



wwPDB EM Validation Summary Report ⓘ

Sep 30, 2026 – 06:45 PM JST

PDB ID : 7D0J / pdb_00007d0j
EMDB ID : EMD-30536
Title : Photosystem I-LHCI-LHCII of Chlamydomonas reinhardtii
Authors : Wang, W.D.; Shen, L.L.; Huang, Z.H.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on : 2020-09-10
Resolution : 3.42 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

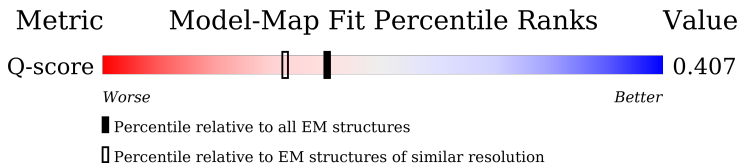
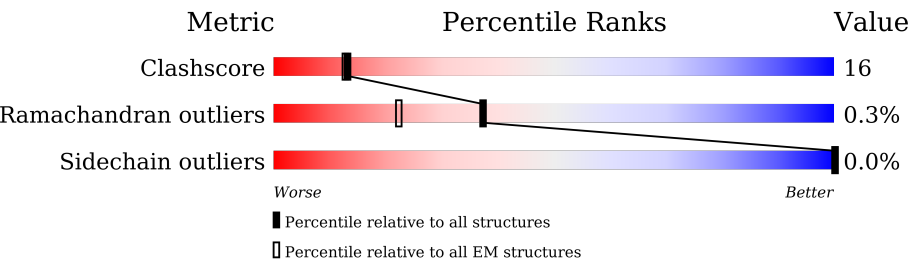
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.51

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 3.42 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	13959 (2.92 - 3.92)

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	740	20% 84% 16%
2	B	734	18% 82% 17%
3	C	80	21% 78% 20% .
4	D	144	56% 78% 22% .

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Mol	Chain	Length	Quality of chain
5	E	63	54% 75% 25%
6	F	165	77% 77% 23%
7	G	91	91% 78% 22%
8	H	100	70% 65% 31% ..
9	I	37	16% 84% 16%
10	J	41	51% 80% 17% .
11	K	85	95% 81% 19%
12	L	159	36% 73% 27%
13	O	93	70% 69% 31%
14	P	219	100% 63% 37%
14	Q	219	100% 69% 31%
14	R	219	100% 68% 32%
14	T	219	100% 67% 33%
14	U	219	100% 68% 32%
15	S	234	100% 69% 30%
16	1	194	69% 77% 23%
16	a	194	98% 67% 32% .
17	2	201	80% 63% 36%
18	3	203	41% 79% 21%
19	4	205	95% 78% 20% .
20	5	225	56% 77% 23%
21	6	230	76% 78% 20% .
22	7	213	44% 82% 17%
23	8	217	62% 81% 19%
24	9	182	87% 73% 26% .

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
25	CLA	P	603	-	-	X	-
25	CLA	P	610	-	-	X	-
25	CLA	P	611	-	-	X	-
25	CLA	P	612	-	-	X	-
25	CLA	Q	603	-	-	X	-
25	CLA	R	603	-	-	X	-
25	CLA	R	610	-	-	X	-
25	CLA	R	612	-	-	X	-
33	CHL	P	609	-	-	X	-
33	CHL	Q	608	-	-	X	-
33	CHL	R	609	-	-	X	-
36	NEX	U	301	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 68860 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
			5811	3799	991	999	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5828	3827	978	1005	18		

- 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
			600	369	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1132	725	200	200	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			496	316	87	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	91	Total	C	N	O	0	0
			678	436	114	128		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	100	Total	C	N	O	S	0	0
			773	479	138	154	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1161	757	189	212	3		

- Molecule 13 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	93	Total	C	N	O	0	0
			720	477	118	125		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	Q	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	R	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	T	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	U	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	233	Total	C	N	O	P S	0	0
			1717	1098	285	328	1 5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
16	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	201	Total	C	N	O	S	0	0
			1545	1002	253	280	10		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	203	Total	C	N	O	S	0	0
			1560	1021	253	278	8		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4	205	Total	C	N	O	S	0	0
			1590	1046	254	285	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	5	225	Total	C	N	O	S	0	0
			1757	1145	294	310	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	7	212	Total	C	N	O	S	0	0
			1644	1067	274	297	6		

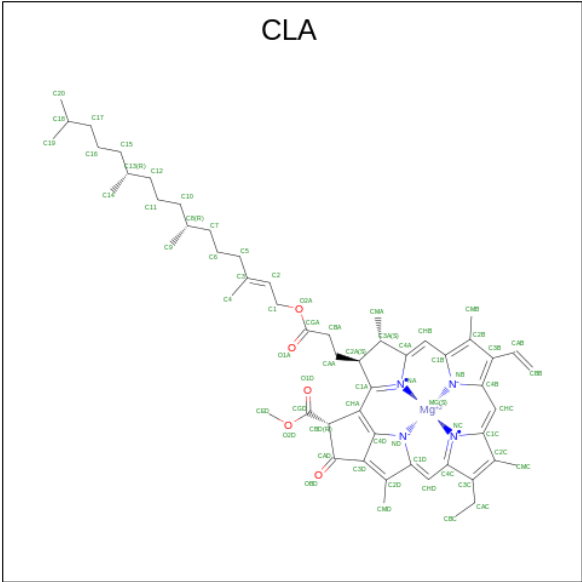
- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	9	182	Total	C	N	O	S	0	0
			1392	903	231	251	7		

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	H	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	K	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	L	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	L	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
25	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	P	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	P	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Q	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	Q	1	Total 48	C 38	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	Q	1	Total 40	C 32	Mg 1	N 4	O 3	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	R	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	R	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	S	1	Total 47	C 37	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	S	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	T	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	T	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	U	1	Total 64	C 54	Mg 1	N 4	O 5	0
25	U	1	Total 54	C 47	Mg 1	N 4	O 2	0
25	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	3	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	5	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 61	C 51	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	6	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
25	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
25	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
25	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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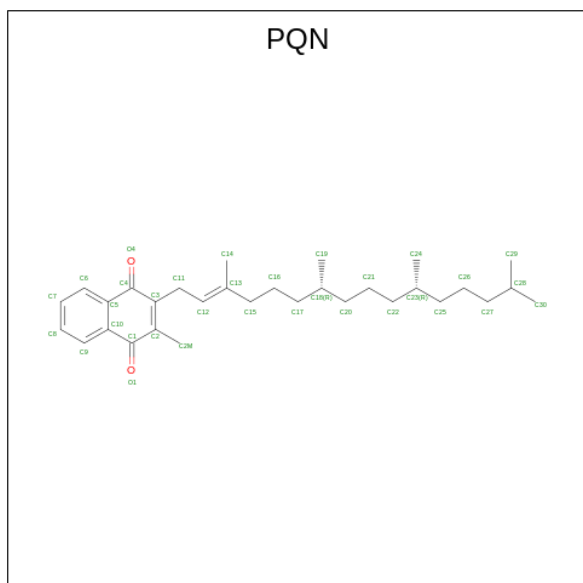
Mol	Chain	Residues	Atoms					AltConf
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
25	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
25	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 57	C 47	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



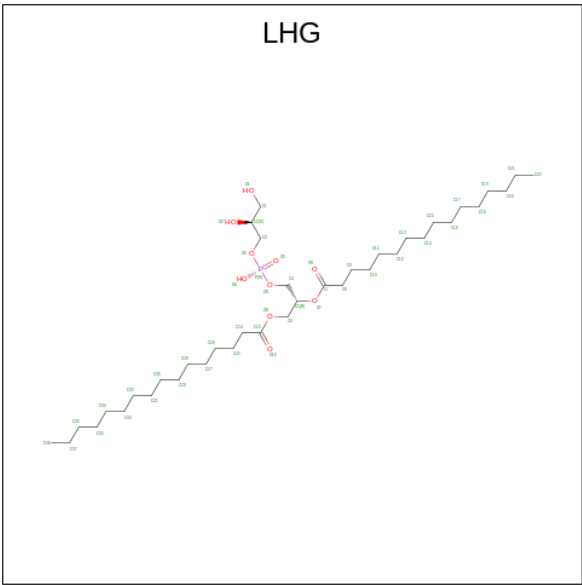
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			33	31	2	

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

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



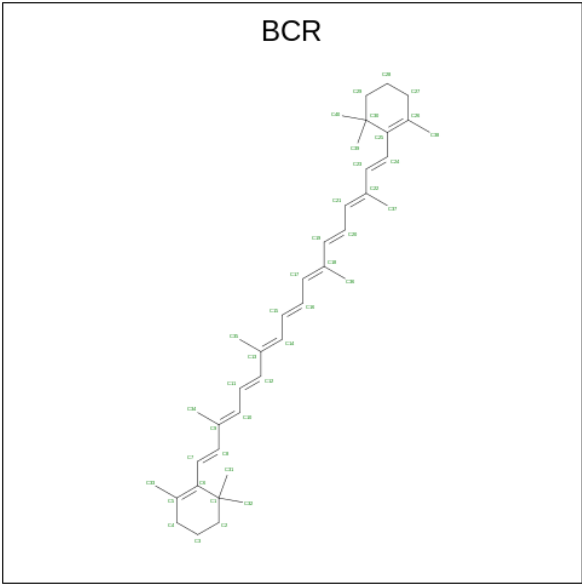
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			38	27	10	1	
27	A	1	Total	C	O	P	0
			48	37	10	1	
27	B	1	Total	C	O	P	0
			38	27	10	1	
27	P	1	Total	C	O	P	0
			49	38	10	1	
27	P	1	Total	C	O	P	0
			49	38	10	1	
27	Q	1	Total	C	O	P	0
			49	38	10	1	
27	R	1	Total	C	O	P	0
			49	38	10	1	
27	S	1	Total	C	O	P	0
			49	38	10	1	
27	T	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	1	1	43	32	10	1	0
27	2	1	49	38	10	1	0
27	4	1	49	38	10	1	0
27	4	1	32	21	10	1	0
27	5	1	45	34	10	1	0
27	5	1	37	26	10	1	0
27	6	1	49	38	10	1	0
27	7	1	37	26	10	1	0
27	8	1	49	38	10	1	0
27	a	1	43	32	10	1	0

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			40	40	

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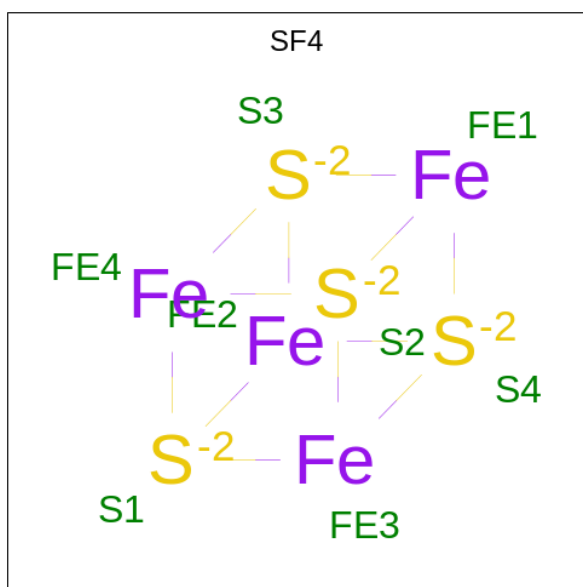
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C 40 40	0
28	A	1	Total C 40 40	0
28	A	1	Total C 40 40	0
28	A	1	Total C 40 40	0
28	A	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	F	1	Total C 40 40	0
28	F	1	Total C 40 40	0
28	G	1	Total C 40 40	0
28	I	1	Total C 40 40	0
28	J	1	Total C 40 40	0
28	J	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	L	1	Total C 40 40	0
28	L	1	Total C 40 40	0

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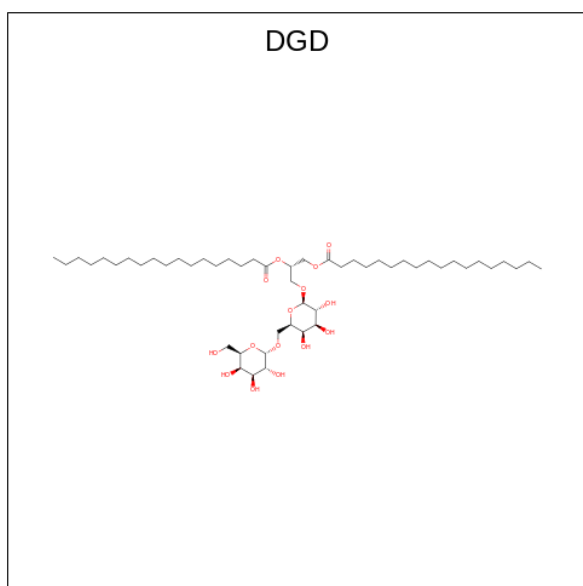
Mol	Chain	Residues	Atoms	AltConf
28	L	1	Total C 40 40	0
28	L	1	Total C 40 40	0
28	O	1	Total C 40 40	0
28	O	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	4	1	Total C 40 40	0
28	4	1	Total C 40 40	0
28	5	1	Total C 40 40	0
28	5	1	Total C 40 40	0
28	6	1	Total C 40 40	0
28	7	1	Total C 40 40	0
28	8	1	Total C 40 40	0
28	8	1	Total C 40 40	0

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



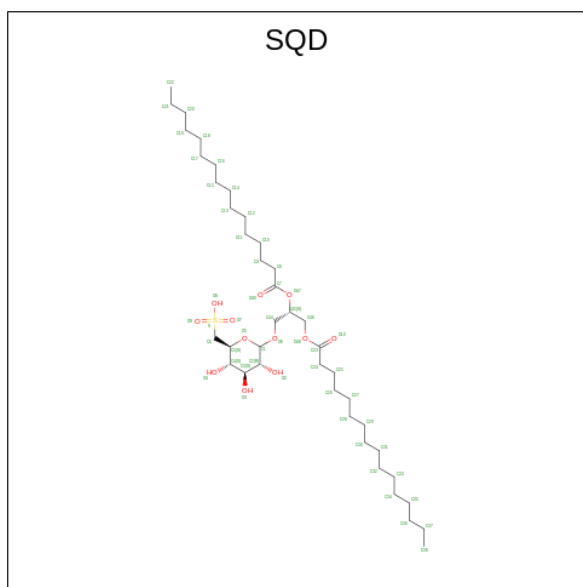
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



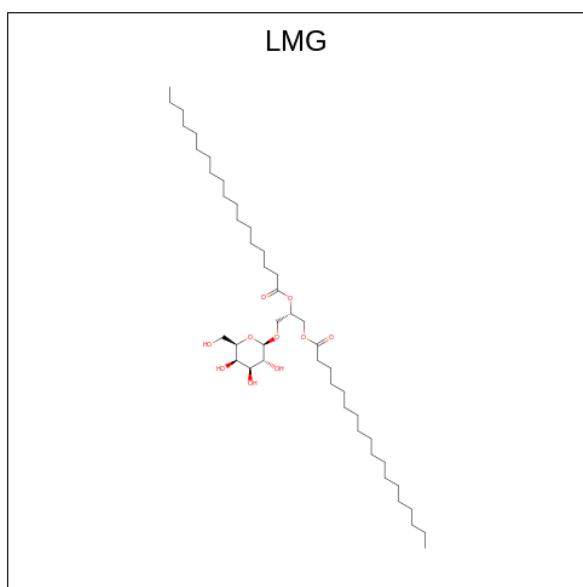
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			66	51	15	
30	B	1	Total	C	O	0
			57	42	15	

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



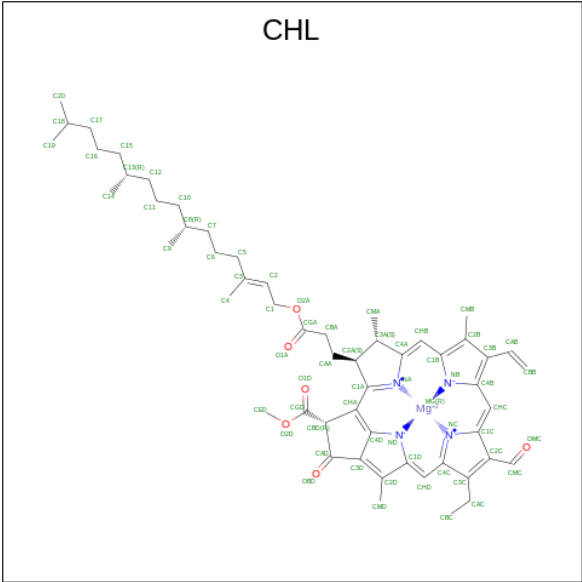
Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	O	S	0
			51	38	12	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
32	H	1	Total	C	O	0
			47	37	10	
32	J	1	Total	C	O	0
			40	30	10	
32	J	1	Total	C	O	0
			35	25	10	
32	J	1	Total	C	O	0
			55	45	10	
32	1	1	Total	C	O	0
			46	36	10	
32	2	1	Total	C	O	0
			41	31	10	
32	4	1	Total	C	O	0
			40	30	10	
32	6	1	Total	C	O	0
			40	30	10	
32	7	1	Total	C	O	0
			35	25	10	
32	7	1	Total	C	O	0
			36	26	10	

- Molecule 33 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
33	P	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	P	1	Total 48	C 37	Mg 1	N 4	O 6	0
33	P	1	Total 50	C 39	Mg 1	N 4	O 6	0
33	P	1	Total 52	C 41	Mg 1	N 4	O 6	0
33	P	1	Total 44	C 35	Mg 1	N 4	O 4	0
33	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
33	P	1	Total 52	C 41	Mg 1	N 4	O 6	0
33	P	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	Q	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	Q	1	Total 42	C 33	Mg 1	N 4	O 4	0
33	Q	1	Total 50	C 39	Mg 1	N 4	O 6	0
33	Q	1	Total 44	C 35	Mg 1	N 4	O 4	0
33	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
33	R	1	Total 51	C 40	Mg 1	N 4	O 6	0

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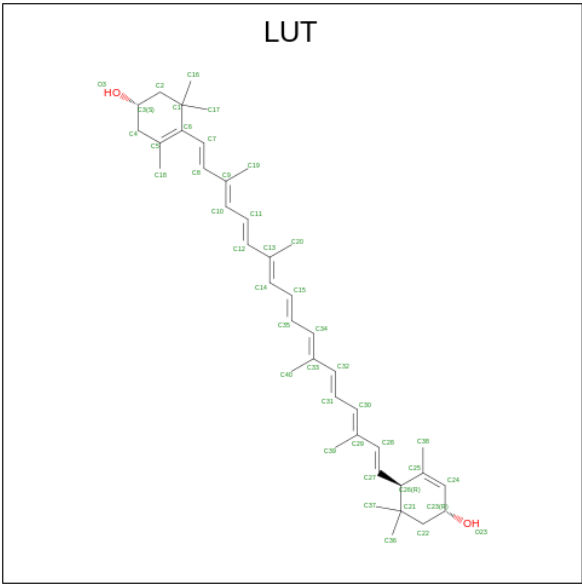
Mol	Chain	Residues	Atoms					AltConf
33	R	1	Total 46	C 35	Mg 1	N 4	O 6	0
33	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
33	R	1	Total 52	C 41	Mg 1	N 4	O 6	0
33	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
33	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
33	S	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	S	1	Total 48	C 37	Mg 1	N 4	O 6	0
33	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
33	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
33	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
33	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
33	S	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	T	1	Total 50	C 39	Mg 1	N 4	O 6	0
33	T	1	Total 48	C 37	Mg 1	N 4	O 6	0
33	T	1	Total 50	C 39	Mg 1	N 4	O 6	0
33	T	1	Total 44	C 35	Mg 1	N 4	O 4	0
33	T	1	Total 52	C 41	Mg 1	N 4	O 6	0
33	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
33	U	1	Total 50	C 39	Mg 1	N 4	O 6	0
33	U	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	U	1	Total 44	C 35	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
33	U	1	Total 48	C 37	Mg 1	N 4	O 6	0
33	1	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
33	3	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	4	1	Total 42	C 33	Mg 1	N 4	O 4	0
33	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
33	4	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	5	1	Total 43	C 34	Mg 1	N 4	O 4	0
33	6	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	6	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
33	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
33	8	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	9	1	Total 42	C 33	Mg 1	N 4	O 4	0
33	9	1	Total 51	C 40	Mg 1	N 4	O 6	0
33	a	1	Total 48	C 37	Mg 1	N 4	O 6	0

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
34	P	1	Total	C	O	0
			42	40	2	
34	P	1	Total	C	O	0
			42	40	2	
34	Q	1	Total	C	O	0
			42	40	2	
34	Q	1	Total	C	O	0
			42	40	2	
34	R	1	Total	C	O	0
			42	40	2	
34	R	1	Total	C	O	0
			42	40	2	
34	S	1	Total	C	O	0
			42	40	2	
34	S	1	Total	C	O	0
			42	40	2	
34	T	1	Total	C	O	0
			42	40	2	
34	T	1	Total	C	O	0
			42	40	2	
34	U	1	Total	C	O	0
			42	40	2	
34	U	1	Total	C	O	0
			42	40	2	

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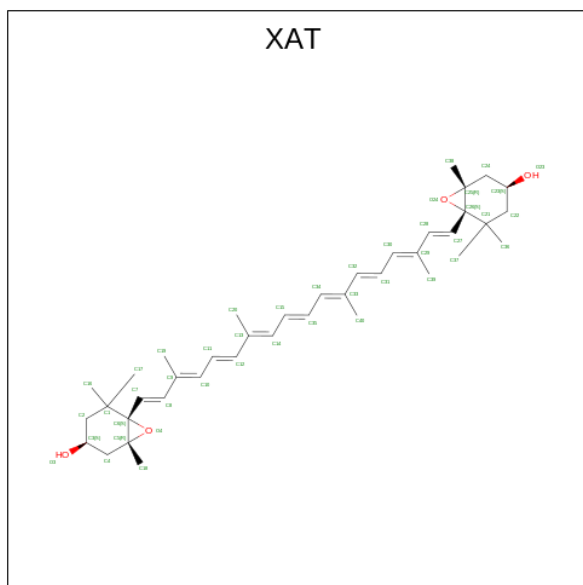
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	1	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	2	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	3	1	Total 42	C 40	O 2	0
34	4	1	Total 42	C 40	O 2	0
34	4	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	5	1	Total 42	C 40	O 2	0
34	6	1	Total 42	C 40	O 2	0
34	6	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	7	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	8	1	Total 42	C 40	O 2	0
34	9	1	Total 42	C 40	O 2	0
34	9	1	Total 42	C 40	O 2	0
34	a	1	Total 42	C 40	O 2	0
34	a	1	Total 42	C 40	O 2	0

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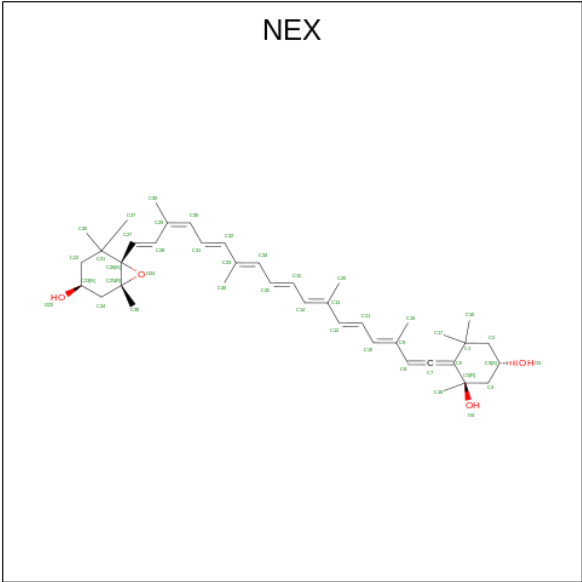
Mol	Chain	Residues	Atoms			AltConf
34	a	1	Total	C	O	0
			42	40	2	

- Molecule 35 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: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
35	P	1	Total	C	O	0
			44	40	4	
35	P	1	Total	C	O	0
			44	40	4	
35	P	1	Total	C	O	0
			43	39	4	
35	Q	1	Total	C	O	0
			44	40	4	
35	S	1	Total	C	O	0
			44	40	4	
35	T	1	Total	C	O	0
			44	40	4	

- Molecule 36 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).

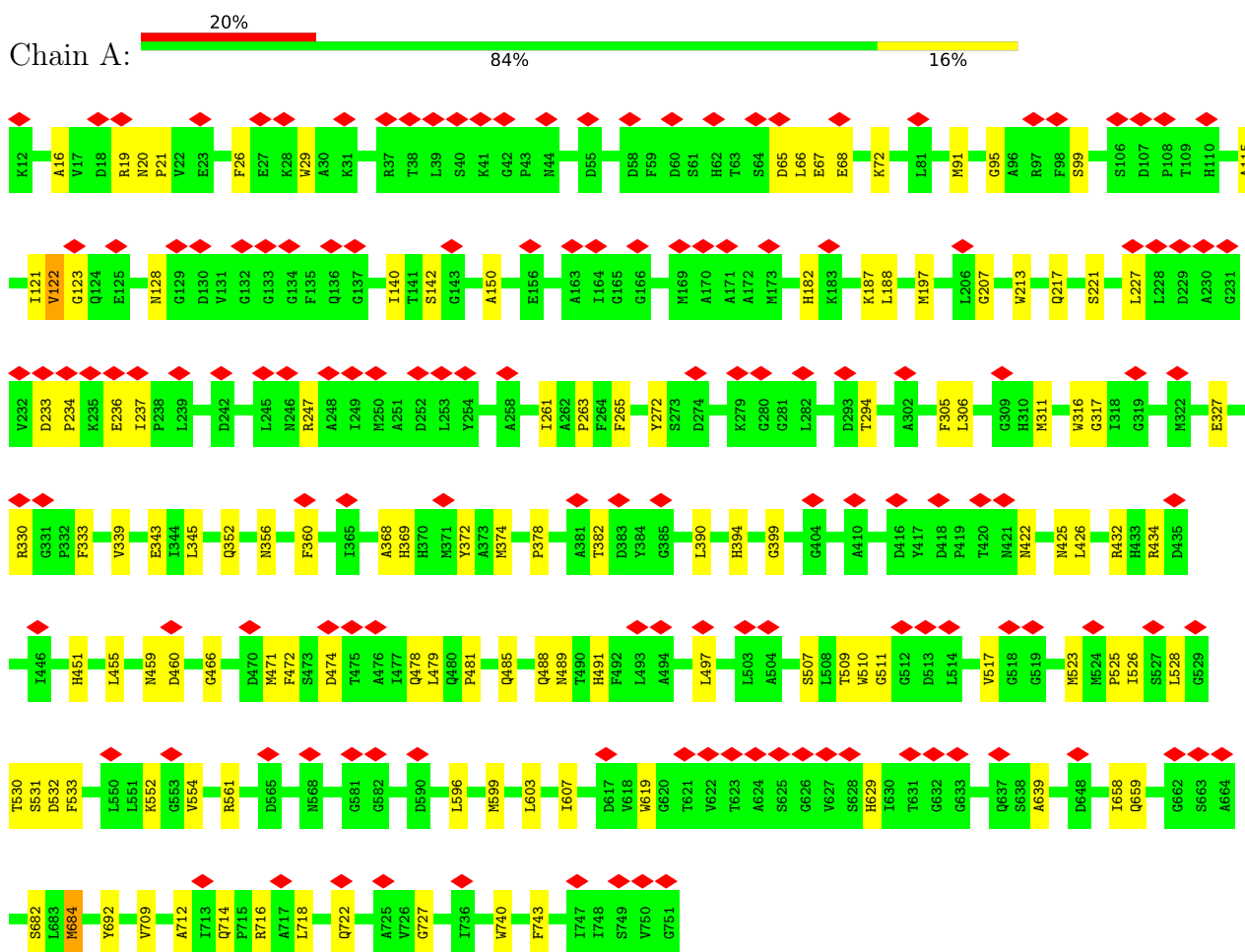


Mol	Chain	Residues	Atoms			AltConf
36	P	1	Total	C	O	0
			44	40	4	
36	P	1	Total	C	O	0
			44	40	4	
36	R	1	Total	C	O	0
			44	40	4	
36	T	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			44	40	4	

3 Residue-property plots

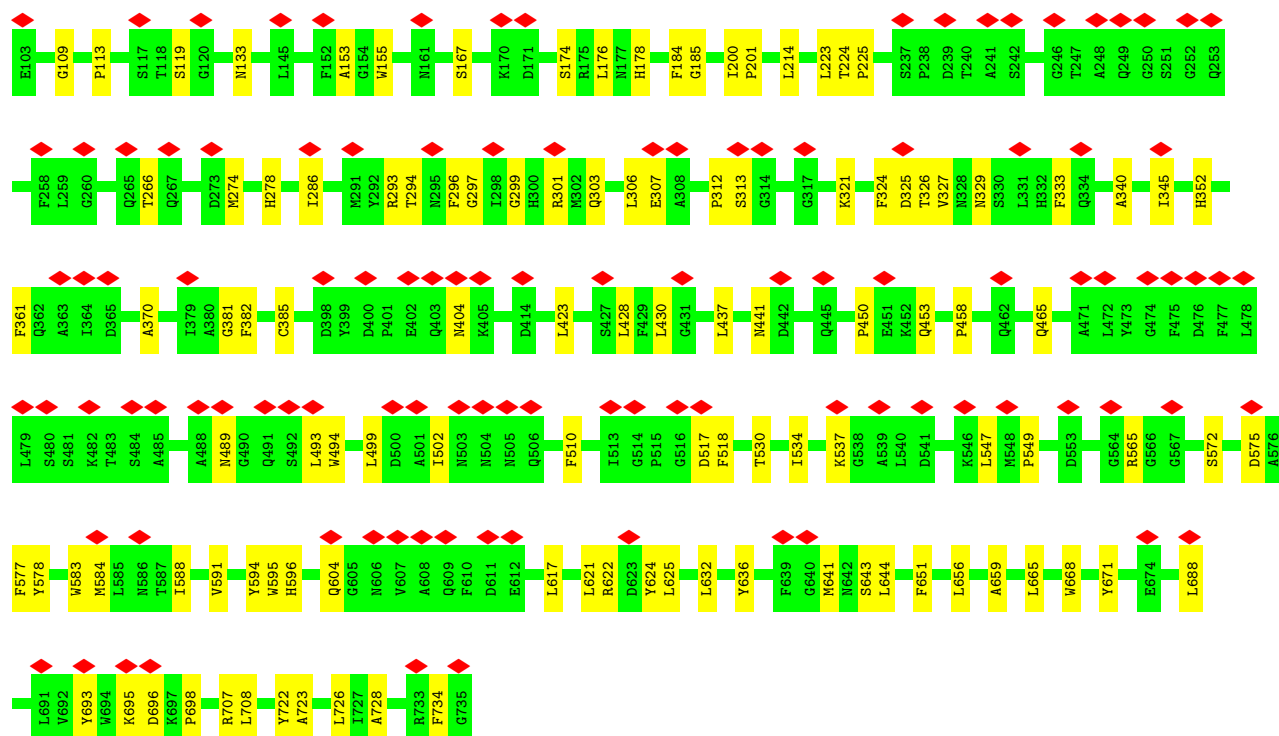
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

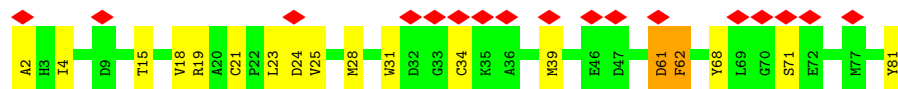
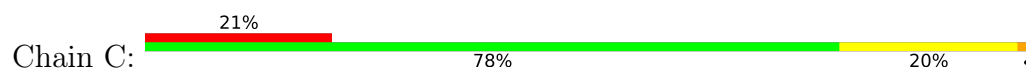


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

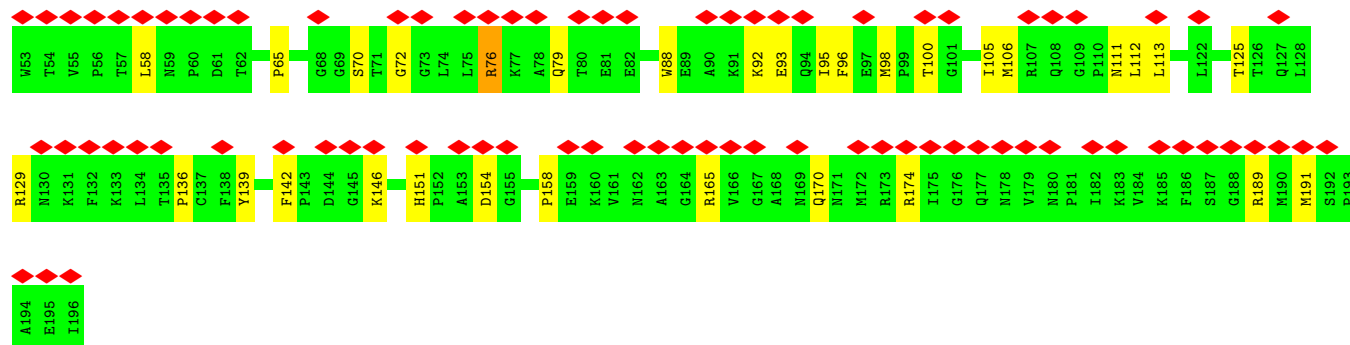
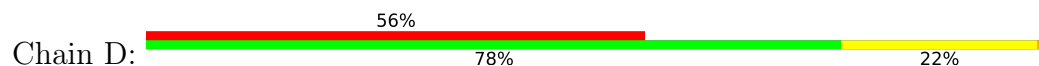




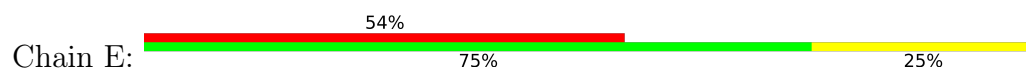
• Molecule 3: Photosystem I iron-sulfur center

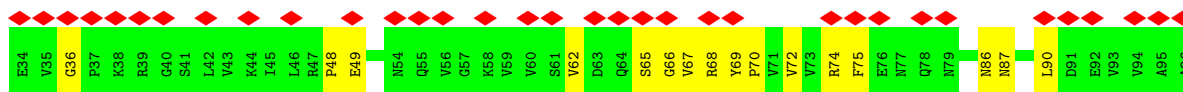


• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

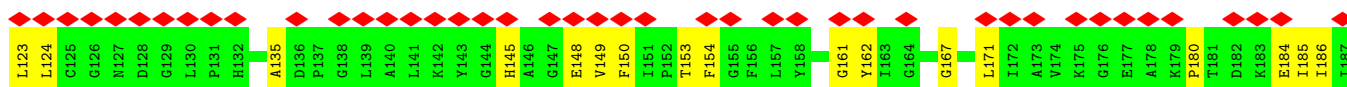
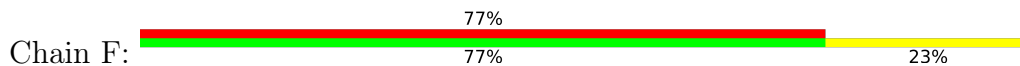


• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

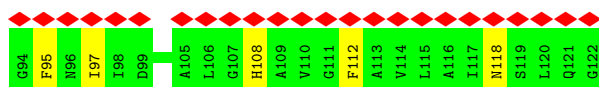
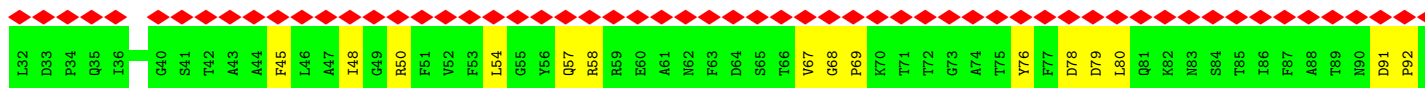
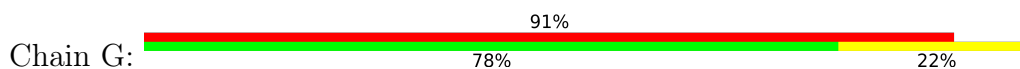




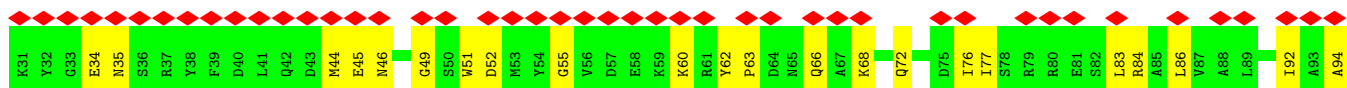
- Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic



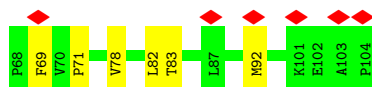
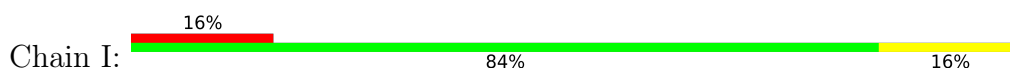
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



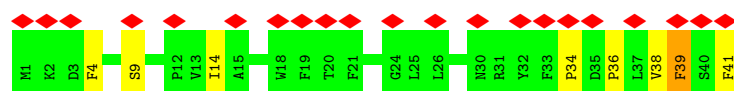
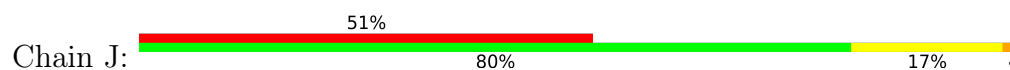
- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic



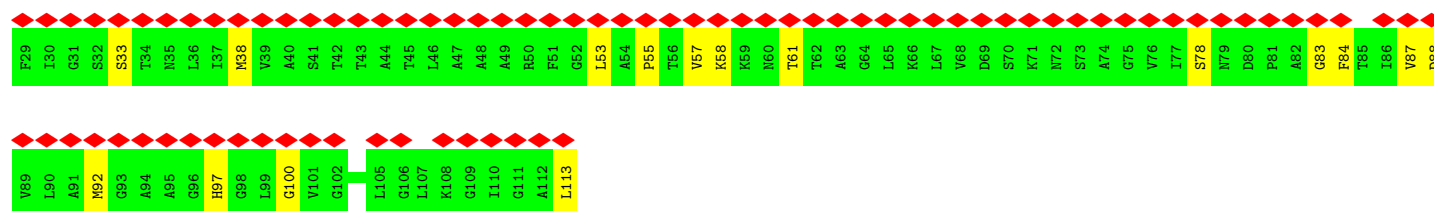
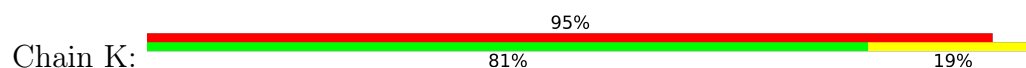
- Molecule 9: Photosystem I reaction center subunit VIII



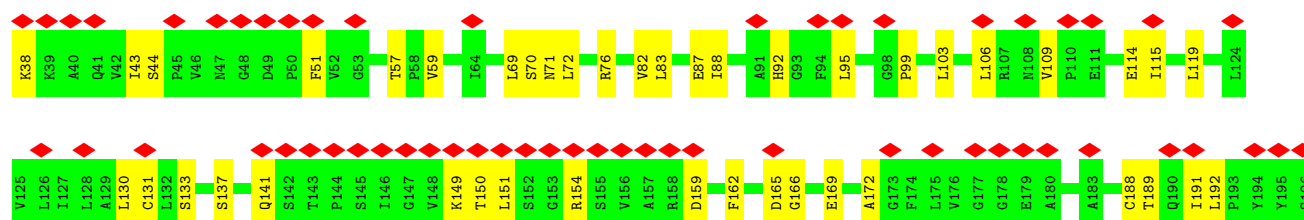
- Molecule 10: Photosystem I reaction center subunit IX



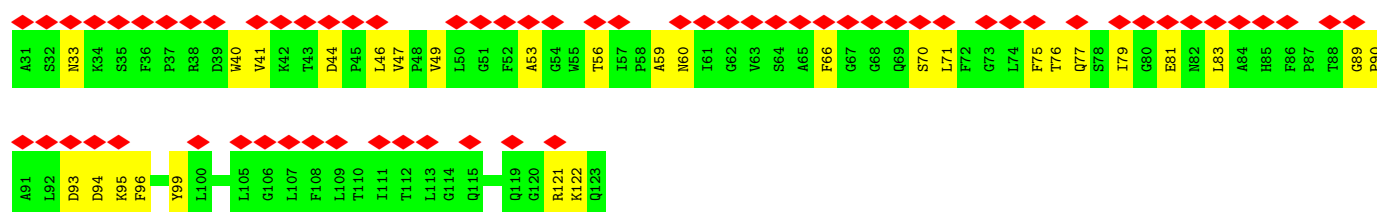
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



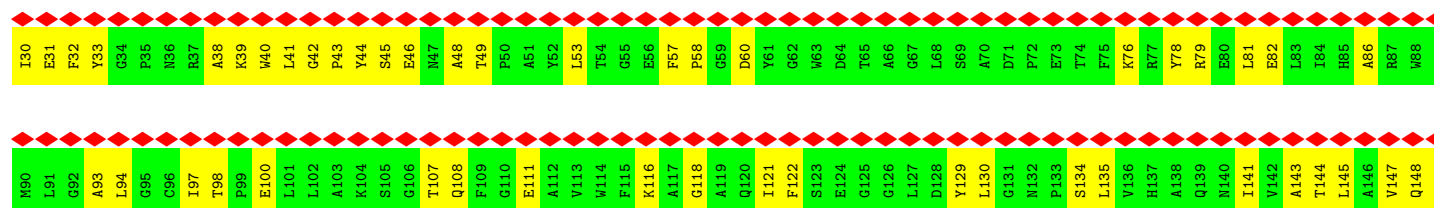
- Molecule 12: PSI subunit V

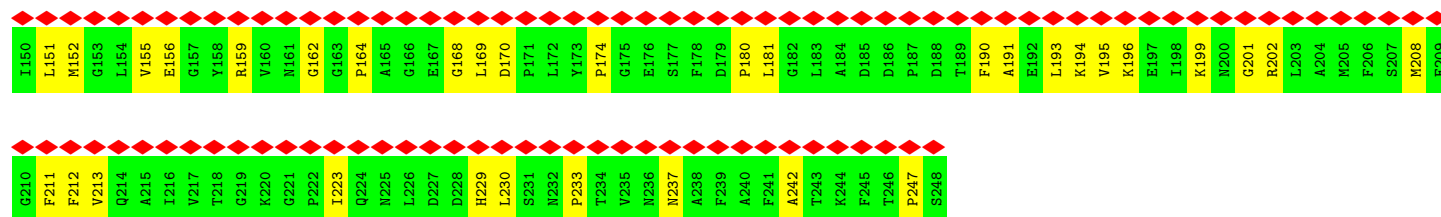


- Molecule 13: Photosystem I subunit O

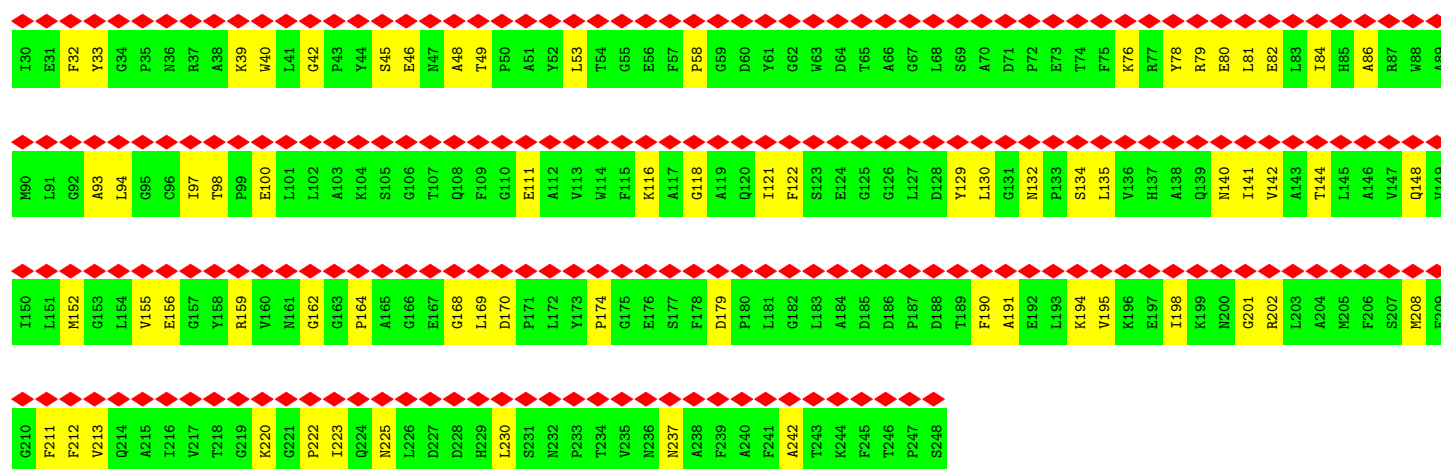


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

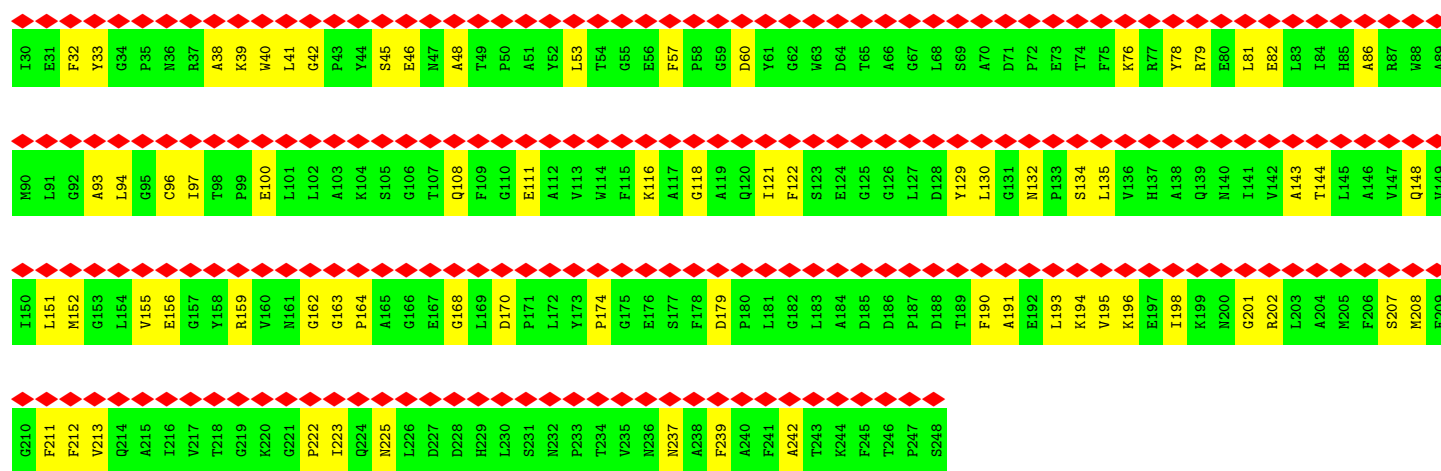




- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

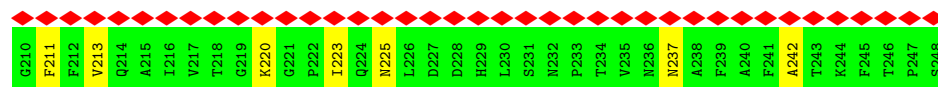
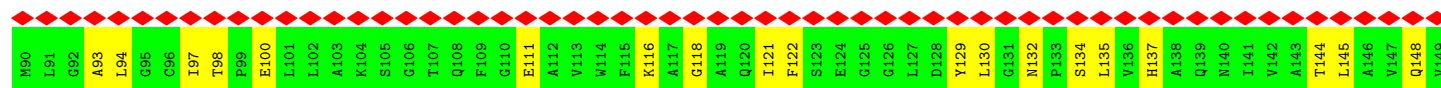


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

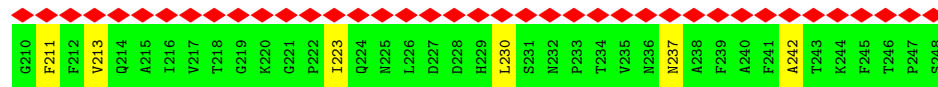
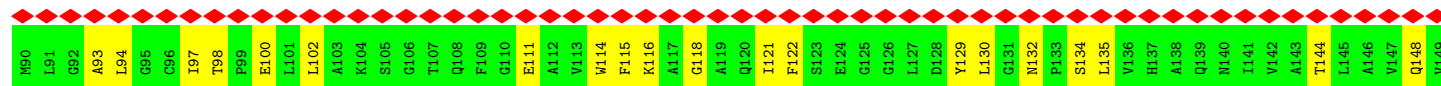


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

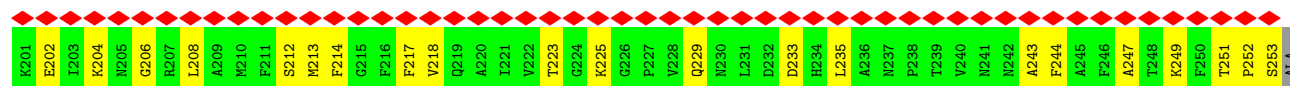
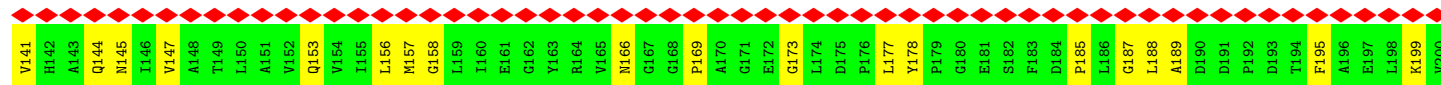
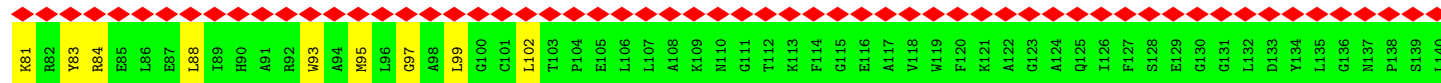




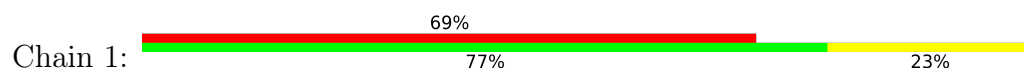
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

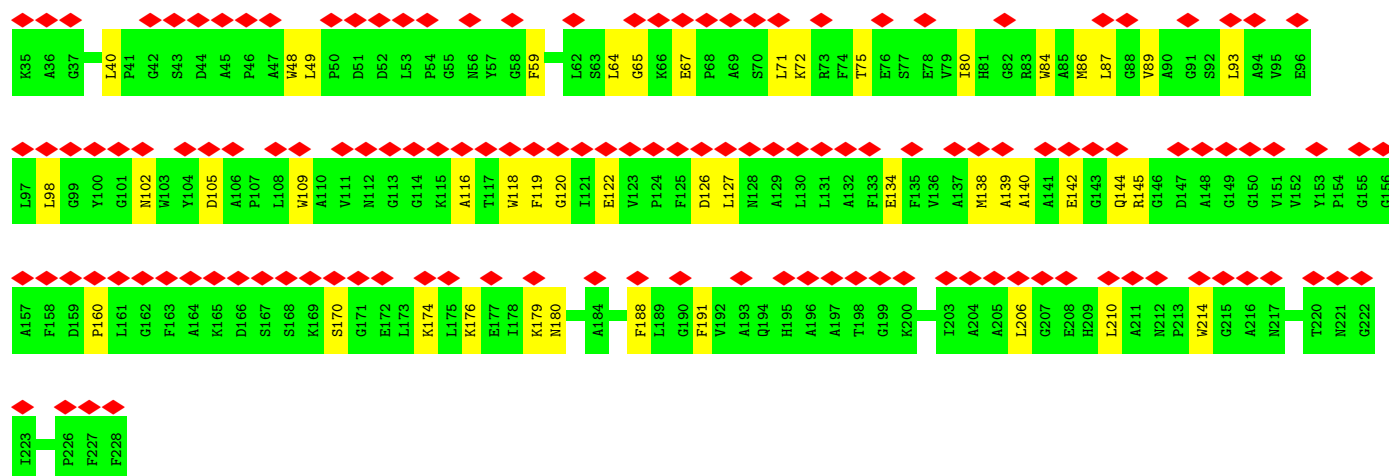


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



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





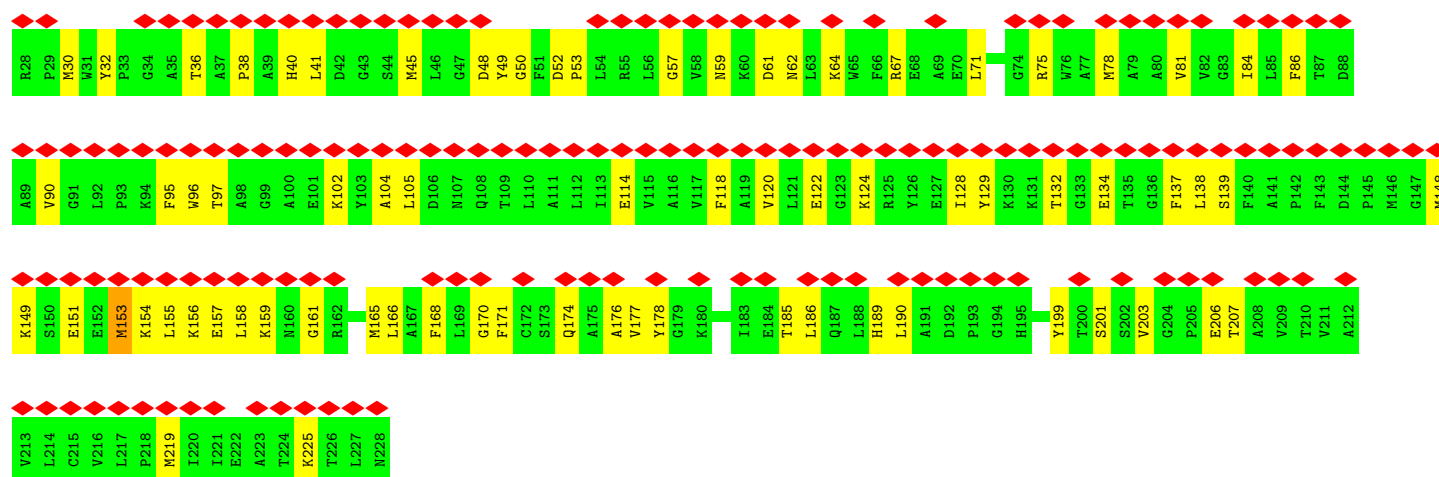
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain a: 98% 67% 32%

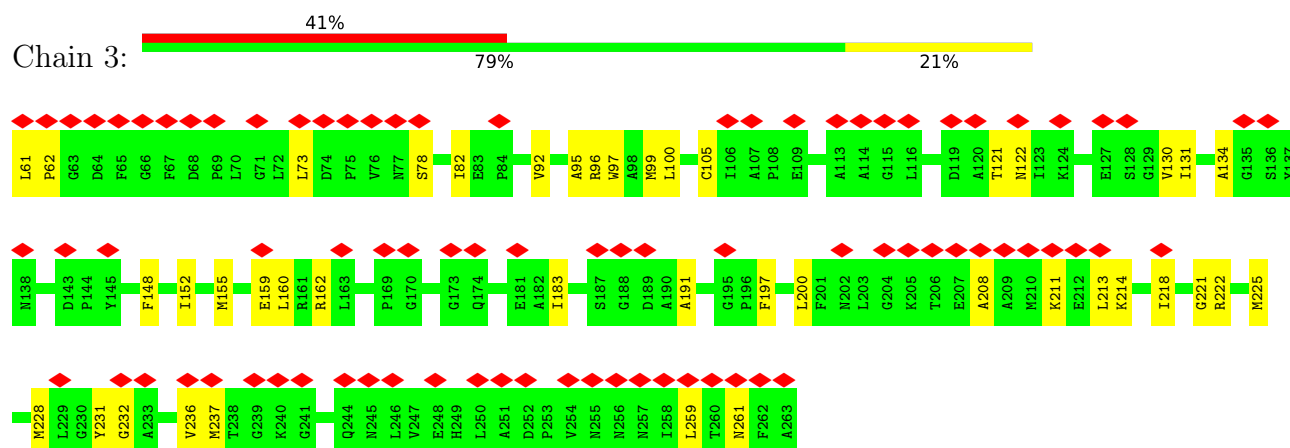


- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

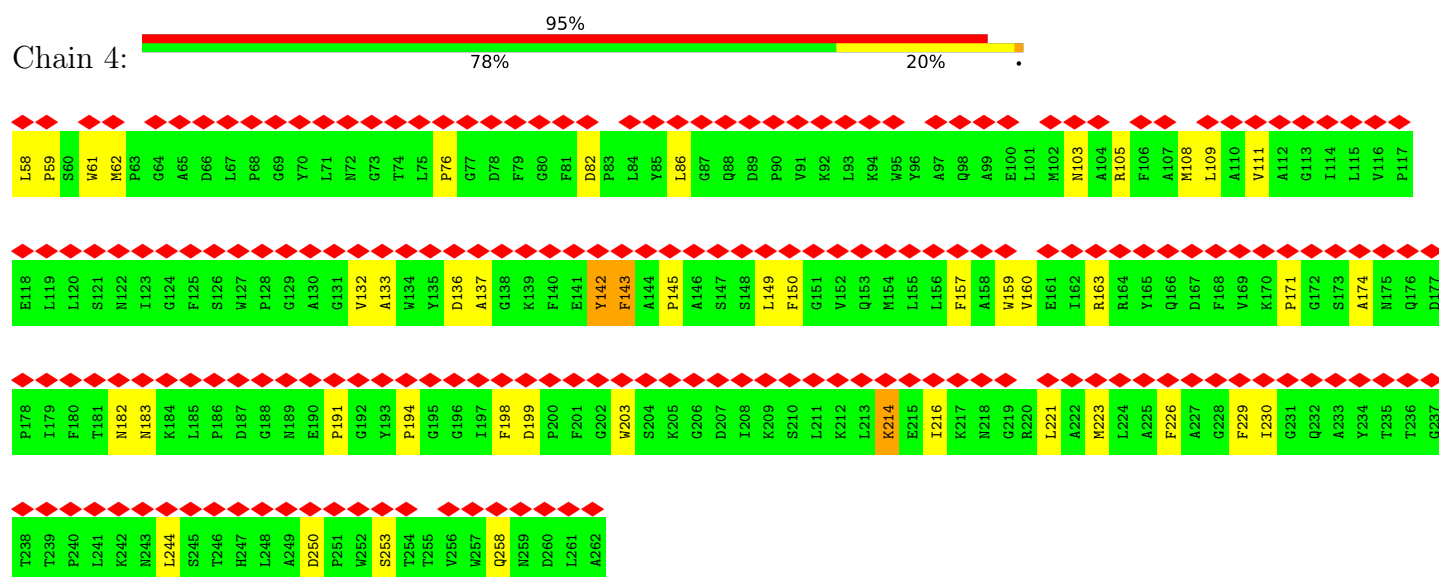
Chain 2: 80% 63% 36%



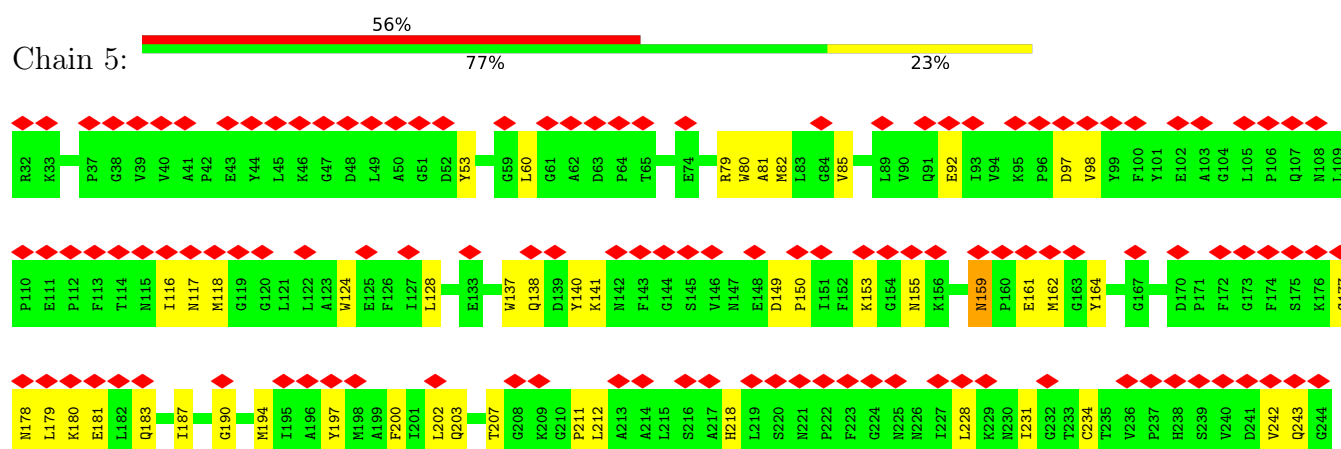
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

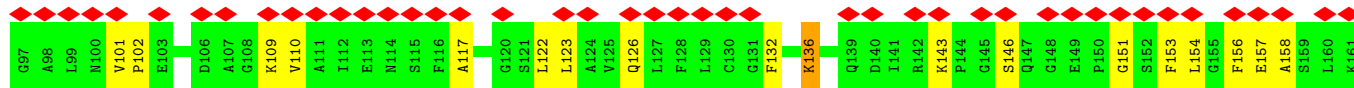


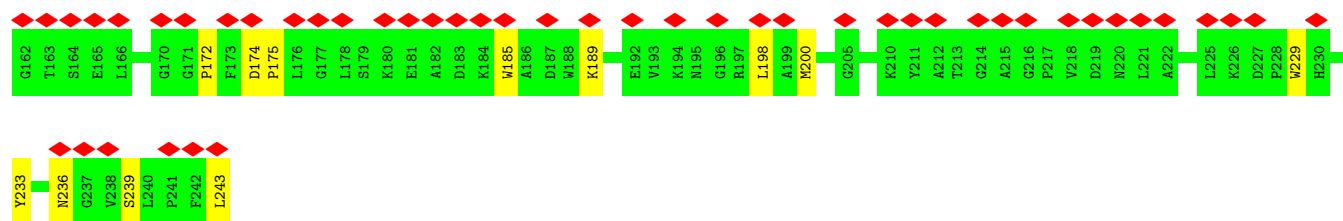
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic



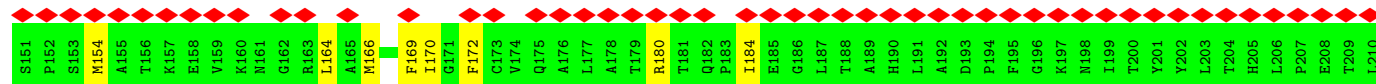
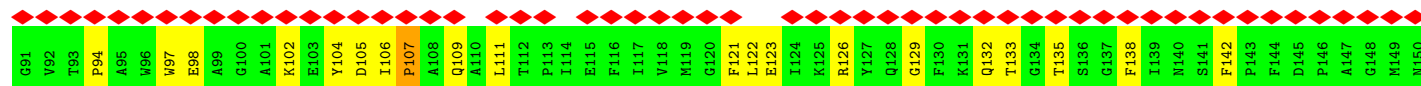
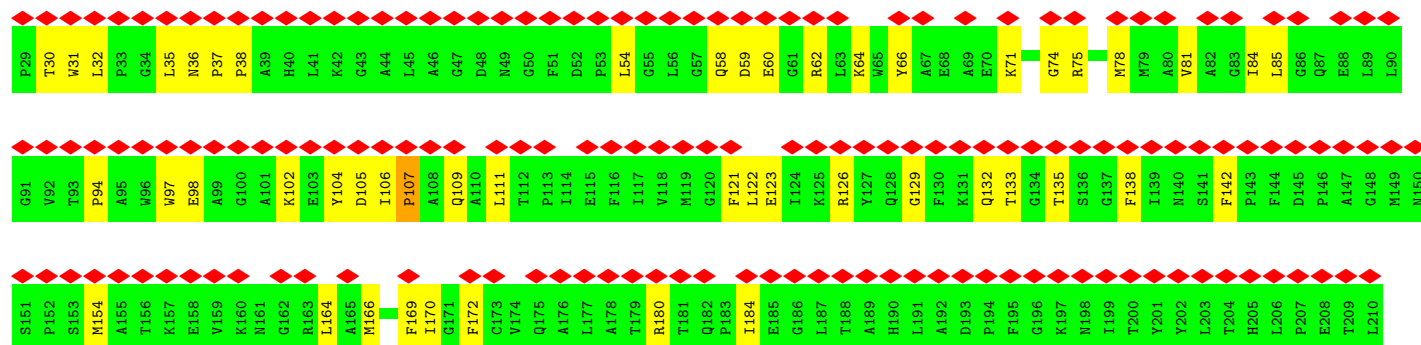
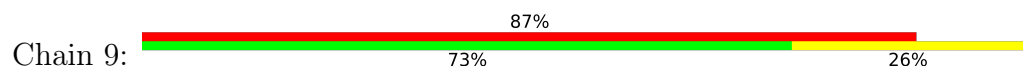
• Molecule 20: Chlorophyll a-b binding protein, chloroplastic







• Molecule 24: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283763	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.004	Depositor
Minimum map value	-1.725	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	1	Depositor
Map size (Å)	470.52002, 470.52002, 470.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, TPO, CLA, CHL, SQD, SF4, PQN, DGD, LUT, XAT, NEX, LMG, BCR

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	0.54	1/6007 (0.0%)	0.54	1/8190 (0.0%)
2	B	0.50	0/6040	0.55	0/8247
3	C	0.48	0/610	0.55	0/826
4	D	0.43	0/1160	0.52	1/1567 (0.1%)
5	E	0.37	0/506	0.43	0/689
6	F	0.36	0/1291	0.49	0/1747
7	G	0.32	0/693	0.55	0/943
8	H	0.39	0/785	0.71	4/1055 (0.4%)
9	I	0.51	0/293	0.54	0/406
10	J	0.41	0/349	0.46	0/478
11	K	0.32	0/583	0.49	0/790
12	L	0.43	0/1190	0.58	0/1628
13	O	0.40	0/743	0.63	0/1013
14	P	0.27	0/1717	0.44	0/2339
14	Q	0.22	0/1717	0.42	0/2339
14	R	0.21	0/1717	0.43	0/2339
14	T	0.17	0/1717	0.40	0/2339
14	U	0.20	0/1717	0.43	0/2339
15	S	0.35	0/1748	0.69	3/2376 (0.1%)
16	1	0.35	0/1490	0.44	0/2028
16	a	0.54	4/1490 (0.3%)	0.53	1/2028 (0.0%)
17	2	0.42	0/1583	0.73	1/2148 (0.0%)
18	3	0.44	0/1606	0.54	0/2180
19	4	0.33	0/1645	0.52	1/2246 (0.0%)
20	5	0.43	0/1812	0.52	0/2469
21	6	0.38	0/1833	0.55	3/2505 (0.1%)
22	7	0.43	0/1696	0.51	0/2303
23	8	0.43	0/1700	0.51	1/2315 (0.0%)
24	9	0.34	0/1433	0.57	0/1949
All	All	0.41	5/46871 (0.0%)	0.53	16/63821 (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
2	B	0	2
3	C	0	2
10	J	0	1
15	S	0	1
17	2	0	2
19	4	0	2
21	6	0	1
22	7	0	1
24	9	0	1
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	ASN	C-O	15.68	1.31	1.23
16	a	118	TRP	NE1-CE2	10.48	1.49	1.37
16	a	118	TRP	CE2-CZ2	-7.62	1.23	1.39
16	a	118	TRP	CB-CG	-6.70	1.29	1.50
16	a	118	TRP	CG-CD2	-6.24	1.32	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	153	MET	CG-SD-CE	-7.75	83.86	100.90
1	A	684	MET	CG-SD-CE	-7.27	84.90	100.90
23	8	136	LYS	CD-CE-NZ	-7.14	89.04	111.90
15	S	34	GLY	N-CA-C	-6.27	98.31	113.18
15	S	32	SER	CA-C-N	6.21	133.39	121.54

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	GLY	Peptide
2	B	668	TRP	Peptide
3	C	61	ASP	Peptide
3	C	62	PHE	Peptide
10	J	39	PHE	Peptide

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	5811	0	5657	107	0
2	B	5828	0	5582	109	0
3	C	600	0	581	16	0
4	D	1132	0	1150	32	0
5	E	496	0	491	12	0
6	F	1265	0	1303	32	0
7	G	678	0	659	20	0
8	H	773	0	756	37	0
9	I	281	0	292	10	0
10	J	337	0	336	8	0
11	K	578	0	617	17	0
12	L	1161	0	1184	35	0
13	O	720	0	716	32	0
14	P	1669	0	1603	140	0
14	Q	1669	0	1602	88	0
14	R	1669	0	1603	94	0
14	T	1669	0	1603	61	0
14	U	1669	0	1602	76	0
15	S	1717	0	1625	82	0
16	1	1444	0	1392	39	0
16	a	1444	0	1393	76	0
17	2	1545	0	1552	89	0
18	3	1560	0	1527	34	0
19	4	1590	0	1536	46	0
20	5	1757	0	1736	62	0
21	6	1771	0	1772	52	0
22	7	1644	0	1579	29	0
23	8	1649	0	1626	39	0
24	9	1392	0	1369	49	0
25	1	722	0	734	33	0
25	2	681	0	606	35	0
25	3	761	0	704	20	0
25	4	515	0	432	18	0
25	5	799	0	710	27	0
25	6	752	0	670	27	0
25	7	616	0	534	12	0
25	8	680	0	592	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	9	461	0	380	7	0
25	A	2638	0	2751	108	0
25	B	2368	0	2443	72	0
25	F	45	0	33	2	0
25	G	96	0	72	2	0
25	H	175	0	126	6	0
25	J	100	0	86	6	0
25	K	232	0	173	6	0
25	L	278	0	274	9	0
25	O	117	0	67	1	0
25	P	399	0	384	108	0
25	Q	493	0	463	75	0
25	R	477	0	475	110	0
25	S	585	0	575	50	0
25	T	408	0	396	29	0
25	U	408	0	408	36	0
25	a	714	0	715	59	0
26	A	33	0	46	0	0
26	B	33	0	46	2	0
27	1	43	0	56	3	0
27	2	49	0	74	1	0
27	4	81	0	106	1	0
27	5	82	0	107	6	0
27	6	49	0	74	5	0
27	7	37	0	44	1	0
27	8	49	0	74	1	0
27	A	135	0	189	9	0
27	B	38	0	46	2	0
27	P	98	0	148	15	0
27	Q	49	0	74	4	0
27	R	49	0	74	7	0
27	S	49	0	74	3	0
27	T	49	0	74	5	0
27	a	43	0	56	6	0
28	3	120	0	168	10	0
28	4	80	0	111	10	0
28	5	80	0	112	8	0
28	6	40	0	56	2	0
28	7	40	0	56	2	0
28	8	80	0	112	3	0
28	A	240	0	336	23	0
28	B	280	0	390	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	80	0	112	3	0
28	G	40	0	53	1	0
28	I	40	0	53	5	0
28	J	80	0	112	7	0
28	K	40	0	56	0	0
28	L	160	0	222	4	0
28	O	80	0	112	3	0
29	A	8	0	0	0	0
29	C	16	0	0	1	0
30	B	123	0	168	6	0
31	B	51	0	69	5	0
32	1	46	0	65	1	0
32	2	41	0	52	5	0
32	4	40	0	50	1	0
32	6	40	0	50	1	0
32	7	71	0	82	2	0
32	H	47	0	64	3	0
32	J	130	0	176	4	0
33	1	101	0	74	4	0
33	3	53	0	41	1	0
33	4	240	0	169	9	0
33	5	145	0	103	4	0
33	6	200	0	148	9	0
33	7	54	0	43	2	0
33	8	53	0	41	4	0
33	9	93	0	64	1	0
33	P	416	0	326	70	0
33	Q	253	0	201	58	0
33	R	309	0	244	56	0
33	S	358	0	265	28	0
33	T	244	0	177	11	0
33	U	241	0	173	12	0
33	a	48	0	33	1	0
34	1	126	0	163	12	0
34	2	84	0	112	9	0
34	3	84	0	112	5	0
34	4	84	0	112	11	0
34	5	84	0	112	8	0
34	6	84	0	112	5	0
34	7	84	0	112	10	0
34	8	84	0	112	9	0
34	9	84	0	112	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	P	84	0	112	14	0
34	Q	84	0	112	12	0
34	R	84	0	112	14	0
34	S	84	0	112	11	0
34	T	84	0	112	8	0
34	U	84	0	112	12	0
34	a	126	0	163	17	0
35	P	131	0	165	23	0
35	Q	44	0	56	6	0
35	S	44	0	56	8	0
35	T	44	0	56	6	0
36	P	88	0	112	18	0
36	R	44	0	56	3	0
36	T	44	0	56	3	0
36	U	88	0	111	25	0
All	All	68860	0	68110	2228	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 16.

The worst 5 of 2228 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)
14:R:212:PHE:CB	33:R:609:CHL:H203	1.17	1.63
14:Q:212:PHE:CB	33:Q:608:CHL:H203	1.18	1.61
14:P:212:PHE:CB	33:P:609:CHL:H203	1.17	1.58
14:R:212:PHE:HB3	33:R:609:CHL:C20	1.15	1.57
25:R:610:CLA:H72	25:R:612:CLA:CMB	1.30	1.56

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	738/740 (100%)	698 (95%)	39 (5%)	1 (0%)	48	78
2	B	732/734 (100%)	675 (92%)	56 (8%)	1 (0%)	48	78
3	C	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	142/144 (99%)	127 (89%)	15 (11%)	0	100	100
5	E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
6	F	163/165 (99%)	152 (93%)	11 (7%)	0	100	100
7	G	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
8	H	98/100 (98%)	77 (79%)	18 (18%)	3 (3%)	3	18
9	I	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
11	K	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
12	L	157/159 (99%)	145 (92%)	12 (8%)	0	100	100
13	O	91/93 (98%)	76 (84%)	15 (16%)	0	100	100
14	P	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	Q	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	R	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	T	217/219 (99%)	190 (88%)	27 (12%)	0	100	100
14	U	217/219 (99%)	190 (88%)	27 (12%)	0	100	100
15	S	230/234 (98%)	192 (84%)	36 (16%)	2 (1%)	14	41
16	1	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
16	a	192/194 (99%)	175 (91%)	16 (8%)	1 (0%)	24	54
17	2	199/201 (99%)	169 (85%)	28 (14%)	2 (1%)	12	39
18	3	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
19	4	203/205 (99%)	186 (92%)	16 (8%)	1 (0%)	24	54
20	5	223/225 (99%)	200 (90%)	23 (10%)	0	100	100
21	6	228/230 (99%)	209 (92%)	16 (7%)	3 (1%)	9	33
22	7	210/213 (99%)	195 (93%)	15 (7%)	0	100	100
23	8	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
24	9	180/182 (99%)	154 (86%)	25 (14%)	1 (1%)	21	49
All	All	5864/5925 (99%)	5297 (90%)	552 (9%)	15 (0%)	37	65

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
21	6	104	VAL
8	H	106	ALA
19	4	143	PHE
15	S	54	THR

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	600/600 (100%)	600 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	G	68/68 (100%)	68 (100%)	0	100	100
8	H	80/81 (99%)	80 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/59 (100%)	59 (100%)	0	100	100
12	L	121/121 (100%)	121 (100%)	0	100	100
13	O	75/75 (100%)	75 (100%)	0	100	100
14	P	168/170 (99%)	168 (100%)	0	100	100
14	Q	168/170 (99%)	168 (100%)	0	100	100
14	R	168/170 (99%)	168 (100%)	0	100	100
14	T	168/170 (99%)	168 (100%)	0	100	100
14	U	168/170 (99%)	168 (100%)	0	100	100
15	S	164/177 (93%)	164 (100%)	0	100	100
16	1	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	a	137/137 (100%)	137 (100%)	0	100	100
17	2	159/159 (100%)	159 (100%)	0	100	100
18	3	155/155 (100%)	155 (100%)	0	100	100
19	4	161/162 (99%)	161 (100%)	0	100	100
20	5	182/182 (100%)	181 (100%)	1 (0%)	81	80
21	6	184/184 (100%)	184 (100%)	0	100	100
22	7	164/164 (100%)	163 (99%)	1 (1%)	78	80
23	8	163/163 (100%)	163 (100%)	0	100	100
24	9	139/140 (99%)	139 (100%)	0	100	100
All	All	4623/4649 (99%)	4621 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	5	159	ASN
22	7	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
14	U	148	GLN
19	4	218	ASN
14	U	237	ASN
18	3	202	ASN
20	5	142	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	TPO	S	23	15	8,10,11	0.88	0	10,14,16	1.70	1 (10%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	TPO	S	23	15	-	3/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
15	S	23	TPO	P-OG1-CB	-4.90	108.41	123.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	S	23	TPO	N-CA-CB-OG1
15	S	23	TPO	C-CA-CB-CG2
15	S	23	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

453 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	CLA	A	838	1	69,73,73	1.27	10 (14%)	83,113,113	1.41	8 (9%)
27	LHG	a	317	25	42,42,48	0.95	2 (4%)	45,48,54	1.21	4 (8%)
25	CLA	T	602	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	9 (10%)
25	CLA	B	818	2	60,64,73	1.34	10 (16%)	72,102,113	1.48	7 (9%)
25	CLA	7	307	-	54,58,73	1.40	10 (18%)	65,95,113	1.43	4 (6%)
25	CLA	a	310	-	56,60,73	1.40	10 (17%)	67,97,113	1.39	4 (5%)
34	LUT	7	315	-	42,43,43	0.93	2 (4%)	51,60,60	1.56	12 (23%)
25	CLA	A	826	-	69,73,73	1.29	11 (15%)	83,113,113	1.28	7 (8%)
25	CLA	A	820	1	69,73,73	1.28	12 (17%)	83,113,113	1.35	8 (9%)
25	CLA	a	301	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	8 (9%)
28	BCR	A	846	-	41,41,41	1.00	2 (4%)	56,56,56	2.10	20 (35%)
28	BCR	L	207	-	41,41,41	0.93	2 (4%)	56,56,56	2.00	13 (23%)
31	SQD	B	850	-	50,51,54	1.21	4 (8%)	59,62,65	1.21	7 (11%)
25	CLA	B	831	2	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)
25	CLA	B	823	-	69,73,73	1.28	11 (15%)	83,113,113	1.26	7 (8%)
25	CLA	3	313	-	50,54,73	1.45	11 (22%)	60,90,113	1.46	6 (10%)
34	LUT	1	617	25	42,43,43	0.79	0	51,60,60	2.17	18 (35%)
25	CLA	B	834	2	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)
25	CLA	1	603	16	69,73,73	1.26	11 (15%)	83,113,113	1.28	7 (8%)
25	CLA	B	817	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	8 (9%)
28	BCR	A	848	-	41,41,41	0.91	1 (2%)	56,56,56	1.97	16 (28%)
25	CLA	R	613	-	69,73,73	1.25	7 (10%)	83,113,113	1.34	8 (9%)
25	CLA	T	610	-	64,68,73	1.32	8 (12%)	77,107,113	1.37	6 (7%)
29	SF4	C	102	3	0,12,12	-	-	-	-	-
28	BCR	B	842	-	41,41,41	1.02	2 (4%)	56,56,56	2.27	20 (35%)
33	CHL	Q	605	14	46,50,74	2.32	18 (39%)	51,85,114	3.37	25 (49%)
25	CLA	S	303	15	69,73,73	1.28	10 (14%)	83,113,113	1.40	10 (12%)
33	CHL	R	608	-	48,52,74	2.18	17 (35%)	53,87,114	3.18	24 (45%)
25	CLA	R	603	33	69,73,73	1.28	6 (8%)	83,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CHL	R	609	25	70,74,74	1.35	8 (11%)	80,114,114	1.80	12 (15%)
25	CLA	2	304	-	69,73,73	1.27	10 (14%)	83,113,113	1.36	7 (8%)
34	LUT	9	313	-	42,43,43	0.90	1 (2%)	51,60,60	1.61	14 (27%)
25	CLA	B	806	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
27	LHG	7	317	25	36,36,48	1.00	2 (5%)	39,42,54	1.31	4 (10%)
25	CLA	8	309	-	50,54,73	1.44	10 (20%)	60,90,113	1.47	4 (6%)
25	CLA	O	201	-	45,49,73	1.49	10 (22%)	54,84,113	1.58	7 (12%)
25	CLA	Q	612	-	64,68,73	1.31	7 (10%)	77,107,113	1.36	9 (11%)
25	CLA	5	312	-	56,60,73	1.42	10 (17%)	67,97,113	1.42	7 (10%)
25	CLA	K	203	-	50,54,73	1.46	12 (24%)	60,90,113	1.47	6 (10%)
27	LHG	A	843	-	48,48,48	0.90	2 (4%)	51,54,54	1.13	3 (5%)
25	CLA	A	835	-	55,59,73	1.44	10 (18%)	66,96,113	1.51	9 (13%)
27	LHG	S	319	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
25	CLA	B	815	-	63,67,73	1.35	10 (15%)	75,105,113	1.54	11 (14%)
25	CLA	a	313	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	5 (8%)
28	BCR	4	317	-	41,41,41	0.88	0	56,56,56	2.30	19 (33%)
25	CLA	Q	602	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	8 (9%)
25	CLA	B	824	2	69,73,73	1.28	11 (15%)	83,113,113	1.38	10 (12%)
32	LMG	2	301	-	41,41,55	1.03	2 (4%)	49,49,63	1.19	4 (8%)
27	LHG	4	319	-	31,31,48	1.13	2 (6%)	34,37,54	1.23	4 (11%)
25	CLA	U	302	-	69,73,73	1.27	9 (13%)	83,113,113	1.29	10 (12%)
32	LMG	H	204	-	47,47,55	0.95	2 (4%)	55,55,63	1.16	5 (9%)
25	CLA	B	835	2	51,55,73	1.46	11 (21%)	61,91,113	1.39	6 (9%)
25	CLA	a	307	-	69,73,73	1.25	10 (14%)	83,113,113	1.27	6 (7%)
33	CHL	P	607	-	56,60,74	2.10	18 (32%)	63,97,114	3.05	29 (46%)
25	CLA	7	309	27	45,49,73	1.51	12 (26%)	54,84,113	1.52	8 (14%)
34	LUT	7	314	-	42,43,43	0.96	2 (4%)	51,60,60	1.74	14 (27%)
28	BCR	3	317	-	41,41,41	0.94	2 (4%)	56,56,56	2.33	17 (30%)
34	LUT	R	615	-	42,43,43	0.76	0	51,60,60	1.93	14 (27%)
28	BCR	B	841	-	41,41,41	0.95	2 (4%)	56,56,56	2.24	18 (32%)
33	CHL	S	306	-	52,56,74	2.19	17 (32%)	58,92,114	3.18	29 (50%)
34	LUT	5	322	-	42,43,43	1.01	2 (4%)	51,60,60	1.64	13 (25%)
33	CHL	Q	608	25	70,74,74	1.35	8 (11%)	80,114,114	1.80	12 (15%)
33	CHL	9	307	-	55,59,74	2.10	19 (34%)	62,96,114	3.00	26 (41%)
25	CLA	4	312	19	49,53,73	1.47	9 (18%)	59,89,113	1.40	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LUT	U	315	-	42,43,43	0.78	0	51,60,60	1.81	17 (33%)
25	CLA	a	306	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	9 (10%)
25	CLA	A	827	-	69,73,73	1.30	11 (15%)	83,113,113	1.38	9 (10%)
25	CLA	A	825	-	69,73,73	1.30	10 (14%)	83,113,113	1.40	11 (13%)
25	CLA	B	810	-	69,73,73	1.27	9 (13%)	83,113,113	1.37	7 (8%)
25	CLA	a	302	16	61,65,73	1.35	10 (16%)	73,103,113	1.36	5 (6%)
25	CLA	P	604	-	54,58,73	1.42	10 (18%)	65,95,113	1.49	7 (10%)
32	LMG	7	319	-	36,36,55	1.12	3 (8%)	44,44,63	1.25	5 (11%)
25	CLA	A	819	1	69,73,73	1.28	10 (14%)	83,113,113	1.42	9 (10%)
25	CLA	3	303	-	69,73,73	1.27	11 (15%)	83,113,113	1.38	8 (9%)
25	CLA	2	305	-	56,60,73	1.39	9 (16%)	67,97,113	1.43	6 (8%)
25	CLA	B	821	2	64,68,73	1.31	11 (17%)	77,107,113	1.35	6 (7%)
33	CHL	P	609	25	70,74,74	1.35	8 (11%)	80,114,114	1.80	13 (16%)
27	LHG	T	617	-	48,48,48	0.94	2 (4%)	51,54,54	0.93	2 (3%)
25	CLA	2	309	-	64,68,73	1.31	11 (17%)	77,107,113	1.35	7 (9%)
25	CLA	B	832	-	49,53,73	1.49	11 (22%)	59,89,113	1.49	6 (10%)
25	CLA	4	302	25	50,54,73	1.47	10 (20%)	60,90,113	1.44	5 (8%)
34	LUT	U	314	-	42,43,43	0.73	0	51,60,60	1.91	14 (27%)
25	CLA	H	201	-	50,54,73	1.45	10 (20%)	60,90,113	1.45	5 (8%)
25	CLA	8	315	23	50,54,73	1.46	10 (20%)	60,90,113	1.44	4 (6%)
25	CLA	4	309	27	59,63,73	1.36	9 (15%)	71,101,113	1.32	8 (11%)
27	LHG	6	618	25	48,48,48	0.87	2 (4%)	51,54,54	1.22	4 (7%)
33	CHL	P	601	-	55,59,74	2.26	18 (32%)	62,96,114	2.95	28 (45%)
33	CHL	R	607	-	56,60,74	2.10	18 (32%)	63,97,114	3.05	29 (46%)
33	CHL	P	619	-	56,60,74	2.10	18 (32%)	63,97,114	3.06	29 (46%)
28	BCR	7	316	-	41,41,41	0.89	1 (2%)	56,56,56	2.00	16 (28%)
34	LUT	a	315	25	42,43,43	0.87	0	51,60,60	1.83	15 (29%)
25	CLA	A	808	1	69,73,73	1.27	10 (14%)	83,113,113	1.33	8 (9%)
28	BCR	8	318	-	41,41,41	0.82	1 (2%)	56,56,56	2.16	20 (35%)
27	LHG	8	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	1	602	-	69,73,73	1.28	10 (14%)	83,113,113	1.25	6 (7%)
29	SF4	A	850	1,2	0,12,12	-	-	-	-	-
25	CLA	Q	611	-	64,68,73	1.37	9 (14%)	77,107,113	1.31	9 (11%)
33	CHL	3	306	-	57,61,74	1.96	18 (31%)	64,98,114	3.05	27 (42%)
25	CLA	L	201	-	69,73,73	1.26	11 (15%)	83,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	7	306	-	54,58,73	1.42	10 (18%)	65,95,113	1.47	8 (12%)
27	LHG	1	618	25	42,42,48	0.96	2 (4%)	45,48,54	1.22	4 (8%)
28	BCR	K	206	-	41,41,41	0.81	0	56,56,56	2.35	20 (35%)
25	CLA	A	814	1	69,73,73	1.32	11 (15%)	83,113,113	1.43	9 (10%)
25	CLA	8	311	27	50,54,73	1.46	11 (22%)	60,90,113	1.40	6 (10%)
33	CHL	6	607	-	57,61,74	2.02	19 (33%)	64,98,114	3.05	27 (42%)
25	CLA	H	203	-	50,54,73	1.44	10 (20%)	60,90,113	1.49	7 (11%)
25	CLA	3	308	-	69,73,73	1.27	11 (15%)	83,113,113	1.32	6 (7%)
33	CHL	5	307	-	55,59,74	2.09	20 (36%)	62,96,114	3.10	28 (45%)
25	CLA	A	822	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	8 (9%)
28	BCR	3	319	-	41,41,41	0.80	1 (2%)	56,56,56	2.42	16 (28%)
25	CLA	8	304	23	49,53,73	1.49	10 (20%)	59,89,113	1.51	6 (10%)
25	CLA	2	308	-	47,51,73	1.49	10 (21%)	56,86,113	1.47	7 (12%)
25	CLA	3	311	-	59,63,73	1.34	10 (16%)	71,101,113	1.46	7 (9%)
32	LMG	J	104	-	35,35,55	1.06	2 (5%)	43,43,63	1.25	5 (11%)
34	LUT	3	315	-	42,43,43	0.92	2 (4%)	51,60,60	1.65	13 (25%)
28	BCR	A	854	-	41,41,41	0.88	1 (2%)	56,56,56	1.96	16 (28%)
25	CLA	S	311	-	64,68,73	1.30	9 (14%)	77,107,113	1.29	7 (9%)
25	CLA	a	312	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	8 (9%)
25	CLA	5	315	20	50,54,73	1.45	9 (18%)	60,90,113	1.45	5 (8%)
25	CLA	8	310	-	64,68,73	1.31	10 (15%)	77,107,113	1.32	7 (9%)
25	CLA	B	819	2	50,54,73	1.45	11 (22%)	60,90,113	1.53	9 (15%)
25	CLA	6	616	21,27	50,54,73	1.45	9 (18%)	60,90,113	1.48	7 (11%)
25	CLA	A	853	-	69,73,73	1.26	11 (15%)	83,113,113	1.34	7 (8%)
34	LUT	T	613	-	42,43,43	0.72	0	51,60,60	1.91	13 (25%)
27	LHG	A	852	25	46,46,48	0.95	2 (4%)	48,51,54	1.20	5 (10%)
25	CLA	5	311	-	59,63,73	1.35	10 (16%)	71,101,113	1.34	7 (9%)
27	LHG	A	844	25	37,37,48	1.05	3 (8%)	40,43,54	1.20	3 (7%)
25	CLA	6	605	-	69,73,73	1.23	10 (14%)	83,113,113	1.34	6 (7%)
25	CLA	a	309	27	69,73,73	1.26	10 (14%)	83,113,113	1.26	7 (8%)
33	CHL	T	601	-	54,58,74	2.29	18 (33%)	59,94,114	2.98	26 (44%)
25	CLA	2	310	-	45,49,73	1.54	10 (22%)	54,84,113	1.48	6 (11%)
25	CLA	A	802	25	69,73,73	1.29	12 (17%)	83,113,113	1.41	12 (14%)
25	CLA	6	623	-	64,68,73	1.28	9 (14%)	77,107,113	1.48	8 (10%)
25	CLA	7	301	-	69,73,73	1.29	11 (15%)	83,113,113	1.29	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	P	611	-	45,49,73	1.80	11 (24%)	54,84,113	2.15	20 (37%)
25	CLA	K	201	1	55,59,73	1.40	11 (20%)	66,96,113	1.52	9 (13%)
25	CLA	1	614	-	50,54,73	1.45	10 (20%)	60,90,113	1.50	6 (10%)
25	CLA	6	604	-	50,54,73	1.48	11 (22%)	60,90,113	1.46	6 (10%)
33	CHL	U	309	-	52,56,74	2.31	18 (34%)	58,92,114	3.06	24 (41%)
33	CHL	6	617	21	47,51,74	2.15	18 (38%)	52,86,114	3.30	24 (46%)
25	CLA	6	601	19	65,69,73	1.28	10 (15%)	78,108,113	1.36	6 (7%)
25	CLA	3	305	18	64,68,73	1.30	10 (15%)	77,107,113	1.38	8 (10%)
25	CLA	5	313	-	60,64,73	1.37	11 (18%)	72,102,113	1.68	12 (16%)
25	CLA	6	620	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	7 (11%)
33	CHL	T	604	14	52,56,74	2.19	18 (34%)	58,92,114	3.17	28 (48%)
34	LUT	S	316	-	42,43,43	0.79	0	51,60,60	1.82	16 (31%)
28	BCR	6	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.23	18 (32%)
36	NEX	P	617	-	38,46,46	1.01	1 (2%)	50,70,70	2.80	18 (36%)
25	CLA	A	815	1,27	64,68,73	1.33	11 (17%)	77,107,113	1.36	6 (7%)
25	CLA	R	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.57	10 (15%)
33	CHL	P	622	-	57,61,74	2.18	18 (31%)	64,98,114	3.08	33 (51%)
25	CLA	2	307	-	54,58,73	1.40	9 (16%)	65,95,113	1.42	7 (10%)
25	CLA	B	809	28,2	69,73,73	1.27	11 (15%)	83,113,113	1.34	7 (8%)
25	CLA	Q	613	-	52,56,73	1.48	8 (15%)	62,92,113	1.46	8 (12%)
25	CLA	B	802	-	69,73,73	1.28	11 (15%)	83,113,113	1.44	8 (9%)
25	CLA	5	306	-	59,63,73	1.35	11 (18%)	71,101,113	1.36	6 (8%)
25	CLA	S	314	-	69,73,73	1.26	8 (11%)	83,113,113	1.33	8 (9%)
25	CLA	A	837	1	69,73,73	1.25	10 (14%)	83,113,113	1.36	8 (9%)
33	CHL	9	306	-	46,50,74	2.22	19 (41%)	51,85,114	3.34	25 (49%)
25	CLA	O	202	-	40,46,73	1.63	11 (27%)	48,80,113	1.60	8 (16%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-
32	LMG	1	619	27	46,46,55	0.98	2 (4%)	54,54,63	1.17	3 (5%)
36	NEX	P	621	-	38,46,46	0.86	0	50,70,70	3.27	27 (54%)
35	XAT	P	616	-	39,47,47	0.93	0	54,74,74	3.03	20 (37%)
25	CLA	3	307	-	54,58,73	1.43	11 (20%)	65,95,113	1.41	7 (10%)
25	CLA	A	803	-	69,73,73	1.30	9 (13%)	83,113,113	1.25	5 (6%)
27	LHG	4	318	25	48,48,48	0.92	2 (4%)	51,54,54	1.09	3 (5%)
25	CLA	3	304	-	46,50,73	1.53	10 (21%)	55,85,113	1.46	5 (9%)
34	LUT	Q	614	-	42,43,43	0.73	0	51,60,60	1.84	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	L	209	-	45,49,73	1.50	10 (22%)	54,84,113	1.67	8 (14%)
25	CLA	A	812	-	69,73,73	1.27	10 (14%)	83,113,113	1.36	9 (10%)
35	XAT	P	623	-	38,46,47	0.97	1 (2%)	52,72,74	3.12	22 (42%)
25	CLA	3	309	-	45,49,73	1.49	11 (24%)	54,84,113	1.53	8 (14%)
25	CLA	B	825	2	69,73,73	1.29	10 (14%)	83,113,113	1.40	9 (10%)
25	CLA	A	813	1	58,62,73	1.40	11 (18%)	69,99,113	1.48	7 (10%)
25	CLA	B	814	2	59,63,73	1.37	11 (18%)	71,101,113	1.43	8 (11%)
25	CLA	5	324	-	69,73,73	1.26	11 (15%)	83,113,113	1.31	5 (6%)
28	BCR	5	320	-	41,41,41	0.82	1 (2%)	56,56,56	1.92	16 (28%)
33	CHL	6	608	-	55,59,74	2.03	18 (32%)	62,96,114	3.25	32 (51%)
25	CLA	K	205	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	5 (8%)
25	CLA	8	308	-	54,58,73	1.40	11 (20%)	65,95,113	1.56	7 (10%)
25	CLA	4	311	19	60,64,73	1.33	9 (15%)	72,102,113	1.44	6 (8%)
25	CLA	A	810	1	69,73,73	1.25	11 (15%)	83,113,113	1.36	8 (9%)
32	LMG	J	107	-	55,55,55	0.90	2 (3%)	63,63,63	1.23	8 (12%)
34	LUT	R	616	-	42,43,43	0.78	0	51,60,60	1.83	18 (35%)
25	CLA	A	811	1	69,73,73	1.26	10 (14%)	83,113,113	1.41	7 (8%)
25	CLA	A	833	1	54,58,73	1.41	11 (20%)	65,95,113	1.52	6 (9%)
25	CLA	U	312	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
33	CHL	5	317	-	47,51,74	2.11	18 (38%)	52,86,114	3.32	24 (46%)
33	CHL	7	305	-	58,62,74	2.00	21 (36%)	65,99,114	3.01	24 (36%)
28	BCR	B	844	-	41,41,41	0.96	2 (4%)	56,56,56	2.11	16 (28%)
34	LUT	6	619	-	42,43,43	0.89	1 (2%)	51,60,60	1.82	14 (27%)
27	LHG	B	847	32	37,37,48	1.03	2 (5%)	40,43,54	1.20	5 (12%)
25	CLA	L	205	12	69,73,73	1.25	10 (14%)	83,113,113	1.39	9 (10%)
33	CHL	T	605	-	54,58,74	2.13	19 (35%)	59,94,114	3.08	24 (40%)
34	LUT	1	616	25	42,43,43	0.95	2 (4%)	51,60,60	1.84	18 (35%)
25	CLA	A	830	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	10 (12%)
30	DGD	B	846	-	67,67,67	0.80	3 (4%)	81,81,81	1.18	5 (6%)
26	PQN	A	841	-	34,34,34	1.37	2 (5%)	42,45,45	1.33	6 (14%)
25	CLA	S	313	-	64,68,73	1.31	8 (12%)	77,107,113	1.31	7 (9%)
25	CLA	6	609	-	54,58,73	1.39	11 (20%)	65,95,113	1.46	7 (10%)
25	CLA	S	320	-	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
25	CLA	T	603	-	54,58,73	1.42	7 (12%)	65,95,113	1.47	6 (9%)
33	CHL	4	322	16	57,61,74	2.02	19 (33%)	64,98,114	3.18	29 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	804	1	69,73,73	1.27	10 (14%)	83,113,113	1.40	8 (9%)
28	BCR	J	101	-	41,41,41	0.90	1 (2%)	56,56,56	2.08	19 (33%)
25	CLA	7	313	22	50,54,73	1.45	10 (20%)	60,90,113	1.44	6 (10%)
25	CLA	K	204	-	49,53,73	1.48	10 (20%)	59,89,113	1.54	7 (11%)
25	CLA	B	837	2	69,73,73	1.27	10 (14%)	83,113,113	1.48	6 (7%)
30	DGD	B	848	-	58,58,67	0.96	4 (6%)	72,72,81	1.37	11 (15%)
25	CLA	5	309	-	54,58,73	1.42	11 (20%)	65,95,113	1.41	8 (12%)
36	NEX	R	617	-	38,46,46	0.98	1 (2%)	50,70,70	2.79	19 (38%)
25	CLA	A	805	1	59,63,73	1.38	11 (18%)	71,101,113	1.44	5 (7%)
33	CHL	5	308	-	55,59,74	1.99	20 (36%)	62,96,114	3.15	30 (48%)
25	CLA	3	301	-	64,68,73	1.32	10 (15%)	77,107,113	1.40	8 (10%)
25	CLA	3	310	-	50,54,73	1.47	10 (20%)	60,90,113	1.48	7 (11%)
25	CLA	R	610	-	68,72,73	1.29	8 (11%)	81,111,113	1.32	9 (11%)
33	CHL	P	605	14	52,56,74	2.22	20 (38%)	58,92,114	3.24	27 (46%)
33	CHL	R	601	-	55,59,74	2.26	18 (32%)	62,96,114	2.94	27 (43%)
25	CLA	9	305	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	6 (9%)
25	CLA	A	817	-	61,65,73	1.36	9 (14%)	73,103,113	1.35	5 (6%)
25	CLA	7	312	22	47,51,73	1.50	11 (23%)	56,86,113	1.51	7 (12%)
34	LUT	9	312	-	42,43,43	0.84	2 (4%)	51,60,60	1.60	13 (25%)
25	CLA	A	801	-	69,73,73	1.28	10 (14%)	83,113,113	1.29	8 (9%)
25	CLA	A	839	1,25	69,73,73	1.26	10 (14%)	83,113,113	1.43	7 (8%)
34	LUT	8	316	-	42,43,43	0.90	1 (2%)	51,60,60	1.78	14 (27%)
25	CLA	9	302	-	50,54,73	1.43	8 (16%)	60,90,113	1.41	5 (8%)
25	CLA	9	311	24	49,53,73	1.50	10 (20%)	59,89,113	1.41	8 (13%)
33	CHL	4	304	-	46,50,74	2.24	16 (34%)	51,85,114	3.20	24 (47%)
27	LHG	P	618	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
28	BCR	L	208	-	41,41,41	0.87	2 (4%)	56,56,56	1.98	18 (32%)
25	CLA	4	310	-	56,60,73	1.46	12 (21%)	67,97,113	1.64	10 (14%)
25	CLA	B	836	-	69,73,73	1.26	11 (15%)	83,113,113	1.33	7 (8%)
25	CLA	2	303	17	69,73,73	1.27	11 (15%)	83,113,113	1.31	7 (8%)
25	CLA	B	812	2	64,68,73	1.31	10 (15%)	77,107,113	1.36	6 (7%)
25	CLA	P	612	-	64,68,73	1.27	7 (10%)	77,107,113	1.59	10 (12%)
25	CLA	A	828	1	69,73,73	1.26	10 (14%)	83,113,113	1.44	7 (8%)
25	CLA	P	610	-	64,68,73	1.31	9 (14%)	77,107,113	1.29	7 (9%)
34	LUT	5	318	-	42,43,43	0.92	2 (4%)	51,60,60	1.68	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	829	-	69,73,73	1.29	11 (15%)	83,113,113	1.41	8 (9%)
25	CLA	B	801	-	69,73,73	1.27	10 (14%)	83,113,113	1.35	7 (8%)
25	CLA	K	202	-	49,53,73	1.47	12 (24%)	59,89,113	1.48	5 (8%)
25	CLA	a	304	-	56,60,73	1.42	9 (16%)	67,97,113	1.30	5 (7%)
25	CLA	7	302	-	50,54,73	1.48	10 (20%)	60,90,113	1.50	7 (11%)
26	PQN	B	839	-	34,34,34	1.35	2 (5%)	42,45,45	1.33	4 (9%)
25	CLA	H	205	12	46,50,73	1.51	11 (23%)	55,85,113	1.81	10 (18%)
25	CLA	R	612	-	64,68,73	1.26	7 (10%)	77,107,113	1.57	10 (12%)
25	CLA	Q	618	-	43,48,73	1.63	10 (23%)	52,82,113	1.75	10 (19%)
33	CHL	1	601	16	57,61,74	1.99	19 (33%)	64,98,114	3.05	28 (43%)
25	CLA	S	312	-	64,68,73	1.30	8 (12%)	77,107,113	1.32	7 (9%)
28	BCR	B	840	28	41,41,41	0.93	1 (2%)	56,56,56	2.11	15 (26%)
28	BCR	F	801	-	41,41,41	0.90	2 (4%)	56,56,56	2.10	17 (30%)
27	LHG	2	317	-	48,48,48	0.90	2 (4%)	51,54,54	0.99	2 (3%)
25	CLA	6	614	-	49,53,73	1.46	10 (20%)	59,89,113	1.48	7 (11%)
25	CLA	8	303	-	66,70,73	1.32	12 (18%)	79,109,113	1.38	6 (7%)
25	CLA	A	818	1	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
25	CLA	B	830	2	69,73,73	1.29	12 (17%)	83,113,113	1.36	9 (10%)
28	BCR	O	205	-	41,41,41	0.82	1 (2%)	56,56,56	2.18	16 (28%)
25	CLA	1	604	34	61,65,73	1.34	12 (19%)	73,103,113	1.34	8 (10%)
27	LHG	5	321	-	36,36,48	1.03	2 (5%)	39,42,54	1.29	5 (12%)
25	CLA	R	614	-	52,56,73	1.44	7 (13%)	62,92,113	1.52	7 (11%)
25	CLA	5	302	20	69,73,73	1.27	11 (15%)	83,113,113	1.37	8 (9%)
25	CLA	2	302	17	50,54,73	1.50	11 (22%)	60,90,113	1.54	7 (11%)
25	CLA	B	820	2	63,67,73	1.31	10 (15%)	75,105,113	1.44	7 (9%)
25	CLA	J	103	-	62,66,73	1.31	10 (16%)	74,104,113	1.41	7 (9%)
25	CLA	U	304	-	54,58,73	1.41	8 (14%)	65,95,113	1.47	8 (12%)
25	CLA	A	816	1	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)
25	CLA	B	829	-	53,57,73	1.41	11 (20%)	62,93,113	1.48	7 (11%)
25	CLA	R	611	-	64,68,73	1.34	7 (10%)	77,107,113	1.57	9 (11%)
28	BCR	A	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.08	17 (30%)
25	CLA	A	834	1	49,53,73	1.49	10 (20%)	59,89,113	1.54	3 (5%)
34	LUT	1	615	-	42,43,43	0.96	2 (4%)	51,60,60	1.87	16 (31%)
28	BCR	J	106	-	41,41,41	0.86	2 (4%)	56,56,56	2.25	18 (32%)
36	NEX	U	301	-	38,46,46	1.08	2 (5%)	50,70,70	2.95	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CHL	4	305	-	55,59,74	2.23	20 (36%)	62,96,114	2.97	26 (41%)
33	CHL	S	308	-	56,60,74	2.08	18 (32%)	63,97,114	3.03	28 (44%)
32	LMG	7	318	-	35,35,55	1.10	2 (5%)	43,43,63	1.11	2 (4%)
25	CLA	6	611	27	59,63,73	1.36	9 (15%)	71,101,113	1.32	5 (7%)
25	CLA	B	803	2	49,53,73	1.47	10 (20%)	59,89,113	1.62	8 (13%)
33	CHL	U	308	-	48,52,74	2.18	17 (35%)	53,87,114	3.18	23 (43%)
25	CLA	1	608	-	69,73,73	1.24	11 (15%)	83,113,113	1.22	6 (7%)
34	LUT	S	317	-	42,43,43	0.77	0	51,60,60	1.65	9 (17%)
25	CLA	9	308	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	9 (13%)
25	CLA	L	206	-	46,50,73	1.51	11 (23%)	55,85,113	1.54	6 (10%)
34	LUT	Q	615	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	16 (31%)
28	BCR	8	301	-	41,41,41	0.78	0	56,56,56	1.88	15 (26%)
25	CLA	T	611	-	64,68,73	1.30	8 (12%)	77,107,113	1.32	6 (7%)
25	CLA	B	838	-	69,73,73	1.27	12 (17%)	83,113,113	1.34	5 (6%)
25	CLA	B	811	-	69,73,73	1.31	10 (14%)	83,113,113	1.44	9 (10%)
25	CLA	4	308	19	64,68,73	1.28	10 (15%)	77,107,113	1.35	6 (7%)
35	XAT	P	620	-	39,47,47	0.89	0	54,74,74	2.97	23 (42%)
33	CHL	S	310	15	56,60,74	2.13	17 (30%)	63,97,114	2.96	26 (41%)
25	CLA	1	610	27	69,73,73	1.26	10 (14%)	83,113,113	1.24	7 (8%)
25	CLA	5	304	20	50,54,73	1.47	10 (20%)	60,90,113	1.50	7 (11%)
25	CLA	A	840	-	69,73,73	1.29	10 (14%)	83,113,113	1.42	10 (12%)
28	BCR	B	843	-	41,41,41	0.86	2 (4%)	56,56,56	1.86	18 (32%)
25	CLA	9	310	24	54,58,73	1.40	10 (18%)	65,95,113	1.49	6 (9%)
33	CHL	8	307	-	57,61,74	2.07	19 (33%)	64,98,114	3.32	30 (46%)
35	XAT	Q	616	-	39,47,47	0.96	1 (2%)	54,74,74	3.04	24 (44%)
25	CLA	7	303	-	60,64,73	1.37	11 (18%)	72,102,113	1.42	6 (8%)
33	CHL	a	305	-	52,56,74	2.21	18 (34%)	58,92,114	2.95	23 (39%)
25	CLA	F	802	-	49,53,73	1.50	11 (22%)	59,89,113	1.45	7 (11%)
25	CLA	7	311	-	69,73,73	1.26	11 (15%)	83,113,113	1.36	7 (8%)
25	CLA	A	824	-	59,63,73	1.36	11 (18%)	71,101,113	1.43	7 (9%)
33	CHL	P	606	-	54,58,74	2.13	18 (33%)	59,94,114	3.09	25 (42%)
25	CLA	7	304	-	46,50,73	1.53	11 (23%)	55,85,113	1.41	6 (10%)
27	LHG	Q	617	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
25	CLA	O	203	-	41,46,73	1.65	10 (24%)	52,81,113	1.63	7 (13%)
25	CLA	8	305	-	50,54,73	1.46	11 (22%)	60,90,113	1.44	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	B	851	-	41,41,41	0.83	2 (4%)	56,56,56	2.12	19 (33%)
25	CLA	5	319	-	50,54,73	1.46	10 (20%)	60,90,113	1.50	7 (11%)
28	BCR	3	318	-	41,41,41	0.84	1 (2%)	56,56,56	2.79	24 (42%)
33	CHL	Q	601	-	55,59,74	2.26	18 (32%)	62,96,114	2.95	27 (43%)
25	CLA	1	609	16	64,68,73	1.26	13 (20%)	77,107,113	1.63	11 (14%)
25	CLA	2	311	-	56,60,73	1.41	10 (17%)	67,97,113	1.41	7 (10%)
25	CLA	2	306	17	45,49,73	1.53	10 (22%)	54,84,113	1.64	9 (16%)
36	NEX	T	616	-	38,46,46	0.98	1 (2%)	50,70,70	2.76	16 (32%)
25	CLA	J	105	-	46,50,73	1.49	10 (21%)	55,85,113	1.51	7 (12%)
25	CLA	5	305	-	54,58,73	1.43	11 (20%)	65,95,113	1.49	8 (12%)
25	CLA	Q	609	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	8 (9%)
34	LUT	2	316	-	42,43,43	0.86	1 (2%)	51,60,60	1.66	13 (25%)
25	CLA	U	303	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	5 (6%)
25	CLA	5	314	-	49,53,73	1.49	10 (20%)	59,89,113	1.44	8 (13%)
33	CHL	R	606	-	54,58,74	2.13	19 (35%)	59,94,114	3.04	26 (44%)
28	BCR	5	323	-	41,41,41	0.96	2 (4%)	56,56,56	3.15	22 (39%)
25	CLA	3	302	-	69,73,73	1.30	10 (14%)	83,113,113	1.34	8 (9%)
25	CLA	U	313	-	49,53,73	1.44	7 (14%)	59,89,113	1.60	8 (13%)
34	LUT	2	315	-	42,43,43	0.83	1 (2%)	51,60,60	1.84	13 (25%)
34	LUT	4	316	-	42,43,43	0.88	2 (4%)	51,60,60	1.53	11 (21%)
34	LUT	a	314	-	42,43,43	0.88	2 (4%)	51,60,60	1.87	16 (31%)
25	CLA	G	202	-	50,54,73	1.47	9 (18%)	60,90,113	1.55	9 (15%)
33	CHL	4	314	19	47,51,74	2.16	18 (38%)	52,86,114	3.25	23 (44%)
25	CLA	9	301	-	58,62,73	1.43	11 (18%)	73,100,113	1.43	9 (12%)
25	CLA	B	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	9 (10%)
25	CLA	4	303	-	54,58,73	1.38	11 (20%)	65,95,113	1.46	7 (10%)
28	BCR	A	845	-	41,41,41	0.83	1 (2%)	56,56,56	2.08	21 (37%)
25	CLA	Q	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.52	7 (10%)
25	CLA	4	301	-	64,68,73	1.30	12 (18%)	77,107,113	1.35	6 (7%)
33	CHL	U	305	14	50,54,74	2.24	18 (36%)	56,90,114	3.16	28 (50%)
28	BCR	A	847	-	41,41,41	0.92	2 (4%)	56,56,56	2.00	18 (32%)
25	CLA	A	807	-	69,73,73	1.30	11 (15%)	83,113,113	1.42	8 (9%)
25	CLA	2	314	-	50,54,73	1.46	10 (20%)	60,90,113	1.39	5 (8%)
33	CHL	T	606	-	48,52,74	2.19	17 (35%)	53,87,114	3.22	25 (47%)
25	CLA	S	301	-	51,55,73	1.48	8 (15%)	61,91,113	1.64	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CHL	S	307	-	54,58,74	2.21	17 (31%)	59,94,114	3.05	24 (40%)
25	CLA	P	613	-	62,66,73	1.33	8 (12%)	74,104,113	1.34	6 (8%)
25	CLA	B	813	2	61,65,73	1.31	11 (18%)	73,103,113	1.37	6 (8%)
25	CLA	Q	610	-	43,48,73	1.56	8 (18%)	52,82,113	1.69	9 (17%)
25	CLA	T	608	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	7 (8%)
33	CHL	U	307	-	57,61,74	2.09	17 (29%)	64,98,114	3.01	27 (42%)
32	LMG	6	602	-	40,40,55	1.03	2 (5%)	48,48,63	1.41	6 (12%)
34	LUT	3	316	-	42,43,43	0.97	2 (4%)	51,60,60	1.65	15 (29%)
25	CLA	a	303	34	61,65,73	1.66	16 (26%)	73,103,113	3.46	21 (28%)
33	CHL	S	321	-	55,59,74	2.12	19 (34%)	62,96,114	3.06	28 (45%)
25	CLA	B	807	-	69,73,73	1.24	10 (14%)	83,113,113	1.52	9 (10%)
25	CLA	R	602	-	69,73,73	1.27	8 (11%)	83,113,113	1.29	9 (10%)
25	CLA	1	613	-	69,73,73	1.27	10 (14%)	83,113,113	1.33	8 (9%)
34	LUT	a	316	25	42,43,43	0.74	0	51,60,60	2.13	15 (29%)
25	CLA	S	315	15	52,56,73	1.42	10 (19%)	62,92,113	1.39	7 (11%)
25	CLA	A	842	27	56,60,73	1.39	10 (17%)	67,97,113	1.70	13 (19%)
25	CLA	S	305	-	54,58,73	1.40	8 (14%)	65,95,113	1.42	6 (9%)
25	CLA	4	307	-	54,58,73	1.42	10 (18%)	65,95,113	1.33	6 (9%)
33	CHL	R	605	14	50,54,74	2.26	19 (38%)	56,90,114	3.23	27 (48%)
36	NEX	U	316	-	38,46,46	0.99	1 (2%)	50,70,70	2.72	18 (36%)
34	LUT	P	614	-	42,43,43	0.74	0	51,60,60	1.92	15 (29%)
33	CHL	S	302	-	57,61,74	2.03	19 (33%)	64,98,114	3.09	29 (45%)
25	CLA	U	311	-	58,62,73	1.38	9 (15%)	64,97,113	1.28	6 (9%)
25	CLA	A	851	-	69,73,73	1.28	11 (15%)	83,113,113	1.26	6 (7%)
25	CLA	B	816	2	64,68,73	1.31	10 (15%)	77,107,113	1.43	8 (10%)
25	CLA	P	602	-	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
33	CHL	4	306	-	55,59,74	2.03	18 (32%)	62,96,114	3.02	26 (41%)
25	CLA	A	823	-	53,57,73	1.42	11 (20%)	62,93,113	1.53	8 (12%)
25	CLA	1	605	-	56,60,73	1.42	9 (16%)	67,97,113	1.40	8 (11%)
33	CHL	6	606	-	57,61,74	1.99	17 (29%)	64,98,114	3.00	28 (43%)
25	CLA	6	615	21	50,54,73	1.47	11 (22%)	60,90,113	1.56	8 (13%)
25	CLA	H	202	-	45,49,73	1.52	9 (20%)	54,84,113	1.66	7 (12%)
25	CLA	5	310	-	64,68,73	1.29	12 (18%)	77,107,113	1.33	8 (10%)
25	CLA	8	313	-	69,73,73	1.26	10 (14%)	83,113,113	1.36	7 (8%)
33	CHL	1	606	-	52,56,74	2.20	20 (38%)	58,92,114	2.95	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	5	316	-	47,51,73	1.51	11 (23%)	56,86,113	1.57	6 (10%)
33	CHL	Q	607	-	48,52,74	2.18	18 (37%)	53,87,114	3.19	24 (45%)
25	CLA	1	607	-	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
32	LMG	4	320	-	40,40,55	1.06	3 (7%)	48,48,63	1.30	6 (12%)
25	CLA	a	308	16	64,68,73	1.25	10 (15%)	77,107,113	1.68	12 (15%)
25	CLA	2	313	-	59,63,73	1.37	10 (16%)	71,101,113	1.47	11 (15%)
28	BCR	F	803	-	41,41,41	0.91	2 (4%)	56,56,56	2.20	20 (35%)
25	CLA	A	831	1	54,58,73	1.42	11 (20%)	65,95,113	1.50	8 (12%)
25	CLA	8	312	25	56,60,73	1.39	10 (17%)	67,97,113	1.40	4 (5%)
25	CLA	1	612	-	69,73,73	1.29	10 (14%)	83,113,113	1.97	14 (16%)
33	CHL	Q	606	-	54,58,74	2.16	17 (31%)	59,94,114	3.13	23 (38%)
34	LUT	8	317	-	42,43,43	0.92	2 (4%)	51,60,60	1.56	12 (23%)
25	CLA	4	313	19	45,49,73	1.51	9 (20%)	54,84,113	1.58	8 (14%)
25	CLA	6	612	-	56,60,73	1.44	10 (17%)	67,97,113	1.37	5 (7%)
34	LUT	6	622	-	42,43,43	0.88	1 (2%)	51,60,60	1.50	11 (21%)
28	BCR	L	203	-	41,41,41	0.90	1 (2%)	56,56,56	2.03	15 (26%)
25	CLA	B	833	-	64,68,73	1.32	11 (17%)	77,107,113	1.35	8 (10%)
25	CLA	2	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.43	9 (10%)
27	LHG	5	301	-	44,44,48	0.96	2 (4%)	47,50,54	1.05	3 (6%)
25	CLA	8	306	-	46,50,73	1.51	10 (21%)	55,85,113	1.46	7 (12%)
28	BCR	4	321	-	41,41,41	0.94	2 (4%)	56,56,56	2.73	24 (42%)
28	BCR	B	845	-	41,41,41	1.03	3 (7%)	56,56,56	2.16	18 (32%)
25	CLA	S	304	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
32	LMG	J	102	-	40,40,55	0.99	2 (5%)	48,48,63	1.11	5 (10%)
25	CLA	7	308	-	64,68,73	1.35	12 (18%)	77,107,113	1.37	8 (10%)
35	XAT	T	615	-	39,47,47	0.92	0	54,74,74	3.00	21 (38%)
25	CLA	A	809	1	69,73,73	1.26	12 (17%)	83,113,113	1.36	8 (9%)
25	CLA	8	302	23	69,73,73	1.25	10 (14%)	83,113,113	1.27	9 (10%)
34	LUT	4	315	-	42,43,43	0.89	1 (2%)	51,60,60	1.94	17 (33%)
25	CLA	A	821	1	49,53,73	1.49	10 (20%)	59,89,113	1.66	10 (16%)
25	CLA	A	832	1	69,73,73	1.27	11 (15%)	83,113,113	1.36	5 (6%)
28	BCR	I	201	25	41,41,41	0.93	2 (4%)	56,56,56	2.42	22 (39%)
25	CLA	6	613	-	60,64,73	1.34	10 (16%)	72,102,113	1.49	7 (9%)
28	BCR	L	204	25	41,41,41	1.01	2 (4%)	56,56,56	2.21	23 (41%)
25	CLA	A	836	1	69,73,73	1.28	11 (15%)	83,113,113	1.40	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	XAT	S	318	-	39,47,47	0.98	1 (2%)	54,74,74	2.87	22 (40%)
25	CLA	7	310	-	56,60,73	1.40	10 (17%)	67,97,113	1.45	6 (8%)
33	CHL	P	608	-	48,52,74	2.18	18 (37%)	53,87,114	3.19	24 (45%)
25	CLA	1	611	-	56,60,73	1.41	11 (19%)	67,97,113	1.39	7 (10%)
25	CLA	8	314	-	59,63,73	1.35	11 (18%)	71,101,113	1.40	9 (12%)
25	CLA	5	303	-	69,73,73	1.28	12 (17%)	83,113,113	1.42	7 (8%)
33	CHL	U	306	-	54,58,74	2.14	18 (33%)	59,94,114	3.08	25 (42%)
25	CLA	B	827	2	69,73,73	1.27	10 (14%)	83,113,113	1.34	9 (10%)
28	BCR	G	203	28	41,41,41	0.84	1 (2%)	56,56,56	2.09	16 (28%)
25	CLA	3	314	-	60,64,73	1.36	10 (16%)	72,102,113	1.42	6 (8%)
25	CLA	B	805	-	69,73,73	1.29	12 (17%)	83,113,113	1.38	5 (6%)
33	CHL	T	607	-	56,60,74	2.19	18 (32%)	63,97,114	2.96	29 (46%)
25	CLA	T	609	-	64,68,73	1.32	8 (12%)	77,107,113	1.43	10 (12%)
25	CLA	B	828	-	54,58,73	1.41	11 (20%)	65,95,113	1.46	6 (9%)
25	CLA	G	201	-	54,58,73	1.41	10 (18%)	65,95,113	1.44	8 (12%)
25	CLA	B	804	2	69,73,73	1.30	11 (15%)	83,113,113	1.40	8 (9%)
27	LHG	P	624	-	48,48,48	0.94	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	a	311	-	69,73,73	1.25	9 (13%)	83,113,113	1.51	8 (9%)
27	LHG	R	618	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	Q	603	33	69,73,73	1.25	7 (10%)	83,113,113	1.38	6 (7%)
25	CLA	U	310	-	68,72,73	1.27	7 (10%)	81,111,113	1.29	8 (9%)
25	CLA	9	304	-	50,54,73	1.47	9 (18%)	60,90,113	1.48	5 (8%)
33	CHL	S	309	-	56,60,74	2.07	18 (32%)	63,97,114	3.06	27 (42%)
34	LUT	P	615	-	42,43,43	0.81	0	51,60,60	1.78	18 (35%)
25	CLA	B	808	2	69,73,73	1.28	11 (15%)	83,113,113	1.35	9 (10%)
25	CLA	6	603	-	69,73,73	1.29	11 (15%)	83,113,113	1.34	7 (8%)
25	CLA	9	303	-	64,68,73	1.31	11 (17%)	77,107,113	1.34	6 (7%)
25	CLA	6	610	-	64,68,73	1.34	9 (14%)	77,107,113	1.36	7 (9%)
25	CLA	B	826	-	69,73,73	1.29	10 (14%)	83,113,113	1.40	9 (10%)
28	BCR	O	204	-	41,41,41	0.86	2 (4%)	56,56,56	2.34	21 (37%)
25	CLA	3	320	22	69,73,73	1.25	12 (17%)	83,113,113	1.36	7 (8%)
25	CLA	P	603	33	69,73,73	1.25	8 (11%)	83,113,113	1.36	7 (8%)
25	CLA	T	612	-	52,56,73	1.44	7 (13%)	62,92,113	1.48	6 (9%)
25	CLA	9	309	-	64,68,73	1.31	9 (14%)	77,107,113	1.40	8 (10%)
25	CLA	A	806	-	69,73,73	1.30	11 (15%)	83,113,113	1.44	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	849	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
25	CLA	L	202	1,28	69,73,73	1.26	11 (15%)	83,113,113	1.32	6 (7%)
34	LUT	T	614	-	42,43,43	0.76	0	51,60,60	1.73	14 (27%)
25	CLA	3	312	18	49,53,73	1.48	9 (18%)	59,89,113	1.48	8 (13%)

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
25	CLA	A	838	1	-	14/39/115/115	-
27	LHG	a	317	25	-	17/47/47/53	-
25	CLA	T	602	-	-	7/39/115/115	-
25	CLA	B	818	2	-	11/29/105/115	-
25	CLA	7	307	-	-	4/21/97/115	-
25	CLA	a	310	-	-	10/24/100/115	-
34	LUT	7	315	-	-	2/29/67/67	0/2/2/2
25	CLA	A	826	-	-	6/39/115/115	-
25	CLA	A	820	1	-	12/39/115/115	-
25	CLA	a	301	-	-	12/39/115/115	-
28	BCR	A	846	-	-	2/29/63/63	0/2/2/2
28	BCR	L	207	-	-	8/29/63/63	0/2/2/2
31	SQD	B	850	-	-	16/46/66/69	0/1/1/1
25	CLA	B	831	2	-	12/39/115/115	-
25	CLA	B	823	-	-	5/39/115/115	-
25	CLA	3	313	-	-	5/17/93/115	-
34	LUT	1	617	25	-	6/29/67/67	0/2/2/2
25	CLA	B	834	2	-	22/39/115/115	-
25	CLA	1	603	16	-	12/39/115/115	-
25	CLA	B	817	-	-	7/39/115/115	-
28	BCR	A	848	-	-	6/29/63/63	0/2/2/2
25	CLA	R	613	-	-	17/39/115/115	-
25	CLA	T	610	-	-	12/33/109/115	-
29	SF4	C	102	3	-	-	0/6/5/5
28	BCR	B	842	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CHL	Q	605	14	-	2/12/88/117	-
25	CLA	S	303	15	-	11/39/115/115	-
33	CHL	R	608	-	-	7/15/91/117	-
25	CLA	R	603	33	-	13/39/115/115	-
33	CHL	R	609	25	-	16/41/117/117	-
25	CLA	2	304	-	-	18/39/115/115	-
34	LUT	9	313	-	-	2/29/67/67	0/2/2/2
25	CLA	B	806	2	-	12/39/115/115	-
27	LHG	7	317	25	-	14/41/41/53	-
25	CLA	8	309	-	-	6/17/93/115	-
25	CLA	O	201	-	-	8/10/86/115	-
25	CLA	Q	612	-	-	13/33/109/115	-
25	CLA	5	312	-	-	7/24/100/115	-
25	CLA	K	203	-	-	8/17/93/115	-
27	LHG	A	843	-	-	18/53/53/53	-
25	CLA	A	835	-	-	8/23/99/115	-
27	LHG	S	319	-	-	10/53/53/53	-
25	CLA	B	815	-	-	17/32/108/115	-
25	CLA	a	313	-	-	6/17/93/115	-
28	BCR	4	317	-	-	8/29/63/63	0/2/2/2
25	CLA	Q	602	-	-	7/39/115/115	-
25	CLA	B	824	2	-	19/39/115/115	-
32	LMG	2	301	-	-	12/36/56/70	0/1/1/1
27	LHG	4	319	-	-	7/36/36/53	-
25	CLA	U	302	-	-	8/39/115/115	-
32	LMG	H	204	-	-	14/42/62/70	0/1/1/1
25	CLA	B	835	2	-	6/18/94/115	-
25	CLA	a	307	-	-	12/39/115/115	-
33	CHL	P	607	-	-	10/25/101/117	-
25	CLA	7	309	27	-	4/10/86/115	-
34	LUT	7	314	-	-	2/29/67/67	0/2/2/2
28	BCR	3	317	-	-	6/29/63/63	0/2/2/2
34	LUT	R	615	-	-	2/29/67/67	0/2/2/2
28	BCR	B	841	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CHL	S	306	-	-	11/20/96/117	-
34	LUT	5	322	-	-	0/29/67/67	0/2/2/2
33	CHL	Q	608	25	-	16/41/117/117	-
33	CHL	9	307	-	-	6/23/99/117	-
25	CLA	4	312	19	-	4/15/91/115	-
34	LUT	U	315	-	-	2/29/67/67	0/2/2/2
25	CLA	a	306	-	-	8/39/115/115	-
25	CLA	A	827	-	-	7/39/115/115	-
25	CLA	A	825	-	-	22/39/115/115	-
25	CLA	B	810	-	-	13/39/115/115	-
25	CLA	a	302	16	-	10/30/106/115	-
25	CLA	P	604	-	-	8/21/97/115	-
32	LMG	7	319	-	-	13/31/51/70	0/1/1/1
25	CLA	A	819	1	-	14/39/115/115	-
25	CLA	3	303	-	-	10/39/115/115	-
25	CLA	2	305	-	-	9/24/100/115	-
25	CLA	B	821	2	-	8/33/109/115	-
33	CHL	P	609	25	-	16/41/117/117	-
27	LHG	T	617	-	-	12/53/53/53	-
25	CLA	2	309	-	-	13/33/109/115	-
25	CLA	B	832	-	-	7/15/91/115	-
25	CLA	4	302	25	-	5/17/93/115	-
34	LUT	U	314	-	-	0/29/67/67	0/2/2/2
25	CLA	H	201	-	-	8/17/93/115	-
25	CLA	8	315	23	-	7/17/93/115	-
25	CLA	4	309	27	-	10/27/103/115	-
27	LHG	6	618	25	-	23/53/53/53	-
33	CHL	P	601	-	-	8/23/99/117	-
33	CHL	R	607	-	-	10/25/101/117	-
33	CHL	P	619	-	-	10/25/101/117	-
28	BCR	7	316	-	-	2/29/63/63	0/2/2/2
34	LUT	a	315	25	-	4/29/67/67	0/2/2/2
25	CLA	A	808	1	-	13/39/115/115	-
28	BCR	8	318	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	8	319	25	-	17/53/53/53	-
25	CLA	1	602	-	-	11/39/115/115	-
29	SF4	A	850	1,2	-	-	0/6/5/5
25	CLA	Q	611	-	-	9/33/109/115	-
33	CHL	3	306	-	-	9/26/102/117	-
25	CLA	L	201	-	-	12/39/115/115	-
25	CLA	7	306	-	-	4/21/97/115	-
27	LHG	1	618	25	-	15/47/47/53	-
28	BCR	K	206	-	-	10/29/63/63	0/2/2/2
25	CLA	A	814	1	-	19/39/115/115	-
25	CLA	8	311	27	-	7/17/93/115	-
33	CHL	6	607	-	-	10/26/102/117	-
25	CLA	H	203	-	-	10/17/93/115	-
25	CLA	3	308	-	-	14/39/115/115	-
33	CHL	5	307	-	-	11/23/99/117	-
25	CLA	A	822	-	-	14/39/115/115	-
28	BCR	3	319	-	-	6/29/63/63	0/2/2/2
25	CLA	8	304	23	-	10/15/91/115	-
25	CLA	2	308	-	-	6/13/89/115	-
25	CLA	3	311	-	-	11/27/103/115	-
32	LMG	J	104	-	-	13/30/50/70	0/1/1/1
34	LUT	3	315	-	-	0/29/67/67	0/2/2/2
28	BCR	A	854	-	-	2/29/63/63	0/2/2/2
25	CLA	S	311	-	-	9/33/109/115	-
25	CLA	a	312	-	-	11/39/115/115	-
25	CLA	5	315	20	-	8/17/93/115	-
25	CLA	8	310	-	-	10/33/109/115	-
25	CLA	B	819	2	-	8/17/93/115	-
25	CLA	6	616	21,27	-	6/17/93/115	-
25	CLA	A	853	-	-	17/39/115/115	-
34	LUT	T	613	-	-	0/29/67/67	0/2/2/2
27	LHG	A	852	25	-	24/49/49/53	-
25	CLA	5	311	-	-	10/27/103/115	-
27	LHG	A	844	25	-	14/42/42/53	-
25	CLA	6	605	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	309	27	-	10/39/115/115	-
33	CHL	T	601	-	-	9/22/98/117	-
25	CLA	2	310	-	-	4/10/86/115	-
25	CLA	A	802	25	-	8/39/115/115	-
25	CLA	6	623	-	-	15/33/109/115	-
25	CLA	7	301	-	-	16/39/115/115	-
25	CLA	P	611	-	-	6/10/86/115	-
25	CLA	K	201	1	-	10/23/99/115	-
25	CLA	1	614	-	-	6/17/93/115	-
25	CLA	6	604	-	-	5/17/93/115	-
33	CHL	U	309	-	-	3/20/96/117	-
33	CHL	6	617	21	-	6/14/90/117	-
25	CLA	6	601	19	-	15/35/111/115	-
25	CLA	3	305	18	-	14/33/109/115	-
25	CLA	5	313	-	-	8/29/105/115	-
25	CLA	6	620	-	-	8/15/91/115	-
33	CHL	T	604	14	-	4/20/96/117	-
34	LUT	S	316	-	-	5/29/67/67	0/2/2/2
28	BCR	6	621	-	-	8/29/63/63	0/2/2/2
36	NEX	P	617	-	-	7/27/83/83	0/3/3/3
25	CLA	A	815	1,27	-	17/33/109/115	-
25	CLA	R	604	-	-	7/21/97/115	-
33	CHL	P	622	-	-	9/26/102/117	-
25	CLA	2	307	-	-	8/21/97/115	-
25	CLA	B	809	28,2	-	15/39/115/115	-
25	CLA	Q	613	-	-	11/19/95/115	-
25	CLA	B	802	-	-	15/39/115/115	-
25	CLA	5	306	-	-	4/27/103/115	-
25	CLA	S	314	-	-	22/39/115/115	-
25	CLA	A	837	1	-	12/39/115/115	-
33	CHL	9	306	-	-	5/12/88/117	-
25	CLA	O	202	-	-	2/6/78/115	-
32	LMG	1	619	27	-	15/41/61/70	0/1/1/1
36	NEX	P	621	-	-	10/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SF4	C	101	3	-	-	0/6/5/5
35	XAT	P	616	-	-	4/31/93/93	0/4/4/4
25	CLA	3	307	-	-	9/21/97/115	-
25	CLA	A	803	-	-	5/39/115/115	-
27	LHG	4	318	25	-	20/53/53/53	-
25	CLA	3	304	-	-	2/12/88/115	-
34	LUT	Q	614	-	-	0/29/67/67	0/2/2/2
25	CLA	L	209	-	-	6/10/86/115	-
25	CLA	A	812	-	-	16/39/115/115	-
35	XAT	P	623	-	-	3/29/91/93	0/4/4/4
25	CLA	3	309	-	-	6/10/86/115	-
25	CLA	B	825	2	-	15/39/115/115	-
25	CLA	A	813	1	-	4/26/102/115	-
25	CLA	B	814	2	-	9/27/103/115	-
25	CLA	5	324	-	-	19/39/115/115	-
28	BCR	5	320	-	-	9/29/63/63	0/2/2/2
33	CHL	6	608	-	-	12/23/99/117	-
25	CLA	K	205	-	-	8/15/91/115	-
25	CLA	8	308	-	-	6/21/97/115	-
25	CLA	4	311	19	-	16/29/105/115	-
25	CLA	A	810	1	-	13/39/115/115	-
32	LMG	J	107	-	-	18/50/70/70	0/1/1/1
34	LUT	R	616	-	-	2/29/67/67	0/2/2/2
25	CLA	A	811	1	-	6/39/115/115	-
25	CLA	A	833	1	-	0/21/97/115	-
25	CLA	U	312	-	-	16/39/115/115	-
33	CHL	5	317	-	-	4/14/90/117	-
33	CHL	7	305	-	-	12/27/103/117	-
28	BCR	B	844	-	-	2/29/63/63	0/2/2/2
34	LUT	6	619	-	-	1/29/67/67	0/2/2/2
27	LHG	B	847	32	-	17/42/42/53	-
25	CLA	L	205	12	-	11/39/115/115	-
33	CHL	T	605	-	-	7/22/98/117	-
34	LUT	1	616	25	-	4/29/67/67	0/2/2/2
25	CLA	A	830	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	B	846	-	-	15/55/95/95	0/2/2/2
26	PQN	A	841	-	-	6/23/43/43	0/2/2/2
25	CLA	S	313	-	-	15/33/109/115	-
25	CLA	6	609	-	-	10/21/97/115	-
25	CLA	S	320	-	-	13/39/115/115	-
25	CLA	T	603	-	-	8/21/97/115	-
33	CHL	4	322	16	-	7/26/102/117	-
25	CLA	A	804	1	-	11/39/115/115	-
28	BCR	J	101	-	-	6/29/63/63	0/2/2/2
25	CLA	7	313	22	-	10/17/93/115	-
25	CLA	K	204	-	-	9/15/91/115	-
25	CLA	B	837	2	-	17/39/115/115	-
30	DGD	B	848	-	-	16/46/86/95	0/2/2/2
25	CLA	5	309	-	-	12/21/97/115	-
36	NEX	R	617	-	-	6/27/83/83	0/3/3/3
25	CLA	A	805	1	-	10/27/103/115	-
33	CHL	5	308	-	-	7/23/99/117	-
25	CLA	3	301	-	-	3/33/109/115	-
25	CLA	3	310	-	-	7/17/93/115	-
25	CLA	R	610	-	-	12/38/114/115	-
33	CHL	P	605	14	-	6/20/96/117	-
33	CHL	R	601	-	-	8/23/99/117	-
25	CLA	9	305	-	-	9/21/97/115	-
25	CLA	A	817	-	-	5/30/106/115	-
25	CLA	7	312	22	-	3/13/89/115	-
34	LUT	9	312	-	-	2/29/67/67	0/2/2/2
25	CLA	A	801	-	-	13/39/115/115	-
25	CLA	A	839	1,25	-	13/39/115/115	-
34	LUT	8	316	-	-	1/29/67/67	0/2/2/2
25	CLA	9	302	-	-	11/17/93/115	-
25	CLA	9	311	24	-	2/15/91/115	-
33	CHL	4	304	-	-	3/12/88/117	-
27	LHG	P	618	-	-	12/53/53/53	-
28	BCR	L	208	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	4	310	-	-	10/24/100/115	-
25	CLA	B	836	-	-	17/39/115/115	-
25	CLA	2	303	17	-	15/39/115/115	-
25	CLA	B	812	2	-	12/33/109/115	-
25	CLA	P	612	-	-	13/33/109/115	-
25	CLA	A	828	1	-	17/39/115/115	-
25	CLA	P	610	-	-	9/33/109/115	-
34	LUT	5	318	-	-	0/29/67/67	0/2/2/2
25	CLA	A	829	-	-	12/39/115/115	-
25	CLA	B	801	-	-	14/39/115/115	-
25	CLA	K	202	-	-	5/15/91/115	-
25	CLA	a	304	-	-	2/24/100/115	-
25	CLA	7	302	-	-	5/17/93/115	-
26	PQN	B	839	-	-	3/23/43/43	0/2/2/2
25	CLA	H	205	12	-	2/12/88/115	-
25	CLA	R	612	-	-	13/33/109/115	-
25	CLA	Q	618	-	-	2/10/82/115	-
33	CHL	1	601	16	-	5/26/102/117	-
25	CLA	S	312	-	-	11/33/109/115	-
28	BCR	B	840	28	-	7/29/63/63	0/2/2/2
28	BCR	F	801	-	-	4/29/63/63	0/2/2/2
27	LHG	2	317	-	-	24/53/53/53	-
25	CLA	6	614	-	-	5/15/91/115	-
25	CLA	8	303	-	-	10/36/112/115	-
25	CLA	A	818	1	-	17/39/115/115	-
25	CLA	B	830	2	-	16/39/115/115	-
28	BCR	O	205	-	-	4/29/63/63	0/2/2/2
25	CLA	1	604	34	-	10/30/106/115	-
27	LHG	5	321	-	-	13/41/41/53	-
25	CLA	R	614	-	-	11/19/95/115	-
25	CLA	5	302	20	-	12/39/115/115	-
25	CLA	2	302	17	-	13/17/93/115	-
25	CLA	B	820	2	-	4/32/108/115	-
25	CLA	J	103	-	-	13/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	U	304	-	-	8/21/97/115	-
25	CLA	A	816	1	-	14/39/115/115	-
25	CLA	B	829	-	-	7/20/96/115	-
25	CLA	R	611	-	-	11/33/109/115	-
28	BCR	A	849	-	-	6/29/63/63	0/2/2/2
25	CLA	A	834	1	-	11/15/91/115	-
34	LUT	1	615	-	-	2/29/67/67	0/2/2/2
28	BCR	J	106	-	-	6/29/63/63	0/2/2/2
36	NEX	U	301	-	-	6/27/83/83	0/3/3/3
33	CHL	4	305	-	-	5/23/99/117	-
33	CHL	S	308	-	-	7/25/101/117	-
32	LMG	7	318	-	-	11/30/50/70	0/1/1/1
25	CLA	6	611	27	-	8/27/103/115	-
25	CLA	B	803	2	-	5/15/91/115	-
33	CHL	U	308	-	-	7/15/91/117	-
25	CLA	1	608	-	-	13/39/115/115	-
34	LUT	S	317	-	-	6/29/67/67	0/2/2/2
25	CLA	9	308	-	-	6/21/97/115	-
25	CLA	L	206	-	-	6/12/88/115	-
34	LUT	Q	615	-	-	2/29/67/67	0/2/2/2
28	BCR	8	301	-	-	3/29/63/63	0/2/2/2
25	CLA	T	611	-	-	13/33/109/115	-
25	CLA	B	838	-	-	11/39/115/115	-
25	CLA	B	811	-	-	17/39/115/115	-
25	CLA	4	308	19	-	14/33/109/115	-
35	XAT	P	620	-	-	4/31/93/93	0/4/4/4
33	CHL	S	310	15	-	7/25/101/117	-
25	CLA	1	610	27	-	10/39/115/115	-
25	CLA	5	304	20	-	5/17/93/115	-
25	CLA	A	840	-	-	17/39/115/115	-
28	BCR	B	843	-	-	5/29/63/63	0/2/2/2
25	CLA	9	310	24	-	12/21/97/115	-
33	CHL	8	307	-	-	11/26/102/117	-
35	XAT	Q	616	-	-	4/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	7	303	-	-	9/29/105/115	-
33	CHL	a	305	-	-	8/20/96/117	-
25	CLA	F	802	-	-	5/15/91/115	-
25	CLA	7	311	-	-	15/39/115/115	-
25	CLA	A	824	-	-	10/27/103/115	-
33	CHL	P	606	-	-	7/22/98/117	-
25	CLA	7	304	-	-	10/12/88/115	-
27	LHG	Q	617	-	-	13/53/53/53	-
25	CLA	O	203	-	-	0/4/80/115	-
25	CLA	8	305	-	-	6/17/93/115	-
28	BCR	B	851	-	-	3/29/63/63	0/2/2/2
25	CLA	5	319	-	-	10/17/93/115	-
28	BCR	3	318	-	-	8/29/63/63	0/2/2/2
33	CHL	Q	601	-	-	8/23/99/117	-
25	CLA	1	609	16	-	7/33/109/115	-
25	CLA	2	311	-	-	10/24/100/115	-
25	CLA	2	306	17	-	2/10/86/115	-
36	NEX	T	616	-	-	7/27/83/83	0/3/3/3
25	CLA	J	105	-	-	8/12/88/115	-
25	CLA	5	305	-	-	4/21/97/115	-
25	CLA	Q	609	-	-	11/39/115/115	-
34	LUT	2	316	-	-	0/29/67/67	0/2/2/2
25	CLA	U	303	-	-	13/39/115/115	-
25	CLA	5	314	-	-	7/15/91/115	-
33	CHL	R	606	-	-	8/22/98/117	-
28	BCR	5	323	-	-	8/29/63/63	0/2/2/2
25	CLA	3	302	-	-	8/39/115/115	-
25	CLA	U	313	-	-	9/15/91/115	-
34	LUT	2	315	-	-	6/29/67/67	0/2/2/2
34	LUT	4	316	-	-	4/29/67/67	0/2/2/2
34	LUT	a	314	-	-	2/29/67/67	0/2/2/2
25	CLA	G	202	-	-	5/17/93/115	-
33	CHL	4	314	19	-	6/14/90/117	-
25	CLA	9	301	-	-	5/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	822	-	-	16/39/115/115	-
25	CLA	4	303	-	-	9/21/97/115	-
28	BCR	A	845	-	-	3/29/63/63	0/2/2/2
25	CLA	Q	604	-	-	8/21/97/115	-
25	CLA	4	301	-	-	13/33/109/115	-
33	CHL	U	305	14	-	8/17/93/117	-
28	BCR	A	847	-	-	2/29/63/63	0/2/2/2
25	CLA	A	807	-	-	23/39/115/115	-
25	CLA	2	314	-	-	7/17/93/115	-
33	CHL	T	606	-	-	7/15/91/117	-
25	CLA	S	301	-	-	9/18/94/115	-
33	CHL	S	307	-	-	6/22/98/117	-
25	CLA	P	613	-	-	11/31/107/115	-
25	CLA	B	813	2	-	8/30/106/115	-
25	CLA	Q	610	-	-	2/10/82/115	-
25	CLA	T	608	-	-	12/39/115/115	-
33	CHL	U	307	-	-	11/26/102/117	-
32	LMG	6	602	-	-	12/35/55/70	0/1/1/1
34	LUT	3	316	-	-	0/29/67/67	0/2/2/2
25	CLA	a	303	34	-	12/30/106/115	-
33	CHL	S	321	-	-	9/23/99/117	-
25	CLA	B	807	-	-	13/39/115/115	-
25	CLA	R	602	-	-	8/39/115/115	-
25	CLA	1	613	-	-	11/39/115/115	-
34	LUT	a	316	25	-	6/29/67/67	0/2/2/2
25	CLA	S	315	15	-	8/19/95/115	-
25	CLA	A	842	27	-	13/24/100/115	-
25	CLA	S	305	-	-	6/21/97/115	-
25	CLA	4	307	-	-	7/21/97/115	-
33	CHL	R	605	14	-	5/17/93/117	-
36	NEX	U	316	-	-	7/27/83/83	0/3/3/3
34	LUT	P	614	-	-	0/29/67/67	0/2/2/2
33	CHL	S	302	-	-	15/26/102/117	-
25	CLA	U	311	-	-	9/27/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	851	-	-	16/39/115/115	-
25	CLA	B	816	2	-	13/33/109/115	-
25	CLA	P	602	-	-	7/39/115/115	-
33	CHL	4	306	-	-	6/23/99/117	-
25	CLA	A	823	-	-	12/20/96/115	-
25	CLA	1	605	-	-	2/24/100/115	-
33	CHL	6	606	-	-	7/26/102/117	-
25	CLA	6	615	21	-	6/17/93/115	-
25	CLA	H	202	-	-	4/10/86/115	-
25	CLA	5	310	-	-	7/33/109/115	-
25	CLA	8	313	-	-	13/39/115/115	-
33	CHL	1	606	-	-	8/20/96/117	-
25	CLA	5	316	-	-	4/13/89/115	-
33	CHL	Q	607	-	-	7/15/91/117	-
25	CLA	1	607	-	-	8/39/115/115	-
32	LMG	4	320	-	-	6/35/55/70	0/1/1/1
25	CLA	a	308	16	-	7/33/109/115	-
25	CLA	2	313	-	-	5/27/103/115	-
28	BCR	F	803	-	-	2/29/63/63	0/2/2/2
25	CLA	A	831	1	-	10/21/97/115	-
25	CLA	8	312	25	-	9/24/100/115	-
25	CLA	1	612	-	-	16/39/115/115	-
33	CHL	Q	606	-	-	7/22/98/117	-
34	LUT	8	317	-	-	1/29/67/67	0/2/2/2
25	CLA	4	313	19	-	2/10/86/115	-
25	CLA	6	612	-	-	5/24/100/115	-
34	LUT	6	622	-	-	1/29/67/67	0/2/2/2
28	BCR	L	203	-	-	4/29/63/63	0/2/2/2
25	CLA	B	833	-	-	5/33/109/115	-
25	CLA	2	312	-	-	14/39/115/115	-
27	LHG	5	301	-	-	19/49/49/53	-
25	CLA	8	306	-	-	5/12/88/115	-
28	BCR	4	321	-	-	7/29/63/63	0/2/2/2
28	BCR	B	845	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	S	304	-	-	14/39/115/115	-
32	LMG	J	102	-	-	8/35/55/70	0/1/1/1
25	CLA	7	308	-	-	12/33/109/115	-
35	XAT	T	615	-	-	4/31/93/93	0/4/4/4
25	CLA	A	809	1	-	15/39/115/115	-
25	CLA	8	302	23	-	15/39/115/115	-
34	LUT	4	315	-	-	1/29/67/67	0/2/2/2
25	CLA	A	821	1	-	3/15/91/115	-
25	CLA	A	832	1	-	15/39/115/115	-
28	BCR	I	201	25	-	7/29/63/63	0/2/2/2
25	CLA	6	613	-	-	11/29/105/115	-
28	BCR	L	204	25	-	7/29/63/63	0/2/2/2
25	CLA	A	836	1	-	16/39/115/115	-
35	XAT	S	318	-	-	4/31/93/93	0/4/4/4
25	CLA	7	310	-	-	9/24/100/115	-
33	CHL	P	608	-	-	7/15/91/117	-
25	CLA	1	611	-	-	10/24/100/115	-
25	CLA	8	314	-	-	9/27/103/115	-
25	CLA	5	303	-	-	13/39/115/115	-
33	CHL	U	306	-	-	7/22/98/117	-
25	CLA	B	827	2	-	9/39/115/115	-
28	BCR	G	203	28	-	1/29/63/63	0/2/2/2
25	CLA	3	314	-	-	15/29/105/115	-
25	CLA	B	805	-	-	16/39/115/115	-
33	CHL	T	607	-	-	6/25/101/117	-
25	CLA	T	609	-	-	14/33/109/115	-
25	CLA	B	828	-	-	5/21/97/115	-
25	CLA	G	201	-	-	5/21/97/115	-
25	CLA	B	804	2	-	15/39/115/115	-
27	LHG	P	624	-	-	12/53/53/53	-
25	CLA	a	311	-	-	15/39/115/115	-
27	LHG	R	618	-	-	13/53/53/53	-
25	CLA	Q	603	33	-	13/39/115/115	-
25	CLA	U	310	-	-	10/38/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	9	304	-	-	6/17/93/115	-
33	CHL	S	309	-	-	6/25/101/117	-
34	LUT	P	615	-	-	2/29/67/67	0/2/2/2
25	CLA	B	808	2	-	10/39/115/115	-
25	CLA	6	603	-	-	13/39/115/115	-
25	CLA	9	303	-	-	12/33/109/115	-
25	CLA	6	610	-	-	10/33/109/115	-
25	CLA	B	826	-	-	18/39/115/115	-
28	BCR	O	204	-	-	5/29/63/63	0/2/2/2
25	CLA	3	320	22	-	18/39/115/115	-
25	CLA	P	603	33	-	13/39/115/115	-
25	CLA	T	612	-	-	11/19/95/115	-
25	CLA	9	309	-	-	12/33/109/115	-
25	CLA	A	806	-	-	19/39/115/115	-
25	CLA	B	849	-	-	15/39/115/115	-
25	CLA	L	202	1,28	-	14/39/115/115	-
34	LUT	T	614	-	-	2/29/67/67	0/2/2/2
25	CLA	3	312	18	-	6/15/91/115	-

The worst 5 of 3923 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	841	PQN	C3-C2	6.71	1.47	1.35
26	B	839	PQN	C3-C2	6.59	1.47	1.35
33	Q	608	CHL	CMC-C2C	5.40	1.56	1.45
33	P	609	CHL	CMC-C2C	5.37	1.56	1.45
33	R	609	CHL	CMC-C2C	5.35	1.56	1.45

The worst 5 of 5047 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	303	CLA	C1-C2-C3	16.98	155.41	126.04
25	1	612	CLA	C4A-NA-C1A	13.26	112.67	106.71
36	P	621	NEX	C16-C1-C6	12.24	121.42	110.47
25	a	303	CLA	C4-C3-C5	-10.98	96.79	115.27
33	S	306	CHL	C2B-C1B-NB	10.73	117.43	110.23

There are no chirality outliers.

5 of 4042 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	801	CLA	CBD-CGD-O2D-CED
25	A	804	CLA	C2B-C3B-CAB-CBB
25	A	804	CLA	C4B-C3B-CAB-CBB
25	A	804	CLA	CAD-CBD-CGD-O1D
25	A	804	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

390 monomers are involved in 1340 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	838	CLA	1	0
27	a	317	LHG	6	0
25	T	602	CLA	6	0
25	B	818	CLA	2	0
25	a	310	CLA	3	0
34	7	315	LUT	2	0
25	A	826	CLA	2	0
25	A	820	CLA	3	0
25	a	301	CLA	6	0
28	A	846	BCR	4	0
28	L	207	BCR	2	0
31	B	850	SQD	5	0
25	B	831	CLA	2	0
25	B	823	CLA	6	0
34	1	617	LUT	3	0
25	B	834	CLA	6	0
25	B	817	CLA	1	0
28	A	848	BCR	3	0
25	R	613	CLA	6	0
25	T	610	CLA	7	0
28	B	842	BCR	4	0
33	Q	605	CHL	2	0
25	S	303	CLA	10	0
33	R	608	CHL	3	0
25	R	603	CLA	29	0
33	R	609	CHL	47	0
25	2	304	CLA	5	0
34	9	313	LUT	7	0
25	B	806	CLA	1	0
27	7	317	LHG	1	0
25	8	309	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Q	612	CLA	5	0
25	K	203	CLA	2	0
27	A	843	LHG	1	0
25	A	835	CLA	1	0
27	S	319	LHG	3	0
25	B	815	CLA	2	0
28	4	317	BCR	8	0
25	Q	602	CLA	6	0
25	B	824	CLA	1	0
32	2	301	LMG	5	0
25	U	302	CLA	6	0
32	H	204	LMG	3	0
25	B	835	CLA	1	0
25	a	307	CLA	6	0
33	P	607	CHL	1	0
25	7	309	CLA	1	0
34	7	314	LUT	8	0
28	3	317	BCR	1	0
34	R	615	LUT	9	0
28	B	841	BCR	1	0
33	S	306	CHL	7	0
34	5	322	LUT	5	0
33	Q	608	CHL	50	0
34	U	315	LUT	8	0
25	a	306	CLA	8	0
25	A	827	CLA	3	0
25	A	825	CLA	5	0
25	B	810	CLA	4	0
25	a	302	CLA	6	0
32	7	319	LMG	2	0
25	A	819	CLA	2	0
25	3	303	CLA	2	0
25	2	305	CLA	1	0
25	B	821	CLA	1	0
33	P	609	CHL	48	0
27	T	617	LHG	5	0
25	2	309	CLA	4	0
25	B	832	CLA	2	0
25	4	302	CLA	1	0
34	U	314	LUT	4	0
25	H	201	CLA	1	0
25	4	309	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	618	LHG	5	0
33	P	601	CHL	2	0
33	R	607	CHL	1	0
33	P	619	CHL	4	0
28	7	316	BCR	2	0
34	a	315	LUT	5	0
25	A	808	CLA	4	0
28	8	318	BCR	3	0
27	8	319	LHG	1	0
25	1	602	CLA	6	0
25	Q	611	CLA	8	0
33	3	306	CHL	1	0
25	L	201	CLA	4	0
27	1	618	LHG	3	0
25	A	814	CLA	6	0
33	6	607	CHL	1	0
25	H	203	CLA	2	0
25	3	308	CLA	3	0
33	5	307	CHL	1	0
25	A	822	CLA	6	0
28	3	319	BCR	7	0
32	J	104	LMG	1	0
34	3	315	LUT	4	0
28	A	854	BCR	7	0
25	a	312	CLA	3	0
25	5	315	CLA	3	0
25	8	310	CLA	3	0
25	A	853	CLA	2	0
34	T	613	LUT	5	0
27	A	852	LHG	6	0
27	A	844	LHG	2	0
25	6	605	CLA	6	0
25	a	309	CLA	3	0
33	T	601	CHL	1	0
25	2	310	CLA	2	0
25	A	802	CLA	7	0
25	6	623	CLA	2	0
25	7	301	CLA	1	0
25	P	611	CLA	22	0
25	K	201	CLA	1	0
33	U	309	CHL	3	0
33	6	617	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	601	CLA	2	0
25	3	305	CLA	3	0
25	5	313	CLA	5	0
25	6	620	CLA	3	0
33	T	604	CHL	1	0
34	S	316	LUT	3	0
28	6	621	BCR	2	0
36	P	617	NEX	3	0
25	A	815	CLA	4	0
33	P	622	CHL	8	0
25	2	307	CLA	1	0
25	B	809	CLA	2	0
25	Q	613	CLA	2	0
25	B	802	CLA	3	0
25	5	306	CLA	2	0
25	S	314	CLA	5	0
25	A	837	CLA	2	0
33	9	306	CHL	1	0
25	O	202	CLA	1	0
29	C	101	SF4	1	0
32	1	619	LMG	1	0
36	P	621	NEX	15	0
35	P	616	XAT	7	0
25	3	307	CLA	2	0
25	A	803	CLA	2	0
27	4	318	LHG	1	0
34	Q	614	LUT	5	0
25	L	209	CLA	1	0
25	A	812	CLA	3	0
35	P	623	XAT	8	0
25	B	825	CLA	3	0
25	A	813	CLA	2	0
25	5	324	CLA	4	0
28	5	320	BCR	4	0
33	6	608	CHL	6	0
25	K	205	CLA	1	0
25	A	810	CLA	5	0
32	J	107	LMG	2	0
34	R	616	LUT	5	0
25	A	811	CLA	4	0
25	A	833	CLA	1	0
25	U	312	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	5	317	CHL	1	0
33	7	305	CHL	2	0
28	B	844	BCR	5	0
34	6	619	LUT	4	0
27	B	847	LHG	2	0
25	L	205	CLA	3	0
33	T	605	CHL	2	0
34	1	616	LUT	1	0
25	A	830	CLA	4	0
30	B	846	DGD	3	0
25	S	313	CLA	1	0
25	6	609	CLA	1	0
25	S	320	CLA	6	0
25	T	603	CLA	1	0
33	4	322	CHL	5	0
25	A	804	CLA	3	0
28	J	101	BCR	2	0
25	7	313	CLA	1	0
25	K	204	CLA	1	0
25	B	837	CLA	4	0
30	B	848	DGD	3	0
36	R	617	NEX	3	0
33	5	308	CHL	2	0
25	3	301	CLA	1	0
25	R	610	CLA	30	0
33	P	605	CHL	2	0
33	R	601	CHL	2	0
25	A	817	CLA	2	0
25	7	312	CLA	2	0
34	9	312	LUT	4	0
25	A	801	CLA	3	0
25	A	839	CLA	3	0
34	8	316	LUT	8	0
25	9	302	CLA	1	0
27	P	618	LHG	9	0
28	L	208	BCR	1	0
25	4	310	CLA	8	0
25	B	836	CLA	3	0
25	2	303	CLA	5	0
25	B	812	CLA	2	0
25	P	612	CLA	41	0
25	A	828	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	610	CLA	29	0
34	5	318	LUT	3	0
25	B	801	CLA	2	0
25	K	202	CLA	1	0
25	a	304	CLA	5	0
26	B	839	PQN	2	0
25	R	612	CLA	62	0
25	Q	618	CLA	12	0
33	1	601	CHL	3	0
25	S	312	CLA	4	0
28	B	840	BCR	3	0
27	2	317	LHG	1	0
25	8	303	CLA	1	0
25	A	818	CLA	3	0
25	B	830	CLA	3	0
28	O	205	BCR	1	0
25	1	604	CLA	3	0
27	5	321	LHG	1	0
25	R	614	CLA	1	0
25	5	302	CLA	2	0
25	2	302	CLA	2	0
25	B	820	CLA	1	0
25	J	103	CLA	6	0
25	U	304	CLA	1	0
25	A	816	CLA	7	0
25	B	829	CLA	1	0
25	R	611	CLA	17	0
28	A	849	BCR	4	0
25	A	834	CLA	1	0
34	1	615	LUT	8	0
28	J	106	BCR	5	0
36	U	301	NEX	21	0
33	S	308	CHL	2	0
25	6	611	CLA	3	0
25	B	803	CLA	1	0
33	U	308	CHL	3	0
25	1	608	CLA	2	0
34	S	317	LUT	8	0
25	9	308	CLA	1	0
25	L	206	CLA	2	0
34	Q	615	LUT	7	0
25	T	611	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	838	CLA	3	0
25	B	811	CLA	2	0
25	4	308	CLA	6	0
35	P	620	XAT	8	0
33	S	310	CHL	7	0
25	1	610	CLA	5	0
25	5	304	CLA	1	0
25	A	840	CLA	3	0
28	B	843	BCR	2	0
33	8	307	CHL	4	0
35	Q	616	XAT	6	0
33	a	305	CHL	1	0
25	F	802	CLA	2	0
25	7	311	CLA	4	0
33	P	606	CHL	4	0
25	7	304	CLA	1	0
27	Q	617	LHG	4	0
28	B	851	BCR	2	0
28	3	318	BCR	2	0
33	Q	601	CHL	1	0
25	1	609	CLA	1	0
25	2	311	CLA	5	0
25	2	306	CLA	2	0
36	T	616	NEX	3	0
25	Q	609	CLA	7	0
34	2	316	LUT	4	0
25	U	303	CLA	6	0
33	R	606	CHL	3	0
28	5	323	BCR	4	0
25	3	302	CLA	4	0
25	U	313	CLA	6	0
34	2	315	LUT	5	0
34	4	316	LUT	2	0
34	a	314	LUT	8	0
25	G	202	CLA	2	0
33	4	314	CHL	3	0
25	9	301	CLA	1	0
25	B	822	CLA	3	0
28	A	845	BCR	5	0
25	Q	604	CLA	3	0
25	4	301	CLA	1	0
33	U	305	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	847	BCR	2	0
25	A	807	CLA	3	0
25	2	314	CLA	3	0
33	T	606	CHL	4	0
25	S	301	CLA	15	0
33	S	307	CHL	1	0
25	P	613	CLA	7	0
25	B	813	CLA	1	0
25	Q	610	CLA	3	0
25	T	608	CLA	7	0
33	U	307	CHL	3	0
32	6	602	LMG	1	0
34	3	316	LUT	1	0
25	a	303	CLA	18	0
33	S	321	CHL	5	0
25	B	807	CLA	3	0
25	R	602	CLA	6	0
25	1	613	CLA	4	0
34	a	316	LUT	4	0
25	S	315	CLA	4	0
25	A	842	CLA	2	0
25	4	307	CLA	1	0
33	R	605	CHL	2	0
36	U	316	NEX	4	0
34	P	614	LUT	5	0
33	S	302	CHL	5	0
25	U	311	CLA	9	0
25	A	851	CLA	4	0
25	B	816	CLA	1	0
25	P	602	CLA	6	0
33	4	306	CHL	2	0
25	A	823	CLA	2	0
25	1	605	CLA	4	0
33	6	606	CHL	3	0
25	6	615	CLA	2	0
25	H	202	CLA	3	0
25	5	310	CLA	1	0
25	8	313	CLA	2	0
33	1	606	CHL	1	0
25	5	316	CLA	1	0
33	Q	607	CHL	3	0
25	1	607	CLA	6	0

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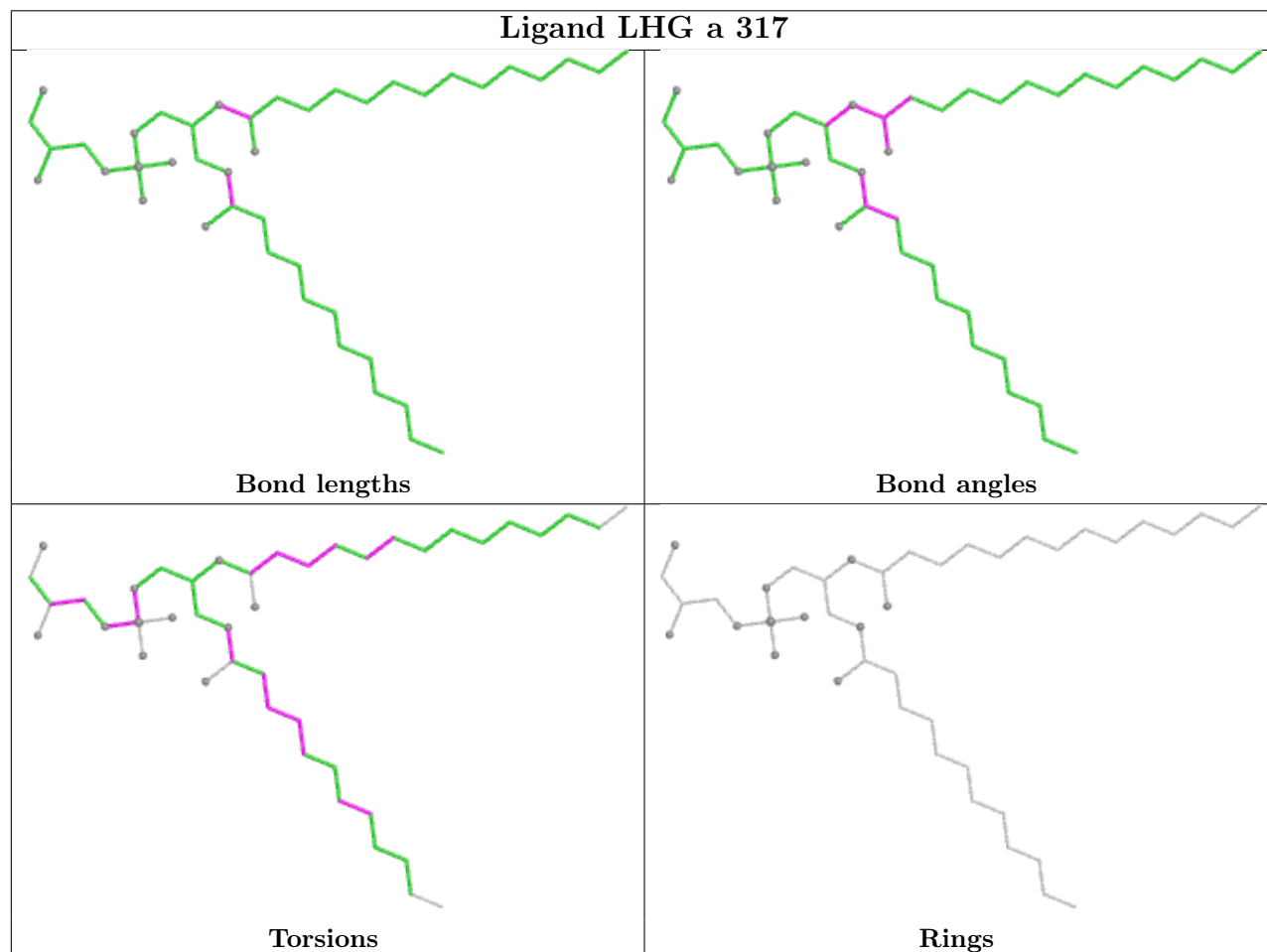
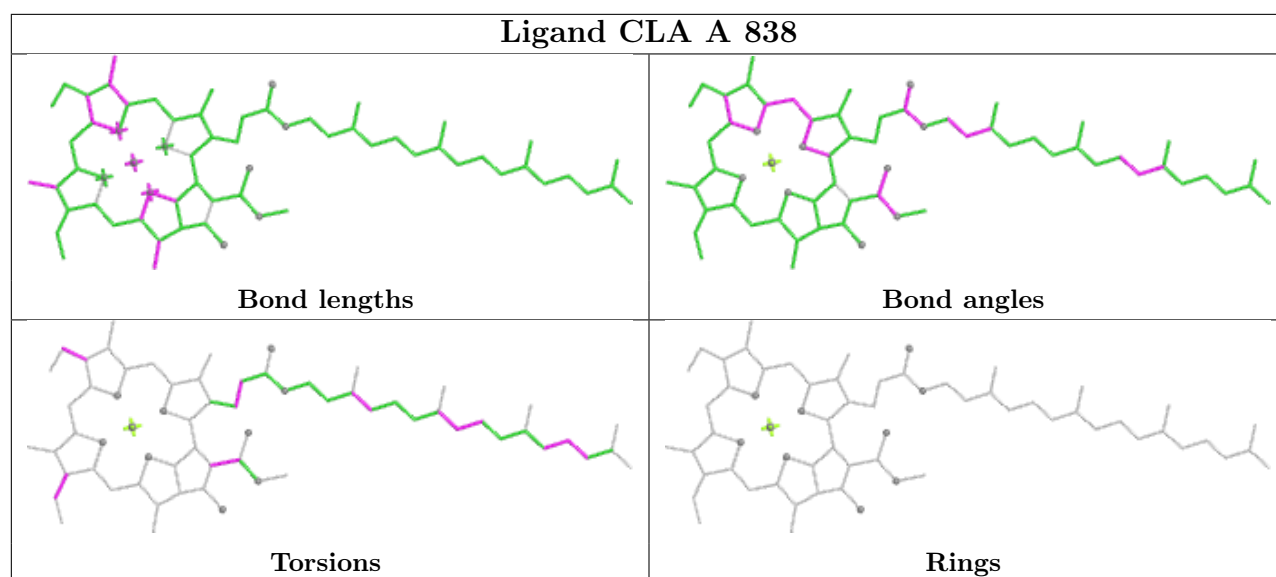
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25	a	308	CLA	2	0
25	2	313	CLA	2	0
28	F	803	BCR	3	0
25	A	831	CLA	1	0
25	1	612	CLA	1	0
33	Q	606	CHL	4	0
34	8	317	LUT	1	0
25	6	612	CLA	1	0
34	6	622	LUT	1	0
25	B	833	CLA	6	0
25	2	312	CLA	5	0
27	5	301	LHG	5	0
25	8	306	CLA	1	0
28	4	321	BCR	2	0
28	B	845	BCR	3	0
25	S	304	CLA	6	0
32	J	102	LMG	1	0
25	7	308	CLA	2	0
35	T	615	XAT	6	0
25	A	809	CLA	3	0
25	8	302	CLA	3	0
34	4	315	LUT	9	0
25	A	821	CLA	1	0
25	A	832	CLA	2	0
28	I	201	BCR	5	0
25	6	613	CLA	1	0
28	L	204	BCR	1	0
25	A	836	CLA	2	0
35	S	318	XAT	8	0
25	7	310	CLA	1	0
33	P	608	CHL	3	0
25	1	611	CLA	4	0
25	8	314	CLA	3	0
25	5	303	CLA	8	0
33	U	306	CHL	2	0
25	B	827	CLA	1	0
28	G	203	BCR	1	0
25	3	314	CLA	3	0
25	B	805	CLA	3	0
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25	T	609	CLA	6	0

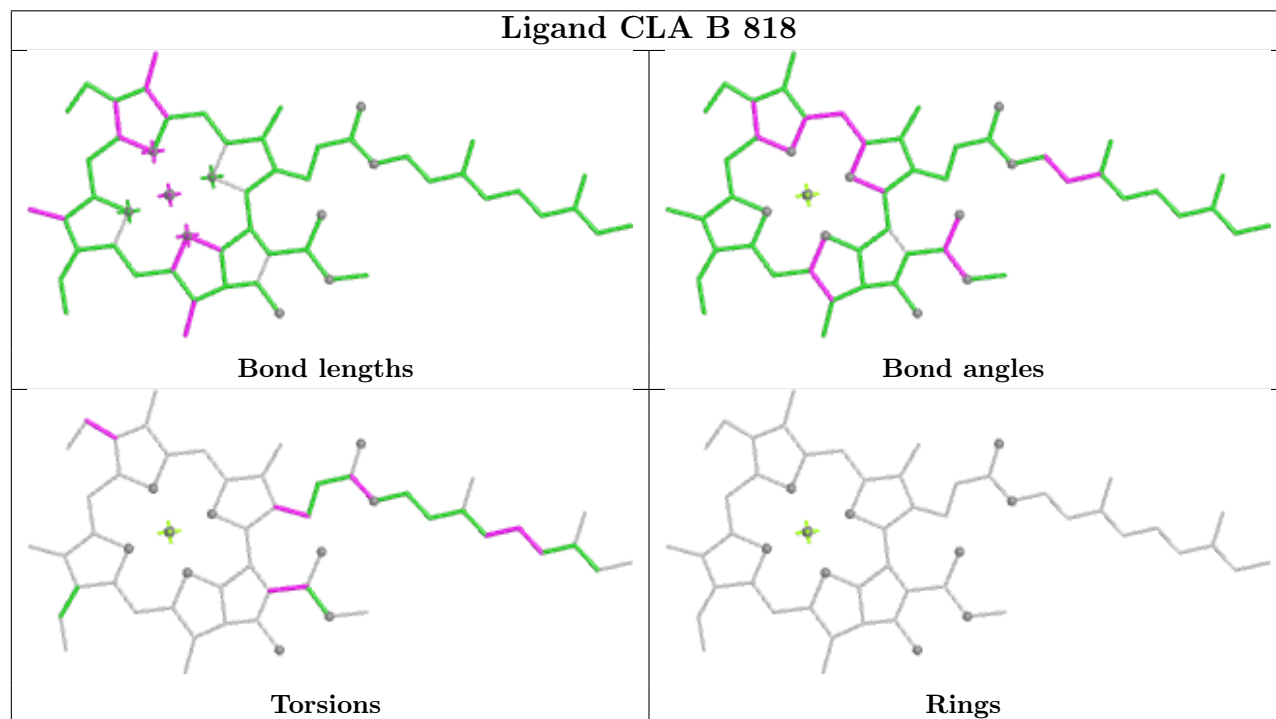
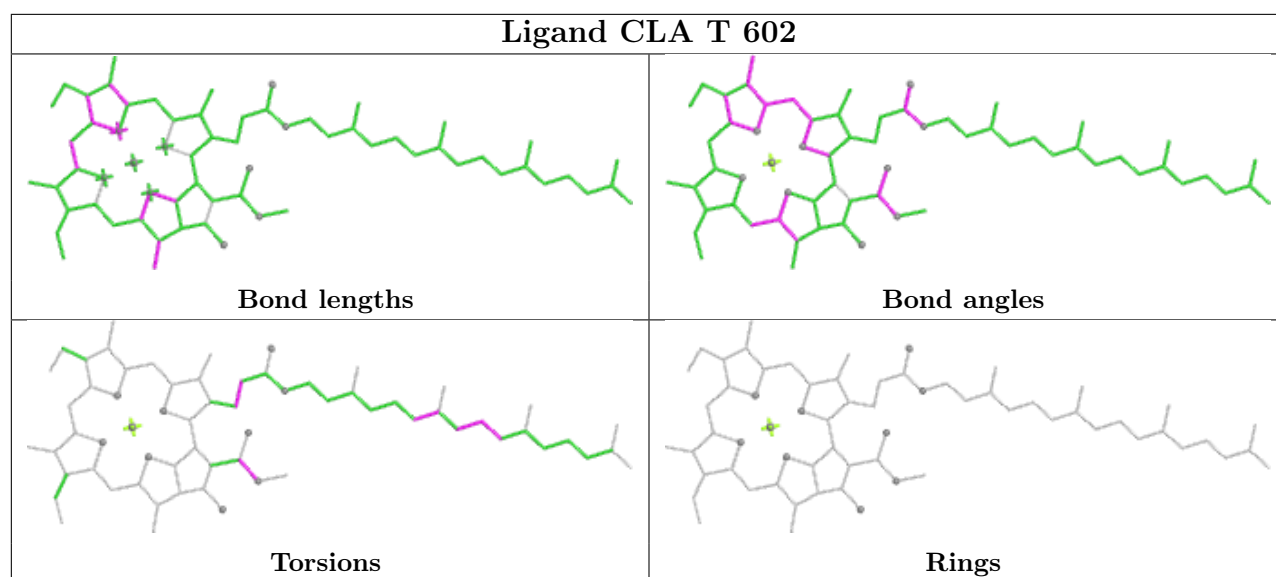
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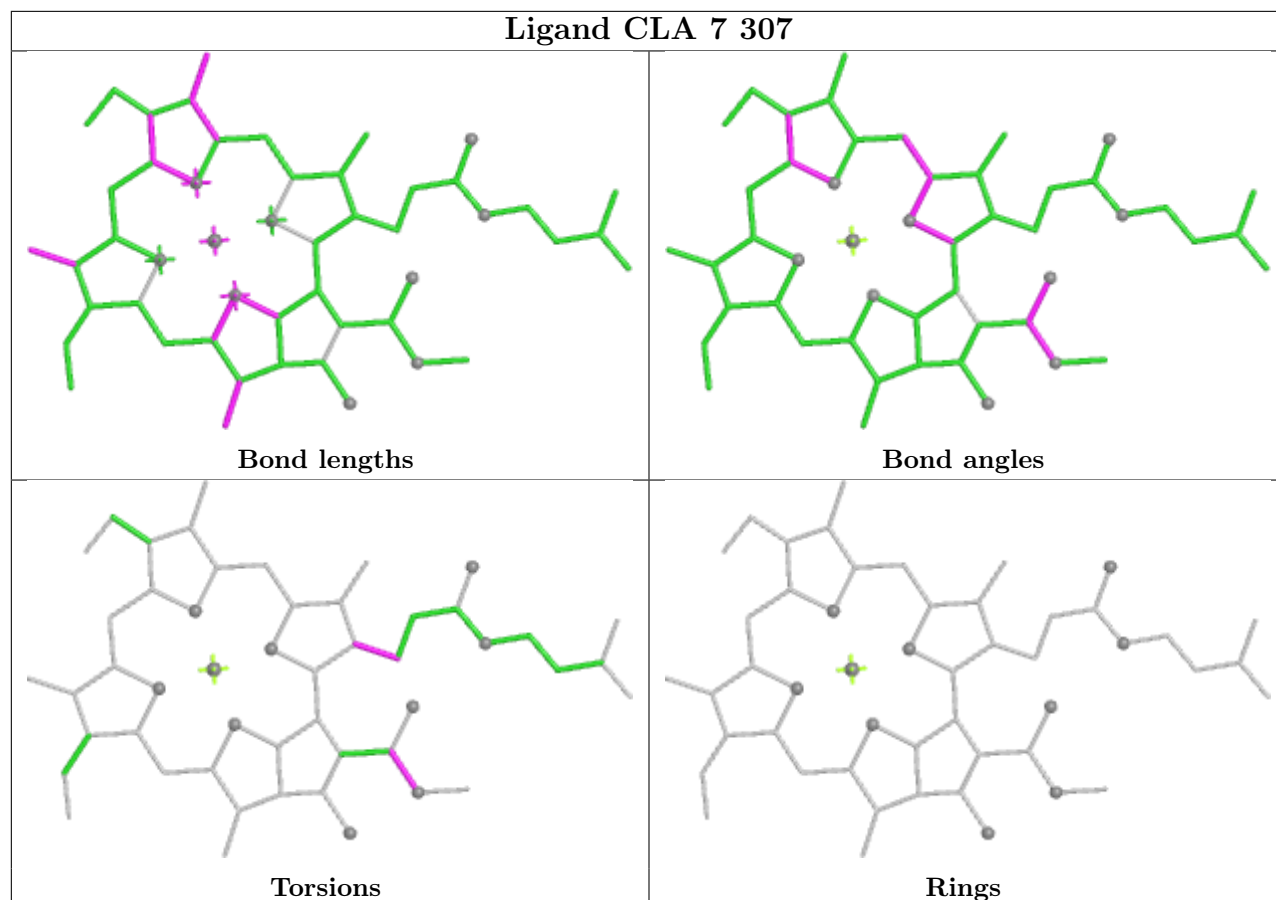
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25	B	804	CLA	1	0
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25	a	311	CLA	2	0
27	R	618	LHG	7	0
25	Q	603	CLA	33	0
25	U	310	CLA	7	0
25	9	304	CLA	2	0
33	S	309	CHL	2	0
34	P	615	LUT	9	0
25	B	808	CLA	1	0
25	6	603	CLA	4	0
25	9	303	CLA	2	0
25	6	610	CLA	3	0
25	B	826	CLA	2	0
28	O	204	BCR	2	0
25	3	320	CLA	3	0
25	P	603	CLA	28	0
25	T	612	CLA	1	0
25	9	309	CLA	1	0
25	A	806	CLA	3	0
25	L	202	CLA	1	0
34	T	614	LUT	3	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.

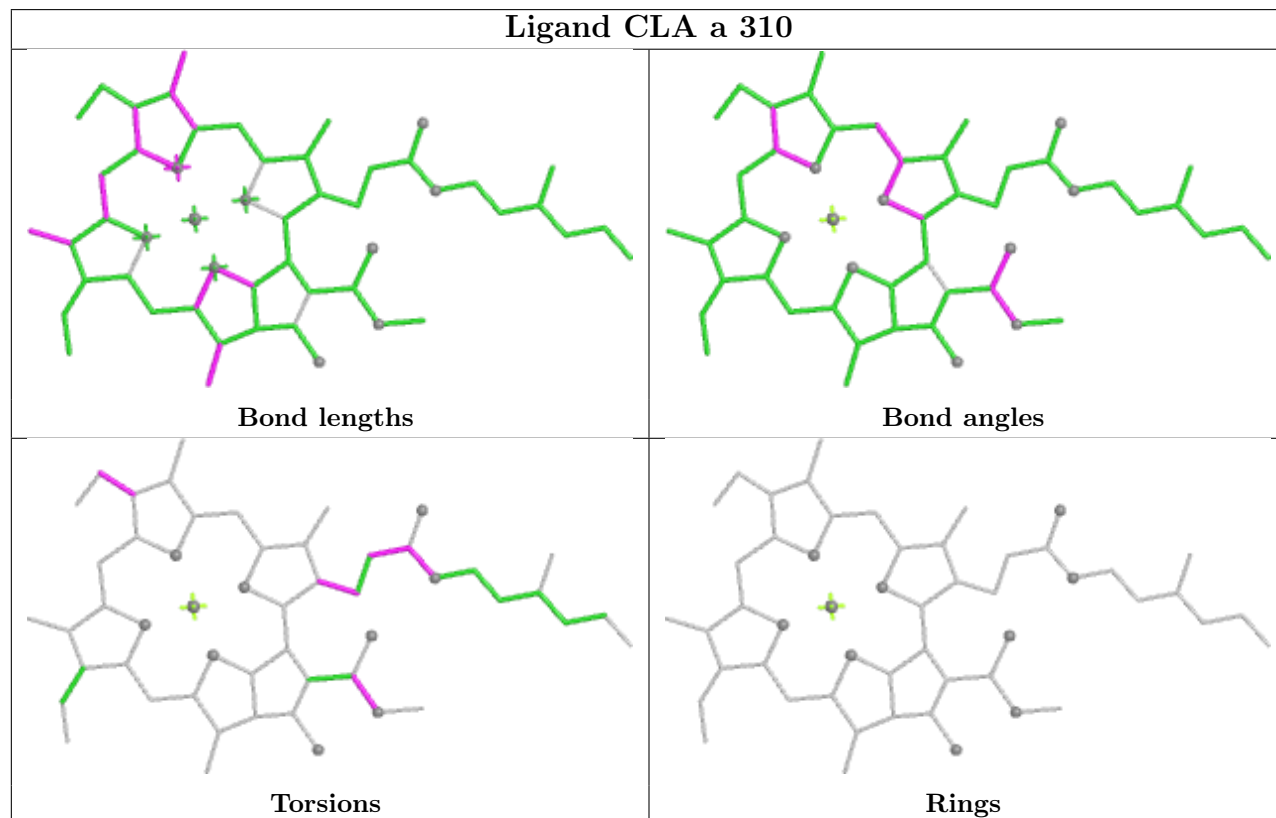


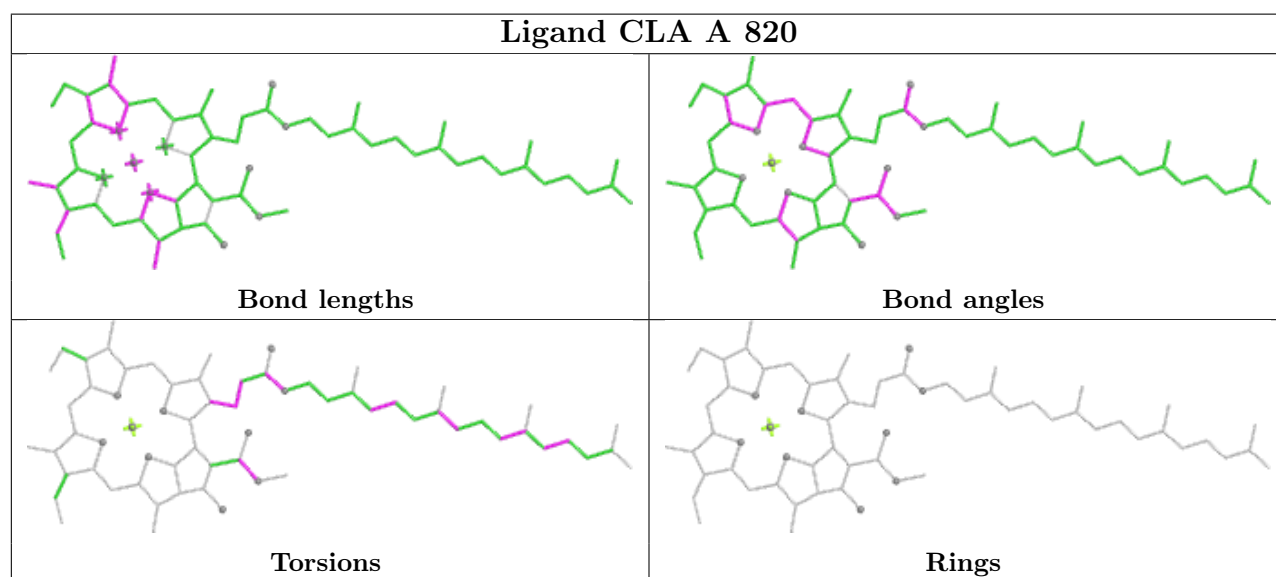
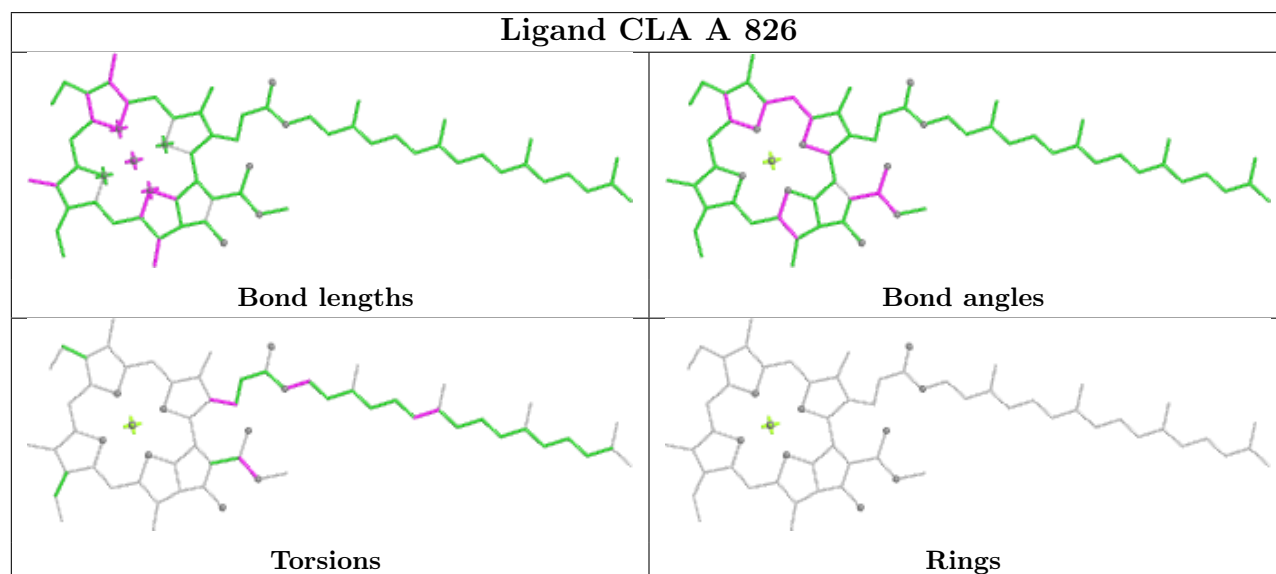
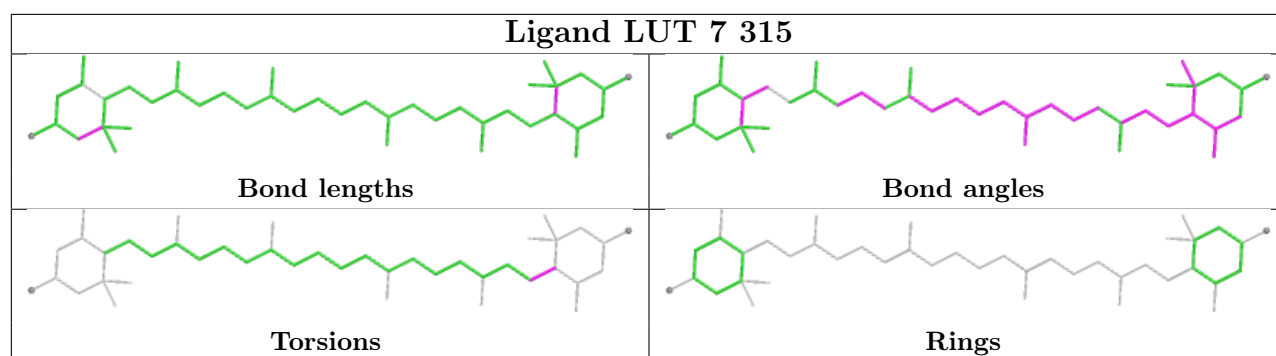


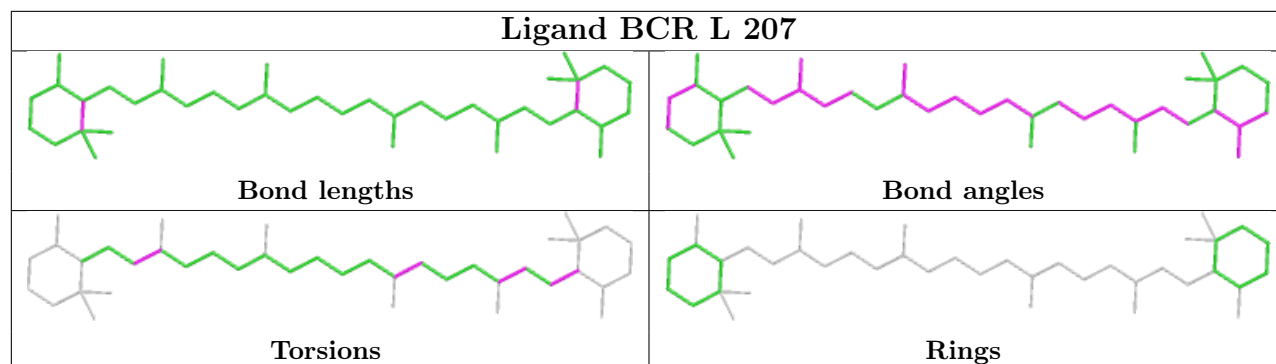
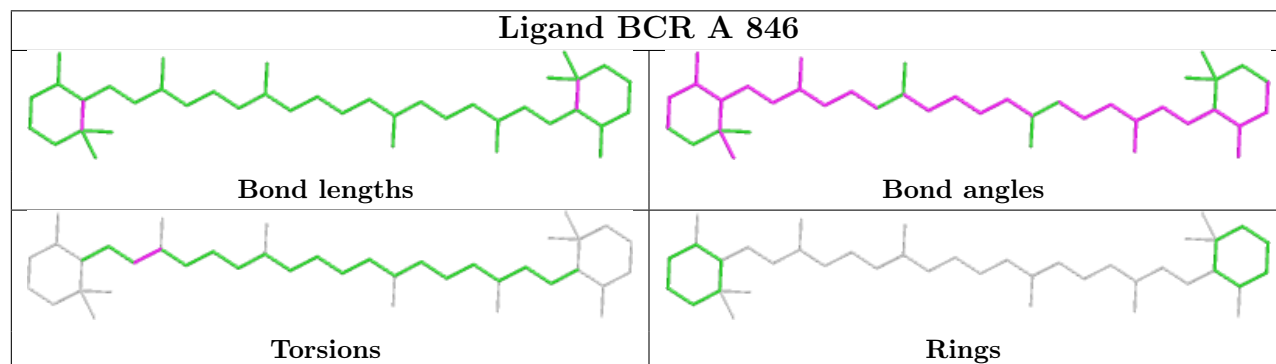
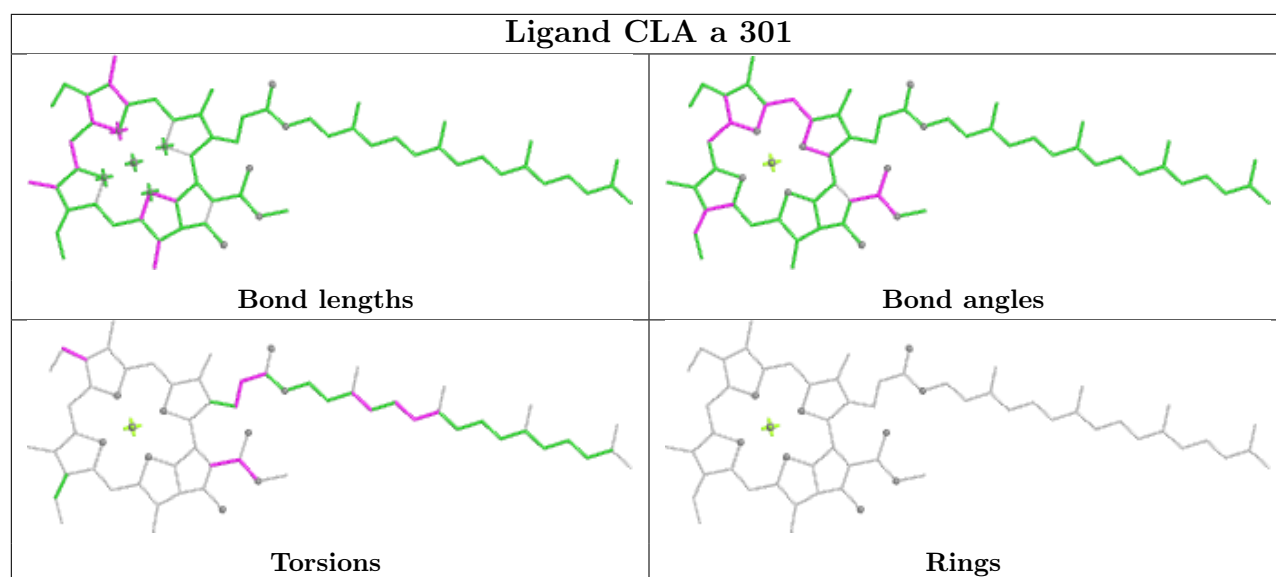
Ligand CLA 7 307

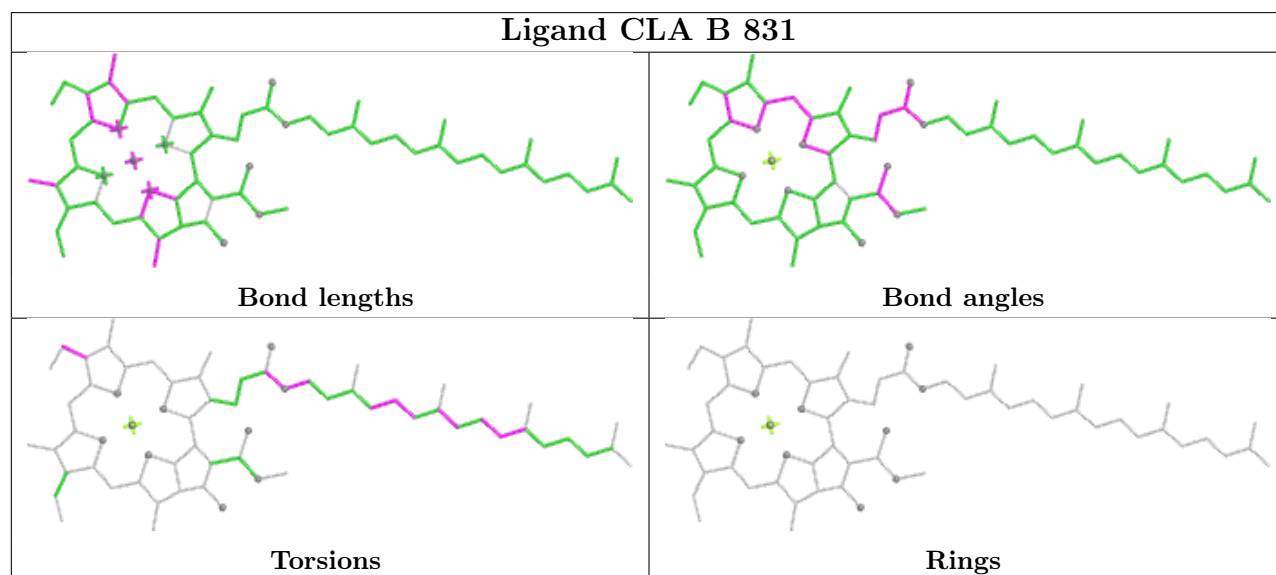
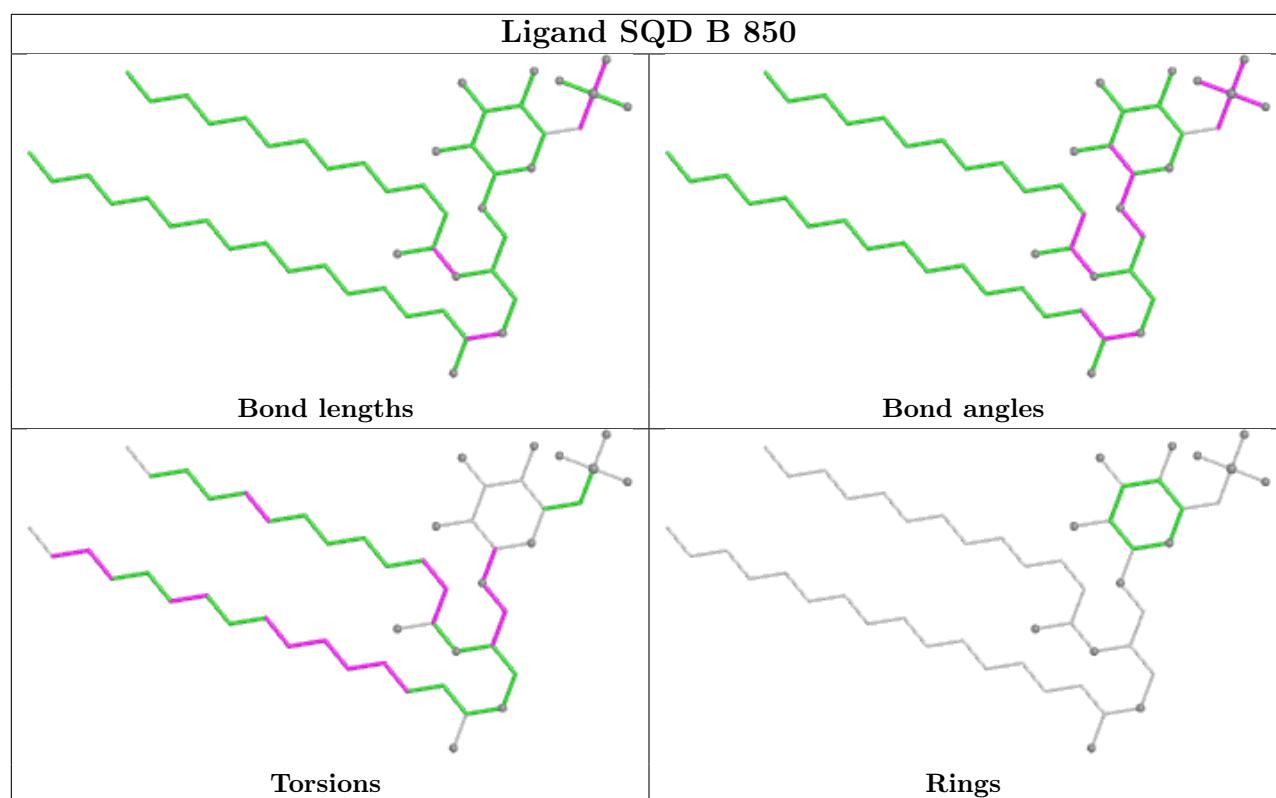


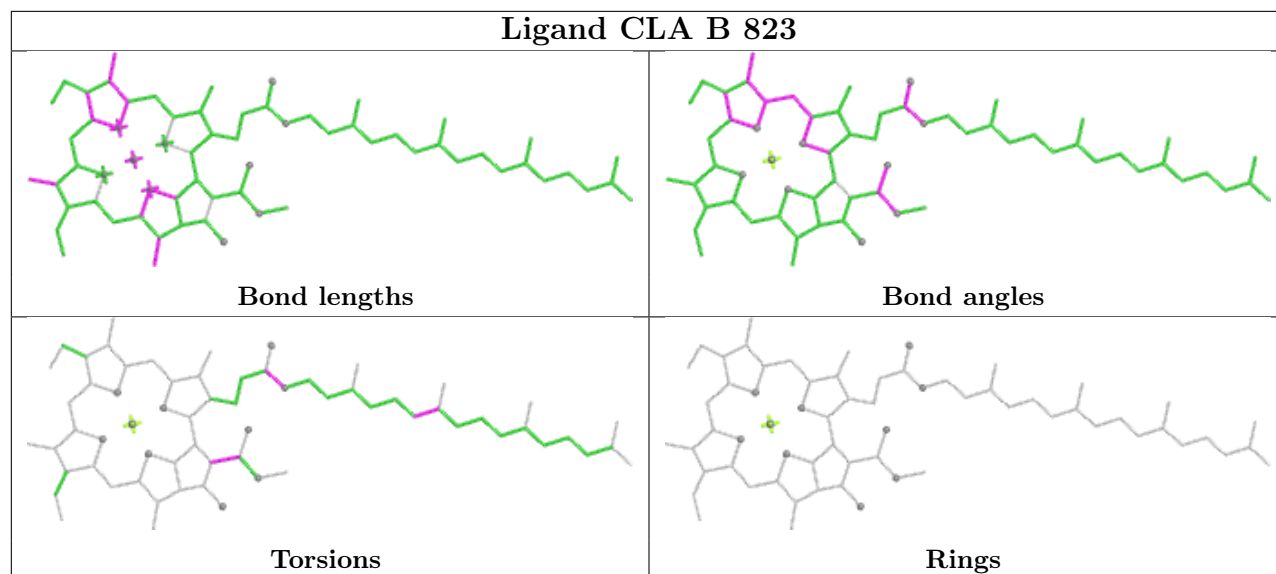
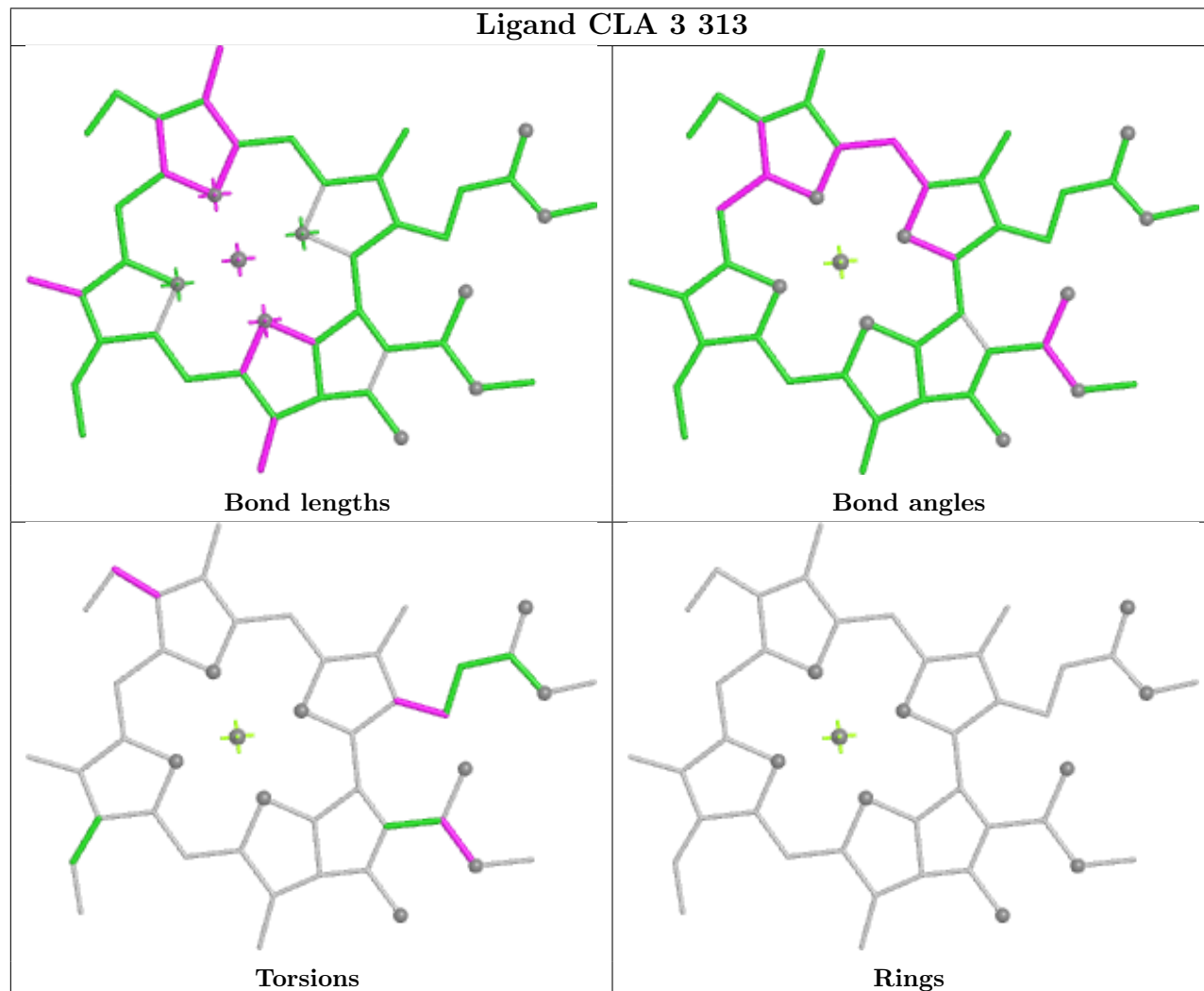
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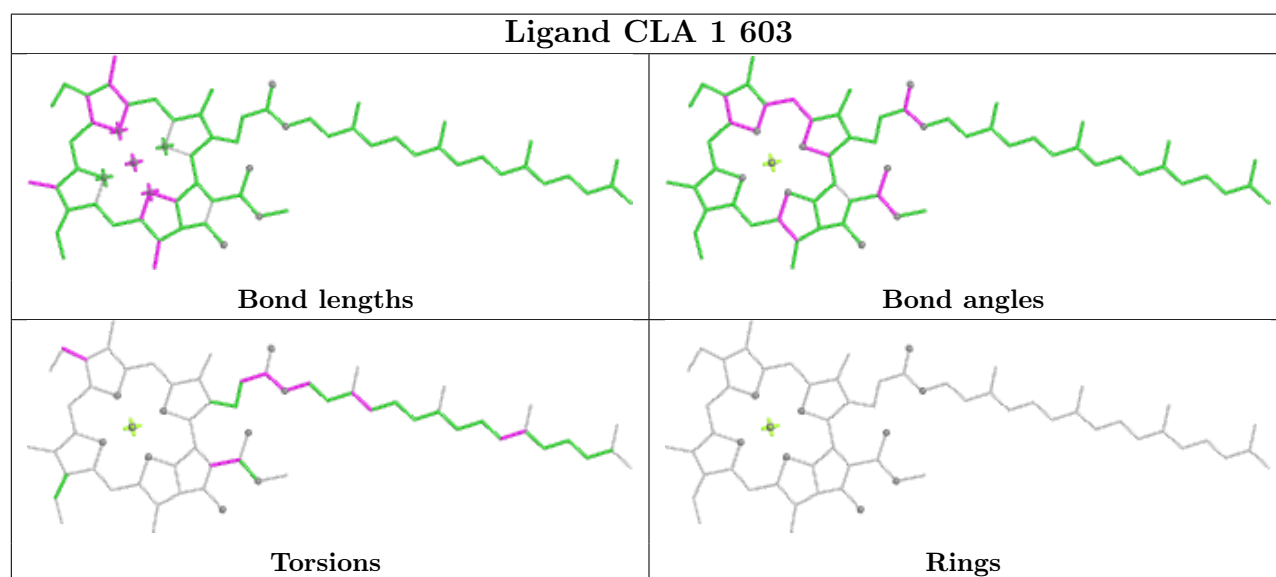
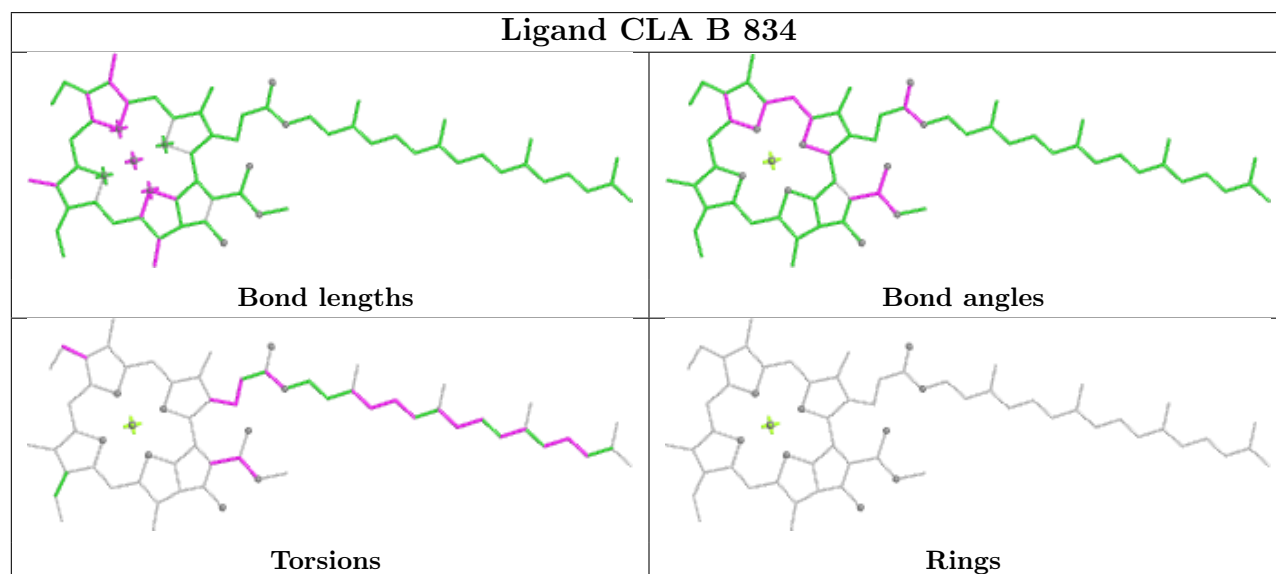
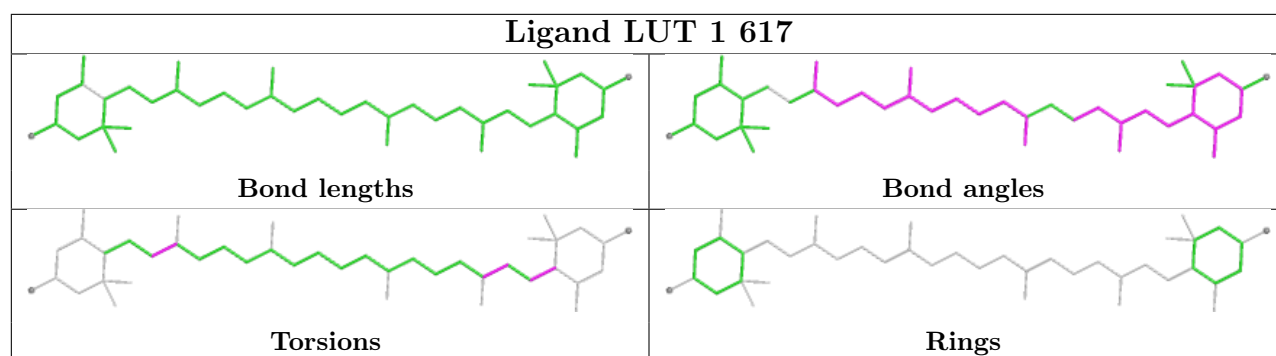


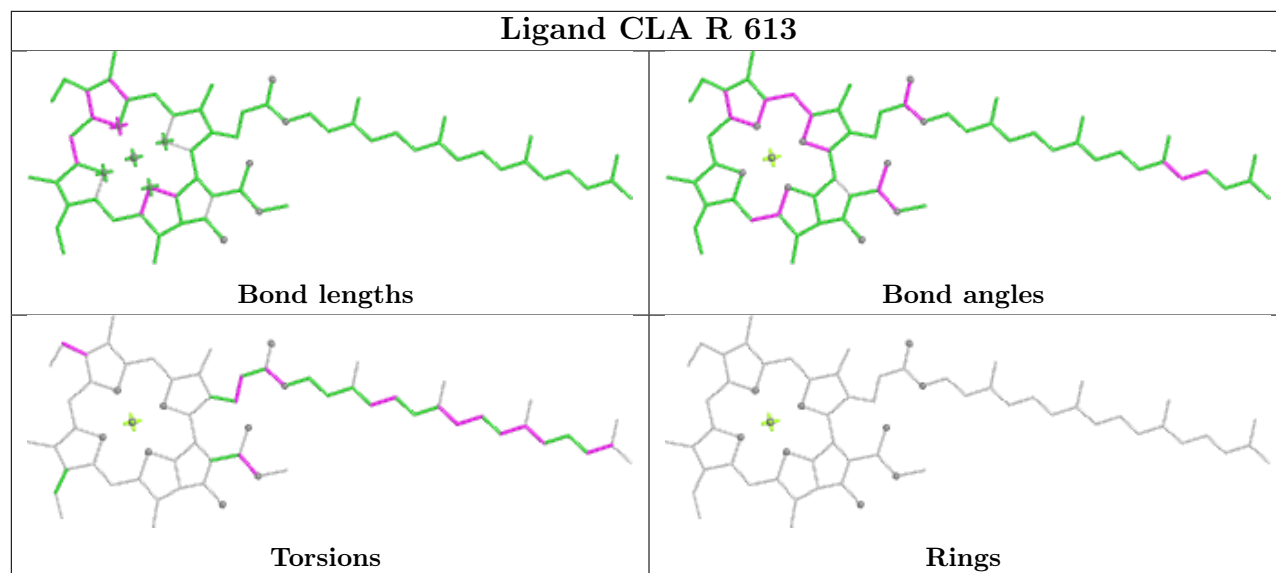
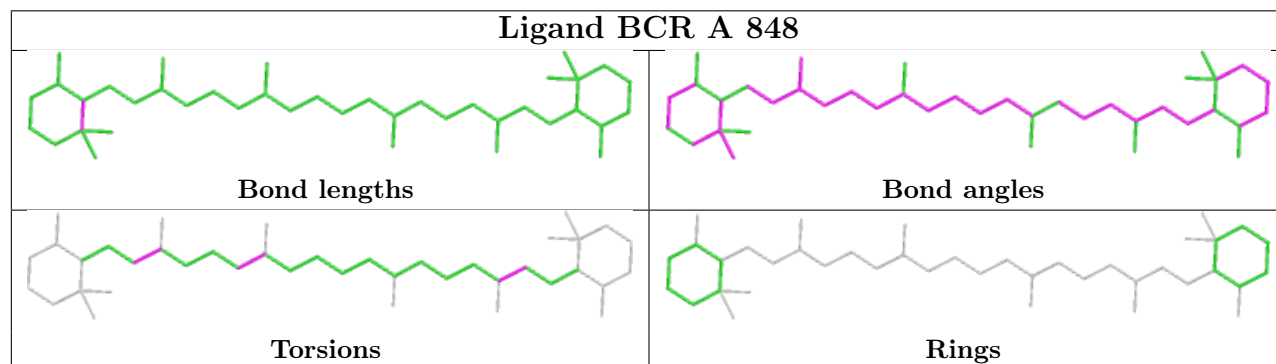
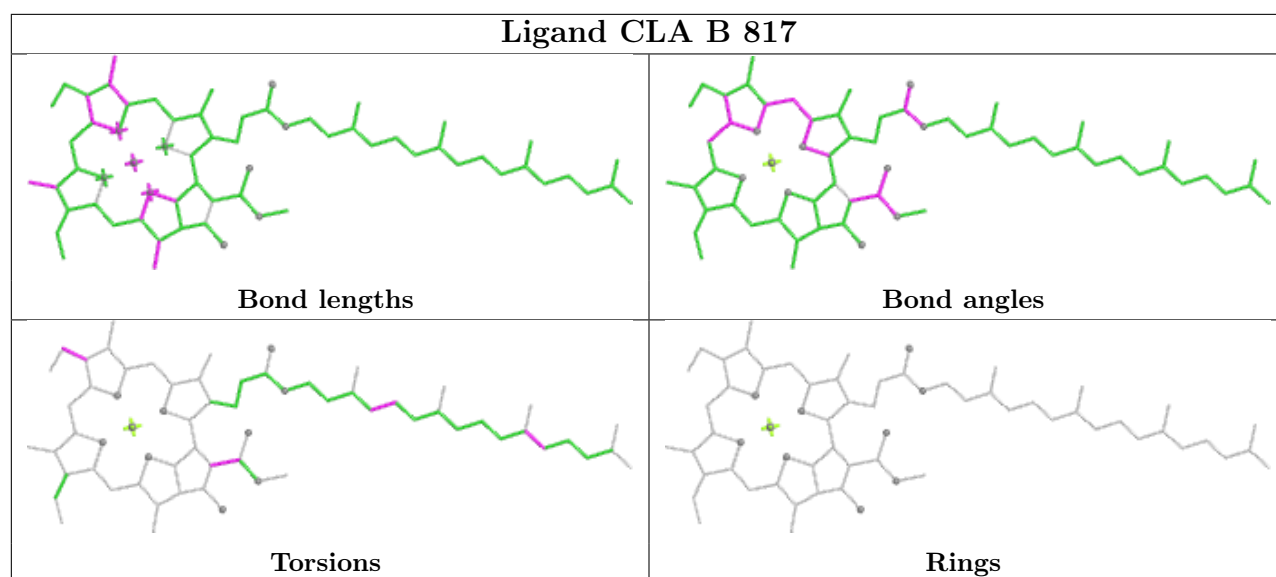


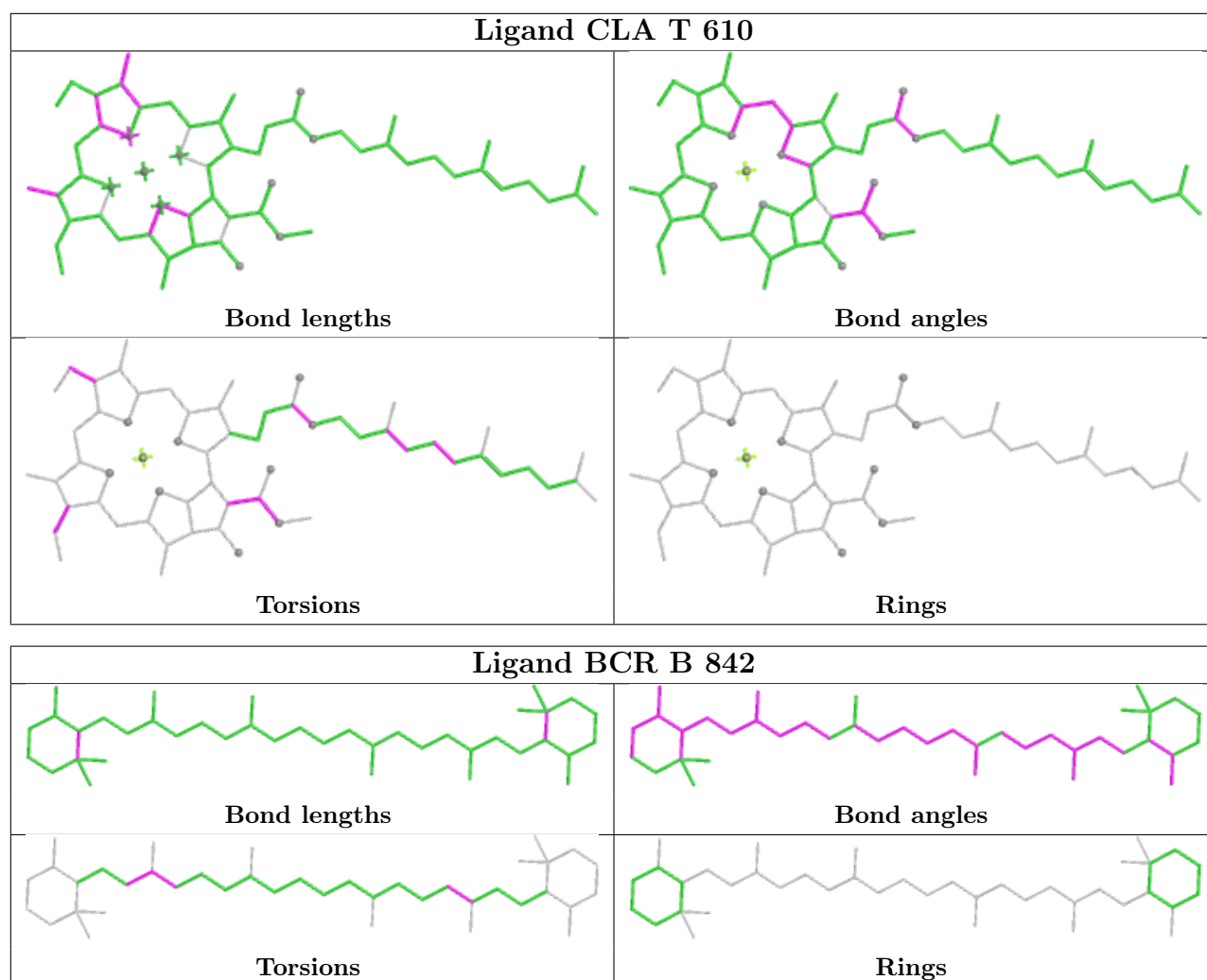


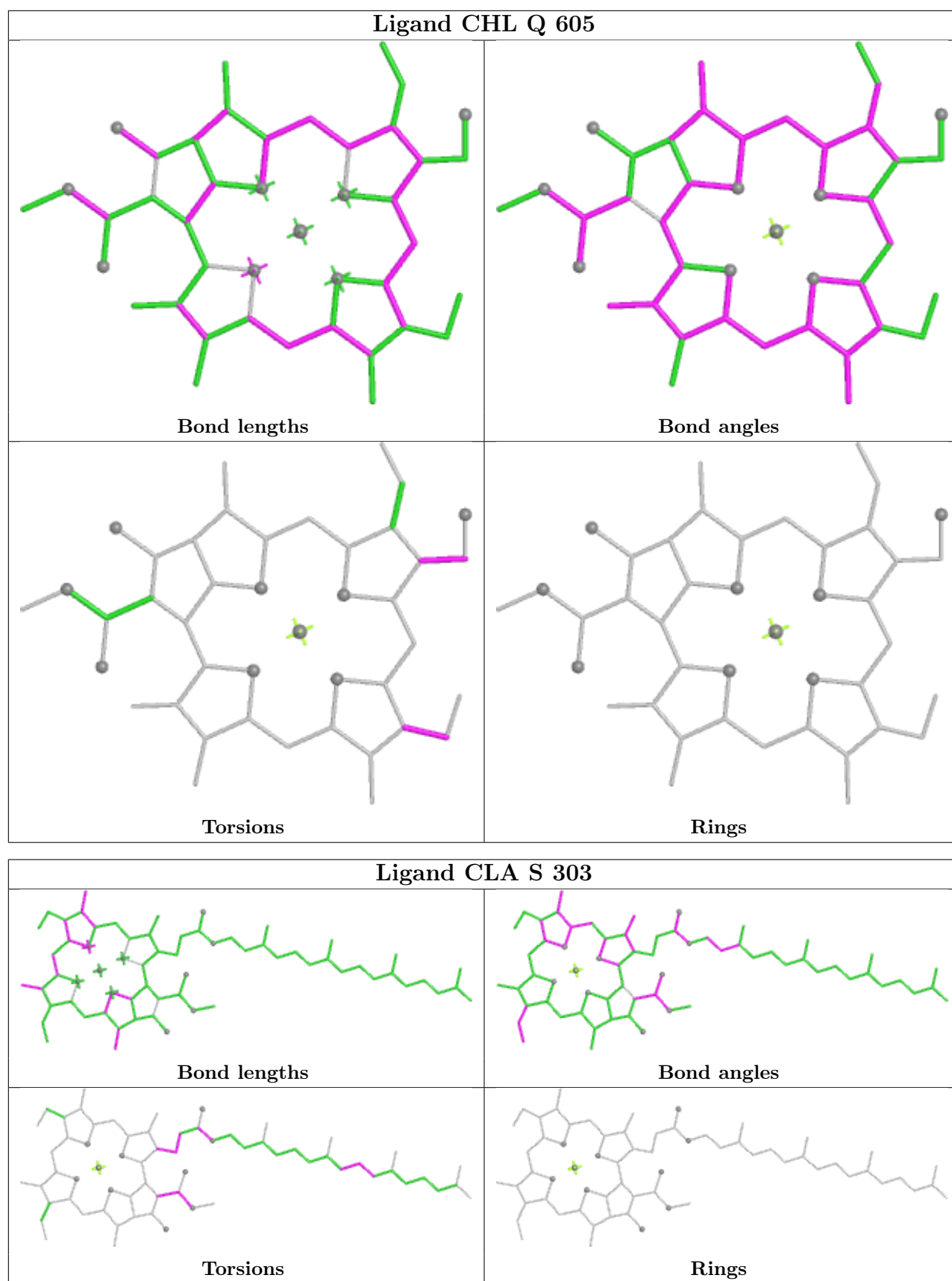


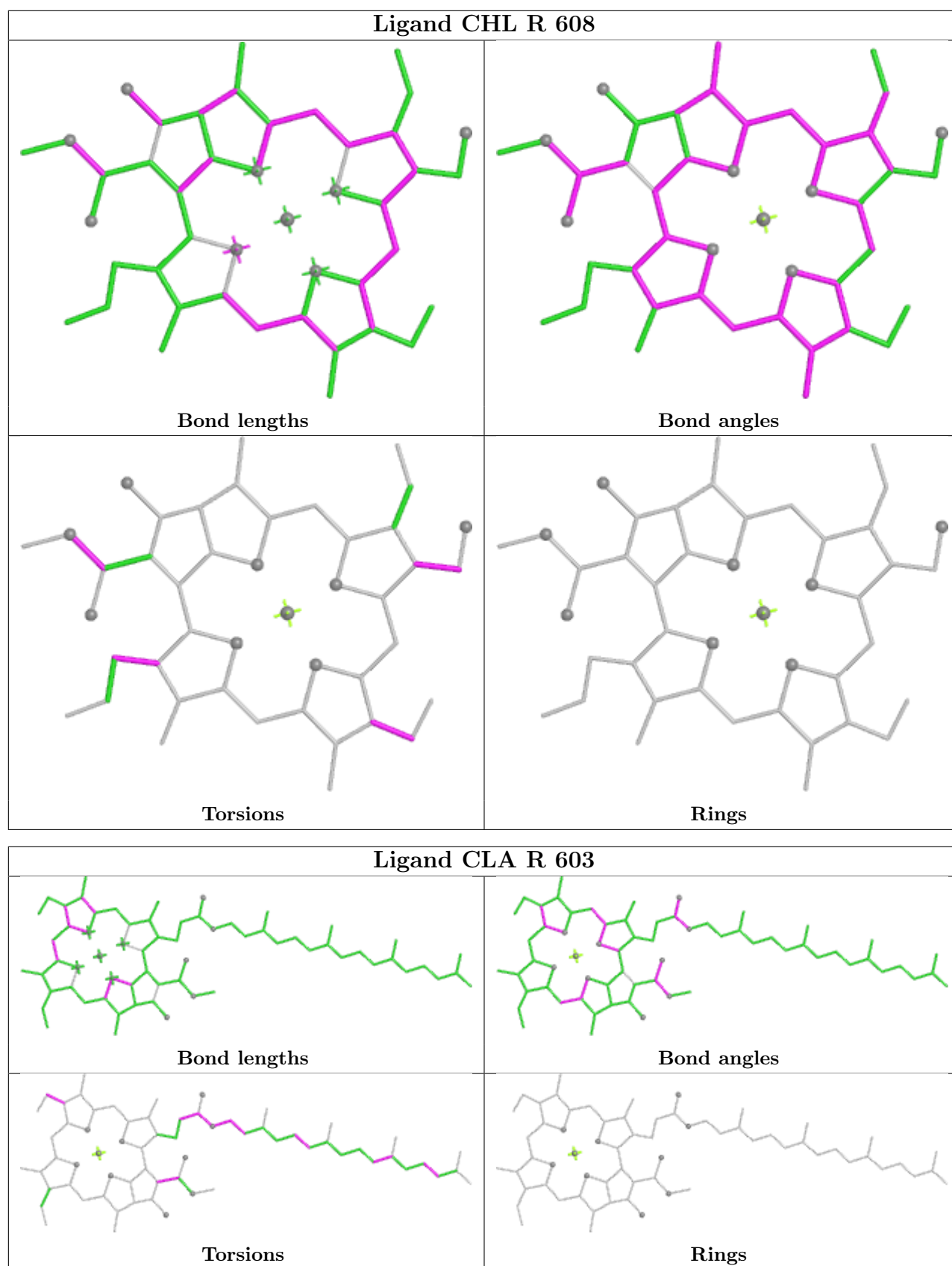
Ligand CLA B 823**Ligand CLA 3 313**

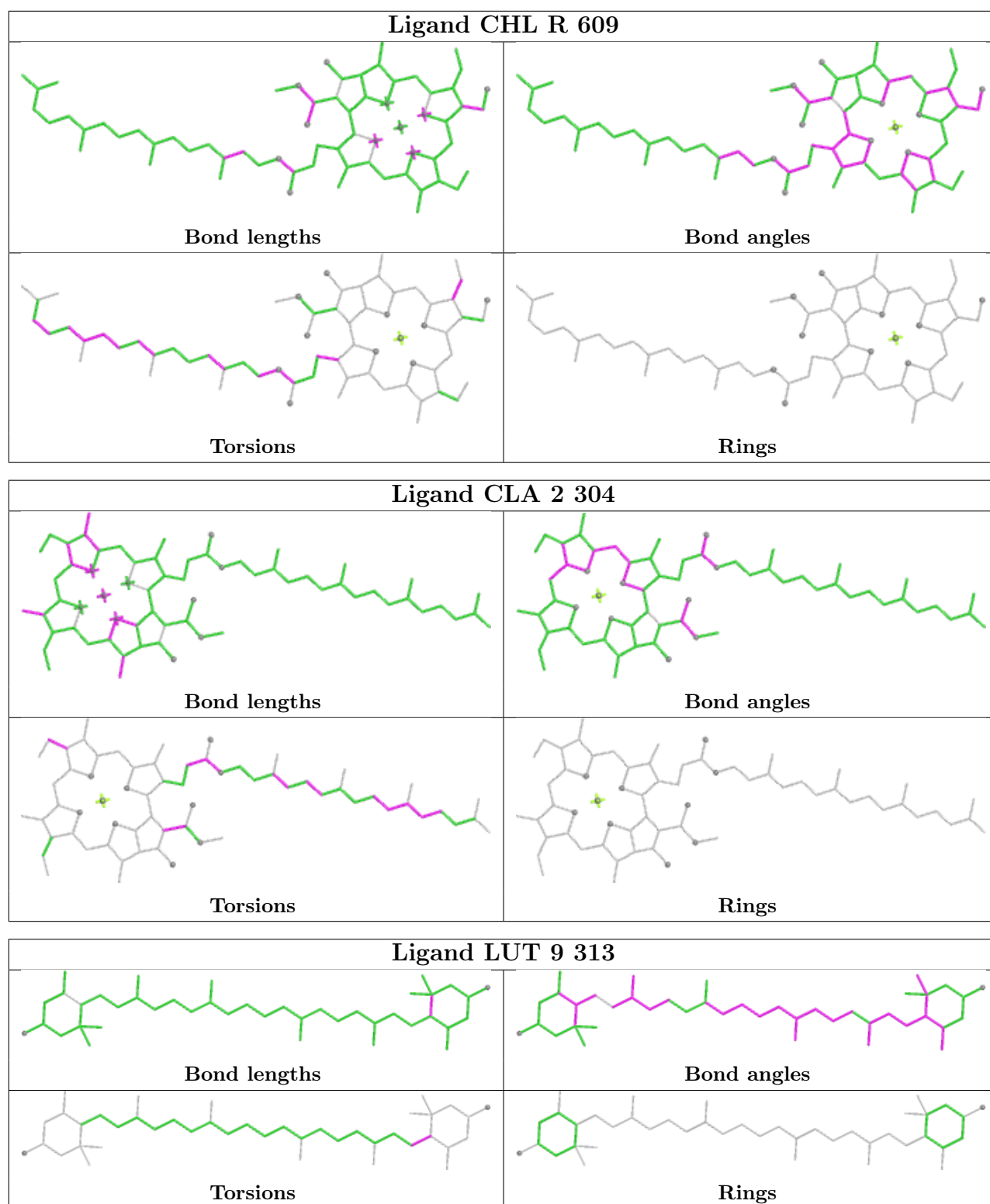


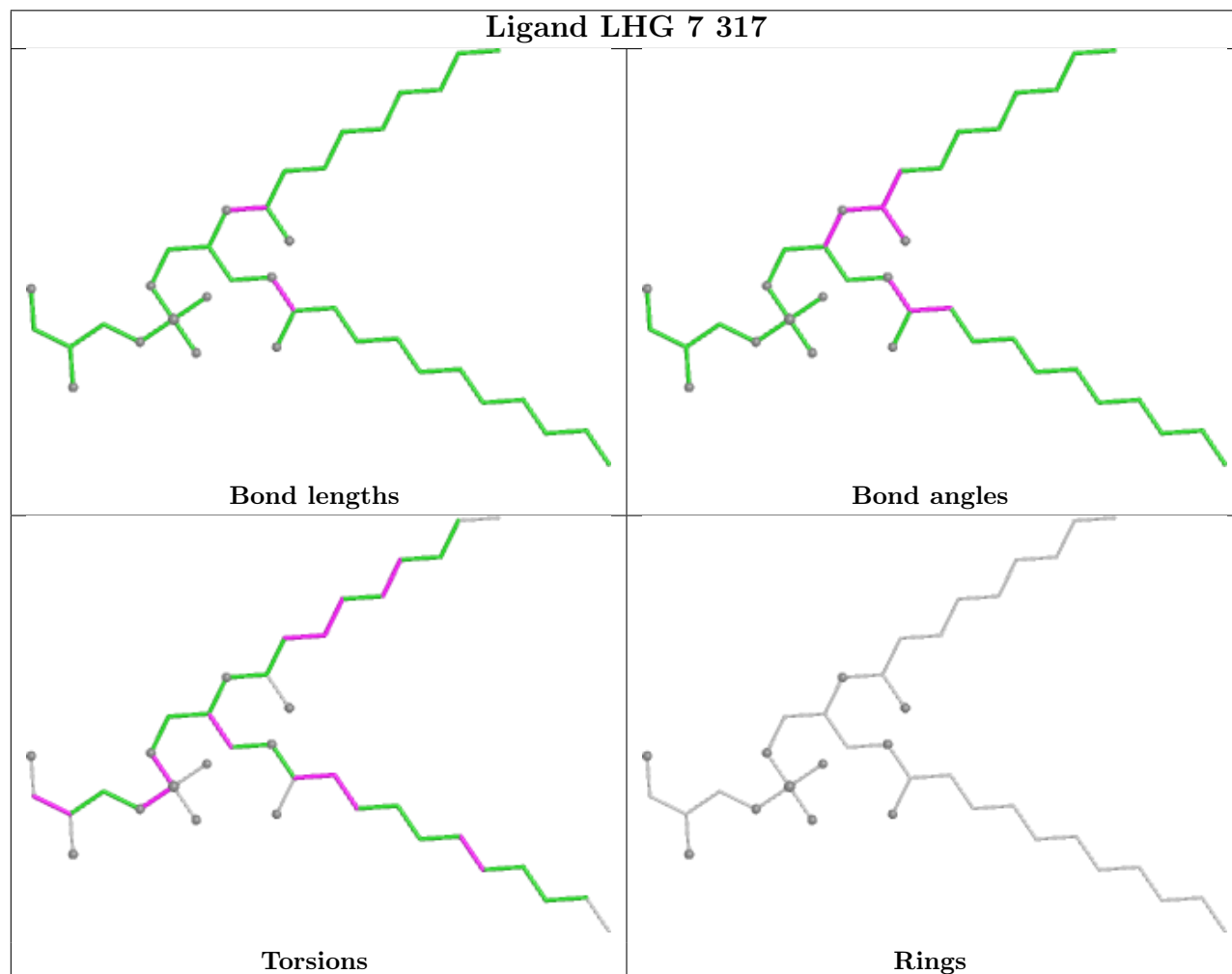
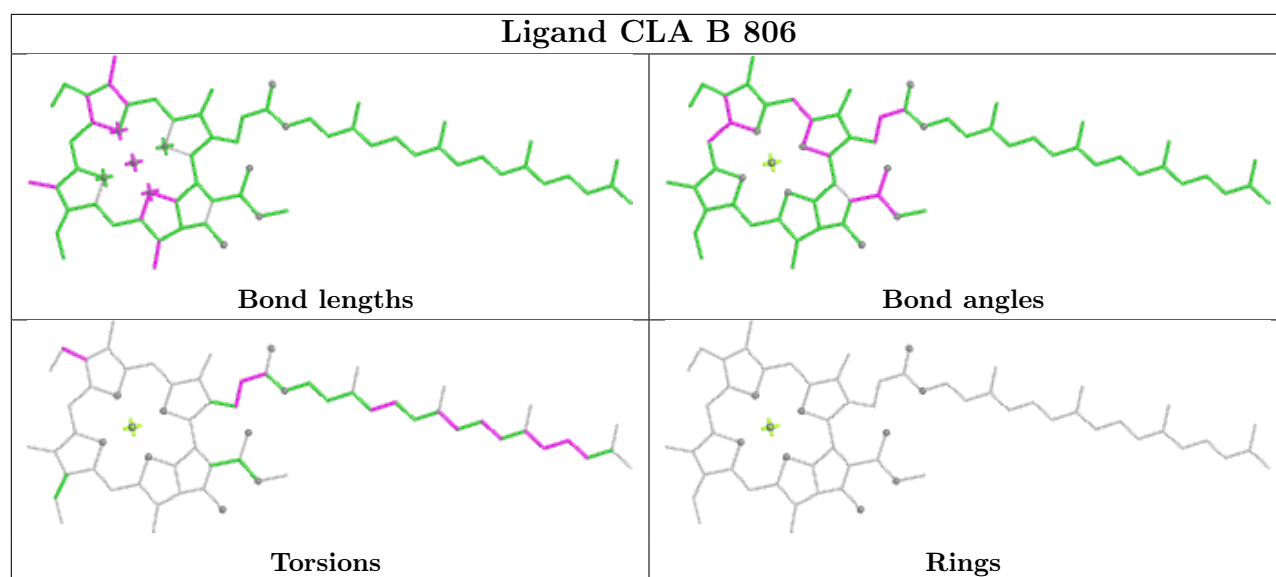




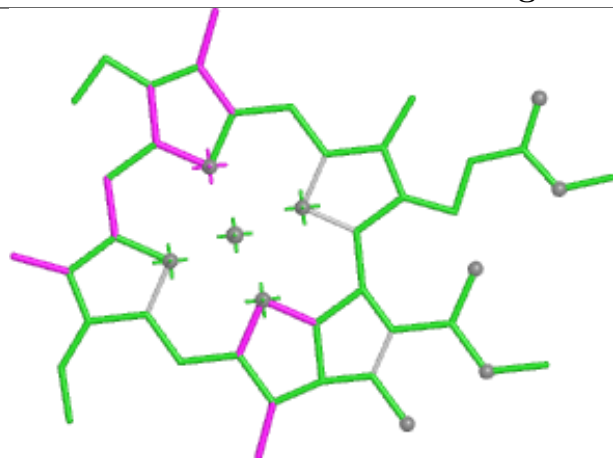




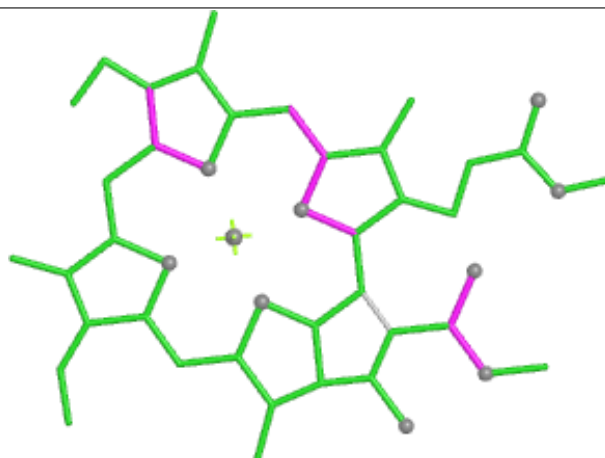




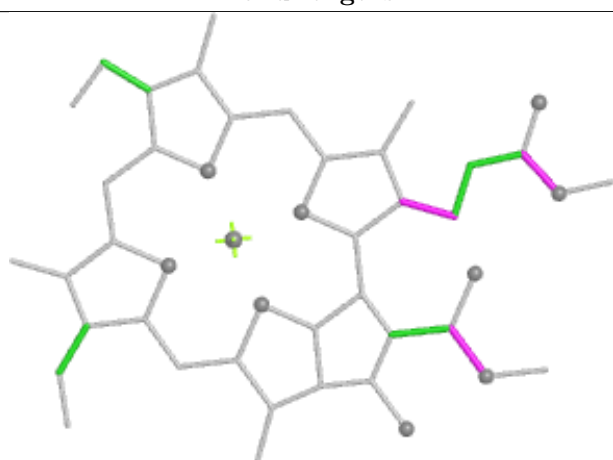
Ligand CLA 8 309



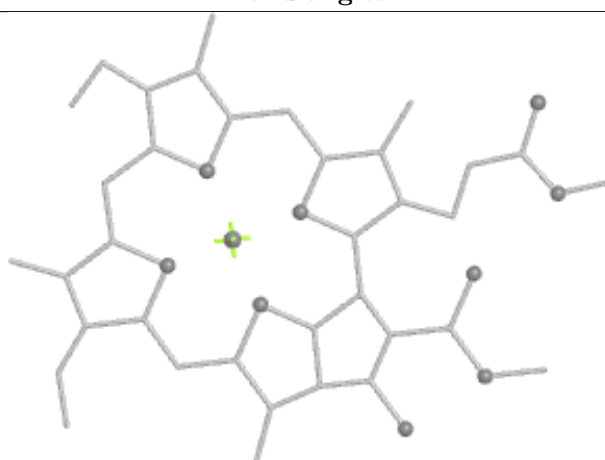
Bond lengths



Bond angles

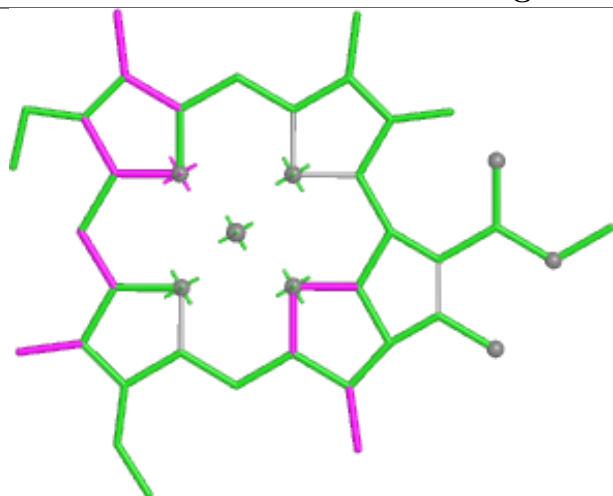


Torsions

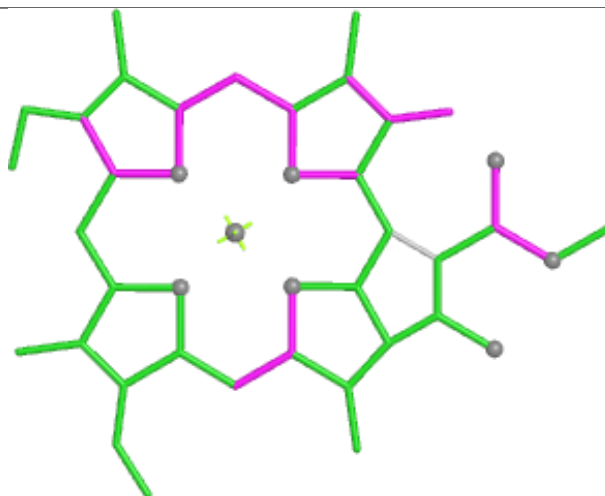


Rings

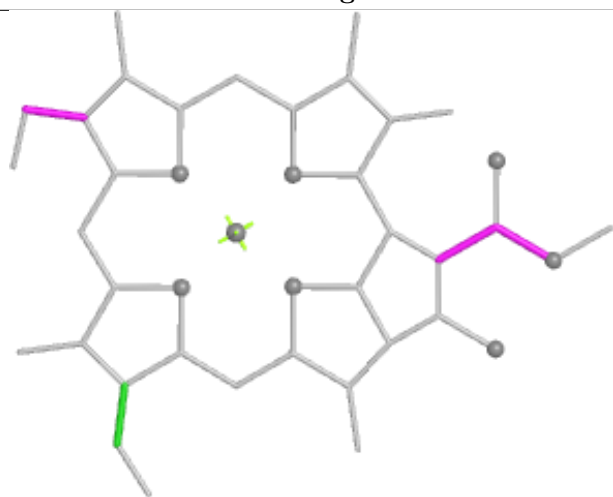
Ligand CLA O 201



Bond lengths



Bond angles

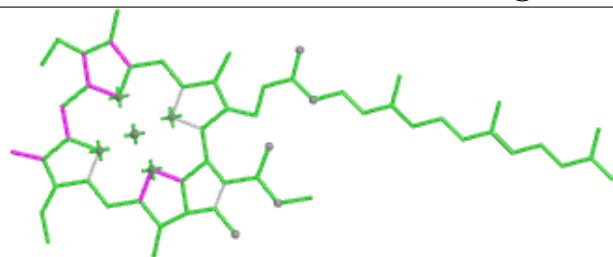


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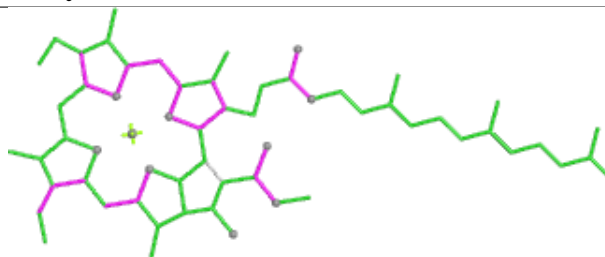


Rings

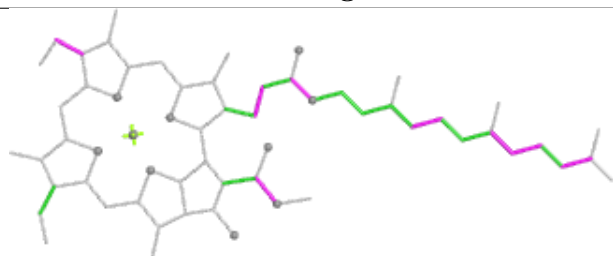
Ligand CLA Q 612



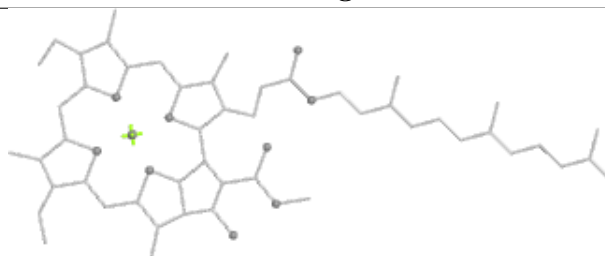
Bond lengths



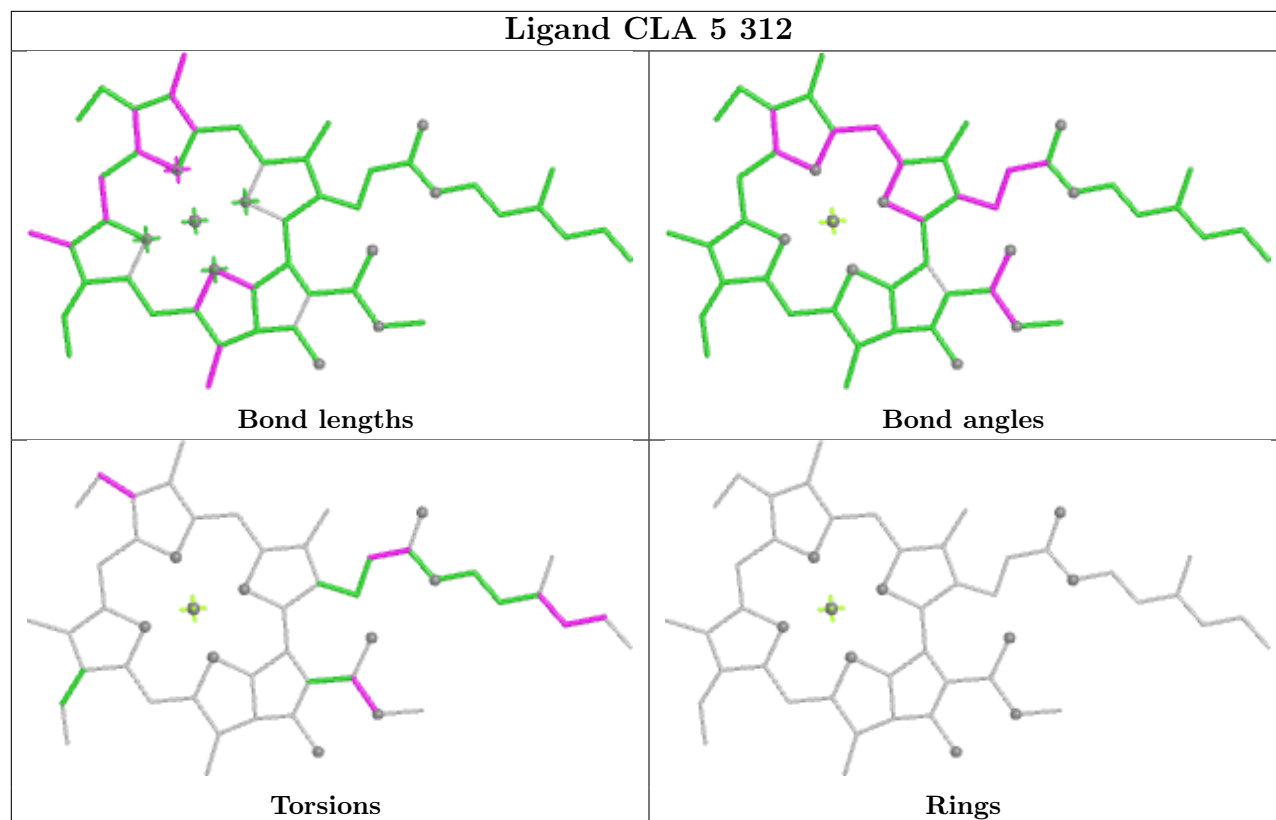
Bond angles



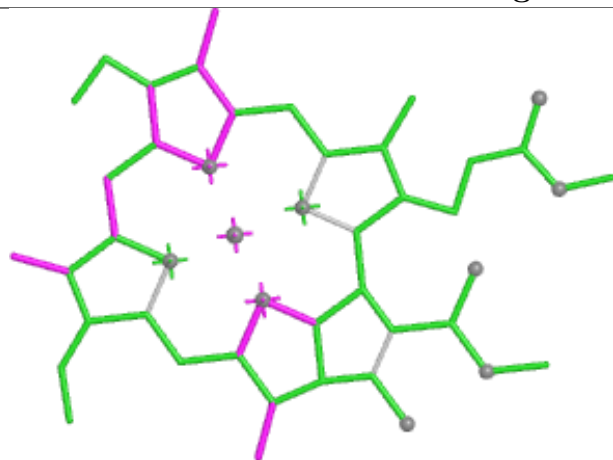
Torsions



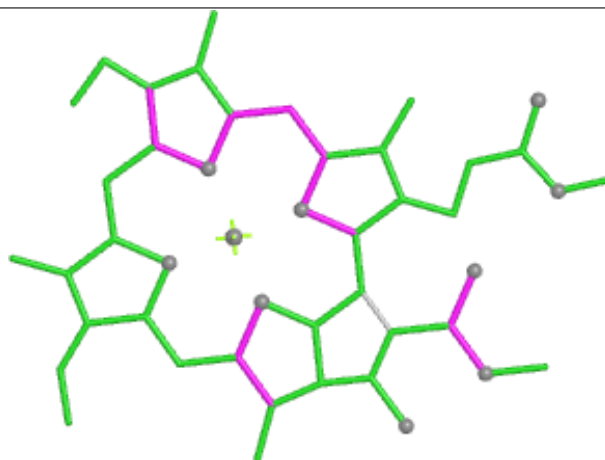
Rings



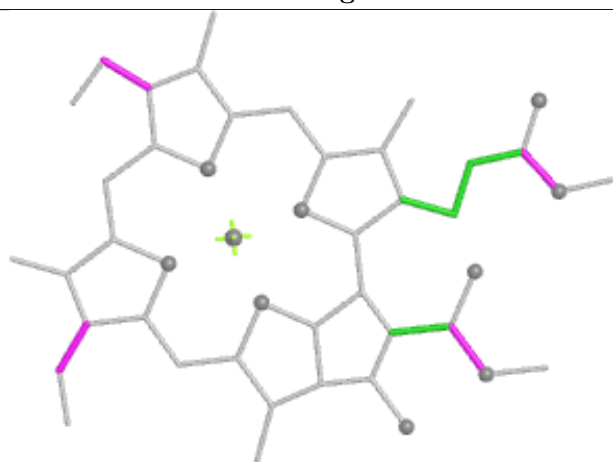
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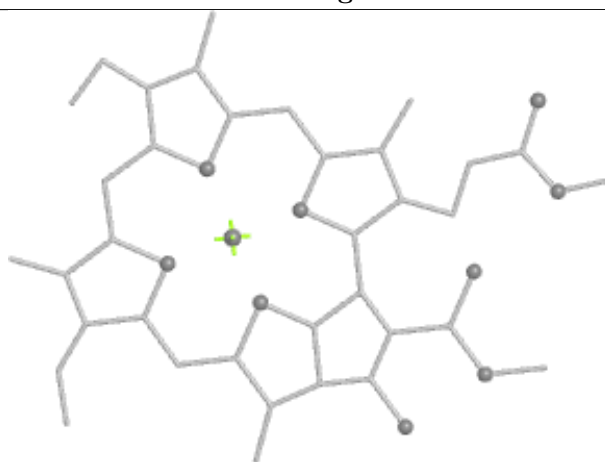
Bond lengths



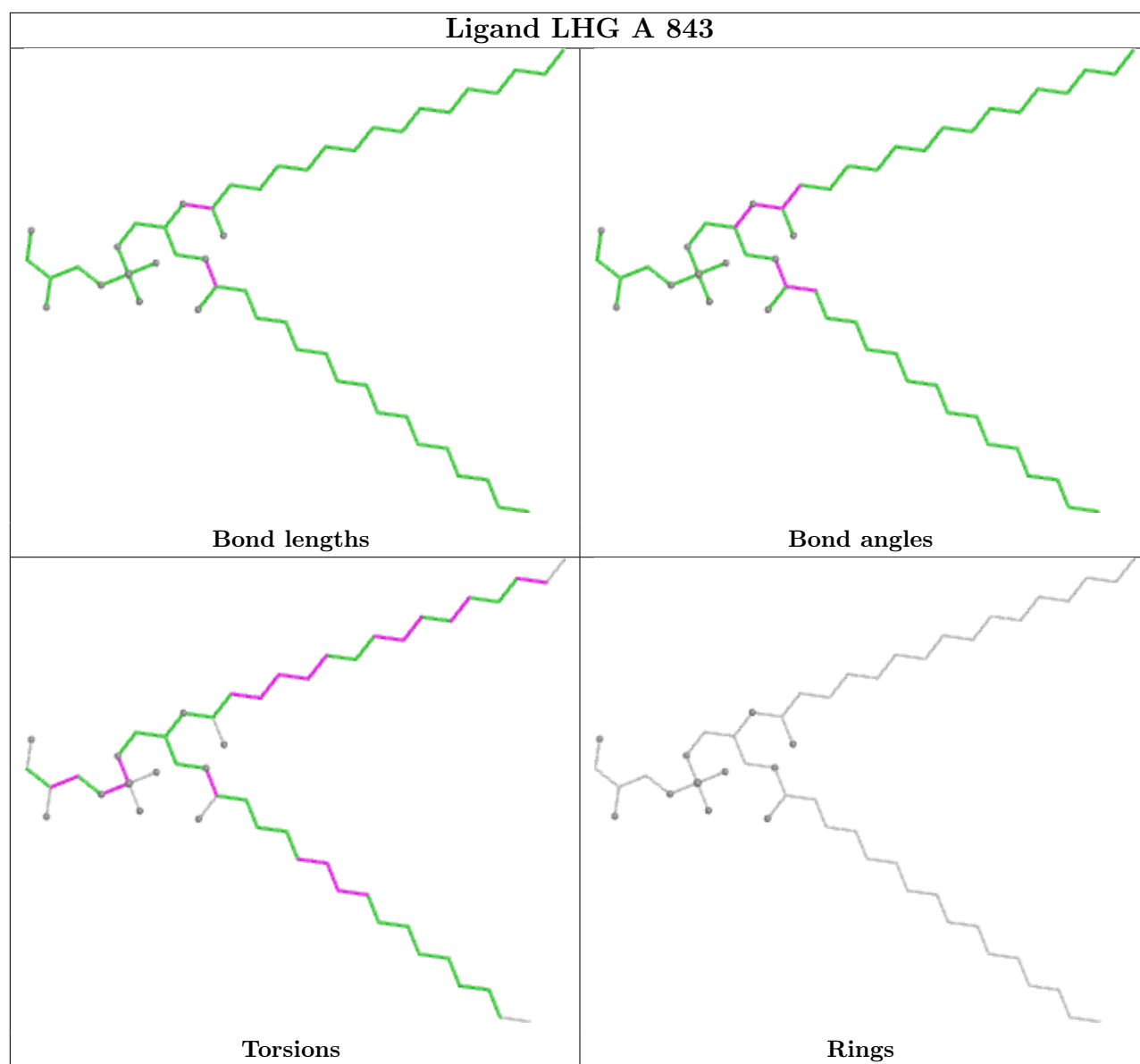
Bond angles

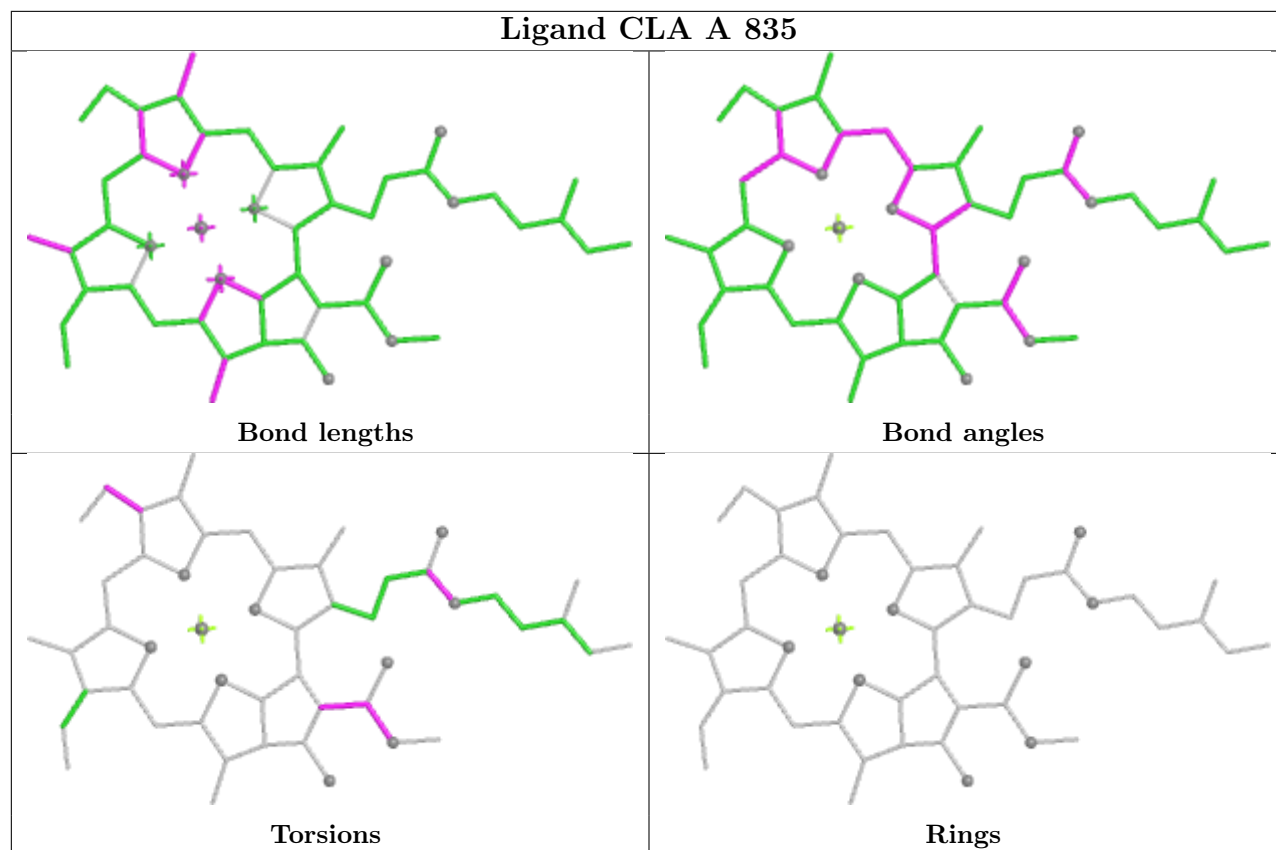


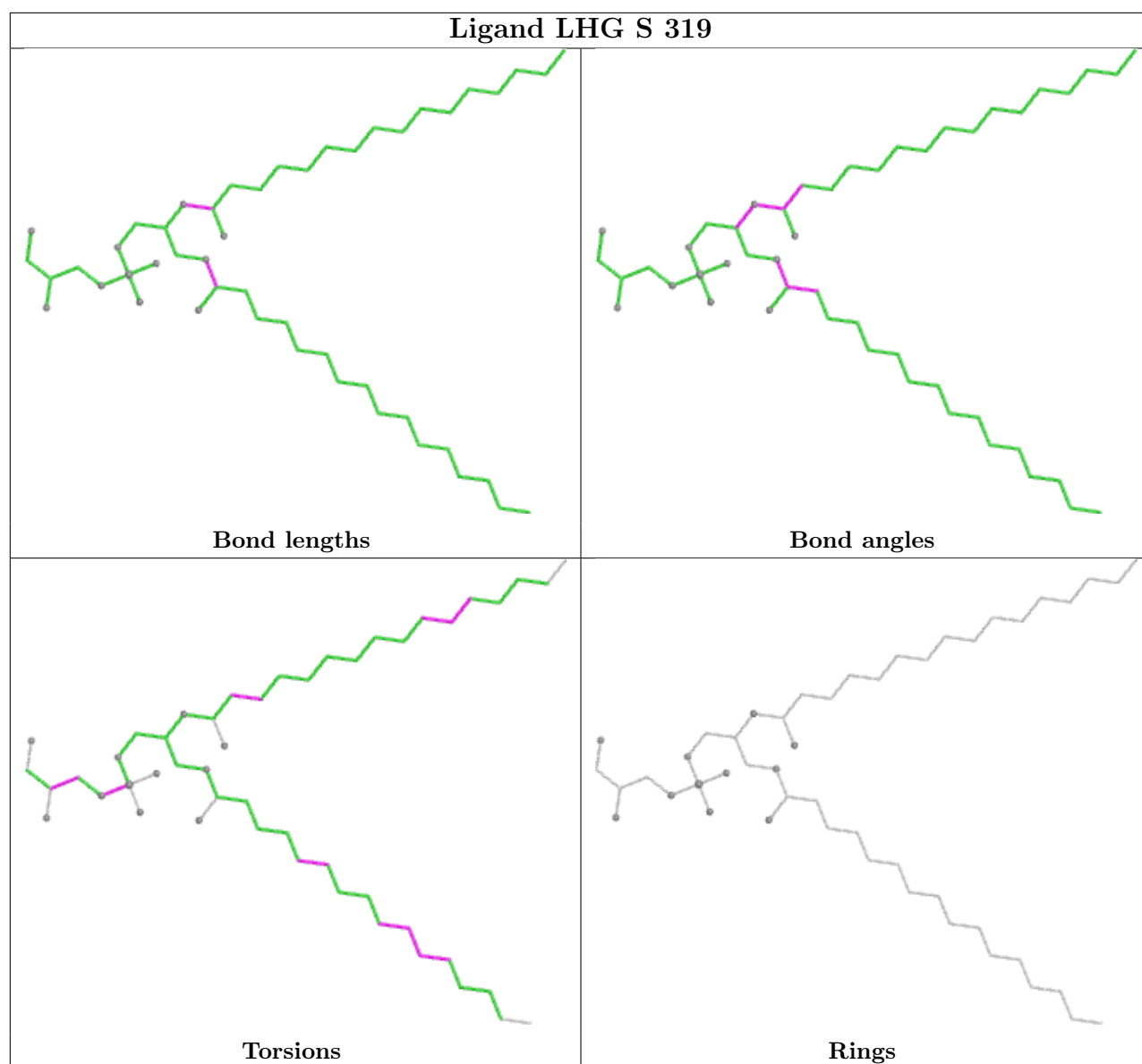
Torsions



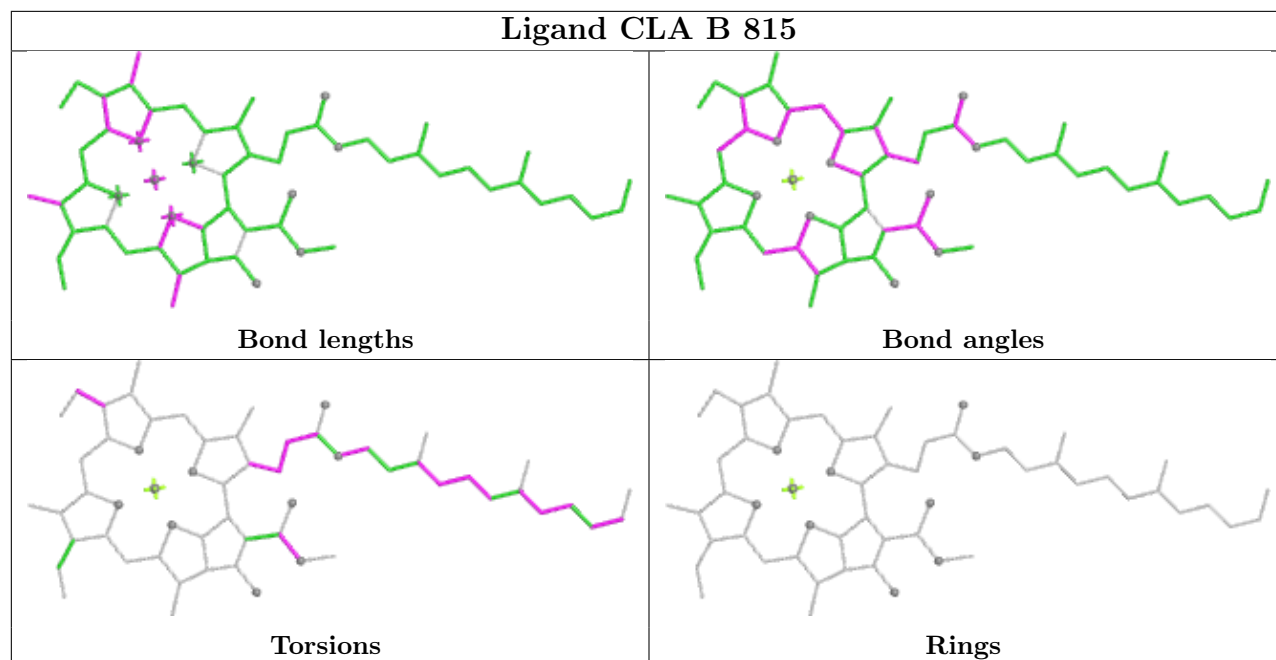
Rings



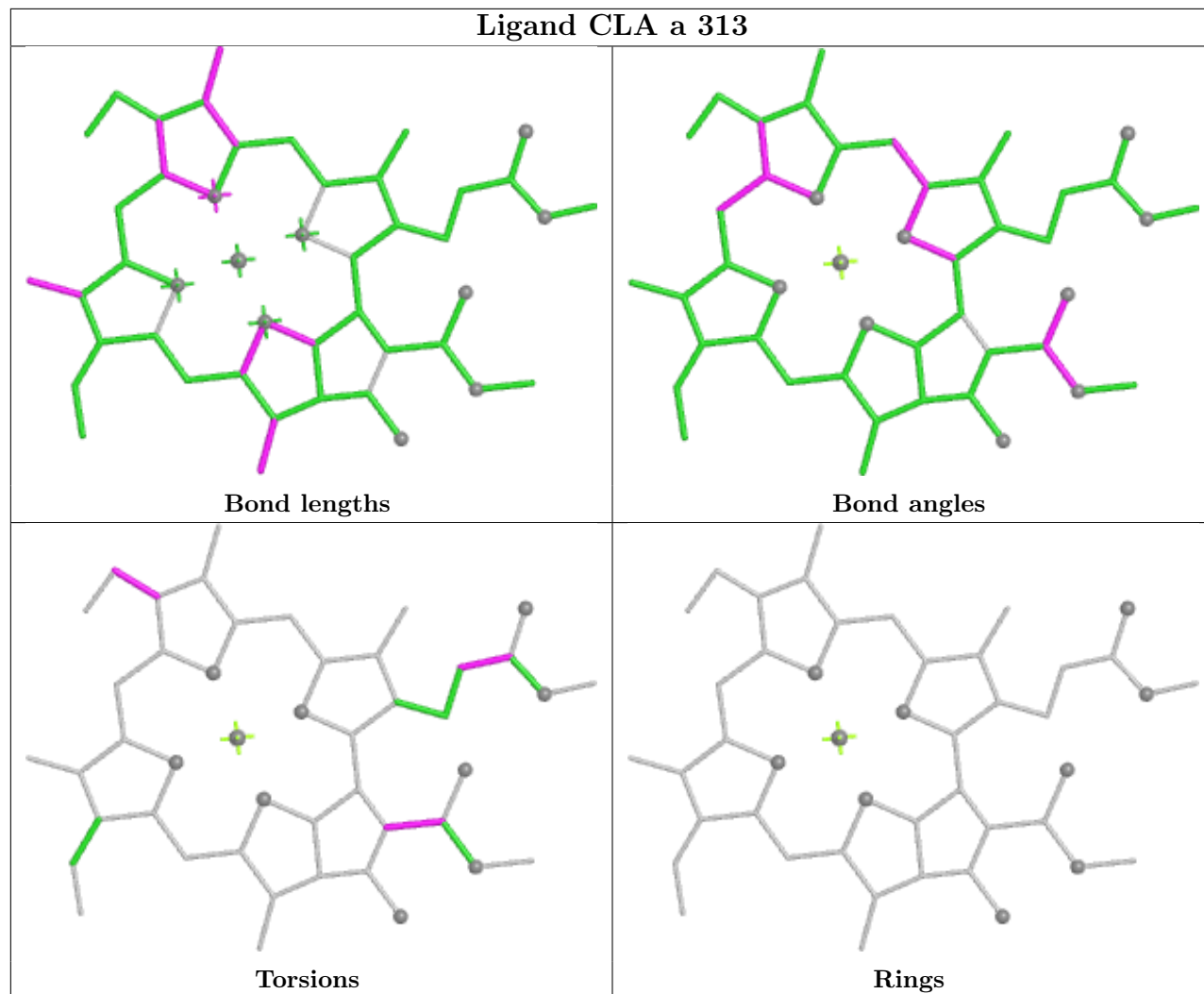


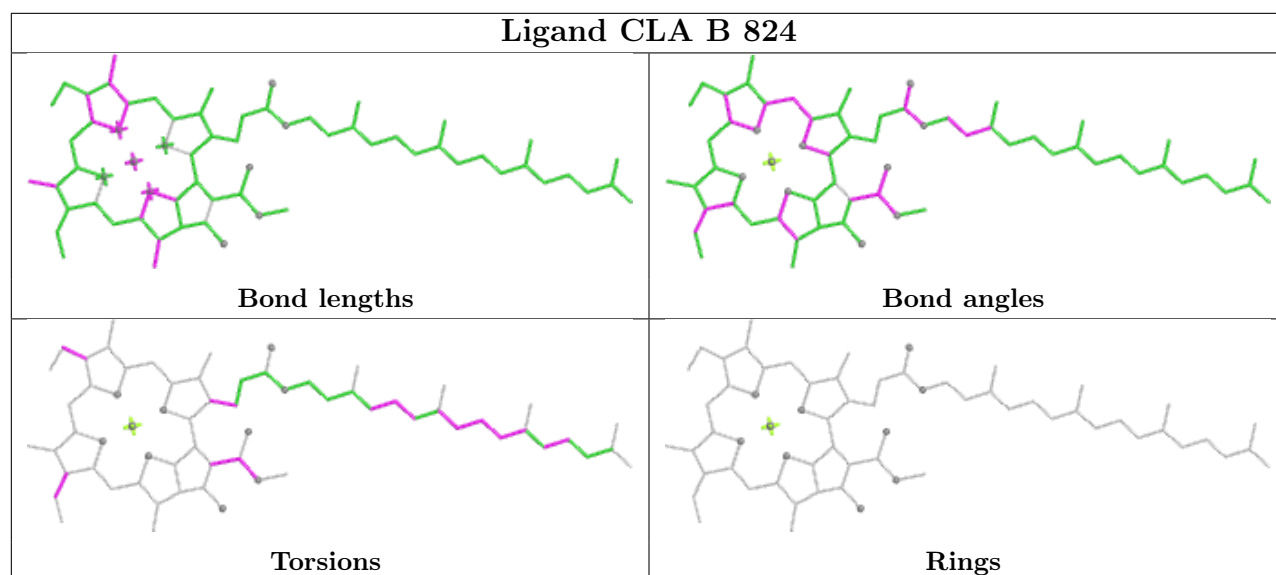
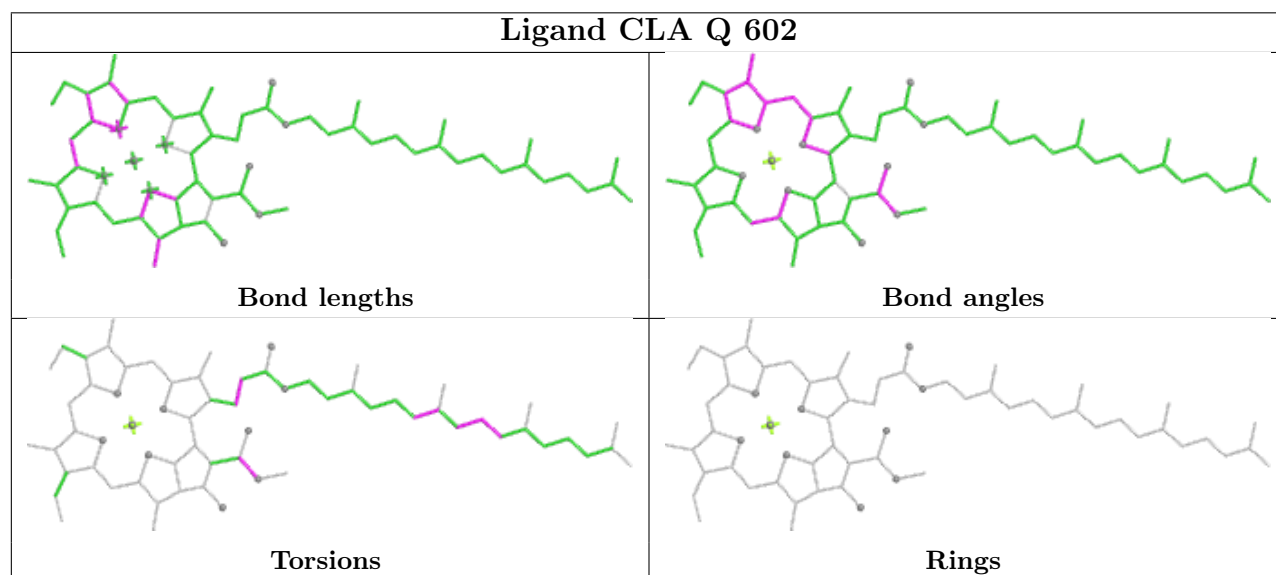
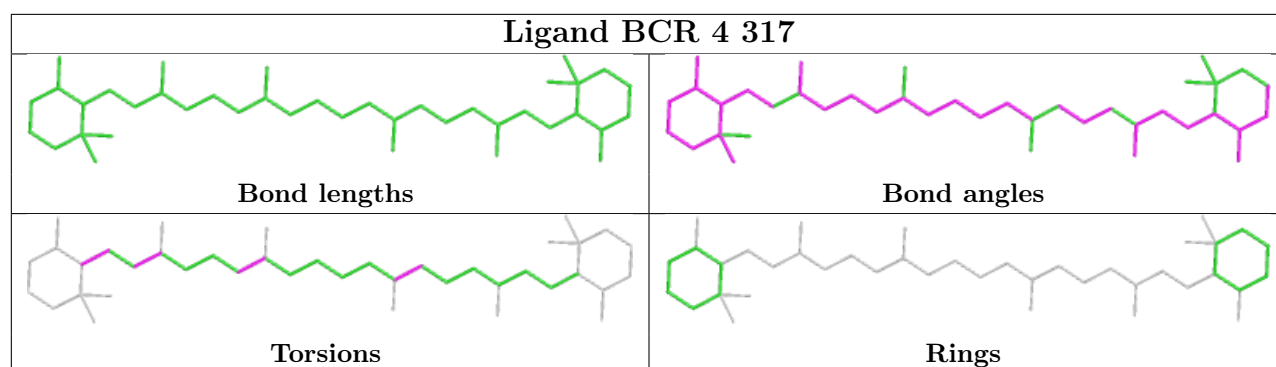


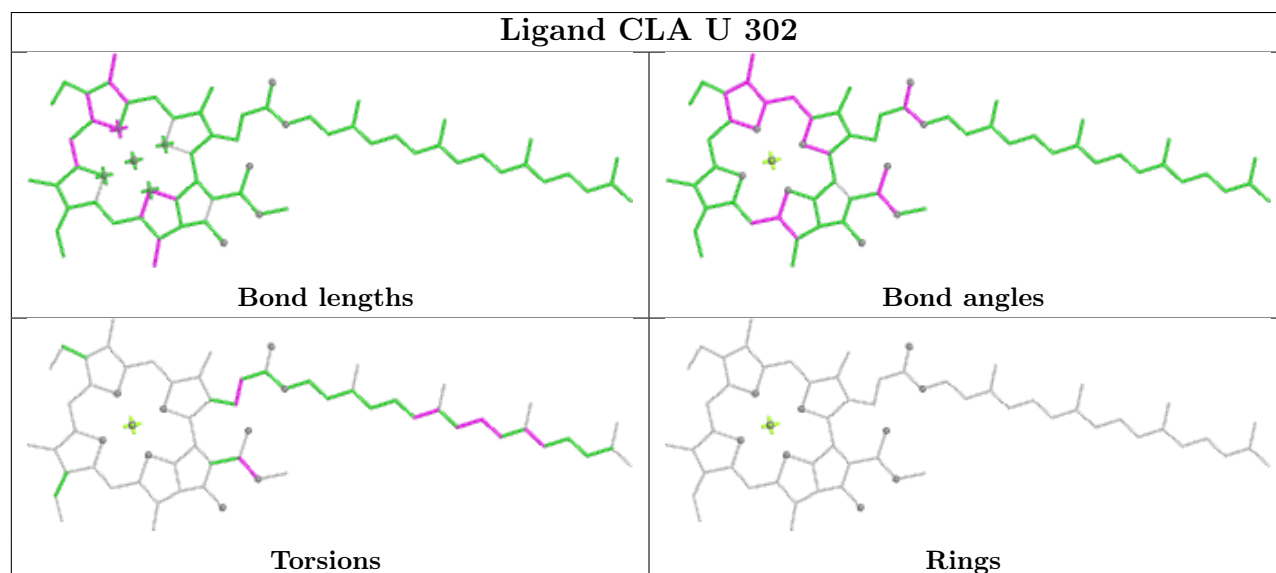
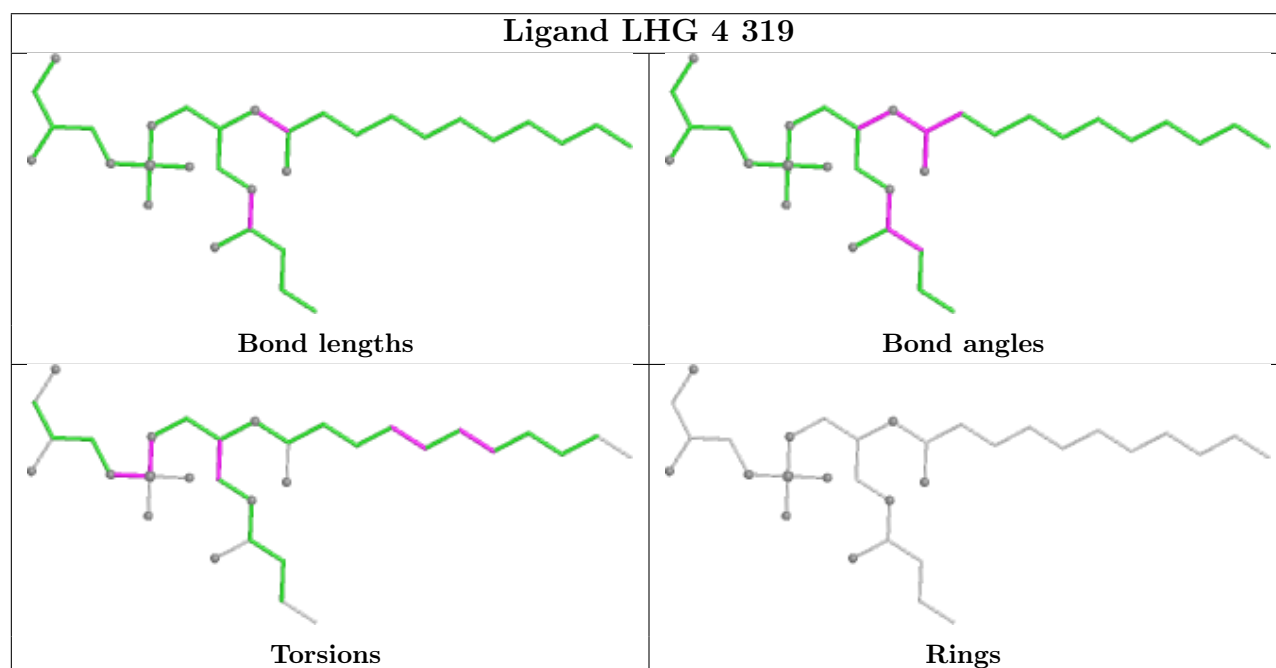
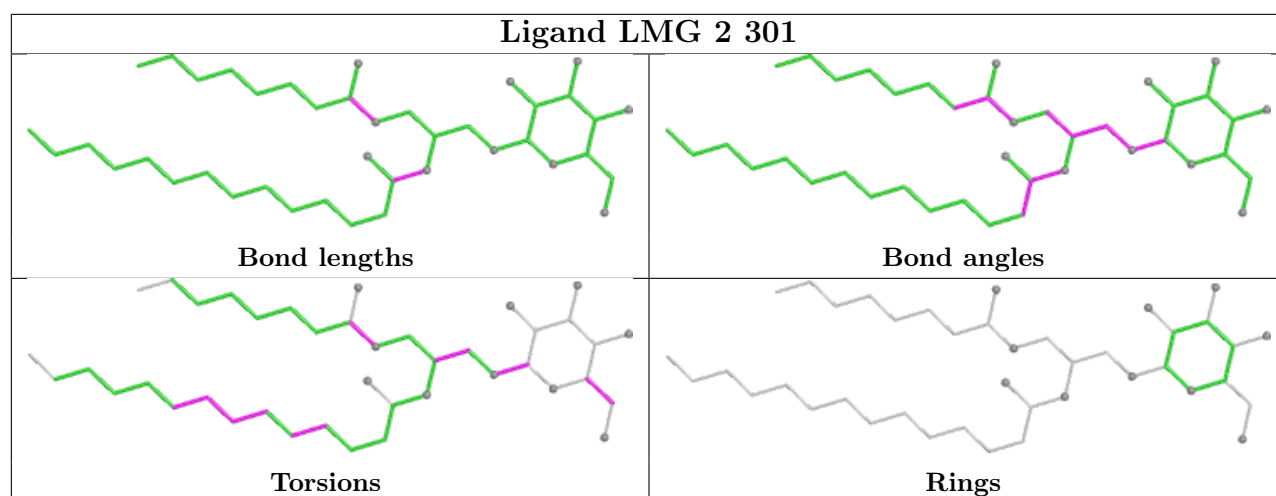
Ligand CLA B 815

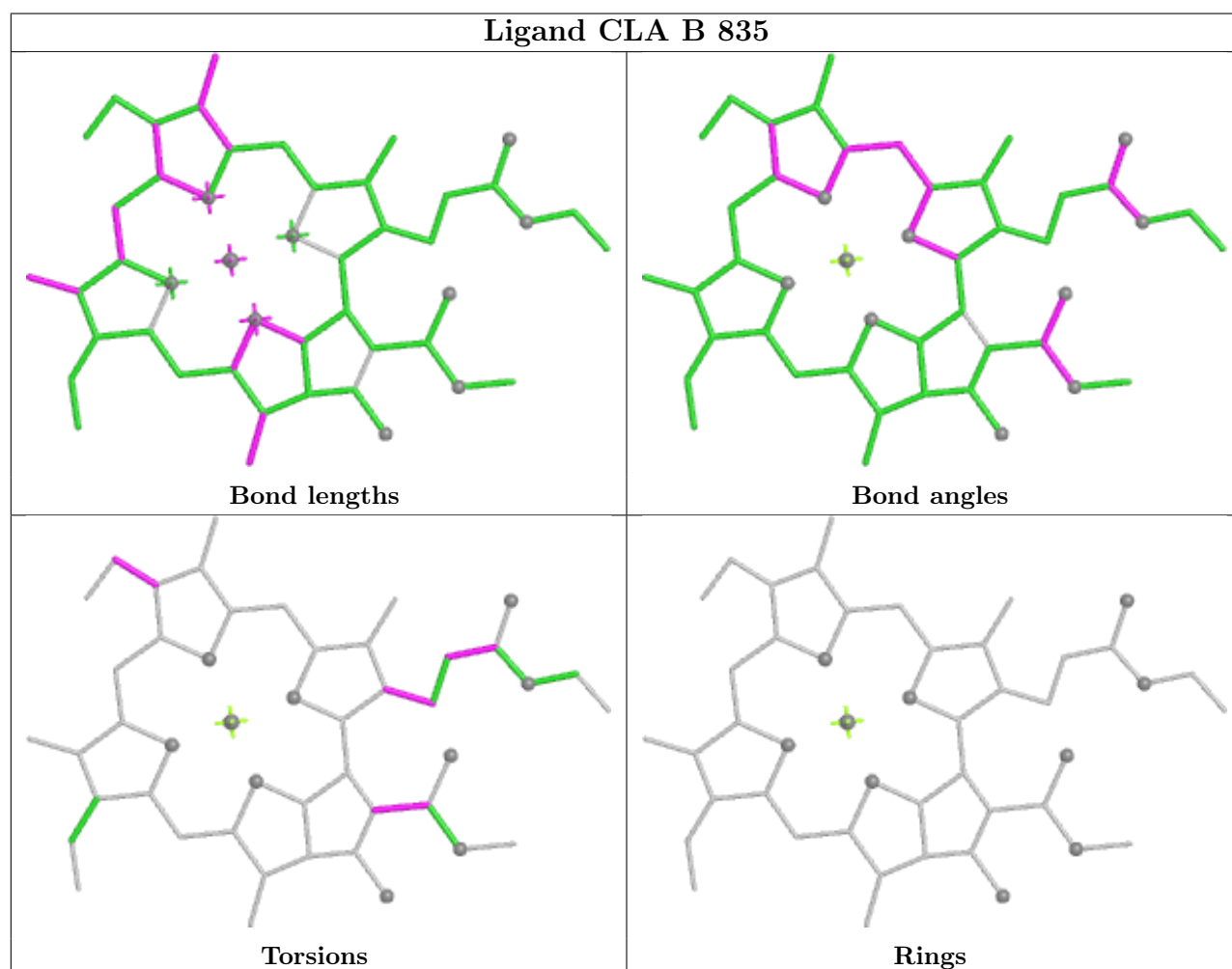
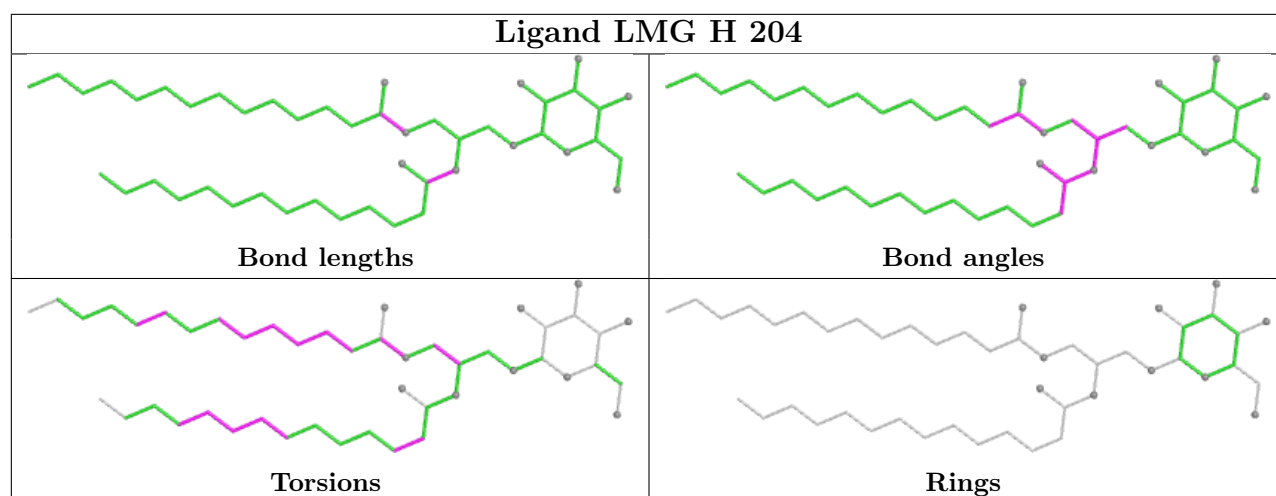


Ligand CLA a 313

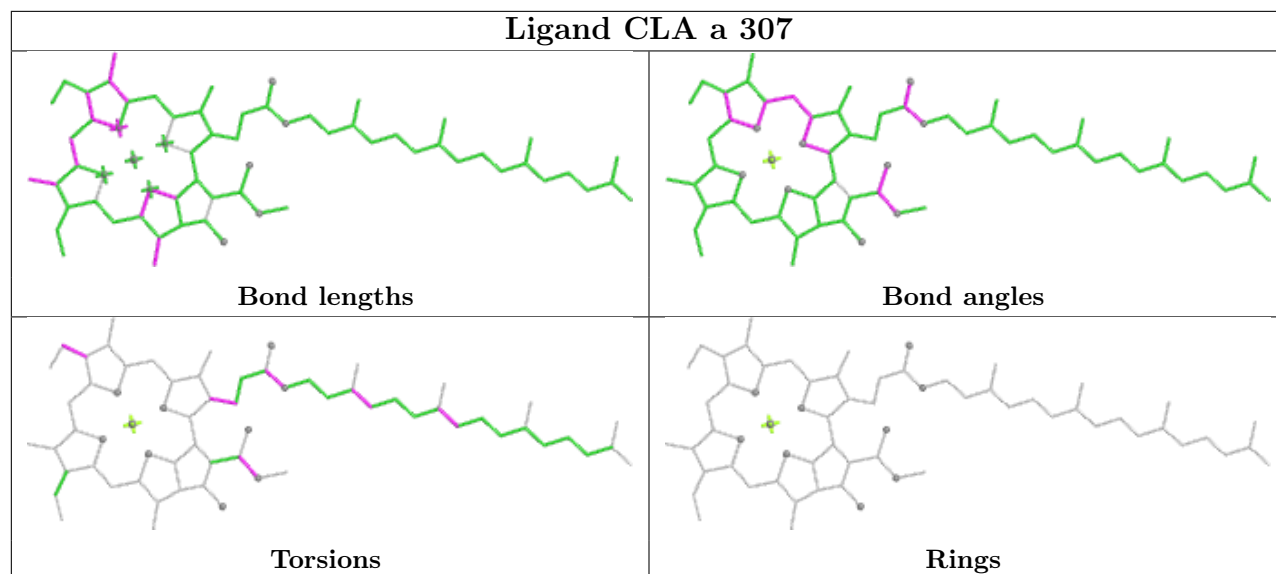




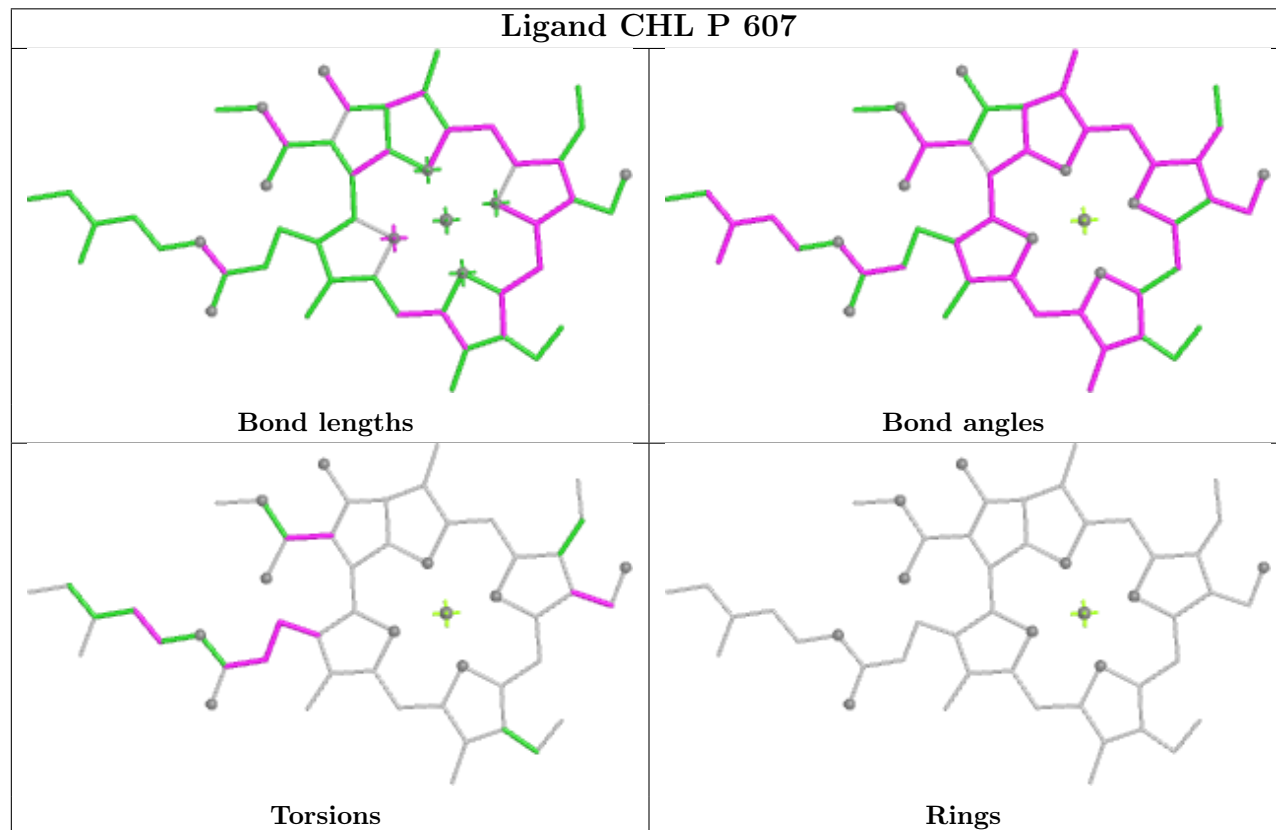




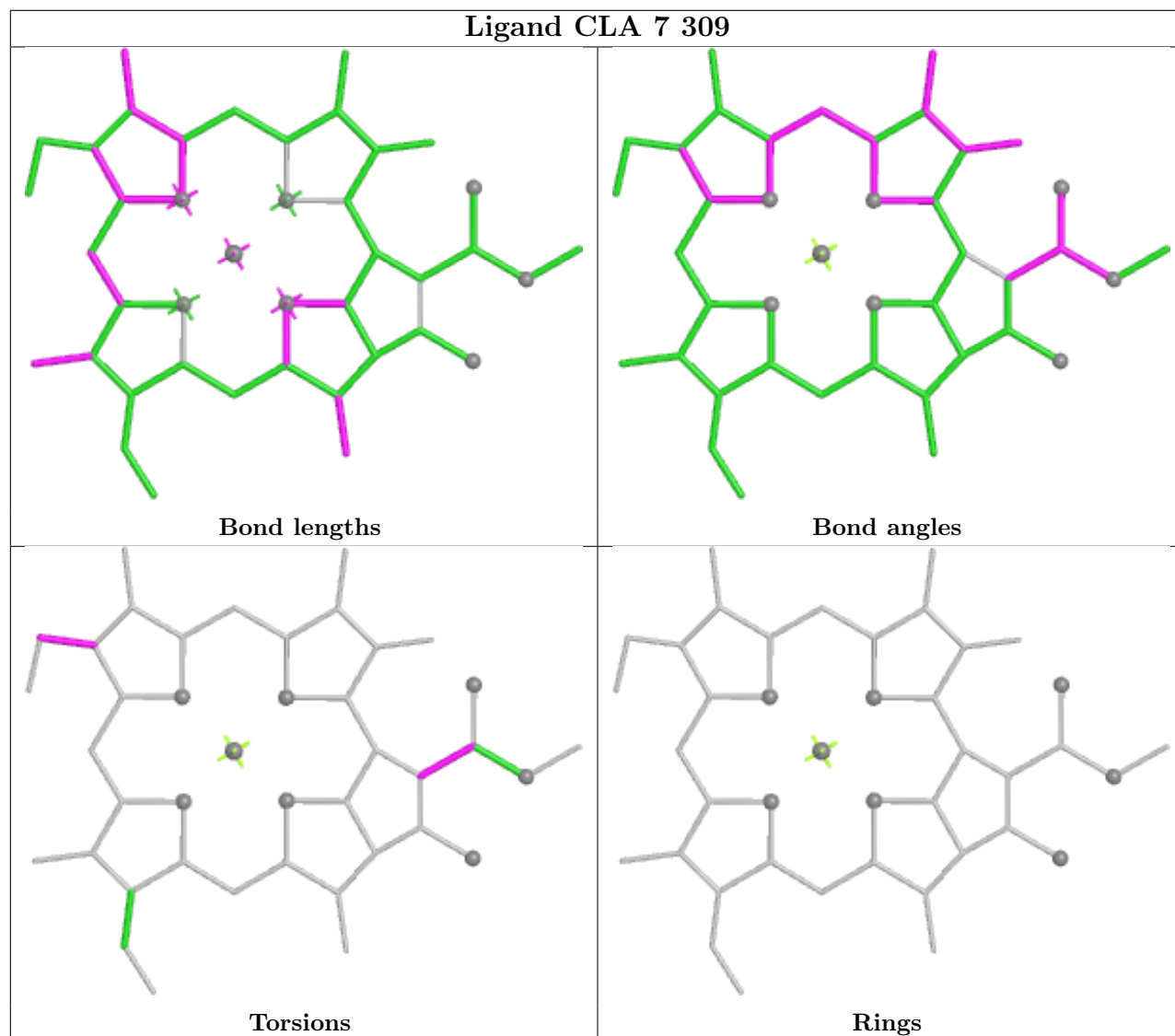
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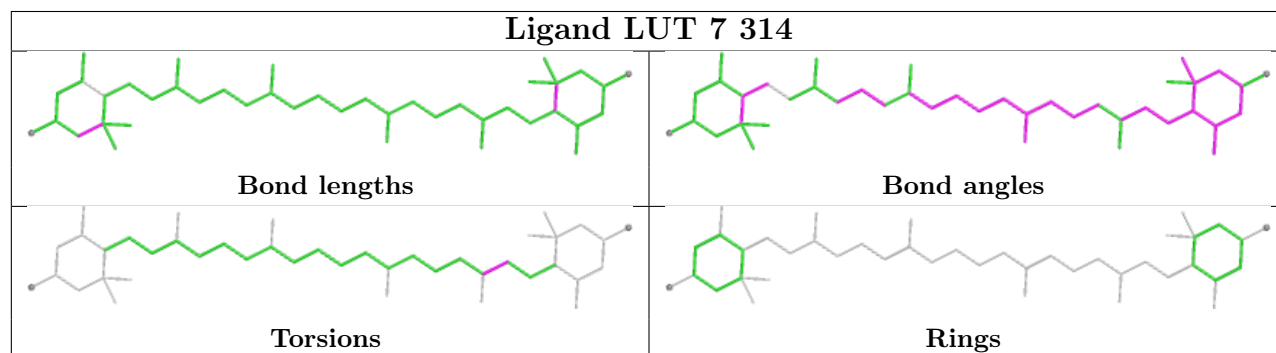
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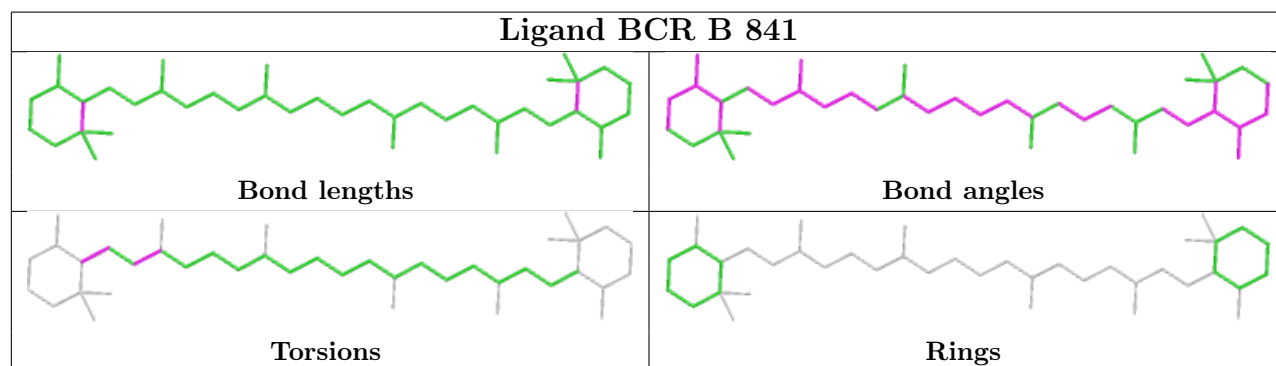
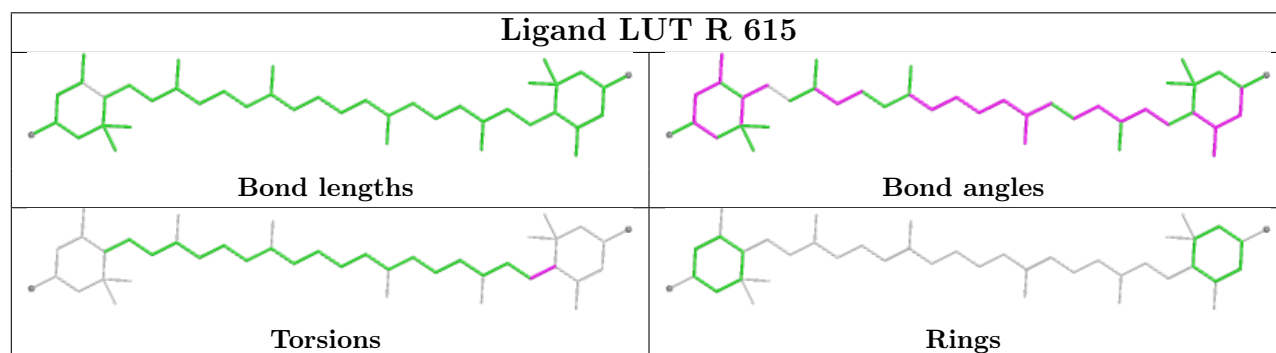
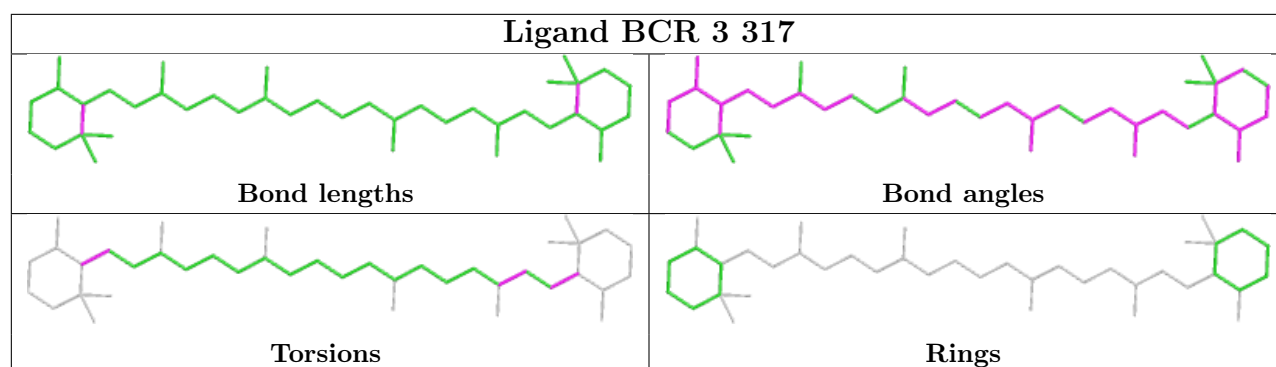


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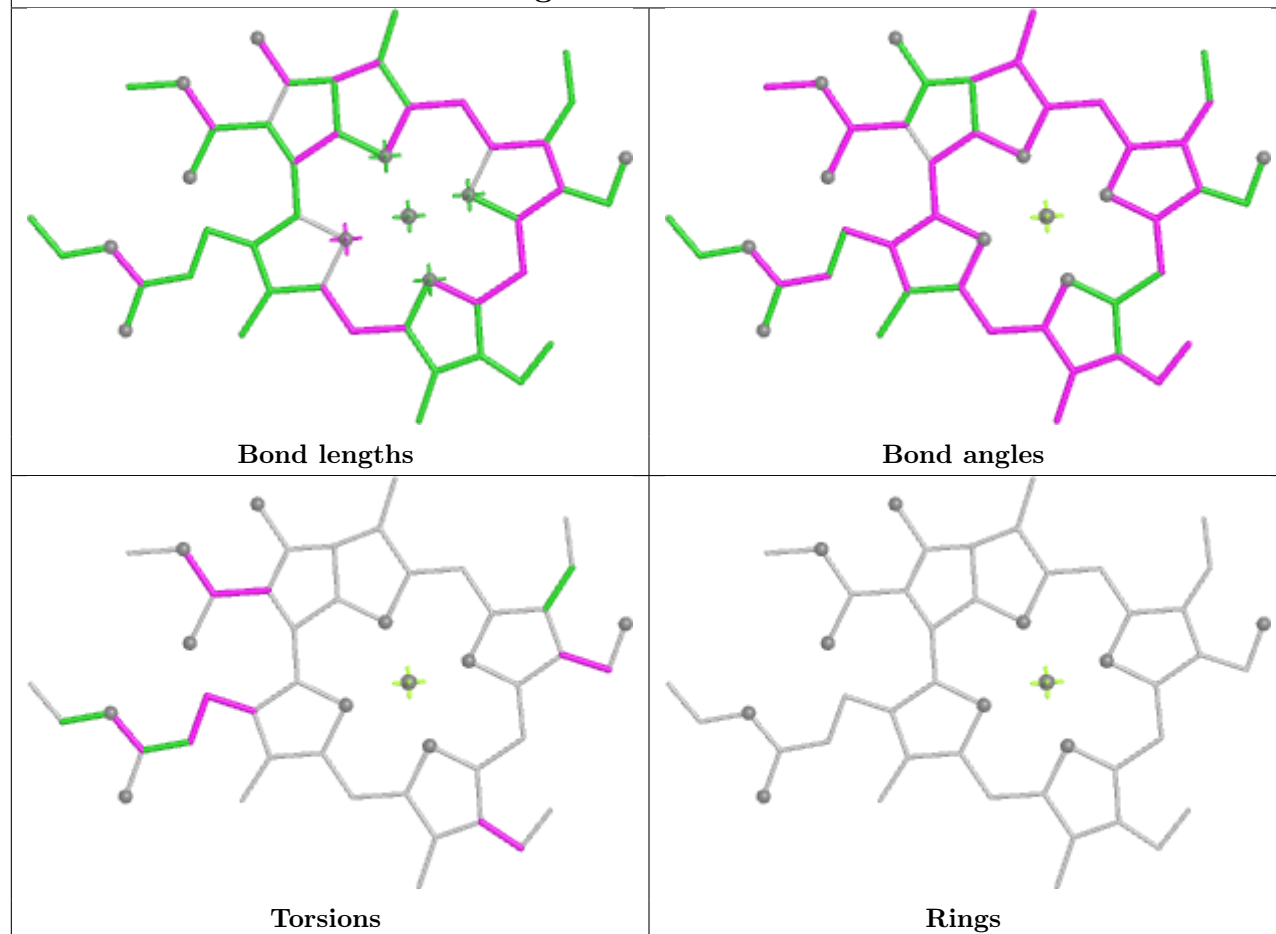


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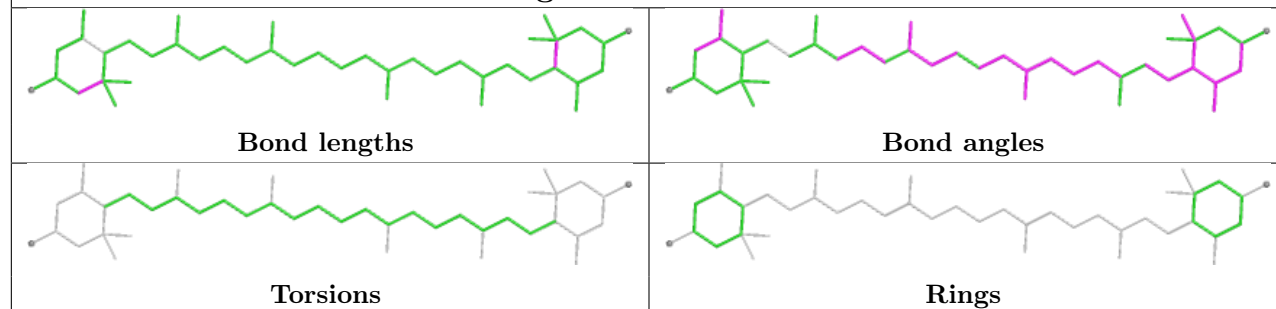


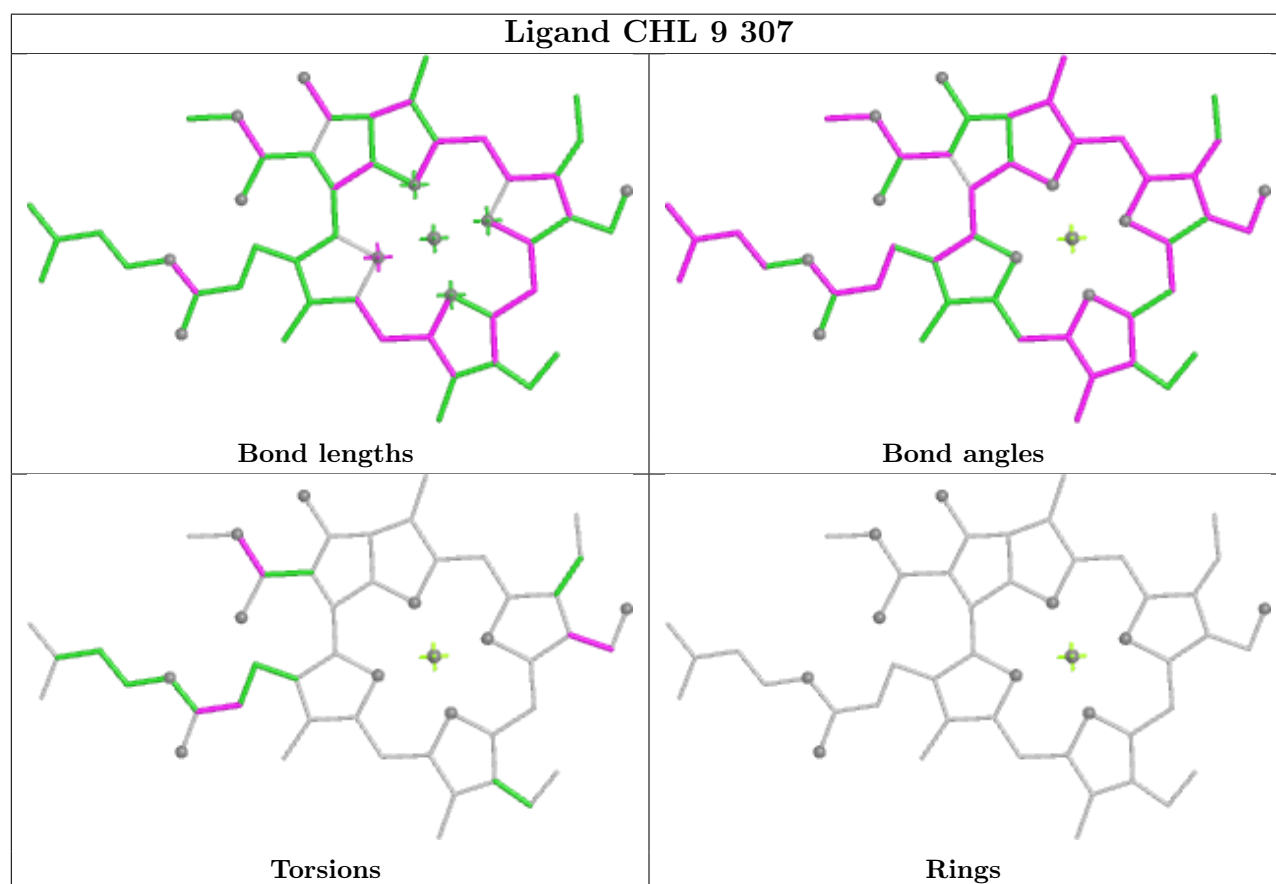
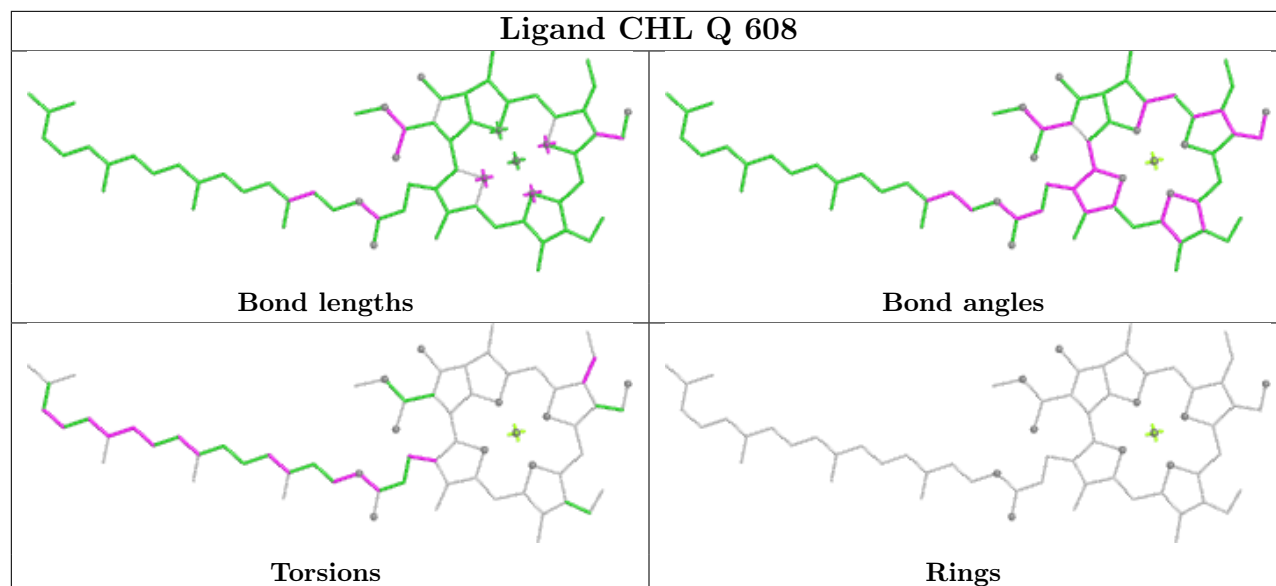


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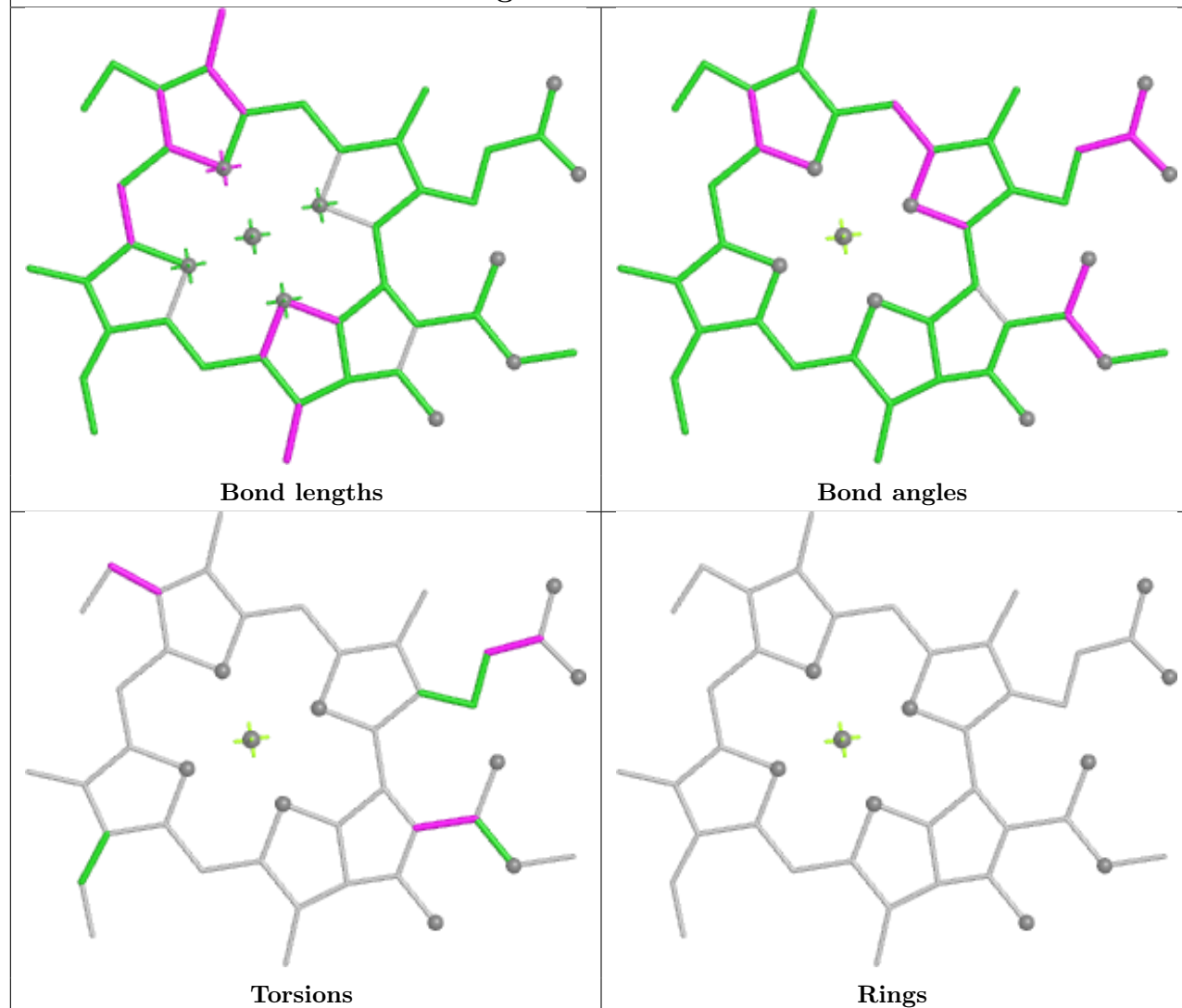


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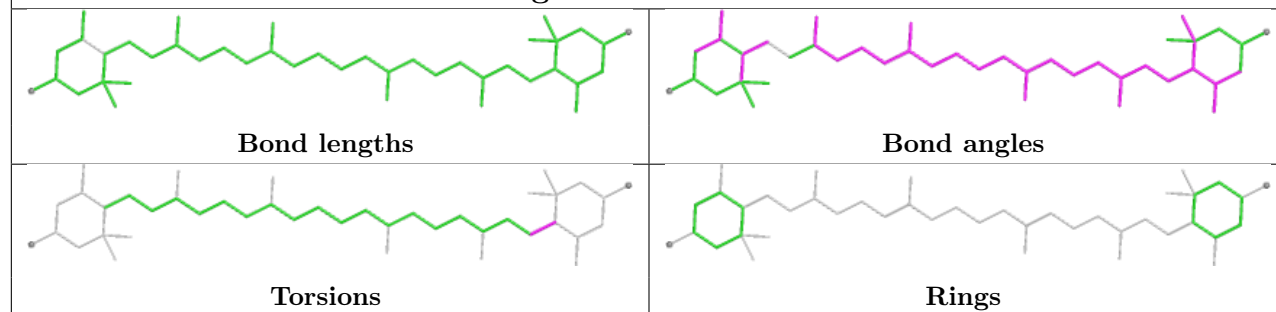


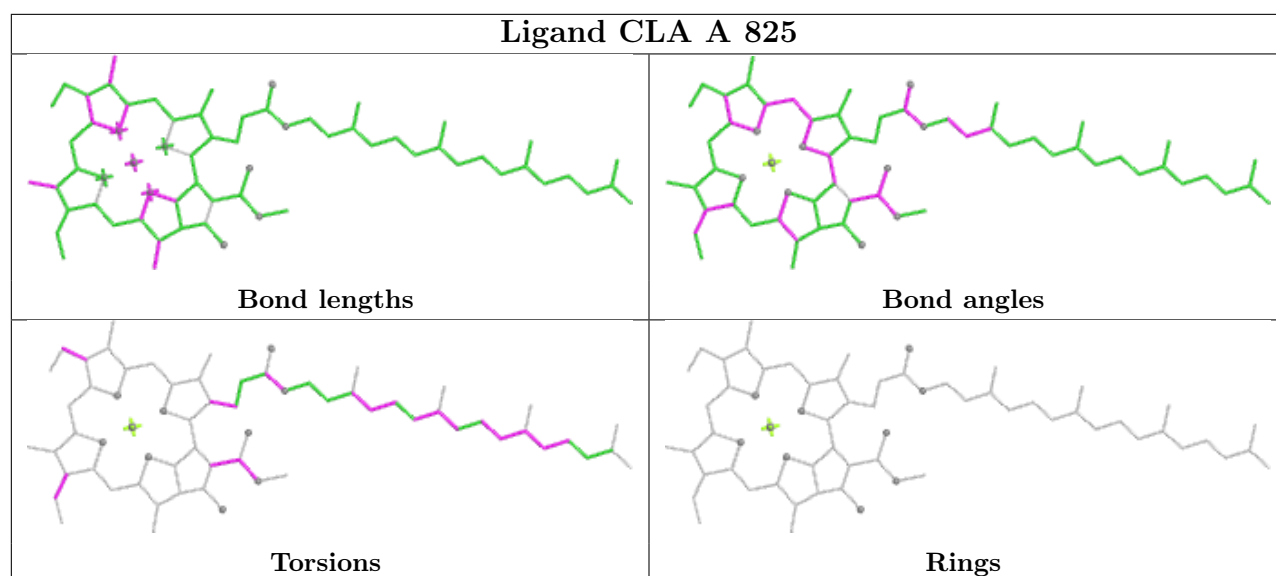
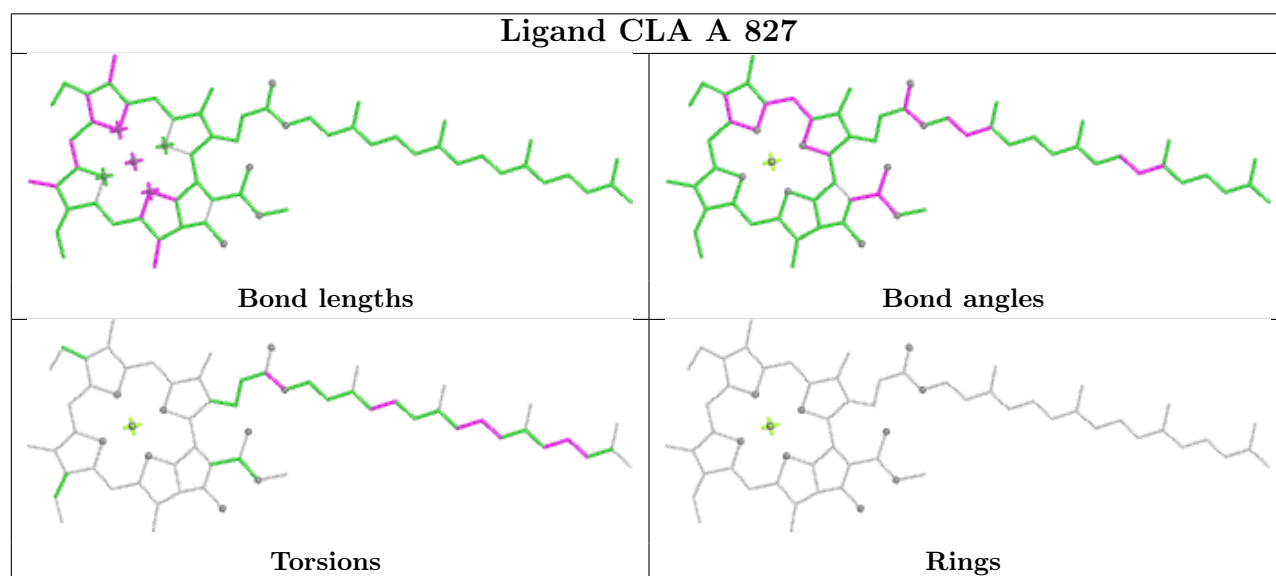
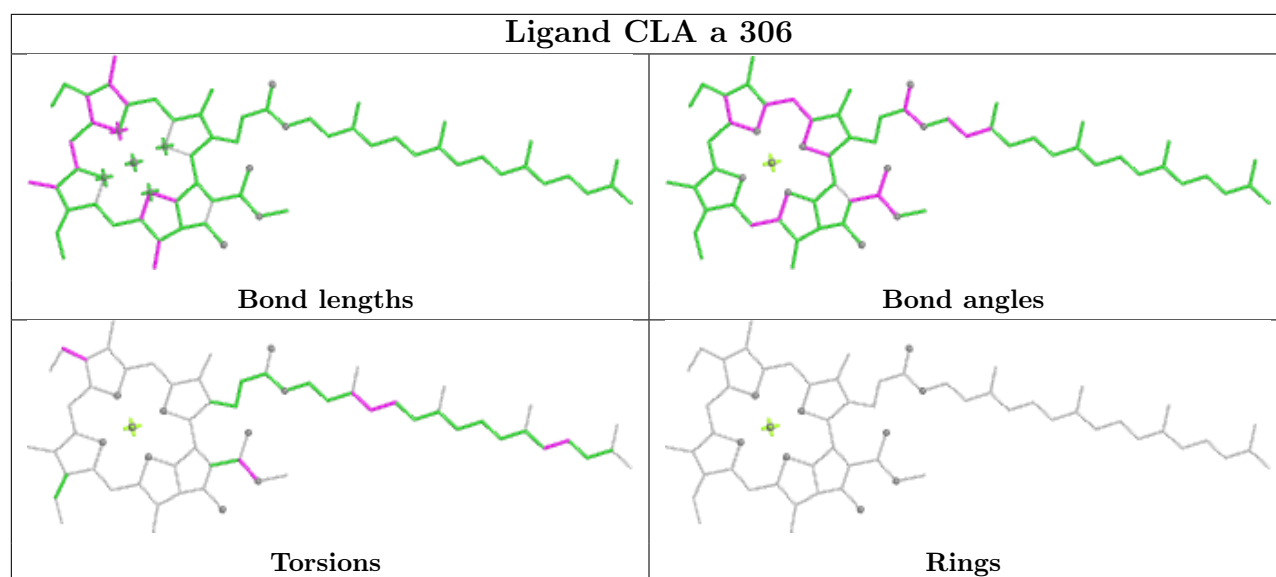


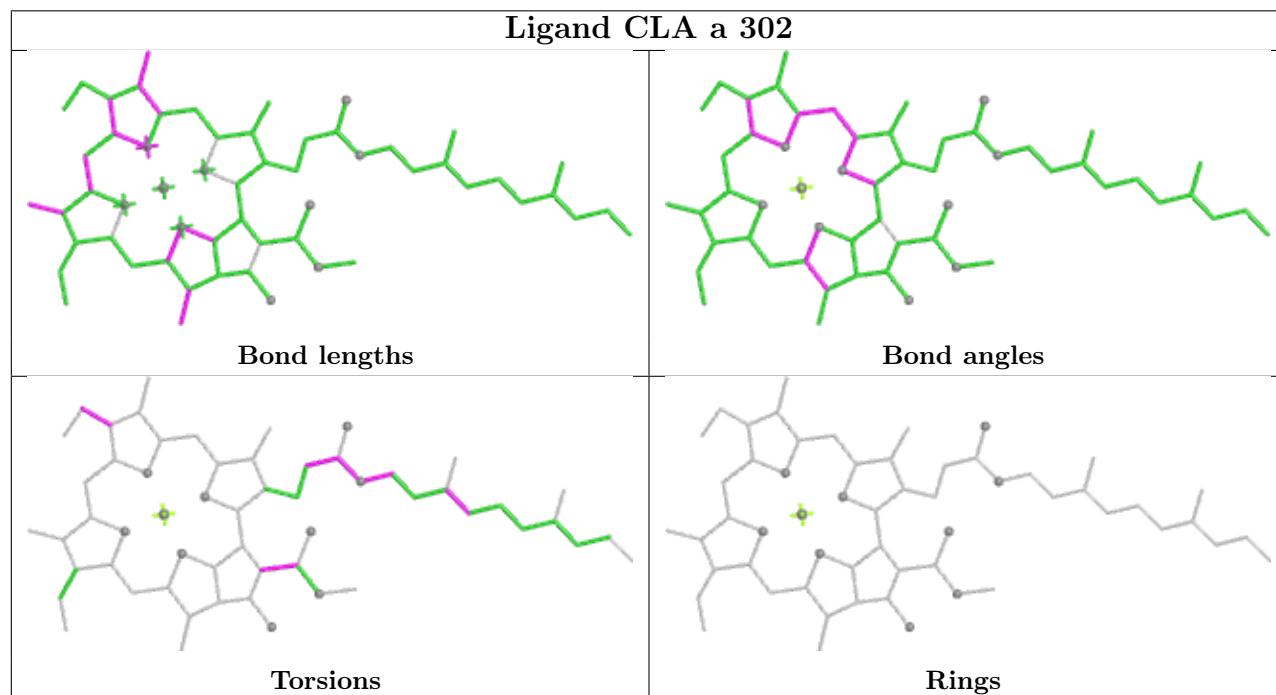
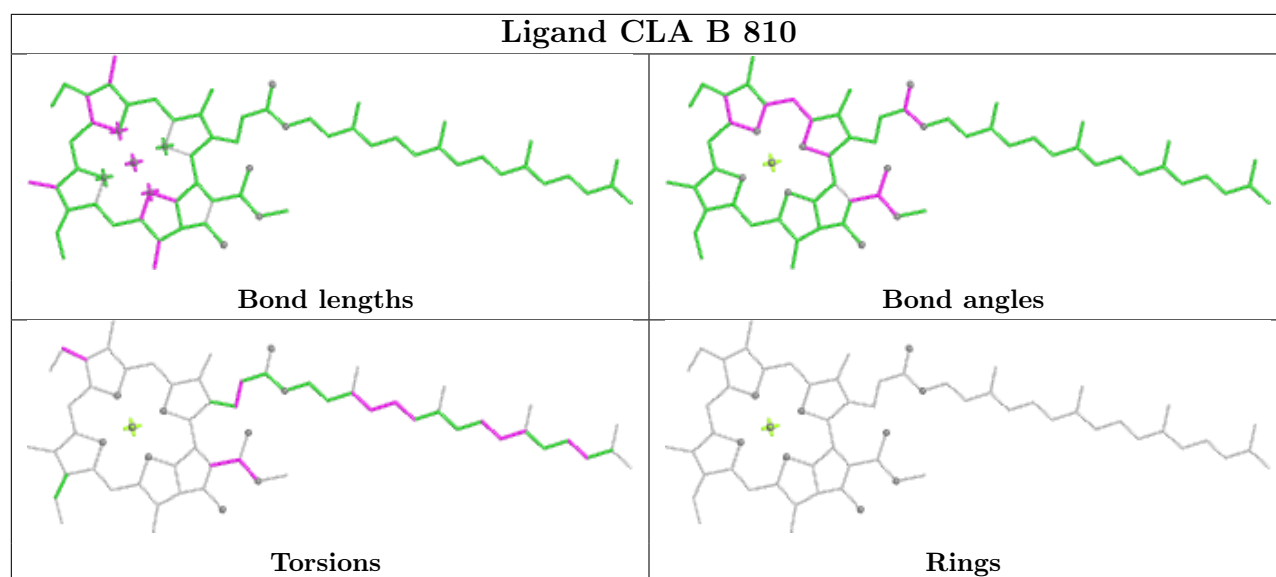
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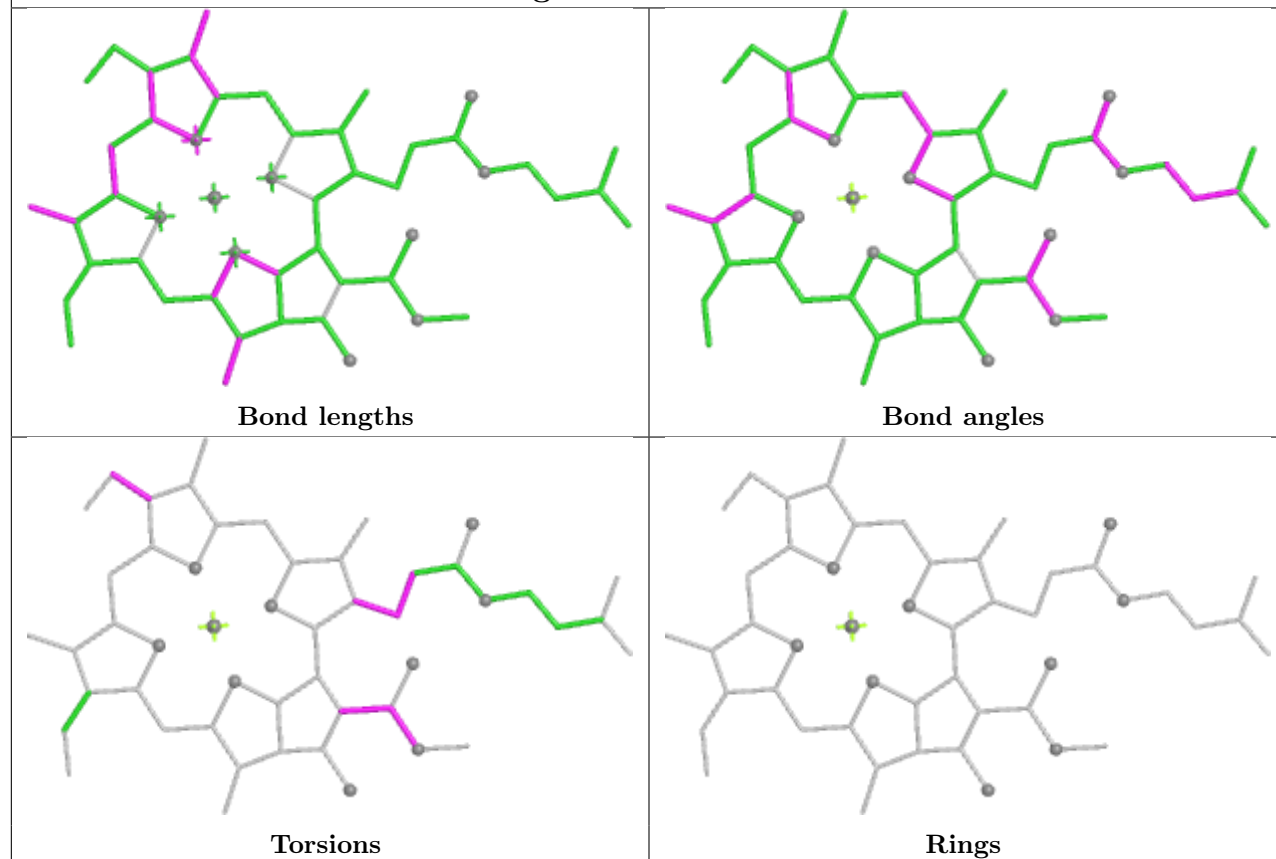
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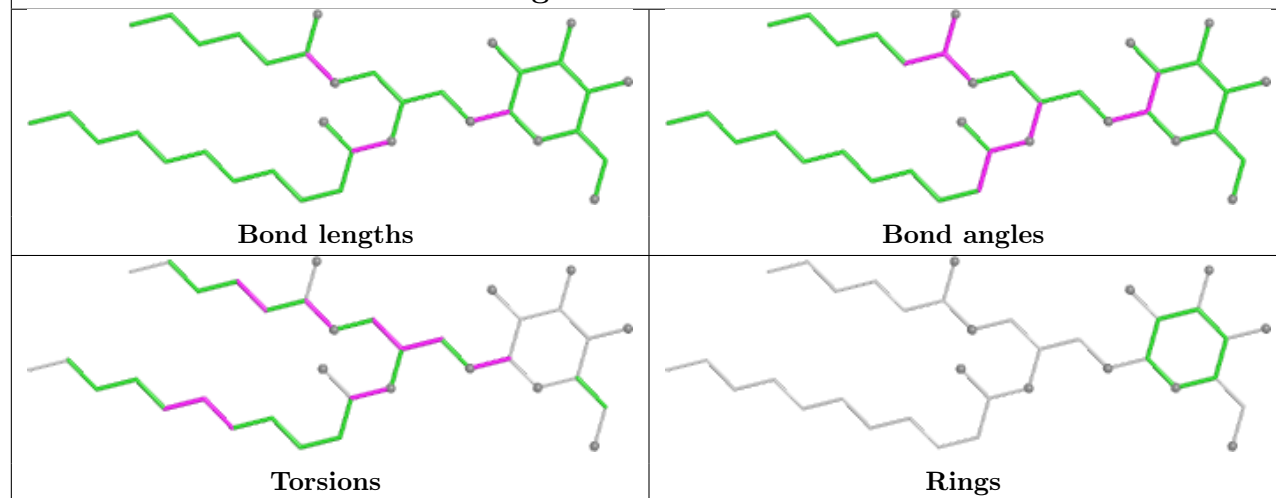


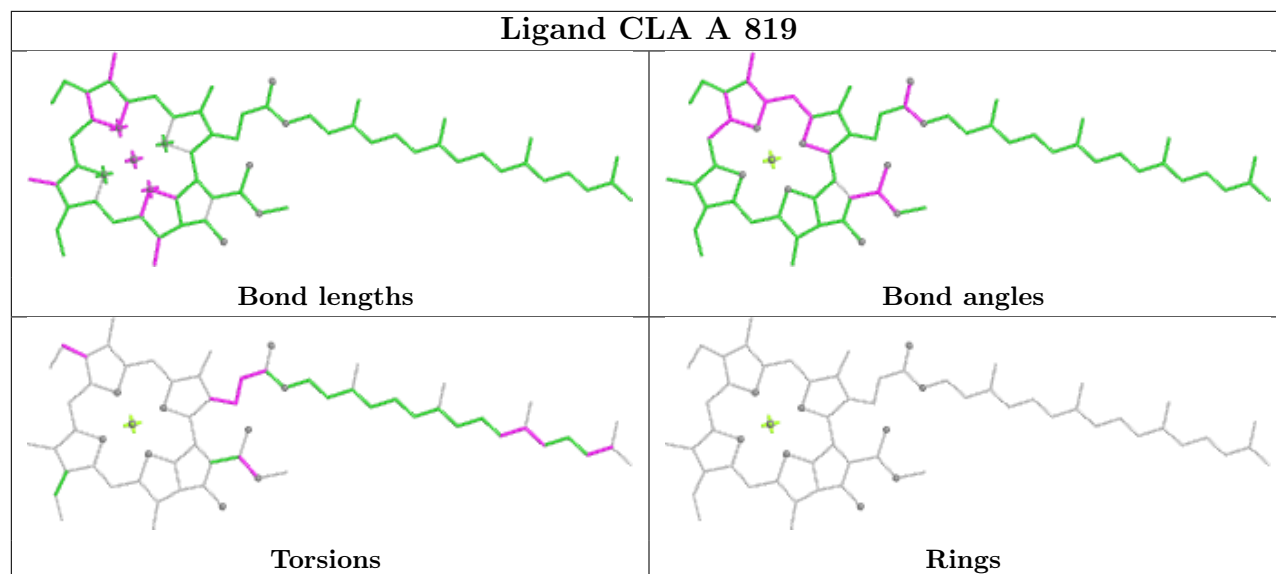
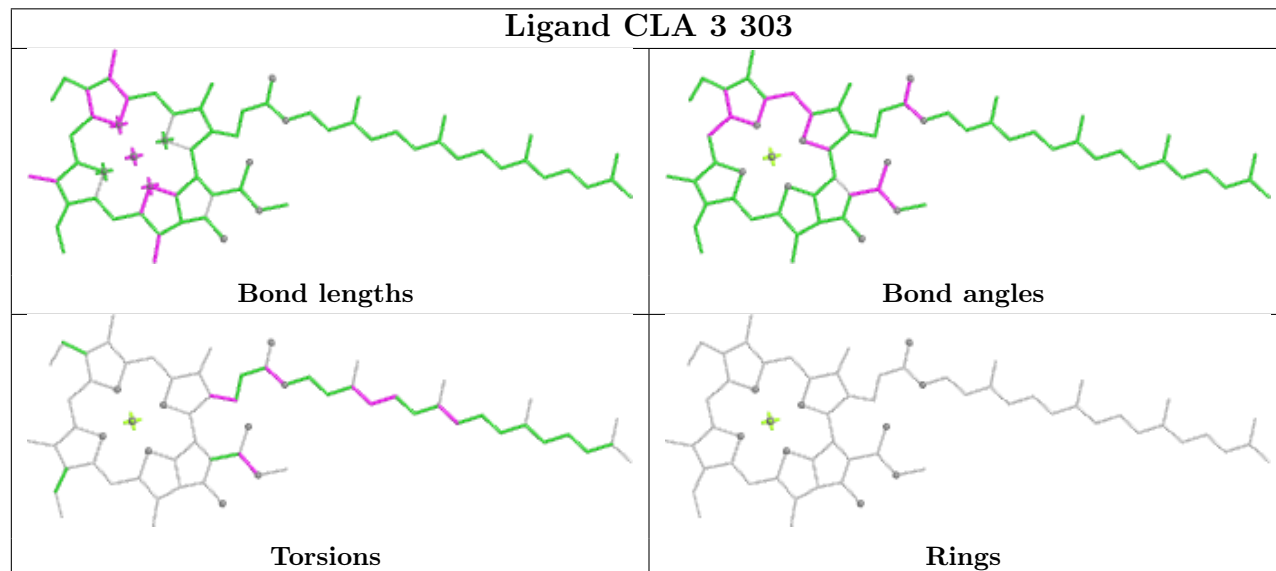


Ligand CLA P 604

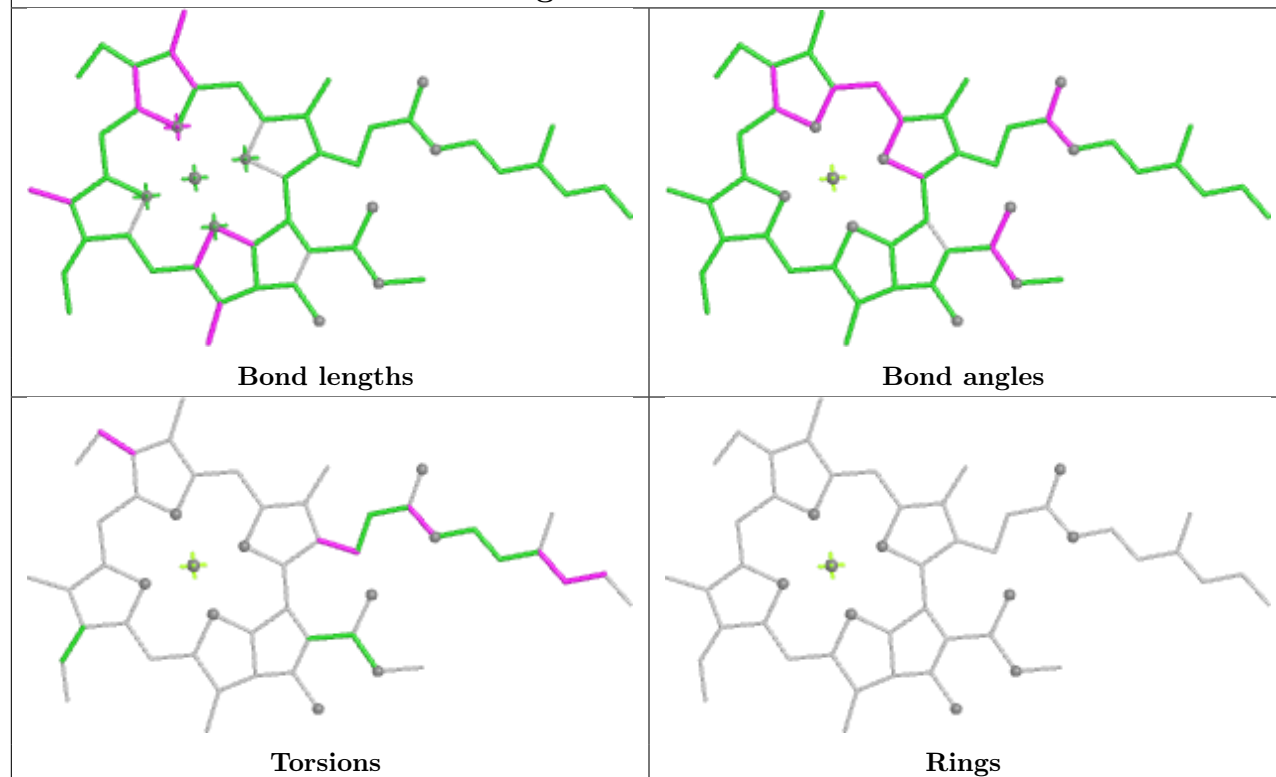


Ligand LMG 7 319

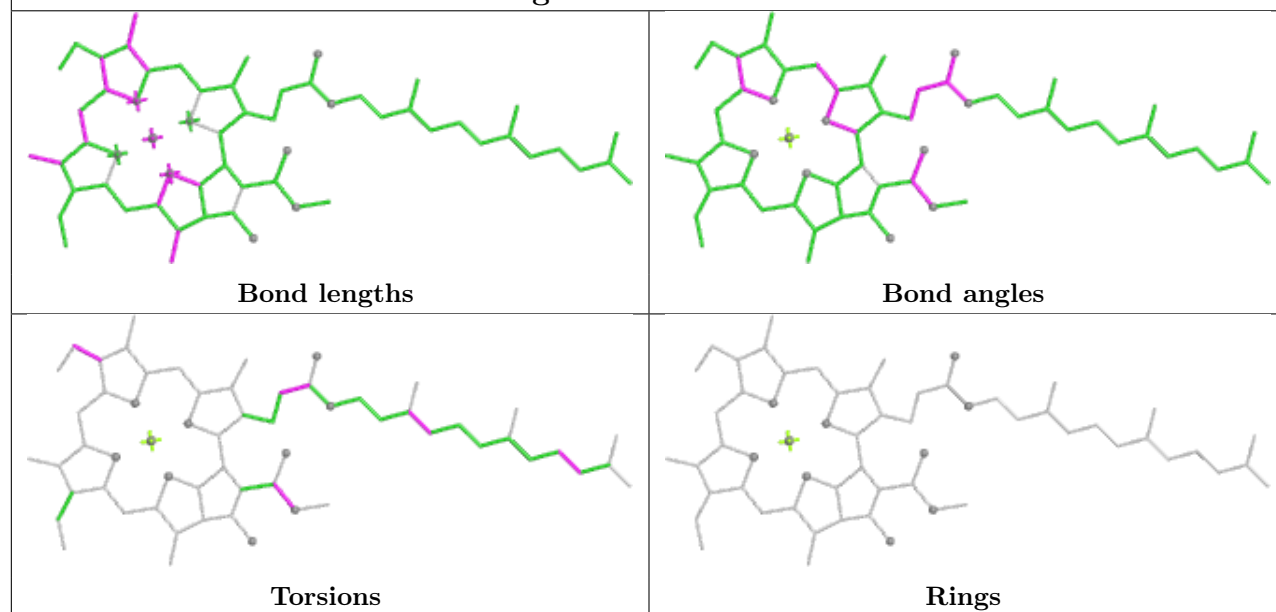


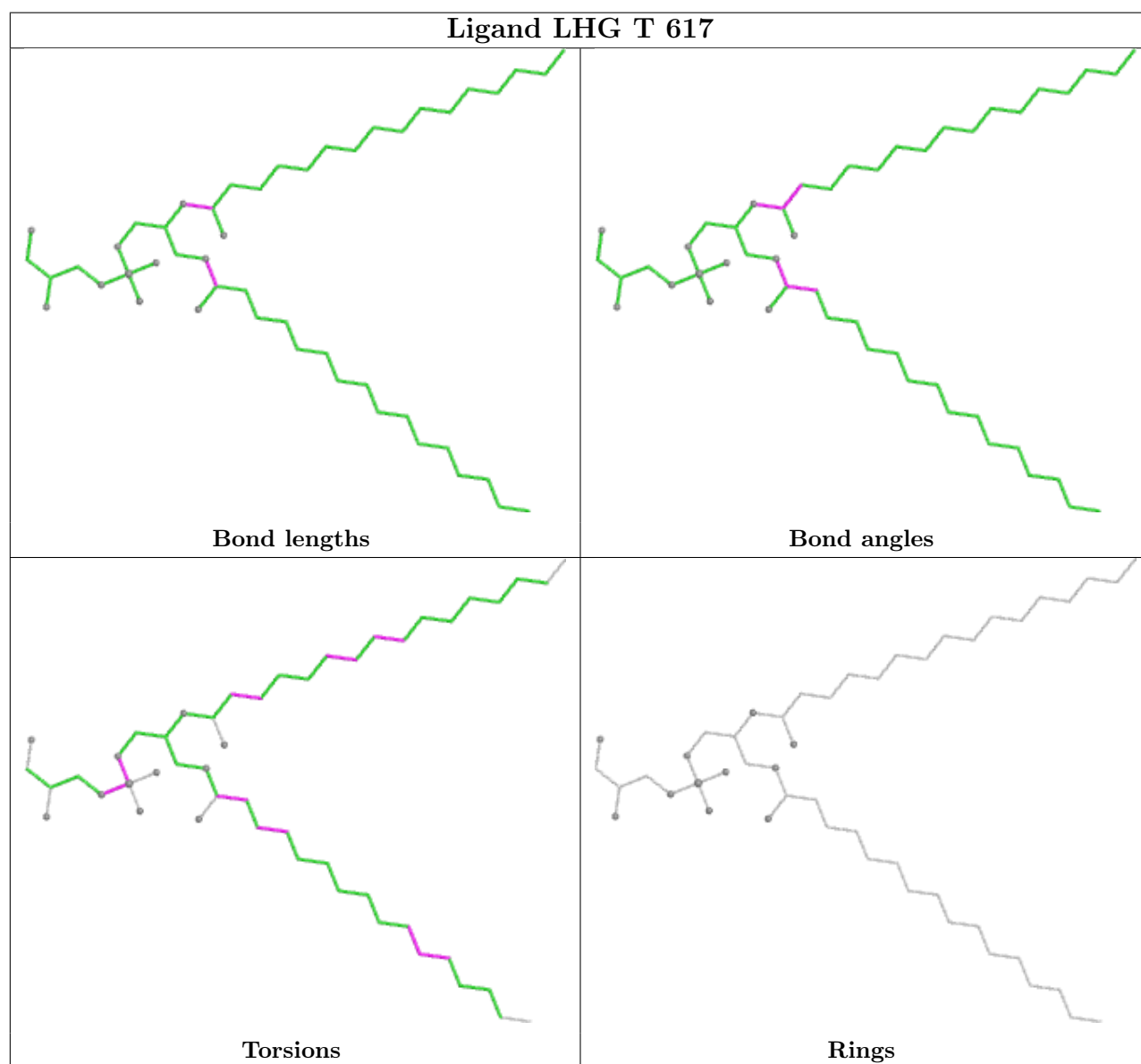
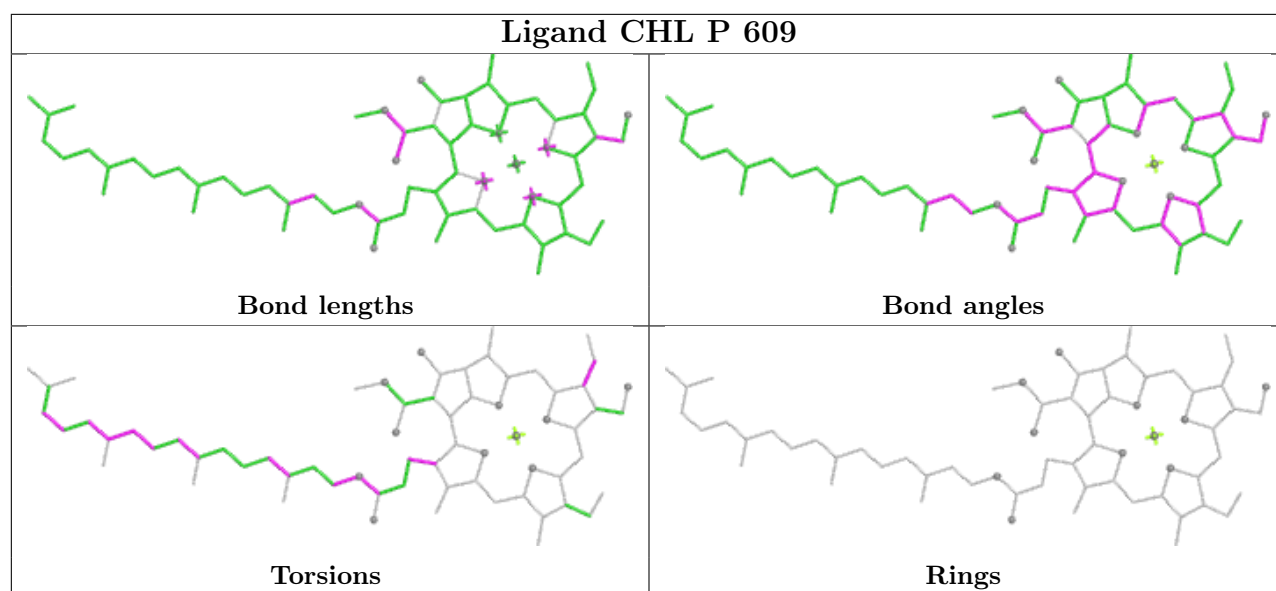
Ligand CLA A 819**Ligand CLA 3 303**

Ligand CLA 2 305

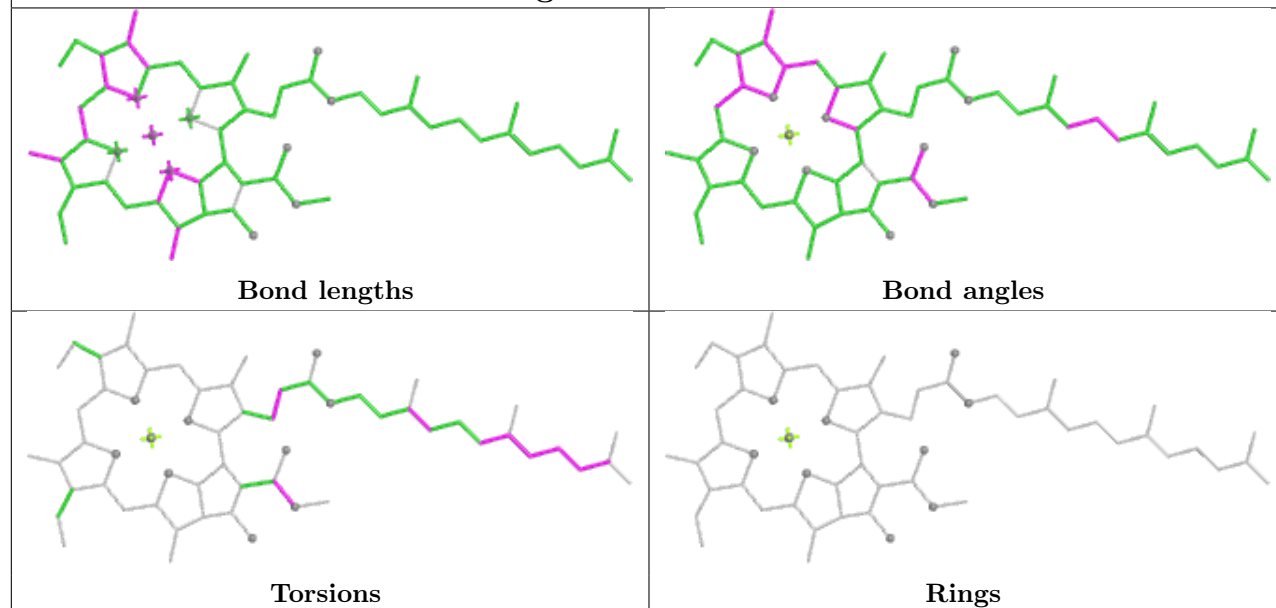


Ligand CLA B 821

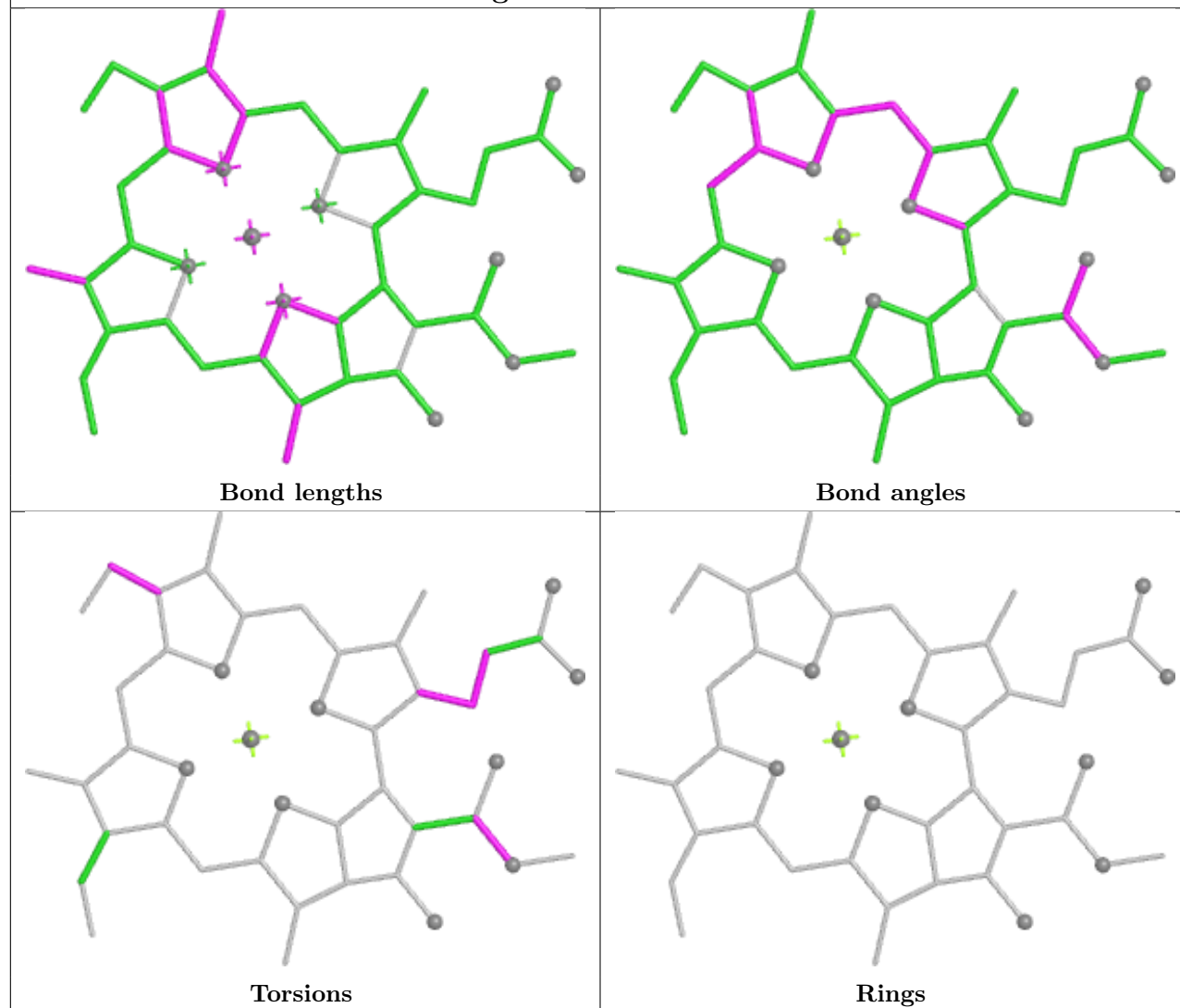




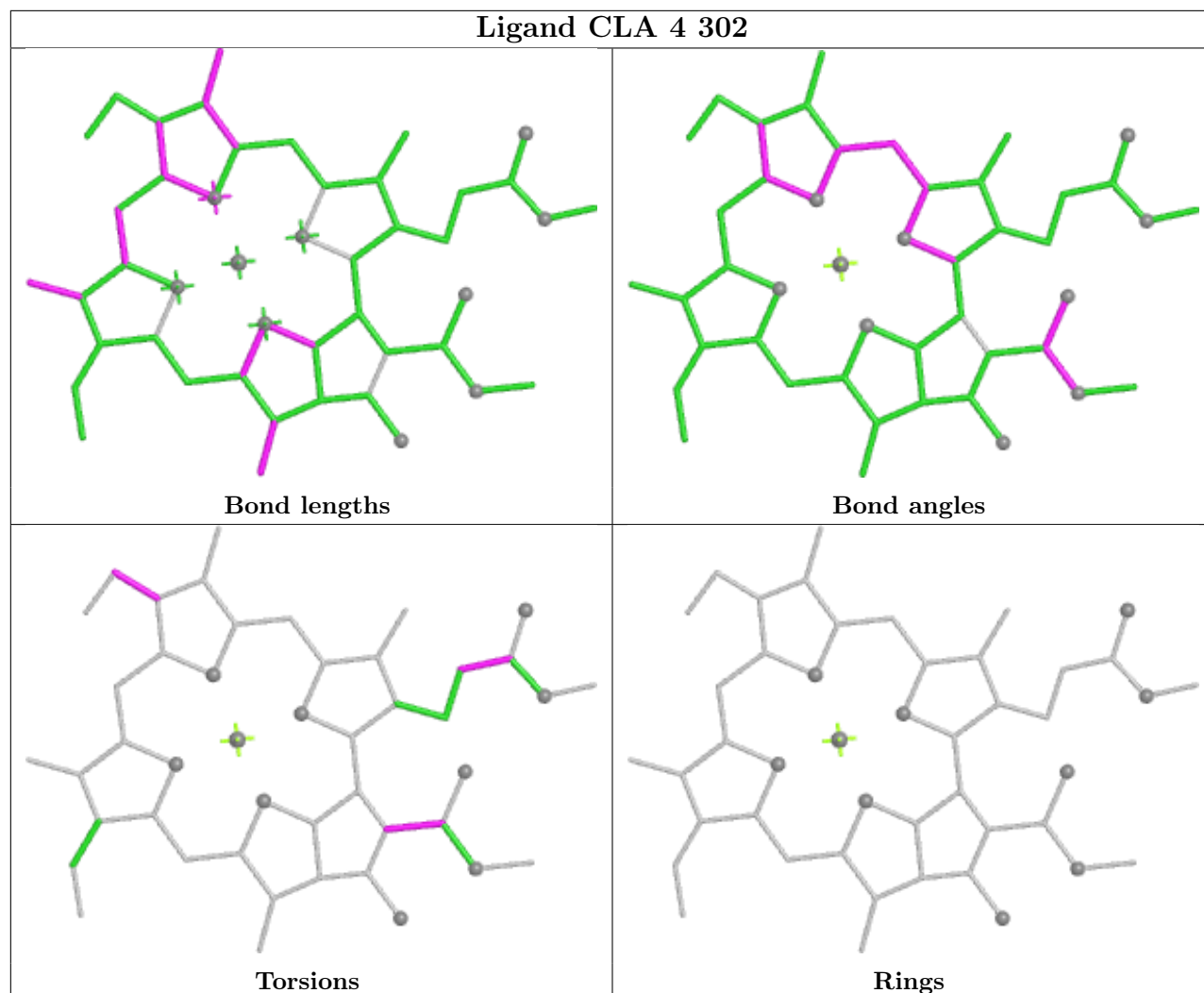
Ligand CLA 2 309



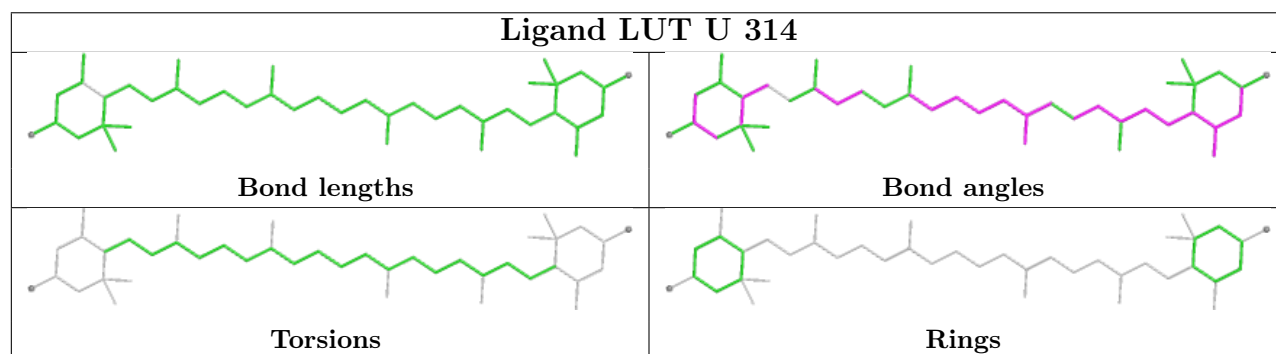
Ligand CLA B 832



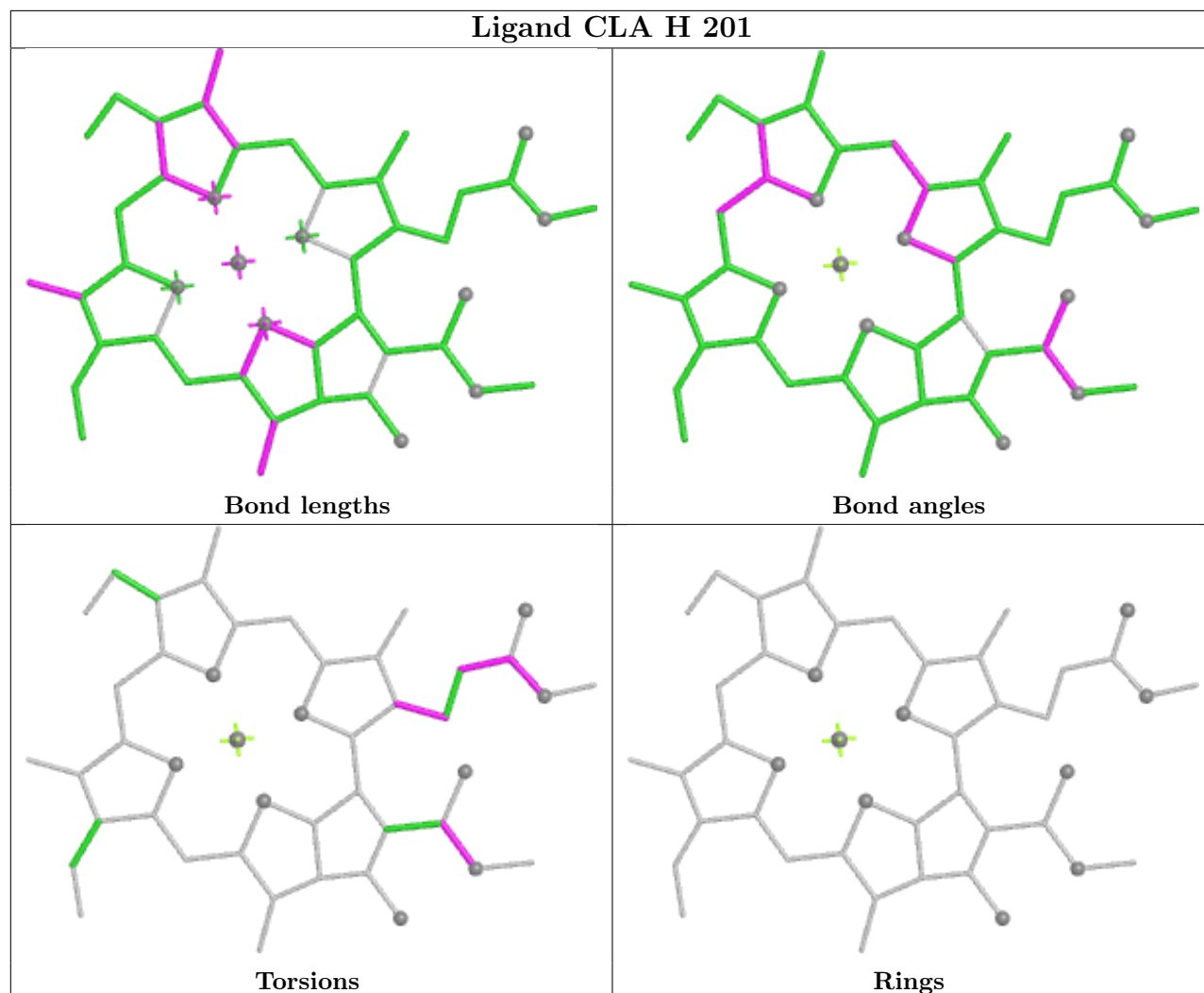
Ligand CLA 4 302



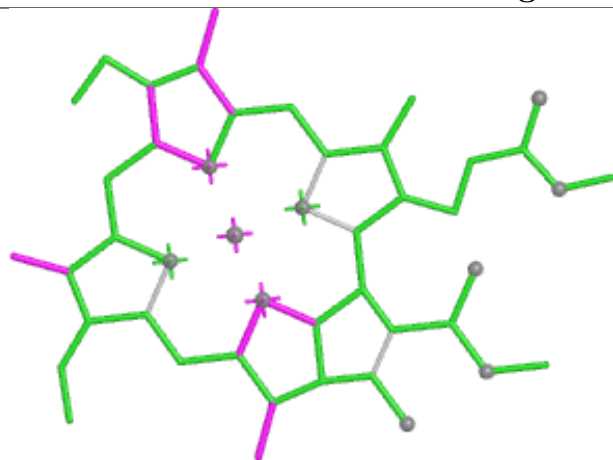
Ligand LUT U 314



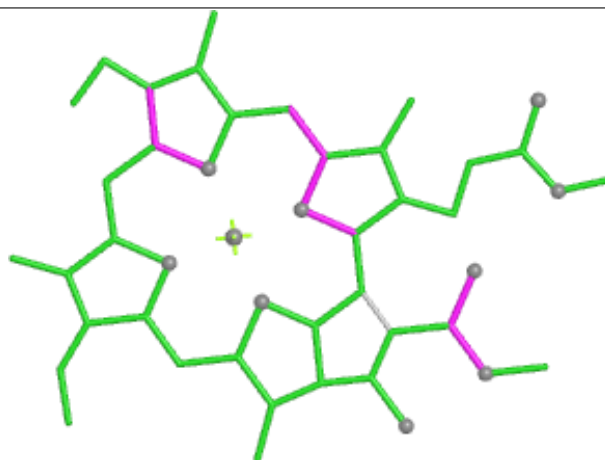
Ligand CLA H 201



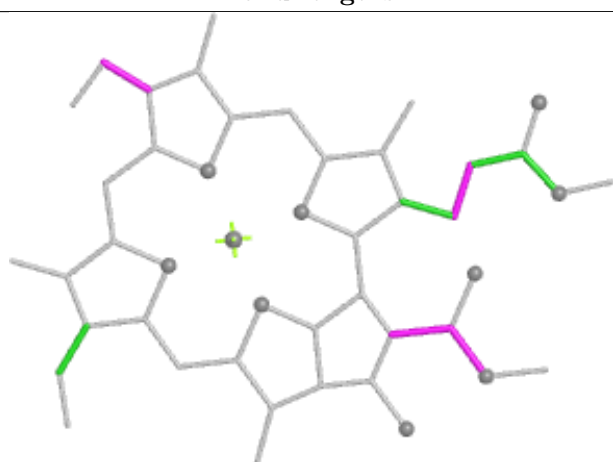
Ligand CLA 8 315



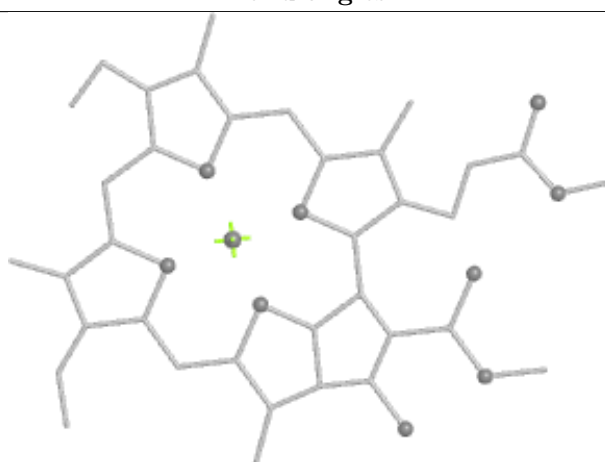
Bond lengths



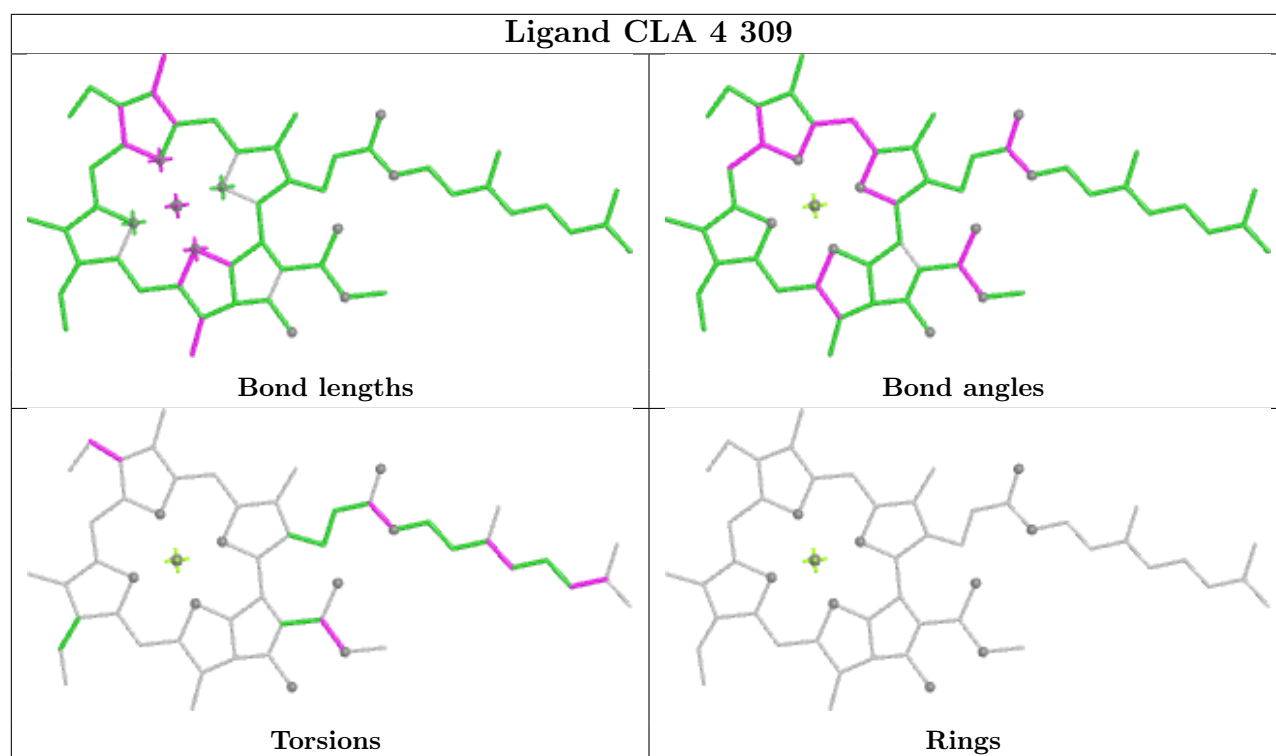
Bond angles

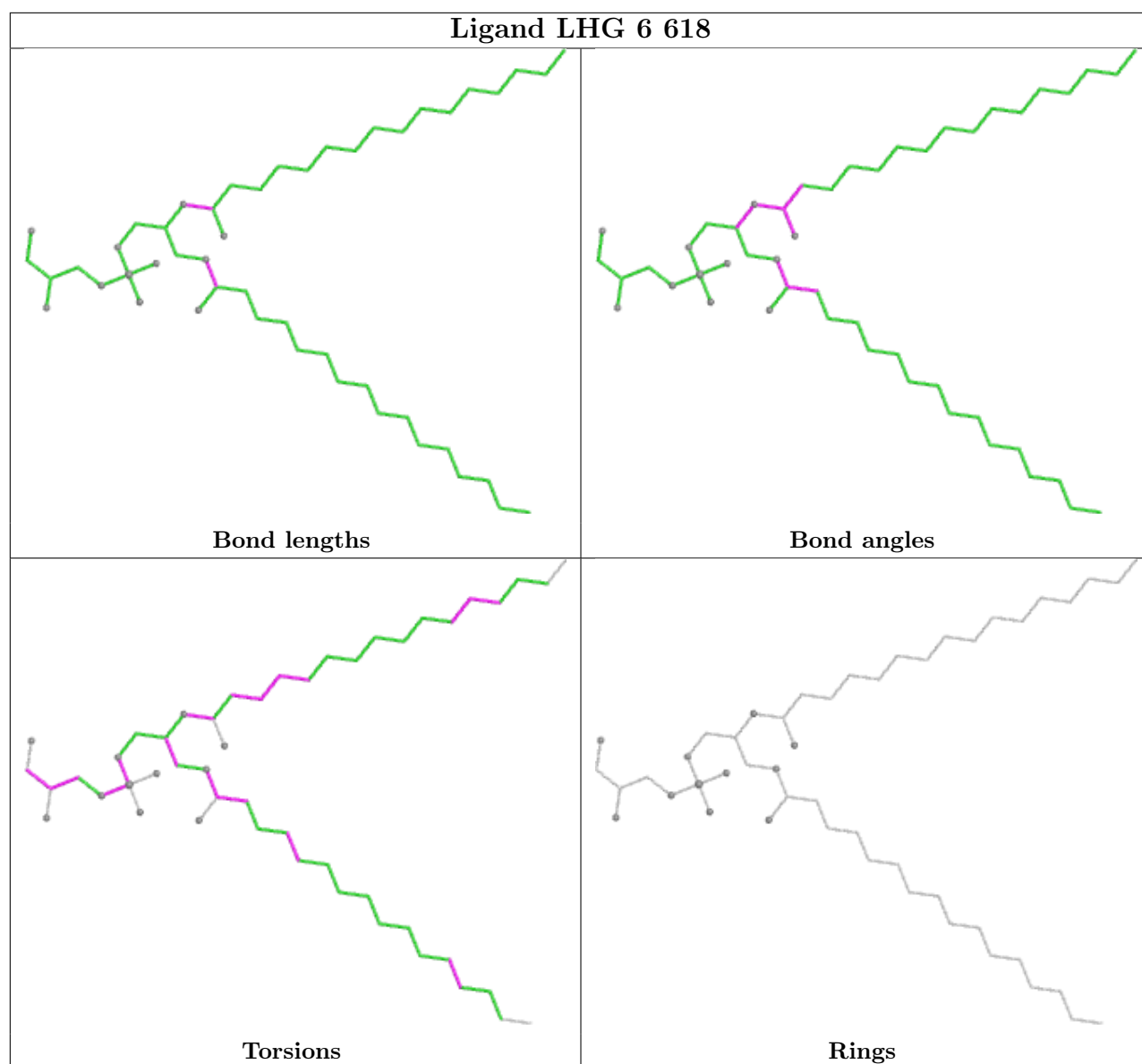


Torsions

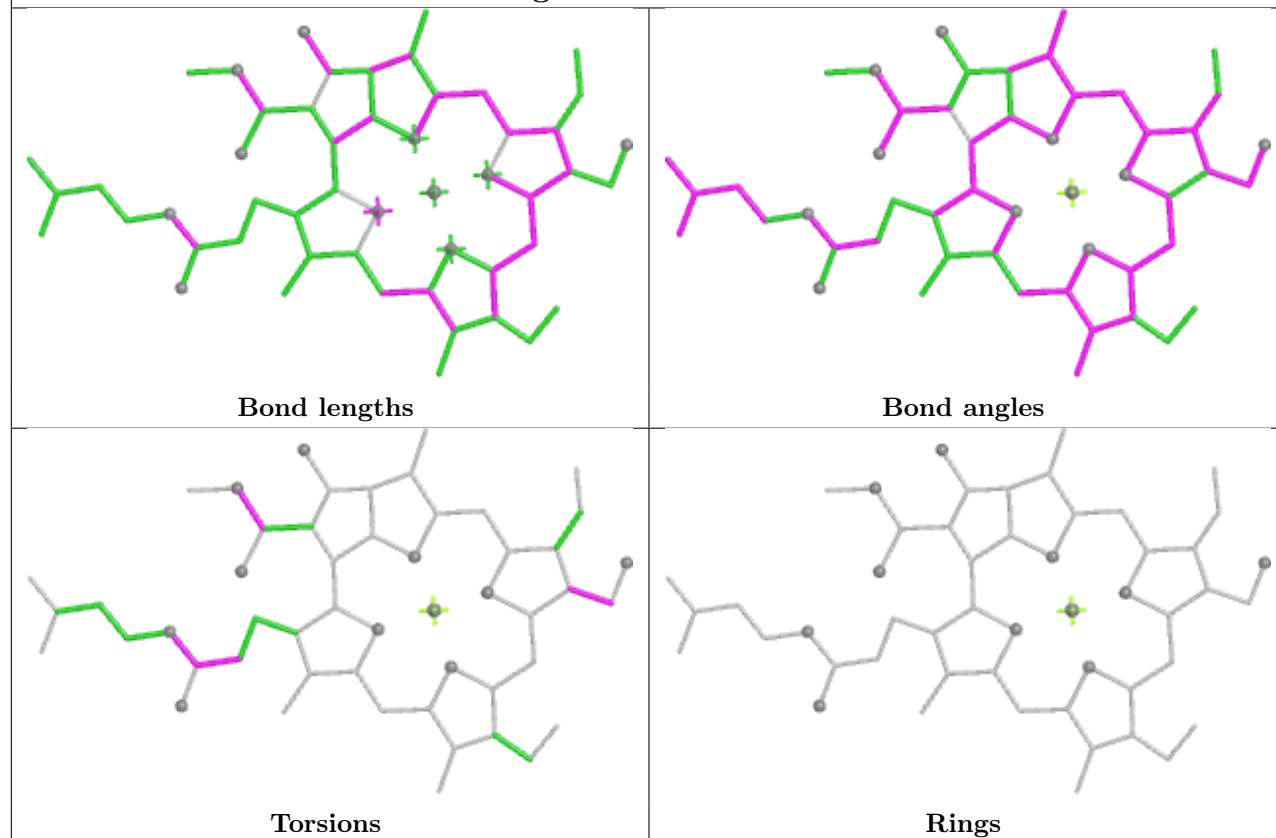


Rings

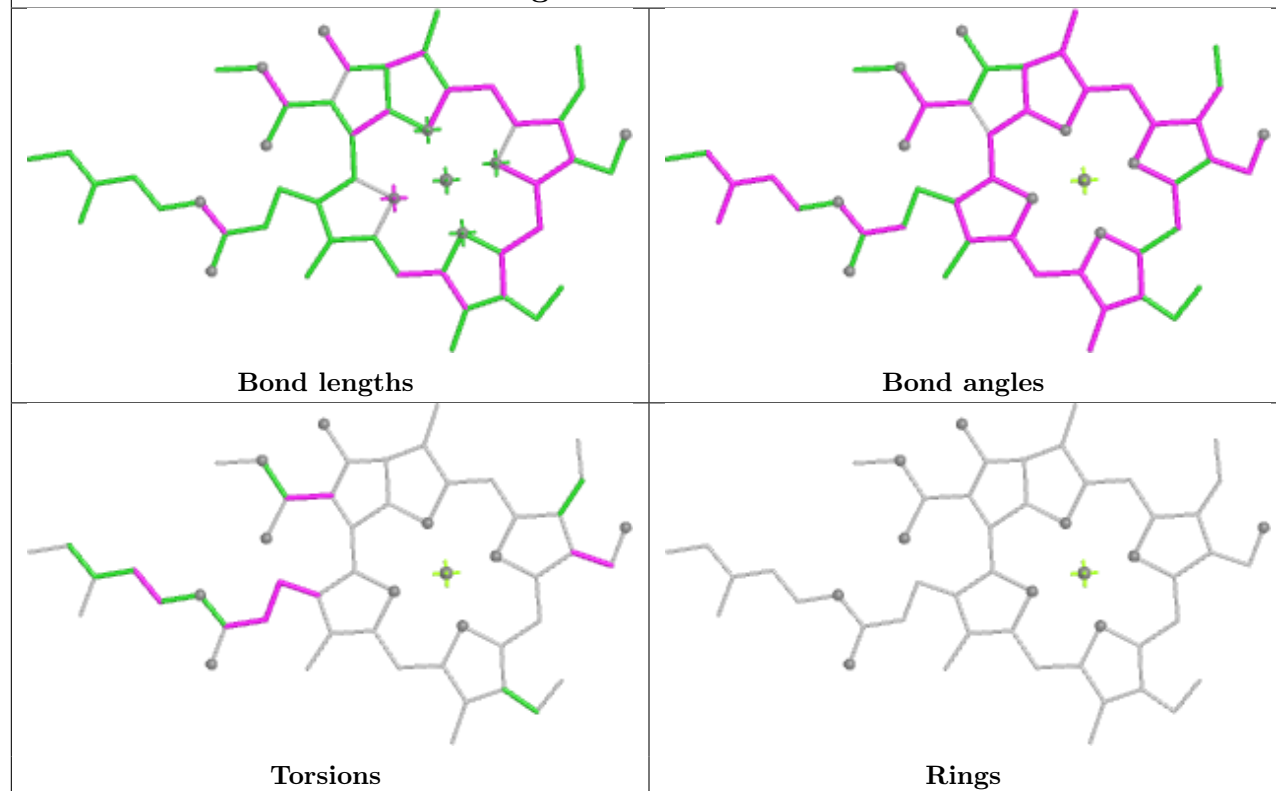


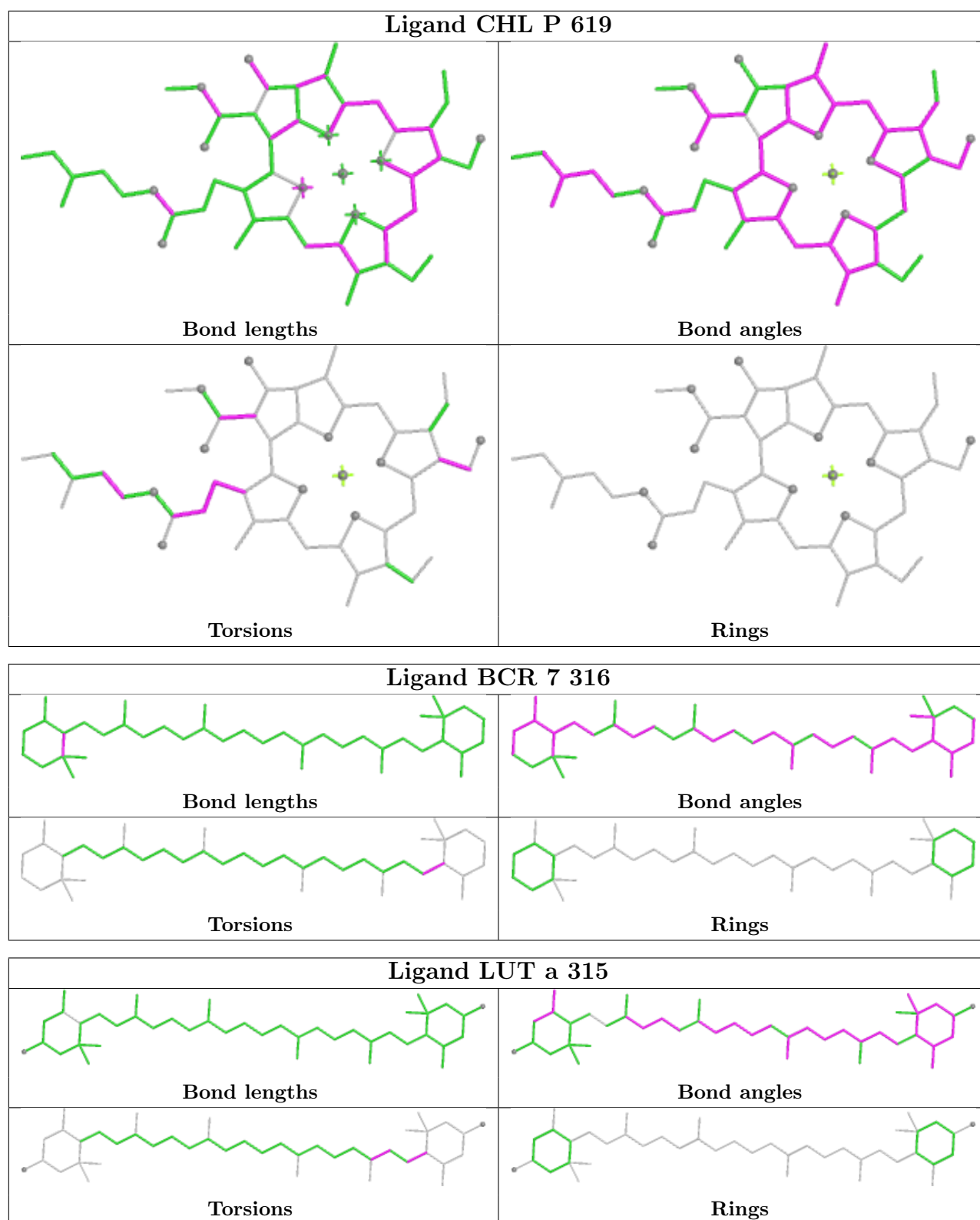


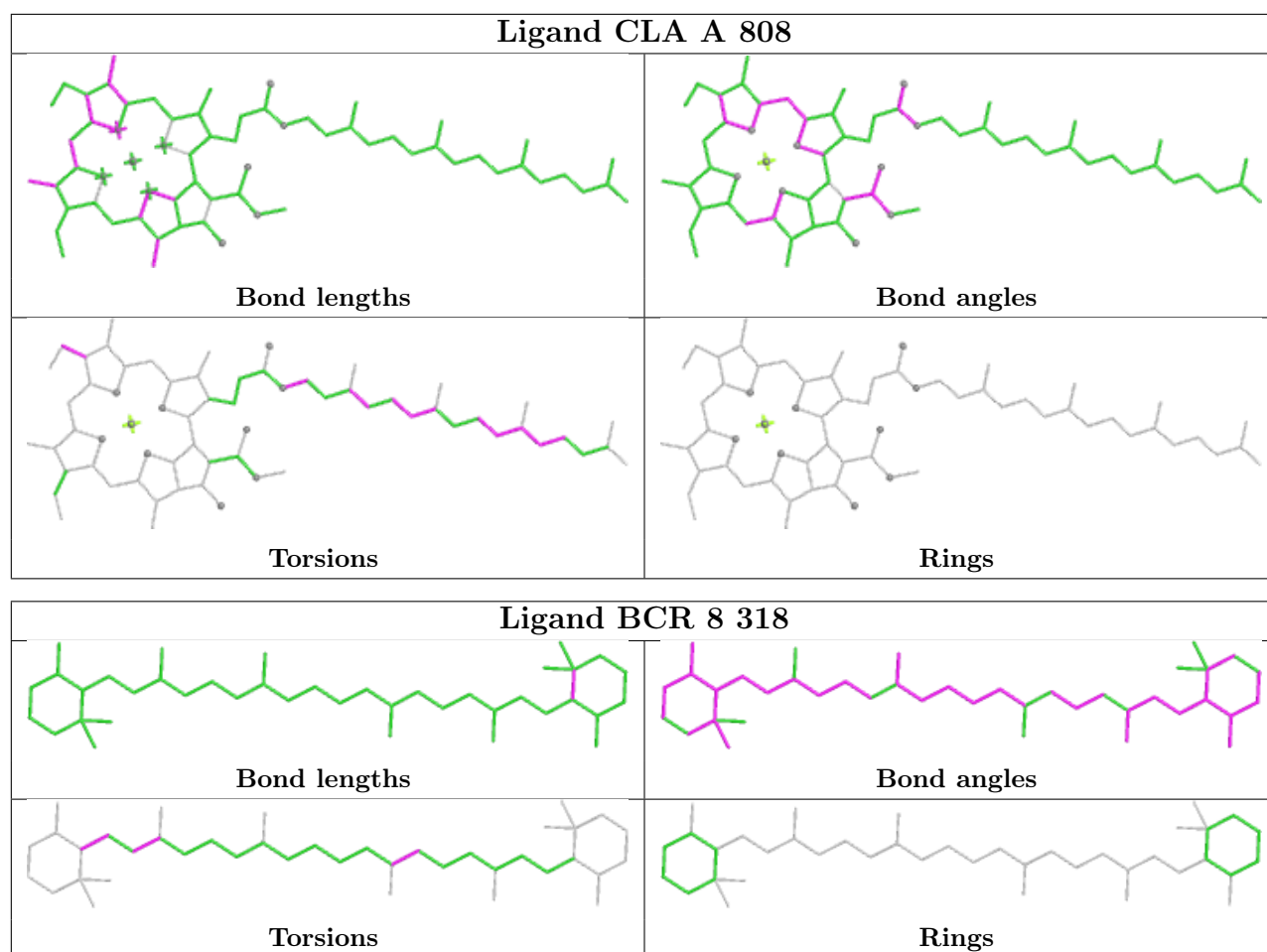
Ligand CHL P 601

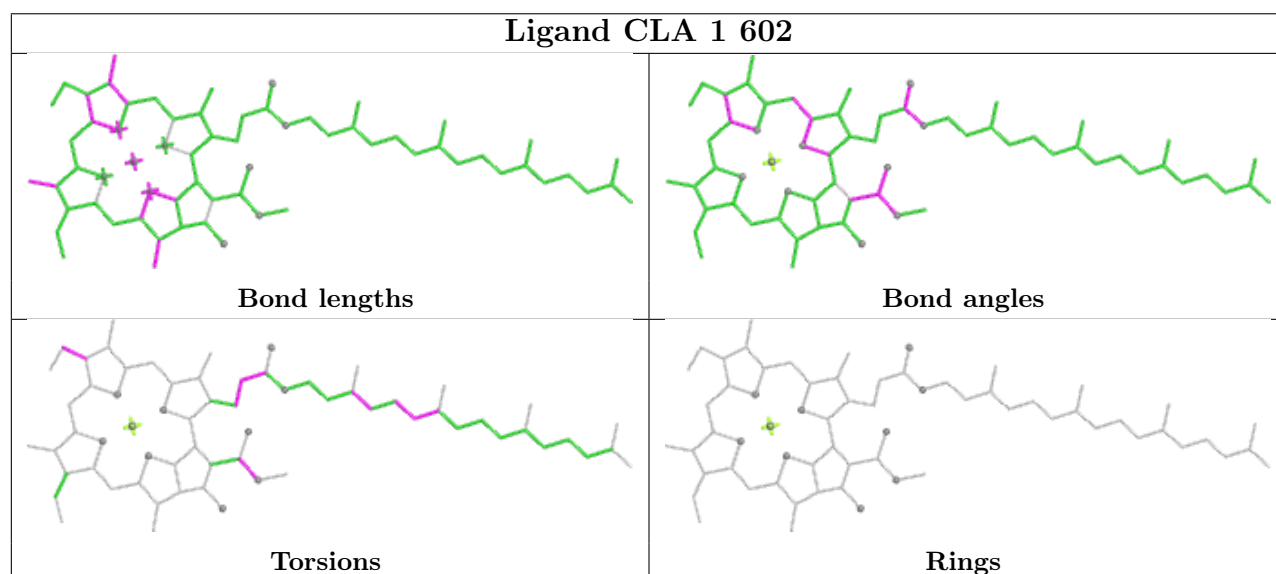
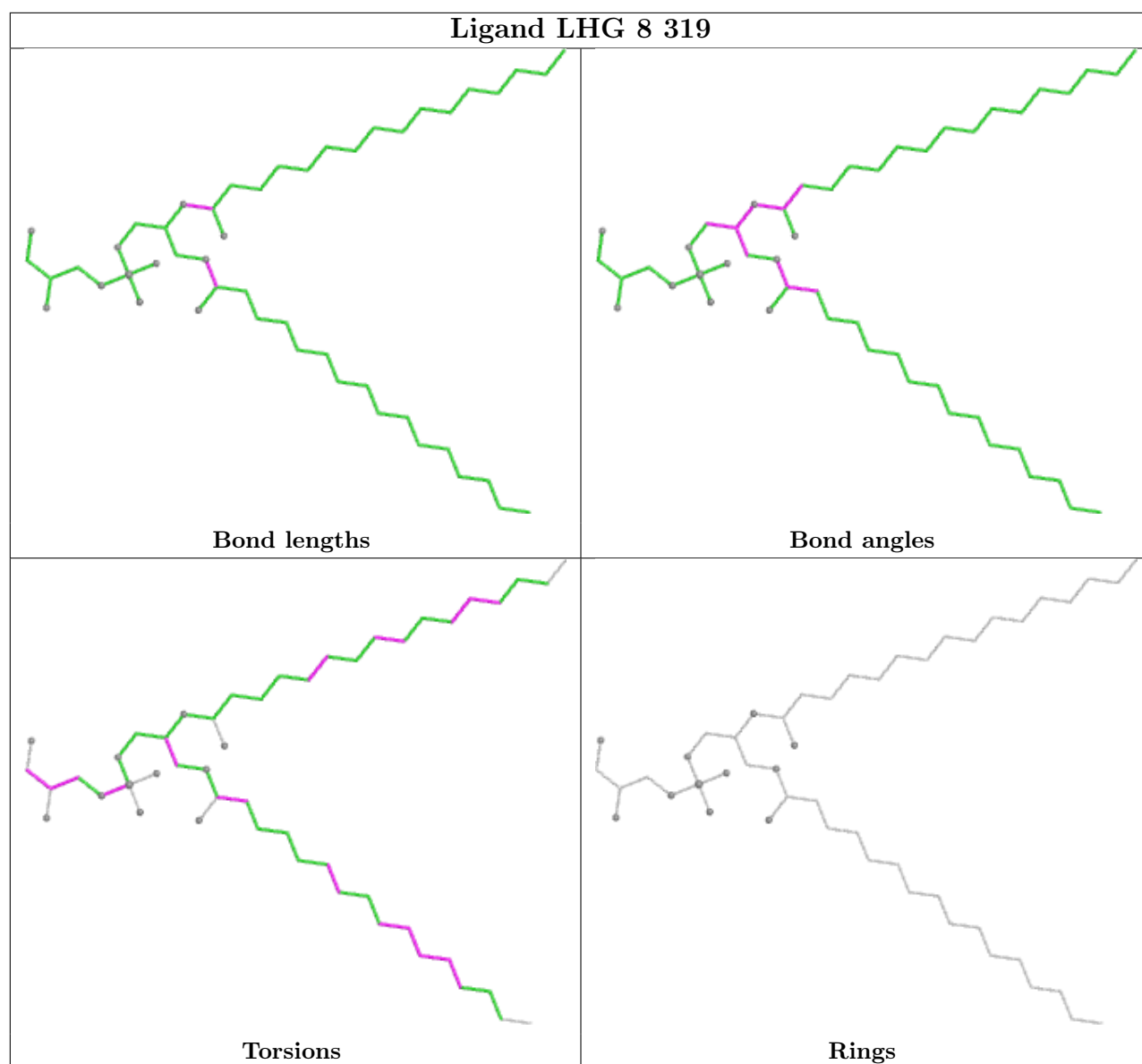


Ligand CHL R 607

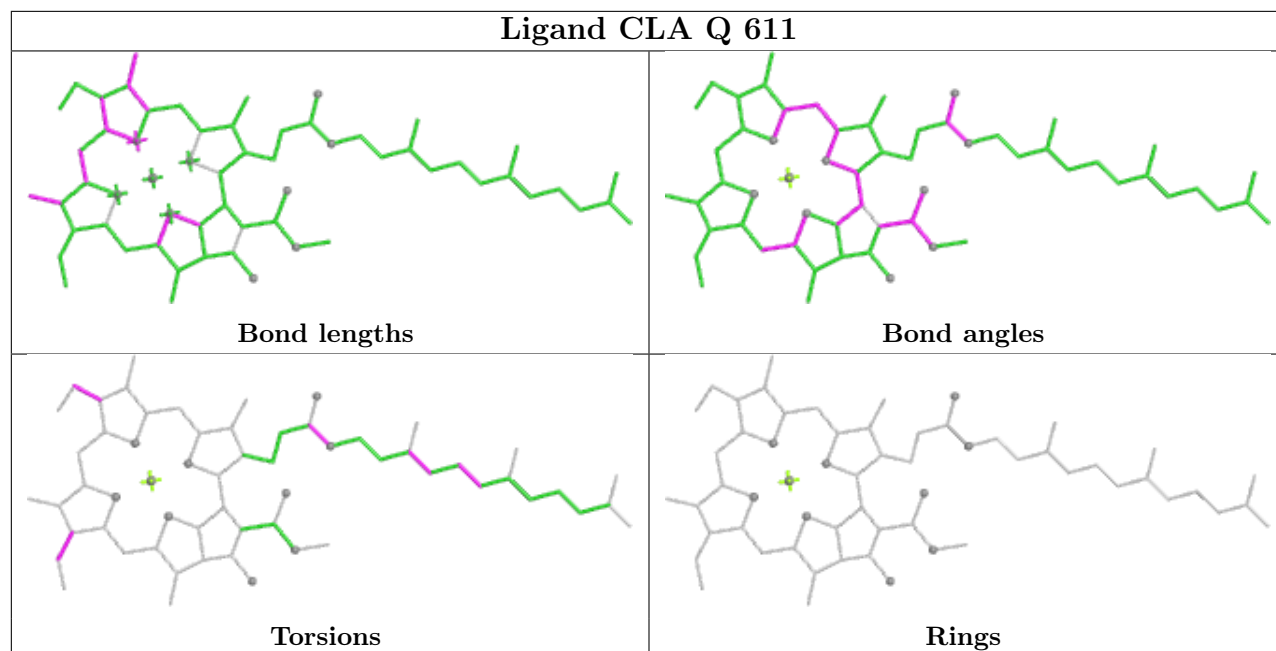




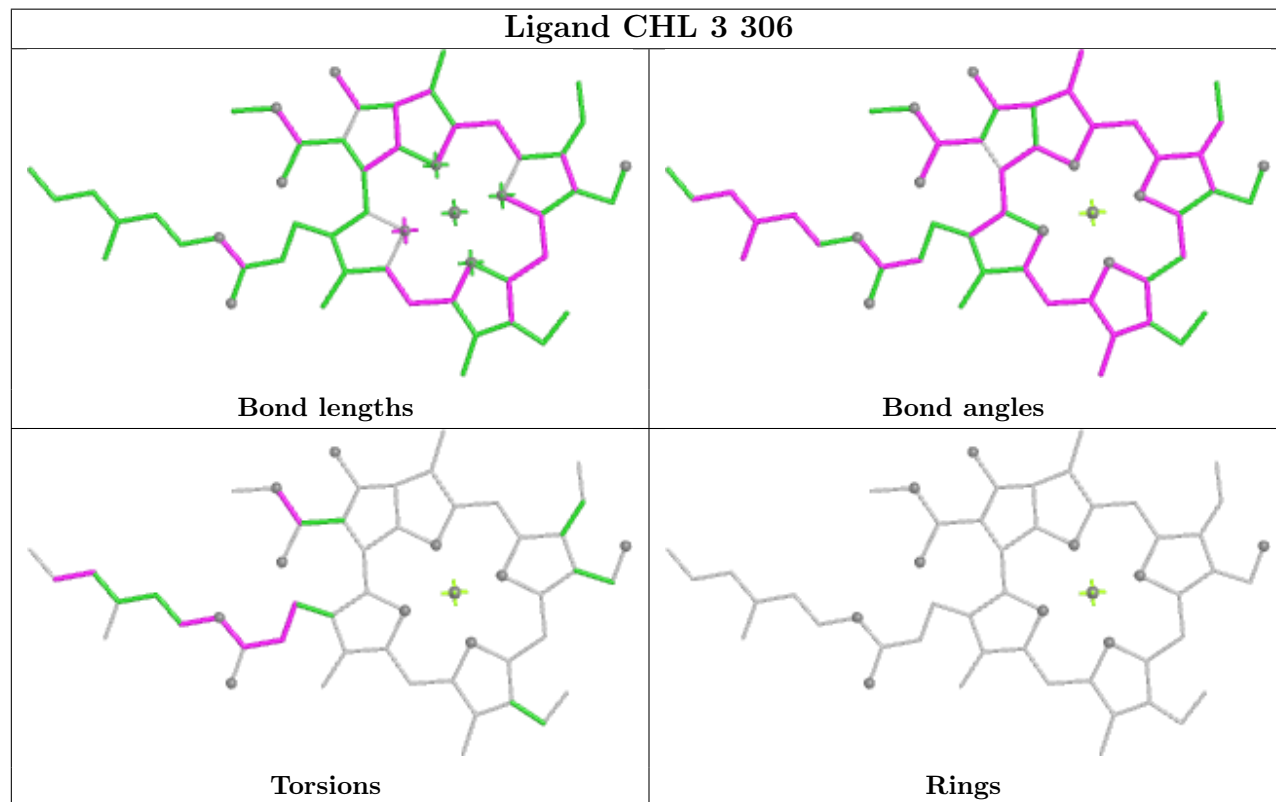




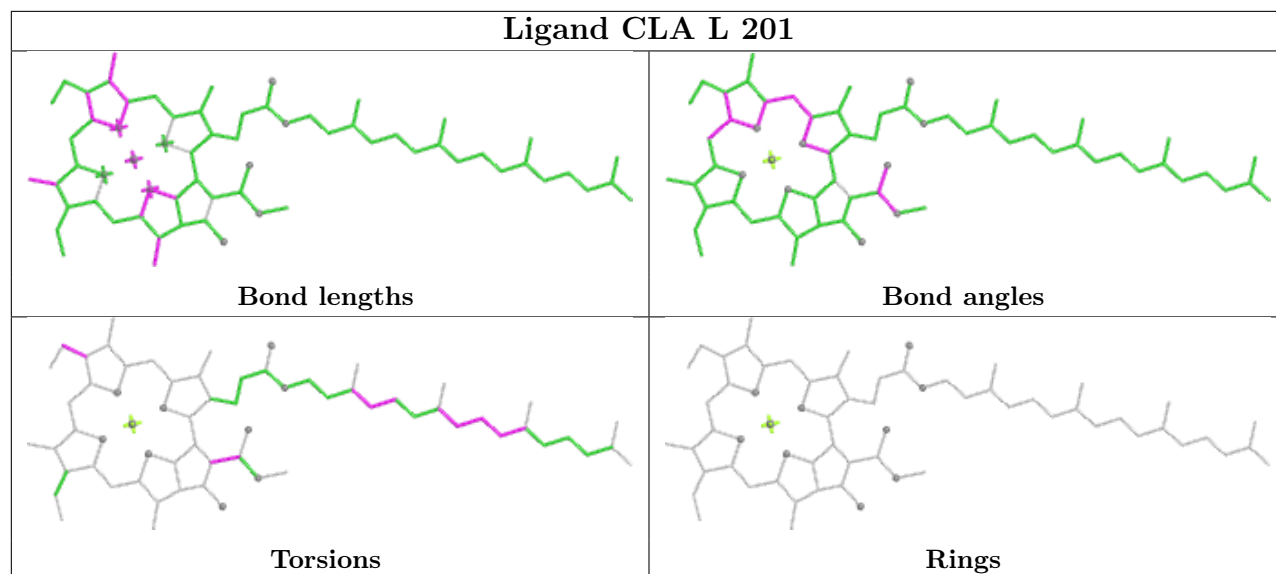
Ligand CLA Q 611



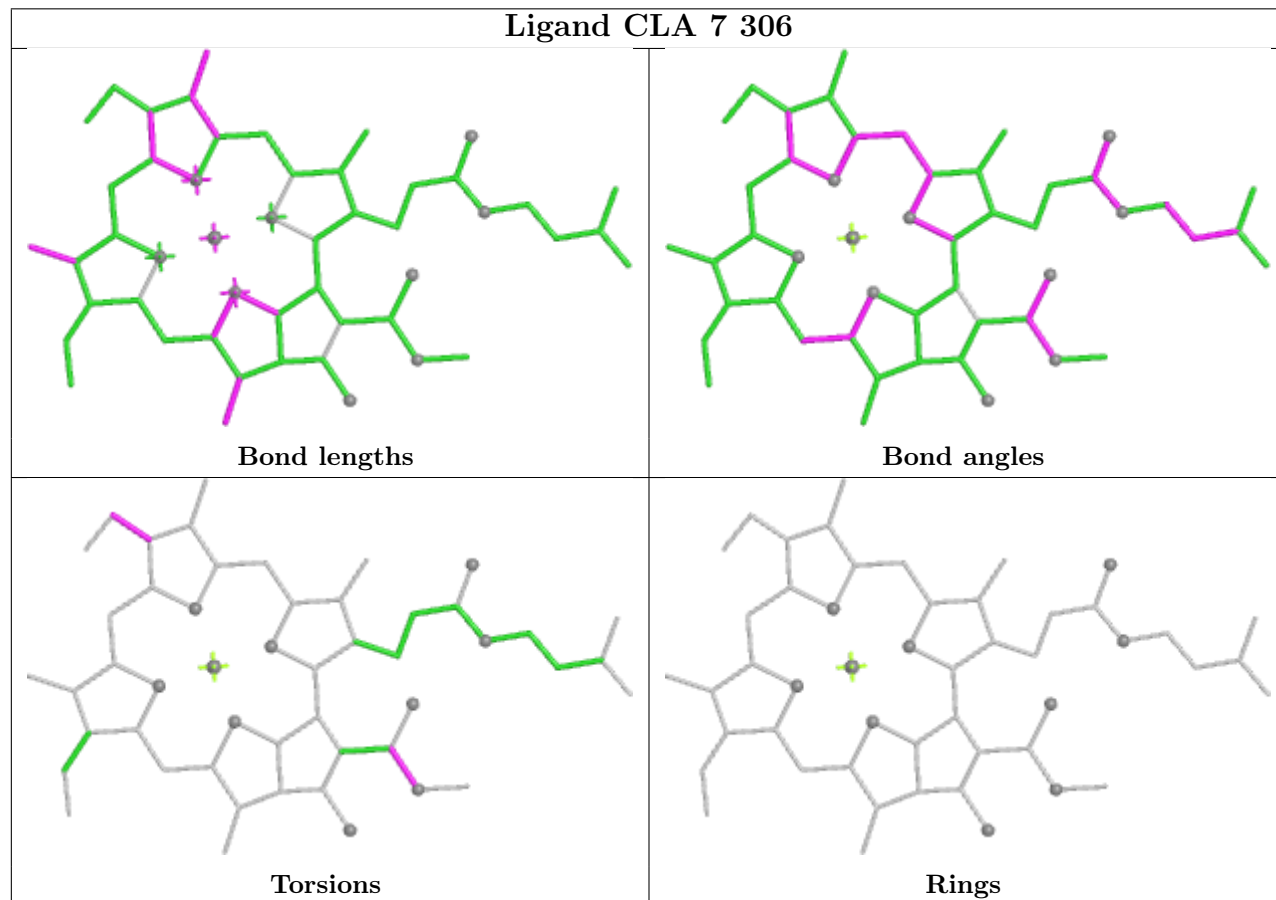
Ligand CHL 3 306

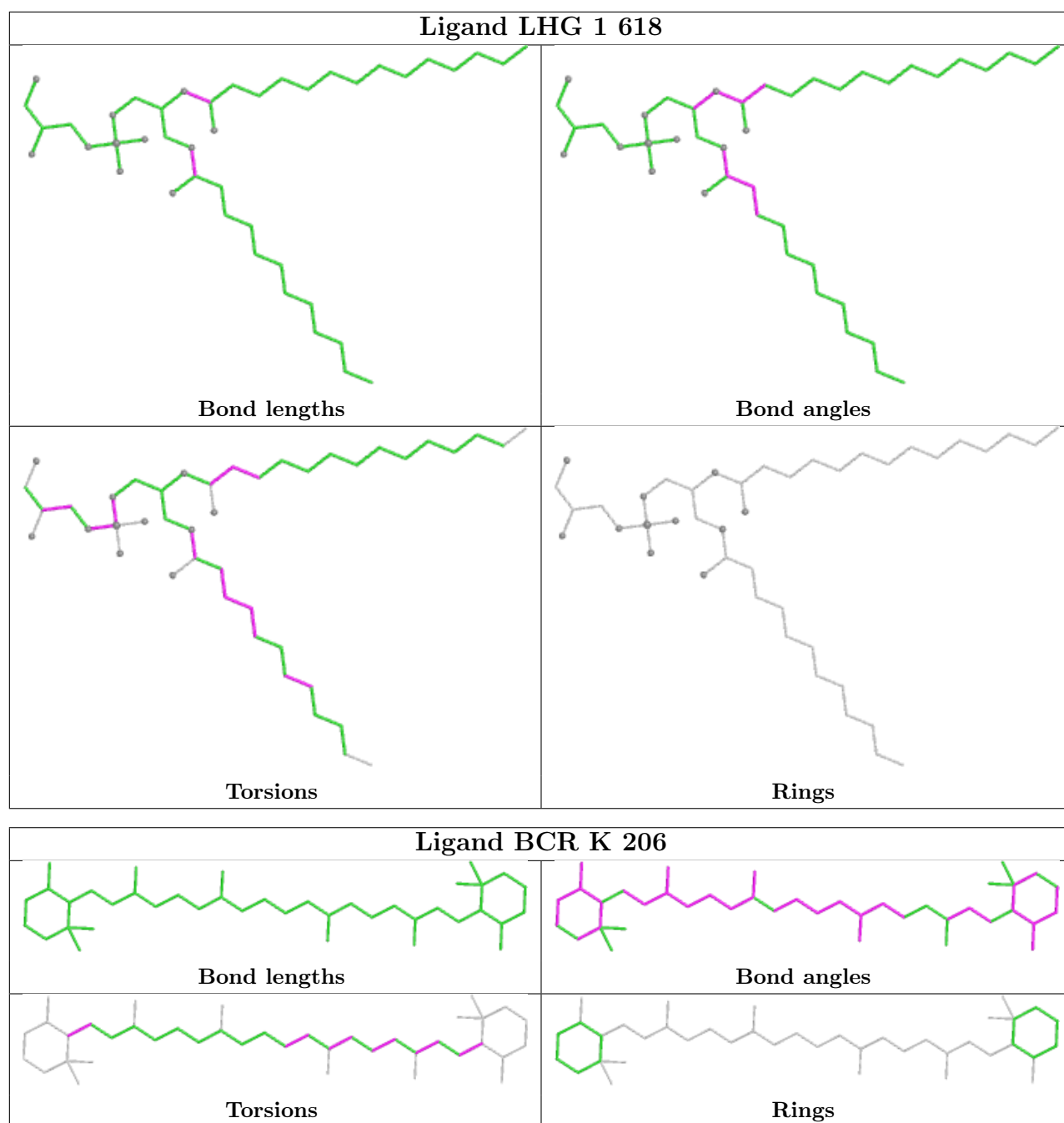


Ligand CLA L 201

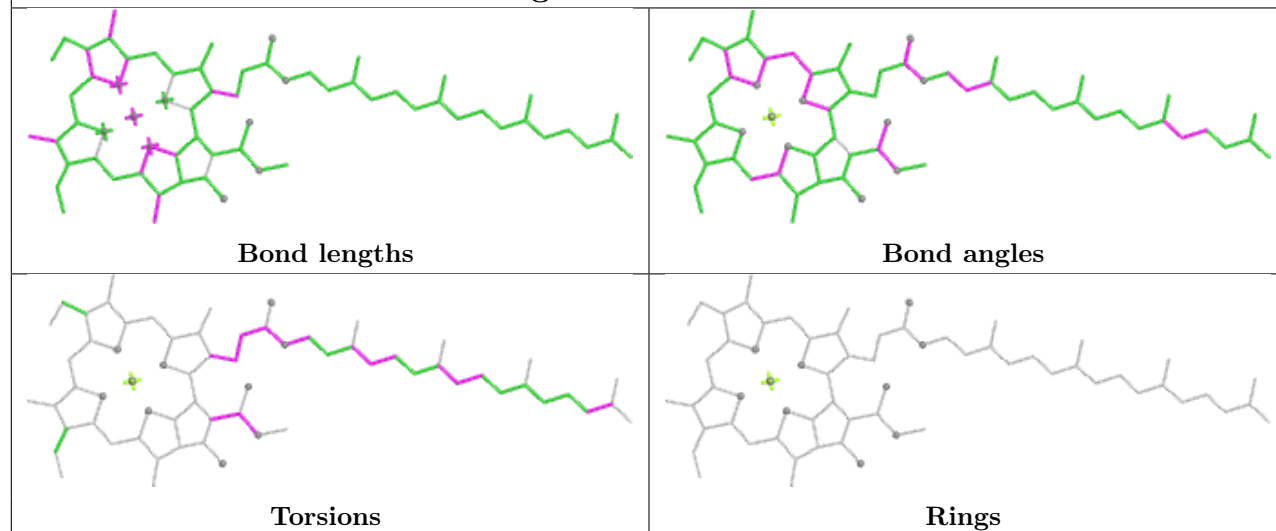


Ligand CLA 7 306

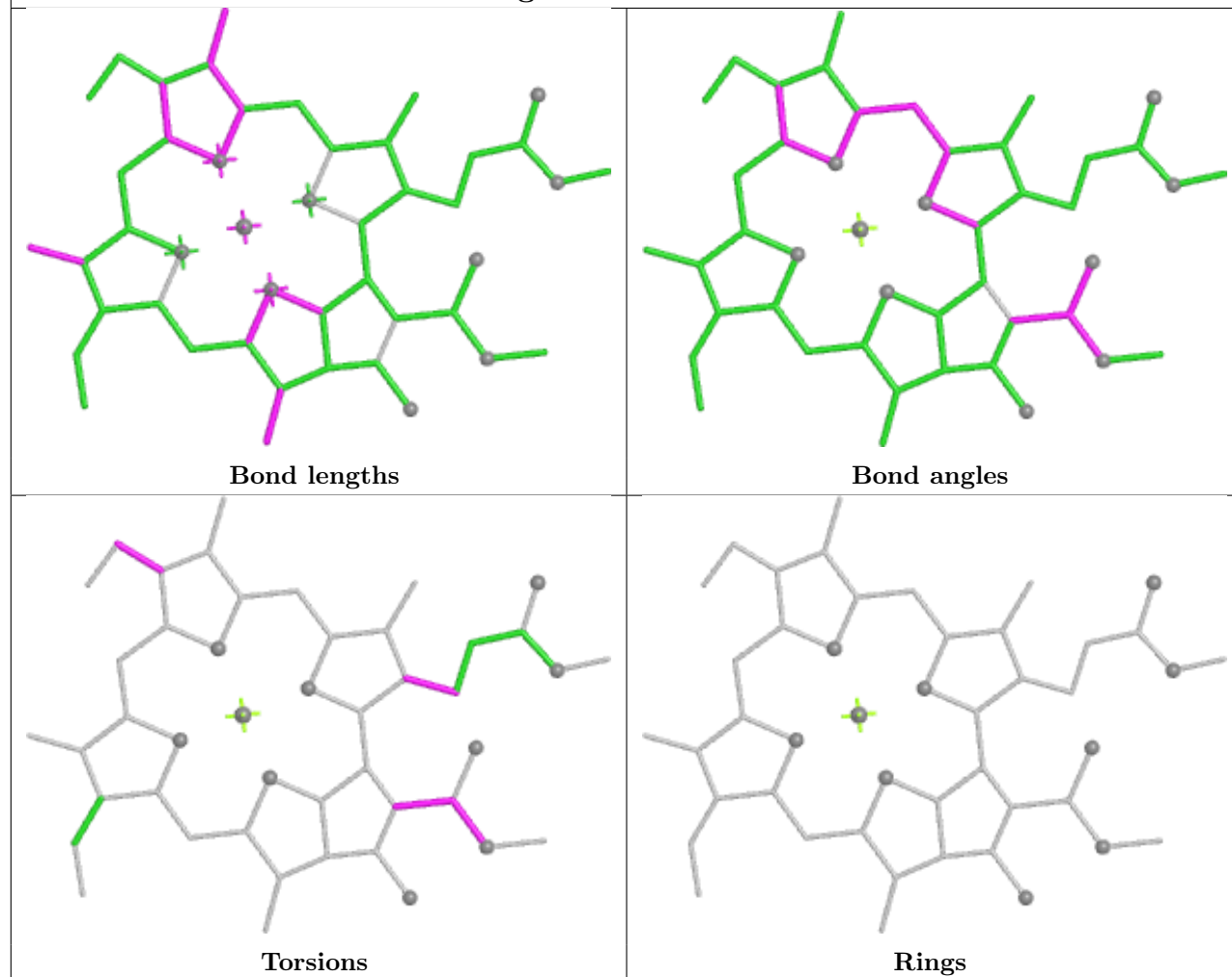


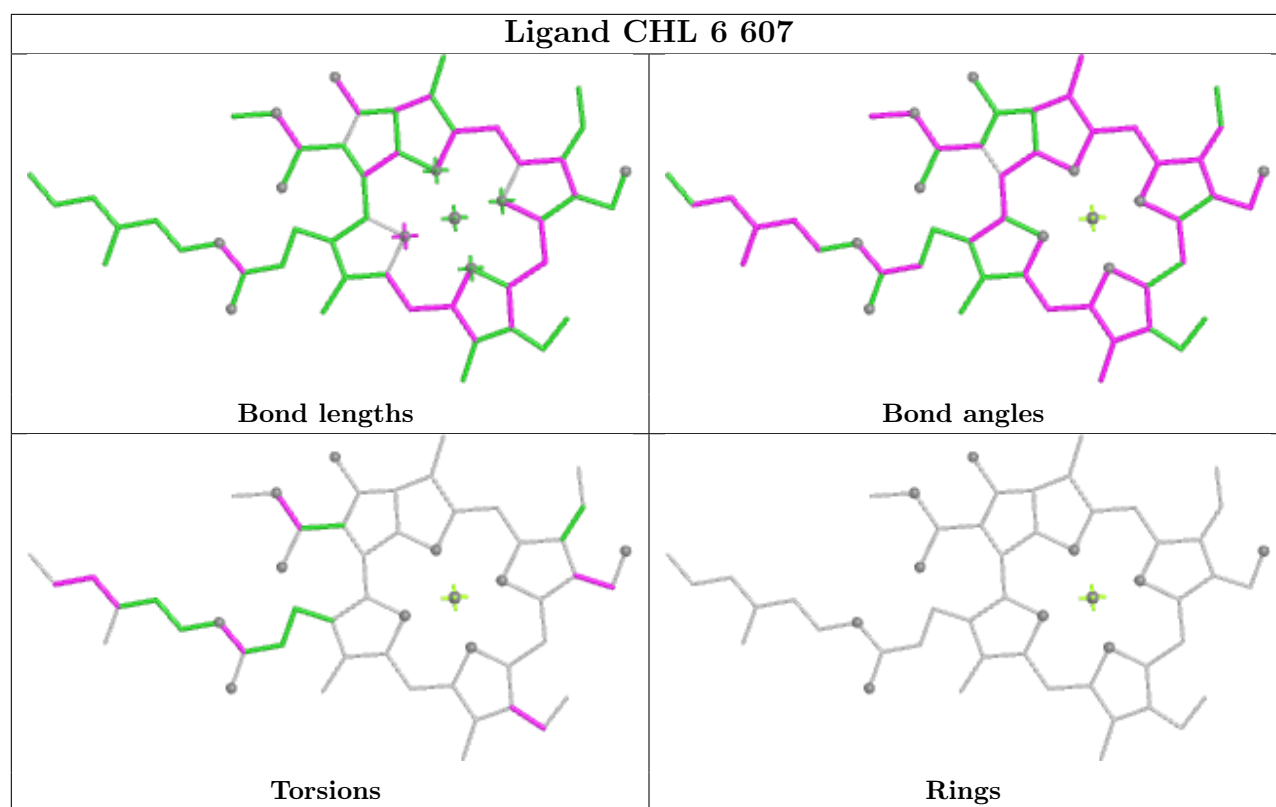


Ligand CLA A 814

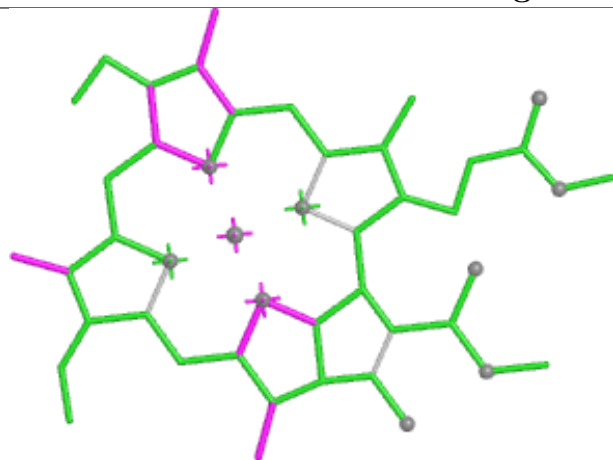


Ligand CLA 8 311

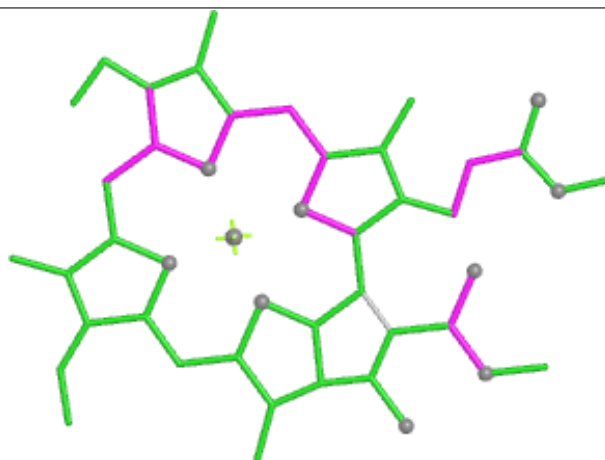




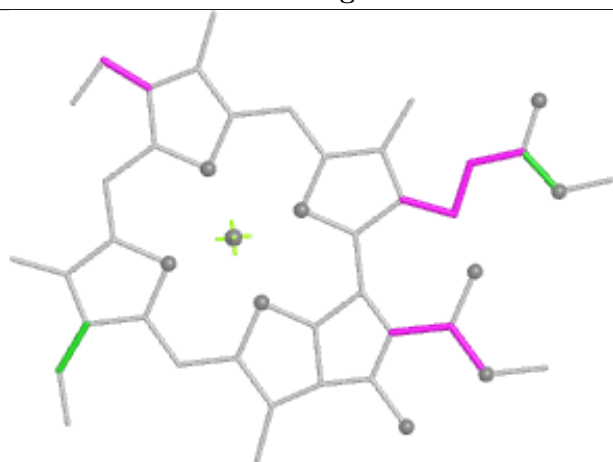
Ligand CLA H 203



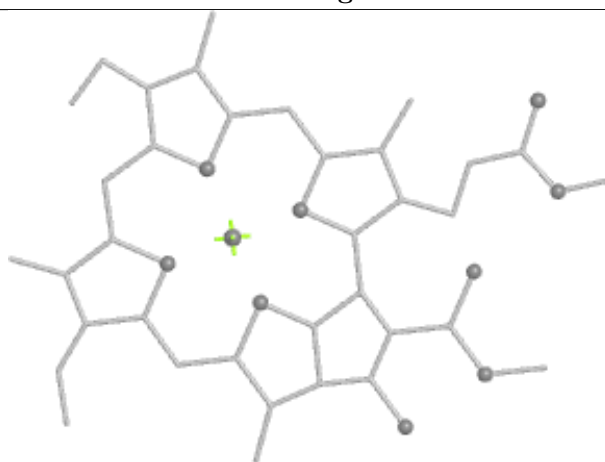
Bond lengths



Bond angles

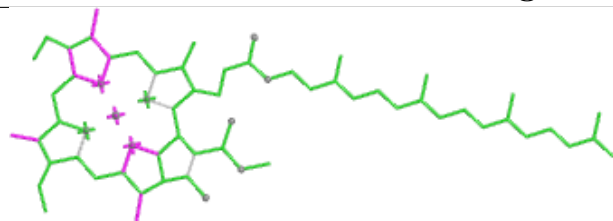


Torsions

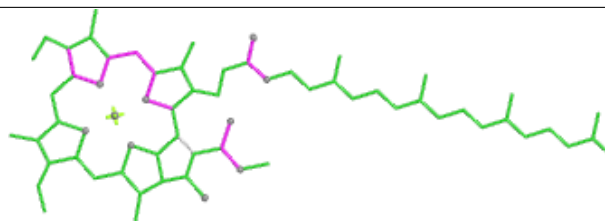


Rings

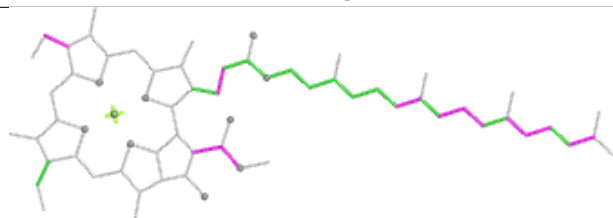
Ligand CLA 3 308



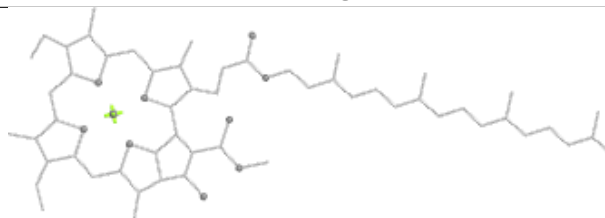
Bond lengths



Bond angles

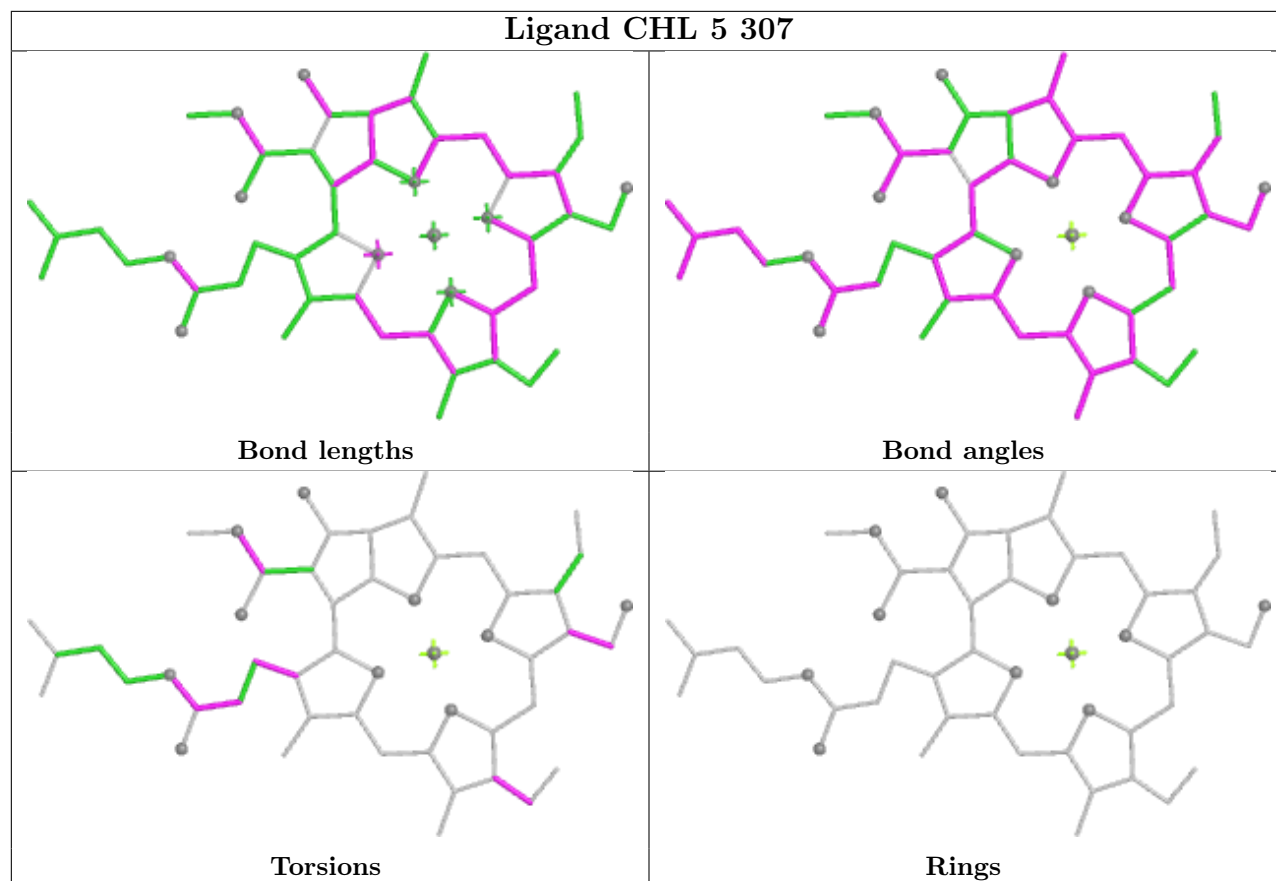


Torsions

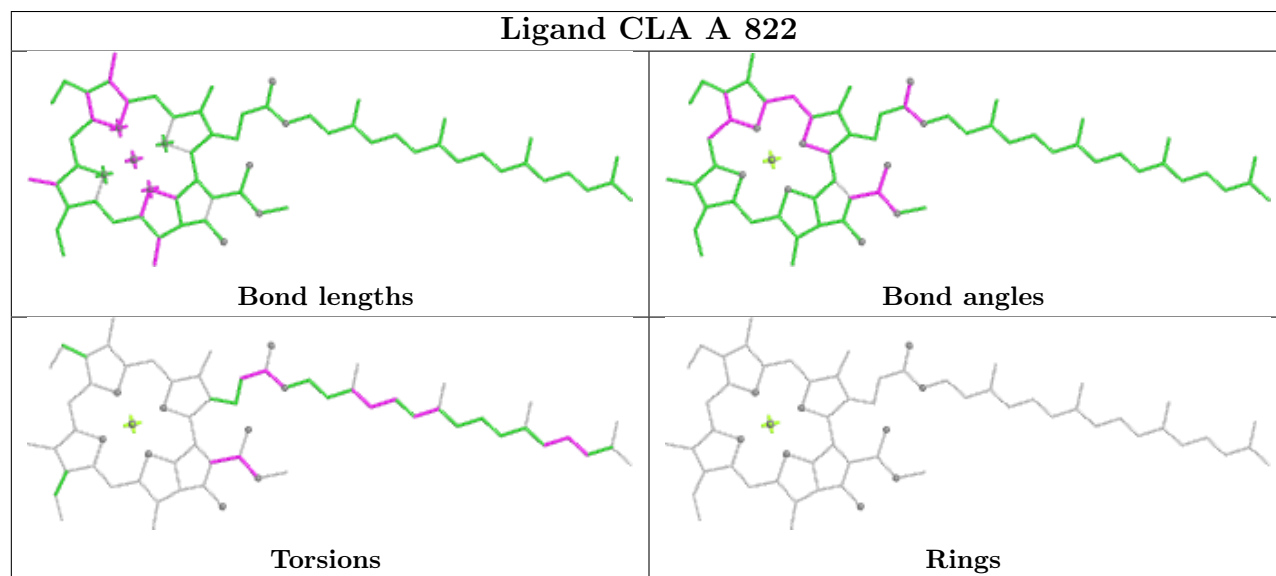


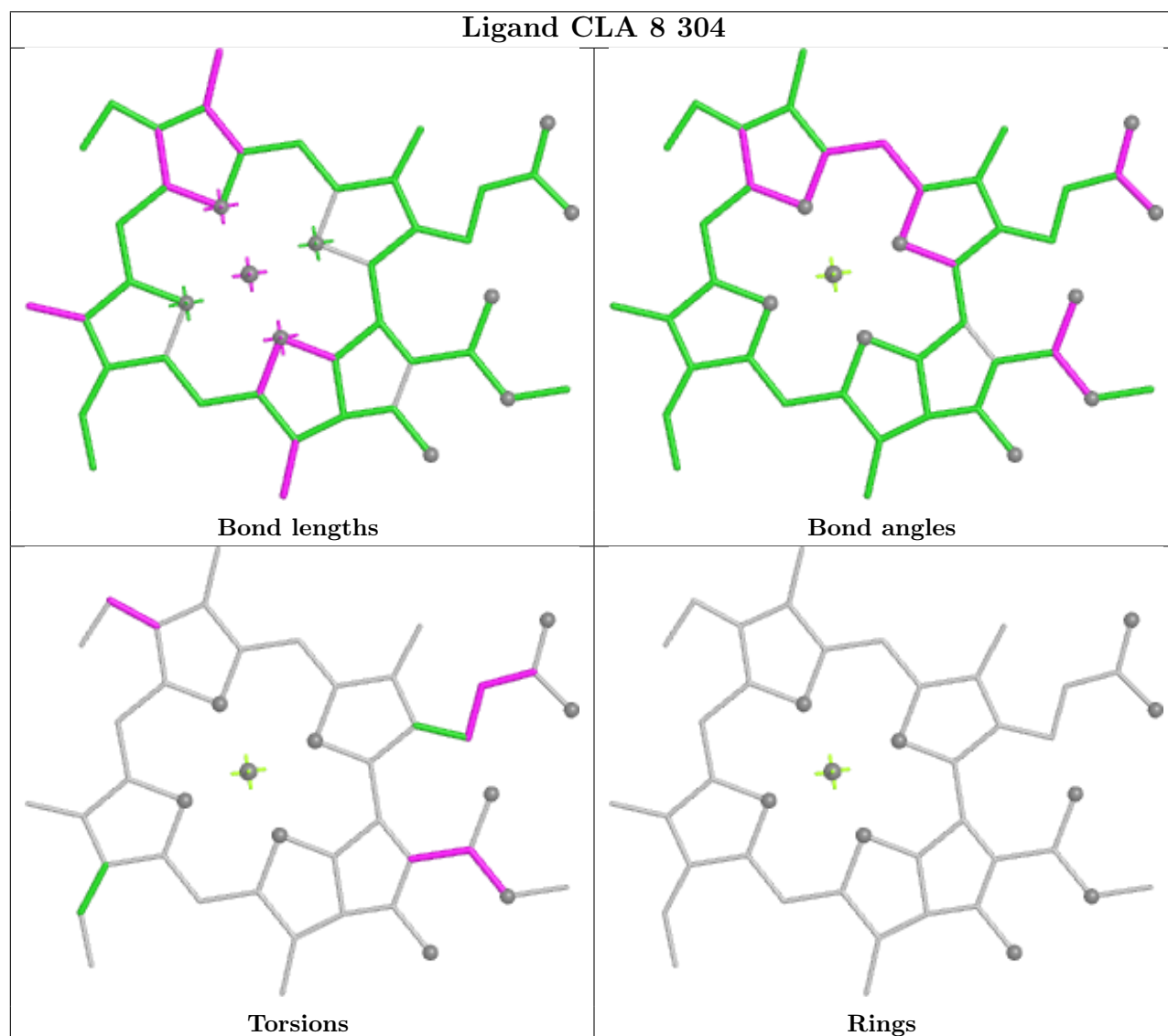
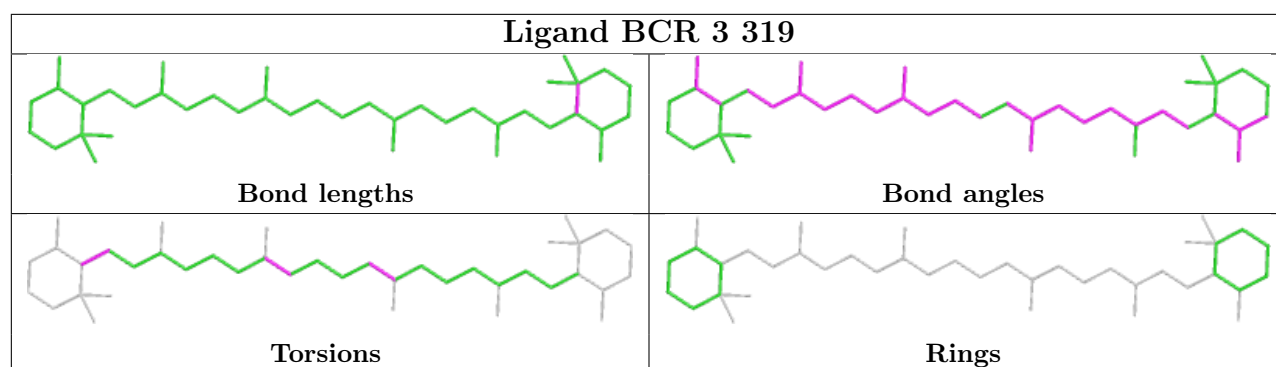
Rings

Ligand CHL 5 307

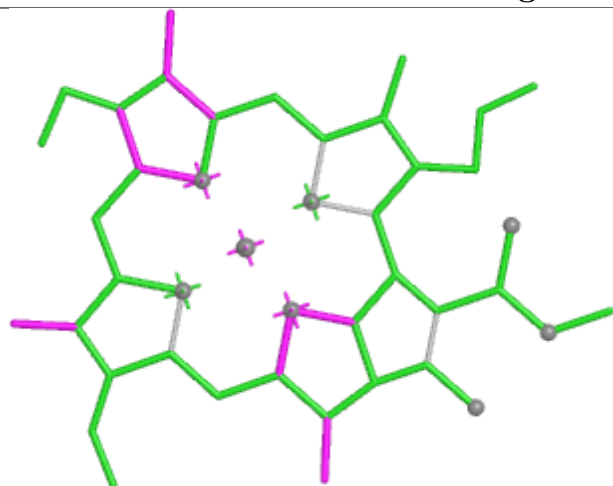


Ligand CLA A 822

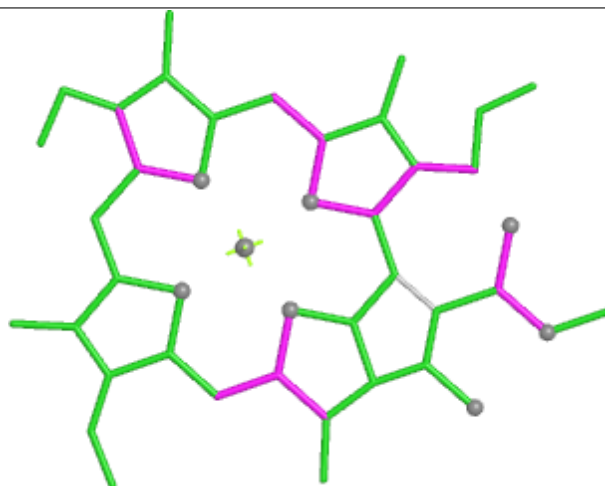




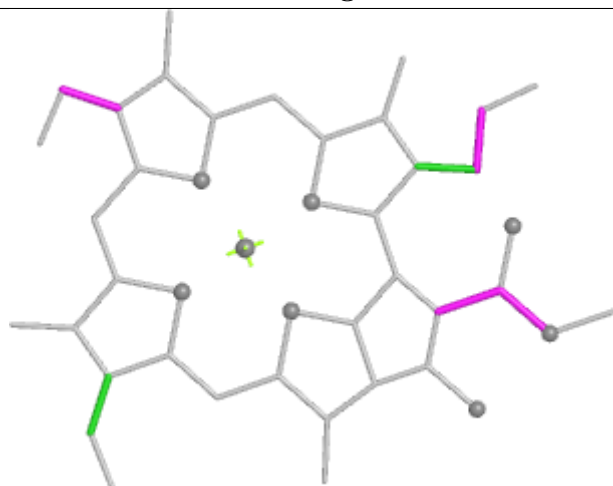
Ligand CLA 2 308



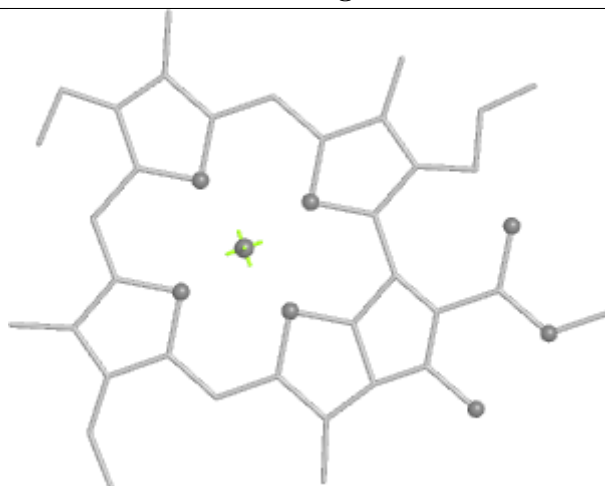
Bond lengths



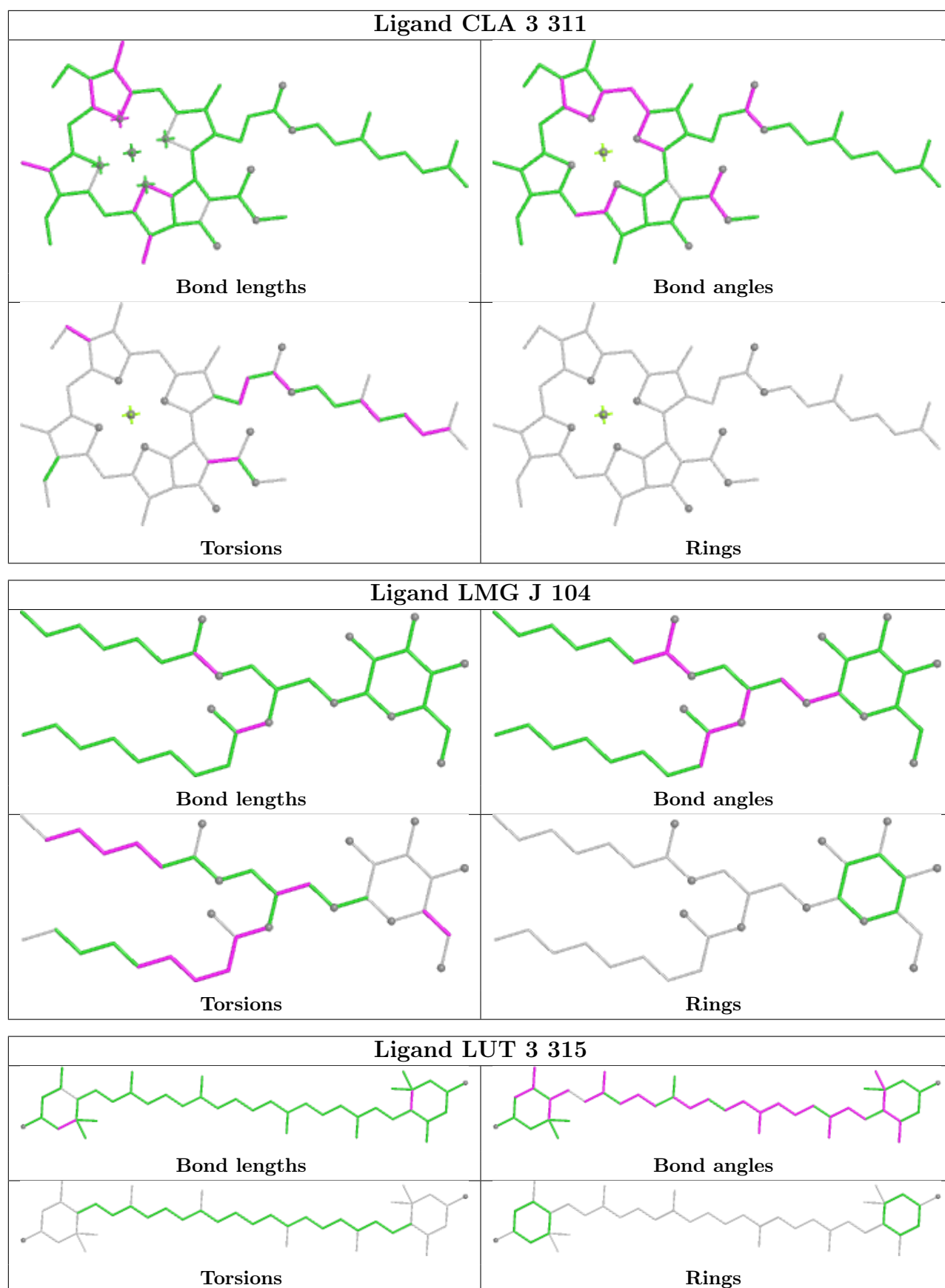
Bond angles

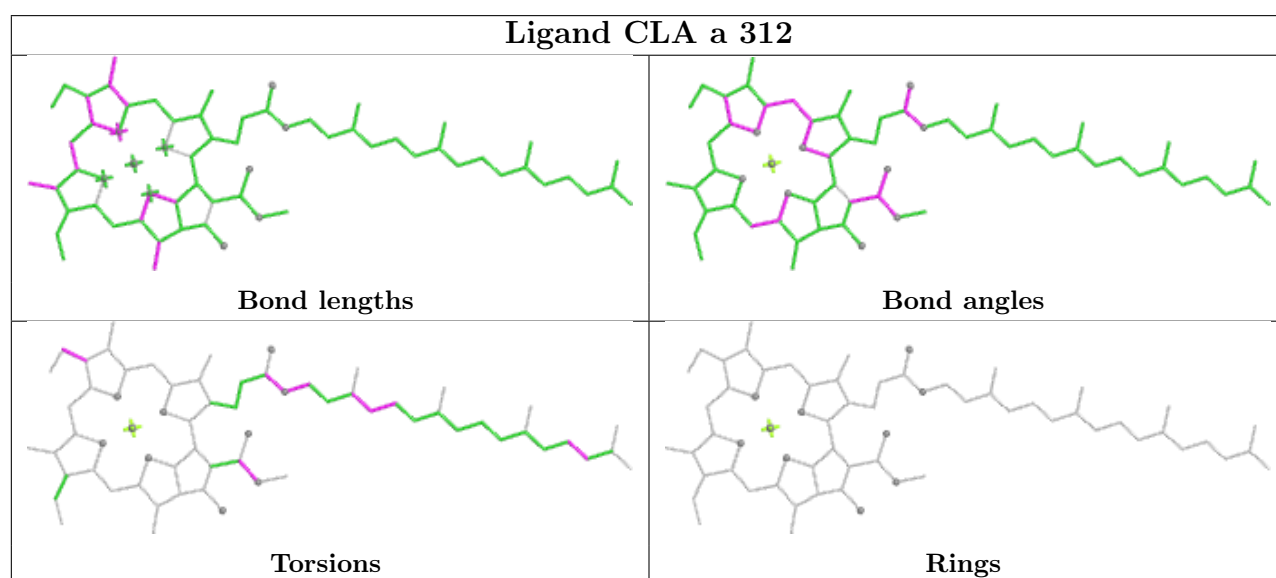
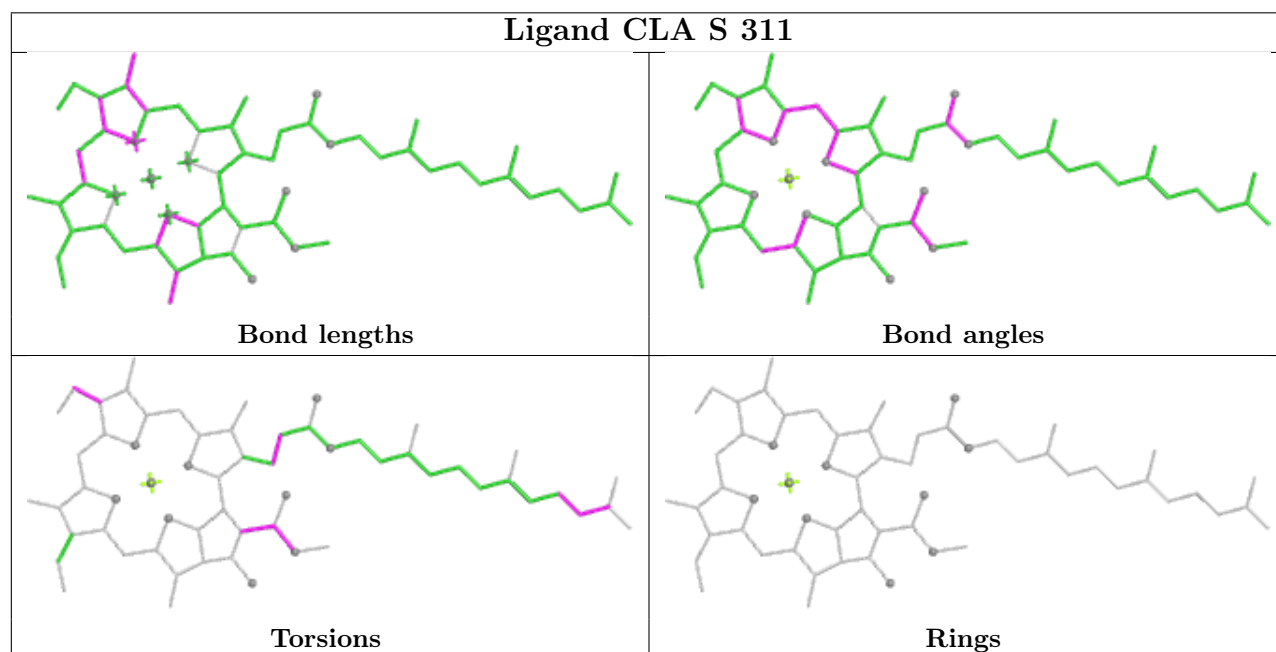
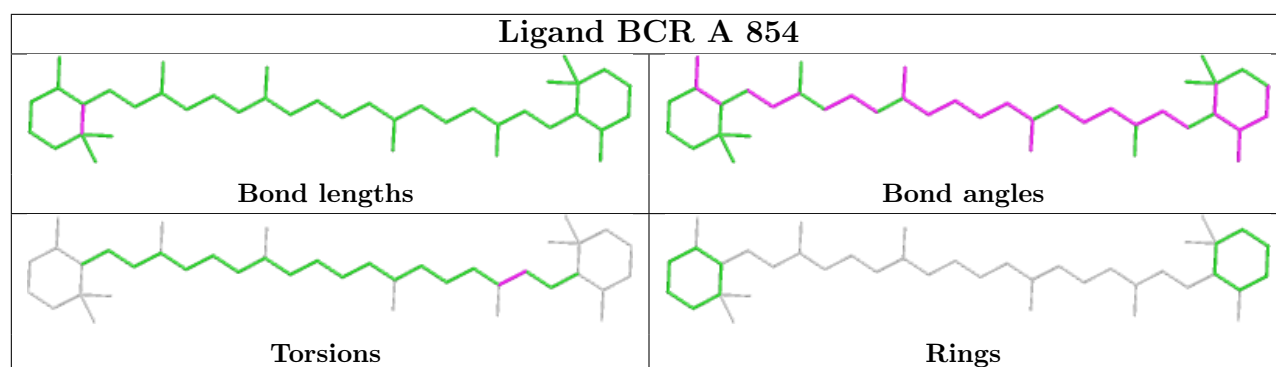


Torsions

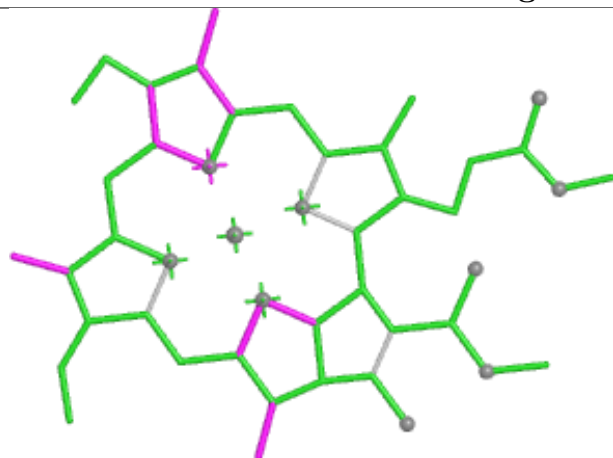


Rings

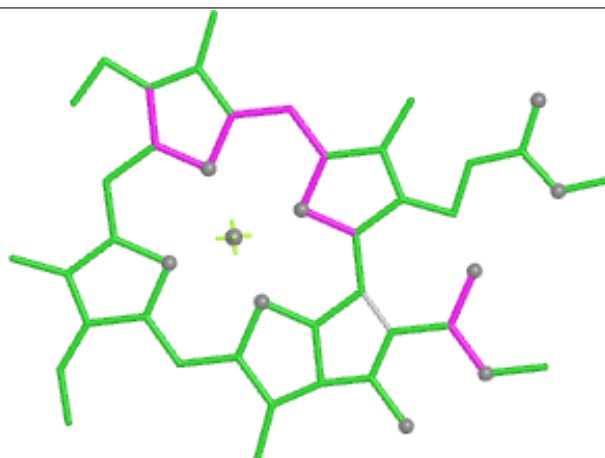




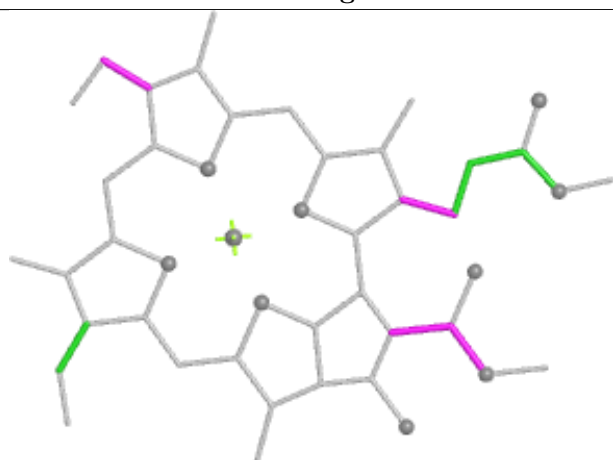
Ligand CLA 5 315



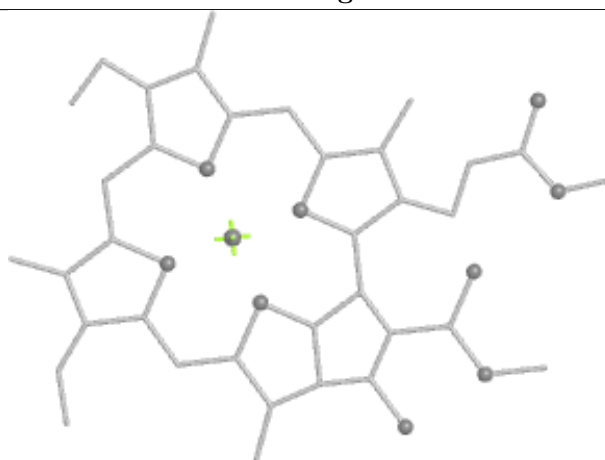
Bond lengths



Bond angles

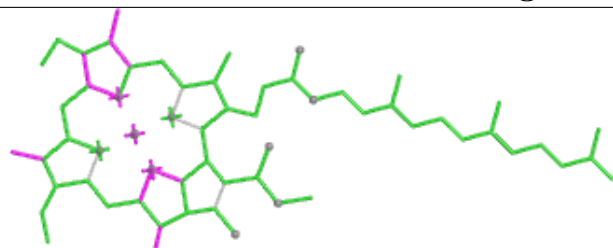


Torsions

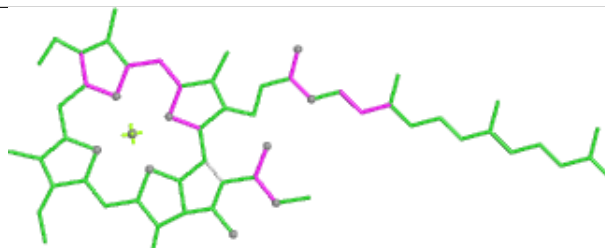


Rings

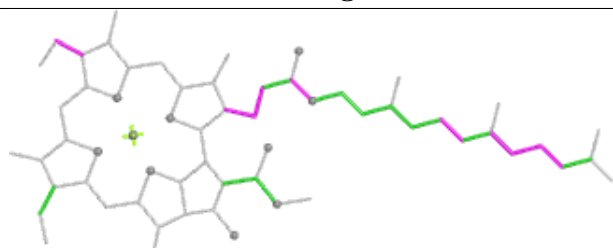
Ligand CLA 8 310



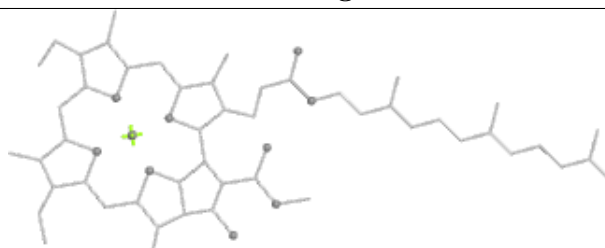
Bond lengths



Bond angles

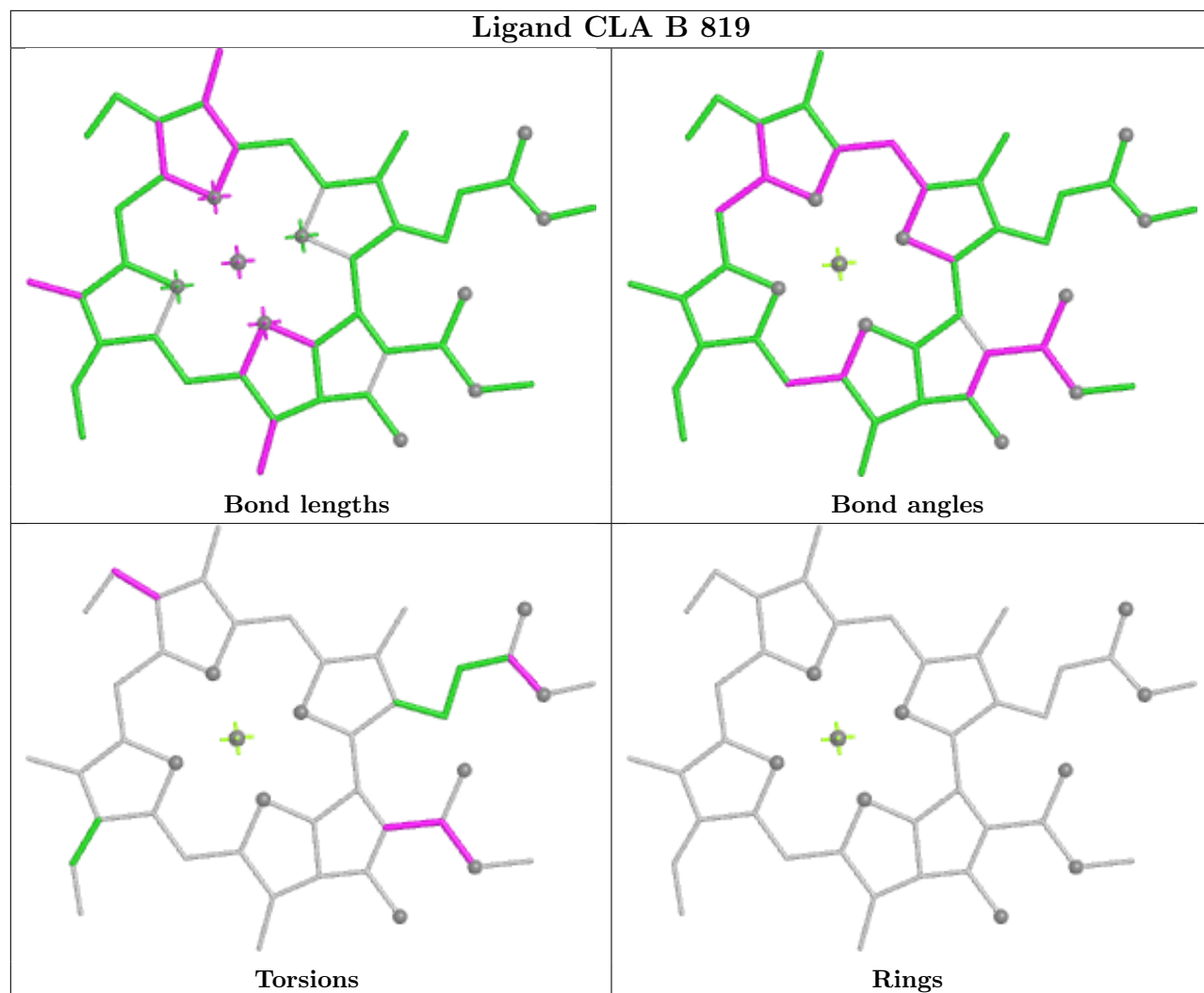


Torsions

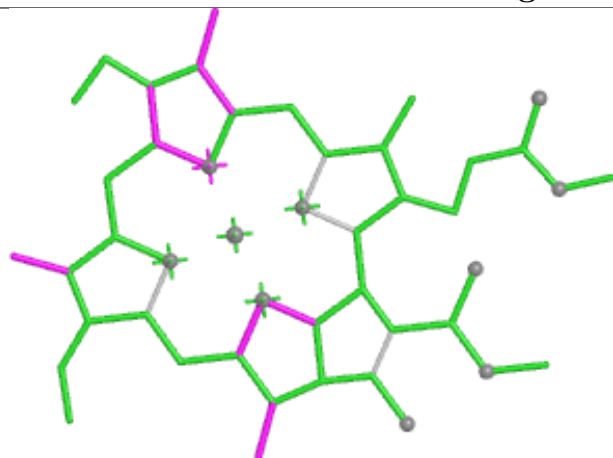


Rings

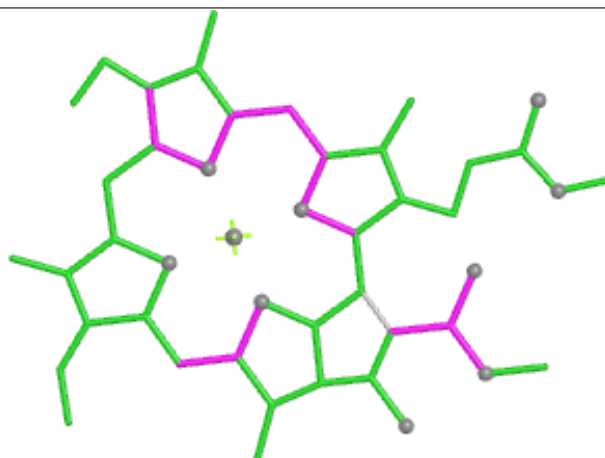
Ligand CLA B 819



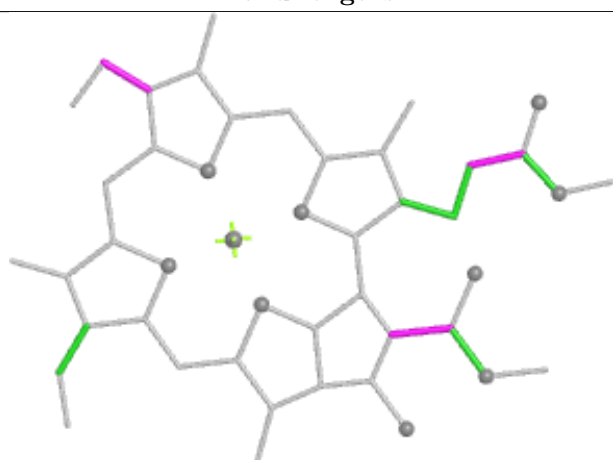
Ligand CLA 6 616



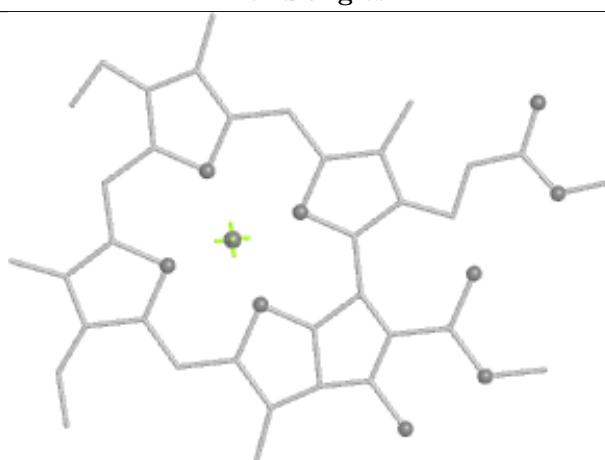
Bond lengths



Bond angles

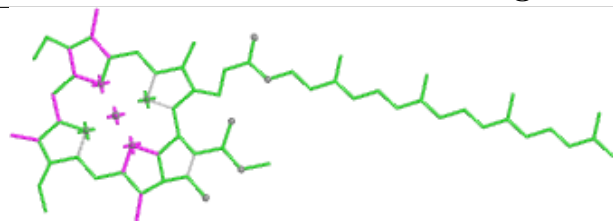


Torsions

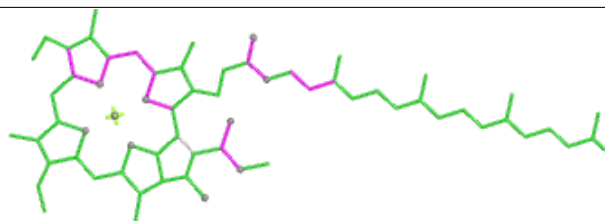


Rings

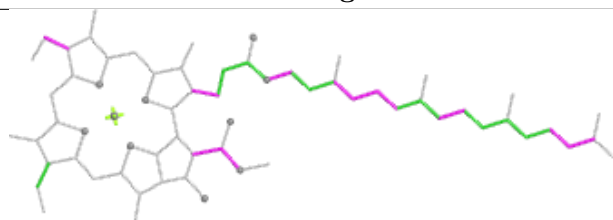
Ligand CLA A 853



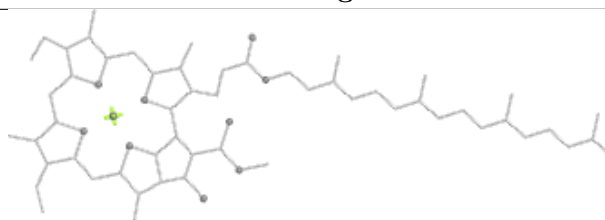
Bond lengths



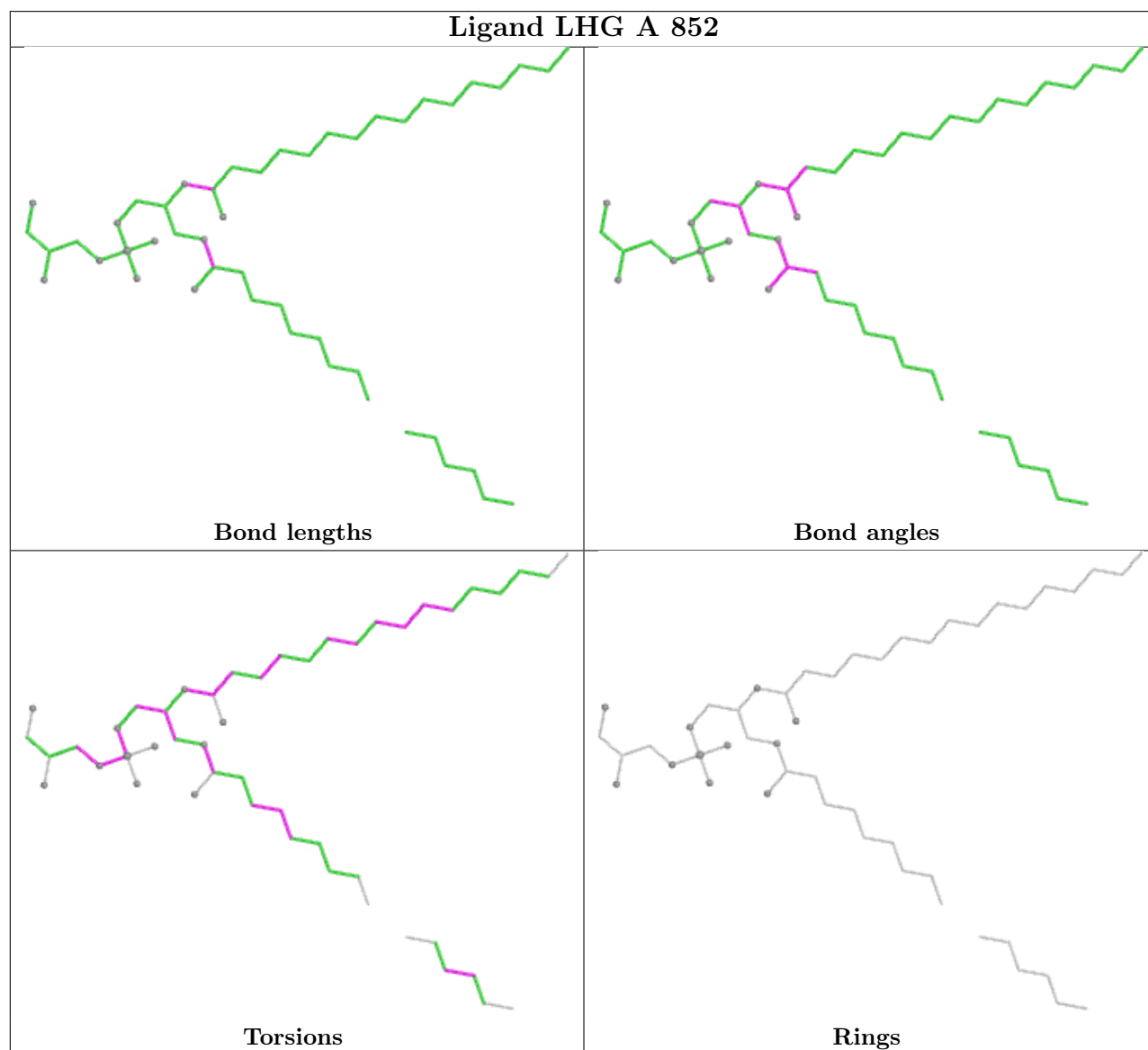
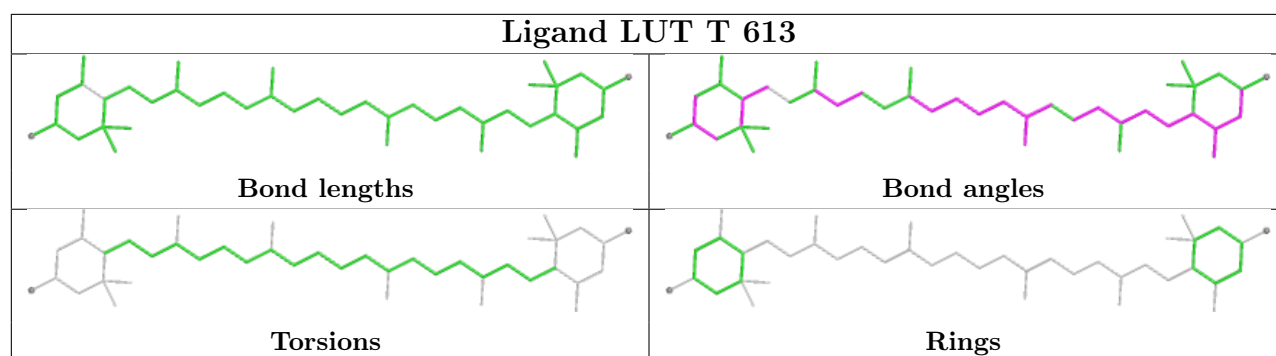
Bond angles

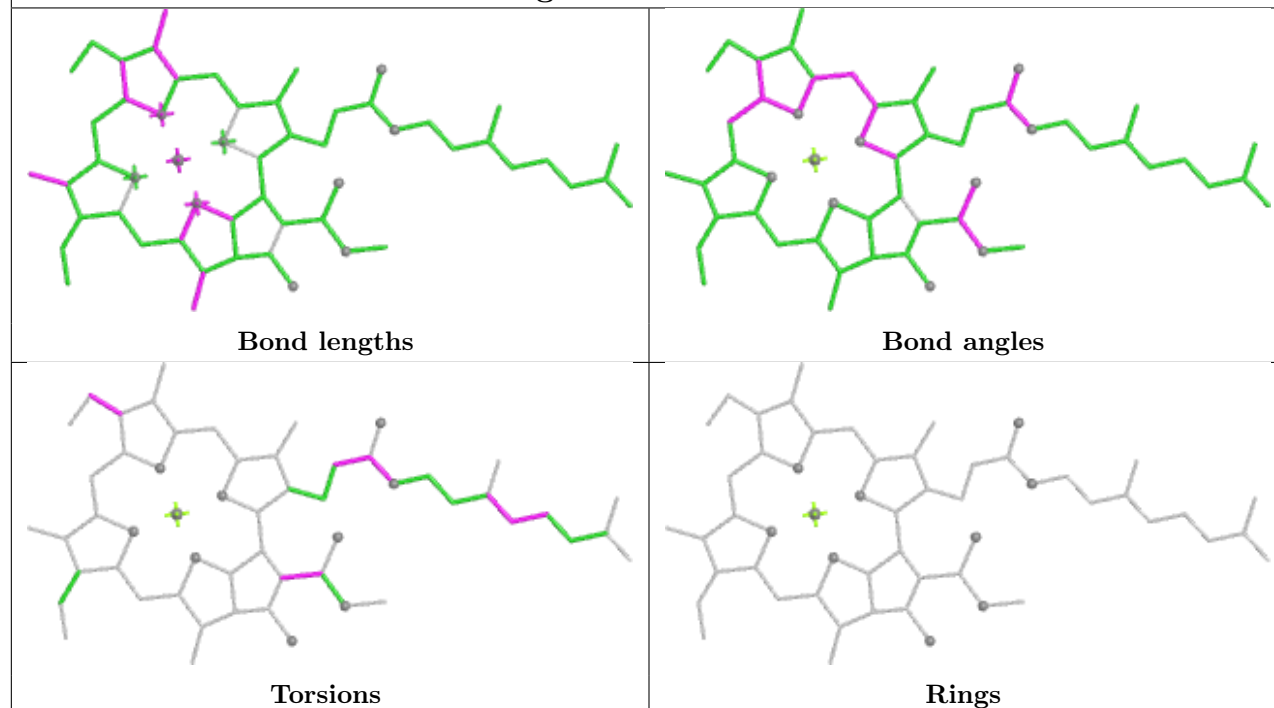
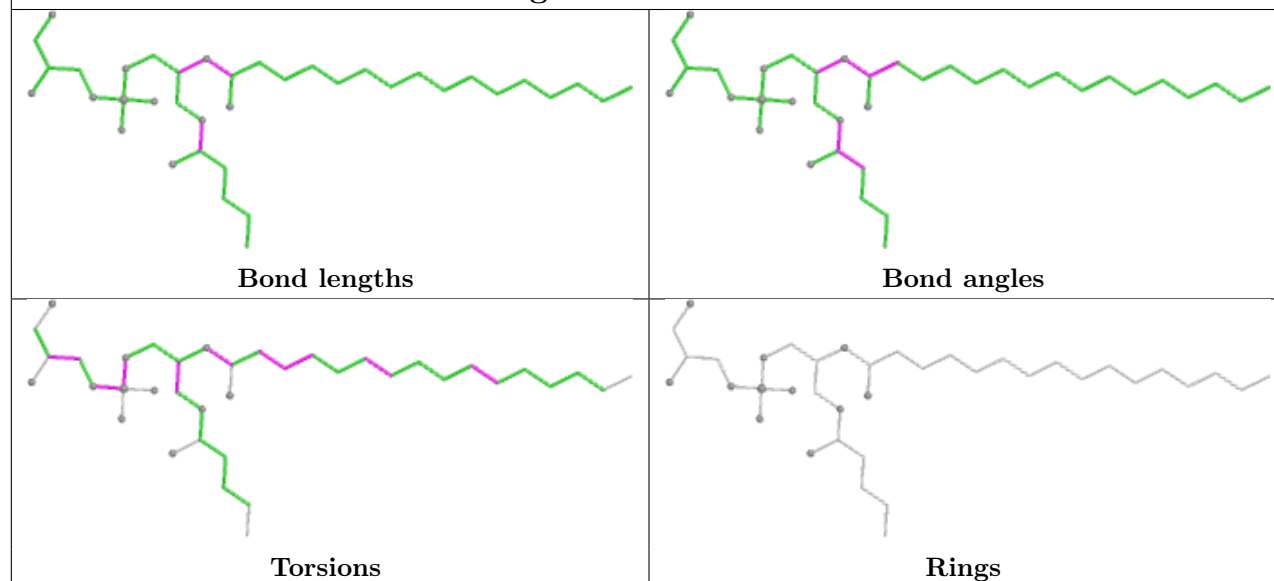


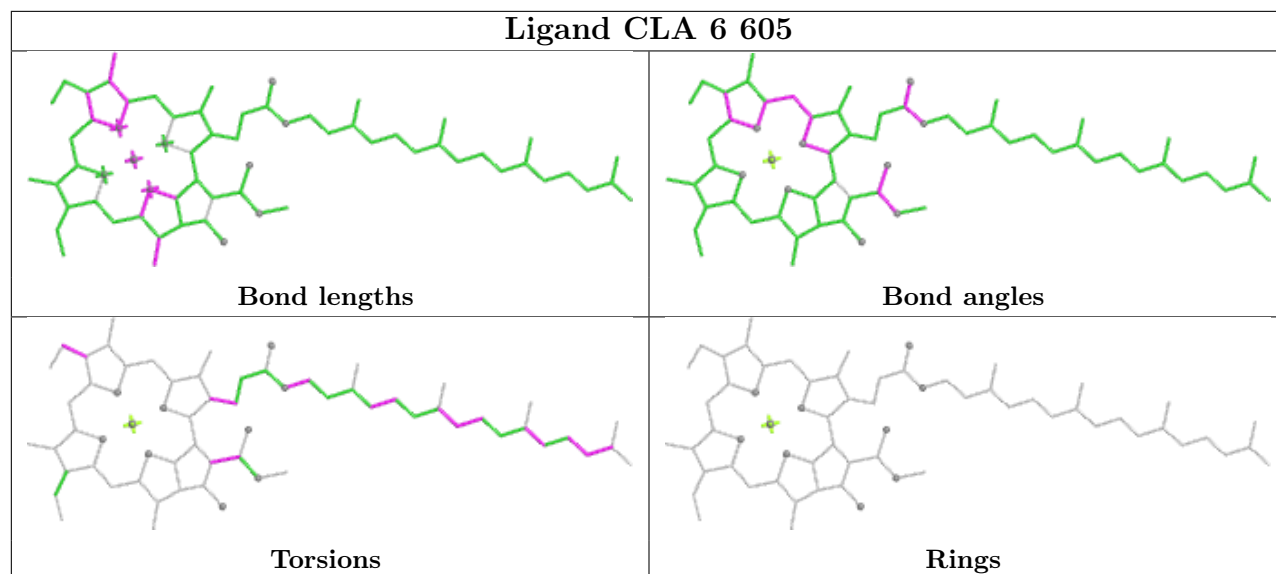
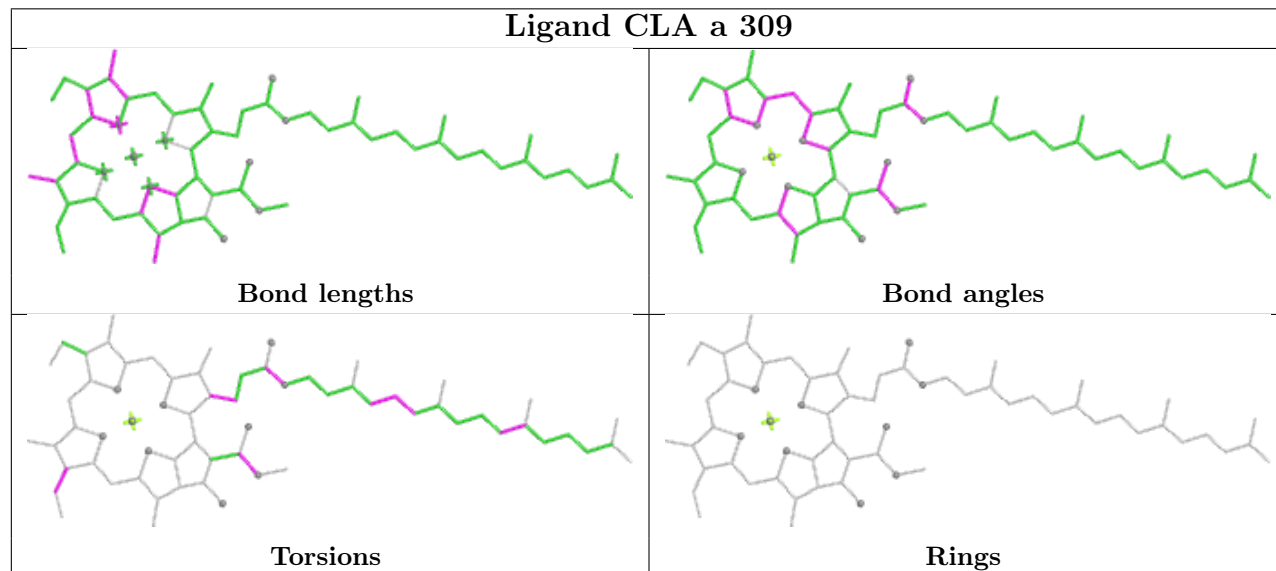
Torsions

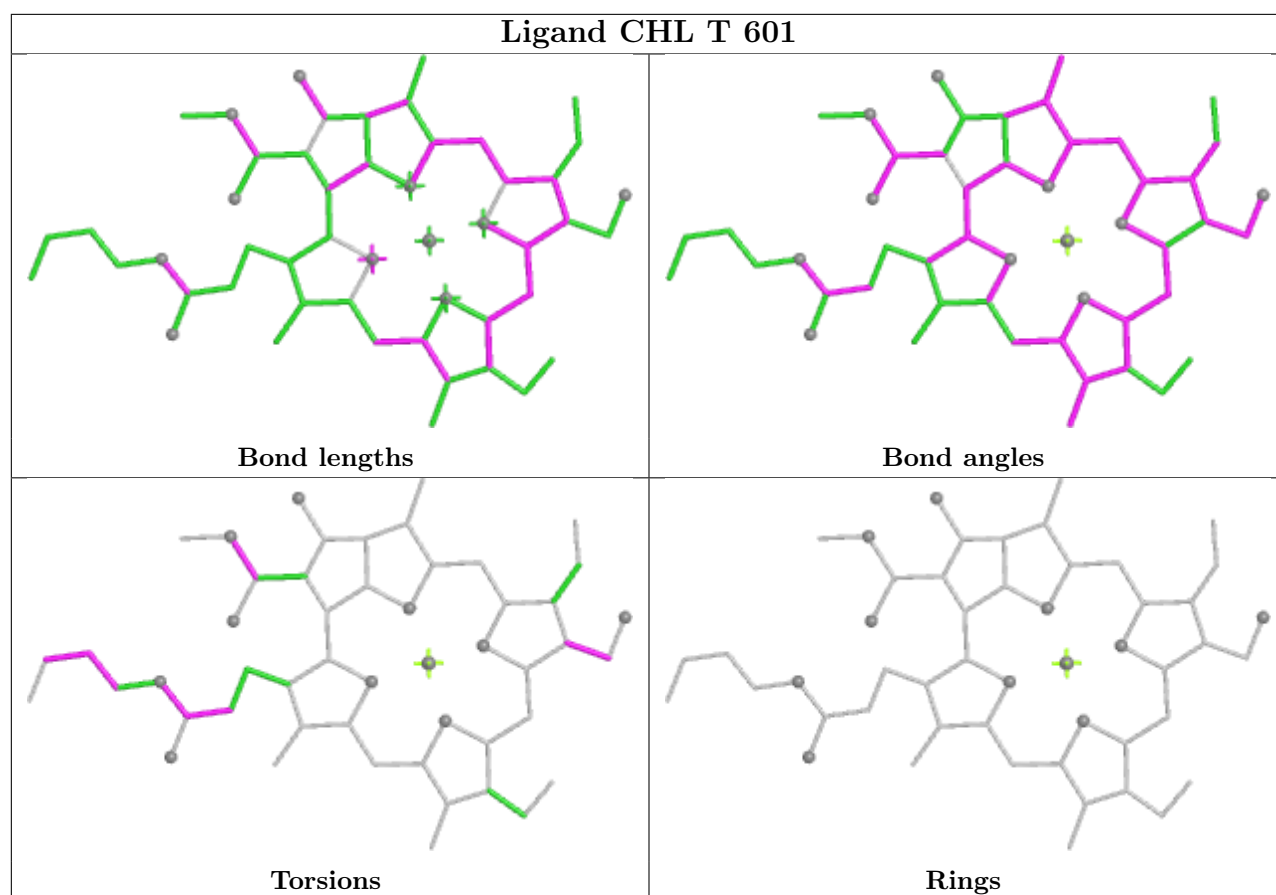


Rings

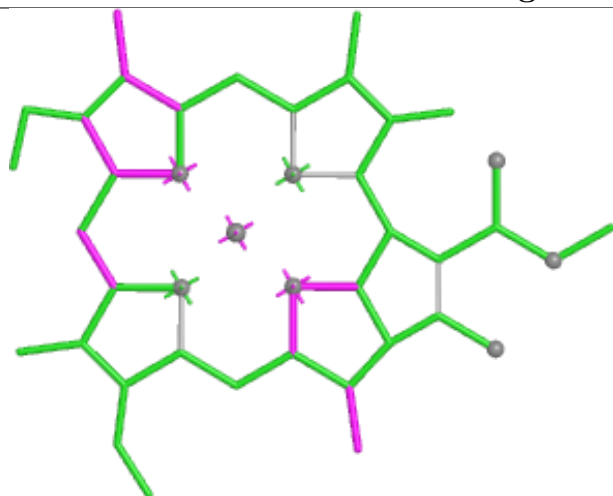


Ligand CLA 5 311**Ligand LHG A 844**

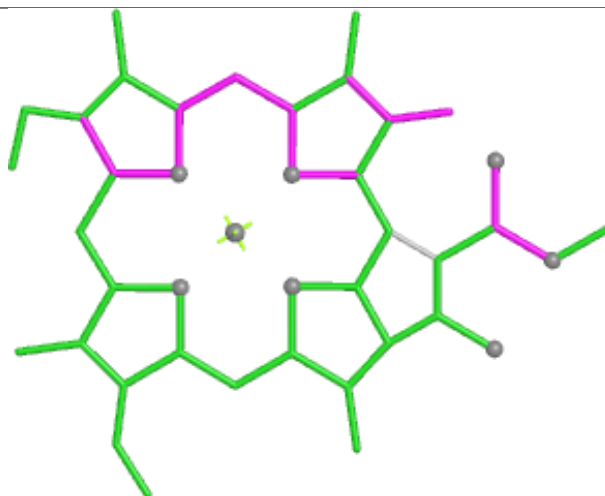
Ligand CLA 6 605**Ligand CLA a 309**



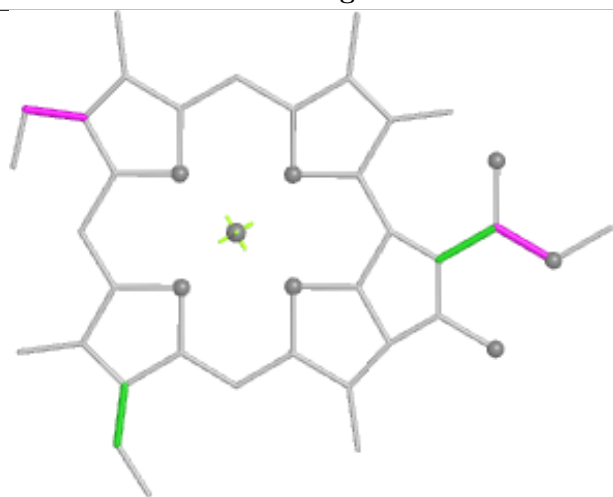
Ligand CLA 2 310



Bond lengths



Bond angles

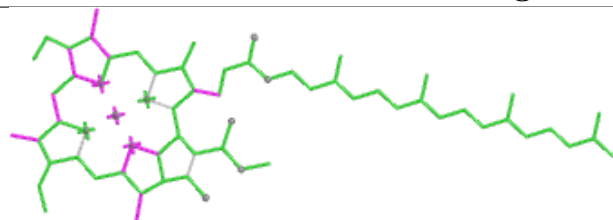


Torsions

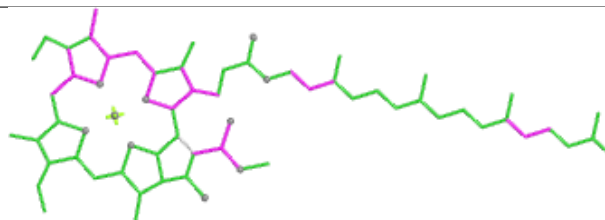


Rings

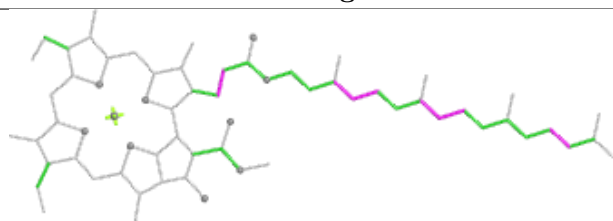
Ligand CLA A 802



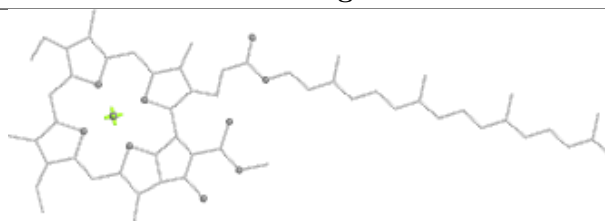
Bond lengths



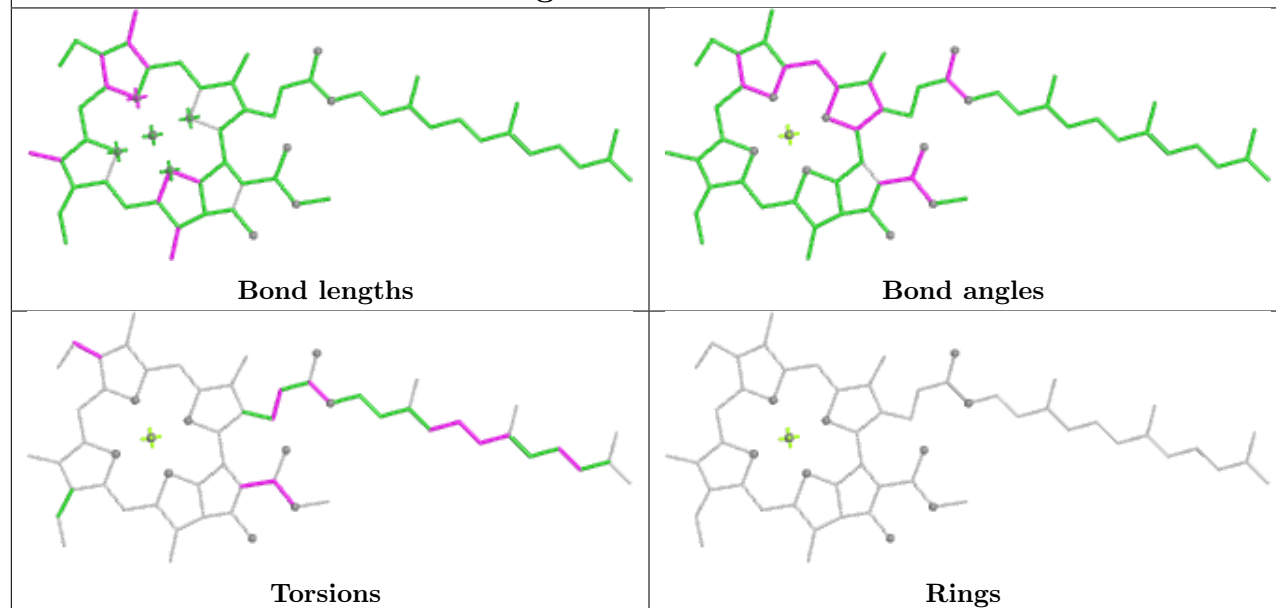
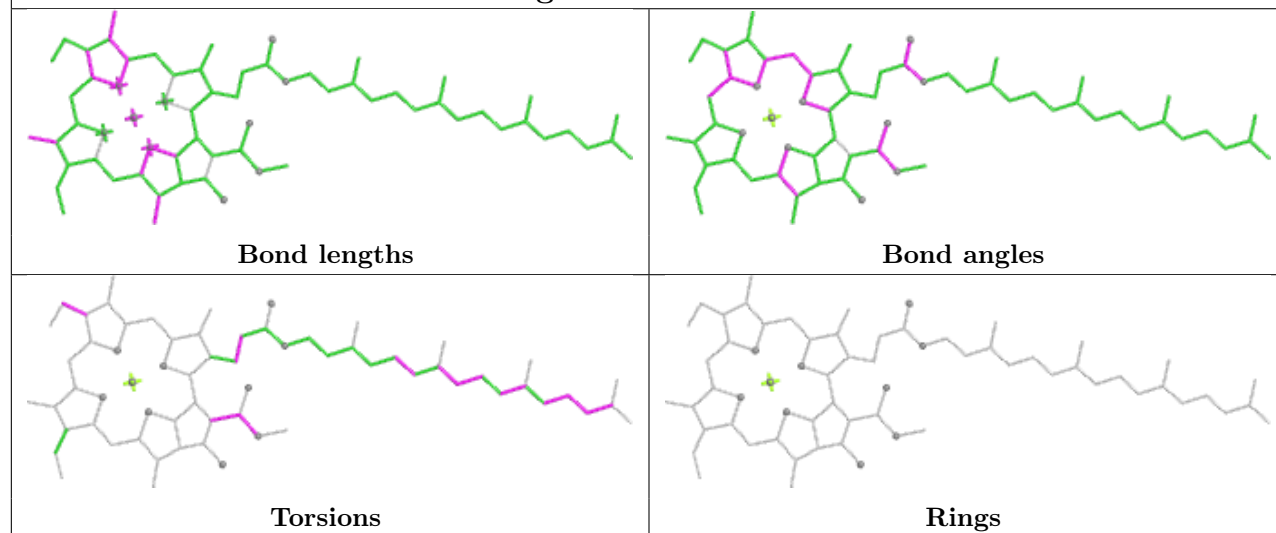
Bond angles



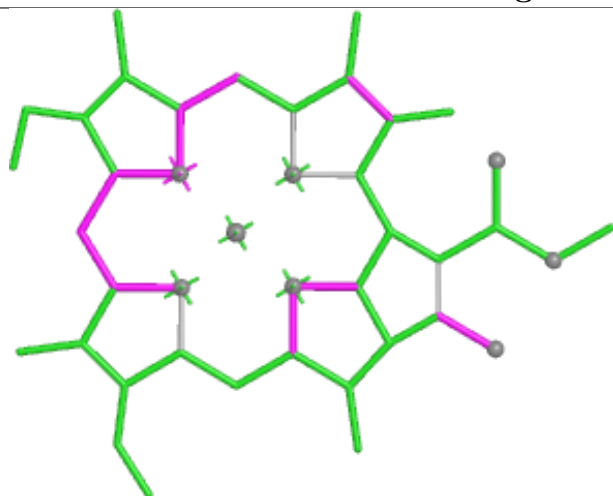
Torsions



Rings

Ligand CLA 6 623**Ligand CLA 7 301**

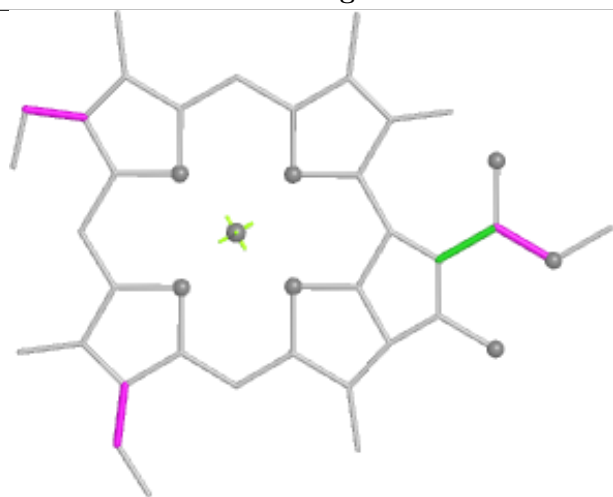
Ligand CLA P 611



Bond lengths



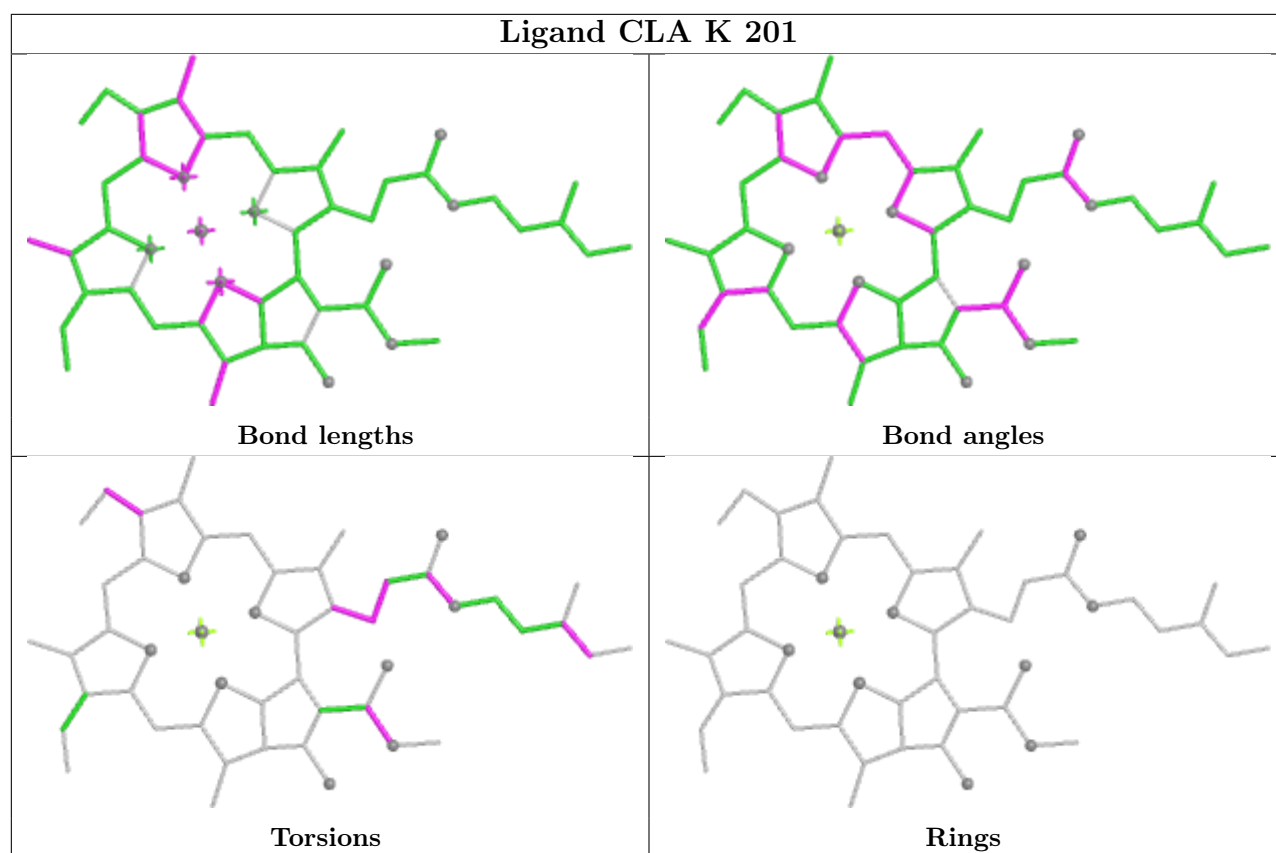
Bond angles



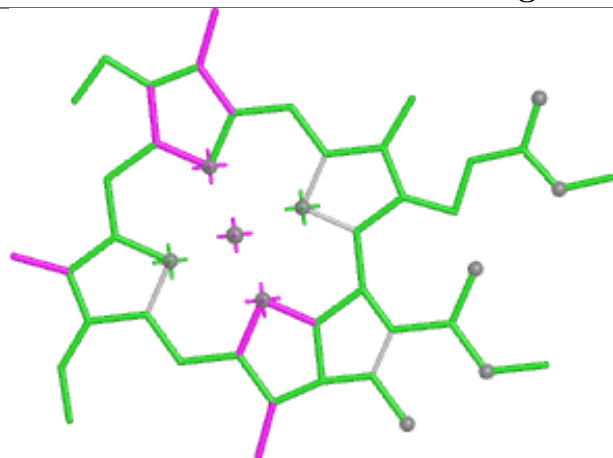
Torsions



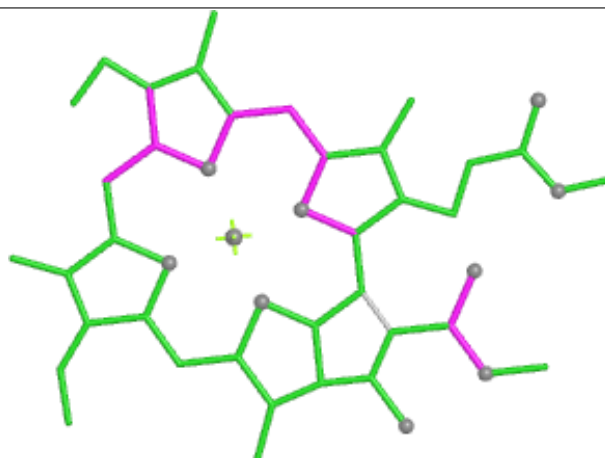
Rings



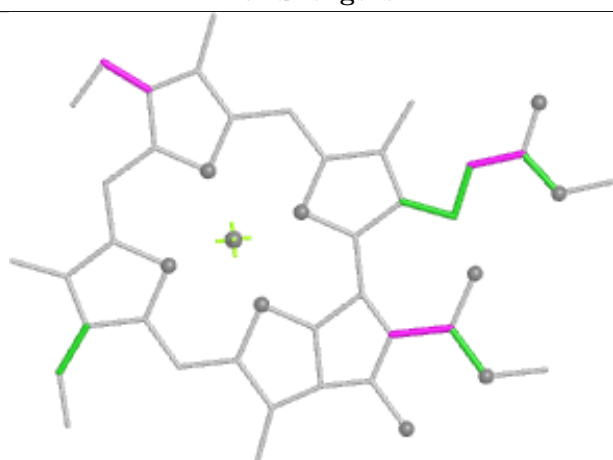
Ligand CLA 1 614



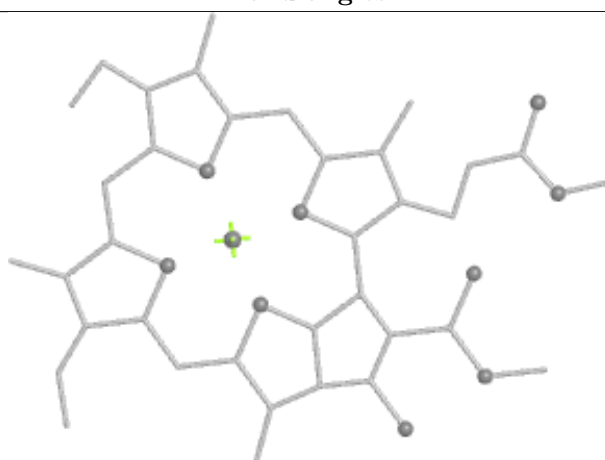
Bond lengths



Bond angles

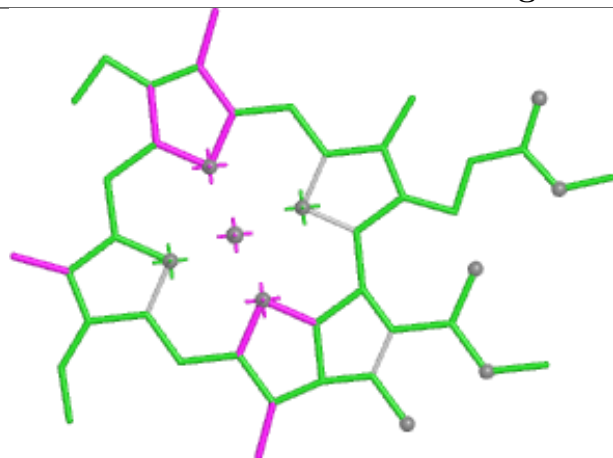


Torsions

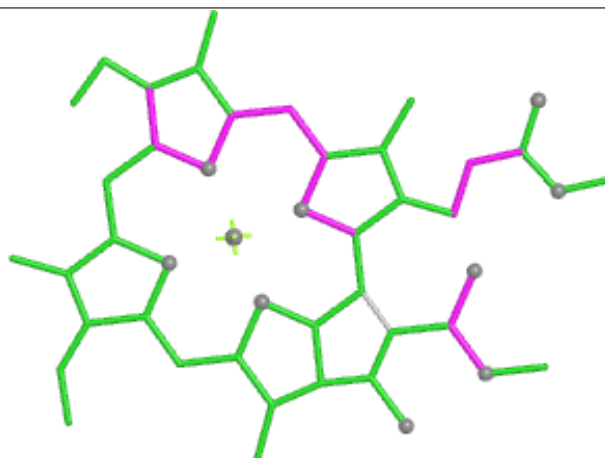


Rings

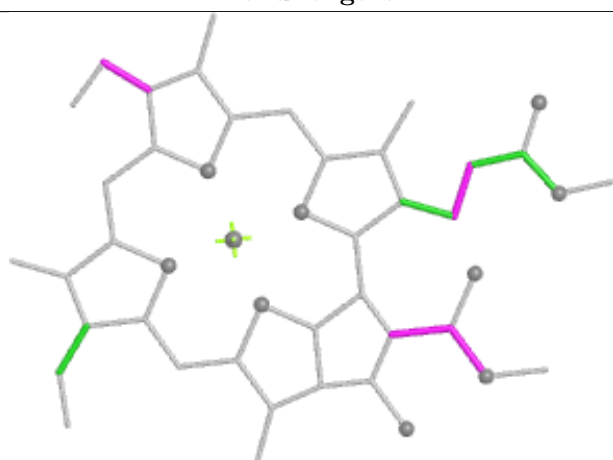
Ligand CLA 6 604



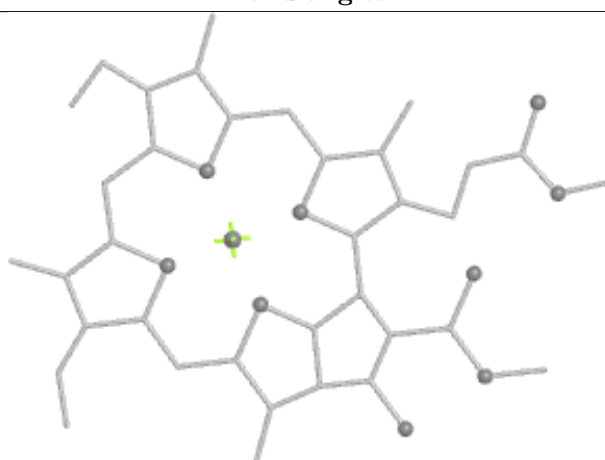
Bond lengths



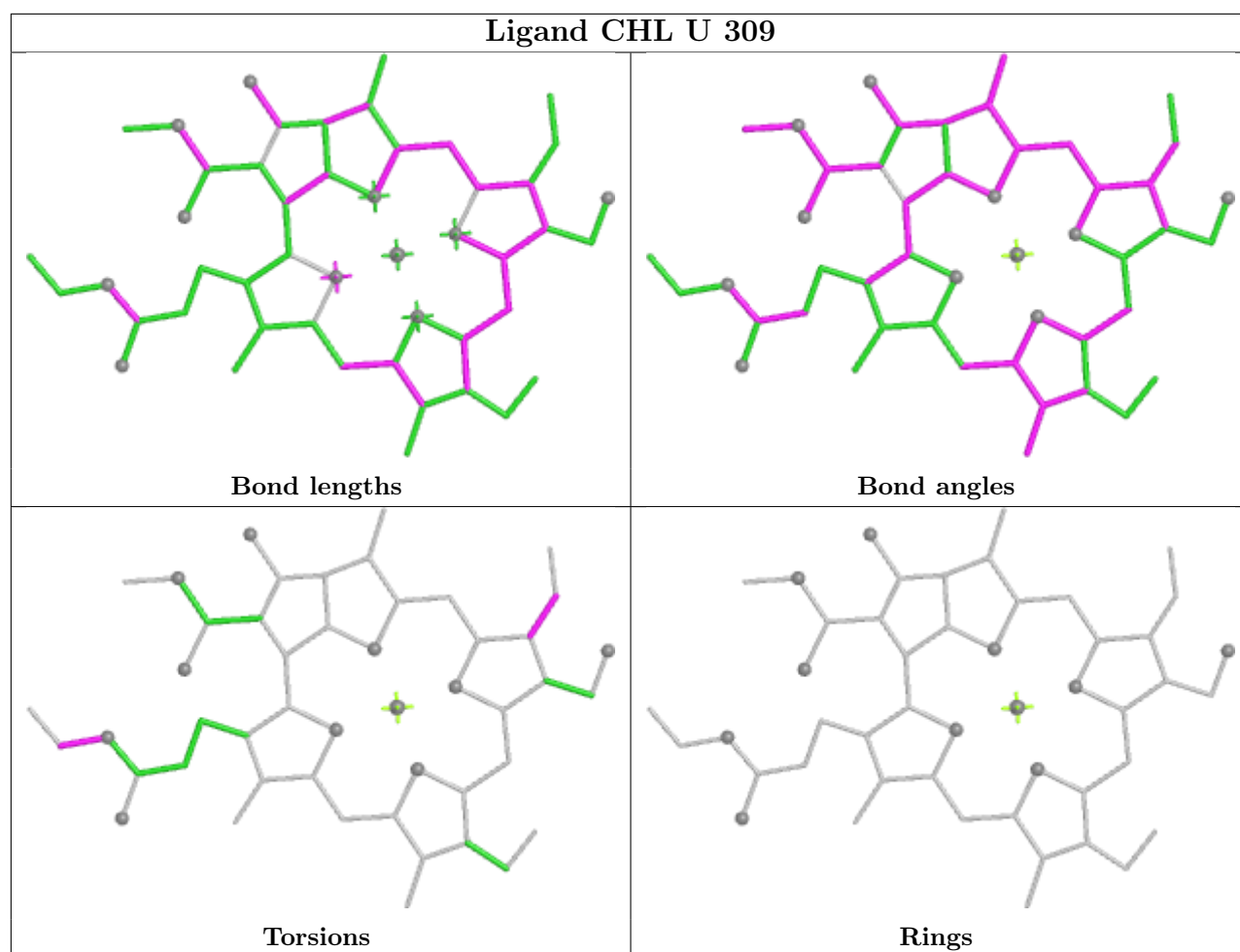
Bond angles



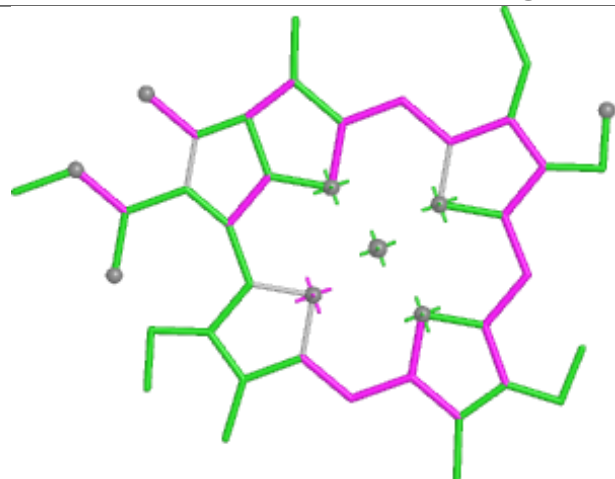
Torsions



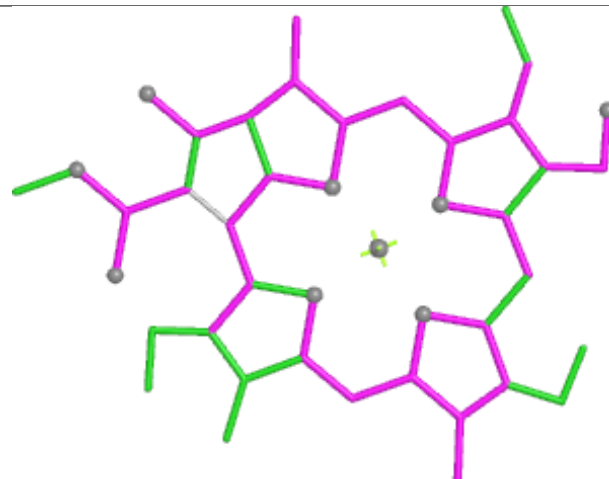
Rings



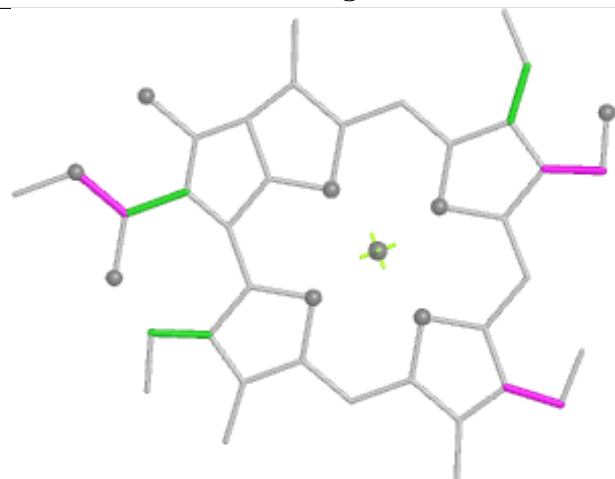
Ligand CHL 6 617



Bond lengths



Bond angles

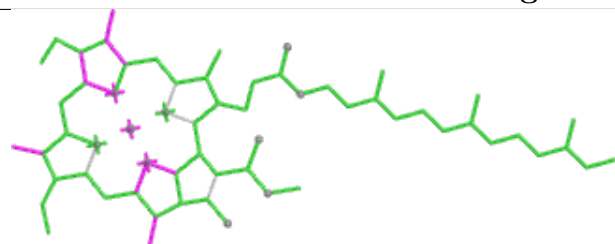


Torsions

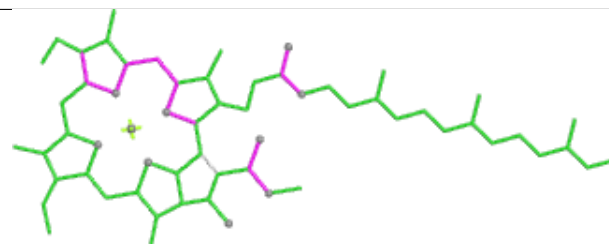


Rings

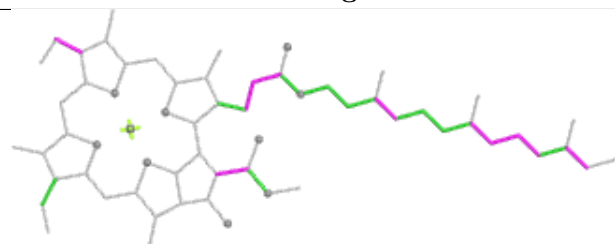
Ligand CLA 6 601



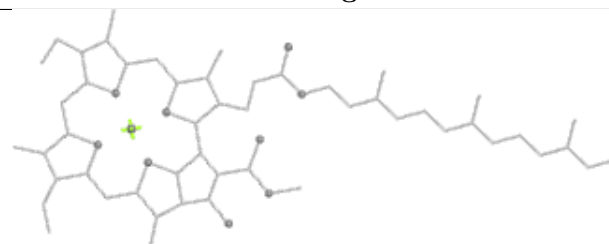
Bond lengths



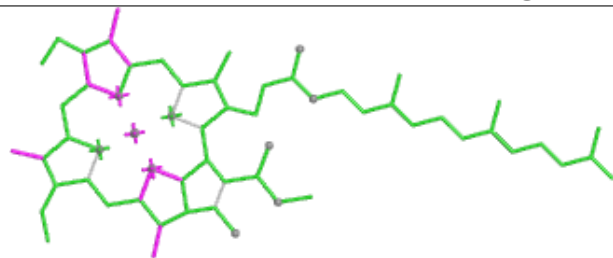
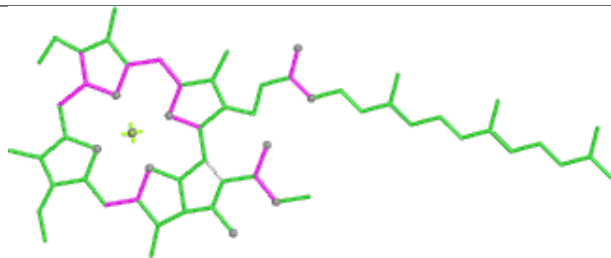
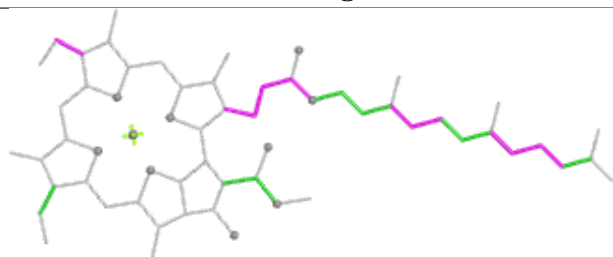
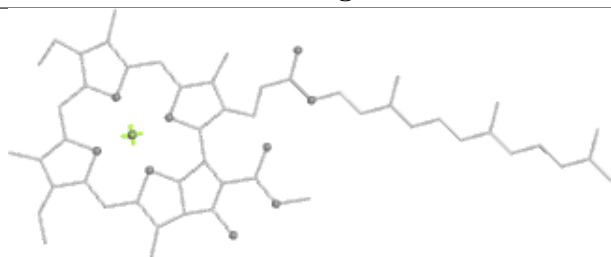
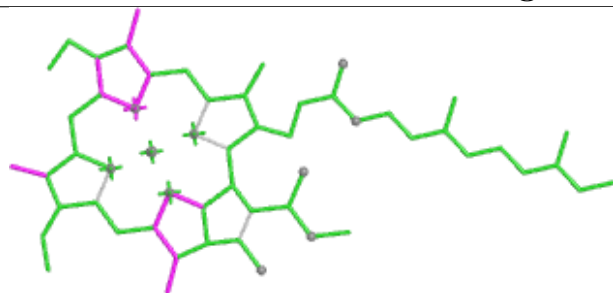
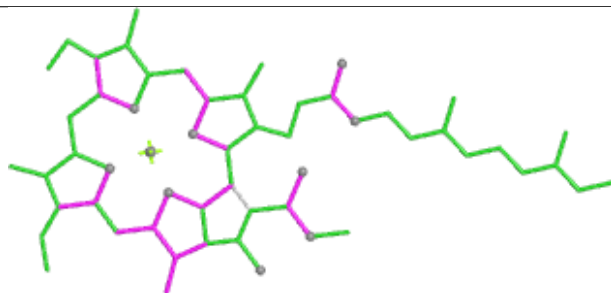
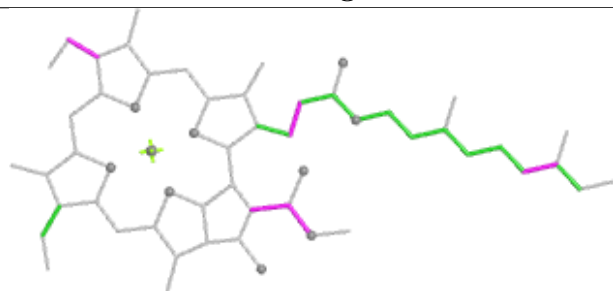
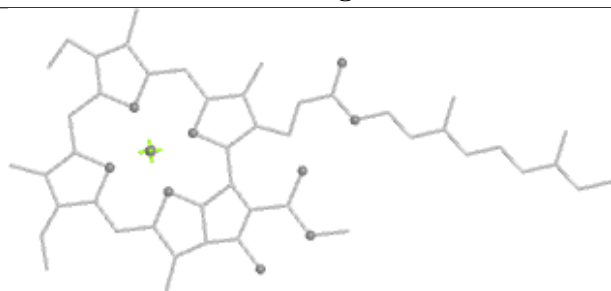
Bond angles



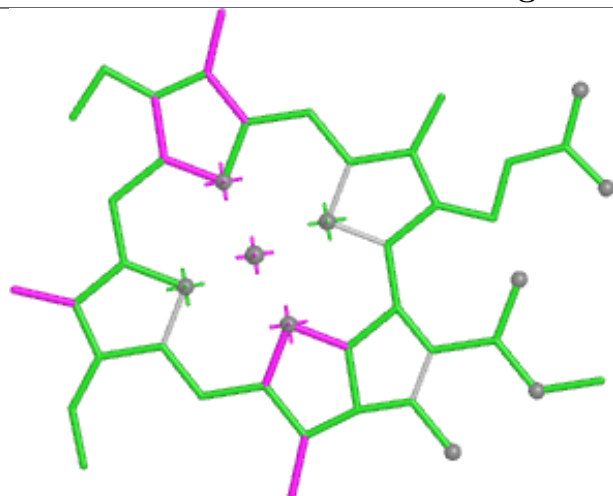
Torsions



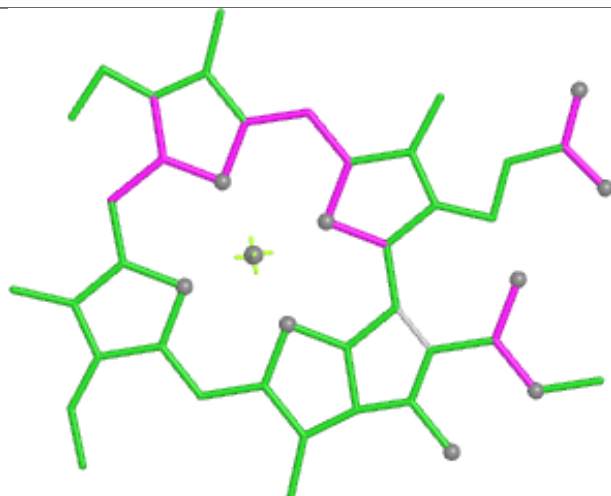
Rings

Ligand CLA 3 305**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 5 313****Bond lengths****Bond angles****Torsions****Rings**

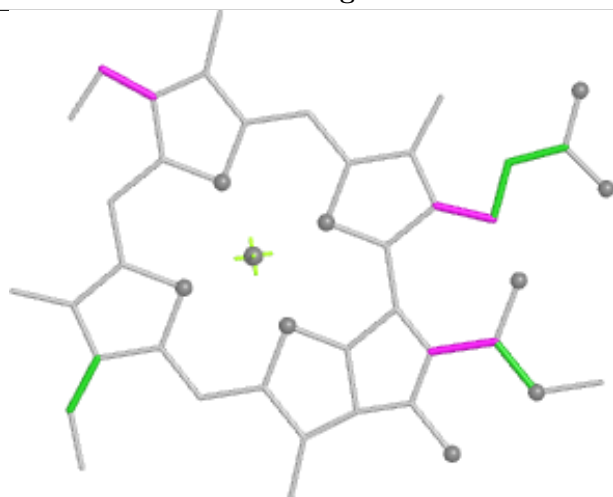
Ligand CLA 6 620



Bond lengths



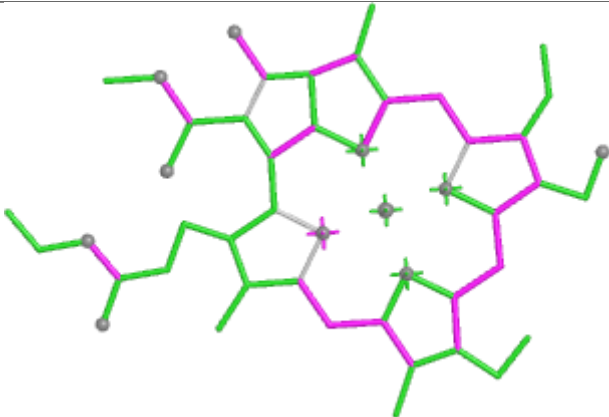
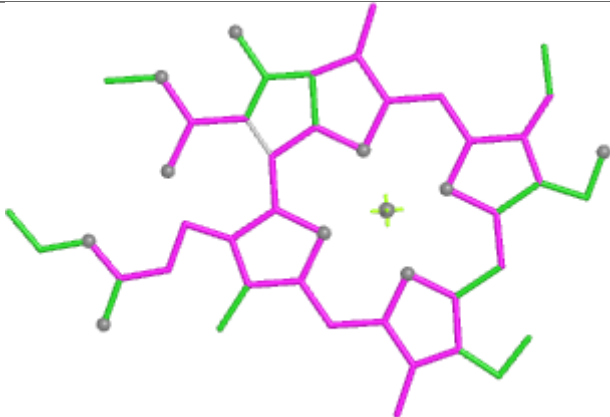
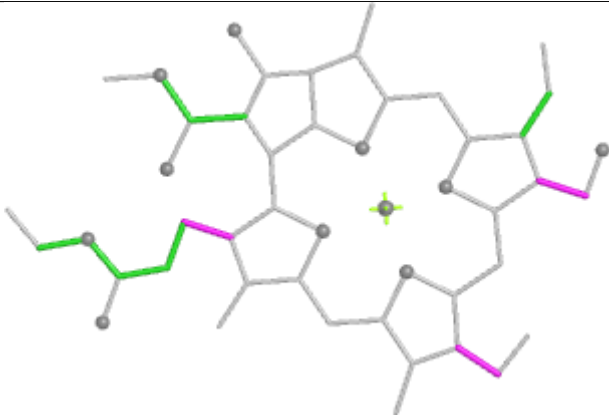
Bond angles

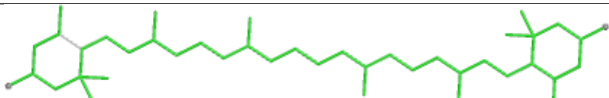
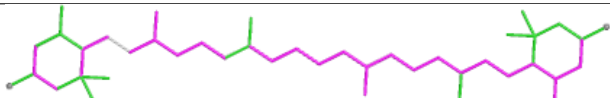
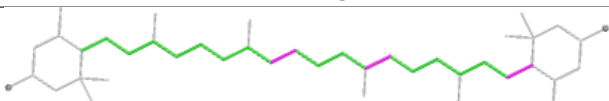


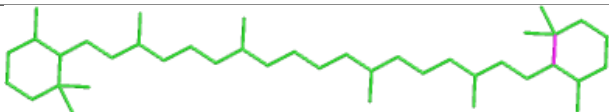
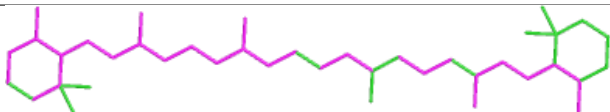
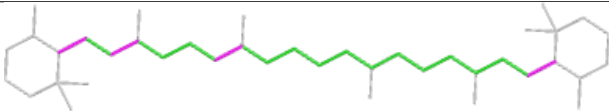
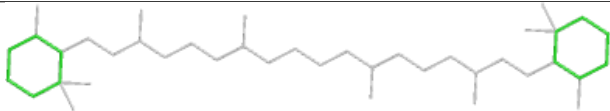
Torsions

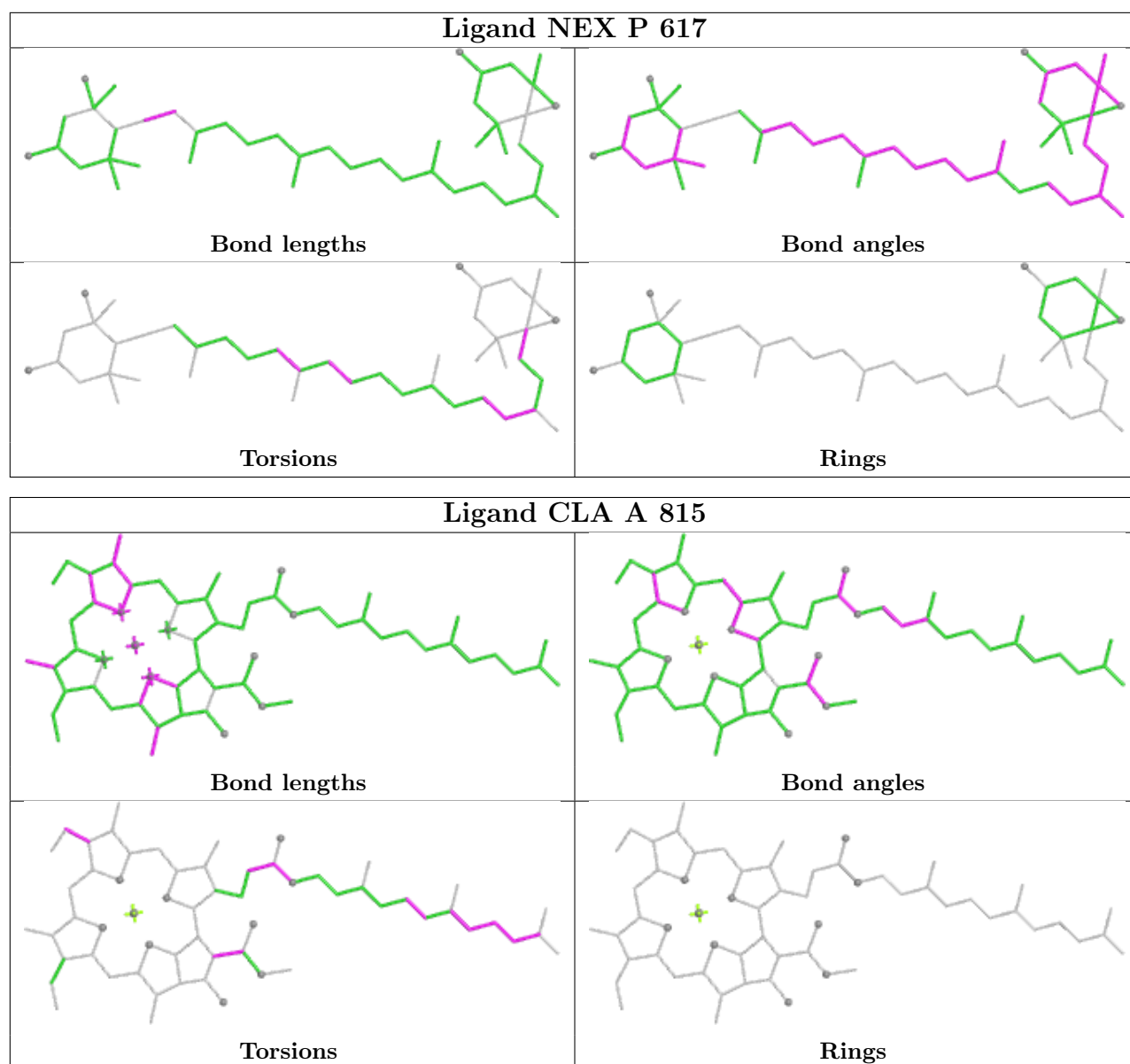


Rings

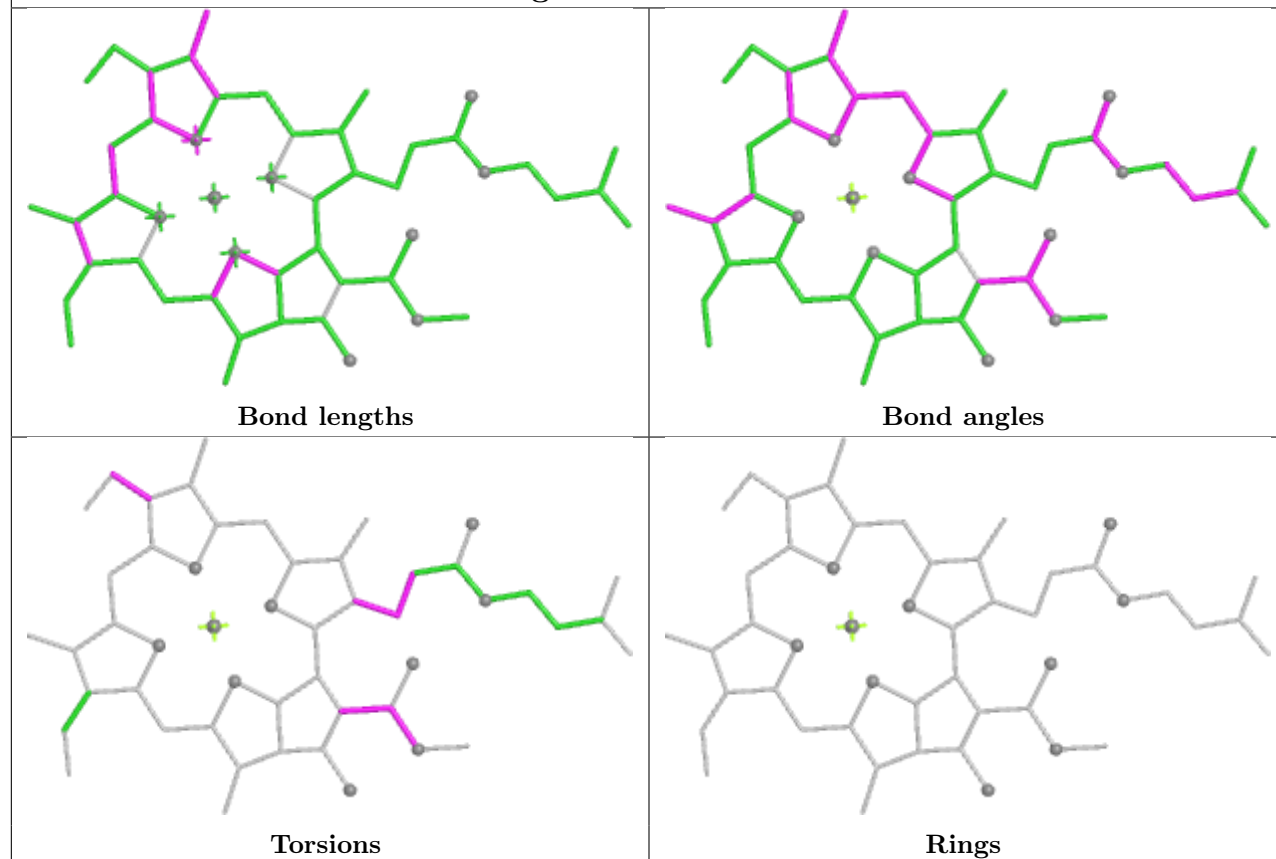
Ligand CHL T 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT S 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

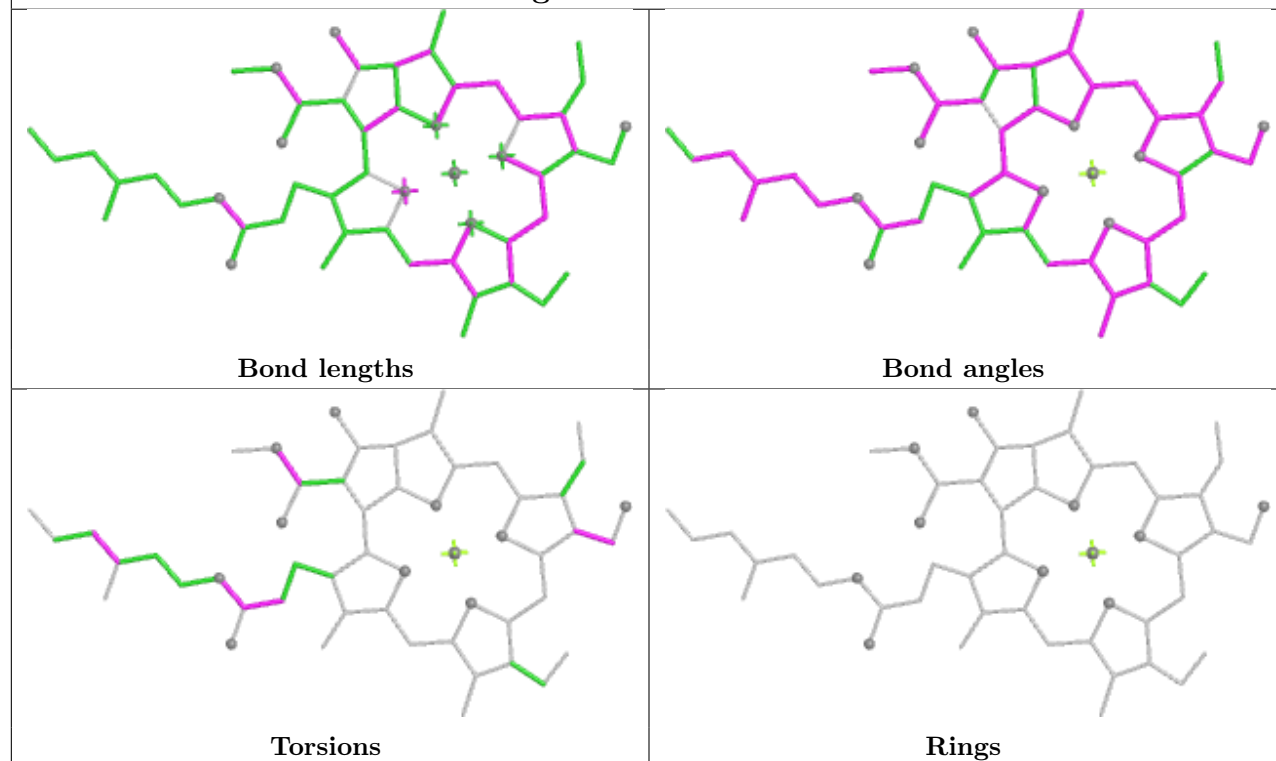
Ligand BCR 6 621	
	
Bond lengths	Bond angles
	
Torsions	Rings



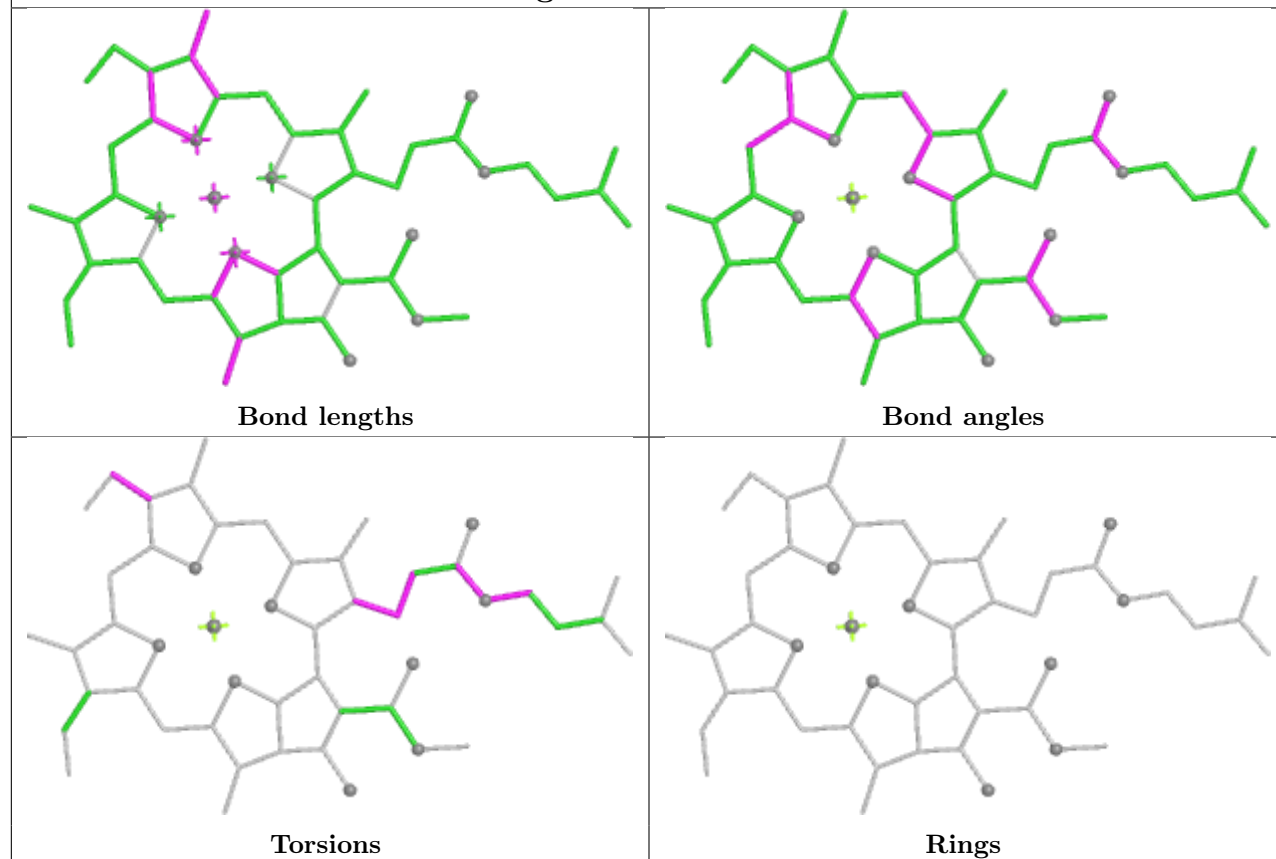
Ligand CLA R 604



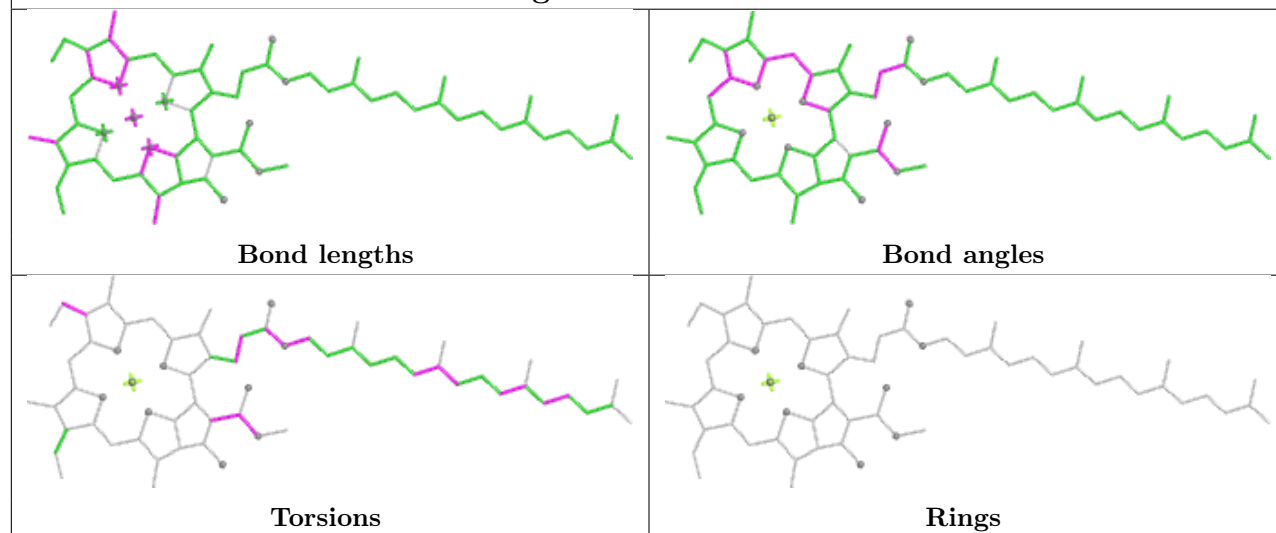
Ligand CHL P 622

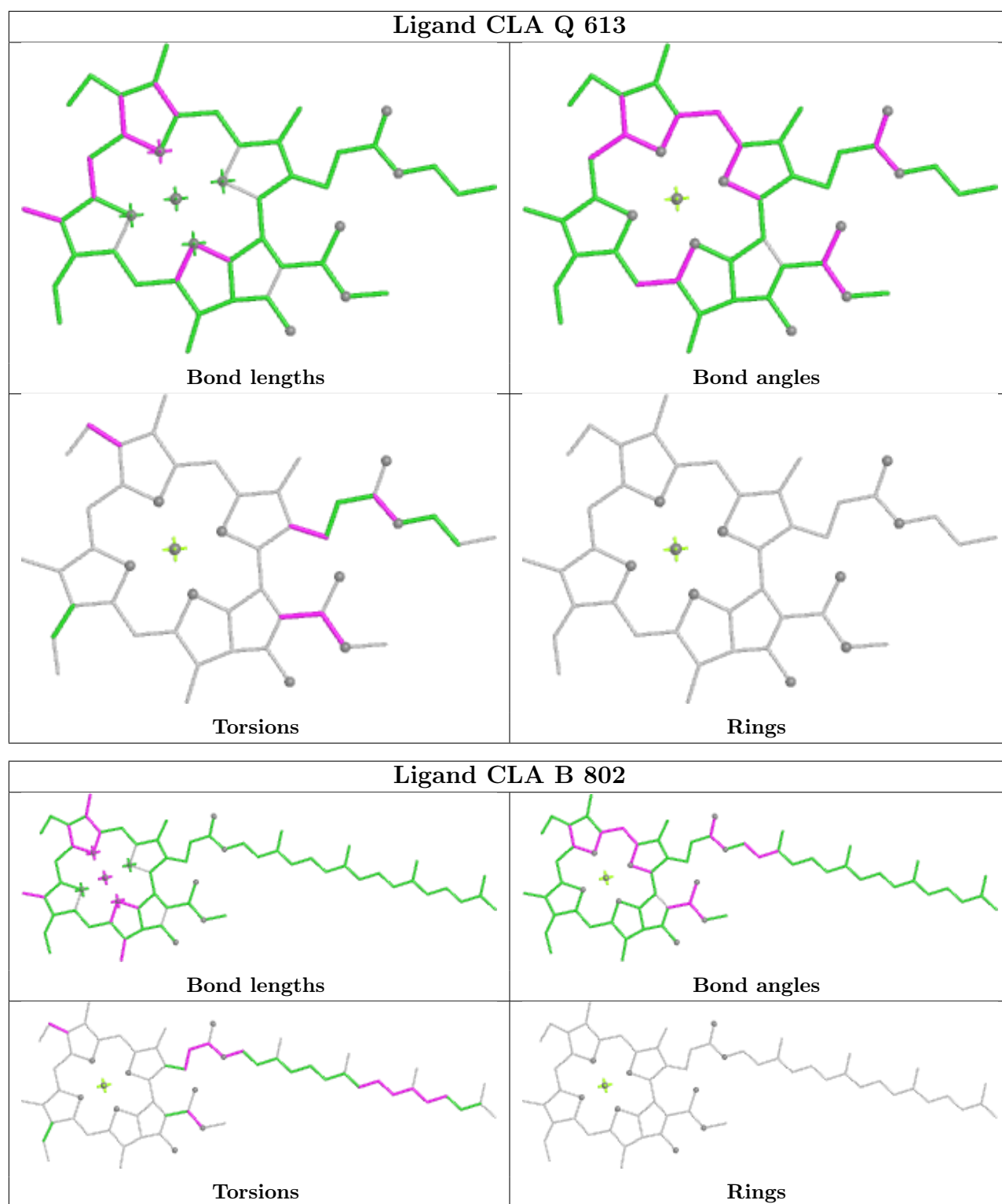


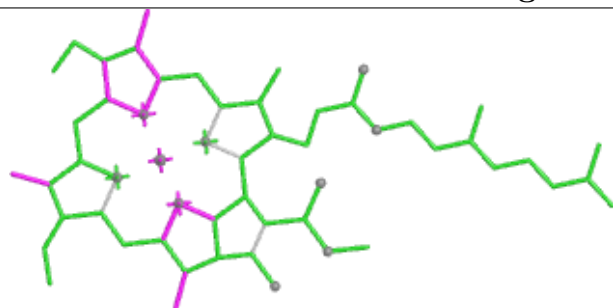
Ligand CLA 2 307



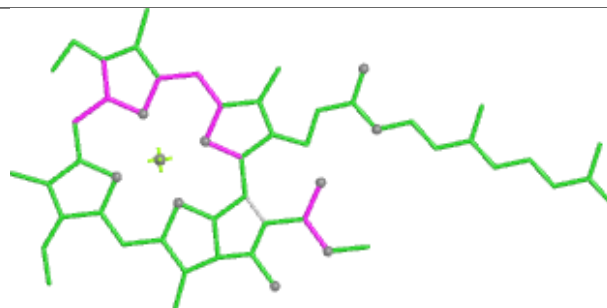
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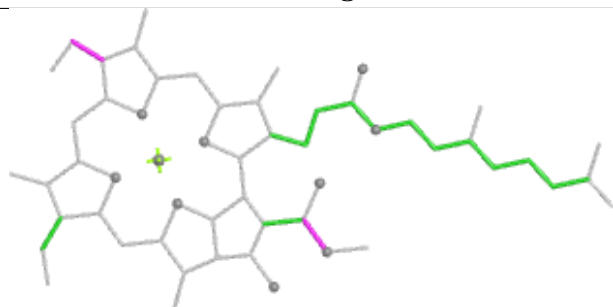


Ligand CLA 5 306

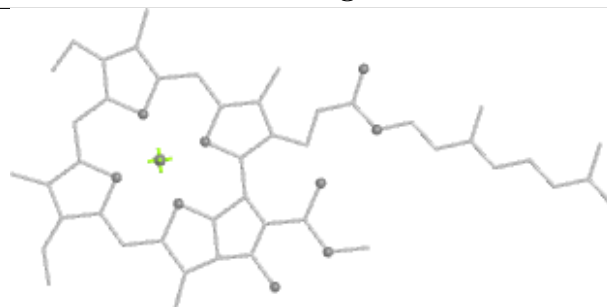
Bond lengths



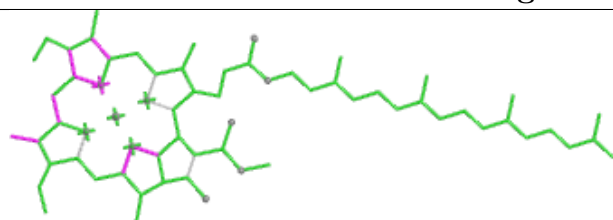
Bond angles



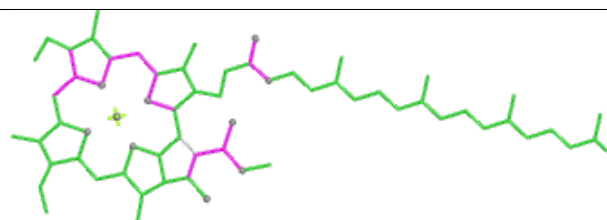
Torsions



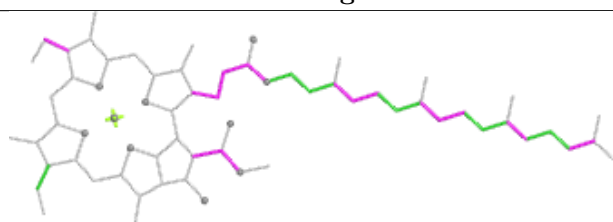
Rings

Ligand CLA S 314

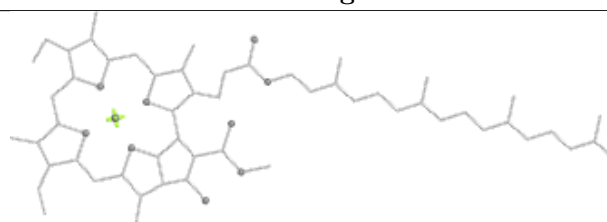
Bond lengths



Bond angles

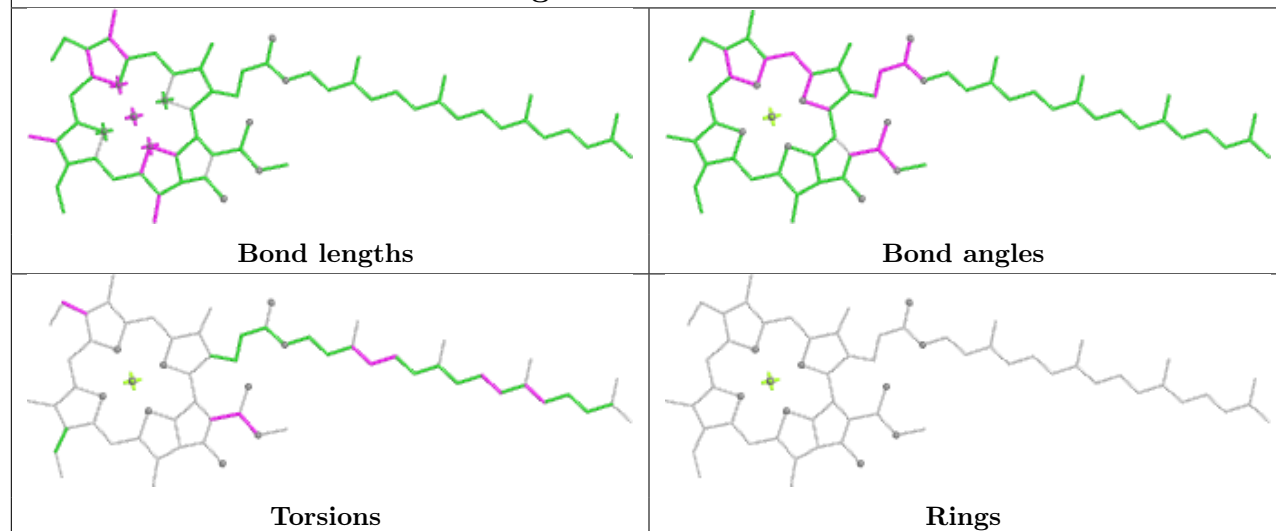


Torsions

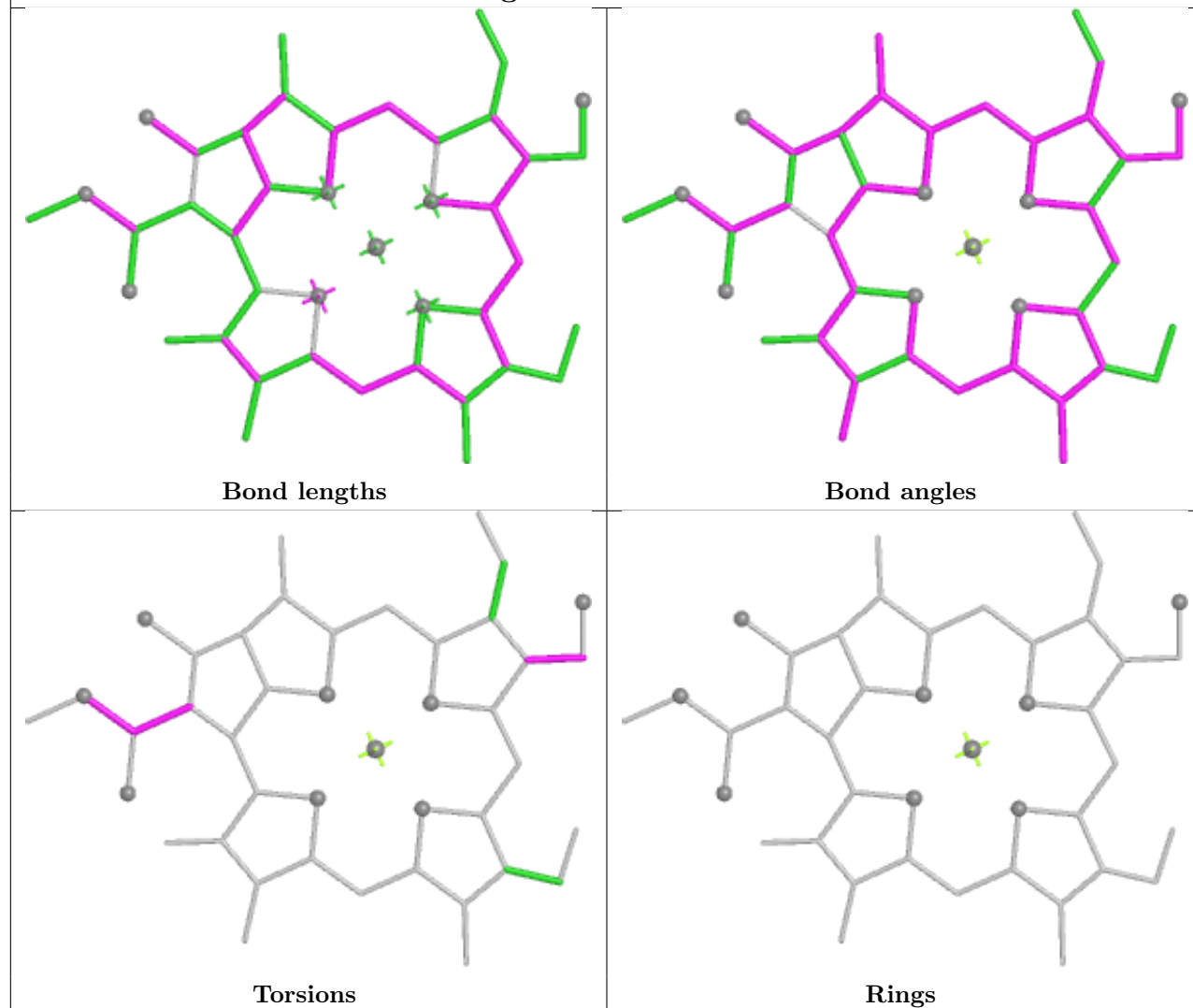


Rings

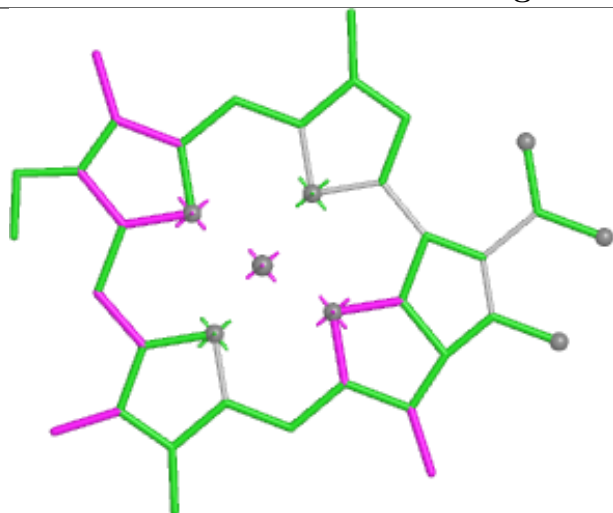
Ligand CLA A 837



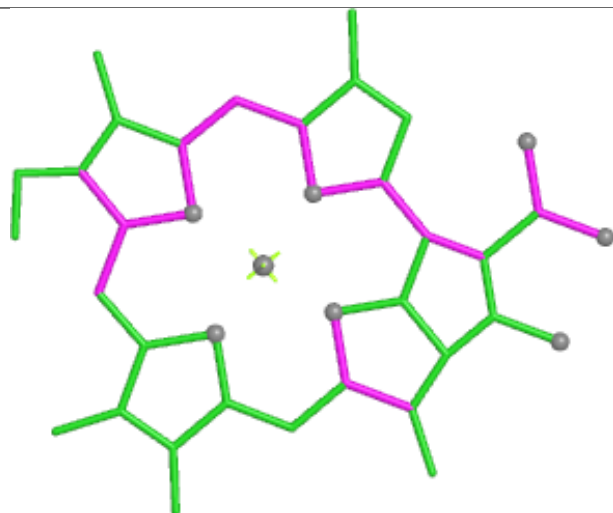
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Ligand CLA O 202



Bond lengths



Bond angles

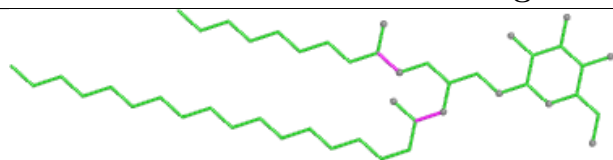


Torsions

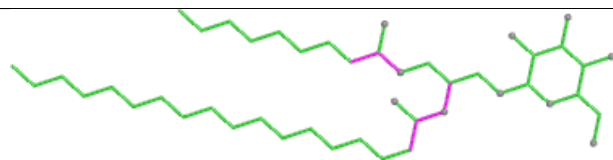


Rings

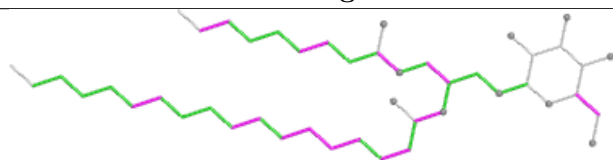
Ligand LMG 1 619



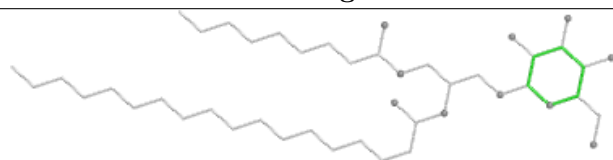
Bond lengths



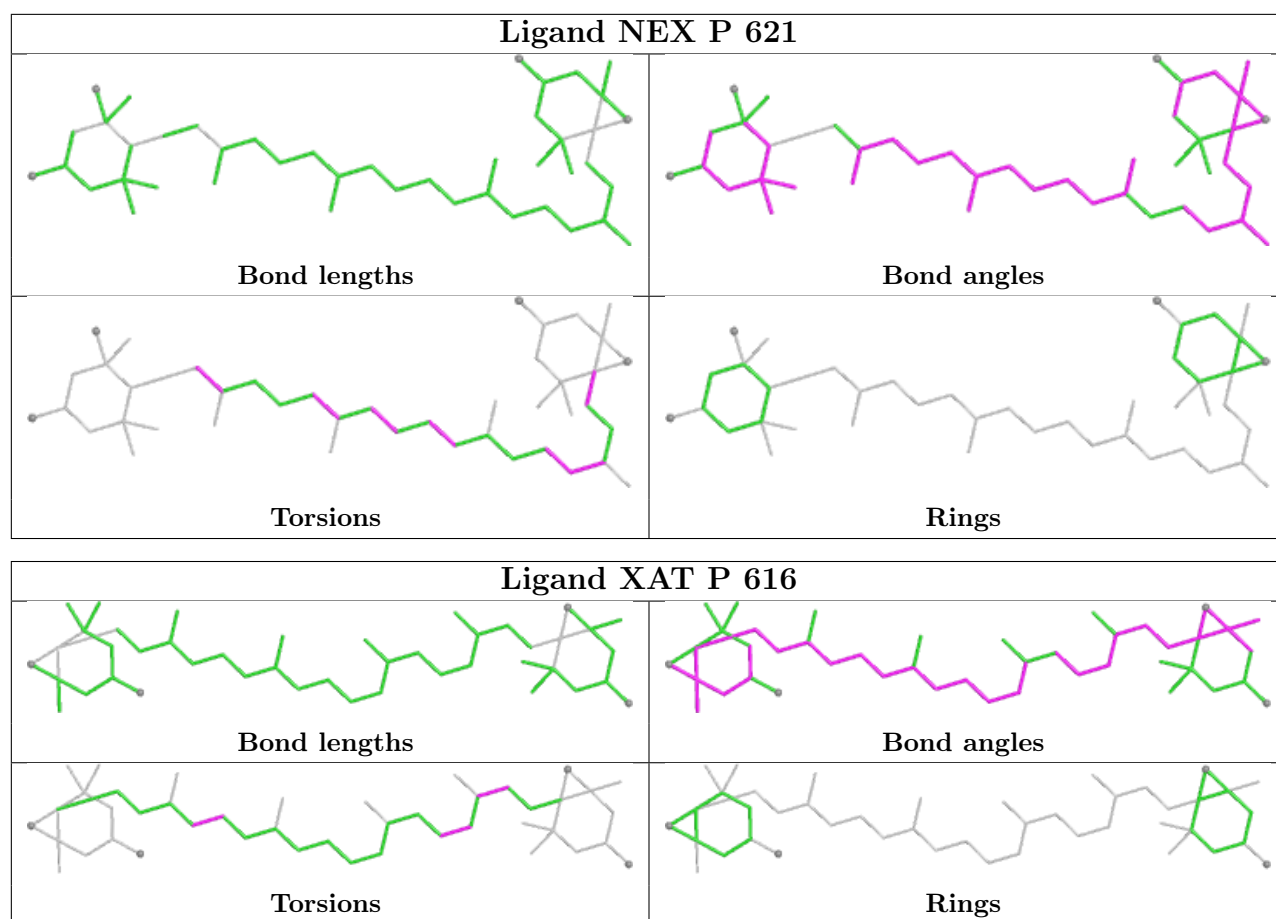
Bond angles



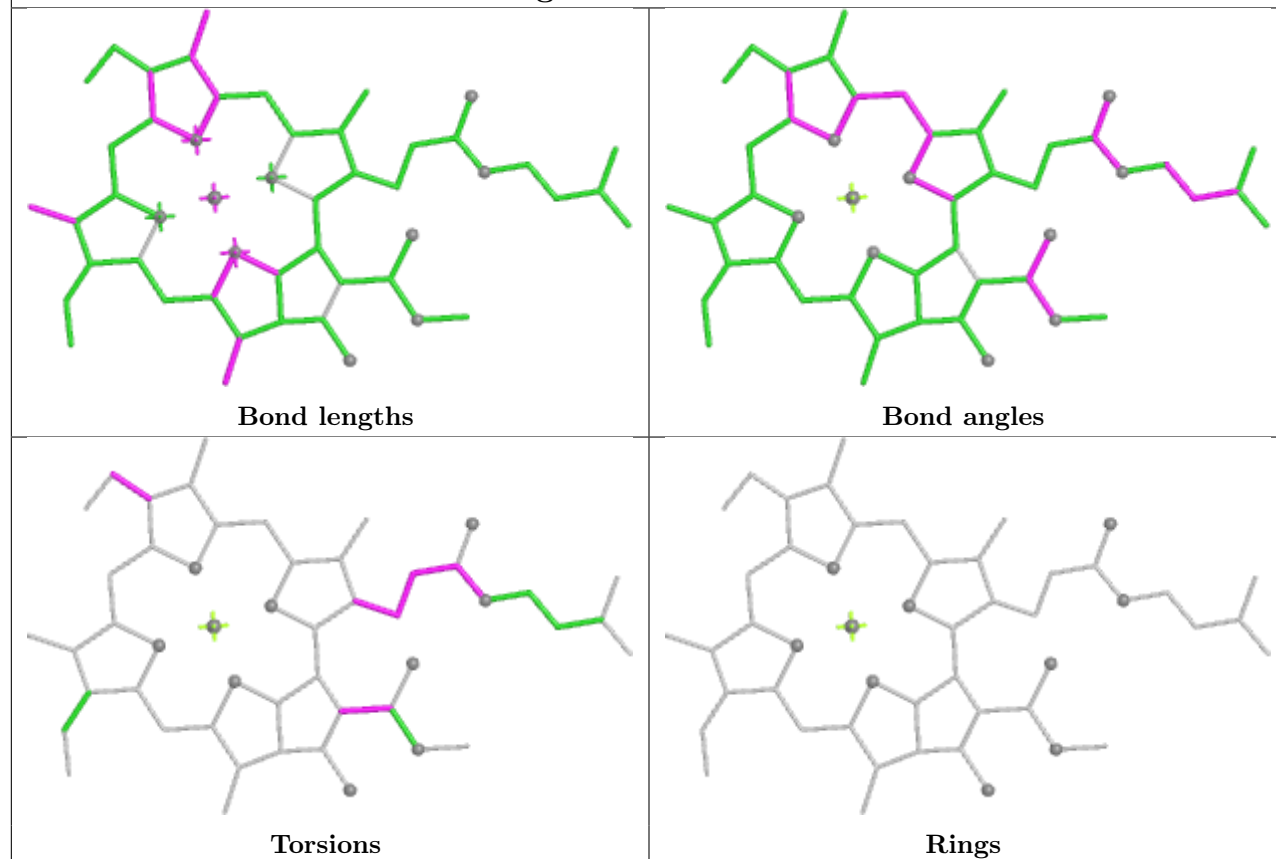
Torsions



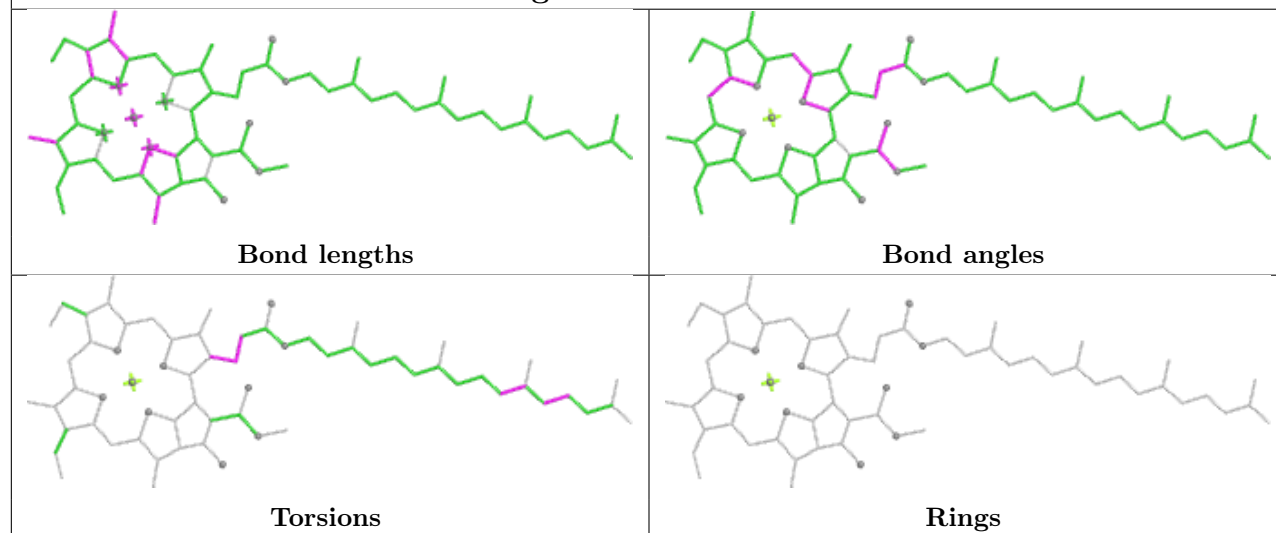
Rings

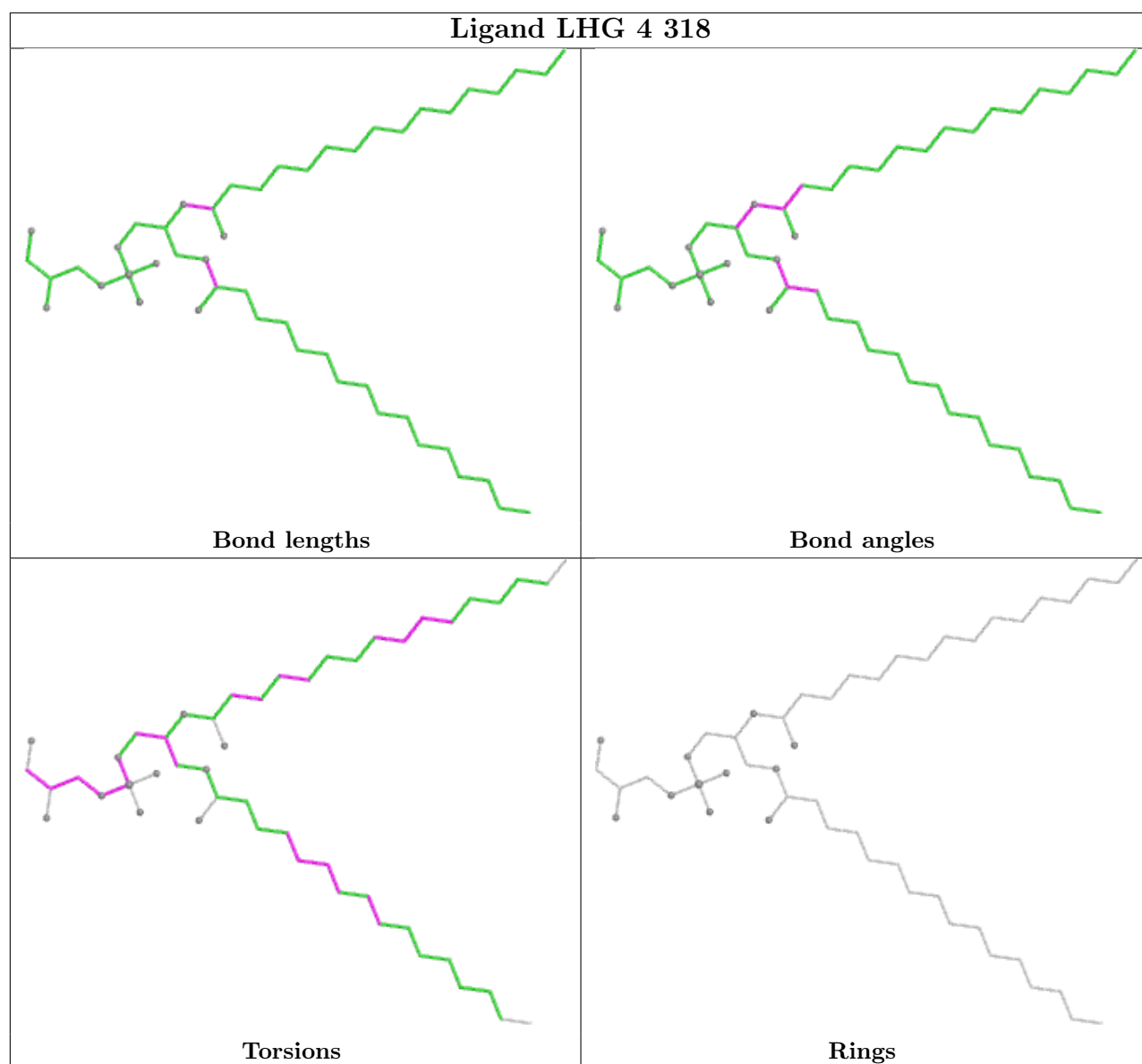


Ligand CLA 3 307

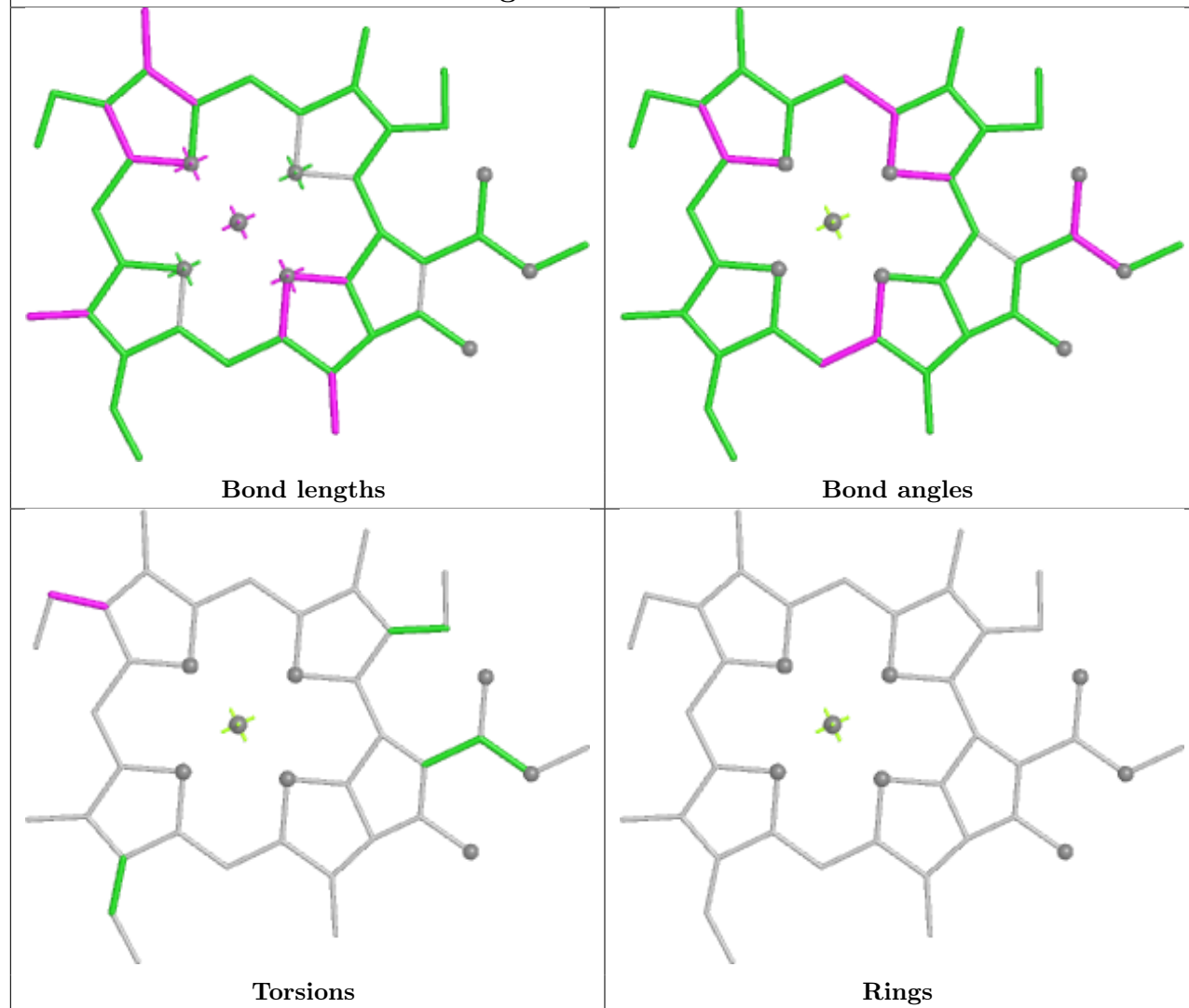


Ligand CLA A 803

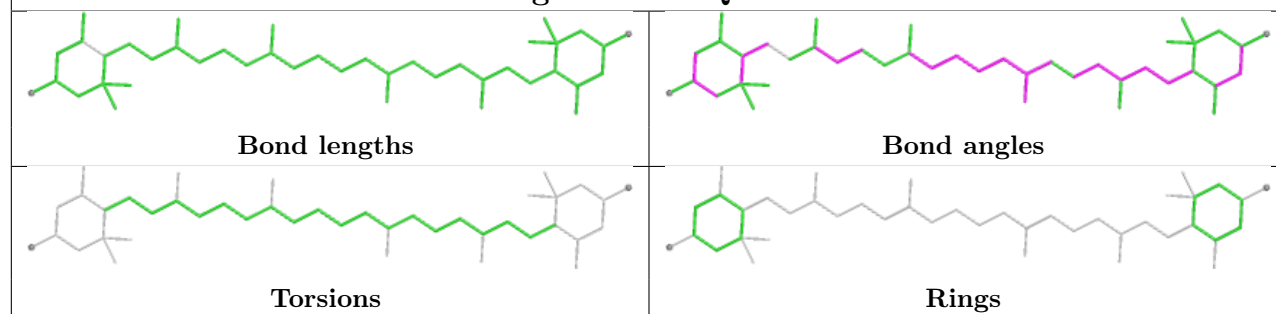




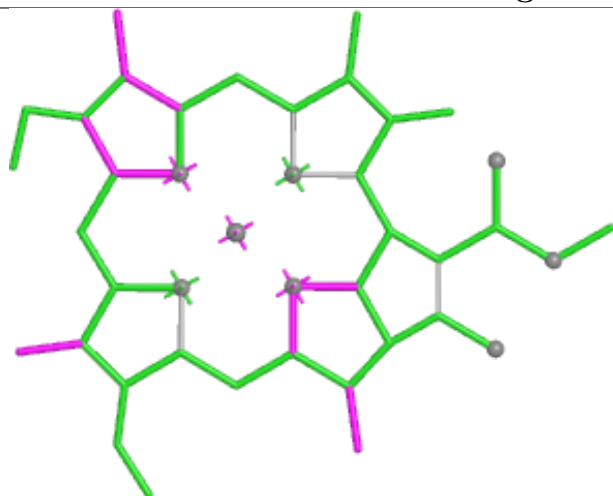
Ligand CLA 3 304



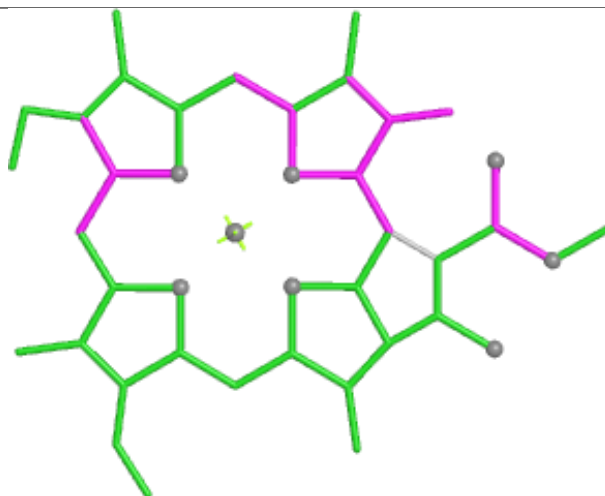
Ligand LUT Q 614



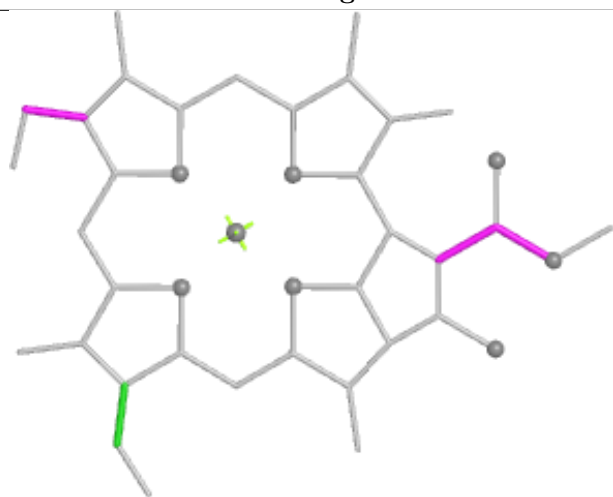
Ligand CLA L 209



Bond lengths



Bond angles

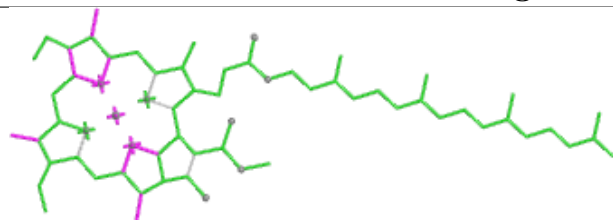


Torsions

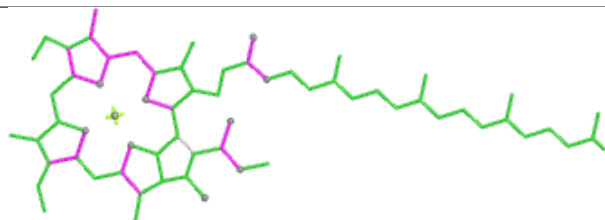


Rings

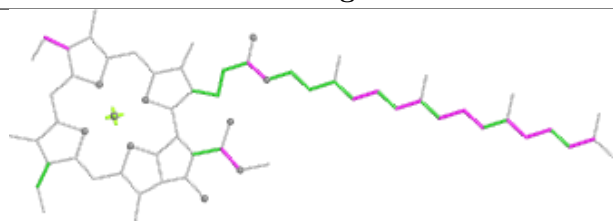
Ligand CLA A 812



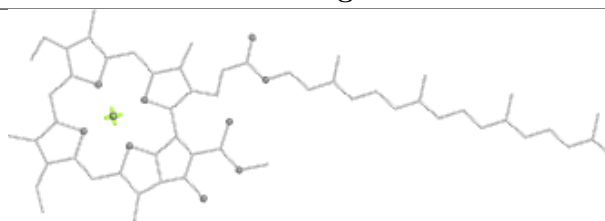
Bond lengths



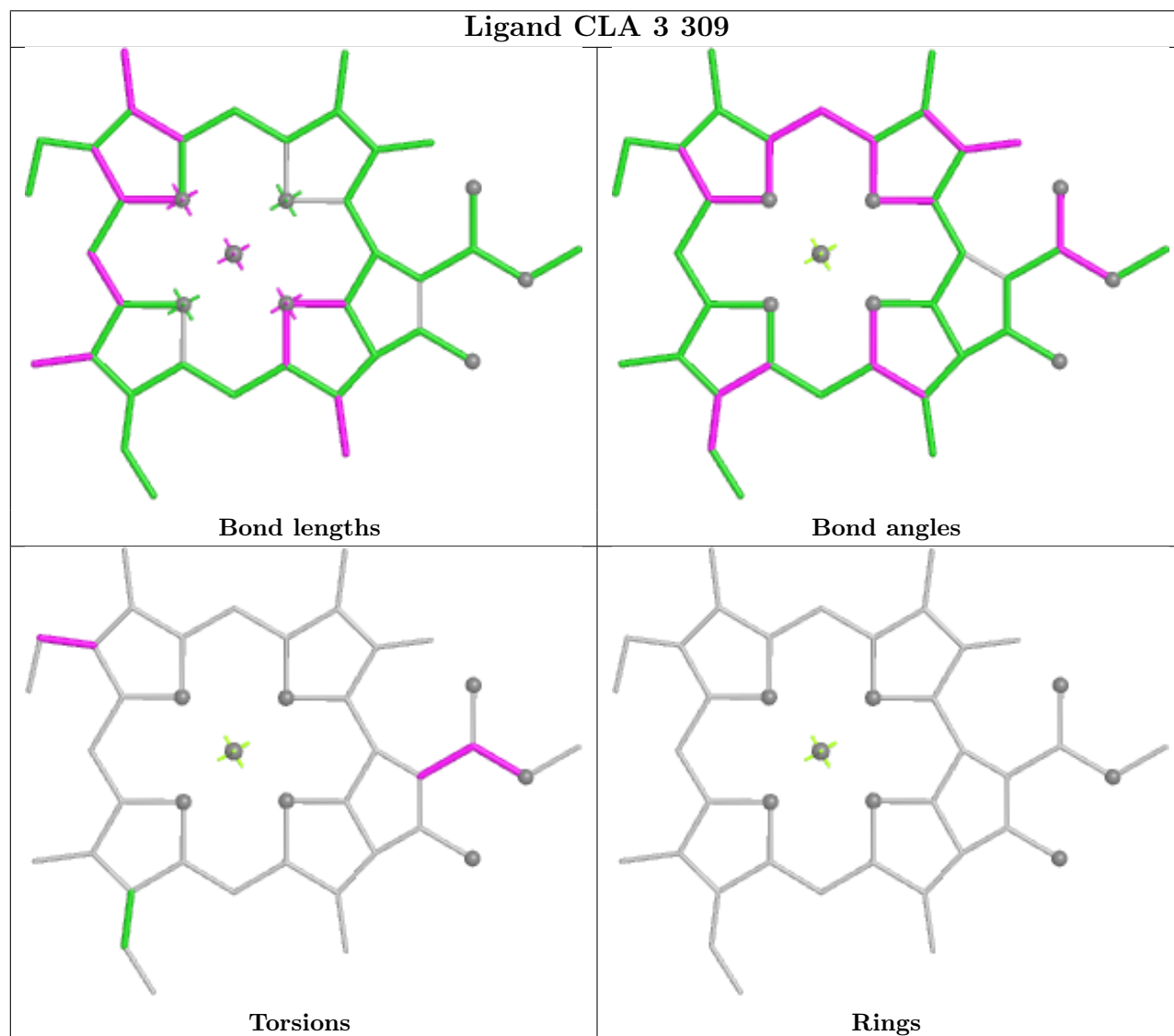
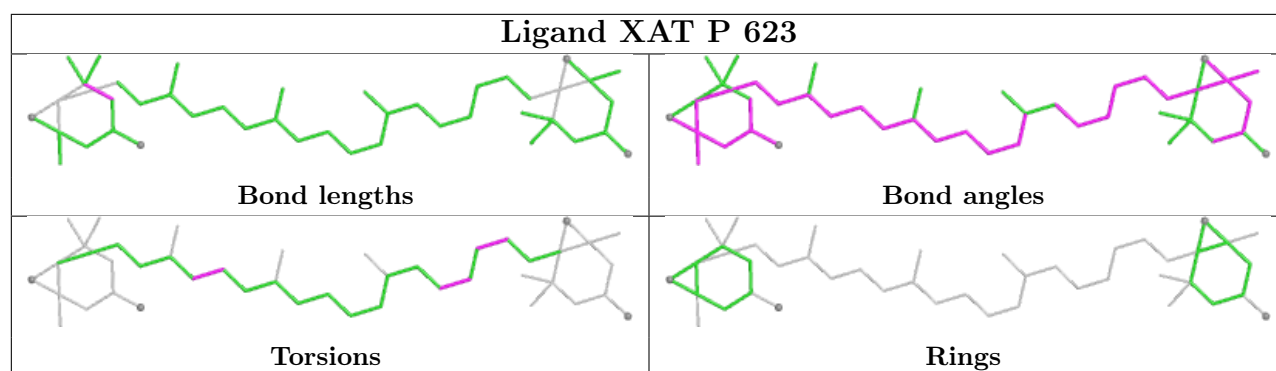
Bond angles

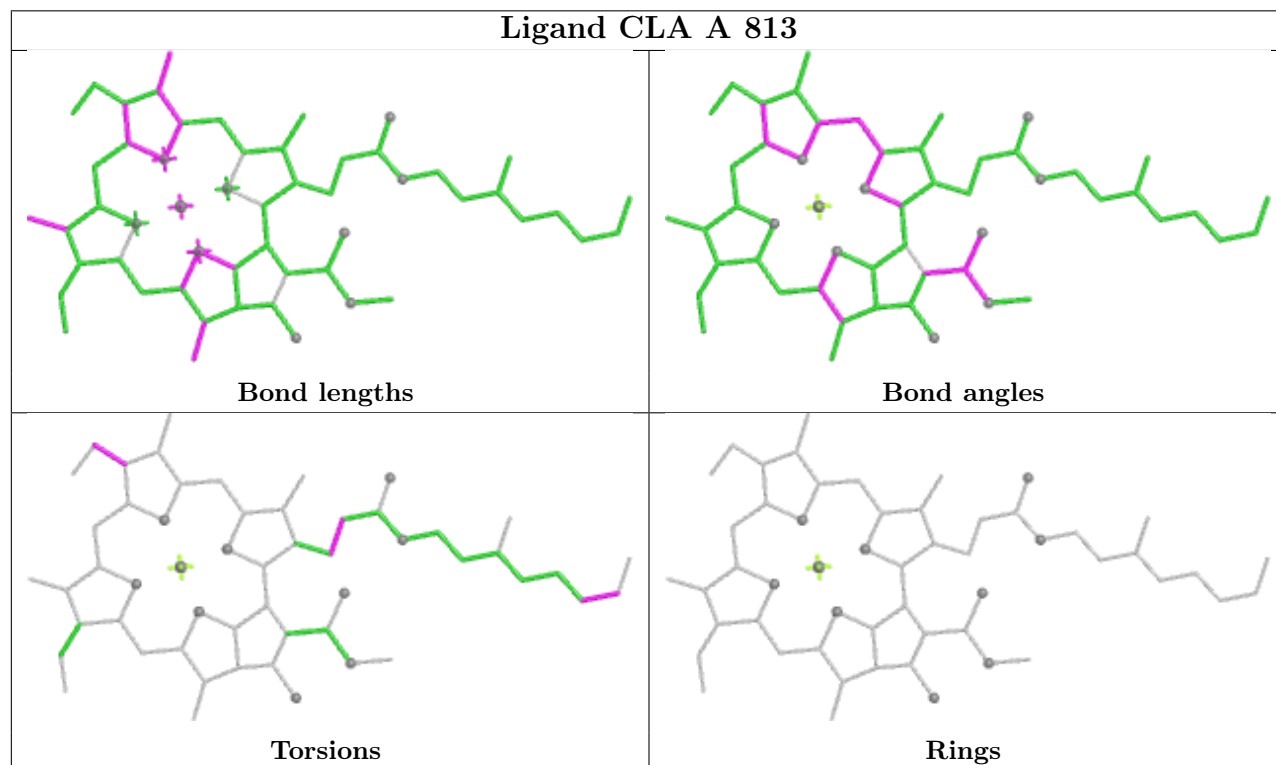
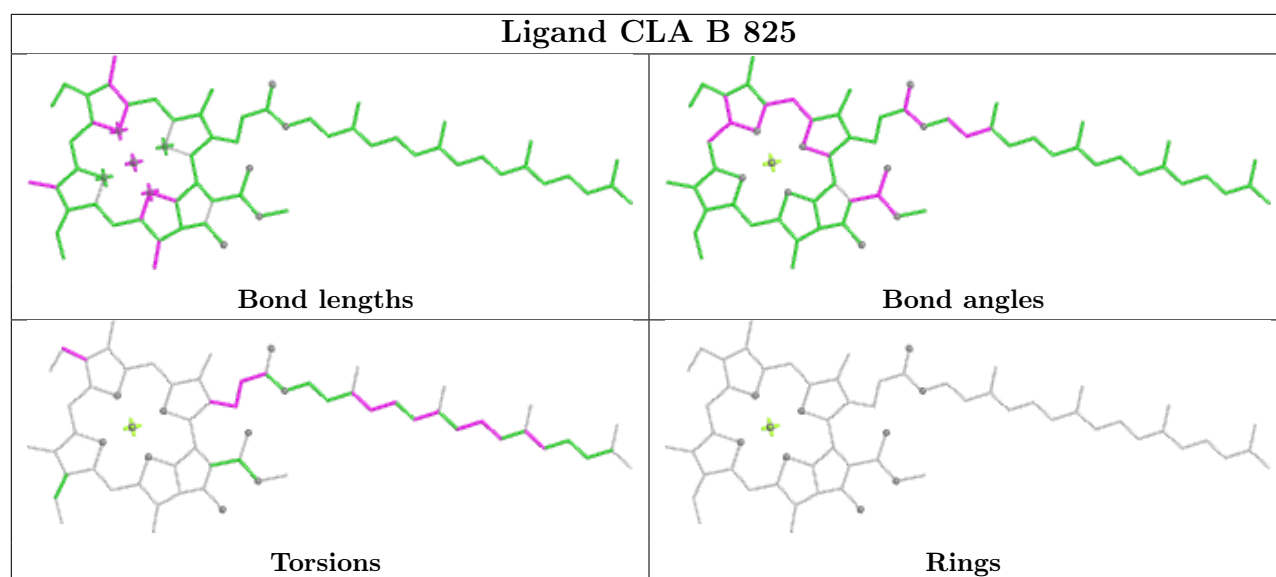


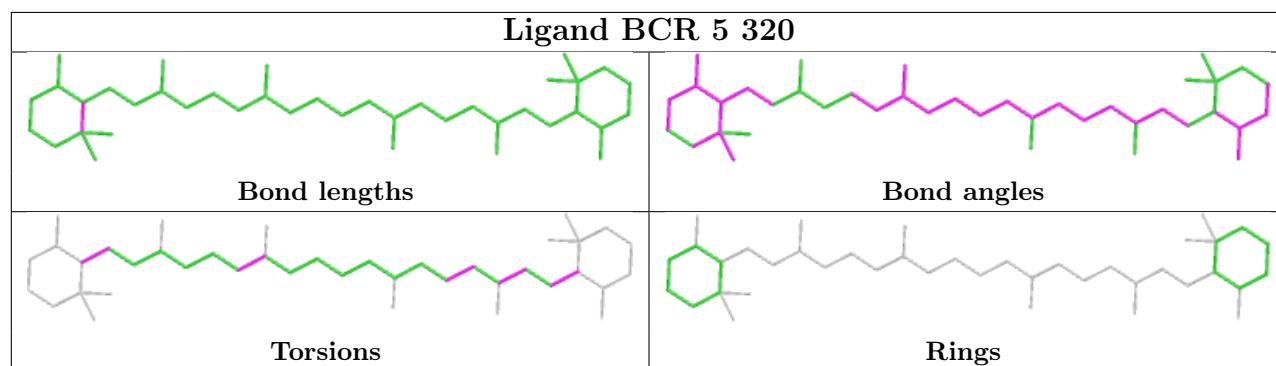
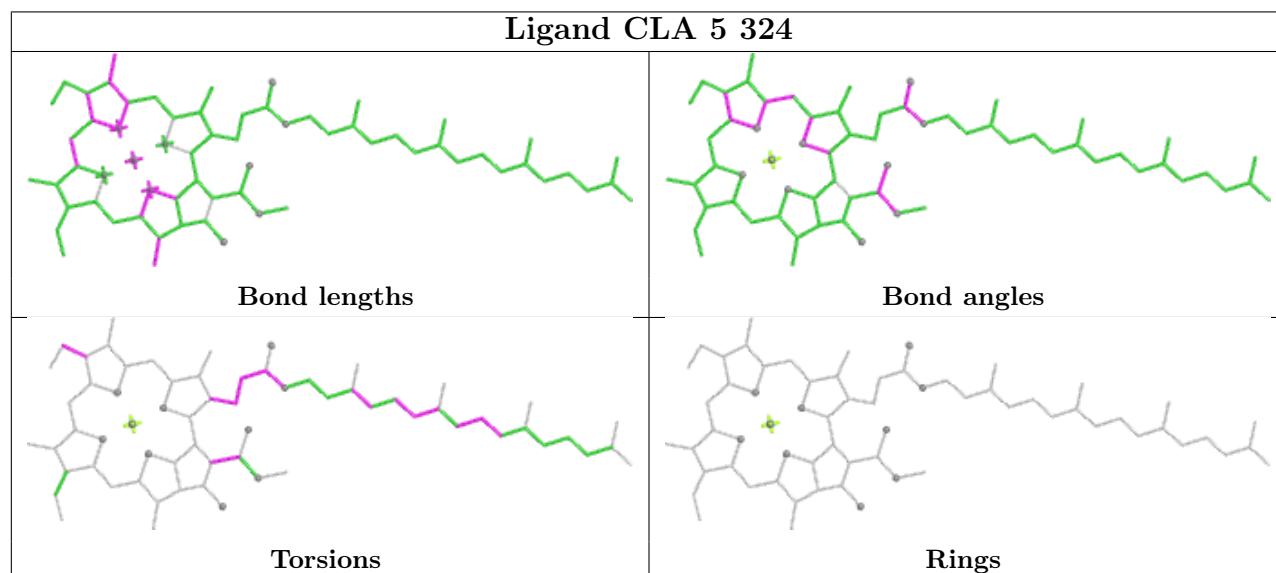
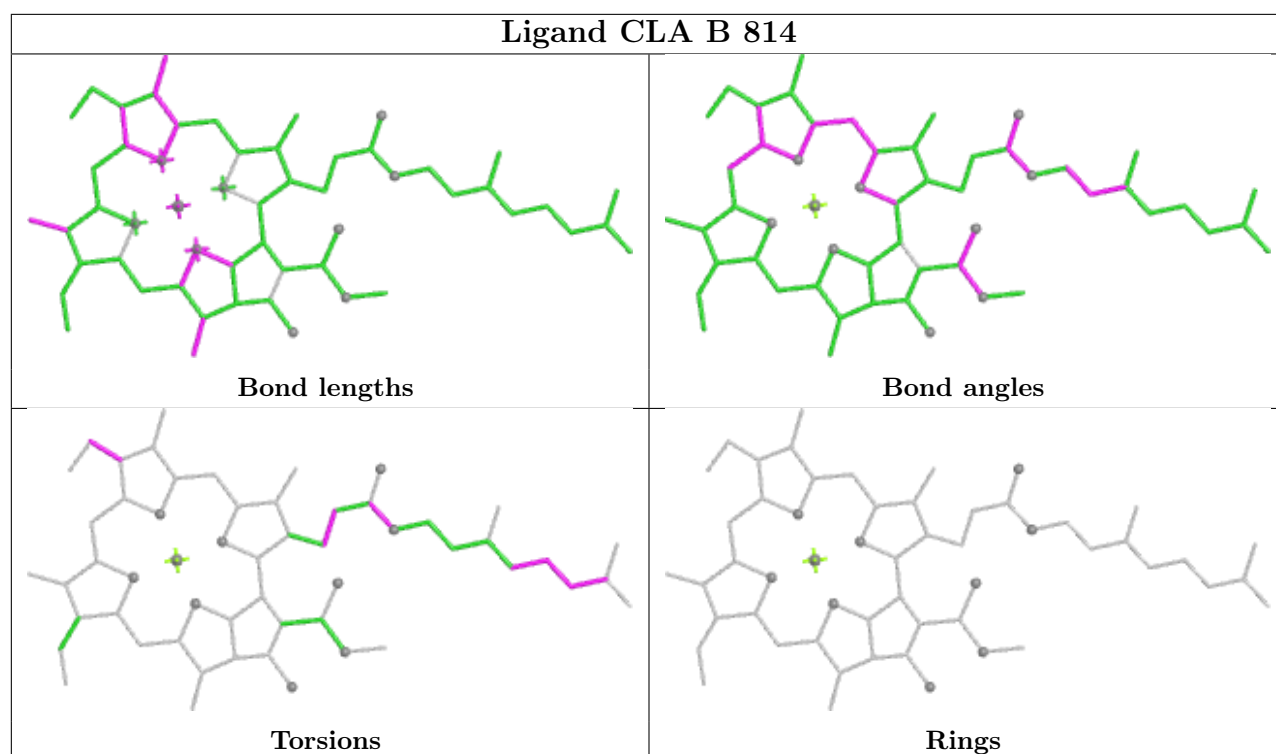
Torsions

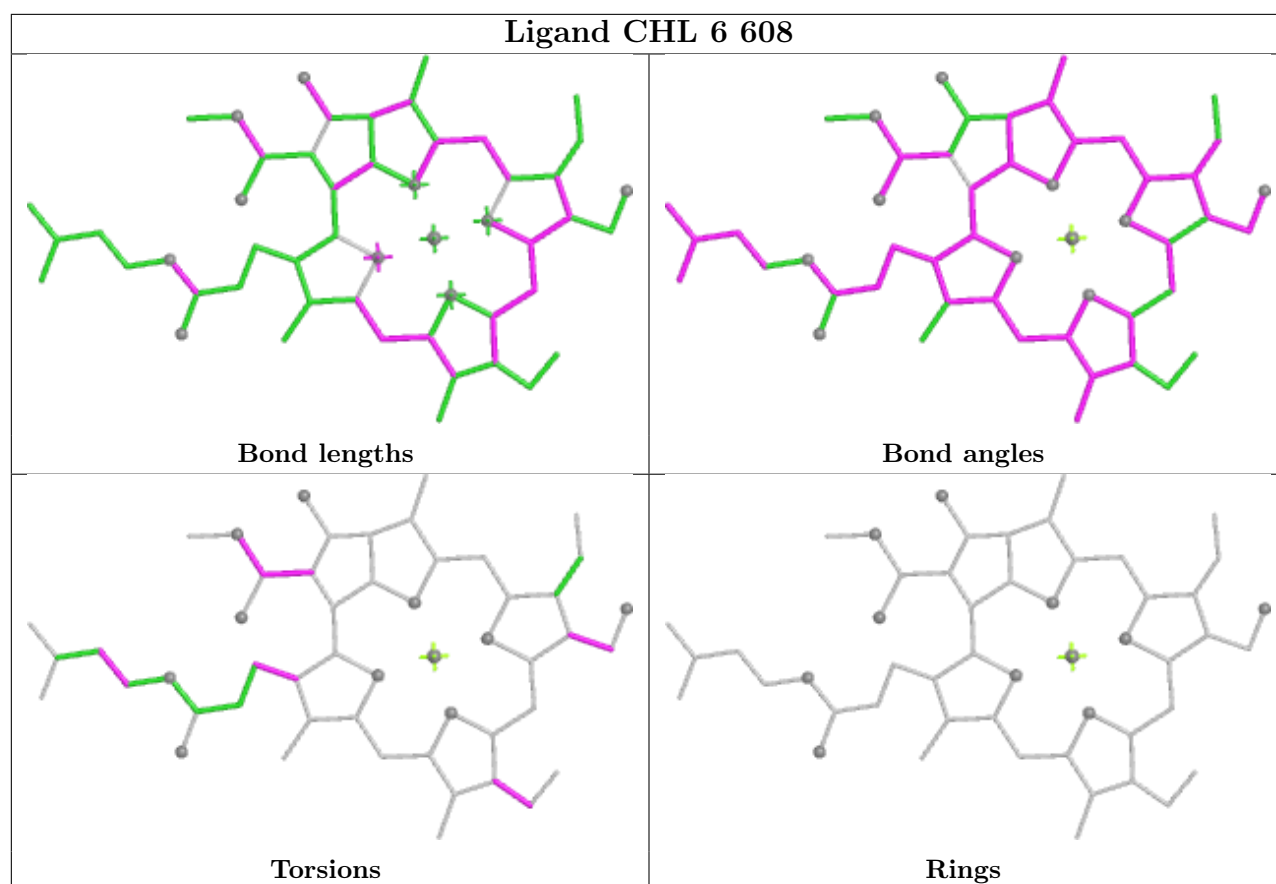


Rings

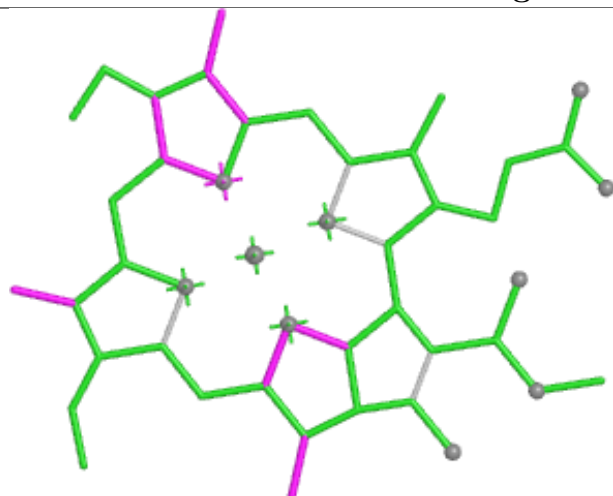




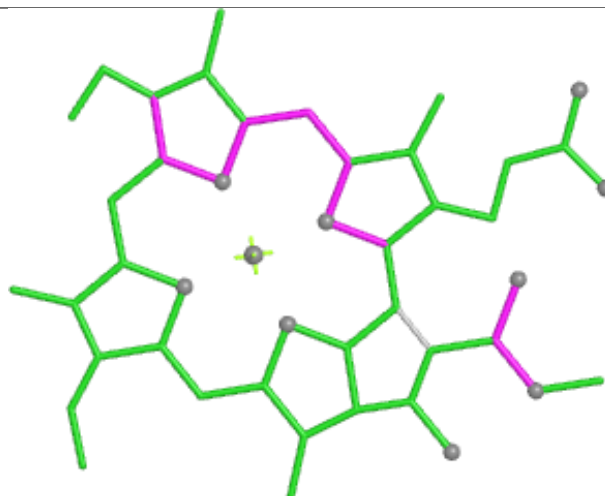




Ligand CLA K 205



Bond lengths



Bond angles

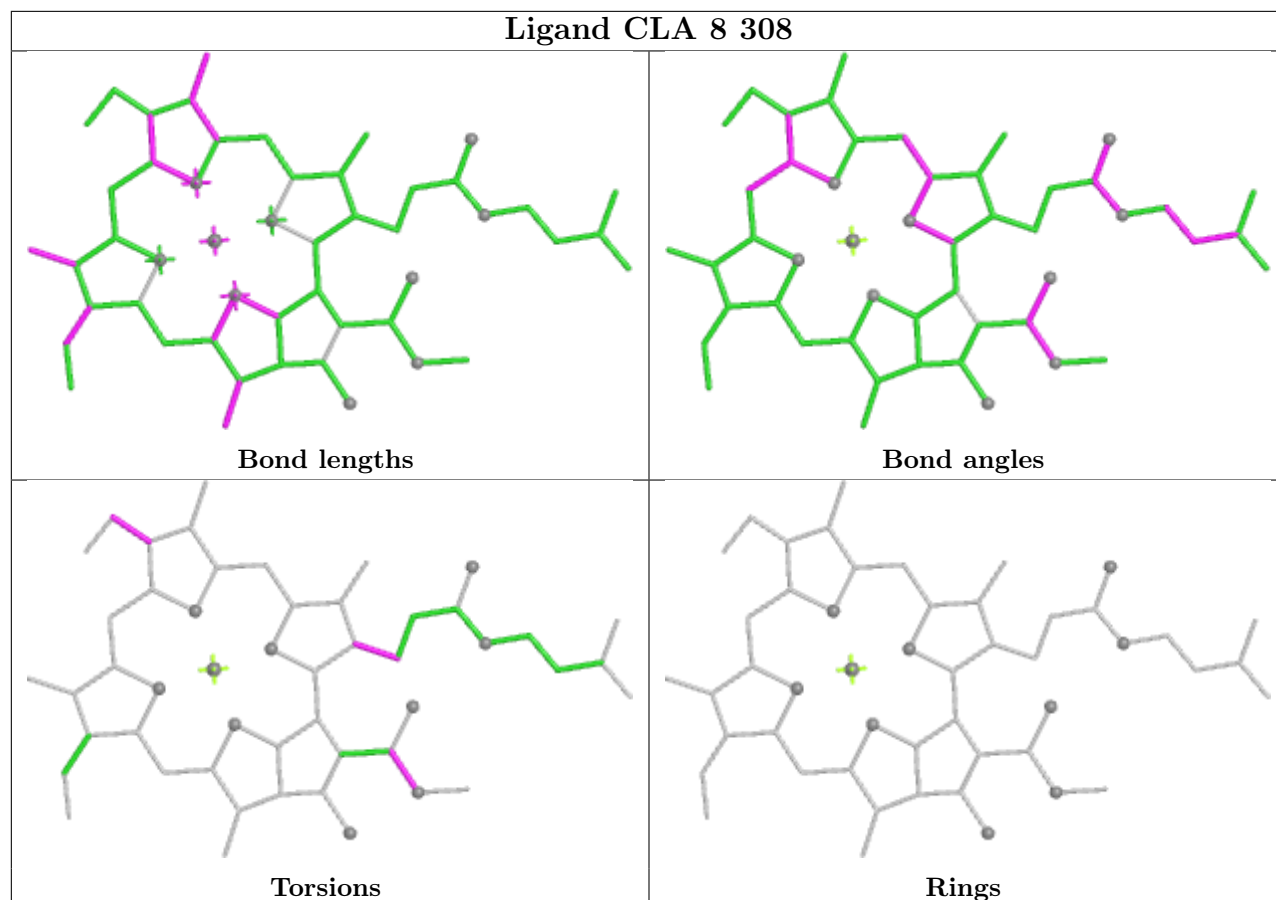


Torsions

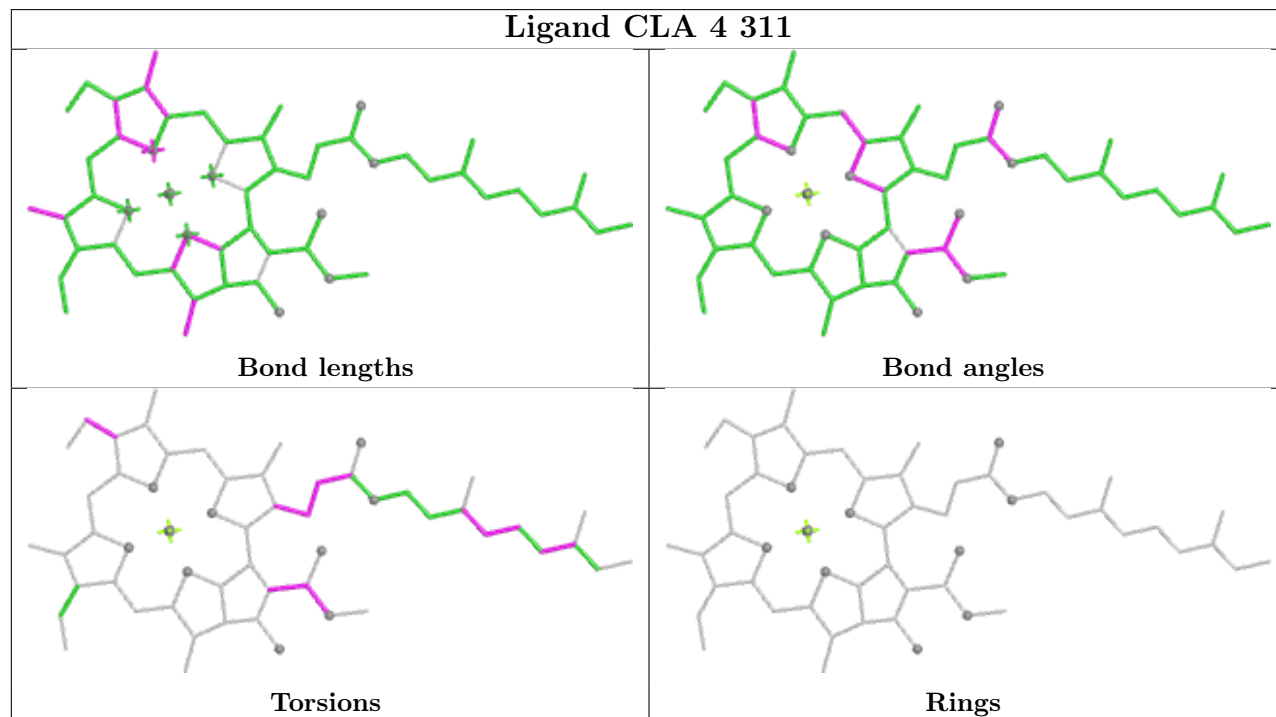


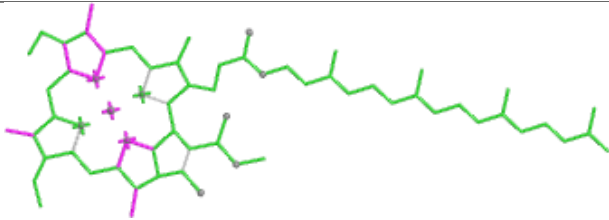
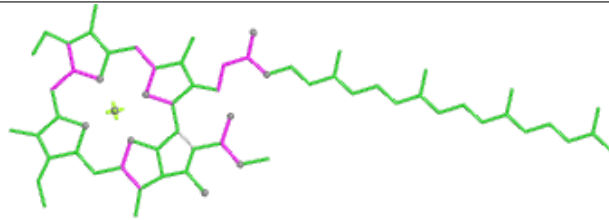
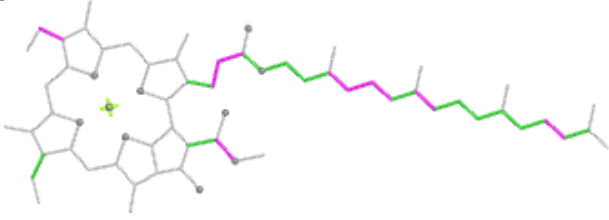
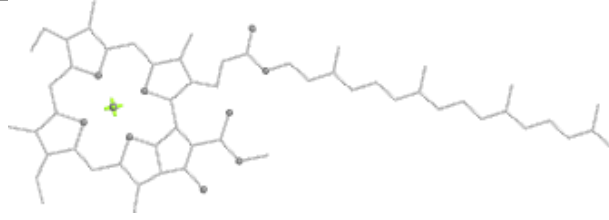
Rings

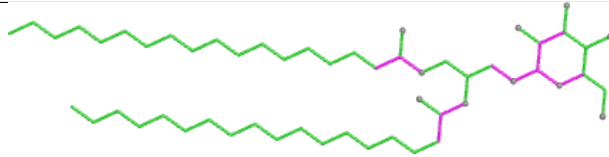
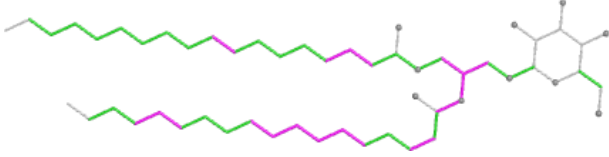
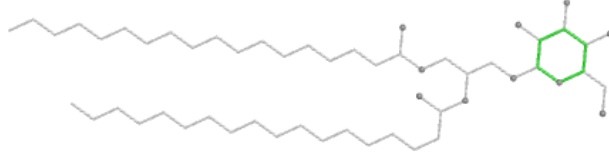
Ligand CLA 8 308

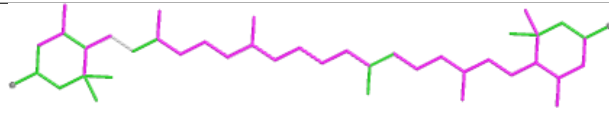
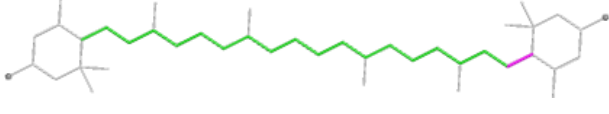
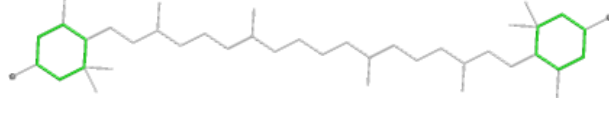


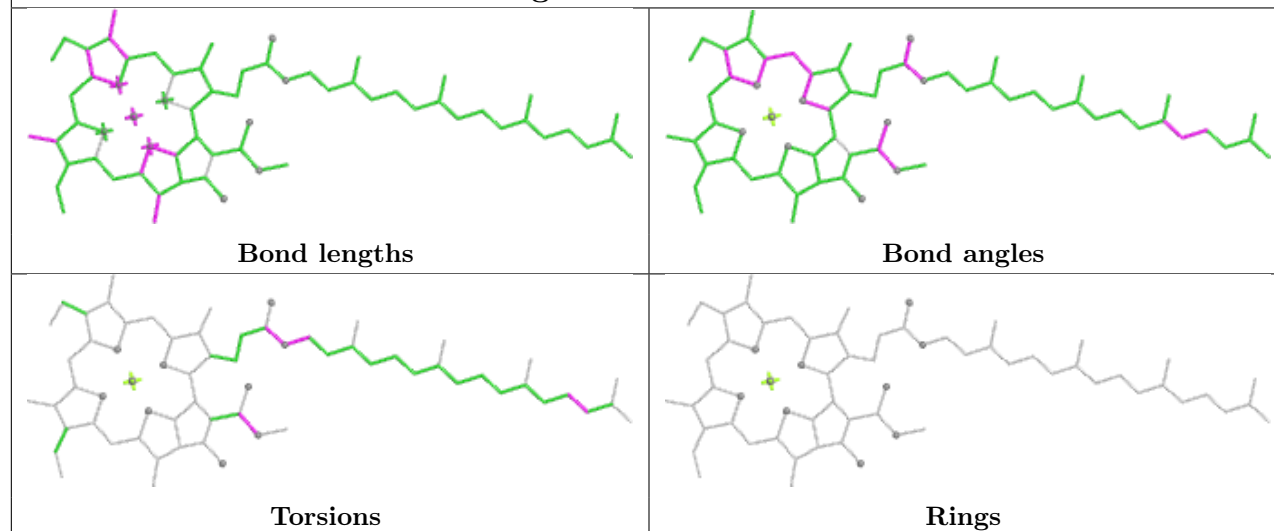
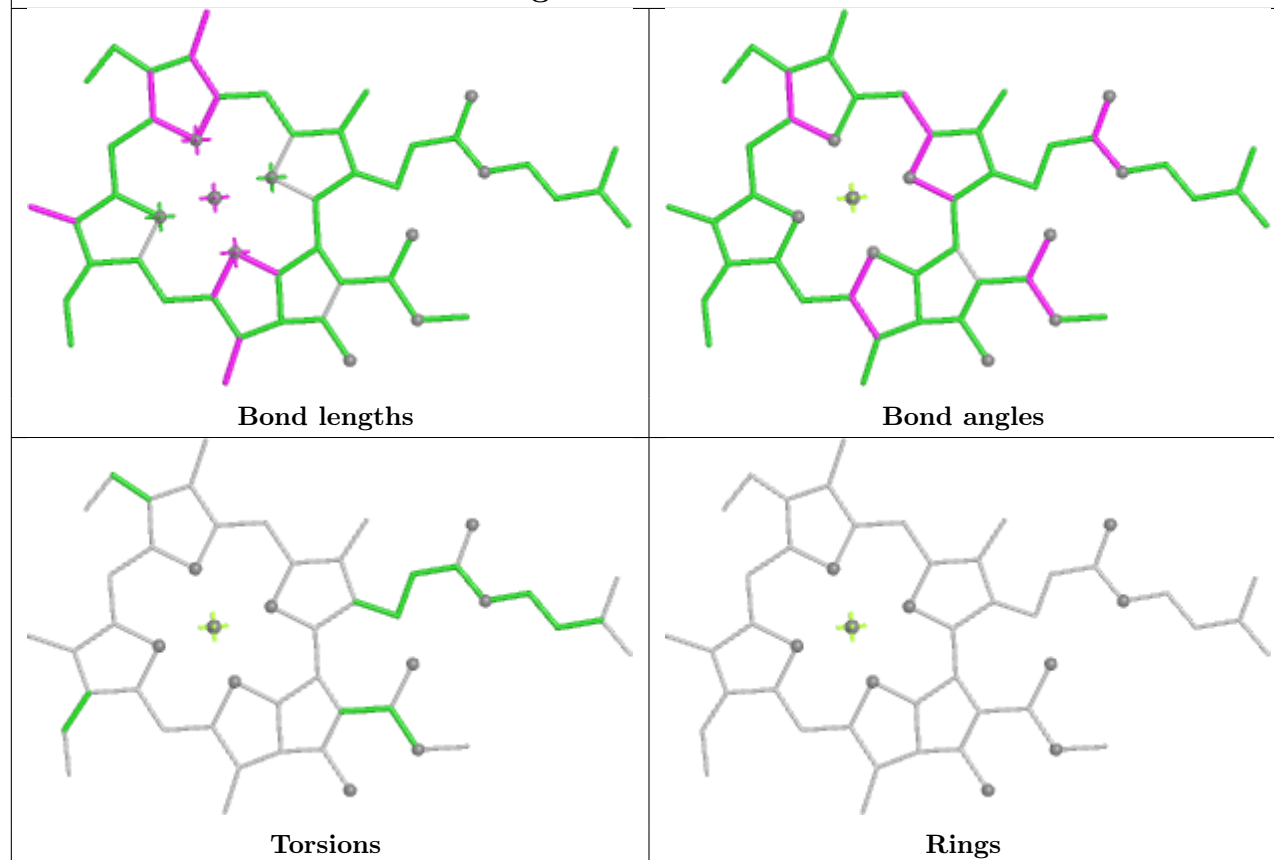
Ligand CLA 4 311

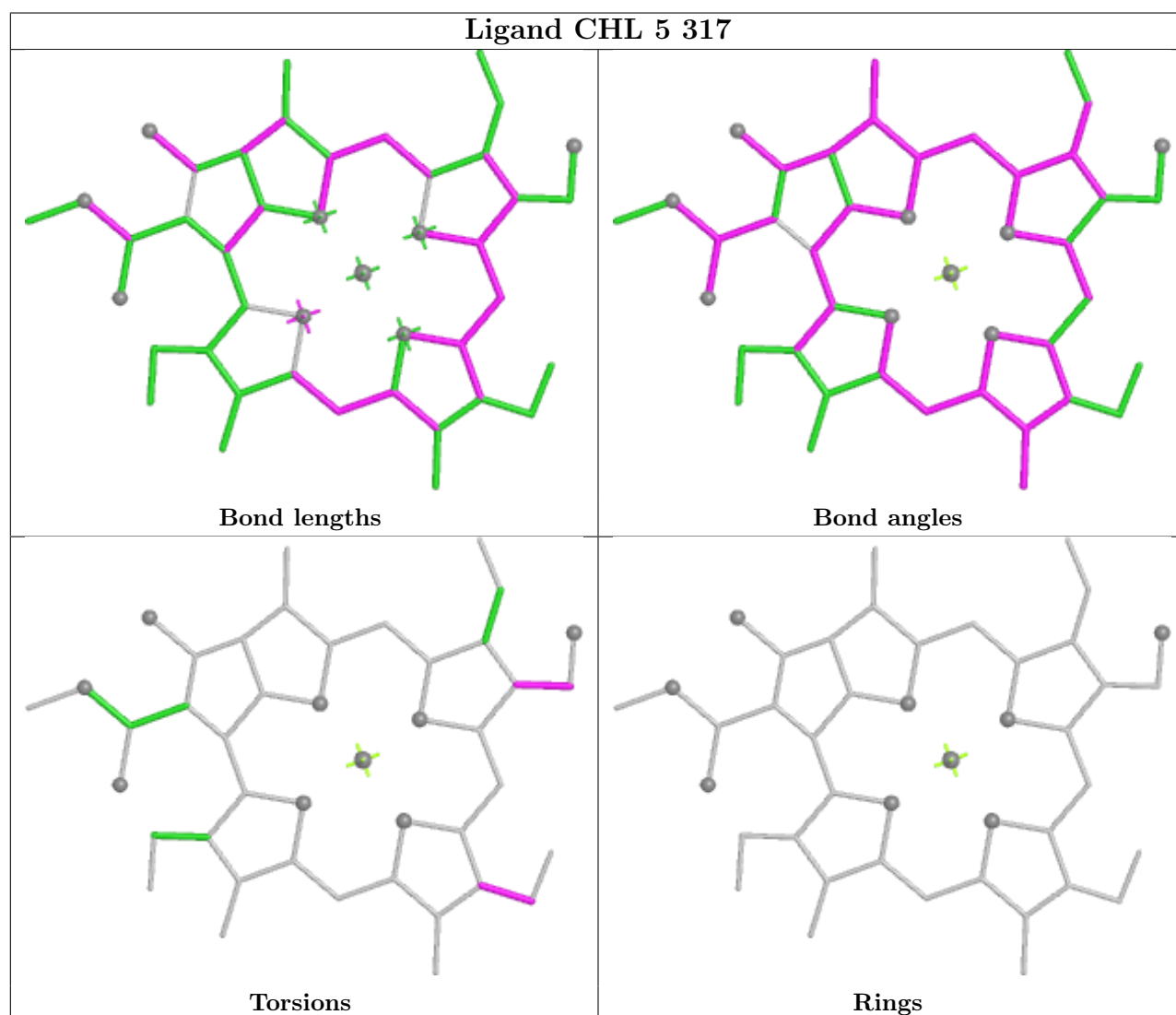
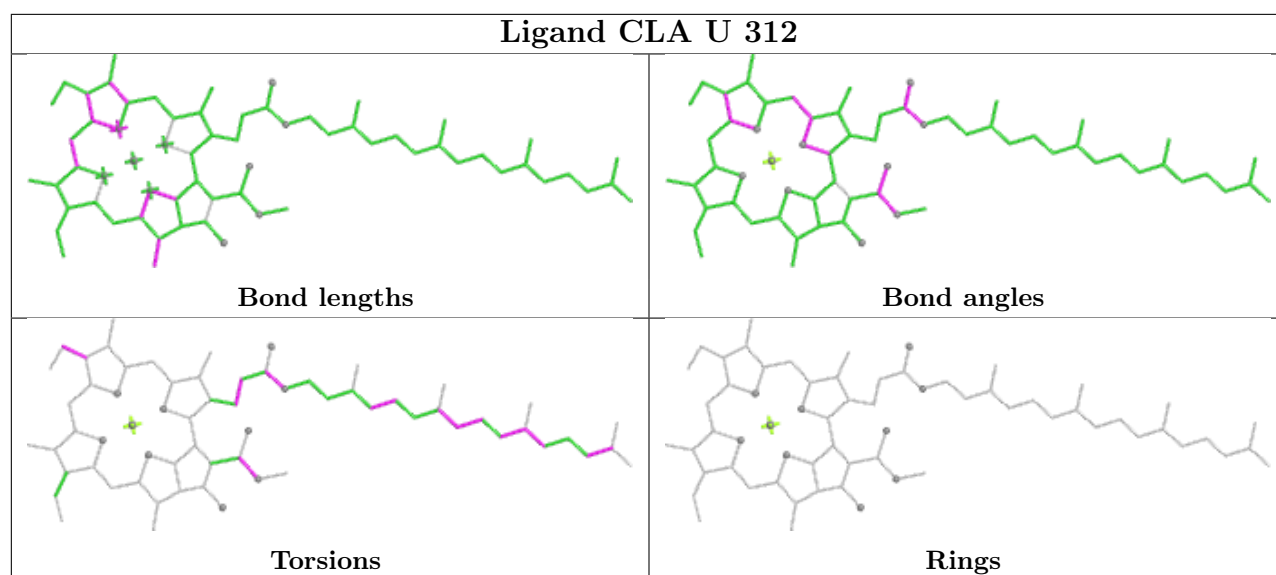


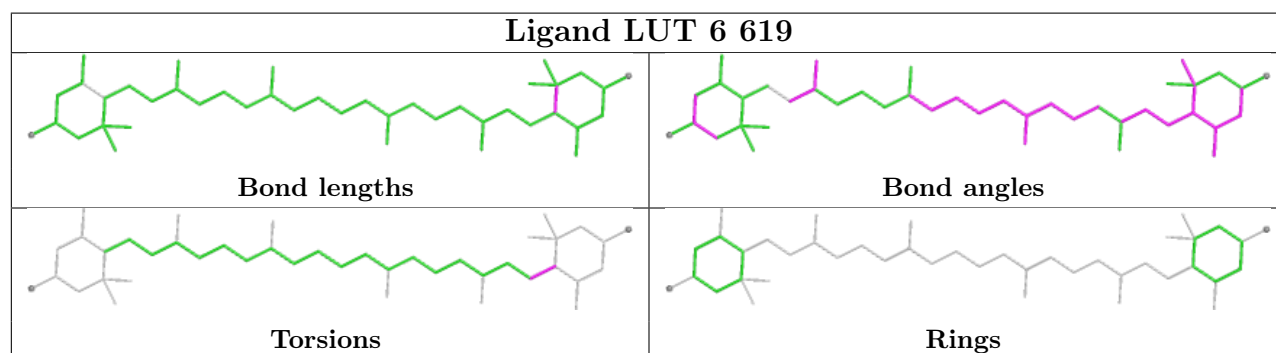
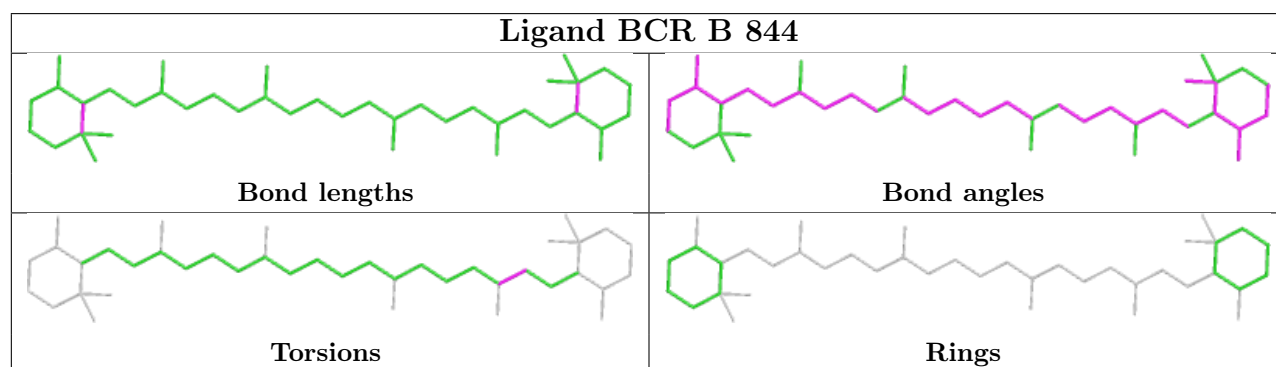
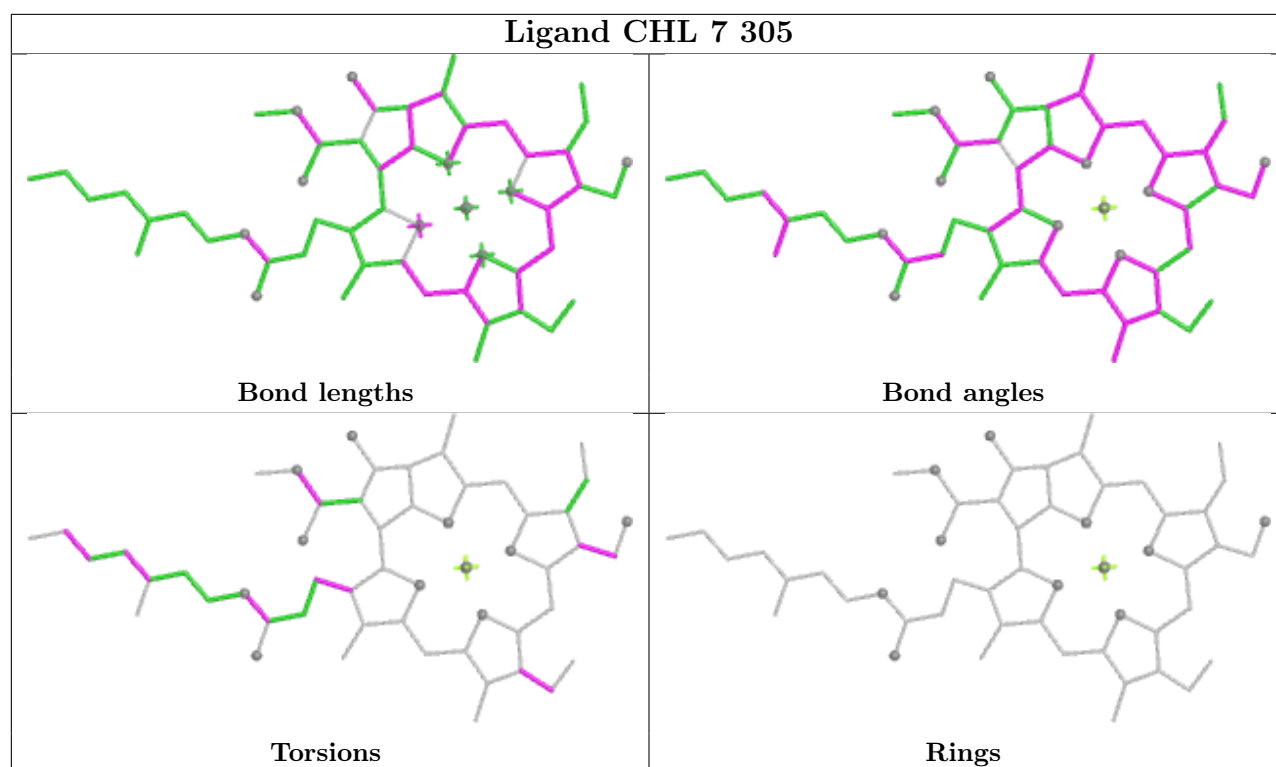
Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

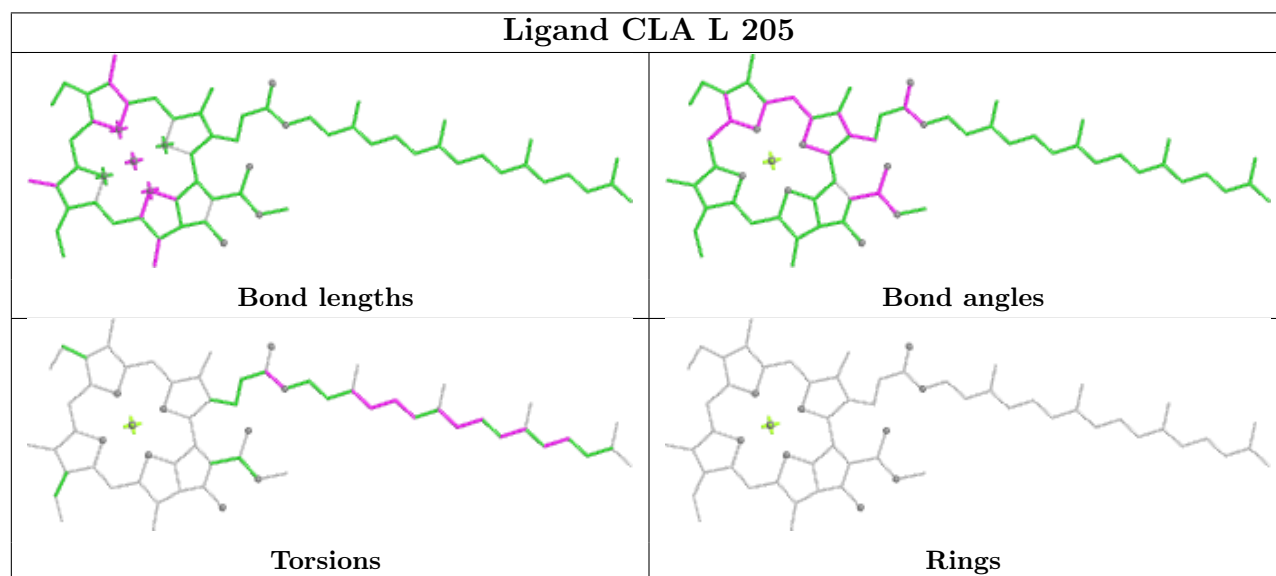
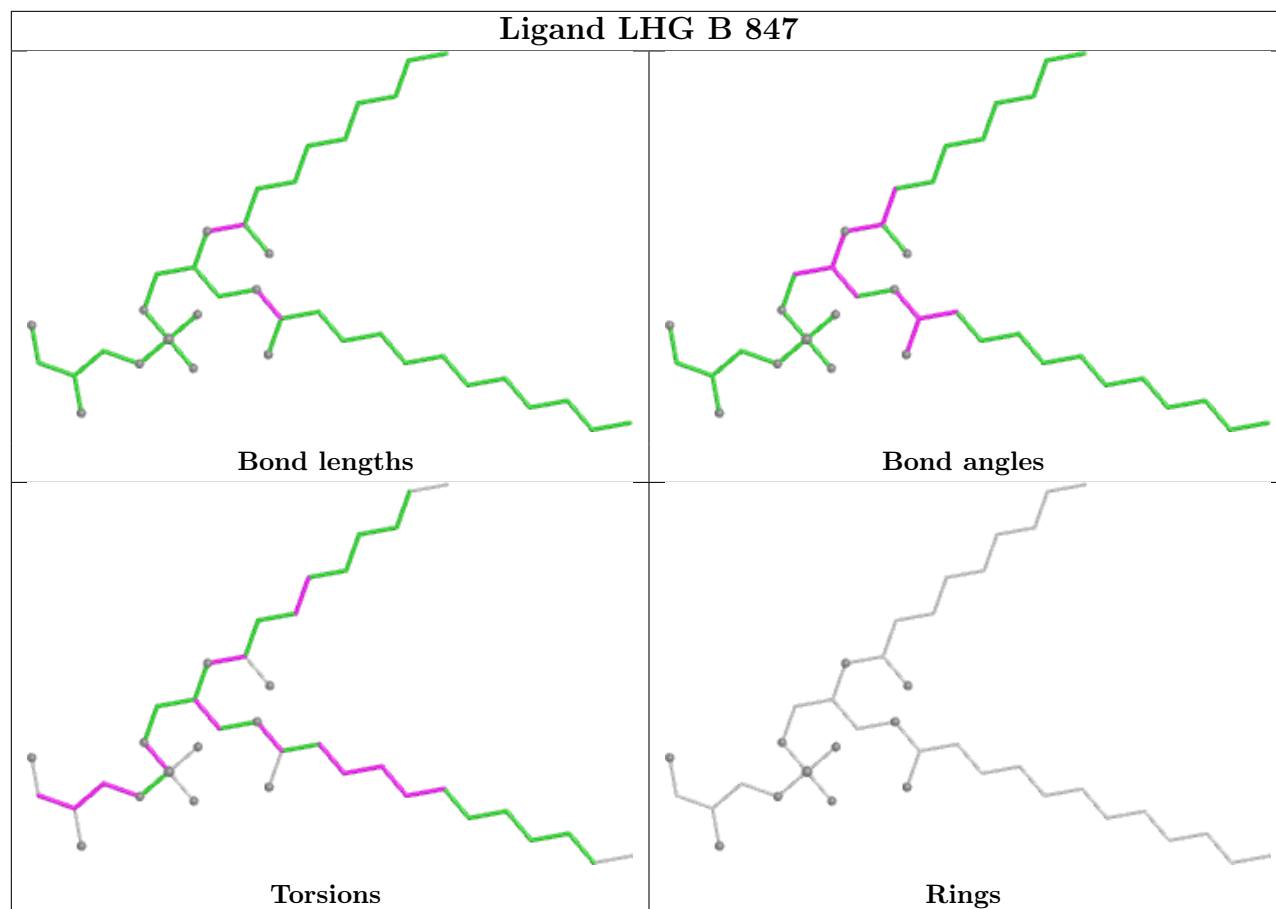
Ligand LMG J 107	
	
Bond lengths	Bond angles
	
Torsions	Rings

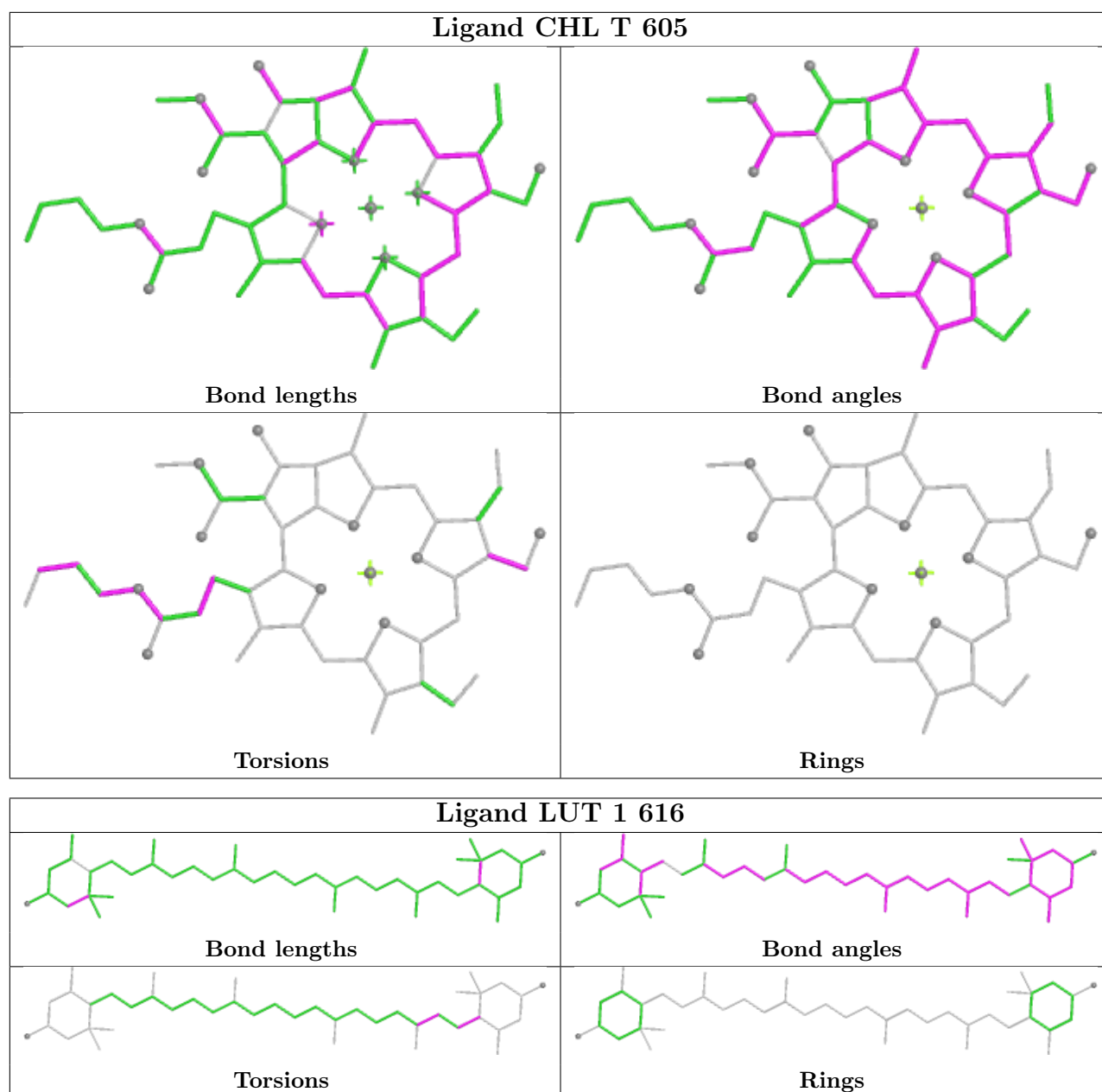
Ligand LUT R 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

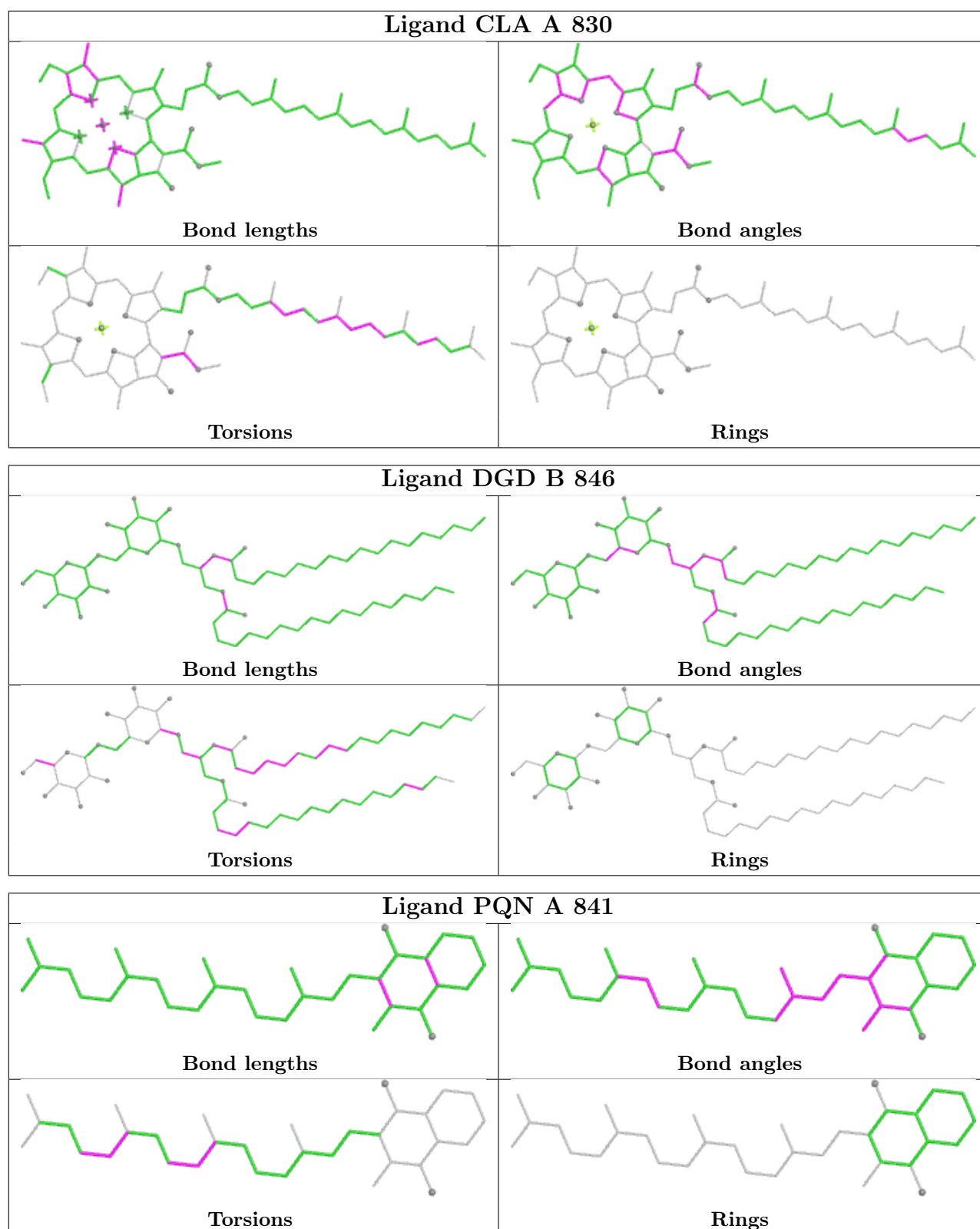
Ligand CLA A 811**Ligand CLA A 833**

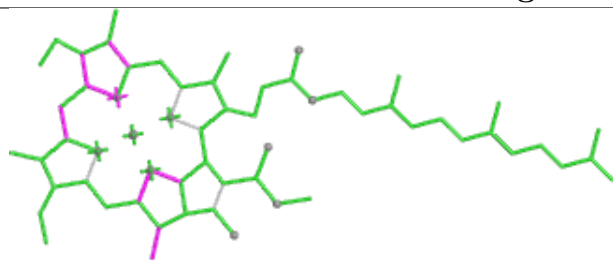
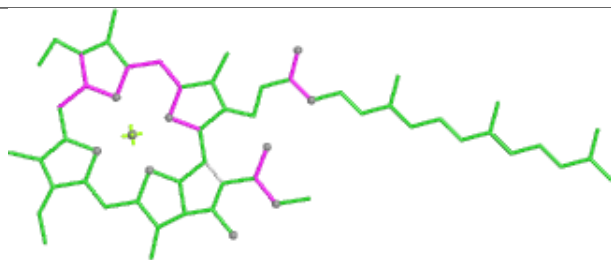
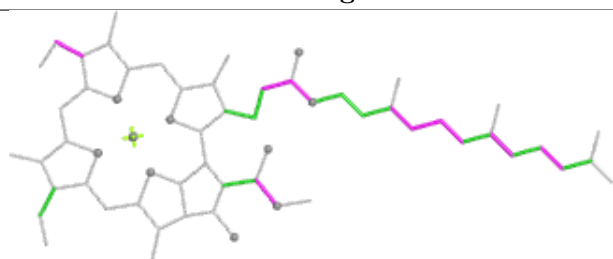
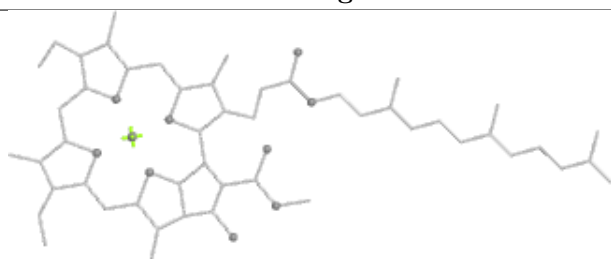
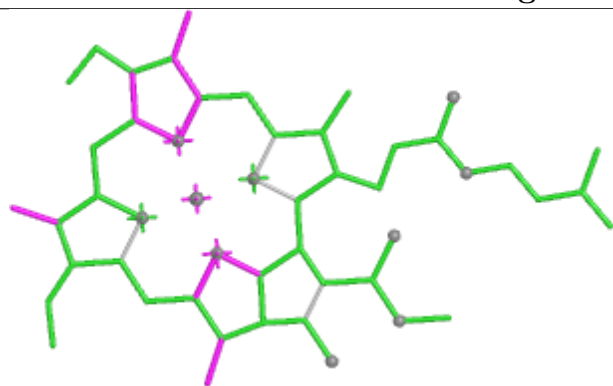
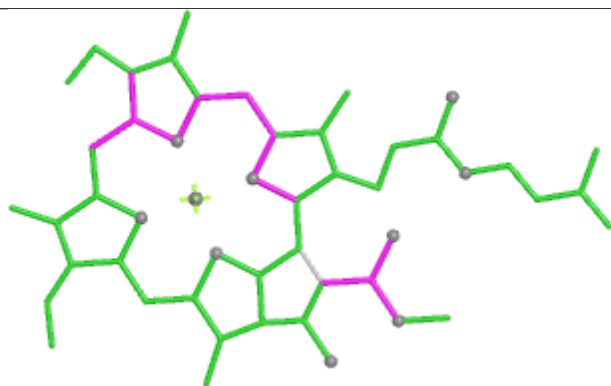
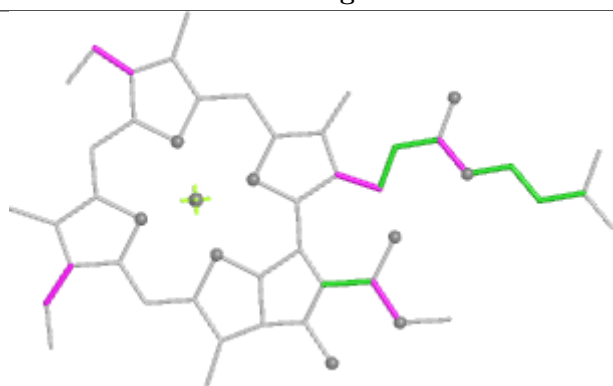
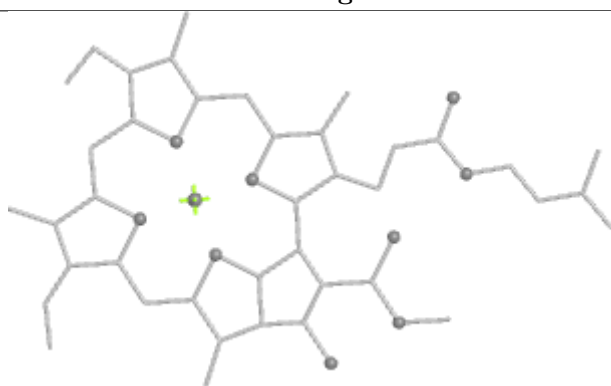


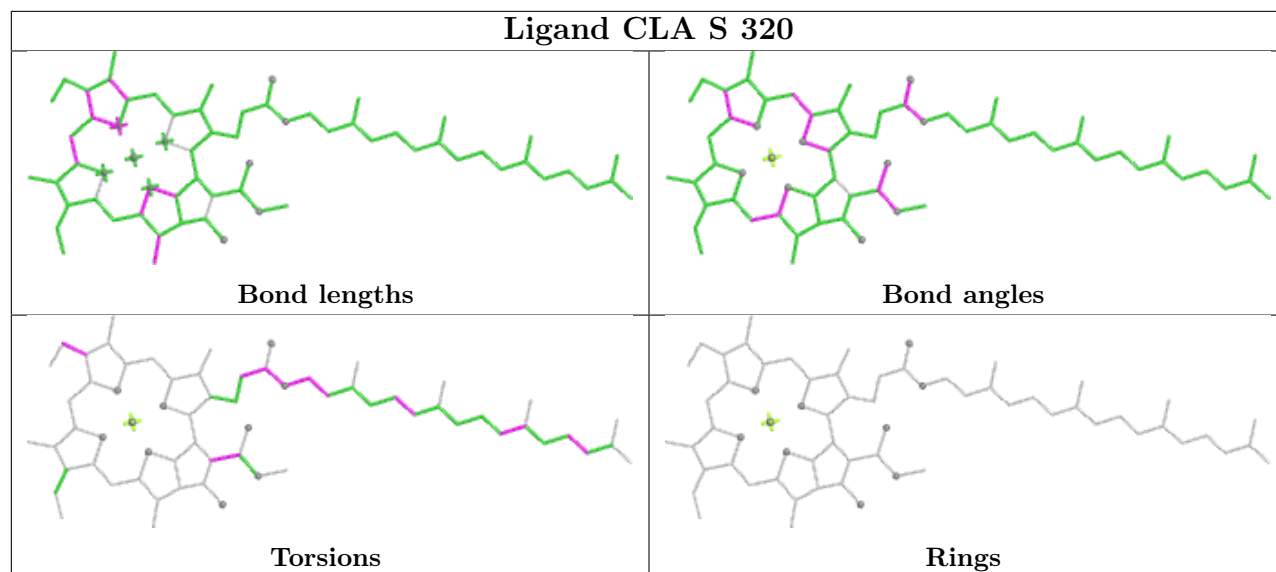
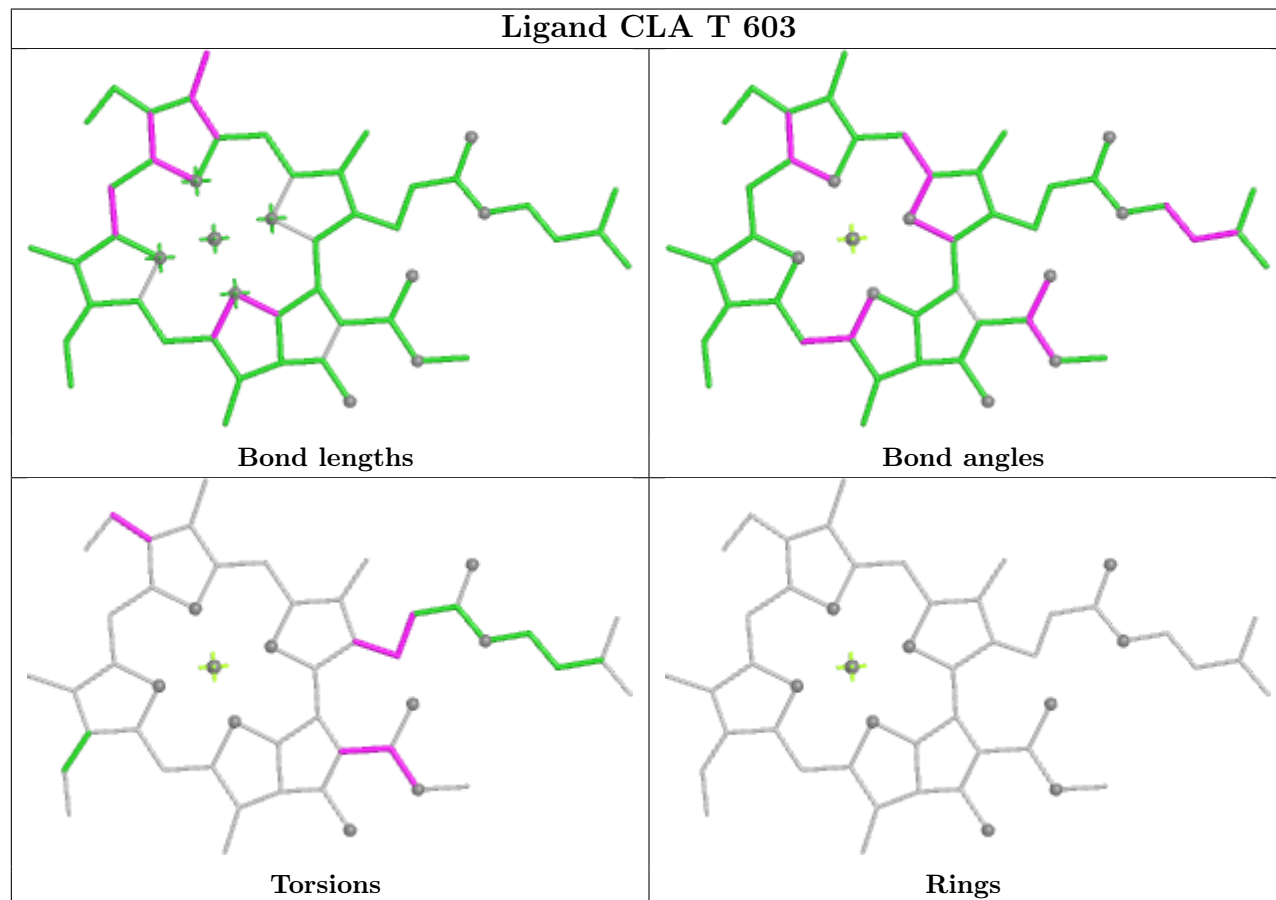


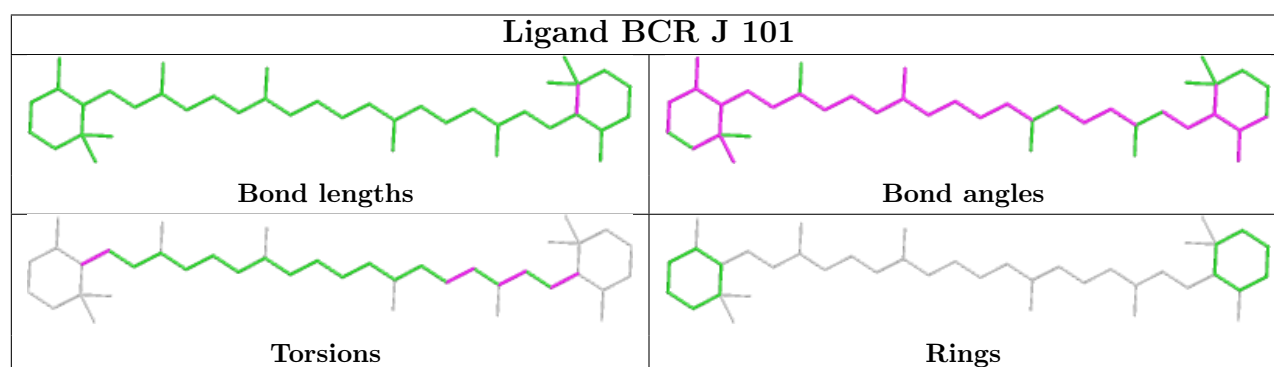
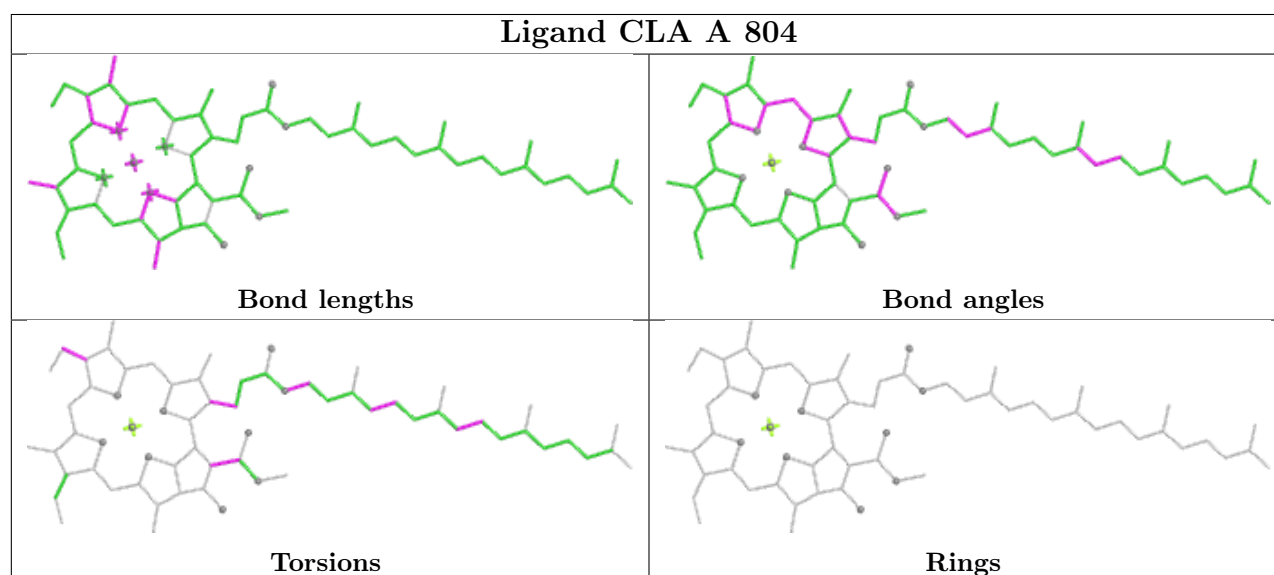
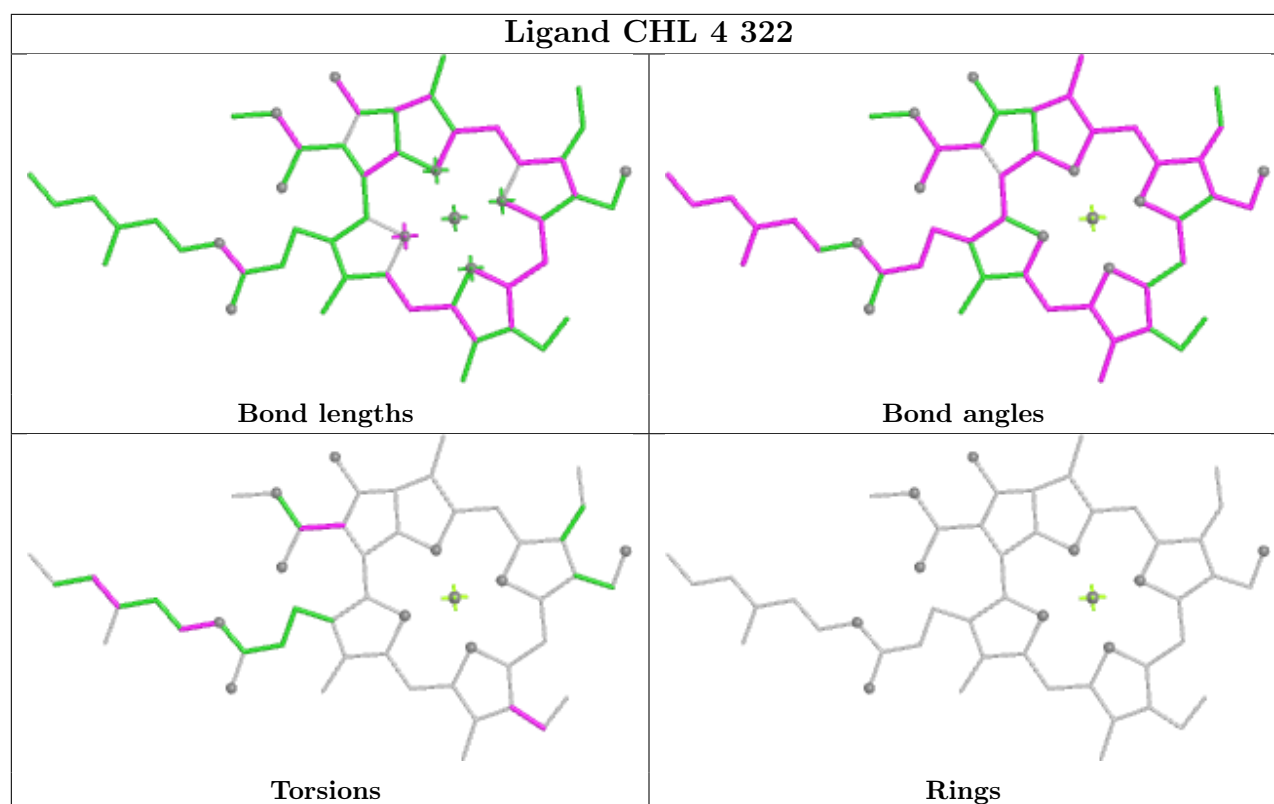




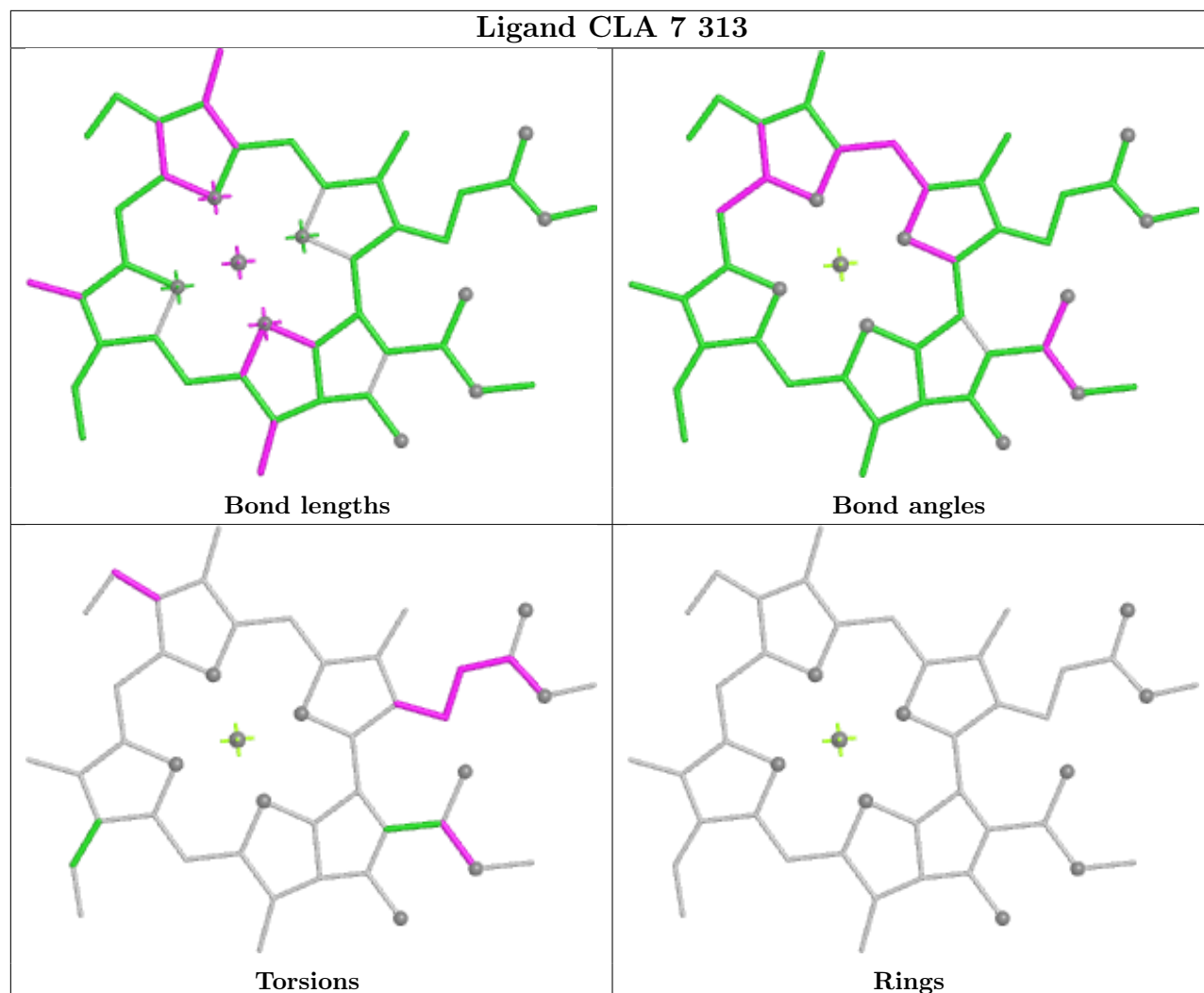


Ligand CLA S 313**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 6 609****Bond lengths****Bond angles****Torsions****Rings**

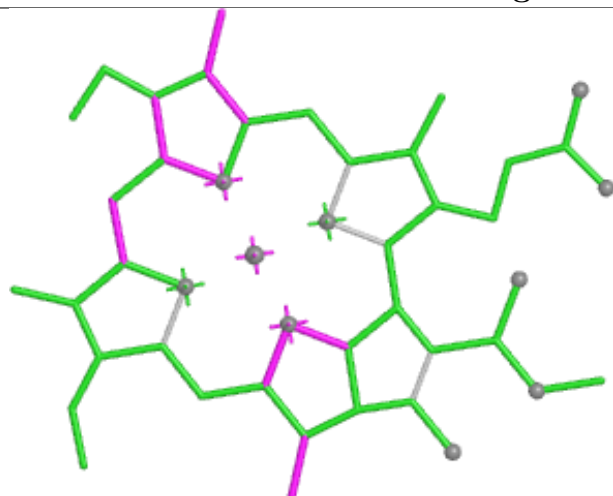
Ligand CLA S 320**Ligand CLA T 603**



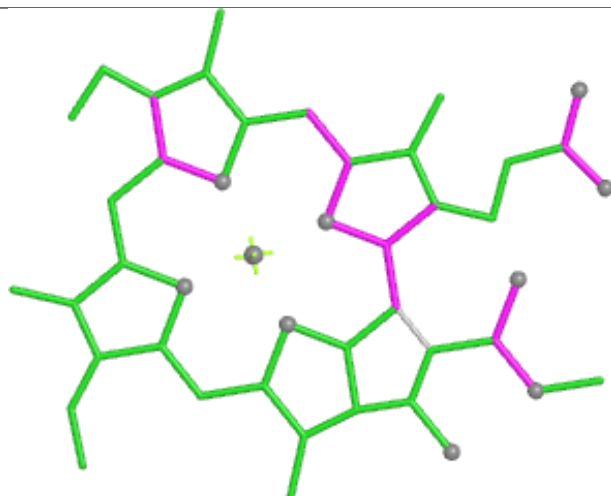
Ligand CLA 7 313



Ligand CLA K 204



Bond lengths



Bond angles

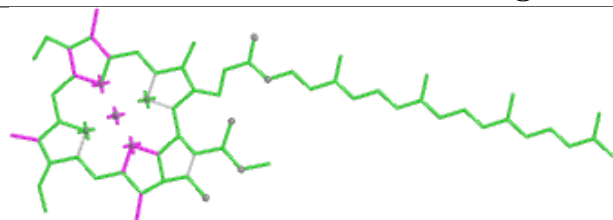


Torsions

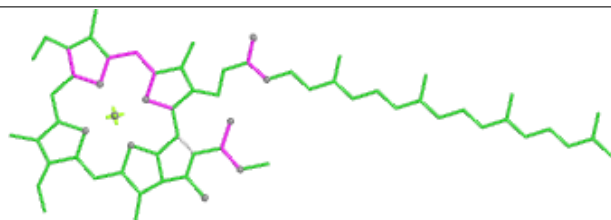


Rings

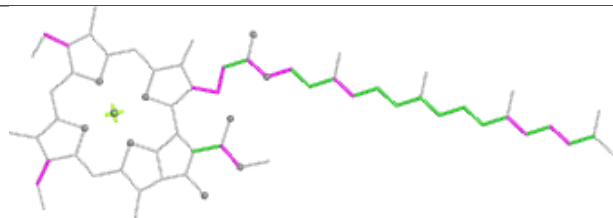
Ligand CLA B 837



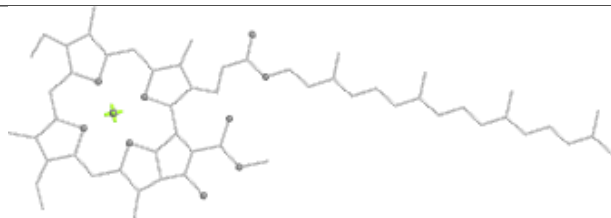
Bond lengths



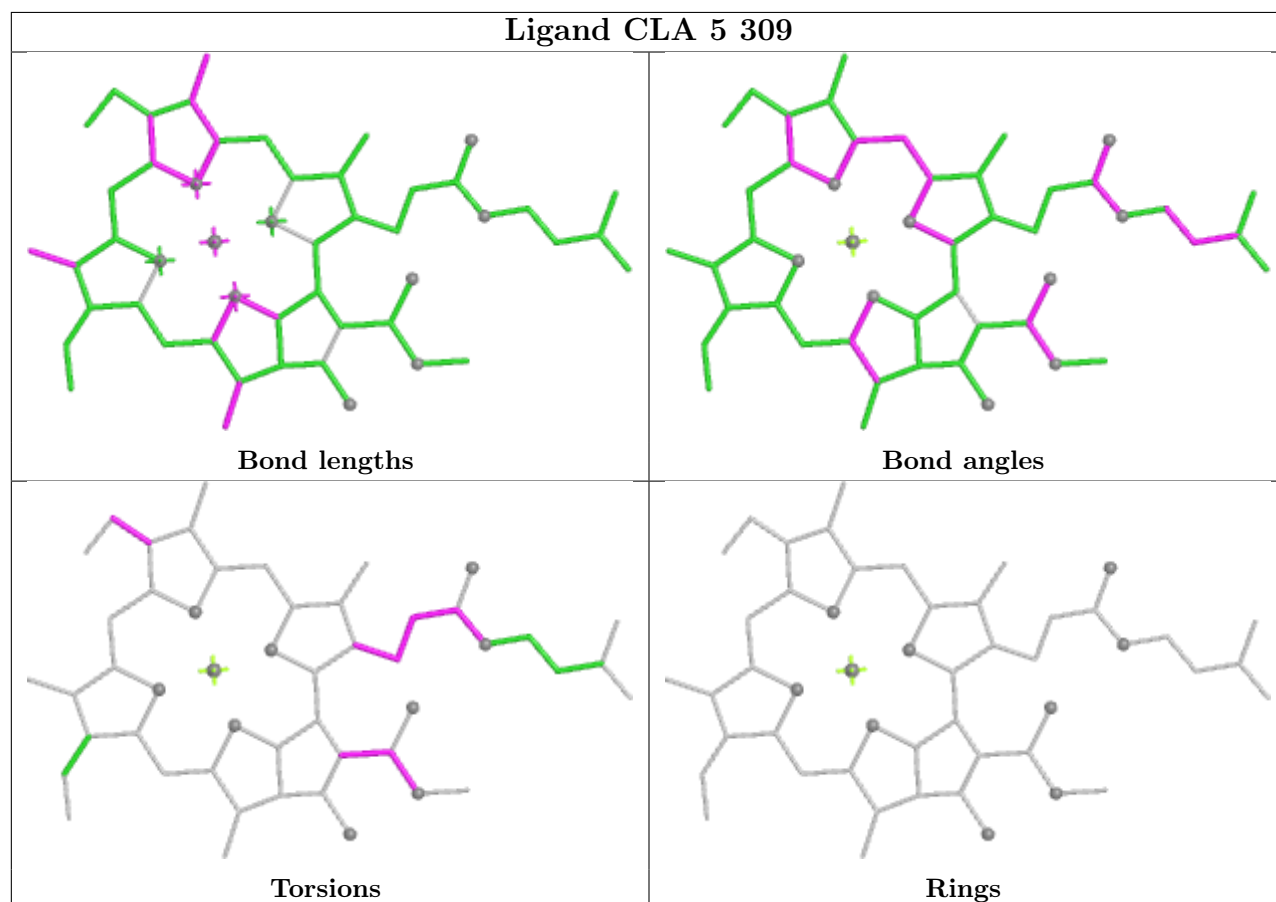
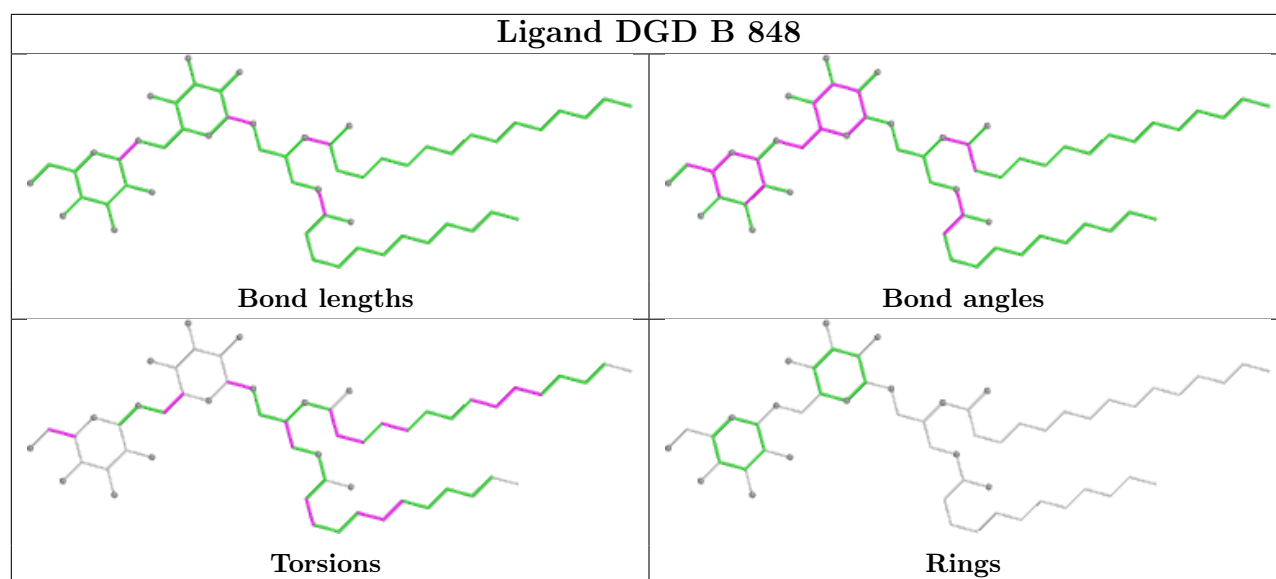
Bond angles

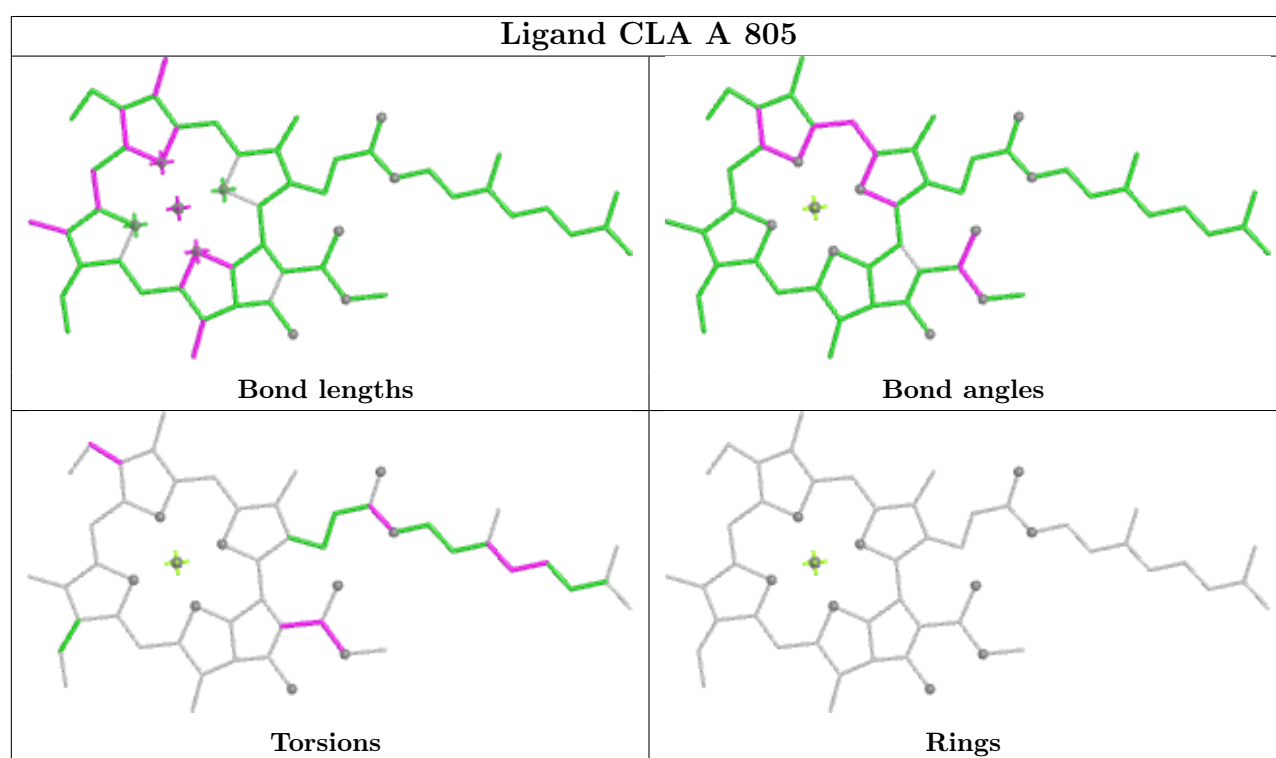
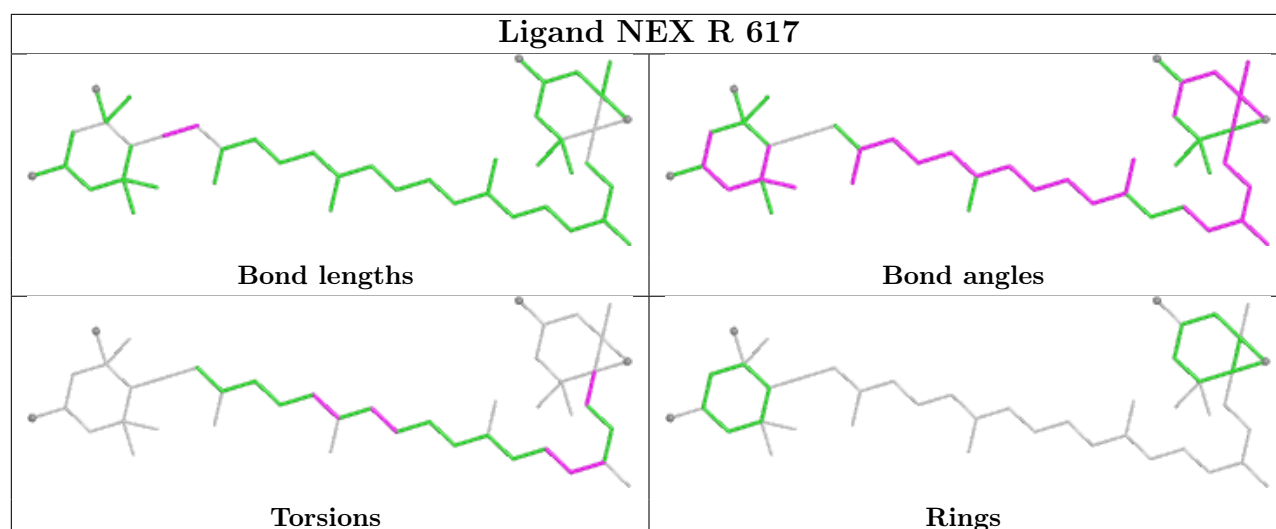


Torsions

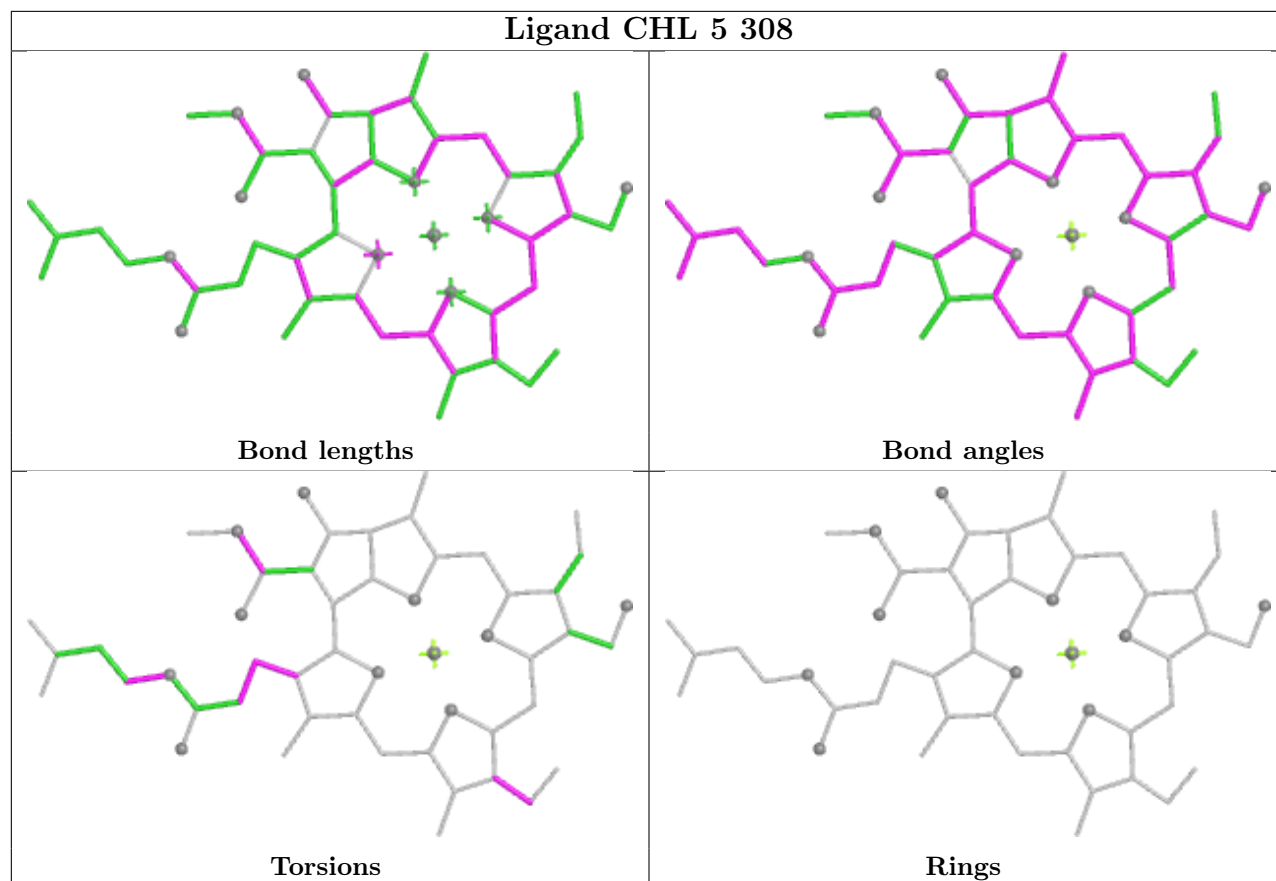


Rings

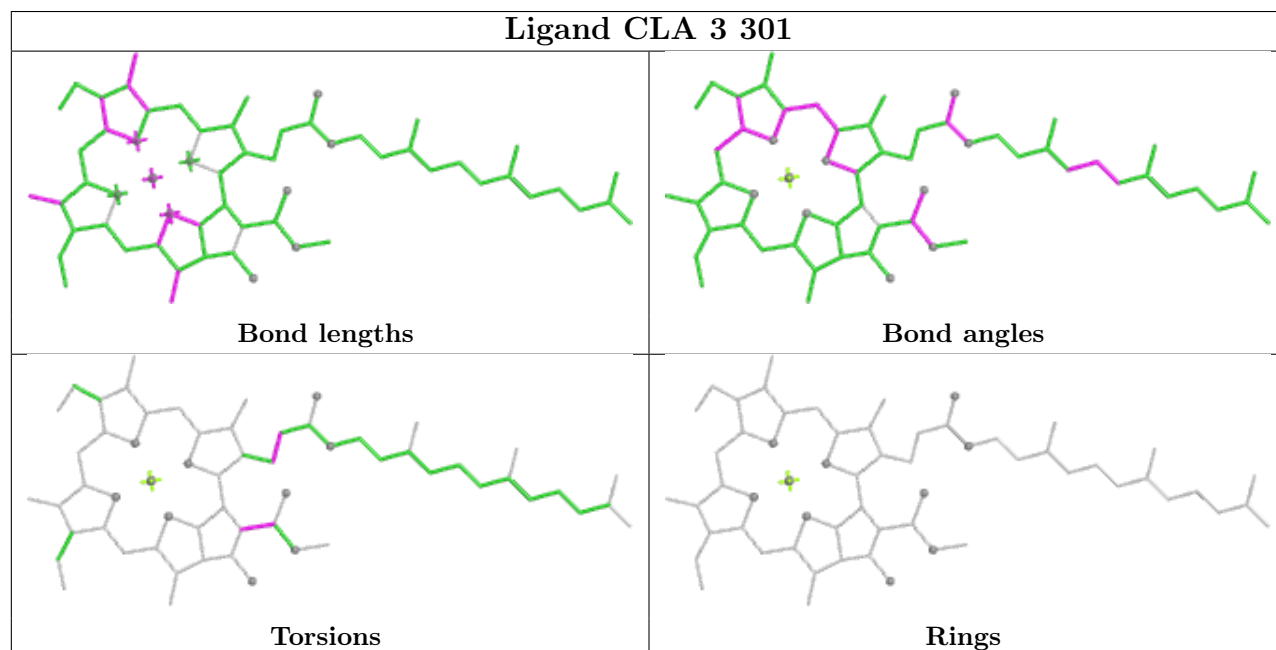




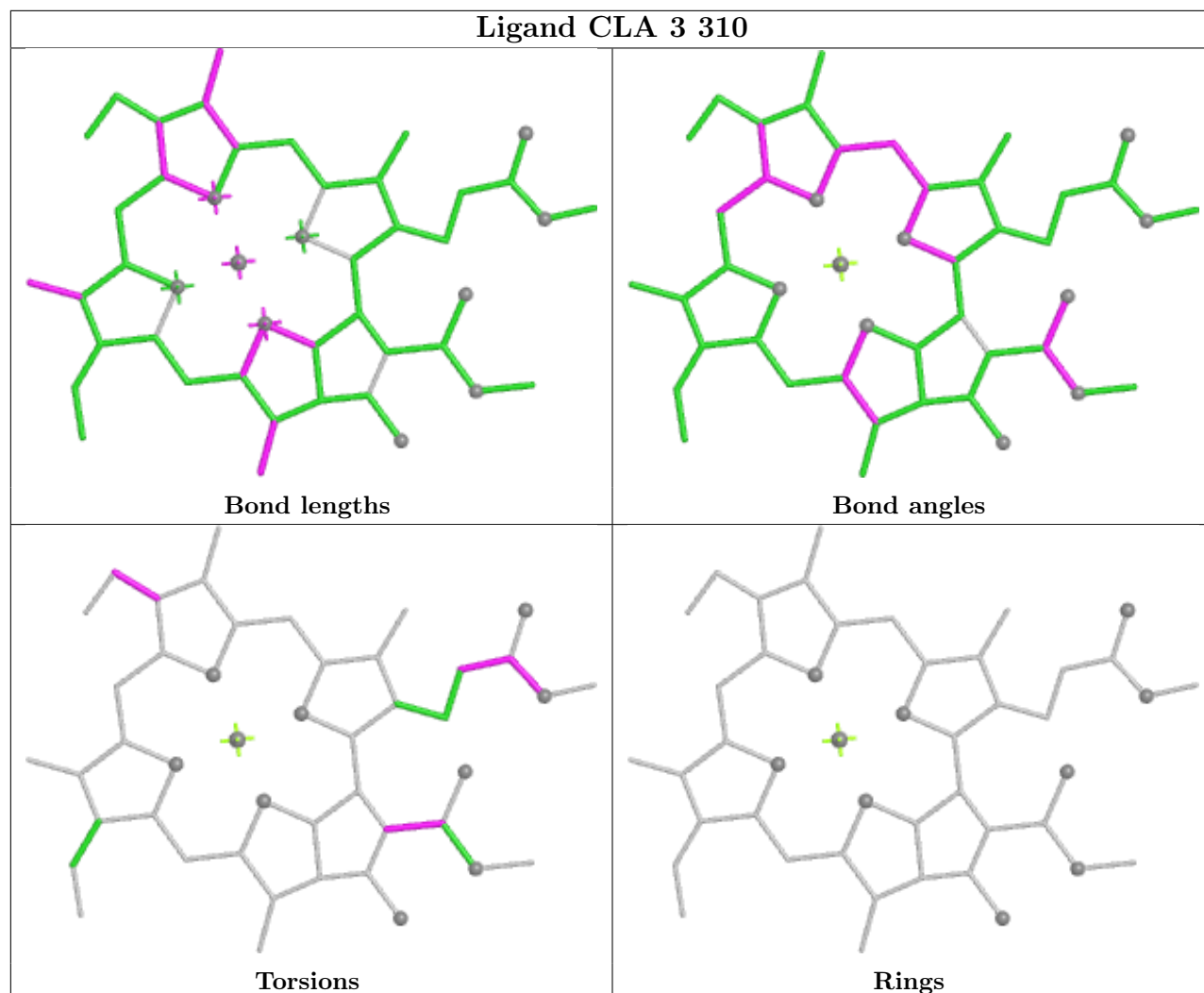
Ligand CHL 5 308



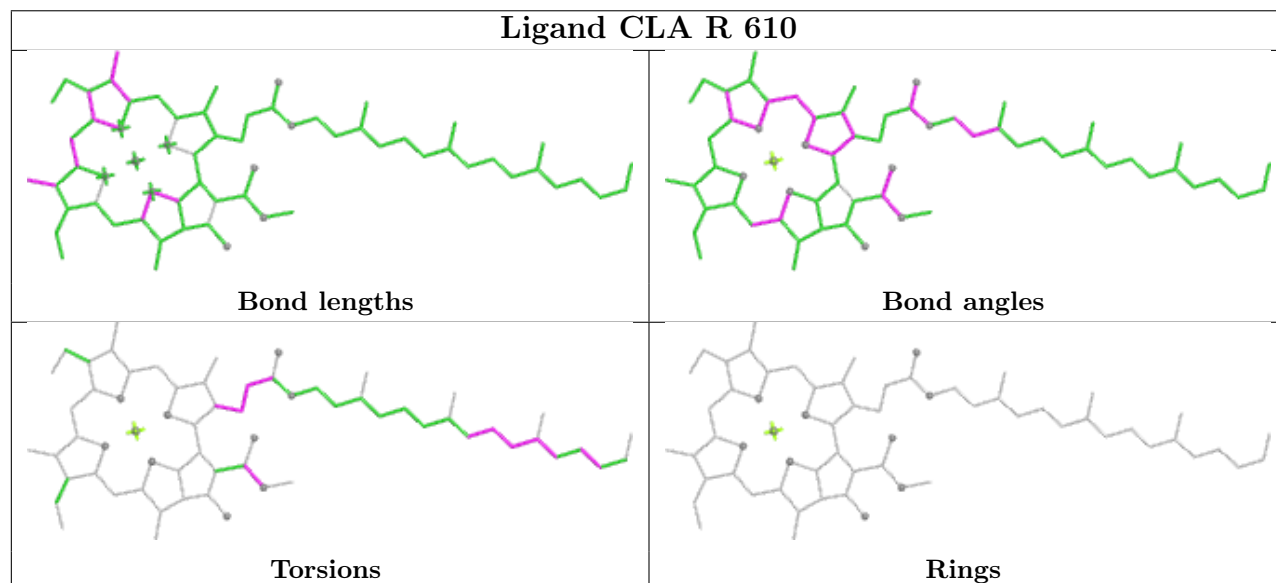
Ligand CLA 3 301



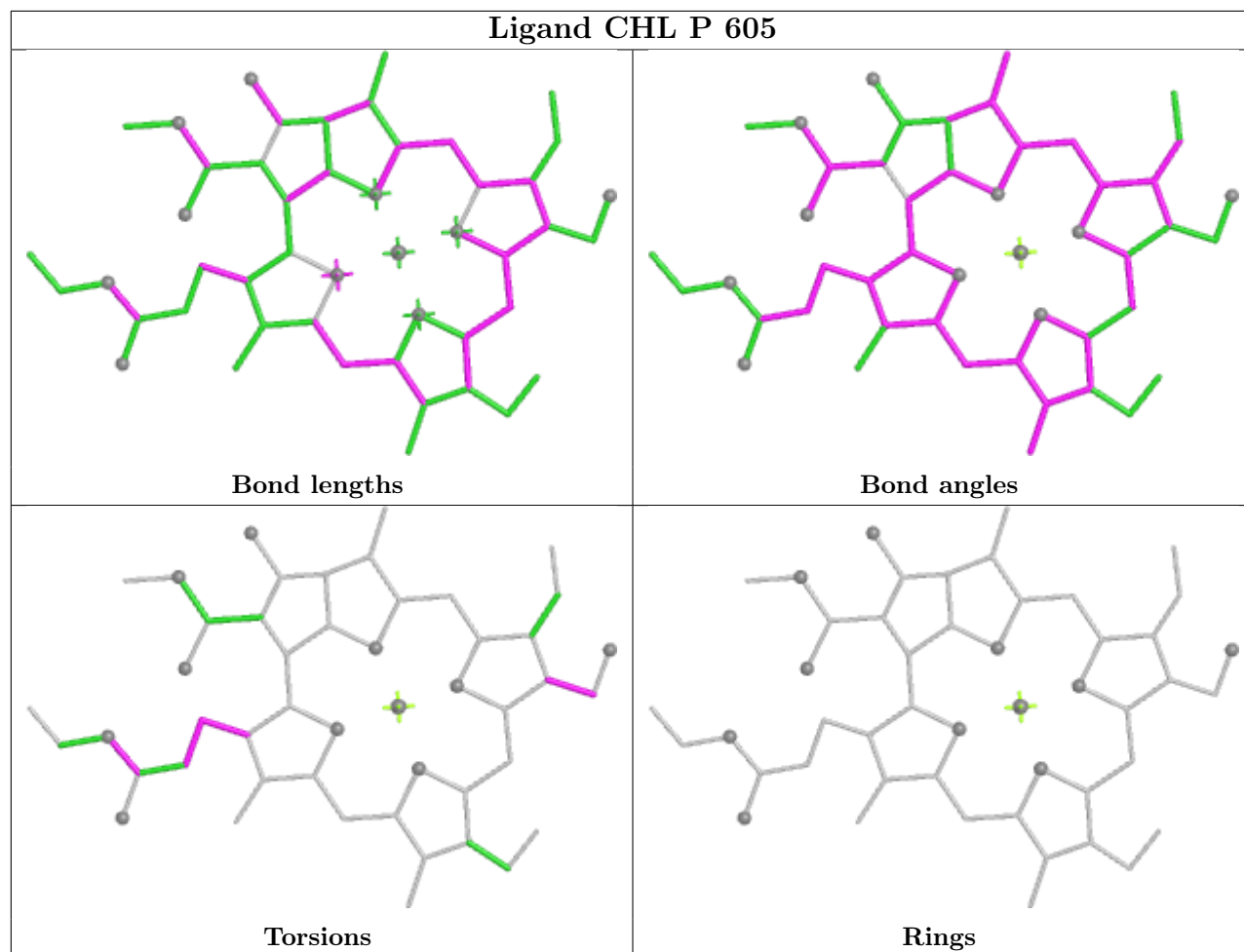
Ligand CLA 3 310



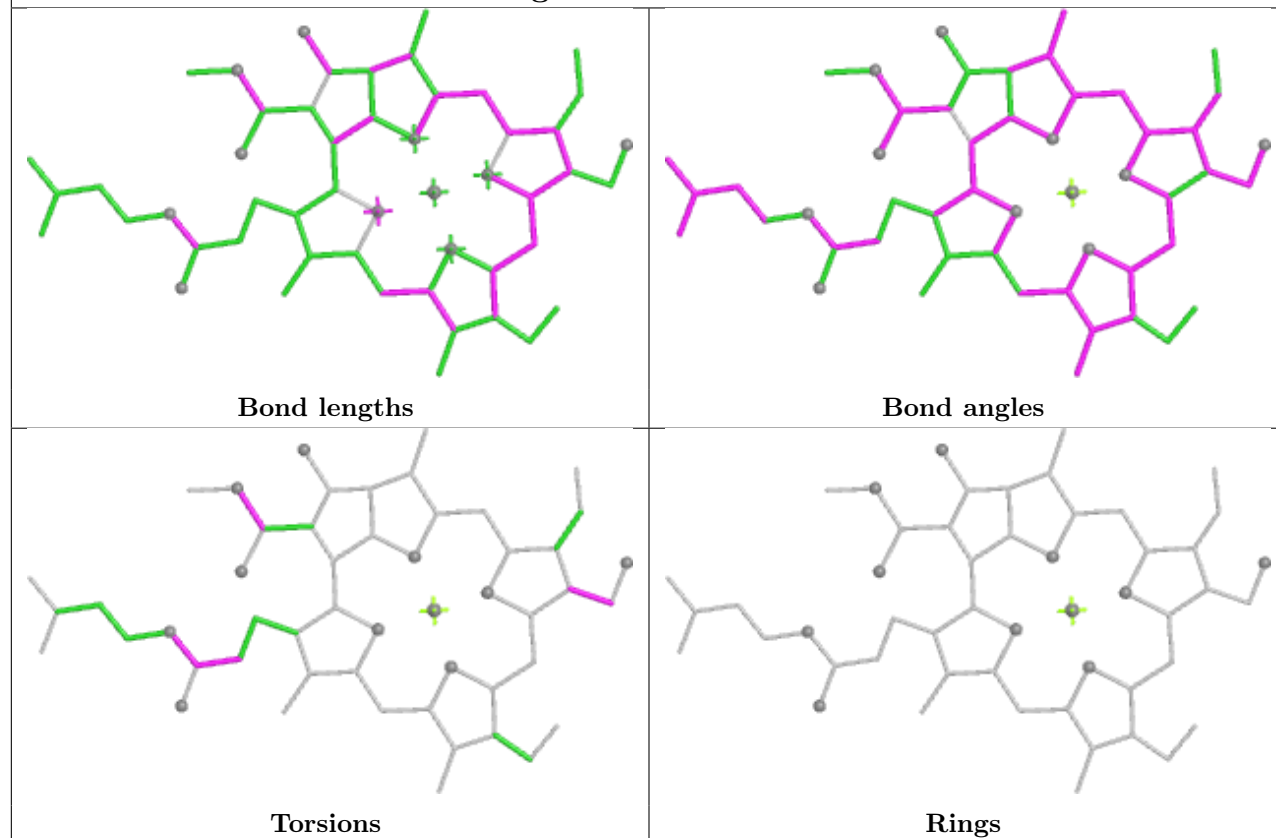
Ligand CLA R 610



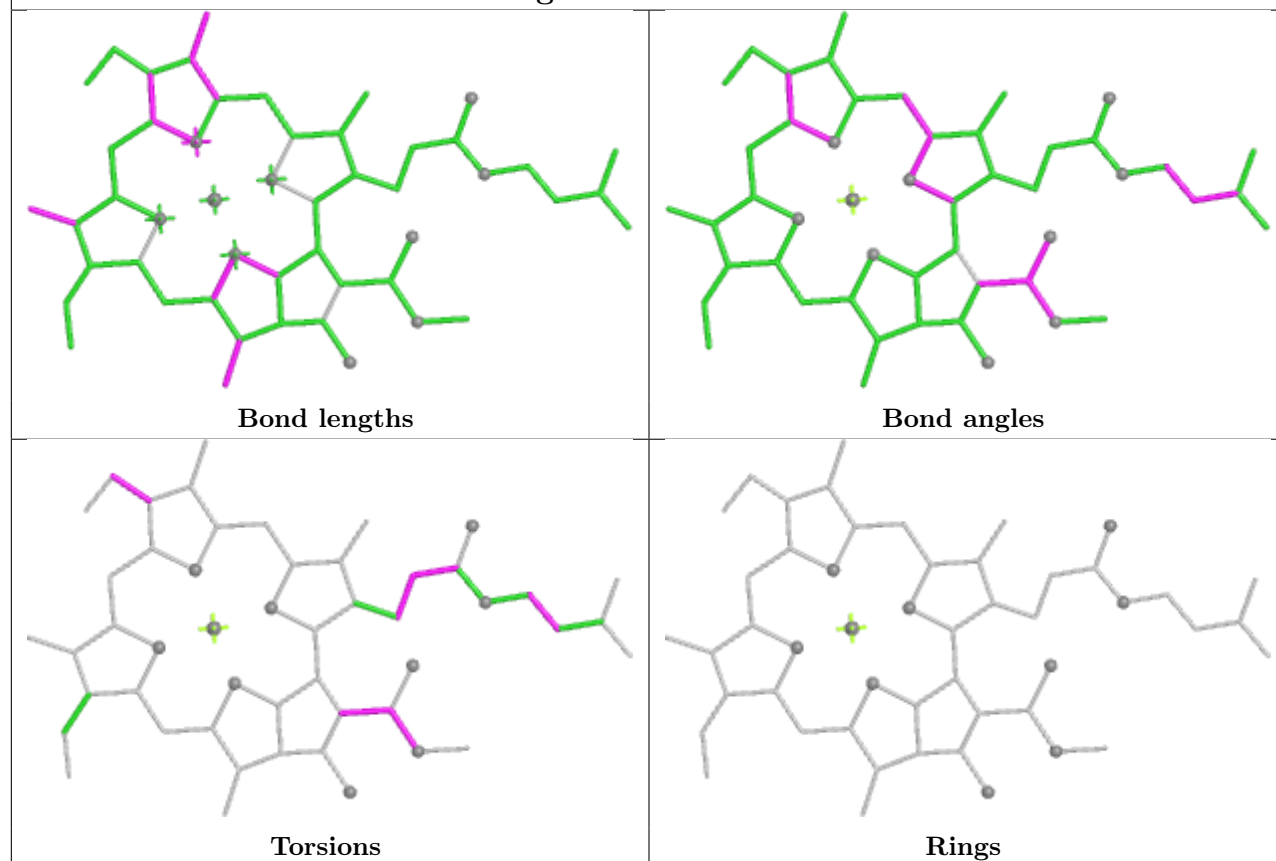
Ligand CHL P 605

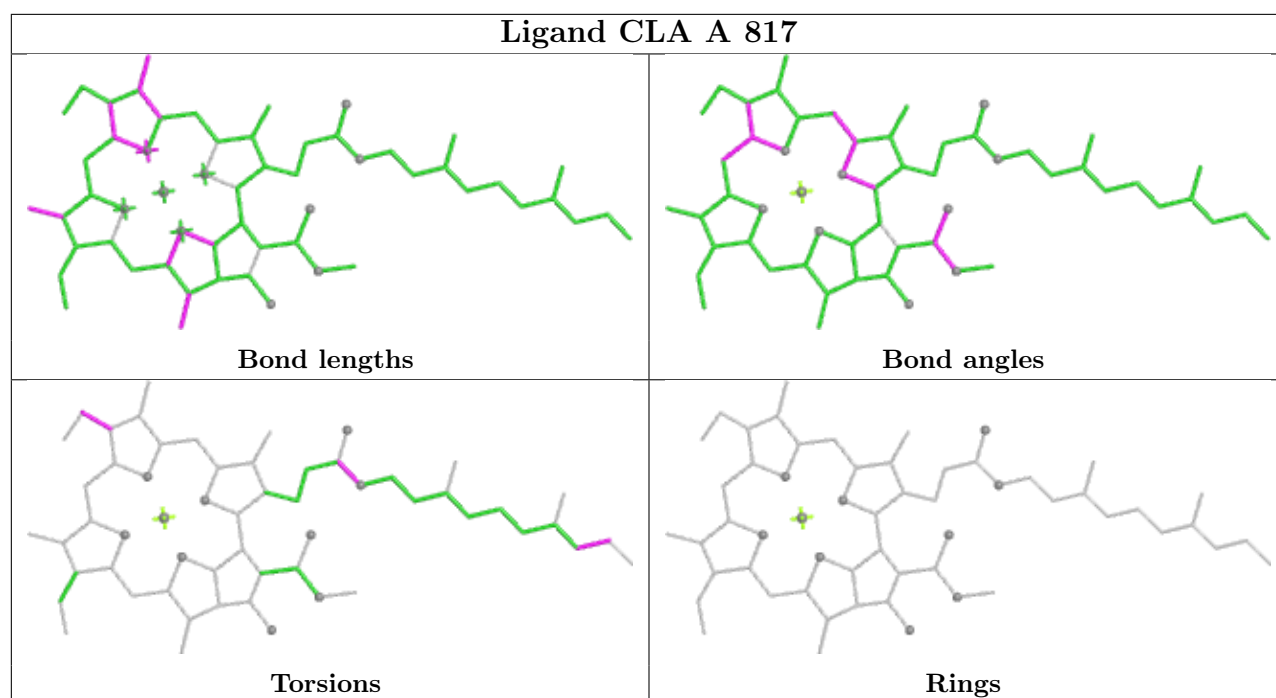


Ligand CHL R 601

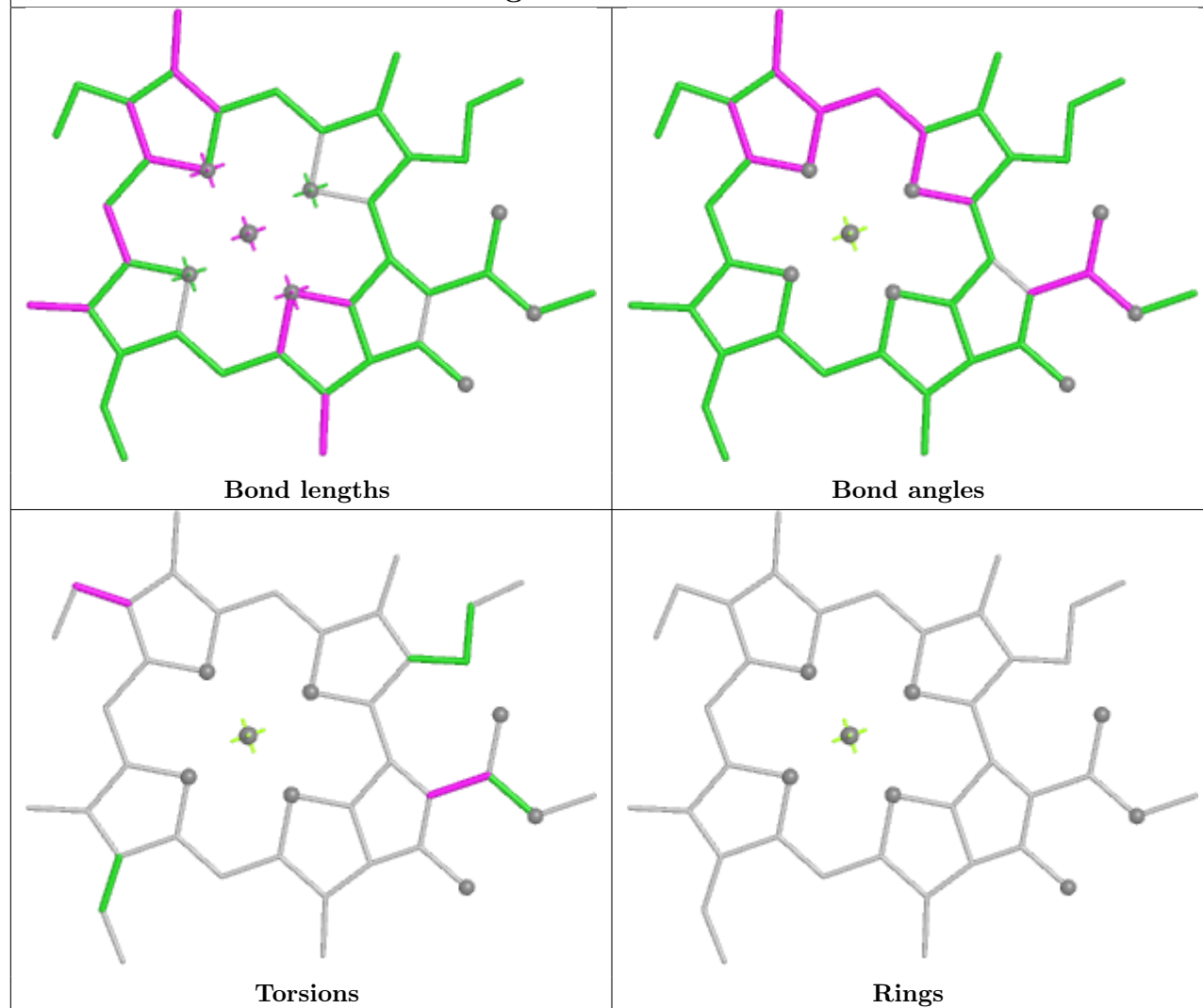


Ligand CLA 9 305

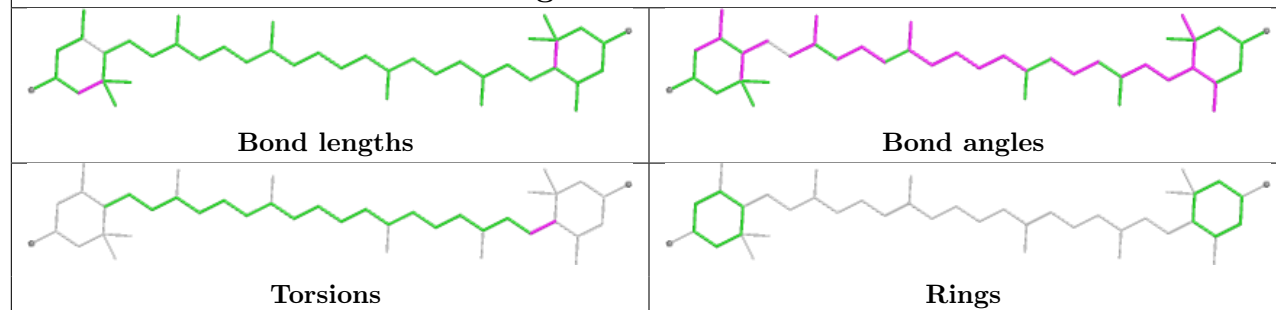


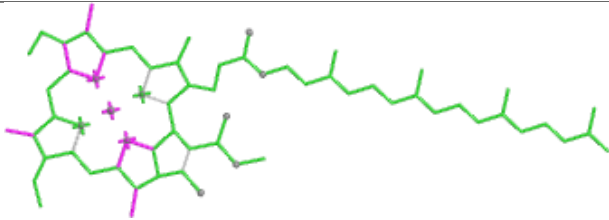
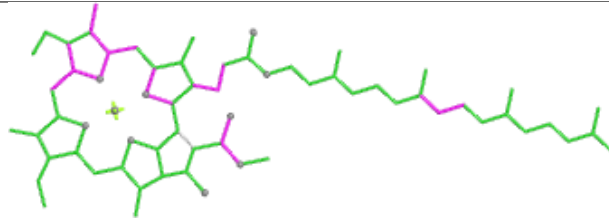
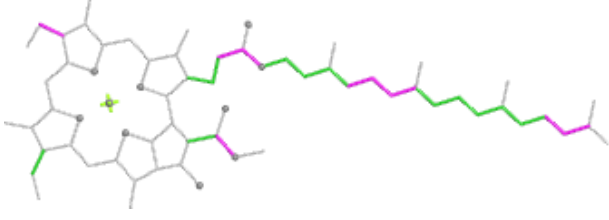
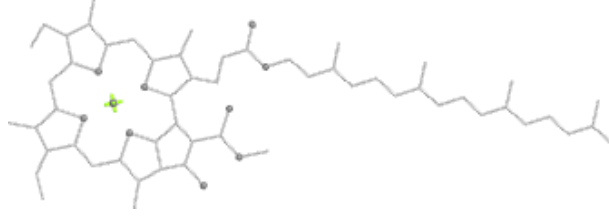


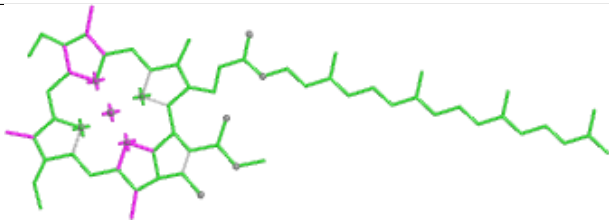
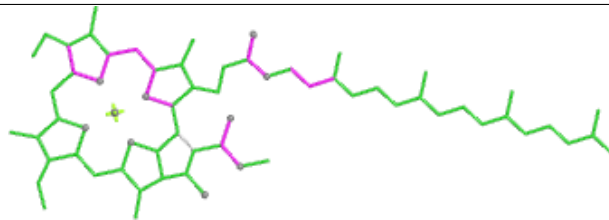
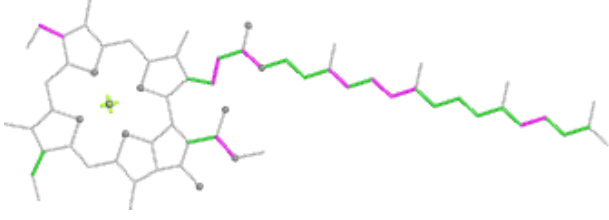
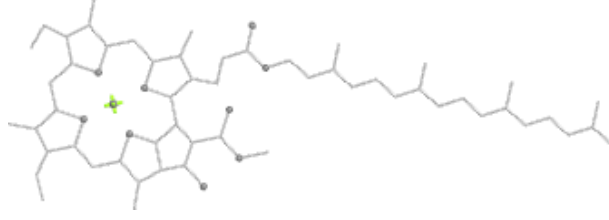
Ligand CLA 7 312

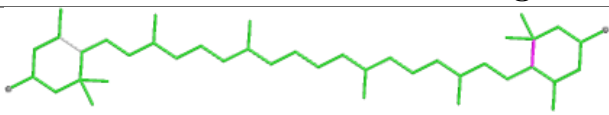
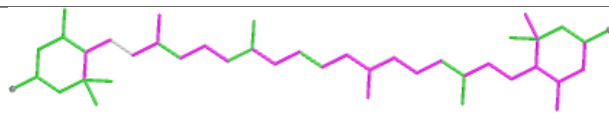
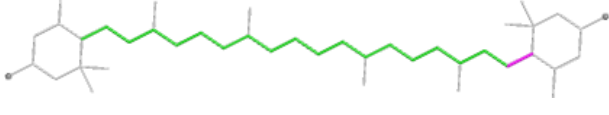
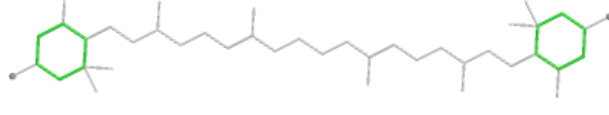


Ligand LUT 9 312

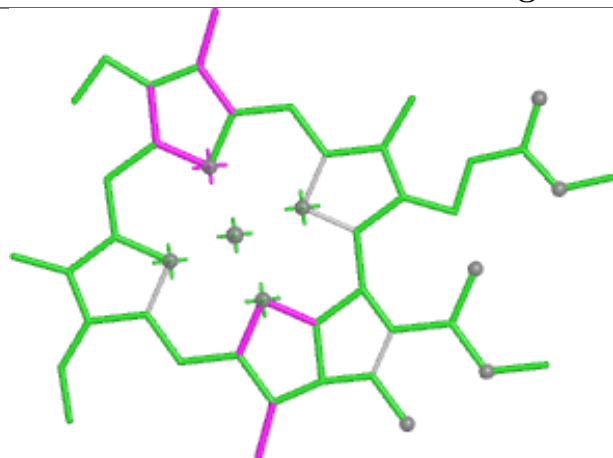


Ligand CLA A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

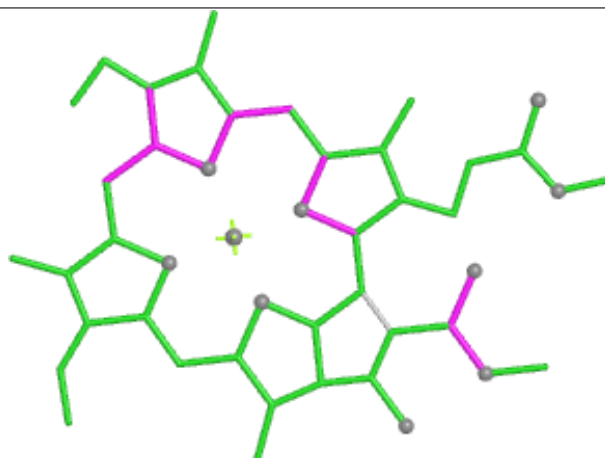
Ligand CLA A 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 8 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

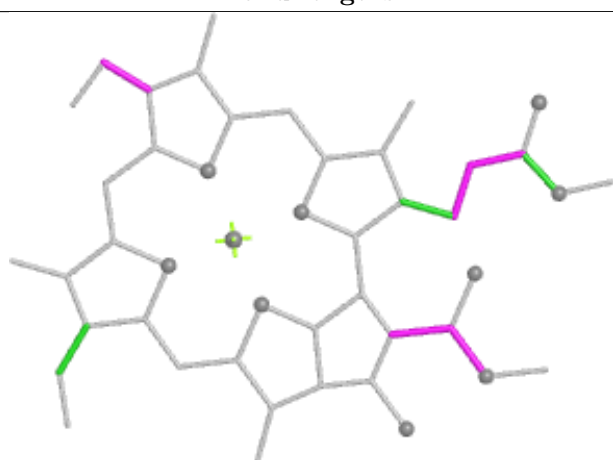
Ligand CLA 9 302



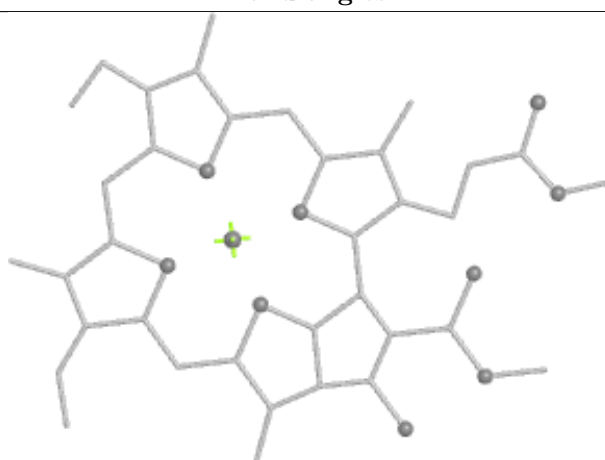
Bond lengths



Bond angles

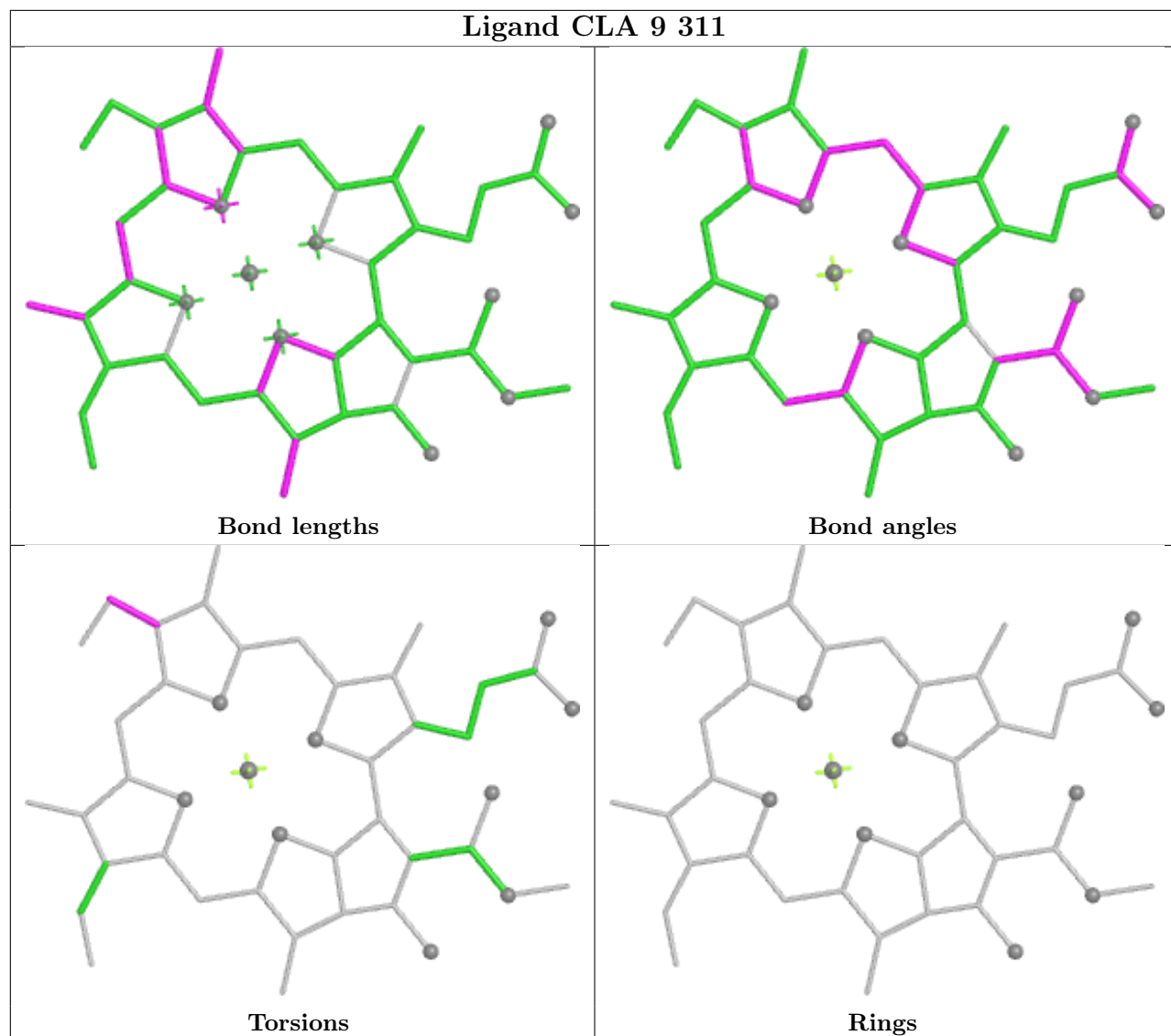


Torsions

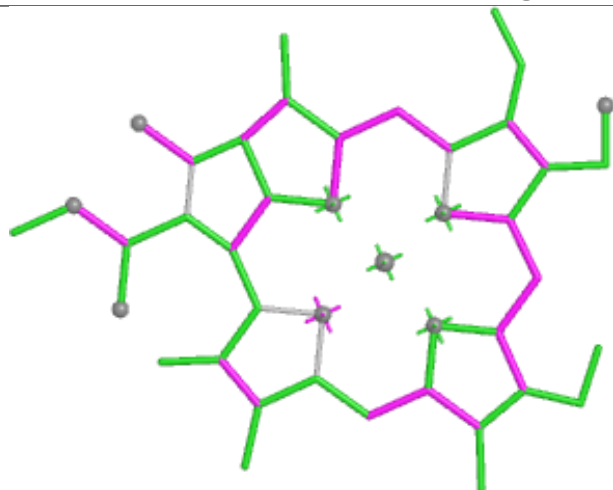


Rings

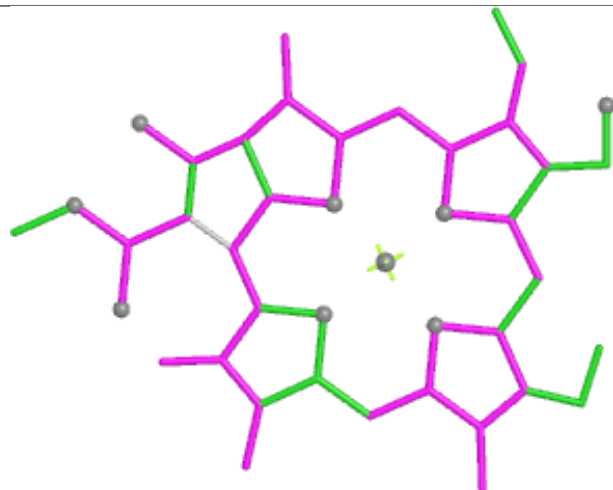
Ligand CLA 9 311



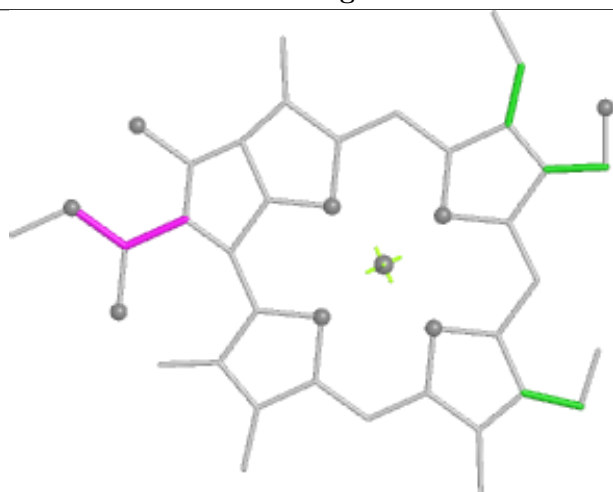
Ligand CHL 4 304



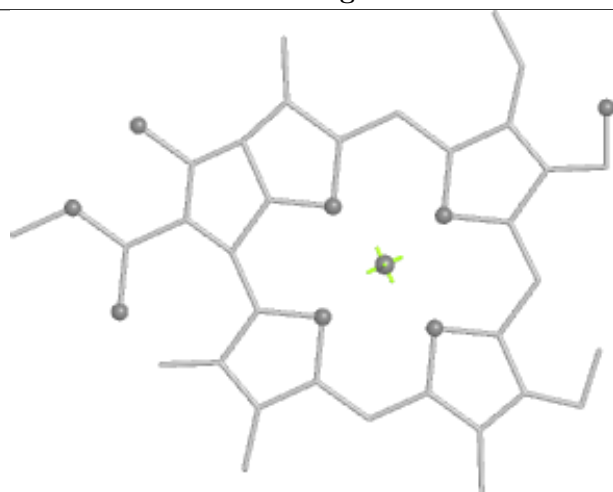
Bond lengths



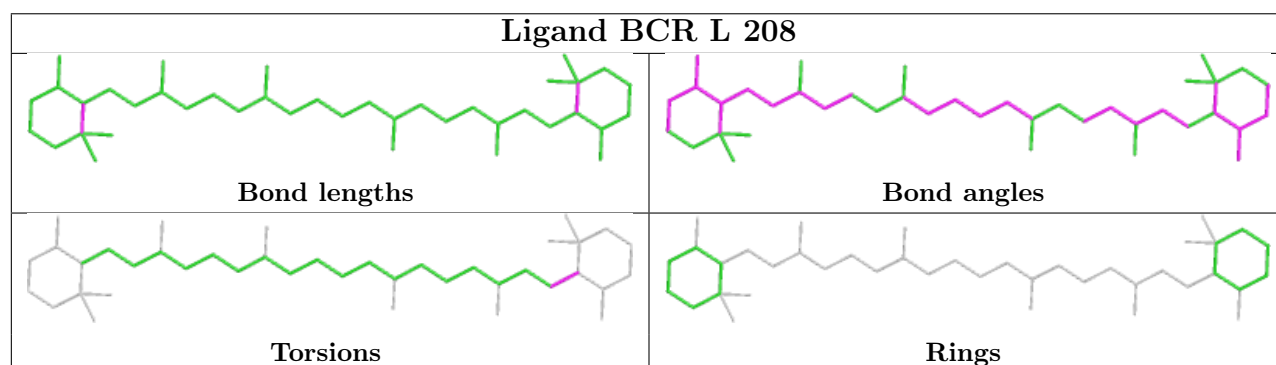
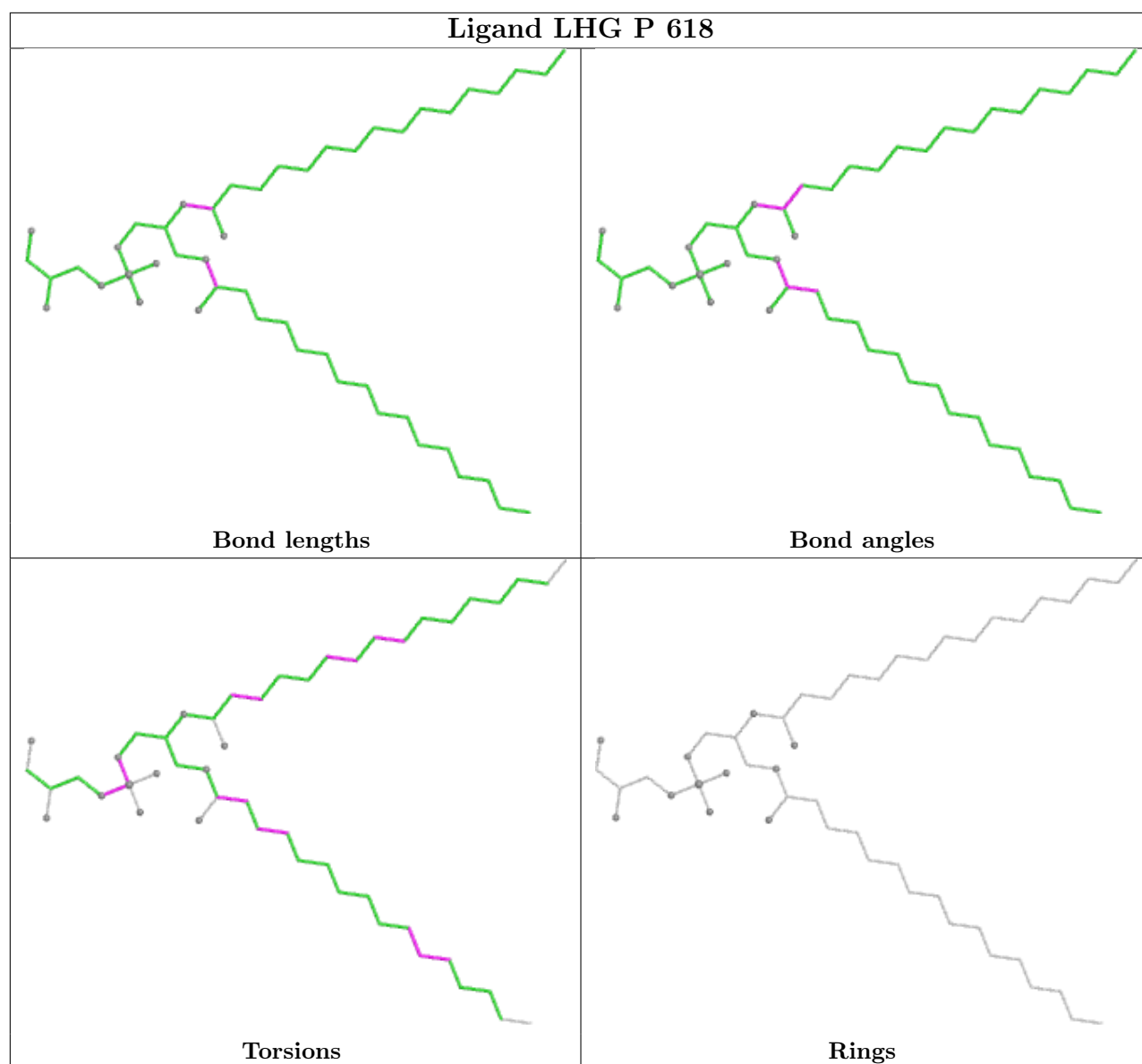
Bond angles

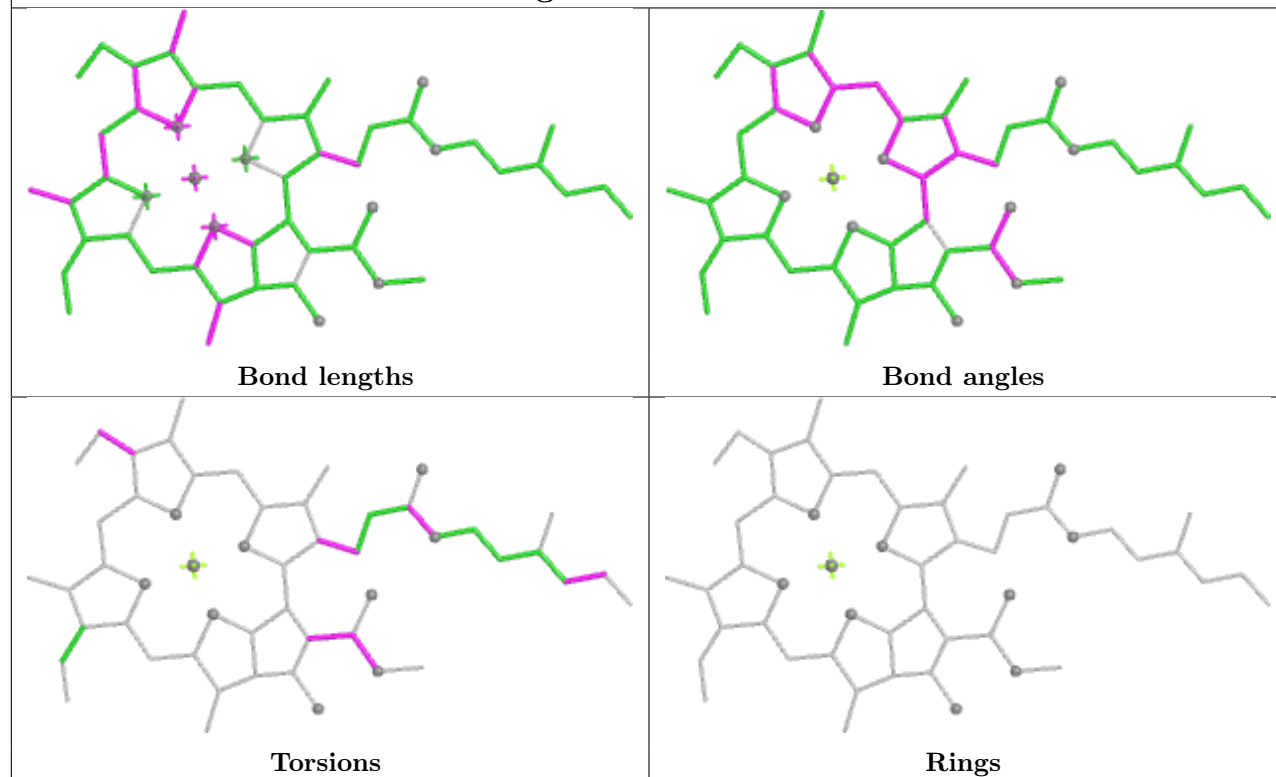
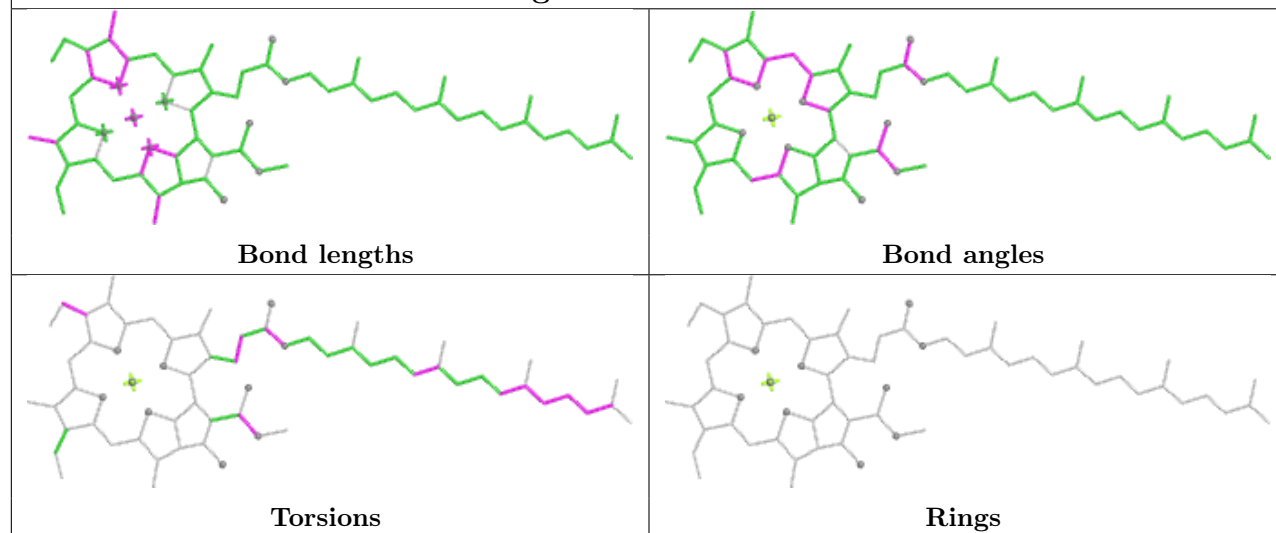


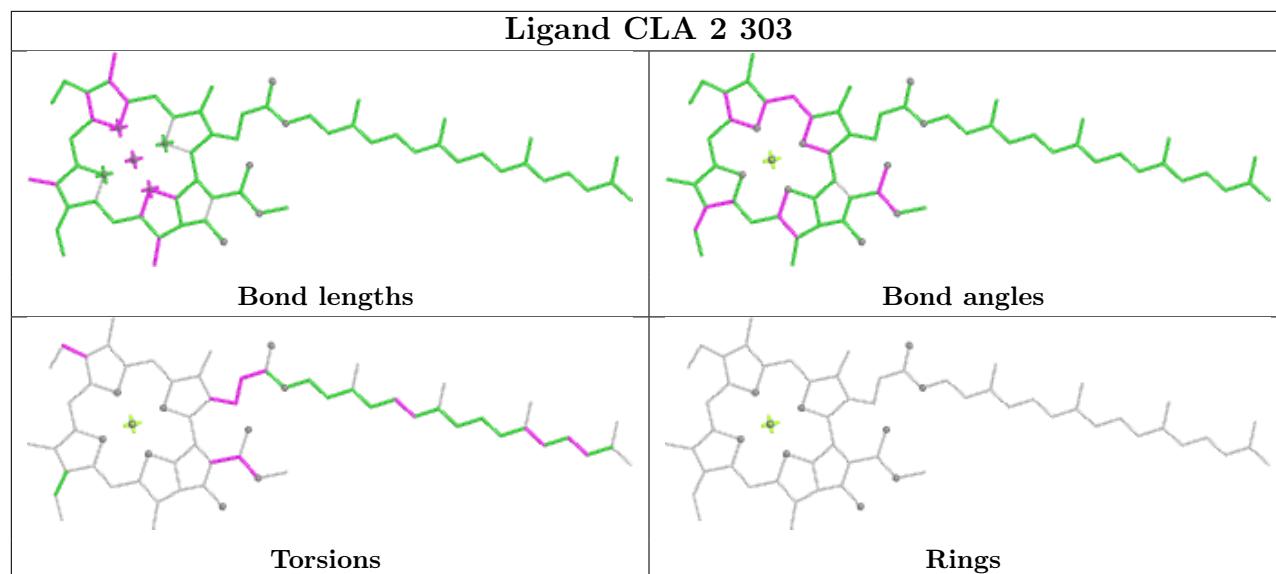
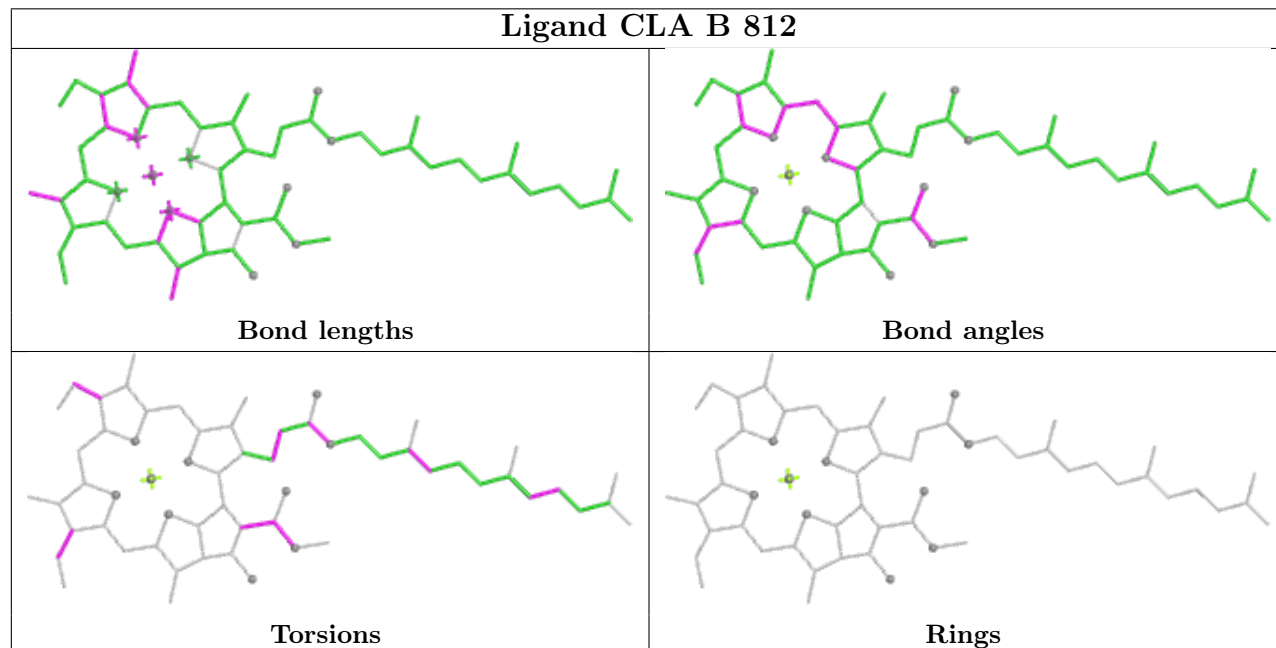
Torsions

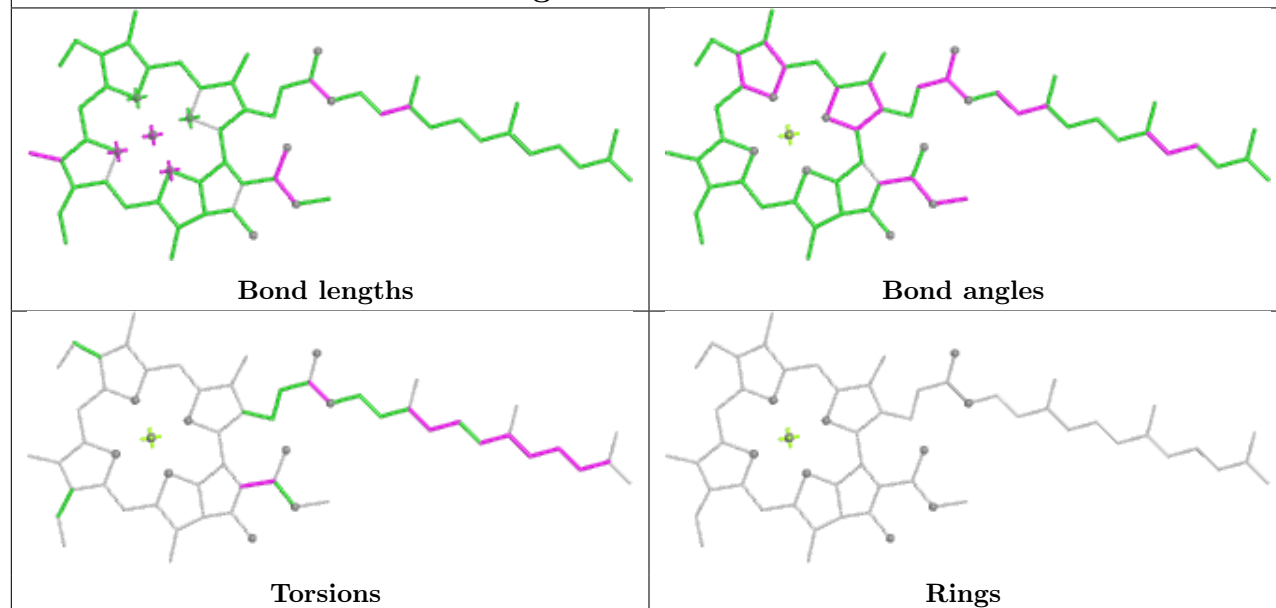
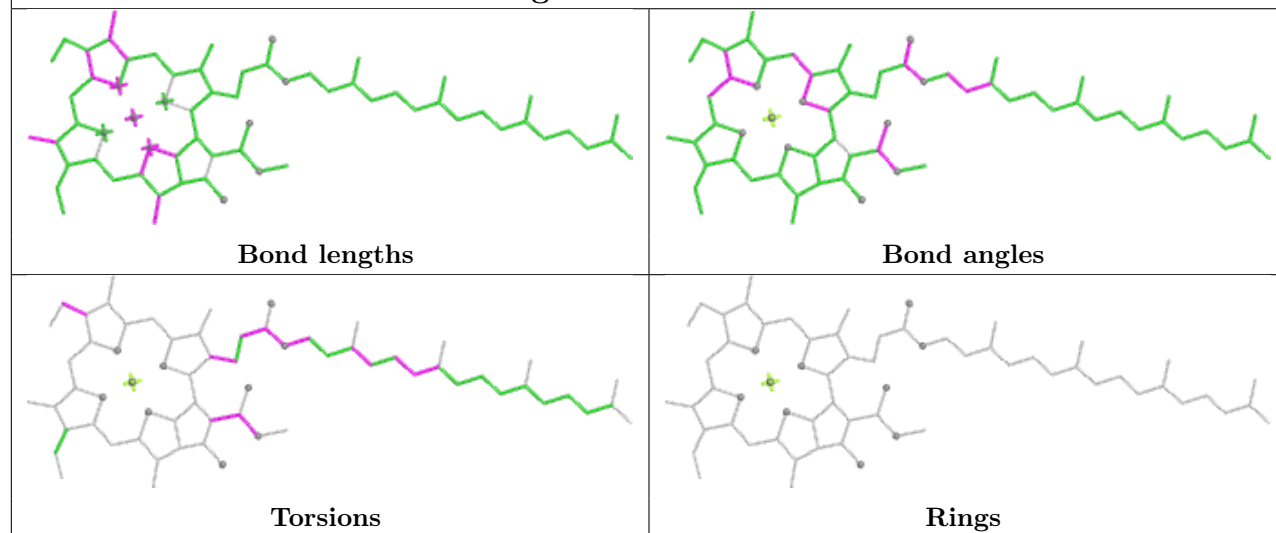


Rings

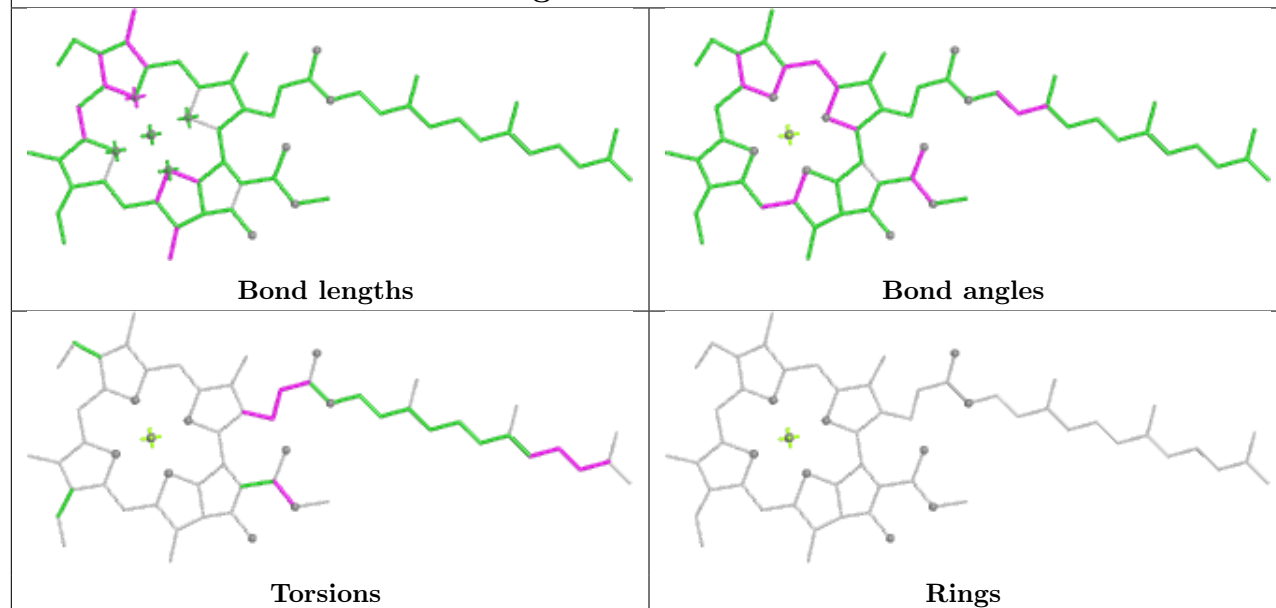


Ligand CLA 4 310**Ligand CLA B 836**

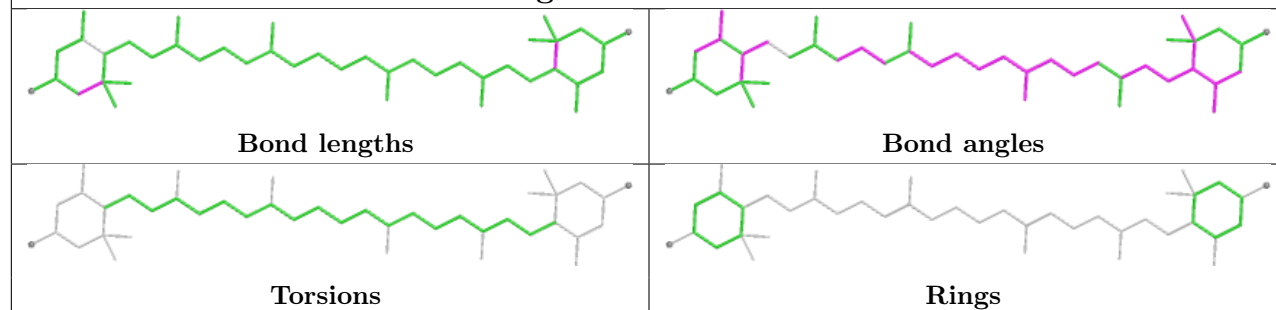
Ligand CLA 2 303**Ligand CLA B 812**

Ligand CLA P 612**Ligand CLA A 828**

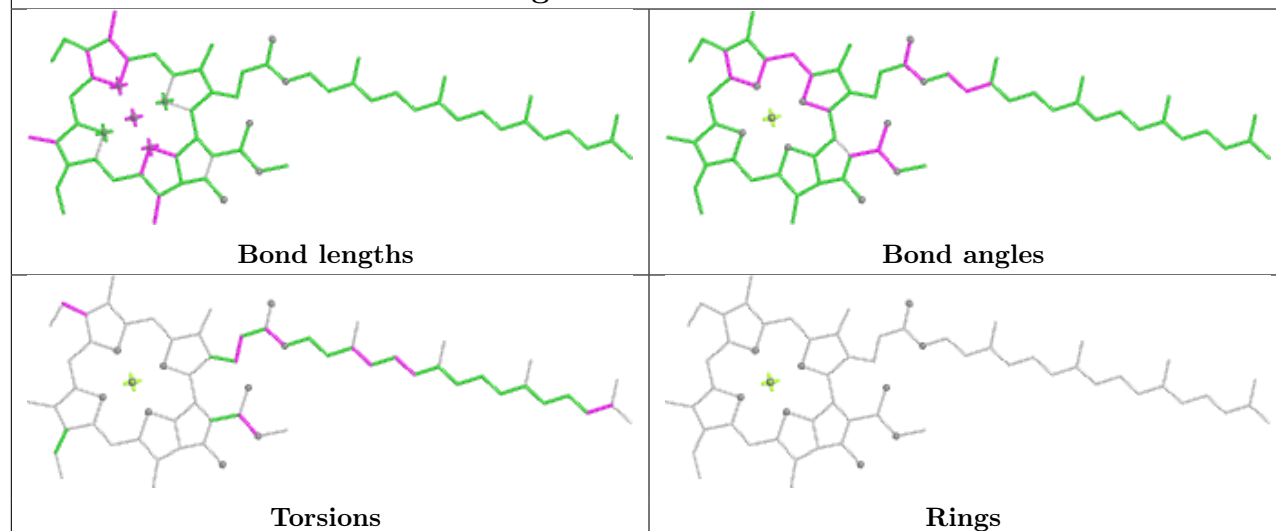
Ligand CLA P 610



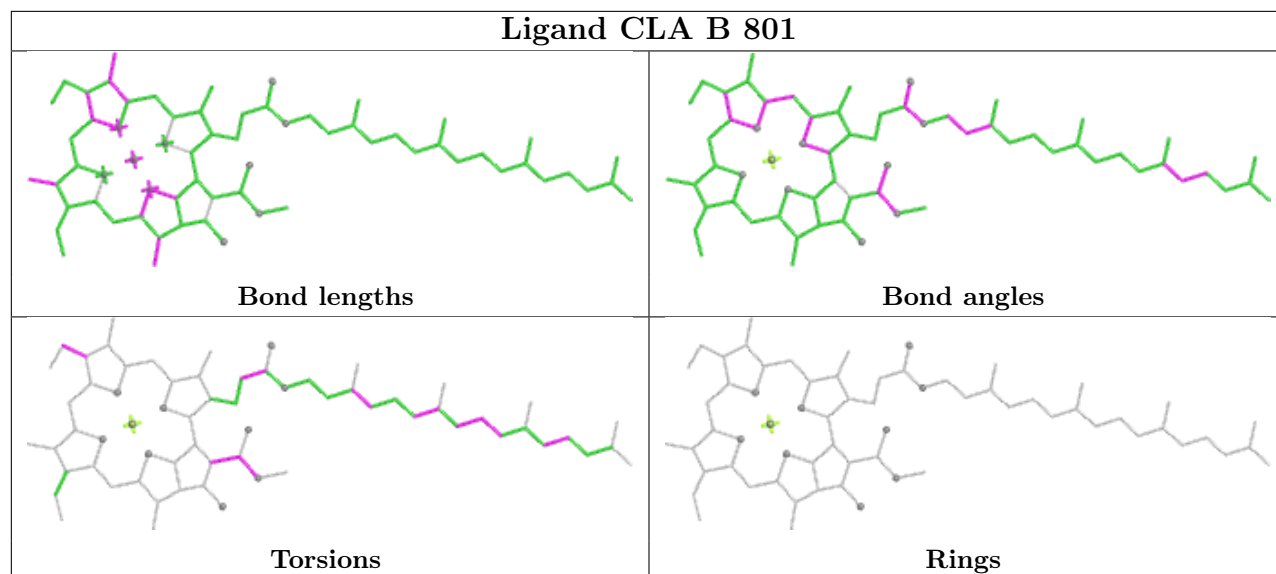
Ligand LUT 5 318



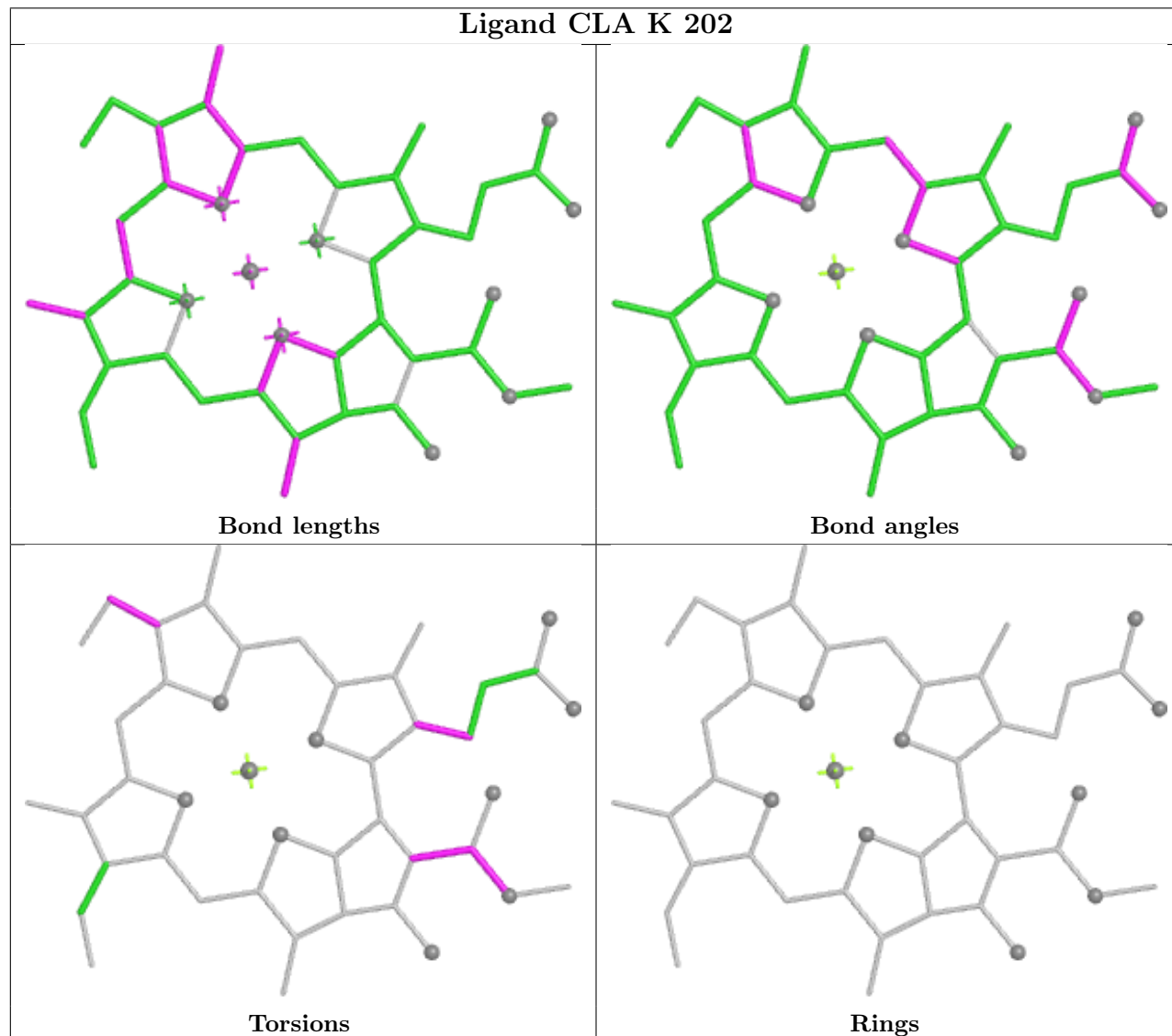
Ligand CLA A 829

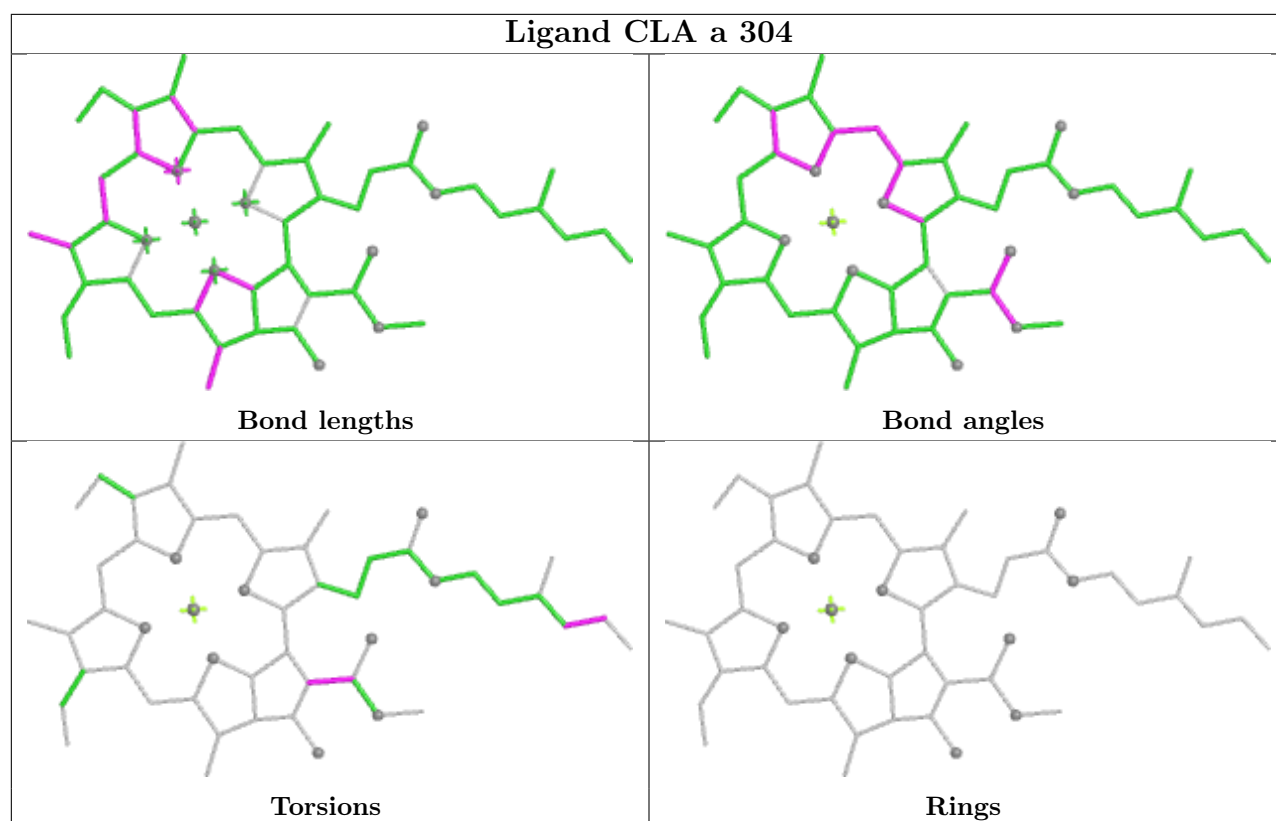


Ligand CLA B 801

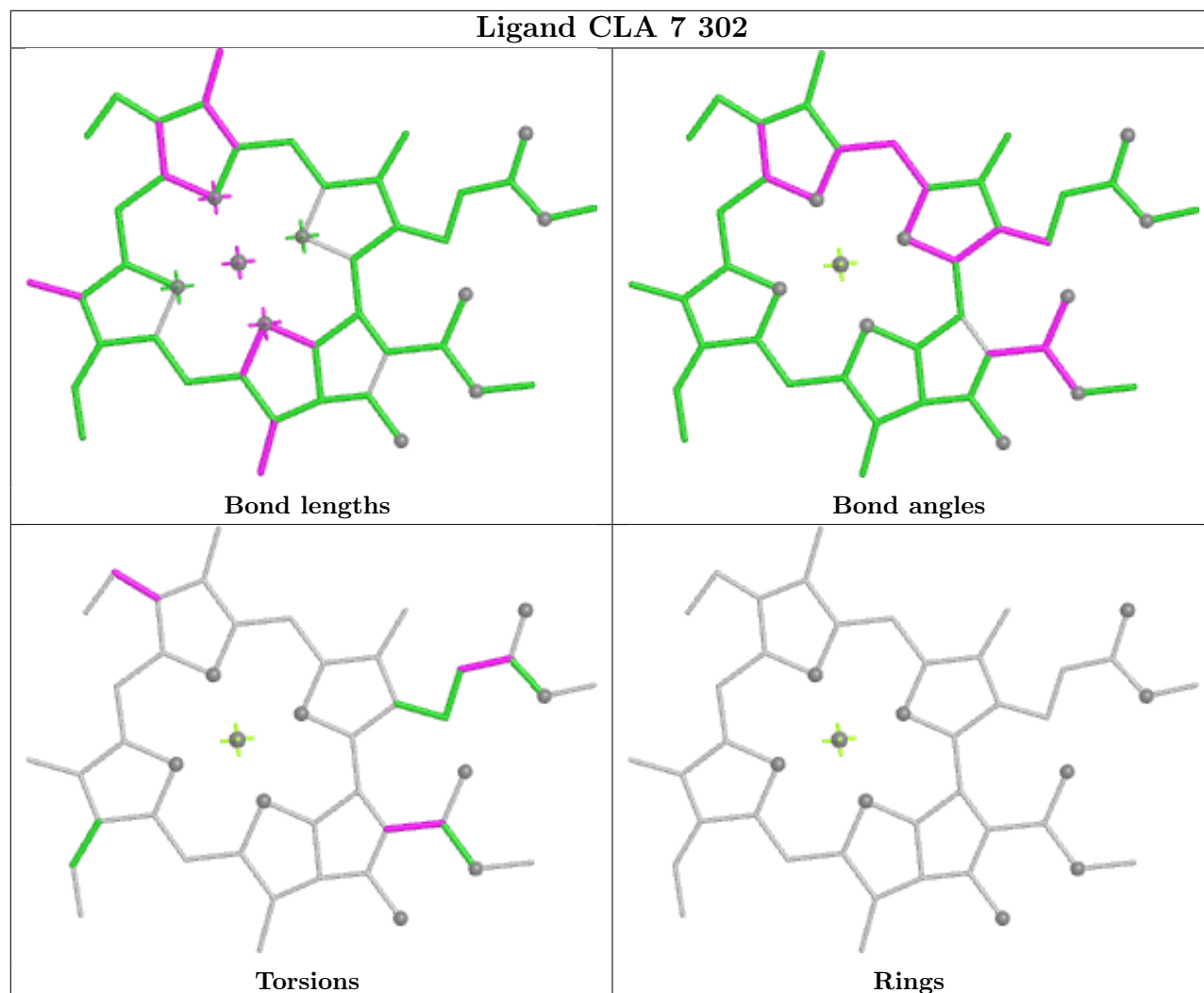


Ligand CLA K 202

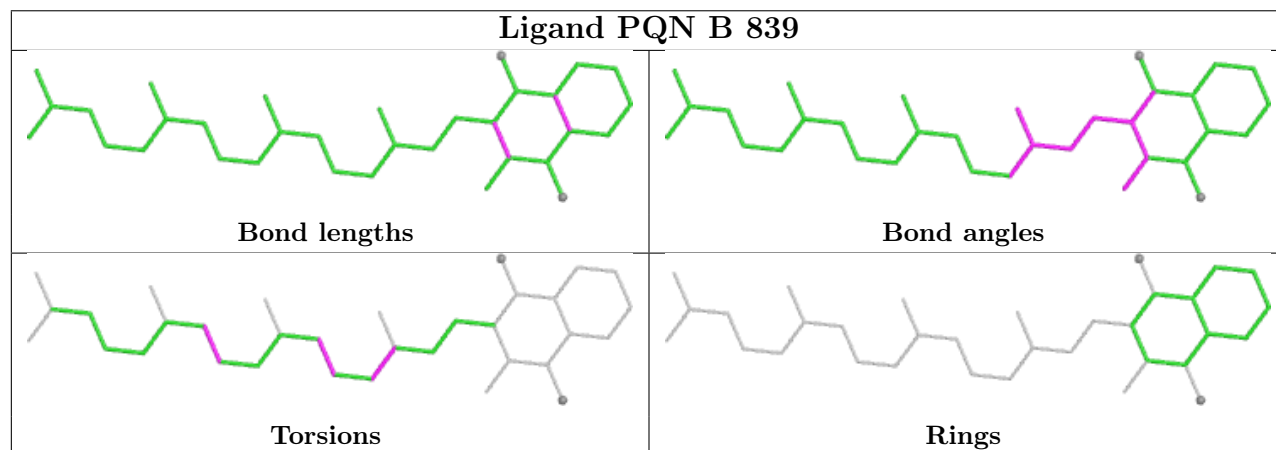




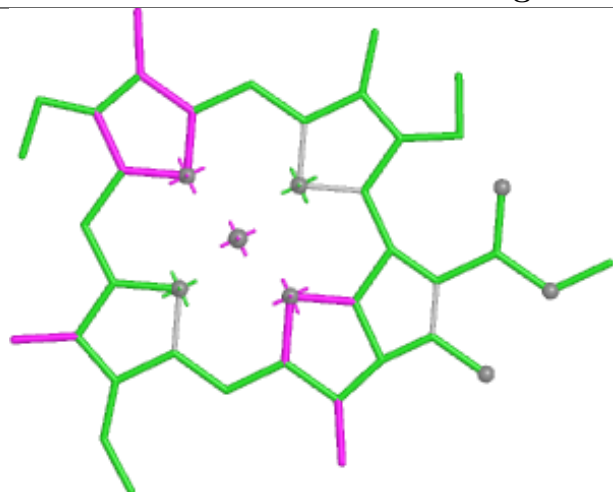
Ligand CLA 7 302



Ligand PQN B 839



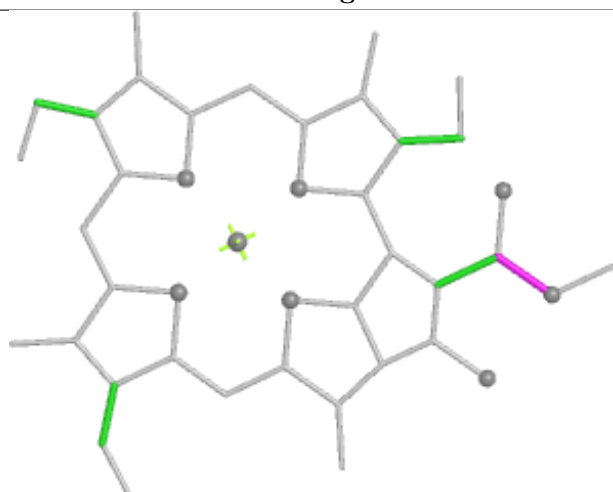
Ligand CLA H 205



Bond lengths



Bond angles

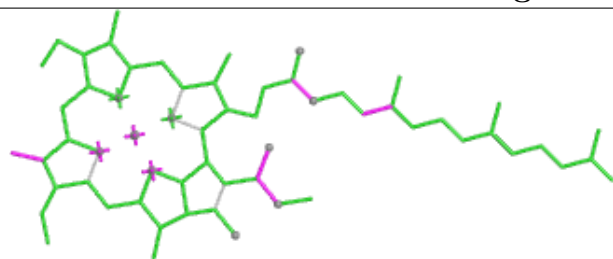


Torsions

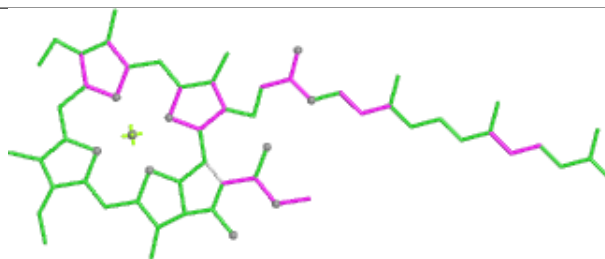


Rings

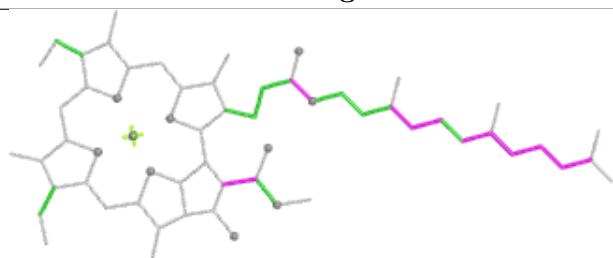
Ligand CLA R 612



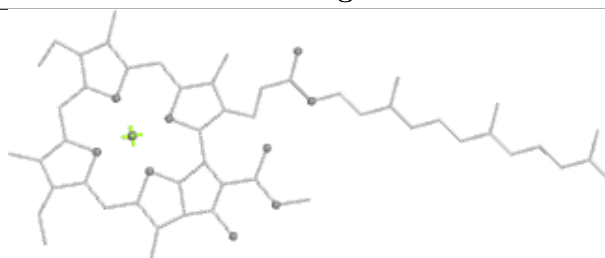
Bond lengths



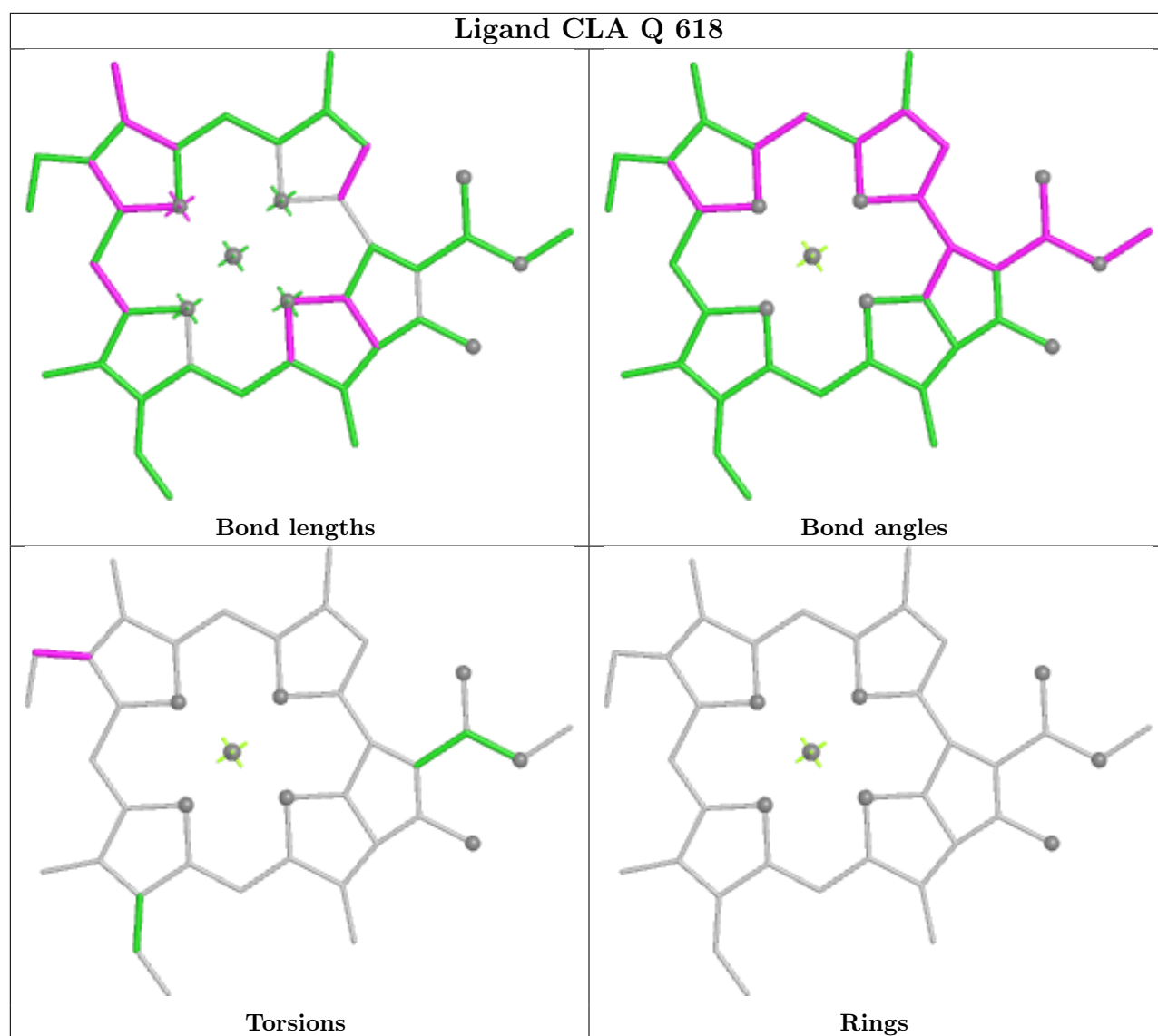
Bond angles

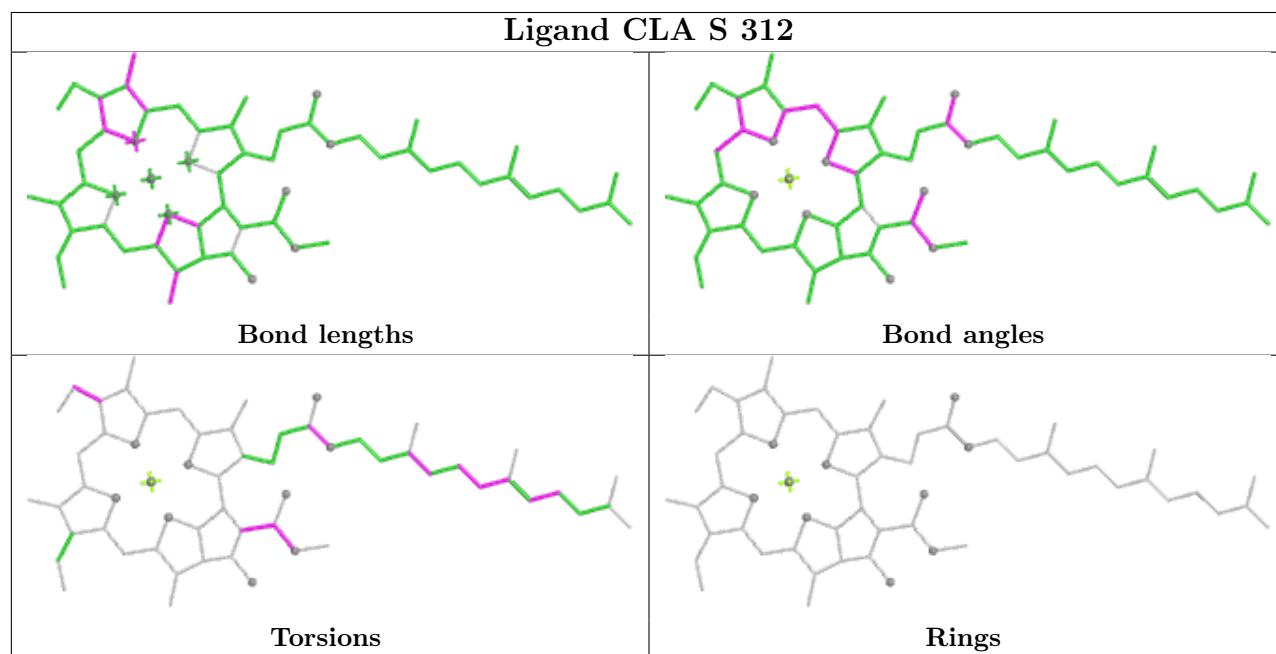
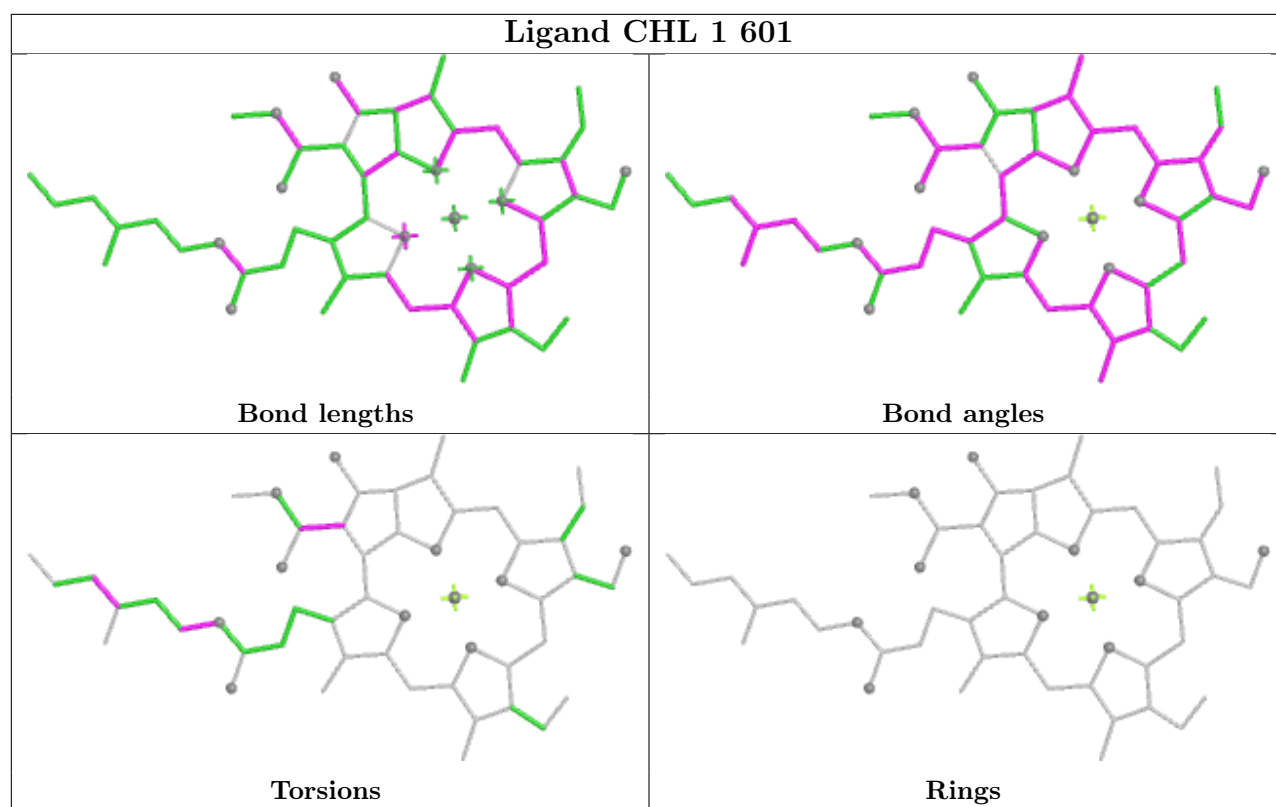


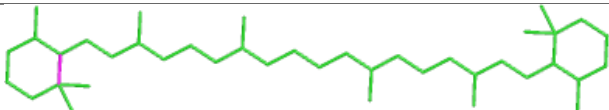
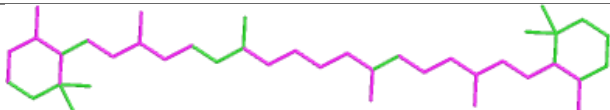
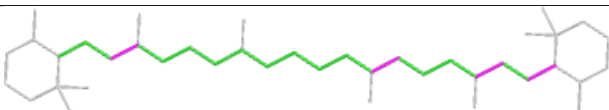
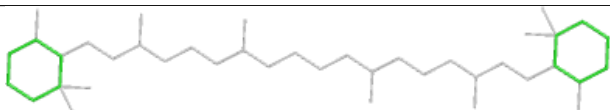
Torsions

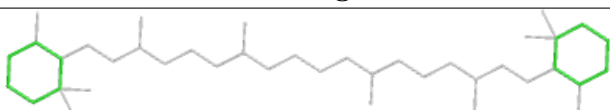


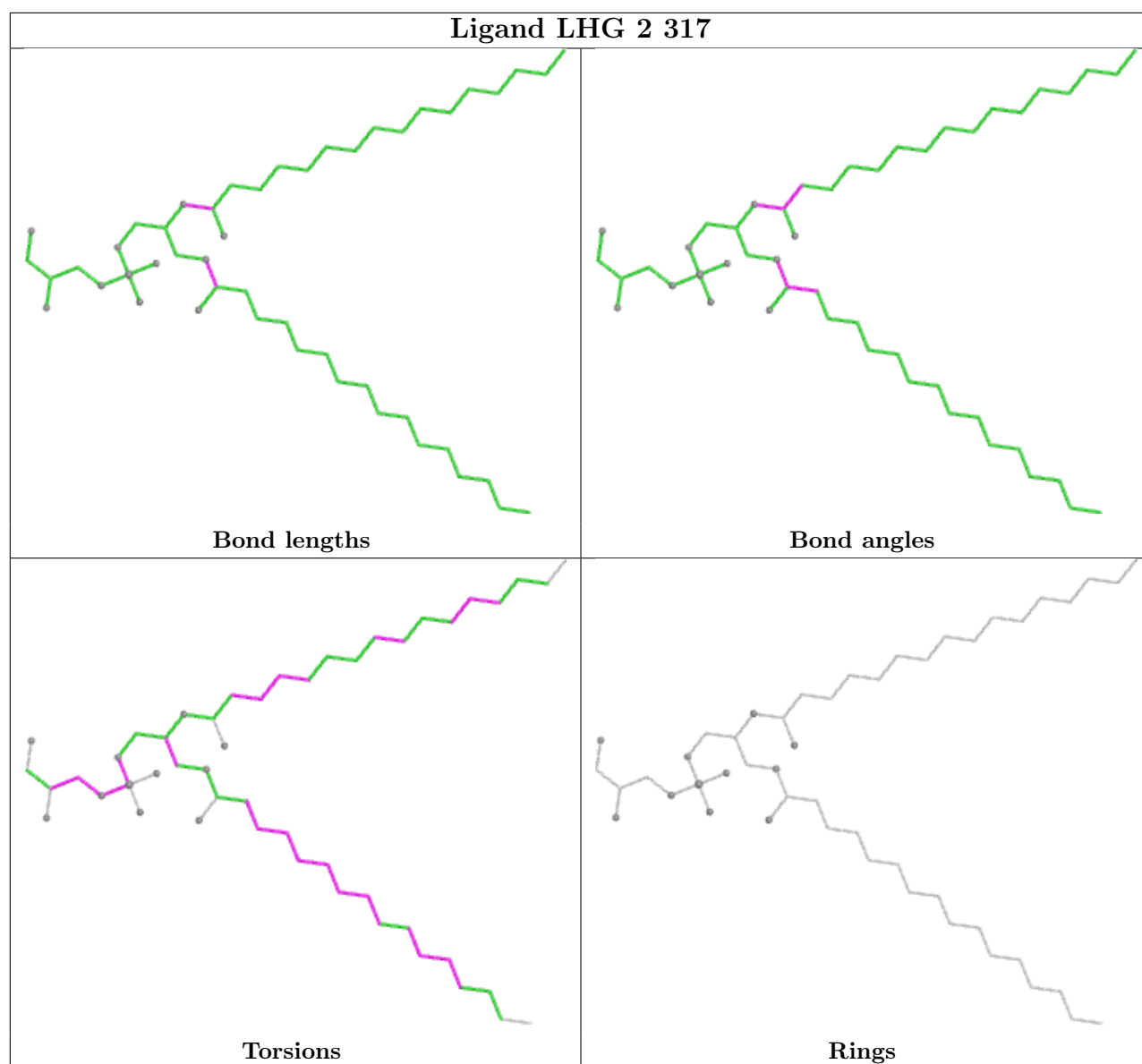
Rings



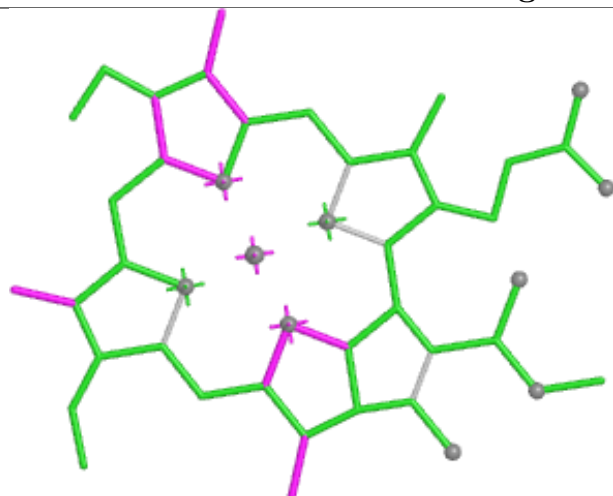


Ligand BCR B 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

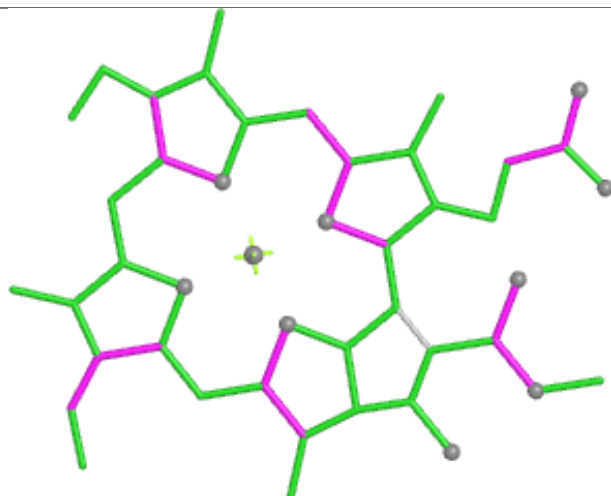
Ligand BCR F 801	
	
Bond lengths	Bond angles
	
Torsions	Rings



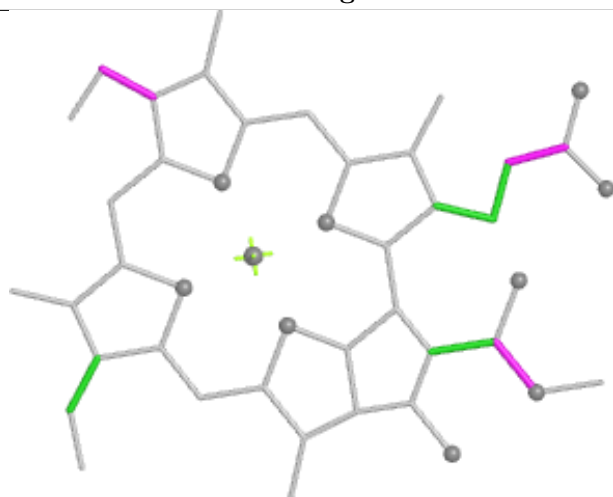
Ligand CLA 6 614



Bond lengths



Bond angles

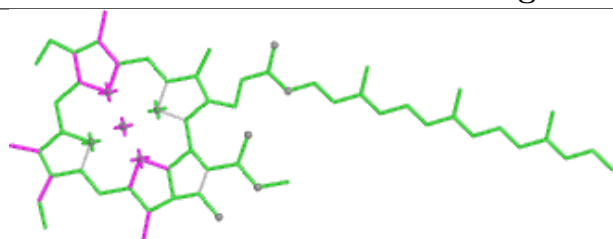


Torsions

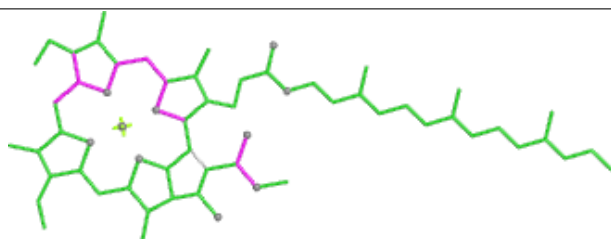


Rings

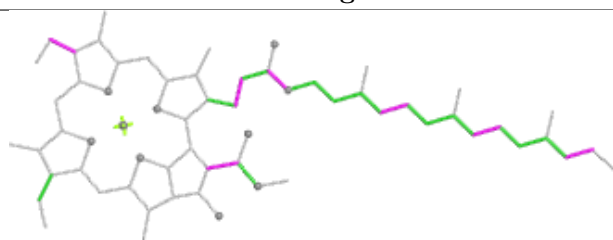
Ligand CLA 8 303



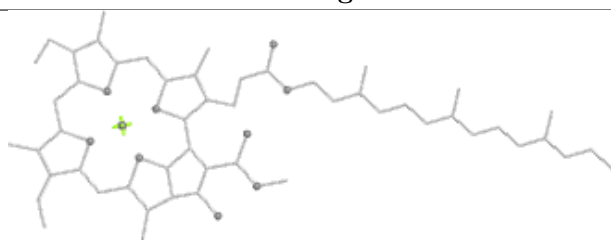
Bond lengths



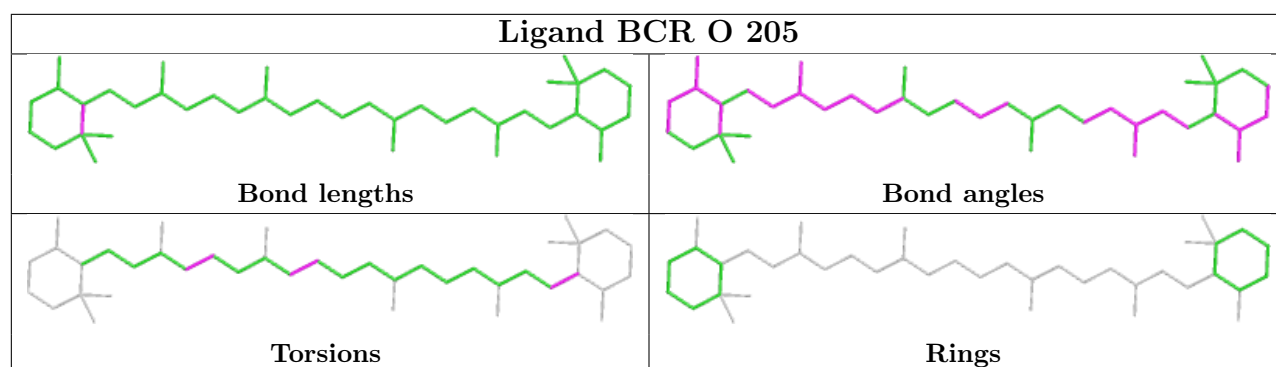
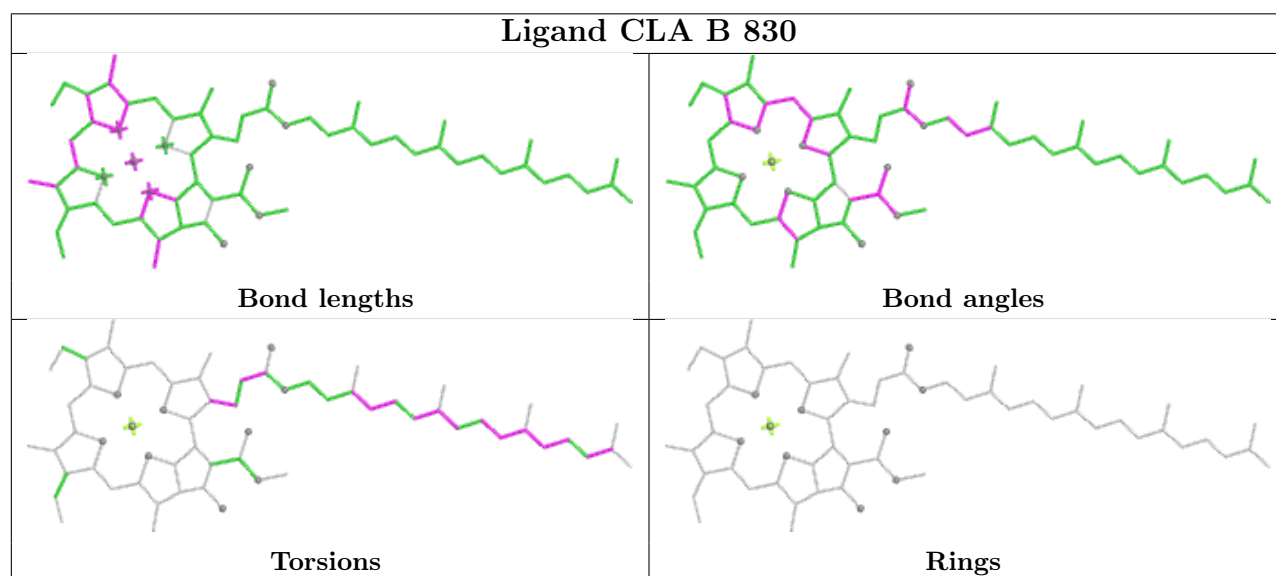
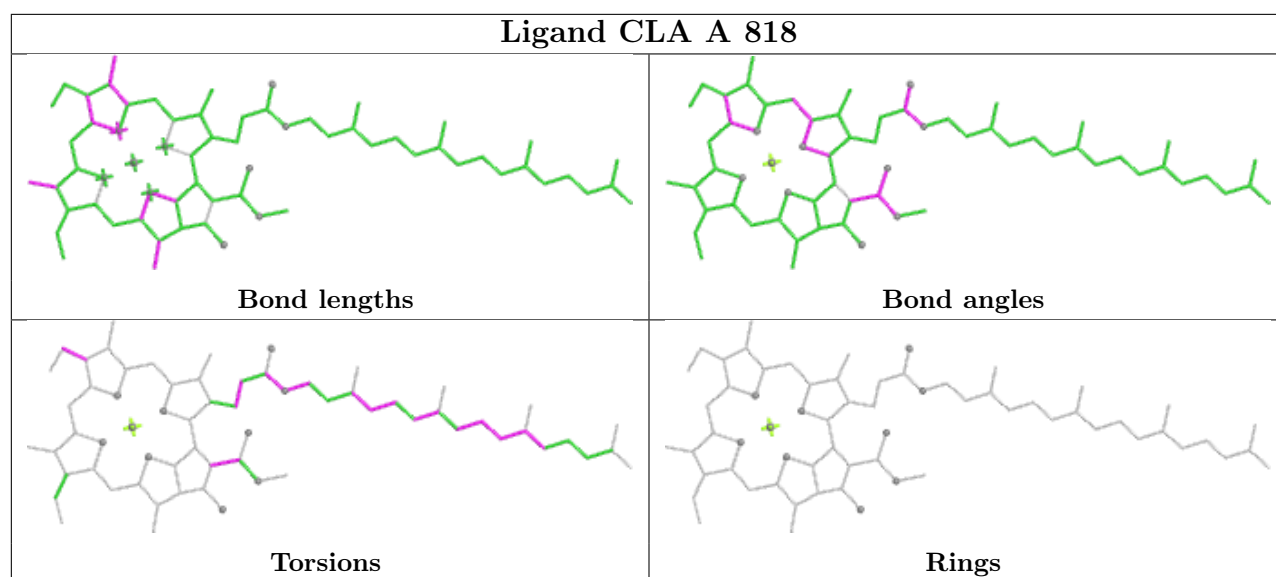
Bond angles



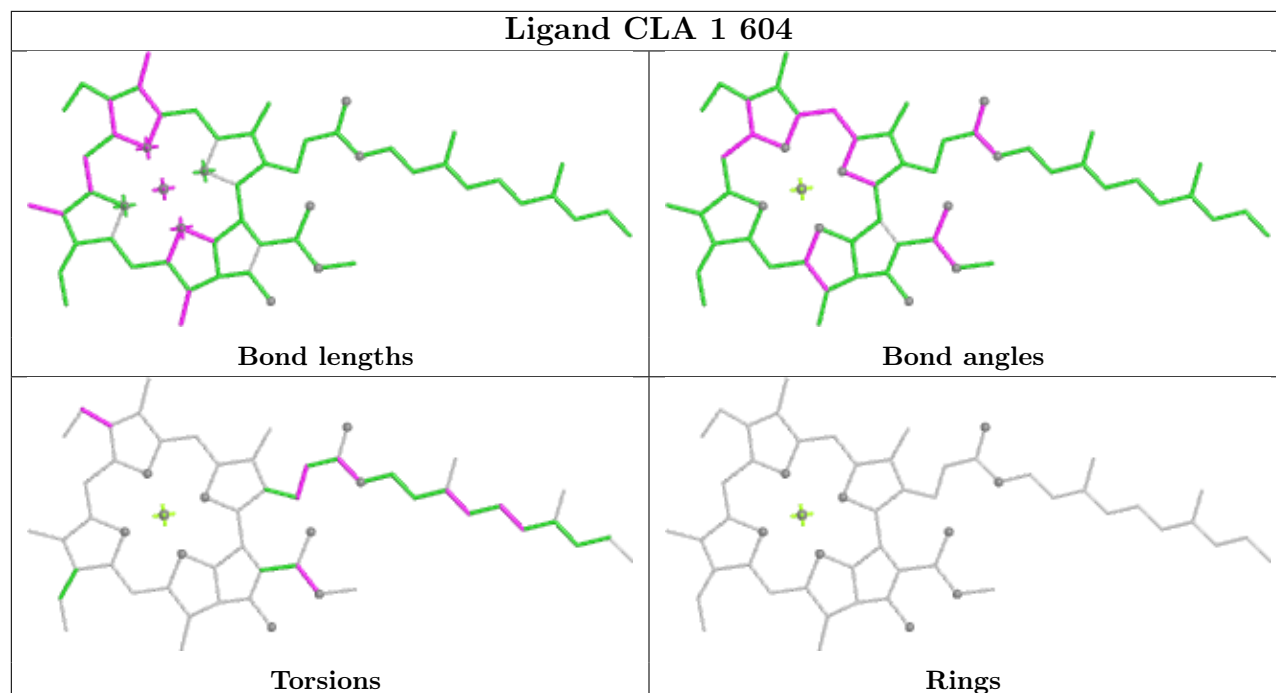
Torsions



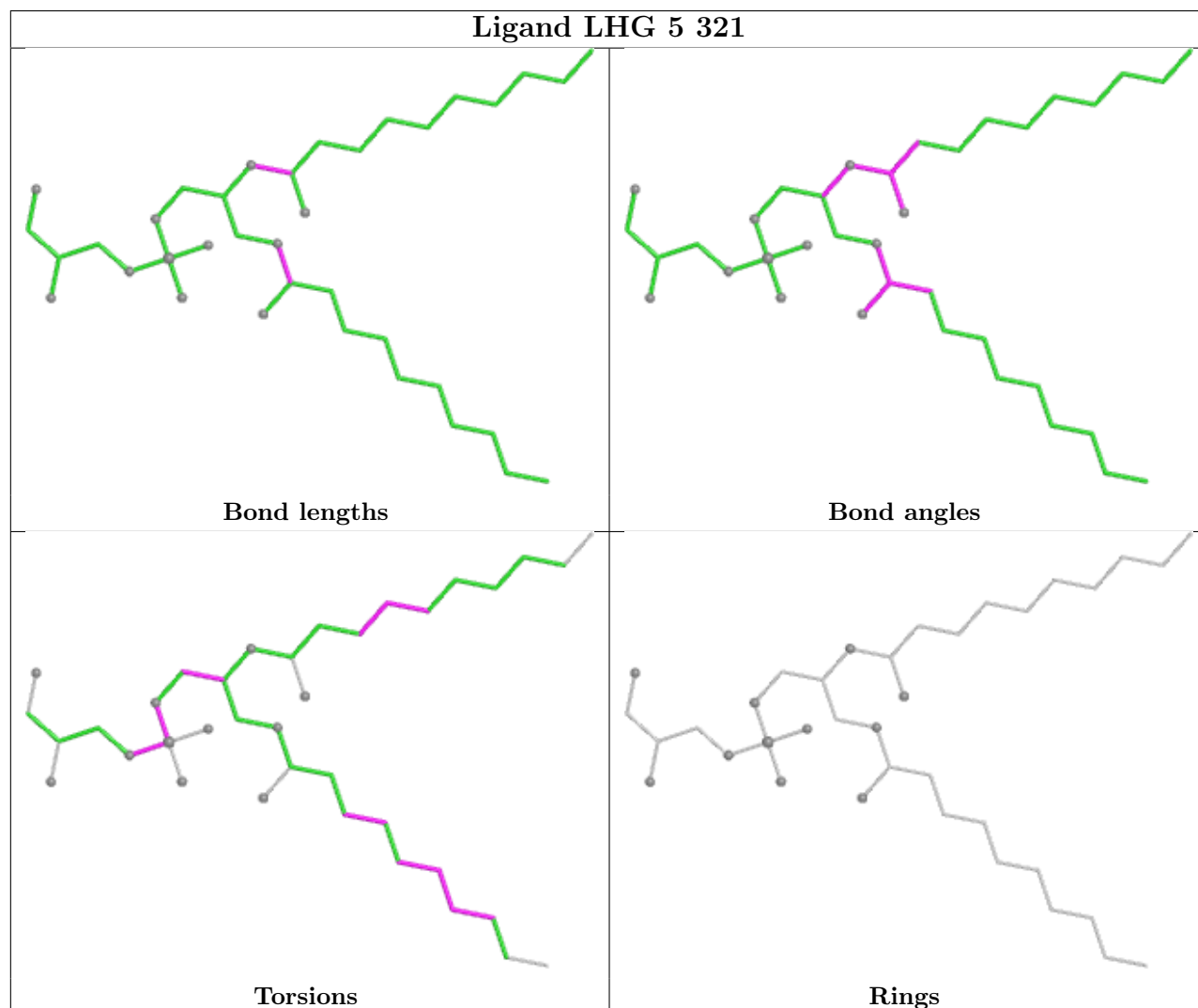
Rings



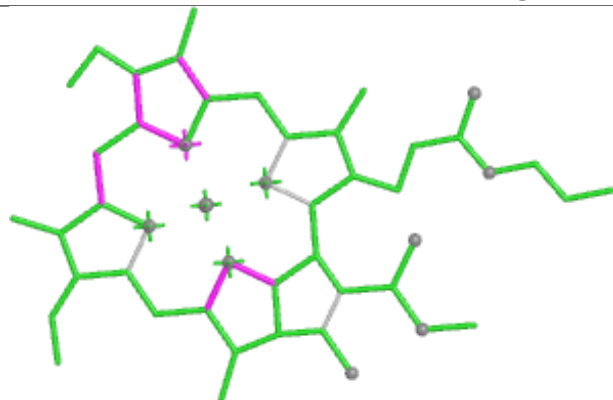
Ligand CLA 1 604



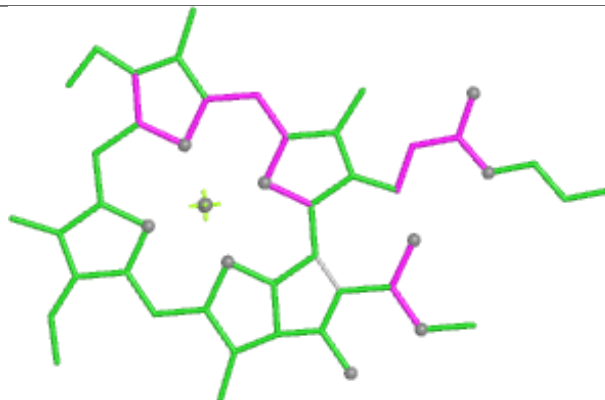
Ligand LHG 5 321



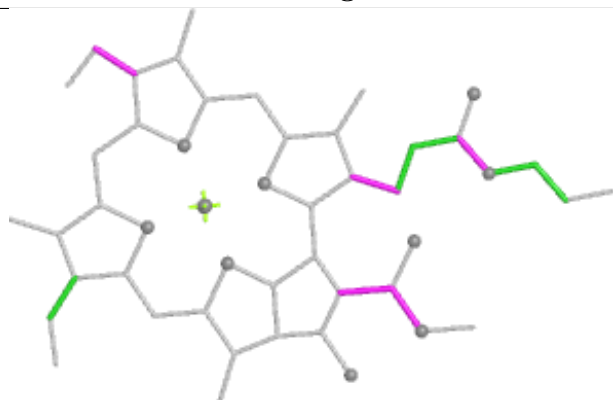
Ligand CLA R 614



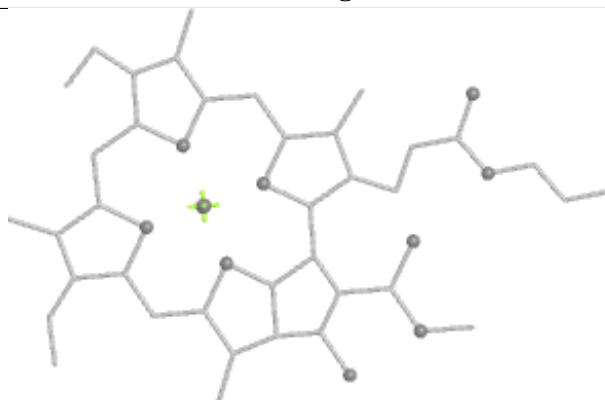
Bond lengths



Bond angles

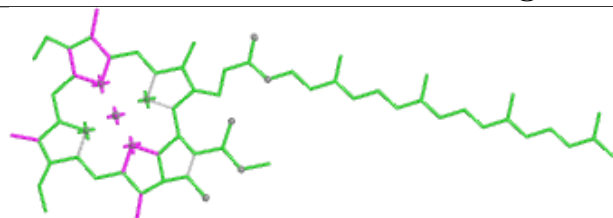


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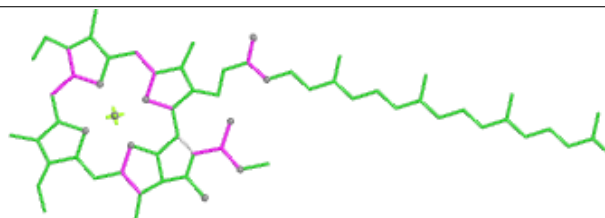


Rings

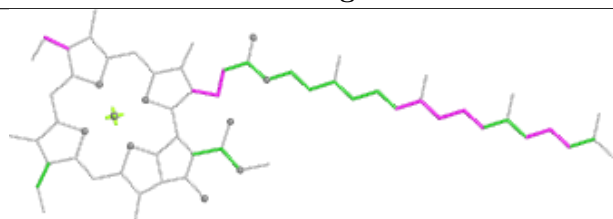
Ligand CLA 5 302



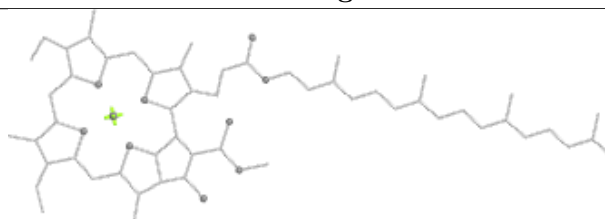
Bond lengths



Bond angles

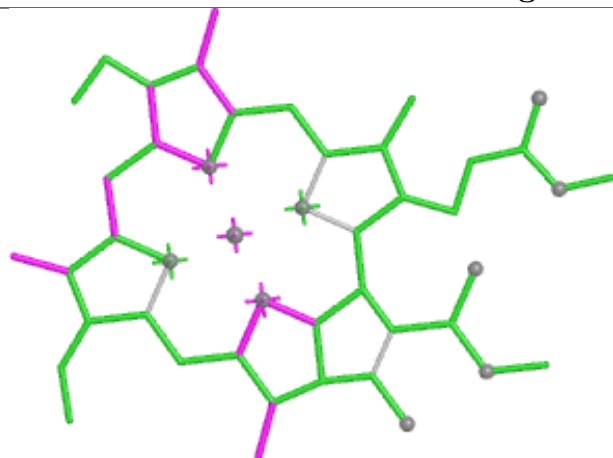


Torsions

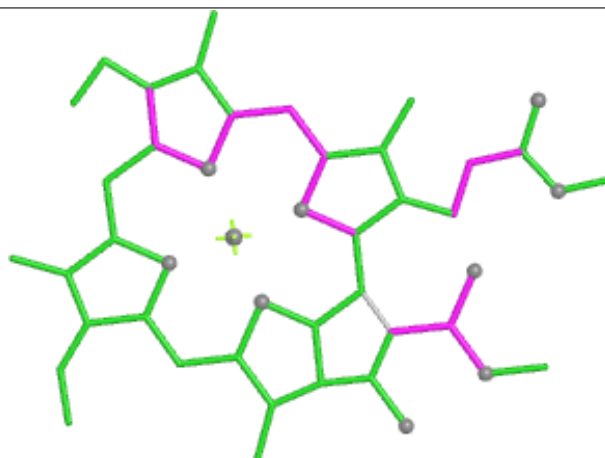


Rings

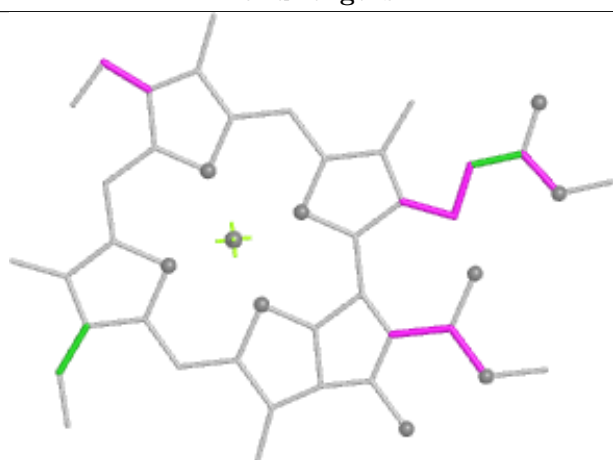
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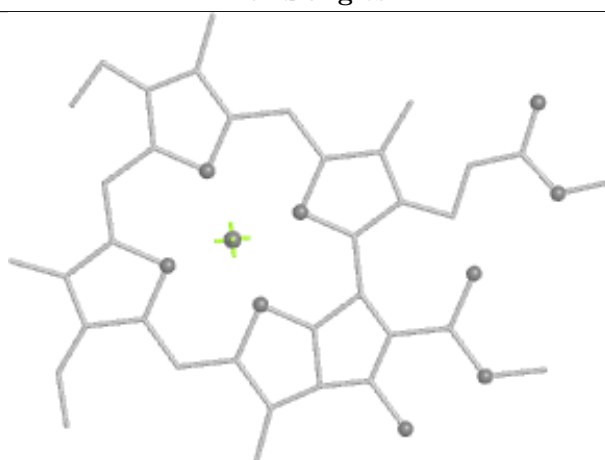
Bond lengths



Bond angles

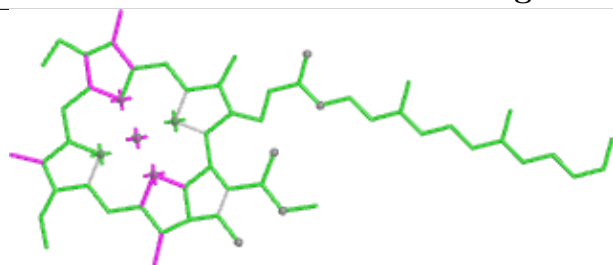


Torsions

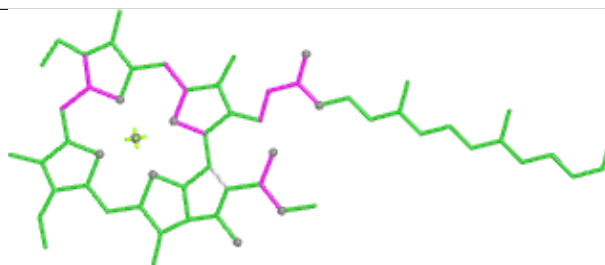


Rings

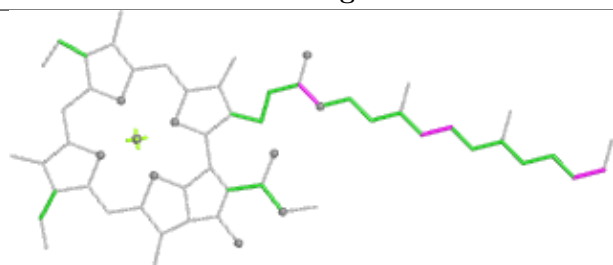
Ligand CLA B 820



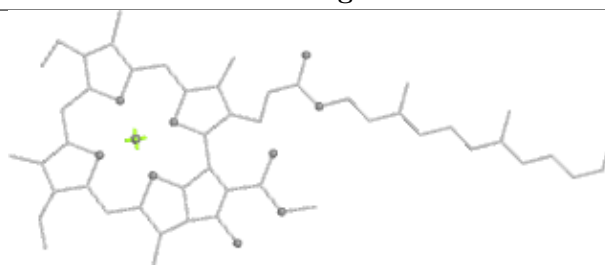
Bond lengths



Bond angles

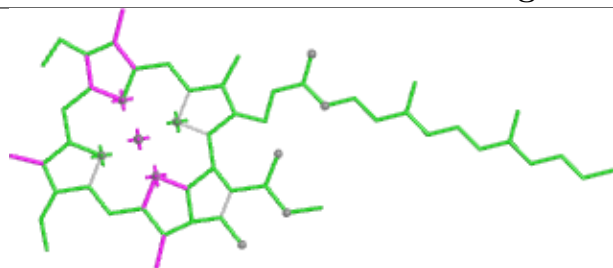


Torsions

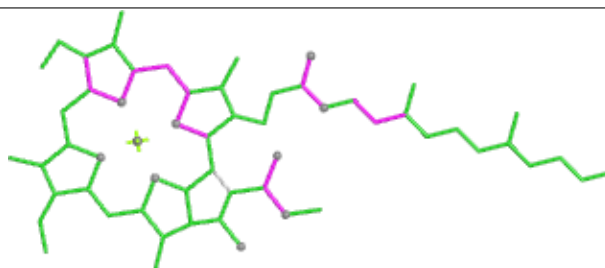


Rings

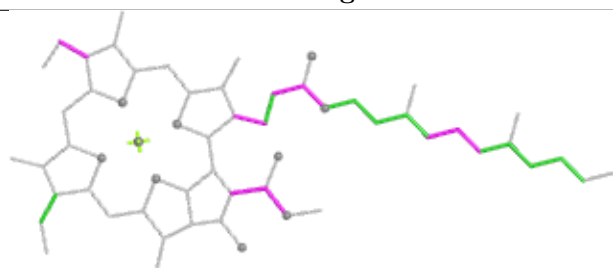
Ligand CLA J 103



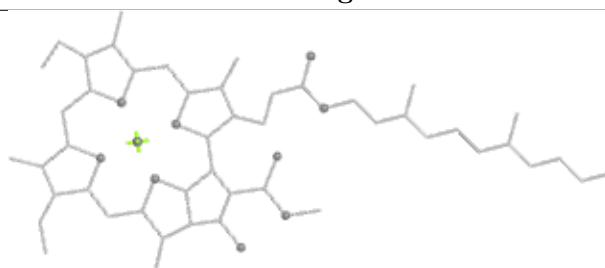
Bond lengths



Bond angles

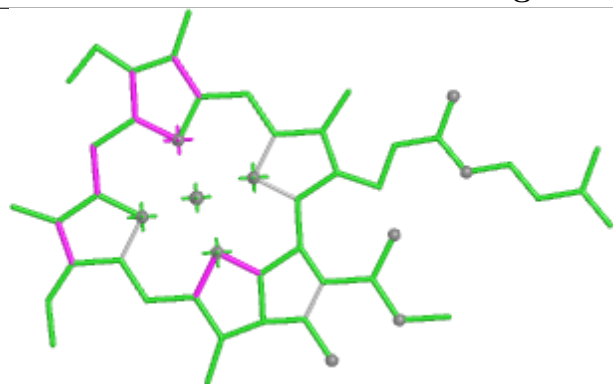


Torsions

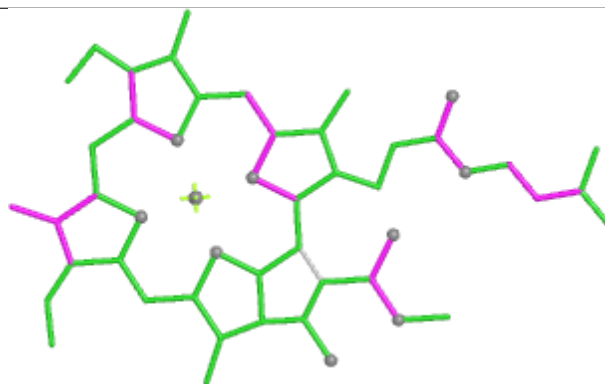


Rings

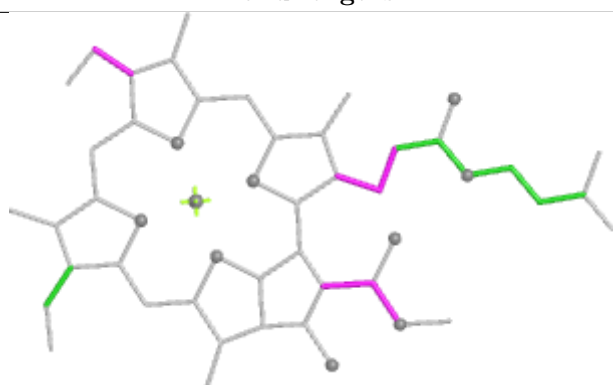
Ligand CLA U 304



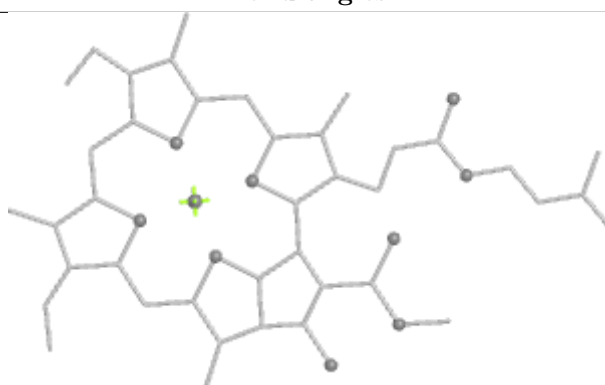
Bond lengths



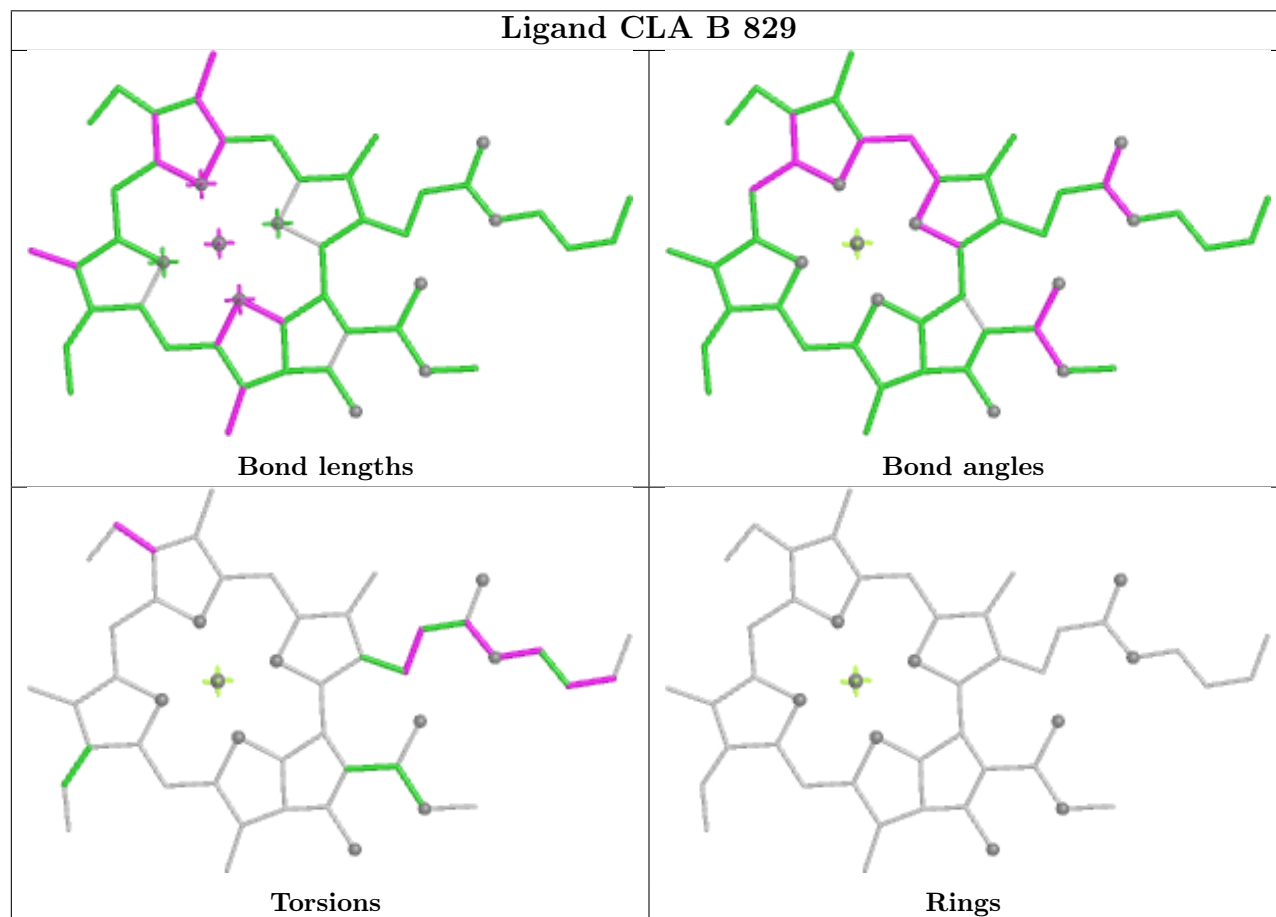
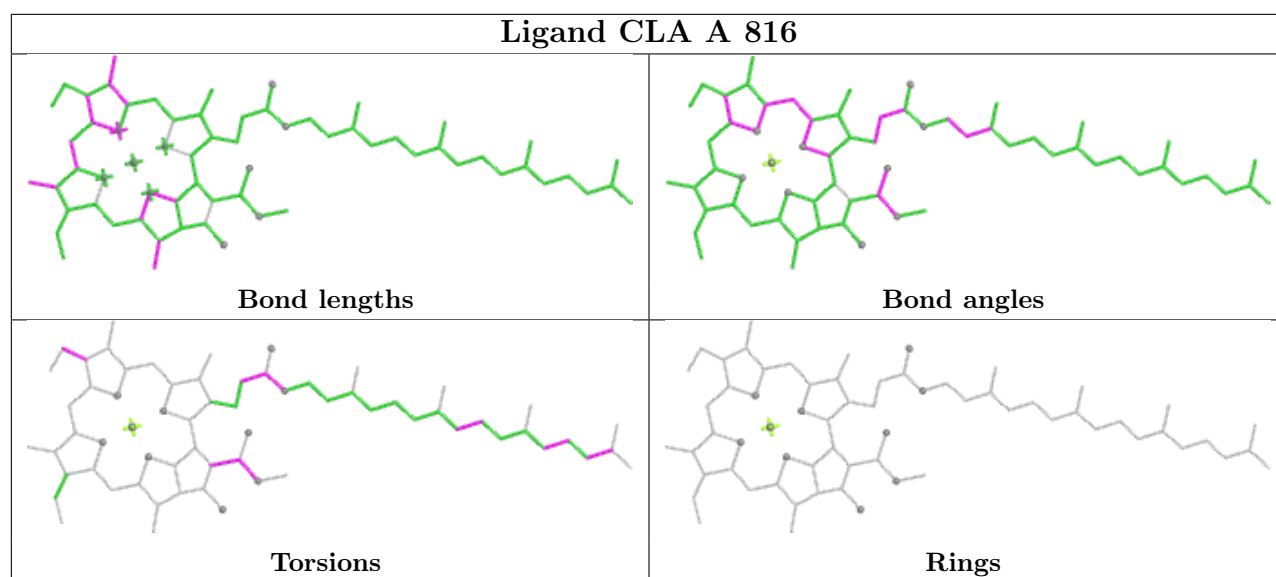
Bond angles

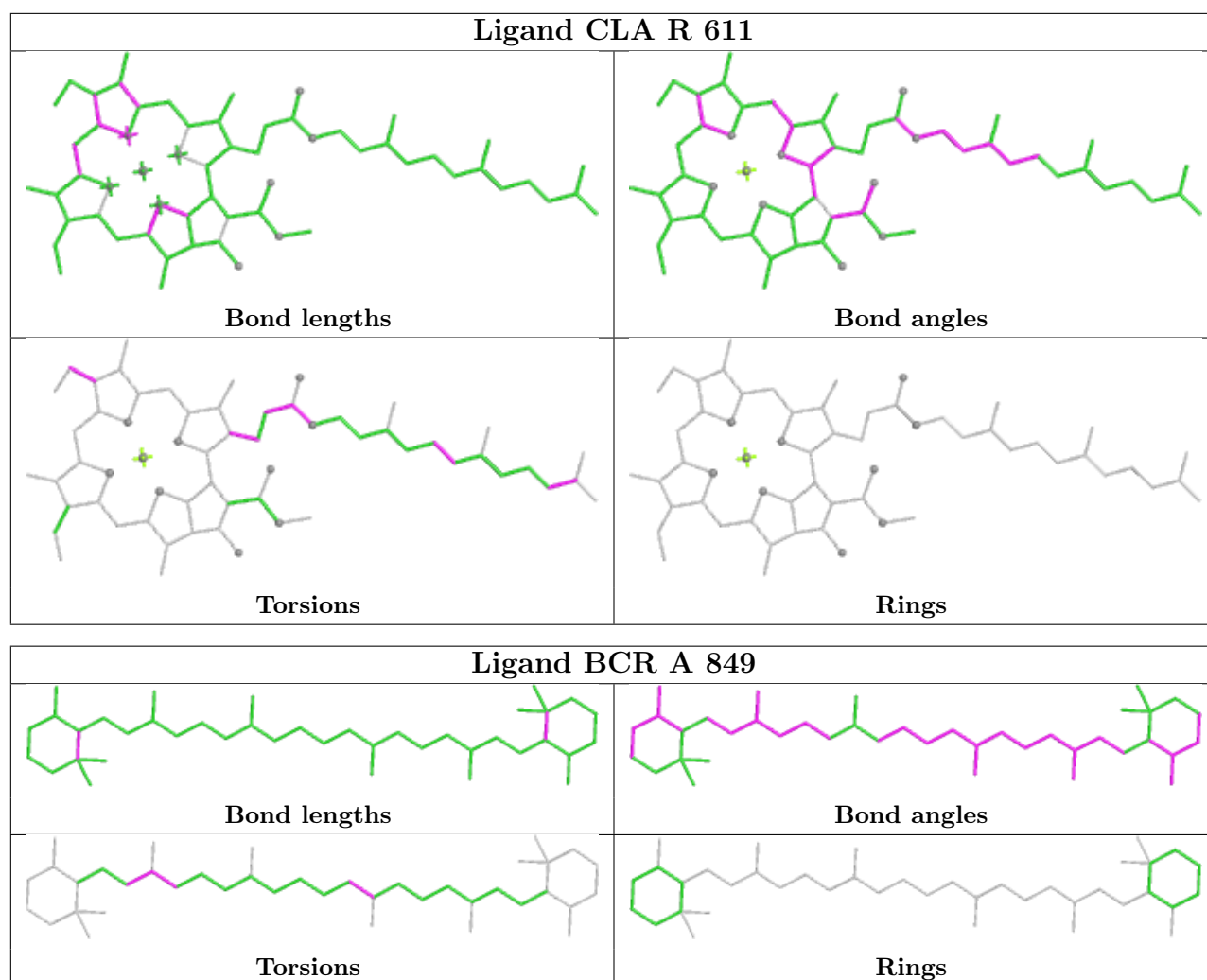


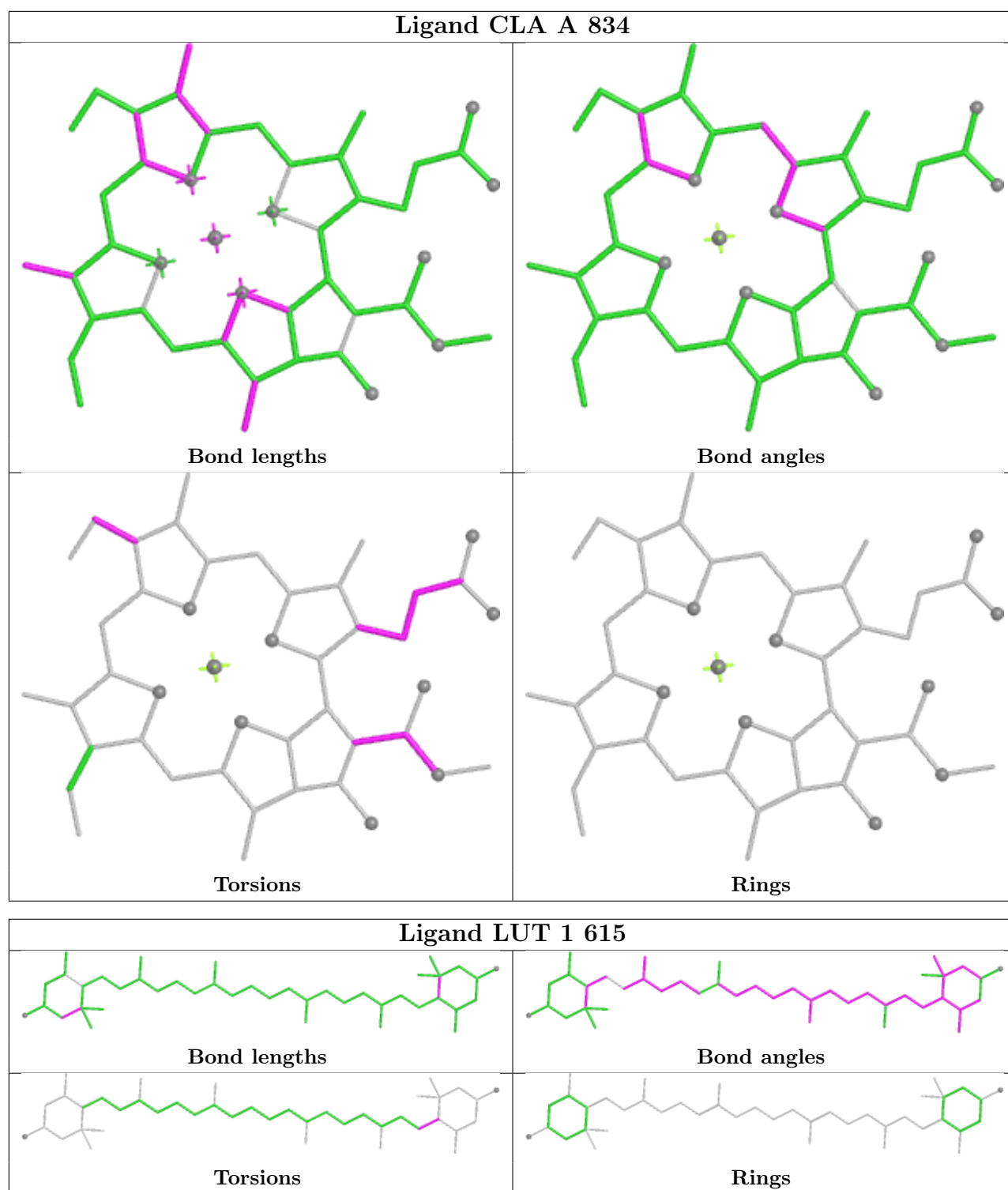
Torsions

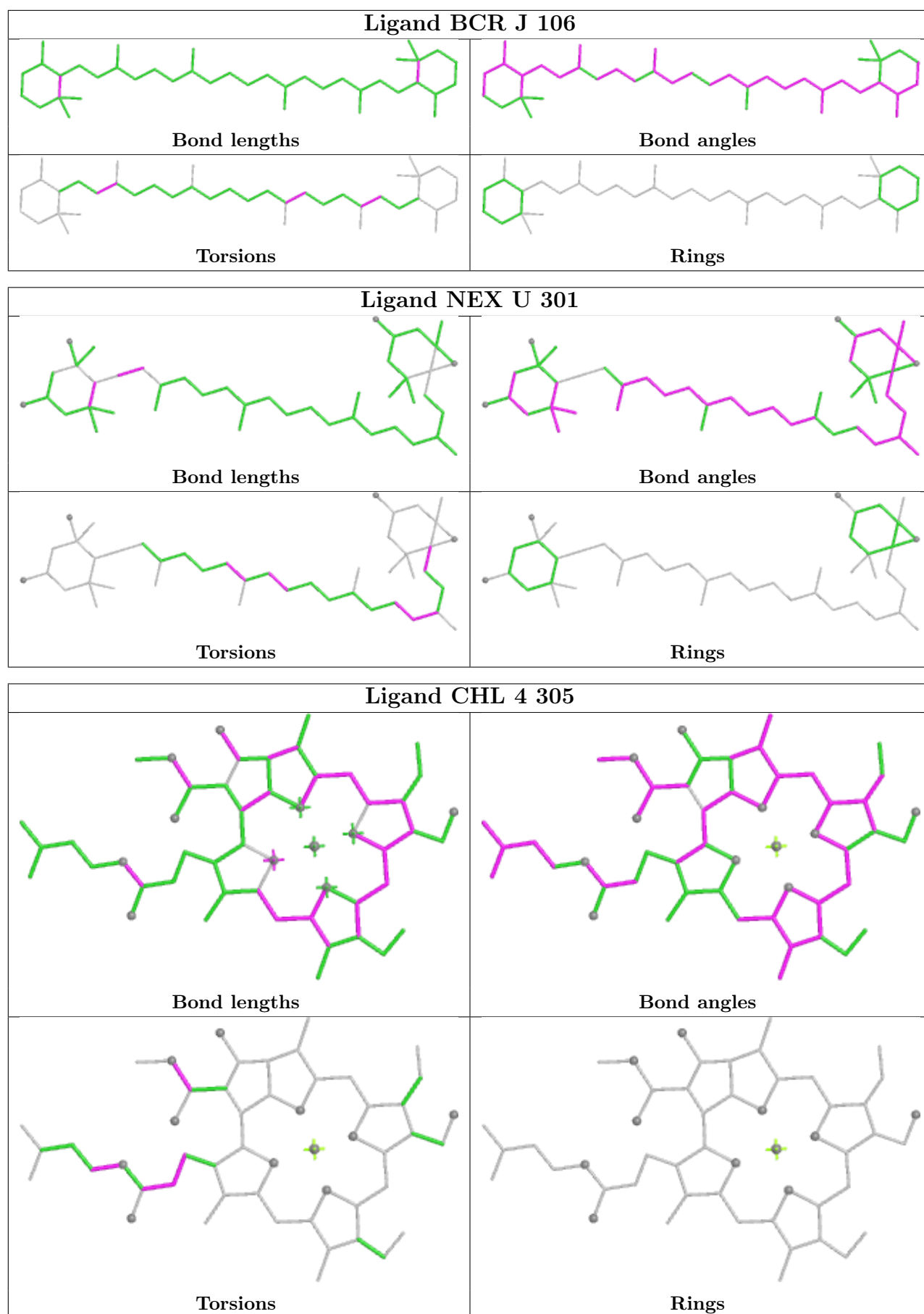


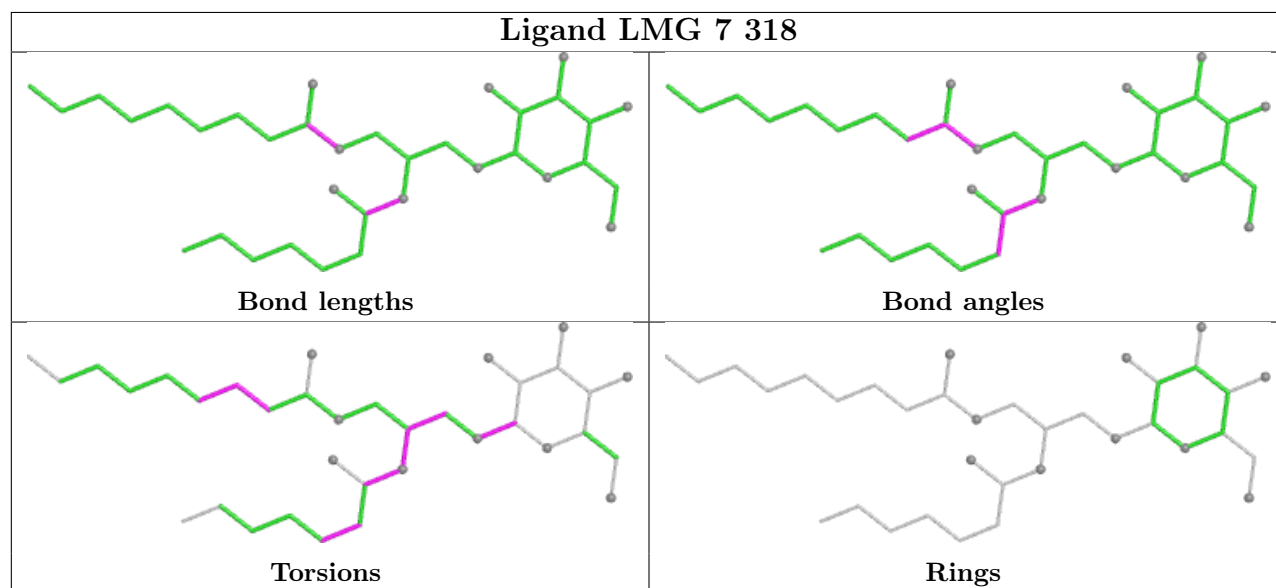
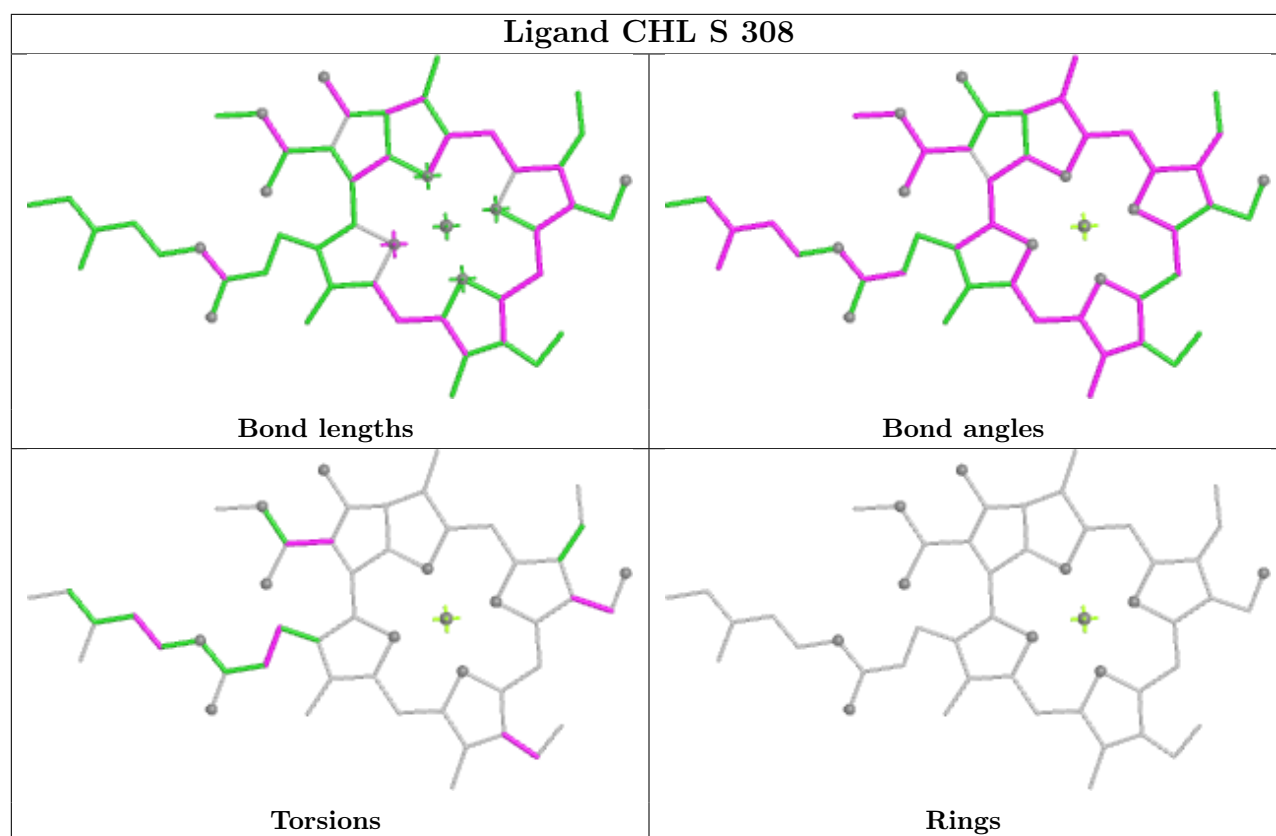
Rings

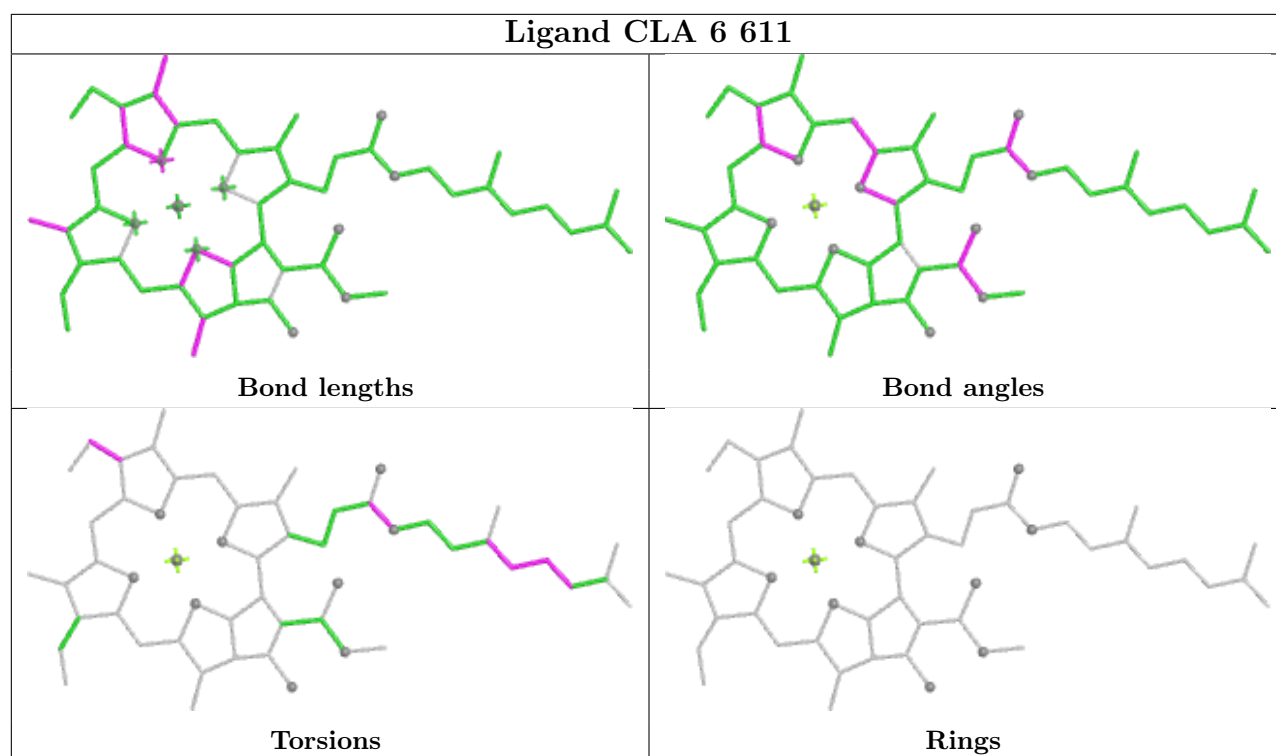




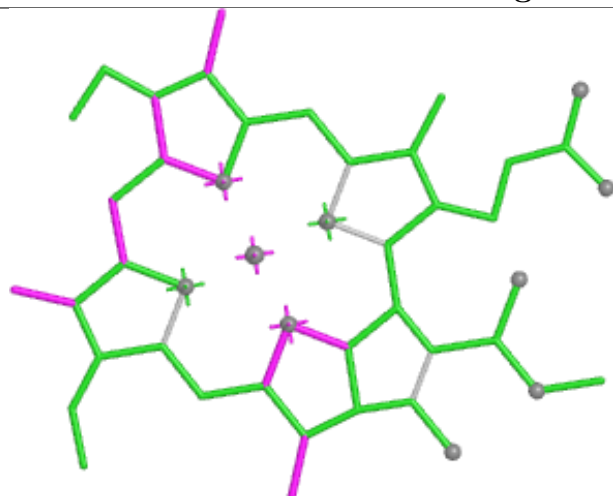




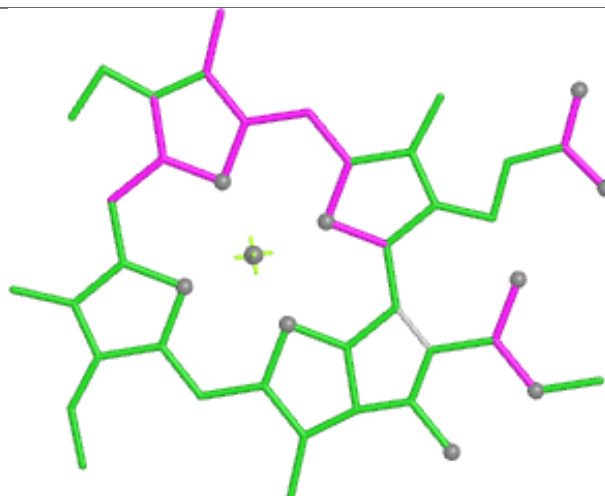




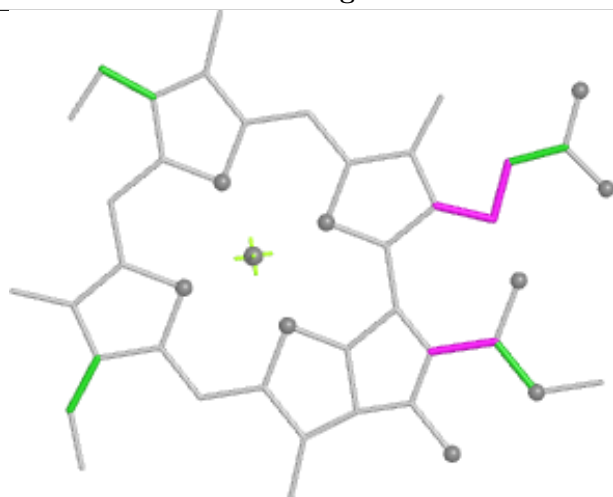
Ligand CLA B 803



Bond lengths



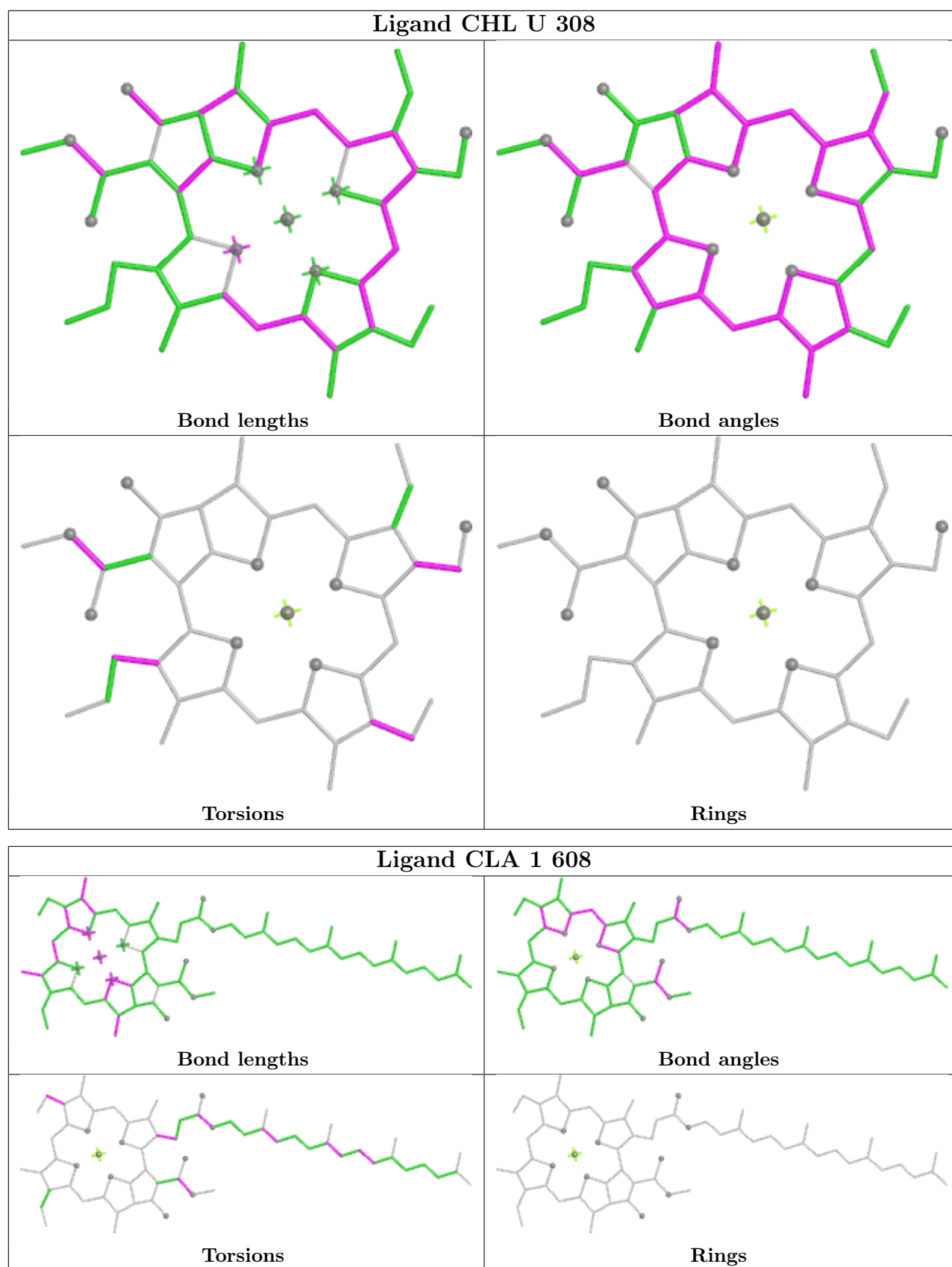
Bond angles

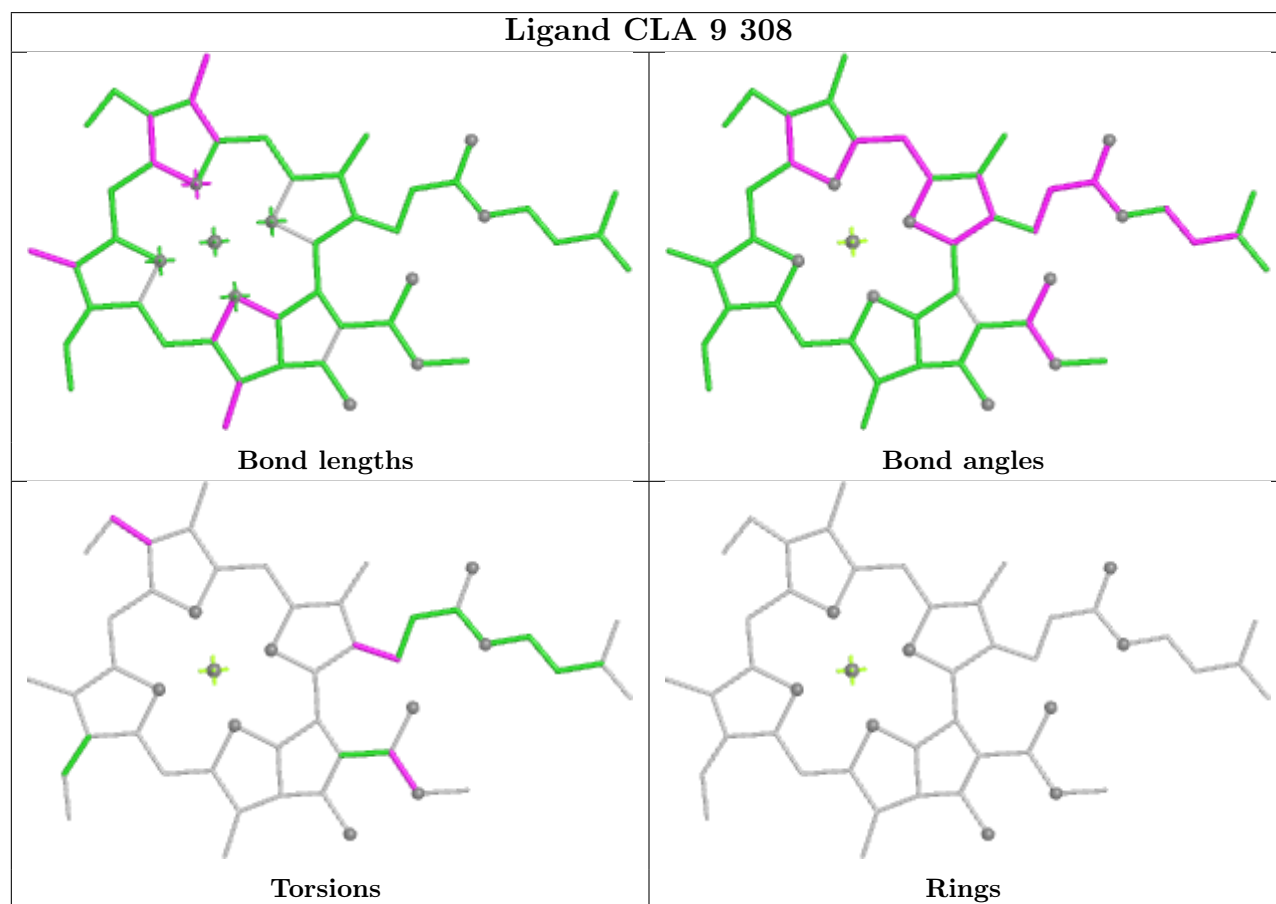
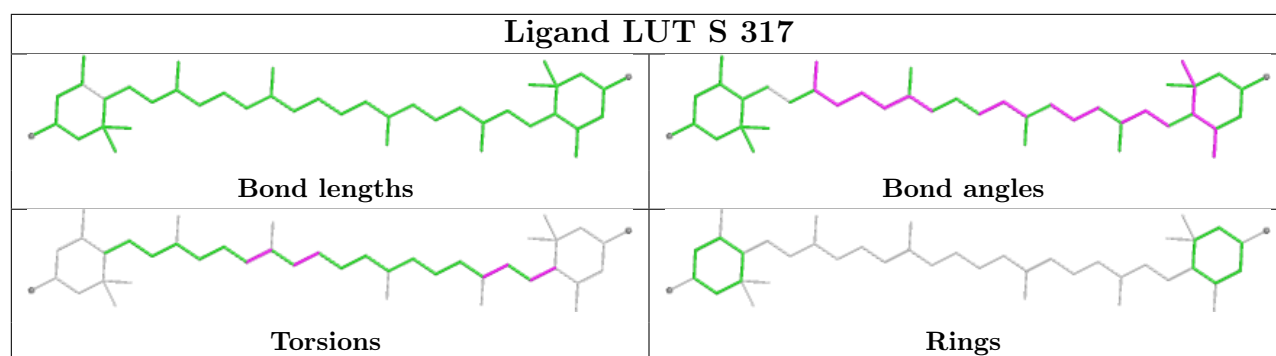


Torsions

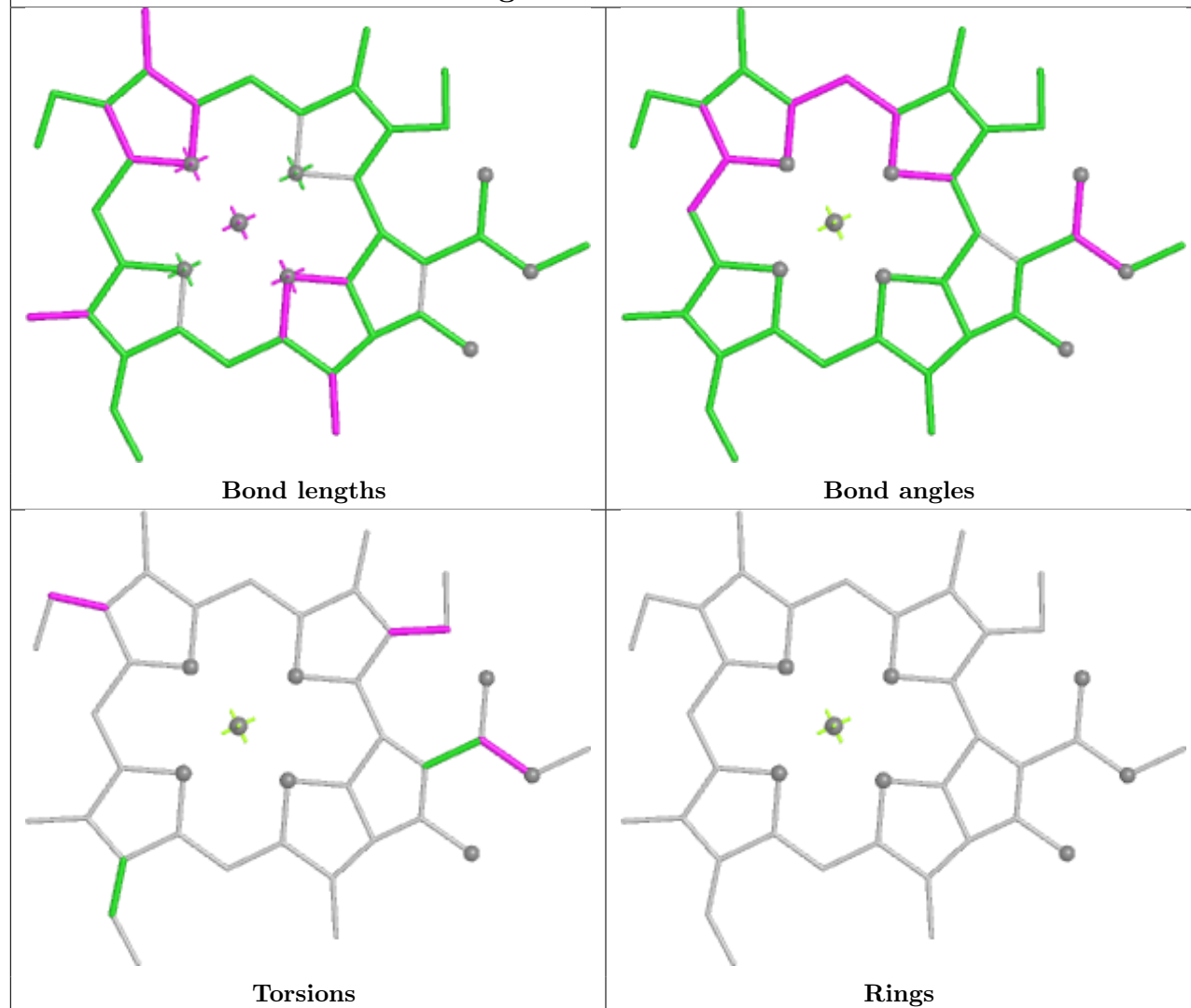


Rings

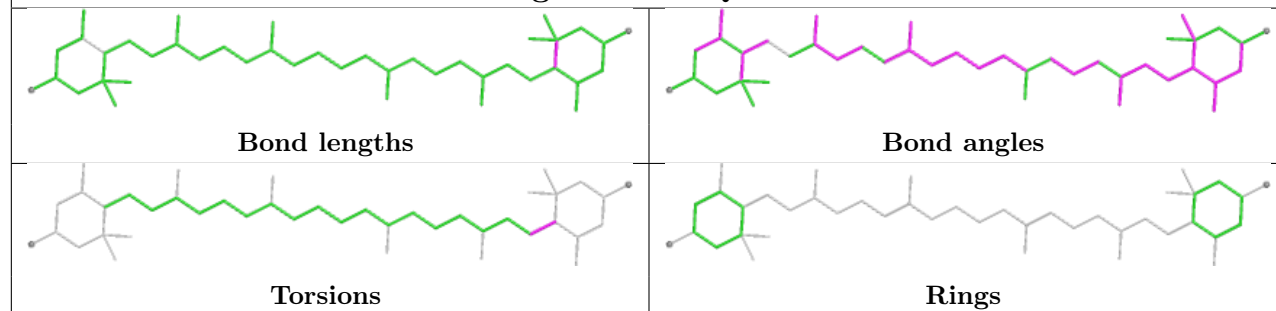


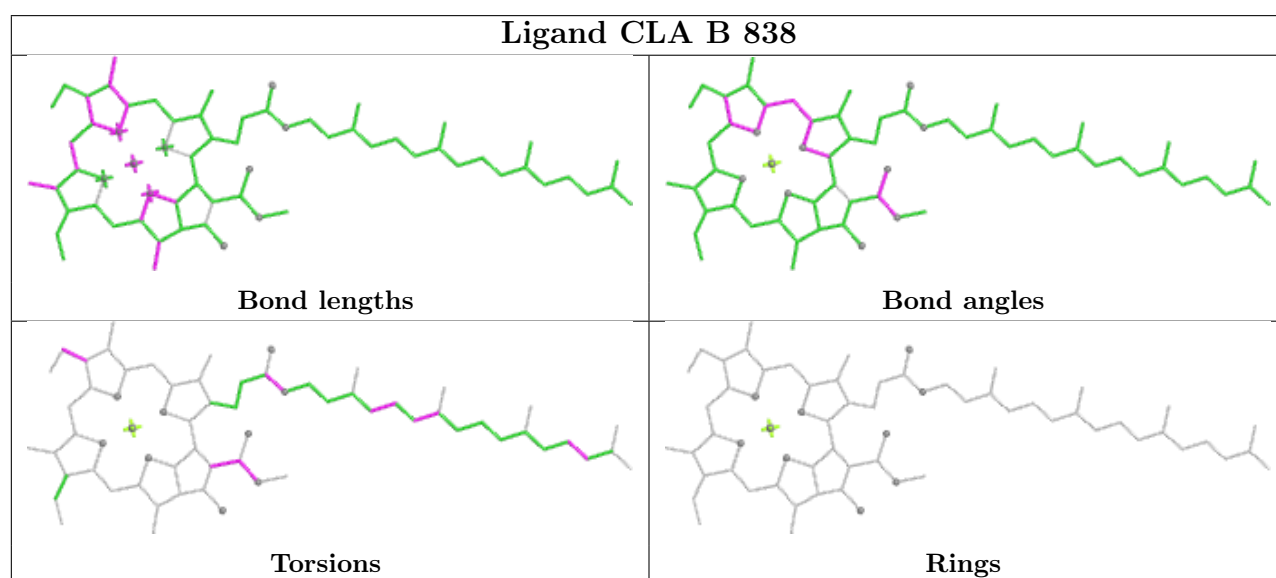
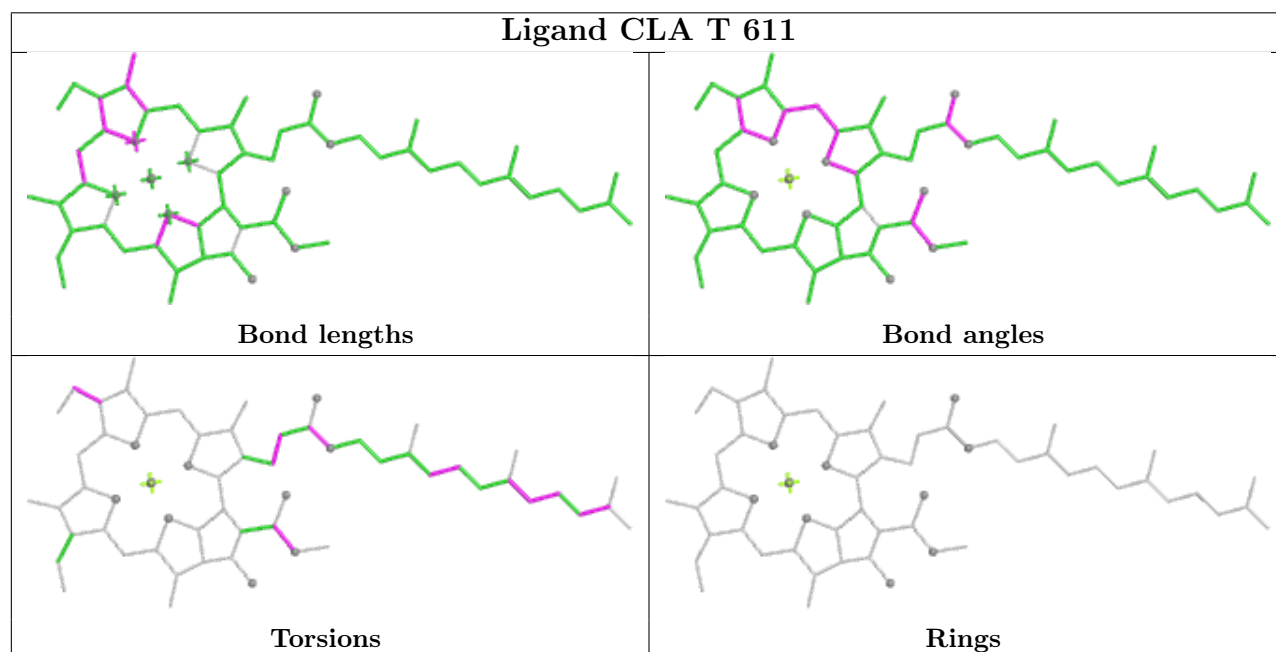
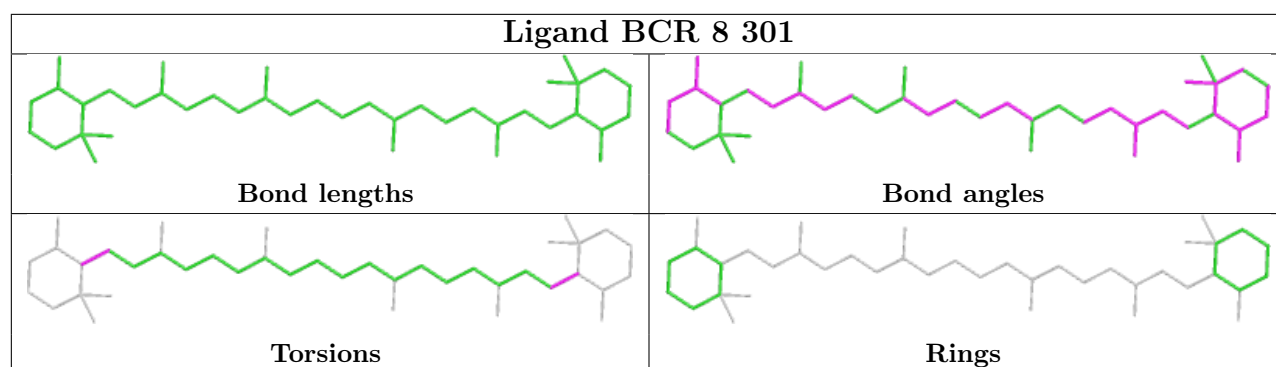


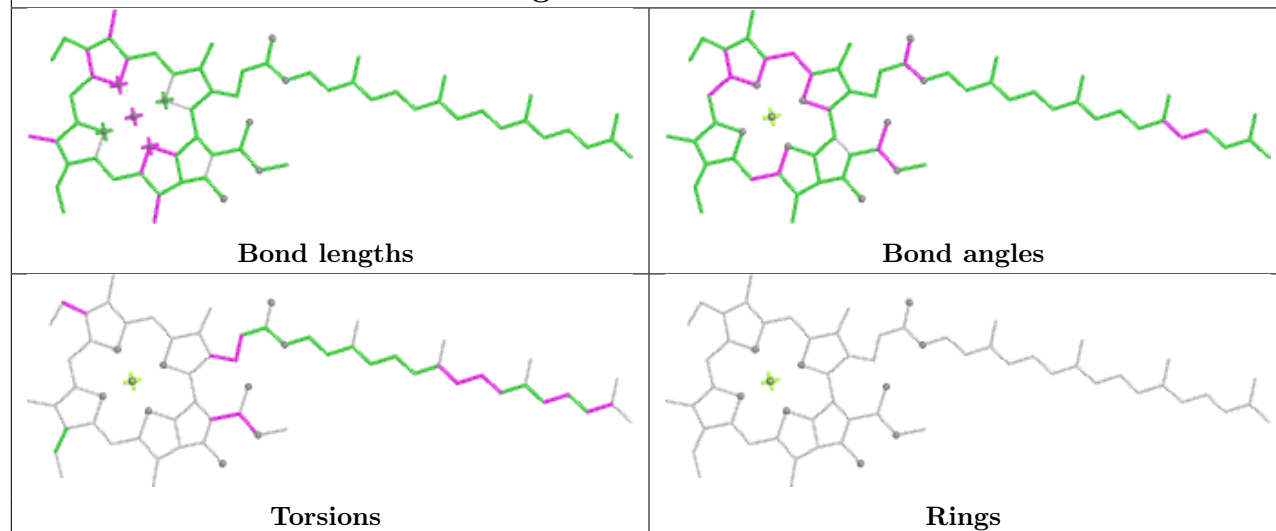
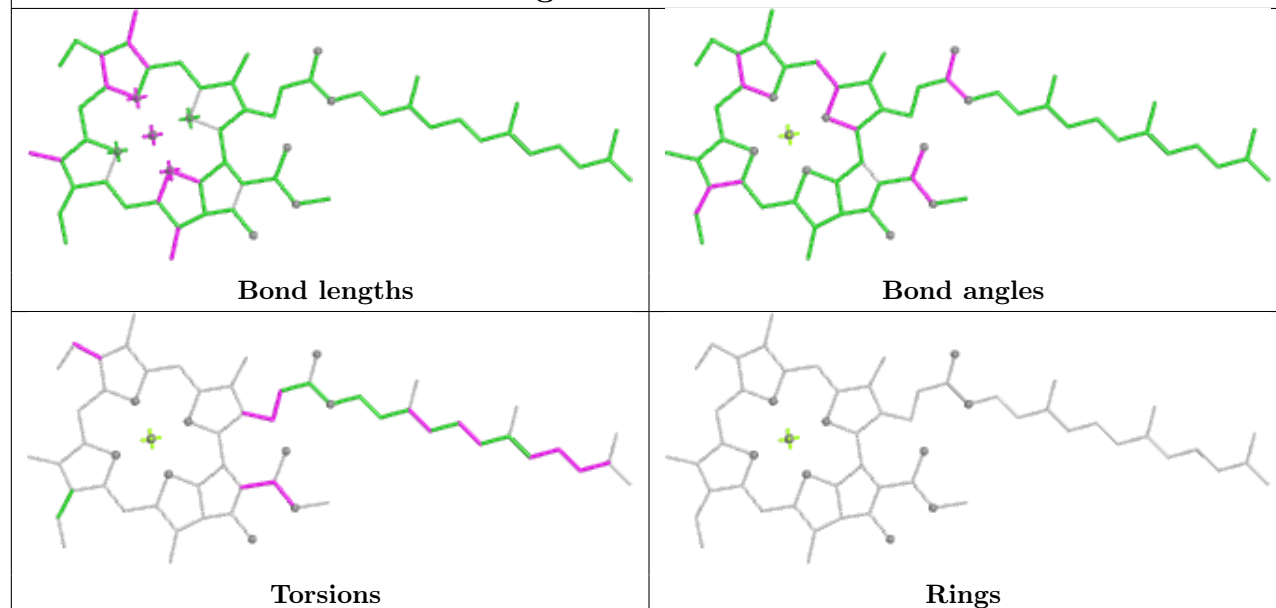
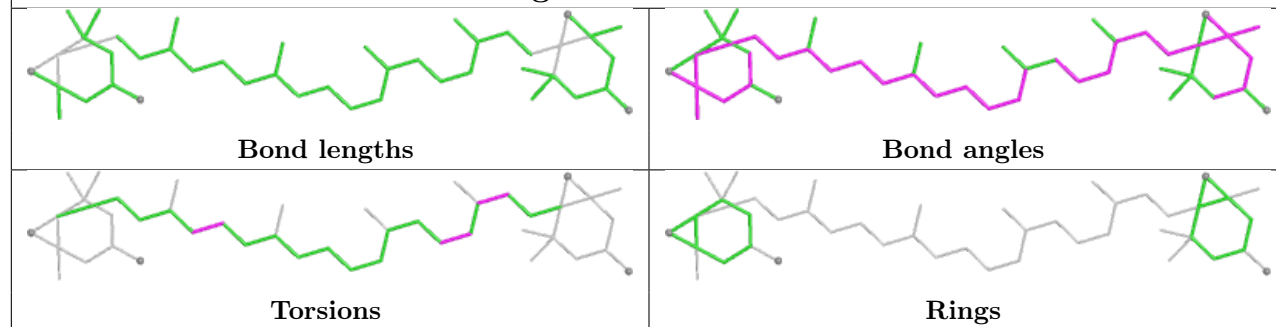
Ligand CLA L 206

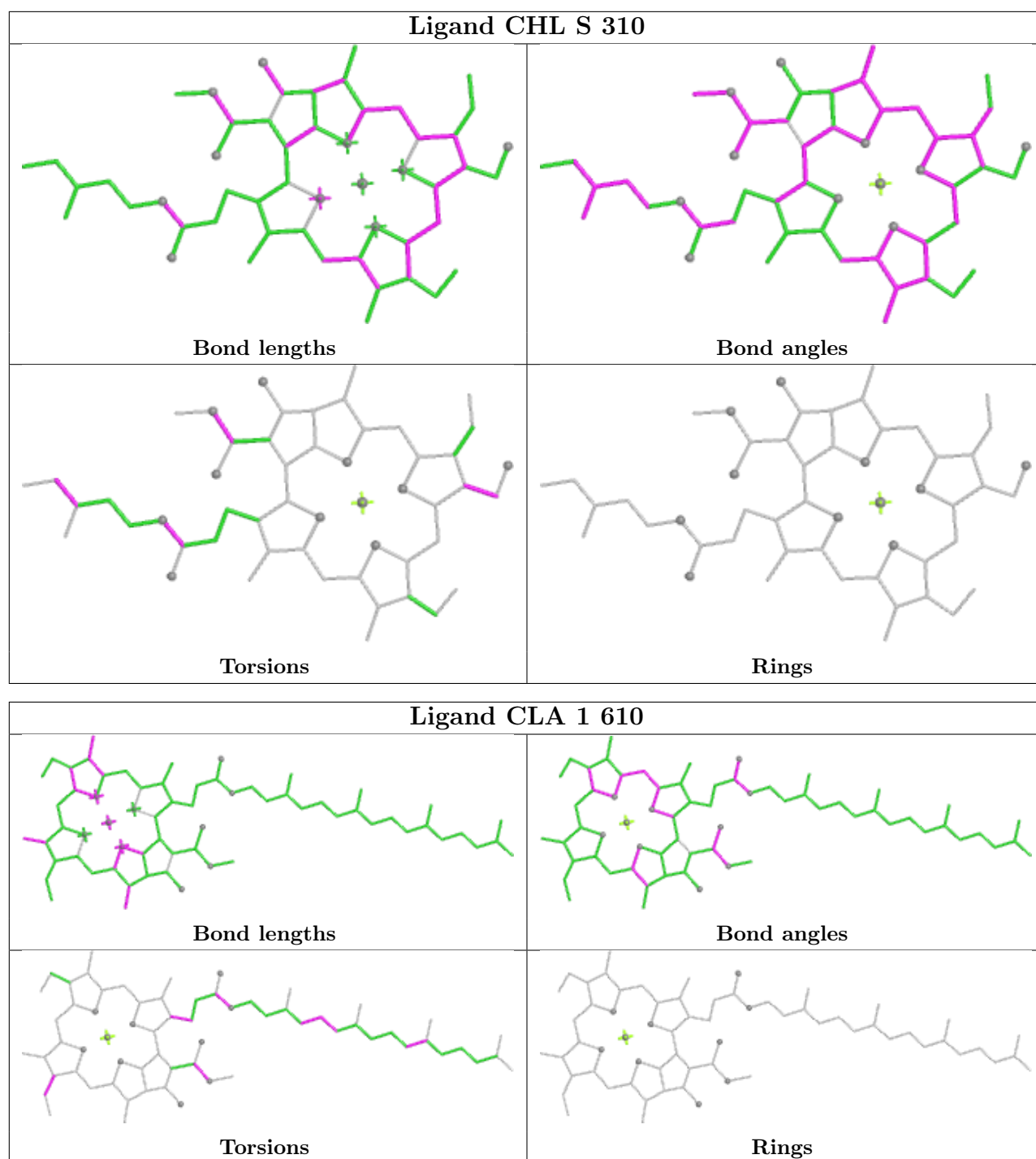


Ligand LUT Q 615

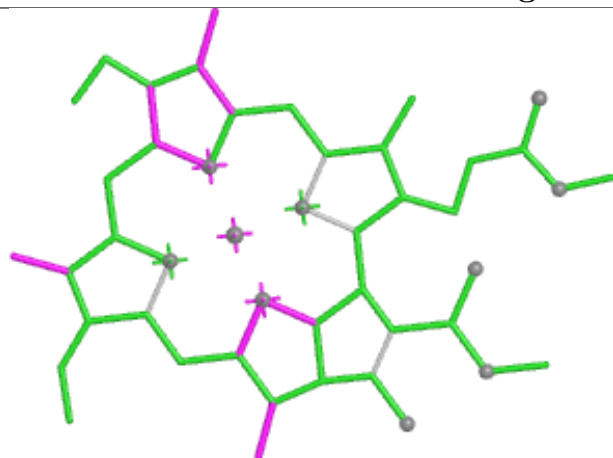




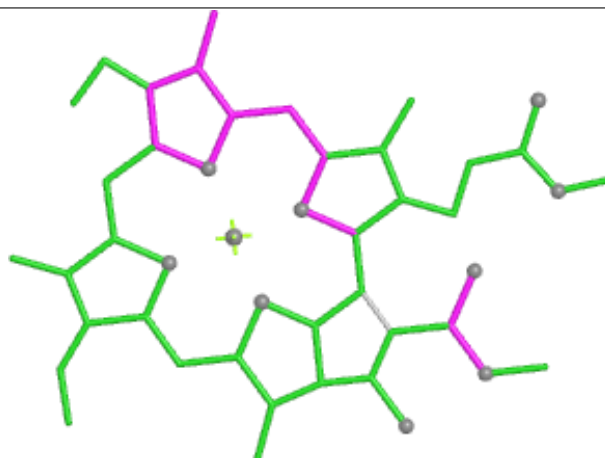
Ligand CLA B 811**Ligand CLA 4 308****Ligand XAT P 620**



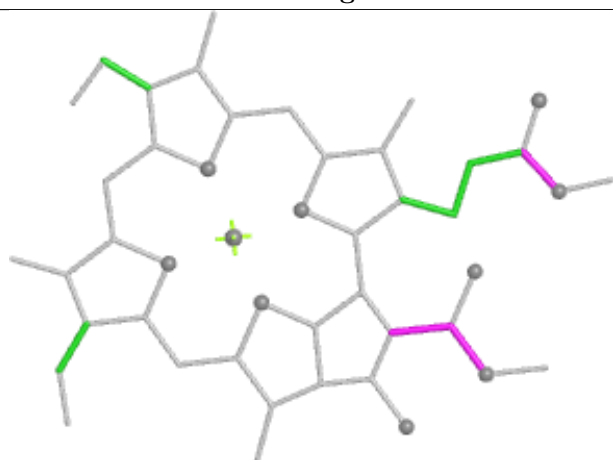
Ligand CLA 5 304



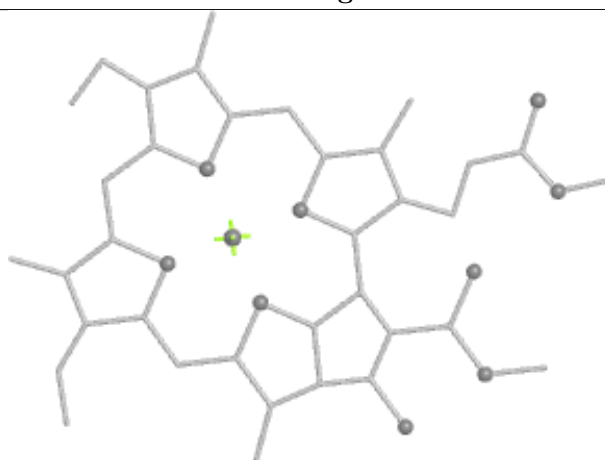
Bond lengths



Bond angles

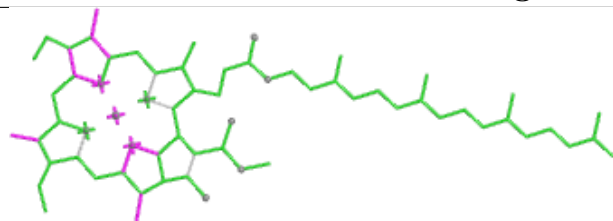


Torsions

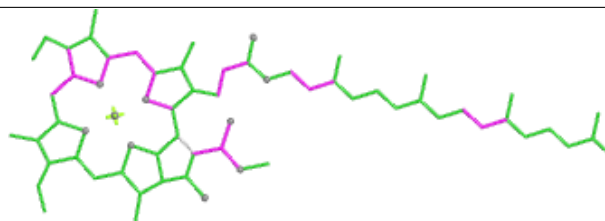


Rings

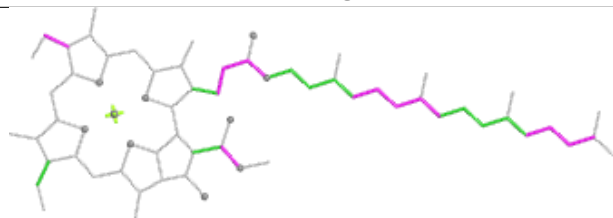
Ligand CLA A 840



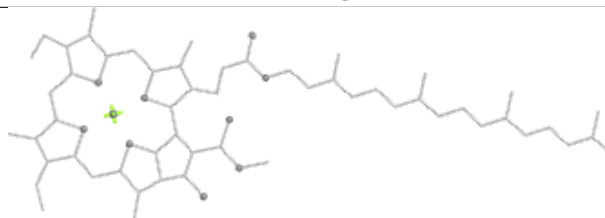
Bond lengths



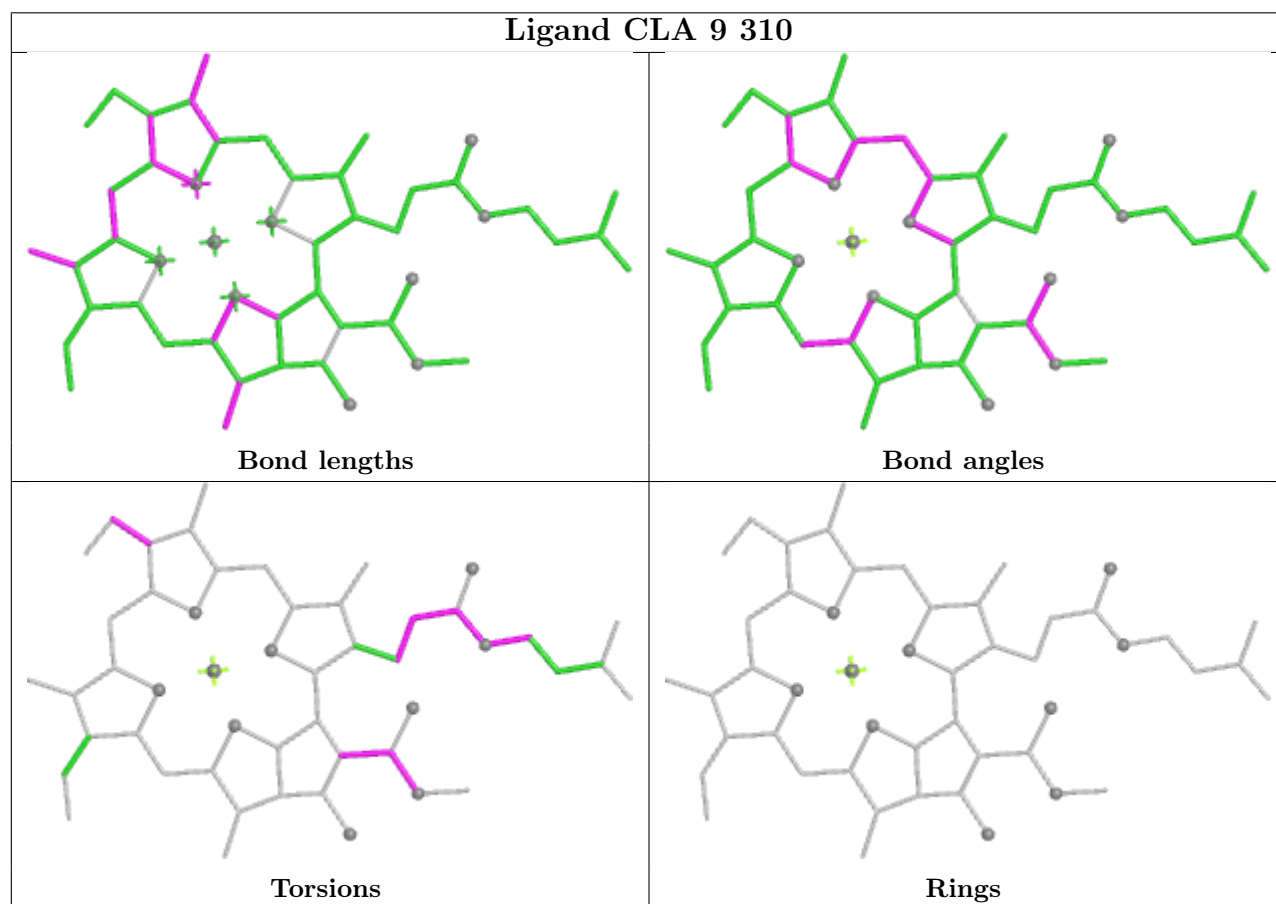
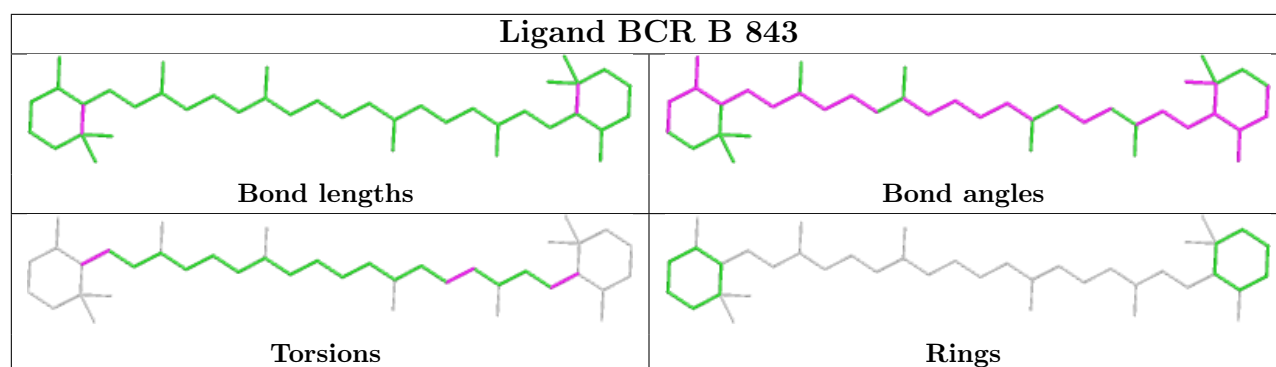
Bond angles



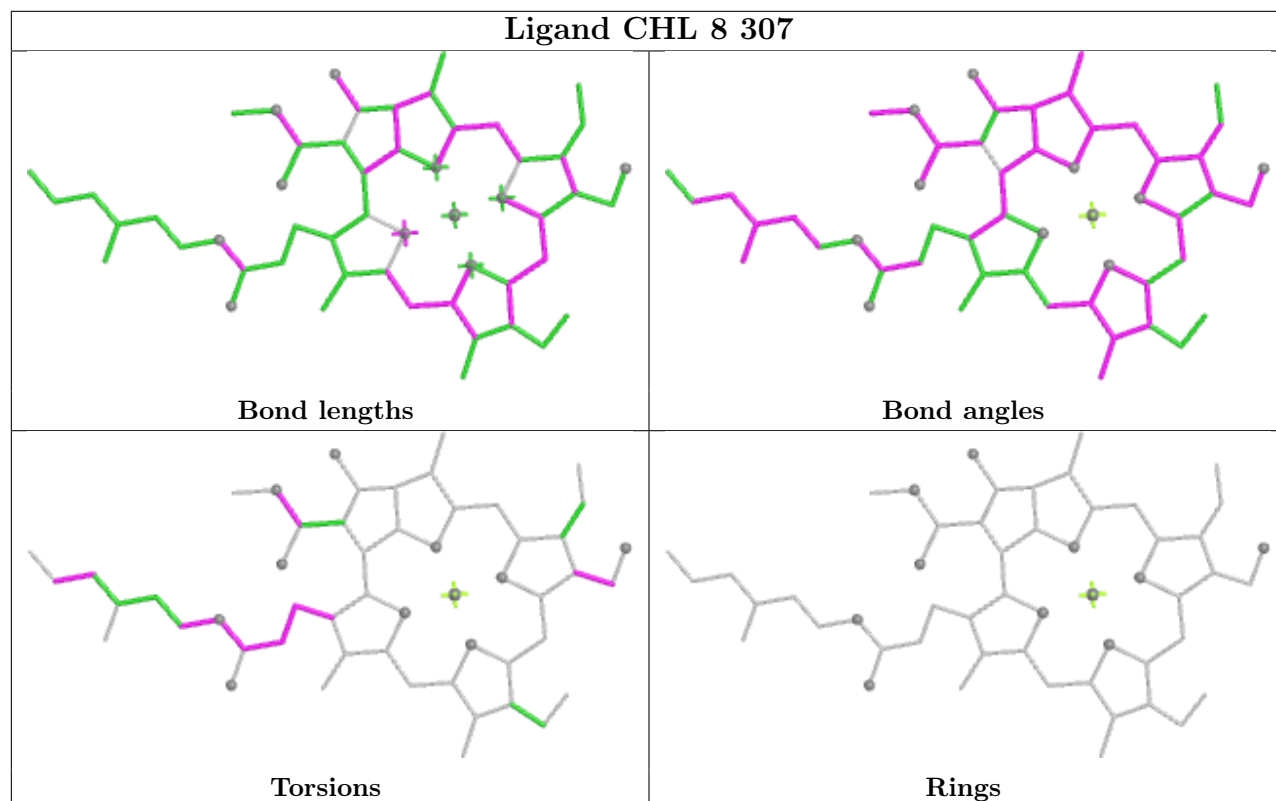
Torsions



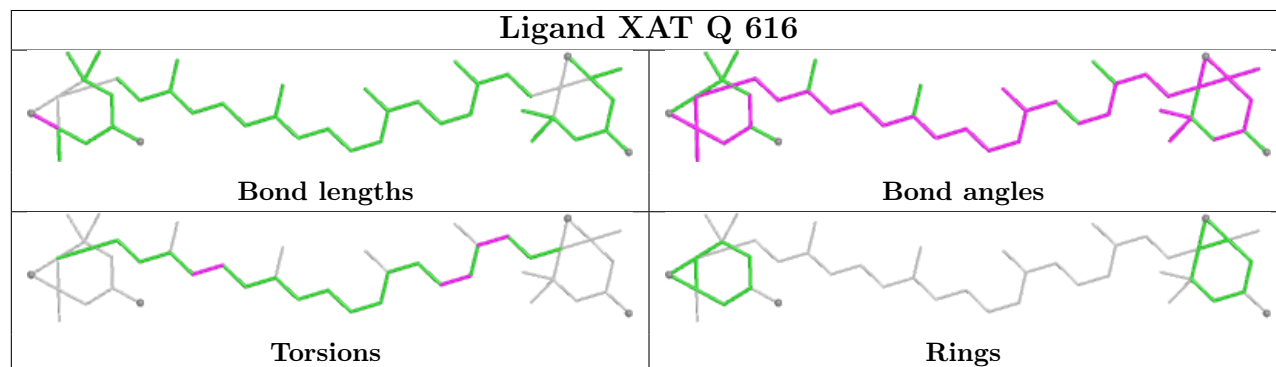
Rings



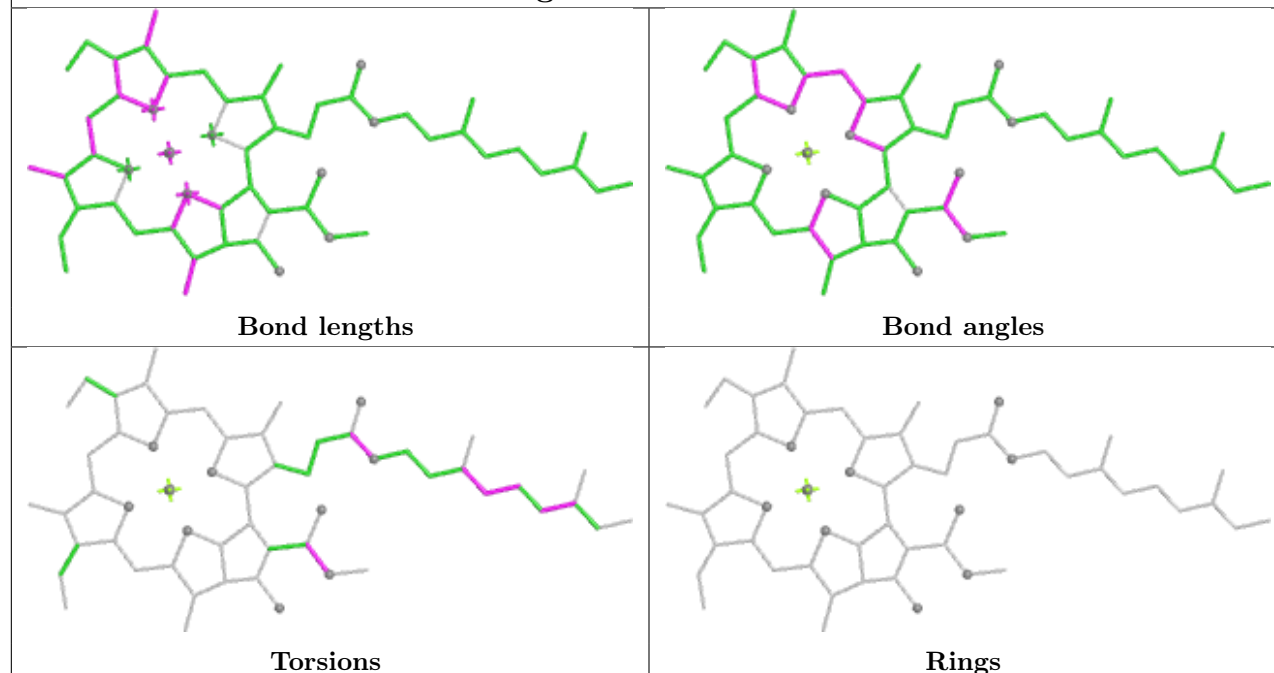
Ligand CHL 8 307



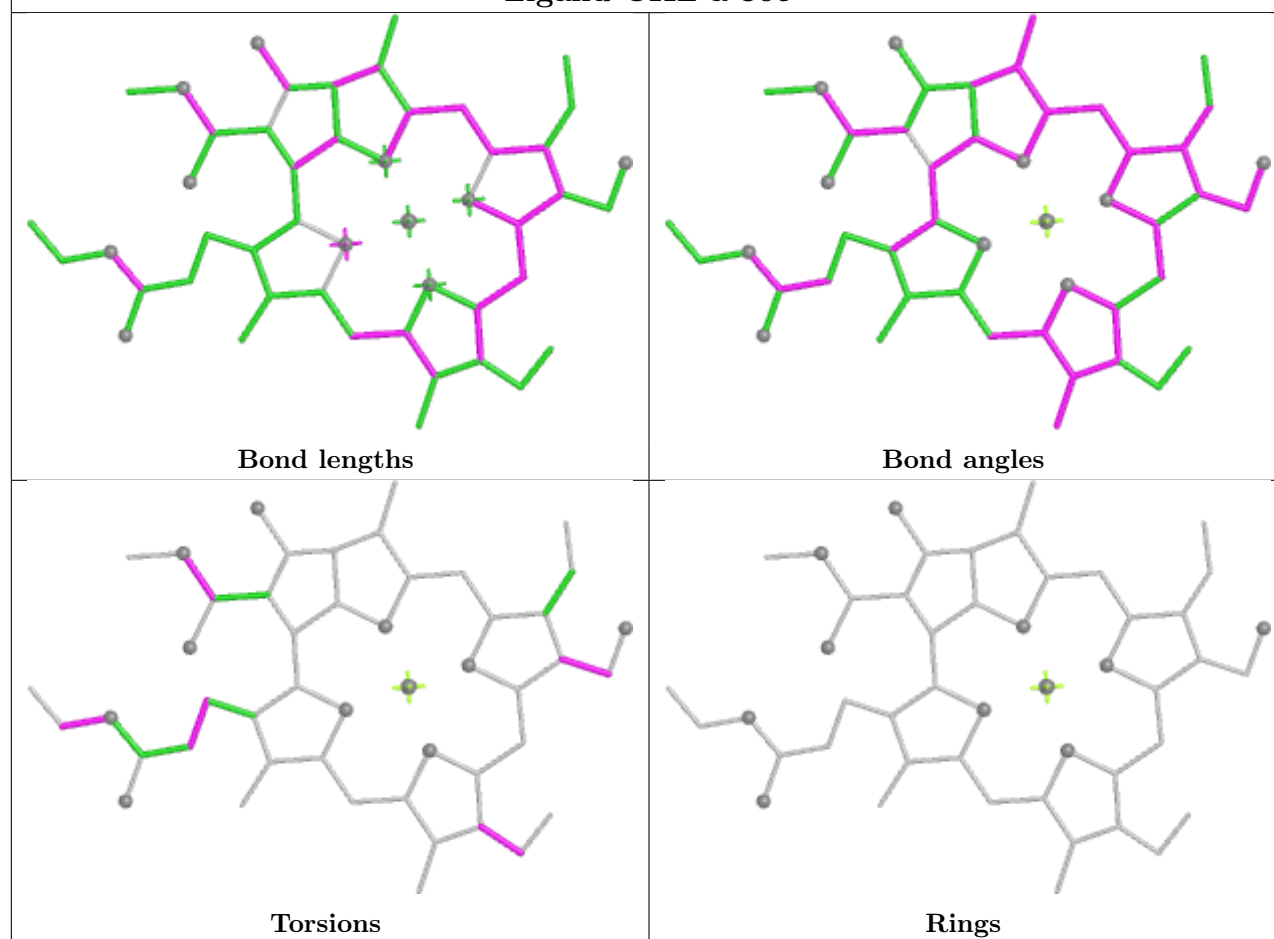
Ligand XAT Q 616



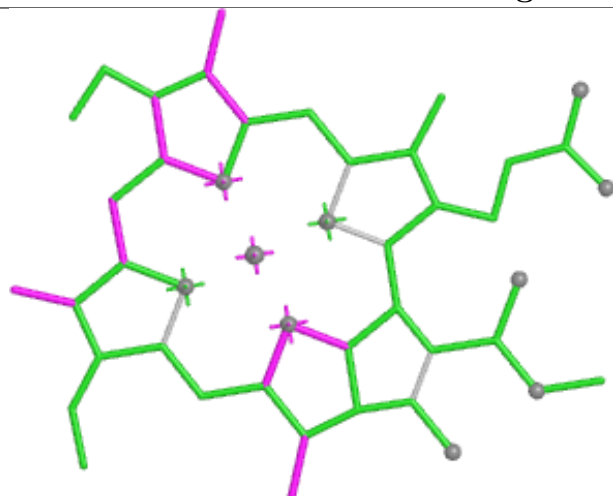
Ligand CLA 7 303



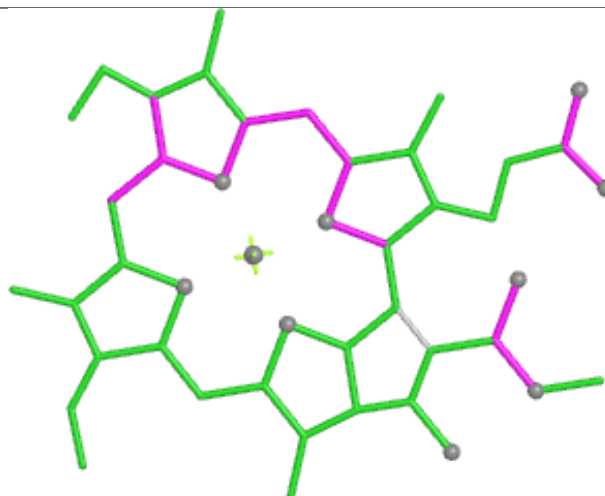
Ligand CHL a 305



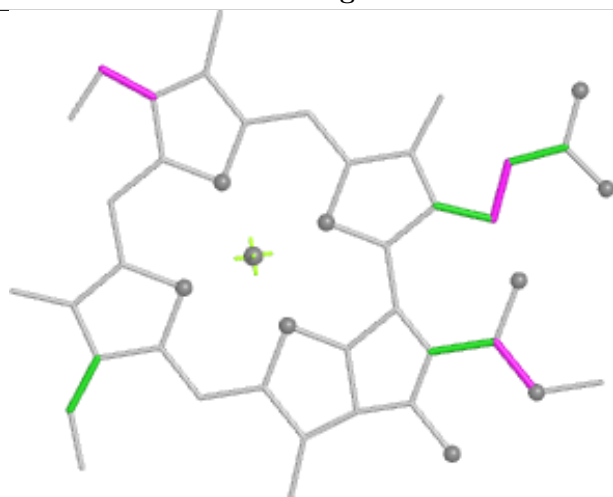
Ligand CLA F 802



Bond lengths



Bond angles

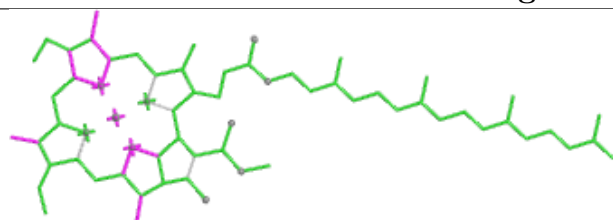


Torsions

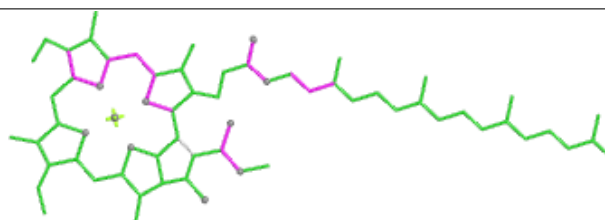


Rings

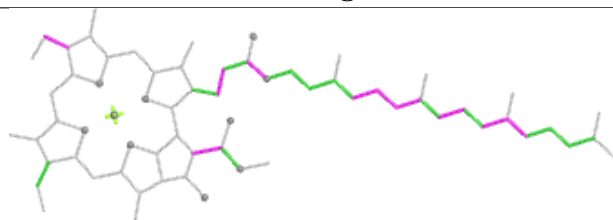
Ligand CLA 7 311



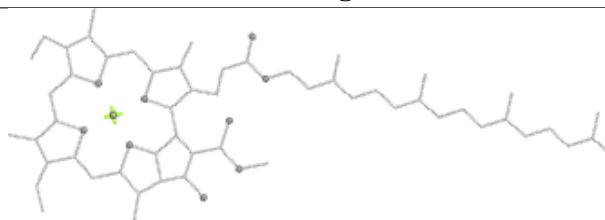
Bond lengths



Bond angles

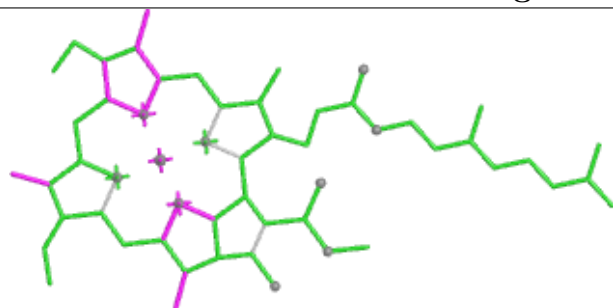


Torsions

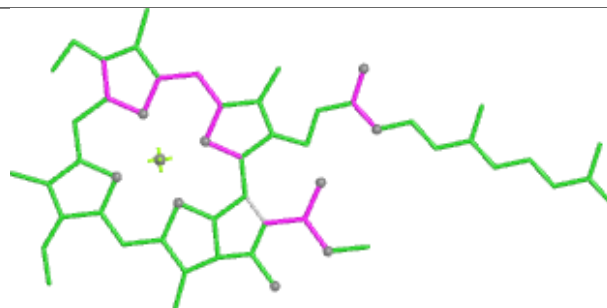


Rings

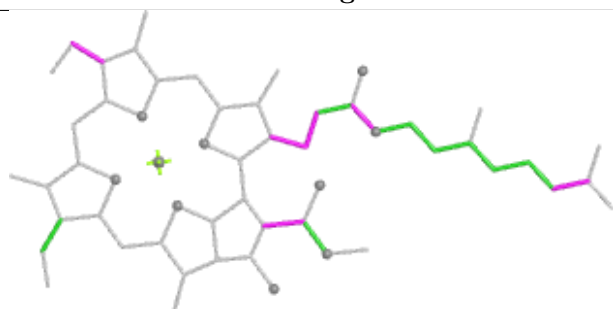
Ligand CLA A 824



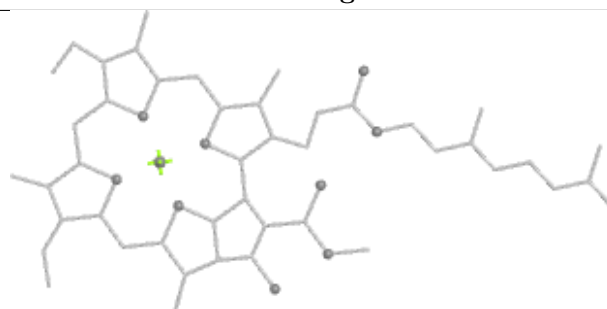
Bond lengths



Bond angles

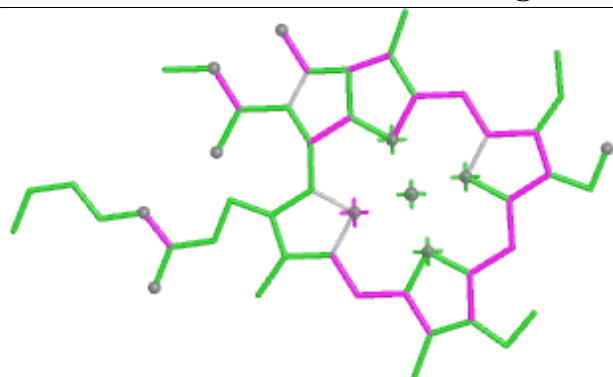


Torsions

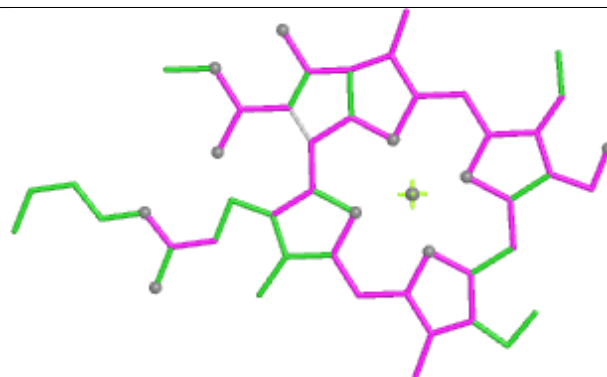


Rings

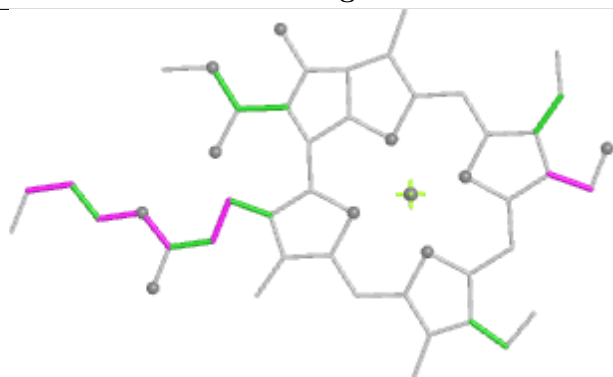
Ligand CHL P 606



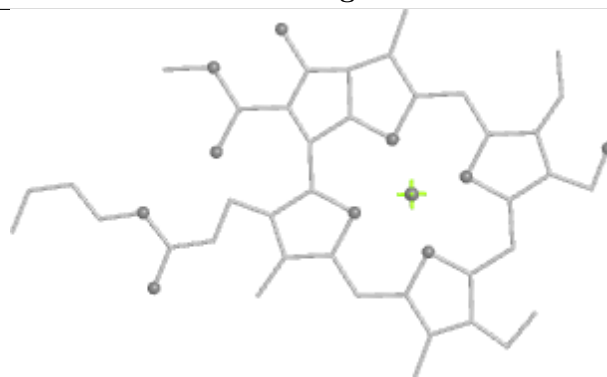
Bond lengths



Bond angles

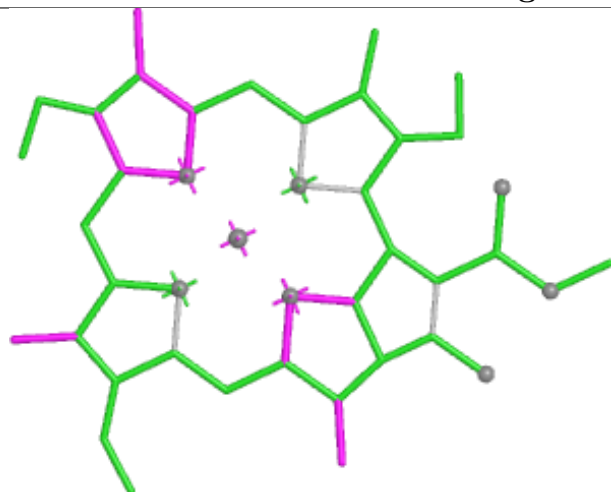


Torsions

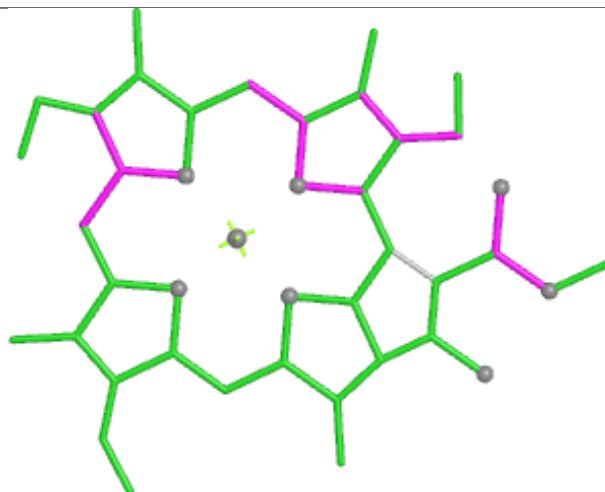


Rings

Ligand CLA 7 304



Bond lengths



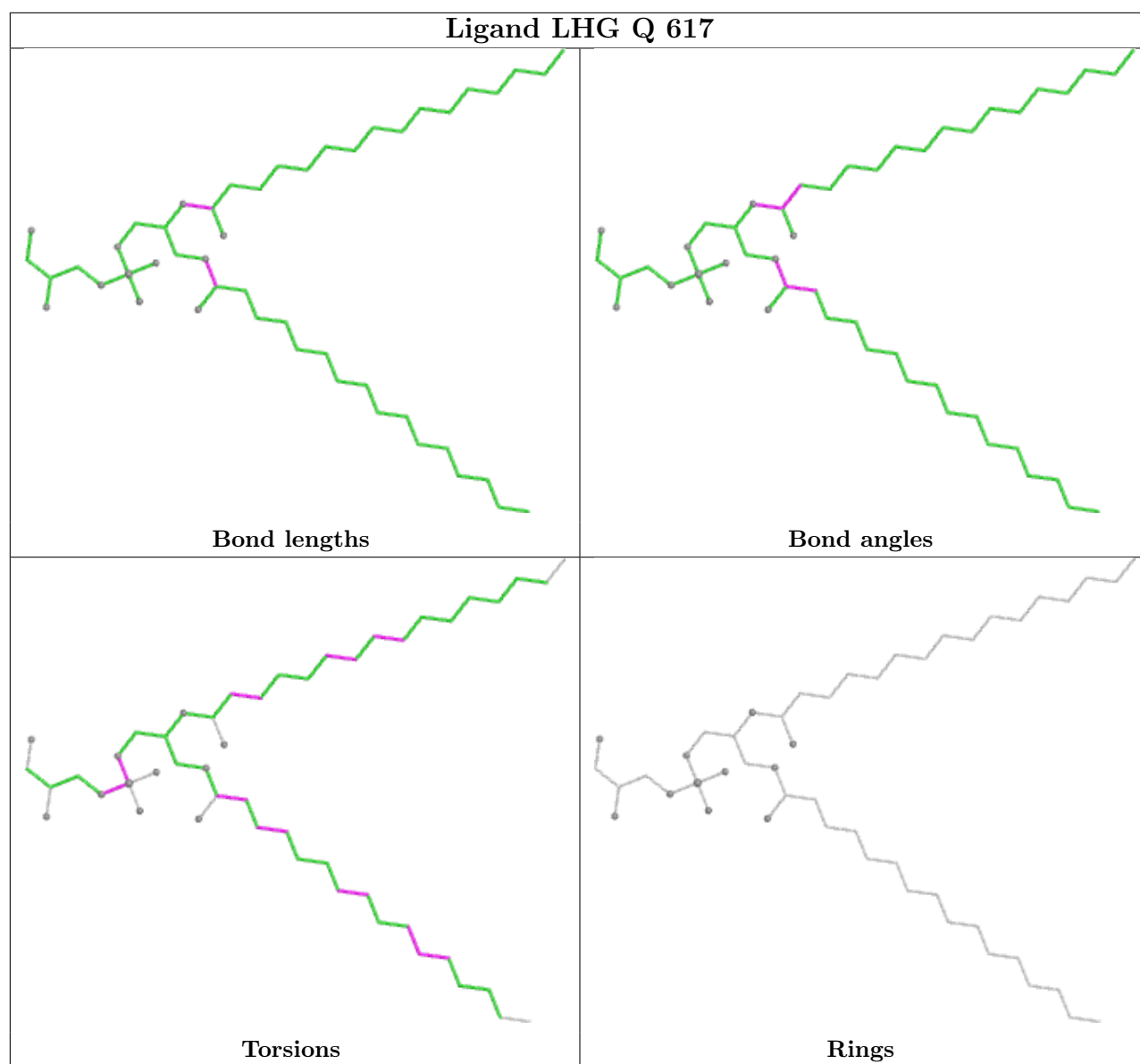
Bond angles



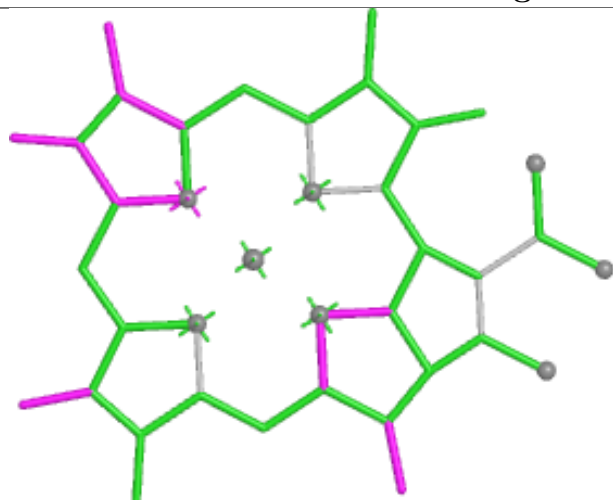
Torsions



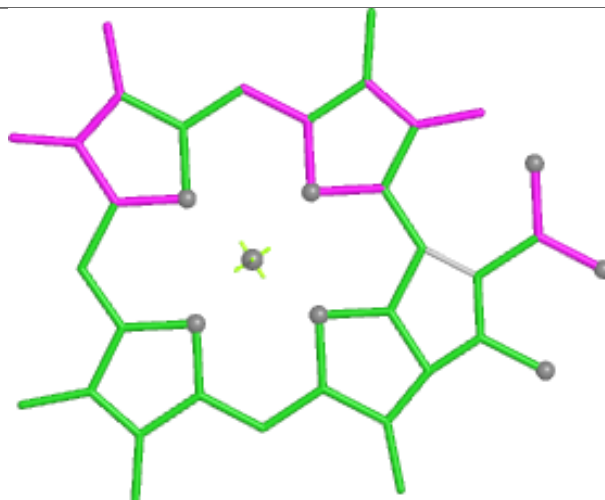
Rings



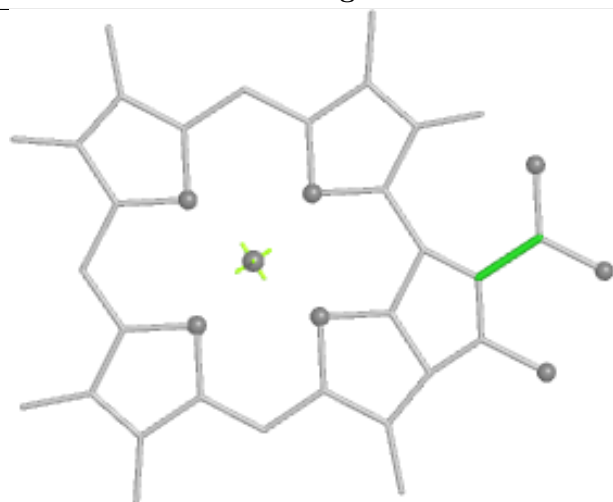
Ligand CLA O 203



Bond lengths



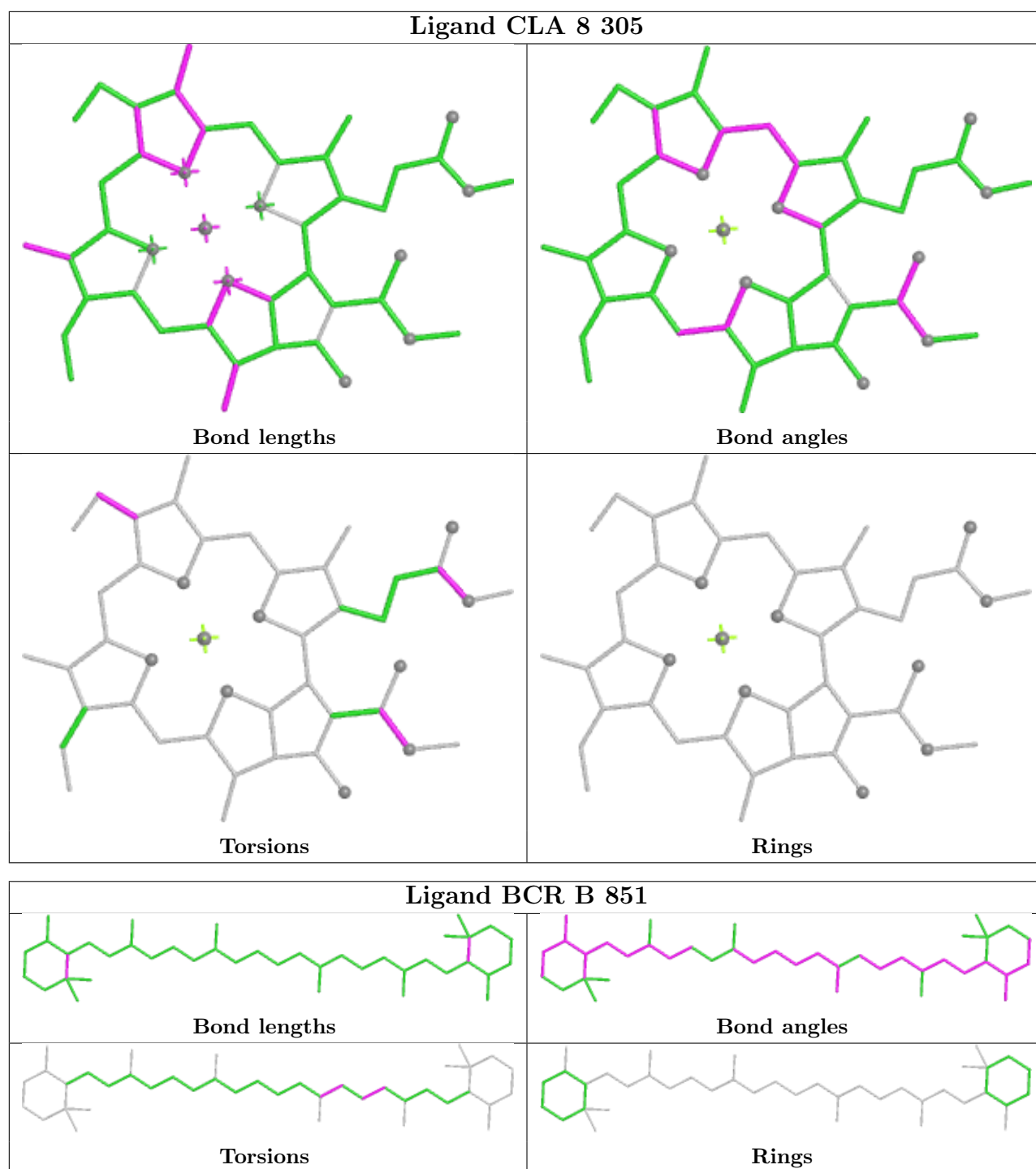
Bond angles



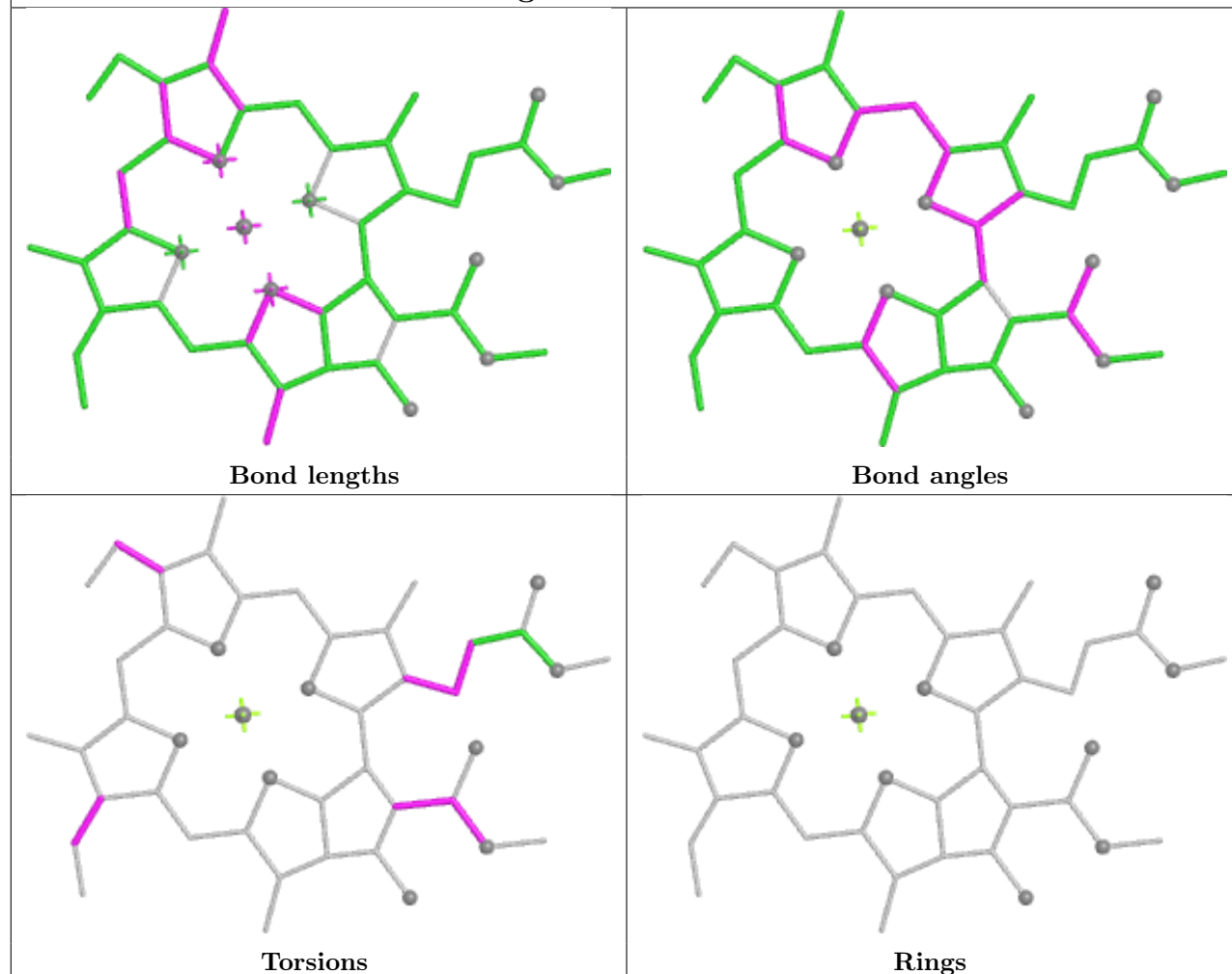
Torsions



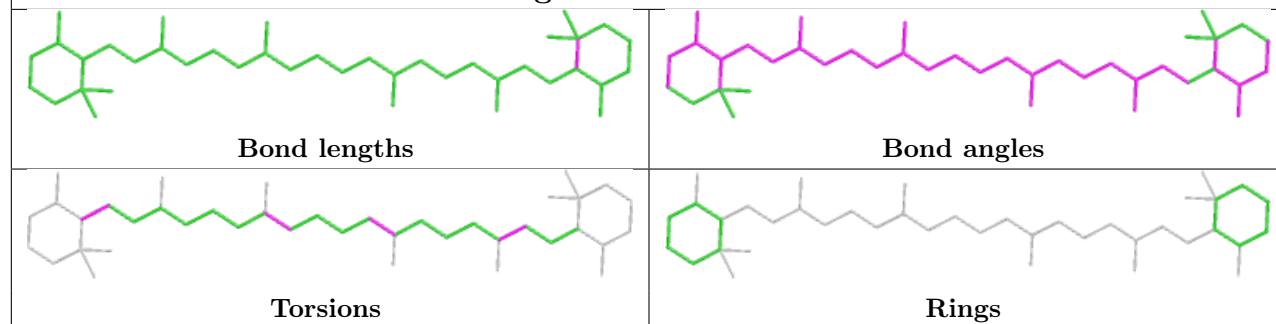
Rings



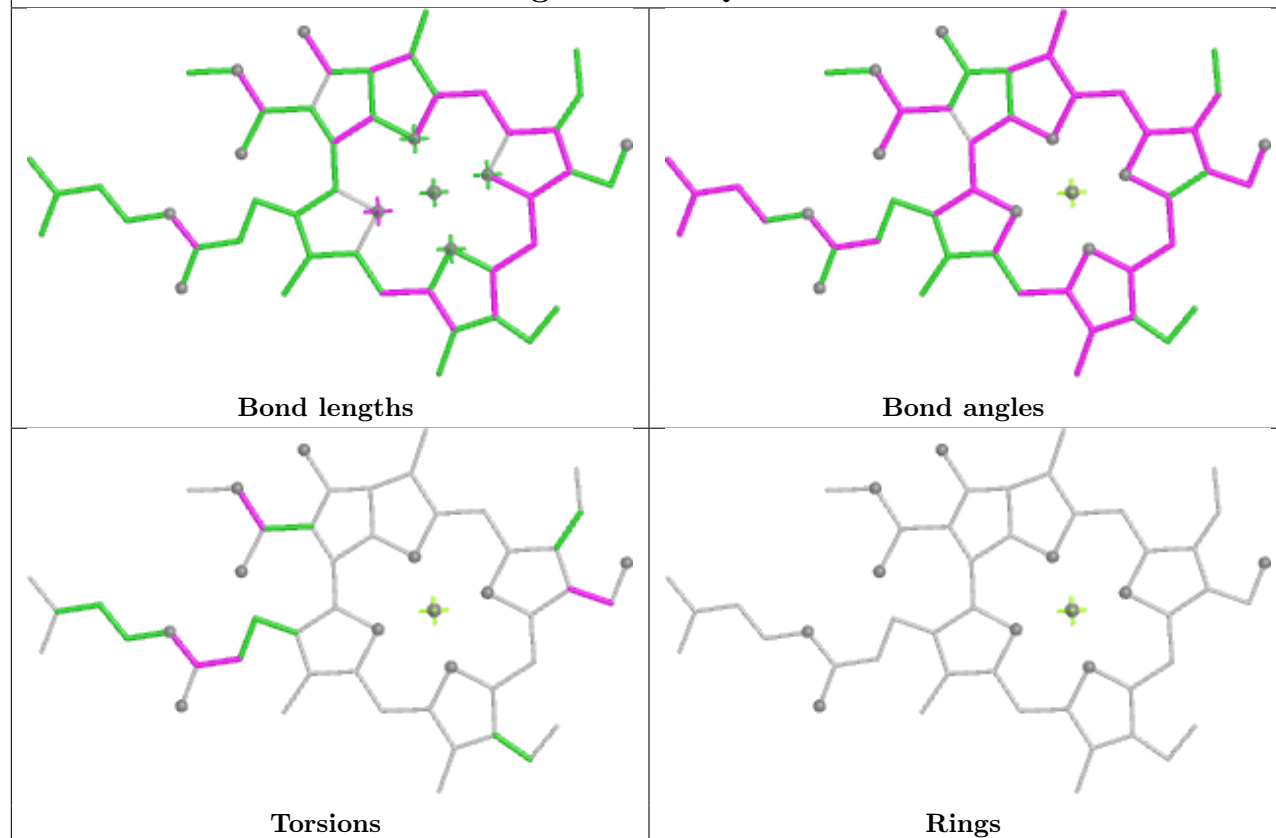
Ligand CLA 5 319



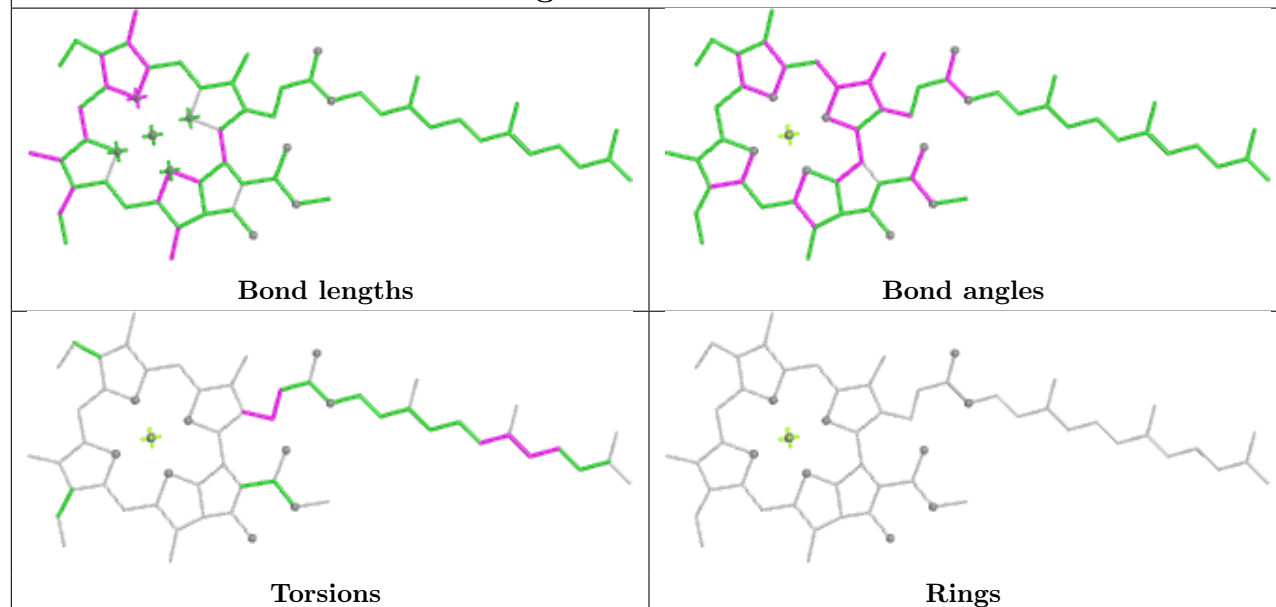
Ligand BCR 3 318

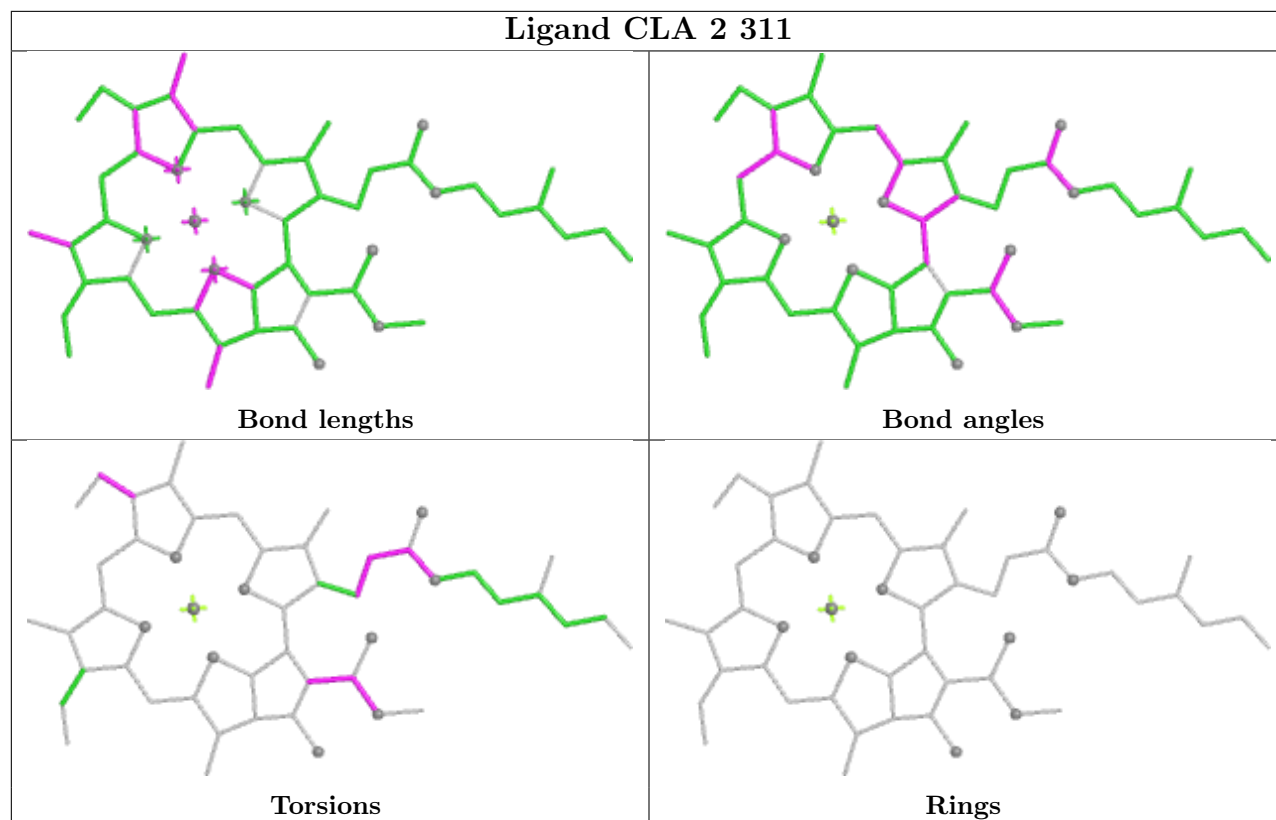


Ligand CHL Q 601

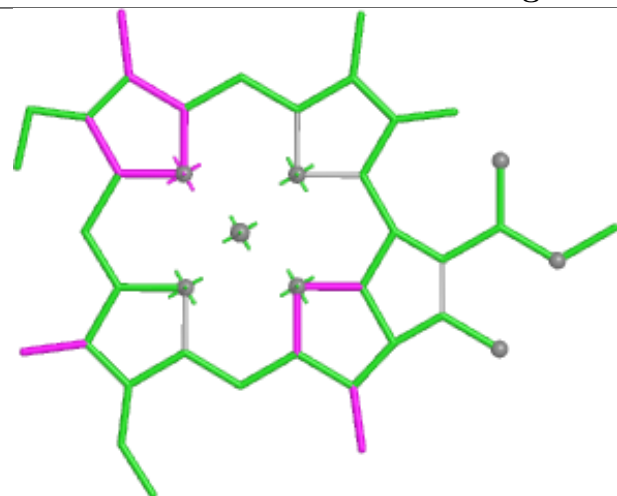


Ligand CLA 1 609





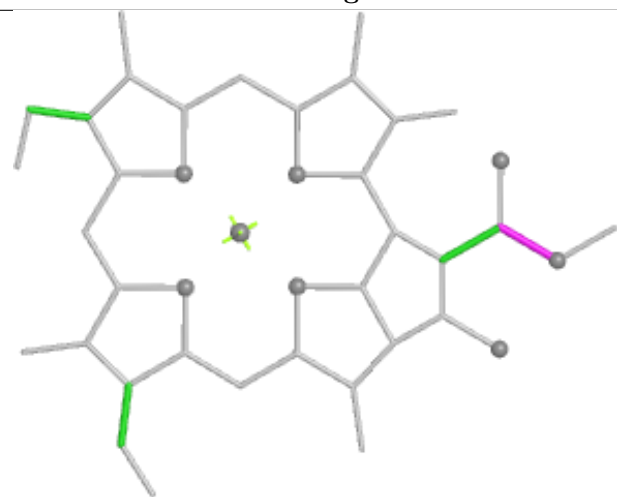
Ligand CLA 2 306



Bond lengths



Bond angles

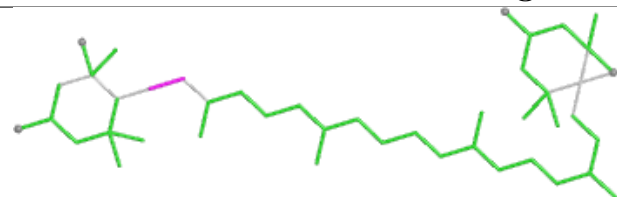


Torsions

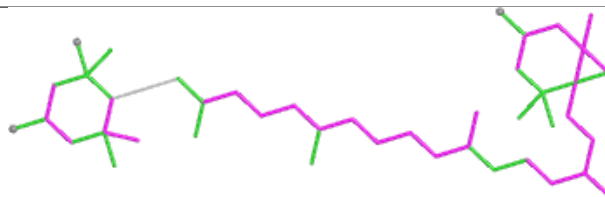


Rings

Ligand NEX T 616



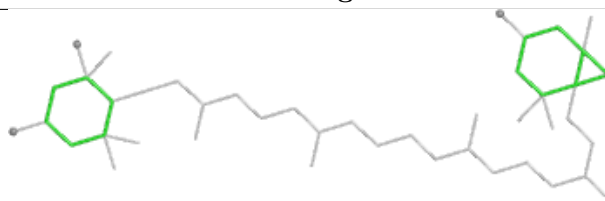
Bond lengths



Bond angles

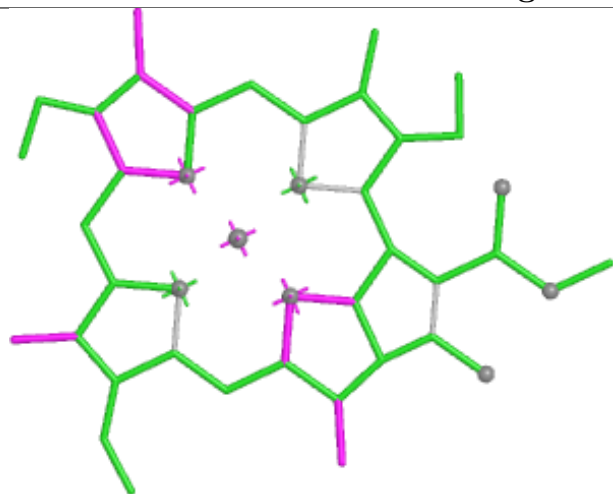


Torsions

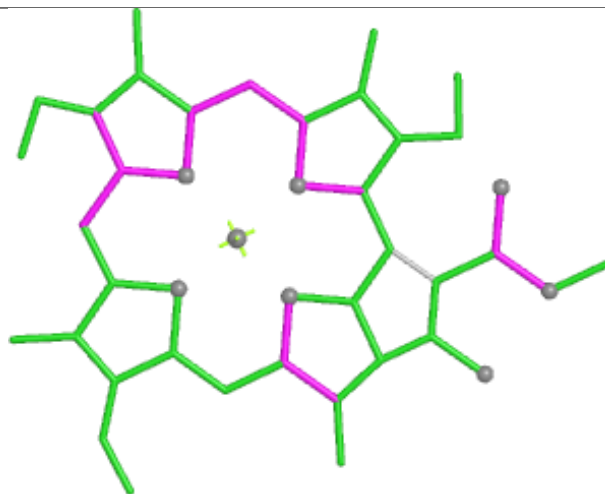


Rings

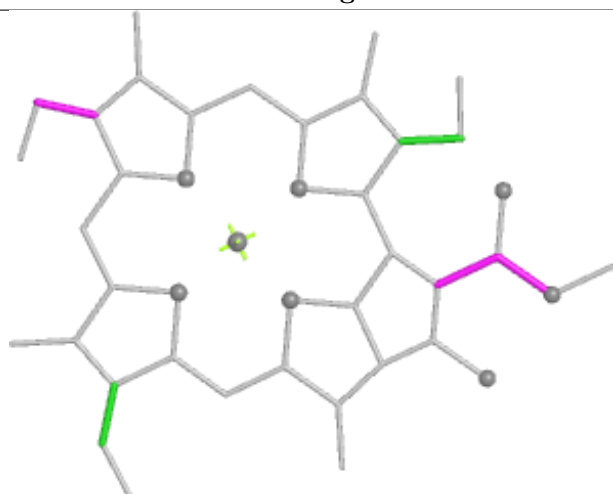
Ligand CLA J 105



Bond lengths



Bond angles

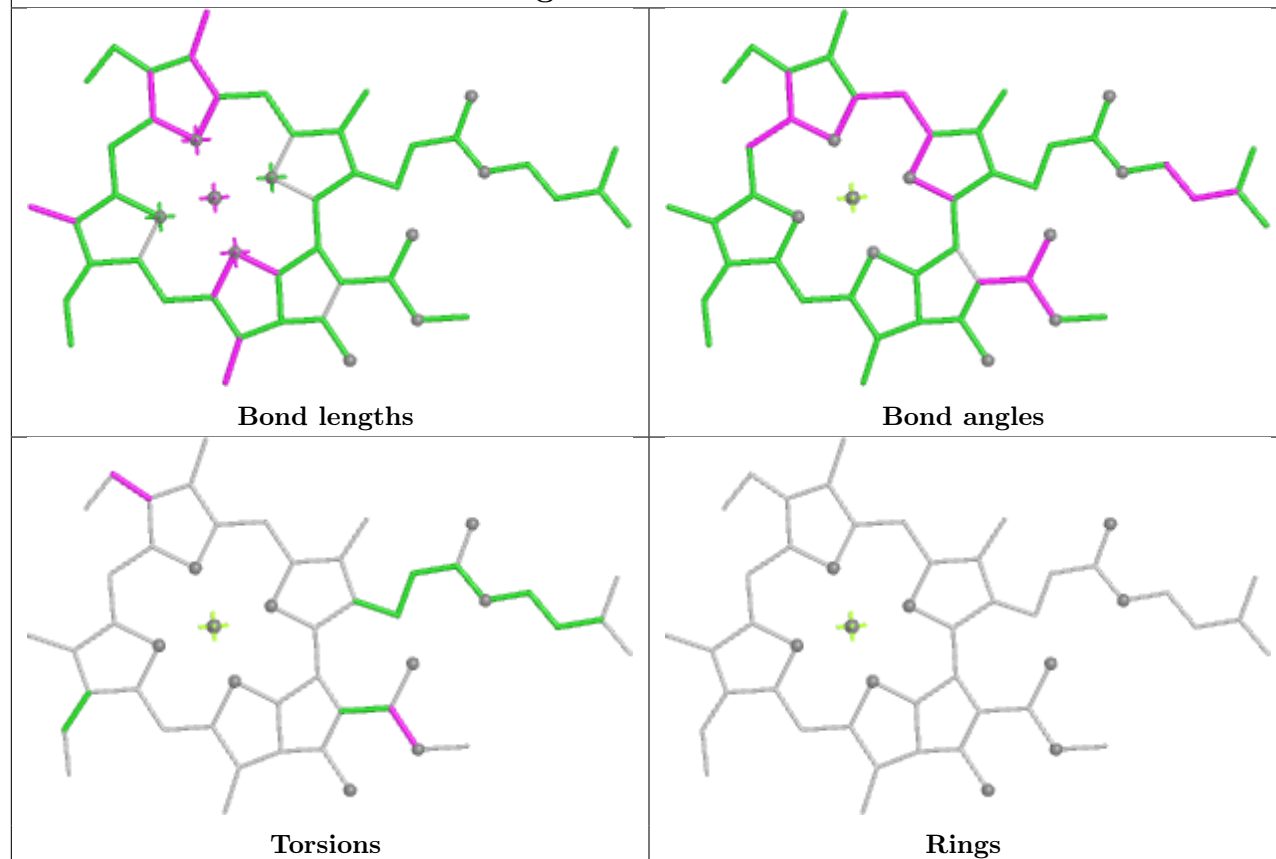


Torsions

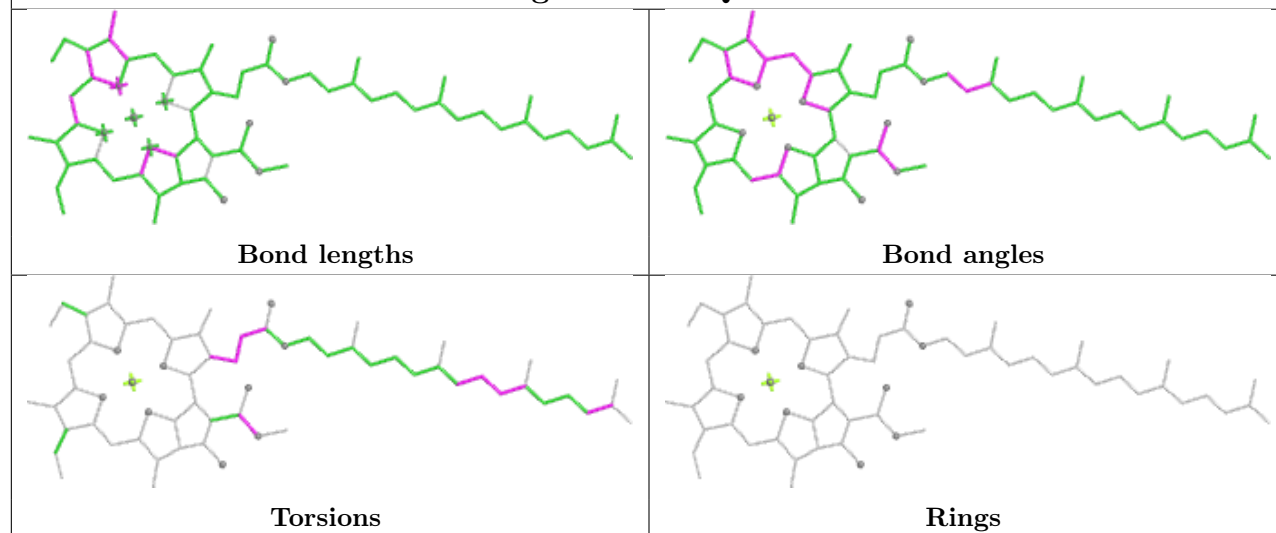


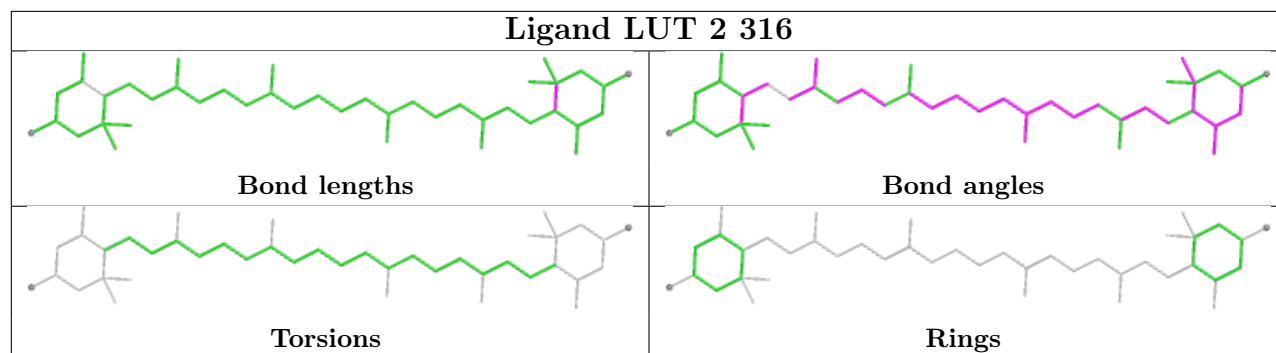
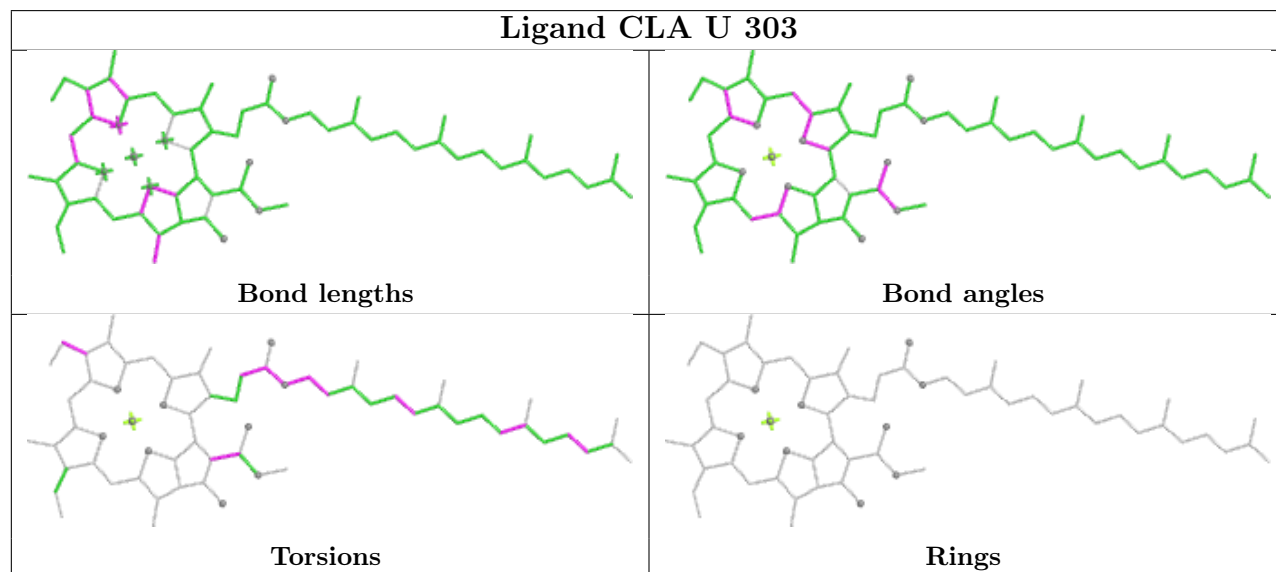
Rings

Ligand CLA 5 305

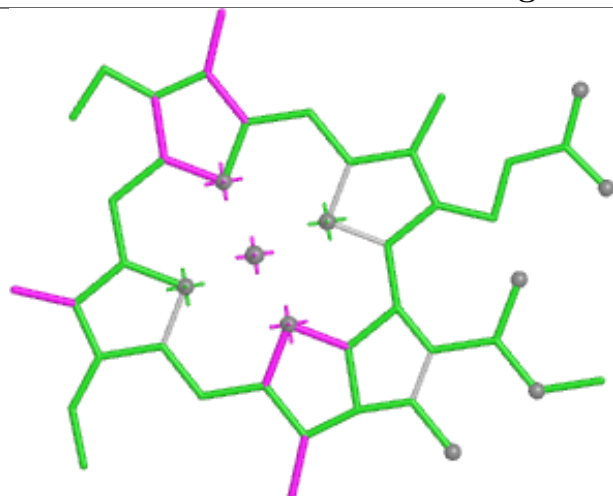


Ligand CLA Q 609

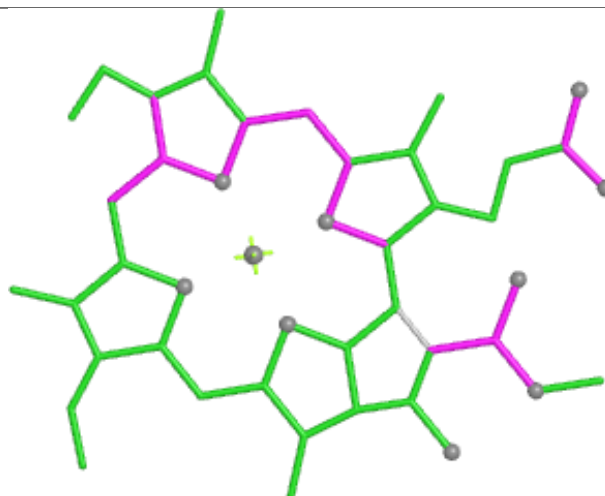


Ligand LUT 2 316**Ligand CLA U 303**

Ligand CLA 5 314



Bond lengths



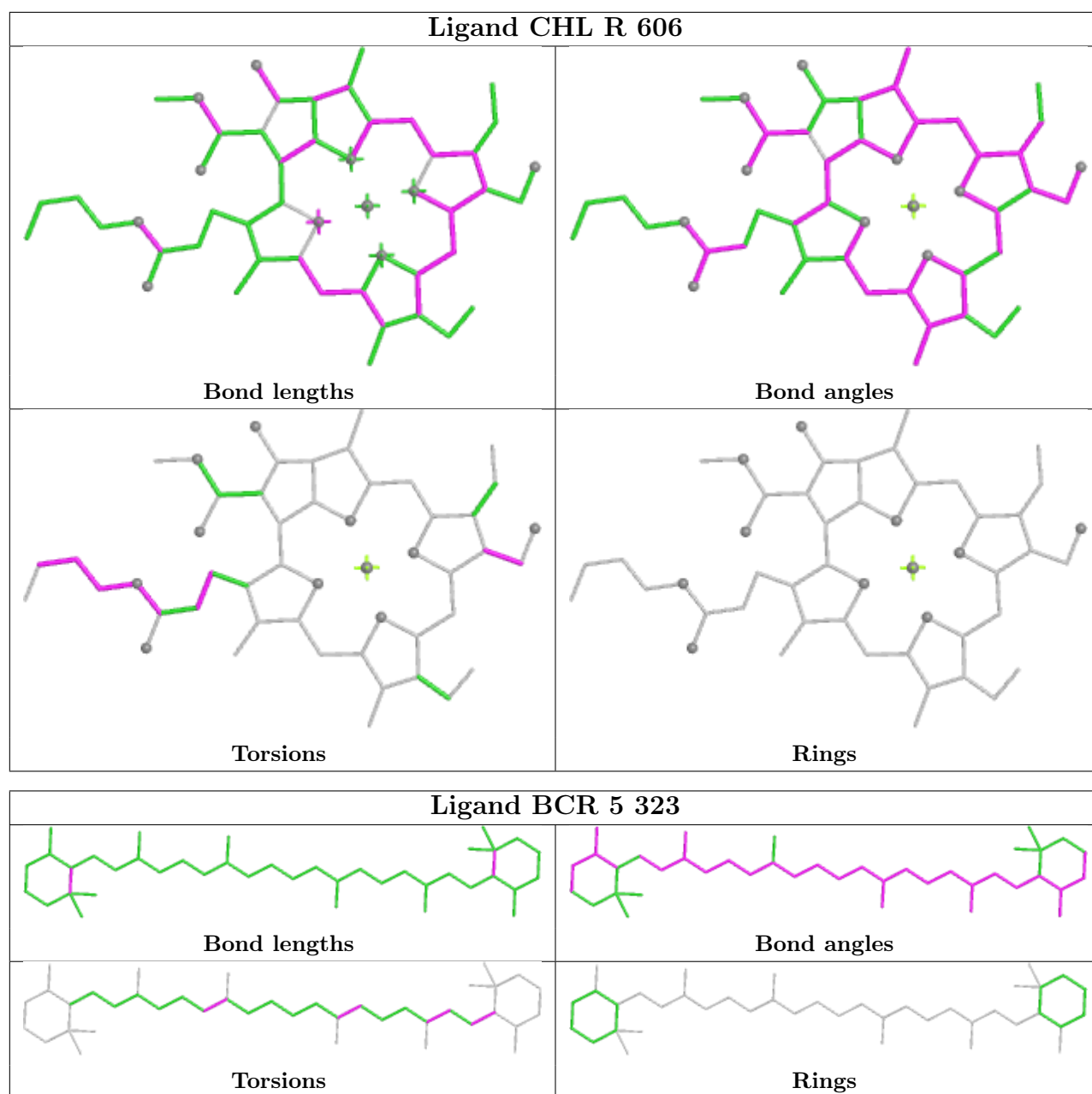
Bond angles



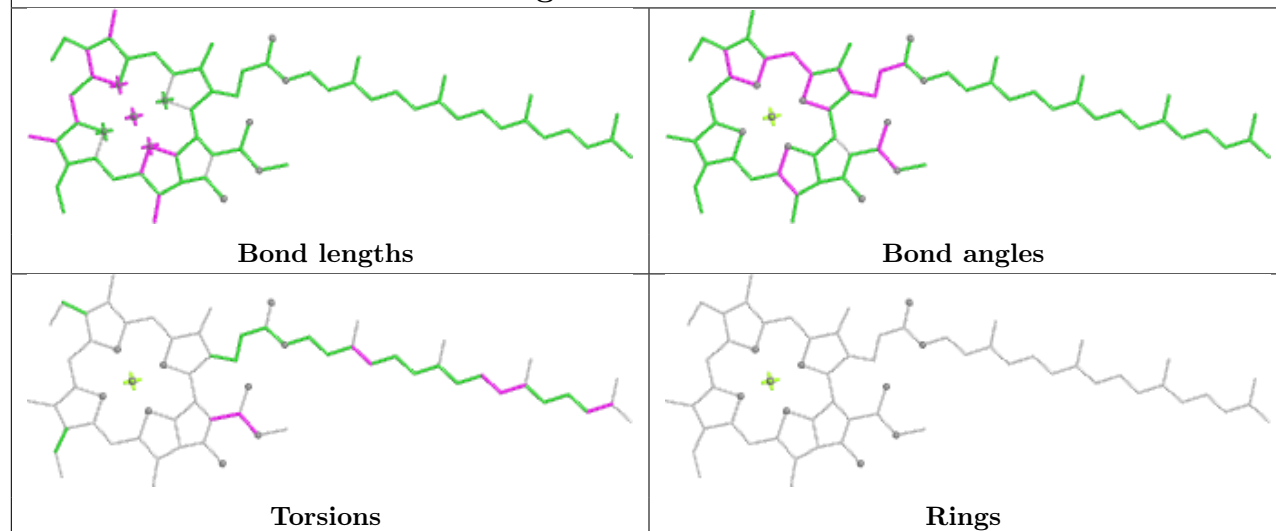
Torsions



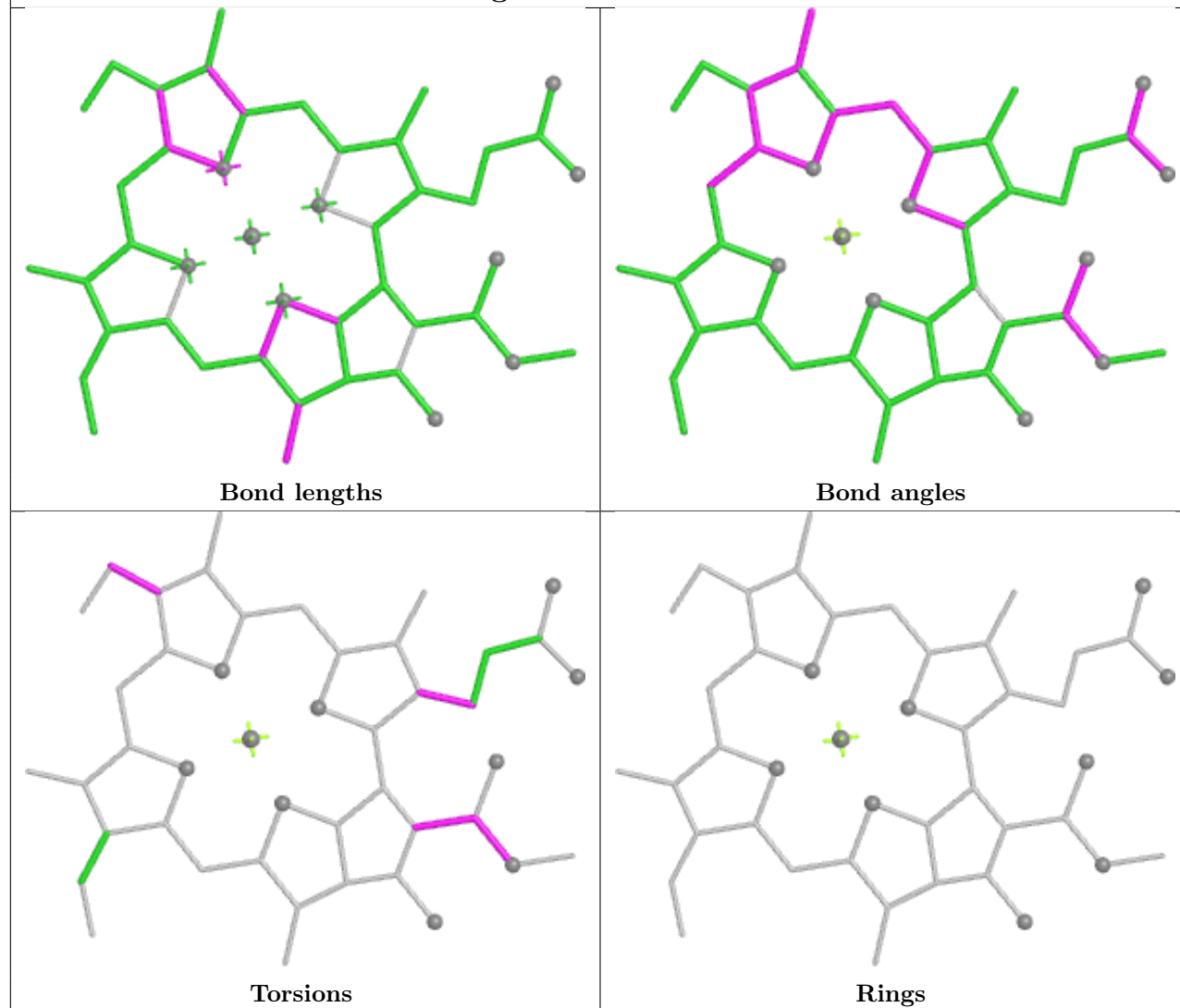
Rings

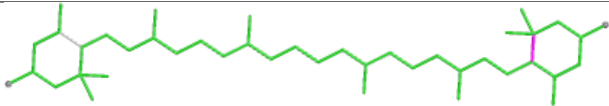
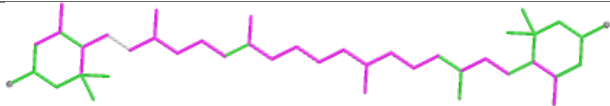
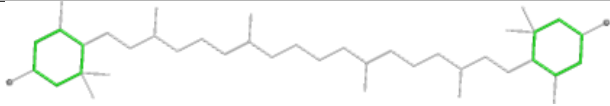


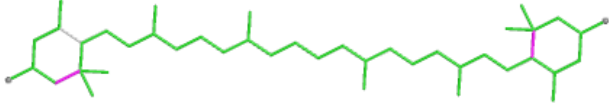
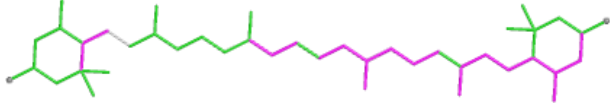
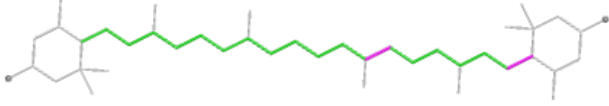
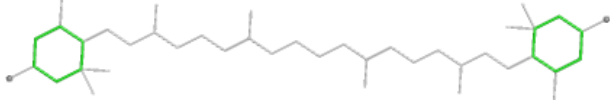
Ligand CLA 3 302

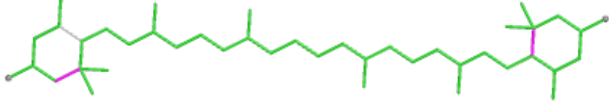
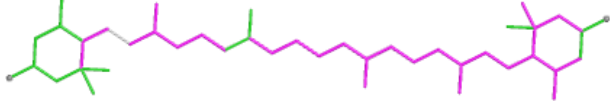
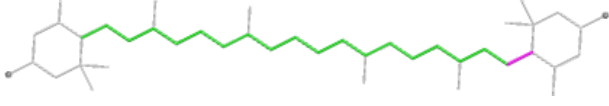
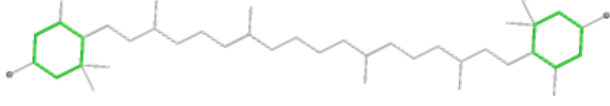


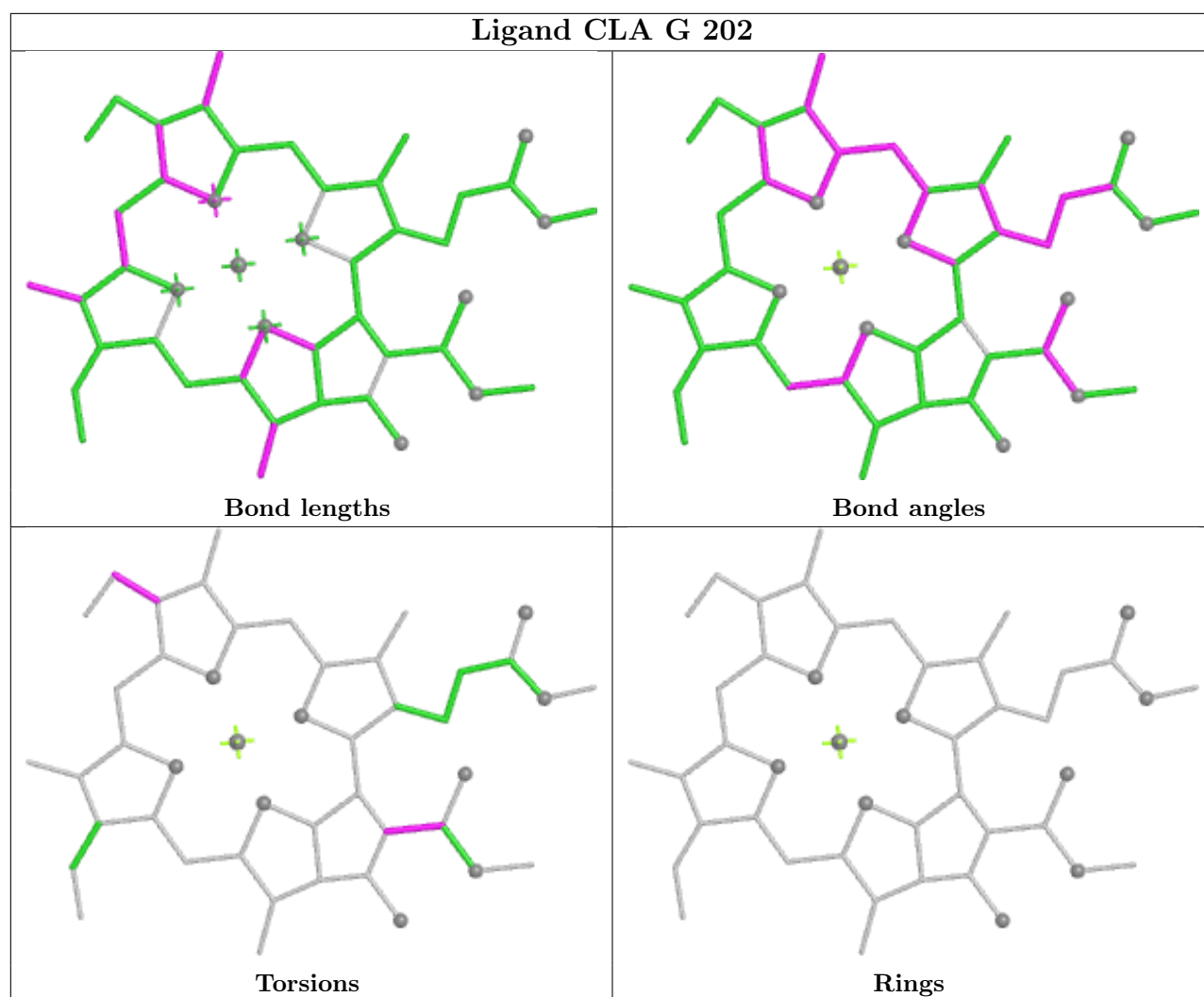
Ligand CLA U 313



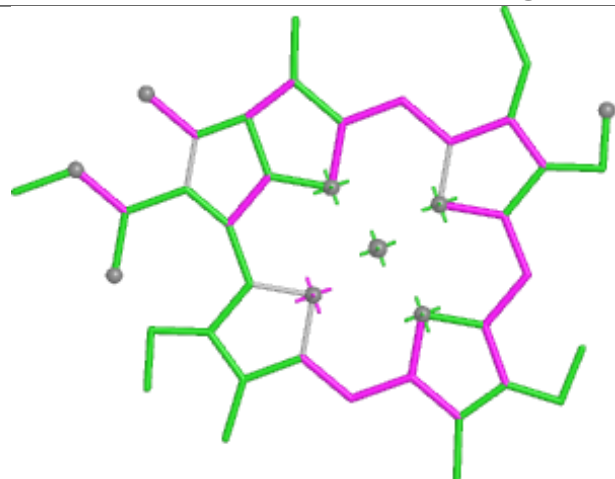
Ligand LUT 2 315	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand LUT 4 316	
	Bond lengths
	Bond angles
	Torsions
	Rings

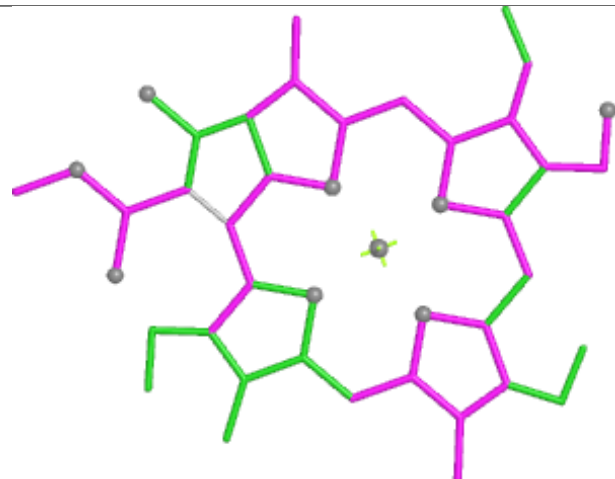
Ligand LUT a 314	
	Bond lengths
	Bond angles
	Torsions
	Rings



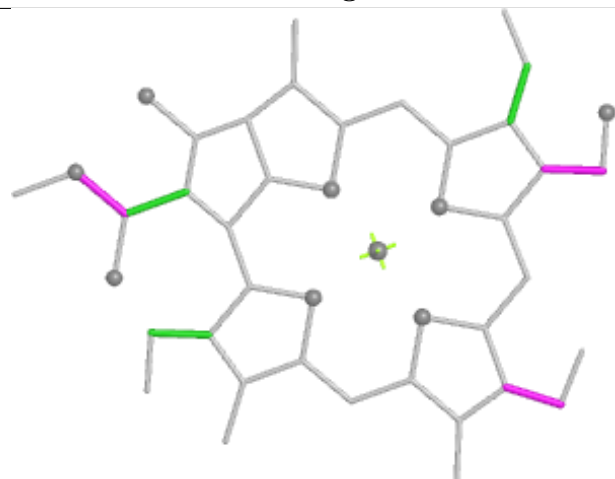
Ligand CHL 4 314



Bond lengths



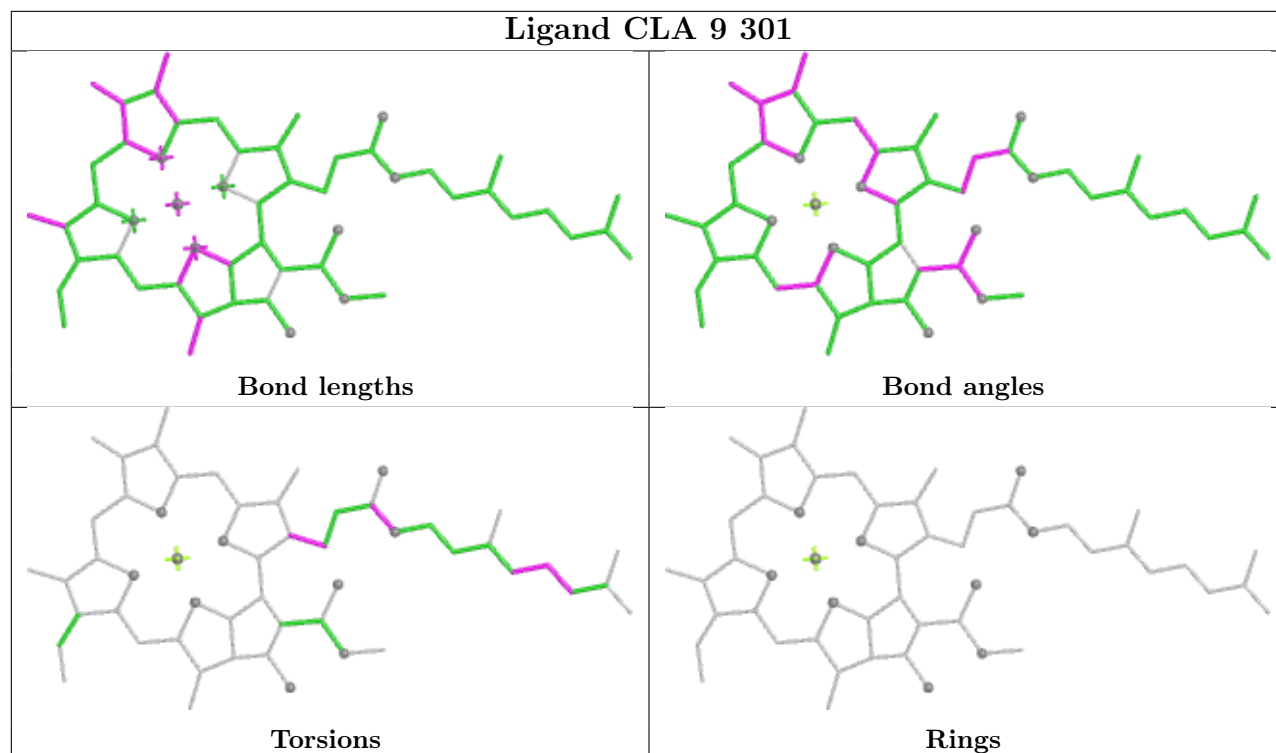
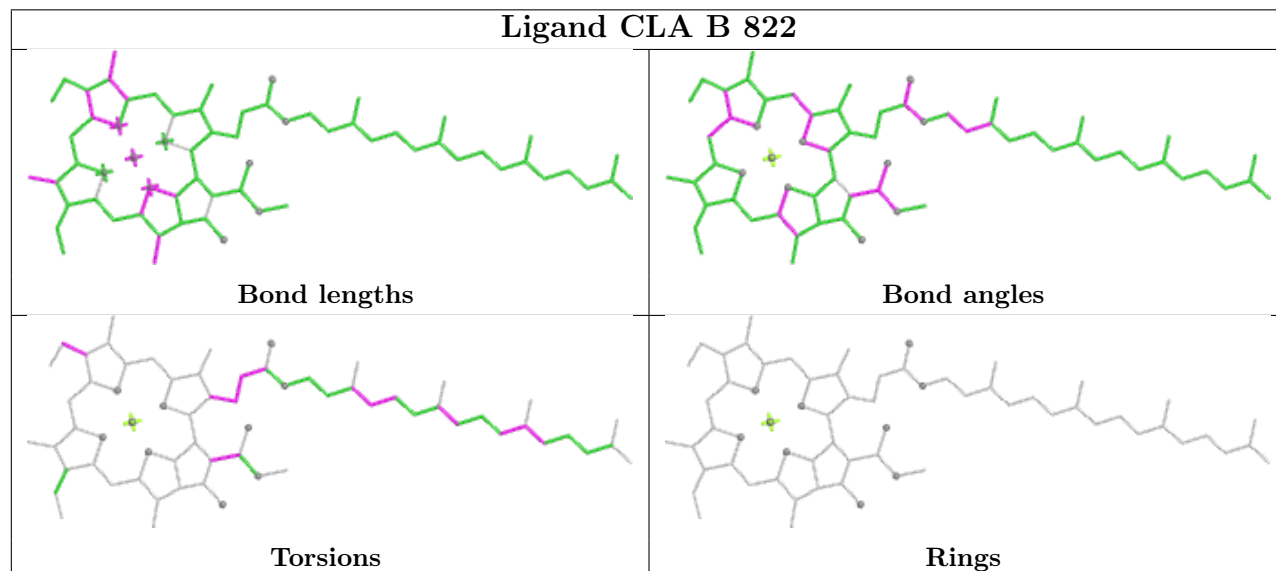
Bond angles



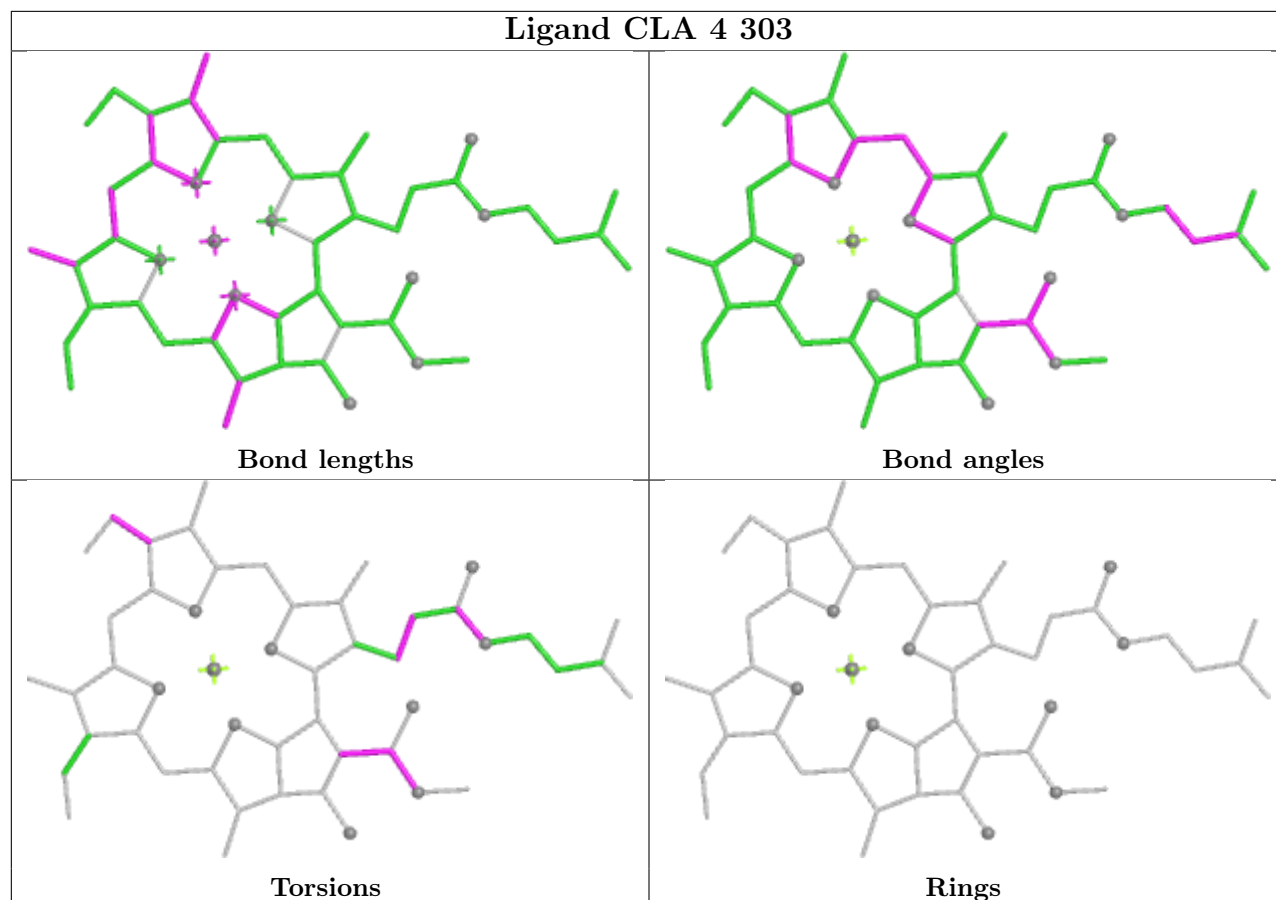
Torsions



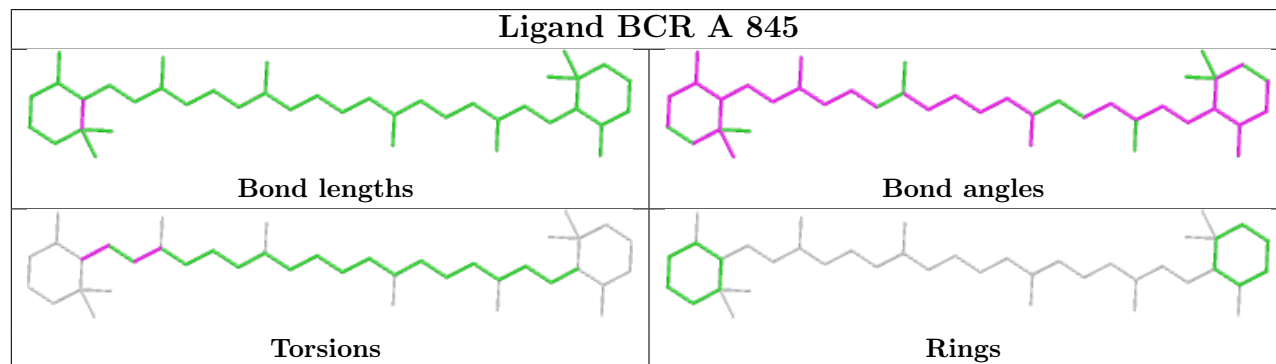
Rings

Ligand CLA 9 301**Ligand CLA B 822**

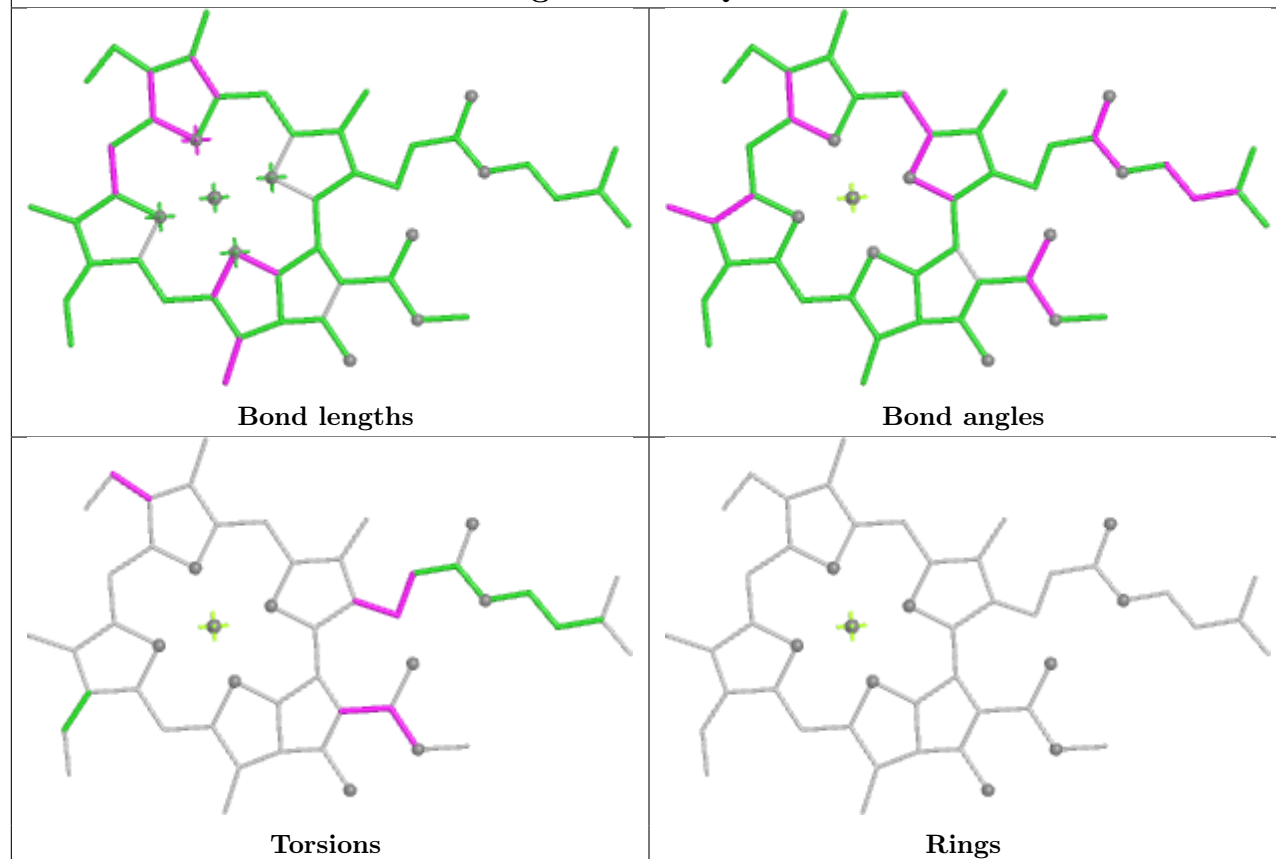
Ligand CLA 4 303



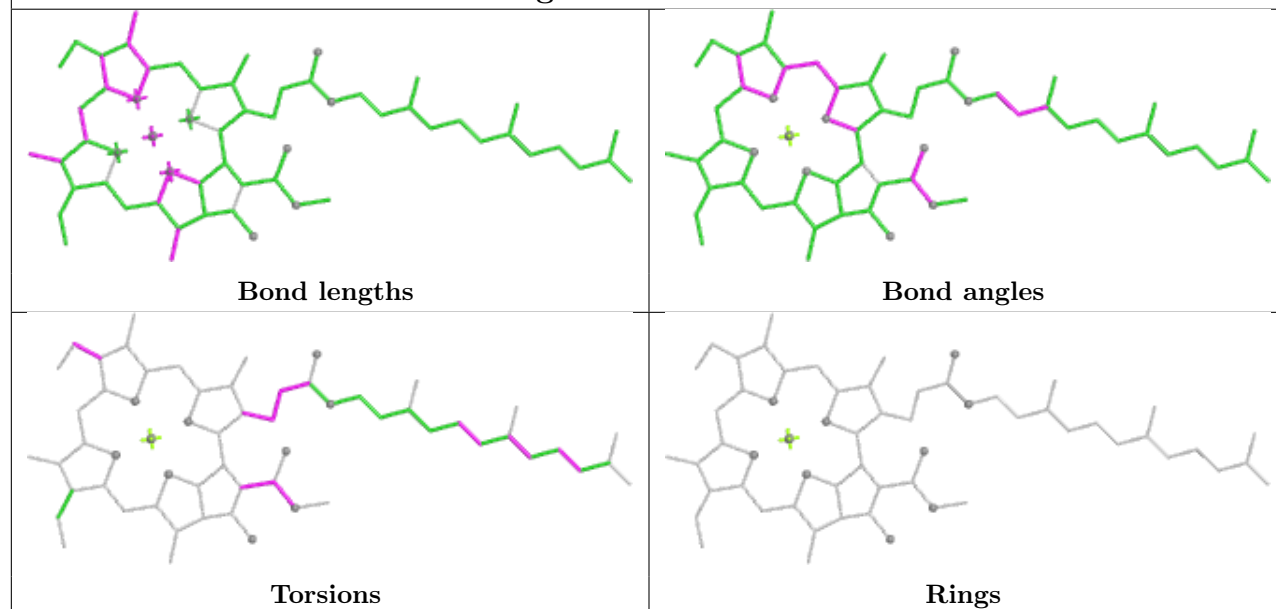
Ligand BCR A 845

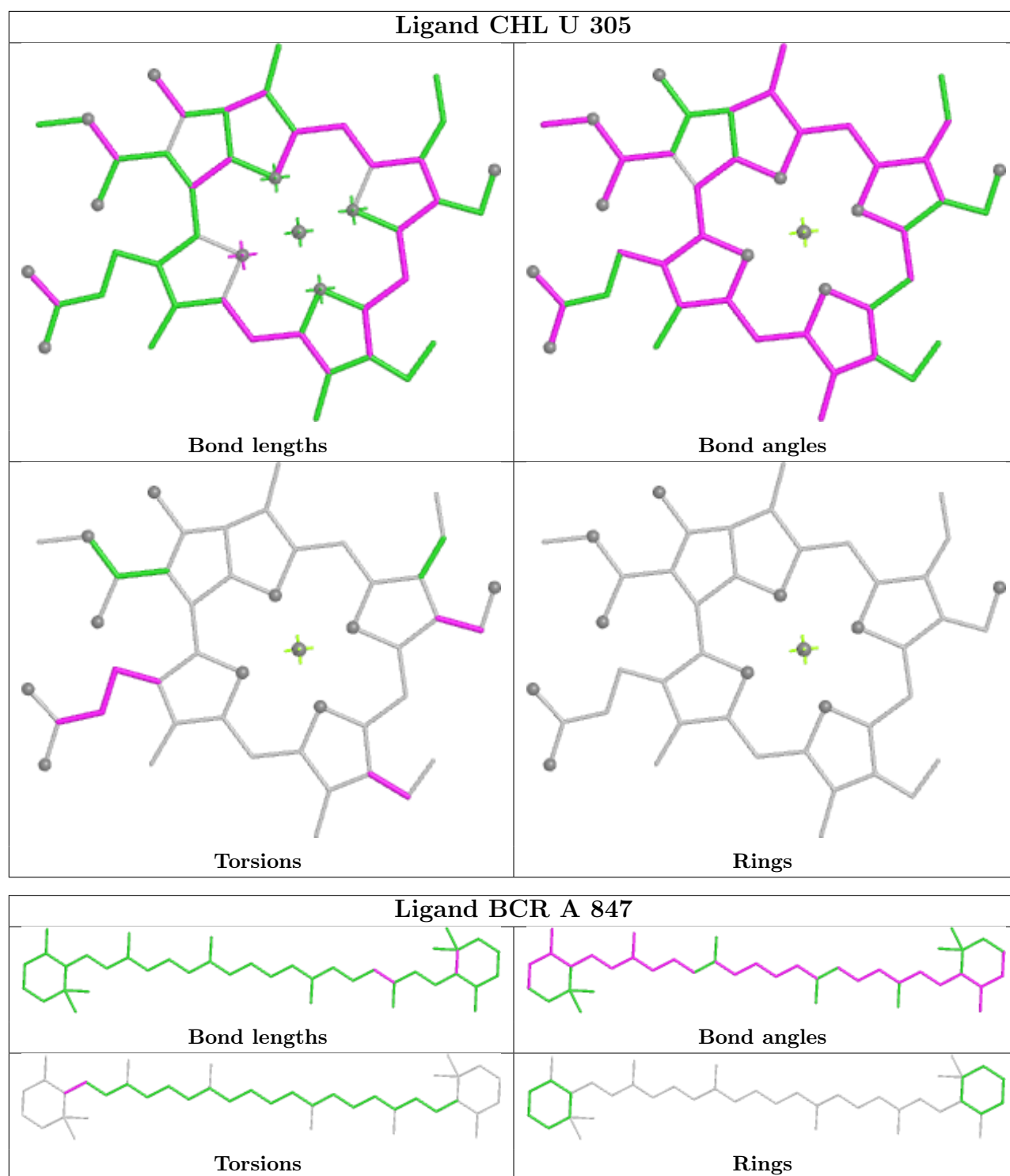


Ligand CLA Q 604

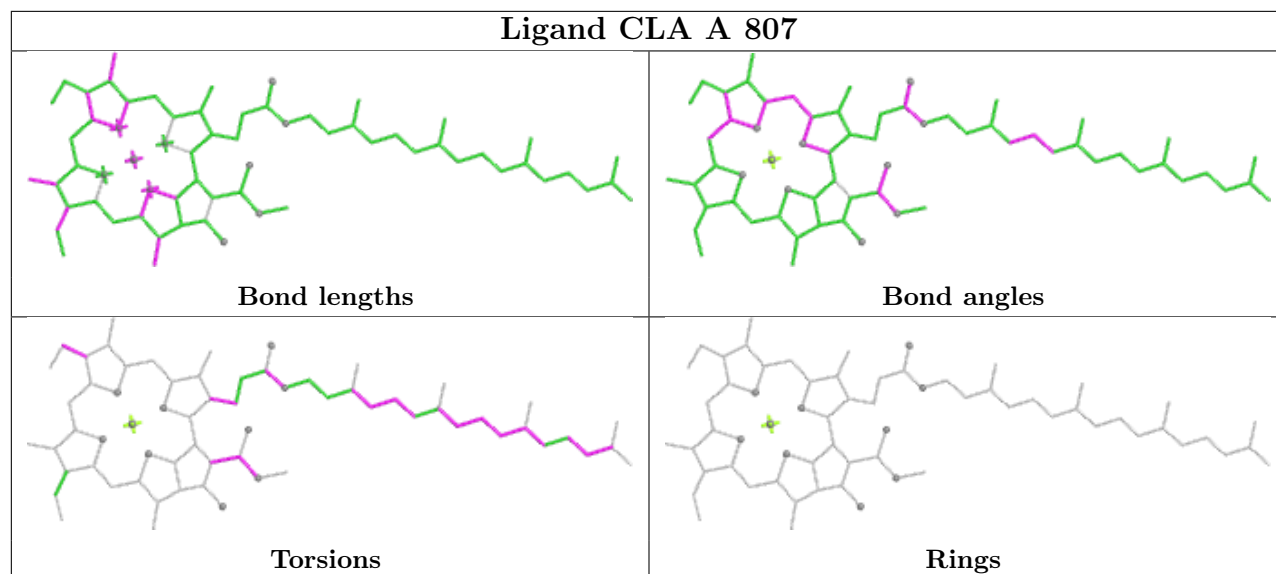


Ligand CLA 4 301

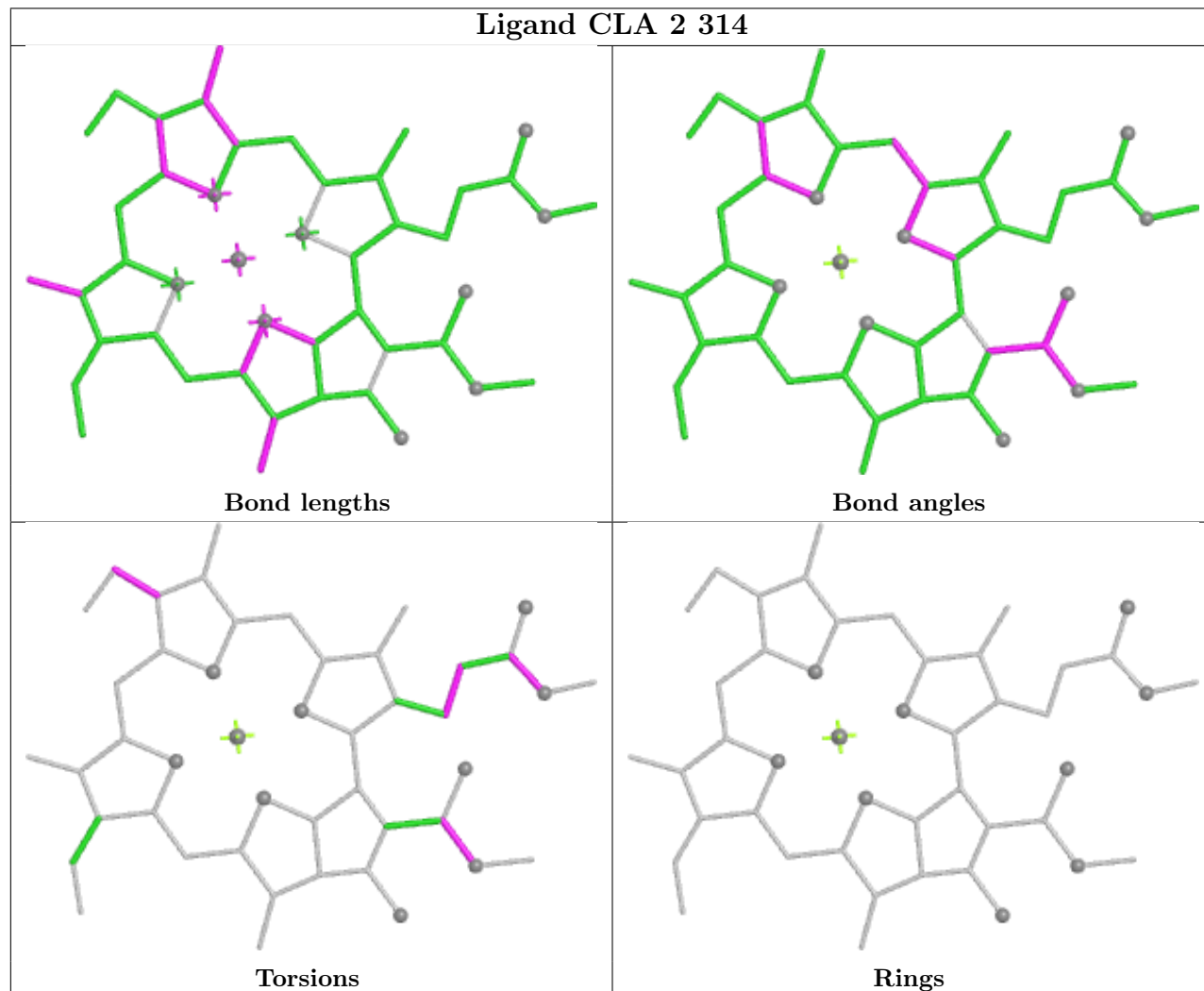




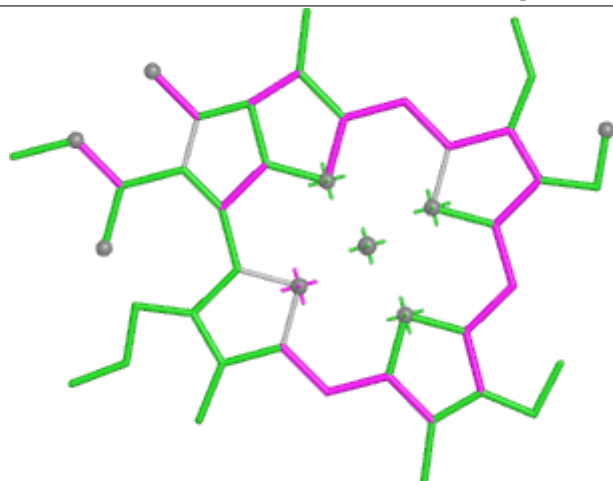
Ligand CLA A 807



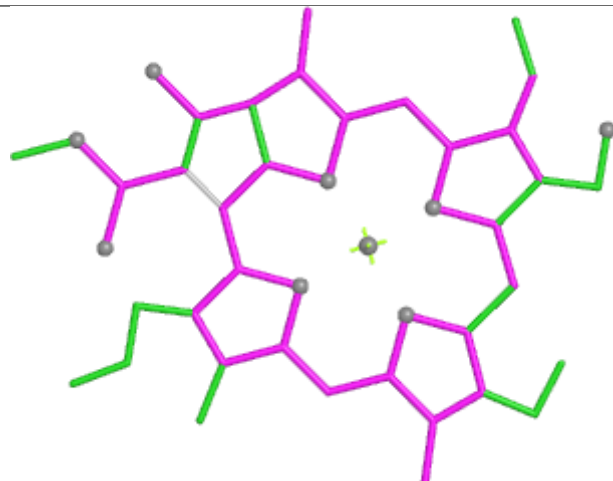
Ligand CLA 2 314



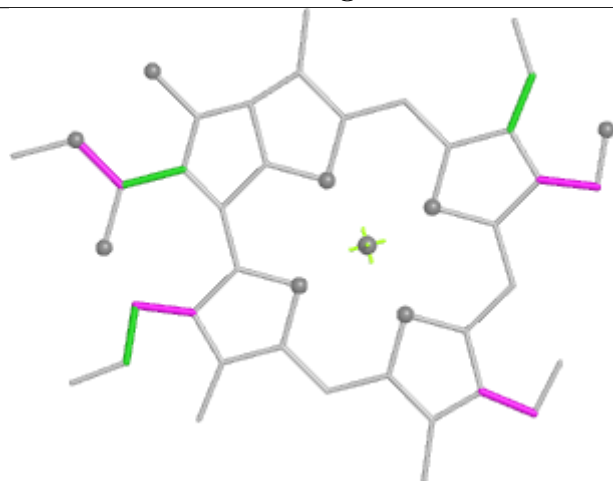
Ligand CHL T 606



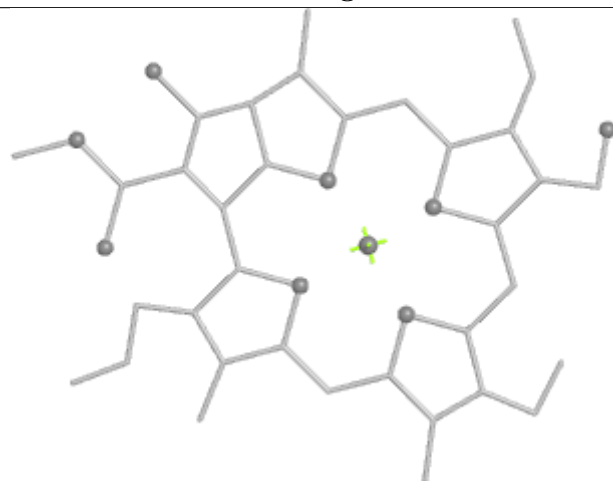
Bond lengths



Bond angles

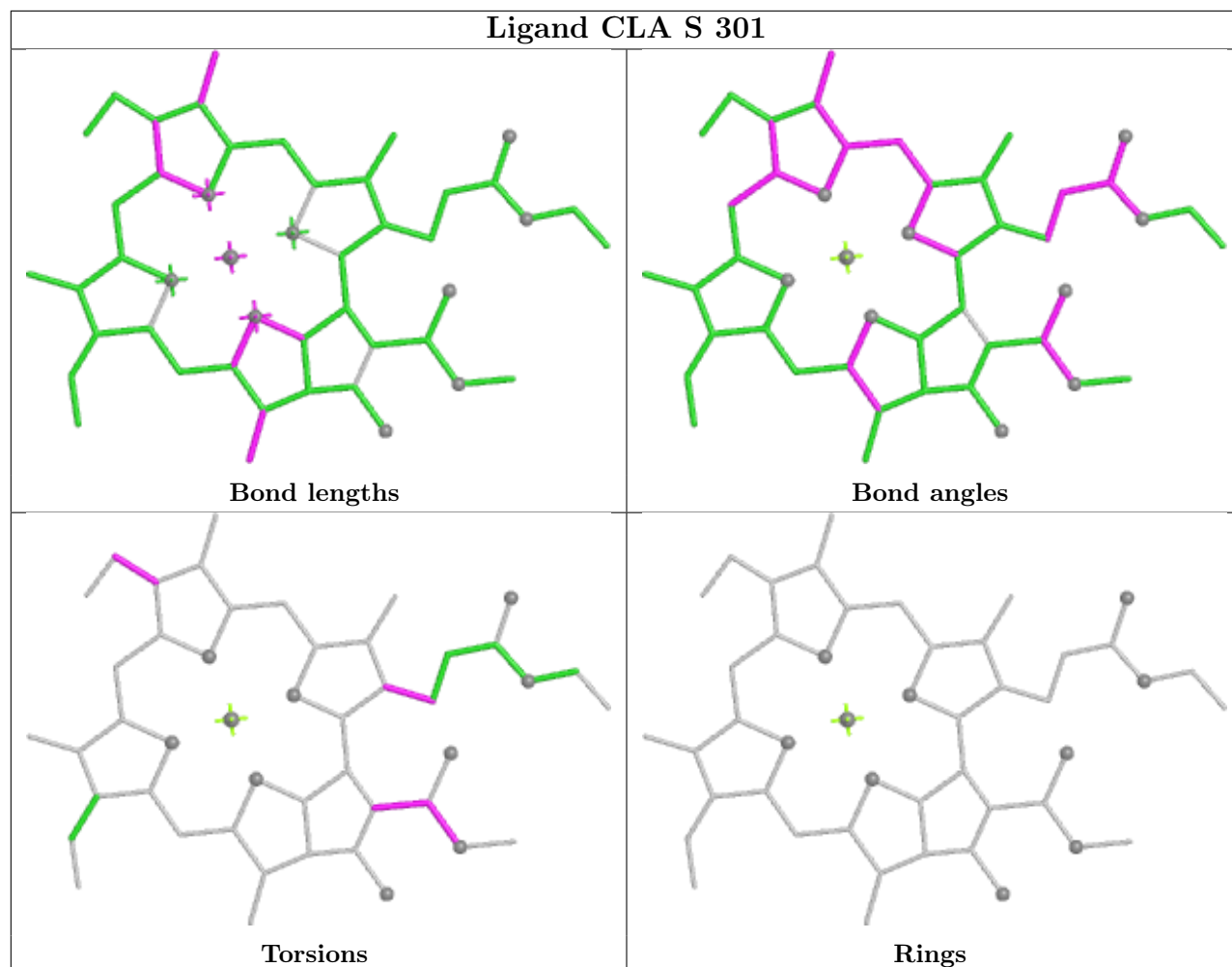


Torsions

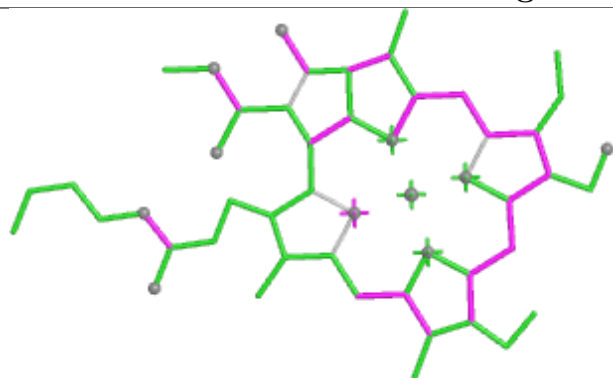


Rings

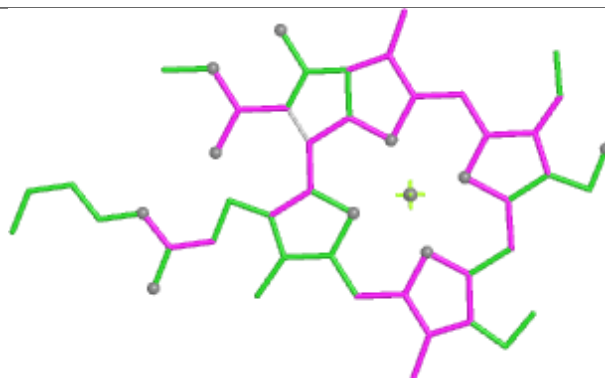
Ligand CLA S 301



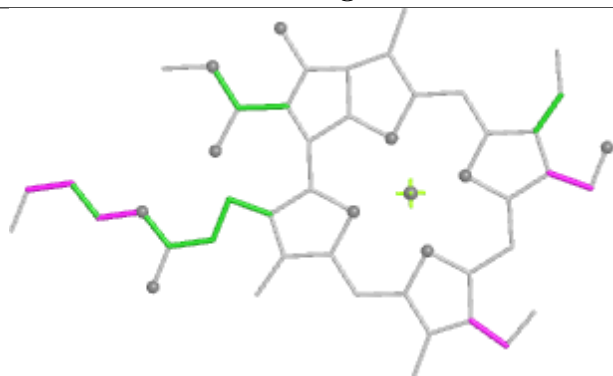
Ligand CHL S 307



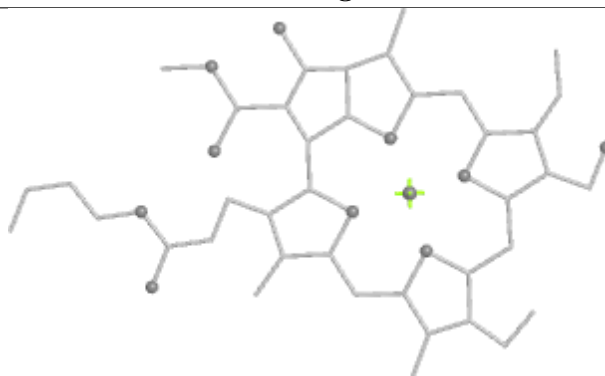
Bond lengths



Bond angles

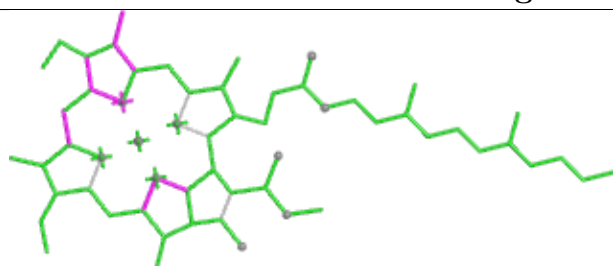


Torsions

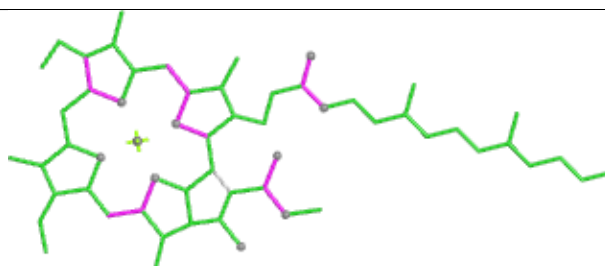


Rings

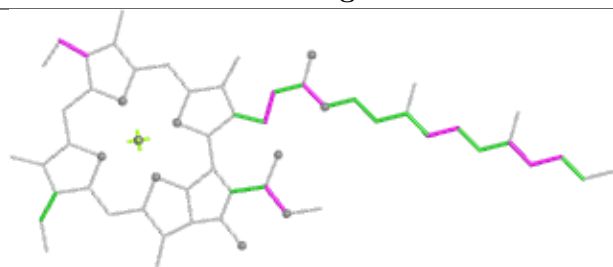
Ligand CLA P 613



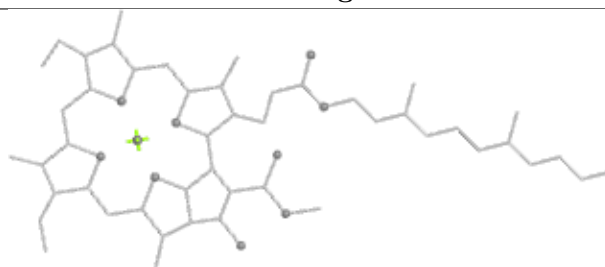
Bond lengths



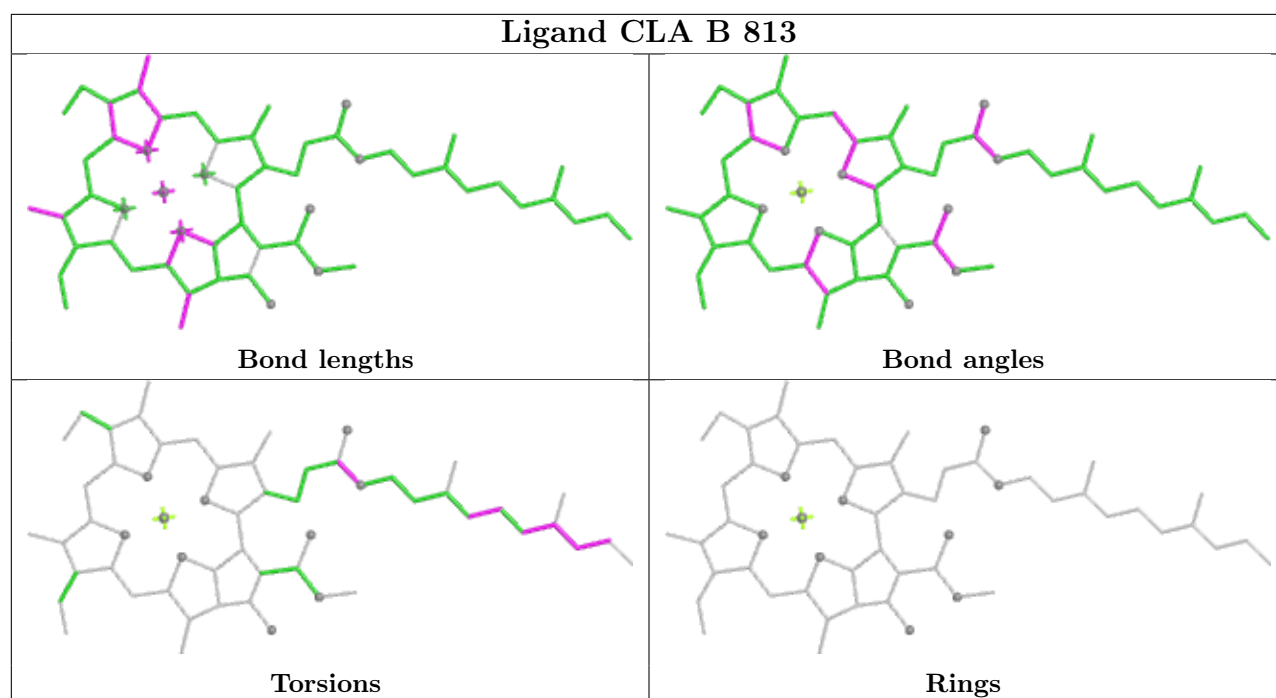
Bond angles



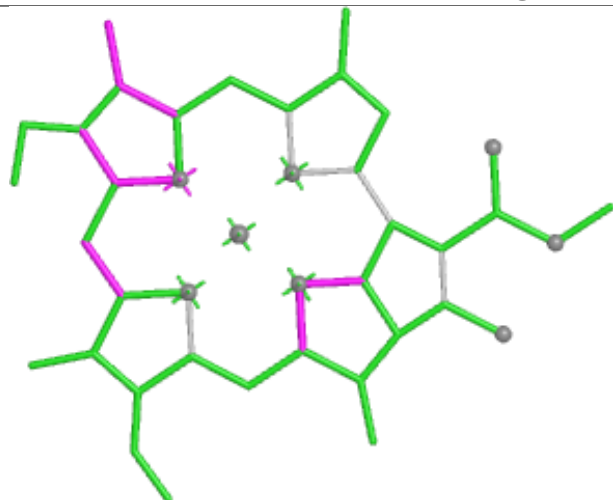
Torsions



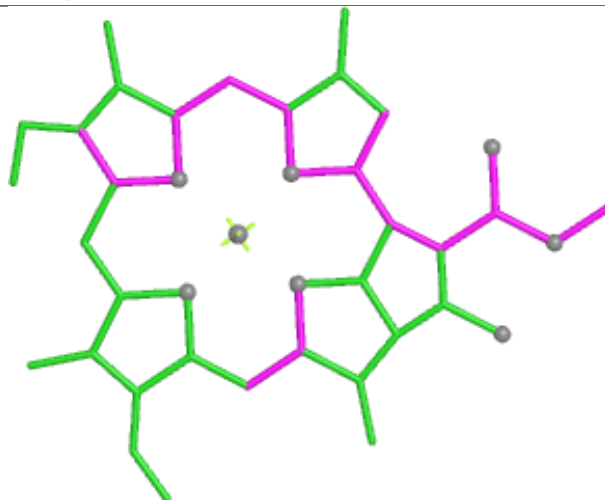
Rings



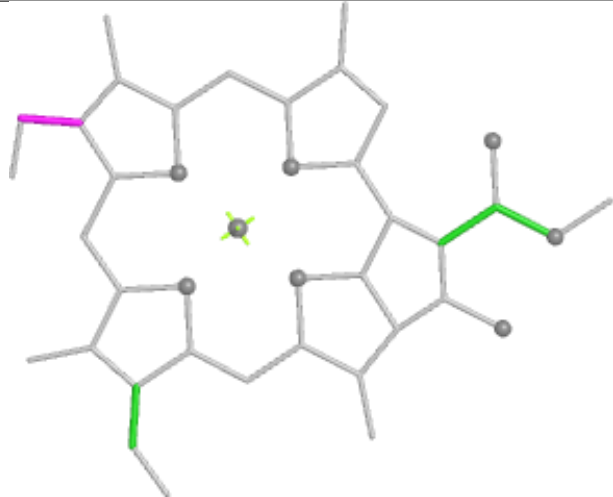
Ligand CLA Q 610



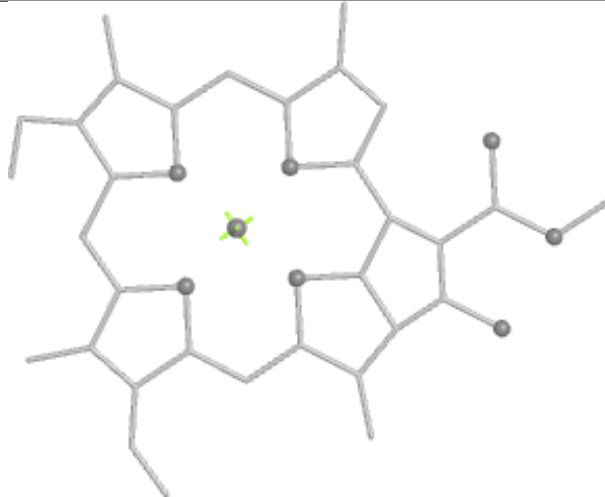
Bond lengths



Bond angles

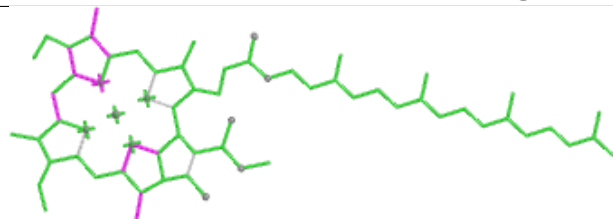


Torsions

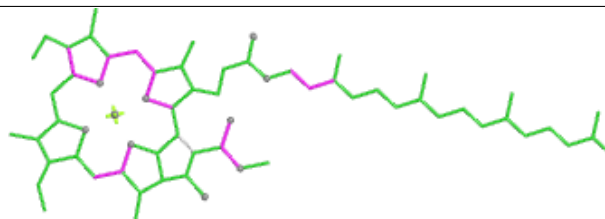


Rings

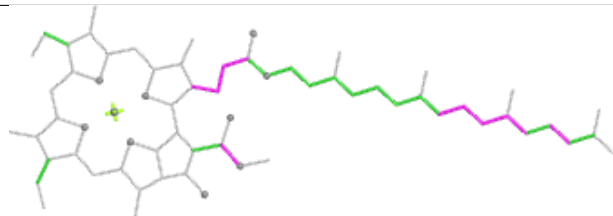
Ligand CLA T 608



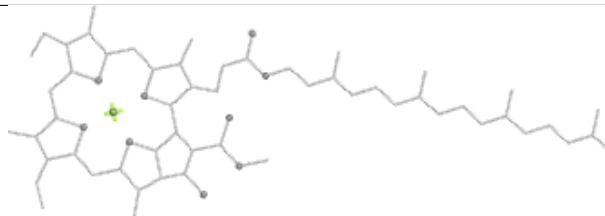
Bond lengths



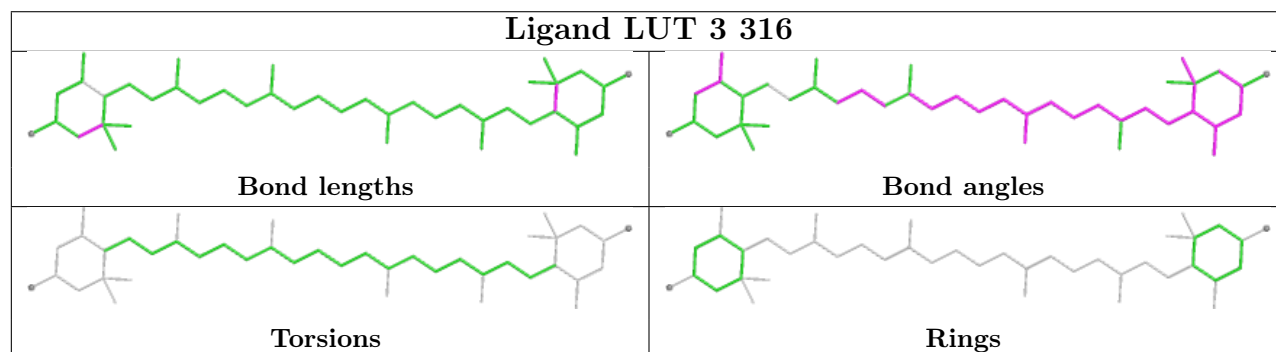
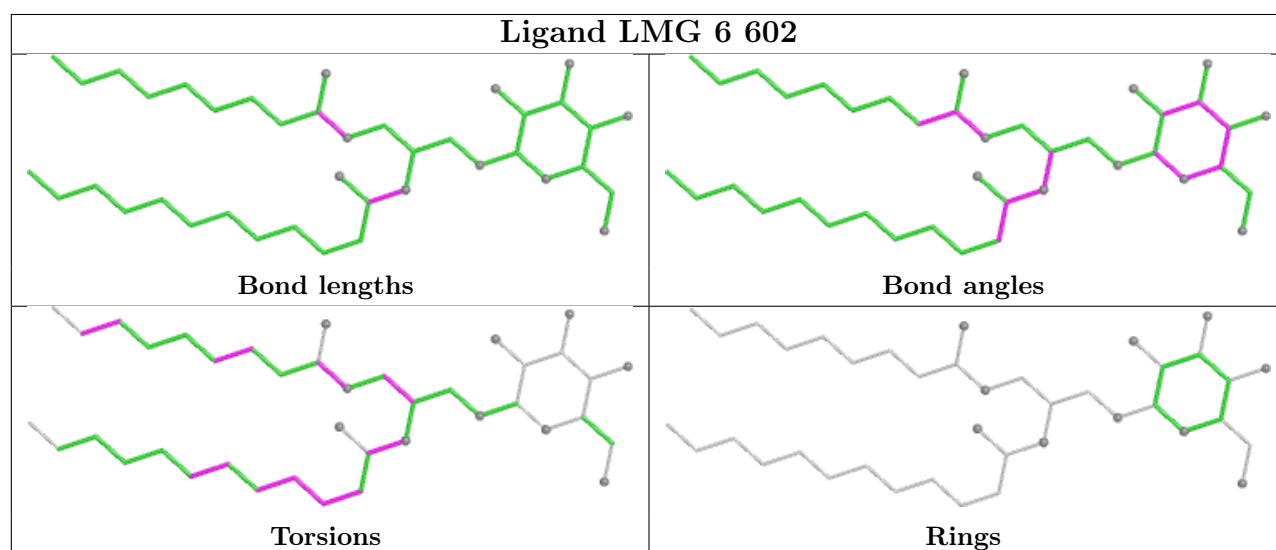
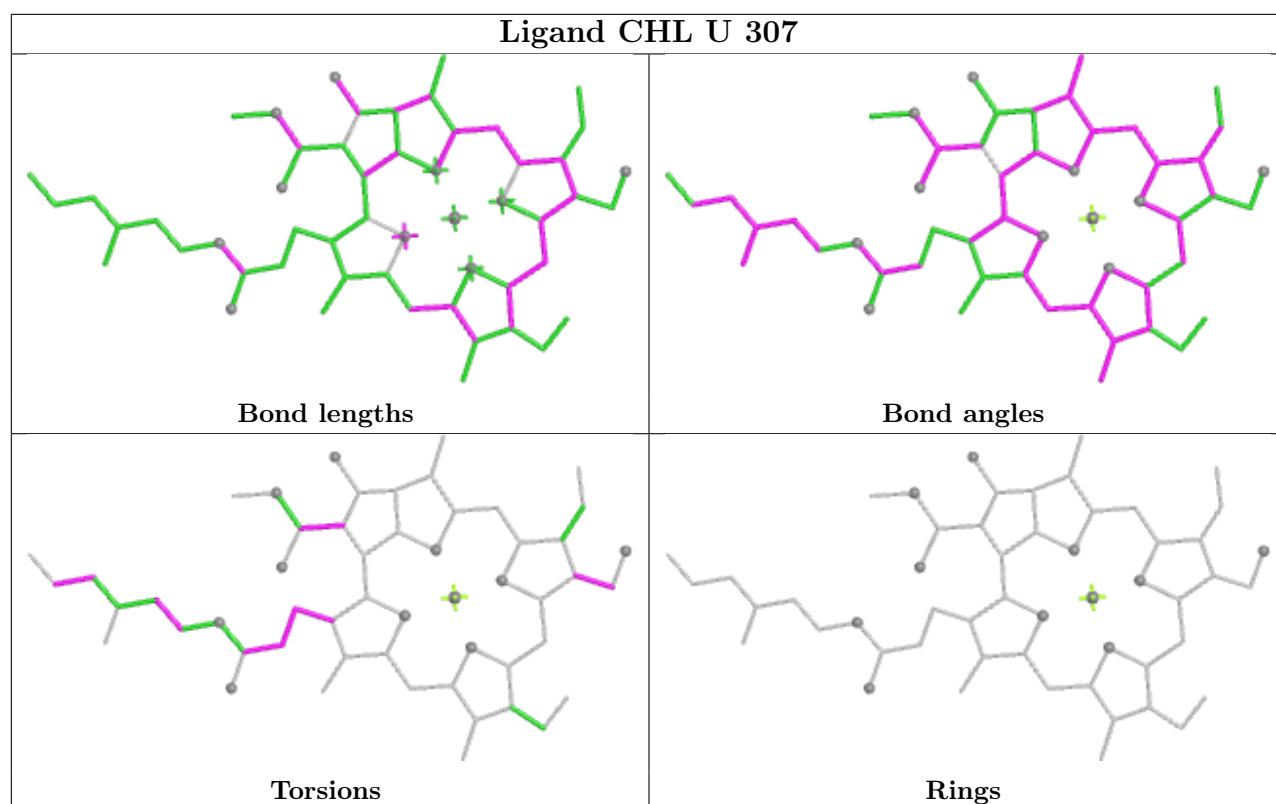
Bond angles

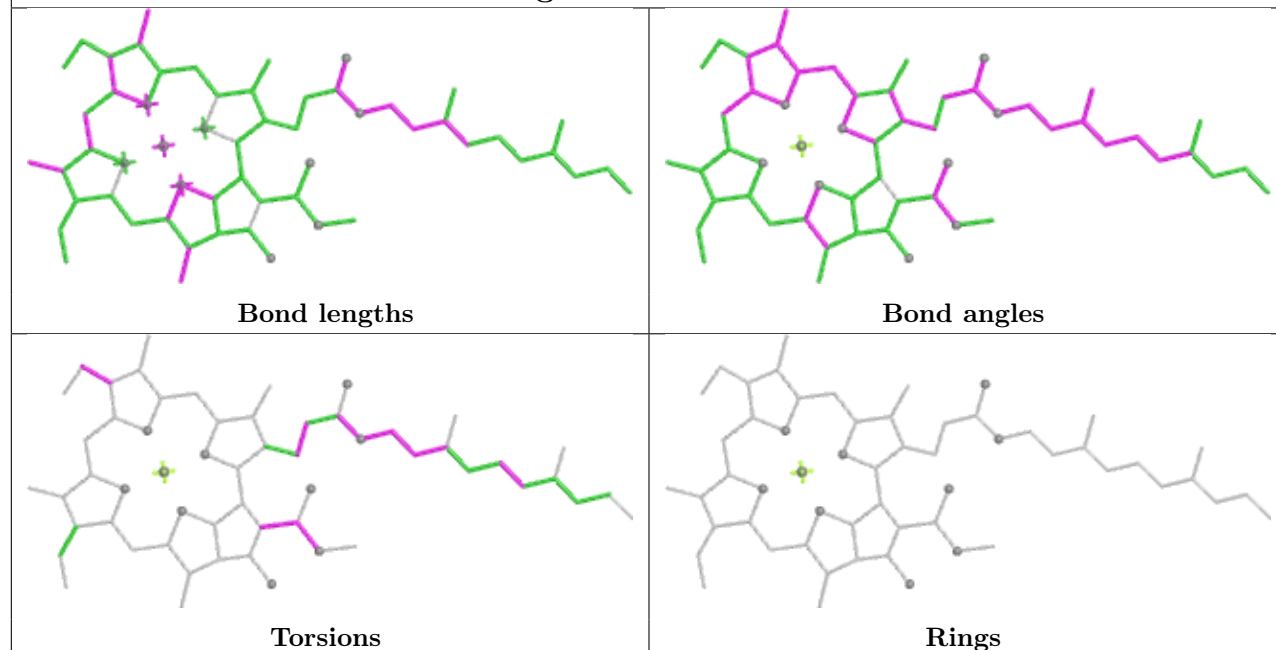
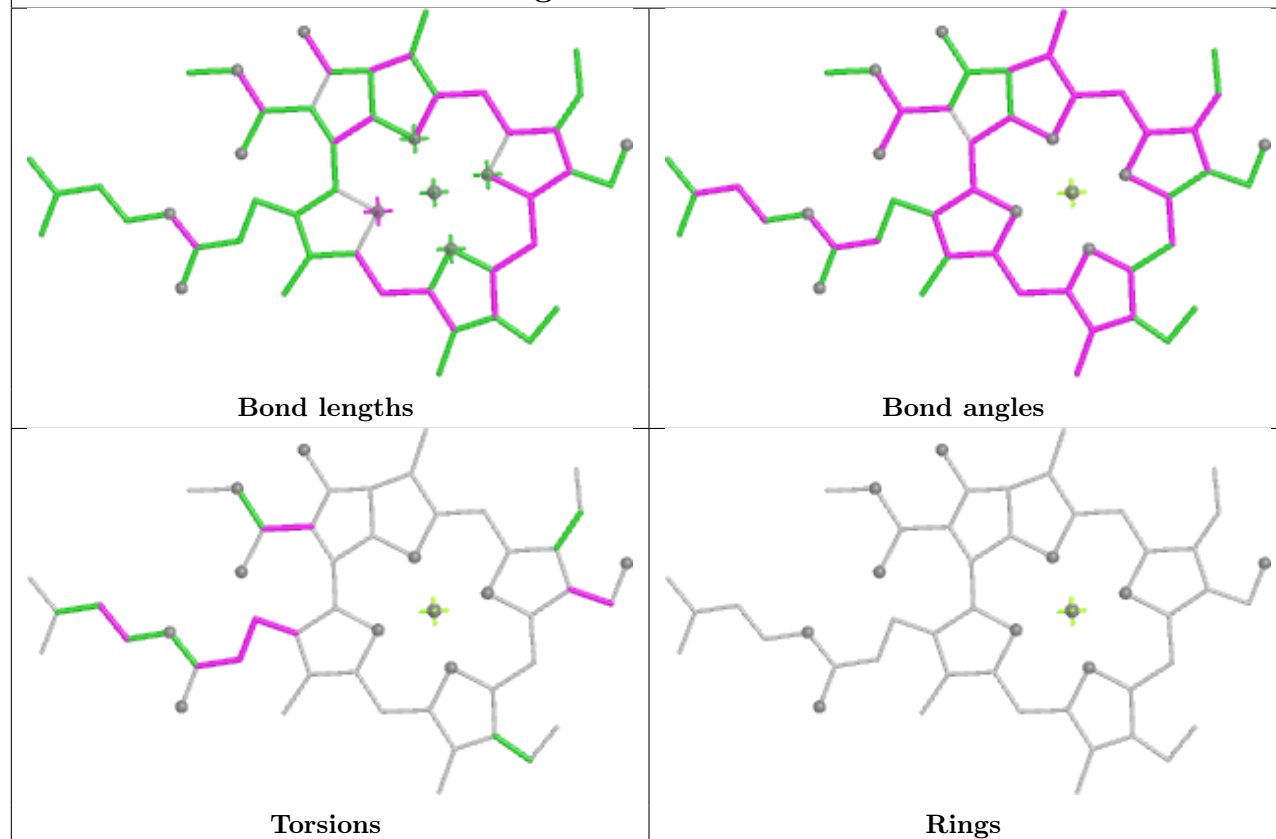


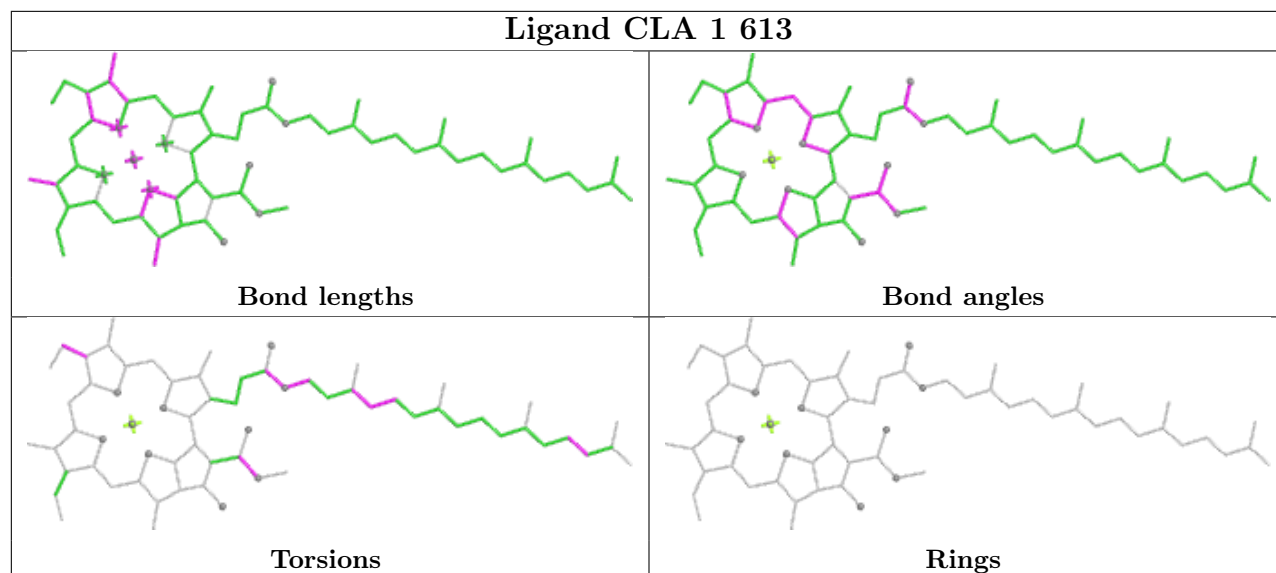
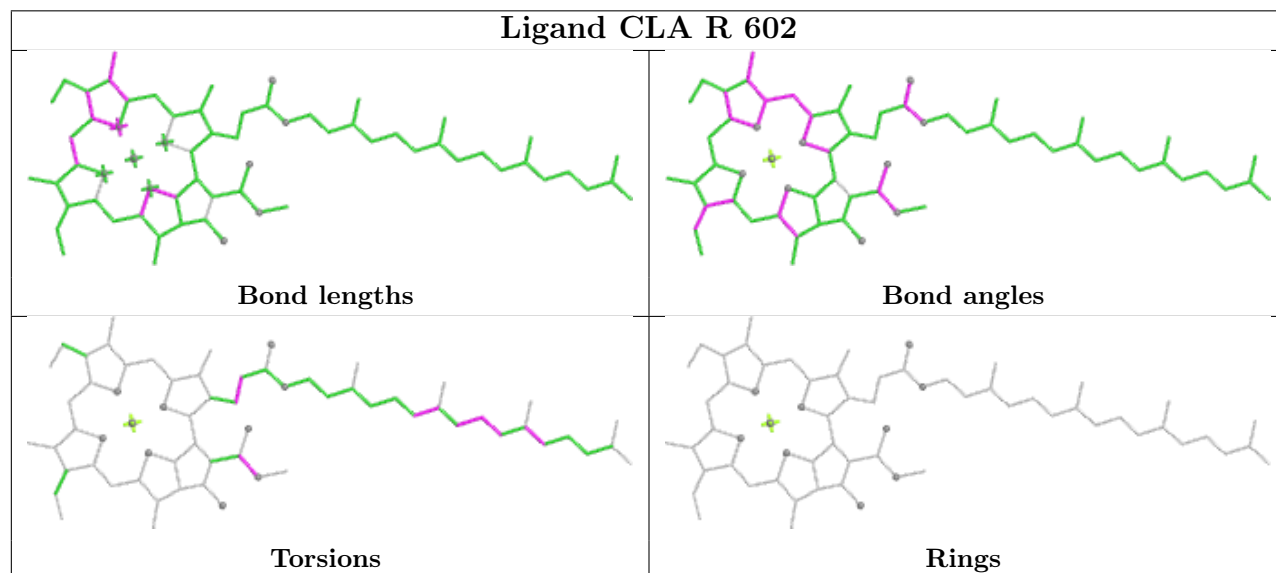
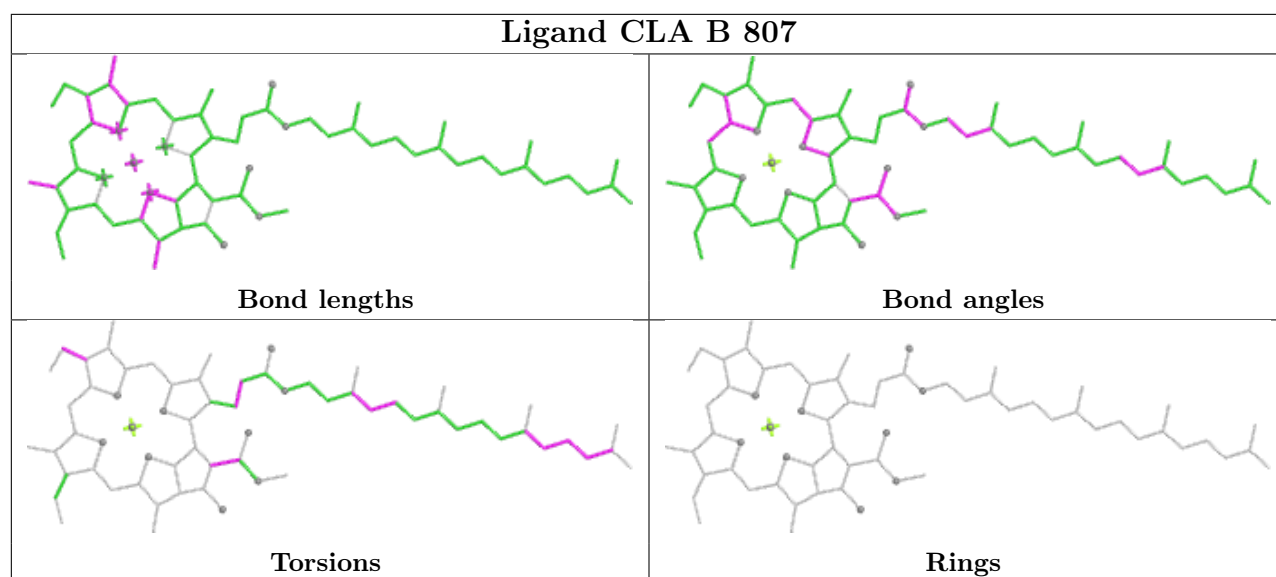
Torsions

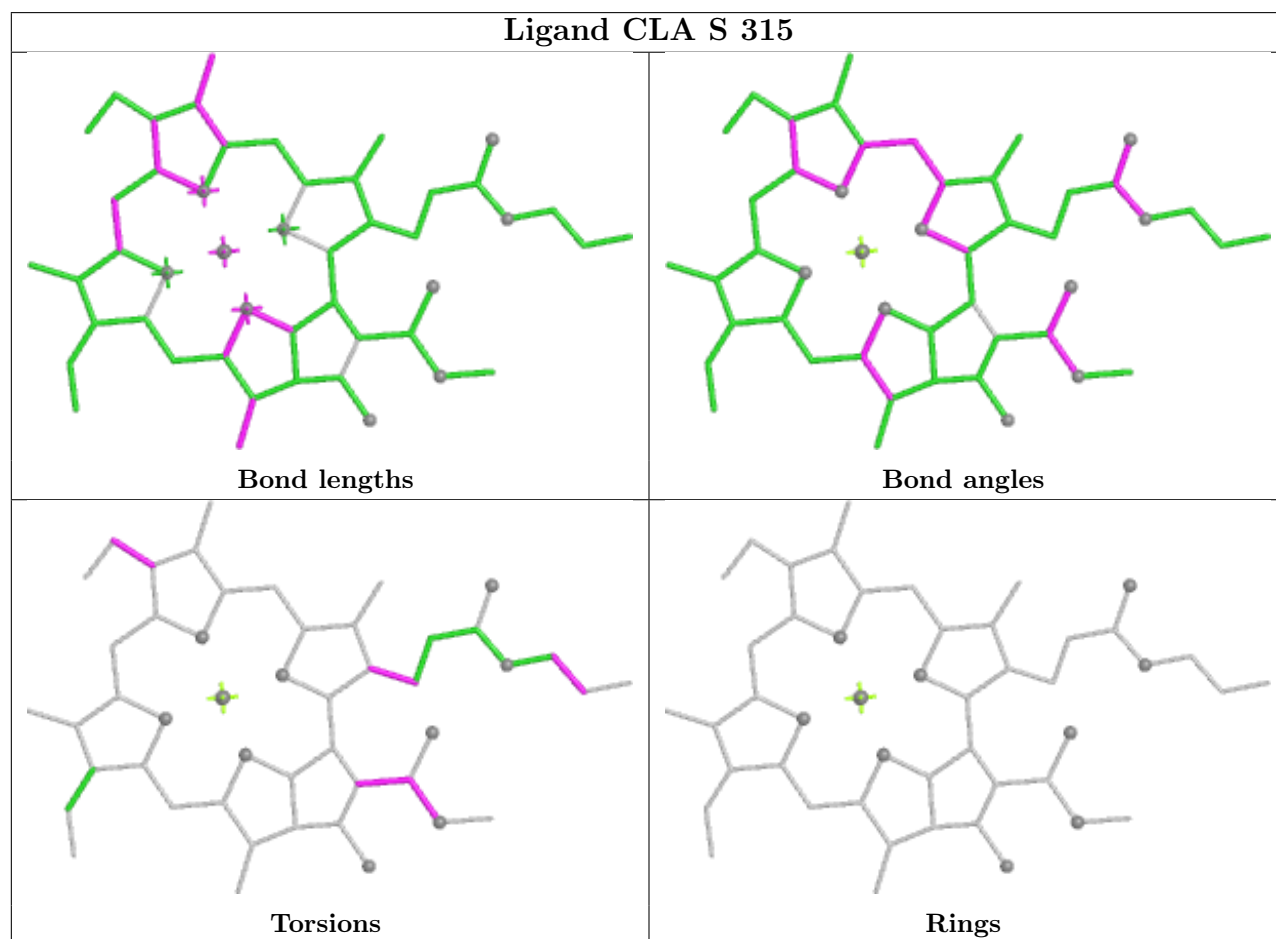
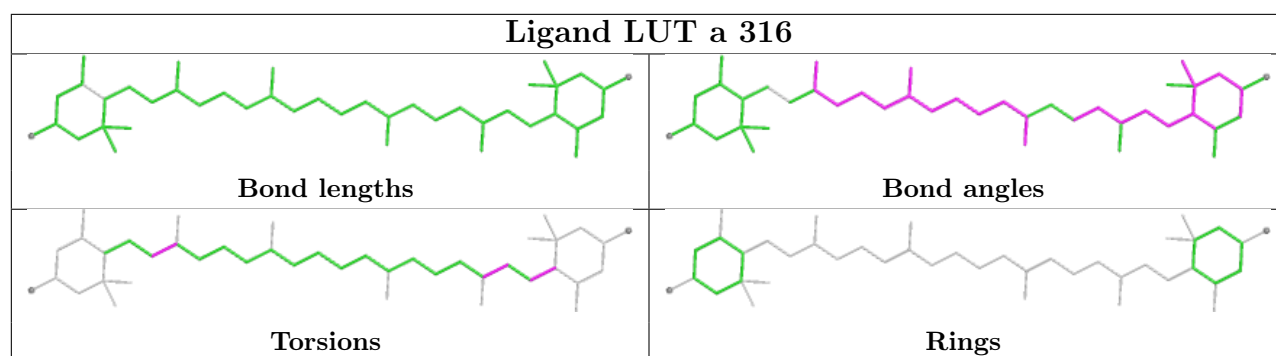


Rings

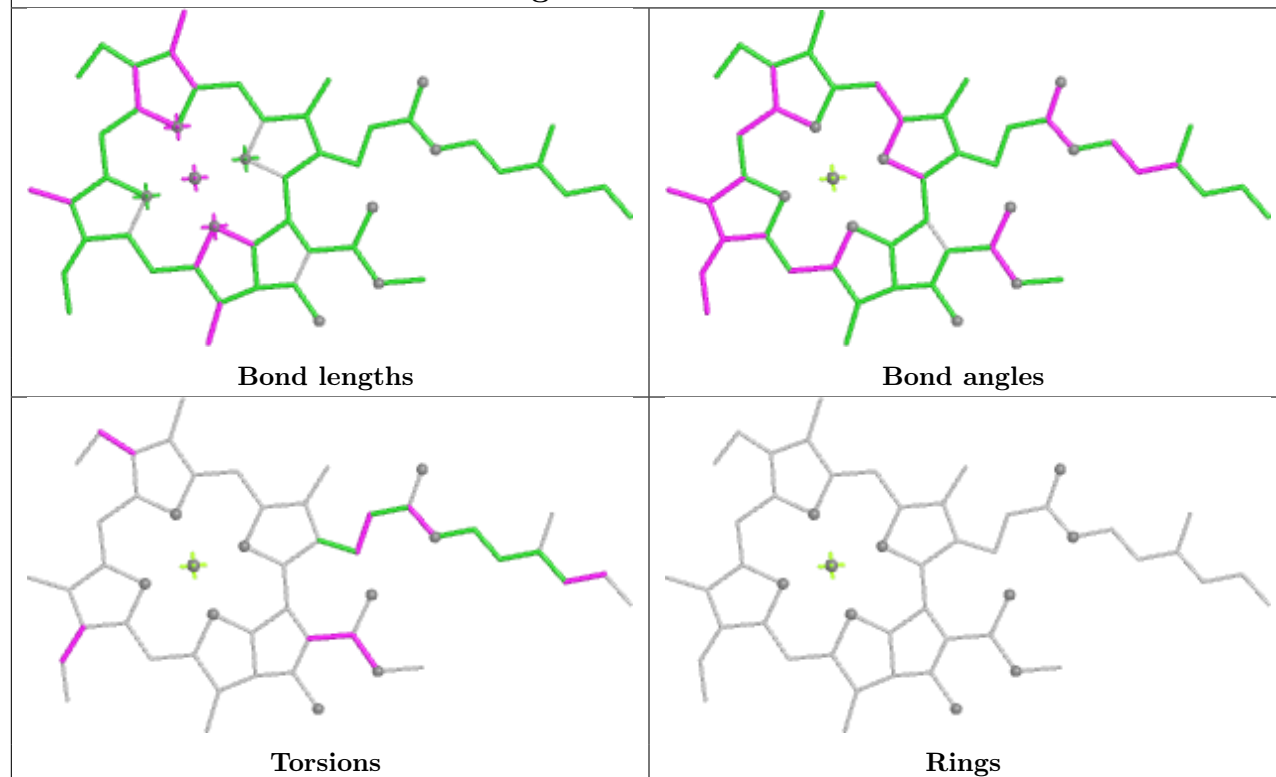


Ligand CLA a 303**Ligand CHL S 321**

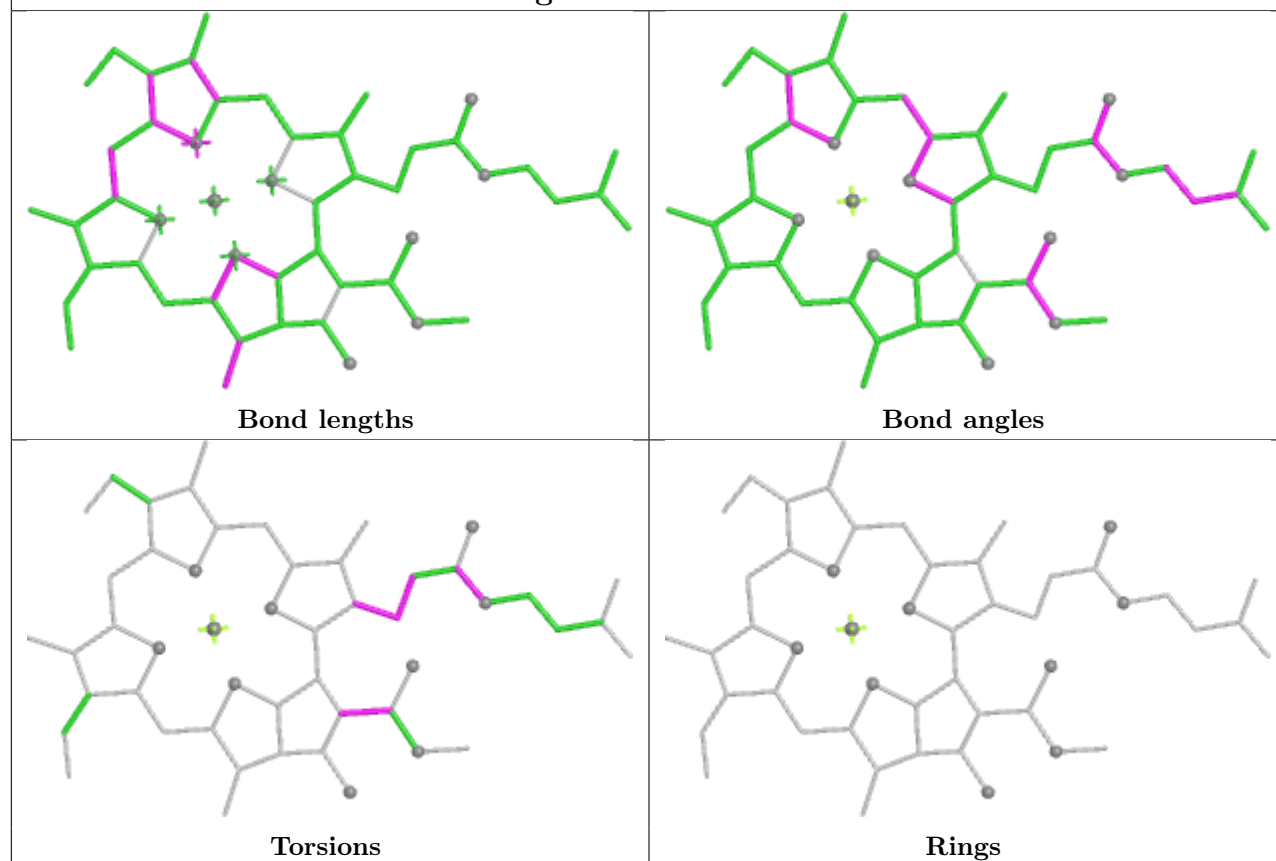




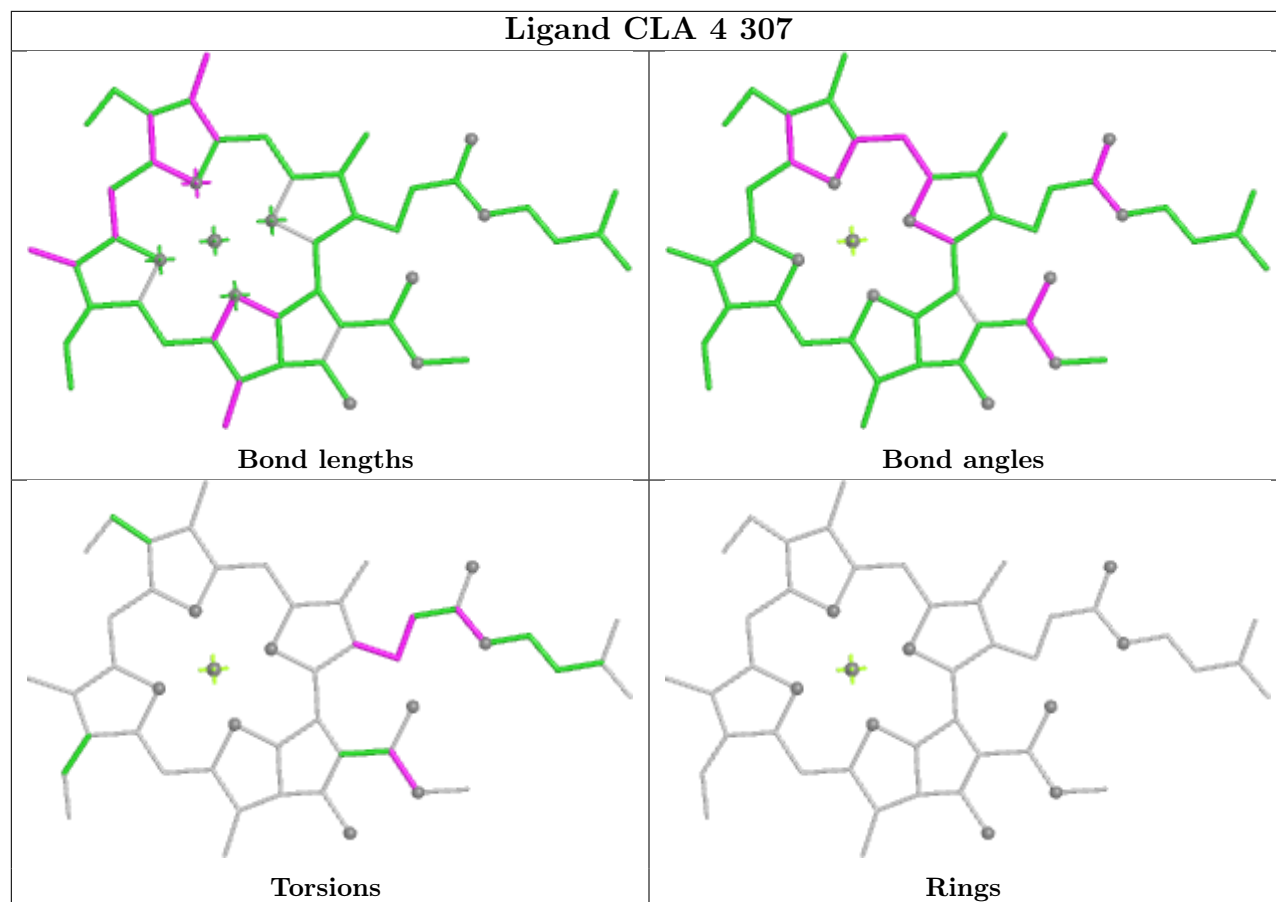
Ligand CLA A 842



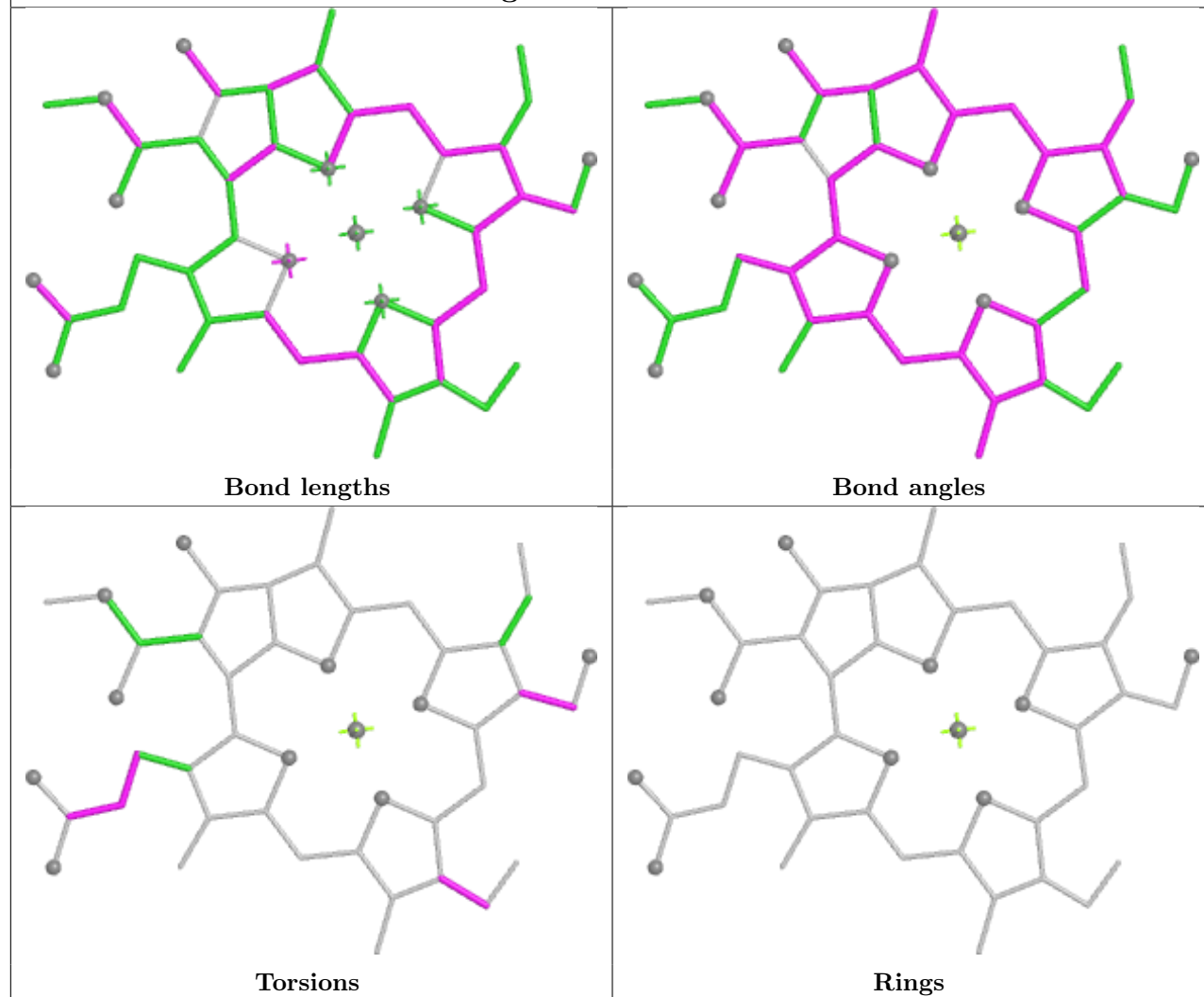
Ligand CLA S 305



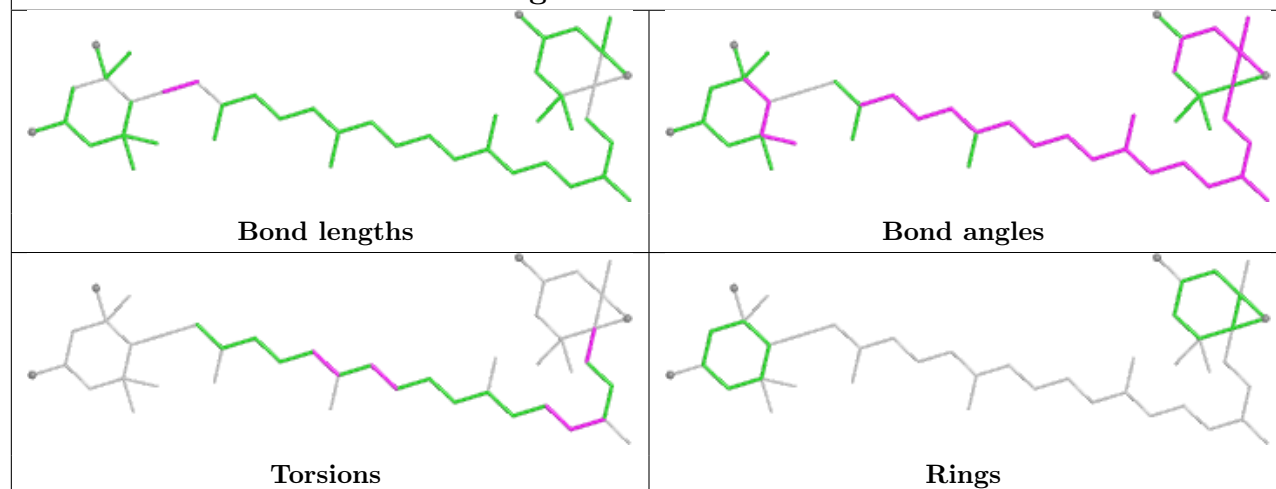
Ligand CLA 4 307

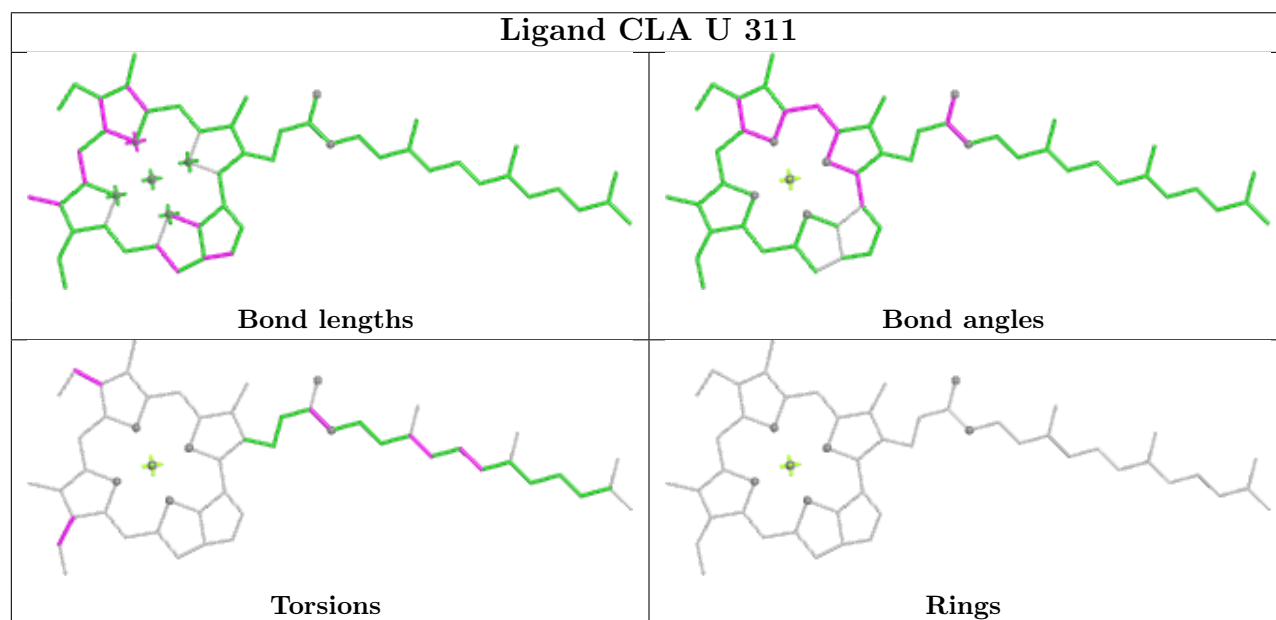
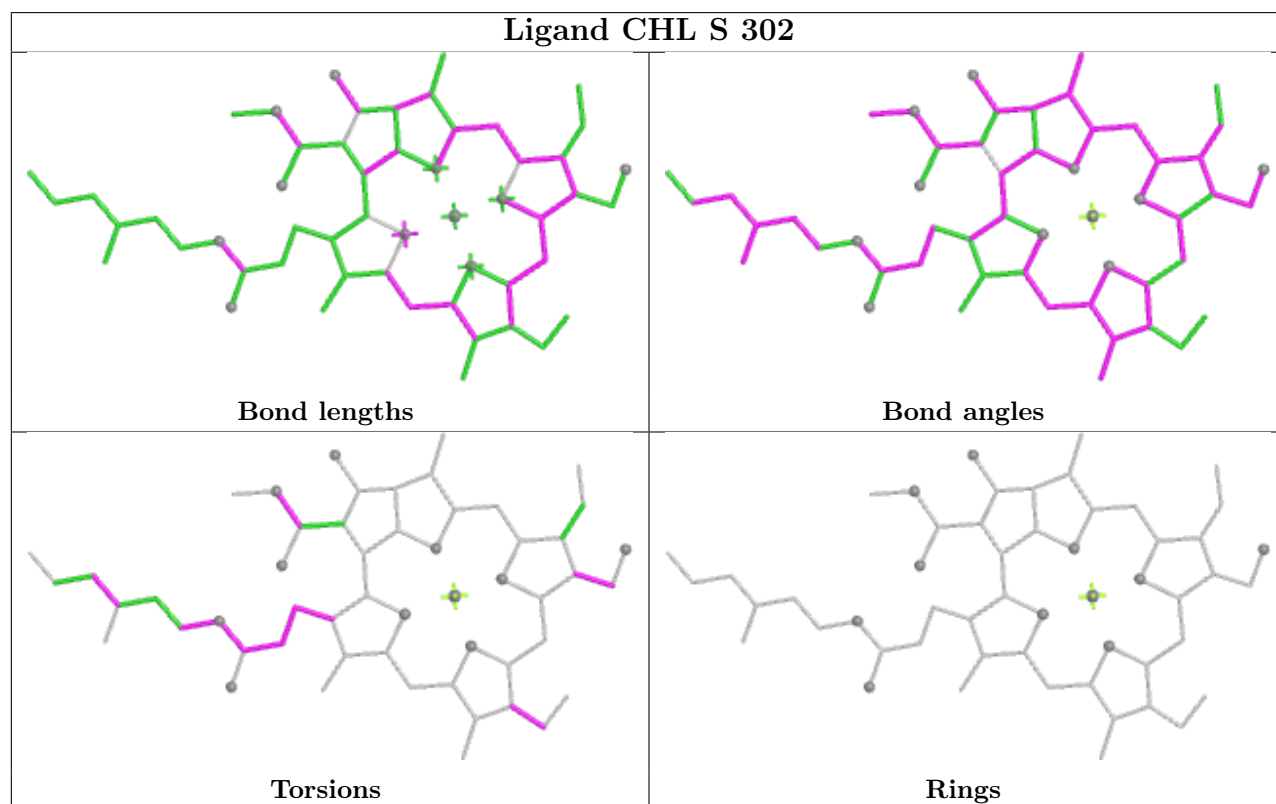
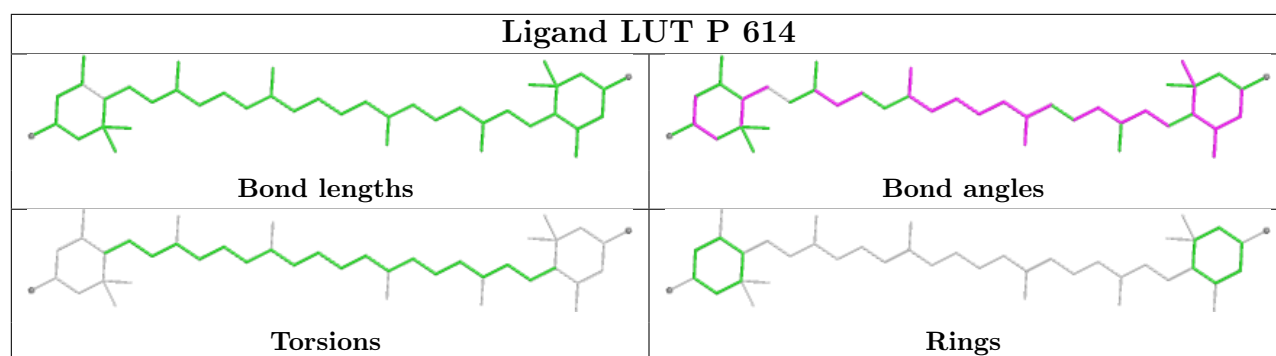


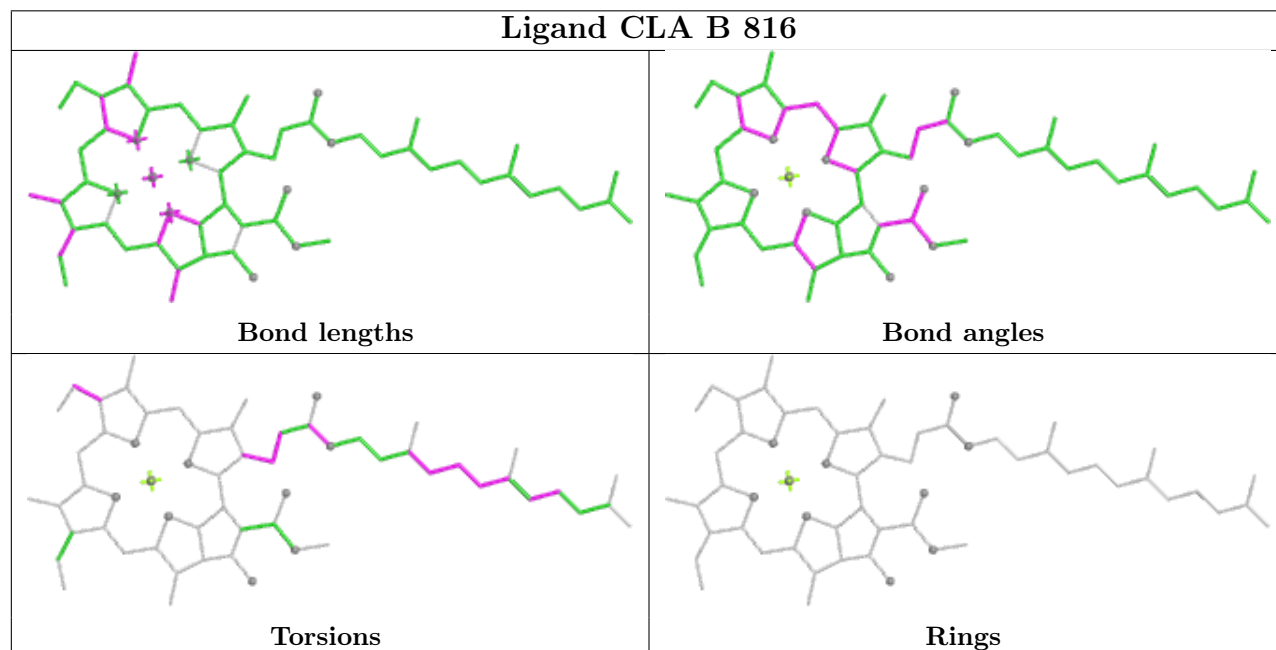
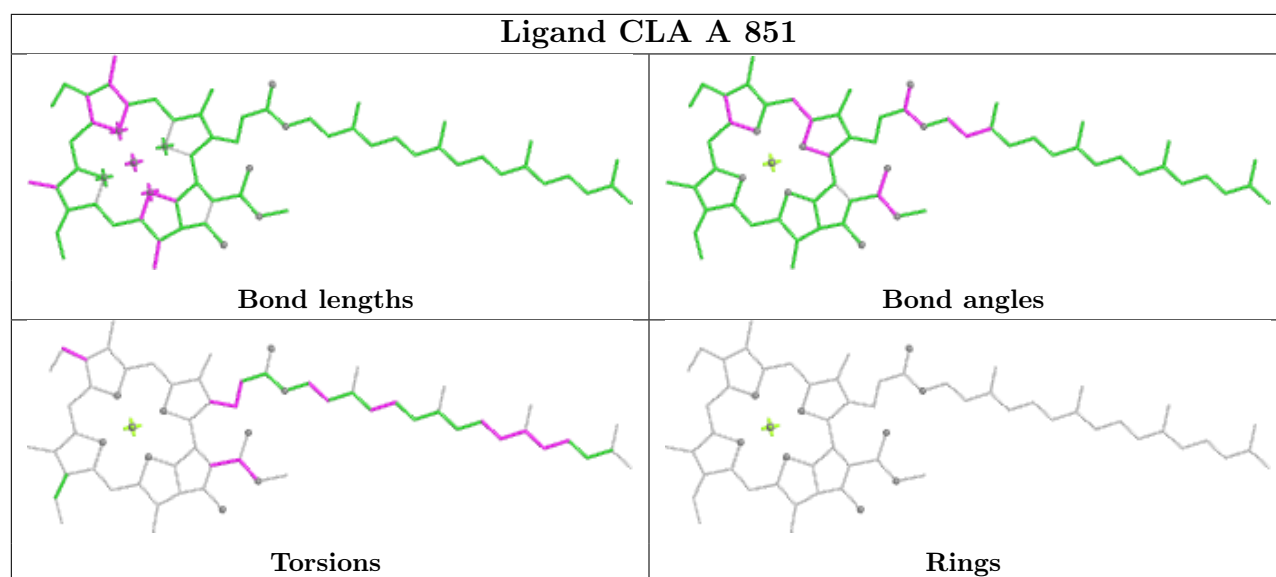
Ligand CHL R 605

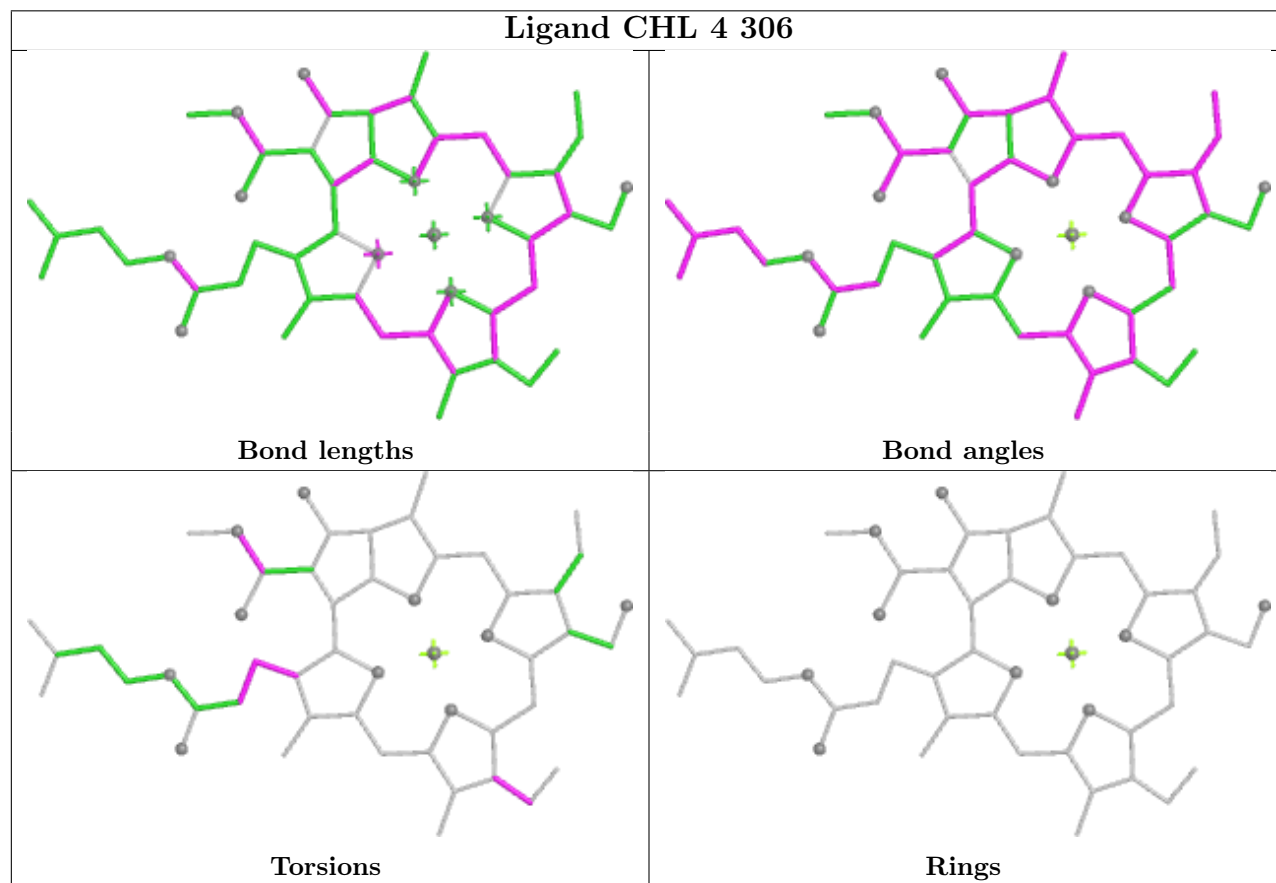
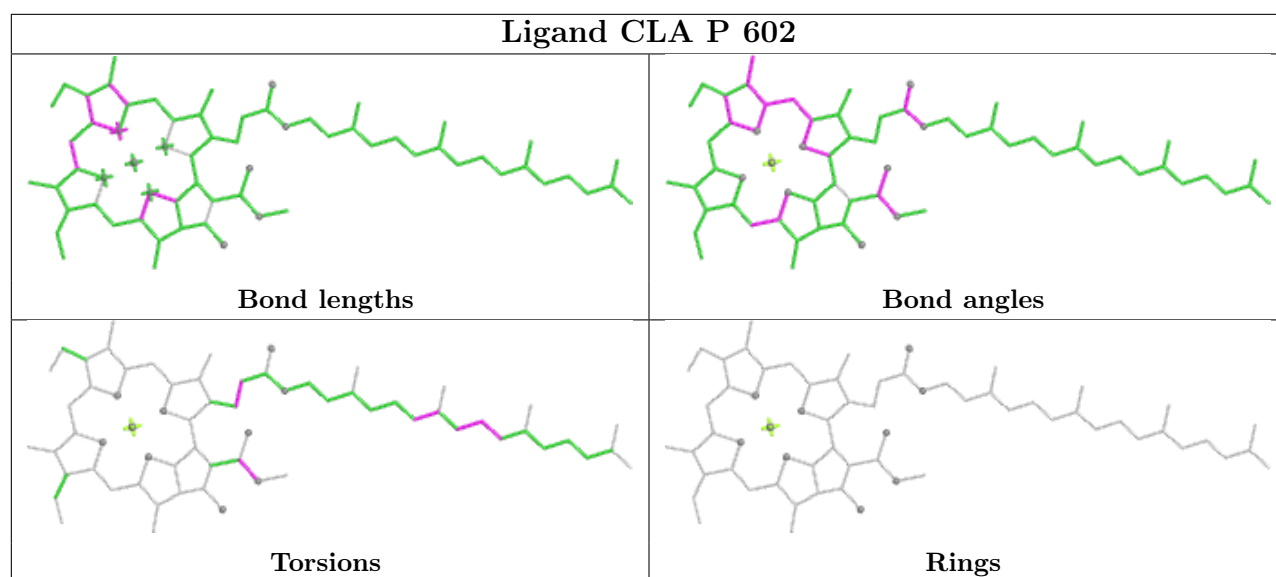


Ligand NEX U 316

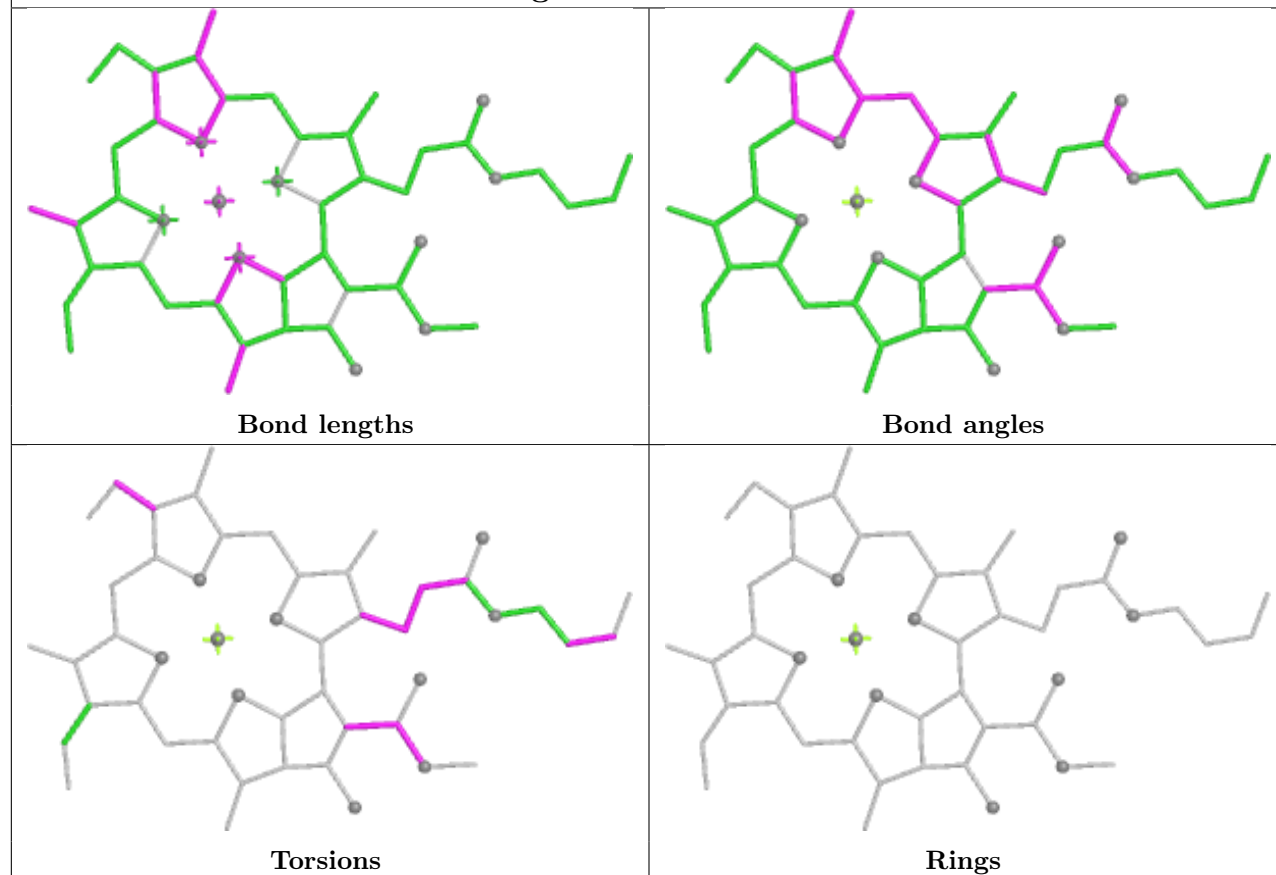




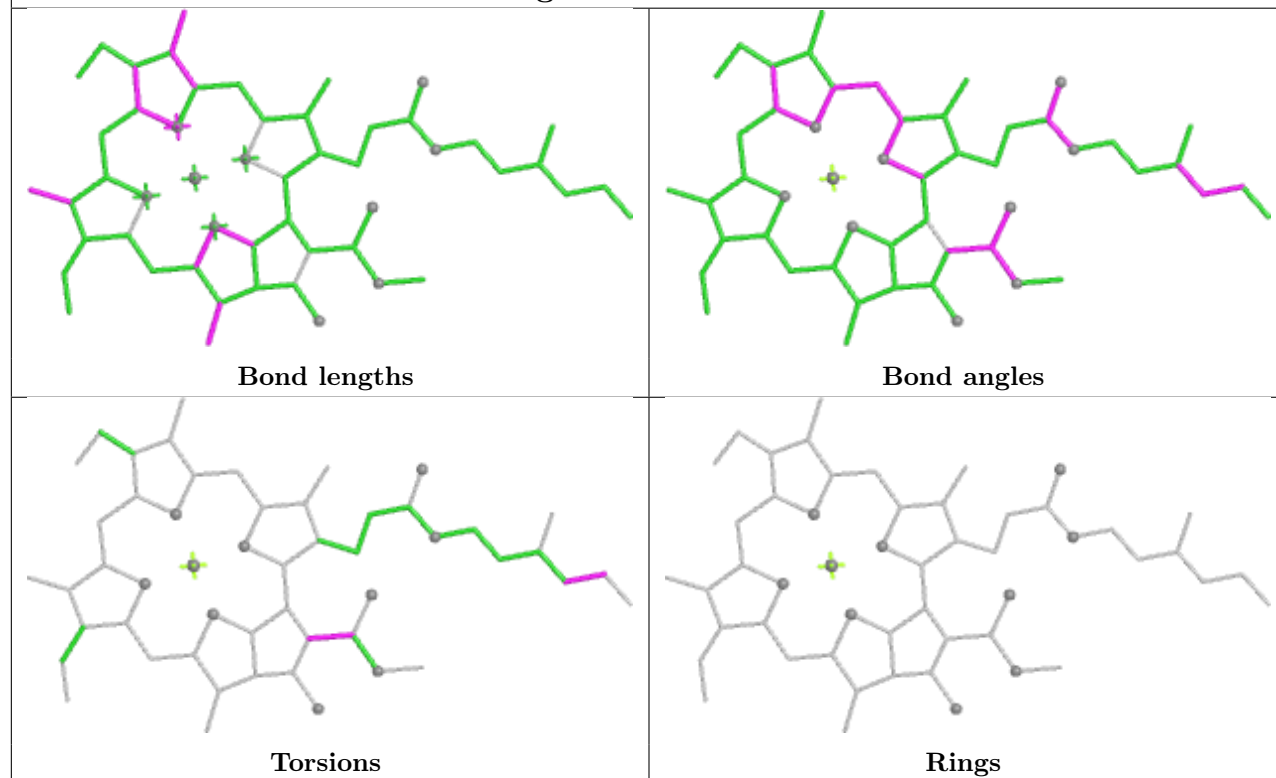


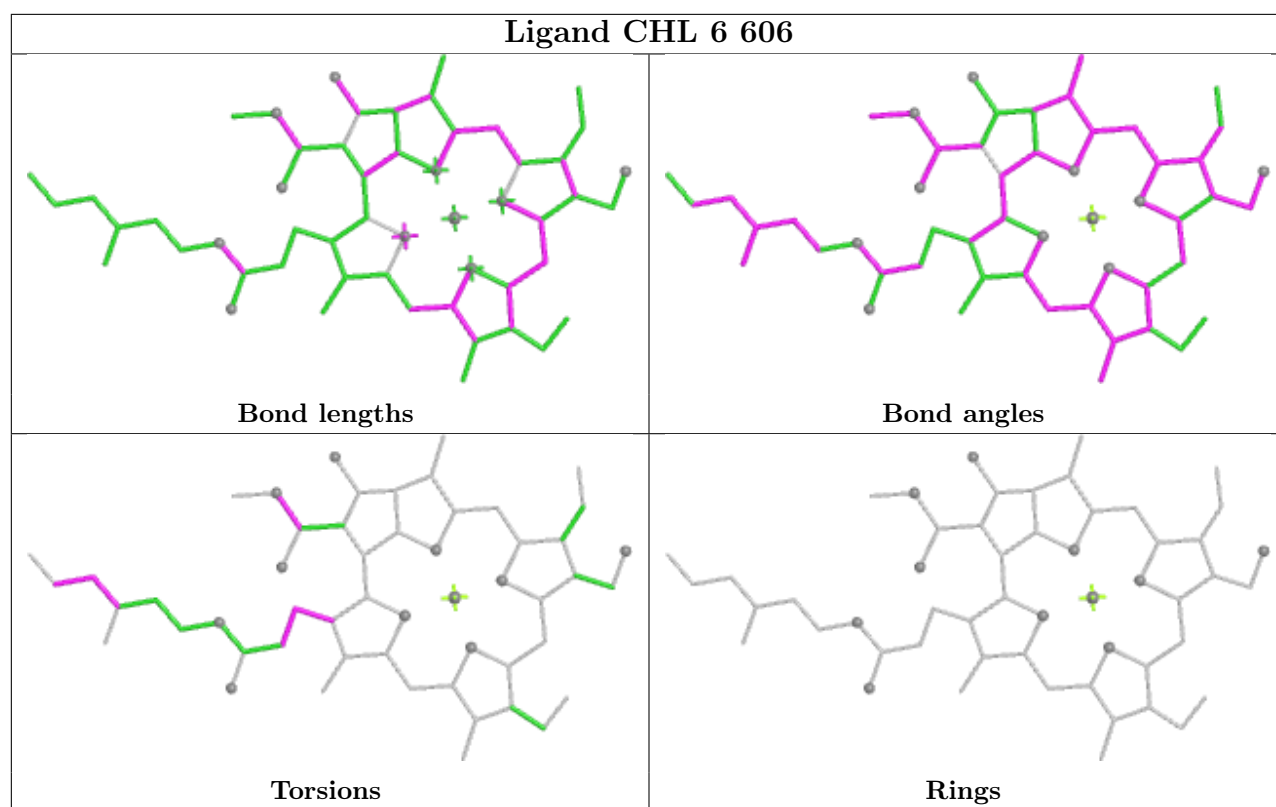


Ligand CLA A 823

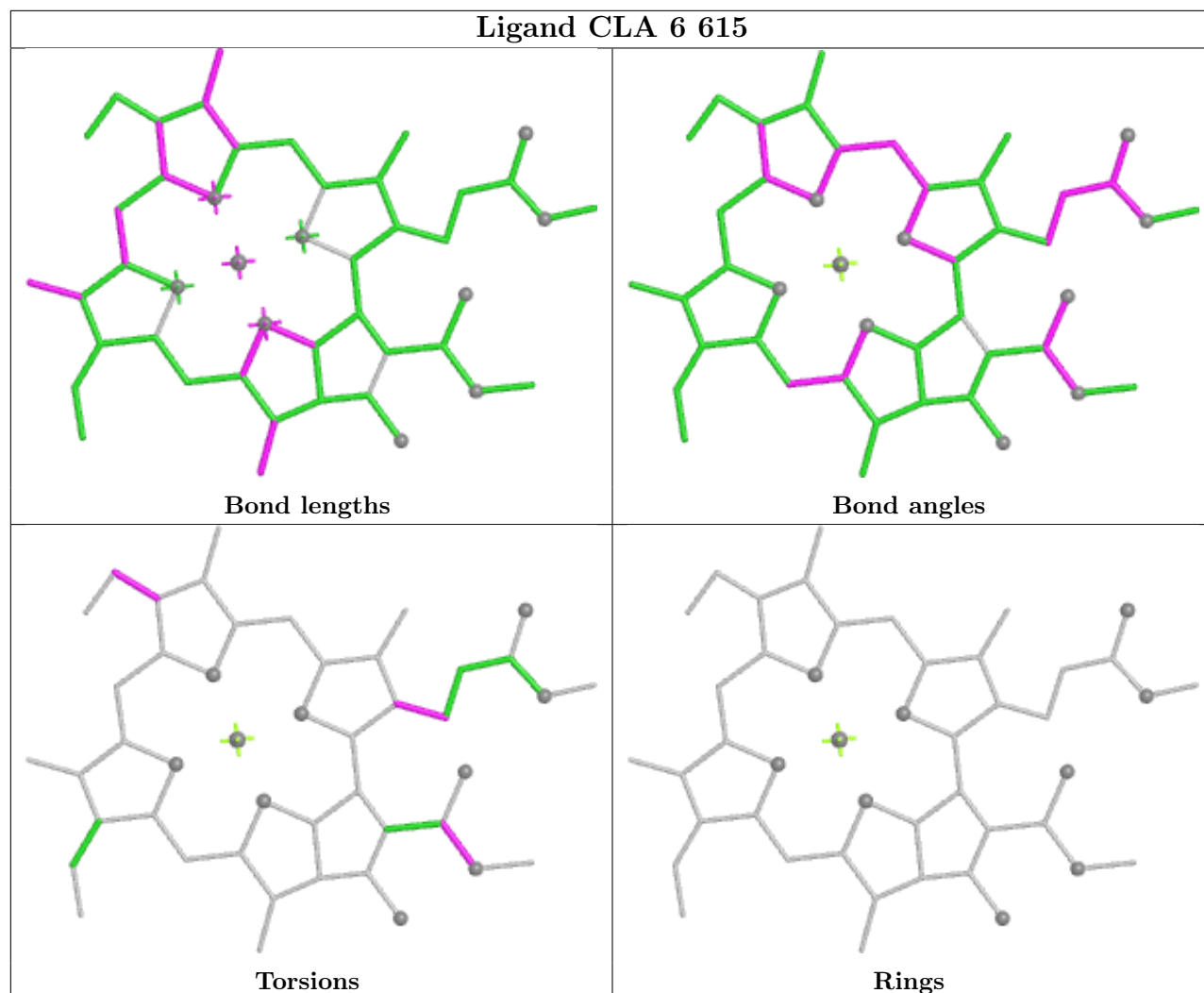


Ligand CLA 1 605

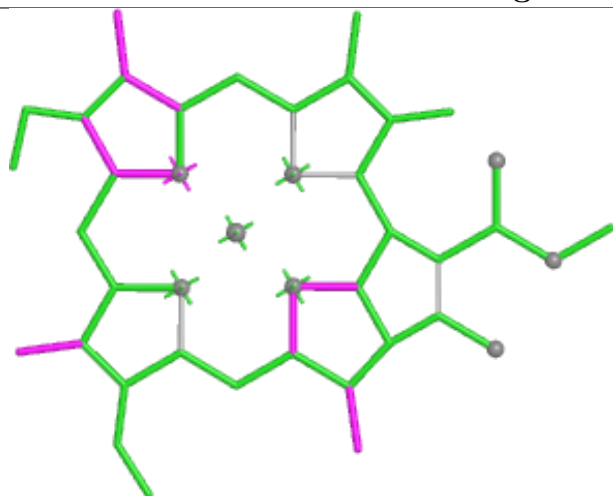




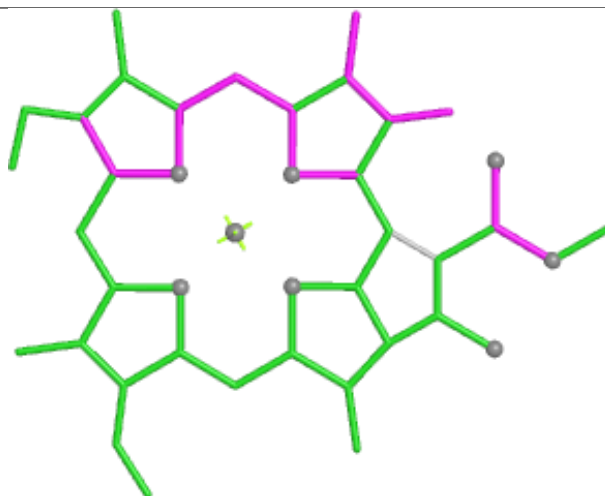
Ligand CLA 6 615



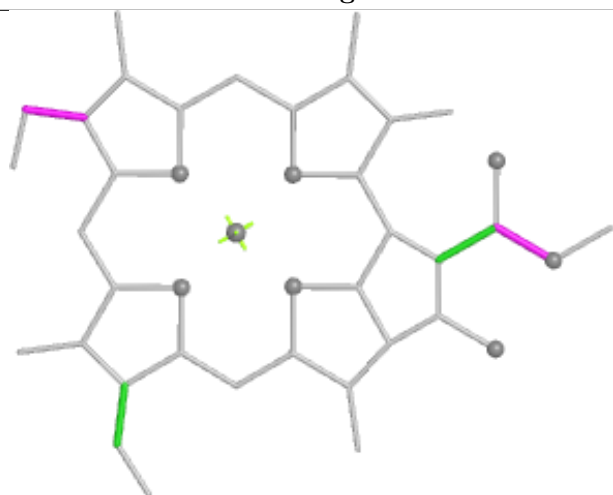
Ligand CLA H 202



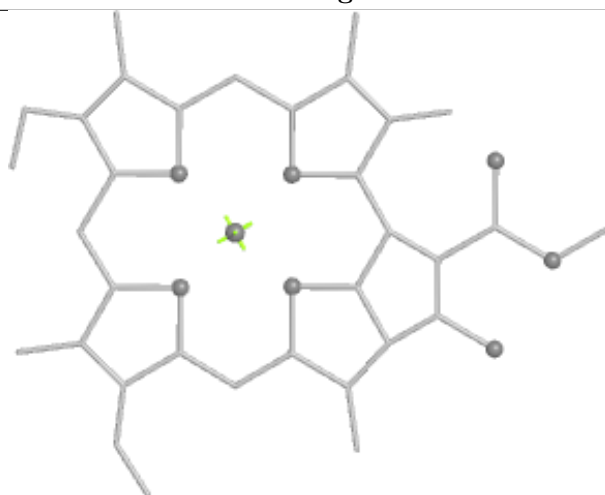
Bond lengths



Bond angles

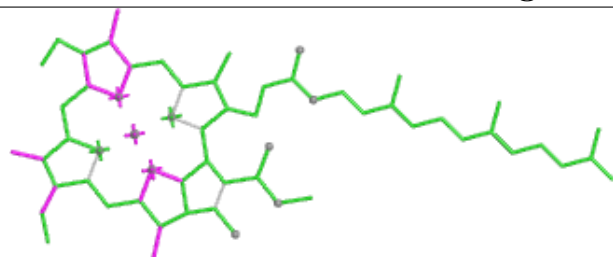


Torsions

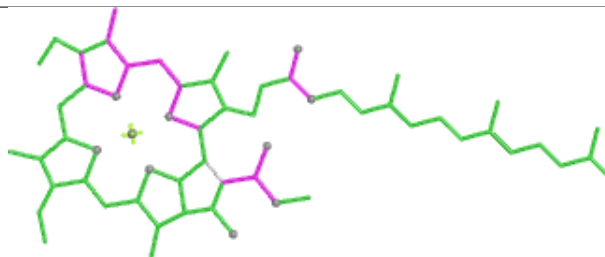


Rings

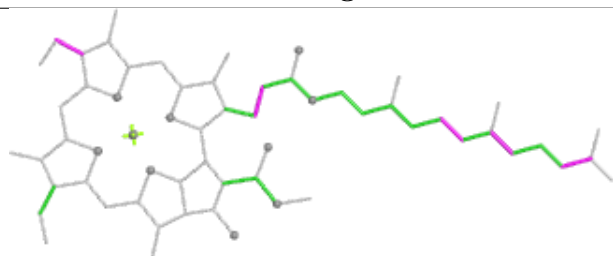
Ligand CLA 5 310



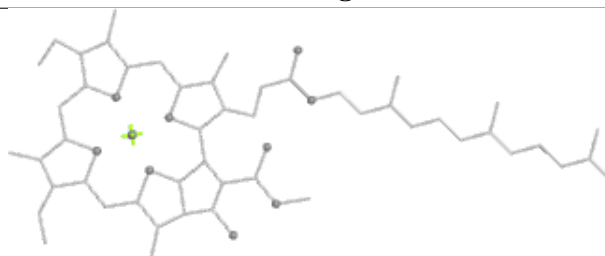
Bond lengths



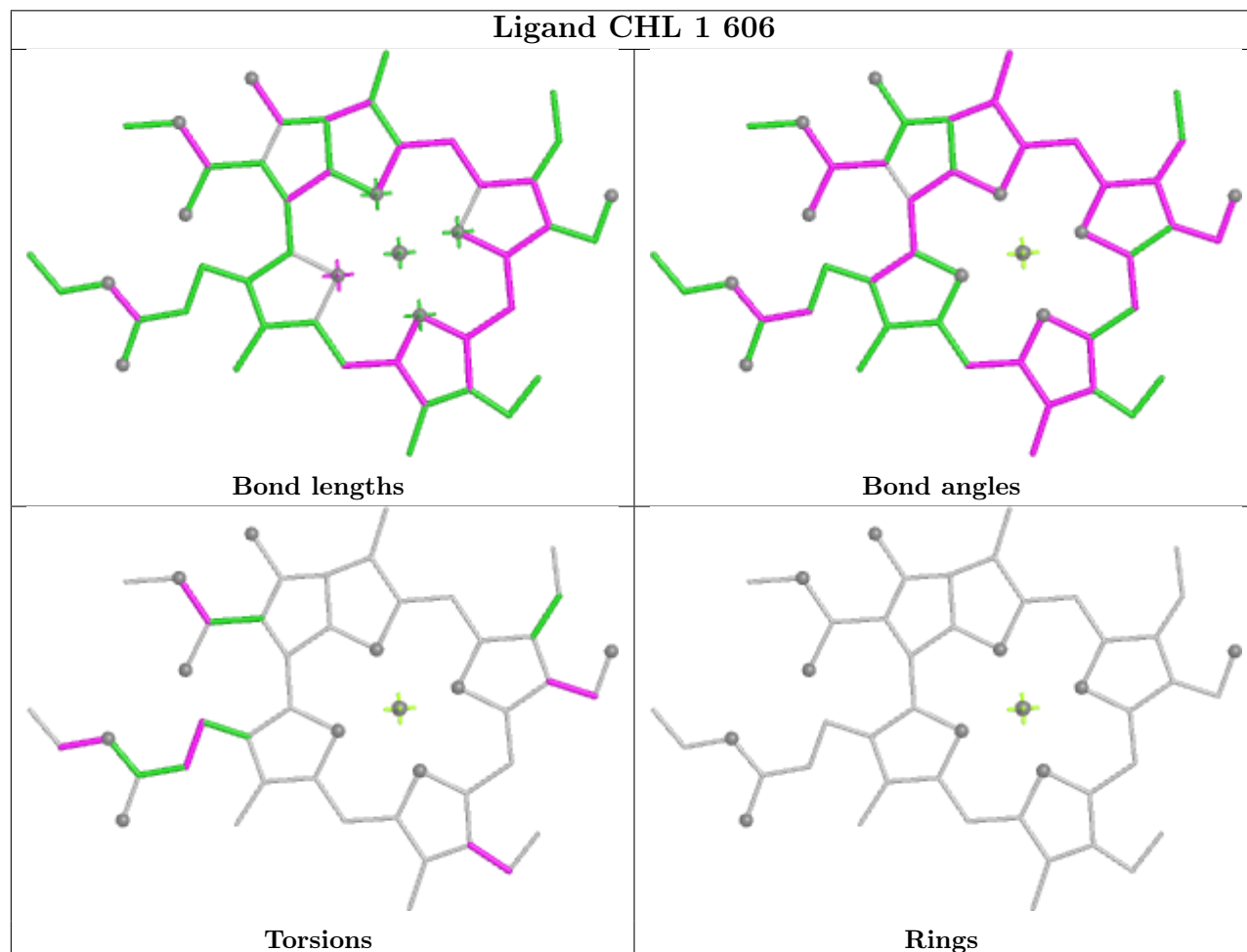
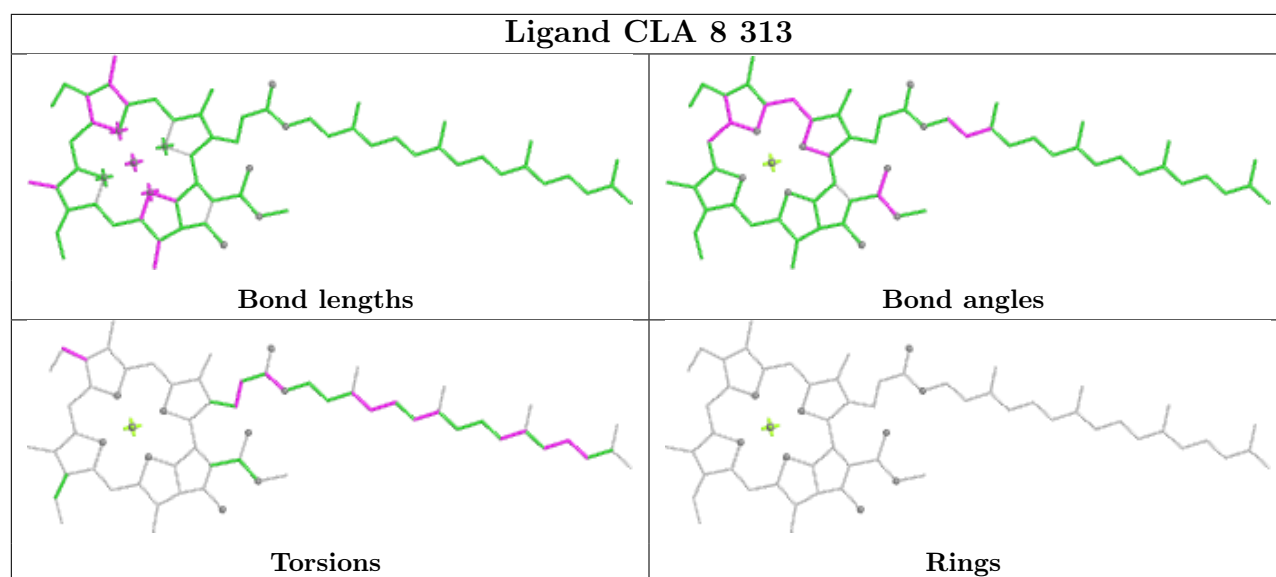
Bond angles



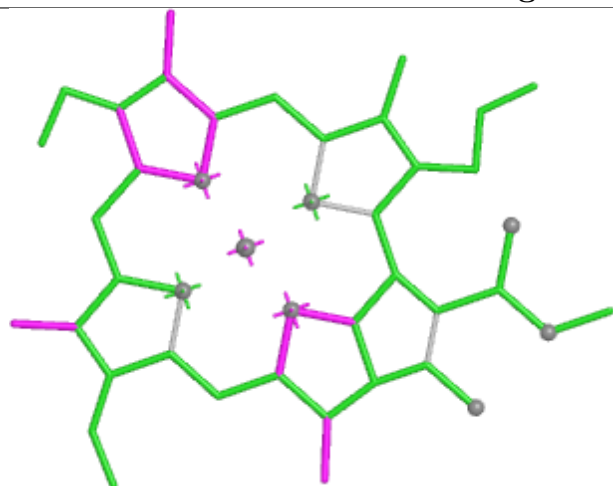
Torsions



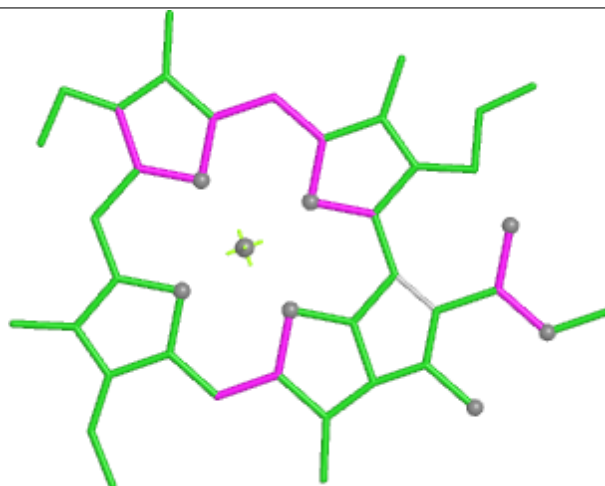
Rings



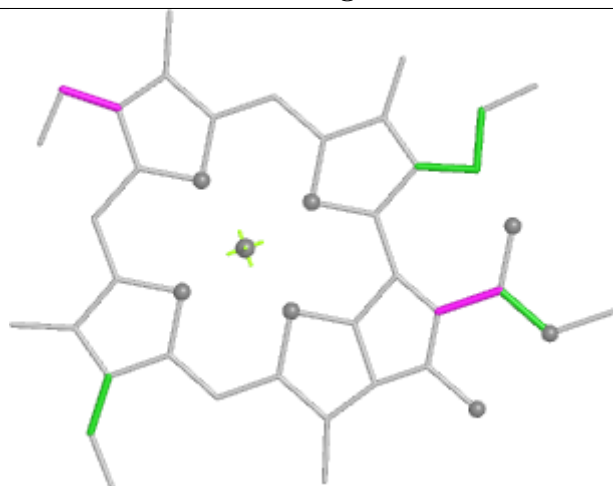
Ligand CLA 5 316



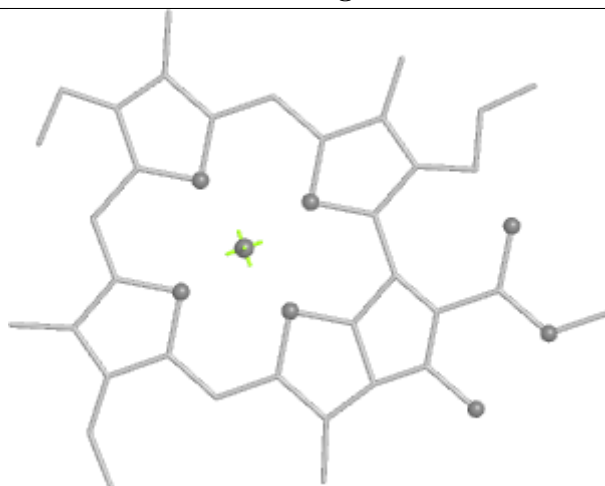
Bond lengths



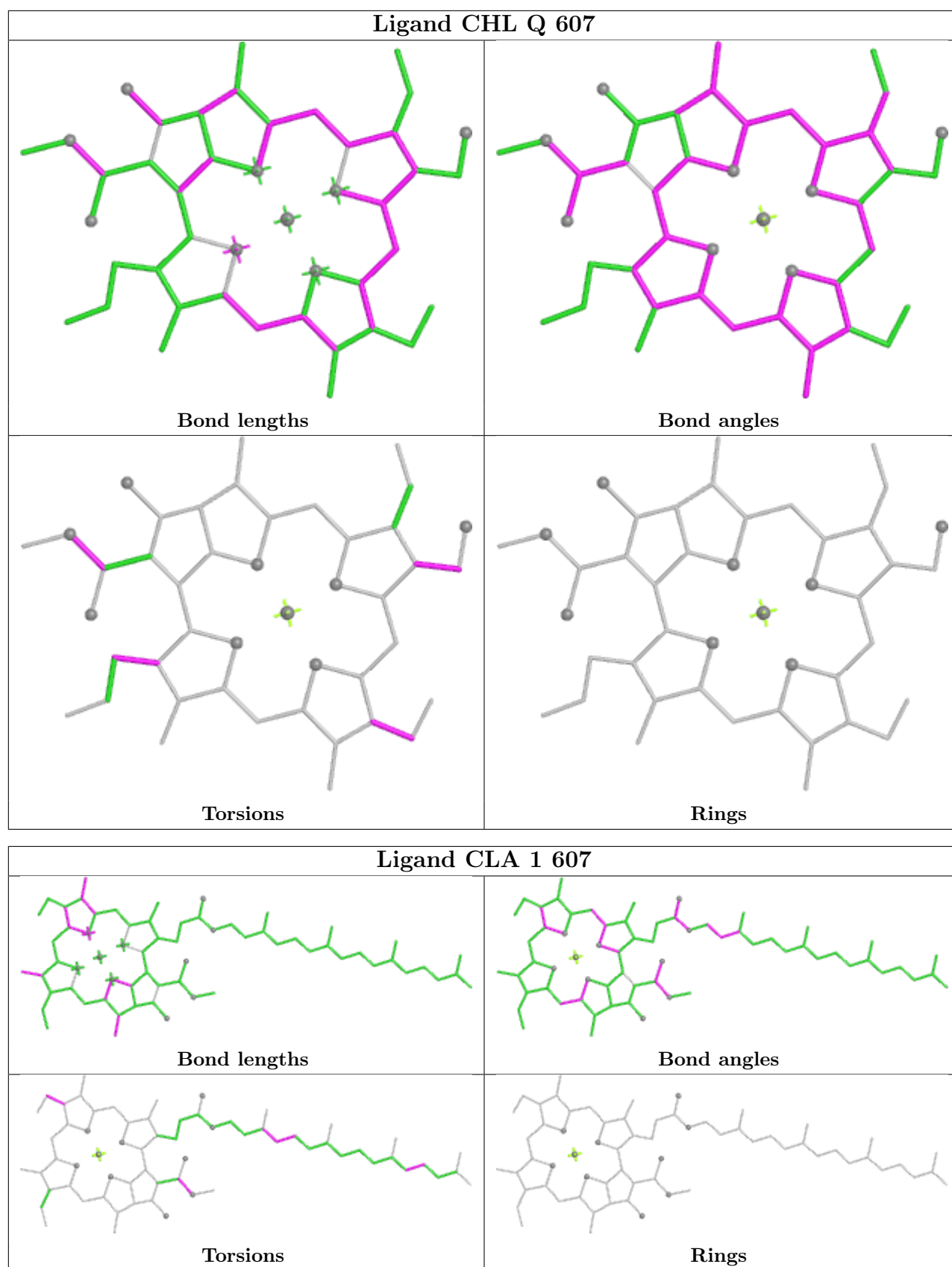
Bond angles

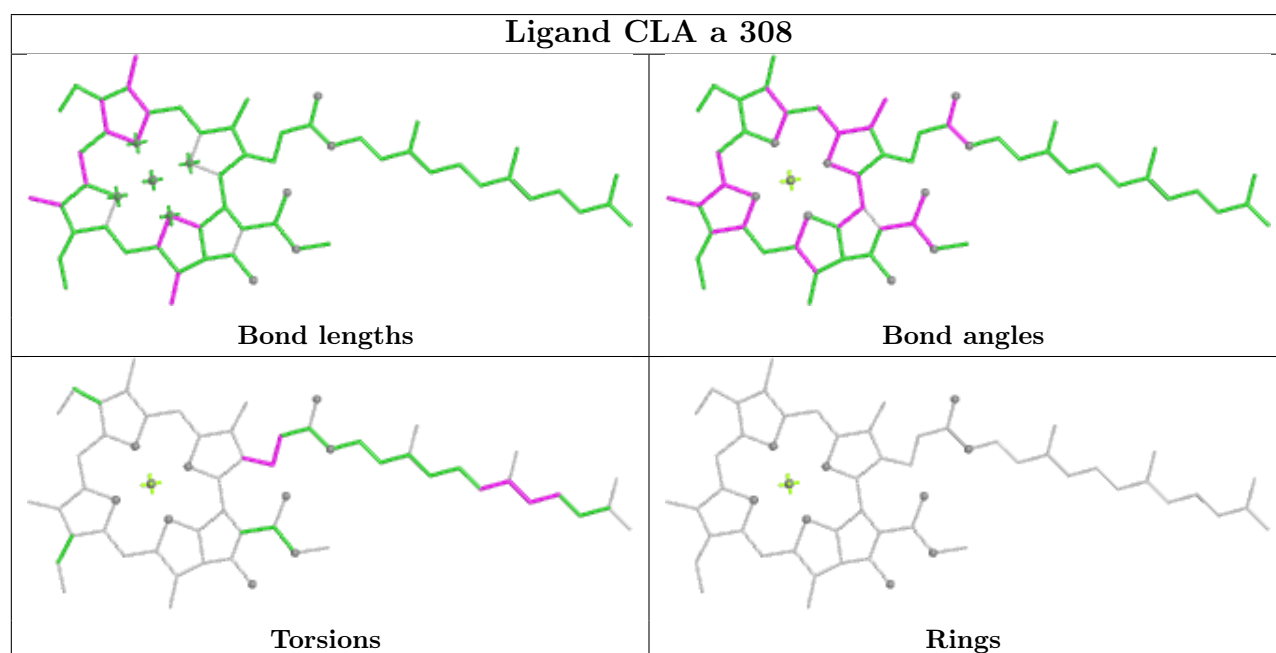
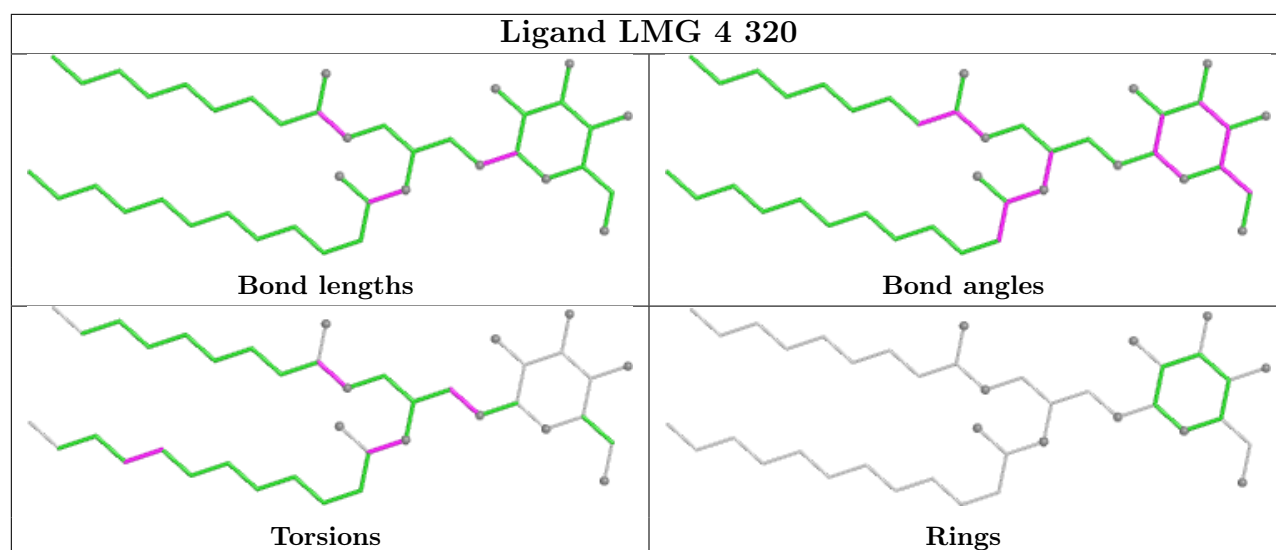


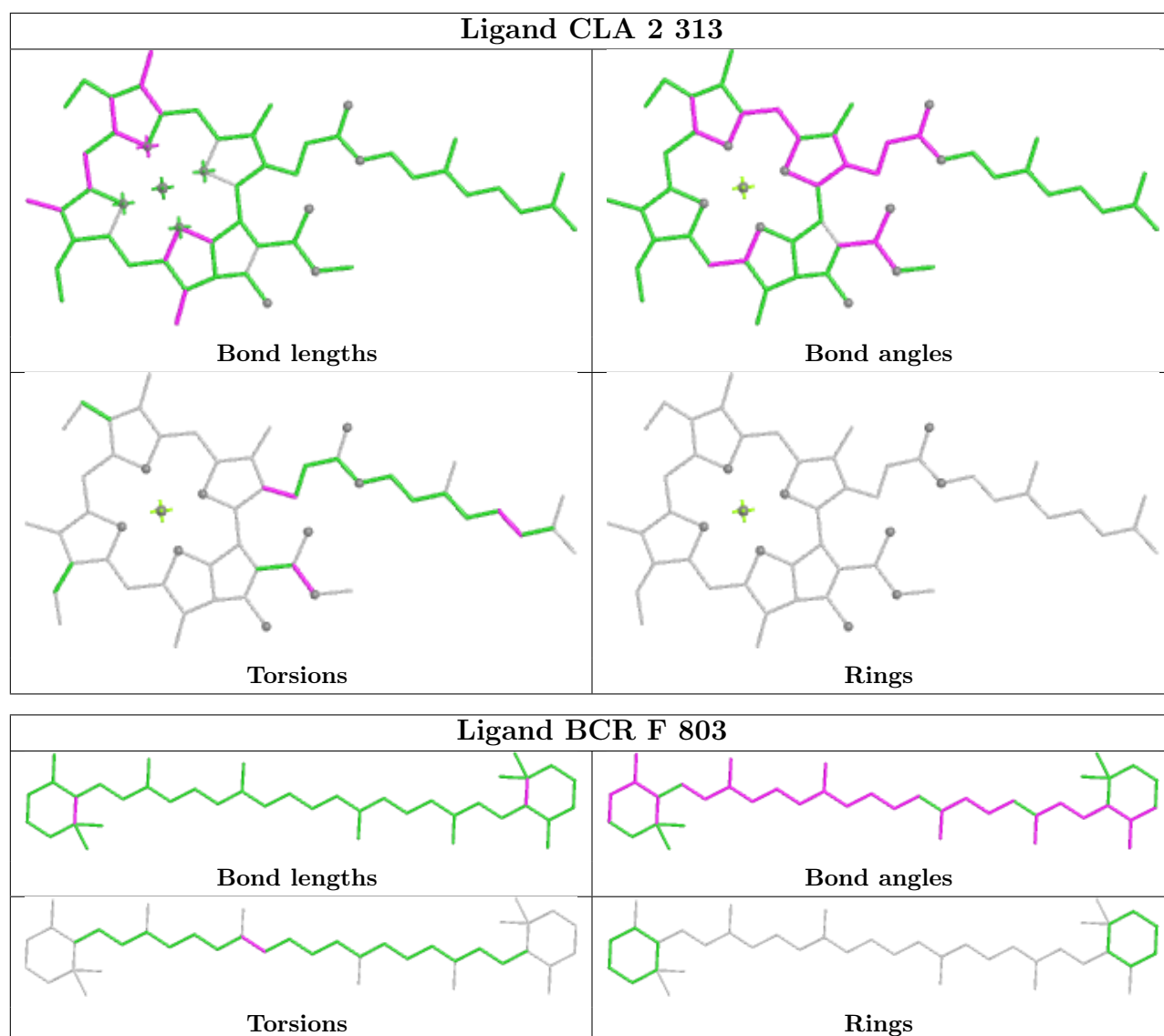
Torsions



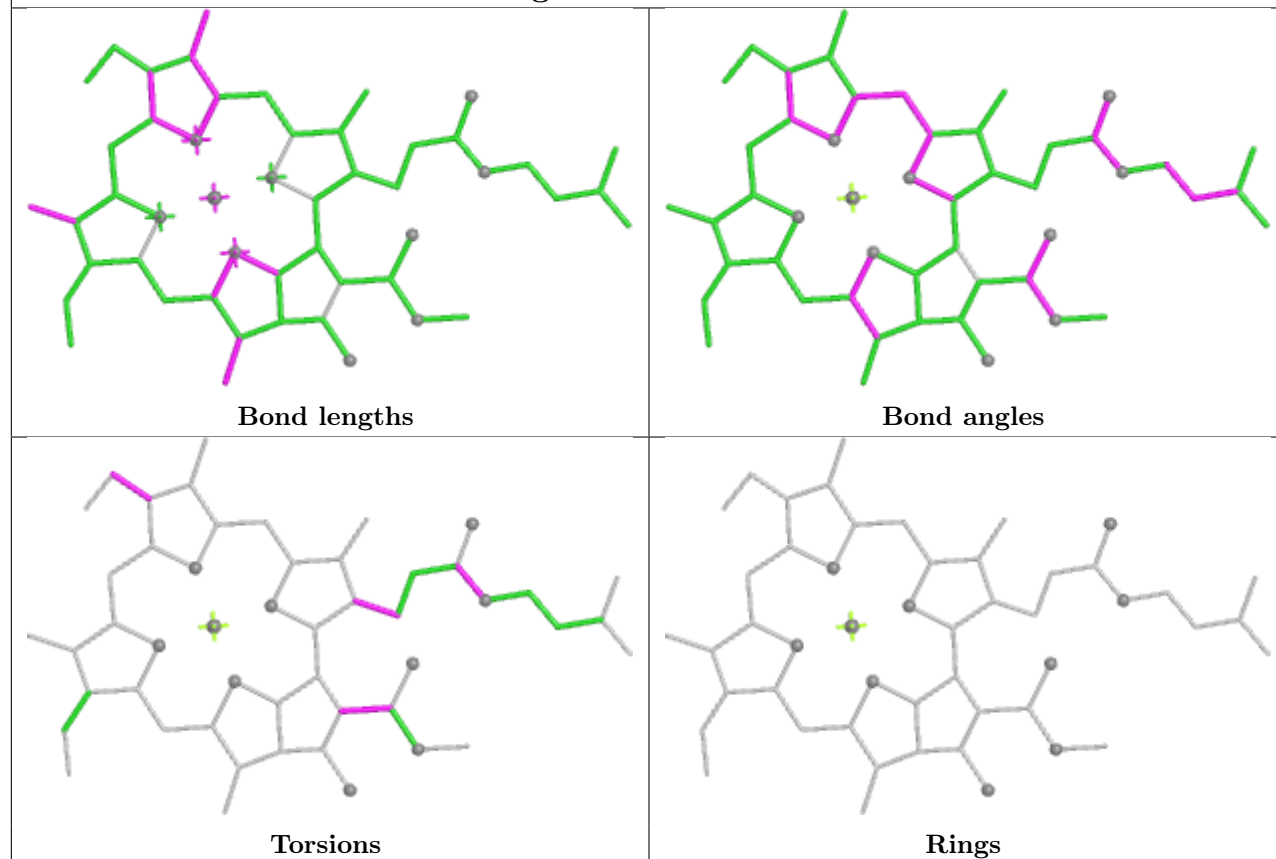
Rings



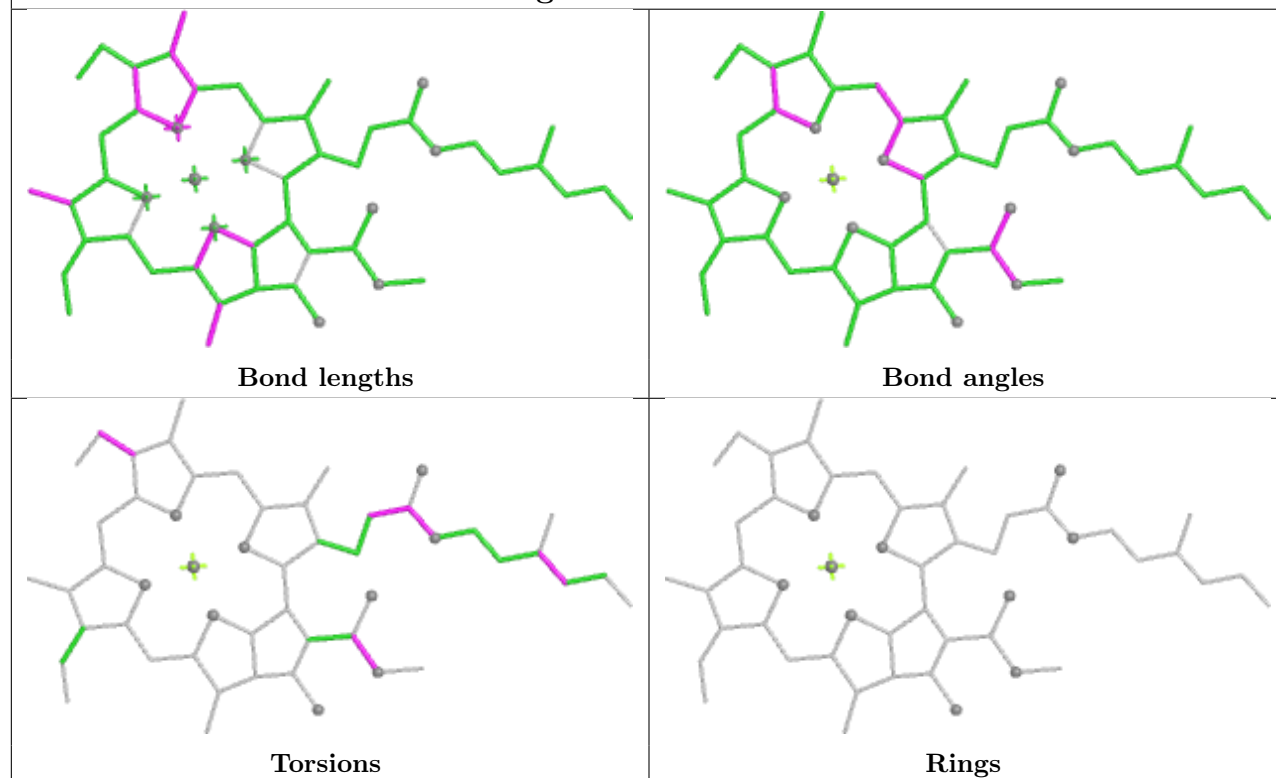




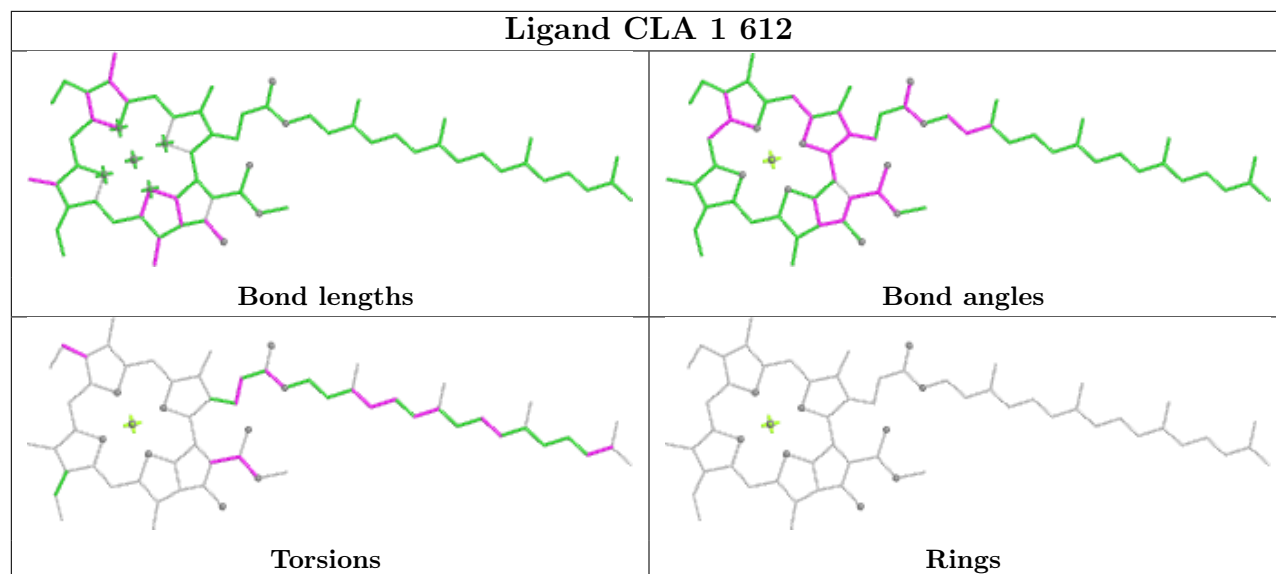
Ligand CLA A 831



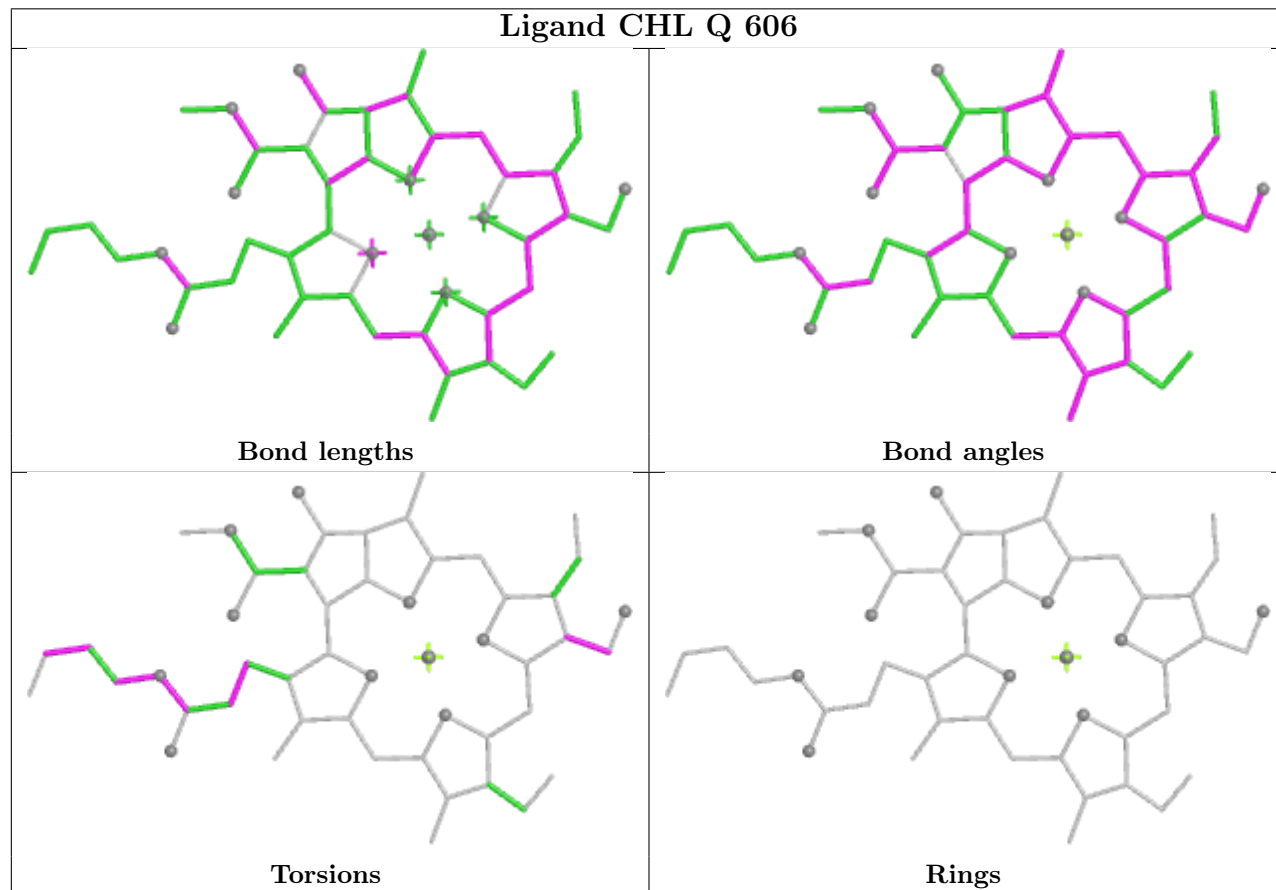
Ligand CLA 8 312

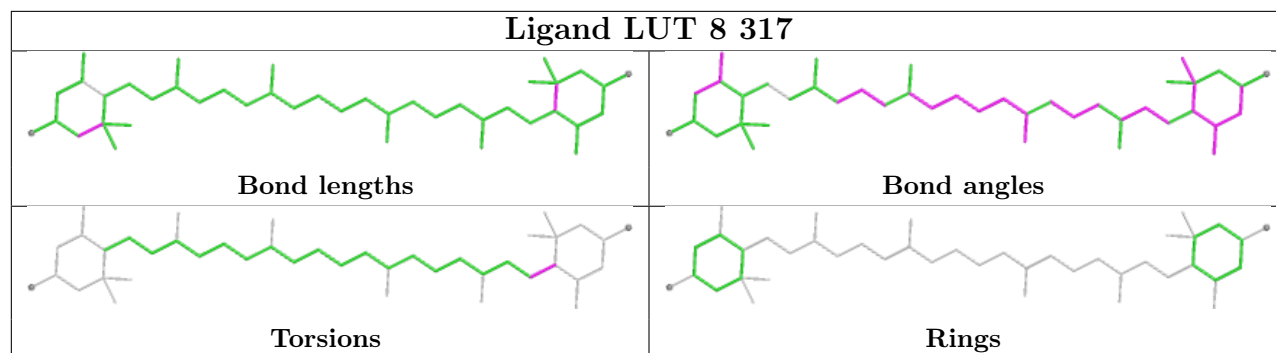
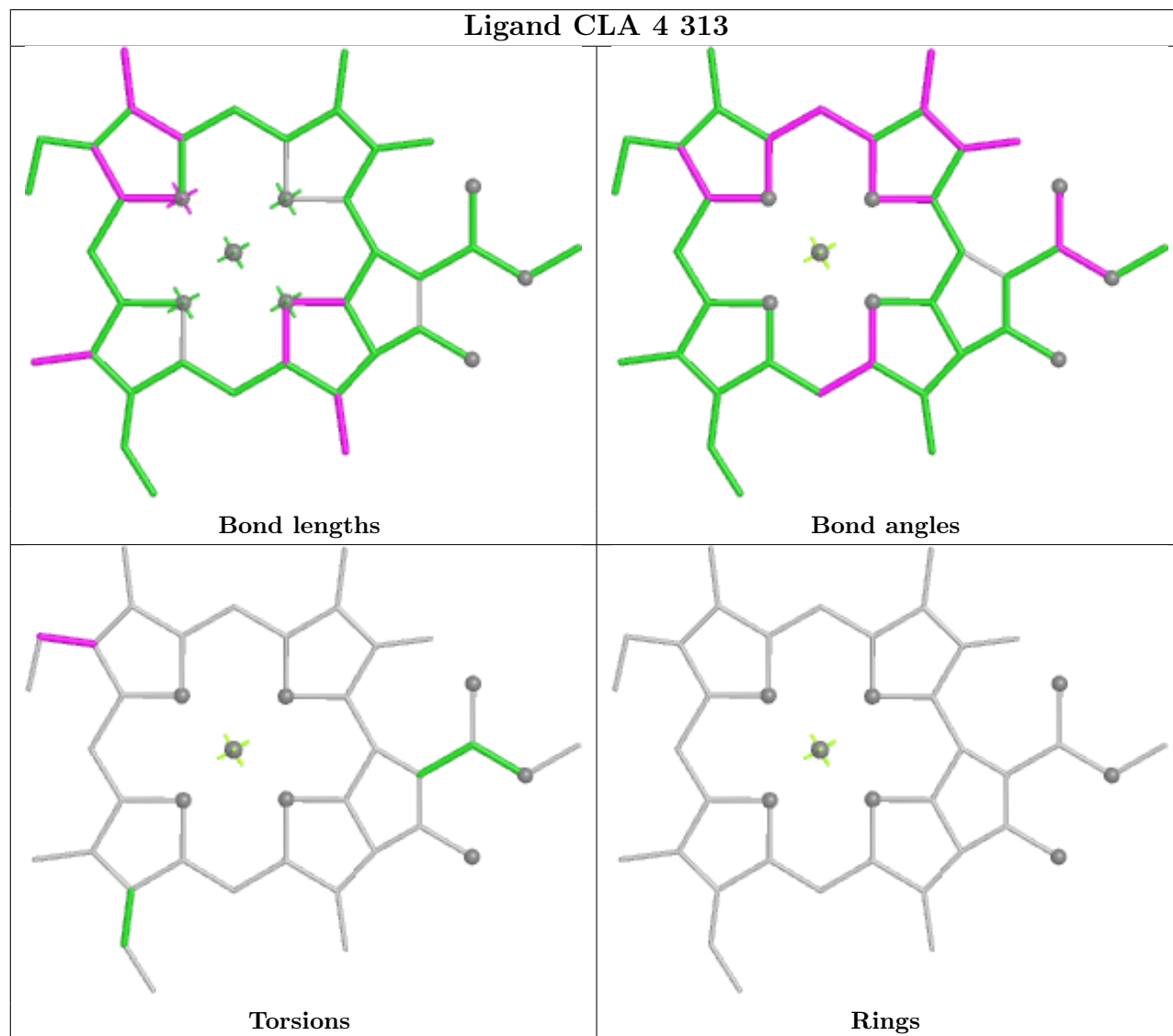


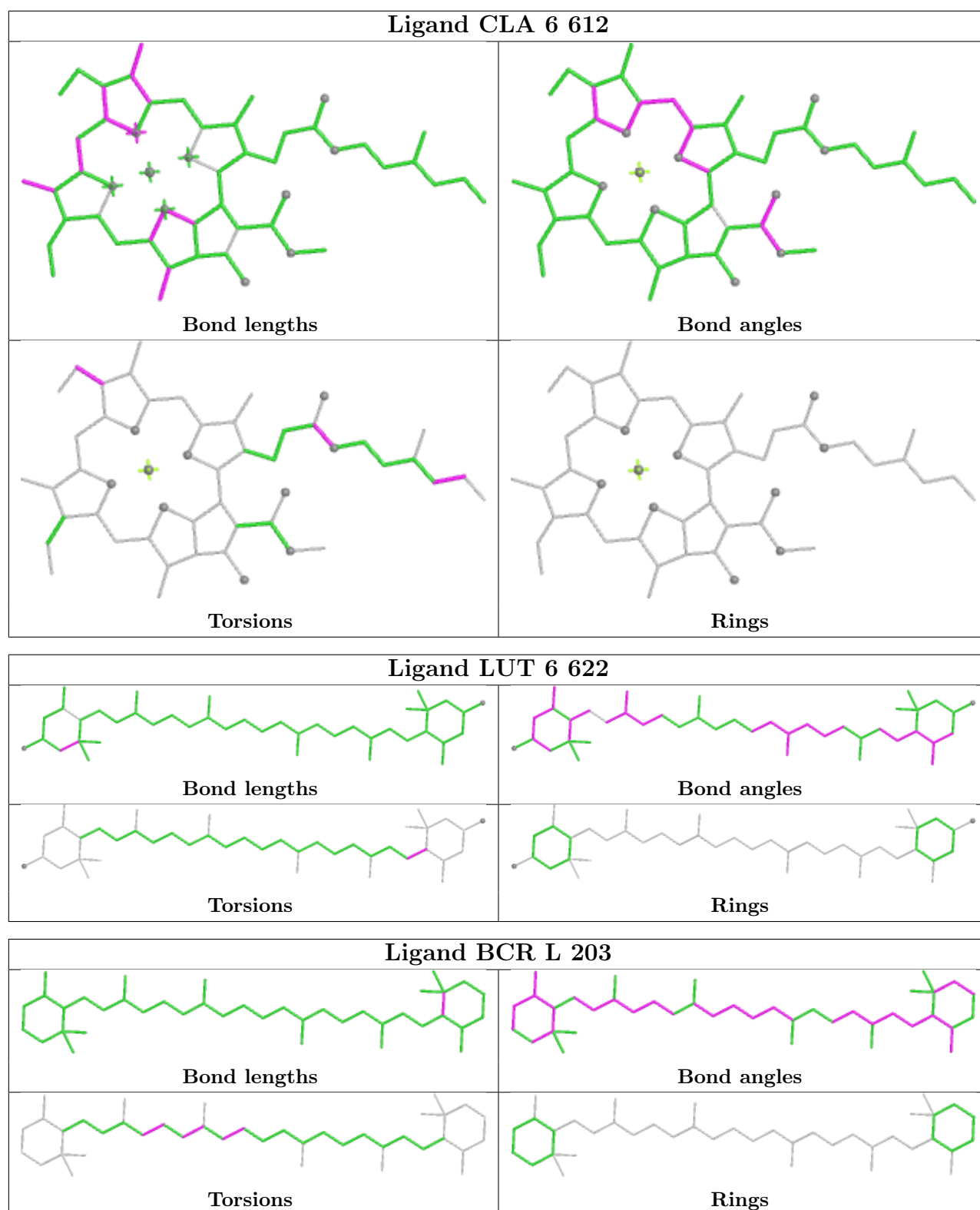
Ligand CLA 1 612

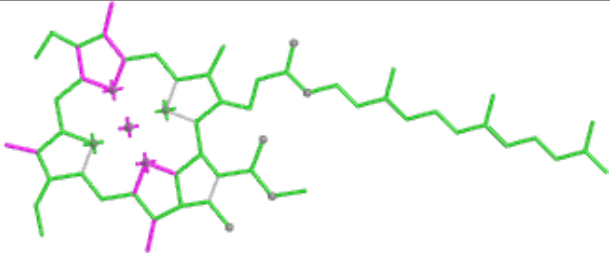
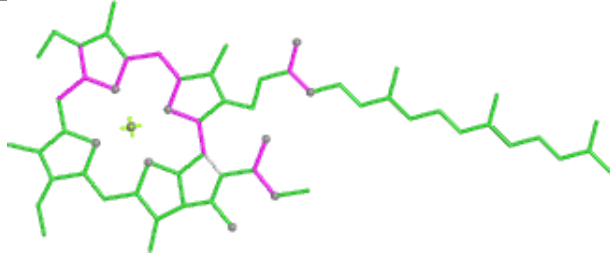
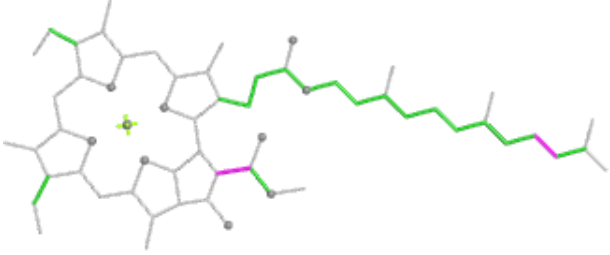
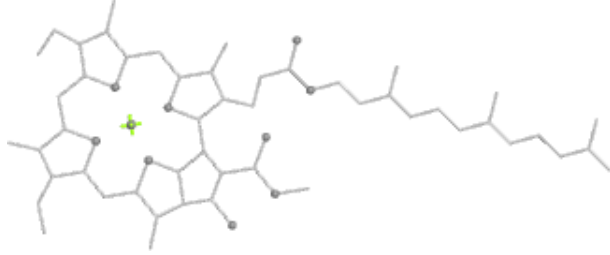
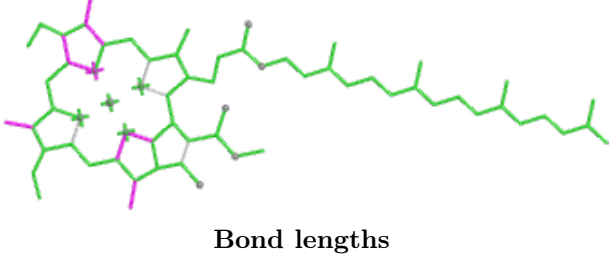
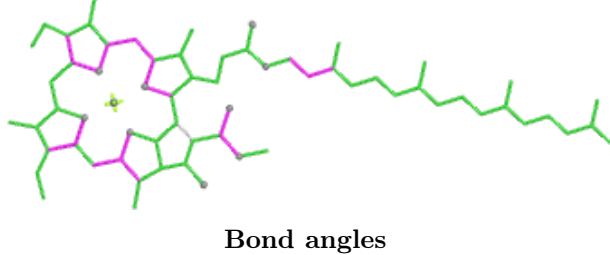
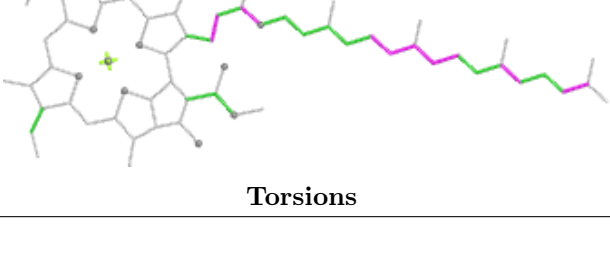
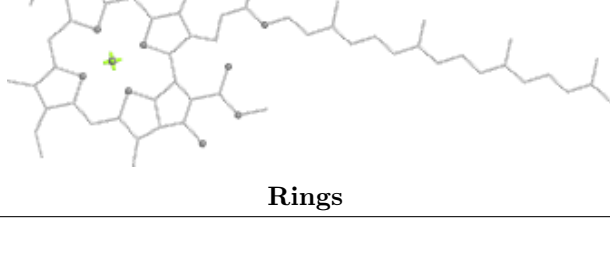


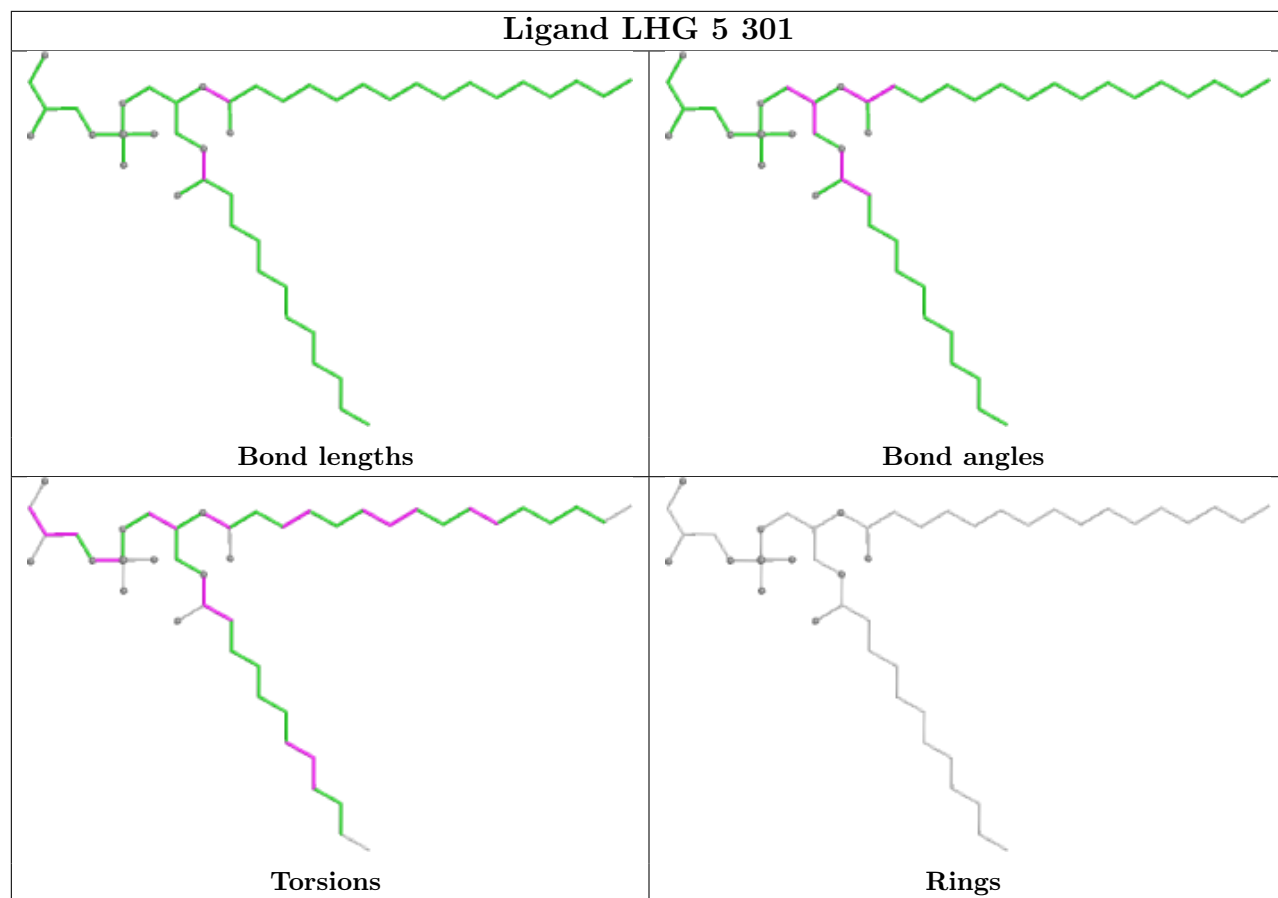
Ligand CHL Q 606



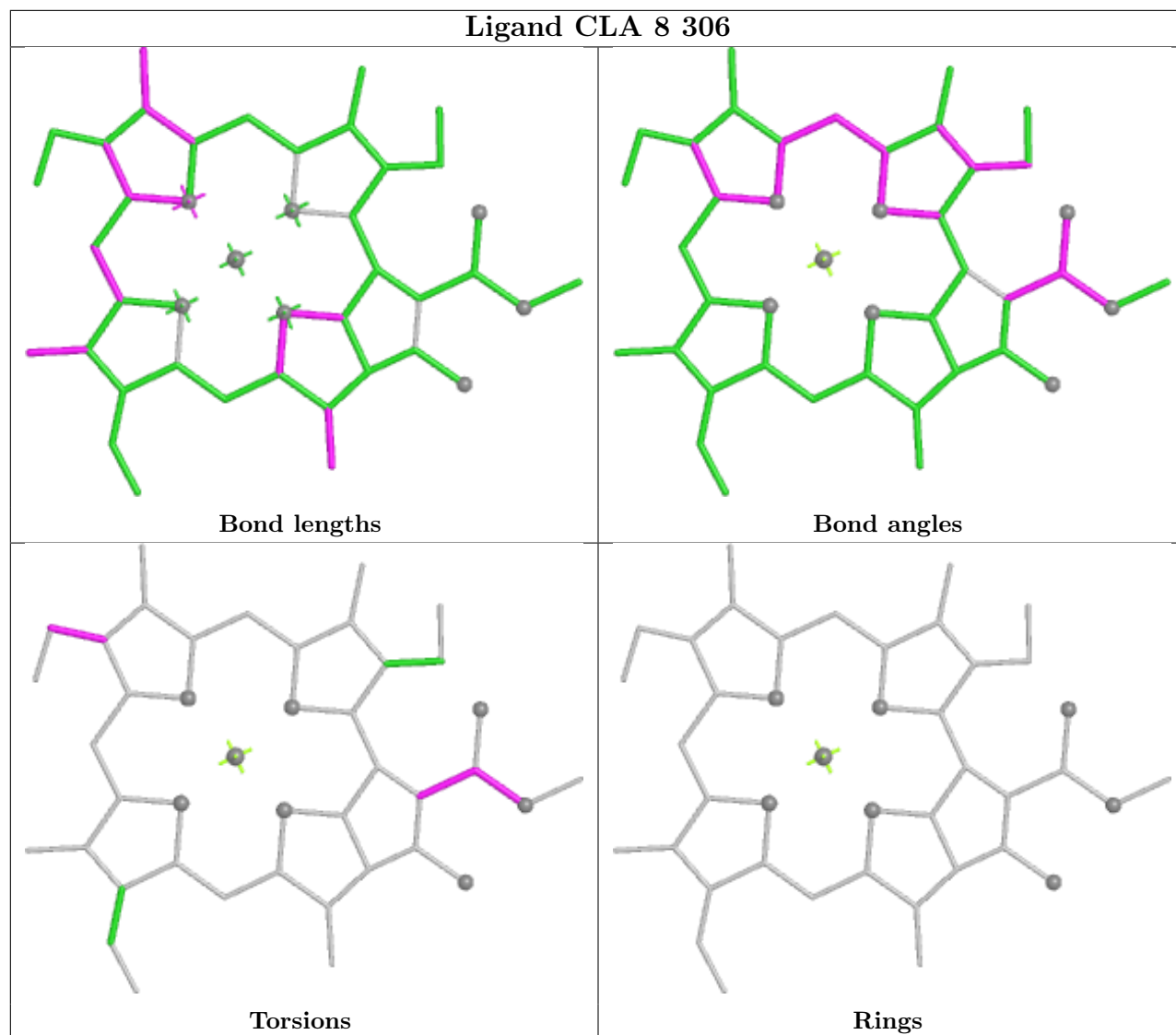
Ligand LUT 8 317**Ligand CLA 4 313**



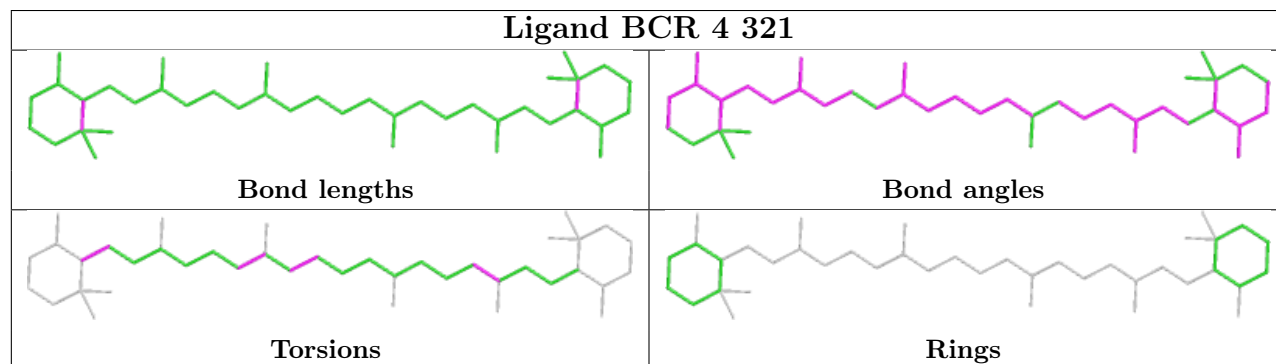
Ligand CLA B 833	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 2 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

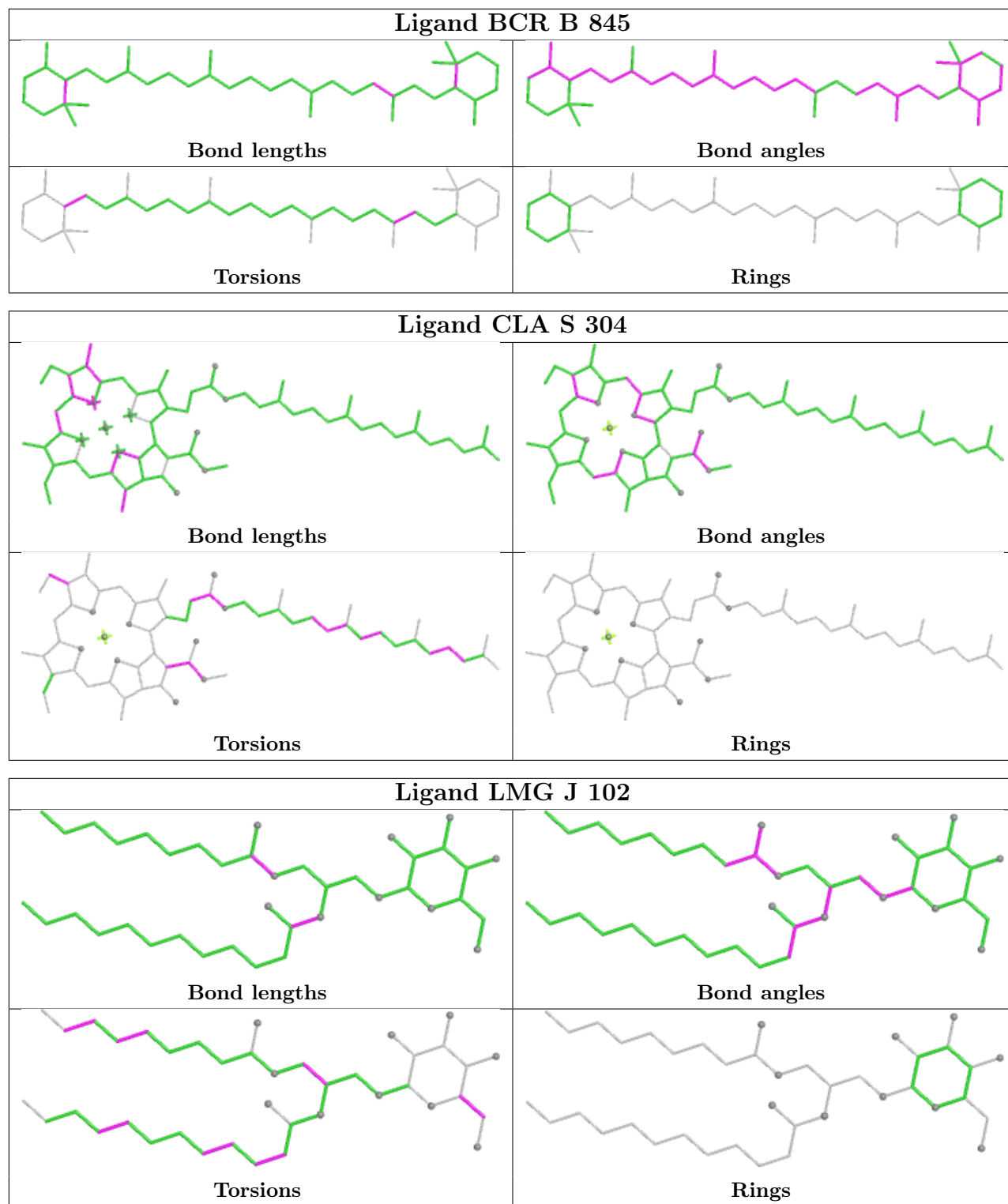


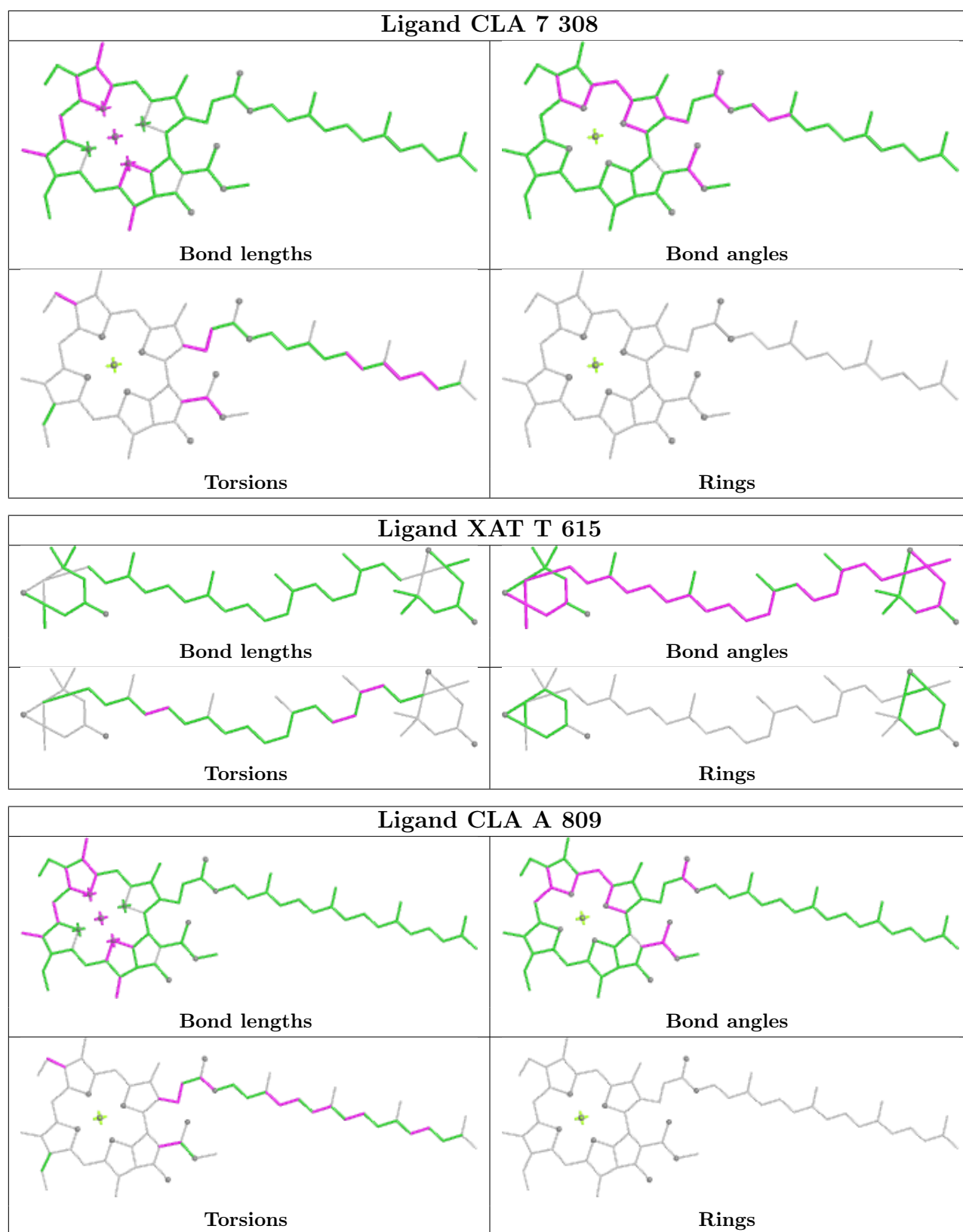
Ligand CLA 8 306

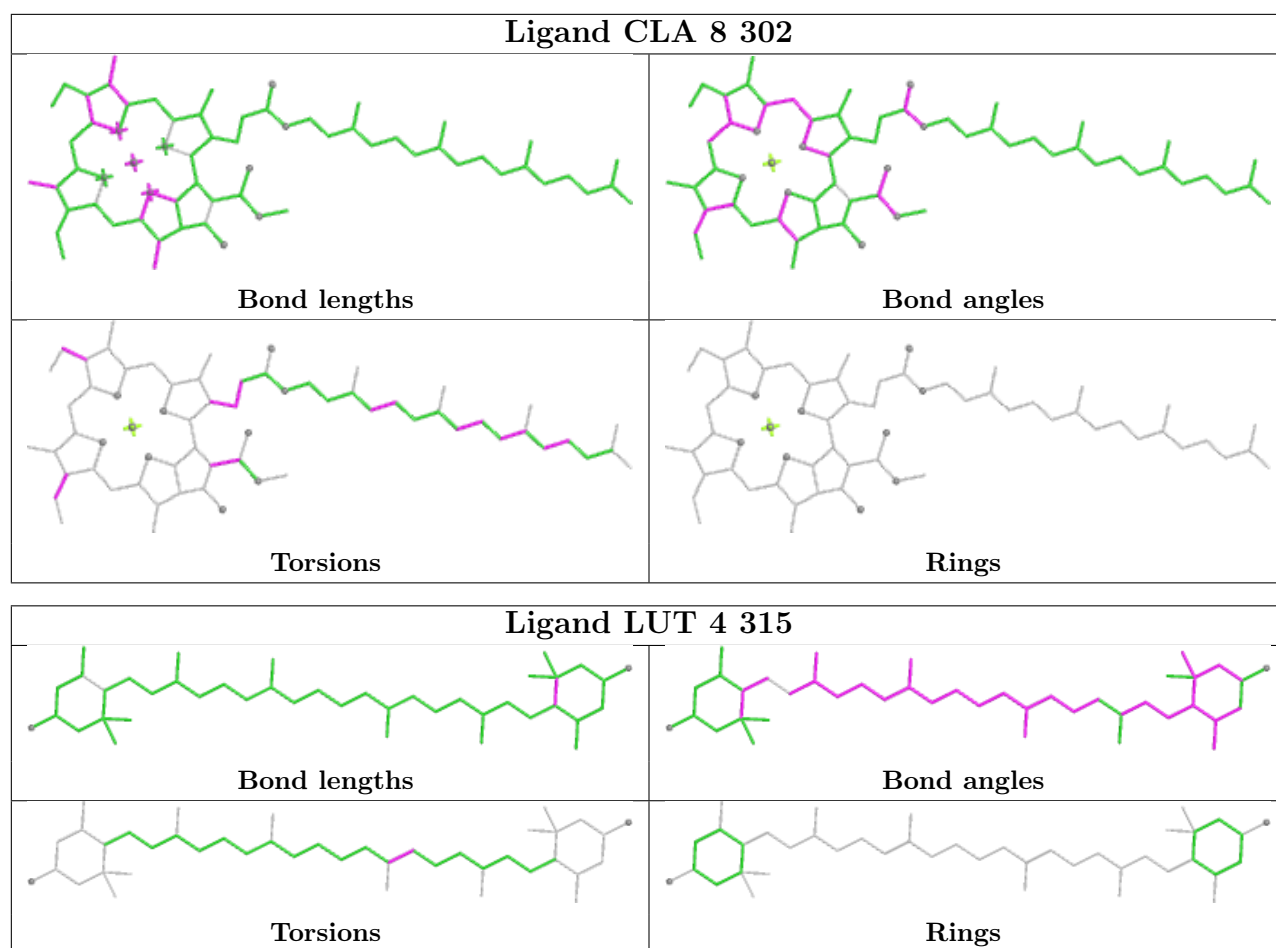


Ligand BCR 4 321

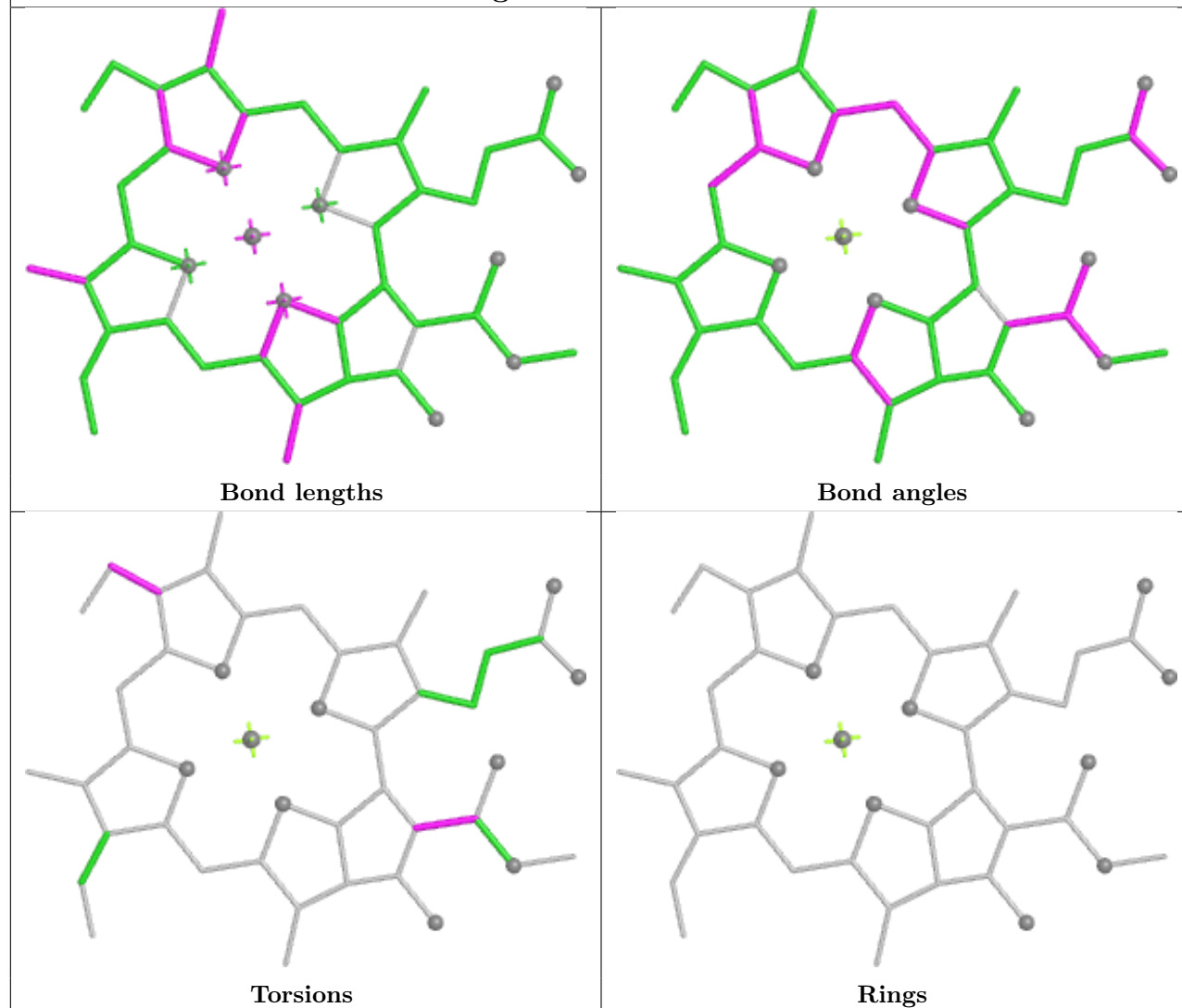




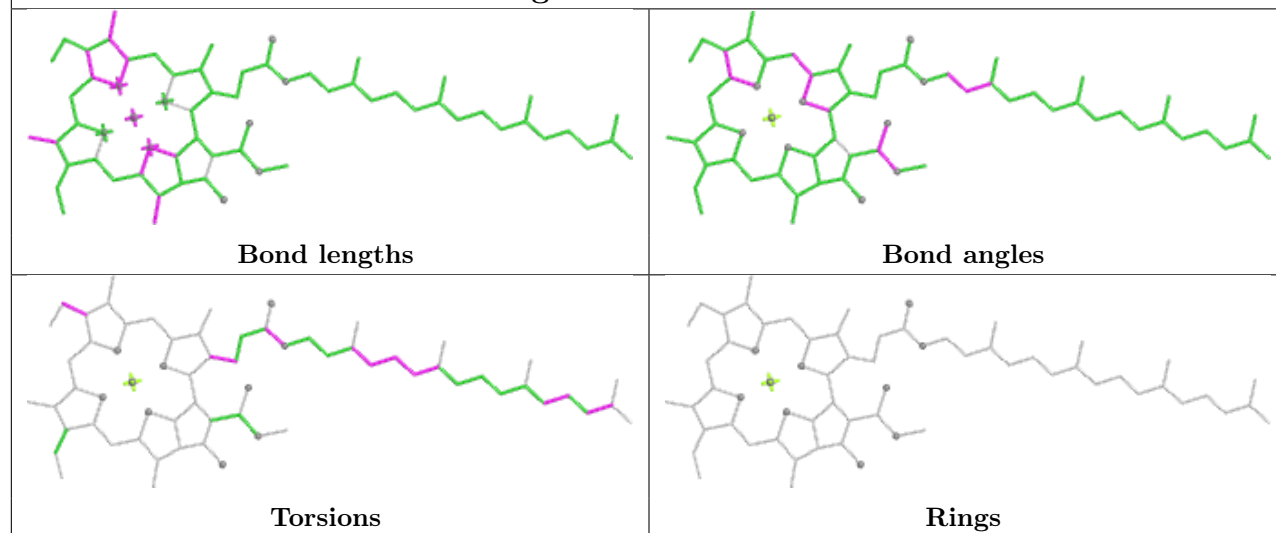


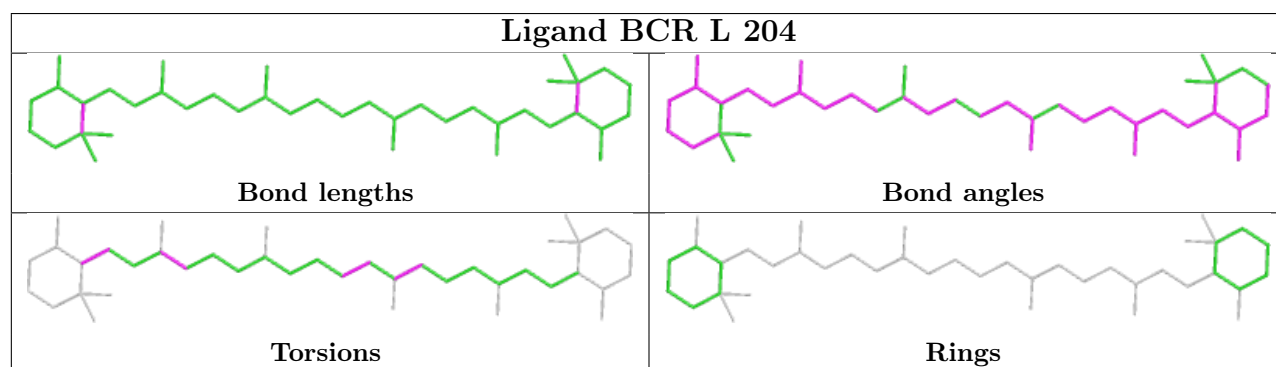
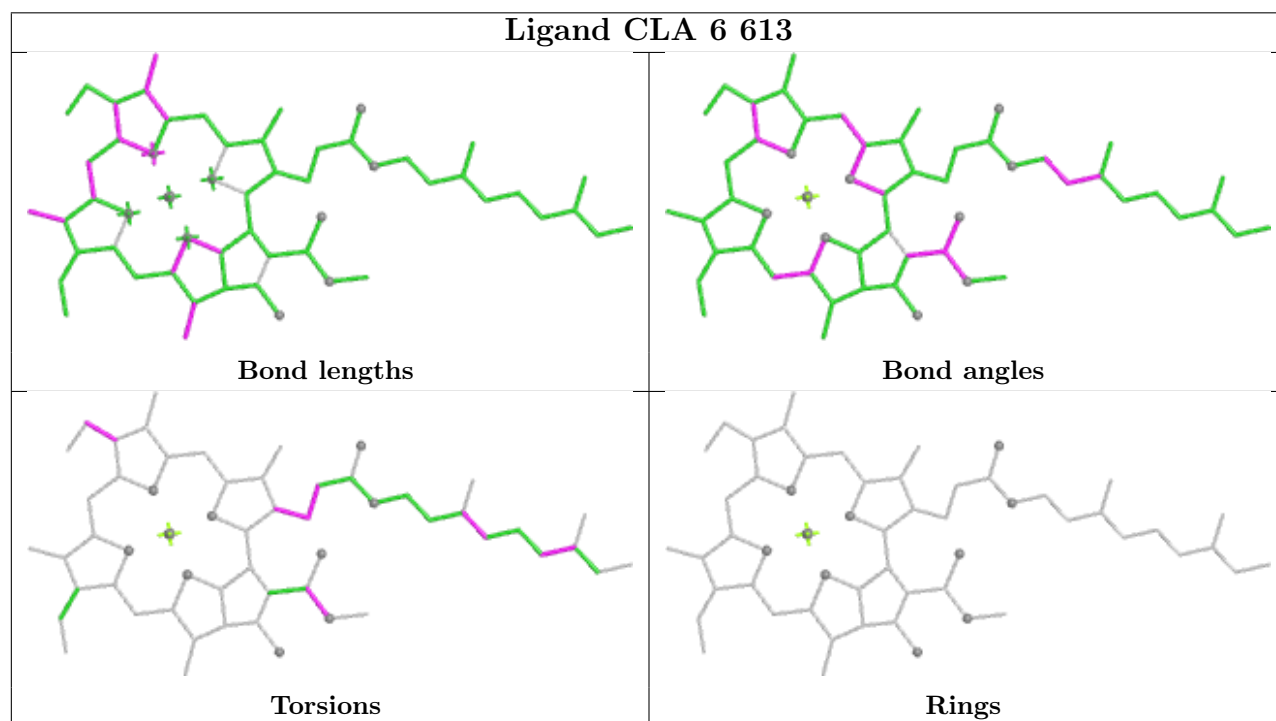
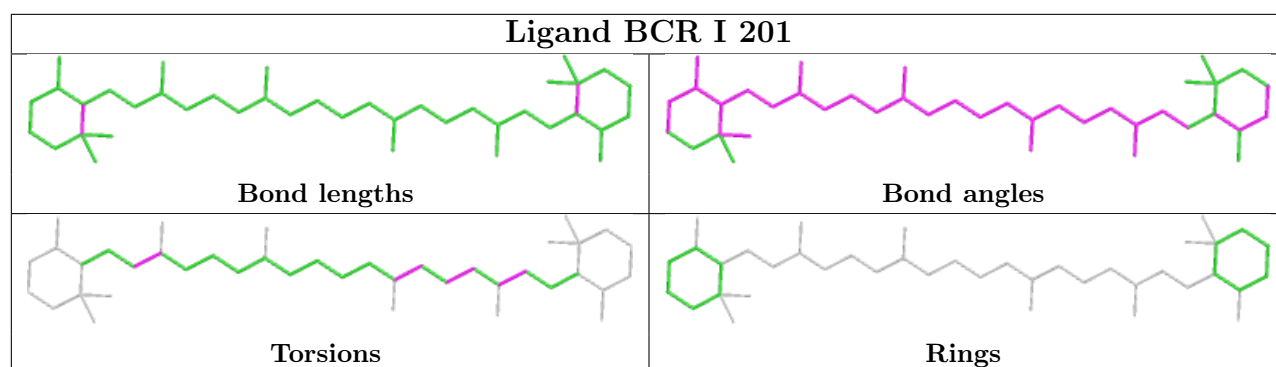


Ligand CLA A 821

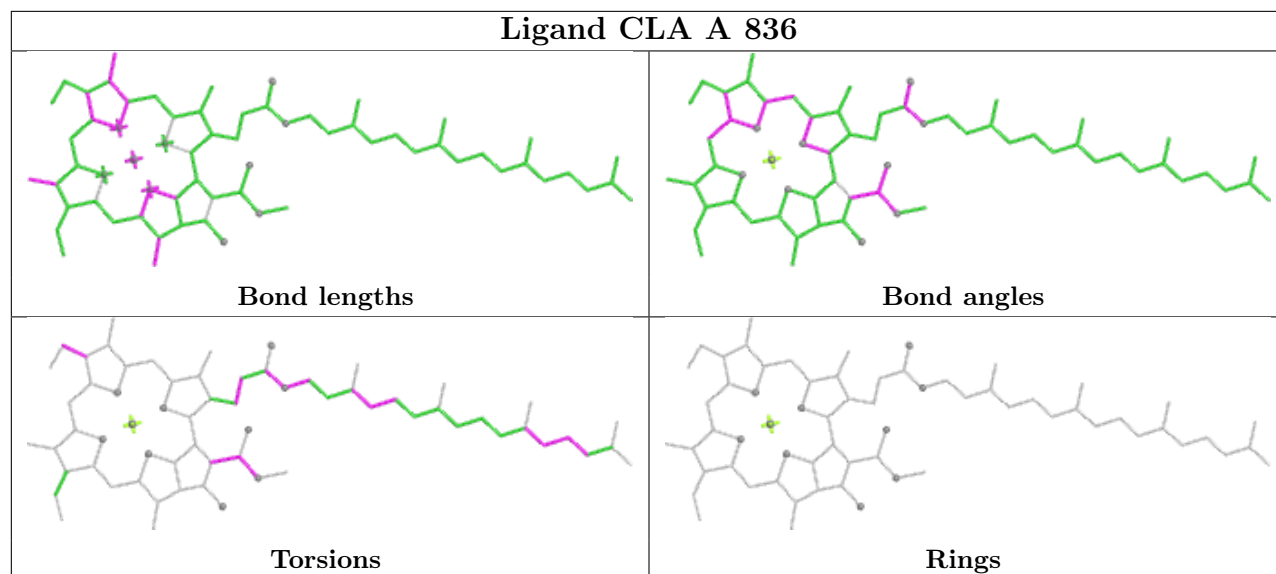


Ligand CLA A 832

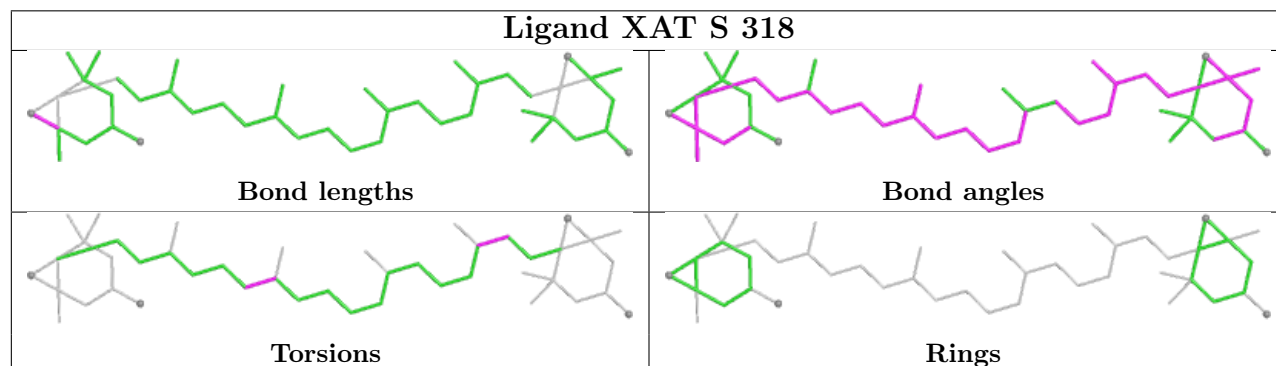




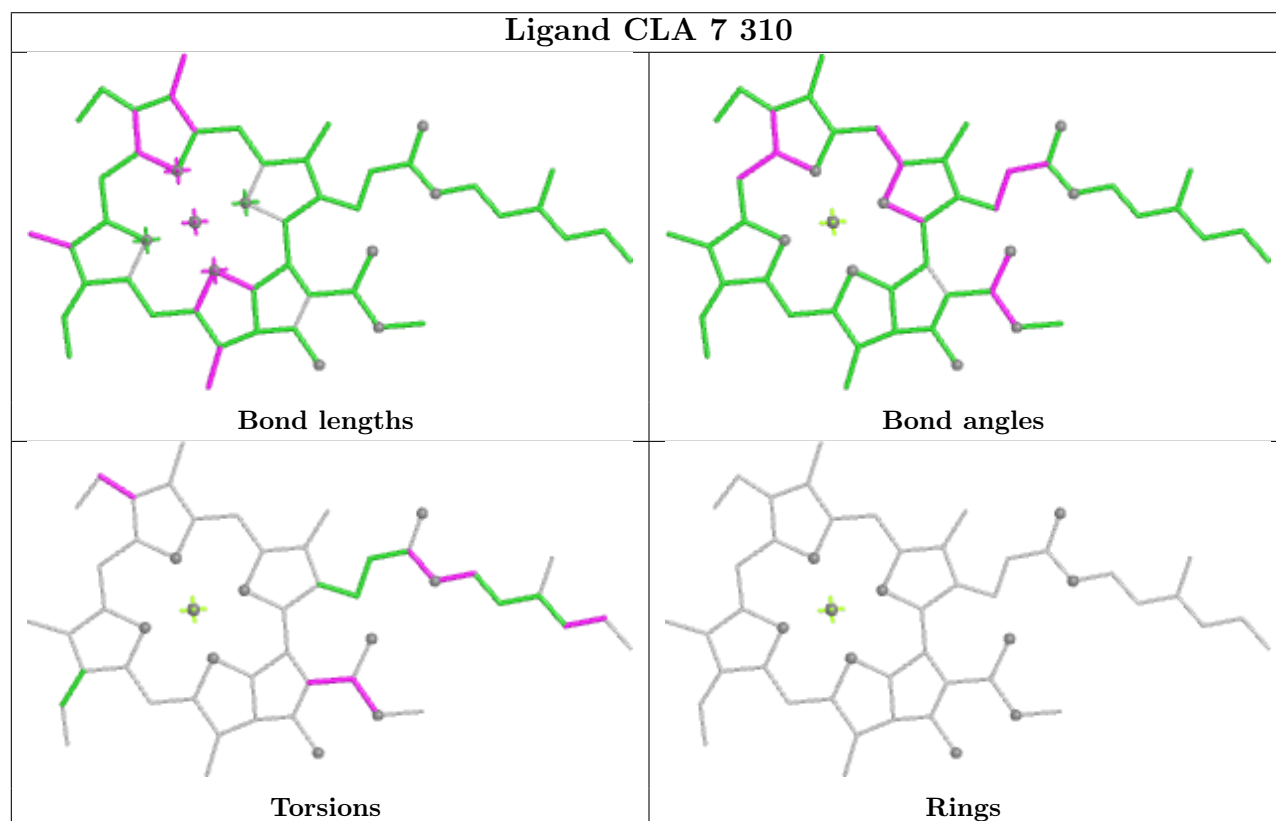
Ligand CLA A 836



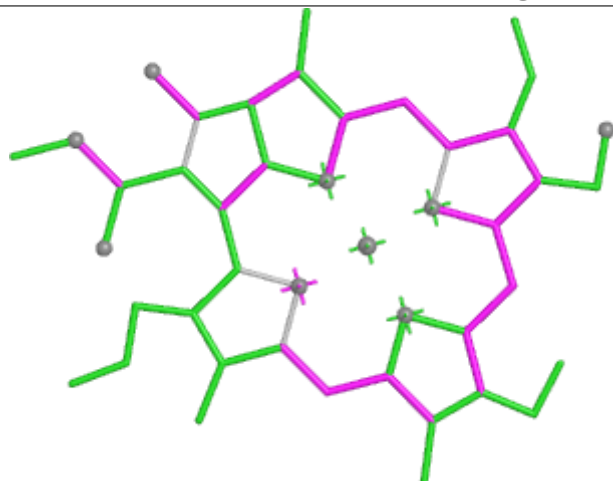
Ligand XAT S 318



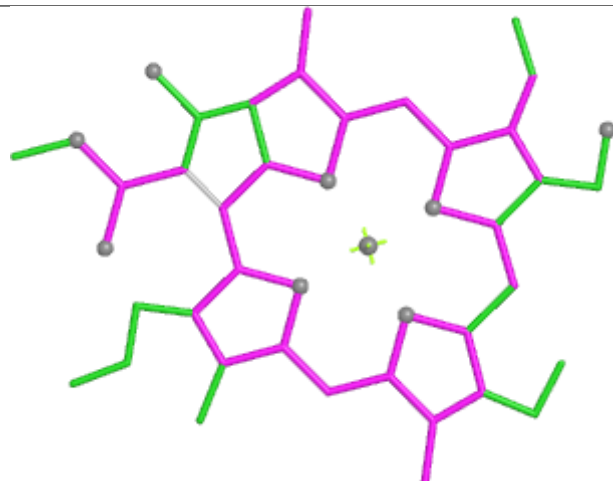
Ligand CLA 7 310



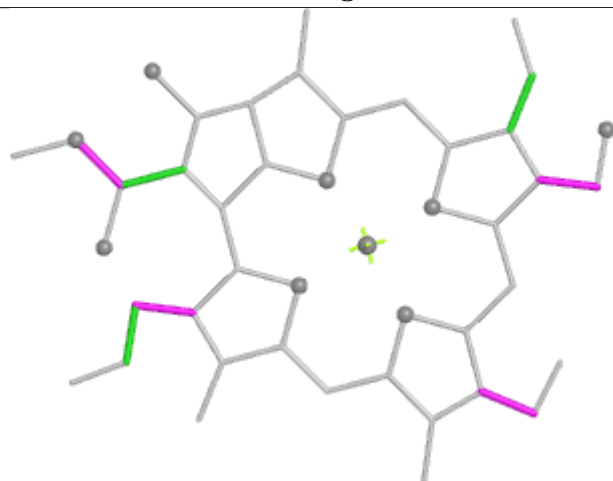
Ligand CHL P 608



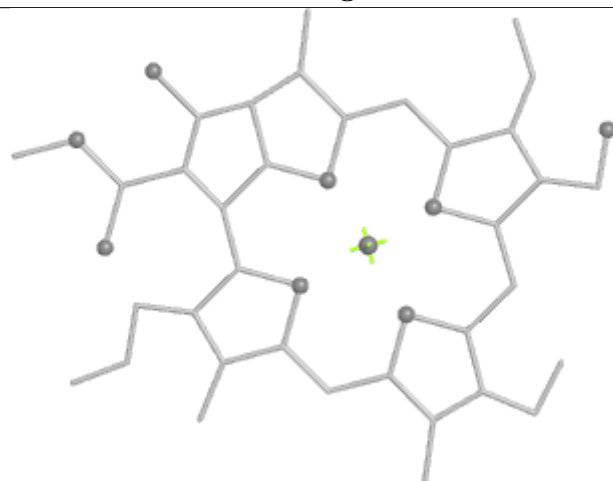
Bond lengths



Bond angles

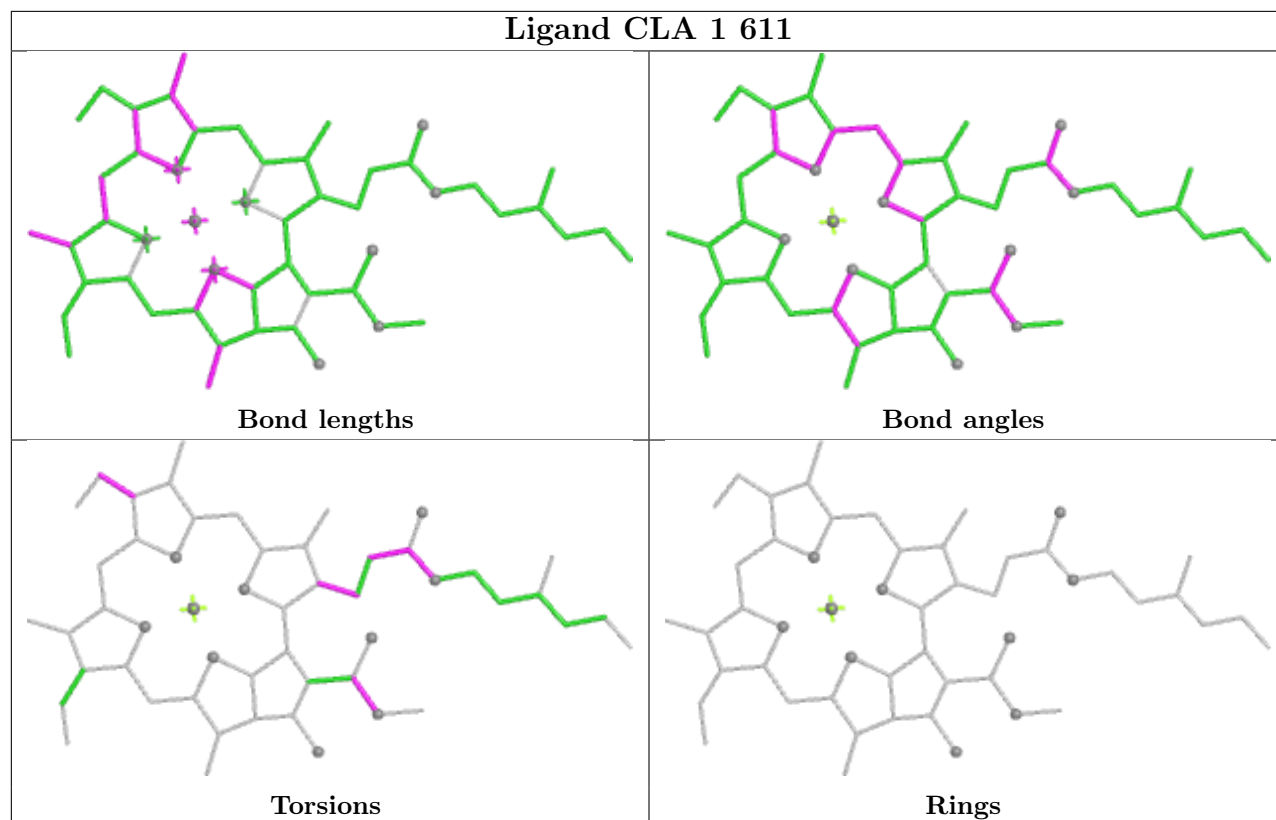


Torsions

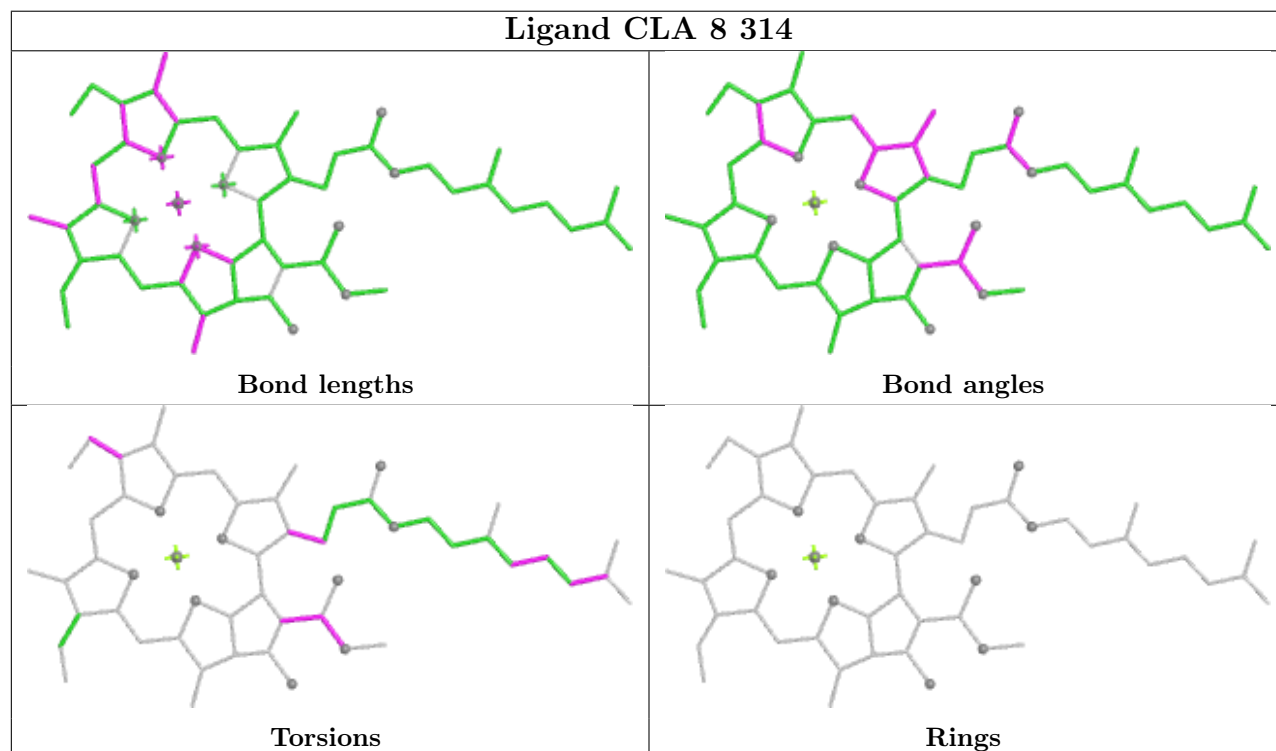


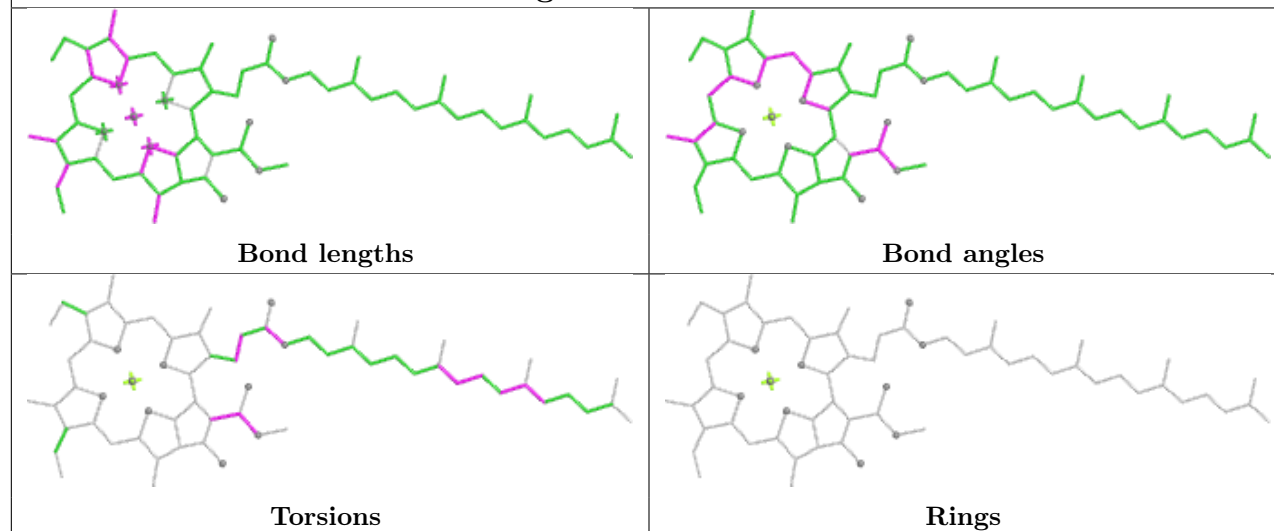
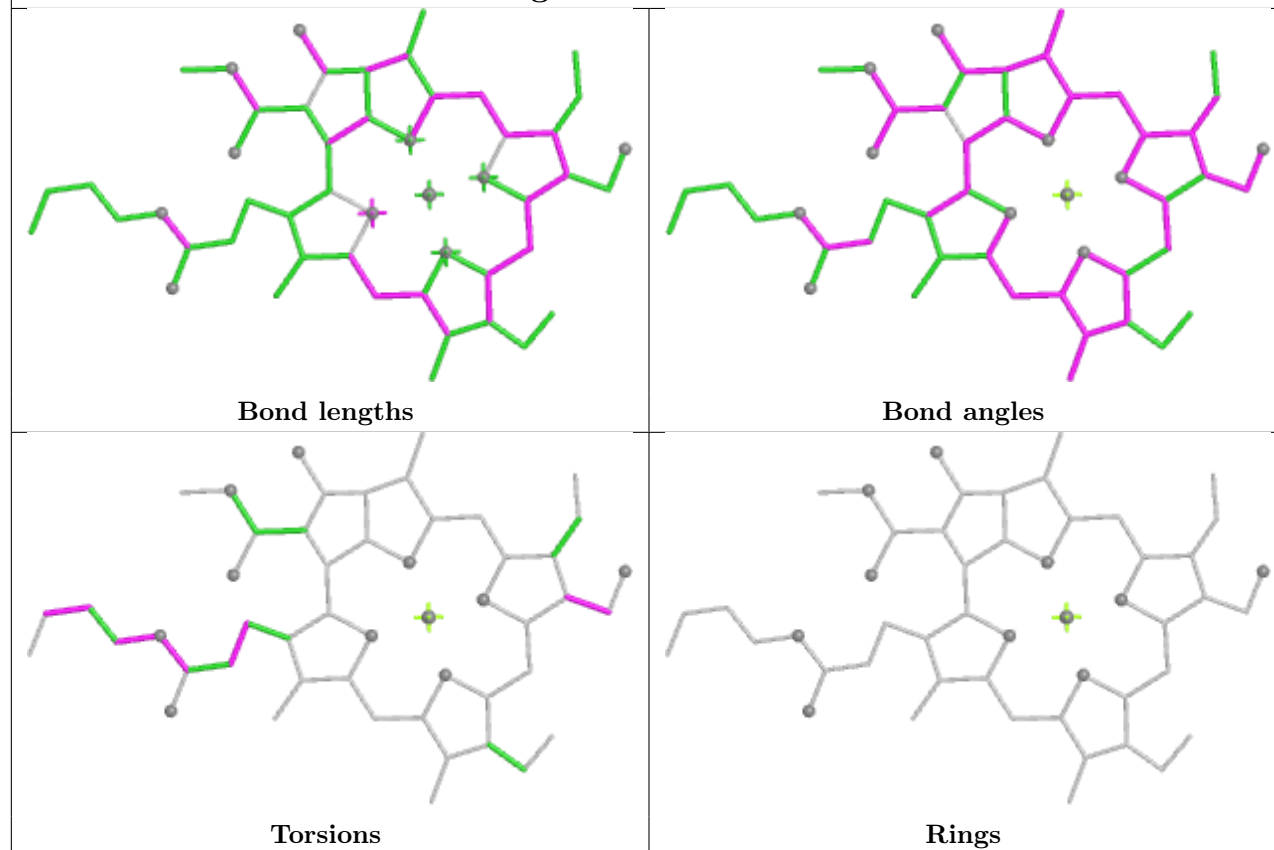
Rings

Ligand CLA 1 611

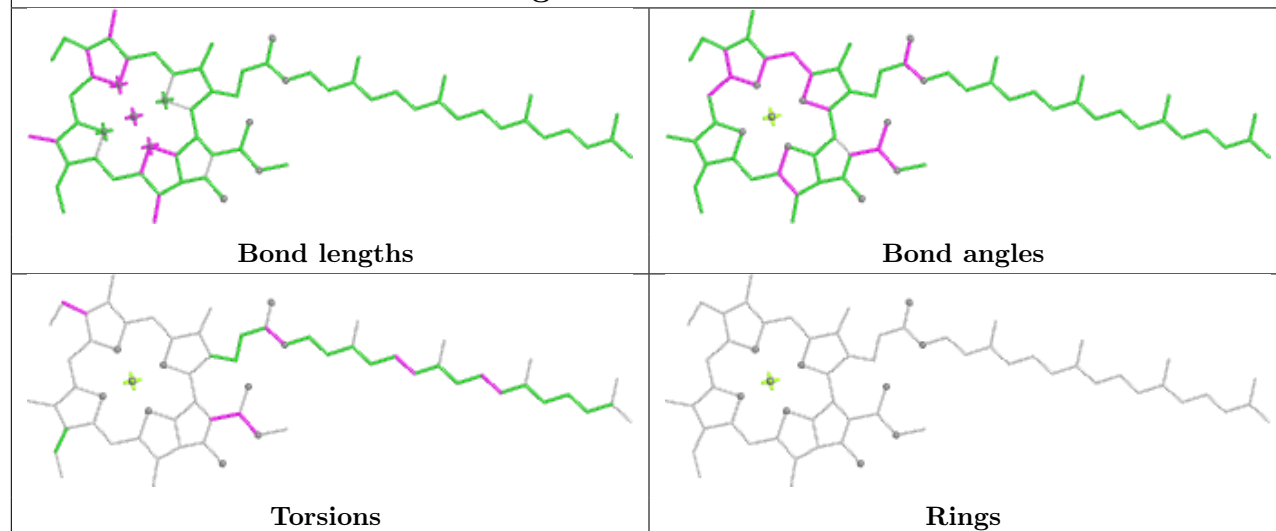


Ligand CLA 8 314

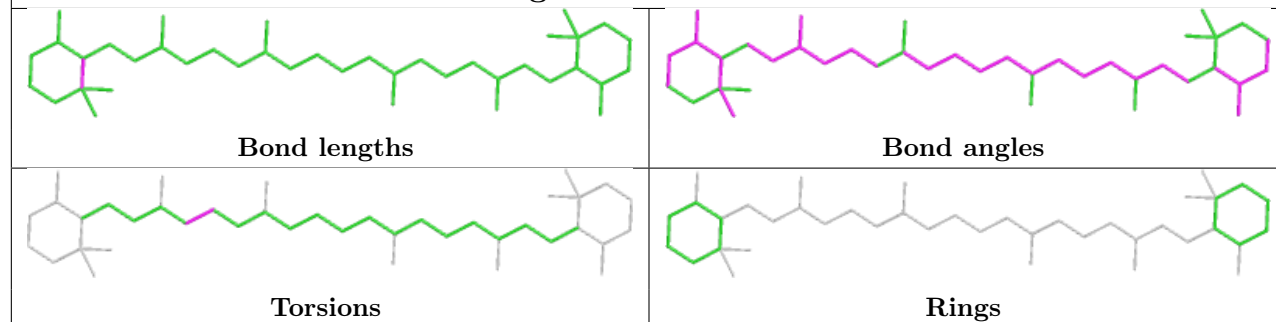


Ligand CLA 5 303**Ligand CHL U 306**

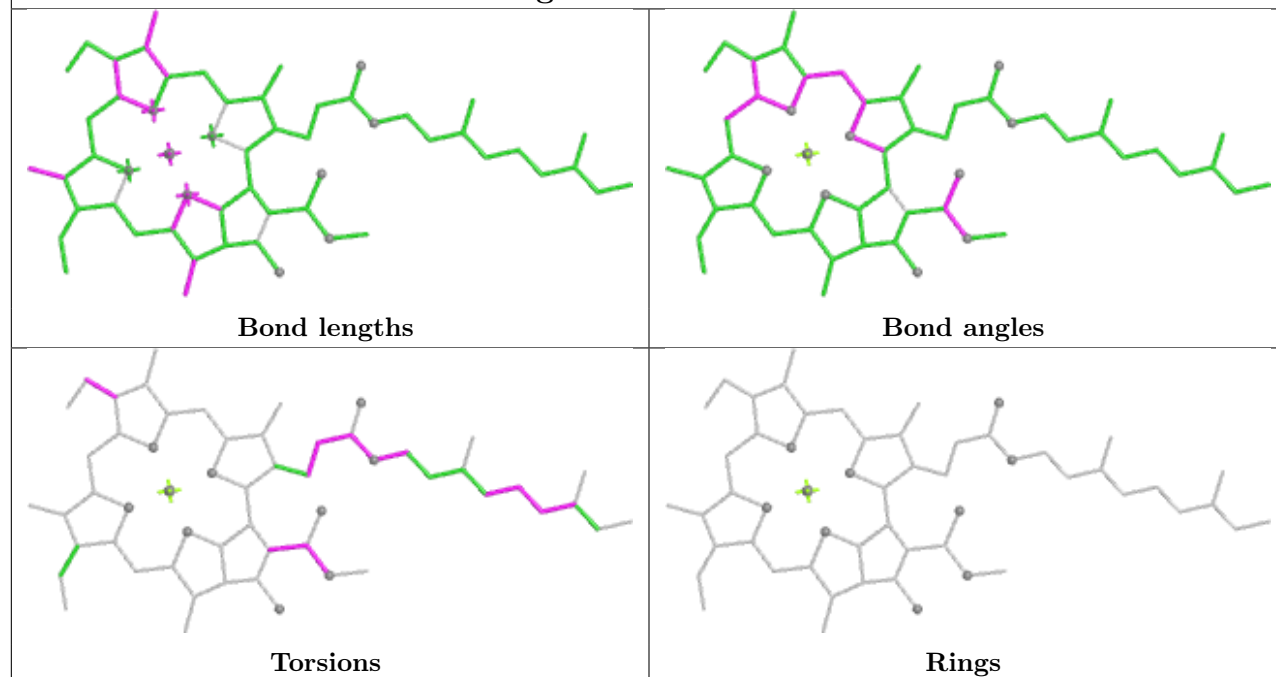
Ligand CLA B 827

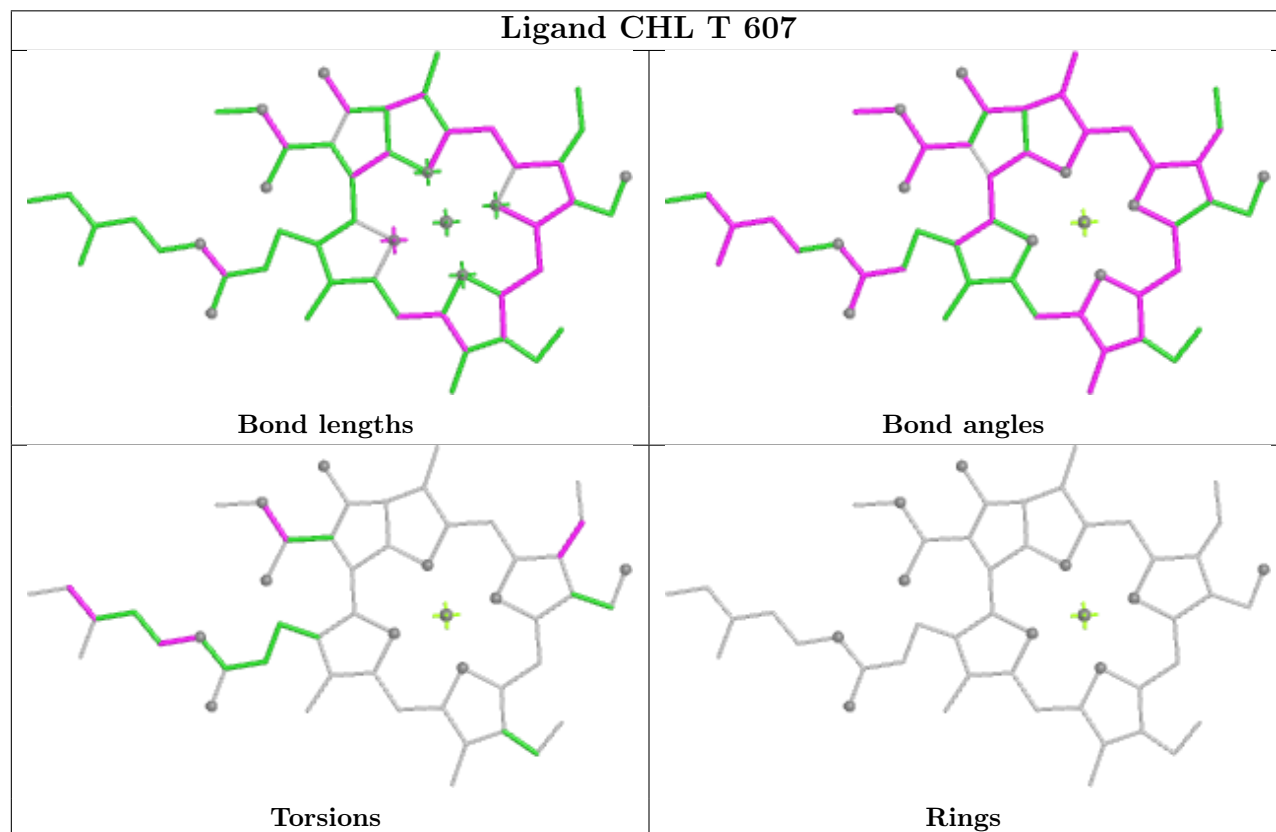
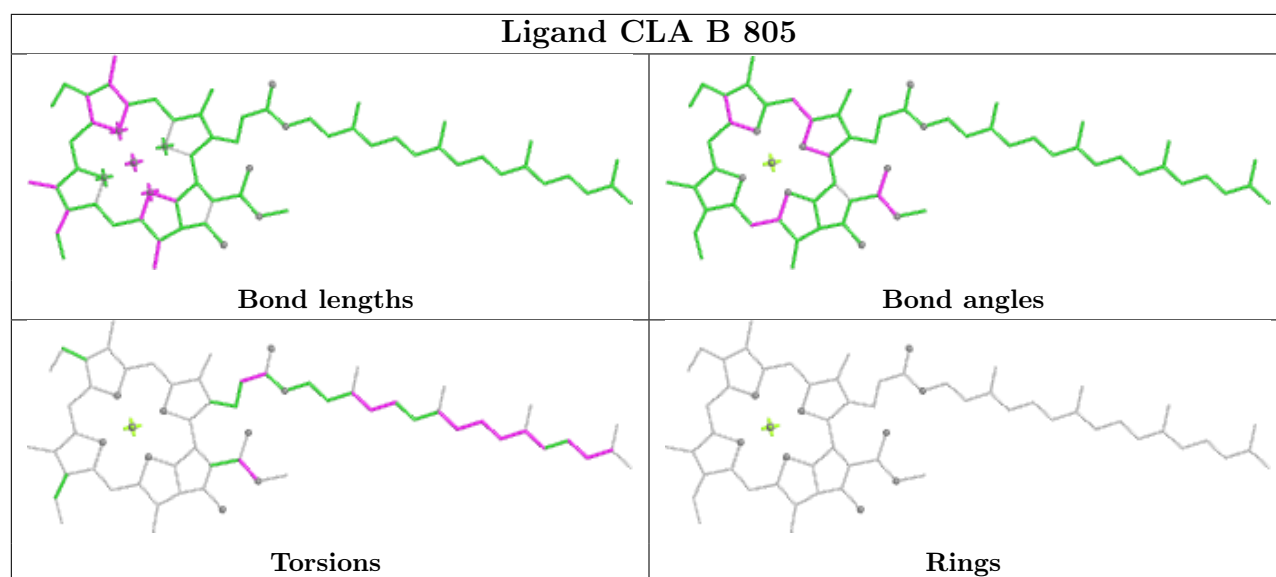


Ligand BCR G 203

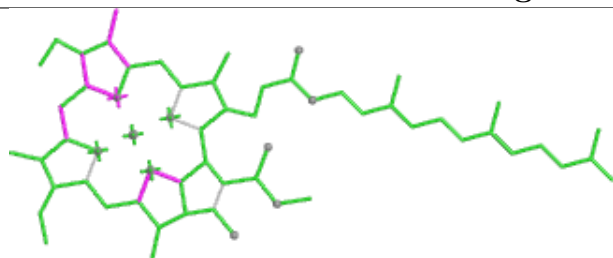


Ligand CLA 3 314

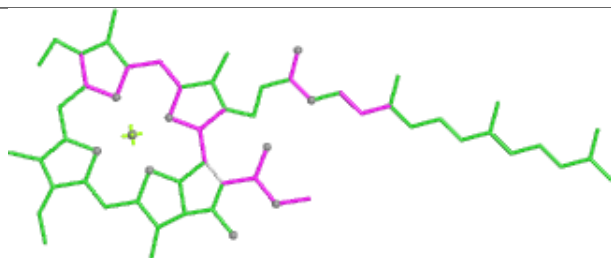




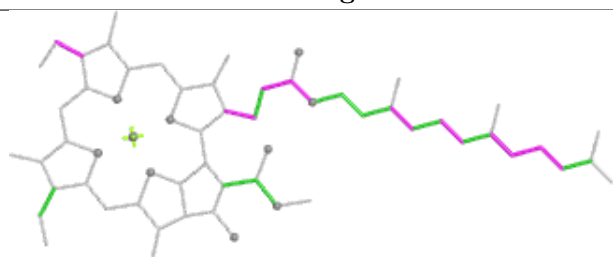
Ligand CLA T 609



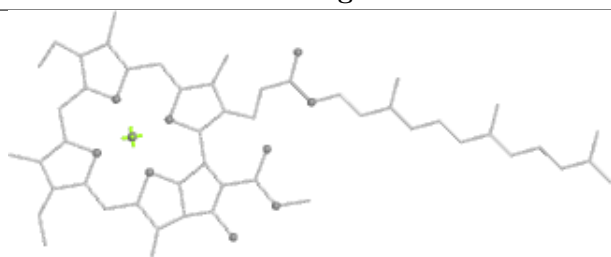
Bond lengths



Bond angles

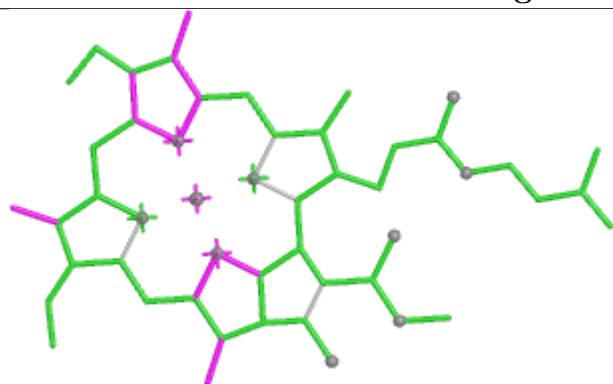


Torsions

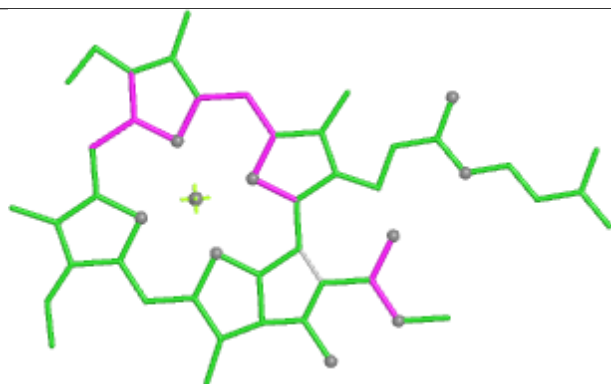


Rings

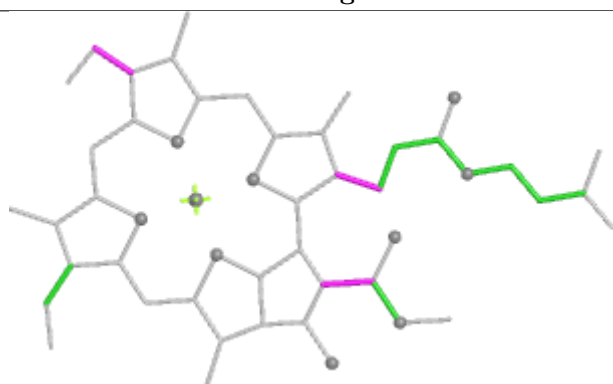
Ligand CLA B 828



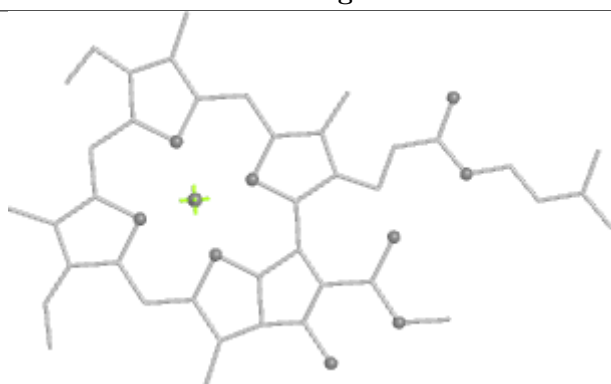
Bond lengths



Bond angles

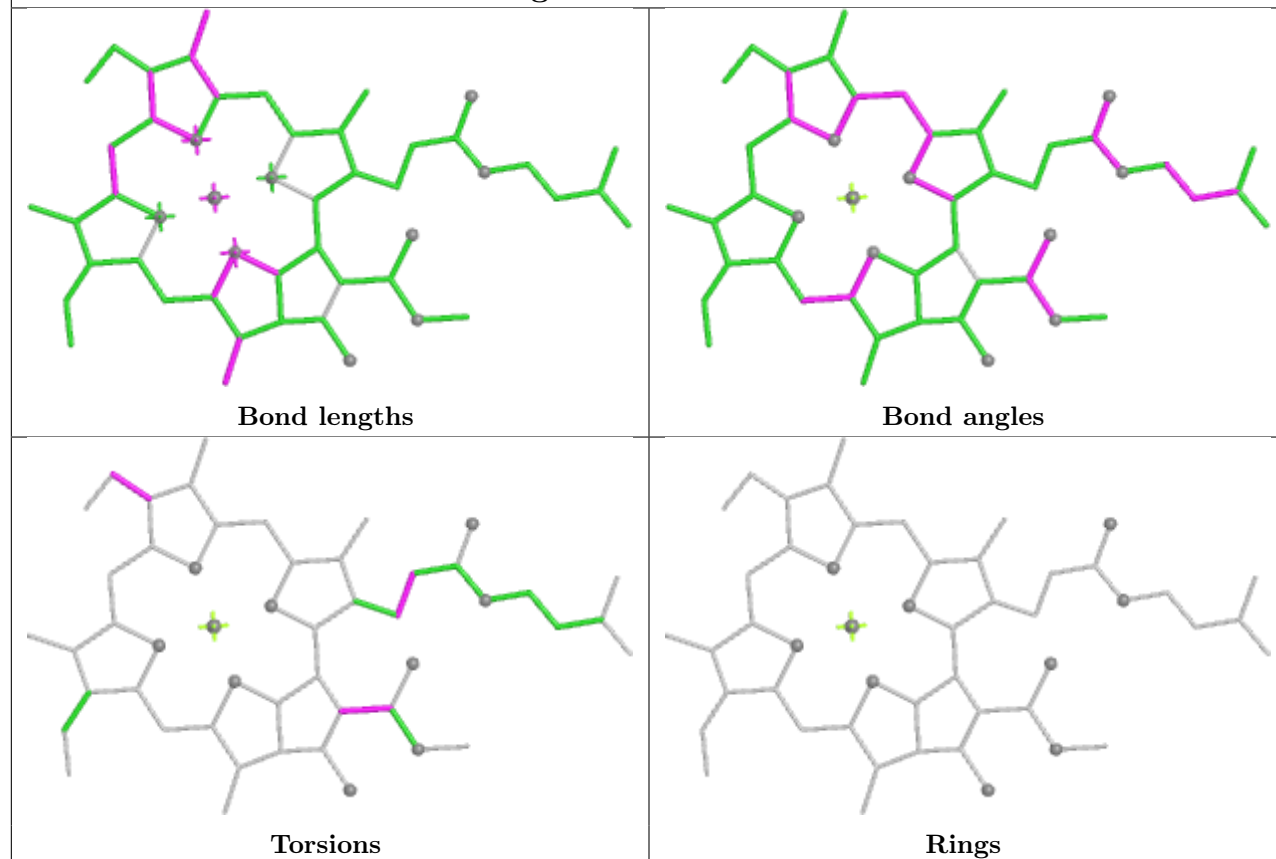


Torsions

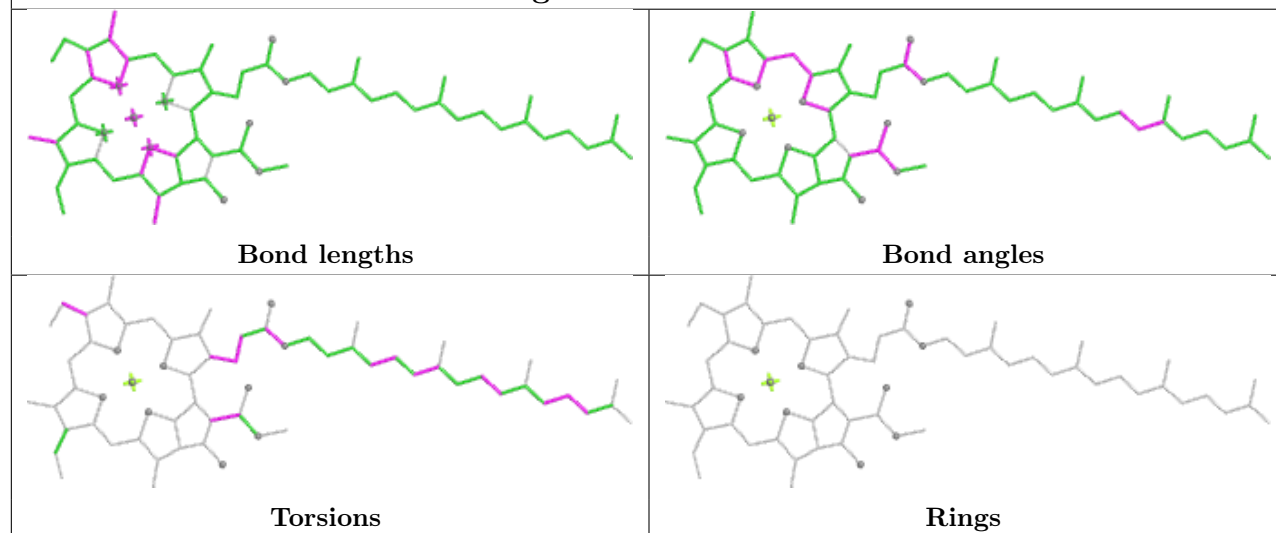


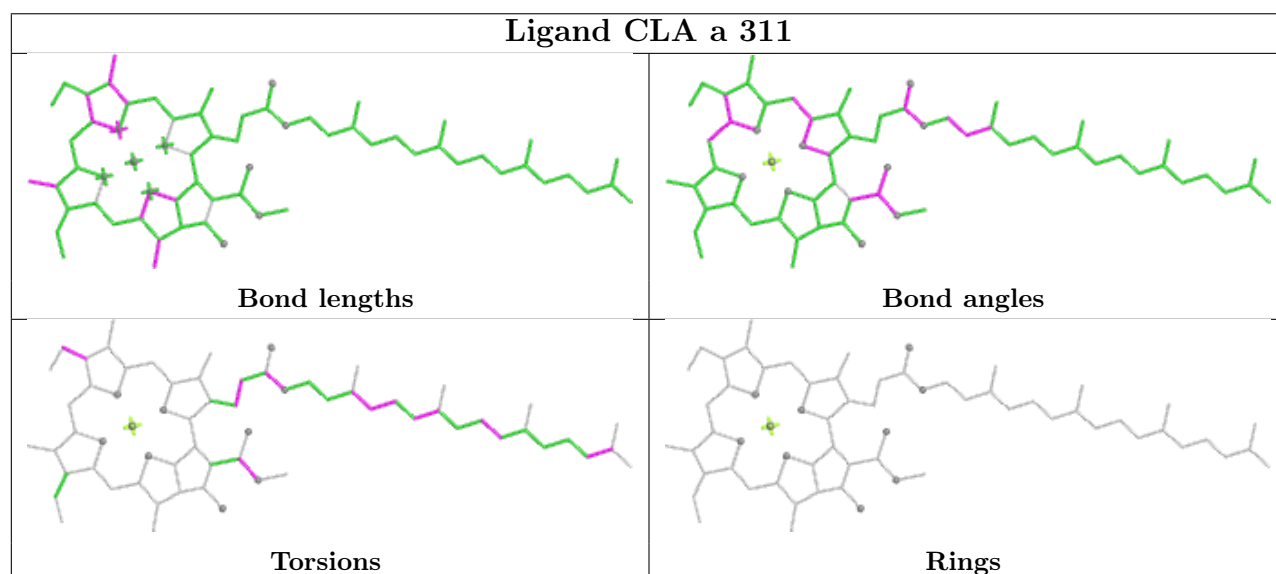
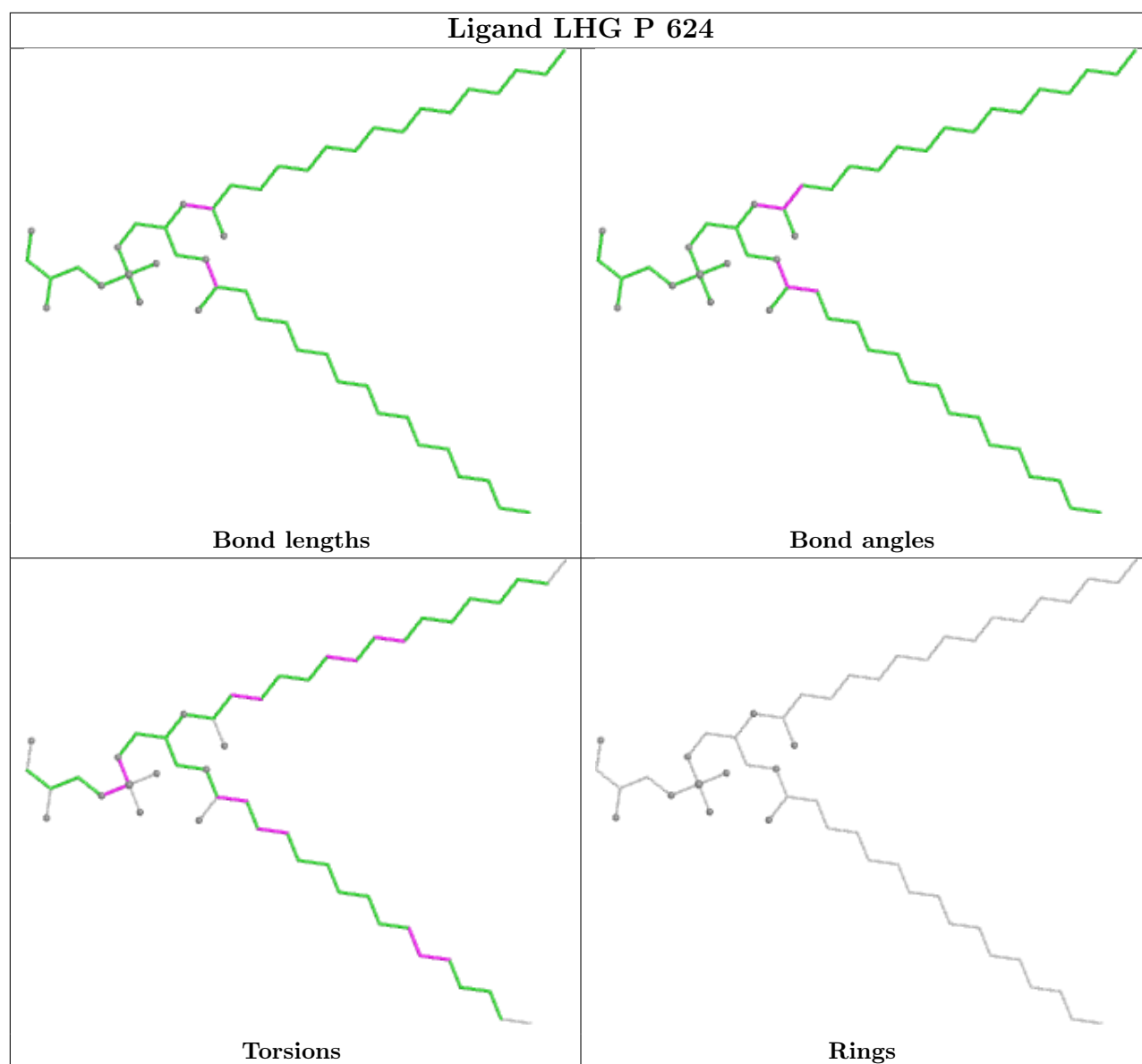
Rings

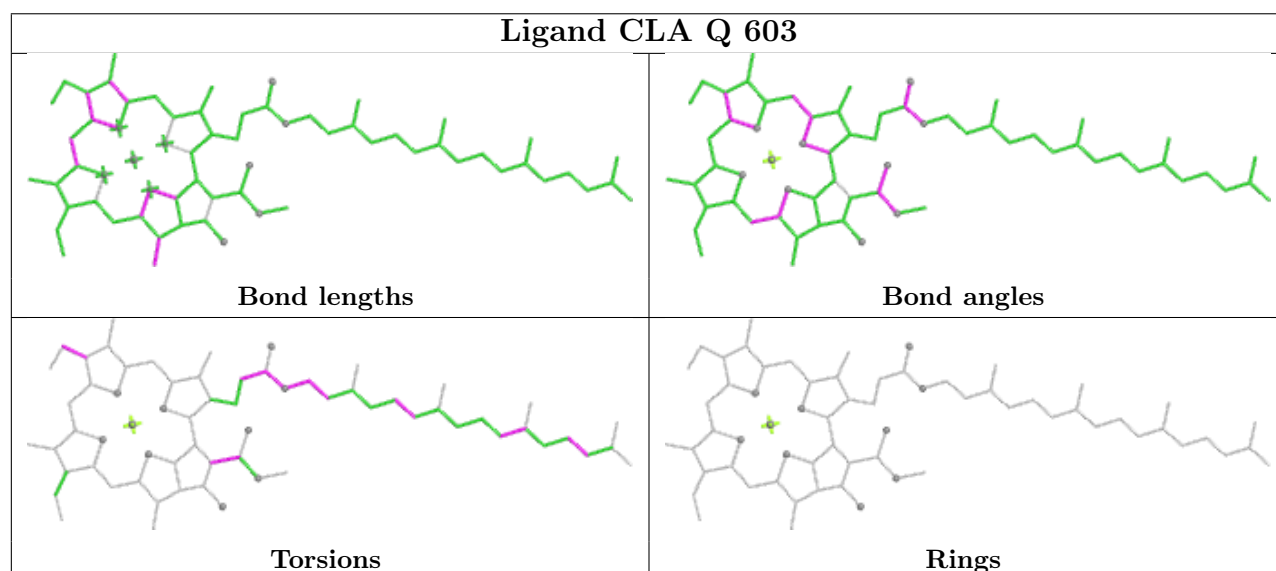
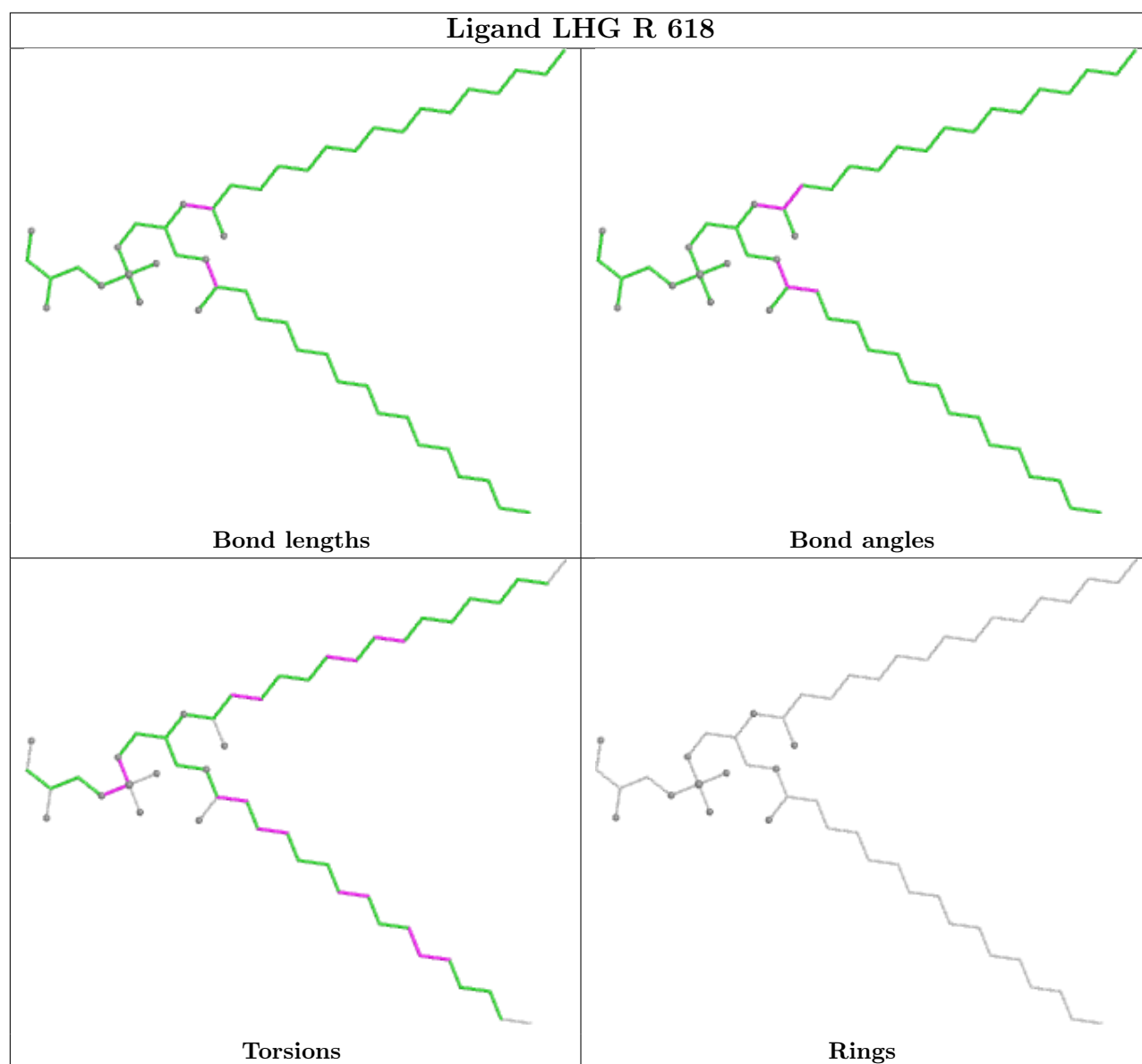
Ligand CLA G 201

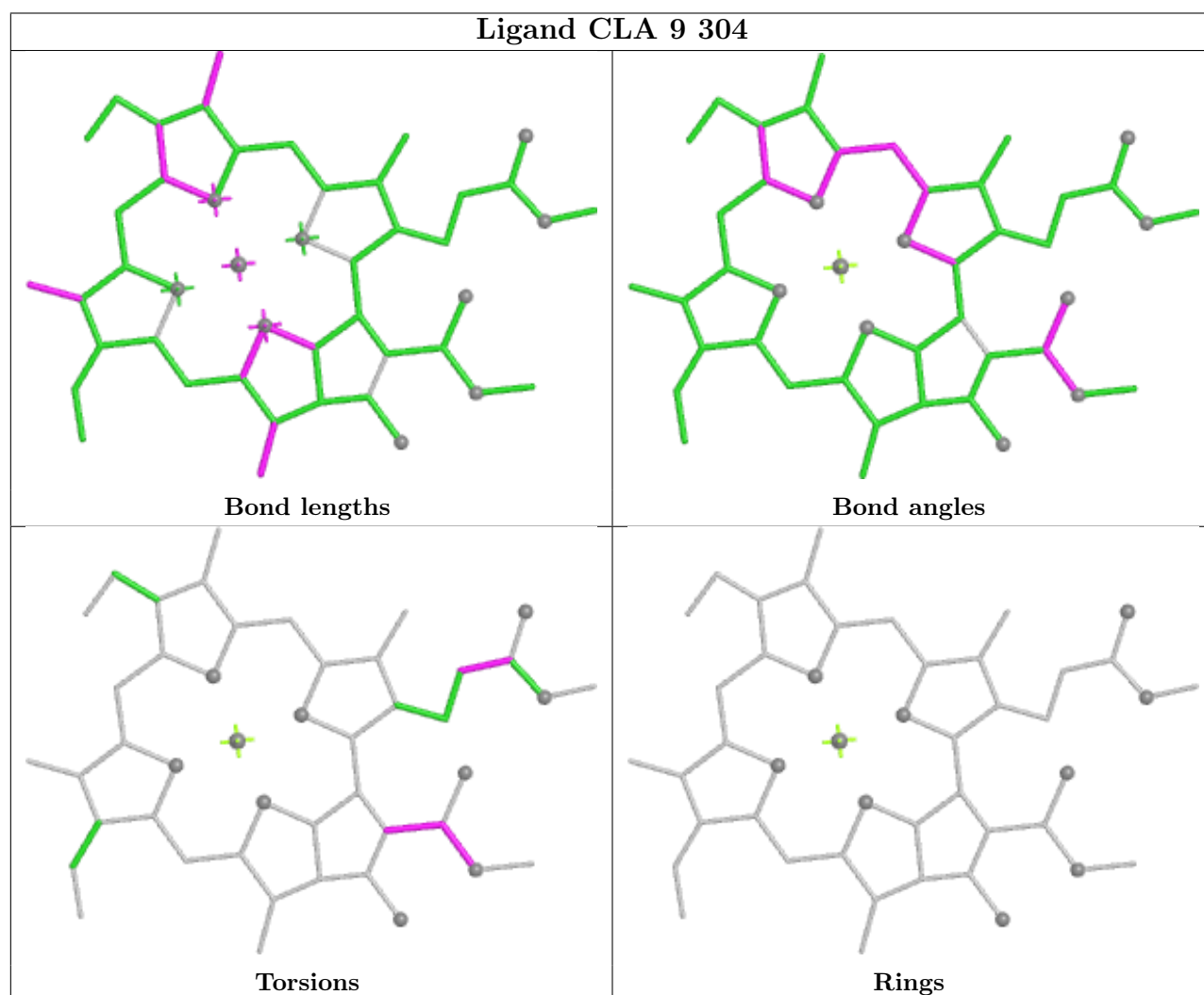
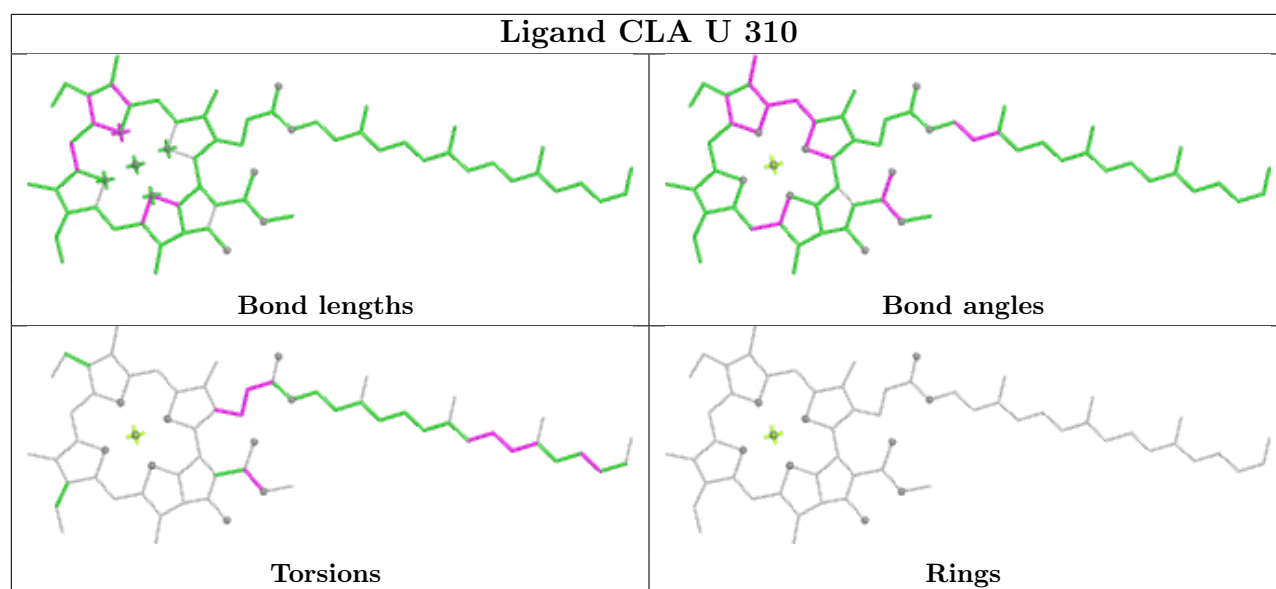


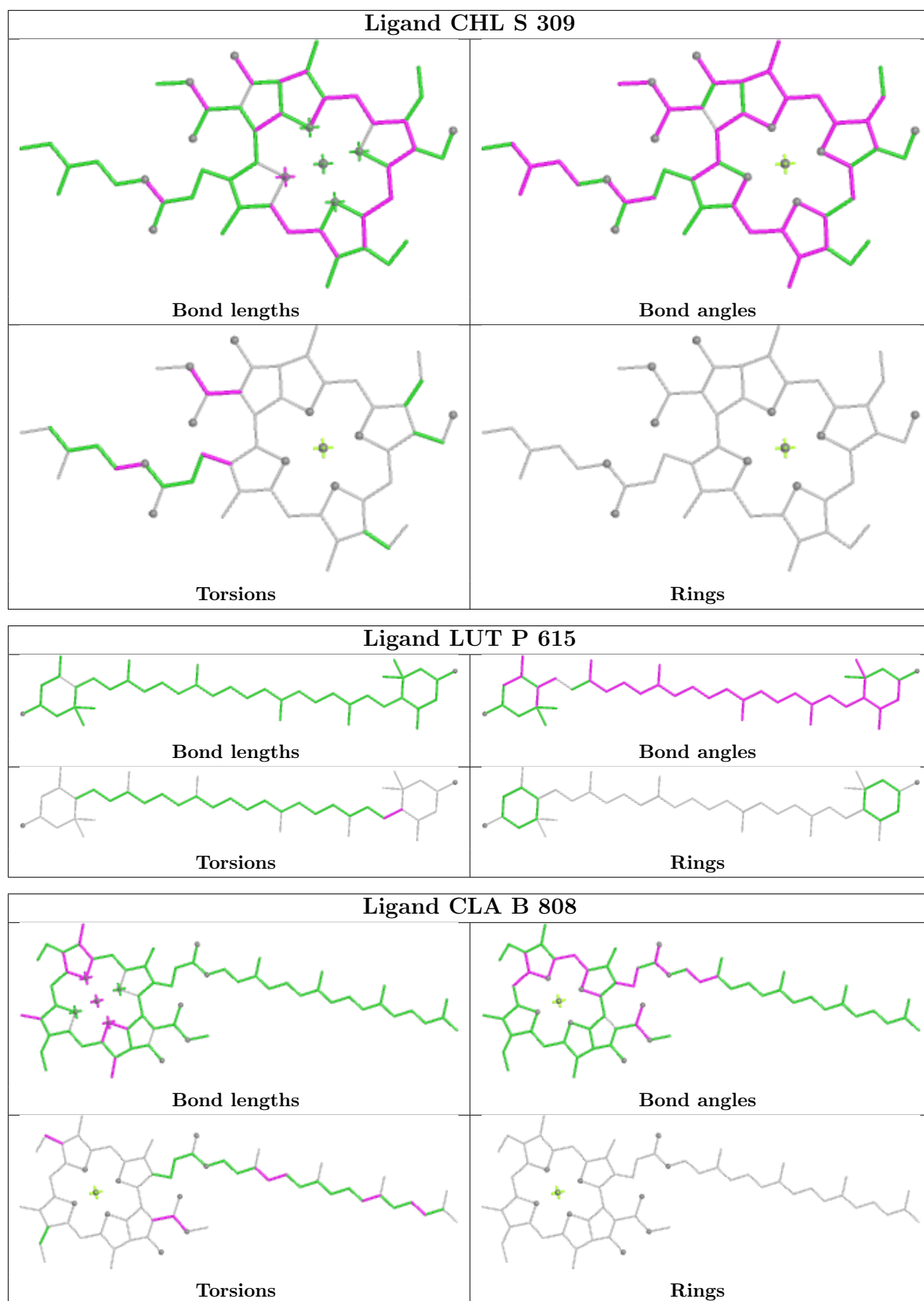
Ligand CLA B 804

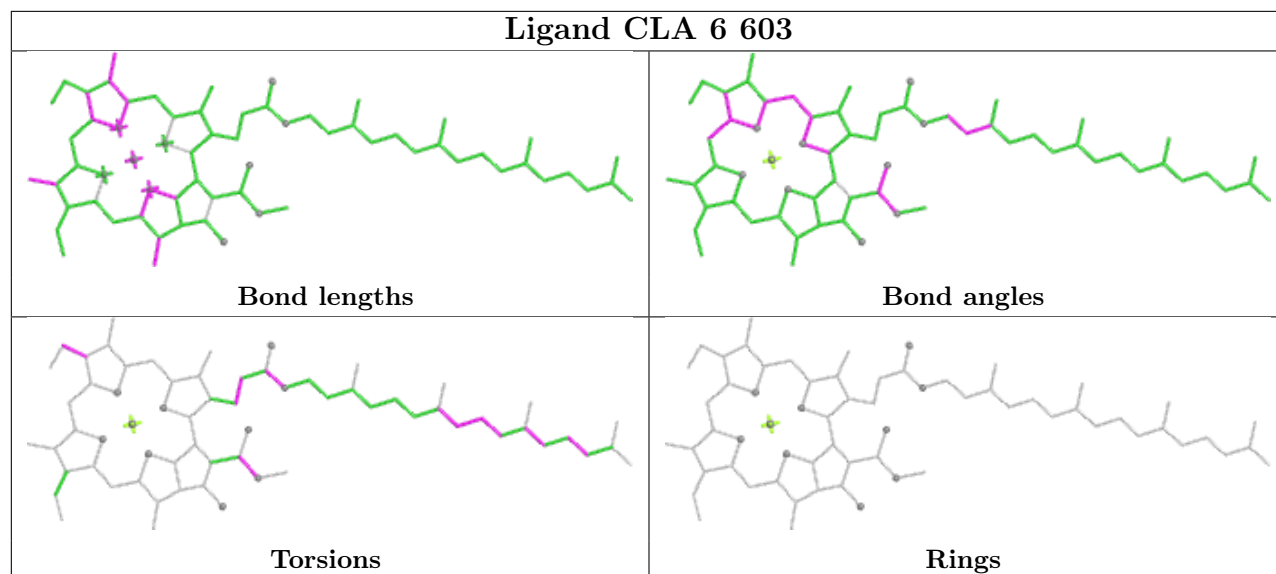
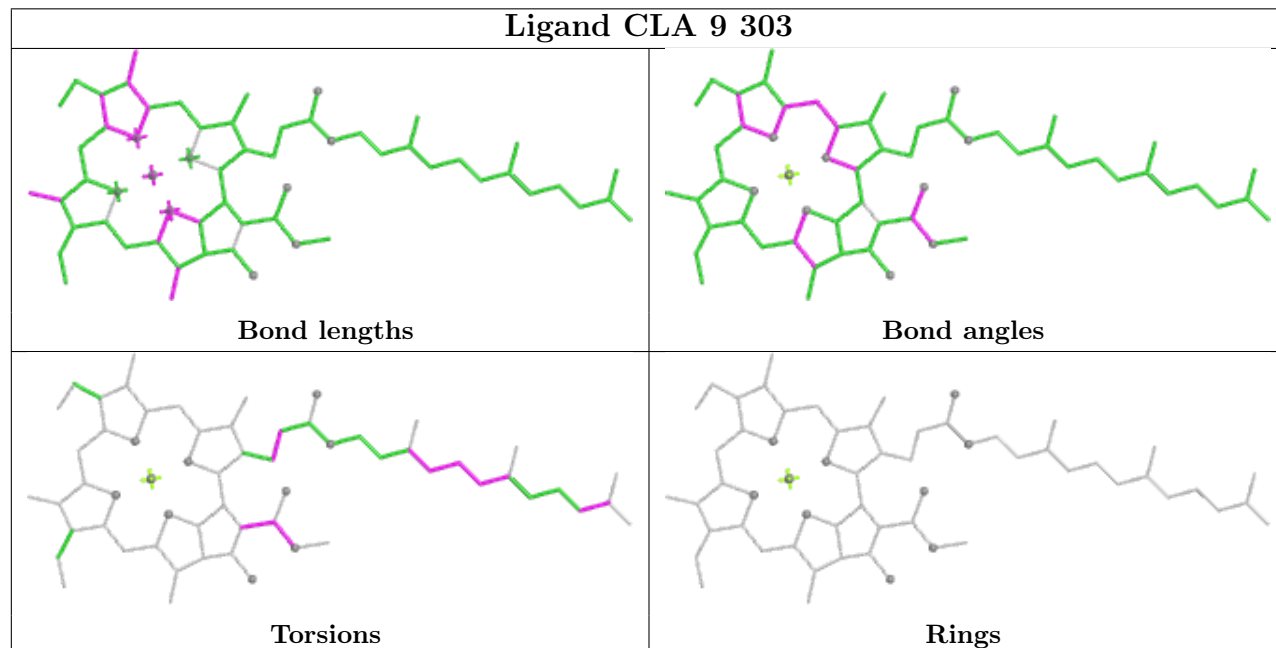


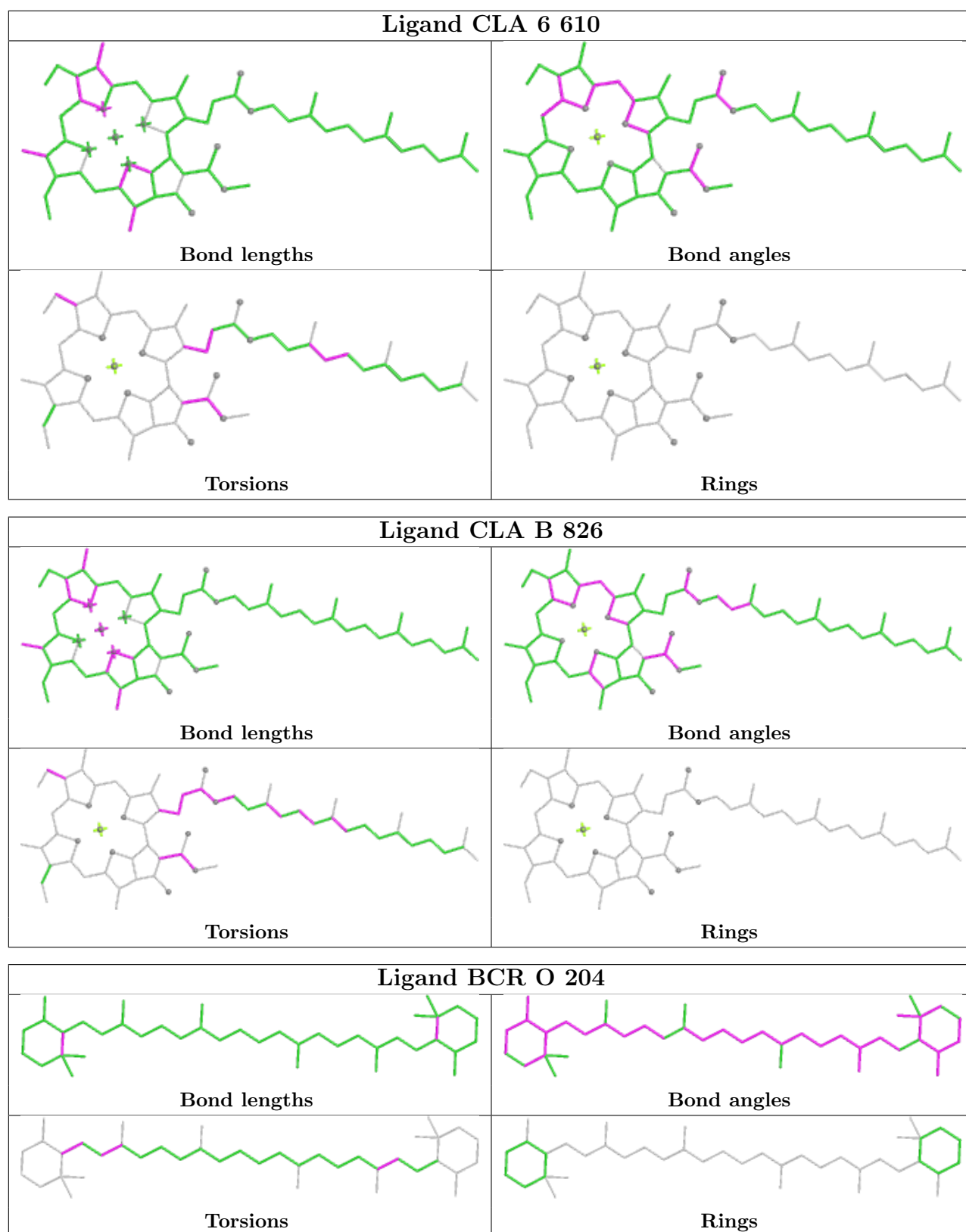


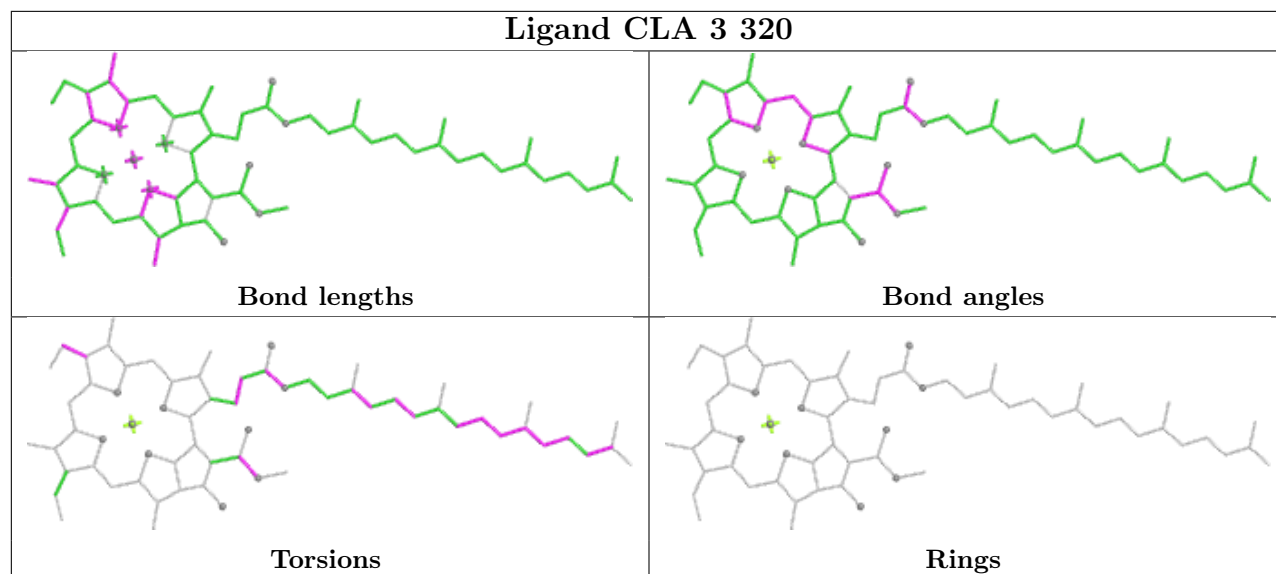
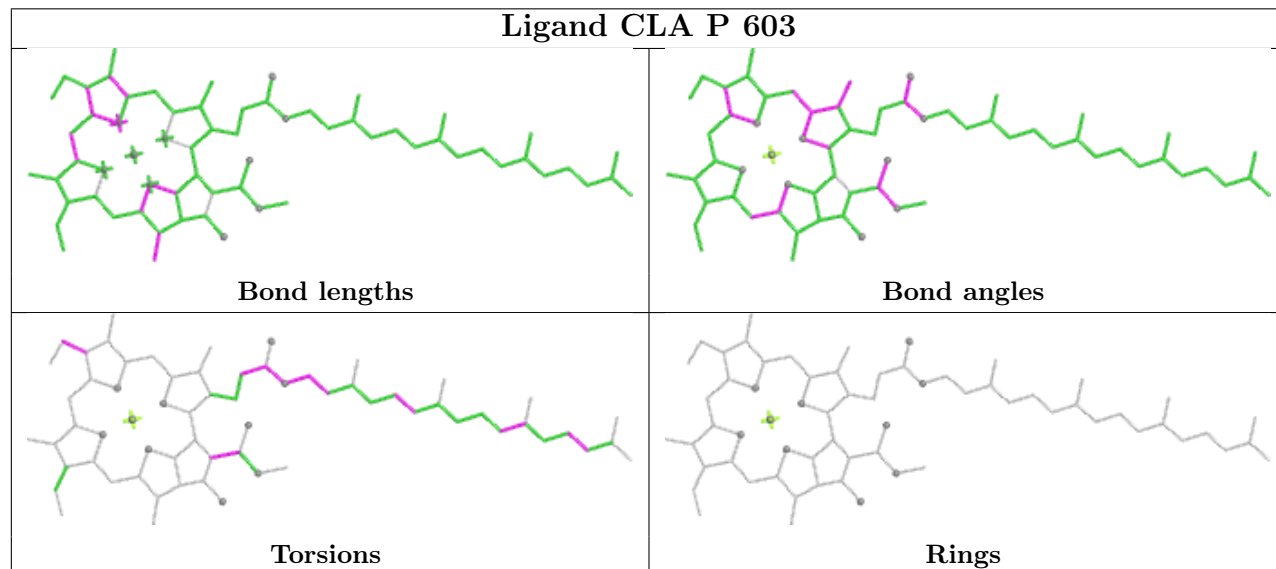




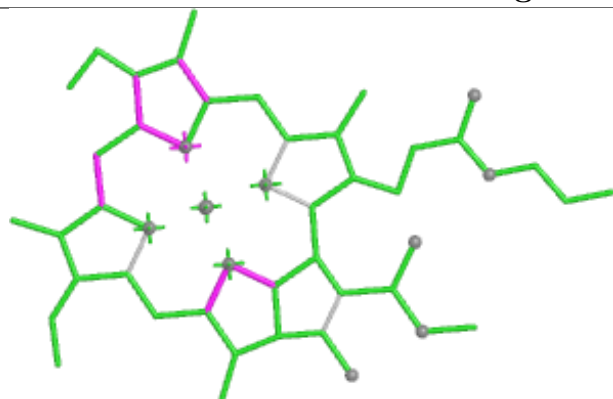


Ligand CLA 6 603**Ligand CLA 9 303**

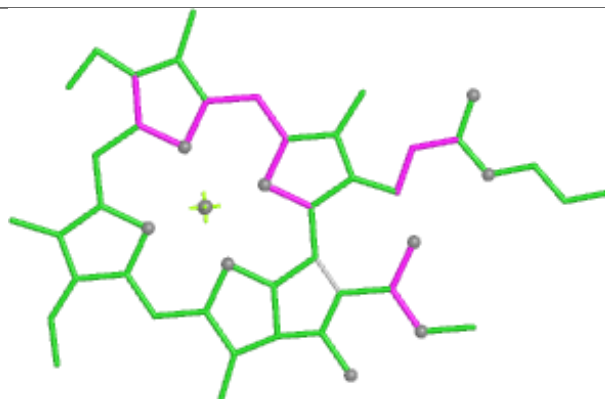


Ligand CLA 3 320**Ligand CLA P 603**

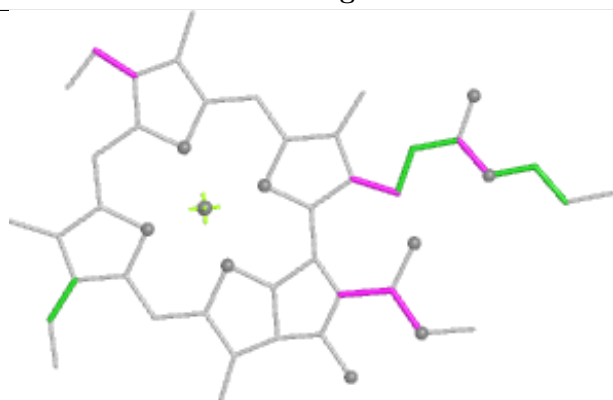
Ligand CLA T 612



Bond lengths



Bond angles

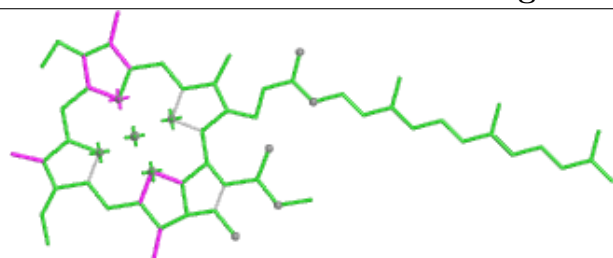


Torsions

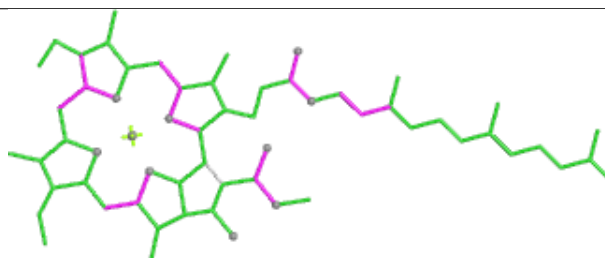


Rings

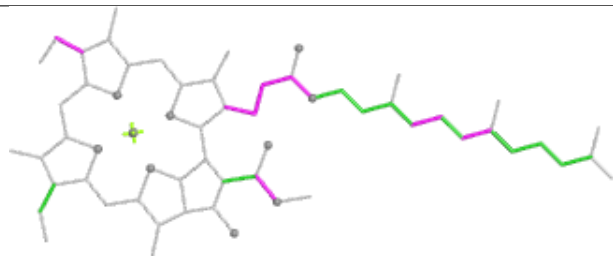
Ligand CLA 9 309



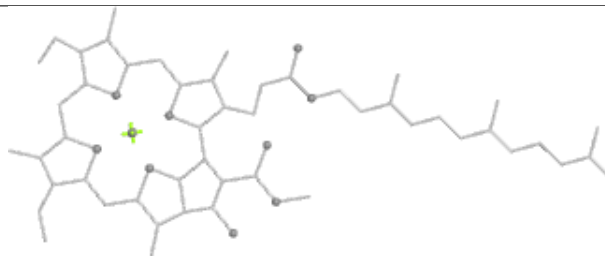
Bond lengths



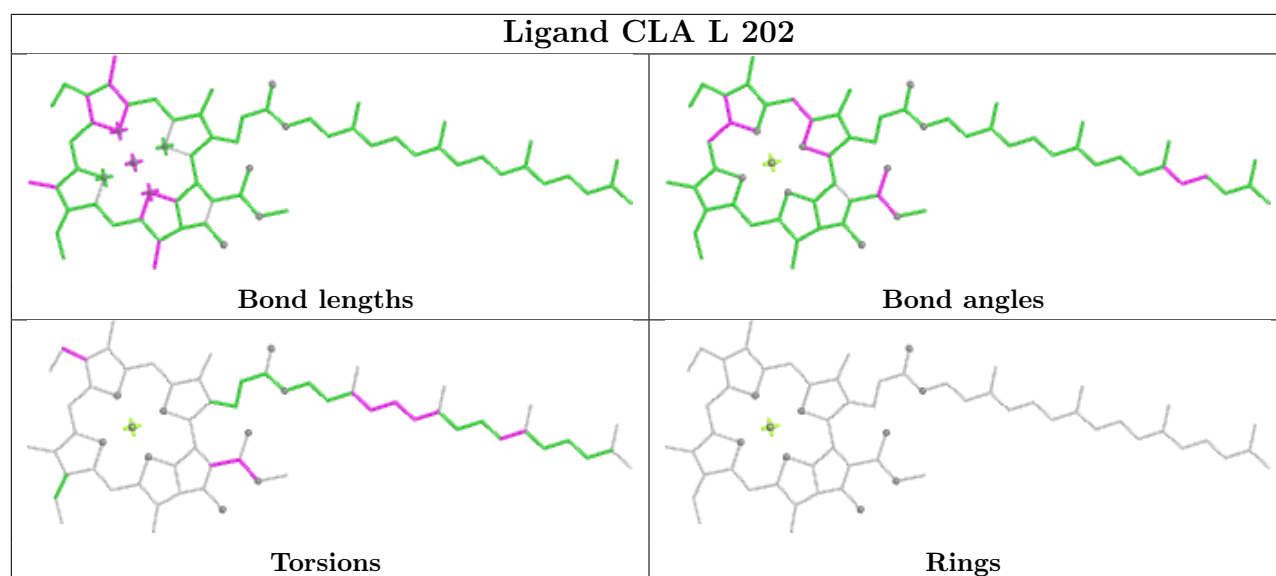
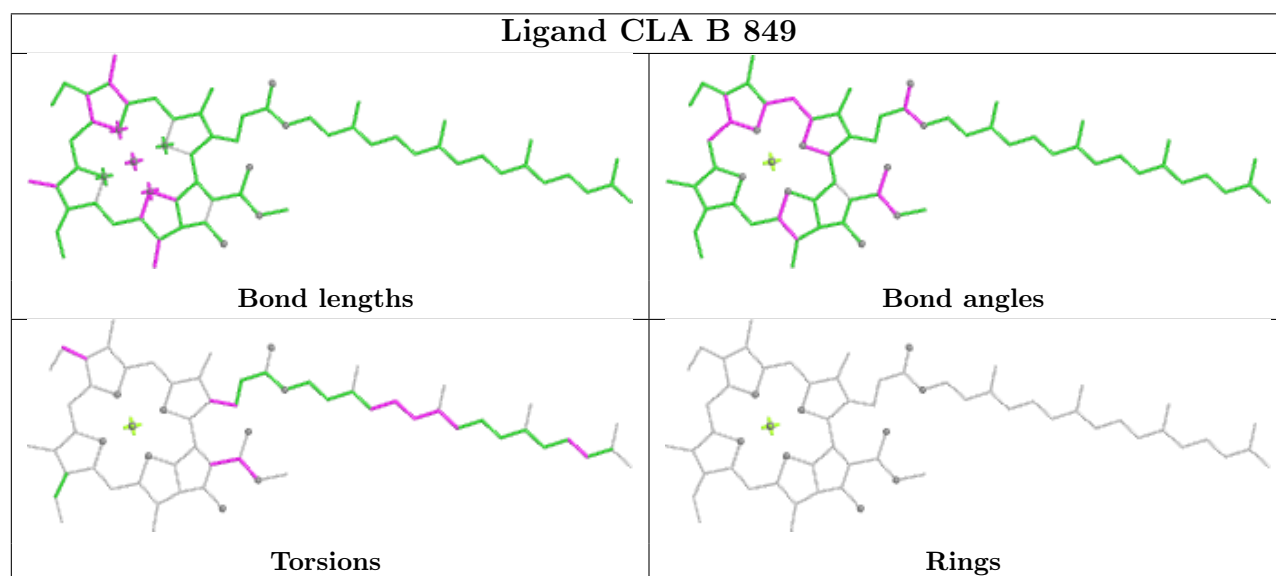
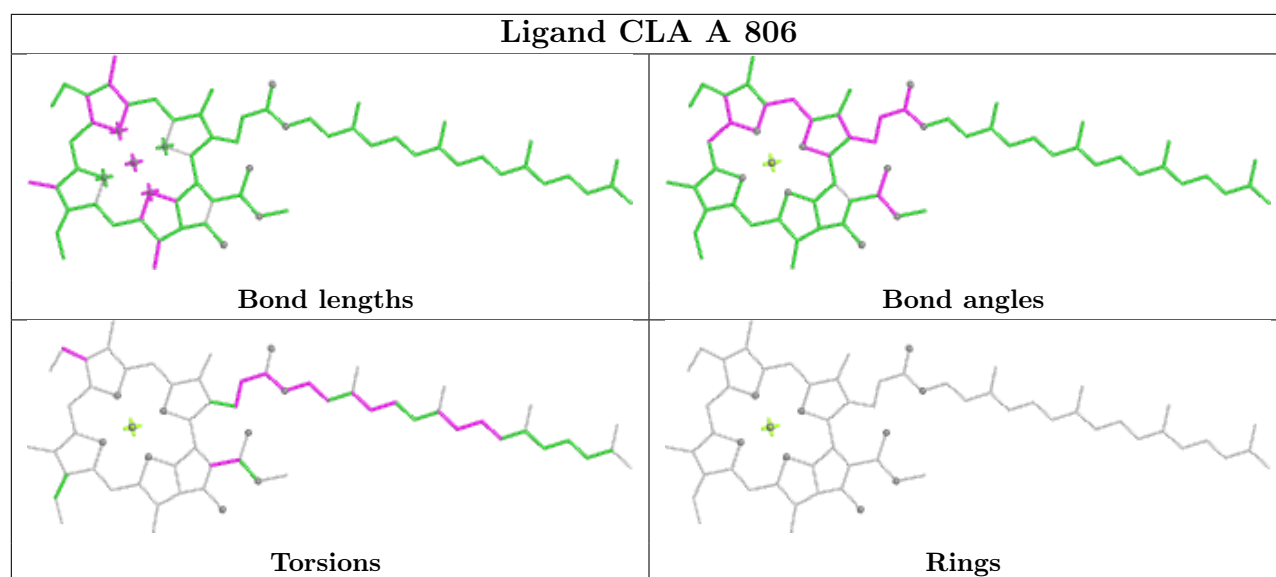
Bond angles

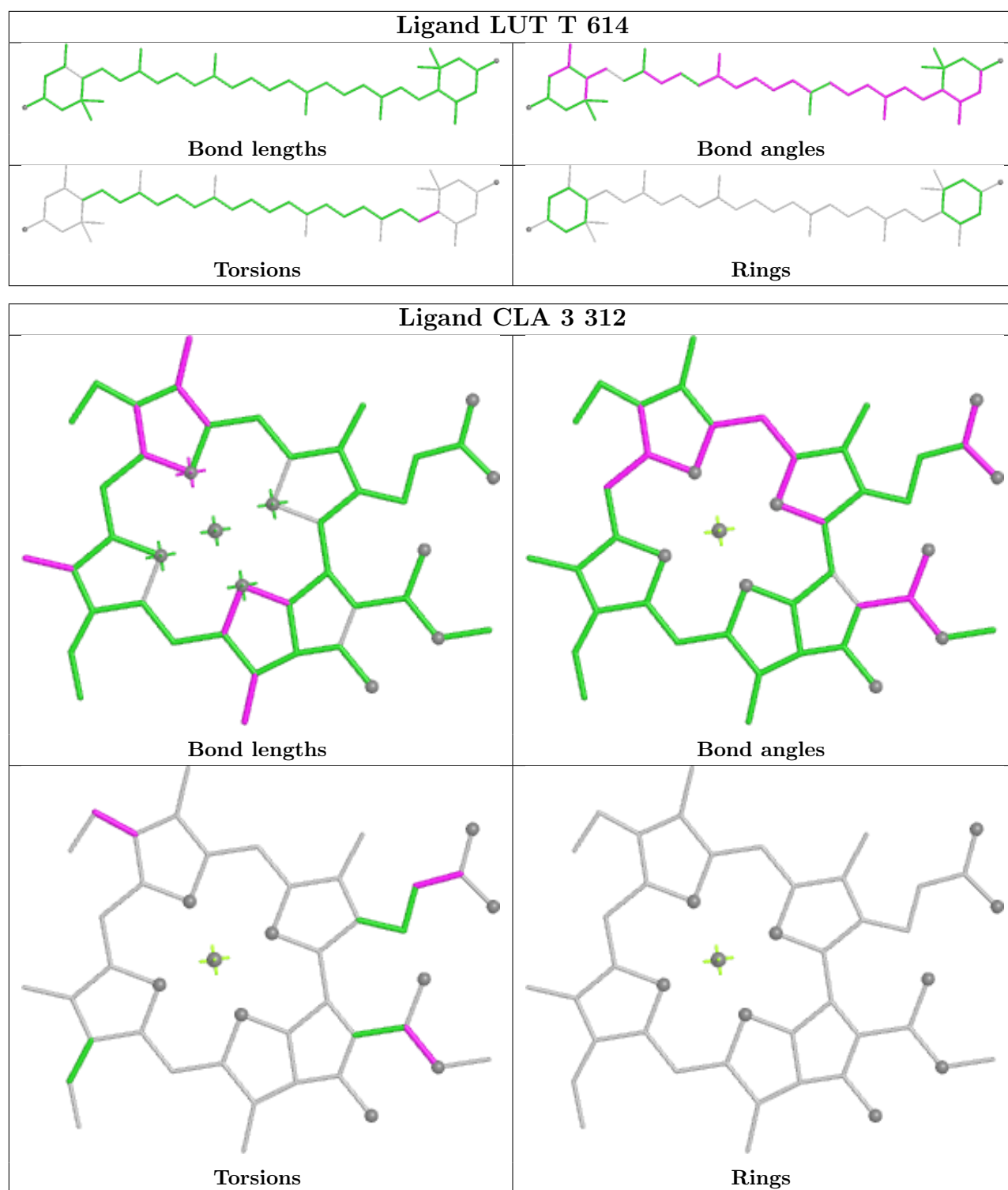


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

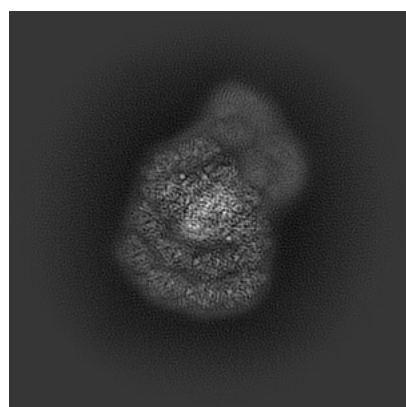
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30536. These allow visual inspection of the internal detail of the map and identification of artifacts.

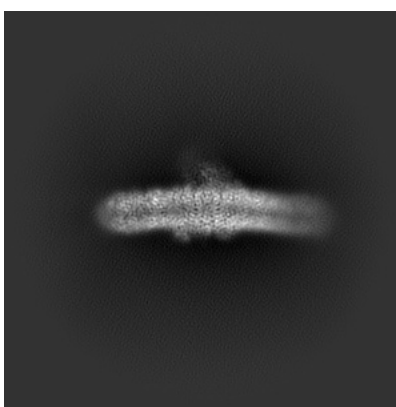
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

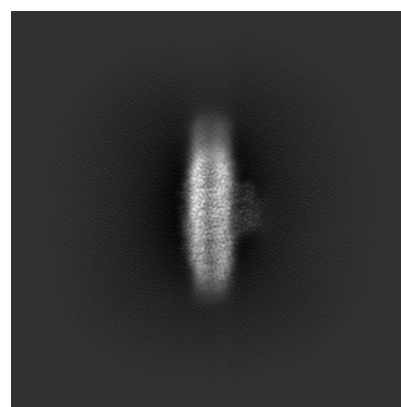
6.1.1 Primary map



X



Y

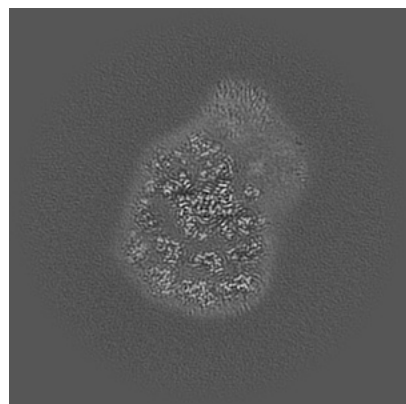


Z

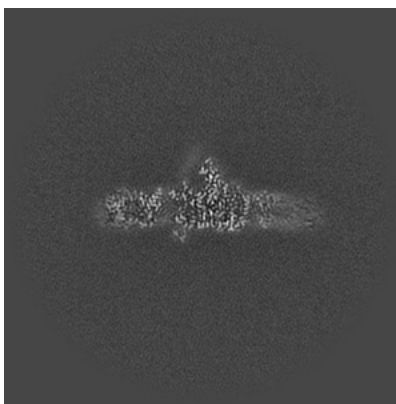
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

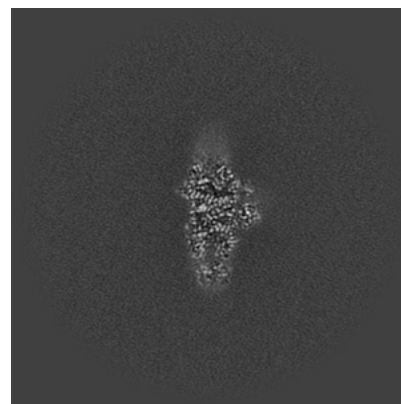
6.2.1 Primary map



X Index: 180



Y Index: 180

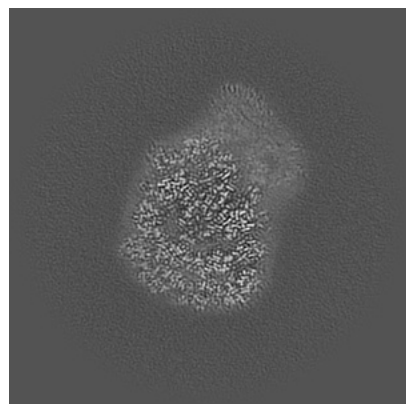


Z Index: 180

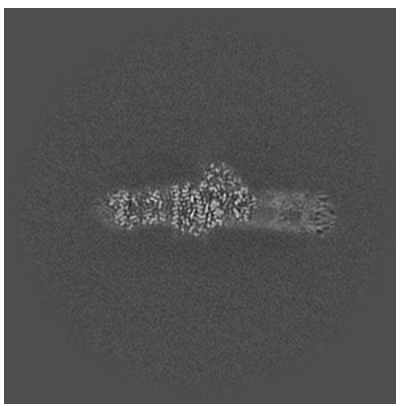
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

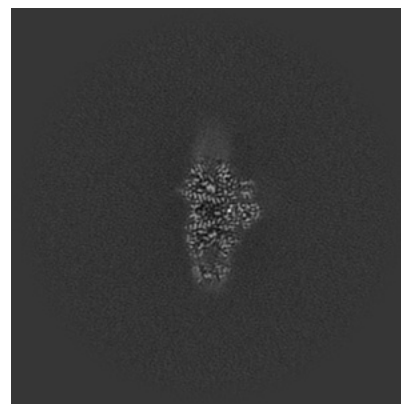
6.3.1 Primary map



X Index: 187



Y Index: 198

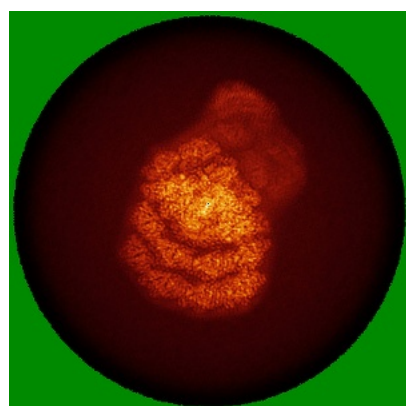


Z Index: 182

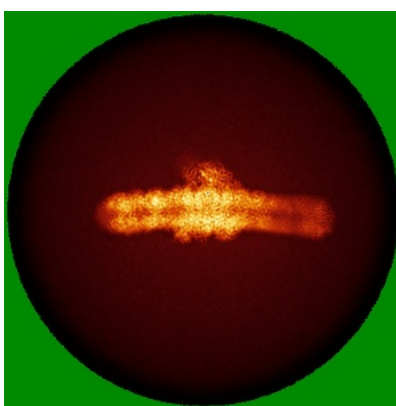
The images above show the largest variance slices of the map in three orthogonal directions.

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

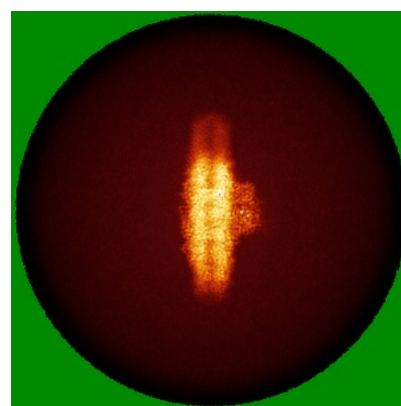
6.4.1 Primary map



X



Y

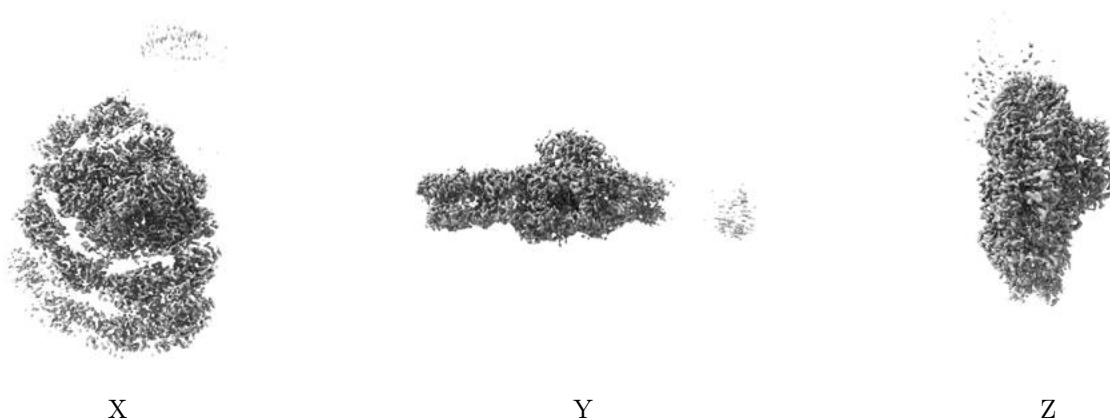


Z

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



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

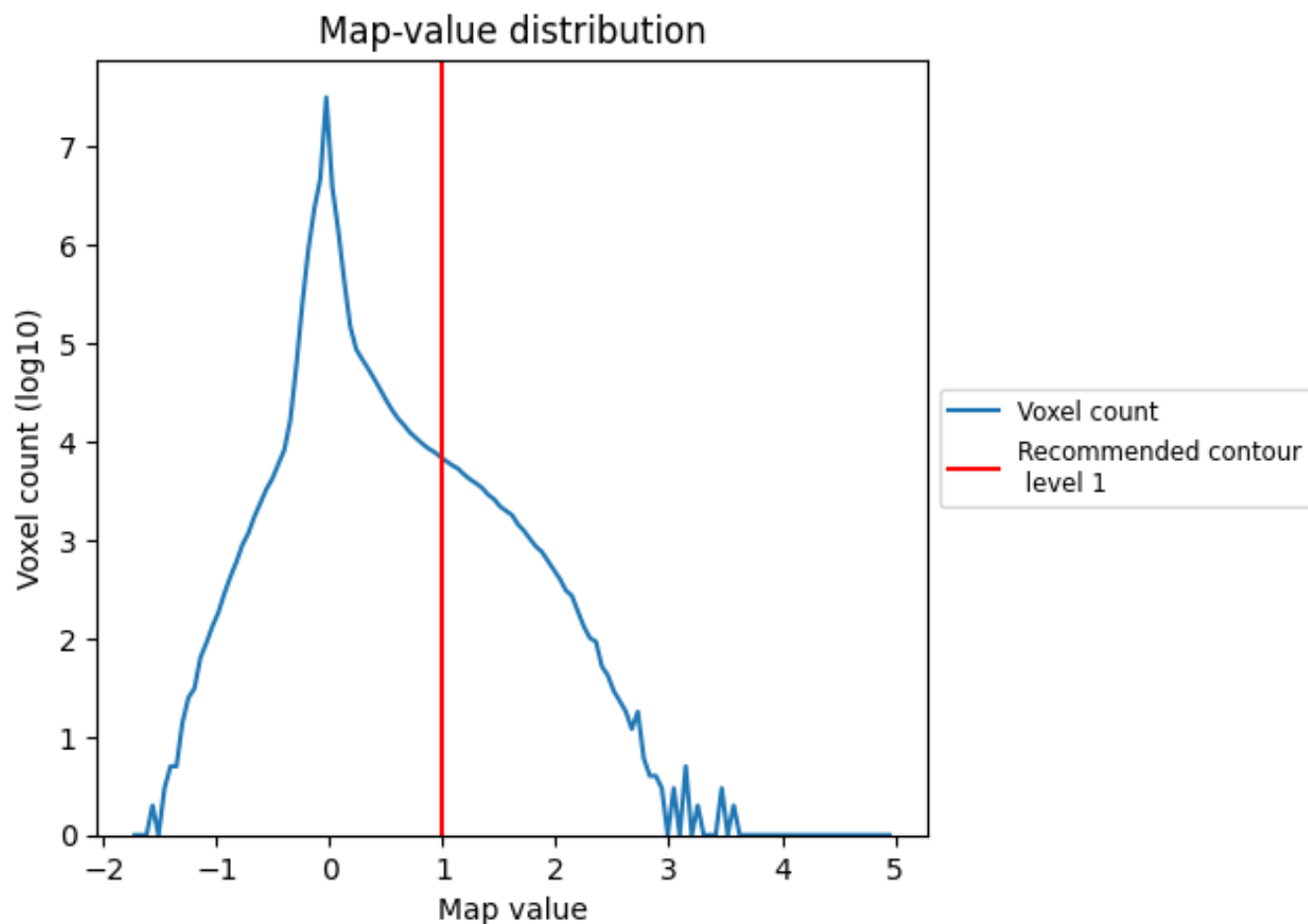
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

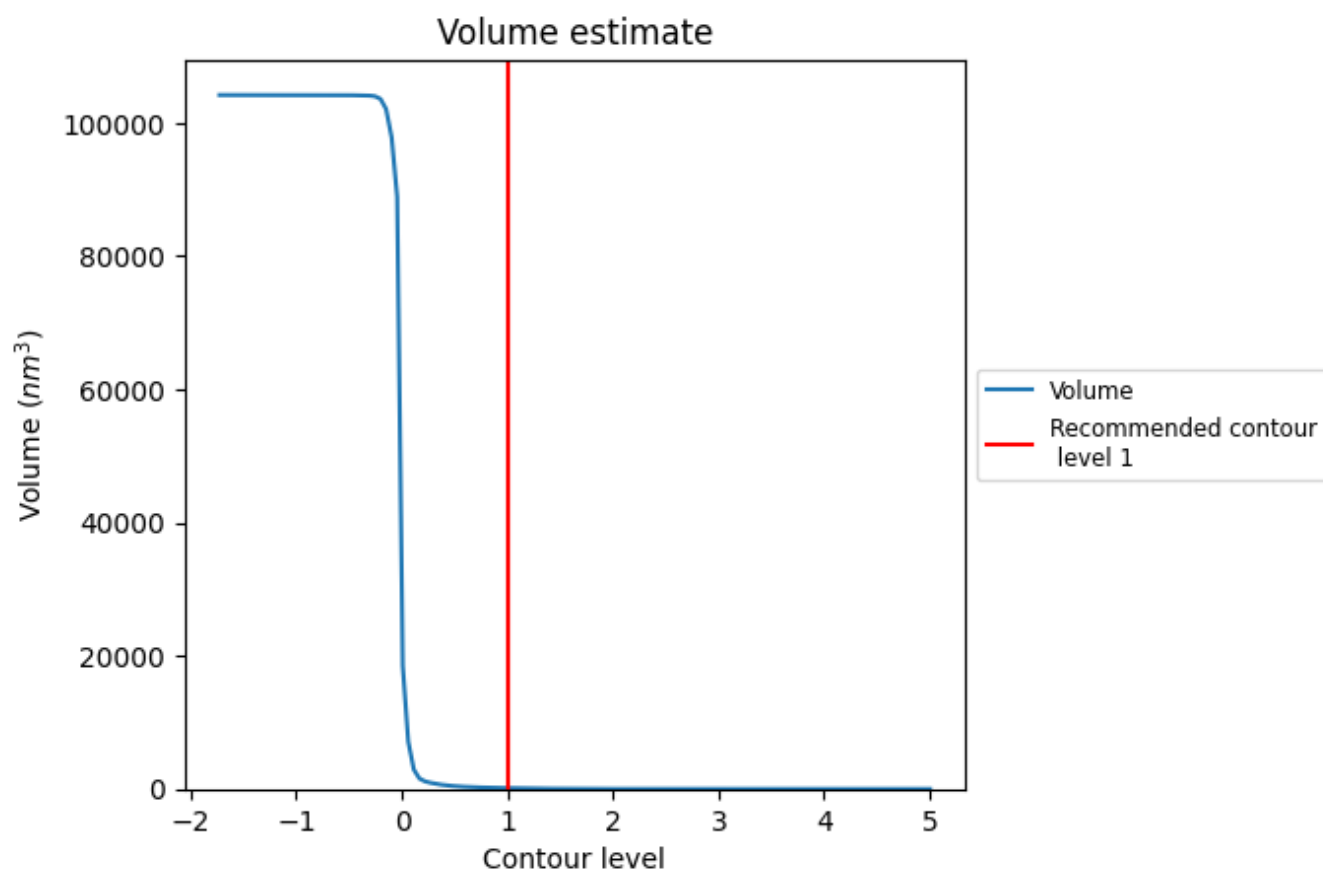
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

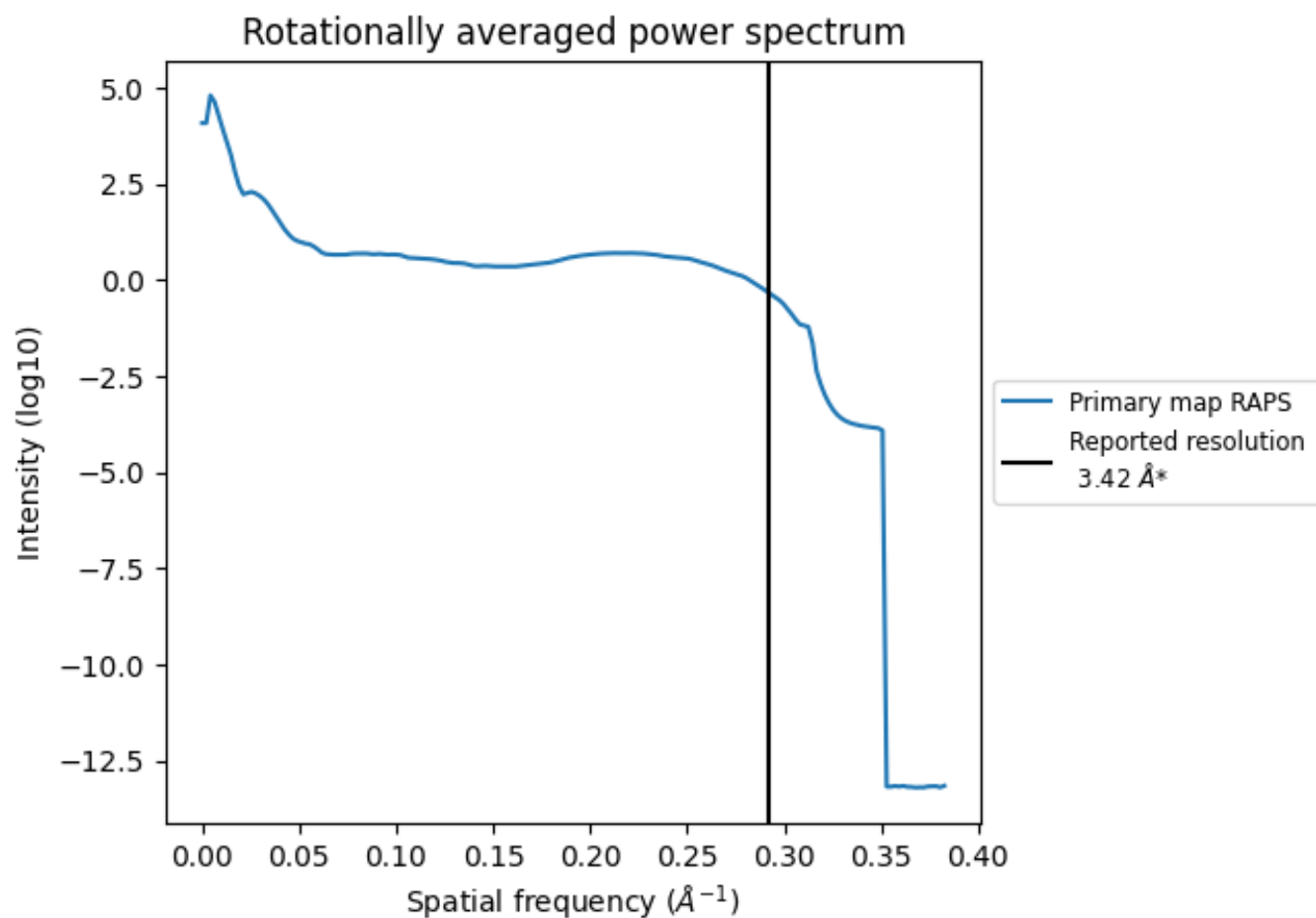
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 0.292 Å⁻¹

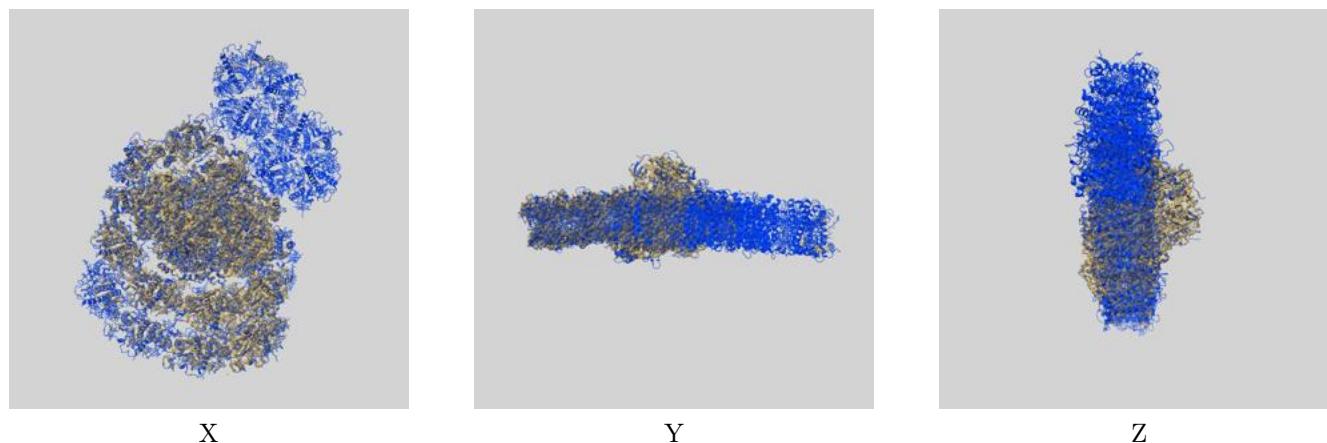
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

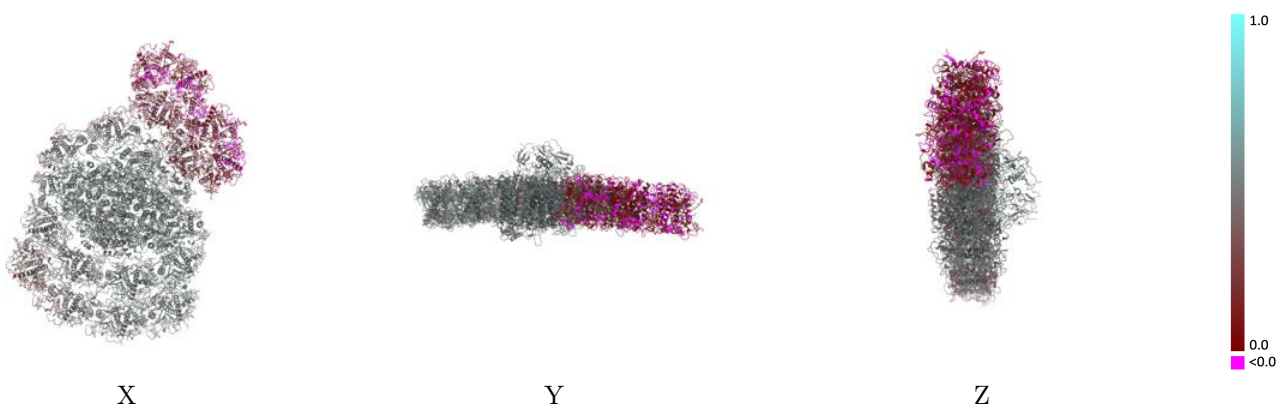
This section contains information regarding the fit between EMDB map EMD-30536 and PDB model 7D0J. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



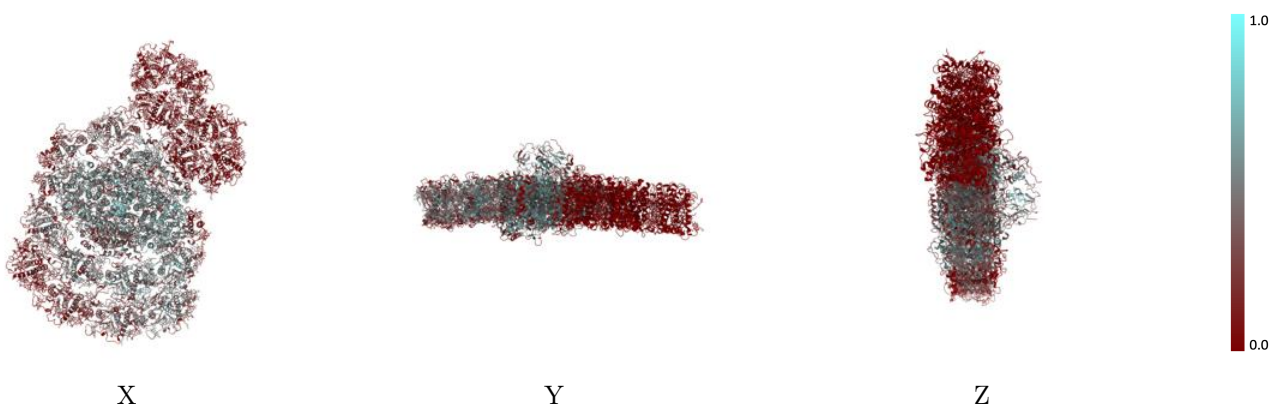
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



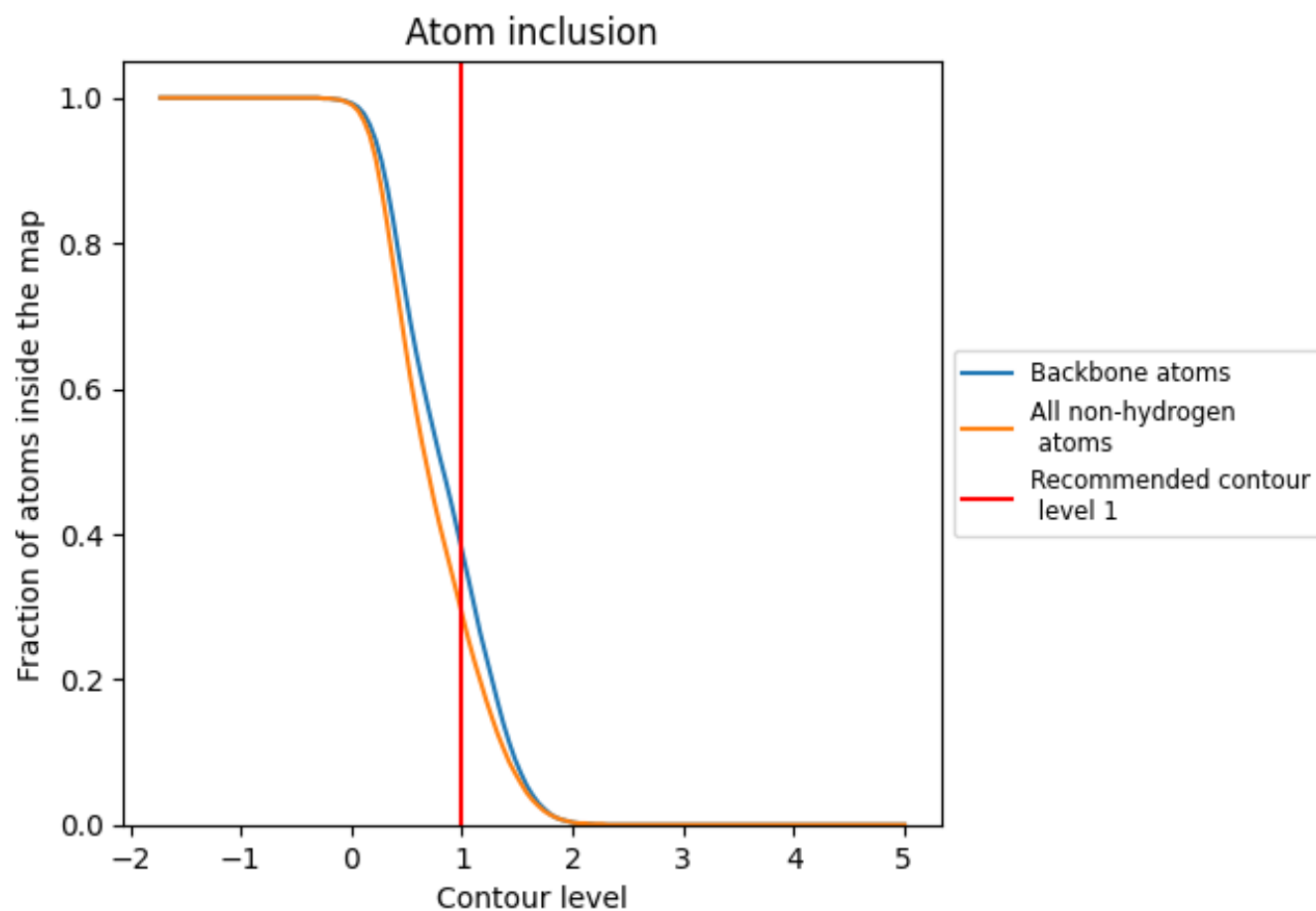
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 29% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2900	 0.4070
1	 0.3150	 0.4760
2	 0.2700	 0.4450
3	 0.4270	 0.5110
4	 0.1240	 0.4380
5	 0.3910	 0.4980
6	 0.2670	 0.4690
7	 0.4370	 0.5110
8	 0.3670	 0.4930
9	 0.2290	 0.4440
A	 0.5310	 0.5300
B	 0.5200	 0.5290
C	 0.5710	 0.5210
D	 0.3740	 0.5140
E	 0.3710	 0.5020
F	 0.2700	 0.4750
G	 0.1380	 0.4410
H	 0.3030	 0.4750
I	 0.4730	 0.5110
J	 0.2900	 0.5190
K	 0.1580	 0.4560
L	 0.4360	 0.5030
O	 0.3060	 0.4670
P	 0.0000	 0.1620
Q	 0.0020	 0.0510
R	 0.0050	 0.0630
S	 0.0030	 0.2360
T	 0.0000	 0.1130
U	 0.0000	 0.1020
a	 0.0570	 0.3750

