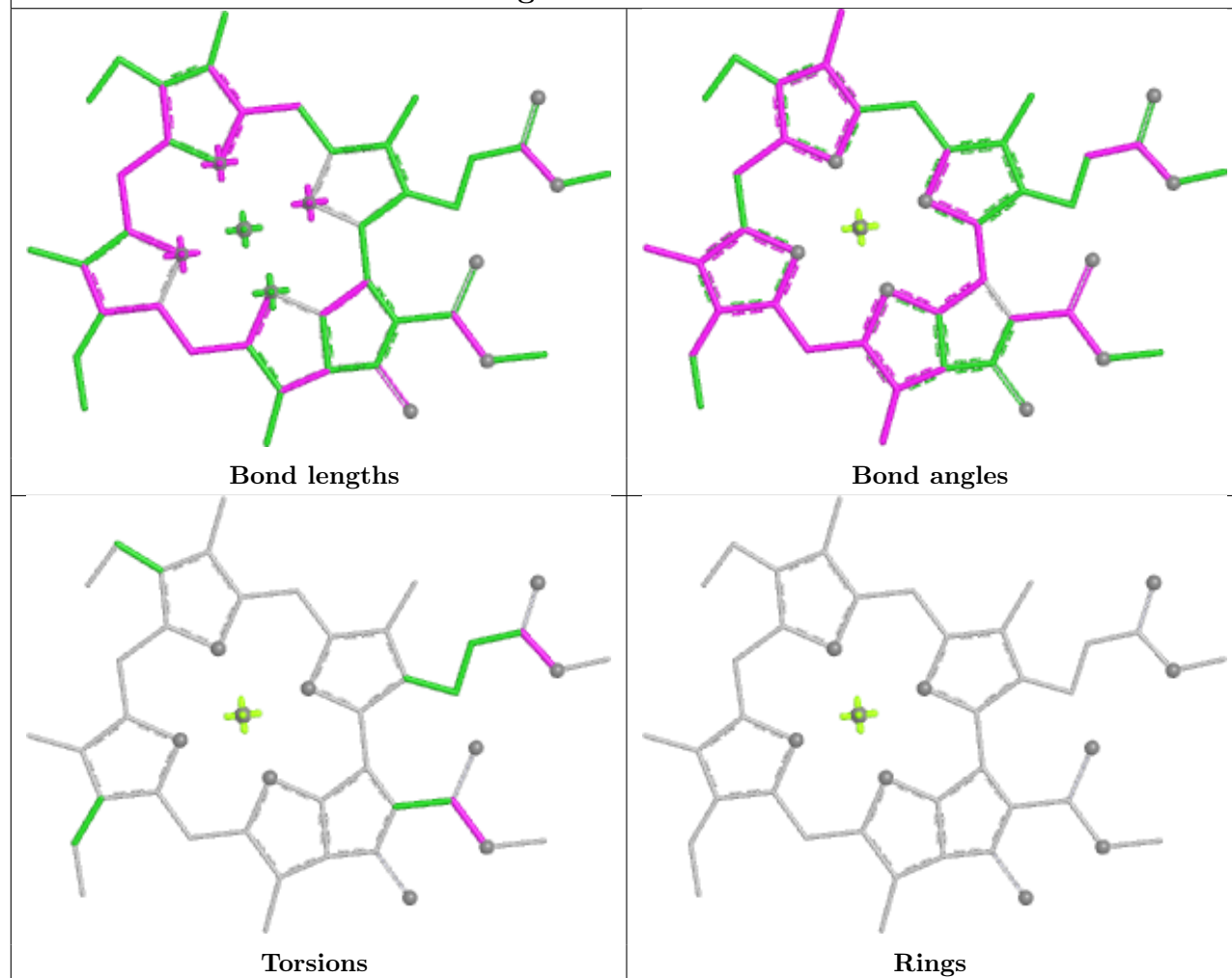




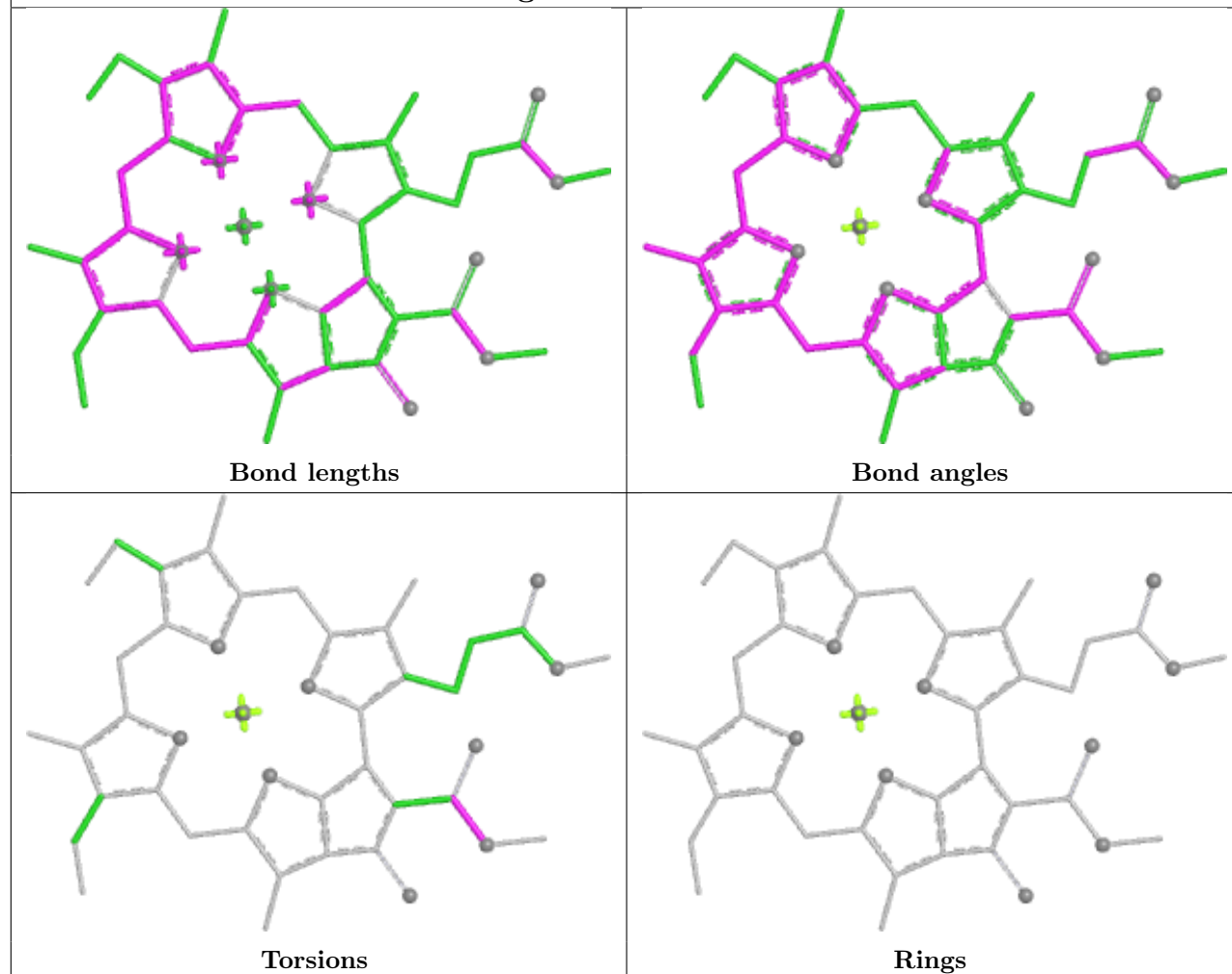
Ligand CLA 7 309



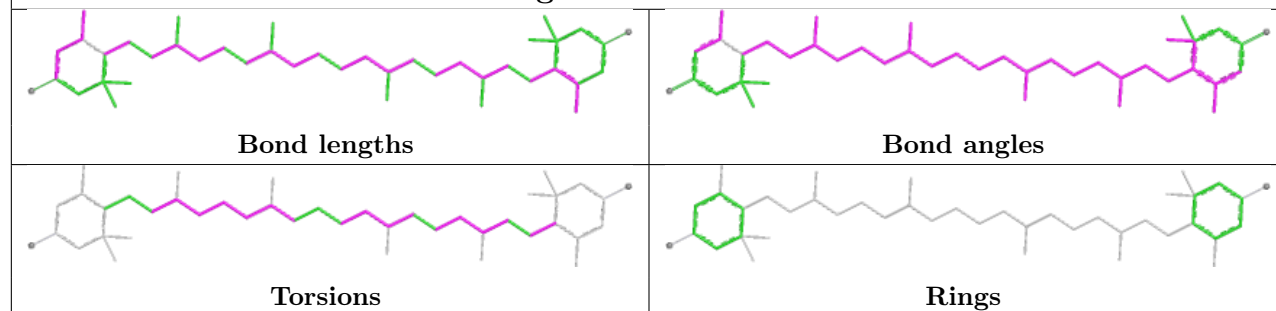
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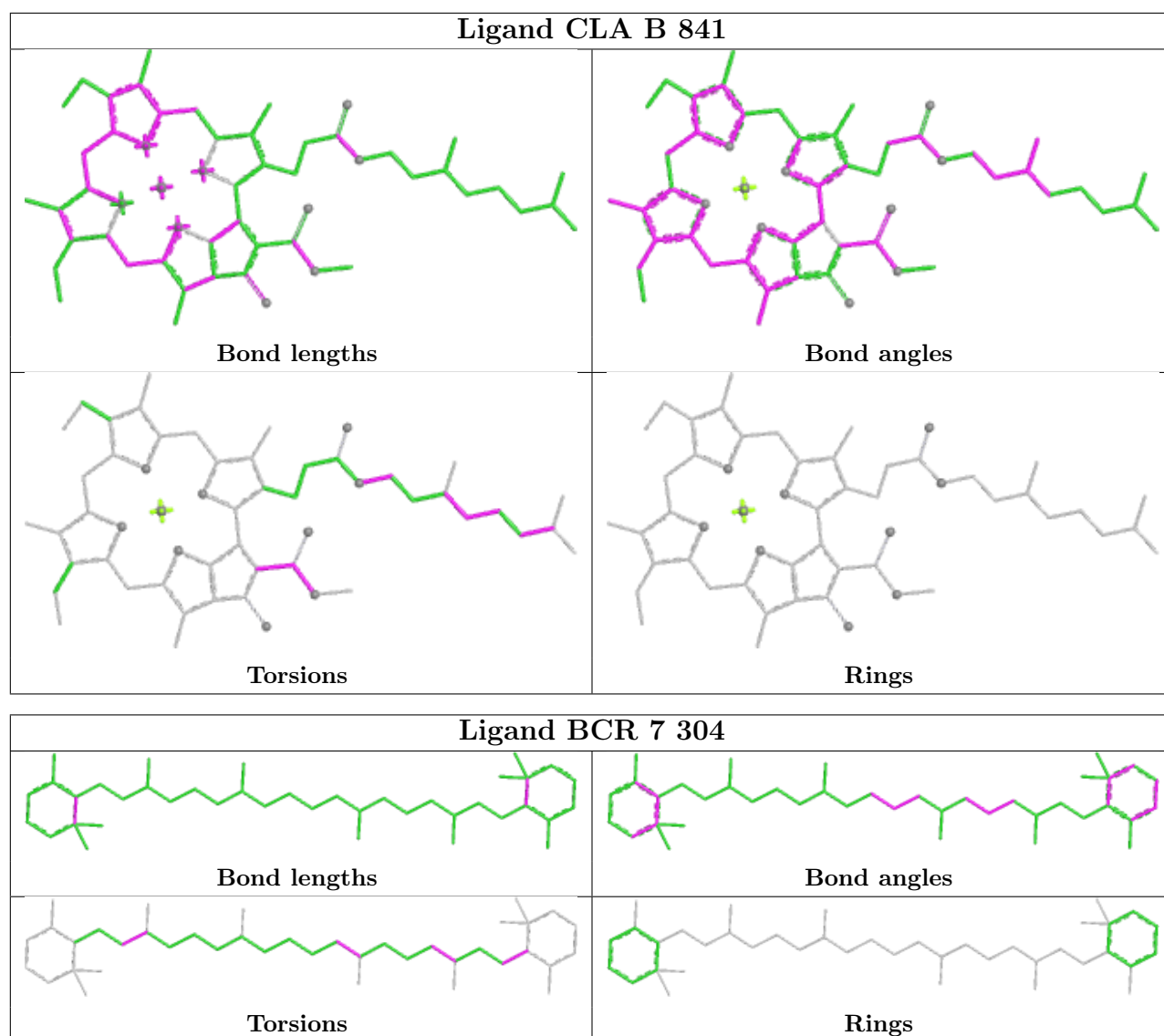


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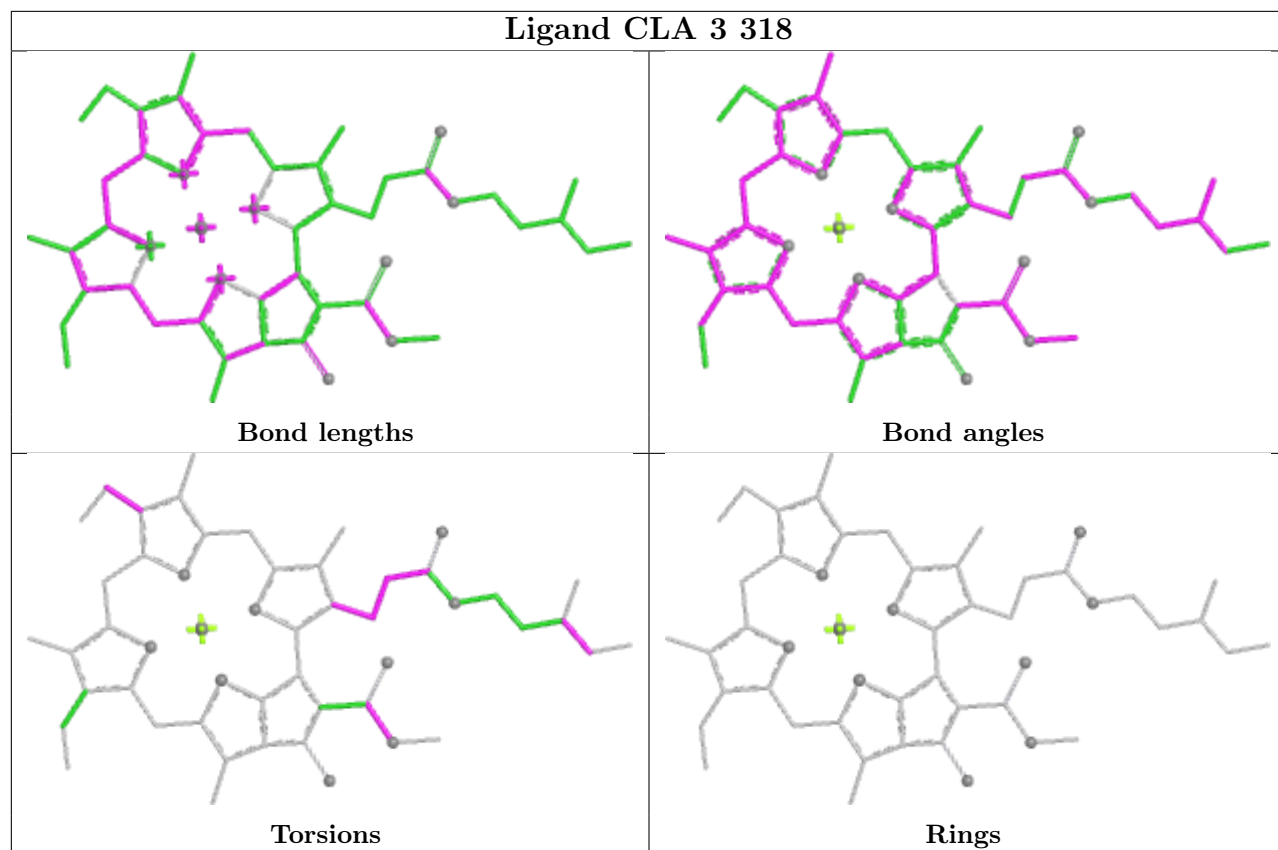


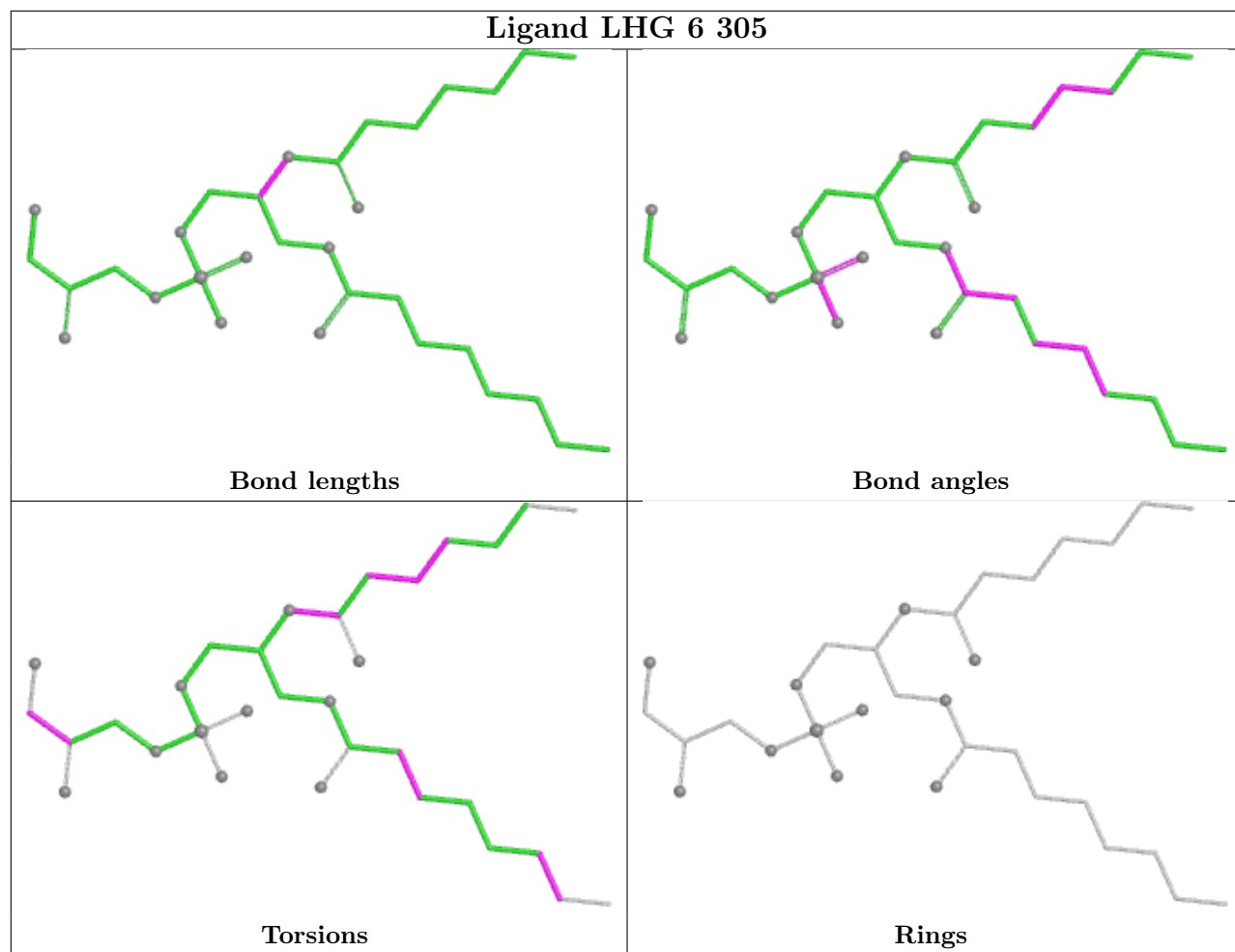
Ligand LUT 9 305



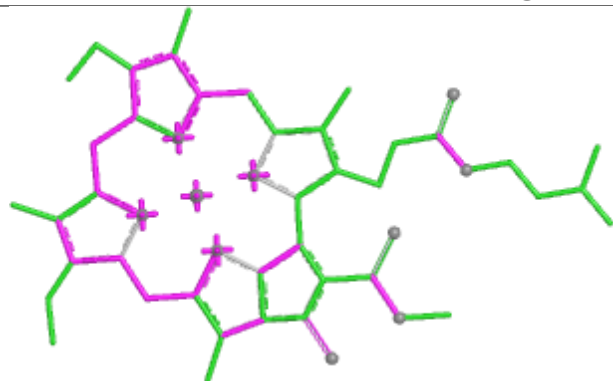


Ligand CLA 3 318

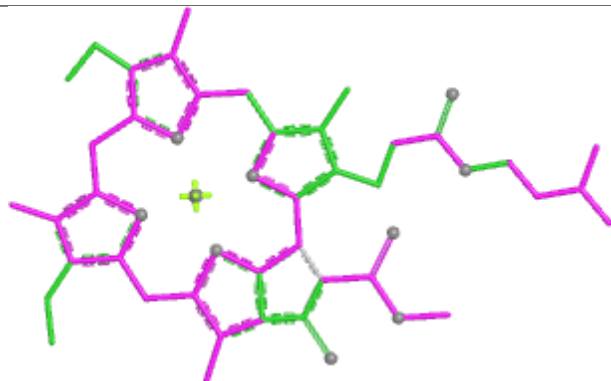




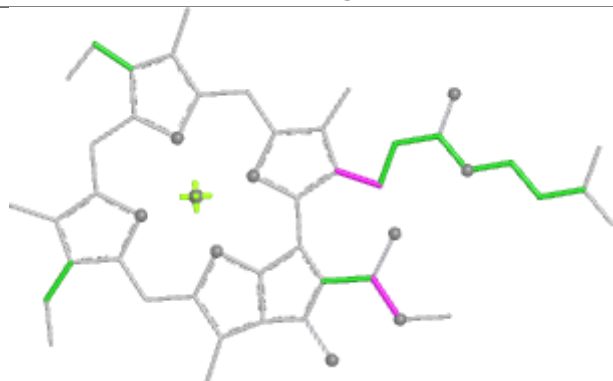
Ligand CLA 6 316



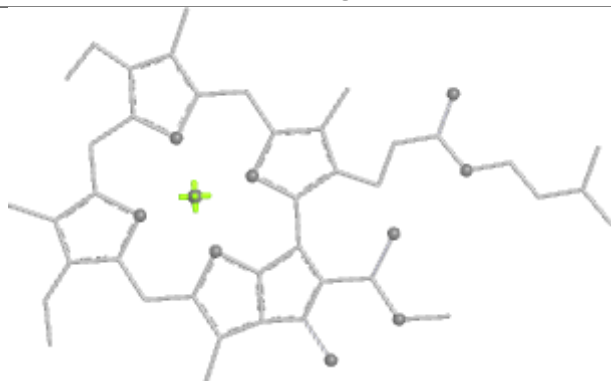
Bond lengths



Bond angles

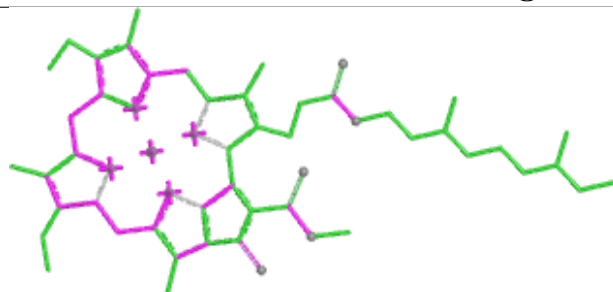


Torsions

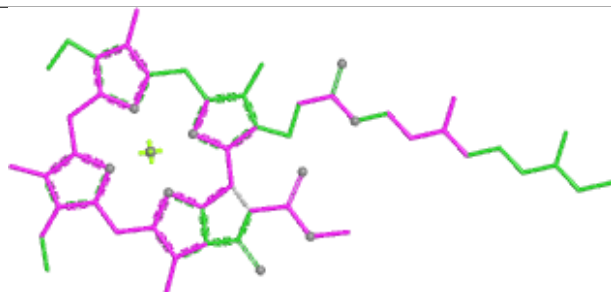


Rings

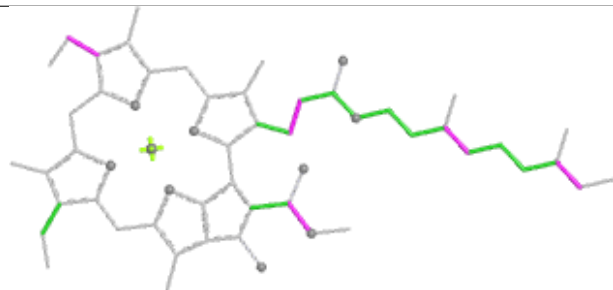
Ligand CLA 4 307



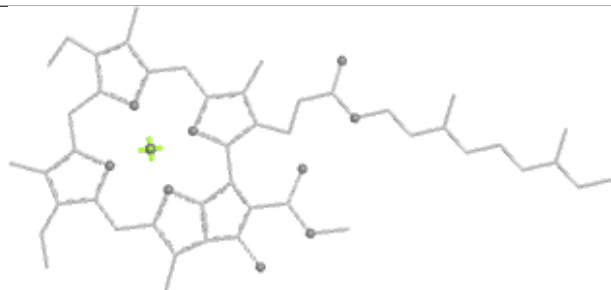
Bond lengths



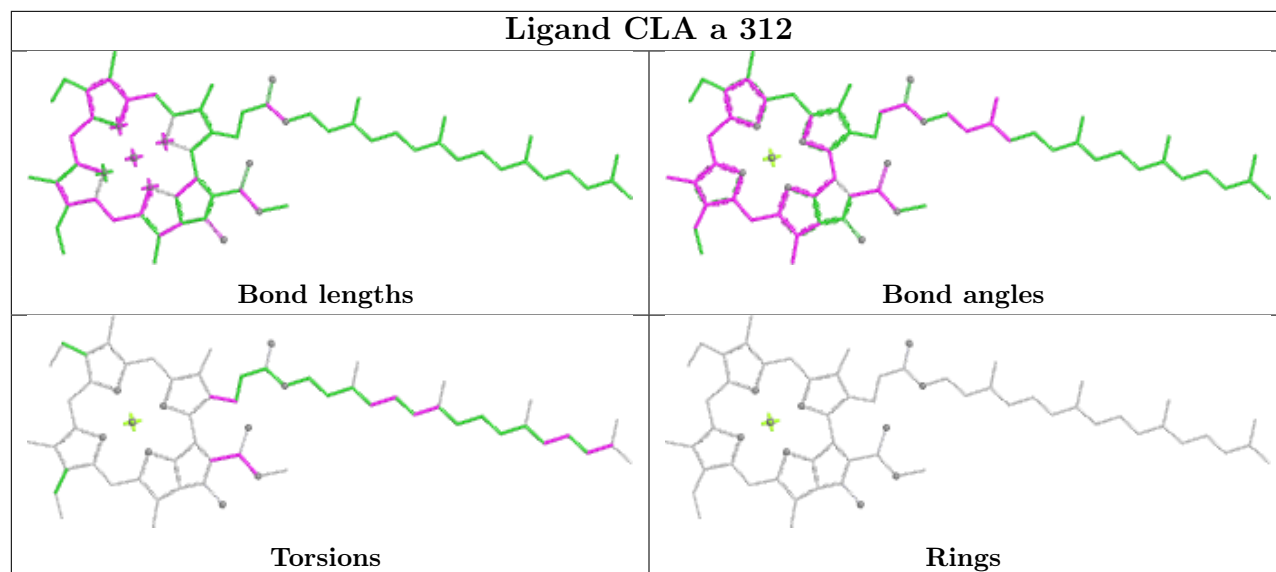
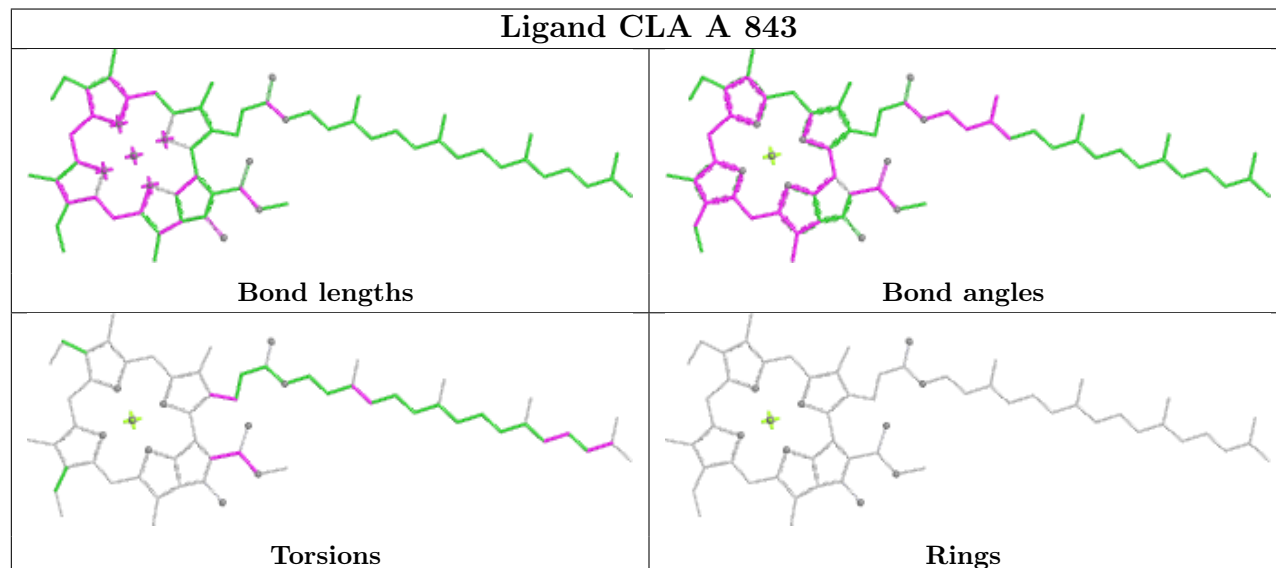
Bond angles

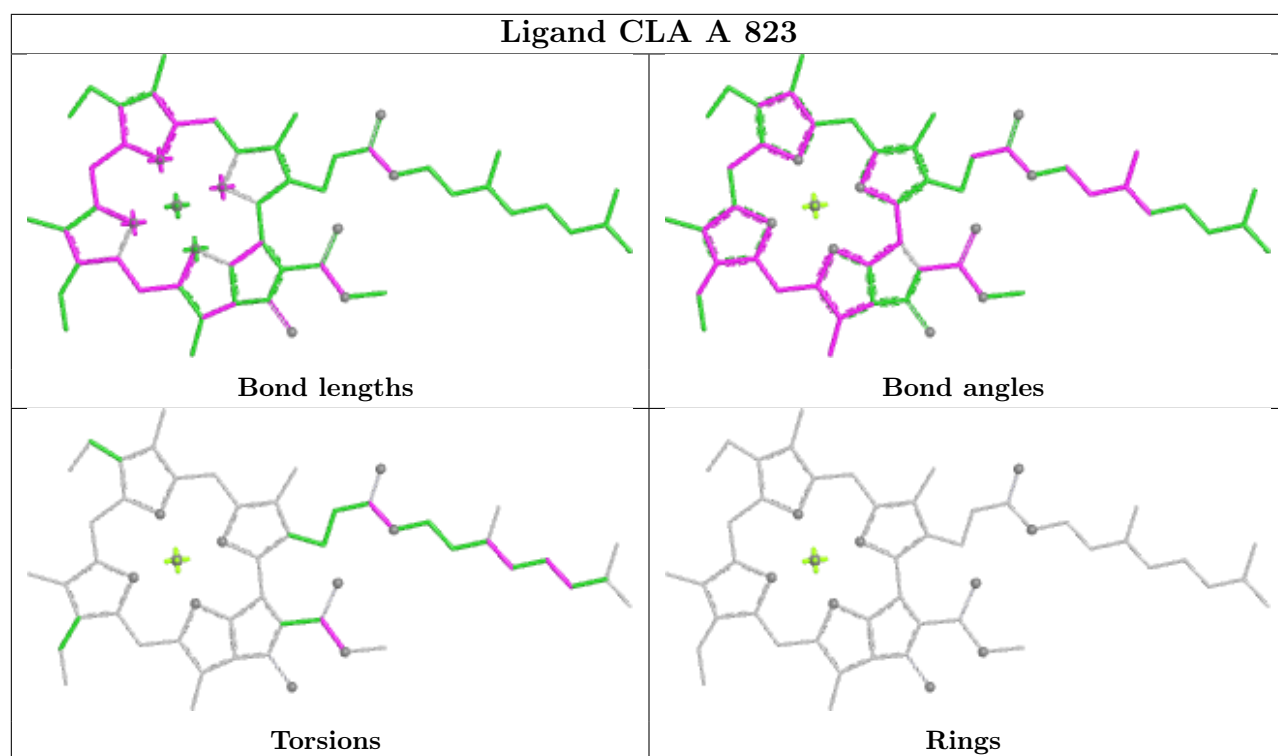


Torsions

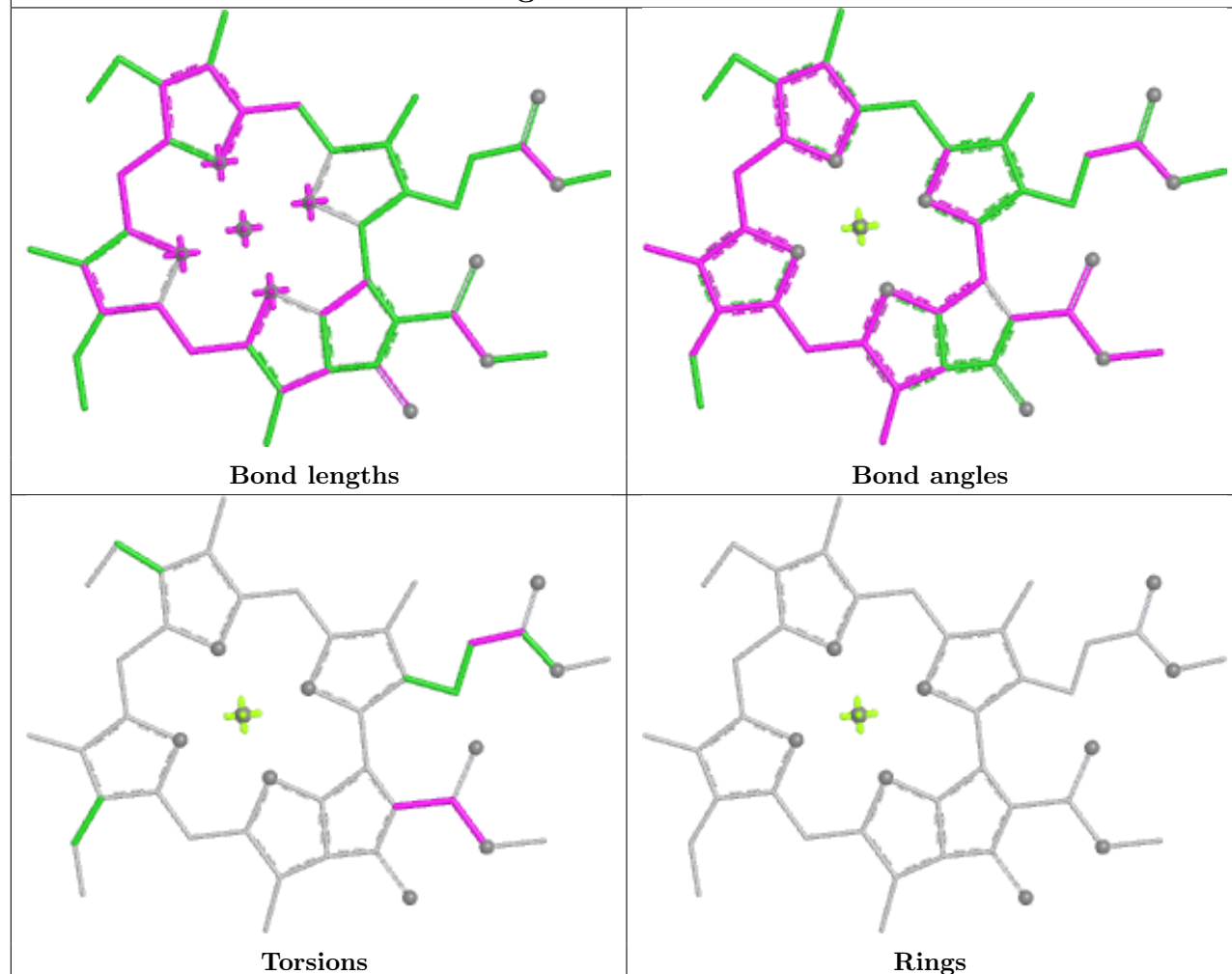


Rings

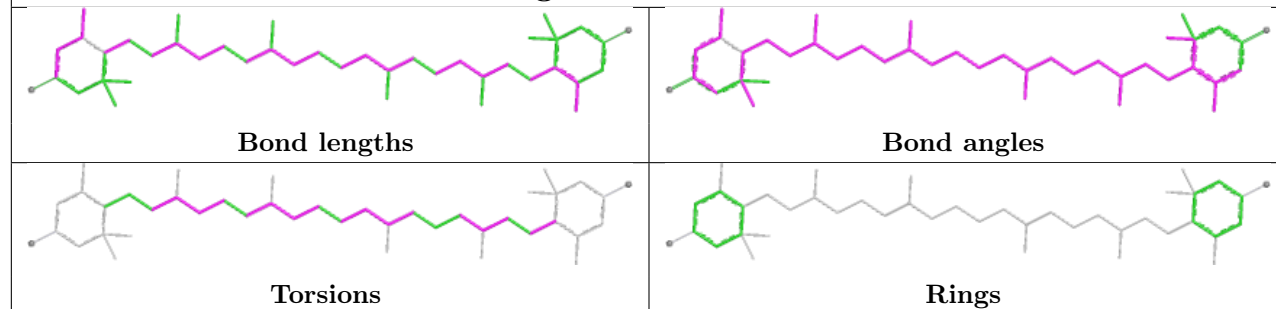
Ligand CLA a 312**Ligand CLA A 843**

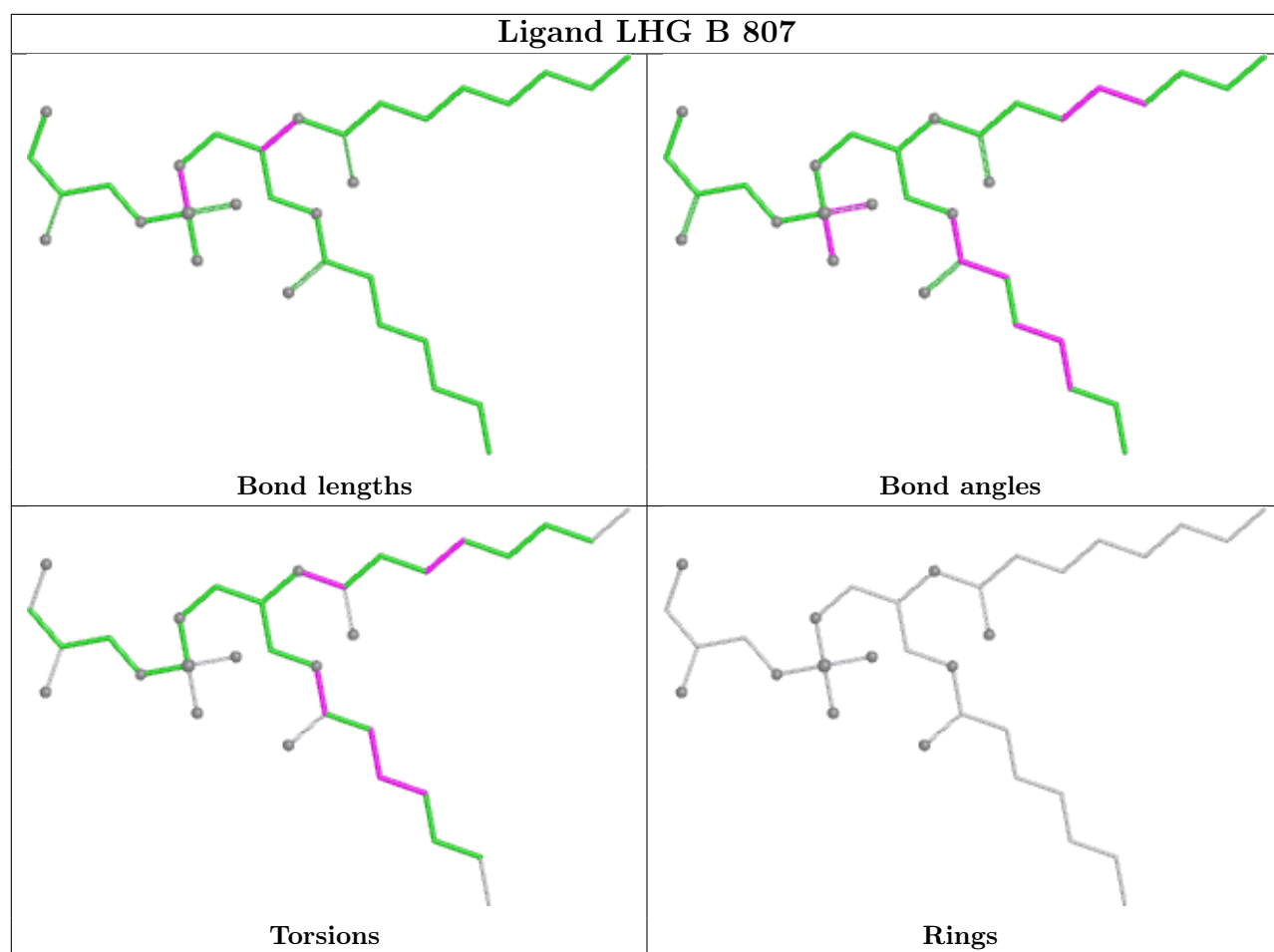


Ligand CLA 6 313

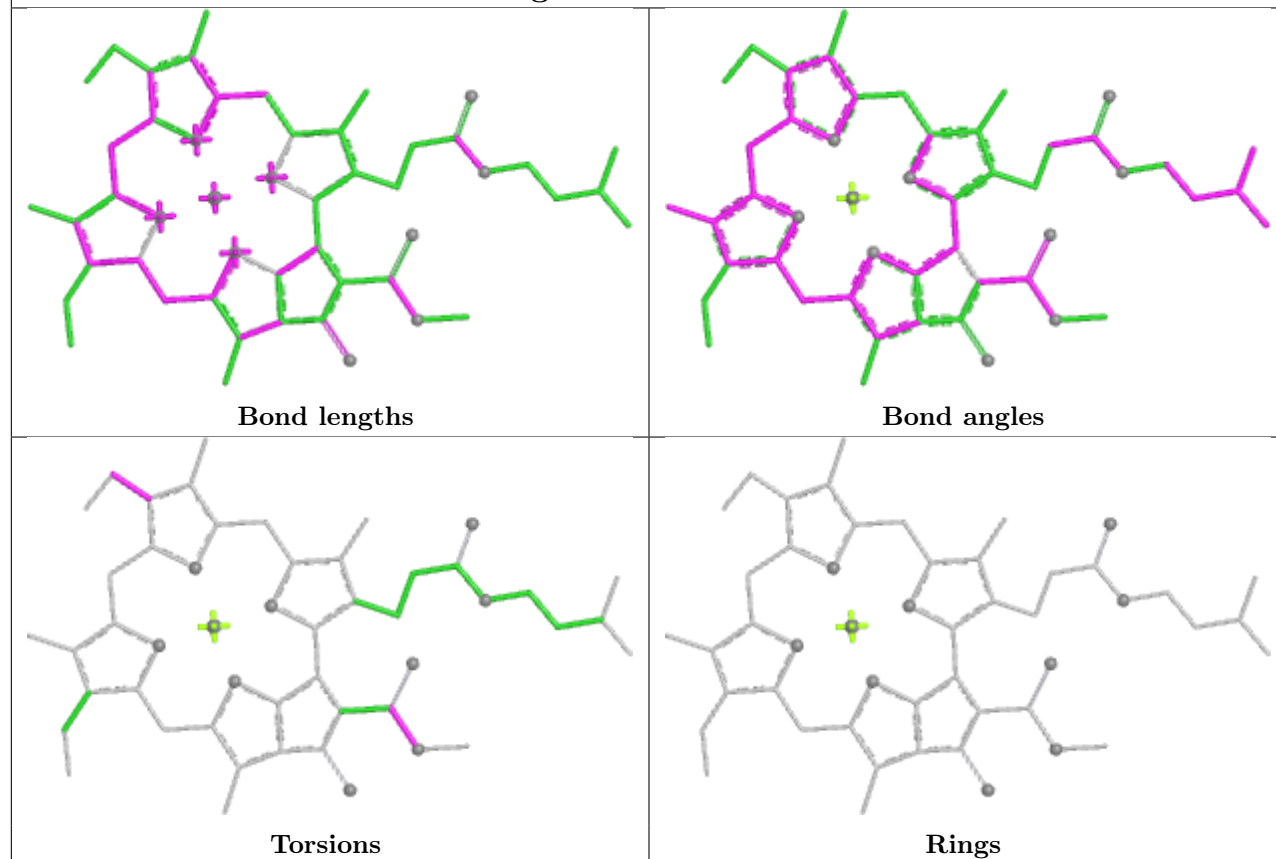


Ligand LUT b 301

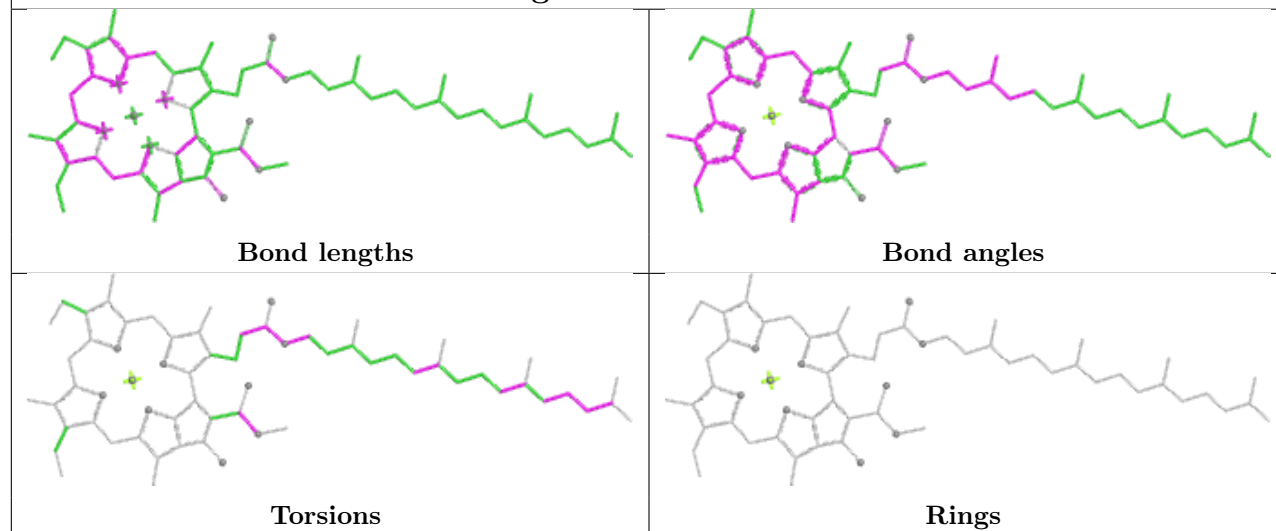


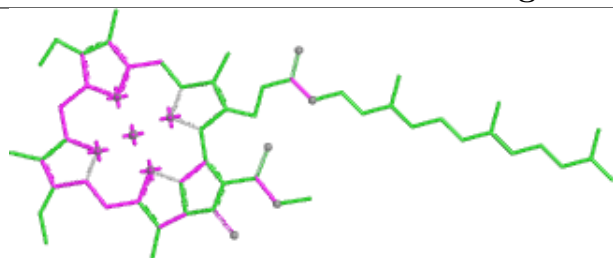
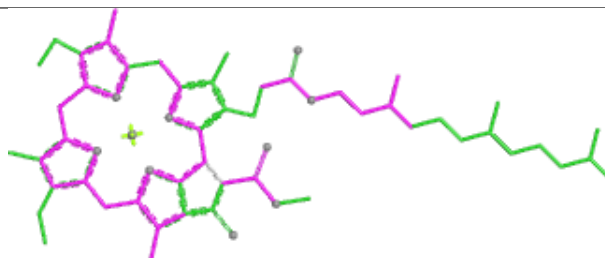
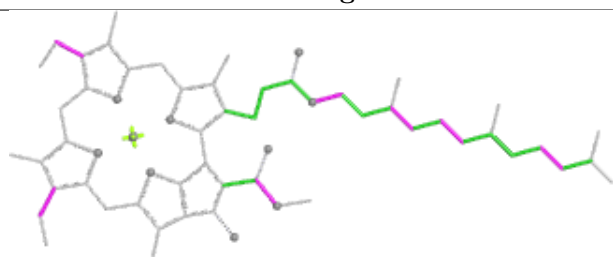
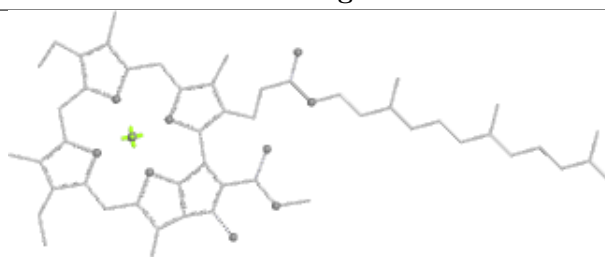
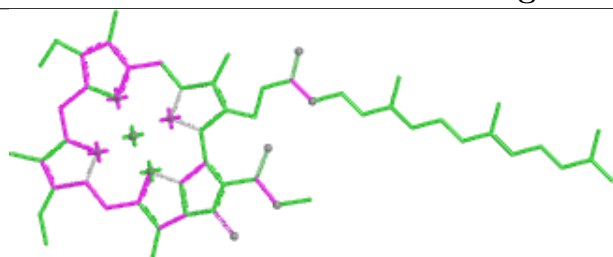
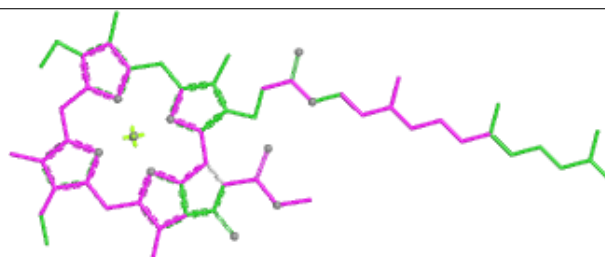
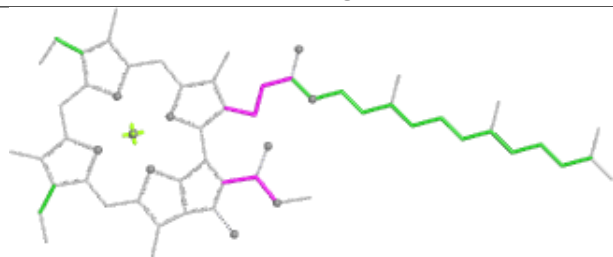
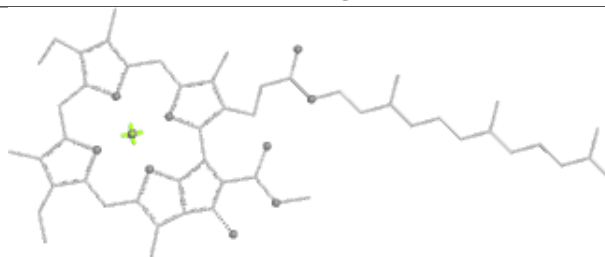


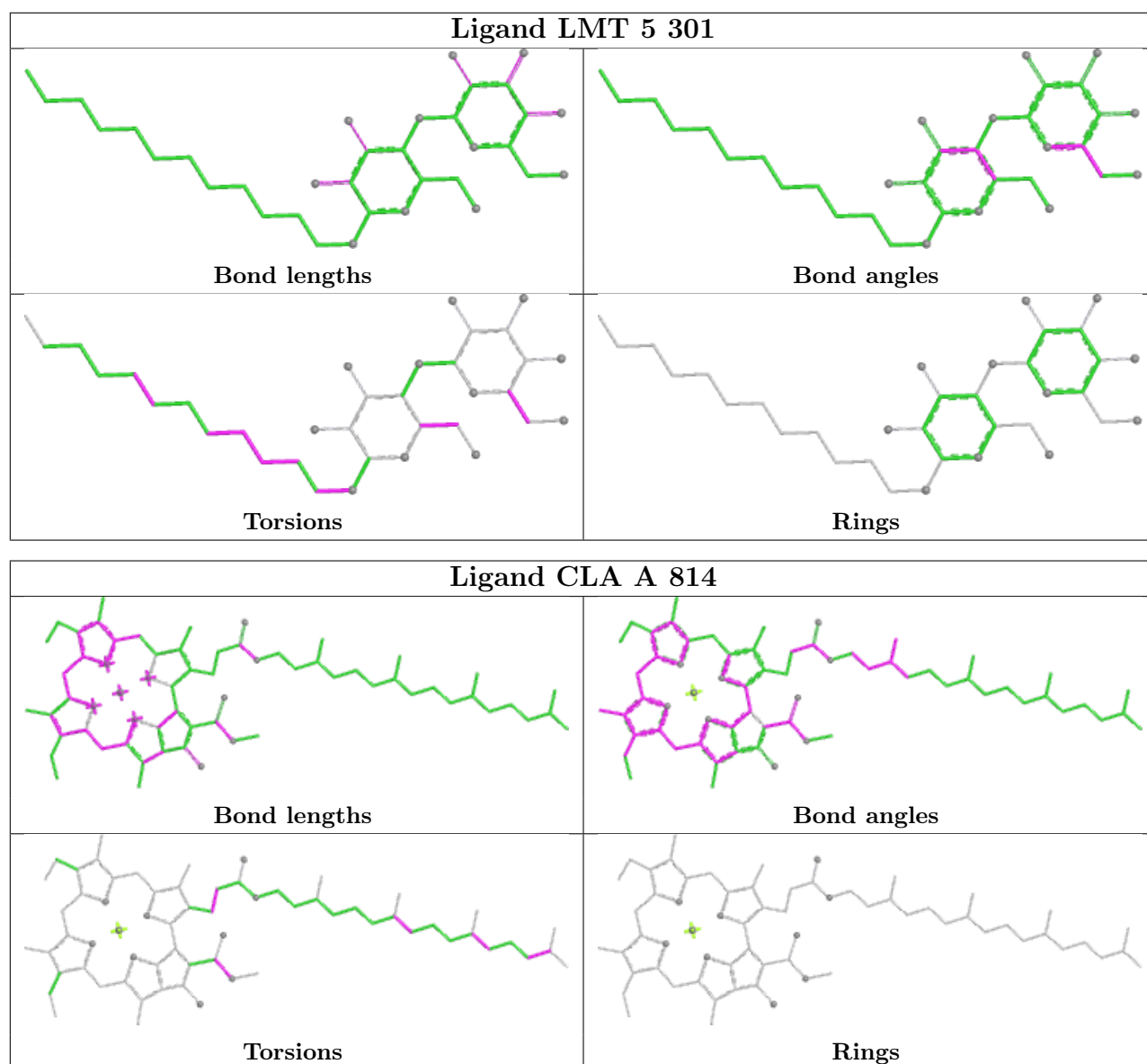
Ligand CLA K 204

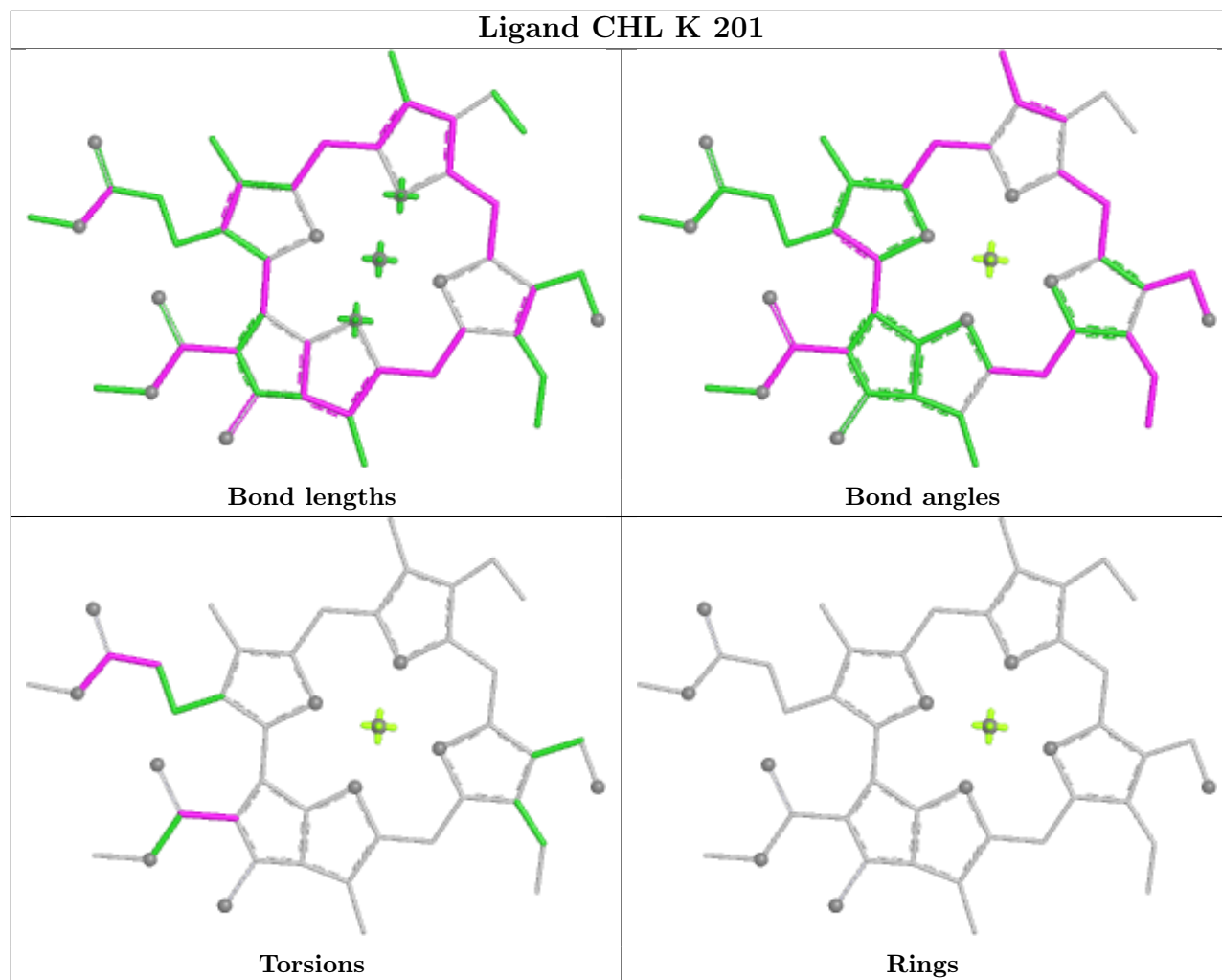


Ligand CLA A 841

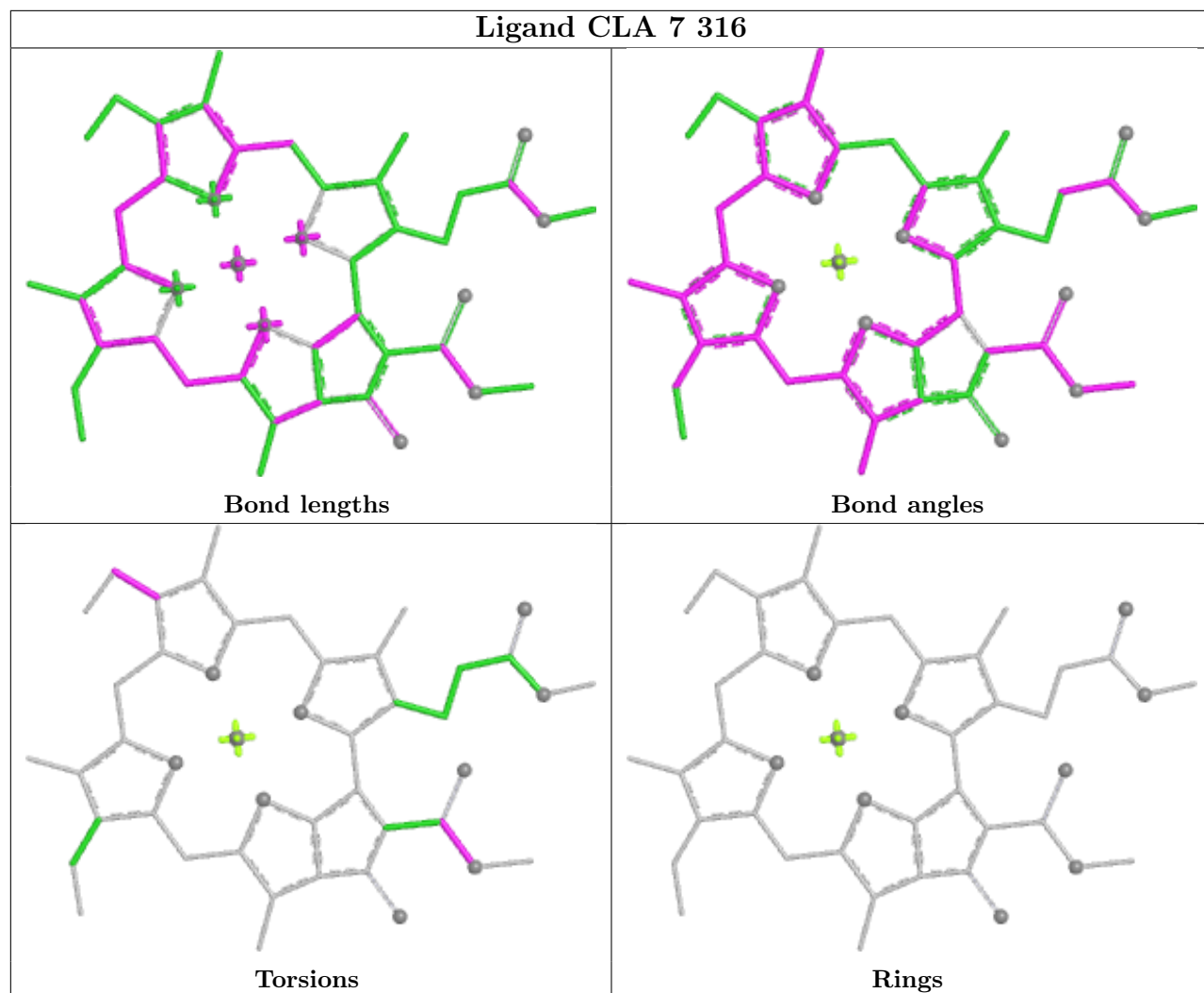


Ligand CLA 3 310**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 4 308****Bond lengths****Bond angles****Torsions****Rings**

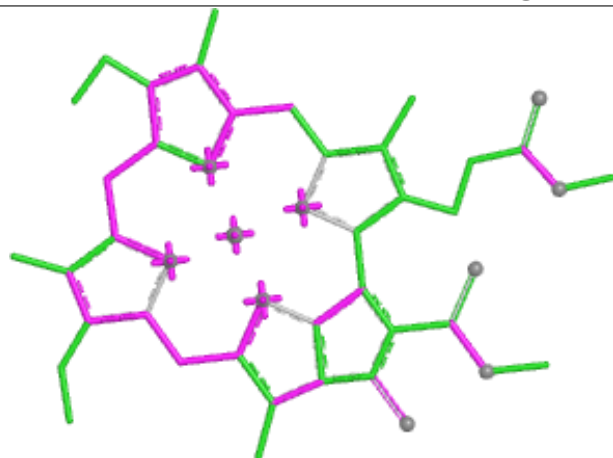




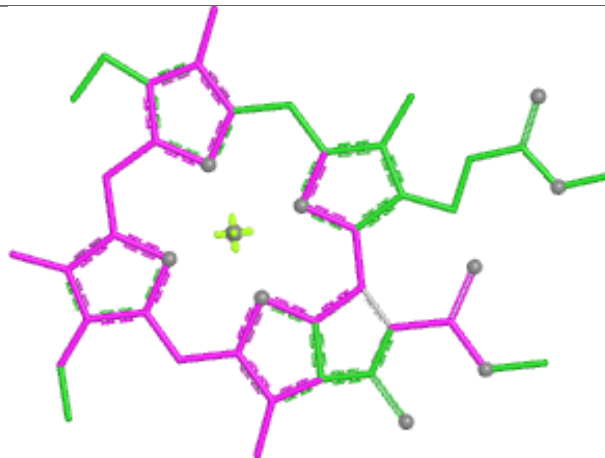
Ligand CLA 7 316



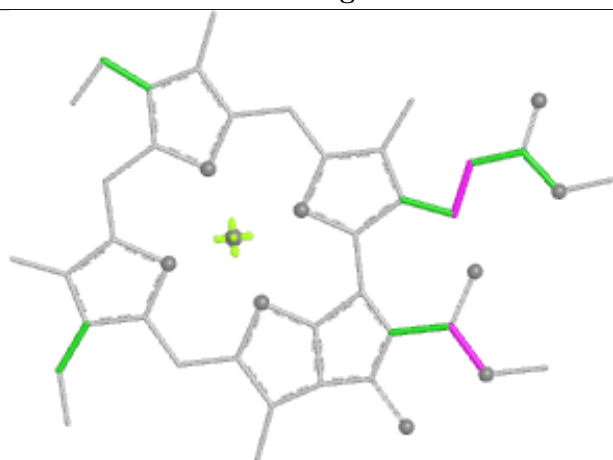
Ligand CLA b 303



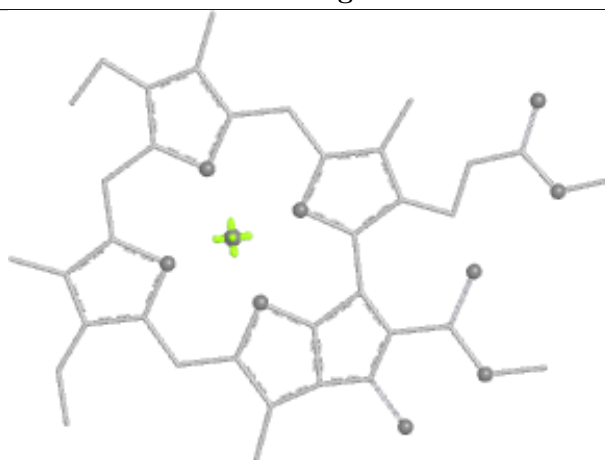
Bond lengths



Bond angles

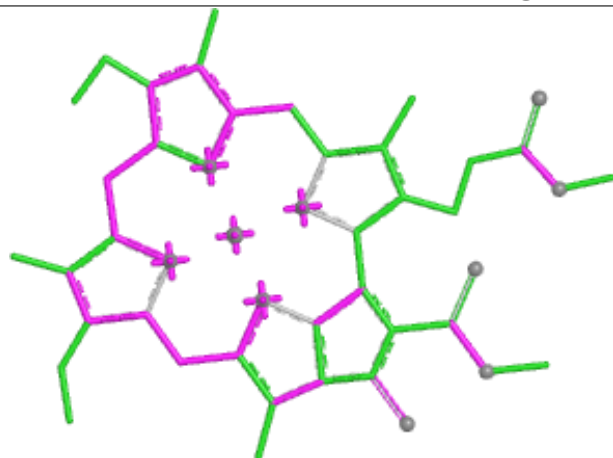


Torsions

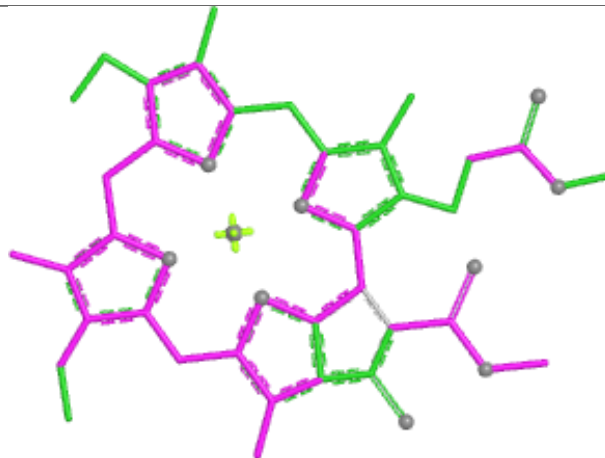


Rings

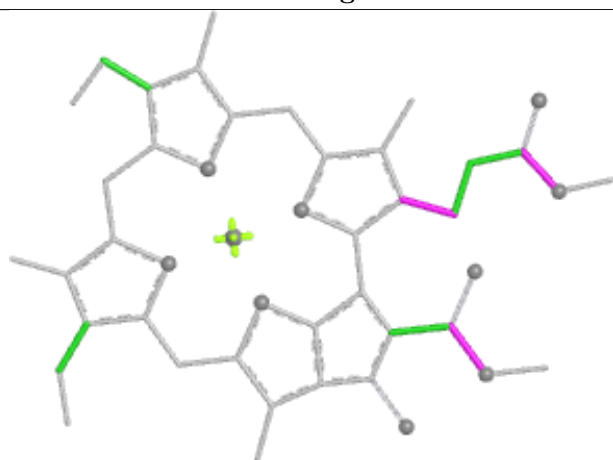
Ligand CLA b 304



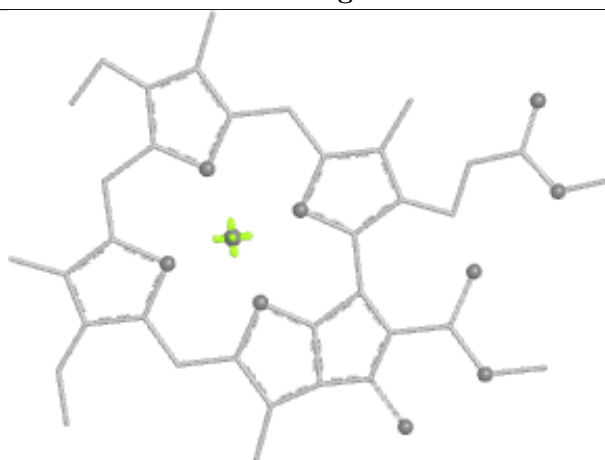
Bond lengths



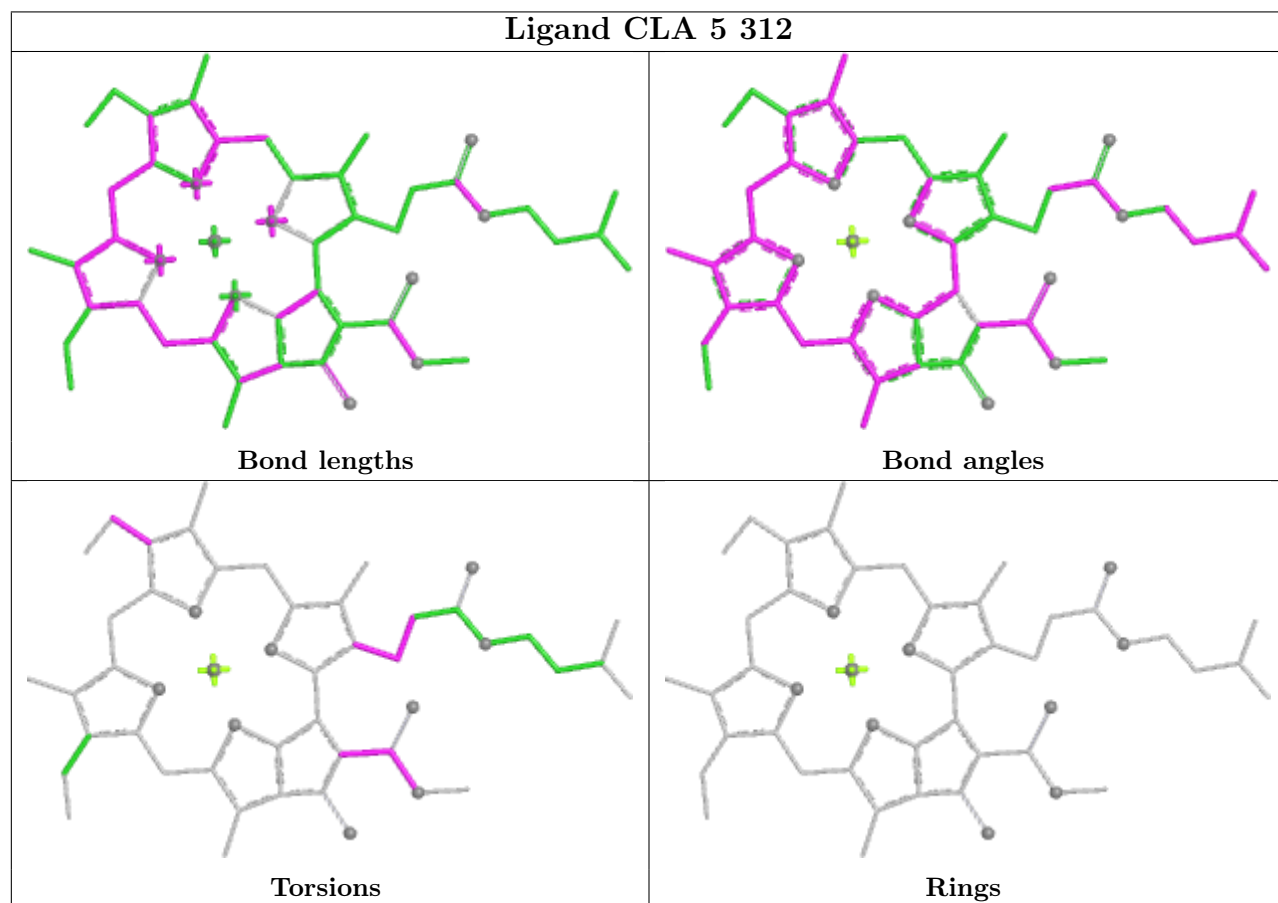
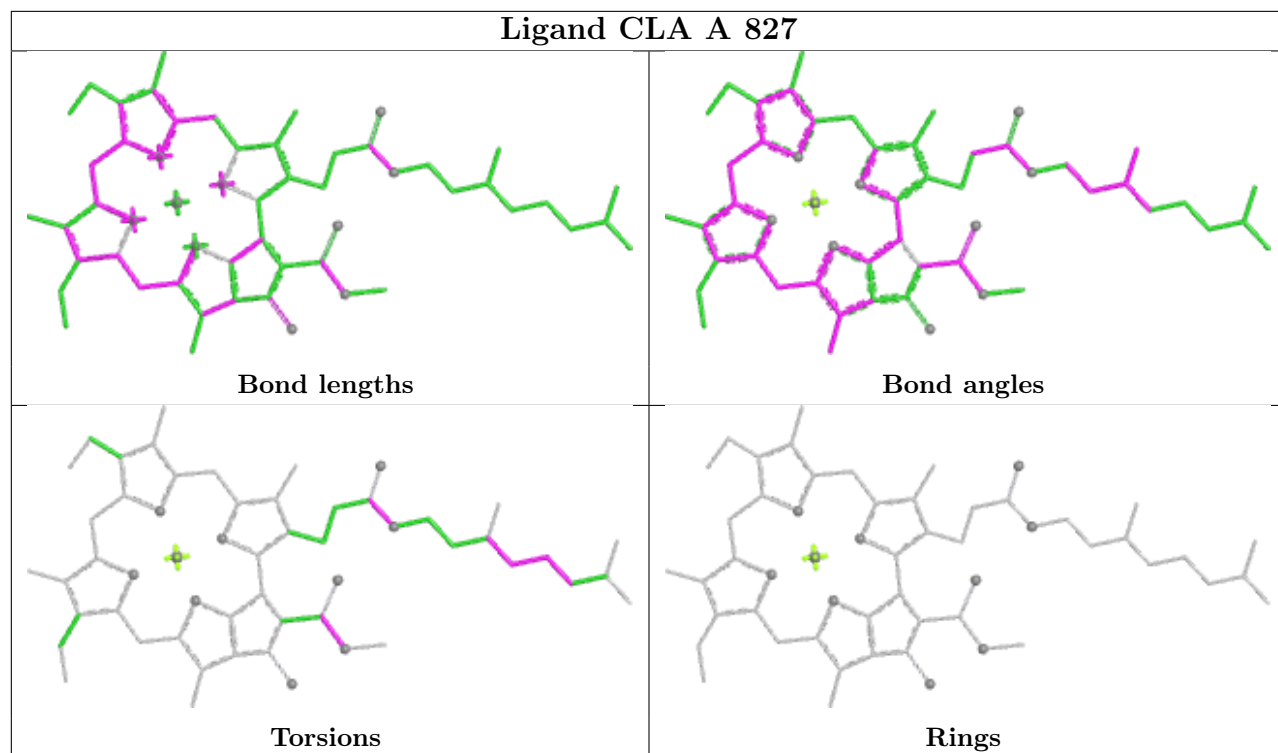
Bond angles



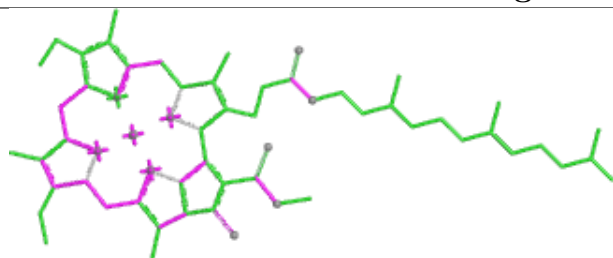
Torsions



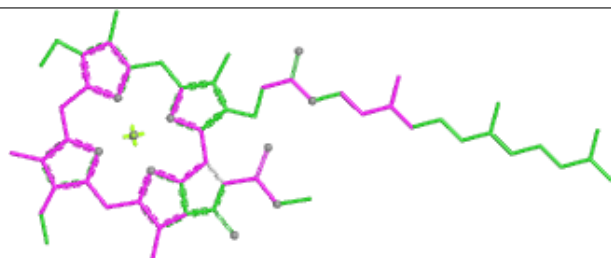
Rings



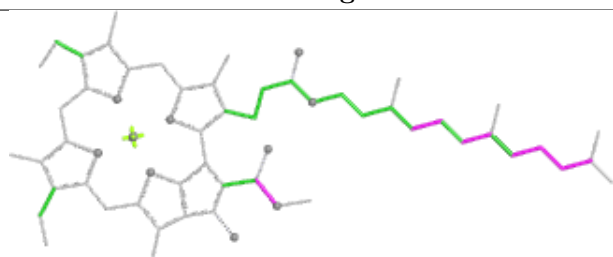
Ligand CLA B 827



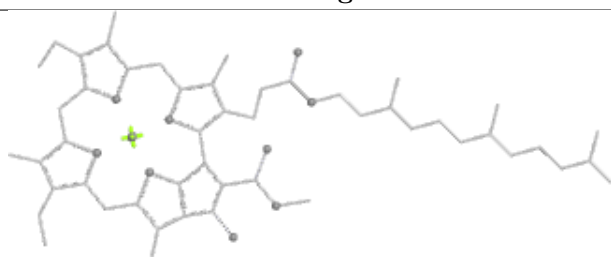
Bond lengths



Bond angles

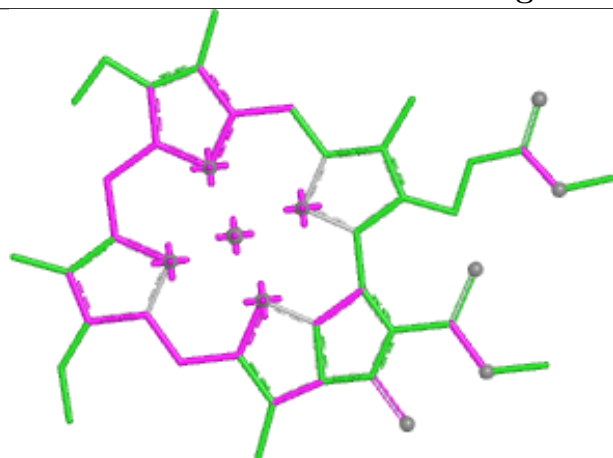


Torsions

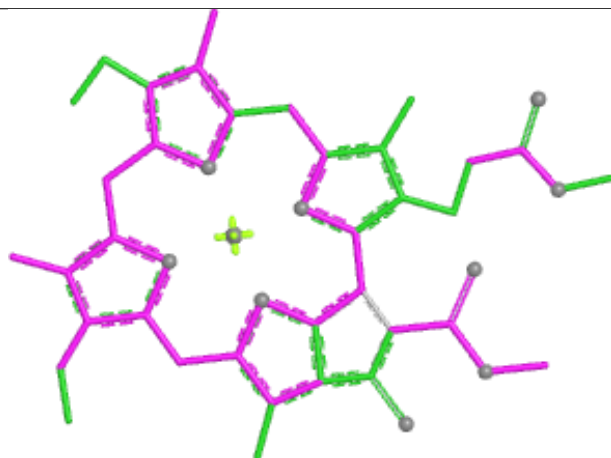


Rings

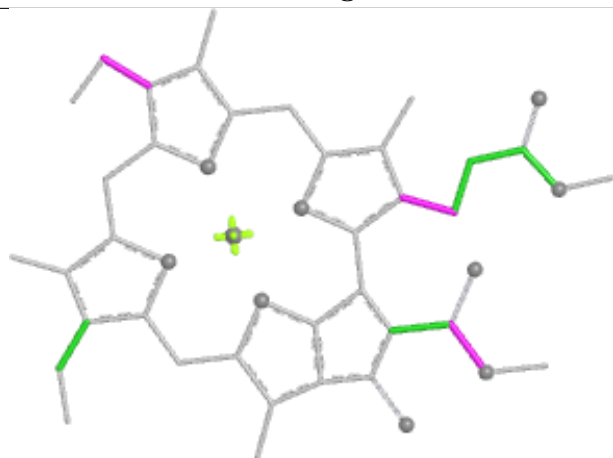
Ligand CLA F 305



Bond lengths



Bond angles

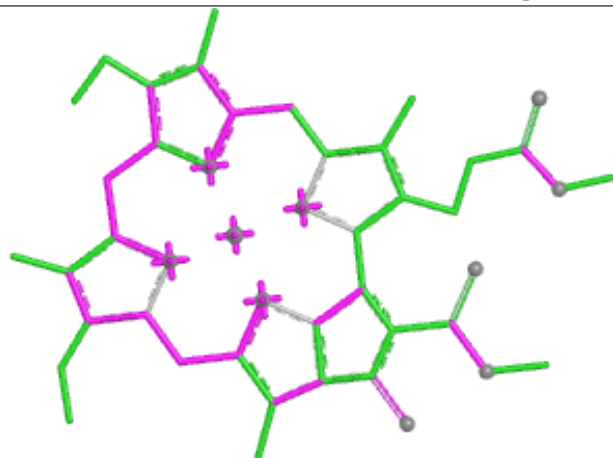


Torsions

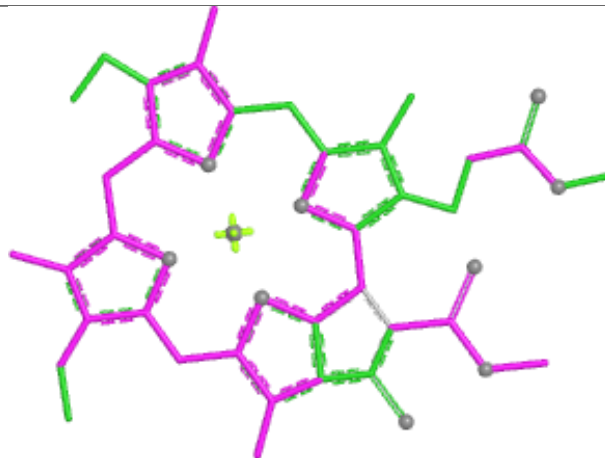


Rings

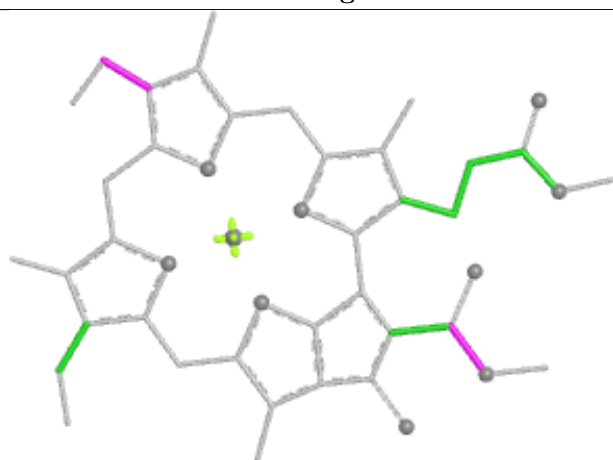
Ligand CLA b 312



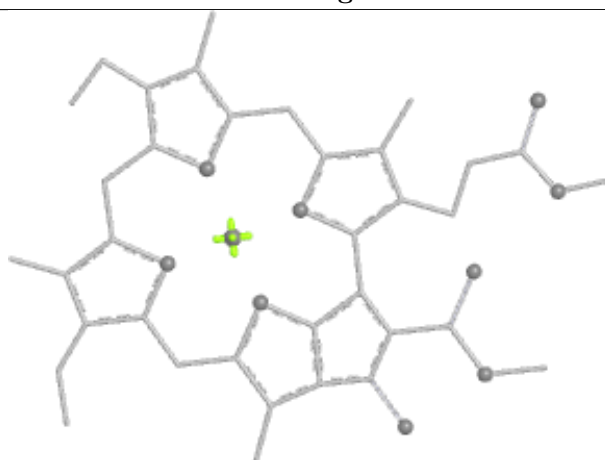
Bond lengths



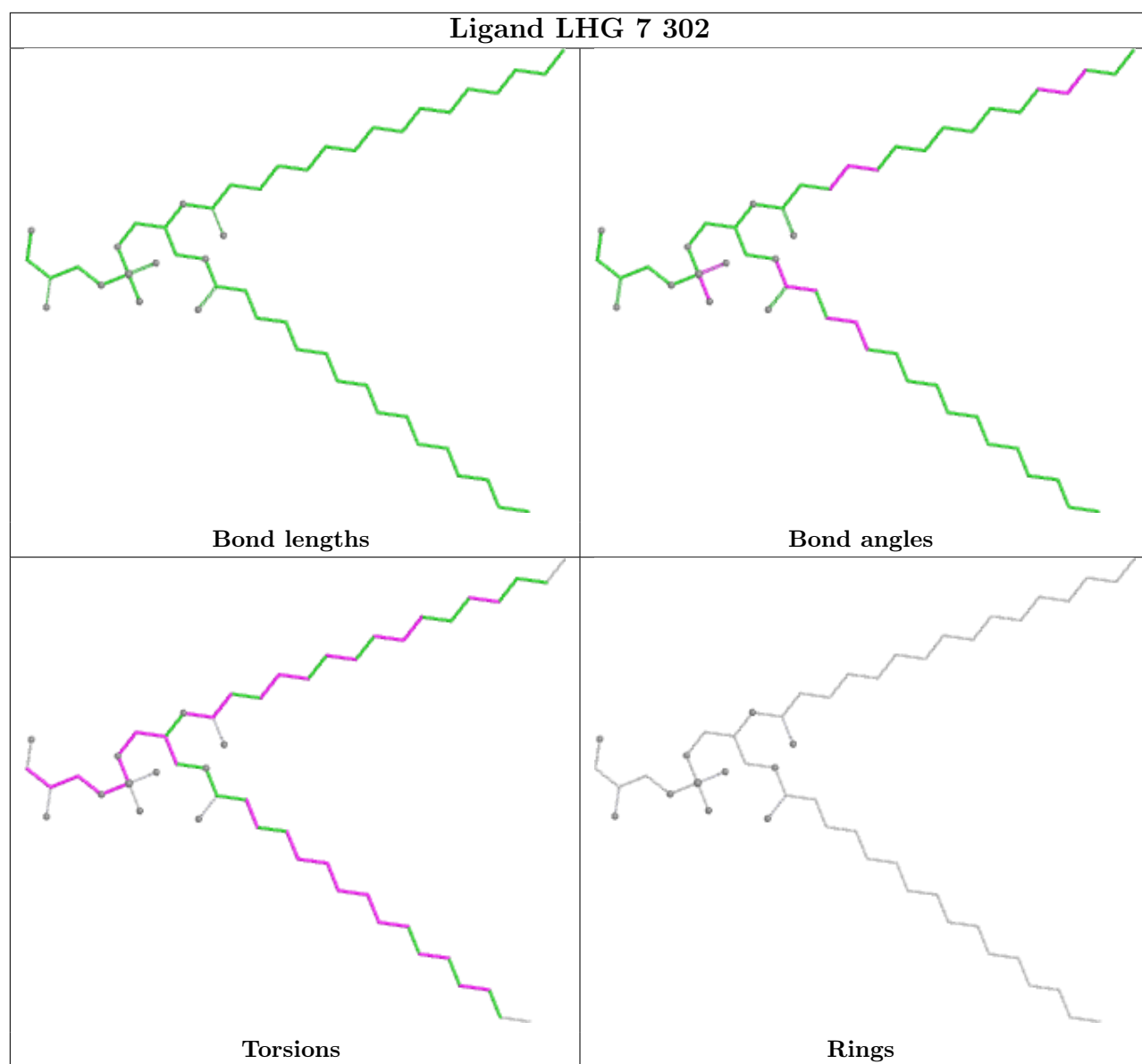
Bond angles

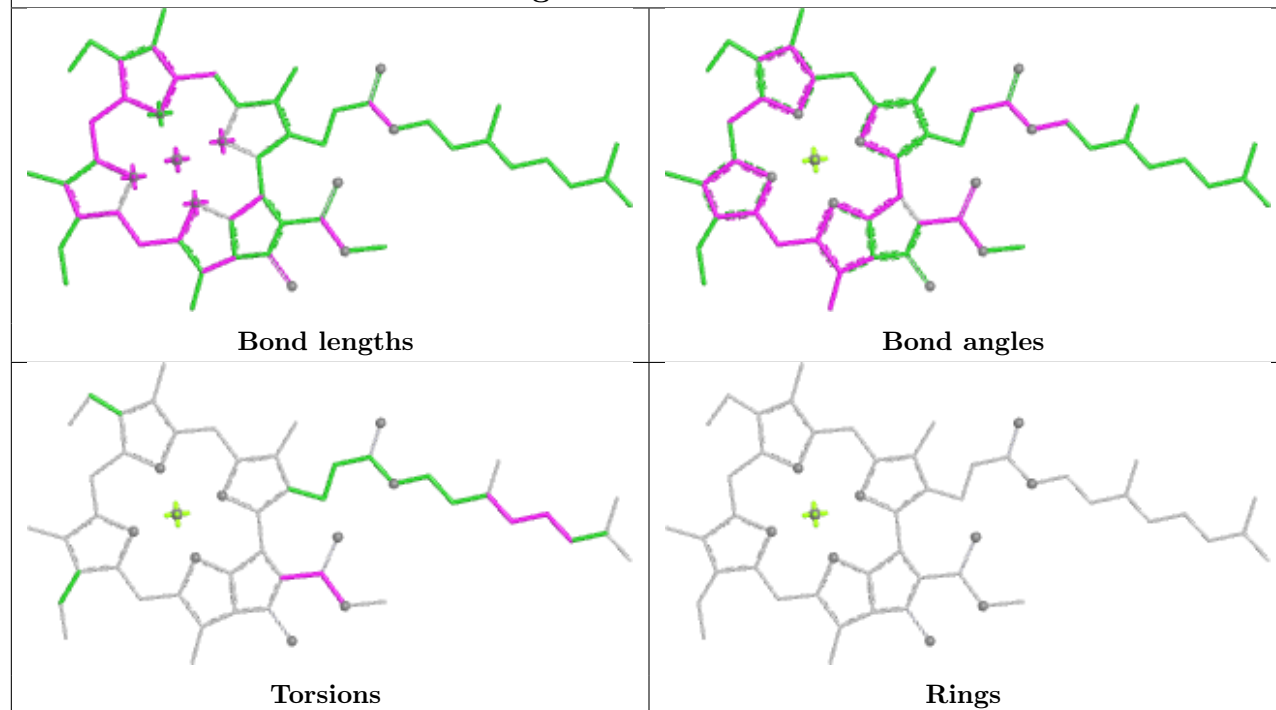
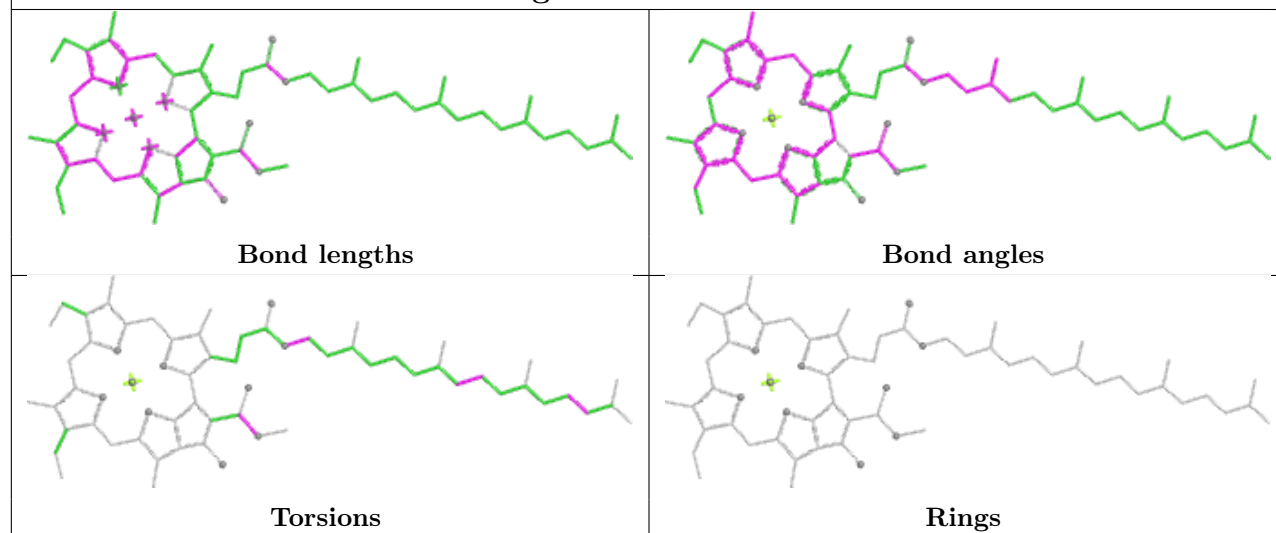


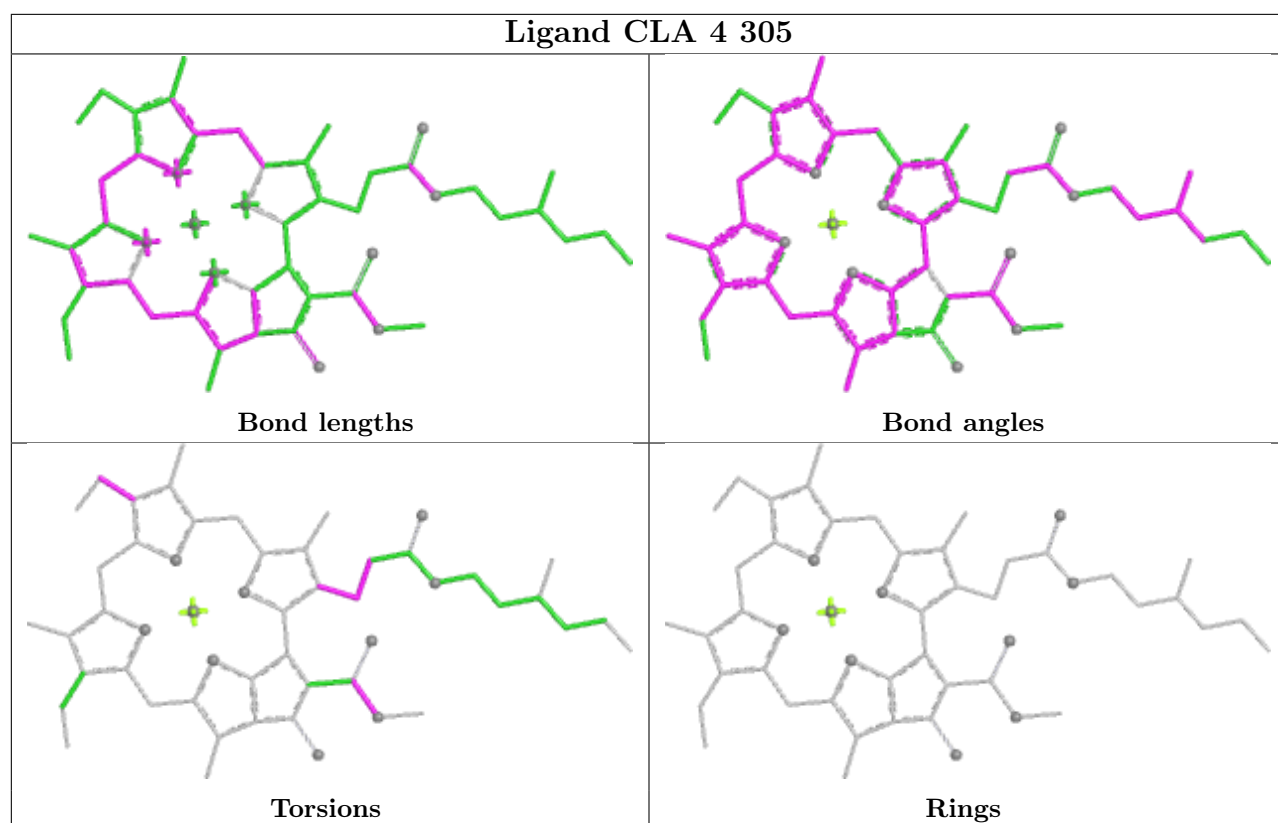
Torsions



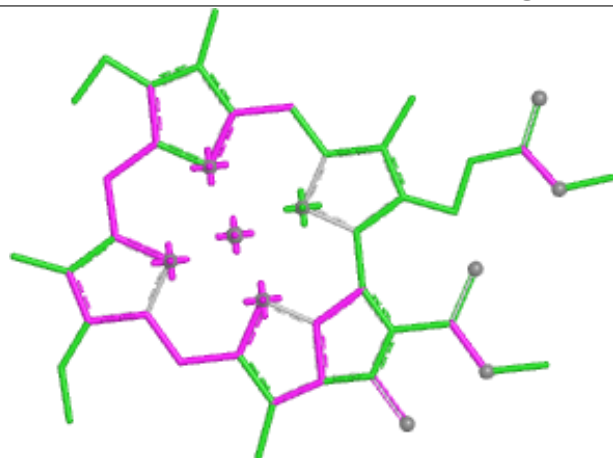
Rings



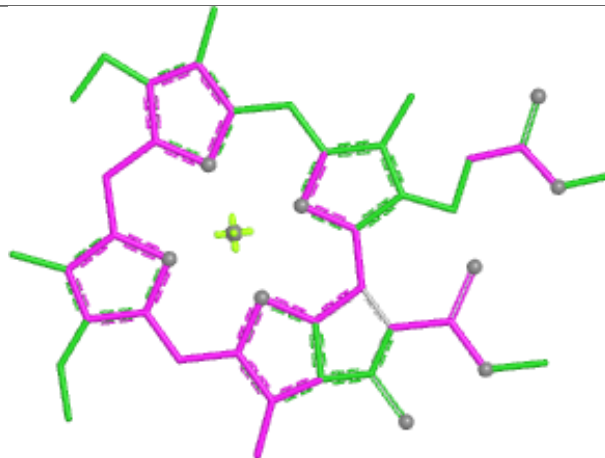
Ligand CLA B 833**Ligand CLA B 811**



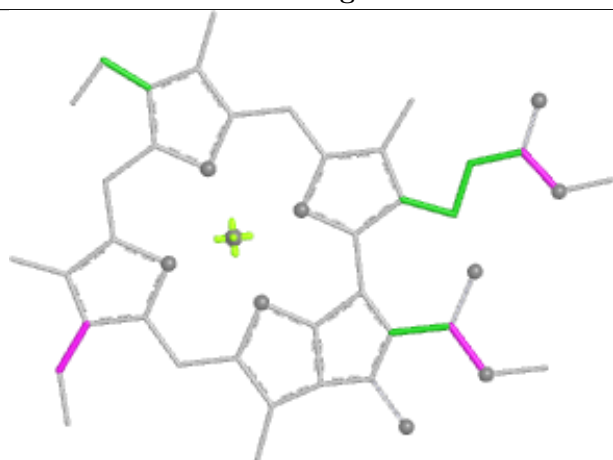
Ligand CLA 2 313



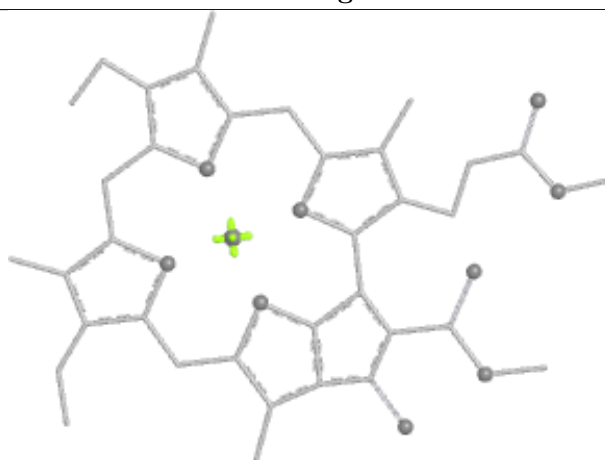
Bond lengths



Bond angles

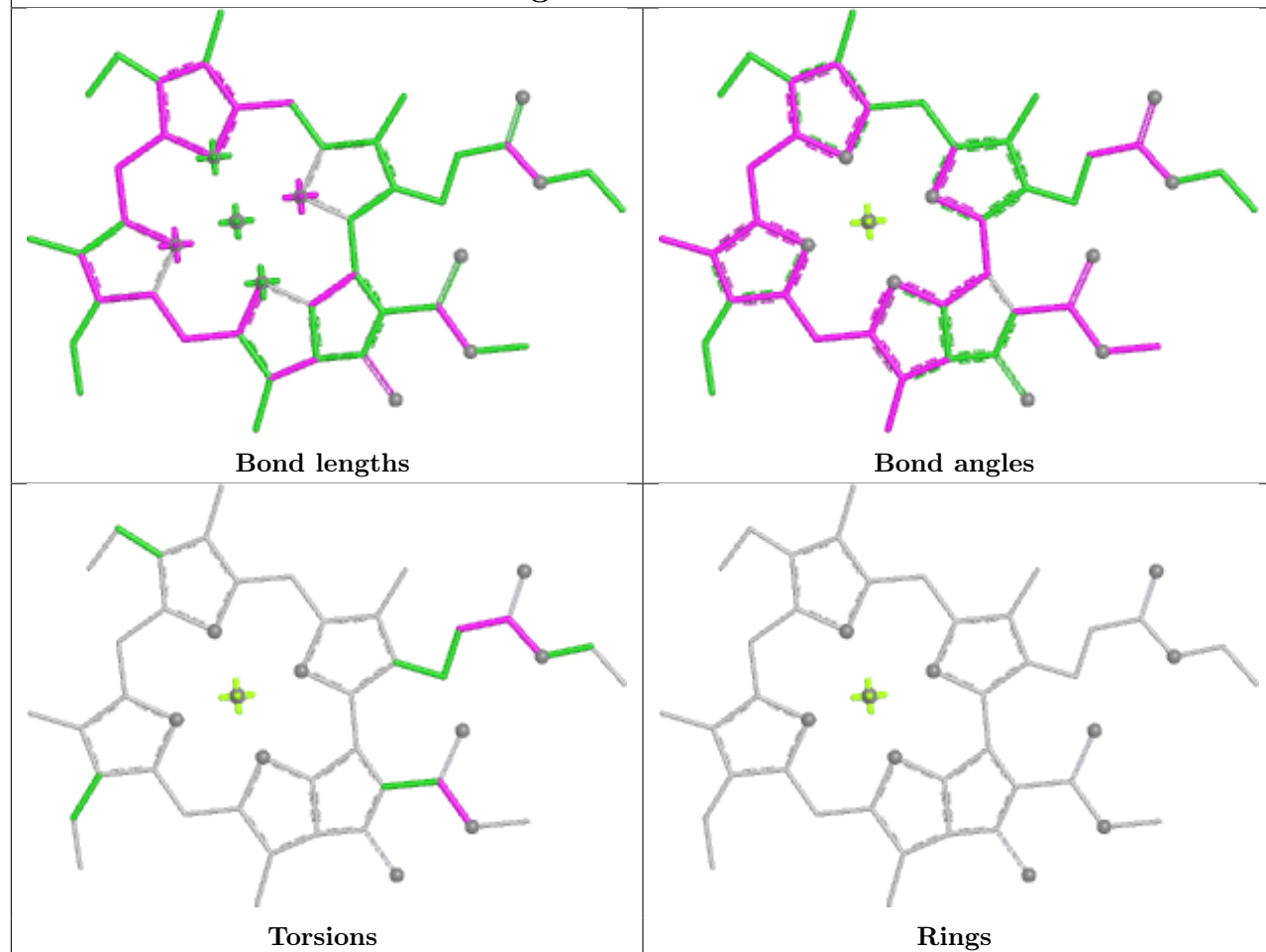


Torsions

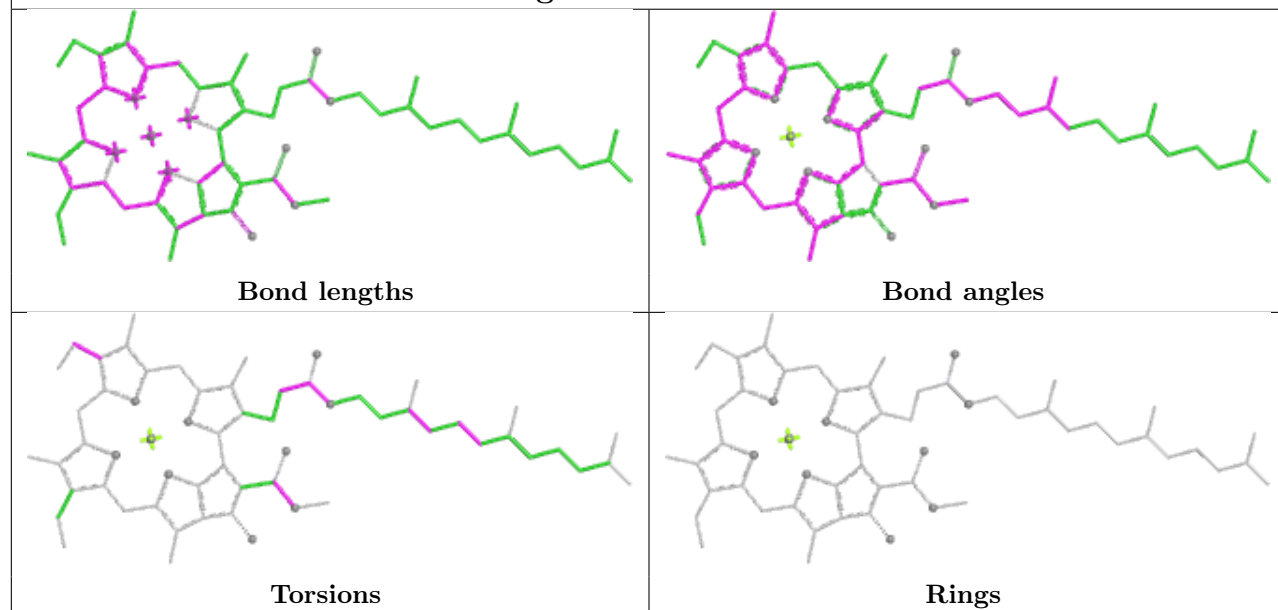


Rings

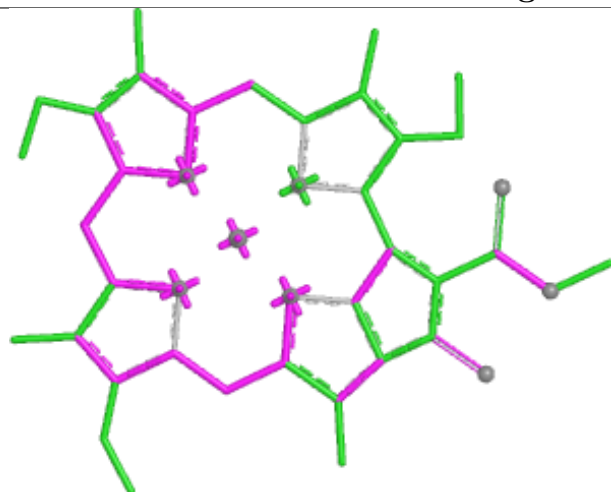
Ligand CLA 7 321



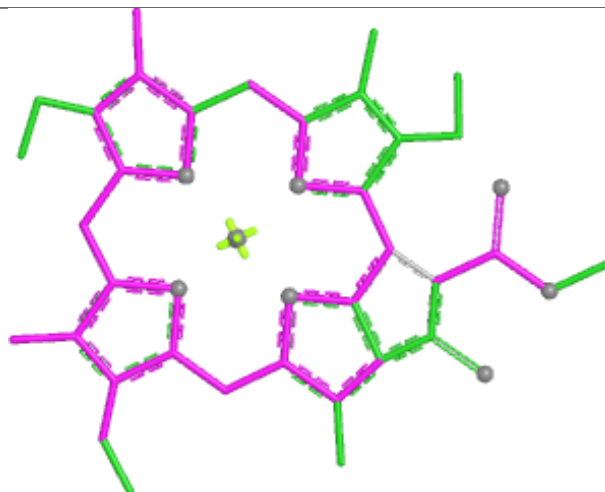
Ligand CLA 4 309



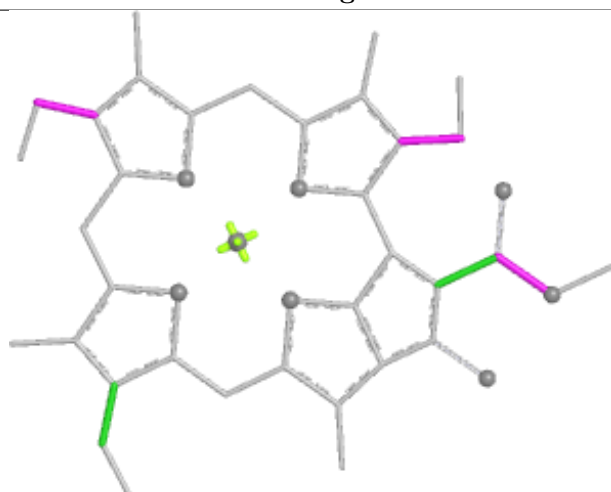
Ligand CLA J 105



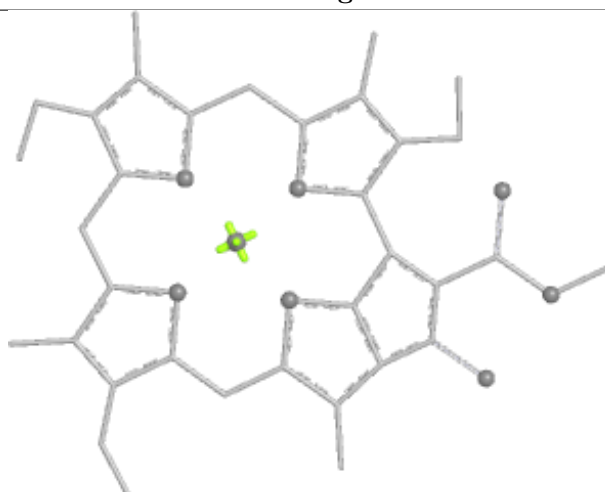
Bond lengths



Bond angles

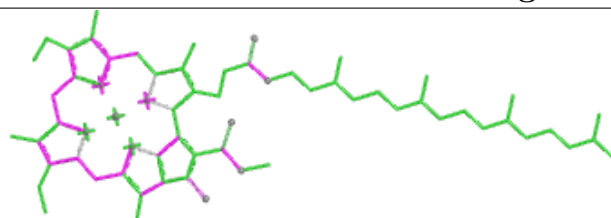


Torsions

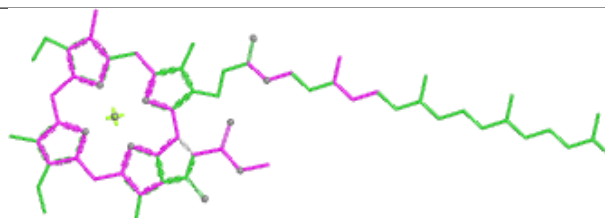


Rings

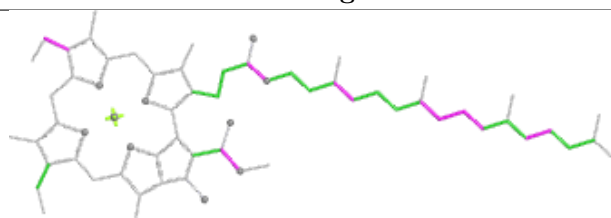
Ligand CLA a 319



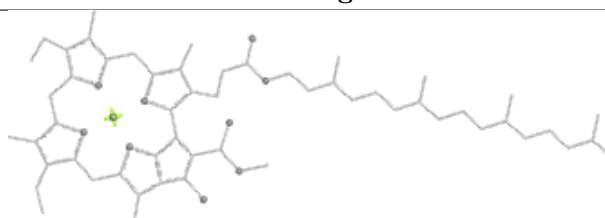
Bond lengths



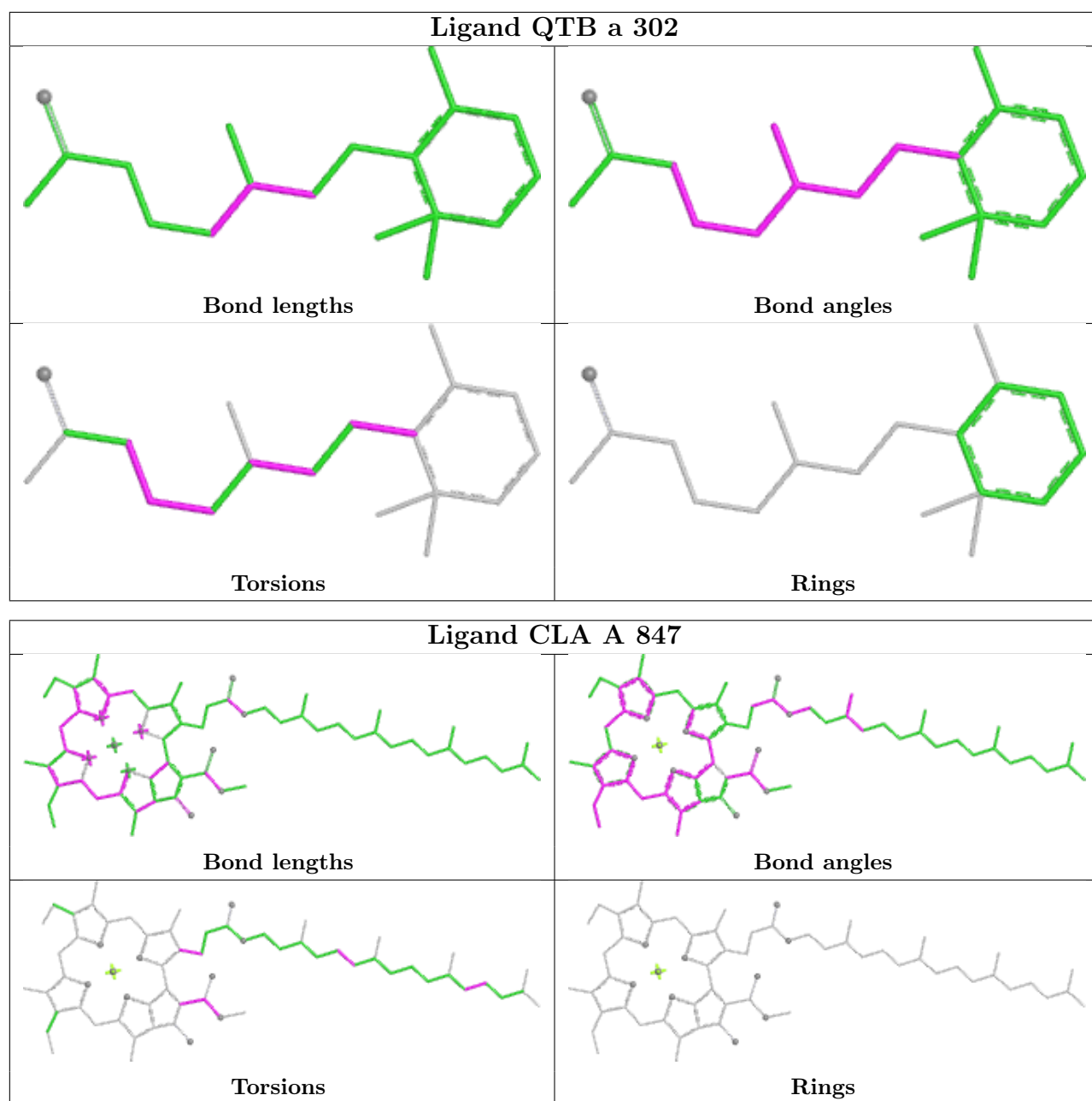
Bond angles



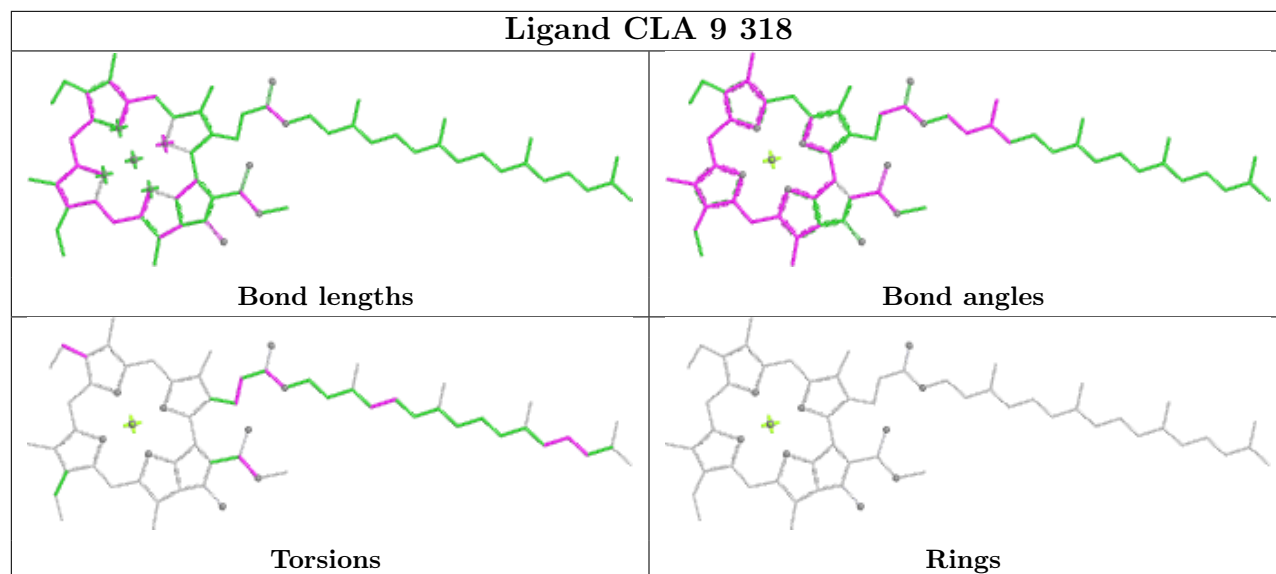
Torsions



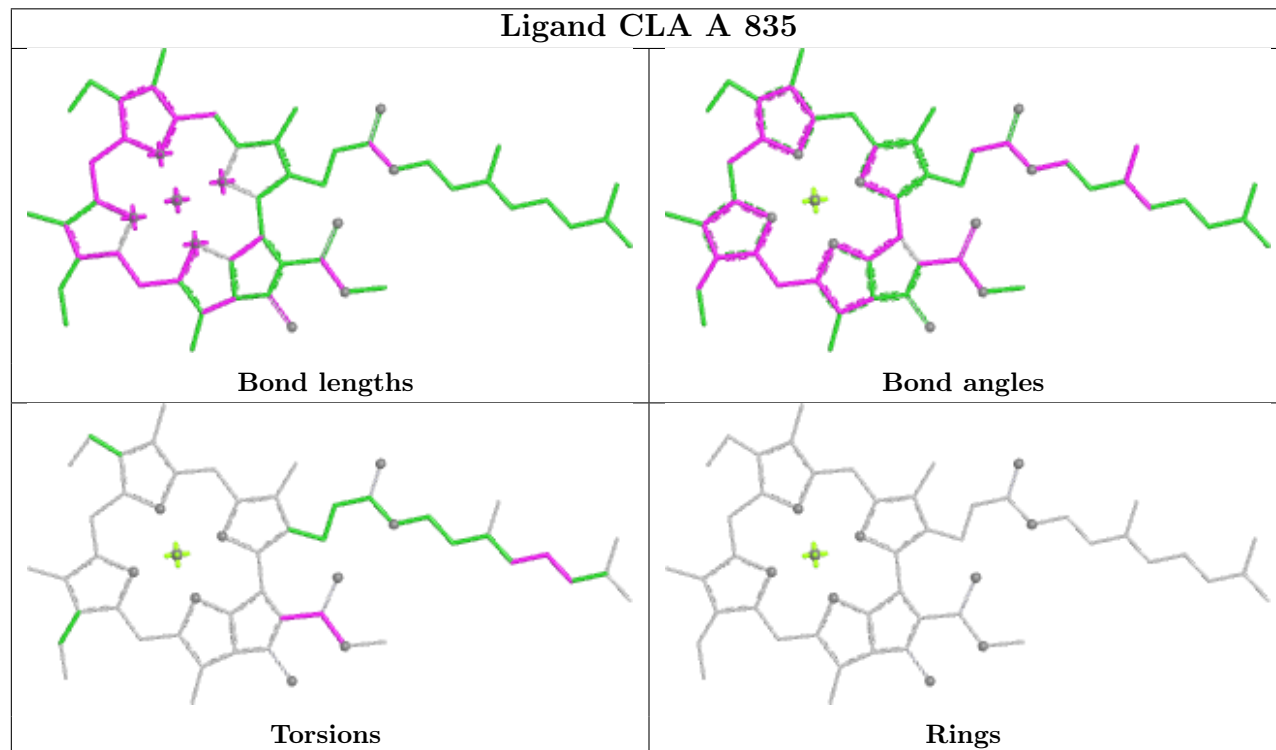
Rings

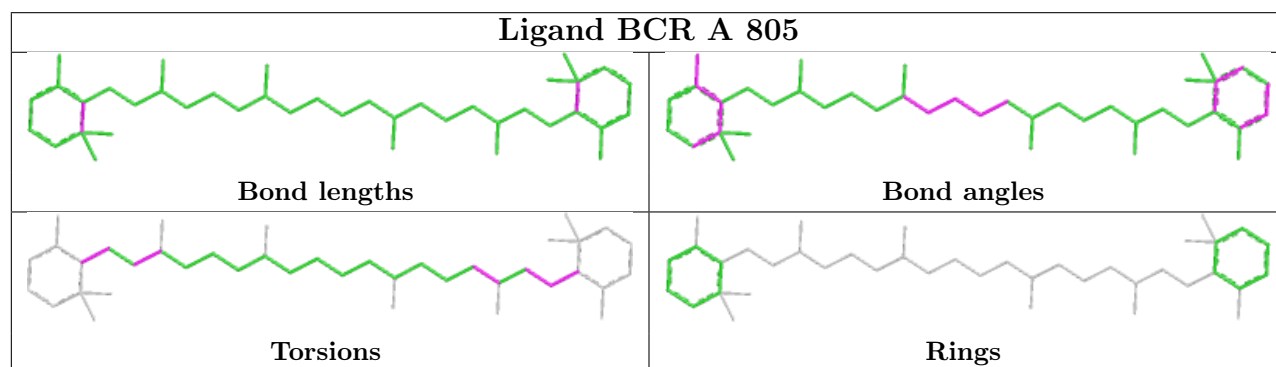
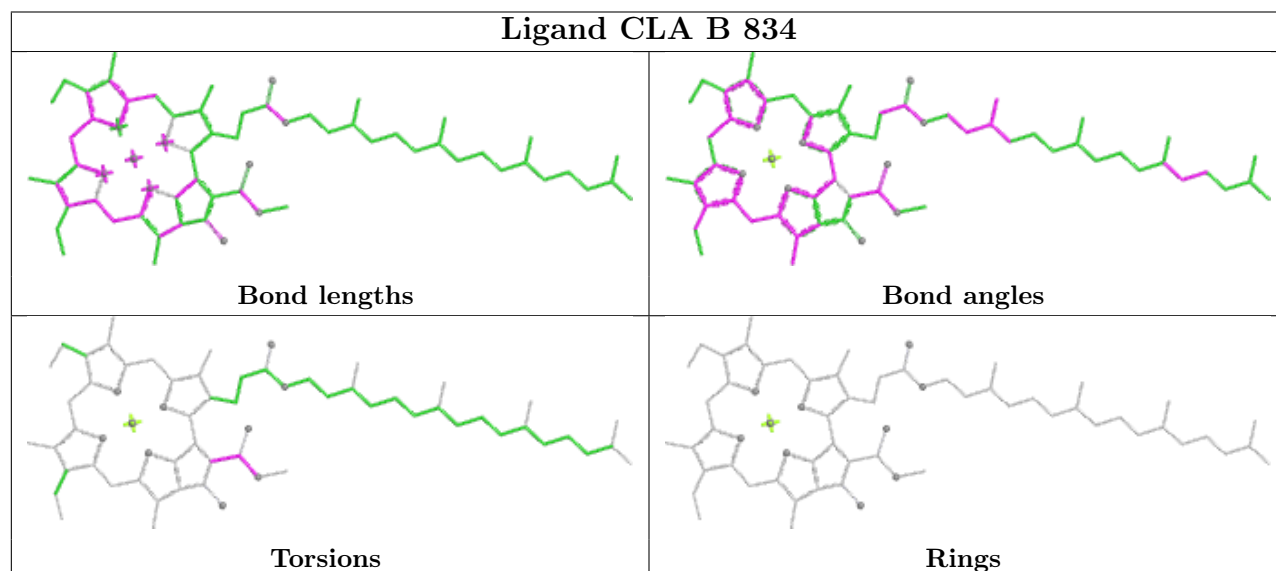
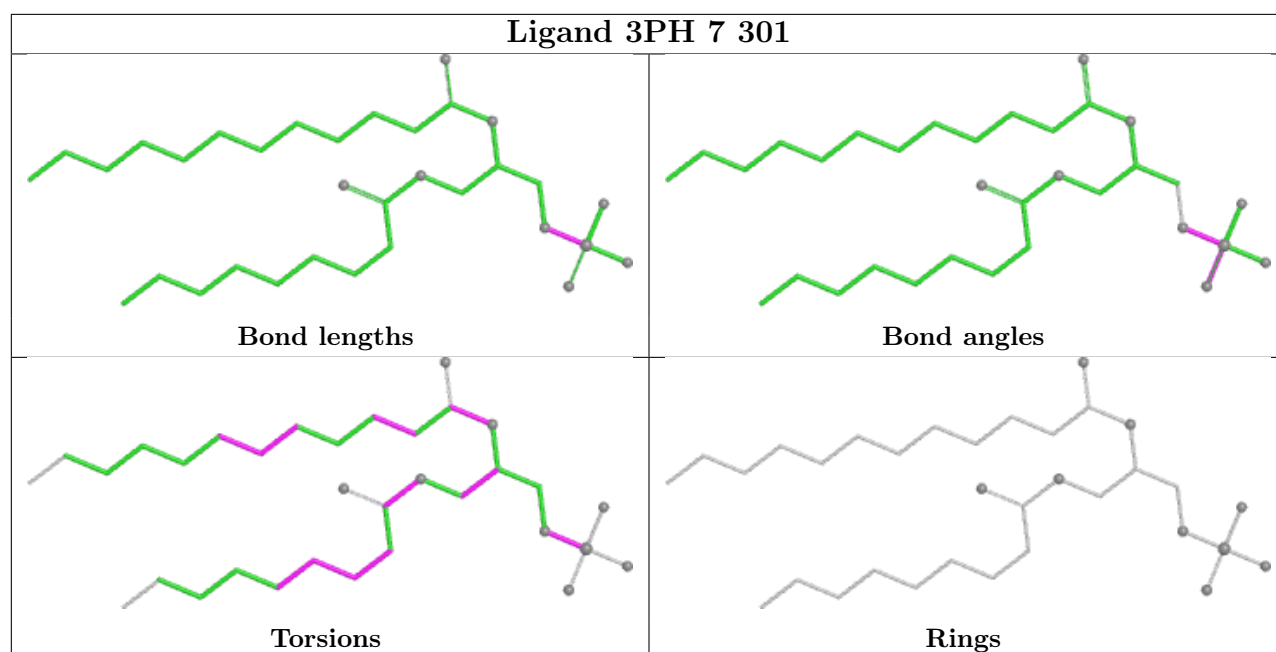


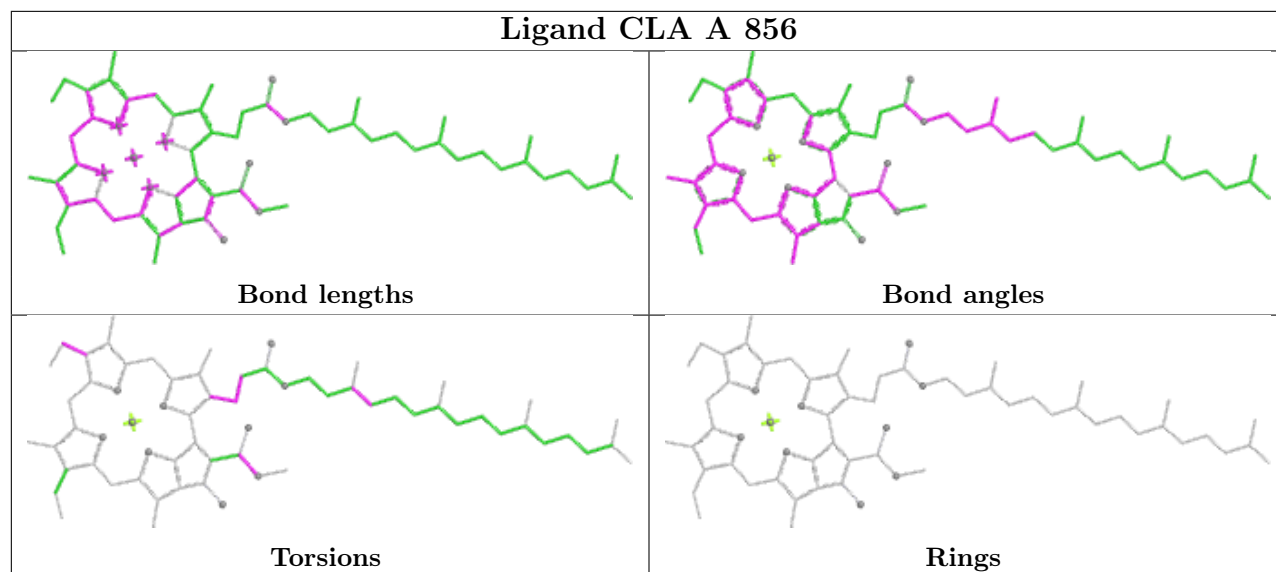
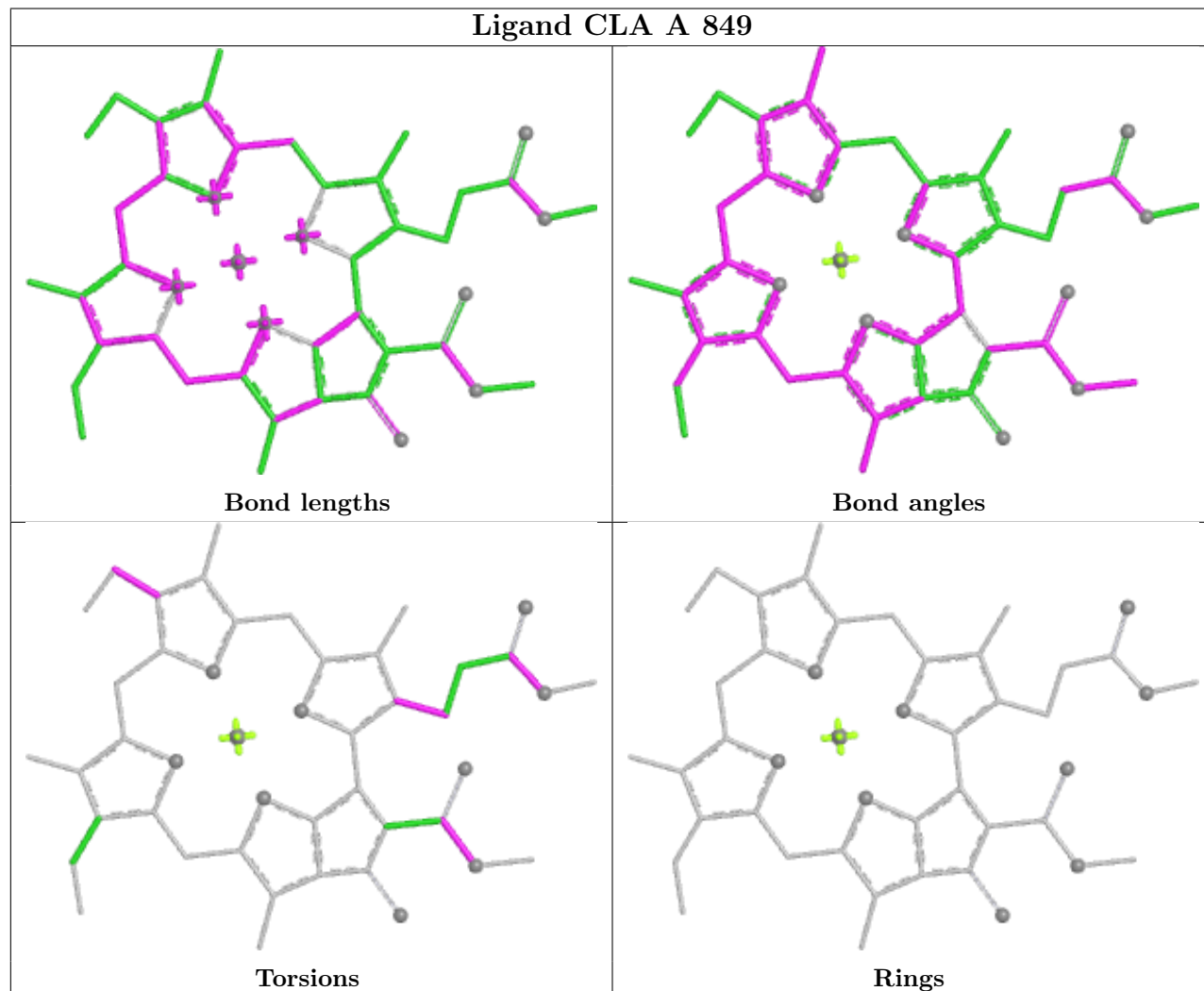
Ligand CLA 9 318

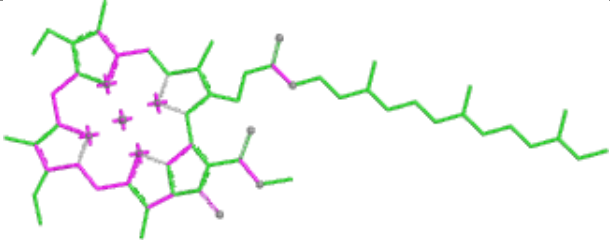
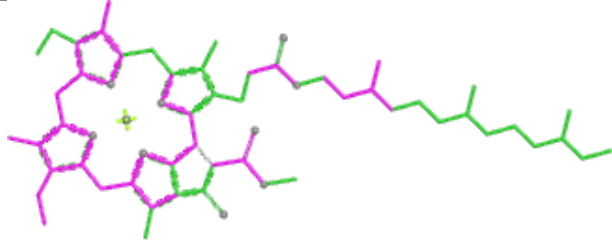
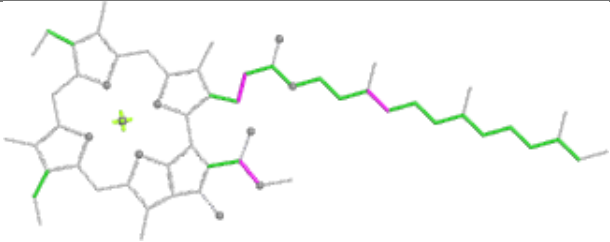
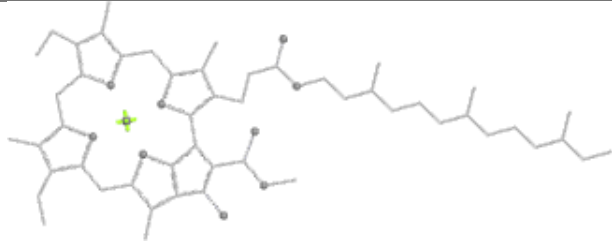
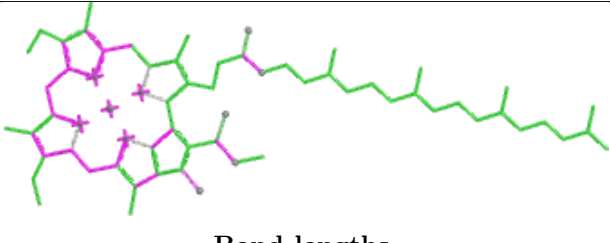
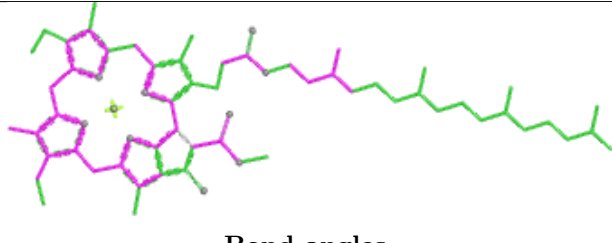
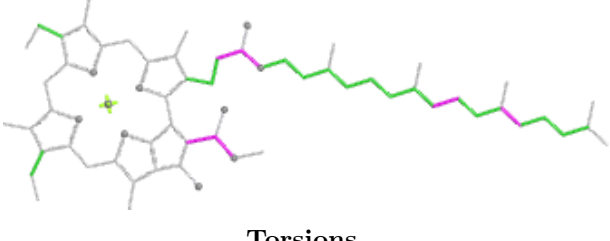
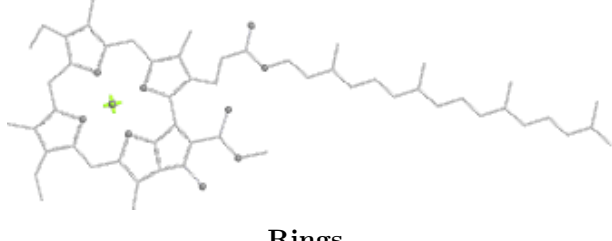
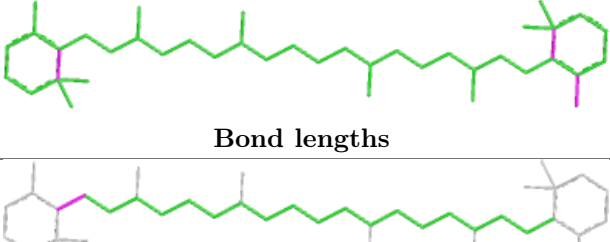
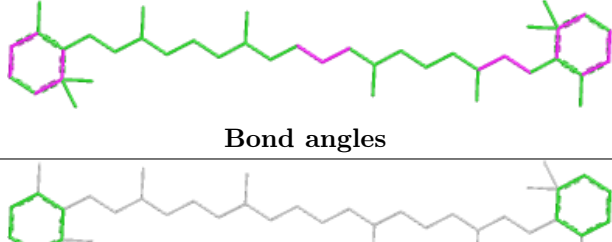
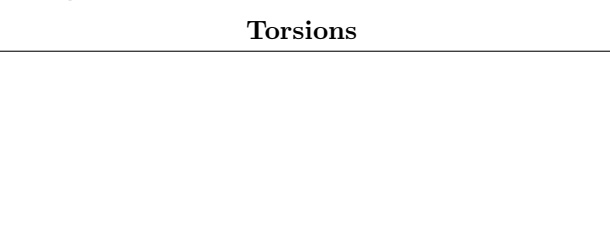
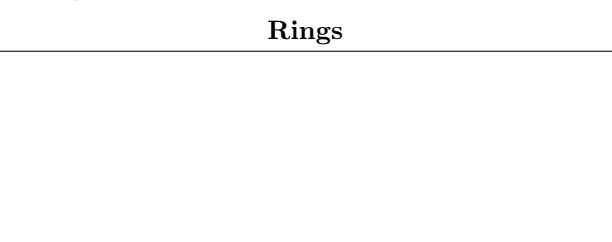


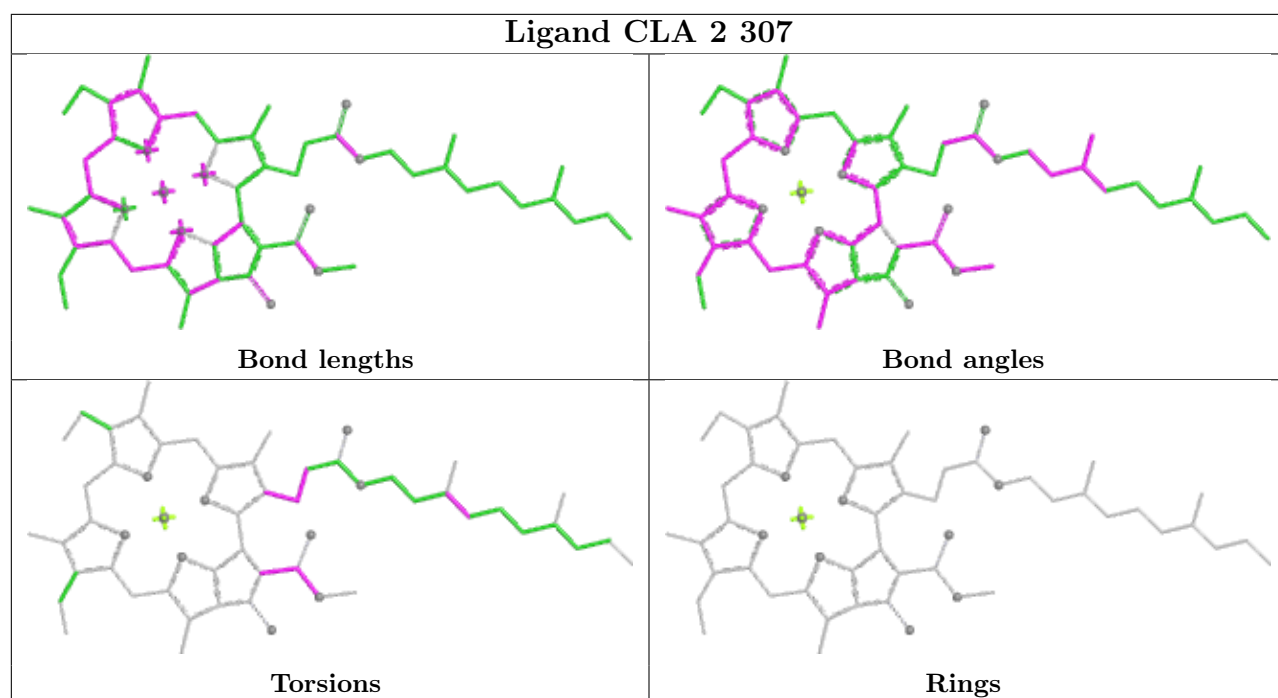
Ligand CLA A 835



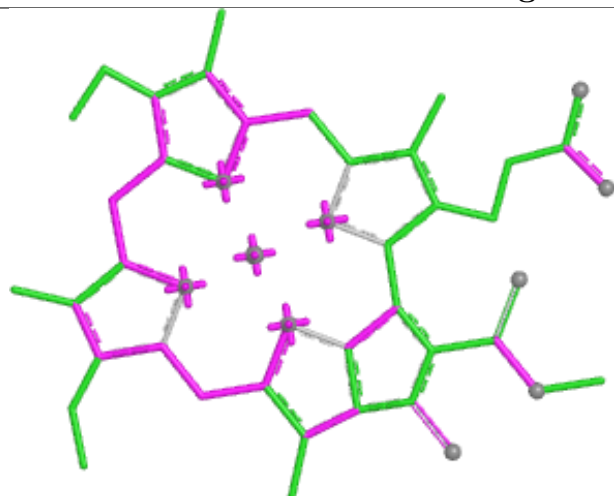


Ligand CLA A 856**Ligand CLA A 849**

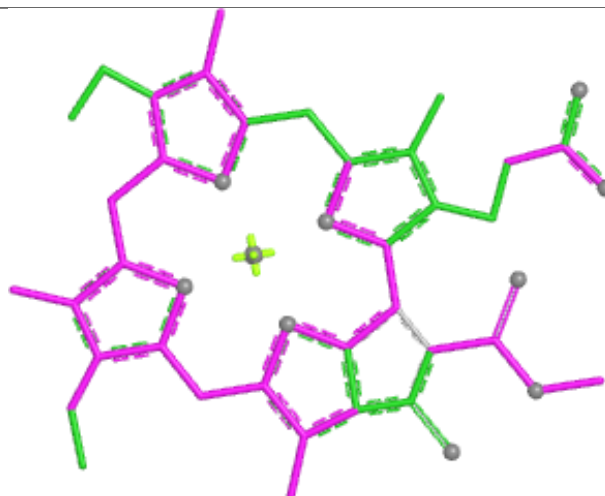
Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR O 201	
 Bond lengths	 Bond angles
 Torsions	 Rings



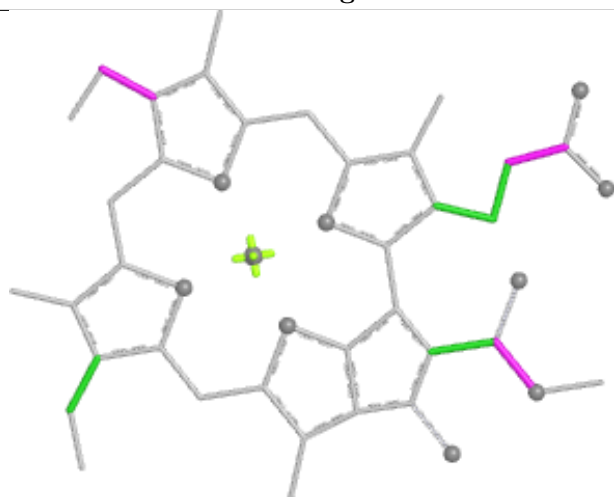
Ligand CLA 4 314



Bond lengths



Bond angles

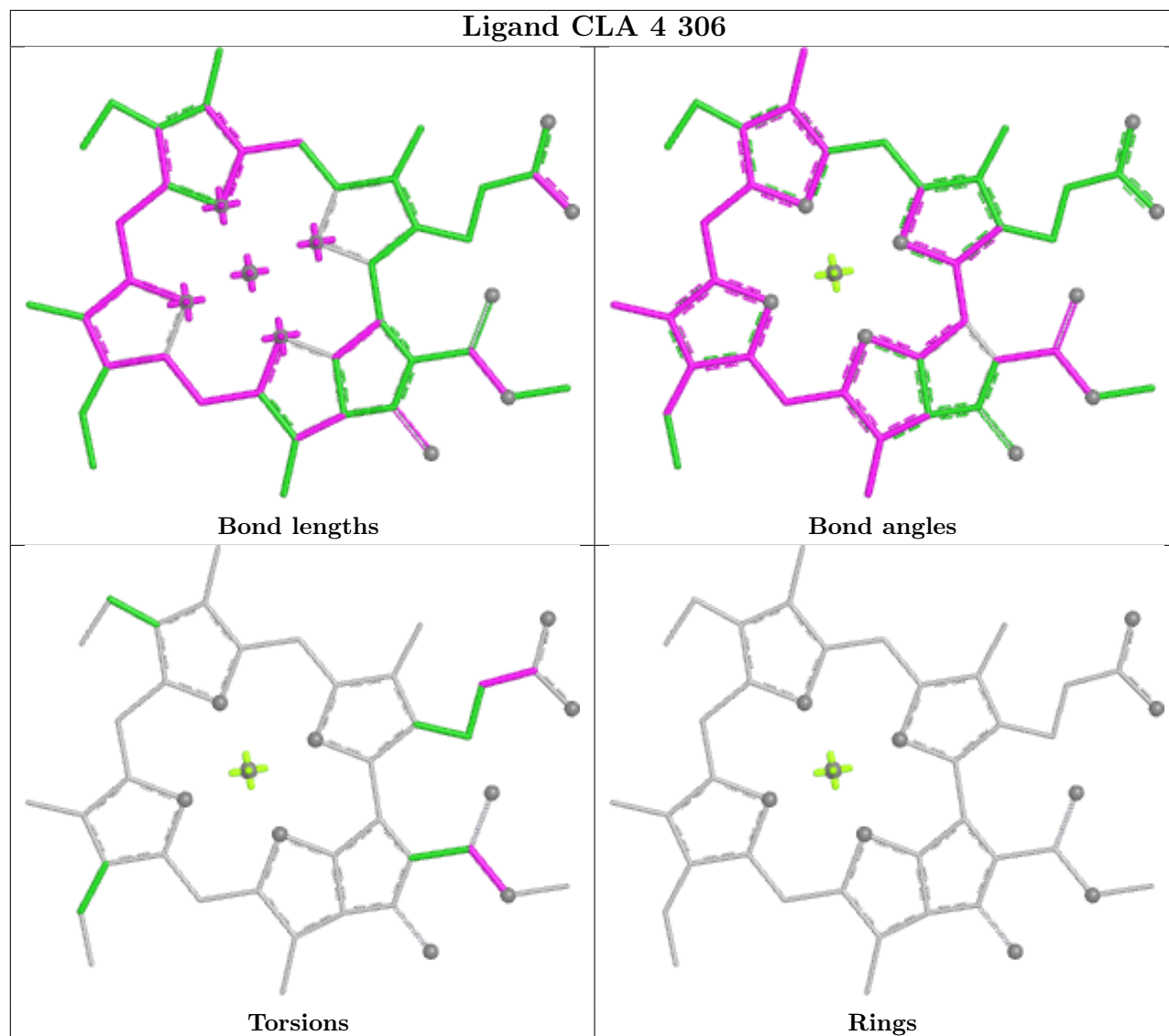


Torsions

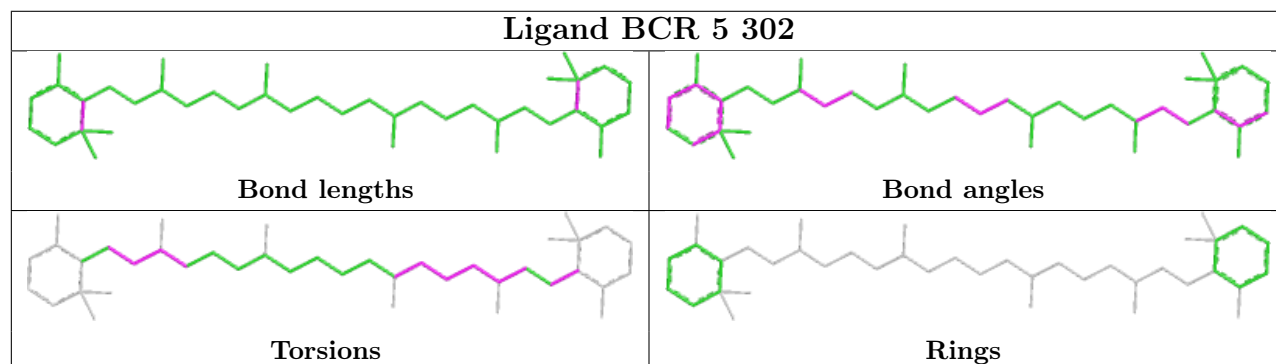


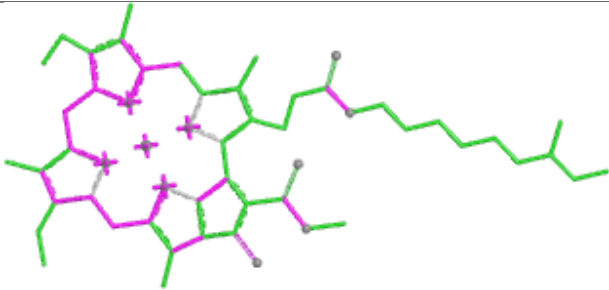
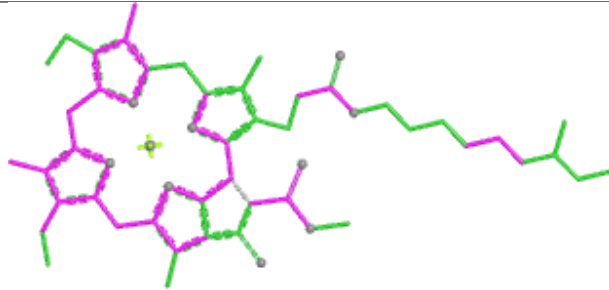
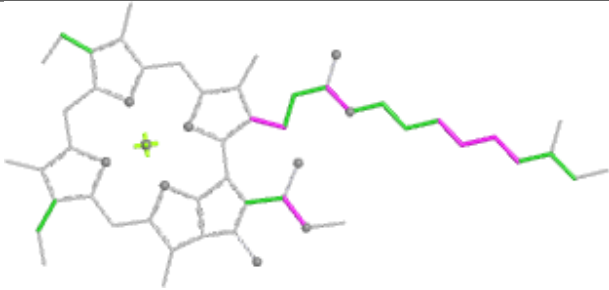
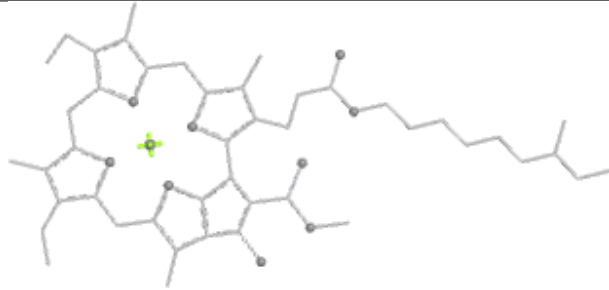
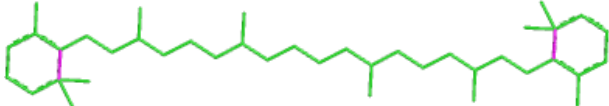
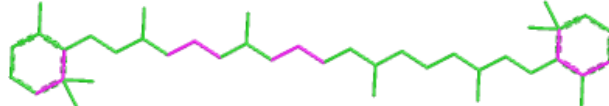
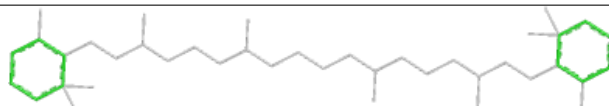
Rings

Ligand CLA 4 306

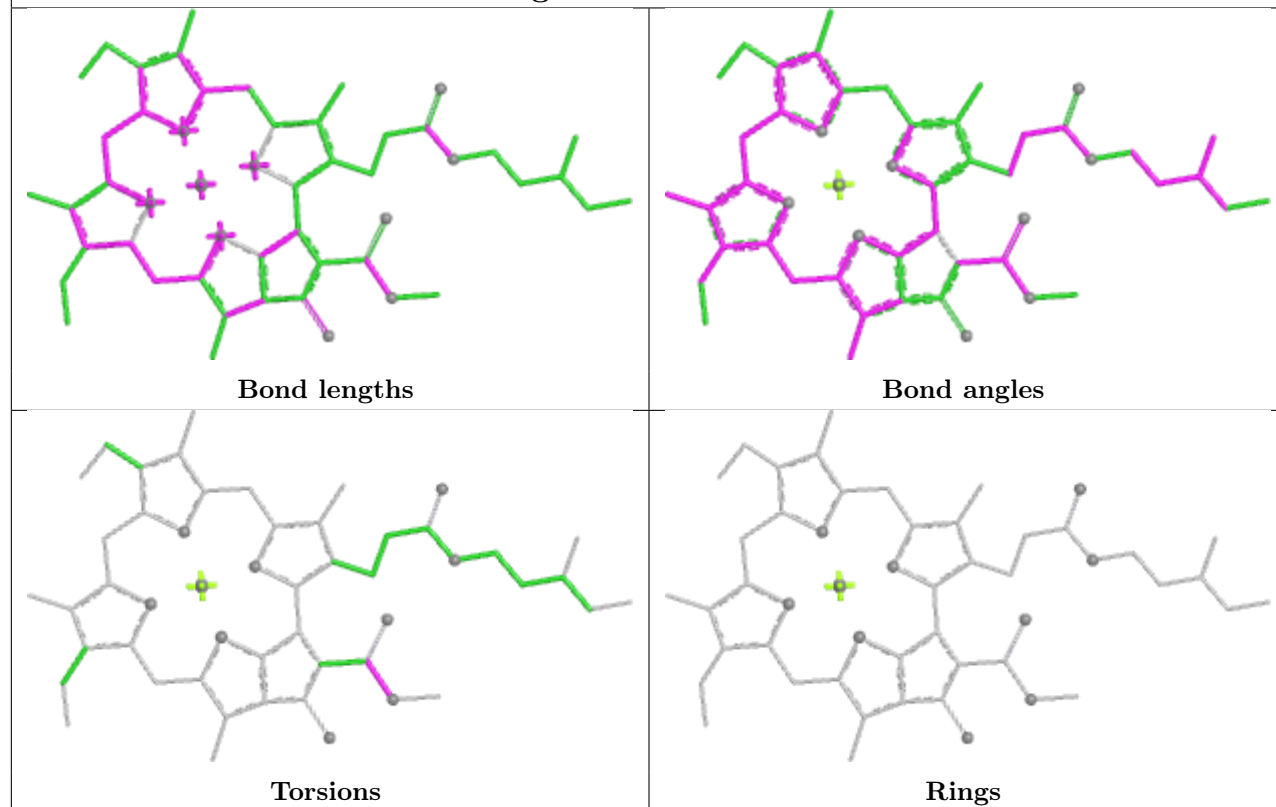


Ligand BCR 5 302

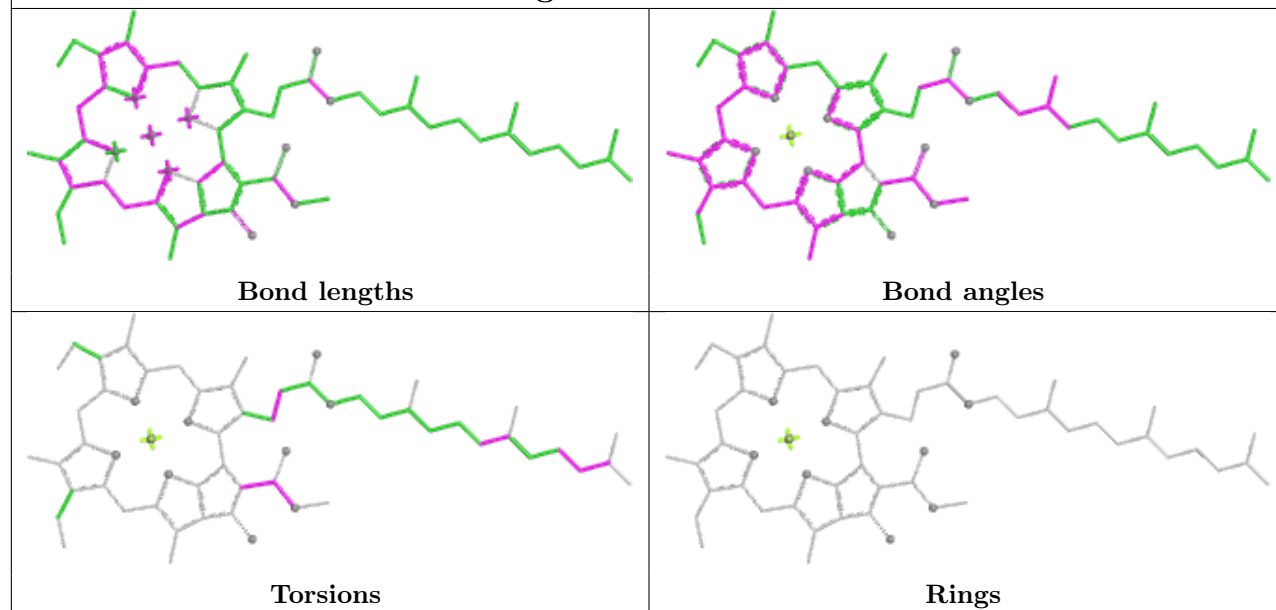


Ligand CLA 7 315	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

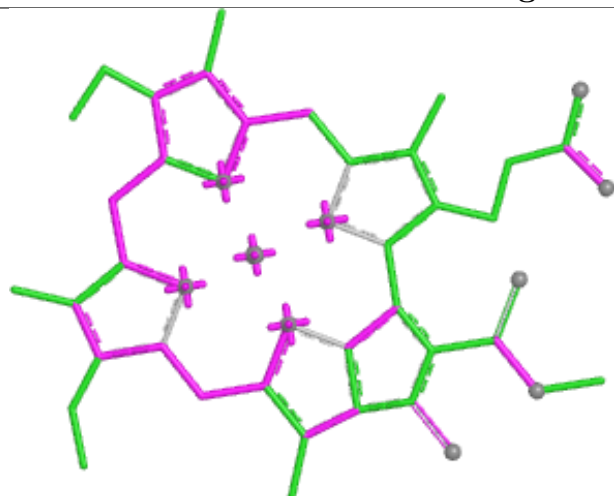
Ligand CLA A 852



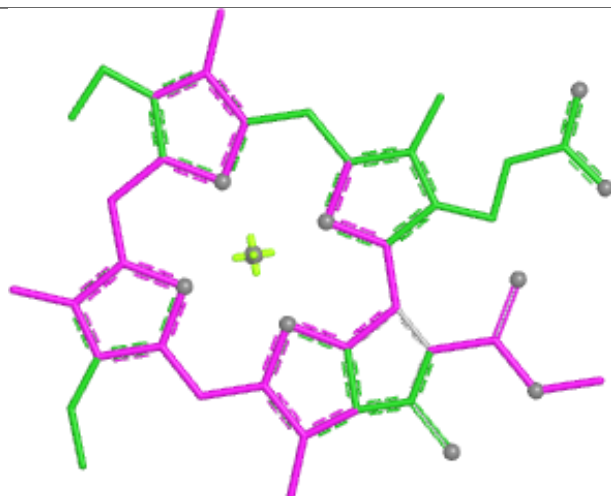
Ligand CLA 9 314



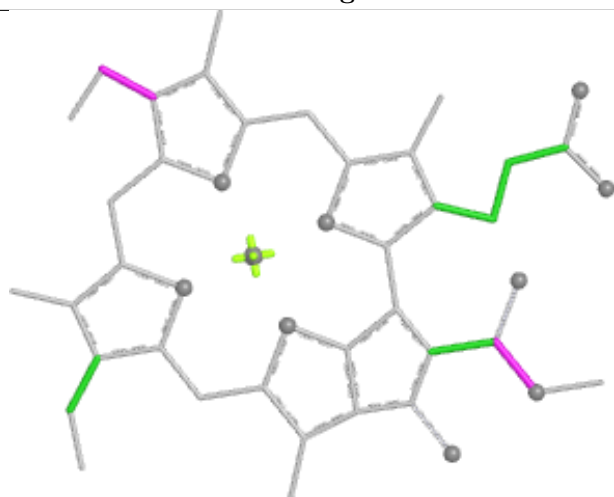
Ligand CLA 3 320



Bond lengths



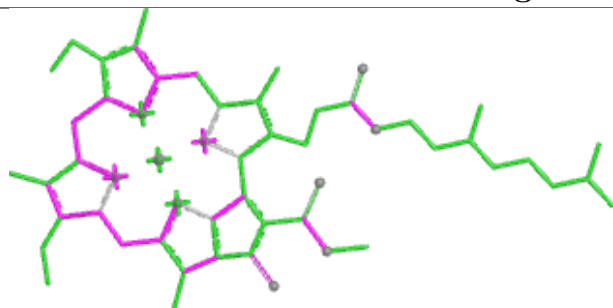
Bond angles



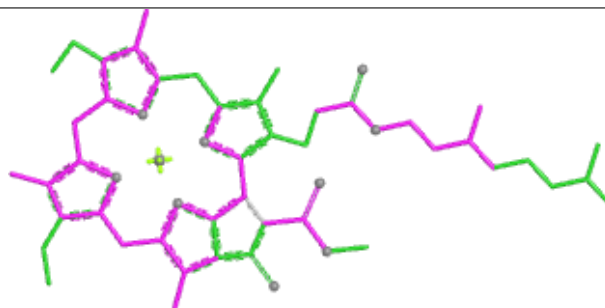
Torsions



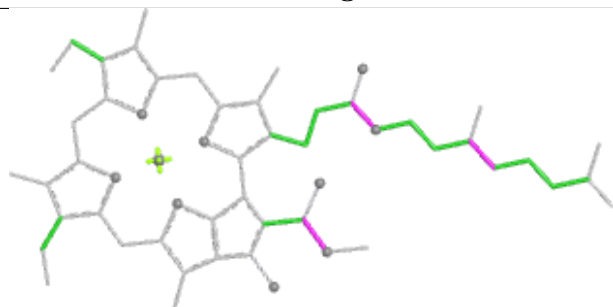
Rings

Ligand CLA B 829

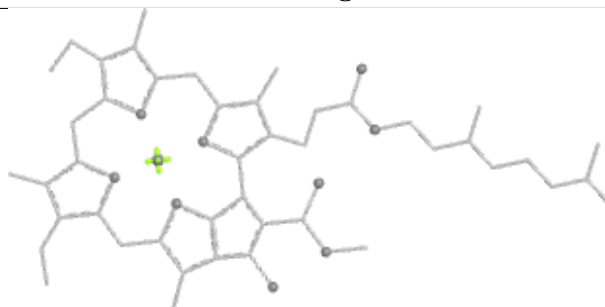
Bond lengths



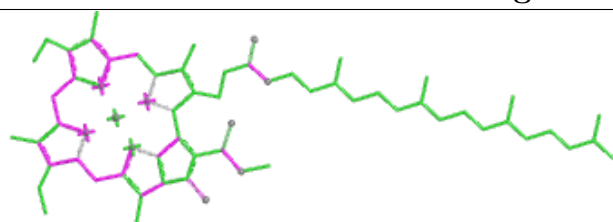
Bond angles



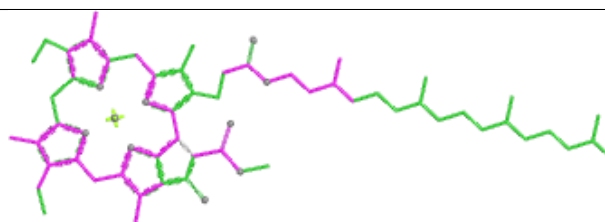
Torsions



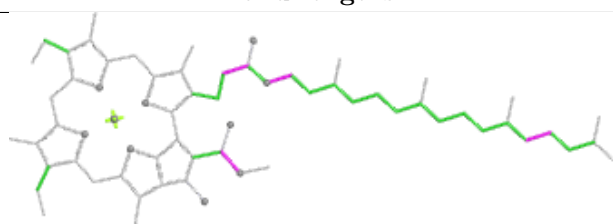
Rings

Ligand CLA A 816

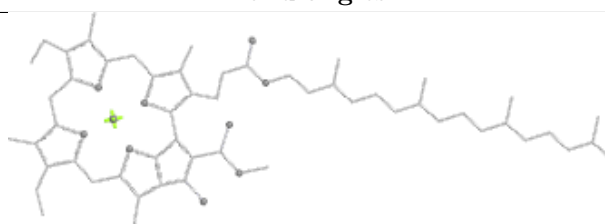
Bond lengths



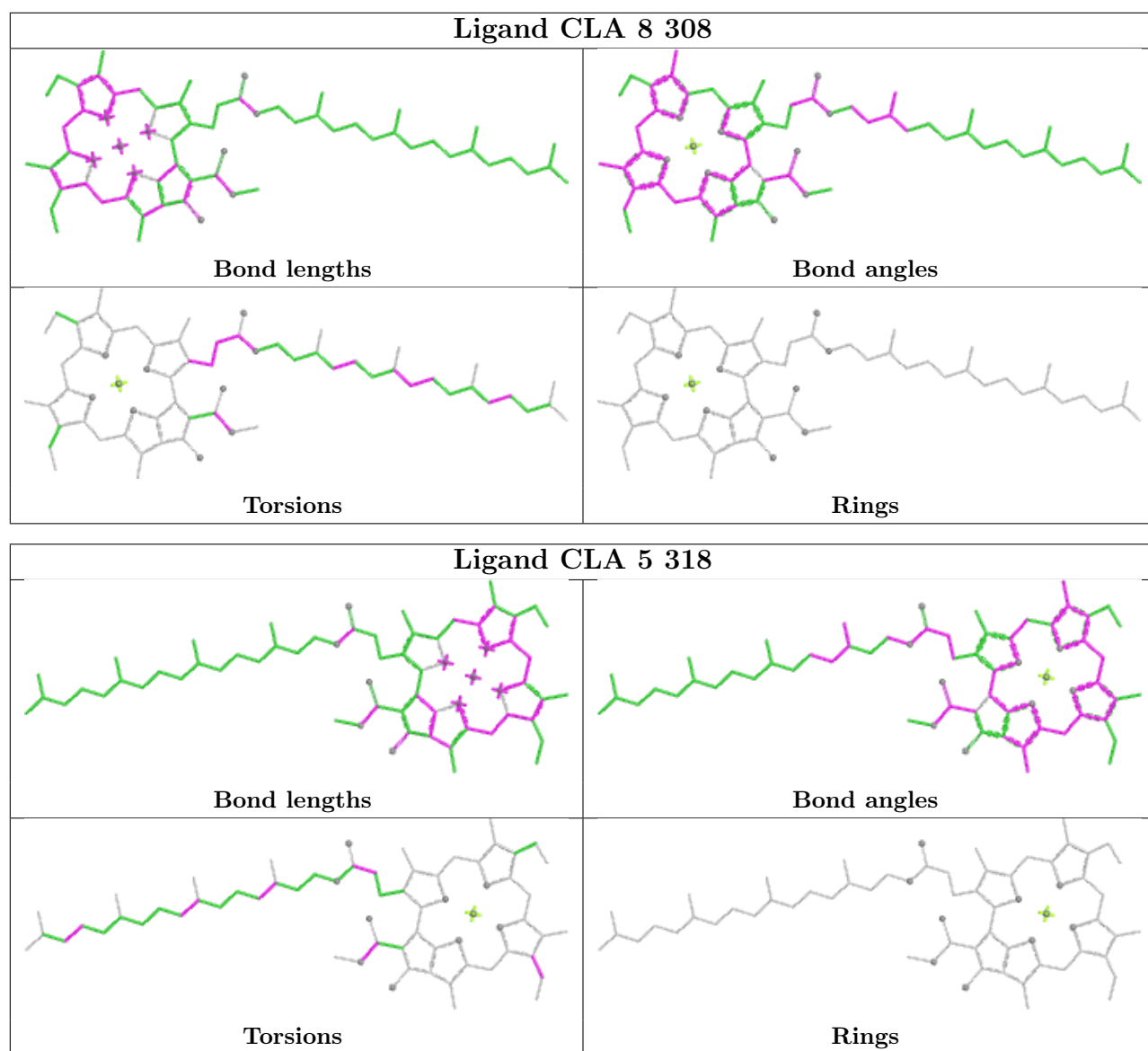
Bond angles



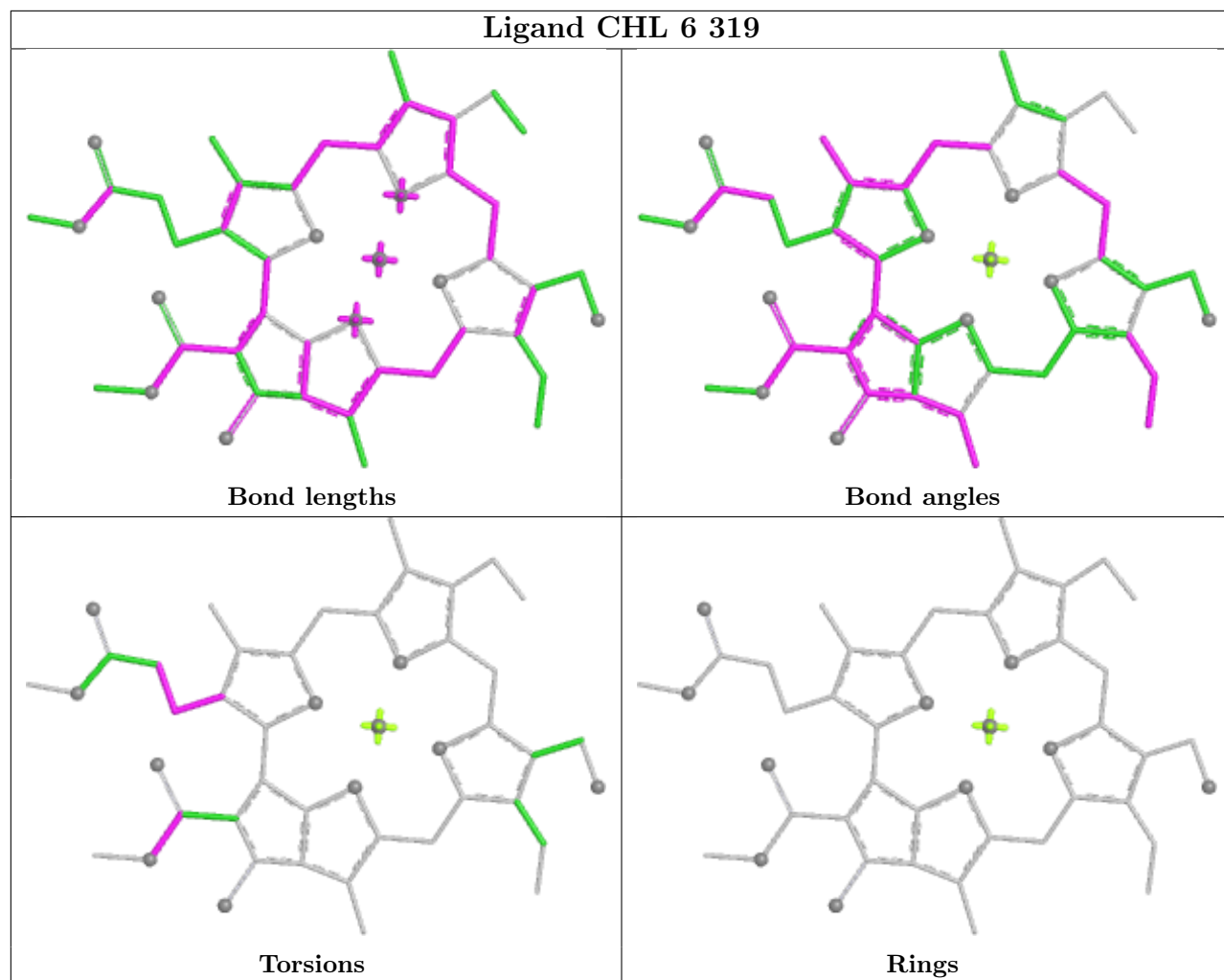
Torsions



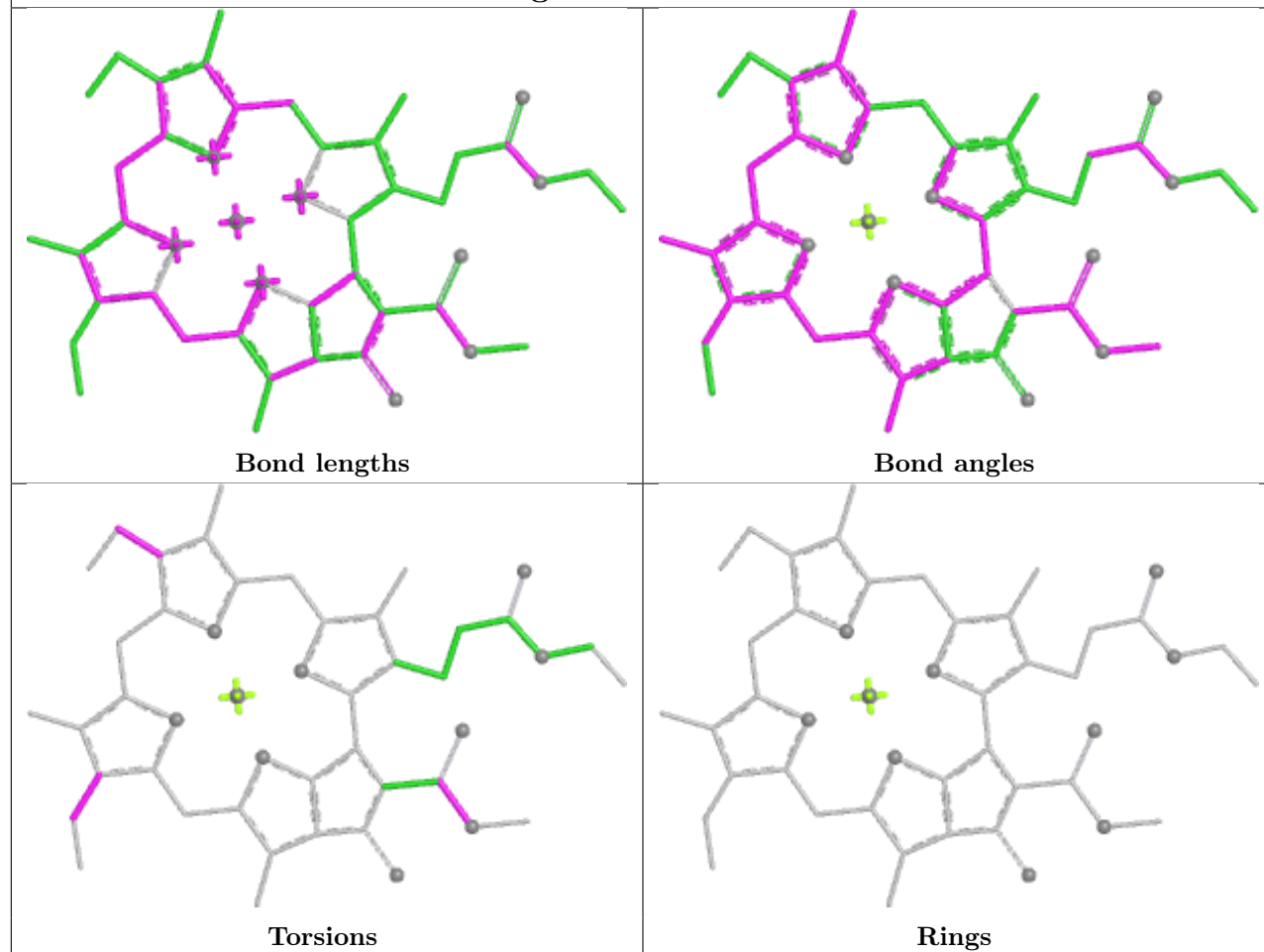
Rings



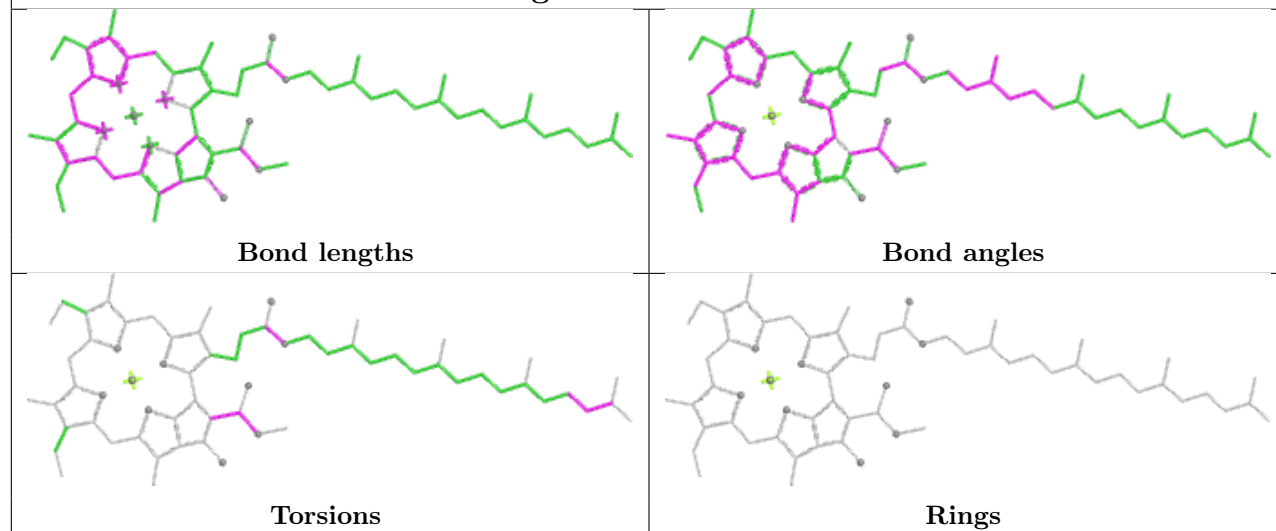
Ligand CHL 6 319

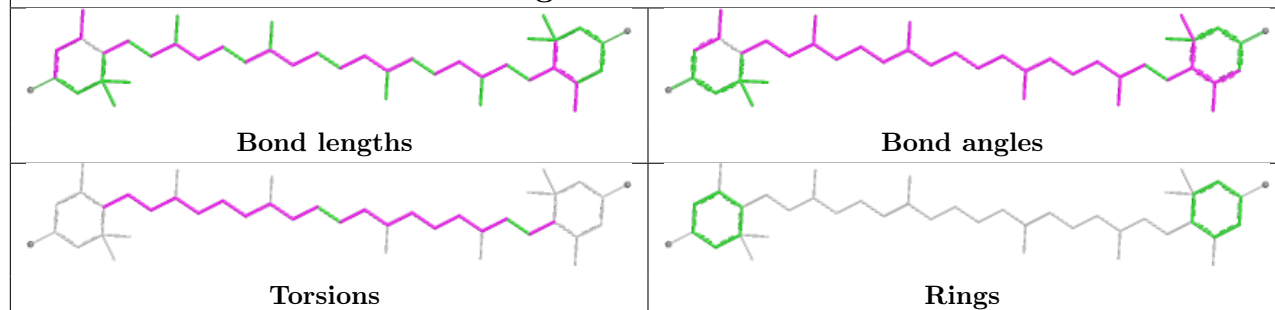
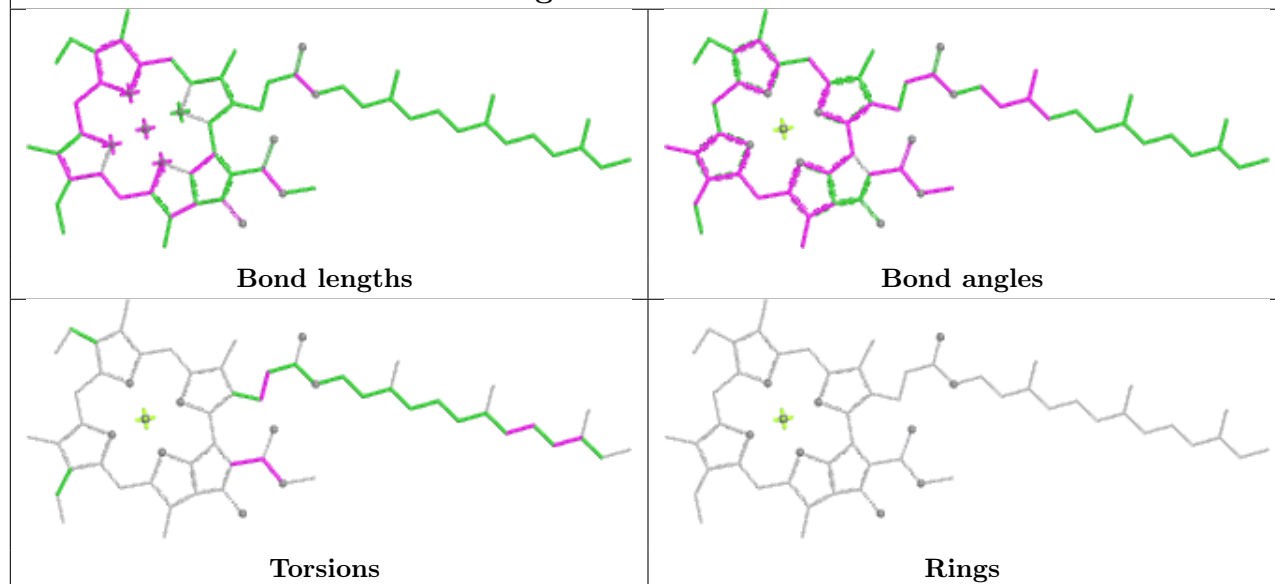
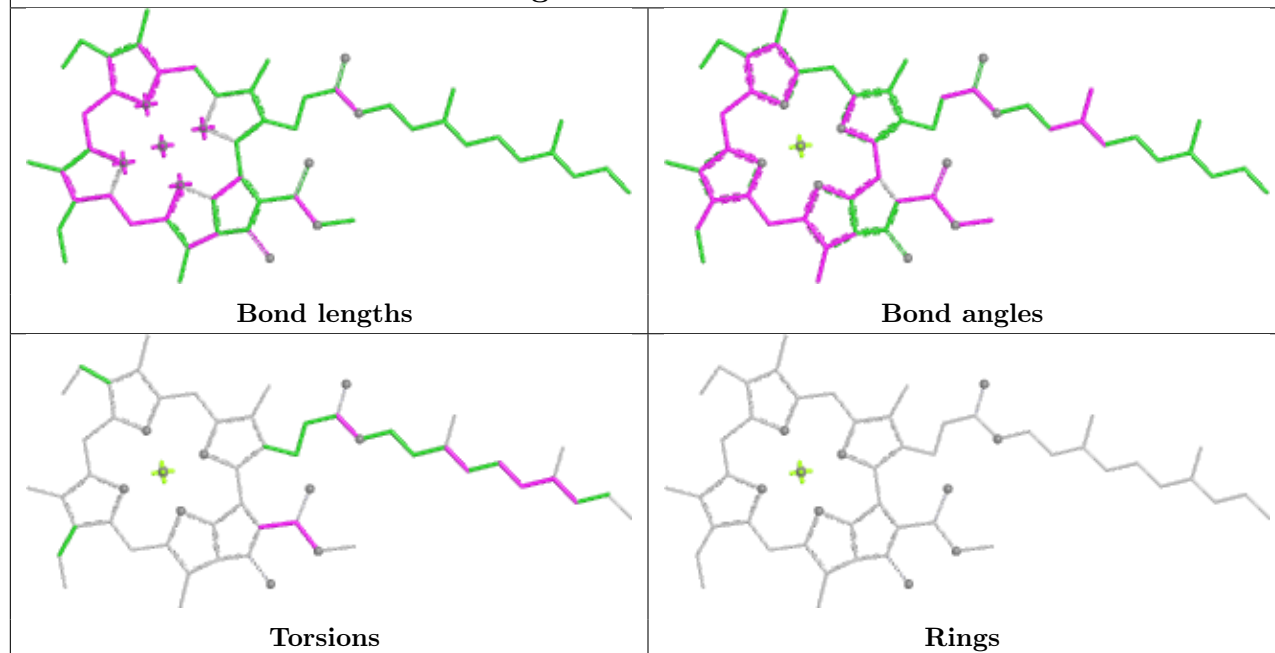


Ligand CLA 6 308

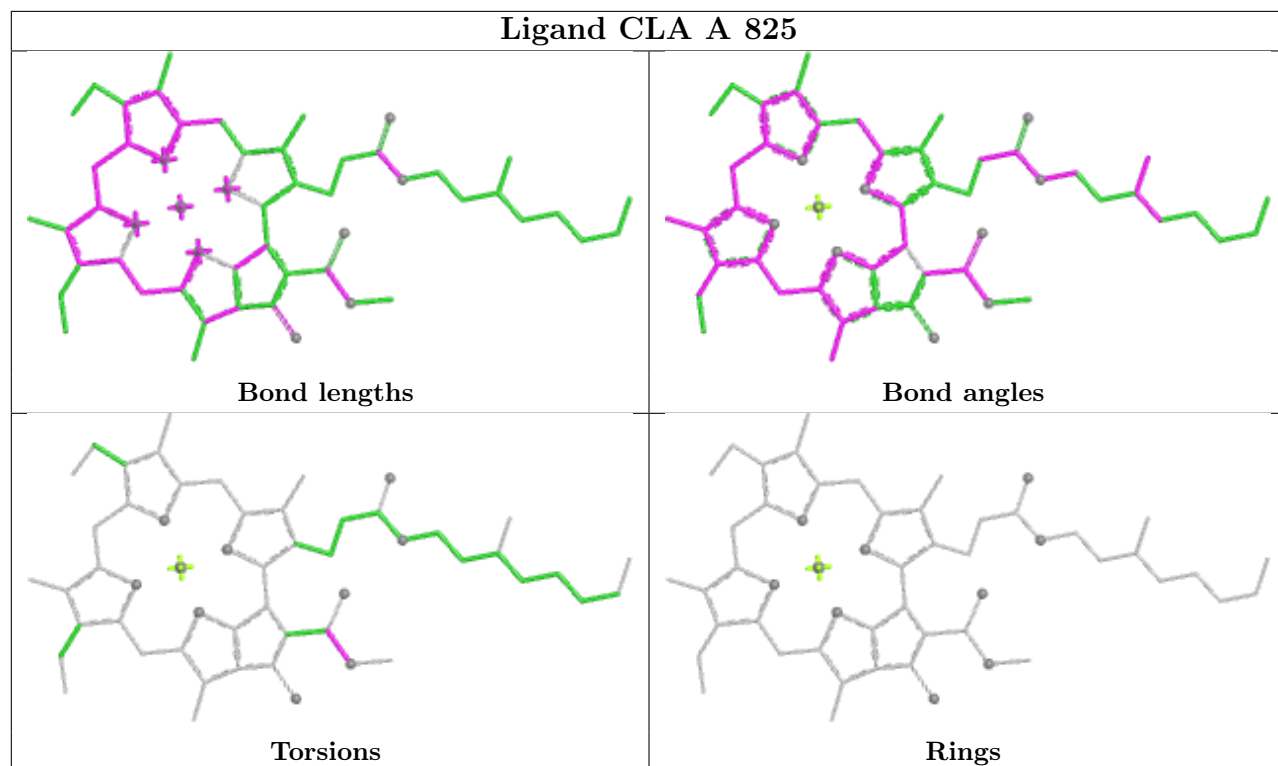


Ligand CLA A 828

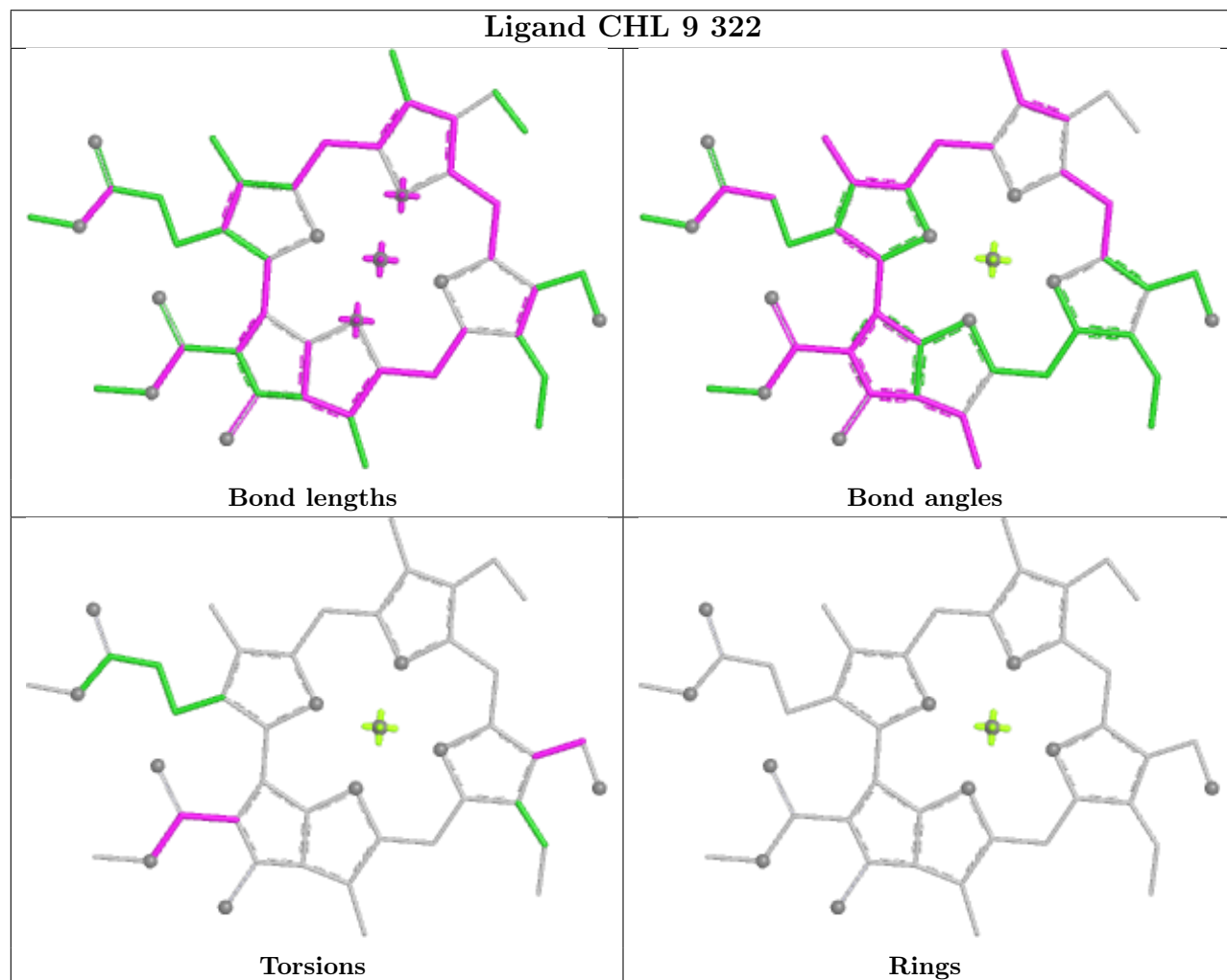


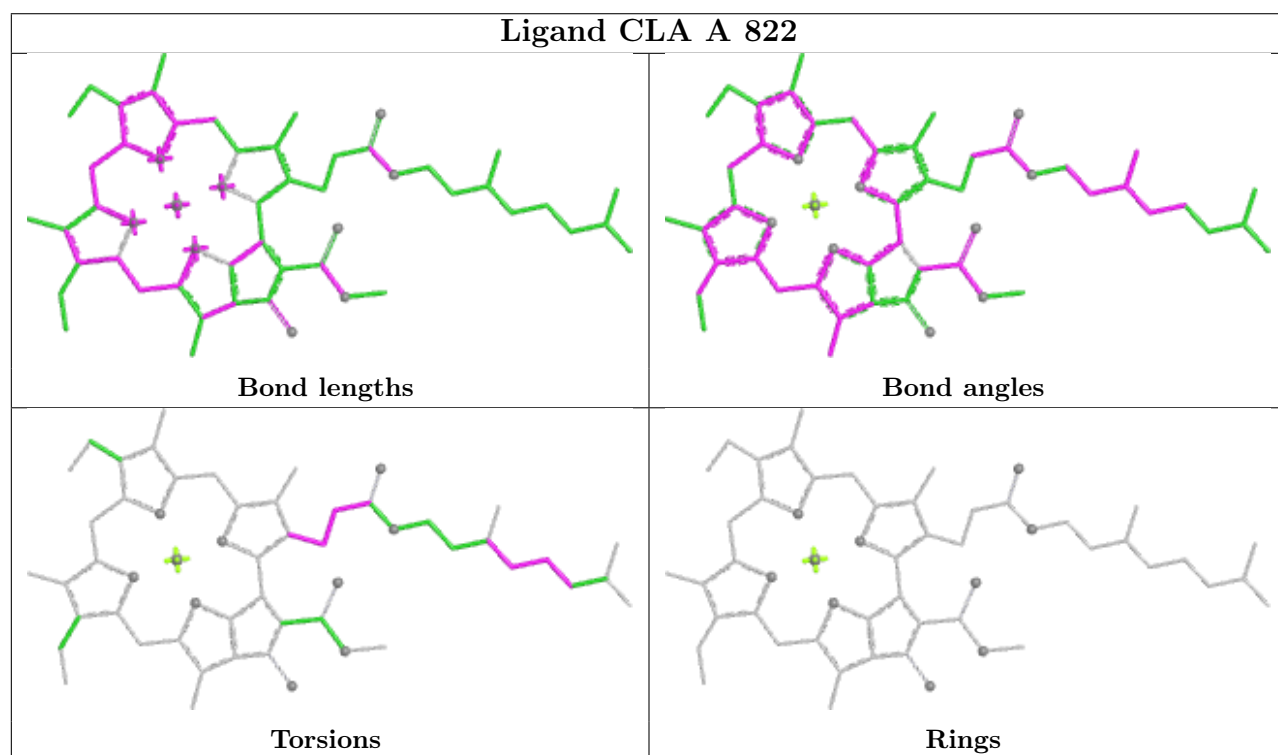
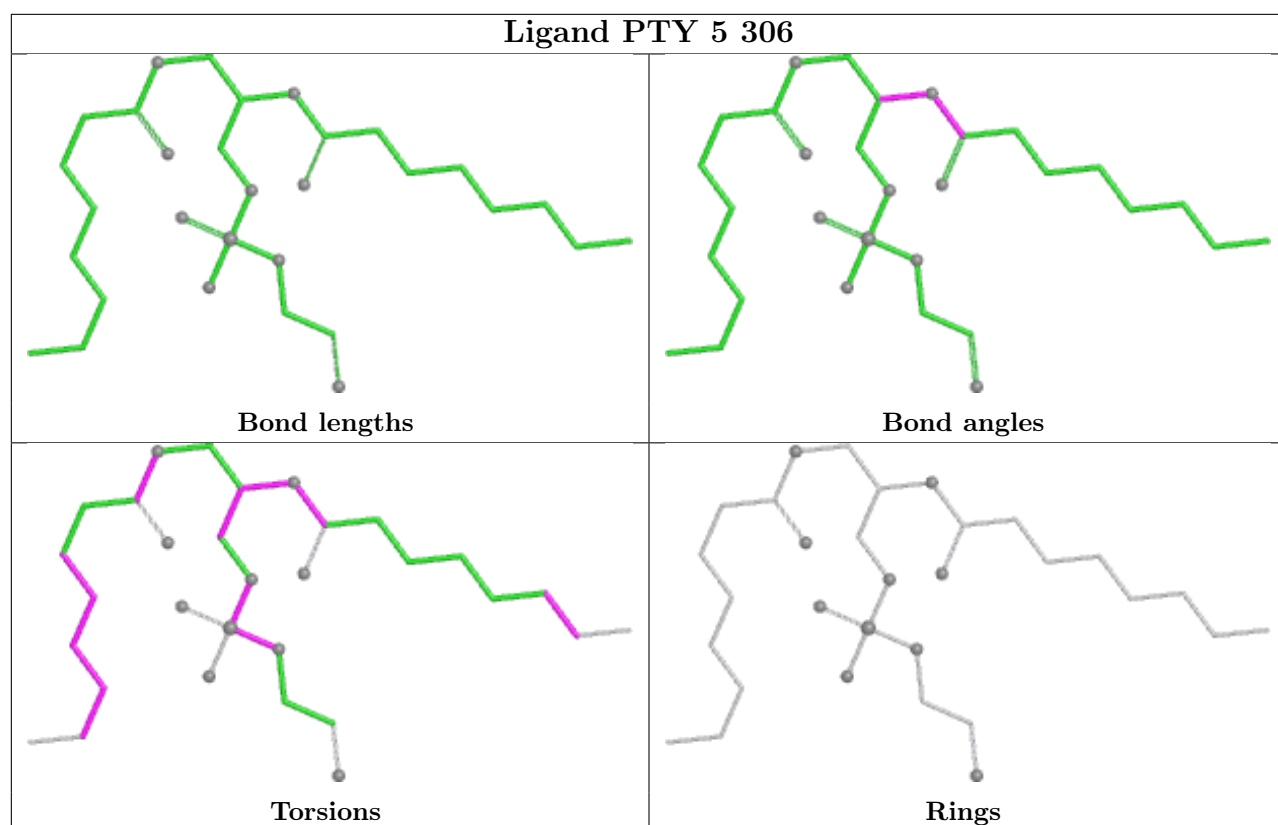
Ligand LUT a 305**Ligand CLA 3 319****Ligand CLA B 824**

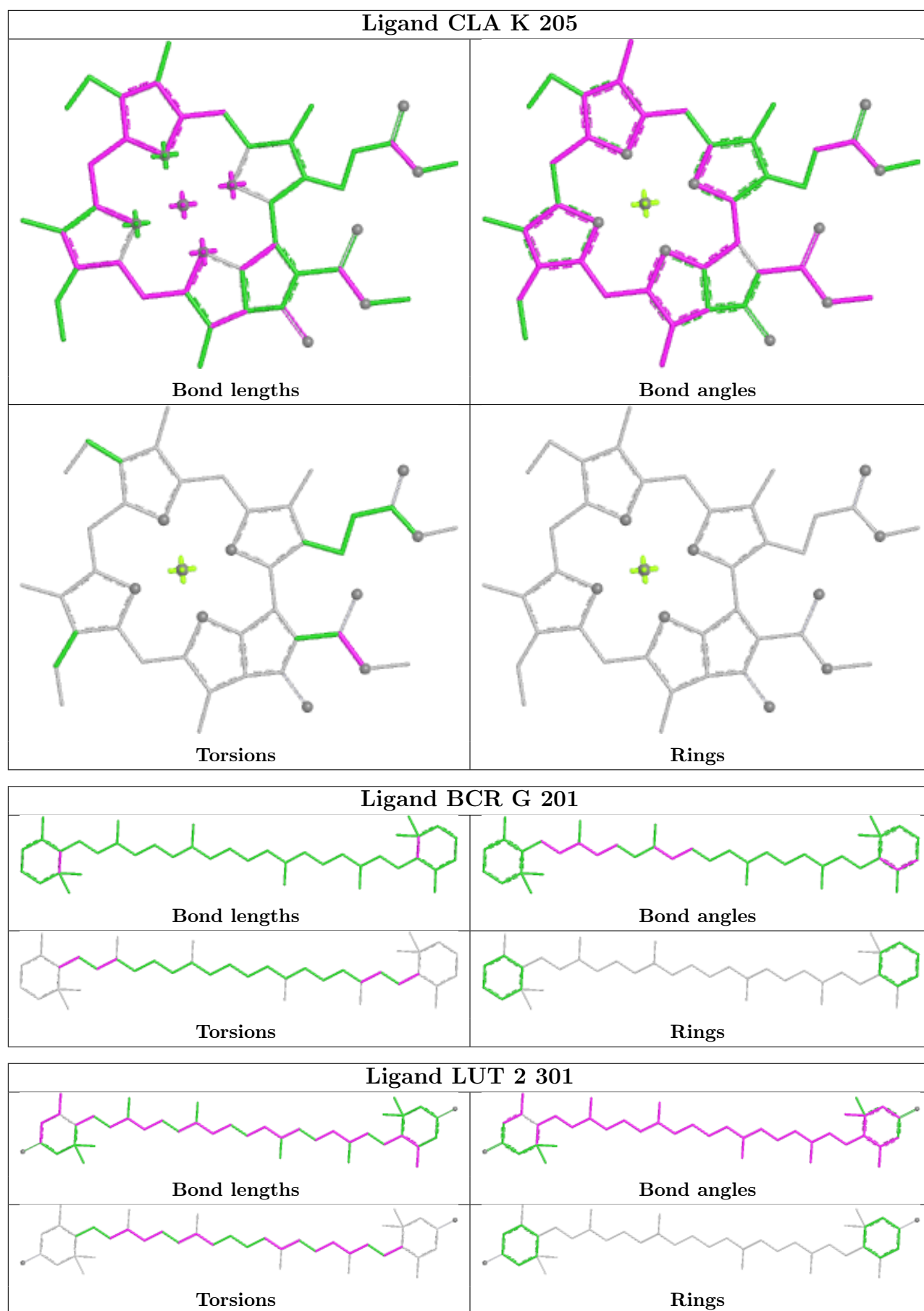
Ligand CLA A 825



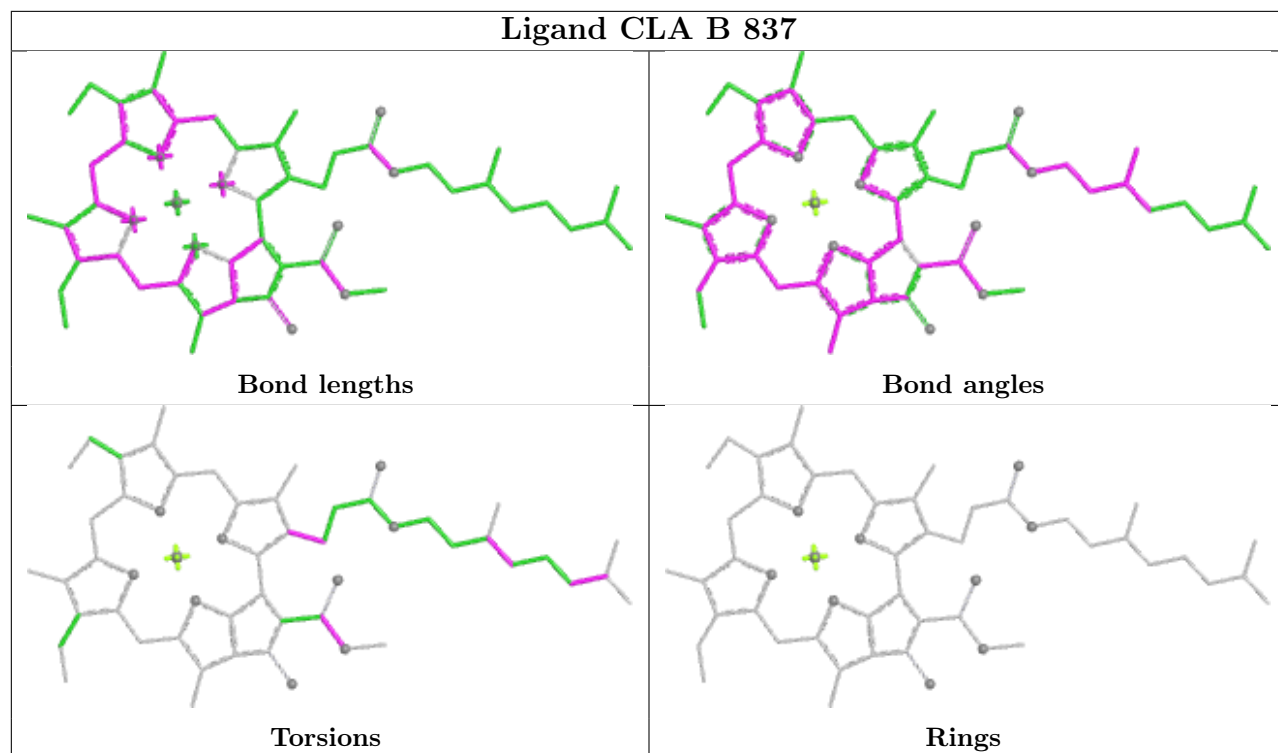
Ligand CHL 9 322



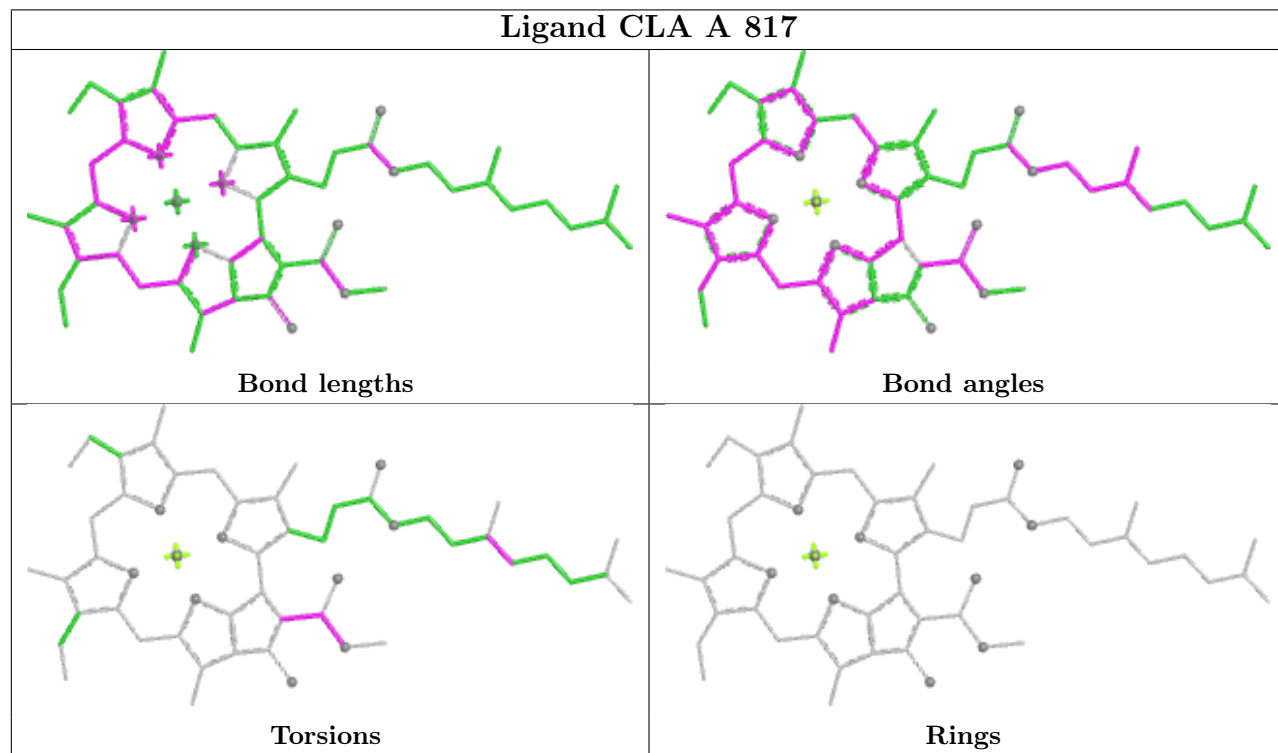




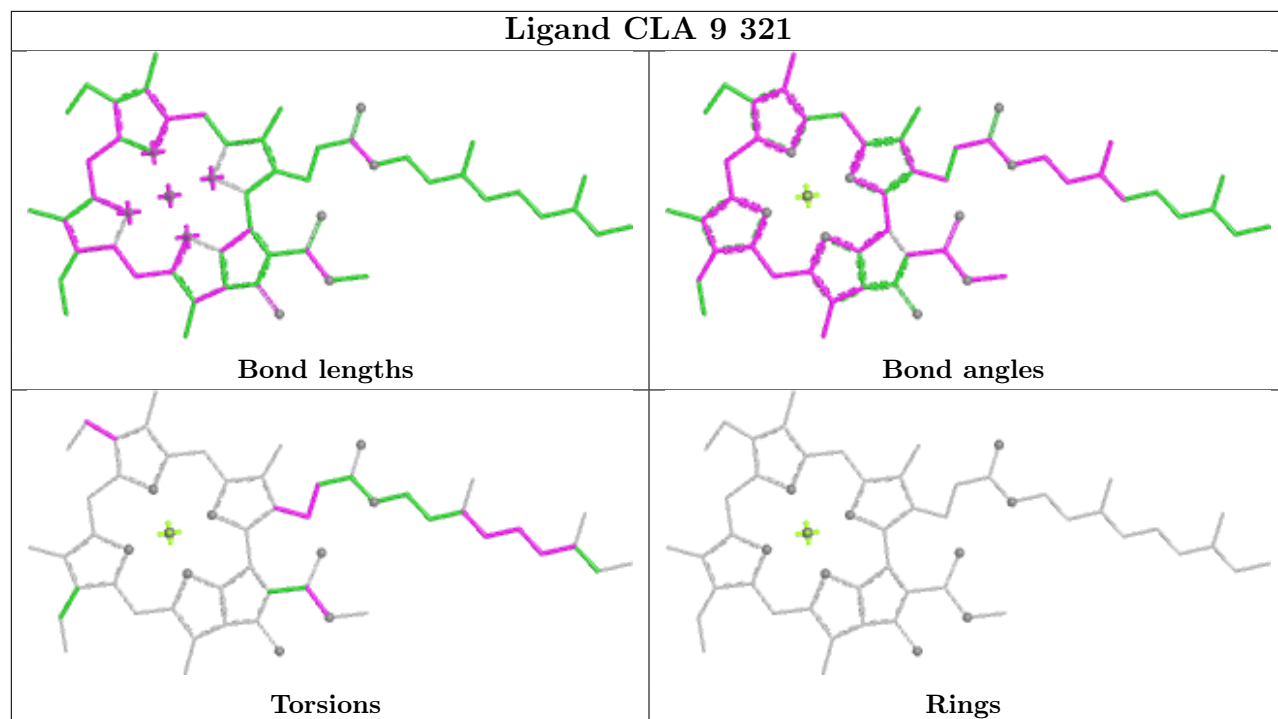
Ligand CLA B 837



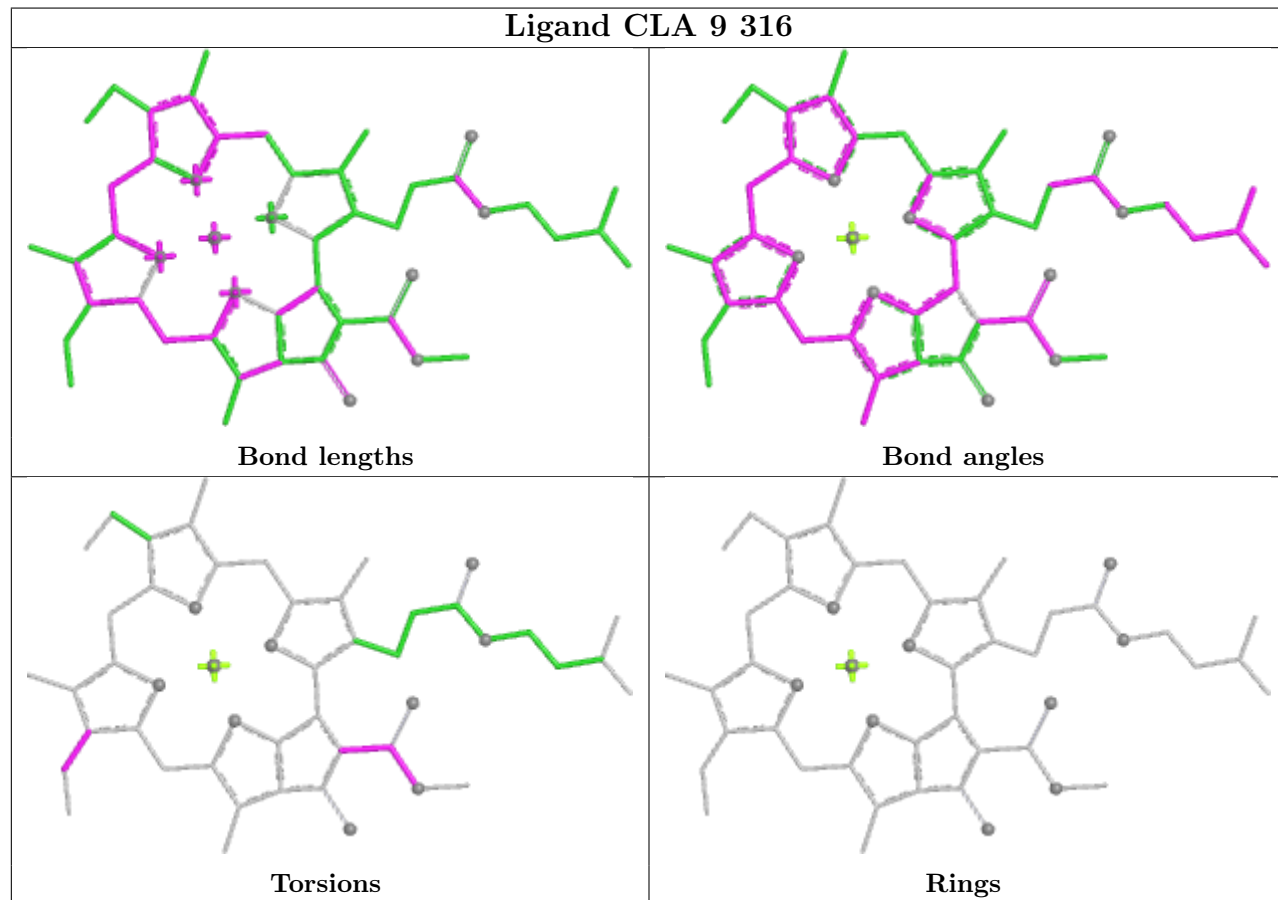
Ligand CLA A 817

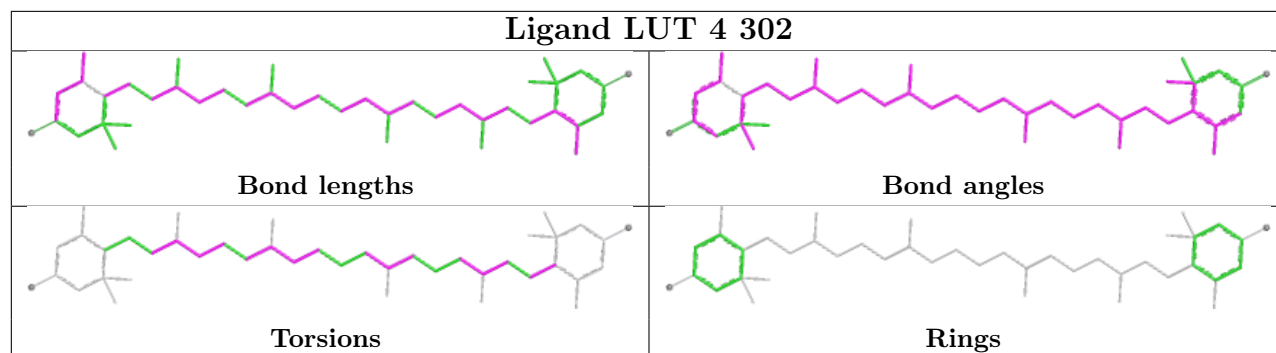
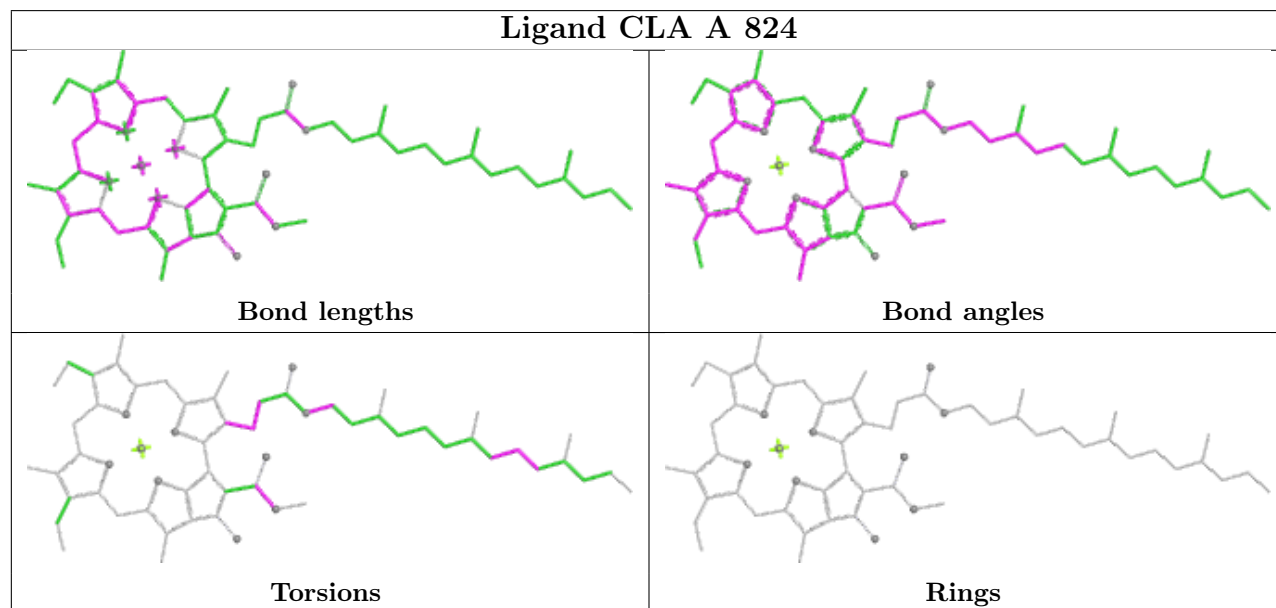


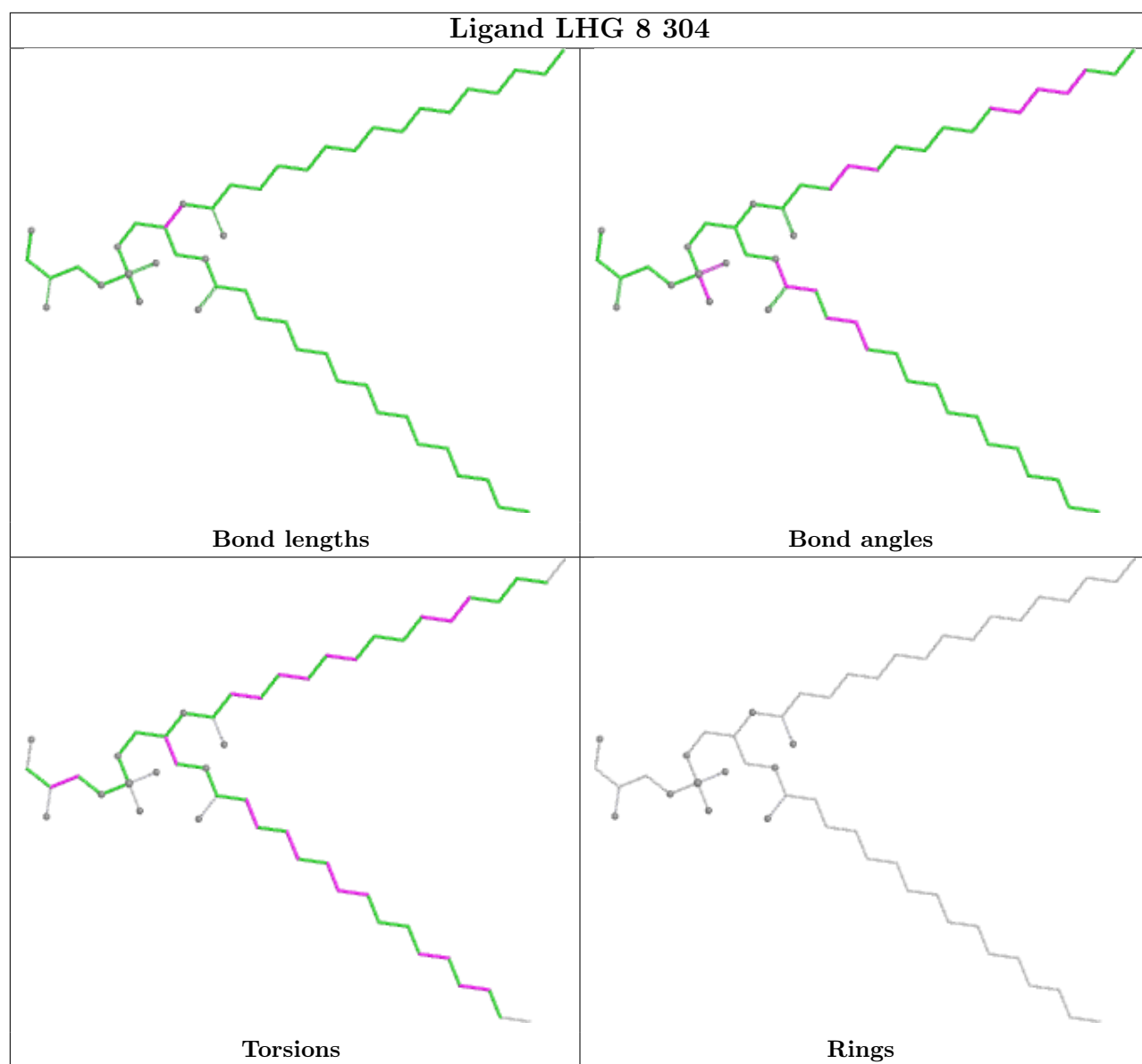
Ligand CLA 9 321

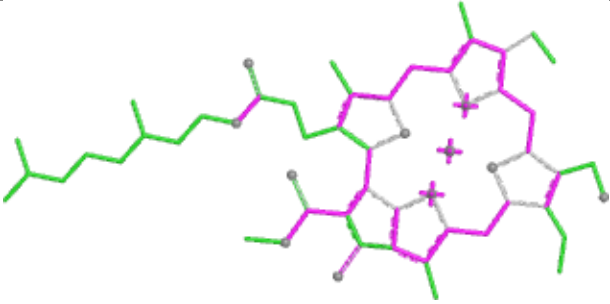
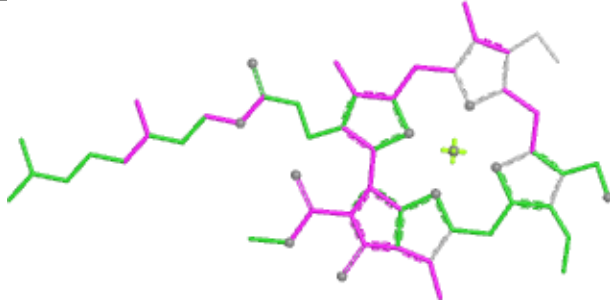
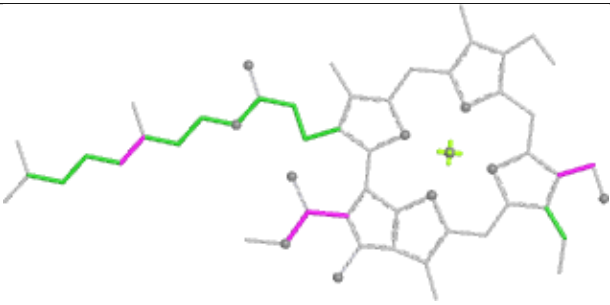
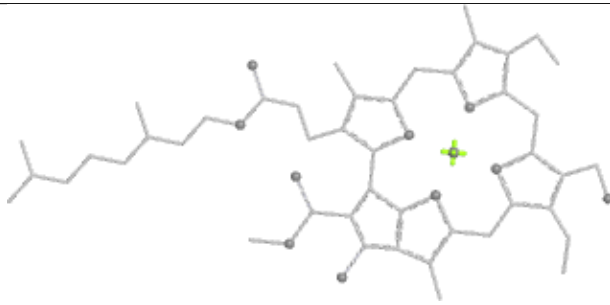
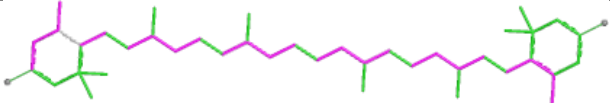
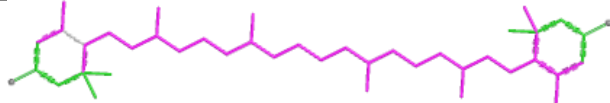
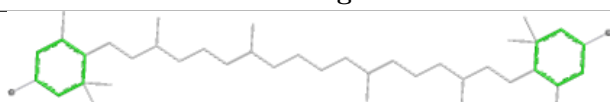
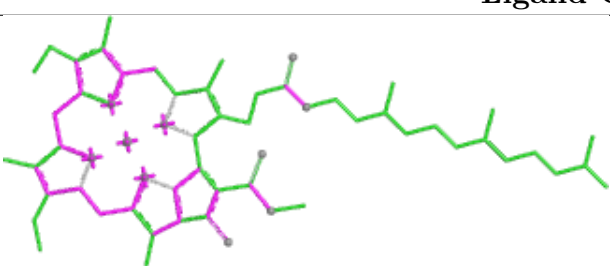
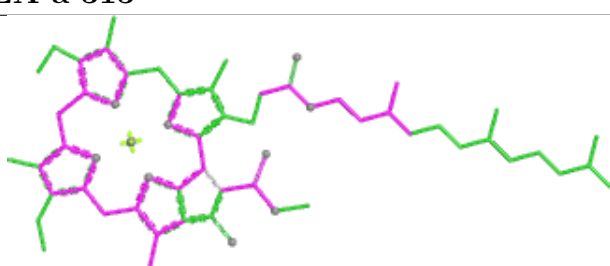
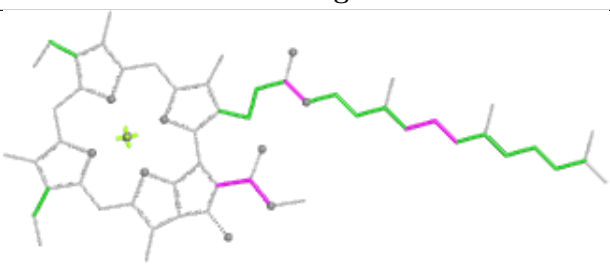
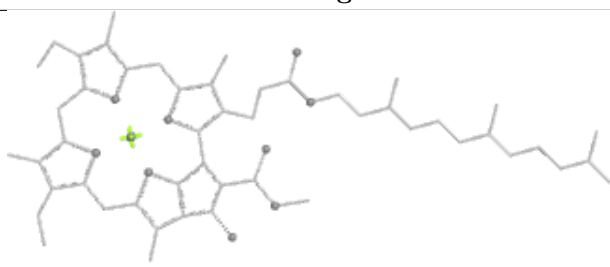


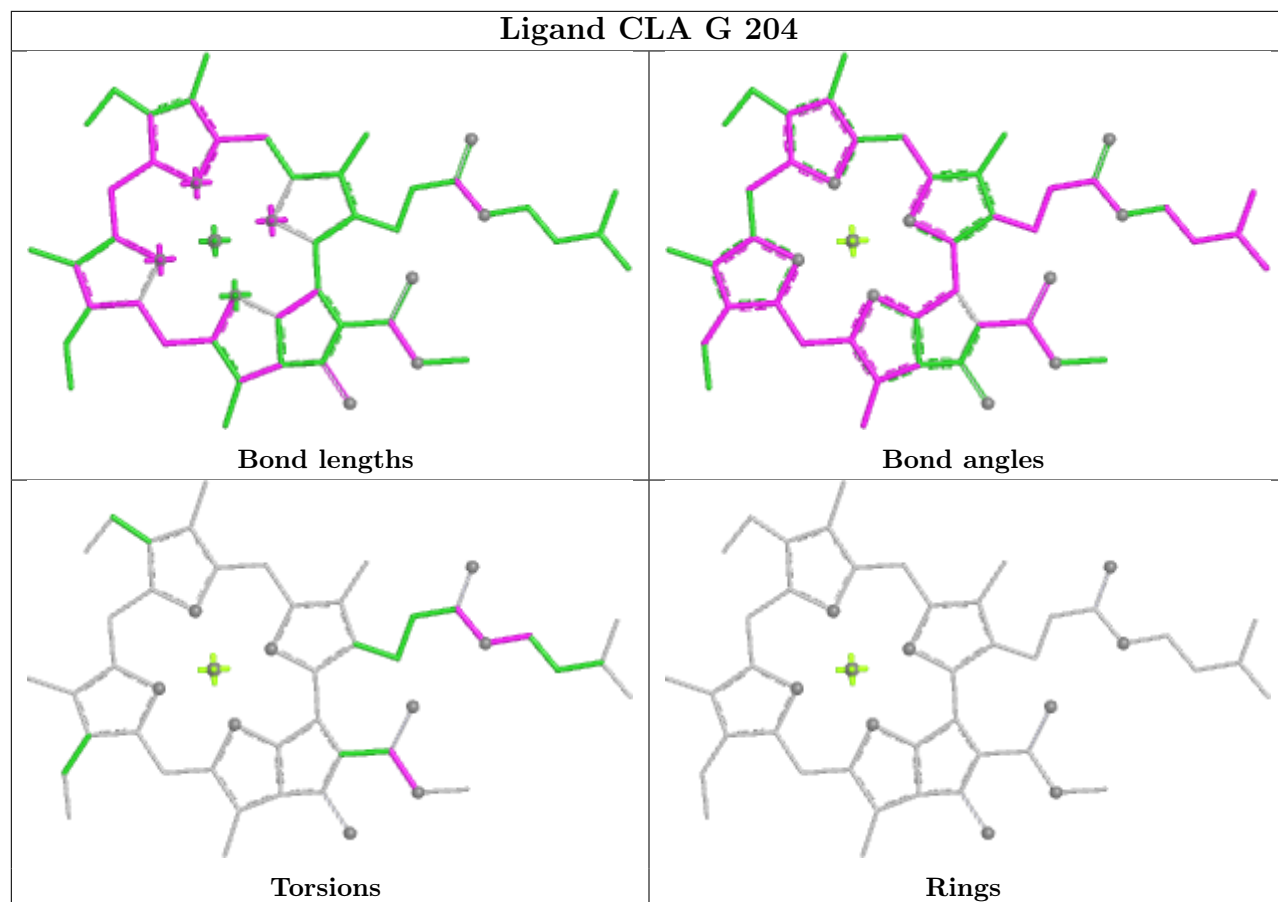
Ligand CLA 9 316



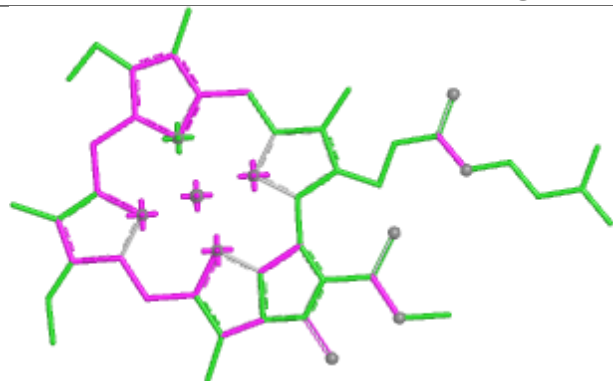
Ligand LUT 4 302**Ligand CLA A 824**



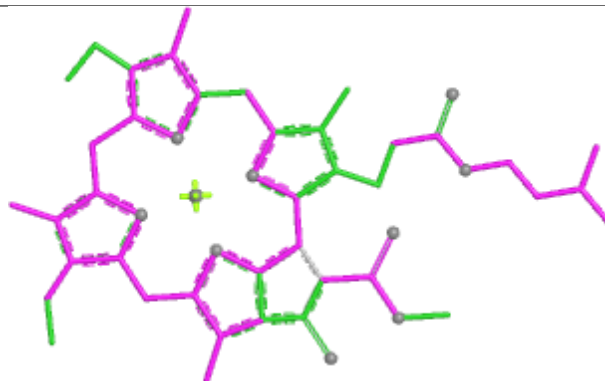
Ligand CHL A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 9 303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 313	
 Bond lengths	 Bond angles
 Torsions	 Rings



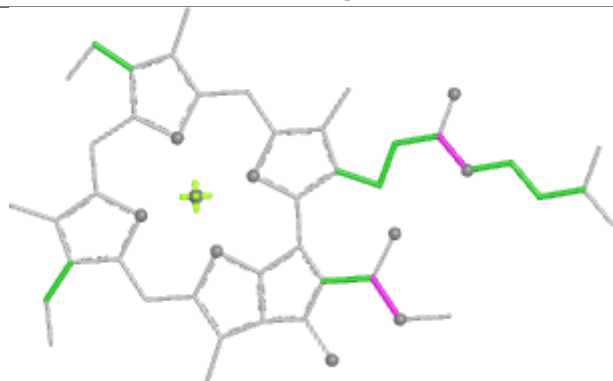
Ligand CLA B 831



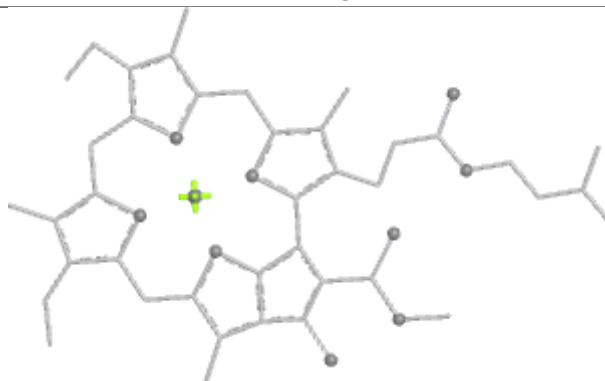
Bond lengths



Bond angles

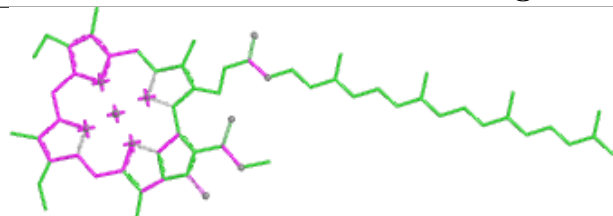


Torsions

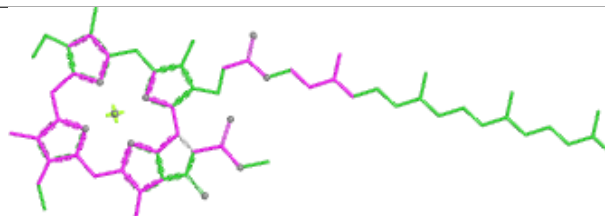


Rings

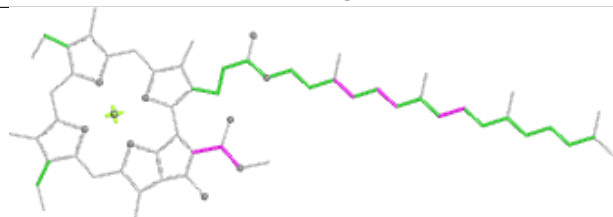
Ligand CLA B 813



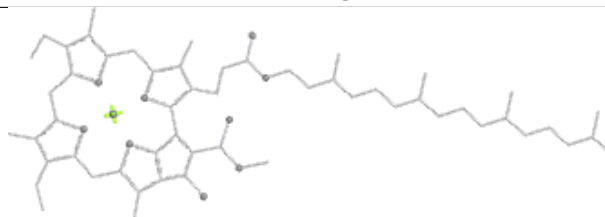
Bond lengths



Bond angles

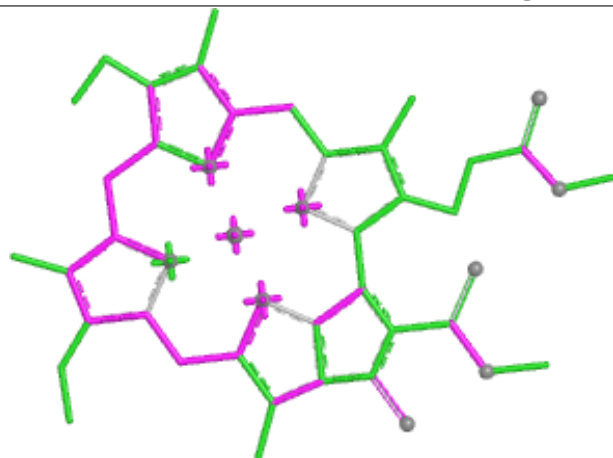


Torsions

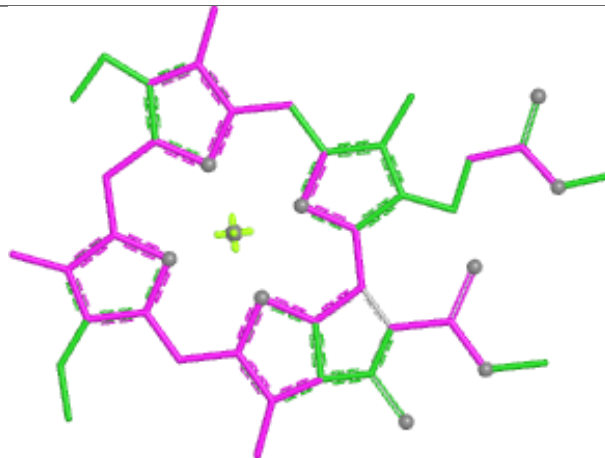


Rings

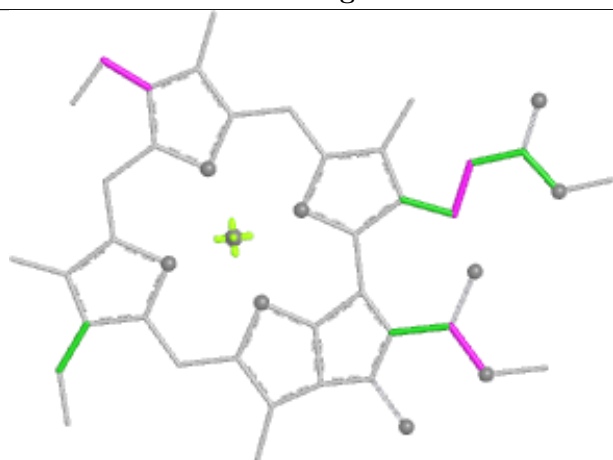
Ligand CLA 2 312



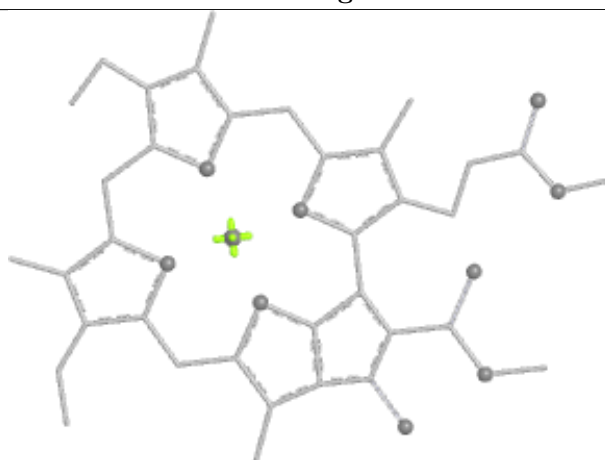
Bond lengths



Bond angles

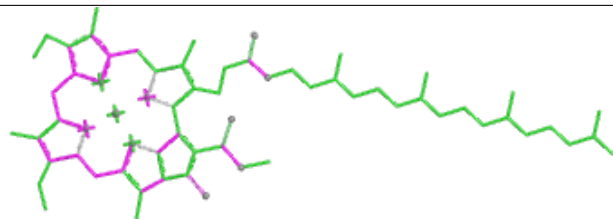


Torsions

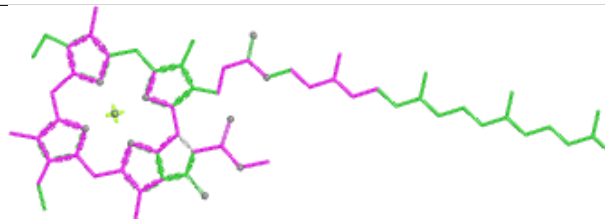


Rings

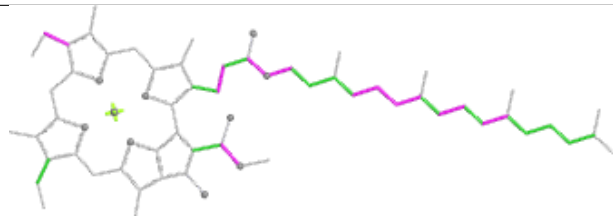
Ligand CLA A 857



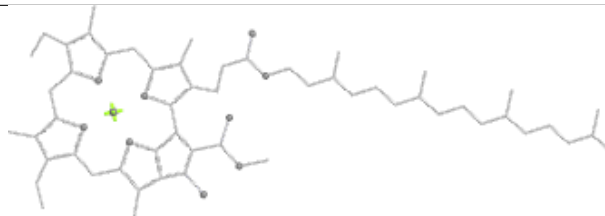
Bond lengths



Bond angles

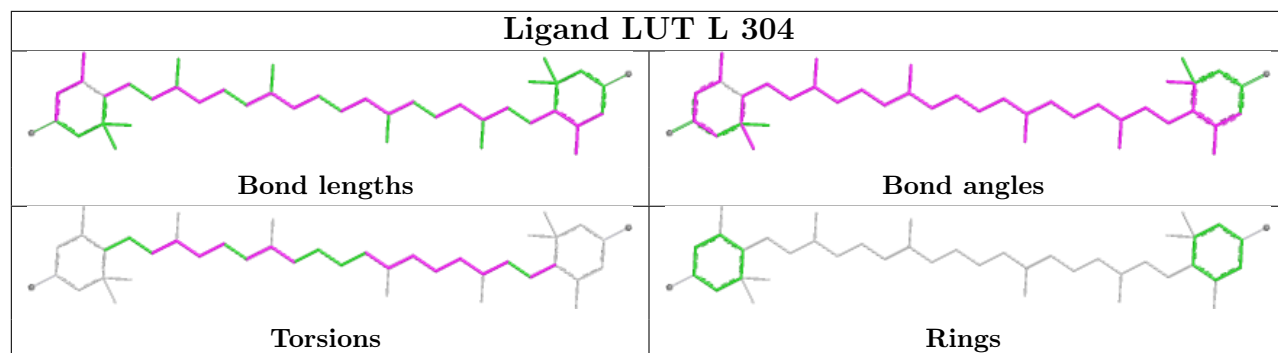


Torsions

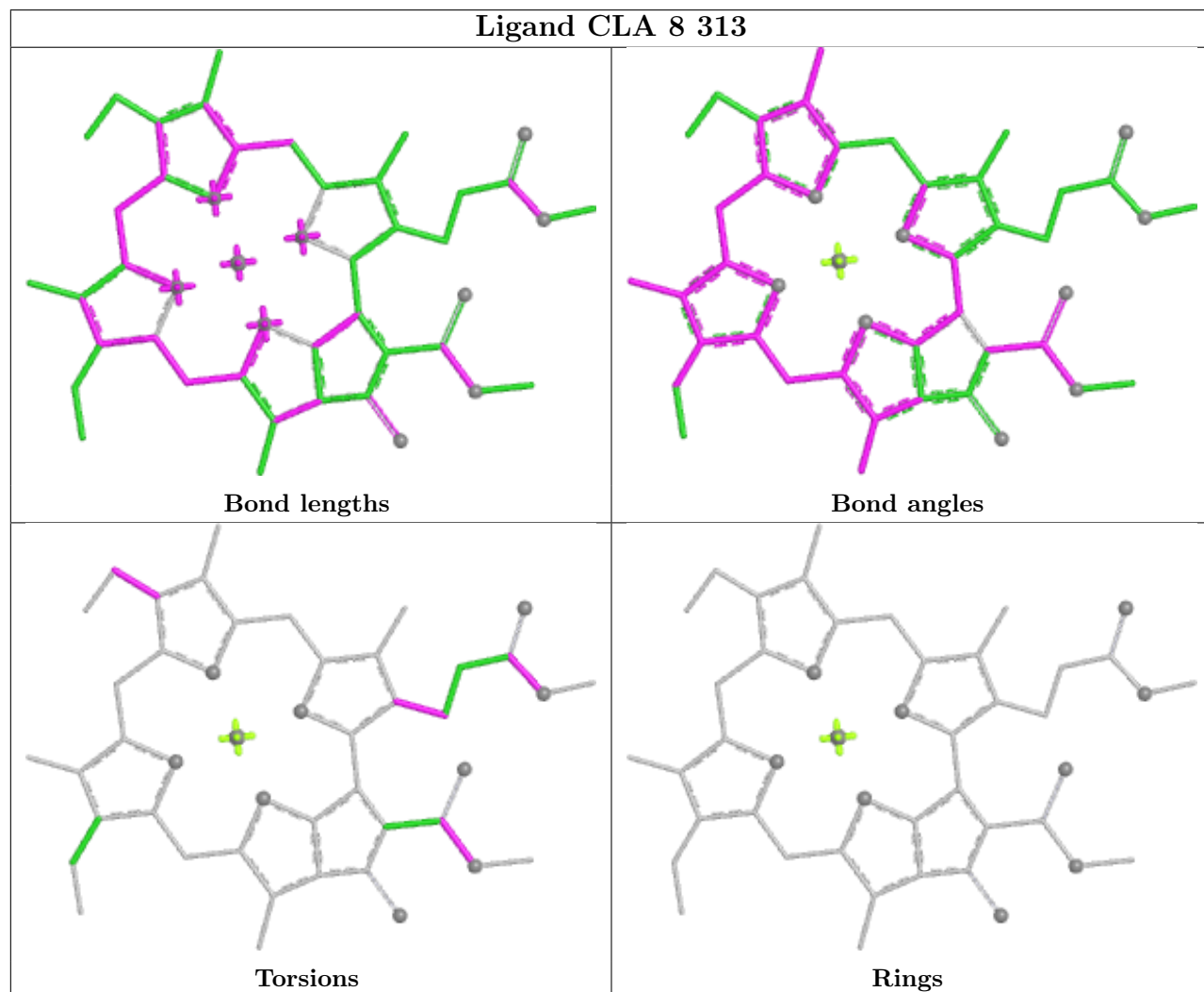


Rings

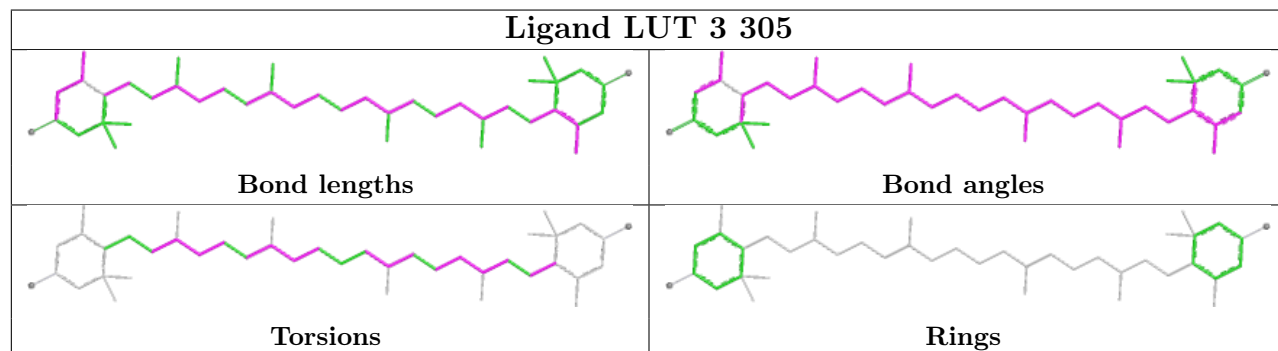
Ligand LUT L 304



Ligand CLA 8 313



Ligand LUT 3 305



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.

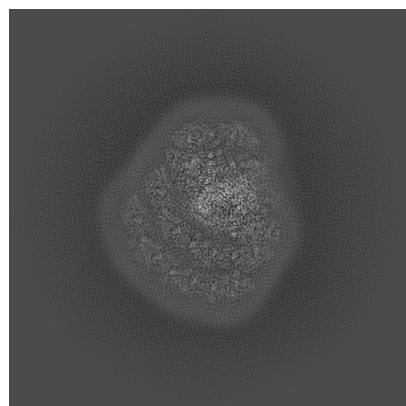
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62511. These allow visual inspection of the internal detail of the map and identification of artifacts.

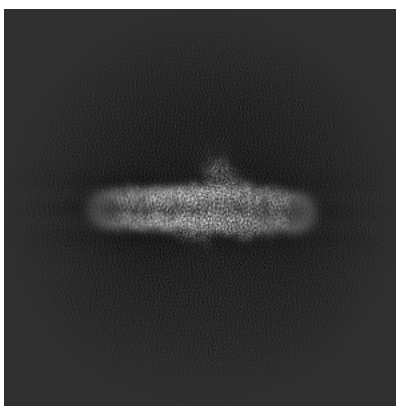
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

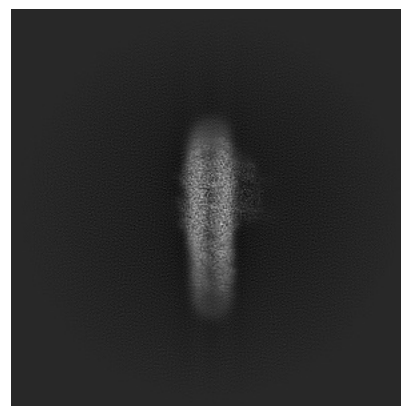
6.1.1 Primary map



X

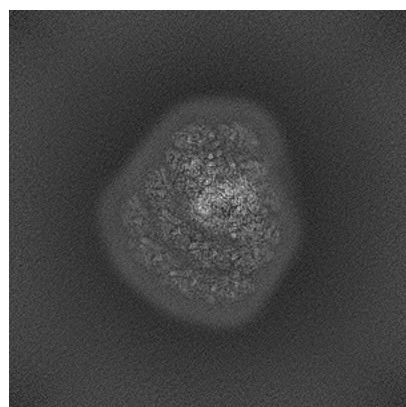


Y

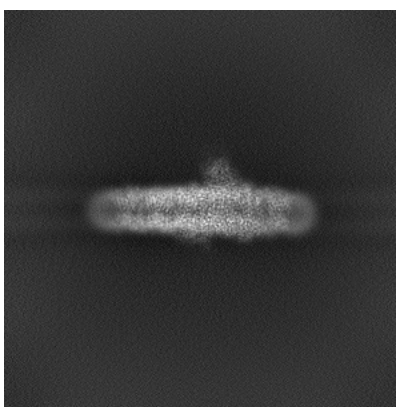


Z

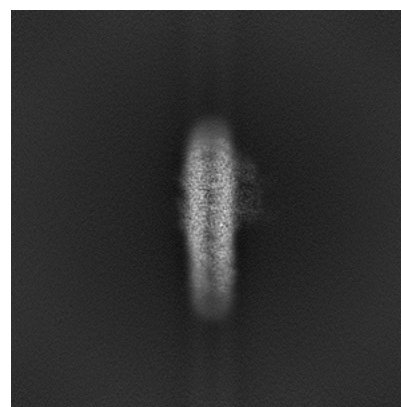
6.1.2 Raw map



X



Y

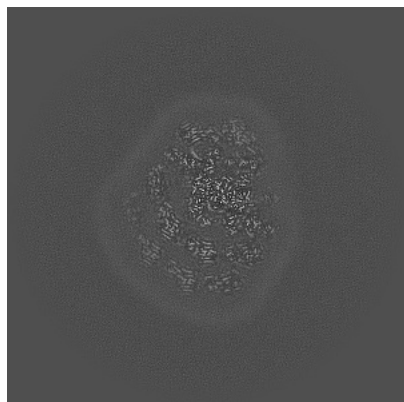


Z

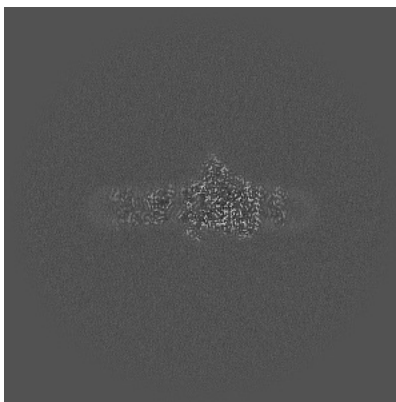
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

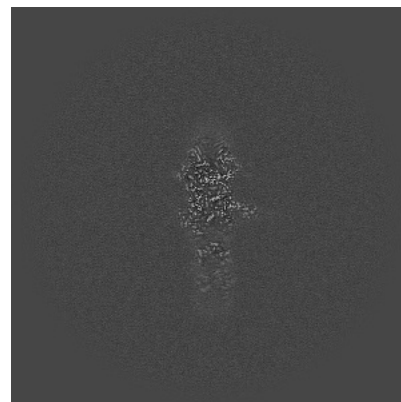
6.2.1 Primary map



X Index: 300

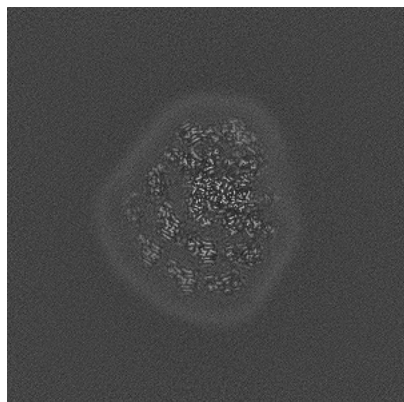


Y Index: 300

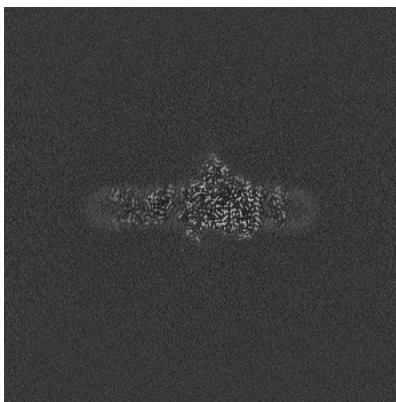


Z Index: 300

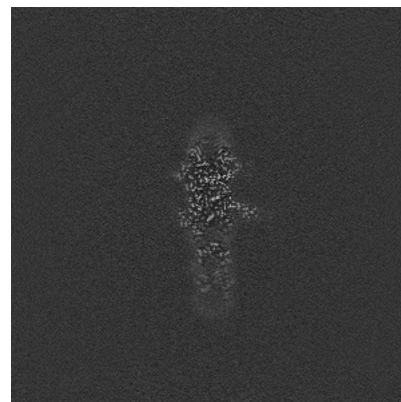
6.2.2 Raw map



X Index: 300



Y Index: 300

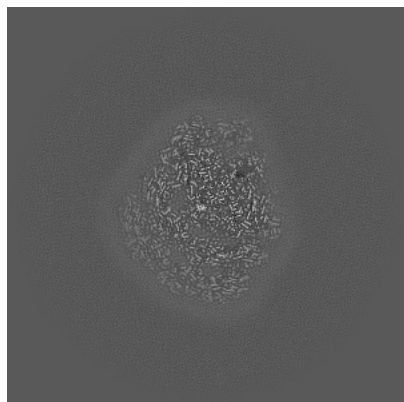


Z Index: 300

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

6.3 Largest variance slices [i](#)

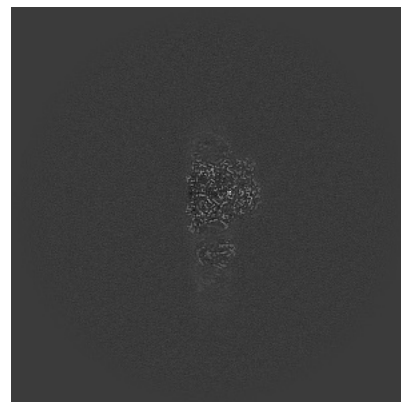
6.3.1 Primary map



X Index: 316

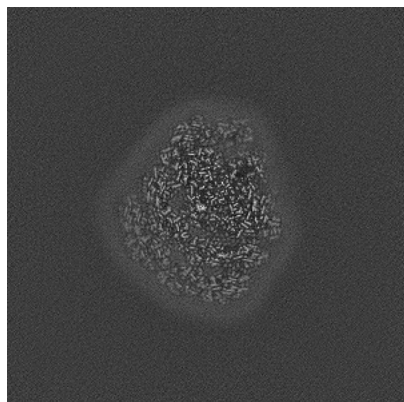


Y Index: 307

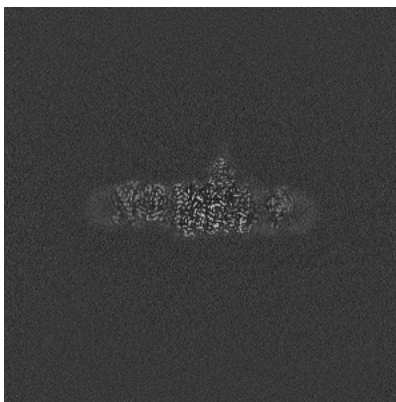


Z Index: 320

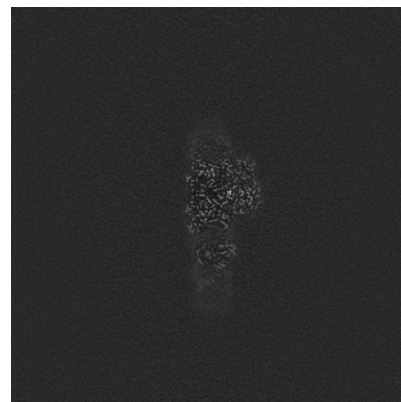
6.3.2 Raw map



X Index: 316



Y Index: 339

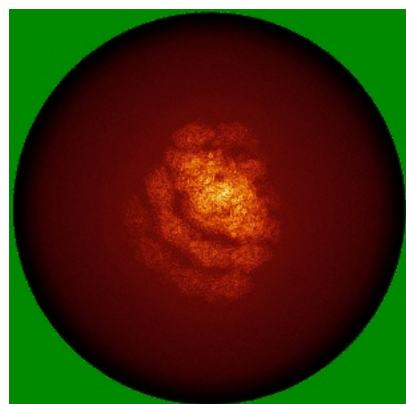


Z Index: 320

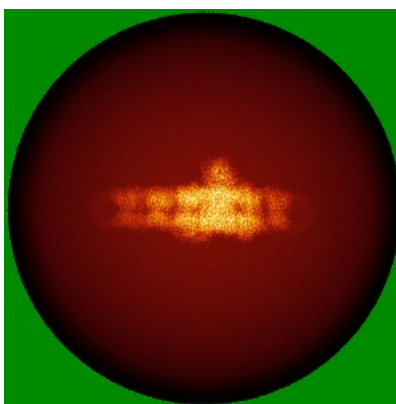
The images above show the largest variance slices of the map in three orthogonal directions.

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

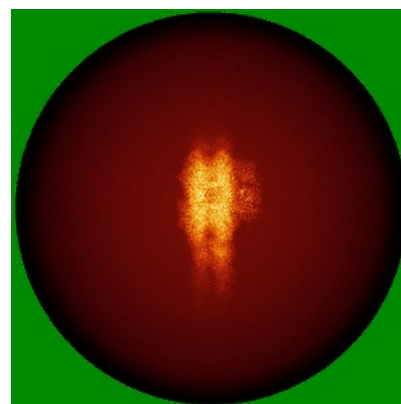
6.4.1 Primary map



X

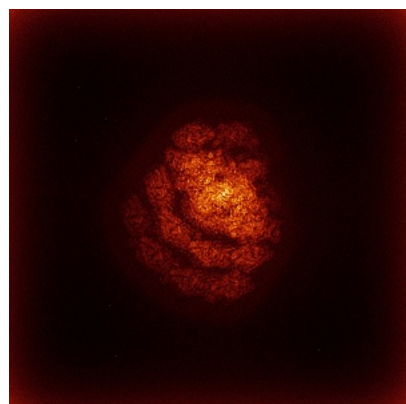


Y

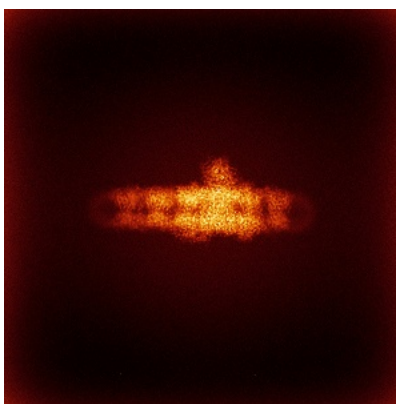


Z

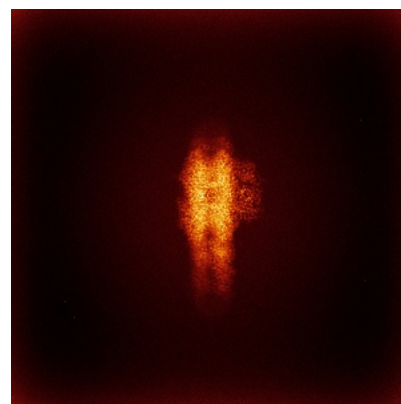
6.4.2 Raw map



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 0.085. 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.

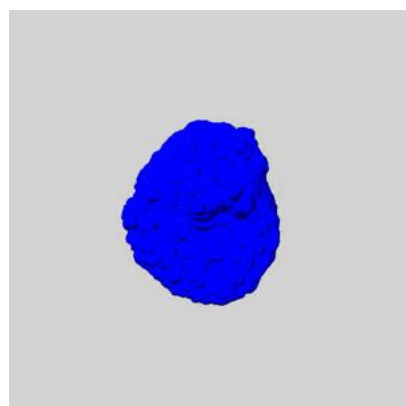
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

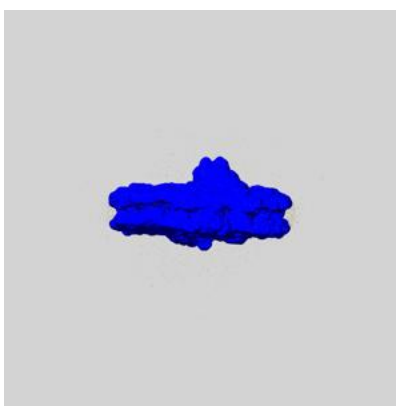
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

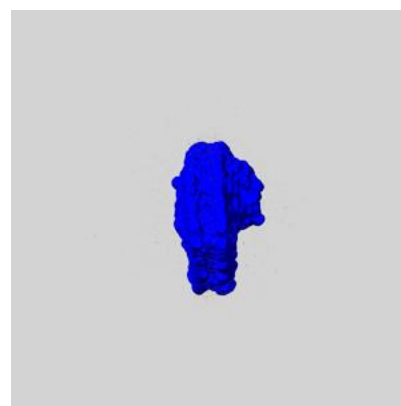
6.6.1 emd_62511_msk_1.map [i](#)



X



Y

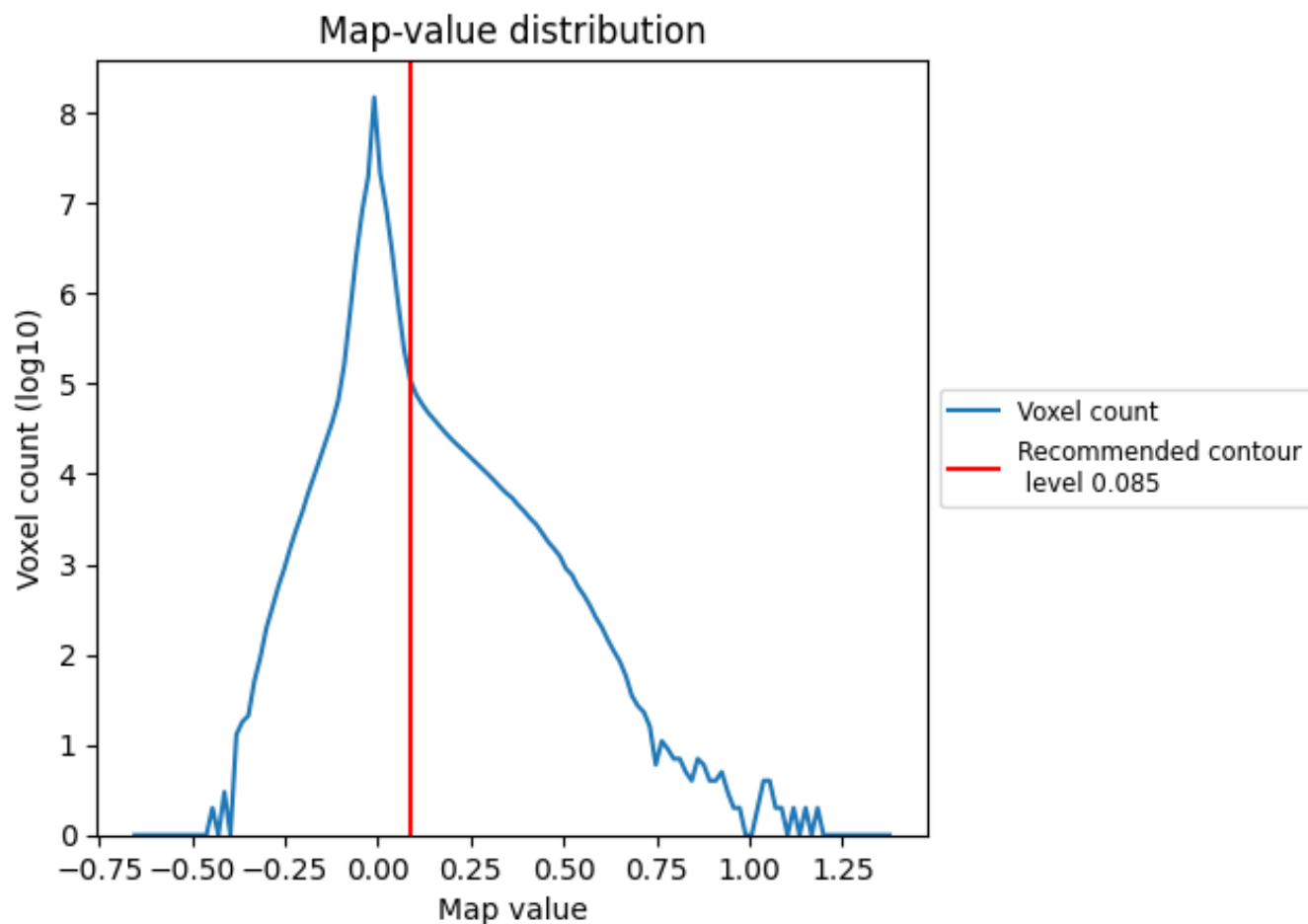


Z

7 Map analysis [i](#)

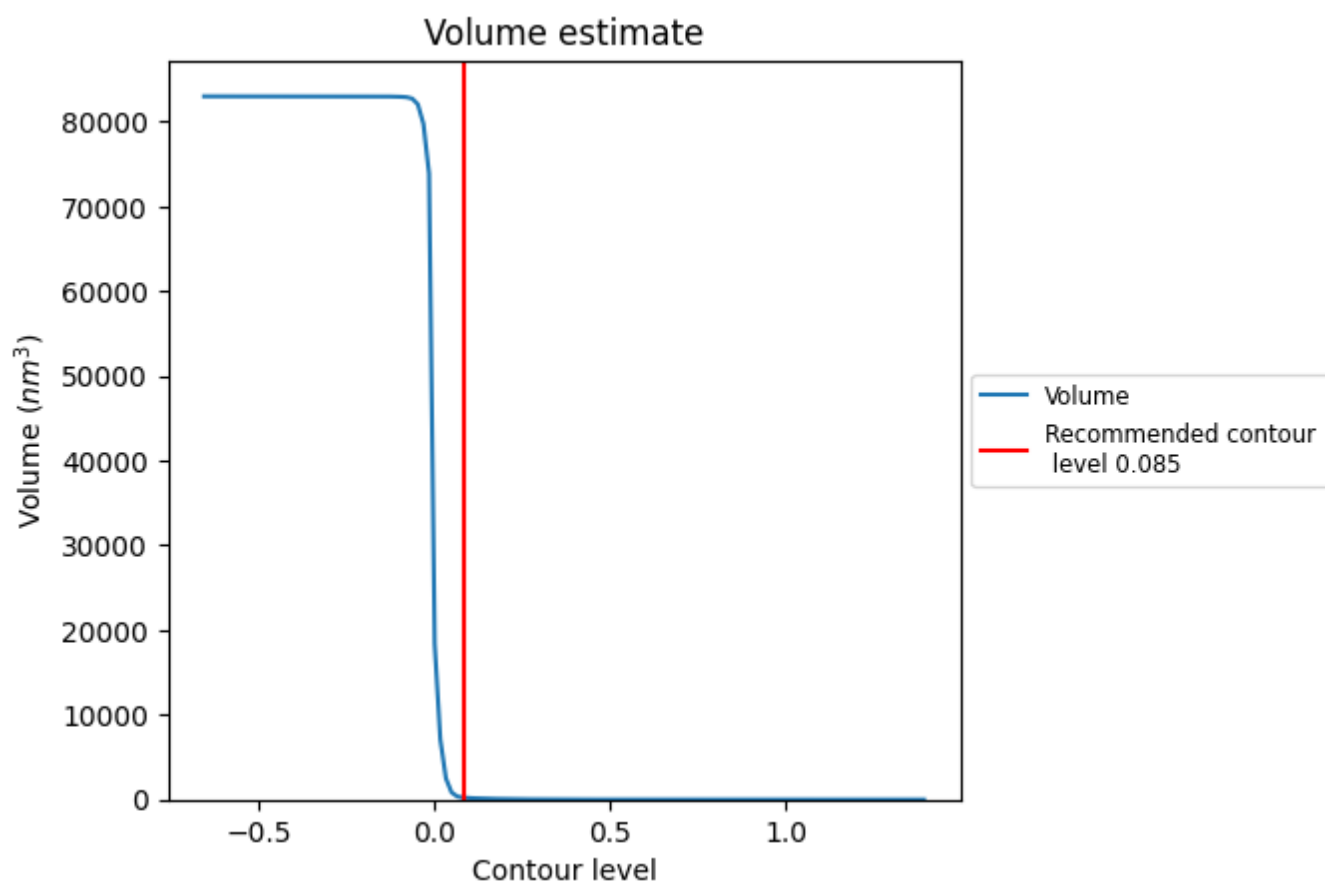
This section contains the results of statistical analysis of the map.

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.

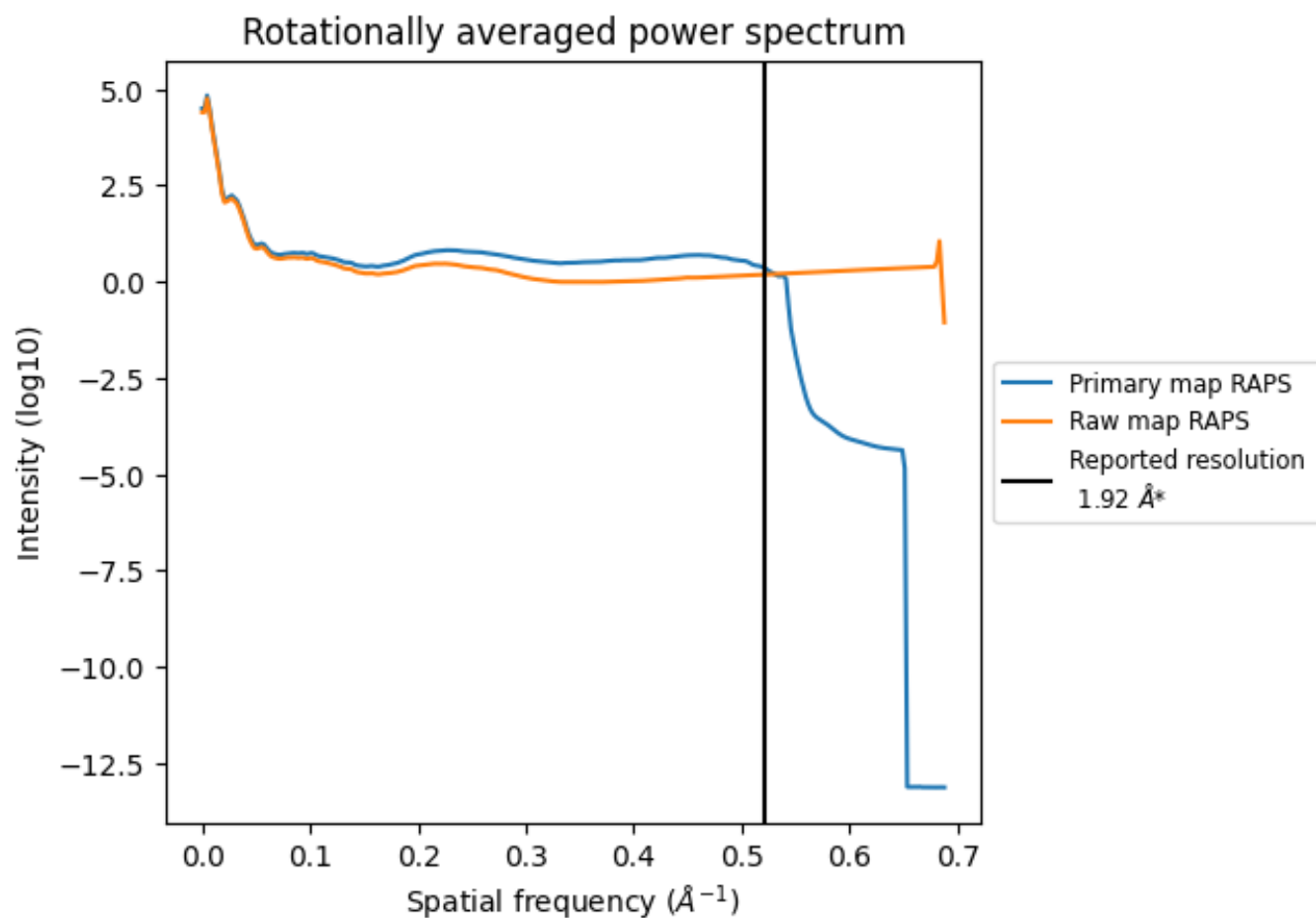
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm^3 ; this corresponds to an approximate mass of 205 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 ⓘ

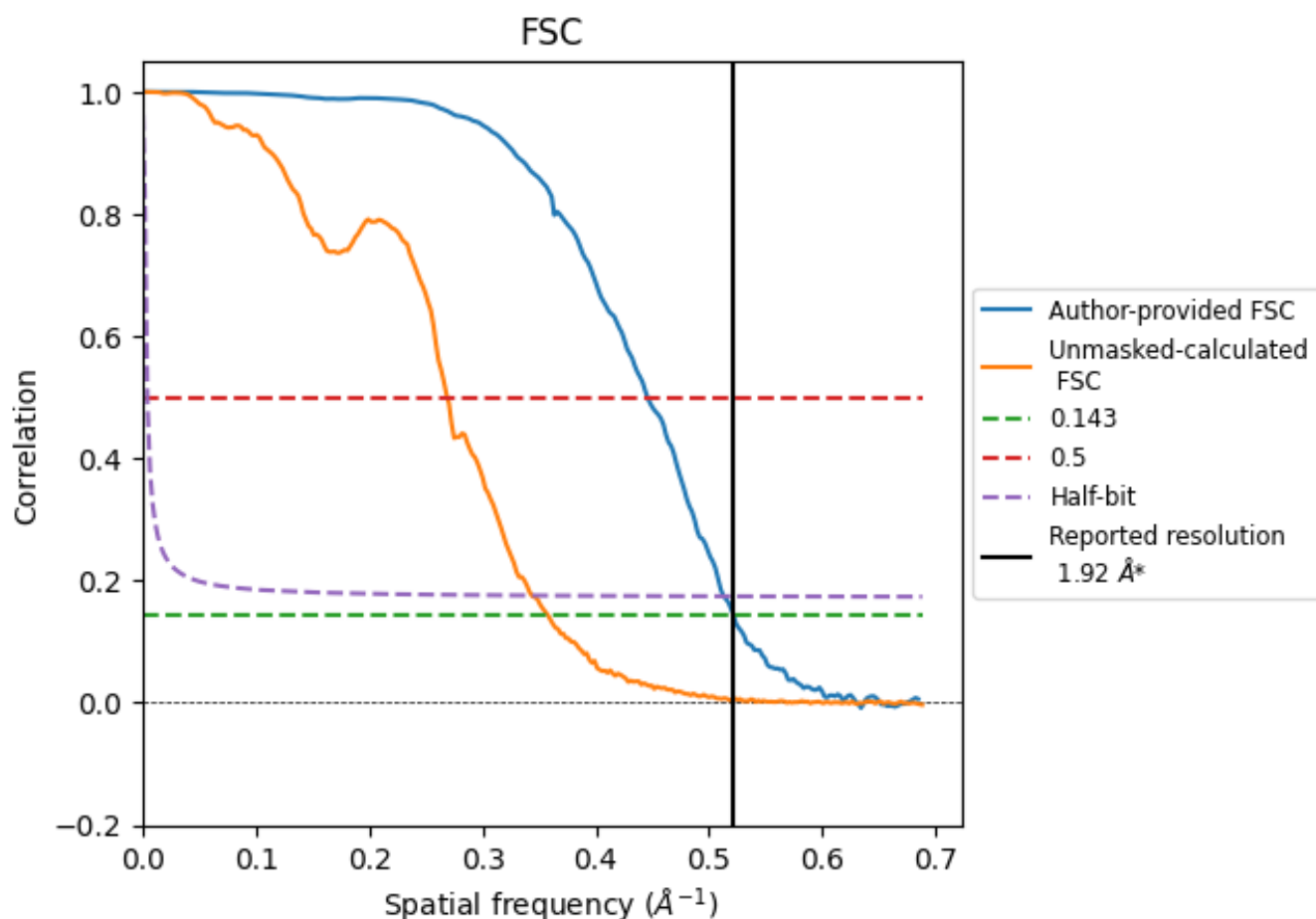


*Reported resolution corresponds to spatial frequency of 0.521 Å⁻¹

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 0.521 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

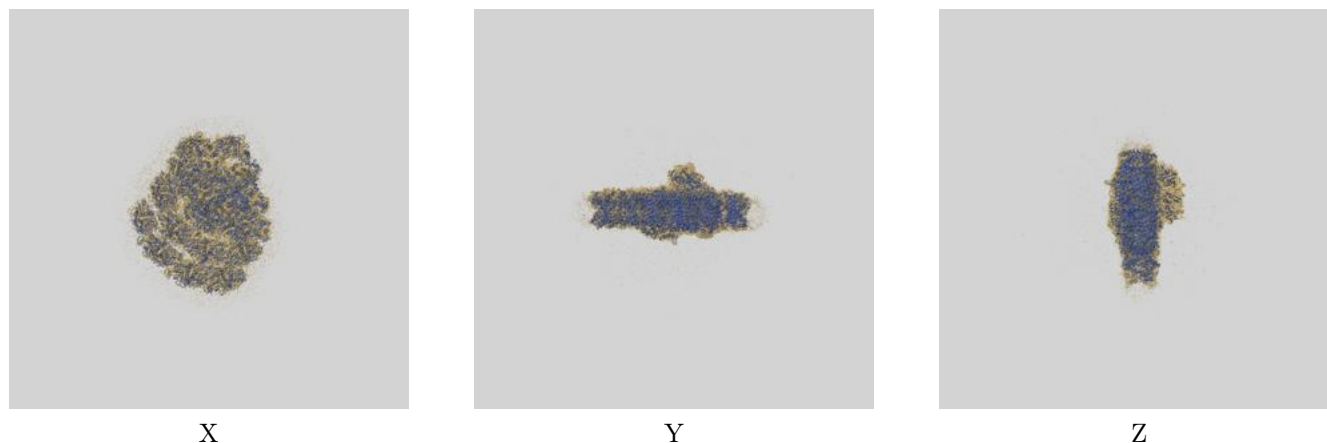
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.92	-	-
Author-provided FSC curve	1.92	2.24	1.95
Unmasked-calculated*	2.79	3.72	2.91

*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 2.79 differs from the reported value 1.92 by more than 10 %

9 Map-model fit [i](#)

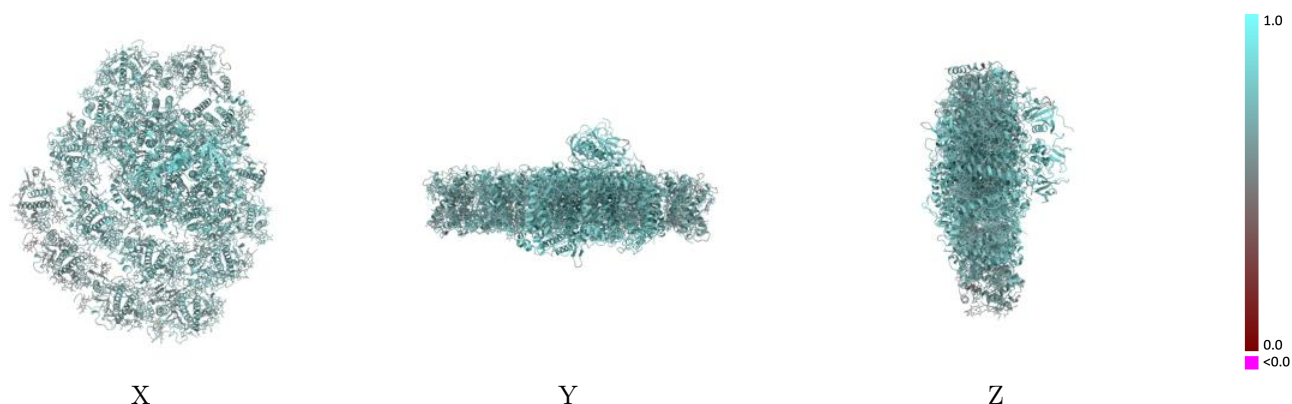
This section contains information regarding the fit between EMDB map EMD-62511 and PDB model 9KQP. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

9.1 Map-model overlay [i](#)



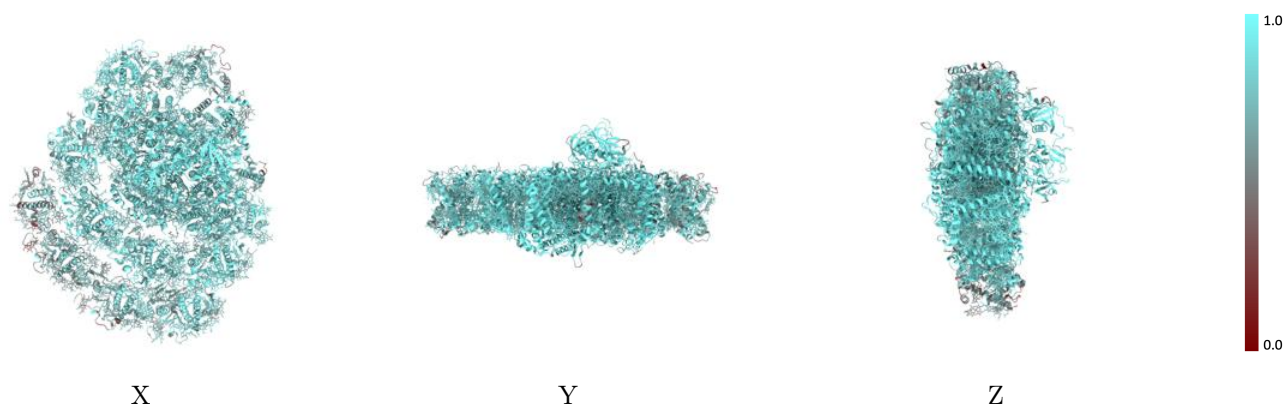
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



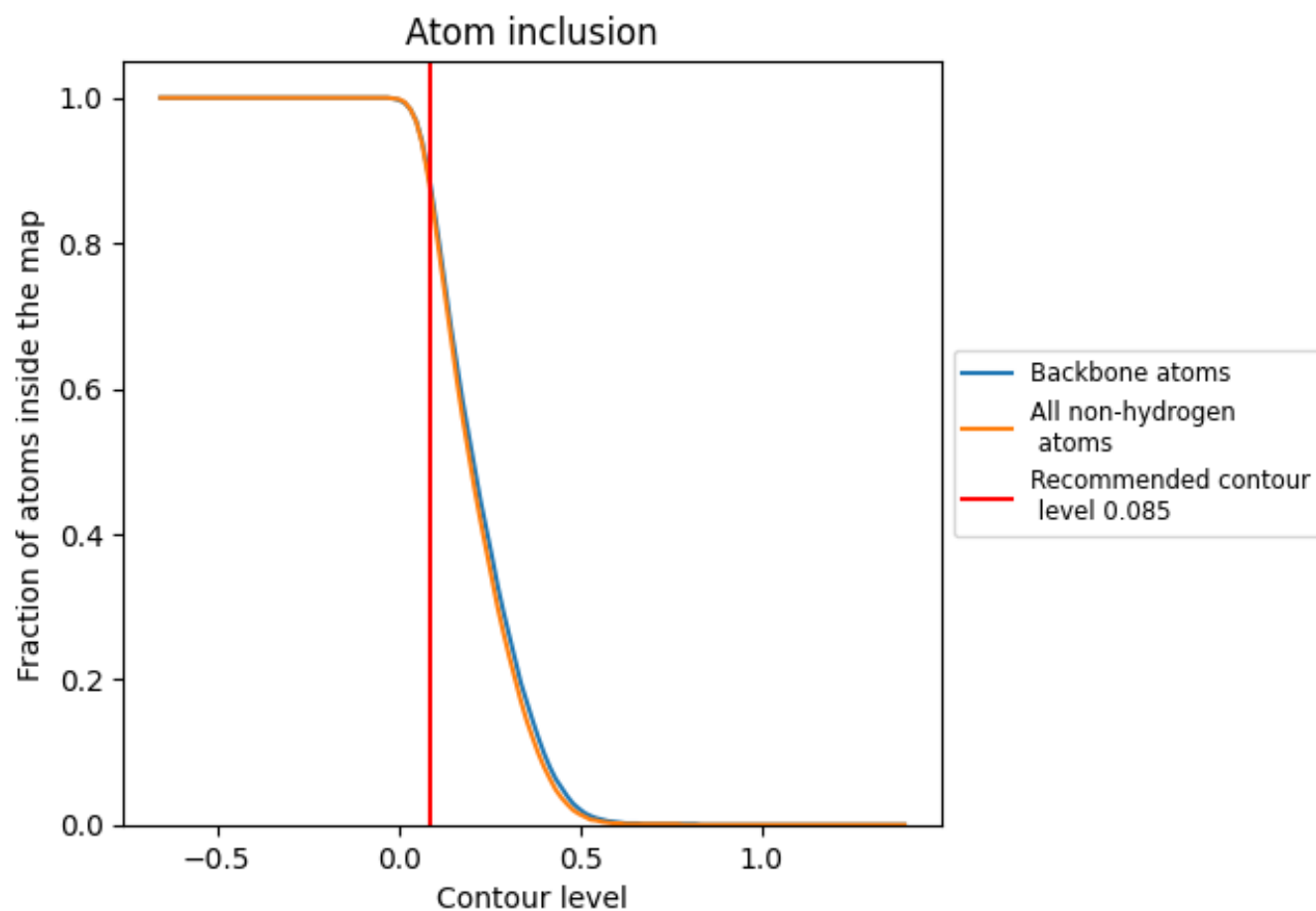
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.7230
2	0.7470	0.6320
3	0.9070	0.7070
4	0.6450	0.5770
5	0.7930	0.6420
6	0.7360	0.6210
7	0.9190	0.7280
8	0.9100	0.7290
9	0.8830	0.6910
A	0.9650	0.7910
B	0.9690	0.7950
C	0.9920	0.8120
D	0.9590	0.7800
E	0.9200	0.7700
F	0.9490	0.7810
G	0.9090	0.7300
H	0.7620	0.6860
I	0.9760	0.7770
J	0.9690	0.7790
K	0.8840	0.6980
L	0.9000	0.7320
M	0.9530	0.7720
O	0.6770	0.6560
a	0.8890	0.7080
b	0.5990	0.5800

1.0

0.0

<0.0