



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:35 PM UTC

PDB ID : 8CMO / pdb_00008cmo
EMDB ID : EMD-16732
Title : Cryo-EM structure of the Photosystem I - LHCI supercomplex from Coelastrella sp.
Authors : Fadeeva, M.; Klaiman, D.; Nelson, N.
Deposited on : 2023-02-20
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

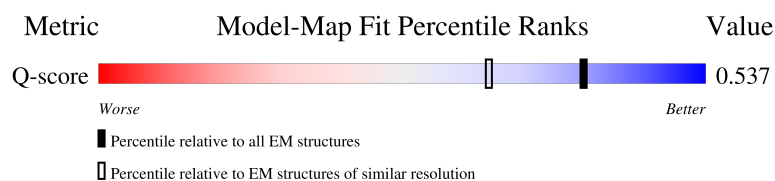
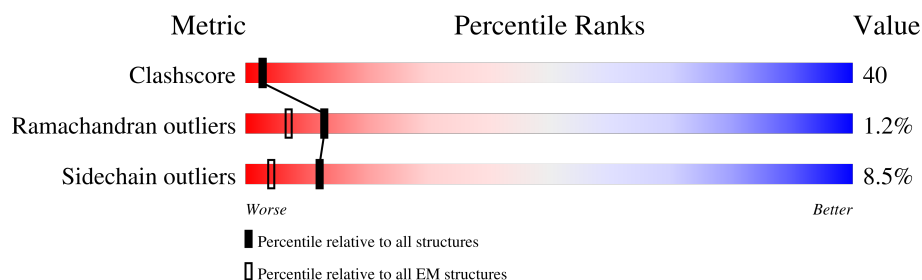
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 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	11740 (2.31 - 3.31)

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	 59% 39% .
2	B	732	 53% 44% .
3	C	80	 48% 51% .
4	D	142	 8% 55% 41% . .

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Mol	Chain	Length	Quality of chain
5	E	61	
6	F	165	
7	G	93	
8	I	41	
9	J	40	
10	K	89	
11	L	123	
12	1	194	
12	Z	194	
13	3	218	
14	7	220	
15	8	214	
16	4	207	
17	5	226	
18	6	226	
19	9	184	
20	2	70	

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
21	CL0	A	801	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	311	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	1	314	X	-	-	-
22	CLA	1	315	X	-	-	-
22	CLA	1	316	X	-	-	-
22	CLA	2	301	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	X	-
22	CLA	3	313	X	-	X	-
22	CLA	3	314	X	-	-	-
22	CLA	3	315	X	-	-	-
22	CLA	3	316	X	-	-	-
22	CLA	3	318	X	-	-	-
22	CLA	3	319	X	-	-	-
22	CLA	3	320	X	-	-	-
22	CLA	3	322	X	-	-	-
22	CLA	4	805	X	-	-	-
22	CLA	4	806	X	-	-	-
22	CLA	4	807	X	-	-	-
22	CLA	4	808	X	-	-	-
22	CLA	4	809	X	-	-	-
22	CLA	4	810	X	-	-	-
22	CLA	4	811	X	-	-	-
22	CLA	4	812	X	-	-	-
22	CLA	4	815	X	-	-	-
22	CLA	4	817	X	-	-	-
22	CLA	4	818	X	-	-	-
22	CLA	5	301	X	-	-	-
22	CLA	5	307	X	-	X	-
22	CLA	5	308	X	-	X	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-
22	CLA	5	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	318	X	-	-	-
22	CLA	5	319	X	-	-	-
22	CLA	5	320	X	-	-	-
22	CLA	5	322	X	-	-	-
22	CLA	5	323	X	-	-	-
22	CLA	5	326	X	-	-	-
22	CLA	6	301	X	-	-	-
22	CLA	6	302	X	-	-	-
22	CLA	6	307	X	-	-	-
22	CLA	6	308	X	-	-	-
22	CLA	6	309	X	-	X	-
22	CLA	6	310	X	-	-	-
22	CLA	6	311	X	-	-	-
22	CLA	6	312	X	-	-	-
22	CLA	6	313	X	-	-	-
22	CLA	6	314	X	-	-	-
22	CLA	6	317	X	-	-	-
22	CLA	6	319	X	-	-	-
22	CLA	6	321	X	-	-	-
22	CLA	6	322	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	308	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-
22	CLA	7	322	X	-	-	-
22	CLA	7	323	X	-	-	-
22	CLA	7	324	X	-	-	-
22	CLA	8	305	X	-	X	-
22	CLA	8	306	X	-	-	-
22	CLA	8	307	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	8	311	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	314	X	-	-	-
22	CLA	8	316	X	-	-	-
22	CLA	9	303	X	-	-	-
22	CLA	9	304	X	-	-	-
22	CLA	9	305	X	-	-	-
22	CLA	9	306	X	-	-	-
22	CLA	9	307	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	X	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	X	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	X	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	X	-
22	CLA	A	822	X	-	X	-
22	CLA	A	823	X	-	X	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	A	855	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	X	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	X	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	X	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	X	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B	842	X	-	X	-
22	CLA	F	301	X	-	-	-
22	CLA	F	302	X	-	-	-
22	CLA	F	304	X	-	X	-
22	CLA	F	305	X	-	-	-
22	CLA	G	201	X	-	-	-
22	CLA	G	202	X	-	-	-
22	CLA	J	103	X	-	-	-
22	CLA	K	202	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	205	X	-	-	-
22	CLA	L	201	X	-	-	-
22	CLA	L	202	X	-	-	-
22	CLA	L	203	X	-	-	-
22	CLA	Z	303	X	-	X	-
22	CLA	Z	304	X	-	-	-
22	CLA	Z	305	X	-	-	-
22	CLA	Z	306	X	-	-	-
22	CLA	Z	307	X	-	-	-
22	CLA	Z	308	X	-	-	-
22	CLA	Z	309	X	-	X	-
22	CLA	Z	310	X	-	-	-
22	CLA	Z	313	X	-	X	-
22	CLA	Z	314	X	-	-	-
22	CLA	Z	315	X	-	-	-
22	CLA	Z	316	X	-	-	-
24	BCR	3	304	-	X	-	-
24	BCR	3	307	-	X	-	-
24	BCR	4	804	-	-	X	-
24	BCR	5	305	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	6	306	-	X	-	-
24	BCR	A	844	-	-	X	-
24	BCR	A	856	-	X	X	-
24	BCR	B	848	-	X	-	-
29	SF4	B	802	-	-	X	-
29	SF4	C	101	-	-	X	-
29	SF4	C	102	-	-	X	-
31	DGD	3	301	-	-	X	-
37	DAO	K	201	-	-	X	-
38	LUT	Z	301	-	-	X	-
39	CHL	1	312	X	-	-	-
39	CHL	2	303	X	-	-	-
39	CHL	3	317	X	-	-	-
39	CHL	4	813	X	-	-	-
39	CHL	4	814	X	-	-	-
39	CHL	4	816	X	-	X	-
39	CHL	4	819	X	-	-	-
39	CHL	5	316	X	-	-	-
39	CHL	5	317	X	-	-	-
39	CHL	5	321	X	-	-	-
39	CHL	6	315	X	-	X	-
39	CHL	6	316	X	-	-	-
39	CHL	6	318	X	-	-	-
39	CHL	6	320	X	-	-	-
39	CHL	7	313	X	-	-	-
39	CHL	8	301	X	-	-	-
39	CHL	8	312	X	-	-	-
39	CHL	8	315	X	-	X	-
39	CHL	9	312	X	-	X	-
39	CHL	9	314	X	-	-	-
39	CHL	Z	311	X	-	-	-
39	CHL	Z	312	X	-	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 50057 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5819	3806	991	1000	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5800	3804	973	1005	18		

- Molecule 3 is a protein called Photosystem I subunit VII PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			603	370	105	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1129	724	196	204	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			484	309	83	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	813	219	230	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	93	Total	C	N	O	S	0	0
			690	440	116	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	41	Total	C	N	O	S	0	0
			308	210	44	53	1		

- Molecule 9 is a protein called Photosystem I subunit IX PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	40	Total	C	N	O	S	0	0
			319	217	47	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	89	Total	C	N	O	S	0	0
			617	390	110	115	2		

- Molecule 11 is a protein called Photosystem I reaction centre subunit XI PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			897	580	148	165	4		

- Molecule 12 is a protein called Light-harvesting protein of photosystem I Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1457	936	248	265	8		
12	Z	194	Total	C	N	O	S	0	0
			1457	936	248	265	8		

- Molecule 13 is a protein called Light-harvesting protein of photosystem I Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	218	Total	C	N	O	S	0	0
			1695	1107	272	309	7		

- Molecule 14 is a protein called Light-harvesting protein of photosystem I Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	220	Total	C	N	O	S	0	0
			1705	1102	283	313	7		

- Molecule 15 is a protein called Light-harvesting protein of photosystem I Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	214	Total	C	N	O	S	0	0
			1602	1032	269	291	10		

- Molecule 16 is a protein called Light-harvesting protein of photosystem I Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1598	1036	272	284	6		

- Molecule 17 is a protein called Light-harvesting protein of photosystem I Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	226	Total	C	N	O	S	0	0
			1764	1136	302	318	8		

- Molecule 18 is a protein called Light-harvesting protein of photosystem I Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	226	Total	C	N	O	S	0	0
			1762	1162	289	303	8		

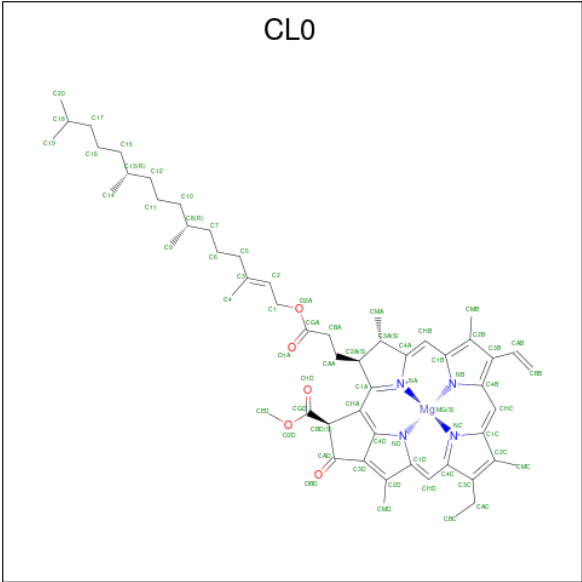
- Molecule 19 is a protein called Light-harvesting protein of photosystem I Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	184	Total	C	N	O	S	0	0
			1416	914	239	254	9		

- Molecule 20 is a protein called Light-harvesting protein of photosystem I Lhca2 partial.

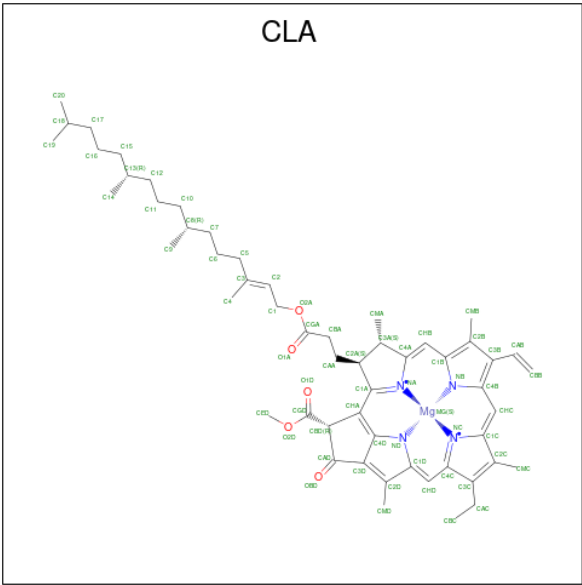
Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	70	Total	C	N	O	S	0	0
			525	336	90	94	5		

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Z	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	Z	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	7	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	8	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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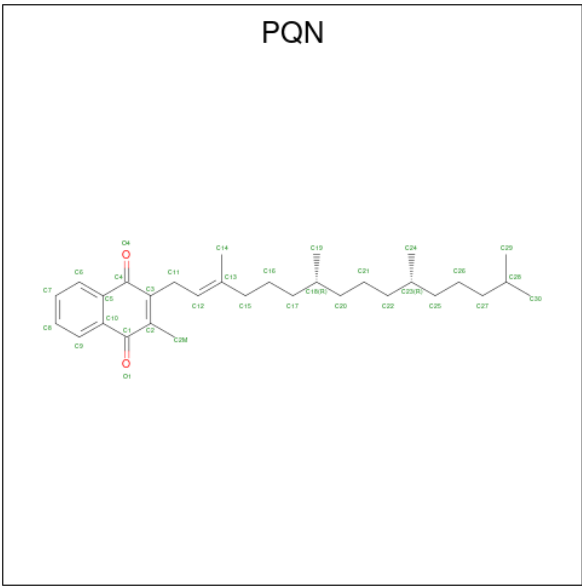
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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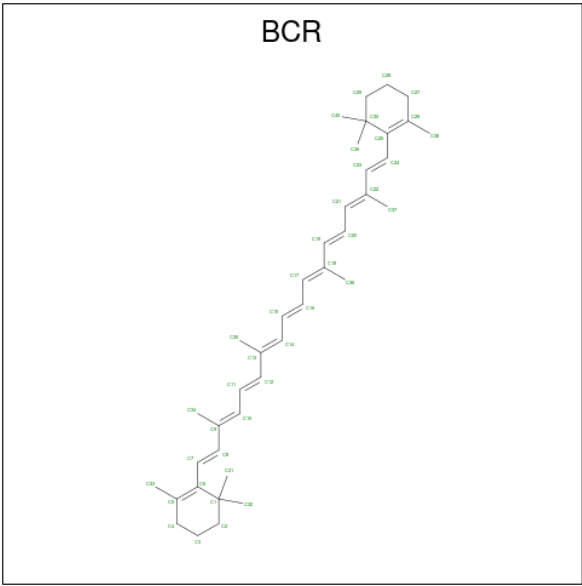
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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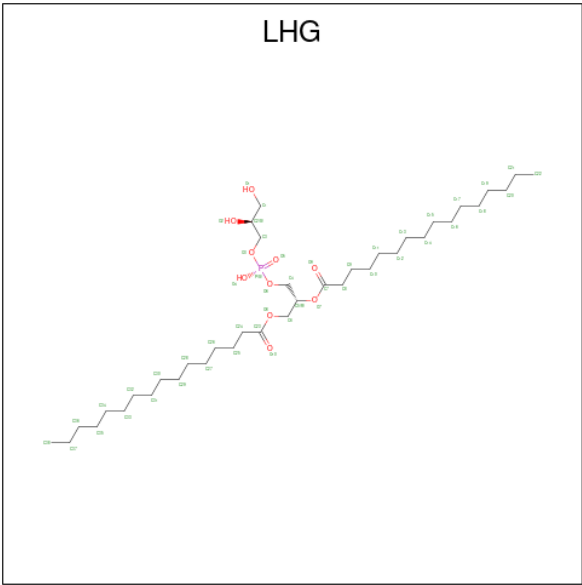
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
24	3	1	Total C 40 40	0
24	7	1	Total C 40 40	0
24	8	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	5	1	Total C 40 40	0
24	5	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	6	1	Total C 40 40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



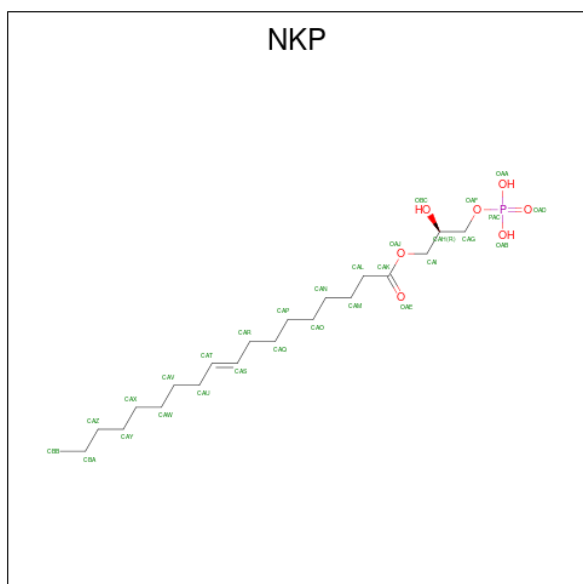
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O P 35 24 10 1	0
25	A	1	Total C O P 49 38 10 1	0
25	B	1	Total C O P 33 22 10 1	0

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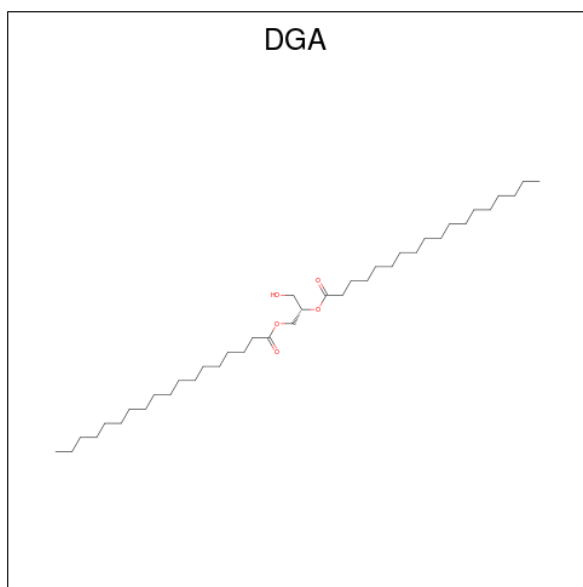
Mol	Chain	Residues	Atoms				AltConf
25	B	1	Total 23	C 12	O 10	P 1	0
25	B	1	Total 20	C 9	O 10	P 1	0
25	1	1	Total 43	C 32	O 10	P 1	0
25	Z	1	Total 43	C 32	O 10	P 1	0
25	3	1	Total 20	C 9	O 10	P 1	0
25	7	1	Total 37	C 26	O 10	P 1	0
25	8	1	Total 38	C 27	O 10	P 1	0
25	4	1	Total 49	C 38	O 10	P 1	0
25	4	1	Total 32	C 21	O 10	P 1	0
25	5	1	Total 37	C 26	O 10	P 1	0
25	6	1	Total 49	C 38	O 10	P 1	0
25	9	1	Total 33	C 22	O 10	P 1	0

- Molecule 26 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: C₂₁H₄₁O₇P).



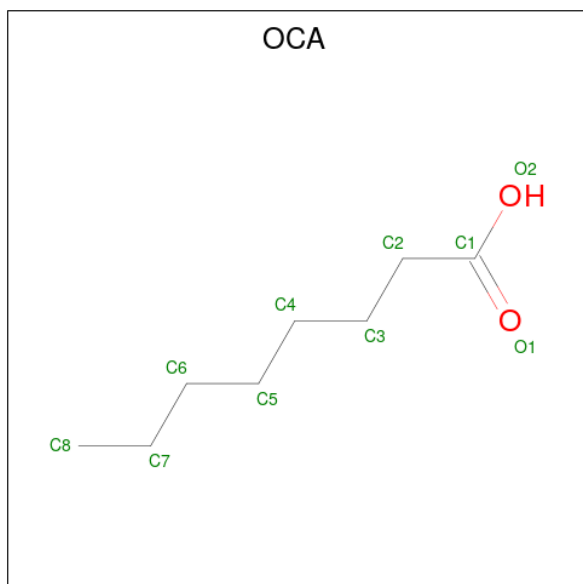
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			23	15	7	1	
26	8	1	Total	C	O	P	0
			29	21	7	1	

- Molecule 27 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



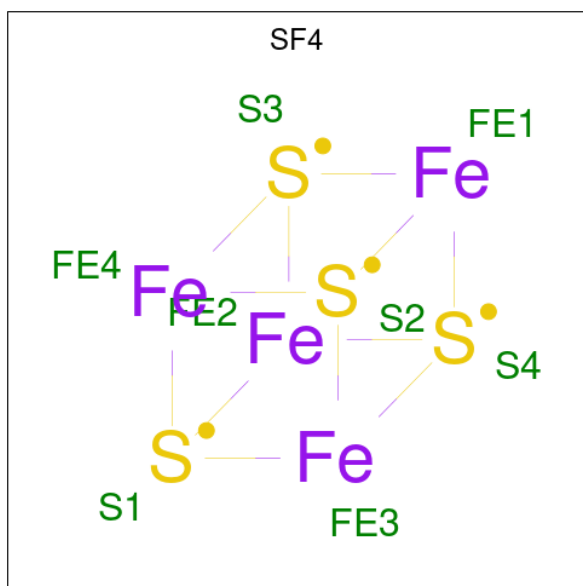
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O		0
			40	35	5		

- Molecule 28 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula: $C_8H_{16}O_2$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			10	8	2	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

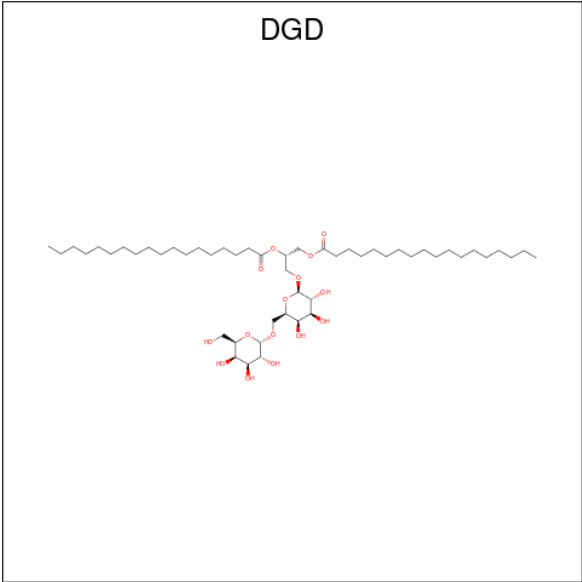


Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

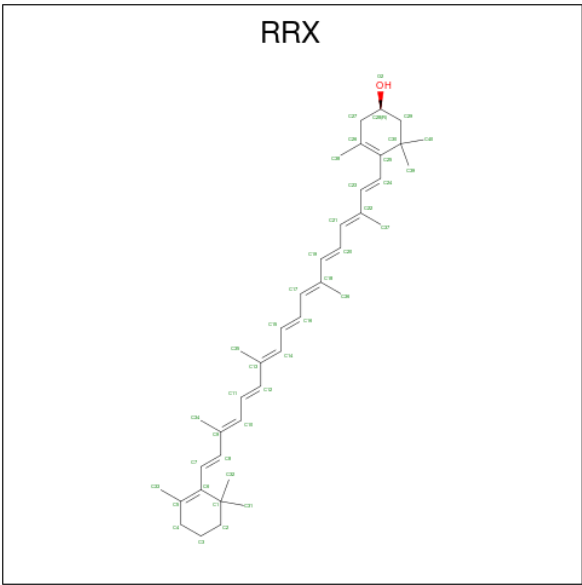
Mol	Chain	Residues	Atoms		AltConf
30	B	1	Total	Ca	0
			1	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



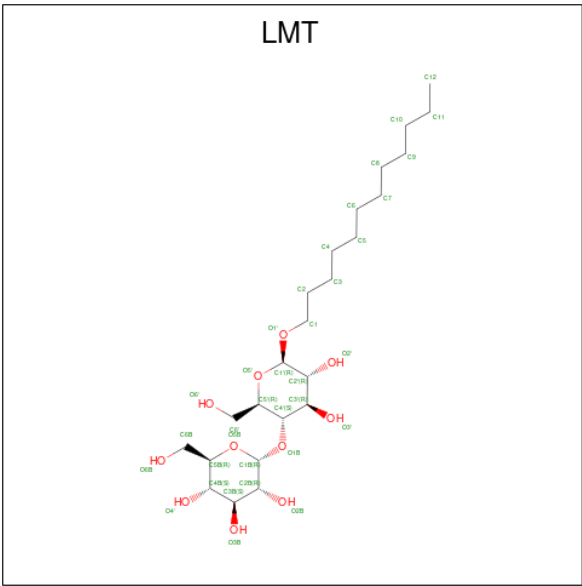
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			61	46	15	
31	1	1	Total	C	O	0
			51	36	15	
31	3	1	Total	C	O	0
			51	36	15	

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



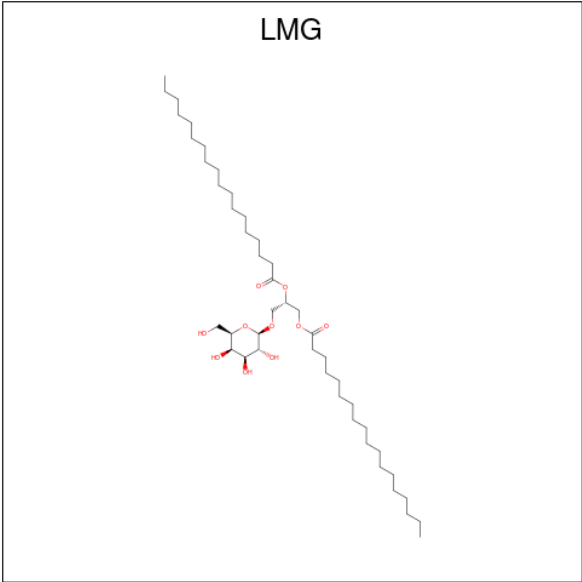
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			41	40	1	

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



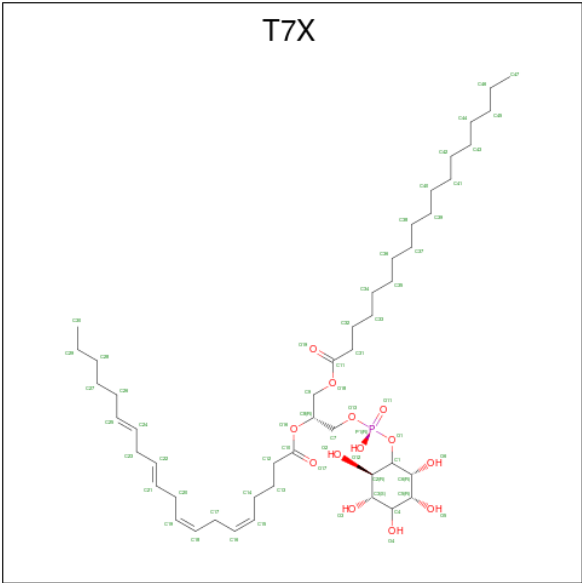
Mol	Chain	Residues	Atoms			AltConf
33	F	1	Total	C	O	0
			35	24	11	
33	G	1	Total	C	O	0
			35	24	11	
33	1	1	Total	C	O	0
			35	24	11	
33	4	1	Total	C	O	0
			35	24	11	
33	4	1	Total	C	O	0
			35	24	11	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
34	F	1	Total	C	O	0
			35	25	10	
34	J	1	Total	C	O	0
			29	19	10	

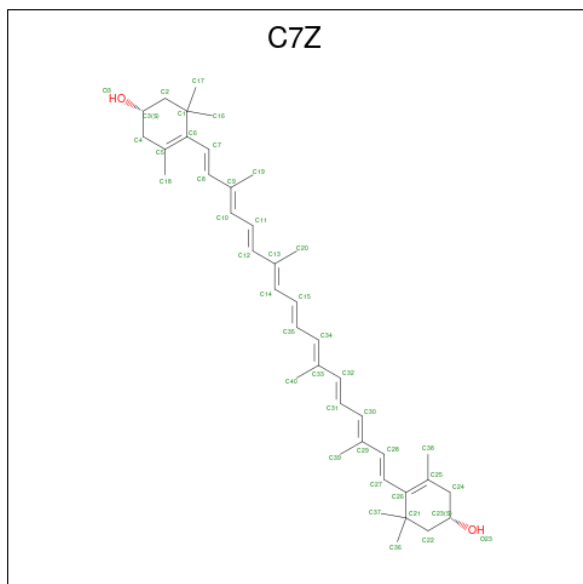
- Molecule 35 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
35	J	1	Total	C	O	P	0
			49	35	13	1	

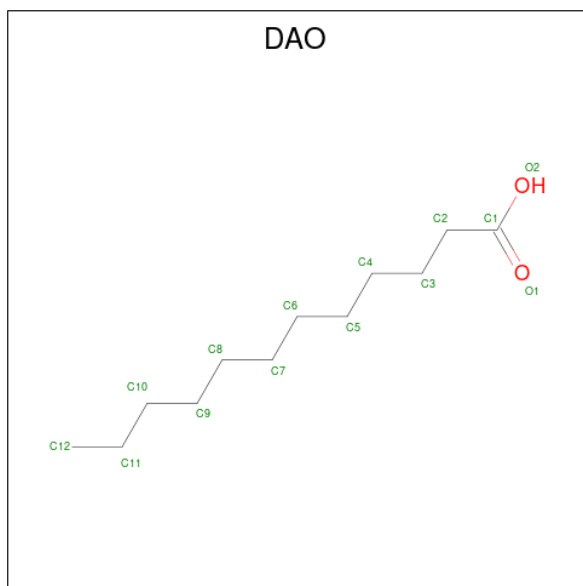
- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},

15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



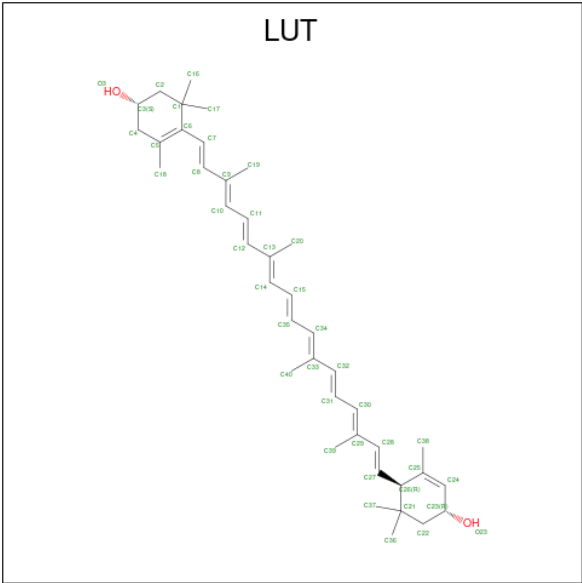
Mol	Chain	Residues	Atoms			AltConf
36	J	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	

- Molecule 37 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			AltConf
37	K	1	Total	C	O	0
			14	12	2	

- Molecule 38 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



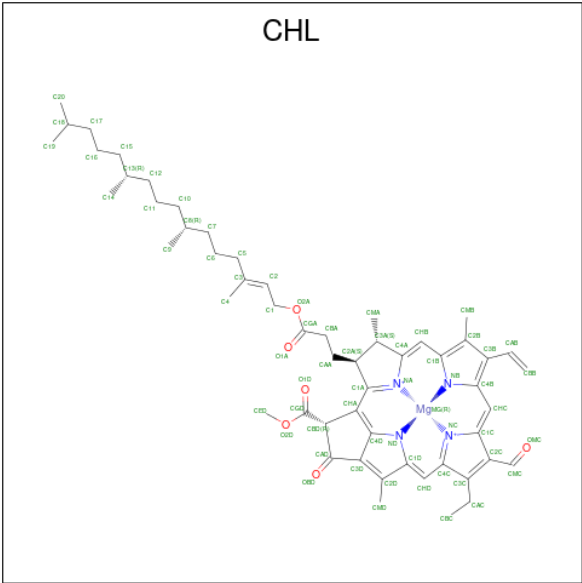
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	C	O	0
			42	40	2	
38	1	1	Total	C	O	0
			42	40	2	
38	Z	1	Total	C	O	0
			42	40	2	
38	Z	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	7	1	Total	C	O	0
			42	40	2	
38	7	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	9	1	Total	C	O	0
			42	40	2	
38	9	1	Total	C	O	0
			42	40	2	

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



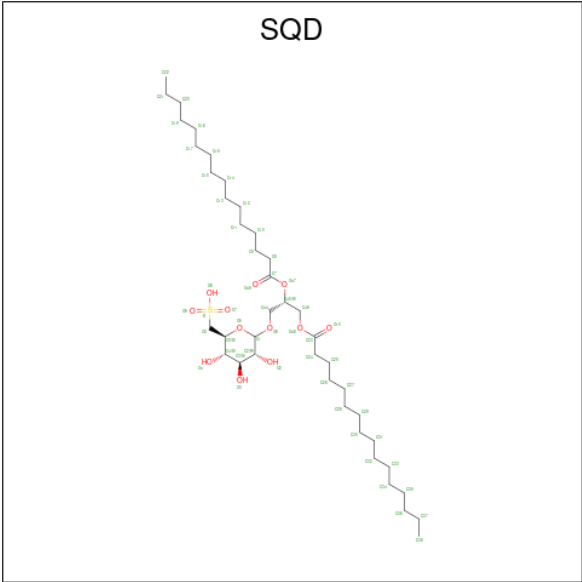
Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	Z	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	Z	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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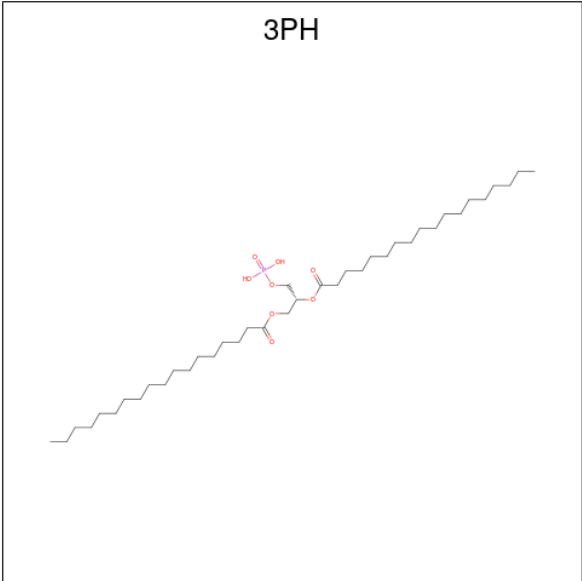
Mol	Chain	Residues	Atoms					AltConf
39	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
39	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
39	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
39	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
39	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
39	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
39	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
40	1	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 41 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



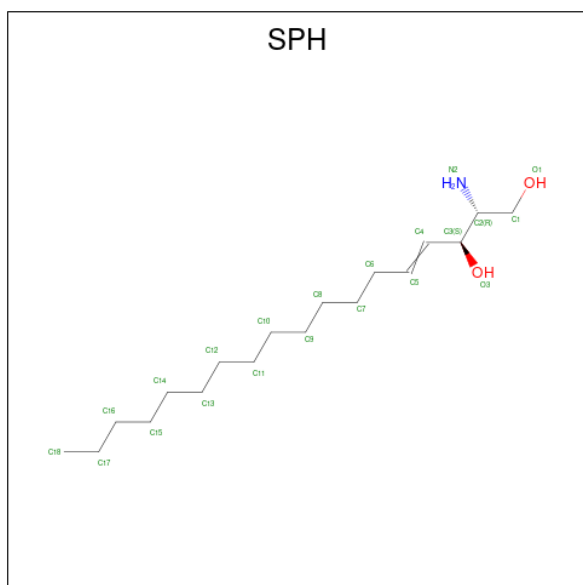
Mol	Chain	Residues	Atoms				AltConf
41	7	1	Total	C	O	P	0
			39	30	8	1	
41	8	1	Total	C	O	P	0
			30	21	8	1	

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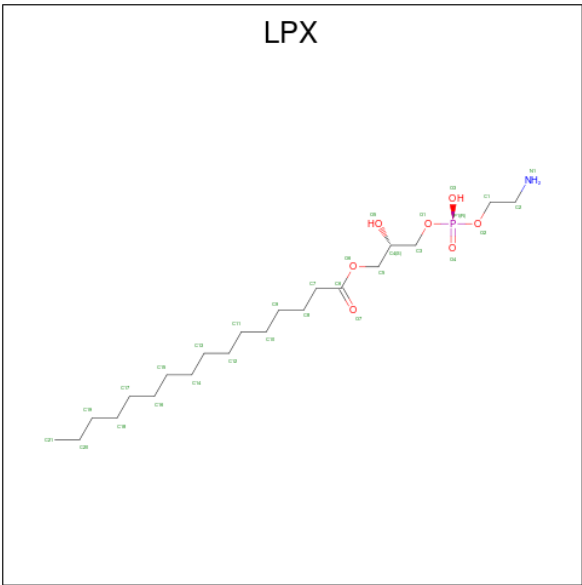
Mol	Chain	Residues	Atoms				AltConf
41	5	1	Total	C	O	P	0
			23	14	8	1	
41	6	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 42 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
42	7	1	Total	C	N	O	0
			21	18	1	2	
42	7	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 43 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
43	8	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	19	Total	O	0
			19	19	
44	B	17	Total	O	0
			17	17	
44	F	3	Total	O	0
			3	3	
44	I	1	Total	O	0
			1	1	
44	J	1	Total	O	0
			1	1	
44	K	1	Total	O	0
			1	1	
44	1	1	Total	O	0
			1	1	
44	Z	1	Total	O	0
			1	1	
44	3	2	Total	O	0
			2	2	
44	7	4	Total	O	0
			4	4	
44	8	4	Total	O	0
			4	4	

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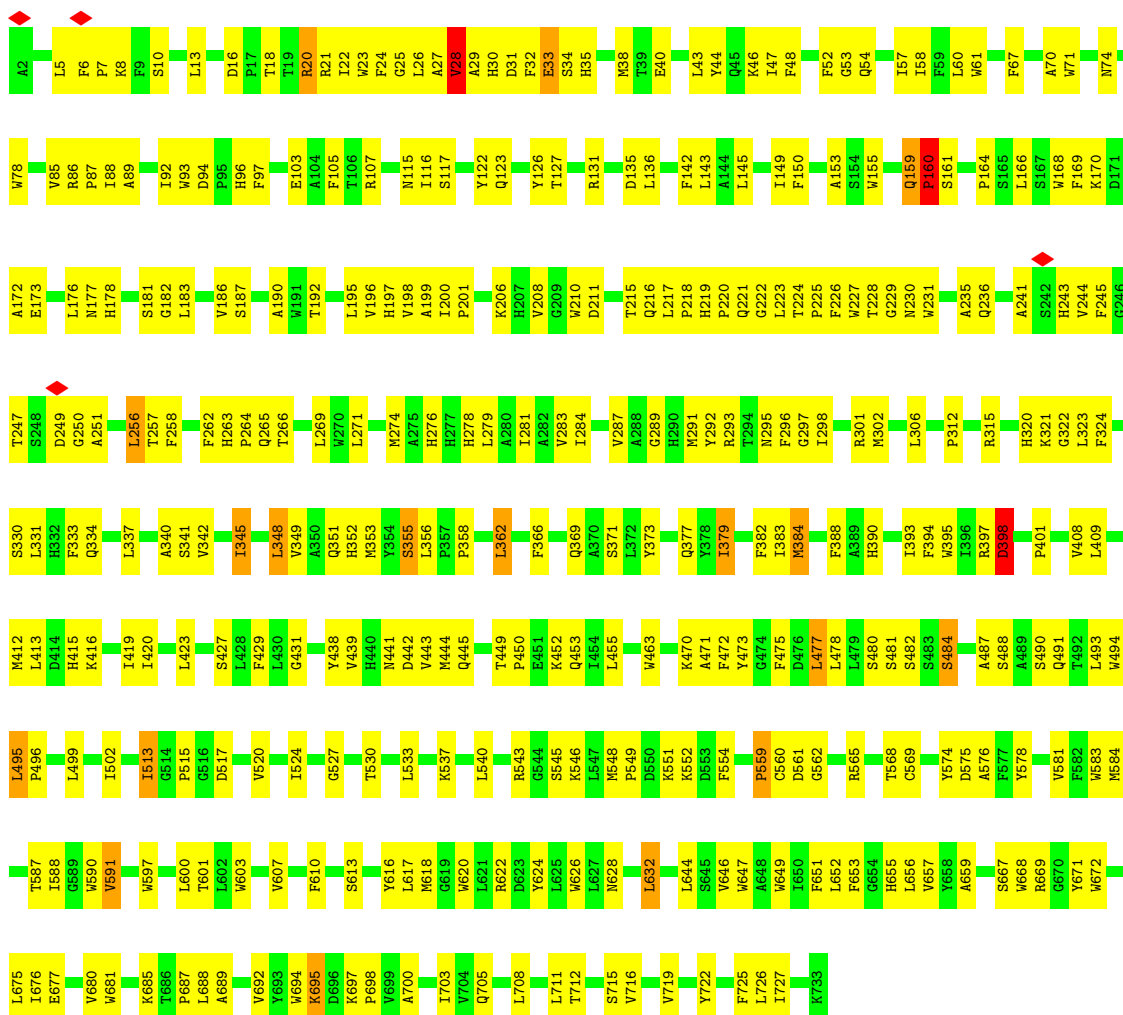
Mol	Chain	Residues	Atoms		AltConf
44	4	5	Total 5	O 5	0
44	5	5	Total 5	O 5	0
44	6	3	Total 3	O 3	0
44	2	1	Total 1	O 1	0

3 Residue-property plots

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

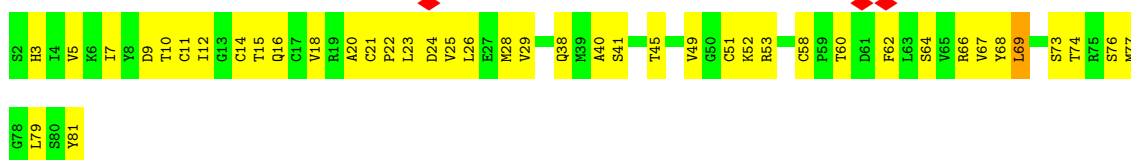
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 PsaA





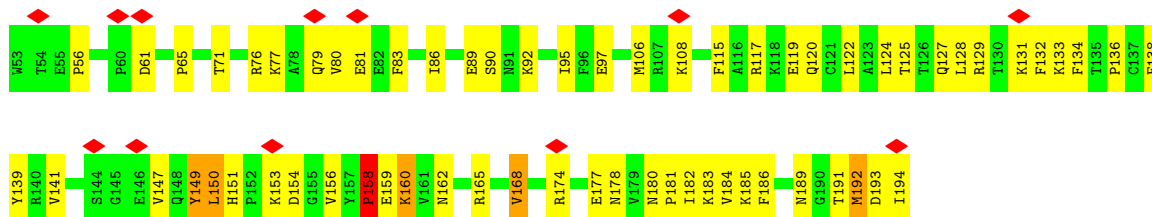
• Molecule 3: Photosystem I subunit VII Psac

Chain C: 48% 51%



• Molecule 4: Photosystem I reaction center subunit II Psad

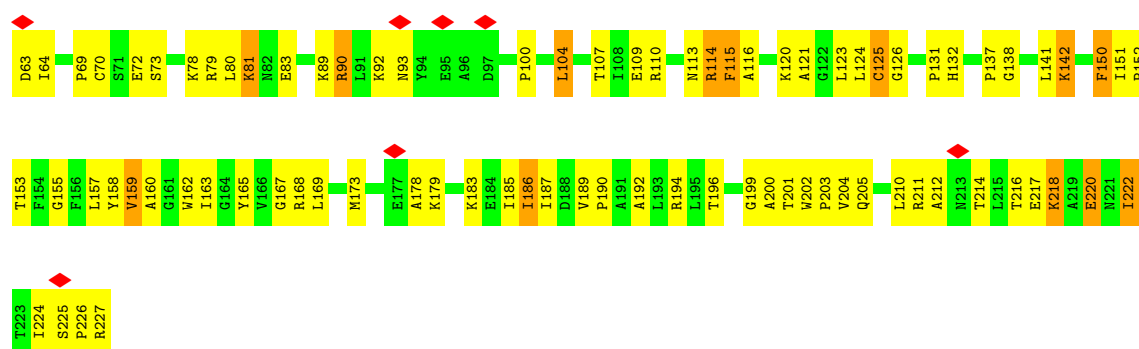
Chain D: 8% 55% 41%



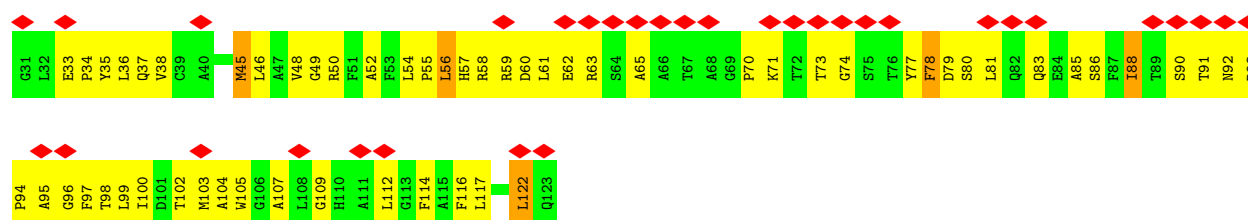
- Molecule 5: Photosystem I reaction center subunit IV PsaE



- Molecule 6: Photosystem I reaction center subunit III PsaF



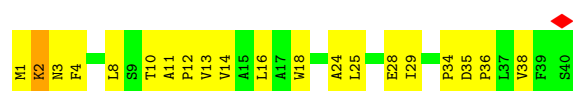
- Molecule 7: Photosystem I reaction center subunit V PsaG



- Molecule 8: Photosystem I reaction center subunit VIII PsaI



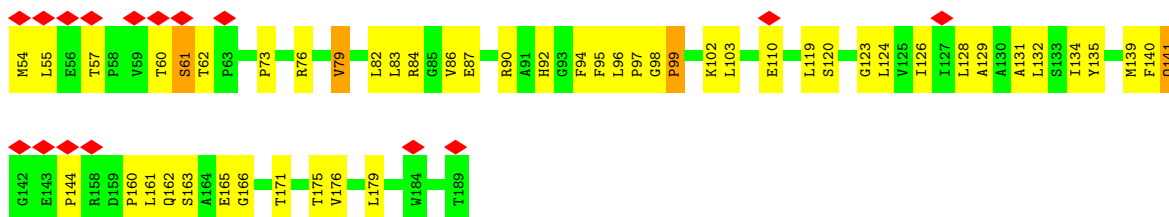
- Molecule 9: Photosystem I subunit IX PsaJ



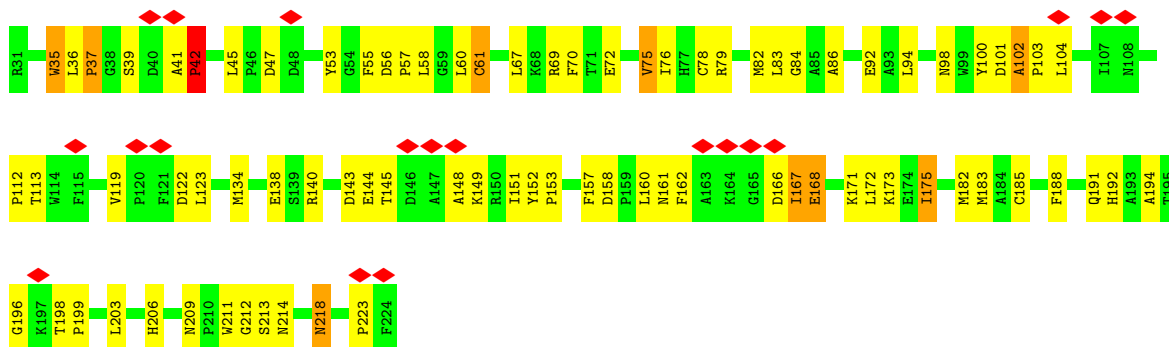
- Molecule 10: Photosystem I reaction center subunit X psaK



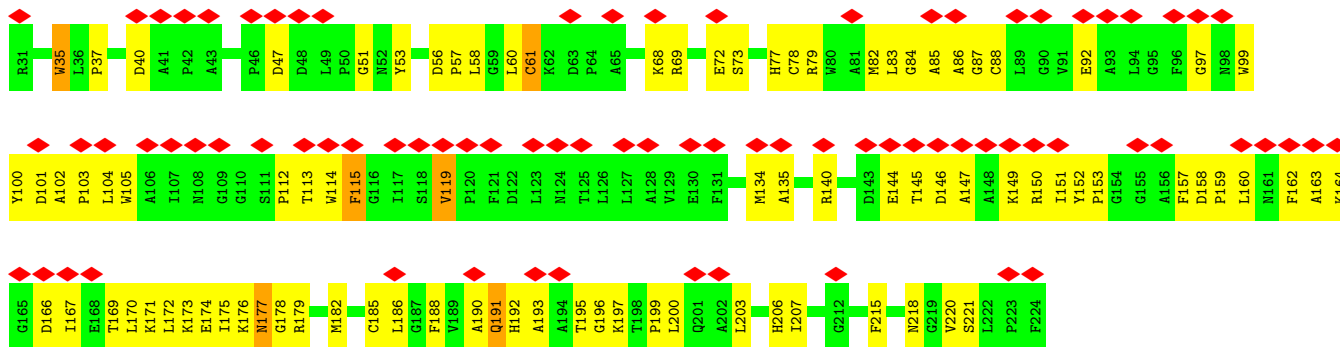
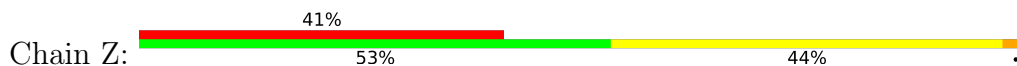
- Molecule 11: Photosystem I reaction centre subunit XI PsaL



- Molecule 12: Light-harvesting protein of photosystem I Lhca1

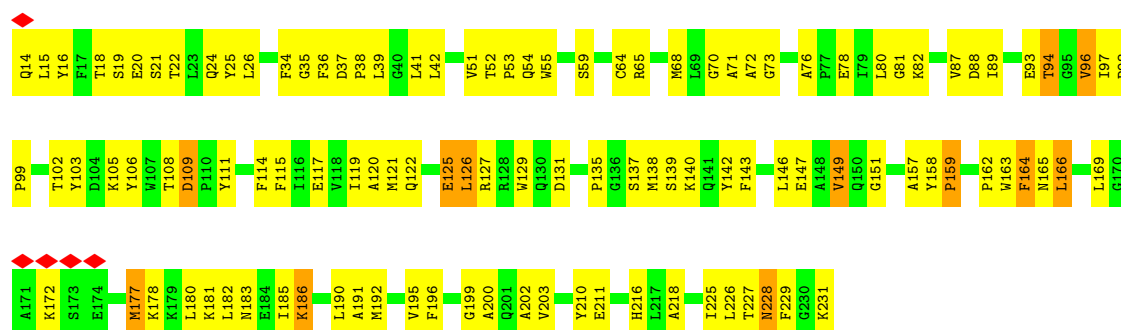


- Molecule 12: Light-harvesting protein of photosystem I Lhca1

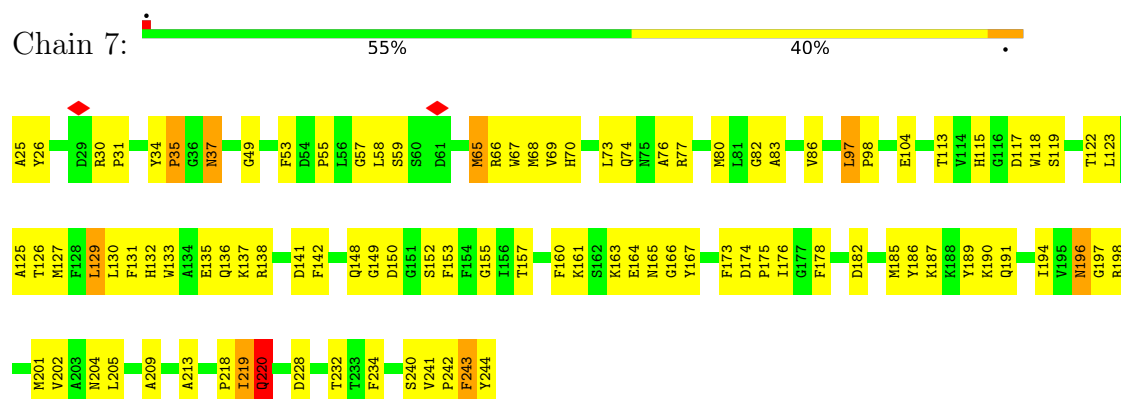


- Molecule 13: Light-harvesting protein of photosystem I Lhca3





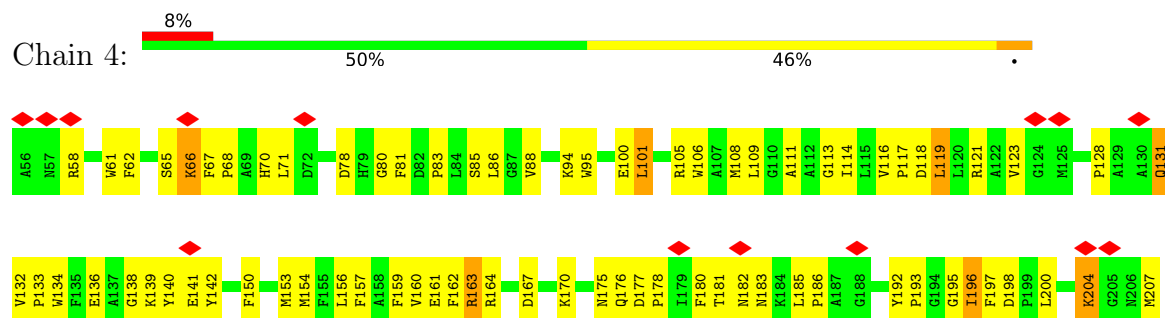
- Molecule 14: Light-harvesting protein of photosystem I Lhca7



- Molecule 15: Light-harvesting protein of photosystem I Lhca8

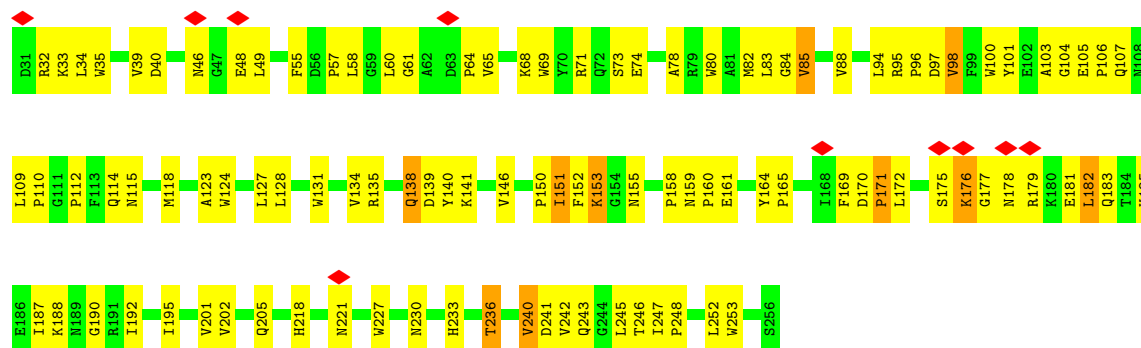


- Molecule 16: Light-harvesting protein of photosystem I Lhca4

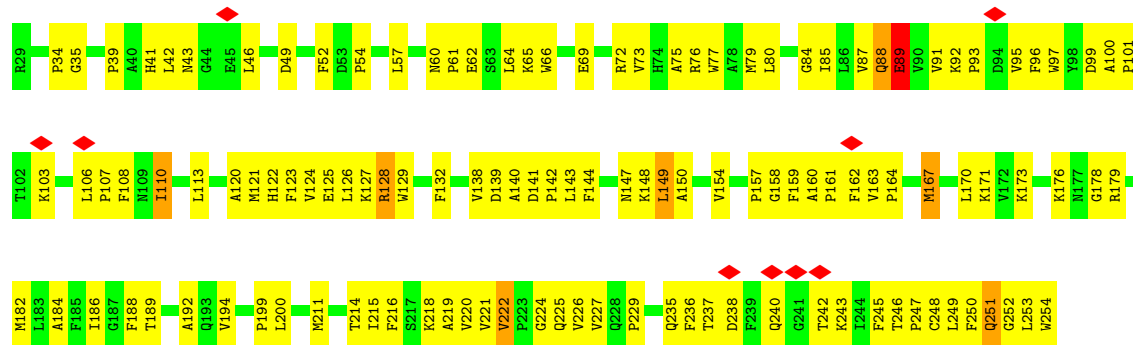




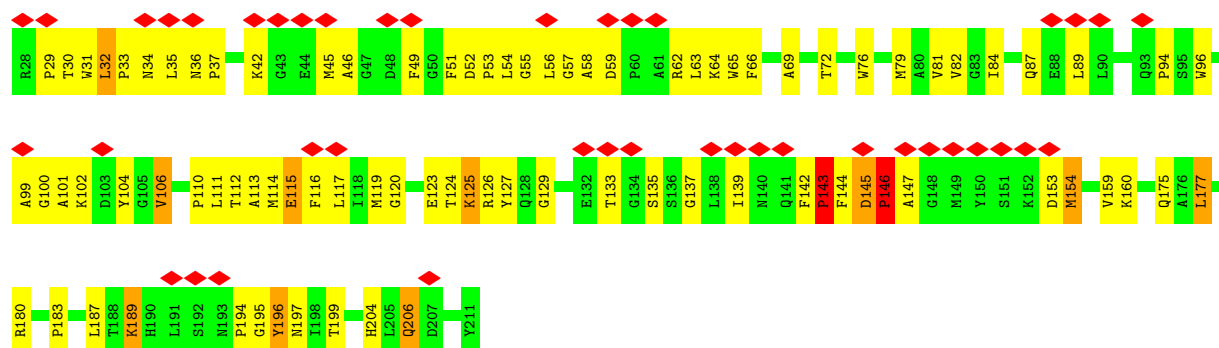
- Molecule 17: Light-harvesting protein of photosystem I Lhca5



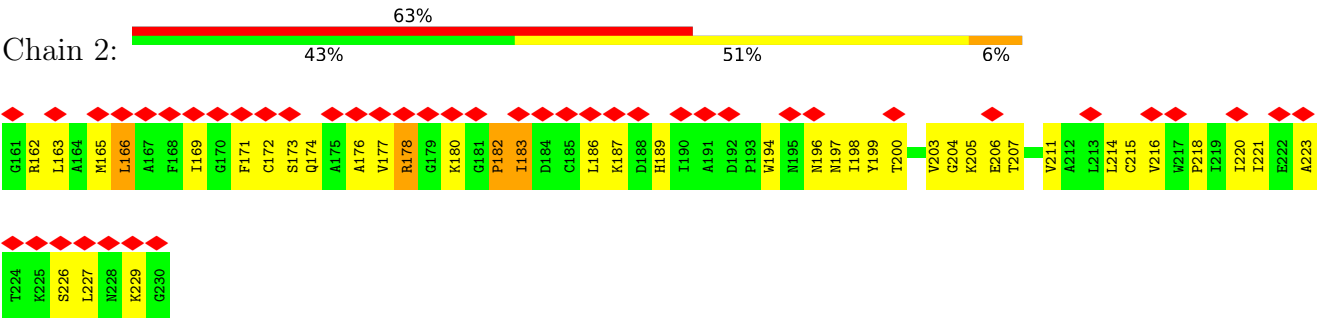
- Molecule 18: Light-harvesting protein of photosystem I Lhca6



- Molecule 19: Light-harvesting protein of photosystem I Lhca9



- Molecule 20: Light-harvesting protein of photosystem I Lhca2 partial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167160	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	150	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	325.5, 325.5, 325.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.651, 0.651, 0.651	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: SF4, SQD, CA, SPH, LPX, NKP, LHG, DGD, LMG, CLA, CHL, T7X, RRX, CL0, PQN, OCA, C7Z, DAO, 3PH, BCR, LUT, LMT, DGA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.91	0/6016	1.13	8/8200 (0.1%)
2	B	0.92	0/6010	1.13	3/8207 (0.0%)
3	C	0.98	0/613	1.15	0/830
4	D	0.89	0/1159	1.17	1/1569 (0.1%)
5	E	0.98	0/495	1.09	0/675
6	F	0.92	0/1292	1.25	3/1755 (0.2%)
7	G	0.95	0/706	1.20	1/960 (0.1%)
8	I	0.97	0/320	1.11	0/443
9	J	0.96	0/329	1.20	0/452
10	K	1.00	0/625	1.27	0/848
11	L	0.97	0/919	1.26	0/1253
12	1	0.91	0/1501	1.28	3/2045 (0.1%)
12	Z	0.78	0/1501	1.03	1/2045 (0.0%)
13	3	0.93	0/1747	1.21	2/2376 (0.1%)
14	7	0.93	0/1765	1.22	1/2407 (0.0%)
15	8	0.94	0/1643	1.24	2/2226 (0.1%)
16	4	0.92	0/1648	1.19	0/2240
17	5	0.92	0/1819	1.21	0/2480
18	6	0.92	0/1824	1.14	1/2488 (0.0%)
19	9	0.85	0/1456	1.30	5/1975 (0.3%)
20	2	0.96	0/535	1.24	0/726
All	All	0.92	0/33923	1.18	31/46200 (0.1%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	143	PRO	CA-N-CD	-11.78	95.51	112.00
12	1	42	PRO	CA-N-CD	-9.96	98.06	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	189	LYS	N-CA-C	-7.90	105.61	114.62
19	9	143	PRO	CB-CA-C	7.80	124.43	111.56
19	9	146	PRO	CA-N-CD	-7.61	101.35	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5666	296	0
2	B	5800	0	5556	372	0
3	C	603	0	587	42	0
4	D	1129	0	1127	46	0
5	E	484	0	477	25	0
6	F	1265	0	1292	75	0
7	G	690	0	671	69	0
8	I	308	0	310	31	0
9	J	319	0	327	23	0
10	K	617	0	635	54	0
11	L	897	0	891	48	0
12	1	1457	0	1406	79	0
12	Z	1457	0	1406	119	0
13	3	1695	0	1641	143	0
14	7	1705	0	1601	104	0
15	8	1602	0	1600	138	0
16	4	1598	0	1569	116	0
17	5	1764	0	1709	126	0
18	6	1762	0	1740	180	0
19	9	1416	0	1392	104	0
20	2	525	0	539	46	0
21	A	65	0	72	7	0
22	1	698	0	678	106	0
22	2	146	0	112	30	0
22	3	749	0	722	153	0
22	4	590	0	511	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	5	910	0	851	191	0
22	6	824	0	800	183	0
22	7	905	0	848	123	0
22	8	555	0	502	111	0
22	9	528	0	451	66	0
22	A	2640	0	2709	508	0
22	B	2340	0	2333	452	0
22	F	240	0	245	60	0
22	G	96	0	70	26	0
22	J	42	0	30	1	0
22	K	205	0	166	28	0
22	L	180	0	180	37	0
22	Z	679	0	631	147	0
23	A	33	0	46	10	0
23	B	33	0	46	5	0
24	3	160	0	224	59	0
24	4	40	0	56	26	0
24	5	80	0	112	30	0
24	6	80	0	112	35	0
24	7	40	0	56	14	0
24	8	40	0	56	14	0
24	A	240	0	336	98	0
24	B	280	0	392	103	0
24	F	40	0	56	14	0
24	G	40	0	56	12	0
24	I	40	0	56	12	0
24	J	40	0	56	18	0
24	K	40	0	55	12	0
24	L	40	0	56	17	0
25	1	43	0	56	8	0
25	3	20	0	12	1	0
25	4	81	0	108	19	0
25	5	37	0	44	7	0
25	6	49	0	74	11	0
25	7	37	0	44	10	0
25	8	38	0	46	7	0
25	9	33	0	36	2	0
25	A	84	0	114	13	0
25	B	76	0	64	15	0
25	Z	43	0	56	9	0
26	8	29	0	39	7	0
26	A	23	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	40	0	65	20	0
28	A	10	0	15	0	0
29	B	8	0	0	8	0
29	C	16	0	0	8	0
30	B	1	0	0	0	0
31	1	51	0	60	10	0
31	3	51	0	60	21	0
31	B	61	0	83	17	0
32	F	41	0	56	19	0
33	1	35	0	46	7	0
33	4	70	0	92	9	0
33	F	35	0	46	5	0
33	G	35	0	46	10	0
34	F	35	0	40	1	0
34	J	29	0	28	10	0
35	J	49	0	0	2	0
36	5	42	0	0	1	0
36	J	42	0	0	2	0
37	K	14	0	23	8	0
38	1	84	0	112	26	0
38	3	84	0	112	28	0
38	4	84	0	112	34	0
38	5	84	0	112	32	0
38	6	84	0	112	24	0
38	7	84	0	112	29	0
38	8	84	0	112	28	0
38	9	84	0	112	33	0
38	Z	84	0	112	36	0
39	1	48	0	32	8	0
39	2	51	0	36	8	0
39	3	66	0	69	14	0
39	4	192	0	130	42	0
39	5	160	0	134	31	0
39	6	206	0	156	51	0
39	7	54	0	42	9	0
39	8	180	0	165	44	0
39	9	108	0	95	35	0
39	Z	99	0	68	23	0
40	1	48	0	62	12	0
41	5	23	0	19	3	0
41	6	29	0	31	5	0
41	7	39	0	51	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	8	30	0	33	4	0
42	7	42	0	74	12	0
43	8	30	0	43	7	0
44	1	1	0	0	0	0
44	2	1	0	0	0	0
44	3	2	0	0	1	0
44	4	5	0	0	0	0
44	5	5	0	0	0	0
44	6	3	0	0	0	0
44	7	4	0	0	0	0
44	8	4	0	0	0	0
44	A	19	0	0	0	0
44	B	17	0	0	0	0
44	F	3	0	0	0	0
44	I	1	0	0	0	0
44	J	1	0	0	0	0
44	K	1	0	0	0	0
44	Z	1	0	0	0	0
All	All	50057	0	49449	4006	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 40.

The worst 5 of 4006 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)
18:6:238:ASP:HA	18:6:243:LYS:HA	1.26	1.13
24:3:306:BCR:H21C	22:3:318:CLA:H91	1.25	1.06
24:5:304:BCR:H19C	22:5:319:CLA:HBA2	1.40	1.04
19:9:53:PRO:HD2	38:9:302:LUT:H23	1.42	1.02
38:6:304:LUT:H28	22:6:310:CLA:H61	1.39	1.02

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	685 (93%)	51 (7%)	2 (0%)	36	64
2	B	730/732 (100%)	683 (94%)	42 (6%)	5 (1%)	18	45
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	140/142 (99%)	124 (89%)	13 (9%)	3 (2%)	5	18
5	E	59/61 (97%)	50 (85%)	8 (14%)	1 (2%)	7	23
6	F	163/165 (99%)	145 (89%)	14 (9%)	4 (2%)	4	15
7	G	91/93 (98%)	73 (80%)	16 (18%)	2 (2%)	5	17
8	I	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
9	J	38/40 (95%)	38 (100%)	0	0	100	100
10	K	87/89 (98%)	78 (90%)	8 (9%)	1 (1%)	11	34
11	L	119/123 (97%)	106 (89%)	11 (9%)	2 (2%)	7	23
12	1	192/194 (99%)	165 (86%)	23 (12%)	4 (2%)	5	18
12	Z	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	24	53
13	3	216/218 (99%)	195 (90%)	18 (8%)	3 (1%)	9	27
14	7	218/220 (99%)	202 (93%)	12 (6%)	4 (2%)	6	22
15	8	212/214 (99%)	181 (85%)	24 (11%)	7 (3%)	3	10
16	4	205/207 (99%)	190 (93%)	15 (7%)	0	100	100
17	5	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	6	22
18	6	224/226 (99%)	212 (95%)	11 (5%)	1 (0%)	30	58
19	9	182/184 (99%)	152 (84%)	23 (13%)	7 (4%)	2	8
20	2	68/70 (97%)	53 (78%)	14 (21%)	1 (2%)	8	26
All	All	4215/4259 (99%)	3826 (91%)	337 (8%)	52 (1%)	13	31

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	154	ASP
12	1	41	ALA
12	1	42	PRO
14	7	219	ILE
15	8	38	ALA

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	602/602 (100%)	574 (95%)	28 (5%)	23	55
2	B	596/596 (100%)	566 (95%)	30 (5%)	22	53
3	C	70/70 (100%)	69 (99%)	1 (1%)	59	84
4	D	122/122 (100%)	107 (88%)	15 (12%)	4	15
5	E	54/54 (100%)	52 (96%)	2 (4%)	30	63
6	F	128/128 (100%)	101 (79%)	27 (21%)	1	3
7	G	69/69 (100%)	63 (91%)	6 (9%)	9	29
8	I	33/33 (100%)	33 (100%)	0	100	100
9	J	35/35 (100%)	34 (97%)	1 (3%)	37	71
10	K	60/60 (100%)	54 (90%)	6 (10%)	7	23
11	L	90/90 (100%)	76 (84%)	14 (16%)	2	8
12	1	144/144 (100%)	125 (87%)	19 (13%)	4	13
12	Z	144/144 (100%)	134 (93%)	10 (7%)	14	39
13	3	173/173 (100%)	159 (92%)	14 (8%)	11	32
14	7	169/169 (100%)	156 (92%)	13 (8%)	12	34
15	8	162/162 (100%)	137 (85%)	25 (15%)	2	9
16	4	162/162 (100%)	141 (87%)	21 (13%)	4	13
17	5	185/185 (100%)	166 (90%)	19 (10%)	7	22
18	6	184/184 (100%)	172 (94%)	12 (6%)	15	42
19	9	143/143 (100%)	125 (87%)	18 (13%)	4	14
20	2	57/57 (100%)	50 (88%)	7 (12%)	4	15
All	All	3382/3382 (100%)	3094 (92%)	288 (8%)	12	30

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	4	257	SER
20	2	205	LYS

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Mol	Chain	Res	Type
17	5	97	ASP
18	6	211	MET
6	F	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
13	3	141	GLN
16	4	98	GLN
13	3	222	ASN
14	7	191	GLN
16	4	242	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 1 is monoatomic - leaving 331 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	BCR	7	303	-	41,41,41	4.92	27 (65%)	56,56,56	2.42	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	A	846	-	41,41,41	4.94	27 (65%)	56,56,56	2.50	20 (35%)
22	CLA	1	314	12	69,73,73	1.34	5 (7%)	82,113,113	1.86	19 (23%)
39	CHL	8	312	-	50,64,74	1.47	9 (18%)	46,102,114	1.83	12 (26%)
25	LHG	3	321	22	19,19,48	0.95	1 (5%)	20,24,54	1.55	1 (5%)
25	LHG	B	803	-	32,32,48	0.47	0	35,38,54	1.20	3 (8%)
24	BCR	B	848	-	41,41,41	4.93	27 (65%)	56,56,56	6.50	24 (42%)
22	CLA	A	815	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	19 (23%)
22	CLA	A	803	-	69,73,73	1.34	7 (10%)	82,113,113	1.91	19 (23%)
22	CLA	3	314	25	64,68,73	1.40	6 (9%)	76,107,113	1.94	18 (23%)
22	CLA	Z	307	-	59,63,73	1.47	7 (11%)	70,101,113	2.08	19 (27%)
22	CLA	B	830	-	69,73,73	1.34	6 (8%)	82,113,113	1.87	18 (21%)
38	LUT	5	302	-	42,43,43	6.39	26 (61%)	51,60,60	2.10	14 (27%)
22	CLA	3	315	-	49,53,73	1.67	6 (12%)	58,89,113	2.10	14 (24%)
22	CLA	1	305	12	49,53,73	1.60	6 (12%)	58,89,113	2.06	18 (31%)
22	CLA	7	314	44	54,58,73	1.51	5 (9%)	64,95,113	2.12	19 (29%)
38	LUT	Z	302	-	42,43,43	6.40	26 (61%)	51,60,60	2.15	13 (25%)
38	LUT	1	302	-	42,43,43	6.42	27 (64%)	51,60,60	2.16	15 (29%)
22	CLA	5	320	-	54,58,73	1.59	7 (12%)	64,95,113	2.08	17 (26%)
22	CLA	A	807	-	64,68,73	1.39	6 (9%)	76,107,113	1.97	19 (25%)
24	BCR	B	846	-	41,41,41	4.94	27 (65%)	56,56,56	2.41	20 (35%)
22	CLA	7	324	-	64,68,73	1.41	6 (9%)	76,107,113	1.96	20 (26%)
22	CLA	4	805	16	64,68,73	1.44	8 (12%)	76,107,113	1.85	17 (22%)
22	CLA	8	309	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	19 (23%)
22	CLA	B	810	-	60,64,73	1.44	5 (8%)	71,102,113	2.08	22 (30%)
22	CLA	B	812	2	63,67,73	1.41	5 (7%)	74,105,113	1.90	18 (24%)
22	CLA	1	308	-	59,63,73	1.46	7 (11%)	70,101,113	2.11	18 (25%)
26	NKP	A	851	-	22,22,28	0.37	0	24,26,32	0.38	0
24	BCR	B	853	-	41,41,41	4.98	27 (65%)	56,56,56	2.40	20 (35%)
22	CLA	6	307	18	64,68,73	1.40	8 (12%)	76,107,113	1.96	18 (23%)
22	CLA	B	832	-	54,58,73	1.52	6 (11%)	64,95,113	2.09	19 (29%)
24	BCR	3	305	-	41,41,41	4.93	27 (65%)	56,56,56	2.23	19 (33%)
42	SPH	7	320	-	19,20,20	0.65	0	18,21,21	1.10	0
22	CLA	K	203	44	59,63,73	1.46	6 (10%)	70,101,113	2.04	20 (28%)
25	LHG	5	324	22	36,36,48	0.44	0	39,42,54	1.14	3 (7%)
22	CLA	Z	314	12	55,59,73	1.50	6 (10%)	64,96,113	2.07	18 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	7	313	44	48,62,74	1.44	9 (18%)	43,99,114	1.88	11 (25%)
22	CLA	K	205	10	59,63,73	1.56	7 (11%)	70,101,113	2.12	17 (24%)
22	CLA	3	309	13	50,54,73	1.59	6 (12%)	59,90,113	2.02	16 (27%)
22	CLA	5	315	17	69,73,73	1.35	6 (8%)	82,113,113	1.90	20 (24%)
24	BCR	A	845	-	41,41,41	4.91	27 (65%)	56,56,56	2.53	22 (39%)
38	LUT	8	302	-	42,43,43	6.34	26 (61%)	51,60,60	2.07	16 (31%)
22	CLA	B	833	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	20 (24%)
22	CLA	Z	315	-	50,54,73	1.58	6 (12%)	59,90,113	2.08	15 (25%)
39	CHL	4	814	44	45,59,74	1.39	8 (17%)	40,96,114	2.01	11 (27%)
22	CLA	7	304	14	64,68,73	1.39	6 (9%)	76,107,113	2.01	21 (27%)
22	CLA	A	826	44	54,58,73	1.52	6 (11%)	64,95,113	2.11	18 (28%)
22	CLA	G	201	-	54,58,73	1.54	6 (11%)	64,95,113	2.12	21 (32%)
22	CLA	6	312	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	21 (25%)
22	CLA	A	827	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	21 (25%)
22	CLA	4	810	44	54,58,73	1.52	5 (9%)	64,95,113	2.11	20 (31%)
22	CLA	8	316	15	50,54,73	1.57	7 (14%)	59,90,113	2.04	15 (25%)
22	CLA	3	310	13	69,73,73	1.36	7 (10%)	82,113,113	1.97	21 (25%)
22	CLA	5	318	17	69,73,73	1.34	5 (7%)	82,113,113	1.86	18 (21%)
22	CLA	A	828	-	69,73,73	1.34	5 (7%)	82,113,113	1.91	17 (20%)
22	CLA	A	802	44	69,73,73	1.35	5 (7%)	82,113,113	1.93	20 (24%)
22	CLA	A	834	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	20 (24%)
22	CLA	8	313	44	54,58,73	1.52	6 (11%)	64,95,113	2.09	18 (28%)
22	CLA	3	312	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	19 (23%)
22	CLA	2	304	44	50,54,73	1.57	6 (12%)	59,90,113	2.05	16 (27%)
39	CHL	5	321	17	37,51,74	1.59	7 (18%)	30,86,114	2.19	9 (30%)
22	CLA	7	312	-	64,68,73	1.40	5 (7%)	76,107,113	1.95	19 (25%)
22	CLA	5	308	17	65,69,73	1.39	6 (9%)	77,108,113	1.94	20 (25%)
39	CHL	4	819	16	37,51,74	1.64	8 (21%)	30,86,114	2.15	9 (30%)
22	CLA	B	808	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	20 (24%)
22	CLA	B	828	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	20 (24%)
22	CLA	7	306	-	69,73,73	1.35	6 (8%)	82,113,113	1.97	19 (23%)
38	LUT	7	302	-	42,43,43	6.40	26 (61%)	51,60,60	2.18	15 (29%)
22	CLA	1	310	25	64,68,73	1.39	6 (9%)	76,107,113	1.95	18 (23%)
22	CLA	A	840	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	18 (21%)
22	CLA	6	311	-	59,63,73	1.46	6 (10%)	70,101,113	1.96	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LUT	4	802	-	42,43,43	6.39	26 (61%)	51,60,60	2.14	14 (27%)
22	CLA	6	321	-	50,54,73	1.58	6 (12%)	59,90,113	2.06	16 (27%)
22	CLA	7	308	14	65,69,73	1.41	7 (10%)	77,108,113	1.93	19 (24%)
24	BCR	5	305	-	41,41,41	4.95	27 (65%)	56,56,56	2.69	25 (44%)
22	CLA	B	809	2	69,73,73	1.35	7 (10%)	82,113,113	1.88	19 (23%)
25	LHG	Z	317	22	42,42,48	0.41	0	45,48,54	1.10	3 (6%)
35	T7X	J	102	-	49,49,61	0.93	4 (8%)	58,61,73	0.94	3 (5%)
22	CLA	6	302	16	64,68,73	1.40	5 (7%)	76,107,113	1.92	19 (25%)
24	BCR	A	856	-	41,41,41	4.91	27 (65%)	56,56,56	2.54	22 (39%)
22	CLA	A	813	-	69,73,73	1.36	5 (7%)	82,113,113	1.92	20 (24%)
39	CHL	6	318	-	50,64,74	1.55	9 (18%)	46,102,114	1.85	13 (28%)
22	CLA	5	311	-	59,63,73	1.47	8 (13%)	70,101,113	2.01	20 (28%)
38	LUT	3	303	-	42,43,43	6.37	26 (61%)	51,60,60	2.10	16 (31%)
22	CLA	8	306	15	55,59,73	1.52	7 (12%)	64,96,113	2.06	18 (28%)
22	CLA	Z	316	12	69,73,73	1.34	6 (8%)	82,113,113	1.88	18 (21%)
25	LHG	7	318	22	36,36,48	0.43	0	39,42,54	1.15	3 (7%)
25	LHG	4	820	22	48,48,48	0.42	0	51,54,54	1.06	4 (7%)
22	CLA	6	313	25	59,63,73	1.47	6 (10%)	70,101,113	2.00	18 (25%)
22	CLA	4	808	16	64,68,73	1.40	7 (10%)	76,107,113	1.95	20 (26%)
22	CLA	5	319	44	59,63,73	1.45	6 (10%)	70,101,113	2.04	20 (28%)
22	CLA	7	315	14	54,58,73	1.52	7 (12%)	64,95,113	2.13	19 (29%)
22	CLA	B	826	44	69,73,73	1.35	6 (8%)	82,113,113	1.91	20 (24%)
22	CLA	9	309	25	59,63,73	1.47	6 (10%)	70,101,113	2.07	16 (22%)
33	LMT	4	801	-	36,36,36	0.36	0	47,47,47	0.73	1 (2%)
38	LUT	1	303	-	42,43,43	6.40	26 (61%)	51,60,60	2.17	14 (27%)
22	CLA	B	834	-	62,66,73	1.43	5 (8%)	73,104,113	2.00	20 (27%)
22	CLA	B	839	-	56,60,73	1.50	6 (10%)	65,97,113	2.09	19 (29%)
22	CLA	B	824	-	63,67,73	1.42	6 (9%)	74,105,113	2.02	20 (27%)
22	CLA	3	313	44	69,73,73	1.33	6 (8%)	82,113,113	1.90	20 (24%)
39	CHL	6	316	-	45,59,74	1.60	9 (20%)	40,96,114	1.97	12 (30%)
42	SPH	7	321	-	19,20,20	0.66	1 (5%)	18,21,21	1.15	1 (5%)
22	CLA	A	842	25	56,60,73	1.50	6 (10%)	65,97,113	2.07	18 (27%)
22	CLA	8	311	25	54,58,73	1.52	6 (11%)	64,95,113	2.07	17 (26%)
38	LUT	7	301	-	42,43,43	6.37	26 (61%)	51,60,60	2.07	15 (29%)
22	CLA	A	838	-	69,73,73	1.34	5 (7%)	82,113,113	1.92	19 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	4	806	16	56,60,73	1.51	7 (12%)	65,97,113	2.11	19 (29%)
22	CLA	G	202	7	50,54,73	1.58	7 (14%)	59,90,113	2.05	17 (28%)
22	CLA	B	814	-	64,68,73	1.39	6 (9%)	76,107,113	1.96	18 (23%)
22	CLA	A	819	-	69,73,73	1.34	6 (8%)	82,113,113	1.86	19 (23%)
22	CLA	1	307	12	64,68,73	1.41	7 (10%)	76,107,113	1.99	18 (23%)
33	LMT	F	307	-	36,36,36	0.38	0	47,47,47	0.64	0
37	DAO	K	201	-	13,13,13	0.61	0	13,13,13	0.57	0
22	CLA	4	817	16	45,49,73	1.66	6 (13%)	54,84,113	2.14	17 (31%)
22	CLA	B	831	-	62,66,73	1.43	7 (11%)	73,104,113	2.01	18 (24%)
22	CLA	1	304	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	19 (23%)
38	LUT	9	302	-	42,43,43	6.39	27 (64%)	51,60,60	1.98	14 (27%)
22	CLA	5	314	-	49,53,73	1.59	6 (12%)	58,89,113	2.05	15 (25%)
22	CLA	B	825	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	20 (24%)
22	CLA	9	313	19	54,58,73	1.52	5 (9%)	64,95,113	2.11	20 (31%)
22	CLA	9	308	-	54,58,73	1.53	5 (9%)	64,95,113	2.08	20 (31%)
22	CLA	B	820	-	64,68,73	1.41	6 (9%)	76,107,113	1.92	19 (25%)
21	CL0	A	801	-	58,73,73	3.23	16 (27%)	60,113,113	2.88	17 (28%)
22	CLA	Z	313	44	69,73,73	1.36	6 (8%)	82,113,113	1.90	19 (23%)
22	CLA	A	804	22	49,53,73	1.59	5 (10%)	58,89,113	2.06	16 (27%)
22	CLA	A	817	-	64,68,73	1.40	6 (9%)	76,107,113	1.99	17 (22%)
22	CLA	A	812	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	19 (23%)
22	CLA	K	204	10	53,57,73	1.54	6 (11%)	61,93,113	2.17	19 (31%)
22	CLA	L	202	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	19 (23%)
22	CLA	B	806	44	69,73,73	1.35	7 (10%)	82,113,113	1.90	20 (24%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-
24	BCR	F	303	-	41,41,41	4.95	27 (65%)	56,56,56	2.23	17 (30%)
41	3PH	5	325	-	22,22,47	1.24	4 (18%)	25,27,52	1.32	2 (8%)
22	CLA	B	842	25	69,73,73	1.35	5 (7%)	82,113,113	1.90	19 (23%)
29	SF4	B	802	-	0,12,12	-	-	-	-	-
40	SQD	1	318	-	46,48,54	0.82	1 (2%)	56,59,65	0.89	2 (3%)
22	CLA	5	310	17	69,73,73	1.35	6 (8%)	82,113,113	1.91	19 (23%)
22	CLA	7	309	-	60,64,73	1.45	6 (10%)	71,102,113	2.05	21 (29%)
39	CHL	5	316	44	60,74,74	1.35	9 (15%)	58,114,114	1.61	13 (22%)
22	CLA	7	307	14	69,73,73	1.35	7 (10%)	82,113,113	1.92	18 (21%)
34	LMG	F	308	-	35,35,55	0.47	0	43,43,63	1.40	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LUT	9	301	-	42,43,43	6.39	26 (61%)	51,60,60	2.05	14 (27%)
22	CLA	3	308	13	69,73,73	1.35	7 (10%)	82,113,113	1.93	19 (23%)
22	CLA	B	841	-	69,73,73	1.35	6 (8%)	82,113,113	1.95	20 (24%)
22	CLA	B	829	-	61,65,73	1.43	6 (9%)	72,103,113	2.00	21 (29%)
25	LHG	B	850	22	22,22,48	0.57	0	25,28,54	1.28	2 (8%)
24	BCR	3	306	-	41,41,41	4.94	27 (65%)	56,56,56	2.31	18 (32%)
28	OCA	A	853	-	9,9,9	0.72	0	9,9,9	0.71	0
22	CLA	A	820	-	64,68,73	1.40	7 (10%)	76,107,113	1.92	19 (25%)
22	CLA	A	818	-	64,68,73	1.40	7 (10%)	76,107,113	2.01	21 (27%)
22	CLA	1	306	-	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
22	CLA	A	835	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	19 (23%)
24	BCR	A	847	-	41,41,41	4.94	27 (65%)	56,56,56	2.41	19 (33%)
25	LHG	A	850	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
22	CLA	A	816	44	60,64,73	1.45	6 (10%)	71,102,113	2.08	21 (29%)
24	BCR	5	304	-	41,41,41	4.93	26 (63%)	56,56,56	2.57	21 (37%)
22	CLA	Z	308	-	65,69,73	1.38	6 (9%)	77,108,113	1.95	20 (25%)
22	CLA	B	836	-	49,53,73	1.59	6 (12%)	58,89,113	2.04	17 (29%)
22	CLA	B	835	-	54,58,73	1.52	7 (12%)	64,95,113	2.16	19 (29%)
39	CHL	1	312	-	42,56,74	1.64	9 (21%)	36,92,114	1.96	11 (30%)
22	CLA	8	305	15	64,68,73	1.40	6 (9%)	76,107,113	1.98	19 (25%)
22	CLA	3	318	13	64,68,73	1.39	6 (9%)	76,107,113	1.96	22 (28%)
22	CLA	B	840	44	69,73,73	1.35	7 (10%)	82,113,113	1.88	18 (21%)
22	CLA	6	309	44	69,73,73	1.35	6 (8%)	82,113,113	1.97	20 (24%)
27	DGA	A	852	-	39,39,43	1.17	3 (7%)	41,41,45	1.34	3 (7%)
22	CLA	1	315	-	50,54,73	1.58	7 (14%)	59,90,113	2.06	15 (25%)
24	BCR	B	845	-	41,41,41	4.93	27 (65%)	56,56,56	2.43	20 (35%)
22	CLA	B	821	44	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
22	CLA	4	811	25	59,63,73	1.45	7 (11%)	70,101,113	2.05	19 (27%)
22	CLA	B	827	44	69,73,73	1.35	6 (8%)	82,113,113	1.92	20 (24%)
22	CLA	6	308	18	56,60,73	1.49	5 (8%)	65,97,113	2.11	21 (32%)
25	LHG	A	849	22	34,34,48	0.44	0	37,40,54	1.16	3 (8%)
22	CLA	A	821	44	69,73,73	1.35	5 (7%)	82,113,113	1.87	18 (21%)
23	PQN	B	843	-	34,34,34	0.39	0	43,45,45	1.18	4 (9%)
25	LHG	1	317	22	42,42,48	0.46	1 (2%)	45,48,54	1.19	3 (6%)
38	LUT	8	303	-	42,43,43	6.39	26 (61%)	51,60,60	2.08	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	837	-	55,59,73	1.51	5 (9%)	64,96,113	2.09	19 (29%)
29	SF4	C	102	3	0,12,12	-	-	-		
22	CLA	2	301	-	59,63,73	1.45	6 (10%)	70,101,113	2.05	18 (25%)
22	CLA	9	305	19	64,68,73	1.46	8 (12%)	76,107,113	2.33	23 (30%)
22	CLA	Z	310	-	54,58,73	1.52	6 (11%)	64,95,113	2.06	20 (31%)
38	LUT	6	303	-	42,43,43	6.43	25 (59%)	51,60,60	2.03	17 (33%)
22	CLA	3	322	14	69,73,73	1.35	7 (10%)	82,113,113	1.87	19 (23%)
22	CLA	3	319	-	59,63,73	1.46	6 (10%)	70,101,113	2.01	19 (27%)
41	3PH	6	324	-	28,28,47	1.11	4 (14%)	31,33,52	1.24	2 (6%)
22	CLA	A	831	-	54,58,73	1.52	6 (11%)	64,95,113	2.10	19 (29%)
22	CLA	7	305	-	54,58,73	1.53	7 (12%)	64,95,113	2.12	19 (29%)
22	CLA	4	812	-	59,63,73	1.46	5 (8%)	70,101,113	2.04	20 (28%)
39	CHL	3	317	-	60,74,74	1.28	8 (13%)	58,114,114	1.65	11 (18%)
22	CLA	4	815	16	54,58,73	1.52	6 (11%)	64,95,113	2.10	18 (28%)
22	CLA	B	813	-	60,64,73	1.44	7 (11%)	71,102,113	2.07	20 (28%)
22	CLA	5	322	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	19 (23%)
22	CLA	8	314	15	50,54,73	1.58	7 (14%)	59,90,113	2.01	16 (27%)
22	CLA	5	313	25	65,69,73	1.39	7 (10%)	77,108,113	1.97	19 (24%)
22	CLA	5	323	44	50,54,73	1.56	5 (10%)	59,90,113	2.12	16 (27%)
24	BCR	6	306	-	41,41,41	4.91	27 (65%)	56,56,56	2.83	22 (39%)
22	CLA	Z	304	12	49,53,73	1.60	6 (12%)	58,89,113	2.00	14 (24%)
22	CLA	1	313	44	69,73,73	1.35	7 (10%)	82,113,113	1.93	21 (25%)
38	LUT	3	302	-	42,43,43	6.38	26 (61%)	51,60,60	2.12	15 (29%)
22	CLA	8	310	44	64,68,73	1.40	6 (9%)	76,107,113	1.98	19 (25%)
22	CLA	4	807	16	69,73,73	1.35	7 (10%)	82,113,113	1.94	20 (24%)
22	CLA	7	316	44	46,50,73	1.64	6 (13%)	53,85,113	2.13	16 (30%)
24	BCR	B	849	-	41,41,41	4.96	28 (68%)	56,56,56	2.37	19 (33%)
22	CLA	A	805	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	20 (24%)
22	CLA	4	809	16	55,59,73	1.52	6 (10%)	64,96,113	2.06	20 (31%)
39	CHL	2	303	-	45,59,74	1.51	7 (15%)	40,96,114	1.96	11 (27%)
22	CLA	3	316	13	56,60,73	1.49	6 (10%)	65,97,113	2.04	19 (29%)
22	CLA	A	811	22	69,73,73	1.34	7 (10%)	82,113,113	1.86	19 (23%)
22	CLA	7	323	15	69,73,73	1.35	5 (7%)	82,113,113	1.91	21 (25%)
22	CLA	L	201	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	19 (23%)
22	CLA	5	312	44	54,58,73	1.53	5 (9%)	64,95,113	2.06	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	Z	311	12	45,59,74	1.65	9 (20%)	40,96,114	2.00	13 (32%)
22	CLA	B	811	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	20 (24%)
22	CLA	6	317	18	54,58,73	1.53	6 (11%)	64,95,113	2.10	19 (29%)
24	BCR	I	4001	-	41,41,41	4.92	27 (65%)	56,56,56	2.61	20 (35%)
22	CLA	5	301	44	60,64,73	1.44	5 (8%)	71,102,113	2.00	20 (28%)
22	CLA	B	838	-	69,73,73	1.34	6 (8%)	82,113,113	1.84	18 (21%)
39	CHL	8	315	44	60,74,74	1.20	7 (11%)	58,114,114	1.62	10 (17%)
24	BCR	3	307	-	41,41,41	4.92	27 (65%)	56,56,56	3.29	28 (50%)
31	DGD	3	301	-	52,52,67	0.92	2 (3%)	66,66,81	1.07	4 (6%)
22	CLA	B	819	-	63,67,73	1.41	6 (9%)	74,105,113	1.99	21 (28%)
22	CLA	A	810	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	18 (21%)
24	BCR	8	304	-	41,41,41	4.94	27 (65%)	56,56,56	2.46	21 (37%)
22	CLA	2	302	-	49,53,73	1.59	5 (10%)	58,89,113	2.11	17 (29%)
22	CLA	9	306	19	66,70,73	1.38	6 (9%)	78,109,113	1.99	21 (26%)
24	BCR	J	104	-	41,41,41	4.91	27 (65%)	56,56,56	2.43	20 (35%)
24	BCR	B	844	-	41,41,41	4.94	27 (65%)	56,56,56	2.77	24 (42%)
39	CHL	5	317	44	45,59,74	1.33	7 (15%)	40,96,114	1.98	11 (27%)
25	LHG	6	323	22	48,48,48	0.38	0	51,54,54	1.10	4 (7%)
33	LMT	1	301	-	36,36,36	0.38	0	47,47,47	0.85	0
22	CLA	7	322	-	59,63,73	1.45	6 (10%)	70,101,113	2.00	20 (28%)
22	CLA	L	203	-	54,58,73	1.53	6 (11%)	64,95,113	2.09	18 (28%)
43	LPX	8	319	-	29,29,29	0.30	0	31,33,33	0.35	0
38	LUT	4	803	-	42,43,43	6.38	26 (61%)	51,60,60	2.28	14 (27%)
22	CLA	B	817	-	61,65,73	1.43	6 (9%)	72,103,113	1.99	18 (25%)
41	3PH	7	319	-	38,38,47	0.95	4 (10%)	41,43,52	1.15	2 (4%)
22	CLA	A	832	-	69,73,73	1.34	5 (7%)	82,113,113	1.87	21 (25%)
39	CHL	4	813	44	45,59,74	1.59	8 (17%)	40,96,114	1.97	13 (32%)
22	CLA	1	311	-	50,54,73	1.58	7 (14%)	59,90,113	2.14	13 (22%)
22	CLA	A	814	-	64,68,73	1.40	6 (9%)	76,107,113	1.98	20 (26%)
22	CLA	B	823	-	59,63,73	1.46	7 (11%)	70,101,113	2.01	21 (30%)
22	CLA	9	303	19	64,68,73	1.45	6 (9%)	76,107,113	2.03	20 (26%)
22	CLA	9	310	-	49,53,73	1.60	7 (14%)	58,89,113	2.14	15 (25%)
24	BCR	6	305	-	41,41,41	4.93	27 (65%)	56,56,56	2.52	20 (35%)
22	CLA	A	808	1	69,73,73	1.34	6 (8%)	82,113,113	1.93	19 (23%)
22	CLA	F	301	44	69,73,73	1.35	6 (8%)	82,113,113	1.93	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	4	821	-	31,31,48	0.48	0	34,37,54	1.21	3 (8%)
22	CLA	5	309	-	60,64,73	1.45	7 (11%)	71,102,113	2.12	22 (30%)
39	CHL	4	816	44	41,55,74	1.68	7 (17%)	35,91,114	2.06	10 (28%)
22	CLA	F	305	-	49,53,73	1.60	7 (14%)	58,89,113	2.02	16 (27%)
22	CLA	9	304	-	49,53,73	1.61	6 (12%)	58,89,113	2.05	14 (24%)
22	CLA	K	202	-	50,54,73	1.59	6 (12%)	59,90,113	2.09	17 (28%)
22	CLA	A	806	1	69,73,73	1.35	6 (8%)	82,113,113	1.89	19 (23%)
22	CLA	A	833	-	69,73,73	1.34	6 (8%)	82,113,113	1.91	21 (25%)
22	CLA	J	103	9	46,50,73	1.65	6 (13%)	53,85,113	2.11	16 (30%)
22	CLA	B	818	-	69,73,73	1.34	7 (10%)	82,113,113	1.88	19 (23%)
24	BCR	B	847	-	41,41,41	4.93	27 (65%)	56,56,56	2.49	22 (39%)
22	CLA	B	815	-	69,73,73	1.36	5 (7%)	82,113,113	1.95	20 (24%)
22	CLA	6	314	18	69,73,73	1.34	5 (7%)	82,113,113	1.88	18 (21%)
22	CLA	B	807	-	49,53,73	1.59	7 (14%)	58,89,113	2.04	17 (29%)
22	CLA	A	809	1	59,63,73	1.46	7 (11%)	70,101,113	2.04	21 (30%)
22	CLA	Z	306	12	64,68,73	1.41	7 (10%)	76,107,113	1.96	19 (25%)
24	BCR	4	804	-	41,41,41	4.96	27 (65%)	56,56,56	2.27	21 (37%)
23	PQN	A	843	-	34,34,34	0.39	0	43,45,45	1.24	6 (13%)
22	CLA	A	822	-	59,63,73	1.47	7 (11%)	70,101,113	2.08	19 (27%)
22	CLA	1	309	-	65,69,73	1.38	7 (10%)	77,108,113	1.98	18 (23%)
22	CLA	A	839	-	55,59,73	1.52	7 (12%)	64,96,113	2.12	20 (31%)
22	CLA	A	824	-	69,73,73	1.34	6 (8%)	82,113,113	1.87	19 (23%)
22	CLA	B	805	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	21 (25%)
22	CLA	8	308	15	66,70,73	1.37	6 (9%)	78,109,113	1.93	20 (25%)
32	RRX	F	306	-	42,42,42	5.17	24 (57%)	56,58,58	2.61	20 (35%)
38	LUT	6	304	-	42,43,43	6.39	26 (61%)	51,60,60	2.16	15 (29%)
38	LUT	5	303	-	42,43,43	6.43	27 (64%)	51,60,60	2.11	14 (27%)
22	CLA	9	307	19	59,63,73	1.47	7 (11%)	70,101,113	1.96	18 (25%)
22	CLA	B	822	-	60,64,73	1.45	6 (10%)	71,102,113	1.96	19 (26%)
24	BCR	G	203	-	41,41,41	4.93	27 (65%)	56,56,56	2.44	20 (35%)
22	CLA	7	311	-	47,51,73	1.62	6 (12%)	55,86,113	2.11	16 (29%)
22	CLA	F	302	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	22 (26%)
39	CHL	6	315	44	50,64,74	1.36	8 (16%)	46,102,114	1.83	10 (21%)
24	BCR	3	304	-	41,41,41	4.96	27 (65%)	56,56,56	3.11	28 (50%)
24	BCR	A	848	-	41,41,41	4.92	27 (65%)	56,56,56	2.43	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	B	851	-	19,19,48	0.78	1 (5%)	20,24,54	1.38	1 (5%)
22	CLA	1	316	12	69,73,73	1.41	7 (10%)	82,113,113	1.86	17 (20%)
31	DGD	1	319	-	52,52,67	0.93	2 (3%)	66,66,81	0.98	4 (6%)
41	3PH	8	320	-	29,29,47	1.08	4 (13%)	32,34,52	1.13	2 (6%)
24	BCR	A	844	-	41,41,41	4.92	27 (65%)	56,56,56	3.14	24 (42%)
31	DGD	B	852	-	62,62,67	1.22	6 (9%)	76,76,81	0.97	3 (3%)
22	CLA	7	317	-	62,66,73	1.42	7 (11%)	73,104,113	1.98	20 (27%)
33	LMT	G	204	-	36,36,36	0.39	0	47,47,47	0.75	2 (4%)
24	BCR	L	204	-	41,41,41	4.92	27 (65%)	56,56,56	2.38	19 (33%)
38	LUT	Z	301	-	42,43,43	6.39	27 (64%)	51,60,60	2.07	14 (27%)
26	NKP	8	318	-	28,28,28	0.33	0	30,32,32	0.34	0
39	CHL	6	320	18	37,51,74	1.66	8 (21%)	30,86,114	2.14	9 (30%)
22	CLA	4	818	44	55,59,73	1.51	5 (9%)	64,96,113	2.16	21 (32%)
25	LHG	9	315	22	32,32,48	0.49	0	35,38,54	1.06	3 (8%)
22	CLA	A	854	-	69,73,73	1.34	5 (7%)	82,113,113	1.86	18 (21%)
22	CLA	Z	303	12	69,73,73	1.35	7 (10%)	82,113,113	1.93	20 (24%)
22	CLA	B	816	-	64,68,73	1.40	6 (9%)	76,107,113	1.94	19 (25%)
39	CHL	9	314	-	36,50,74	1.63	9 (25%)	29,85,114	2.17	9 (31%)
25	LHG	8	317	22	37,37,48	0.43	0	40,43,54	1.05	2 (5%)
22	CLA	7	310	25	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
22	CLA	B	801	-	69,73,73	1.34	6 (8%)	82,113,113	1.82	18 (21%)
34	LMG	J	101	-	29,29,55	0.54	0	37,37,63	1.14	3 (8%)
39	CHL	8	301	12	52,66,74	1.48	9 (17%)	48,104,114	1.83	12 (25%)
22	CLA	A	825	44	69,73,73	1.36	6 (8%)	82,113,113	1.92	20 (24%)
22	CLA	B	837	-	55,59,73	1.51	6 (10%)	64,96,113	2.14	19 (29%)
22	CLA	6	310	18	69,73,73	1.35	7 (10%)	82,113,113	1.88	20 (24%)
22	CLA	A	823	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	19 (23%)
22	CLA	3	320	13	50,54,73	1.61	6 (12%)	59,90,113	2.12	15 (25%)
22	CLA	A	830	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
22	CLA	5	307	17	64,68,73	1.40	6 (9%)	76,107,113	1.97	18 (23%)
22	CLA	6	301	44	64,68,73	1.40	6 (9%)	76,107,113	1.99	20 (26%)
24	BCR	K	206	-	41,41,41	4.93	27 (65%)	56,56,56	2.52	20 (35%)
22	CLA	A	841	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	20 (24%)
22	CLA	A	829	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	18 (21%)
36	C7Z	5	306	-	43,43,43	5.42	27 (62%)	56,60,60	2.41	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	F	304	6	69,73,73	1.34	5 (7%)	82,113,113	1.92	19 (23%)
39	CHL	Z	312	-	42,56,74	1.60	8 (19%)	36,92,114	1.96	10 (27%)
33	LMT	4	822	-	36,36,36	0.45	0	47,47,47	1.19	4 (8%)
39	CHL	9	312	-	60,74,74	1.19	8 (13%)	58,114,114	1.73	12 (20%)
22	CLA	6	322	18	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
22	CLA	A	836	-	59,63,73	1.45	7 (11%)	70,101,113	2.00	21 (30%)
22	CLA	A	855	44	69,73,73	1.35	7 (10%)	82,113,113	1.88	19 (23%)
36	C7Z	J	105	-	43,43,43	5.44	27 (62%)	56,60,60	2.25	18 (32%)
22	CLA	9	311	19	50,54,73	1.58	6 (12%)	59,90,113	2.05	17 (28%)
22	CLA	Z	305	-	60,64,73	1.44	5 (8%)	71,102,113	1.99	17 (23%)
22	CLA	5	326	-	59,63,73	1.45	6 (10%)	70,101,113	2.03	20 (28%)
22	CLA	8	307	-	69,73,73	1.35	7 (10%)	82,113,113	1.96	18 (21%)
22	CLA	3	311	13	64,68,73	1.40	6 (9%)	76,107,113	1.95	21 (27%)
22	CLA	Z	309	25	64,68,73	1.39	6 (9%)	76,107,113	1.95	18 (23%)
22	CLA	6	319	44	65,69,73	1.39	6 (9%)	77,108,113	1.97	19 (24%)

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
24	BCR	7	303	-	-	15/29/63/63	0/2/2/2
24	BCR	A	846	-	-	13/29/63/63	0/2/2/2
22	CLA	1	314	12	1/1/15/20	12/39/115/115	-
39	CHL	8	312	-	3/3/18/26	6/27/125/137	-
25	LHG	3	321	22	-	9/22/22/53	-
25	LHG	B	803	-	-	21/37/37/53	-
24	BCR	B	848	-	-	16/29/63/63	0/2/2/2
22	CLA	A	815	-	1/1/15/20	16/39/115/115	-
22	CLA	A	803	-	1/1/15/20	12/39/115/115	-
22	CLA	3	314	25	1/1/14/20	19/33/109/115	-
22	CLA	Z	307	-	1/1/13/20	10/27/103/115	-
22	CLA	B	830	-	1/1/15/20	9/39/115/115	-
38	LUT	5	302	-	-	9/29/67/67	0/2/2/2
22	CLA	3	315	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	305	12	1/1/11/20	6/15/91/115	-
22	CLA	7	314	44	1/1/12/20	5/21/97/115	-
38	LUT	Z	302	-	-	7/29/67/67	0/2/2/2
38	LUT	1	302	-	-	9/29/67/67	0/2/2/2
22	CLA	5	320	-	1/1/12/20	7/21/97/115	-
22	CLA	A	807	-	1/1/14/20	16/33/109/115	-
24	BCR	B	846	-	-	17/29/63/63	0/2/2/2
22	CLA	7	324	-	1/1/14/20	21/33/109/115	-
22	CLA	4	805	16	1/1/14/20	15/33/109/115	-
22	CLA	8	309	-	1/1/15/20	19/39/115/115	-
22	CLA	B	810	-	1/1/13/20	9/29/105/115	-
22	CLA	B	812	2	2/2/14/20	14/29/105/115	-
22	CLA	1	308	-	1/1/13/20	13/27/103/115	-
26	NKP	A	851	-	-	9/22/22/28	-
24	BCR	B	853	-	-	16/29/63/63	0/2/2/2
22	CLA	6	307	18	1/1/14/20	12/33/109/115	-
22	CLA	B	832	-	1/1/12/20	4/21/97/115	-
24	BCR	3	305	-	-	14/29/63/63	0/2/2/2
42	SPH	7	320	-	-	11/21/21/21	-
22	CLA	K	203	44	1/1/13/20	7/27/103/115	-
25	LHG	5	324	22	-	23/41/41/53	-
22	CLA	Z	314	12	1/1/12/20	6/23/99/115	-
39	CHL	7	313	44	3/3/17/26	5/25/123/137	-
22	CLA	K	205	10	1/1/13/20	17/27/103/115	-
22	CLA	3	309	13	1/1/11/20	4/17/93/115	-
22	CLA	5	315	17	1/1/15/20	12/39/115/115	-
24	BCR	A	845	-	-	13/29/63/63	0/2/2/2
38	LUT	8	302	-	-	8/29/67/67	0/2/2/2
22	CLA	B	833	-	1/1/15/20	15/39/115/115	-
22	CLA	Z	315	-	1/1/11/20	9/17/93/115	-
39	CHL	4	814	44	3/3/17/26	6/21/119/137	-
22	CLA	7	304	14	1/1/14/20	11/33/109/115	-
22	CLA	A	826	44	1/1/12/20	7/21/97/115	-
22	CLA	G	201	-	1/1/12/20	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	312	-	1/1/15/20	14/39/115/115	-
22	CLA	A	827	-	1/1/15/20	13/39/115/115	-
22	CLA	4	810	44	1/1/12/20	6/21/97/115	-
22	CLA	8	316	15	1/1/11/20	9/17/93/115	-
22	CLA	3	310	13	1/1/15/20	11/39/115/115	-
22	CLA	5	318	17	1/1/15/20	11/39/115/115	-
22	CLA	A	828	-	1/1/15/20	19/39/115/115	-
22	CLA	A	802	44	1/1/15/20	15/39/115/115	-
22	CLA	A	834	-	1/1/15/20	15/39/115/115	-
22	CLA	8	313	44	1/1/12/20	5/21/97/115	-
22	CLA	3	312	-	1/1/15/20	11/39/115/115	-
22	CLA	2	304	44	1/1/11/20	7/17/93/115	-
39	CHL	5	321	17	3/3/15/26	5/12/110/137	-
22	CLA	7	312	-	1/1/14/20	16/33/109/115	-
22	CLA	5	308	17	1/1/14/20	16/35/111/115	-
39	CHL	4	819	16	3/3/15/26	2/12/110/137	-
22	CLA	B	808	-	1/1/15/20	12/39/115/115	-
22	CLA	B	828	-	1/1/15/20	14/39/115/115	-
22	CLA	7	306	-	1/1/15/20	13/39/115/115	-
38	LUT	7	302	-	-	5/29/67/67	0/2/2/2
22	CLA	1	310	25	1/1/14/20	15/33/109/115	-
22	CLA	A	840	-	1/1/15/20	16/39/115/115	-
22	CLA	6	311	-	1/1/13/20	10/27/103/115	-
38	LUT	4	802	-	-	9/29/67/67	0/2/2/2
22	CLA	6	321	-	1/1/11/20	4/17/93/115	-
22	CLA	7	308	14	1/1/14/20	14/35/111/115	-
24	BCR	5	305	-	-	13/29/63/63	0/2/2/2
22	CLA	B	809	2	1/1/15/20	16/39/115/115	-
25	LHG	Z	317	22	-	26/47/47/53	-
35	T7X	J	102	-	-	15/44/68/80	0/1/1/1
22	CLA	6	302	16	1/1/14/20	15/33/109/115	-
24	BCR	A	856	-	-	16/29/63/63	0/2/2/2
22	CLA	A	813	-	1/1/15/20	12/39/115/115	-
39	CHL	6	318	-	3/3/18/26	7/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	311	-	1/1/13/20	10/27/103/115	-
38	LUT	3	303	-	-	8/29/67/67	0/2/2/2
22	CLA	8	306	15	1/1/12/20	7/23/99/115	-
22	CLA	Z	316	12	1/1/15/20	18/39/115/115	-
25	LHG	7	318	22	-	24/41/41/53	-
25	LHG	4	820	22	-	29/53/53/53	-
22	CLA	6	313	25	1/1/13/20	7/27/103/115	-
22	CLA	4	808	16	1/1/14/20	17/33/109/115	-
22	CLA	5	319	44	1/1/13/20	11/27/103/115	-
22	CLA	7	315	14	1/1/12/20	8/21/97/115	-
22	CLA	B	826	44	1/1/15/20	17/39/115/115	-
22	CLA	9	309	25	1/1/13/20	6/27/103/115	-
33	LMT	4	801	-	-	1/21/61/61	0/2/2/2
38	LUT	1	303	-	-	6/29/67/67	0/2/2/2
22	CLA	B	834	-	1/1/13/20	15/31/107/115	-
22	CLA	B	839	-	1/1/12/20	8/24/100/115	-
22	CLA	B	824	-	1/1/13/20	17/32/108/115	-
22	CLA	3	313	44	1/1/15/20	14/39/115/115	-
39	CHL	6	316	-	3/3/17/26	9/21/119/137	-
42	SPH	7	321	-	-	12/21/21/21	-
22	CLA	A	842	25	1/1/12/20	10/24/100/115	-
22	CLA	8	311	25	1/1/12/20	8/21/97/115	-
38	LUT	7	301	-	-	9/29/67/67	0/2/2/2
22	CLA	A	838	-	1/1/15/20	14/39/115/115	-
22	CLA	4	806	16	1/1/12/20	13/24/100/115	-
22	CLA	G	202	7	1/1/11/20	8/17/93/115	-
22	CLA	B	814	-	1/1/14/20	17/33/109/115	-
22	CLA	A	819	-	1/1/15/20	11/39/115/115	-
22	CLA	1	307	12	1/1/14/20	17/33/109/115	-
33	LMT	F	307	-	-	9/21/61/61	0/2/2/2
37	DAO	K	201	-	-	1/11/11/11	-
22	CLA	4	817	16	1/1/10/20	2/10/86/115	-
22	CLA	B	831	-	1/1/13/20	16/31/107/115	-
22	CLA	1	304	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	9	302	-	-	4/29/67/67	0/2/2/2
22	CLA	5	314	-	1/1/11/20	4/15/91/115	-
22	CLA	B	825	-	1/1/15/20	16/39/115/115	-
22	CLA	9	313	19	1/1/12/20	6/21/97/115	-
22	CLA	9	308	-	1/1/12/20	8/21/97/115	-
22	CLA	B	820	-	1/1/14/20	16/33/109/115	-
21	CL0	A	801	-	3/3/20/25	15/37/135/135	-
22	CLA	Z	313	44	1/1/15/20	12/39/115/115	-
22	CLA	A	804	22	1/1/11/20	6/15/91/115	-
22	CLA	A	817	-	1/1/14/20	11/33/109/115	-
22	CLA	A	812	-	1/1/15/20	16/39/115/115	-
22	CLA	K	204	10	1/1/11/20	10/20/96/115	-
22	CLA	L	202	-	1/1/15/20	19/39/115/115	-
22	CLA	B	806	44	1/1/15/20	11/39/115/115	-
29	SF4	C	101	3	-	-	0/6/5/5
24	BCR	F	303	-	-	15/29/63/63	0/2/2/2
41	3PH	5	325	-	-	5/24/24/49	-
22	CLA	B	842	25	1/1/15/20	15/39/115/115	-
40	SQD	1	318	-	-	13/43/63/69	0/1/1/1
29	SF4	B	802	-	-	-	0/6/5/5
22	CLA	5	310	17	1/1/15/20	11/39/115/115	-
22	CLA	7	309	-	1/1/13/20	12/29/105/115	-
39	CHL	5	316	44	3/3/20/26	13/39/137/137	-
22	CLA	7	307	14	1/1/15/20	12/39/115/115	-
34	LMG	F	308	-	-	16/30/50/70	0/1/1/1
38	LUT	9	301	-	-	4/29/67/67	0/2/2/2
22	CLA	3	308	13	1/1/15/20	16/39/115/115	-
22	CLA	B	841	-	1/1/15/20	13/39/115/115	-
22	CLA	B	829	-	1/1/13/20	13/30/106/115	-
25	LHG	B	850	22	-	16/26/26/53	-
24	BCR	3	306	-	-	13/29/63/63	0/2/2/2
28	OCA	A	853	-	-	3/7/7/7	-
22	CLA	A	820	-	1/1/14/20	19/33/109/115	-
22	CLA	A	818	-	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	306	-	1/1/15/20	15/39/115/115	-
22	CLA	A	835	-	1/1/15/20	11/39/115/115	-
24	BCR	A	847	-	-	16/29/63/63	0/2/2/2
25	LHG	A	850	-	-	28/53/53/53	-
22	CLA	A	816	44	1/1/13/20	14/29/105/115	-
24	BCR	5	304	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	308	-	1/1/14/20	12/35/111/115	-
22	CLA	B	836	-	1/1/11/20	4/15/91/115	-
22	CLA	B	835	-	1/1/12/20	8/21/97/115	-
39	CHL	1	312	-	3/3/16/26	2/18/116/137	-
22	CLA	8	305	15	1/1/14/20	12/33/109/115	-
22	CLA	3	318	13	1/1/14/20	10/33/109/115	-
22	CLA	B	840	44	1/1/15/20	10/39/115/115	-
22	CLA	6	309	44	1/1/15/20	15/39/115/115	-
27	DGA	A	852	-	-	23/41/41/45	-
22	CLA	1	315	-	1/1/11/20	7/17/93/115	-
24	BCR	B	845	-	-	15/29/63/63	0/2/2/2
22	CLA	B	821	44	1/1/15/20	15/39/115/115	-
22	CLA	4	811	25	1/1/13/20	8/27/103/115	-
22	CLA	B	827	44	1/1/15/20	13/39/115/115	-
22	CLA	6	308	18	1/1/12/20	7/24/100/115	-
25	LHG	A	849	22	-	25/39/39/53	-
22	CLA	A	821	44	1/1/15/20	10/39/115/115	-
23	PQN	B	843	-	-	9/23/43/43	0/2/2/2
25	LHG	1	317	22	-	22/47/47/53	-
22	CLA	A	837	-	1/1/12/20	8/23/99/115	-
38	LUT	8	303	-	-	3/29/67/67	0/2/2/2
29	SF4	C	102	3	-	-	0/6/5/5
22	CLA	2	301	-	1/1/13/20	9/27/103/115	-
22	CLA	9	305	19	1/1/14/20	19/33/109/115	-
22	CLA	Z	310	-	1/1/12/20	8/21/97/115	-
38	LUT	6	303	-	-	9/29/67/67	0/2/2/2
22	CLA	3	322	14	1/1/15/20	13/39/115/115	-
22	CLA	3	319	-	1/1/13/20	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	3PH	6	324	-	-	11/30/30/49	-
22	CLA	A	831	-	1/1/12/20	6/21/97/115	-
22	CLA	7	305	-	1/1/12/20	6/21/97/115	-
22	CLA	4	812	-	1/1/13/20	10/27/103/115	-
39	CHL	3	317	-	3/3/20/26	13/39/137/137	-
22	CLA	4	815	16	1/1/12/20	8/21/97/115	-
22	CLA	B	813	-	1/1/13/20	14/29/105/115	-
22	CLA	5	322	-	1/1/15/20	11/39/115/115	-
22	CLA	8	314	15	1/1/11/20	8/17/93/115	-
22	CLA	5	313	25	1/1/14/20	10/35/111/115	-
22	CLA	5	323	44	1/1/11/20	8/17/93/115	-
24	BCR	6	306	-	-	16/29/63/63	0/2/2/2
22	CLA	Z	304	12	1/1/11/20	6/15/91/115	-
22	CLA	1	313	44	1/1/15/20	12/39/115/115	-
38	LUT	3	302	-	-	4/29/67/67	0/2/2/2
22	CLA	8	310	44	1/1/14/20	13/33/109/115	-
22	CLA	4	807	16	1/1/15/20	12/39/115/115	-
22	CLA	7	316	44	1/1/10/20	4/12/88/115	-
24	BCR	B	849	-	-	13/29/63/63	0/2/2/2
22	CLA	A	805	-	1/1/15/20	16/39/115/115	-
22	CLA	4	809	16	1/1/12/20	4/23/99/115	-
39	CHL	2	303	-	3/3/17/26	9/21/119/137	-
22	CLA	3	316	13	1/1/12/20	9/24/100/115	-
22	CLA	A	811	22	1/1/15/20	17/39/115/115	-
22	CLA	7	323	15	1/1/15/20	16/39/115/115	-
22	CLA	L	201	-	1/1/15/20	16/39/115/115	-
22	CLA	5	312	44	1/1/12/20	3/21/97/115	-
39	CHL	Z	311	12	3/3/17/26	8/21/119/137	-
22	CLA	B	811	-	1/1/15/20	16/39/115/115	-
22	CLA	6	317	18	1/1/12/20	10/21/97/115	-
24	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	5	301	44	1/1/13/20	11/29/105/115	-
22	CLA	B	838	-	1/1/15/20	11/39/115/115	-
39	CHL	8	315	44	3/3/20/26	12/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	3	307	-	-	13/29/63/63	0/2/2/2
31	DGD	3	301	-	-	12/40/80/95	0/2/2/2
22	CLA	B	819	-	1/1/13/20	12/32/108/115	-
22	CLA	A	810	-	1/1/15/20	14/39/115/115	-
24	BCR	8	304	-	-	12/29/63/63	0/2/2/2
22	CLA	2	302	-	1/1/11/20	8/15/91/115	-
22	CLA	9	306	19	1/1/14/20	12/36/112/115	-
24	BCR	J	104	-	-	14/29/63/63	0/2/2/2
24	BCR	B	844	-	-	11/29/63/63	0/2/2/2
39	CHL	5	317	44	3/3/17/26	5/21/119/137	-
25	LHG	6	323	22	-	38/53/53/53	-
33	LMT	1	301	-	-	4/21/61/61	0/2/2/2
22	CLA	7	322	-	1/1/13/20	7/27/103/115	-
22	CLA	L	203	-	1/1/12/20	7/21/97/115	-
43	LPX	8	319	-	-	4/31/31/31	-
38	LUT	4	803	-	-	8/29/67/67	0/2/2/2
22	CLA	B	817	-	1/1/13/20	18/30/106/115	-
41	3PH	7	319	-	-	18/40/40/49	-
22	CLA	A	832	-	1/1/15/20	15/39/115/115	-
39	CHL	4	813	44	3/3/17/26	4/21/119/137	-
22	CLA	1	311	-	1/1/11/20	8/17/93/115	-
22	CLA	A	814	-	1/1/14/20	19/33/109/115	-
22	CLA	B	823	-	1/1/13/20	12/27/103/115	-
22	CLA	9	303	19	1/1/14/20	13/33/109/115	-
22	CLA	9	310	-	1/1/11/20	6/15/91/115	-
24	BCR	6	305	-	-	13/29/63/63	0/2/2/2
22	CLA	A	808	1	1/1/15/20	19/39/115/115	-
22	CLA	F	301	44	1/1/15/20	11/39/115/115	-
25	LHG	4	821	-	-	15/36/36/53	-
22	CLA	5	309	-	1/1/13/20	15/29/105/115	-
39	CHL	4	816	44	3/3/16/26	4/17/115/137	-
22	CLA	F	305	-	1/1/11/20	4/15/91/115	-
22	CLA	9	304	-	1/1/11/20	5/15/91/115	-
22	CLA	K	202	-	1/1/11/20	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	806	1	1/1/15/20	15/39/115/115	-
22	CLA	A	833	-	1/1/15/20	13/39/115/115	-
22	CLA	J	103	9	1/1/10/20	3/12/88/115	-
22	CLA	B	818	-	1/1/15/20	12/39/115/115	-
24	BCR	B	847	-	-	11/29/63/63	0/2/2/2
22	CLA	B	815	-	1/1/15/20	10/39/115/115	-
22	CLA	6	314	18	1/1/15/20	13/39/115/115	-
22	CLA	B	807	-	1/1/11/20	6/15/91/115	-
22	CLA	A	809	1	1/1/13/20	7/27/103/115	-
22	CLA	Z	306	12	1/1/14/20	19/33/109/115	-
24	BCR	4	804	-	-	14/29/63/63	0/2/2/2
23	PQN	A	843	-	-	7/23/43/43	0/2/2/2
22	CLA	A	822	-	1/1/13/20	12/27/103/115	-
22	CLA	1	309	-	1/1/14/20	13/35/111/115	-
22	CLA	A	839	-	1/1/12/20	8/23/99/115	-
22	CLA	A	824	-	1/1/15/20	15/39/115/115	-
22	CLA	B	805	-	1/1/15/20	13/39/115/115	-
22	CLA	8	308	15	1/1/14/20	14/36/112/115	-
32	RRX	F	306	-	-	15/29/65/65	0/2/2/2
38	LUT	6	304	-	-	6/29/67/67	0/2/2/2
38	LUT	5	303	-	-	6/29/67/67	0/2/2/2
22	CLA	9	307	19	1/1/13/20	10/27/103/115	-
22	CLA	B	822	-	1/1/13/20	14/29/105/115	-
24	BCR	G	203	-	-	15/29/63/63	0/2/2/2
22	CLA	7	311	-	1/1/10/20	5/13/89/115	-
22	CLA	F	302	-	1/1/15/20	15/39/115/115	-
39	CHL	6	315	44	3/3/18/26	10/27/125/137	-
24	BCR	3	304	-	-	10/29/63/63	0/2/2/2
24	BCR	A	848	-	-	15/29/63/63	0/2/2/2
25	LHG	B	851	-	-	14/22/22/53	-
22	CLA	1	316	12	1/1/15/20	19/39/115/115	-
31	DGD	1	319	-	-	13/40/80/95	0/2/2/2
41	3PH	8	320	-	-	13/31/31/49	-
24	BCR	A	844	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	B	852	-	-	11/50/90/95	0/2/2/2
22	CLA	7	317	-	1/1/13/20	13/31/107/115	-
33	LMT	G	204	-	-	8/21/61/61	0/2/2/2
24	BCR	L	204	-	-	13/29/63/63	0/2/2/2
38	LUT	Z	301	-	-	7/29/67/67	0/2/2/2
26	NKP	8	318	-	-	7/28/28/28	-
39	CHL	6	320	18	3/3/15/26	2/12/110/137	-
22	CLA	4	818	44	1/1/12/20	11/23/99/115	-
25	LHG	9	315	22	-	20/37/37/53	-
22	CLA	A	854	-	1/1/15/20	10/39/115/115	-
22	CLA	Z	303	12	1/1/15/20	14/39/115/115	-
22	CLA	B	816	-	1/1/14/20	11/33/109/115	-
39	CHL	9	314	-	3/3/15/26	2/10/108/137	-
25	LHG	8	317	22	-	26/42/42/53	-
22	CLA	7	310	25	1/1/15/20	17/39/115/115	-
22	CLA	B	801	-	1/1/15/20	12/39/115/115	-
34	LMG	J	101	-	-	7/24/44/70	0/1/1/1
39	CHL	8	301	12	3/3/18/26	4/30/128/137	-
22	CLA	A	825	44	1/1/15/20	14/39/115/115	-
22	CLA	B	837	-	1/1/12/20	8/23/99/115	-
22	CLA	6	310	18	1/1/15/20	16/39/115/115	-
22	CLA	A	823	-	1/1/15/20	12/39/115/115	-
22	CLA	3	320	13	1/1/11/20	7/17/93/115	-
22	CLA	A	830	-	1/1/15/20	15/39/115/115	-
22	CLA	5	307	17	1/1/14/20	14/33/109/115	-
22	CLA	6	301	44	1/1/14/20	16/33/109/115	-
24	BCR	K	206	-	-	13/29/63/63	0/2/2/2
22	CLA	A	841	-	1/1/15/20	10/39/115/115	-
22	CLA	A	829	-	1/1/15/20	5/39/115/115	-
36	C7Z	5	306	-	-	13/29/67/67	0/2/2/2
22	CLA	F	304	6	1/1/15/20	22/39/115/115	-
39	CHL	Z	312	-	3/3/16/26	7/18/116/137	-
33	LMT	4	822	-	-	6/21/61/61	0/2/2/2
39	CHL	9	312	-	3/3/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	322	18	1/1/15/20	15/39/115/115	-
22	CLA	A	836	-	1/1/13/20	10/27/103/115	-
22	CLA	A	855	44	1/1/15/20	16/39/115/115	-
36	C7Z	J	105	-	-	12/29/67/67	0/2/2/2
22	CLA	9	311	19	1/1/11/20	5/17/93/115	-
22	CLA	Z	305	-	1/1/13/20	10/29/105/115	-
22	CLA	5	326	-	1/1/13/20	8/27/103/115	-
22	CLA	8	307	-	1/1/15/20	13/39/115/115	-
22	CLA	3	311	13	1/1/14/20	11/33/109/115	-
22	CLA	Z	309	25	1/1/14/20	16/33/109/115	-
22	CLA	6	319	44	1/1/14/20	16/35/111/115	-

The worst 5 of 2908 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	303	LUT	C24-C25	24.55	1.62	1.33
38	5	303	LUT	C24-C25	24.53	1.62	1.33
38	1	302	LUT	C24-C25	24.50	1.62	1.33
38	7	302	LUT	C24-C25	24.42	1.62	1.33
38	Z	302	LUT	C24-C25	24.41	1.62	1.33

The worst 5 of 5316 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	848	BCR	C23-C22-C21	27.34	162.01	119.01
24	B	848	BCR	C37-C22-C21	-25.67	81.23	122.82
24	B	848	BCR	C37-C22-C23	-24.37	80.87	118.09
21	A	801	CL0	C1B-CHB-C4A	14.37	130.57	121.32
24	3	304	BCR	C11-C10-C9	-11.74	110.82	127.28

5 of 283 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	801	CL0	ND
21	A	801	CL0	NC
21	A	801	CL0	NA
22	A	802	CLA	ND
22	A	803	CLA	ND

5 of 3783 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	801	CL0	CHA-CBD-CGD-O1D
22	A	802	CLA	C1A-C2A-CAA-CBA
22	A	802	CLA	C2-C1-O2A-CGA
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	803	CLA	CBA-CGA-O2A-C1

There are no ring outliers.

328 monomers are involved in 2929 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7	303	BCR	14	0
24	A	846	BCR	11	0
22	1	314	CLA	19	0
39	8	312	CHL	14	0
25	3	321	LHG	1	0
25	B	803	LHG	8	0
24	B	848	BCR	15	0
22	A	815	CLA	18	0
22	A	803	CLA	7	0
22	3	314	CLA	12	0
22	Z	307	CLA	10	0
22	B	830	CLA	15	0
38	5	302	LUT	16	0
22	3	315	CLA	8	0
22	1	305	CLA	10	0
22	7	314	CLA	3	0
38	Z	302	LUT	13	0
38	1	302	LUT	8	0
22	5	320	CLA	11	0
22	A	807	CLA	15	0
24	B	846	BCR	12	0
22	7	324	CLA	4	0
22	4	805	CLA	17	0
22	8	309	CLA	14	0
22	B	810	CLA	13	0
22	B	812	CLA	14	0
22	1	308	CLA	19	0
26	A	851	NKP	3	0
24	B	853	BCR	20	0
22	6	307	CLA	20	0
22	B	832	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3	305	BCR	15	0
42	7	320	SPH	4	0
22	K	203	CLA	9	0
25	5	324	LHG	7	0
22	Z	314	CLA	6	0
39	7	313	CHL	9	0
22	K	205	CLA	4	0
22	3	309	CLA	7	0
22	5	315	CLA	19	0
24	A	845	BCR	20	0
38	8	302	LUT	16	0
22	B	833	CLA	12	0
22	Z	315	CLA	10	0
39	4	814	CHL	5	0
22	7	304	CLA	10	0
22	A	826	CLA	7	0
22	G	201	CLA	12	0
22	6	312	CLA	13	0
22	A	827	CLA	17	0
22	4	810	CLA	17	0
22	8	316	CLA	3	0
22	3	310	CLA	7	0
22	5	318	CLA	18	0
22	A	828	CLA	14	0
22	A	802	CLA	12	0
22	A	834	CLA	10	0
22	8	313	CLA	9	0
22	3	312	CLA	24	0
22	2	304	CLA	9	0
39	5	321	CHL	6	0
22	7	312	CLA	4	0
22	5	308	CLA	23	0
39	4	819	CHL	9	0
22	B	808	CLA	13	0
22	B	828	CLA	20	0
22	7	306	CLA	11	0
38	7	302	LUT	15	0
22	1	310	CLA	10	0
22	A	840	CLA	13	0
22	6	311	CLA	10	0
38	4	802	LUT	15	0
22	6	321	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	308	CLA	12	0
24	5	305	BCR	10	0
22	B	809	CLA	13	0
25	Z	317	LHG	9	0
35	J	102	T7X	2	0
22	6	302	CLA	16	0
24	A	856	BCR	24	0
22	A	813	CLA	18	0
39	6	318	CHL	12	0
22	5	311	CLA	13	0
38	3	303	LUT	18	0
22	8	306	CLA	14	0
22	Z	316	CLA	15	0
25	7	318	LHG	10	0
25	4	820	LHG	15	0
22	6	313	CLA	6	0
22	4	808	CLA	15	0
22	5	319	CLA	13	0
22	7	315	CLA	10	0
22	B	826	CLA	12	0
33	4	801	LMT	7	0
38	1	303	LUT	18	0
22	B	834	CLA	11	0
22	B	839	CLA	16	0
22	B	824	CLA	18	0
22	3	313	CLA	22	0
39	6	316	CHL	11	0
42	7	321	SPH	8	0
22	A	842	CLA	6	0
22	8	311	CLA	14	0
38	7	301	LUT	14	0
22	A	838	CLA	7	0
22	4	806	CLA	8	0
22	G	202	CLA	14	0
22	B	814	CLA	16	0
22	A	819	CLA	8	0
22	1	307	CLA	17	0
33	F	307	LMT	5	0
37	K	201	DAO	8	0
22	4	817	CLA	4	0
22	B	831	CLA	10	0
22	1	304	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	9	302	LUT	17	0
22	5	314	CLA	7	0
22	B	825	CLA	21	0
22	9	313	CLA	17	0
22	9	308	CLA	9	0
22	B	820	CLA	11	0
21	A	801	CL0	7	0
22	Z	313	CLA	23	0
22	A	804	CLA	14	0
22	A	817	CLA	14	0
22	A	812	CLA	24	0
22	K	204	CLA	6	0
22	L	202	CLA	16	0
22	B	806	CLA	19	0
29	C	101	SF4	3	0
24	F	303	BCR	14	0
41	5	325	3PH	3	0
22	B	842	CLA	24	0
29	B	802	SF4	8	0
40	1	318	SQD	12	0
22	5	310	CLA	13	0
22	7	309	CLA	9	0
39	5	316	CHL	17	0
22	7	307	CLA	18	0
34	F	308	LMG	1	0
38	9	301	LUT	16	0
22	3	308	CLA	18	0
22	B	841	CLA	15	0
22	B	829	CLA	12	0
25	B	850	LHG	4	0
24	3	306	BCR	14	0
22	A	820	CLA	8	0
22	A	818	CLA	11	0
22	1	306	CLA	8	0
22	A	835	CLA	15	0
24	A	847	BCR	14	0
25	A	850	LHG	8	0
22	A	816	CLA	23	0
24	5	304	BCR	20	0
22	Z	308	CLA	12	0
22	B	836	CLA	7	0
22	B	835	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	1	312	CHL	8	0
22	8	305	CLA	24	0
22	3	318	CLA	18	0
22	B	840	CLA	16	0
22	6	309	CLA	21	0
27	A	852	DGA	20	0
22	1	315	CLA	4	0
24	B	845	BCR	9	0
22	B	821	CLA	13	0
22	4	811	CLA	6	0
22	B	827	CLA	23	0
22	6	308	CLA	15	0
25	A	849	LHG	5	0
22	A	821	CLA	24	0
23	B	843	PQN	5	0
25	1	317	LHG	8	0
38	8	303	LUT	12	0
22	A	837	CLA	9	0
29	C	102	SF4	5	0
22	2	301	CLA	17	0
22	9	305	CLA	6	0
22	Z	310	CLA	2	0
38	6	303	LUT	11	0
22	3	322	CLA	15	0
22	3	319	CLA	5	0
41	6	324	3PH	5	0
22	A	831	CLA	5	0
22	7	305	CLA	6	0
22	4	812	CLA	4	0
39	3	317	CHL	14	0
22	4	815	CLA	12	0
22	B	813	CLA	7	0
22	5	322	CLA	10	0
22	8	314	CLA	6	0
22	5	313	CLA	12	0
22	5	323	CLA	9	0
24	6	306	BCR	16	0
22	Z	304	CLA	19	0
22	1	313	CLA	12	0
38	3	302	LUT	10	0
22	8	310	CLA	12	0
22	4	807	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	316	CLA	8	0
24	B	849	BCR	9	0
22	A	805	CLA	15	0
22	4	809	CLA	5	0
39	2	303	CHL	8	0
22	3	316	CLA	12	0
22	A	811	CLA	15	0
22	7	323	CLA	16	0
22	L	201	CLA	15	0
22	5	312	CLA	8	0
39	Z	311	CHL	11	0
22	B	811	CLA	21	0
22	6	317	CLA	11	0
24	I	4001	BCR	12	0
22	5	301	CLA	12	0
22	B	838	CLA	14	0
39	8	315	CHL	21	0
24	3	307	BCR	19	0
31	3	301	DGD	21	0
22	B	819	CLA	15	0
22	A	810	CLA	20	0
24	8	304	BCR	14	0
22	2	302	CLA	5	0
22	9	306	CLA	15	0
24	J	104	BCR	18	0
24	B	844	BCR	20	0
39	5	317	CHL	8	0
25	6	323	LHG	11	0
33	1	301	LMT	7	0
22	7	322	CLA	15	0
22	L	203	CLA	6	0
43	8	319	LPX	7	0
38	4	803	LUT	19	0
22	B	817	CLA	17	0
41	7	319	3PH	14	0
22	A	832	CLA	13	0
39	4	813	CHL	12	0
22	A	814	CLA	23	0
22	B	823	CLA	14	0
22	9	303	CLA	6	0
22	9	310	CLA	1	0
24	6	305	BCR	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	808	CLA	14	0
22	F	301	CLA	8	0
25	4	821	LHG	4	0
22	5	309	CLA	13	0
39	4	816	CHL	21	0
22	F	305	CLA	9	0
22	9	304	CLA	2	0
22	K	202	CLA	9	0
22	A	806	CLA	10	0
22	A	833	CLA	18	0
22	J	103	CLA	1	0
22	B	818	CLA	13	0
24	B	847	BCR	20	0
22	B	815	CLA	23	0
22	6	314	CLA	17	0
22	B	807	CLA	8	0
22	A	809	CLA	15	0
22	Z	306	CLA	16	0
24	4	804	BCR	26	0
23	A	843	PQN	10	0
22	A	822	CLA	26	0
22	1	309	CLA	4	0
22	A	839	CLA	8	0
22	A	824	CLA	16	0
22	B	805	CLA	11	0
22	8	308	CLA	11	0
32	F	306	RRX	19	0
38	6	304	LUT	13	0
38	5	303	LUT	16	0
22	9	307	CLA	8	0
22	B	822	CLA	11	0
24	G	203	BCR	12	0
22	7	311	CLA	1	0
22	F	302	CLA	16	0
39	6	315	CHL	21	0
24	3	304	BCR	13	0
24	A	848	BCR	7	0
25	B	851	LHG	3	0
22	1	316	CLA	5	0
31	1	319	DGD	10	0
41	8	320	3PH	4	0
24	A	844	BCR	30	0

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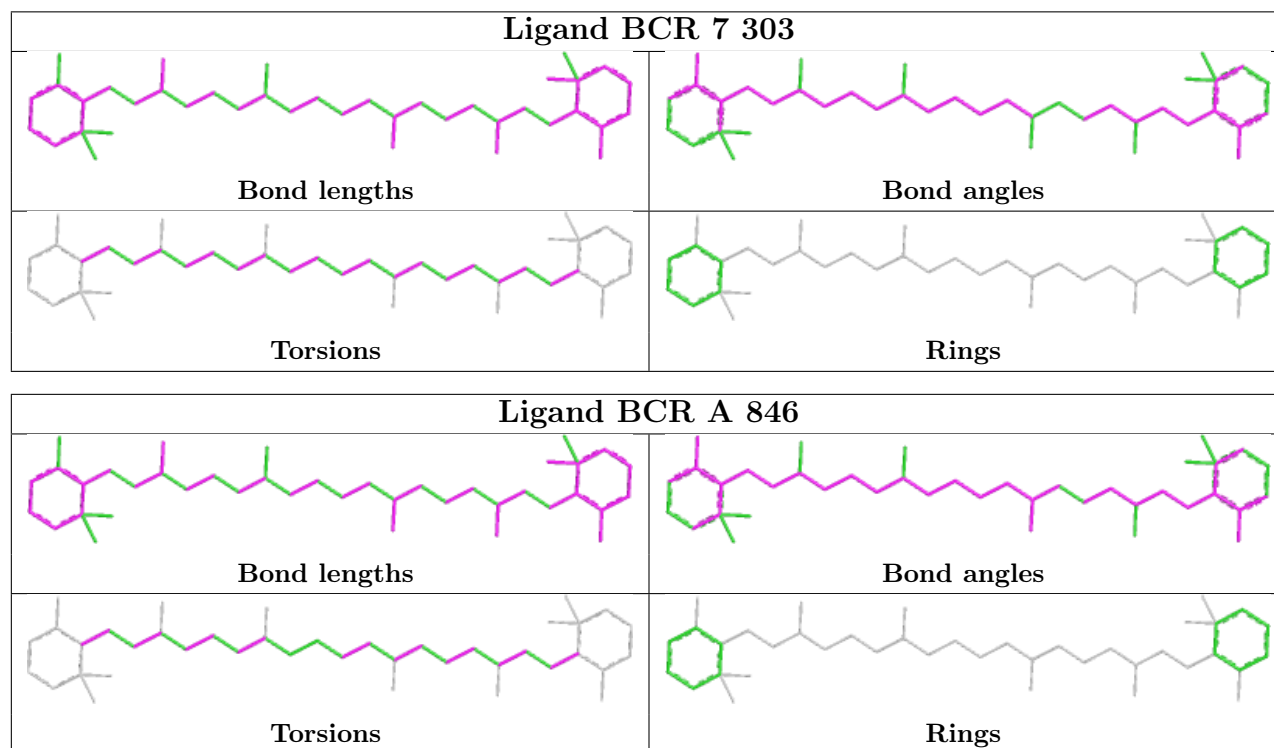
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	852	DGD	17	0
22	7	317	CLA	4	0
33	G	204	LMT	10	0
24	L	204	BCR	17	0
38	Z	301	LUT	23	0
26	8	318	NKP	7	0
39	6	320	CHL	13	0
22	4	818	CLA	9	0
25	9	315	LHG	2	0
22	A	854	CLA	10	0
22	Z	303	CLA	29	0
22	B	816	CLA	12	0
39	9	314	CHL	13	0
25	8	317	LHG	7	0
22	7	310	CLA	13	0
22	B	801	CLA	13	0
34	J	101	LMG	10	0
39	8	301	CHL	11	0
22	A	825	CLA	18	0
22	B	837	CLA	1	0
22	6	310	CLA	15	0
22	A	823	CLA	28	0
22	3	320	CLA	10	0
22	A	830	CLA	9	0
22	5	307	CLA	24	0
22	6	301	CLA	20	0
24	K	206	BCR	12	0
22	A	841	CLA	16	0
22	A	829	CLA	16	0
36	5	306	C7Z	1	0
22	F	304	CLA	27	0
39	Z	312	CHL	12	0
33	4	822	LMT	2	0
39	9	312	CHL	24	0
22	6	322	CLA	17	0
22	A	836	CLA	13	0
22	A	855	CLA	14	0
36	J	105	C7Z	2	0
22	9	311	CLA	5	0
22	Z	305	CLA	14	0
22	5	326	CLA	17	0
22	8	307	CLA	15	0

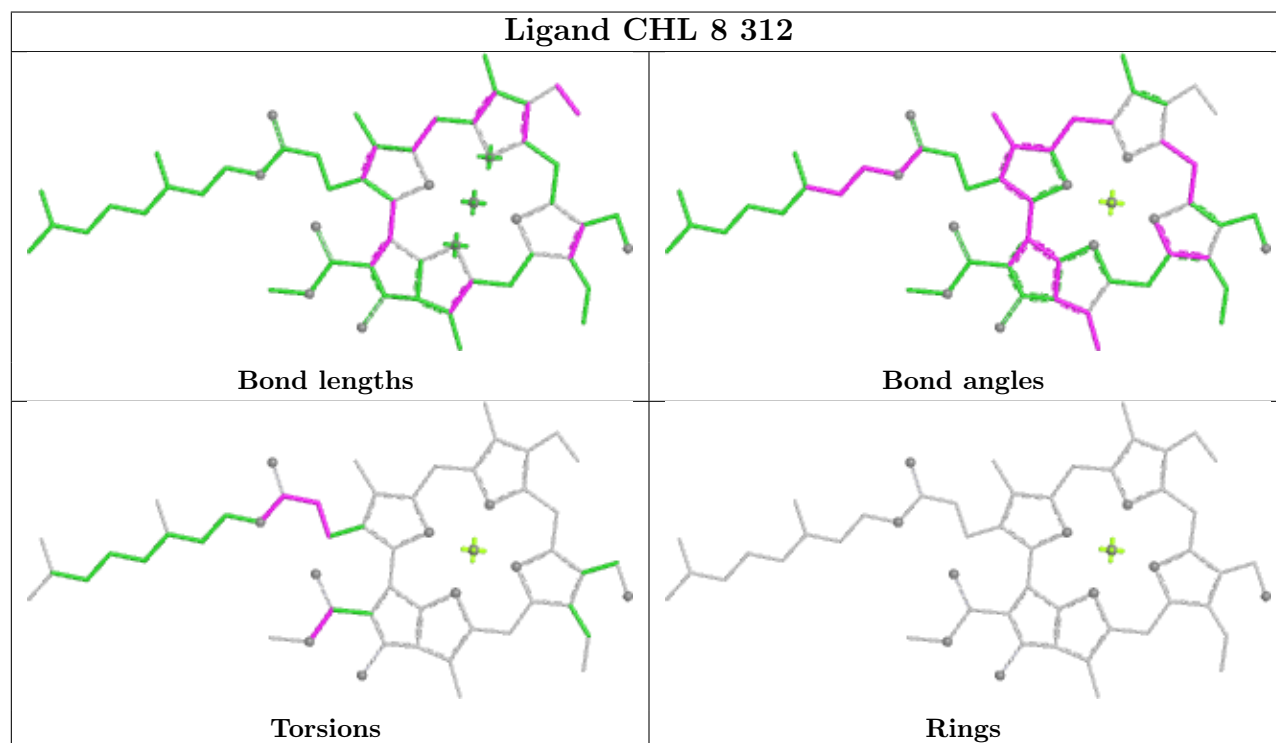
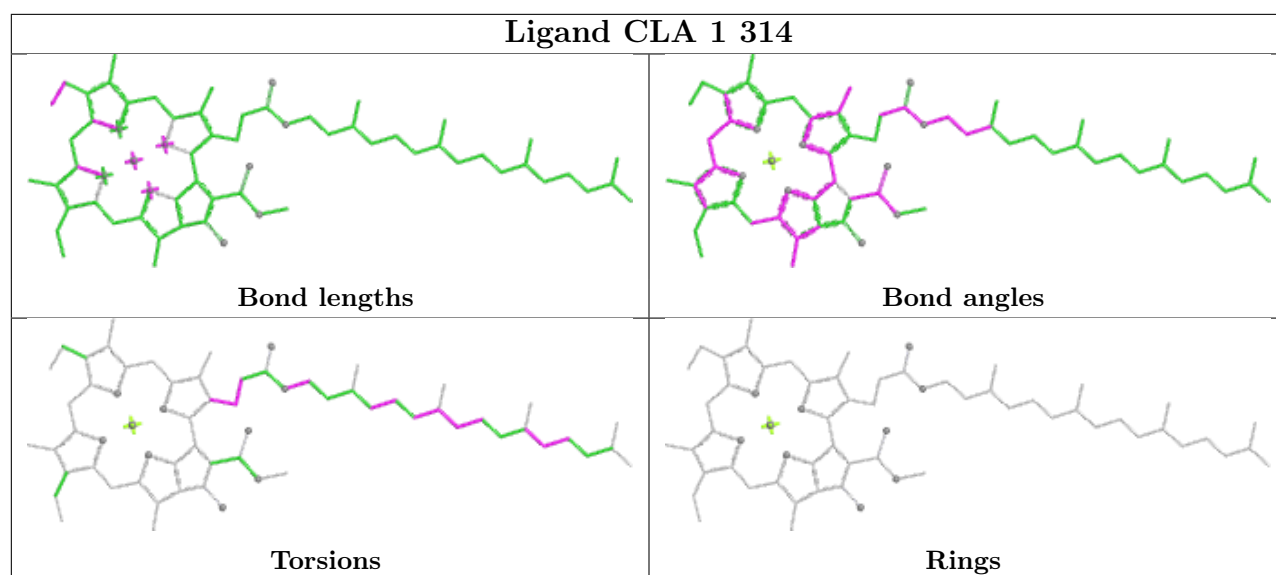
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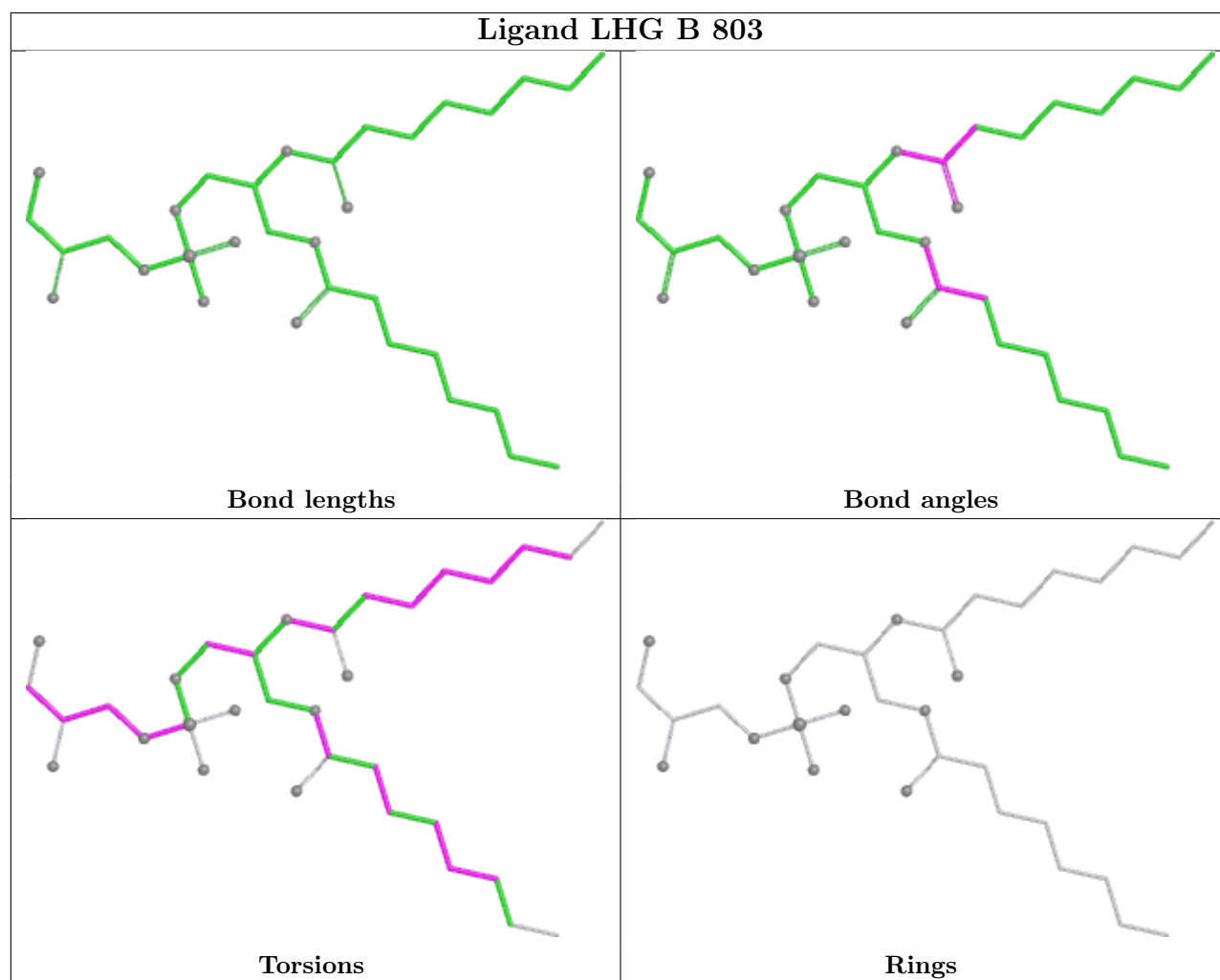
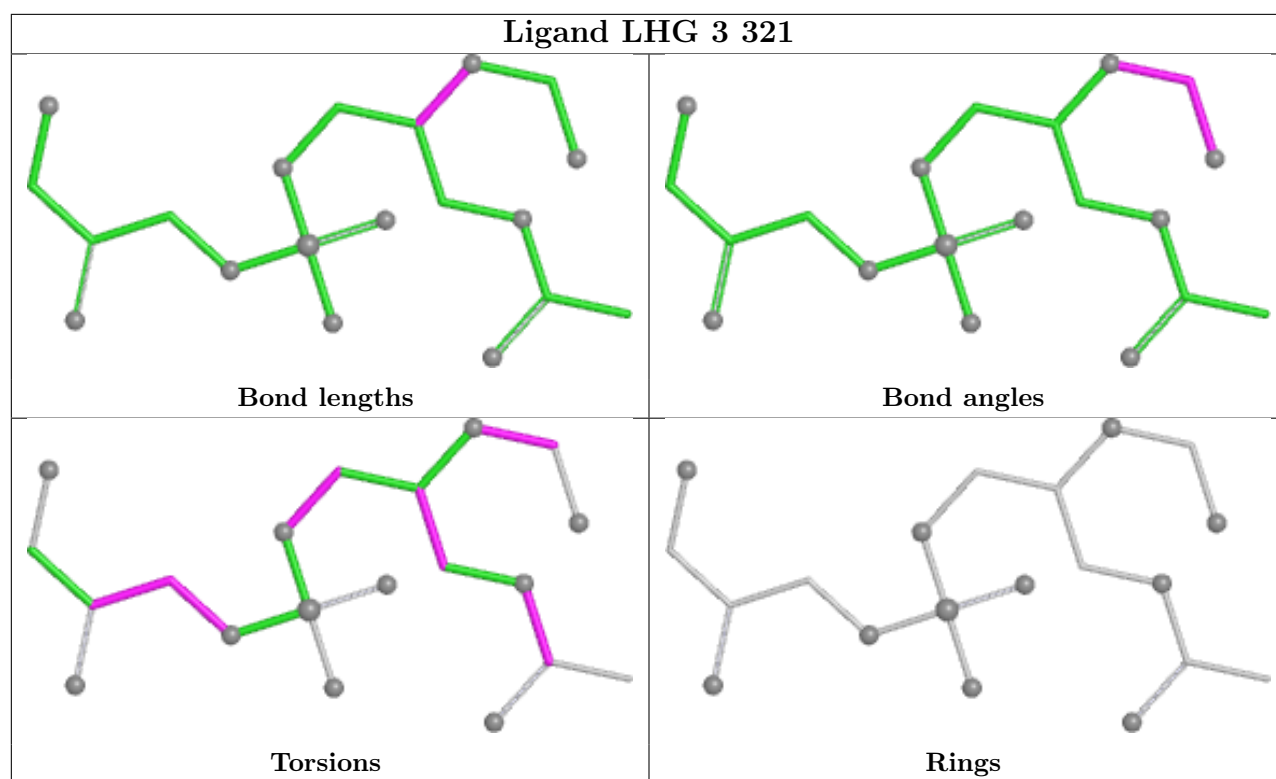
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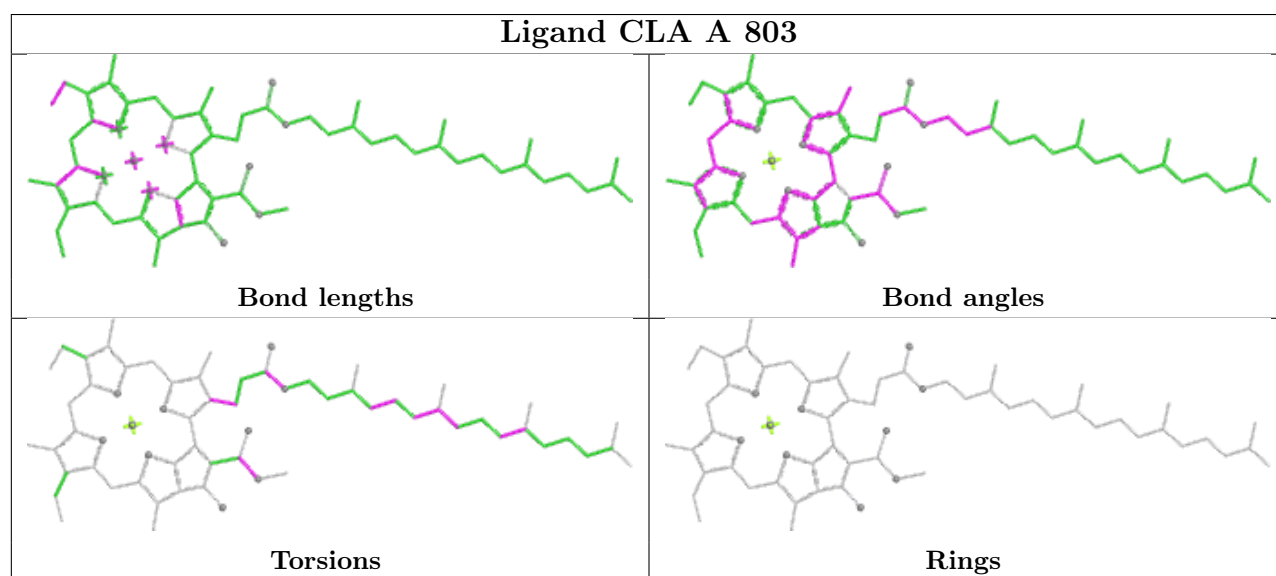
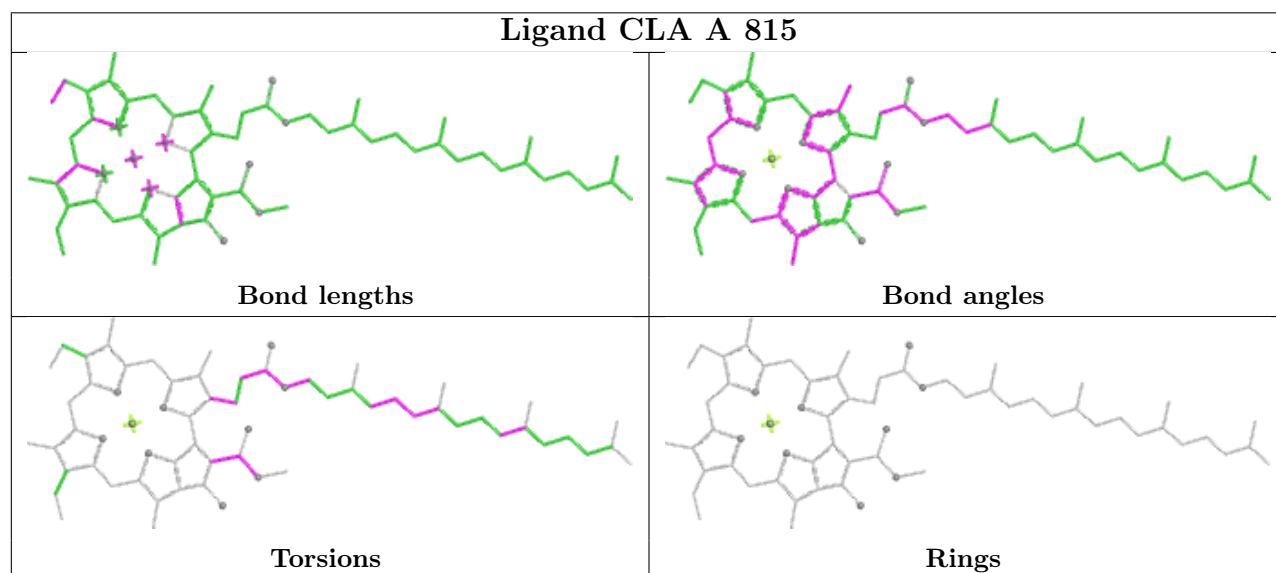
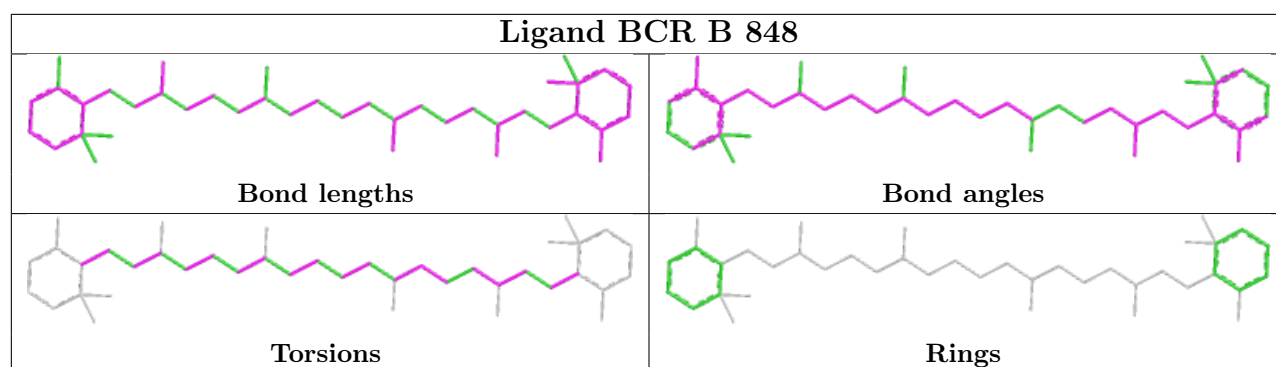
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	311	CLA	14	0
22	Z	309	CLA	21	0
22	6	319	CLA	11	0

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.

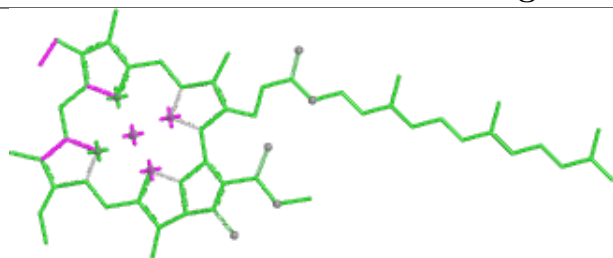




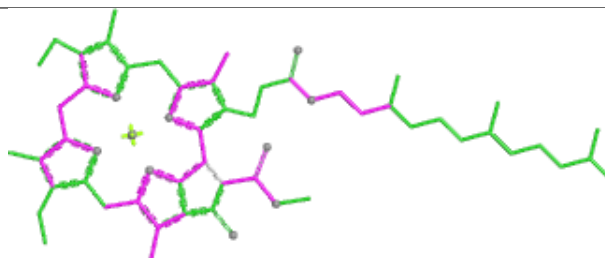




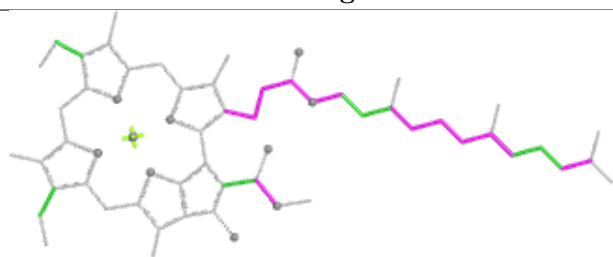
Ligand CLA 3 314



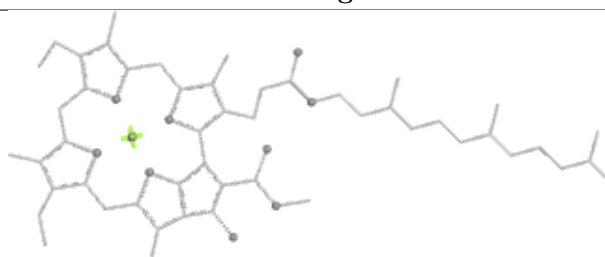
Bond lengths



Bond angles

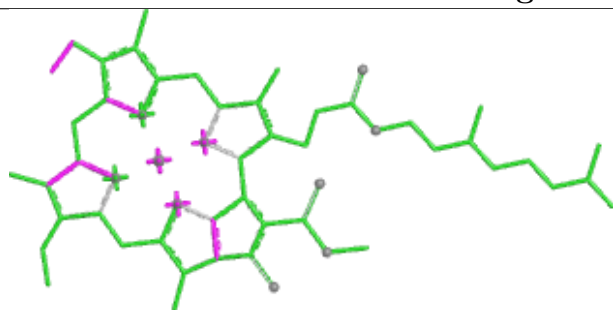


Torsions

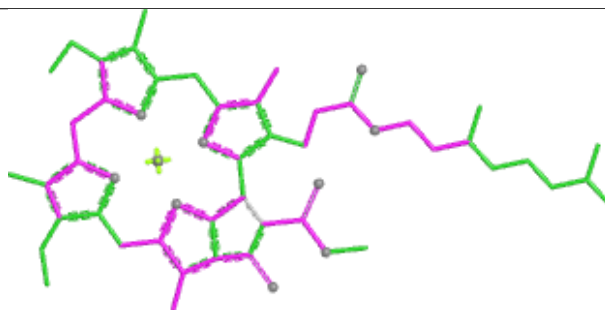


Rings

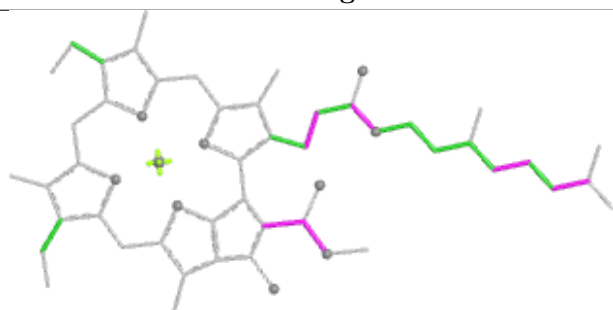
Ligand CLA Z 307



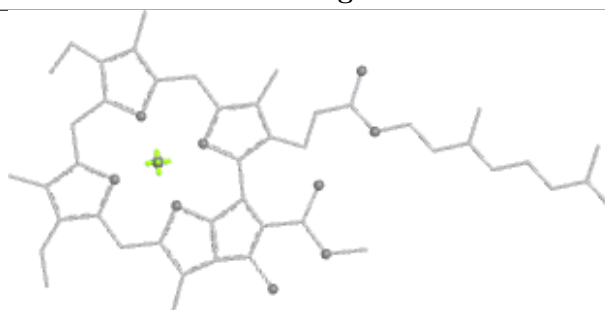
Bond lengths



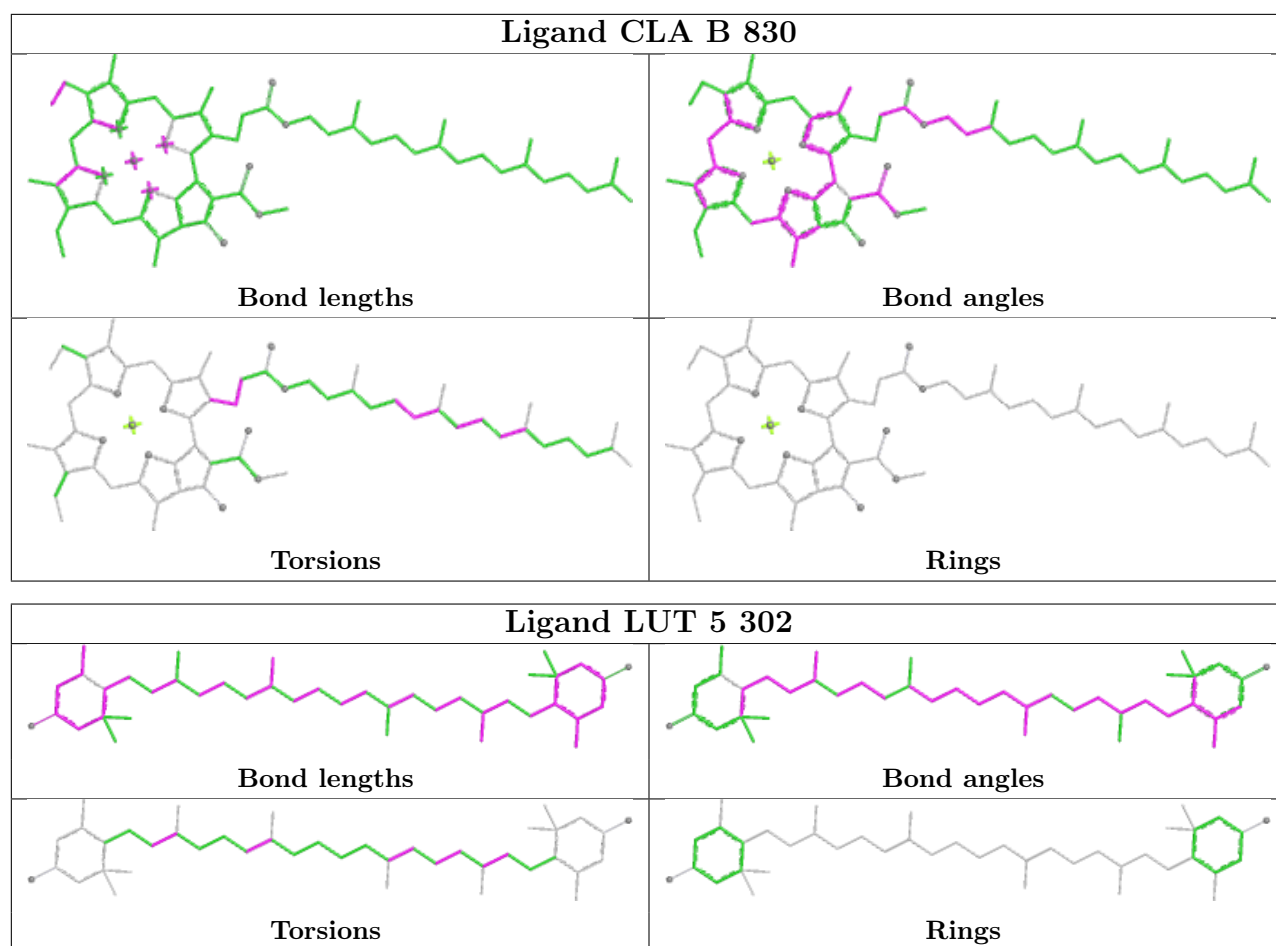
Bond angles



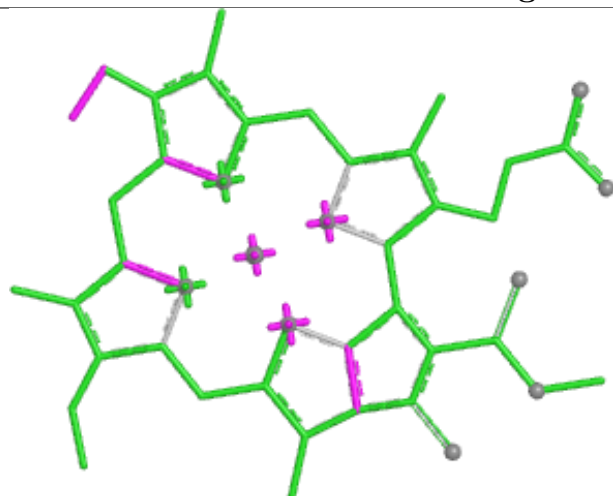
Torsions



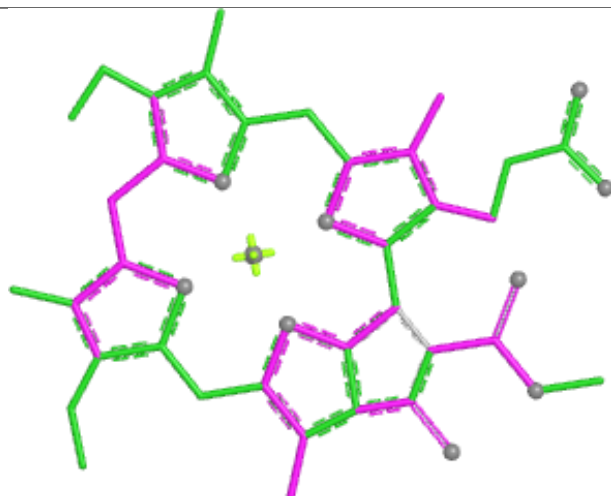
Rings



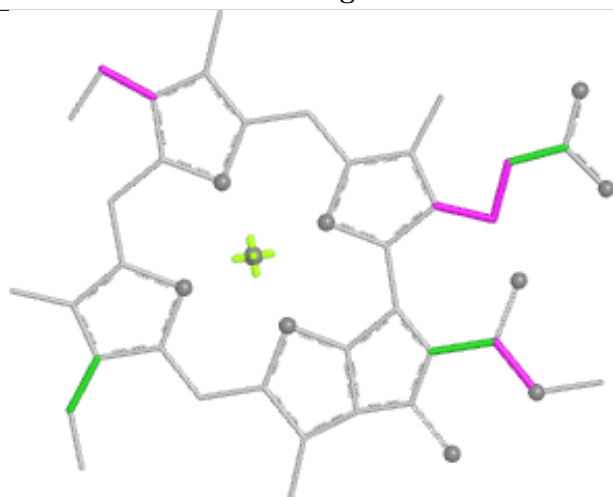
Ligand CLA 3 315



Bond lengths



Bond angles

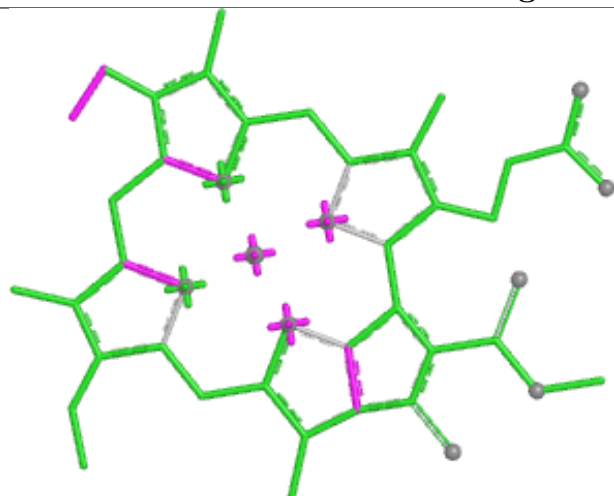


Torsions

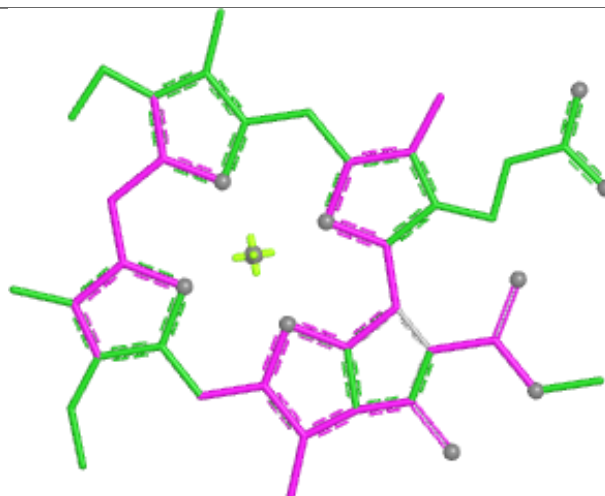


Rings

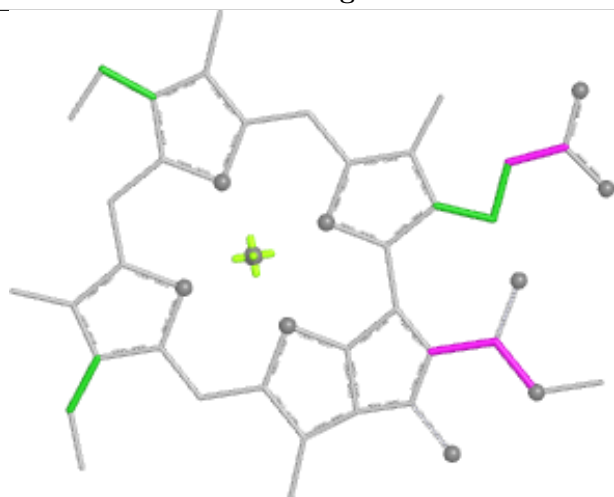
Ligand CLA 1 305



Bond lengths



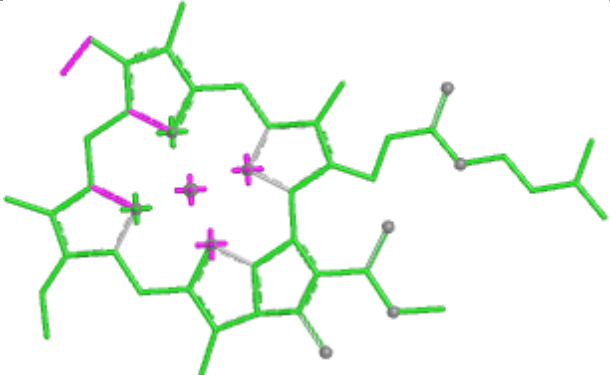
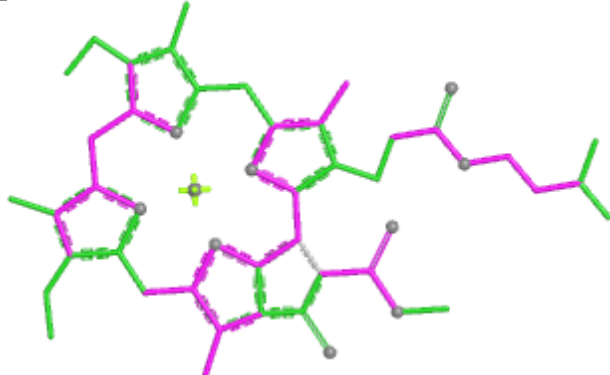
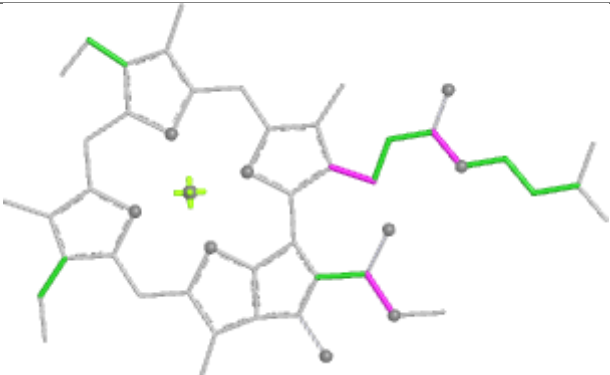
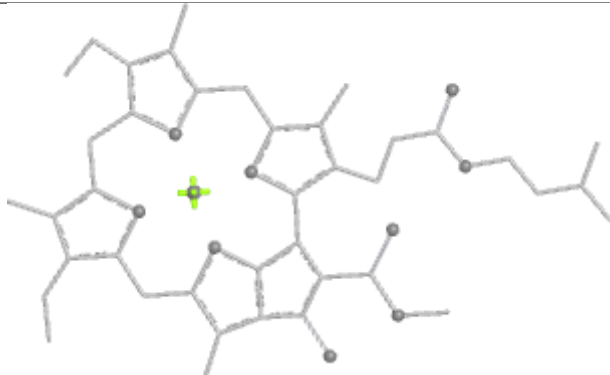
Bond angles

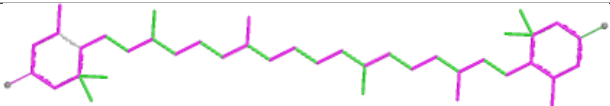
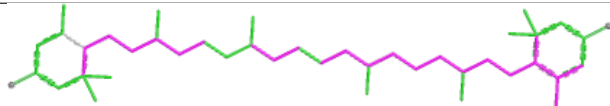
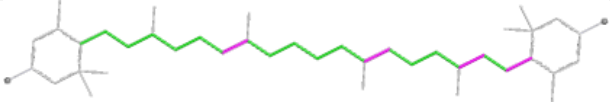
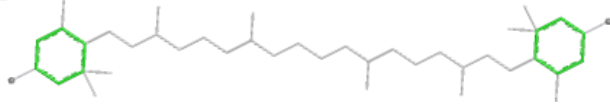


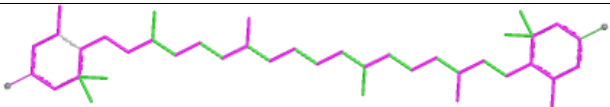
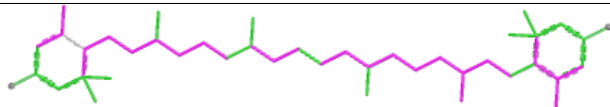
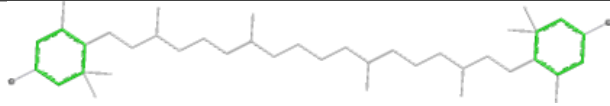
Torsions



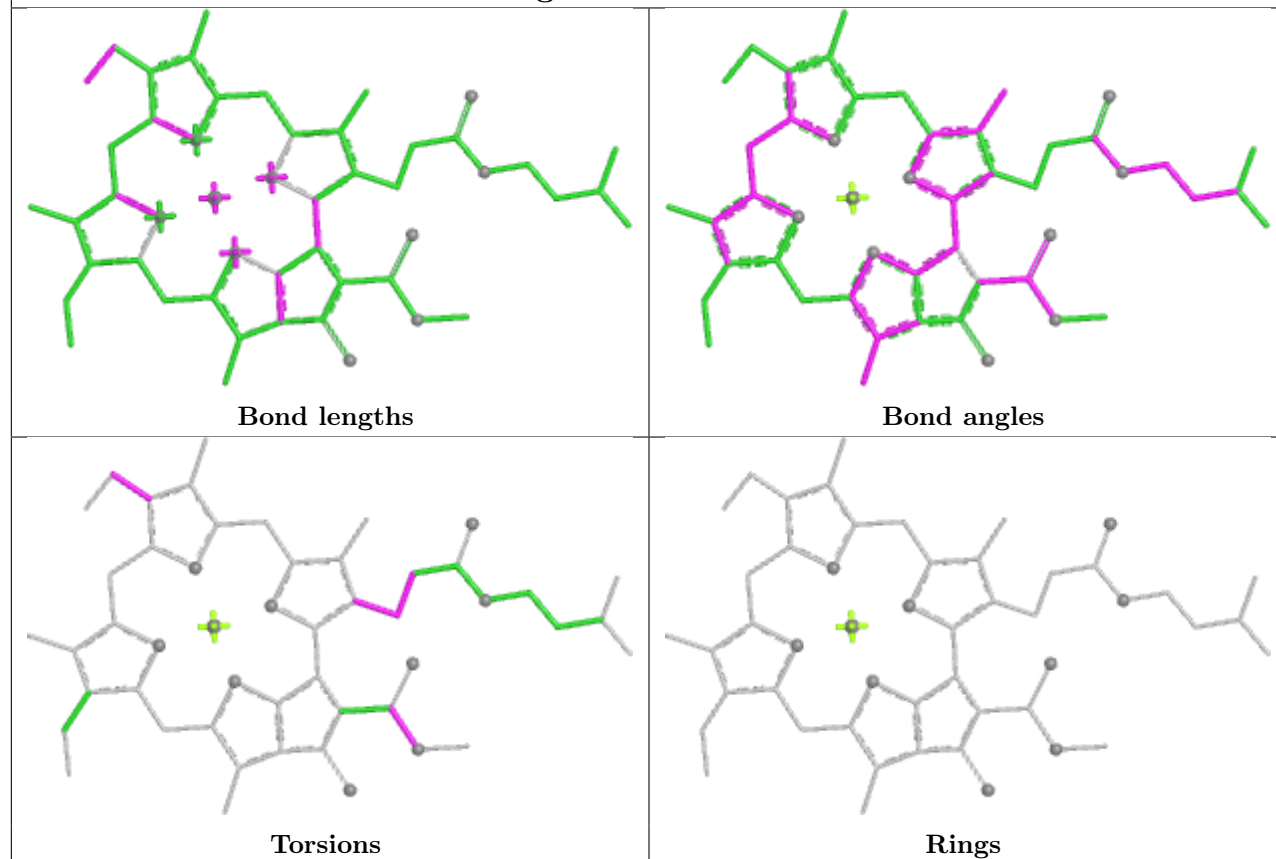
Rings

Ligand CLA 7 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

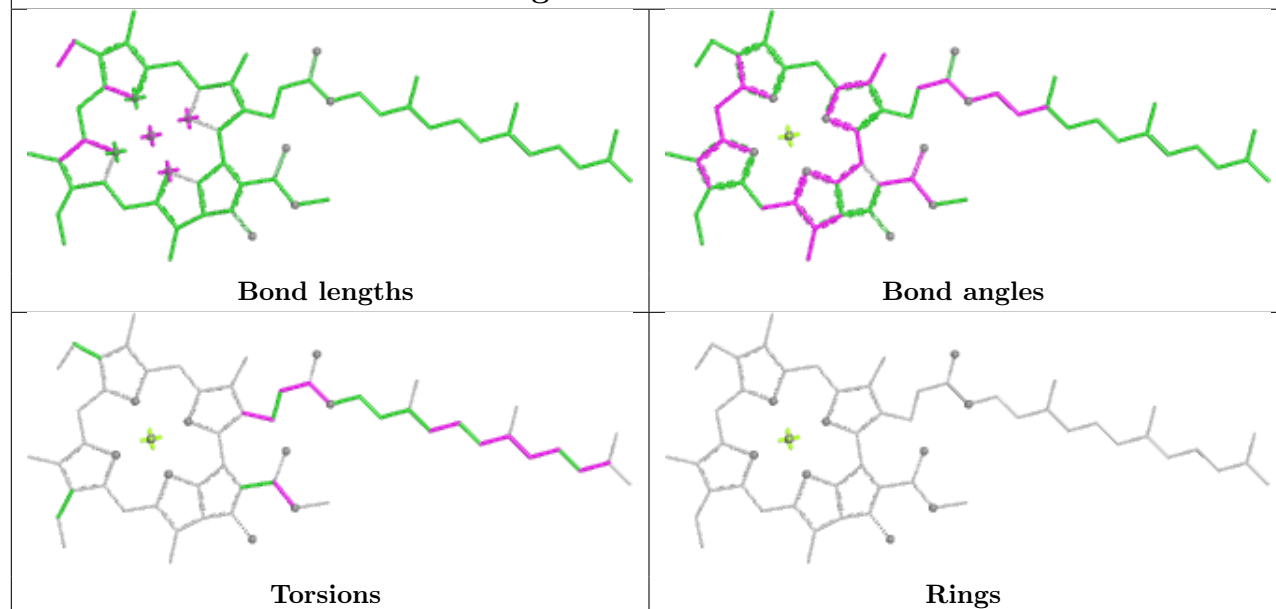
Ligand LUT Z 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

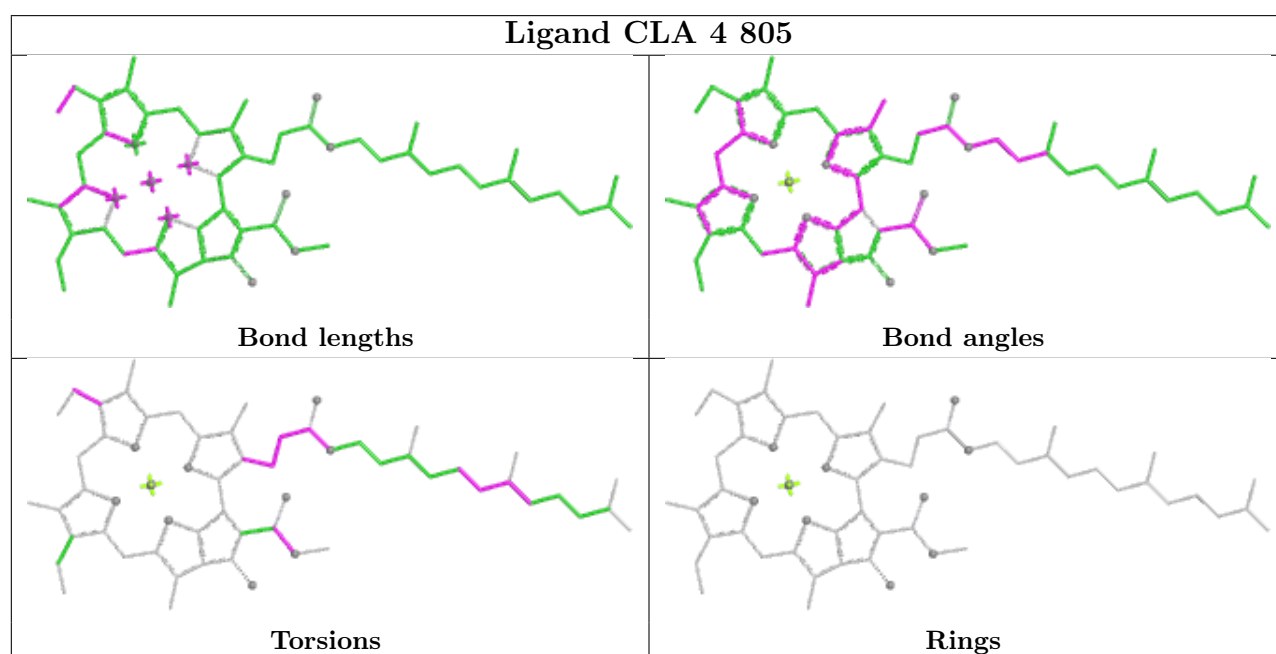
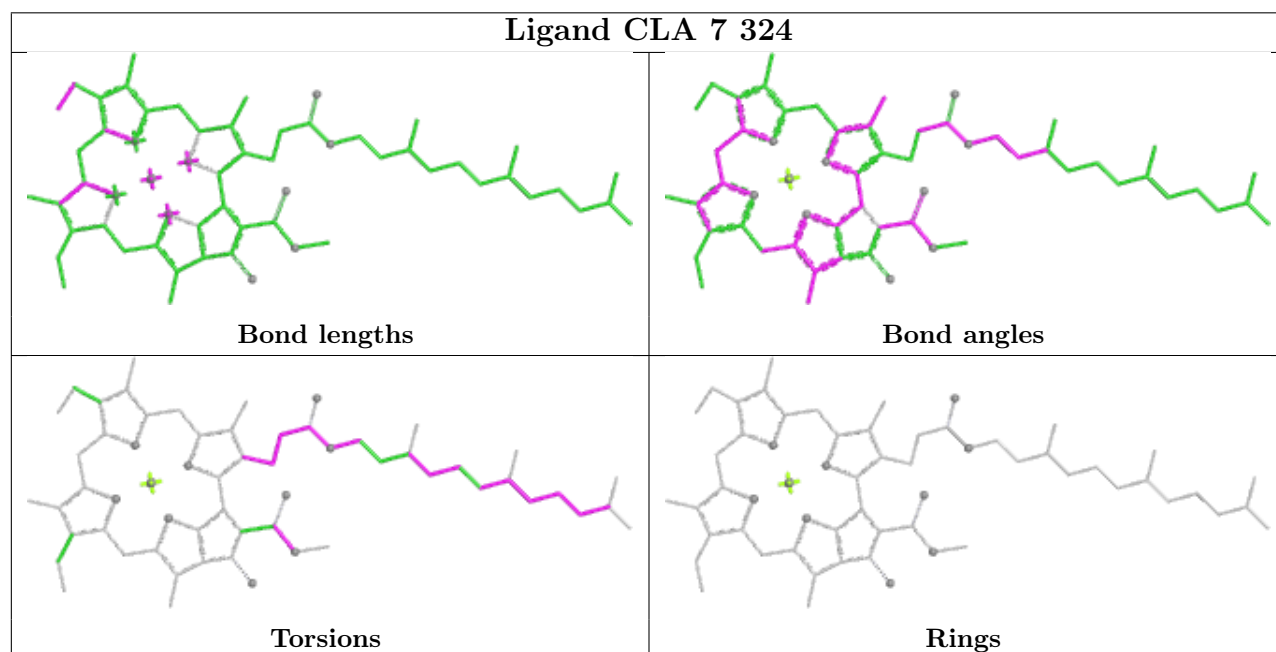
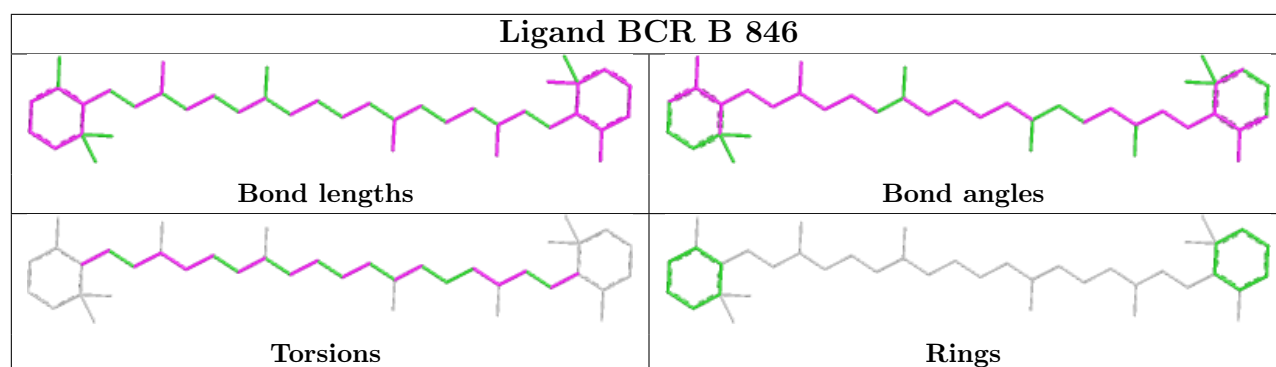
Ligand LUT 1 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

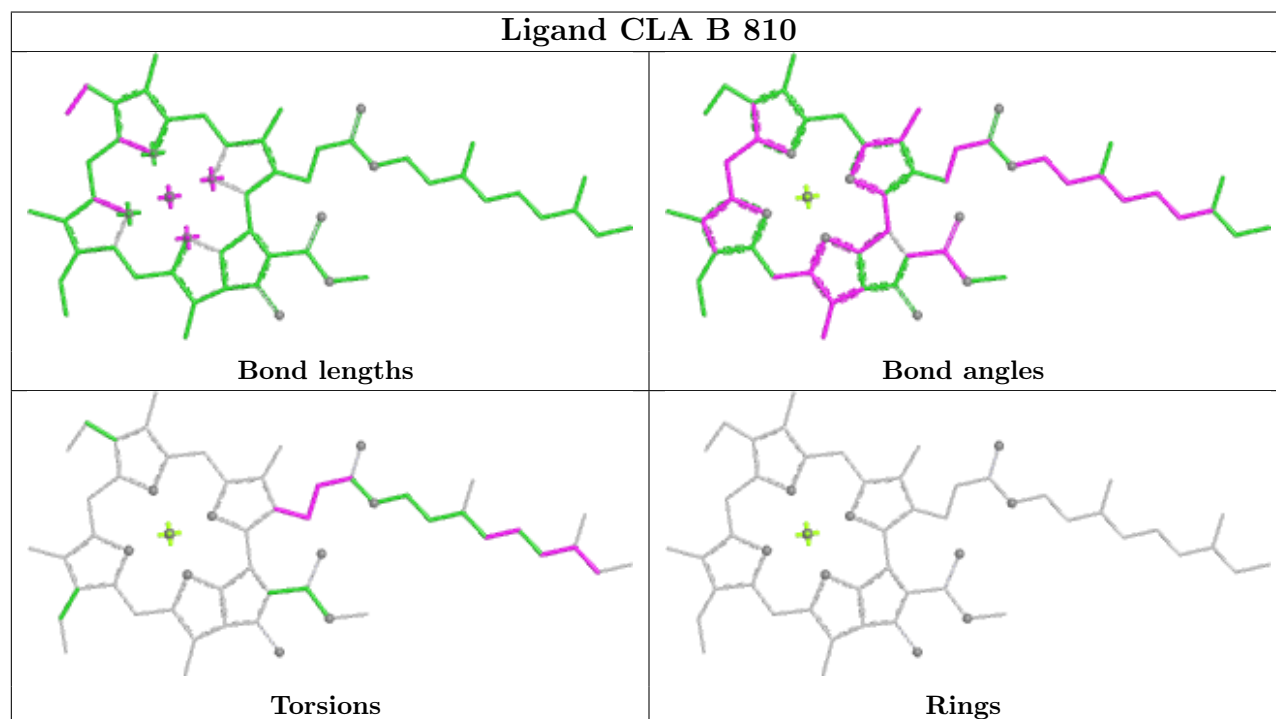
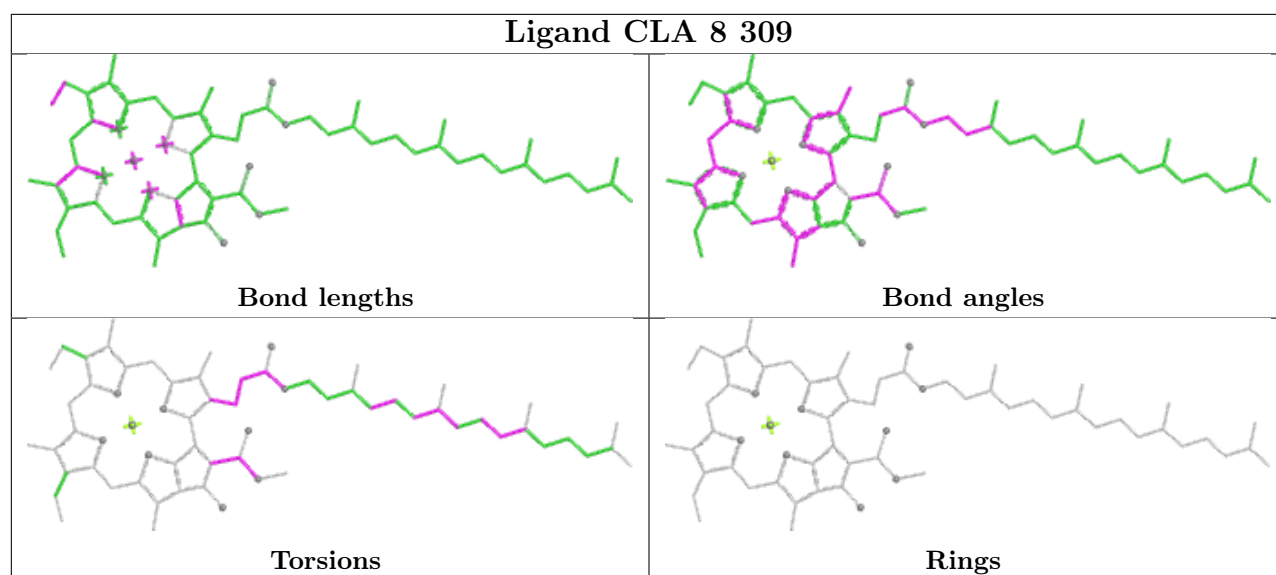
Ligand CLA 5 320

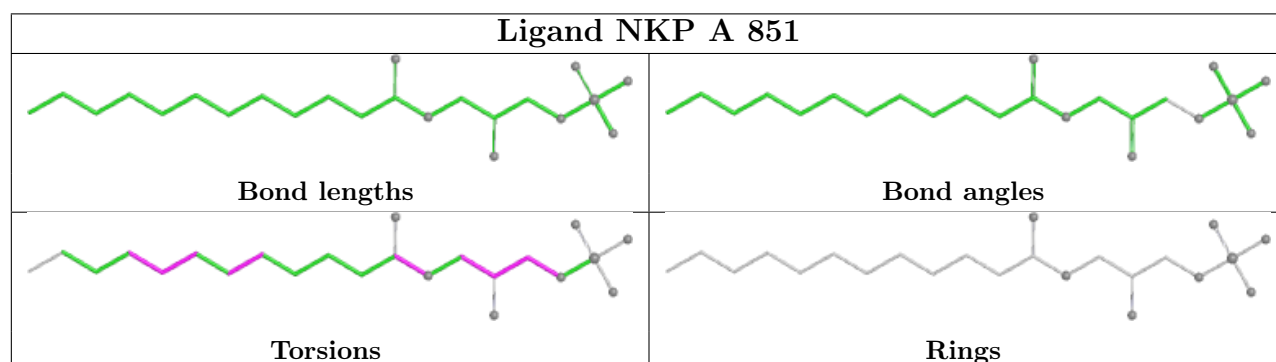
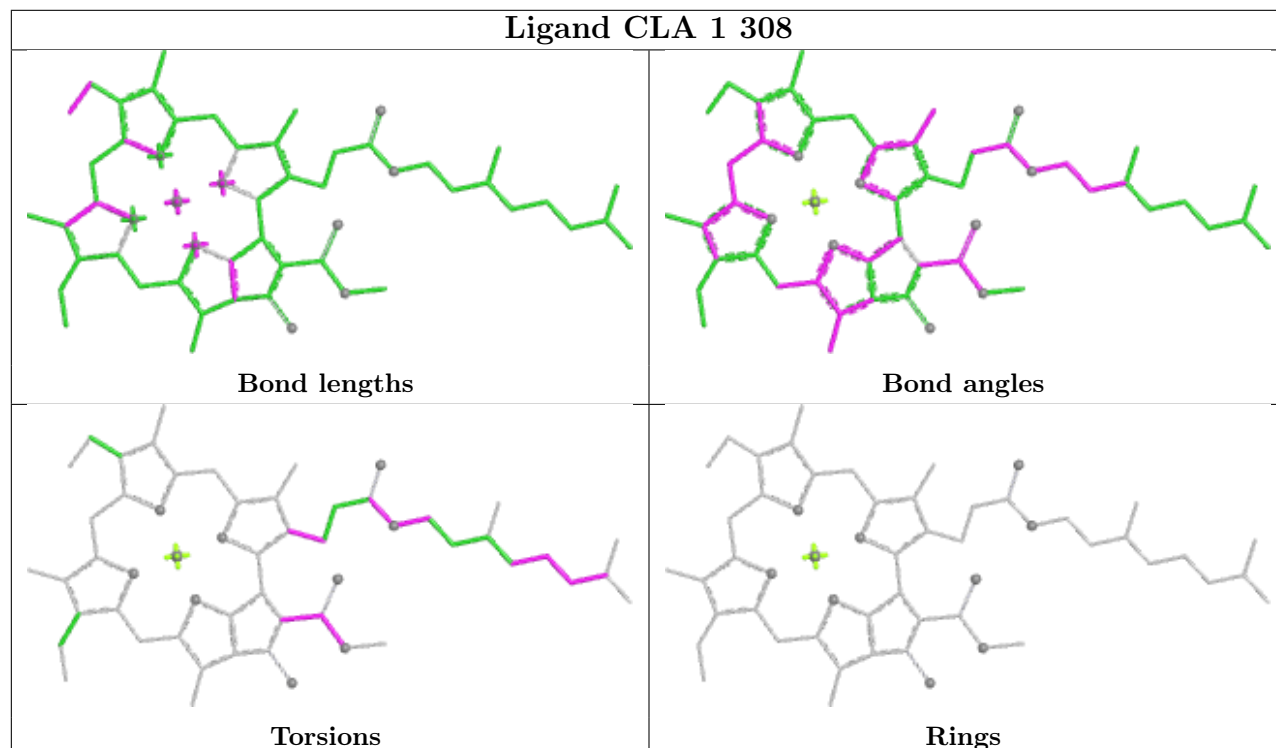
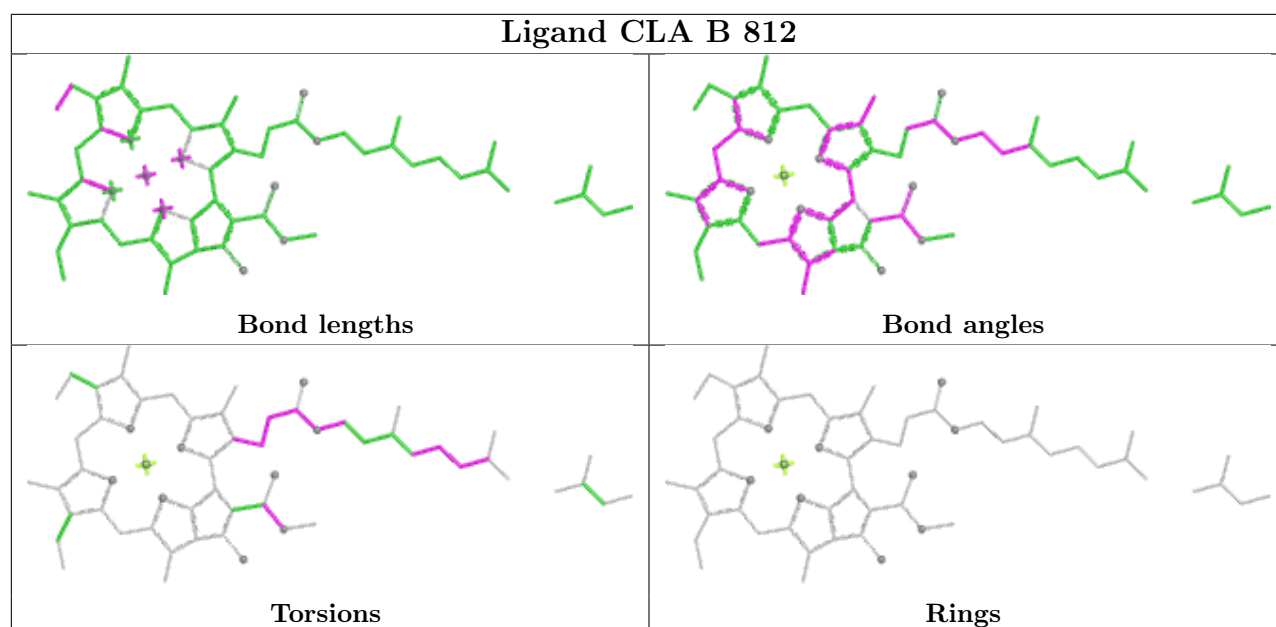


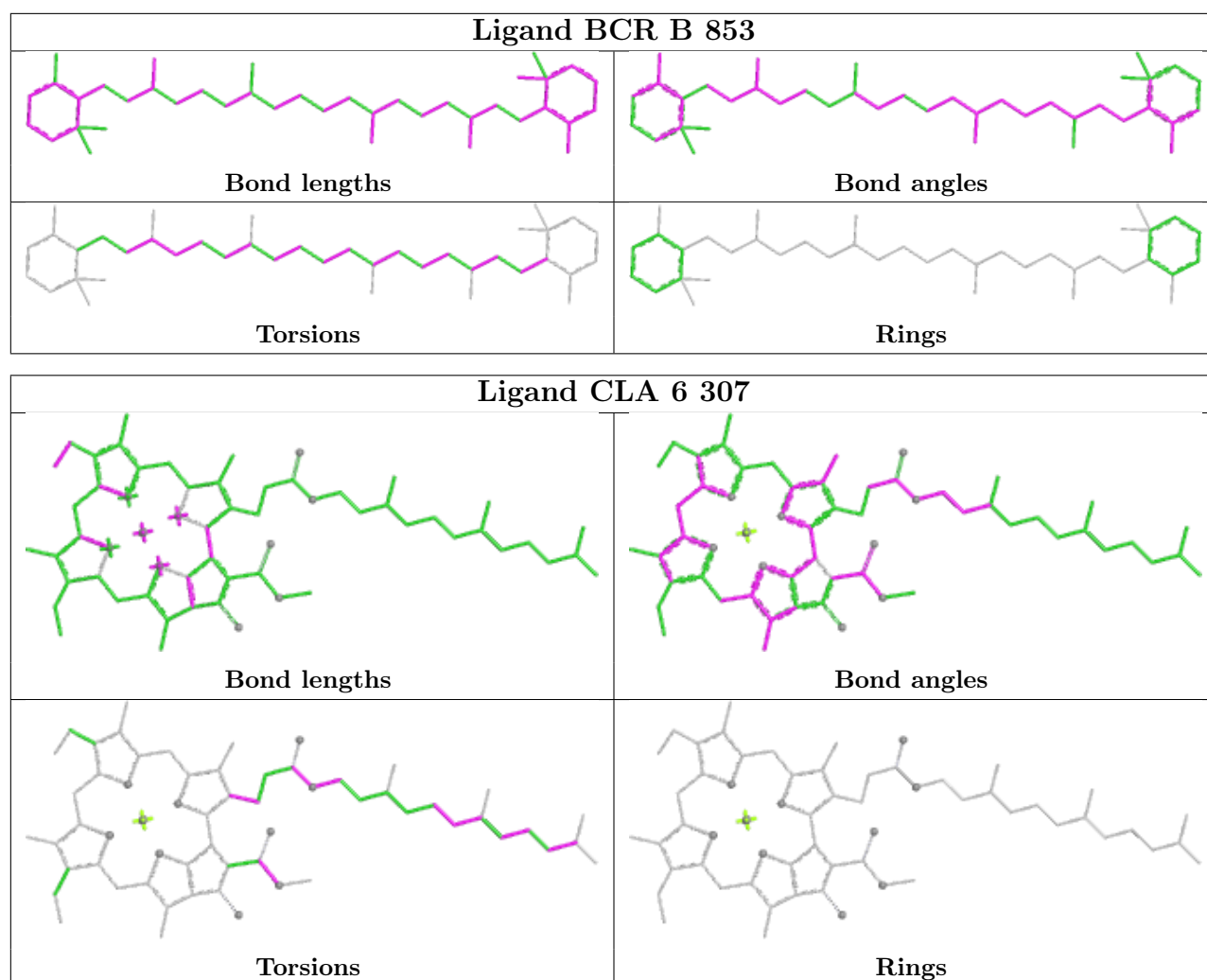
Ligand CLA A 807

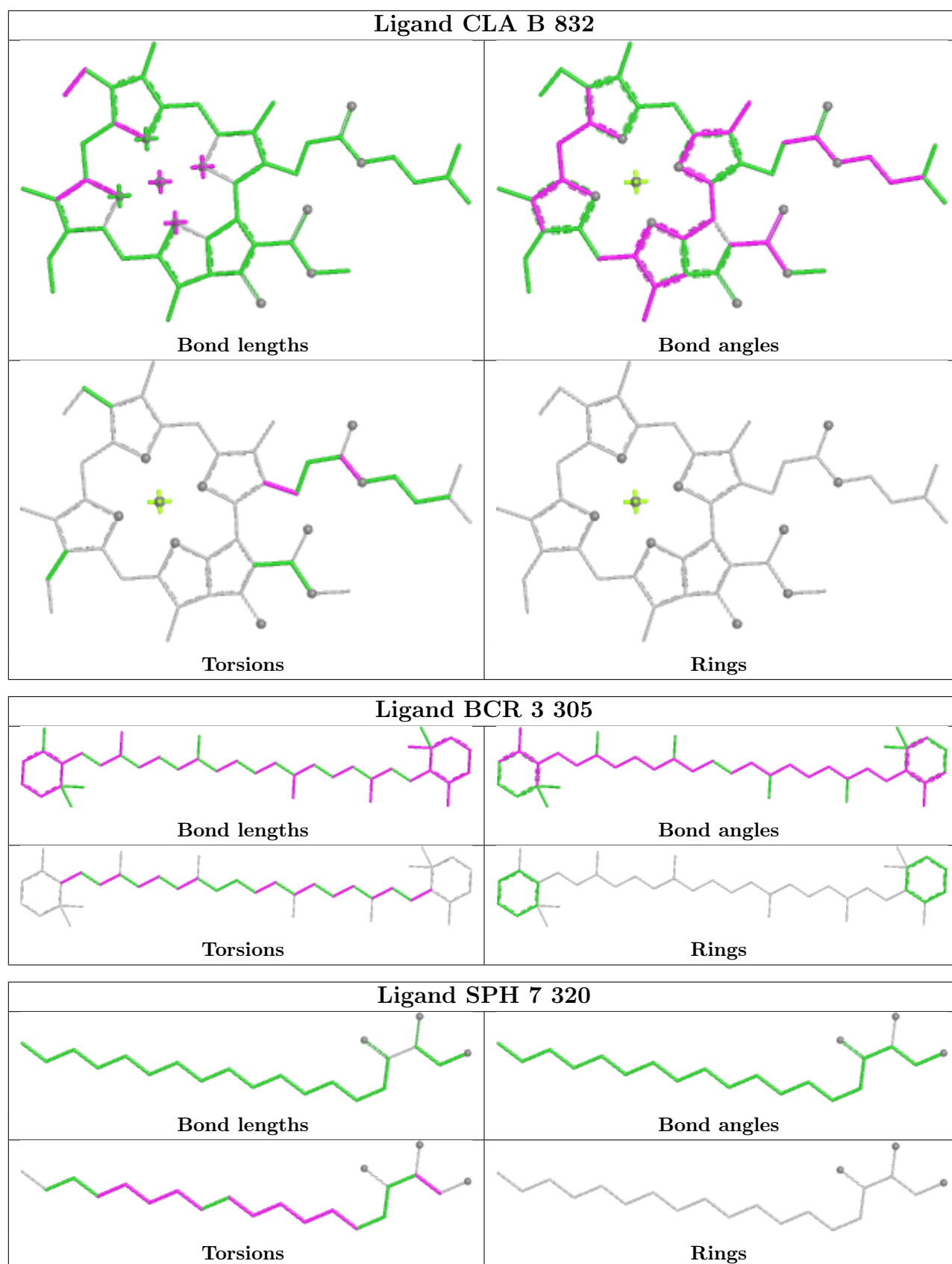


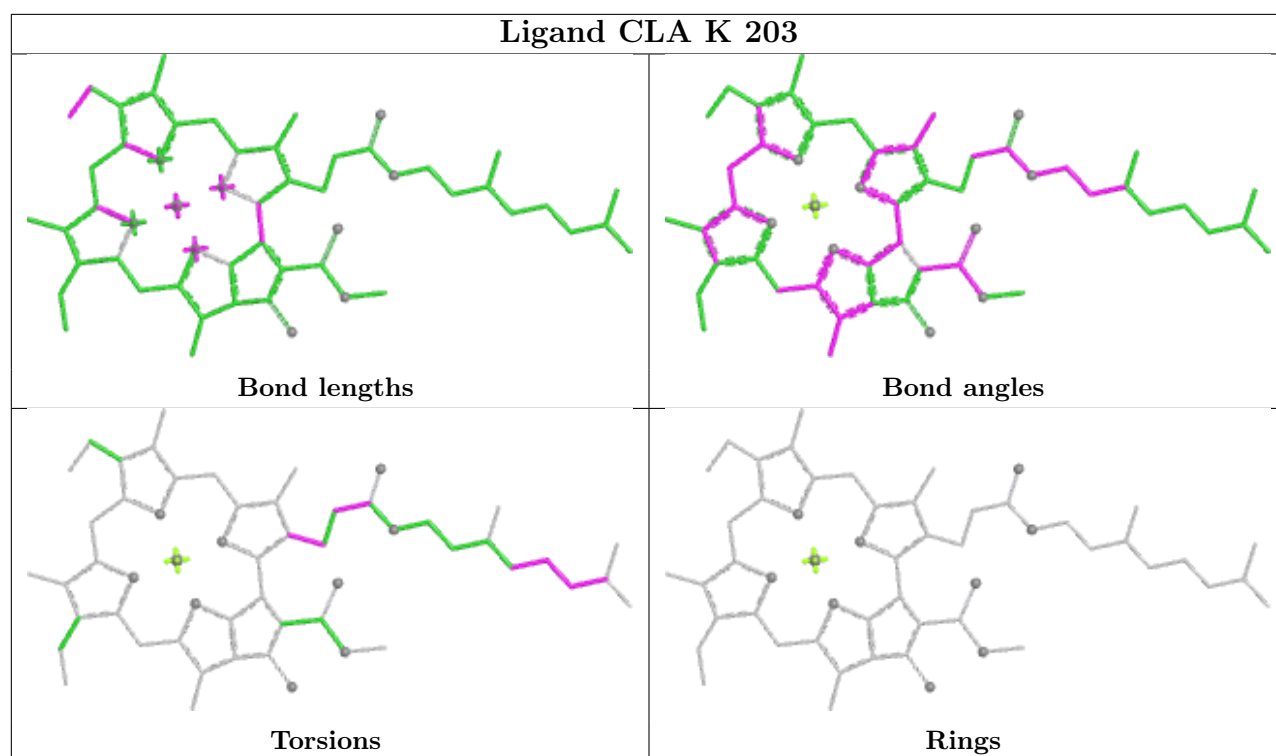


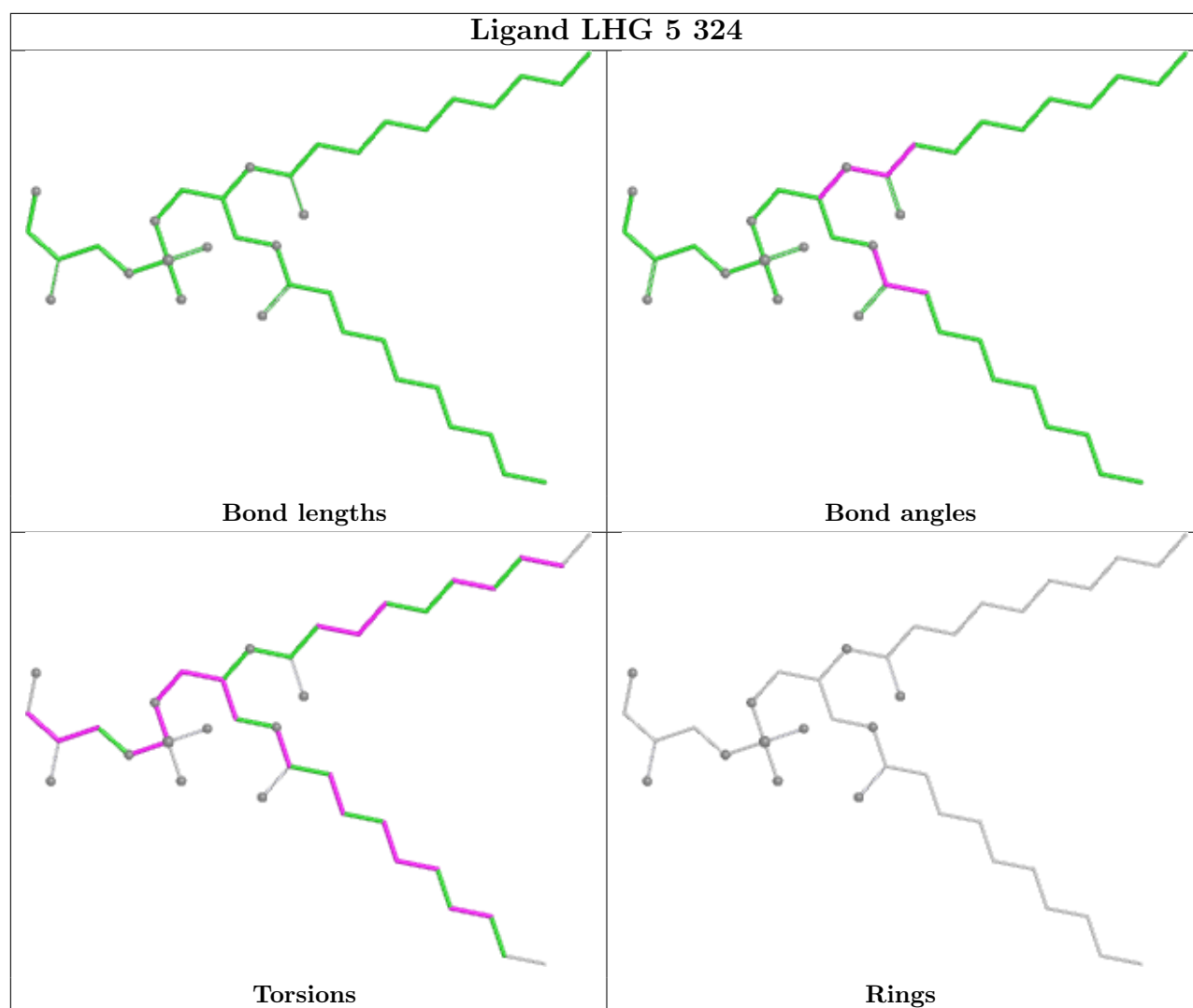




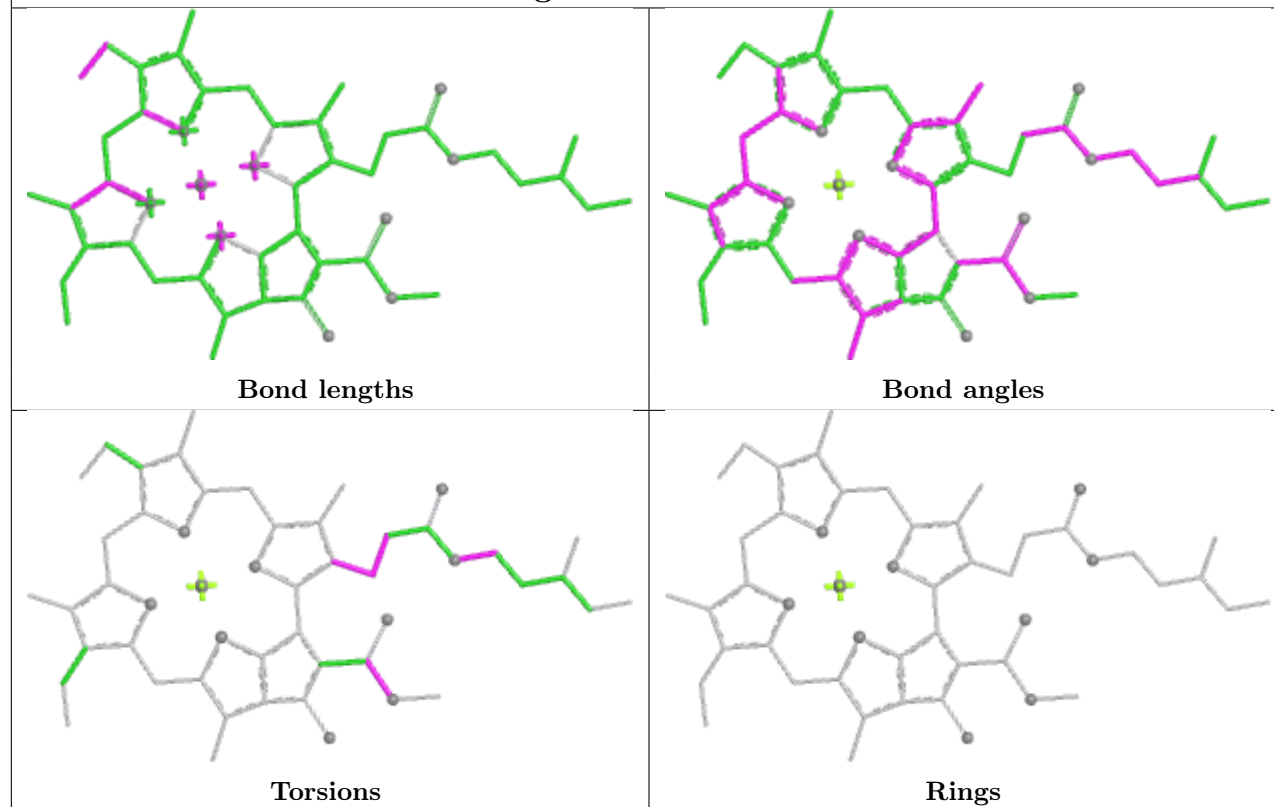




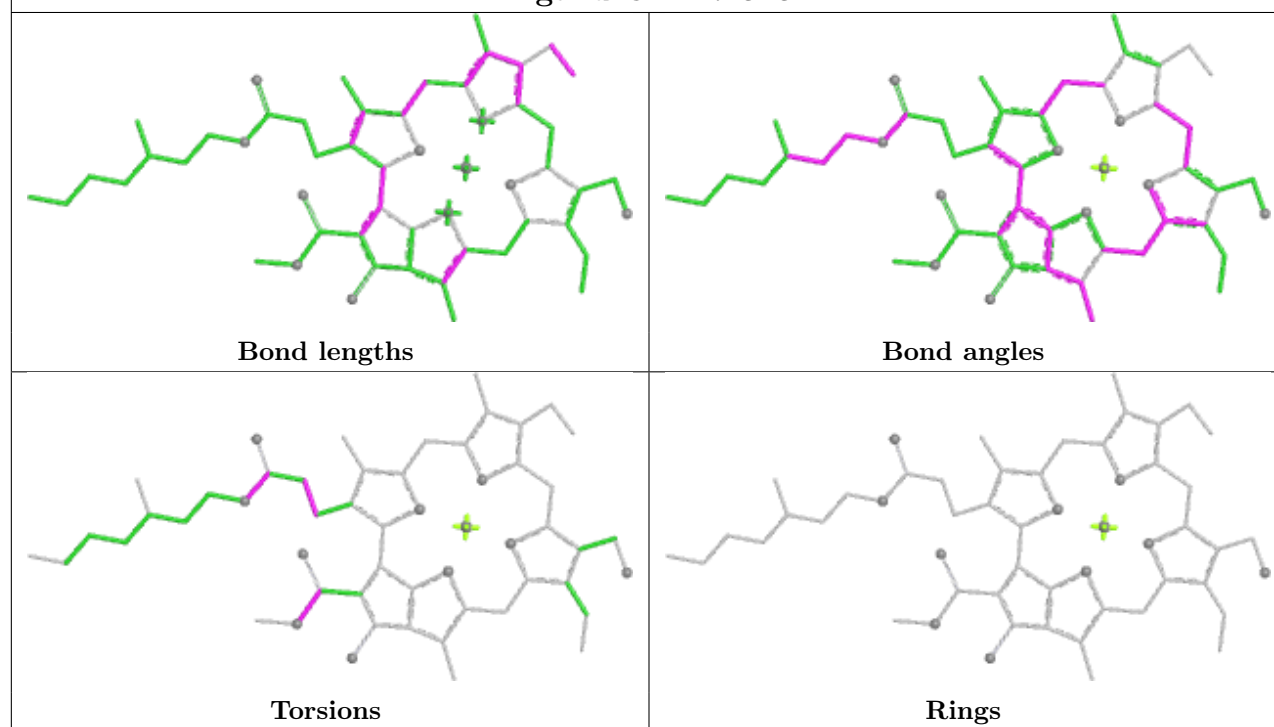


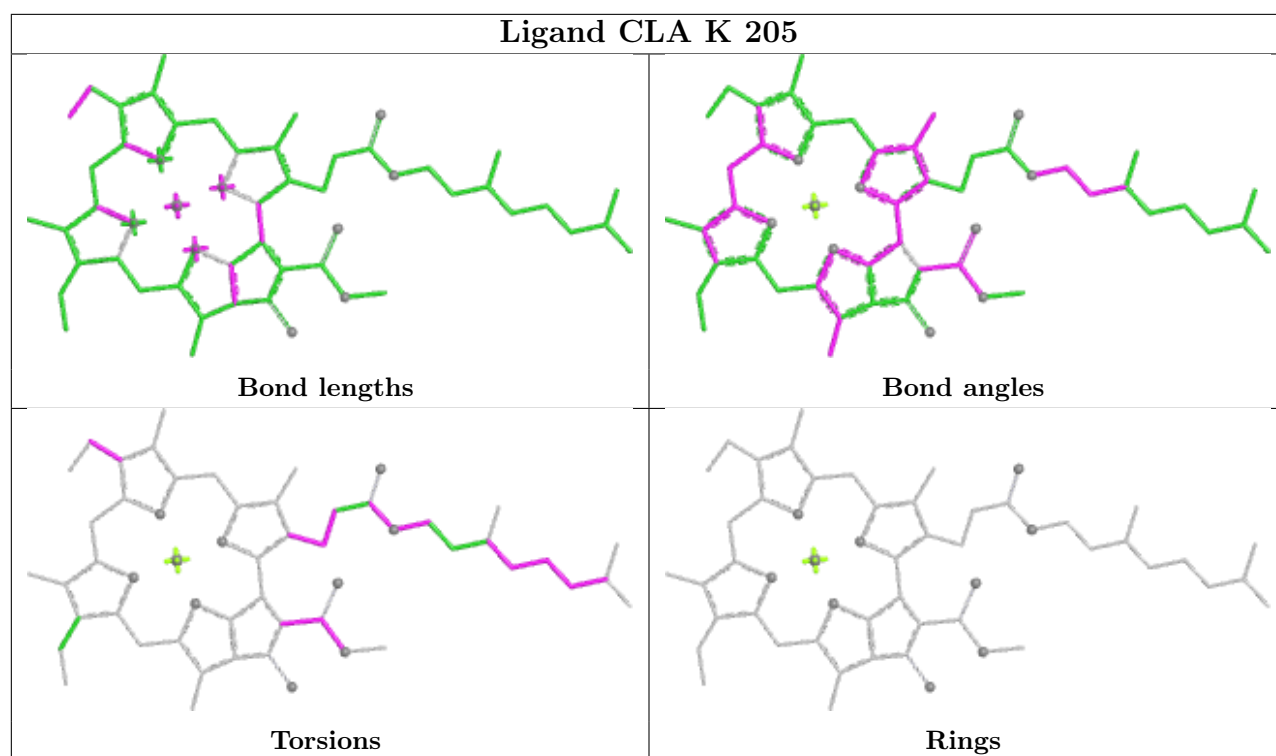


Ligand CLA Z 314

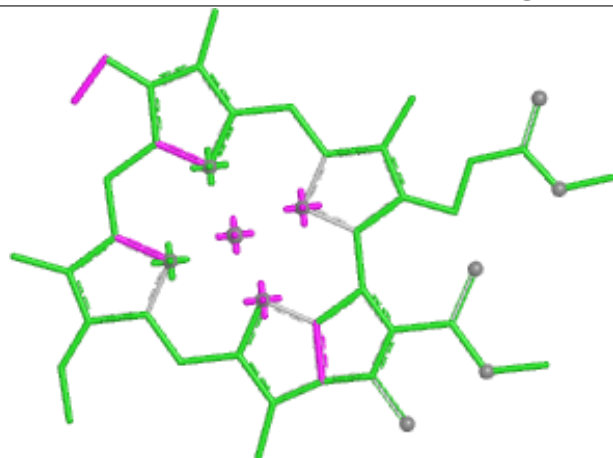


Ligand CHL 7 313

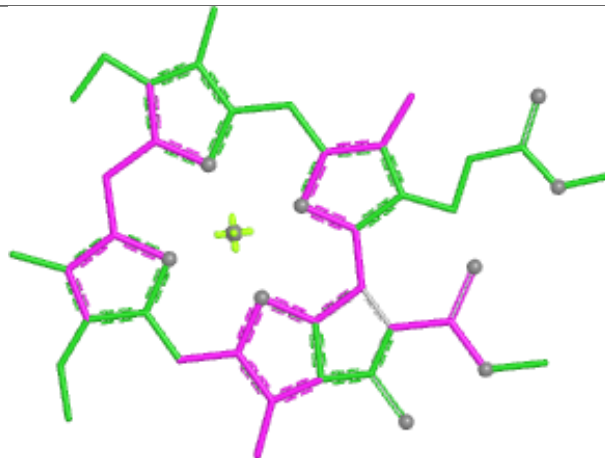




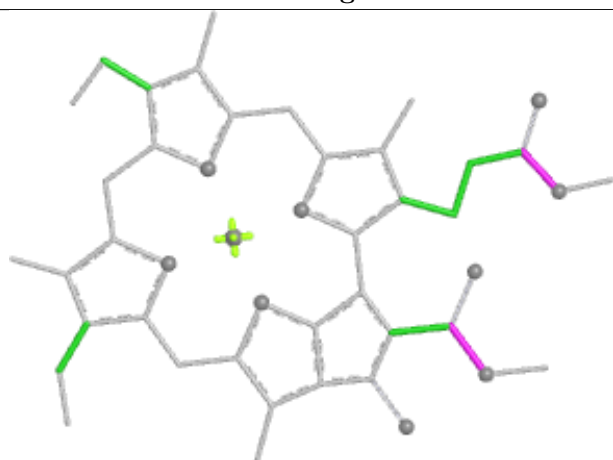
Ligand CLA 3 309



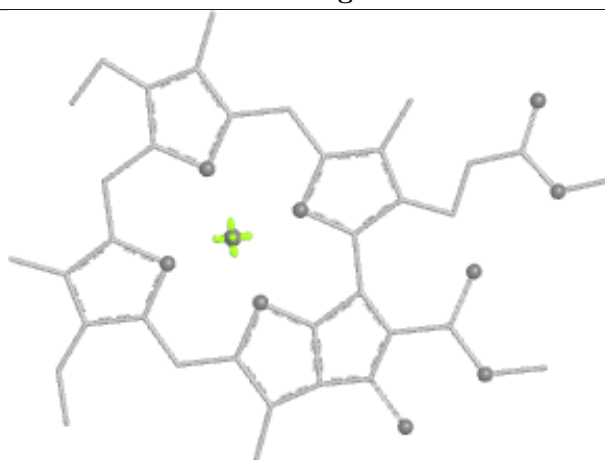
Bond lengths



Bond angles

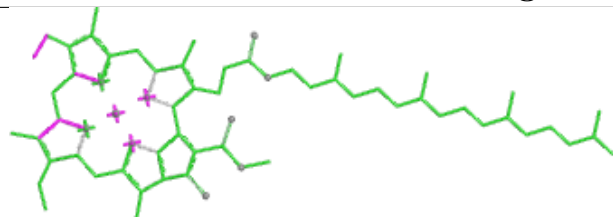


Torsions

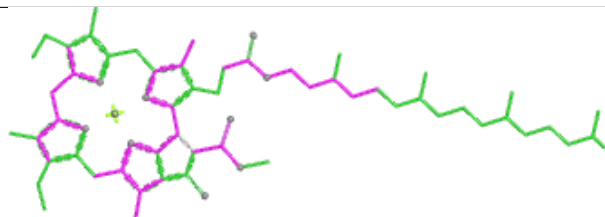


Rings

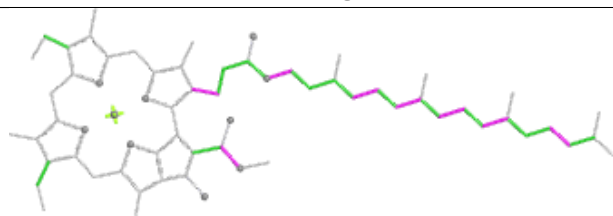
Ligand CLA 5 315



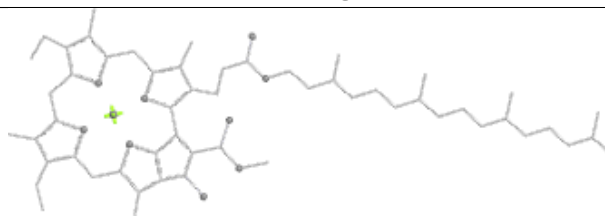
Bond lengths



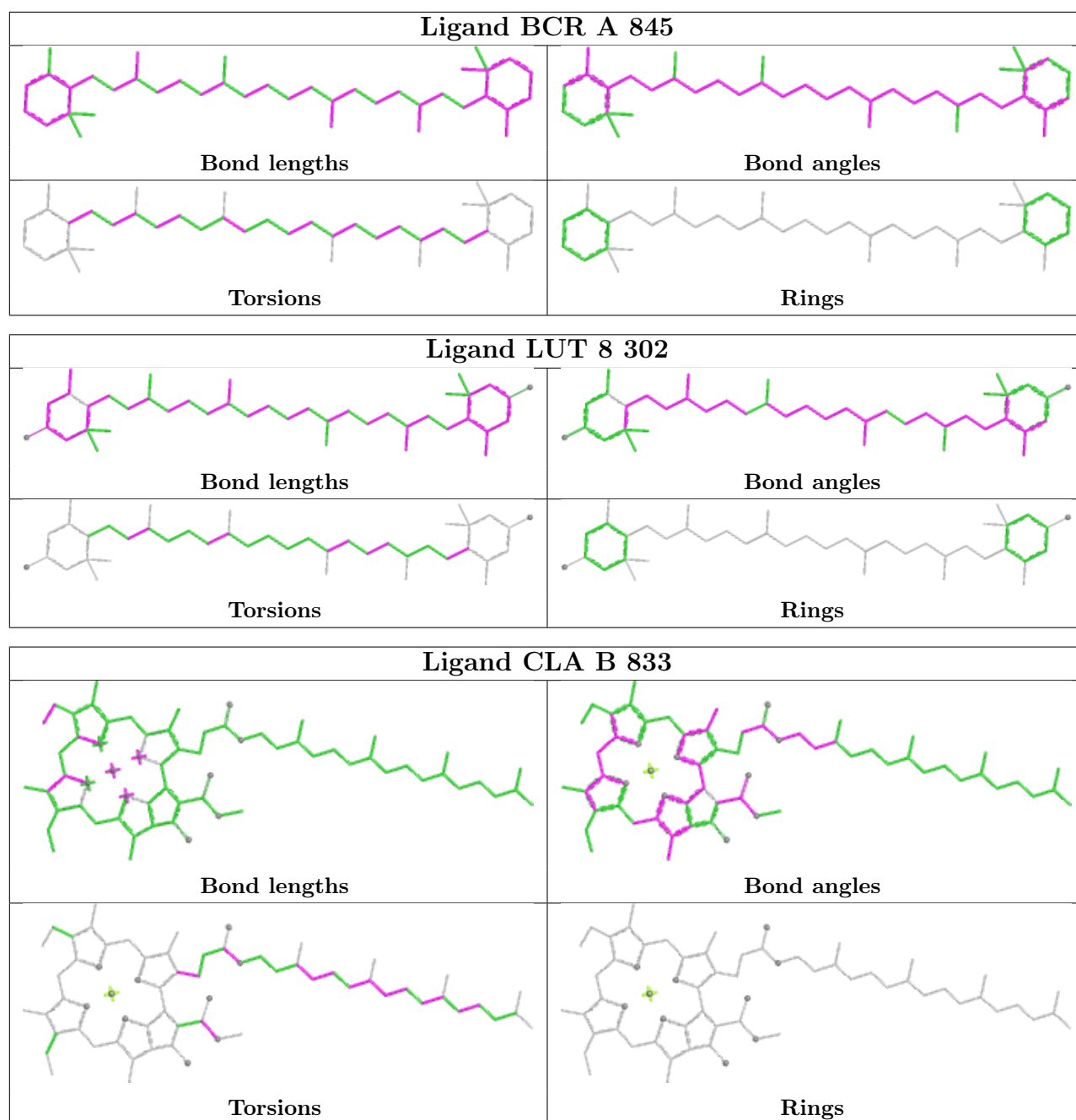
Bond angles



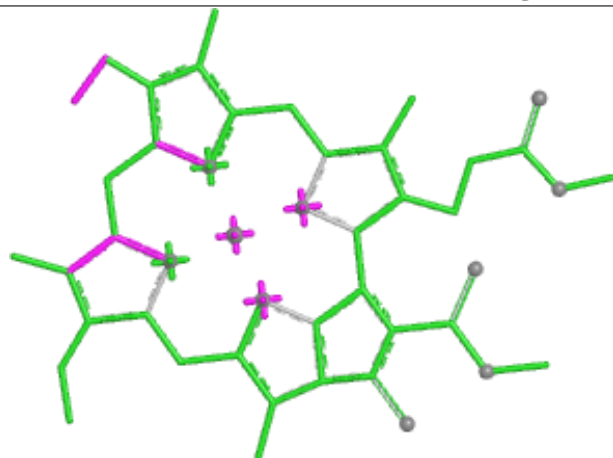
Torsions



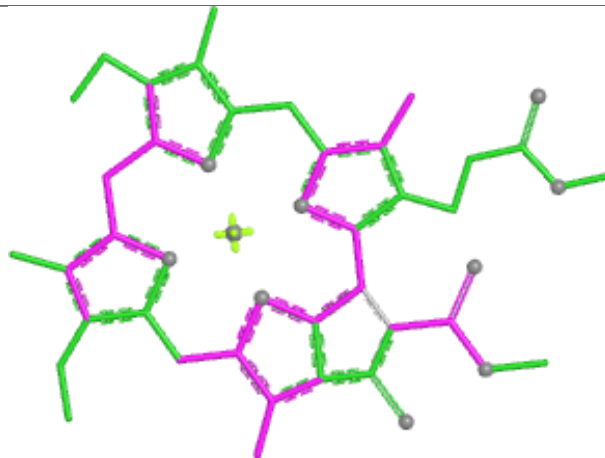
Rings



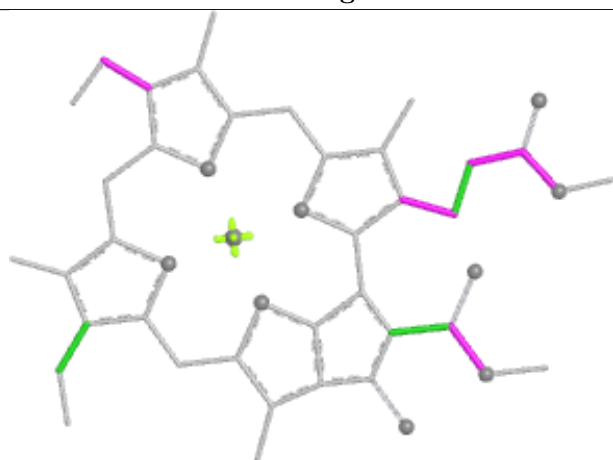
Ligand CLA Z 315



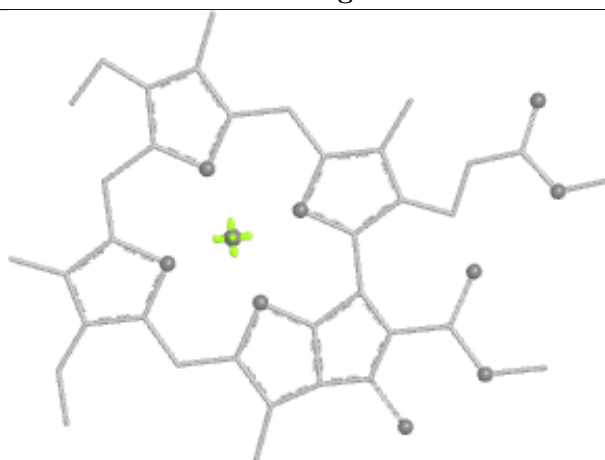
Bond lengths



Bond angles

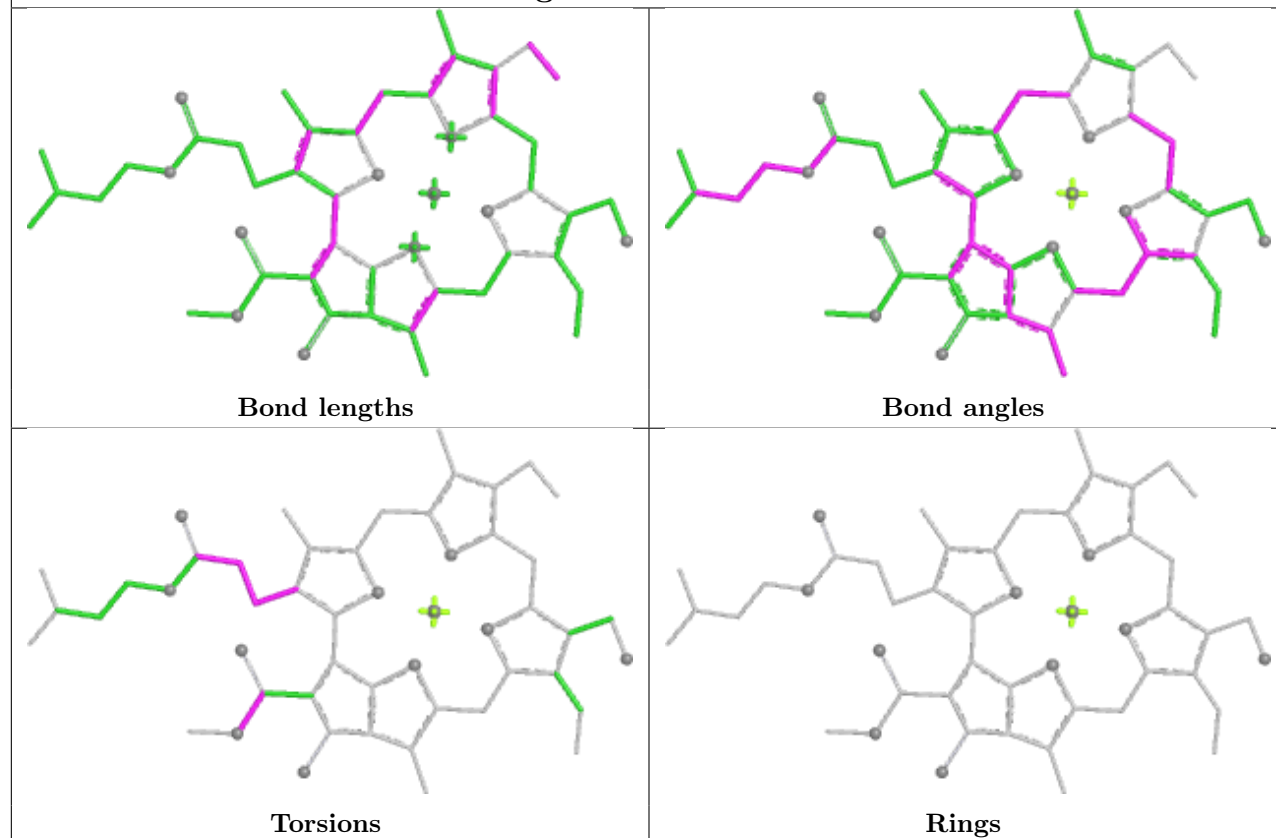


Torsions

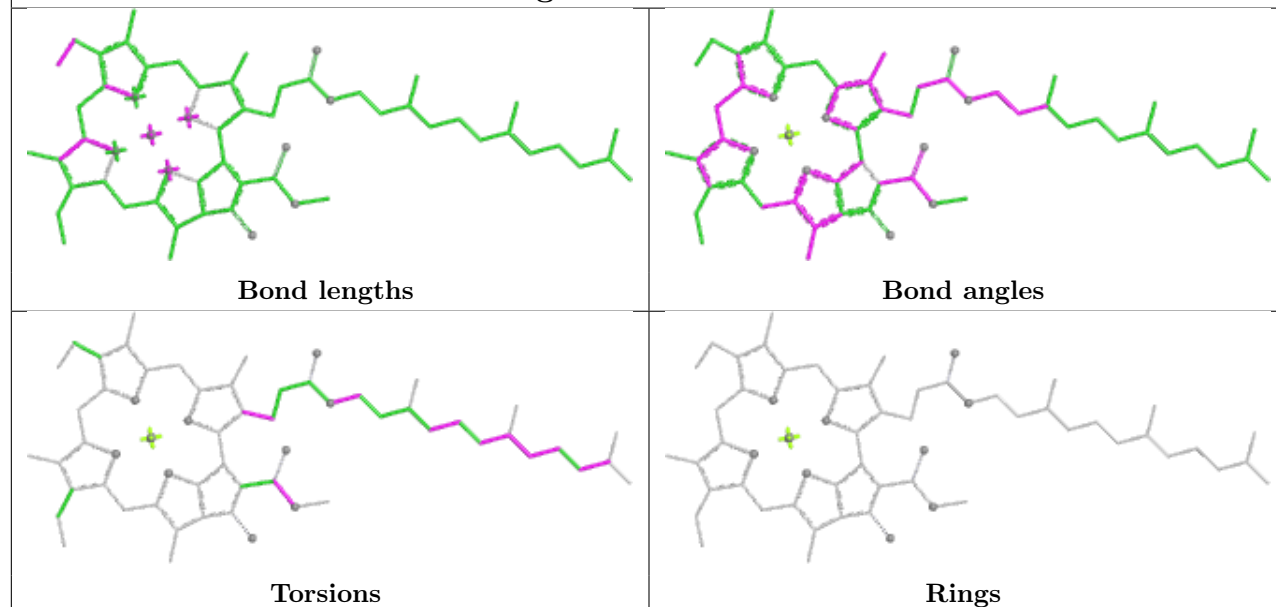


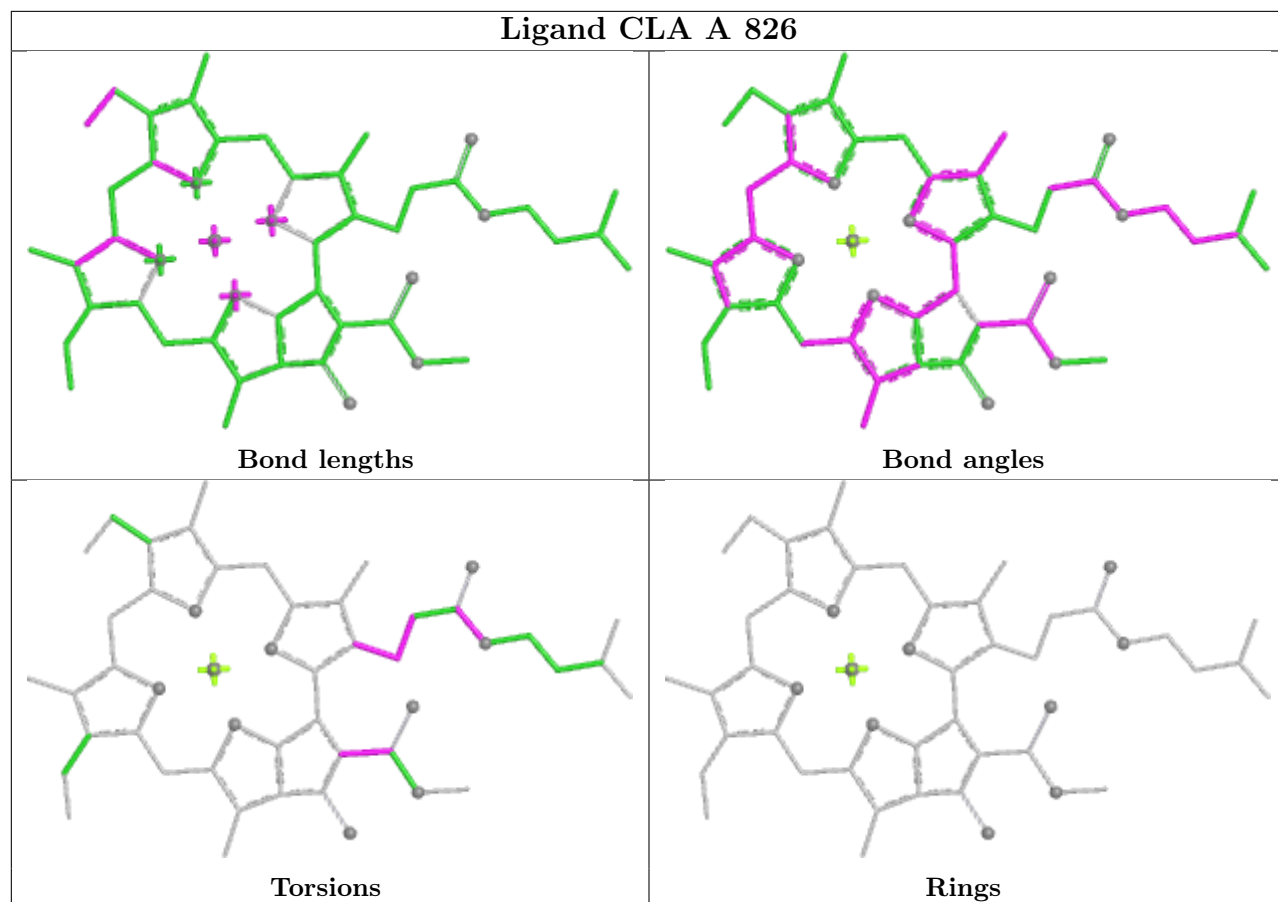
Rings

Ligand CHL 4 814

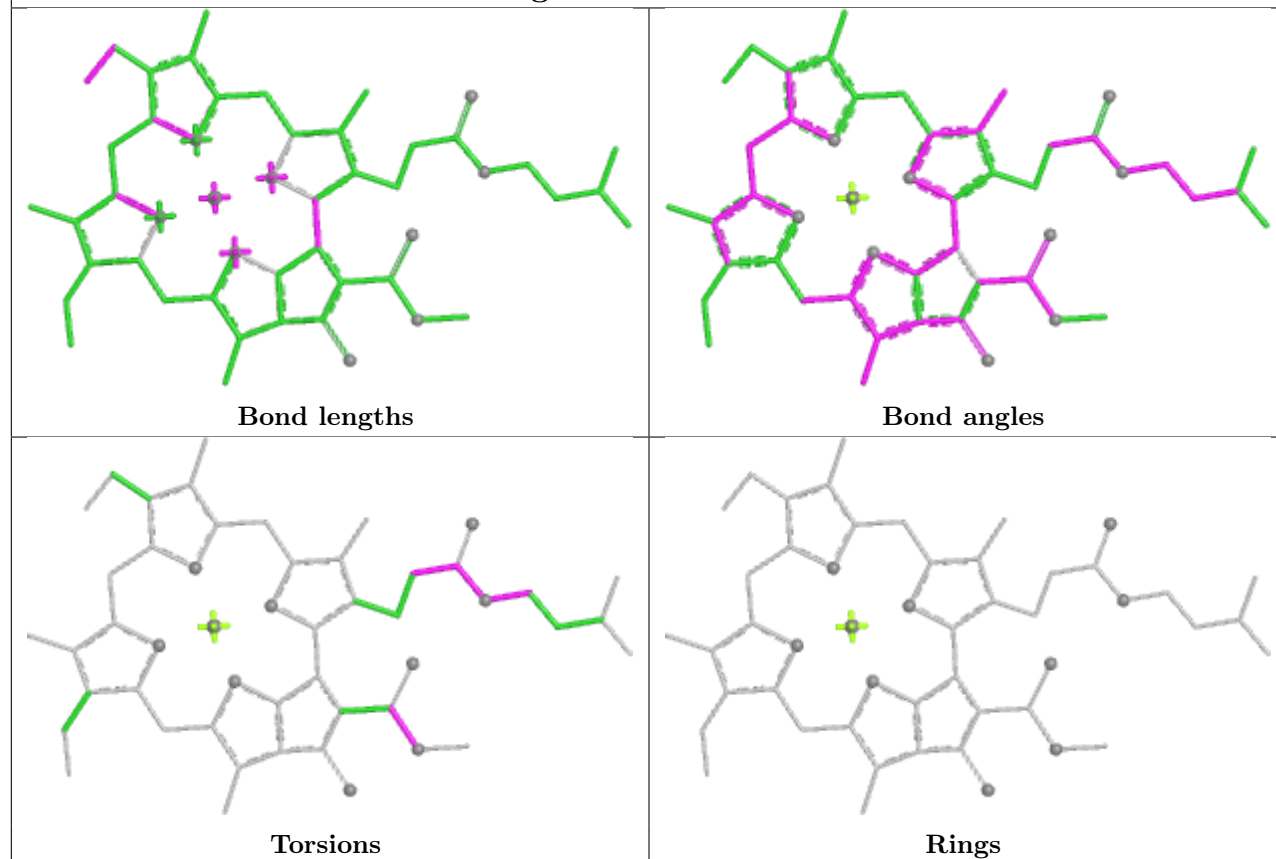


Ligand CLA 7 304

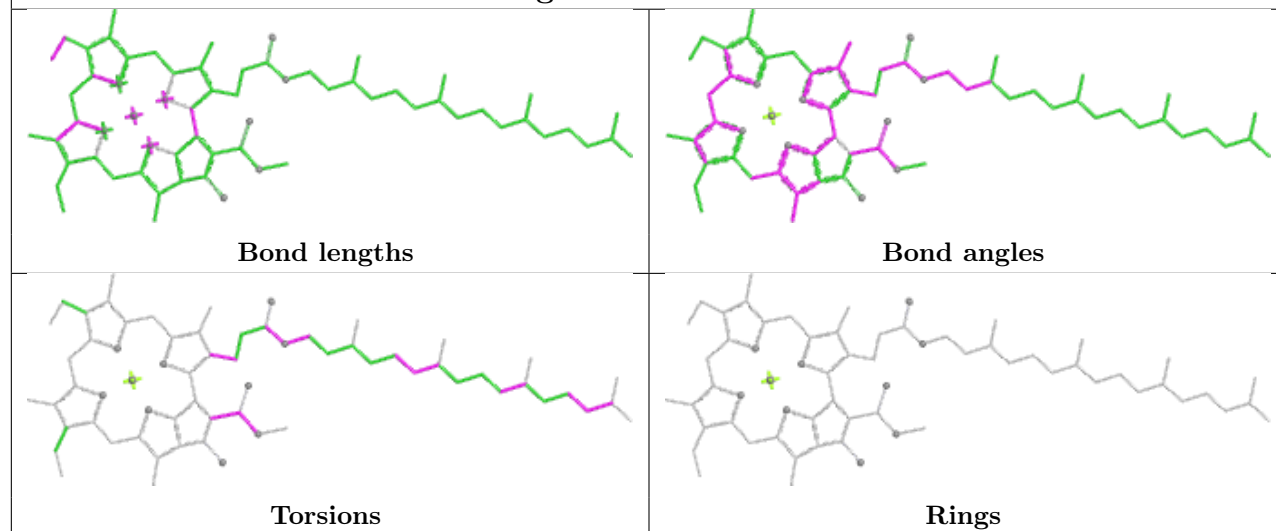




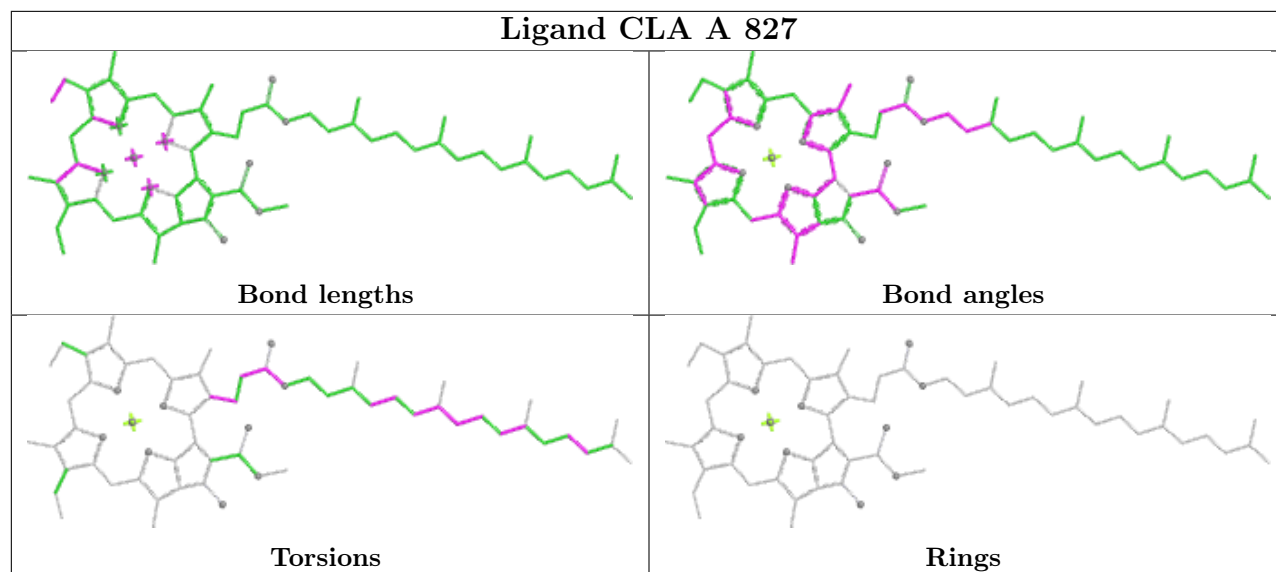
Ligand CLA G 201



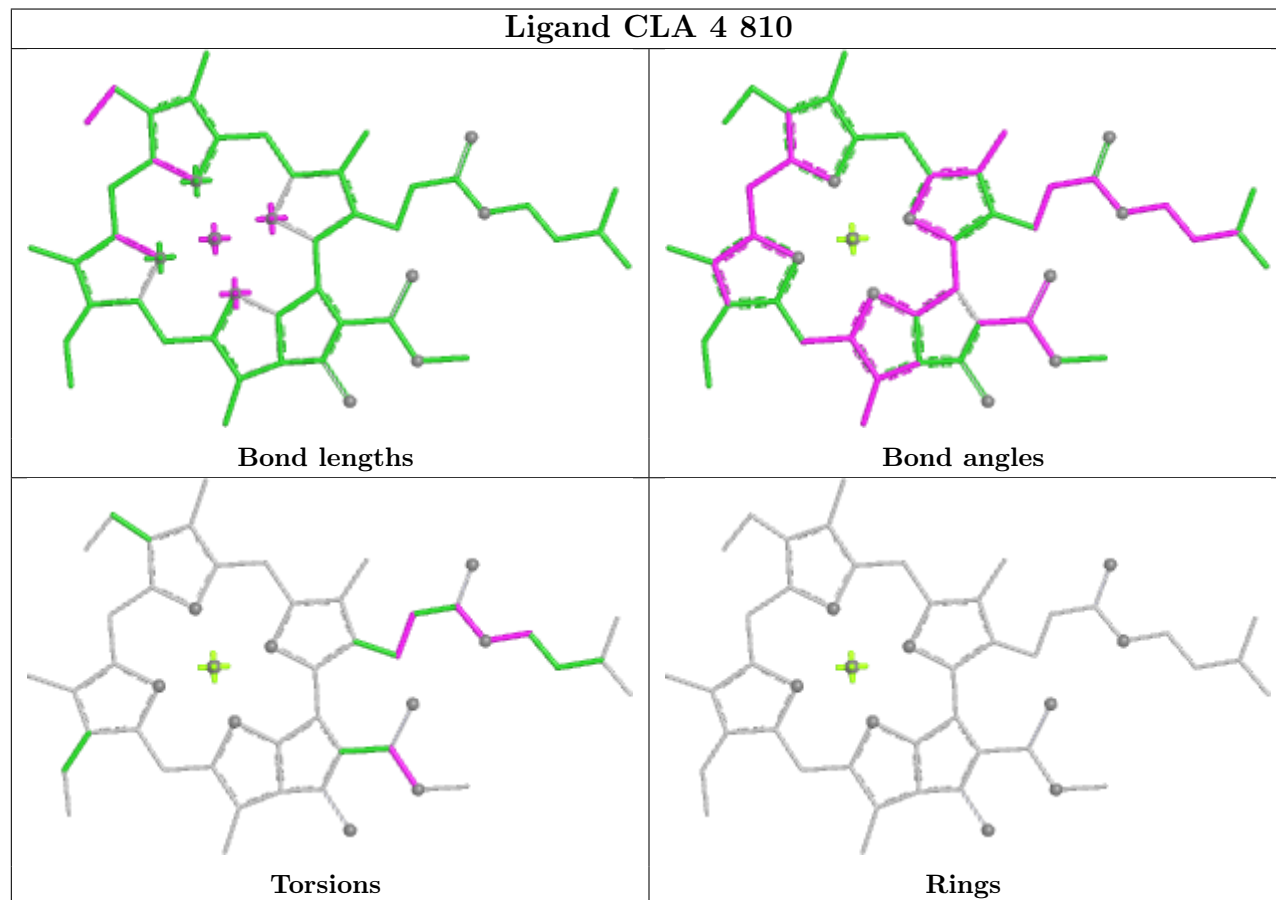
Ligand CLA 6 312



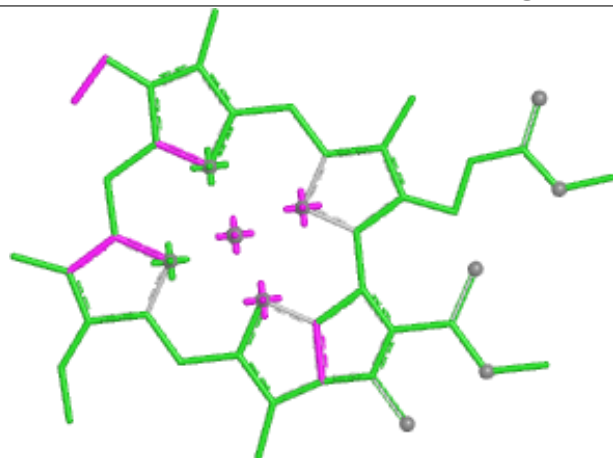
Ligand CLA A 827



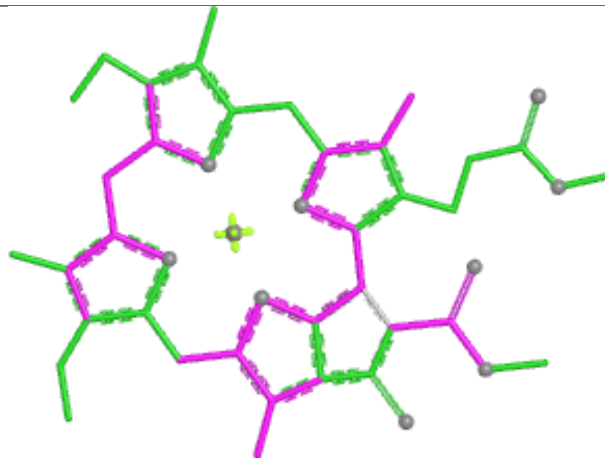
Ligand CLA 4 810



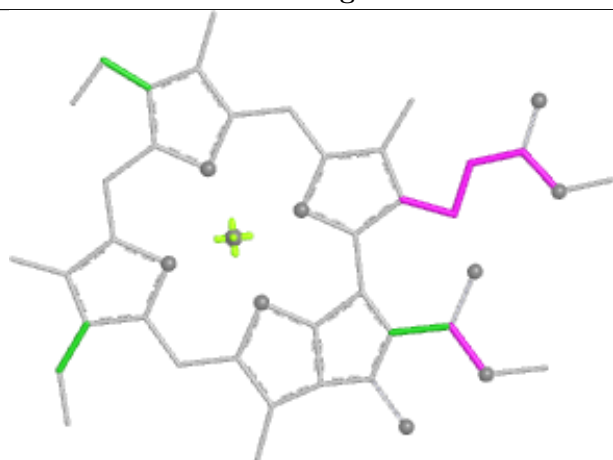
Ligand CLA 8 316



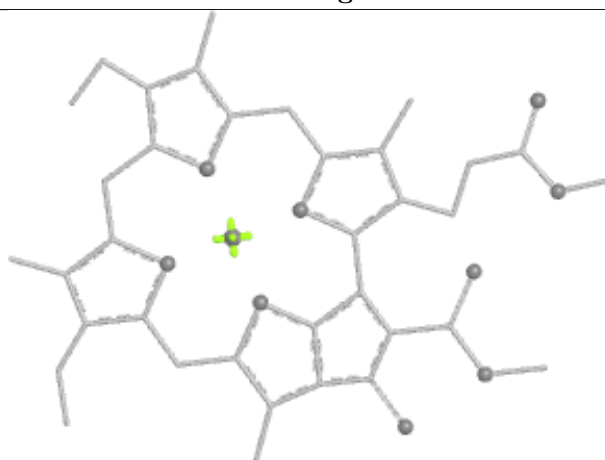
Bond lengths



Bond angles

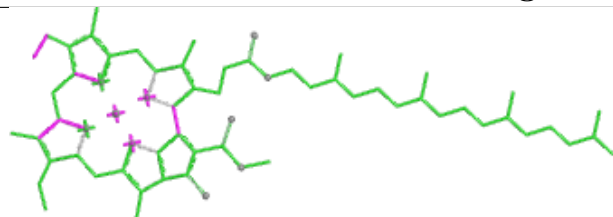


Torsions

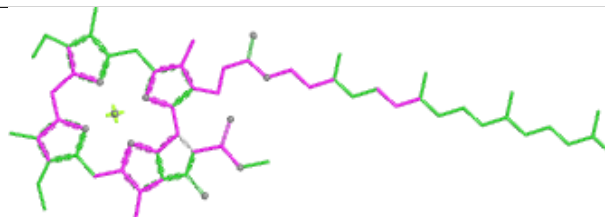


Rings

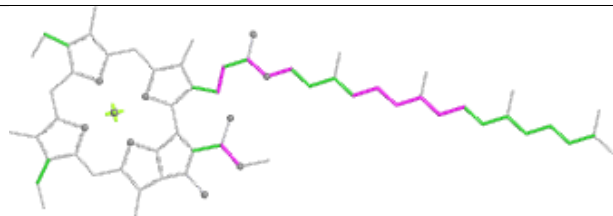
Ligand CLA 3 310



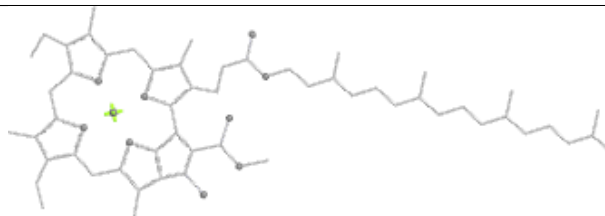
Bond lengths



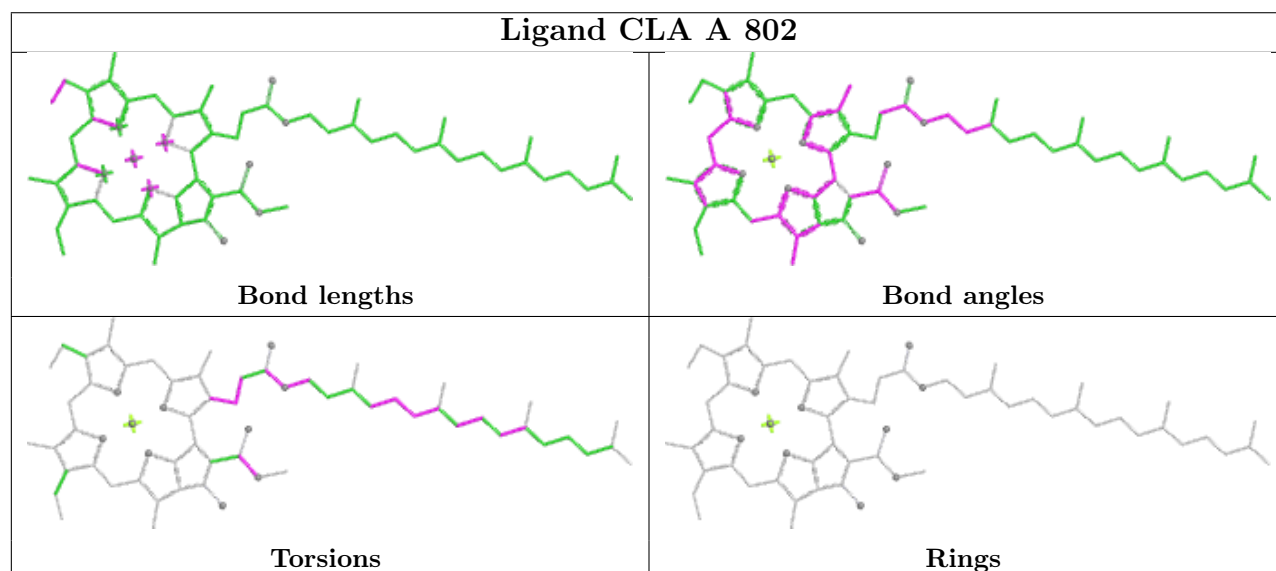
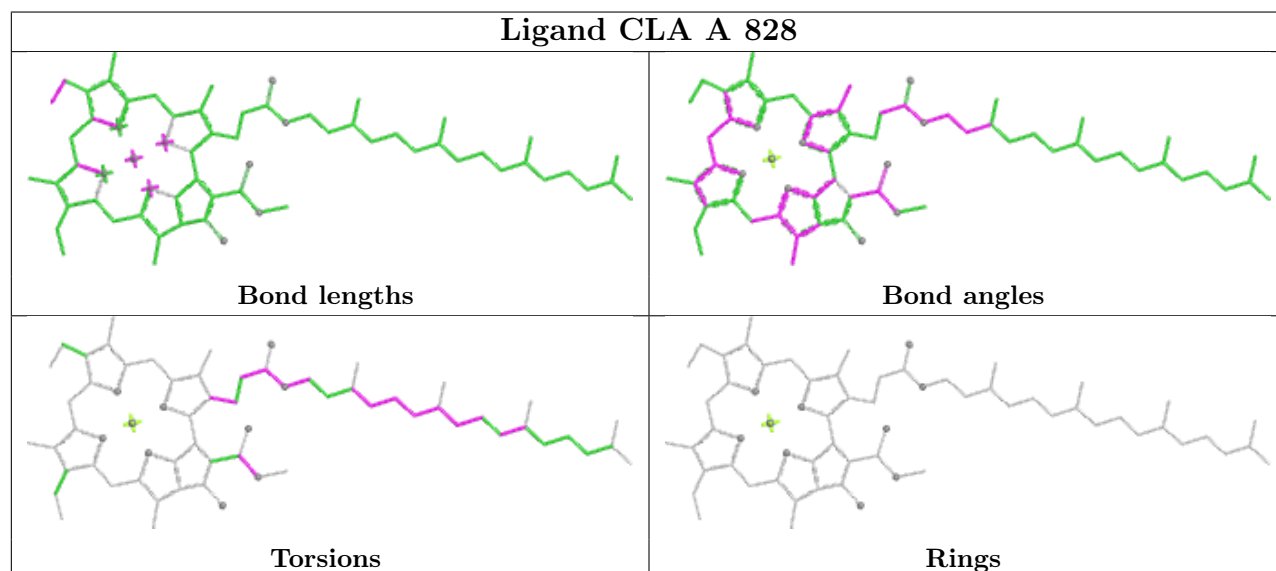
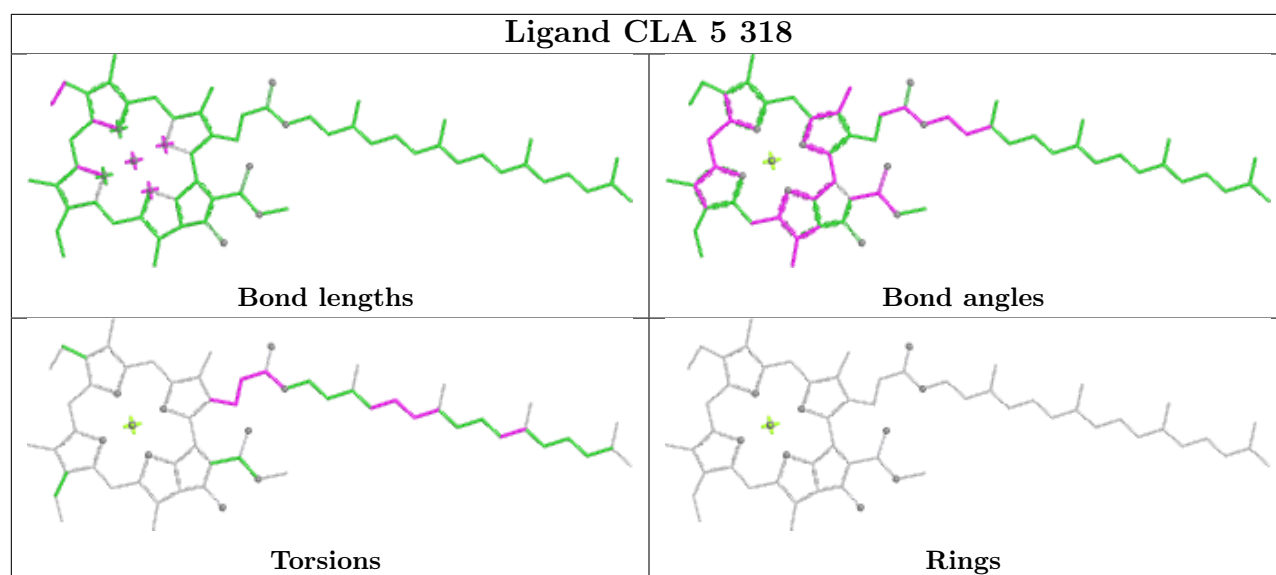
Bond angles



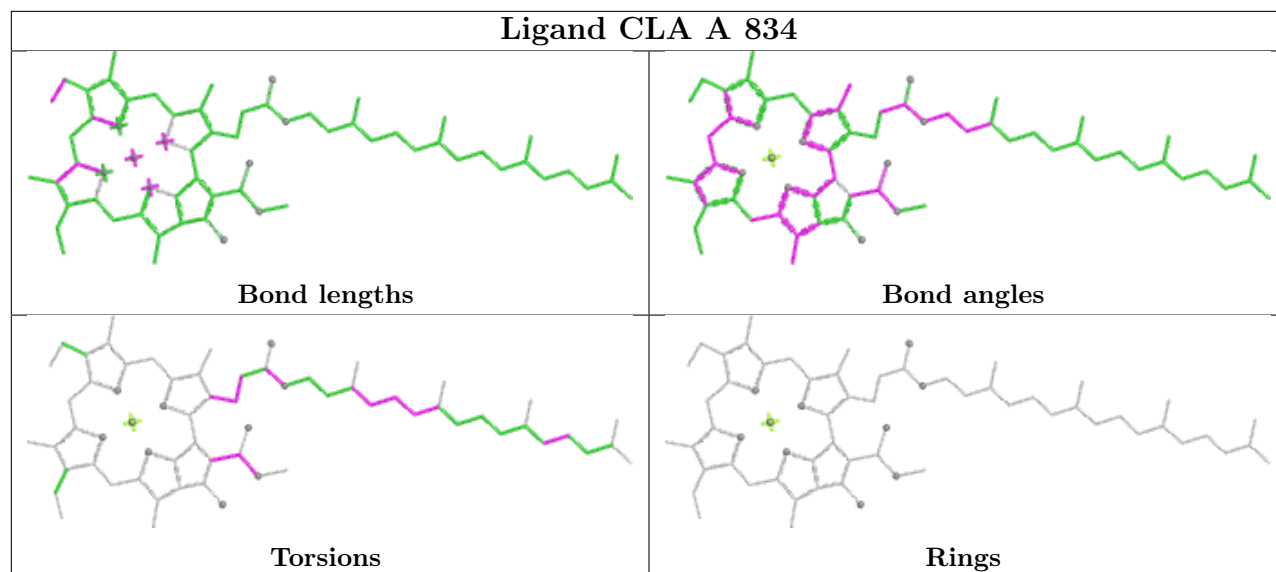
Torsions



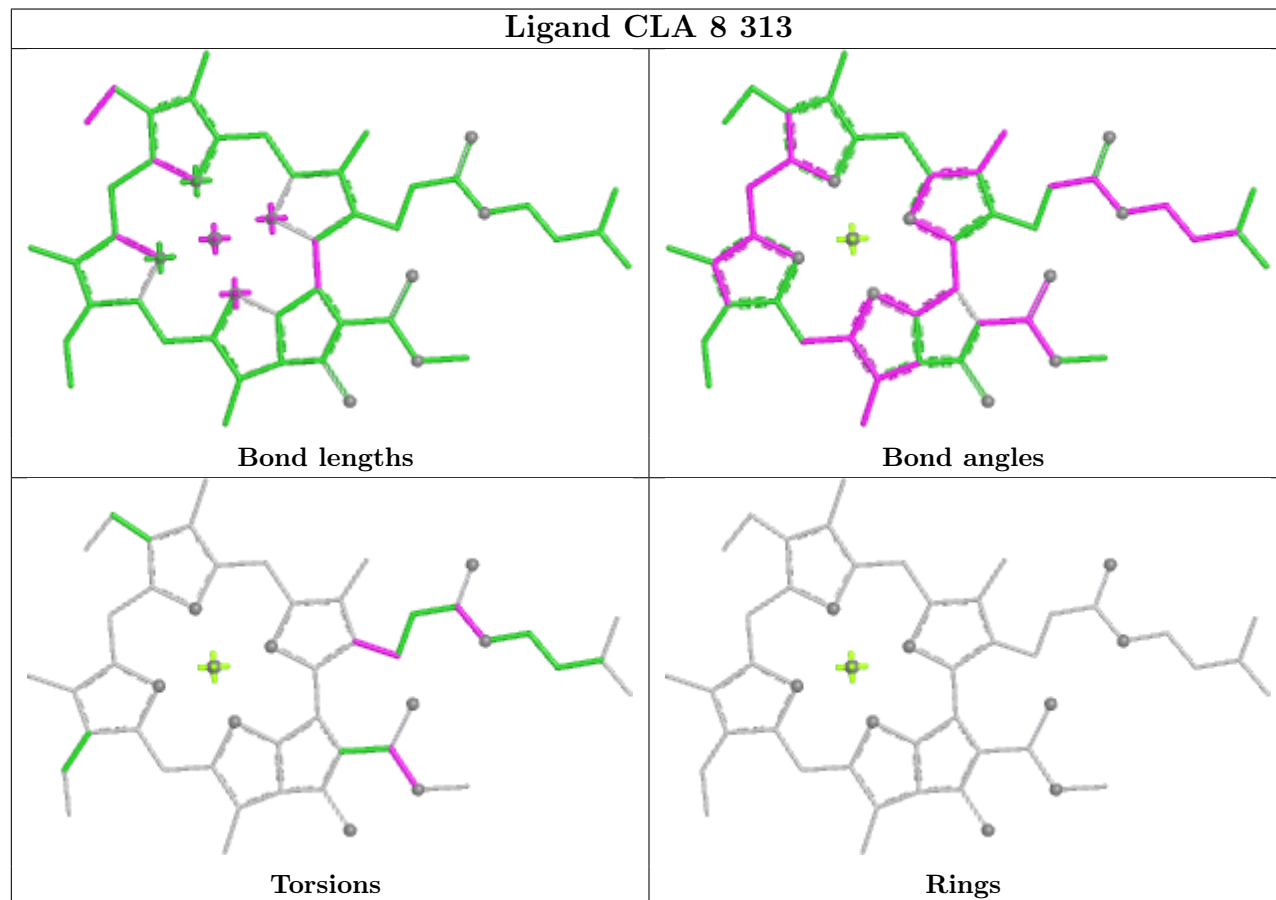
Rings

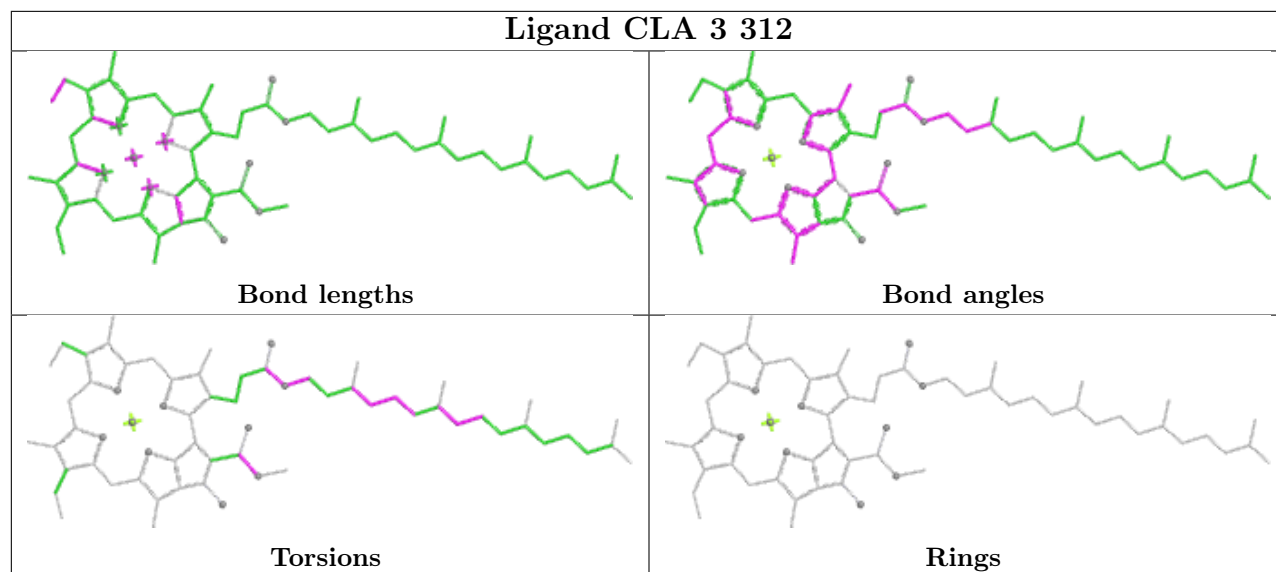
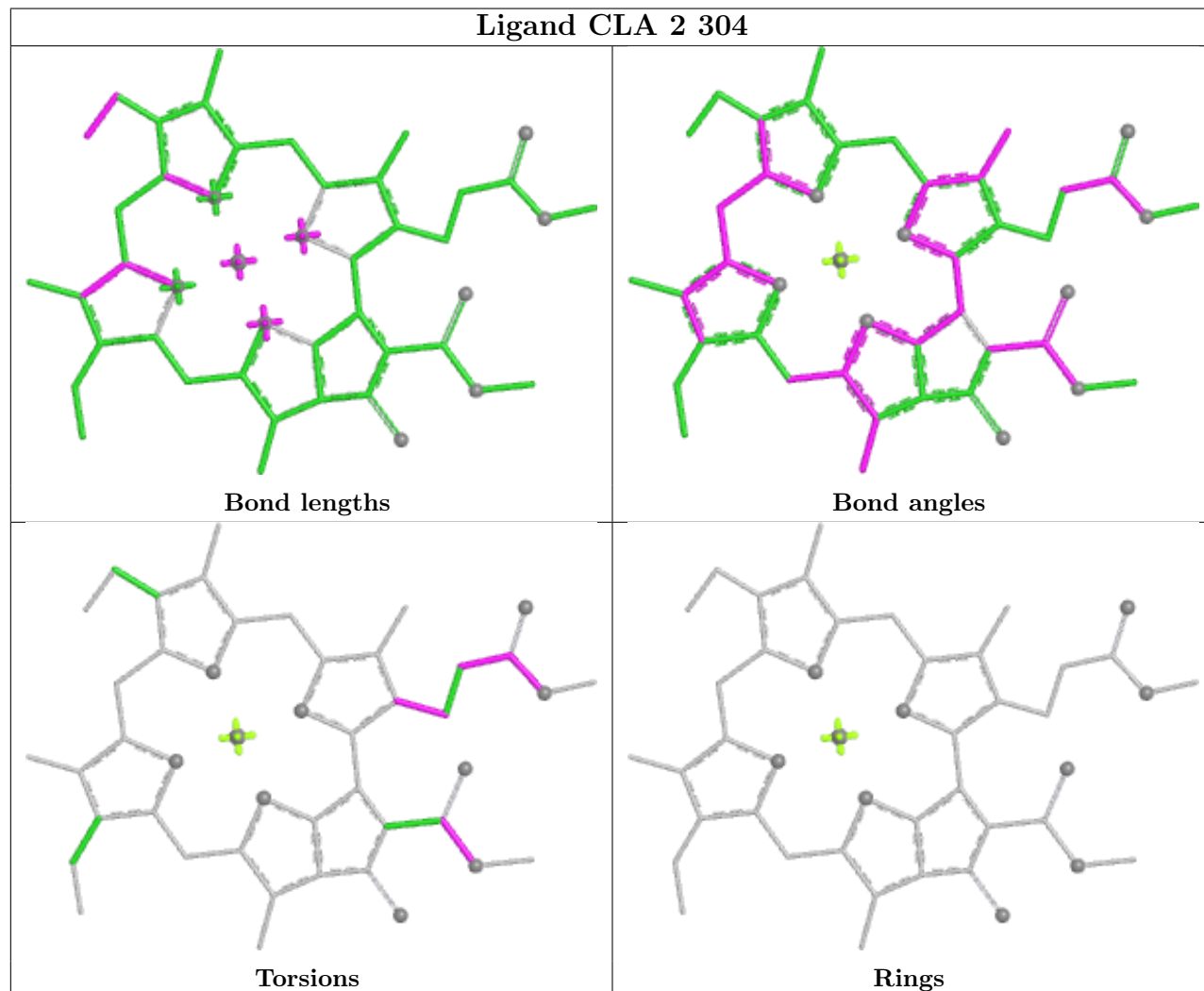


Ligand CLA A 834

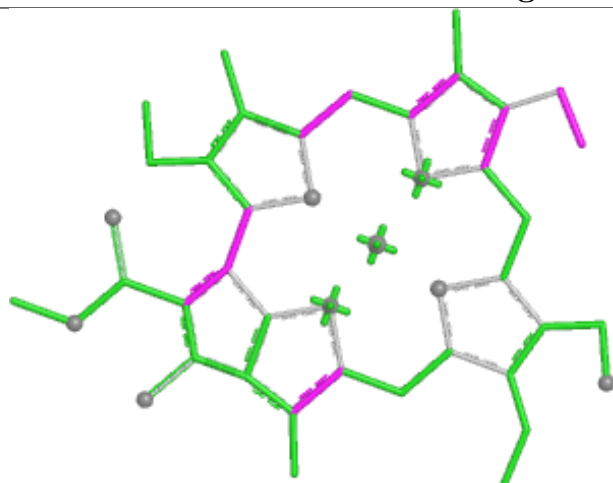


Ligand CLA 8 313

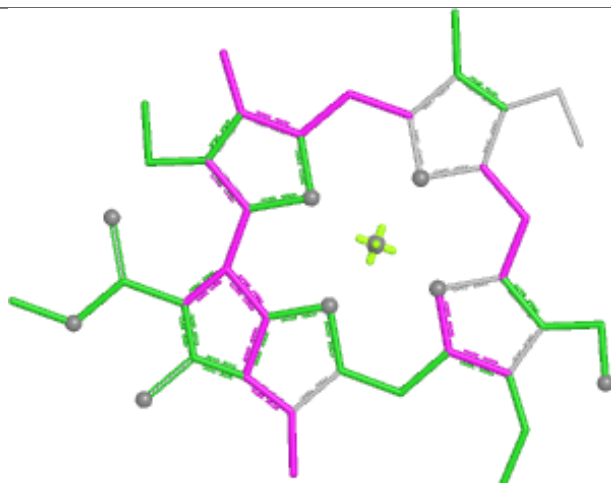


Ligand CLA 3 312**Ligand CLA 2 304**

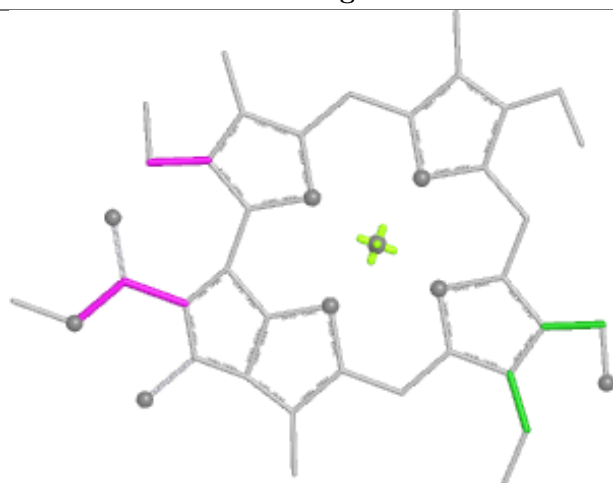
Ligand CHL 5 321



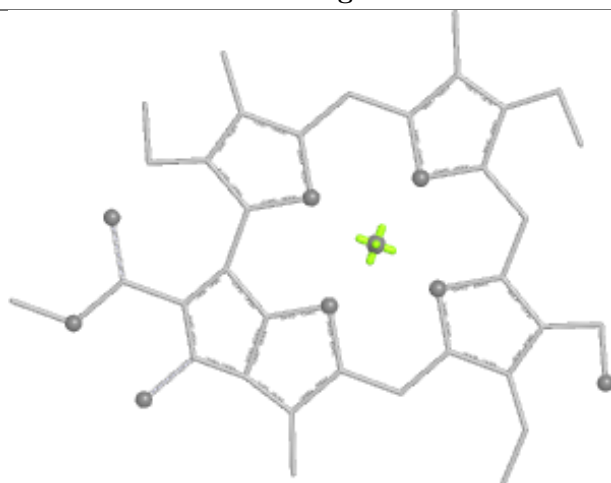
Bond lengths



Bond angles

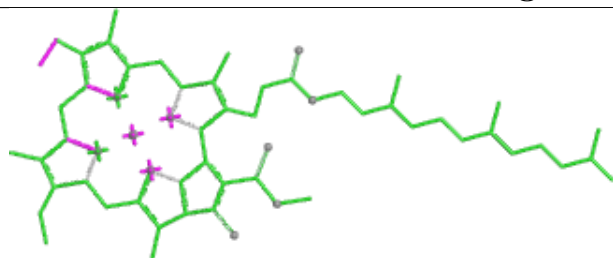


Torsions

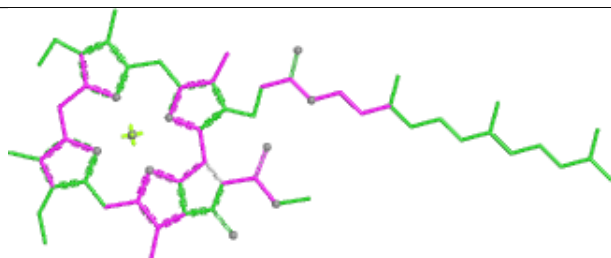


Rings

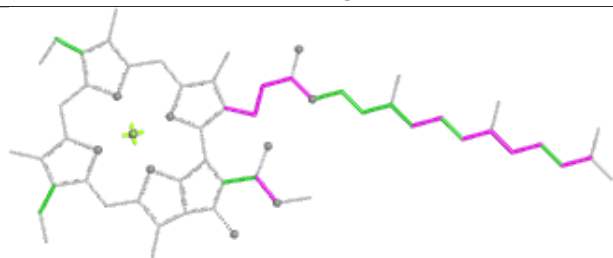
Ligand CLA 7 312



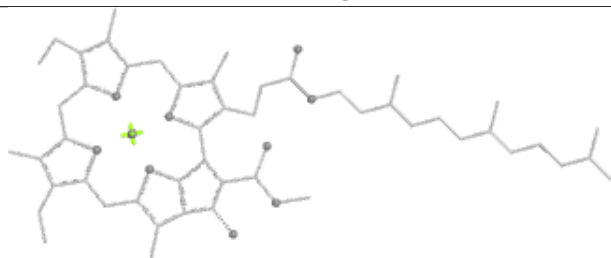
Bond lengths



Bond angles

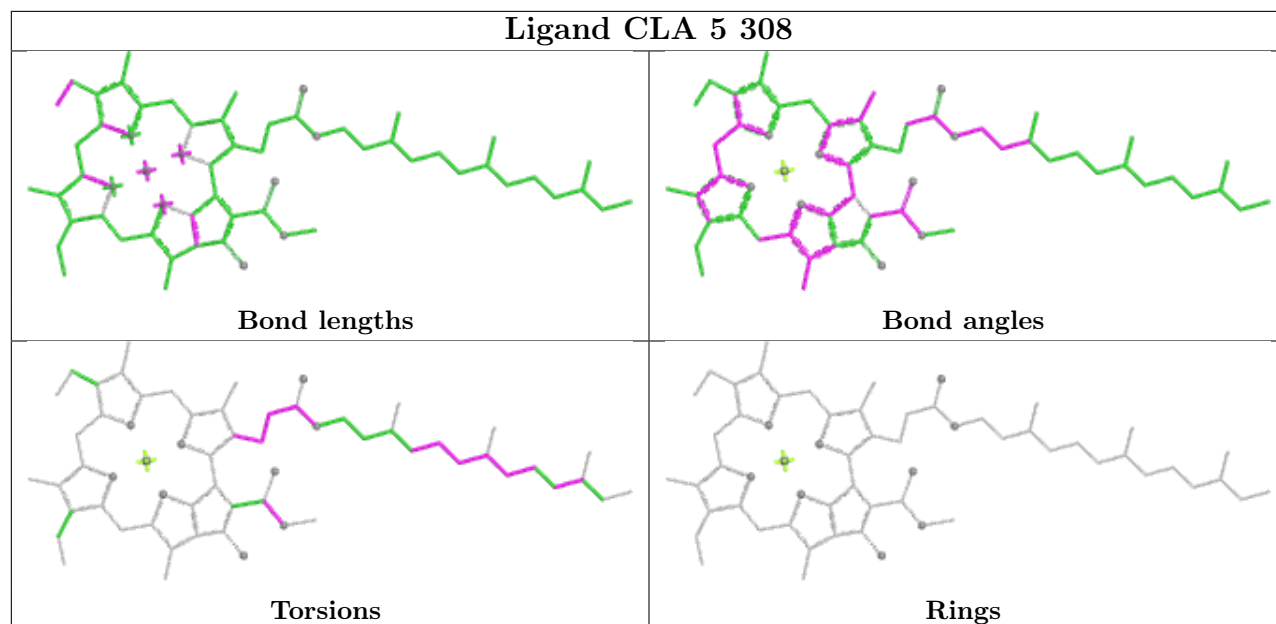


Torsions

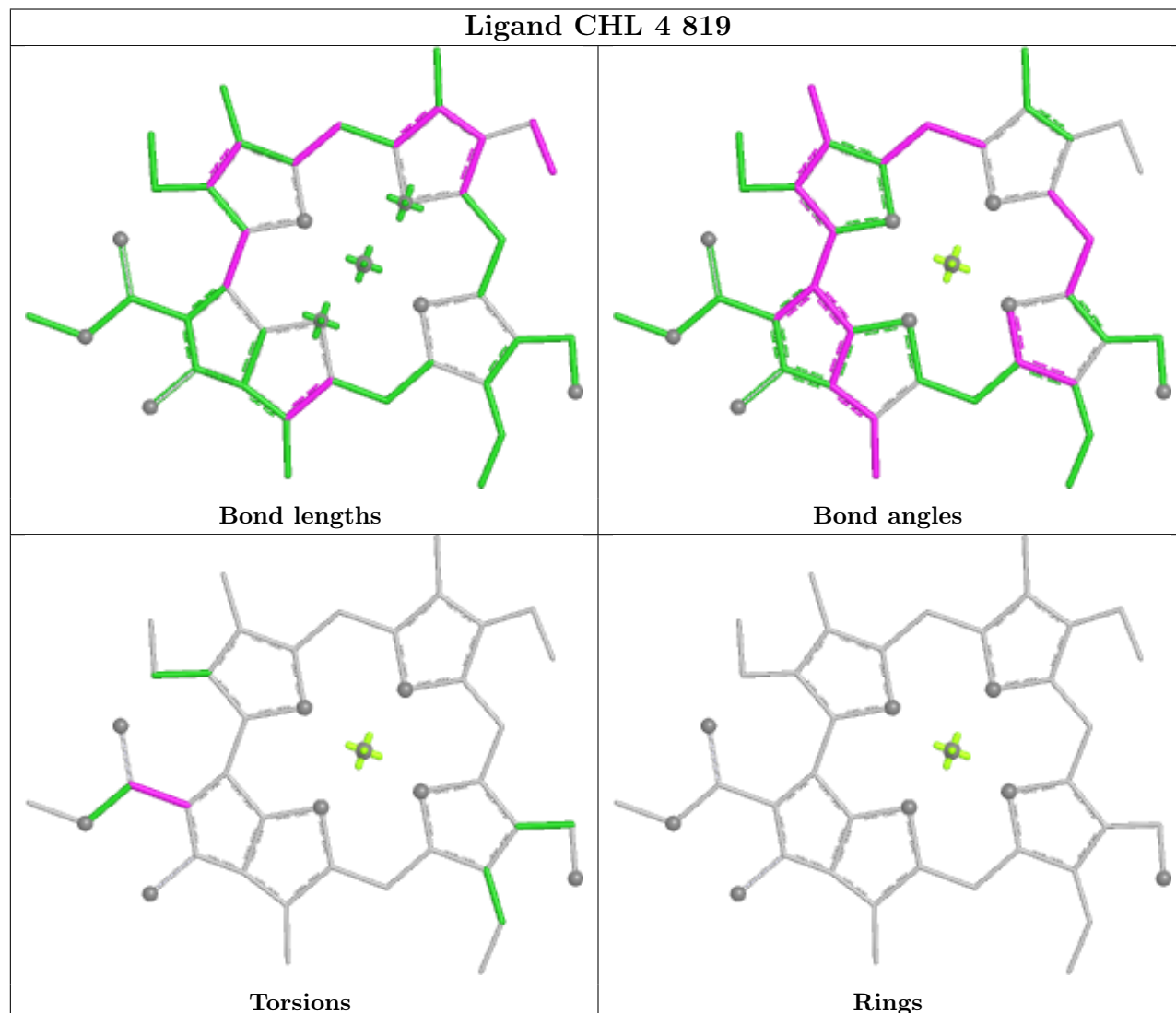


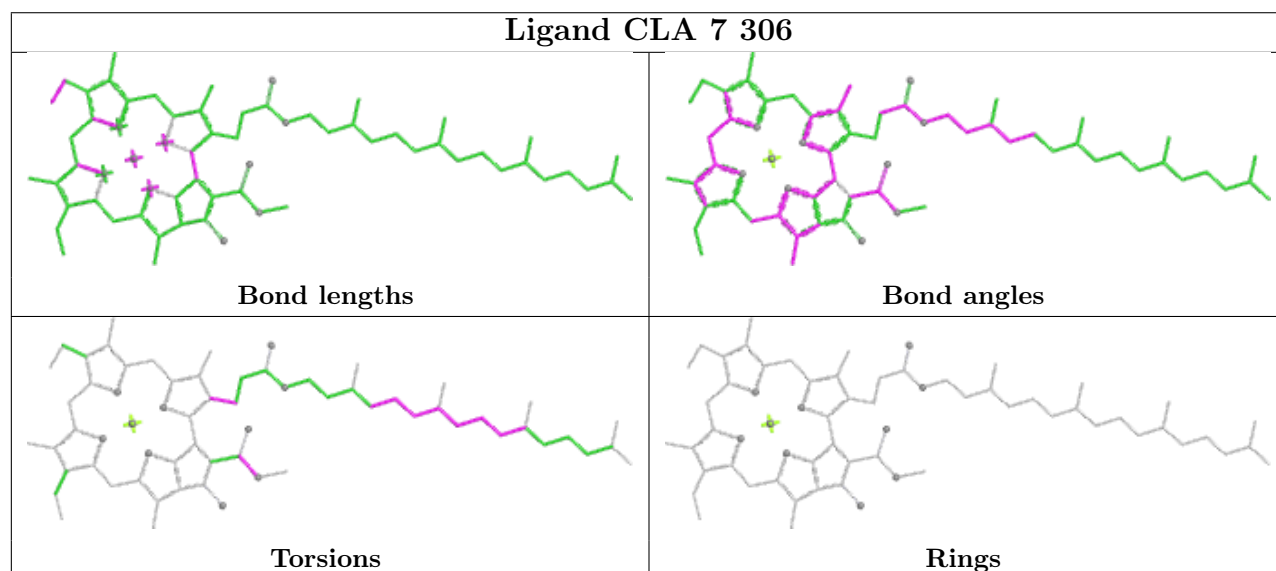
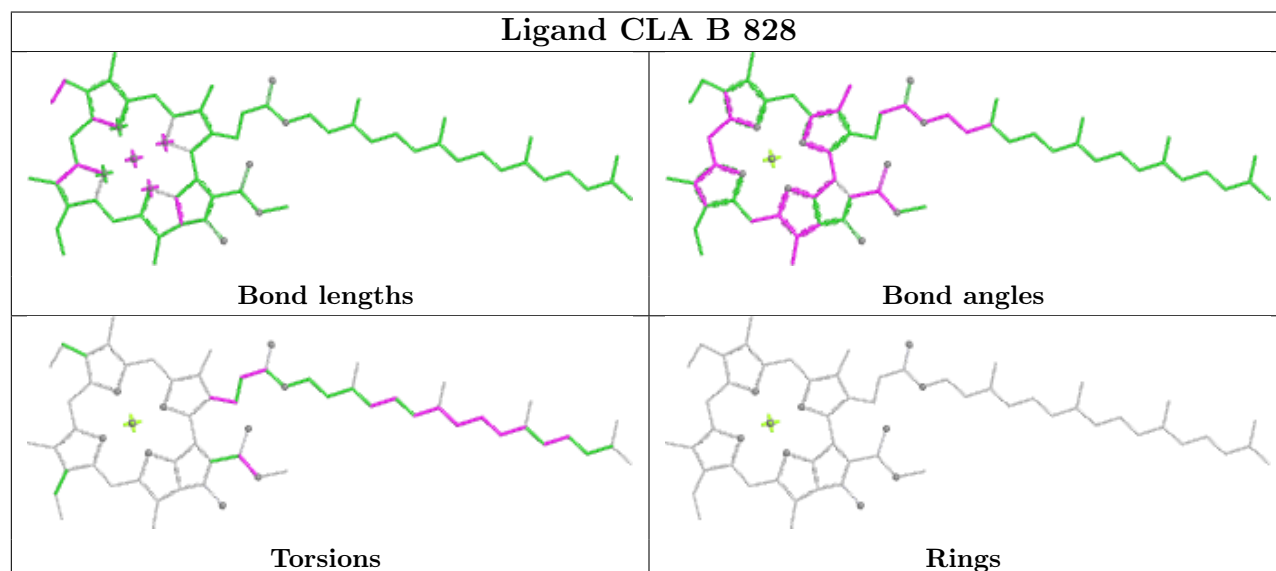
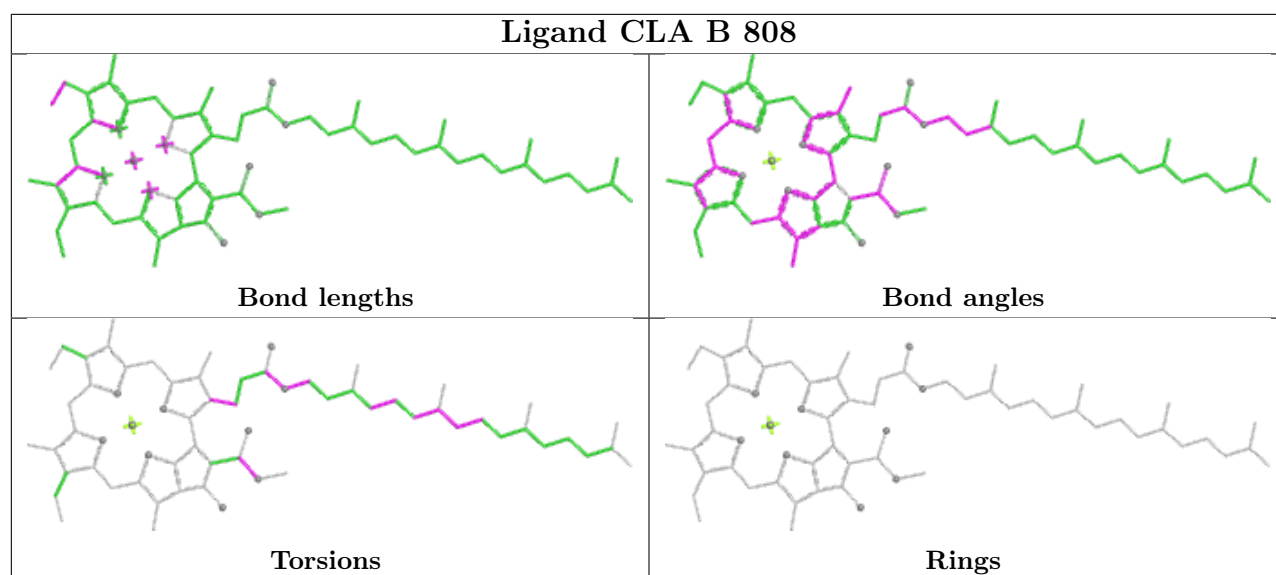
Rings

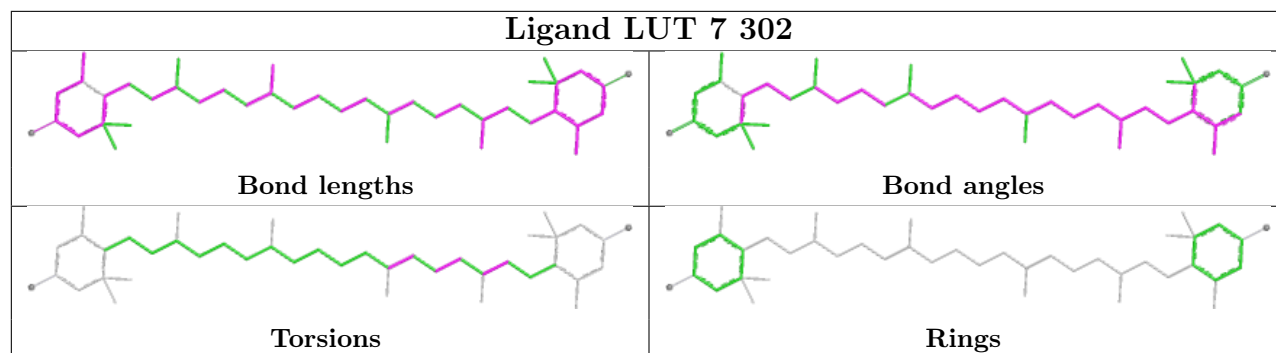
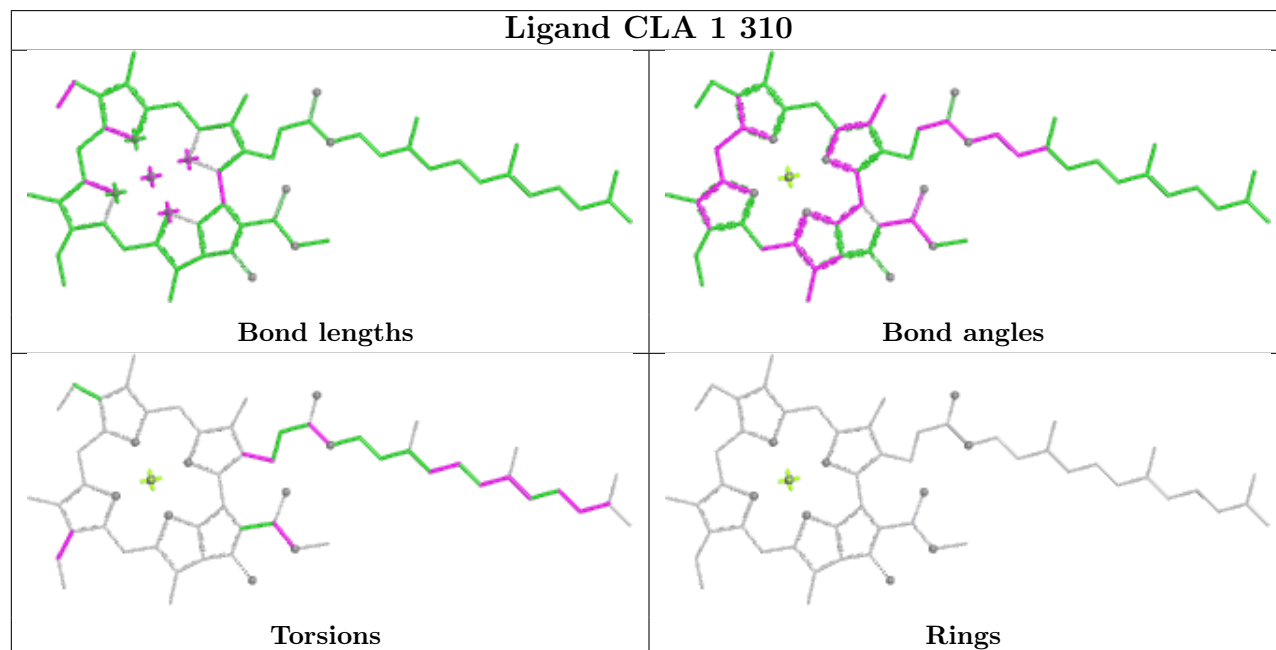
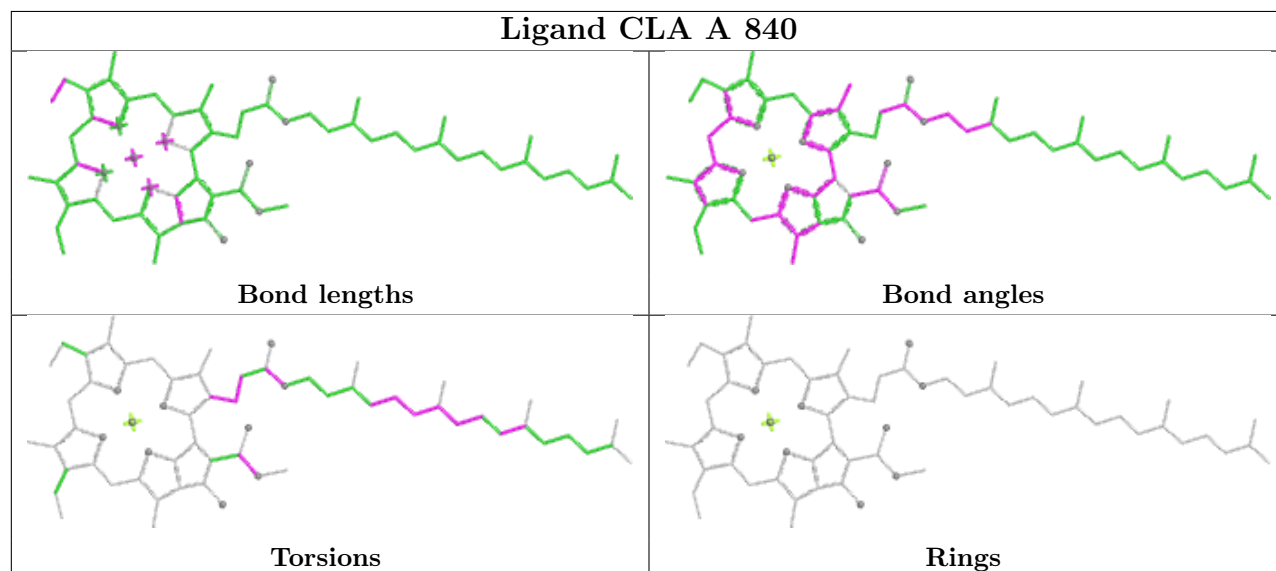
Ligand CLA 5 308

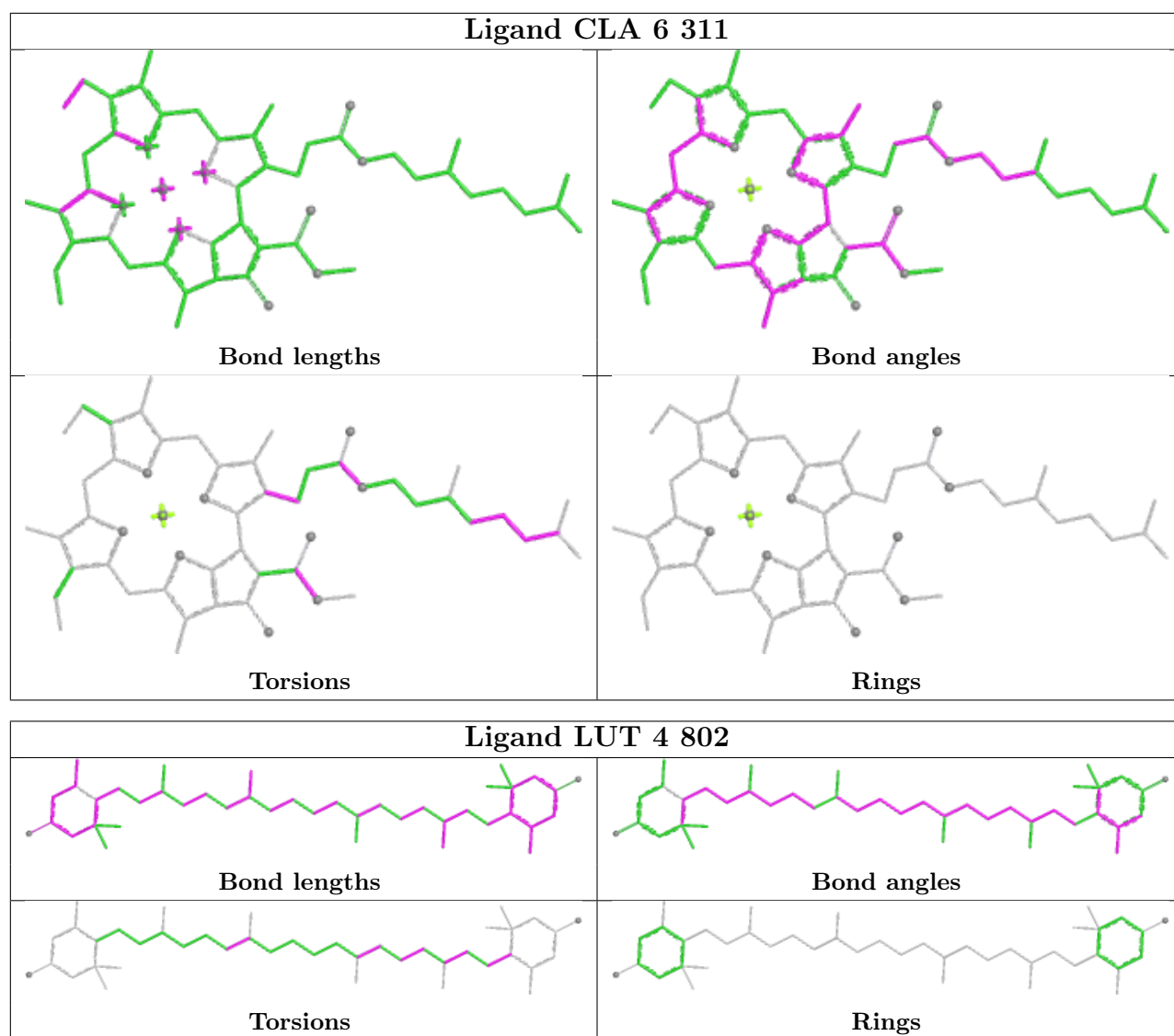


Ligand CHL 4 819

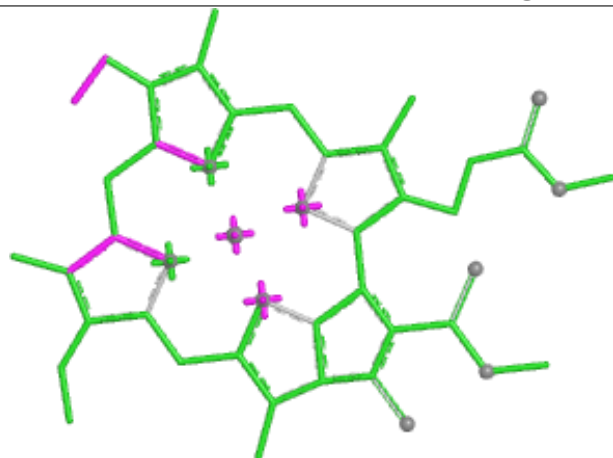




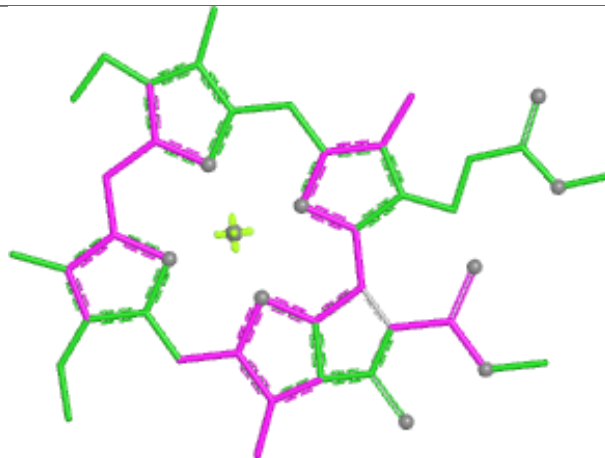
Ligand LUT 7 302**Ligand CLA 1 310****Ligand CLA A 840**



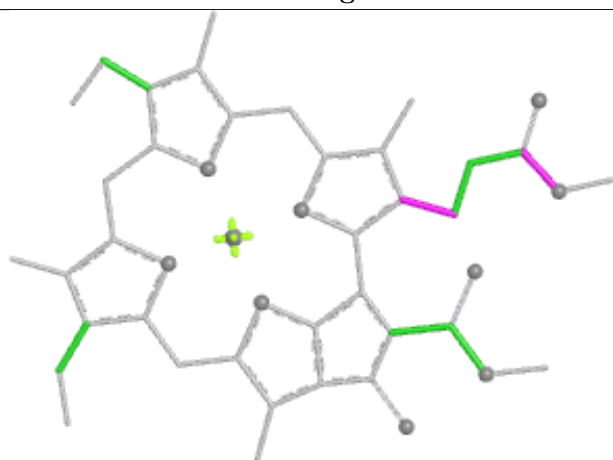
Ligand CLA 6 321



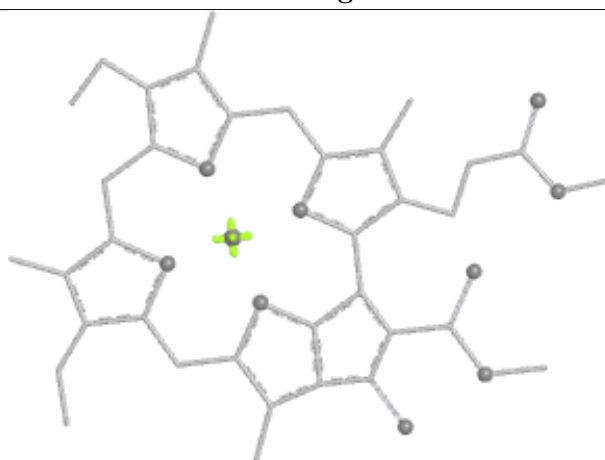
Bond lengths



Bond angles

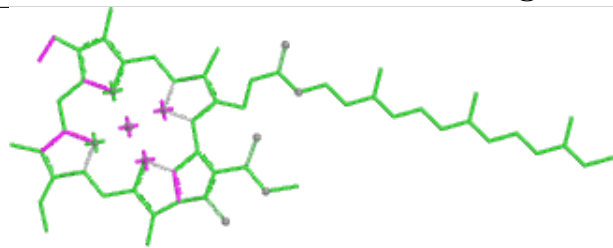


Torsions

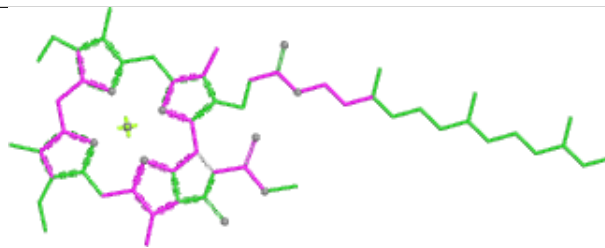


Rings

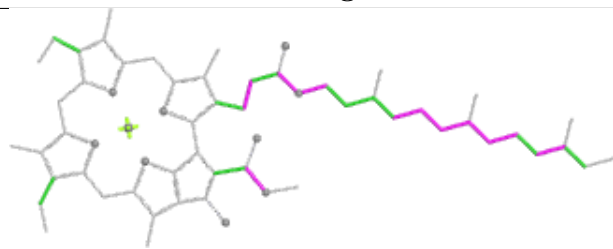
Ligand CLA 7 308



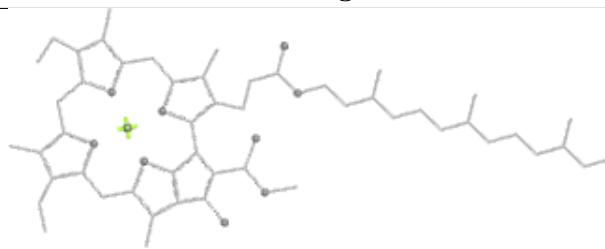
Bond lengths



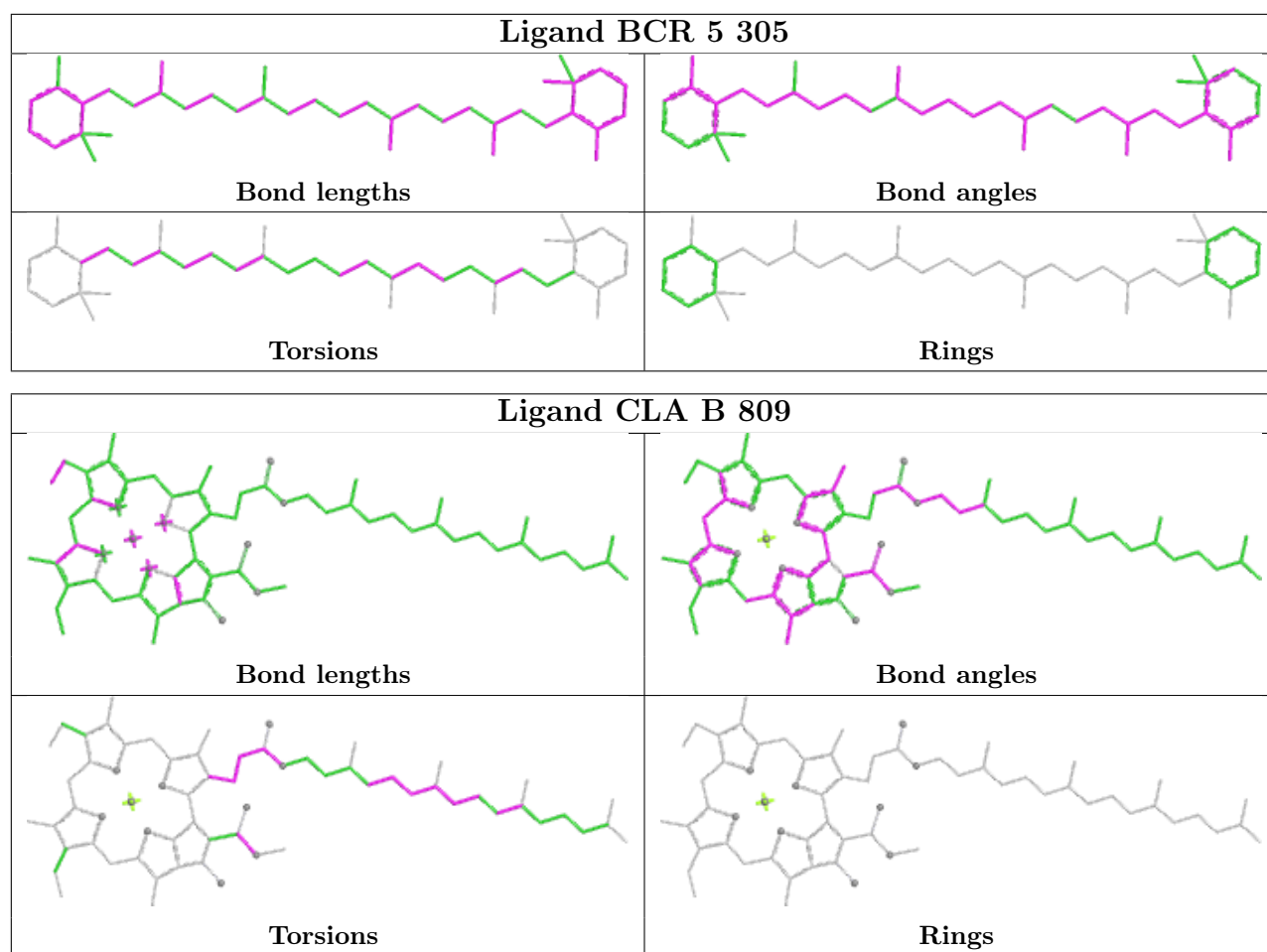
Bond angles

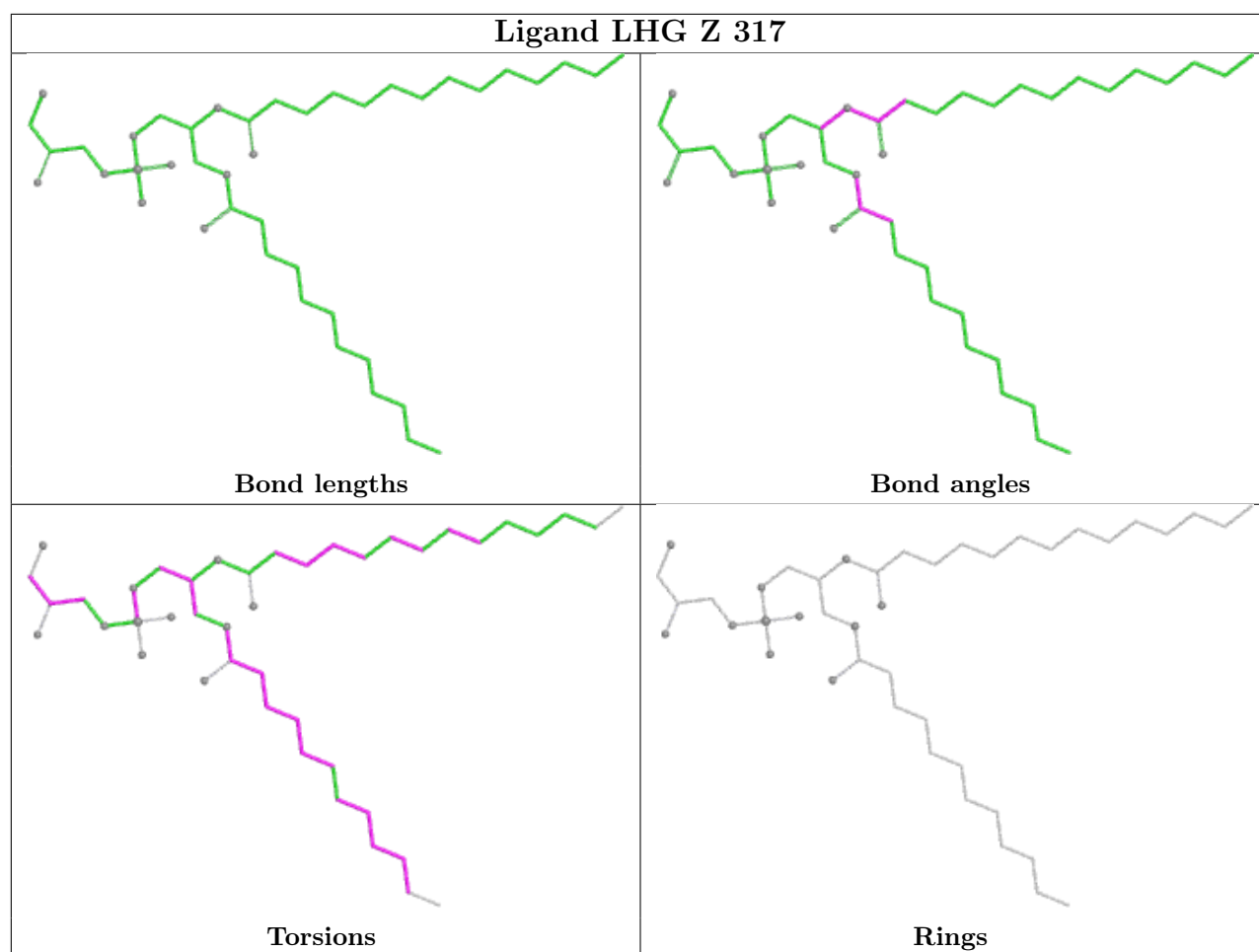


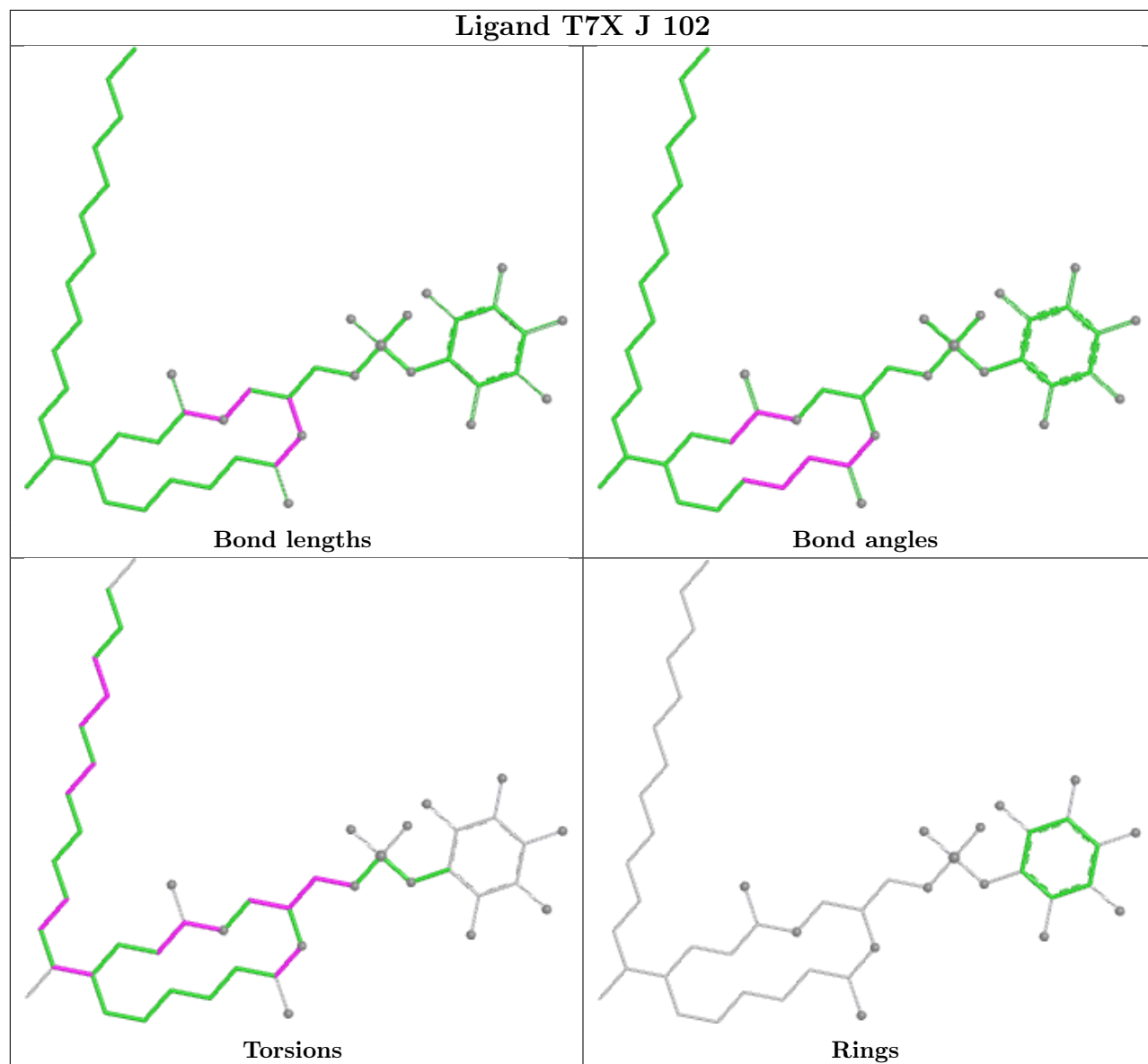
Torsions

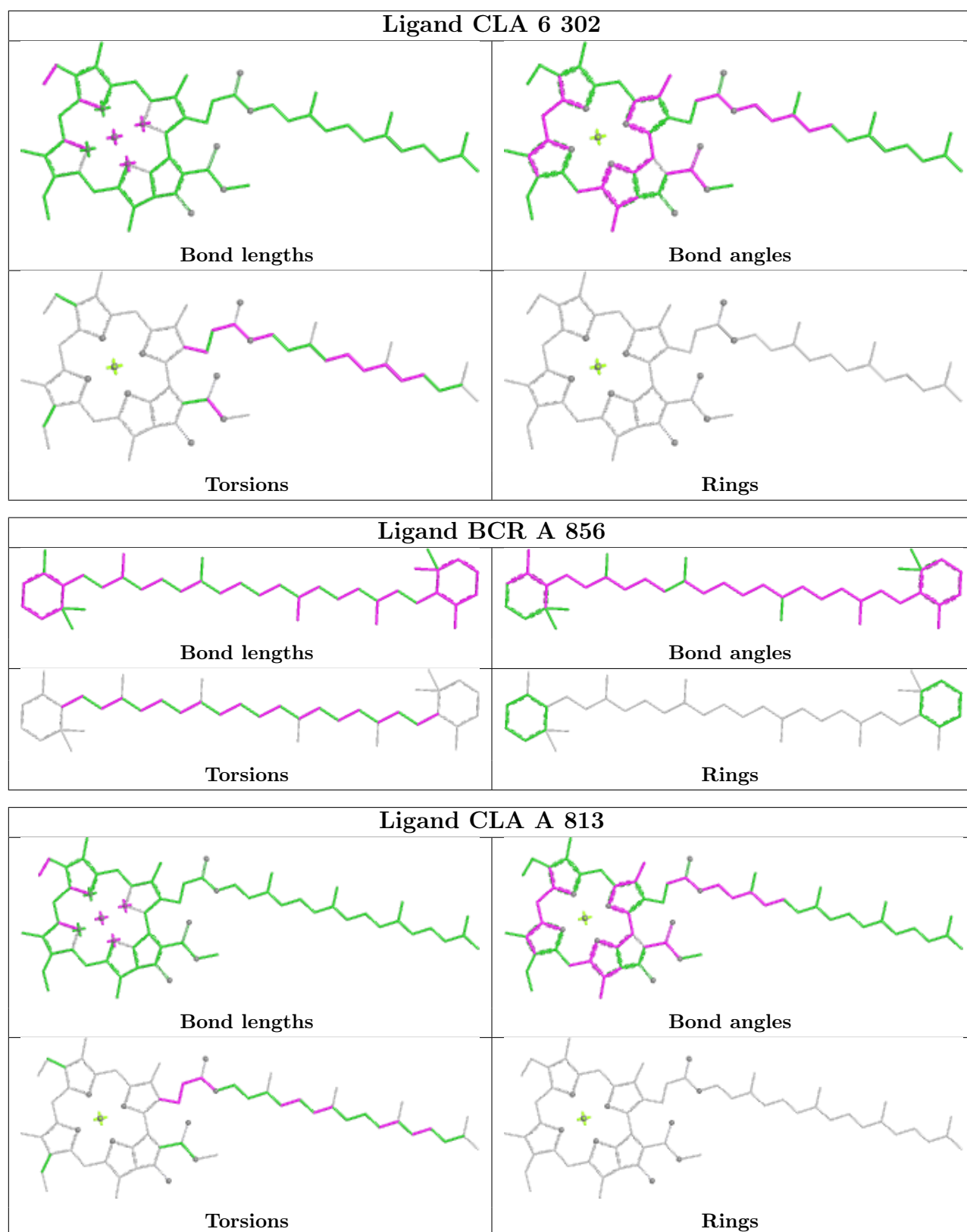


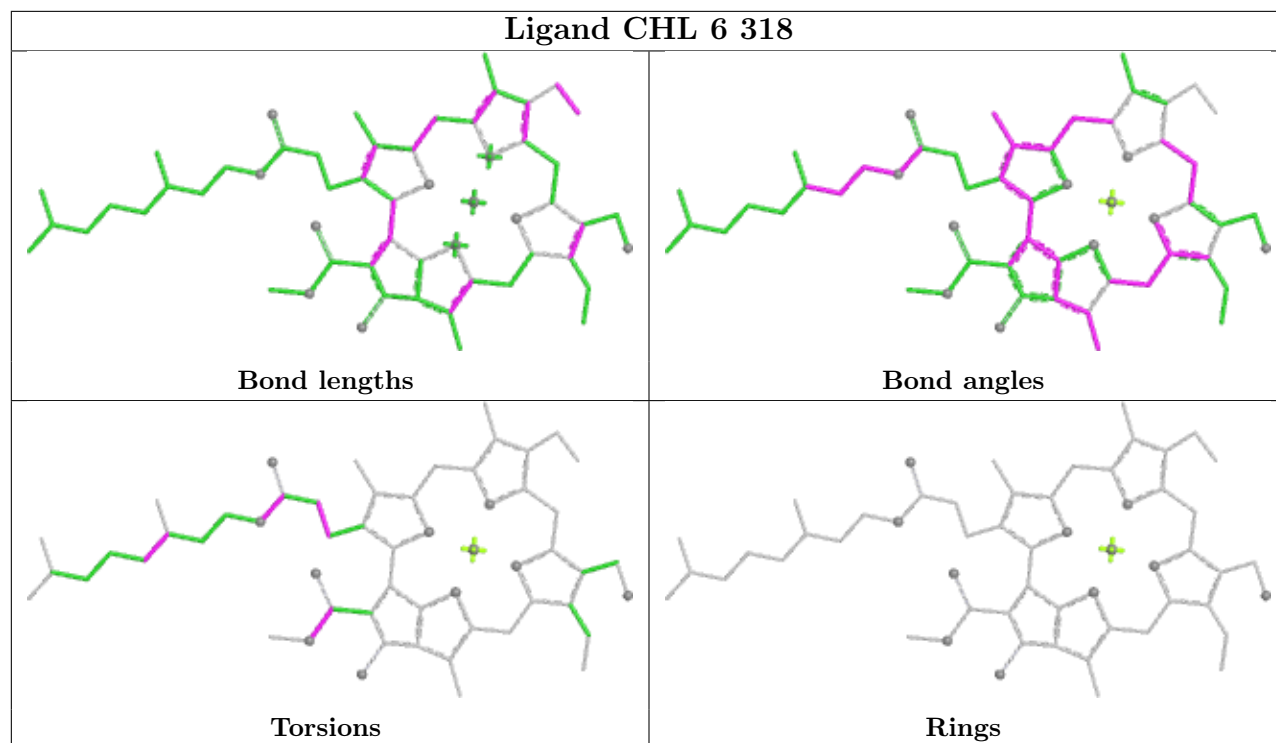
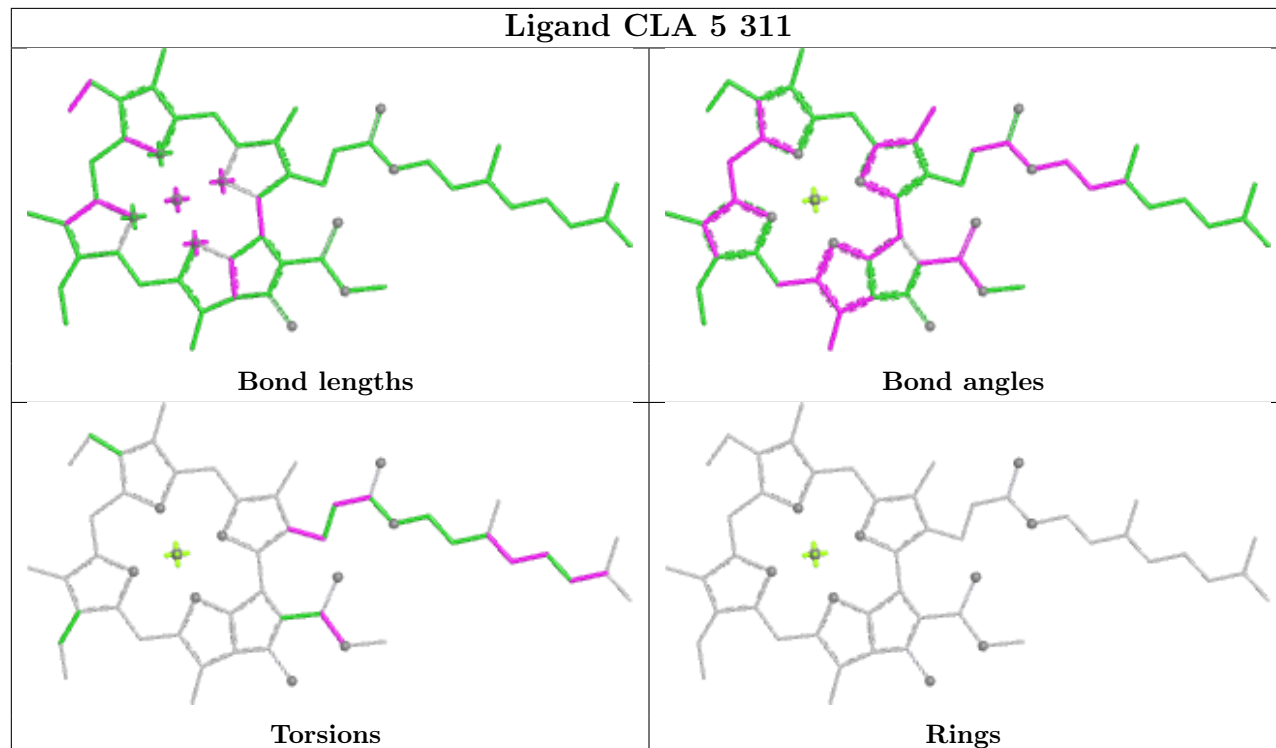
Rings

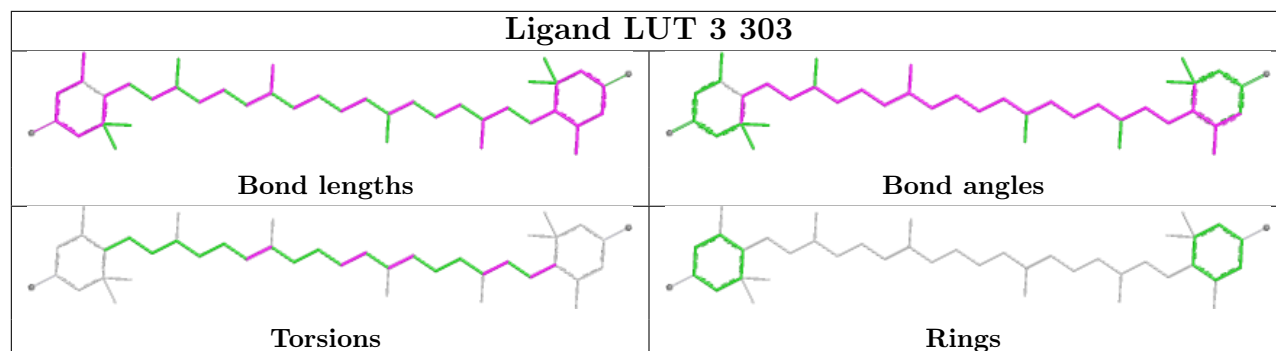
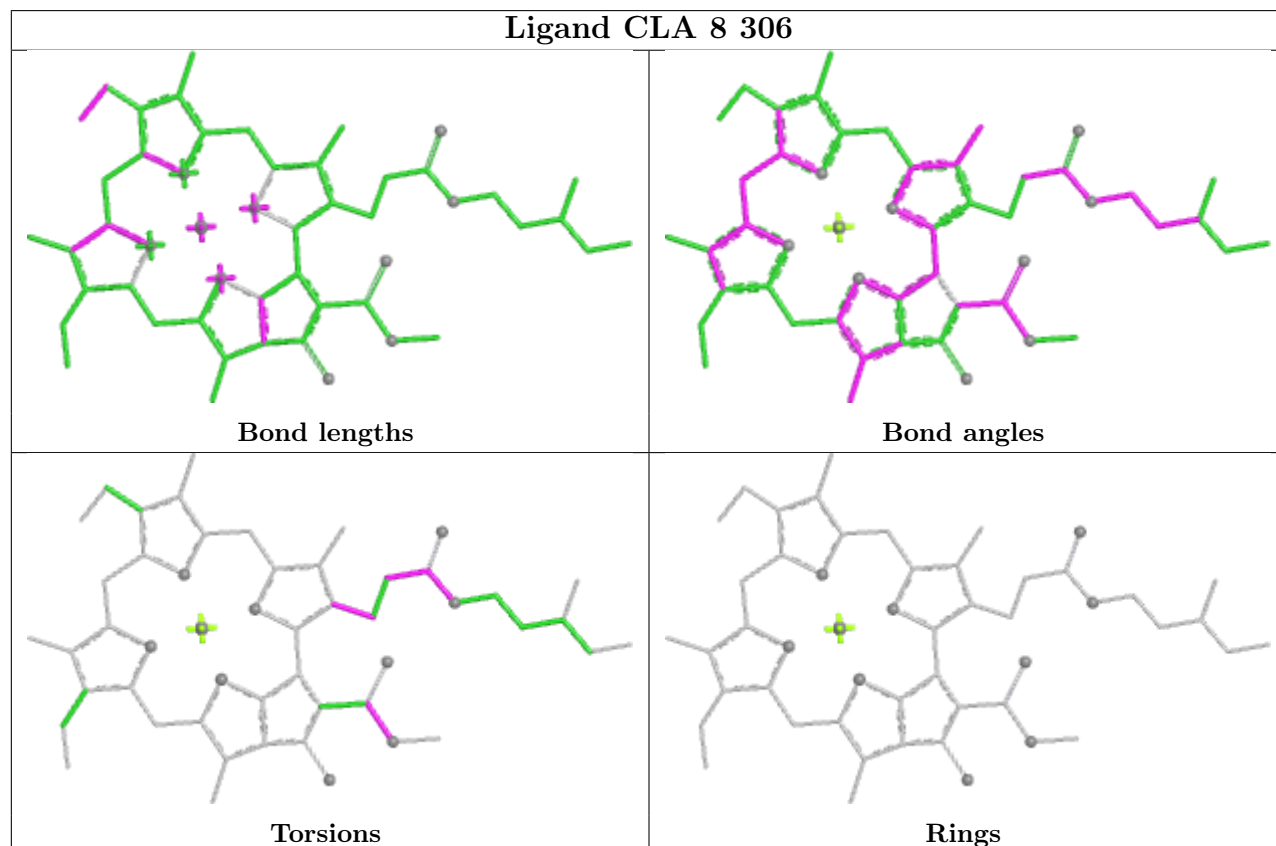
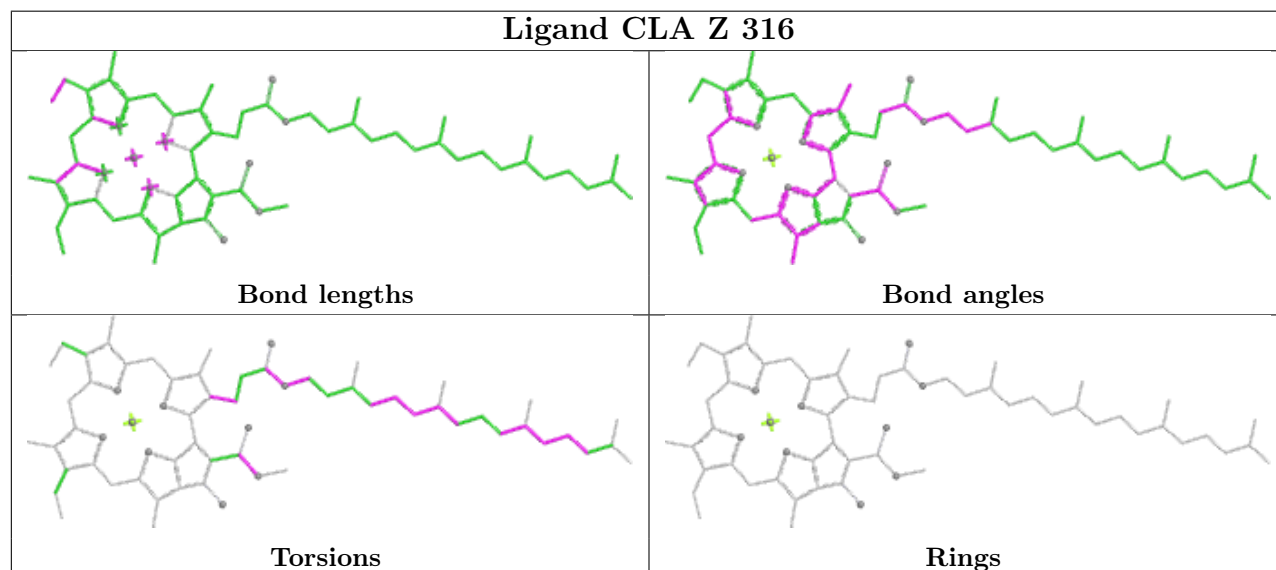


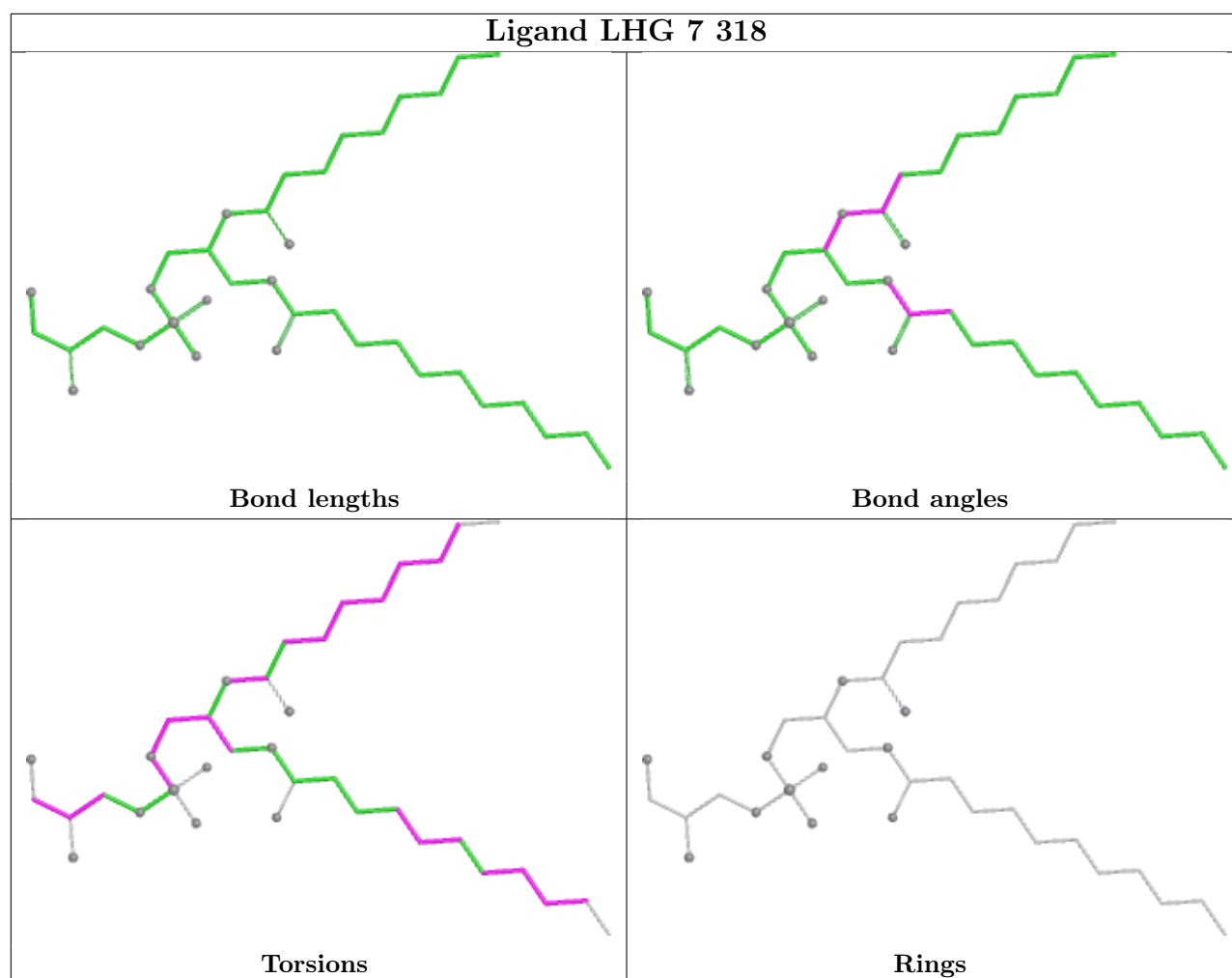


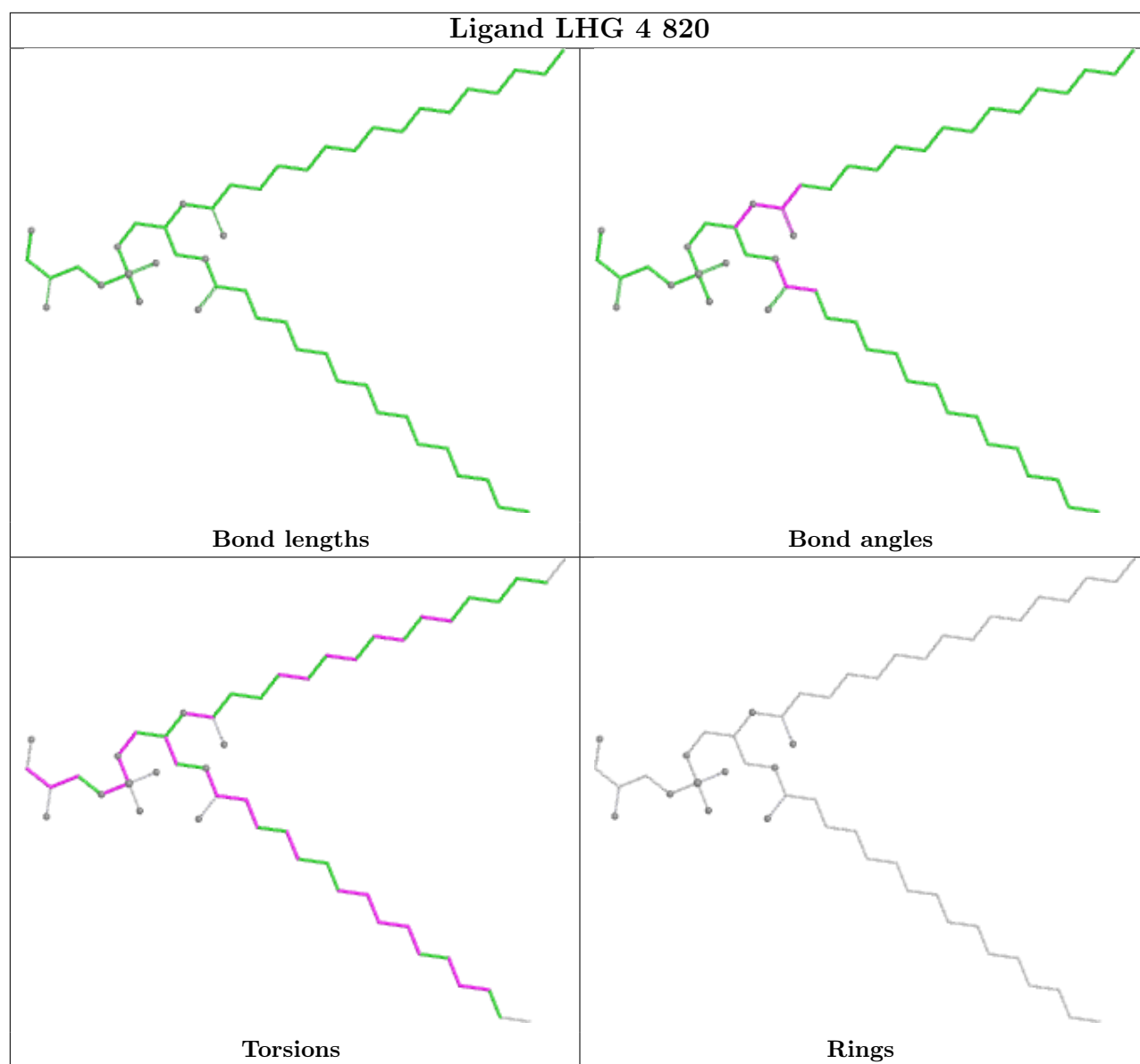


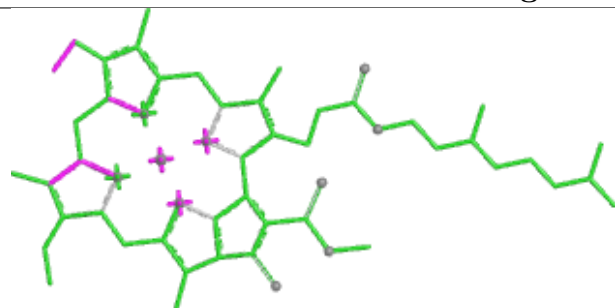


Ligand CHL 6 318**Ligand CLA 5 311**

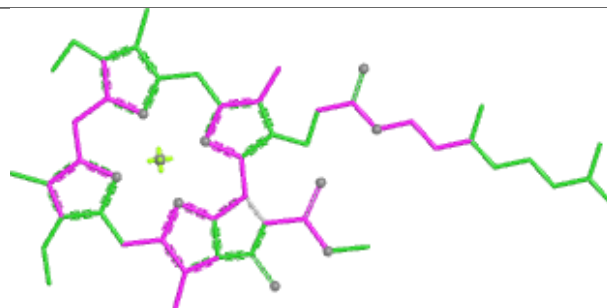
Ligand LUT 3 303**Ligand CLA 8 306****Ligand CLA Z 316**



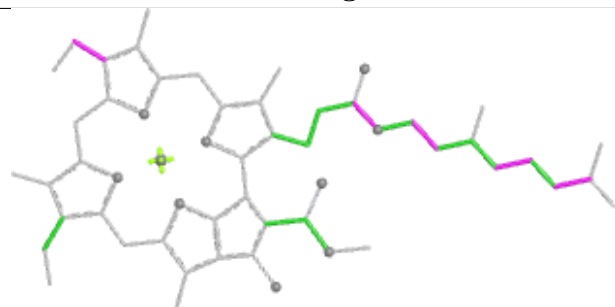


Ligand CLA 6 313

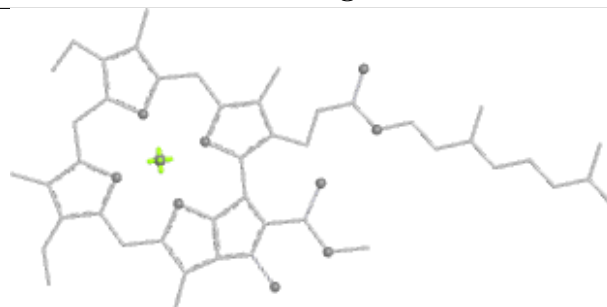
Bond lengths



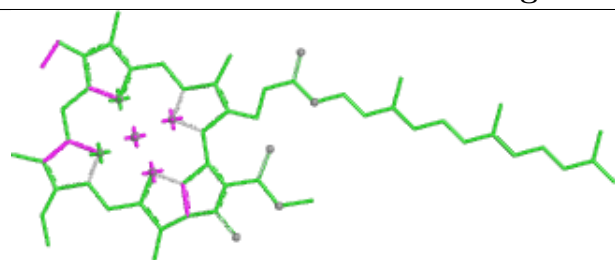
Bond angles



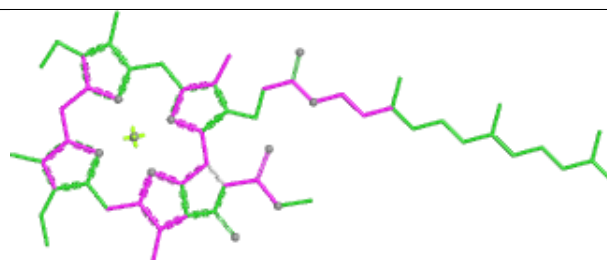
Torsions



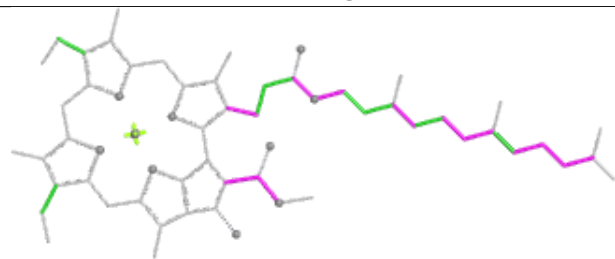
Rings

Ligand CLA 4 808

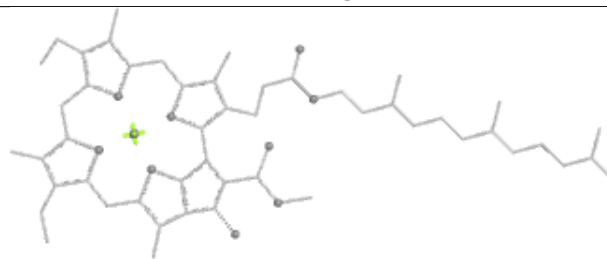
Bond lengths



Bond angles

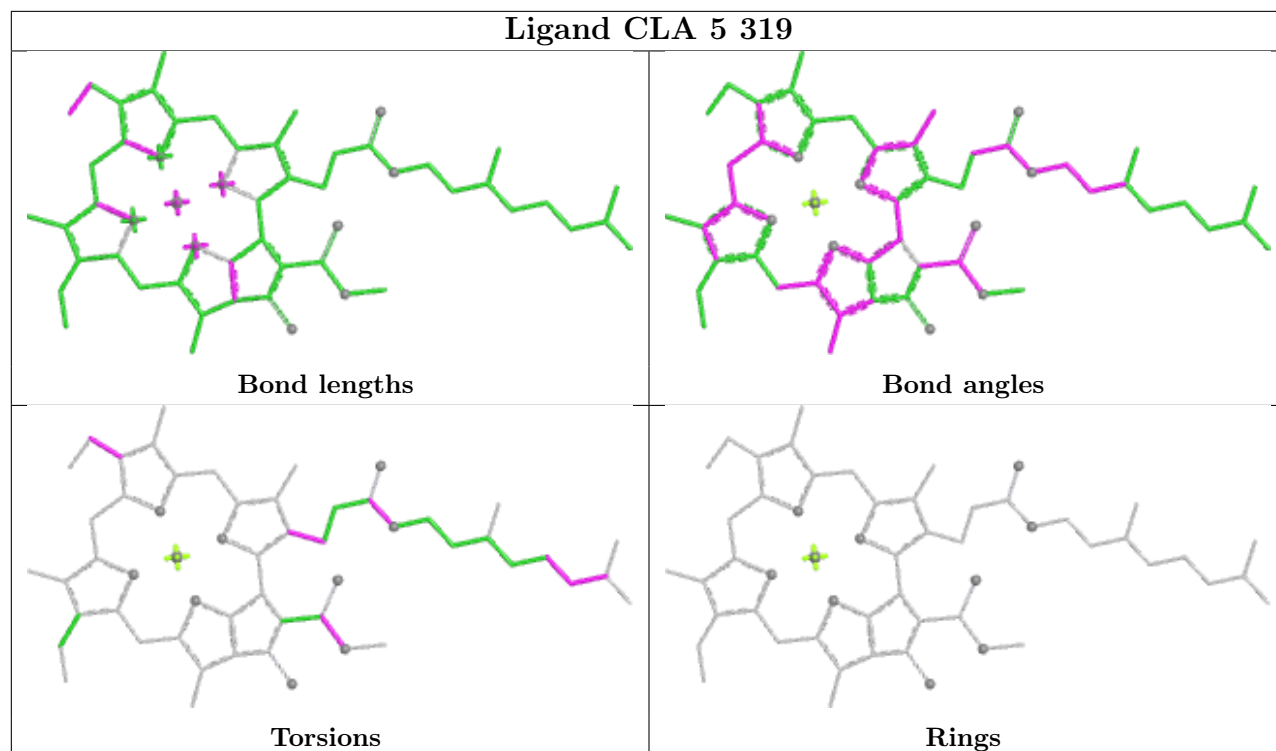


Torsions

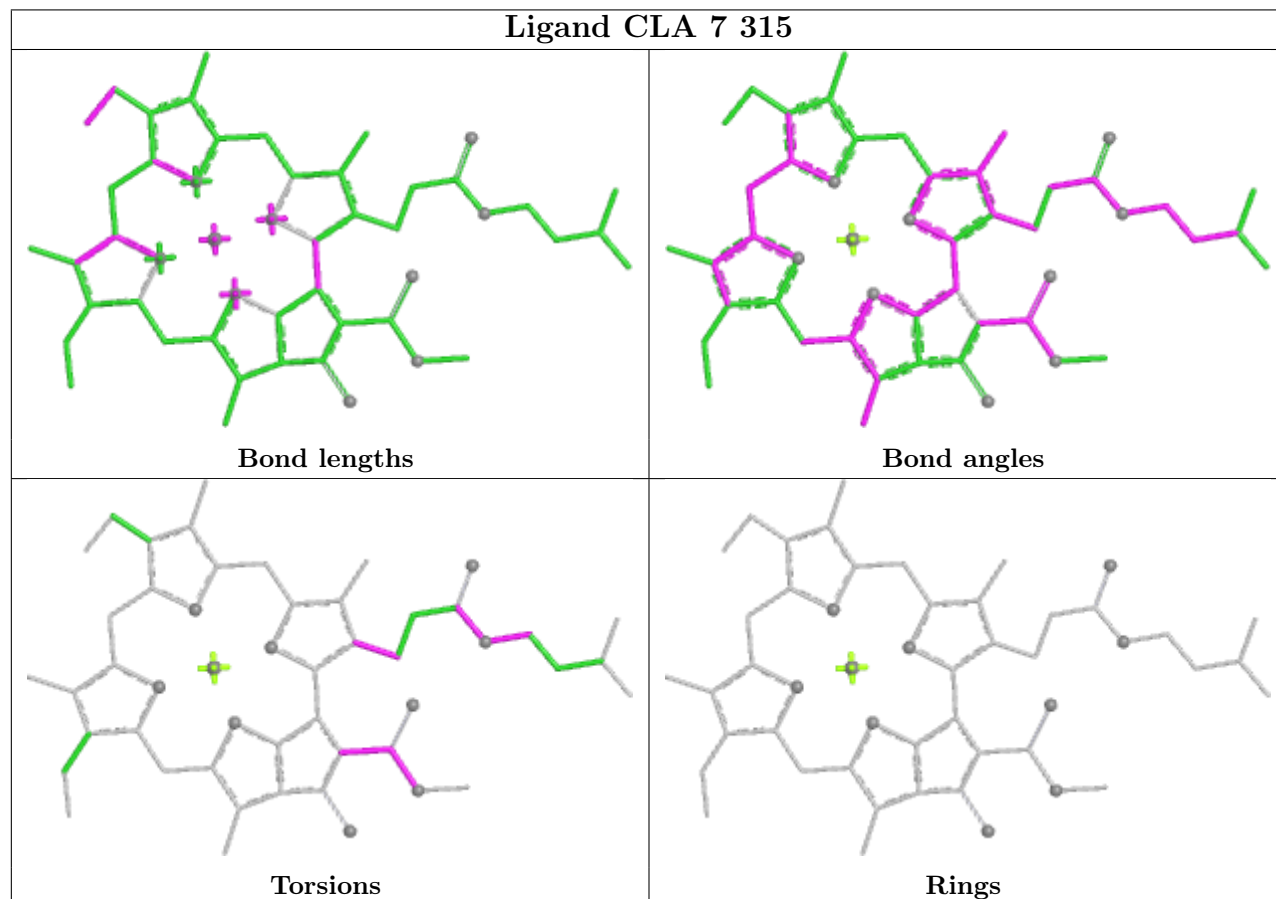


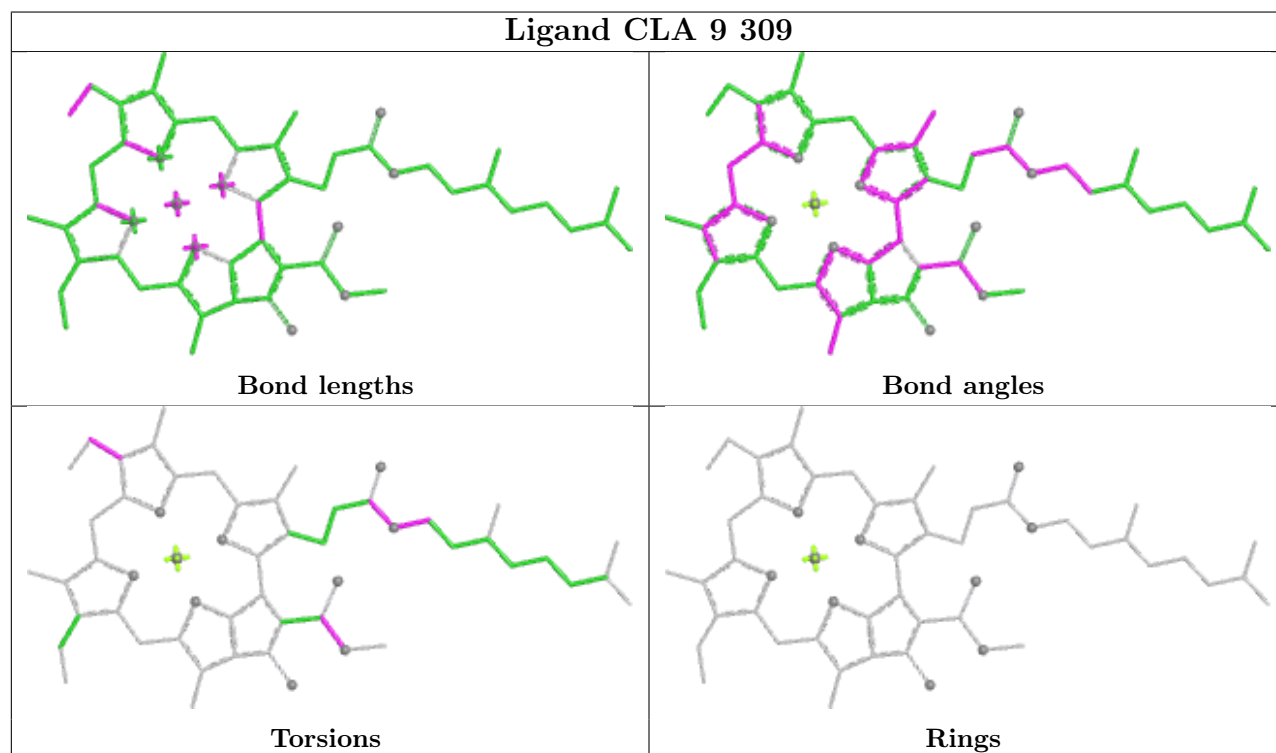
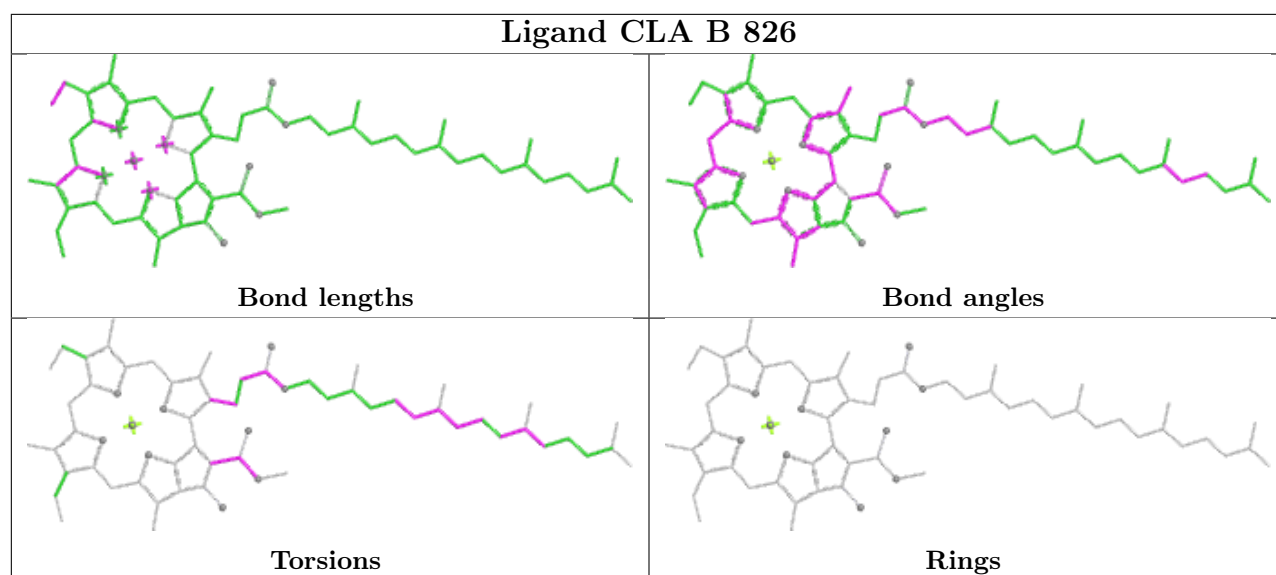
Rings

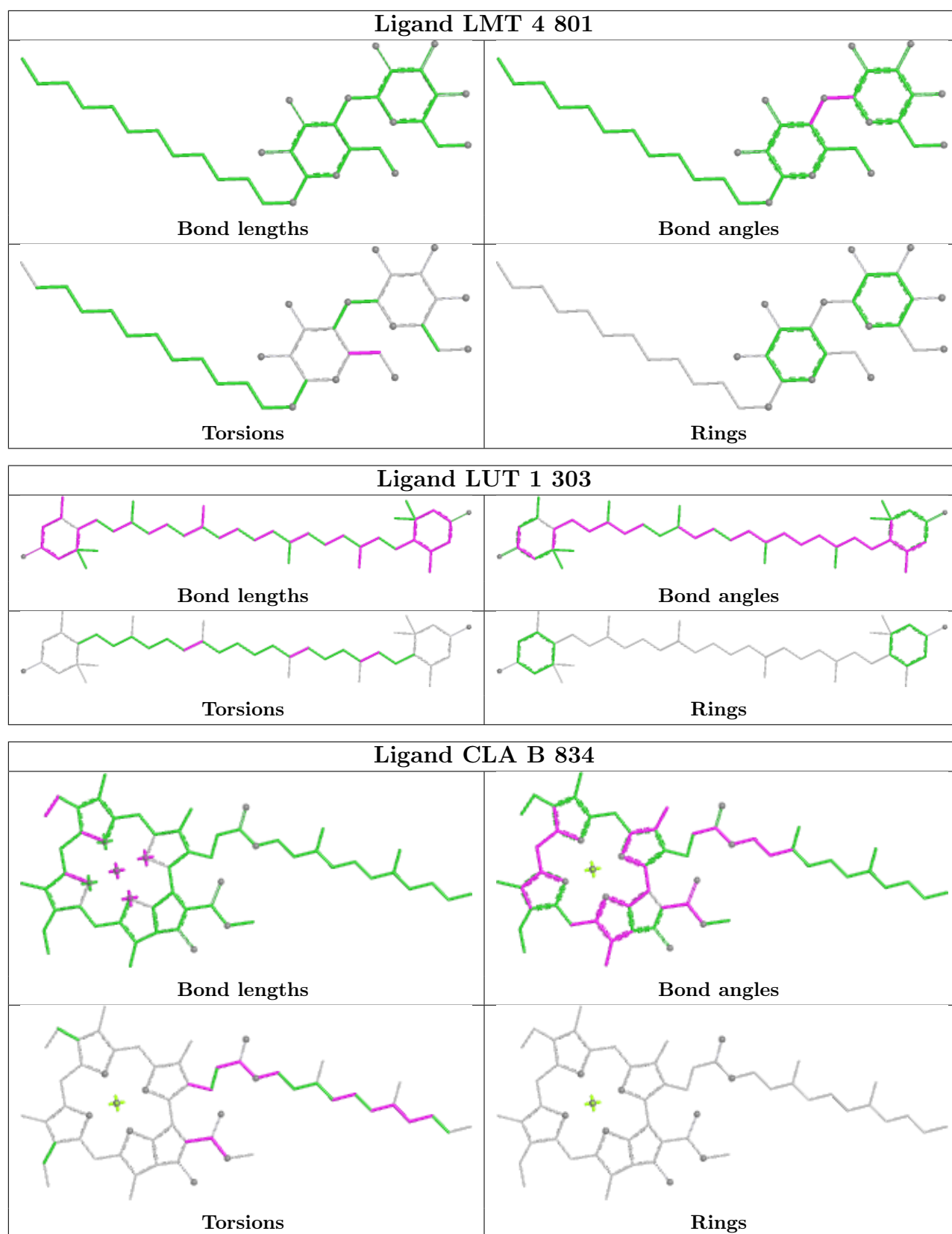
Ligand CLA 5 319

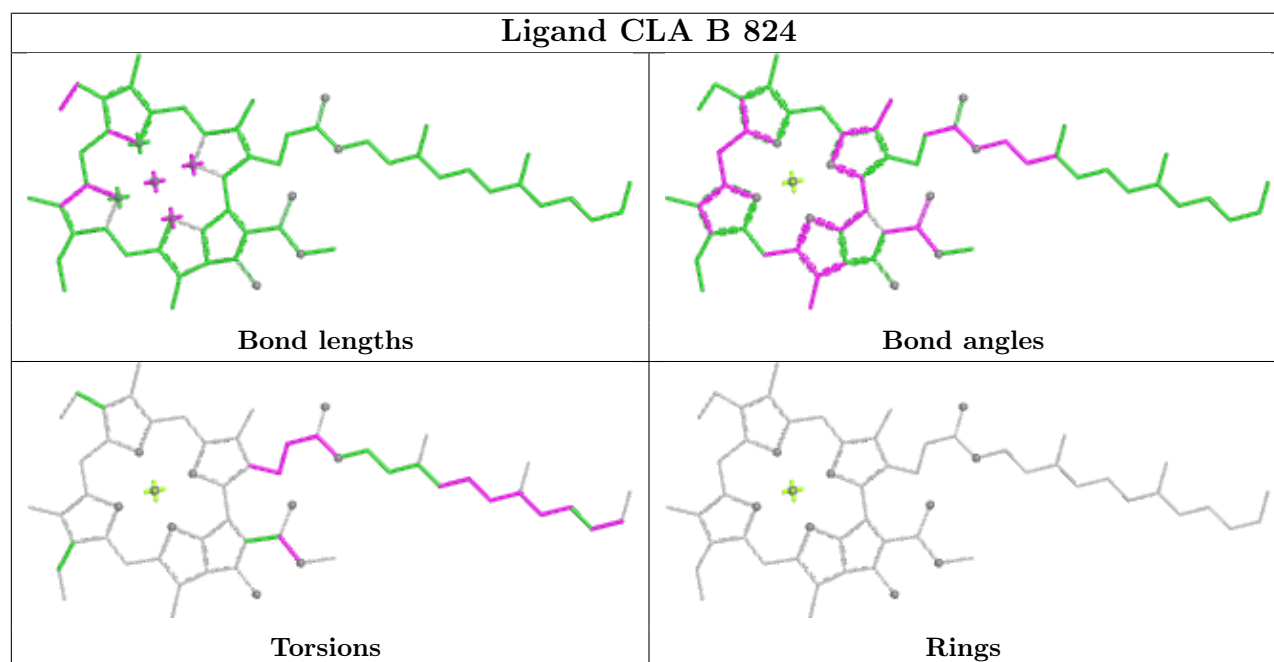
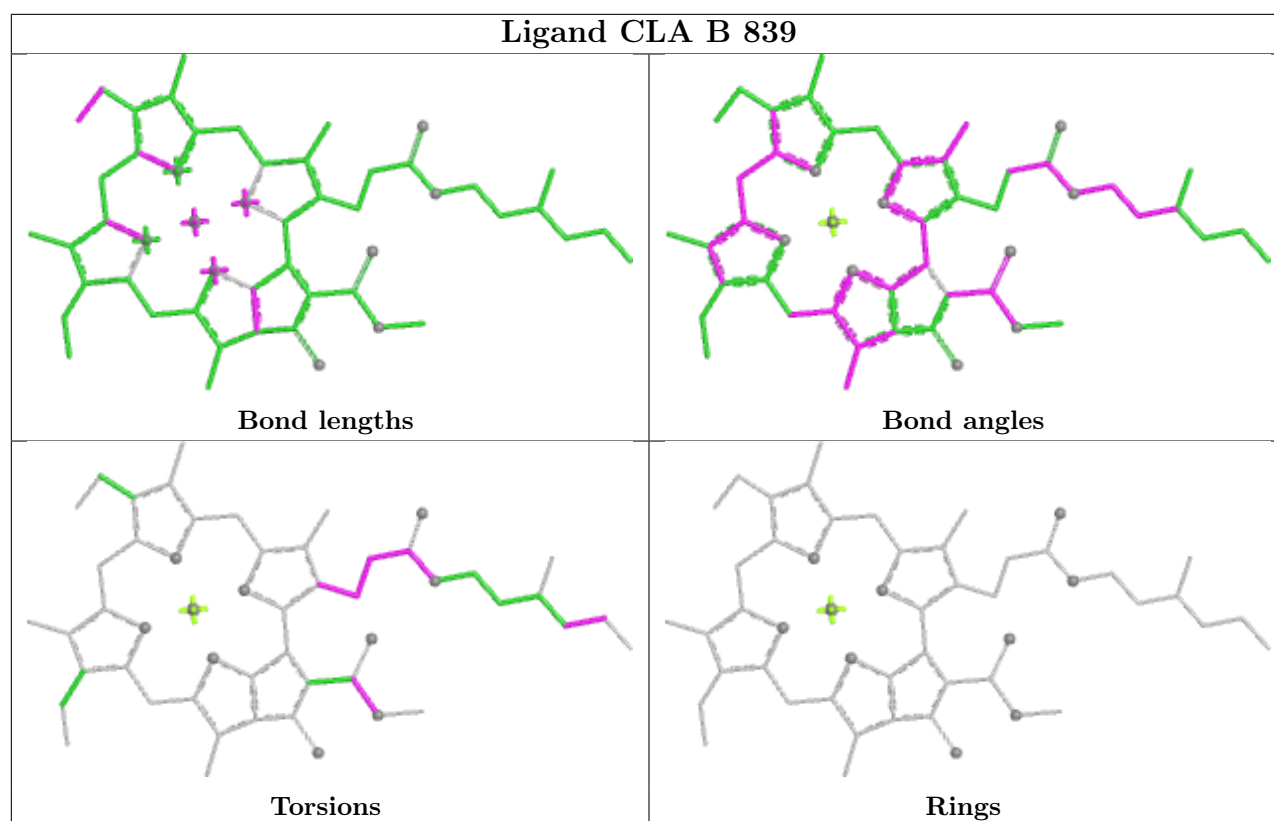


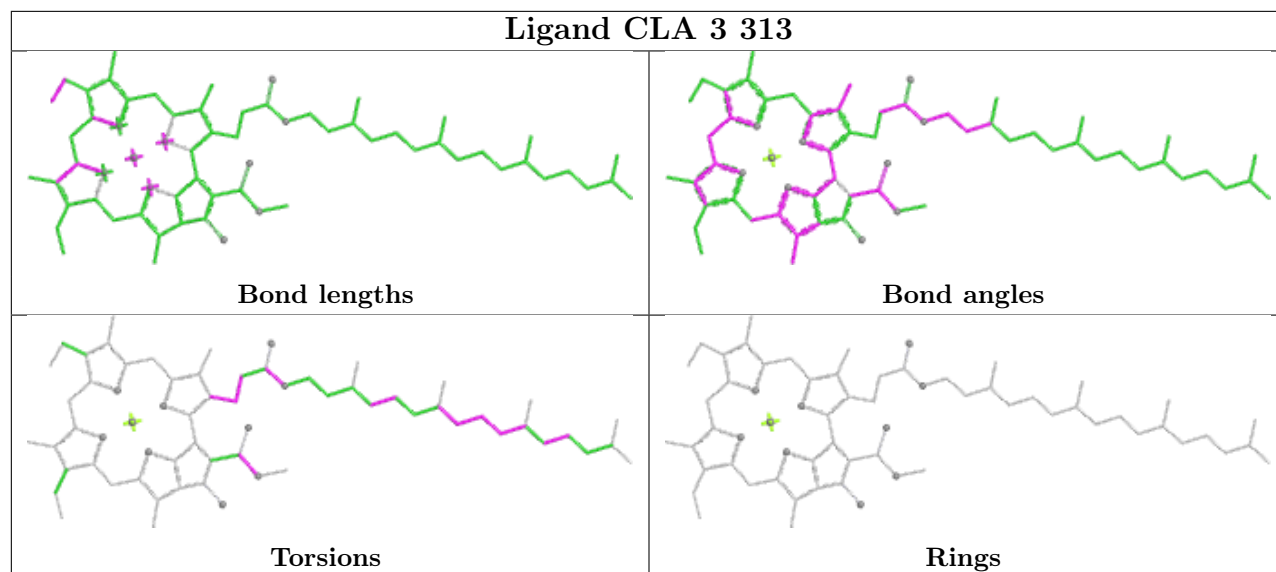
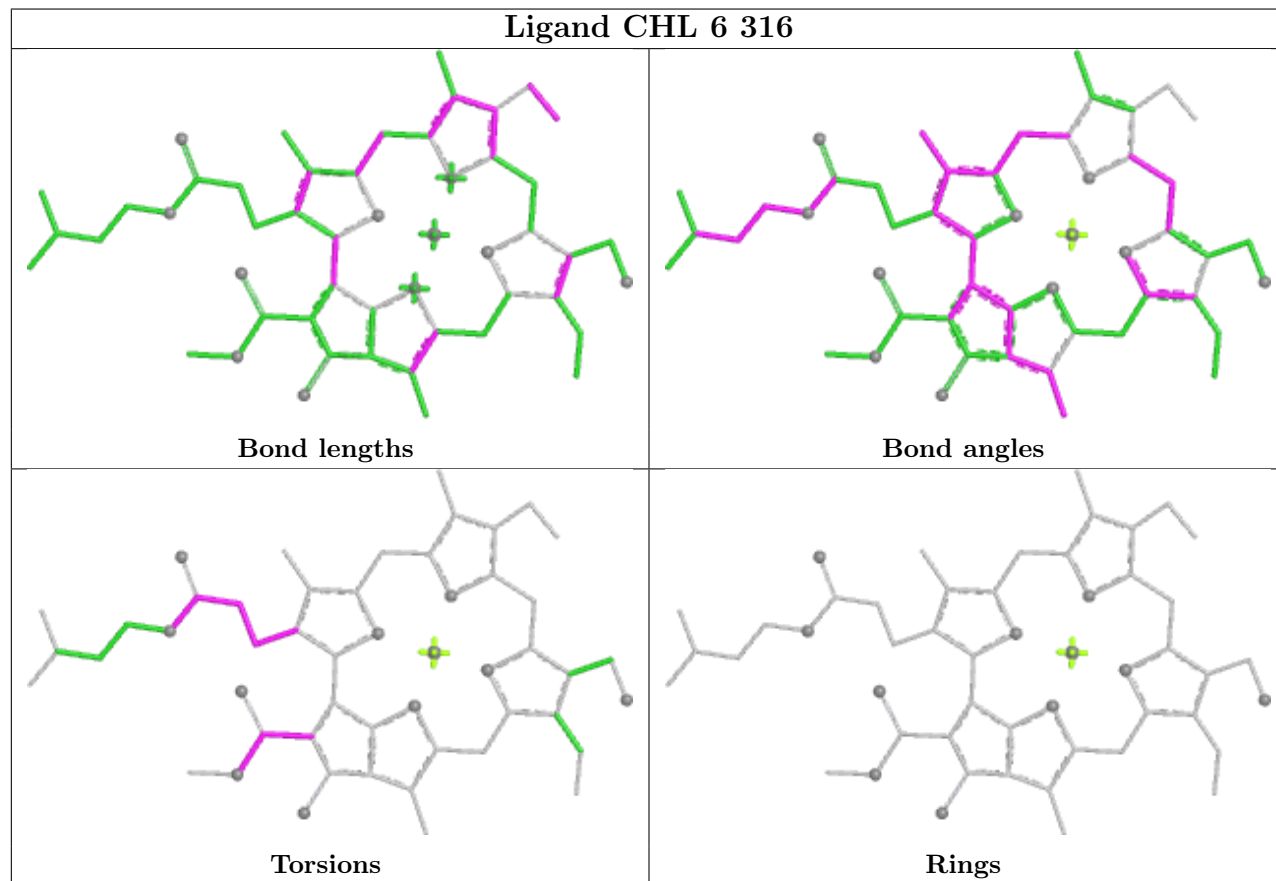
Ligand CLA 7 315

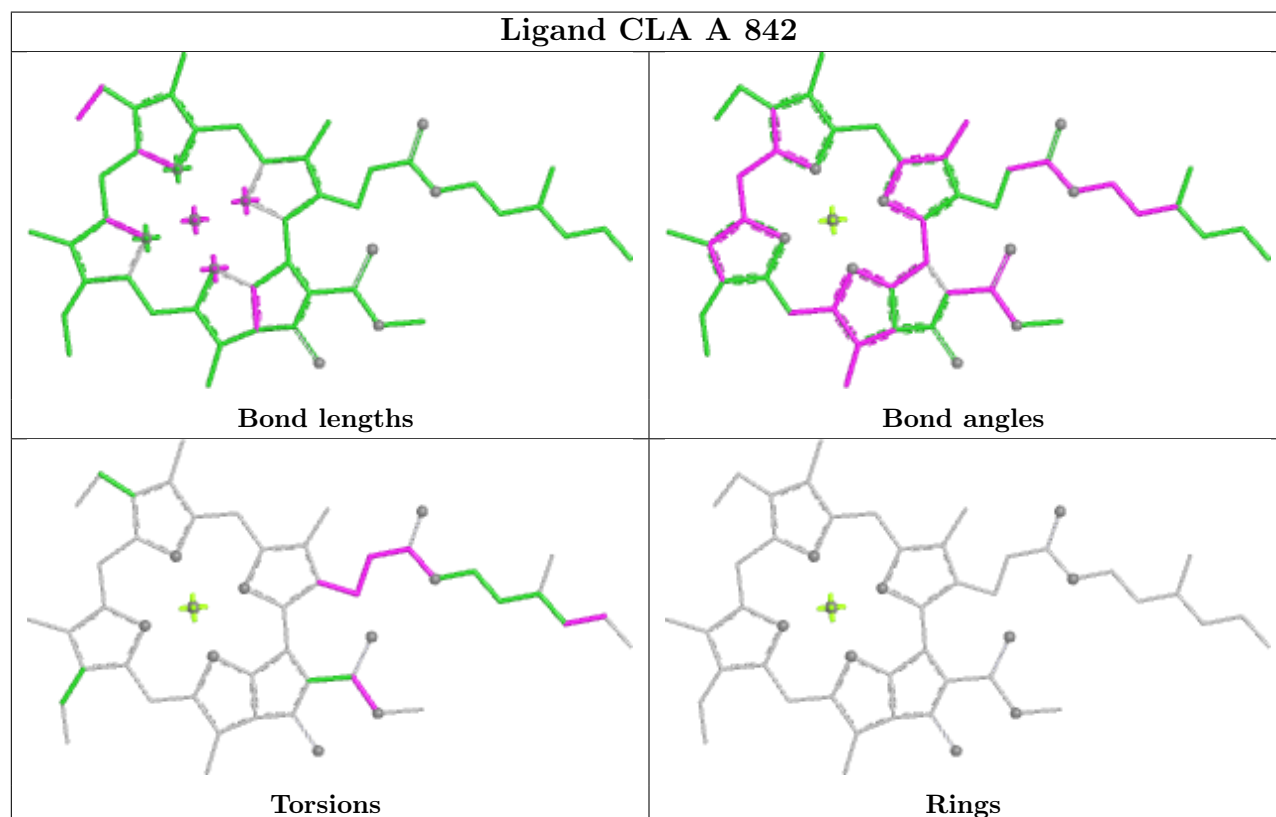
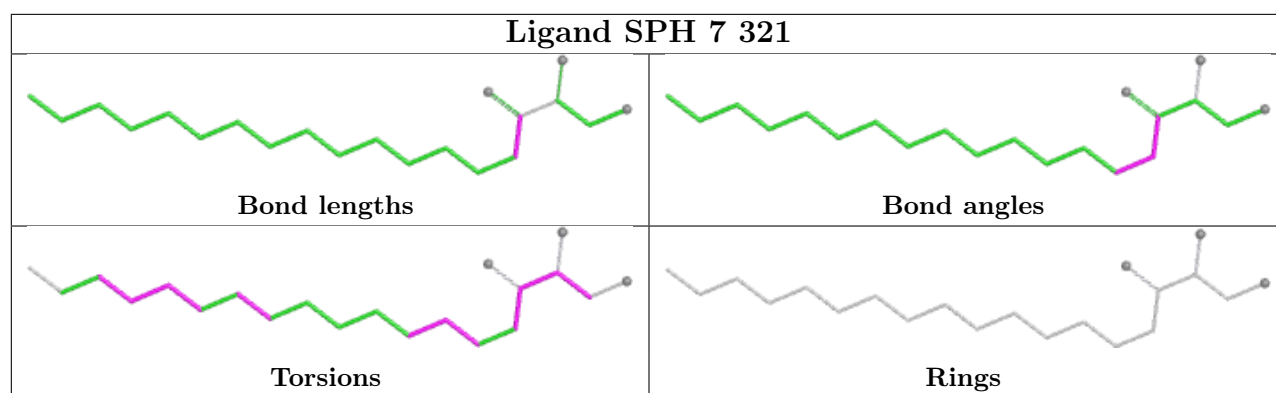


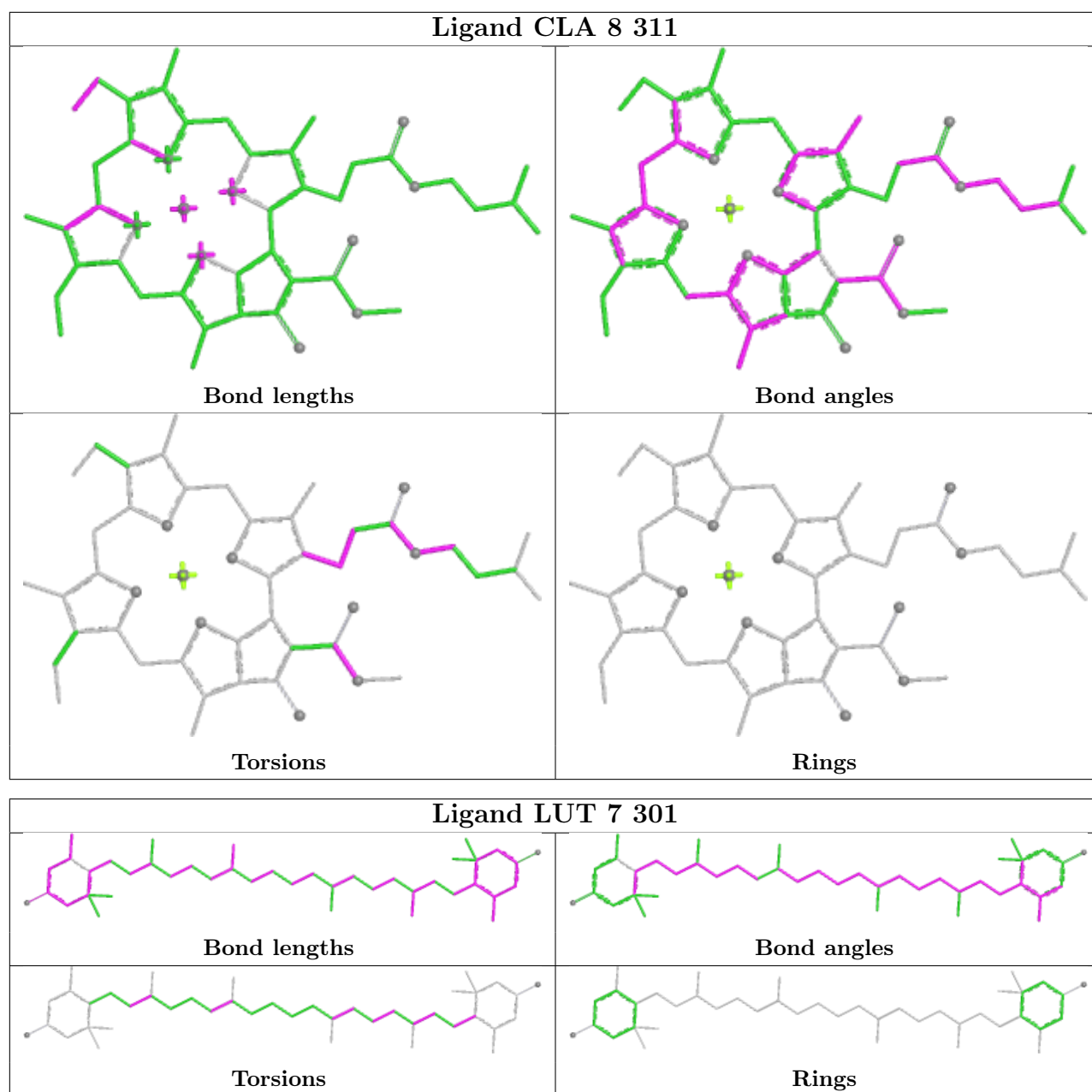


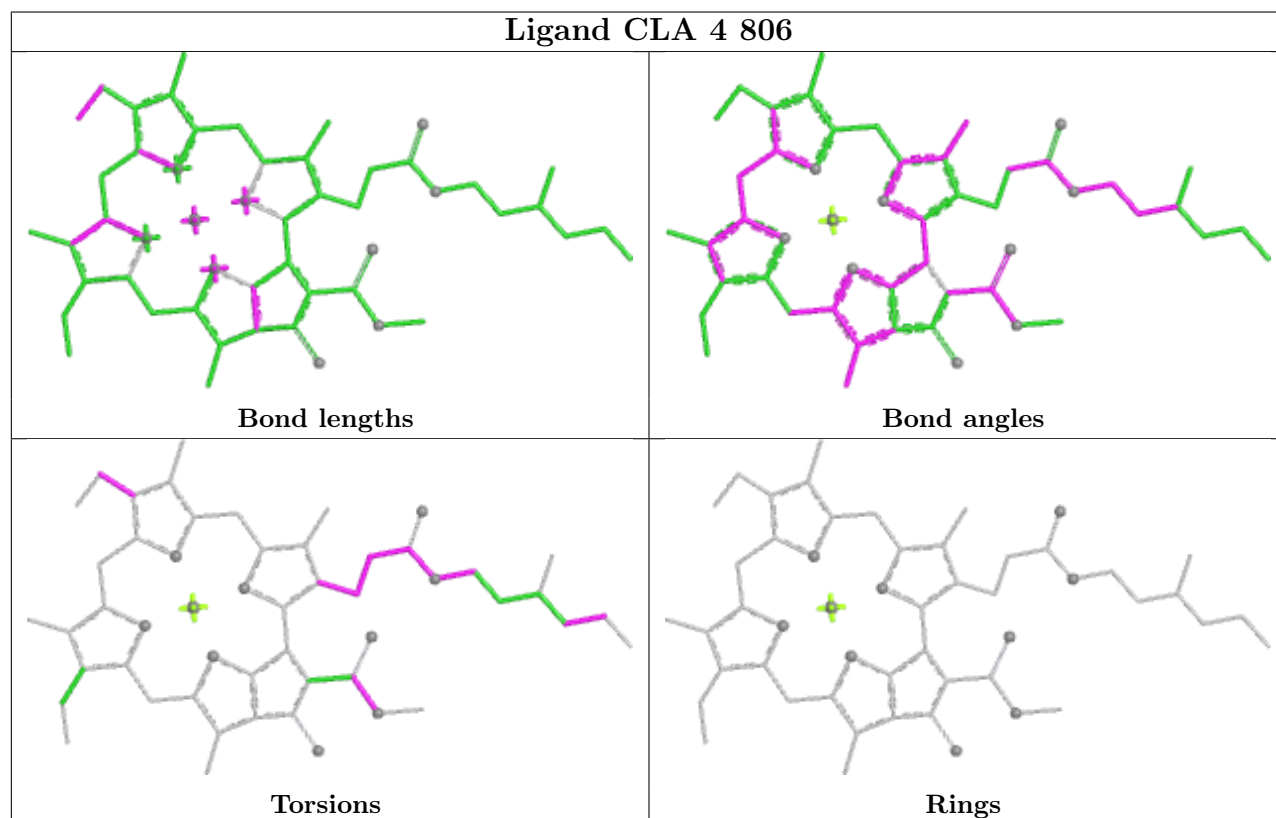
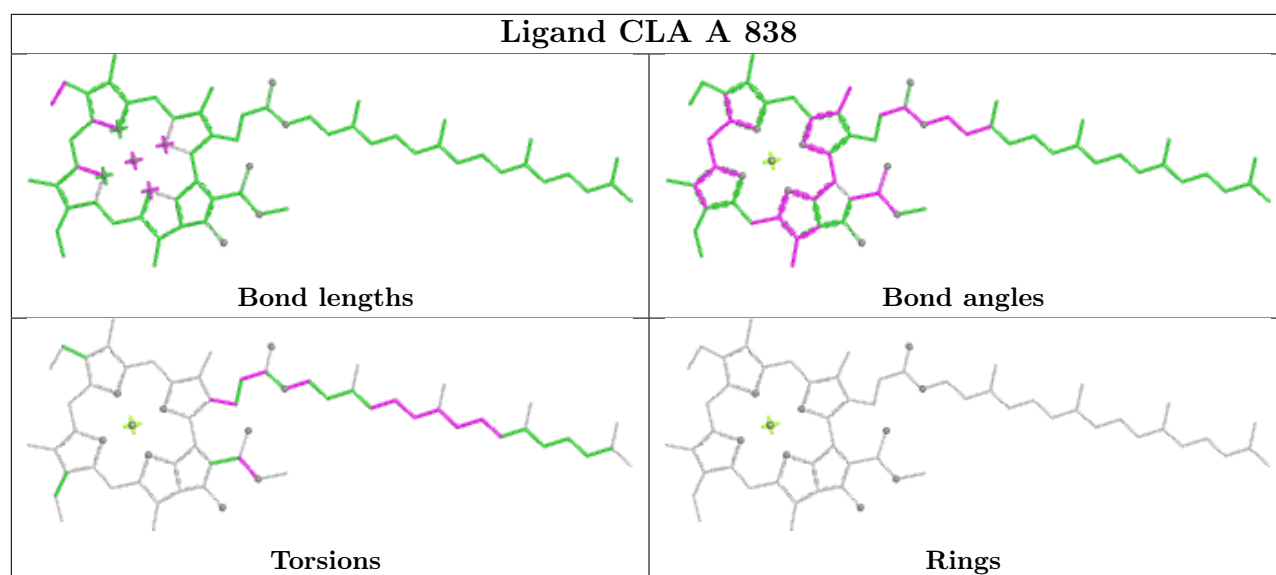




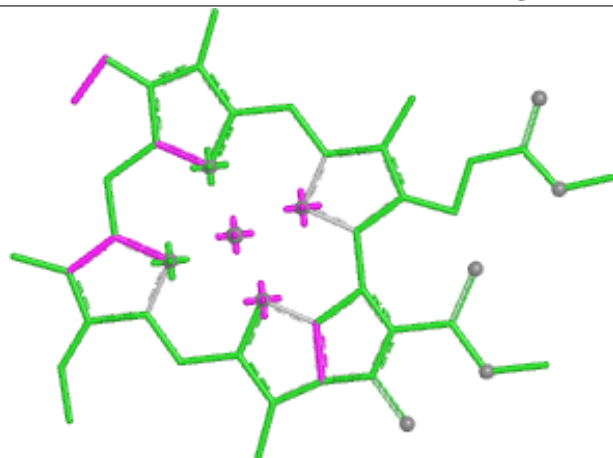
Ligand CLA 3 313**Ligand CHL 6 316**



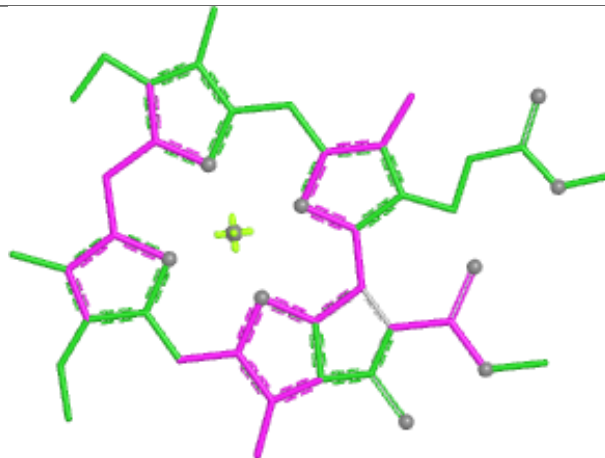




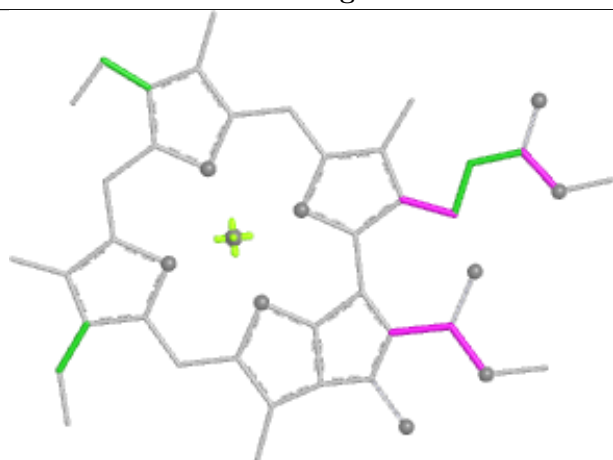
Ligand CLA G 202



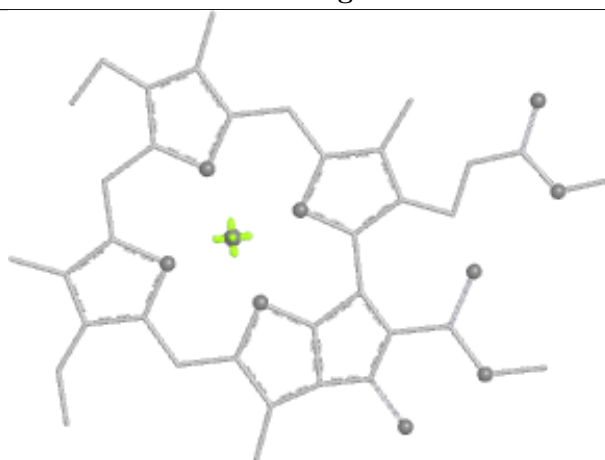
Bond lengths



Bond angles

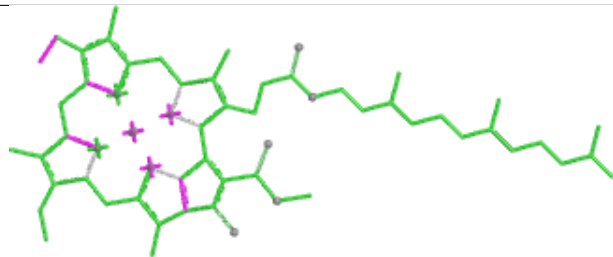


Torsions

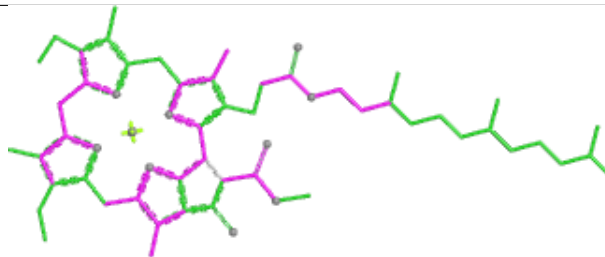


Rings

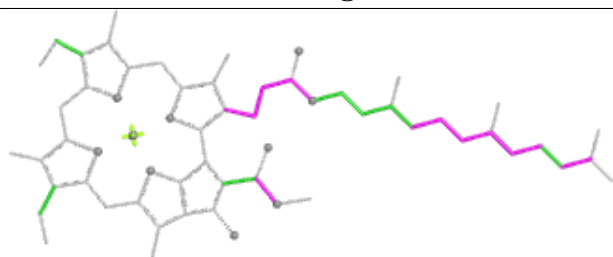
Ligand CLA B 814



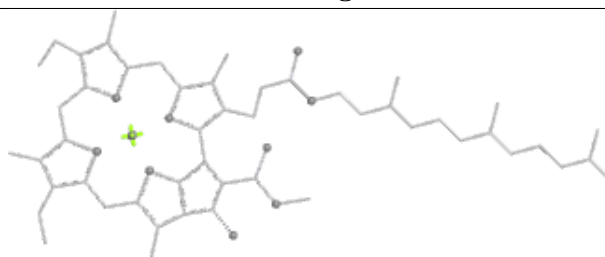
Bond lengths



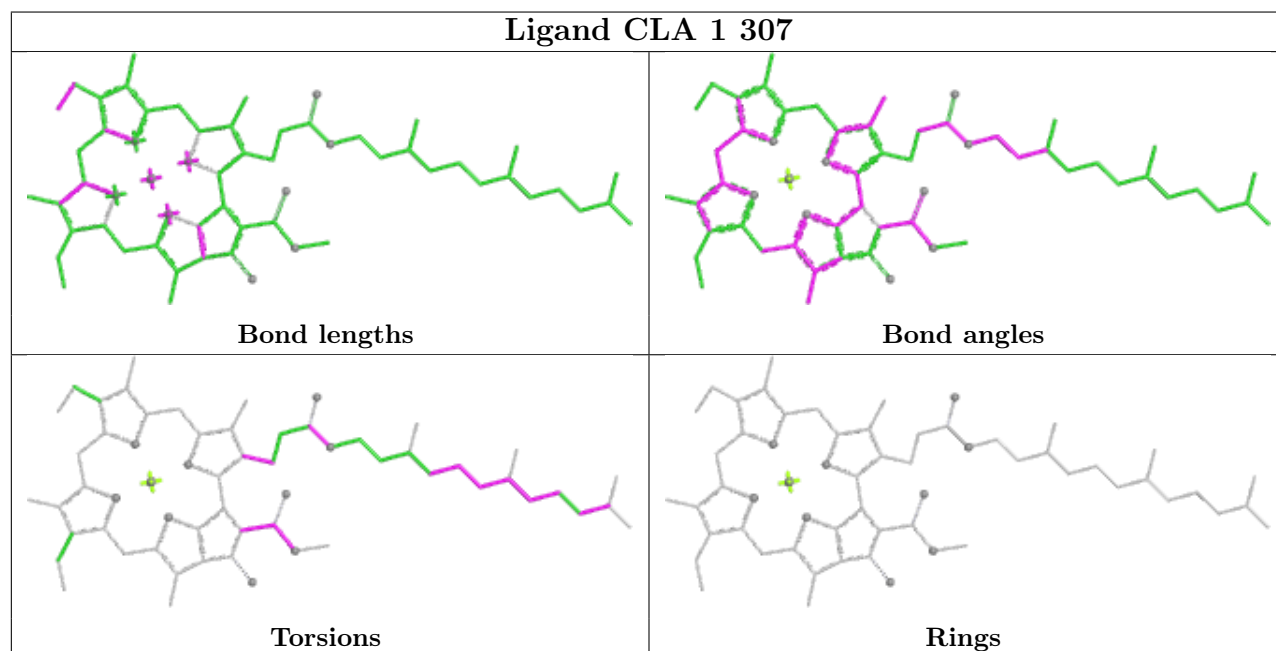
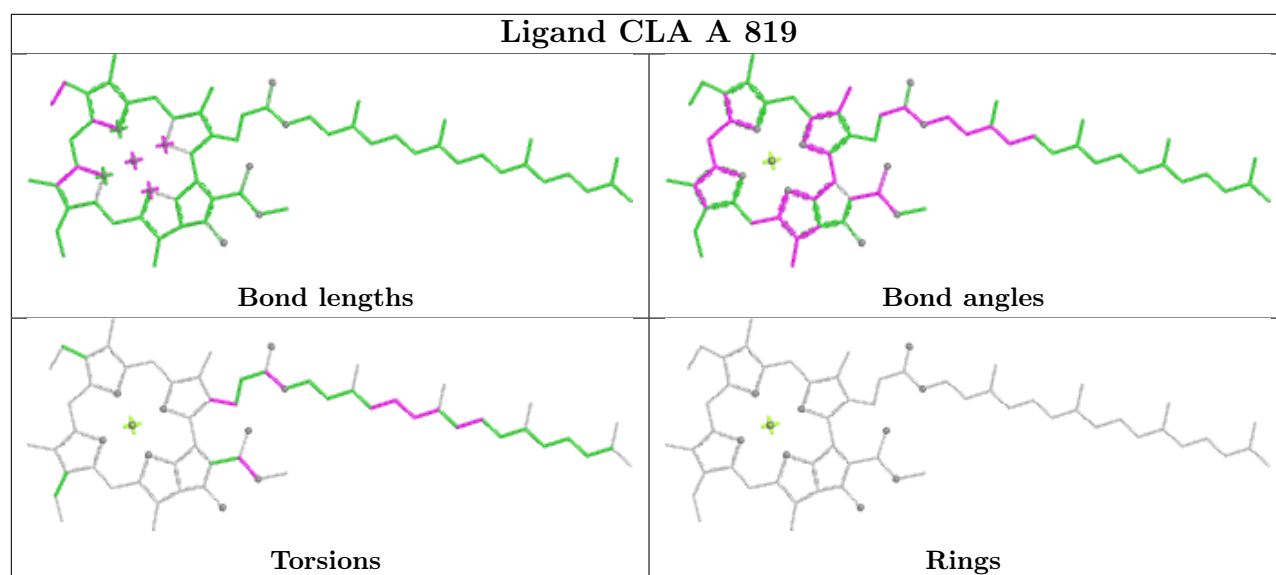
Bond angles

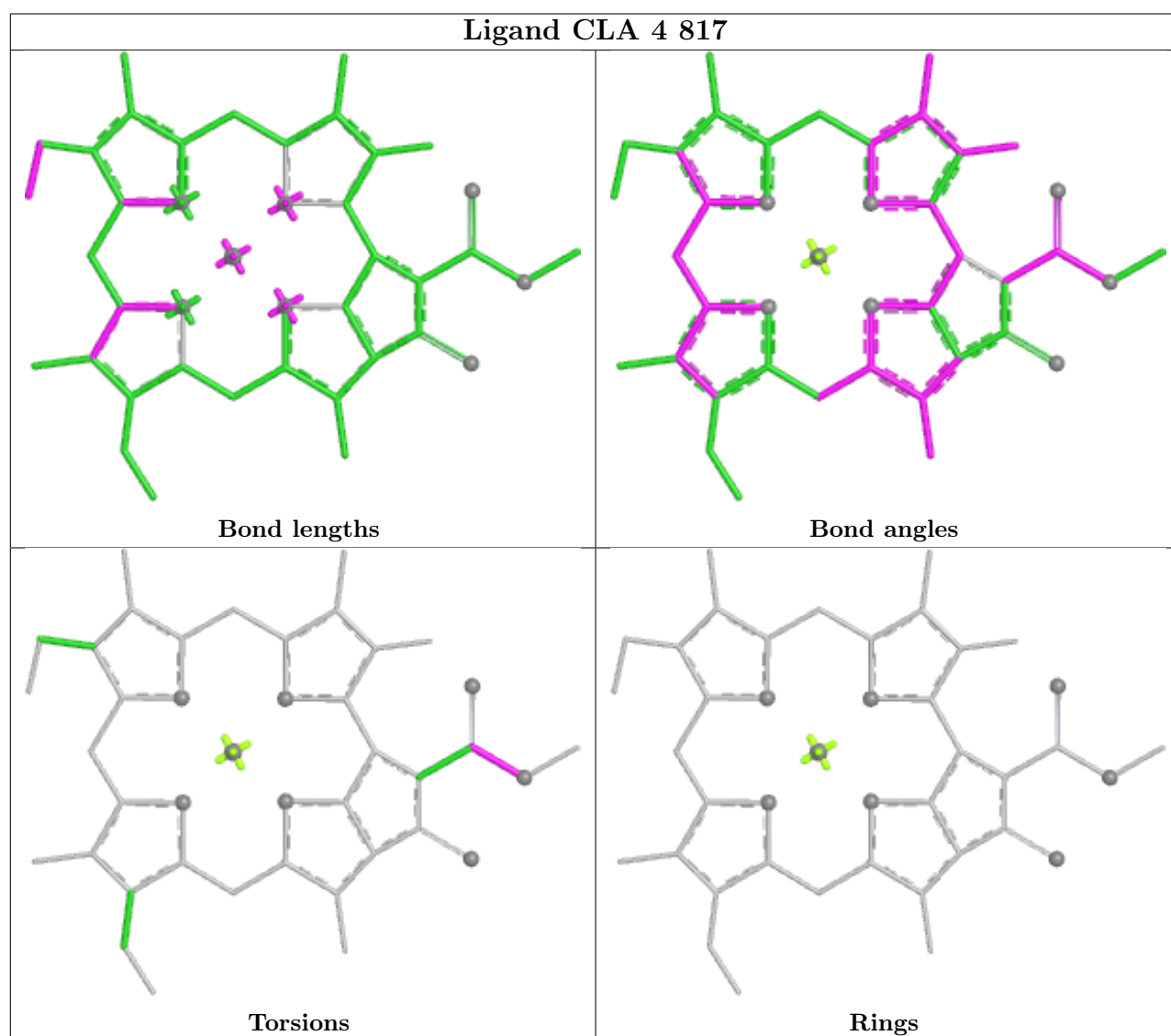
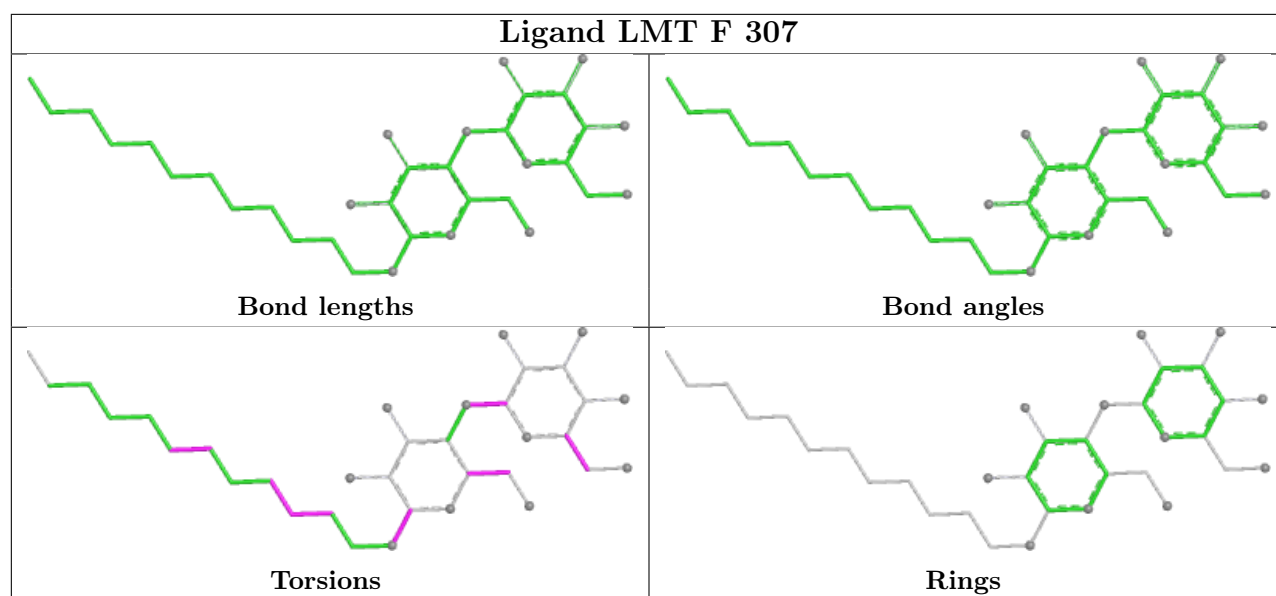


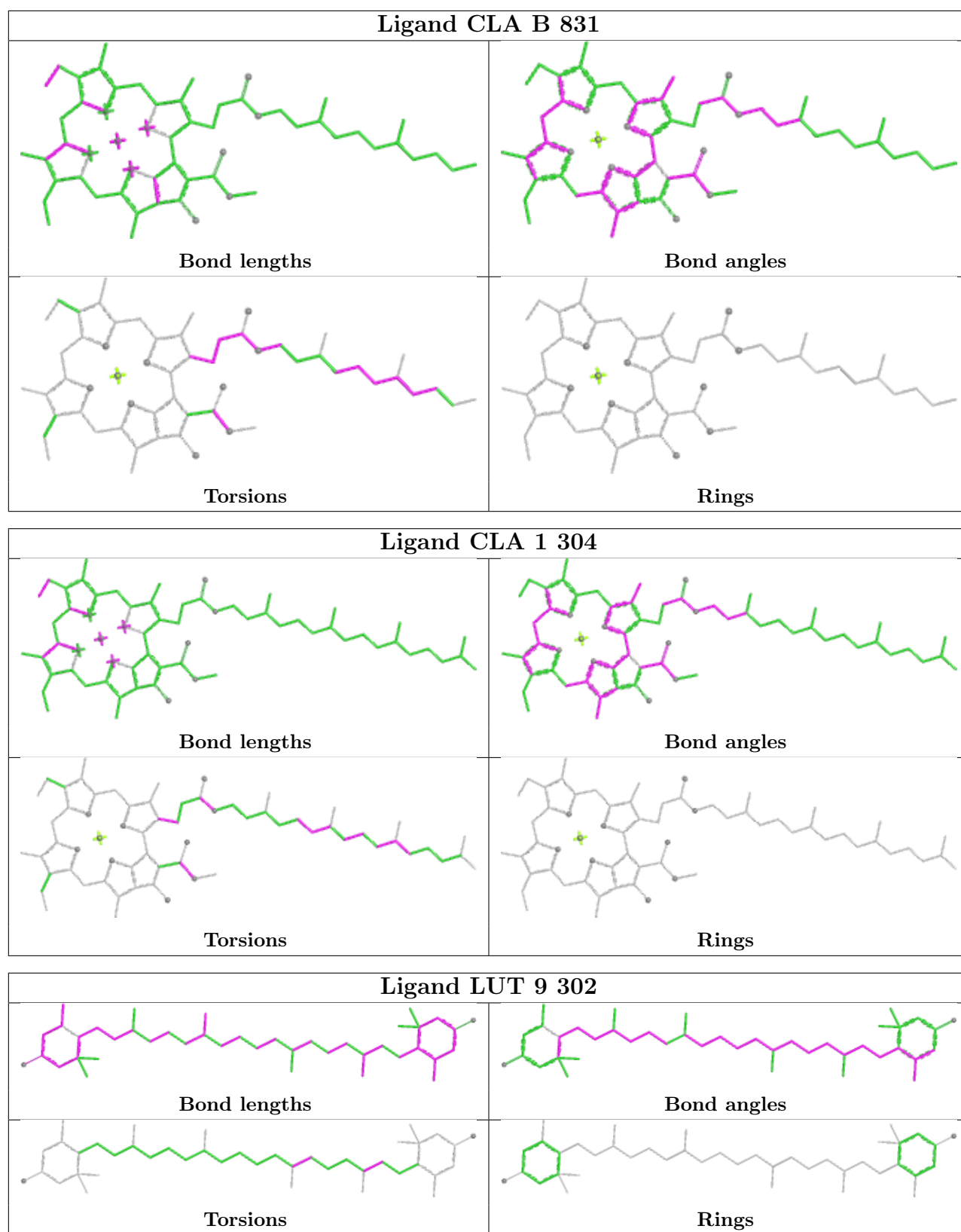
Torsions



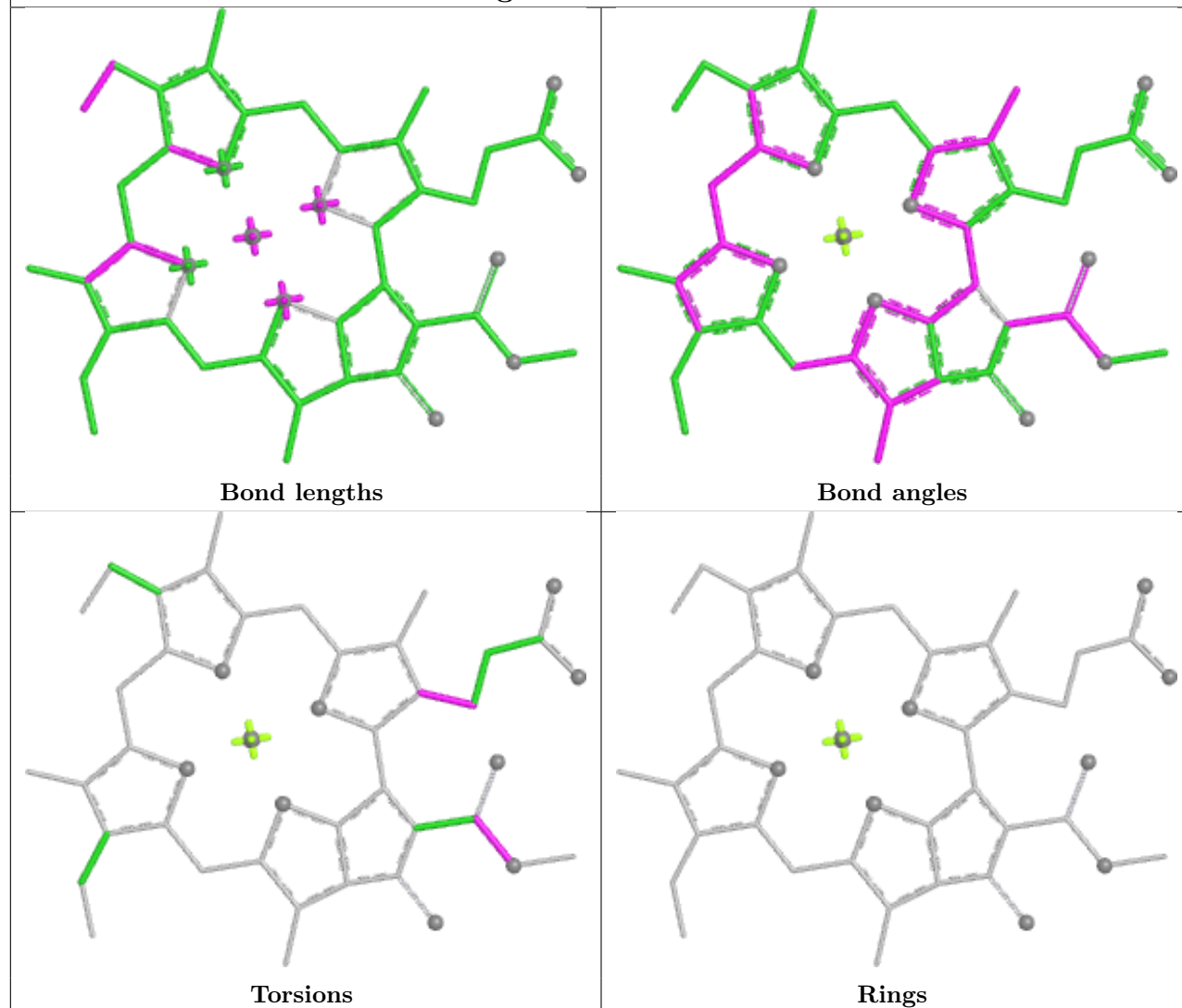
Rings



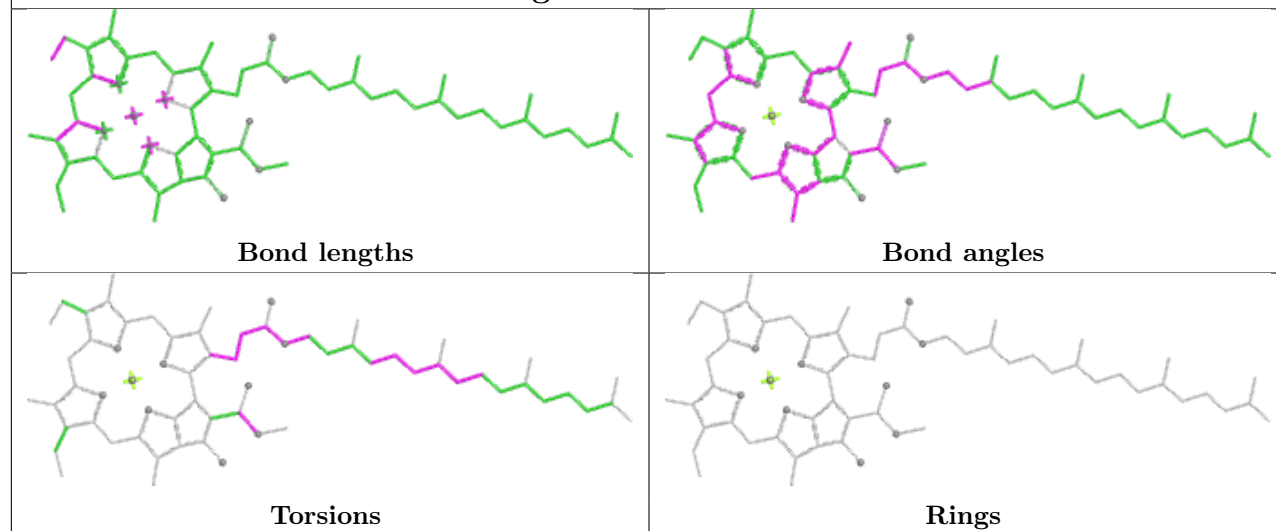


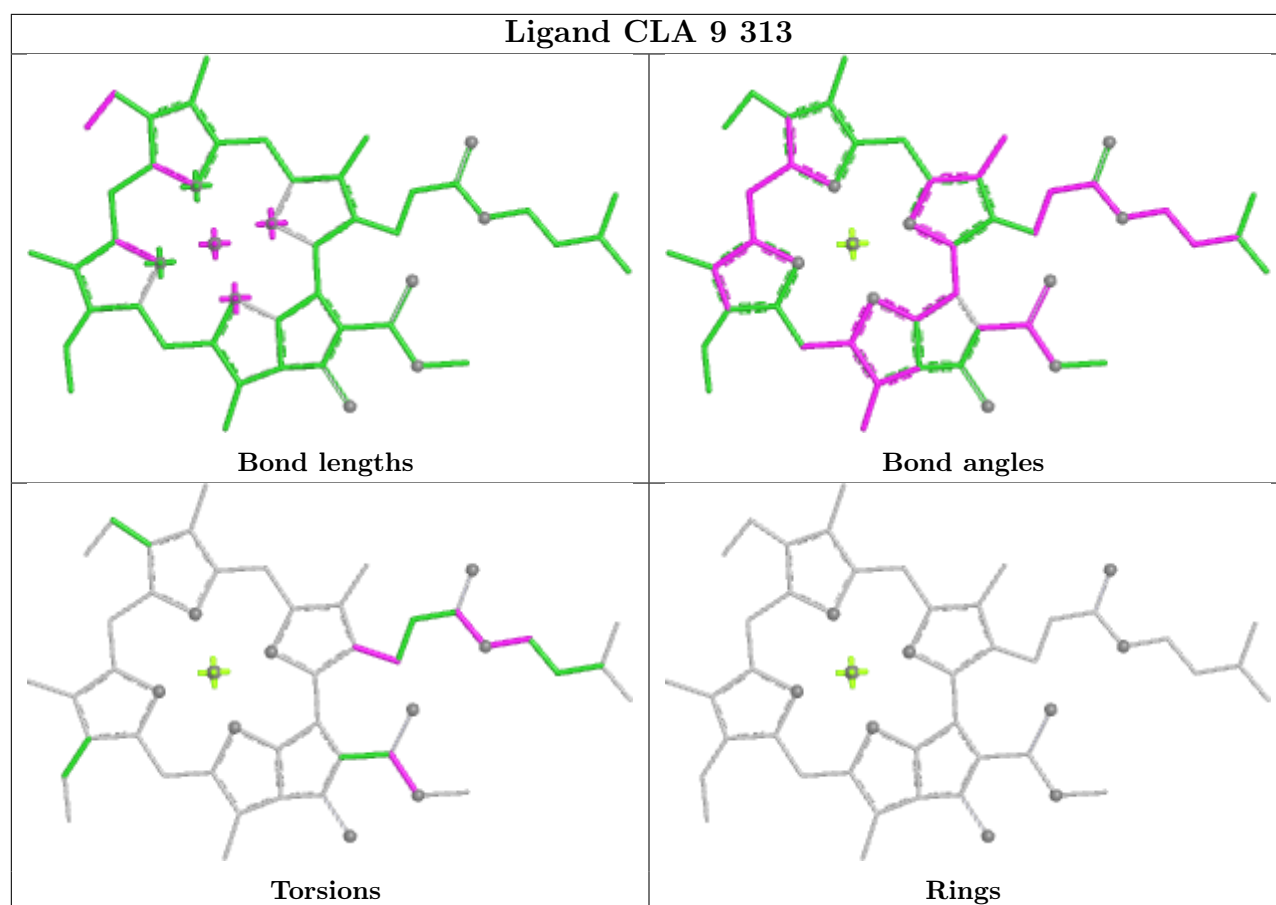


Ligand CLA 5 314

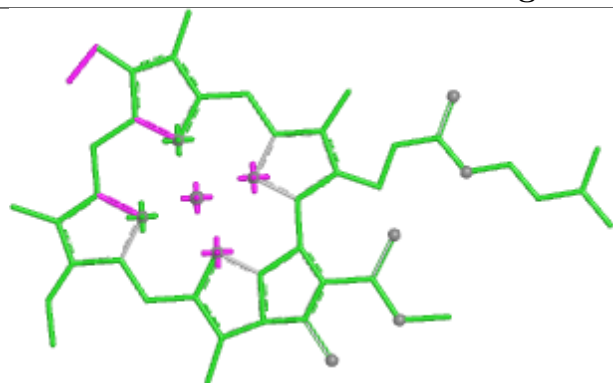


Ligand CLA B 825

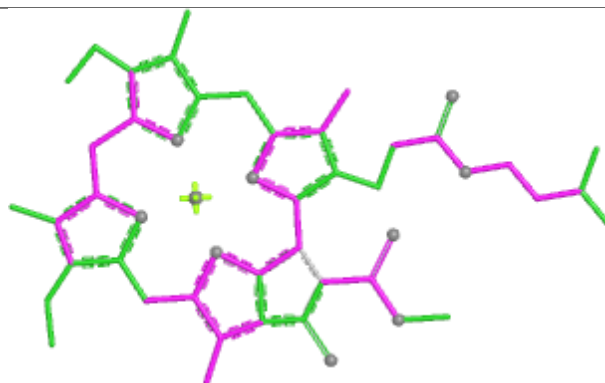




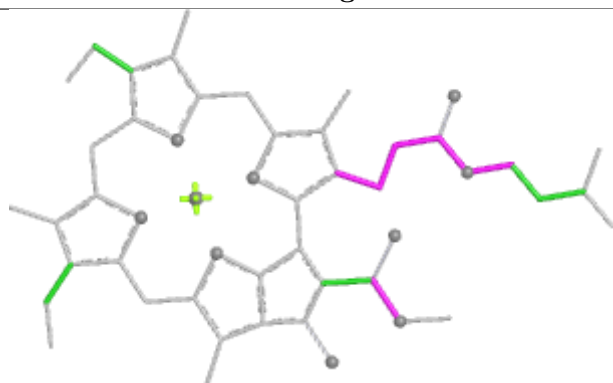
Ligand CLA 9 308



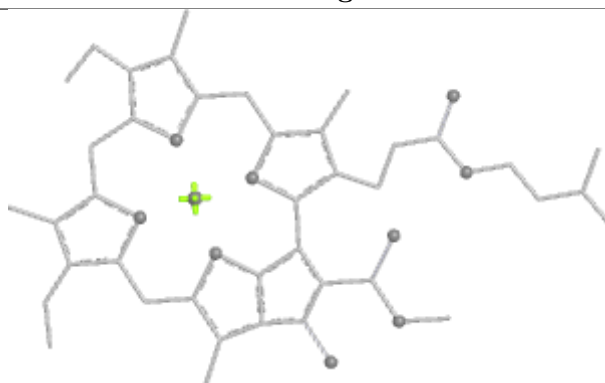
Bond lengths



Bond angles

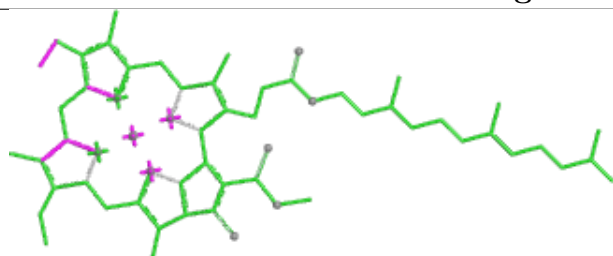


Torsions

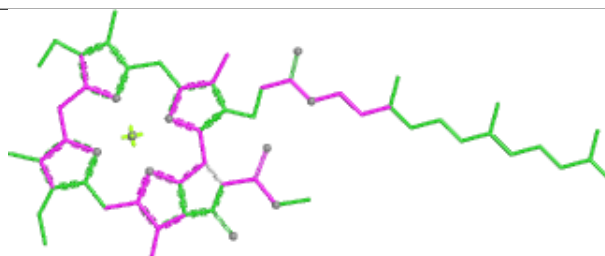


Rings

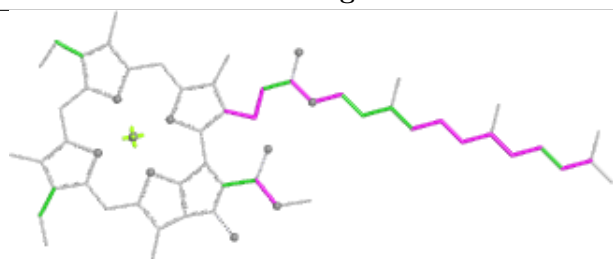
Ligand CLA B 820



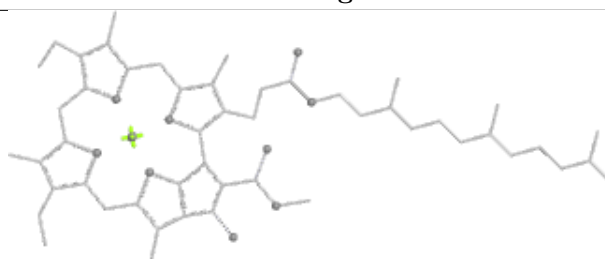
Bond lengths



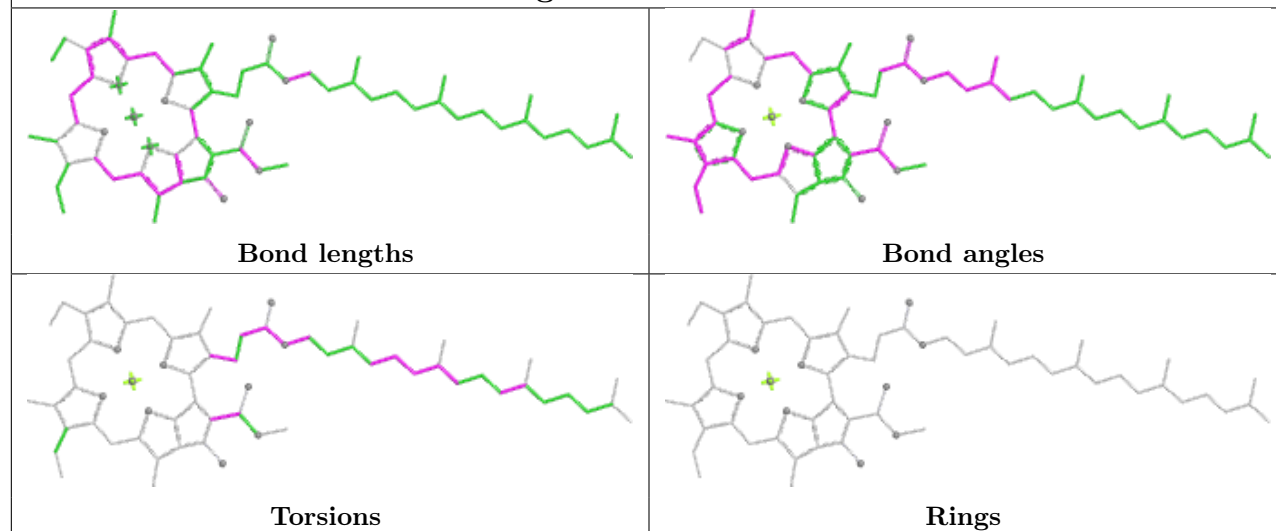
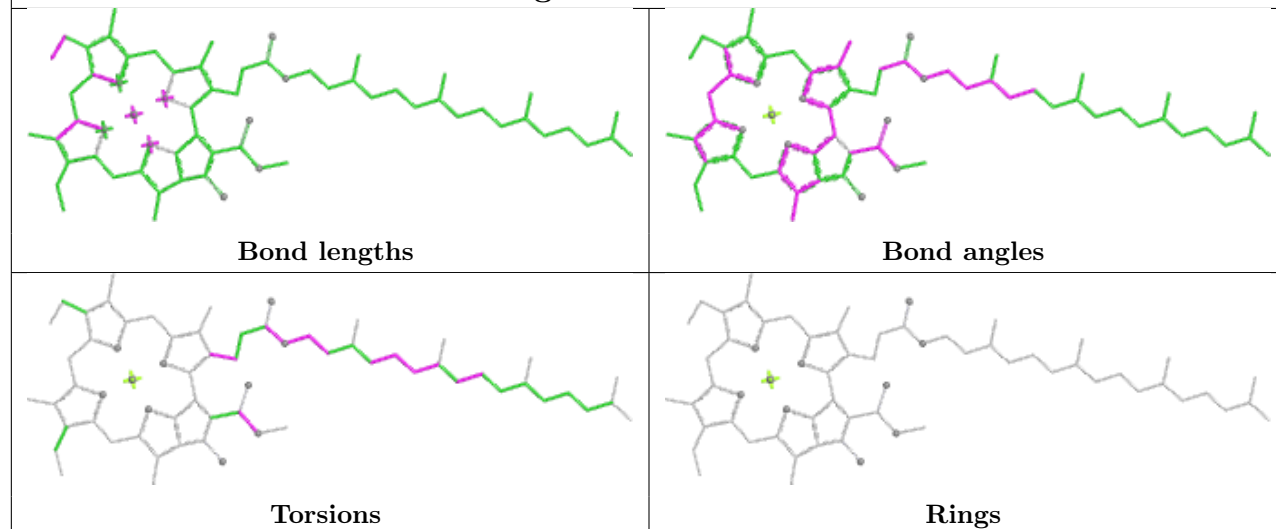
Bond angles



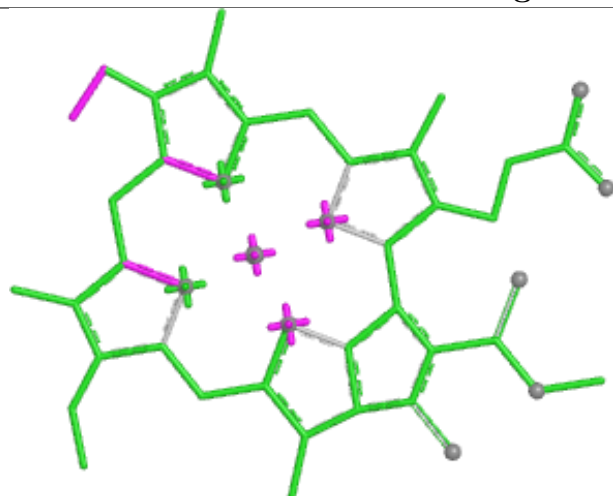
Torsions



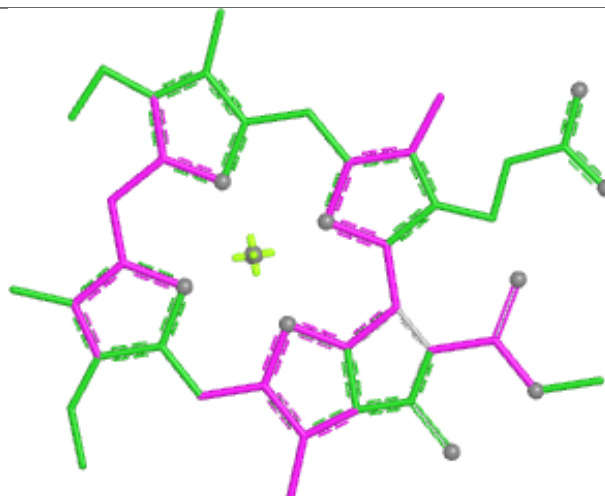
Rings

Ligand CL0 A 801**Ligand CLA Z 313**

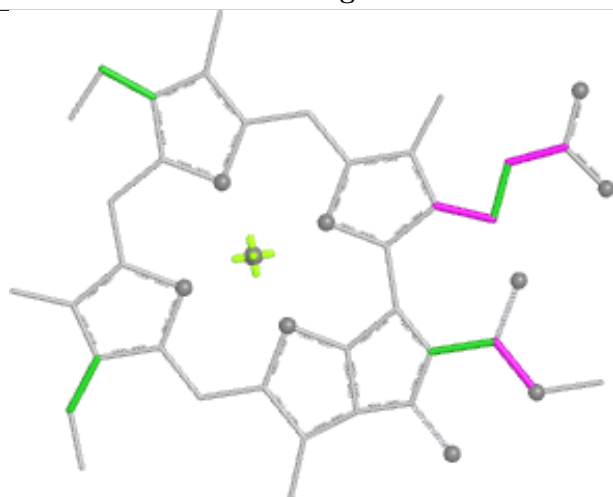
Ligand CLA A 804



Bond lengths



Bond angles

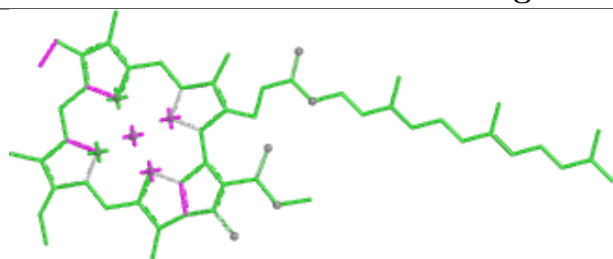


Torsions

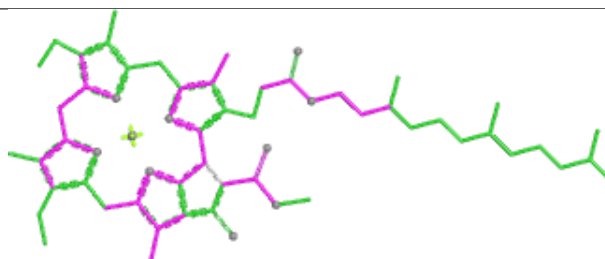


Rings

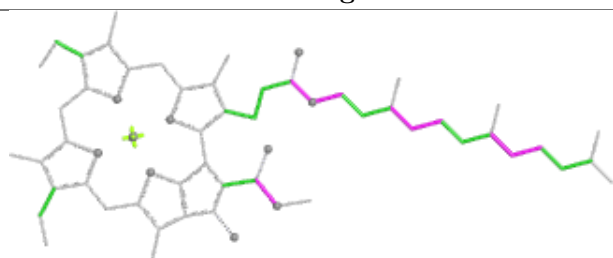
Ligand CLA A 817



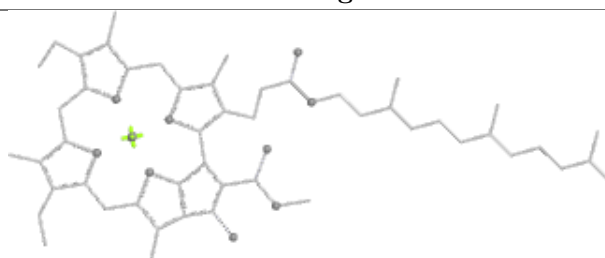
Bond lengths



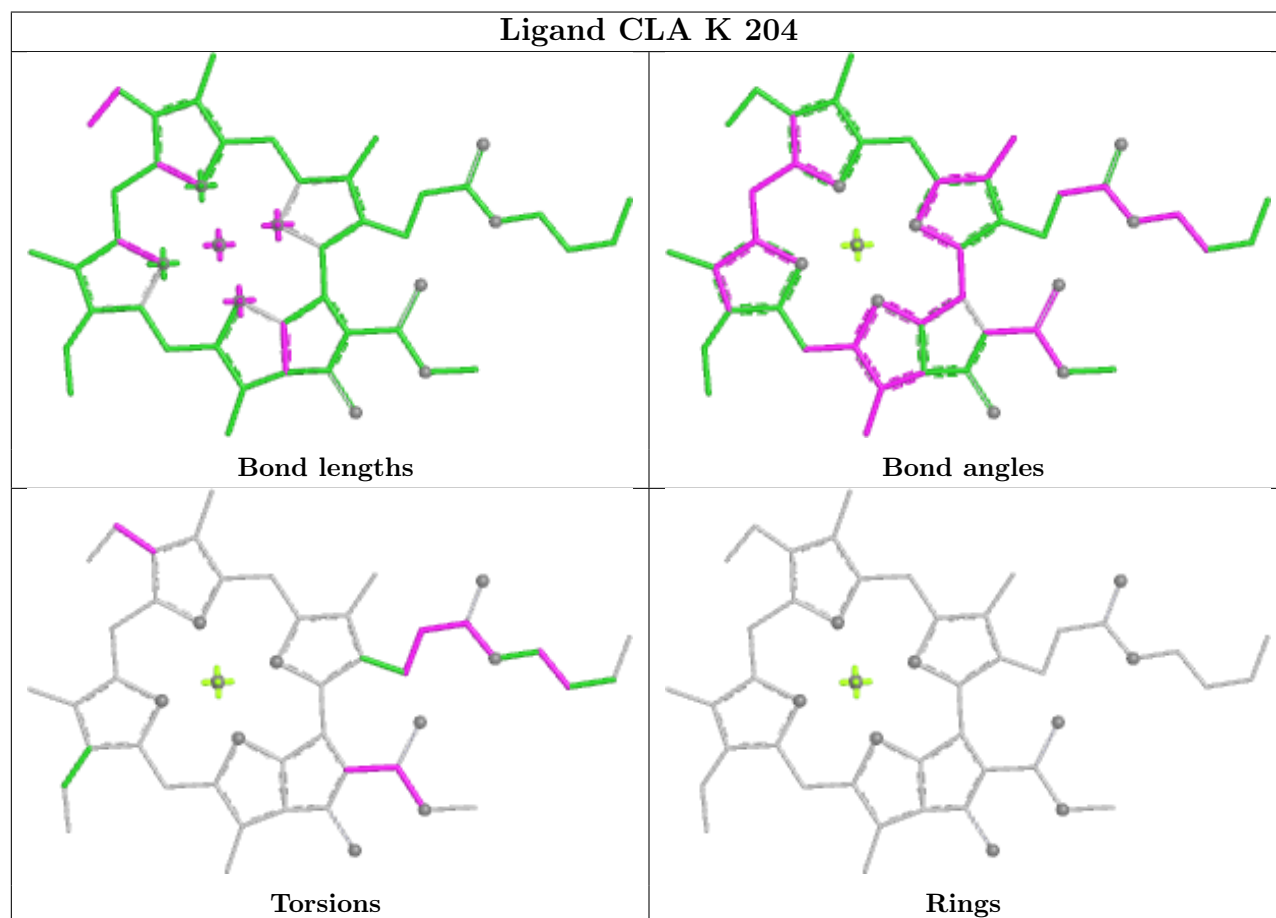
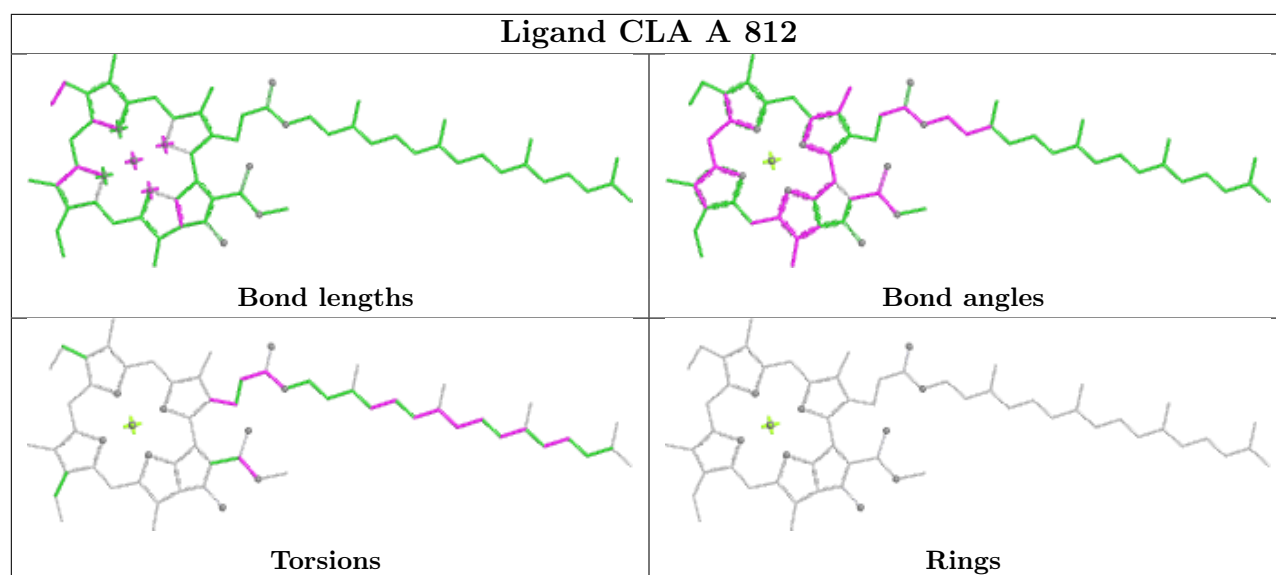
Bond angles

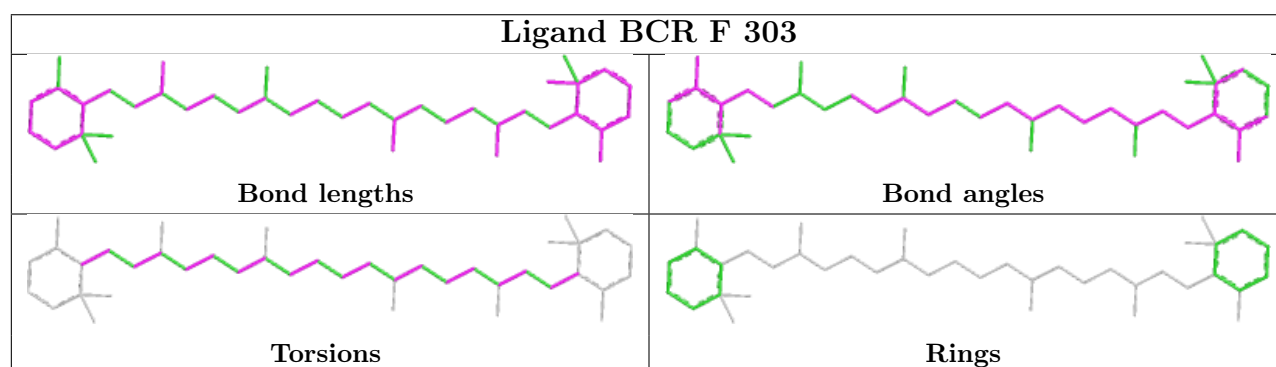
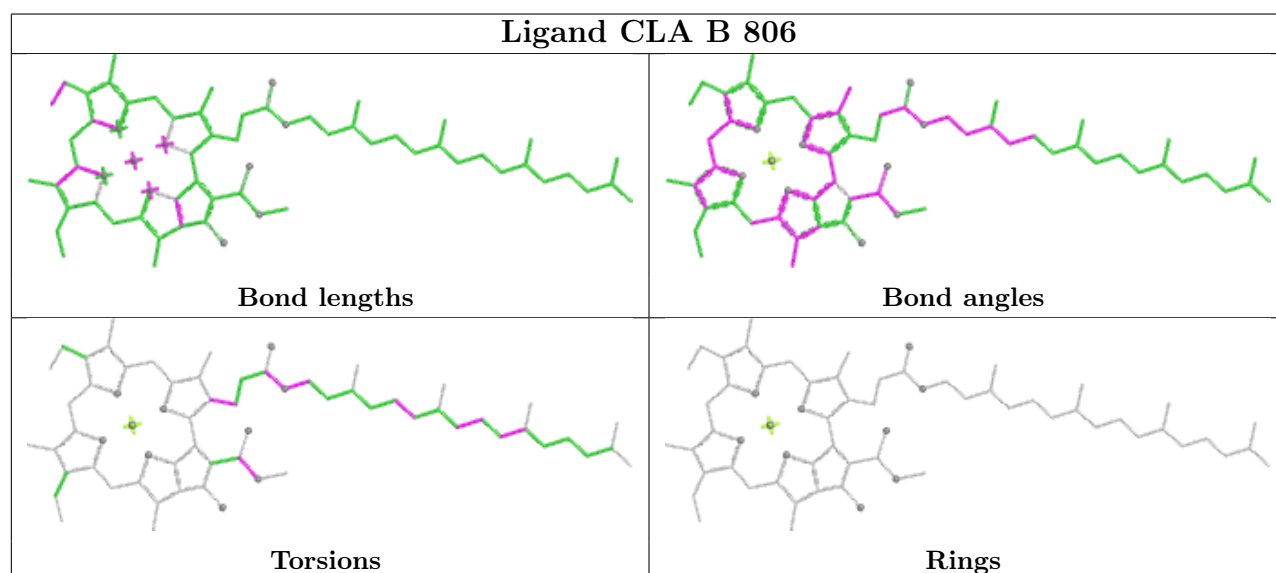
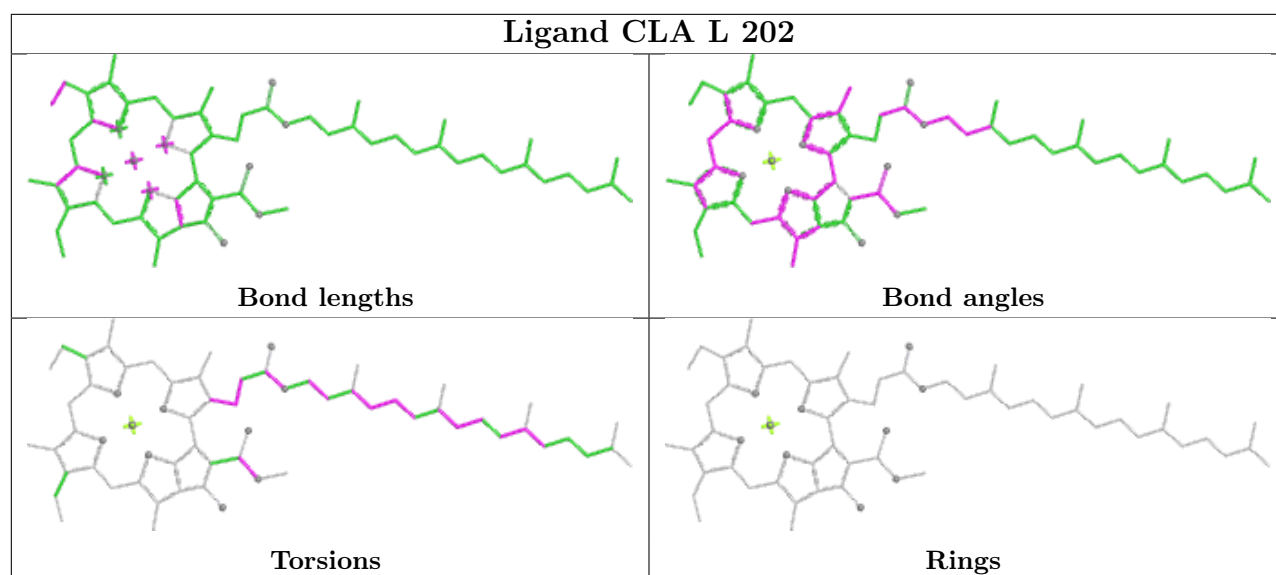


Torsions

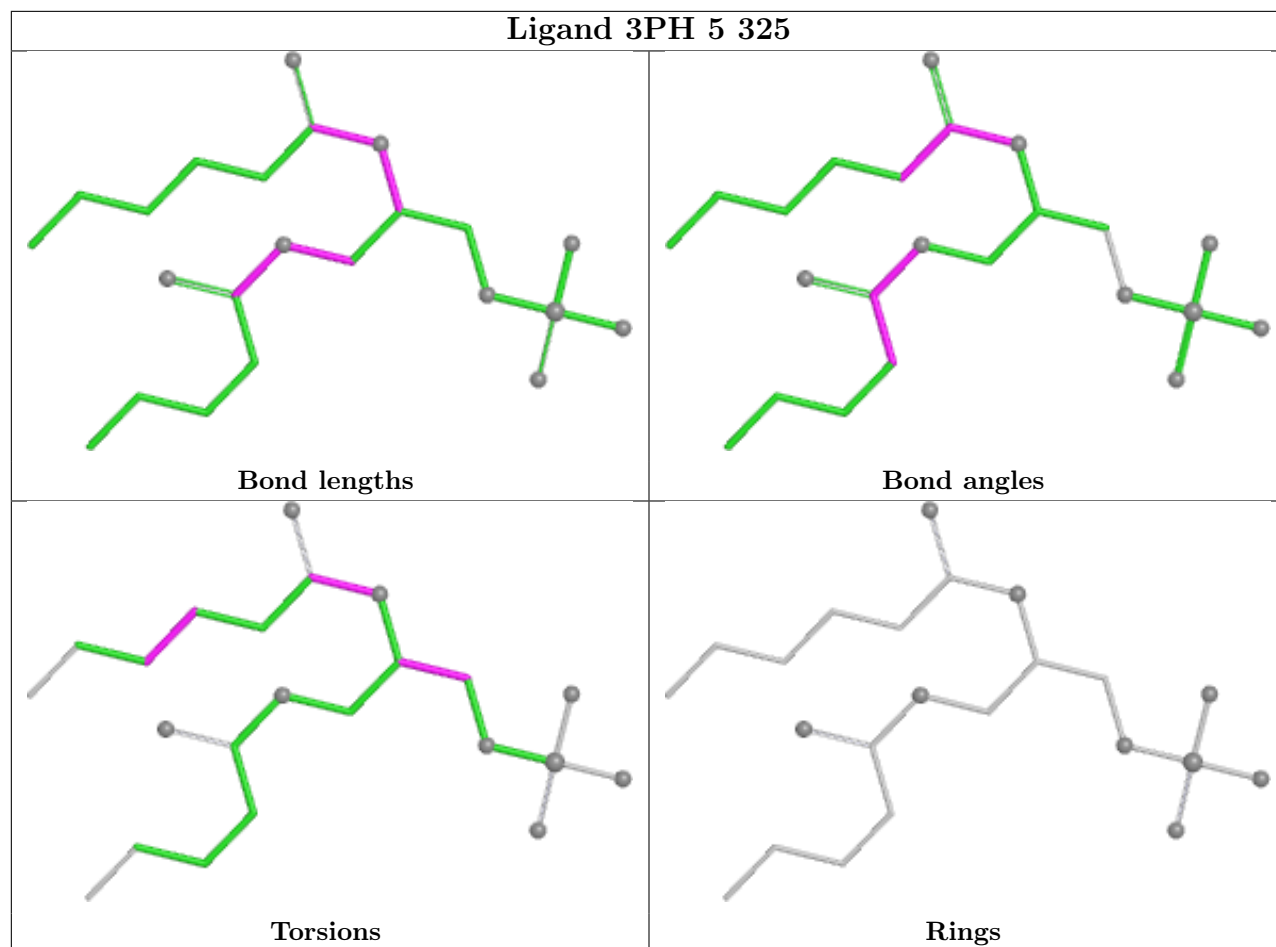


Rings

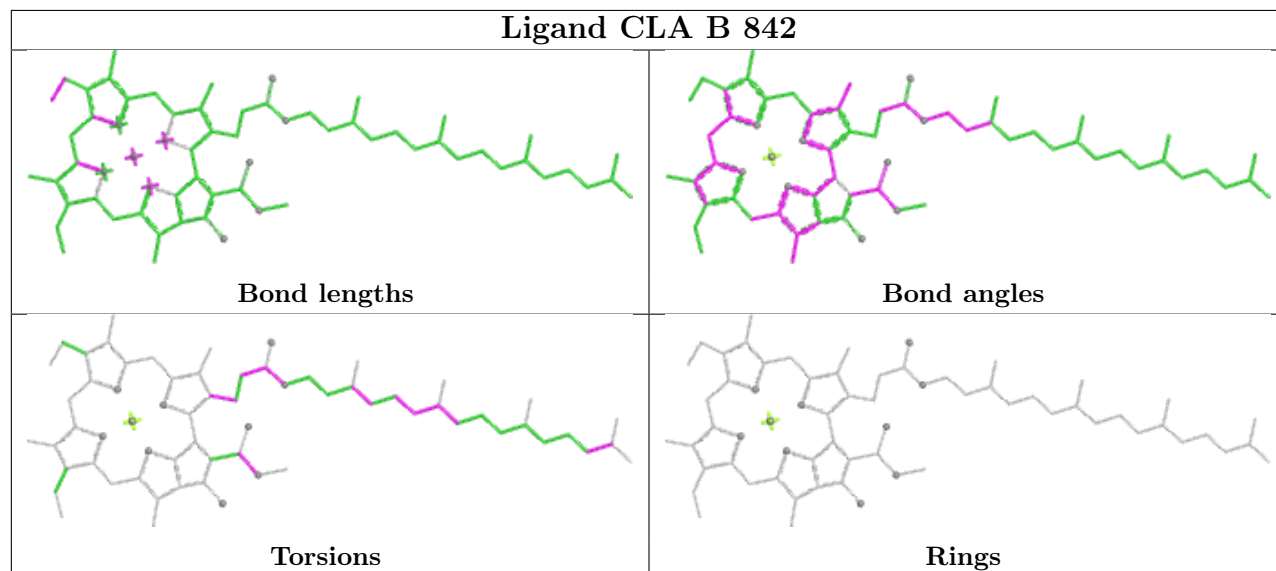


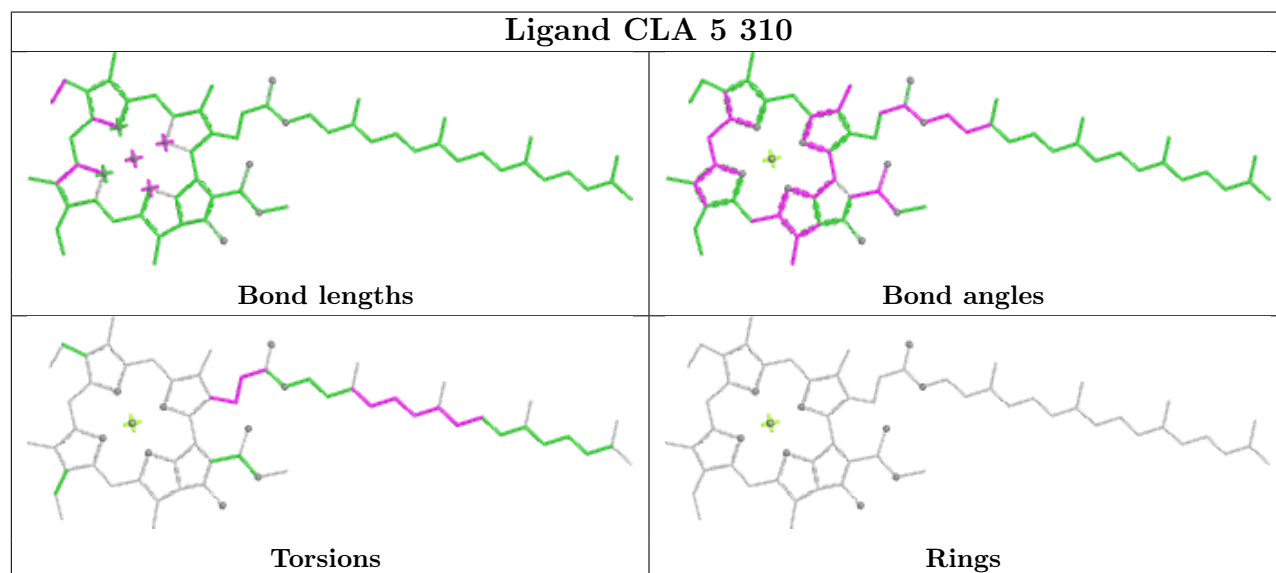
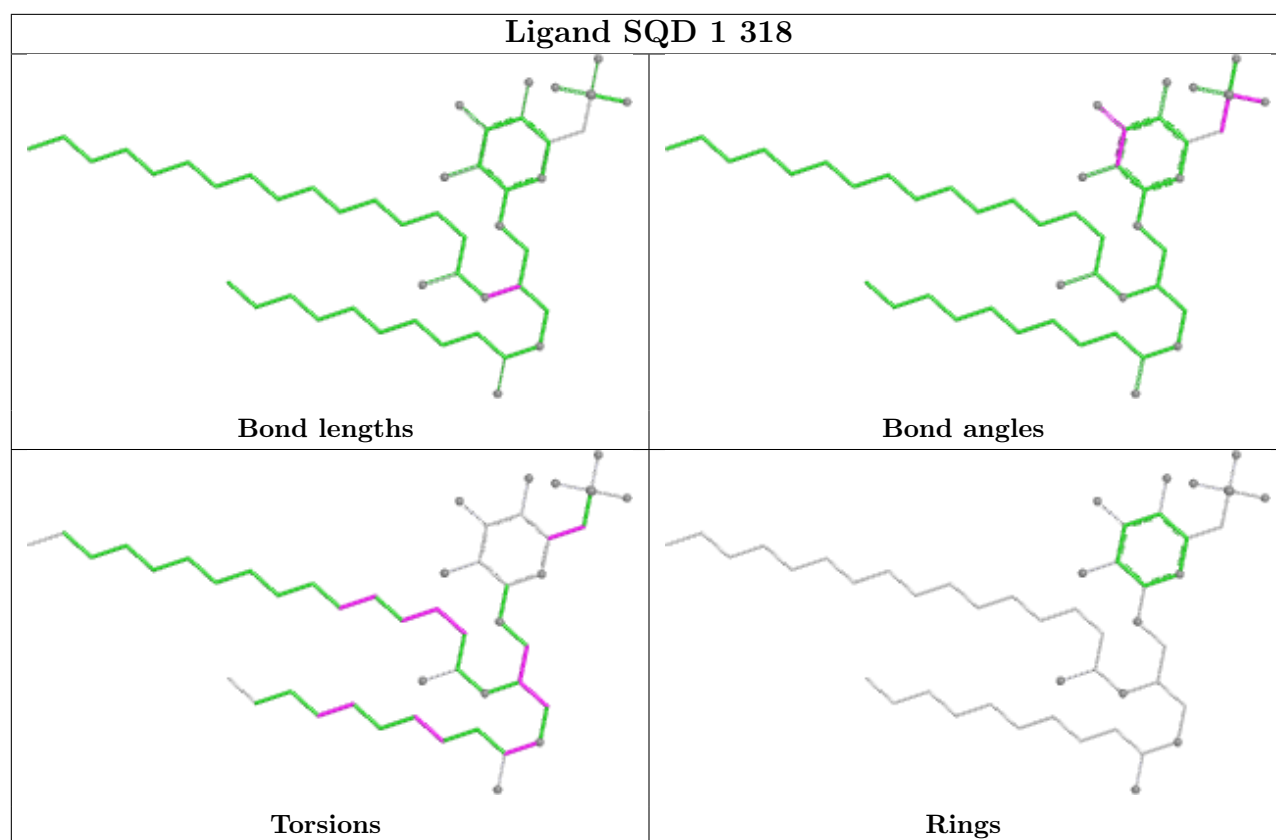


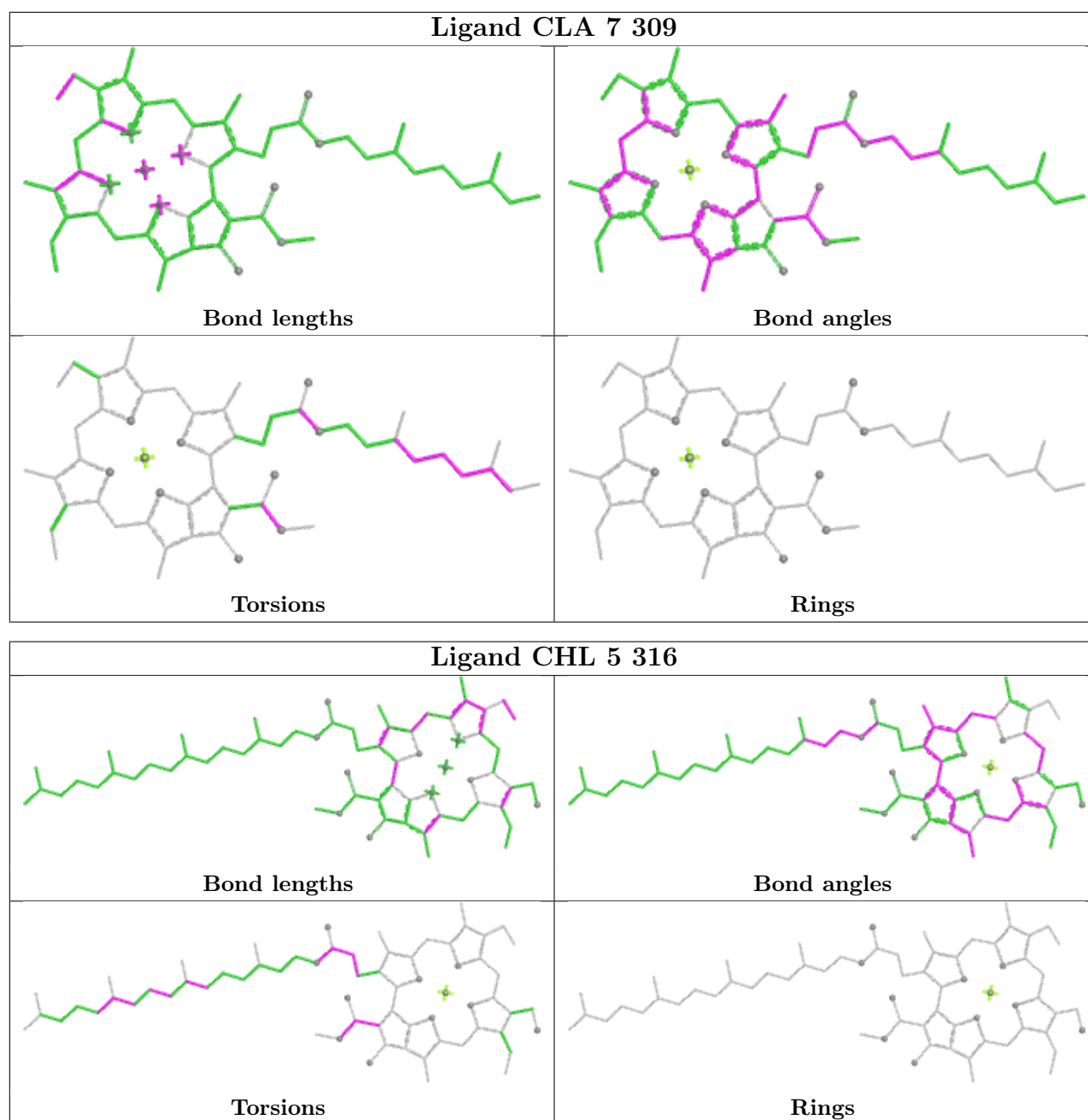
Ligand 3PH 5 325

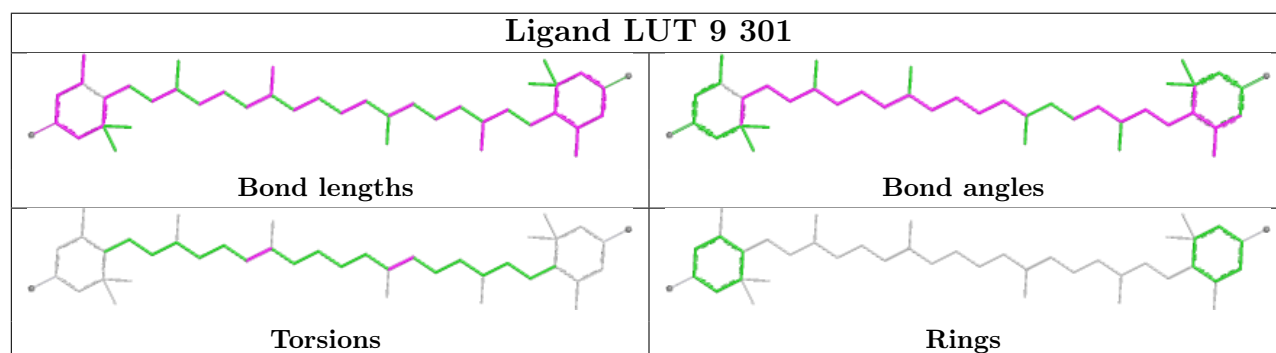
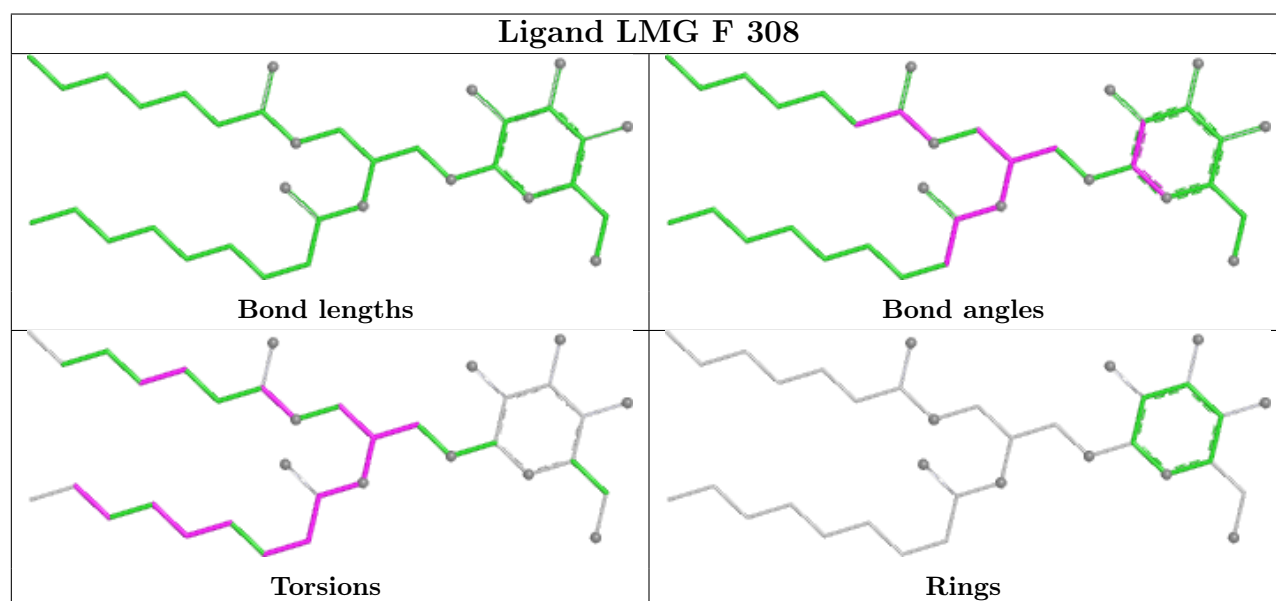
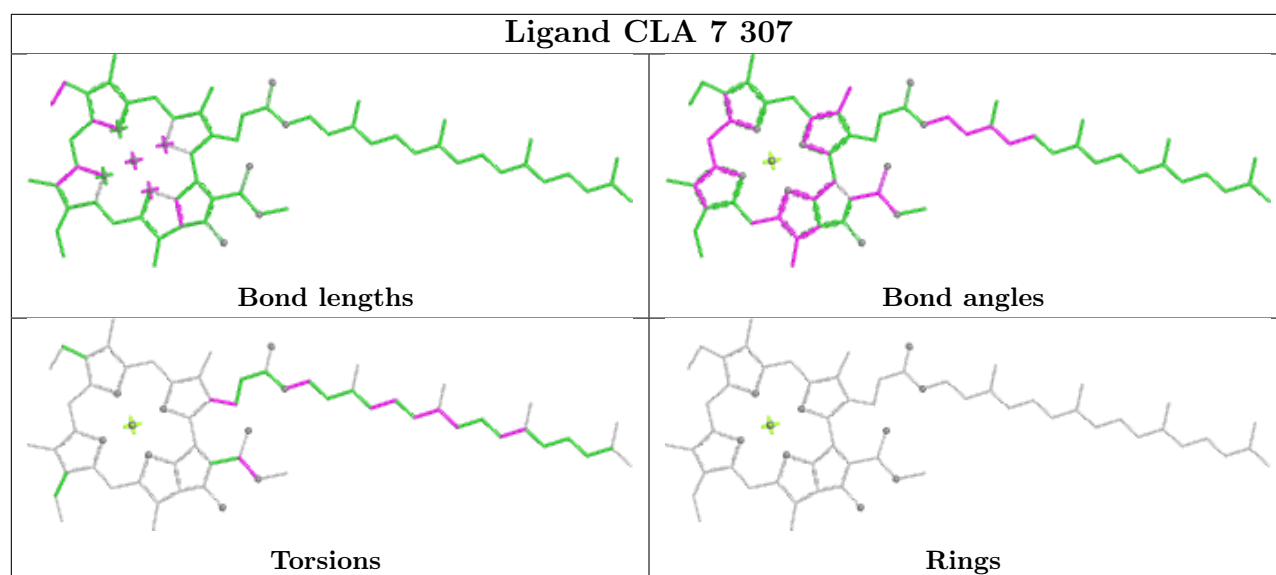


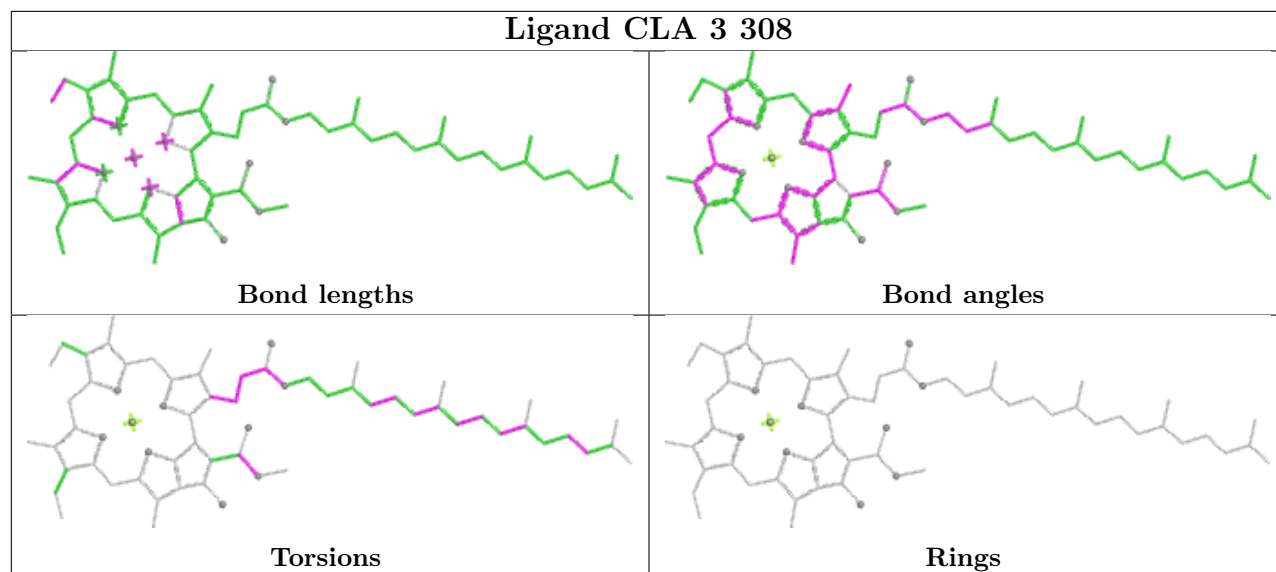
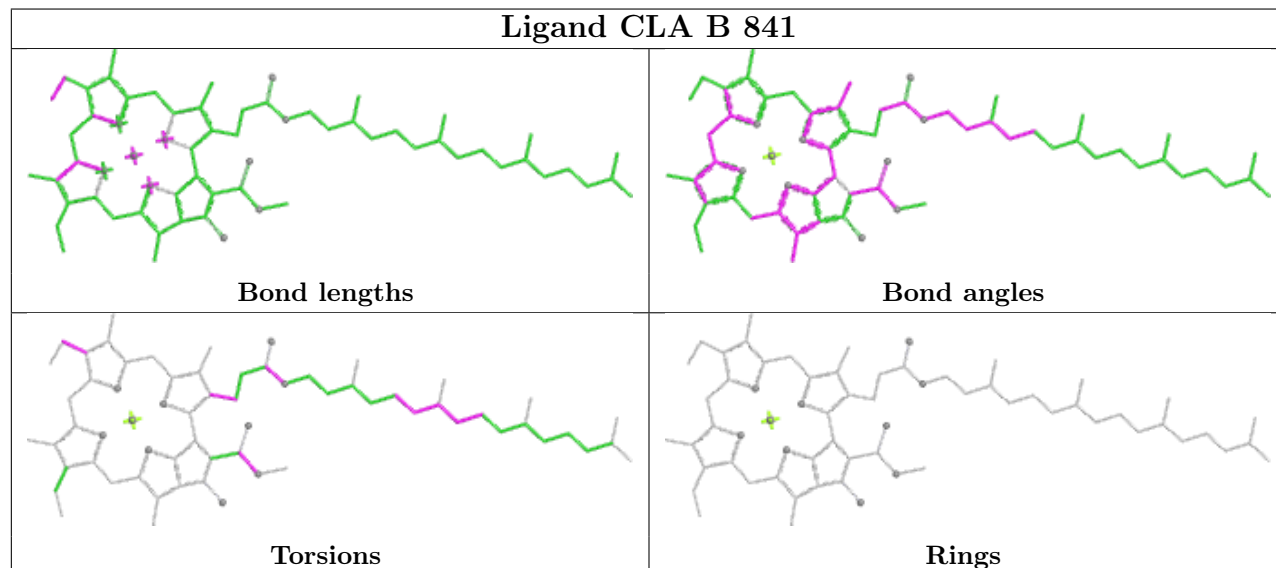
Ligand CLA B 842

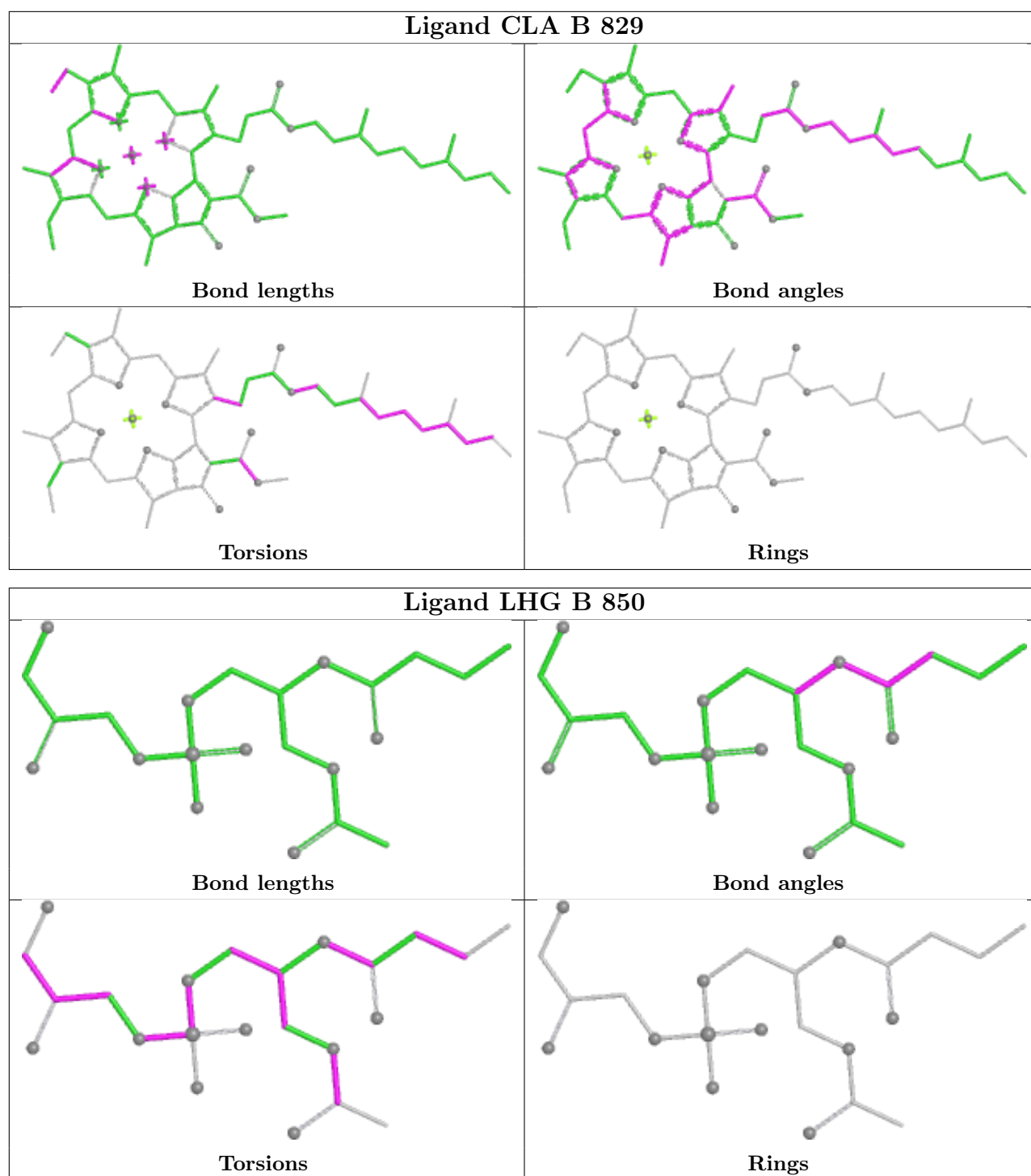


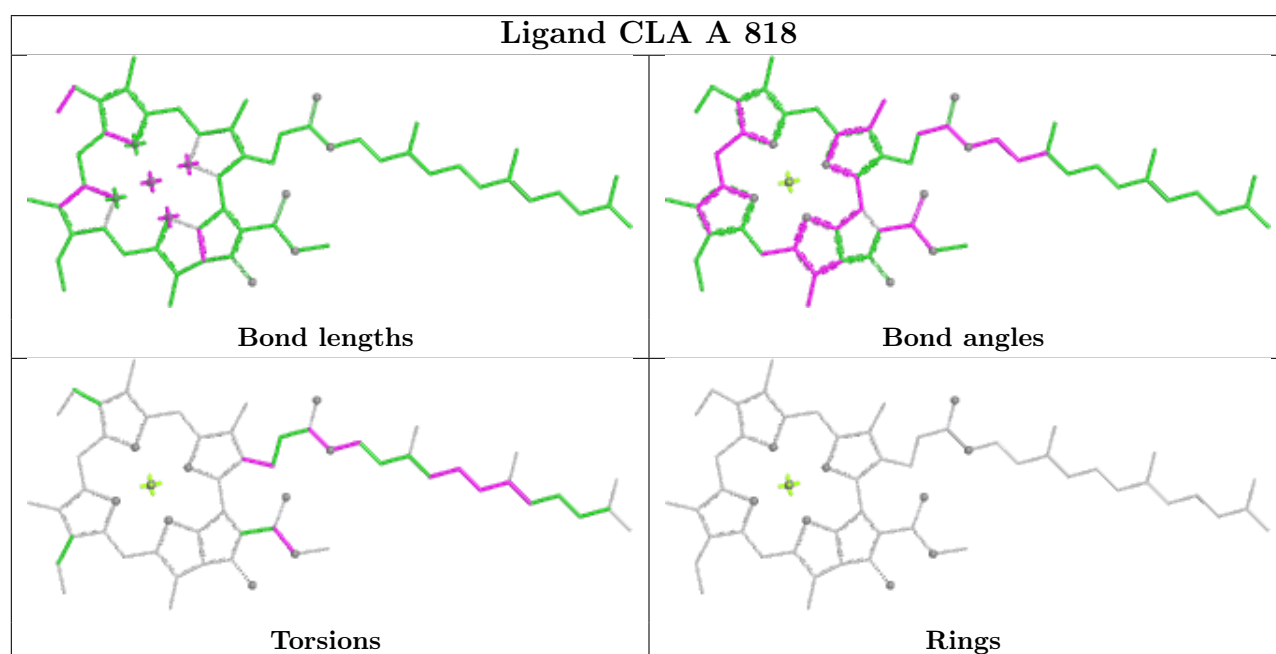
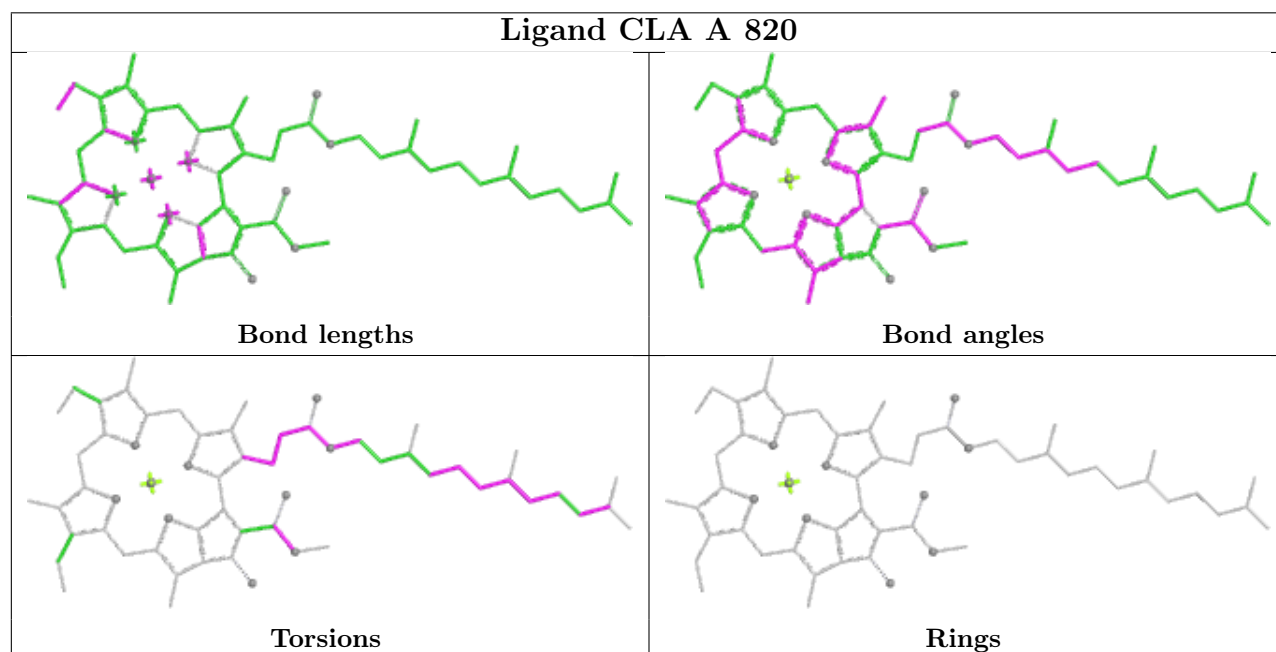
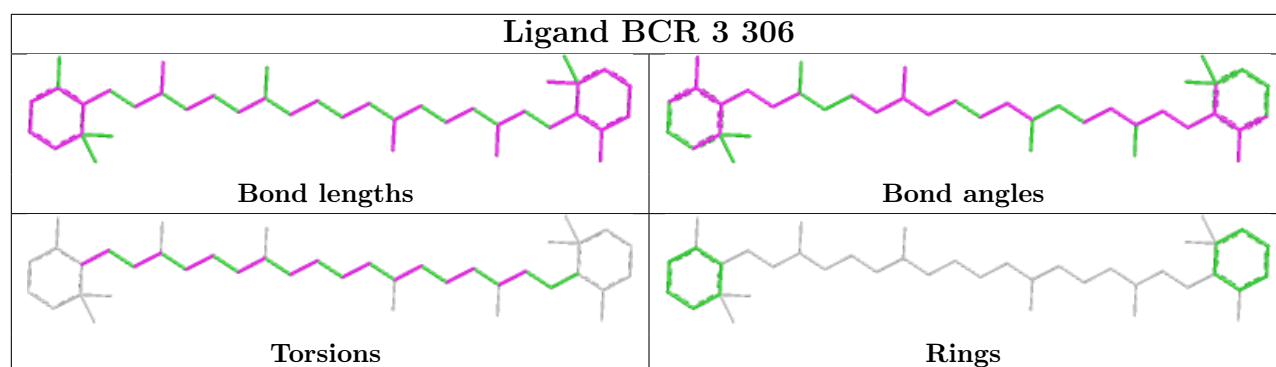


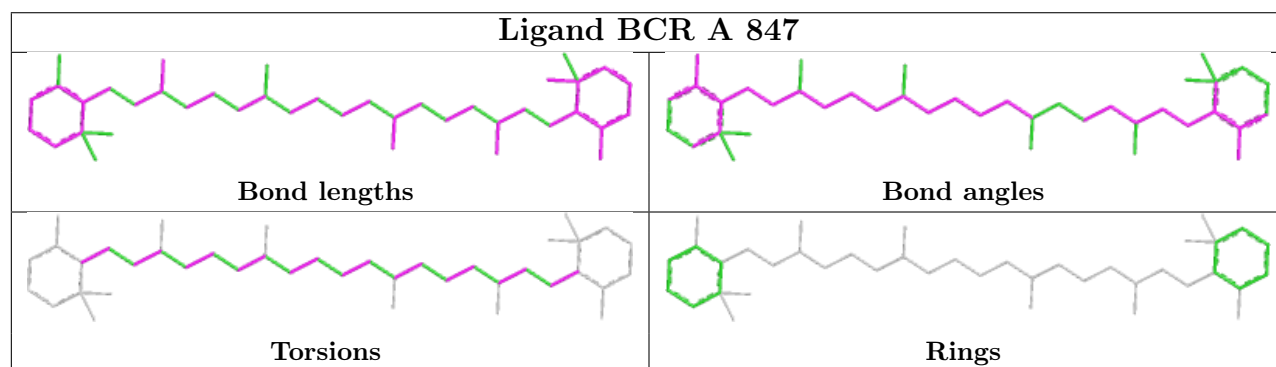
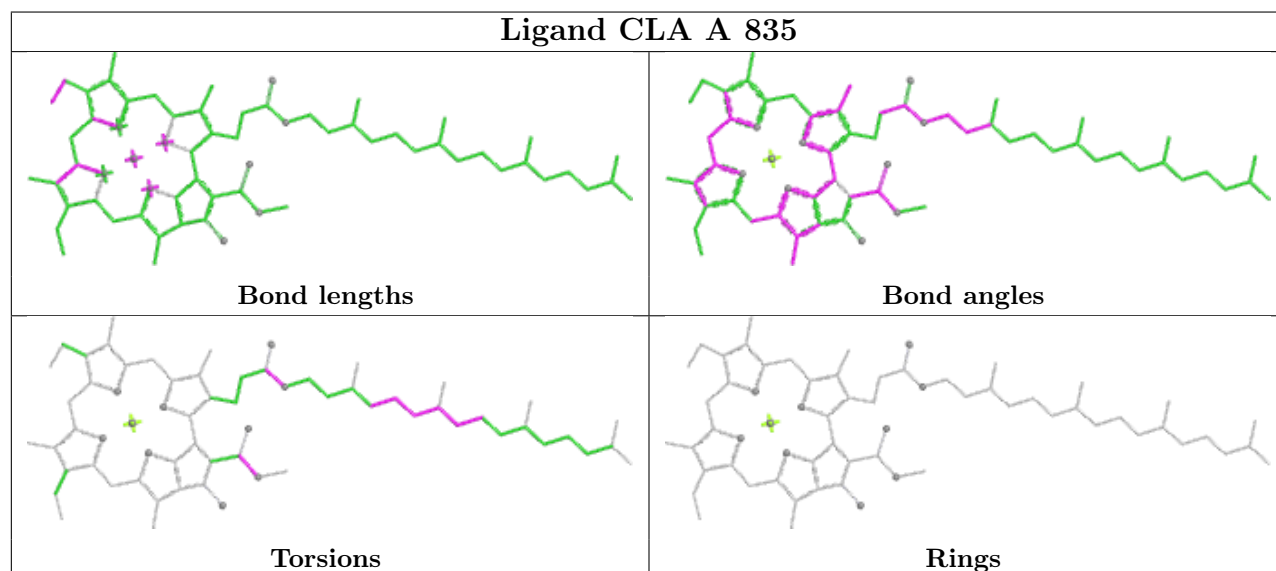
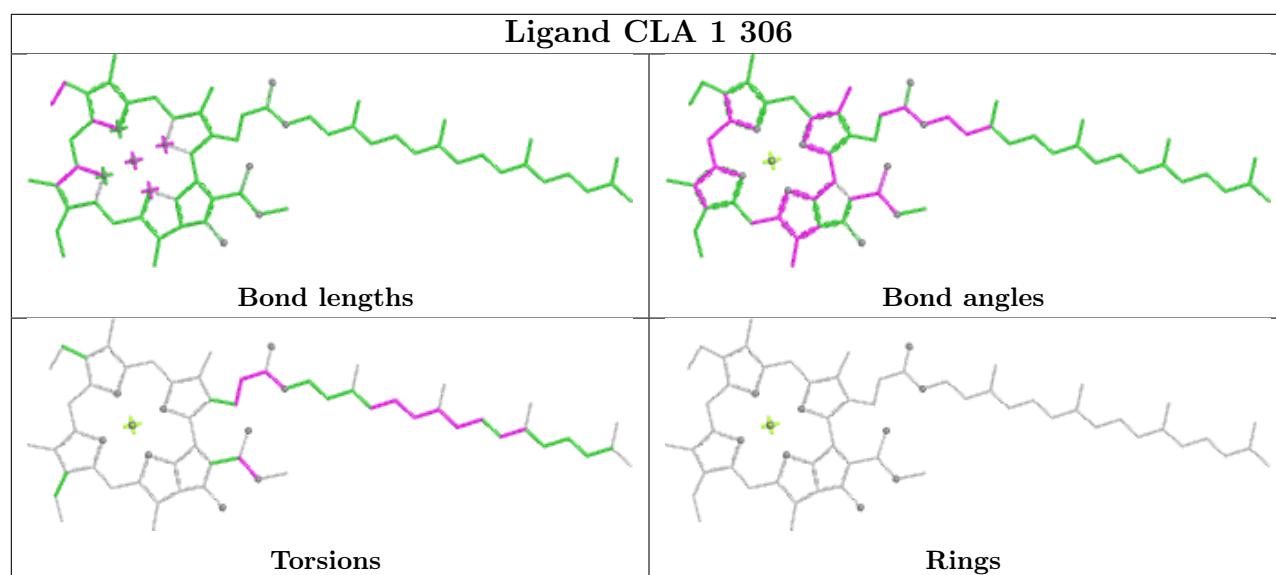


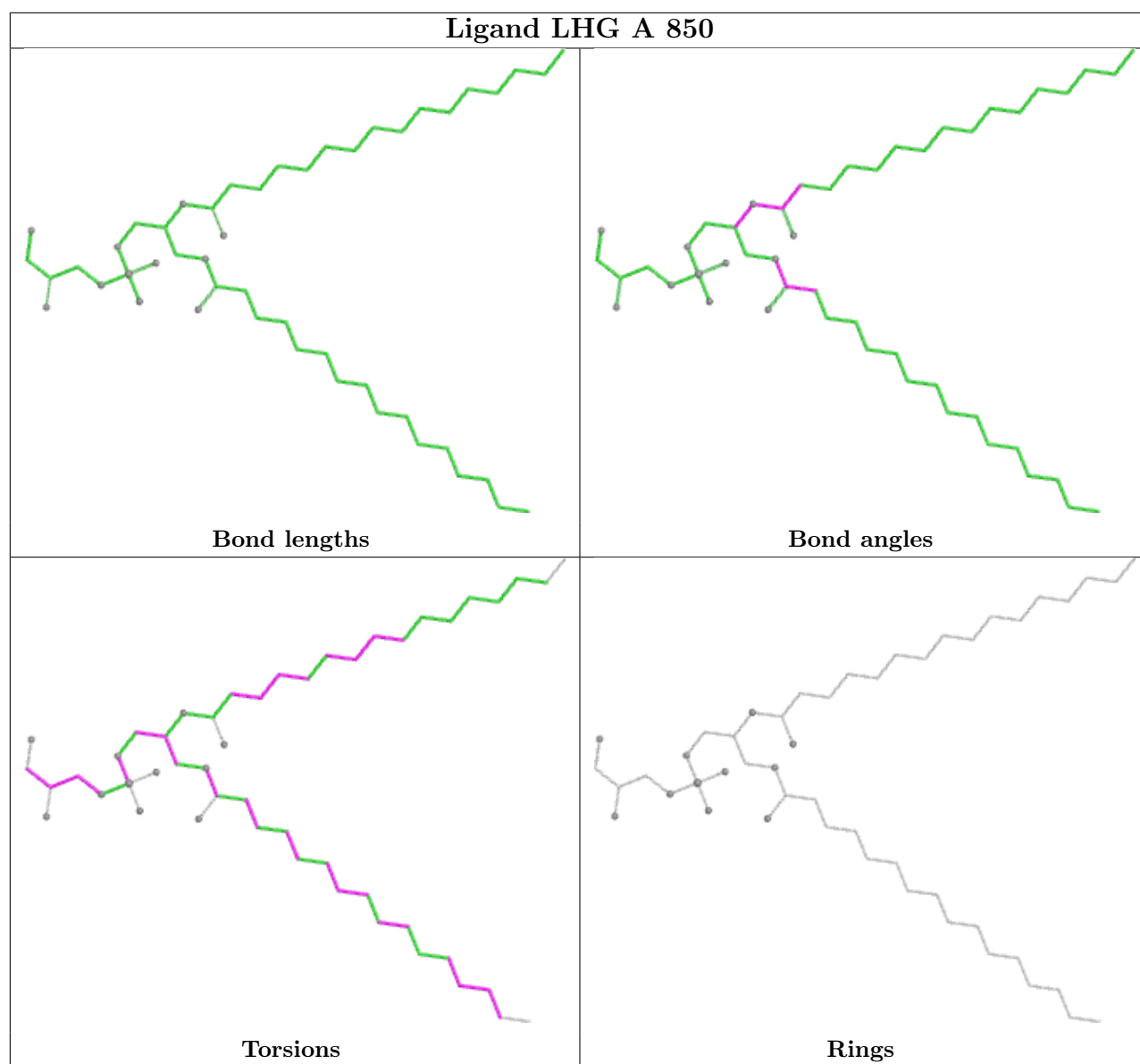


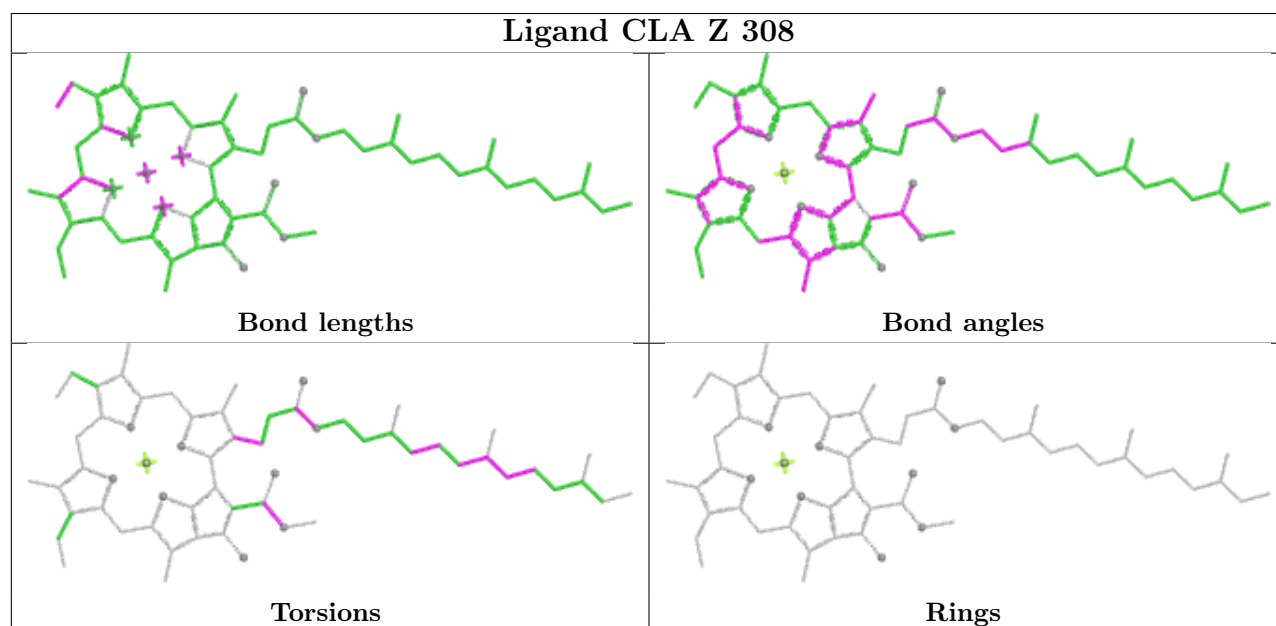
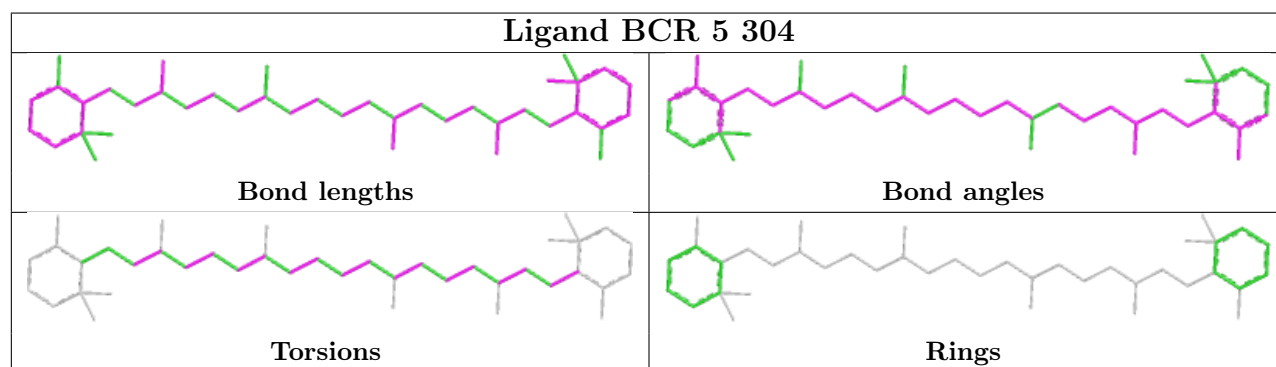
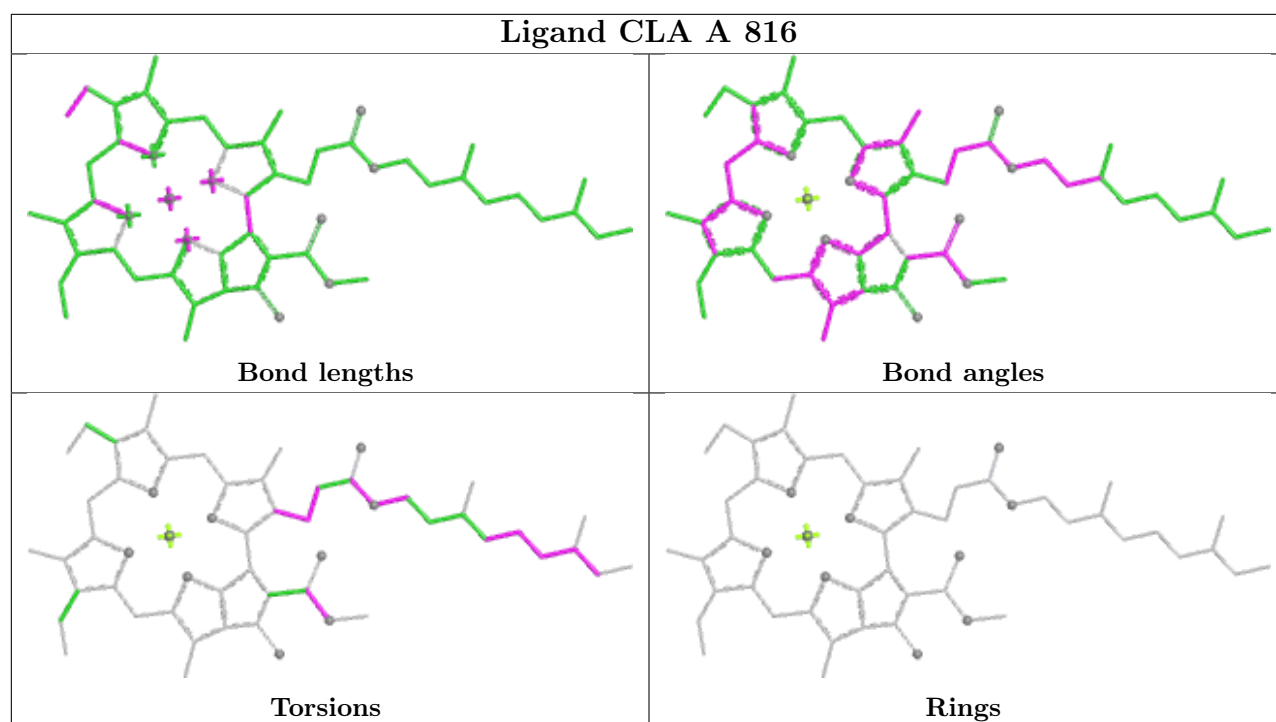
Ligand CLA 3 308**Ligand CLA B 841**



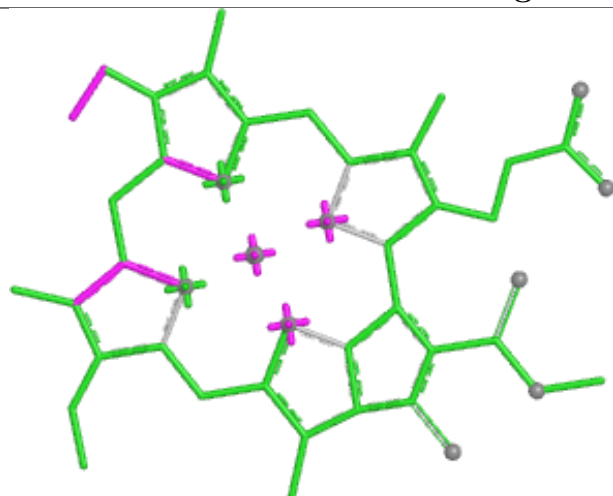




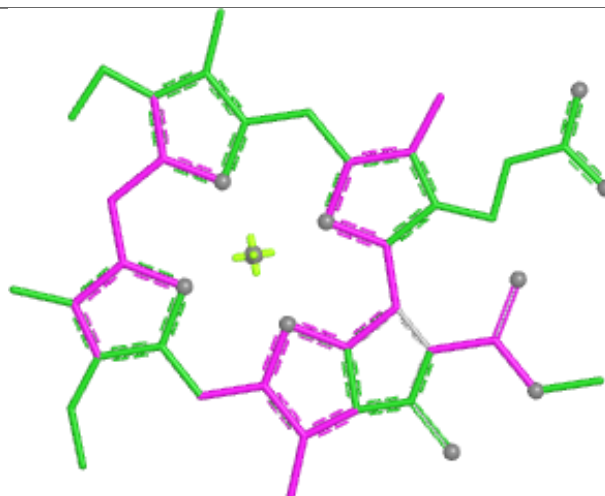




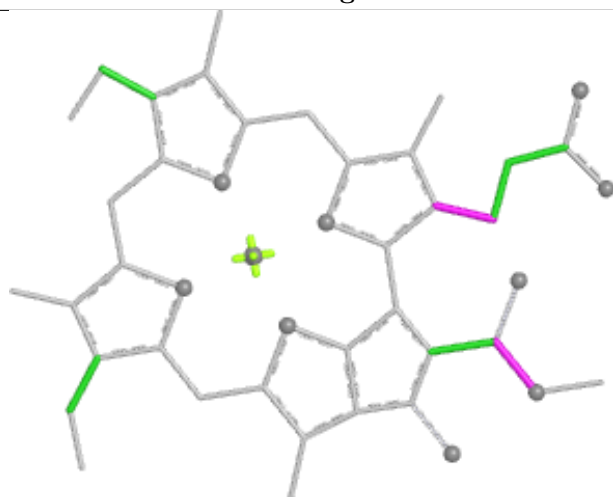
Ligand CLA B 836



Bond lengths



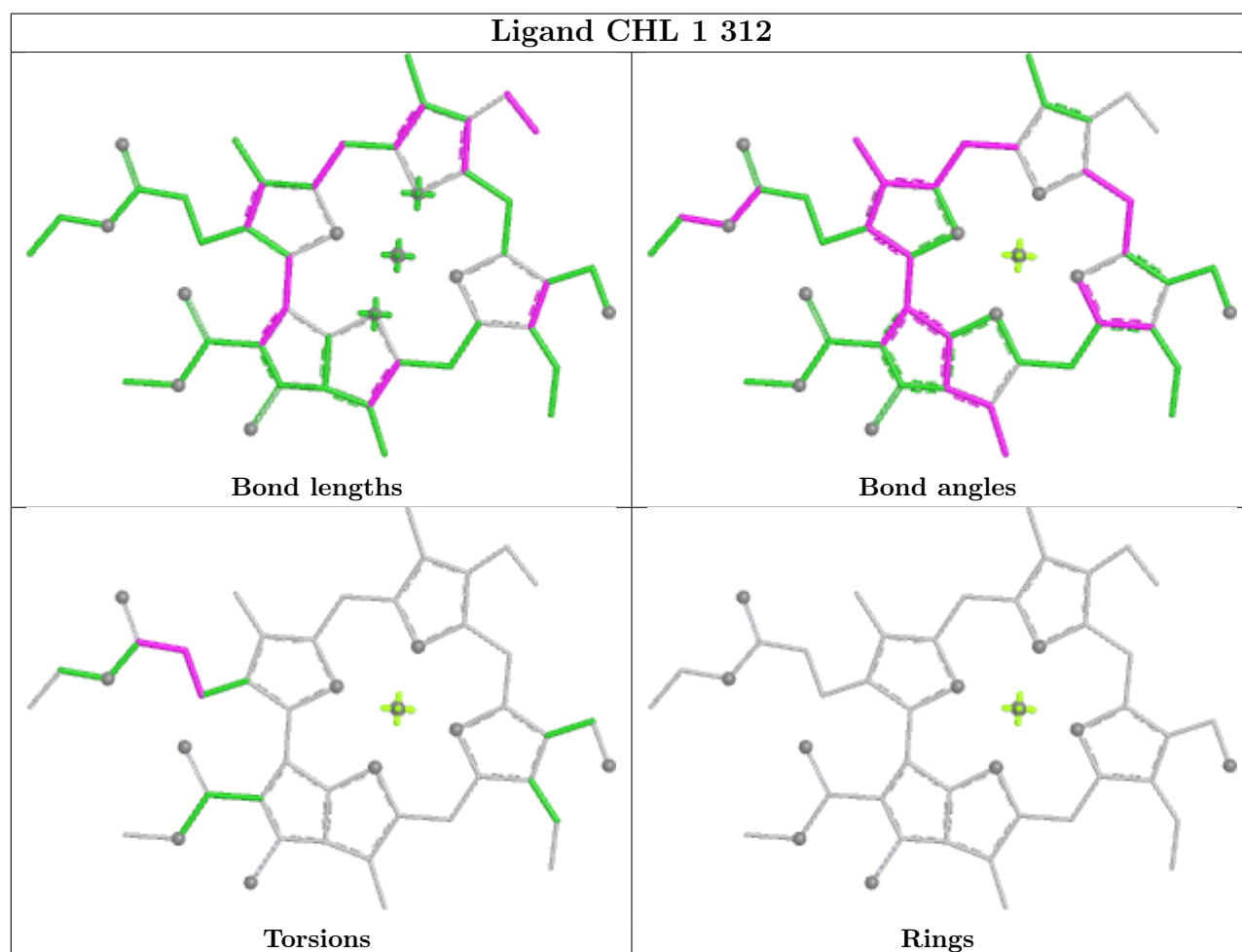
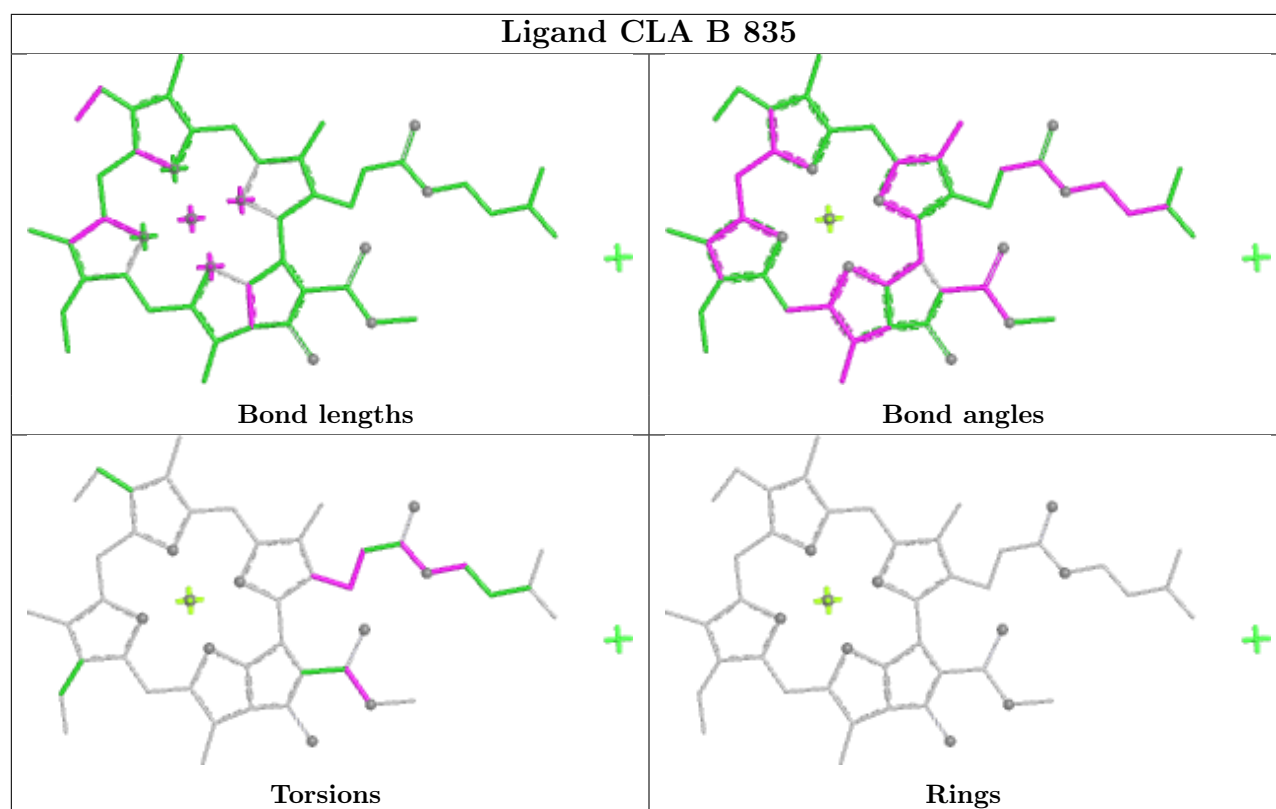
Bond angles

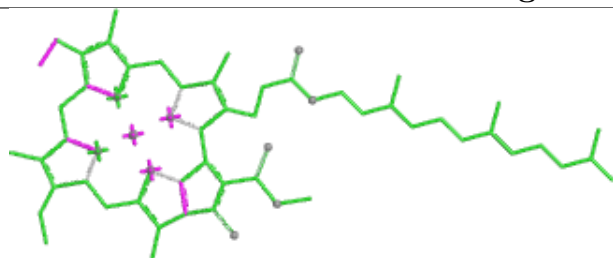
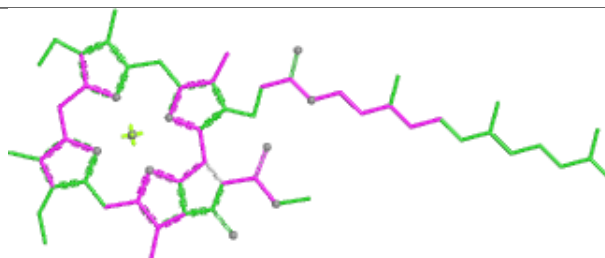
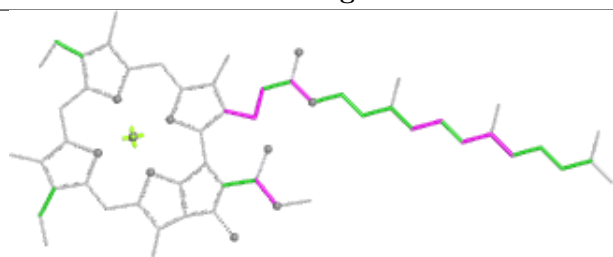
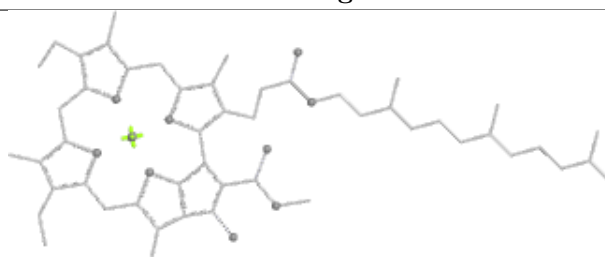
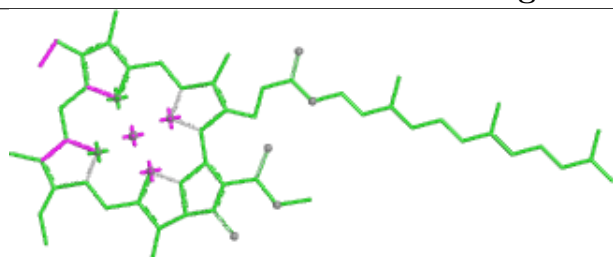
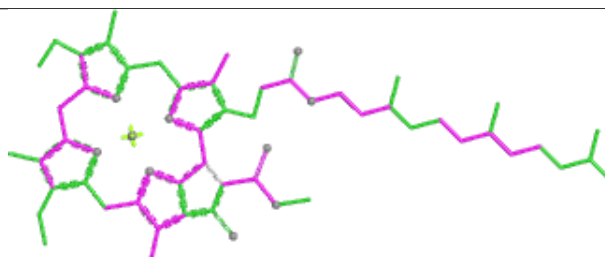
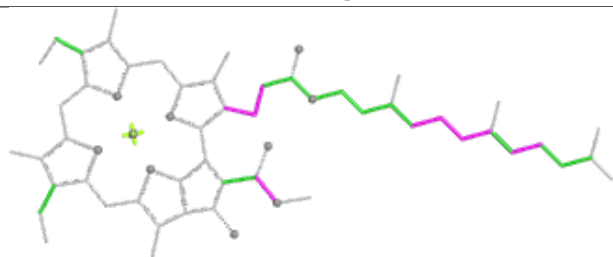
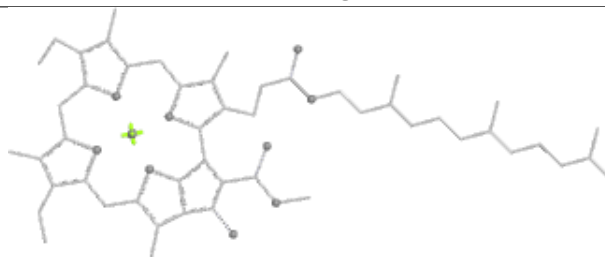


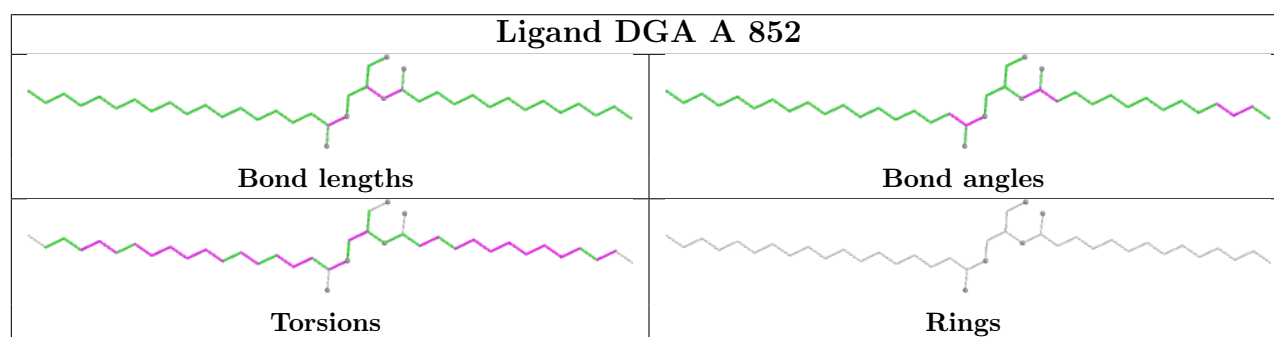
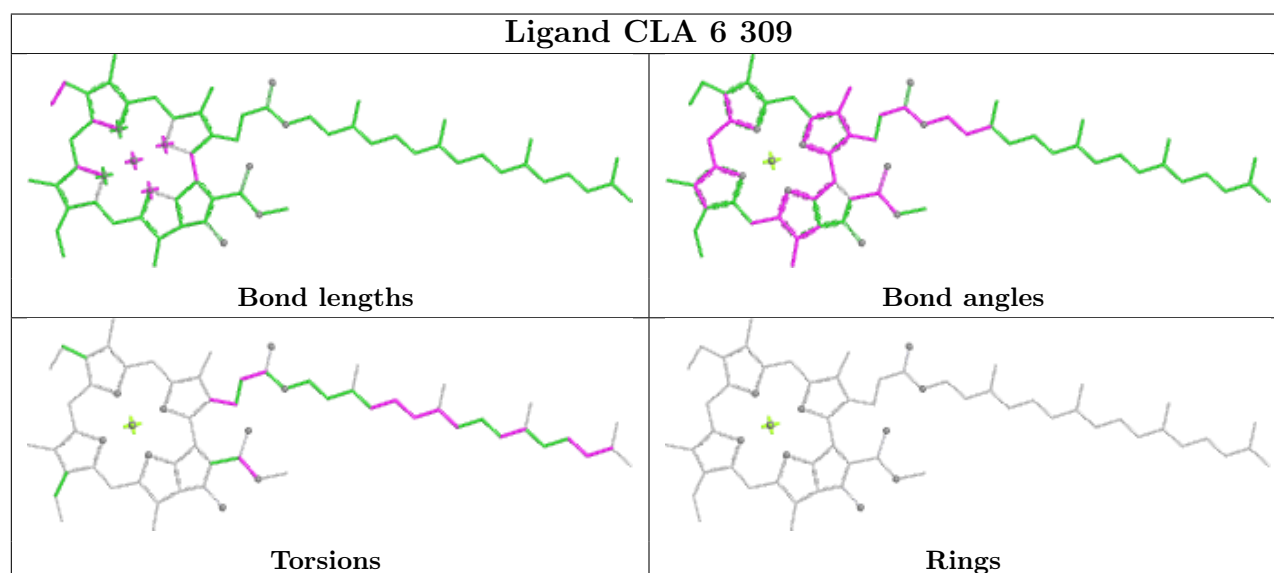
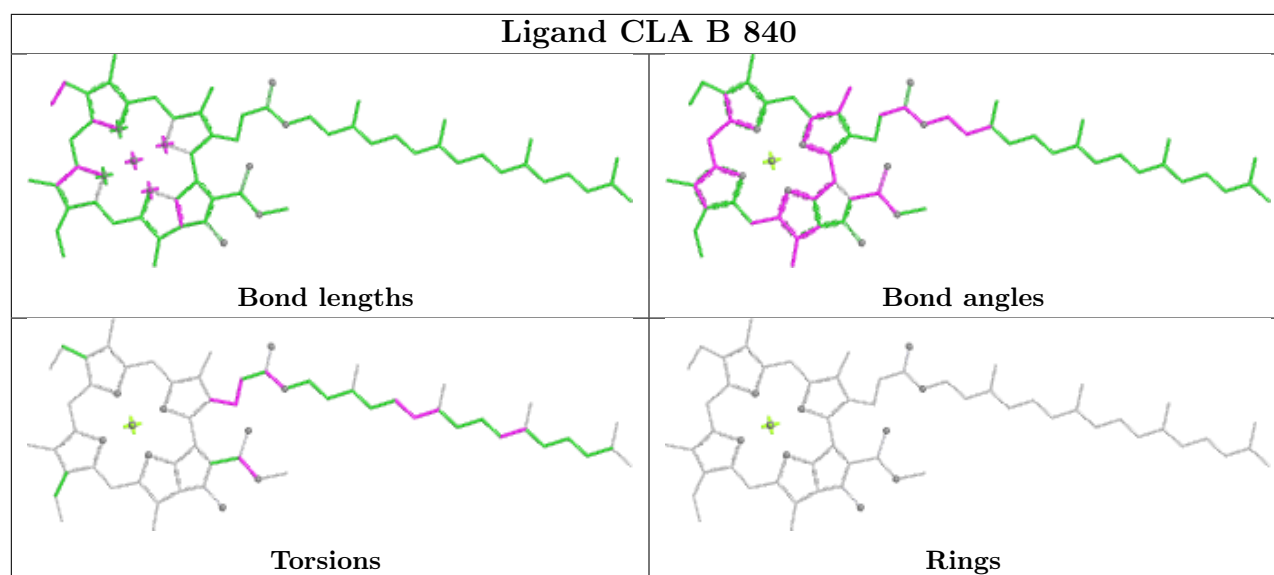
Torsions



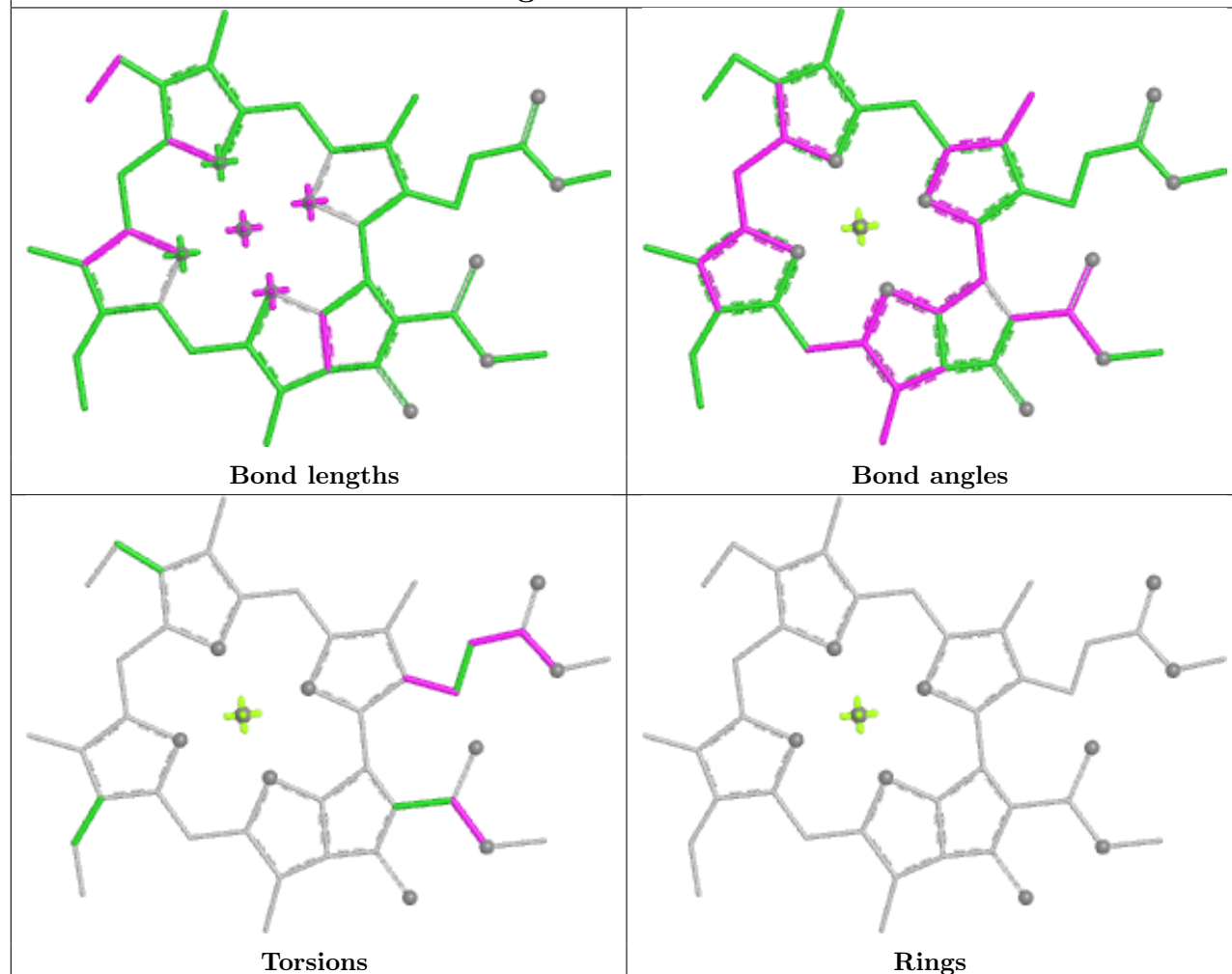
Rings



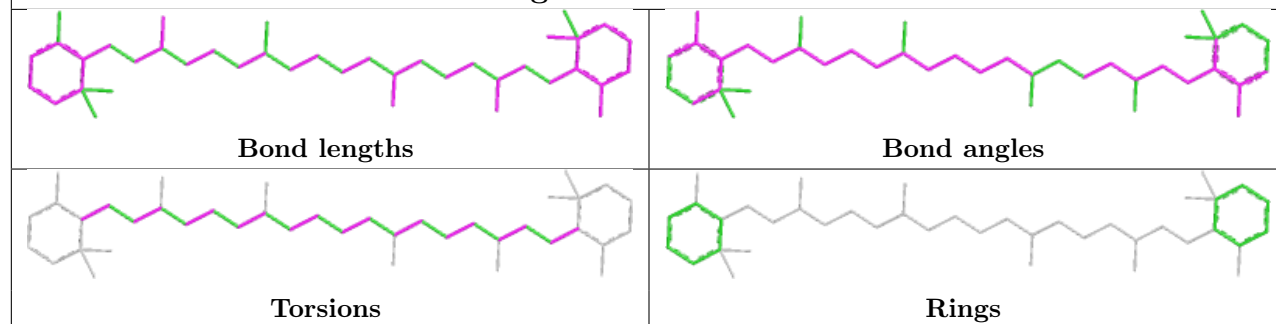
Ligand CLA 8 305**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 3 318****Bond lengths****Bond angles****Torsions****Rings**

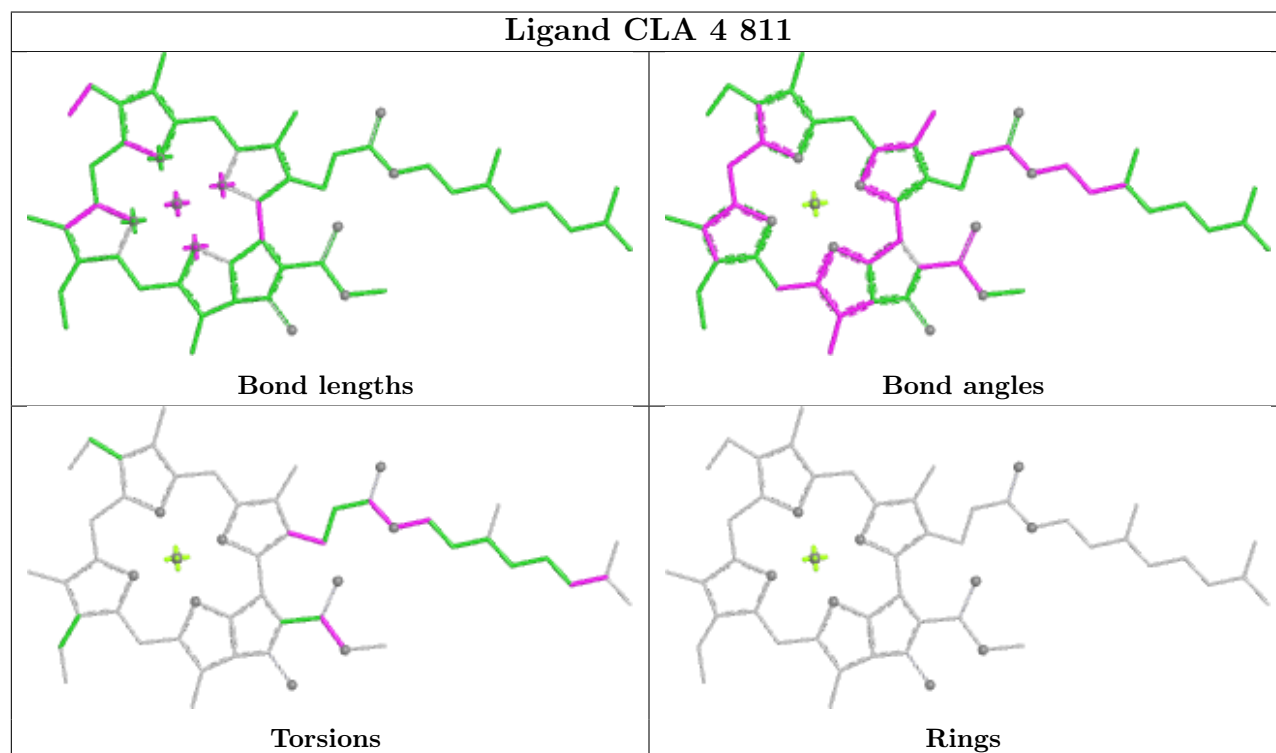
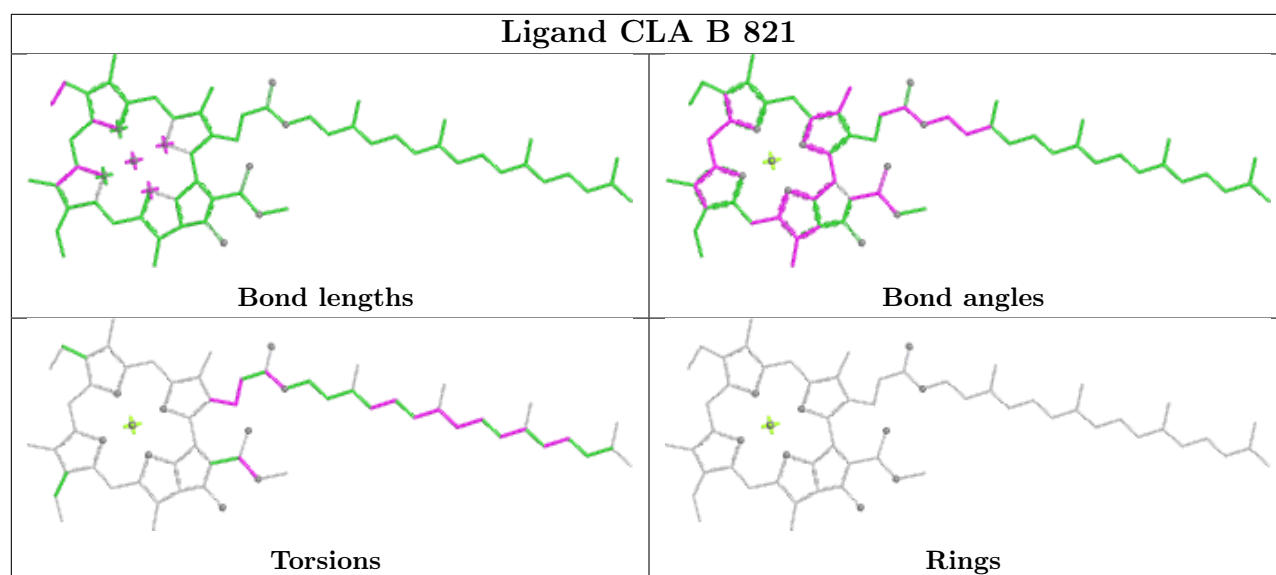


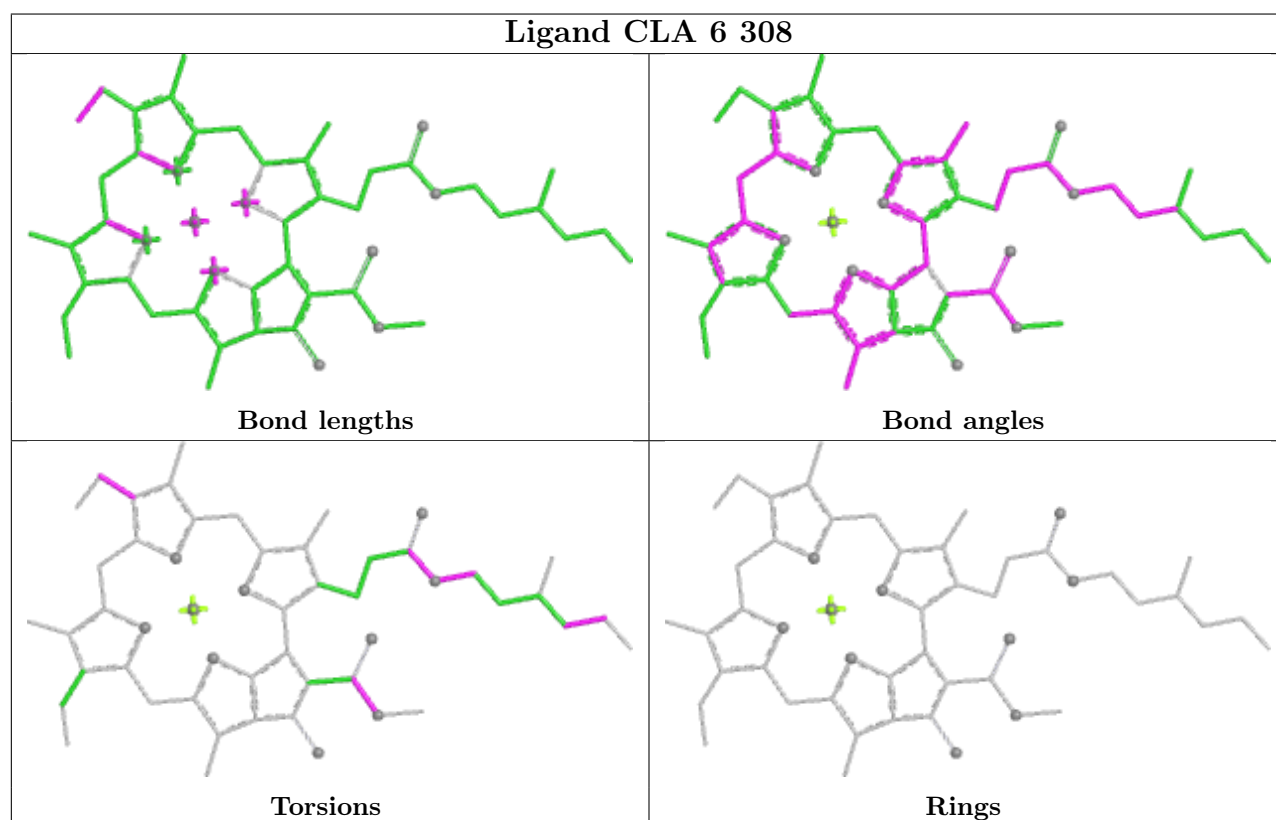
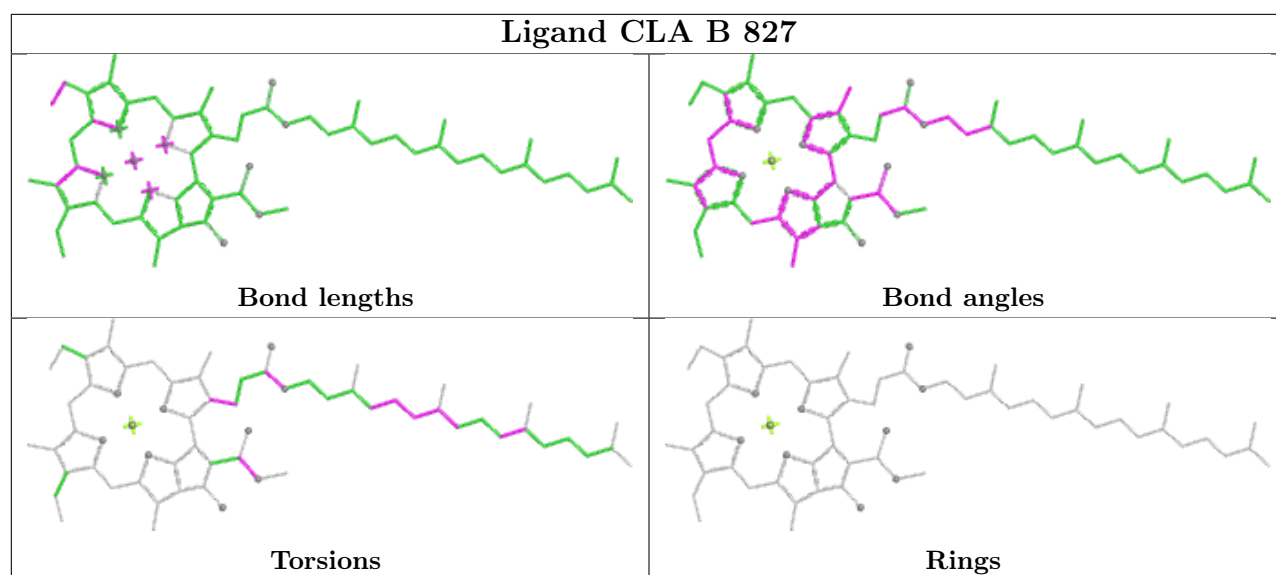
Ligand CLA 1 315

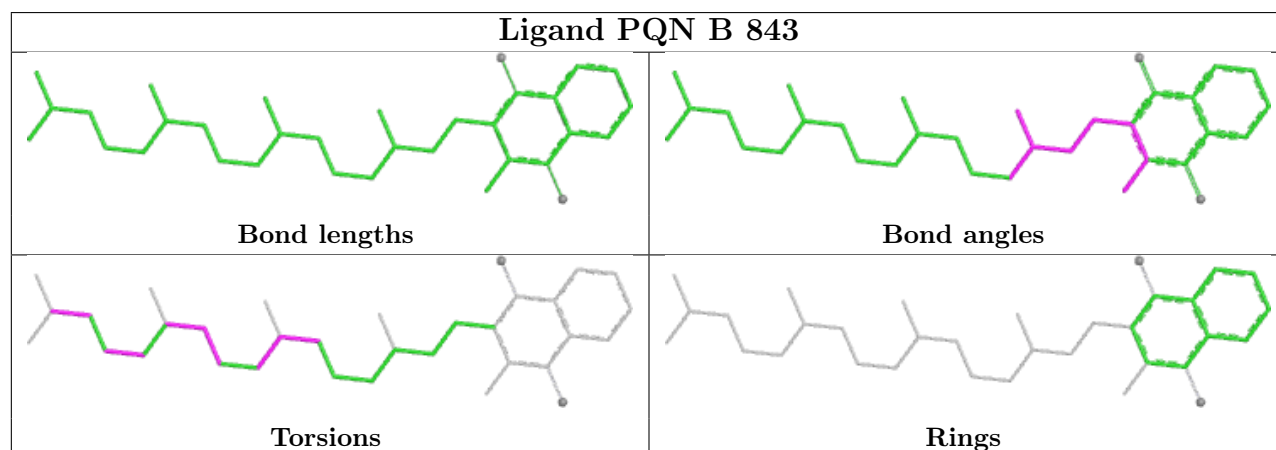
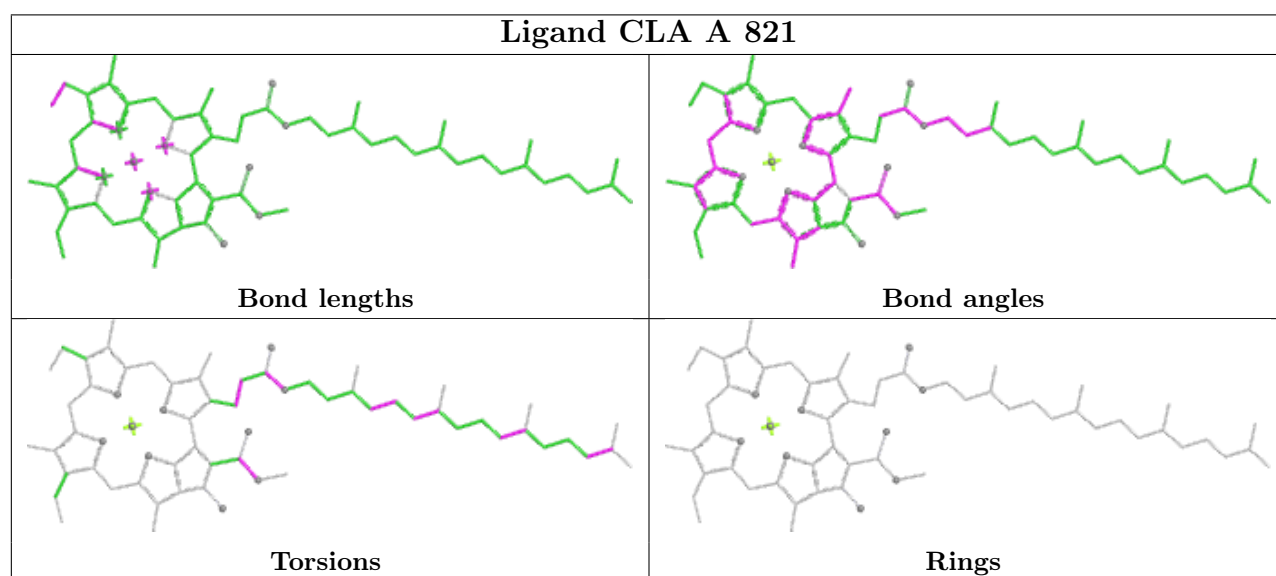
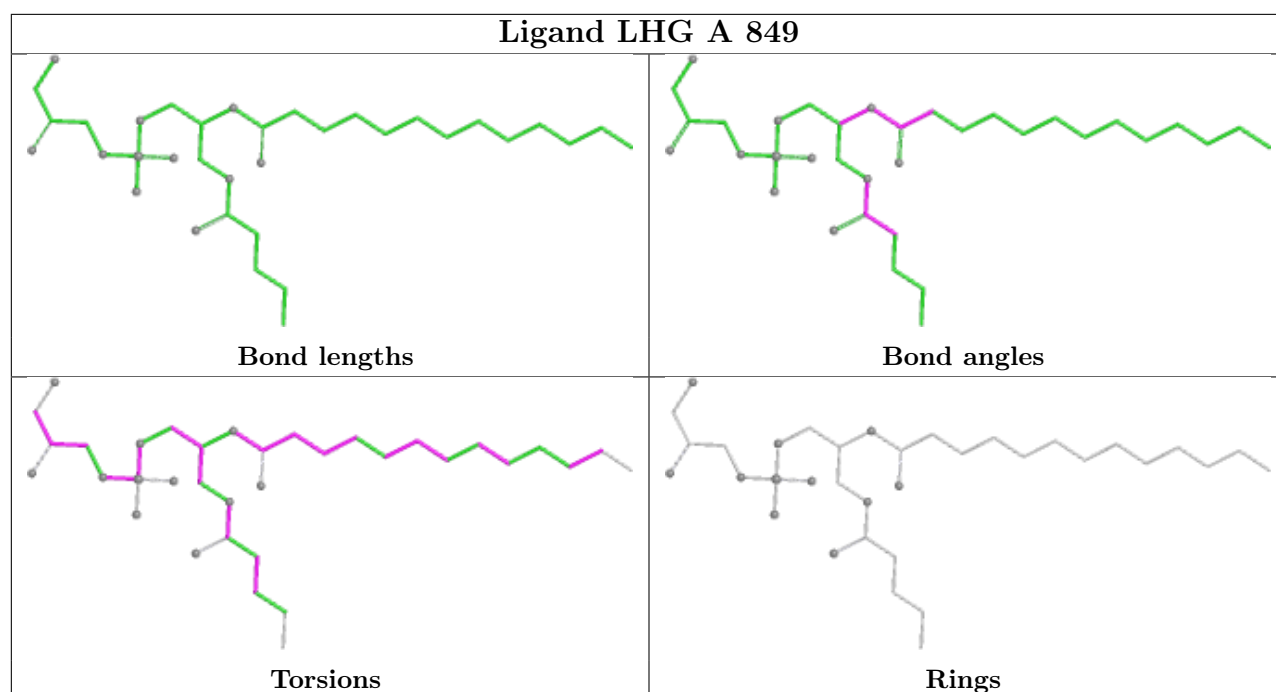


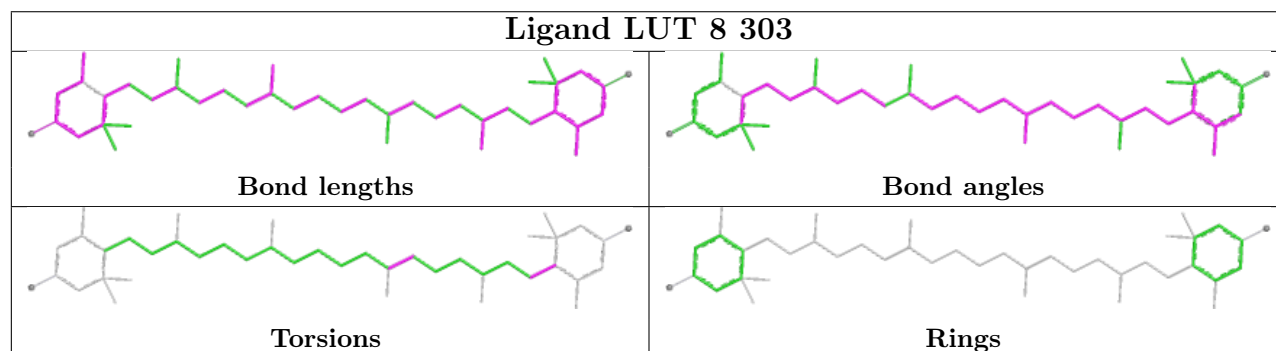
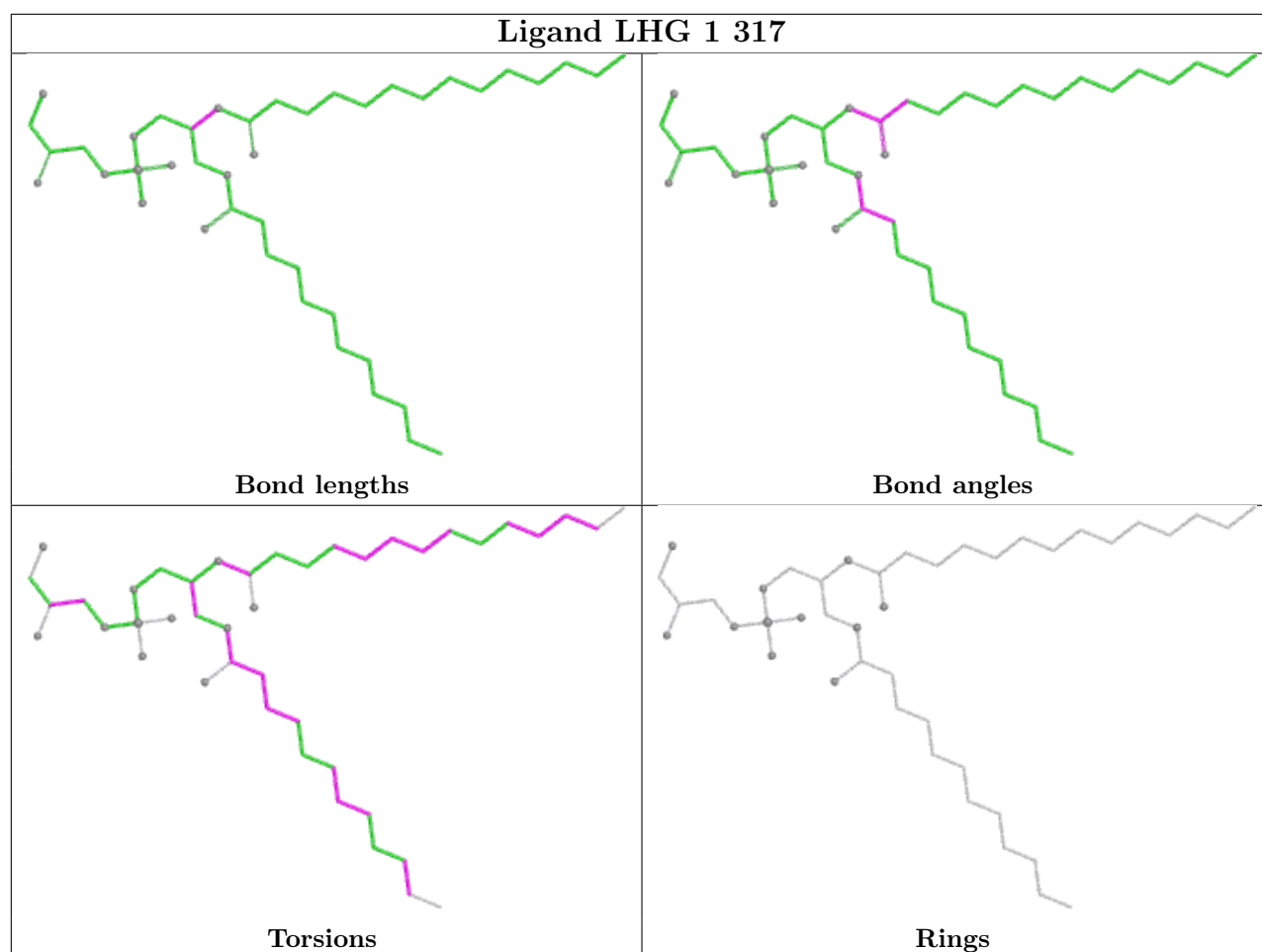
Ligand BCR B 845



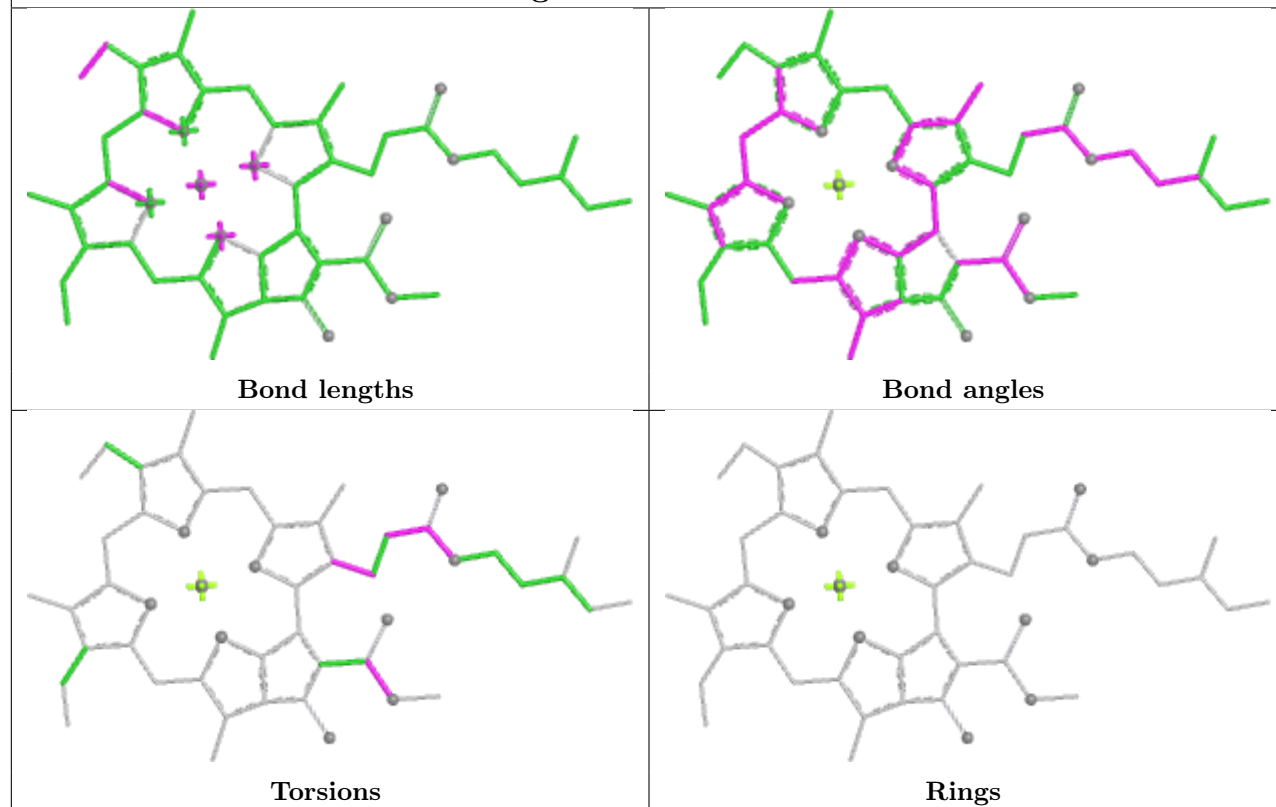




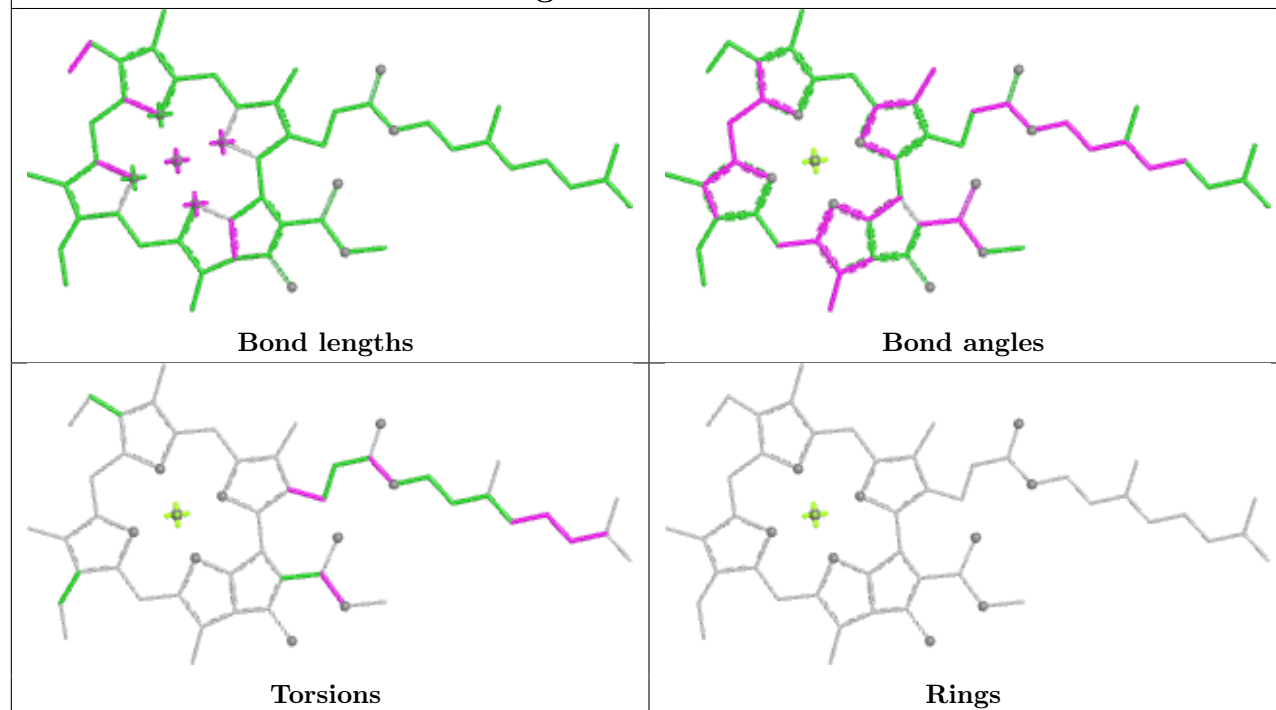




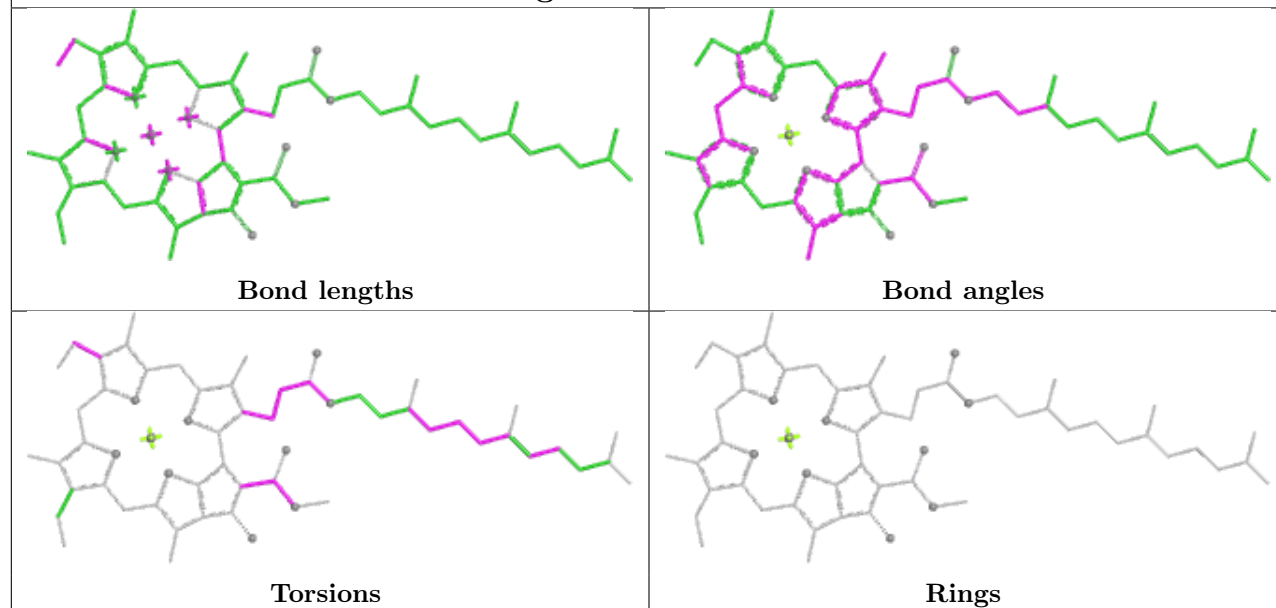
Ligand CLA A 837



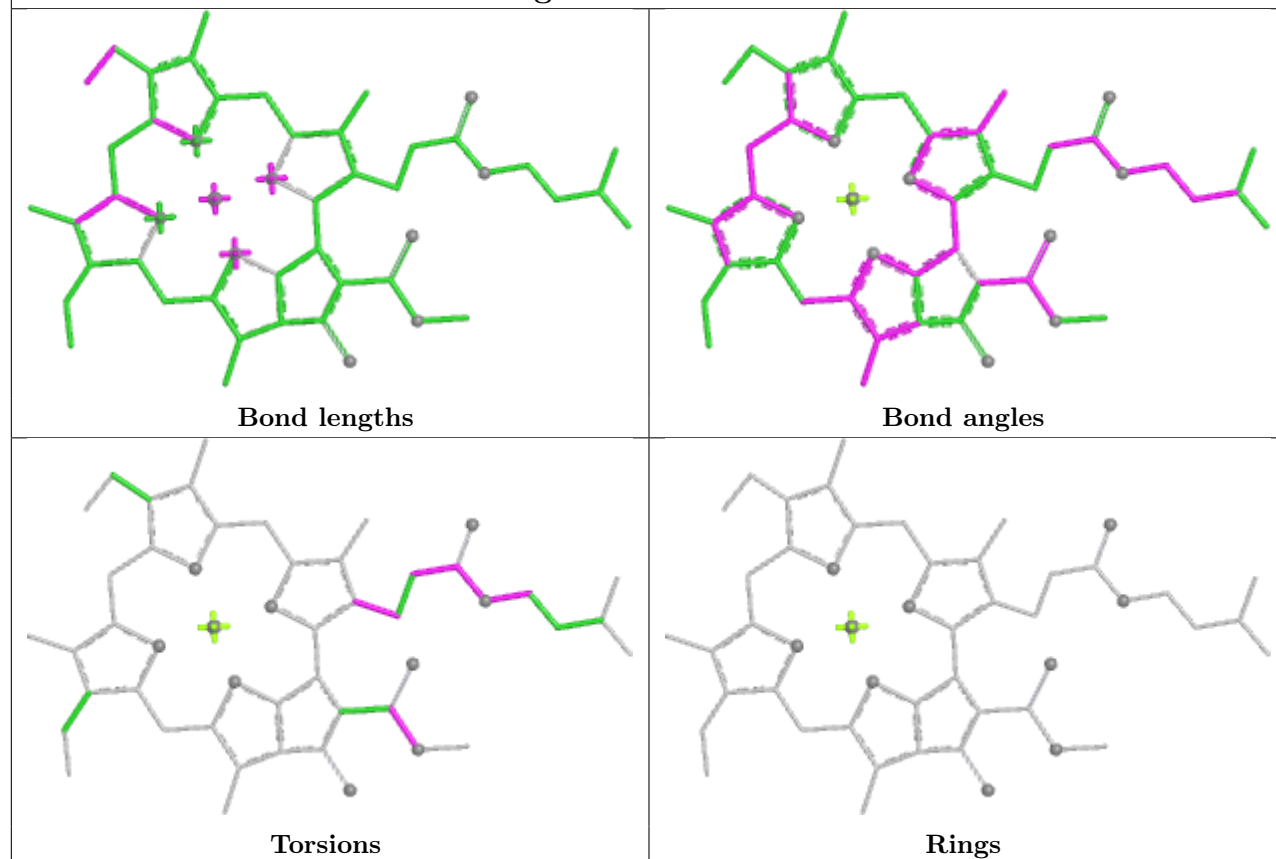
Ligand CLA 2 301

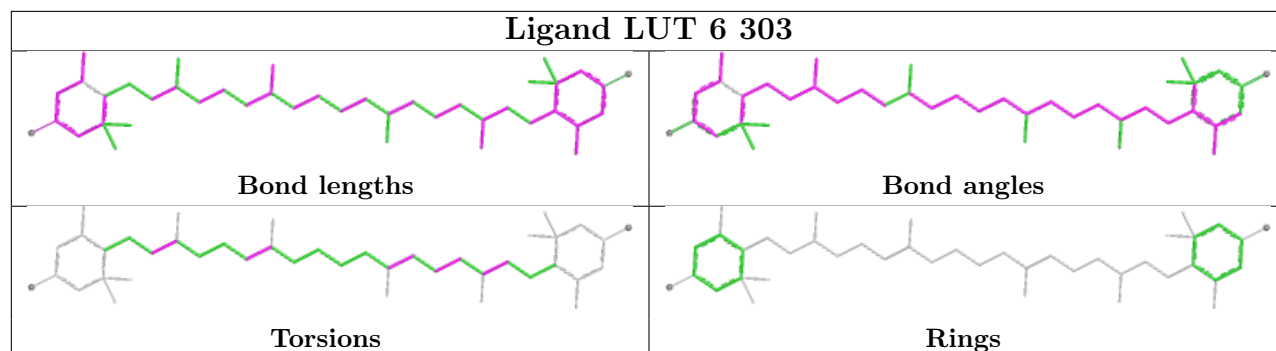
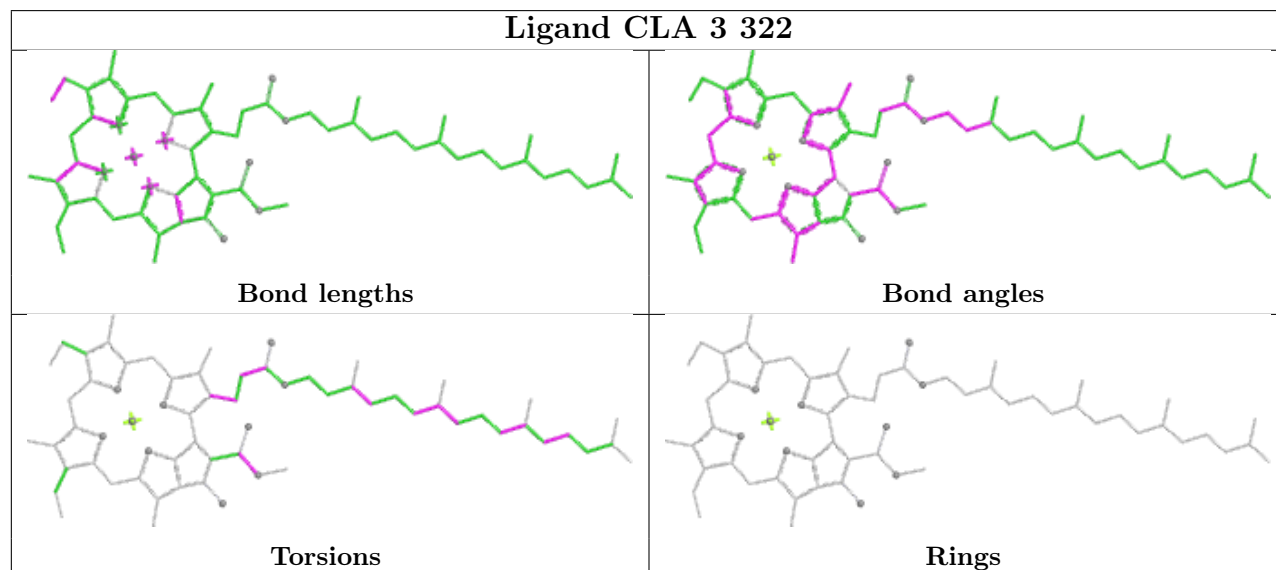
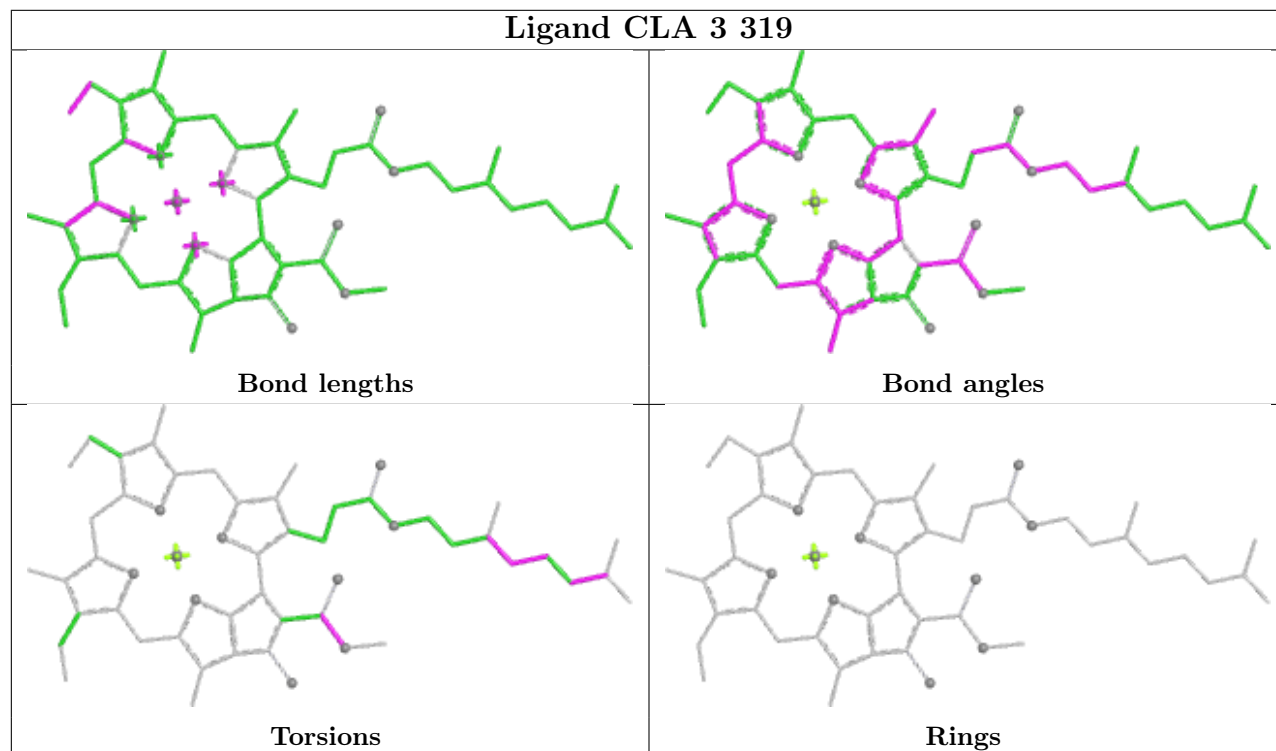


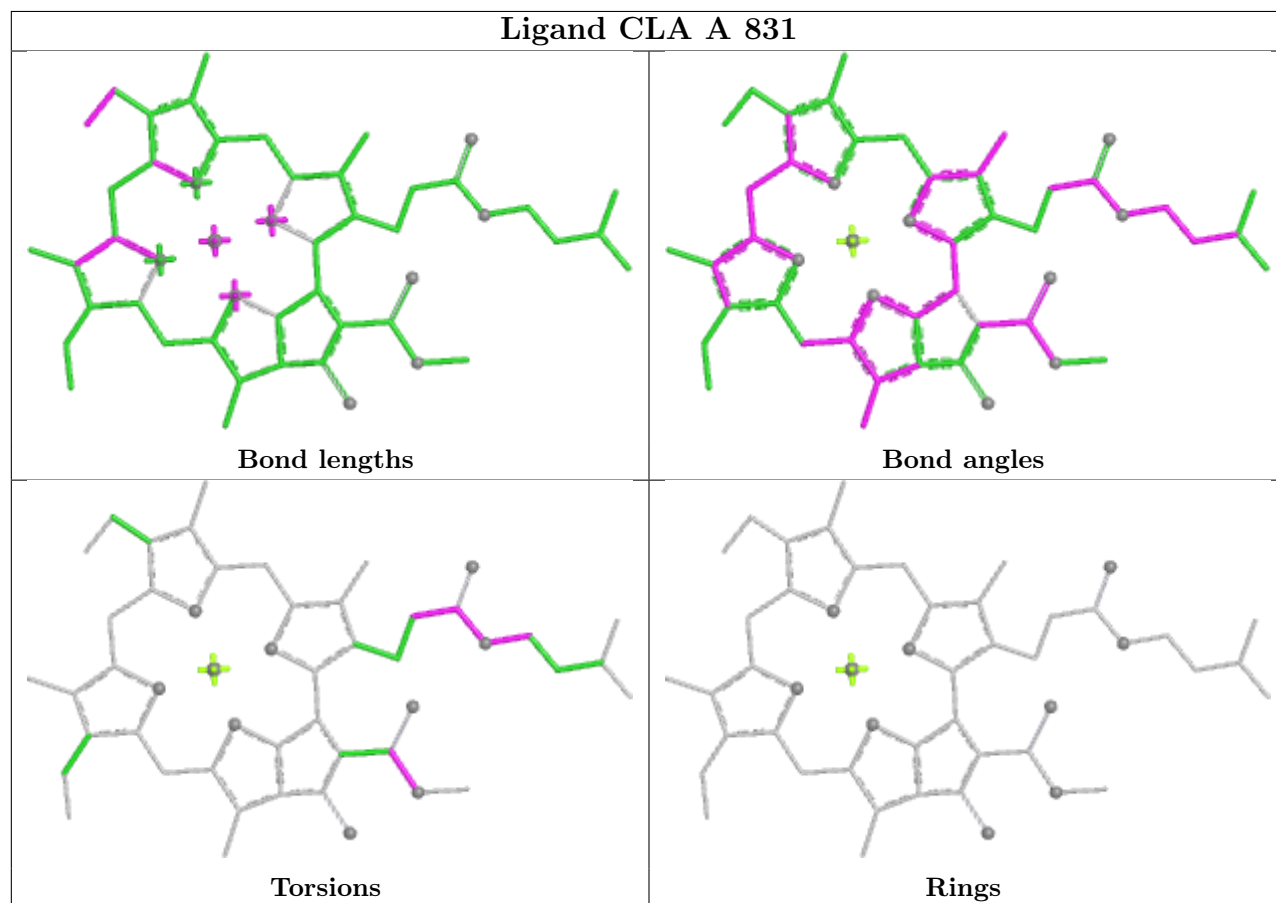
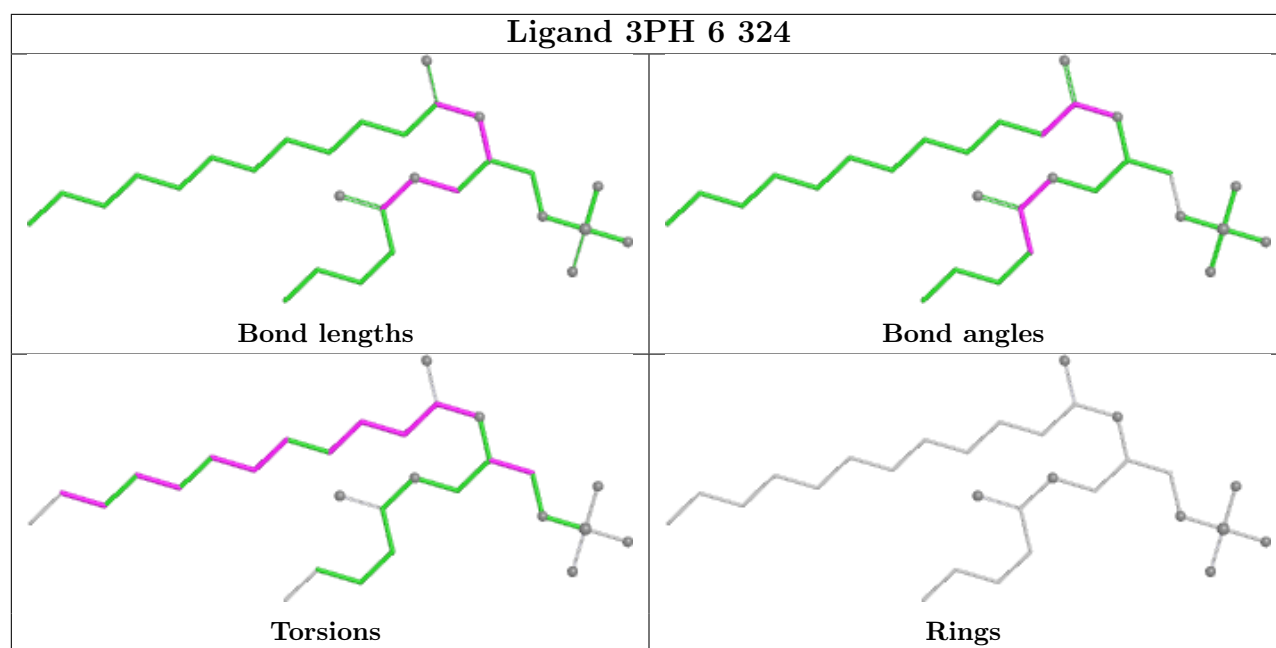
Ligand CLA 9 305



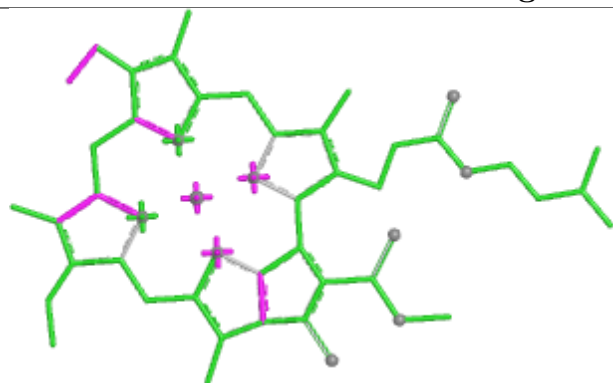
Ligand CLA Z 310



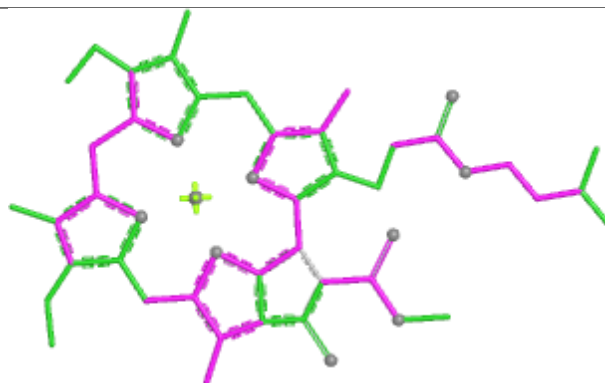
Ligand LUT 6 303**Ligand CLA 3 322****Ligand CLA 3 319**



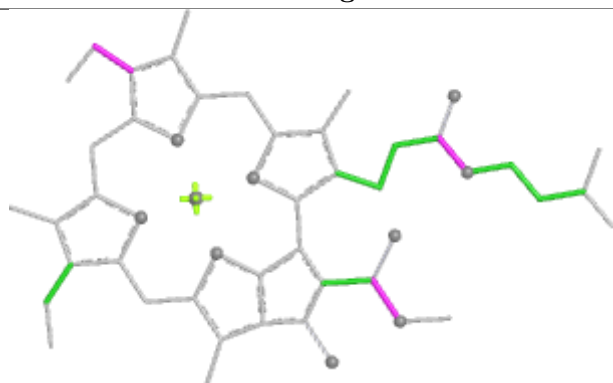
Ligand CLA 7 305



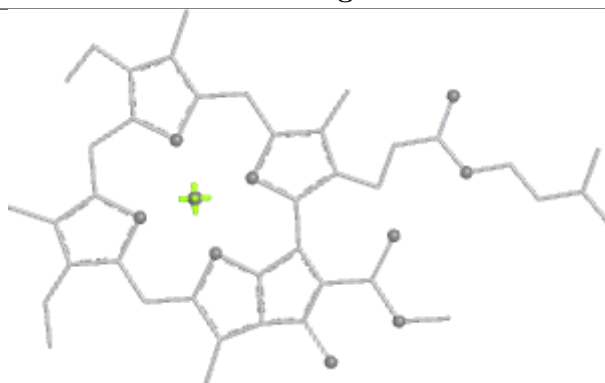
Bond lengths



Bond angles

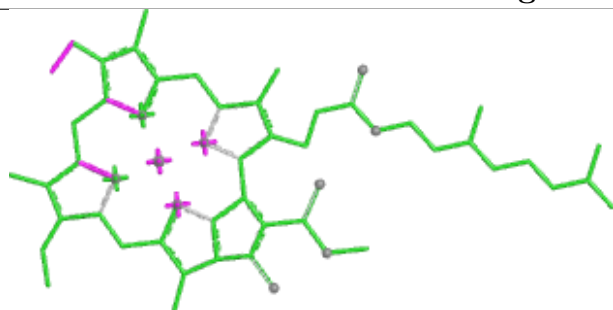


Torsions

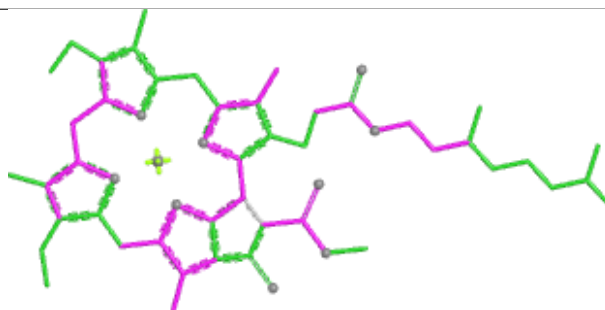


Rings

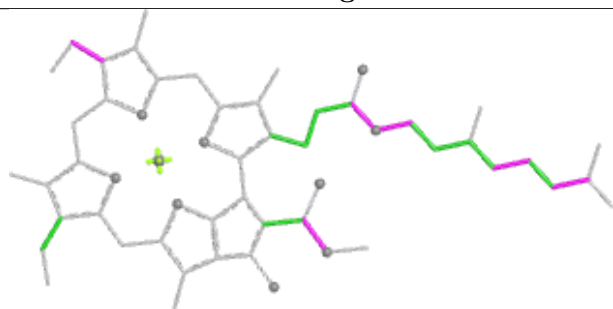
Ligand CLA 4 812



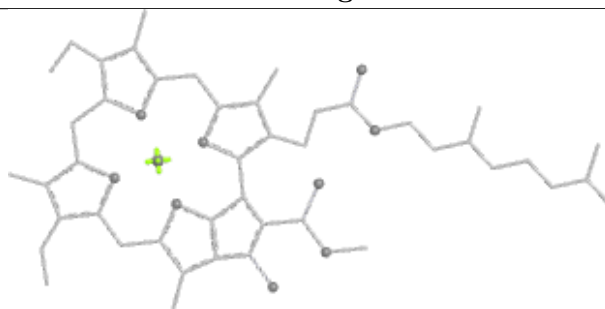
Bond lengths



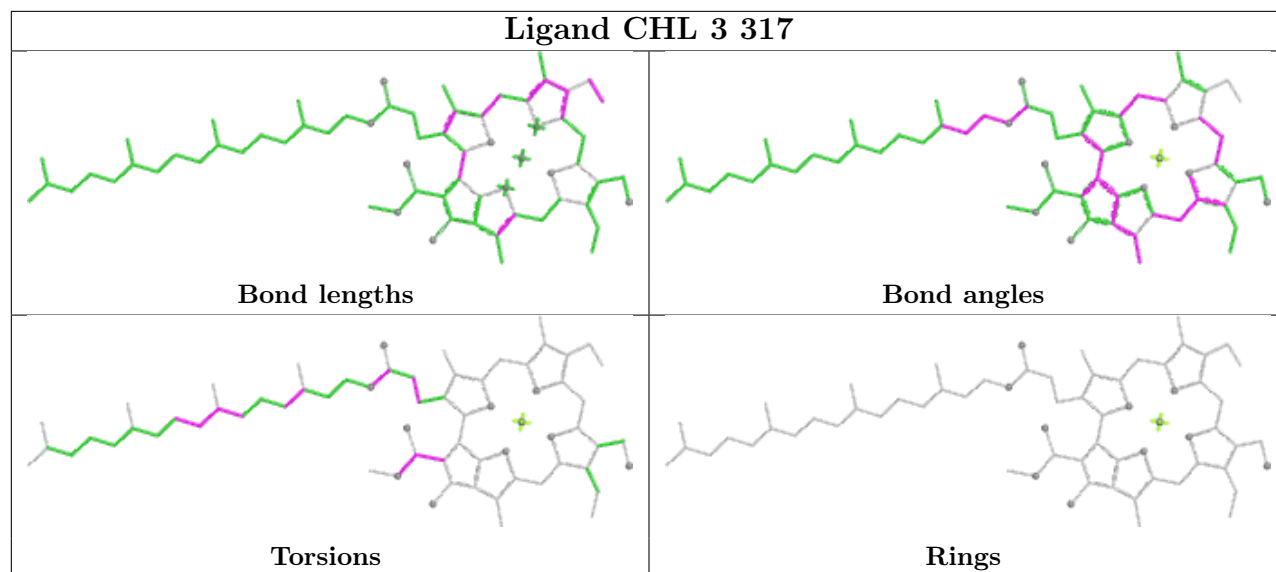
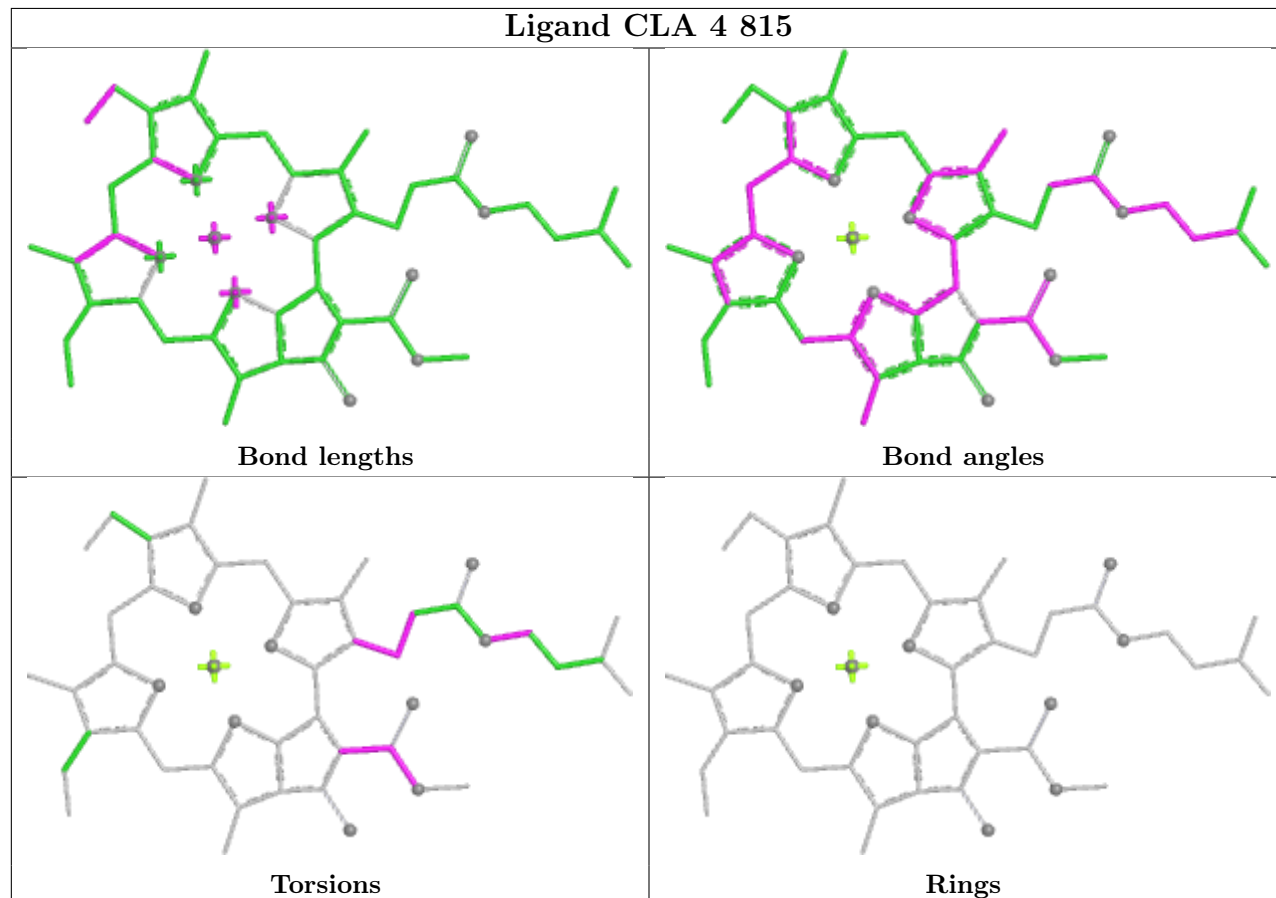
Bond angles

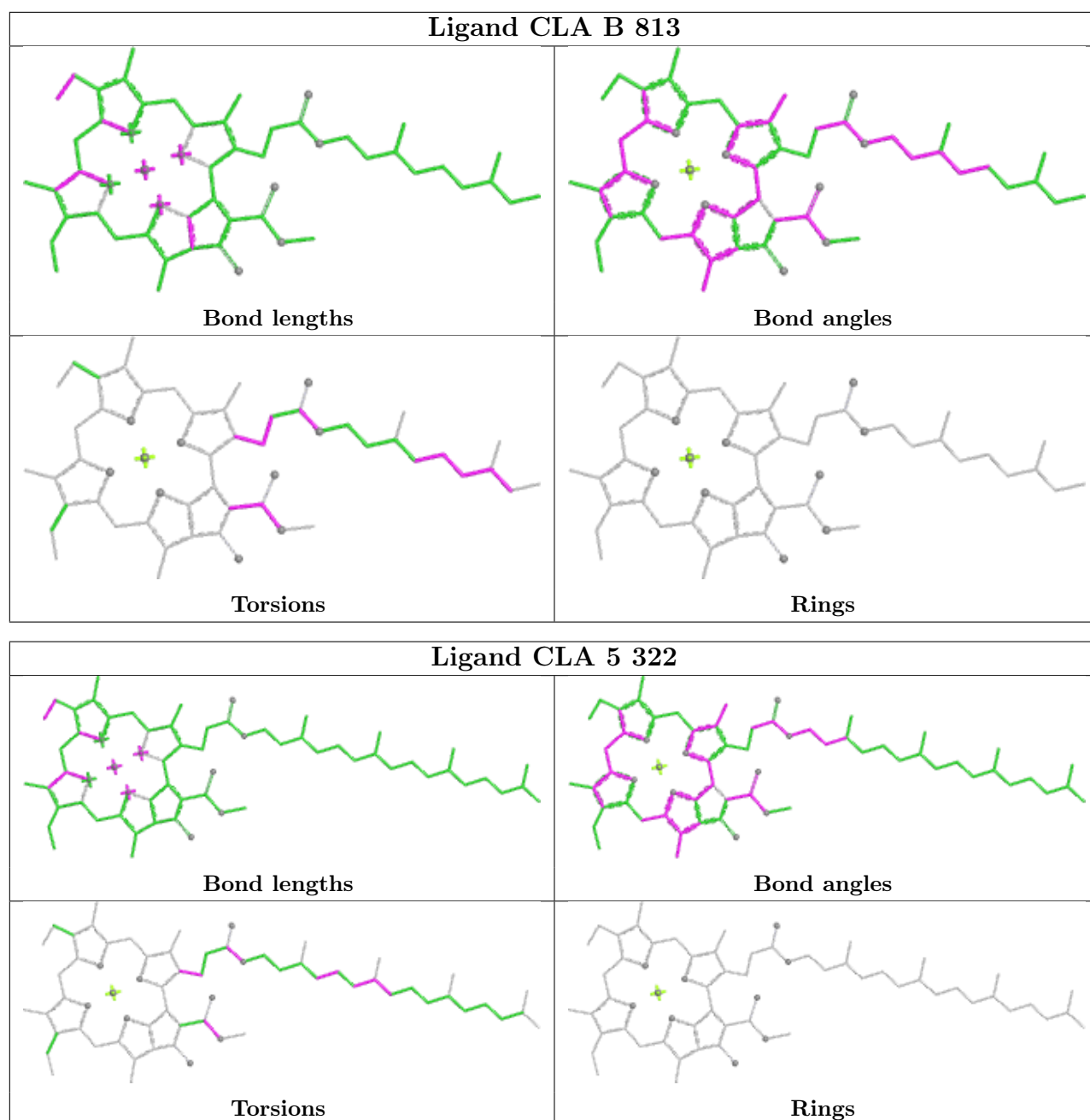


Torsions

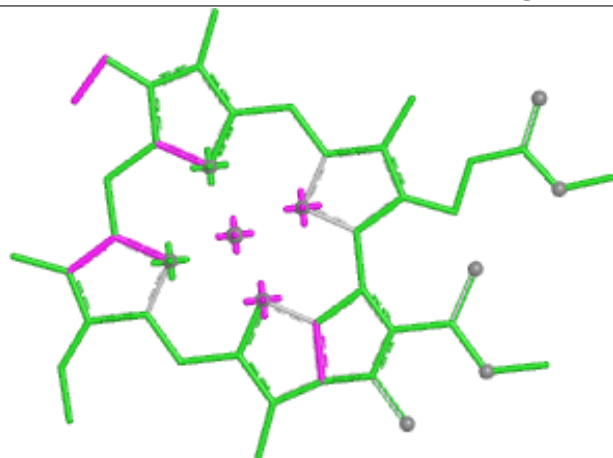


Rings

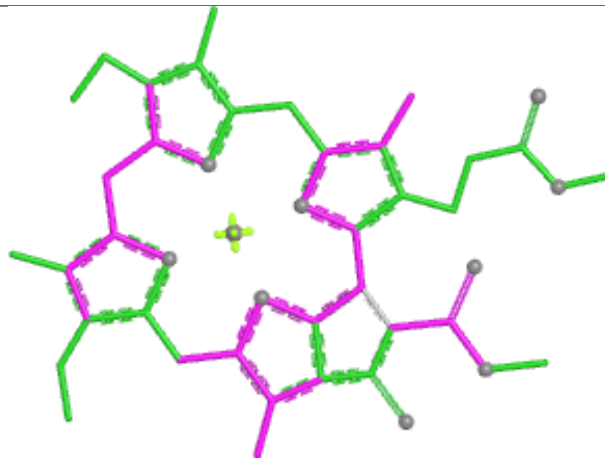
Ligand CHL 3 317**Ligand CLA 4 815**



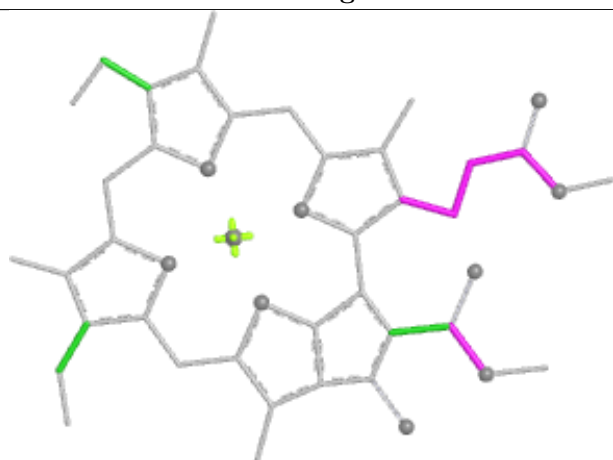
Ligand CLA 8 314



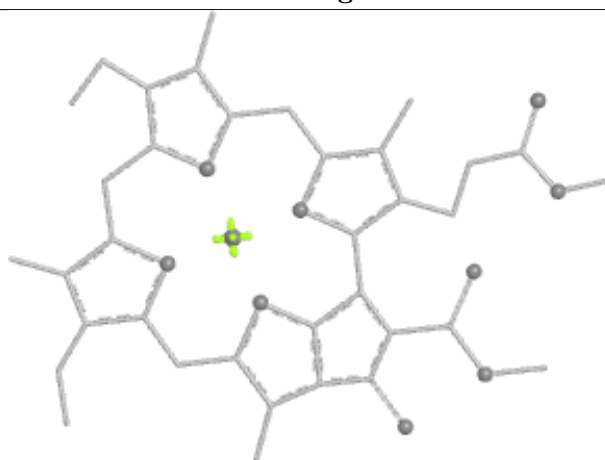
Bond lengths



Bond angles

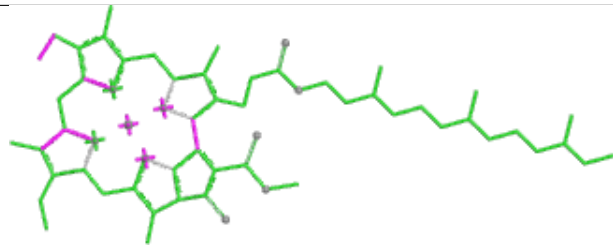


Torsions

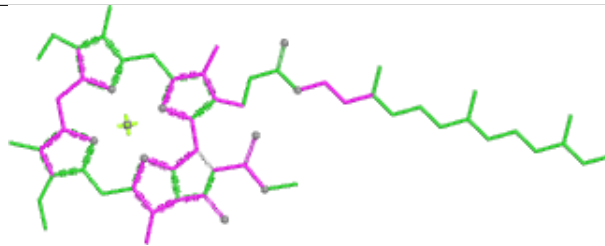


Rings

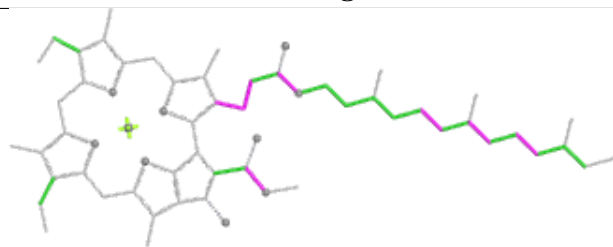
Ligand CLA 5 313



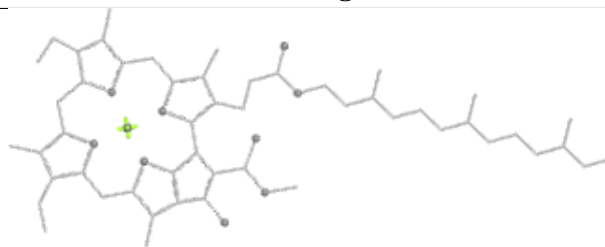
Bond lengths



Bond angles

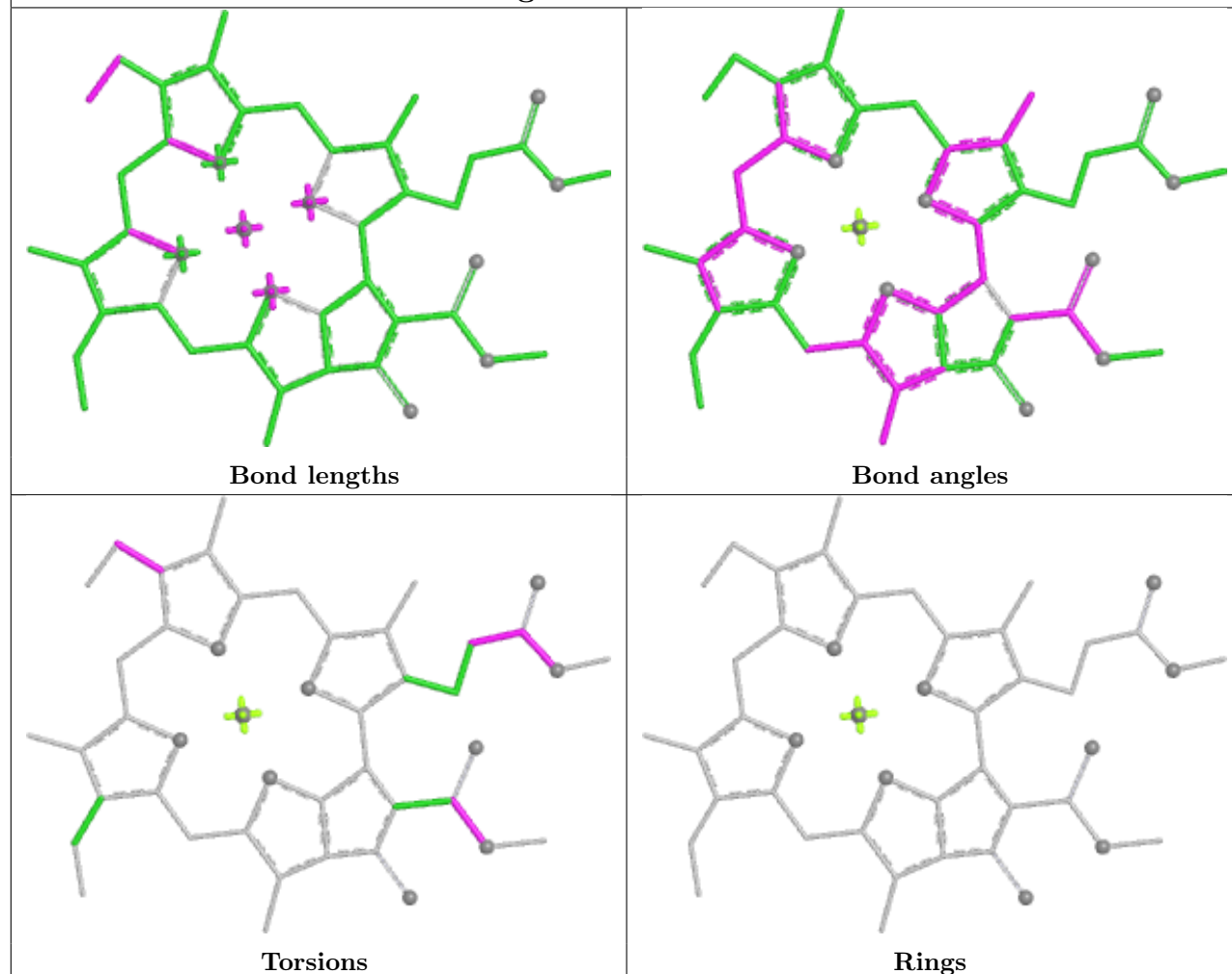


Torsions

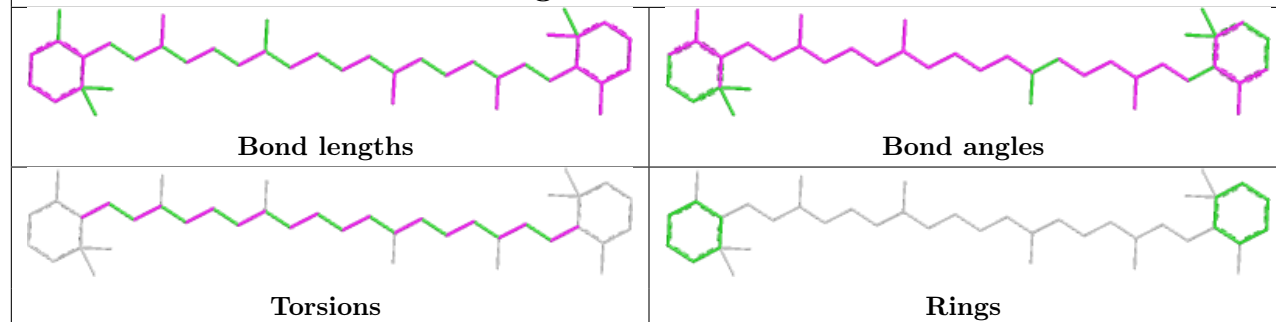


Rings

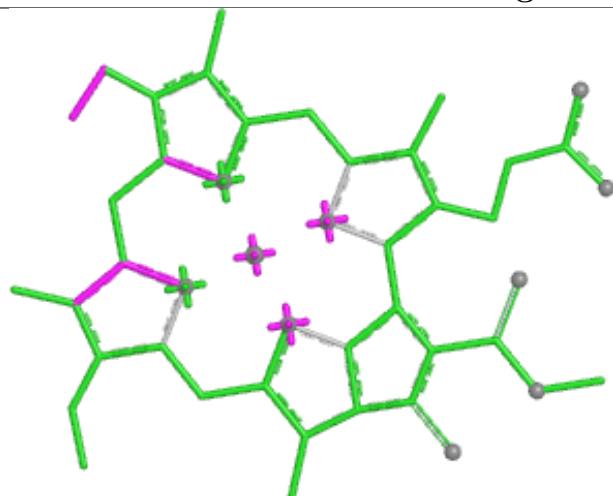
Ligand CLA 5 323



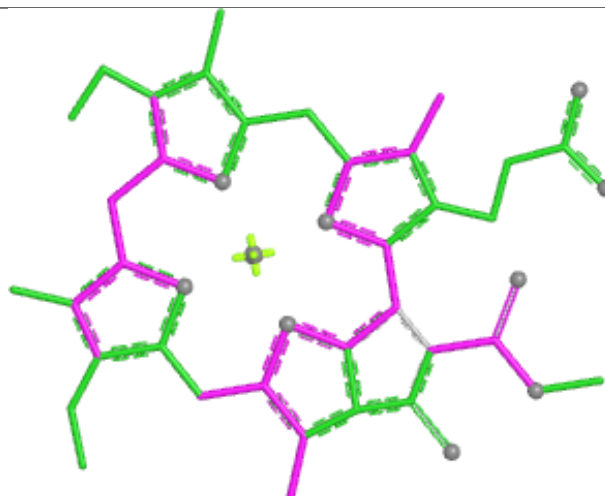
Ligand BCR 6 306



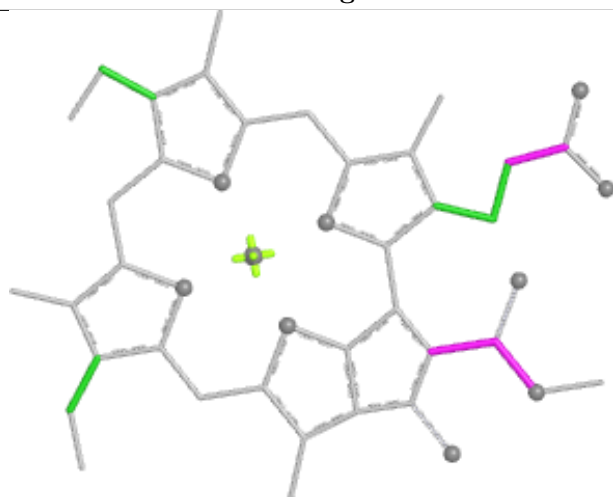
Ligand CLA Z 304



Bond lengths



Bond angles

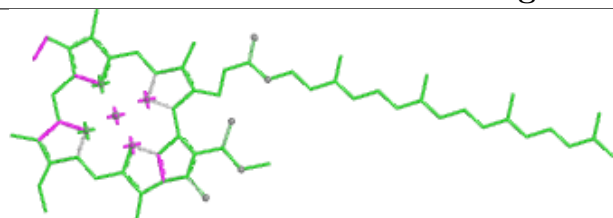


Torsions

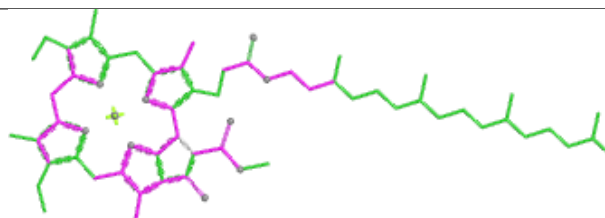


Rings

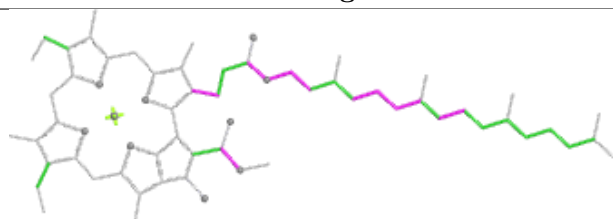
Ligand CLA 1 313



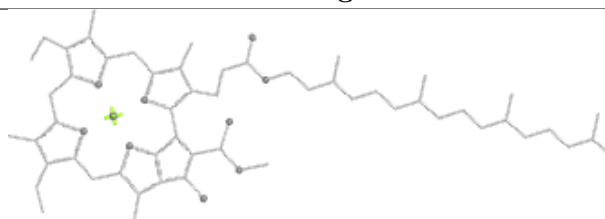
Bond lengths



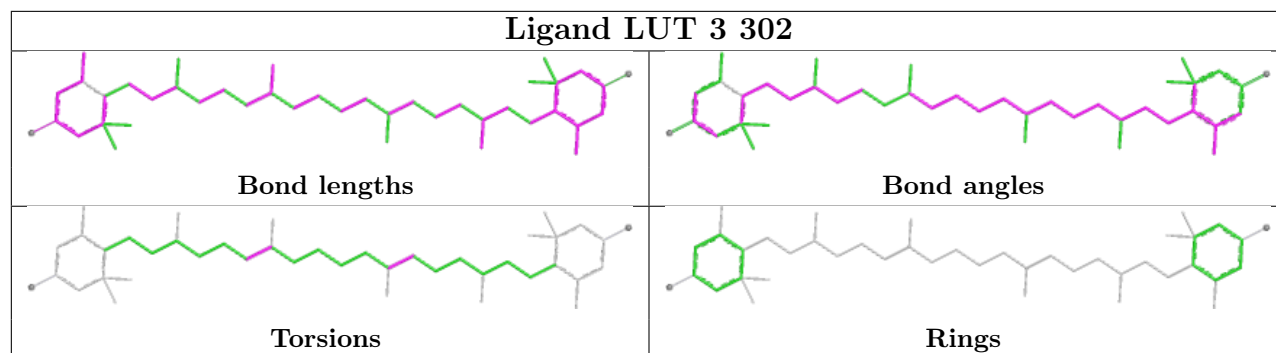
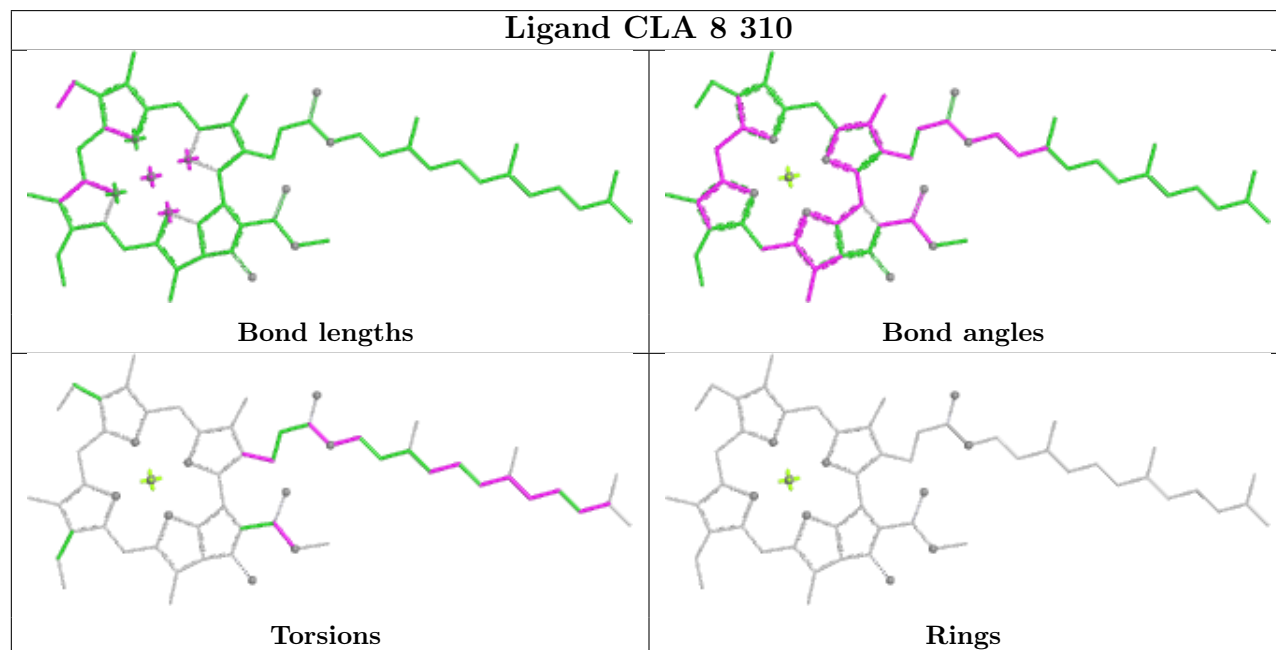
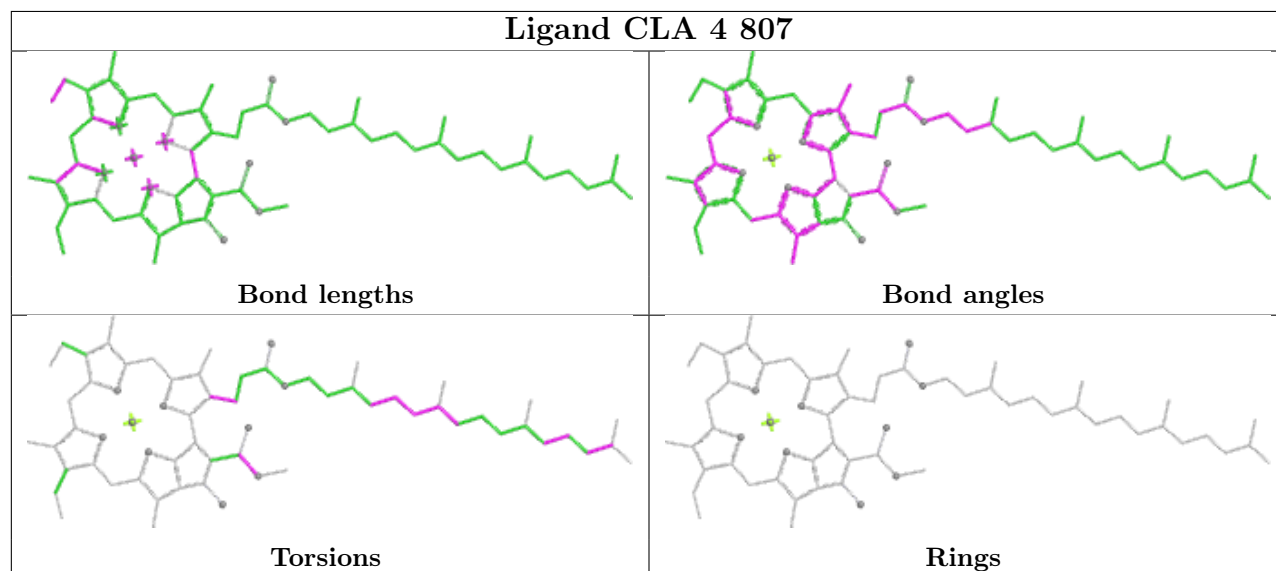
Bond angles



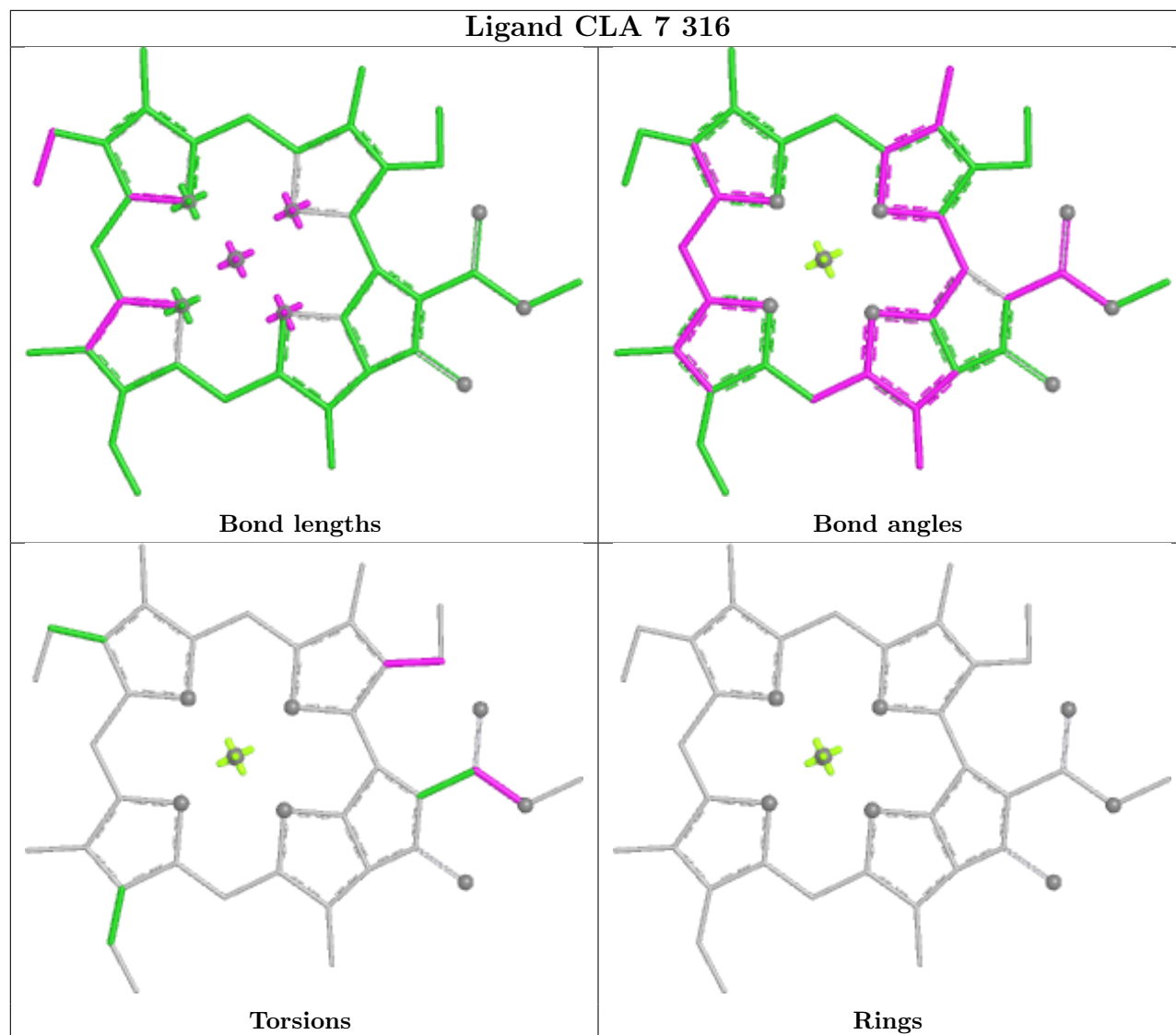
Torsions



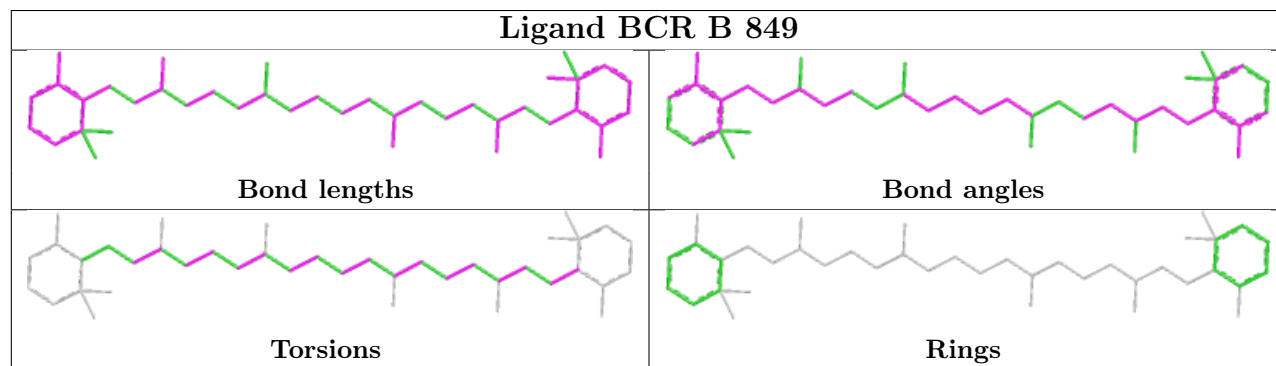
Rings

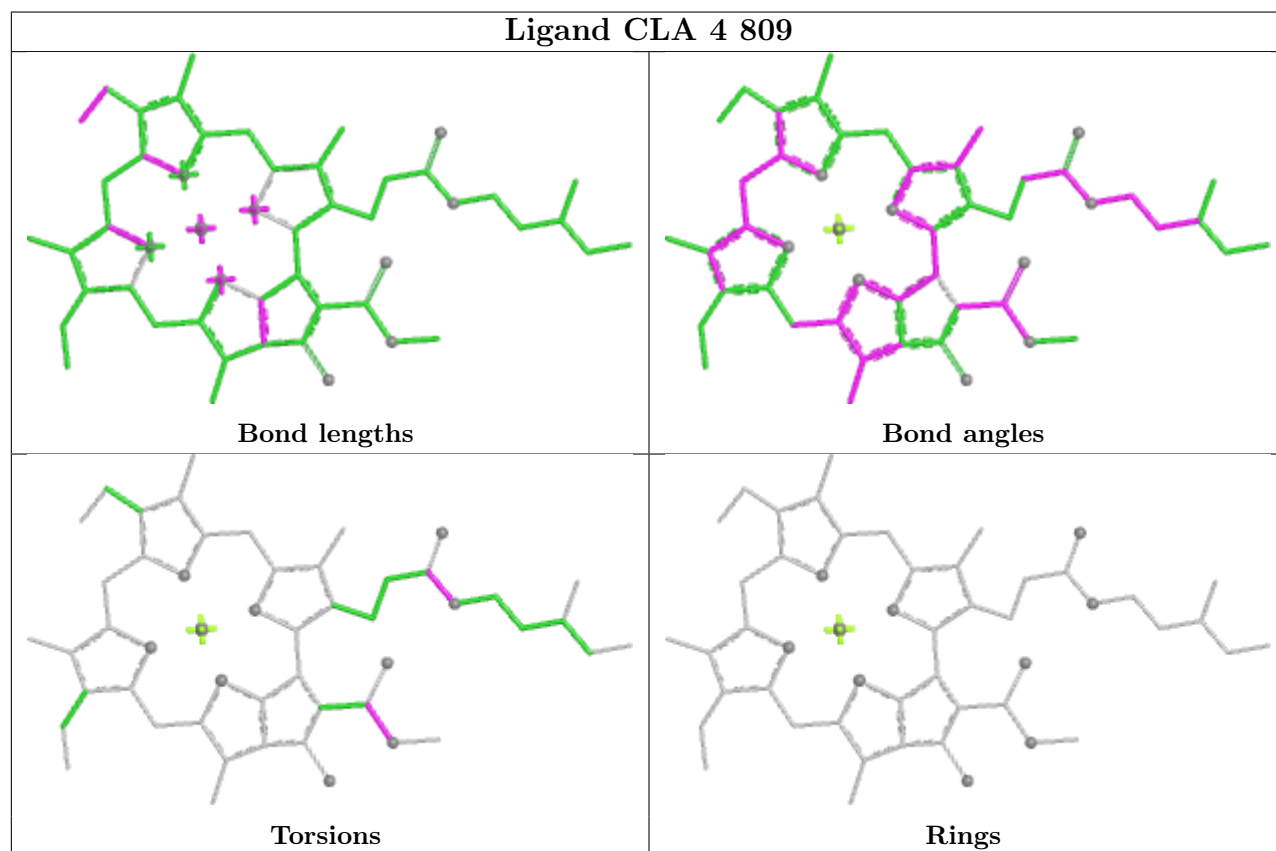
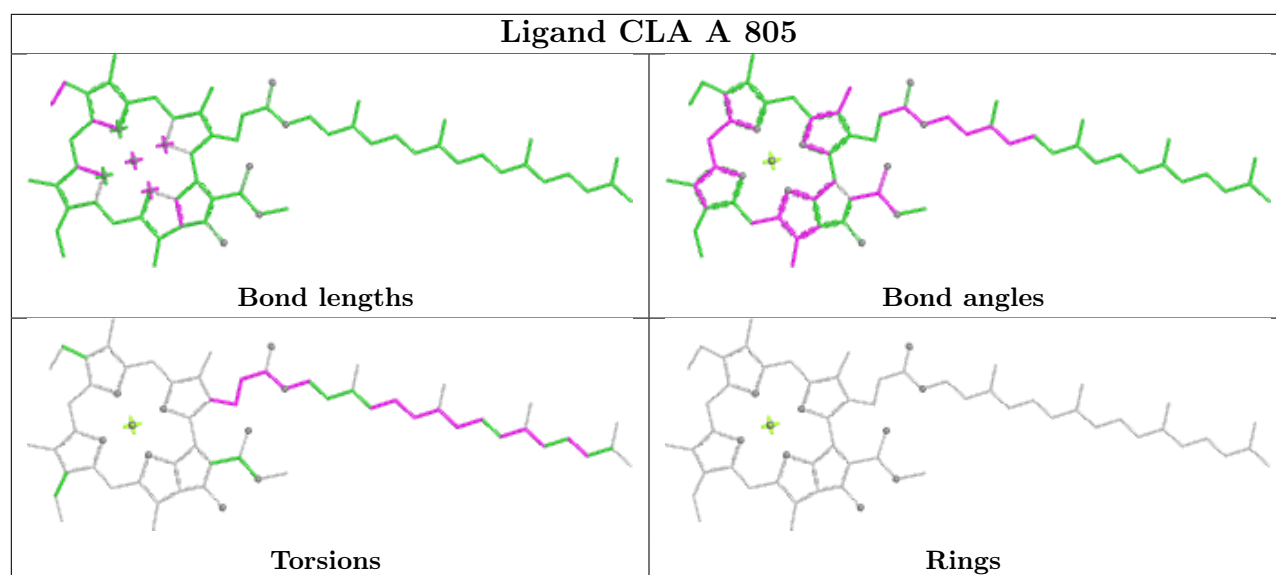
Ligand LUT 3 302**Ligand CLA 8 310****Ligand CLA 4 807**

Ligand CLA 7 316

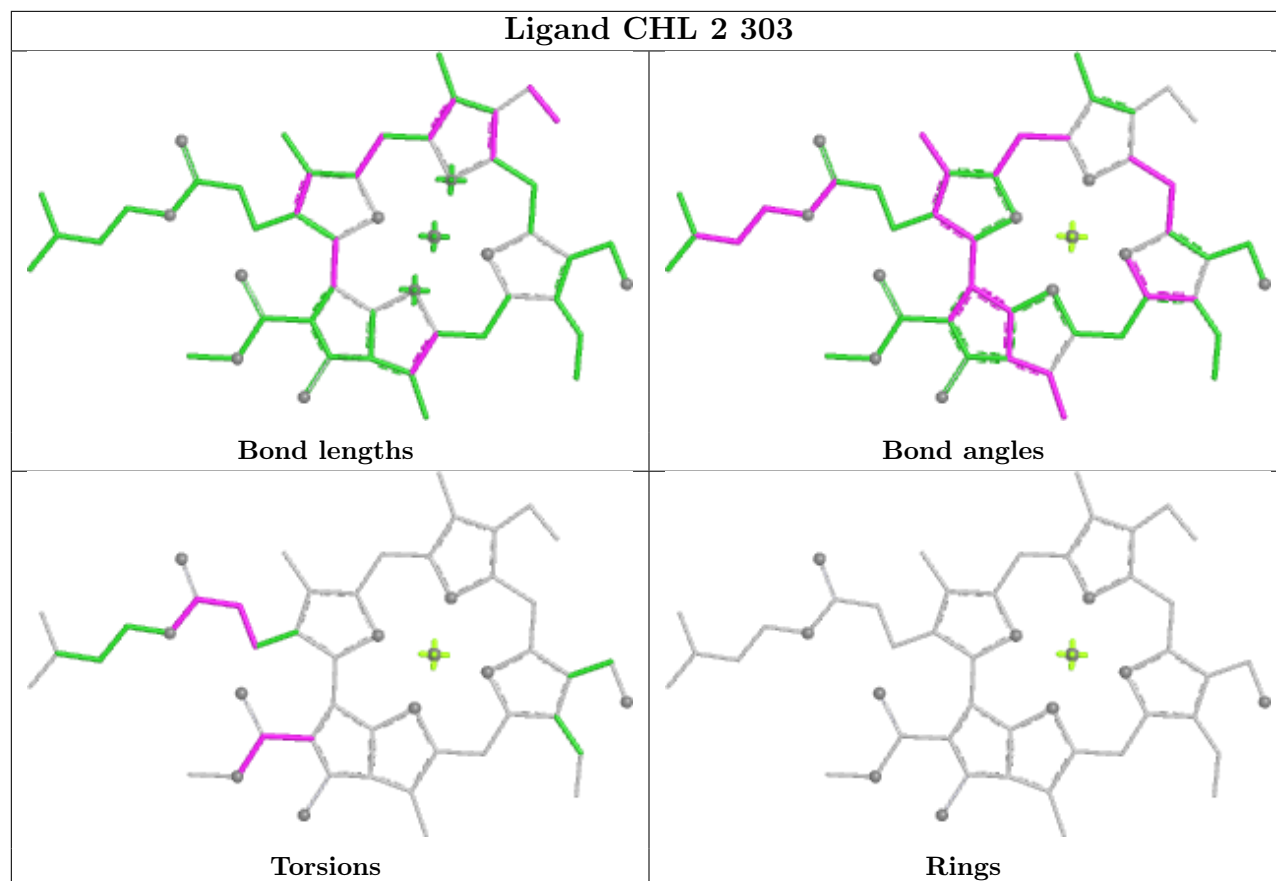


Ligand BCR B 849

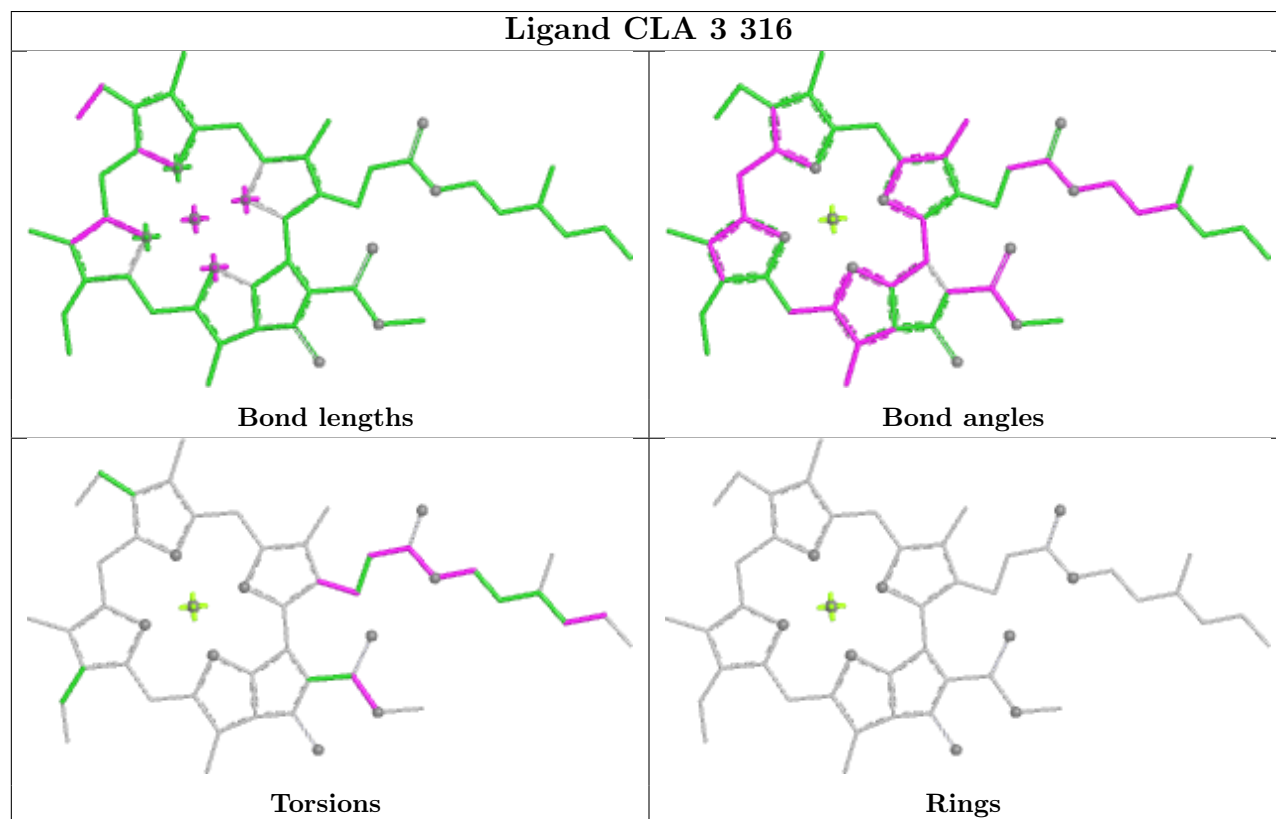


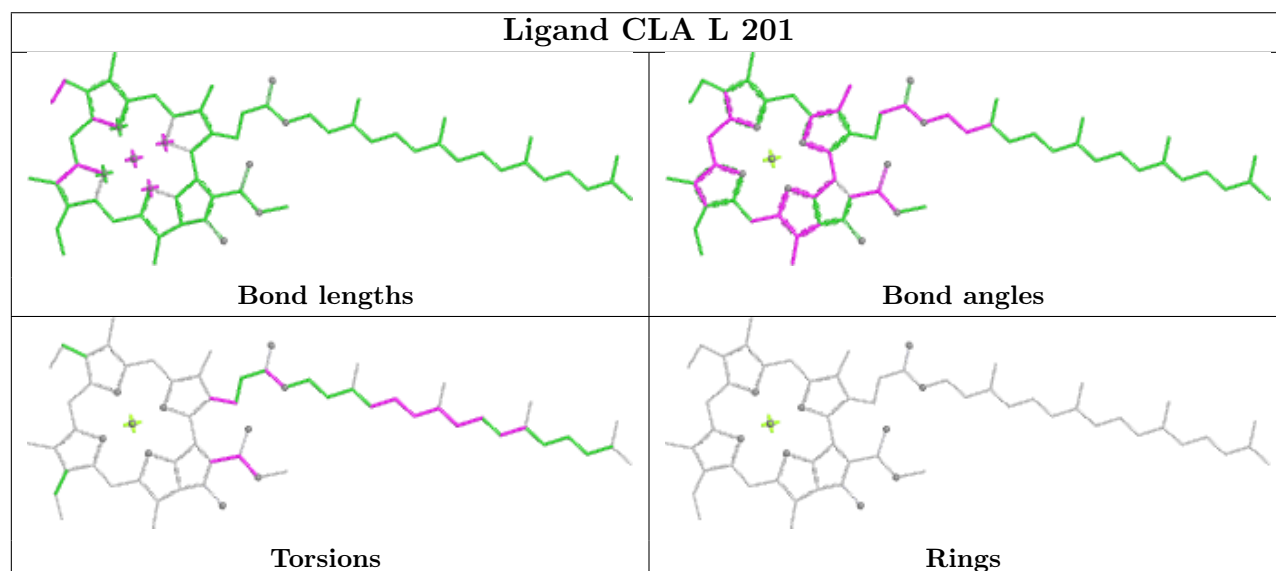
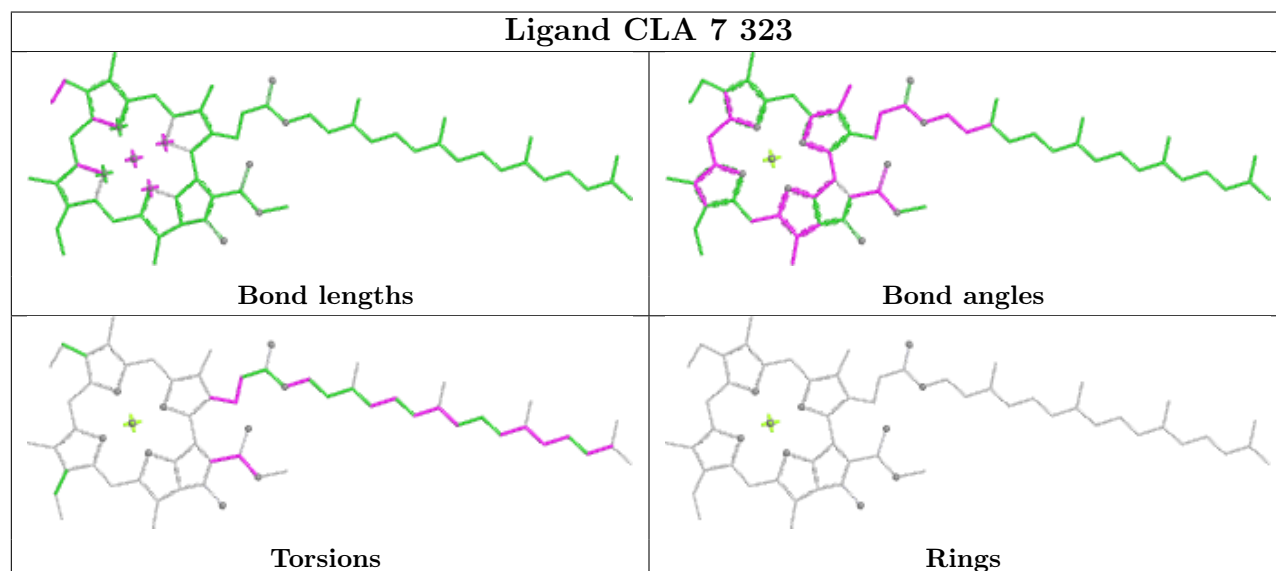
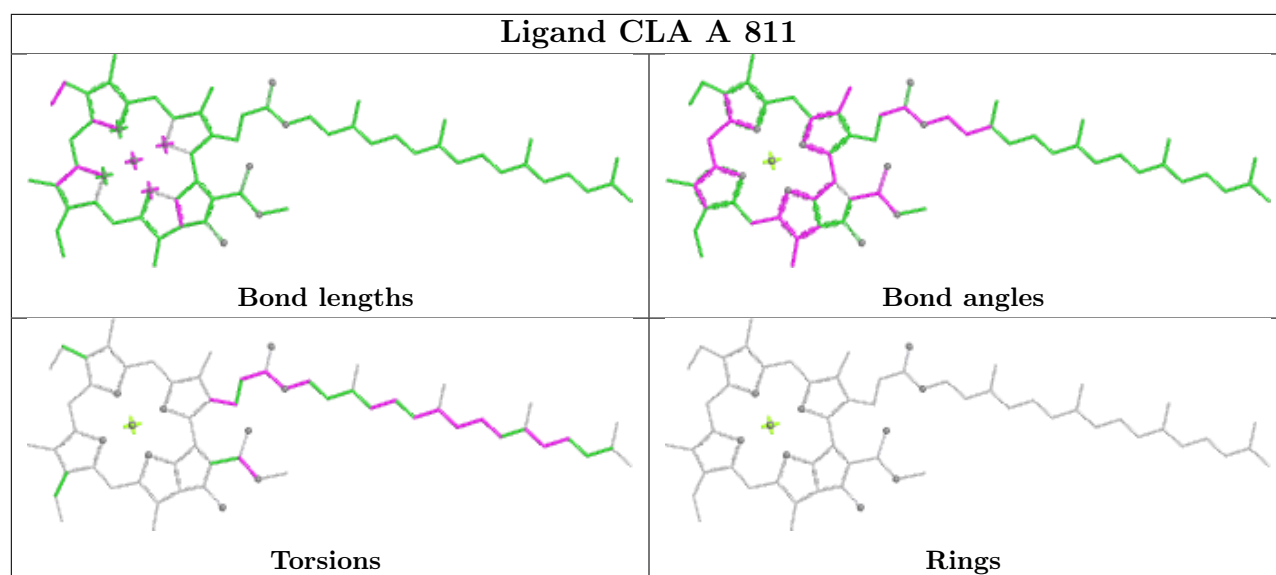


Ligand CHL 2 303

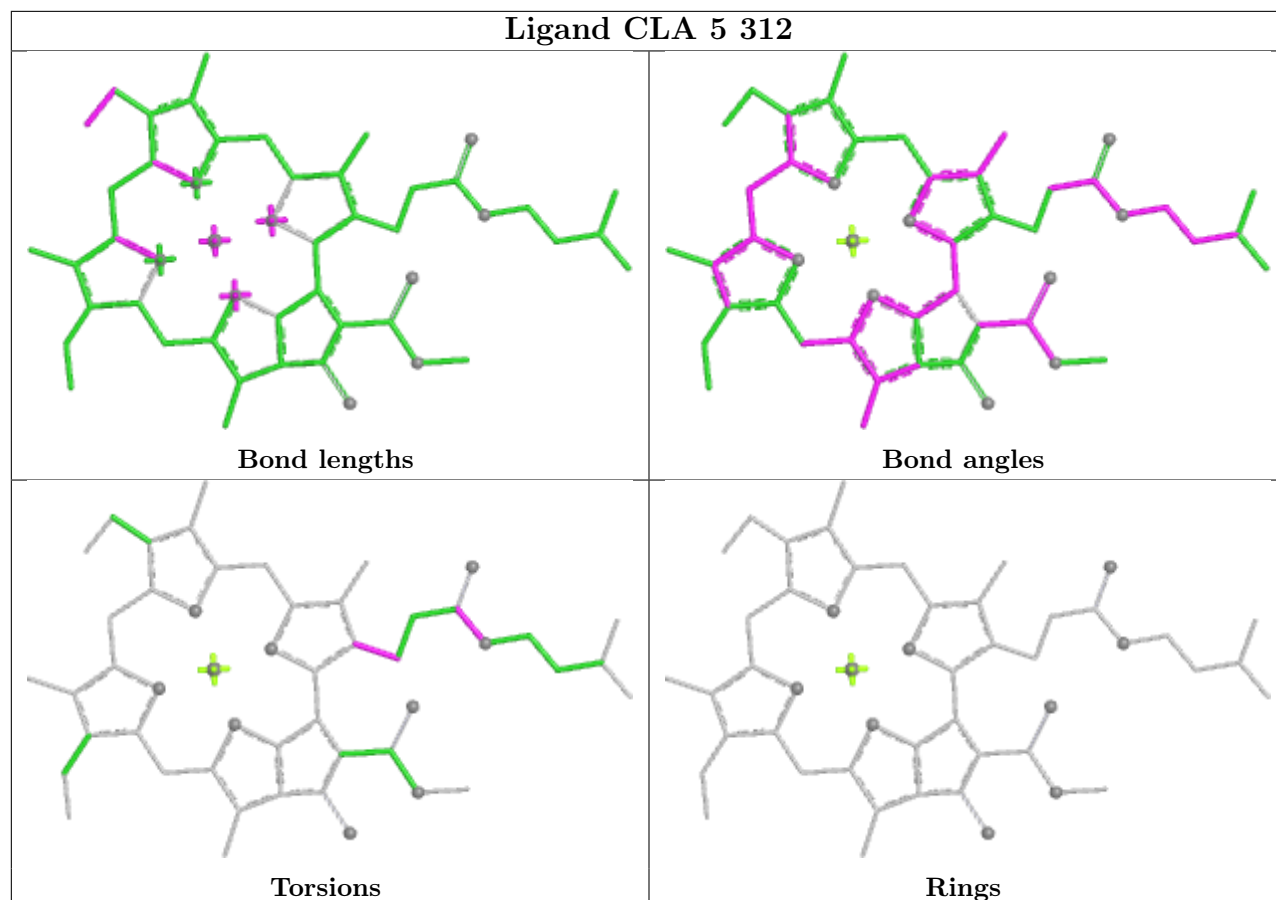


Ligand CLA 3 316

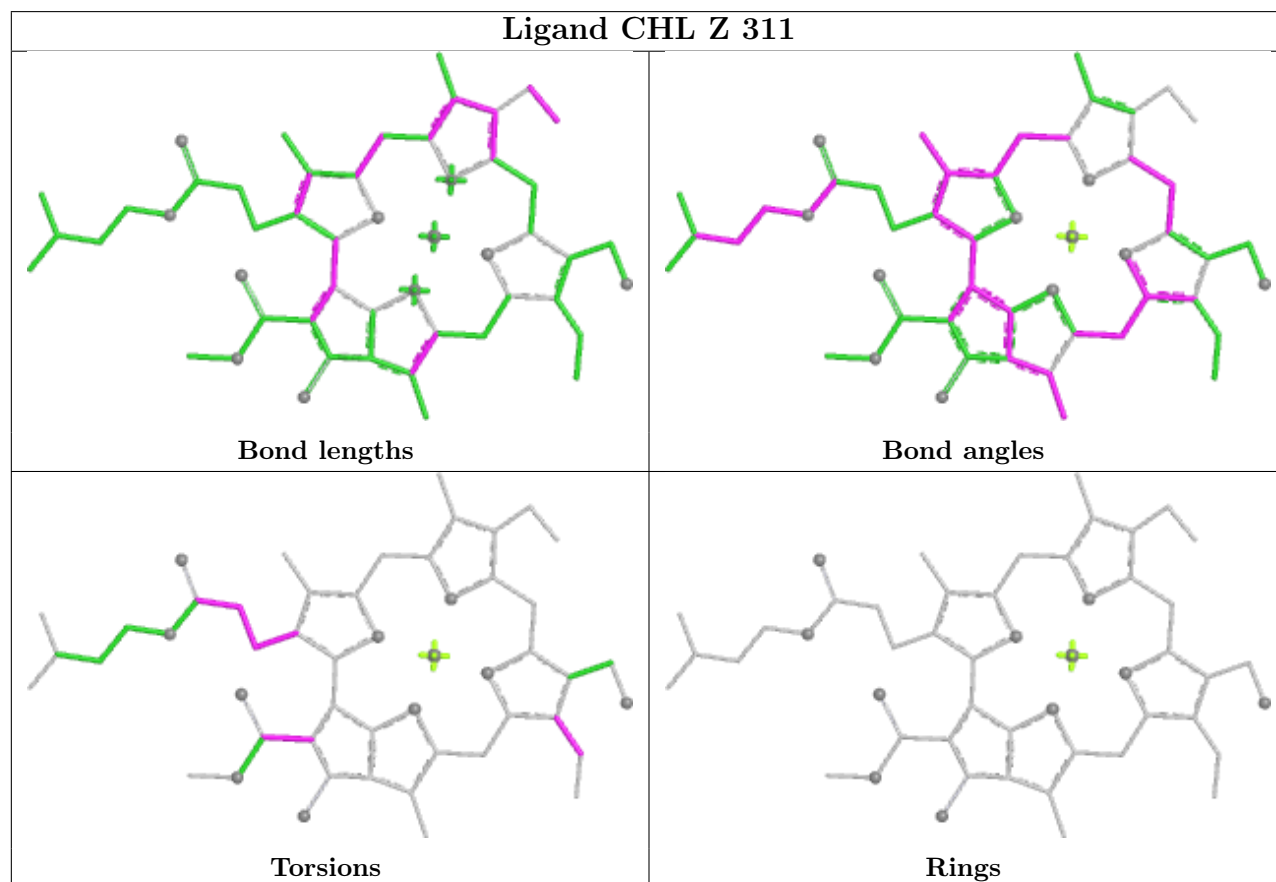


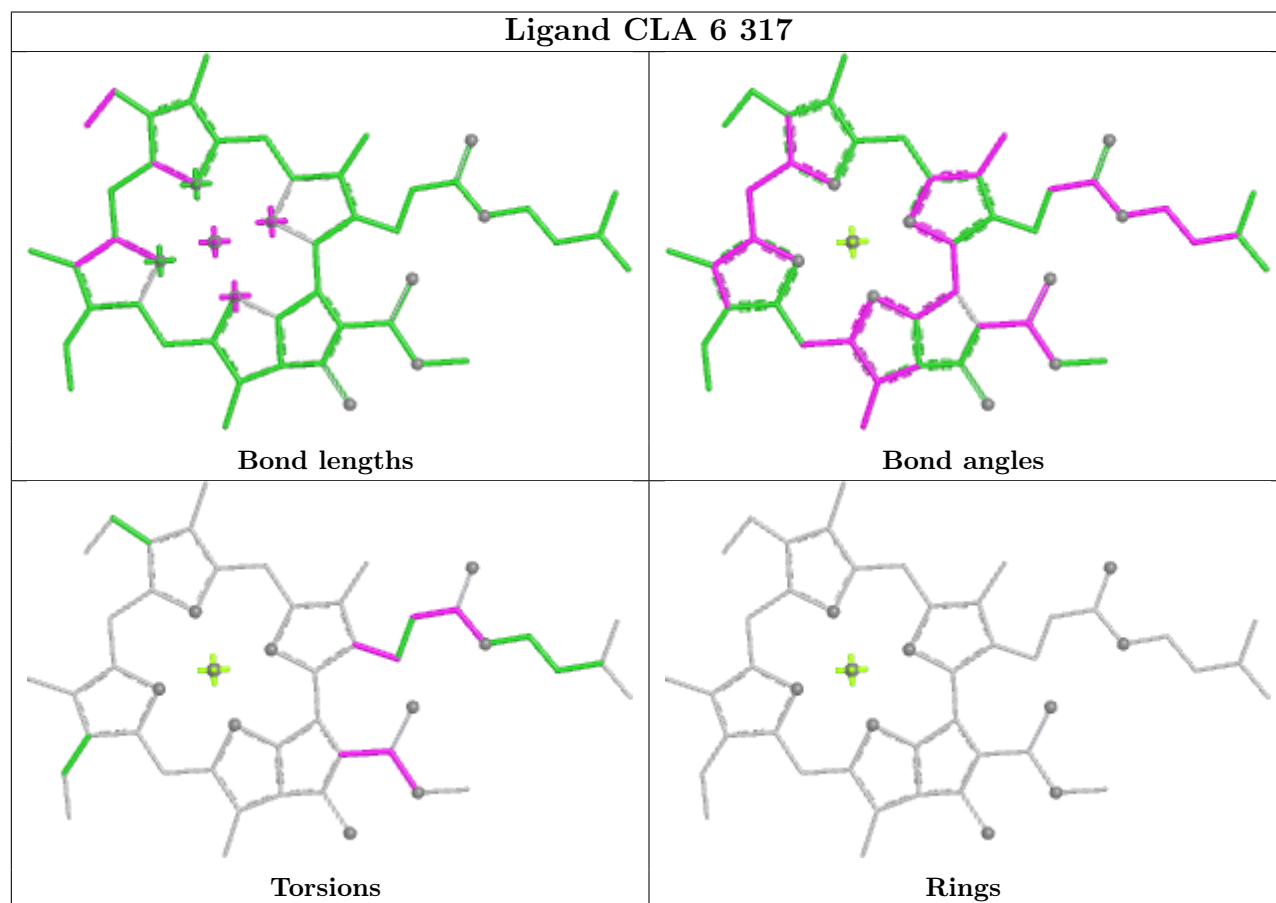
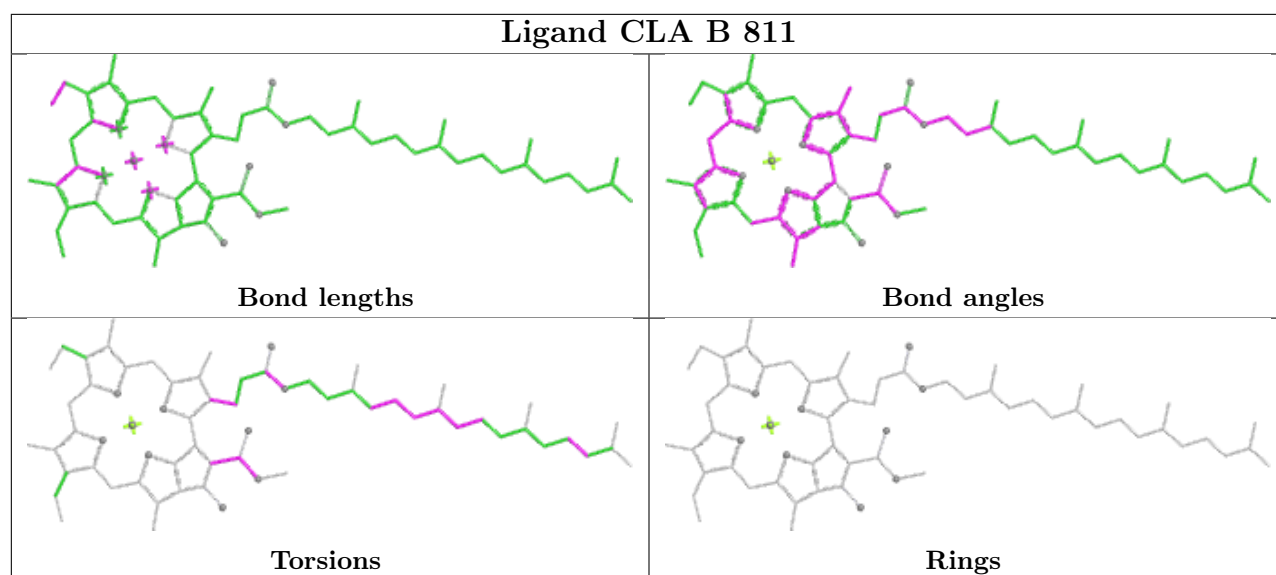


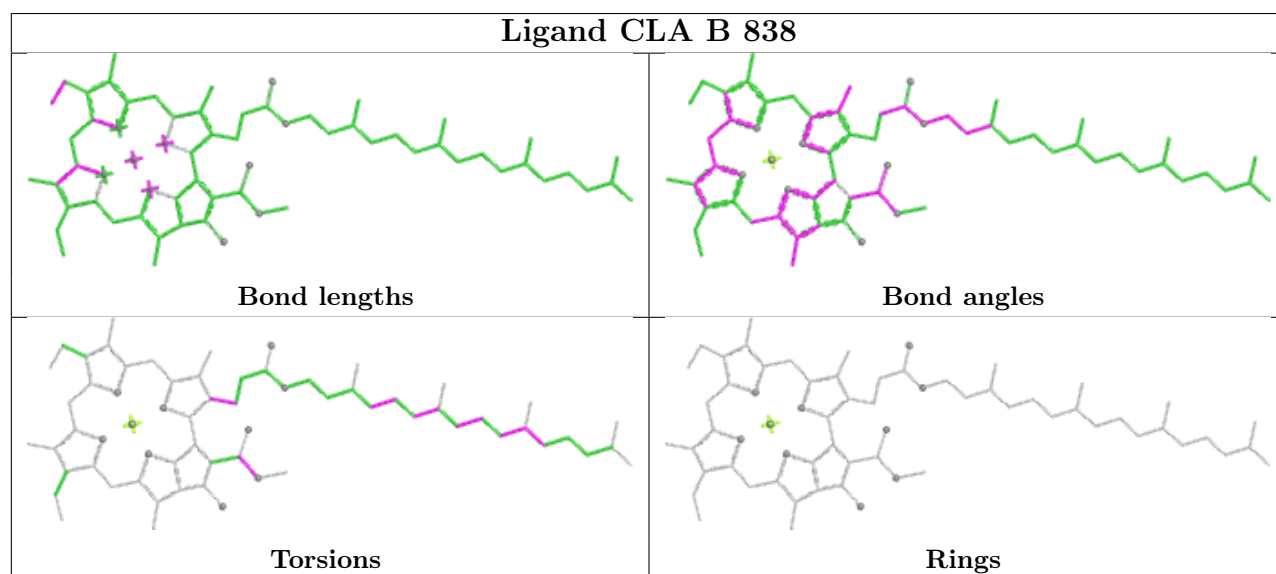
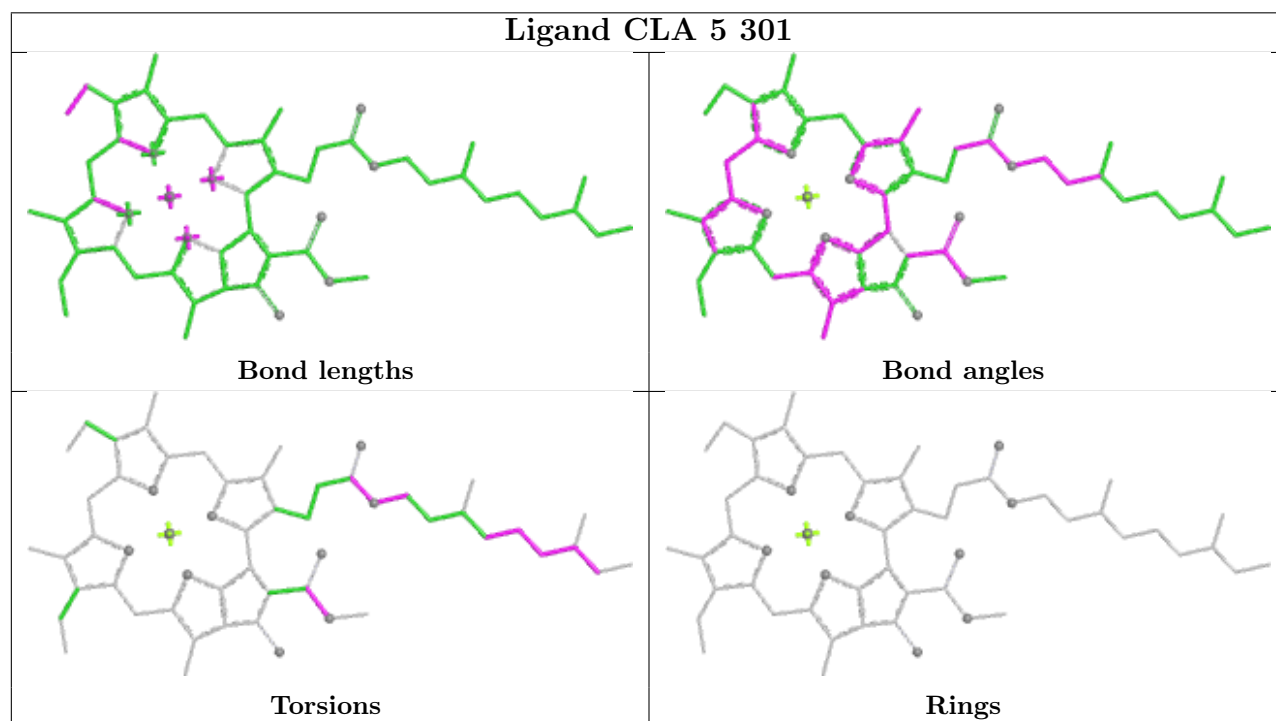
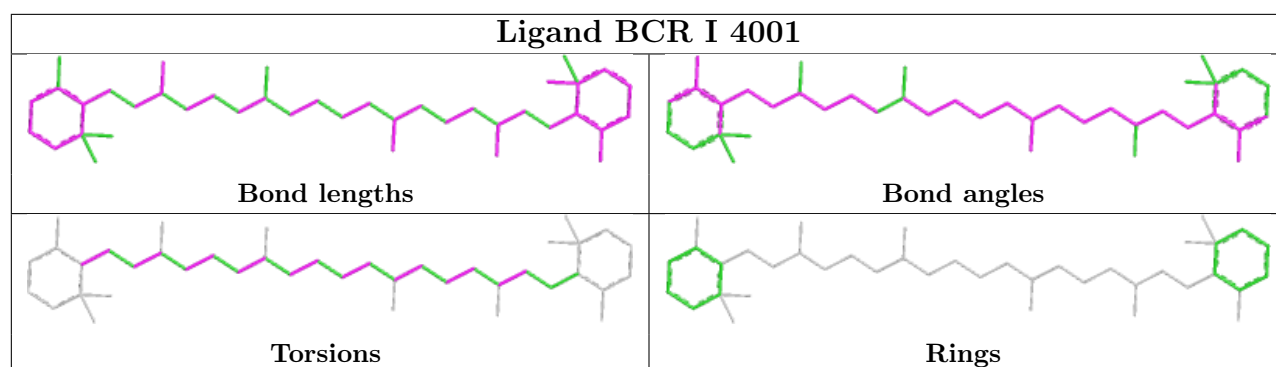
Ligand CLA 5 312

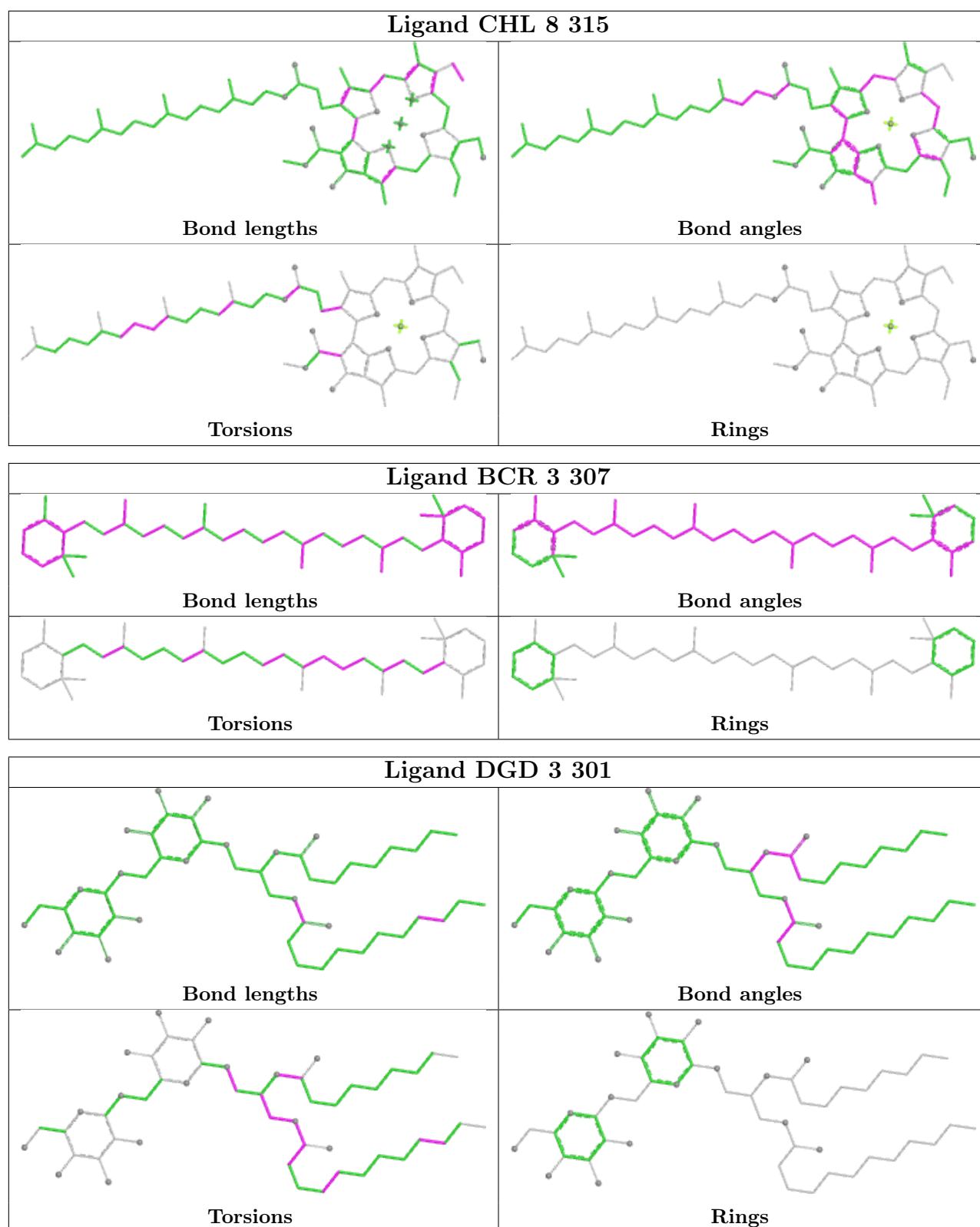


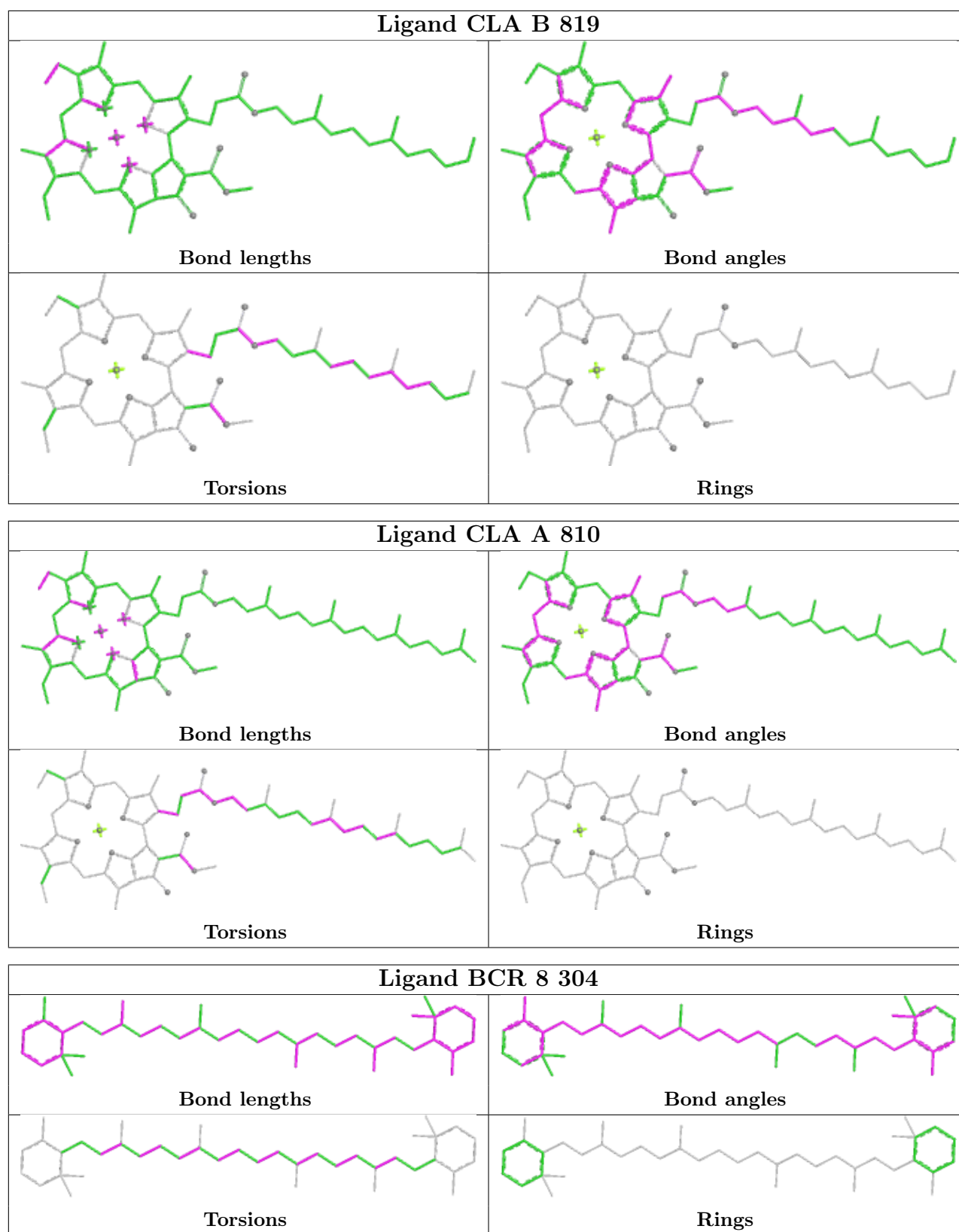
Ligand CHL Z 311



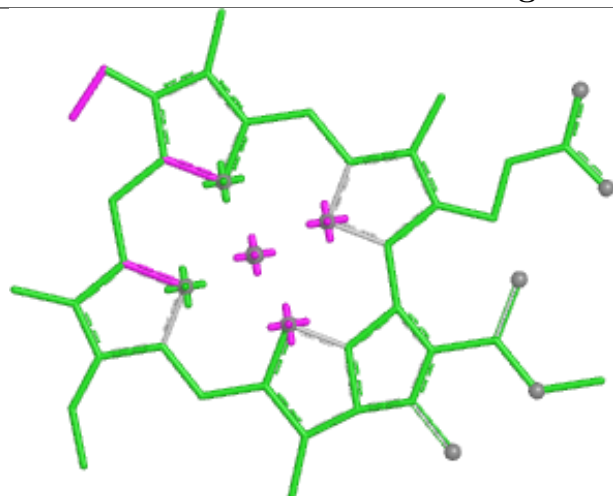




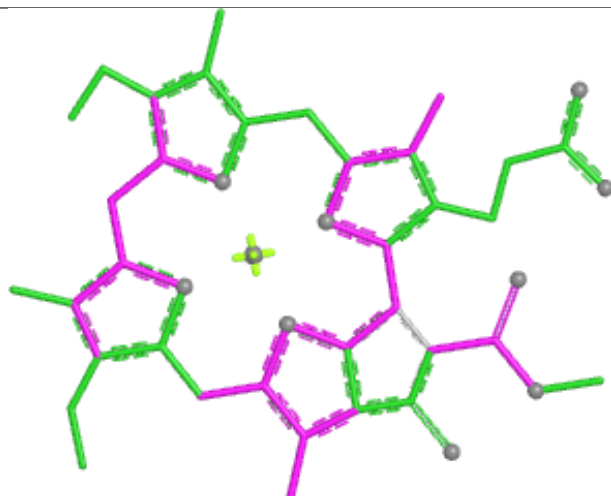




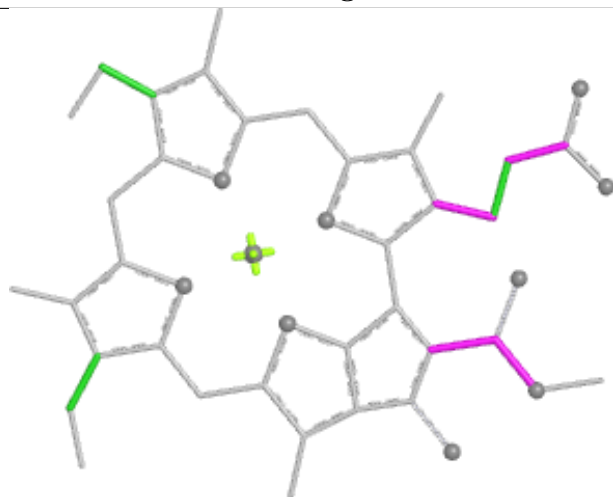
Ligand CLA 2 302



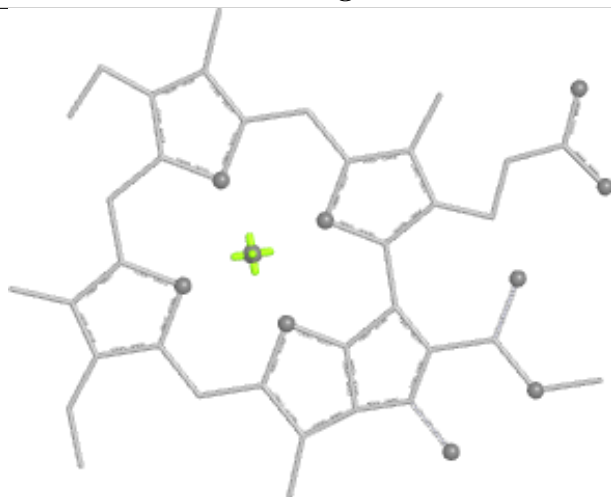
Bond lengths



Bond angles

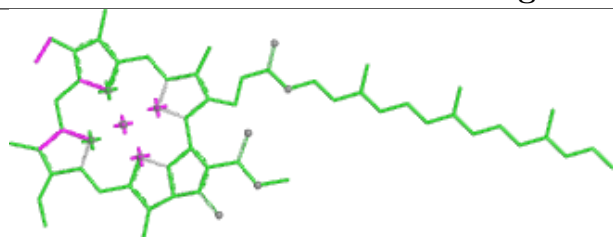


Torsions

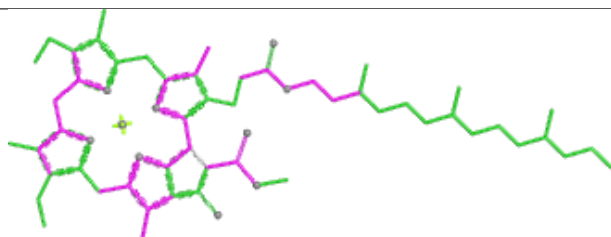


Rings

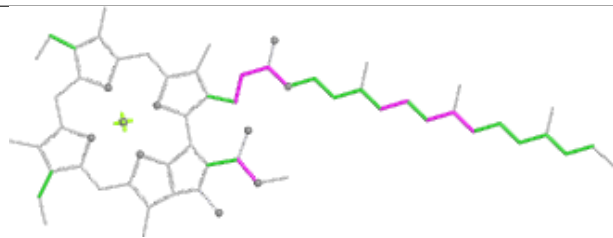
Ligand CLA 9 306



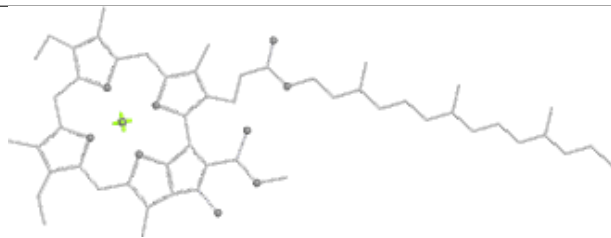
Bond lengths



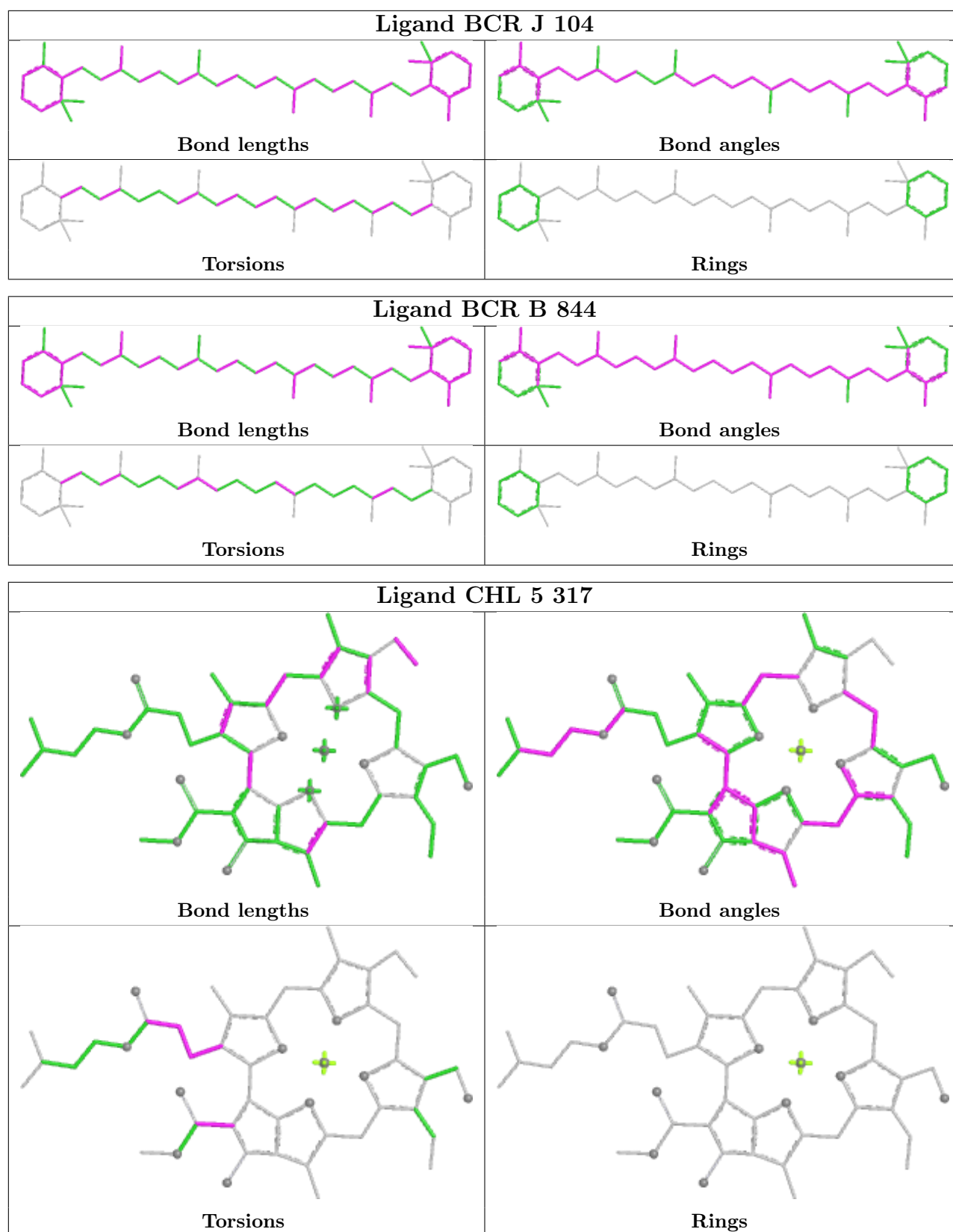
Bond angles

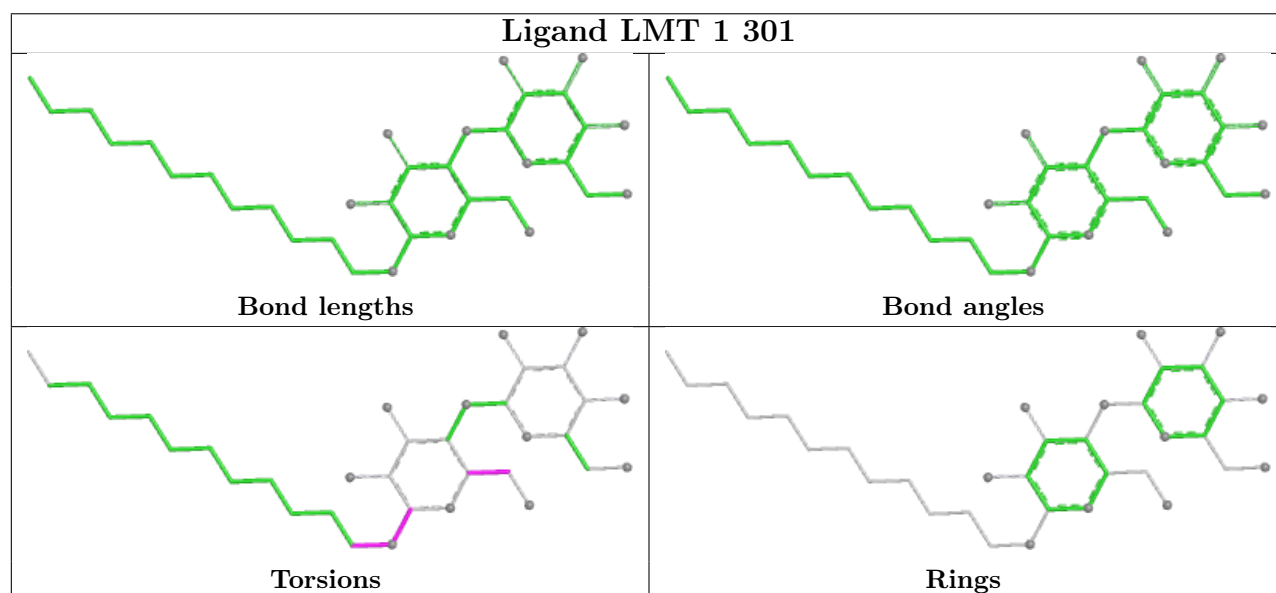
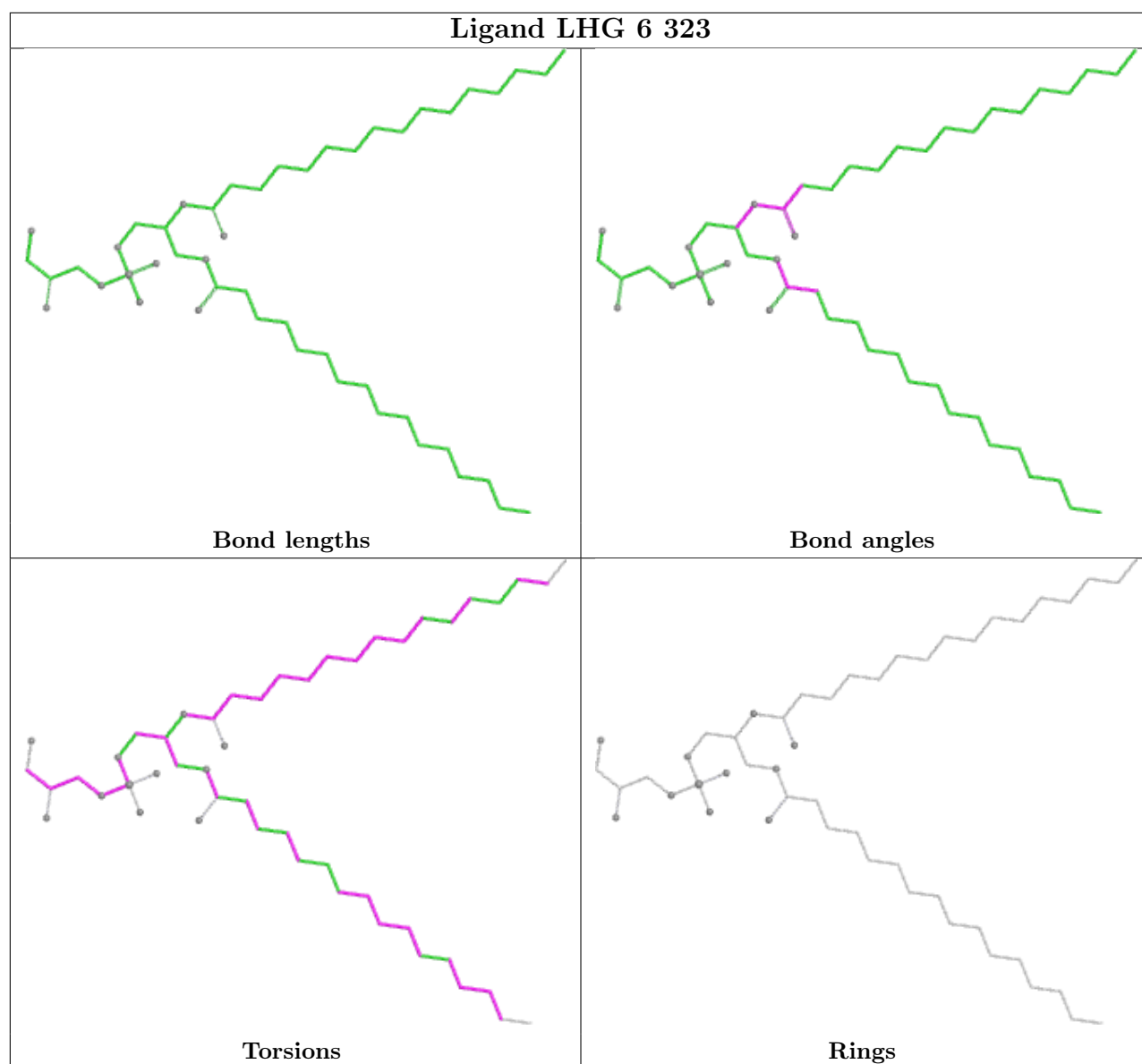


Torsions

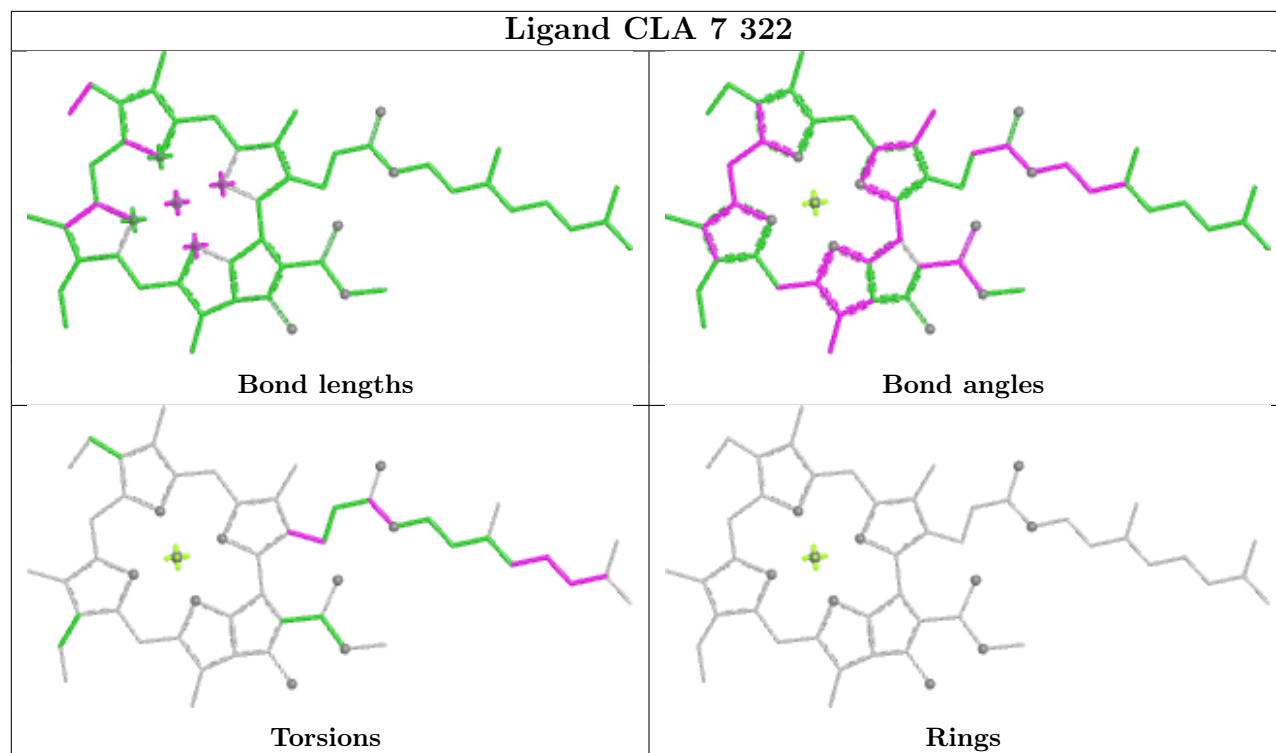


Rings

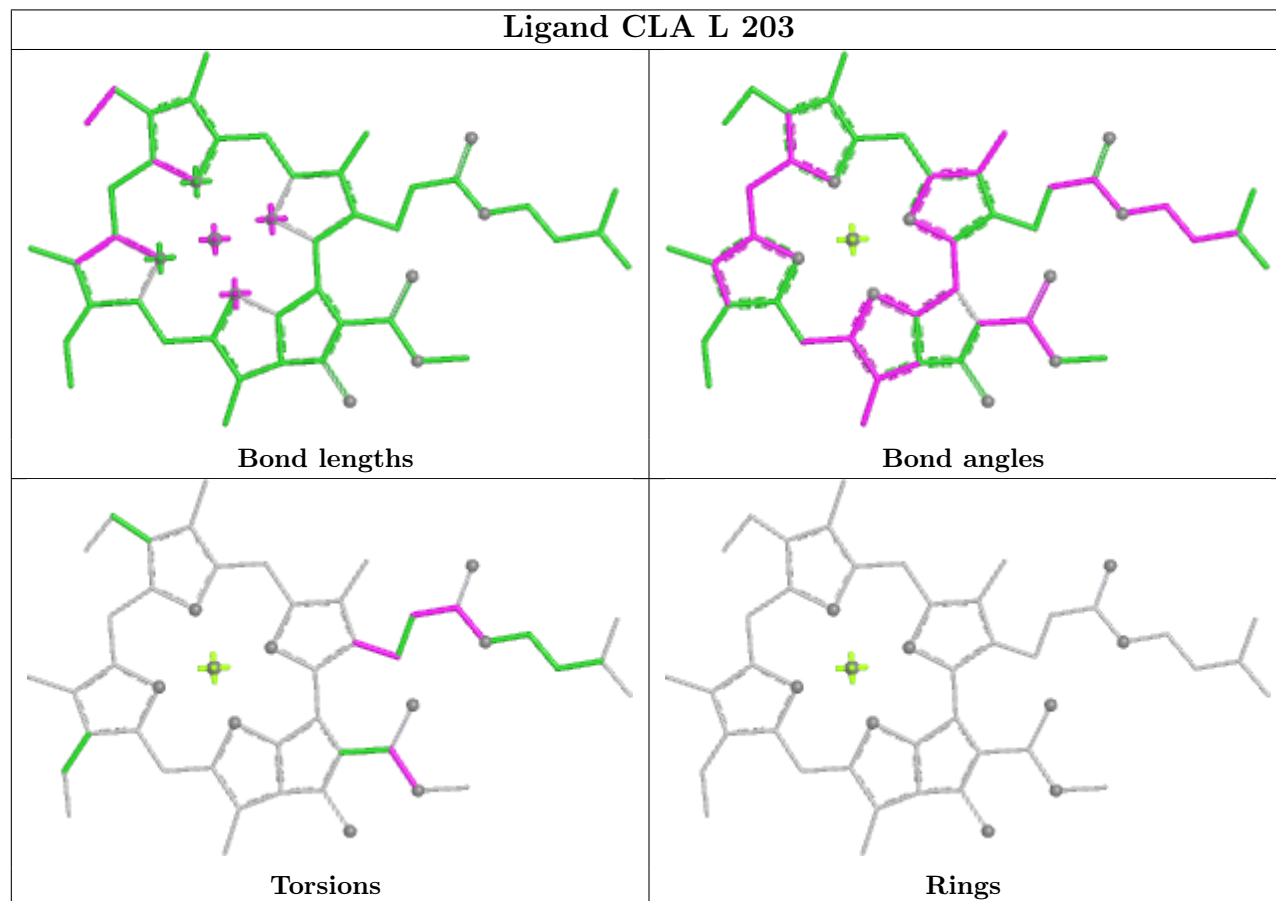


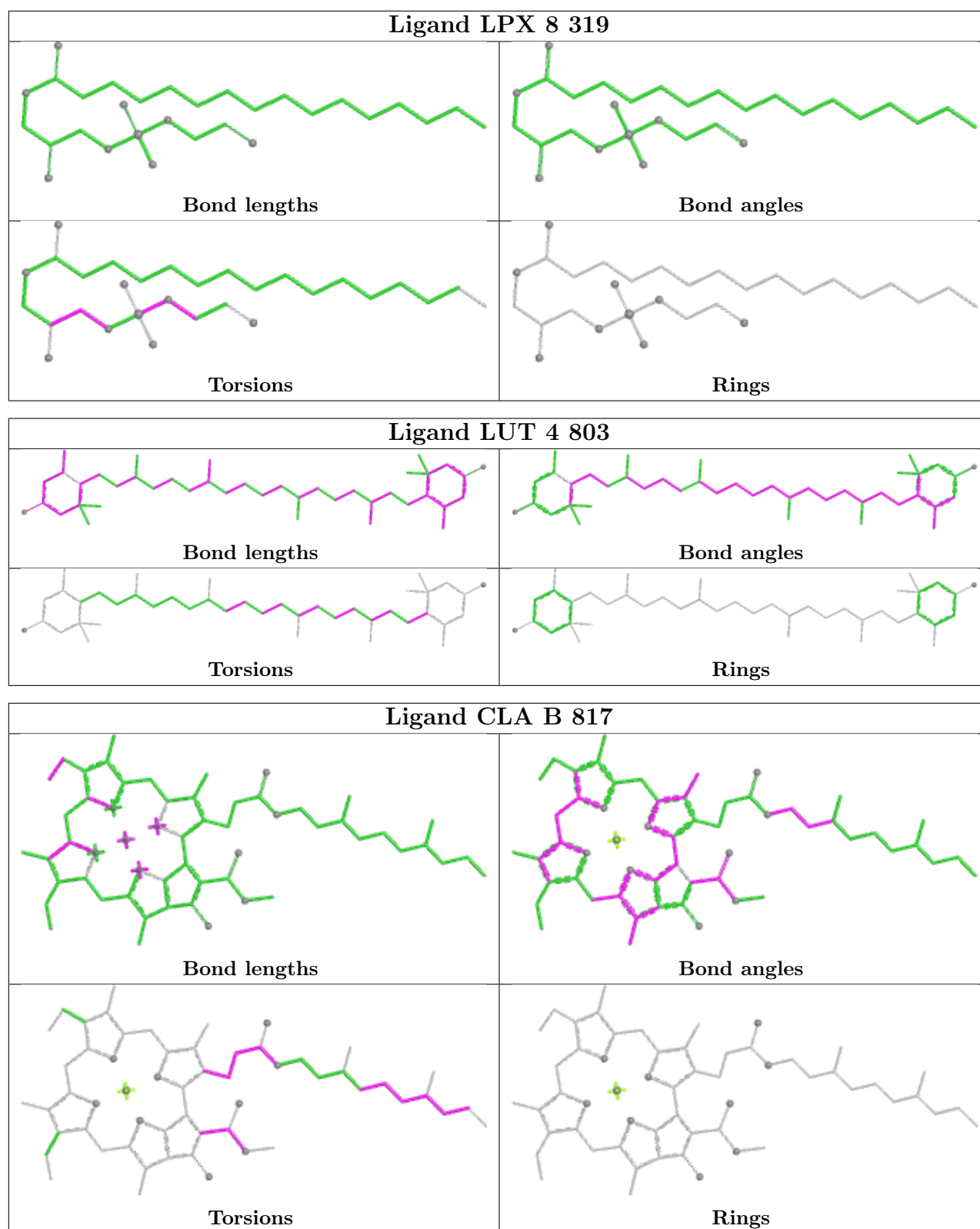


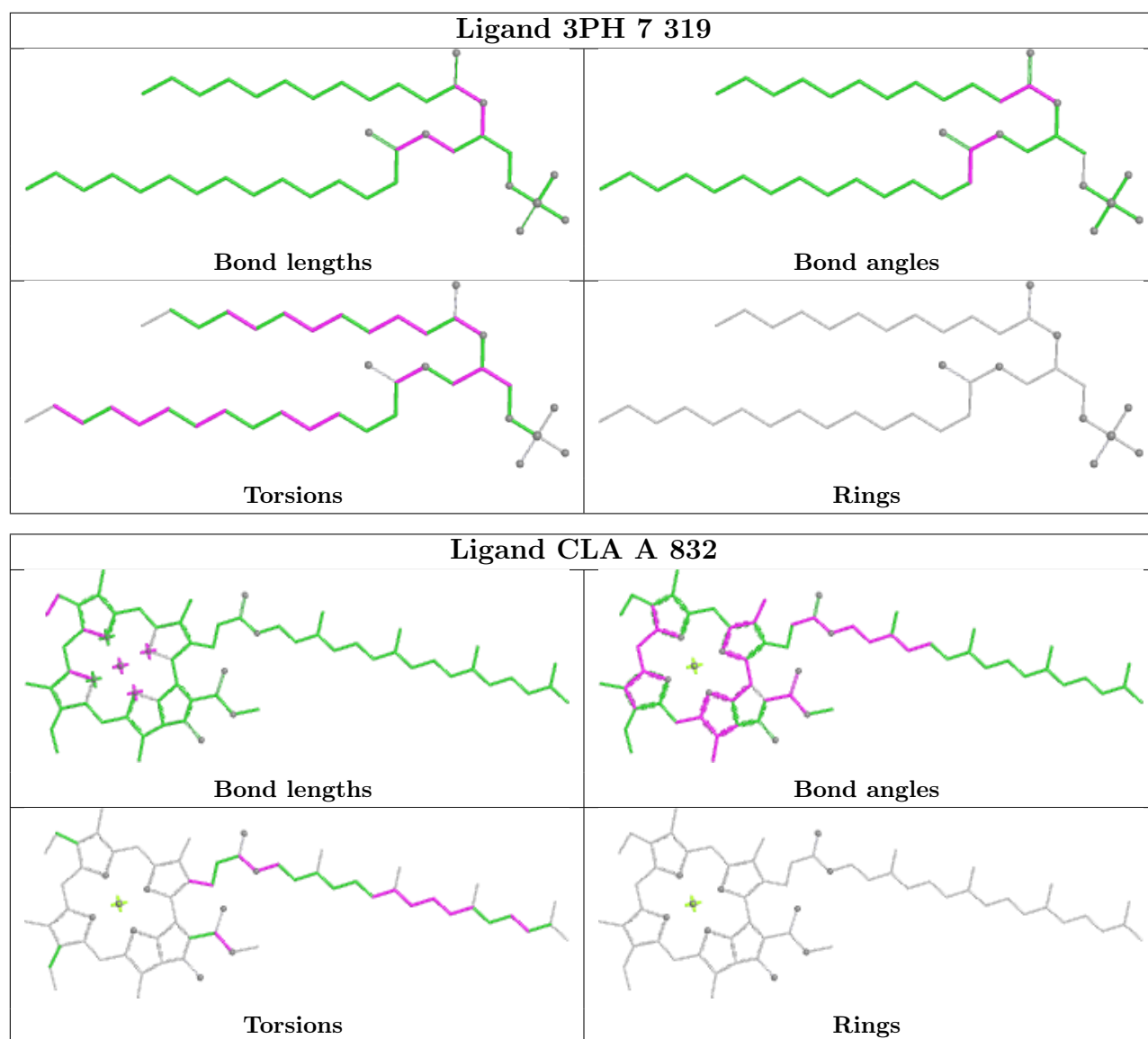
Ligand CLA 7 322

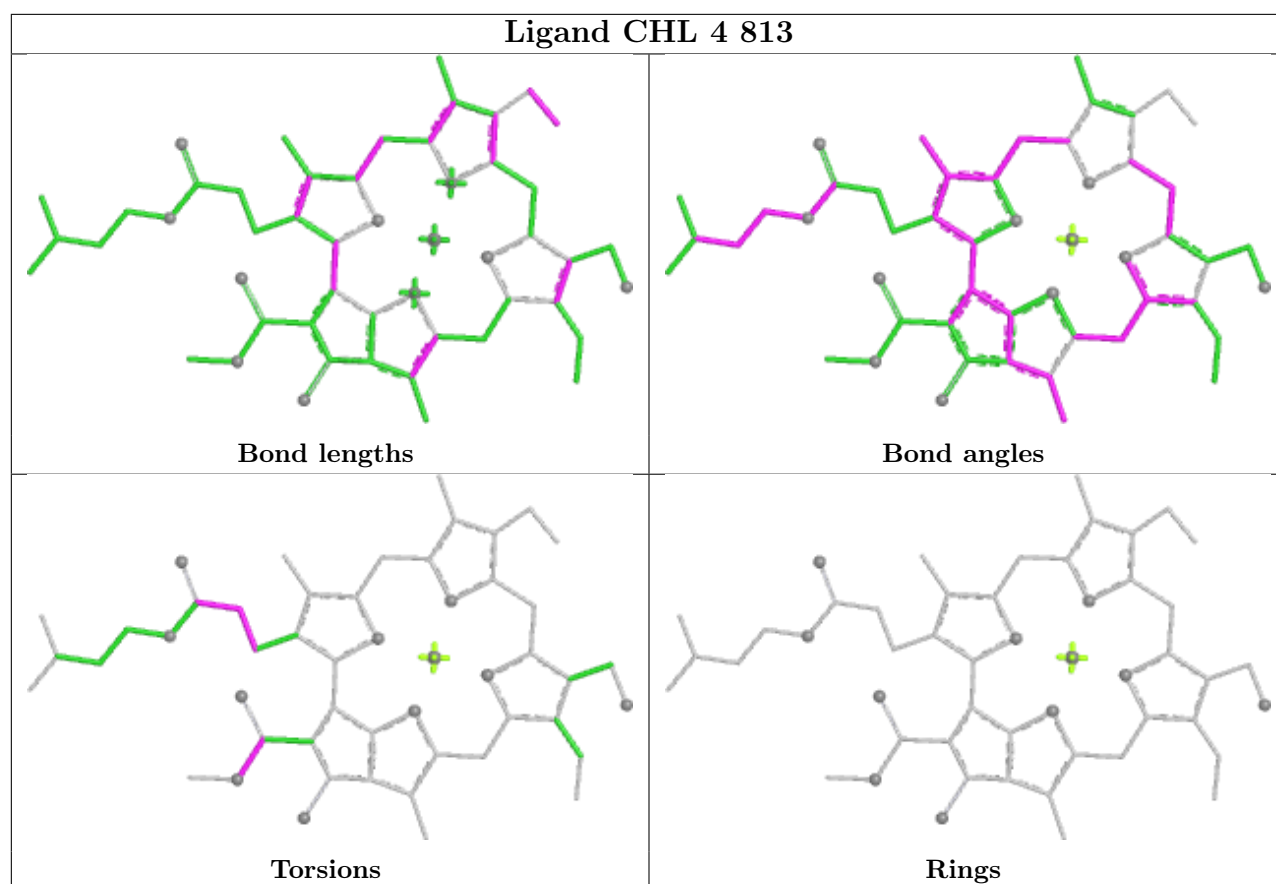


Ligand CLA L 203

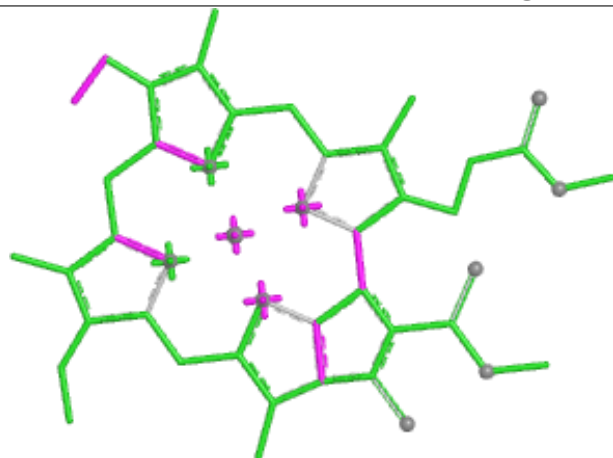




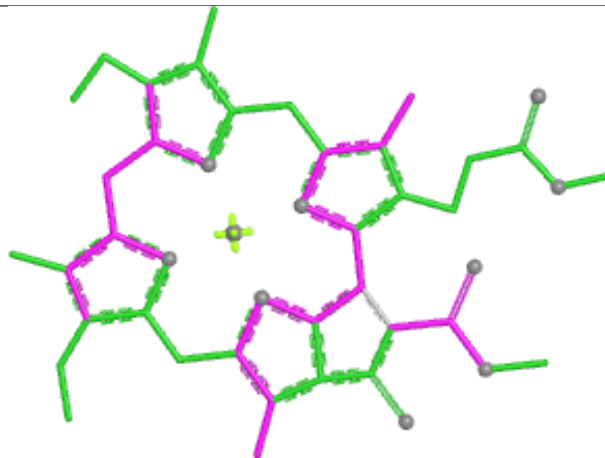




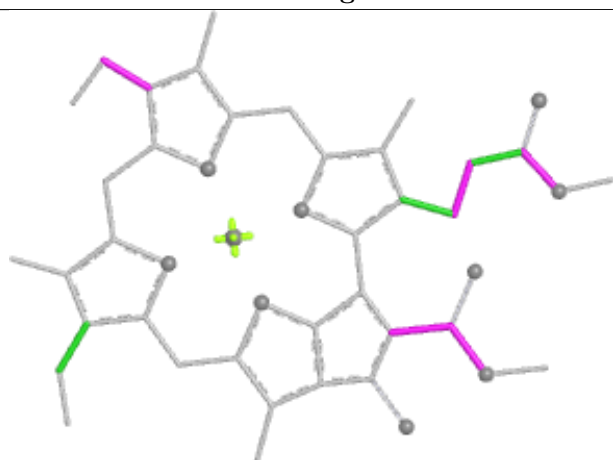
Ligand CLA 1 311



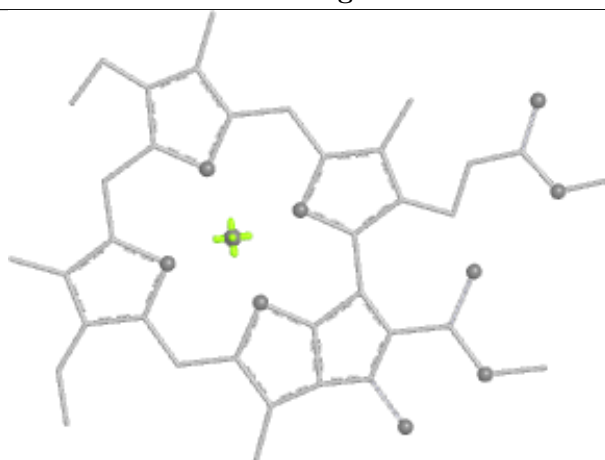
Bond lengths



Bond angles

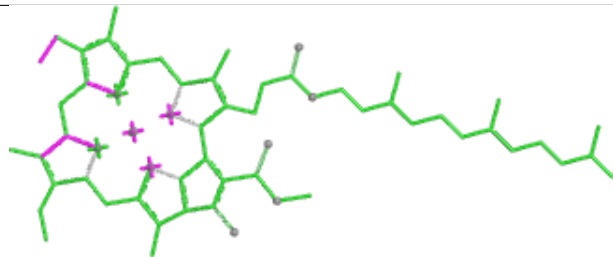


Torsions

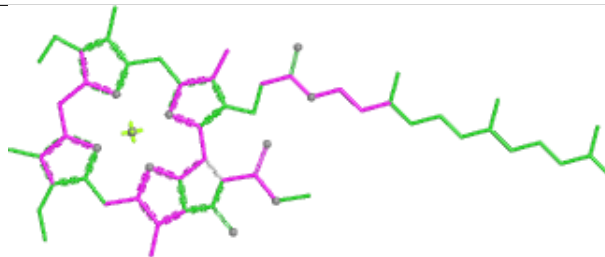


Rings

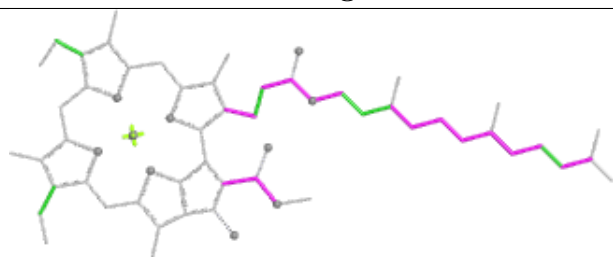
Ligand CLA A 814



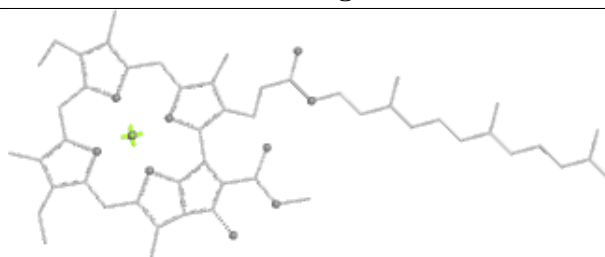
Bond lengths



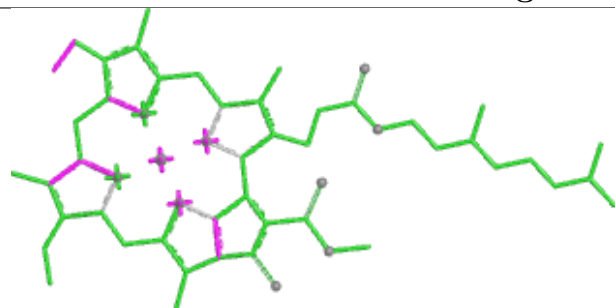
Bond angles



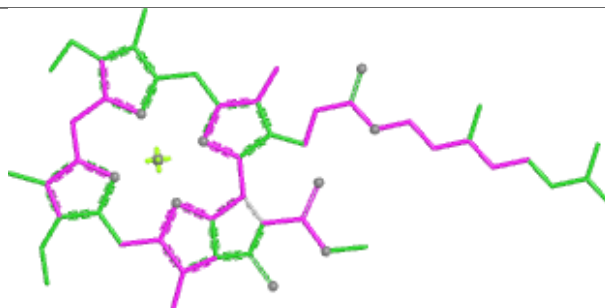
Torsions



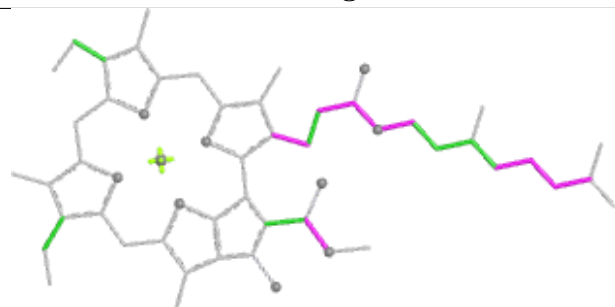
Rings

Ligand CLA B 823

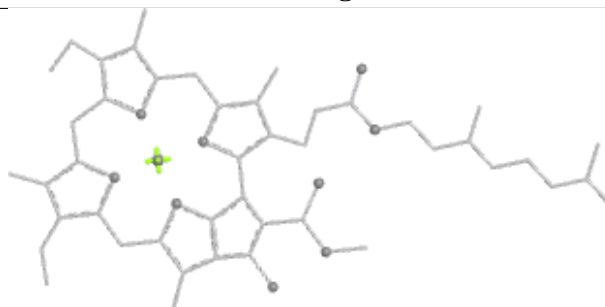
Bond lengths



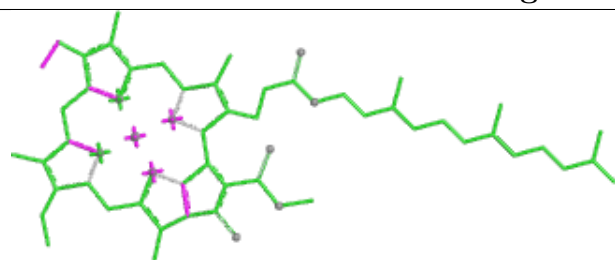
Bond angles



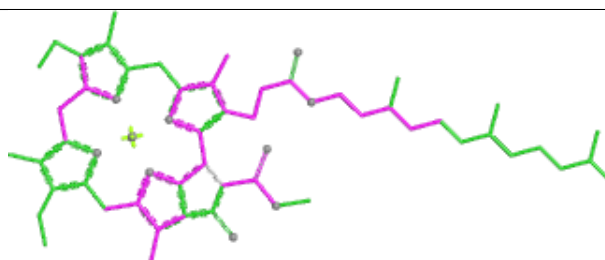
Torsions



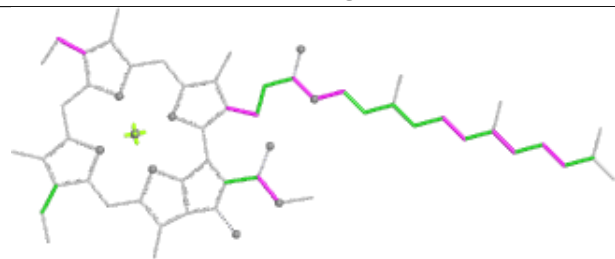
Rings

Ligand CLA 9 303

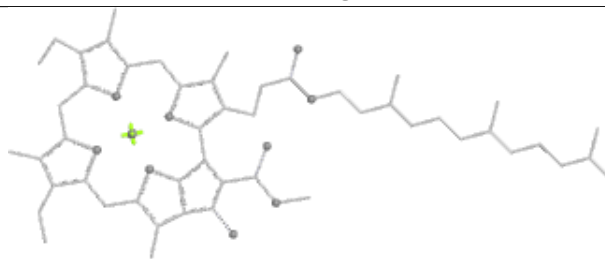
Bond lengths



Bond angles

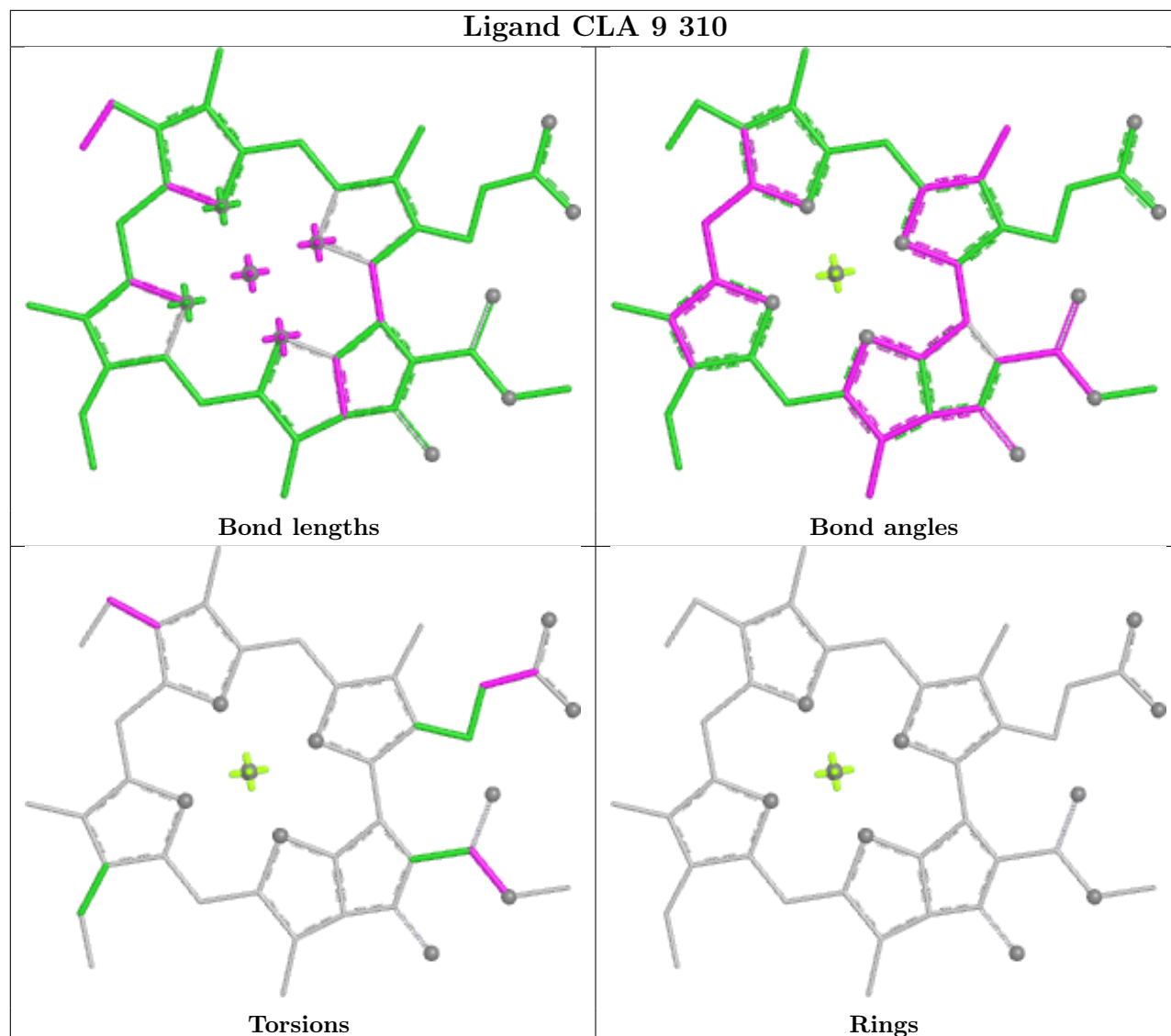


Torsions

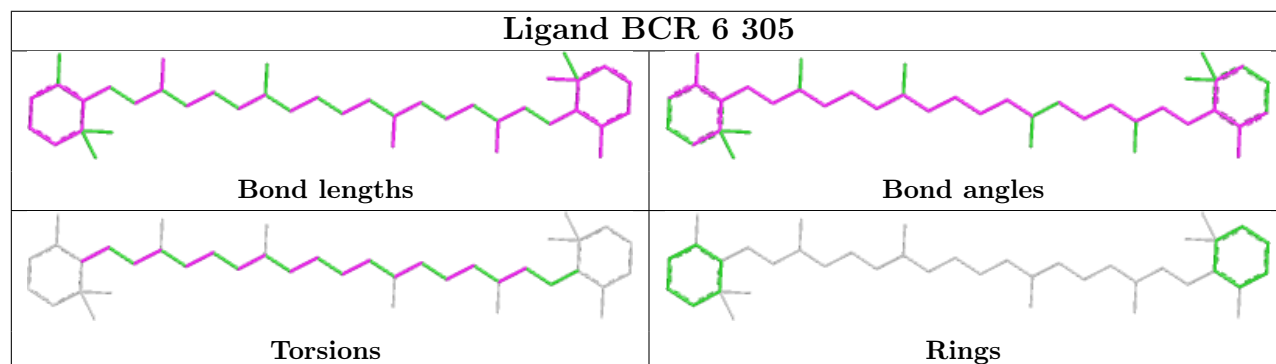


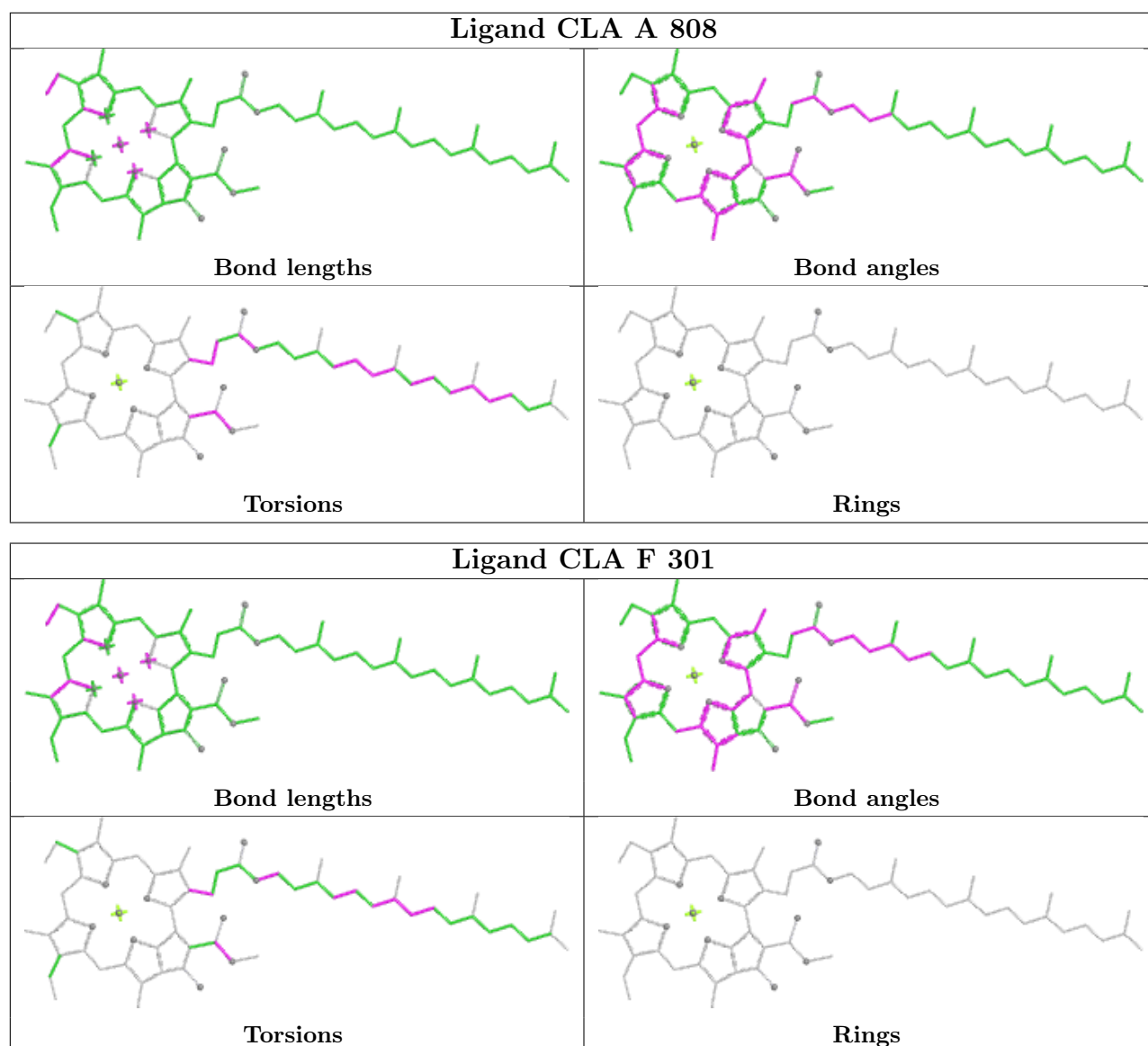
Rings

Ligand CLA 9 310

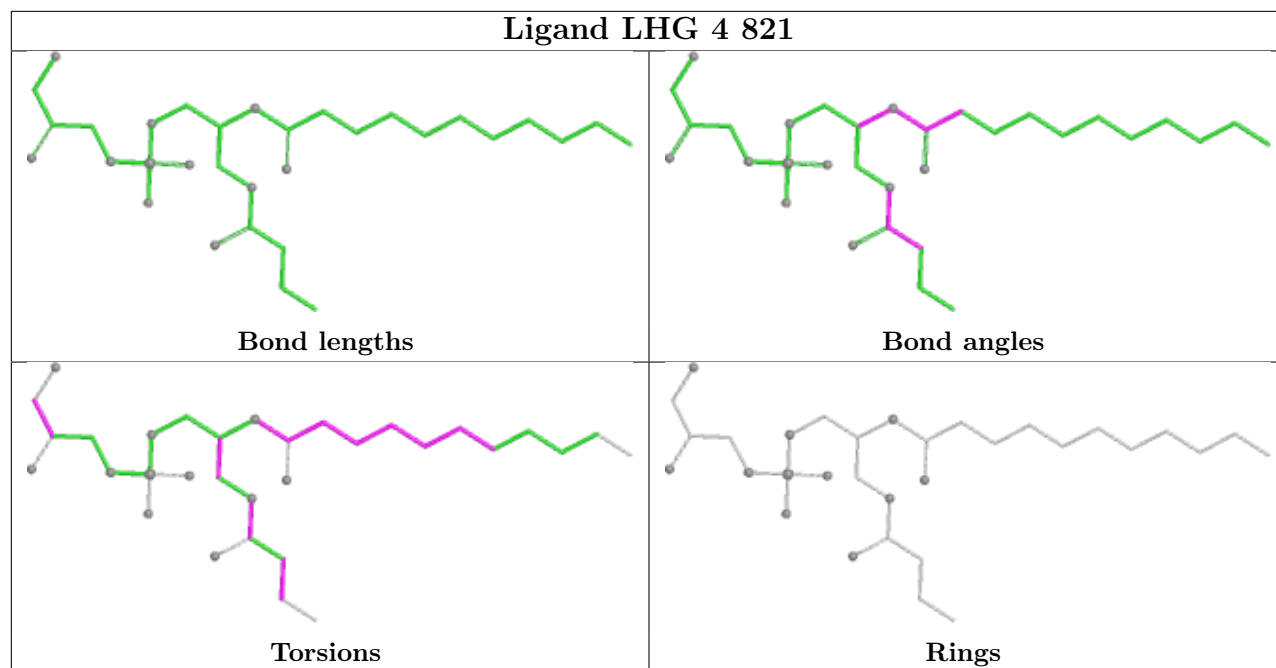


Ligand BCR 6 305

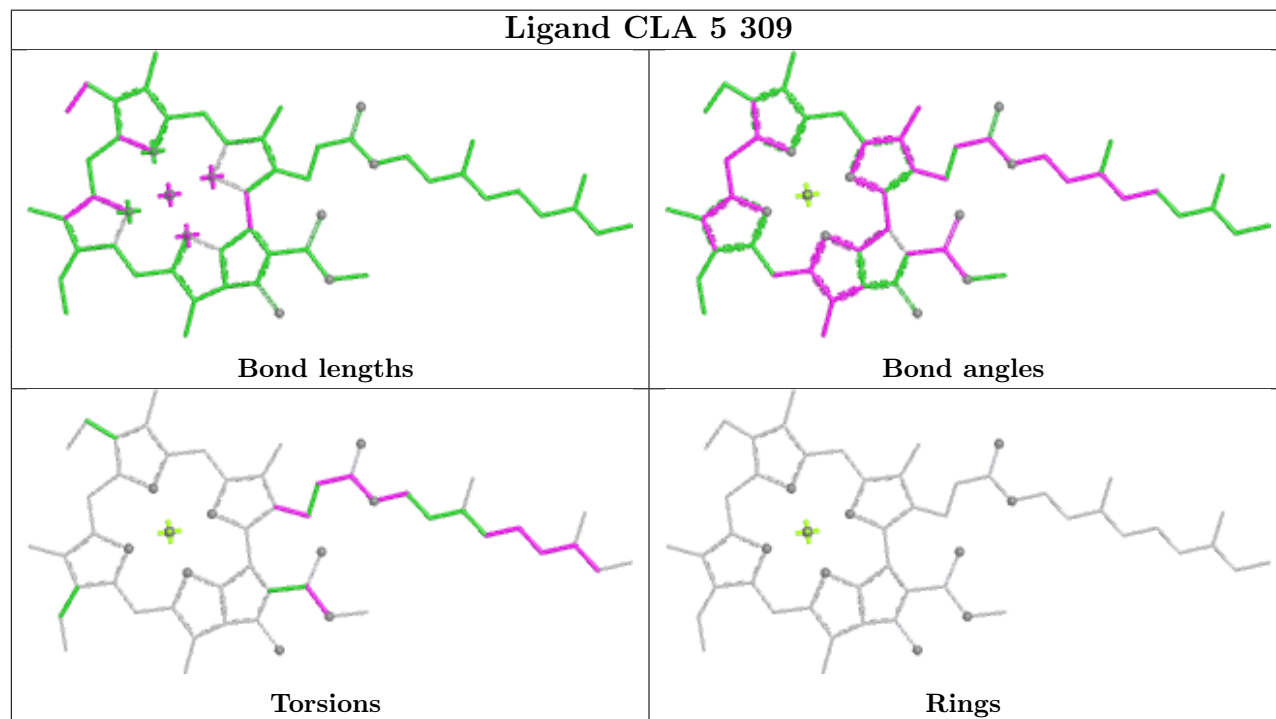




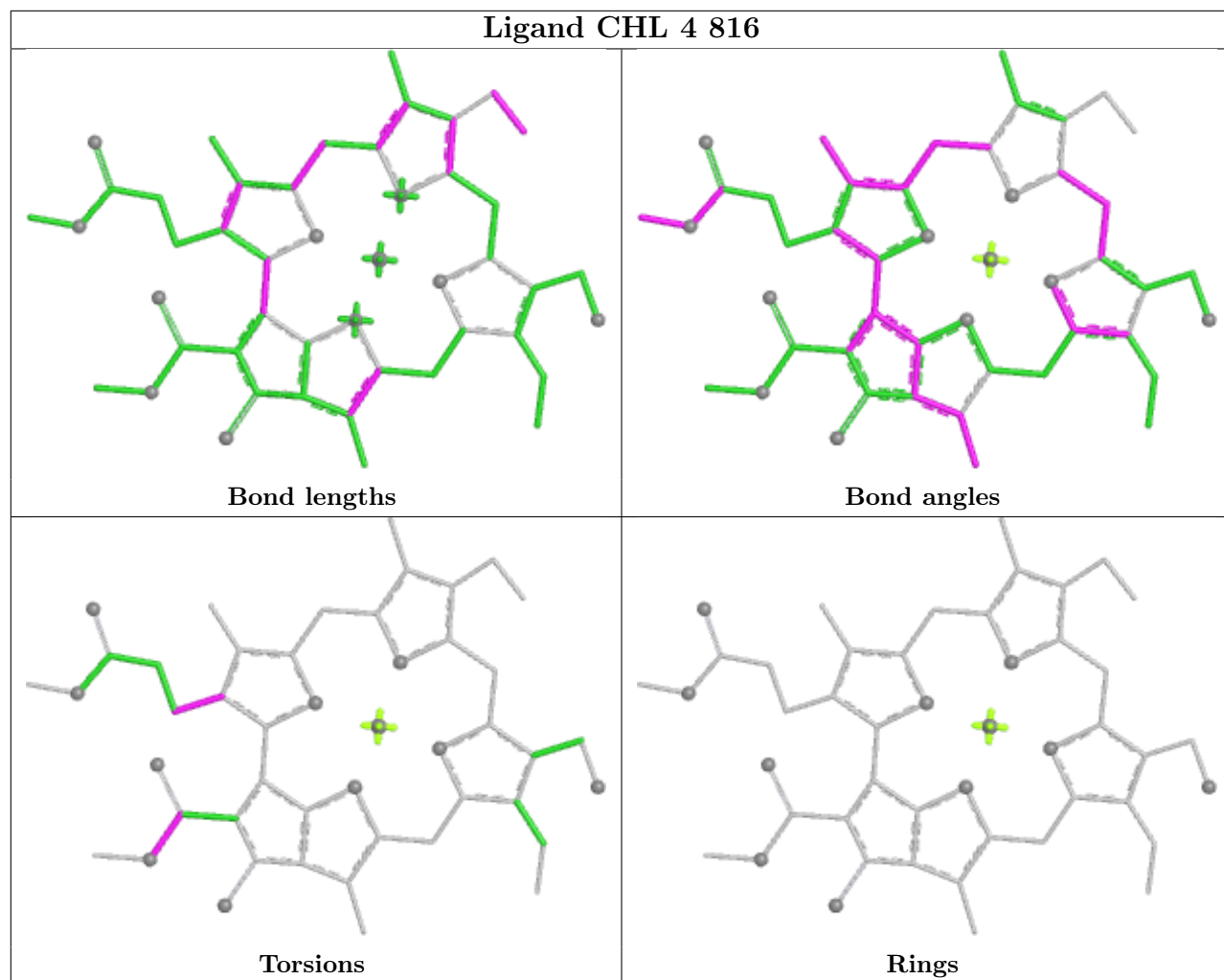
Ligand LHG 4 821



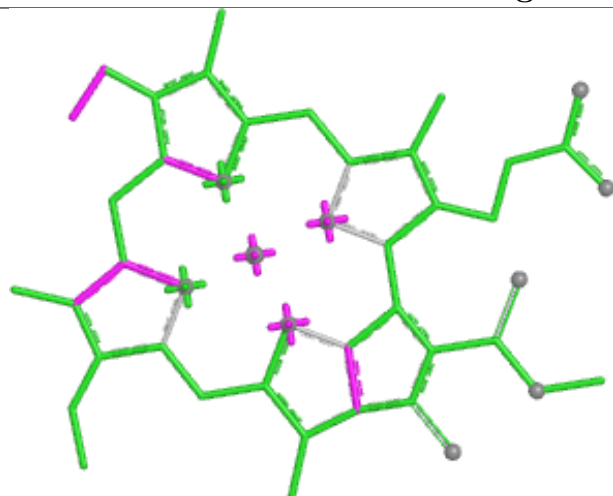
Ligand CLA 5 309



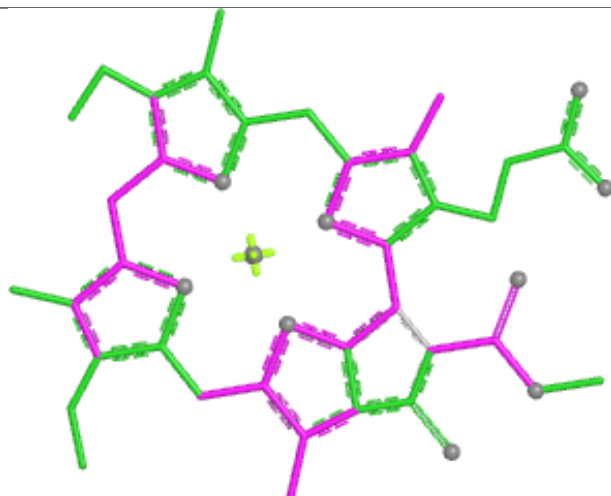
Ligand CHL 4 816



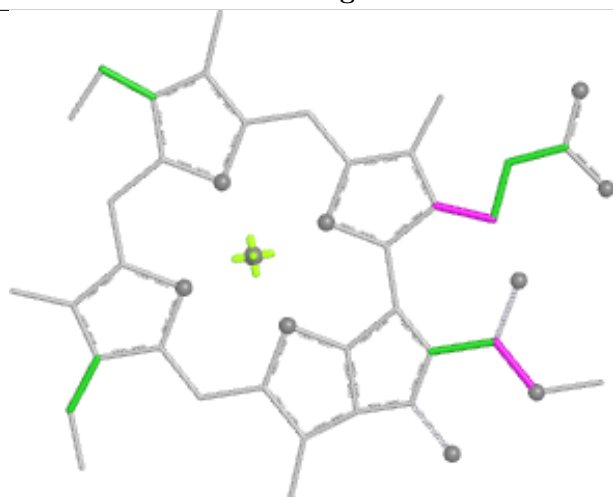
Ligand CLA F 305



Bond lengths



Bond angles

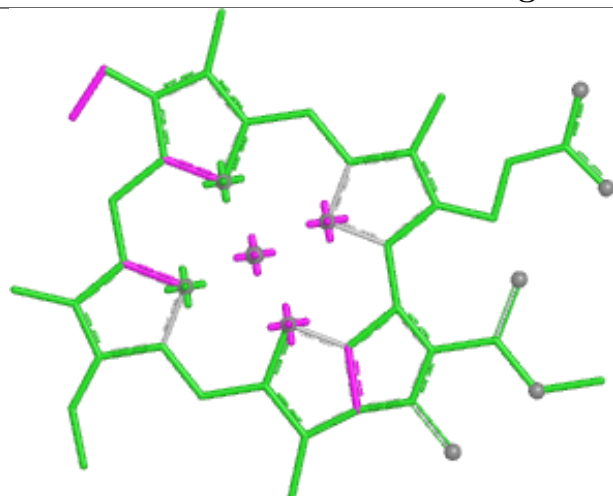


Torsions

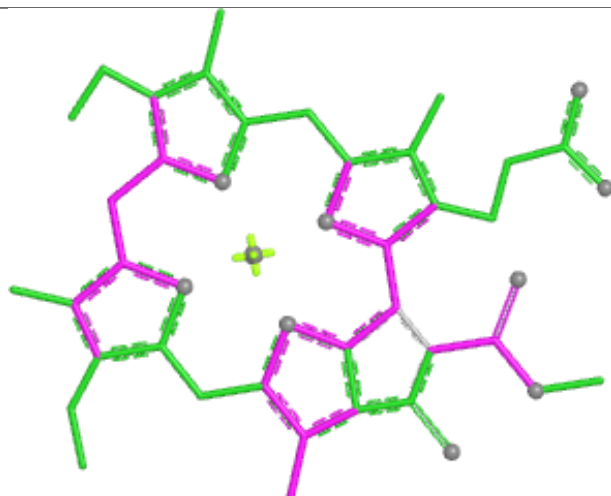


Rings

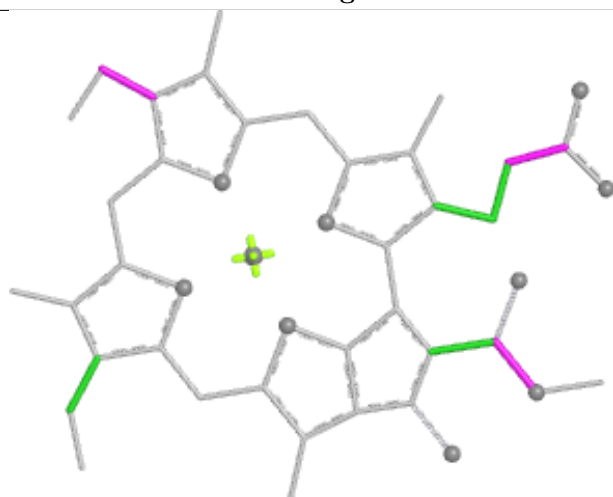
Ligand CLA 9 304



Bond lengths



Bond angles

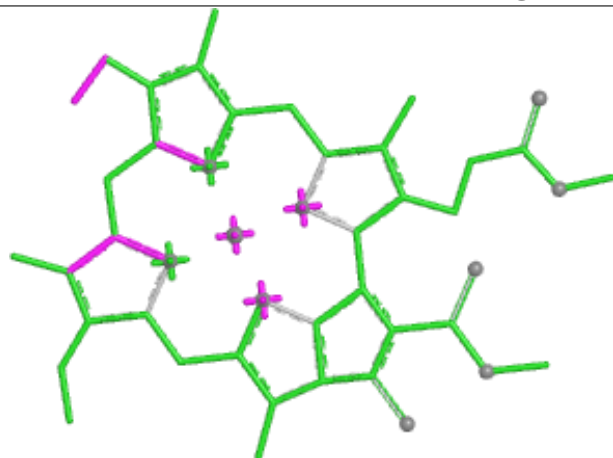


Torsions

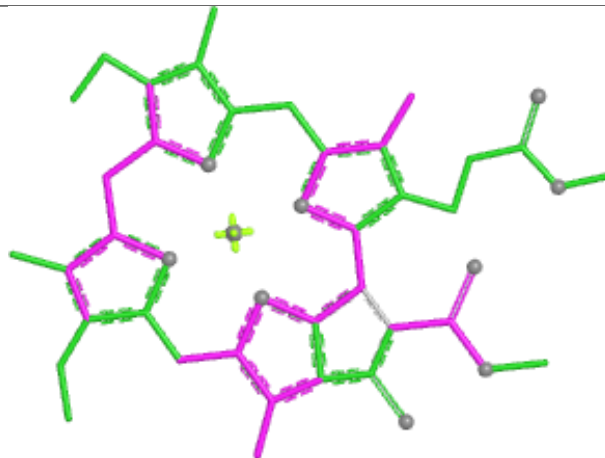


Rings

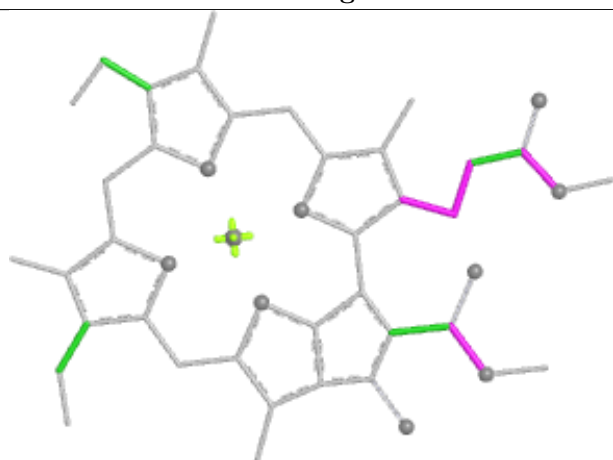
Ligand CLA K 202



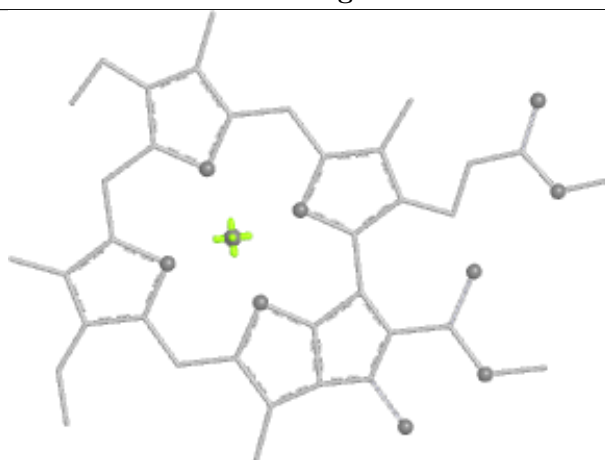
Bond lengths



Bond angles

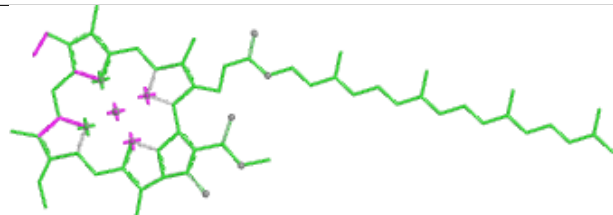


Torsions

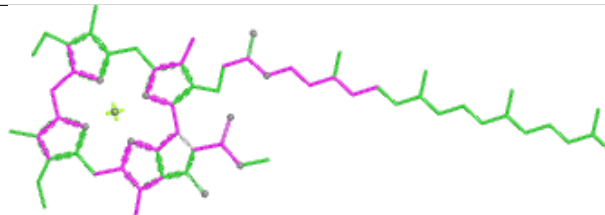


Rings

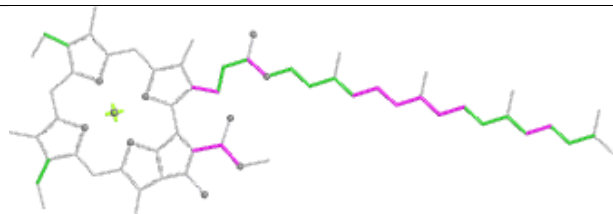
Ligand CLA A 806



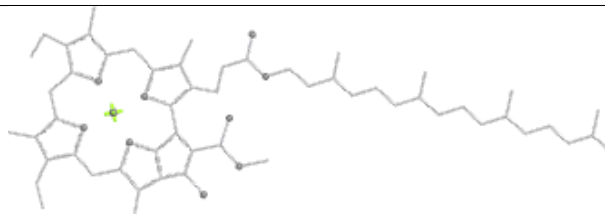
Bond lengths



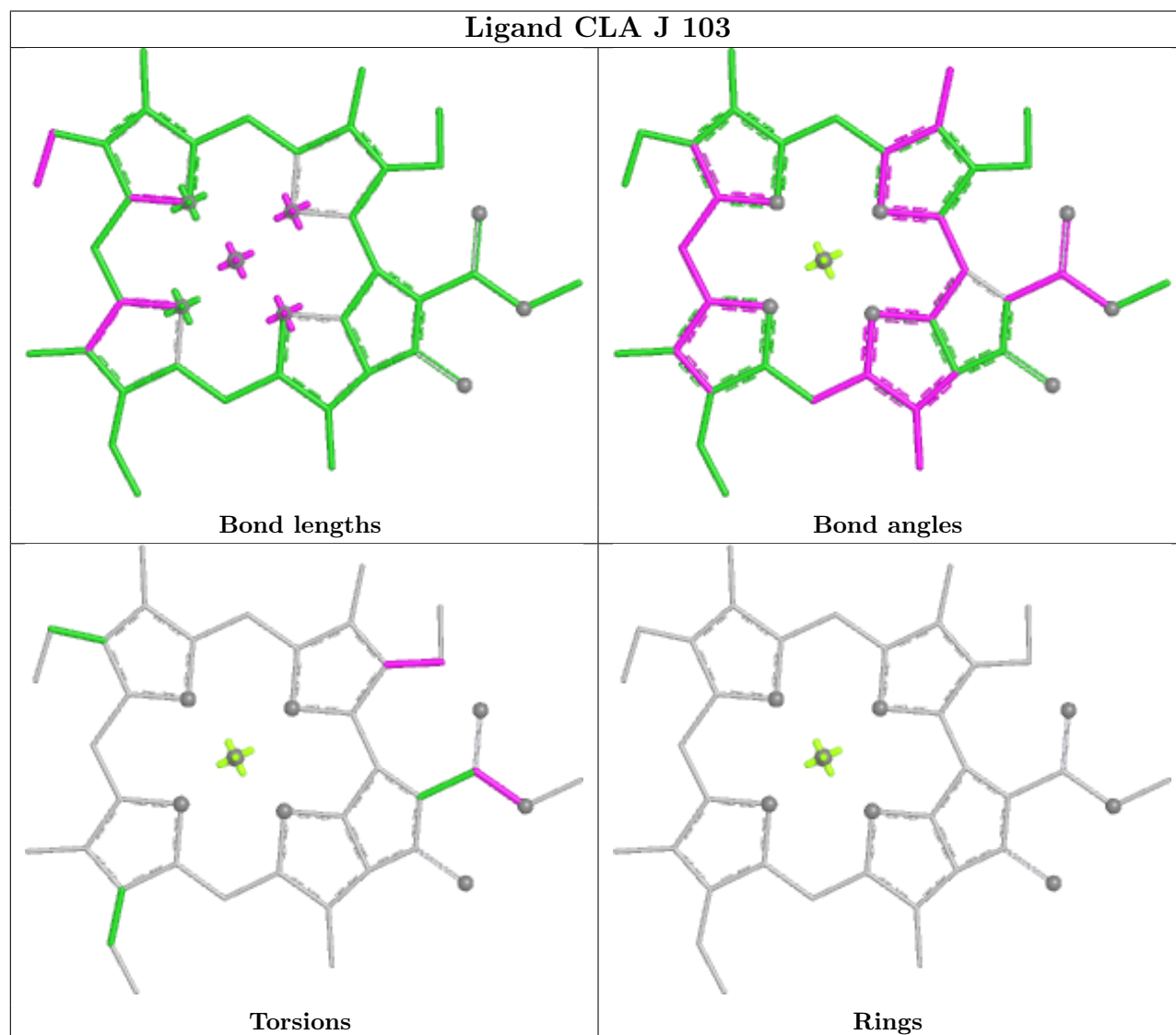
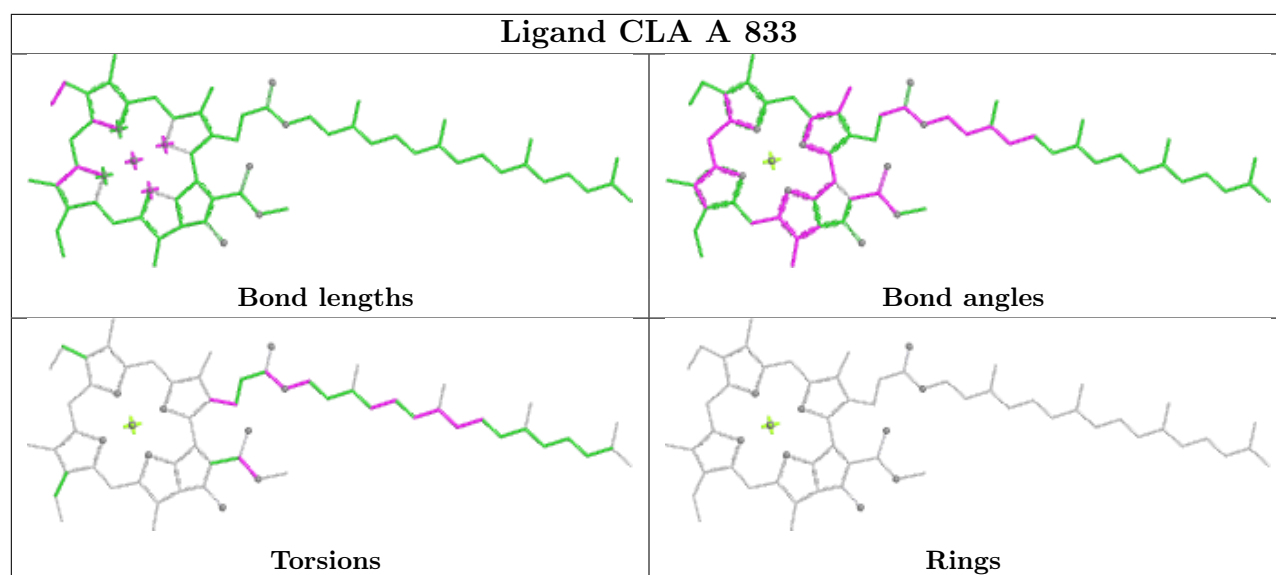
Bond angles

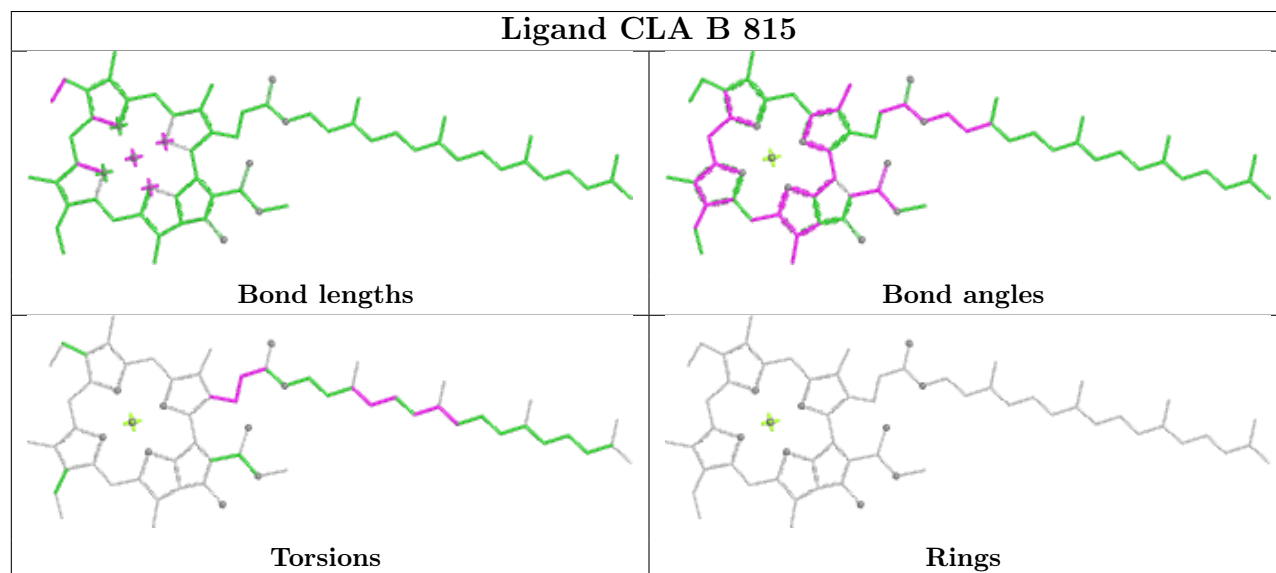
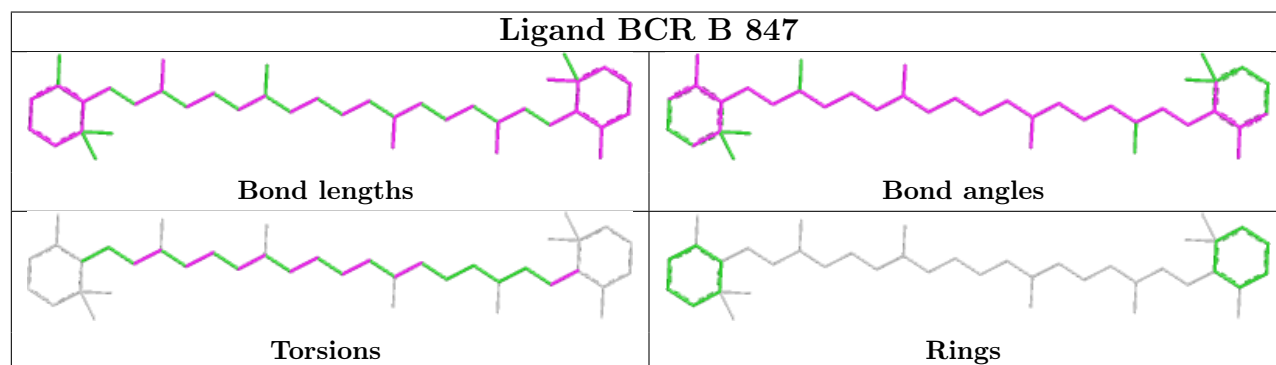
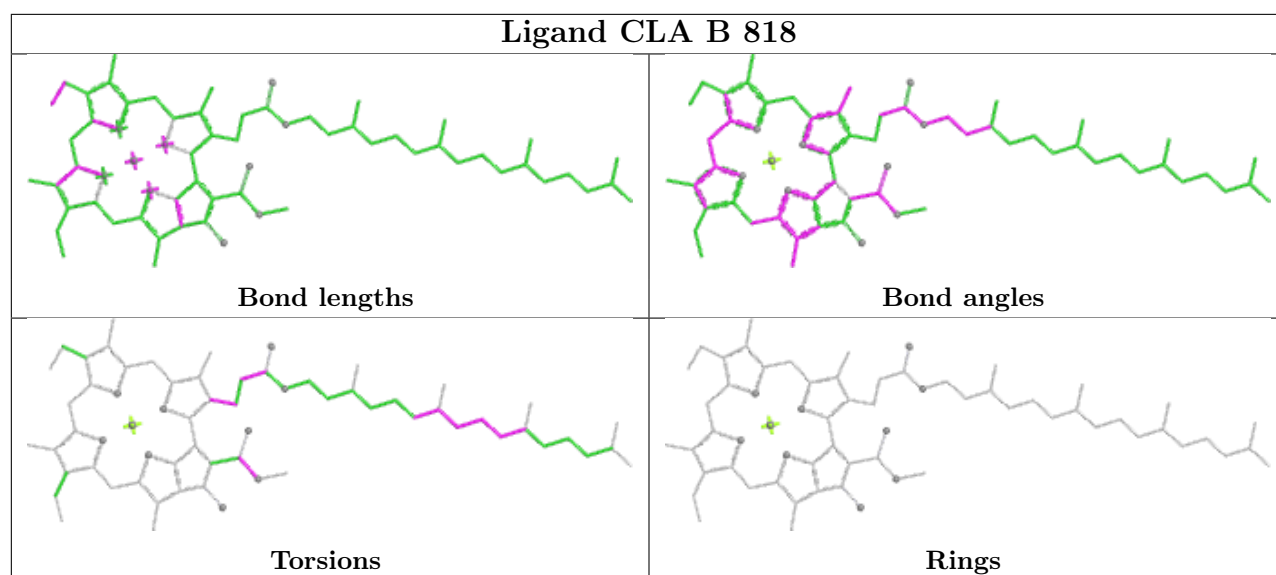


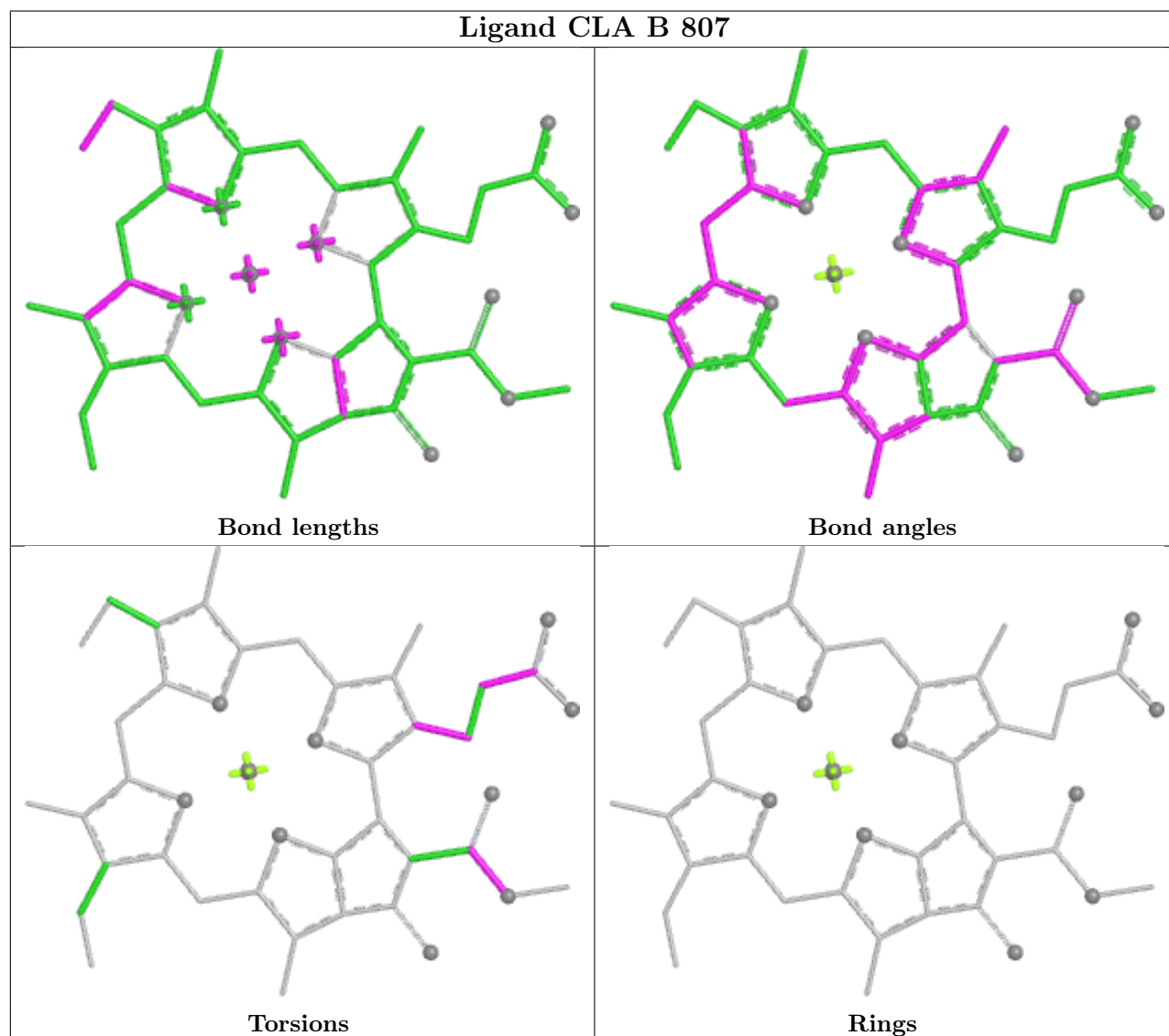
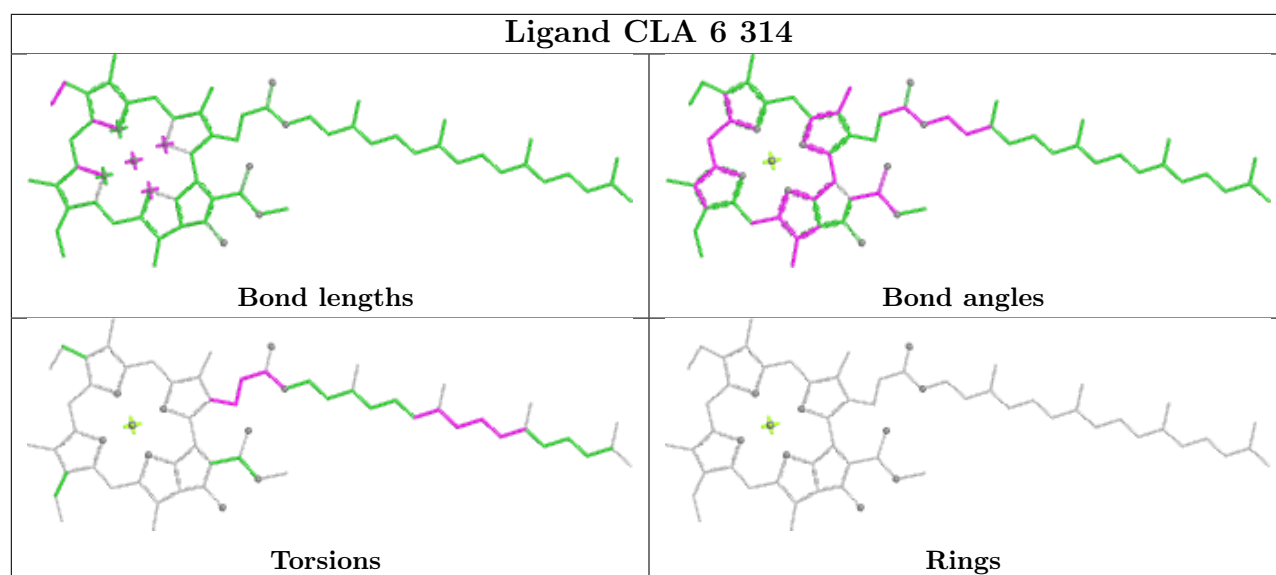
Torsions

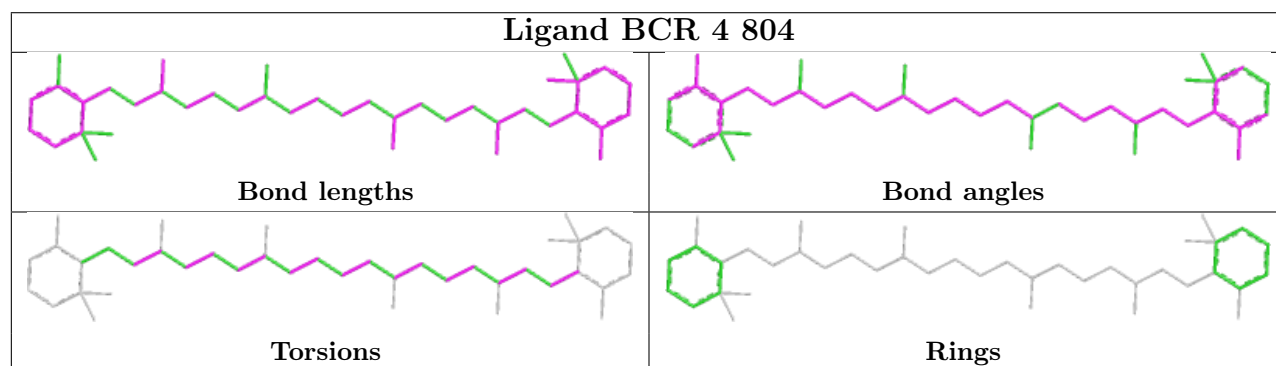
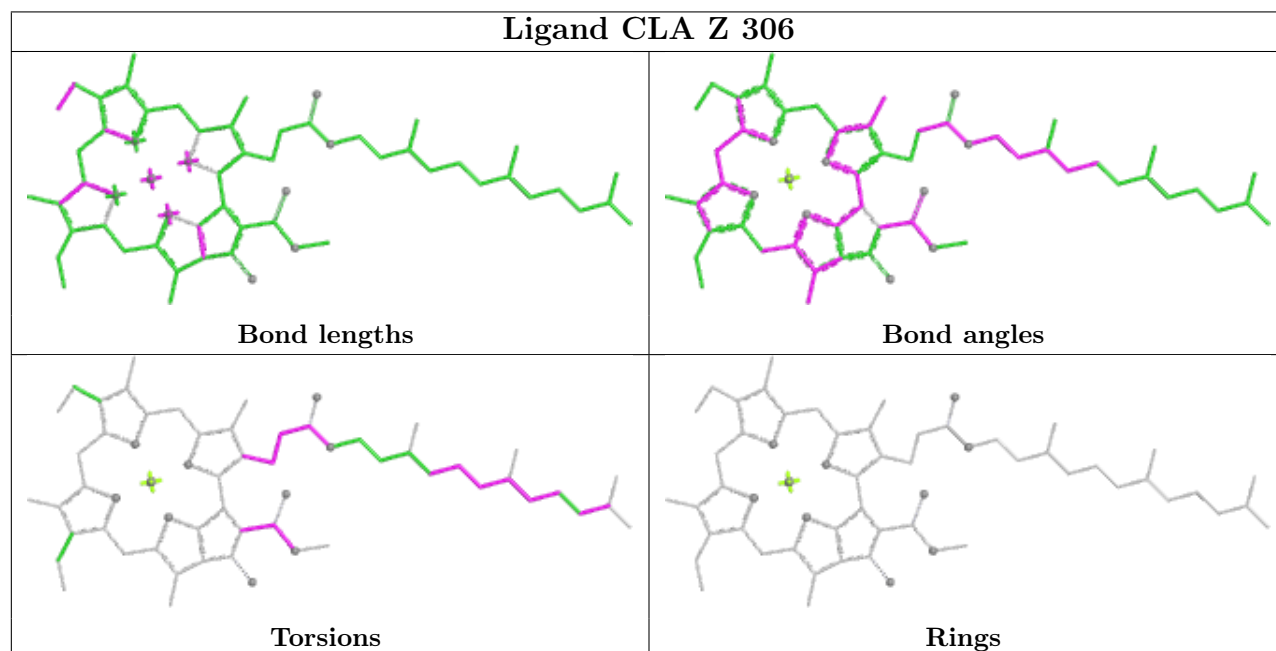
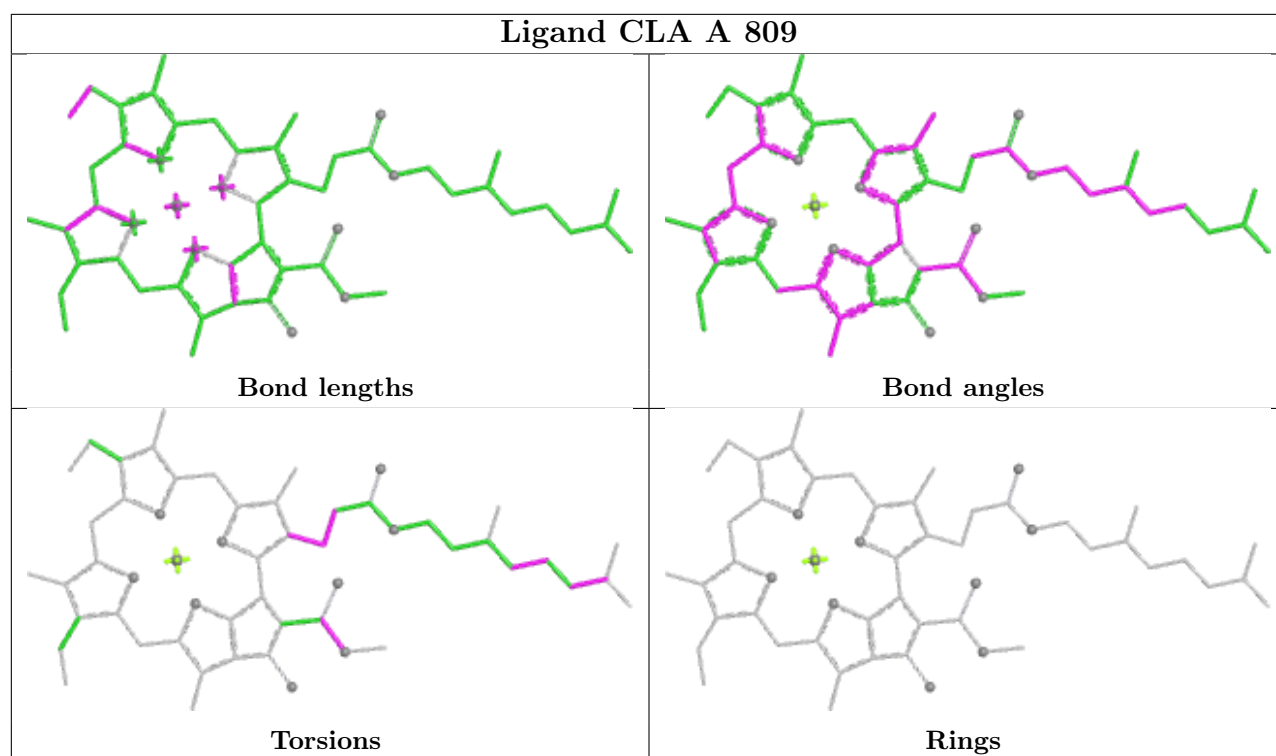


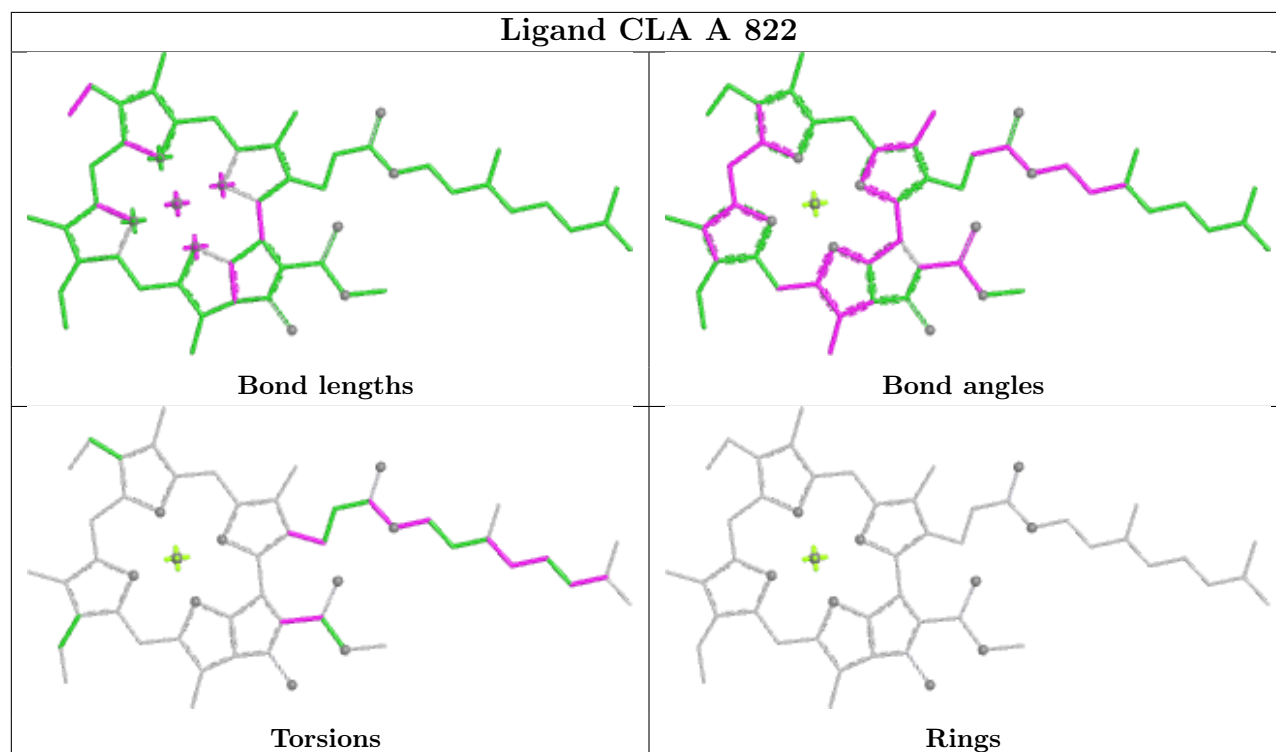
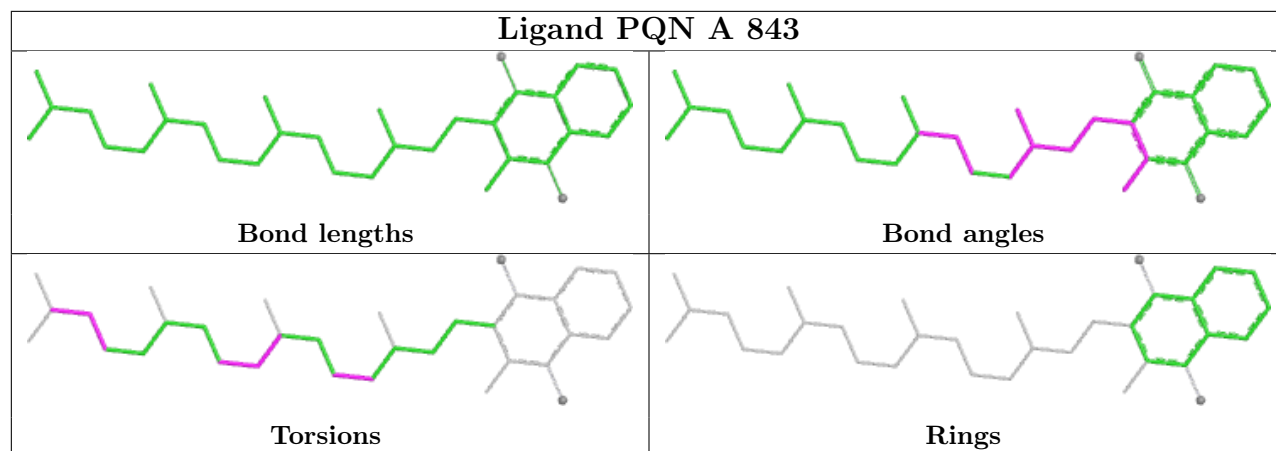
Rings



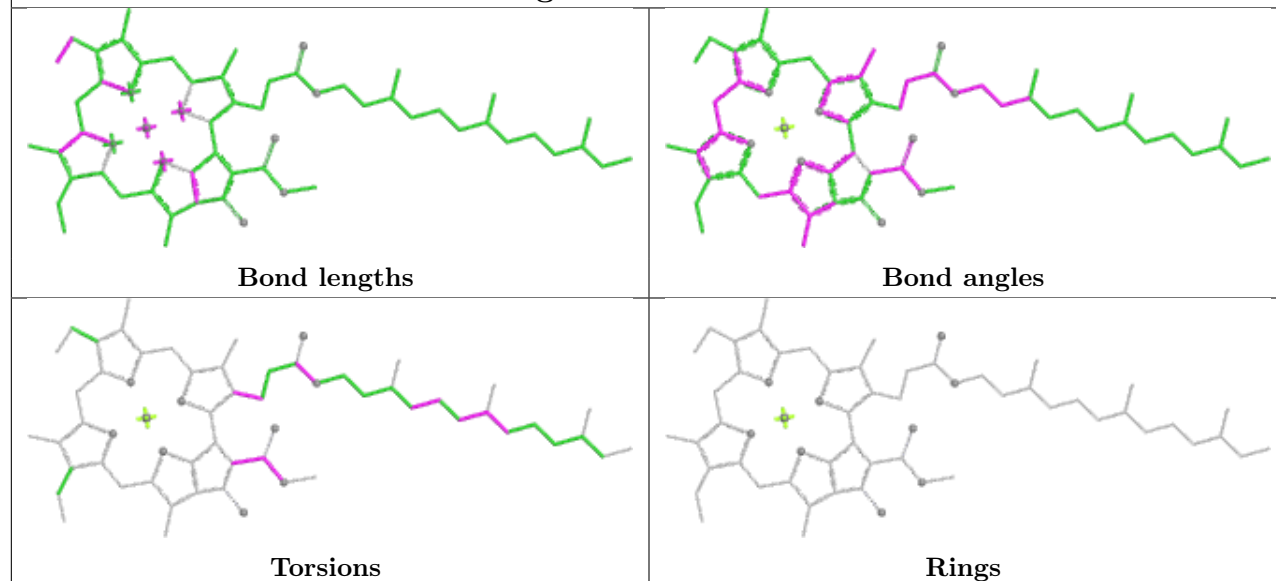




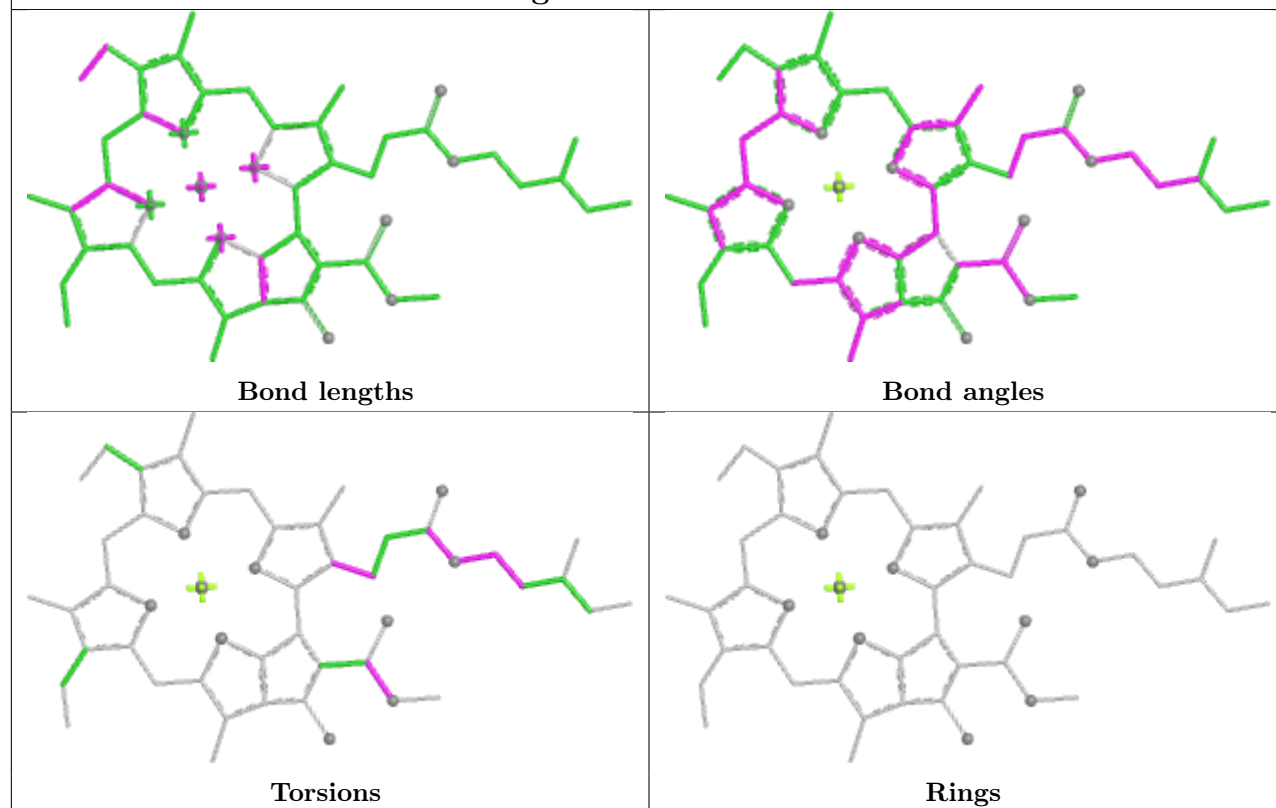


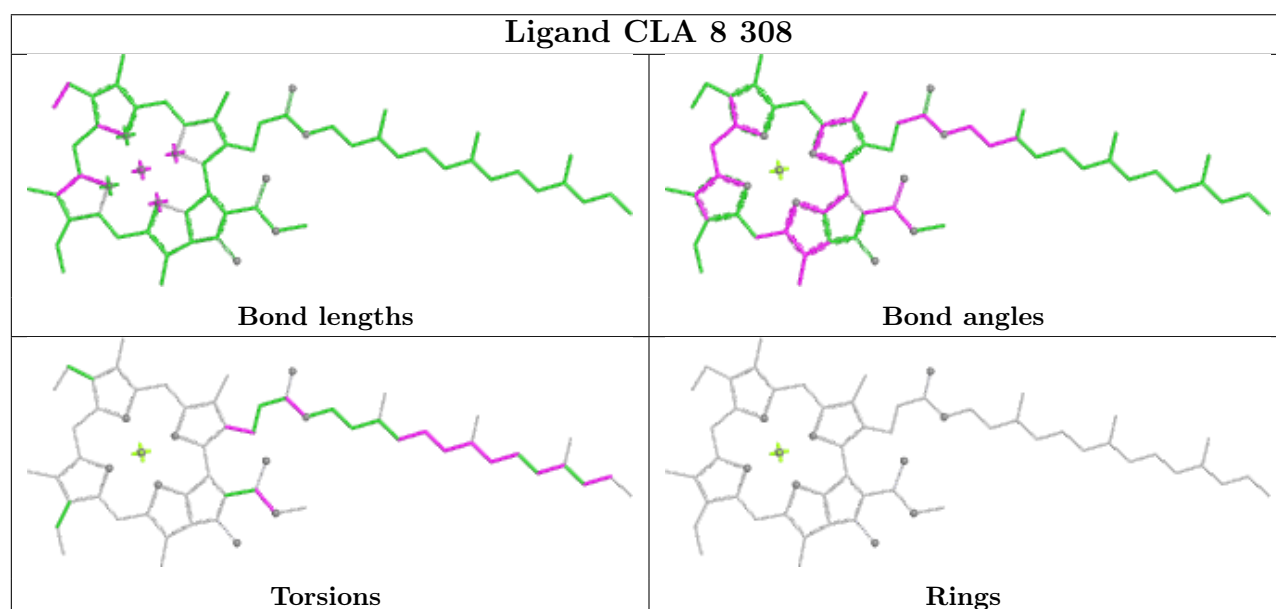
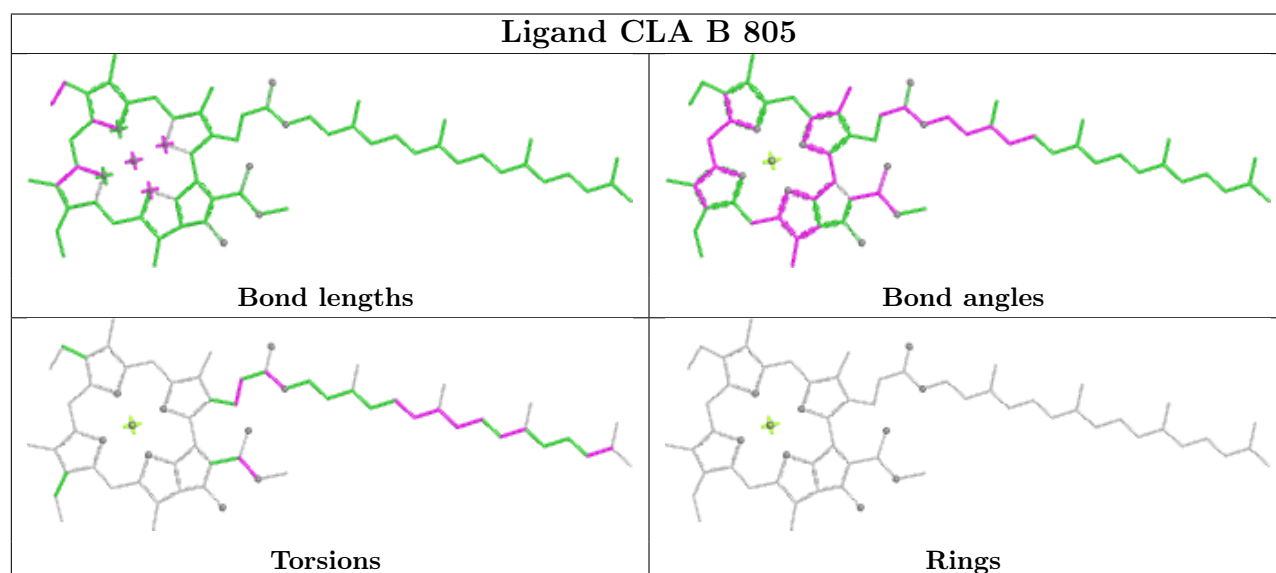
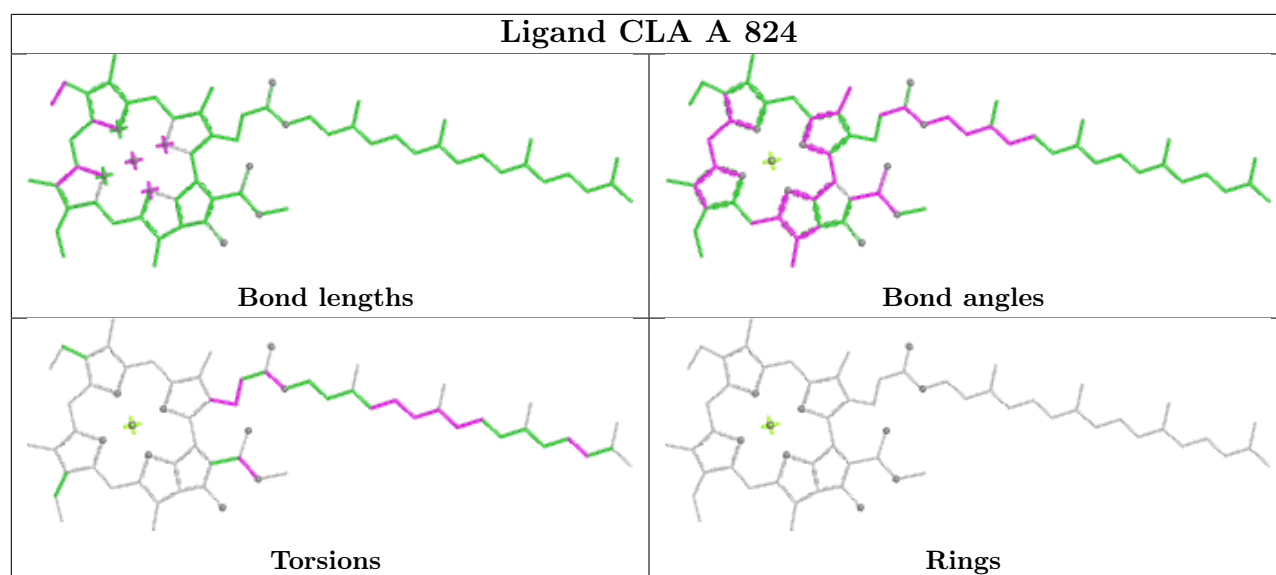


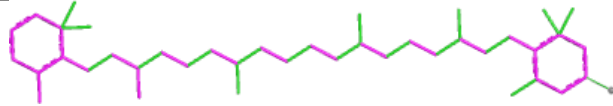
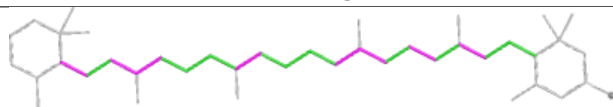
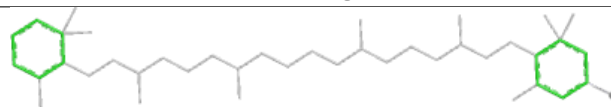
Ligand CLA 1 309

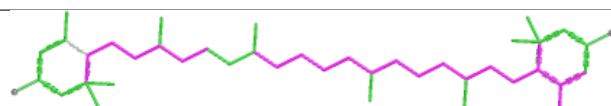
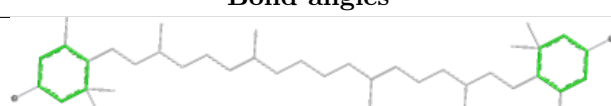


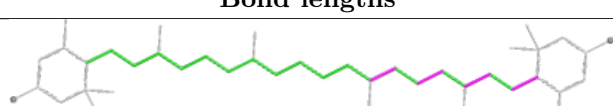
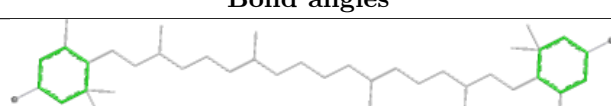
Ligand CLA A 839



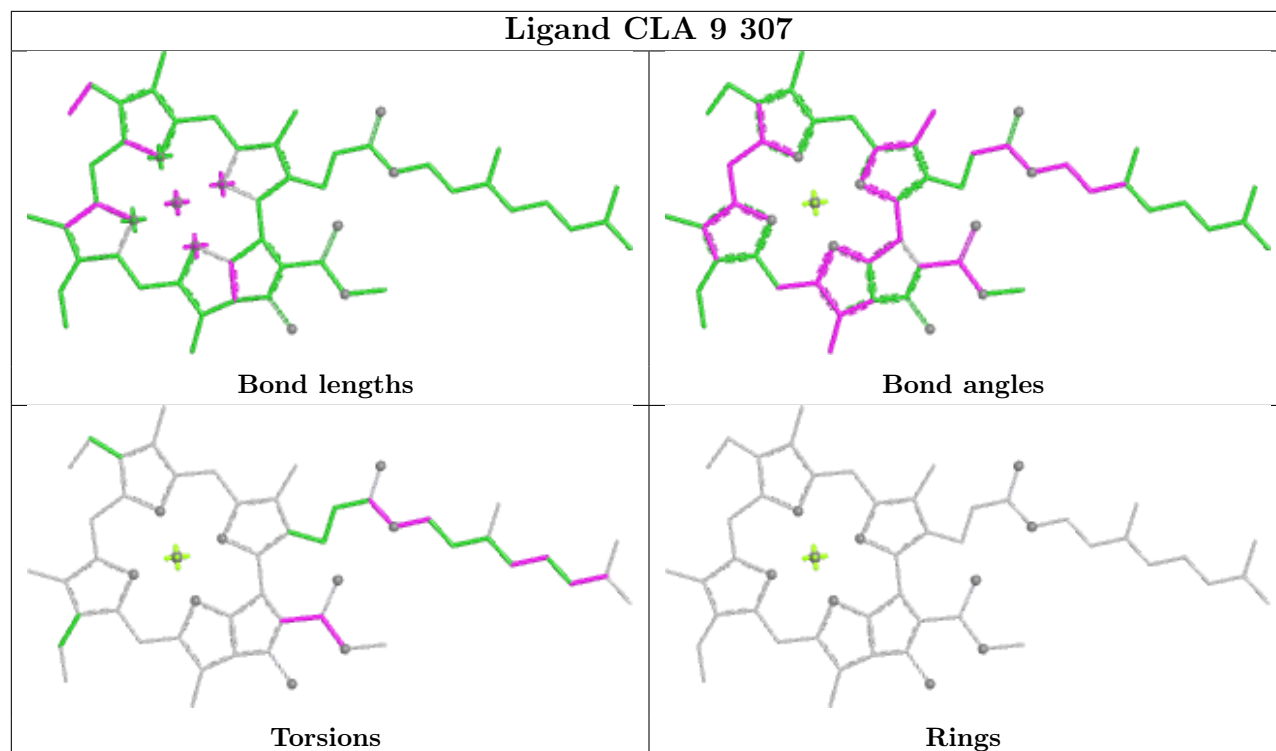


Ligand RRX F 306	
	Bond lengths
	Bond angles
	Torsions
	Rings

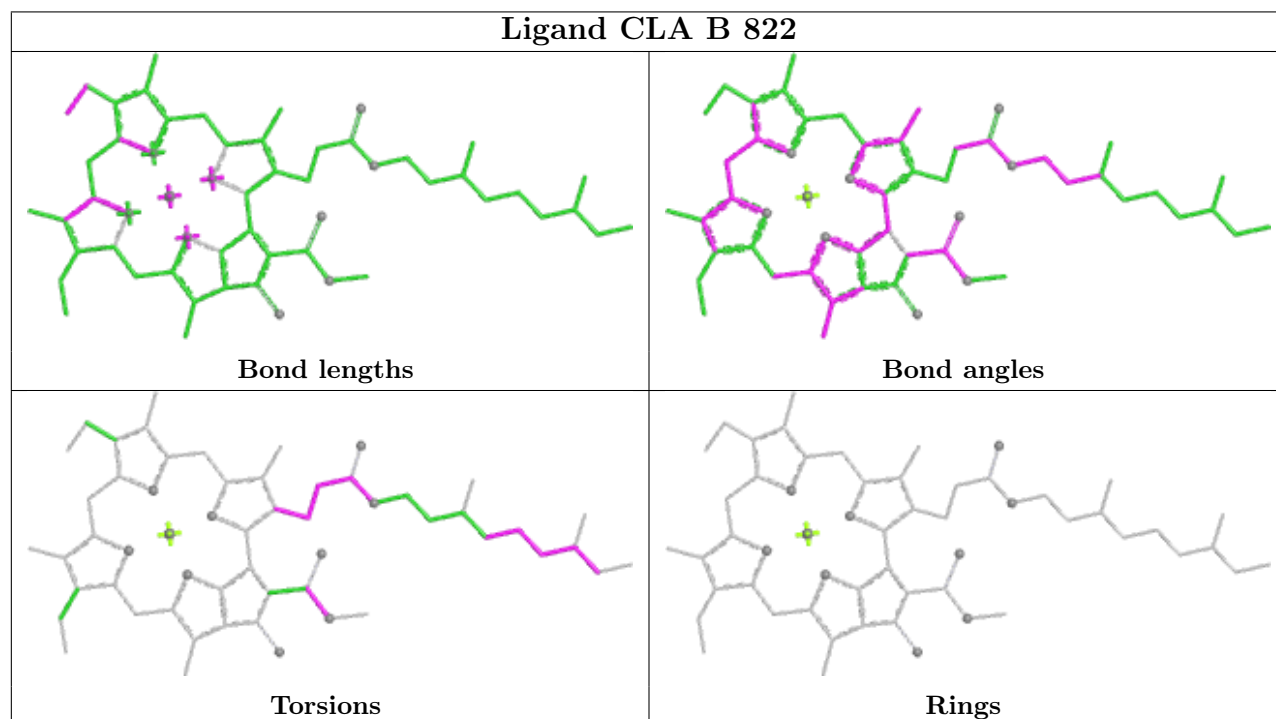
Ligand LUT 6 304	
	Bond lengths
	Bond angles
	Torsions
	Rings

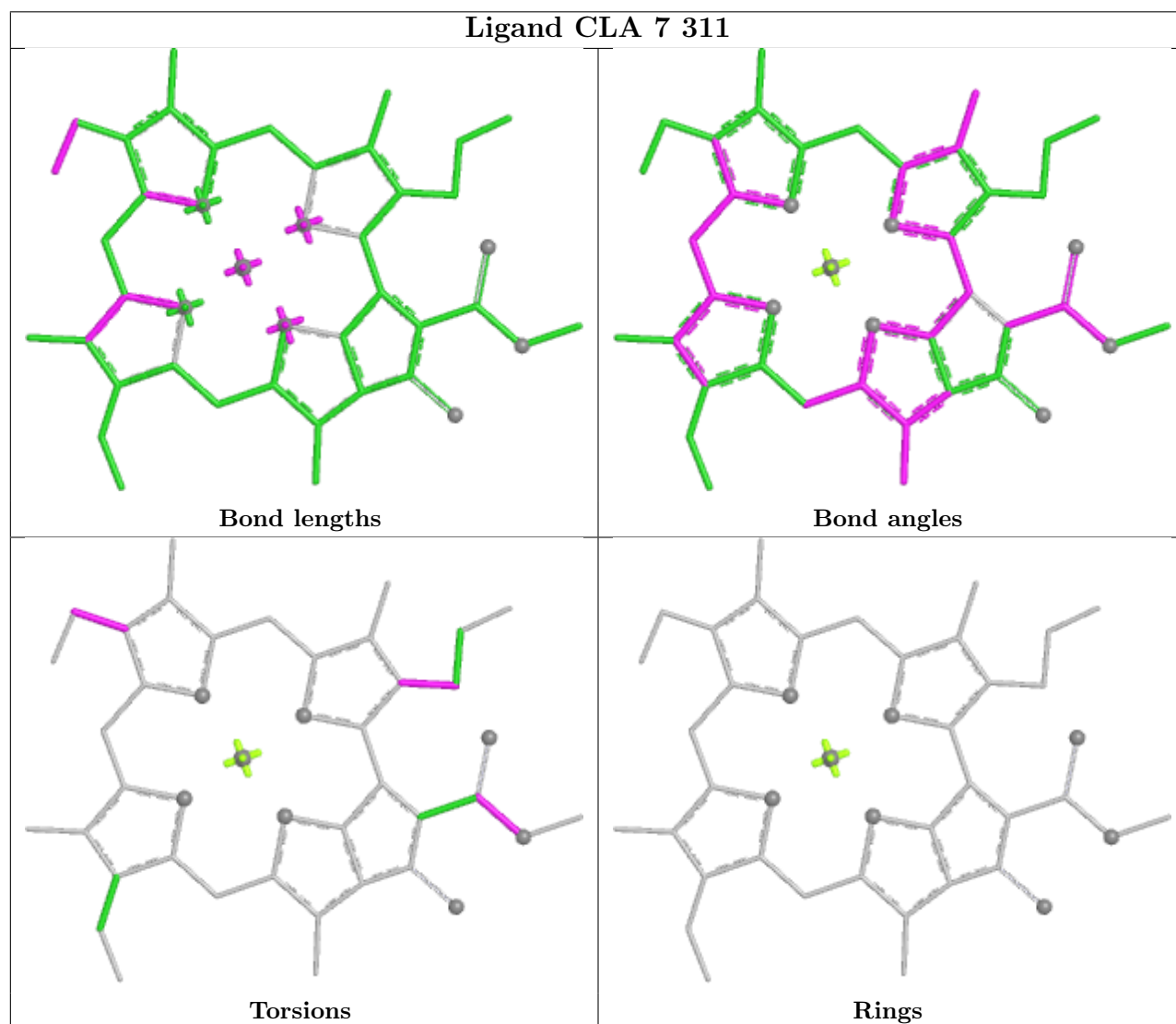
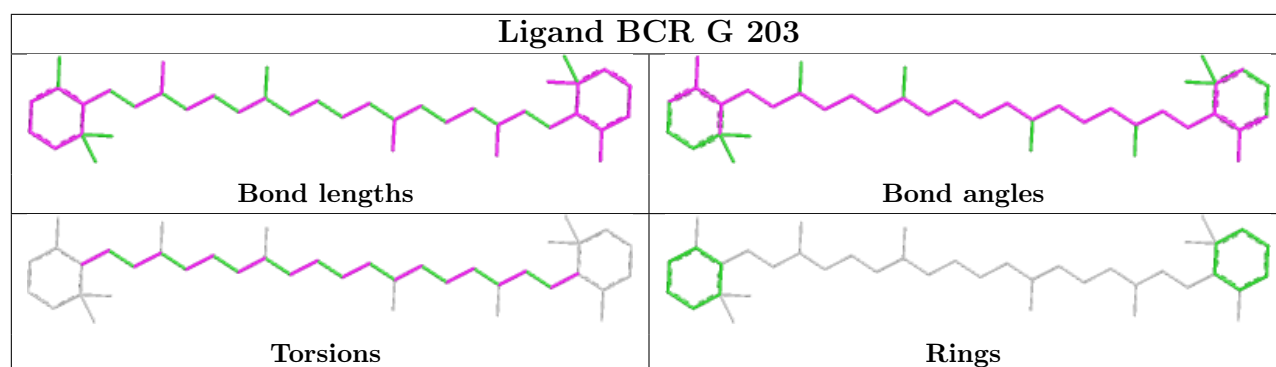
Ligand LUT 5 303	
	Bond lengths
	Bond angles
	Torsions
	Rings

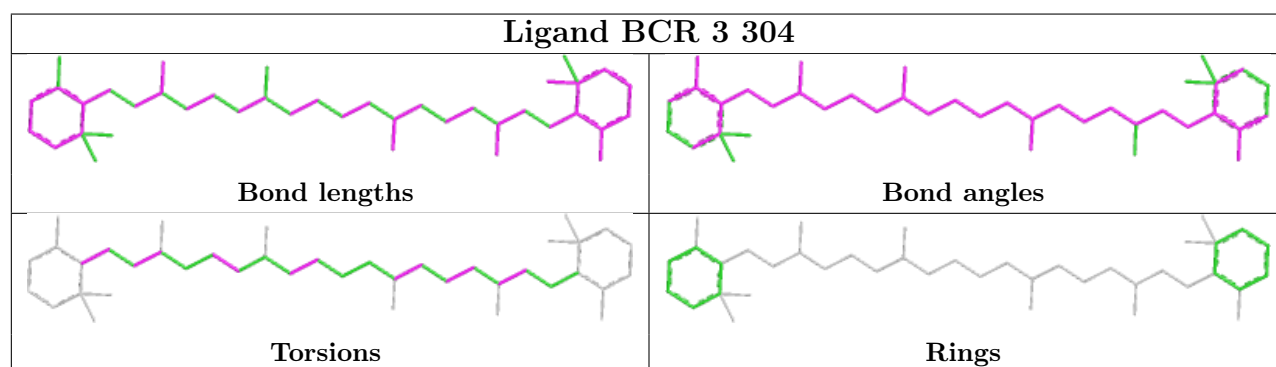
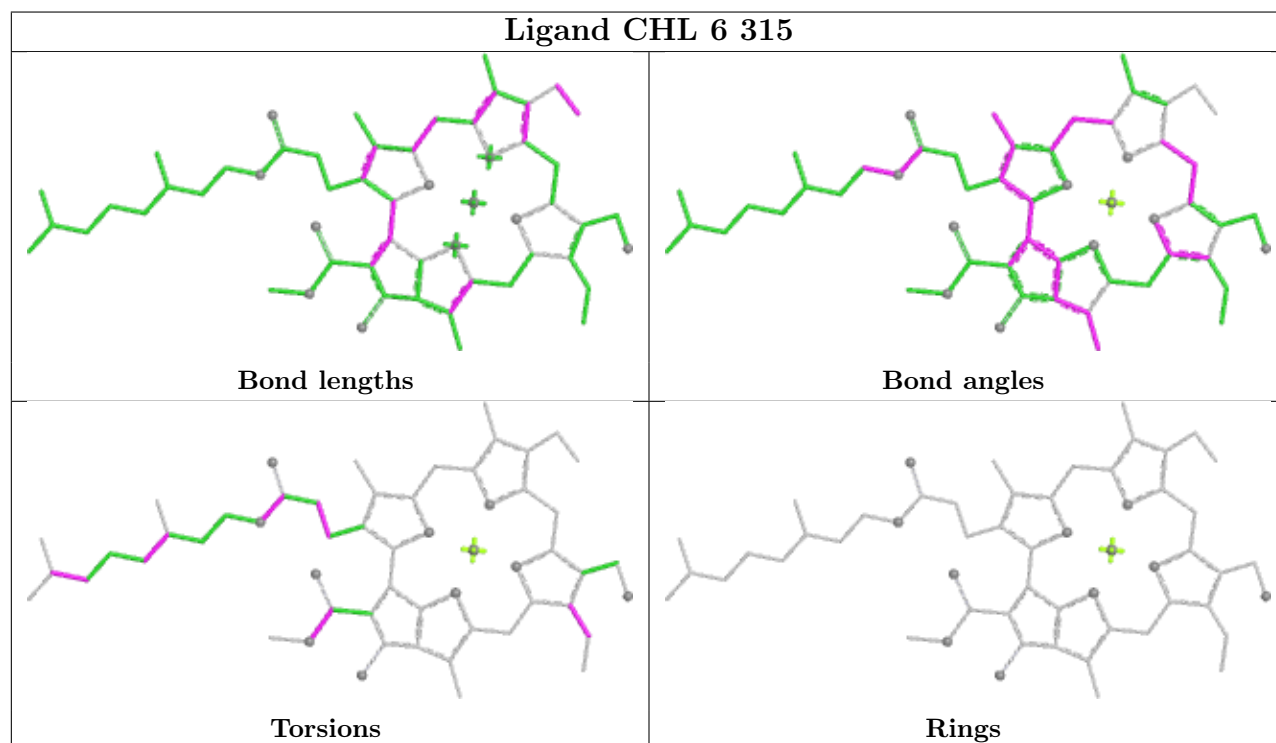
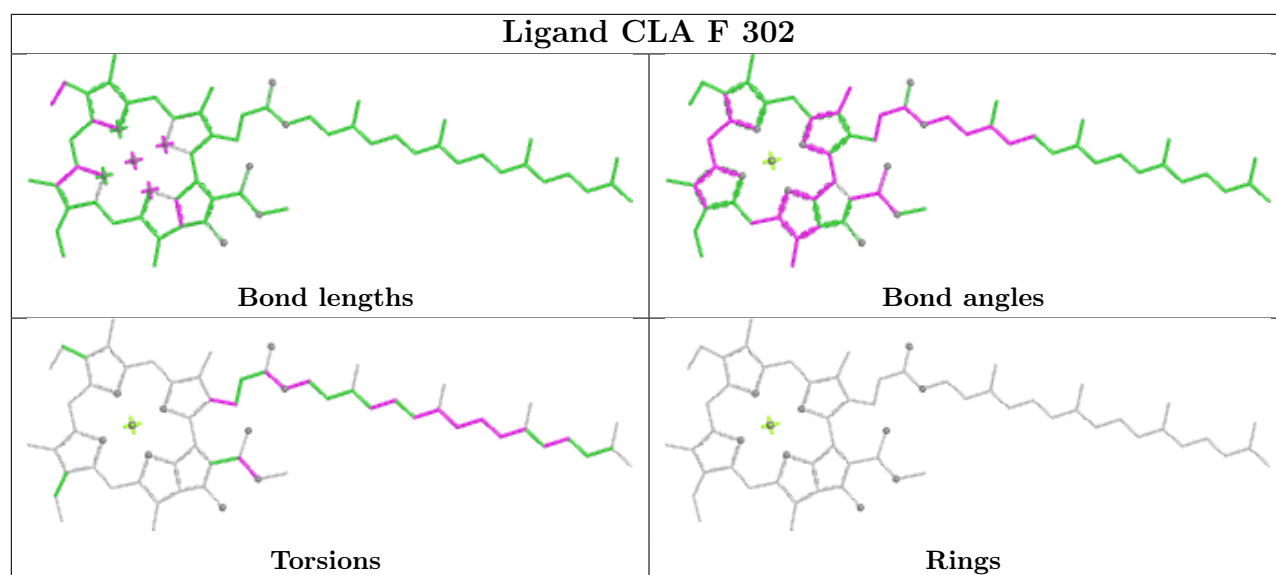
Ligand CLA 9 307

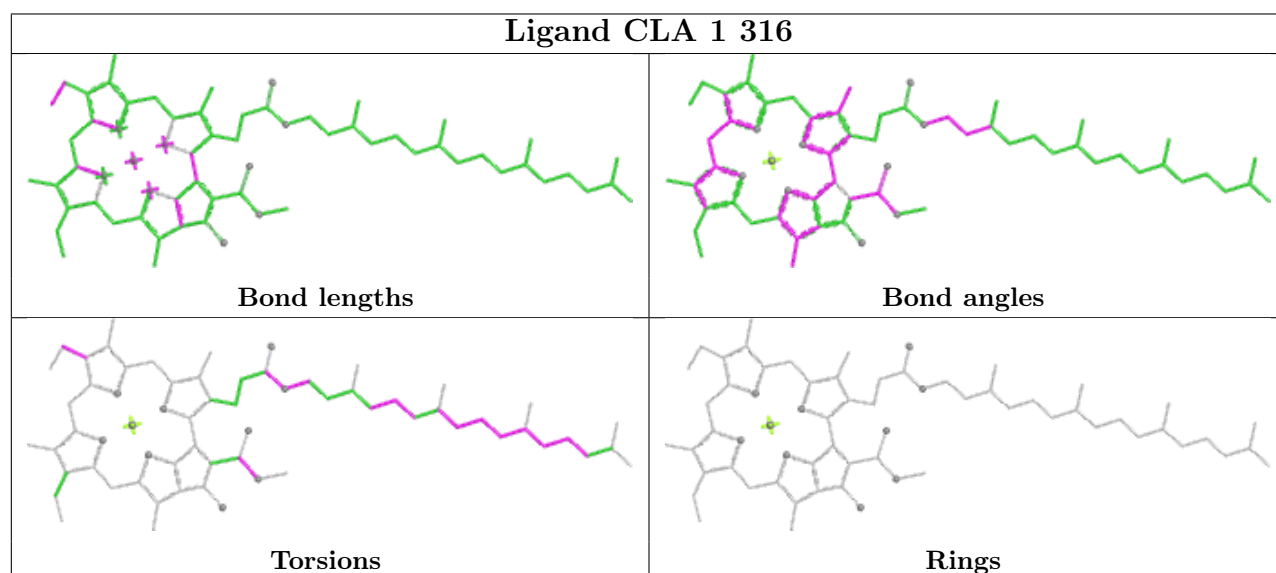
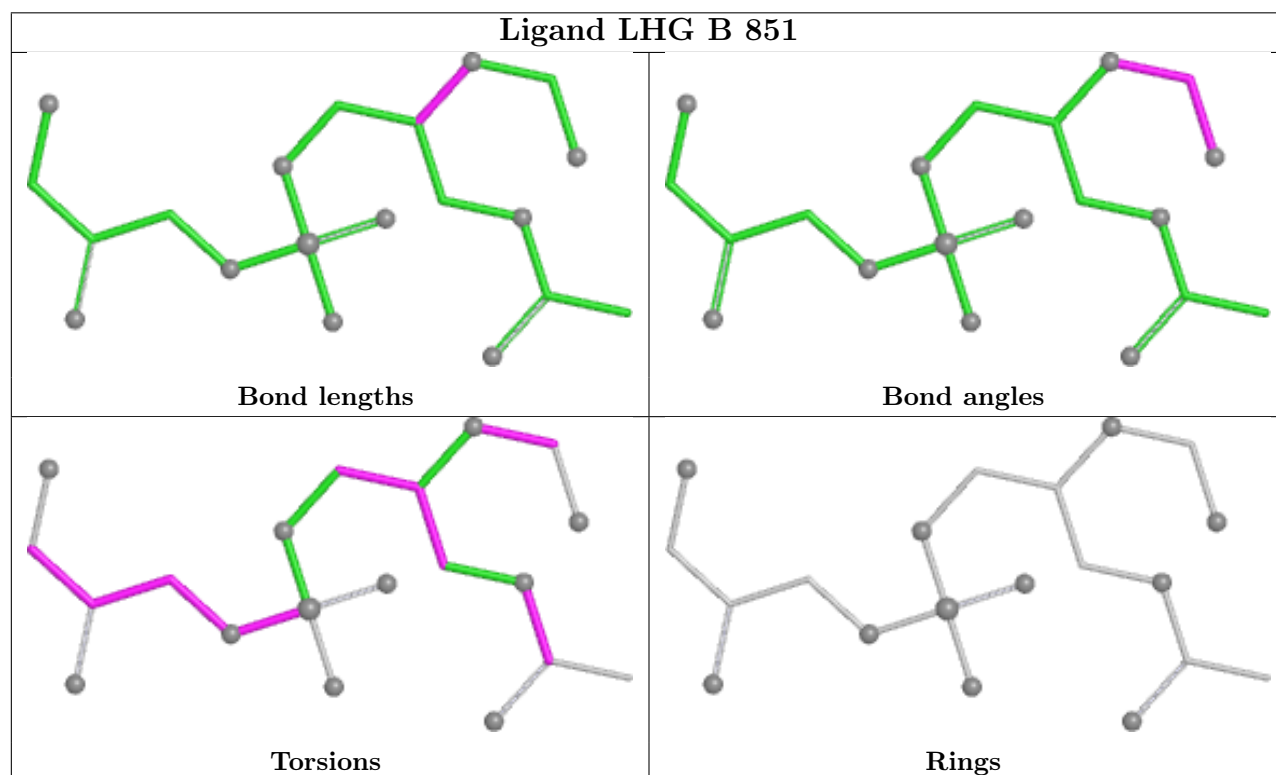
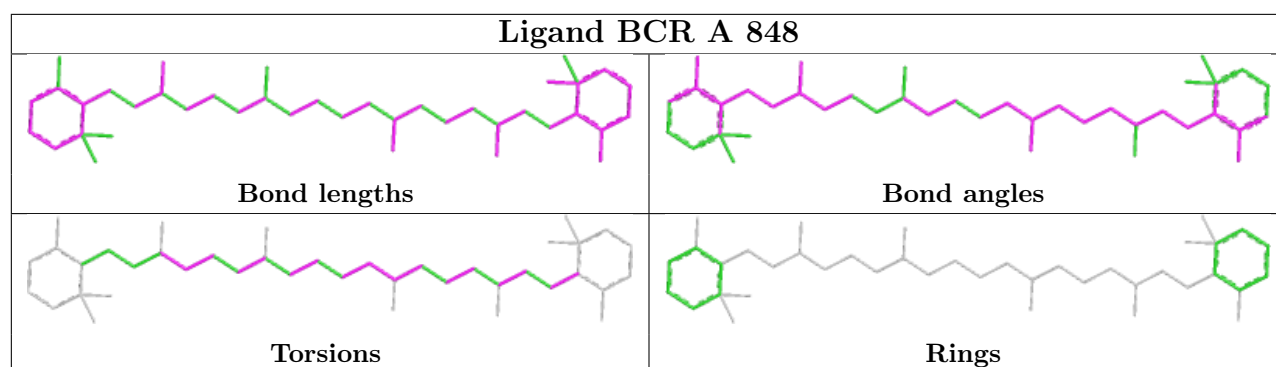


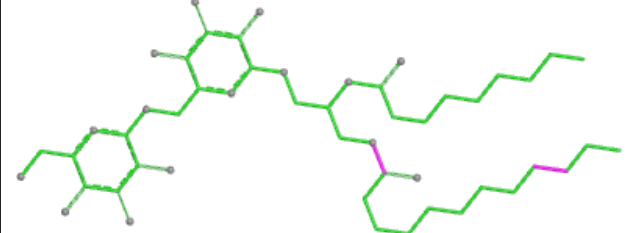
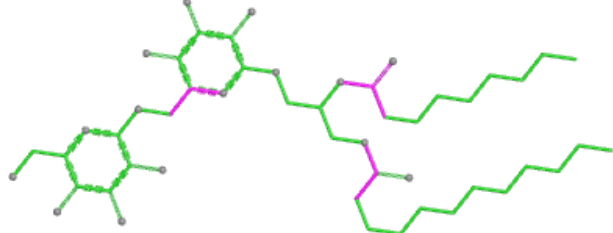
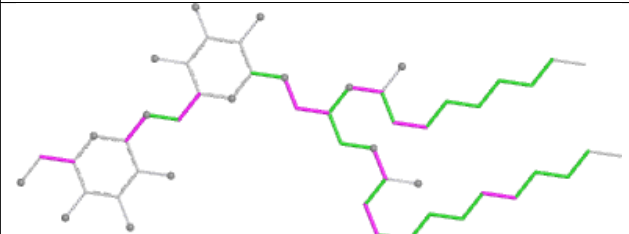
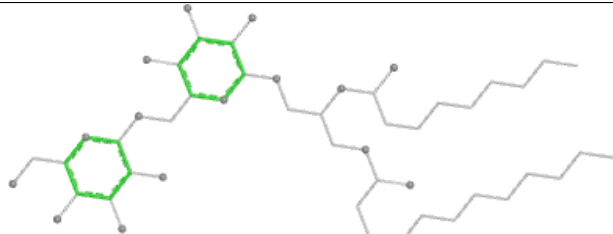
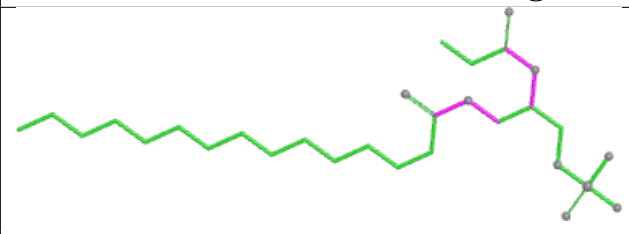
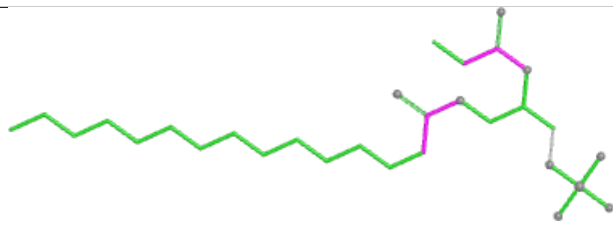
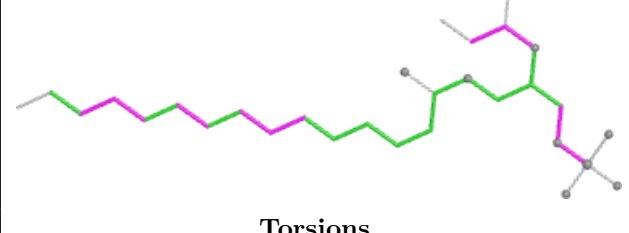
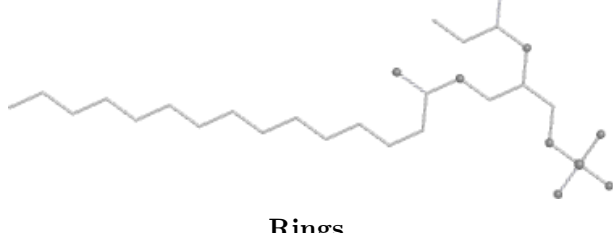
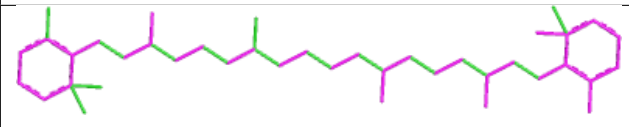
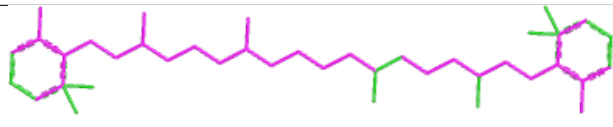
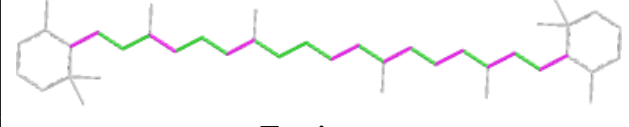
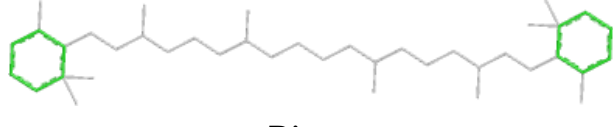
Ligand CLA B 822

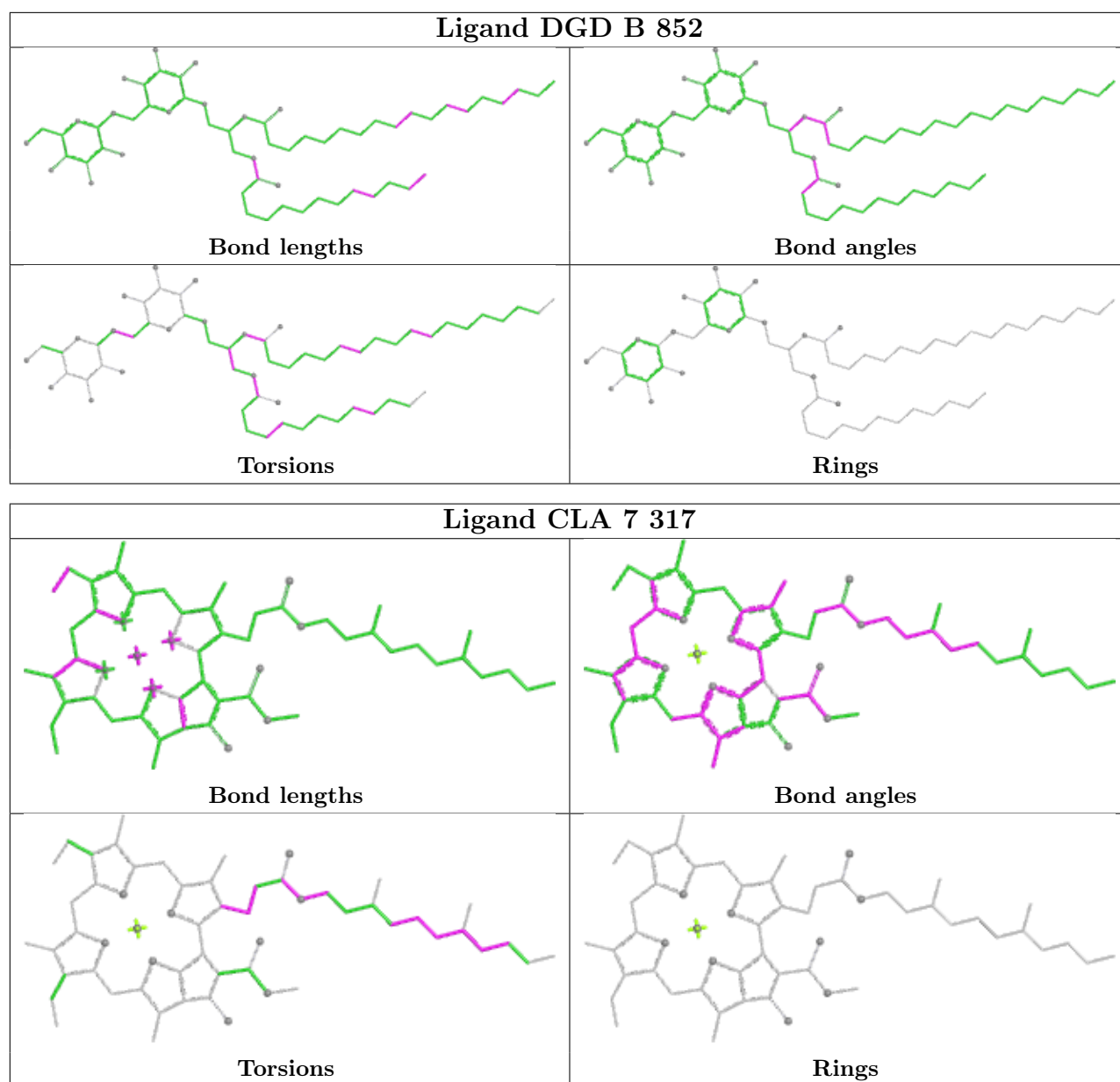


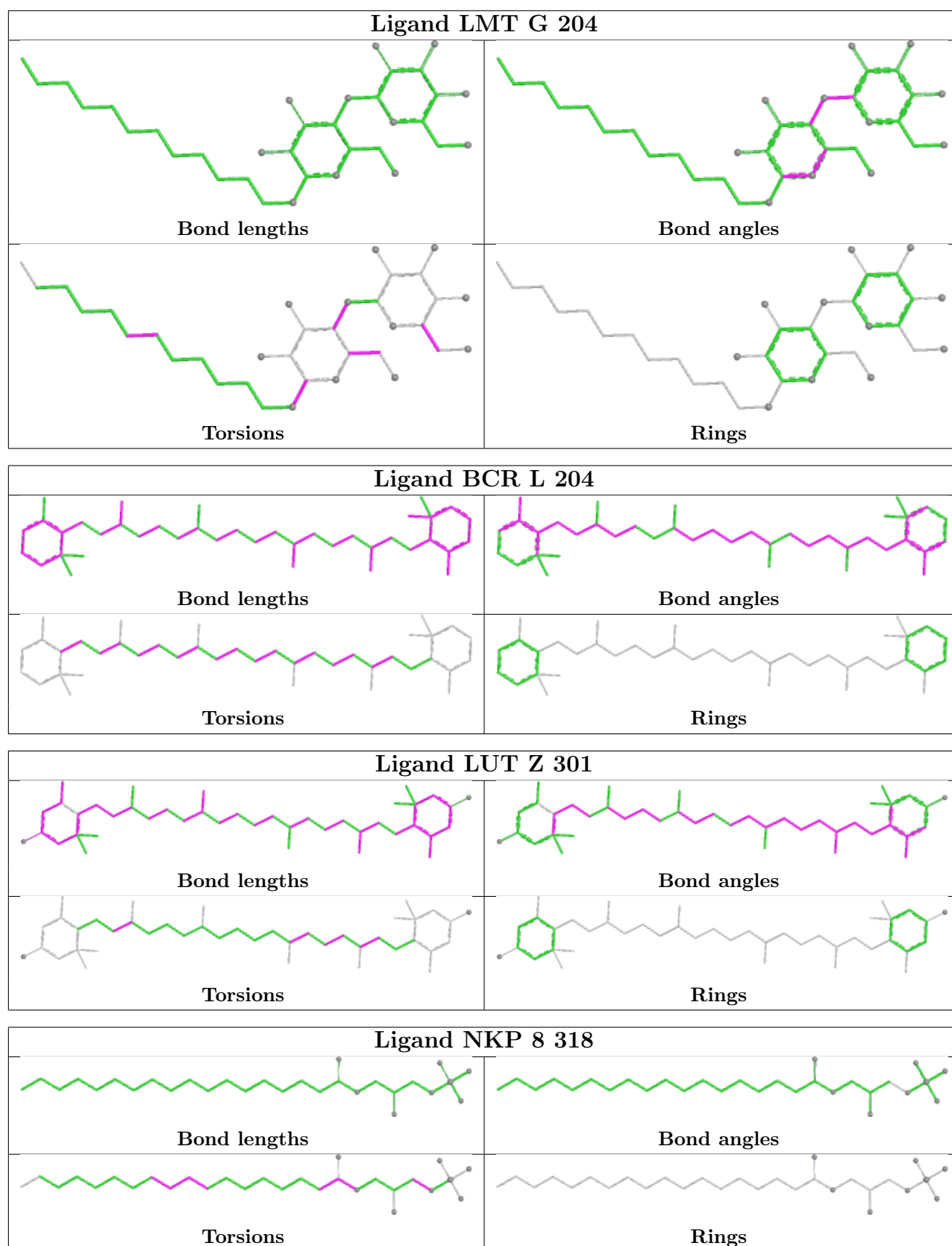




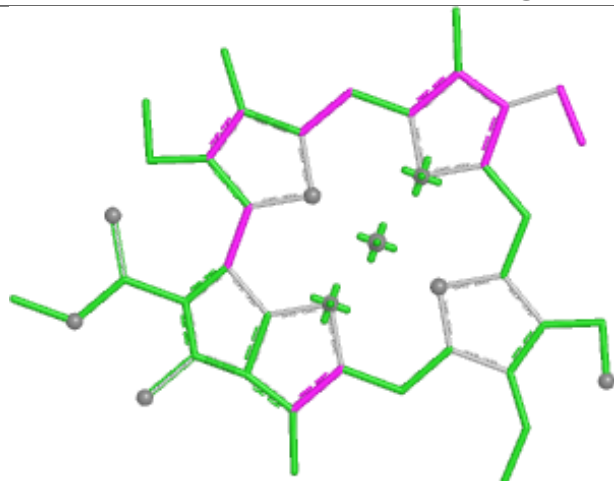


Ligand DGD 1 319	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand 3PH 8 320	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

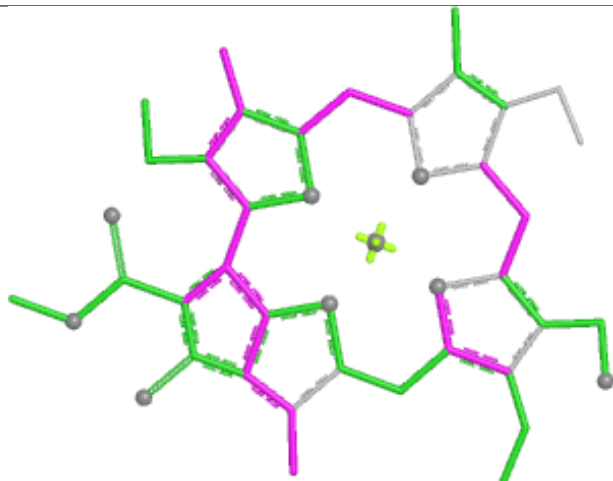




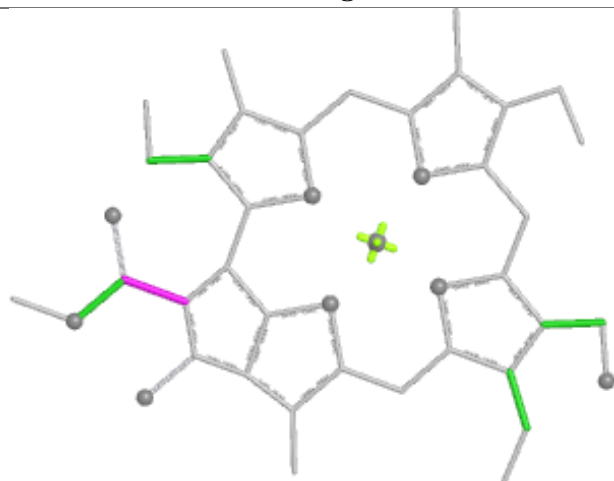
Ligand CHL 6 320



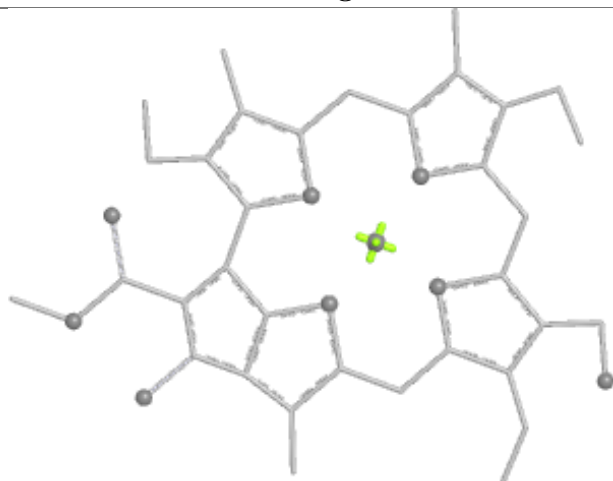
Bond lengths



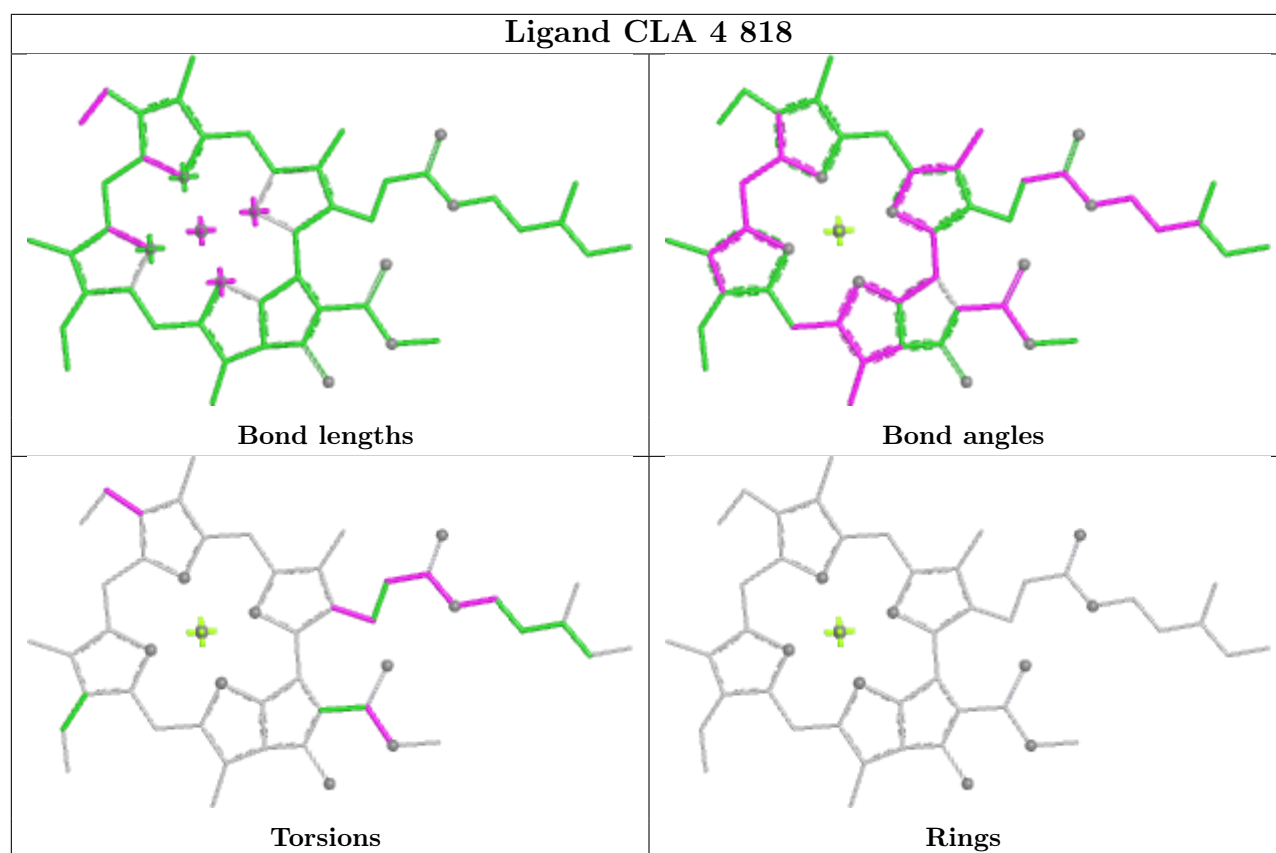
Bond angles

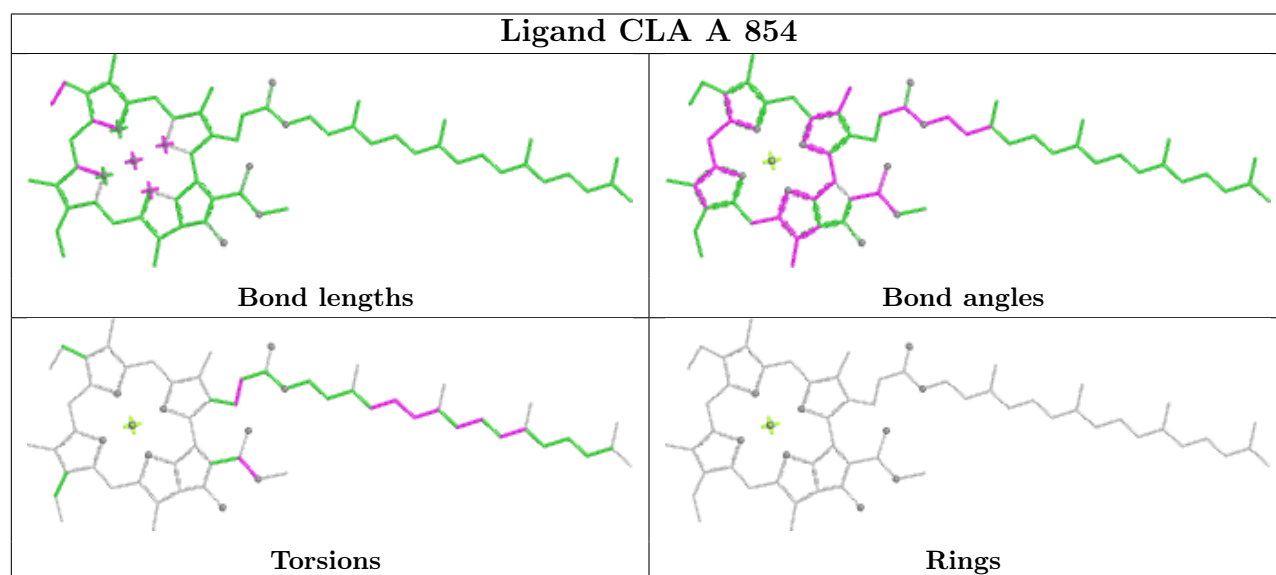
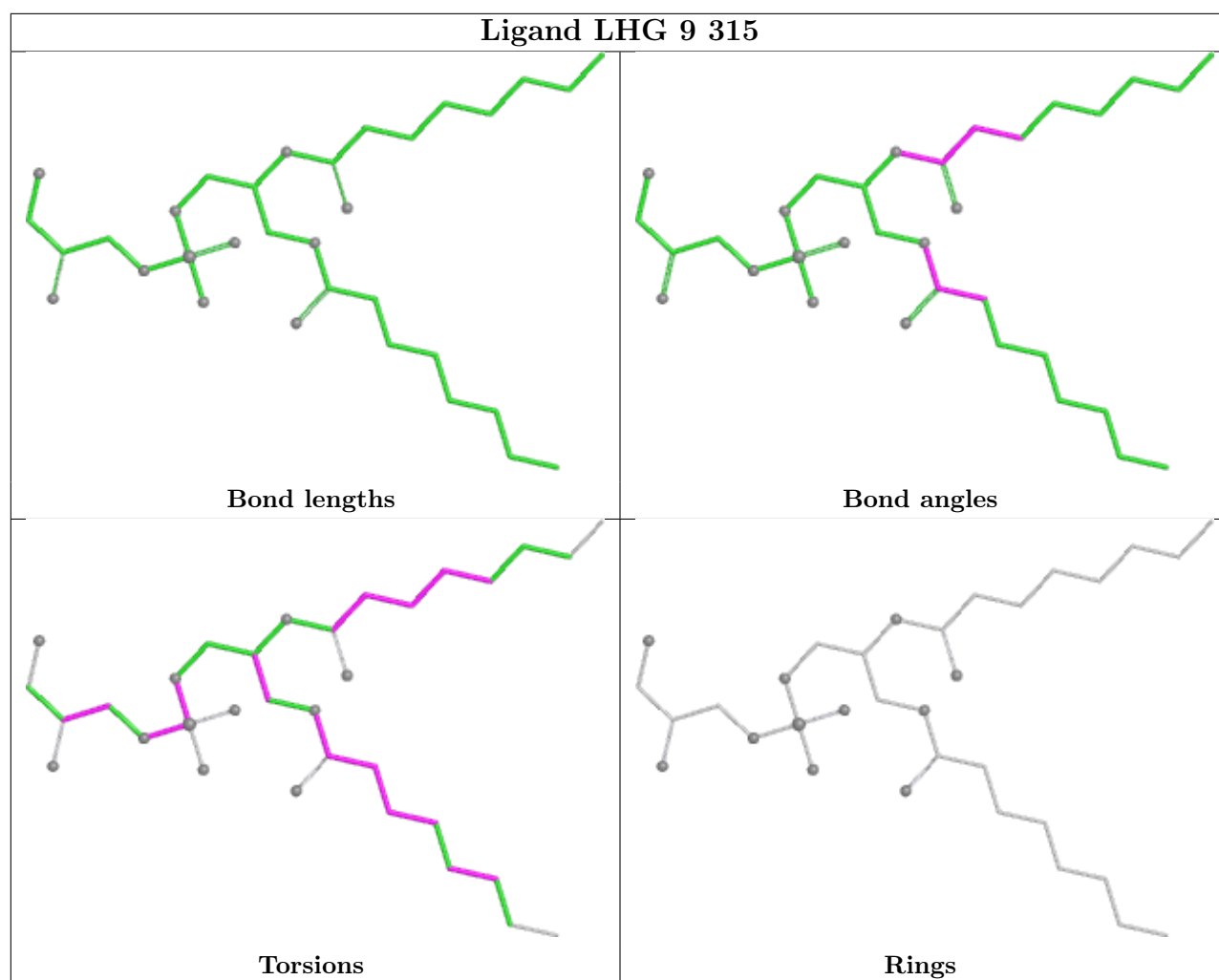


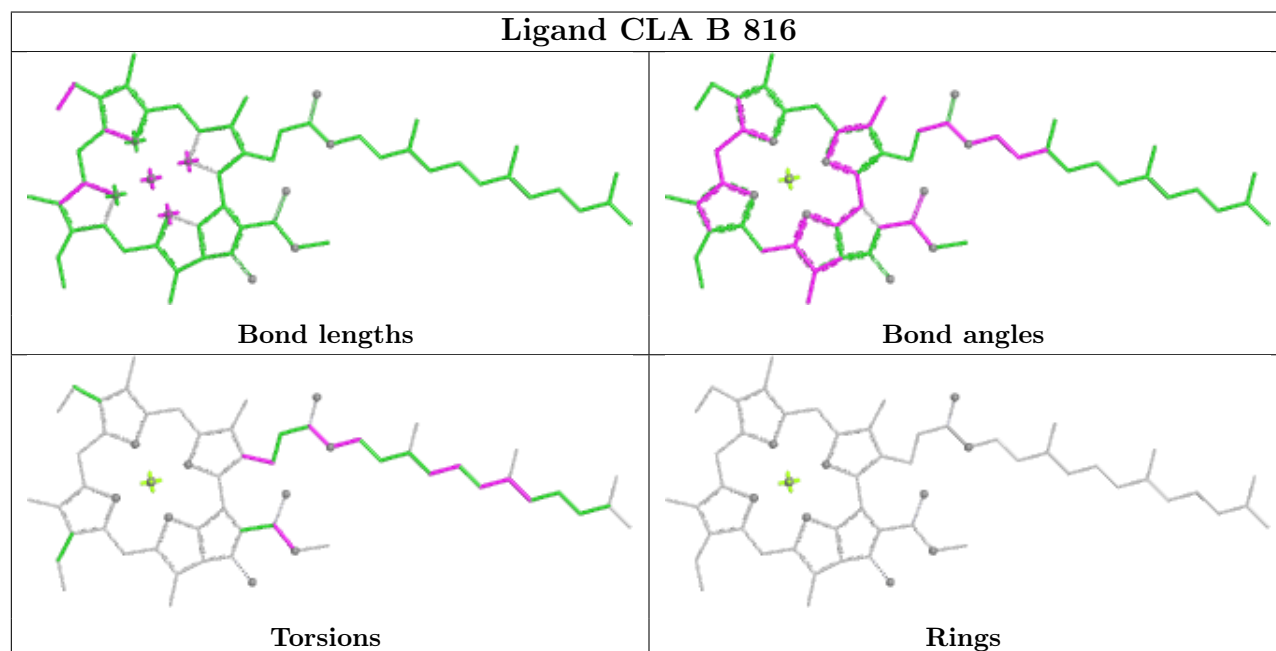
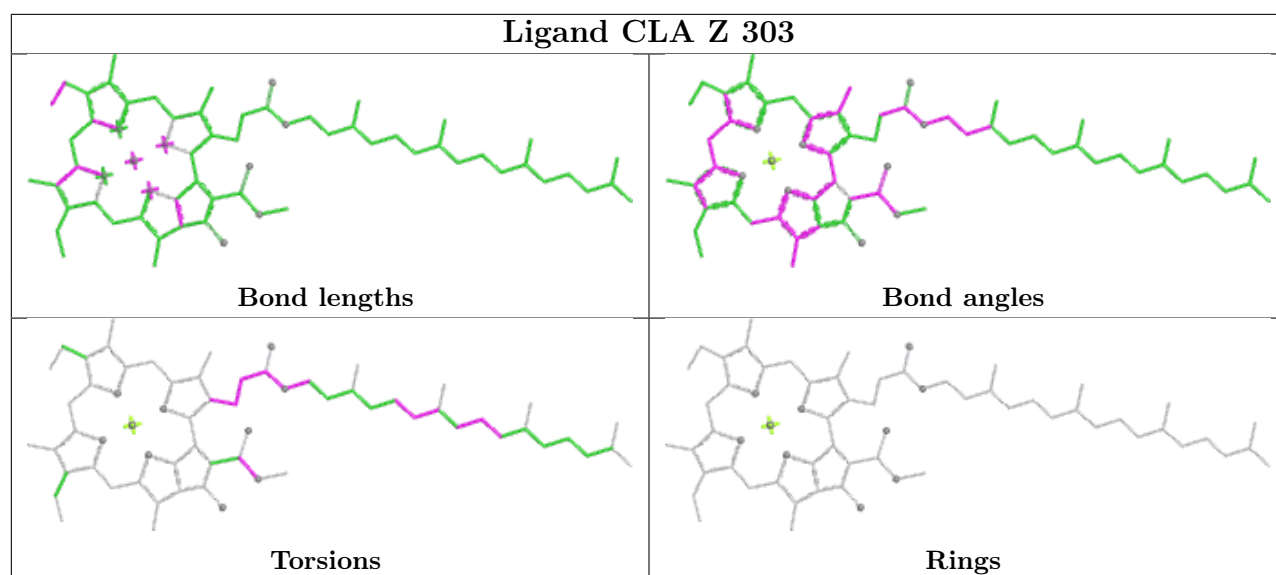
Torsions



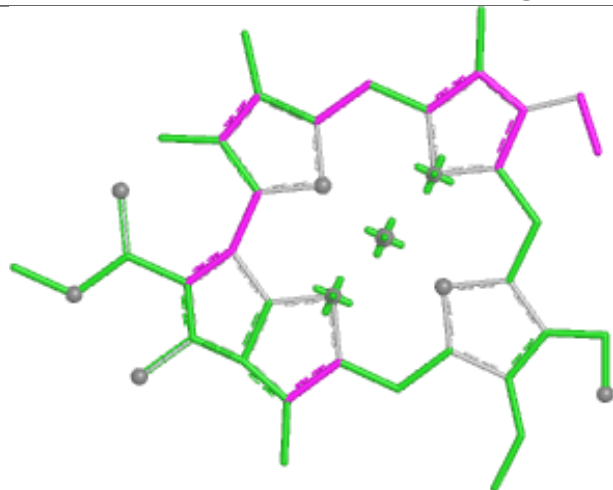
Rings



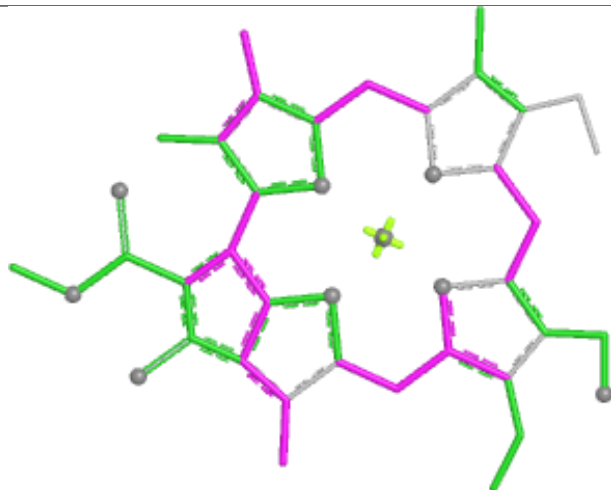




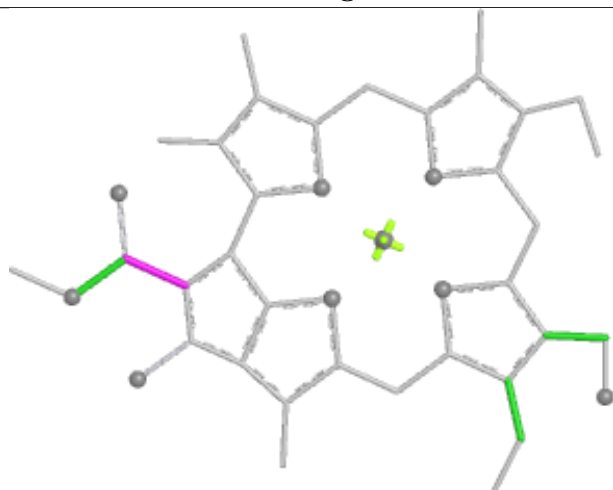
Ligand CHL 9 314



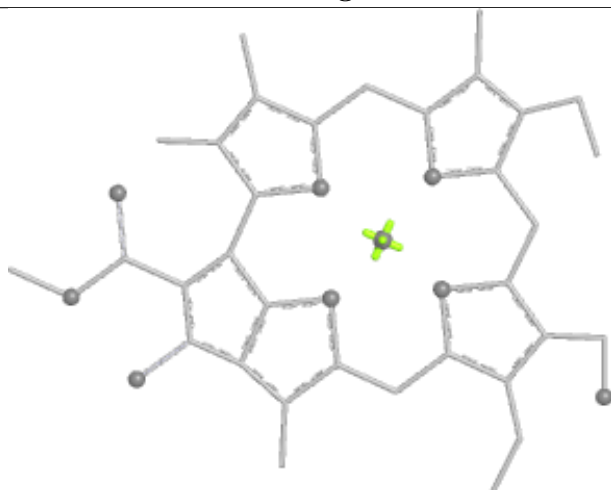
Bond lengths



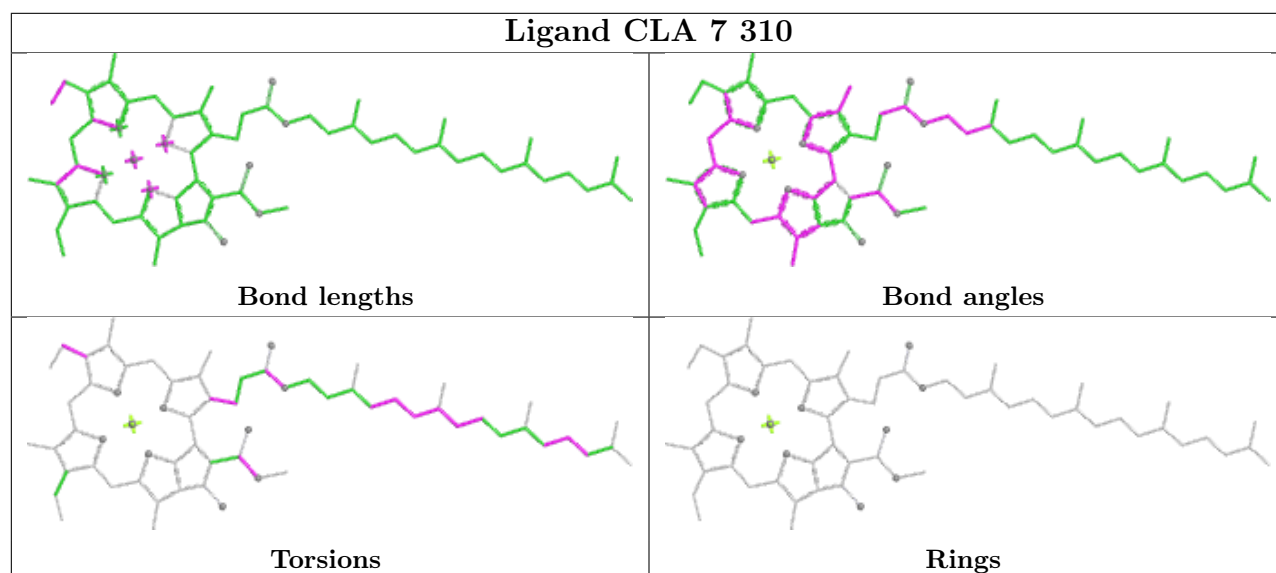
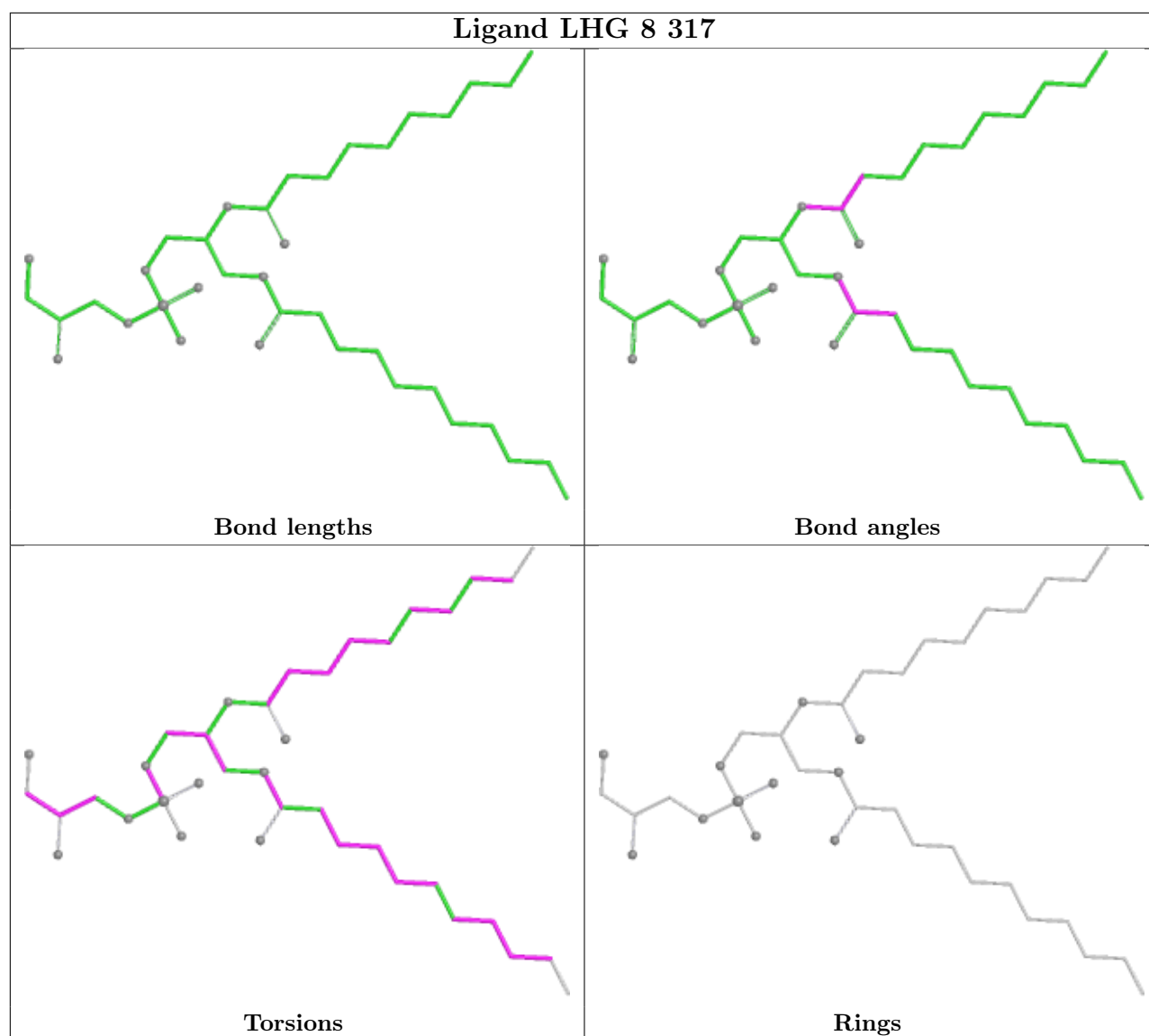
Bond angles

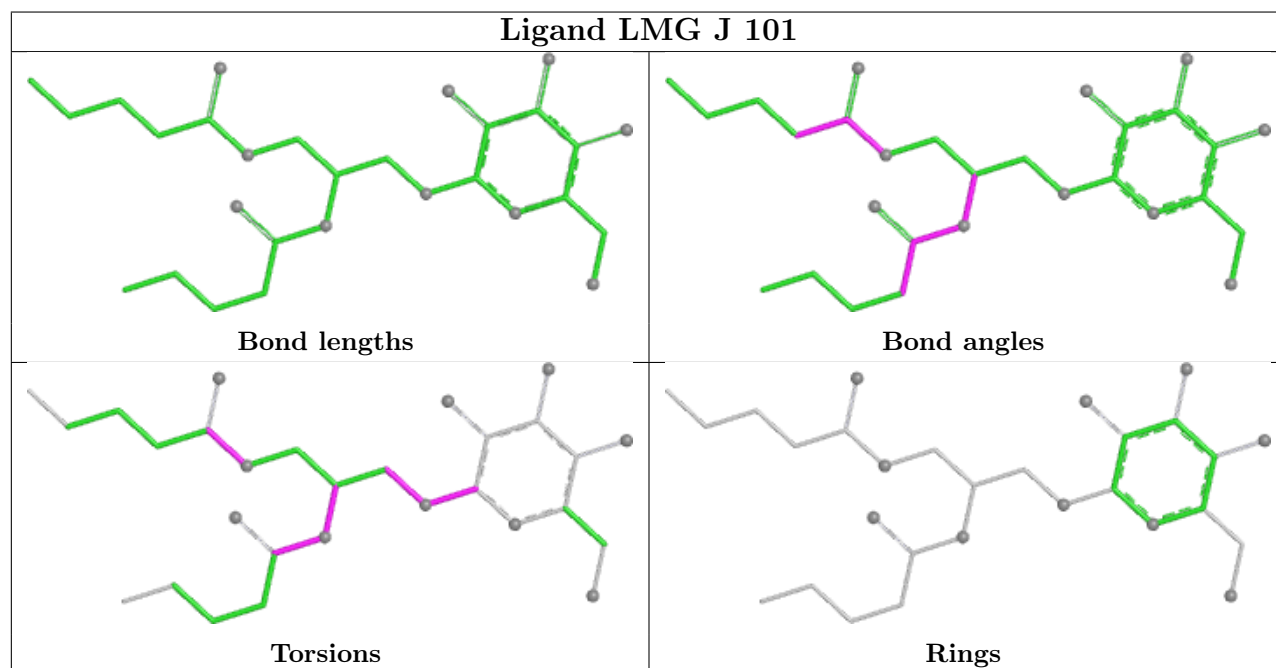
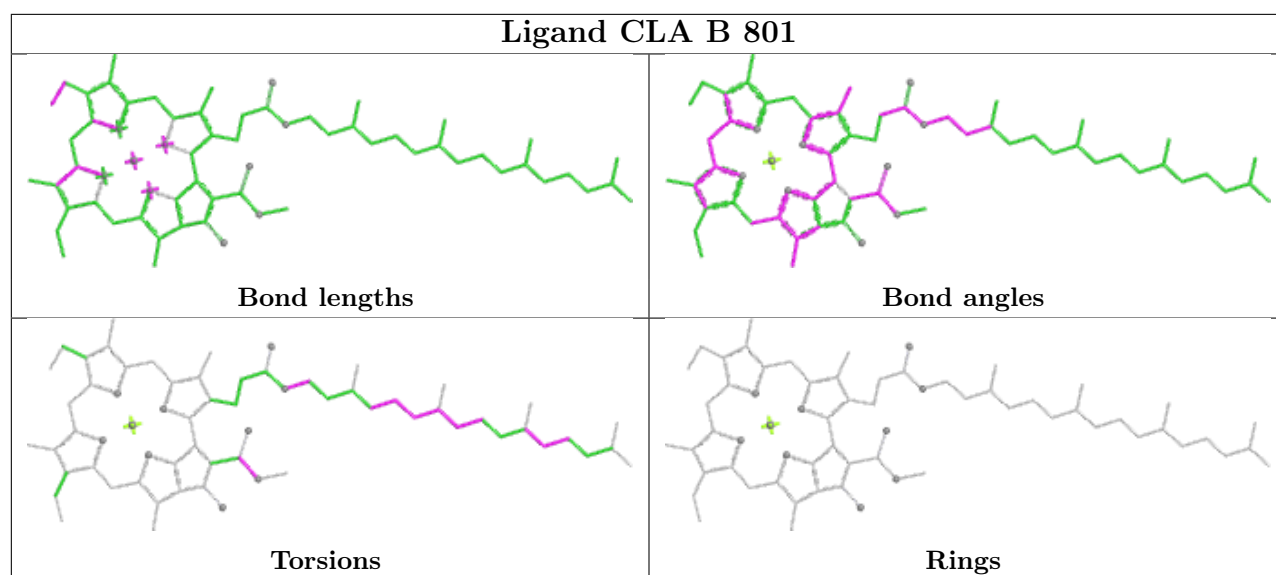


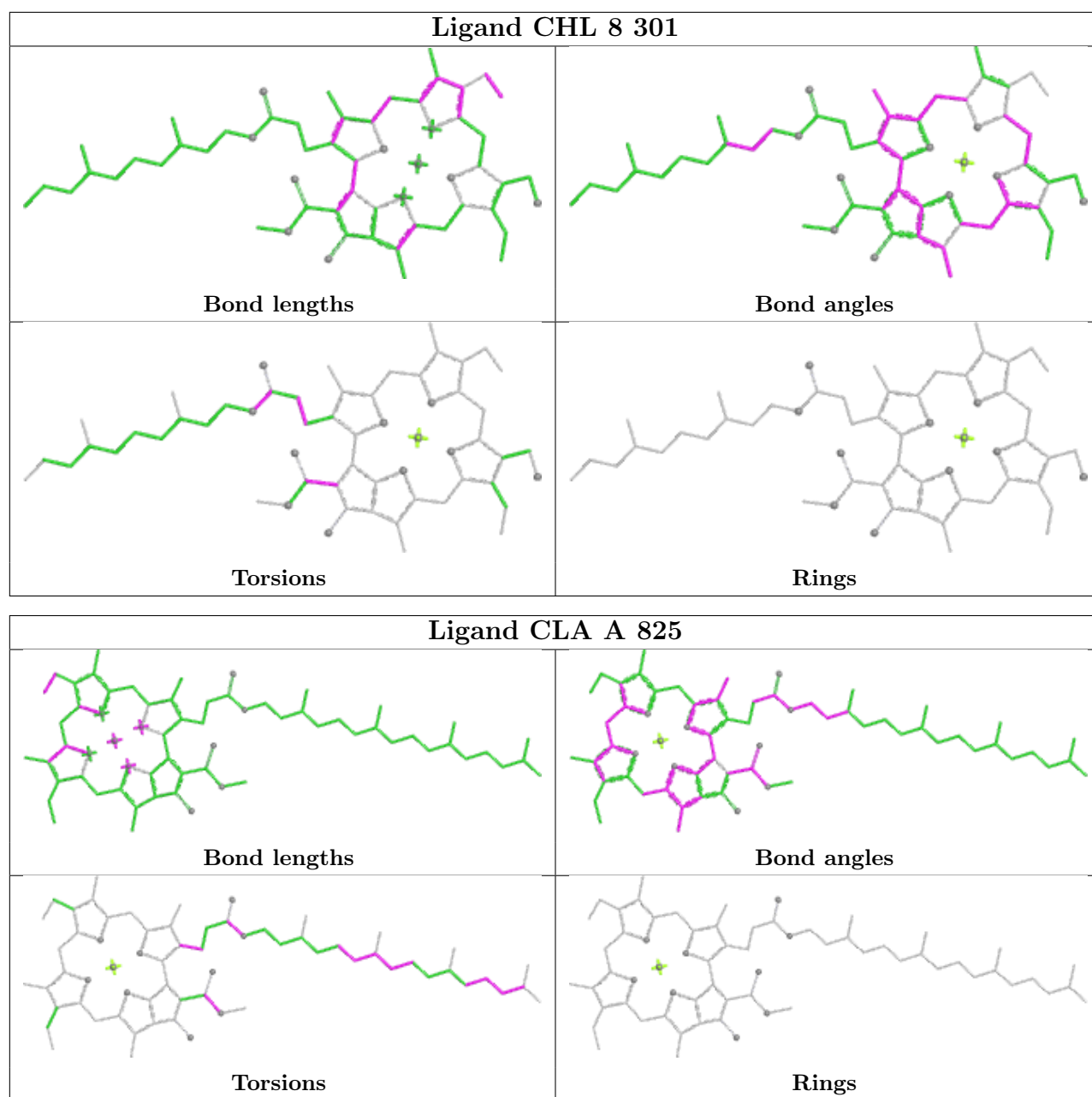
Torsions



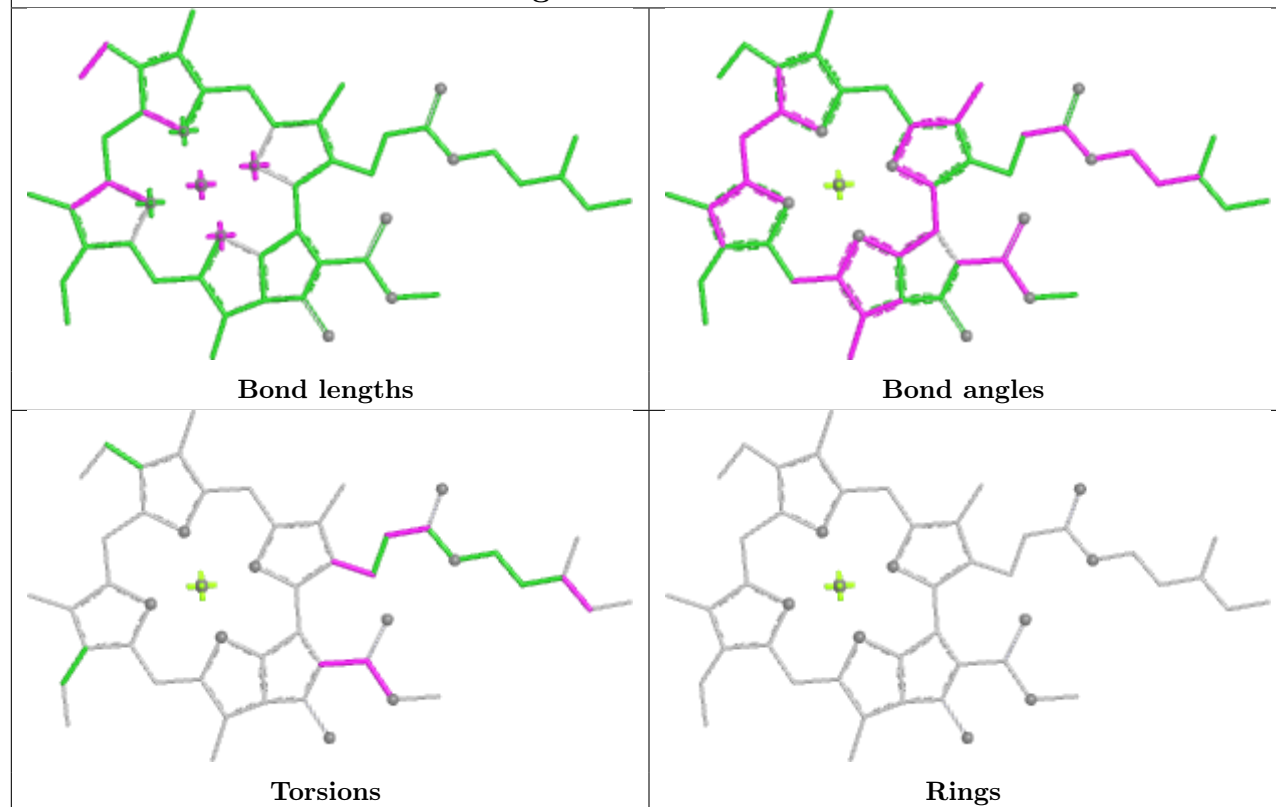
Rings



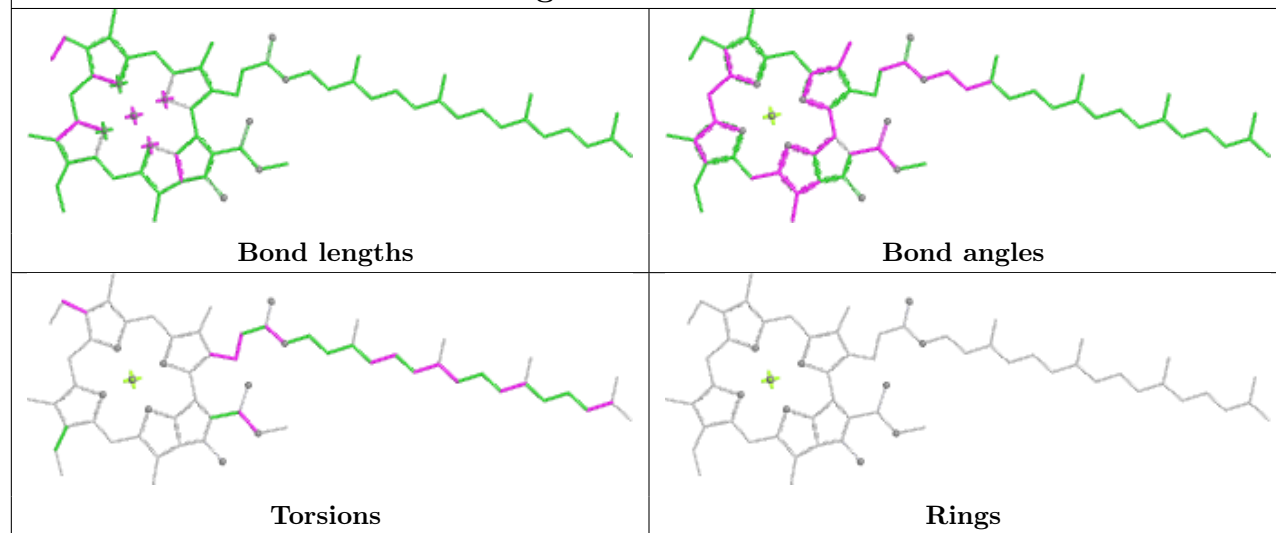


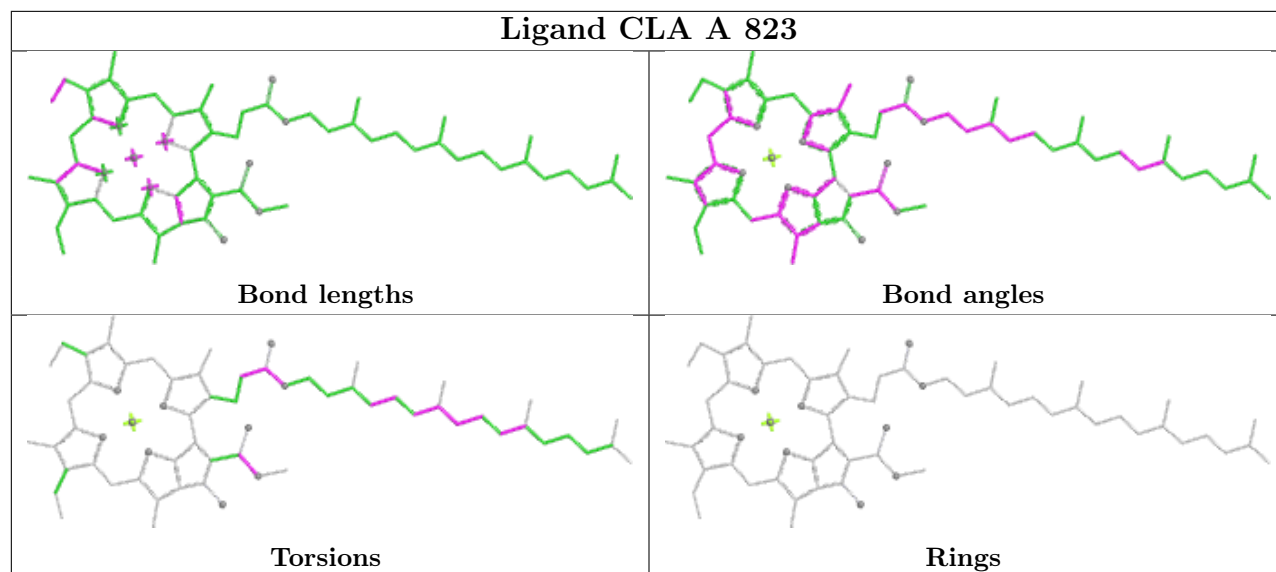
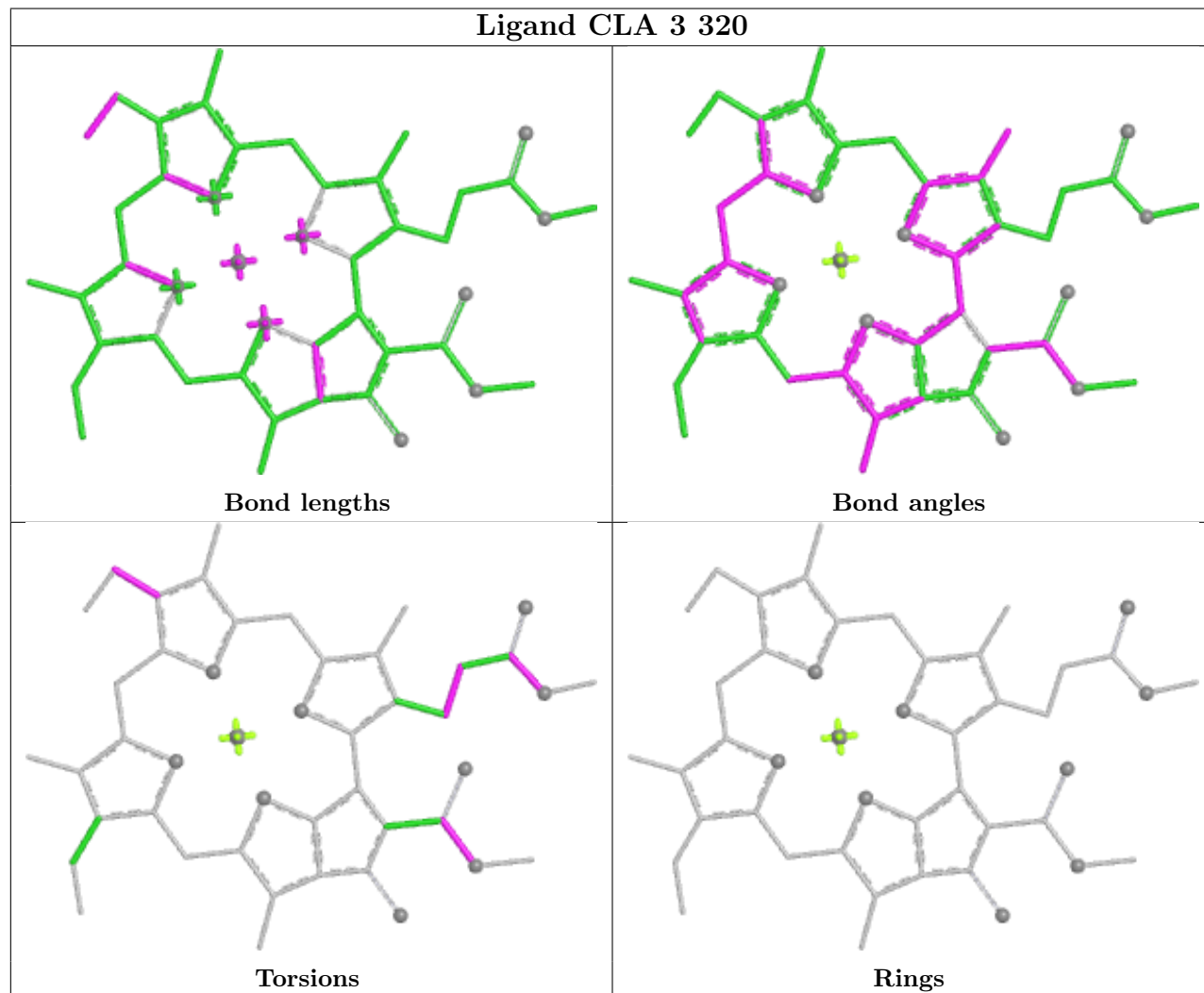


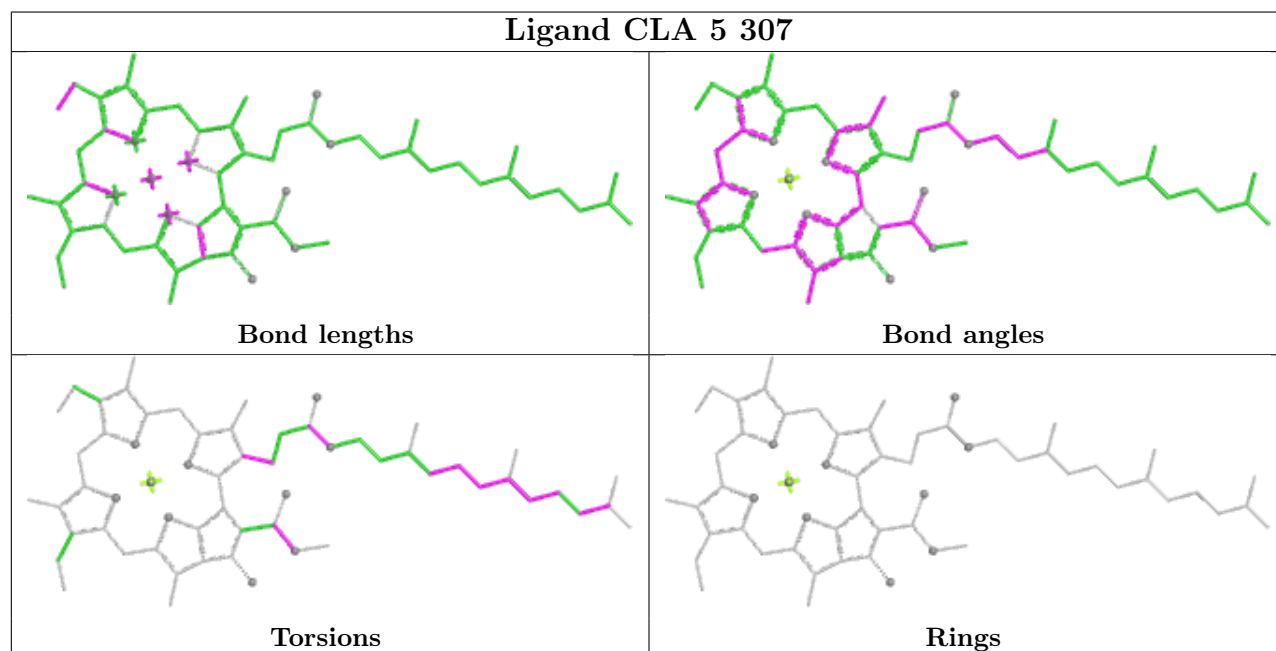
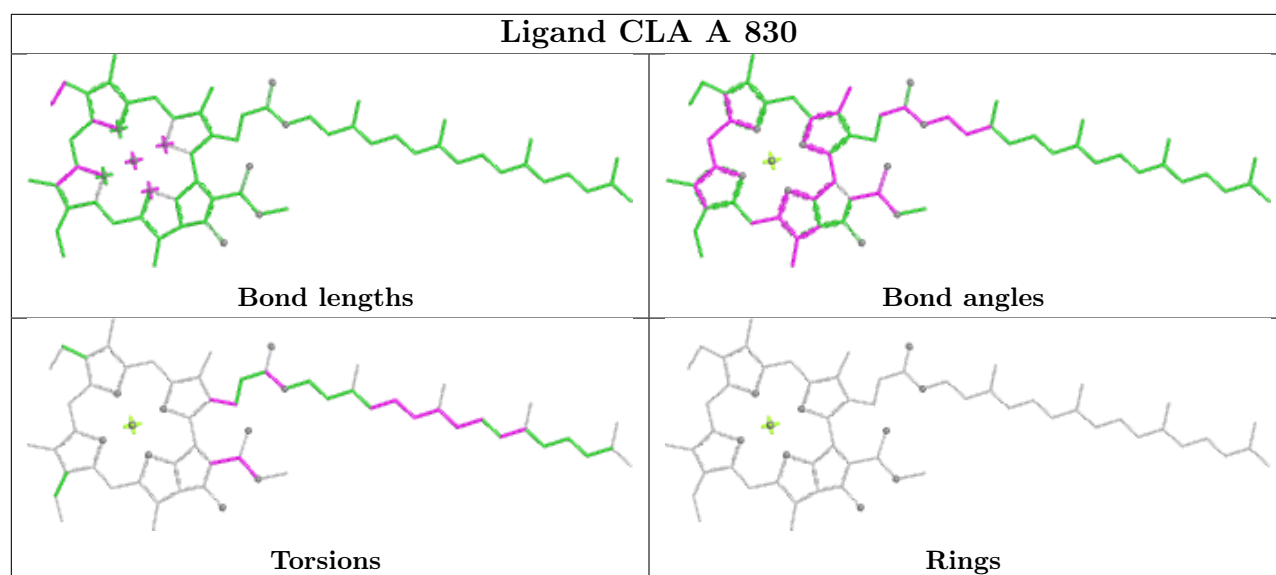
Ligand CLA B 837

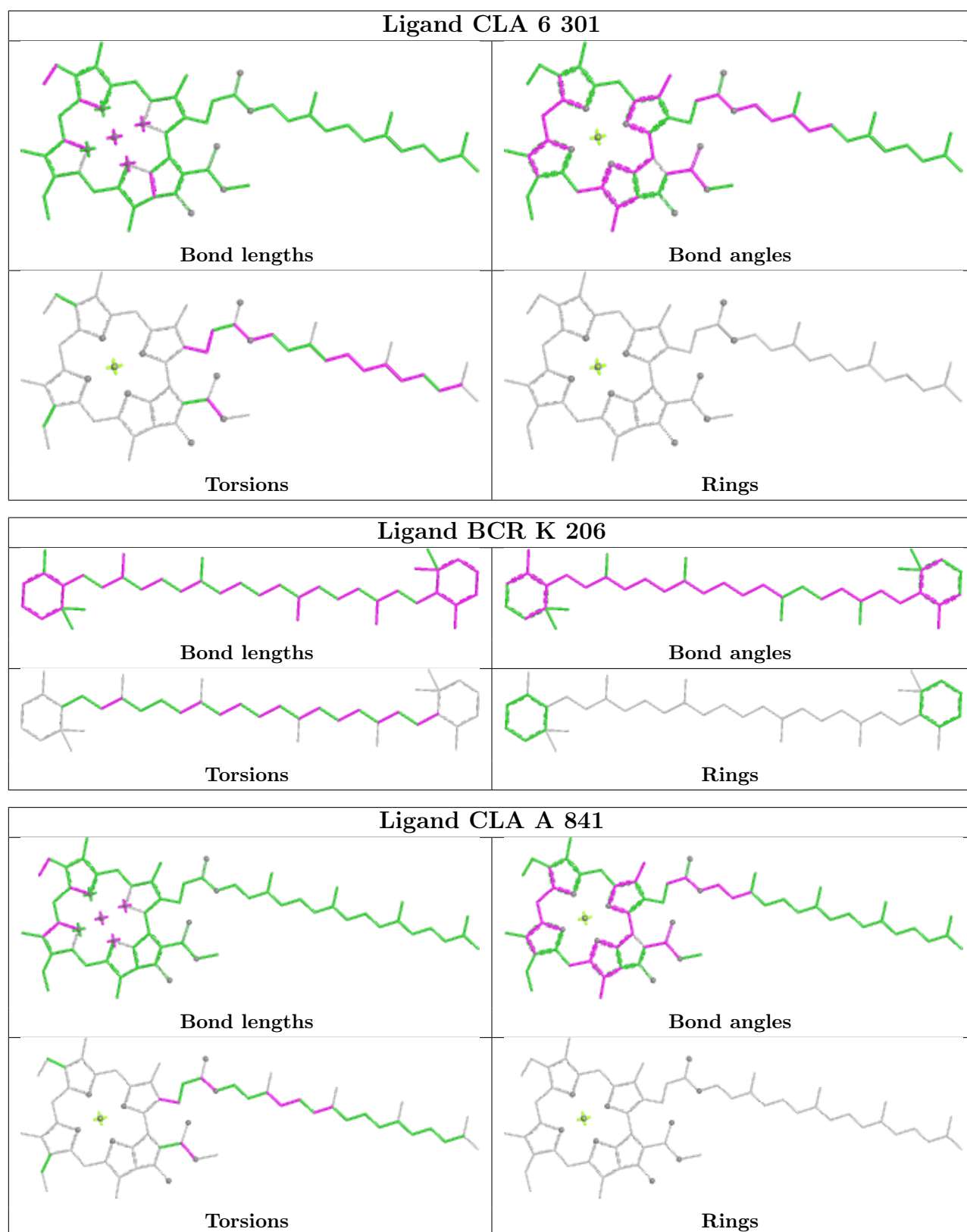


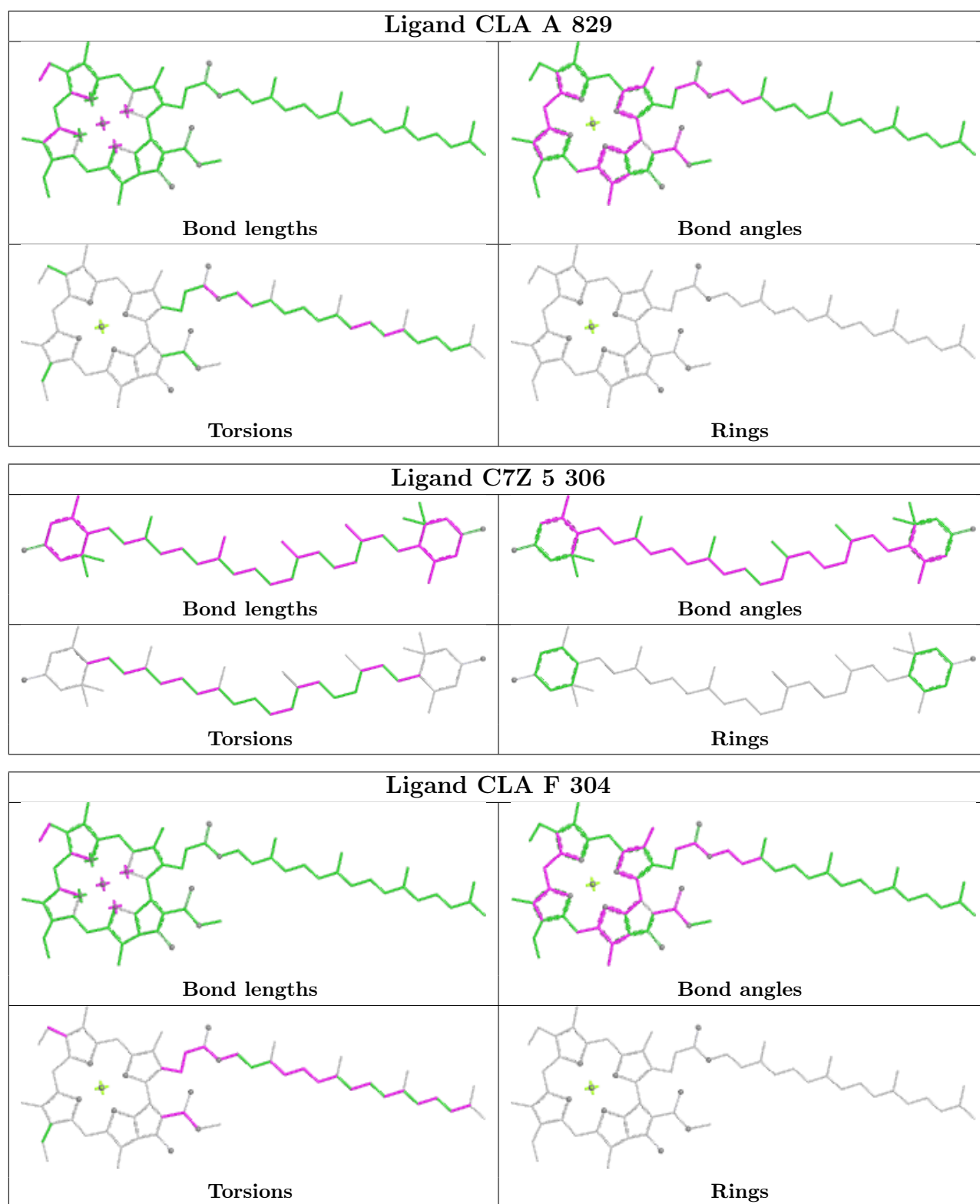
Ligand CLA 6 310

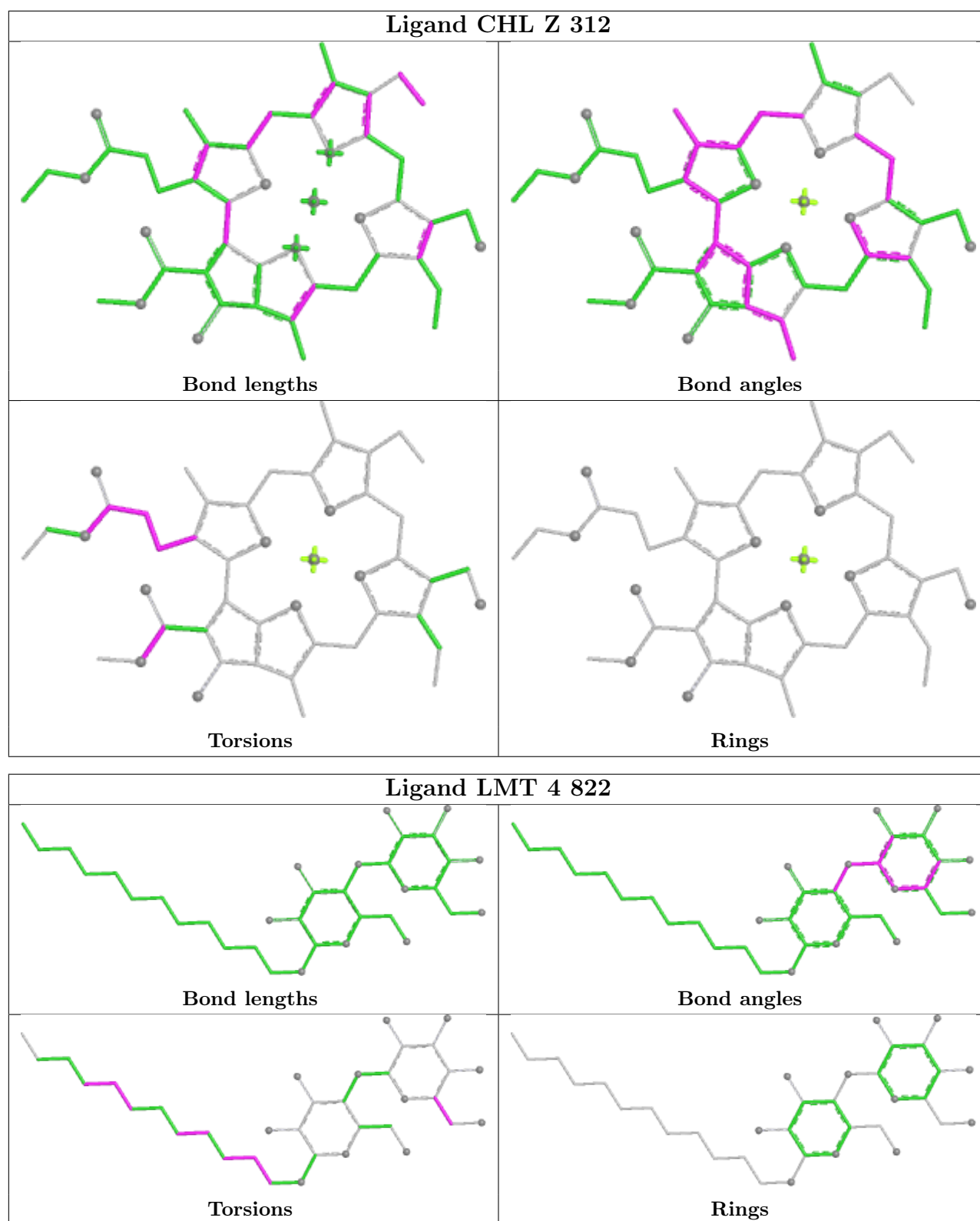


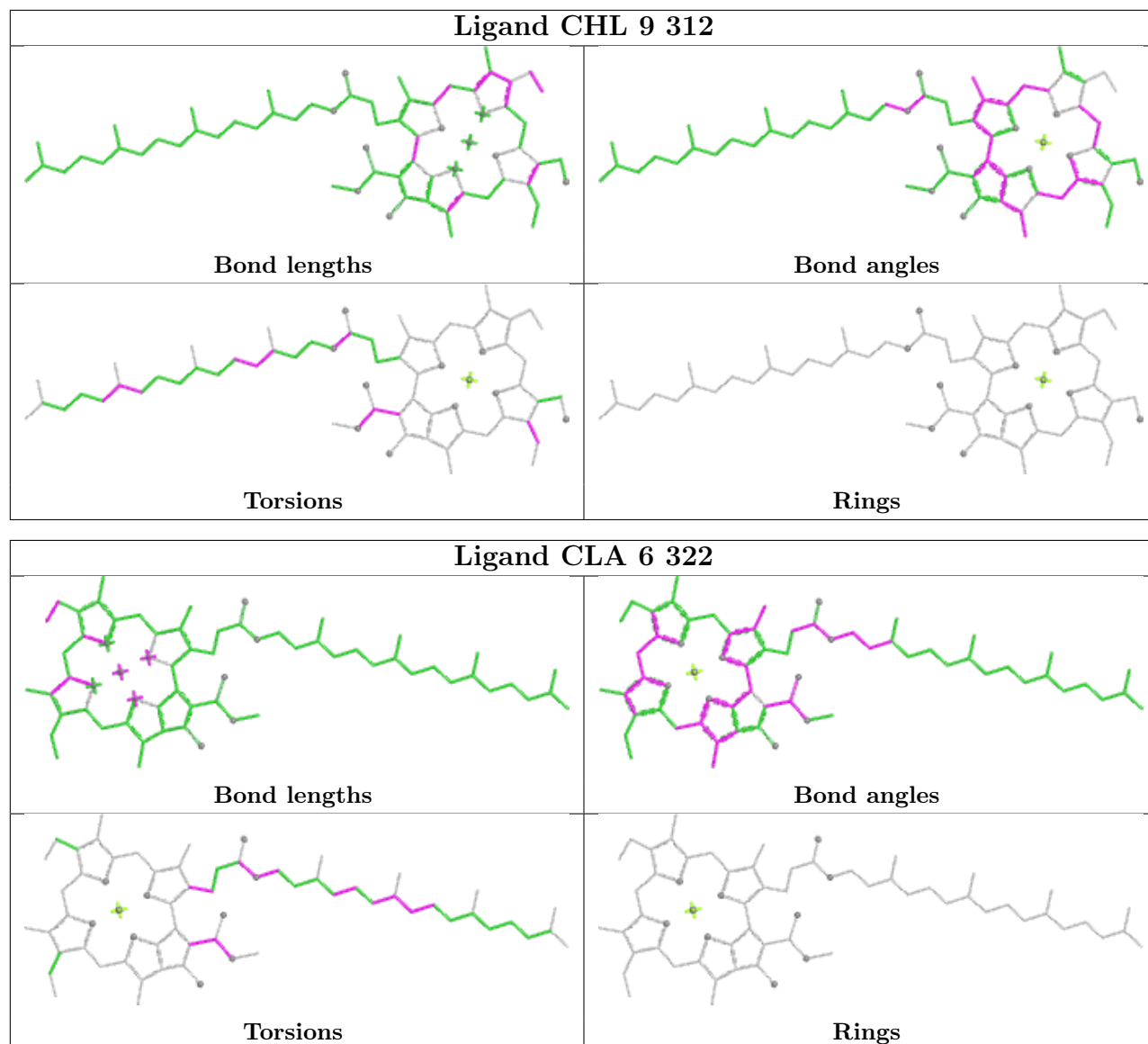
Ligand CLA A 823**Ligand CLA 3 320**

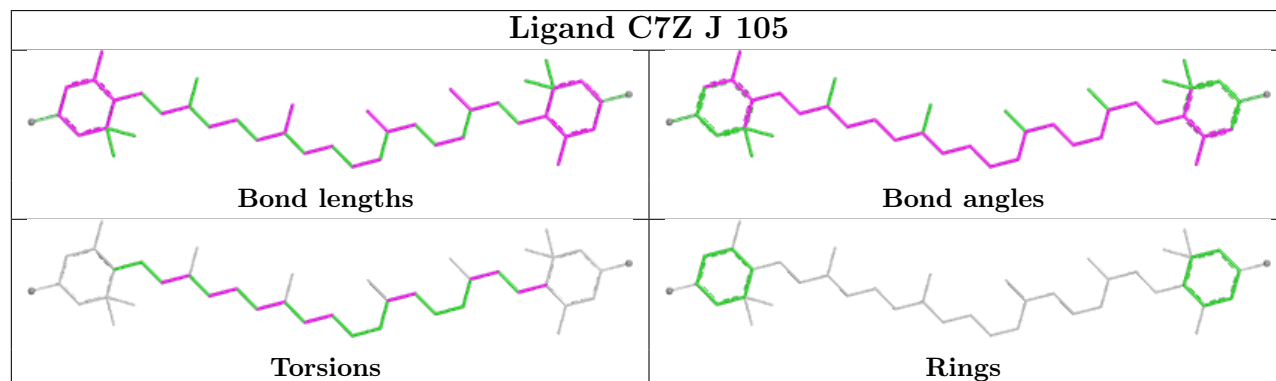
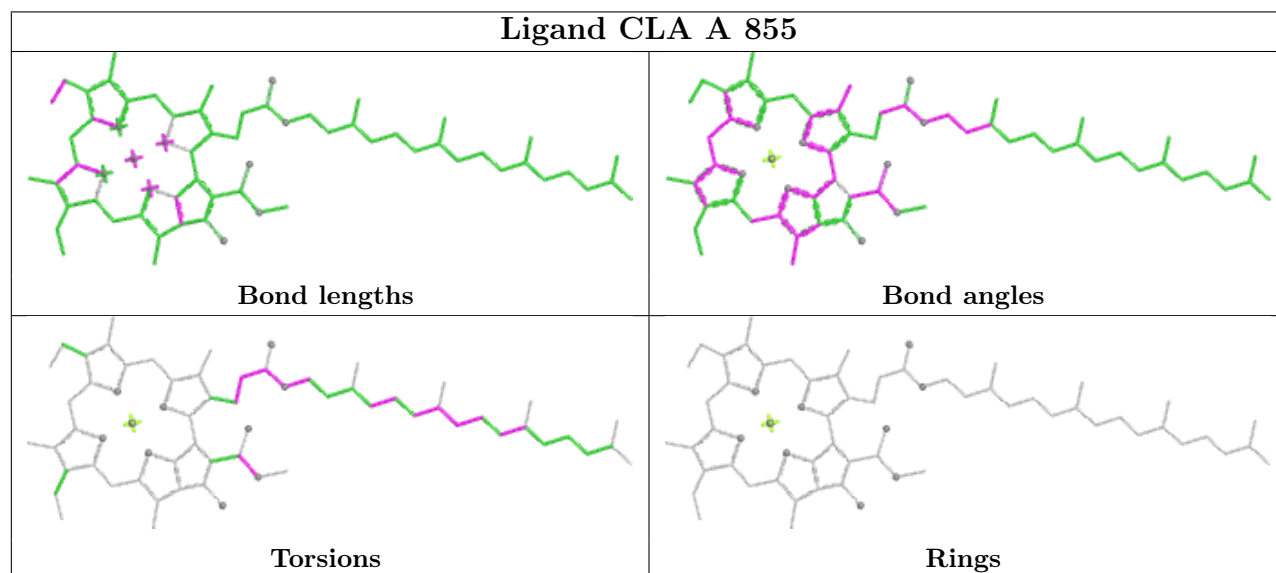
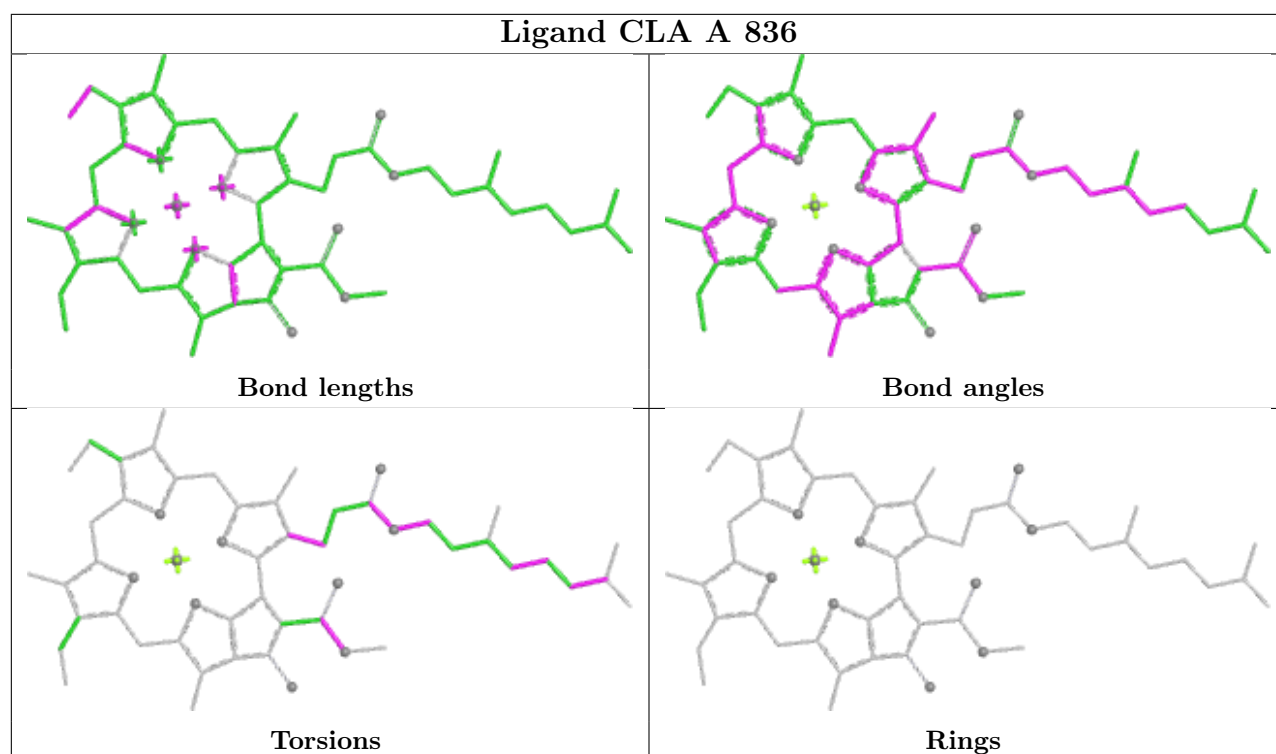




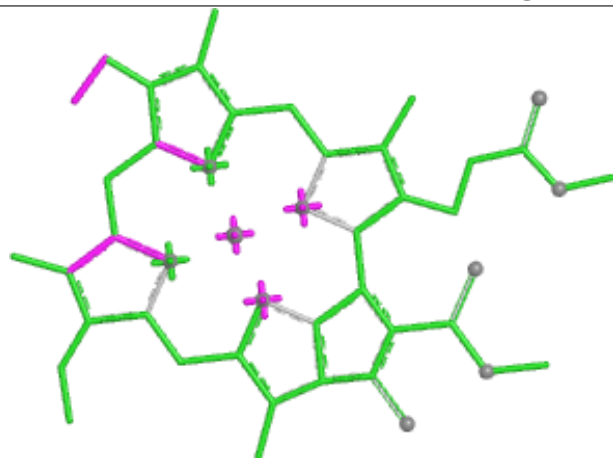




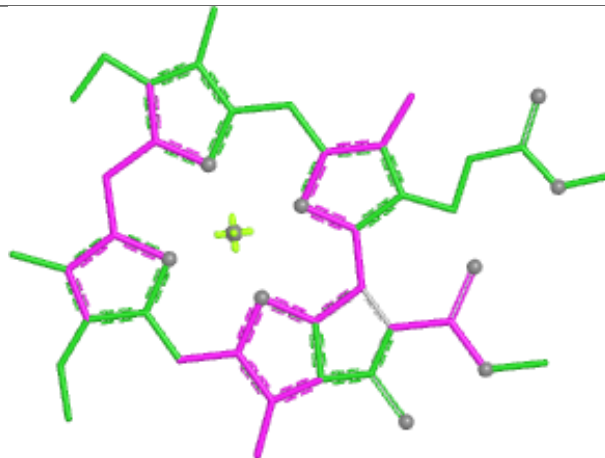




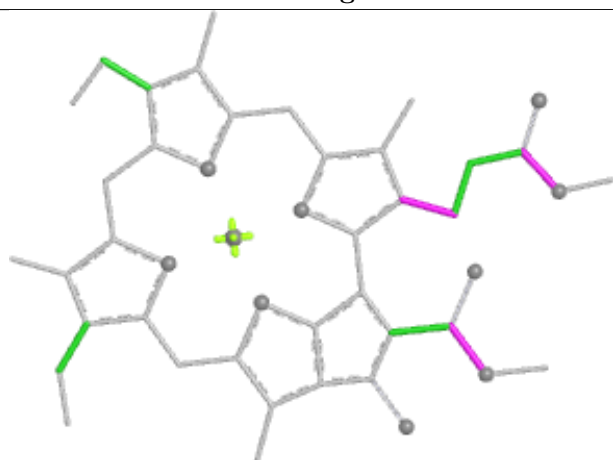
Ligand CLA 9 311



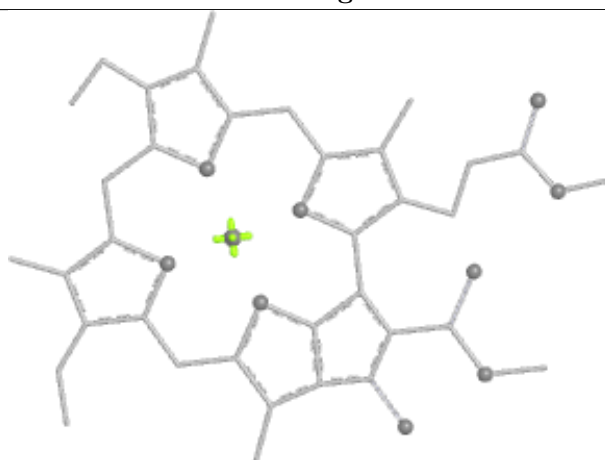
Bond lengths



Bond angles

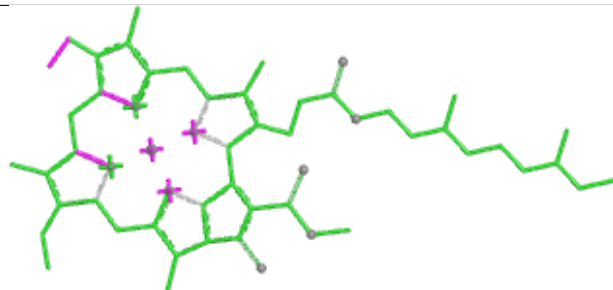


Torsions

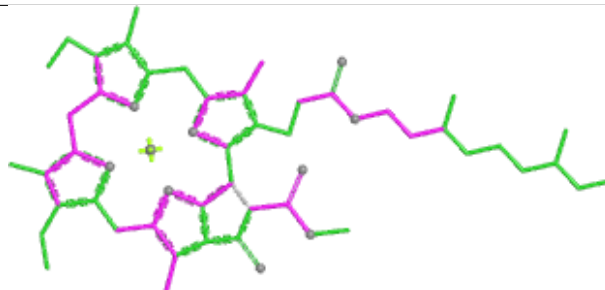


Rings

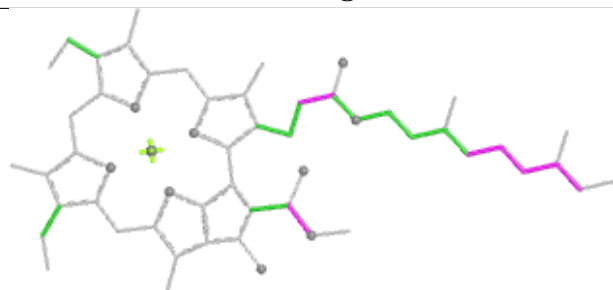
Ligand CLA Z 305



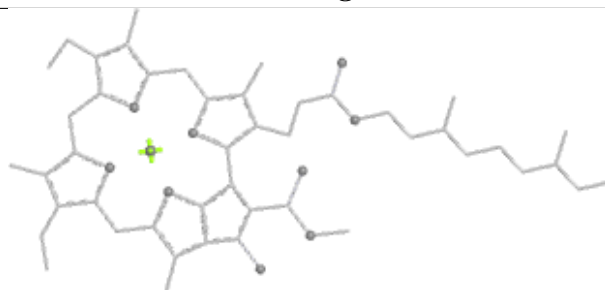
Bond lengths



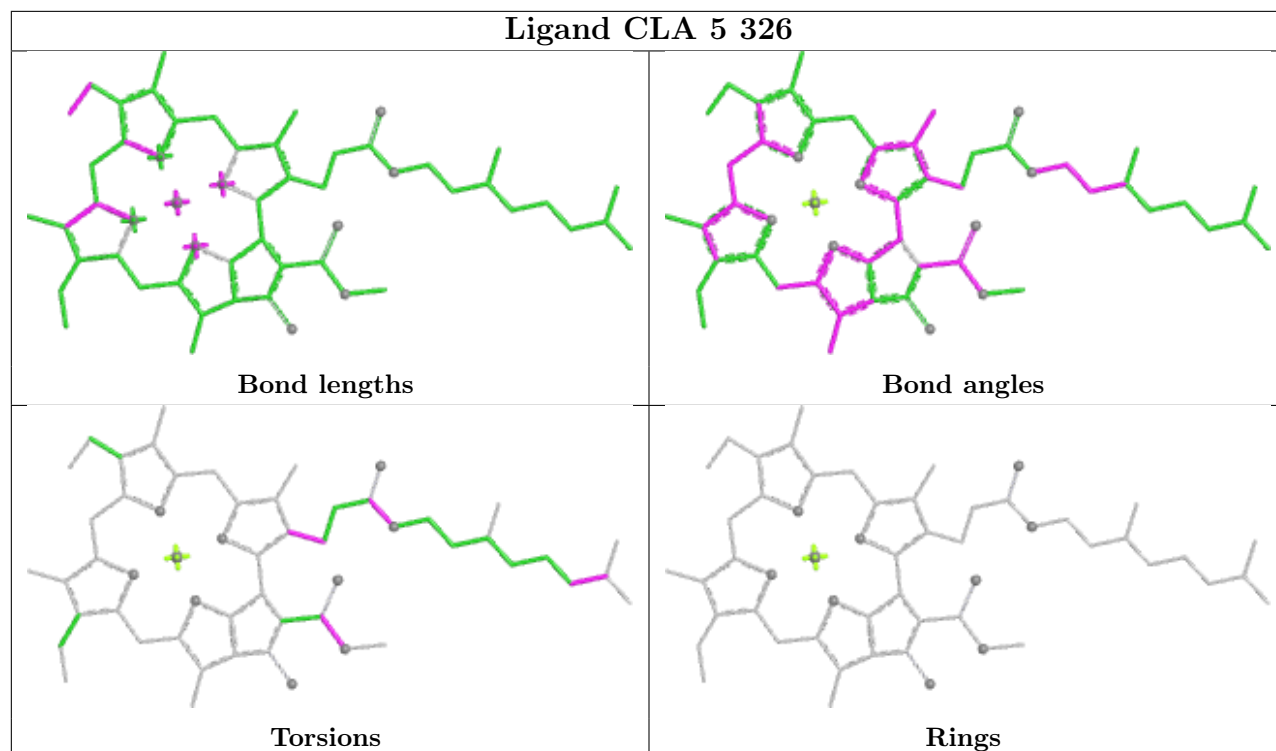
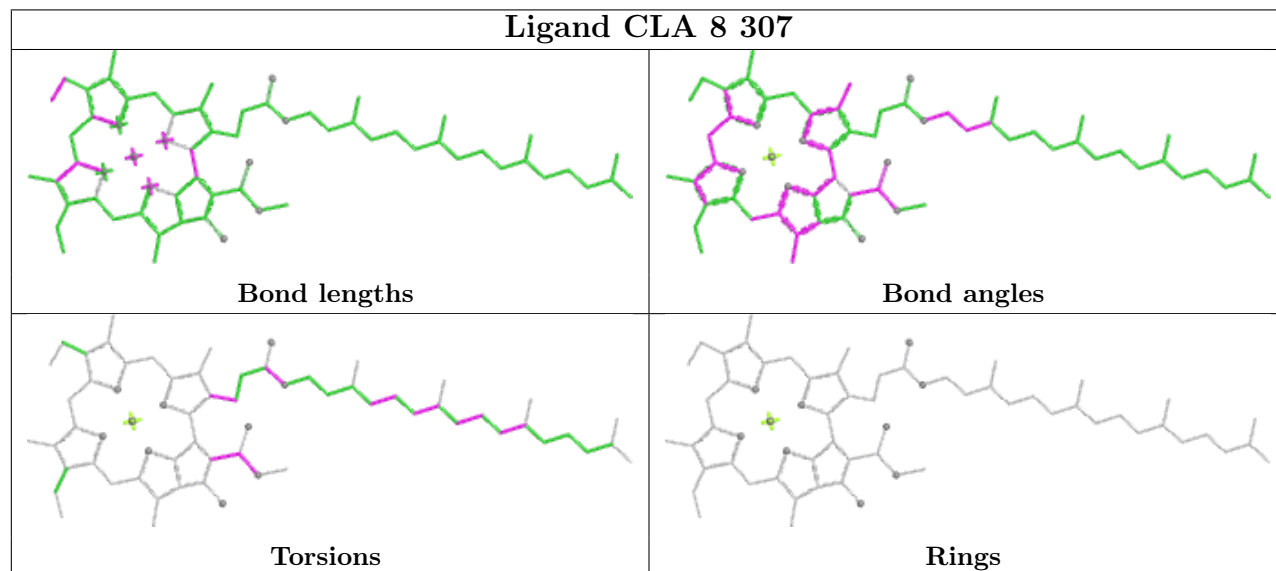
Bond angles

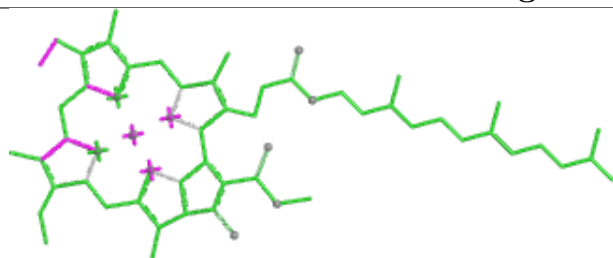
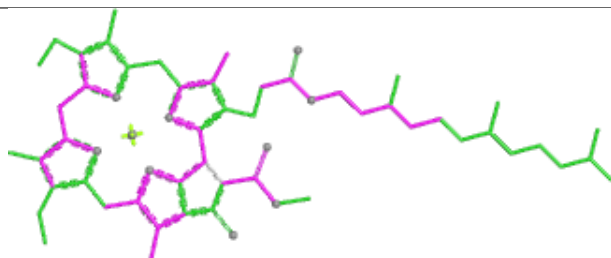
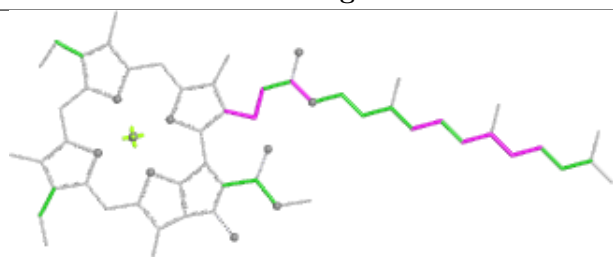
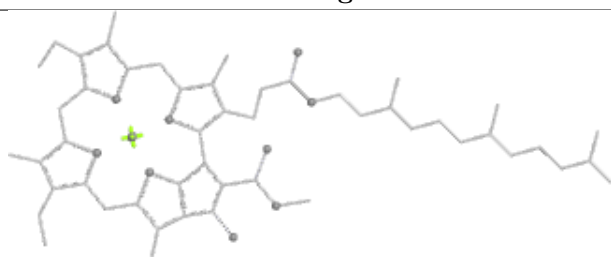
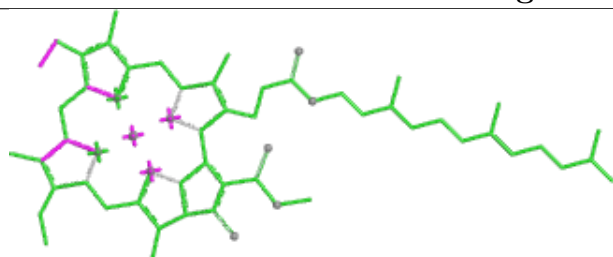
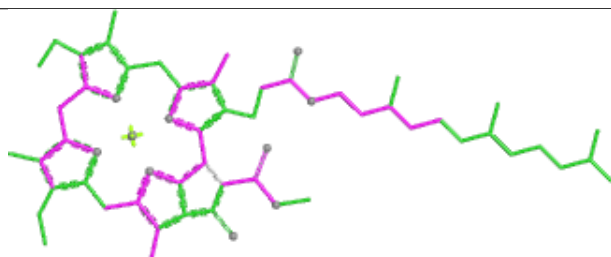
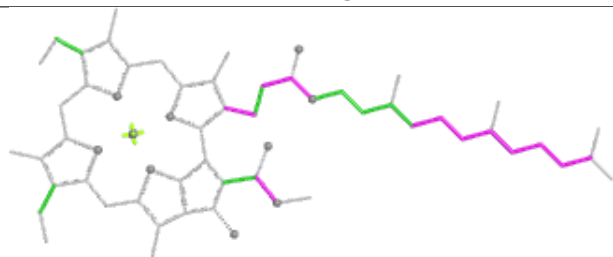
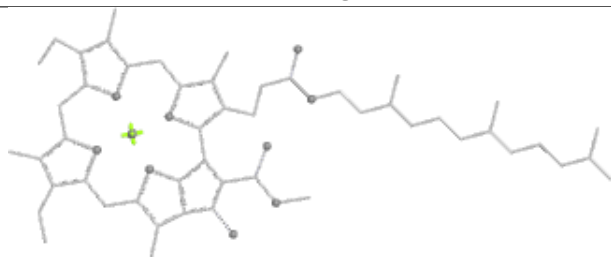


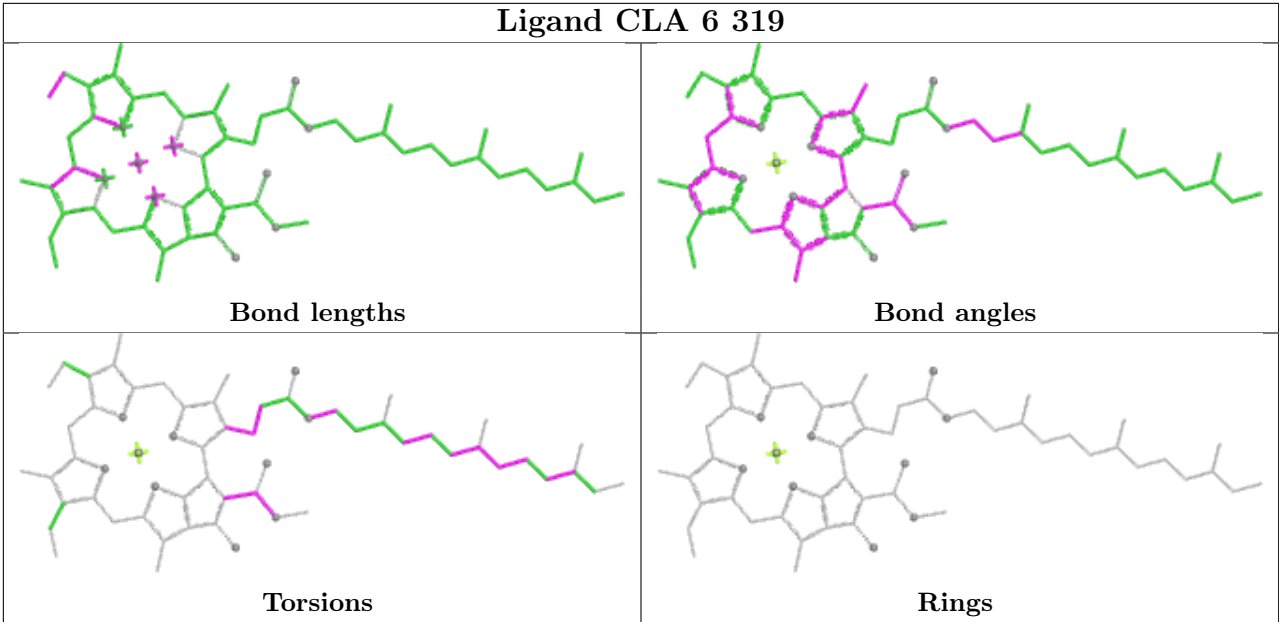
Torsions



Rings

Ligand CLA 5 326**Ligand CLA 8 307**

Ligand CLA 3 311**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA Z 309****Bond lengths****Bond angles****Torsions****Rings**



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	144:PRO	C	158:ARG	N	6.44

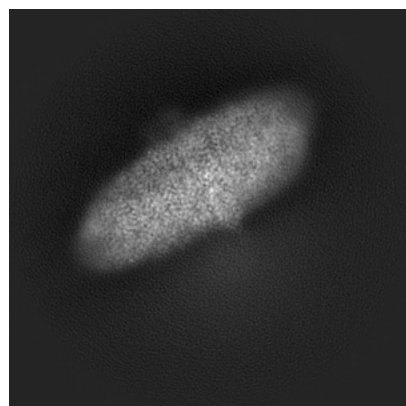
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16732. These allow visual inspection of the internal detail of the map and identification of artifacts.

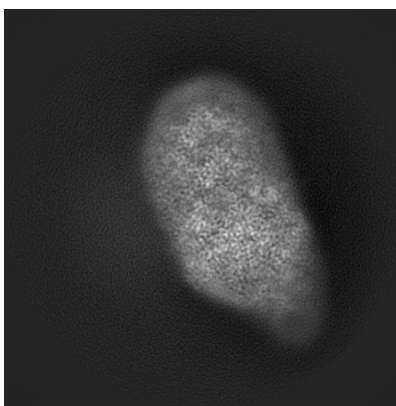
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

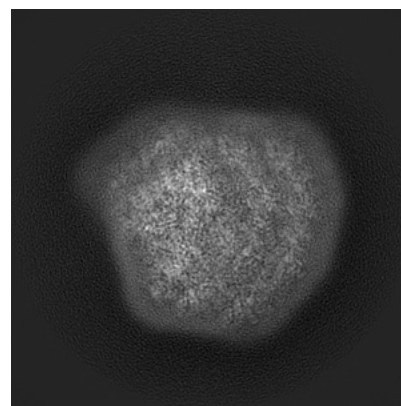
6.1.1 Primary map



X

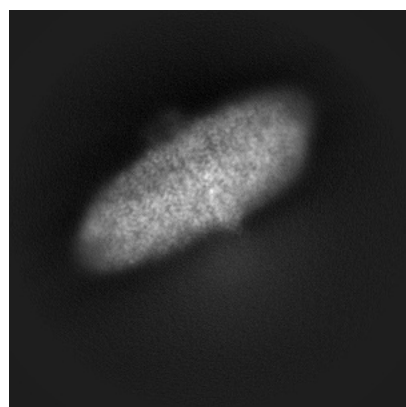


Y

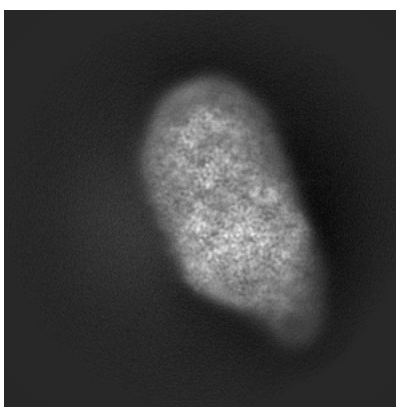


Z

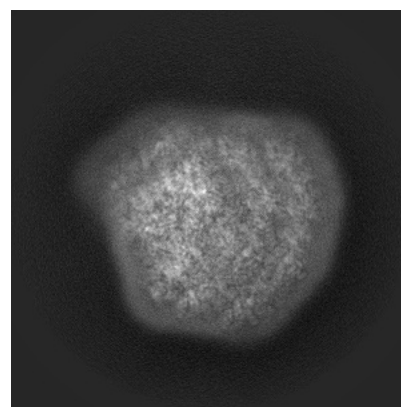
6.1.2 Raw map



X



Y

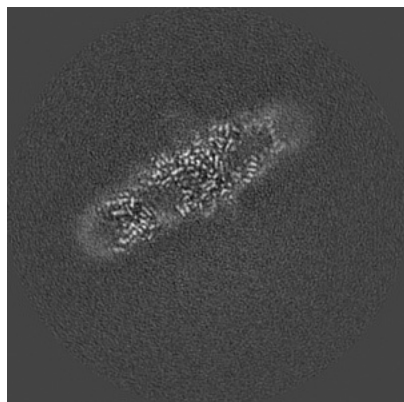


Z

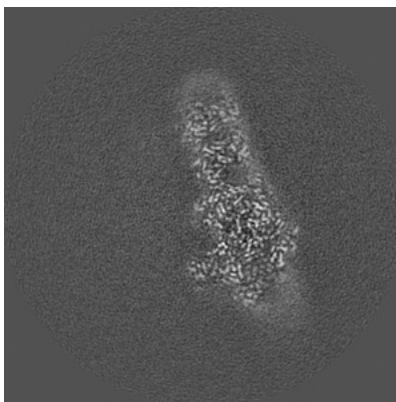
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

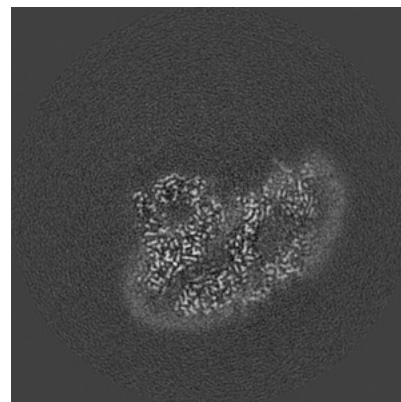
6.2.1 Primary map



X Index: 250

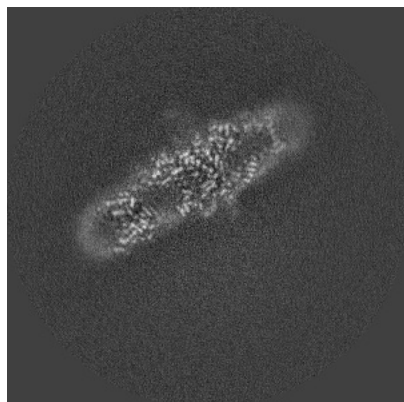


Y Index: 250

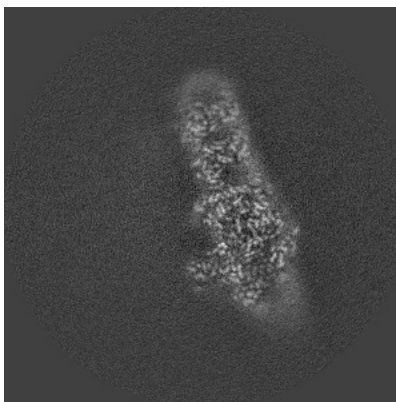


Z Index: 250

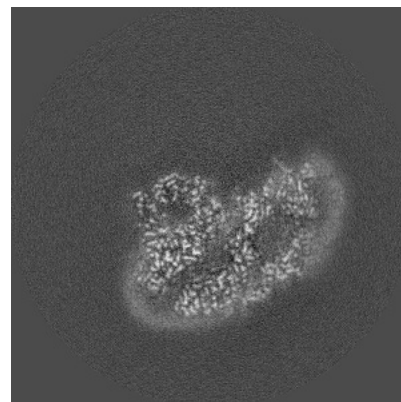
6.2.2 Raw map



X Index: 250



Y Index: 250

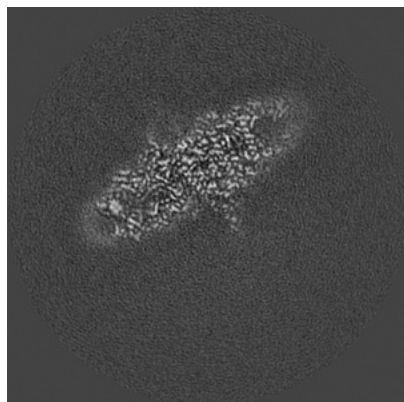


Z Index: 250

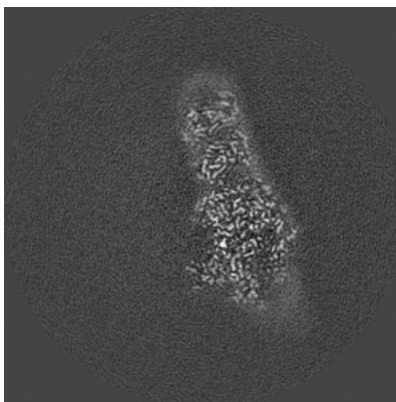
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

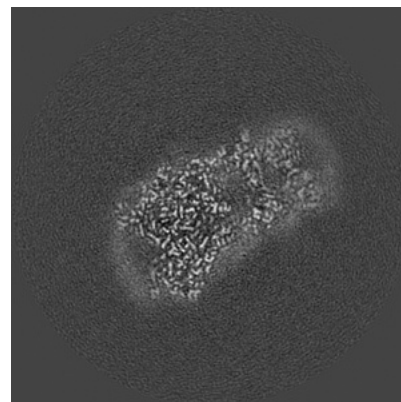
6.3.1 Primary map



X Index: 218

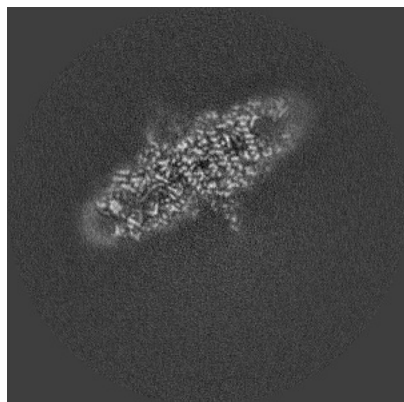


Y Index: 252

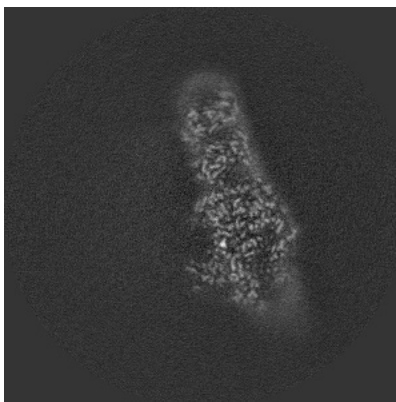


Z Index: 289

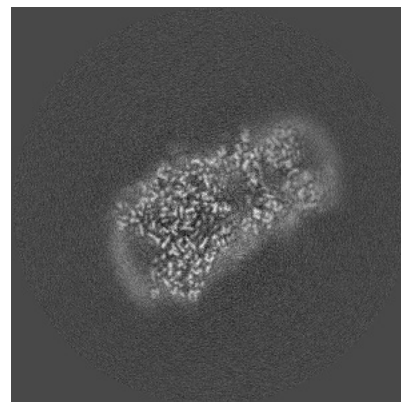
6.3.2 Raw map



X Index: 218



Y Index: 252

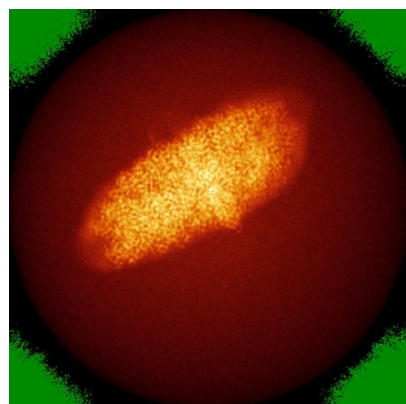


Z Index: 289

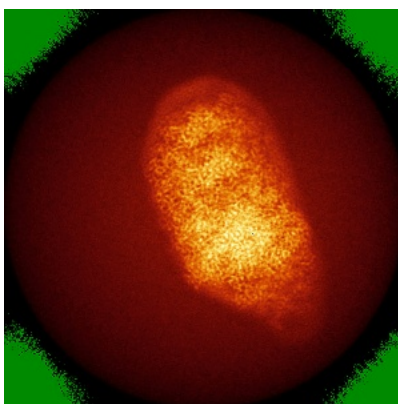
The images above show the largest variance slices of the map in three orthogonal directions.

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

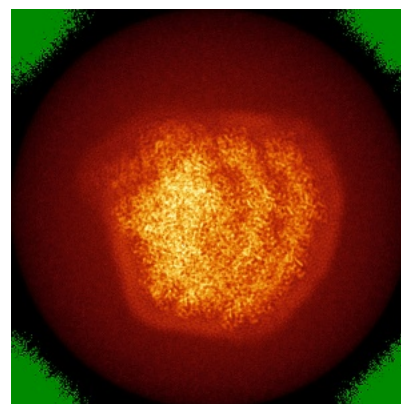
6.4.1 Primary map



X

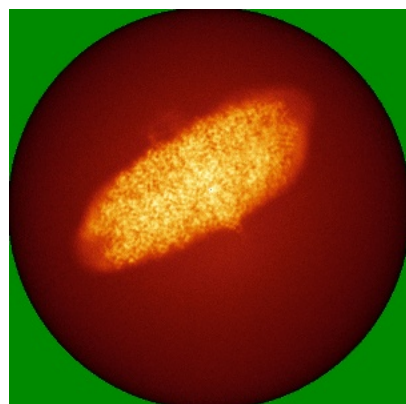


Y

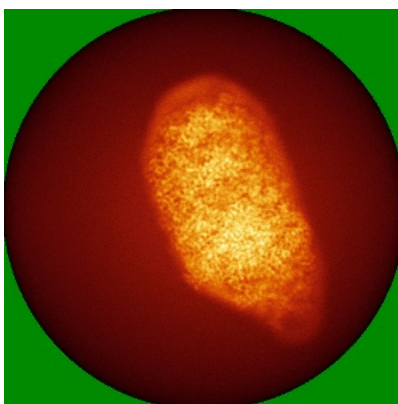


Z

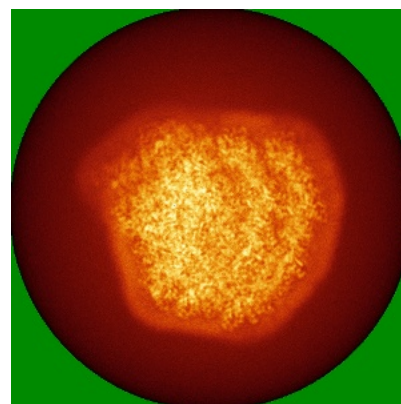
6.4.2 Raw map



X



Y



Z

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

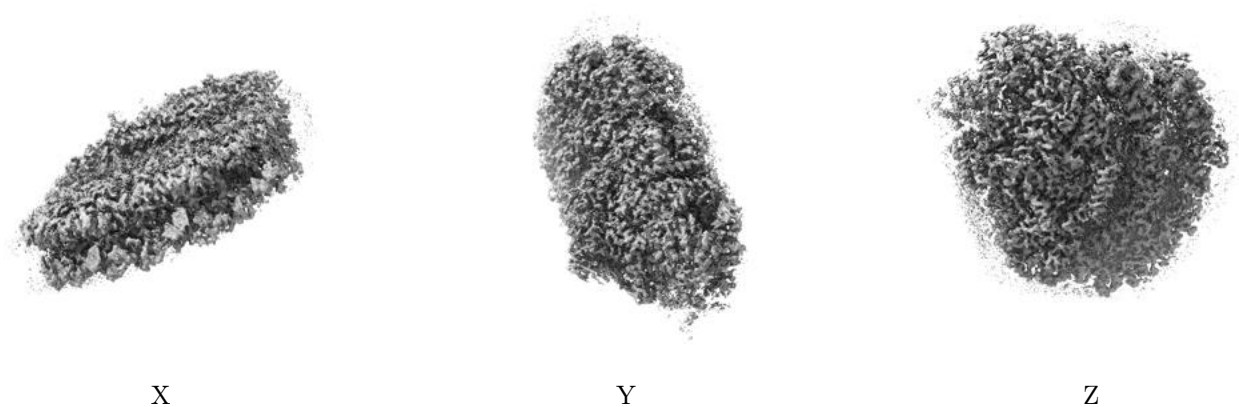
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

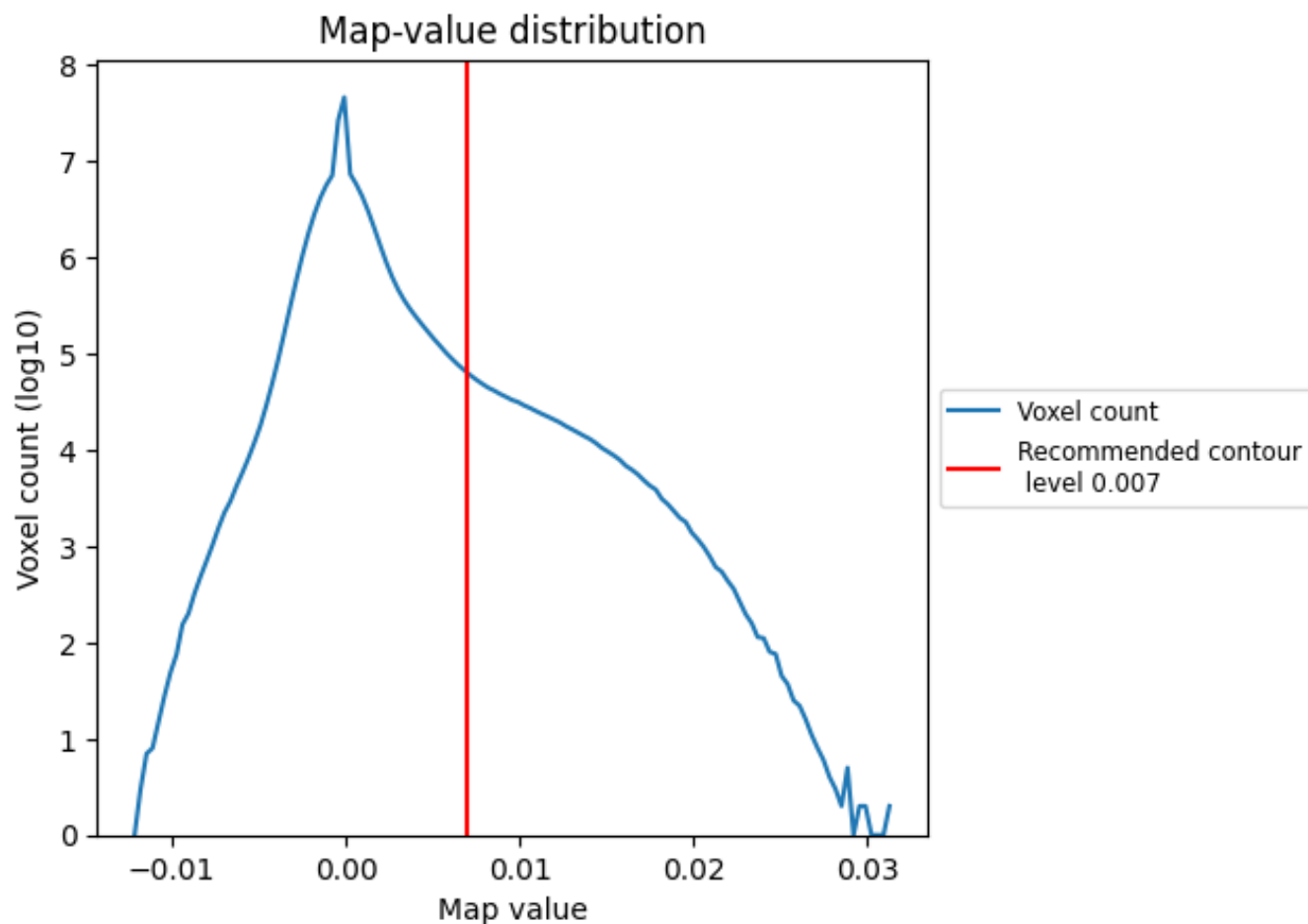
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

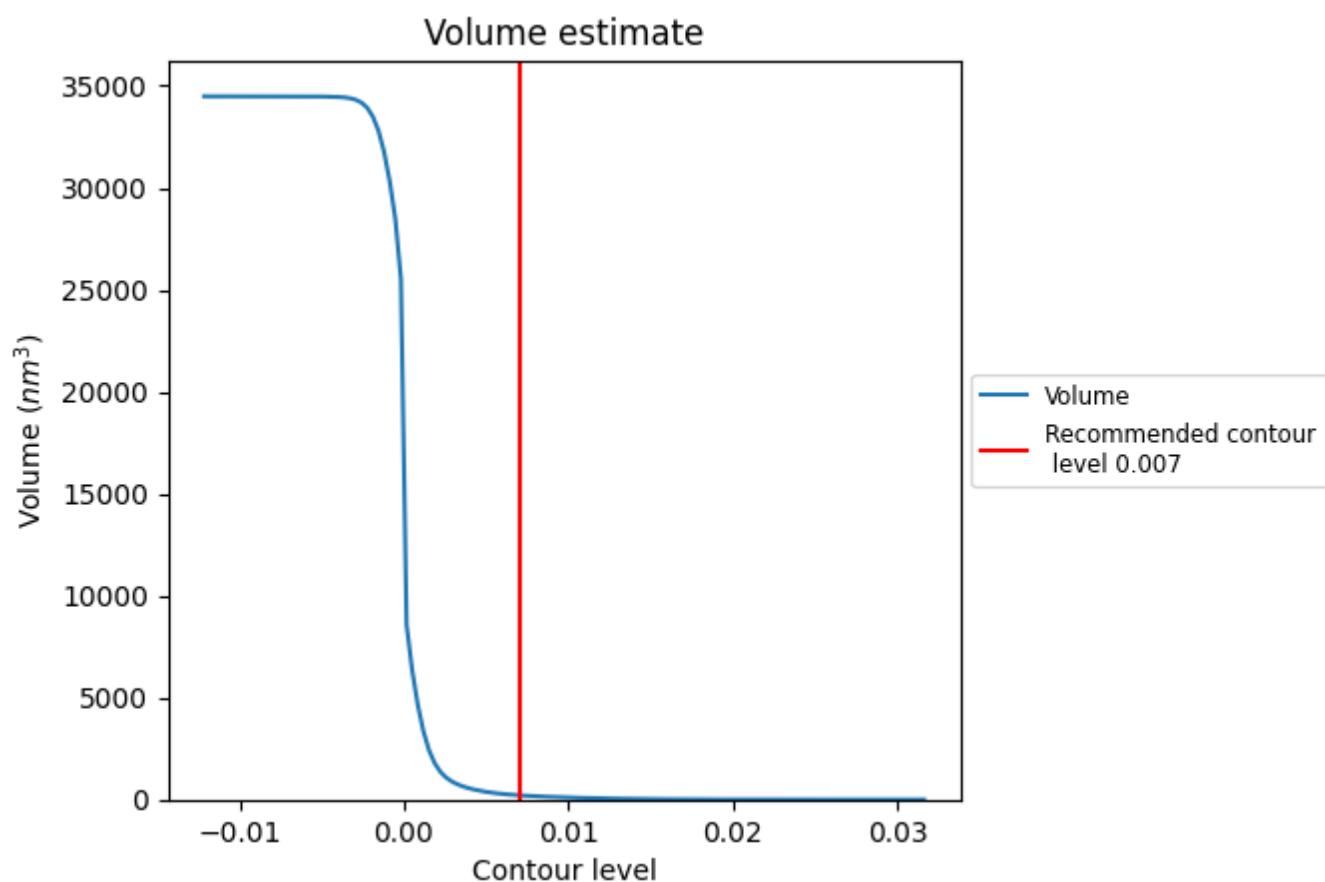
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

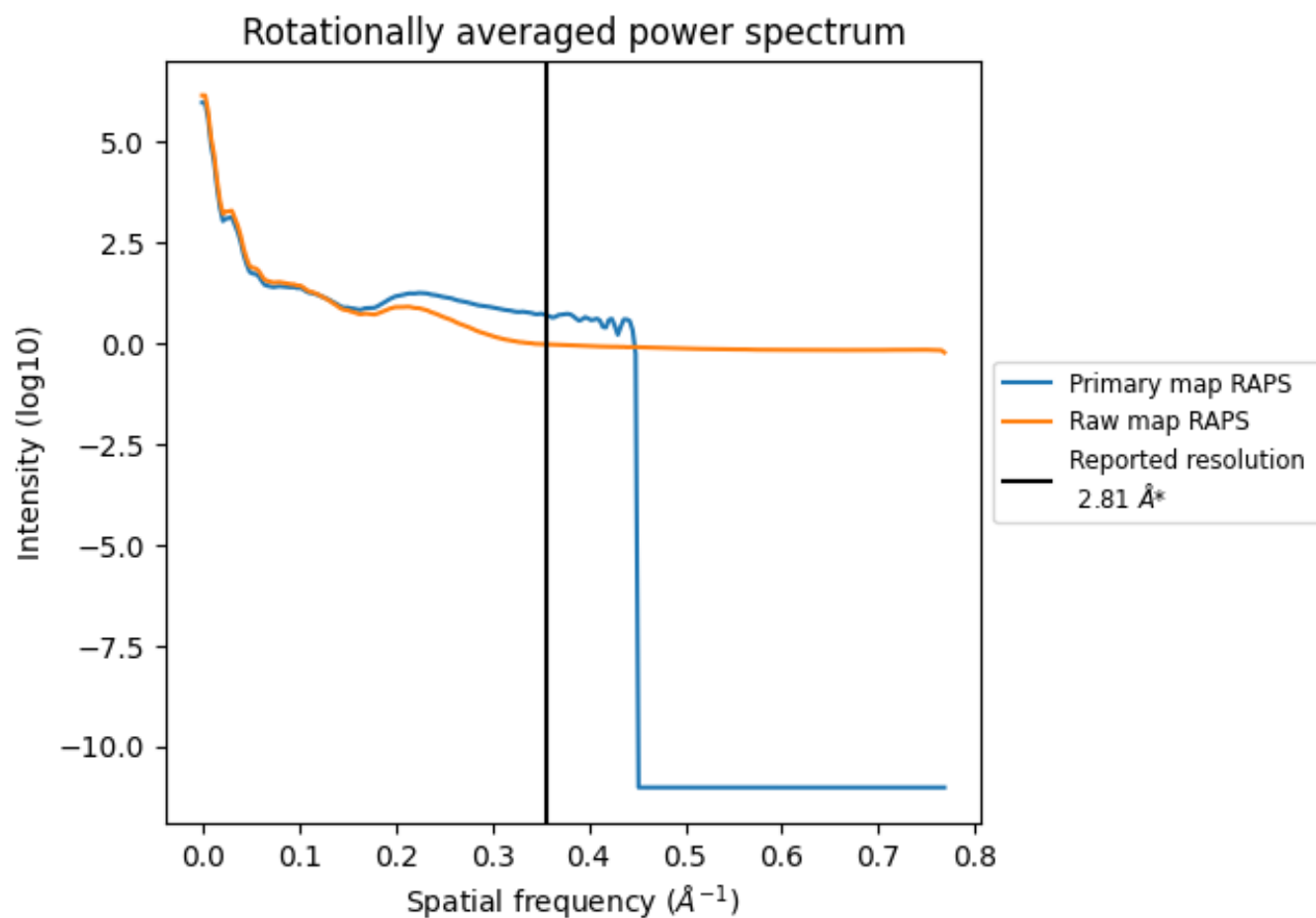
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

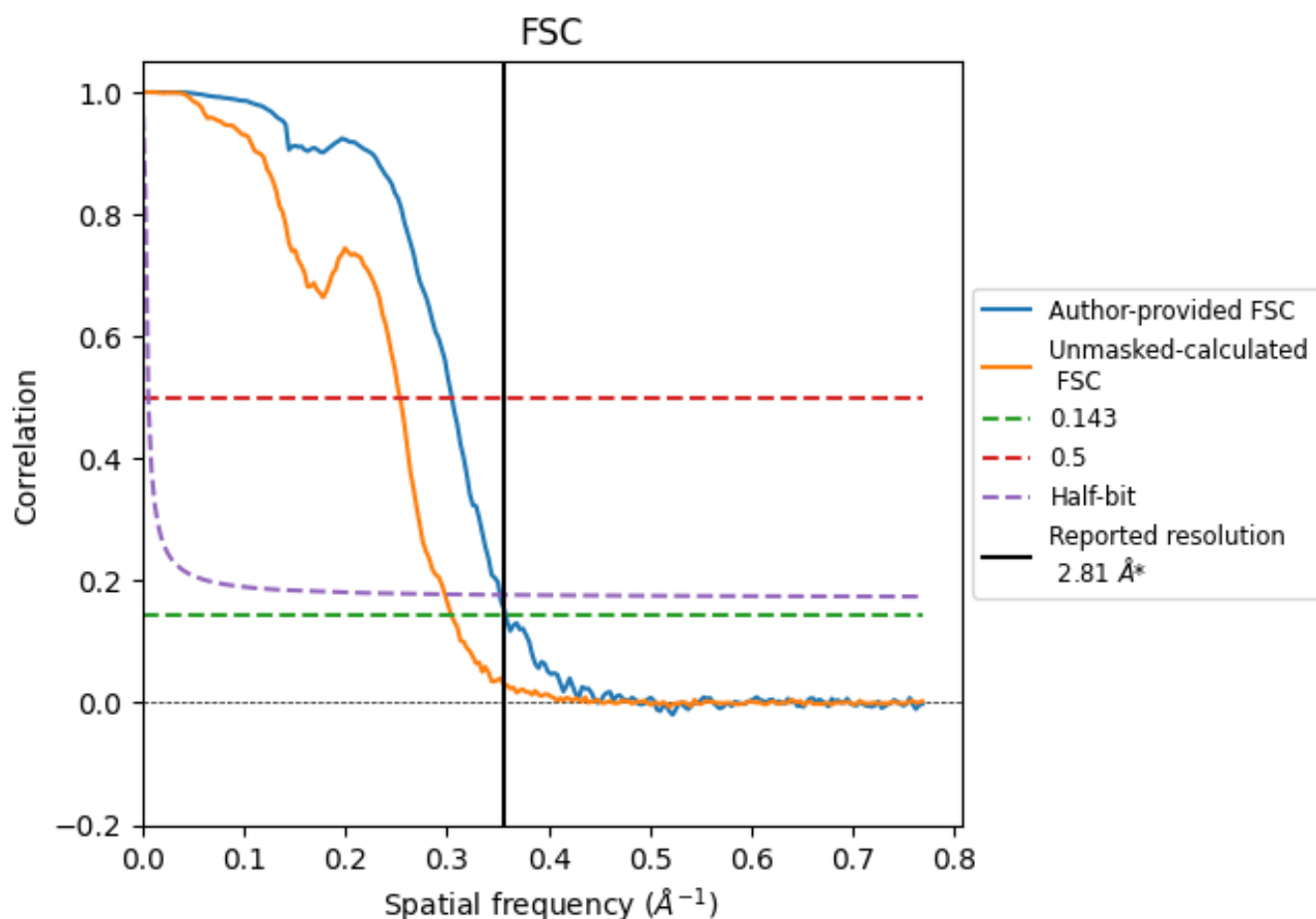


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

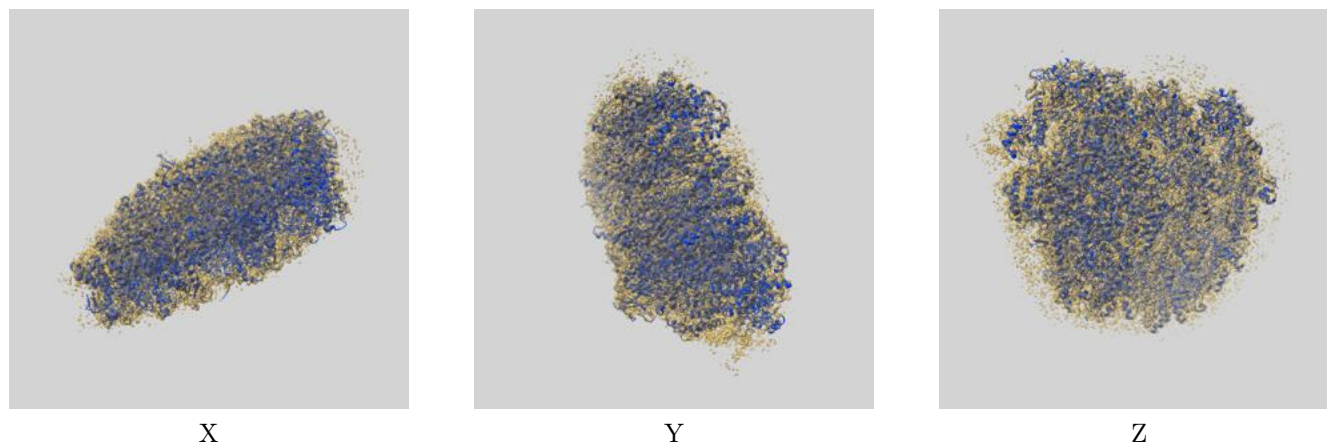
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.79	3.28	2.84
Unmasked-calculated*	3.28	3.94	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.81 by more than 10 %

9 Map-model fit [i](#)

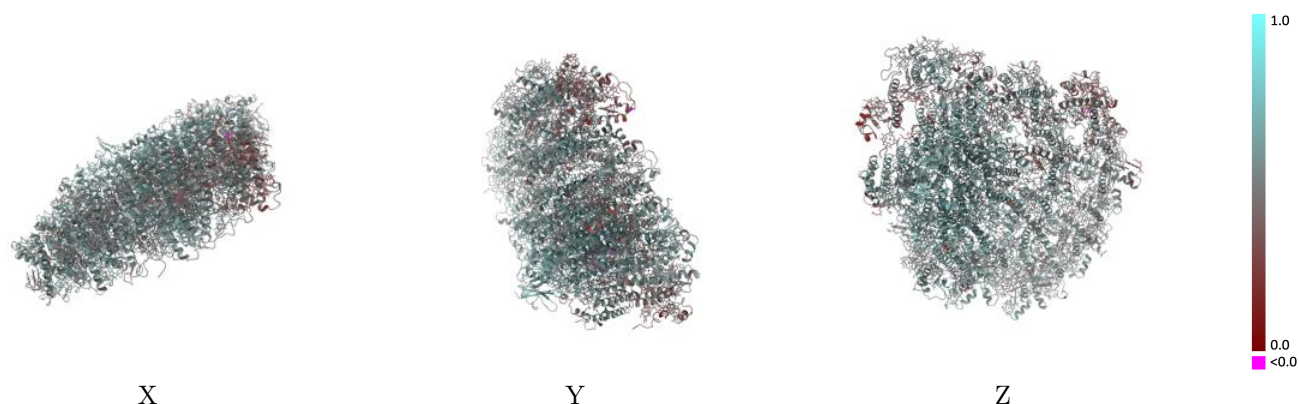
This section contains information regarding the fit between EMDB map EMD-16732 and PDB model 8CMO. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



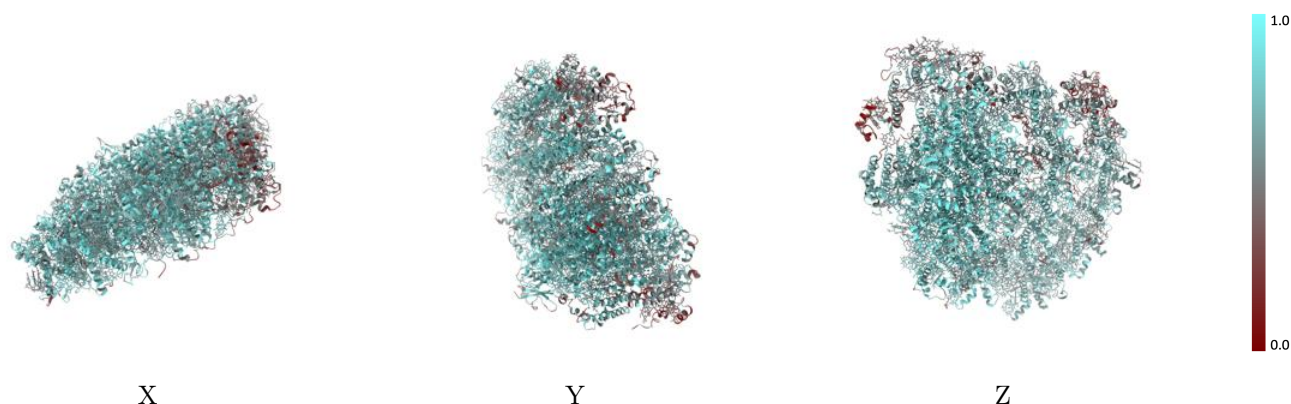
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



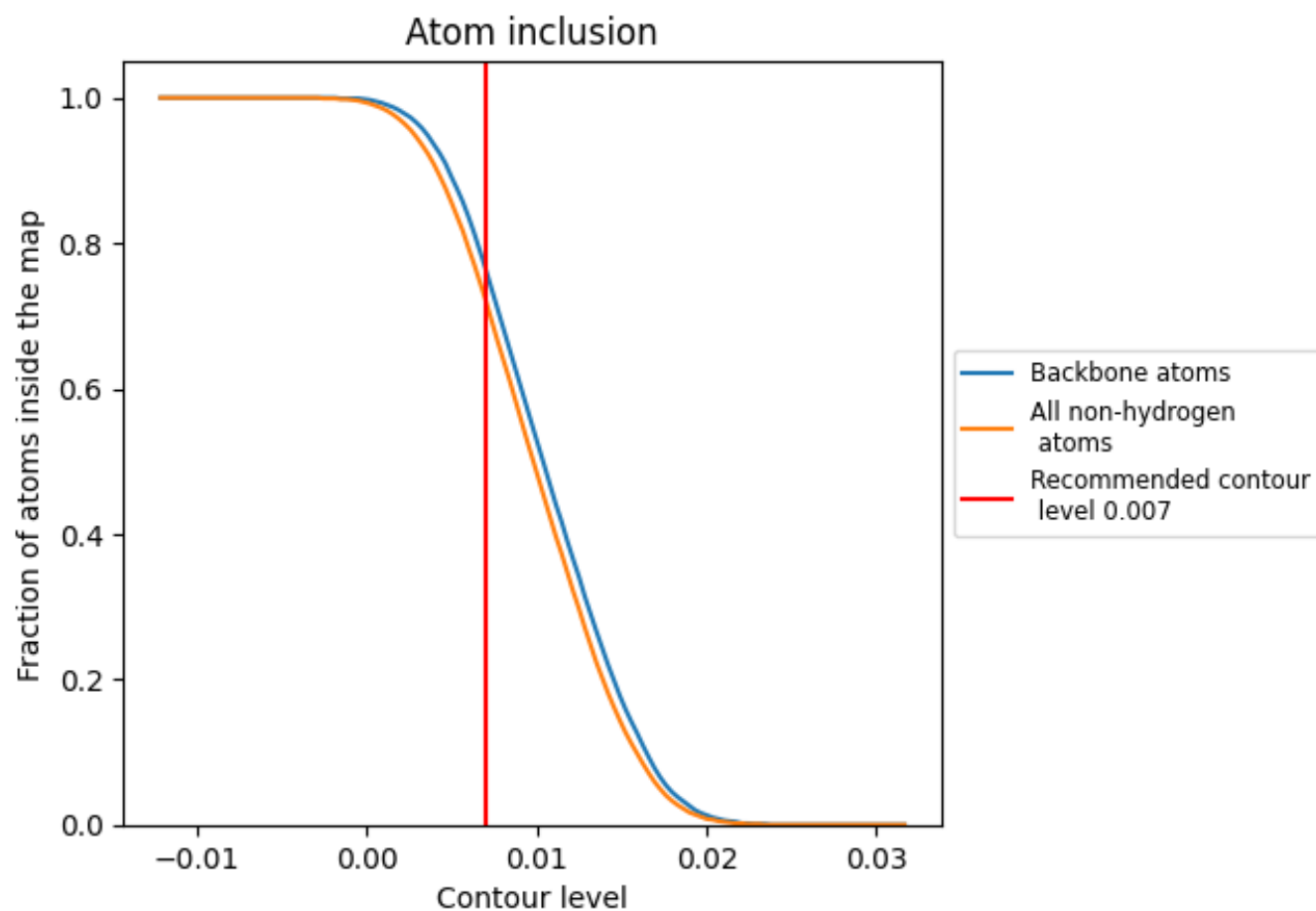
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.5370
1	0.6350	0.4980
2	0.3310	0.3380
3	0.7710	0.5610
4	0.6470	0.5050
5	0.6780	0.5150
6	0.6810	0.5140
7	0.7840	0.5510
8	0.7410	0.5310
9	0.5380	0.4770
A	0.8270	0.5920
B	0.8210	0.5830
C	0.7720	0.6020
D	0.6520	0.5660
E	0.6830	0.5660
F	0.6980	0.5310
G	0.4660	0.4150
I	0.6720	0.5270
J	0.7000	0.5310
K	0.7110	0.5230
L	0.6550	0.5030
Z	0.4730	0.4100

