



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 04:11 AM JST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

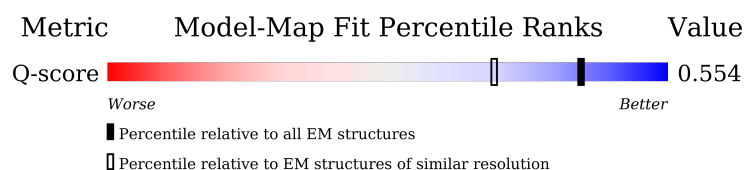
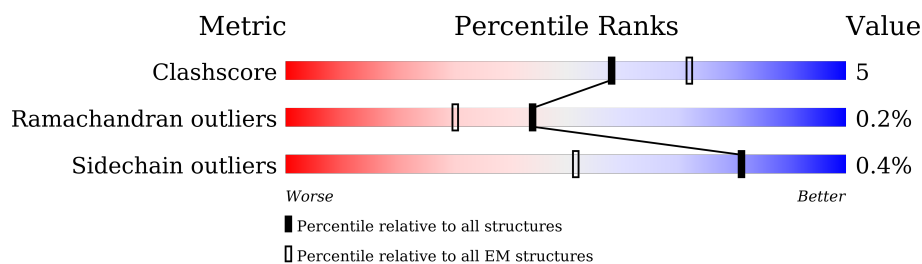
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	209	
2	B	209	
3	C	205	
4	D	245	

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 73546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called iFCPI-7.

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

- Molecule 2 is a protein called iFCPI-1.

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

- Molecule 3 is a protein called iFCPI-11.

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

- Molecule 4 is a protein called iFCPI-6.

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

- Molecule 5 is a protein called iFCPI-5.

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

- Molecule 6 is a protein called iFCPI-8.

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

- Molecule 7 is a protein called iFCPI-13.

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

- Molecule 8 is a protein called iFCPI-10.

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

- Molecule 9 is a protein called iFCPI-3.

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

- Molecule 10 is a protein called iFCPI-9.

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

- Molecule 11 is a protein called iFCPI-4.

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

- Molecule 12 is a protein called iFCPI-12.

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

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

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

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

- Molecule 14 is a protein called iFCPI-17.

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

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

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

- Molecule 16 is a protein called iFCPI-18.

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

- Molecule 17 is a protein called iFCPI-22.

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

- Molecule 18 is a protein called iFCPI-2.

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

- Molecule 19 is a protein called L-iFP.

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

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

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

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

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

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

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

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

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

- Molecule 24 is a protein called PsaE.

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

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

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

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

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

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

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

- Molecule 28 is a protein called PsaK.

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

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

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

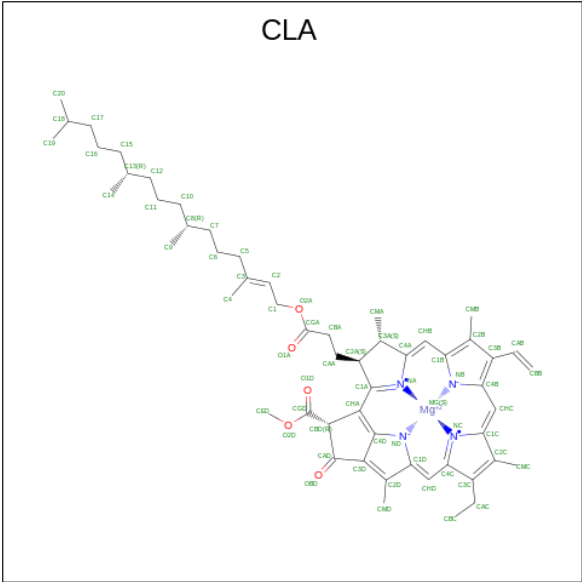
- Molecule 30 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 31 is a protein called PsaR.

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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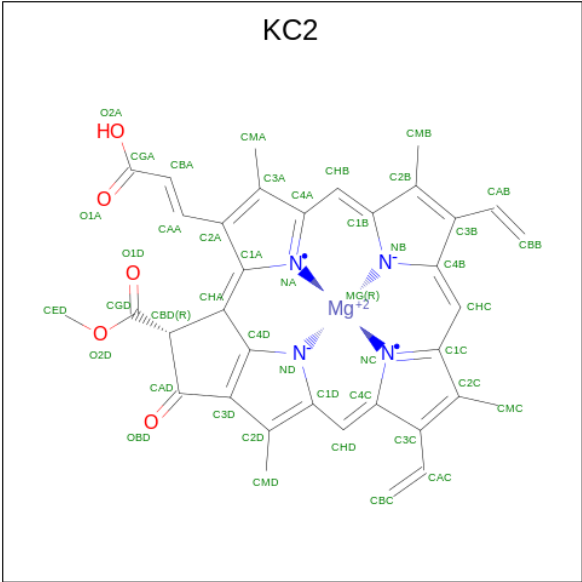
Mol	Chain	Residues	Atoms					AltConf
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
32	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
32	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
32	b	1	Total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

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

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



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

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

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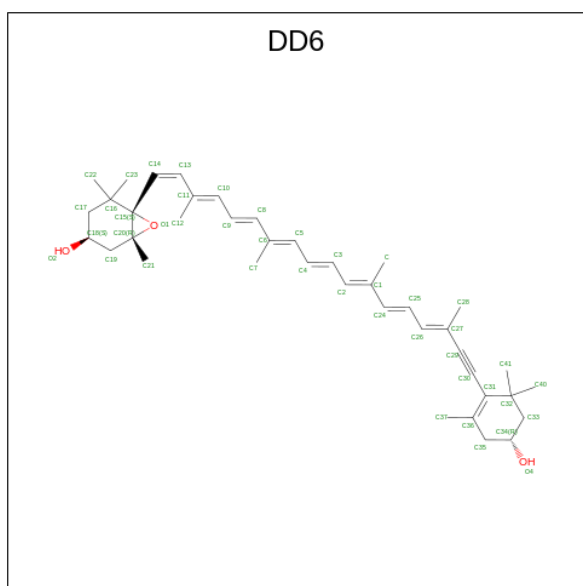
Mol	Chain	Residues	Atoms					AltConf
33	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	P	1	Total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

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

- Molecule 34 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



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

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

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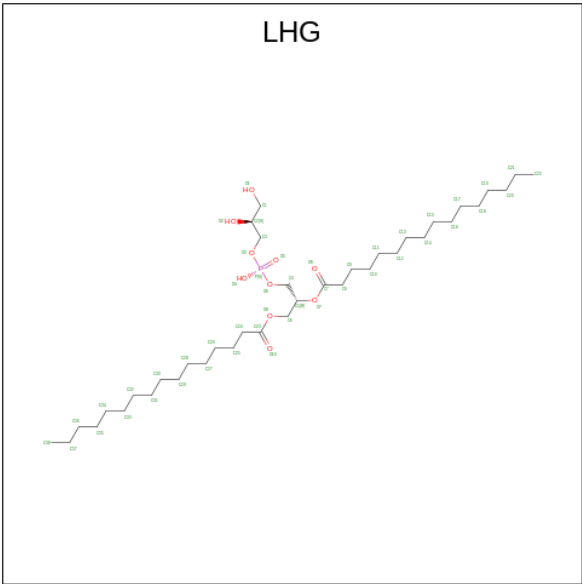
Mol	Chain	Residues	Atoms			AltConf
34	I	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	J	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	K	1	Total 43	C 40	O 3	0
34	L	1	Total 43	C 40	O 3	0
34	M	1	Total 43	C 40	O 3	0
34	N	1	Total 43	C 40	O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

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

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



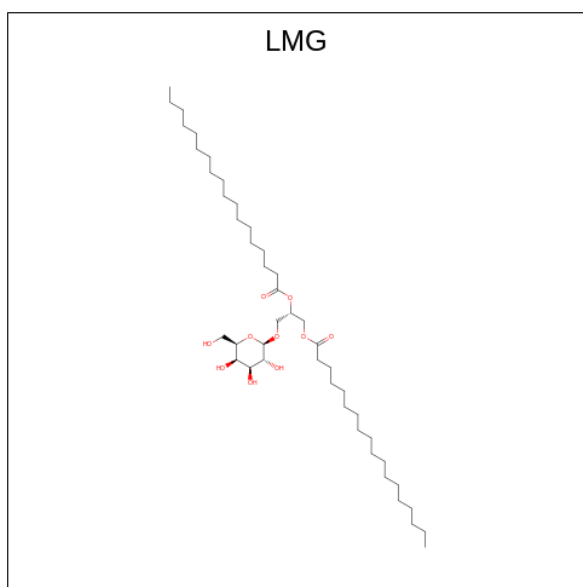
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			40	29	10	1	
35	B	1	Total	C	O	P	0
			31	20	10	1	
35	D	1	Total	C	O	P	0
			48	37	10	1	
35	E	1	Total	C	O	P	0
			46	35	10	1	
35	E	1	Total	C	O	P	0
			46	35	10	1	
35	F	1	Total	C	O	P	0
			41	30	10	1	

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

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



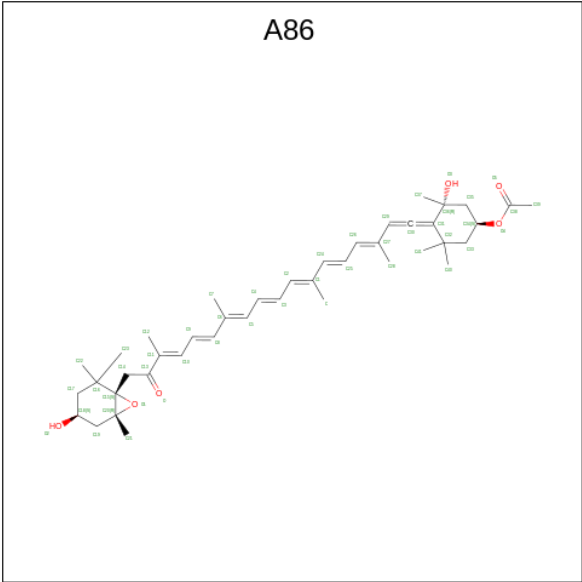
Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			36	26	10	

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

- Molecule 37 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆) (labeled as "Ligand of Interest" by depositor).



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

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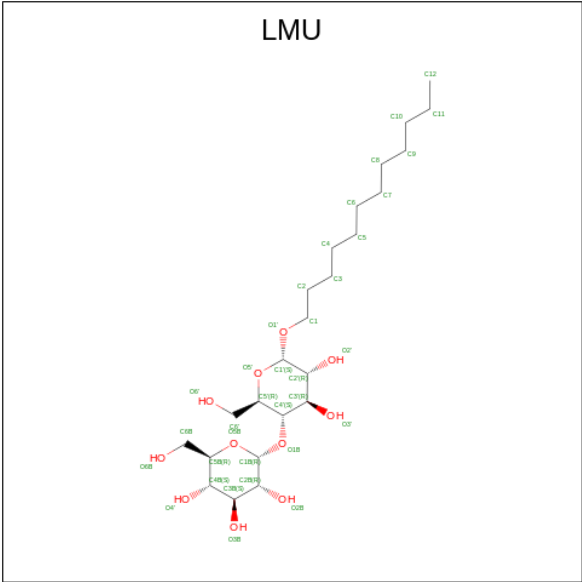
Mol	Chain	Residues	Atoms			AltConf
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	L	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0
			48	42	6	
37	M	1	Total	C	O	0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

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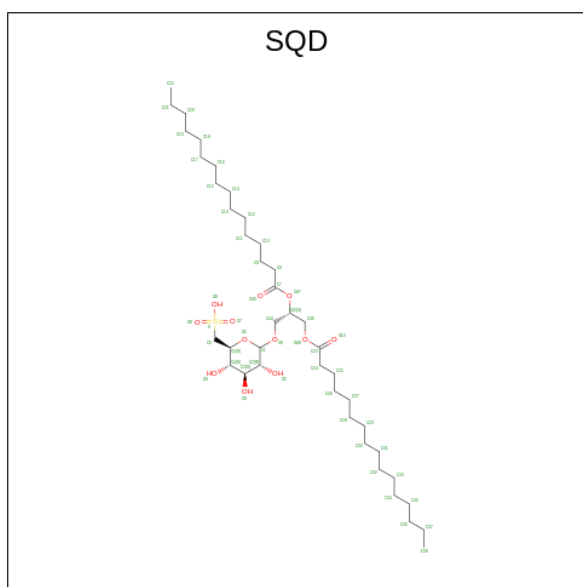
Mol	Chain	Residues	Atoms			AltConf
37	Q	1	Total	C	O	0
			48	42	6	
37	R	1	Total	C	O	0
			48	42	6	
37	R	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0
			48	42	6	
37	S	1	Total	C	O	0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

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



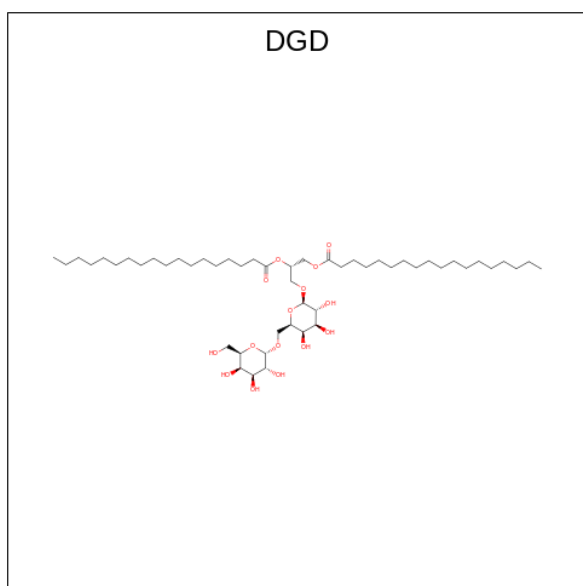
Mol	Chain	Residues	Atoms			AltConf
38	D	1	Total	C	O	0
			35	24	11	
38	I	1	Total	C	O	0
			35	24	11	
38	J	1	Total	C	O	0
			35	24	11	
38	V	1	Total	C	O	0
			34	23	11	
38	j	1	Total	C	O	0
			34	23	11	

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



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

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



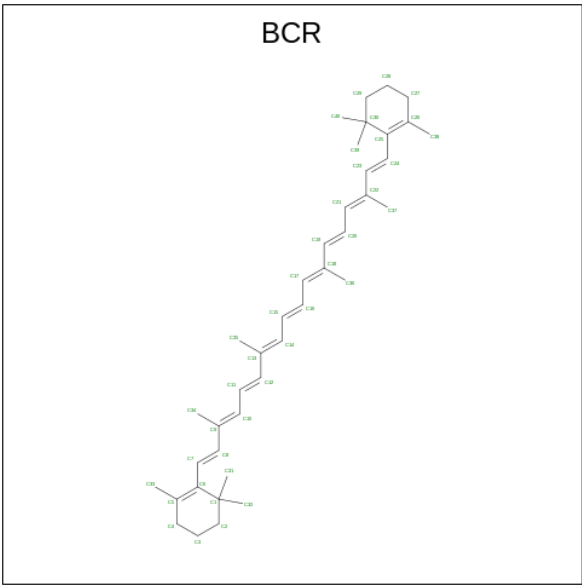
Mol	Chain	Residues	Atoms			AltConf
40	Q	1	Total	C	O	0
			56	41	15	

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

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



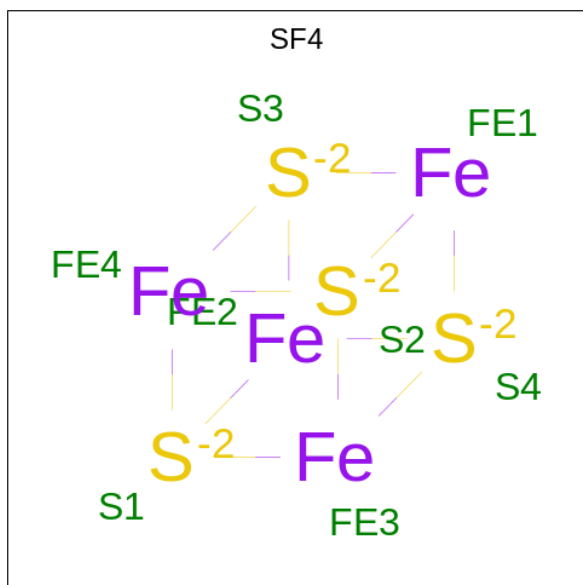
Mol	Chain	Residues	Atoms		AltConf
41	U	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	a	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	
41	b	1	Total	C	0
			40	40	

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

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



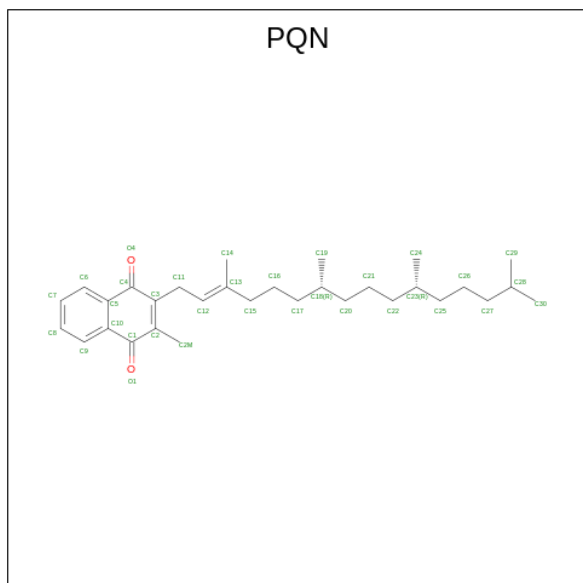
Mol	Chain	Residues	Atoms	AltConf
42	a	1	Total Fe S 8 4 4	0

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

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



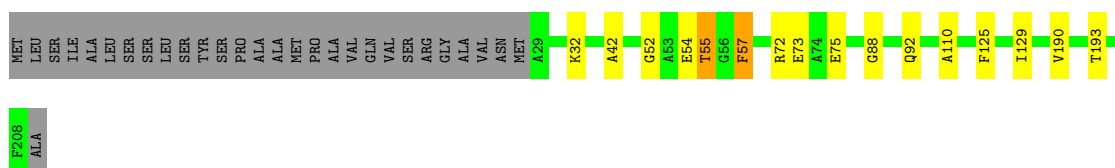
Mol	Chain	Residues	Atoms			AltConf
43	a	1	Total	C	O	0
			33	31	2	
43	b	1	Total	C	O	0
			33	31	2	

3 Residue-property plots [i](#)

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

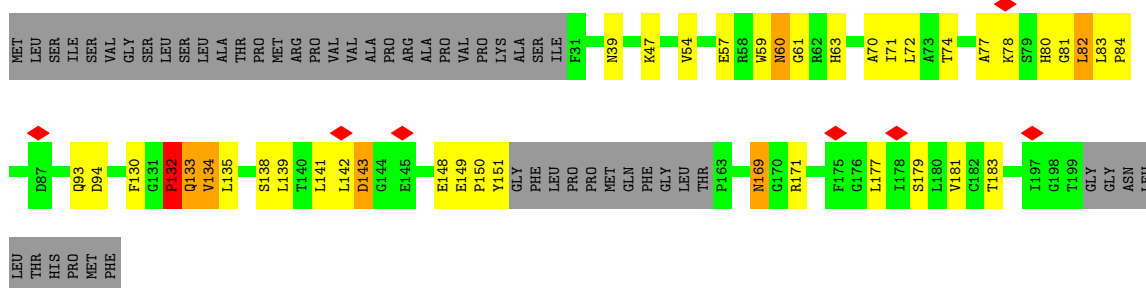
• Molecule 1: iFCPI-7

Chain A: 



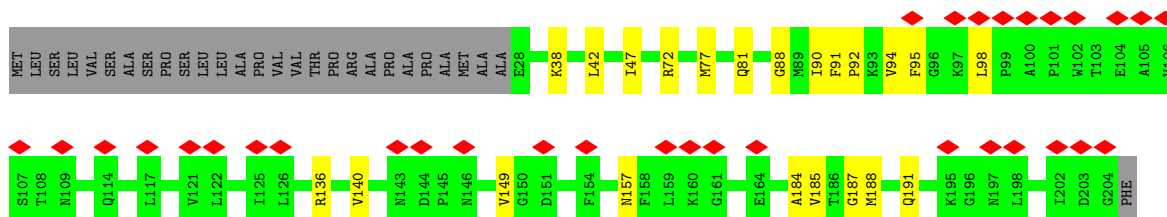
• Molecule 2: iFCPI-1

Chain B: 



• Molecule 3: iFCPI-11

Chain C: 



• Molecule 4: iFCPI-6

Chain D: 

MET ALA PRO LEU LEU ARG THR LEU THR ALA VAL SER VAL GLY VAL ALA THR ALA LEU THR THR GLY ALA THR PRO PRO ALA LEU ALA ARG PRO MET MET THR THR HIS ASP ALA LEU ARG PHE LEU ARG MET ASP GLU ALA ALA PRO PRO ALA LYS PRO ALA GLU ALA ALA GLU GLU ALA ALA PRO

ALA PRO PRO PRO ALA PRO F68 E73 V68 R108 E111 H132 F136 H144 D145 A152 M153 S154 Q155 MET L156 L157 L158 V159 T168 I171 T174 L175 R180 D188 G191 F192 G193 M199 N229 L234 L245

• Molecule 5: iFCPI-5

Chain E: 75% 10% 15%

MET LEU LEU SER LEU ALA SER PRO ALA PRO LEU LEU SER PHE ALA GLY PRO PRO LEU LEU SER GLY VAL ALA HIS ARG THR THR GLY ALA LEU ASN MET MET SER ALA K31 D45 G46 A49 M57 R69 E72 A76 D90 V95 P96 D182 M183 G171 V182 L187 Y194

T195 Y196 M197 G198 M199 S200 D201 L206

• Molecule 6: iFCPI-8

Chain F: 78% 9% 12%

MET LEU SER VAL VAL SER ALA PRO THR THR LEU ALA PHE ALA GLY ALA GLY VAL VAL ALA ARG VAL VAL PRO GLN ARG ALA VAL GLN MET MET SER A30 D35 E36 A39 I48 R52 N96 D99 R104 E105 F174 D175 L176 W177 L178 G179 R184 G187 M188 L189

L195 K205 R215 M222 G236 Y239 SER

• Molecule 7: iFCPI-13

Chain G: 71% 13% 16%

MET LEU SER LEU ALA SER PRO LEU SER SER THR ALA PHE VAL VAL ALA PRO ILE PRO PRO ALA ALA ARG ARG GLY VAL ARG ALA ALA ALA MET MET G31 V36 D57 E58 G59 N60 R65 A66 A67 H71 G88 T89 H90 F91 E92 G93 M94 A109 G110 L113 G114 A115 A116

K117 V118 V135 E138 M139 E145 P153 V154 V155 M177 I189 P197 PHE

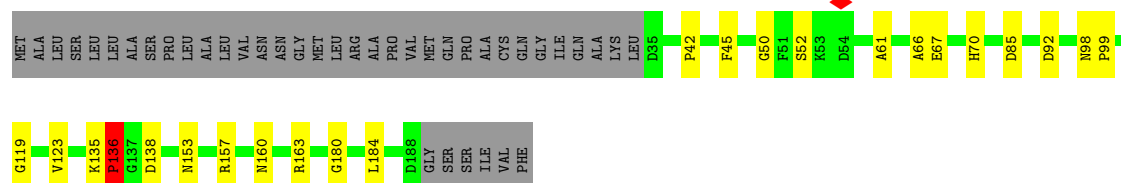
• Molecule 8: iFCPI-10

Chain H: 5% 67% 17% 16%

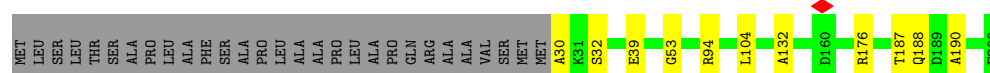
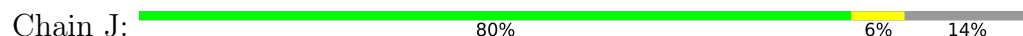
MET LEU THR SER LEU GLN SER SER LEU SER ASN ALA GLY VAL ALA PRO ALA ALA ARG VAL VAL ARG MET GLN ALA PRO MET MET VAL K31 S32 K43 L44 D45 S62 F63 W67 L73 K74 R77 I78 D90 G91 G92 F93 F97 H100 S103 Q115

A128 Y131 I134 M135 M138 G147 D152 P153 F154 K155 D158 T159 P160 E161 A164 K169 E170 H173 F181 V185 T186 Q187 L190 H193 G194 F195 P196 Y197 LEU

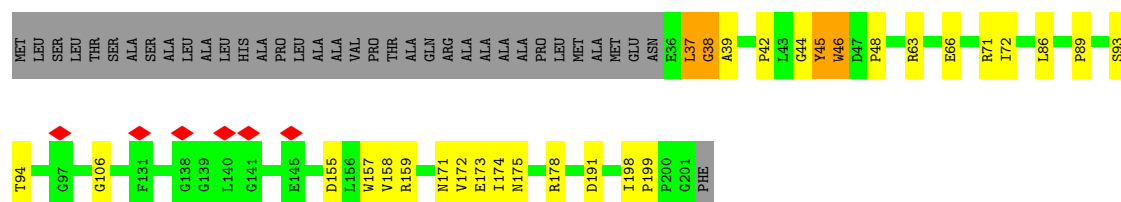
• Molecule 9: iFCPI-3



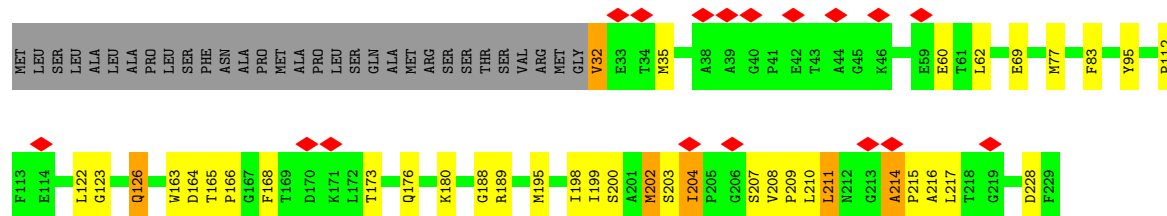
• Molecule 10: iFCPI-9



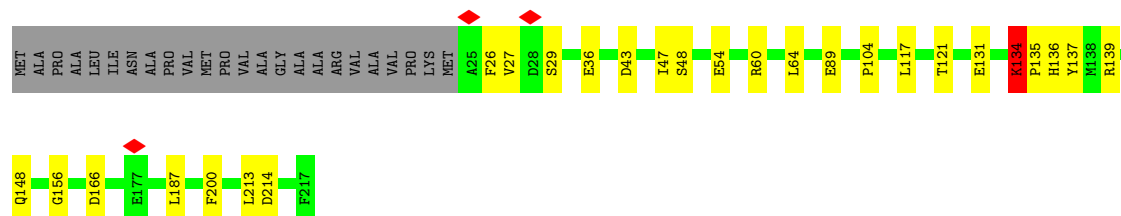
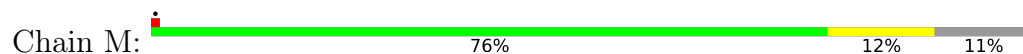
• Molecule 11: iFCPI-4



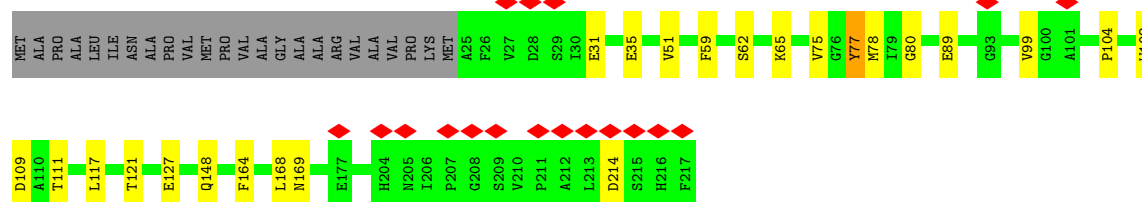
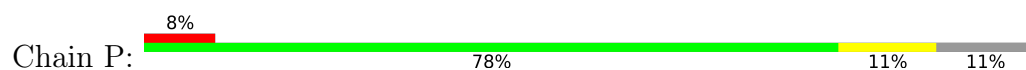
• Molecule 12: iFCPI-12



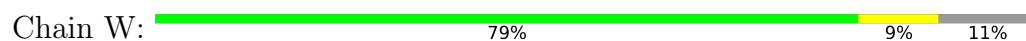
• Molecule 13: iFCPI-15/14/16



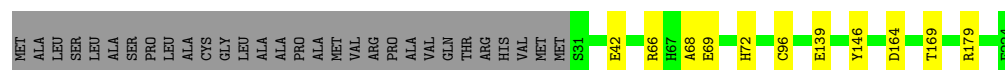
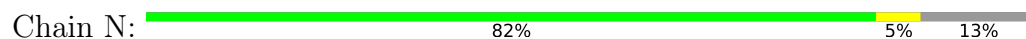
• Molecule 13: iFCPI-15/14/16



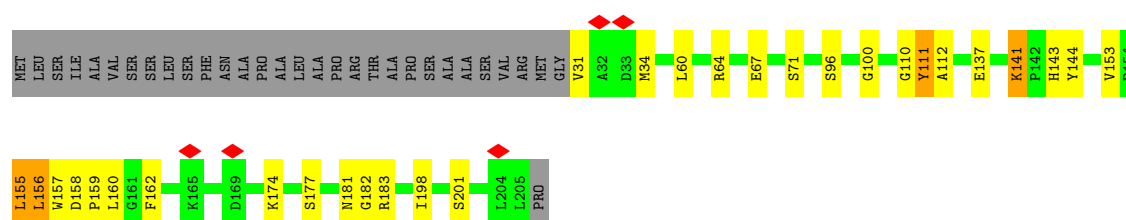
- Molecule 13: iFCPI-15/14/16



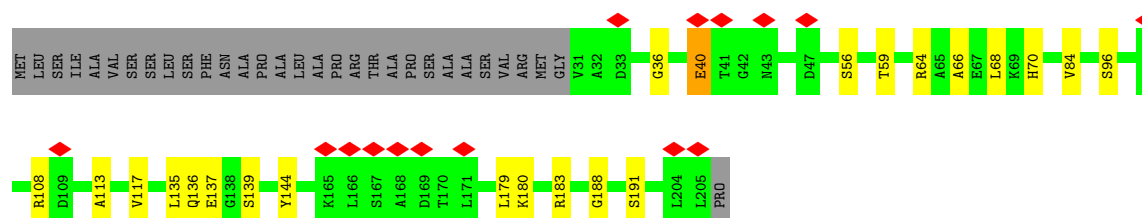
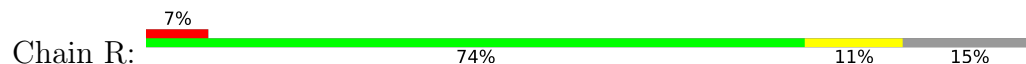
- Molecule 14: iFCPI-17



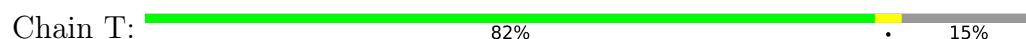
- Molecule 15: iFCPI-20/19/21

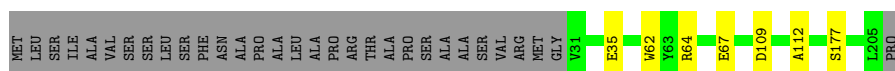


- Molecule 15: iFCPI-20/19/21



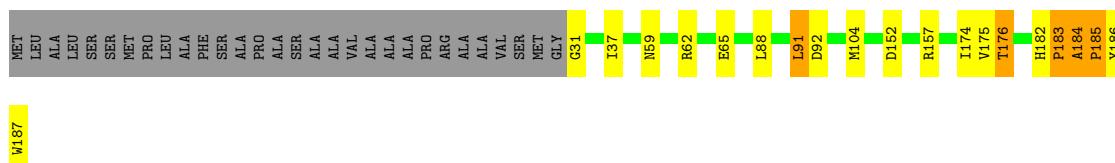
- Molecule 15: iFCPI-20/19/21





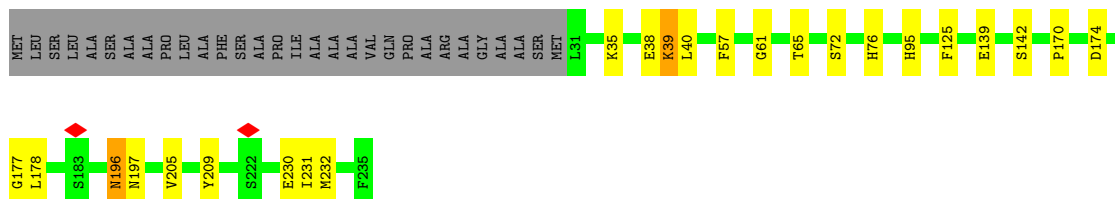
- Molecule 16: iFCPI-18

Chain Q: 73% 8% 16%



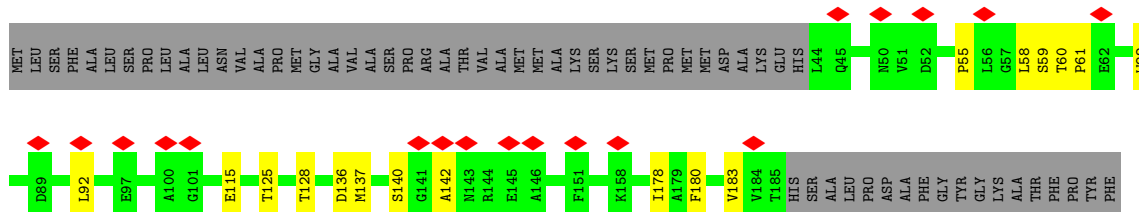
- Molecule 17: iFCPI-22

Chain S: 77% 9% 13%



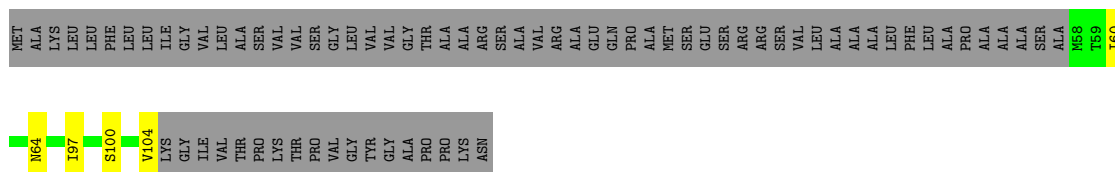
- Molecule 18: iFCPI-2

Chain U: 9% 62% 8% 30%



- Molecule 19: L-iFP

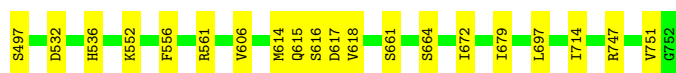
Chain V: 34% 61% 5%



- Molecule 20: Photosystem I P700 chlorophyll a apoprotein A1

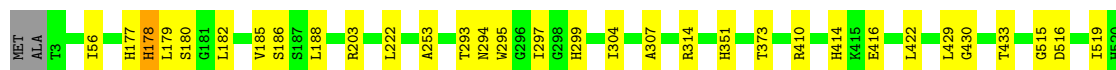
Chain a: 92% 6% 2%





- Molecule 21: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 92% 7%



- Molecule 22: Photosystem I iron-sulfur center

Chain c: 89% 10%



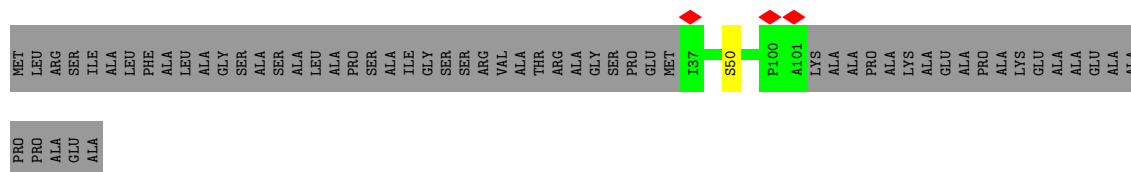
- Molecule 23: Photosystem I reaction center subunit II

Chain d: 89% 8%



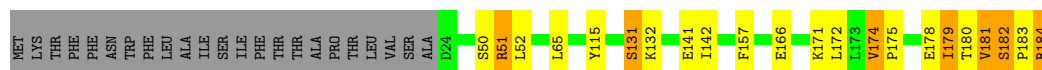
- Molecule 24: PsaE

Chain e: 52% 48%



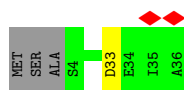
- Molecule 25: Photosystem I reaction center subunit III

Chain f: 76% 8% 12%



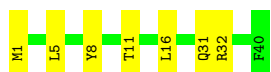
- Molecule 26: Photosystem I reaction center subunit VIII

Chain i: 6% 89% 8%



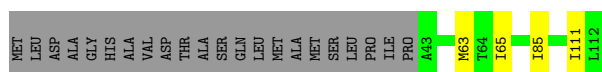
- Molecule 27: Photosystem I reaction center subunit IX

Chain j: 82% 18%



- Molecule 28: PsaK

Chain k: 72% . 24%



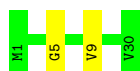
- Molecule 29: Photosystem I reaction center subunit XI

Chain l: 94% 5% .



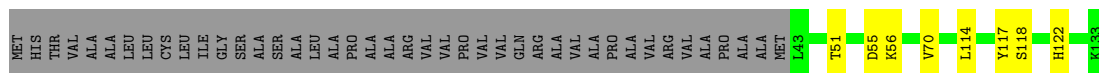
- Molecule 30: Photosystem I reaction center subunit XII

Chain m: 93% 7%



- Molecule 31: PsaR

Chain r: 62% 6% 32%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.577	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.065	Depositor
Map value standard deviation	0.129	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DD6, SF4, CLA, LMG, DGD, SQD, LMU, PQN, BCR, KC2, A86, LHG

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

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

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

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

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1403	0	1381	14	0
2	B	1194	0	1157	35	0
3	C	1346	0	1366	16	0
4	D	1392	0	1340	20	0
5	E	1316	0	1319	11	0
6	F	1573	0	1548	22	0
7	G	1235	0	1231	24	0

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 651 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:497:SER:OG	35:a:851:LHG:C4	1.80	1.27
20:a:497:SER:OG	35:a:851:LHG:HC41	1.10	1.25
33:I:309:KC2:O1A	36:I:201:LMG:O3	1.52	1.20
34:A:313:DD6:C28	36:N:301:LMG:H322	1.77	1.14
37:S:315:A86:C39	36:S:322:LMG:H291	1.79	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

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

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	GLY

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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

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

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

517 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	CLA	H	308	8	45,49,73	2.32	10 (22%)	54,84,113	1.87	9 (16%)
32	CLA	P	311	-	64,68,73	1.80	9 (14%)	77,107,113	1.44	10 (12%)
37	A86	G	311	-	44,50,50	0.56	1 (2%)	51,76,76	0.88	2 (3%)
37	A86	P	313	-	44,50,50	0.57	1 (2%)	51,76,76	1.28	2 (3%)
32	CLA	Q	310	-	50,54,73	2.10	9 (18%)	60,90,113	1.67	9 (15%)
37	A86	W	318	-	44,50,50	0.36	0	51,76,76	1.34	4 (7%)
39	SQD	H	315	-	42,43,54	1.32	4 (9%)	51,54,65	1.39	6 (11%)
32	CLA	Q	309	-	49,53,73	2.06	9 (18%)	59,89,113	1.63	5 (8%)
32	CLA	b	820	-	68,72,73	1.78	9 (13%)	81,111,113	1.46	7 (8%)
37	A86	T	313	-	44,50,50	0.78	1 (2%)	51,76,76	1.05	2 (3%)
36	LMG	P	318	-	45,45,55	0.97	2 (4%)	53,53,63	1.15	4 (7%)
37	A86	P	316	-	44,50,50	0.44	0	51,76,76	1.61	5 (9%)
33	KC2	O	302	-	49,53,53	1.89	4 (8%)	62,89,89	1.34	9 (14%)
32	CLA	L	314	-	49,53,73	2.12	9 (18%)	59,89,113	1.61	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	BCR	a	843	-	41,41,41	0.16	0	56,56,56	0.41	0
32	CLA	A	304	-	69,73,73	1.74	9 (13%)	83,113,113	1.41	9 (10%)
33	KC2	W	314	13,36	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
32	CLA	C	309	-	47,51,73	2.16	9 (19%)	56,86,113	1.63	7 (12%)
34	DD6	H	313	-	39,45,45	0.21	0	52,67,67	0.92	4 (7%)
32	CLA	S	304	-	46,50,73	2.14	9 (19%)	55,85,113	1.62	7 (12%)
34	DD6	I	312	-	39,45,45	0.20	0	52,67,67	0.68	1 (1%)
36	LMG	D	302	-	30,30,55	1.17	3 (10%)	38,38,63	1.40	5 (13%)
34	DD6	E	319	-	39,45,45	0.18	0	52,67,67	0.80	3 (5%)
34	DD6	J	314	-	39,45,45	0.25	0	52,67,67	0.65	1 (1%)
32	CLA	P	305	13	64,68,73	1.81	9 (14%)	77,107,113	1.44	7 (9%)
32	CLA	M	306	13	66,70,73	1.81	9 (13%)	79,109,113	1.45	7 (8%)
32	CLA	R	308	15	64,68,73	1.80	9 (14%)	77,107,113	1.49	9 (11%)
33	KC2	S	302	17	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
32	CLA	J	301	10	49,53,73	2.09	9 (18%)	59,89,113	1.57	7 (11%)
37	A86	Q	311	-	44,50,50	0.44	0	51,76,76	0.89	2 (3%)
33	KC2	E	313	-	49,53,53	1.88	4 (8%)	62,89,89	1.34	8 (12%)
34	DD6	Q	312	-	39,45,45	0.18	0	52,67,67	0.77	1 (1%)
42	SF4	c	101	22	0,12,12	-	-	-	-	-
32	CLA	b	805	-	69,73,73	1.69	9 (13%)	83,113,113	1.32	8 (9%)
32	CLA	M	312	-	64,68,73	1.82	9 (14%)	77,107,113	1.46	7 (9%)
32	CLA	N	309	14	54,58,73	2.04	9 (16%)	65,95,113	1.69	9 (13%)
32	CLA	k	203	-	59,63,73	1.88	9 (15%)	71,101,113	1.55	10 (14%)
37	A86	Q	316	-	44,50,50	0.57	1 (2%)	51,76,76	0.45	0
33	KC2	R	303	-	49,53,53	1.91	4 (8%)	62,89,89	1.35	8 (12%)
32	CLA	b	813	-	49,53,73	2.07	9 (18%)	59,89,113	1.61	7 (11%)
32	CLA	W	306	-	59,63,73	1.90	9 (15%)	71,101,113	1.52	7 (9%)
34	DD6	H	311	-	39,45,45	0.23	0	52,67,67	1.03	4 (7%)
34	DD6	C	310	-	39,45,45	0.19	0	52,67,67	0.81	2 (3%)
33	KC2	L	313	-	49,53,53	1.88	4 (8%)	62,89,89	1.36	6 (9%)
34	DD6	O	313	-	39,45,45	0.18	0	52,67,67	1.22	4 (7%)
34	DD6	V	202	-	39,45,45	0.19	0	52,67,67	0.96	3 (5%)
32	CLA	J	307	10	59,63,73	1.93	10 (16%)	71,101,113	1.69	9 (12%)
32	CLA	b	808	21	69,73,73	1.72	9 (13%)	83,113,113	1.34	7 (8%)
32	CLA	F	309	-	59,63,73	1.88	9 (15%)	71,101,113	1.47	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	H	307	-	64,68,73	1.85	9 (14%)	77,107,113	1.49	8 (10%)
32	CLA	E	314	-	54,58,73	2.01	9 (16%)	65,95,113	1.59	8 (12%)
32	CLA	r	202	-	49,53,73	2.09	9 (18%)	59,89,113	1.63	6 (10%)
35	LHG	I	318	32	36,36,48	1.05	2 (5%)	39,42,54	1.29	4 (10%)
32	CLA	L	307	-	61,65,73	1.87	9 (14%)	73,103,113	1.50	8 (10%)
33	KC2	M	307	-	49,53,53	1.91	4 (8%)	62,89,89	1.31	8 (12%)
33	KC2	K	309	11	49,53,53	1.89	4 (8%)	62,89,89	1.36	10 (16%)
32	CLA	D	311	4	69,73,73	1.74	9 (13%)	83,113,113	1.38	8 (9%)
32	CLA	B	309	-	59,63,73	1.88	9 (15%)	71,101,113	1.41	6 (8%)
33	KC2	P	301	-	49,53,53	1.89	4 (8%)	62,89,89	1.33	9 (14%)
32	CLA	a	810	-	66,70,73	1.76	9 (13%)	79,109,113	1.43	8 (10%)
43	PQN	b	847	-	34,34,34	0.42	0	42,45,45	0.67	1 (2%)
41	BCR	k	204	-	41,41,41	0.14	0	56,56,56	0.38	0
36	LMG	l	201	33	49,49,55	0.89	2 (4%)	57,57,63	1.48	12 (21%)
32	CLA	G	306	7	60,64,73	1.91	9 (15%)	72,102,113	1.64	10 (13%)
32	CLA	b	835	-	64,68,73	1.79	9 (14%)	77,107,113	1.50	9 (11%)
32	CLA	D	309	4	49,53,73	2.10	9 (18%)	59,89,113	1.65	7 (11%)
32	CLA	H	309	-	49,53,73	2.16	9 (18%)	59,89,113	1.66	8 (13%)
37	A86	D	322	-	44,50,50	0.47	1 (2%)	51,76,76	0.92	2 (3%)
32	CLA	a	836	20	59,63,73	1.90	9 (15%)	71,101,113	1.47	7 (9%)
32	CLA	E	312	-	64,68,73	1.82	9 (14%)	77,107,113	1.43	7 (9%)
32	CLA	U	305	18	49,53,73	2.15	9 (18%)	59,89,113	1.76	10 (16%)
34	DD6	E	317	-	39,45,45	0.20	0	52,67,67	0.94	3 (5%)
32	CLA	L	309	-	49,53,73	2.13	9 (18%)	59,89,113	1.65	7 (11%)
36	LMG	W	320	33,37	39,39,55	1.05	2 (5%)	47,47,63	1.13	3 (6%)
32	CLA	U	302	18	49,53,73	2.12	9 (18%)	59,89,113	1.63	9 (15%)
32	CLA	C	305	-	64,68,73	1.92	9 (14%)	77,107,113	1.57	9 (11%)
33	KC2	W	305	13	49,53,53	1.85	4 (8%)	62,89,89	1.36	7 (11%)
32	CLA	a	833	-	69,73,73	1.72	9 (13%)	83,113,113	1.40	7 (8%)
32	CLA	R	309	15	45,49,73	2.29	10 (22%)	54,84,113	1.83	7 (12%)
32	CLA	R	307	15	49,53,73	2.08	9 (18%)	59,89,113	1.63	7 (11%)
34	DD6	G	312	-	39,45,45	0.24	0	52,67,67	0.86	4 (7%)
41	BCR	l	205	-	41,41,41	0.11	0	56,56,56	0.33	0
33	KC2	I	309	9,36	49,53,53	1.87	4 (8%)	62,89,89	1.37	8 (12%)
32	CLA	F	311	-	49,53,73	2.10	9 (18%)	59,89,113	1.69	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DD6	D	317	-	39,45,45	0.17	0	52,67,67	1.01	3 (5%)
35	LHG	F	321	-	39,39,48	0.69	2 (5%)	42,45,54	1.16	2 (4%)
34	DD6	M	316	-	39,45,45	0.18	0	52,67,67	0.79	1 (1%)
34	DD6	R	314	-	39,45,45	0.18	0	52,67,67	0.83	1 (1%)
35	LHG	a	851	-	37,37,48	1.01	2 (5%)	40,43,54	1.27	5 (12%)
32	CLA	M	305	-	54,58,73	1.96	9 (16%)	65,95,113	1.54	11 (16%)
32	CLA	Q	305	16	55,59,73	1.94	9 (16%)	66,96,113	1.54	6 (9%)
33	KC2	T	311	15	49,53,53	1.88	4 (8%)	62,89,89	1.38	10 (16%)
32	CLA	Q	303	16	64,68,73	1.88	10 (15%)	77,107,113	1.65	9 (11%)
34	DD6	I	313	-	39,45,45	0.19	0	52,67,67	0.79	2 (3%)
32	CLA	a	815	20	54,58,73	1.93	9 (16%)	65,95,113	1.53	7 (10%)
32	CLA	T	310	-	59,63,73	1.91	9 (15%)	71,101,113	1.56	8 (11%)
32	CLA	b	837	21	69,73,73	1.77	9 (13%)	83,113,113	1.52	7 (8%)
32	CLA	J	312	-	62,66,73	1.88	9 (14%)	74,104,113	1.45	8 (10%)
32	CLA	K	301	-	49,53,73	2.11	9 (18%)	59,89,113	1.62	7 (11%)
36	LMG	A	318	-	40,40,55	0.95	2 (5%)	48,48,63	1.28	6 (12%)
32	CLA	H	306	8	54,58,73	2.01	9 (16%)	65,95,113	1.57	6 (9%)
33	KC2	N	302	14	49,53,53	1.89	4 (8%)	62,89,89	1.33	8 (12%)
37	A86	W	316	36	44,50,50	0.62	1 (2%)	51,76,76	0.69	1 (1%)
32	CLA	L	311	-	43,48,73	2.30	9 (20%)	52,82,113	1.97	10 (19%)
32	CLA	a	841	20	69,73,73	1.72	9 (13%)	83,113,113	1.38	7 (8%)
32	CLA	S	309	-	64,68,73	1.79	9 (14%)	77,107,113	1.47	9 (11%)
35	LHG	E	321	-	45,45,48	0.92	2 (4%)	48,51,54	1.15	3 (6%)
34	DD6	Q	314	-	39,45,45	0.17	0	52,67,67	0.67	2 (3%)
32	CLA	a	832	-	64,68,73	1.80	9 (14%)	77,107,113	1.48	5 (6%)
32	CLA	S	311	-	54,58,73	2.02	9 (16%)	65,95,113	1.65	8 (12%)
32	CLA	T	308	15	64,68,73	1.84	9 (14%)	77,107,113	1.57	14 (18%)
34	DD6	K	315	-	39,45,45	0.18	0	52,67,67	1.18	3 (5%)
35	LHG	F	318	-	40,40,48	0.71	1 (2%)	43,46,54	1.11	2 (4%)
33	KC2	A	310	1	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
36	LMG	D	321	-	40,40,55	0.82	0	48,48,63	1.29	6 (12%)
33	KC2	J	310	10	49,53,53	1.90	4 (8%)	62,89,89	1.33	8 (12%)
34	DD6	H	312	-	39,45,45	0.20	0	52,67,67	0.90	3 (5%)
32	CLA	Q	301	33	64,68,73	1.86	9 (14%)	77,107,113	1.48	7 (9%)
32	CLA	b	818	-	69,73,73	1.77	9 (13%)	83,113,113	1.42	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	l	203	35	69,73,73	1.79	9 (13%)	83,113,113	1.32	7 (8%)
32	CLA	O	305	15	69,73,73	1.70	9 (13%)	83,113,113	1.40	8 (9%)
35	LHG	a	850	32	29,29,48	0.84	0	32,35,54	1.23	3 (9%)
32	CLA	M	308	13	61,65,73	1.89	9 (14%)	73,103,113	1.55	11 (15%)
32	CLA	I	305	9	60,64,73	1.91	9 (15%)	72,102,113	1.58	8 (11%)
32	CLA	R	304	-	49,53,73	2.10	9 (18%)	59,89,113	1.66	8 (13%)
32	CLA	B	301	-	43,48,73	2.25	9 (20%)	52,82,113	1.86	9 (17%)
32	CLA	G	301	-	49,53,73	2.15	9 (18%)	59,89,113	1.64	7 (11%)
32	CLA	a	817	20	65,69,73	1.78	9 (13%)	78,108,113	1.44	8 (10%)
32	CLA	b	828	21	65,69,73	1.82	9 (13%)	78,108,113	1.50	8 (10%)
35	LHG	D	320	-	47,47,48	0.64	0	50,53,54	1.17	3 (6%)
32	CLA	B	303	-	49,53,73	2.10	9 (18%)	59,89,113	1.57	5 (8%)
37	A86	K	312	-	44,50,50	0.50	1 (2%)	51,76,76	0.74	1 (1%)
41	BCR	a	844	-	41,41,41	0.16	0	56,56,56	0.40	0
32	CLA	H	310	-	50,54,73	2.12	9 (18%)	60,90,113	1.59	7 (11%)
34	DD6	N	321	-	39,45,45	0.16	0	52,67,67	0.89	1 (1%)
33	KC2	L	302	12	49,53,53	1.91	4 (8%)	62,89,89	1.33	9 (14%)
32	CLA	a	820	-	69,73,73	1.75	9 (13%)	83,113,113	1.48	9 (10%)
37	A86	M	315	-	44,50,50	0.36	0	51,76,76	1.19	3 (5%)
32	CLA	D	306	4	64,68,73	1.78	9 (14%)	77,107,113	1.48	10 (12%)
33	KC2	R	311	15	49,53,53	1.88	4 (8%)	62,89,89	1.33	9 (14%)
32	CLA	b	821	21	59,63,73	1.87	9 (15%)	71,101,113	1.55	7 (9%)
32	CLA	K	304	11	49,53,73	2.11	9 (18%)	59,89,113	1.67	7 (11%)
37	A86	N	315	-	44,50,50	0.54	1 (2%)	51,76,76	0.79	1 (1%)
32	CLA	a	852	-	69,73,73	1.75	9 (13%)	83,113,113	1.31	9 (10%)
32	CLA	R	310	-	59,63,73	1.89	9 (15%)	71,101,113	1.48	6 (8%)
33	KC2	T	304	15	49,53,53	1.87	4 (8%)	62,89,89	1.35	8 (12%)
37	A86	M	314	-	44,50,50	0.60	1 (2%)	51,76,76	0.82	2 (3%)
32	CLA	a	822	-	66,70,73	1.76	9 (13%)	79,109,113	1.43	10 (12%)
37	A86	N	317	-	44,50,50	0.61	1 (2%)	51,76,76	0.84	2 (3%)
34	DD6	P	315	-	39,45,45	0.25	0	52,67,67	0.89	4 (7%)
32	CLA	I	303	9	59,63,73	1.93	9 (15%)	71,101,113	1.64	9 (12%)
37	A86	R	313	-	44,50,50	0.56	1 (2%)	51,76,76	1.01	2 (3%)
32	CLA	l	202	-	49,53,73	2.07	9 (18%)	59,89,113	1.65	7 (11%)
32	CLA	F	322	-	64,68,73	1.86	9 (14%)	77,107,113	1.52	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	b	806	-	69,73,73	1.77	9 (13%)	83,113,113	1.40	7 (8%)
37	A86	N	316	-	44,50,50	0.56	1 (2%)	51,76,76	1.37	3 (5%)
32	CLA	H	301	8	49,53,73	2.15	9 (18%)	59,89,113	1.75	9 (15%)
35	LHG	E	301	-	45,45,48	0.65	1 (2%)	48,51,54	1.10	2 (4%)
32	CLA	a	823	-	69,73,73	1.73	9 (13%)	83,113,113	1.41	8 (9%)
34	DD6	Q	313	-	39,45,45	0.21	0	52,67,67	0.64	1 (1%)
37	A86	r	204	-	44,50,50	0.44	1 (2%)	51,76,76	1.00	2 (3%)
35	LHG	a	849	-	47,47,48	0.63	1 (2%)	50,53,54	1.16	3 (6%)
36	LMG	L	320	-	37,37,55	0.82	1 (2%)	45,45,63	1.24	5 (11%)
32	CLA	f	201	-	64,68,73	1.79	9 (14%)	77,107,113	1.36	7 (9%)
38	LMU	D	324	-	36,36,36	0.38	0	47,47,47	0.85	0
32	CLA	U	307	-	49,53,73	2.15	9 (18%)	59,89,113	1.70	8 (13%)
32	CLA	W	313	-	64,68,73	1.86	9 (14%)	77,107,113	1.51	8 (10%)
34	DD6	E	318	-	39,45,45	0.17	0	52,67,67	0.73	3 (5%)
36	LMG	S	322	33	33,33,55	1.10	2 (6%)	41,41,63	1.27	3 (7%)
35	LHG	B	308	-	30,30,48	1.11	2 (6%)	33,36,54	1.20	4 (12%)
32	CLA	R	301	-	49,53,73	2.15	9 (18%)	59,89,113	1.74	8 (13%)
33	KC2	N	307	14	49,53,53	1.89	4 (8%)	62,89,89	1.34	7 (11%)
32	CLA	J	308	-	49,53,73	2.15	9 (18%)	59,89,113	1.73	8 (13%)
37	A86	H	314	-	44,50,50	0.38	0	51,76,76	1.15	3 (5%)
33	KC2	K	303	11	49,53,53	1.90	4 (8%)	62,89,89	1.34	9 (14%)
32	CLA	U	306	-	49,53,73	2.13	9 (18%)	59,89,113	1.63	7 (11%)
36	LMG	A	317	-	36,36,55	1.07	2 (5%)	44,44,63	1.32	4 (9%)
32	CLA	l	204	29	69,73,73	1.79	9 (13%)	83,113,113	1.48	11 (13%)
32	CLA	b	832	-	69,73,73	1.77	9 (13%)	83,113,113	1.43	6 (7%)
33	KC2	R	302	15	49,53,53	1.91	4 (8%)	62,89,89	1.37	9 (14%)
32	CLA	E	308	5	69,73,73	1.73	9 (13%)	83,113,113	1.35	7 (8%)
33	KC2	M	313	13,36	49,53,53	1.88	4 (8%)	62,89,89	1.34	9 (14%)
37	A86	S	314	-	44,50,50	0.30	0	51,76,76	1.65	6 (11%)
32	CLA	Q	308	-	49,53,73	2.12	9 (18%)	59,89,113	1.65	8 (13%)
32	CLA	b	810	21	64,68,73	1.77	9 (14%)	77,107,113	1.34	6 (7%)
32	CLA	a	812	20	59,63,73	1.88	9 (15%)	71,101,113	1.67	10 (14%)
32	CLA	b	802	-	69,73,73	1.70	9 (13%)	83,113,113	1.47	8 (9%)
32	CLA	K	308	11	69,73,73	1.78	9 (13%)	83,113,113	1.41	7 (8%)
32	CLA	a	819	20	69,73,73	1.72	9 (13%)	83,113,113	1.37	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	C	306	3	69,73,73	1.81	9 (13%)	83,113,113	1.48	8 (9%)
37	A86	L	316	-	44,50,50	0.44	1 (2%)	51,76,76	1.50	2 (3%)
32	CLA	A	302	35	64,68,73	1.81	9 (14%)	77,107,113	1.37	5 (6%)
35	LHG	M	319	-	45,45,48	0.64	0	48,51,54	1.18	4 (8%)
34	DD6	A	315	-	39,45,45	0.19	0	52,67,67	0.90	3 (5%)
32	CLA	K	307	11	45,49,73	2.26	10 (22%)	54,84,113	1.67	9 (16%)
32	CLA	a	814	20	69,73,73	1.70	9 (13%)	83,113,113	1.53	11 (13%)
32	CLA	D	315	-	49,53,73	2.05	9 (18%)	59,89,113	1.70	7 (11%)
32	CLA	G	308	-	58,62,73	1.94	9 (15%)	69,99,113	1.53	7 (10%)
34	DD6	J	315	-	39,45,45	0.18	0	52,67,67	0.88	2 (3%)
35	LHG	A	316	-	39,39,48	0.70	1 (2%)	42,45,54	1.16	2 (4%)
33	KC2	C	303	-	49,53,53	1.91	4 (8%)	62,89,89	1.32	7 (11%)
35	LHG	W	319	32	45,45,48	0.72	1 (2%)	48,51,54	1.16	4 (8%)
32	CLA	P	308	13	49,53,73	2.08	9 (18%)	59,89,113	1.58	7 (11%)
32	CLA	W	312	13	64,68,73	1.82	9 (14%)	77,107,113	1.42	7 (9%)
32	CLA	O	308	-	49,53,73	2.13	9 (18%)	59,89,113	1.68	8 (13%)
33	KC2	N	303	14	49,53,53	1.88	4 (8%)	62,89,89	1.38	9 (14%)
32	CLA	I	308	-	59,63,73	1.93	9 (15%)	71,101,113	1.58	7 (9%)
33	KC2	N	304	14	49,53,53	1.84	4 (8%)	62,89,89	1.37	9 (14%)
32	CLA	A	305	1	65,69,73	1.82	9 (13%)	78,108,113	1.46	7 (8%)
32	CLA	F	306	6	59,63,73	1.91	9 (15%)	71,101,113	1.50	8 (11%)
32	CLA	a	838	-	69,73,73	1.72	9 (13%)	83,113,113	1.46	9 (10%)
32	CLA	b	817	21	59,63,73	1.87	9 (15%)	71,101,113	1.50	7 (9%)
37	A86	O	312	-	44,50,50	0.47	1 (2%)	51,76,76	0.92	3 (5%)
32	CLA	B	306	-	49,53,73	2.11	9 (18%)	59,89,113	1.65	7 (11%)
32	CLA	b	804	21	69,73,73	1.75	9 (13%)	83,113,113	1.50	10 (12%)
33	KC2	P	306	-	49,53,53	1.90	4 (8%)	62,89,89	1.31	8 (12%)
37	A86	J	313	-	44,50,50	0.47	1 (2%)	51,76,76	1.82	5 (9%)
32	CLA	D	312	4	59,63,73	1.92	9 (15%)	71,101,113	1.52	9 (12%)
32	CLA	a	840	-	69,73,73	1.74	9 (13%)	83,113,113	1.44	8 (9%)
32	CLA	b	814	-	49,53,73	2.05	9 (18%)	59,89,113	1.60	7 (11%)
32	CLA	E	306	5	64,68,73	1.86	9 (14%)	77,107,113	1.47	7 (9%)
32	CLA	T	305	-	49,53,73	2.14	9 (18%)	59,89,113	1.68	9 (15%)
41	BCR	f	202	-	41,41,41	0.11	0	56,56,56	0.38	0
32	CLA	C	302	-	45,49,73	2.27	10 (22%)	54,84,113	1.79	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	k	202	-	59,63,73	1.90	9 (15%)	71,101,113	1.46	5 (7%)
36	LMG	M	320	33	40,40,55	1.08	2 (5%)	48,48,63	1.09	3 (6%)
33	KC2	H	303	-	49,53,53	1.91	4 (8%)	62,89,89	1.33	7 (11%)
32	CLA	I	317	35	69,73,73	1.73	9 (13%)	83,113,113	1.40	6 (7%)
32	CLA	K	310	-	49,53,73	2.14	9 (18%)	59,89,113	1.73	8 (13%)
32	CLA	G	307	-	43,48,73	2.26	9 (20%)	52,82,113	1.93	9 (17%)
42	SF4	c	102	-	0,12,12	-	-	-	-	-
36	LMG	E	302	-	40,40,55	1.11	4 (10%)	48,48,63	1.55	8 (16%)
32	CLA	N	311	14	64,68,73	1.80	9 (14%)	77,107,113	1.40	8 (10%)
33	KC2	L	303	-	49,53,53	1.87	4 (8%)	62,89,89	1.36	9 (14%)
32	CLA	I	306	9	69,73,73	1.75	9 (13%)	83,113,113	1.43	6 (7%)
32	CLA	D	314	4	56,60,73	1.84	9 (16%)	67,97,113	1.51	10 (14%)
32	CLA	a	825	20	69,73,73	1.71	9 (13%)	83,113,113	1.30	7 (8%)
37	A86	M	317	-	44,50,50	0.73	1 (2%)	51,76,76	0.55	1 (1%)
32	CLA	C	304	3	47,51,73	2.21	9 (19%)	56,86,113	1.85	10 (17%)
33	KC2	S	303	17	49,53,53	1.86	4 (8%)	62,89,89	1.36	9 (14%)
41	BCR	a	845	-	41,41,41	0.15	0	56,56,56	0.37	0
43	PQN	a	848	-	34,34,34	0.39	0	42,45,45	0.99	1 (2%)
32	CLA	D	305	-	62,66,73	1.84	9 (14%)	74,104,113	1.49	7 (9%)
32	CLA	A	308	-	59,63,73	1.87	9 (15%)	71,101,113	1.45	6 (8%)
32	CLA	W	310	13	64,68,73	1.81	9 (14%)	77,107,113	1.43	8 (10%)
32	CLA	f	203	25	49,53,73	2.08	9 (18%)	59,89,113	1.64	5 (8%)
37	A86	U	308	-	44,50,50	0.65	1 (2%)	51,76,76	1.16	3 (5%)
32	CLA	E	315	-	50,54,73	2.07	9 (18%)	60,90,113	1.62	8 (13%)
37	A86	P	319	-	44,50,50	0.49	1 (2%)	51,76,76	0.80	2 (3%)
32	CLA	I	307	-	49,53,73	2.10	9 (18%)	59,89,113	1.71	8 (13%)
32	CLA	V	201	-	62,66,73	1.86	9 (14%)	74,104,113	1.45	7 (9%)
41	BCR	b	844	-	41,41,41	0.14	0	56,56,56	0.49	0
33	KC2	P	312	13	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
32	CLA	P	309	-	65,69,73	1.81	10 (15%)	78,108,113	1.44	7 (8%)
32	CLA	b	836	-	69,73,73	1.74	9 (13%)	83,113,113	1.45	7 (8%)
37	A86	K	311	-	44,50,50	0.60	1 (2%)	51,76,76	0.83	2 (3%)
41	BCR	r	203	-	41,41,41	0.14	0	56,56,56	0.42	0
42	SF4	a	847	-	0,12,12	-	-	-	-	-
32	CLA	Q	307	16	66,70,73	1.78	9 (13%)	79,109,113	1.39	7 (8%)
34	DD6	I	310	-	39,45,45	0.15	0	52,67,67	0.88	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DD6	S	321	-	39,45,45	0.46	0	52,67,67	1.56	5 (9%)
32	CLA	T	309	-	49,53,73	2.12	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	F	304	-	59,63,73	1.91	9 (15%)	71,101,113	1.55	9 (12%)
32	CLA	b	833	-	66,70,73	1.78	9 (13%)	79,109,113	1.51	7 (8%)
32	CLA	a	809	-	64,68,73	1.80	9 (14%)	77,107,113	1.49	7 (9%)
32	CLA	U	301	18	43,48,73	2.25	9 (20%)	52,82,113	1.81	9 (17%)
32	CLA	r	201	-	64,68,73	1.89	9 (14%)	77,107,113	1.54	9 (11%)
37	A86	D	323	-	44,50,50	0.38	0	51,76,76	0.90	3 (5%)
32	CLA	a	828	-	62,66,73	1.81	9 (14%)	74,104,113	1.53	9 (12%)
32	CLA	a	802	-	67,71,73	1.75	9 (13%)	80,110,113	1.47	11 (13%)
34	DD6	D	316	-	39,45,45	0.20	0	52,67,67	0.93	3 (5%)
37	A86	O	311	-	44,50,50	0.33	0	51,76,76	0.96	2 (3%)
32	CLA	F	301	-	43,48,73	2.25	9 (20%)	52,82,113	1.86	9 (17%)
33	KC2	K	302	11	49,53,53	1.87	4 (8%)	62,89,89	1.36	7 (11%)
35	LHG	P	317	-	45,45,48	0.63	0	48,51,54	1.16	4 (8%)
32	CLA	U	303	18	49,53,73	2.10	9 (18%)	59,89,113	1.73	9 (15%)
32	CLA	G	304	-	59,63,73	1.89	9 (15%)	71,101,113	1.49	8 (11%)
37	A86	S	318	-	44,50,50	0.45	1 (2%)	51,76,76	0.92	3 (5%)
37	A86	W	315	-	44,50,50	0.57	1 (2%)	51,76,76	1.11	2 (3%)
33	KC2	Q	317	32	49,53,53	1.85	4 (8%)	62,89,89	1.42	8 (12%)
41	BCR	b	841	-	41,41,41	0.13	0	56,56,56	0.41	0
32	CLA	O	307	15	64,68,73	1.83	9 (14%)	77,107,113	1.47	8 (10%)
32	CLA	b	812	21	69,73,73	1.72	9 (13%)	83,113,113	1.40	7 (8%)
34	DD6	N	319	-	39,45,45	0.16	0	52,67,67	0.98	3 (5%)
32	CLA	D	313	-	62,66,73	1.84	9 (14%)	74,104,113	1.47	7 (9%)
38	LMU	J	318	-	36,36,36	0.69	0	47,47,47	1.01	1 (2%)
36	LMG	D	303	-	36,36,55	1.03	2 (5%)	44,44,63	1.48	7 (15%)
41	BCR	i	101	-	41,41,41	0.20	0	56,56,56	0.53	0
37	A86	C	311	-	44,50,50	0.67	1 (2%)	51,76,76	1.00	3 (5%)
32	CLA	A	307	1	64,68,73	1.84	9 (14%)	77,107,113	1.49	8 (10%)
34	DD6	J	316	-	39,45,45	0.19	0	52,67,67	0.73	3 (5%)
36	LMG	j	104	-	38,38,55	1.09	3 (7%)	46,46,63	1.48	6 (13%)
36	LMG	T	301	-	37,37,55	0.93	1 (2%)	45,45,63	1.27	6 (13%)
41	BCR	a	854	-	41,41,41	0.17	0	56,56,56	0.44	0
32	CLA	a	818	20	64,68,73	1.83	9 (14%)	77,107,113	1.66	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	L	312	-	64,68,73	1.81	9 (14%)	77,107,113	1.40	7 (9%)
33	KC2	L	305	12	49,53,53	1.89	4 (8%)	62,89,89	1.37	8 (12%)
32	CLA	a	803	20	67,71,73	1.75	9 (13%)	80,110,113	1.48	8 (10%)
33	KC2	W	304	13	49,53,53	1.87	4 (8%)	62,89,89	1.35	9 (14%)
36	LMG	N	301	-	40,40,55	1.07	2 (5%)	48,48,63	1.16	4 (8%)
32	CLA	H	305	8	49,53,73	2.09	9 (18%)	59,89,113	1.75	8 (13%)
34	DD6	A	314	-	39,45,45	0.19	0	52,67,67	0.70	1 (1%)
32	CLA	a	830	20	69,73,73	1.78	9 (13%)	83,113,113	1.43	9 (10%)
32	CLA	Q	306	16	66,70,73	1.80	9 (13%)	79,109,113	1.49	9 (11%)
32	CLA	I	301	-	69,73,73	1.74	9 (13%)	83,113,113	1.38	5 (6%)
37	A86	P	314	-	44,50,50	0.43	1 (2%)	51,76,76	1.19	3 (5%)
32	CLA	f	204	-	51,55,73	2.06	9 (17%)	61,91,113	1.60	8 (13%)
34	DD6	A	313	-	39,45,45	0.15	0	52,67,67	0.80	2 (3%)
32	CLA	E	305	5	59,63,73	1.89	9 (15%)	71,101,113	1.48	7 (9%)
33	KC2	M	321	15	49,53,53	1.87	4 (8%)	62,89,89	1.39	7 (11%)
37	A86	M	318	-	44,50,50	0.42	1 (2%)	51,76,76	0.85	4 (7%)
33	KC2	G	309	7	49,53,53	1.88	4 (8%)	62,89,89	1.39	8 (12%)
33	KC2	L	306	12	49,53,53	1.89	4 (8%)	62,89,89	1.35	9 (14%)
41	BCR	j	102	-	41,41,41	0.16	0	56,56,56	0.48	0
32	CLA	b	838	-	69,73,73	1.82	9 (13%)	83,113,113	1.52	8 (9%)
37	A86	S	320	-	44,50,50	0.47	1 (2%)	51,76,76	0.58	0
32	CLA	M	309	13	49,53,73	2.06	9 (18%)	59,89,113	1.63	6 (10%)
32	CLA	H	304	-	49,53,73	2.15	9 (18%)	59,89,113	1.80	9 (15%)
32	CLA	b	819	-	69,73,73	1.71	9 (13%)	83,113,113	1.32	8 (9%)
34	DD6	T	314	-	39,45,45	0.19	0	52,67,67	0.85	3 (5%)
32	CLA	a	835	20	69,73,73	1.72	9 (13%)	83,113,113	1.37	6 (7%)
36	LMG	D	325	-	35,35,55	1.06	2 (5%)	43,43,63	1.48	7 (16%)
41	BCR	b	842	-	41,41,41	0.23	0	56,56,56	0.57	1 (1%)
32	CLA	a	831	20	64,68,73	1.82	9 (14%)	77,107,113	1.45	6 (7%)
33	KC2	M	304	13	49,53,53	1.91	4 (8%)	62,89,89	1.33	6 (9%)
32	CLA	j	101	27	49,53,73	2.09	9 (18%)	59,89,113	1.59	6 (10%)
33	KC2	U	304	18	49,53,53	1.87	4 (8%)	62,89,89	1.36	7 (11%)
33	KC2	F	302	6	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
32	CLA	b	816	-	66,70,73	1.77	9 (13%)	79,109,113	1.37	7 (8%)
32	CLA	V	203	19	59,63,73	1.88	9 (15%)	71,101,113	1.47	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	C	307	3	64,68,73	1.83	9 (14%)	77,107,113	1.54	10 (12%)
40	DGD	b	846	-	57,57,67	0.88	2 (3%)	71,71,81	1.31	6 (8%)
32	CLA	A	309	1	69,73,73	1.74	9 (13%)	83,113,113	1.39	7 (8%)
32	CLA	A	306	1	69,73,73	1.74	9 (13%)	83,113,113	1.34	6 (7%)
32	CLA	E	303	5	49,53,73	2.05	9 (18%)	59,89,113	1.61	6 (10%)
32	CLA	J	306	10	59,63,73	1.85	9 (15%)	71,101,113	1.53	8 (11%)
37	A86	F	317	-	44,50,50	0.52	1 (2%)	51,76,76	0.63	2 (3%)
33	KC2	G	302	-	49,53,53	1.88	4 (8%)	62,89,89	1.33	7 (11%)
32	CLA	D	308	4	59,63,73	1.92	9 (15%)	71,101,113	1.59	8 (11%)
33	KC2	Q	302	-	49,53,53	1.87	4 (8%)	62,89,89	1.32	8 (12%)
32	CLA	F	308	6	50,54,73	2.12	9 (18%)	60,90,113	1.61	7 (11%)
34	DD6	B	307	-	39,45,45	0.19	0	52,67,67	0.78	3 (5%)
32	CLA	W	307	13	49,53,73	2.10	9 (18%)	59,89,113	1.61	7 (11%)
33	KC2	F	310	6,36	49,53,53	1.86	4 (8%)	62,89,89	1.35	9 (14%)
34	DD6	F	316	-	39,45,45	0.21	0	52,67,67	1.38	3 (5%)
32	CLA	F	307	6	64,68,73	1.81	9 (14%)	77,107,113	1.45	8 (10%)
32	CLA	G	303	7	59,63,73	1.89	9 (15%)	71,101,113	1.63	11 (15%)
37	A86	L	318	-	44,50,50	0.67	1 (2%)	51,76,76	1.09	2 (3%)
32	CLA	Q	304	-	54,58,73	1.97	9 (16%)	65,95,113	1.59	9 (13%)
32	CLA	N	313	-	64,68,73	1.83	9 (14%)	77,107,113	1.48	8 (10%)
32	CLA	T	306	15	64,68,73	1.80	9 (14%)	77,107,113	1.37	6 (7%)
37	A86	L	317	-	44,50,50	0.51	1 (2%)	51,76,76	1.20	3 (5%)
34	DD6	D	318	-	39,45,45	0.19	0	52,67,67	0.61	0
32	CLA	a	806	-	64,68,73	1.80	9 (14%)	77,107,113	1.43	8 (10%)
32	CLA	b	803	21	69,73,73	1.71	9 (13%)	83,113,113	1.33	6 (7%)
32	CLA	W	309	13	69,73,73	1.74	9 (13%)	83,113,113	1.38	7 (8%)
32	CLA	J	302	-	49,53,73	2.09	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	b	827	21	54,58,73	1.99	9 (16%)	65,95,113	1.53	7 (10%)
37	A86	R	312	-	44,50,50	0.56	1 (2%)	51,76,76	0.77	1 (1%)
32	CLA	b	815	21	69,73,73	1.69	9 (13%)	83,113,113	1.41	8 (9%)
39	SQD	k	206	-	35,36,54	1.46	5 (14%)	44,47,65	1.49	7 (15%)
37	A86	S	316	-	44,50,50	0.62	1 (2%)	51,76,76	1.21	3 (5%)
33	KC2	N	308	14	49,53,53	1.87	4 (8%)	62,89,89	1.33	8 (12%)
32	CLA	E	307	5	59,63,73	1.85	9 (15%)	71,101,113	1.48	6 (8%)
34	DD6	L	319	-	39,45,45	0.20	0	52,67,67	1.23	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	L	308	12	49,53,73	2.10	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	b	824	21	62,66,73	1.82	9 (14%)	74,104,113	1.43	6 (8%)
33	KC2	W	308	-	49,53,53	1.85	4 (8%)	62,89,89	1.36	9 (14%)
32	CLA	D	307	4	65,69,73	1.81	9 (13%)	78,108,113	1.57	10 (12%)
32	CLA	O	304	-	49,53,73	2.14	9 (18%)	59,89,113	1.74	9 (15%)
32	CLA	b	811	21	54,58,73	1.95	9 (16%)	65,95,113	1.58	8 (12%)
34	DD6	F	314	-	39,45,45	0.23	0	52,67,67	0.86	3 (5%)
33	KC2	R	305	15	49,53,53	1.90	4 (8%)	62,89,89	1.36	6 (9%)
32	CLA	a	834	20	69,73,73	1.73	9 (13%)	83,113,113	1.37	6 (7%)
32	CLA	b	831	-	64,68,73	1.77	9 (14%)	77,107,113	1.37	7 (9%)
41	BCR	b	845	-	41,41,41	0.16	0	56,56,56	0.29	0
32	CLA	a	807	-	69,73,73	1.78	9 (13%)	83,113,113	1.50	9 (10%)
33	KC2	P	302	13	49,53,53	1.91	4 (8%)	62,89,89	1.37	9 (14%)
32	CLA	a	808	20	54,58,73	2.01	9 (16%)	65,95,113	1.59	8 (12%)
32	CLA	P	310	-	45,49,73	2.29	10 (22%)	54,84,113	1.80	7 (12%)
32	CLA	W	311	13	69,73,73	1.73	9 (13%)	83,113,113	1.35	7 (8%)
34	DD6	I	311	-	39,45,45	0.17	0	52,67,67	0.70	1 (1%)
37	A86	G	310	-	44,50,50	0.38	0	51,76,76	1.25	2 (3%)
32	CLA	A	301	1	49,53,73	2.05	9 (18%)	59,89,113	1.59	8 (13%)
32	CLA	a	853	-	69,73,73	1.73	9 (13%)	83,113,113	1.43	10 (12%)
32	CLA	V	204	-	54,58,73	1.98	9 (16%)	65,95,113	1.54	6 (9%)
33	KC2	O	303	15	49,53,53	1.86	4 (8%)	62,89,89	1.31	8 (12%)
41	BCR	b	843	-	41,41,41	0.12	0	56,56,56	0.55	0
32	CLA	E	309	5	62,66,73	1.81	9 (14%)	74,104,113	1.51	8 (10%)
32	CLA	A	303	1	66,70,73	1.77	9 (13%)	79,109,113	1.43	7 (8%)
34	DD6	E	316	-	39,45,45	0.19	0	52,67,67	0.95	3 (5%)
32	CLA	b	826	-	53,57,73	2.05	9 (16%)	62,93,113	1.68	9 (14%)
37	A86	M	322	-	44,50,50	0.43	1 (2%)	51,76,76	0.65	1 (1%)
32	CLA	a	837	20	59,63,73	1.93	9 (15%)	71,101,113	1.59	9 (12%)
40	DGD	Q	318	-	57,57,67	0.92	2 (3%)	71,71,81	1.15	6 (8%)
32	CLA	P	304	-	49,53,73	2.13	9 (18%)	59,89,113	1.68	10 (16%)
32	CLA	a	813	20	49,53,73	2.13	9 (18%)	59,89,113	1.76	8 (13%)
34	DD6	Q	315	-	39,45,45	0.18	0	52,67,67	0.74	2 (3%)
32	CLA	a	839	20	59,63,73	1.88	9 (15%)	71,101,113	1.55	8 (11%)
32	CLA	b	822	21	69,73,73	1.69	9 (13%)	83,113,113	1.41	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	M	311	13	49,53,73	2.13	9 (18%)	59,89,113	1.74	8 (13%)
32	CLA	S	305	17	67,71,73	1.78	9 (13%)	80,110,113	1.38	6 (7%)
32	CLA	T	302	15	49,53,73	2.15	9 (18%)	59,89,113	1.66	8 (13%)
35	LHG	I	314	-	45,45,48	0.64	0	48,51,54	1.18	2 (4%)
37	A86	S	319	-	44,50,50	0.37	0	51,76,76	0.94	2 (3%)
32	CLA	b	825	21	64,68,73	1.78	10 (15%)	77,107,113	1.44	6 (7%)
34	DD6	N	318	-	39,45,45	0.18	0	52,67,67	0.88	2 (3%)
37	A86	S	315	-	44,50,50	0.55	1 (2%)	51,76,76	1.37	3 (5%)
33	KC2	S	312	17,36	49,53,53	1.74	4 (8%)	62,89,89	1.34	7 (11%)
32	CLA	b	830	21	65,69,73	1.82	9 (13%)	78,108,113	1.64	11 (14%)
37	A86	N	320	-	44,50,50	0.62	1 (2%)	51,76,76	0.55	1 (1%)
37	A86	W	302	-	44,50,50	0.45	1 (2%)	51,76,76	0.68	1 (1%)
33	KC2	P	303	13	49,53,53	1.90	4 (8%)	62,89,89	1.31	6 (9%)
35	LHG	f	205	-	46,46,48	0.59	0	49,52,54	1.10	2 (4%)
32	CLA	R	306	15	49,53,73	2.09	9 (18%)	59,89,113	1.70	7 (11%)
32	CLA	O	309	-	66,70,73	1.79	9 (13%)	79,109,113	1.45	8 (10%)
32	CLA	b	823	-	69,73,73	1.71	9 (13%)	83,113,113	1.40	8 (9%)
34	DD6	F	315	-	39,45,45	0.19	0	52,67,67	1.01	3 (5%)
32	CLA	E	311	5	49,53,73	2.11	9 (18%)	59,89,113	1.71	8 (13%)
32	CLA	C	301	3	49,53,73	2.10	9 (18%)	59,89,113	1.59	8 (13%)
32	CLA	N	312	-	45,49,73	2.23	10 (22%)	54,84,113	1.69	7 (12%)
32	CLA	S	313	17	49,53,73	2.11	9 (18%)	59,89,113	1.67	7 (11%)
34	DD6	j	103	-	39,45,45	0.18	0	52,67,67	0.83	1 (1%)
33	KC2	T	303	-	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
32	CLA	D	304	4	64,68,73	1.83	9 (14%)	77,107,113	1.45	7 (9%)
36	LMG	F	319	33	40,40,55	1.01	2 (5%)	48,48,63	1.08	2 (4%)
34	DD6	D	301	-	39,45,45	0.20	0	52,67,67	0.78	2 (3%)
32	CLA	D	310	4	69,73,73	1.76	9 (13%)	83,113,113	1.52	11 (13%)
32	CLA	O	306	15	49,53,73	2.09	9 (18%)	59,89,113	1.63	8 (13%)
32	CLA	b	834	21	64,68,73	1.82	9 (14%)	77,107,113	1.47	7 (9%)
32	CLA	B	304	-	50,54,73	2.15	9 (18%)	60,90,113	1.71	9 (15%)
32	CLA	N	310	14	59,63,73	1.92	9 (15%)	71,101,113	1.59	6 (8%)
32	CLA	N	305	-	54,58,73	2.03	9 (16%)	65,95,113	1.62	8 (12%)
32	CLA	I	302	9	59,63,73	1.87	9 (15%)	71,101,113	1.50	8 (11%)
32	CLA	B	302	2	49,53,73	2.04	9 (18%)	59,89,113	1.61	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	M	310	13	66,70,73	1.74	9 (13%)	79,109,113	1.38	6 (7%)
32	CLA	E	304	-	64,68,73	1.87	9 (14%)	77,107,113	1.51	7 (9%)
32	CLA	J	304	10	59,63,73	1.94	10 (16%)	71,101,113	1.63	11 (15%)
32	CLA	I	304	9	49,53,73	2.10	9 (18%)	59,89,113	1.66	8 (13%)
36	LMG	F	320	-	33,33,55	1.11	3 (9%)	41,41,63	1.27	4 (9%)
32	CLA	L	304	-	49,53,73	2.05	9 (18%)	59,89,113	1.60	9 (15%)
33	KC2	O	310	15	49,53,53	1.88	4 (8%)	62,89,89	1.34	9 (14%)
38	LMU	I	315	-	36,36,36	0.35	0	47,47,47	1.18	5 (10%)
38	LMU	V	205	-	35,35,36	0.48	0	46,46,47	1.16	3 (6%)
37	A86	F	313	-	44,50,50	0.44	1 (2%)	51,76,76	0.93	3 (5%)
32	CLA	J	305	10	56,60,73	1.96	9 (16%)	67,97,113	1.51	8 (11%)
34	DD6	K	313	-	39,45,45	0.19	0	52,67,67	0.64	2 (3%)
32	CLA	a	805	20	69,73,73	1.82	12 (17%)	83,113,113	1.53	11 (13%)
37	A86	K	314	-	44,50,50	0.58	1 (2%)	51,76,76	1.15	4 (7%)
32	CLA	G	305	7	49,53,73	2.05	9 (18%)	59,89,113	1.57	8 (13%)
32	CLA	B	305	-	49,53,73	2.16	9 (18%)	59,89,113	1.75	8 (13%)
32	CLA	S	308	17	48,52,73	2.18	10 (20%)	58,87,113	1.96	10 (17%)
37	A86	M	301	-	44,50,50	0.47	1 (2%)	51,76,76	0.64	2 (3%)
32	CLA	E	310	5	49,53,73	2.07	9 (18%)	59,89,113	1.57	6 (10%)
41	BCR	l	206	-	41,41,41	0.23	0	56,56,56	0.92	3 (5%)
32	CLA	C	308	3	49,53,73	2.12	9 (18%)	59,89,113	1.78	11 (18%)
33	KC2	K	305	11	49,53,53	1.87	4 (8%)	62,89,89	1.38	7 (11%)
37	A86	T	315	-	44,50,50	0.54	1 (2%)	51,76,76	0.52	1 (1%)
32	CLA	a	821	20	59,63,73	1.88	9 (15%)	71,101,113	1.47	6 (8%)
33	KC2	J	303	10	49,53,53	1.87	4 (8%)	62,89,89	1.34	7 (11%)
32	CLA	a	804	20	62,66,73	1.82	9 (14%)	74,104,113	1.49	8 (10%)
32	CLA	b	809	21	49,53,73	2.07	9 (18%)	59,89,113	1.61	6 (10%)
34	DD6	J	317	-	39,45,45	0.18	0	52,67,67	0.97	3 (5%)
33	KC2	I	316	12	49,53,53	1.88	4 (8%)	62,89,89	1.34	9 (14%)
34	DD6	A	312	-	39,45,45	0.21	0	52,67,67	0.94	4 (7%)
32	CLA	L	310	-	43,48,73	2.26	9 (20%)	52,82,113	1.94	8 (15%)
33	KC2	N	314	14	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
32	CLA	H	302	-	45,49,73	2.33	10 (22%)	54,84,113	1.85	8 (14%)
32	CLA	b	807	21	64,68,73	1.87	9 (14%)	77,107,113	1.60	8 (10%)
37	A86	C	312	-	44,50,50	0.41	1 (2%)	51,76,76	1.25	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	KC2	N	306	14	49,53,53	1.86	4 (8%)	62,89,89	1.34	9 (14%)
33	KC2	S	306	17	49,53,53	1.86	4 (8%)	62,89,89	1.32	8 (12%)
32	CLA	O	301	15	49,53,73	2.16	9 (18%)	59,89,113	1.69	8 (13%)
33	KC2	M	303	13	49,53,53	1.89	4 (8%)	62,89,89	1.29	5 (8%)
36	LMG	E	322	-	40,40,55	1.08	2 (5%)	48,48,63	1.34	3 (6%)
32	CLA	a	801	-	69,73,73	1.69	9 (13%)	83,113,113	1.38	10 (12%)
32	CLA	S	310	17	49,53,73	2.08	9 (18%)	59,89,113	1.63	7 (11%)
37	A86	L	315	-	44,50,50	0.51	1 (2%)	51,76,76	1.03	3 (5%)
32	CLA	P	307	13	49,53,73	2.10	9 (18%)	59,89,113	1.67	7 (11%)
41	BCR	U	310	-	41,41,41	0.15	0	56,56,56	0.39	0
32	CLA	a	842	-	59,63,73	1.89	9 (15%)	71,101,113	1.46	6 (8%)
32	CLA	k	201	28	59,63,73	1.88	9 (15%)	71,101,113	1.49	7 (9%)
32	CLA	a	816	20	49,53,73	2.06	9 (18%)	59,89,113	1.64	6 (10%)
34	DD6	D	319	-	39,45,45	0.18	0	52,67,67	0.87	3 (5%)
32	CLA	A	311	-	49,53,73	2.09	9 (18%)	59,89,113	1.69	6 (10%)
32	CLA	F	303	6	66,70,73	1.78	9 (13%)	79,109,113	1.39	8 (10%)
32	CLA	J	311	-	49,53,73	2.08	9 (18%)	59,89,113	1.72	7 (11%)
32	CLA	L	301	-	49,53,73	2.12	9 (18%)	59,89,113	1.63	7 (11%)
32	CLA	b	801	-	64,68,73	1.83	9 (14%)	77,107,113	1.57	8 (10%)
37	A86	F	312	-	44,50,50	0.57	1 (2%)	51,76,76	1.34	3 (5%)
34	DD6	W	317	-	39,45,45	0.20	0	52,67,67	0.67	2 (3%)
32	CLA	J	309	-	49,53,73	2.08	9 (18%)	59,89,113	1.62	7 (11%)
32	CLA	b	839	21	69,73,73	1.72	9 (13%)	83,113,113	1.32	6 (7%)
41	BCR	a	846	-	41,41,41	0.15	0	56,56,56	0.38	0
32	CLA	T	307	15	54,58,73	2.00	9 (16%)	65,95,113	1.55	7 (10%)
32	CLA	S	307	-	56,60,73	1.98	9 (16%)	67,97,113	1.86	12 (17%)
32	CLA	S	301	-	49,53,73	2.16	9 (18%)	59,89,113	1.77	9 (15%)
37	A86	T	312	-	44,50,50	0.81	1 (2%)	51,76,76	1.12	3 (5%)
32	CLA	a	827	-	69,73,73	1.73	9 (13%)	83,113,113	1.45	9 (10%)
34	DD6	U	309	-	39,45,45	0.19	0	52,67,67	0.97	4 (7%)
38	LMU	j	105	-	35,35,36	0.27	0	46,46,47	1.09	3 (6%)
32	CLA	a	826	20	69,73,73	1.71	9 (13%)	83,113,113	1.34	6 (7%)
41	BCR	m	101	-	41,41,41	0.14	0	56,56,56	0.43	0
32	CLA	b	840	-	65,69,73	1.79	9 (13%)	78,108,113	1.37	6 (7%)
32	CLA	K	306	-	64,68,73	1.80	9 (14%)	77,107,113	1.54	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	KC2	W	301	15	49,53,53	1.87	4 (8%)	62,89,89	1.36	9 (14%)
34	DD6	k	205	-	39,45,45	0.18	0	52,67,67	0.84	4 (7%)
33	KC2	M	302	13	49,53,53	1.87	4 (8%)	62,89,89	1.33	8 (12%)
32	CLA	a	811	20	59,63,73	1.90	9 (15%)	71,101,113	1.52	8 (11%)
32	CLA	b	829	21	59,63,73	1.89	9 (15%)	71,101,113	1.53	7 (9%)
32	CLA	a	824	-	65,69,73	1.76	9 (13%)	78,108,113	1.44	7 (8%)
37	A86	S	317	-	44,50,50	0.49	1 (2%)	51,76,76	1.42	2 (3%)
41	BCR	r	205	-	41,41,41	0.16	0	56,56,56	0.36	0
32	CLA	F	305	-	53,57,73	2.04	9 (16%)	64,94,113	1.69	8 (12%)
32	CLA	a	829	-	64,68,73	1.85	9 (14%)	77,107,113	1.48	7 (9%)
36	LMG	E	320	-	31,31,55	1.12	2 (6%)	39,39,63	1.54	7 (17%)
33	KC2	W	303	13	49,53,53	1.87	4 (8%)	62,89,89	1.34	9 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	H	308	8	-	3/10/86/115	-
32	CLA	P	311	-	-	13/33/109/115	-
37	A86	G	311	-	-	4/34/90/90	1/3/3/3
37	A86	P	313	-	-	7/34/90/90	1/3/3/3
32	CLA	Q	310	-	-	4/17/93/115	-
37	A86	W	318	-	-	6/34/90/90	0/3/3/3
39	SQD	H	315	-	-	23/38/58/69	0/1/1/1
32	CLA	Q	309	-	-	3/15/91/115	-
32	CLA	b	820	-	-	7/38/114/115	-
37	A86	T	313	-	-	9/34/90/90	0/3/3/3
36	LMG	P	318	-	-	20/40/60/70	0/1/1/1
37	A86	P	316	-	-	7/34/90/90	0/3/3/3
33	KC2	O	302	-	-	8/15/71/71	-
32	CLA	L	314	-	-	7/15/91/115	-
41	BCR	a	843	-	-	4/29/63/63	0/2/2/2
32	CLA	A	304	-	-	10/39/115/115	-
33	KC2	W	314	13,36	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	C	309	-	-	3/13/89/115	-
34	DD6	H	313	-	-	2/26/80/80	0/3/3/3
32	CLA	S	304	-	-	2/12/88/115	-
34	DD6	I	312	-	-	0/26/80/80	0/3/3/3
36	LMG	D	302	-	-	9/25/45/70	0/1/1/1
34	DD6	E	319	-	-	0/26/80/80	0/3/3/3
34	DD6	J	314	-	-	2/26/80/80	0/3/3/3
32	CLA	P	305	13	-	12/33/109/115	-
32	CLA	M	306	13	-	3/36/112/115	-
32	CLA	R	308	15	-	3/33/109/115	-
33	KC2	S	302	17	-	4/15/71/71	-
32	CLA	J	301	10	-	3/15/91/115	-
37	A86	Q	311	-	-	8/34/90/90	0/3/3/3
33	KC2	E	313	-	-	8/15/71/71	-
34	DD6	Q	312	-	-	1/26/80/80	0/3/3/3
42	SF4	c	101	22	-	-	0/6/5/5
32	CLA	b	805	-	-	6/39/115/115	-
32	CLA	M	312	-	-	10/33/109/115	-
32	CLA	N	309	14	-	4/21/97/115	-
32	CLA	k	203	-	-	9/27/103/115	-
37	A86	Q	316	-	-	6/34/90/90	0/3/3/3
33	KC2	R	303	-	-	5/15/71/71	-
32	CLA	b	813	-	-	4/15/91/115	-
32	CLA	W	306	-	-	6/27/103/115	-
34	DD6	H	311	-	-	0/26/80/80	0/3/3/3
34	DD6	C	310	-	-	0/26/80/80	0/3/3/3
33	KC2	L	313	-	-	8/15/71/71	-
34	DD6	O	313	-	1/1/12/24	0/26/80/80	0/3/3/3
34	DD6	V	202	-	-	4/26/80/80	0/3/3/3
32	CLA	J	307	10	-	6/27/103/115	-
32	CLA	b	808	21	-	9/39/115/115	-
32	CLA	F	309	-	-	5/27/103/115	-
32	CLA	H	307	-	-	12/33/109/115	-
32	CLA	E	314	-	-	2/21/97/115	-
32	CLA	r	202	-	-	1/15/91/115	-
35	LHG	I	318	32	-	16/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	L	307	-	-	2/30/106/115	-
33	KC2	M	307	-	-	3/15/71/71	-
33	KC2	K	309	11	-	8/15/71/71	-
32	CLA	D	311	4	-	6/39/115/115	-
32	CLA	B	309	-	-	5/27/103/115	-
33	KC2	P	301	-	-	9/15/71/71	-
32	CLA	a	810	-	-	14/36/112/115	-
43	PQN	b	847	-	-	1/23/43/43	0/2/2/2
41	BCR	k	204	-	-	4/29/63/63	0/2/2/2
36	LMG	l	201	33	-	23/44/64/70	0/1/1/1
32	CLA	G	306	7	-	11/29/105/115	-
32	CLA	b	835	-	-	7/33/109/115	-
32	CLA	D	309	4	-	2/15/91/115	-
32	CLA	H	309	-	-	7/15/91/115	-
37	A86	D	322	-	-	4/34/90/90	0/3/3/3
32	CLA	a	836	20	-	9/27/103/115	-
32	CLA	E	312	-	-	8/33/109/115	-
32	CLA	U	305	18	-	7/15/91/115	-
34	DD6	E	317	-	-	0/26/80/80	0/3/3/3
32	CLA	L	309	-	-	5/15/91/115	-
36	LMG	W	320	33,37	-	13/34/54/70	0/1/1/1
32	CLA	U	302	18	-	4/15/91/115	-
32	CLA	C	305	-	-	8/33/109/115	-
33	KC2	W	305	13	-	4/15/71/71	-
32	CLA	a	833	-	-	4/39/115/115	-
32	CLA	R	309	15	-	3/10/86/115	-
32	CLA	R	307	15	-	2/15/91/115	-
34	DD6	G	312	-	-	1/26/80/80	0/3/3/3
41	BCR	l	205	-	-	4/29/63/63	0/2/2/2
33	KC2	I	309	9,36	-	8/15/71/71	-
32	CLA	F	311	-	-	0/15/91/115	-
34	DD6	D	317	-	-	0/26/80/80	0/3/3/3
35	LHG	F	321	-	-	16/44/44/53	-
34	DD6	M	316	-	-	1/26/80/80	0/3/3/3
34	DD6	R	314	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	a	851	-	-	8/42/42/53	-
32	CLA	M	305	-	-	3/21/97/115	-
32	CLA	Q	305	16	-	5/23/99/115	-
33	KC2	T	311	15	-	5/15/71/71	-
32	CLA	Q	303	16	-	6/33/109/115	-
34	DD6	I	313	-	-	0/26/80/80	0/3/3/3
32	CLA	a	815	20	-	1/21/97/115	-
32	CLA	T	310	-	-	4/27/103/115	-
32	CLA	b	837	21	-	13/39/115/115	-
32	CLA	J	312	-	-	12/31/107/115	-
32	CLA	K	301	-	-	4/15/91/115	-
36	LMG	A	318	-	-	9/35/55/70	0/1/1/1
32	CLA	H	306	8	-	3/21/97/115	-
33	KC2	N	302	14	-	5/15/71/71	-
37	A86	W	316	36	-	5/34/90/90	0/3/3/3
32	CLA	L	311	-	-	2/10/82/115	-
32	CLA	a	841	20	-	11/39/115/115	-
32	CLA	S	309	-	-	15/33/109/115	-
35	LHG	E	321	-	-	18/50/50/53	-
34	DD6	Q	314	-	-	1/26/80/80	0/3/3/3
32	CLA	a	832	-	-	5/33/109/115	-
34	DD6	K	315	-	1/1/12/24	1/26/80/80	0/3/3/3
32	CLA	S	311	-	-	5/21/97/115	-
32	CLA	T	308	15	-	7/33/109/115	-
35	LHG	F	318	-	-	15/45/45/53	-
33	KC2	A	310	1	-	5/15/71/71	-
36	LMG	D	321	-	-	16/35/55/70	0/1/1/1
33	KC2	J	310	10	-	8/15/71/71	-
34	DD6	H	312	-	-	2/26/80/80	0/3/3/3
32	CLA	Q	301	33	-	6/33/109/115	-
32	CLA	b	818	-	-	9/39/115/115	-
32	CLA	l	203	35	-	16/39/115/115	-
32	CLA	O	305	15	-	8/39/115/115	-
35	LHG	a	850	32	-	13/34/34/53	-
32	CLA	M	308	13	-	9/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	I	305	9	-	6/29/105/115	-
32	CLA	R	304	-	-	5/15/91/115	-
32	CLA	B	301	-	-	3/10/82/115	-
32	CLA	G	301	-	-	6/15/91/115	-
32	CLA	a	817	20	-	9/35/111/115	-
32	CLA	b	828	21	-	7/35/111/115	-
35	LHG	D	320	-	-	23/52/52/53	-
32	CLA	B	303	-	-	3/15/91/115	-
37	A86	K	312	-	-	7/34/90/90	0/3/3/3
41	BCR	a	844	-	-	2/29/63/63	0/2/2/2
32	CLA	H	310	-	-	3/17/93/115	-
34	DD6	N	321	-	-	2/26/80/80	0/3/3/3
33	KC2	L	302	12	-	4/15/71/71	-
32	CLA	a	820	-	-	10/39/115/115	-
37	A86	M	315	-	-	4/34/90/90	0/3/3/3
32	CLA	D	306	4	-	9/33/109/115	-
33	KC2	R	311	15	-	4/15/71/71	-
32	CLA	b	821	21	-	3/27/103/115	-
32	CLA	K	304	11	-	5/15/91/115	-
37	A86	N	315	-	-	2/34/90/90	0/3/3/3
32	CLA	a	852	-	-	11/39/115/115	-
32	CLA	R	310	-	-	6/27/103/115	-
33	KC2	T	304	15	-	3/15/71/71	-
37	A86	M	314	-	-	4/34/90/90	1/3/3/3
32	CLA	a	822	-	-	10/36/112/115	-
37	A86	N	317	-	-	8/34/90/90	0/3/3/3
34	DD6	P	315	-	-	0/26/80/80	0/3/3/3
32	CLA	I	303	9	-	6/27/103/115	-
37	A86	R	313	-	-	4/34/90/90	0/3/3/3
32	CLA	l	202	-	-	5/15/91/115	-
32	CLA	F	322	-	-	10/33/109/115	-
32	CLA	b	806	-	-	10/39/115/115	-
37	A86	N	316	-	-	14/34/90/90	0/3/3/3
32	CLA	H	301	8	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	E	301	-	-	18/50/50/53	-
32	CLA	a	823	-	-	5/39/115/115	-
34	DD6	Q	313	-	-	0/26/80/80	0/3/3/3
37	A86	r	204	-	-	8/34/90/90	0/3/3/3
35	LHG	a	849	-	-	22/52/52/53	-
36	LMG	L	320	-	-	13/32/52/70	0/1/1/1
32	CLA	f	201	-	-	4/33/109/115	-
38	LMU	D	324	-	-	11/21/61/61	0/2/2/2
32	CLA	U	307	-	-	5/15/91/115	-
32	CLA	W	313	-	-	5/33/109/115	-
34	DD6	E	318	-	-	1/26/80/80	0/3/3/3
36	LMG	S	322	33	-	13/28/48/70	0/1/1/1
35	LHG	B	308	-	-	18/35/35/53	-
32	CLA	R	301	-	-	4/15/91/115	-
33	KC2	N	307	14	-	4/15/71/71	-
32	CLA	J	308	-	-	6/15/91/115	-
37	A86	H	314	-	-	5/34/90/90	0/3/3/3
33	KC2	K	303	11	-	8/15/71/71	-
32	CLA	U	306	-	-	8/15/91/115	-
36	LMG	A	317	-	-	15/31/51/70	0/1/1/1
32	CLA	l	204	29	-	15/39/115/115	-
32	CLA	b	832	-	-	9/39/115/115	-
33	KC2	R	302	15	-	5/15/71/71	-
32	CLA	E	308	5	-	11/39/115/115	-
33	KC2	M	313	13,36	-	7/15/71/71	-
37	A86	S	314	-	-	6/34/90/90	0/3/3/3
32	CLA	Q	308	-	-	5/15/91/115	-
32	CLA	b	810	21	-	5/33/109/115	-
32	CLA	a	812	20	-	7/27/103/115	-
32	CLA	b	802	-	-	3/39/115/115	-
32	CLA	K	308	11	-	12/39/115/115	-
32	CLA	a	819	20	-	14/39/115/115	-
32	CLA	C	306	3	-	14/39/115/115	-
37	A86	L	316	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	A	302	35	-	4/33/109/115	-
35	LHG	M	319	-	-	18/50/50/53	-
34	DD6	A	315	-	-	3/26/80/80	0/3/3/3
32	CLA	K	307	11	-	4/10/86/115	-
32	CLA	a	814	20	-	10/39/115/115	-
32	CLA	D	315	-	-	4/15/91/115	-
32	CLA	G	308	-	-	6/26/102/115	-
34	DD6	J	315	-	-	1/26/80/80	0/3/3/3
35	LHG	A	316	-	-	21/44/44/53	-
33	KC2	C	303	-	-	9/15/71/71	-
35	LHG	W	319	32	-	18/50/50/53	-
32	CLA	P	308	13	-	2/15/91/115	-
32	CLA	W	312	13	-	12/33/109/115	-
32	CLA	O	308	-	-	6/15/91/115	-
33	KC2	N	303	14	-	7/15/71/71	-
32	CLA	I	308	-	-	8/27/103/115	-
33	KC2	N	304	14	-	8/15/71/71	-
32	CLA	A	305	1	-	6/35/111/115	-
32	CLA	F	306	6	-	5/27/103/115	-
32	CLA	a	838	-	-	5/39/115/115	-
32	CLA	b	817	21	-	11/27/103/115	-
37	A86	O	312	-	1/1/14/25	4/34/90/90	0/3/3/3
32	CLA	B	306	-	-	4/15/91/115	-
32	CLA	b	804	21	-	19/39/115/115	-
33	KC2	P	306	-	-	5/15/71/71	-
37	A86	J	313	-	-	8/34/90/90	0/3/3/3
32	CLA	D	312	4	-	6/27/103/115	-
32	CLA	a	840	-	-	7/39/115/115	-
32	CLA	b	814	-	-	6/15/91/115	-
32	CLA	E	306	5	-	7/33/109/115	-
32	CLA	T	305	-	-	12/15/91/115	-
41	BCR	f	202	-	-	2/29/63/63	0/2/2/2
32	CLA	C	302	-	-	0/10/86/115	-
32	CLA	k	202	-	-	10/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	M	320	33	-	9/35/55/70	0/1/1/1
33	KC2	H	303	-	-	8/15/71/71	-
32	CLA	I	317	35	-	3/39/115/115	-
32	CLA	K	310	-	-	6/15/91/115	-
32	CLA	G	307	-	-	2/10/82/115	-
42	SF4	c	102	-	-	-	0/6/5/5
36	LMG	E	302	-	-	19/35/55/70	0/1/1/1
32	CLA	N	311	14	-	7/33/109/115	-
33	KC2	L	303	-	-	4/15/71/71	-
32	CLA	I	306	9	-	7/39/115/115	-
32	CLA	D	314	4	-	7/24/100/115	-
32	CLA	a	825	20	-	2/39/115/115	-
37	A86	M	317	-	-	7/34/90/90	1/3/3/3
32	CLA	C	304	3	-	4/13/89/115	-
33	KC2	S	303	17	-	6/15/71/71	-
41	BCR	a	845	-	-	4/29/63/63	0/2/2/2
43	PQN	a	848	-	-	8/23/43/43	0/2/2/2
32	CLA	D	305	-	-	9/31/107/115	-
32	CLA	A	308	-	-	3/27/103/115	-
32	CLA	W	310	13	-	12/33/109/115	-
32	CLA	f	203	25	-	2/15/91/115	-
37	A86	U	308	-	-	2/34/90/90	1/3/3/3
32	CLA	E	315	-	-	5/17/93/115	-
37	A86	P	319	-	-	4/34/90/90	0/3/3/3
32	CLA	I	307	-	-	6/15/91/115	-
32	CLA	V	201	-	-	6/31/107/115	-
41	BCR	b	844	-	-	4/29/63/63	0/2/2/2
33	KC2	P	312	13	-	7/15/71/71	-
32	CLA	P	309	-	-	7/35/111/115	-
32	CLA	b	836	-	-	9/39/115/115	-
37	A86	K	311	-	-	8/34/90/90	0/3/3/3
41	BCR	r	203	-	-	5/29/63/63	0/2/2/2
42	SF4	a	847	-	-	-	0/6/5/5
32	CLA	Q	307	16	-	8/36/112/115	-
34	DD6	I	310	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	S	321	-	1/1/12/24	5/26/80/80	0/3/3/3
32	CLA	T	309	-	-	4/15/91/115	-
32	CLA	F	304	-	-	3/27/103/115	-
32	CLA	b	833	-	-	10/36/112/115	-
32	CLA	a	809	-	-	8/33/109/115	-
32	CLA	U	301	18	-	3/10/82/115	-
32	CLA	r	201	-	-	8/33/109/115	-
37	A86	D	323	-	-	10/34/90/90	0/3/3/3
32	CLA	a	828	-	-	7/31/107/115	-
32	CLA	a	802	-	-	10/37/113/115	-
34	DD6	D	316	-	-	1/26/80/80	0/3/3/3
37	A86	O	311	-	-	4/34/90/90	0/3/3/3
32	CLA	F	301	-	-	2/10/82/115	-
33	KC2	K	302	11	-	6/15/71/71	-
35	LHG	P	317	-	-	20/50/50/53	-
32	CLA	U	303	18	-	3/15/91/115	-
32	CLA	G	304	-	-	4/27/103/115	-
37	A86	S	318	-	-	4/34/90/90	0/3/3/3
37	A86	W	315	-	-	7/34/90/90	0/3/3/3
33	KC2	Q	317	32	-	8/15/71/71	-
41	BCR	b	841	-	-	0/29/63/63	0/2/2/2
32	CLA	O	307	15	-	7/33/109/115	-
32	CLA	b	812	21	-	11/39/115/115	-
34	DD6	N	319	-	-	1/26/80/80	0/3/3/3
32	CLA	D	313	-	-	11/31/107/115	-
38	LMU	J	318	-	-	4/21/61/61	0/2/2/2
36	LMG	D	303	-	-	16/31/51/70	0/1/1/1
41	BCR	i	101	-	-	3/29/63/63	0/2/2/2
37	A86	C	311	-	-	8/34/90/90	0/3/3/3
32	CLA	A	307	1	-	5/33/109/115	-
34	DD6	J	316	-	-	0/26/80/80	0/3/3/3
36	LMG	j	104	-	-	21/33/53/70	0/1/1/1
36	LMG	T	301	-	-	14/32/52/70	0/1/1/1
41	BCR	a	854	-	-	5/29/63/63	0/2/2/2
32	CLA	a	818	20	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	L	312	-	-	8/33/109/115	-
33	KC2	L	305	12	-	11/15/71/71	-
32	CLA	a	803	20	-	8/37/113/115	-
33	KC2	W	304	13	-	5/15/71/71	-
36	LMG	N	301	-	-	19/35/55/70	0/1/1/1
32	CLA	H	305	8	-	5/15/91/115	-
34	DD6	A	314	-	-	1/26/80/80	0/3/3/3
32	CLA	a	830	20	-	11/39/115/115	-
32	CLA	Q	306	16	-	14/36/112/115	-
32	CLA	I	301	-	-	12/39/115/115	-
37	A86	P	314	-	-	4/34/90/90	0/3/3/3
32	CLA	f	204	-	-	1/18/94/115	-
34	DD6	A	313	-	-	3/26/80/80	0/3/3/3
32	CLA	E	305	5	-	1/27/103/115	-
33	KC2	M	321	15	-	5/15/71/71	-
37	A86	M	318	-	-	4/34/90/90	0/3/3/3
33	KC2	G	309	7	-	9/15/71/71	-
33	KC2	L	306	12	-	6/15/71/71	-
41	BCR	j	102	-	-	5/29/63/63	0/2/2/2
32	CLA	b	838	-	-	10/39/115/115	-
37	A86	S	320	-	-	6/34/90/90	0/3/3/3
32	CLA	M	309	13	-	7/15/91/115	-
32	CLA	H	304	-	-	7/15/91/115	-
32	CLA	b	819	-	-	4/39/115/115	-
34	DD6	T	314	-	-	1/26/80/80	0/3/3/3
32	CLA	a	835	20	-	11/39/115/115	-
36	LMG	D	325	-	-	9/30/50/70	0/1/1/1
41	BCR	b	842	-	-	6/29/63/63	0/2/2/2
32	CLA	a	831	20	-	4/33/109/115	-
33	KC2	M	304	13	-	6/15/71/71	-
32	CLA	j	101	27	-	4/15/91/115	-
33	KC2	U	304	18	-	6/15/71/71	-
33	KC2	F	302	6	-	8/15/71/71	-
32	CLA	b	816	-	-	8/36/112/115	-
32	CLA	V	203	19	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	C	307	3	-	9/33/109/115	-
40	DGD	b	846	-	-	21/45/85/95	0/2/2/2
32	CLA	A	309	1	-	12/39/115/115	-
32	CLA	A	306	1	-	9/39/115/115	-
32	CLA	E	303	5	-	4/15/91/115	-
32	CLA	J	306	10	-	7/27/103/115	-
37	A86	F	317	-	-	7/34/90/90	0/3/3/3
33	KC2	G	302	-	-	9/15/71/71	-
32	CLA	D	308	4	-	4/27/103/115	-
33	KC2	Q	302	-	-	7/15/71/71	-
32	CLA	F	308	6	-	3/17/93/115	-
34	DD6	B	307	-	-	2/26/80/80	0/3/3/3
32	CLA	W	307	13	-	7/15/91/115	-
33	KC2	F	310	6,36	-	8/15/71/71	-
34	DD6	F	316	-	-	3/26/80/80	0/3/3/3
32	CLA	F	307	6	-	5/33/109/115	-
32	CLA	G	303	7	-	10/27/103/115	-
37	A86	L	318	-	-	4/34/90/90	0/3/3/3
32	CLA	Q	304	-	-	3/21/97/115	-
32	CLA	N	313	-	-	9/33/109/115	-
32	CLA	T	306	15	-	5/33/109/115	-
37	A86	L	317	-	-	10/34/90/90	0/3/3/3
34	DD6	D	318	-	-	2/26/80/80	0/3/3/3
32	CLA	a	806	-	-	7/33/109/115	-
32	CLA	b	803	21	-	9/39/115/115	-
32	CLA	W	309	13	-	6/39/115/115	-
32	CLA	J	302	-	-	2/15/91/115	-
32	CLA	b	827	21	-	4/21/97/115	-
37	A86	R	312	-	-	3/34/90/90	0/3/3/3
32	CLA	b	815	21	-	7/39/115/115	-
39	SQD	k	206	-	-	13/31/51/69	0/1/1/1
37	A86	S	316	-	-	2/34/90/90	0/3/3/3
33	KC2	N	308	14	-	5/15/71/71	-
32	CLA	E	307	5	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	L	319	-	-	2/26/80/80	0/3/3/3
32	CLA	L	308	12	-	4/15/91/115	-
32	CLA	b	824	21	-	8/31/107/115	-
33	KC2	W	308	-	-	6/15/71/71	-
32	CLA	D	307	4	-	6/35/111/115	-
32	CLA	O	304	-	-	2/15/91/115	-
32	CLA	b	811	21	-	6/21/97/115	-
34	DD6	F	314	-	-	1/26/80/80	0/3/3/3
33	KC2	R	305	15	-	5/15/71/71	-
32	CLA	a	834	20	-	7/39/115/115	-
32	CLA	b	831	-	-	14/33/109/115	-
41	BCR	b	845	-	-	2/29/63/63	0/2/2/2
32	CLA	a	807	-	-	9/39/115/115	-
33	KC2	P	302	13	-	9/15/71/71	-
32	CLA	a	808	20	-	3/21/97/115	-
32	CLA	P	310	-	-	3/10/86/115	-
32	CLA	W	311	13	-	13/39/115/115	-
34	DD6	I	311	-	-	1/26/80/80	0/3/3/3
37	A86	G	310	-	-	10/34/90/90	0/3/3/3
32	CLA	A	301	1	-	5/15/91/115	-
32	CLA	a	853	-	-	10/39/115/115	-
32	CLA	V	204	-	-	3/21/97/115	-
33	KC2	O	303	15	-	6/15/71/71	-
41	BCR	b	843	-	-	2/29/63/63	0/2/2/2
32	CLA	E	309	5	-	10/31/107/115	-
32	CLA	A	303	1	-	11/36/112/115	-
34	DD6	E	316	-	-	0/26/80/80	0/3/3/3
32	CLA	b	826	-	-	4/20/96/115	-
37	A86	M	322	-	-	4/34/90/90	0/3/3/3
32	CLA	a	837	20	-	7/27/103/115	-
40	DGD	Q	318	-	-	27/45/85/95	0/2/2/2
32	CLA	P	304	-	-	6/15/91/115	-
32	CLA	a	813	20	-	6/15/91/115	-
34	DD6	Q	315	-	-	1/26/80/80	0/3/3/3
32	CLA	a	839	20	-	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	b	822	21	-	7/39/115/115	-
32	CLA	M	311	13	-	7/15/91/115	-
32	CLA	S	305	17	-	6/37/113/115	-
32	CLA	T	302	15	-	6/15/91/115	-
35	LHG	I	314	-	-	22/50/50/53	-
37	A86	S	319	-	-	7/34/90/90	0/3/3/3
32	CLA	b	825	21	-	8/33/109/115	-
34	DD6	N	318	-	-	2/26/80/80	0/3/3/3
37	A86	S	315	-	-	3/34/90/90	1/3/3/3
33	KC2	S	312	17,36	-	4/15/71/71	-
32	CLA	b	830	21	-	7/35/111/115	-
37	A86	N	320	-	-	0/34/90/90	0/3/3/3
37	A86	W	302	-	-	1/34/90/90	0/3/3/3
33	KC2	P	303	13	-	3/15/71/71	-
35	LHG	f	205	-	-	26/51/51/53	-
32	CLA	R	306	15	-	4/15/91/115	-
32	CLA	O	309	-	-	7/36/112/115	-
32	CLA	b	823	-	-	10/39/115/115	-
34	DD6	F	315	-	-	3/26/80/80	0/3/3/3
32	CLA	E	311	5	-	3/15/91/115	-
32	CLA	C	301	3	-	3/15/91/115	-
32	CLA	N	312	-	-	6/10/86/115	-
32	CLA	S	313	17	-	6/15/91/115	-
34	DD6	j	103	-	-	1/26/80/80	0/3/3/3
33	KC2	T	303	-	-	8/15/71/71	-
32	CLA	D	304	4	-	10/33/109/115	-
36	LMG	F	319	33	-	16/35/55/70	0/1/1/1
34	DD6	D	301	-	-	2/26/80/80	0/3/3/3
32	CLA	D	310	4	-	6/39/115/115	-
32	CLA	O	306	15	-	5/15/91/115	-
32	CLA	b	834	21	-	3/33/109/115	-
32	CLA	B	304	-	-	7/17/93/115	-
32	CLA	N	310	14	-	7/27/103/115	-
32	CLA	N	305	-	-	6/21/97/115	-
32	CLA	I	302	9	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	B	302	2	-	6/15/91/115	-
32	CLA	M	310	13	-	4/36/112/115	-
32	CLA	E	304	-	-	4/33/109/115	-
32	CLA	J	304	10	-	5/27/103/115	-
32	CLA	I	304	9	-	5/15/91/115	-
36	LMG	F	320	-	-	7/28/48/70	0/1/1/1
32	CLA	L	304	-	-	2/15/91/115	-
33	KC2	O	310	15	-	6/15/71/71	-
38	LMU	I	315	-	-	6/21/61/61	0/2/2/2
38	LMU	V	205	-	-	6/20/60/61	0/2/2/2
37	A86	F	313	-	-	5/34/90/90	0/3/3/3
32	CLA	J	305	10	-	3/24/100/115	-
34	DD6	K	313	-	-	0/26/80/80	0/3/3/3
32	CLA	a	805	20	-	15/39/115/115	-
37	A86	K	314	-	-	4/34/90/90	0/3/3/3
32	CLA	G	305	7	-	5/15/91/115	-
32	CLA	B	305	-	-	5/15/91/115	-
32	CLA	S	308	17	-	4/15/91/115	-
37	A86	M	301	-	-	6/34/90/90	0/3/3/3
32	CLA	E	310	5	-	7/15/91/115	-
41	BCR	l	206	-	-	5/29/63/63	0/2/2/2
32	CLA	C	308	3	-	4/15/91/115	-
33	KC2	K	305	11	-	4/15/71/71	-
37	A86	T	315	-	-	4/34/90/90	0/3/3/3
32	CLA	a	821	20	-	7/27/103/115	-
33	KC2	J	303	10	-	8/15/71/71	-
32	CLA	a	804	20	-	4/31/107/115	-
32	CLA	b	809	21	-	5/15/91/115	-
34	DD6	J	317	-	1/1/12/24	0/26/80/80	0/3/3/3
33	KC2	I	316	12	-	8/15/71/71	-
34	DD6	A	312	-	-	0/26/80/80	0/3/3/3
32	CLA	L	310	-	-	4/10/82/115	-
33	KC2	N	314	14	-	6/15/71/71	-
32	CLA	H	302	-	-	5/10/86/115	-
32	CLA	b	807	21	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	C	312	-	-	6/34/90/90	0/3/3/3
33	KC2	N	306	14	-	4/15/71/71	-
33	KC2	S	306	17	-	6/15/71/71	-
32	CLA	O	301	15	-	5/15/91/115	-
33	KC2	M	303	13	-	2/15/71/71	-
36	LMG	E	322	-	-	12/35/55/70	0/1/1/1
32	CLA	a	801	-	-	5/39/115/115	-
32	CLA	S	310	17	-	9/15/91/115	-
37	A86	L	315	-	-	4/34/90/90	0/3/3/3
32	CLA	P	307	13	-	0/15/91/115	-
41	BCR	U	310	-	-	4/29/63/63	0/2/2/2
32	CLA	a	842	-	-	8/27/103/115	-
32	CLA	k	201	28	-	9/27/103/115	-
32	CLA	a	816	20	-	7/15/91/115	-
34	DD6	D	319	-	-	2/26/80/80	0/3/3/3
32	CLA	A	311	-	-	7/15/91/115	-
32	CLA	F	303	6	-	10/36/112/115	-
32	CLA	J	311	-	-	2/15/91/115	-
32	CLA	L	301	-	-	7/15/91/115	-
32	CLA	b	801	-	-	6/33/109/115	-
37	A86	F	312	-	-	2/34/90/90	0/3/3/3
34	DD6	W	317	-	-	1/26/80/80	0/3/3/3
32	CLA	J	309	-	-	2/15/91/115	-
32	CLA	b	839	21	-	12/39/115/115	-
41	BCR	a	846	-	-	2/29/63/63	0/2/2/2
32	CLA	T	307	15	-	4/21/97/115	-
32	CLA	S	307	-	-	2/24/100/115	-
32	CLA	S	301	-	-	3/15/91/115	-
37	A86	T	312	-	-	4/34/90/90	0/3/3/3
32	CLA	a	827	-	-	11/39/115/115	-
34	DD6	U	309	-	-	0/26/80/80	0/3/3/3
38	LMU	j	105	-	-	12/20/60/61	0/2/2/2
32	CLA	a	826	20	-	16/39/115/115	-
41	BCR	m	101	-	-	1/29/63/63	0/2/2/2
32	CLA	b	840	-	-	9/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	K	306	-	-	10/33/109/115	-
33	KC2	W	301	15	-	5/15/71/71	-
34	DD6	k	205	-	-	1/26/80/80	0/3/3/3
33	KC2	M	302	13	-	6/15/71/71	-
32	CLA	a	811	20	-	5/27/103/115	-
32	CLA	b	829	21	-	8/27/103/115	-
32	CLA	a	824	-	-	7/35/111/115	-
37	A86	S	317	-	-	6/34/90/90	0/3/3/3
41	BCR	r	205	-	-	2/29/63/63	0/2/2/2
32	CLA	F	305	-	-	1/19/95/115	-
32	CLA	a	829	-	-	7/33/109/115	-
36	LMG	E	320	-	-	13/26/46/70	0/1/1/1
33	KC2	W	303	13	-	6/15/71/71	-

The worst 5 of 2897 bond length outliers are listed below:

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

The worst 5 of 3137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	S	307	CLA	C4A-NA-C1A	-8.62	102.83	106.71
37	S	317	A86	O1-C20-C19	8.49	119.76	113.38
32	a	818	CLA	C4A-NA-C1A	-8.34	102.95	106.71
34	S	321	DD6	O1-C20-C19	-8.32	107.14	113.38
32	S	308	CLA	C1C-NC-C4C	-8.20	103.02	106.71

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	J	317	DD6	C20
34	K	315	DD6	C20
34	O	313	DD6	C20
34	S	321	DD6	C20

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Mol	Chain	Res	Type	Atom
37	O	312	A86	C36

5 of 3346 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	304	CLA	C1A-C2A-CAA-CBA
32	A	304	CLA	C3A-C2A-CAA-CBA
32	A	305	CLA	C2B-C3B-CAB-CBB
32	A	305	CLA	C4B-C3B-CAB-CBB
32	A	309	CLA	CHA-CBD-CGD-O1D

5 of 6 ring outliers are listed below:

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

163 monomers are involved in 261 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	P	311	CLA	2	0
39	H	315	SQD	16	0
37	T	313	A86	1	0
36	P	318	LMG	7	0
37	P	316	A86	1	0
33	O	302	KC2	1	0
41	a	843	BCR	1	0
33	W	314	KC2	1	0
34	I	312	DD6	1	0
32	R	308	CLA	1	0
42	c	101	SF4	1	0
32	k	203	CLA	6	0
37	Q	316	A86	2	0
32	W	306	CLA	1	0
33	K	309	KC2	2	0
32	a	810	CLA	1	0
41	k	204	BCR	1	0
36	l	201	LMG	5	0
32	b	835	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	H	309	CLA	1	0
37	D	322	A86	1	0
32	a	836	CLA	1	0
32	U	305	CLA	2	0
32	L	309	CLA	2	0
36	W	320	LMG	11	0
32	C	305	CLA	2	0
32	a	833	CLA	1	0
33	I	309	KC2	4	0
35	F	321	LHG	1	0
34	M	316	DD6	3	0
35	a	851	LHG	7	0
32	Q	303	CLA	1	0
32	J	312	CLA	4	0
32	K	301	CLA	2	0
36	A	318	LMG	1	0
32	H	306	CLA	1	0
37	W	316	A86	1	0
32	L	311	CLA	3	0
32	a	832	CLA	2	0
35	F	318	LHG	1	0
33	A	310	KC2	2	0
32	a	817	CLA	1	0
32	b	828	CLA	1	0
32	a	820	CLA	1	0
37	M	315	A86	1	0
33	R	311	KC2	1	0
32	K	304	CLA	1	0
32	a	852	CLA	1	0
32	a	822	CLA	1	0
32	I	303	CLA	1	0
37	R	313	A86	1	0
32	H	301	CLA	1	0
32	a	823	CLA	2	0
38	D	324	LMU	2	0
36	S	322	LMG	8	0
35	B	308	LHG	2	0
37	H	314	A86	1	0
33	K	303	KC2	1	0
32	U	306	CLA	1	0
36	A	317	LMG	1	0
33	M	313	KC2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	L	316	A86	1	0
32	a	814	CLA	1	0
32	D	315	CLA	2	0
32	W	312	CLA	7	0
33	N	303	KC2	1	0
32	a	838	CLA	1	0
32	b	817	CLA	2	0
32	b	814	CLA	1	0
36	M	320	LMG	9	0
32	N	311	CLA	1	0
32	D	314	CLA	1	0
37	M	317	A86	3	0
32	W	310	CLA	5	0
33	P	312	KC2	2	0
34	S	321	DD6	2	0
32	F	304	CLA	2	0
32	b	833	CLA	4	0
32	a	828	CLA	3	0
32	a	802	CLA	1	0
34	D	316	DD6	1	0
35	P	317	LHG	1	0
41	b	841	BCR	1	0
38	J	318	LMU	3	0
32	A	307	CLA	1	0
36	j	104	LMG	1	0
36	T	301	LMG	2	0
32	a	803	CLA	1	0
36	N	301	LMG	5	0
32	H	305	CLA	2	0
32	I	301	CLA	2	0
34	A	313	DD6	2	0
37	M	318	A86	1	0
33	G	309	KC2	1	0
32	M	309	CLA	1	0
36	D	325	LMG	1	0
32	j	101	CLA	1	0
33	F	302	KC2	1	0
32	b	816	CLA	1	0
32	A	309	CLA	2	0
32	D	308	CLA	1	0
33	F	310	KC2	1	0
32	F	307	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	D	318	DD6	1	0
32	W	309	CLA	1	0
32	b	827	CLA	1	0
37	R	312	A86	1	0
39	k	206	SQD	6	0
34	L	319	DD6	1	0
32	D	307	CLA	1	0
32	O	304	CLA	4	0
32	b	811	CLA	1	0
32	a	834	CLA	1	0
32	b	831	CLA	1	0
41	b	845	BCR	3	0
32	a	807	CLA	1	0
32	W	311	CLA	1	0
34	I	311	DD6	1	0
32	A	301	CLA	3	0
41	b	843	BCR	2	0
32	A	303	CLA	1	0
32	b	826	CLA	2	0
40	Q	318	DGD	3	0
32	b	822	CLA	1	0
32	M	311	CLA	3	0
32	S	305	CLA	1	0
32	T	302	CLA	1	0
37	S	315	A86	2	0
33	S	312	KC2	5	0
32	b	830	CLA	1	0
37	W	302	A86	1	0
35	f	205	LHG	1	0
32	N	312	CLA	4	0
32	D	304	CLA	1	0
36	F	319	LMG	5	0
32	b	834	CLA	1	0
32	N	310	CLA	1	0
32	M	310	CLA	1	0
36	F	320	LMG	13	0
38	I	315	LMU	3	0
38	V	205	LMU	3	0
37	F	313	A86	1	0
32	a	805	CLA	1	0
37	M	301	A86	1	0
41	l	206	BCR	1	0

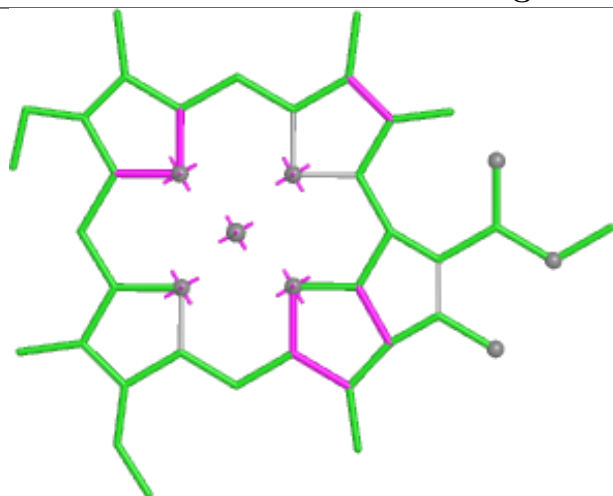
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	C	308	CLA	1	0
32	a	821	CLA	1	0
34	J	317	DD6	1	0
32	L	310	CLA	5	0
33	N	314	KC2	1	0
32	b	807	CLA	1	0
37	L	315	A86	3	0
32	P	307	CLA	1	0
41	U	310	BCR	1	0
32	k	201	CLA	1	0
37	F	312	A86	1	0
34	W	317	DD6	1	0
41	a	846	BCR	1	0
32	T	307	CLA	1	0
34	U	309	DD6	1	0
32	K	306	CLA	1	0
34	k	205	DD6	1	0
32	a	824	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

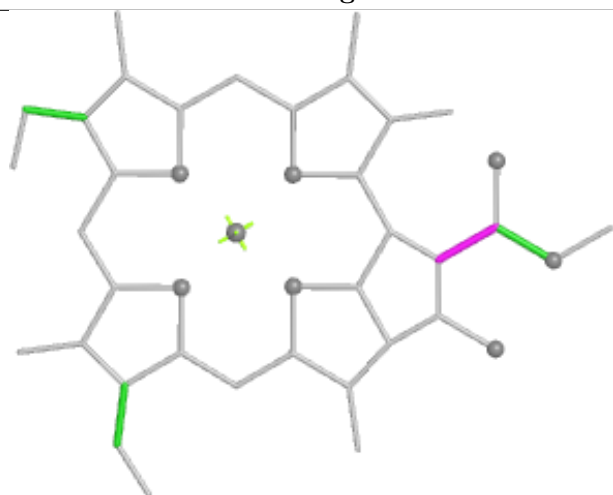
Ligand CLA H 308



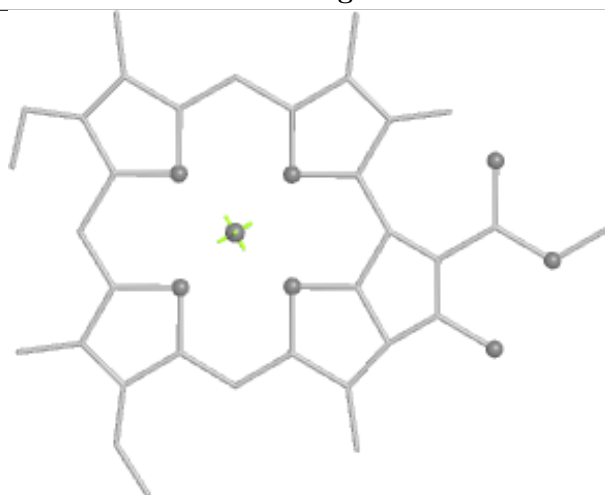
Bond lengths



Bond angles

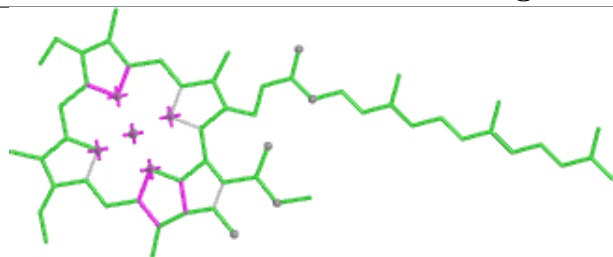


Torsions

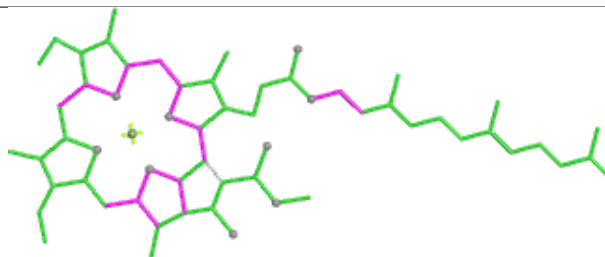


Rings

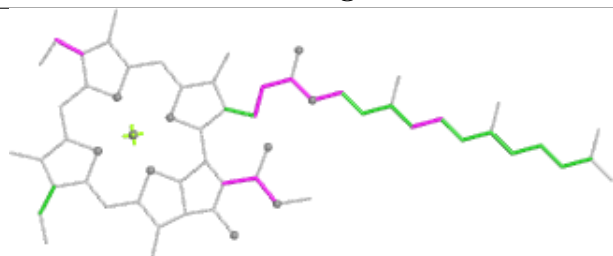
Ligand CLA P 311



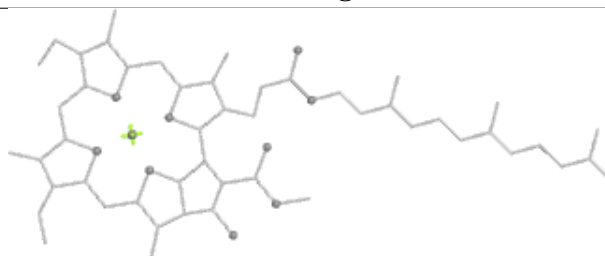
Bond lengths



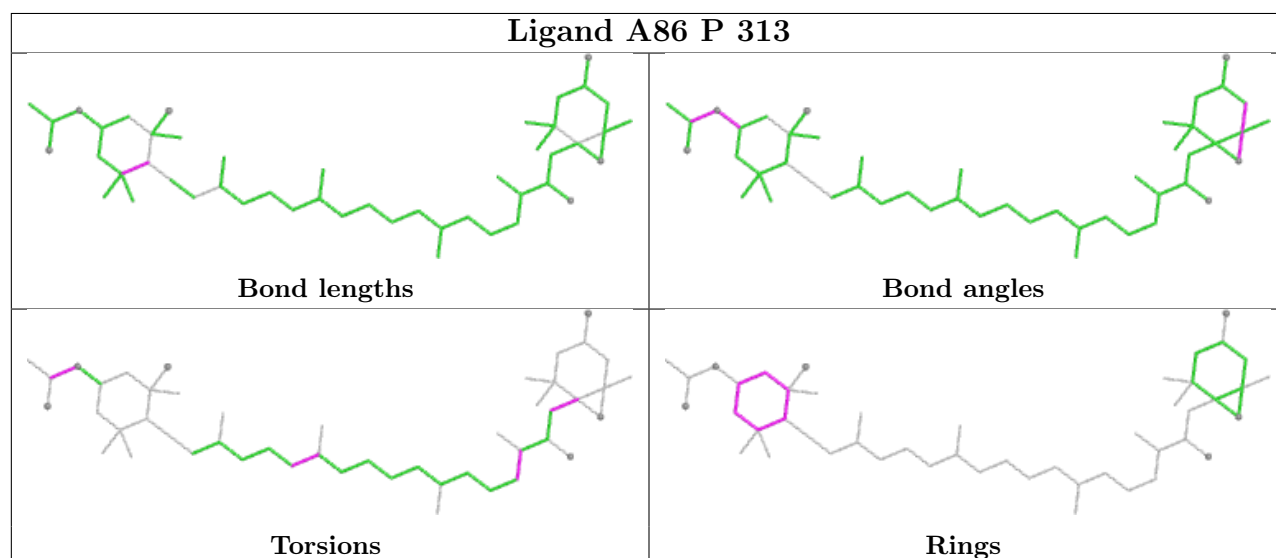
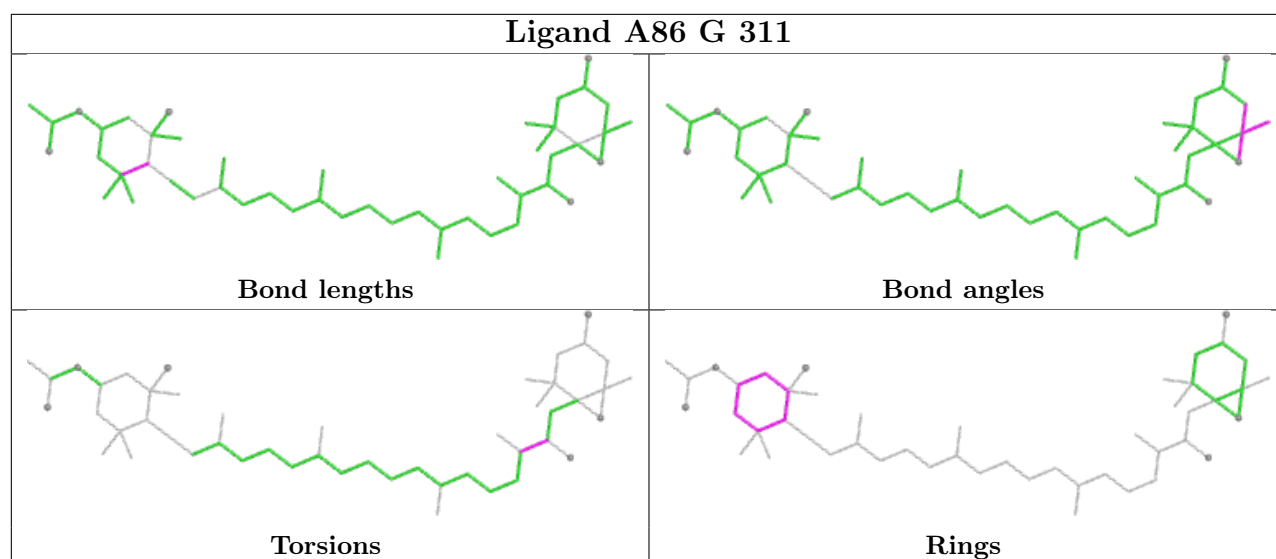
Bond angles



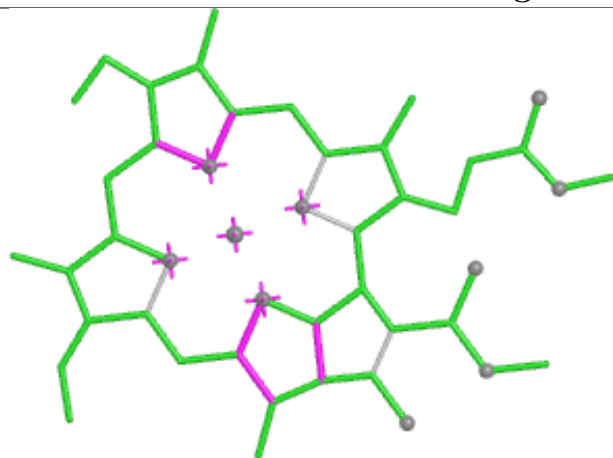
Torsions



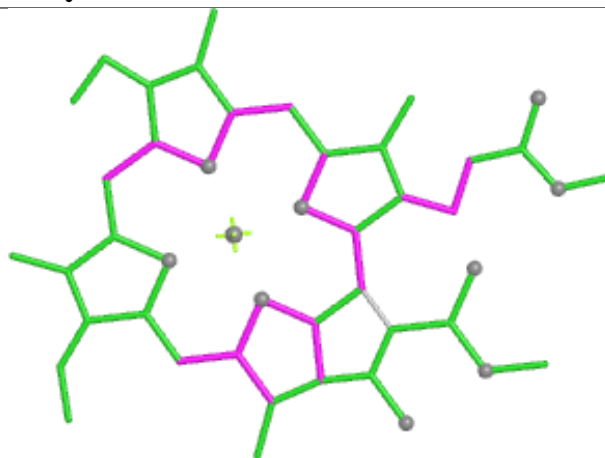
Rings



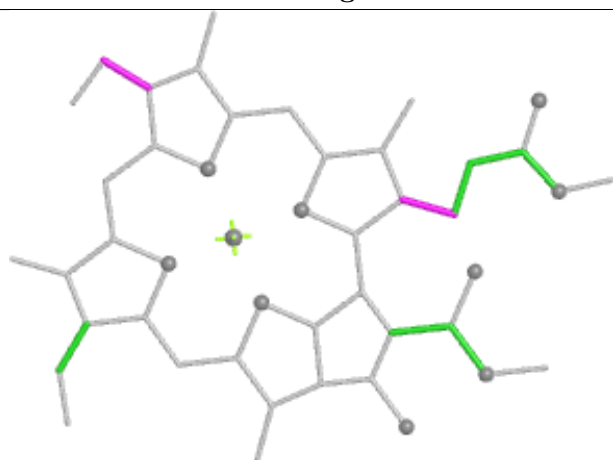
Ligand CLA Q 310



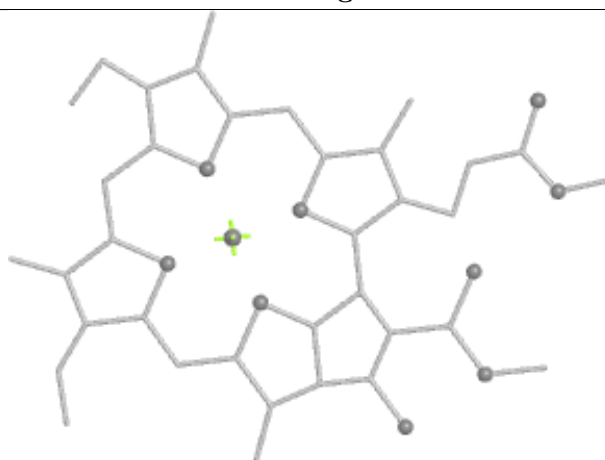
Bond lengths



Bond angles

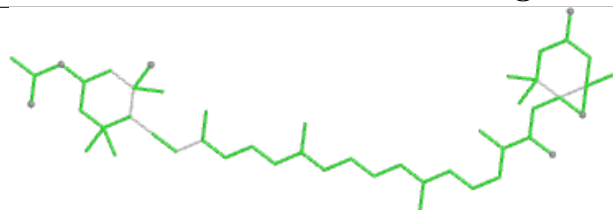


Torsions

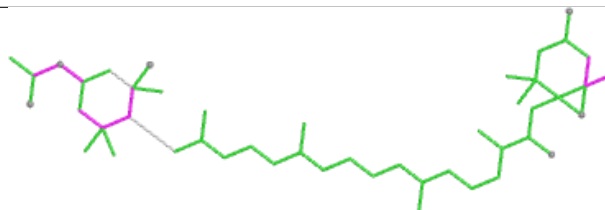


Rings

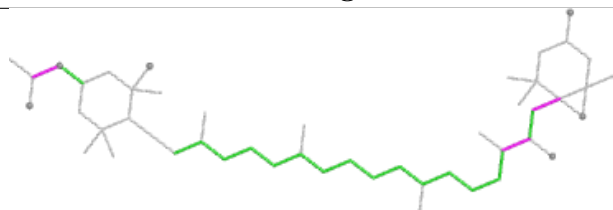
Ligand A86 W 318



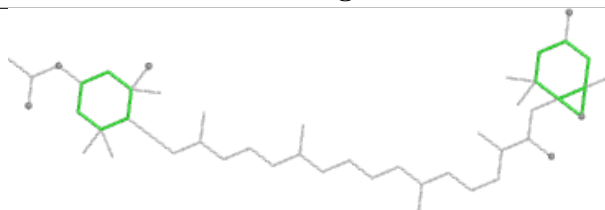
Bond lengths



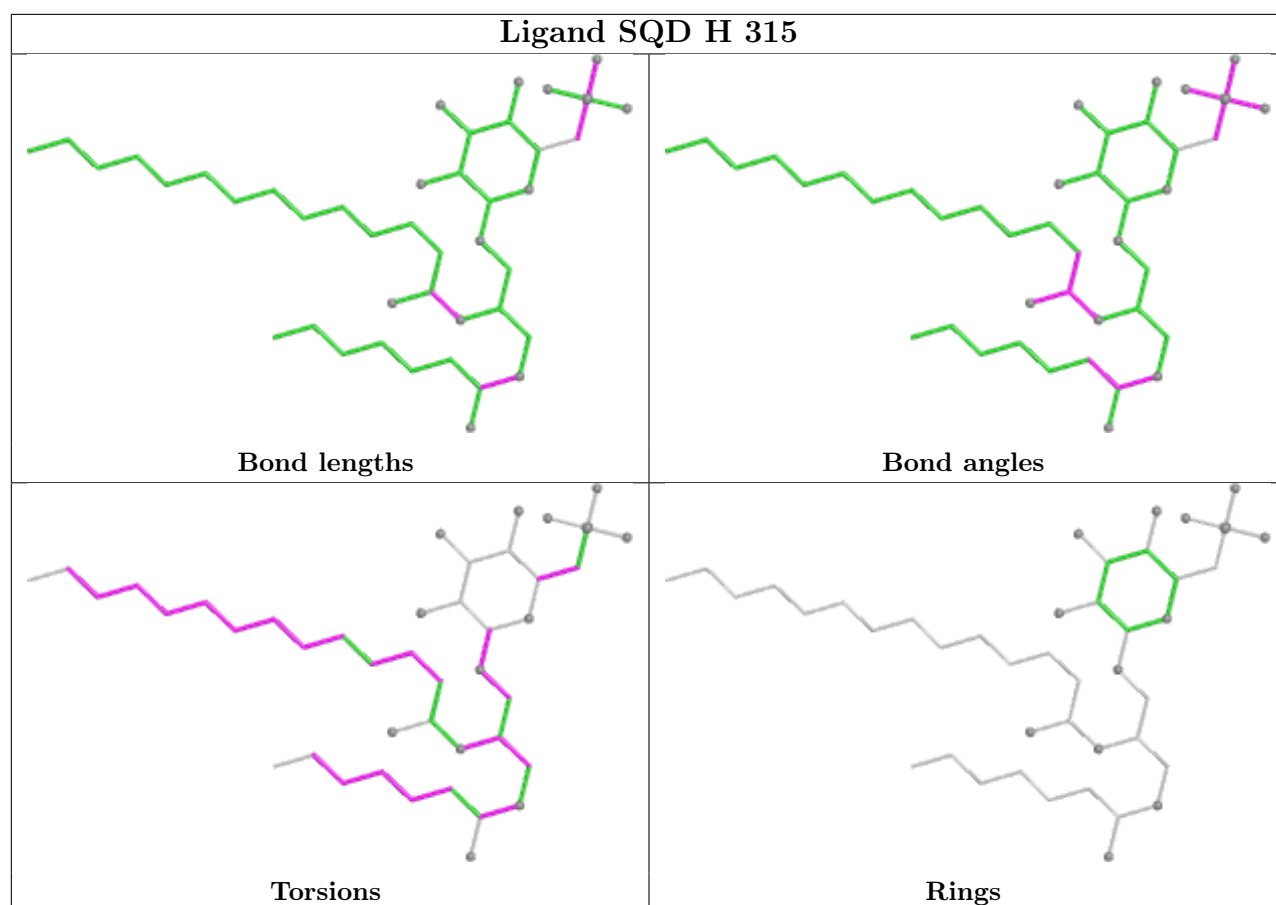
Bond angles

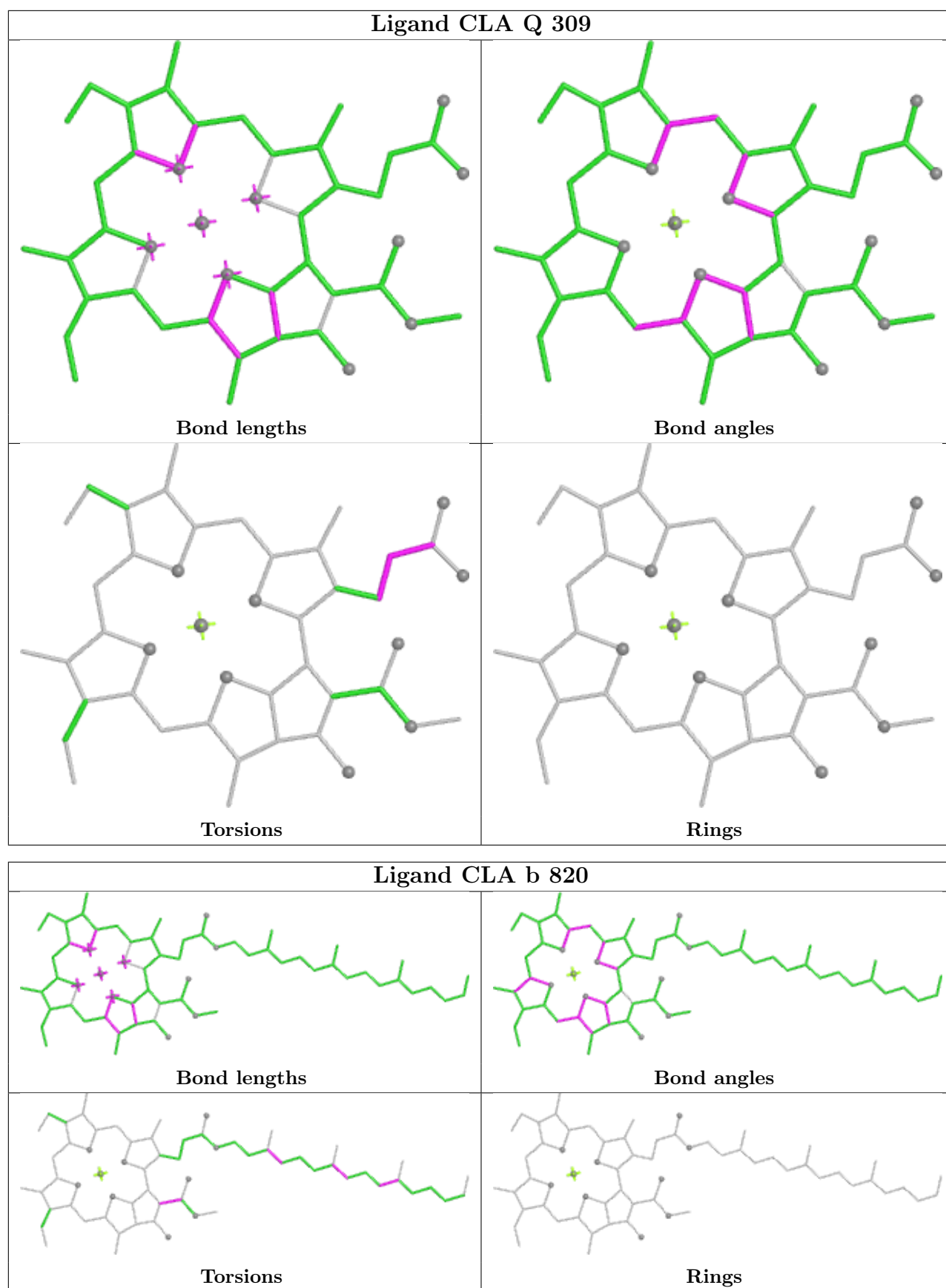


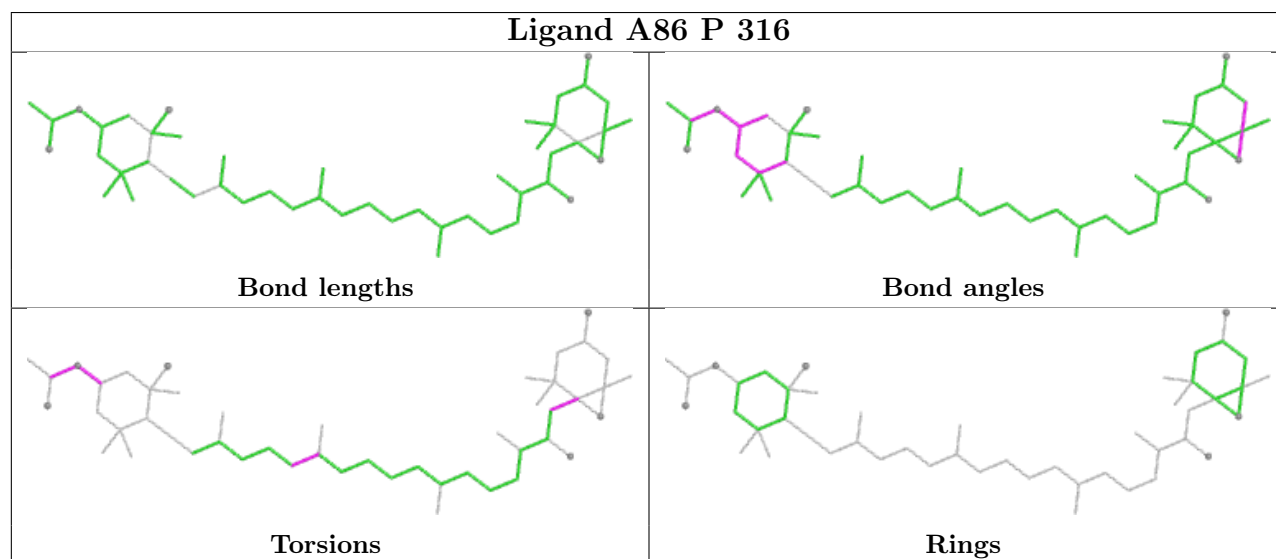
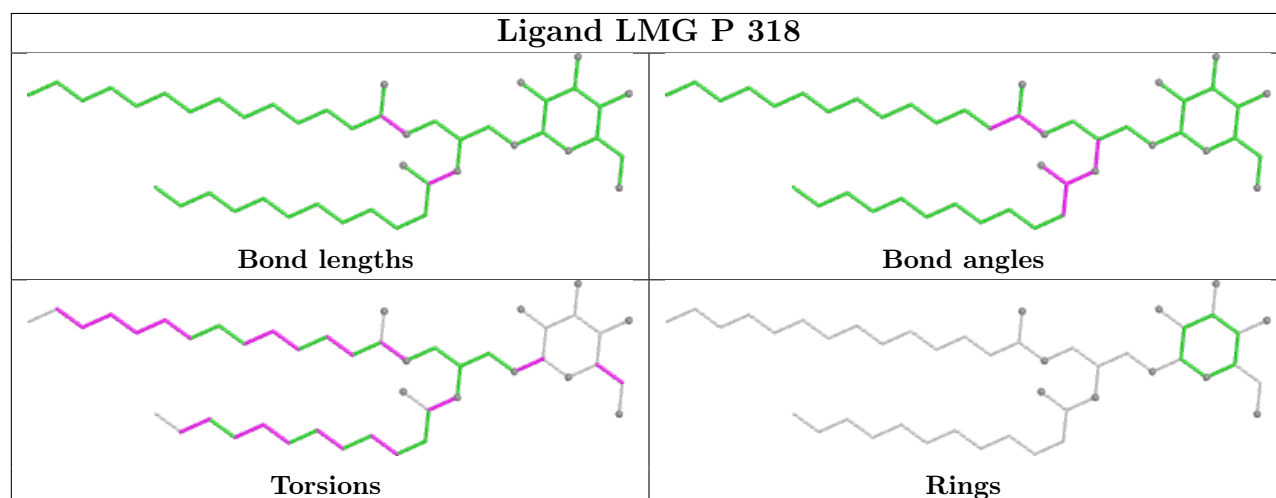
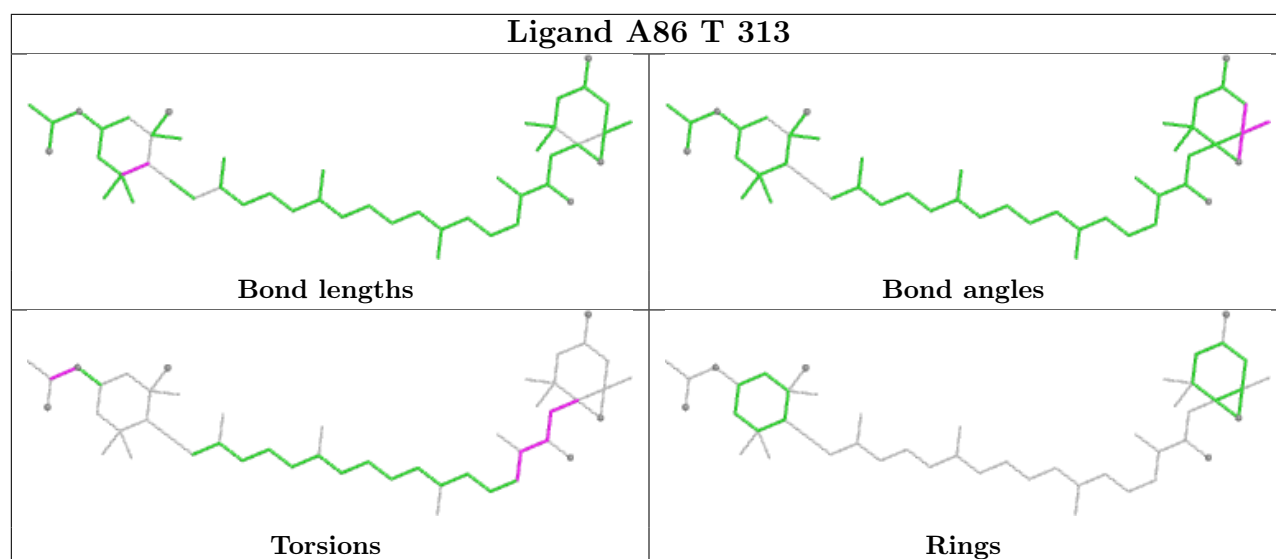
Torsions



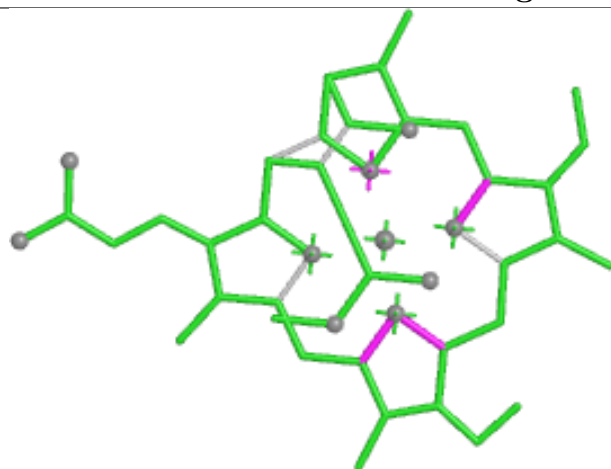
Rings



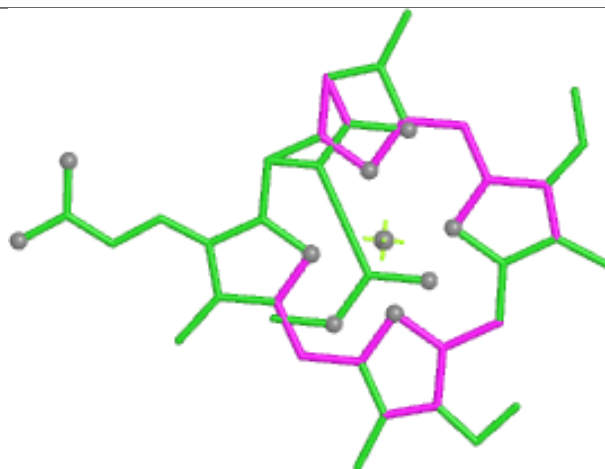




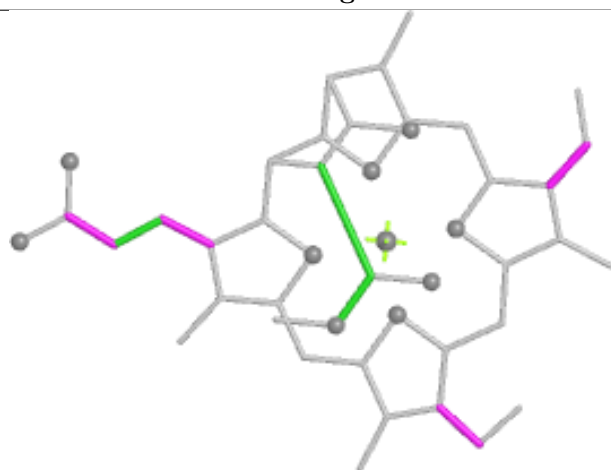
Ligand KC2 O 302



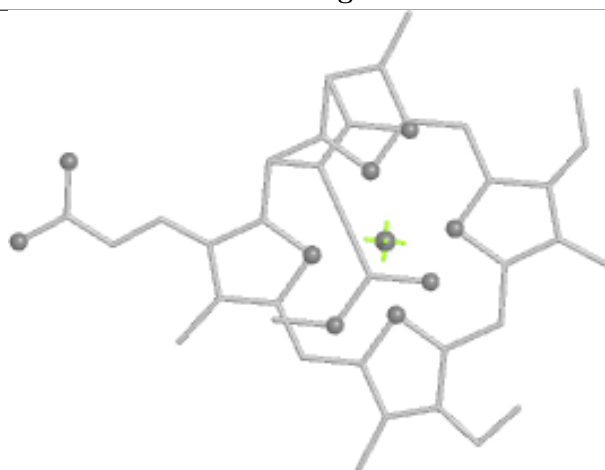
Bond lengths



Bond angles

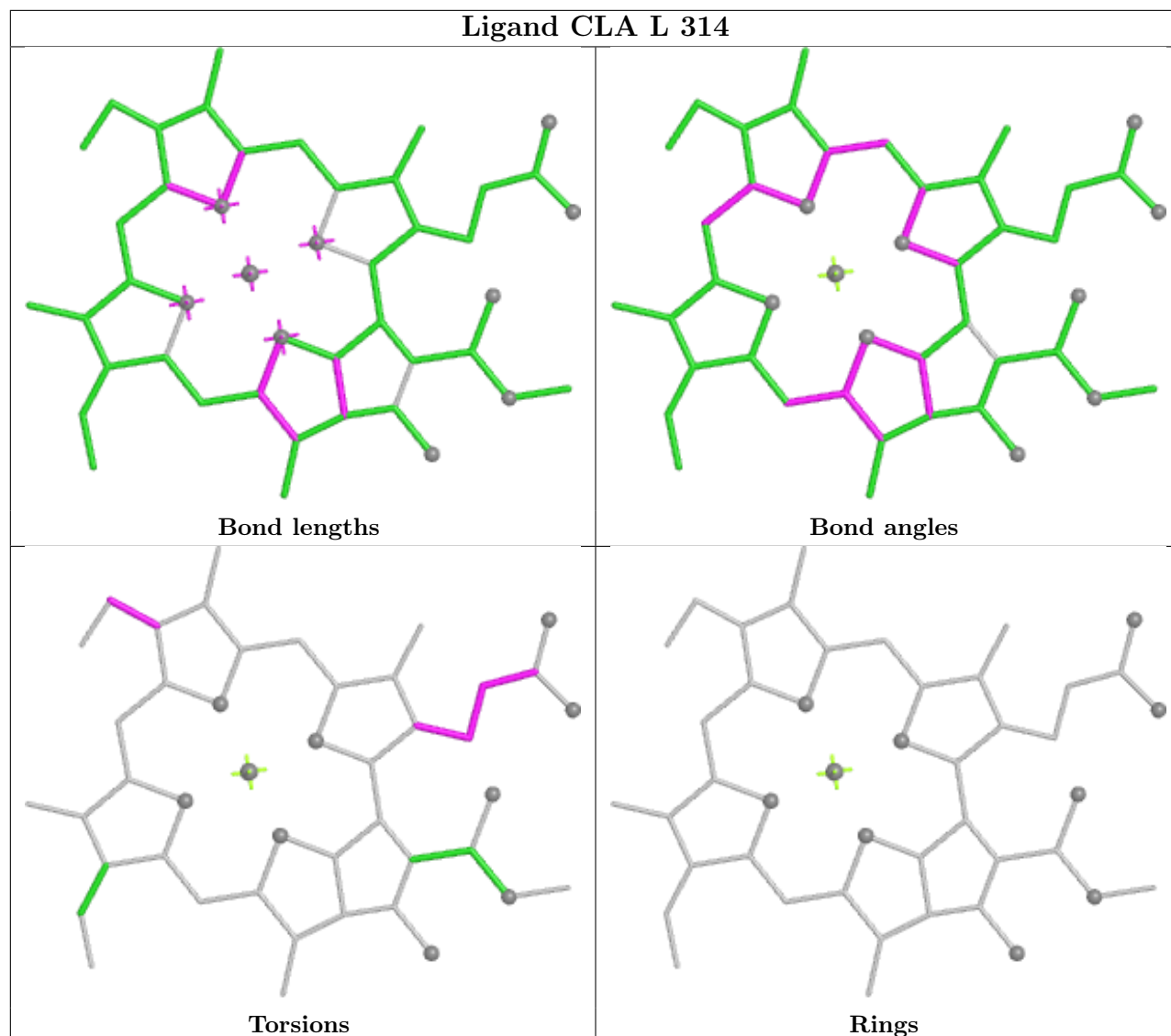


Torsions

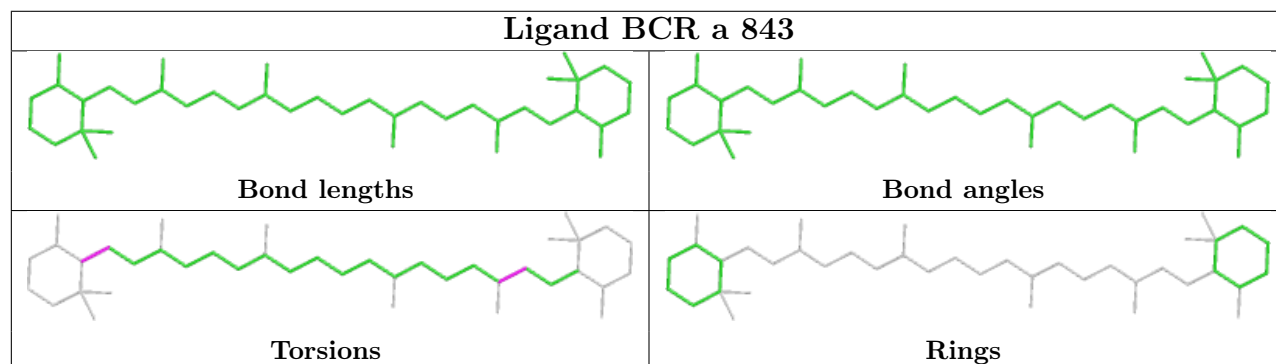


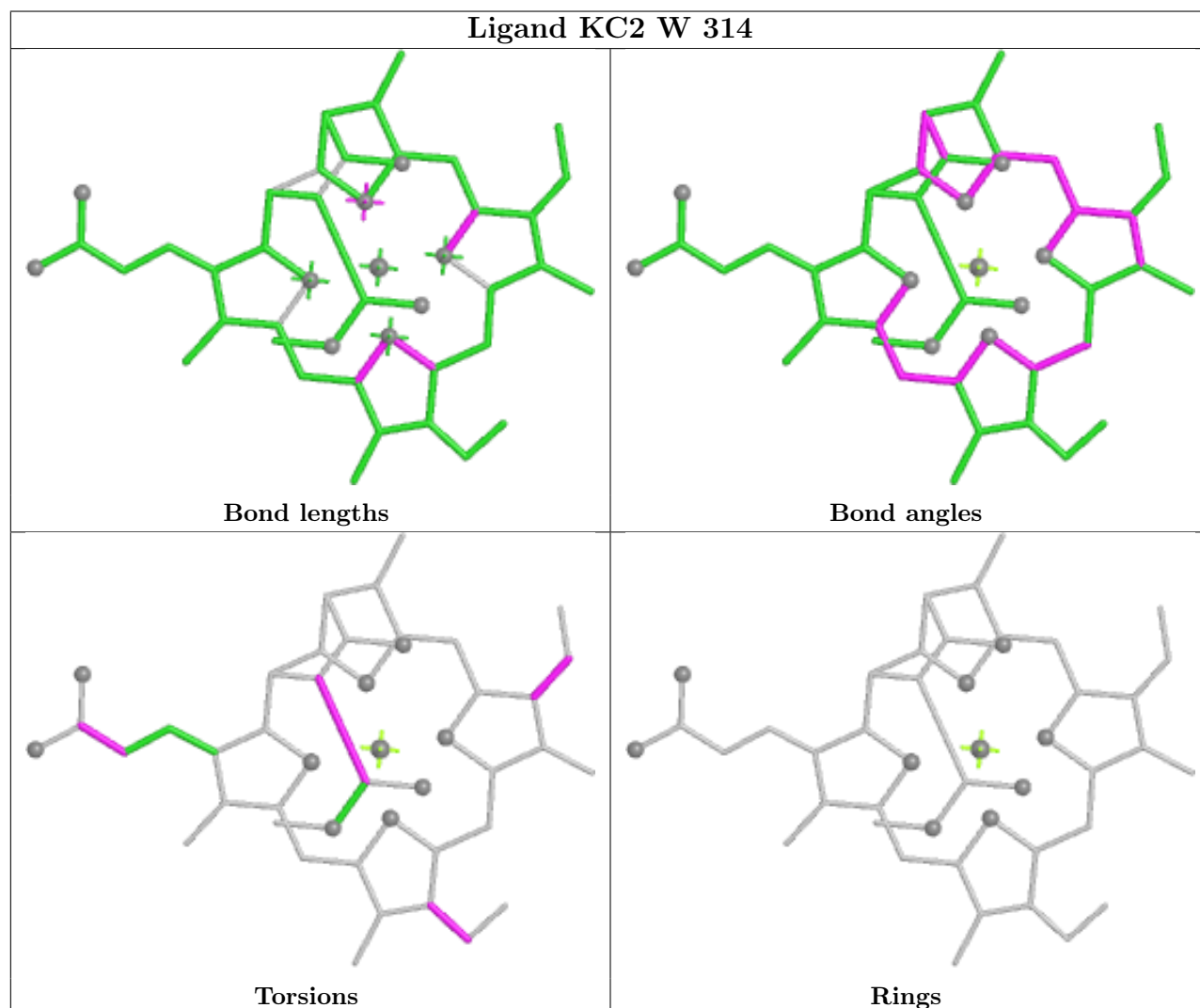
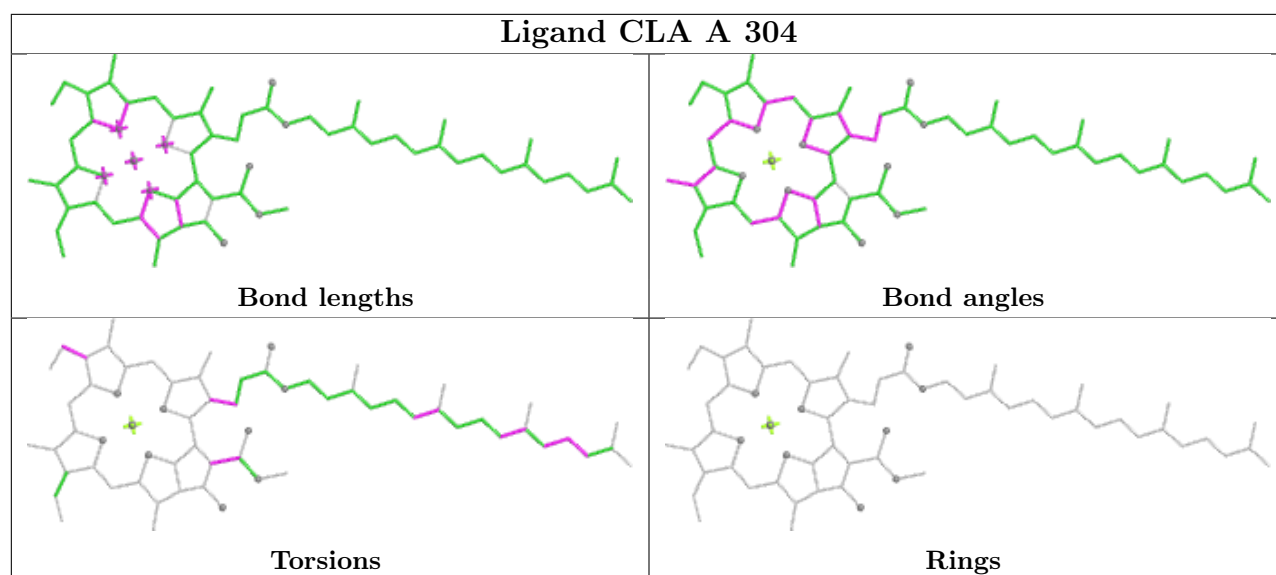
Rings

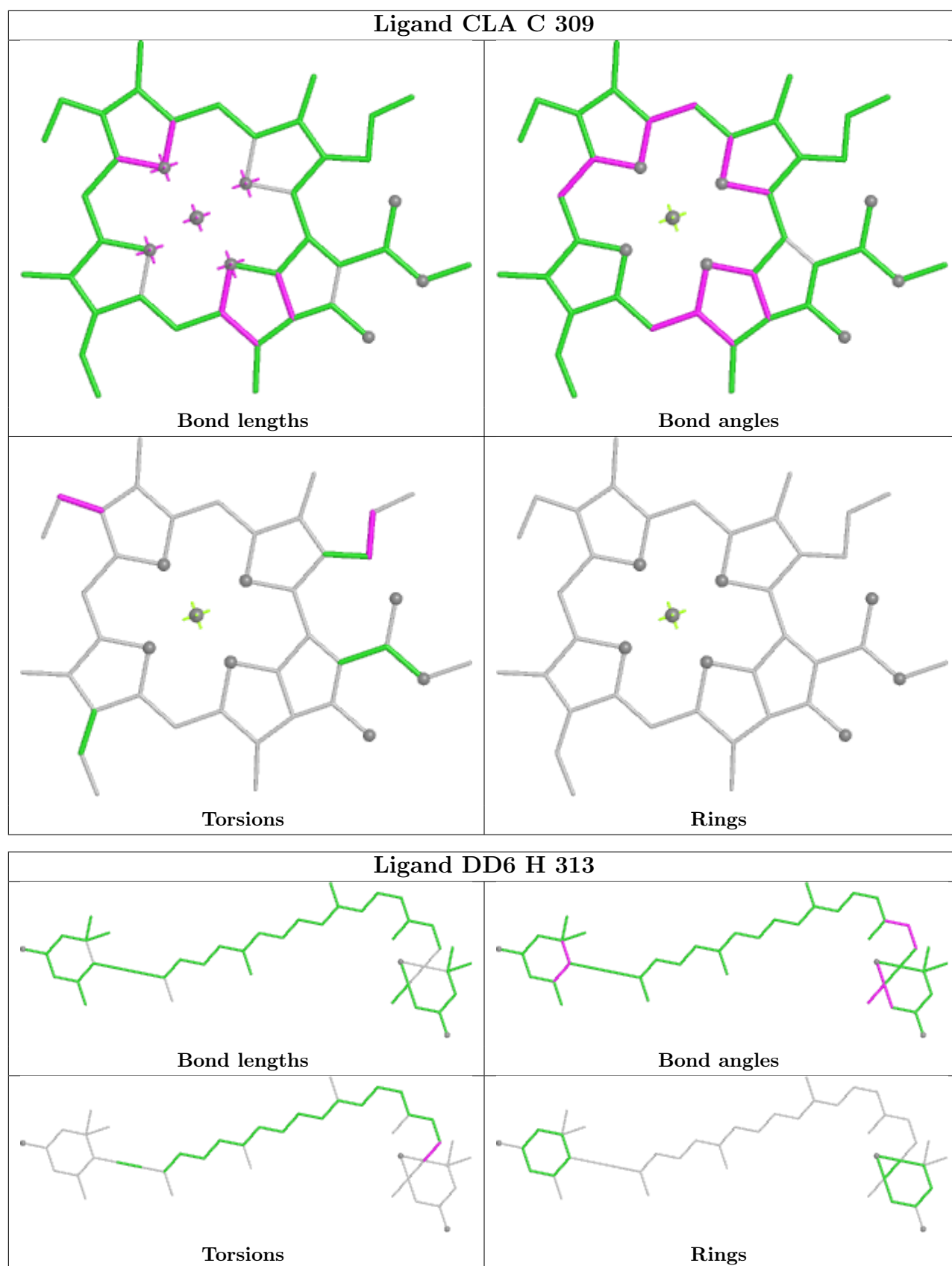
Ligand CLA L 314



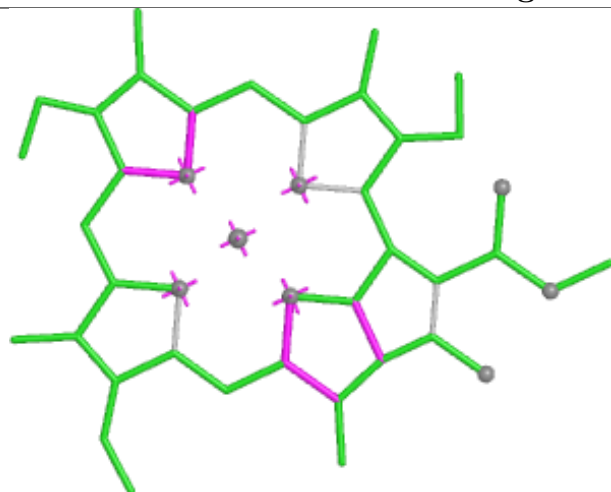
Ligand BCR a 843



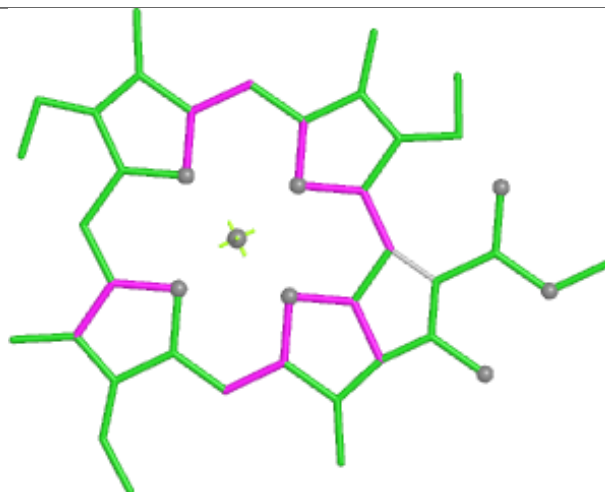




Ligand CLA S 304



Bond lengths



Bond angles

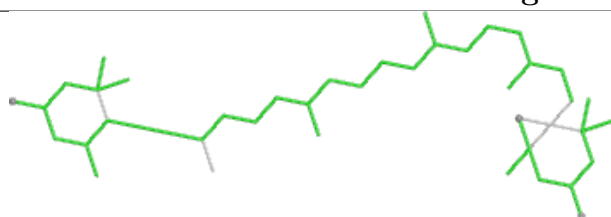


Torsions

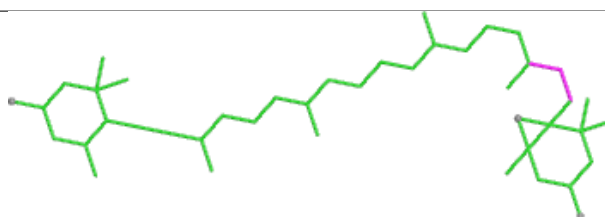


Rings

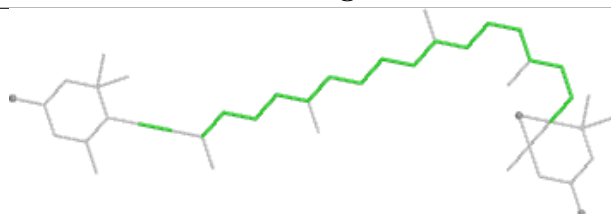
Ligand DD6 I 312



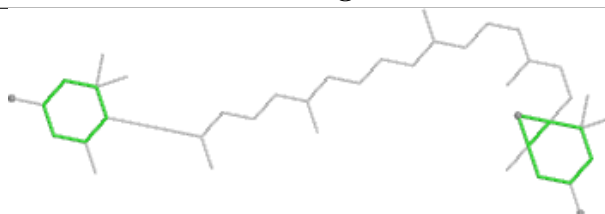
Bond lengths



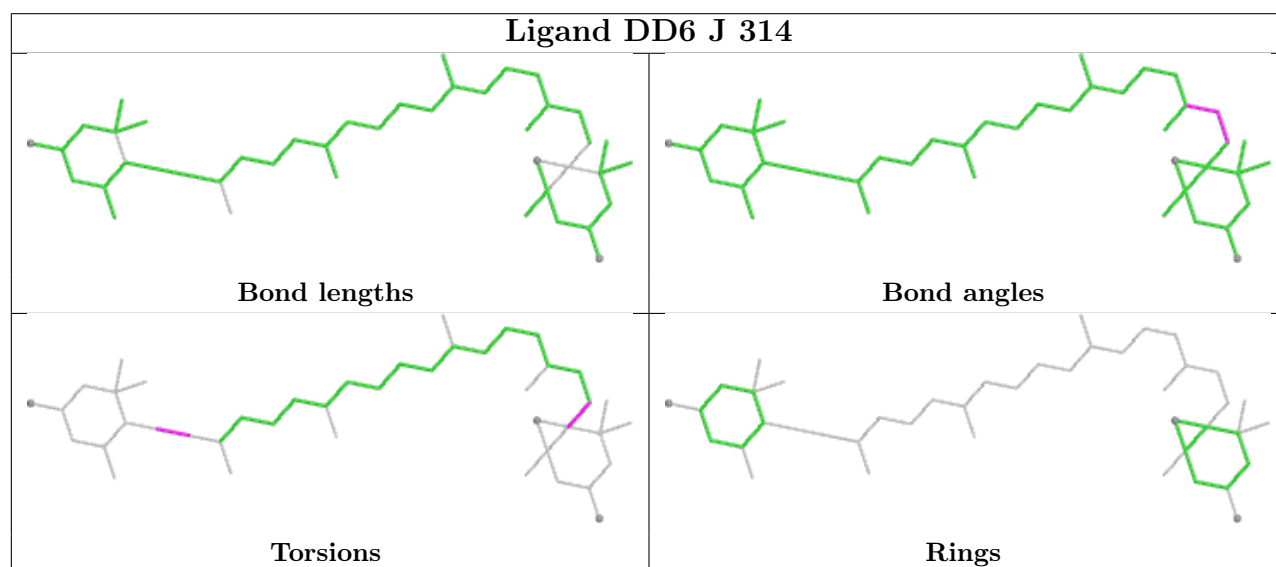
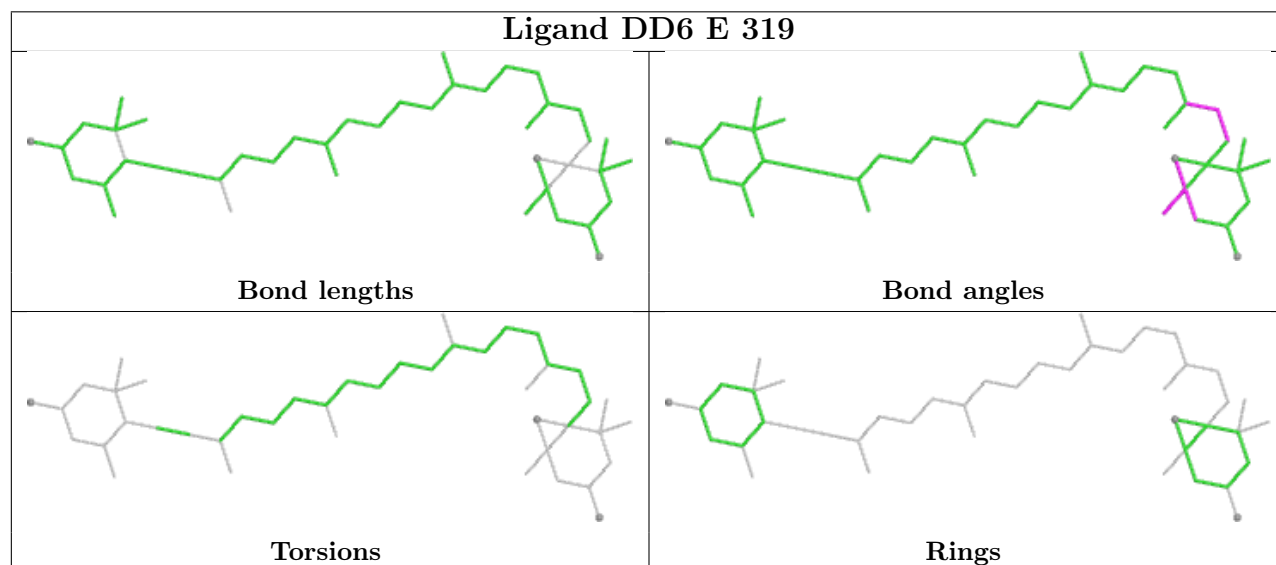
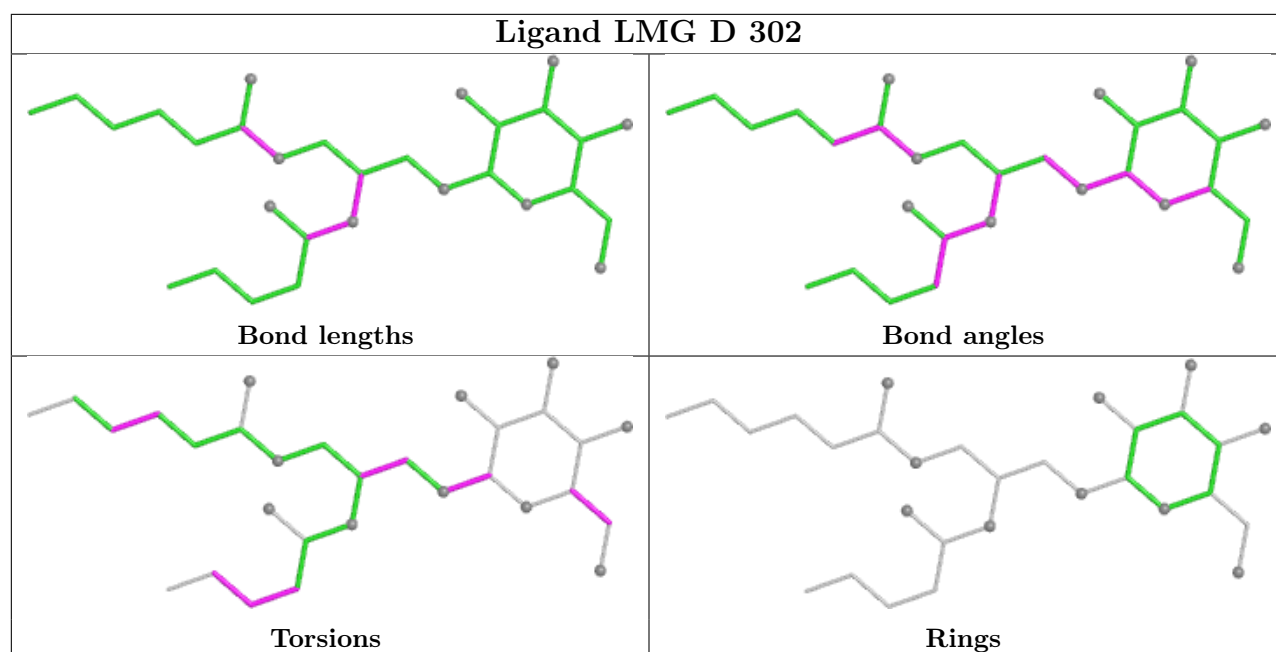
Bond angles

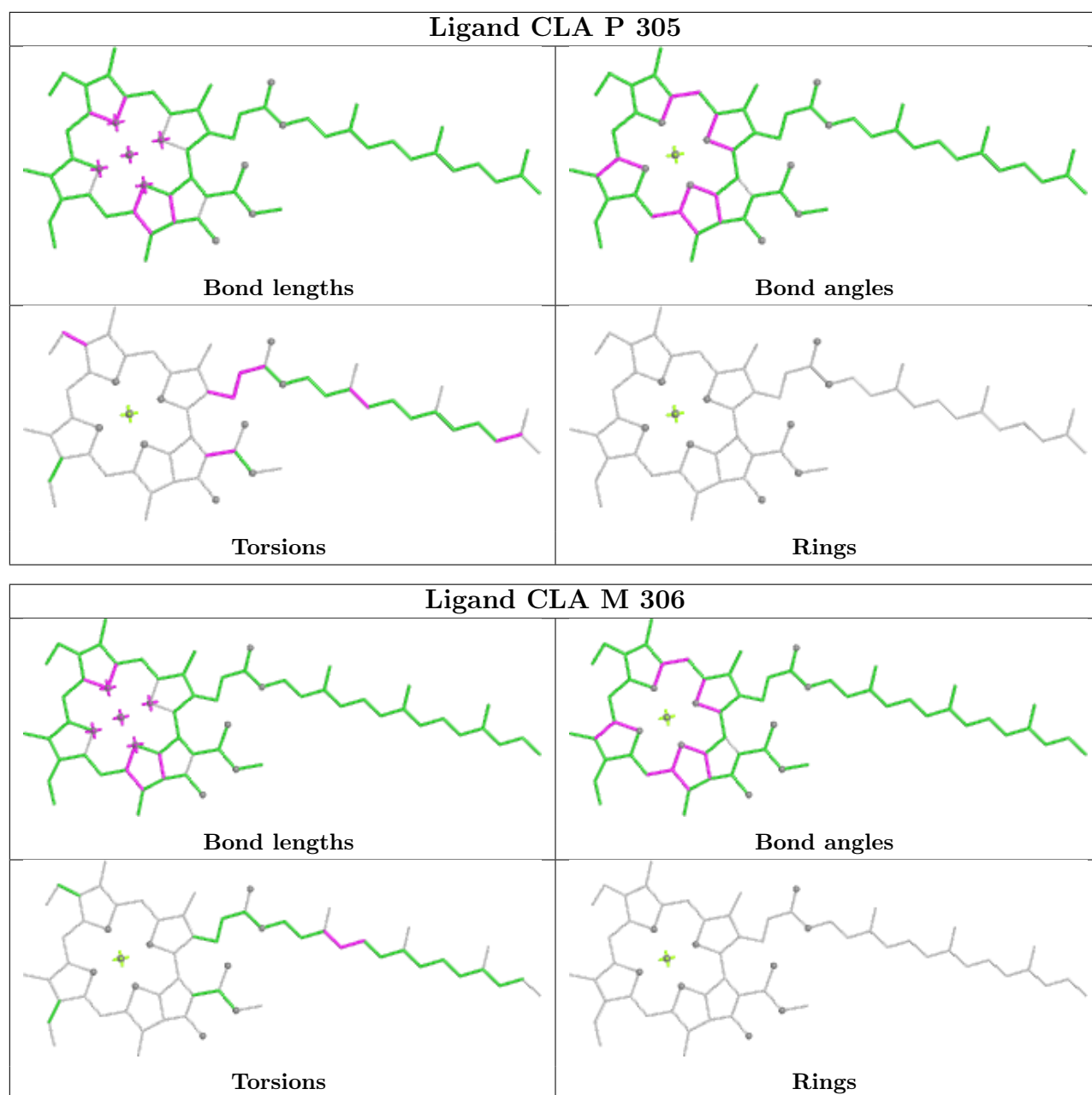


Torsions

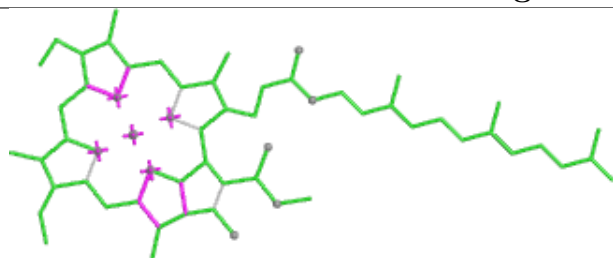


Rings

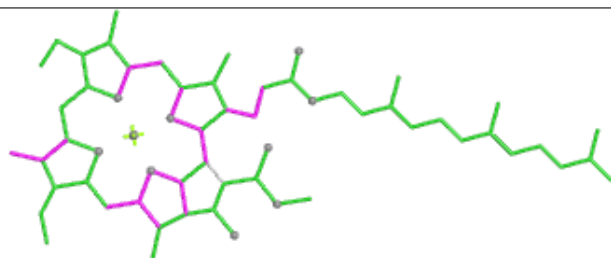




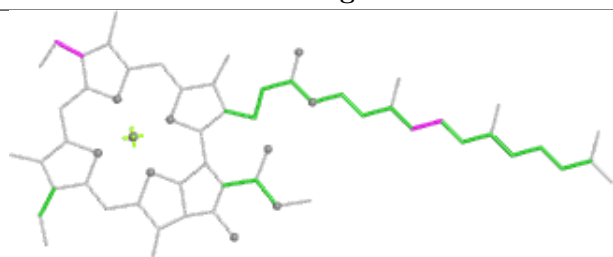
Ligand CLA R 308



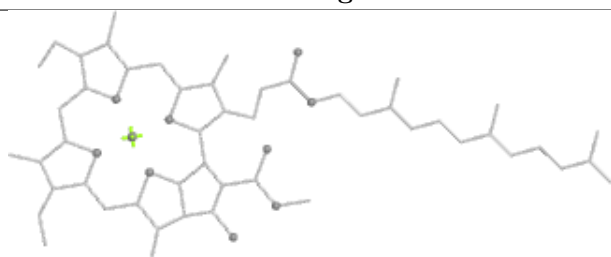
Bond lengths



Bond angles

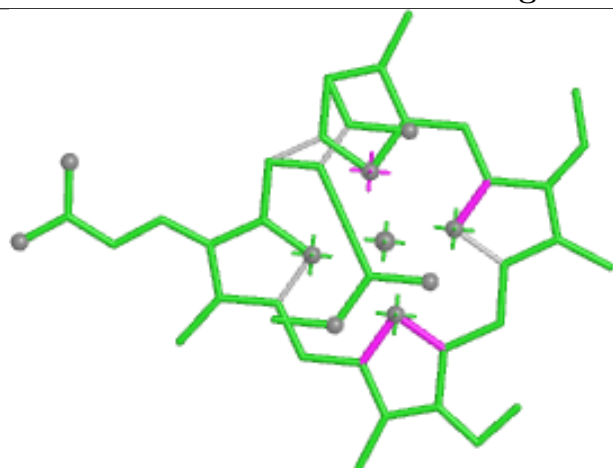


Torsions

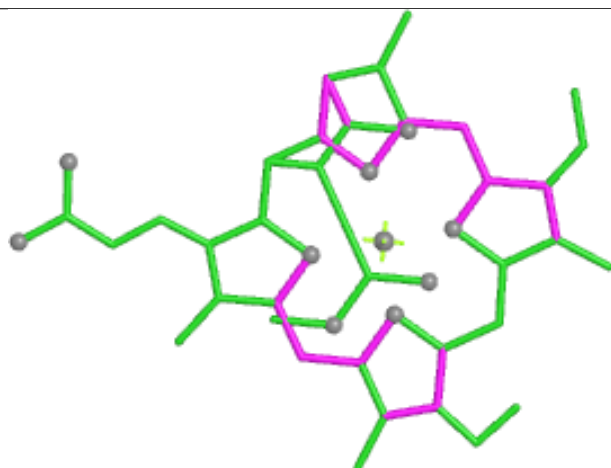


Rings

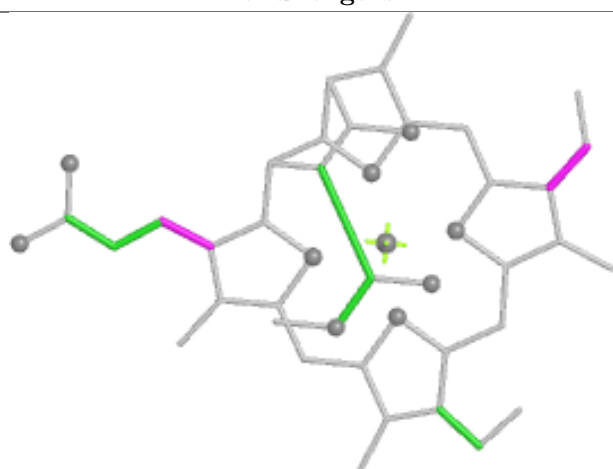
Ligand KC2 S 302



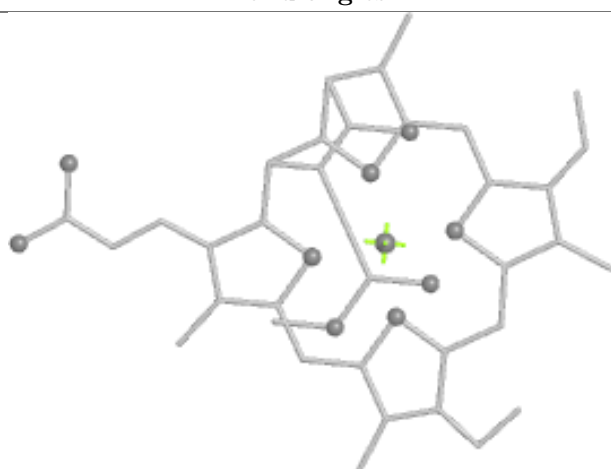
Bond lengths



Bond angles

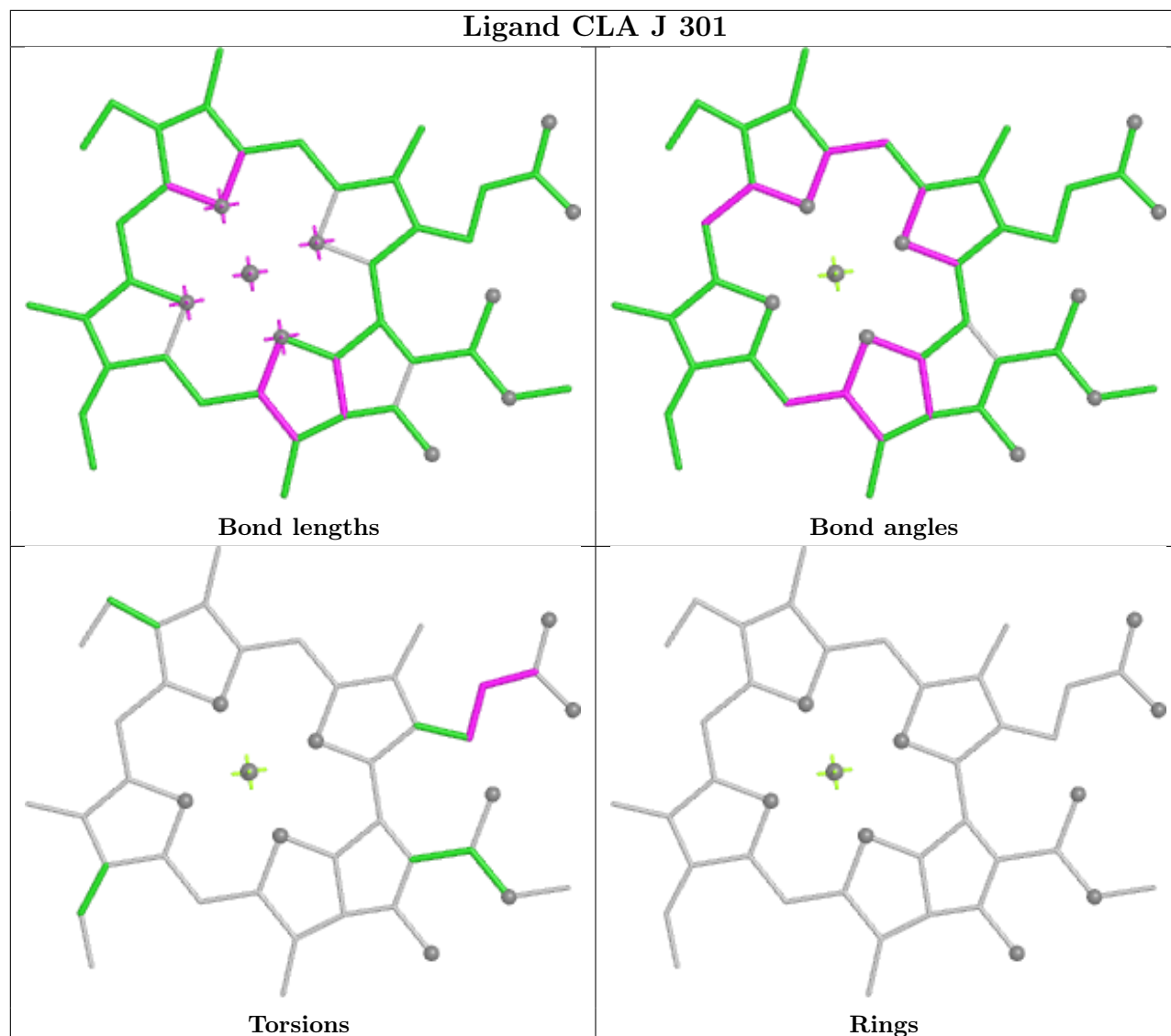


Torsions

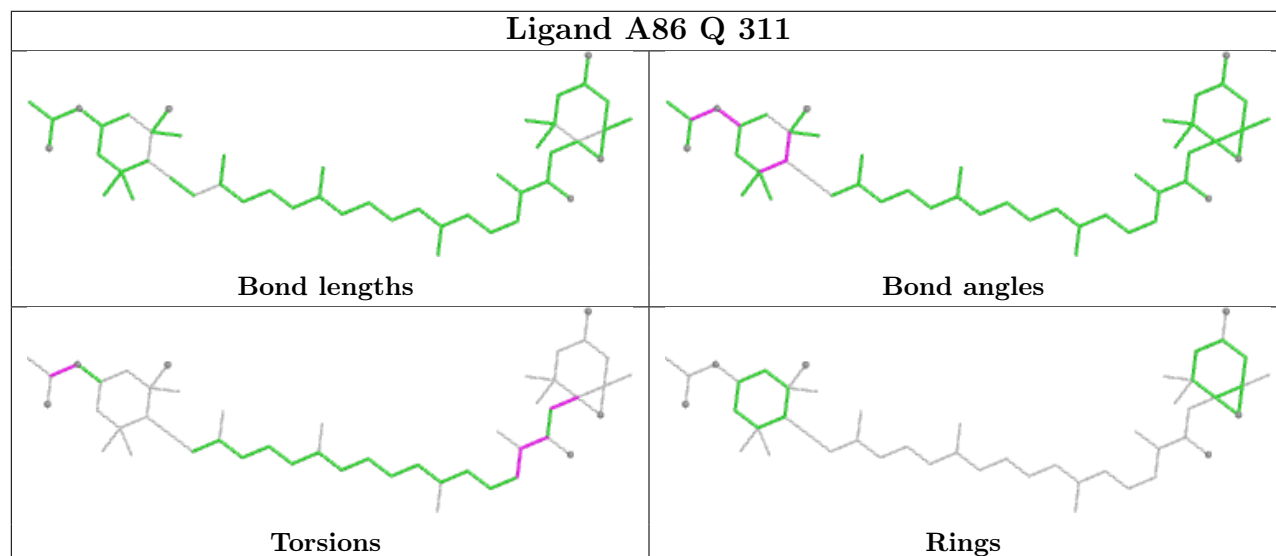


Rings

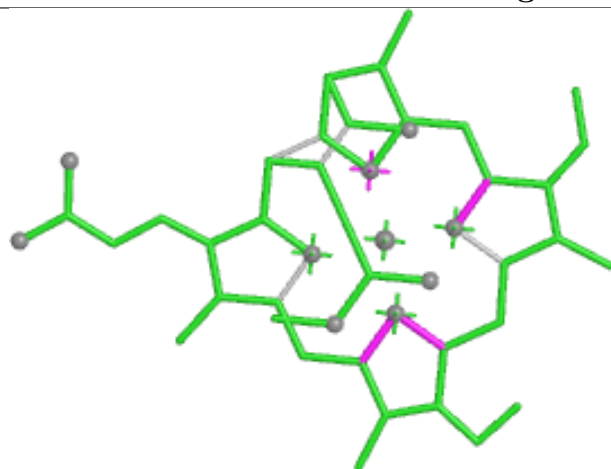
Ligand CLA J 301



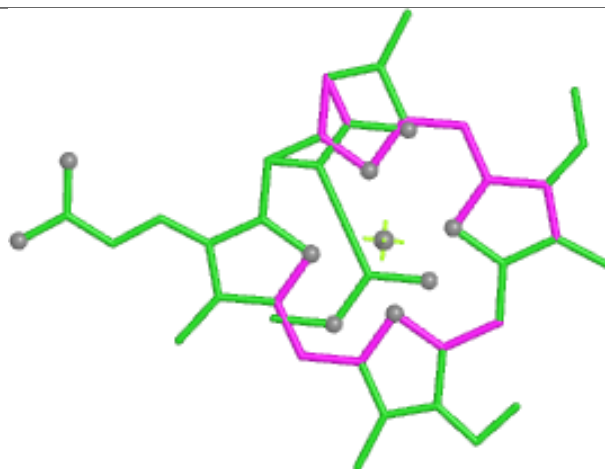
Ligand A86 Q 311



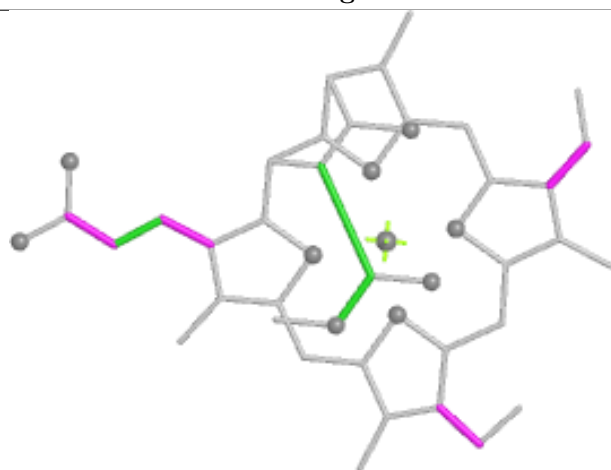
Ligand KC2 E 313



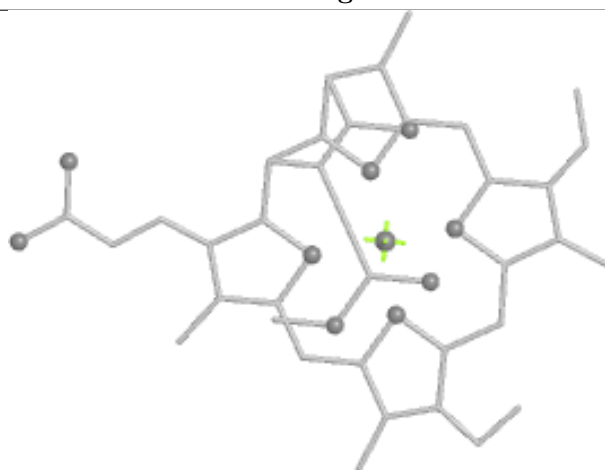
Bond lengths



Bond angles



Torsions



Rings

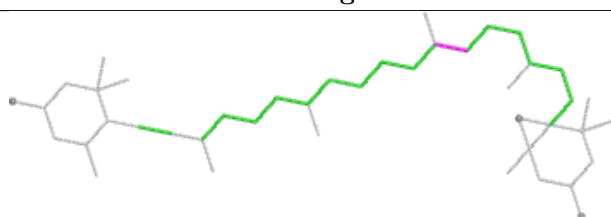
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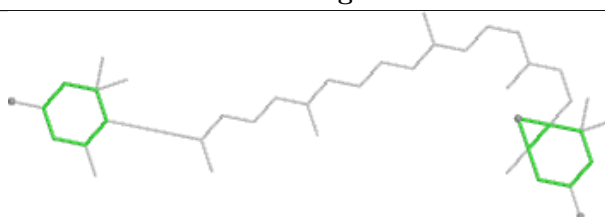
Bond lengths



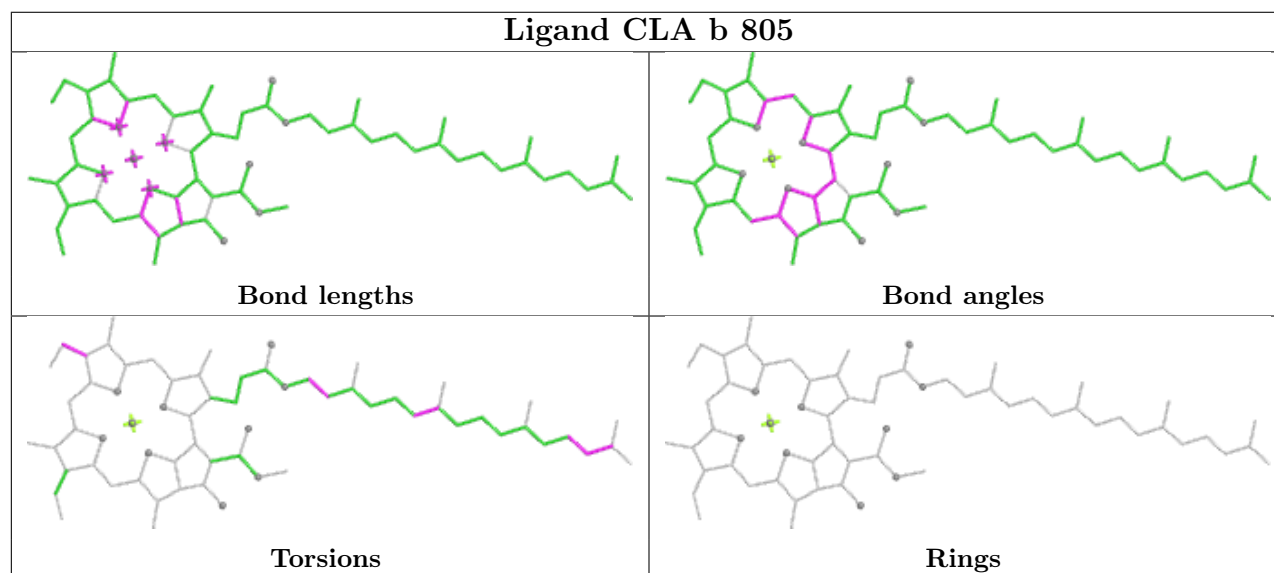
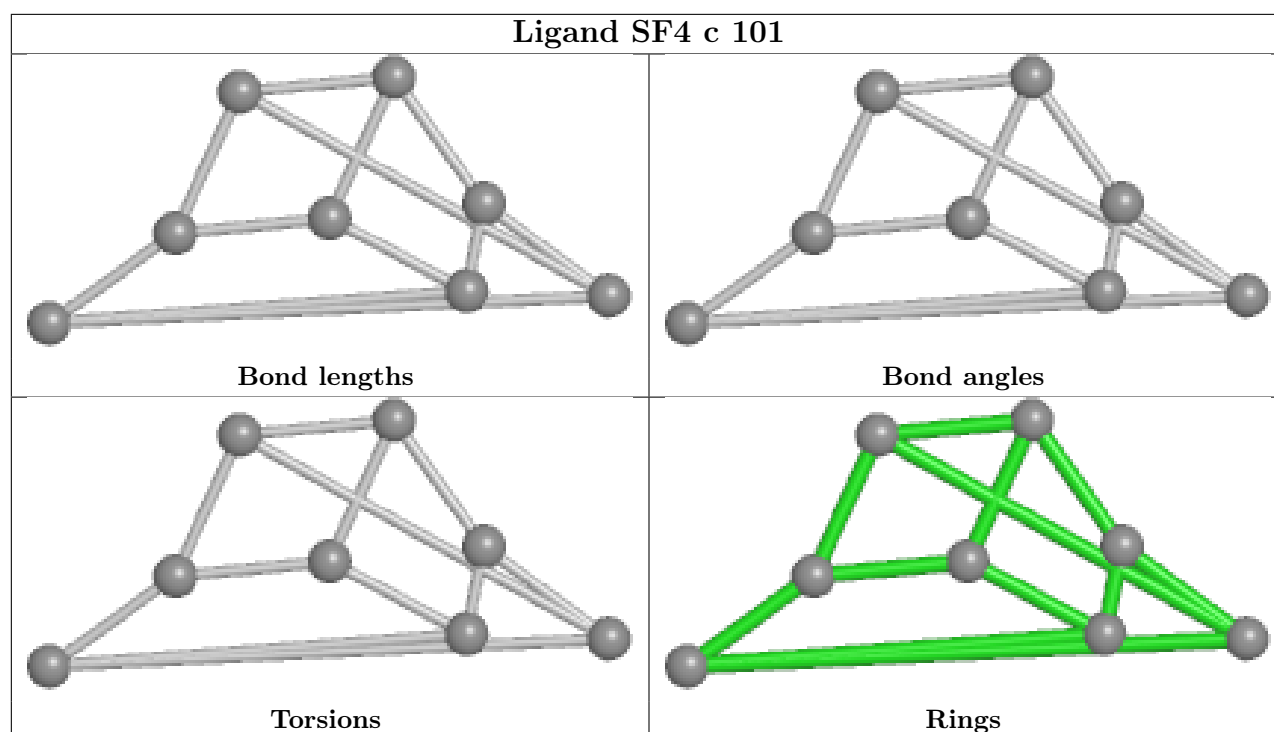
Bond angles

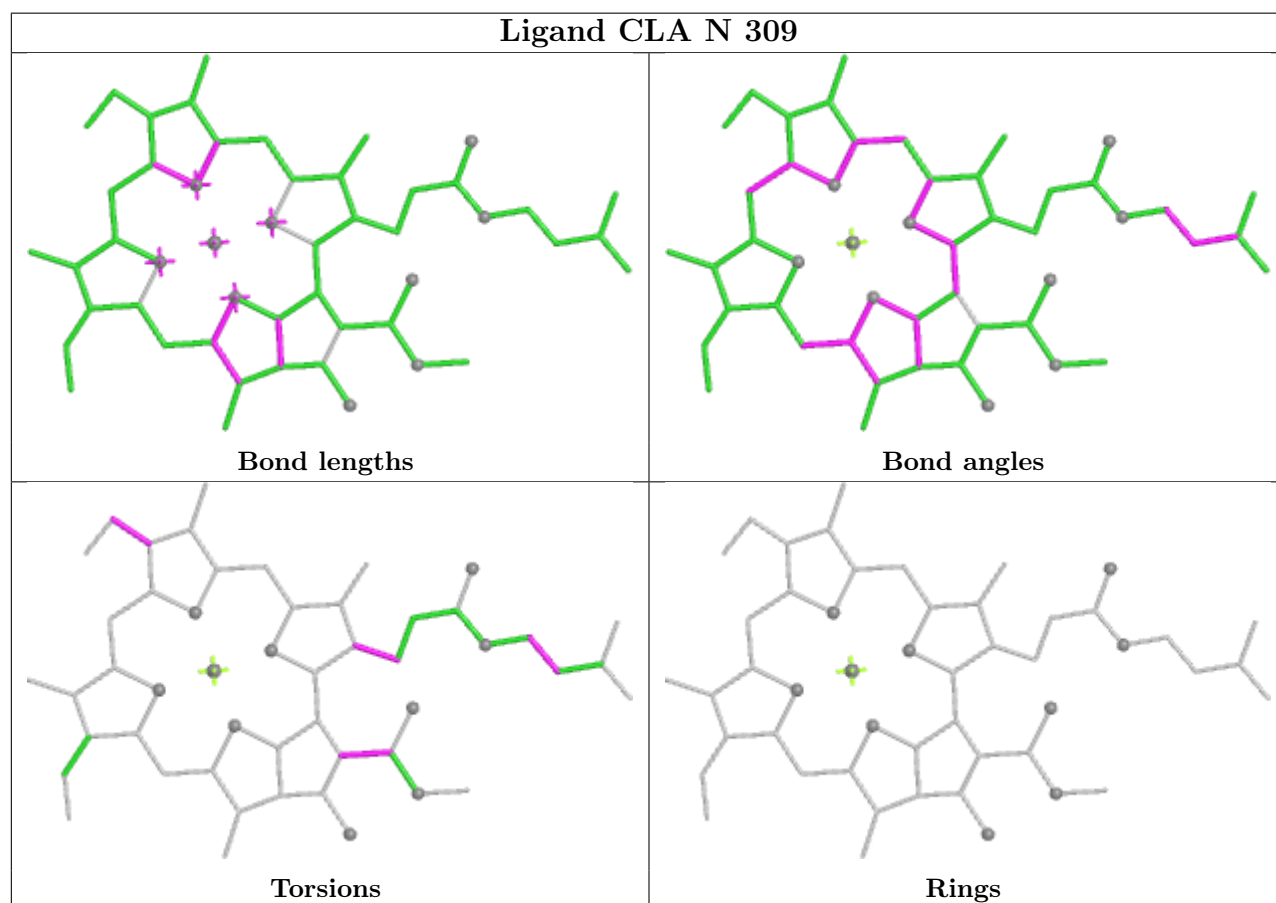
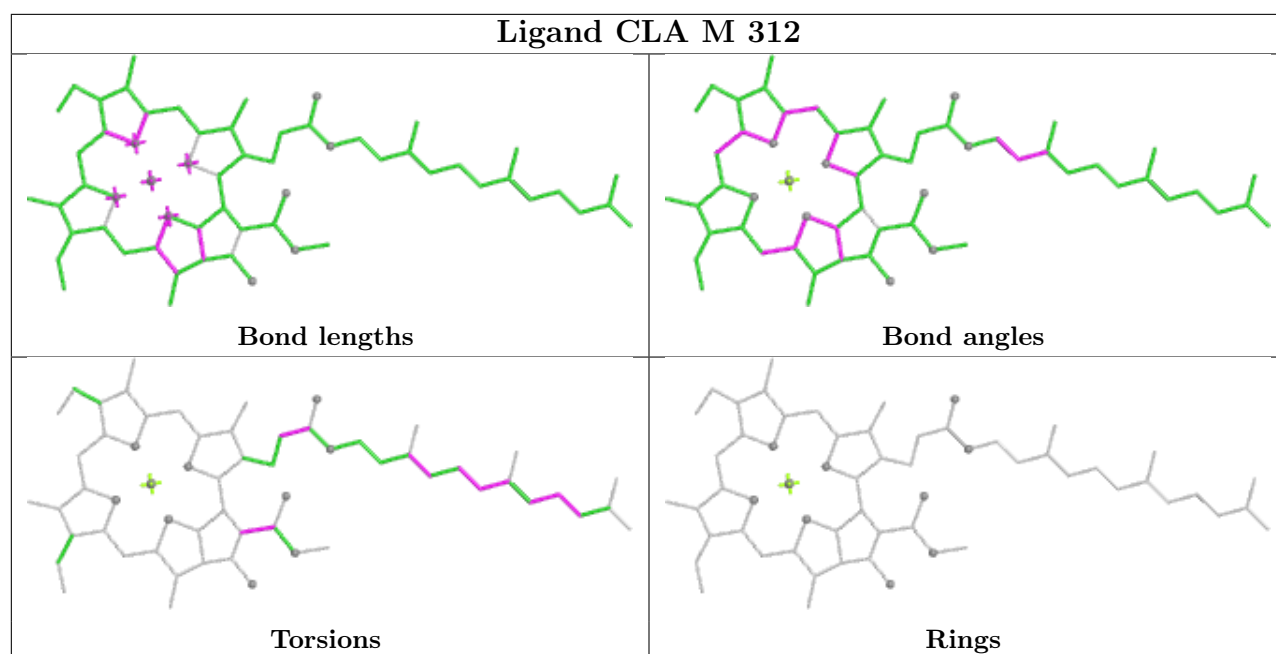


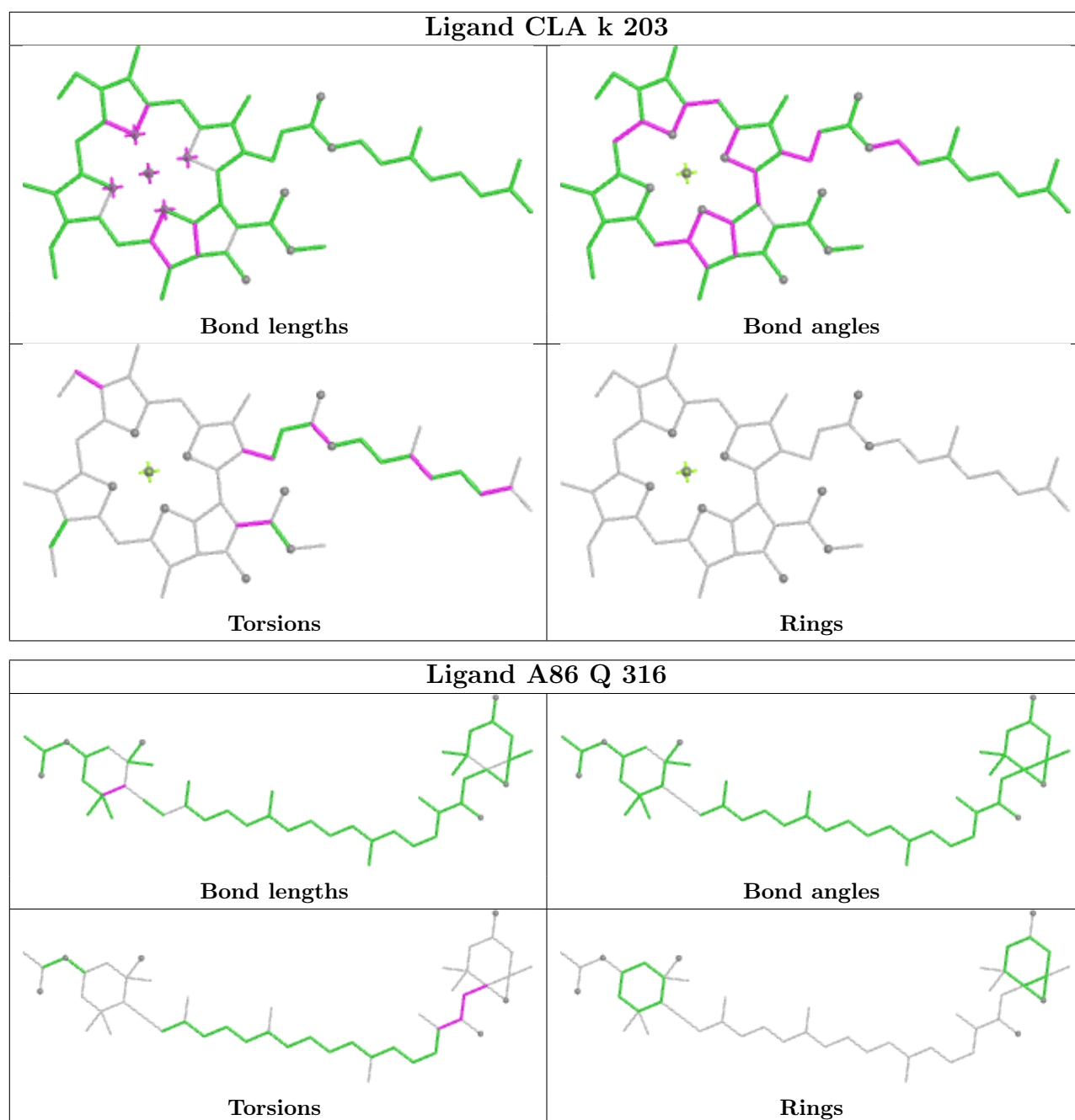
Torsions



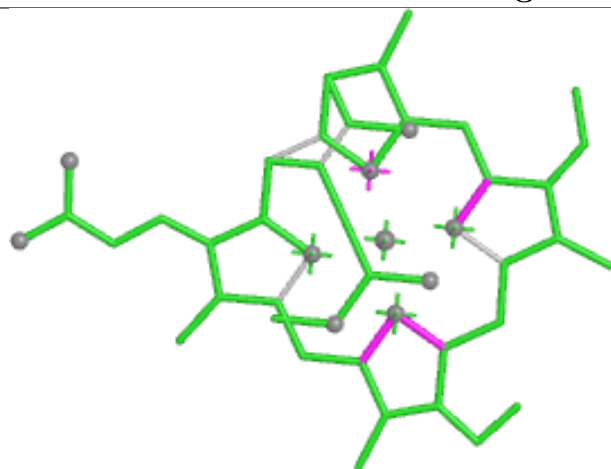
Rings



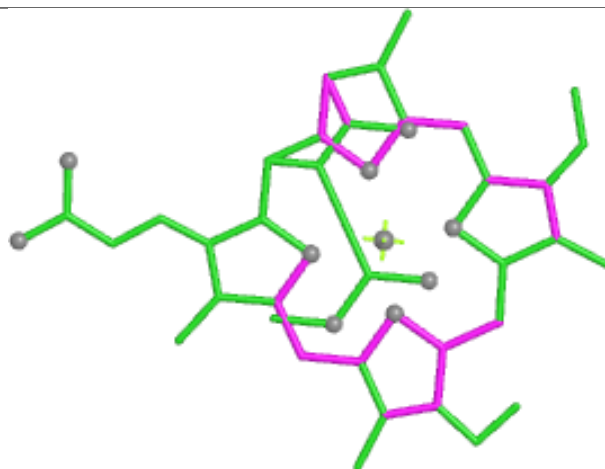




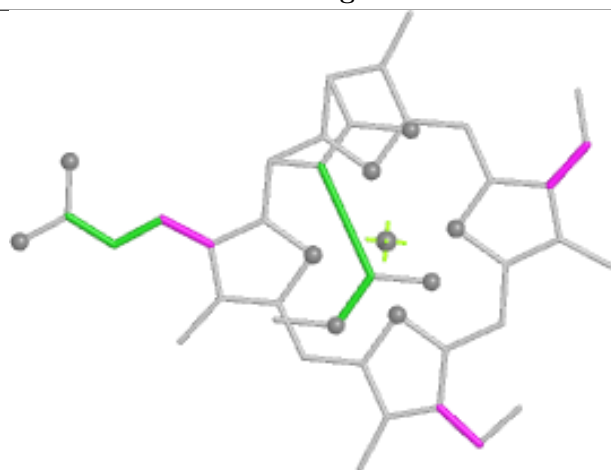
Ligand KC2 R 303



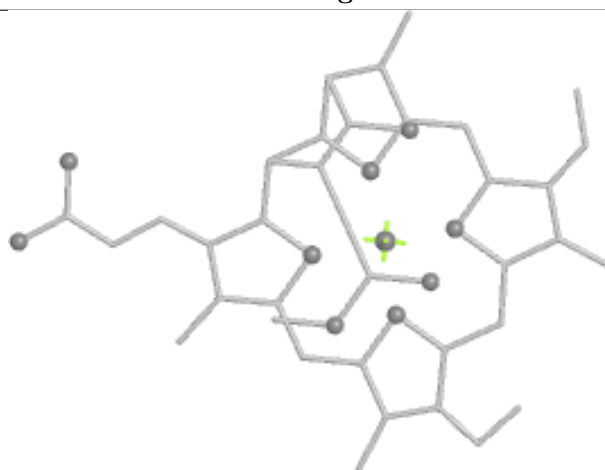
Bond lengths



Bond angles

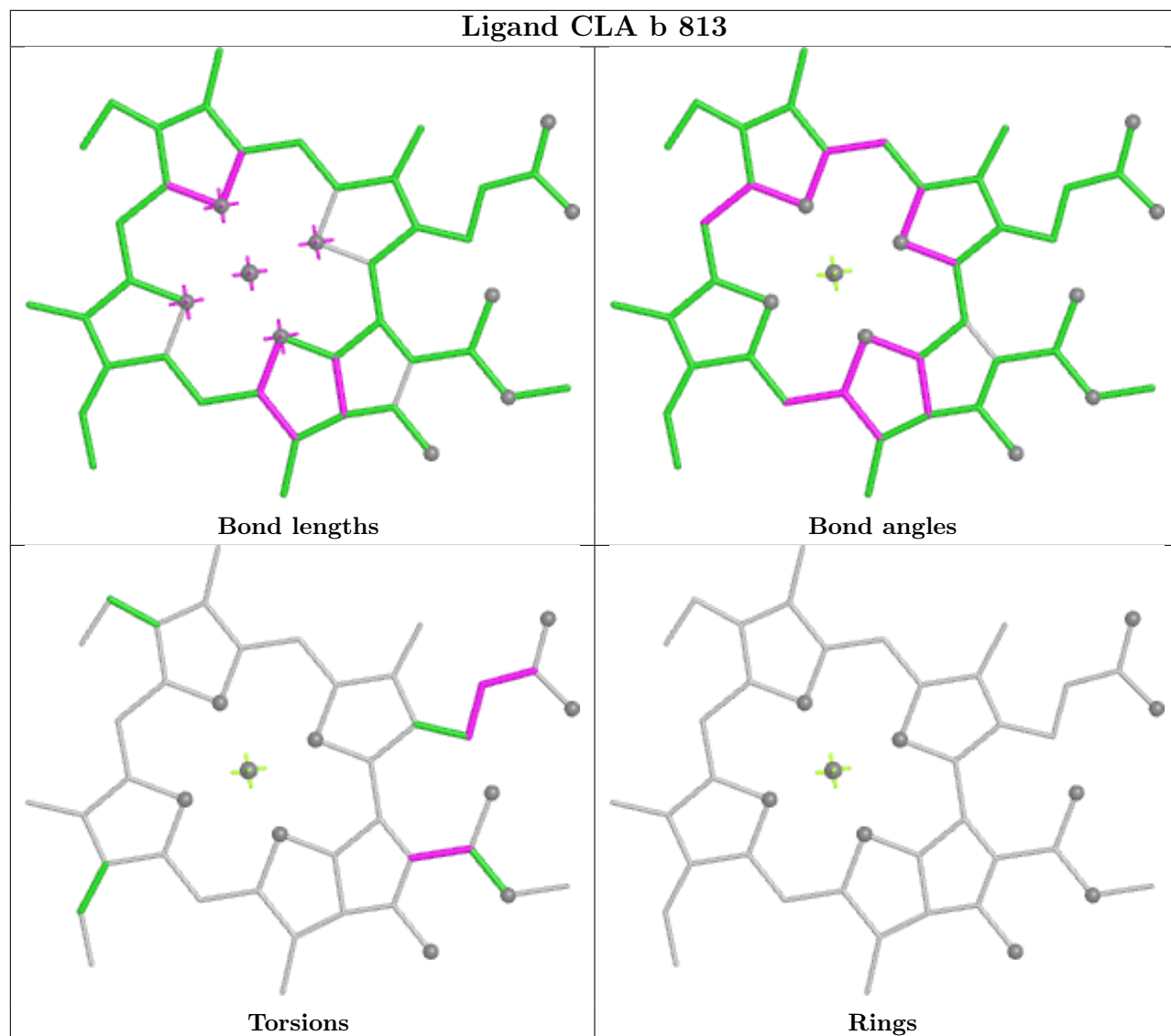


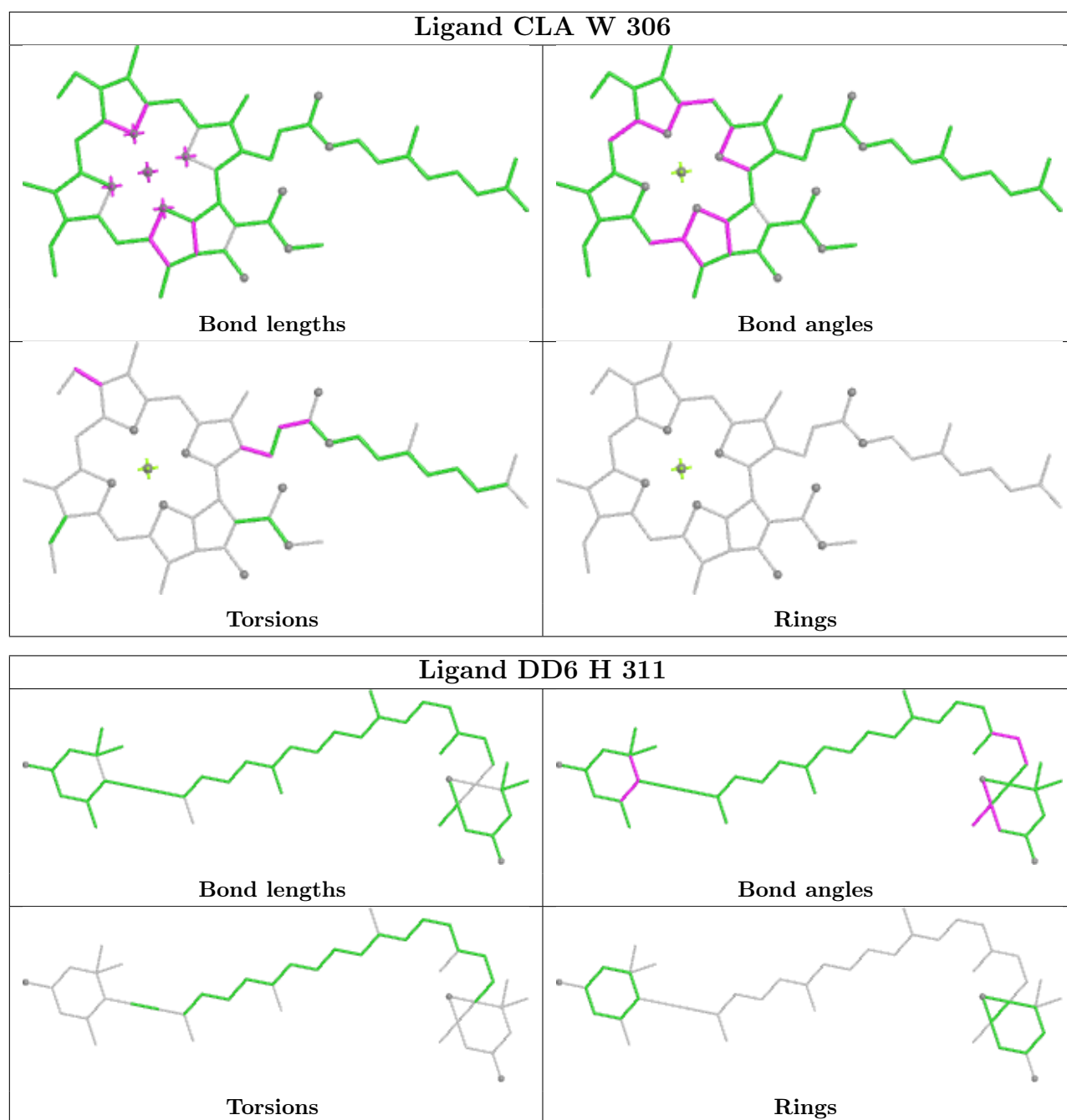
Torsions

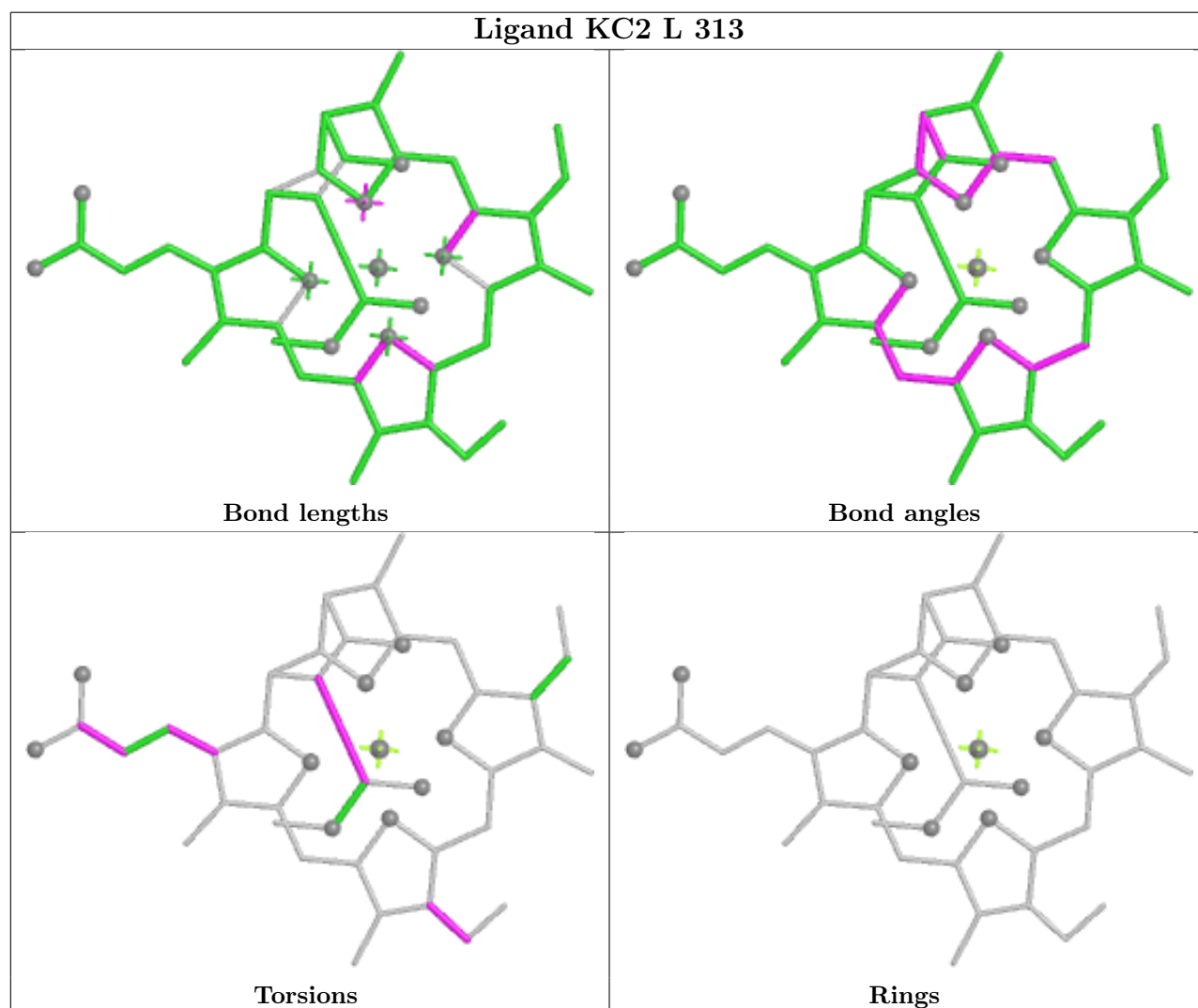
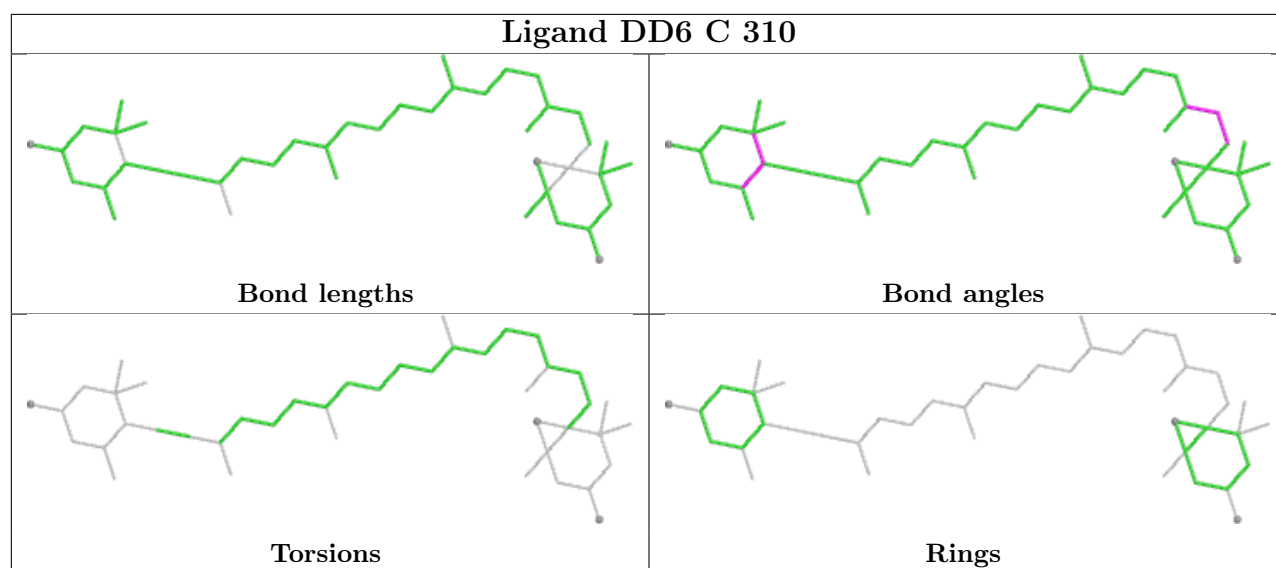


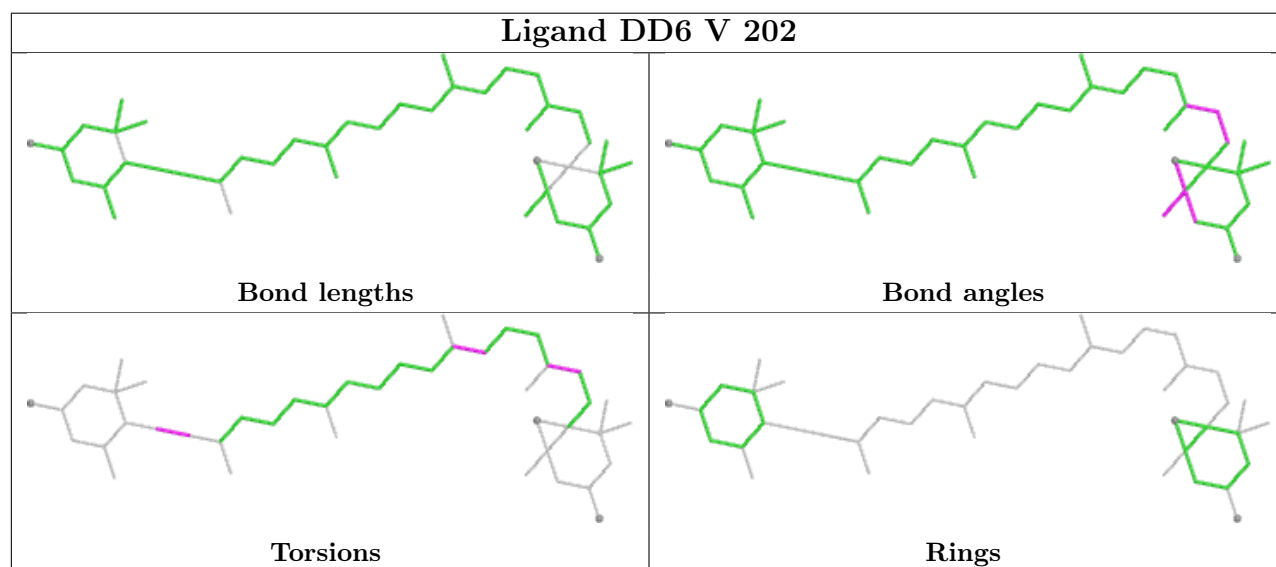
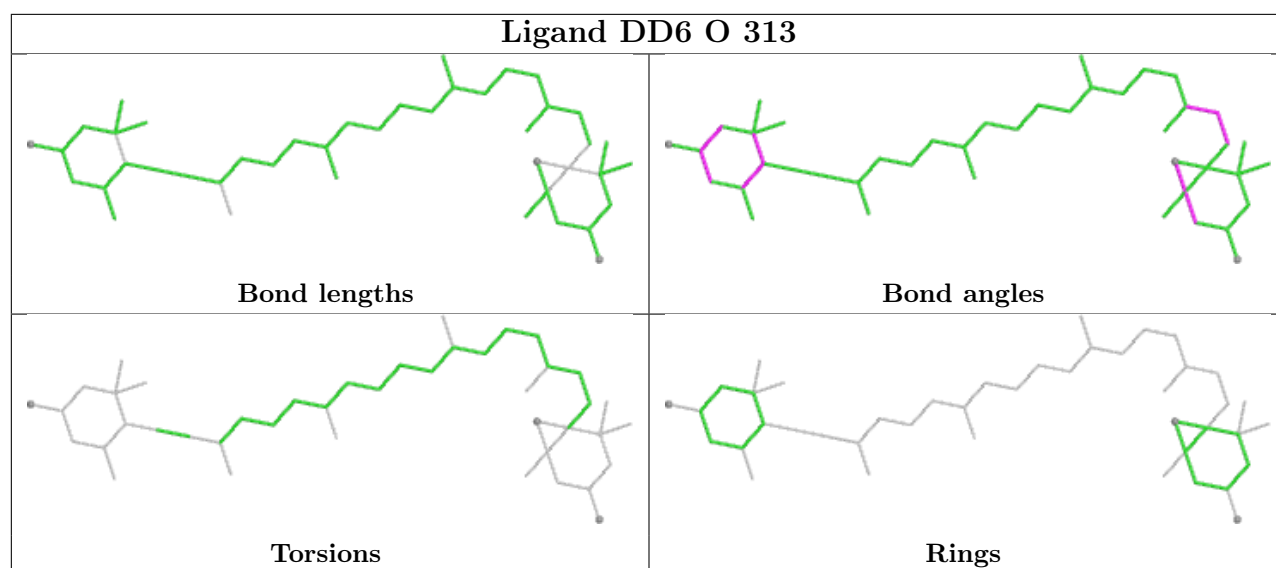
Rings

Ligand CLA b 813

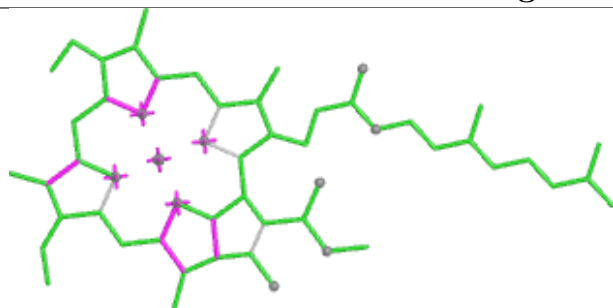




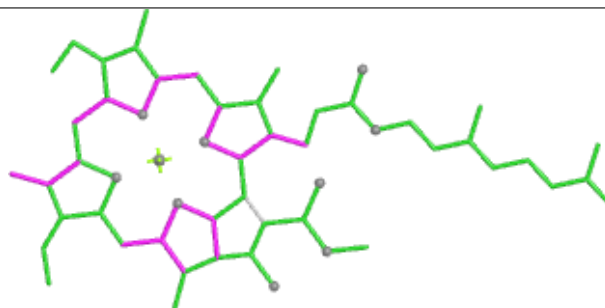




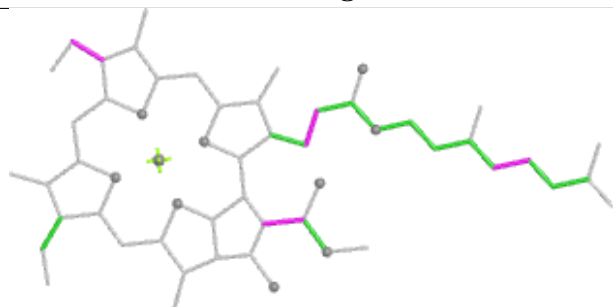
Ligand CLA J 307



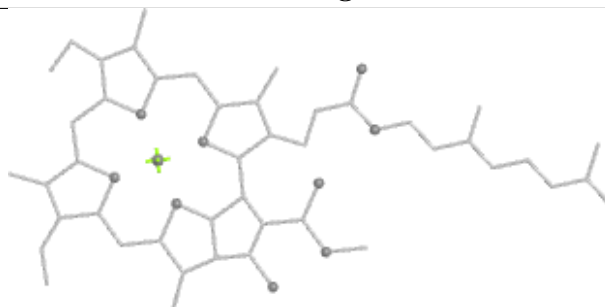
Bond lengths



Bond angles

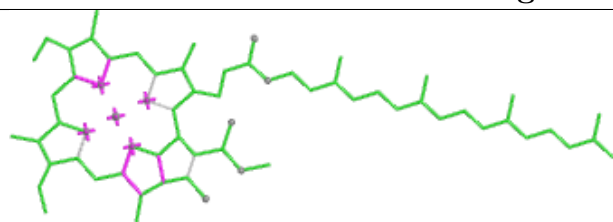


Torsions

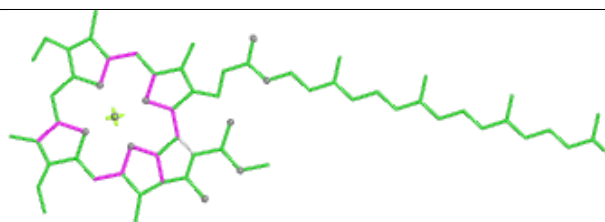


Rings

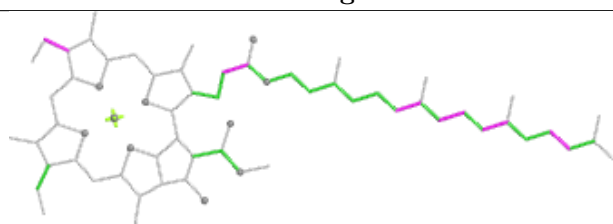
Ligand CLA b 808



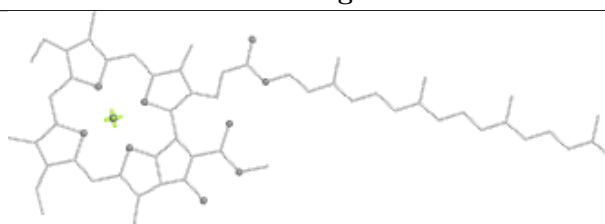
Bond lengths



Bond angles

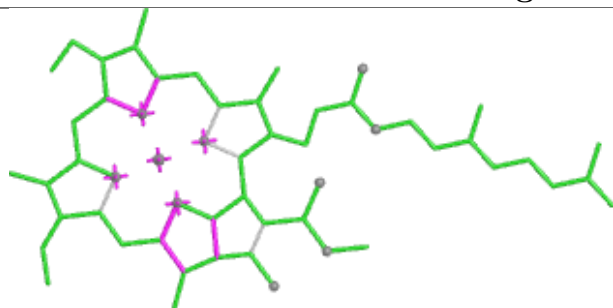


Torsions

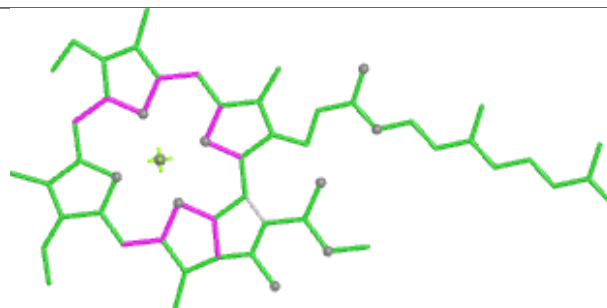


Rings

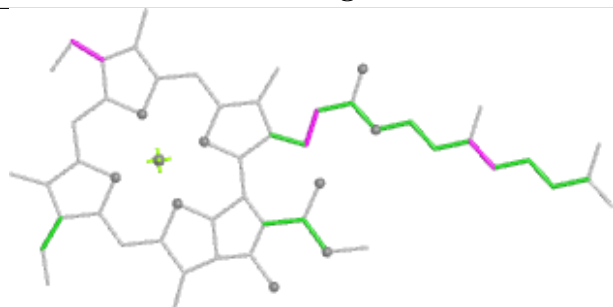
Ligand CLA F 309



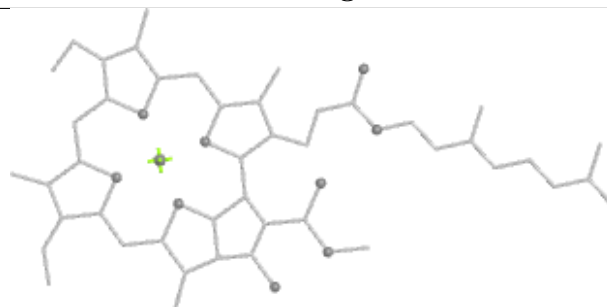
Bond lengths



Bond angles

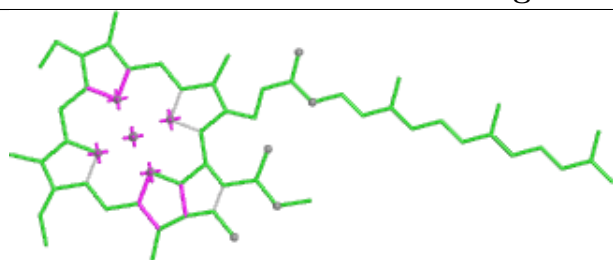


Torsions

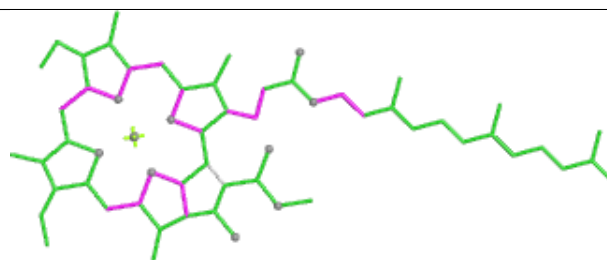


Rings

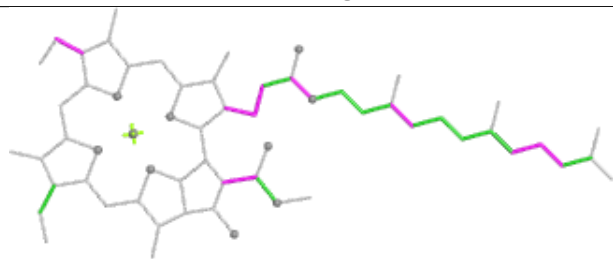
Ligand CLA H 307



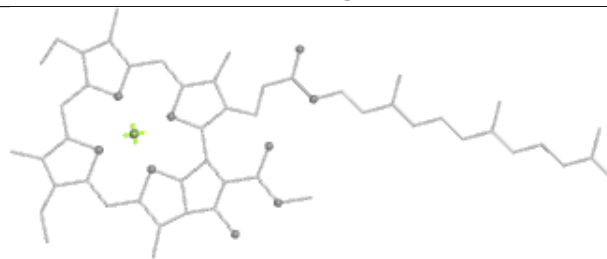
Bond lengths



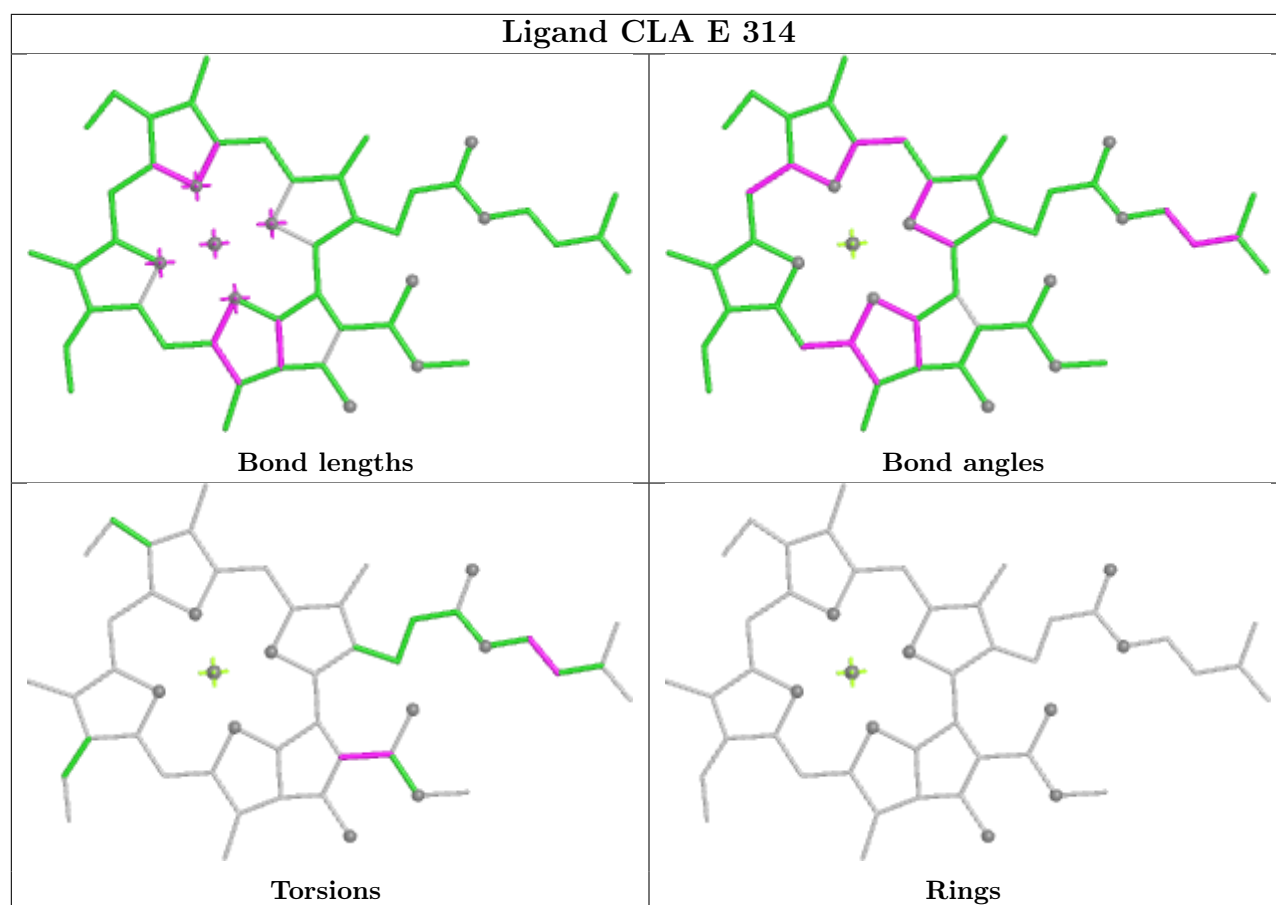
Bond angles



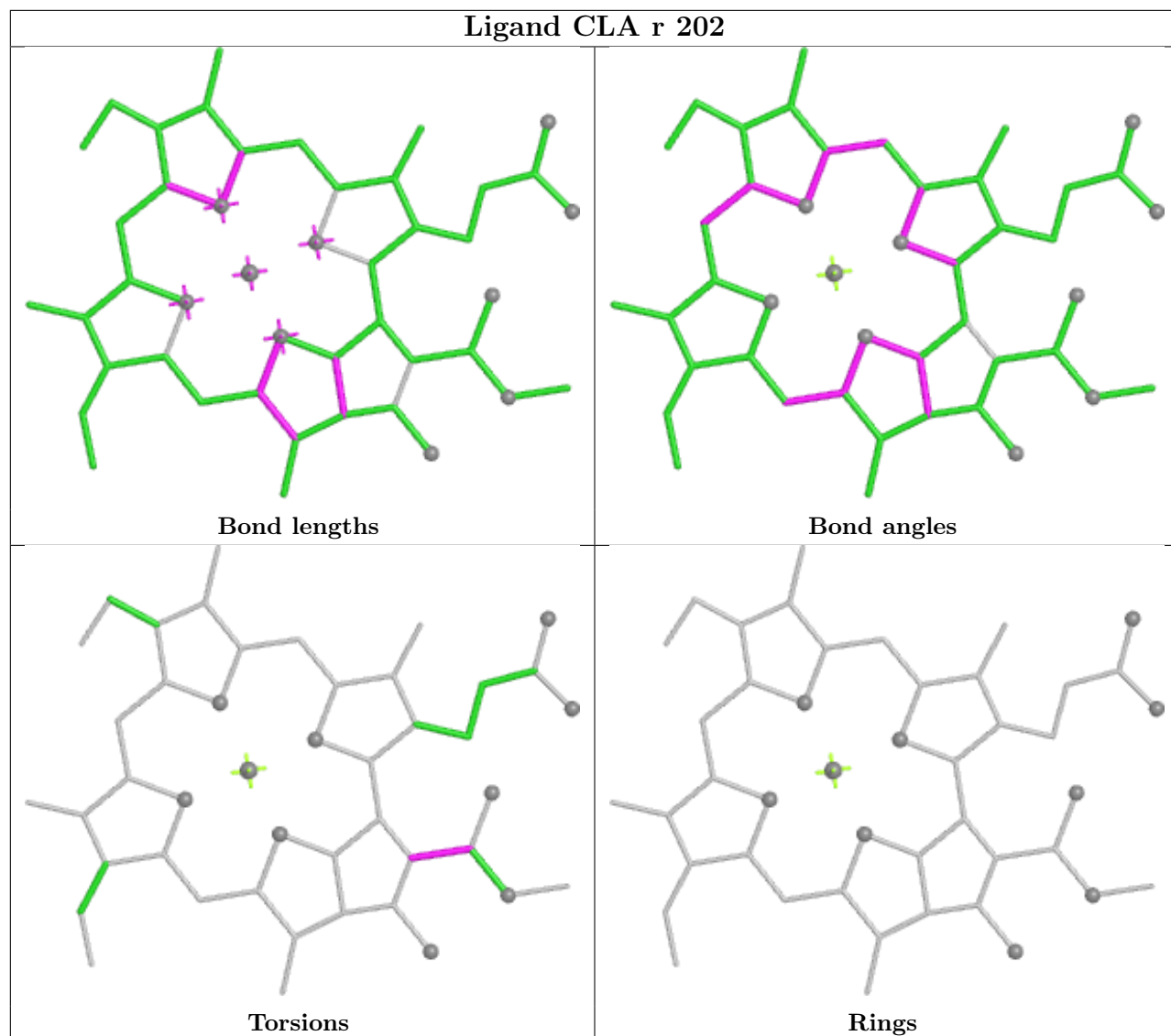
Torsions

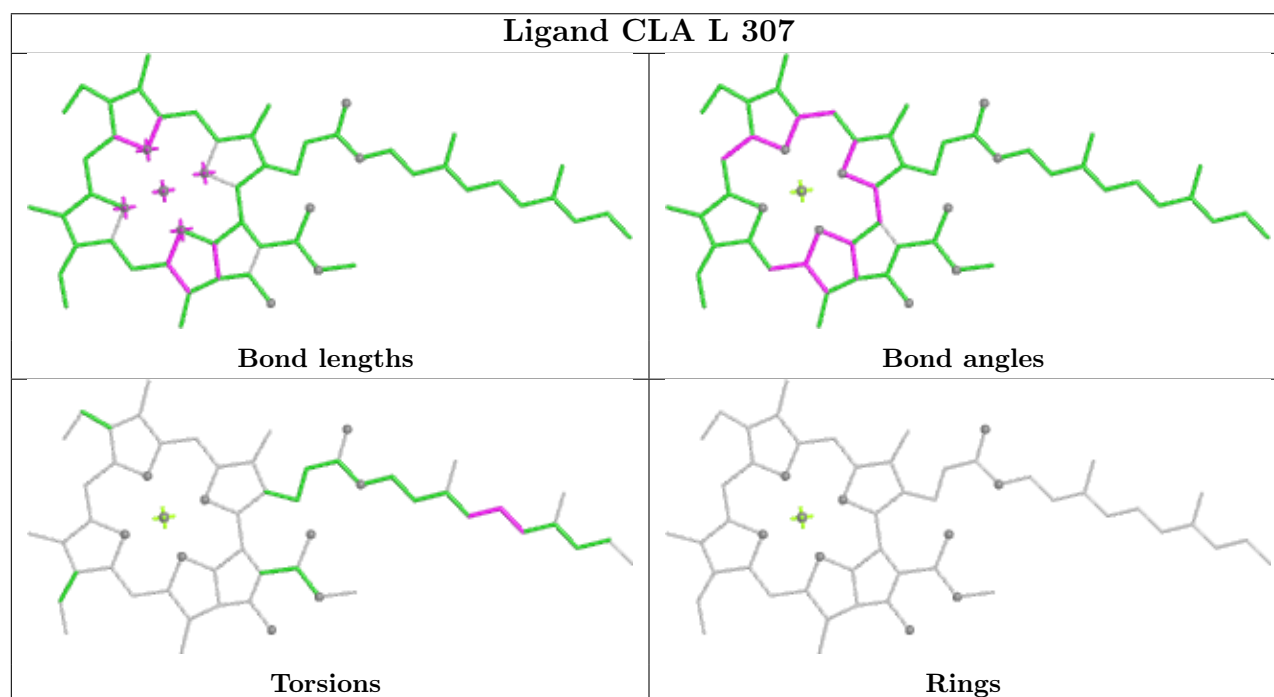
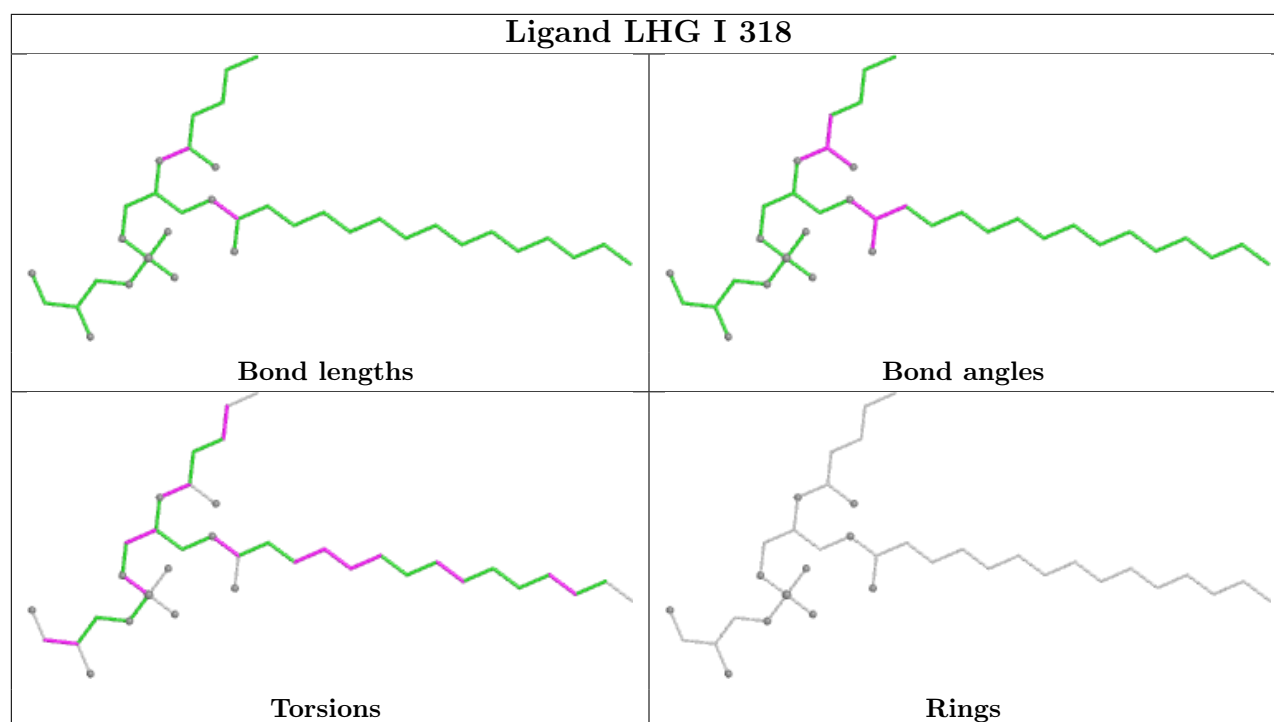


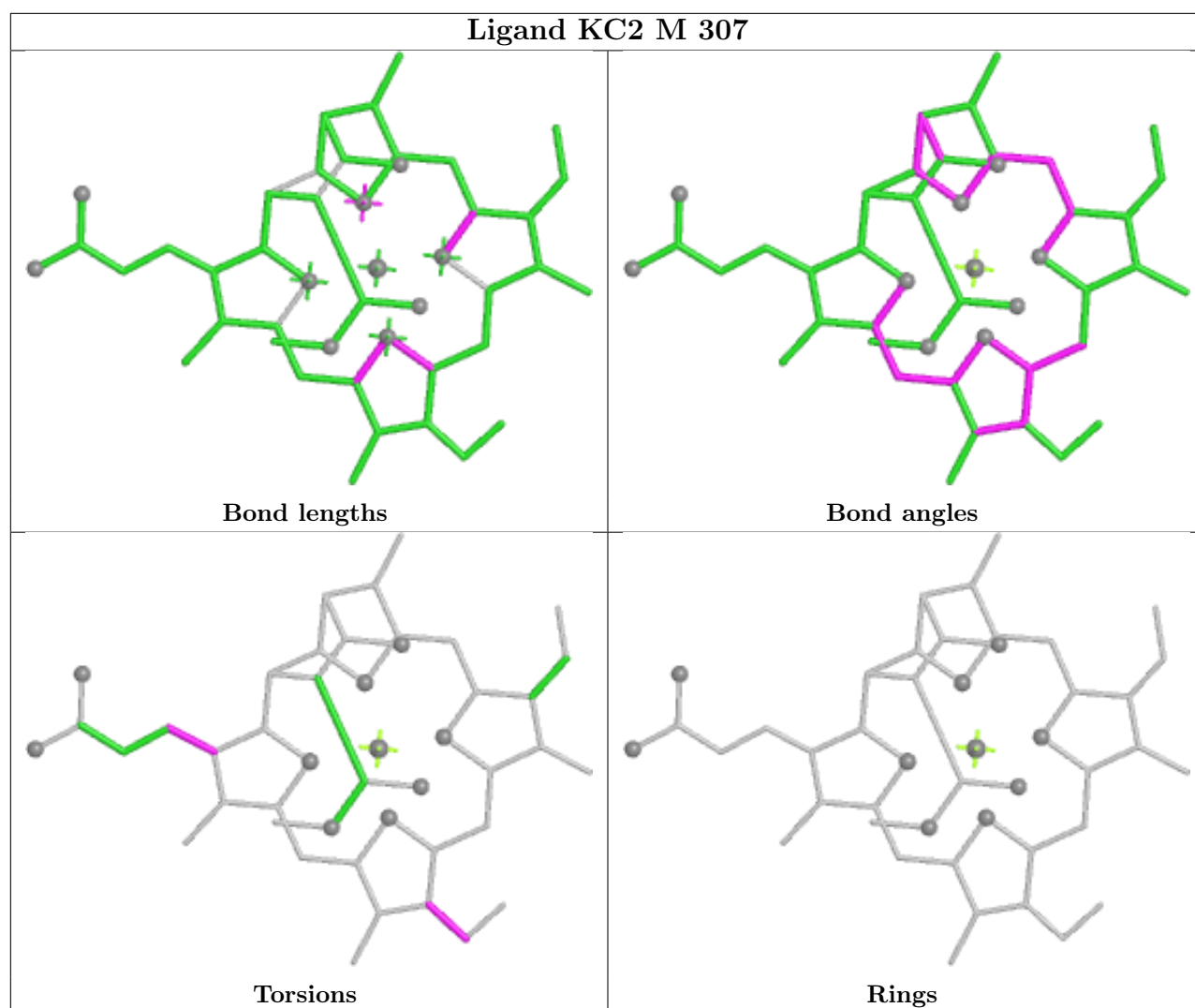
Rings



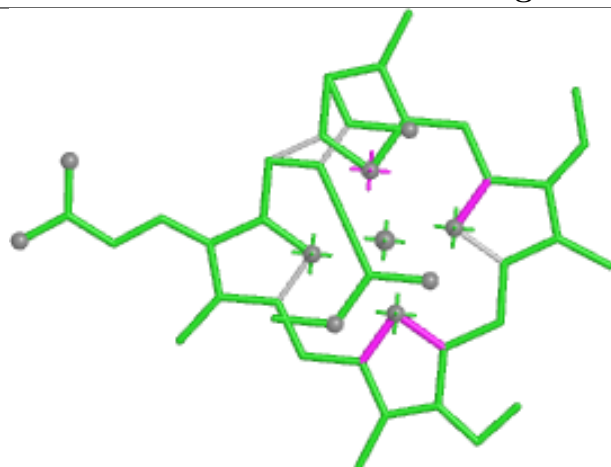
Ligand CLA r 202



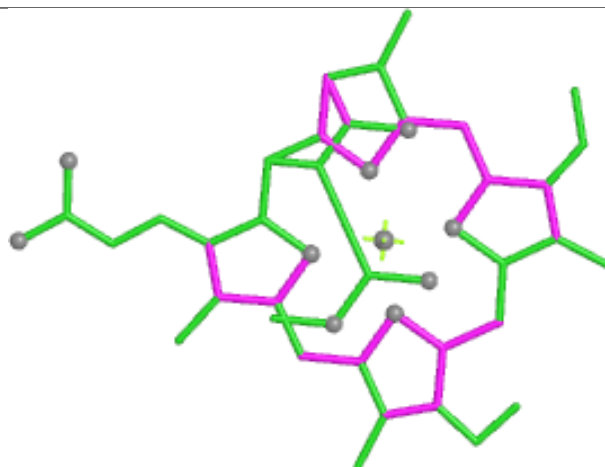




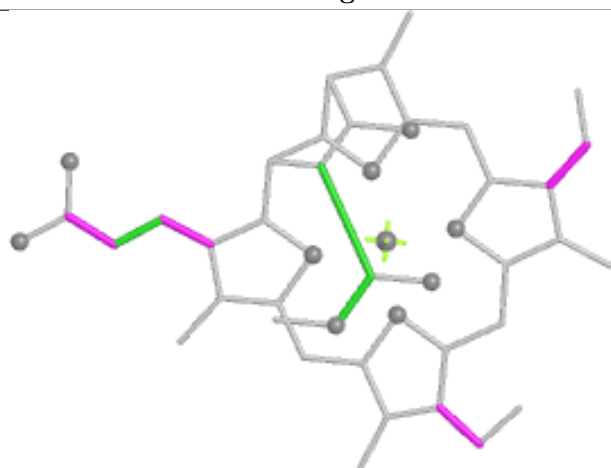
Ligand KC2 K 309



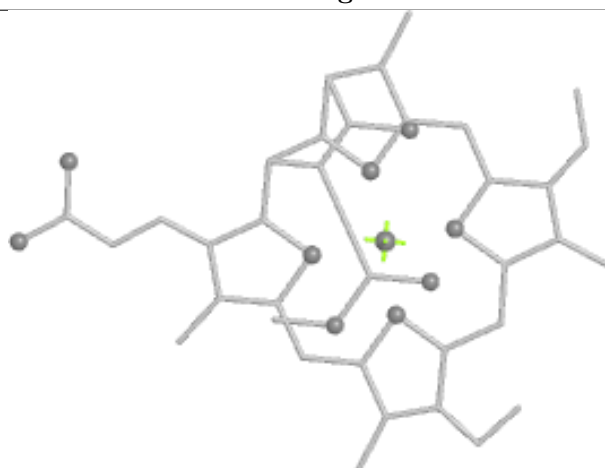
Bond lengths



Bond angles

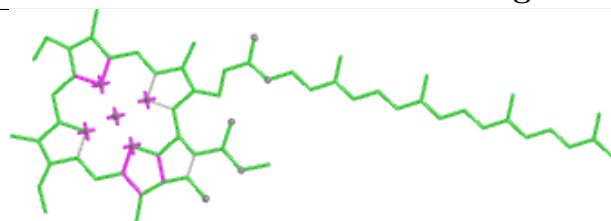


Torsions

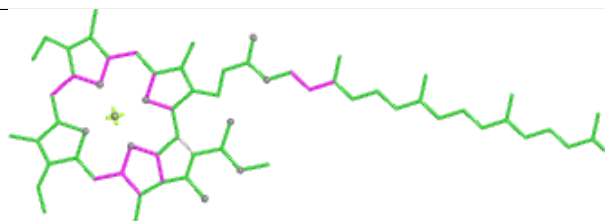


Rings

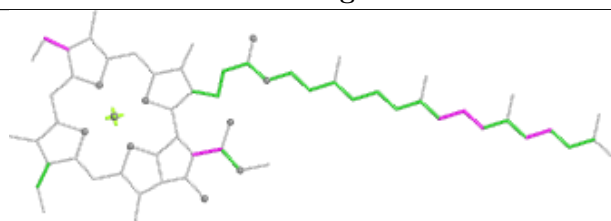
Ligand CLA D 311



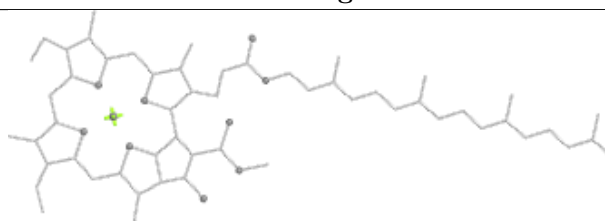
Bond lengths



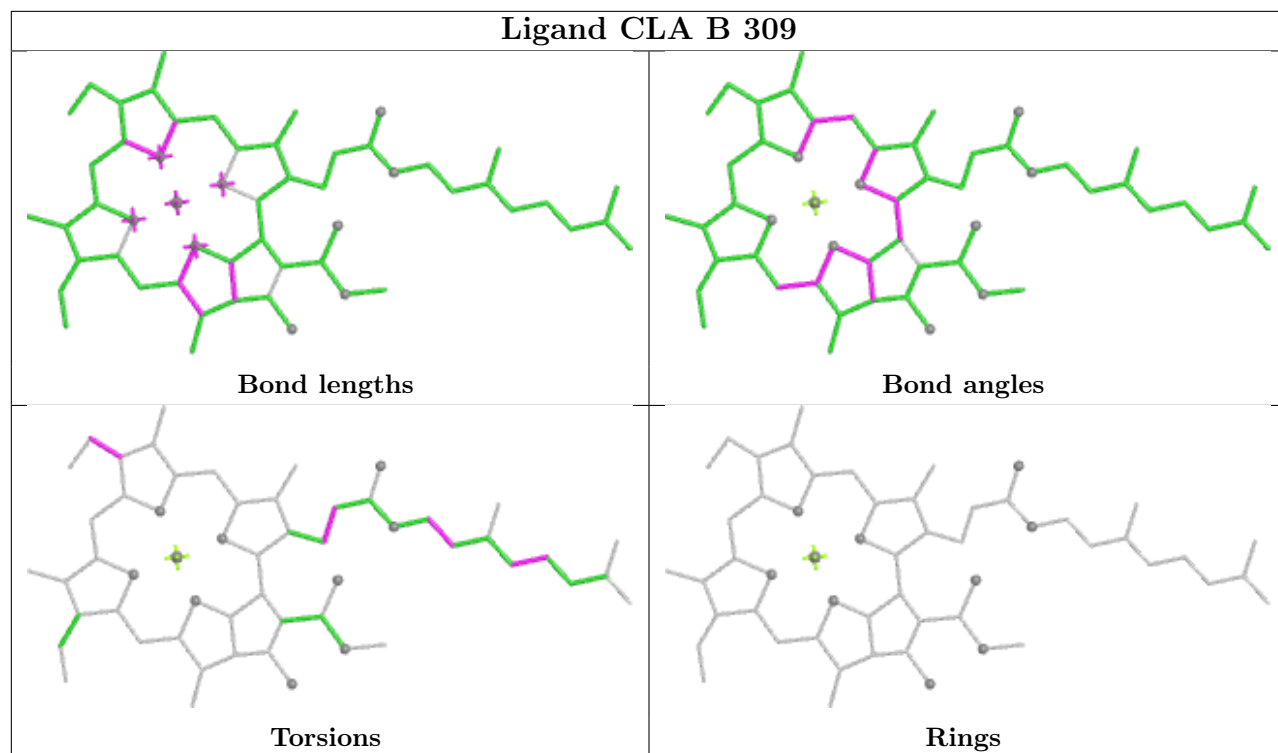
Bond angles



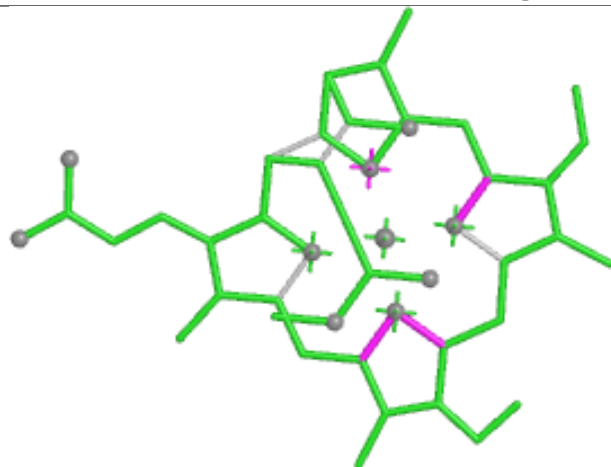
Torsions



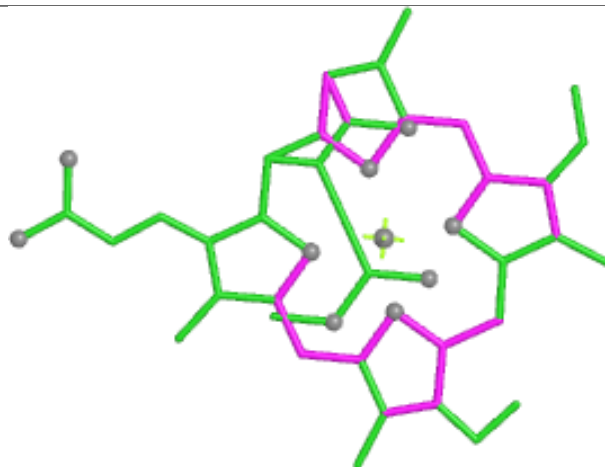
Rings



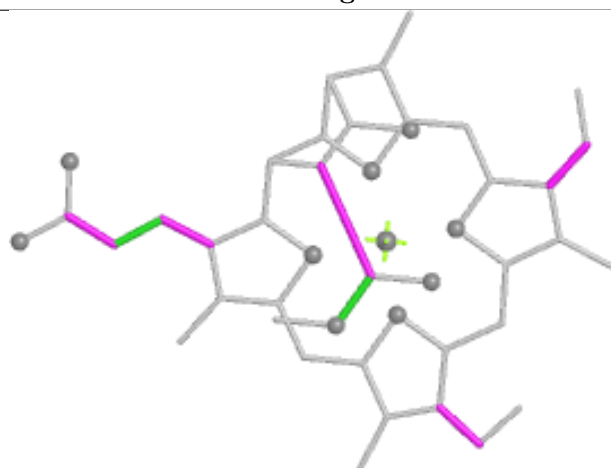
Ligand KC2 P 301



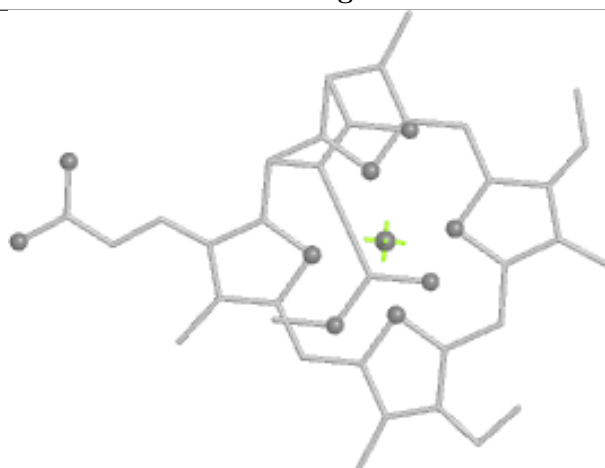
Bond lengths



Bond angles

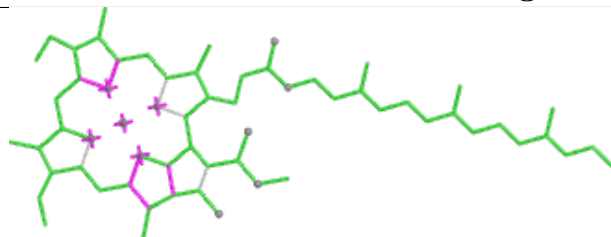


Torsions

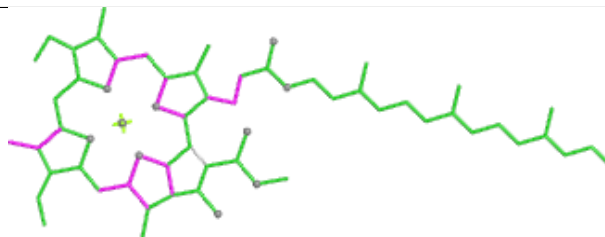


Rings

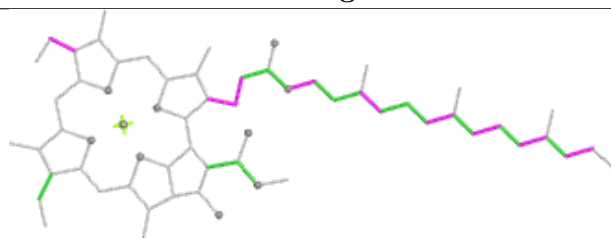
Ligand CLA a 810



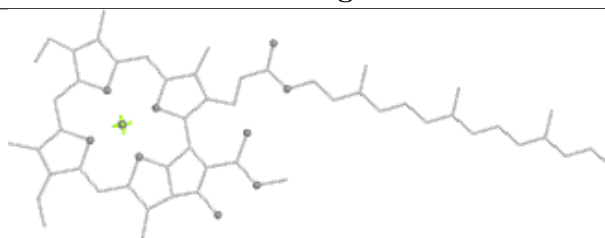
Bond lengths



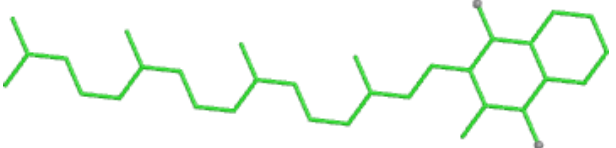
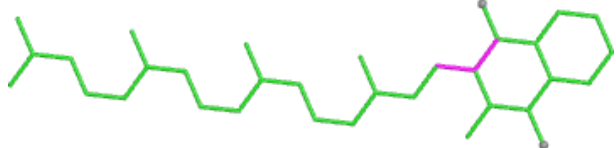
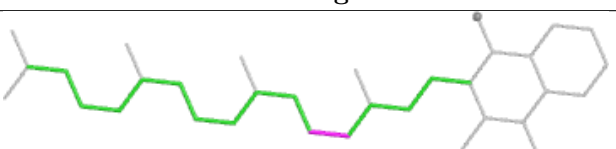
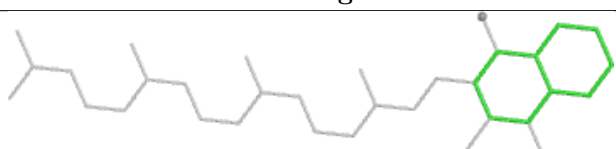
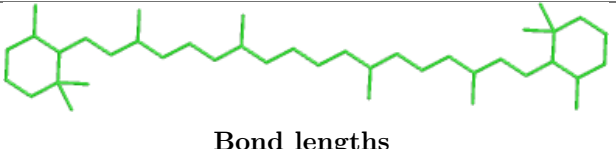
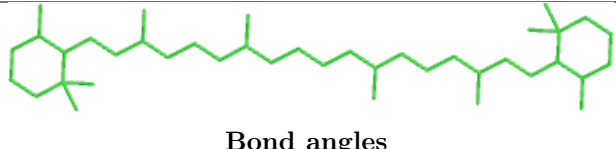
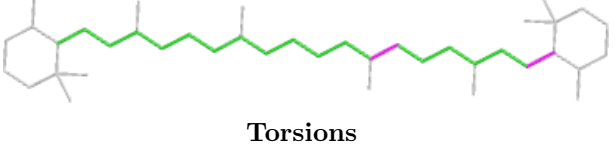
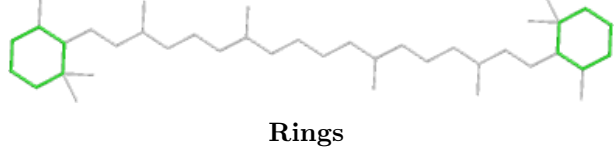
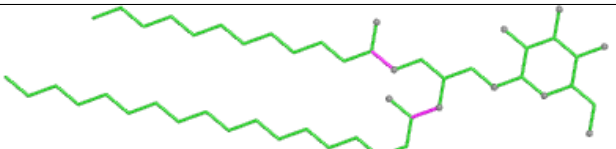
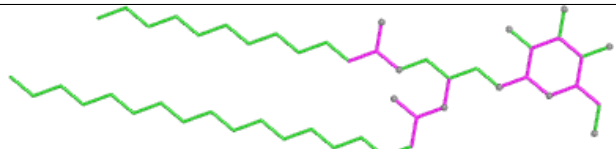
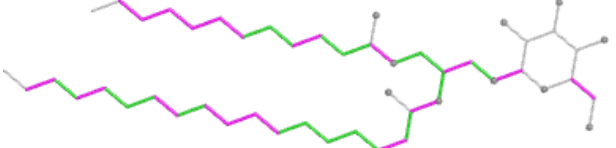
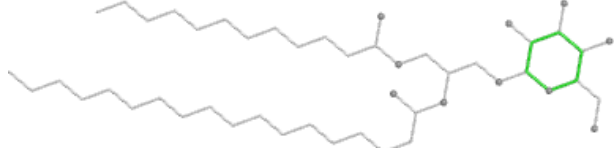
Bond angles

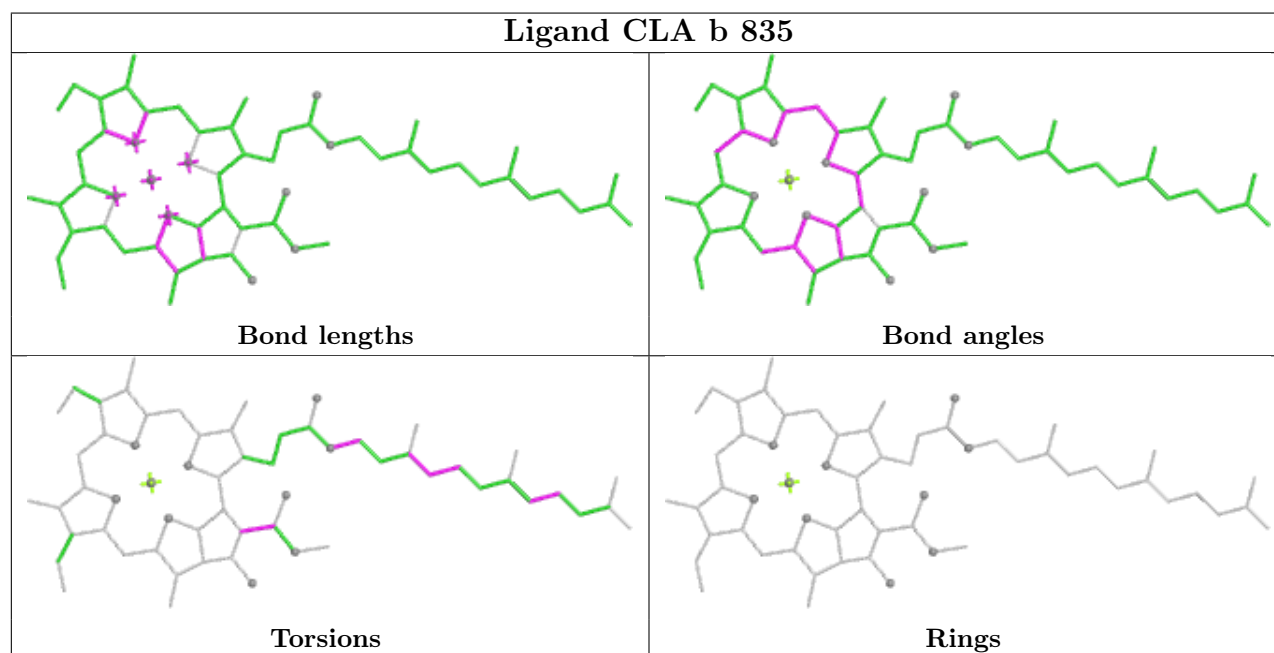
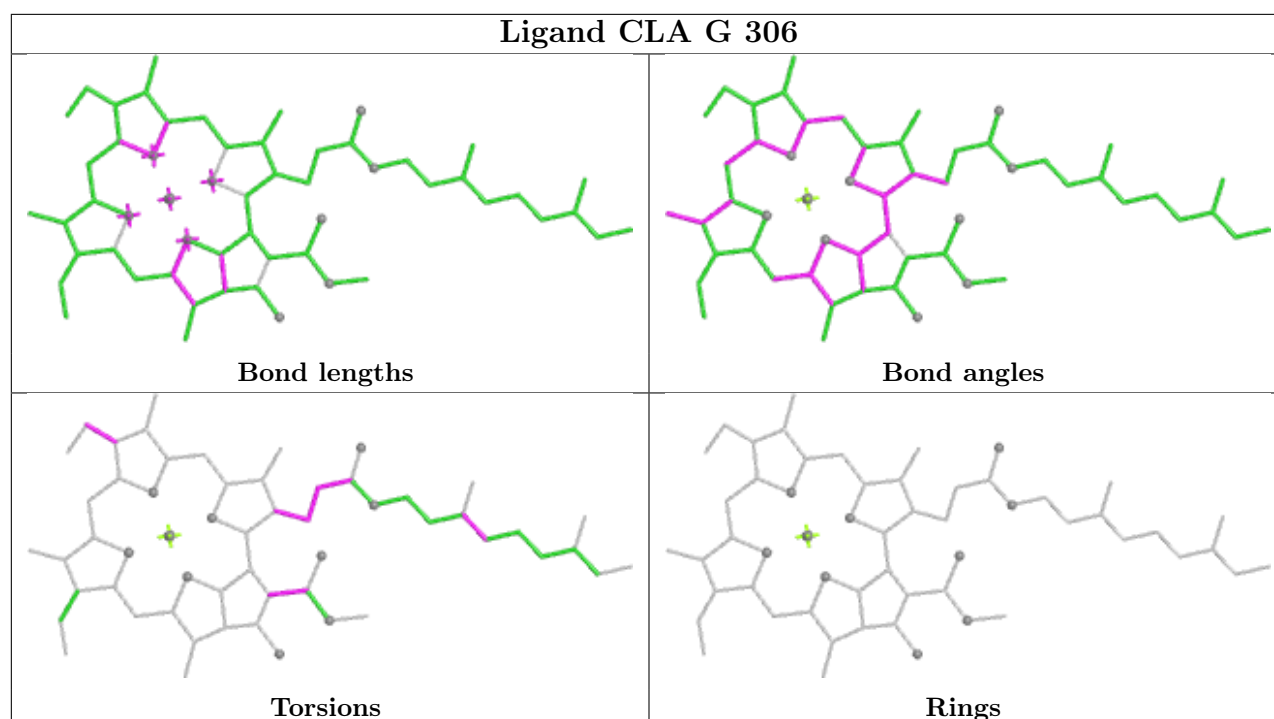


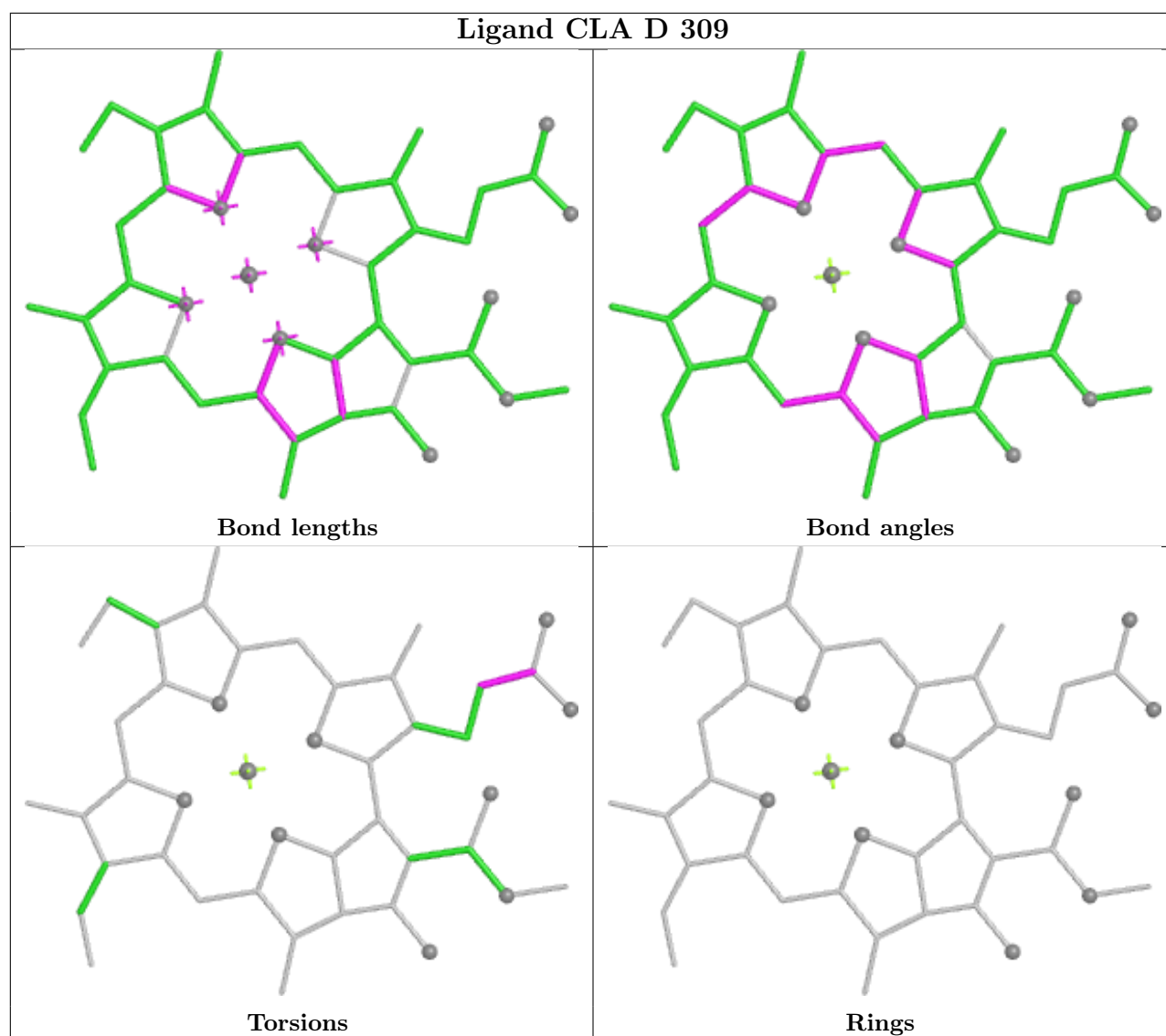
Torsions

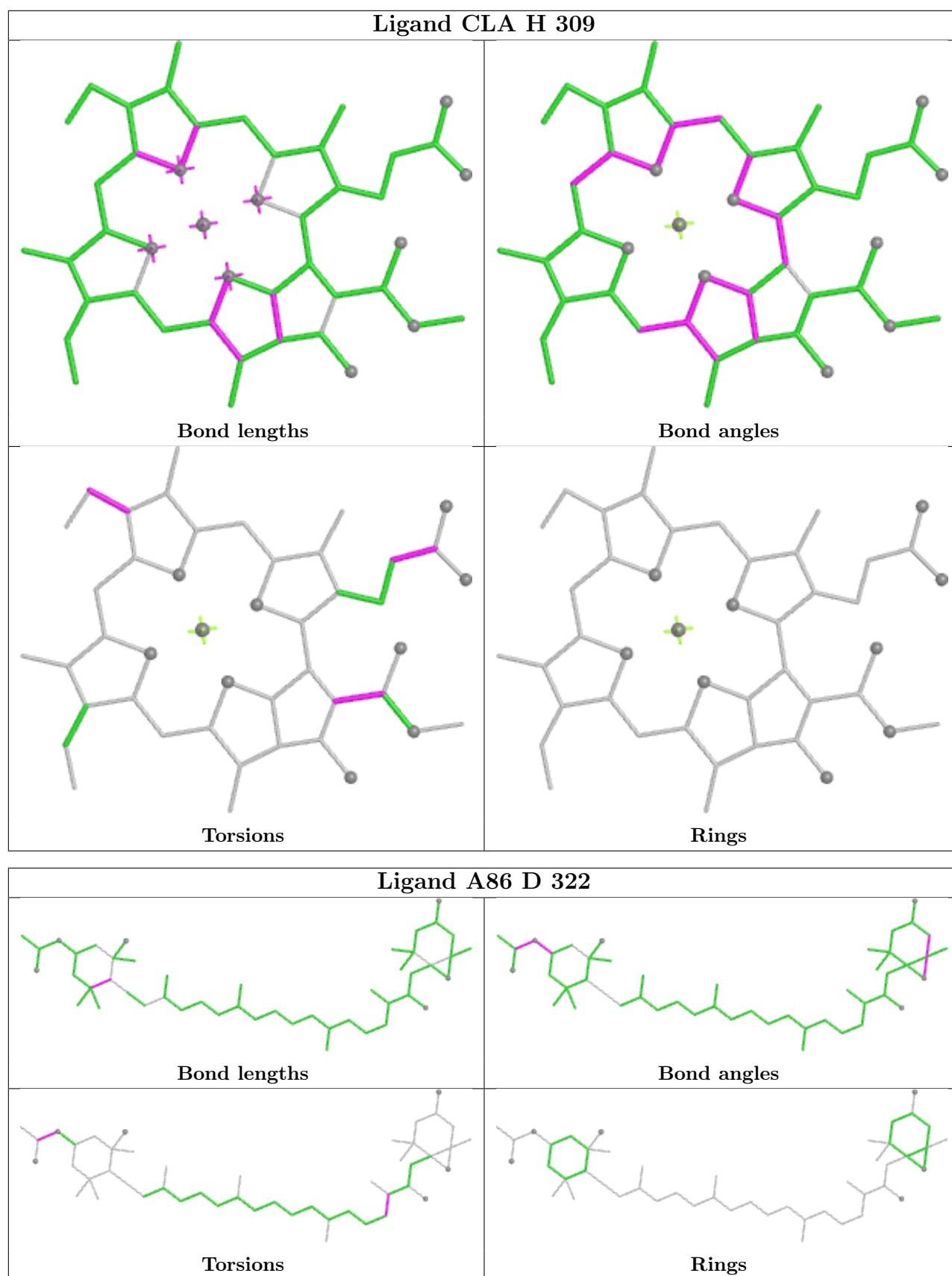


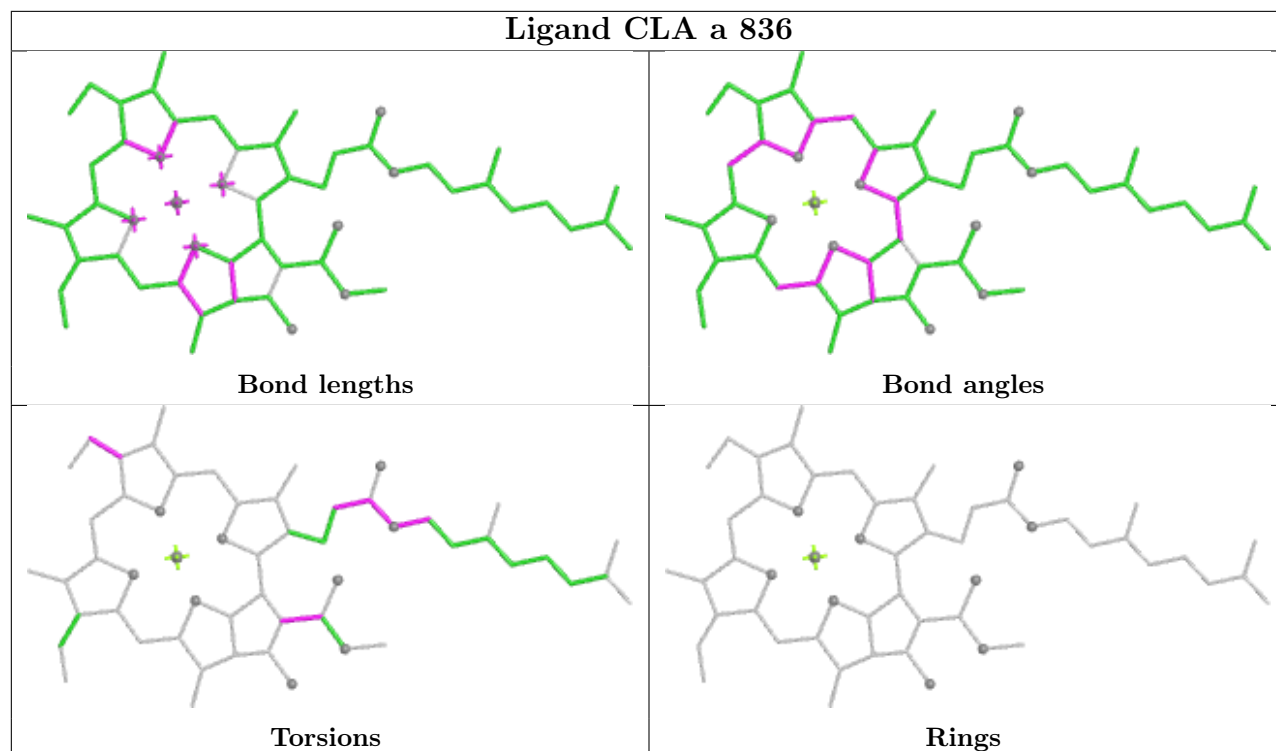
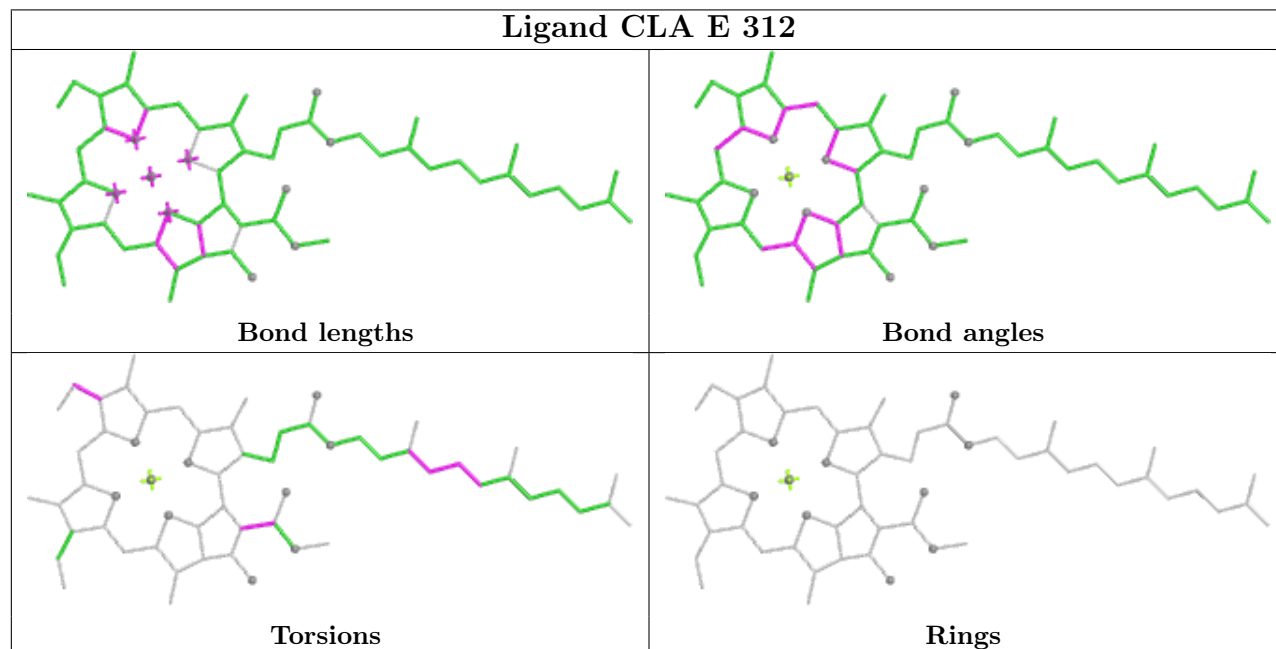
Rings

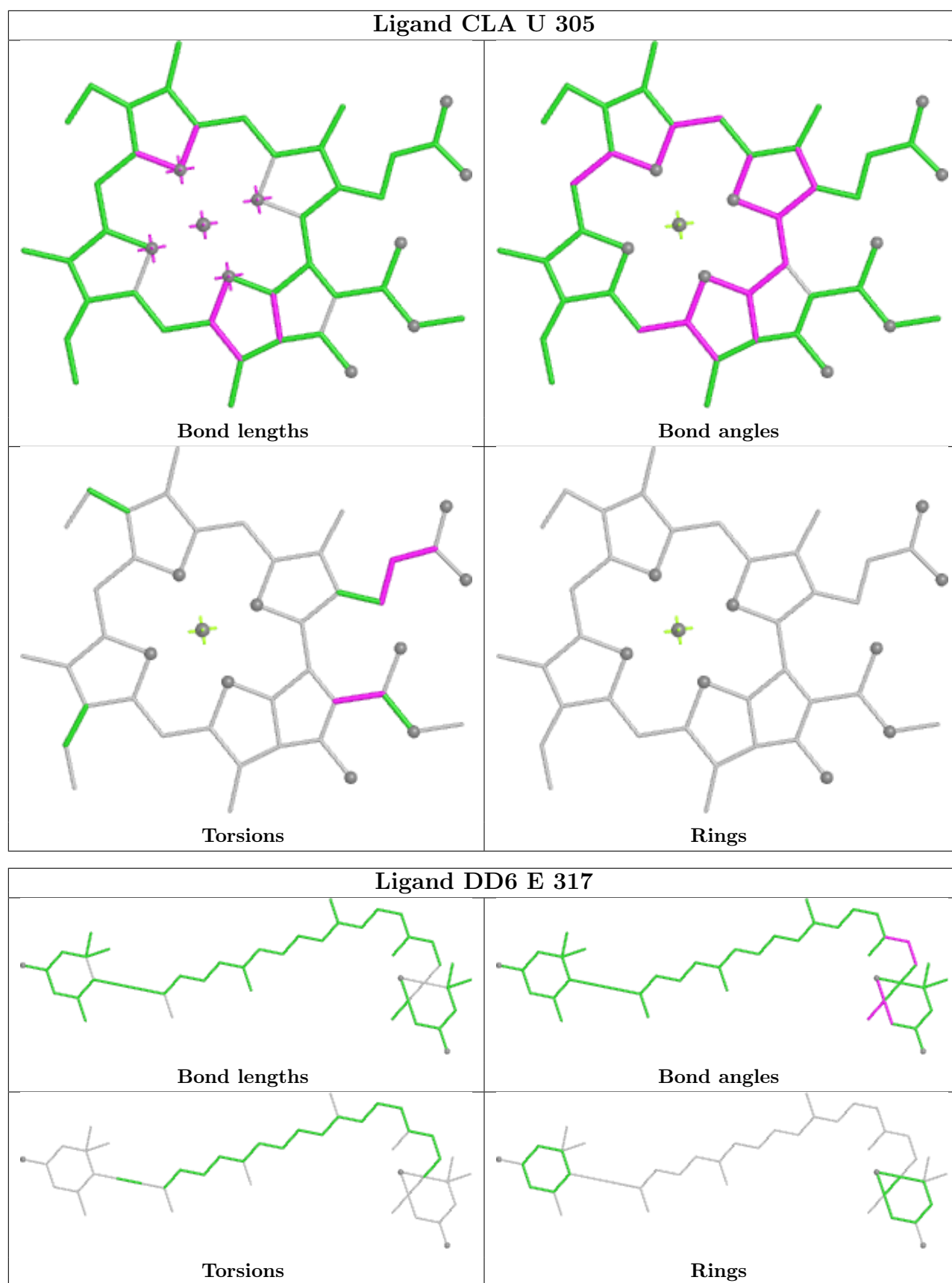
Ligand PQN b 847	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 204	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG l 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

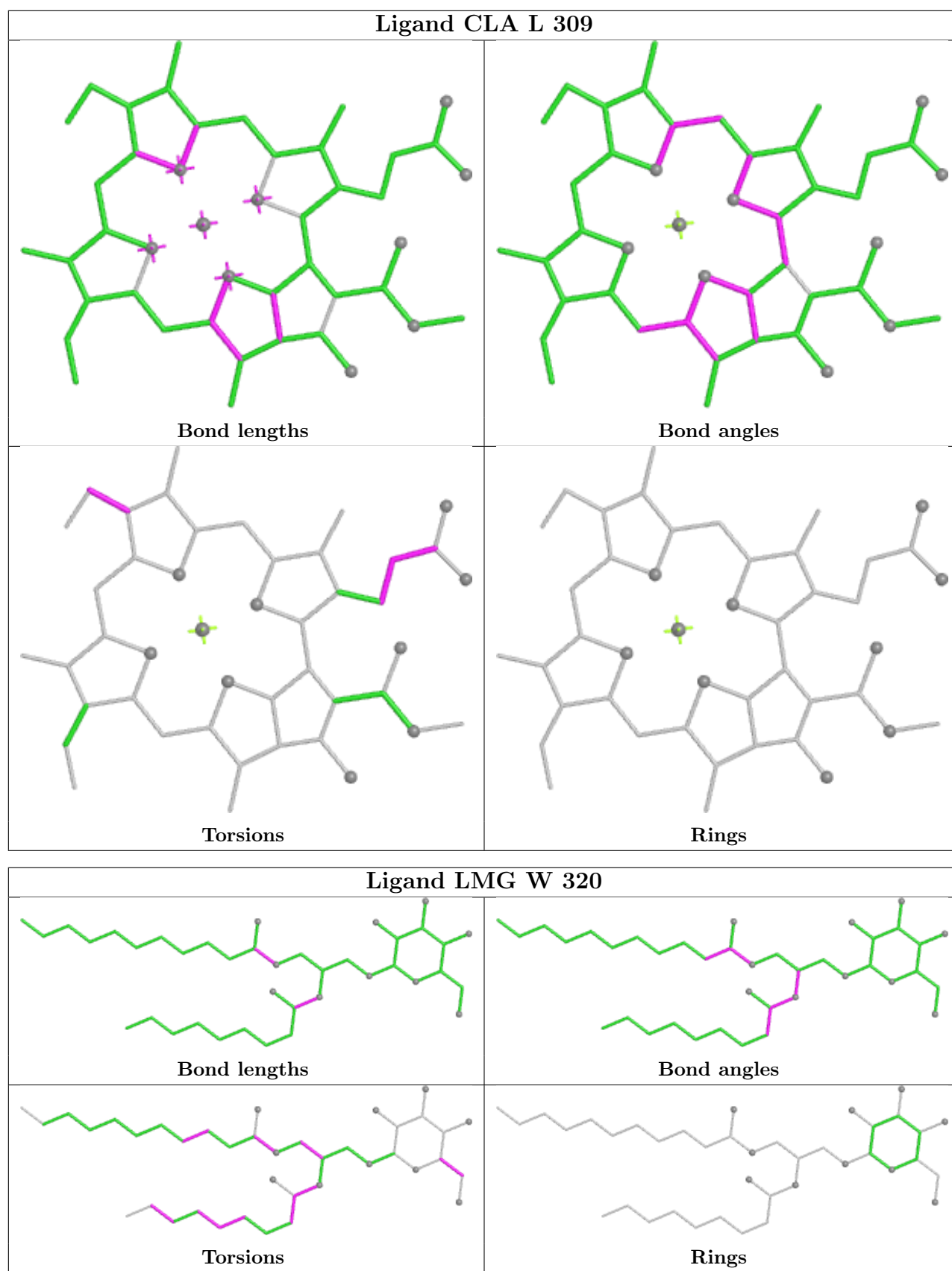


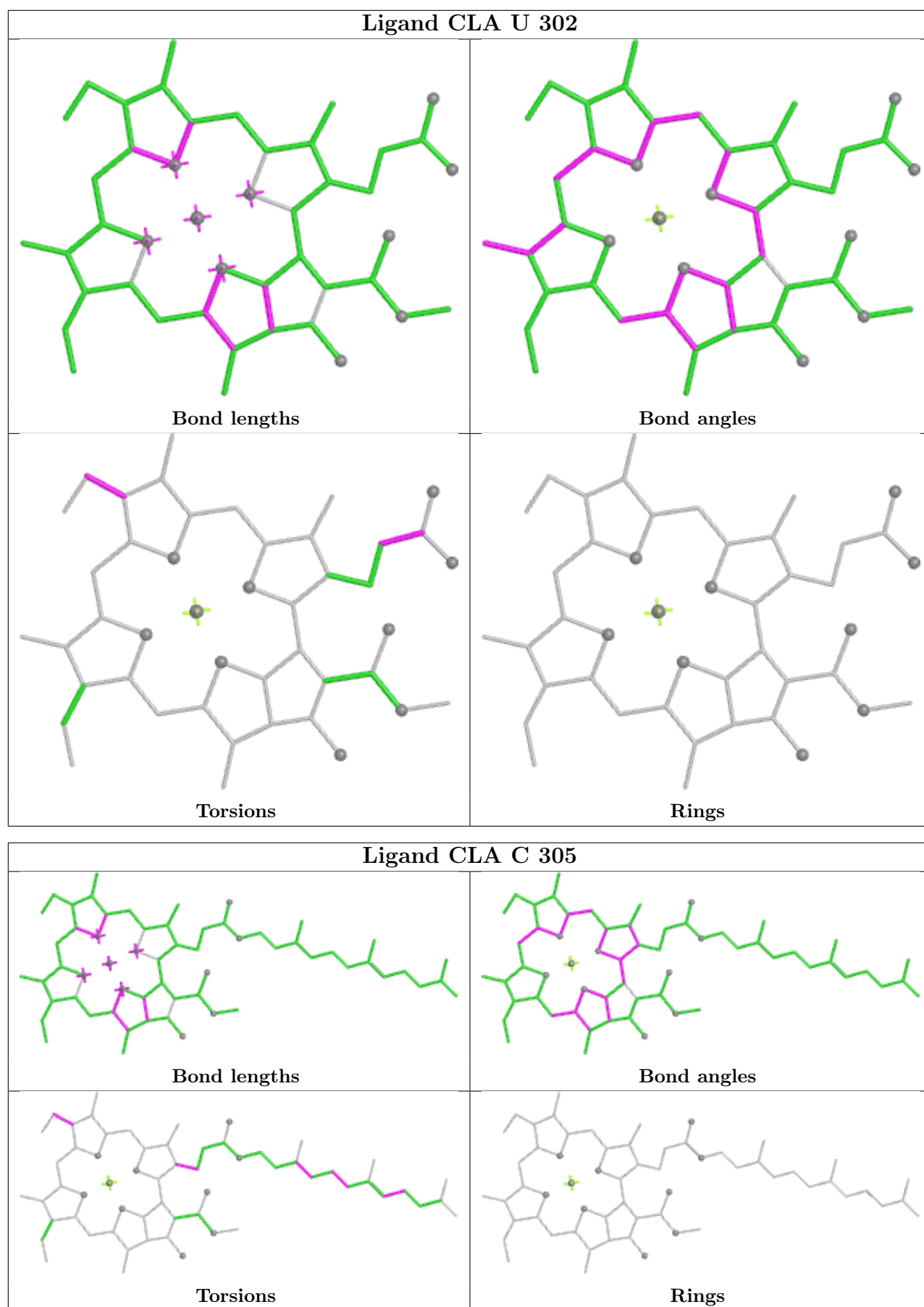


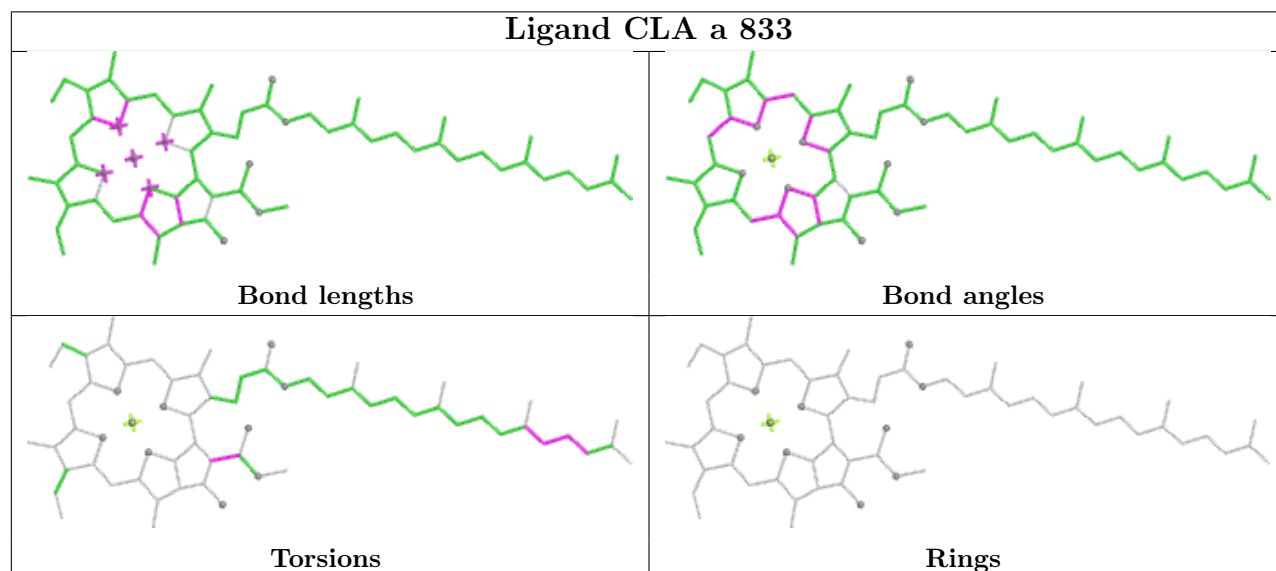
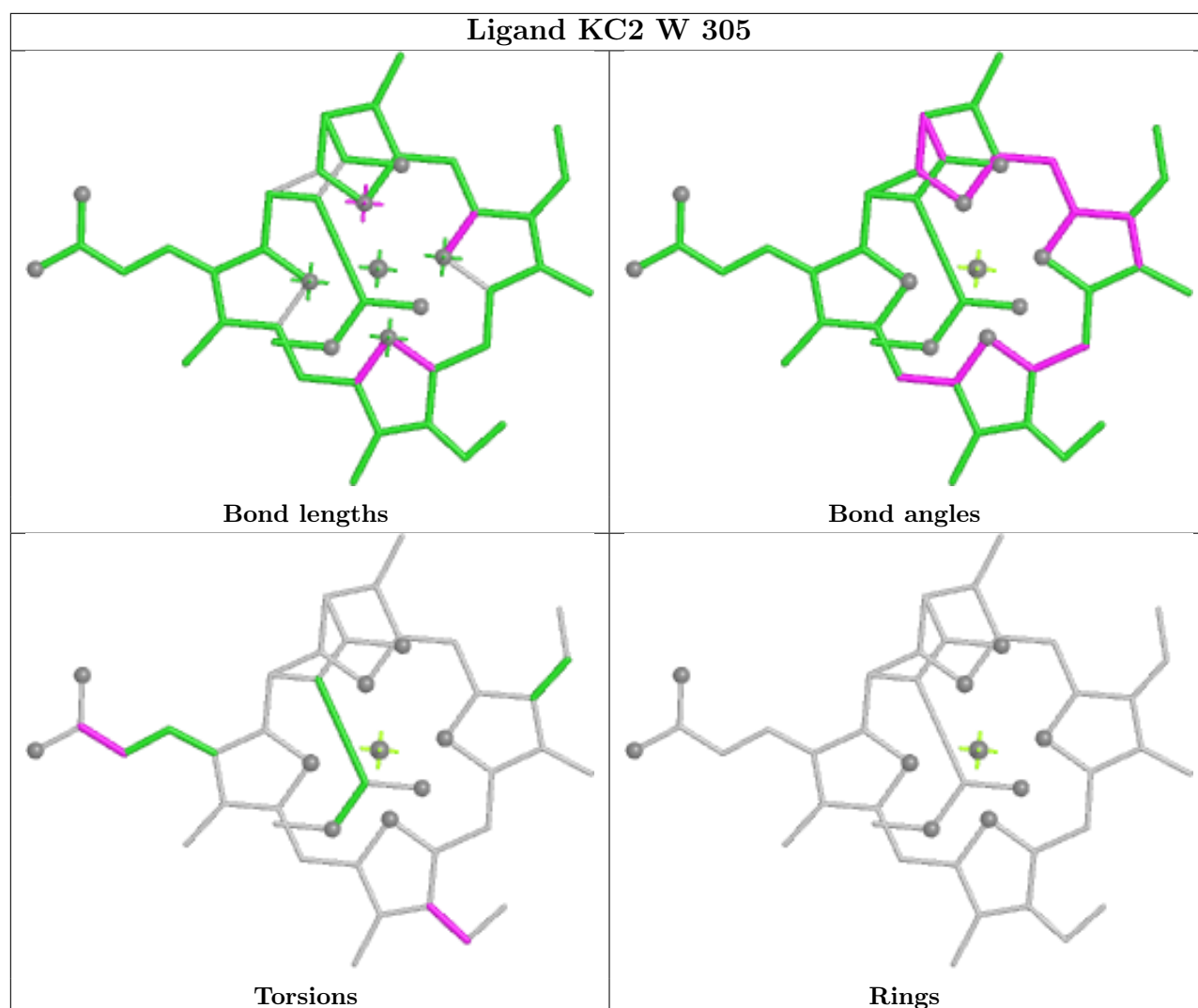


Ligand CLA a 836**Ligand CLA E 312**

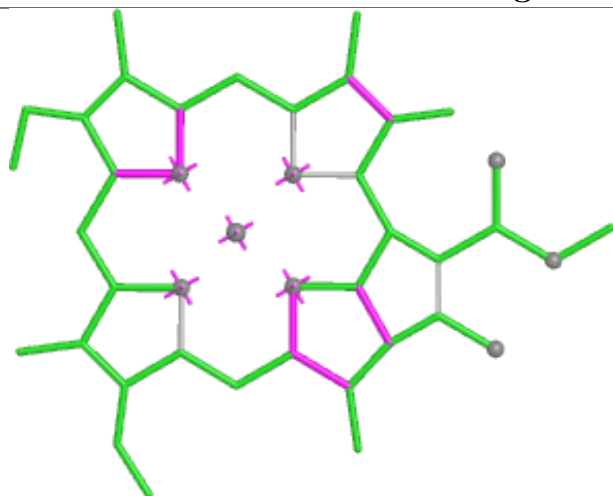




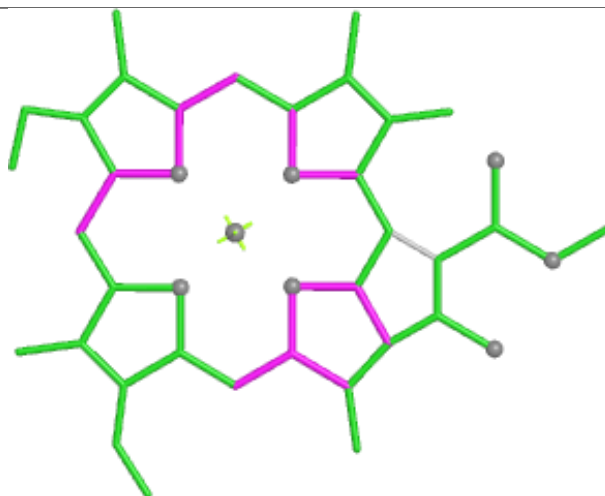




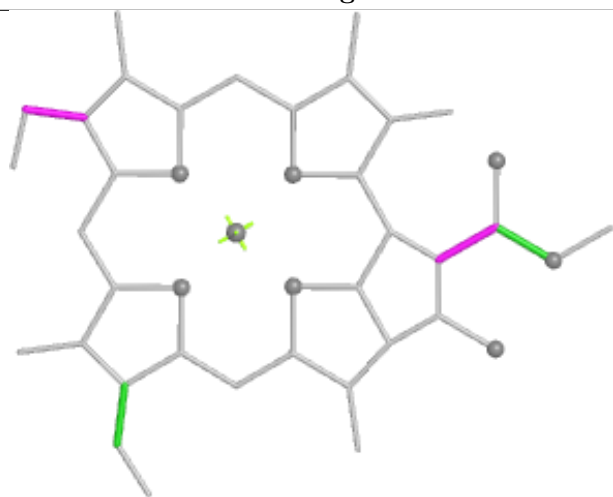
Ligand CLA R 309



Bond lengths



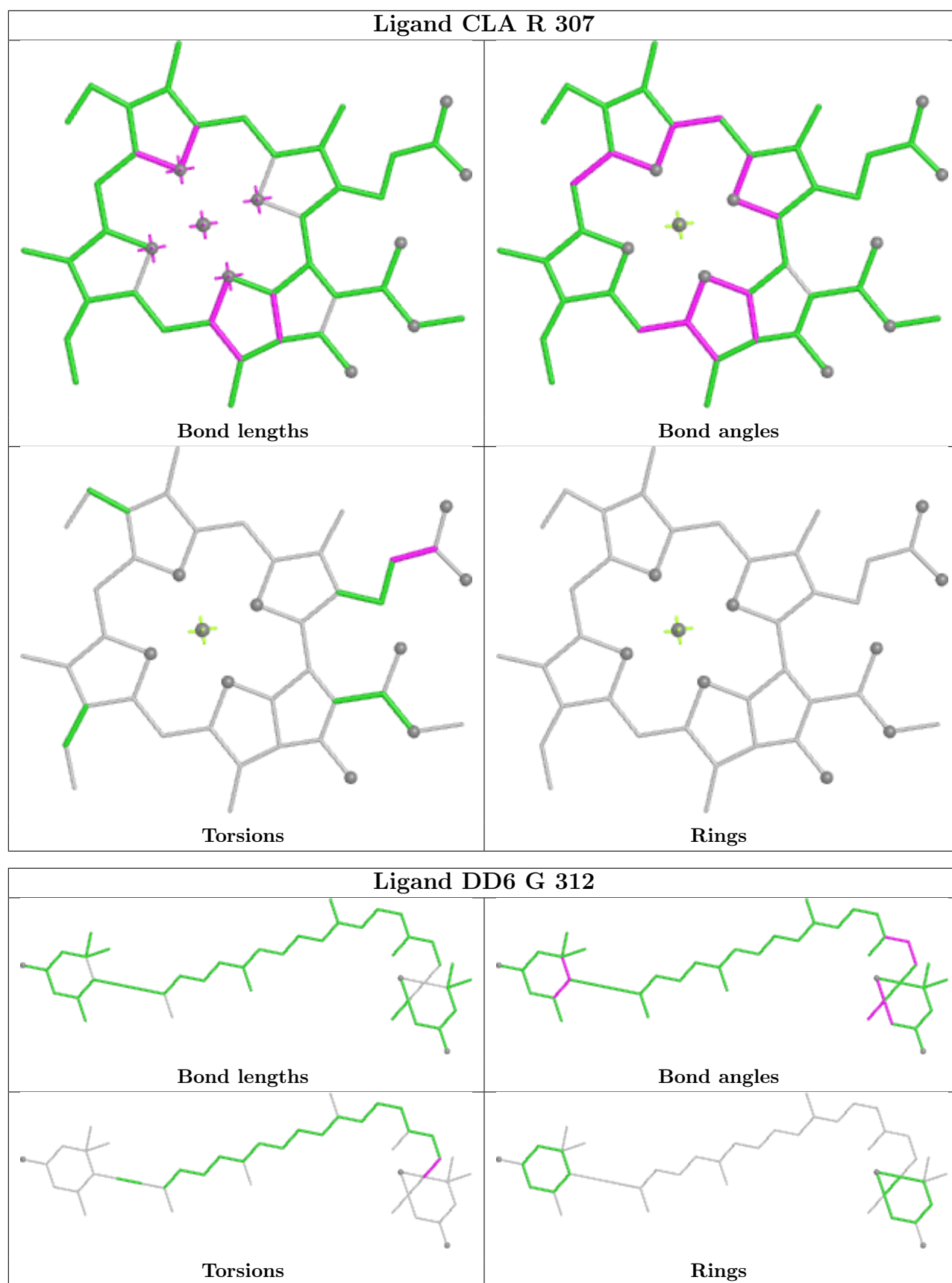
Bond angles

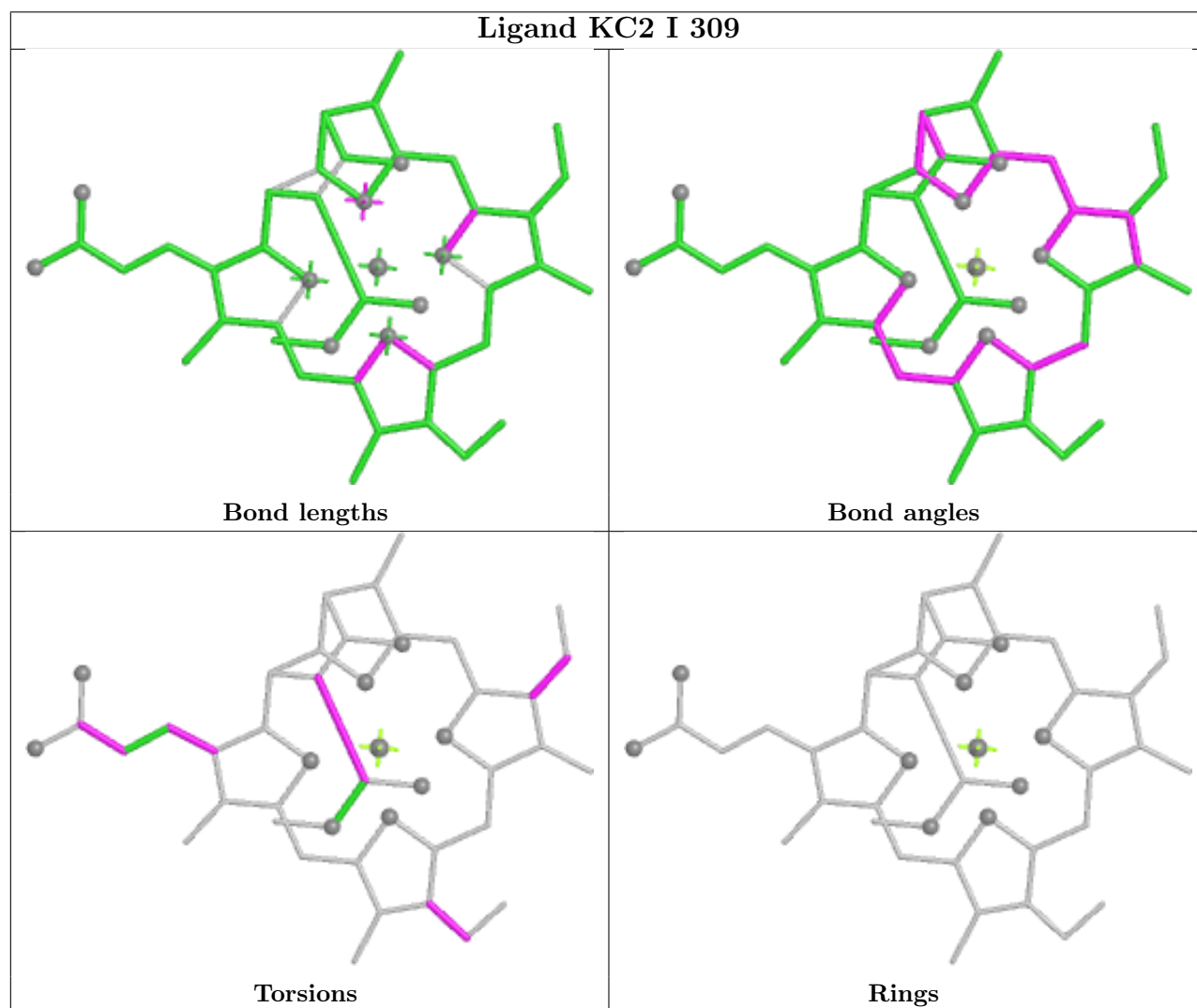
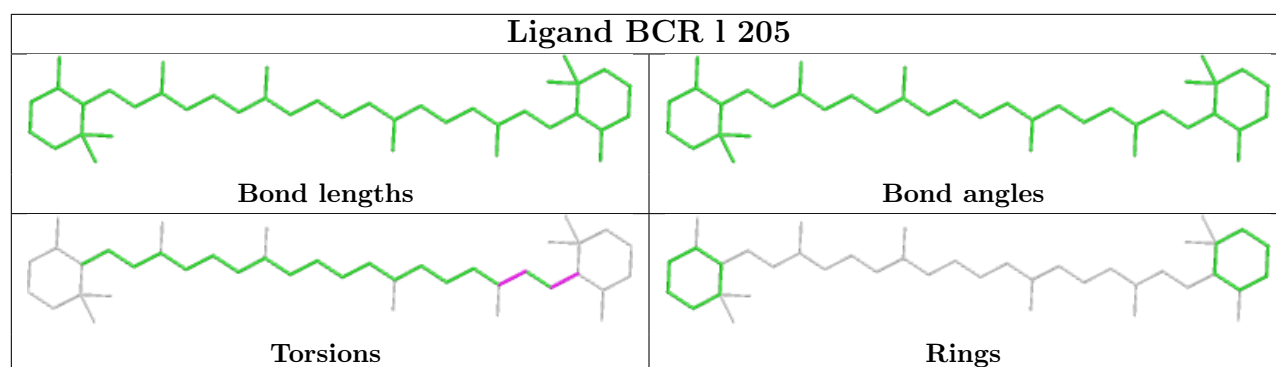


Torsions

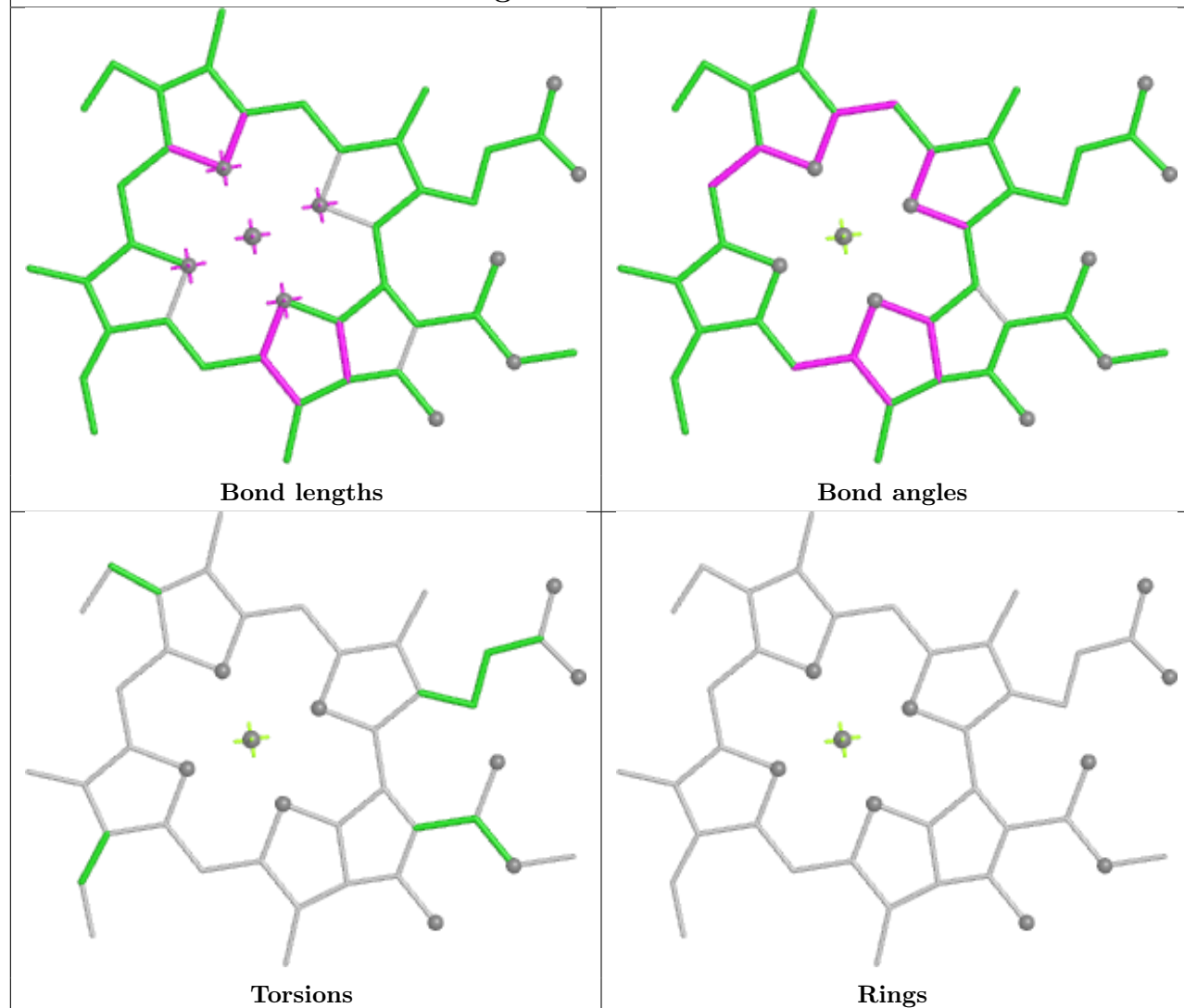


Rings

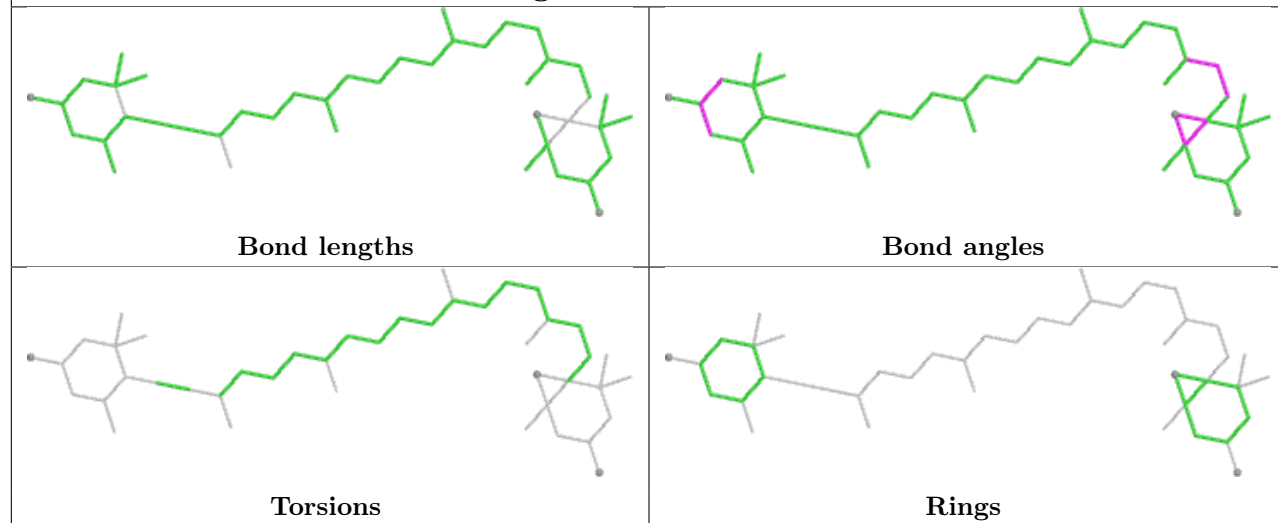


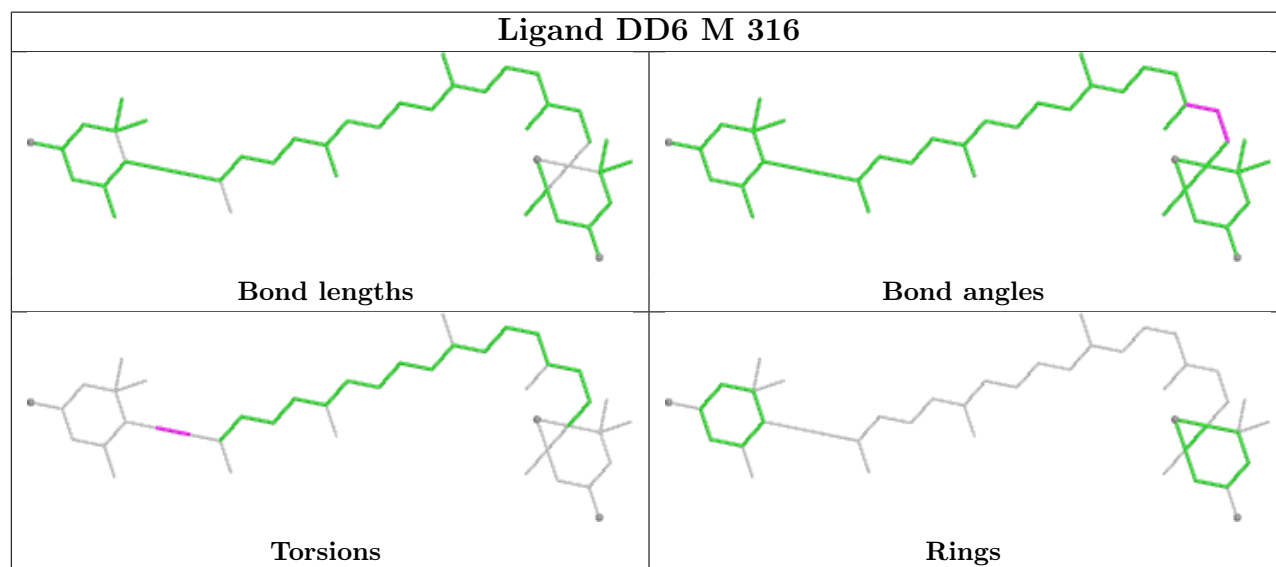
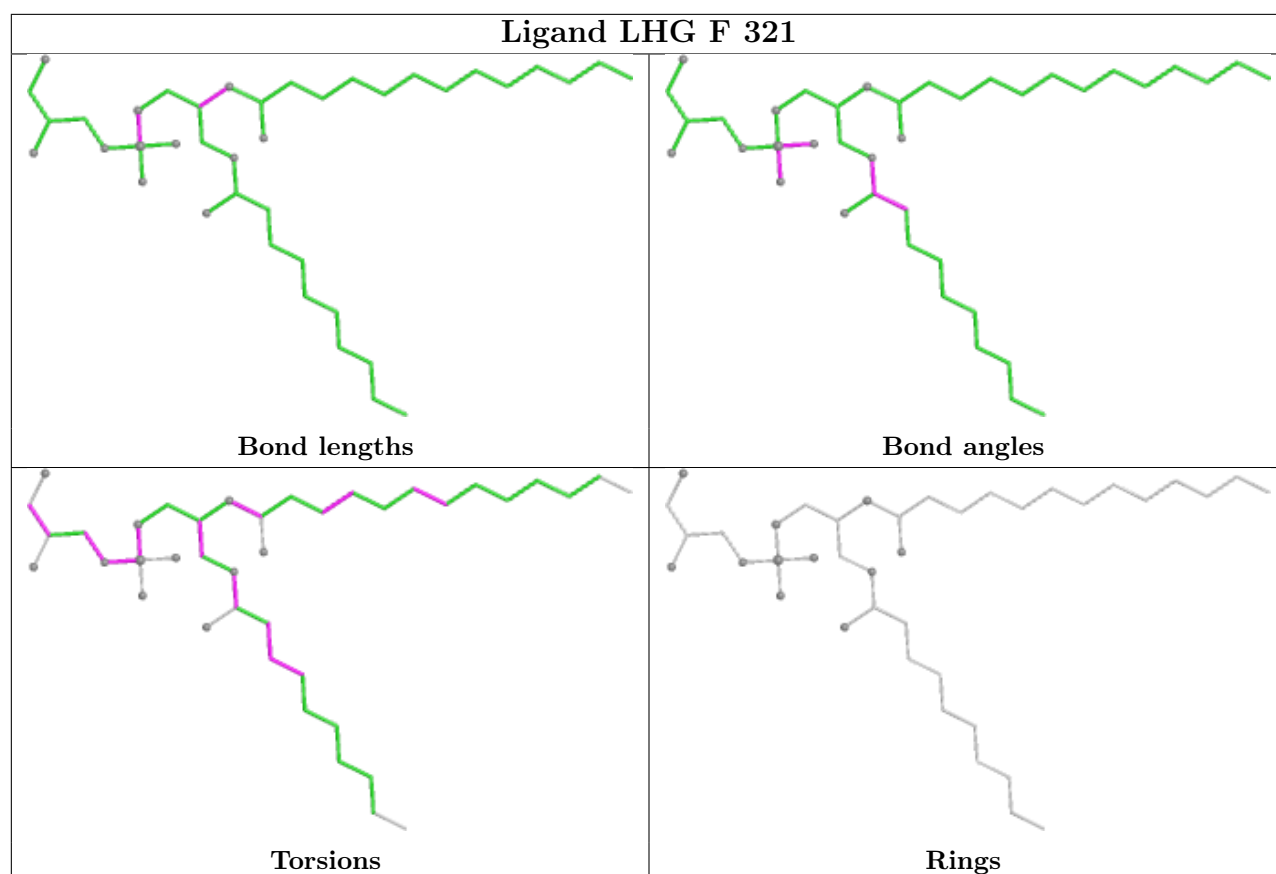


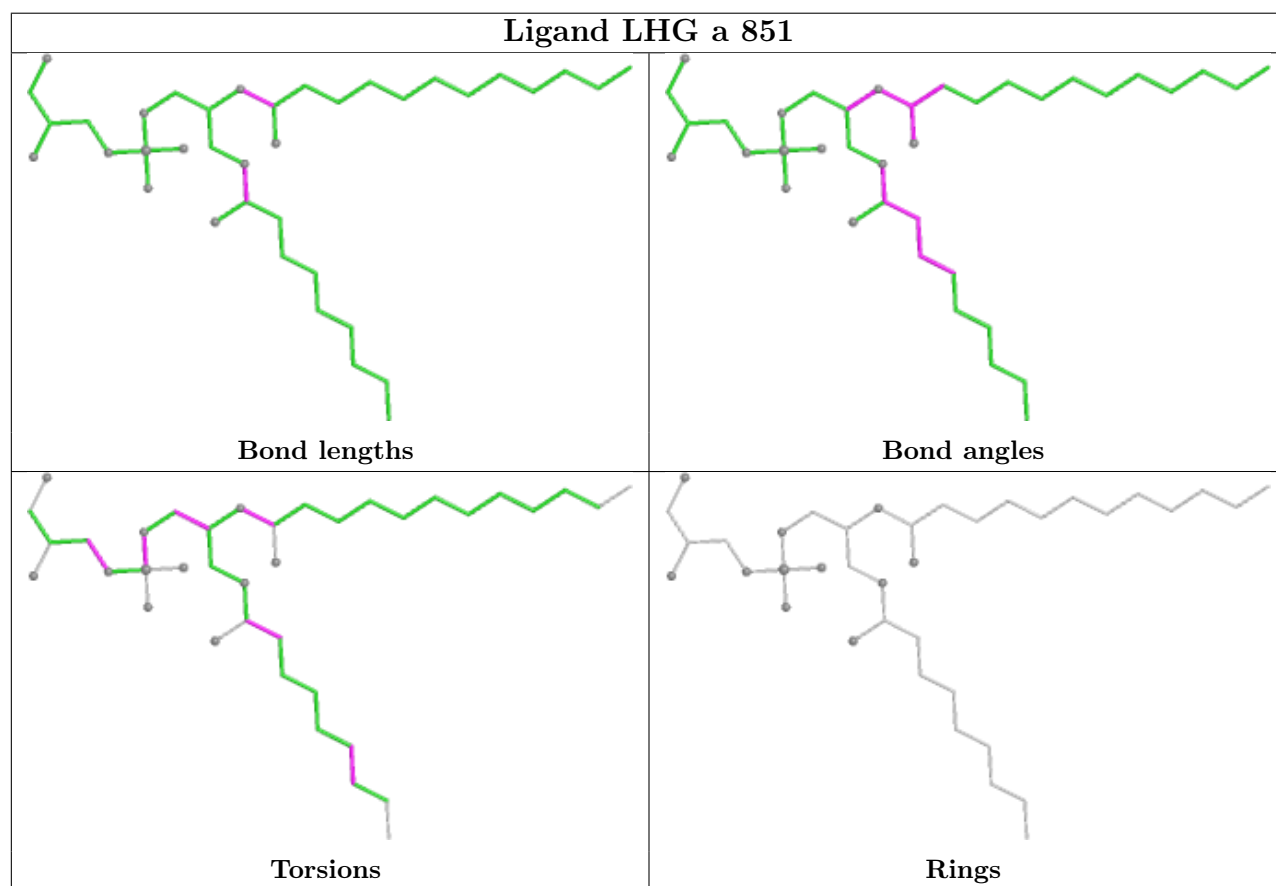
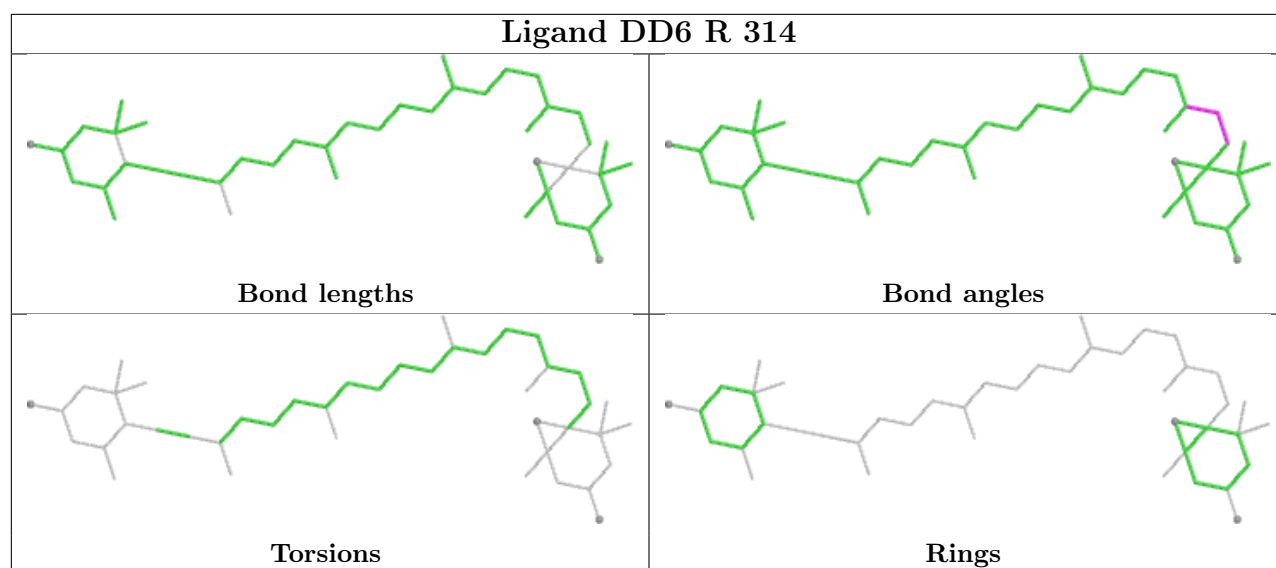
Ligand CLA F 311

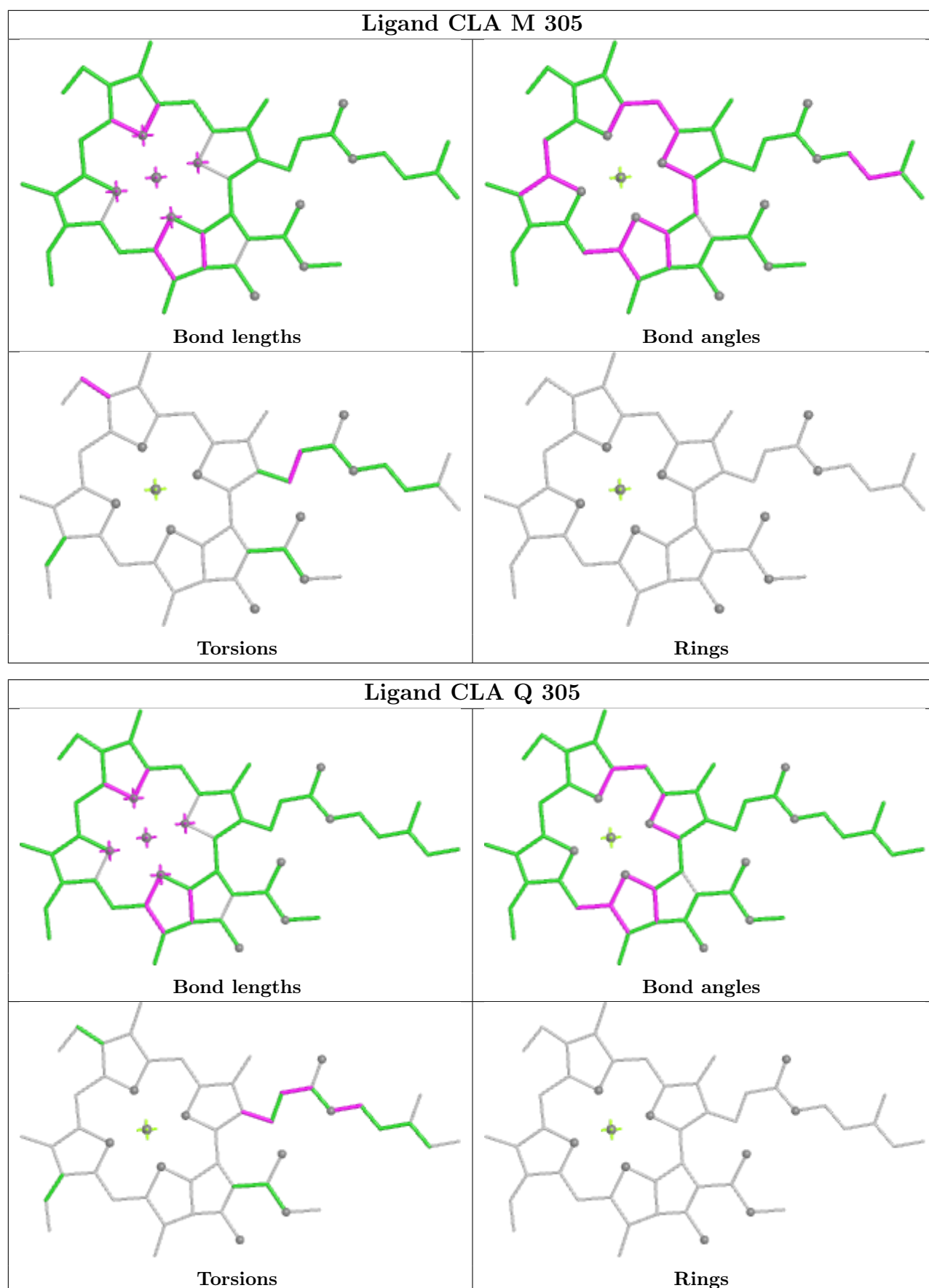


Ligand DD6 D 317

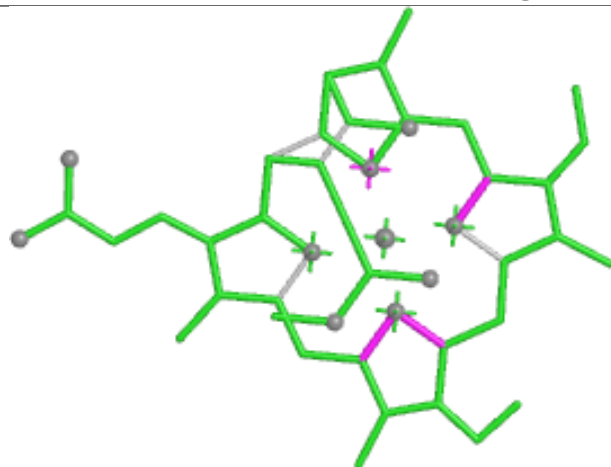




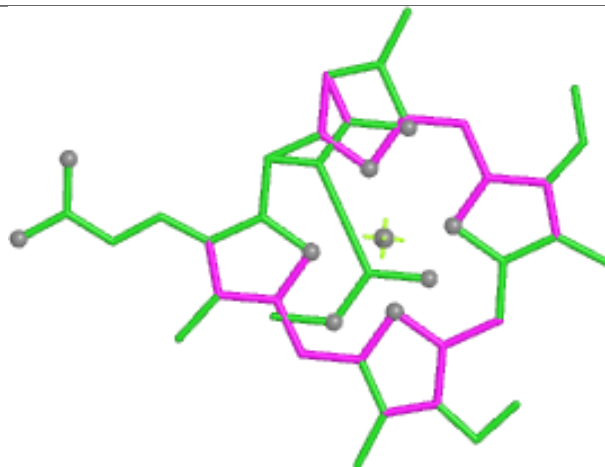




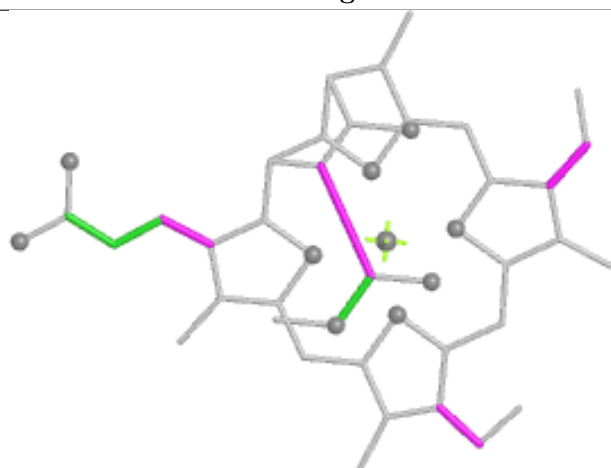
Ligand KC2 T 311



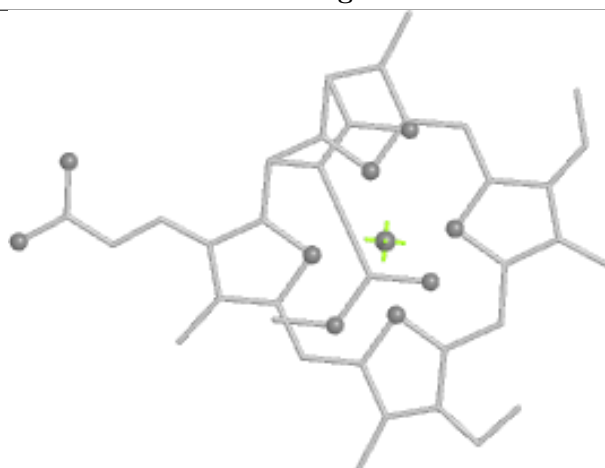
Bond lengths



Bond angles

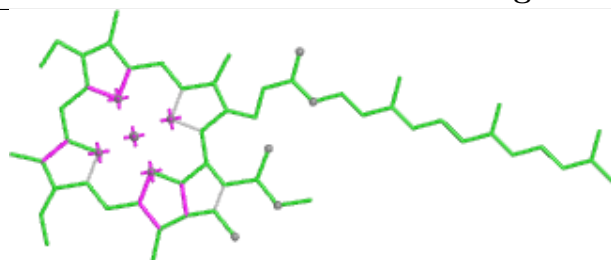


Torsions

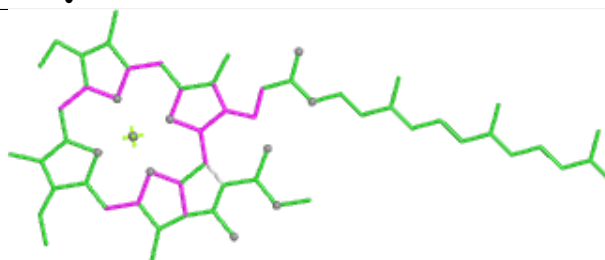


Rings

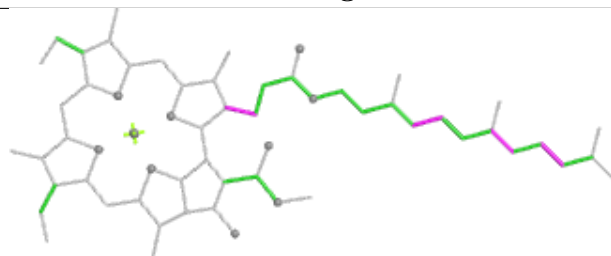
Ligand CLA Q 303



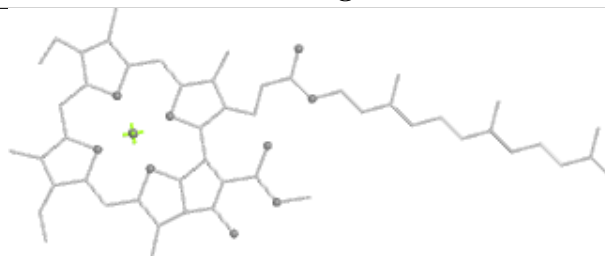
Bond lengths



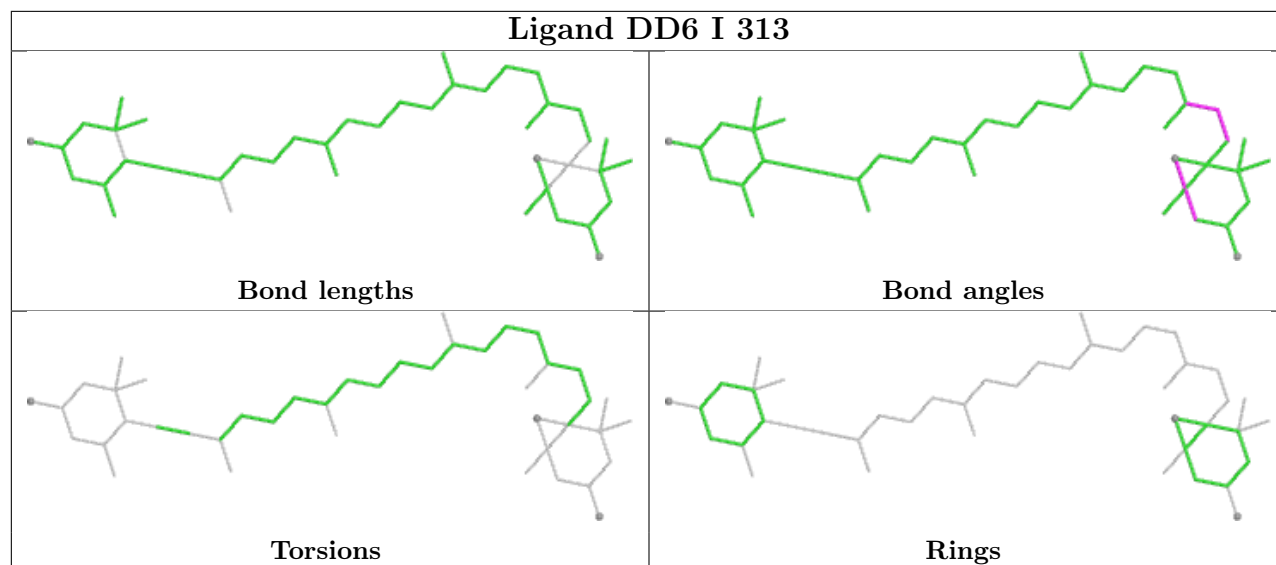
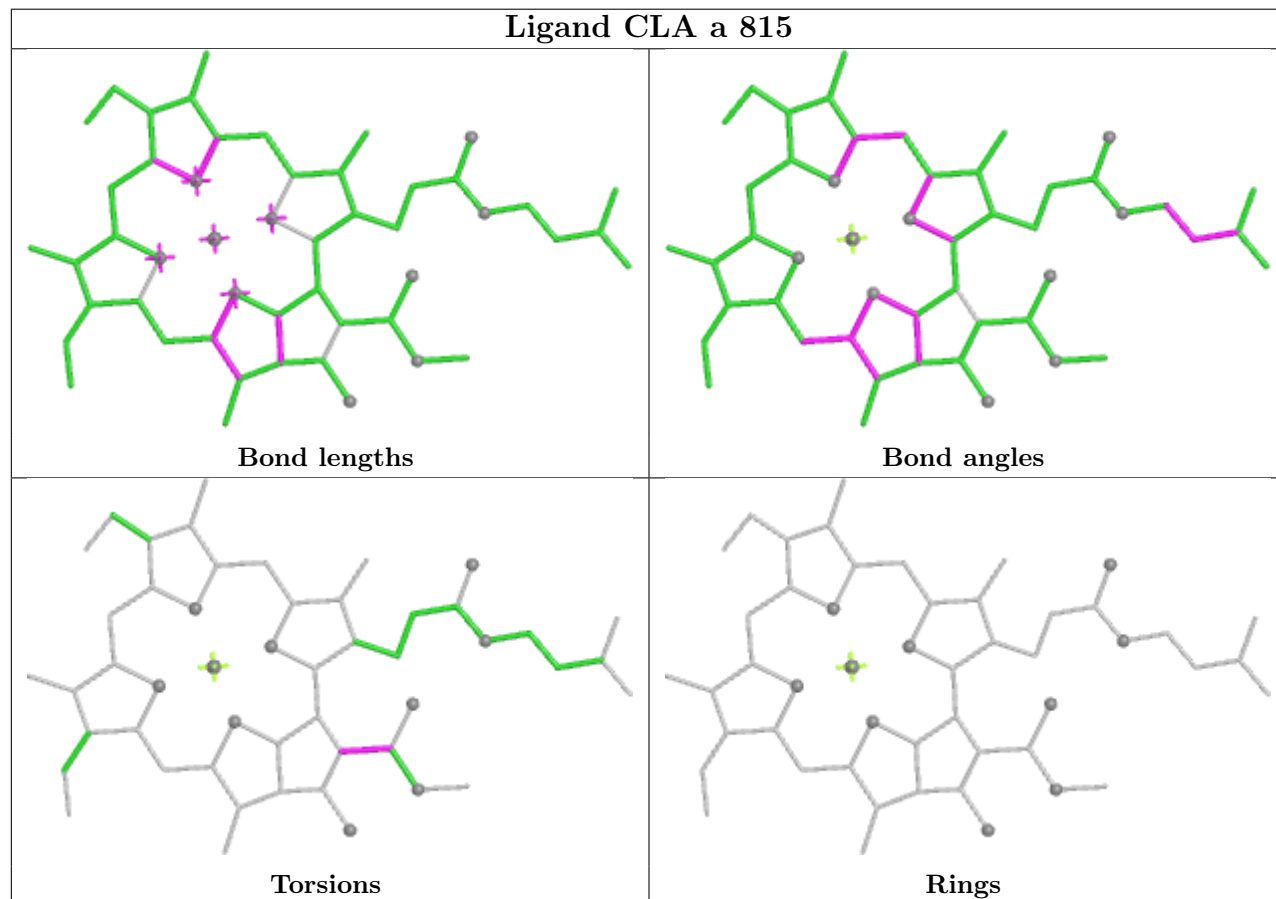
Bond angles

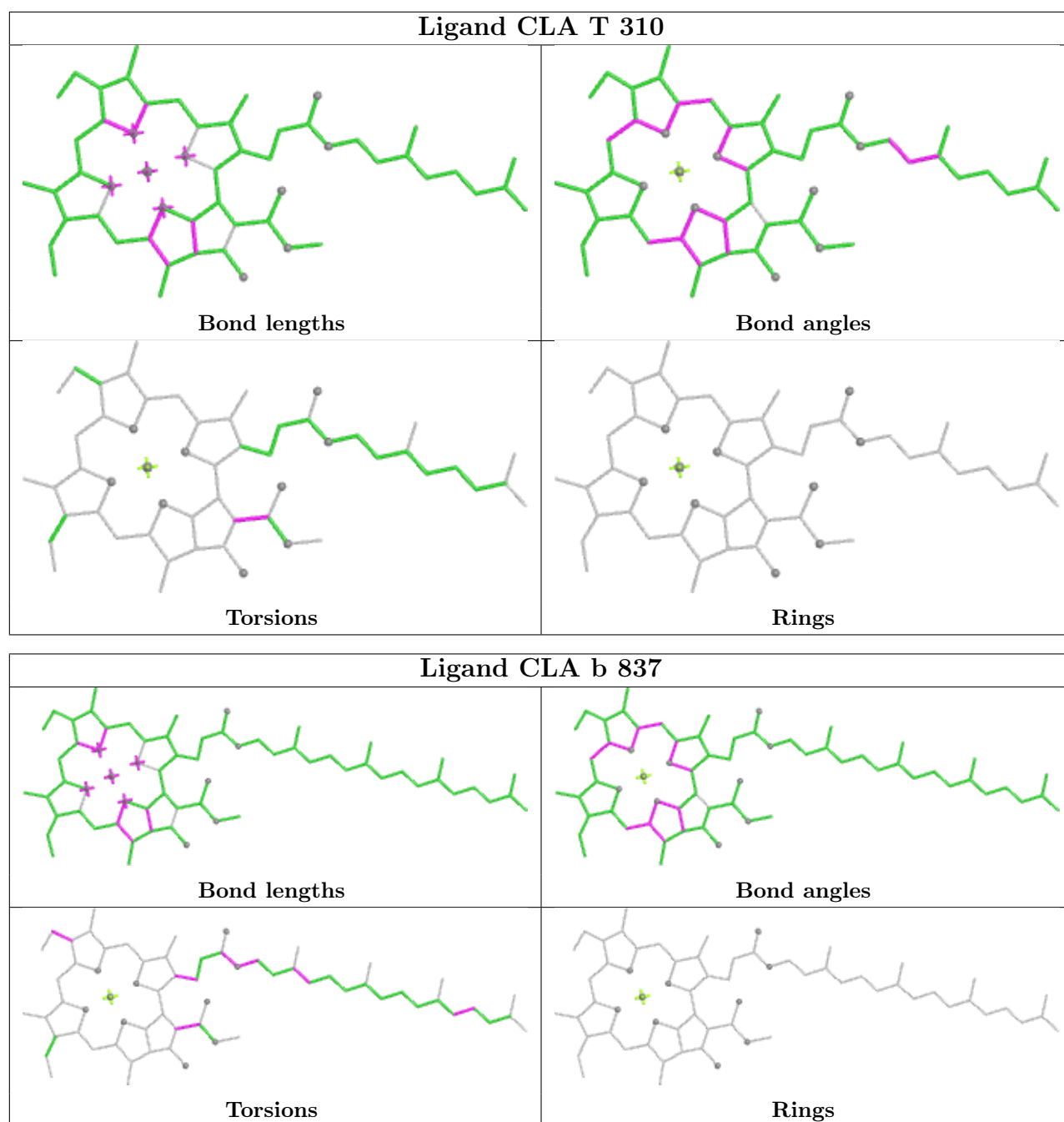


Torsions

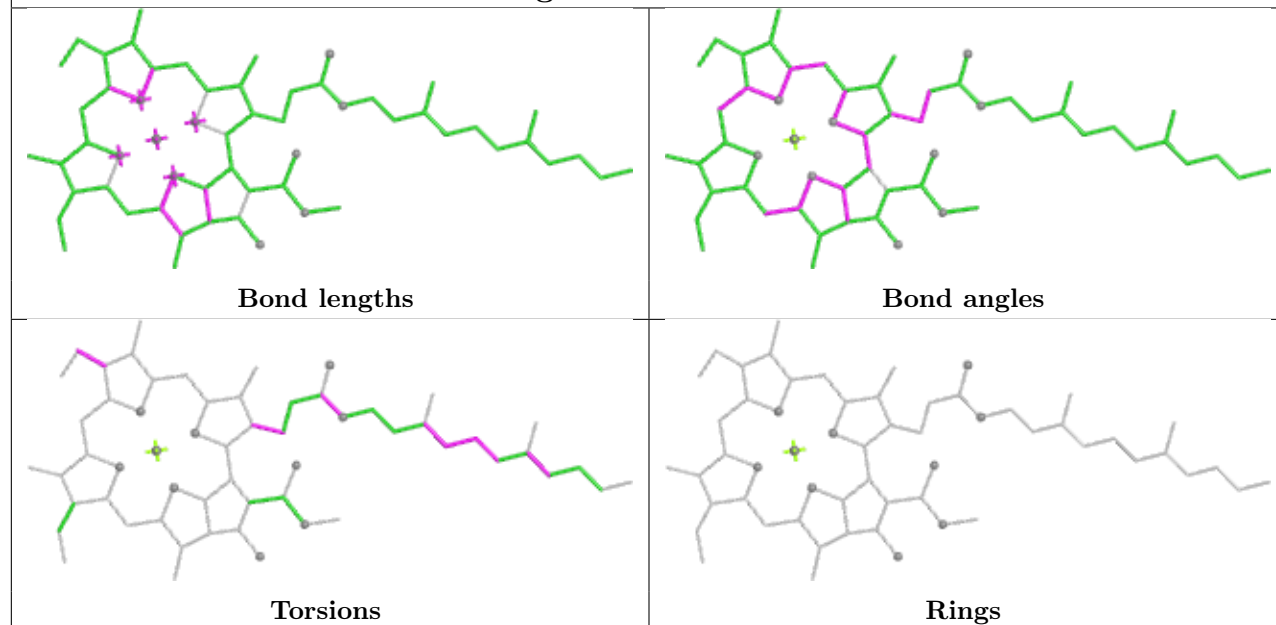


Rings

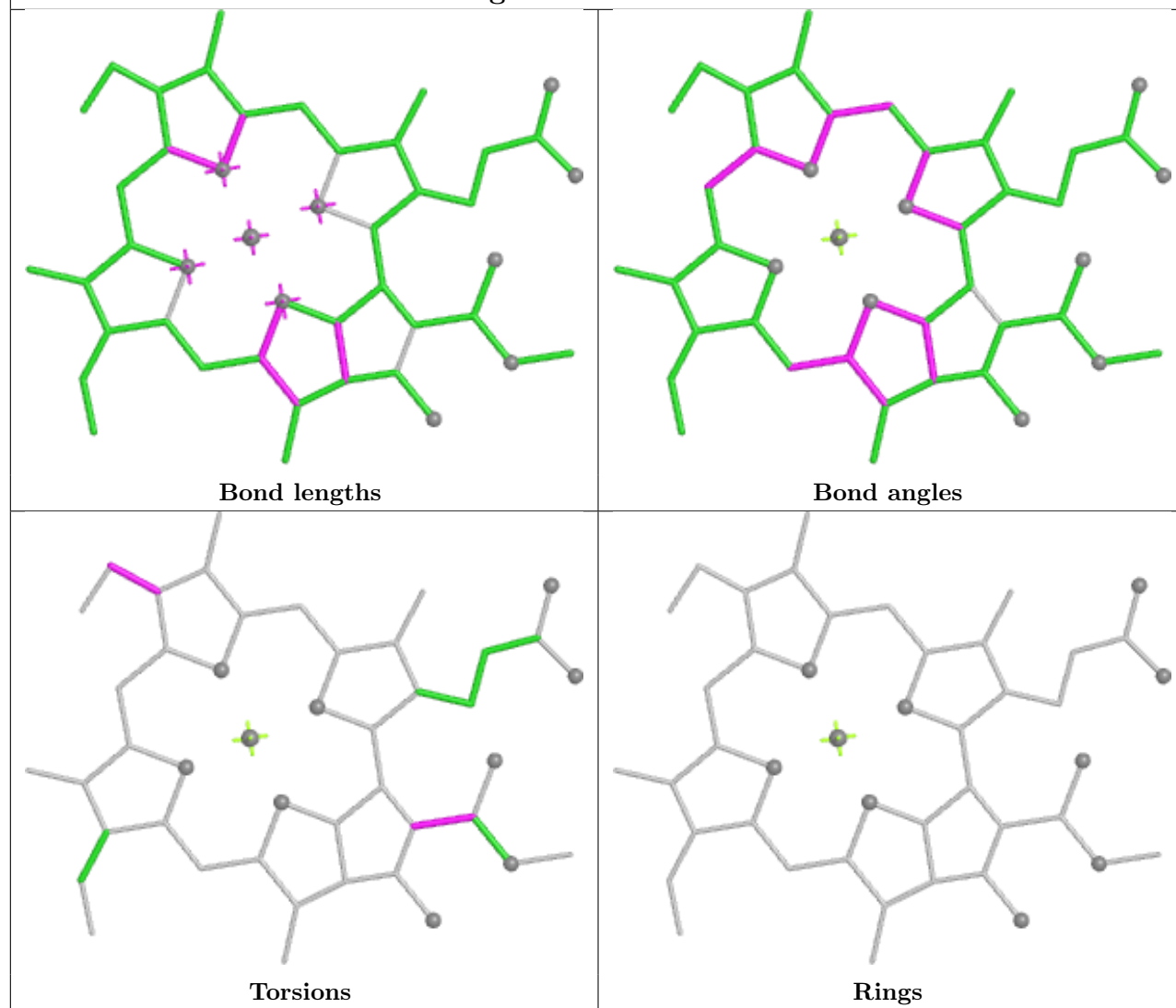
Ligand DD6 I 313**Ligand CLA a 815**

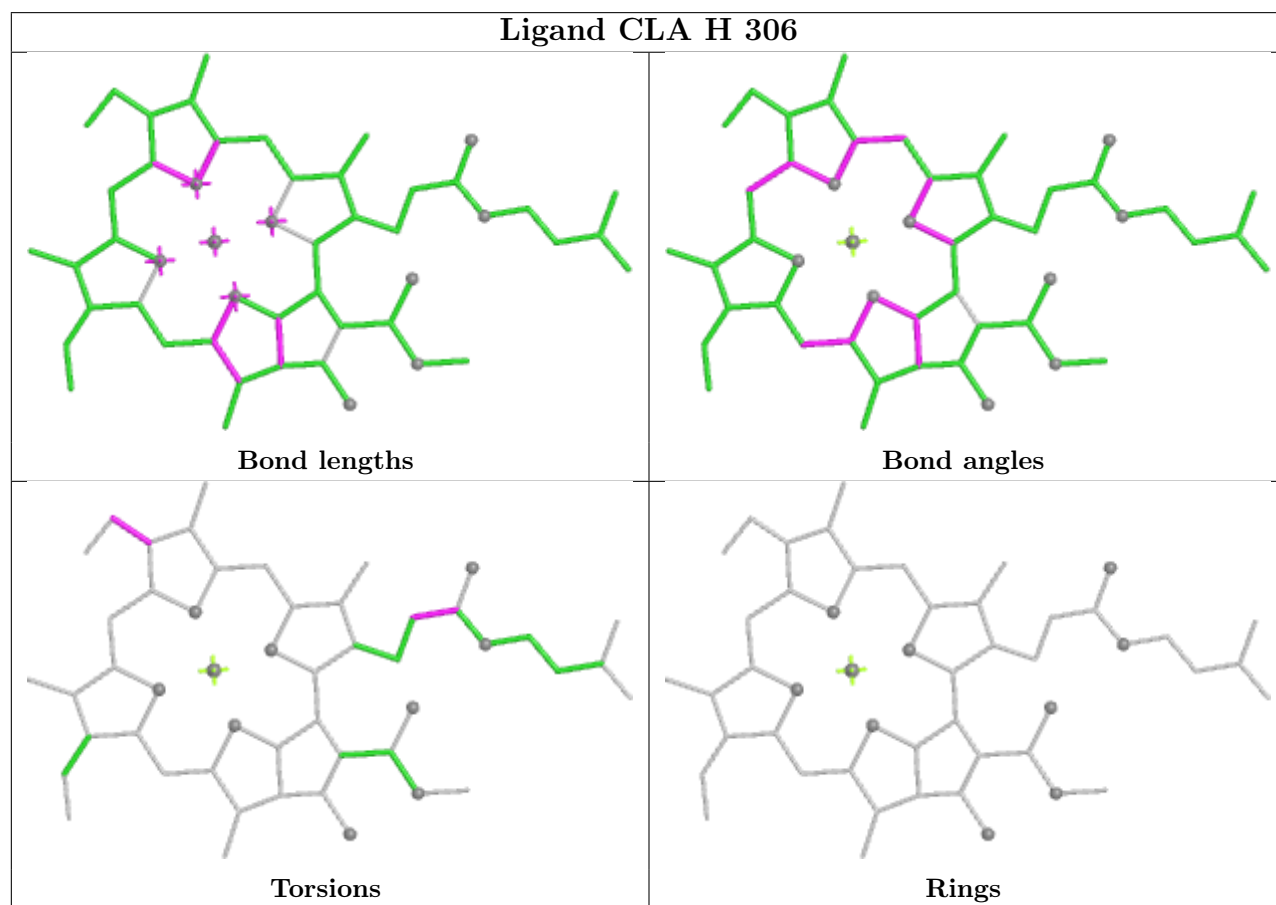
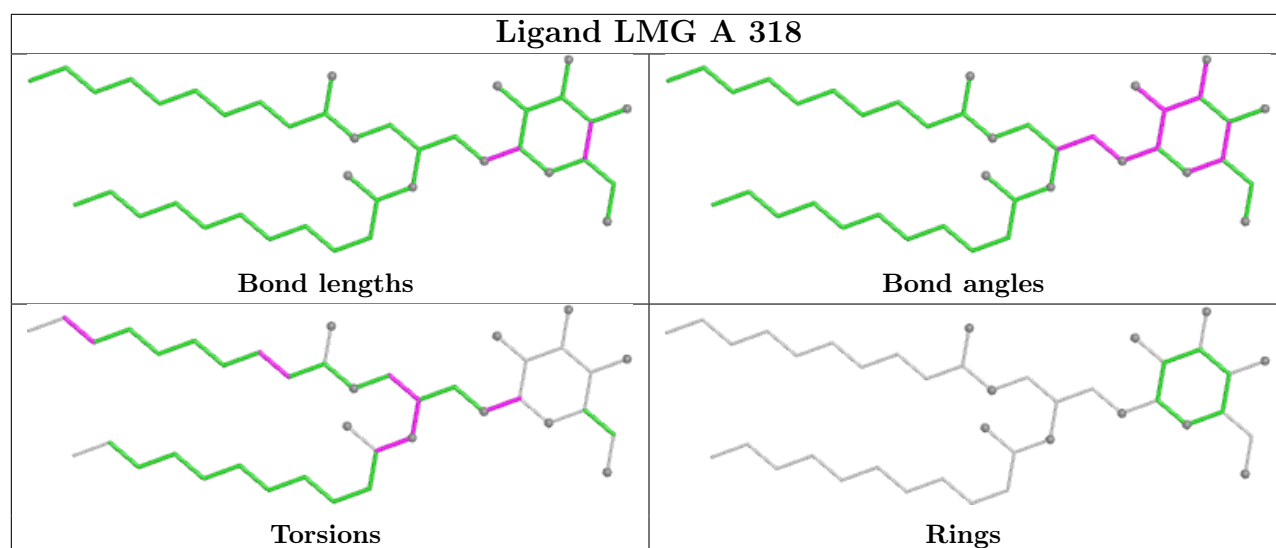


Ligand CLA J 312

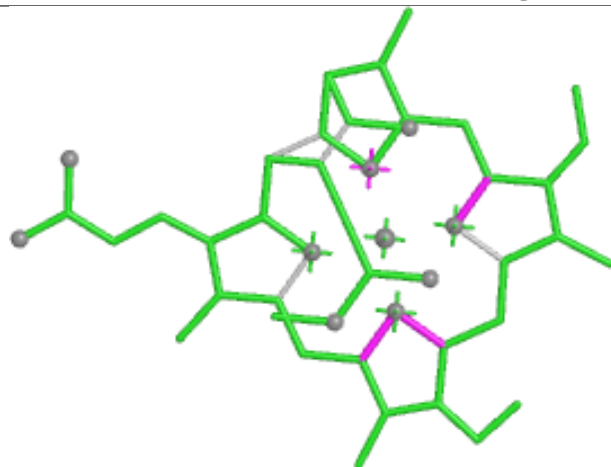


Ligand CLA K 301

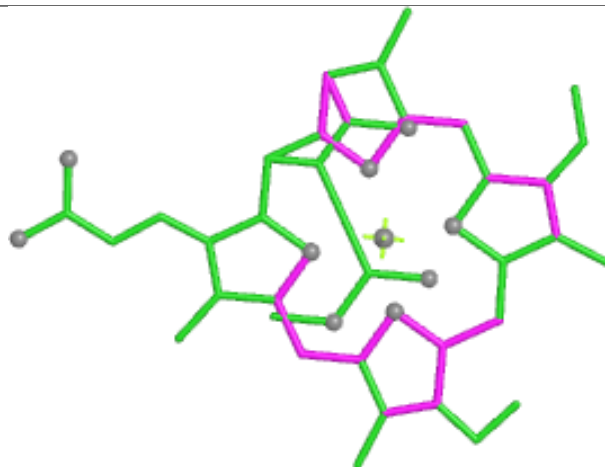




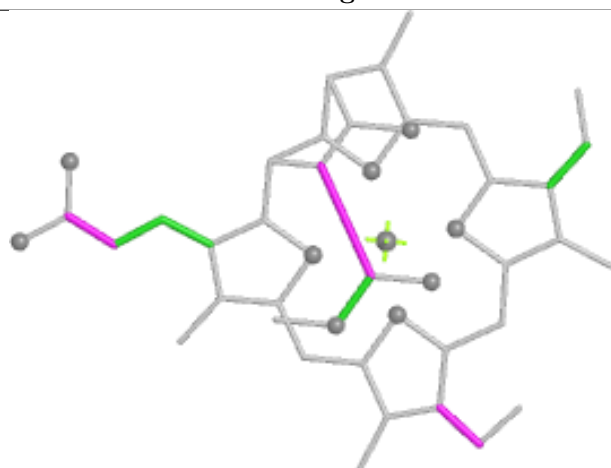
Ligand KC2 N 302



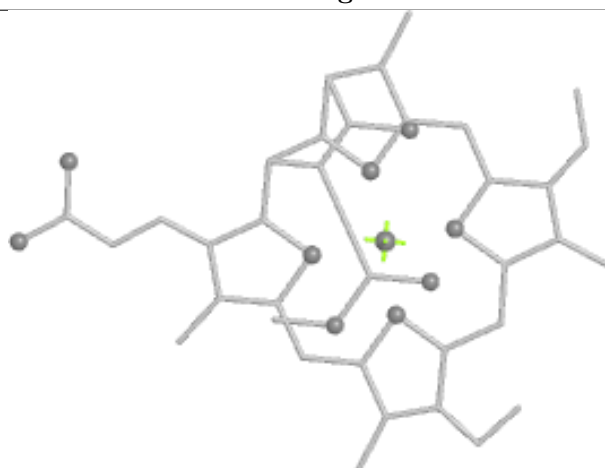
Bond lengths



Bond angles

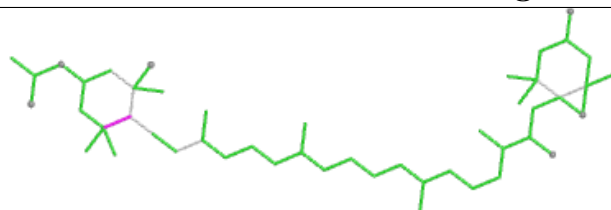


Torsions

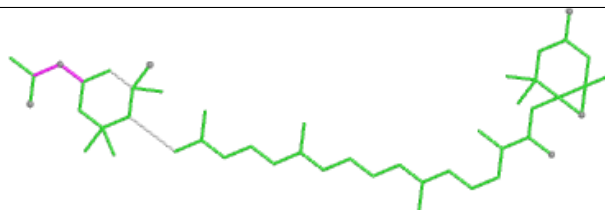


Rings

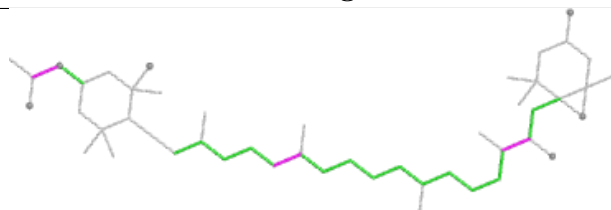
Ligand A86 W 316



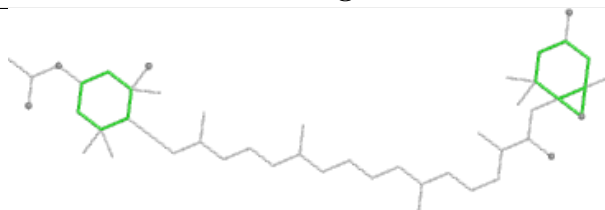
Bond lengths



Bond angles

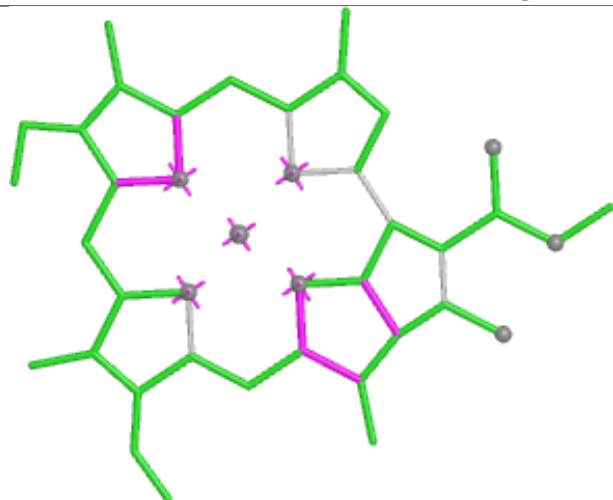


Torsions

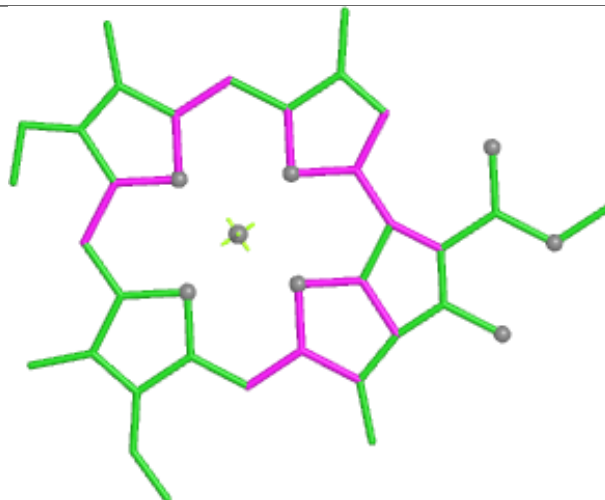


Rings

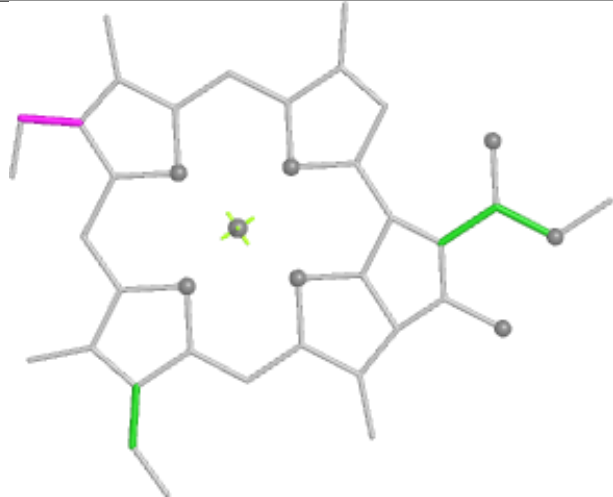
Ligand CLA L 311



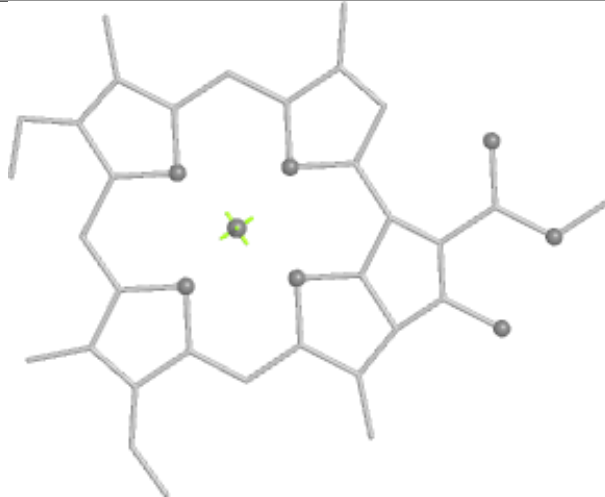
Bond lengths



Bond angles

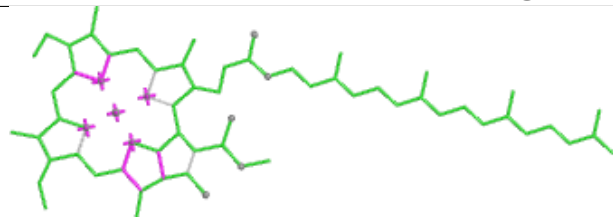


Torsions

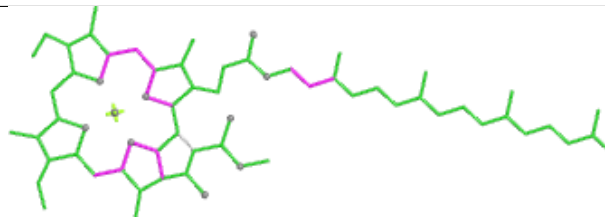


Rings

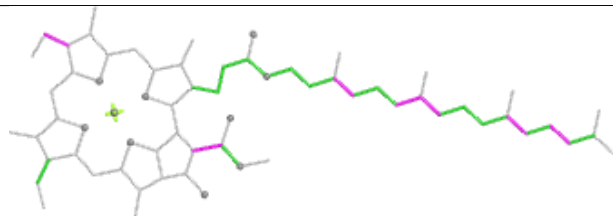
Ligand CLA a 841



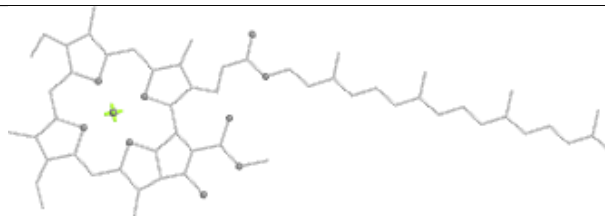
Bond lengths



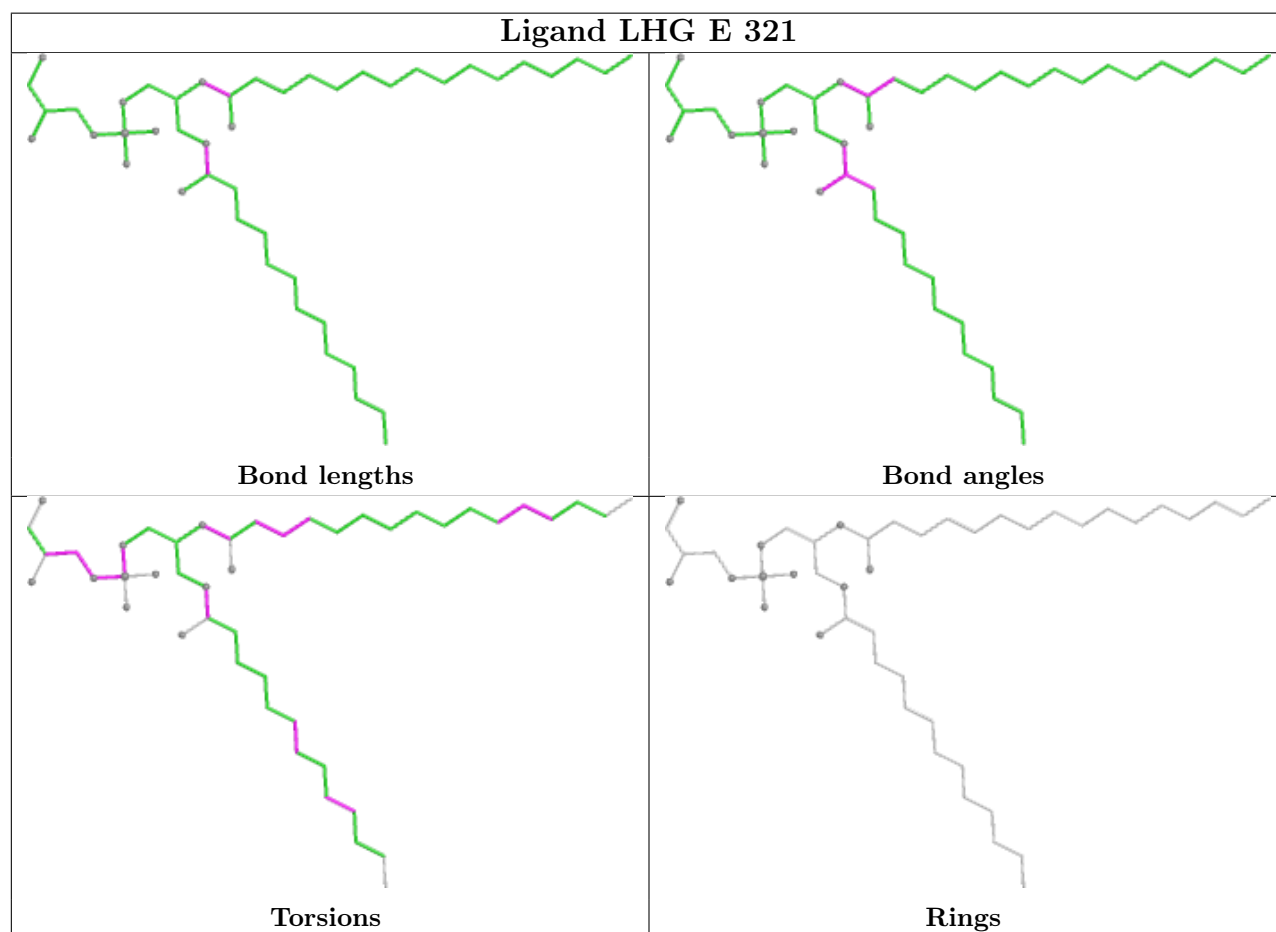
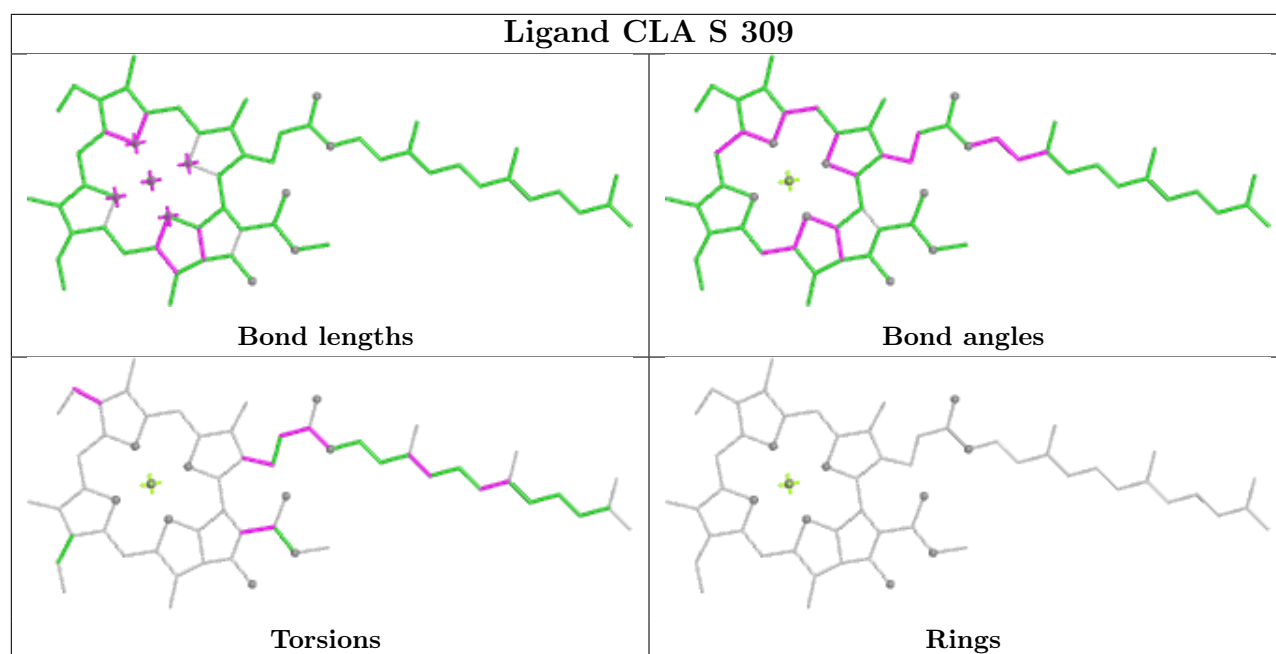
Bond angles

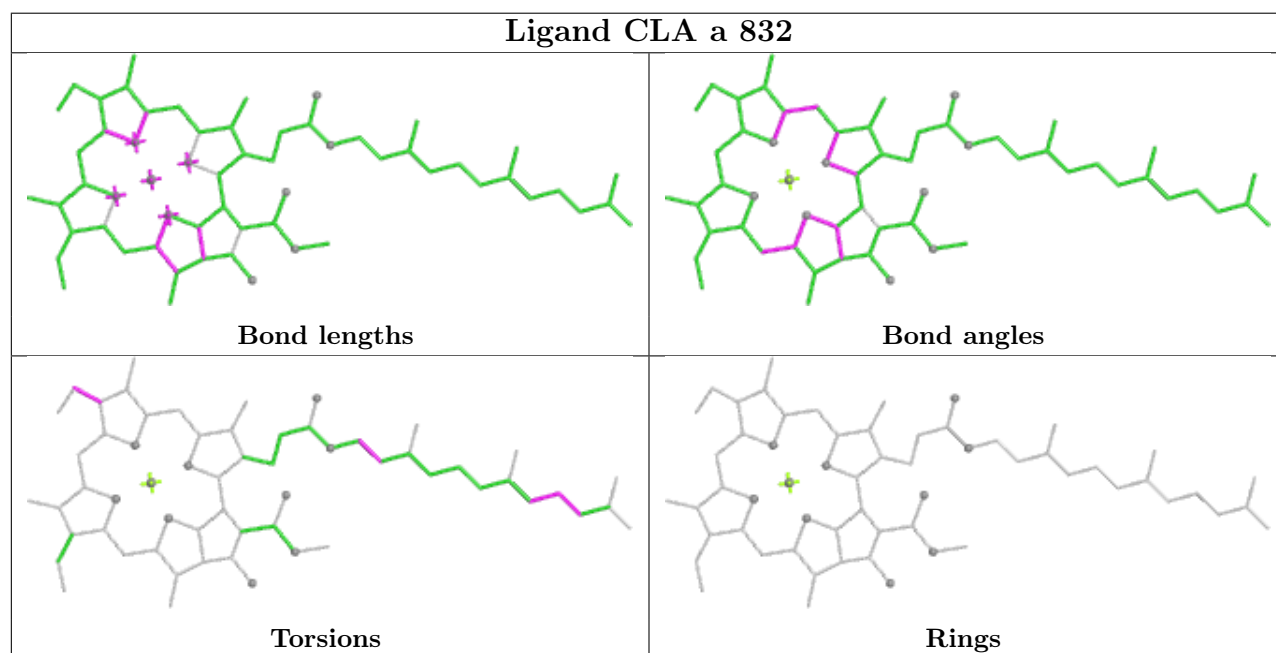
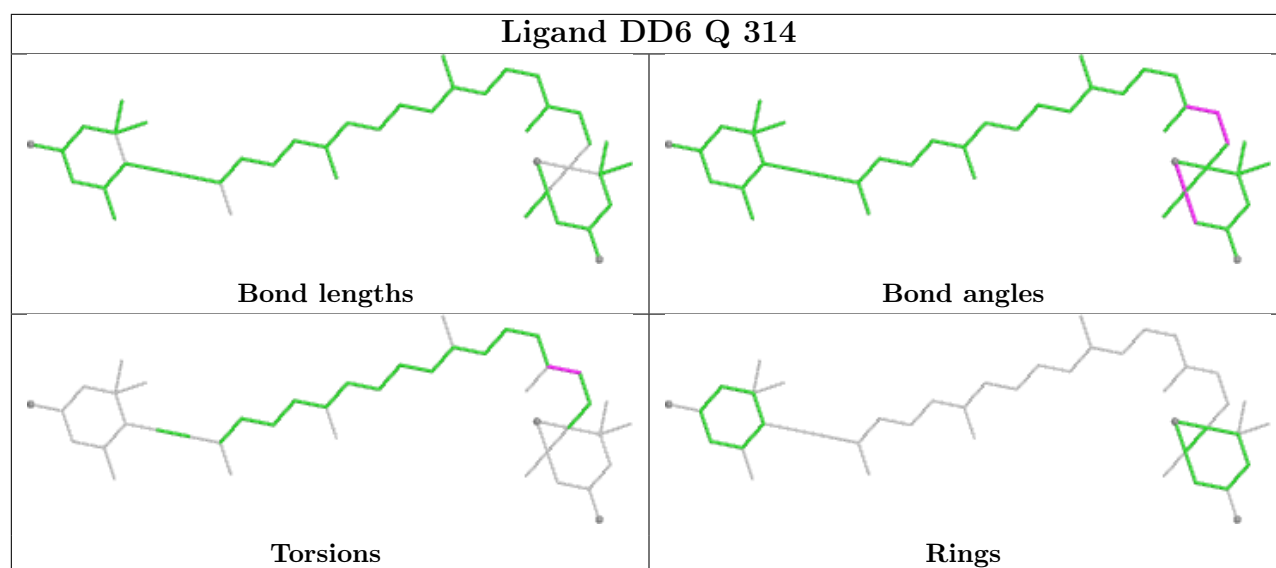


Torsions

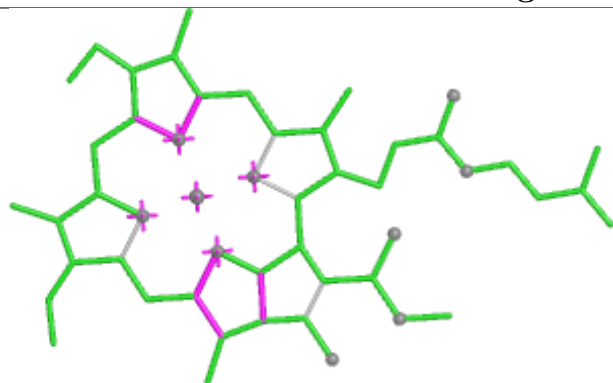


Rings

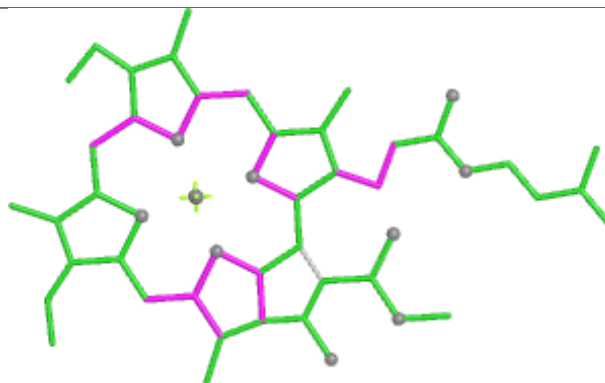




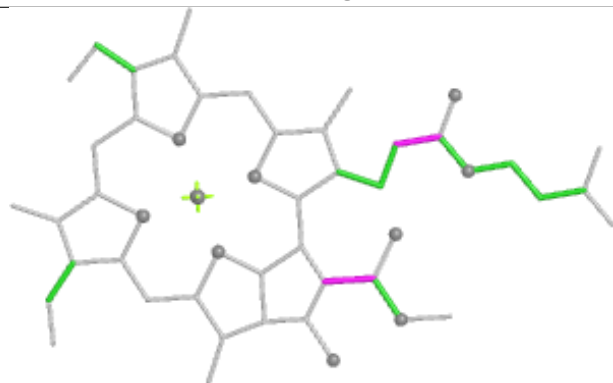
Ligand CLA S 311



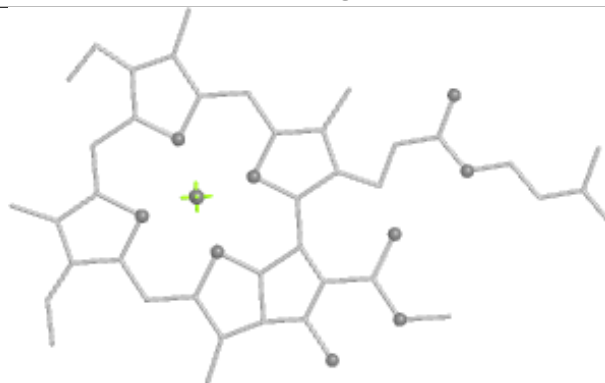
Bond lengths



Bond angles

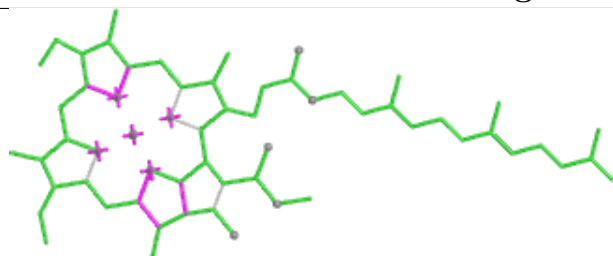


Torsions

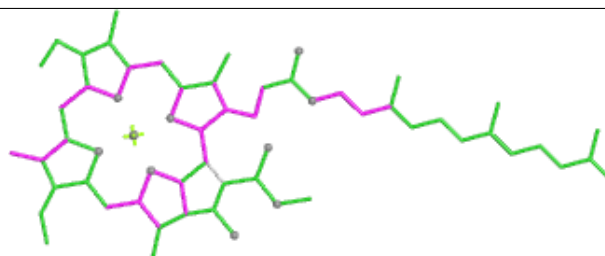


Rings

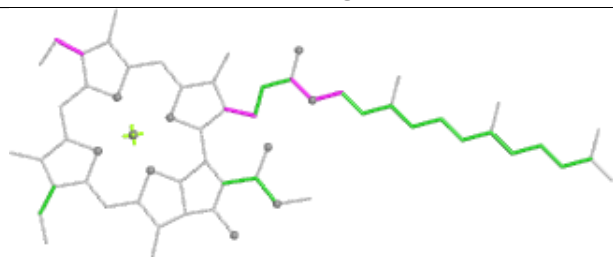
Ligand CLA T 308



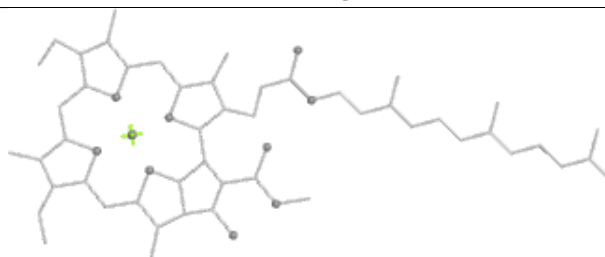
Bond lengths



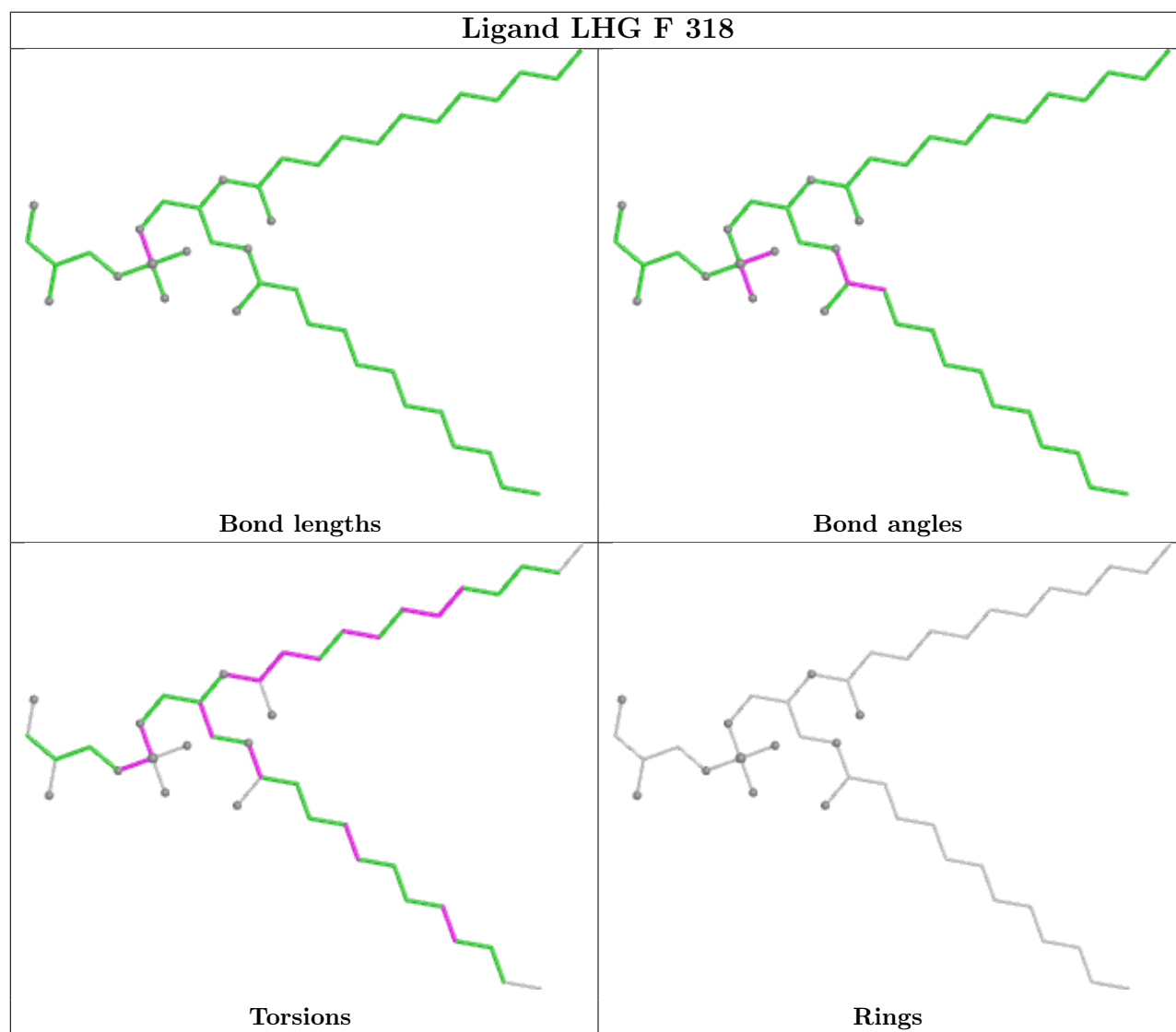
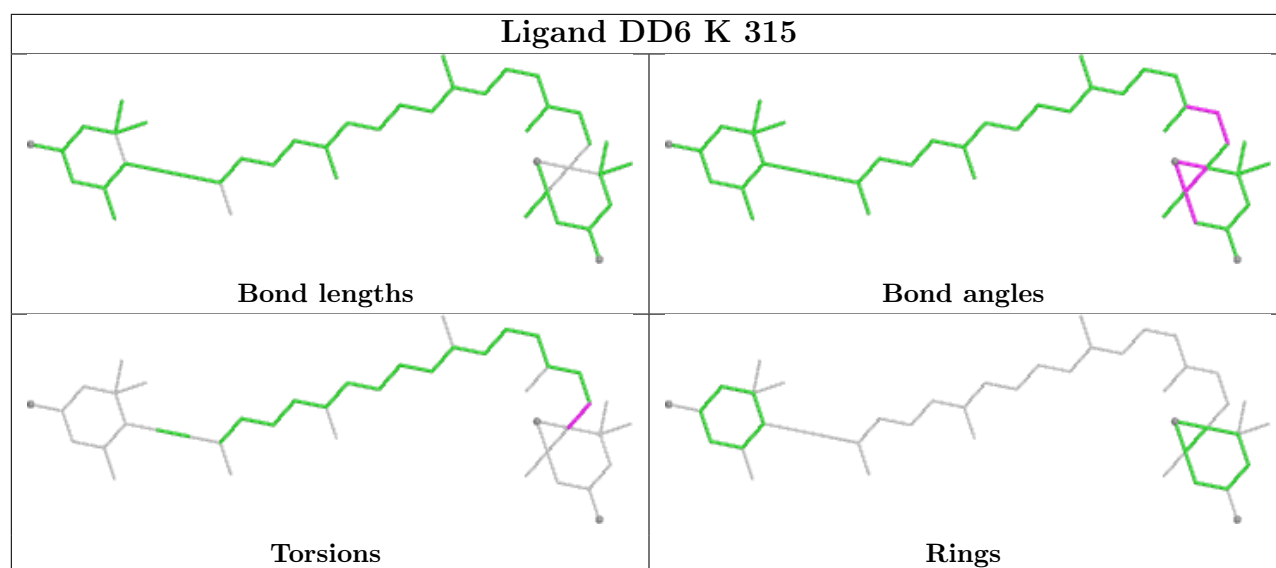
Bond angles



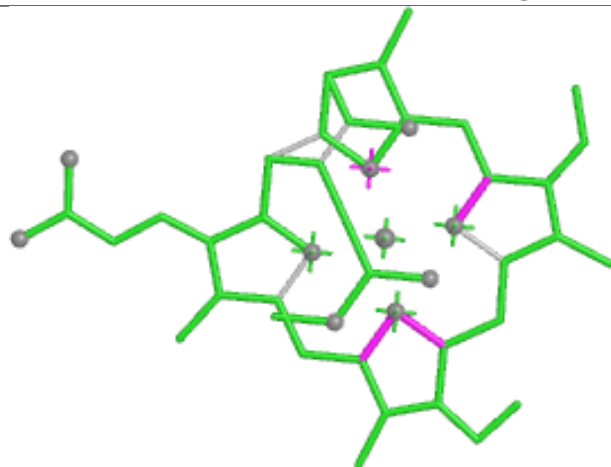
Torsions



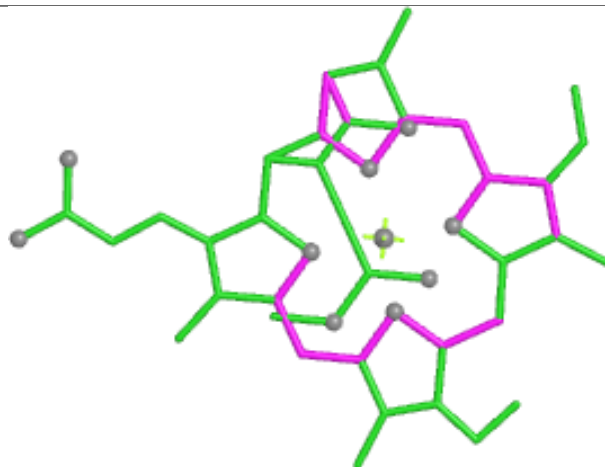
Rings



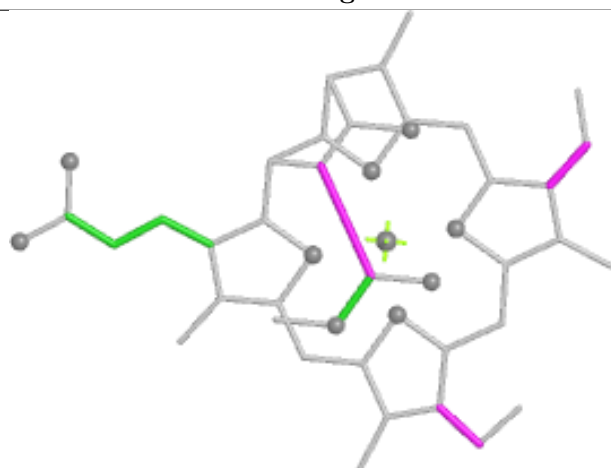
Ligand KC2 A 310



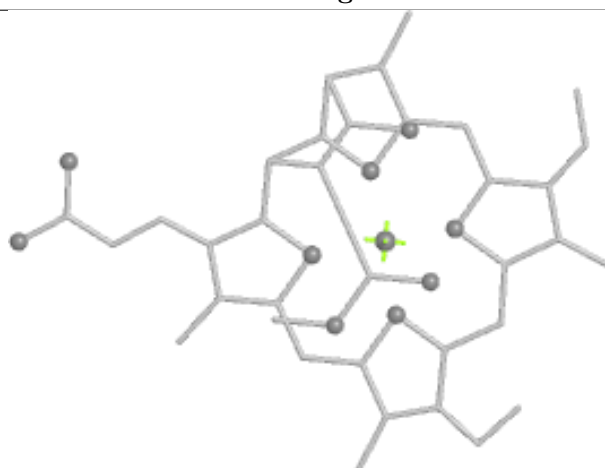
Bond lengths



Bond angles

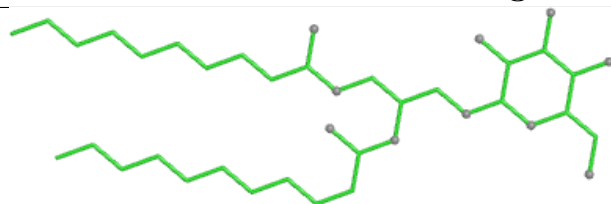


Torsions

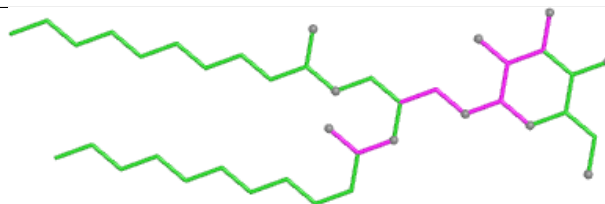


Rings

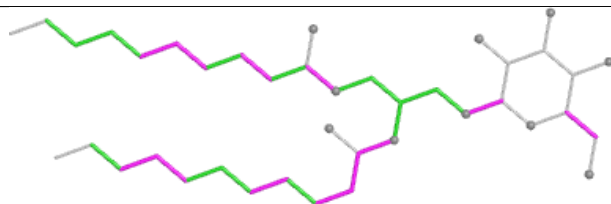
Ligand LMG D 321



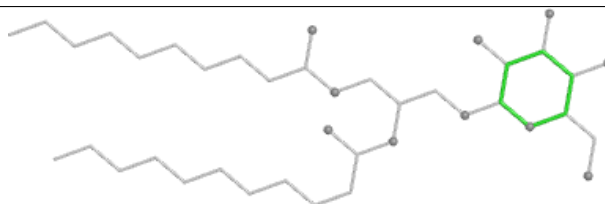
Bond lengths



Bond angles

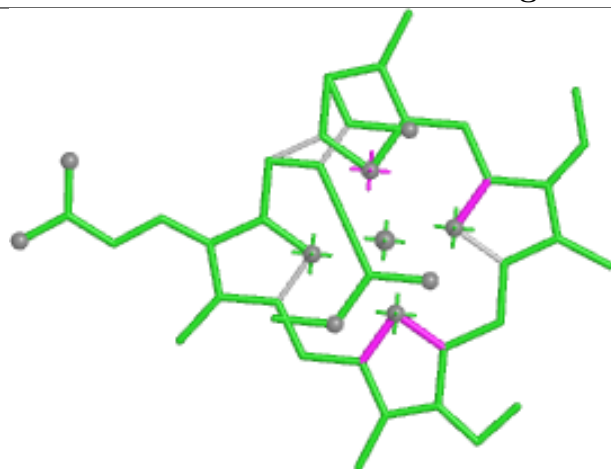


Torsions

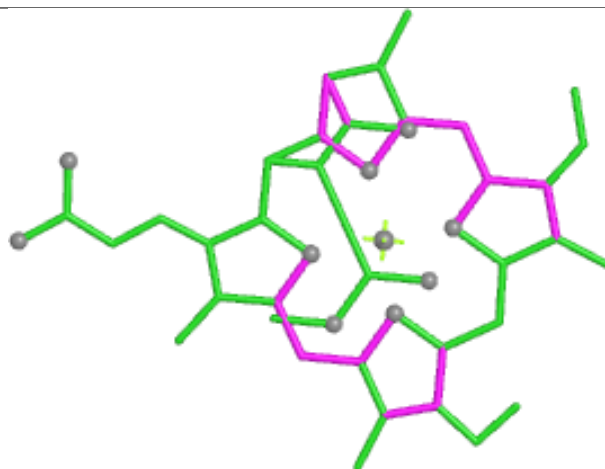


Rings

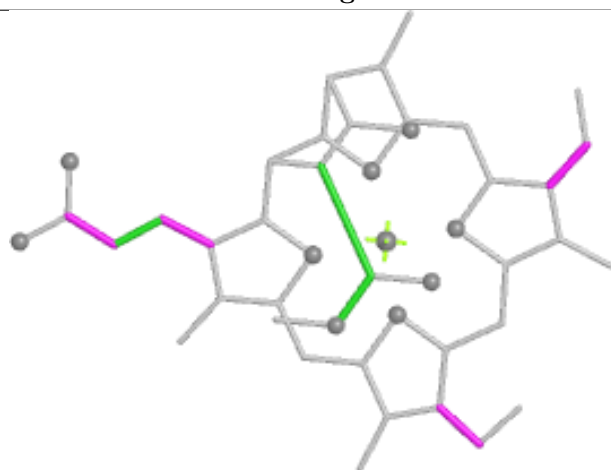
Ligand KC2 J 310



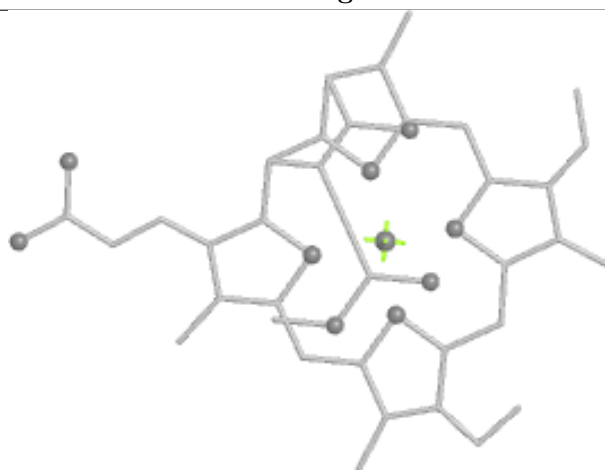
Bond lengths



Bond angles



Torsions



Rings

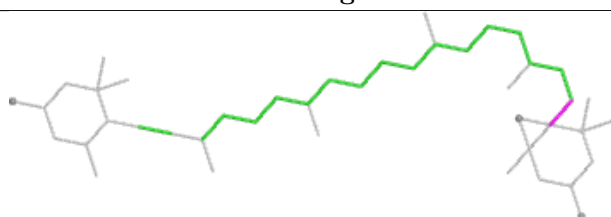
Ligand DD6 H 312



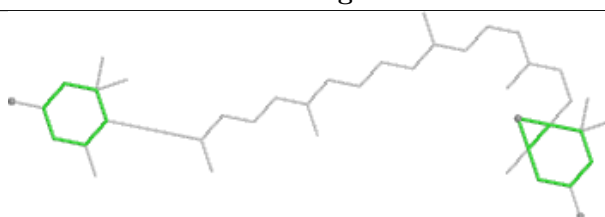
Bond lengths



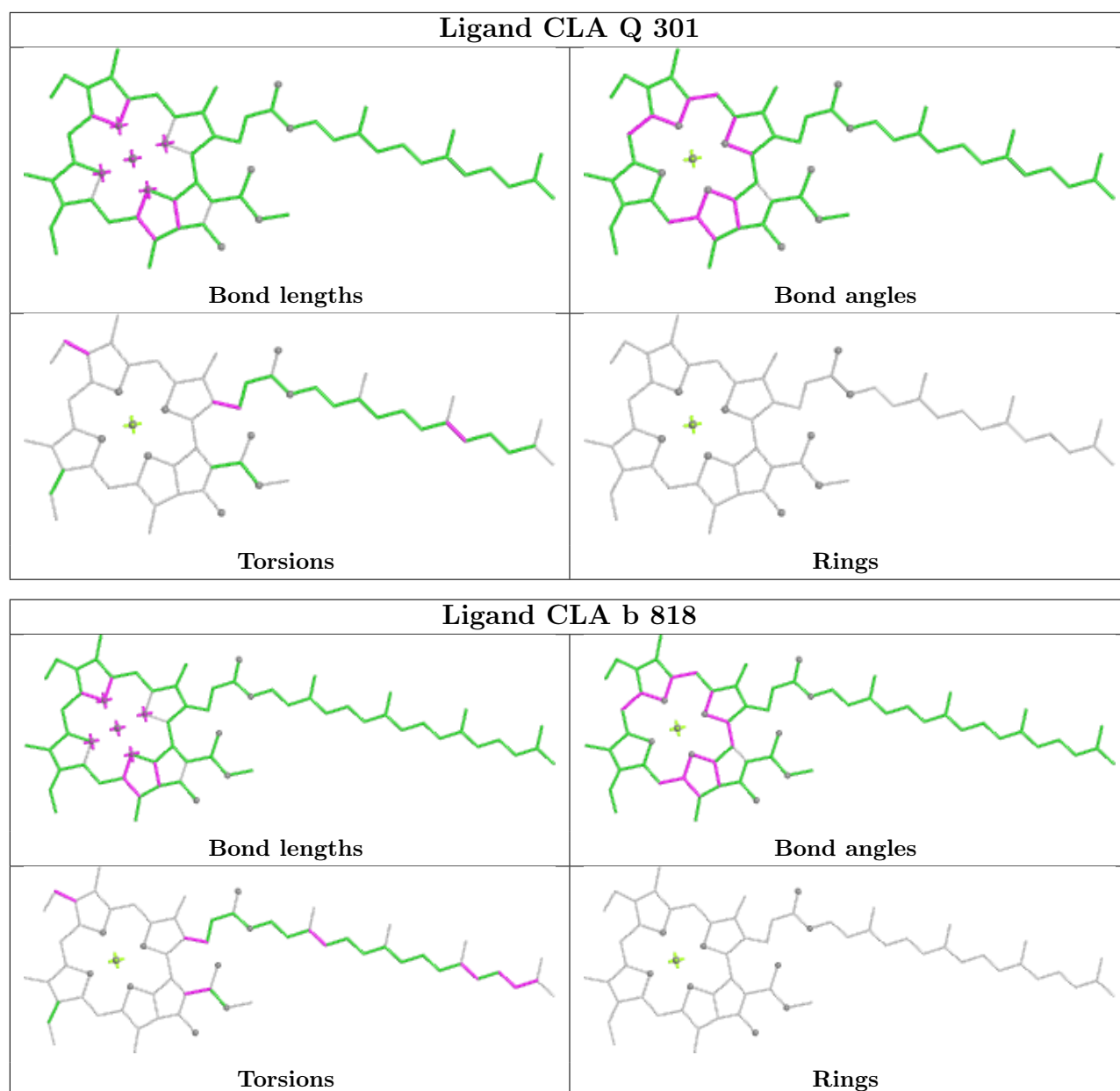
Bond angles

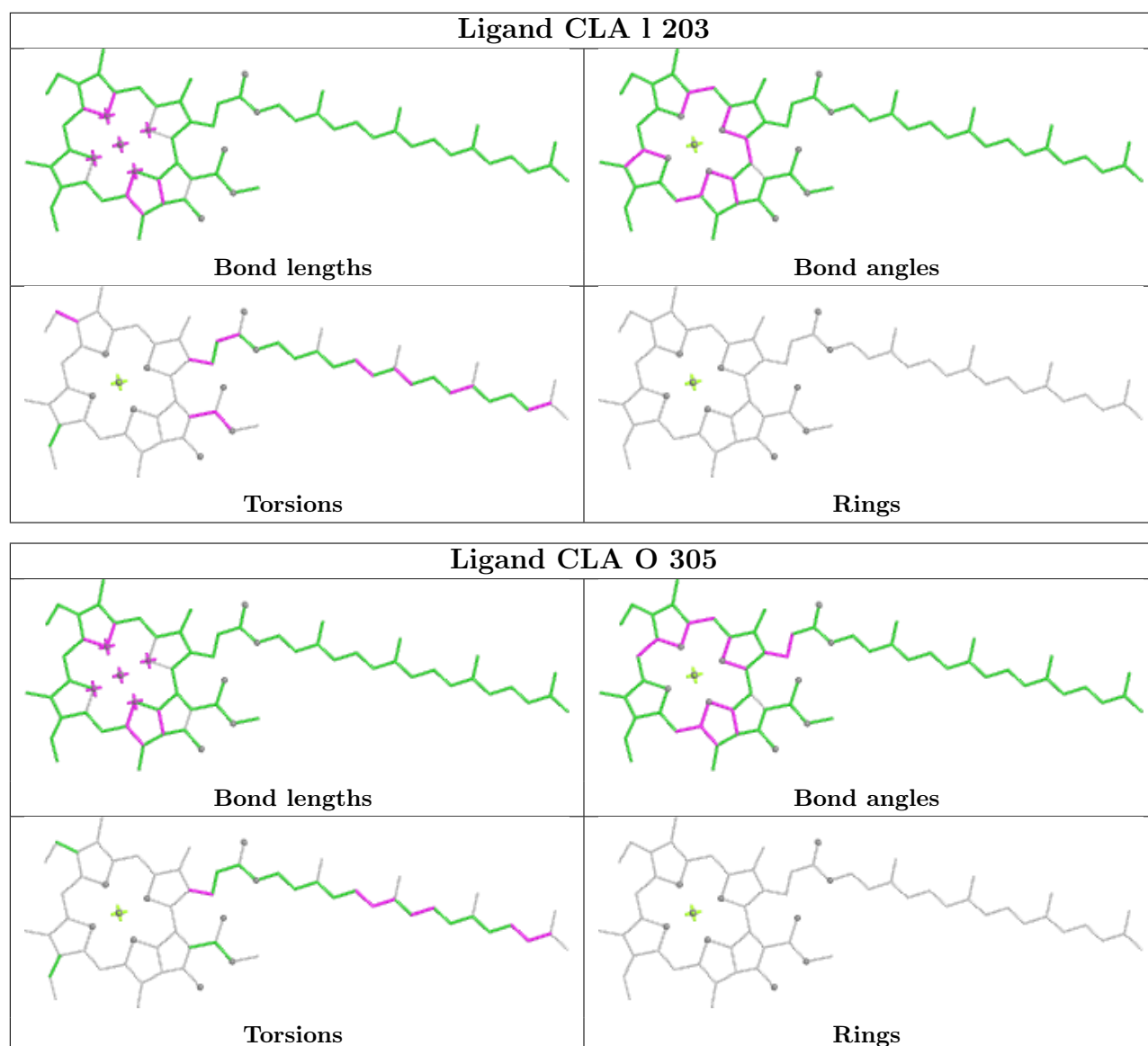


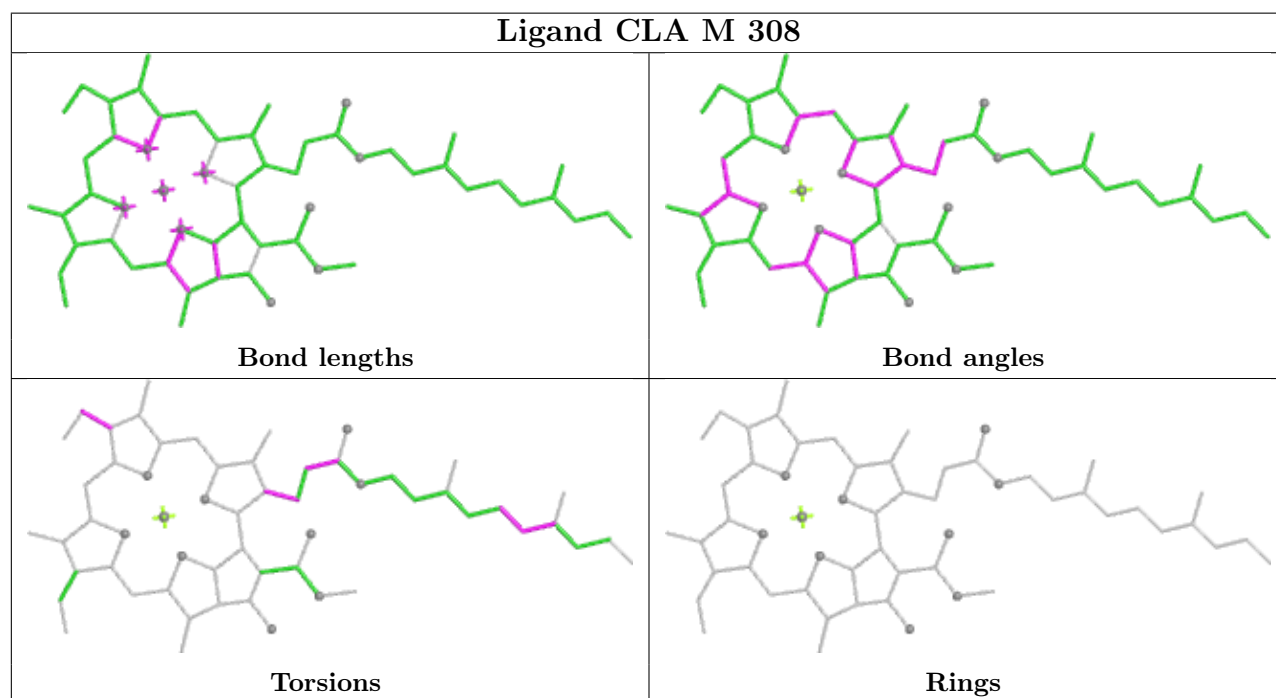
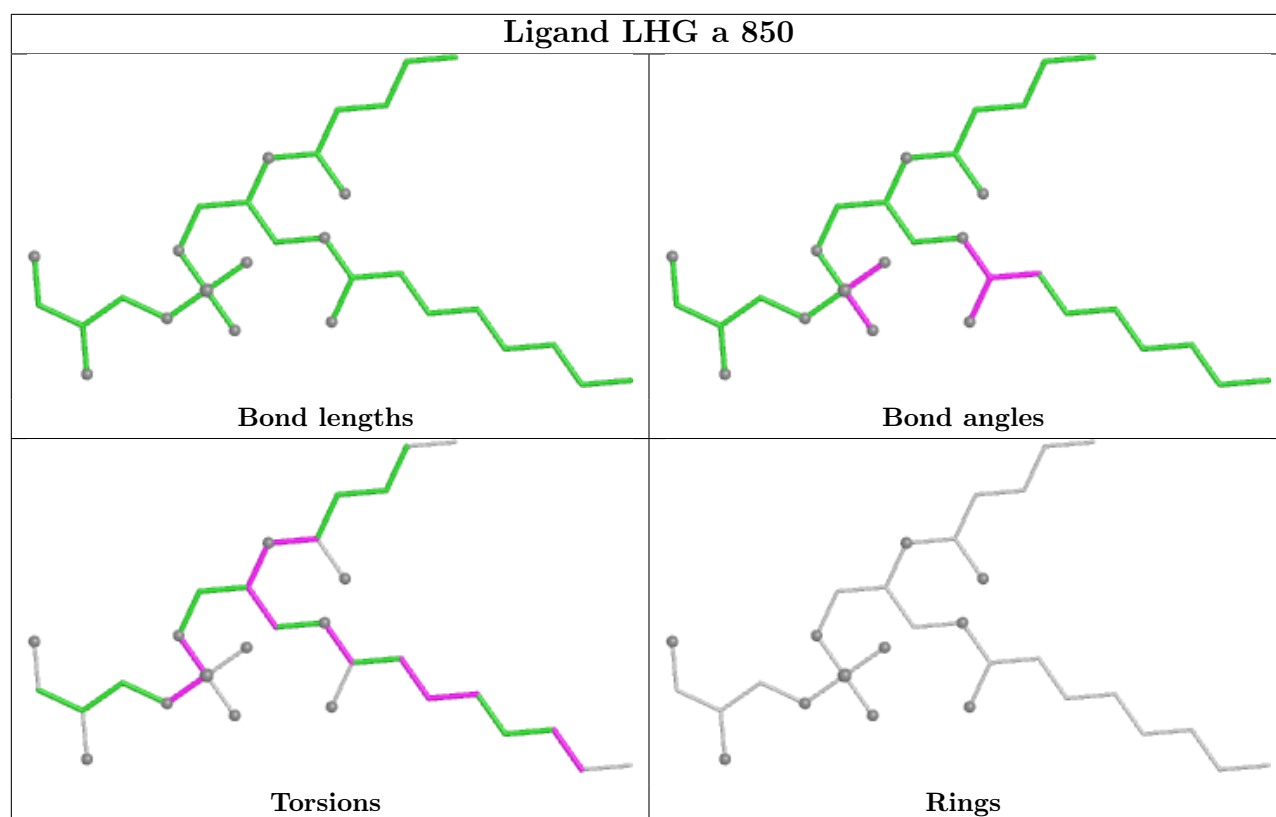
Torsions

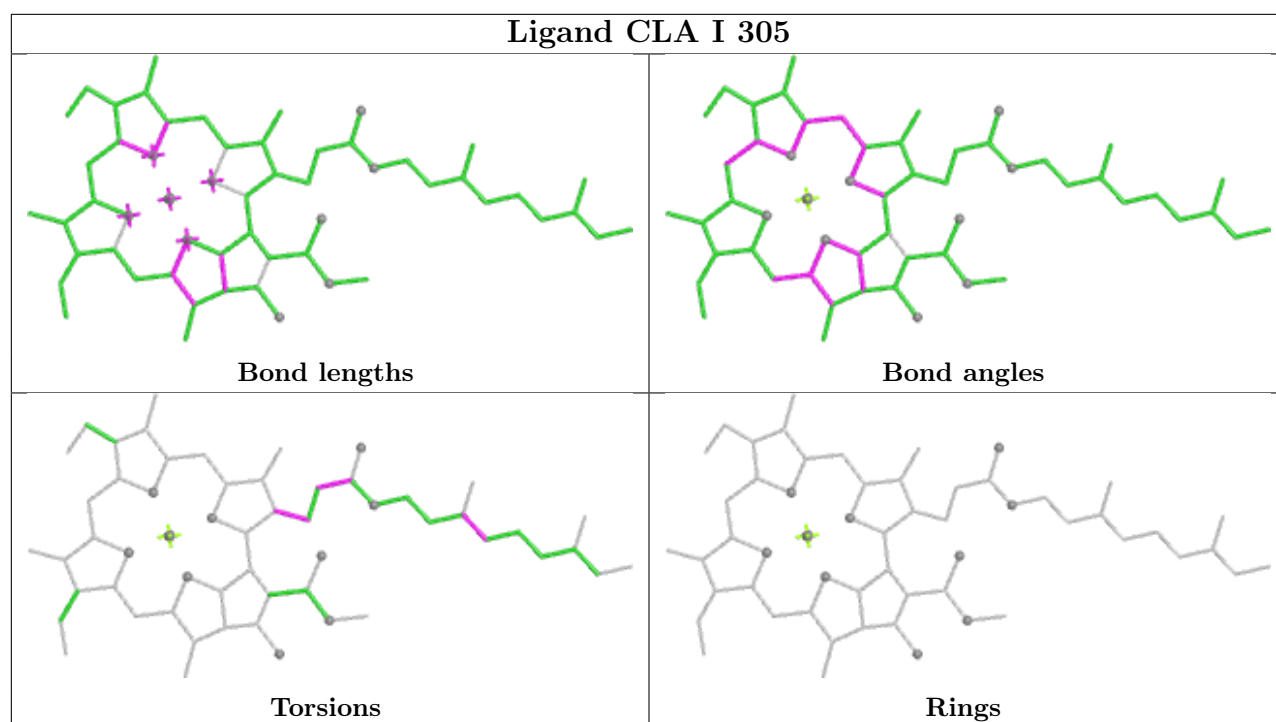


Rings

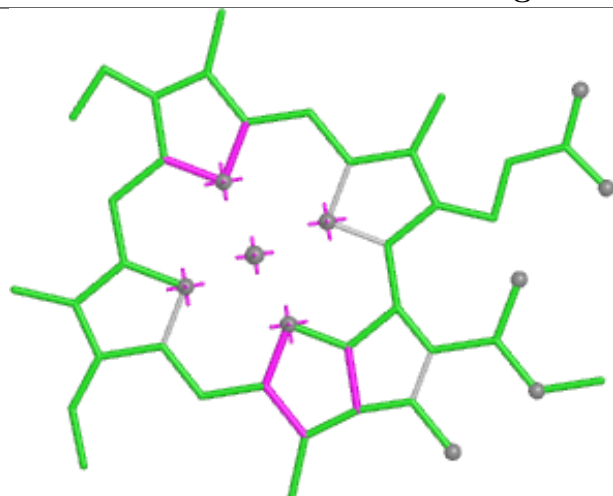




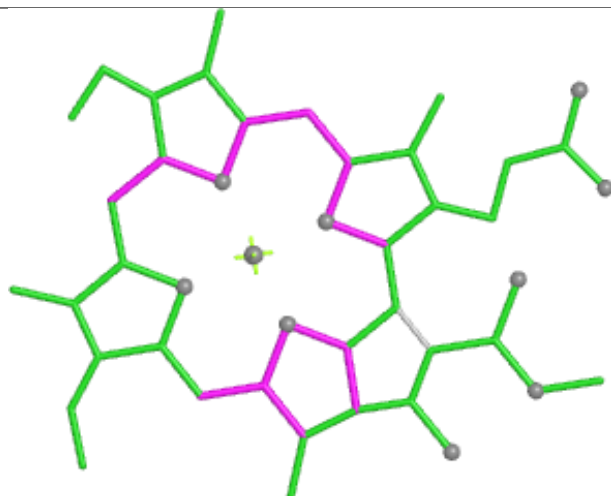




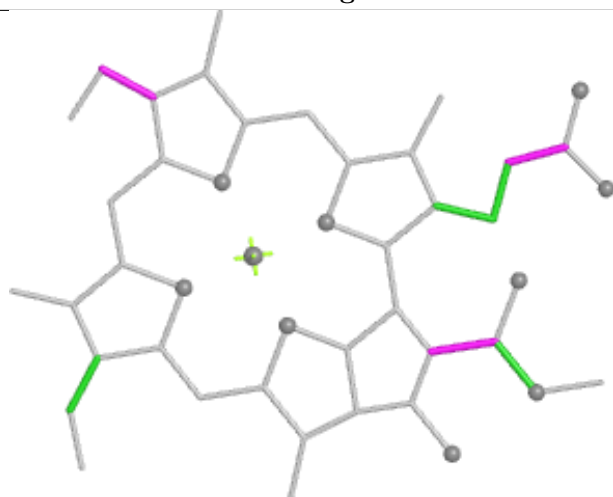
Ligand CLA R 304



Bond lengths



Bond angles

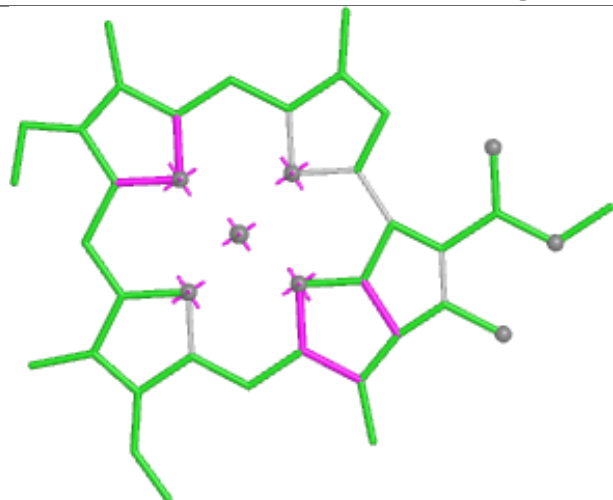


Torsions

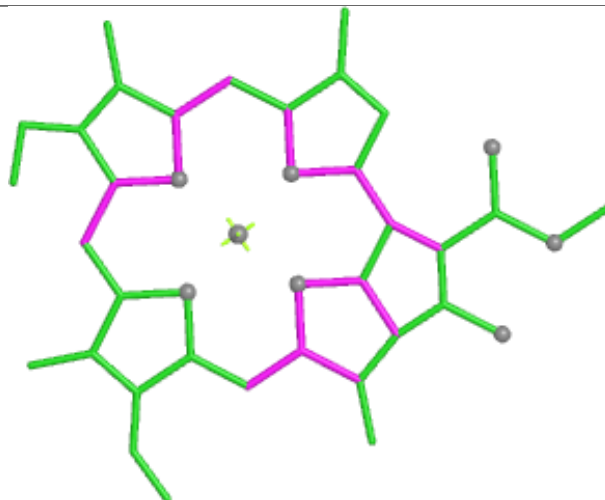


Rings

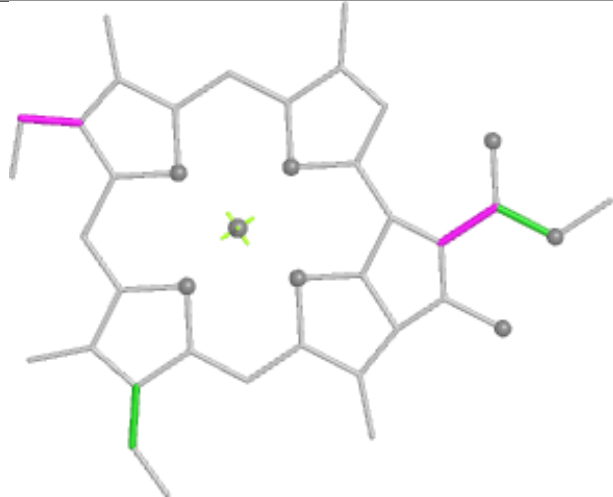
Ligand CLA B 301



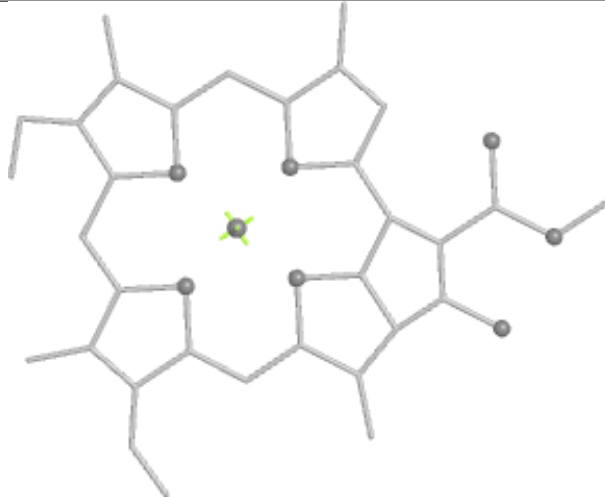
Bond lengths



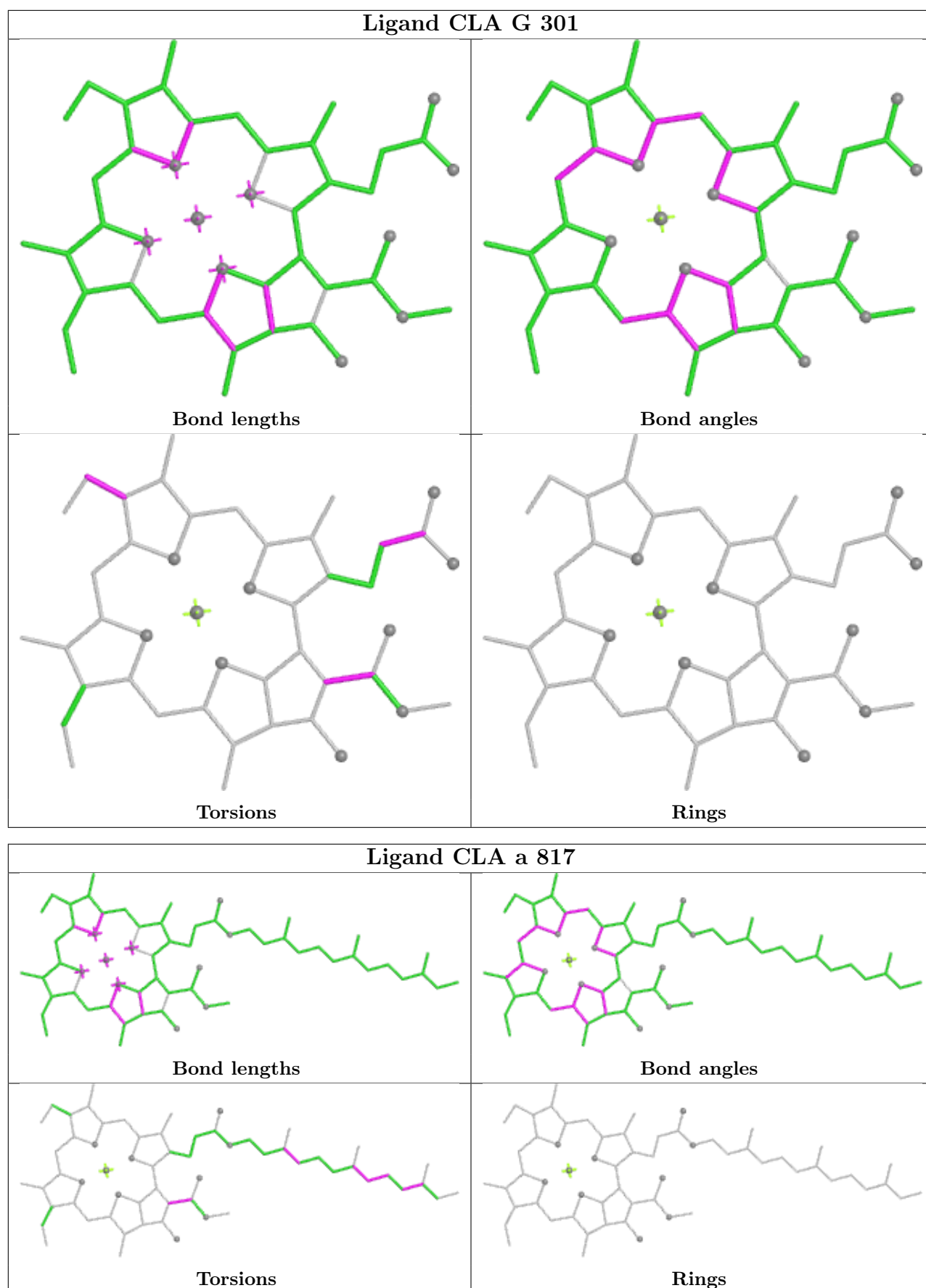
Bond angles

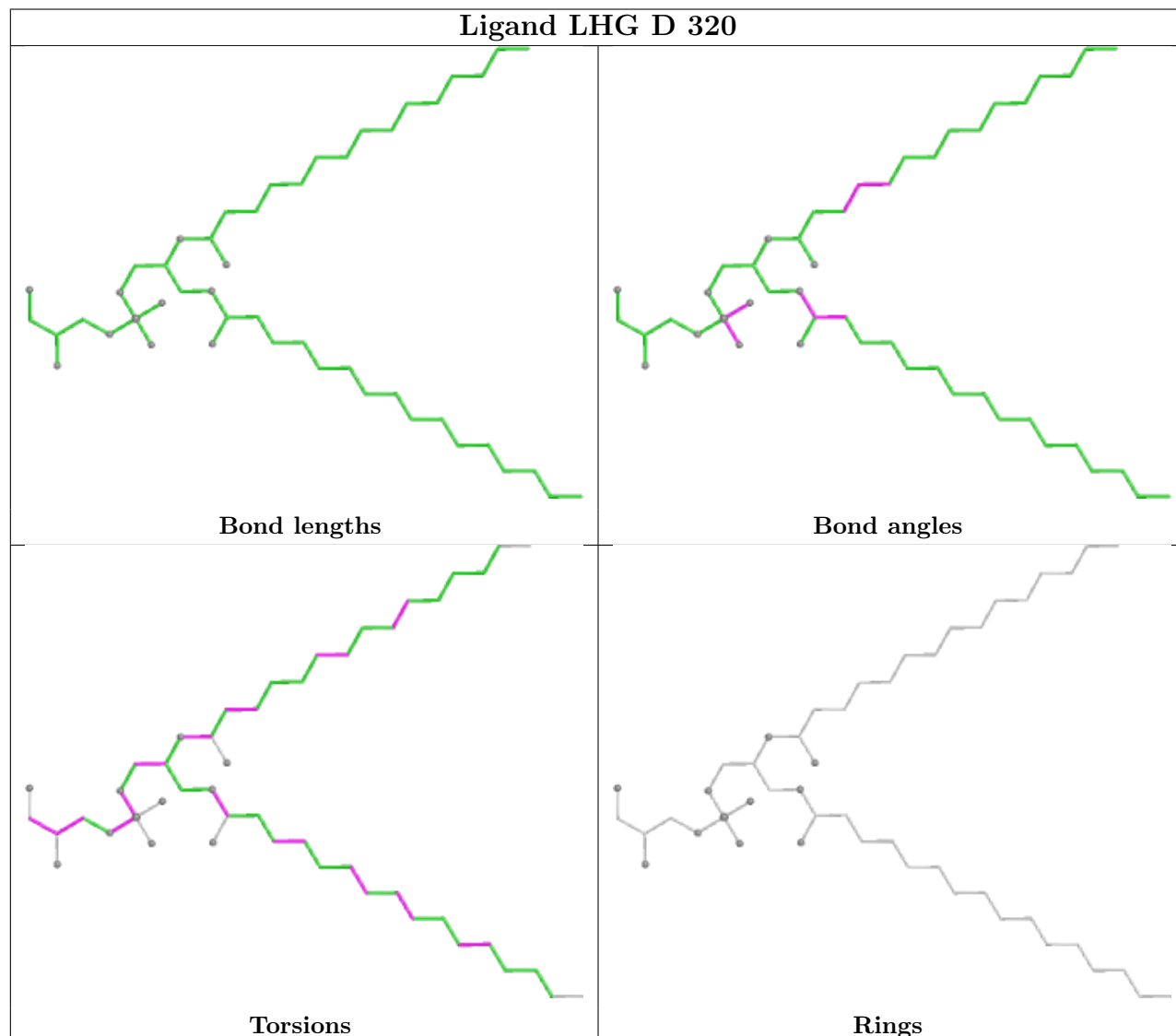
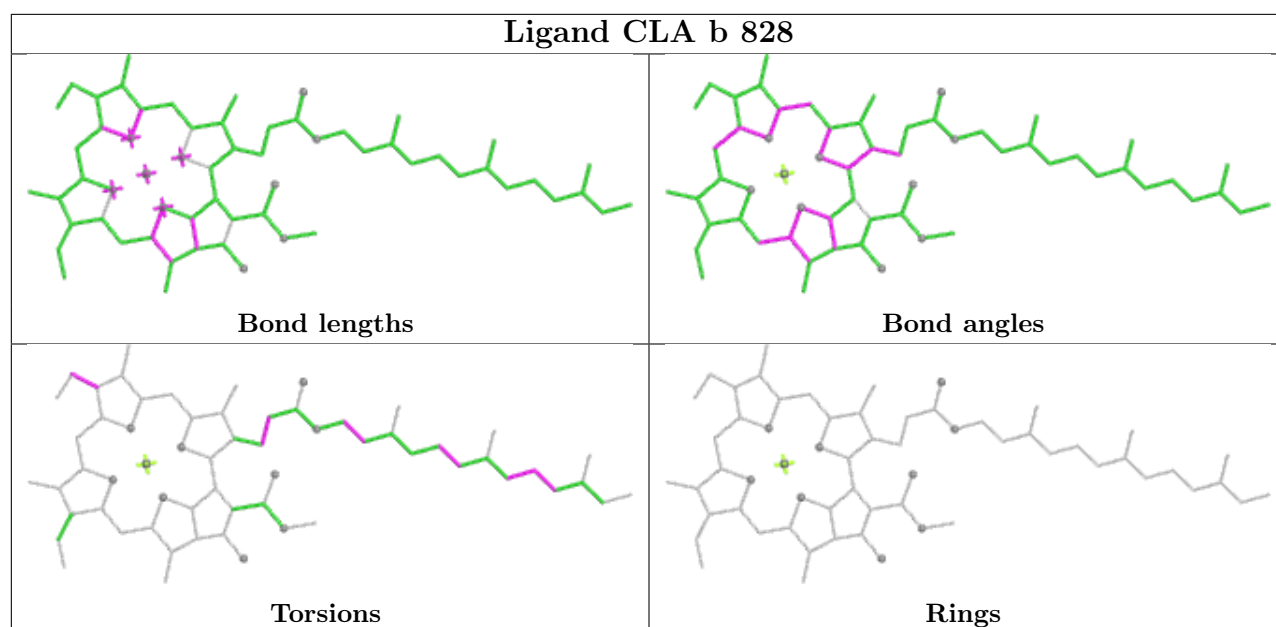


Torsions

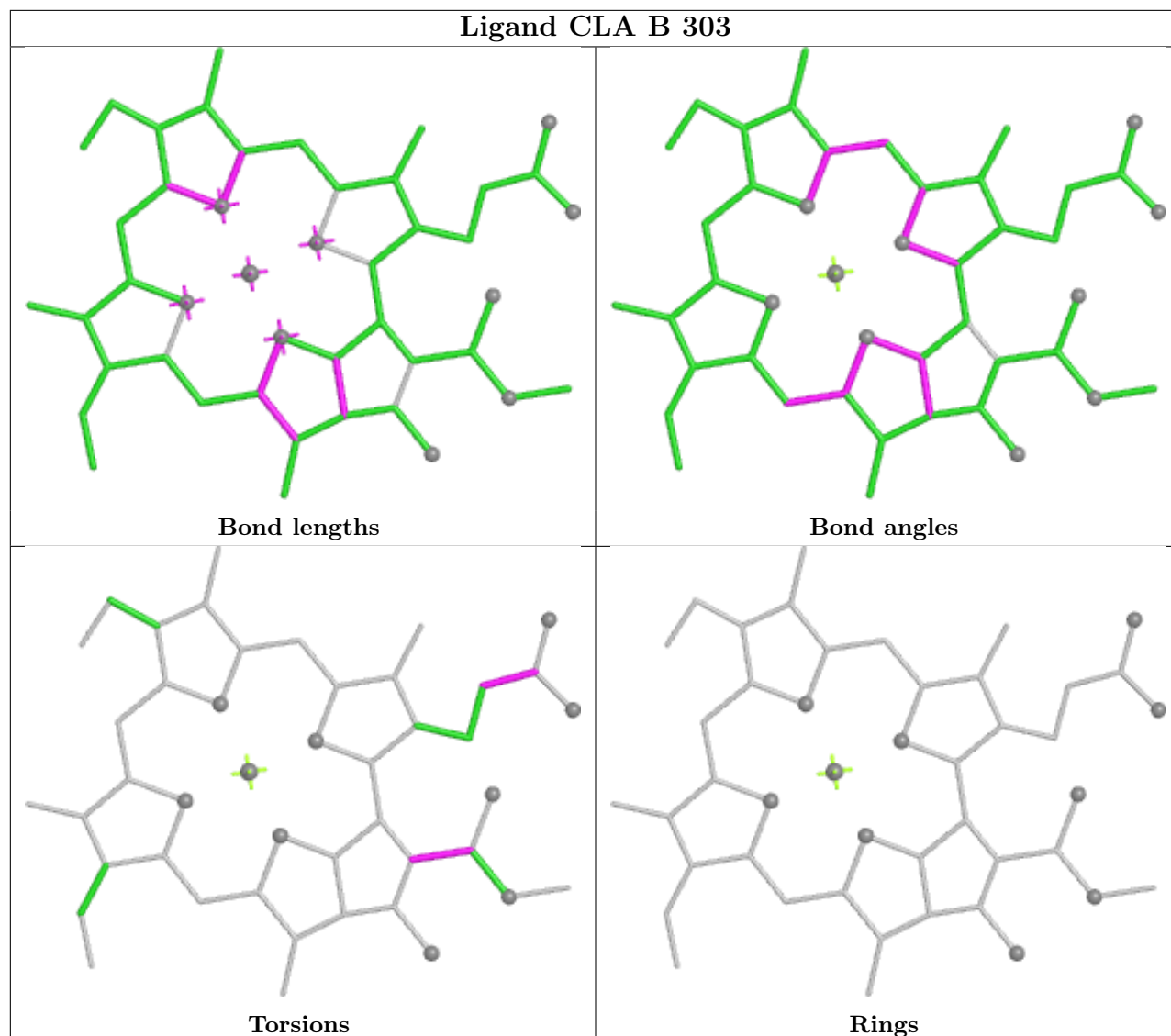


Rings

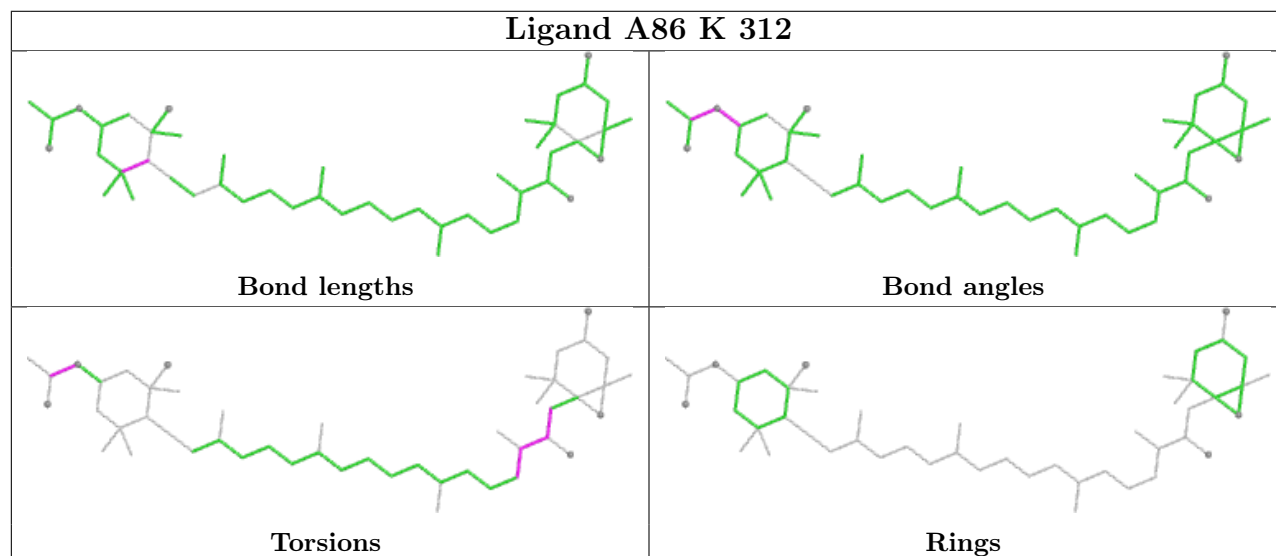


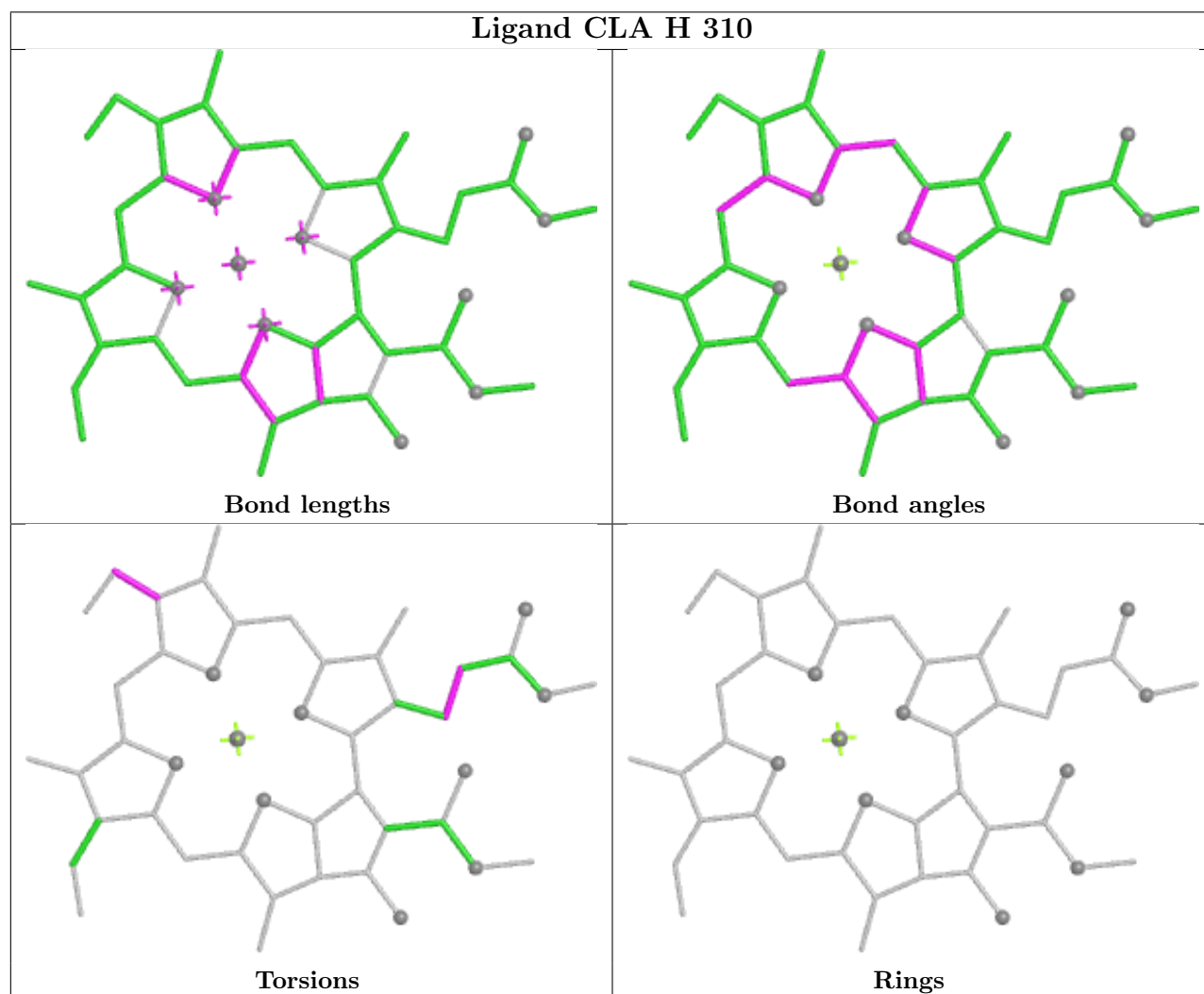
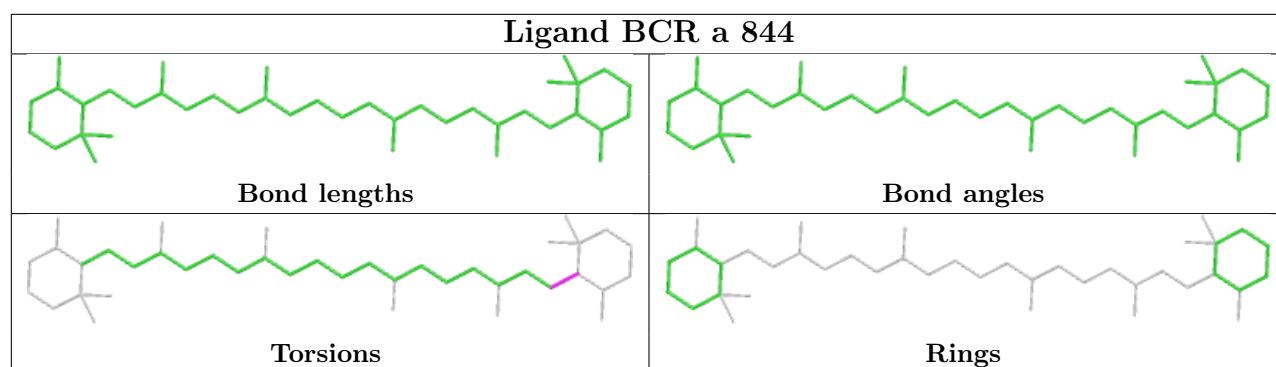


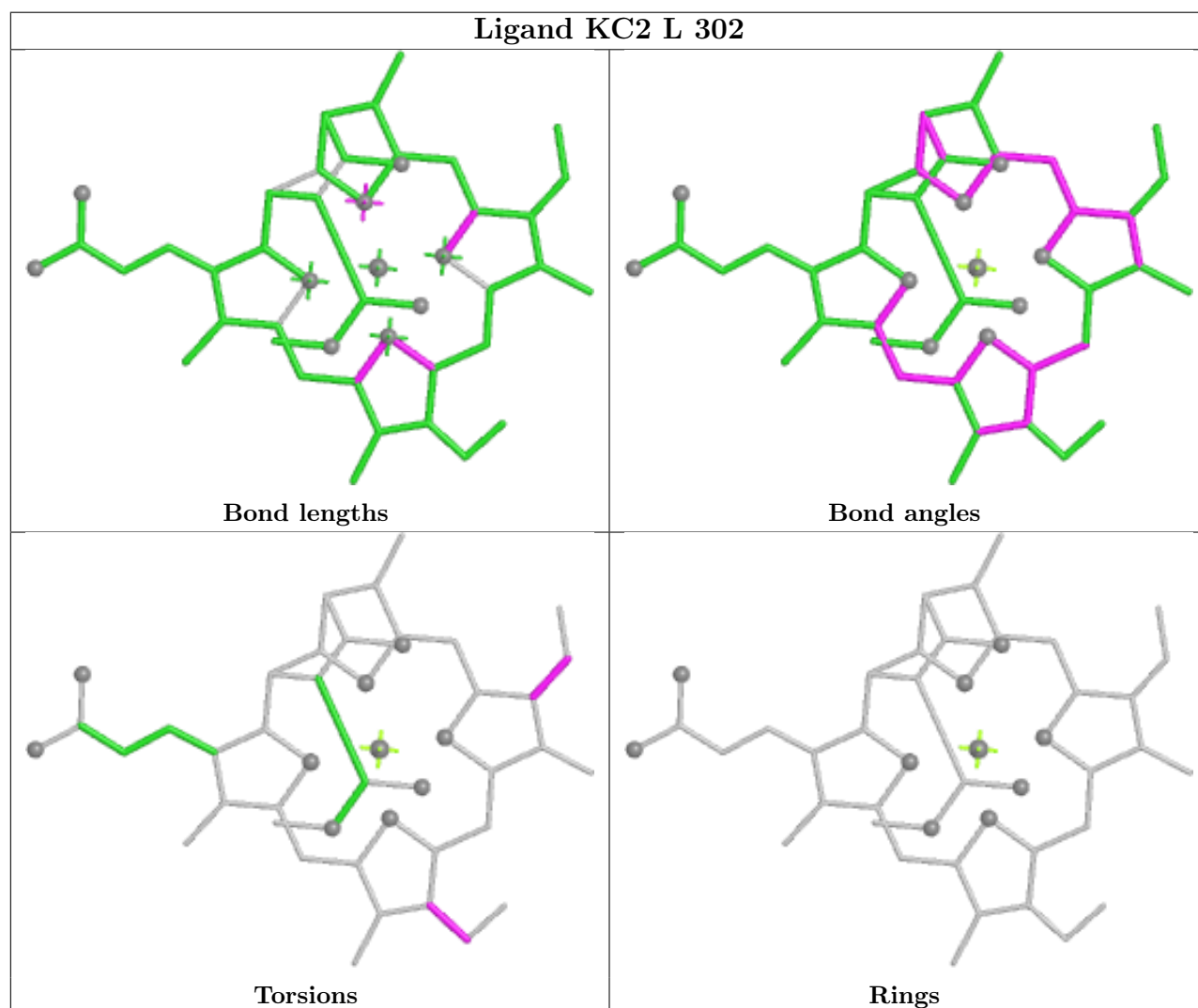
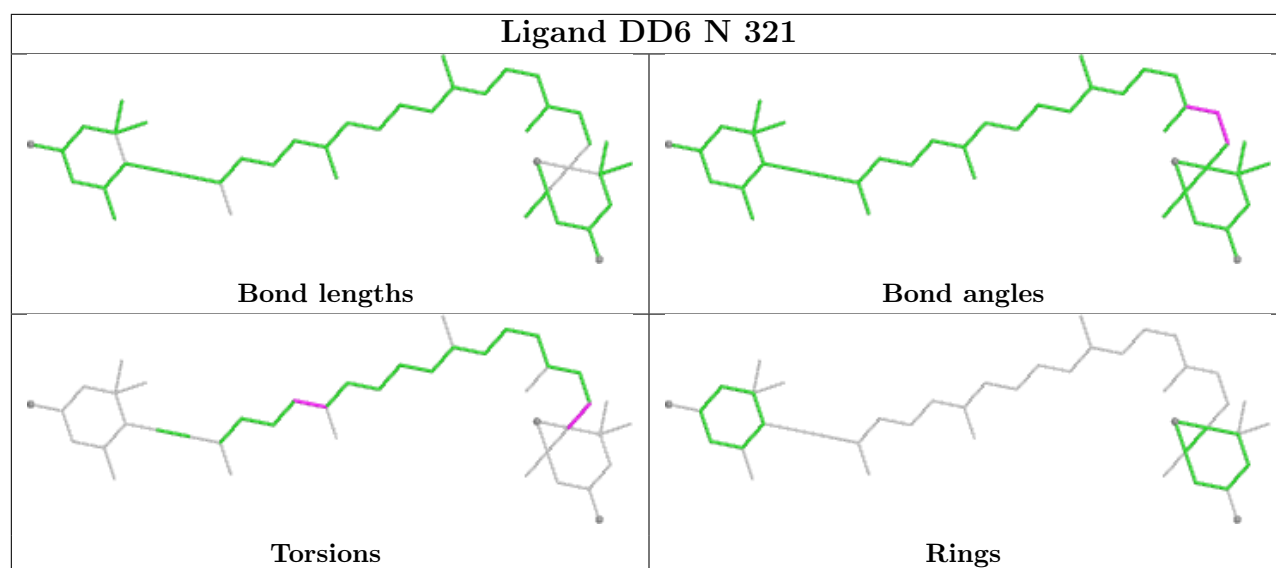
Ligand CLA B 303

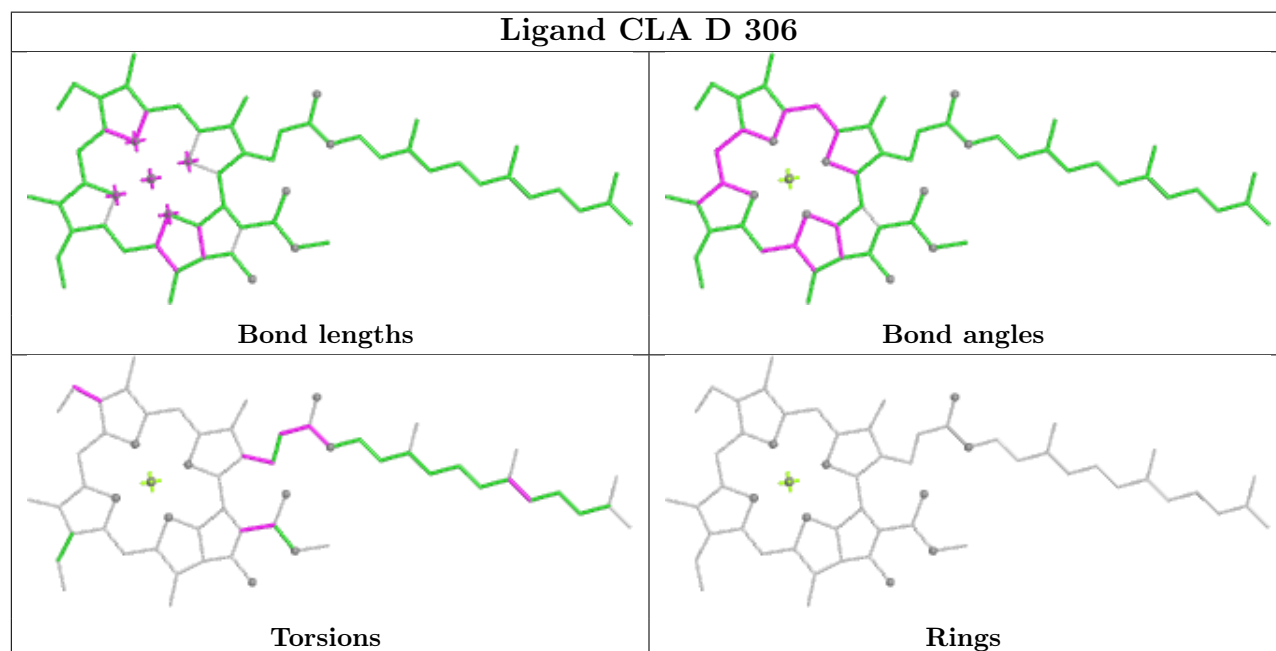
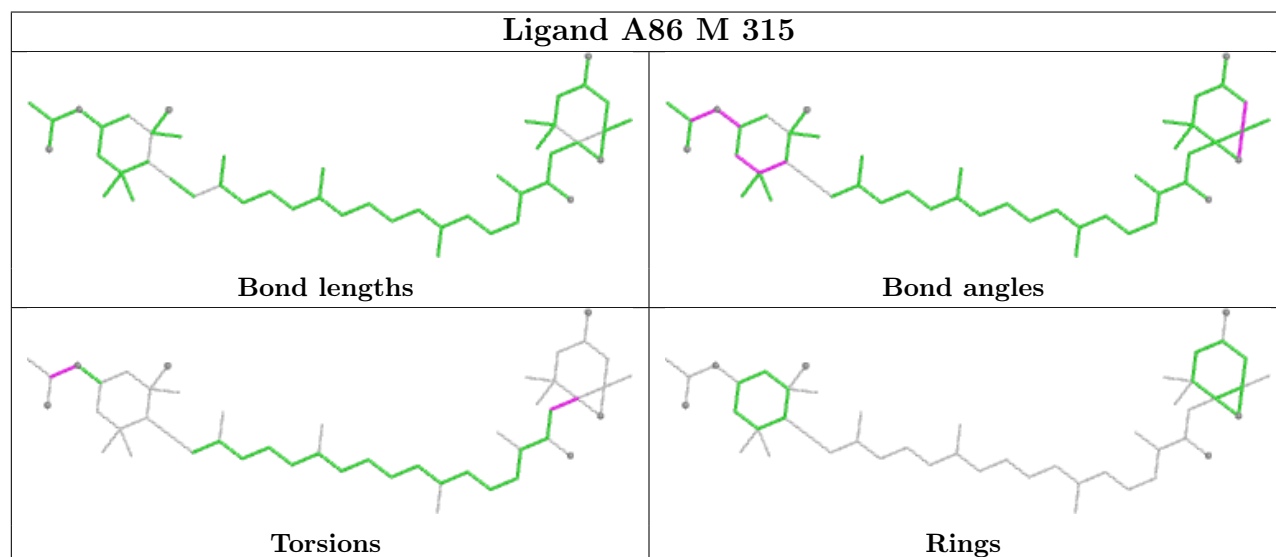
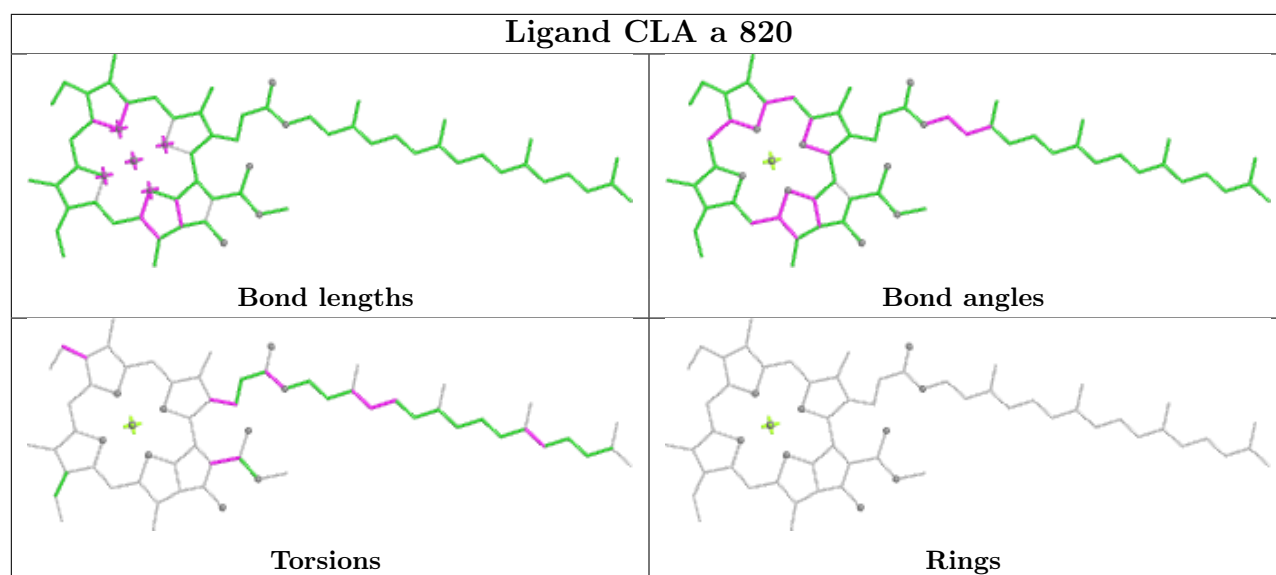


Ligand A86 K 312

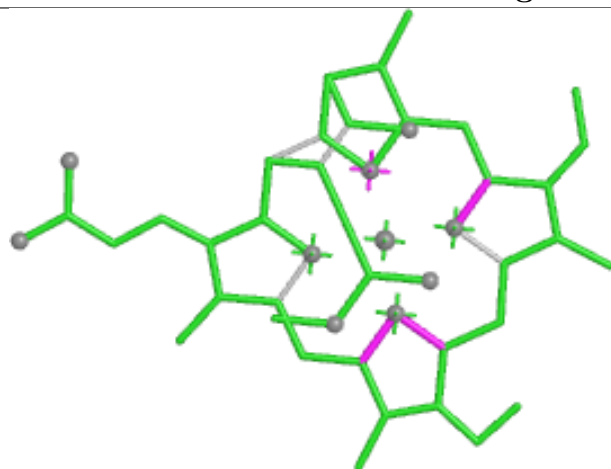




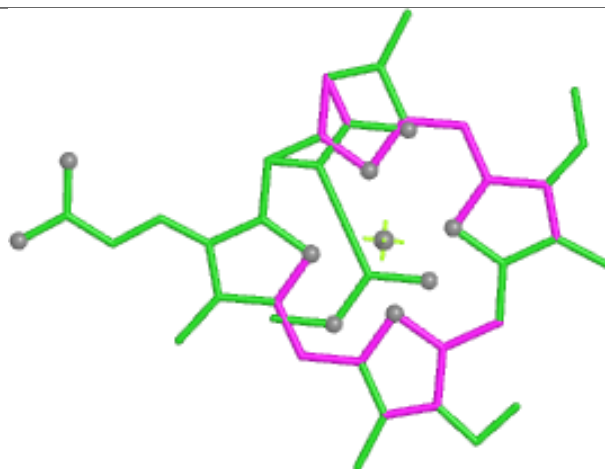




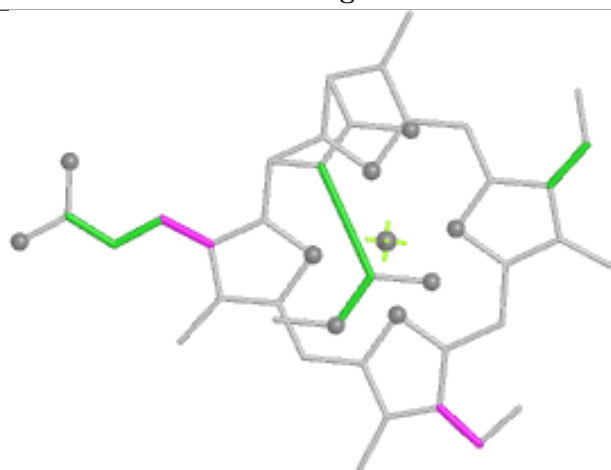
Ligand KC2 R 311



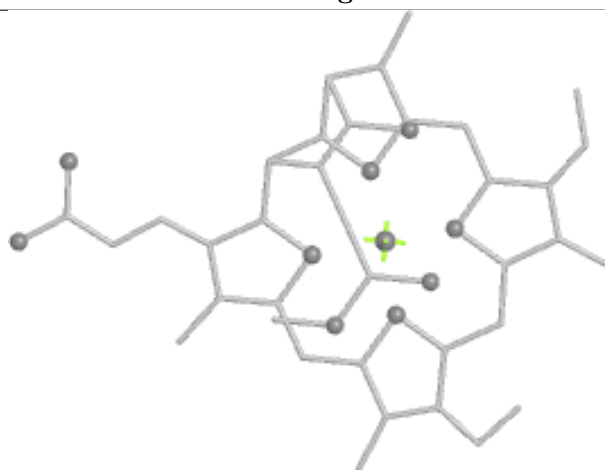
Bond lengths



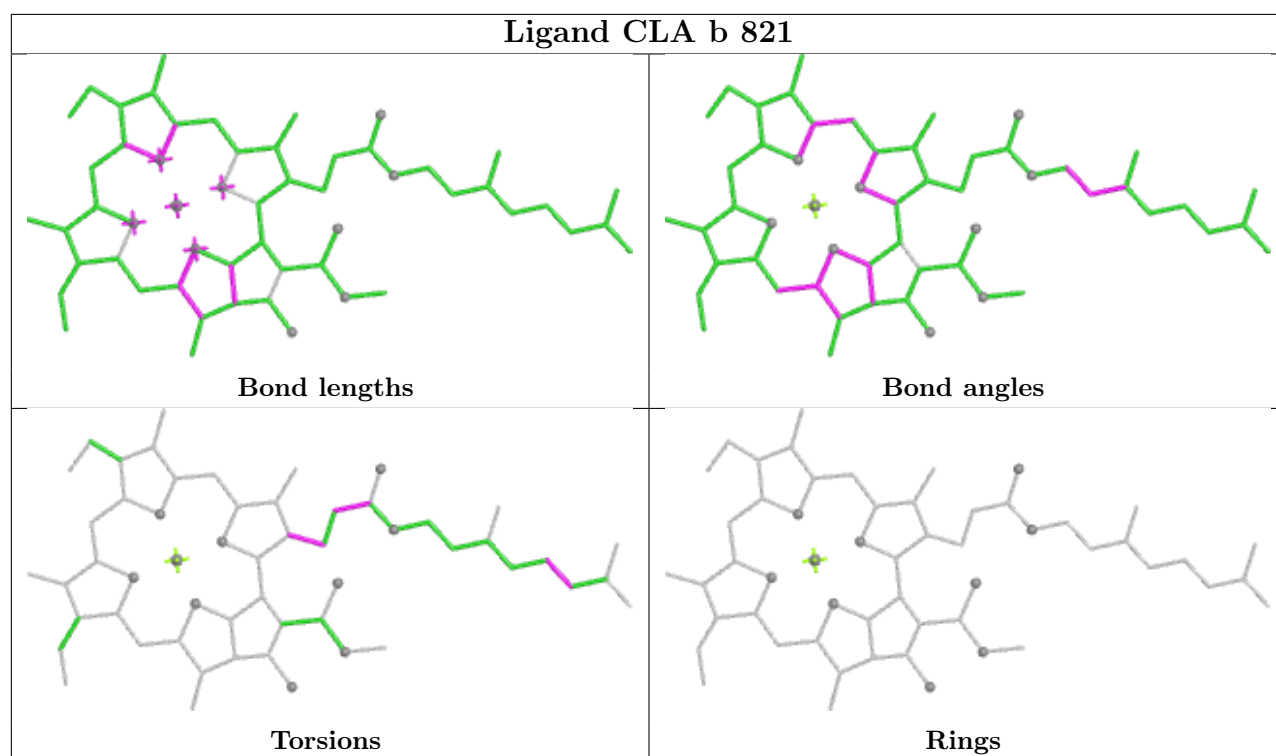
Bond angles

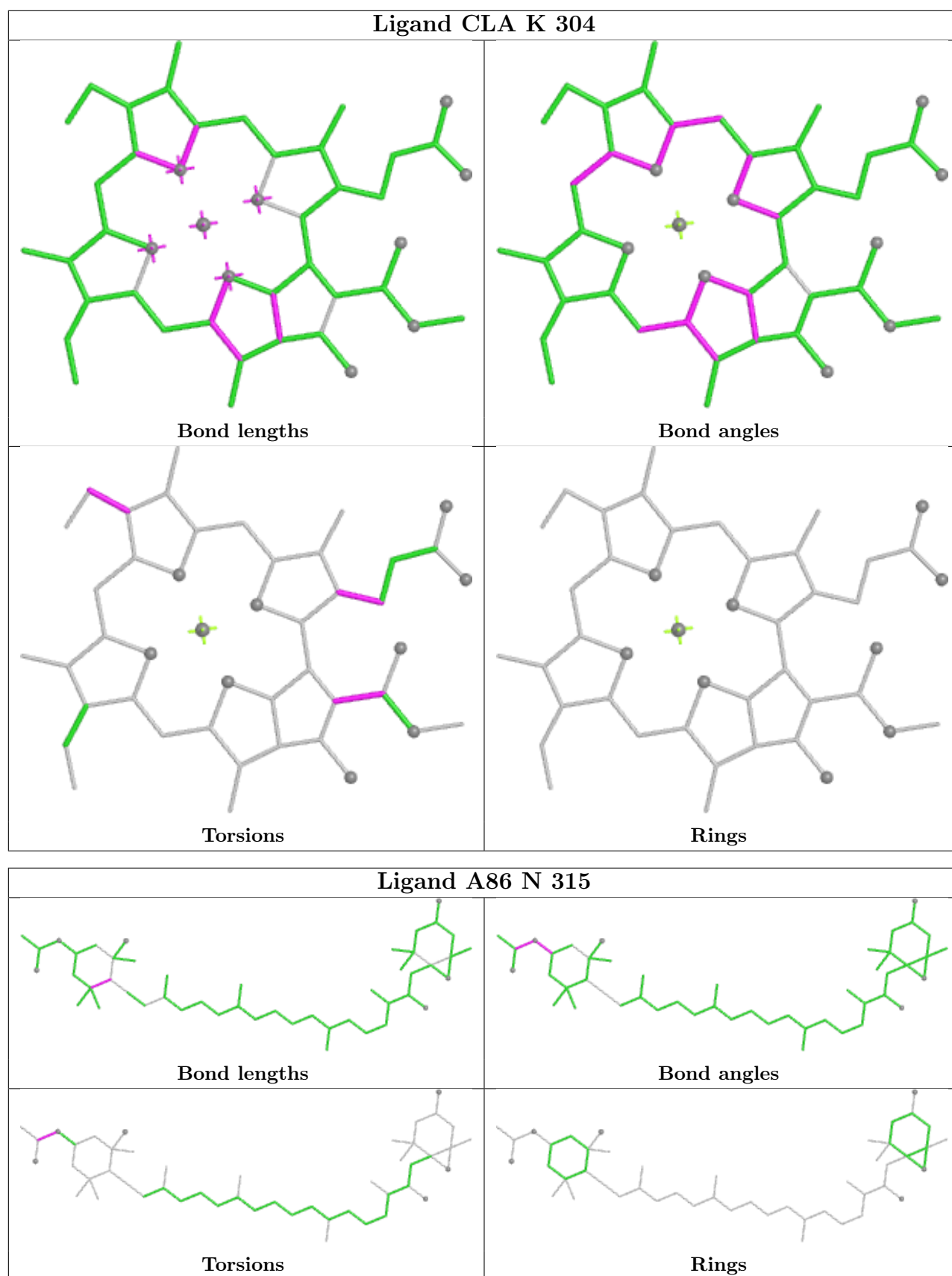


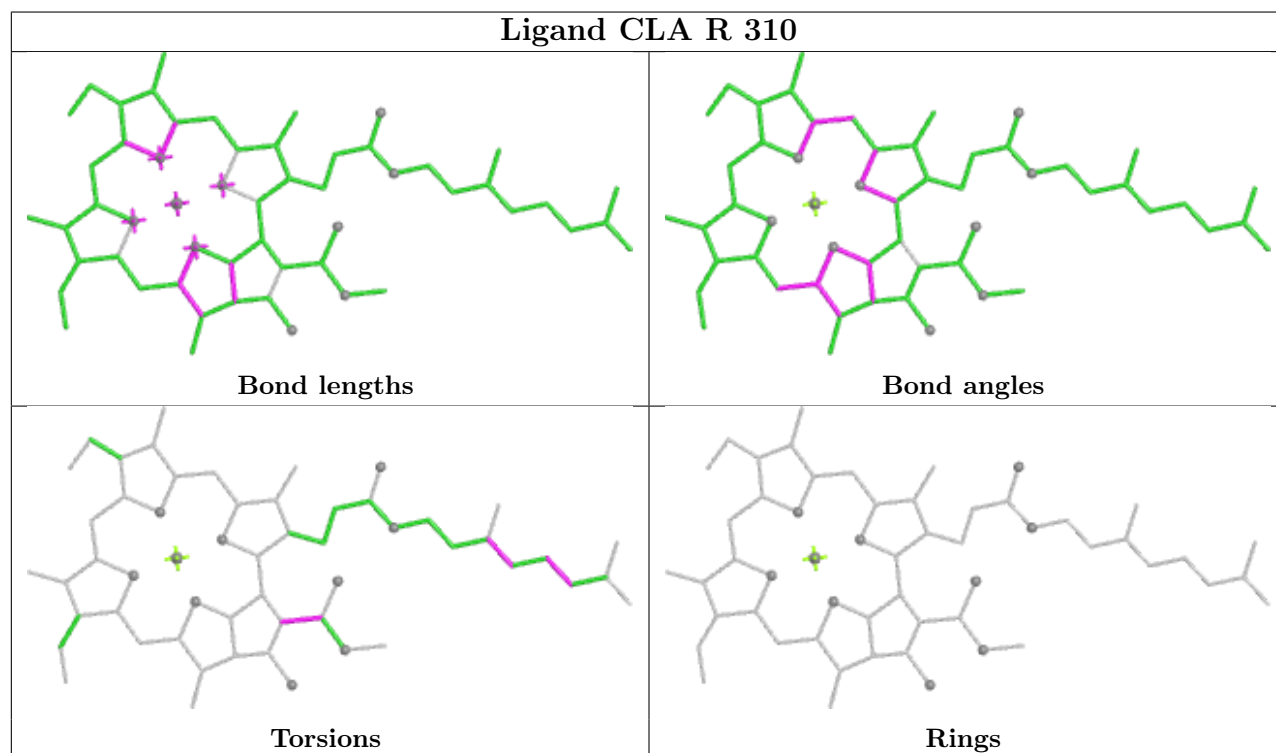
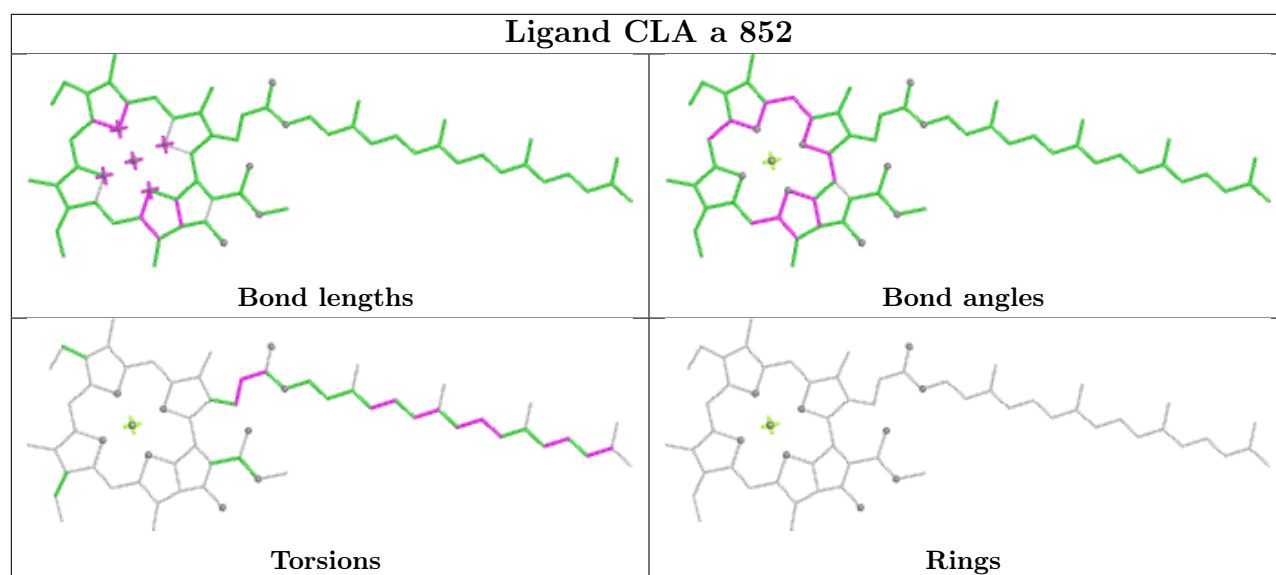
Torsions



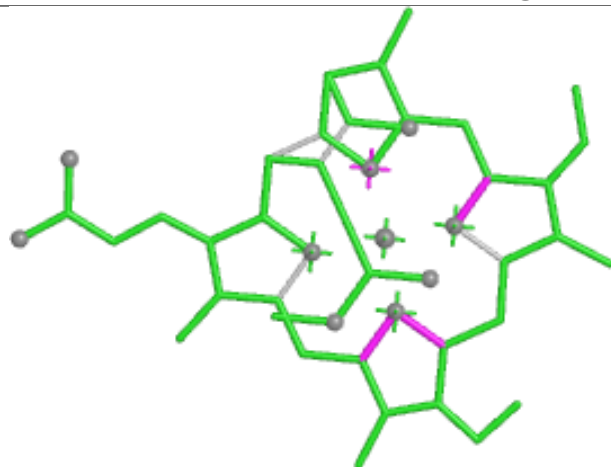
Rings



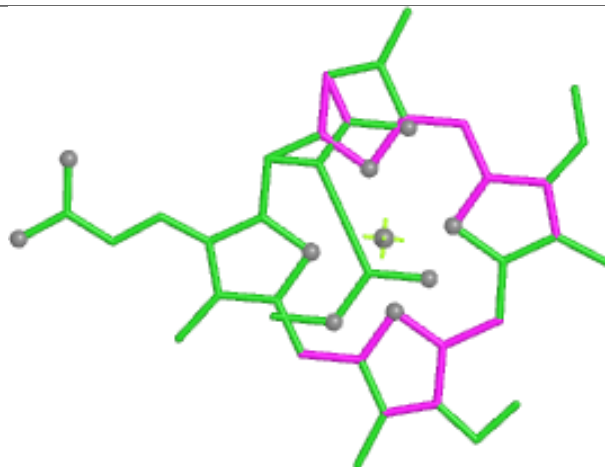




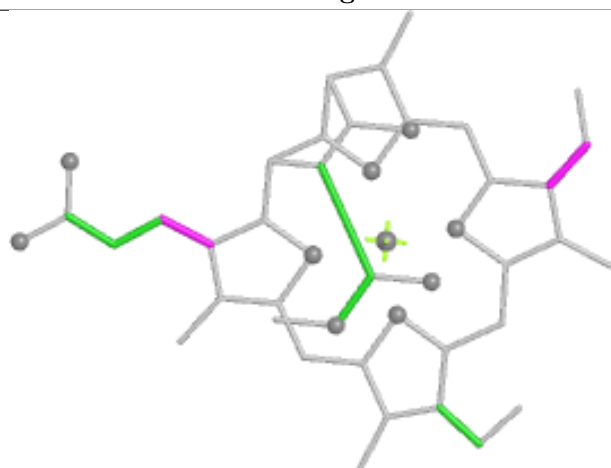
Ligand KC2 T 304



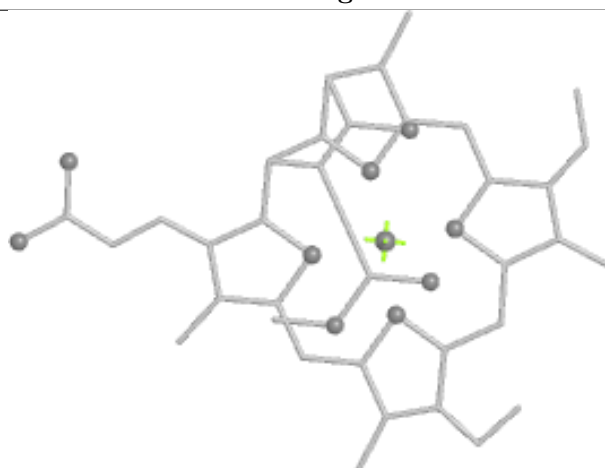
Bond lengths



Bond angles

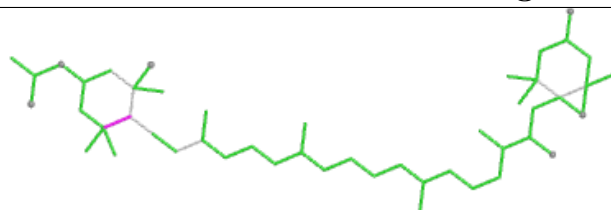


Torsions

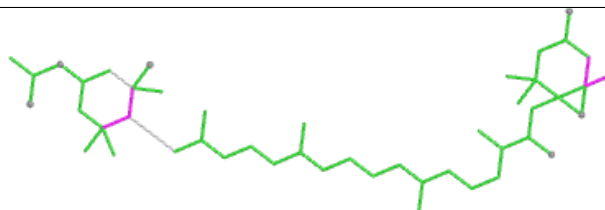


Rings

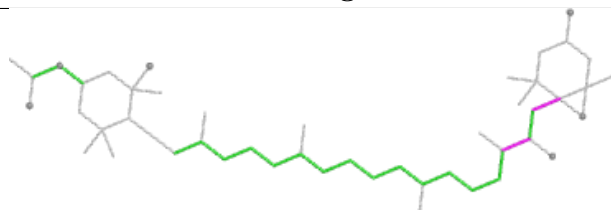
Ligand A86 M 314



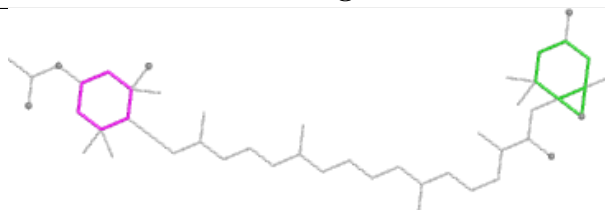
Bond lengths



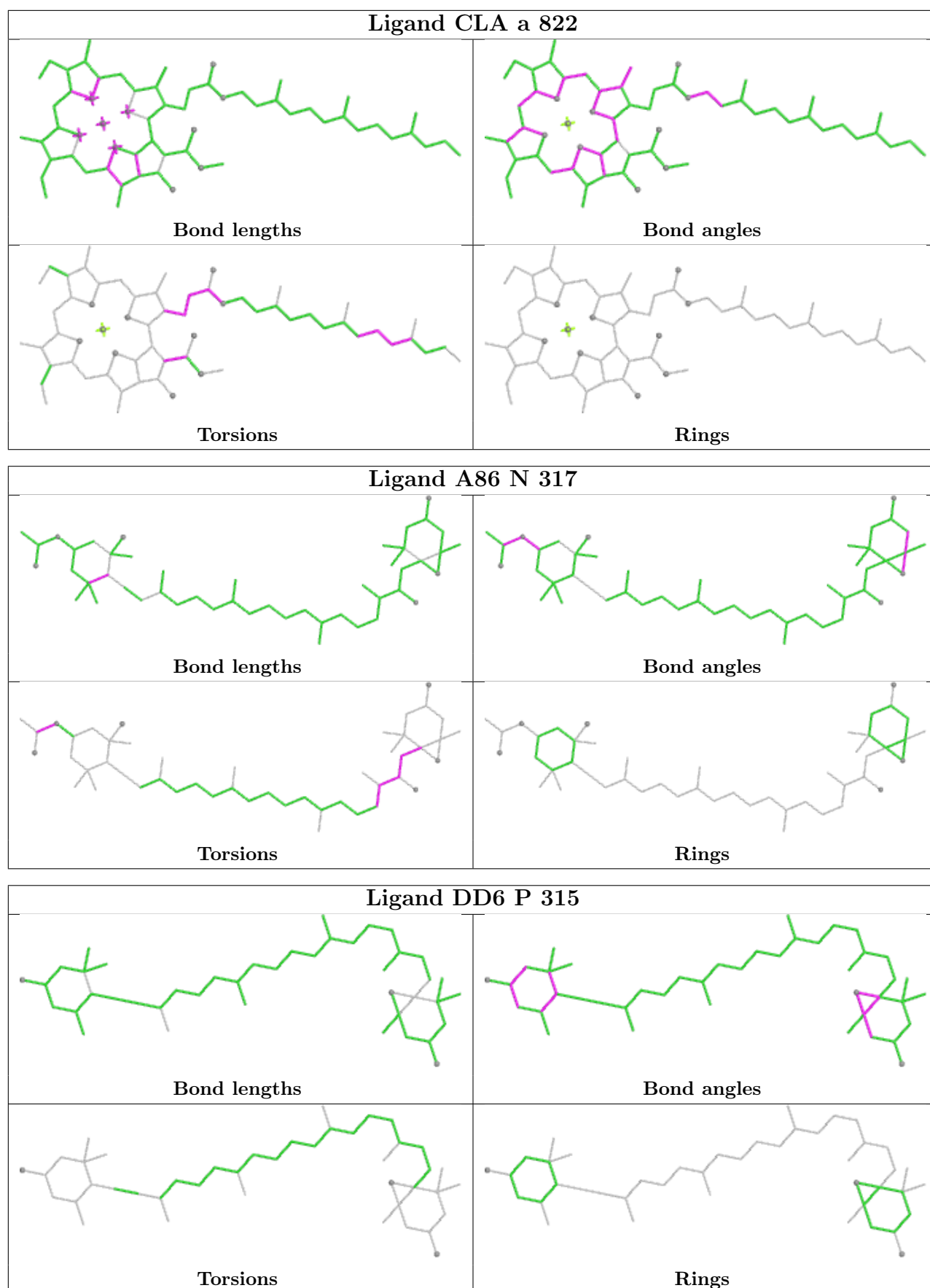
Bond angles

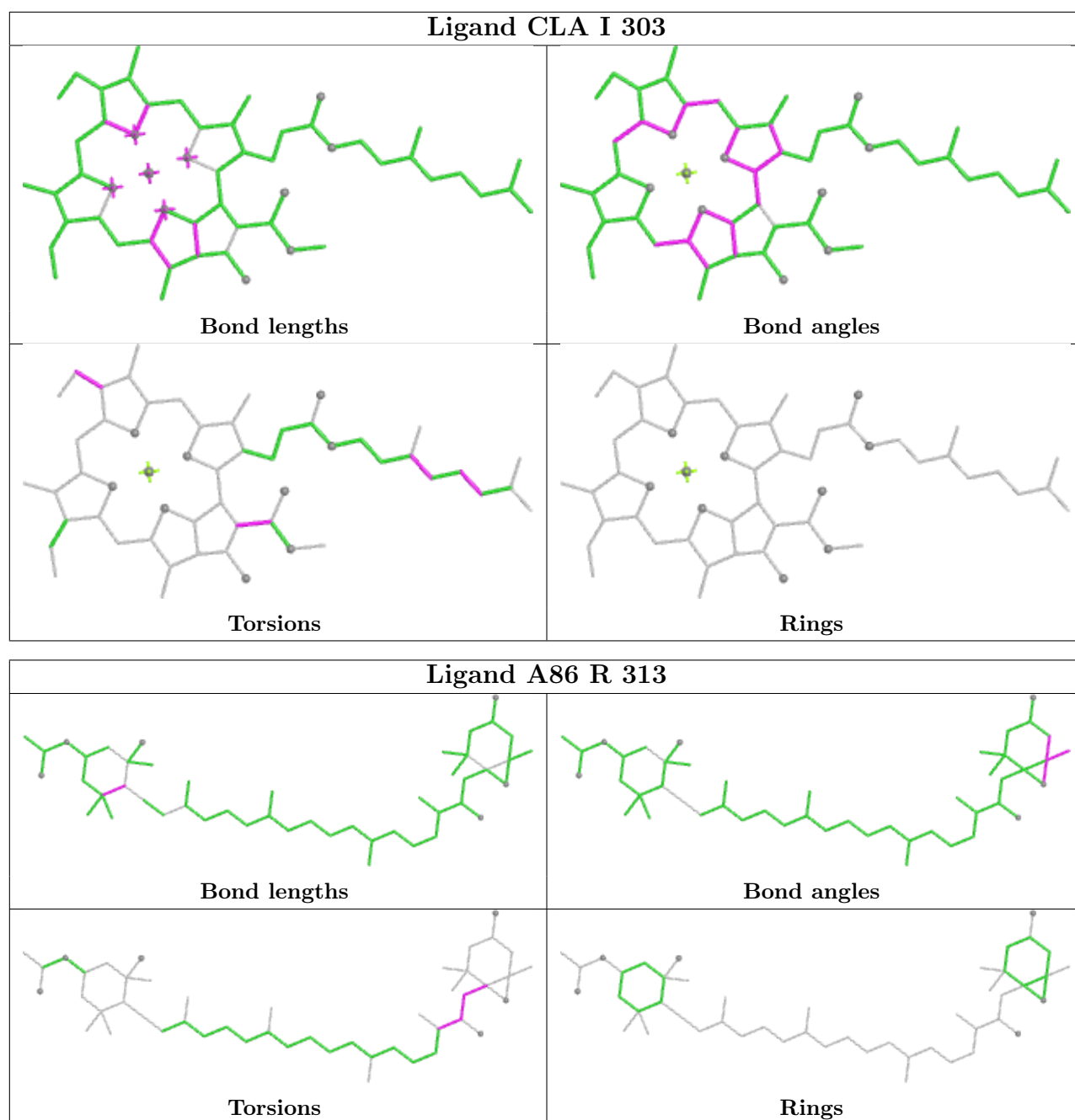


Torsions

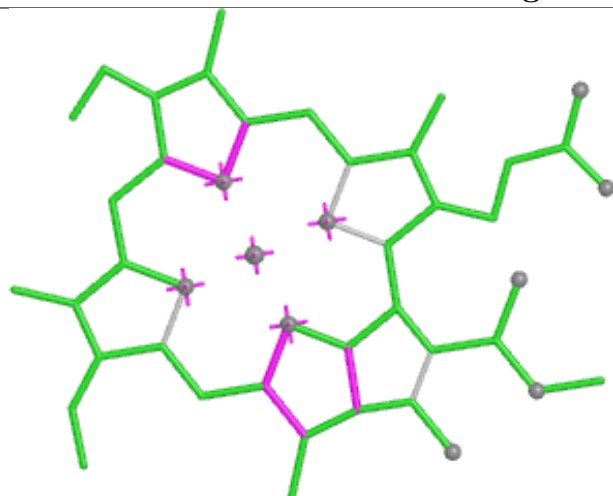


Rings

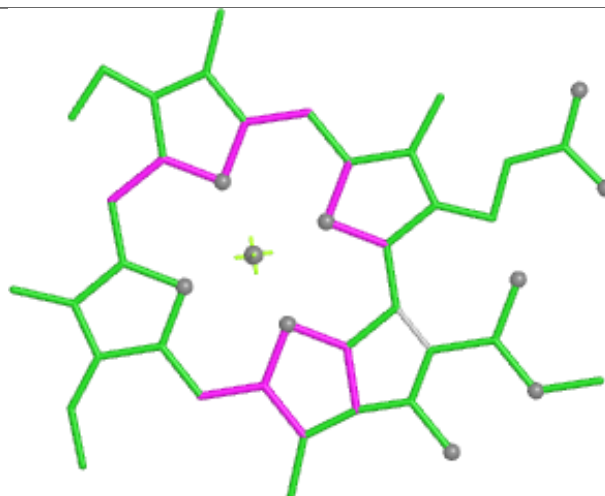




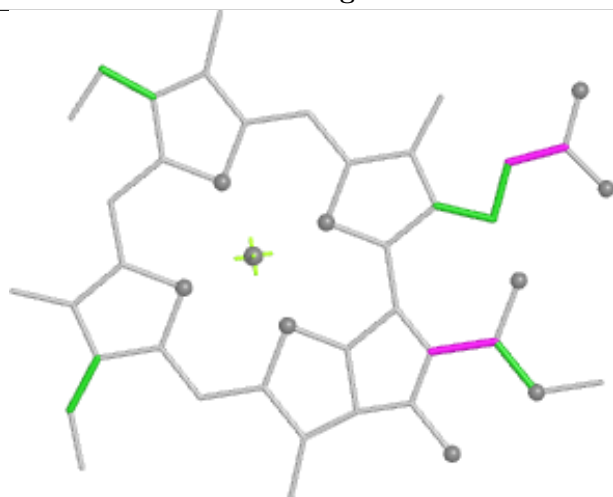
Ligand CLA I 202



Bond lengths



Bond angles

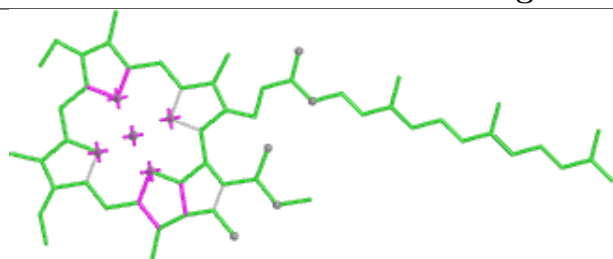


Torsions

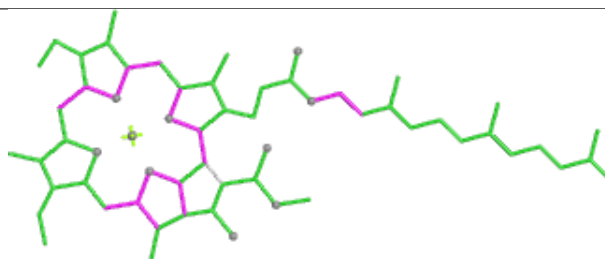


Rings

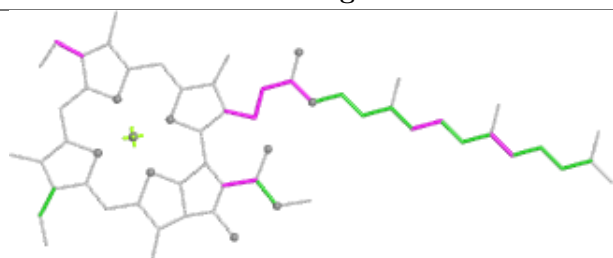
Ligand CLA F 322



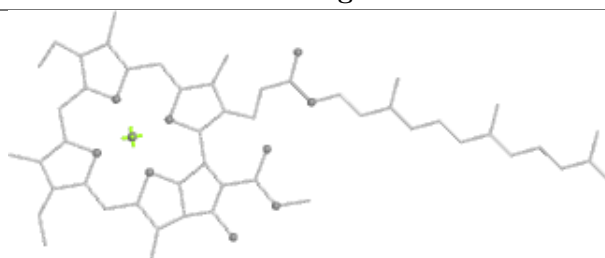
Bond lengths



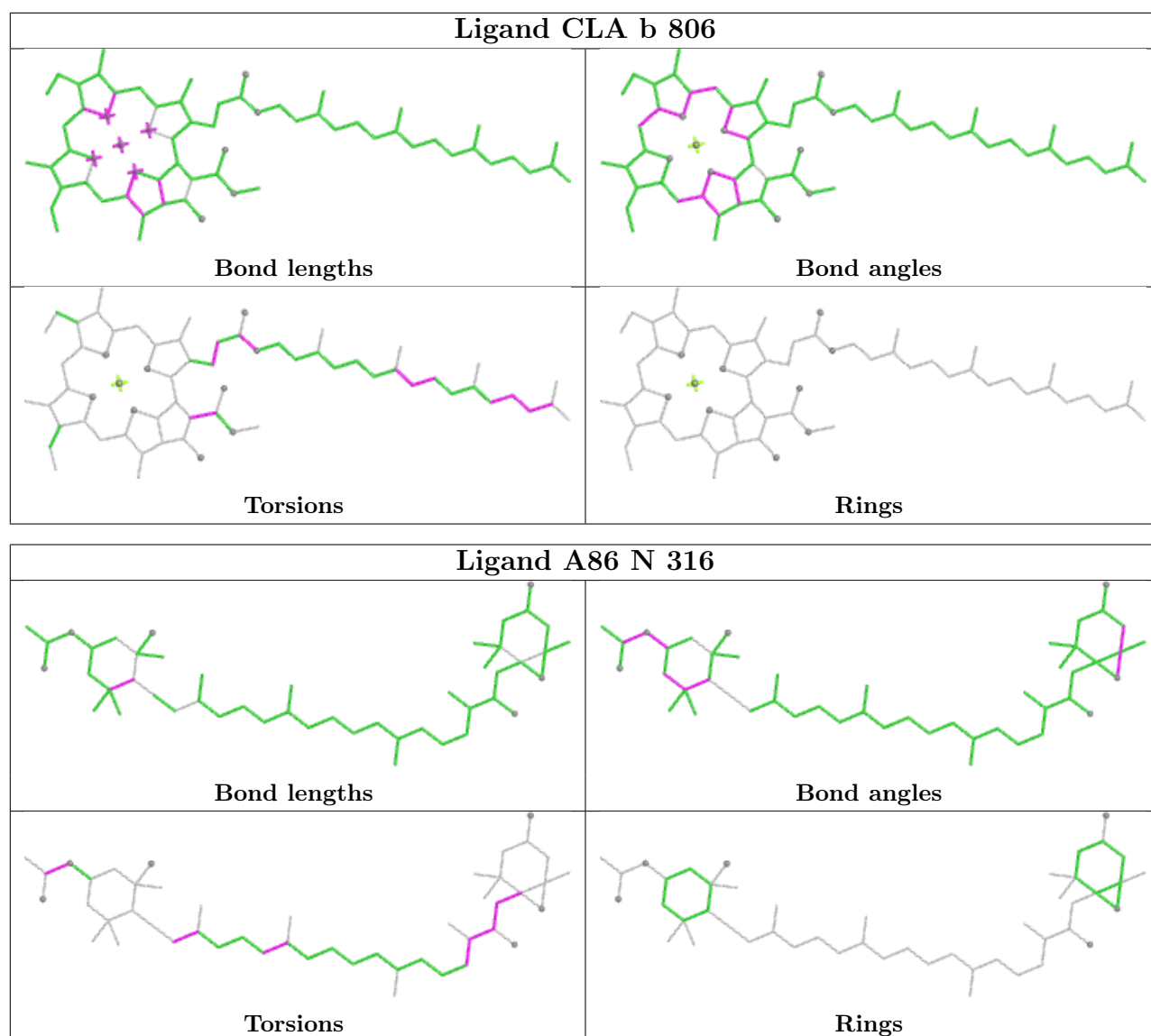
Bond angles

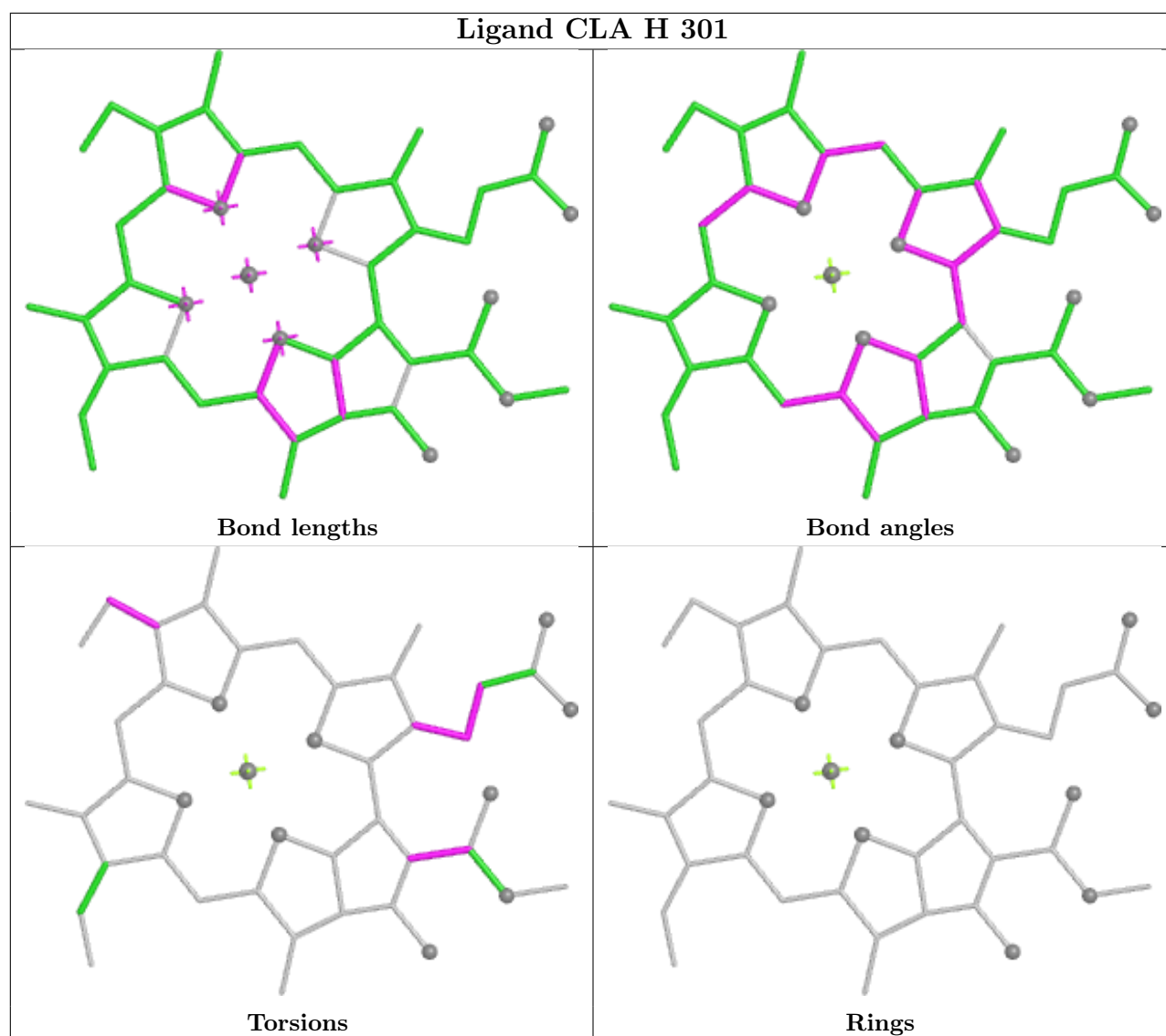


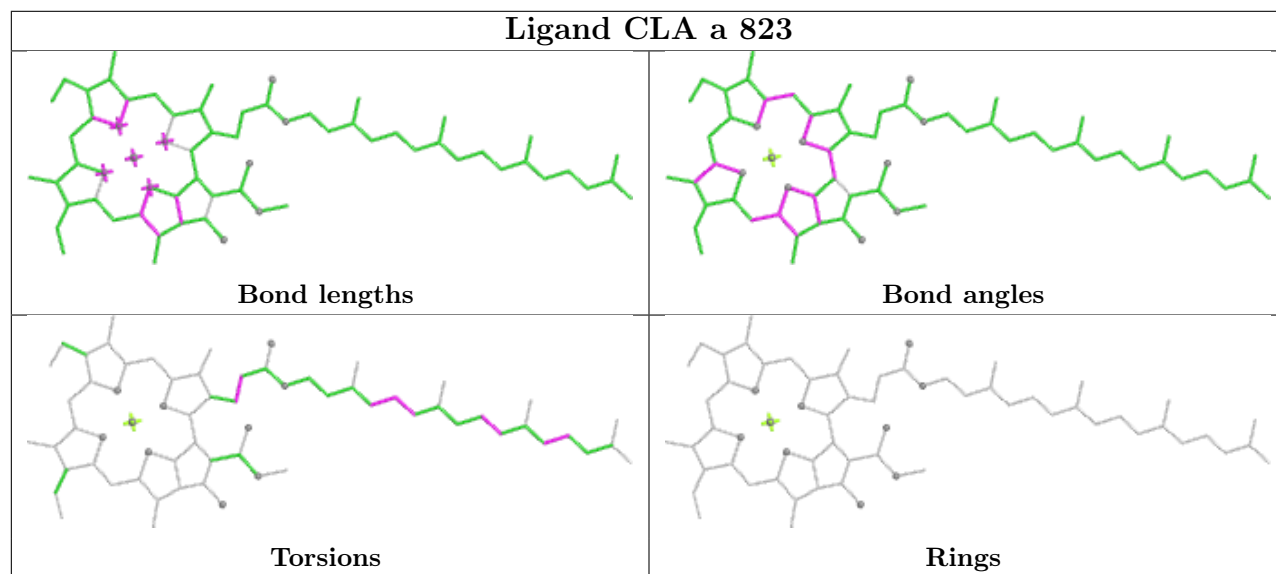
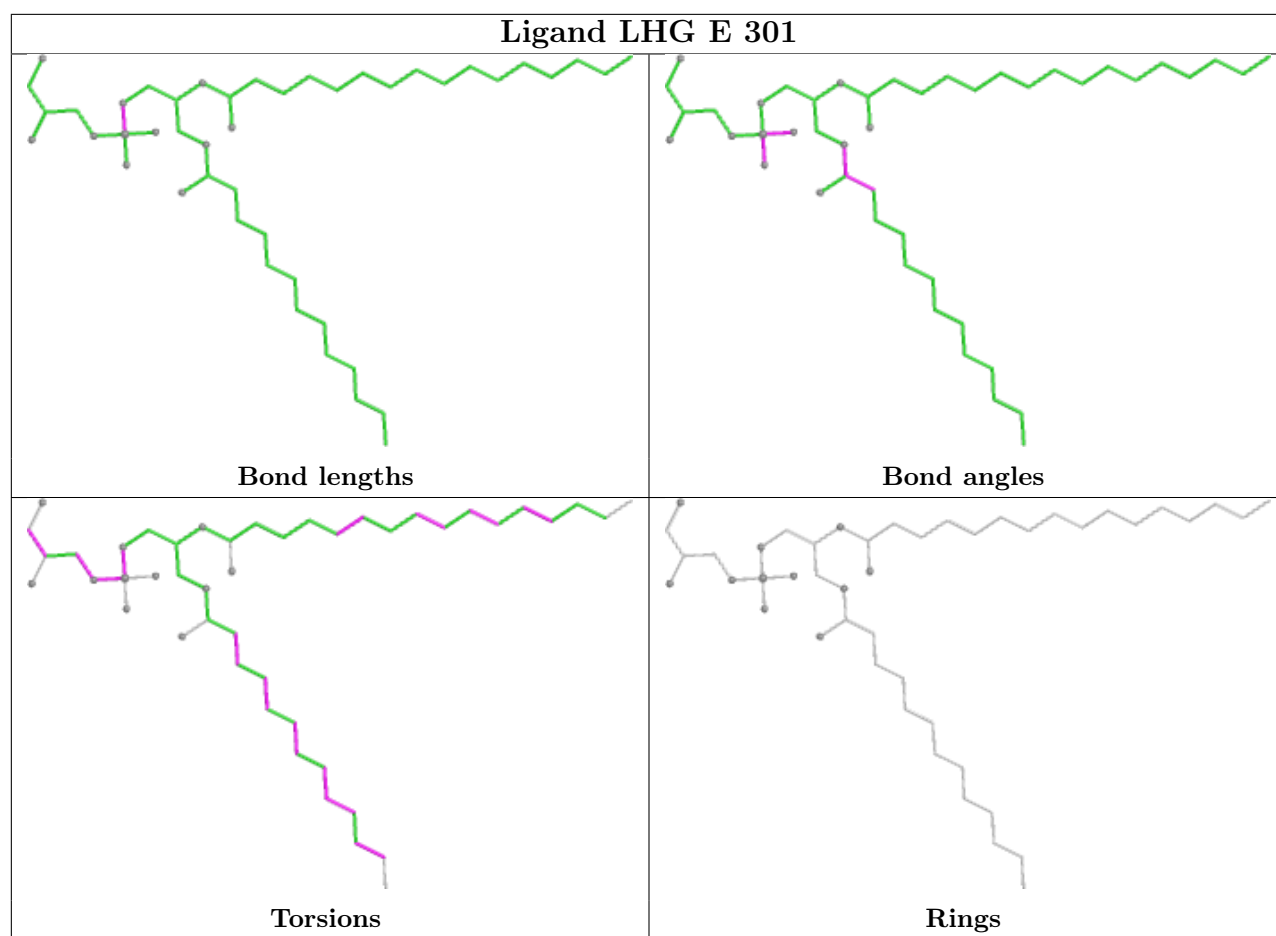
Torsions

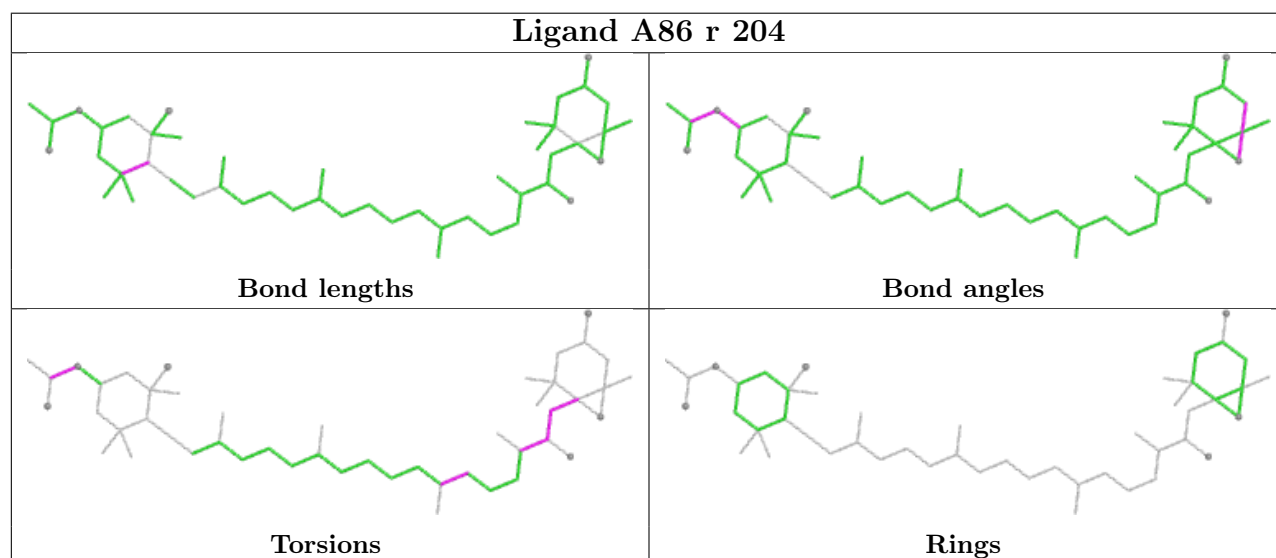
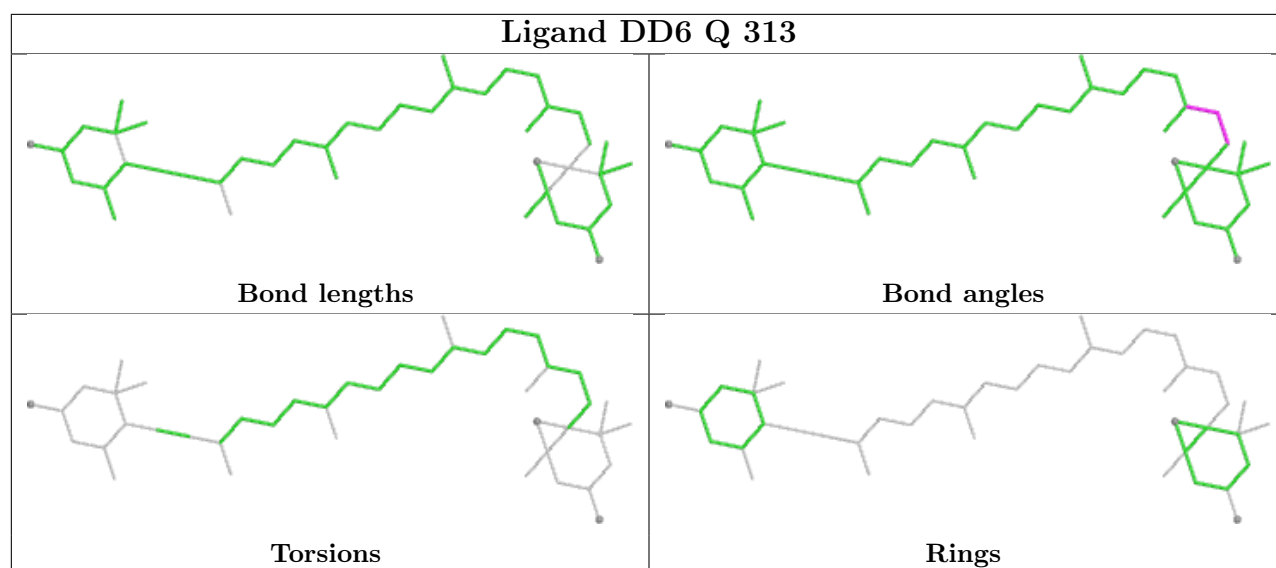


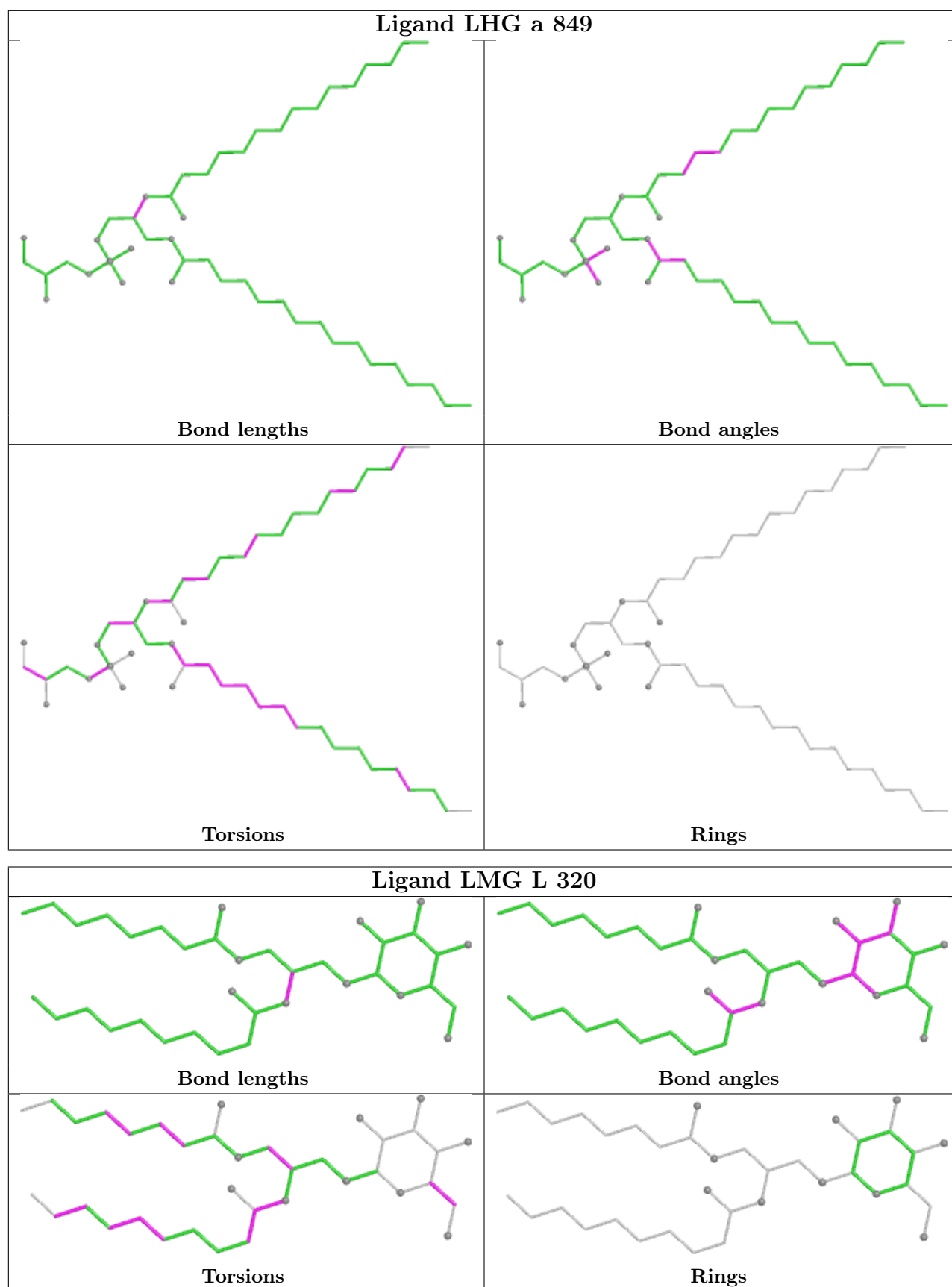
Rings

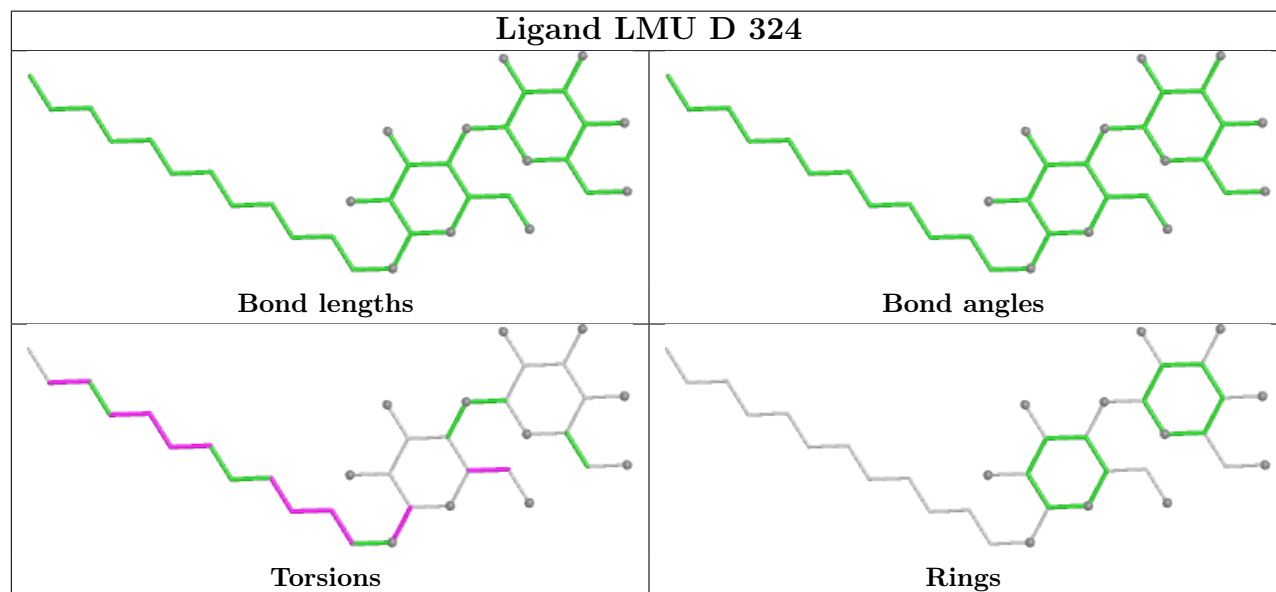
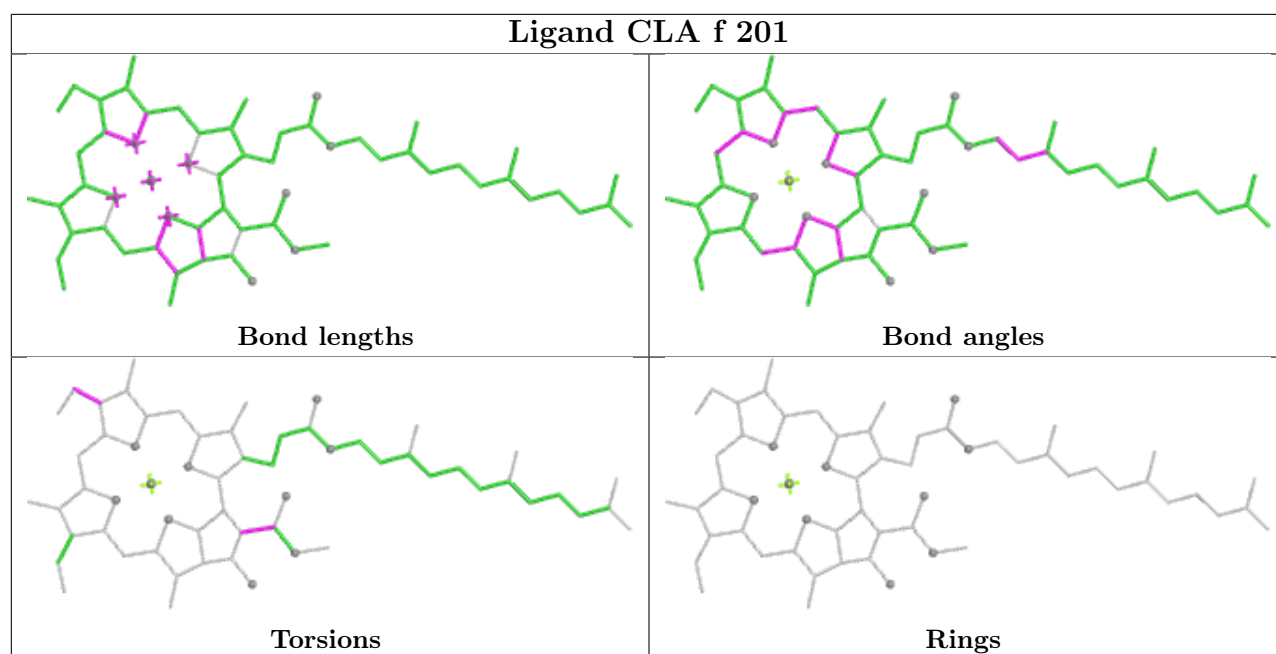


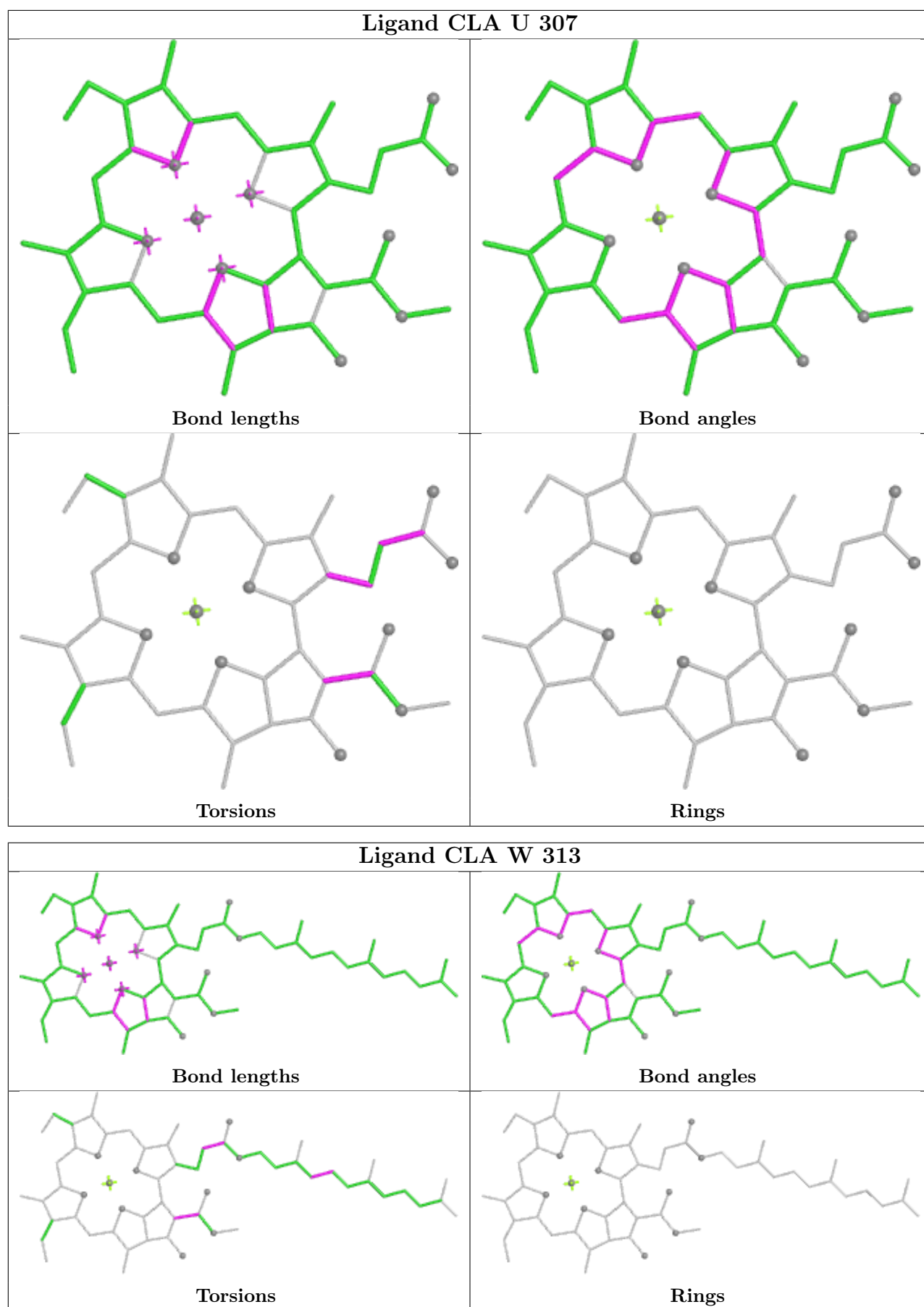


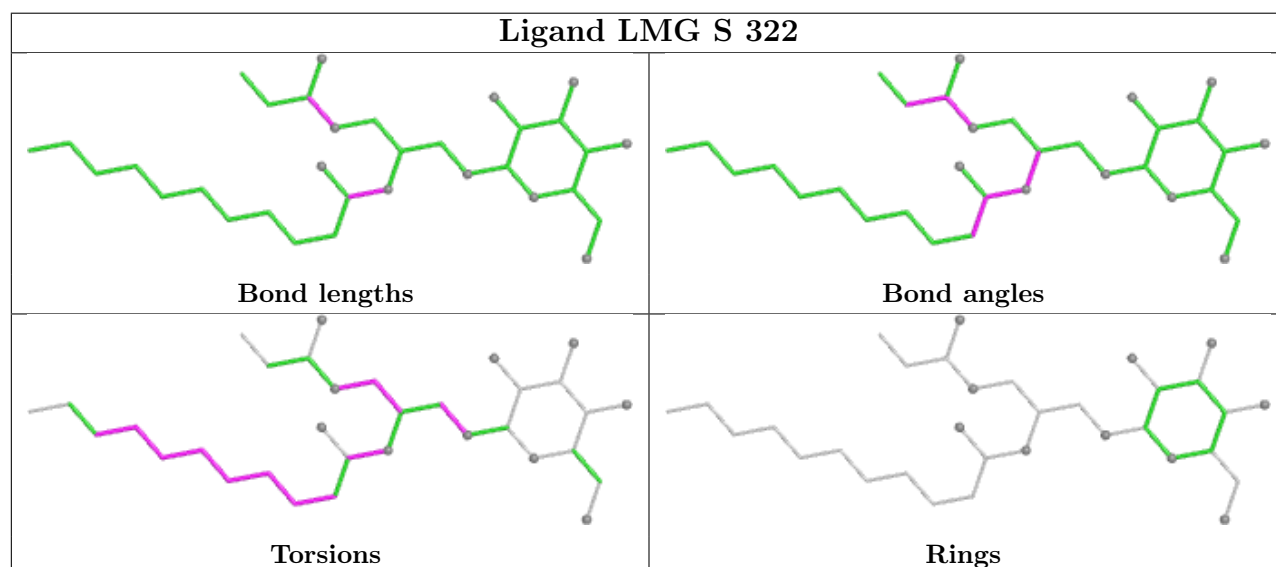
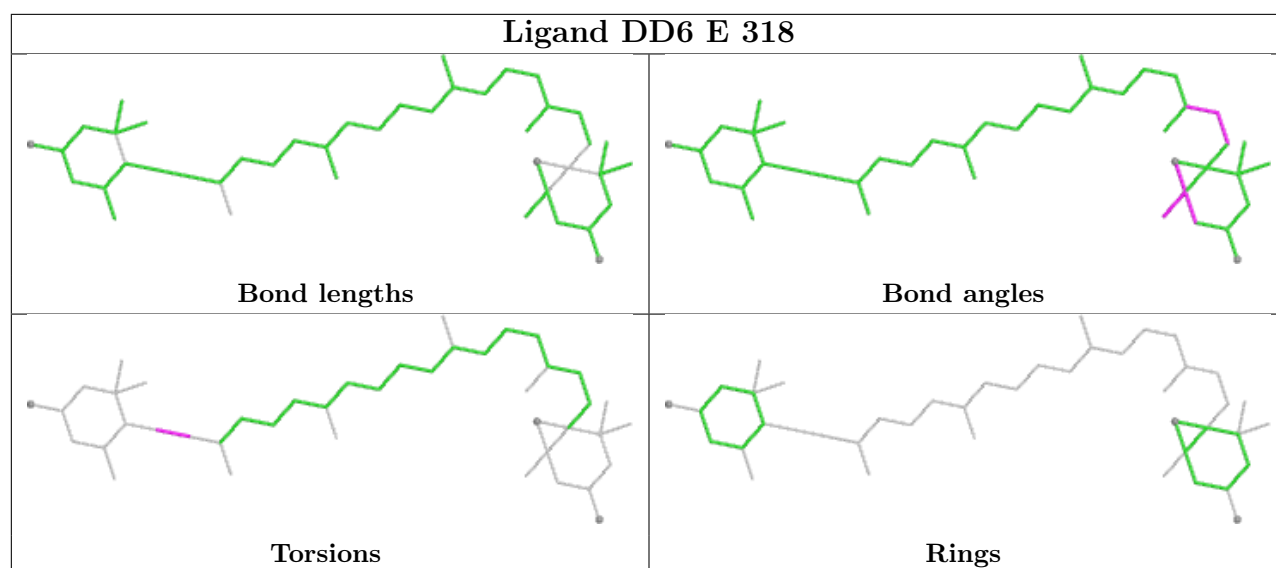


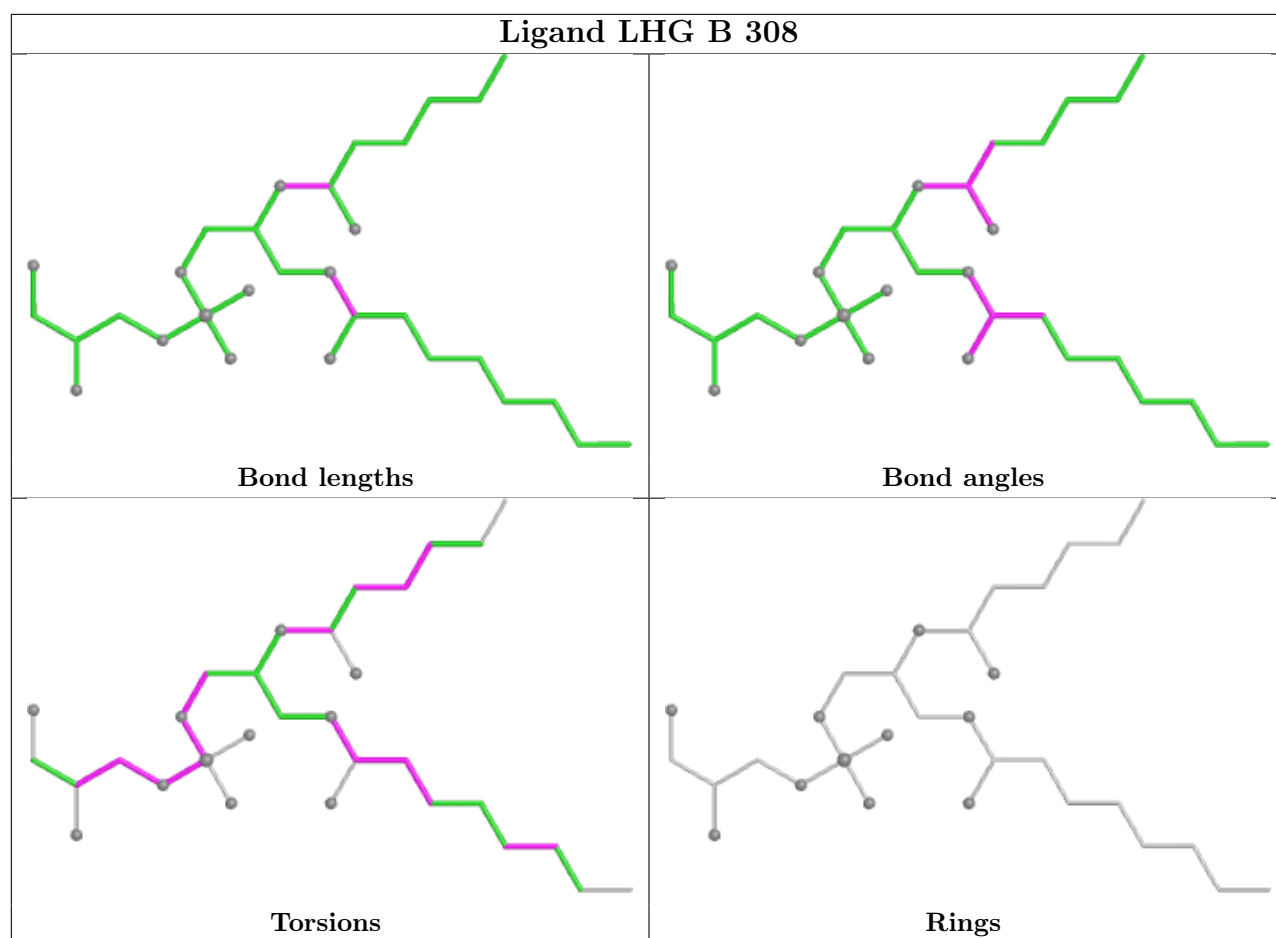


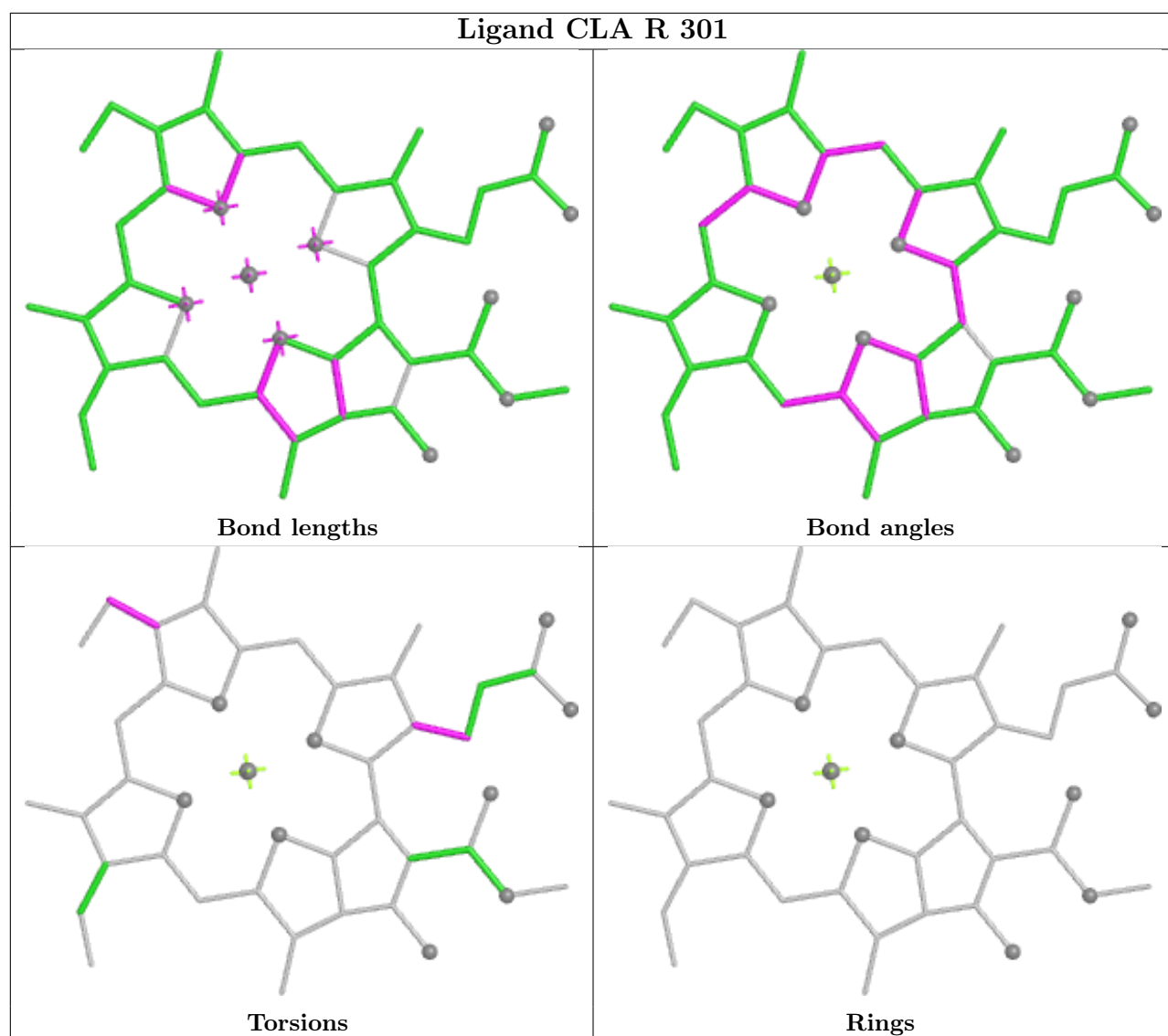




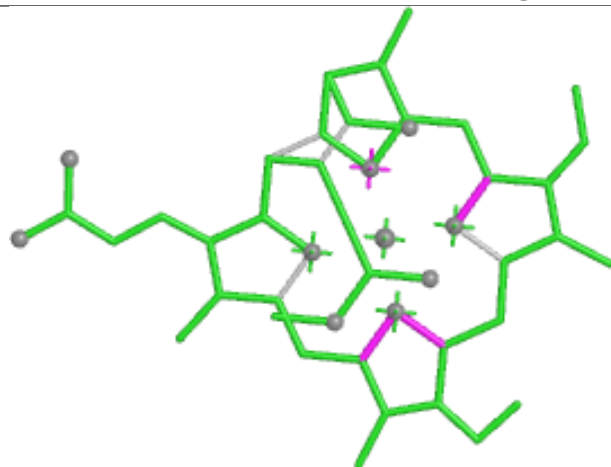




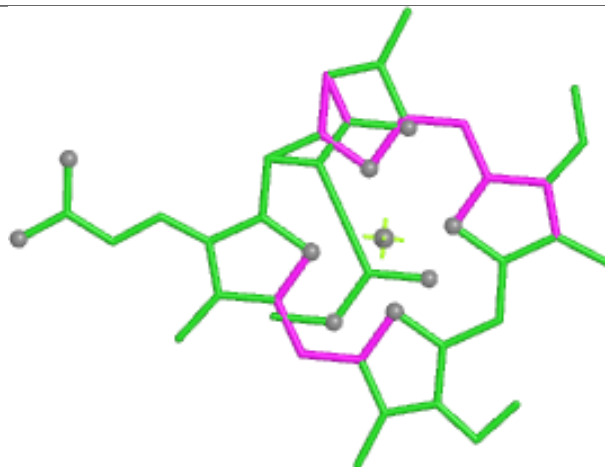




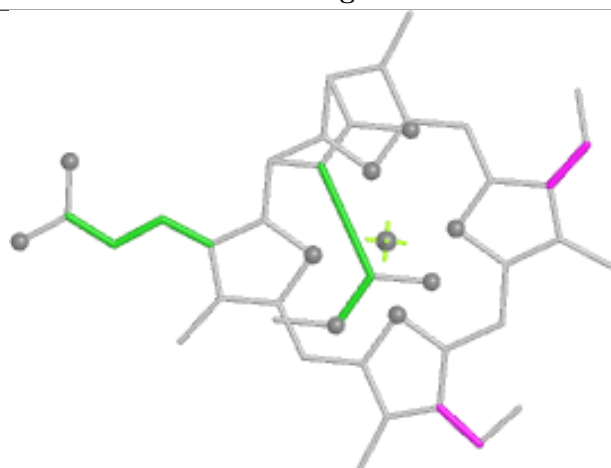
Ligand KC2 N 307



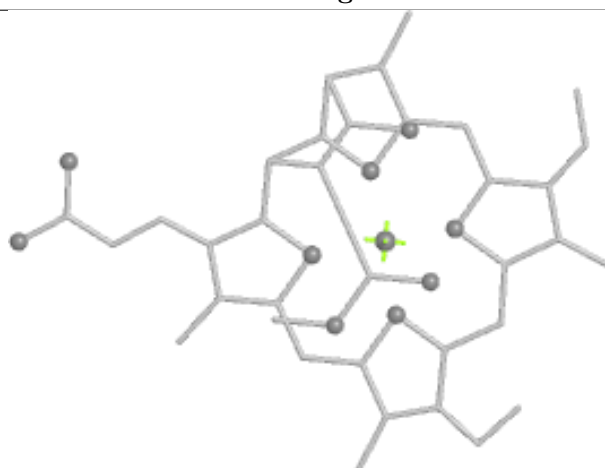
Bond lengths



Bond angles

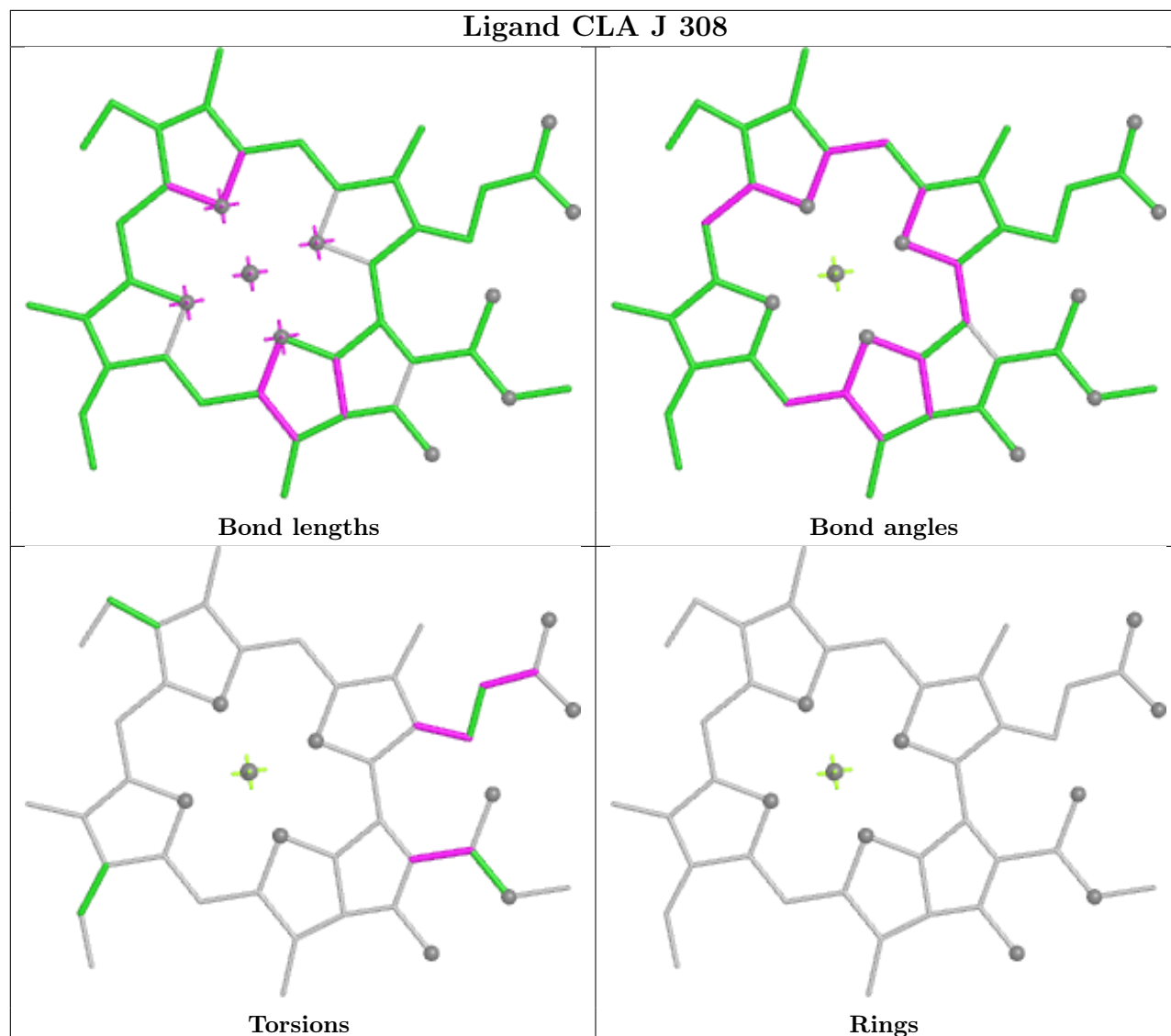


Torsions

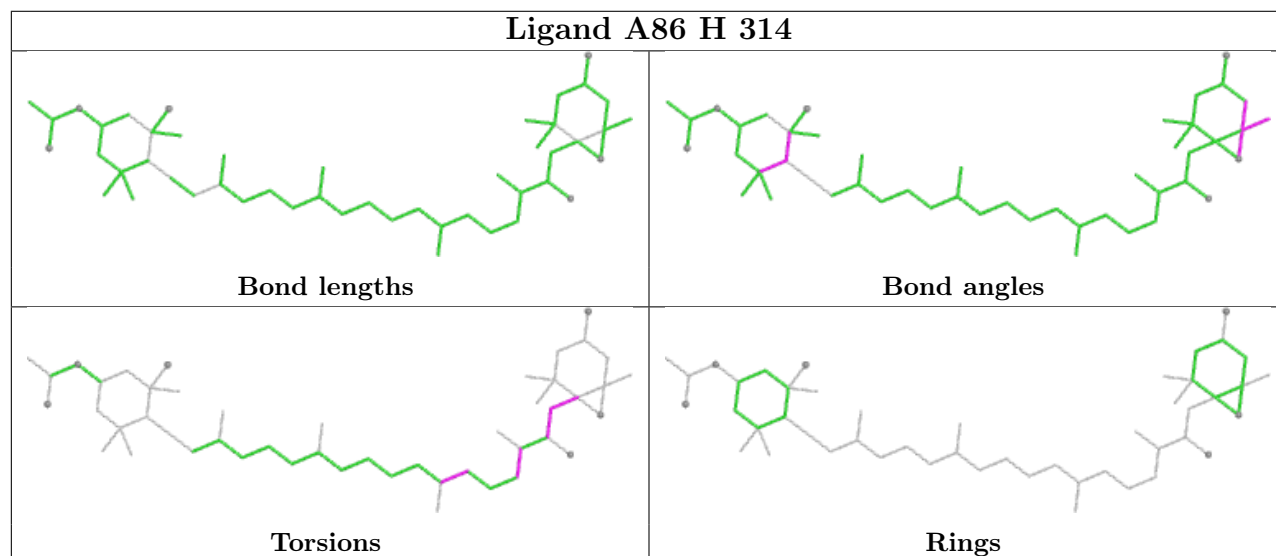


Rings

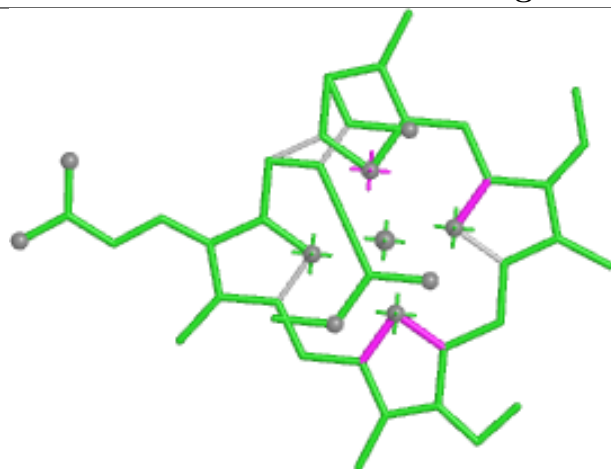
Ligand CLA J 308



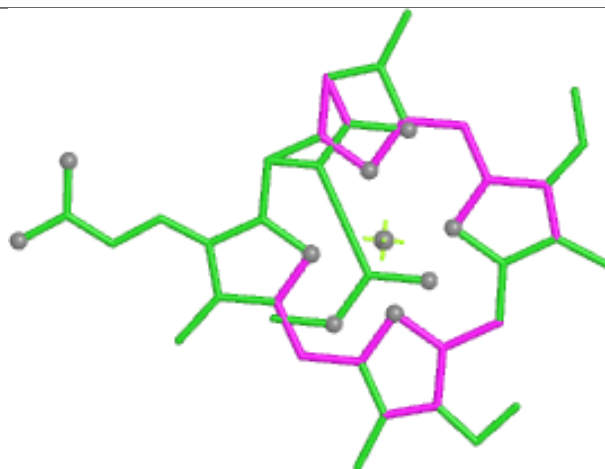
Ligand A86 H 314



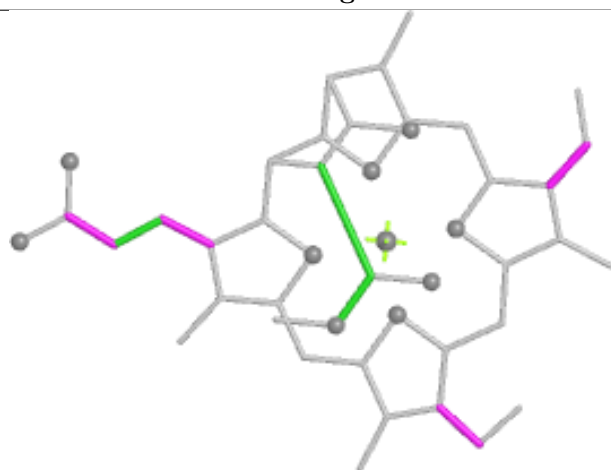
Ligand KC2 K 303



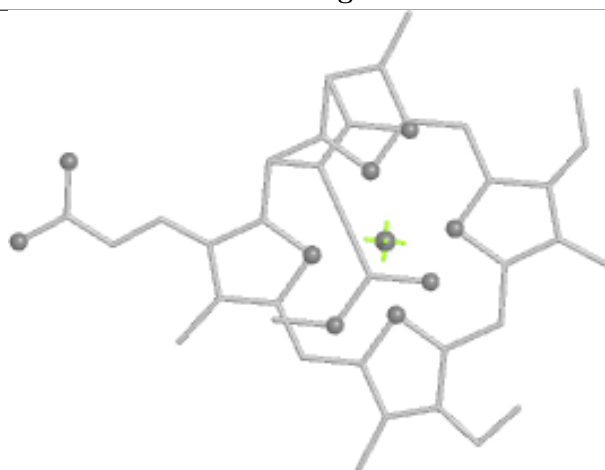
Bond lengths



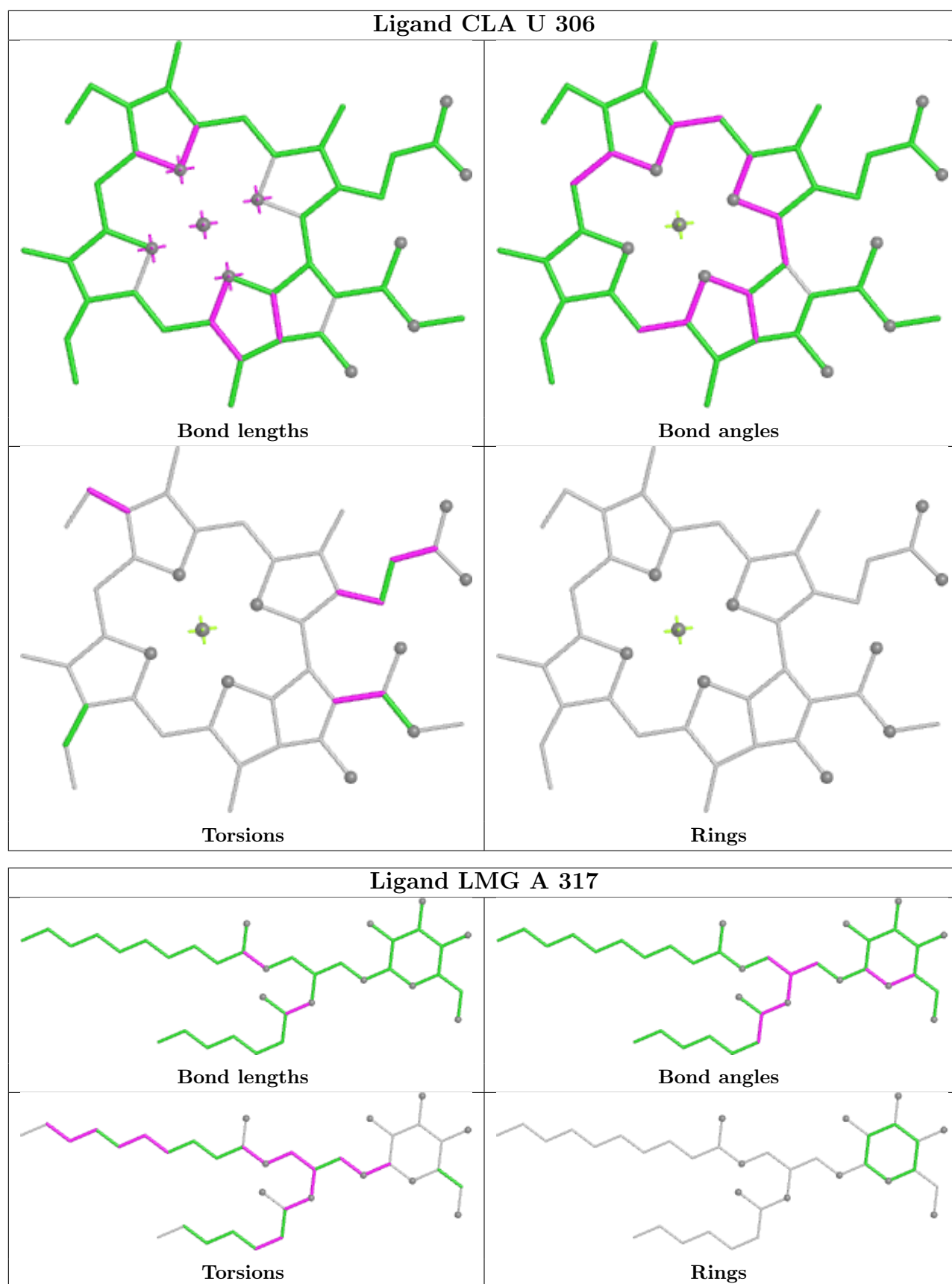
Bond angles

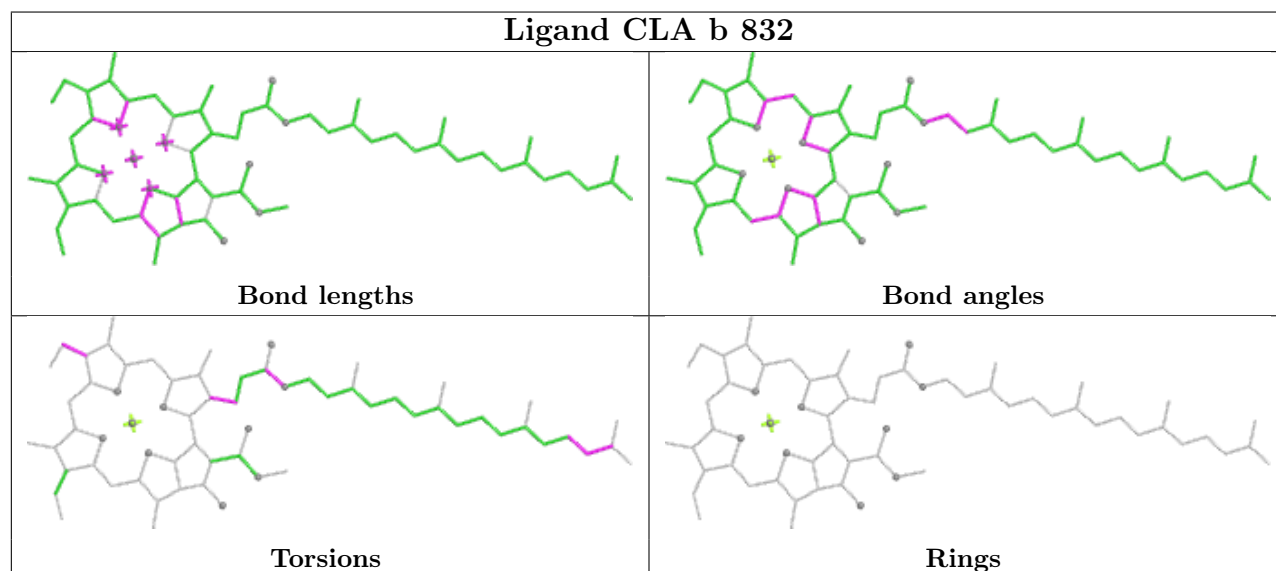
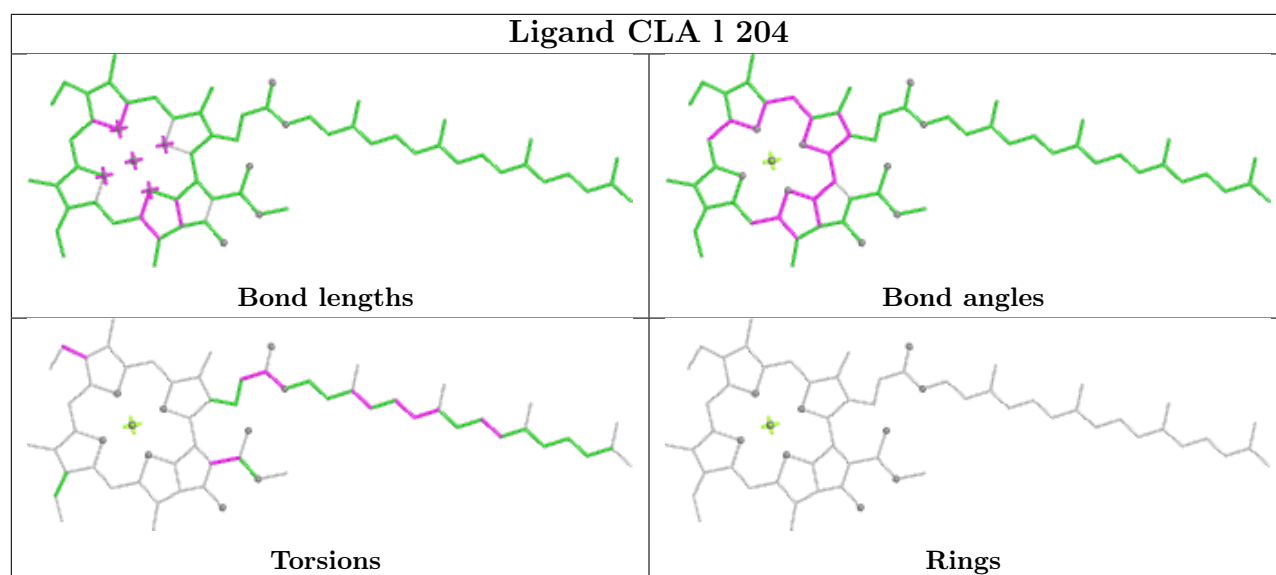


Torsions

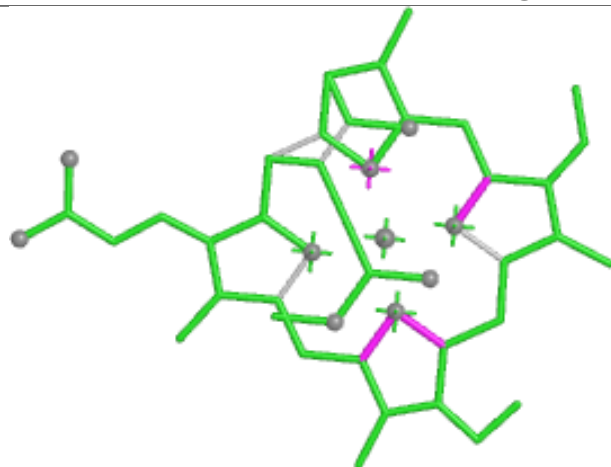


Rings

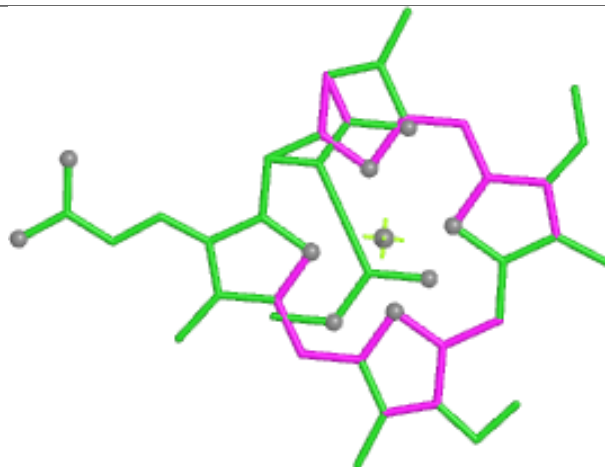




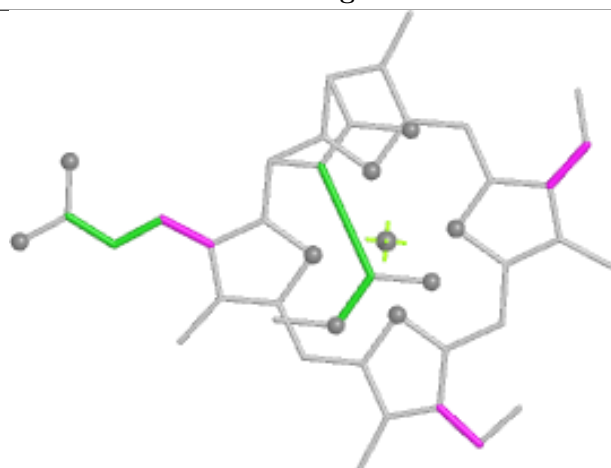
Ligand KC2 R 302



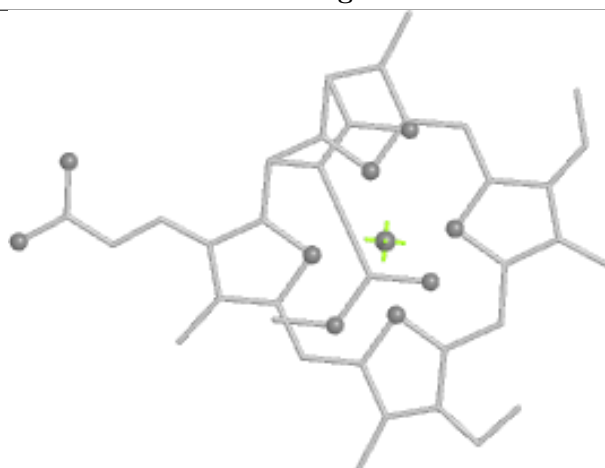
Bond lengths



Bond angles

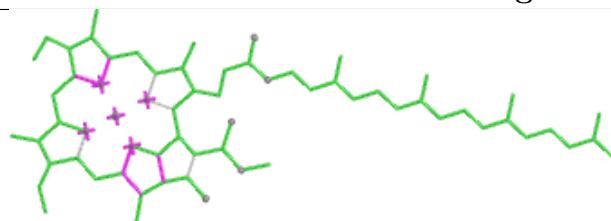


Torsions

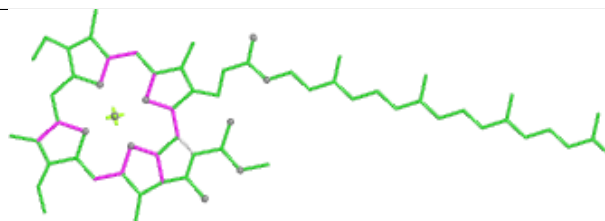


Rings

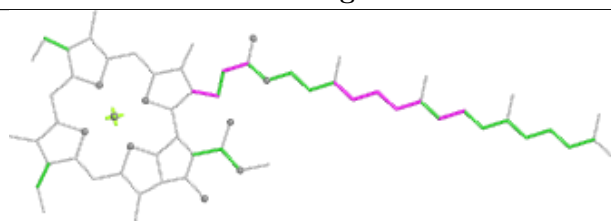
Ligand CLA E 308



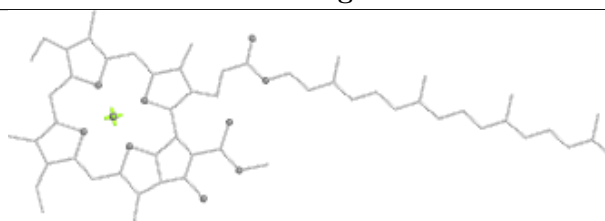
Bond lengths



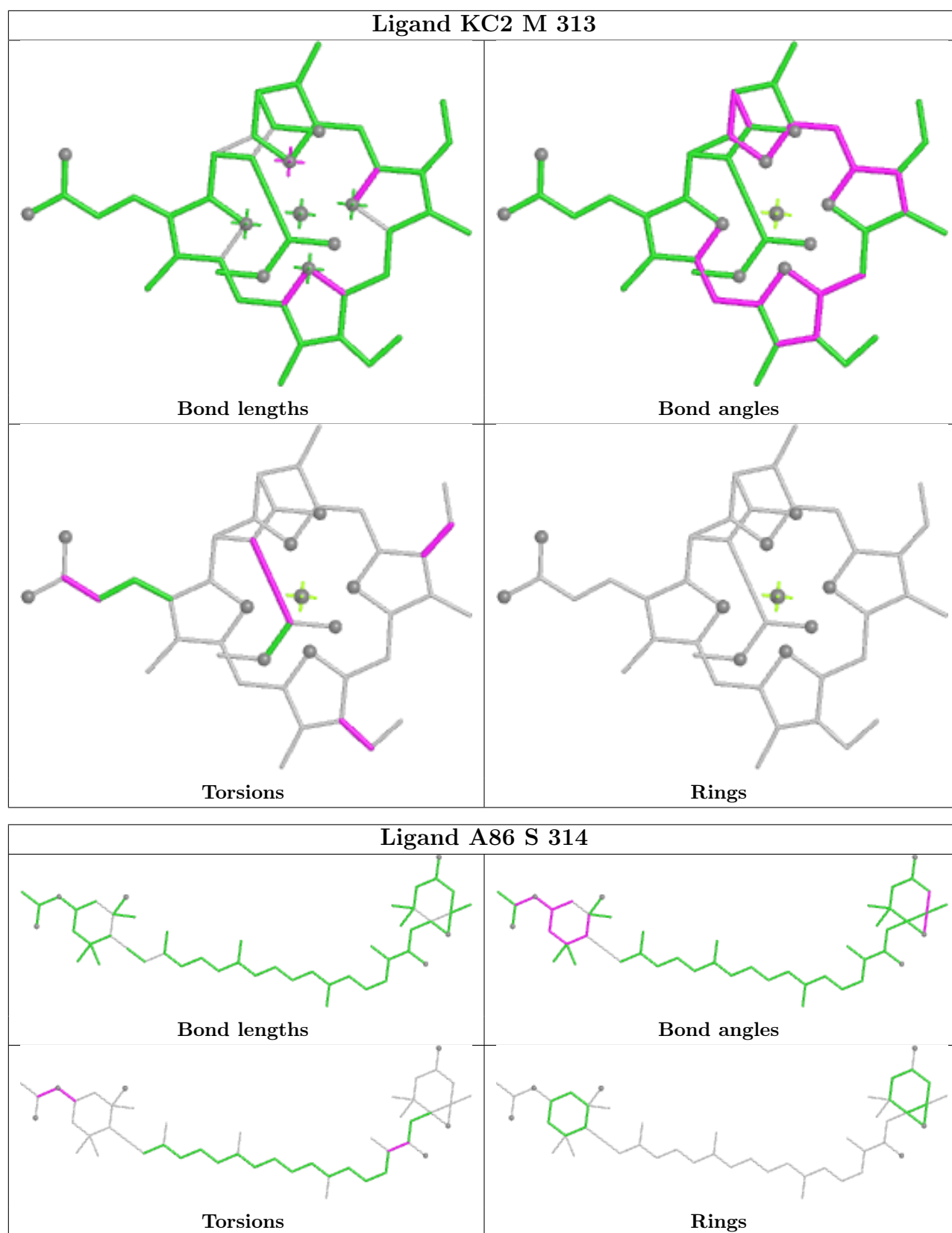
Bond angles



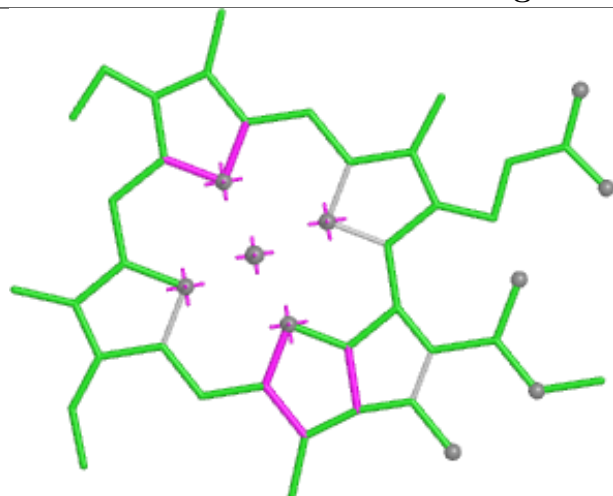
Torsions



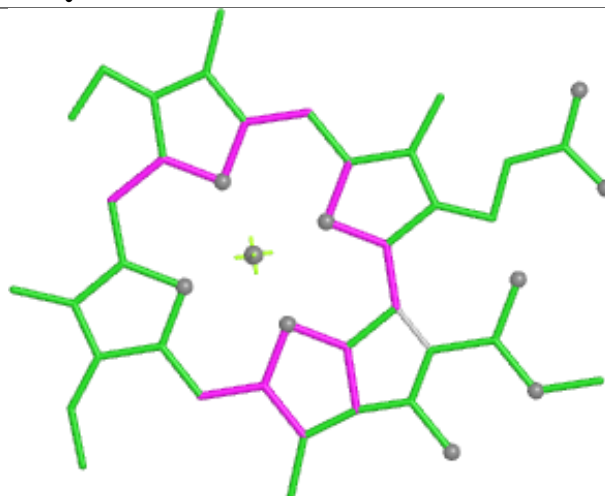
Rings



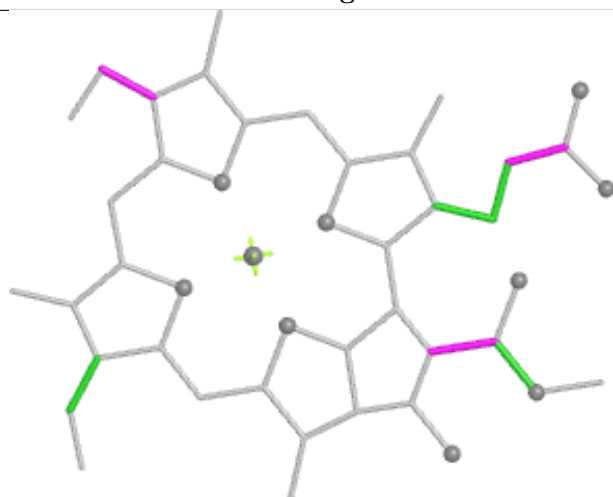
Ligand CLA Q 308



Bond lengths



Bond angles

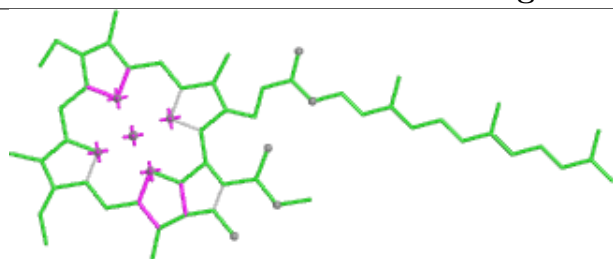


Torsions

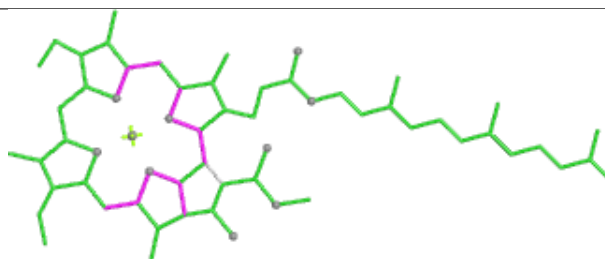


Rings

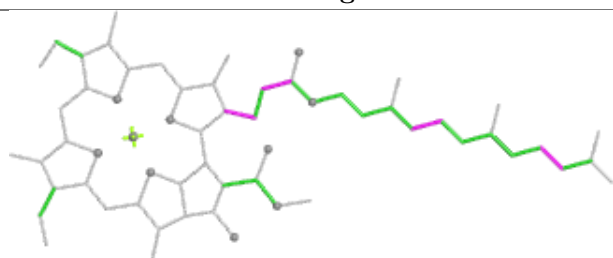
Ligand CLA b 810



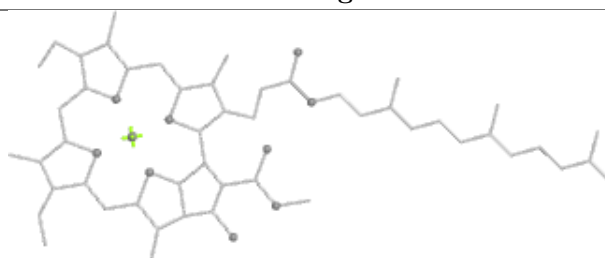
Bond lengths



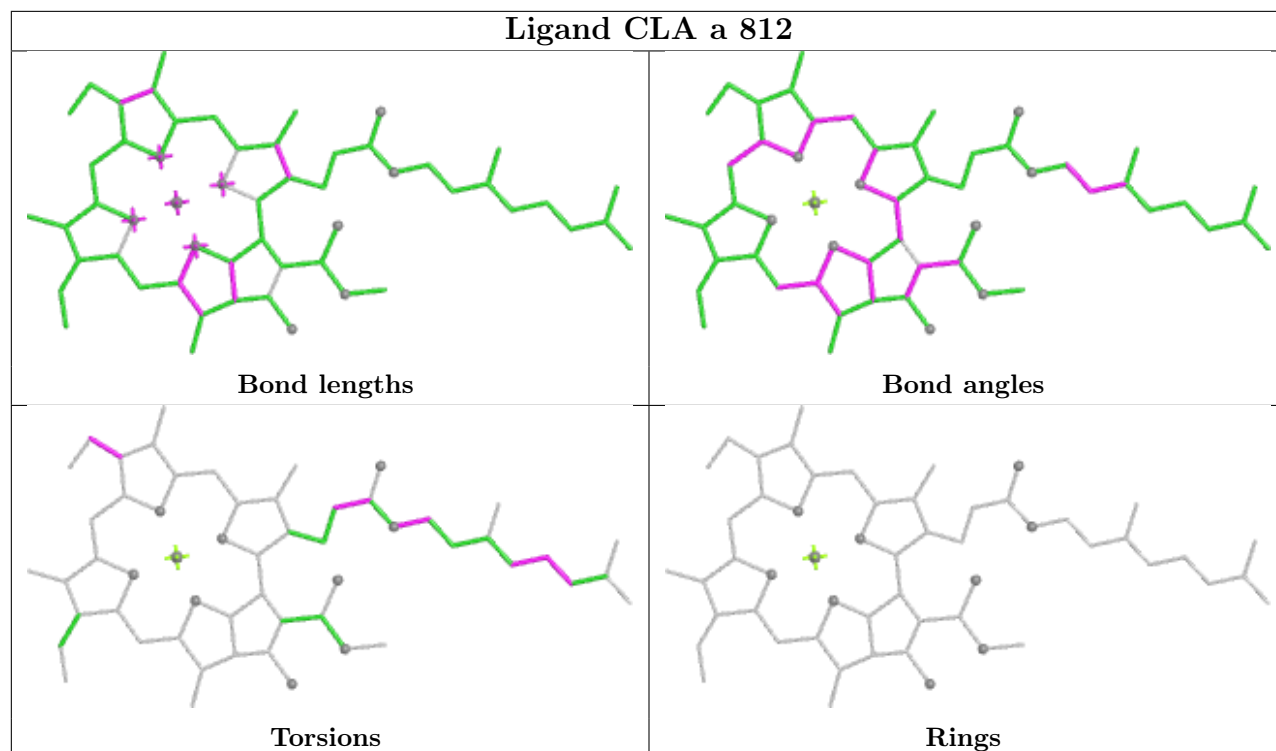
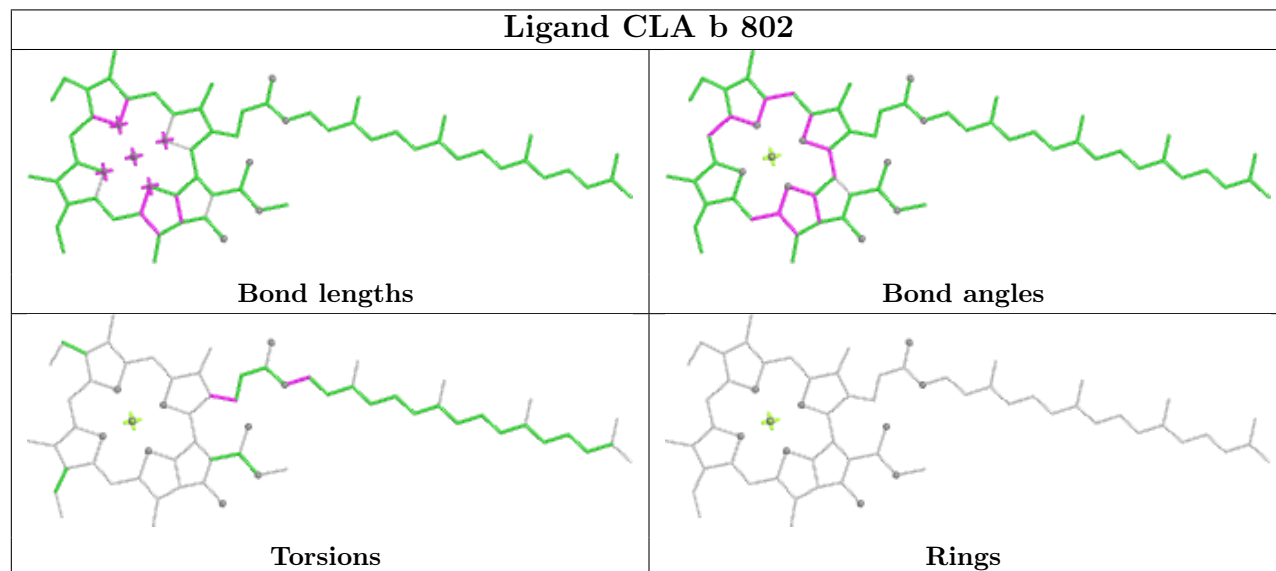
Bond angles

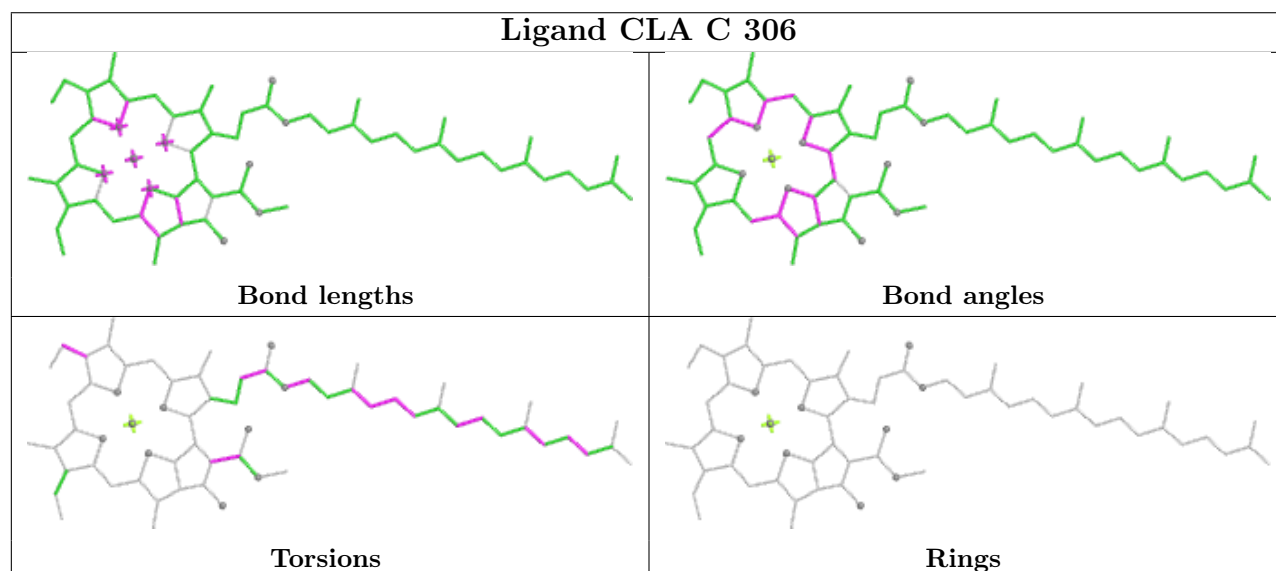
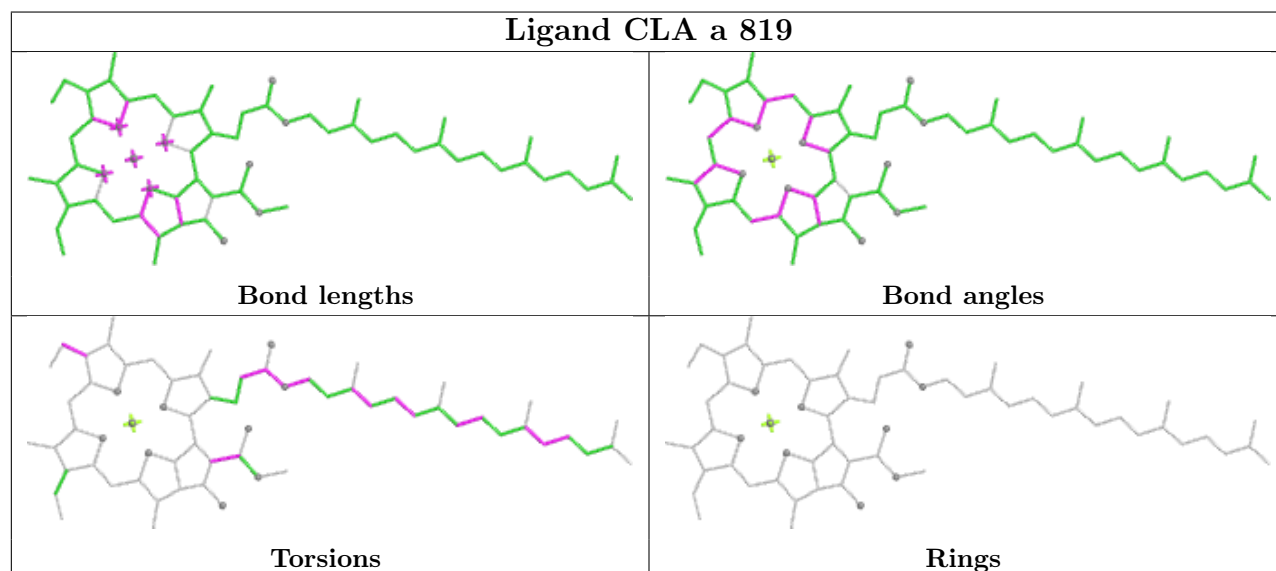
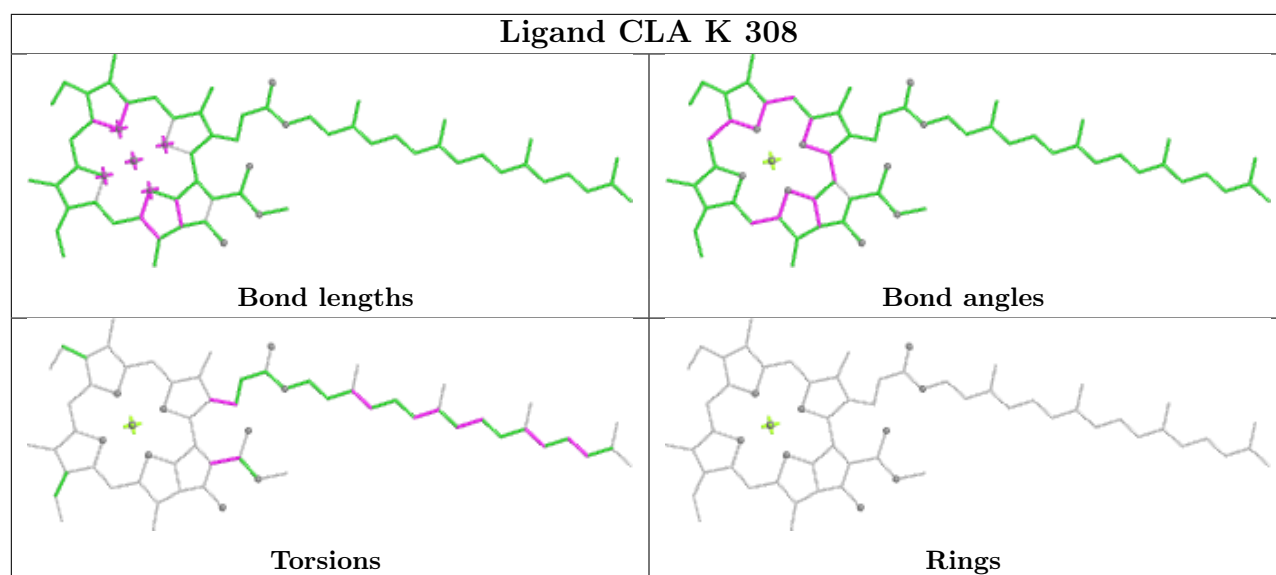


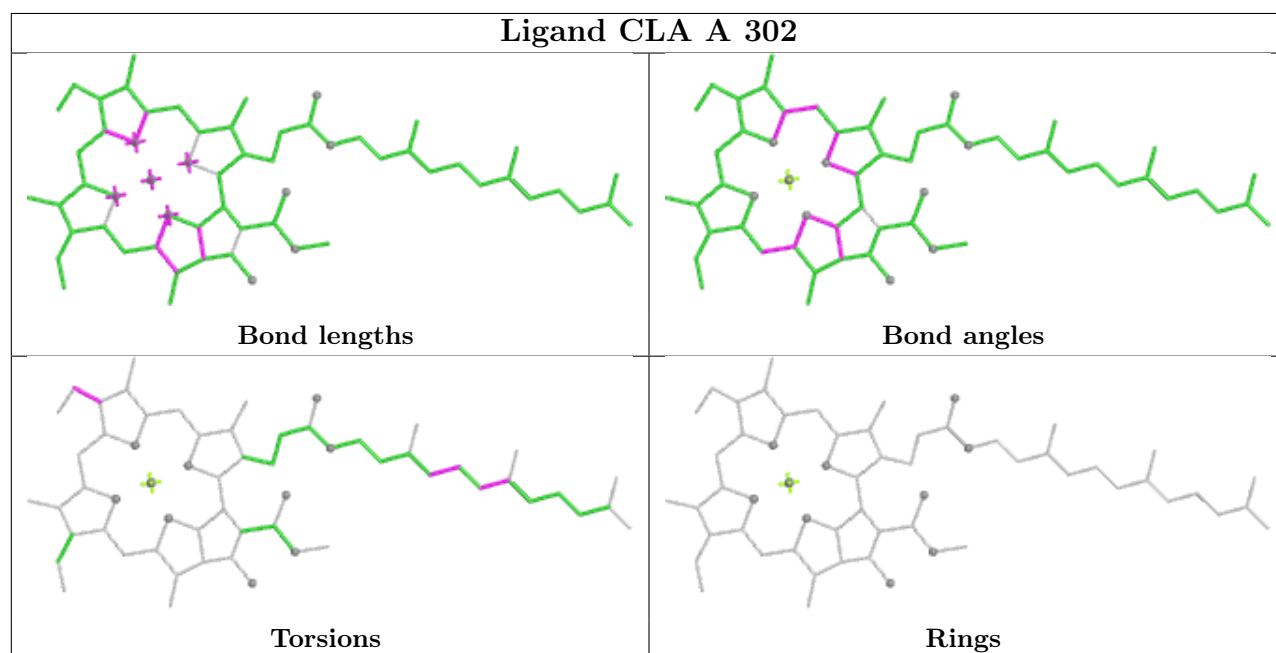
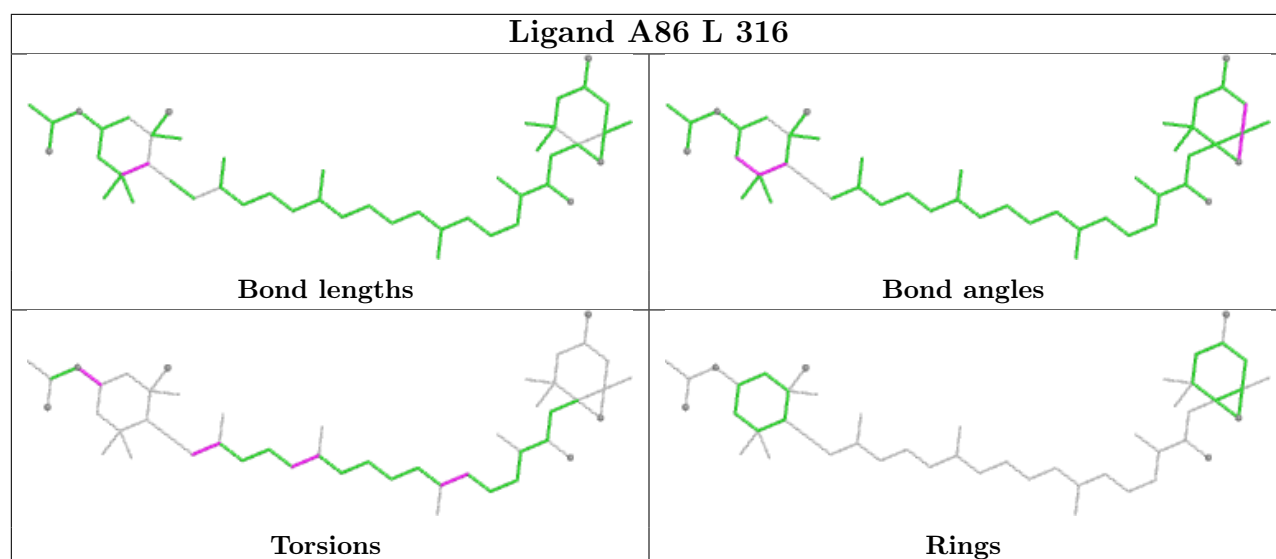
Torsions

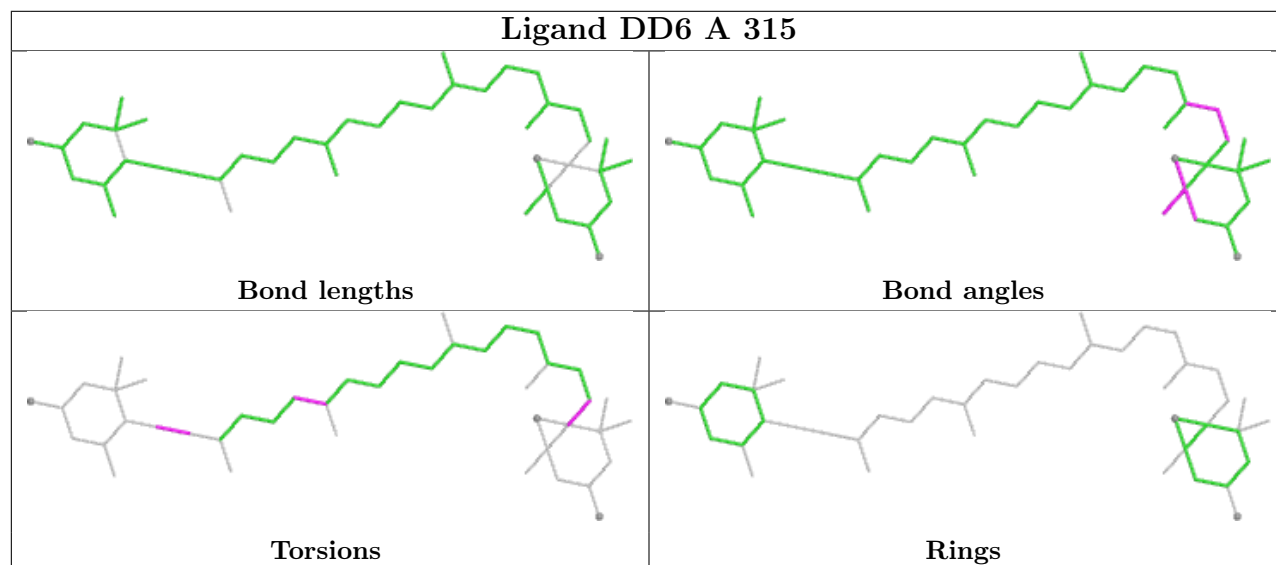
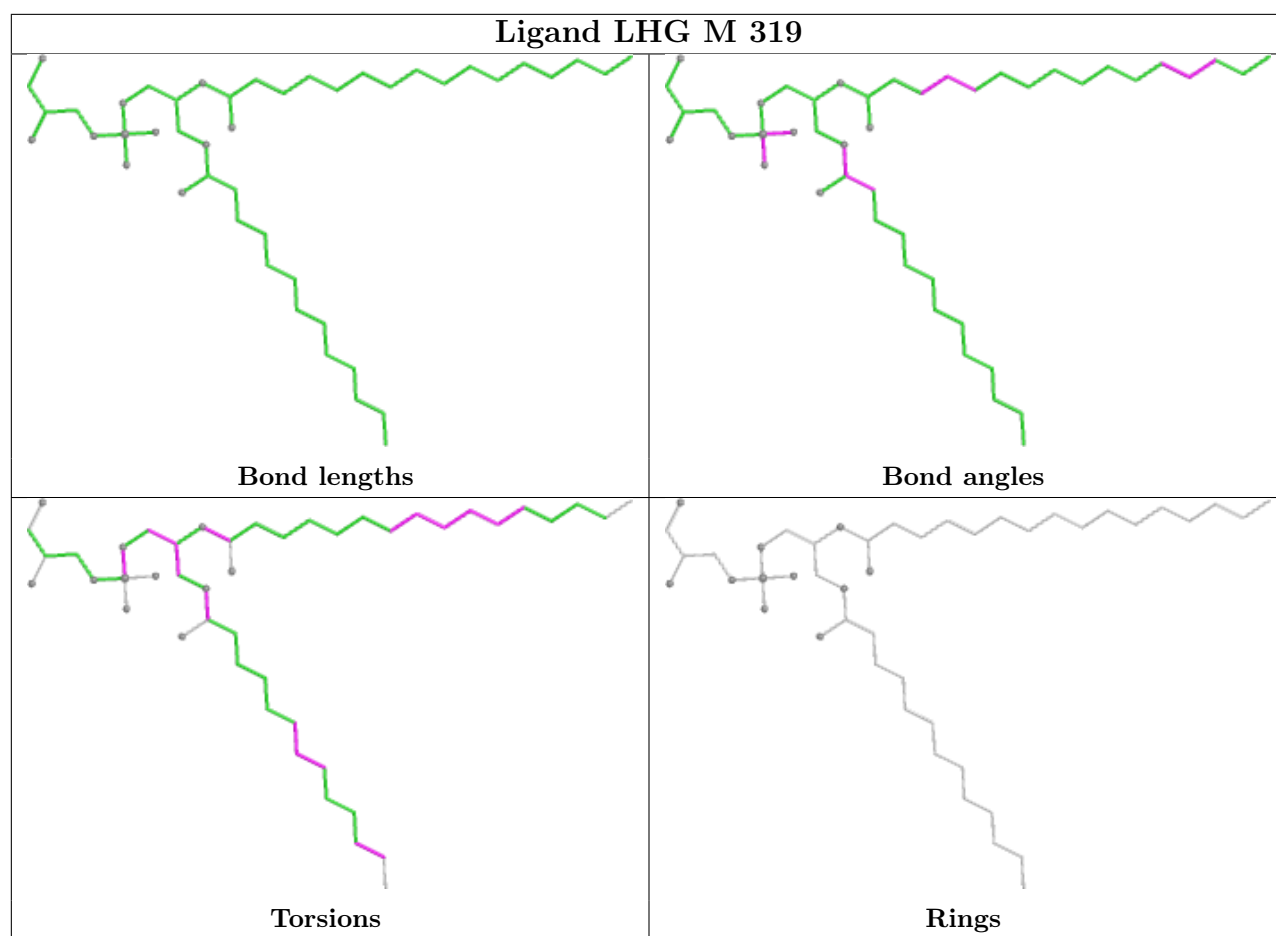


Rings

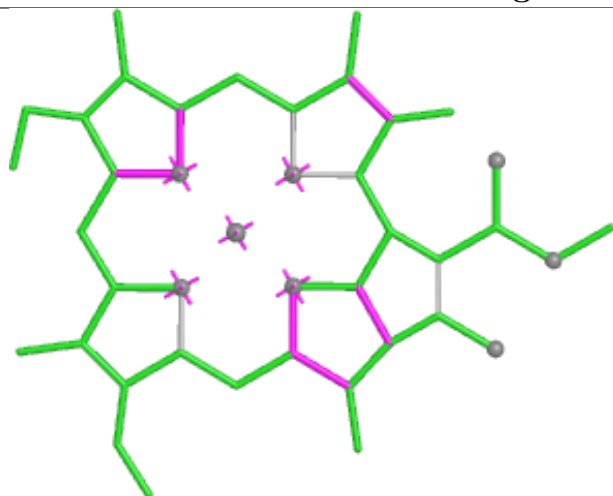
Ligand CLA a 812**Ligand CLA b 802**



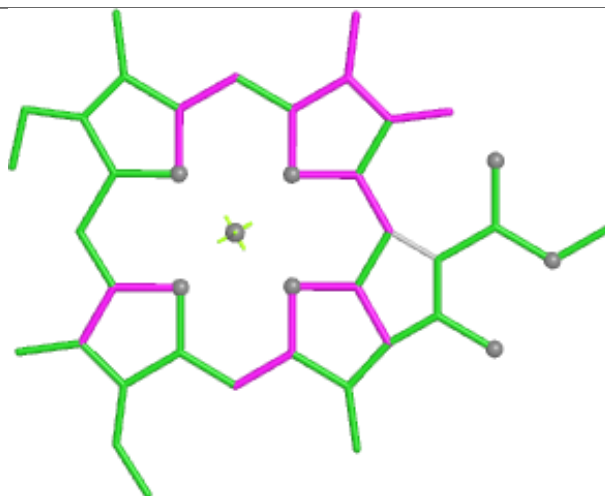




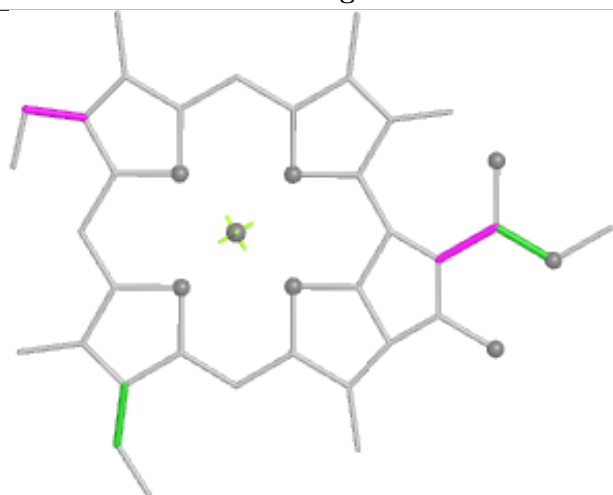
Ligand CLA K 307



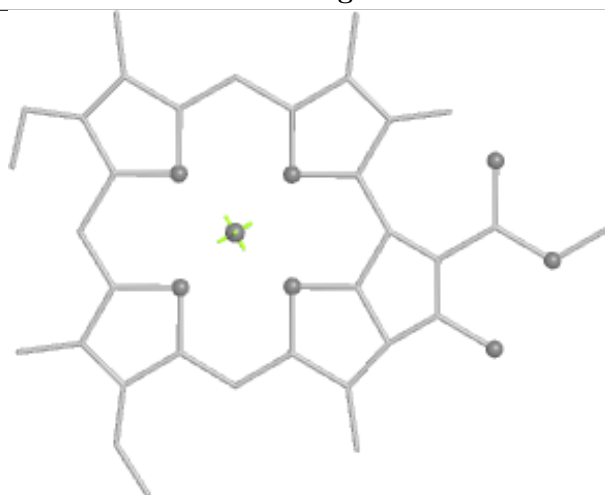
Bond lengths



Bond angles

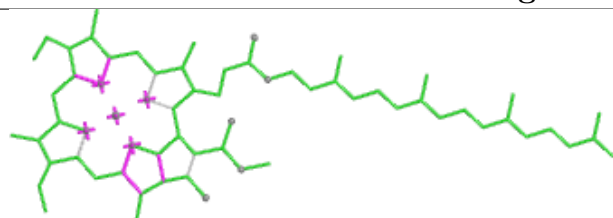


Torsions

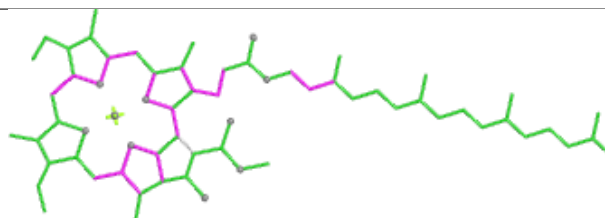


Rings

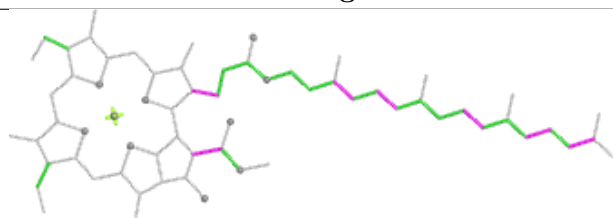
Ligand CLA a 814



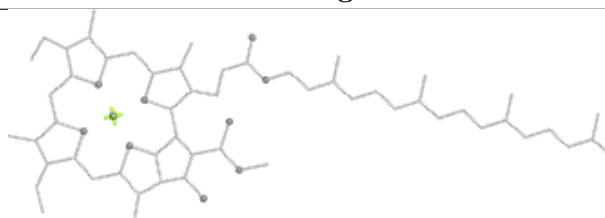
Bond lengths



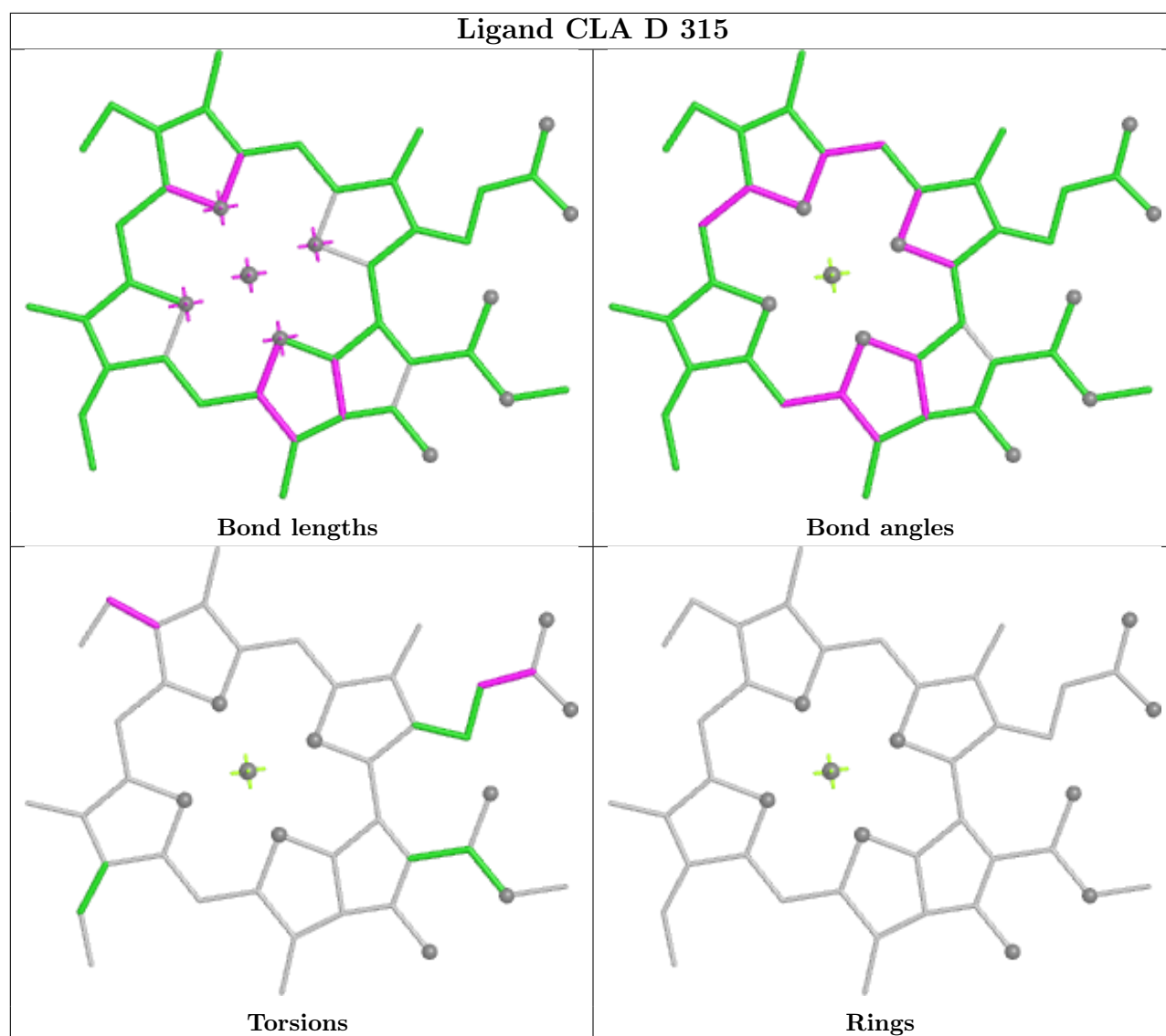
Bond angles

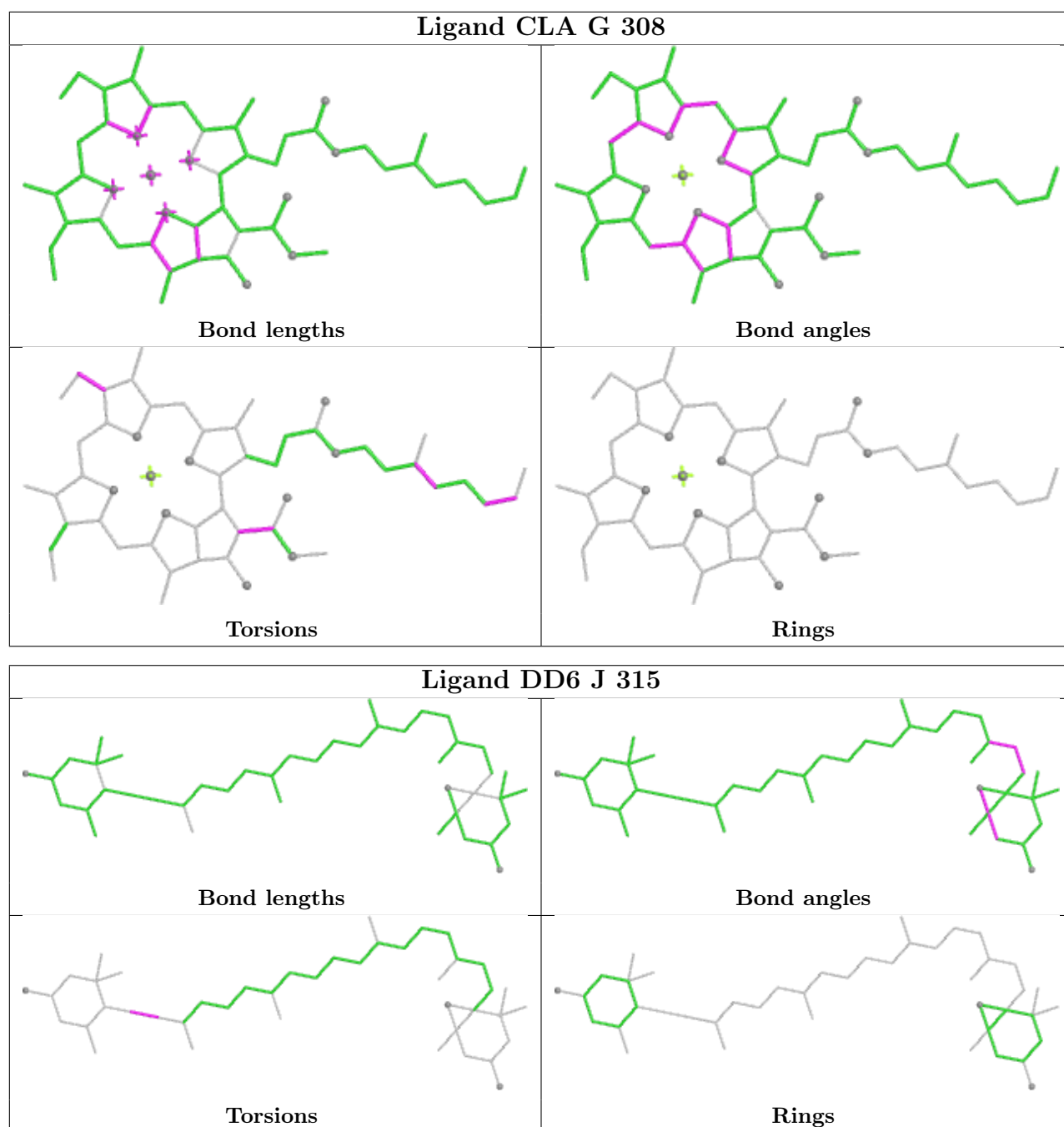


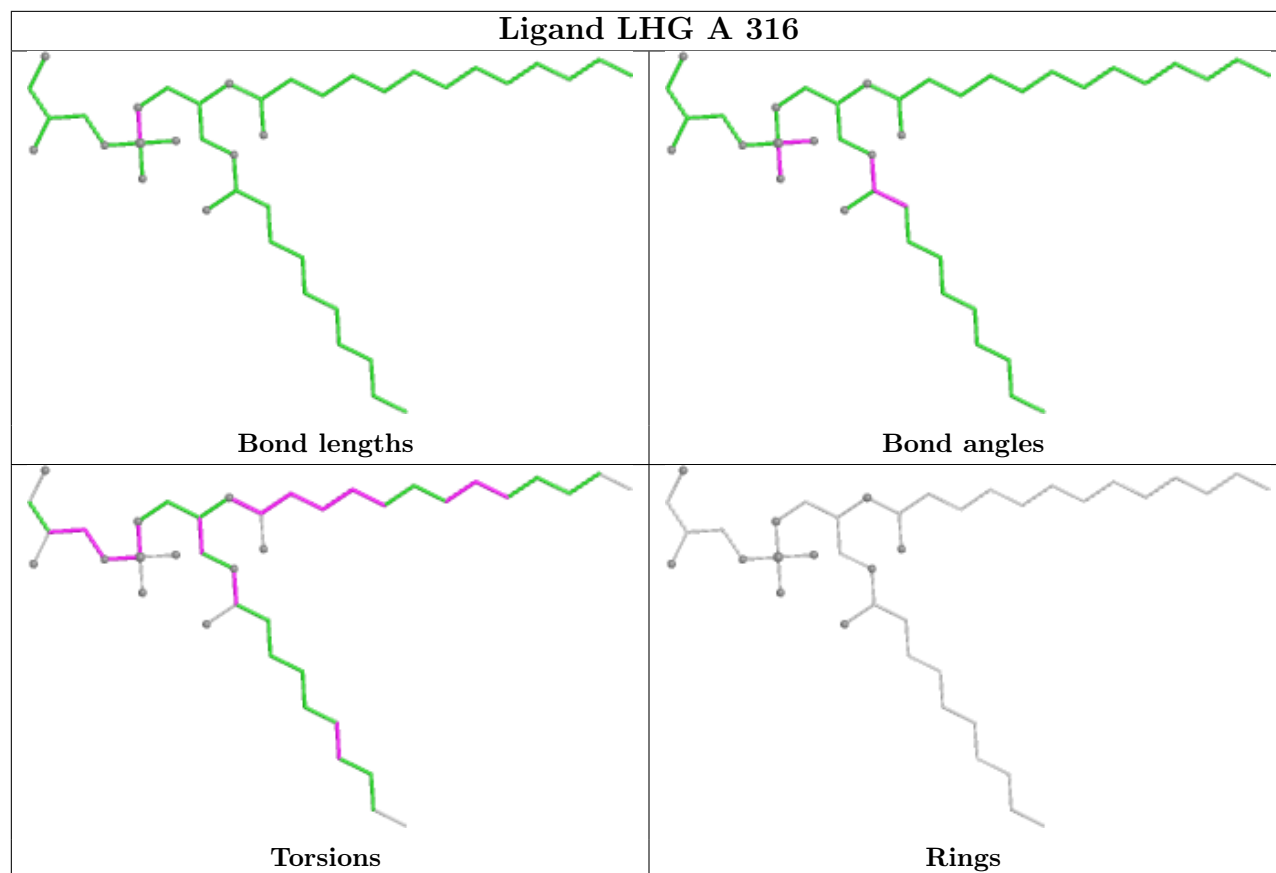
Torsions



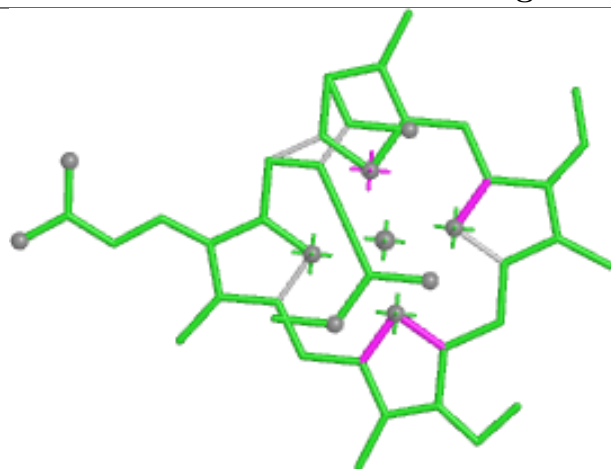
Rings



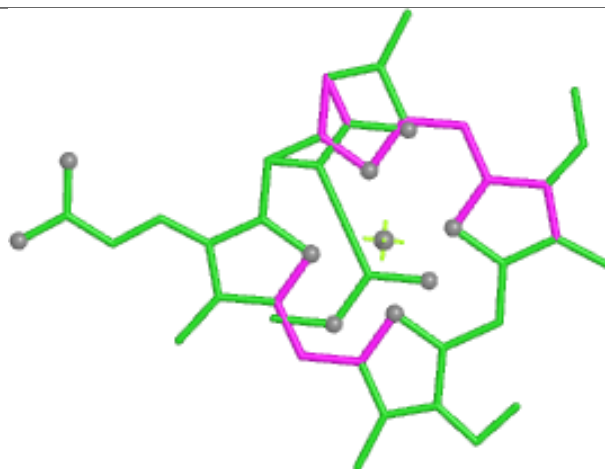




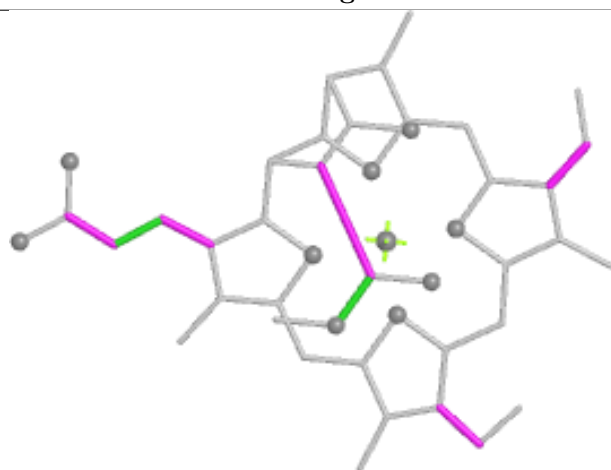
Ligand KC2 C 303



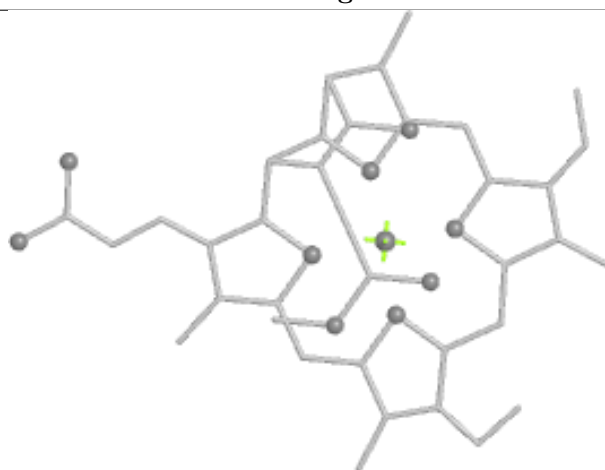
Bond lengths



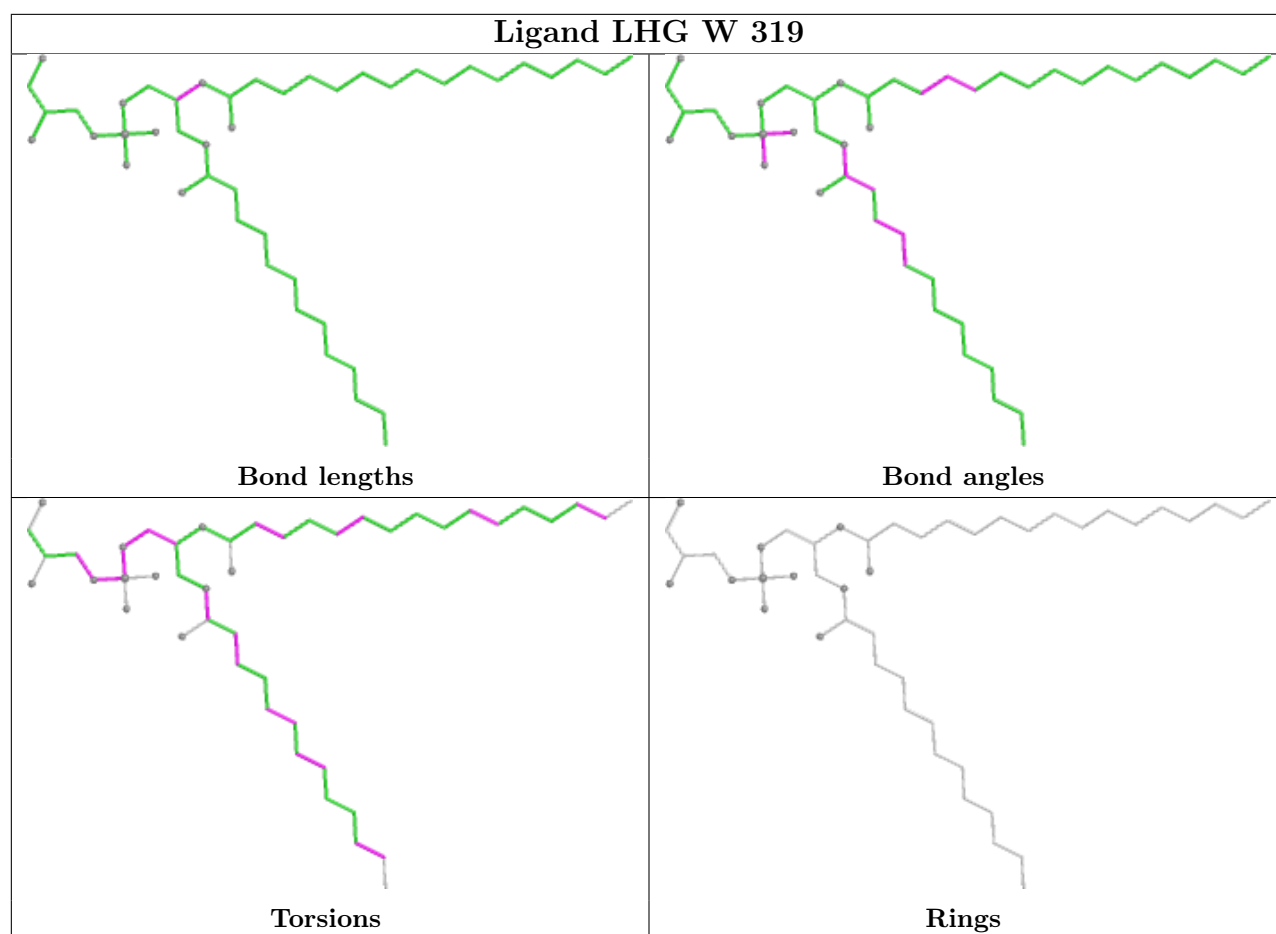
Bond angles



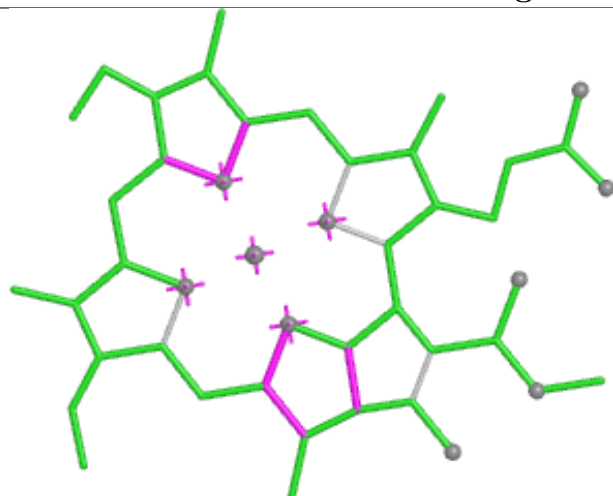
Torsions



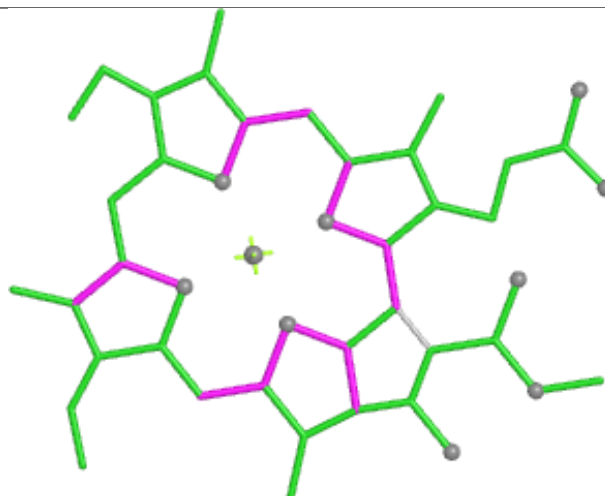
Rings



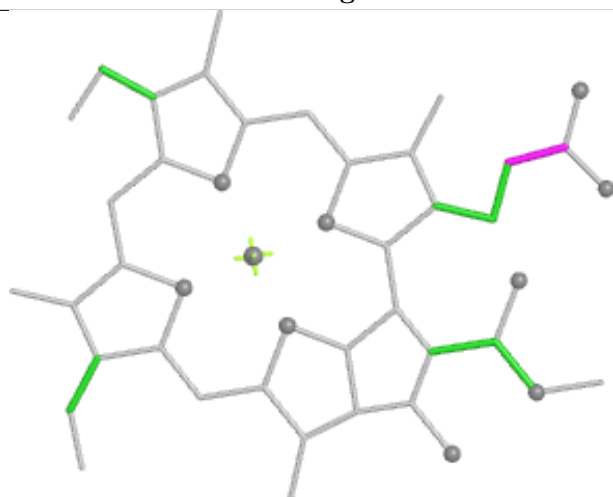
Ligand CLA P 308



Bond lengths



Bond angles

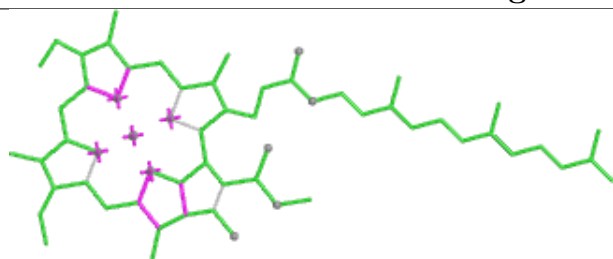


Torsions

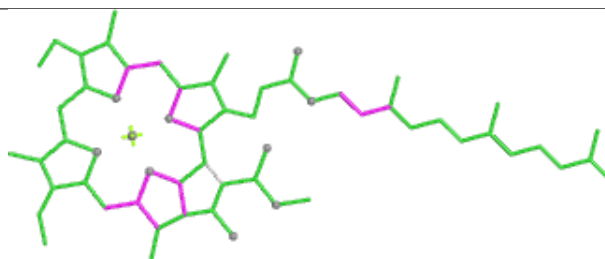


Rings

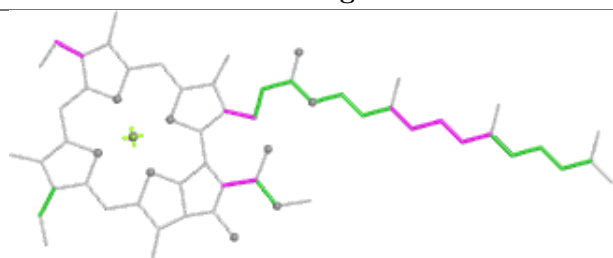
Ligand CLA W 312



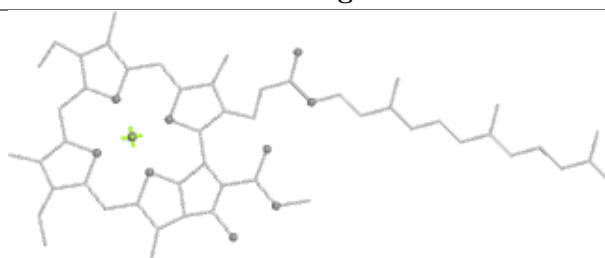
Bond lengths



Bond angles

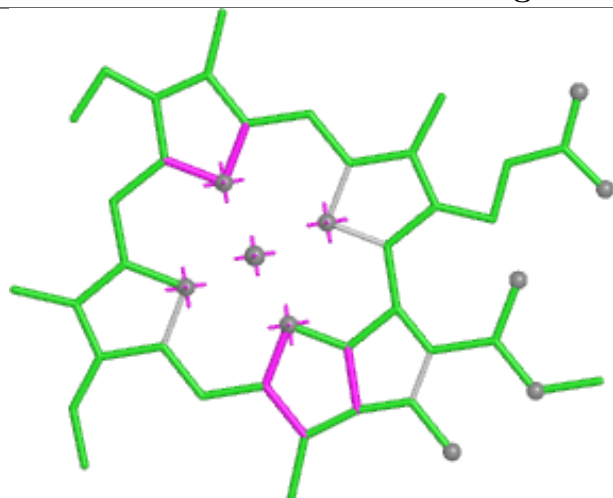


Torsions

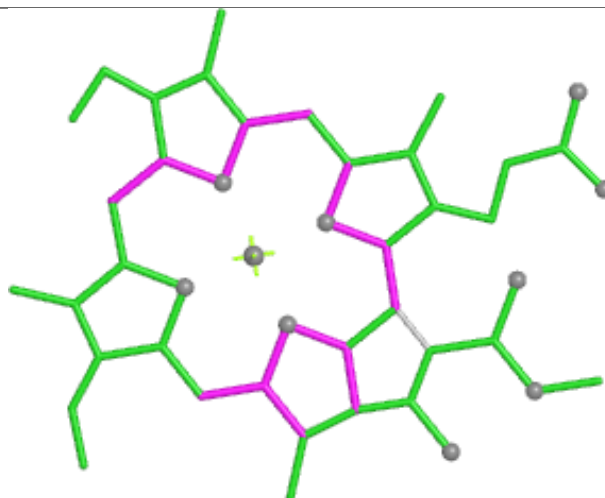


Rings

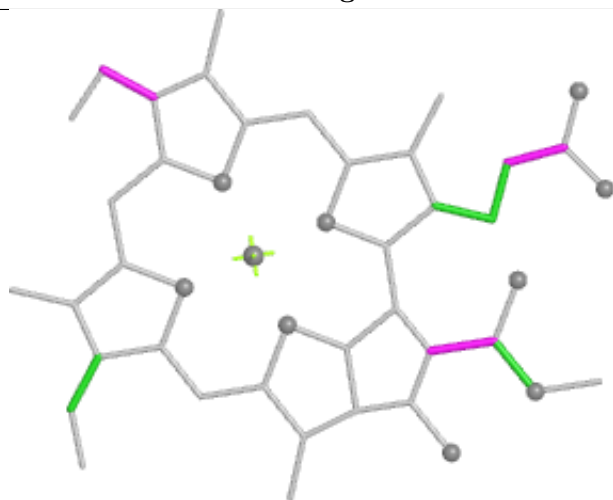
Ligand CLA O 308



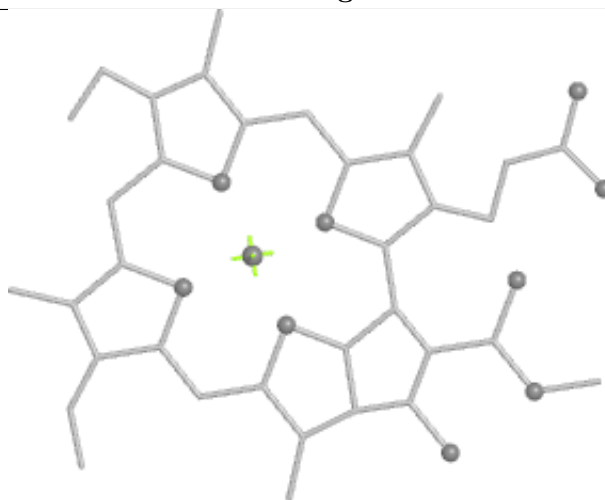
Bond lengths



Bond angles

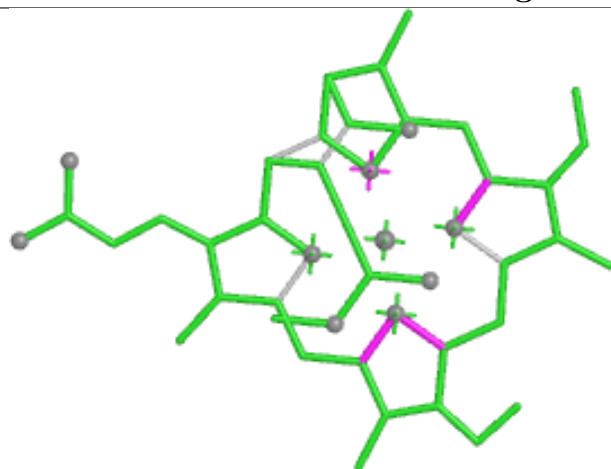


Torsions

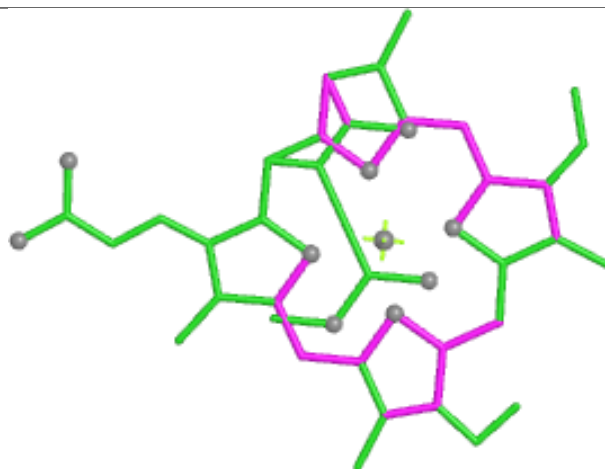


Rings

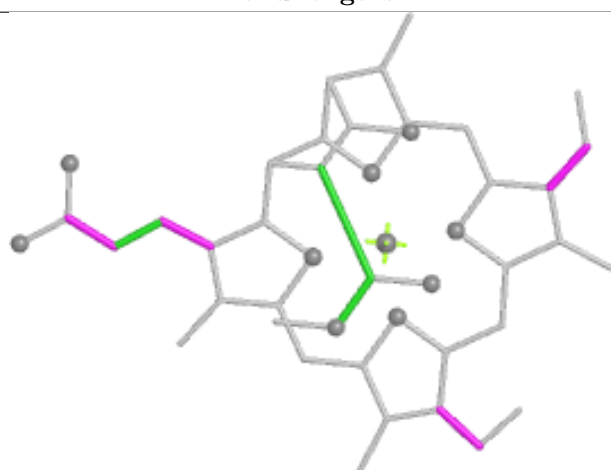
Ligand KC2 N 303



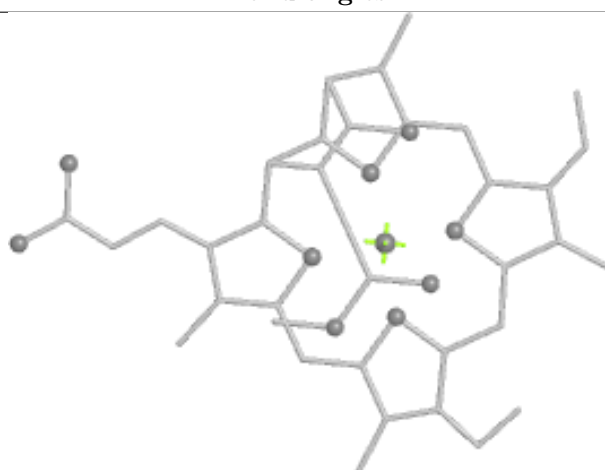
Bond lengths



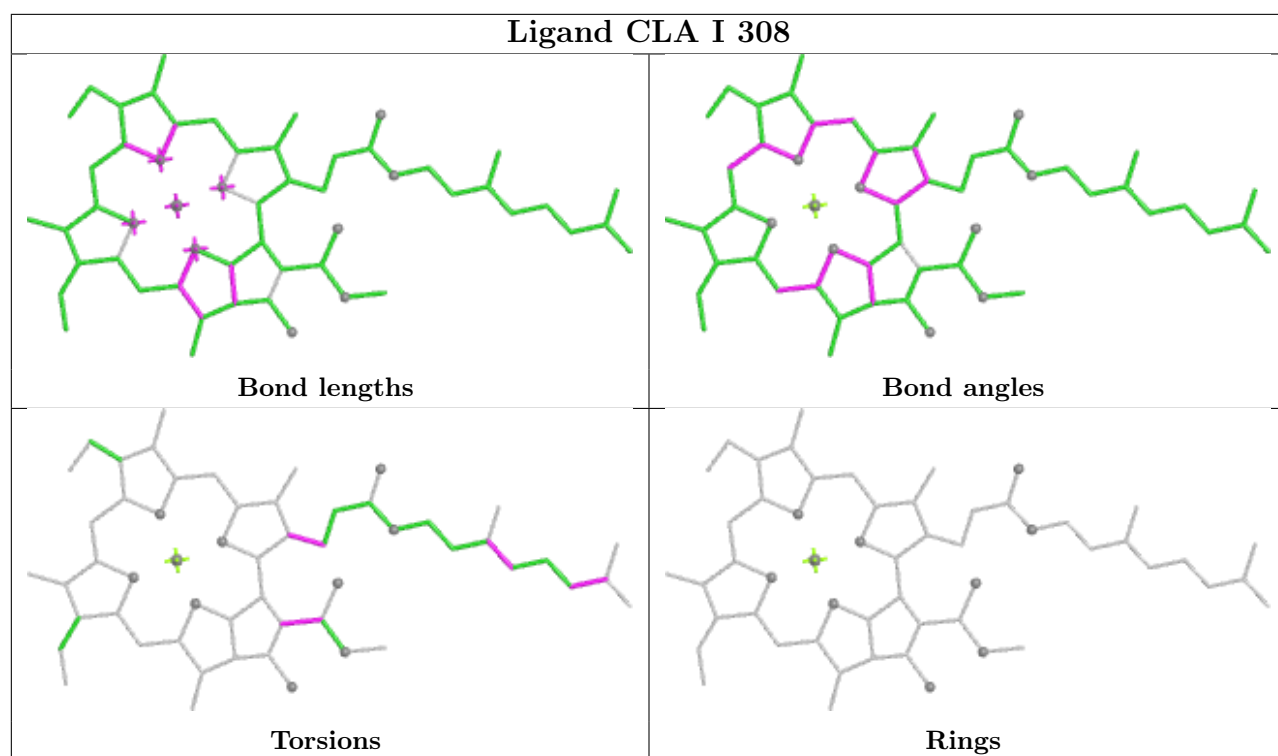
Bond angles



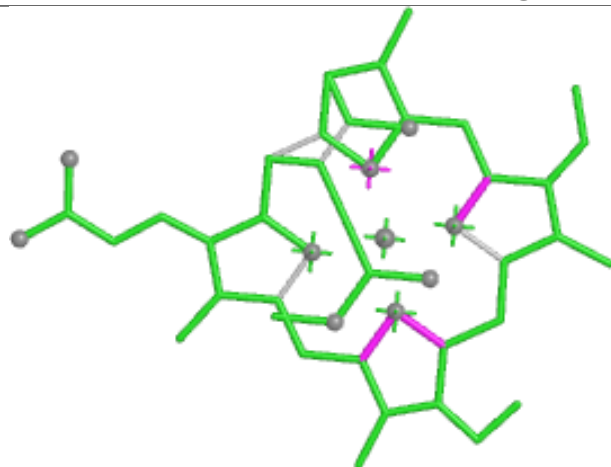
Torsions



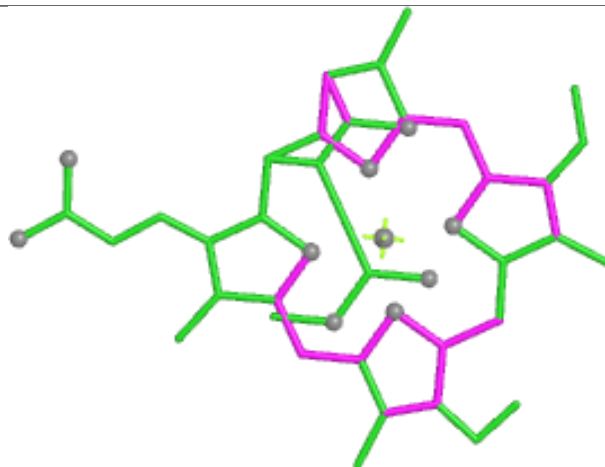
Rings



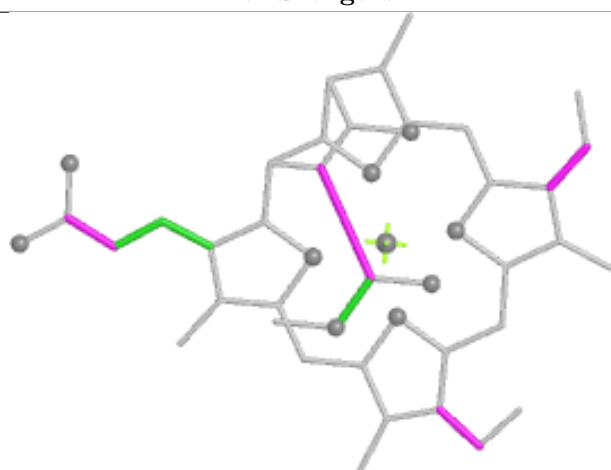
Ligand KC2 N 304



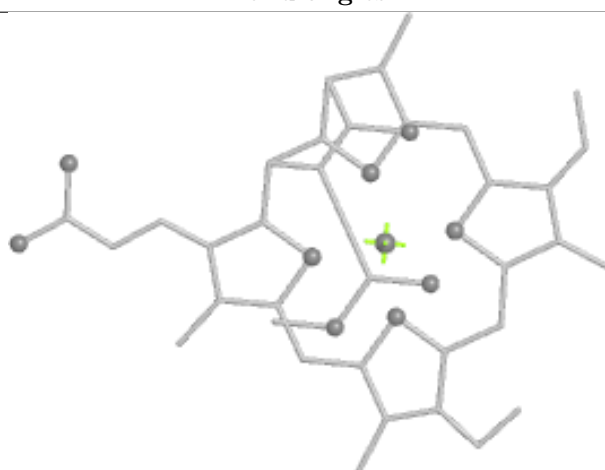
Bond lengths



Bond angles

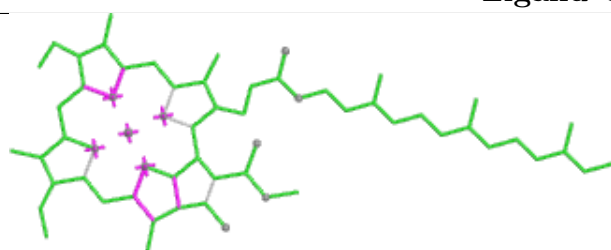


Torsions

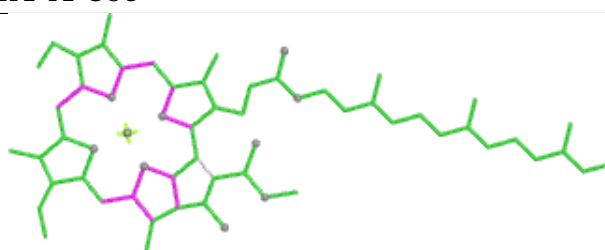


Rings

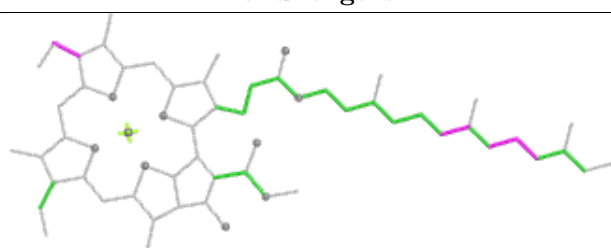
Ligand CLA A 305



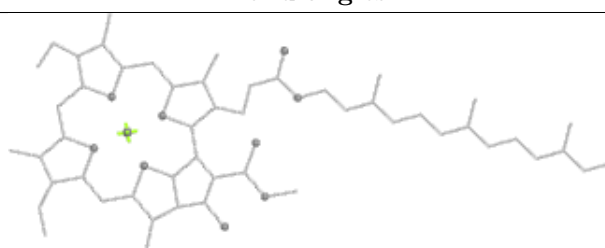
Bond lengths



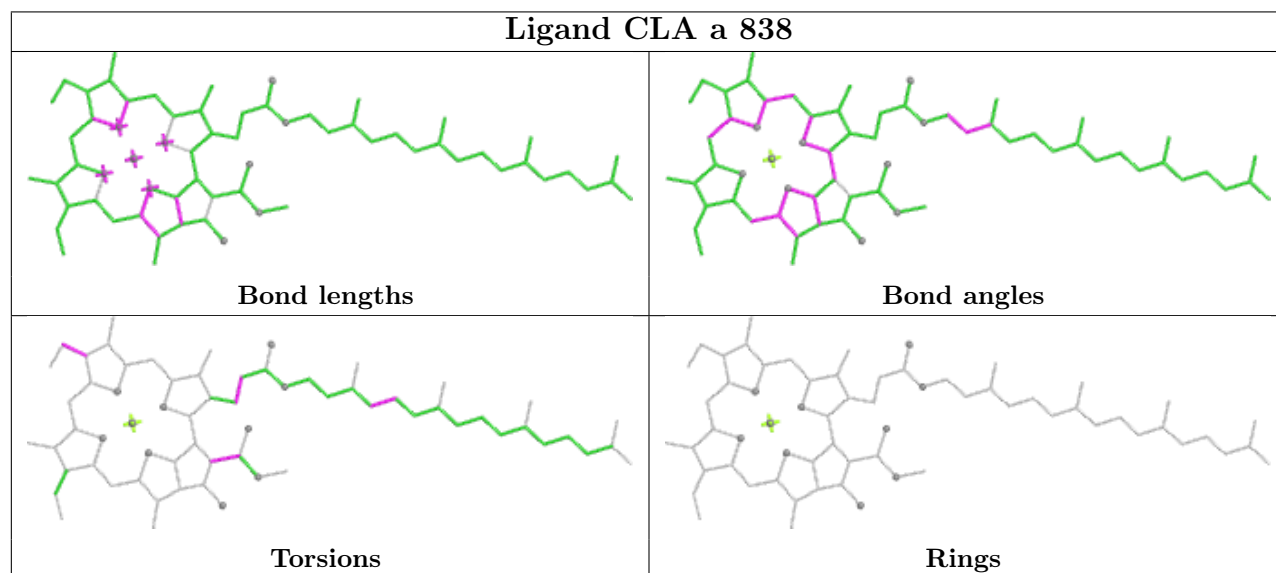
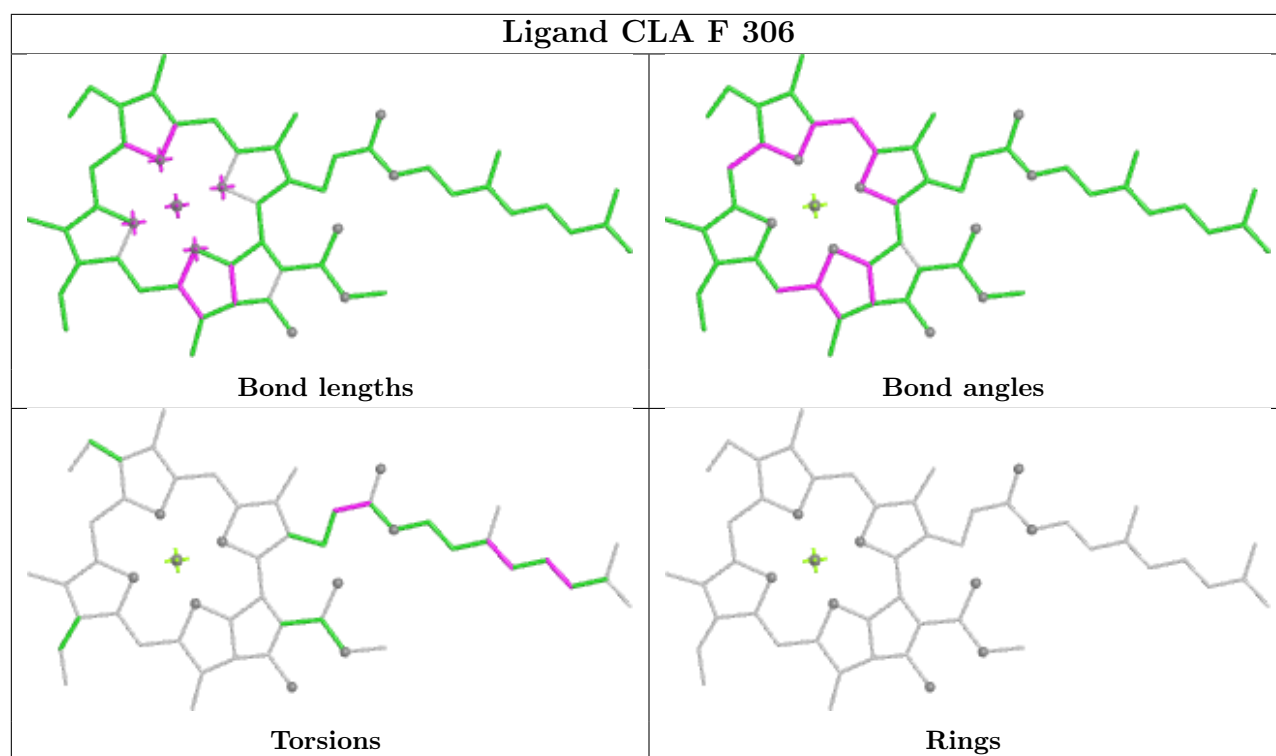
Bond angles

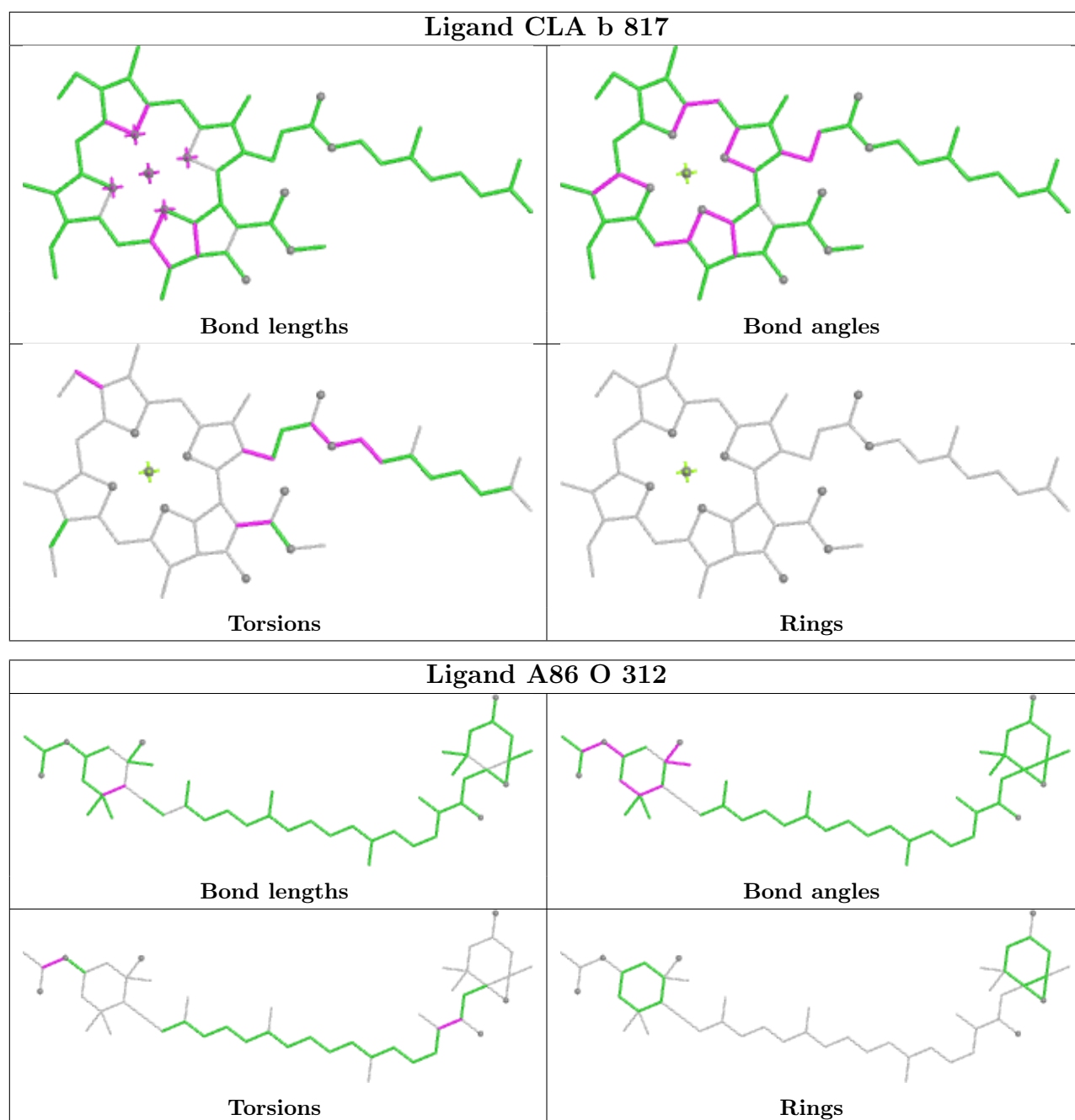


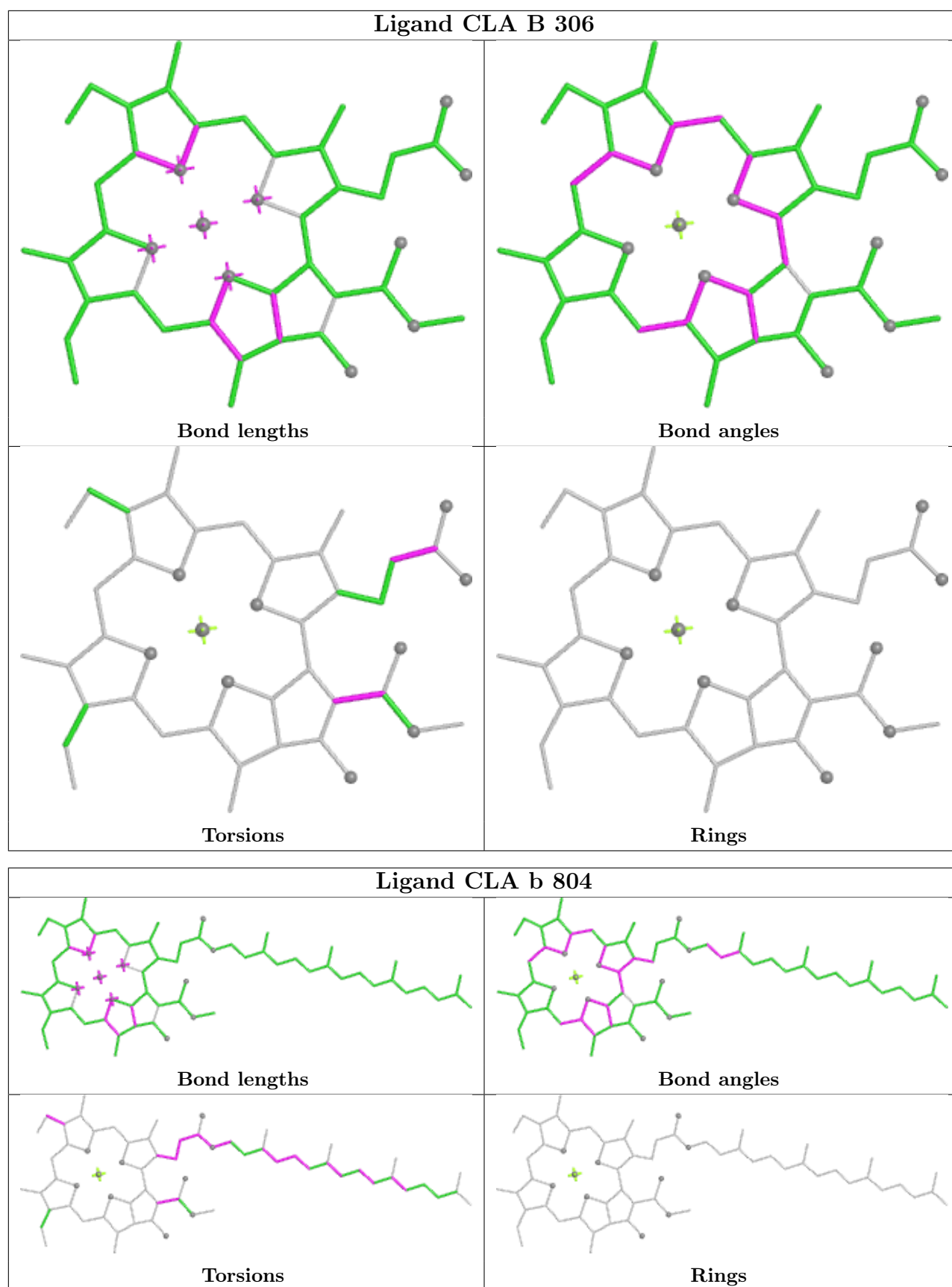
Torsions



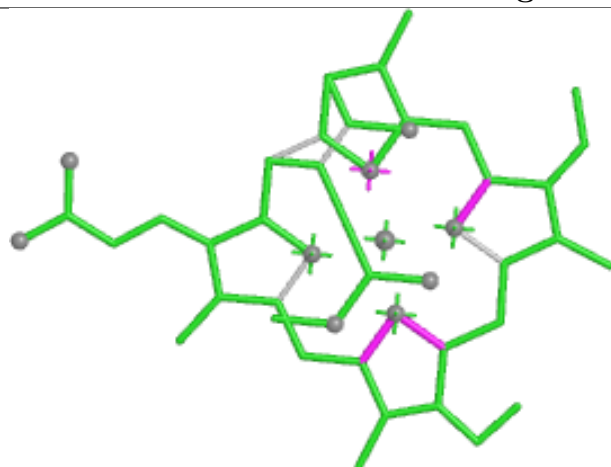
Rings



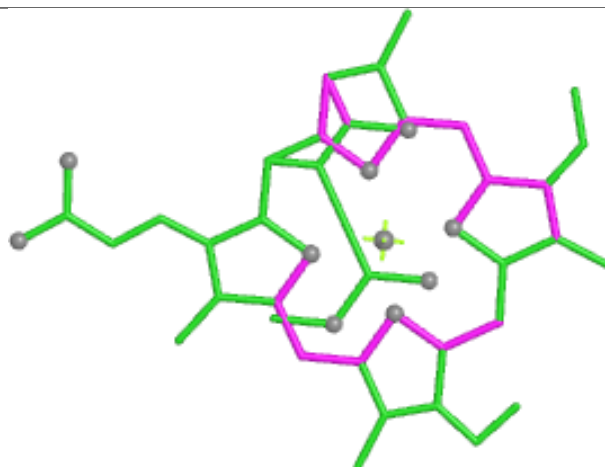




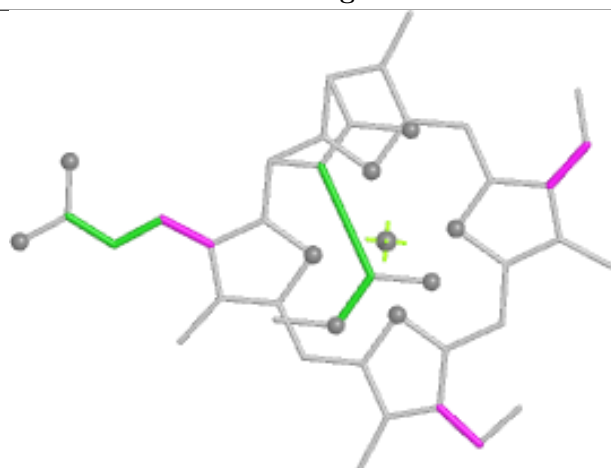
Ligand KC2 P 306



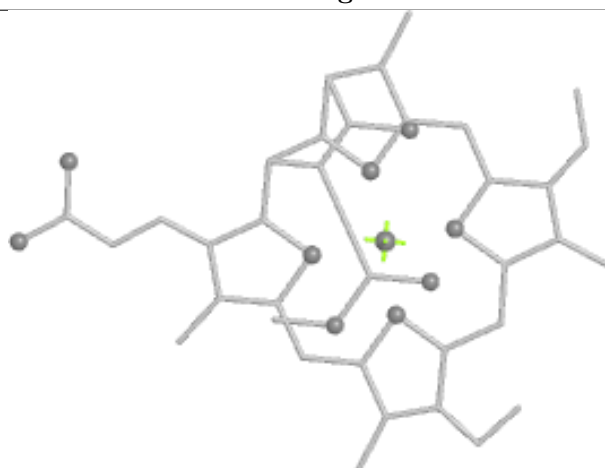
Bond lengths



Bond angles

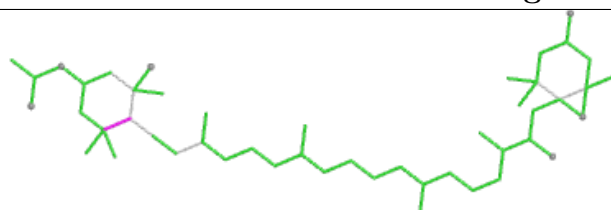


Torsions

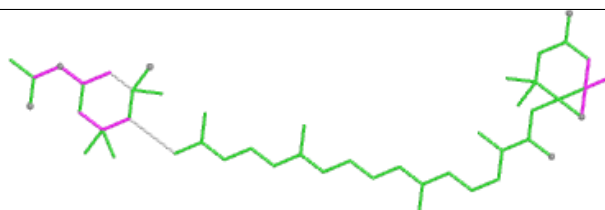


Rings

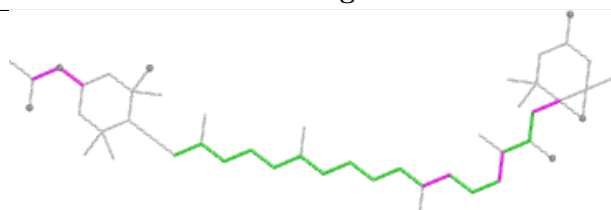
Ligand A86 J 313



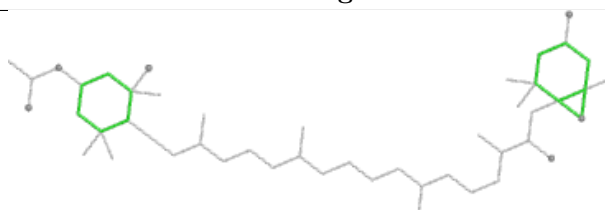
Bond lengths



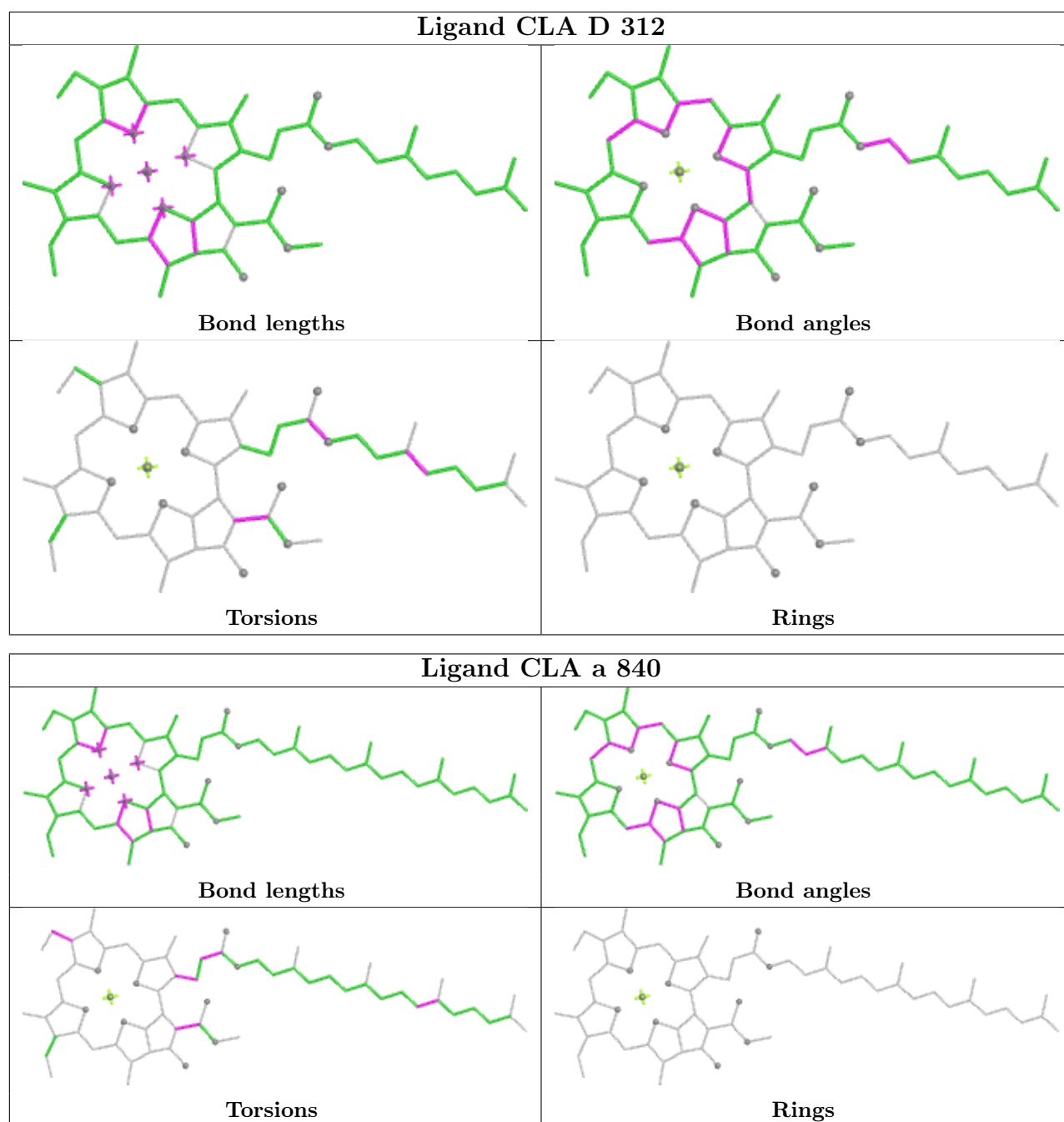
Bond angles



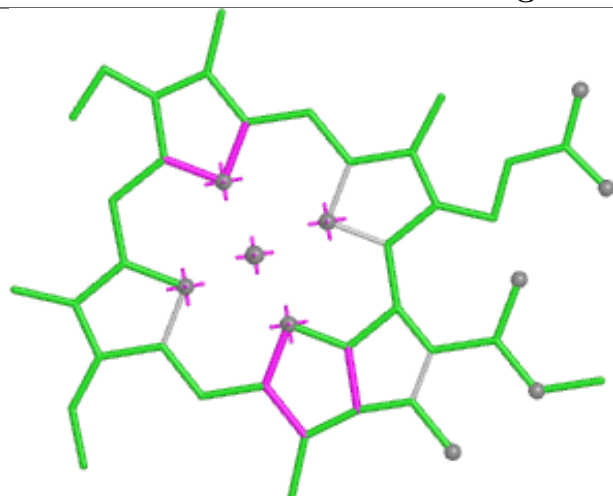
Torsions



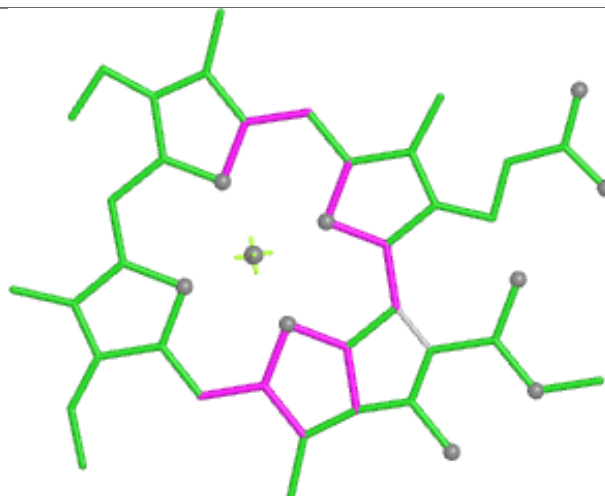
Rings



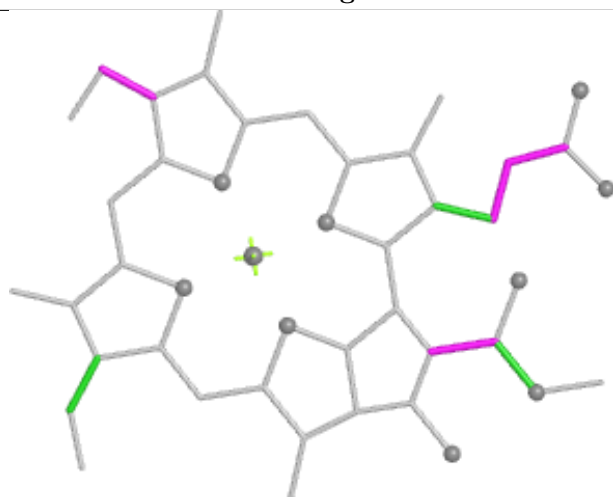
Ligand CLA b 814



Bond lengths



Bond angles

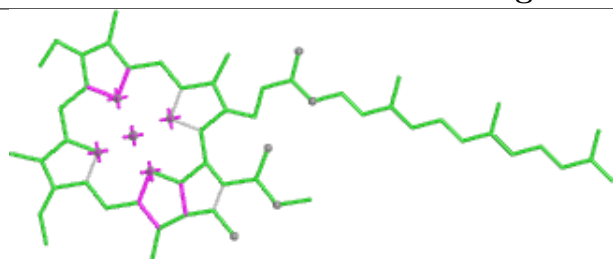


Torsions

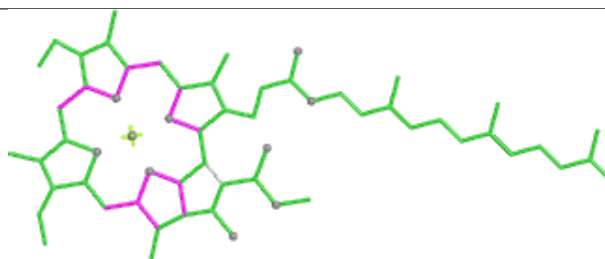


Rings

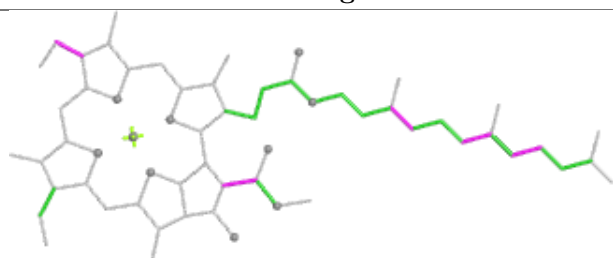
Ligand CLA E 306



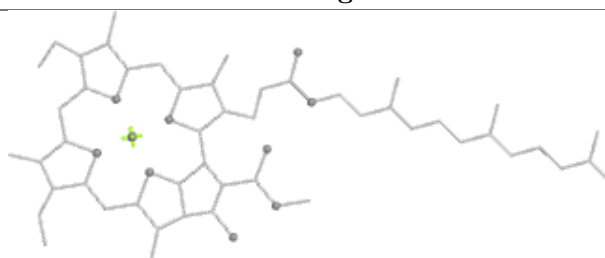
Bond lengths



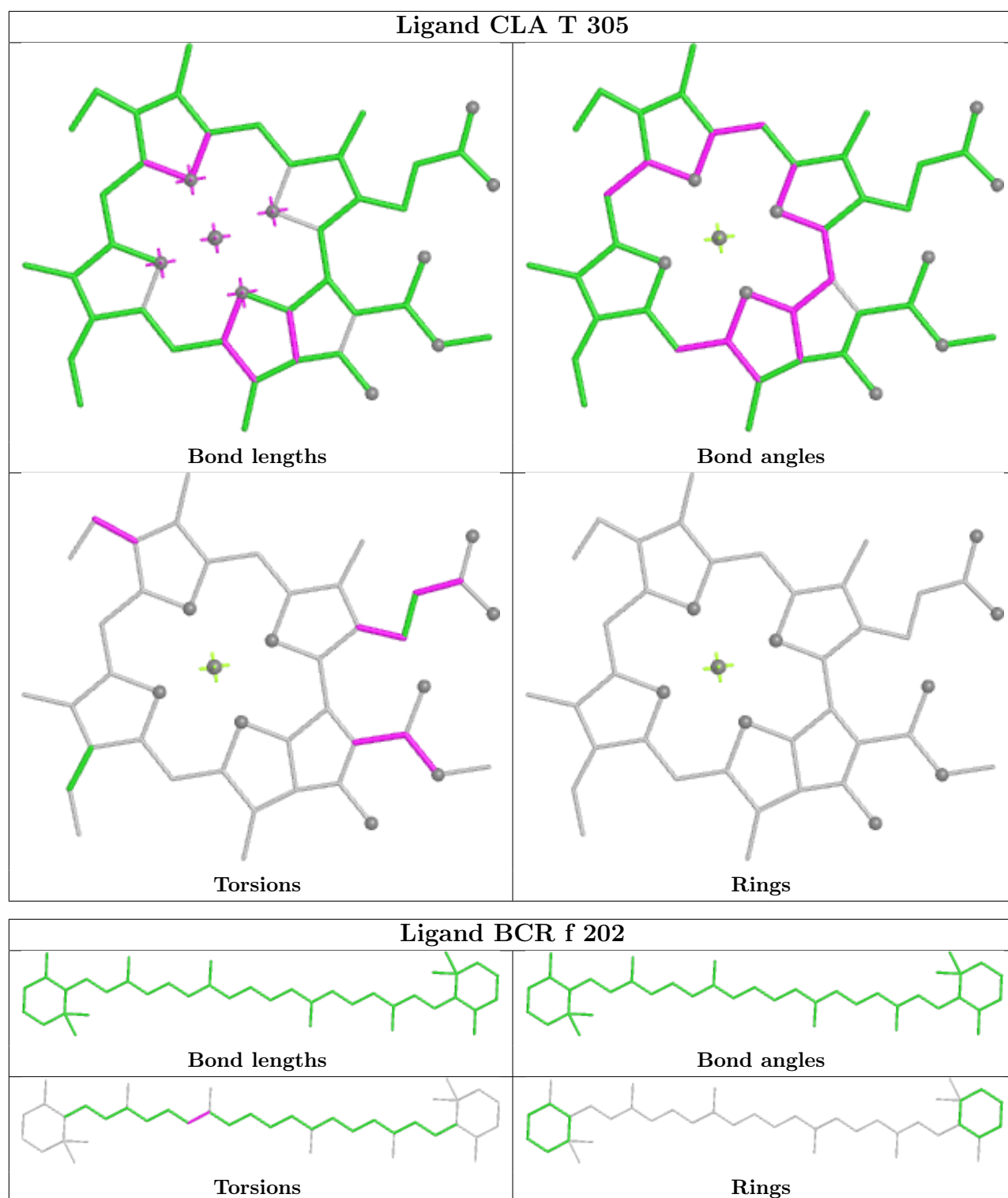
Bond angles

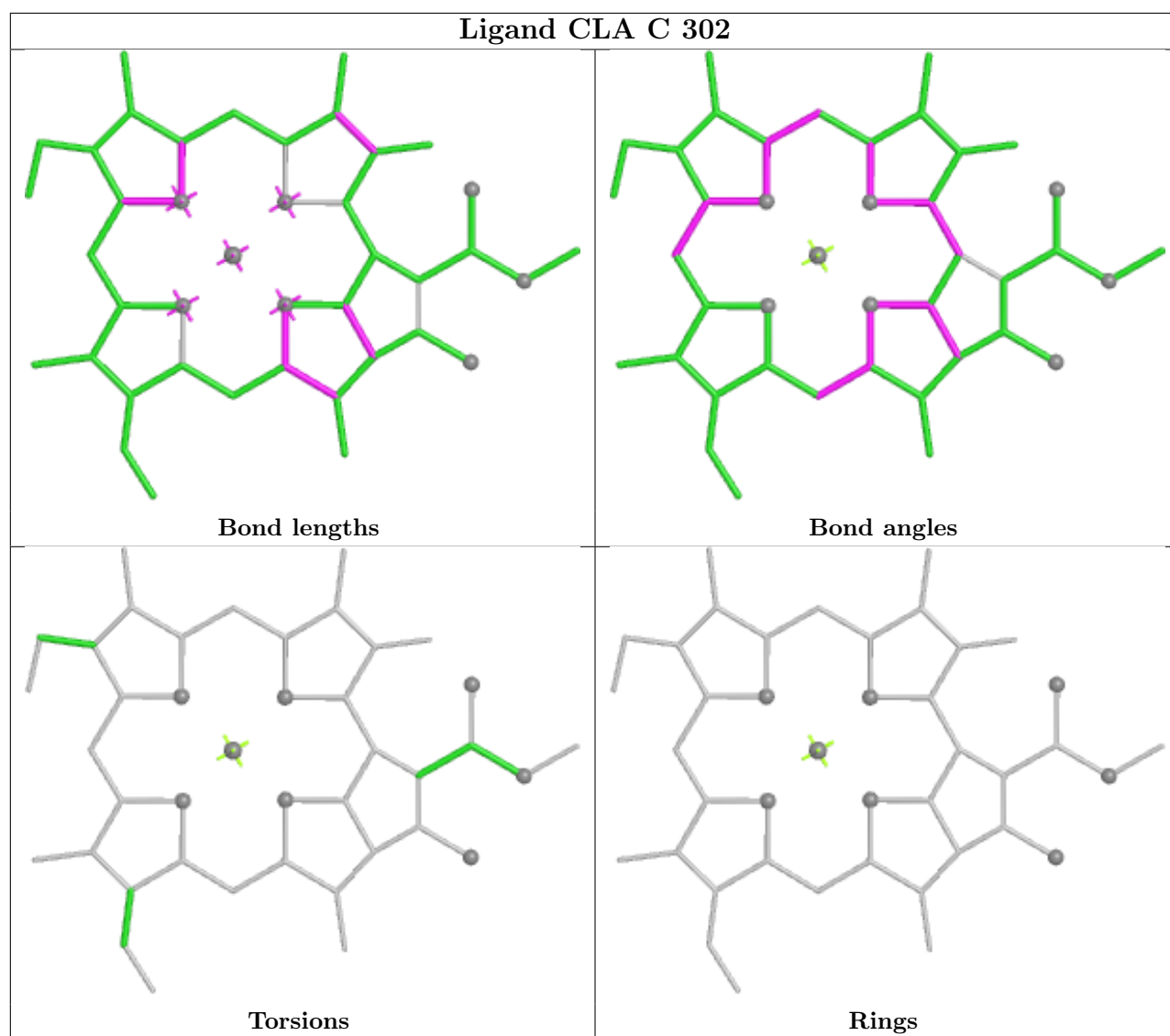


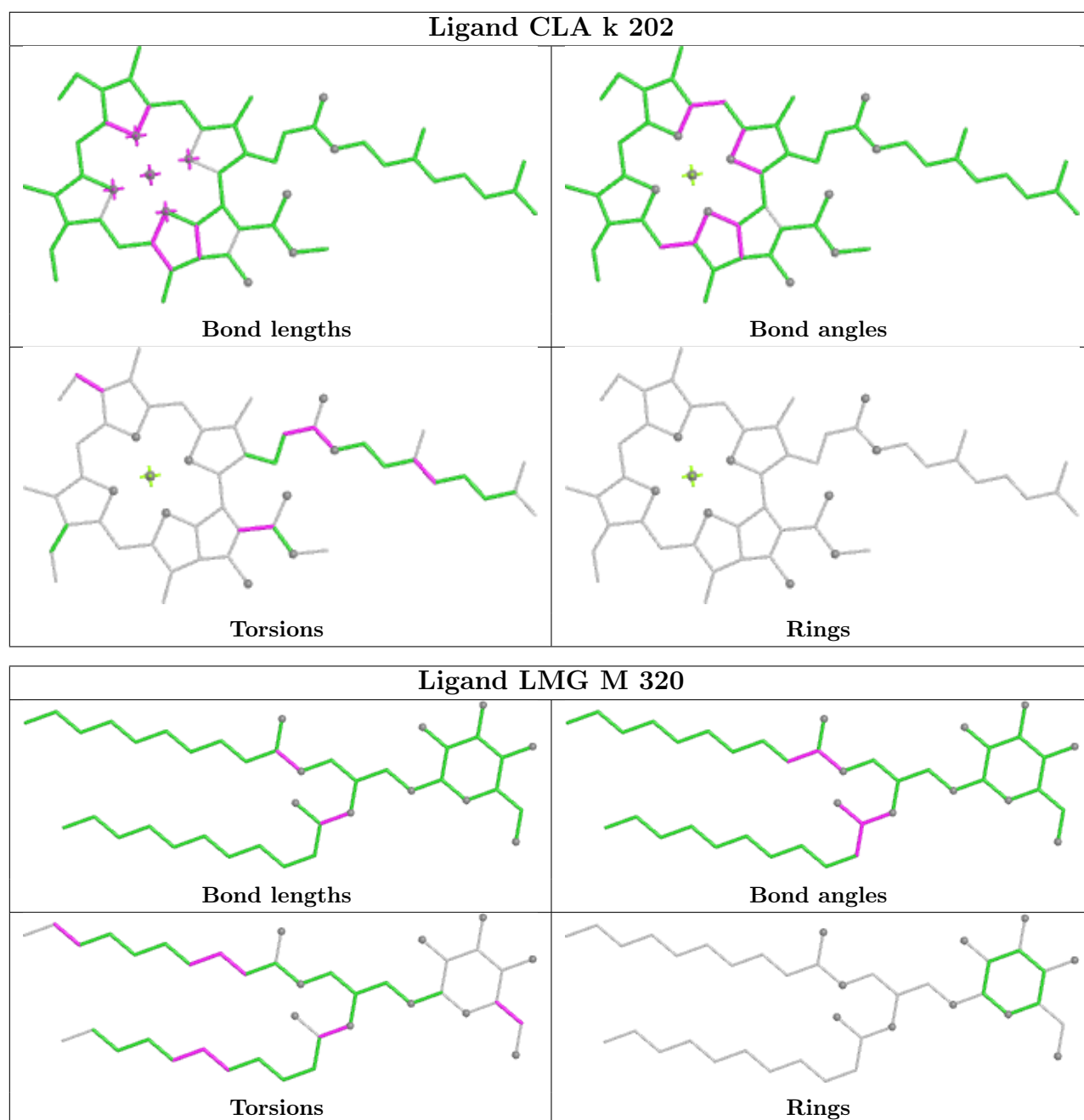
Torsions



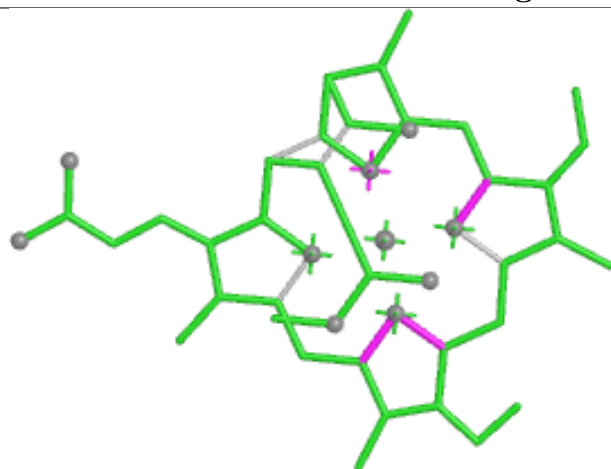
Rings



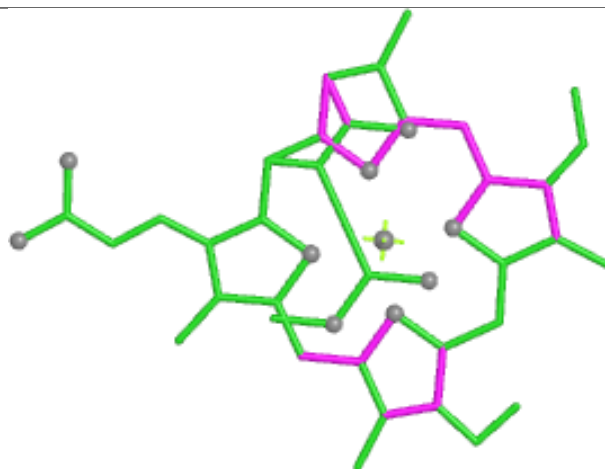




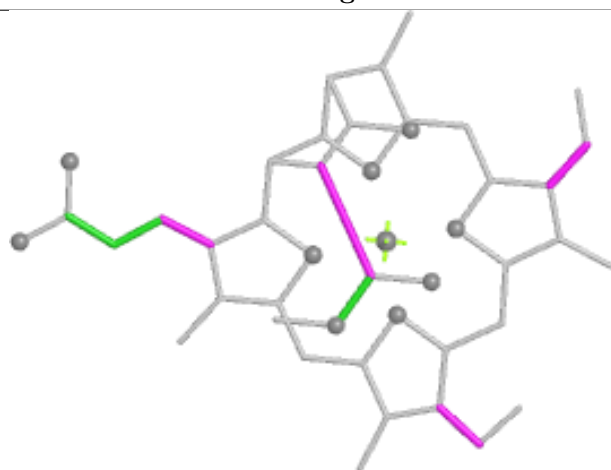
Ligand KC2 H 303



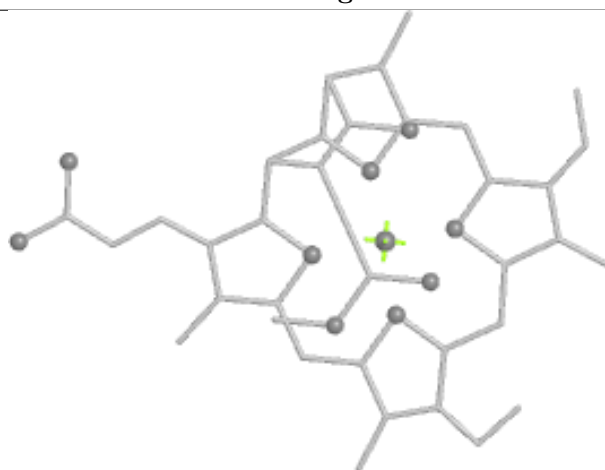
Bond lengths



Bond angles

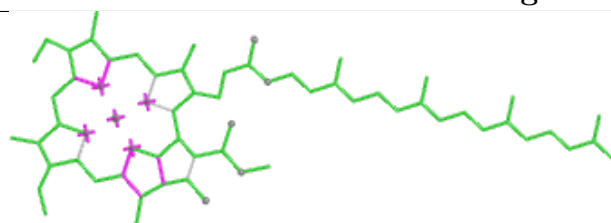


Torsions

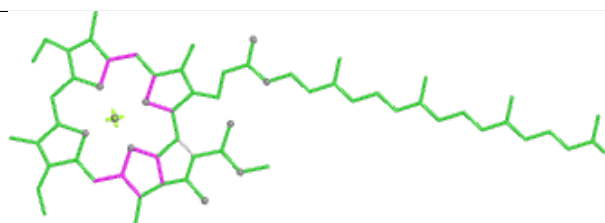


Rings

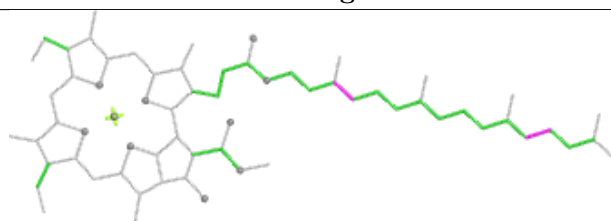
Ligand CLA I 317



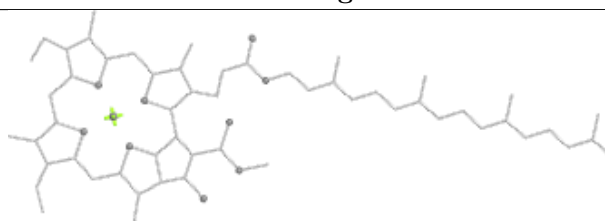
Bond lengths



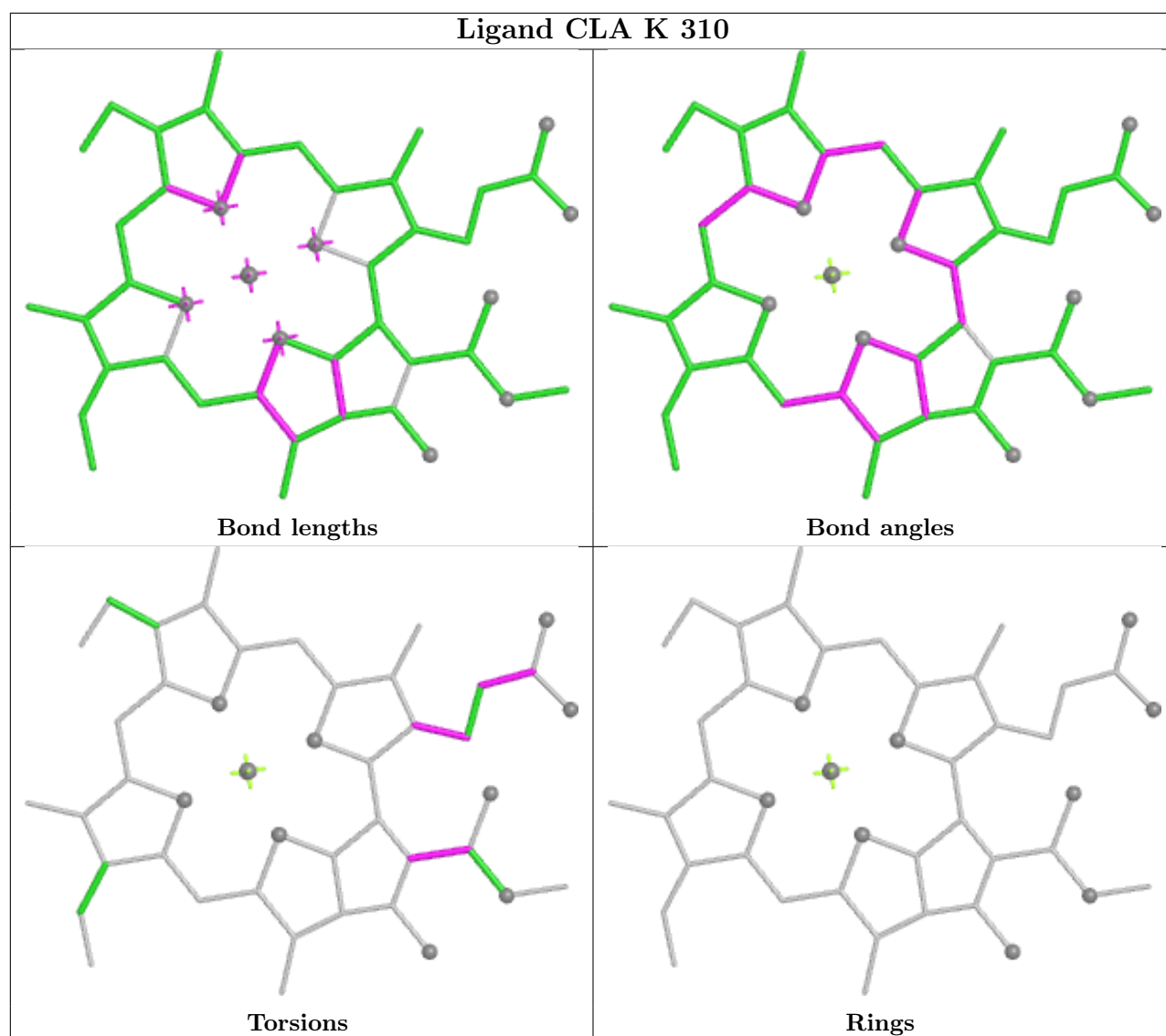
Bond angles

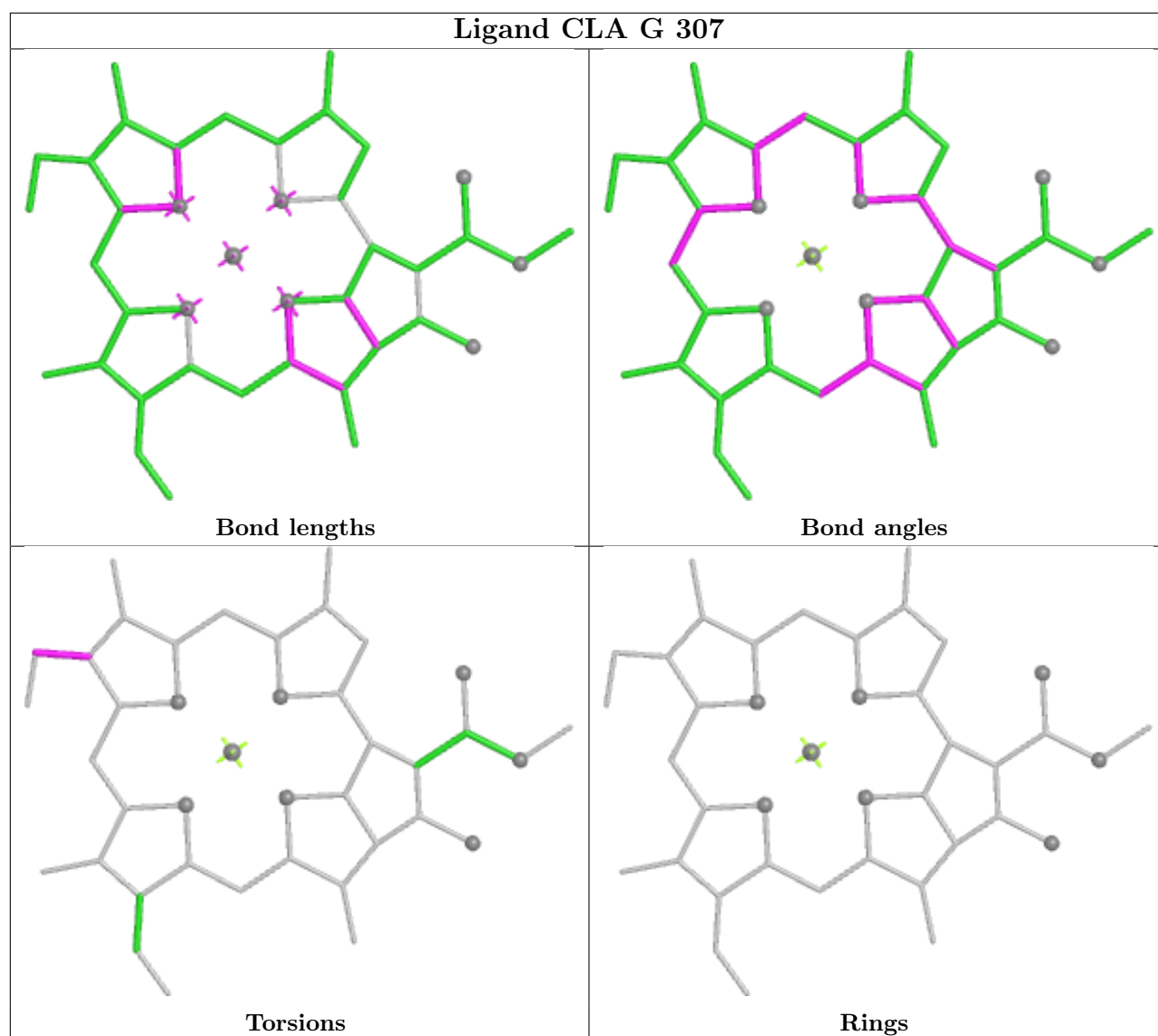


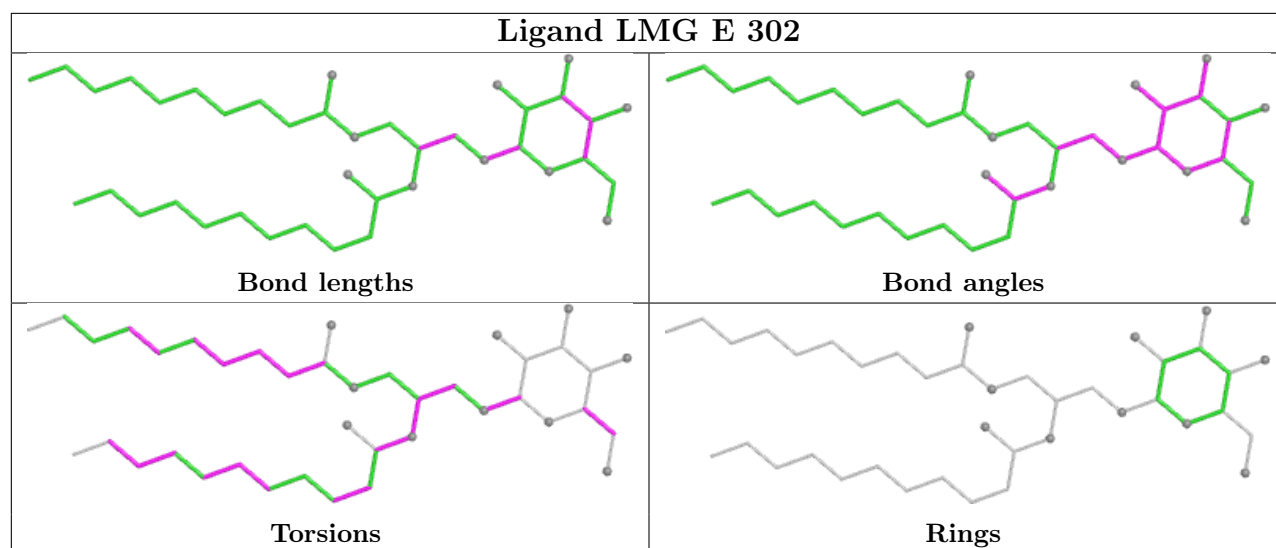
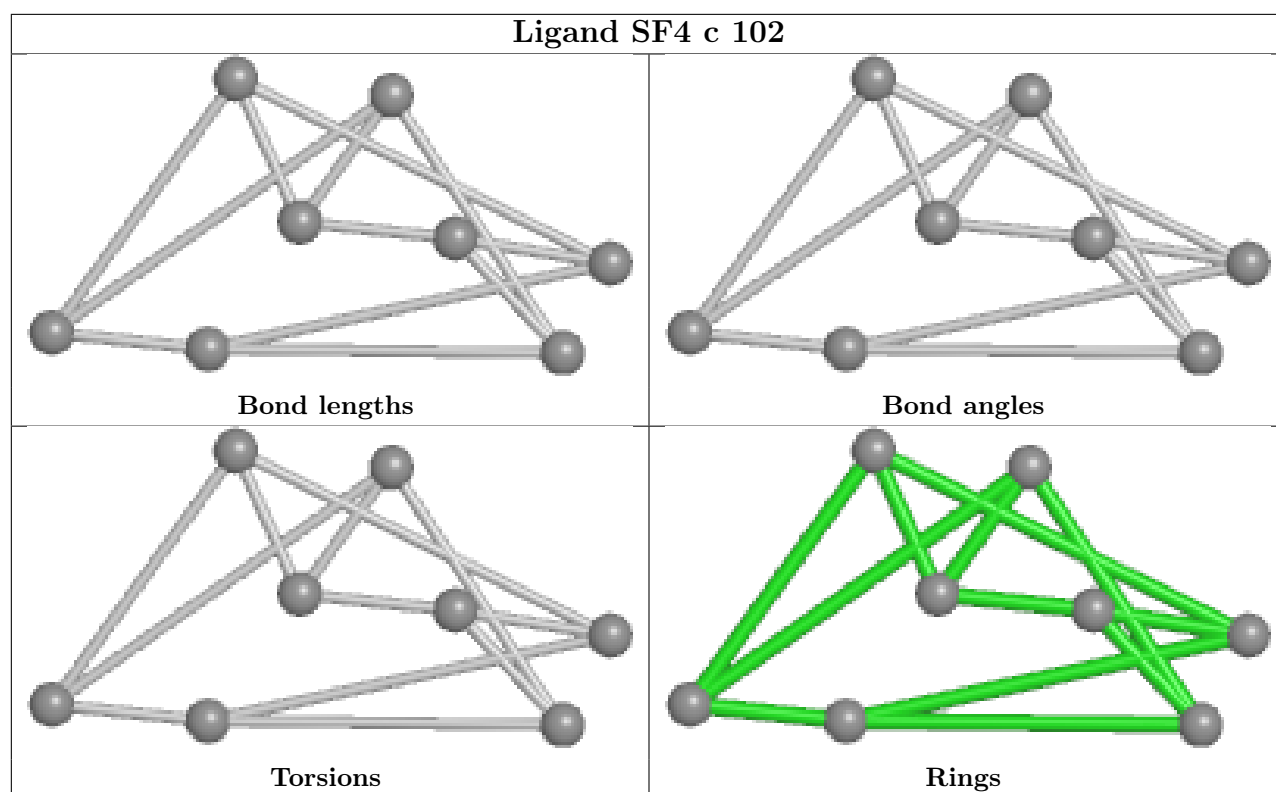
Torsions



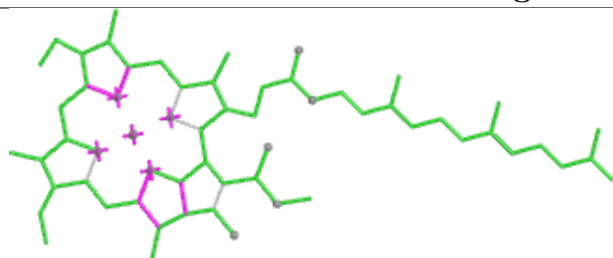
Rings



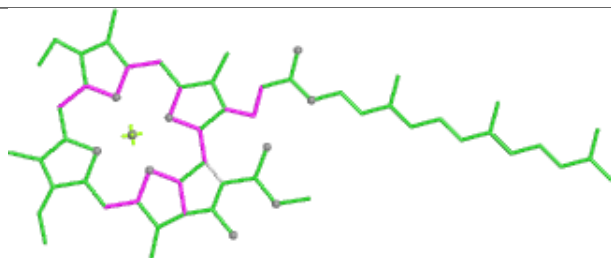




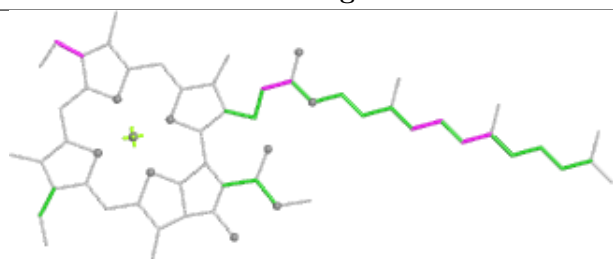
Ligand CLA N 311



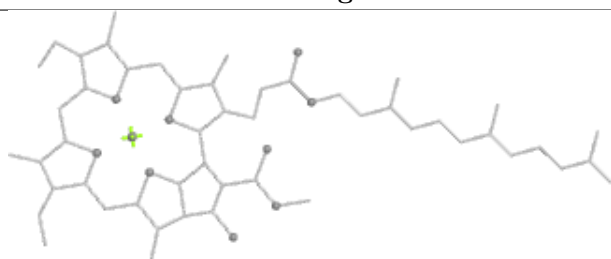
Bond lengths



Bond angles

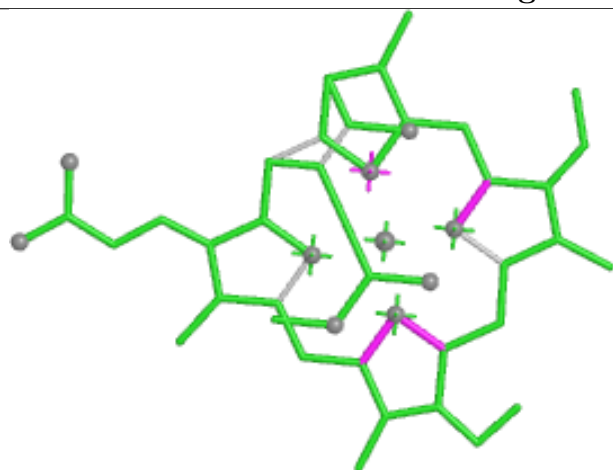


Torsions

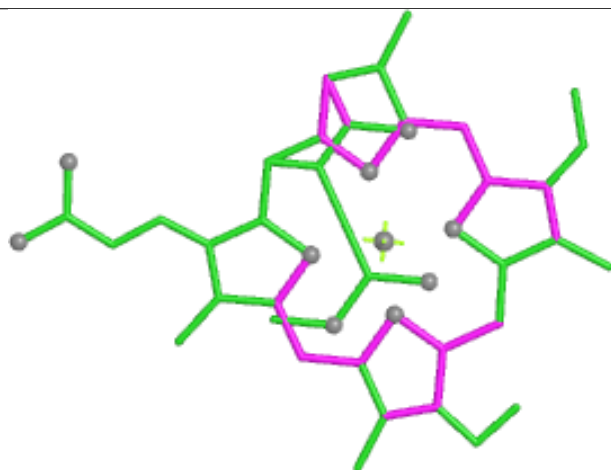


Rings

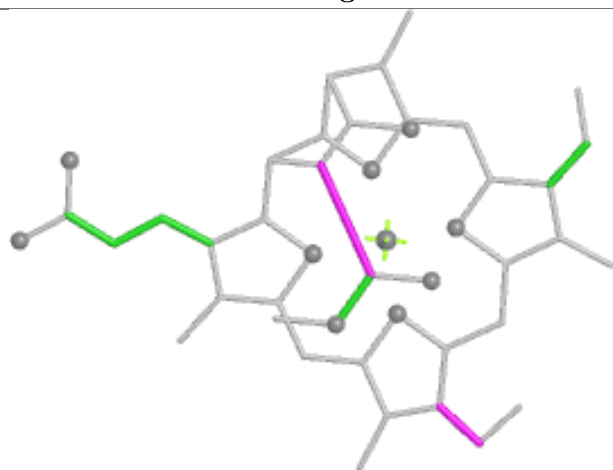
Ligand KC2 L 303



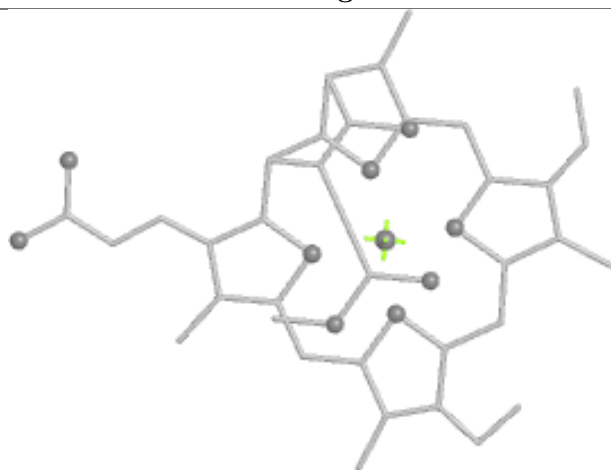
Bond lengths



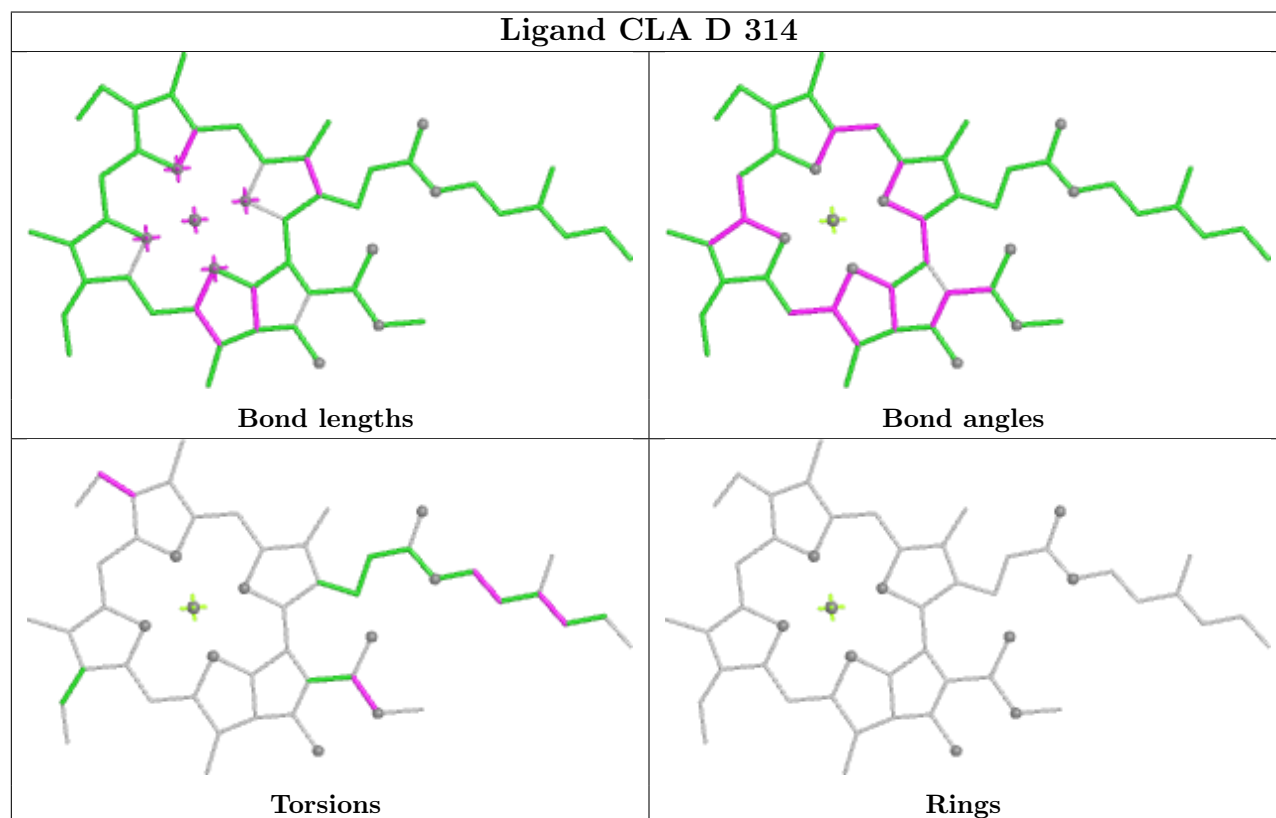
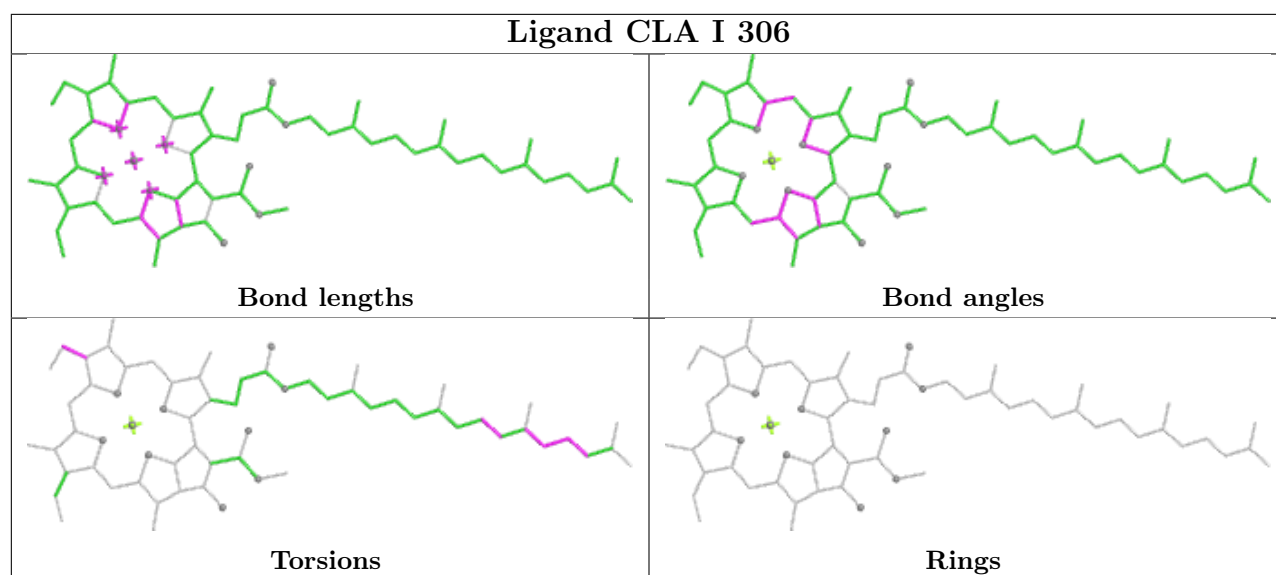
Bond angles

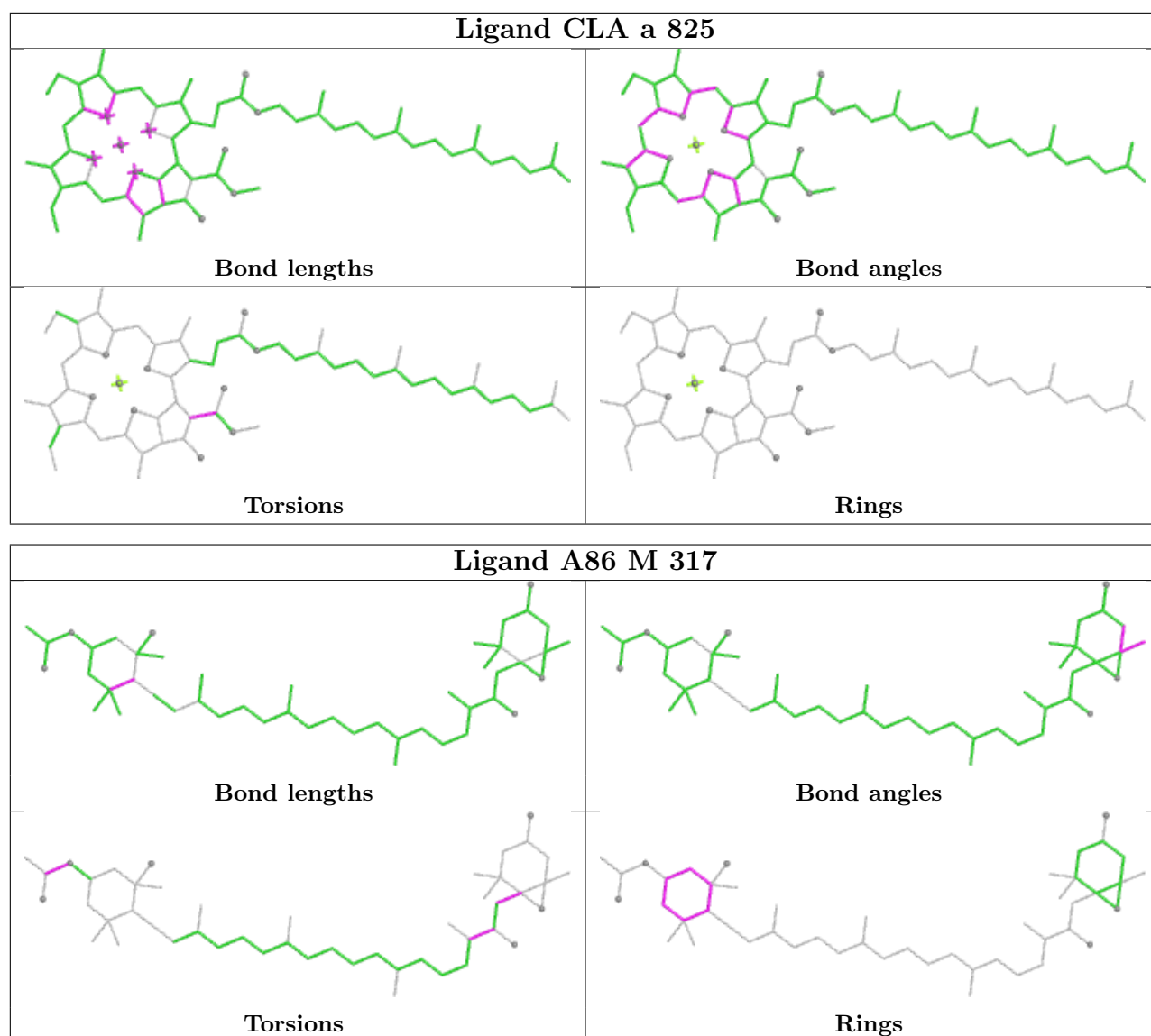


Torsions

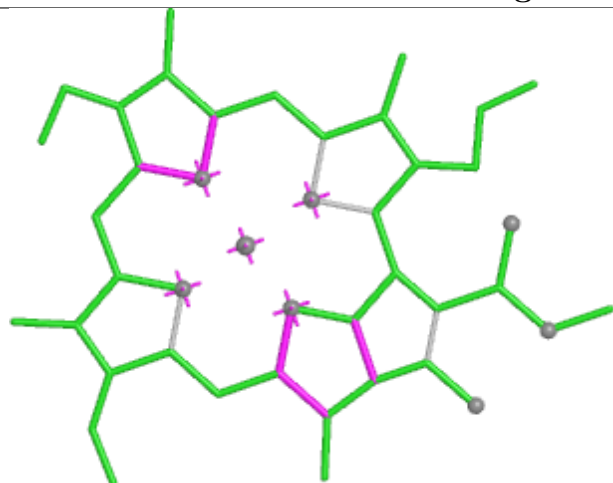


Rings

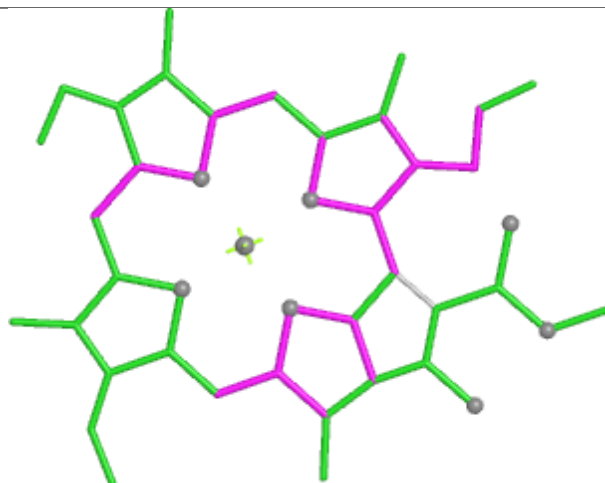




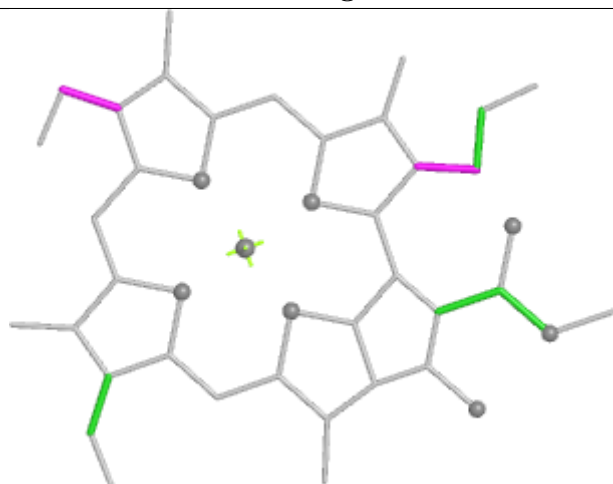
Ligand CLA C 304



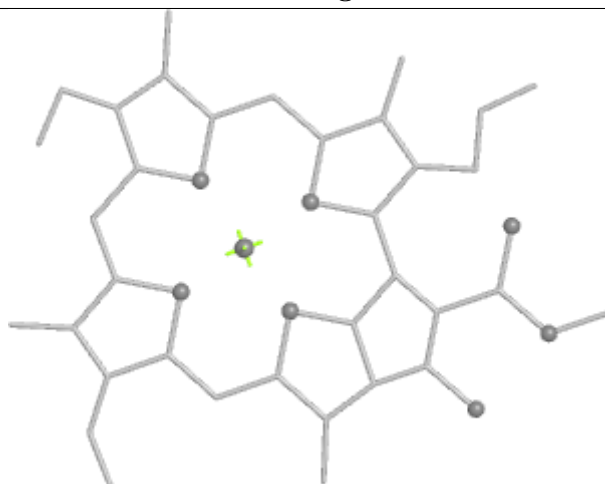
Bond lengths



Bond angles

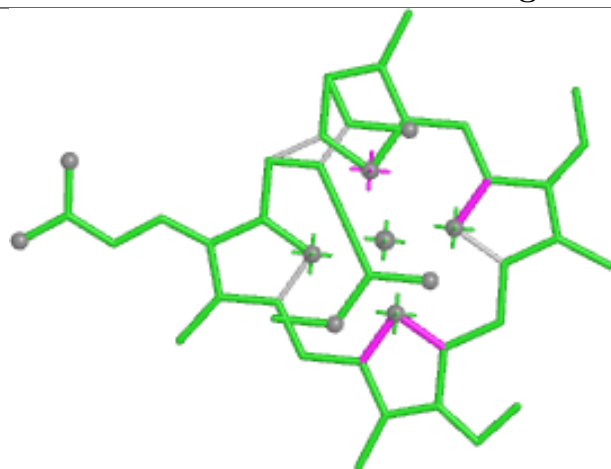


Torsions

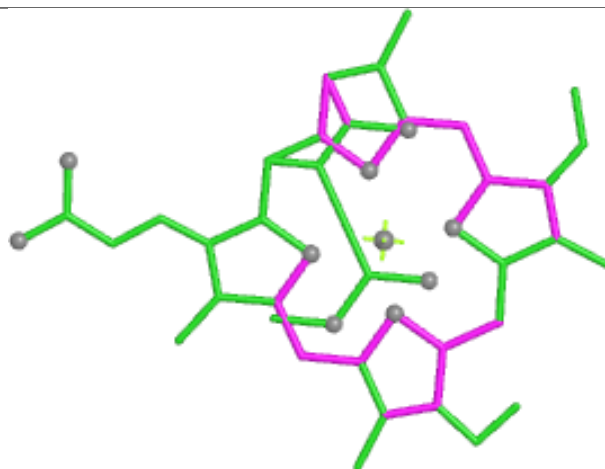


Rings

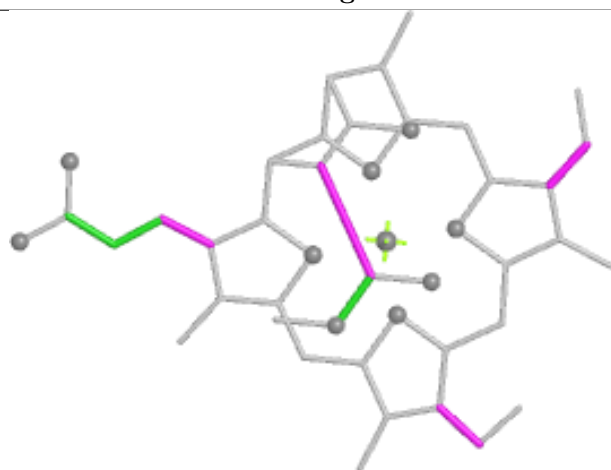
Ligand KC2 S 303



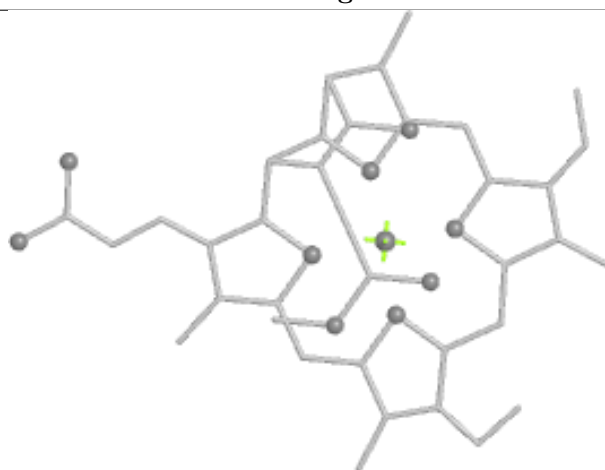
Bond lengths



Bond angles



Torsions

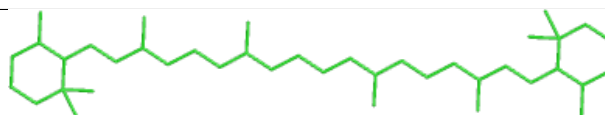


Rings

Ligand BCR a 845



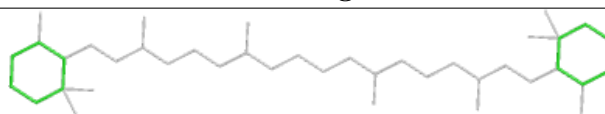
Bond lengths



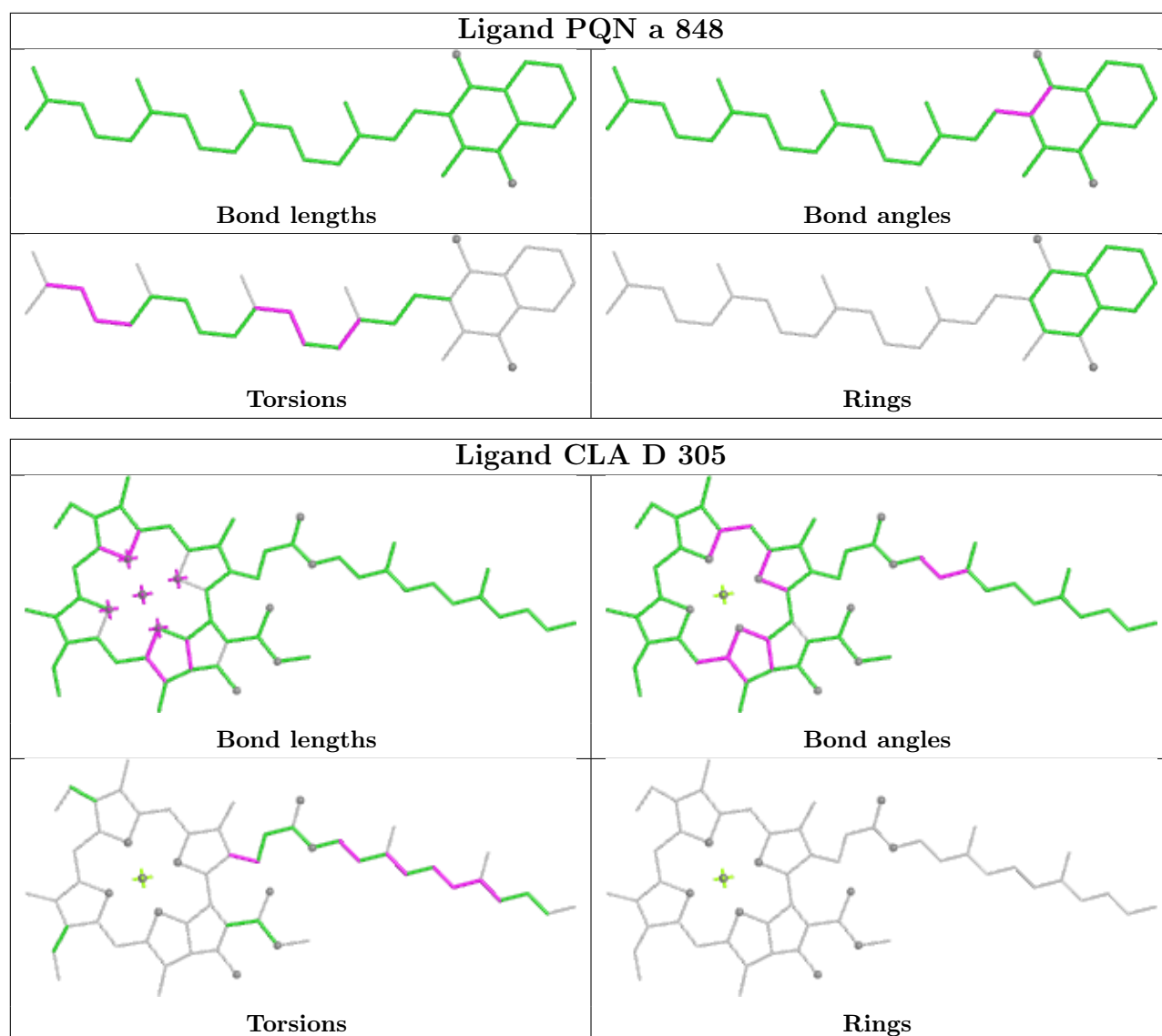
Bond angles



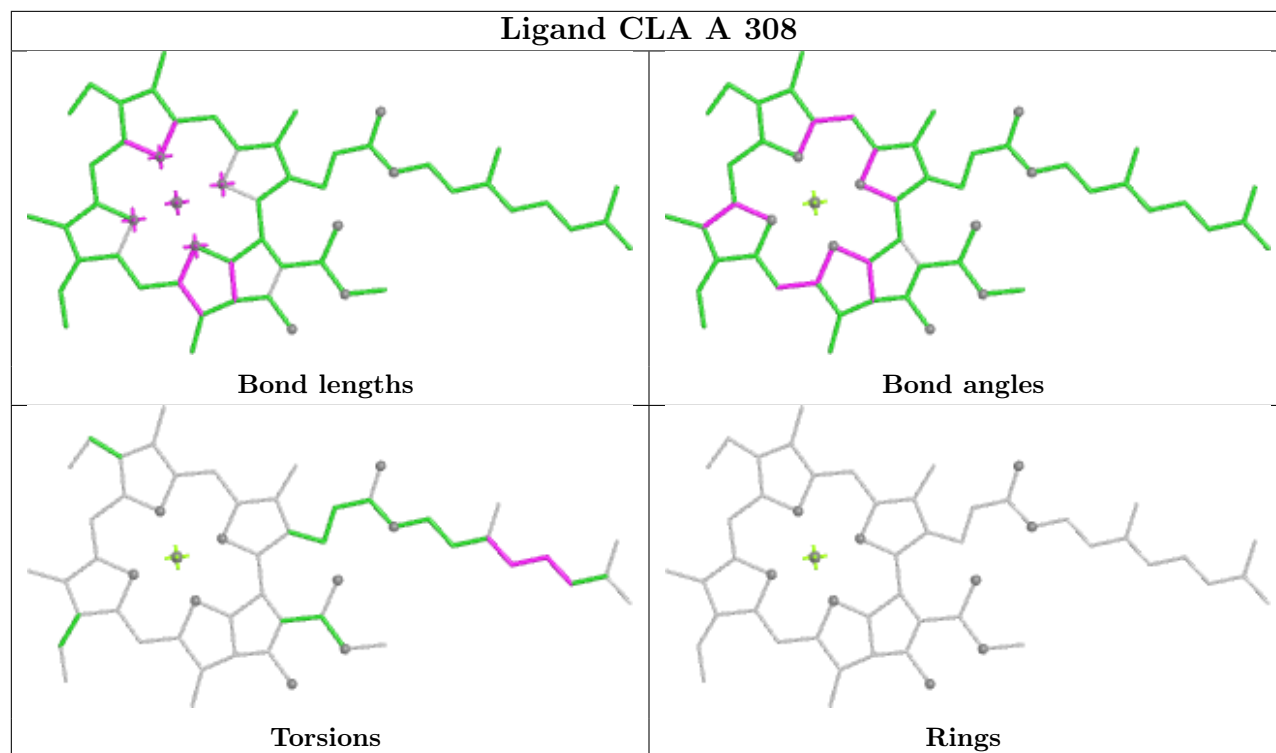
Torsions



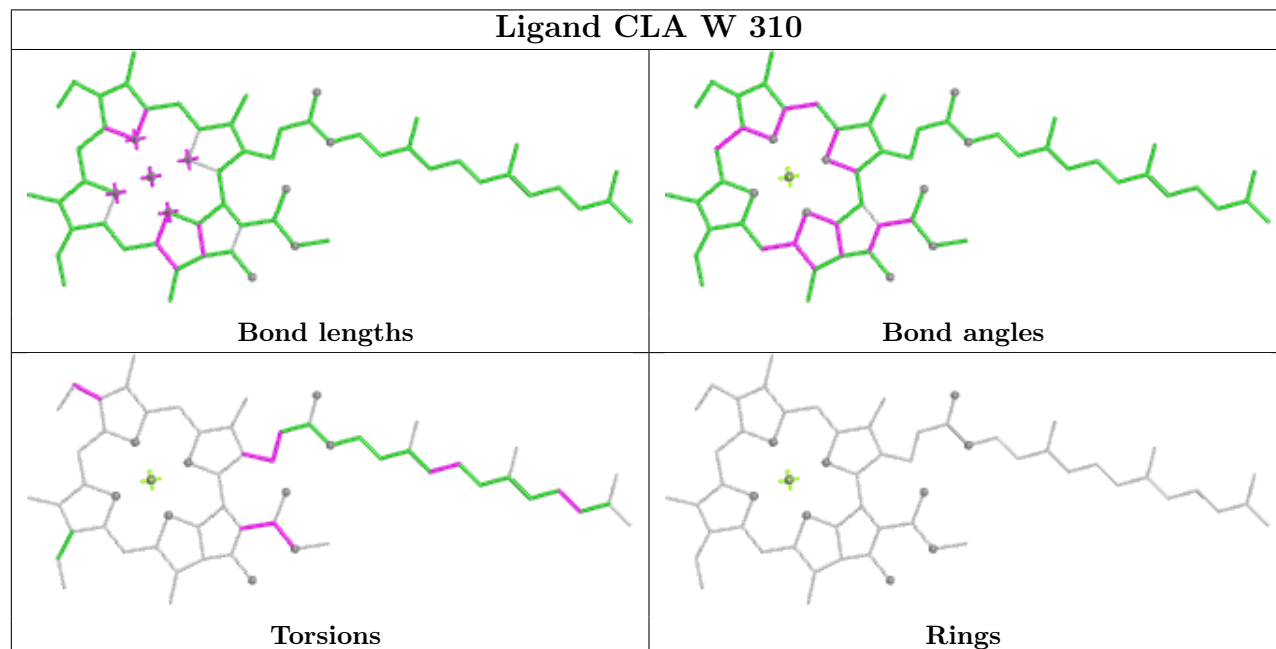
Rings

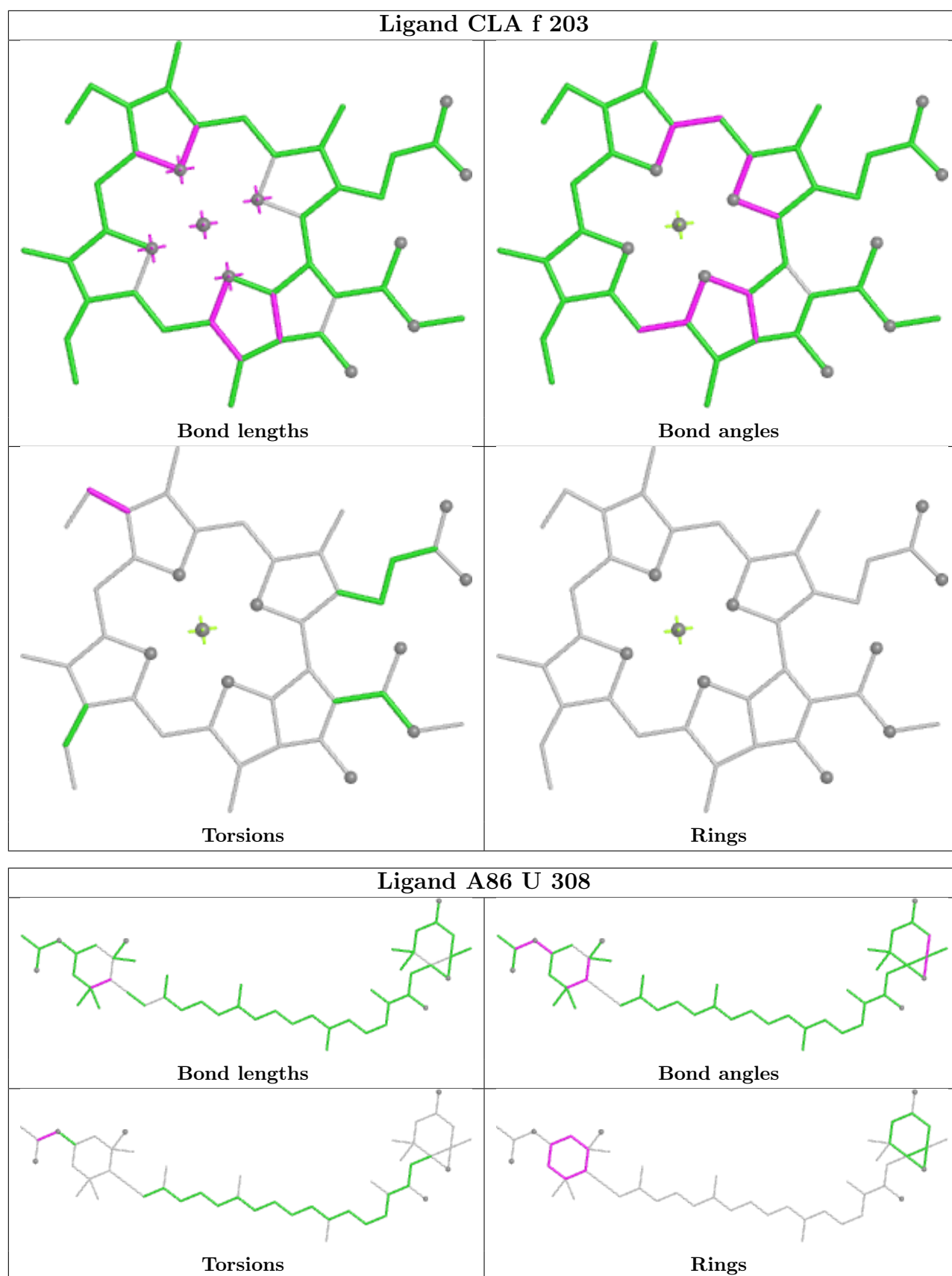


Ligand CLA A 308

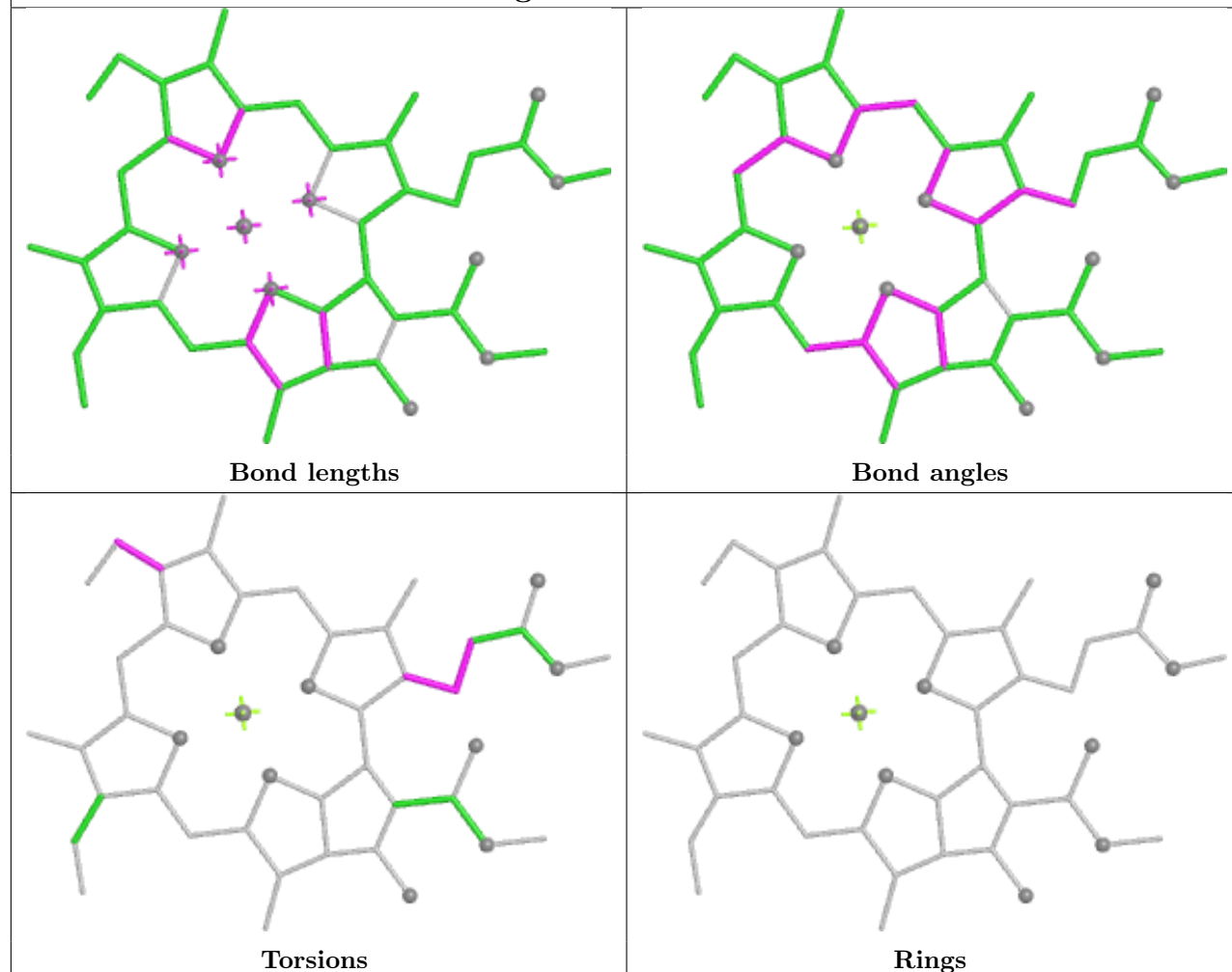


Ligand CLA W 310

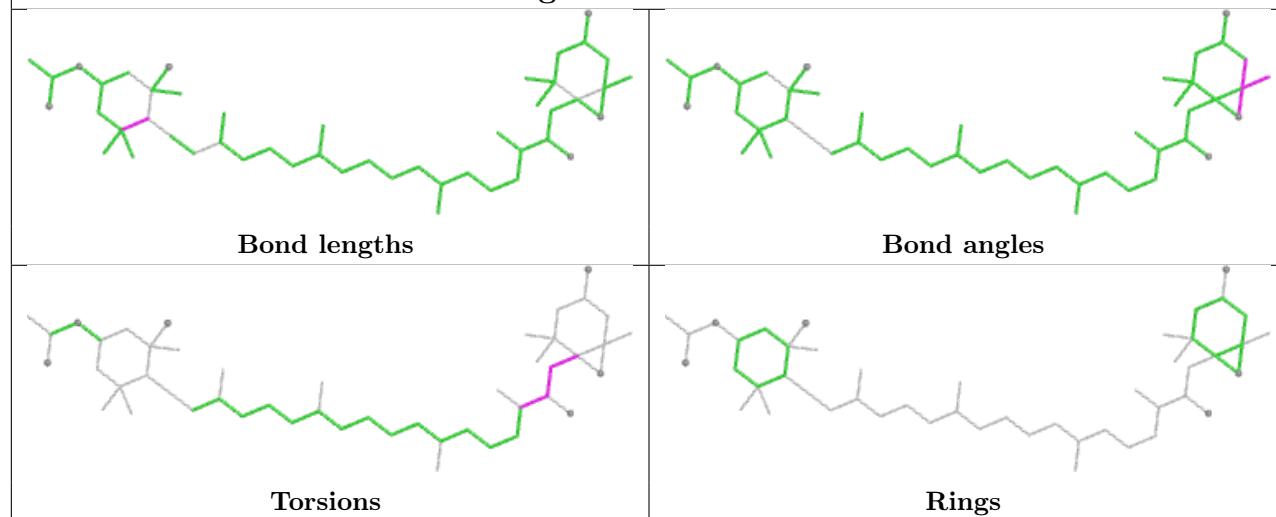




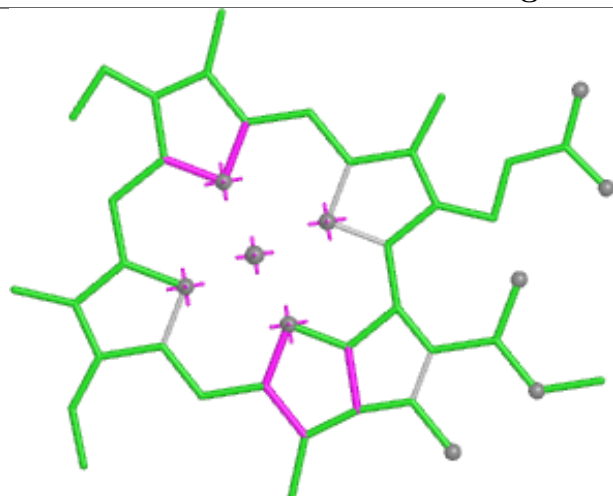
Ligand CLA E 315



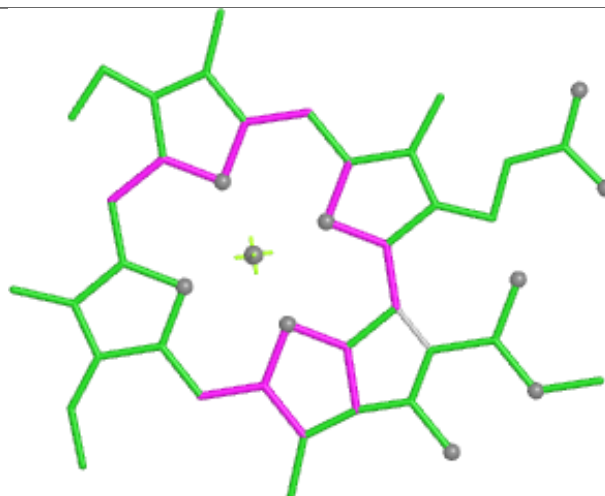
Ligand A86 P 319



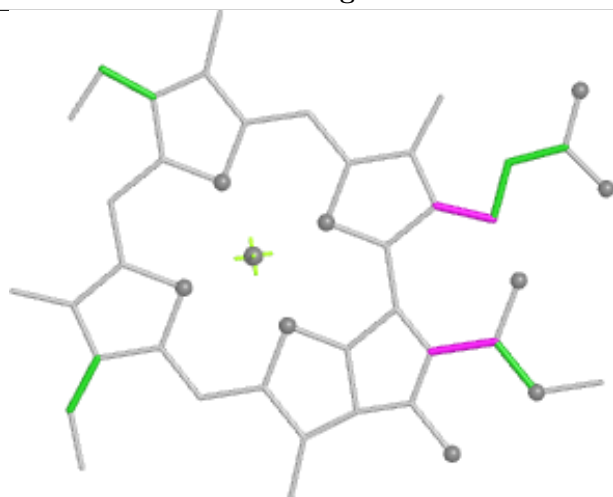
Ligand CLA I 307



Bond lengths



Bond angles

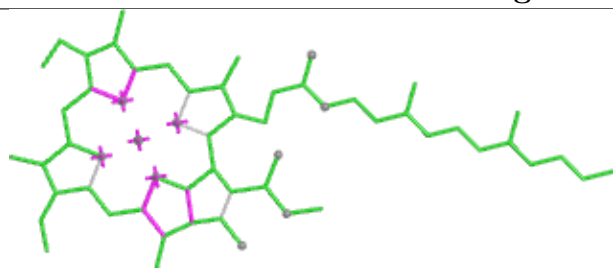


Torsions

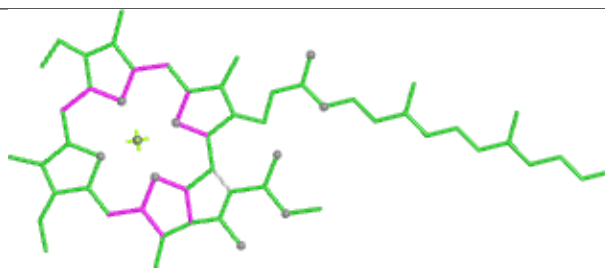


Rings

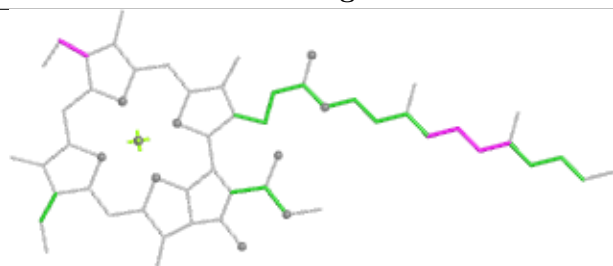
Ligand CLA V 201



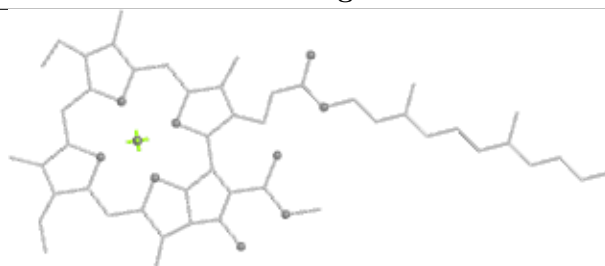
Bond lengths



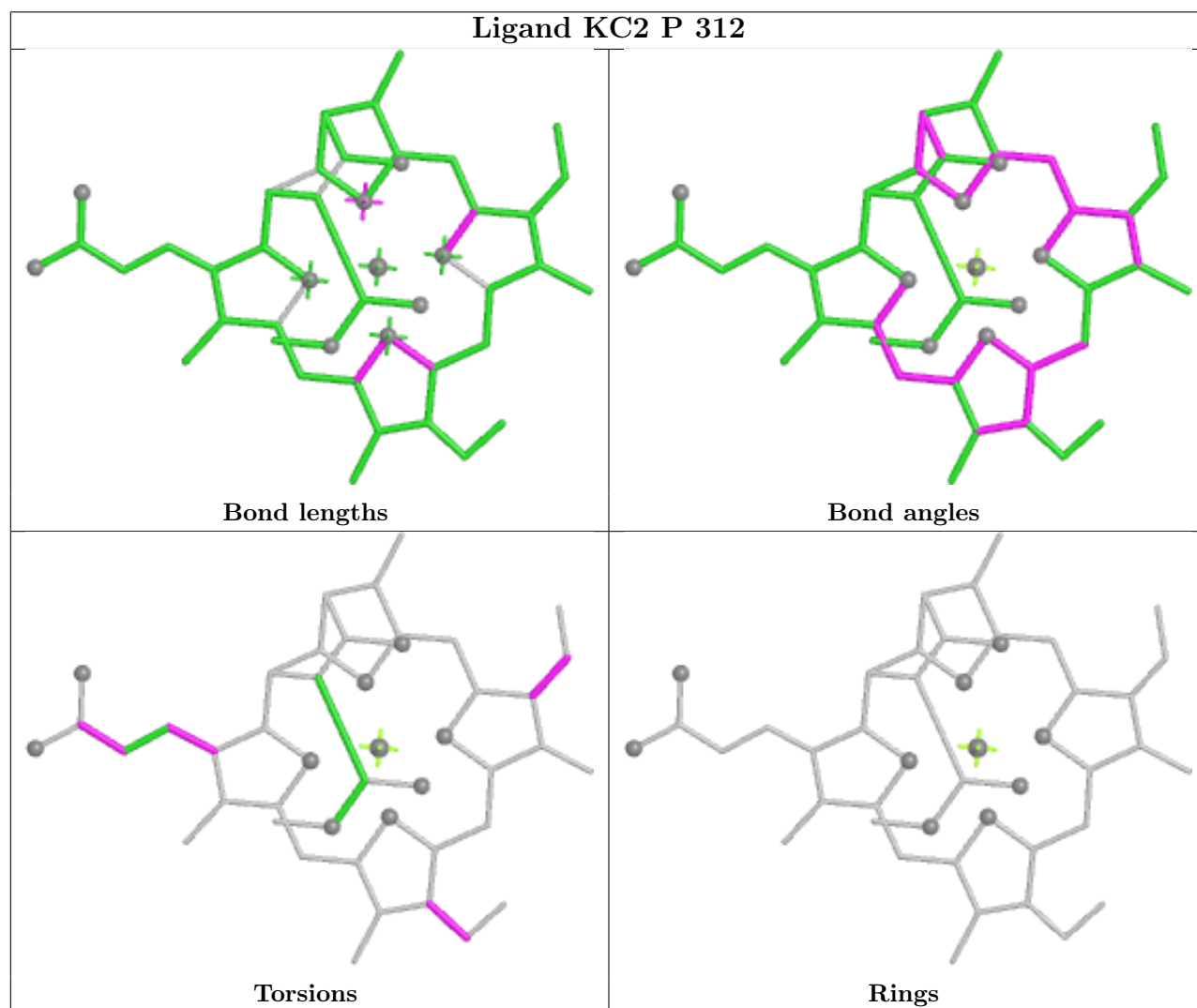
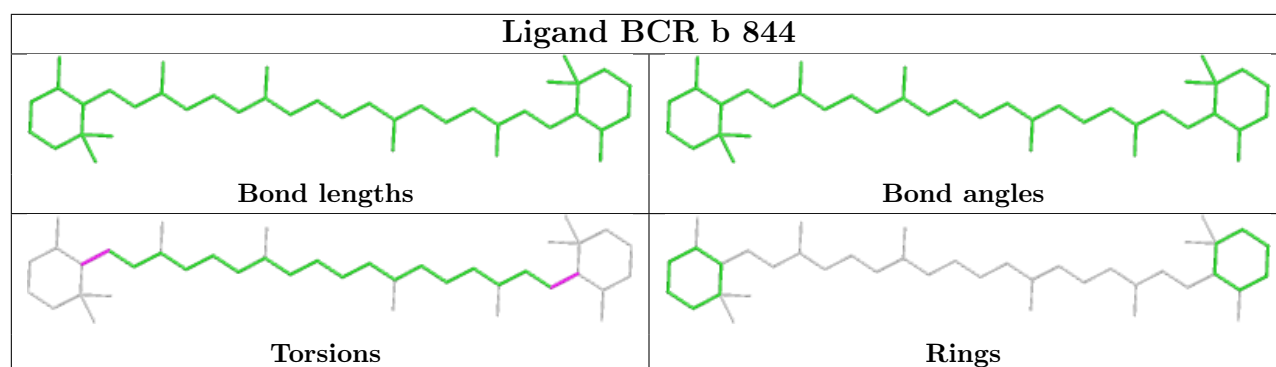
Bond angles

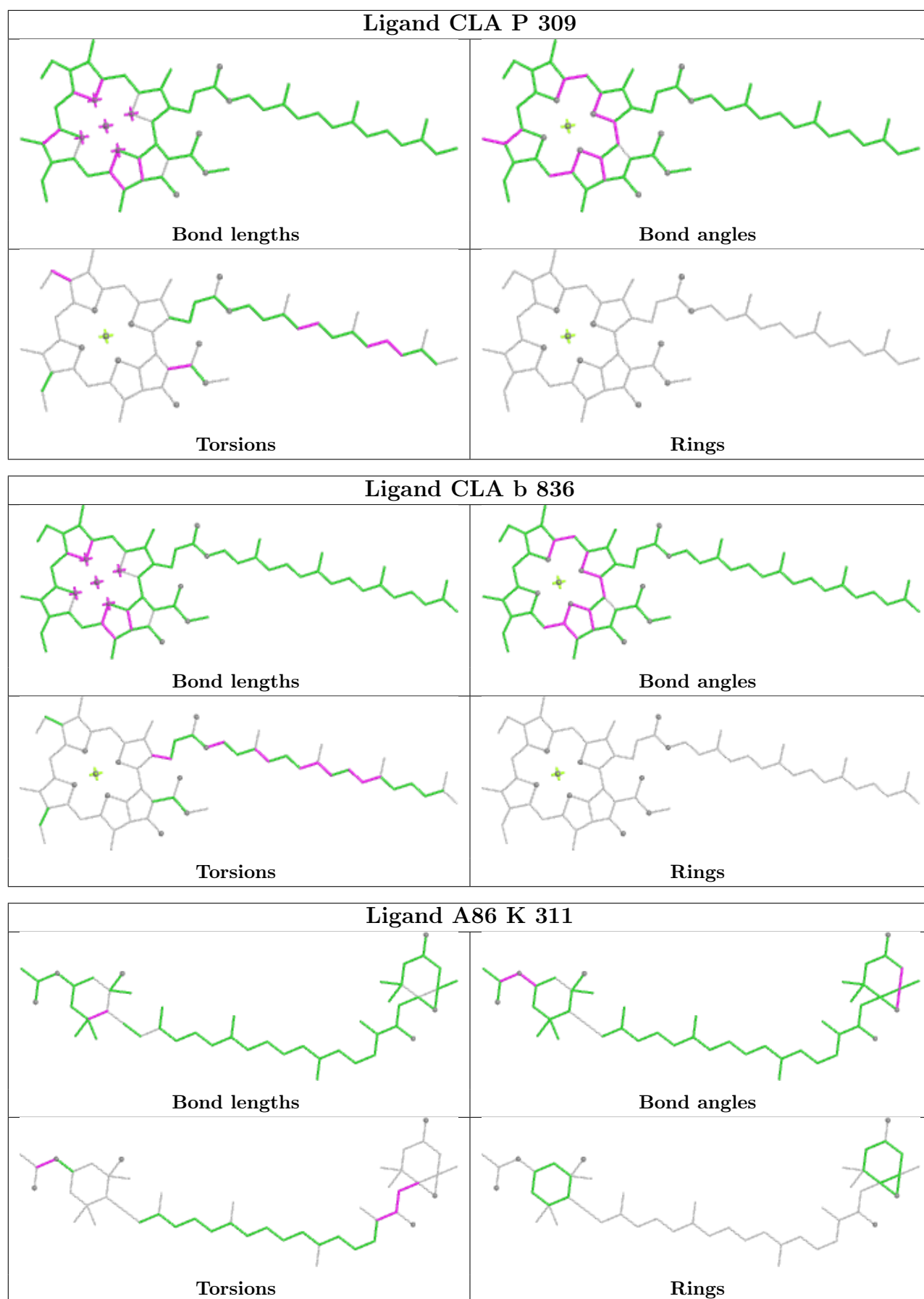


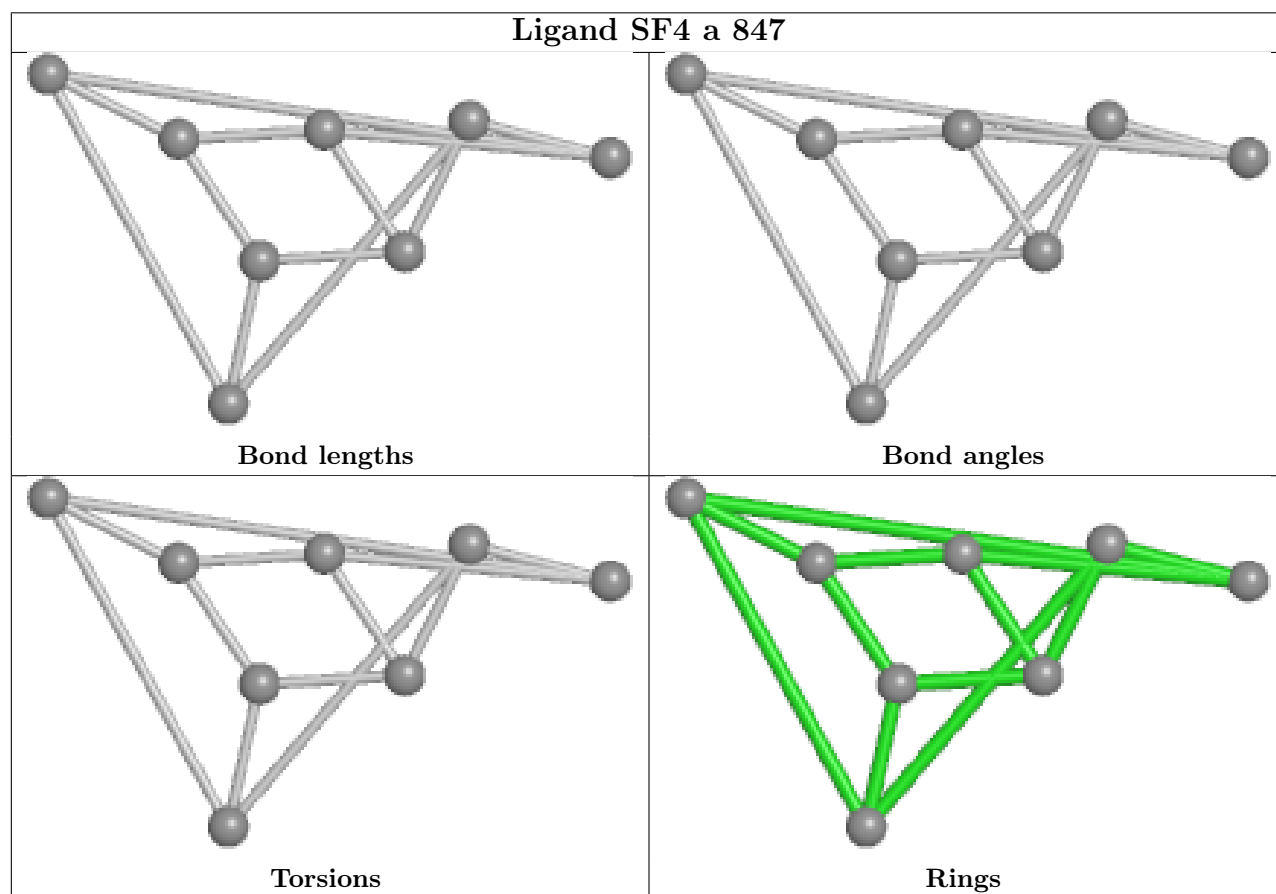
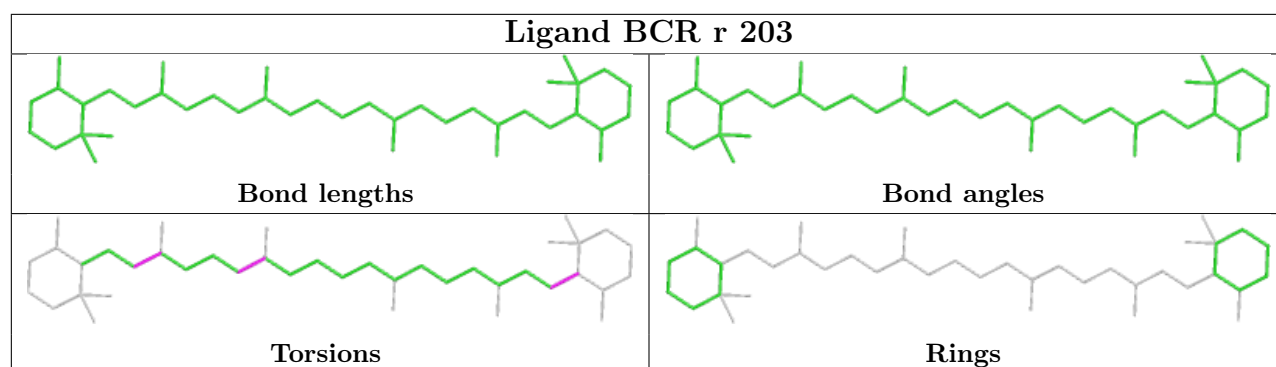
Torsions

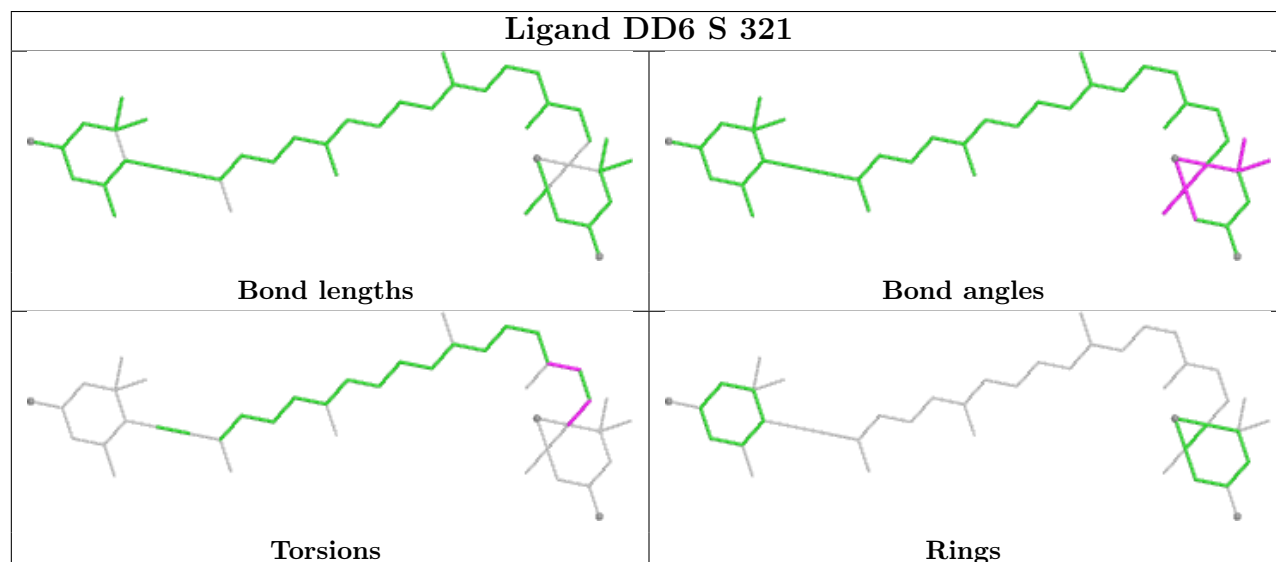
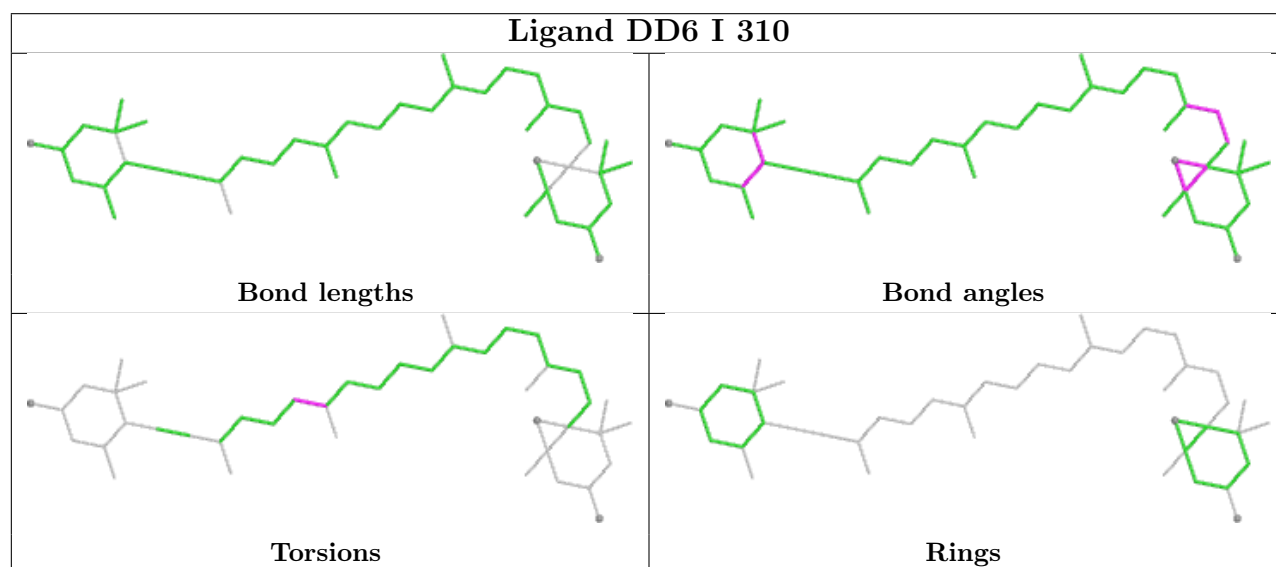
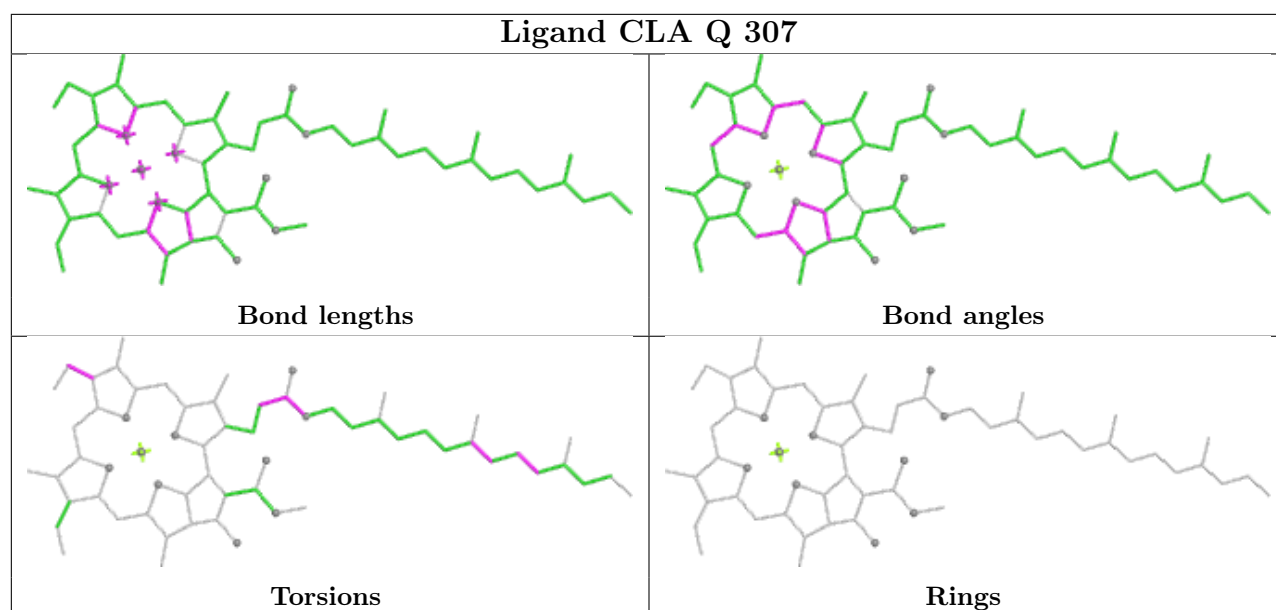


Rings

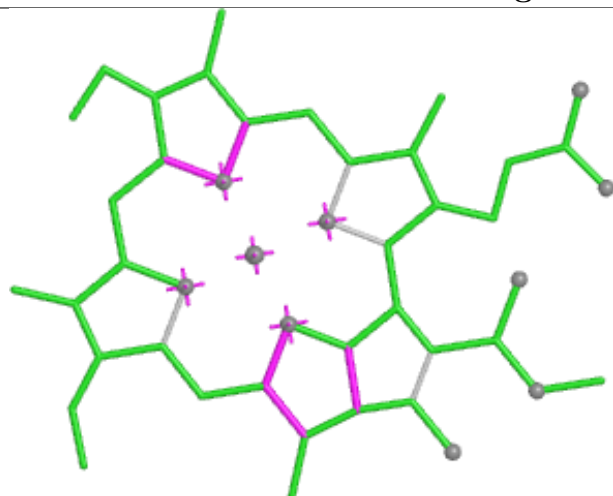




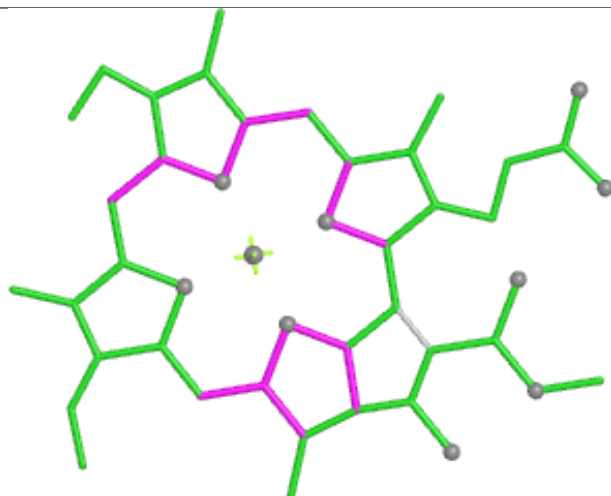




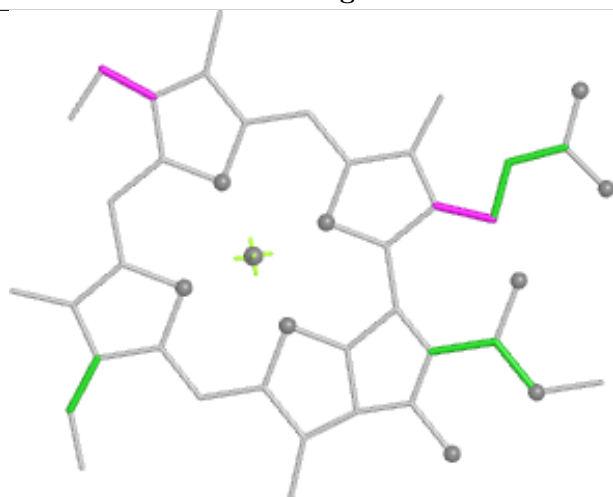
Ligand CLA T 309



Bond lengths



Bond angles

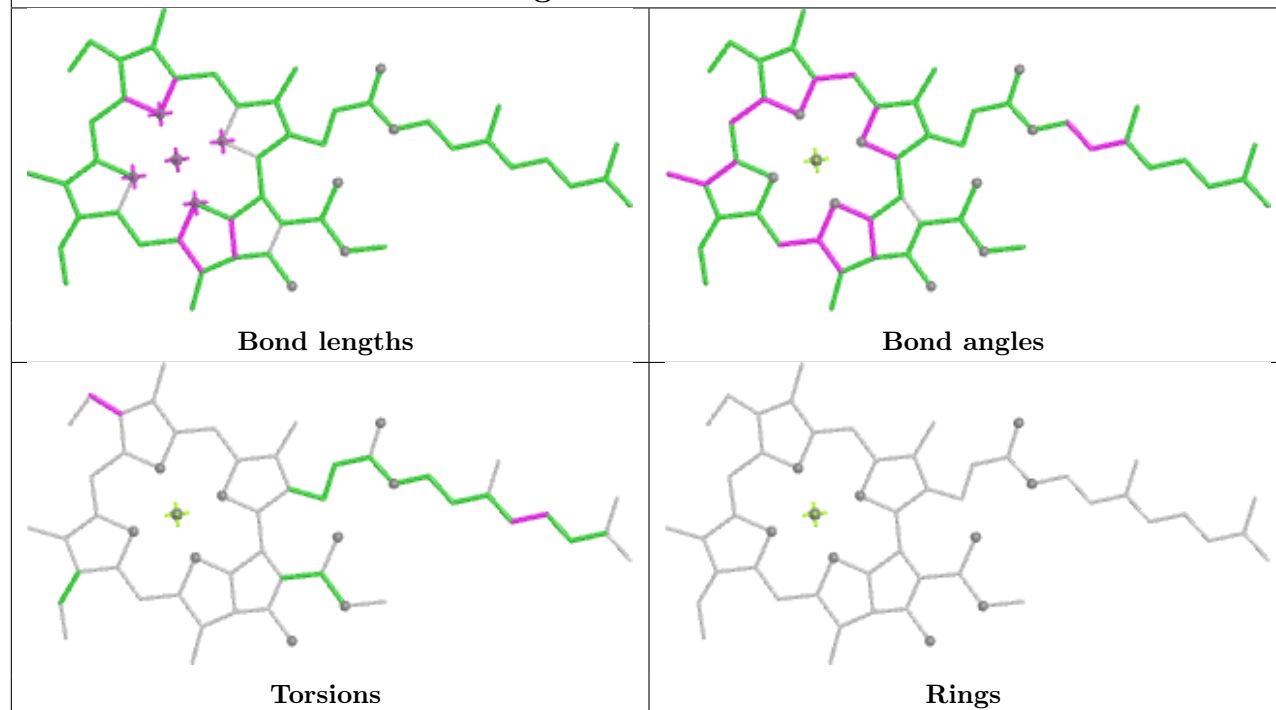


Torsions

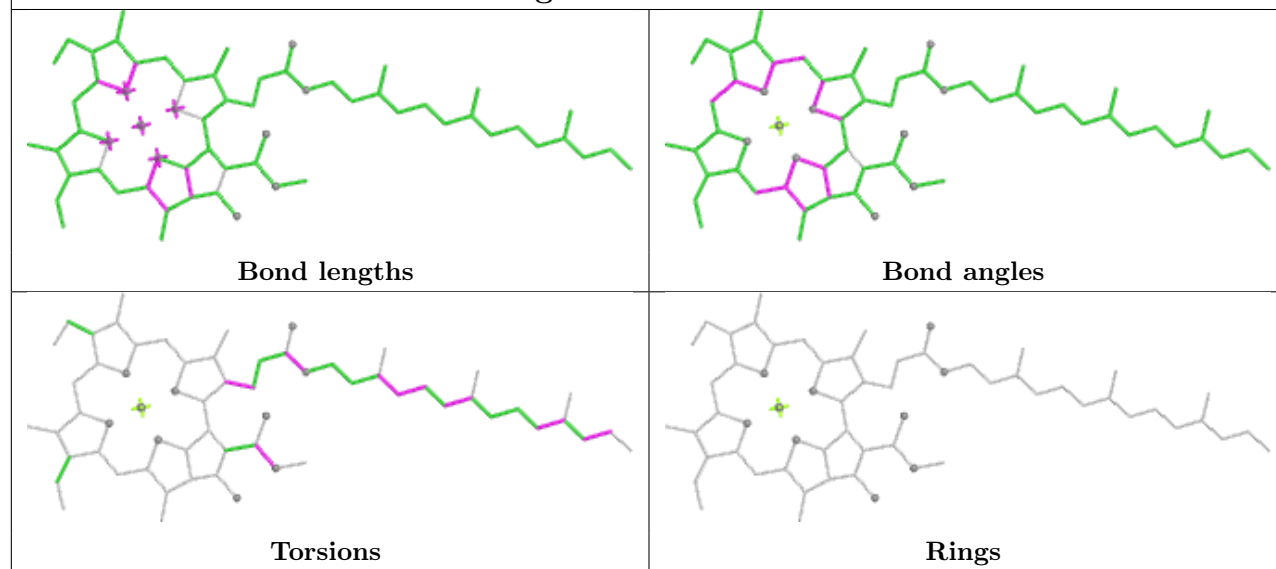


Rings

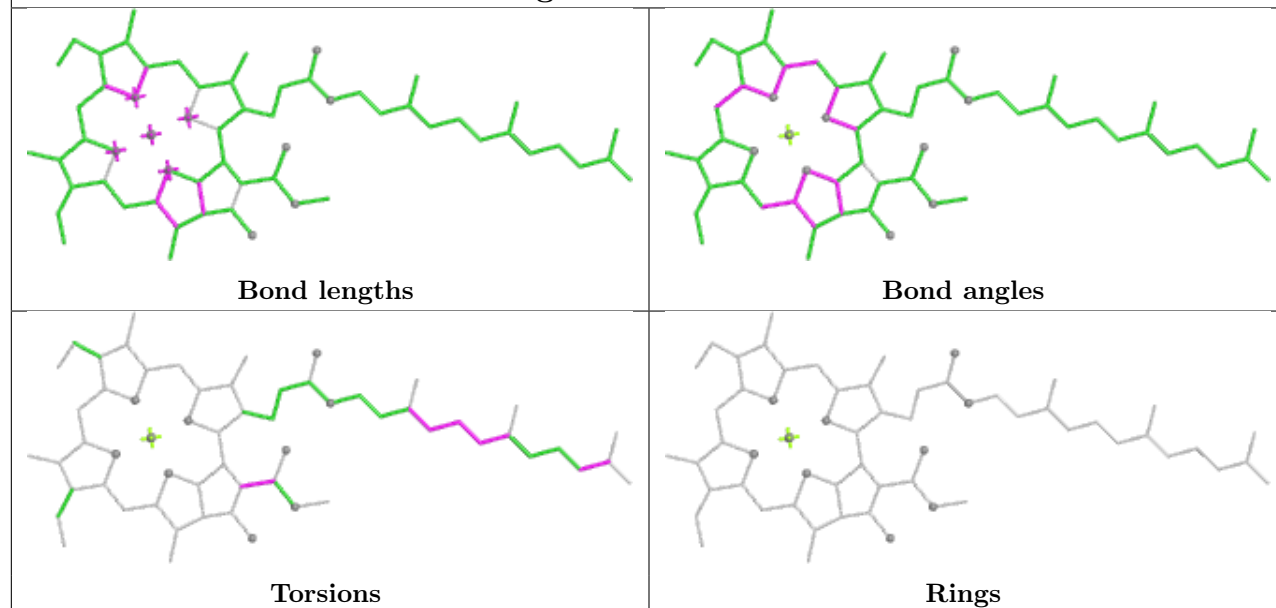
Ligand CLA F 304



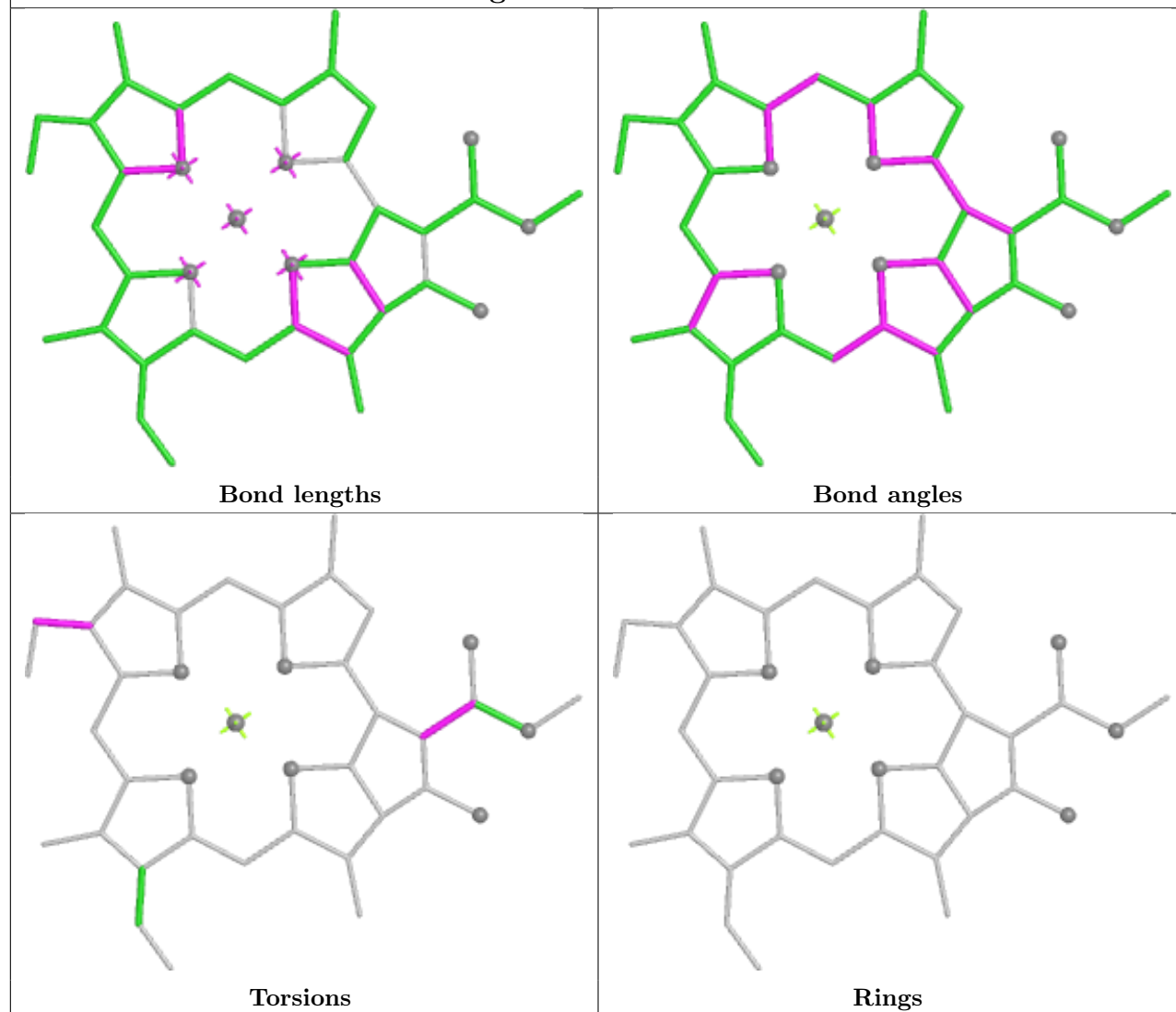
Ligand CLA b 833

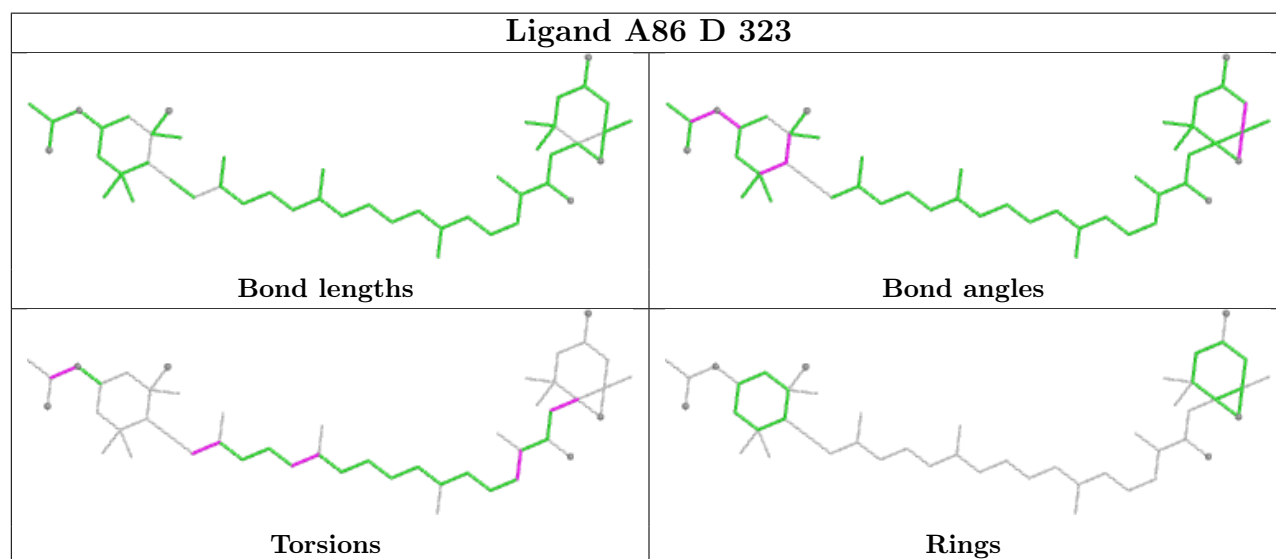
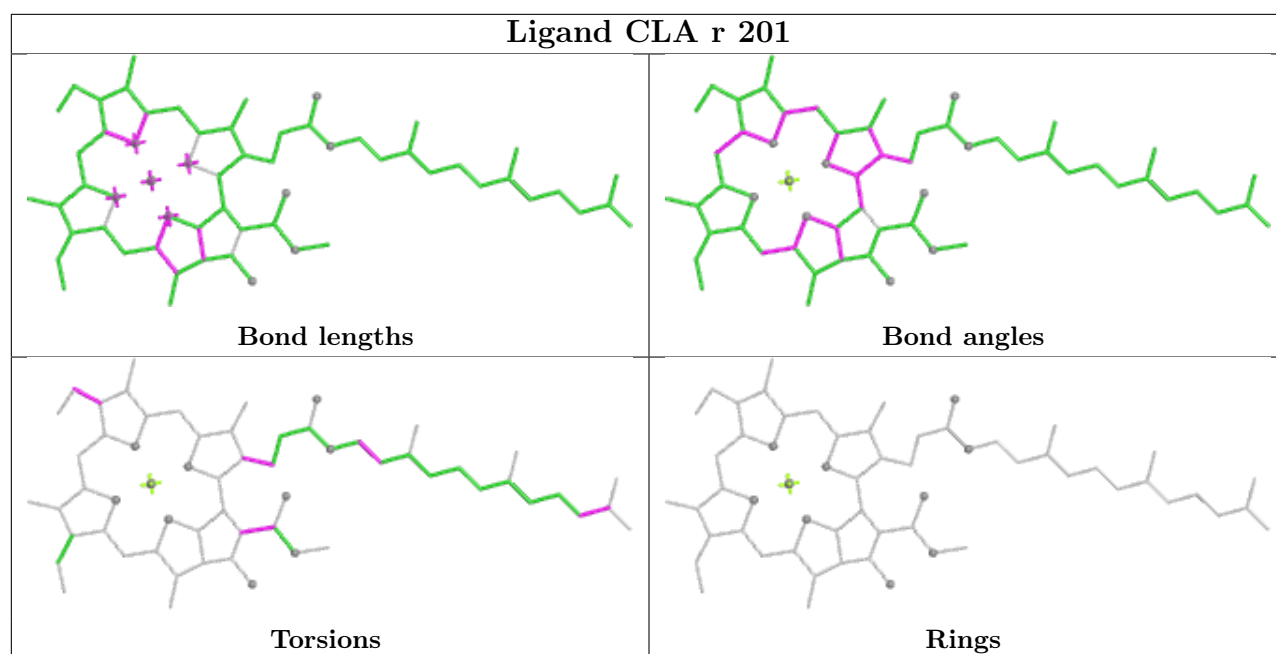


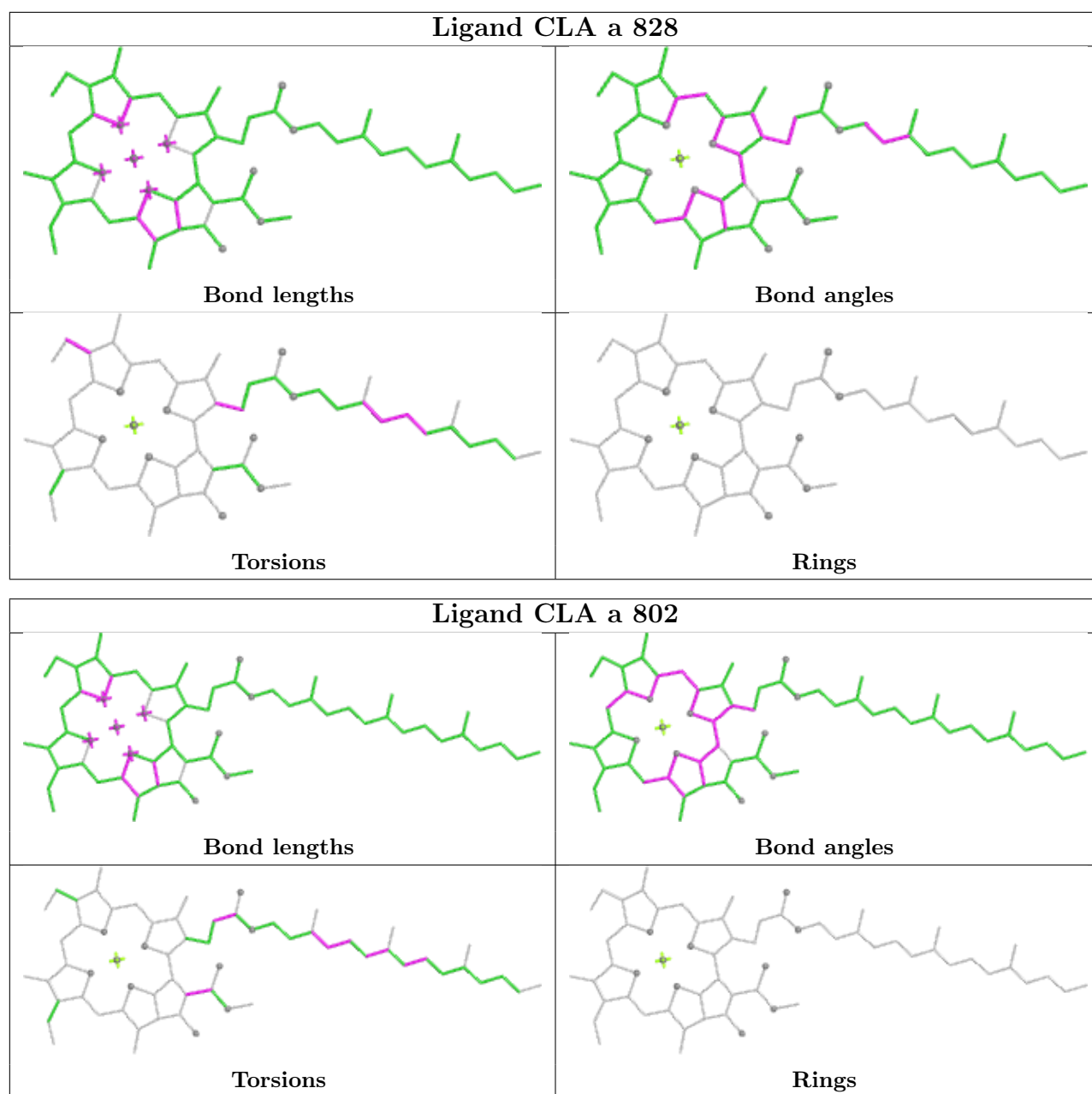
Ligand CLA a 809

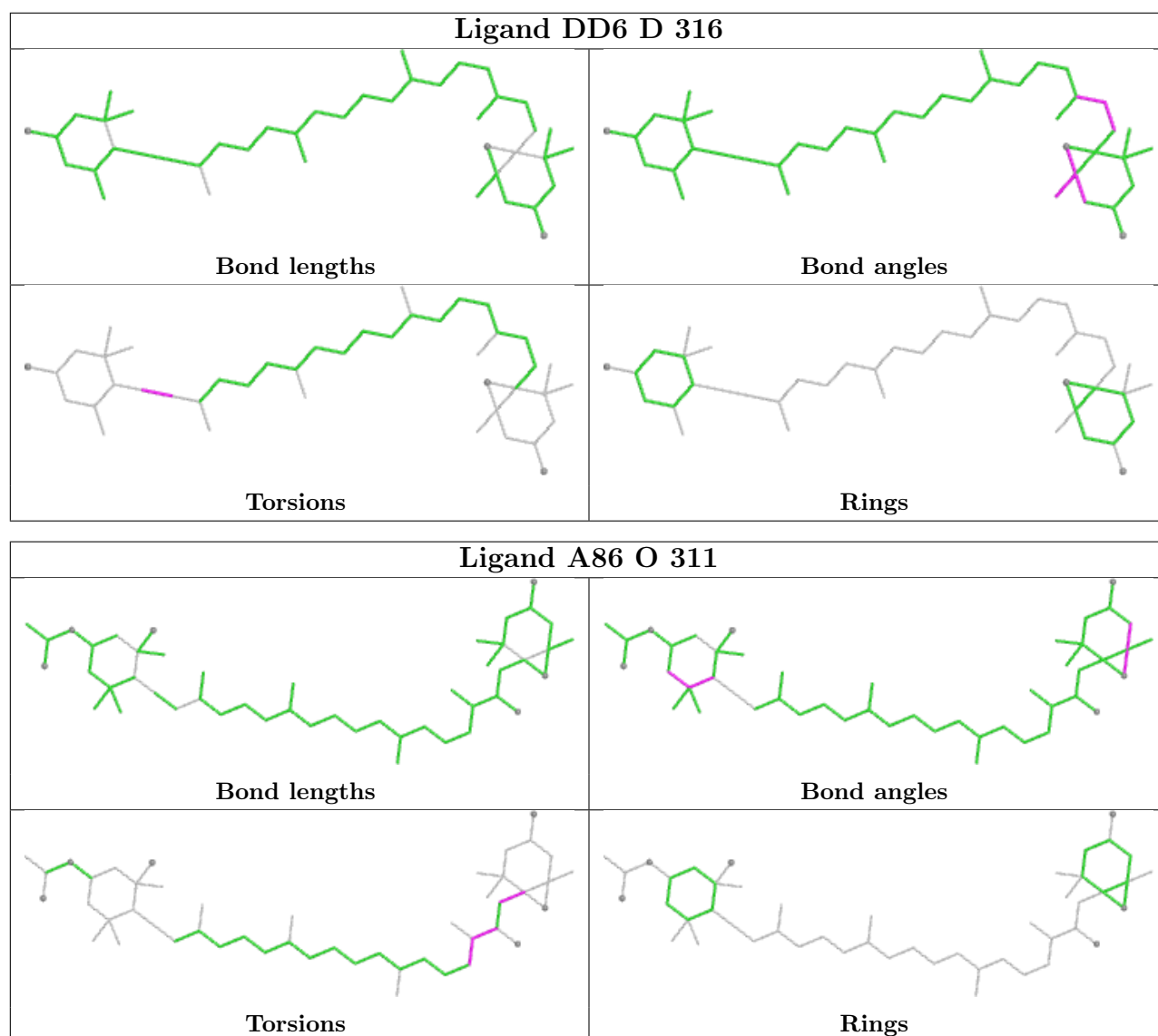


Ligand CLA U 301

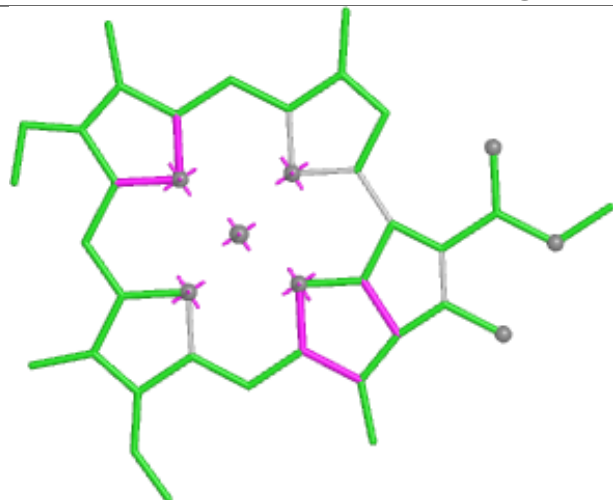




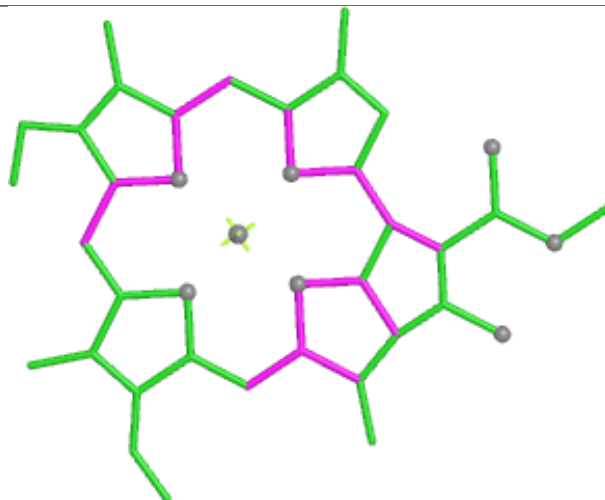




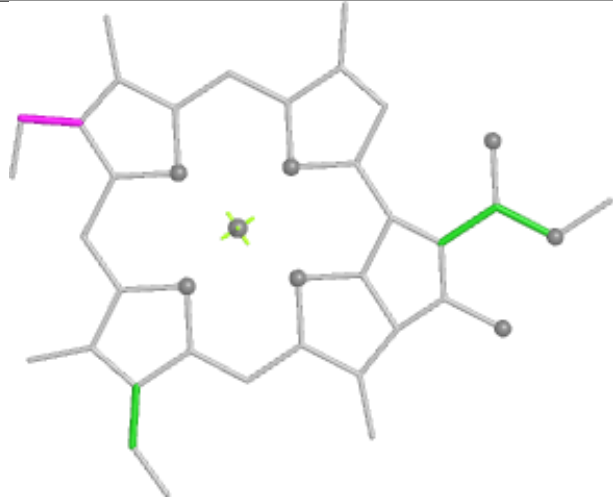
Ligand CLA F 301



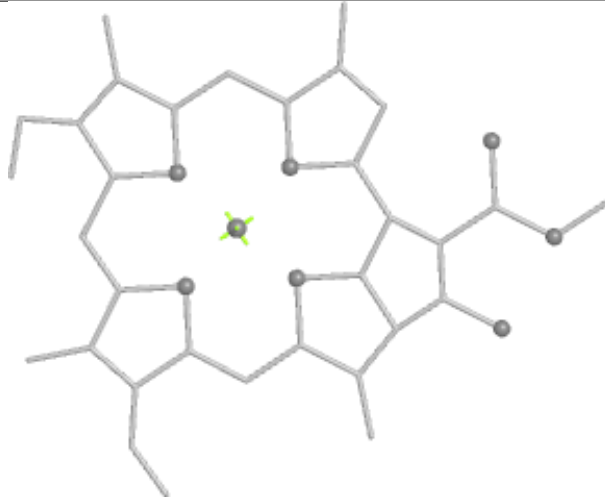
Bond lengths



Bond angles

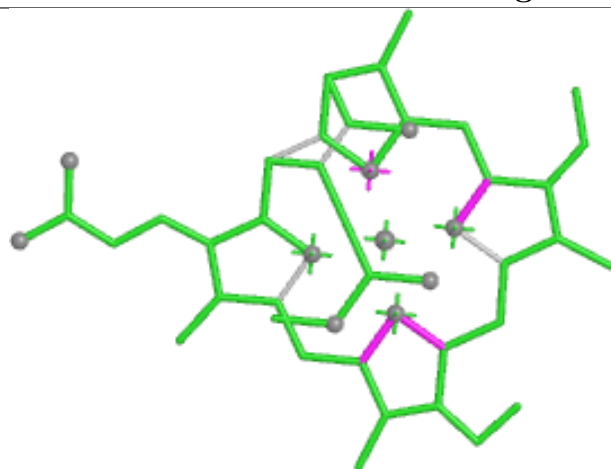


Torsions

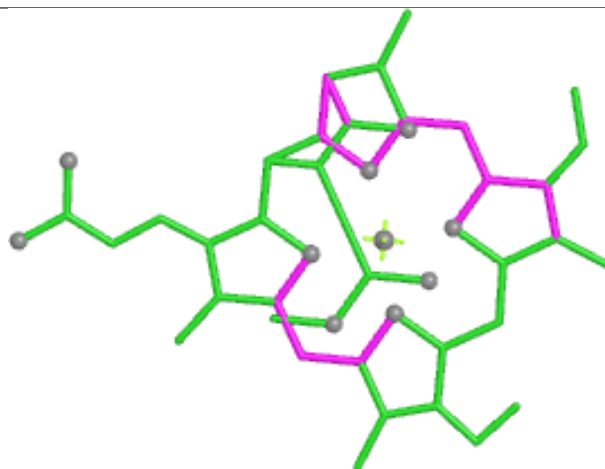


Rings

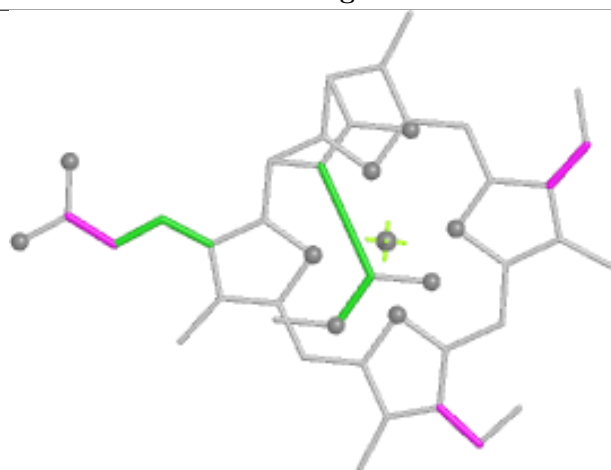
Ligand KC2 K 302



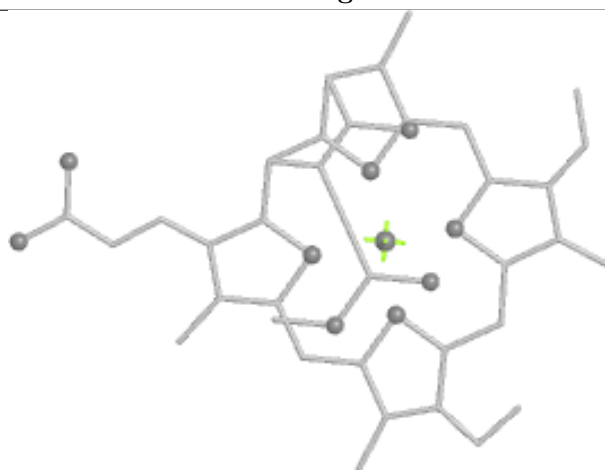
Bond lengths



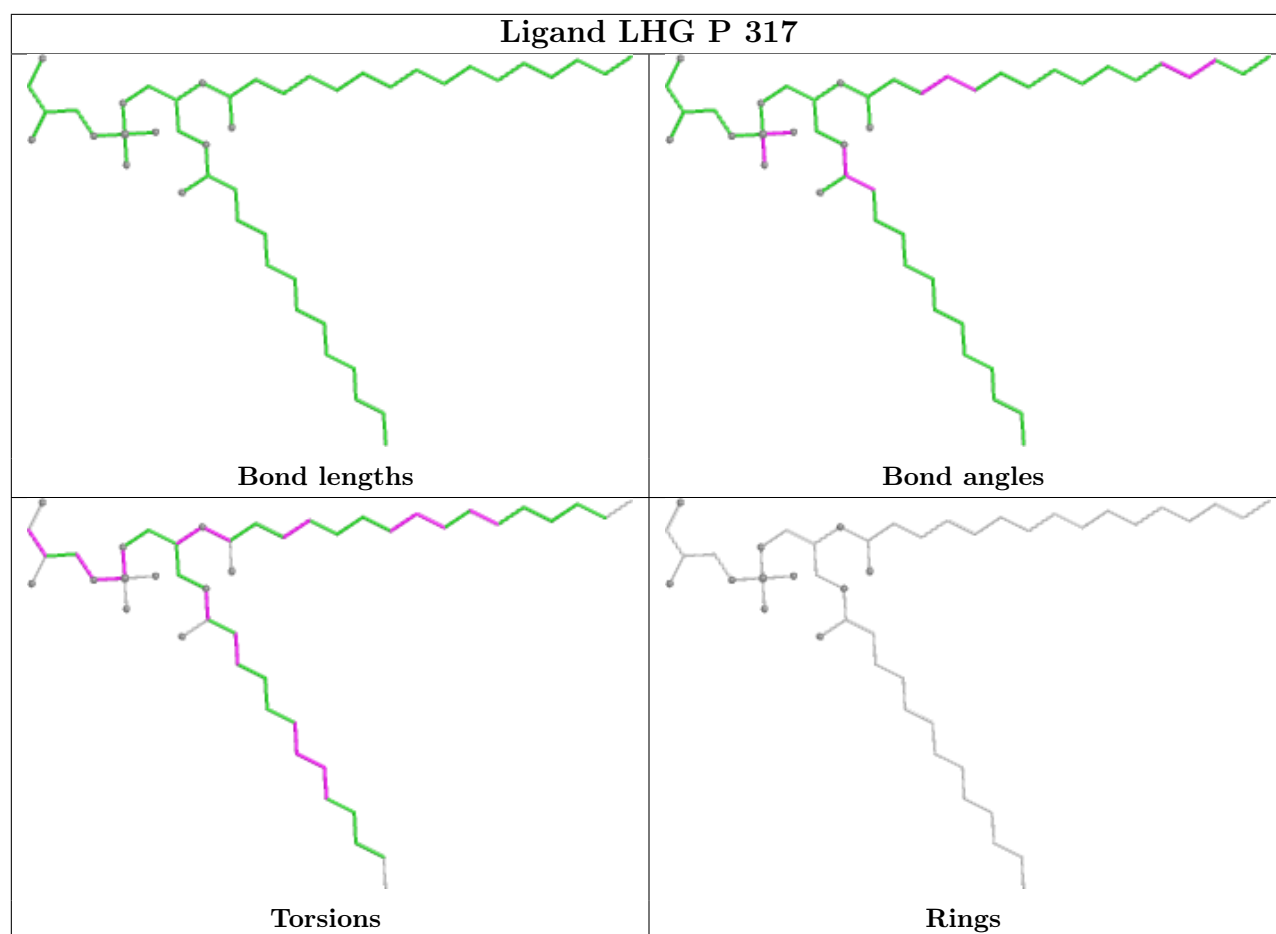
Bond angles



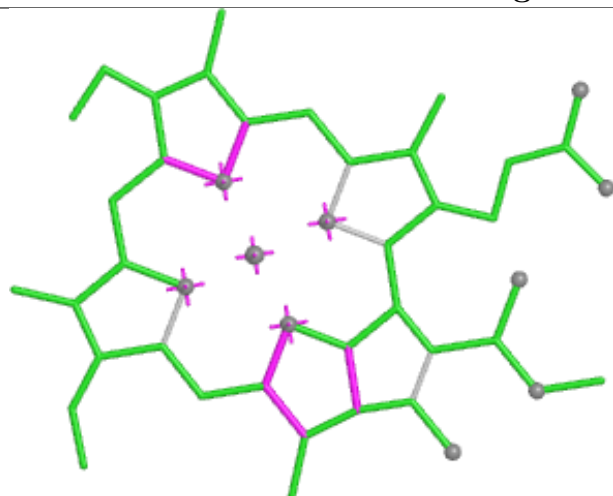
Torsions



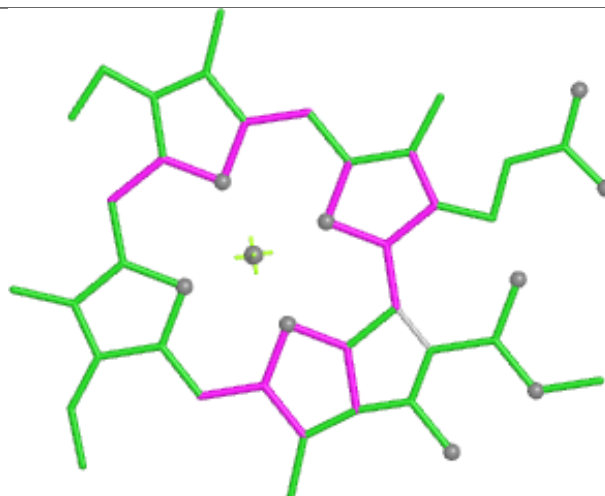
Rings



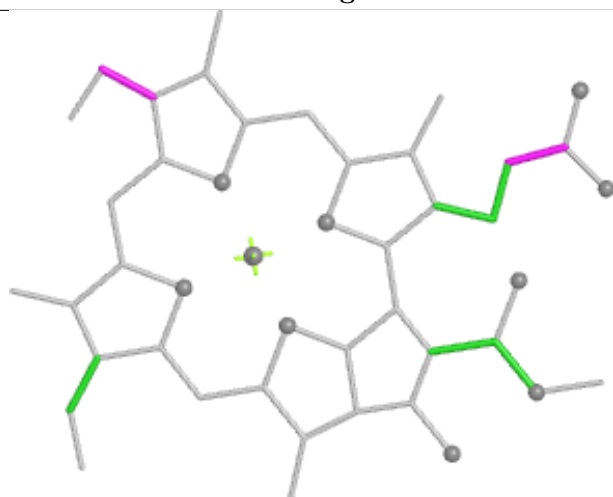
Ligand CLA U 303



Bond lengths



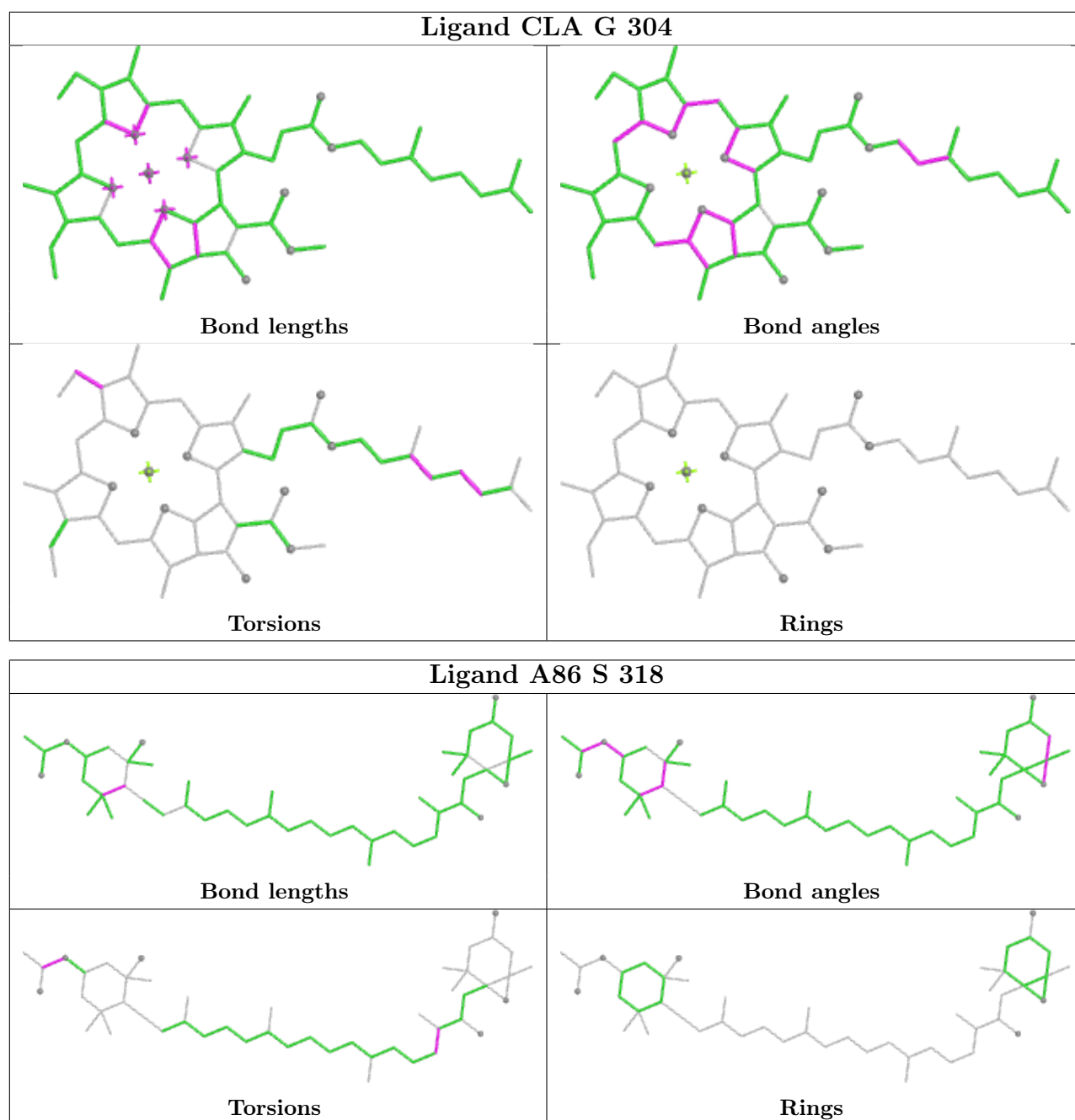
Bond angles

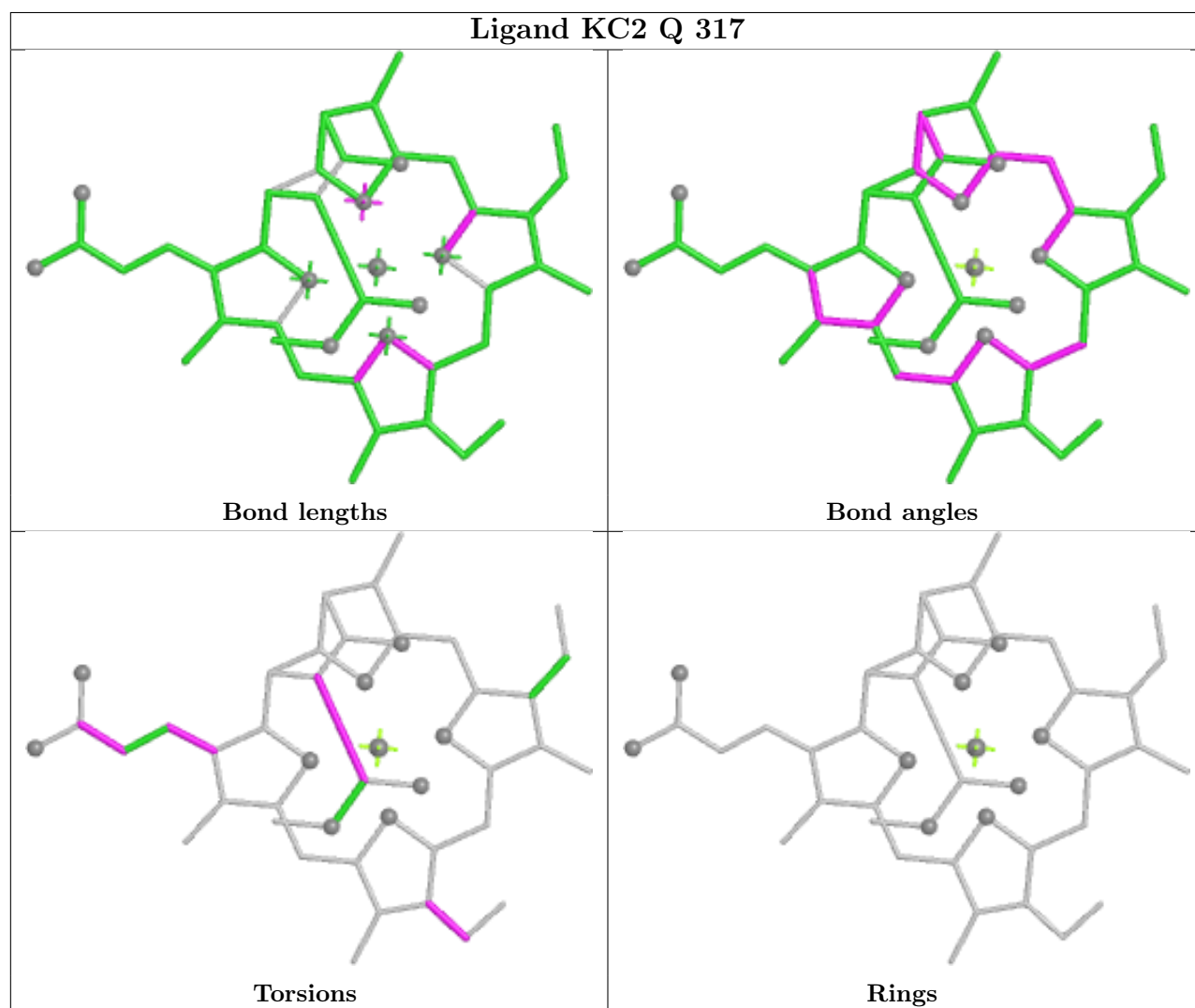
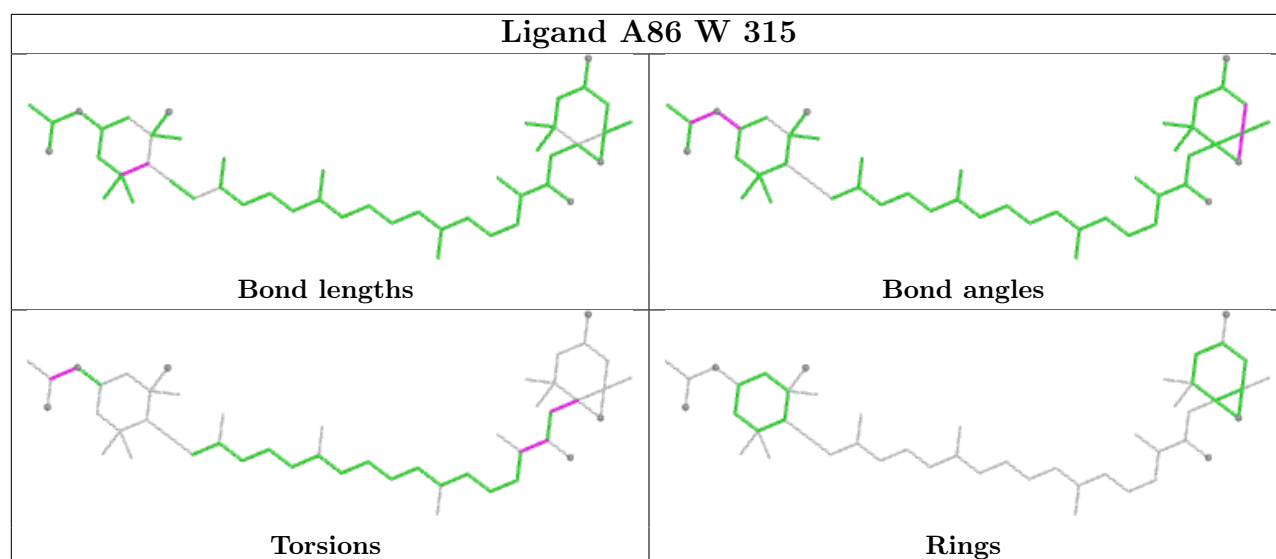


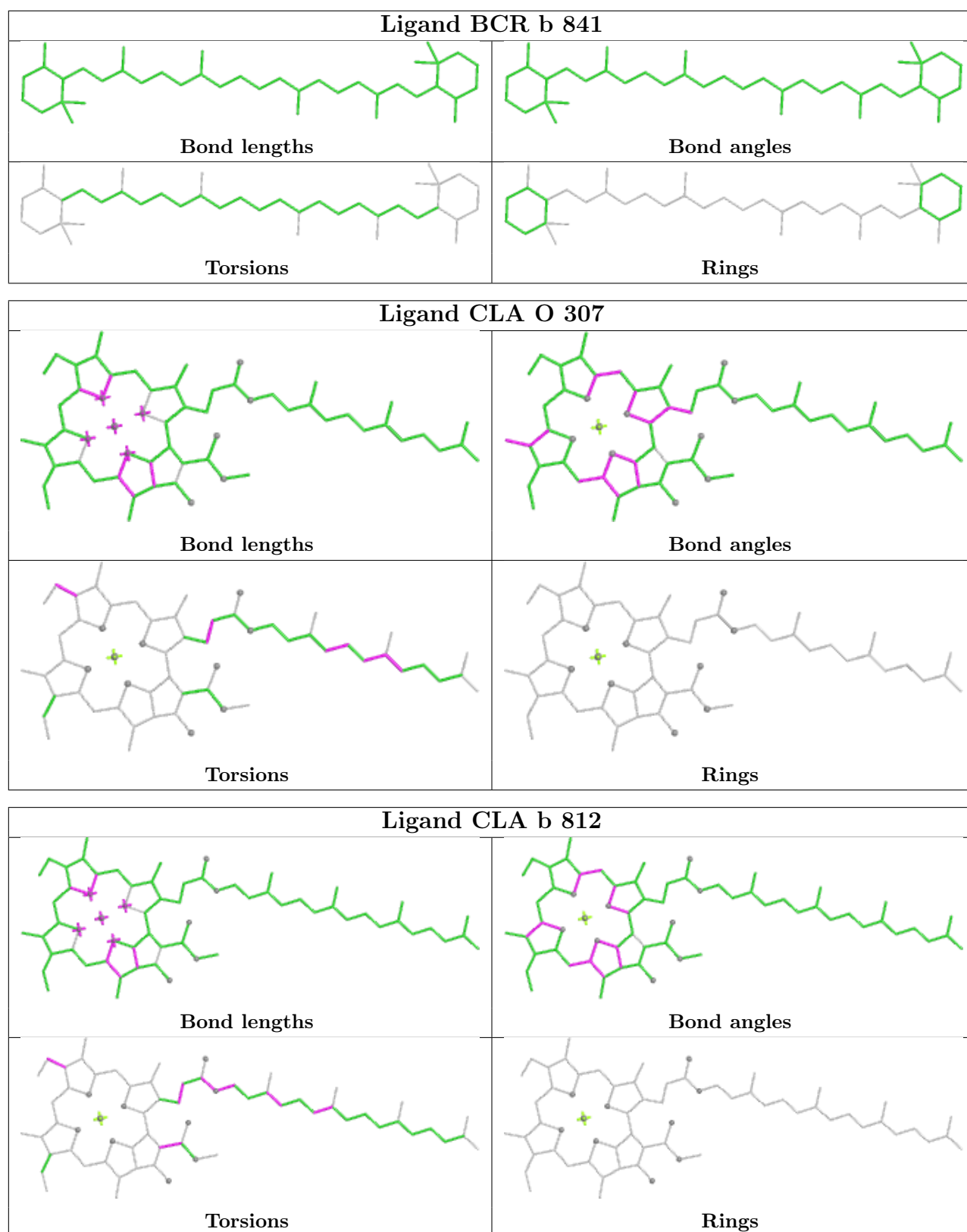
Torsions

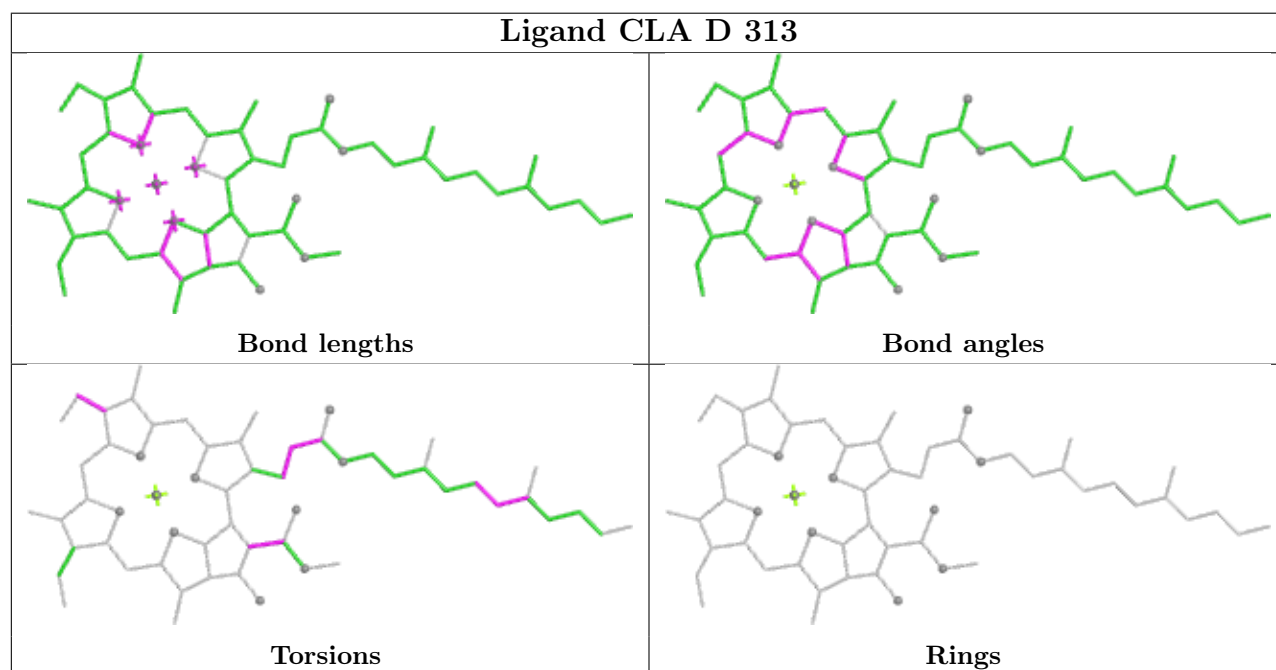
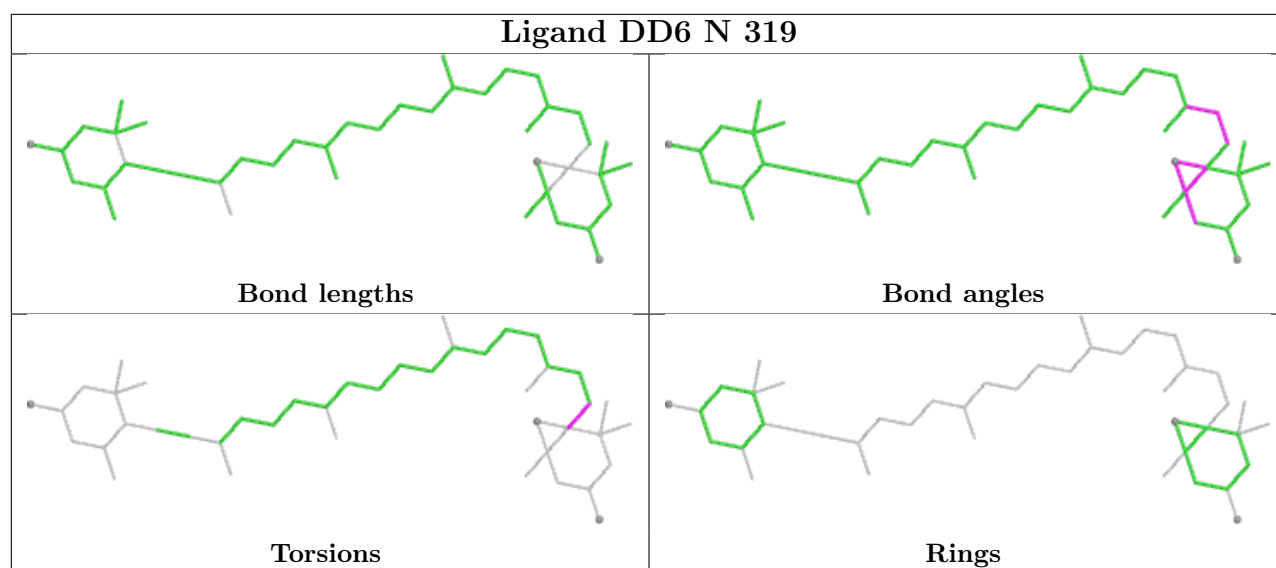


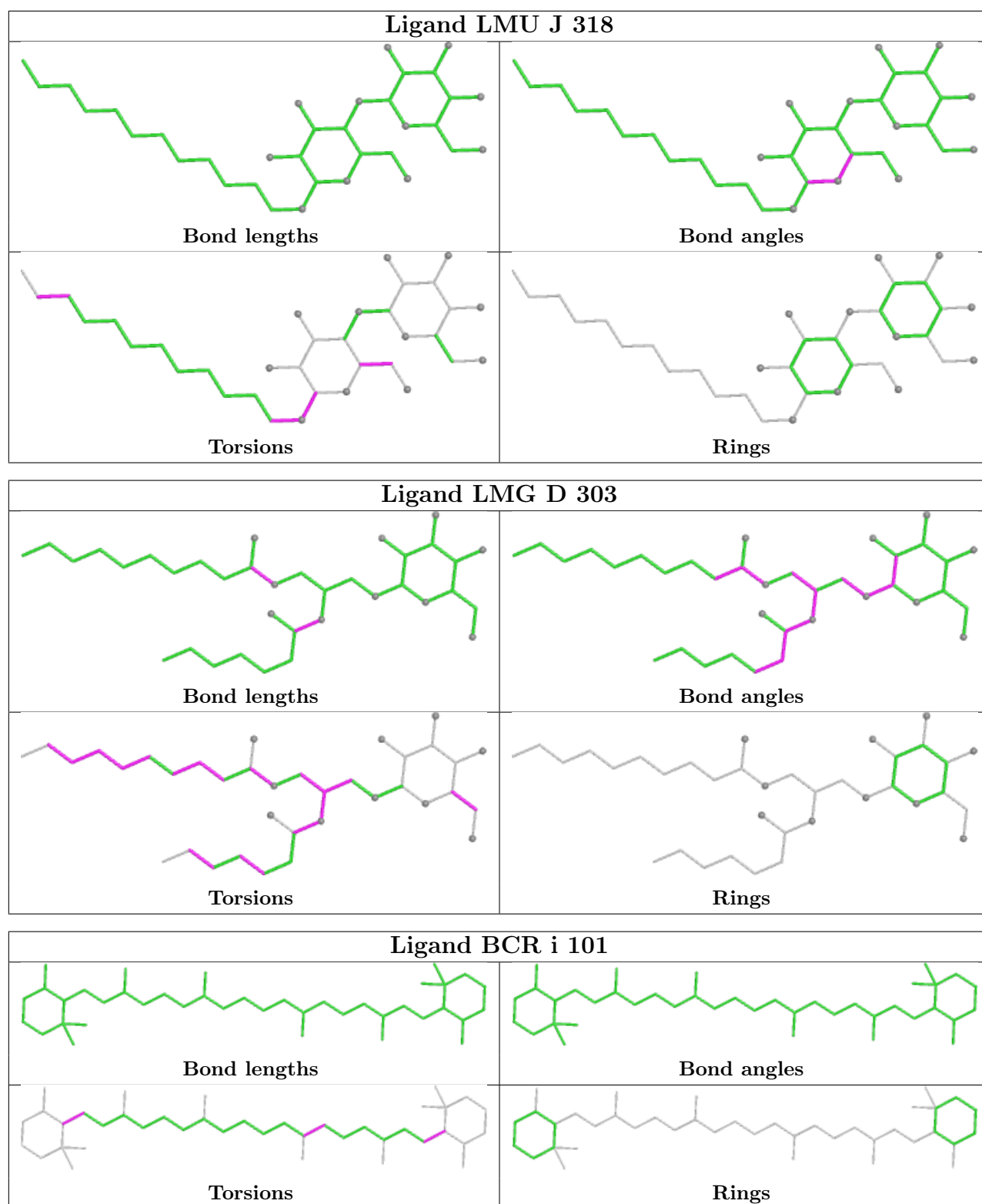
Rings

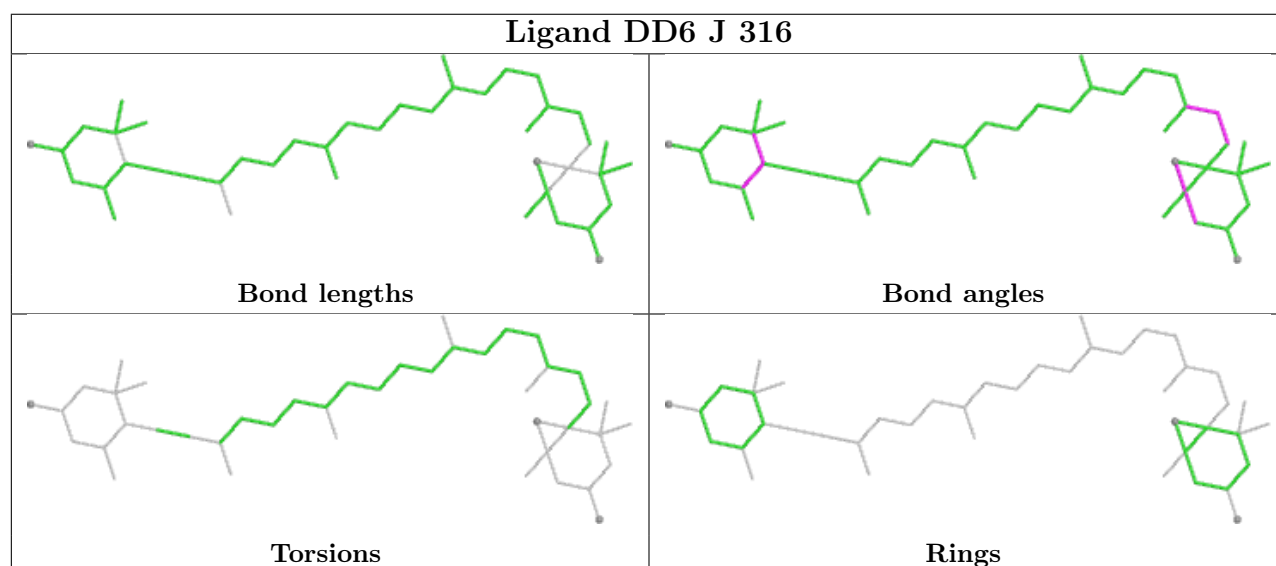
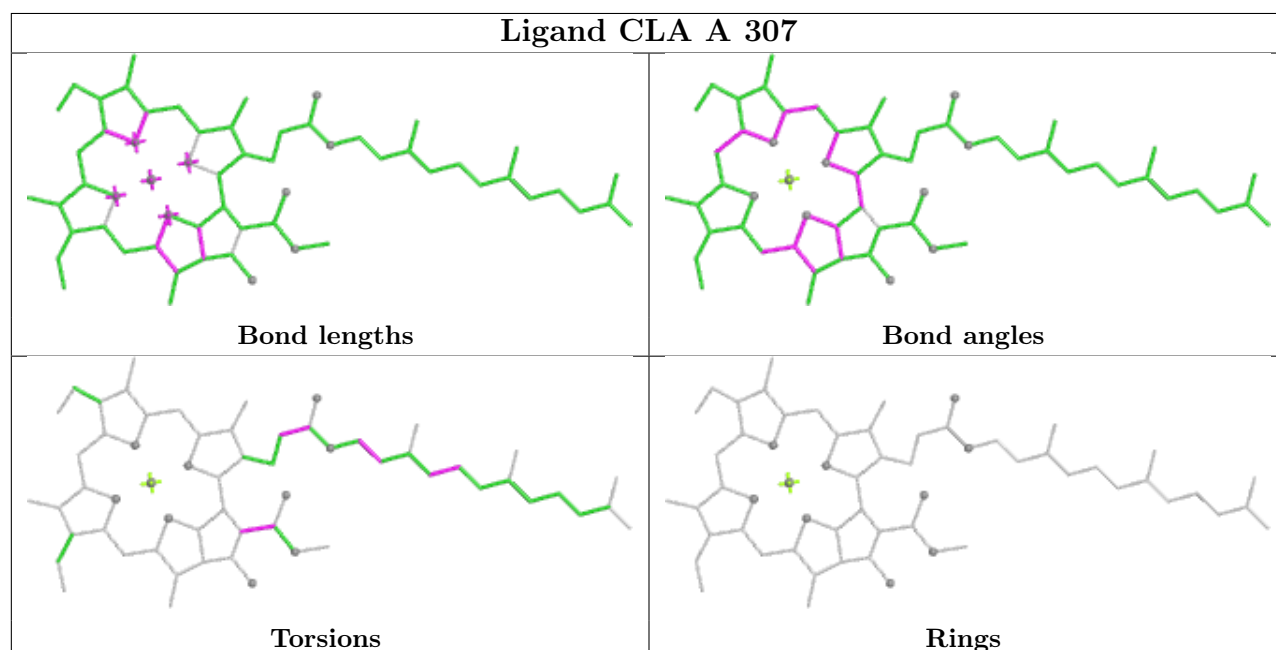
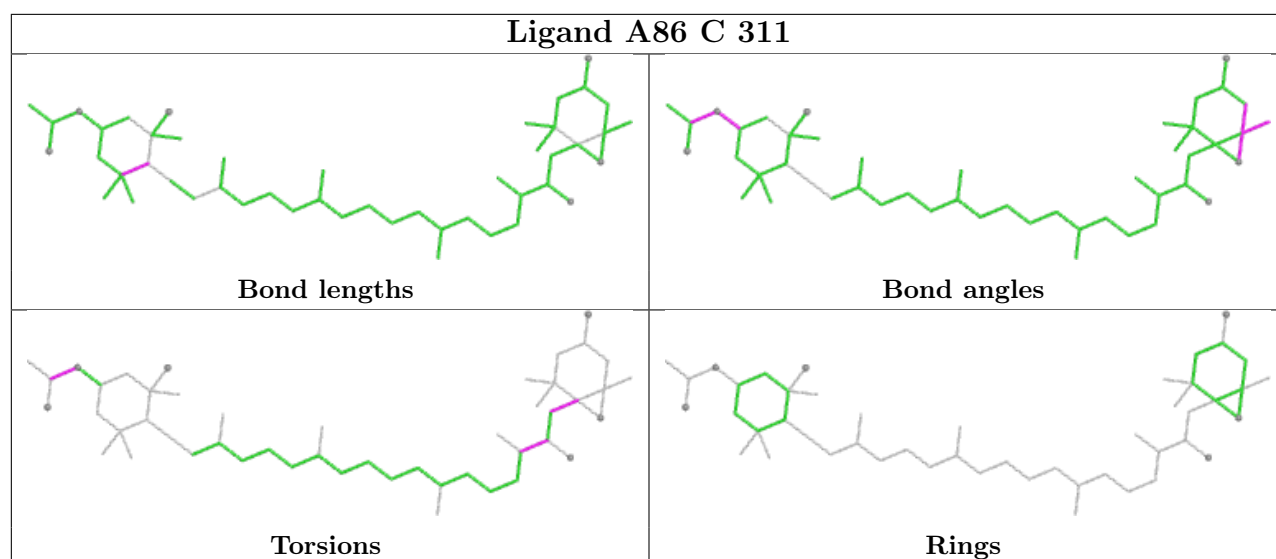


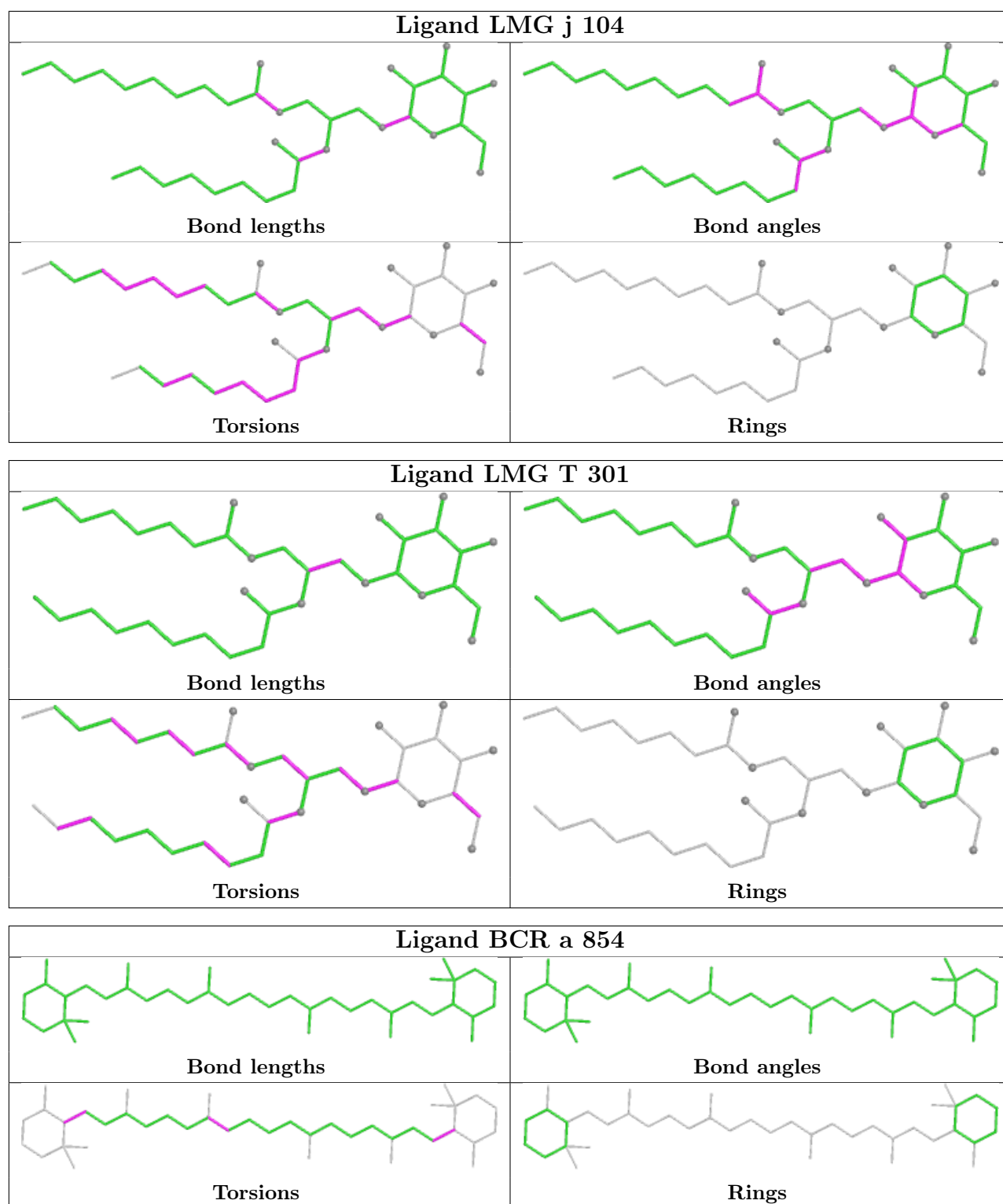


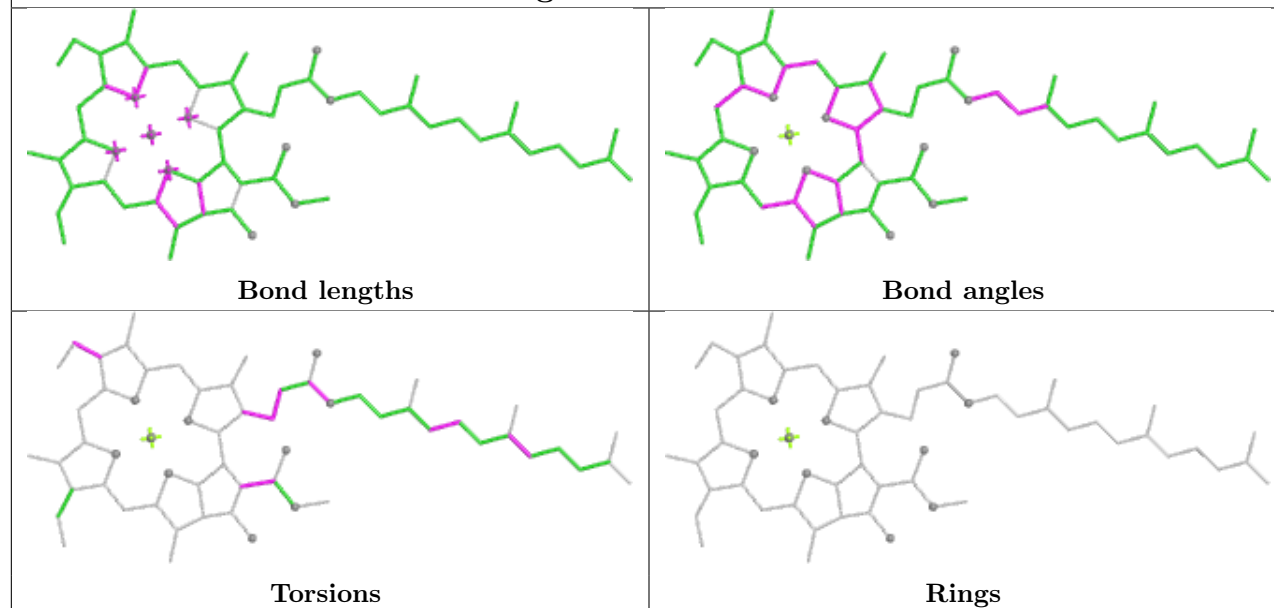
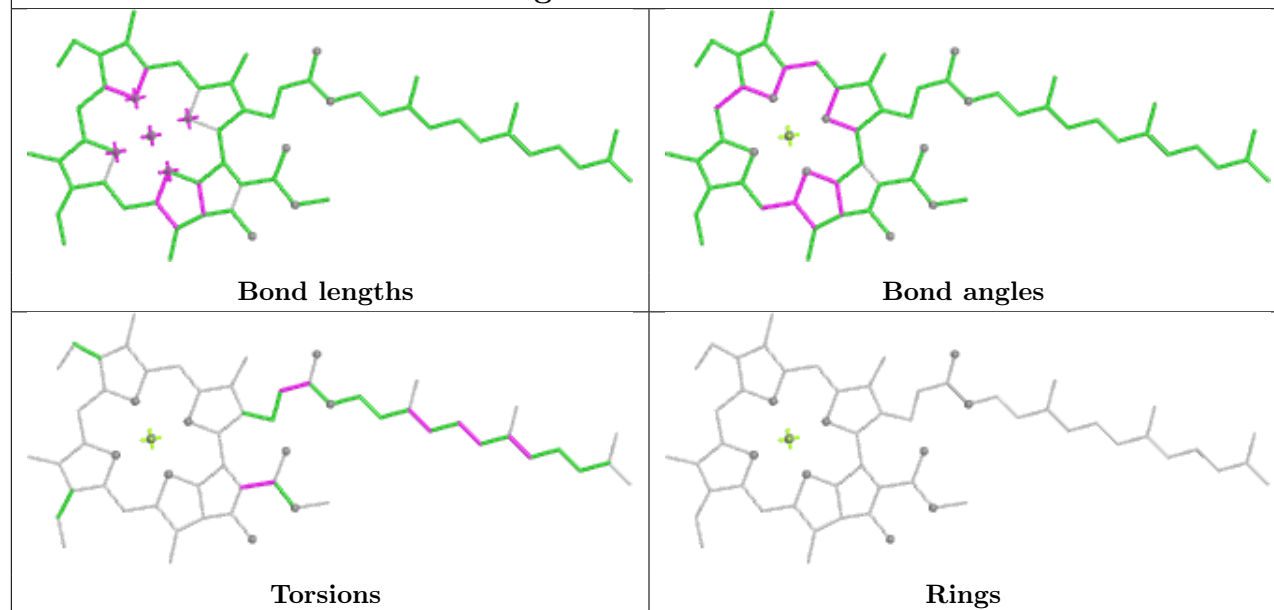




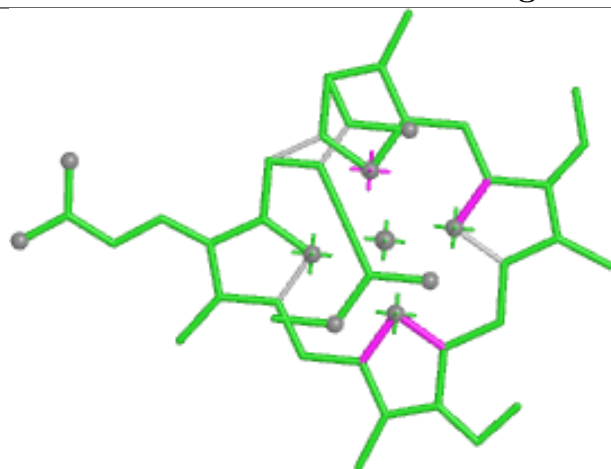




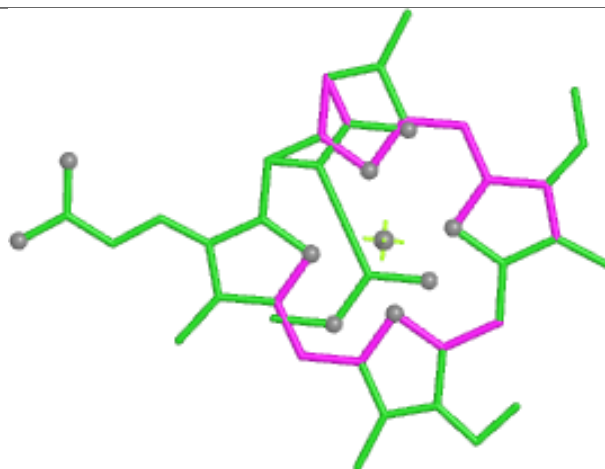


Ligand CLA a 818**Ligand CLA L 312**

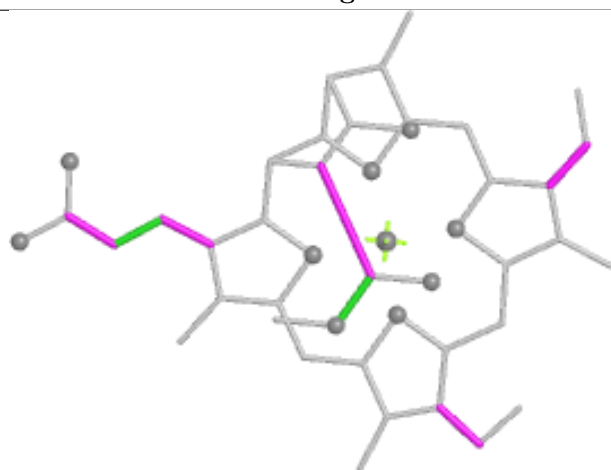
Ligand KC2 L 305



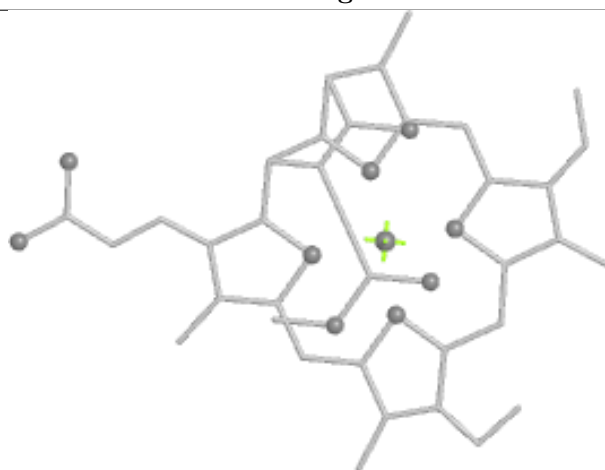
Bond lengths



Bond angles

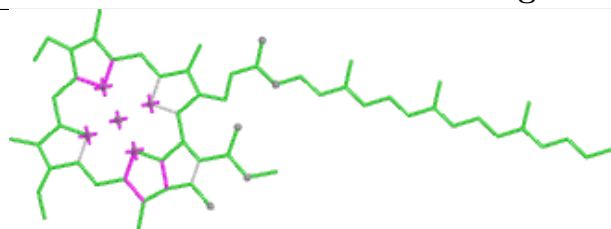


Torsions

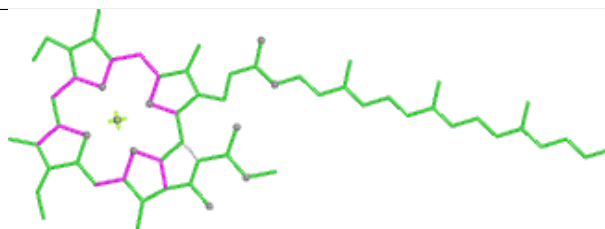


Rings

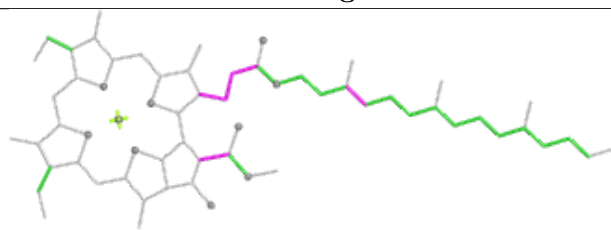
Ligand CLA a 803



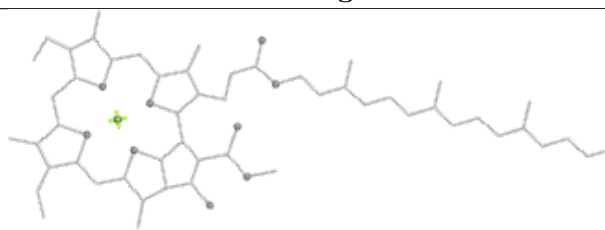
Bond lengths



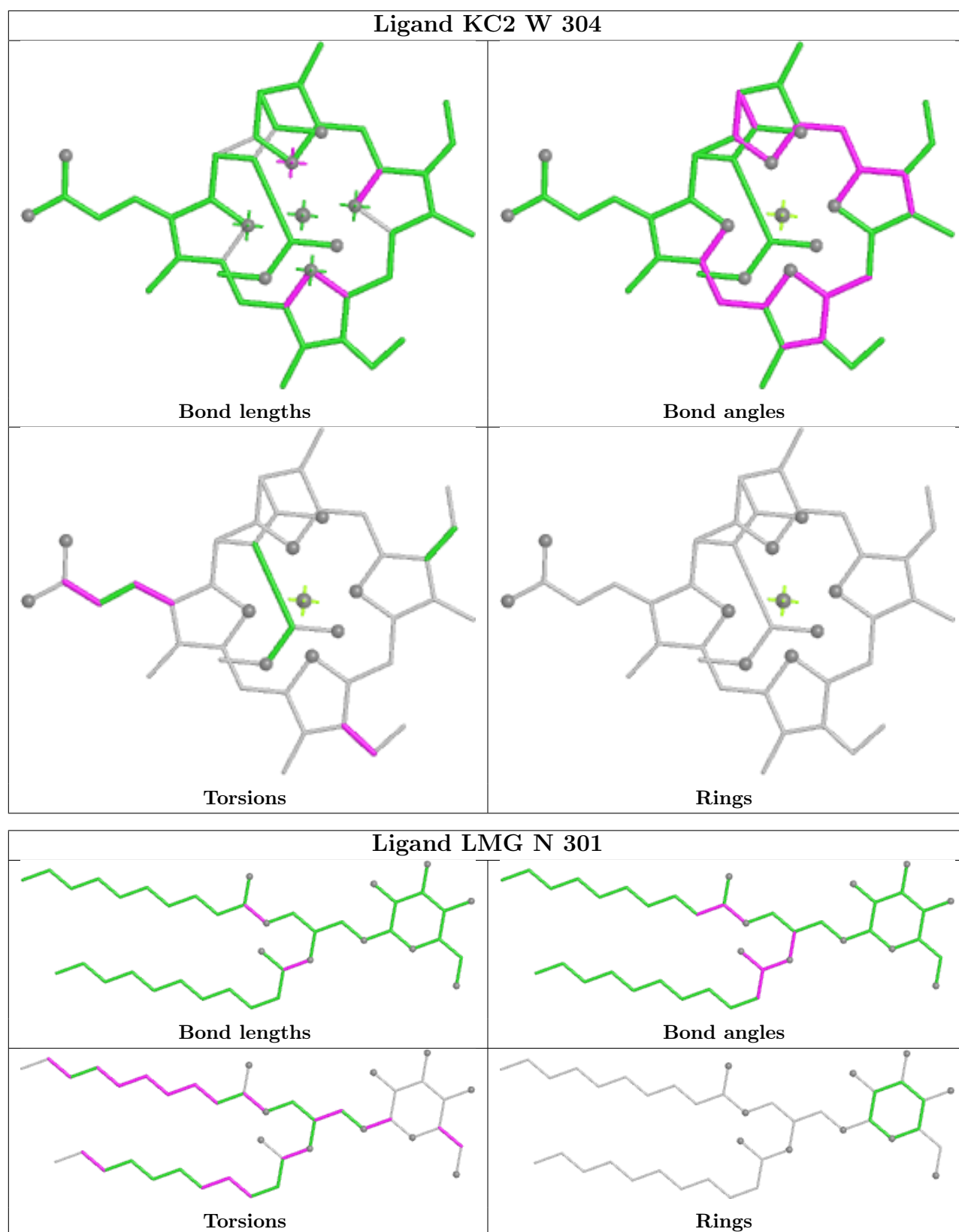
Bond angles

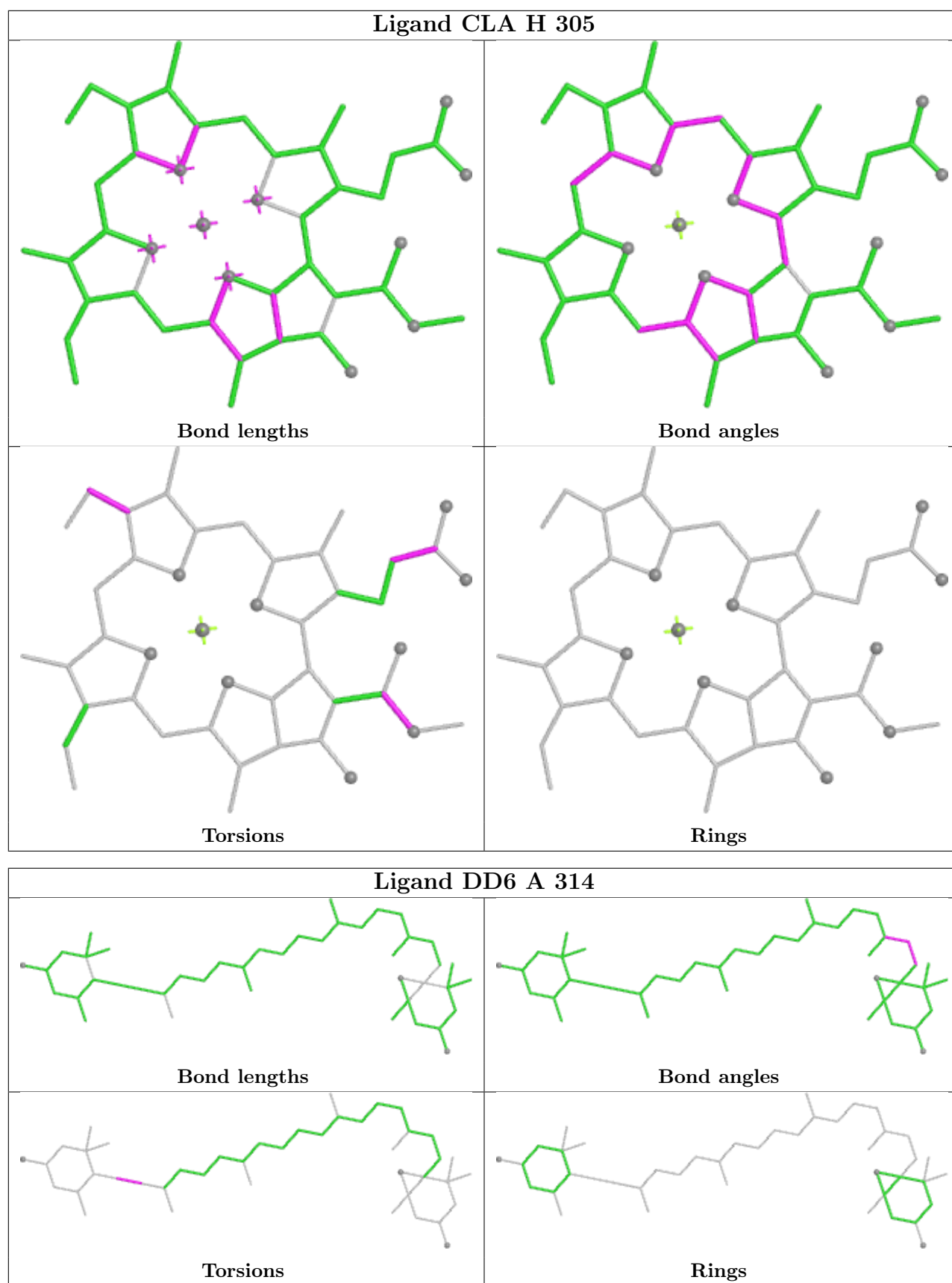


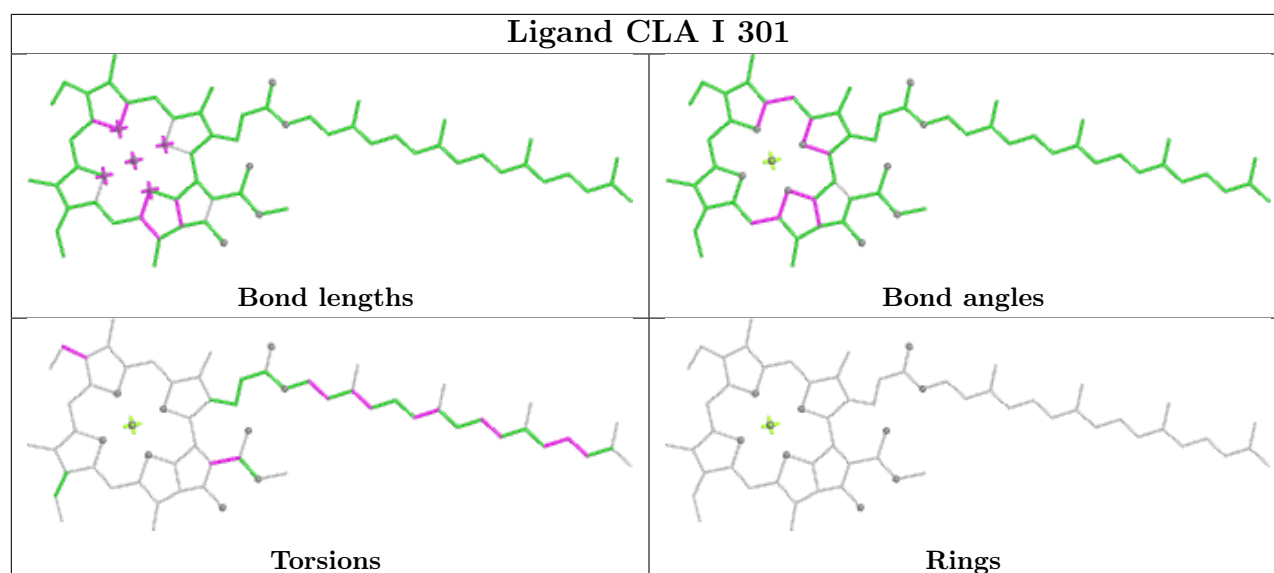
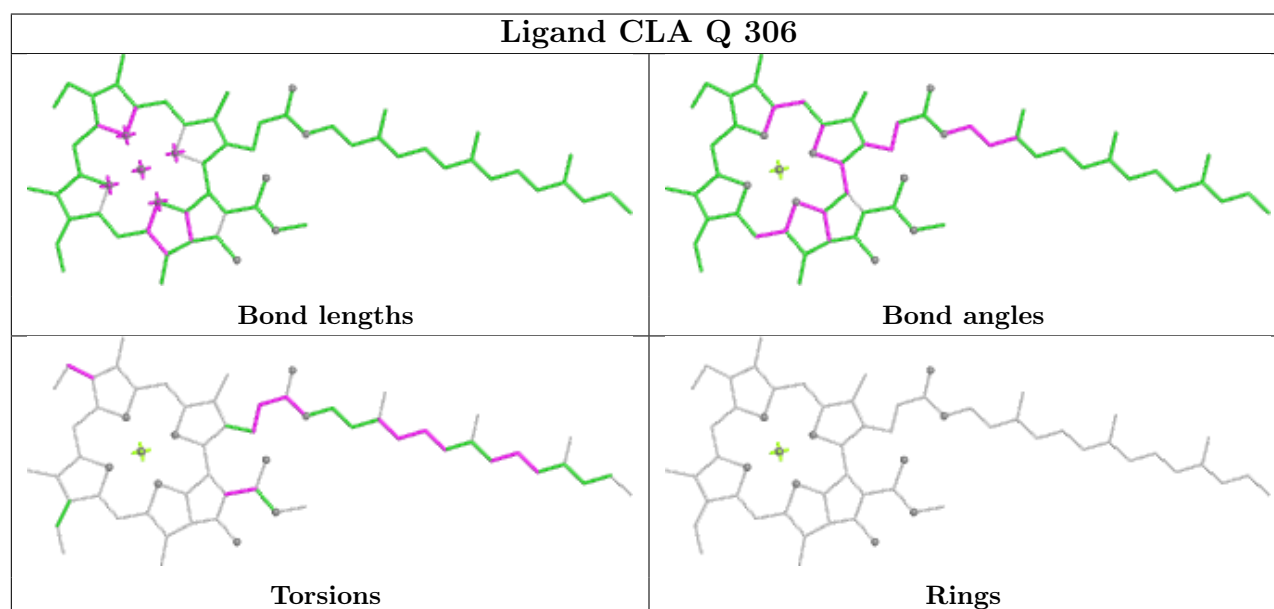
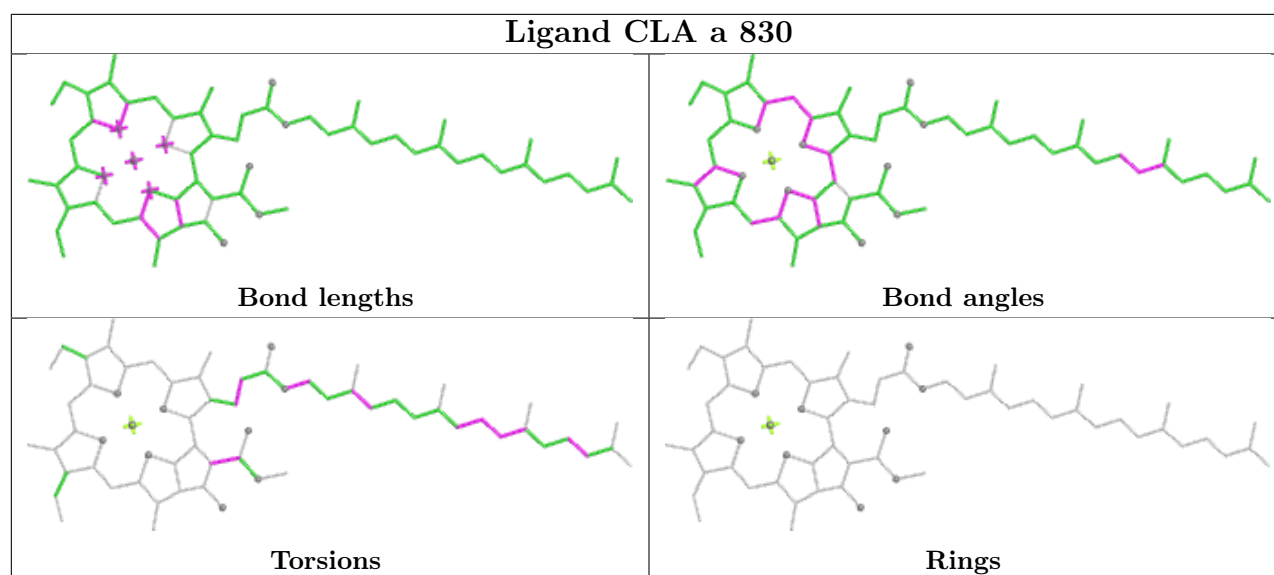
Torsions

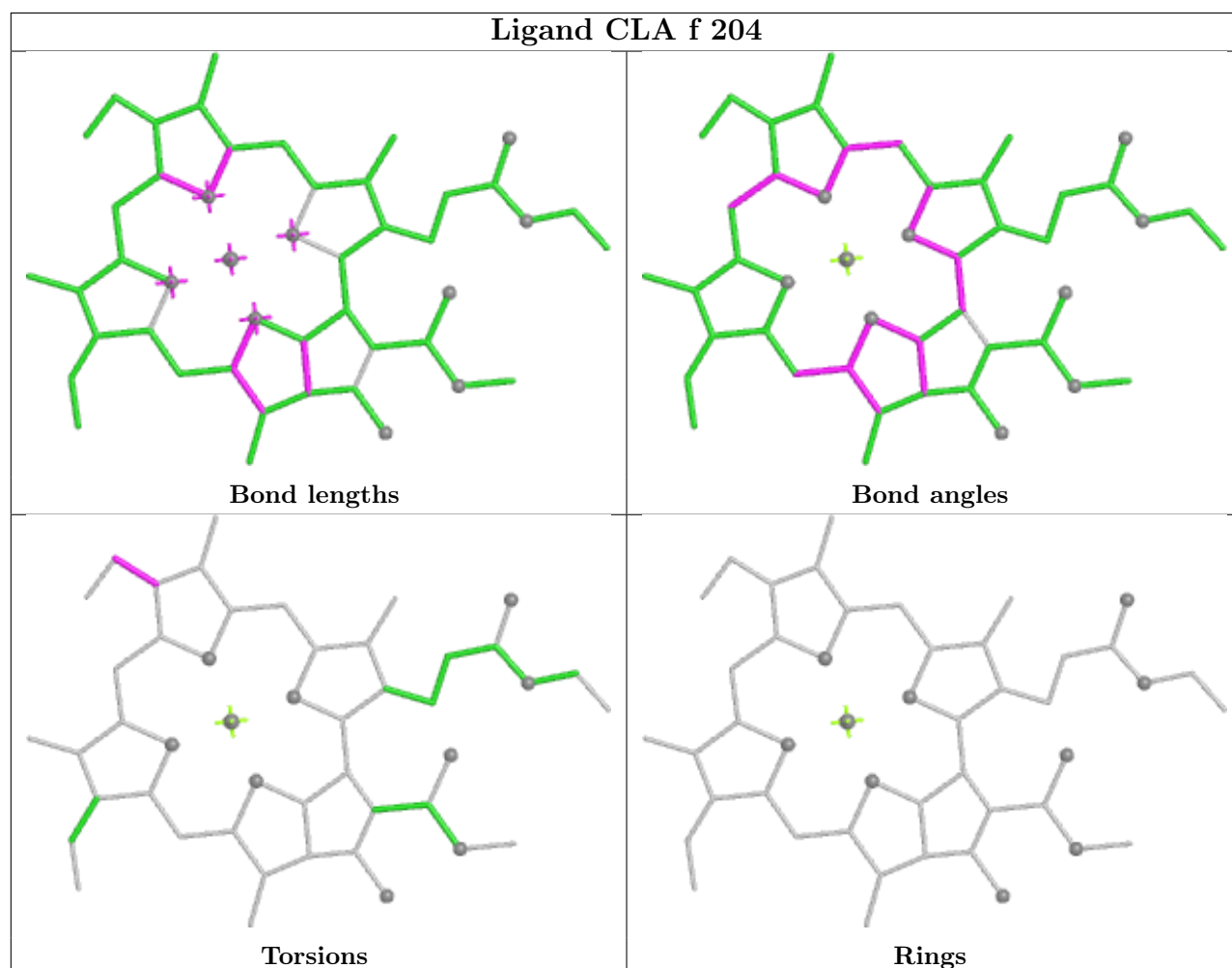
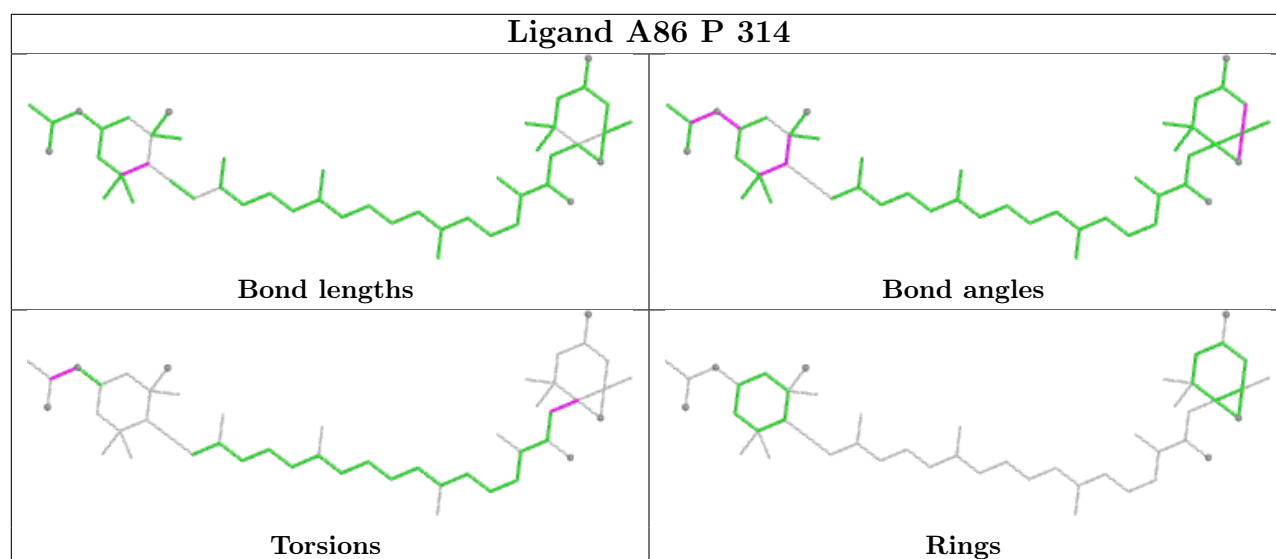


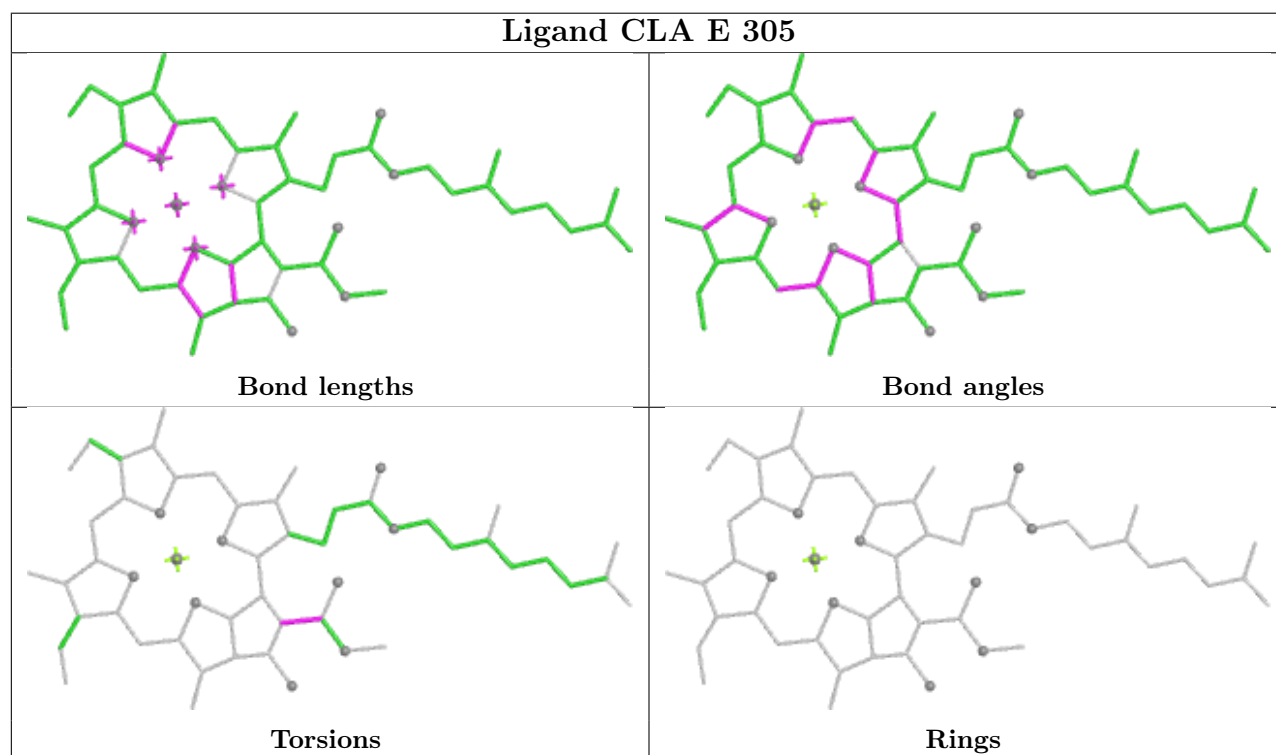
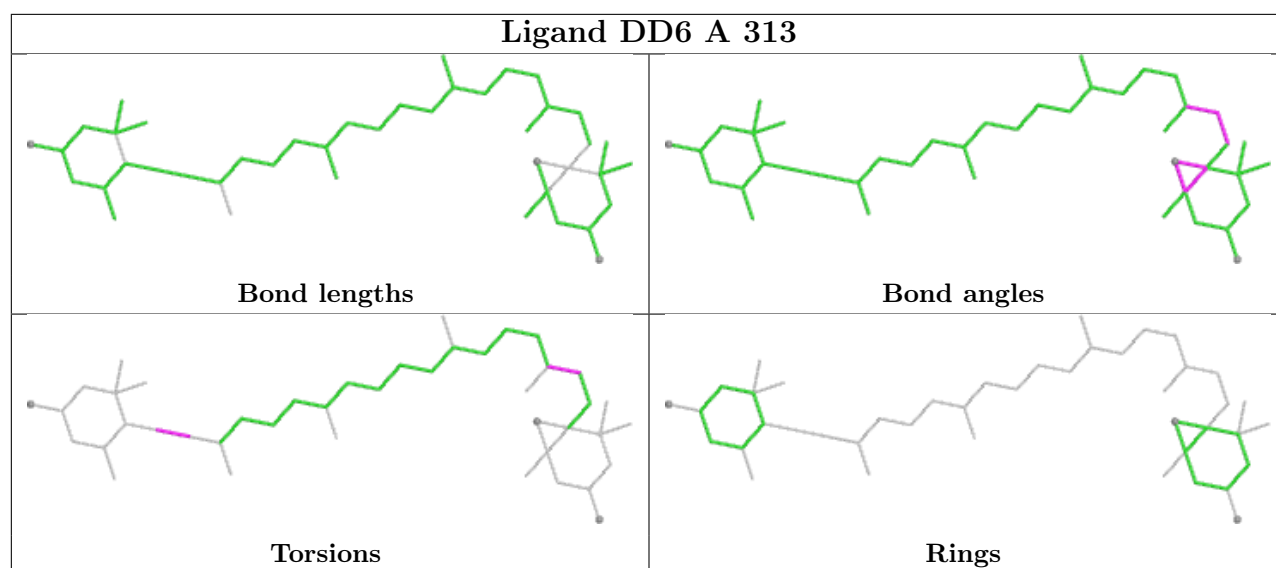
Rings

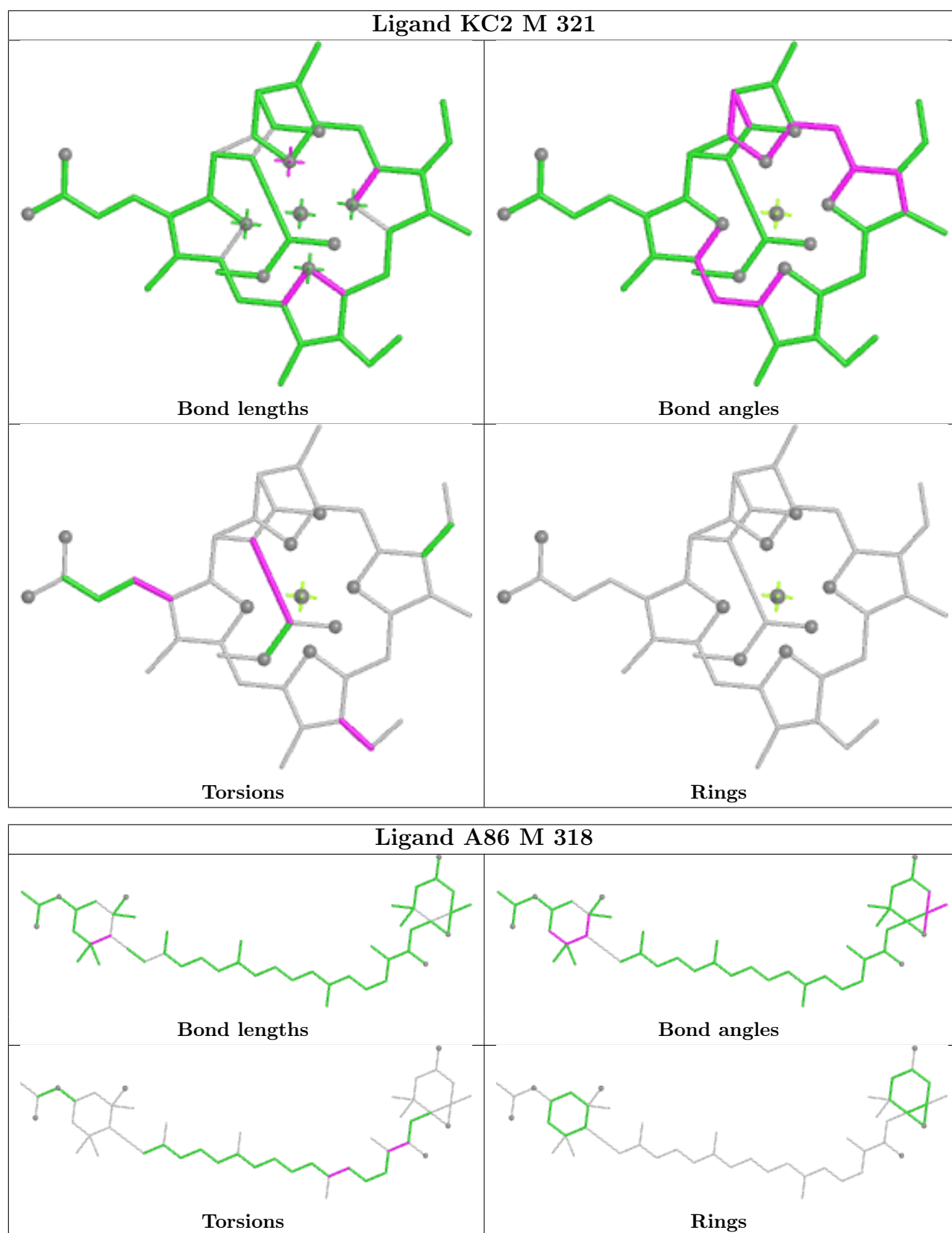




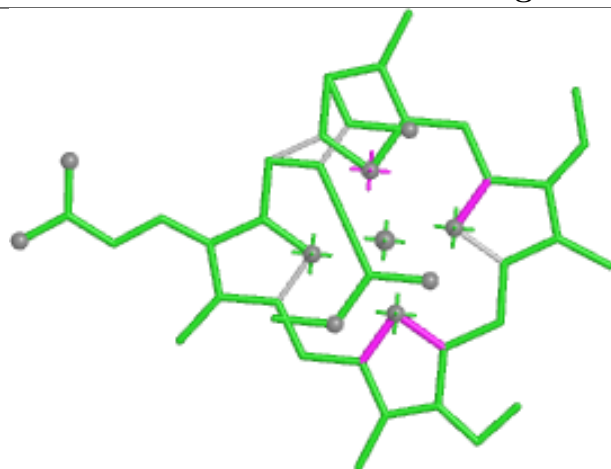




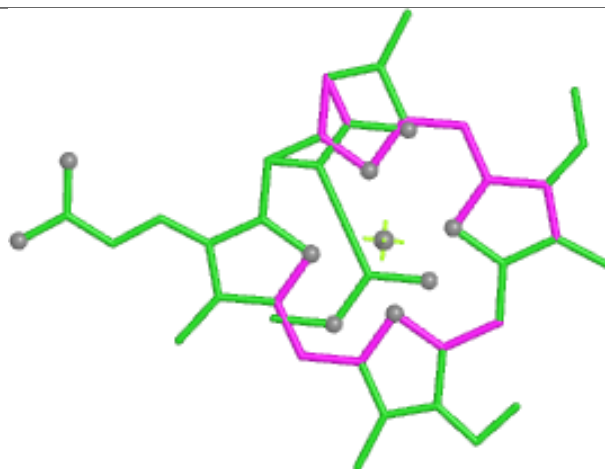




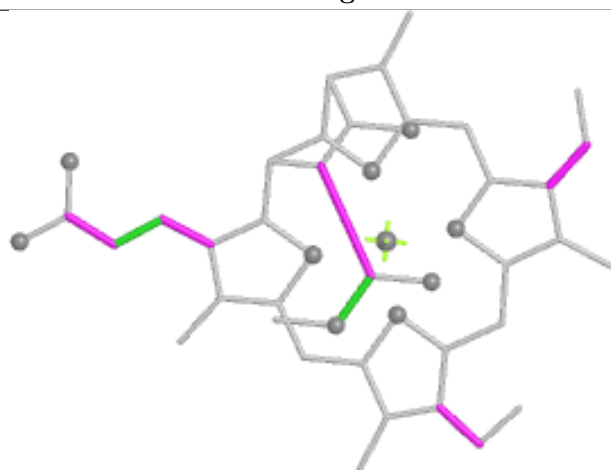
Ligand KC2 G 309



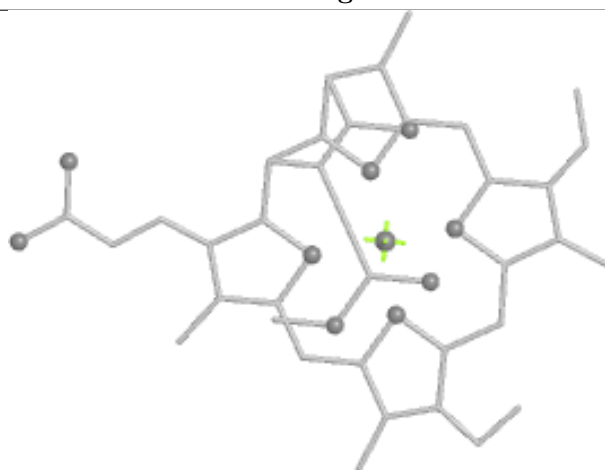
Bond lengths



Bond angles

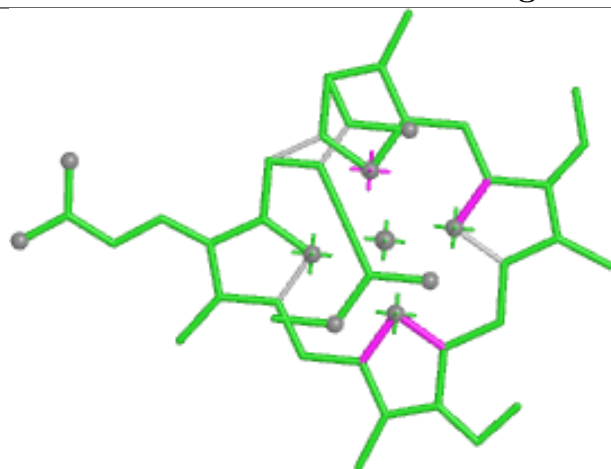


Torsions

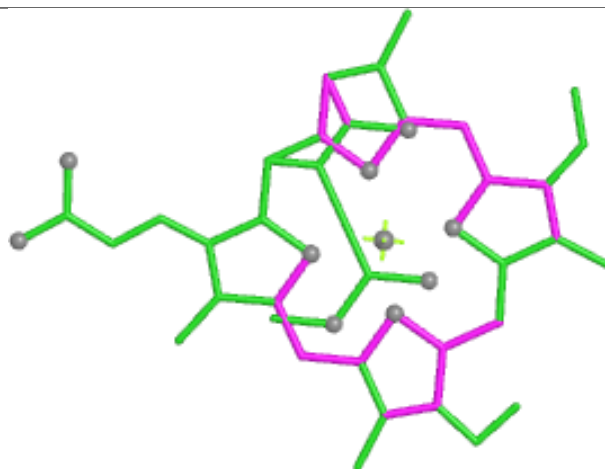


Rings

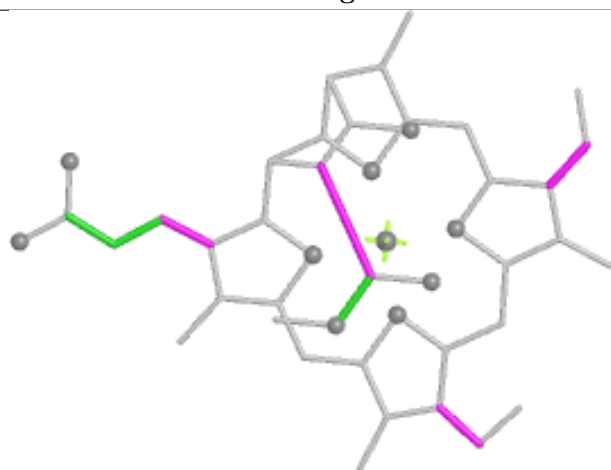
Ligand KC2 L 306



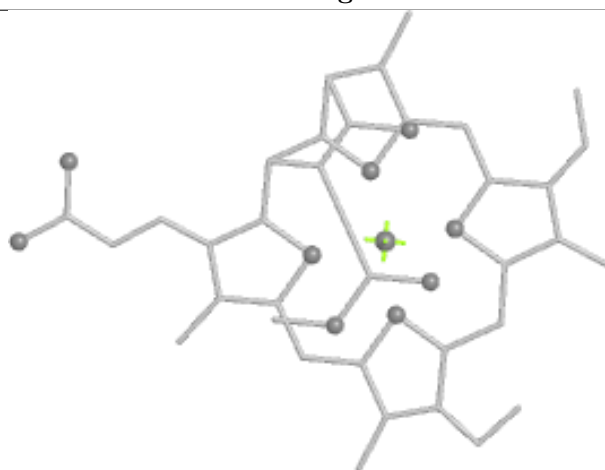
Bond lengths



Bond angles



Torsions

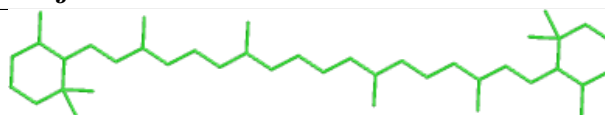


Rings

Ligand BCR j 102



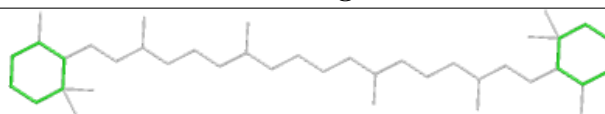
Bond lengths



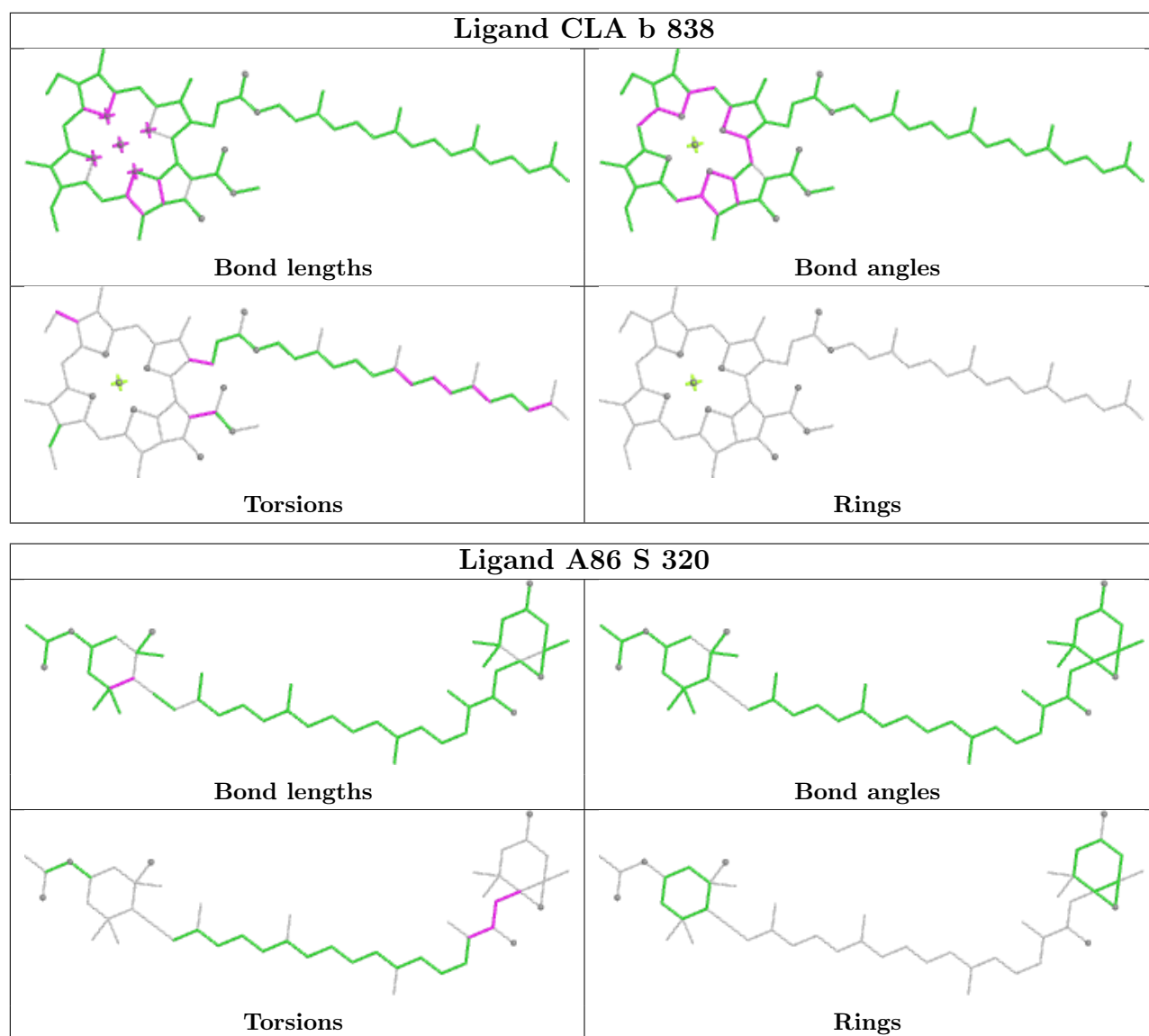
Bond angles

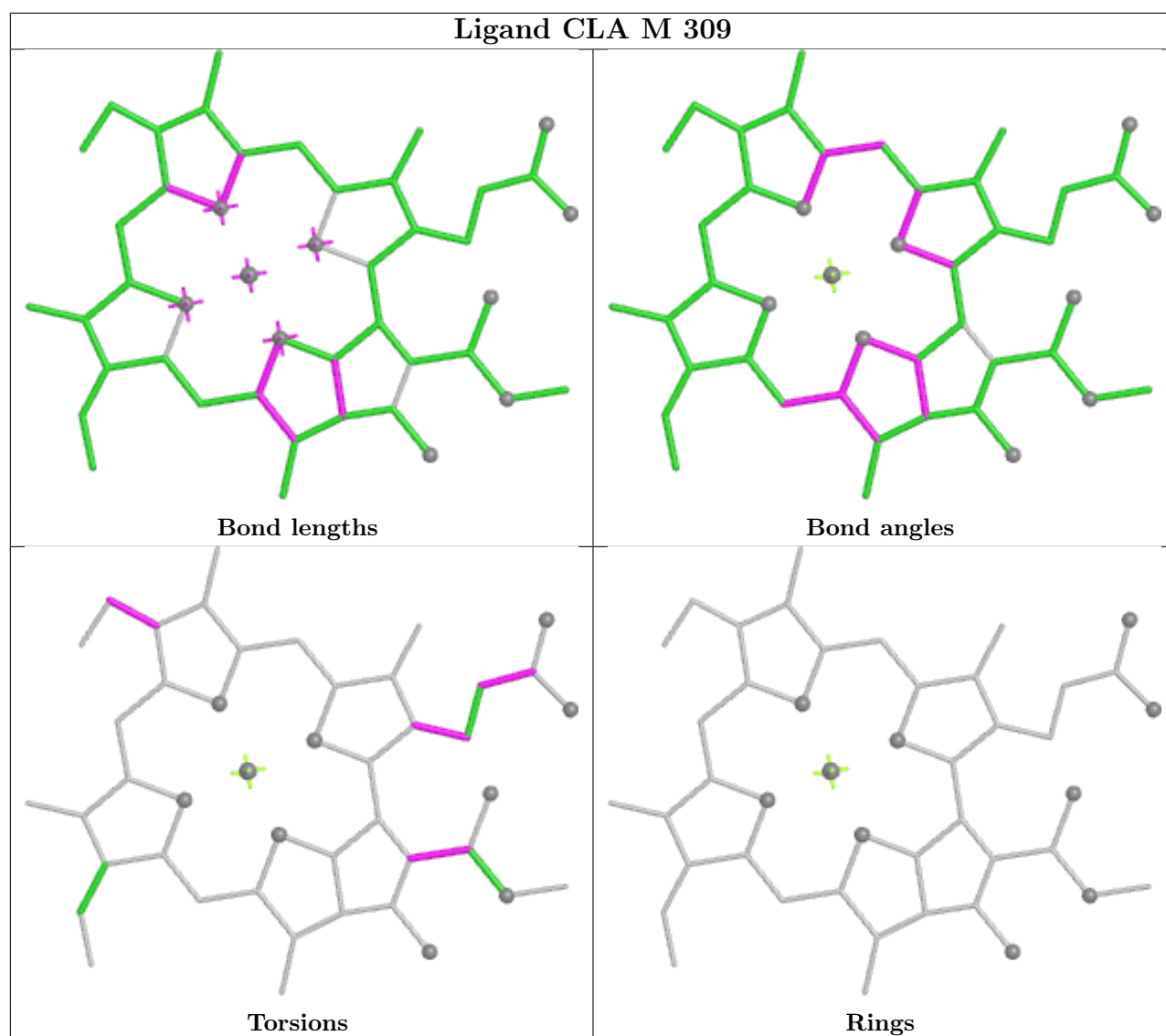


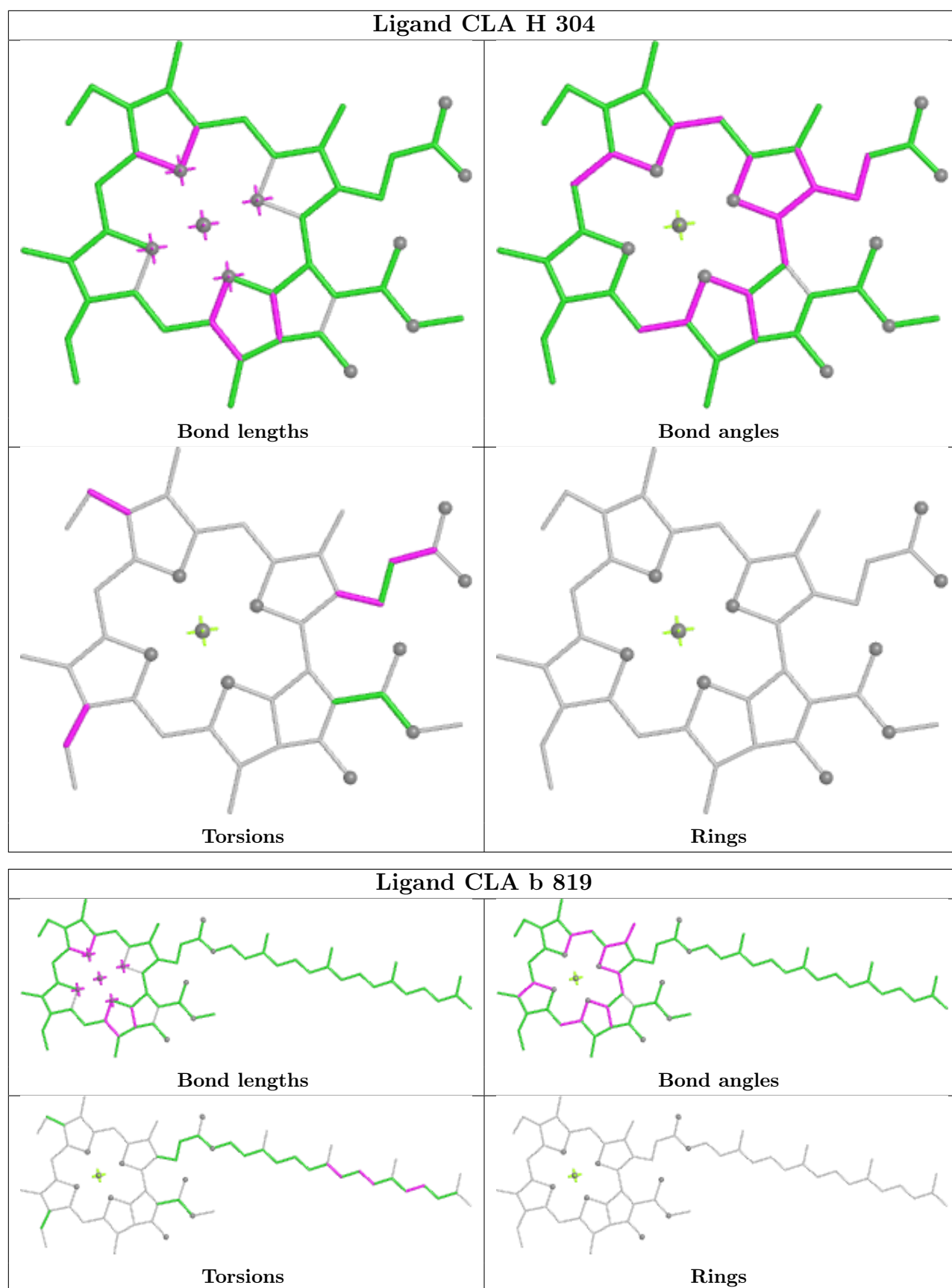
Torsions

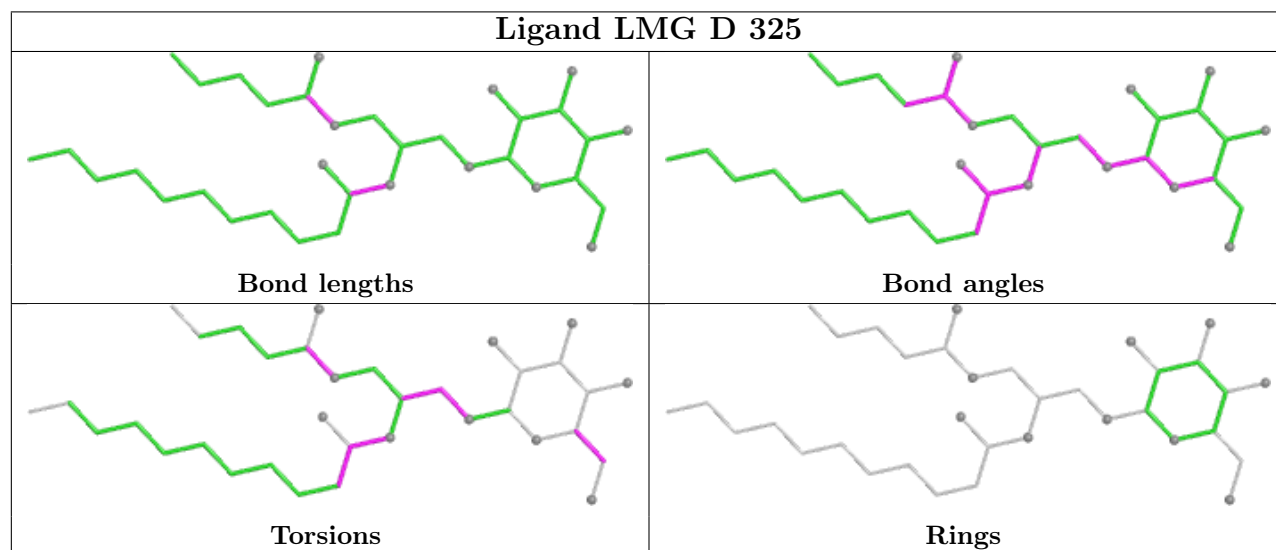
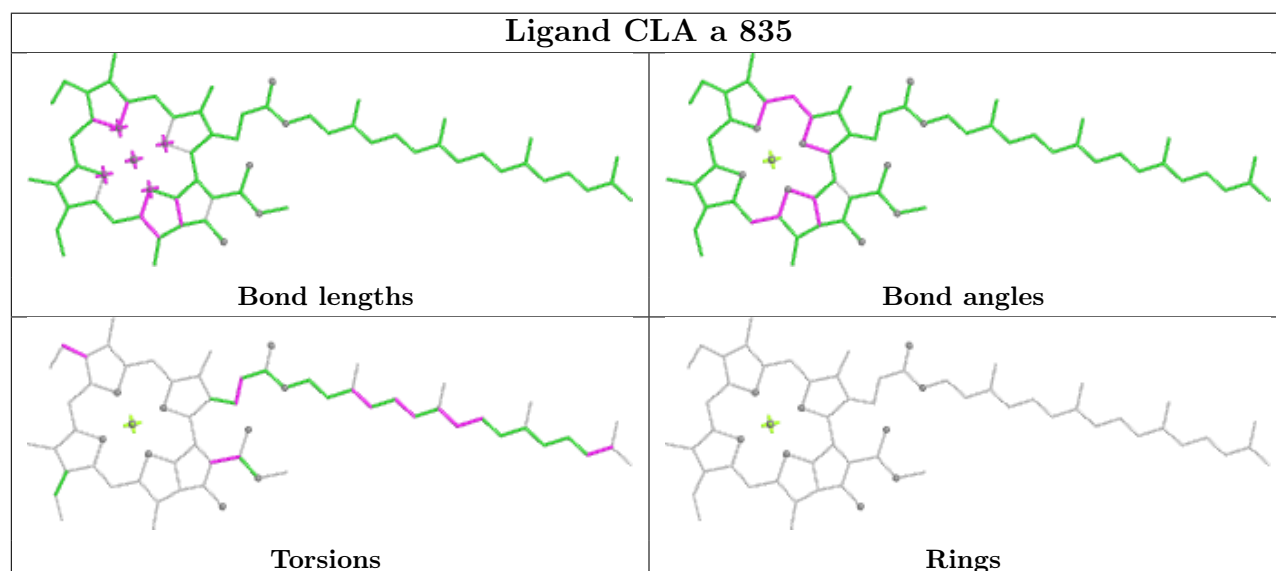
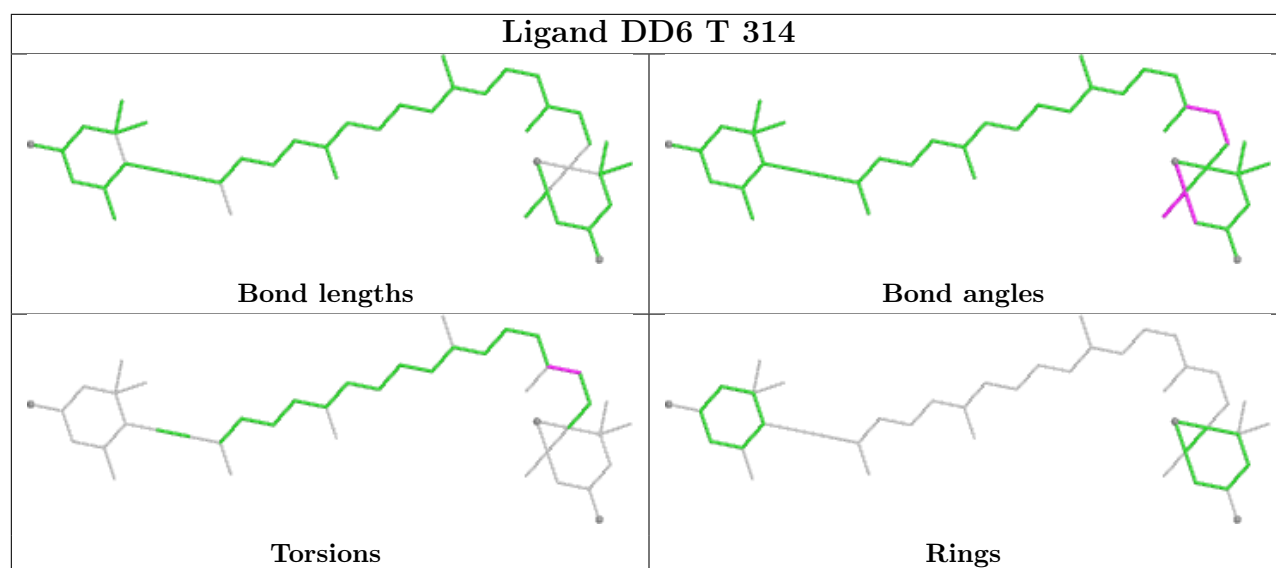


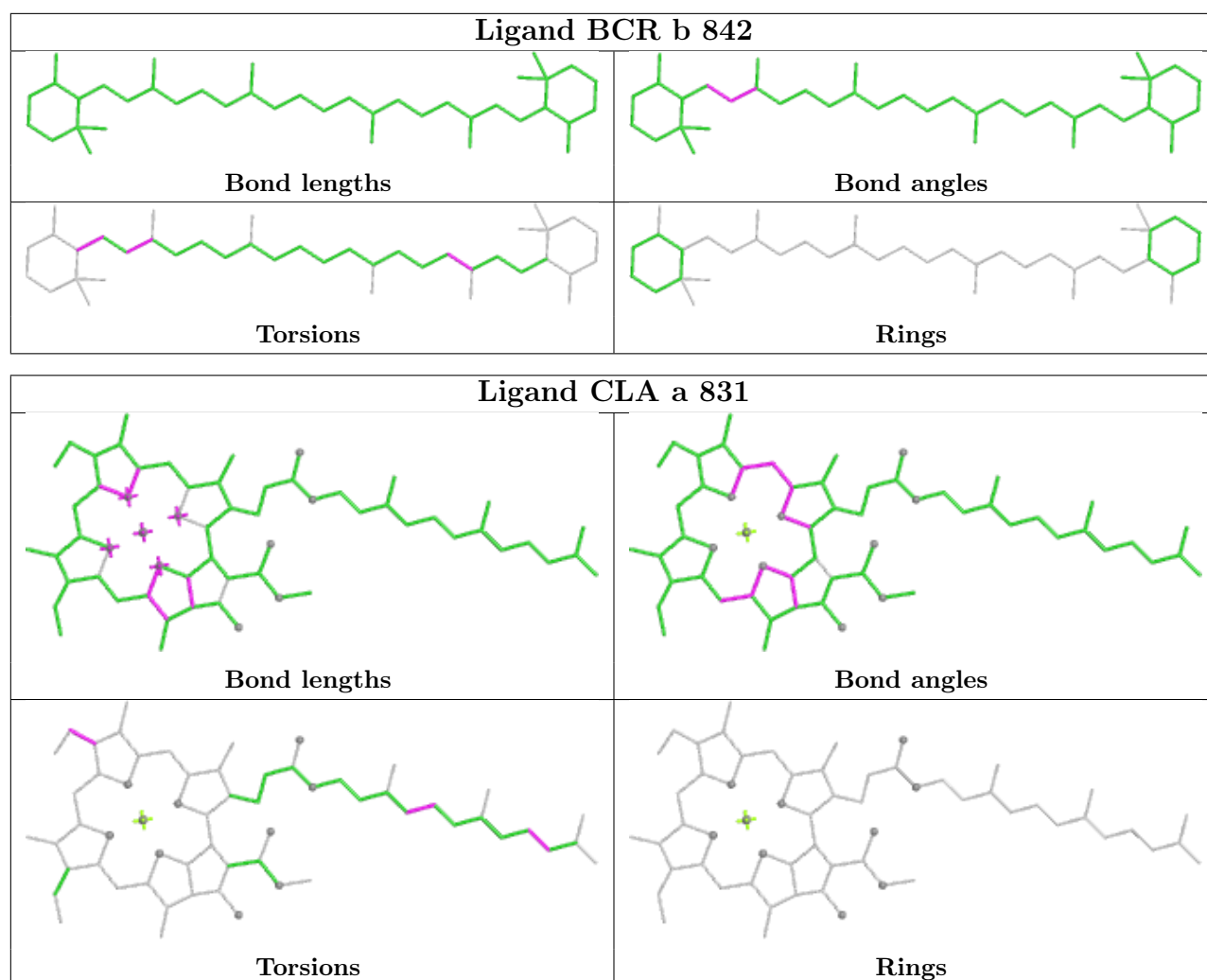
Rings

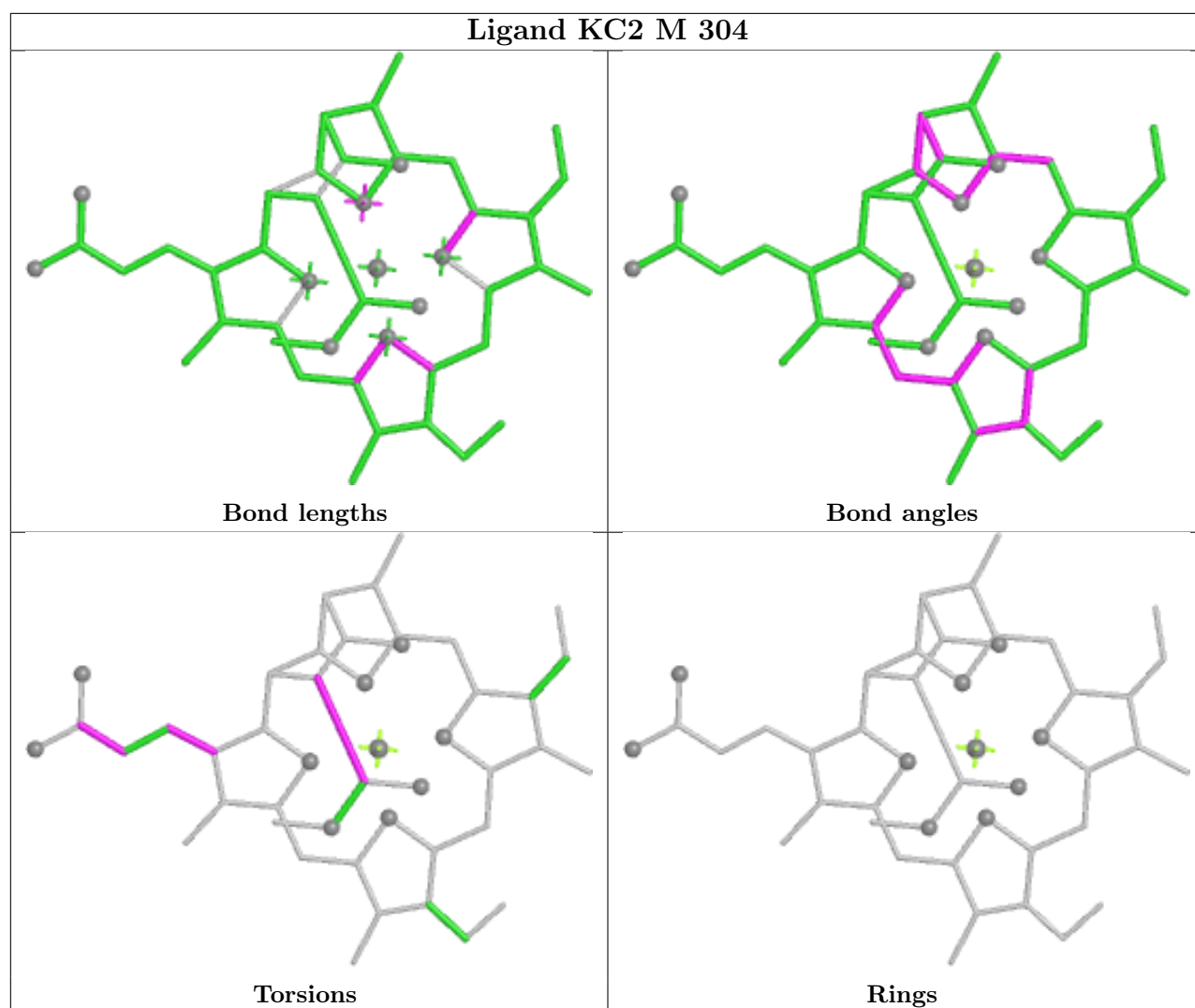




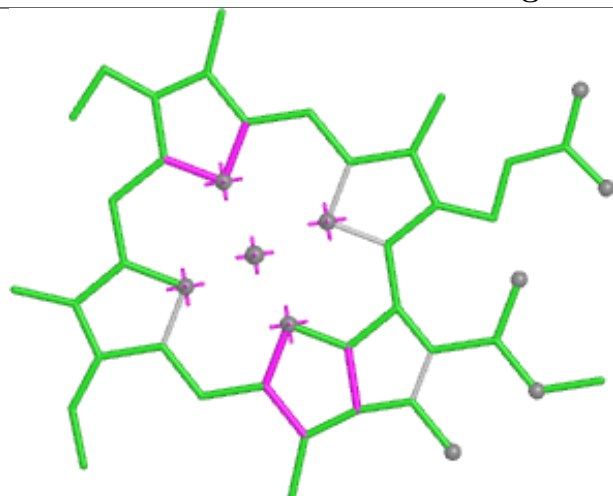




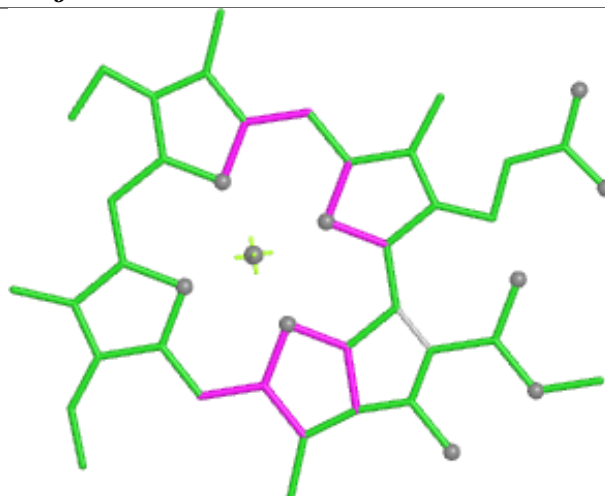




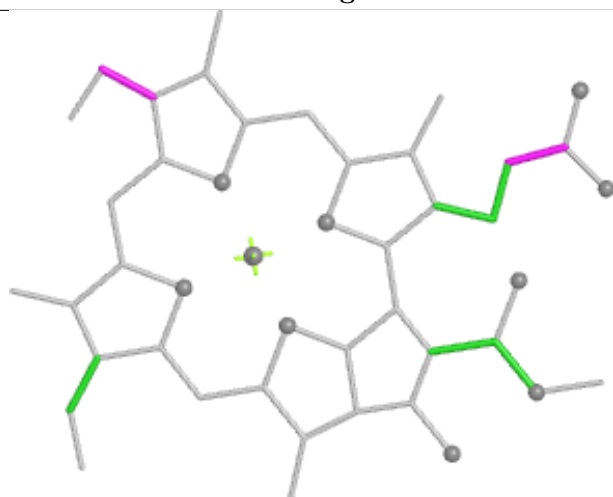
Ligand CLA j 101



Bond lengths



Bond angles

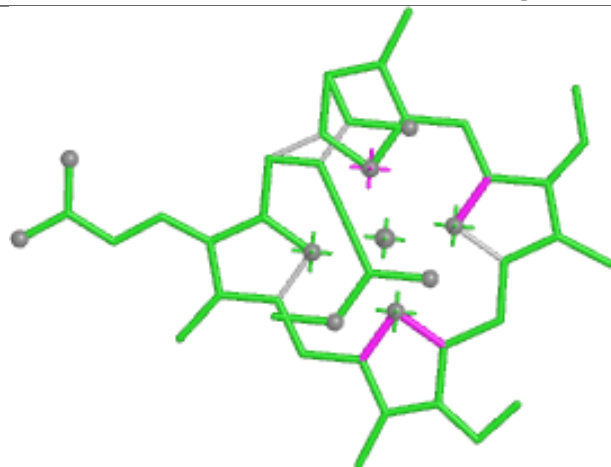


Torsions

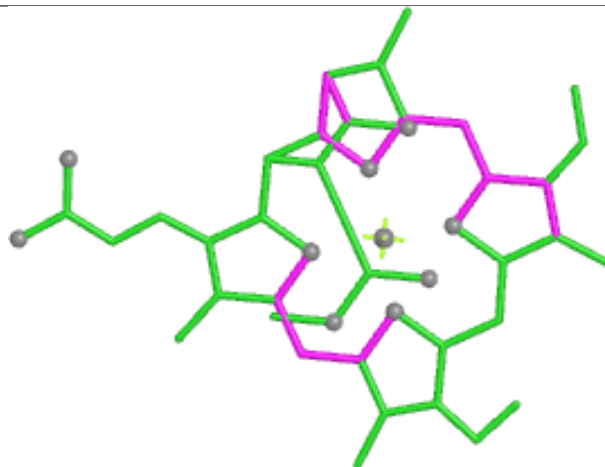


Rings

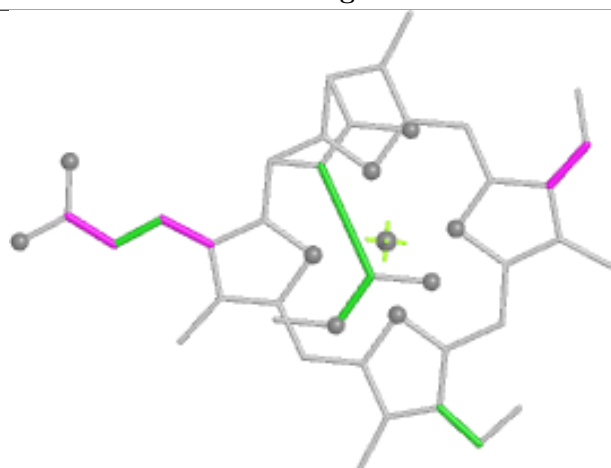
Ligand KC2 U 304



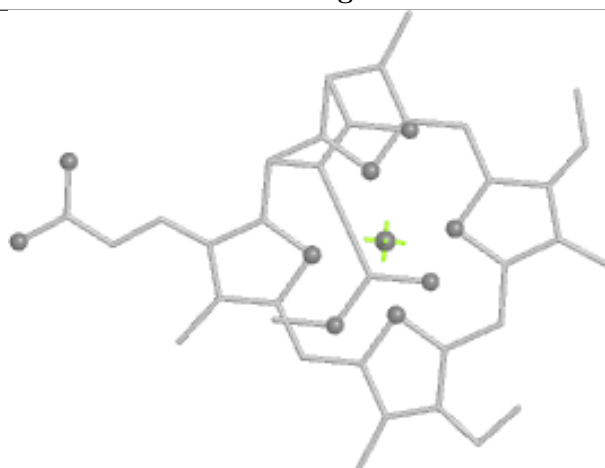
Bond lengths



Bond angles

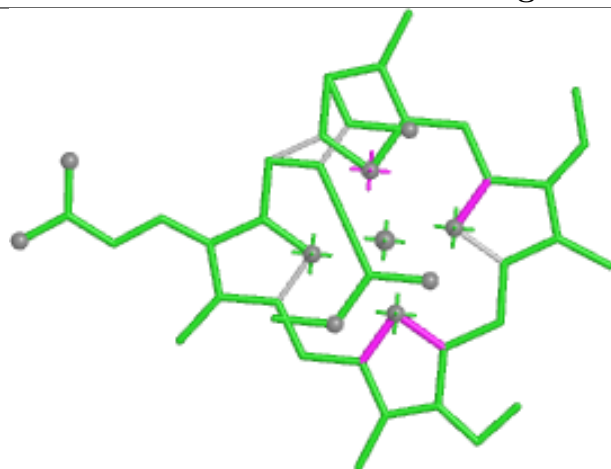


Torsions

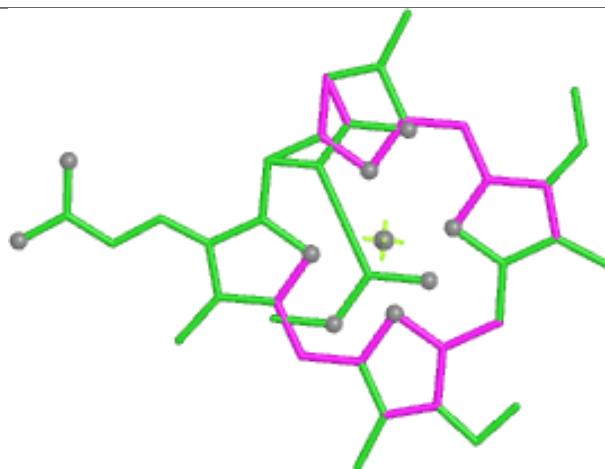


Rings

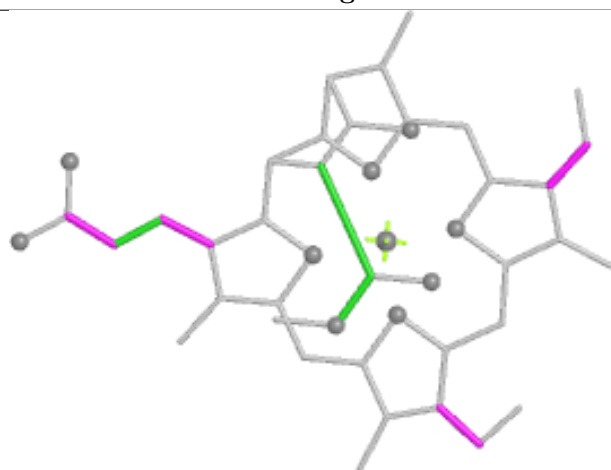
Ligand KC2 F 302



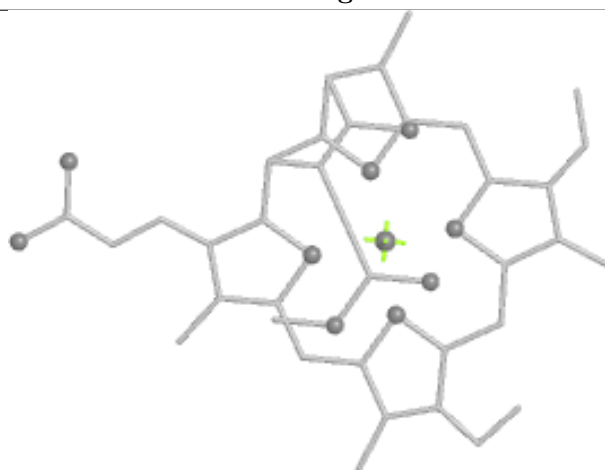
Bond lengths



Bond angles

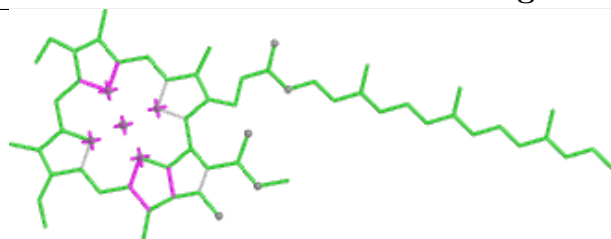


Torsions

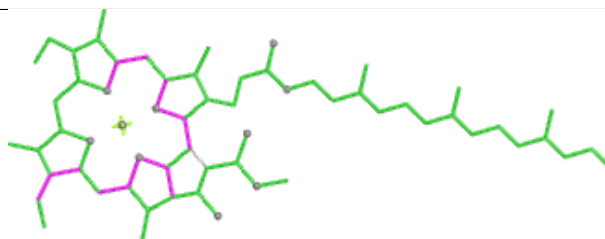


Rings

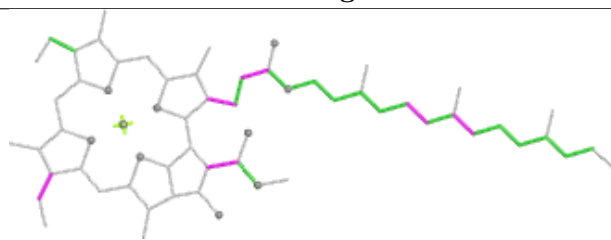
Ligand CLA b 816



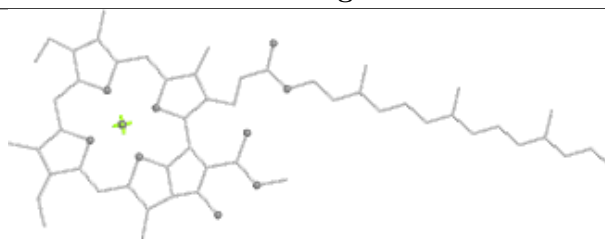
Bond lengths



Bond angles

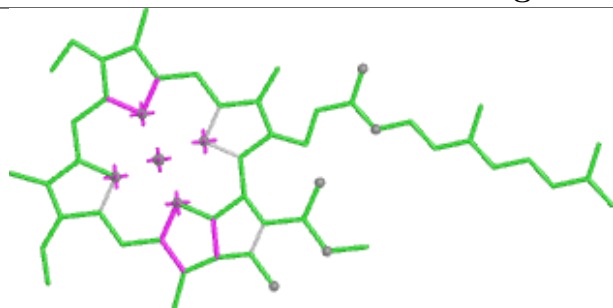


Torsions

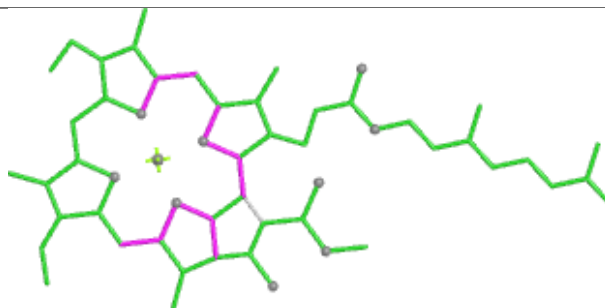


Rings

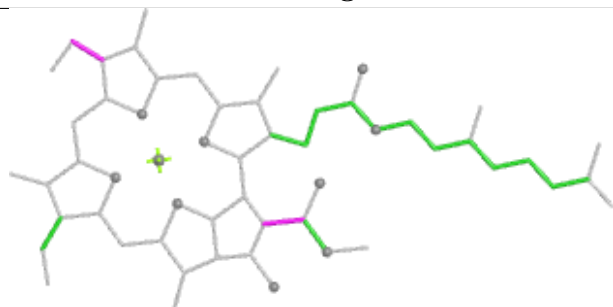
Ligand CLA V 203



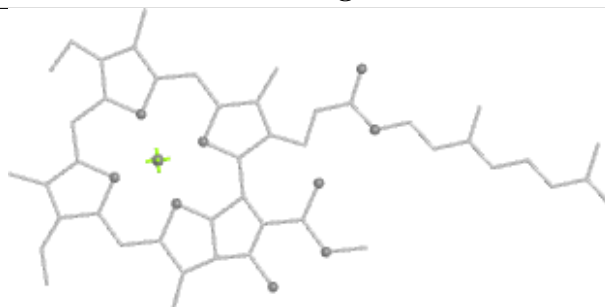
Bond lengths



Bond angles

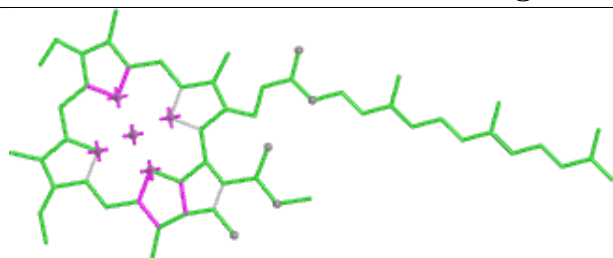


Torsions

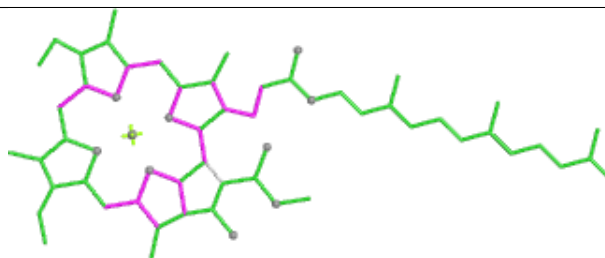


Rings

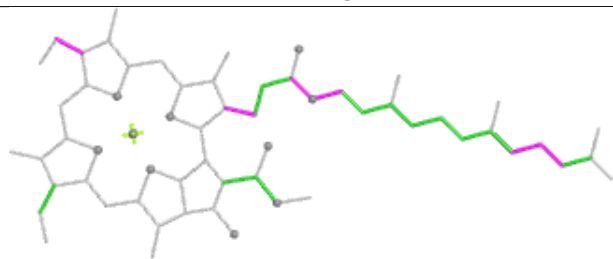
Ligand CLA C 307



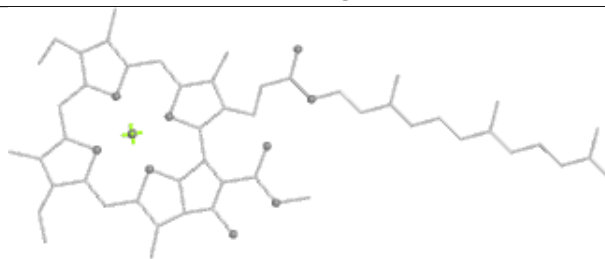
Bond lengths



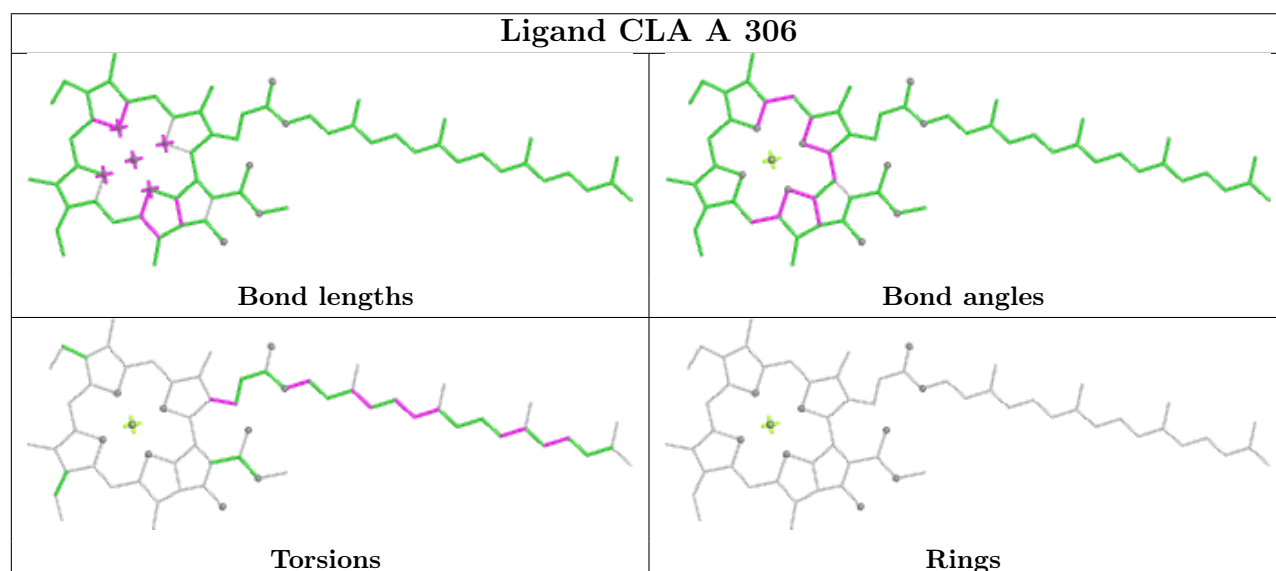
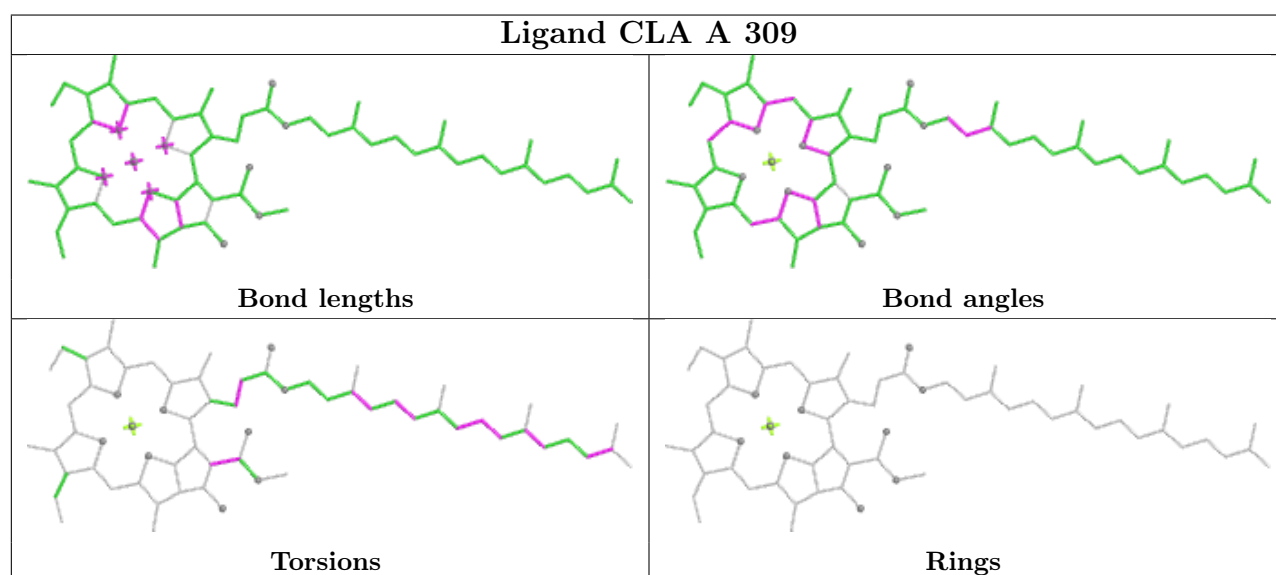
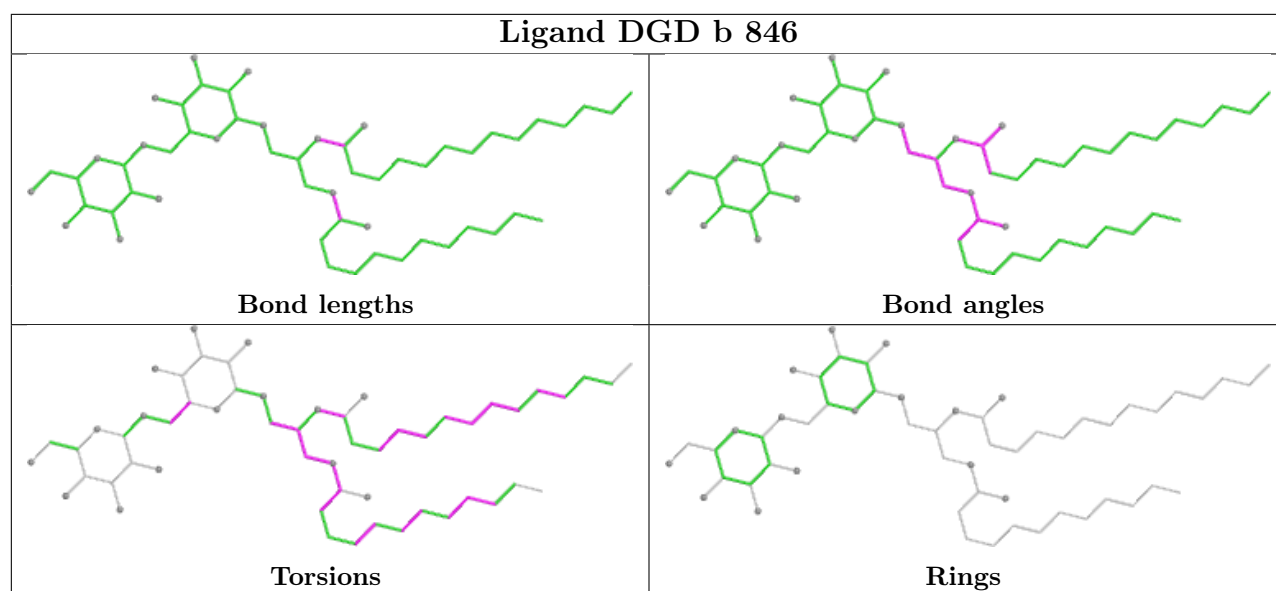
Bond angles



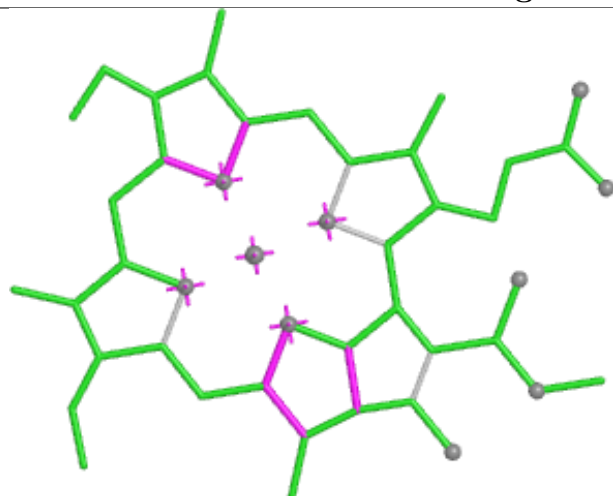
Torsions



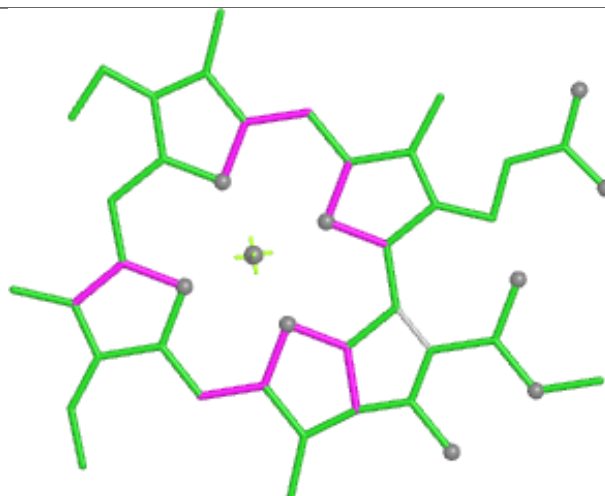
Rings



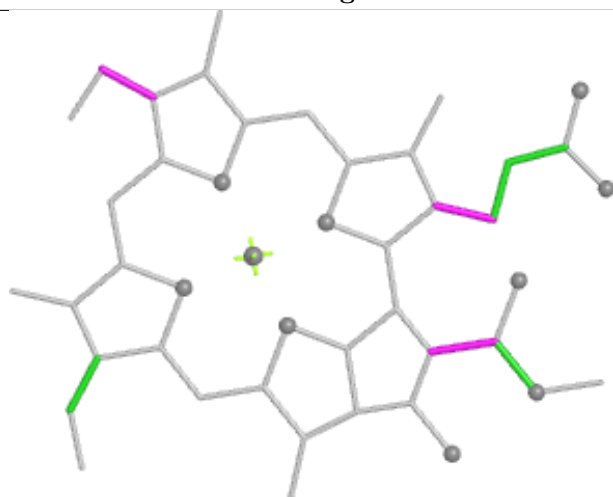
Ligand CLA E 303



Bond lengths



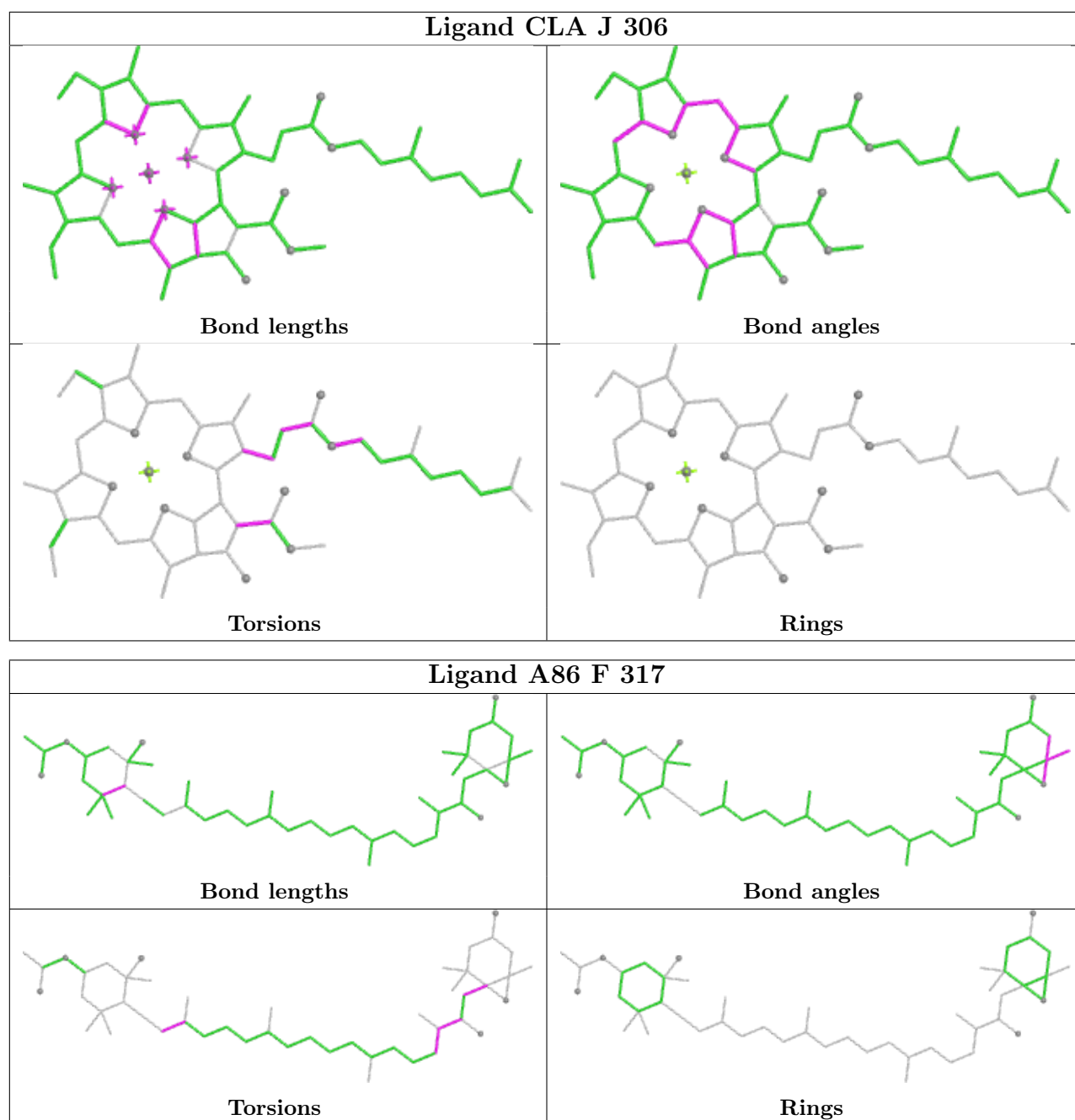
Bond angles



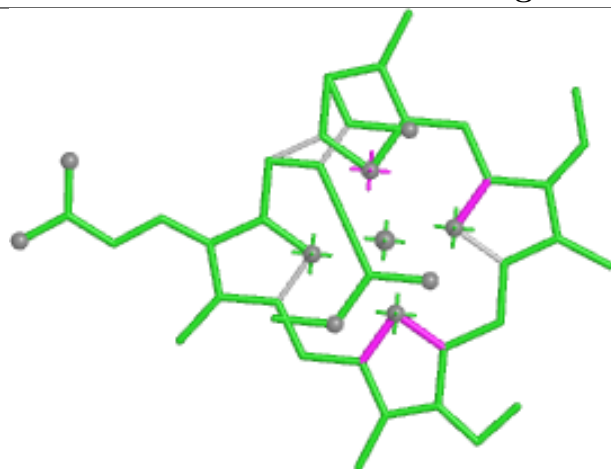
Torsions



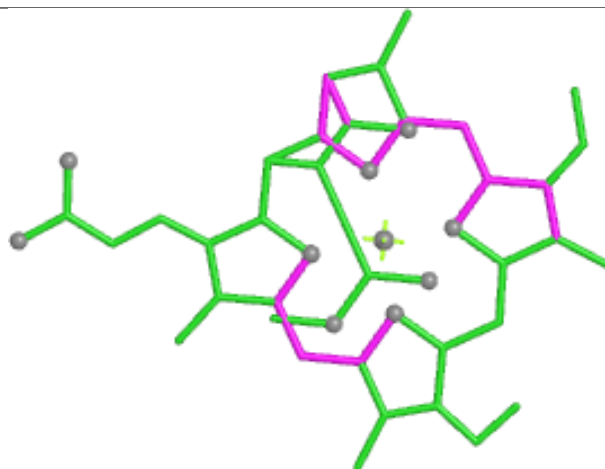
Rings



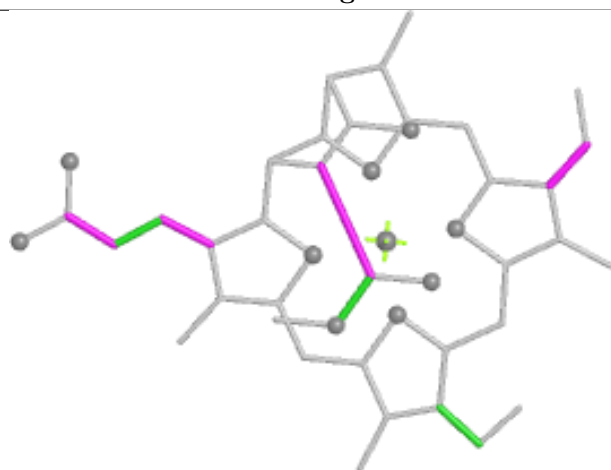
Ligand KC2 G 302



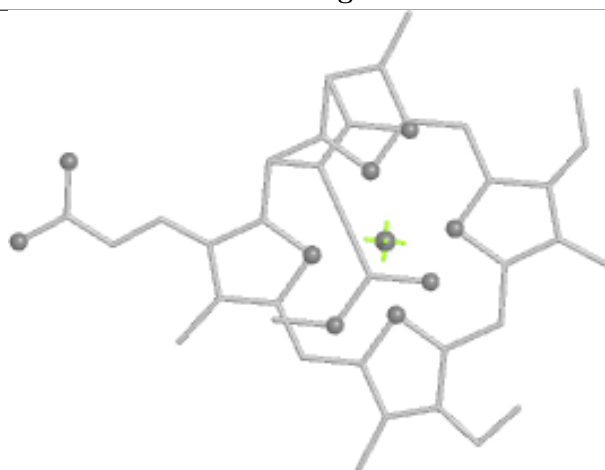
Bond lengths



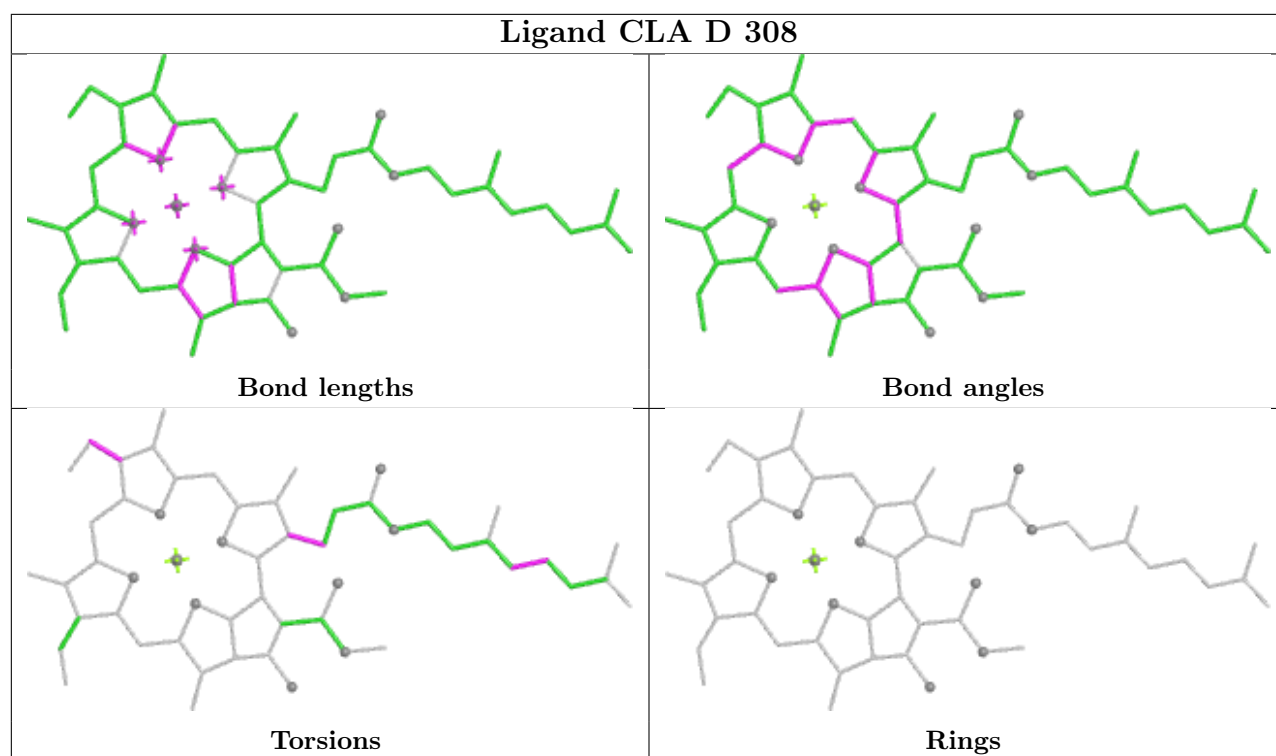
Bond angles



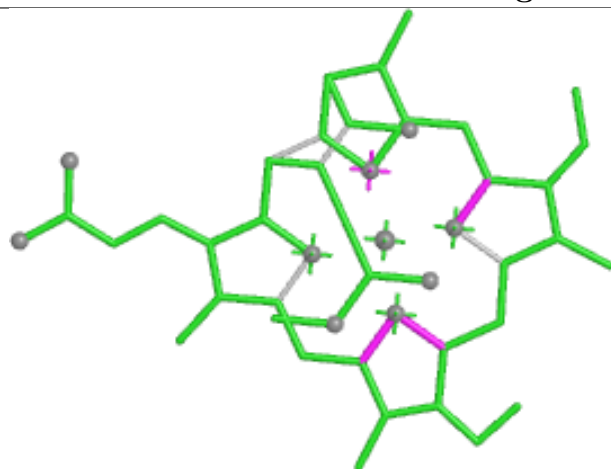
Torsions



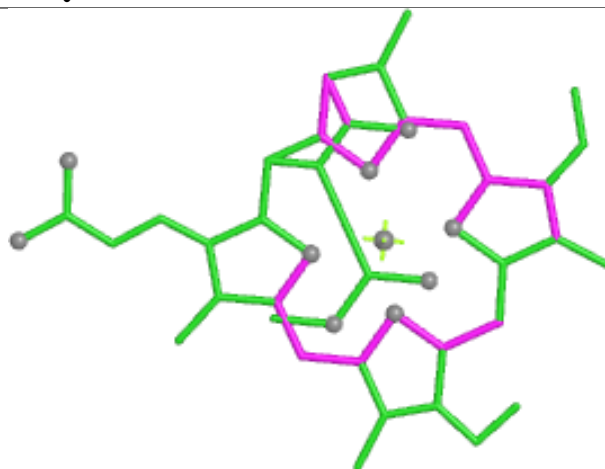
Rings



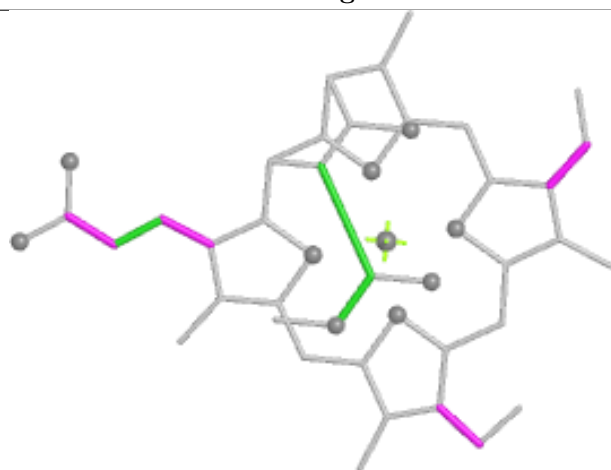
Ligand KC2 Q 302



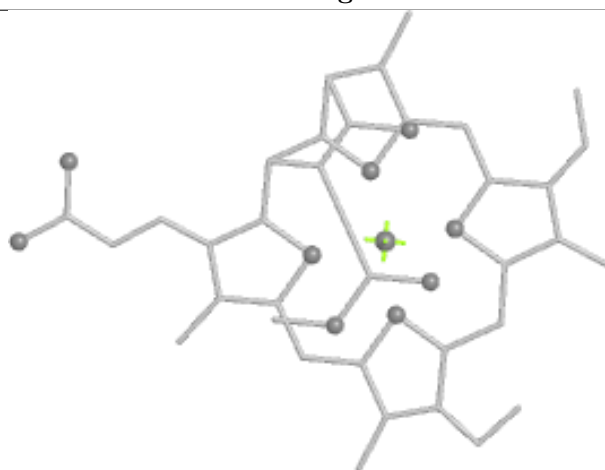
Bond lengths



Bond angles

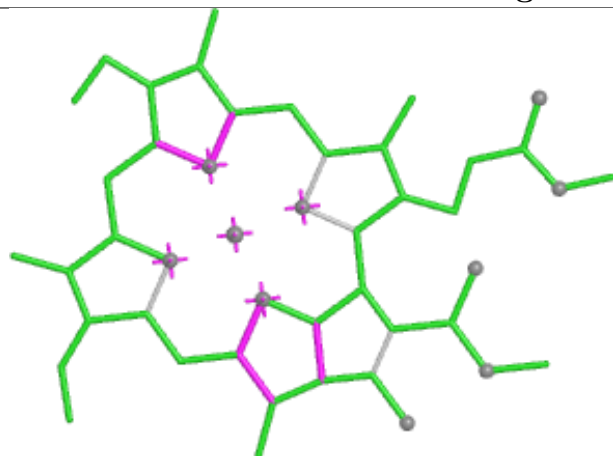


Torsions

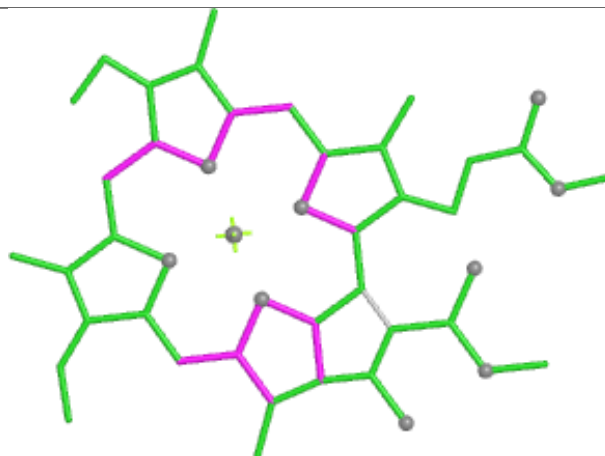


Rings

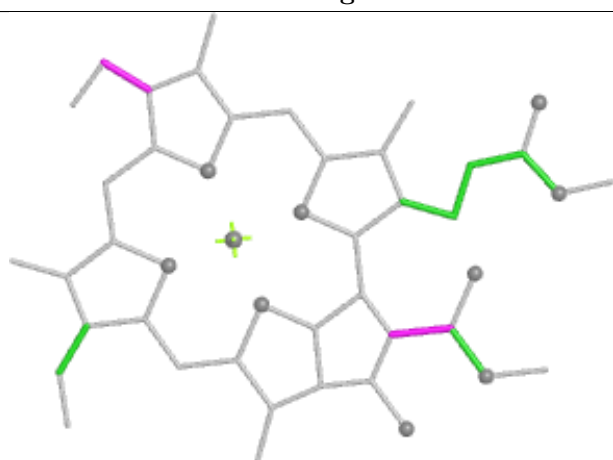
Ligand CLA F 308



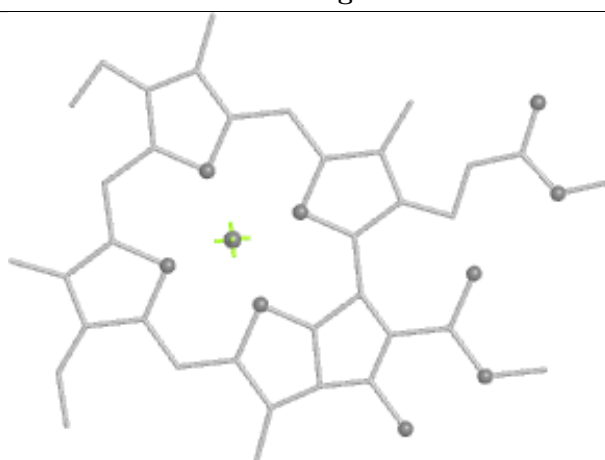
Bond lengths



Bond angles

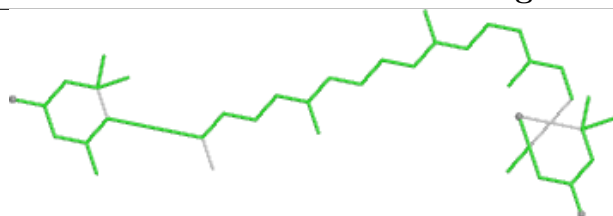


Torsions



Rings

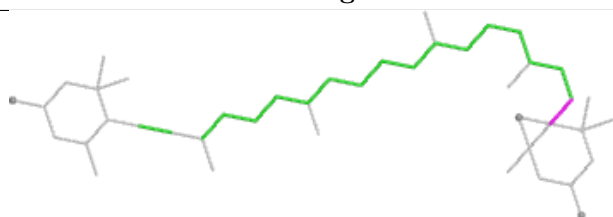
Ligand DD6 B 307



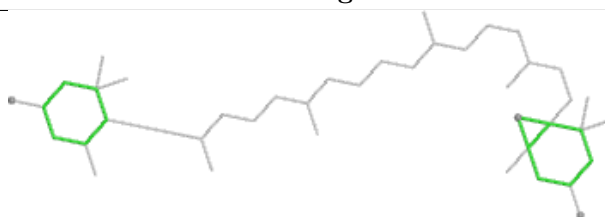
Bond lengths



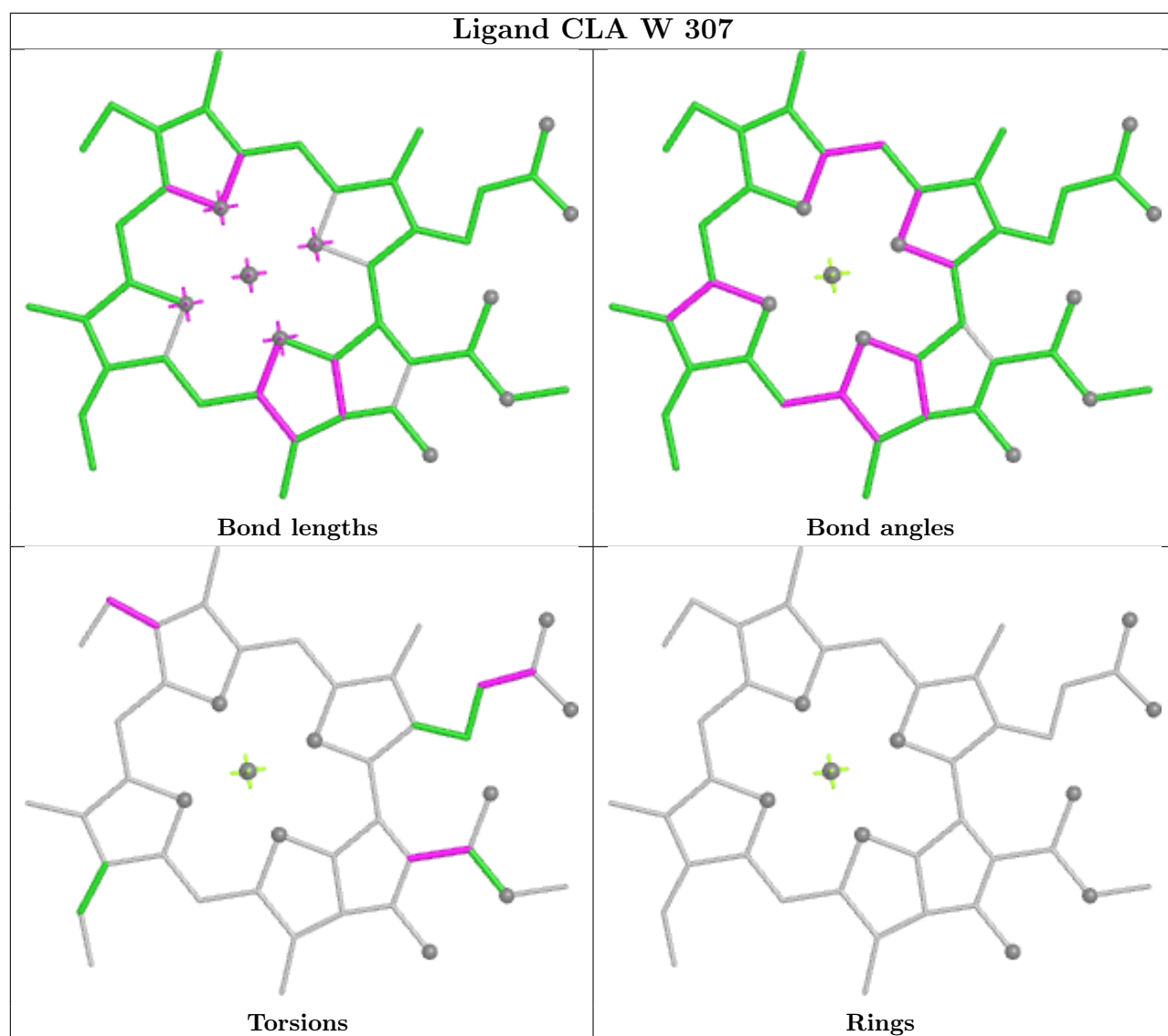
Bond angles



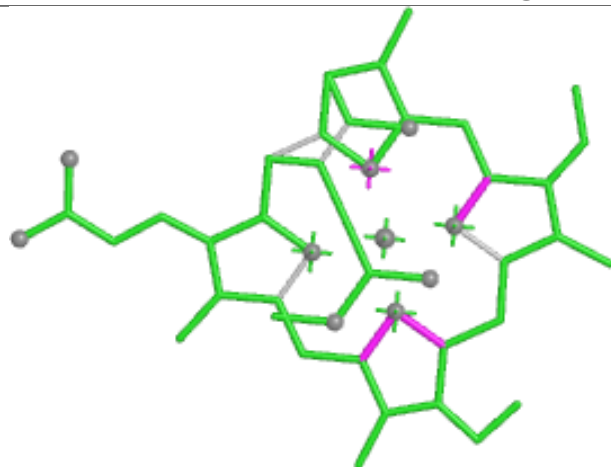
Torsions



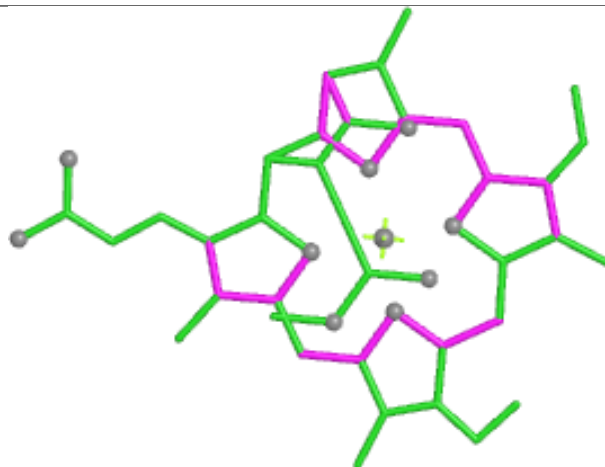
Rings



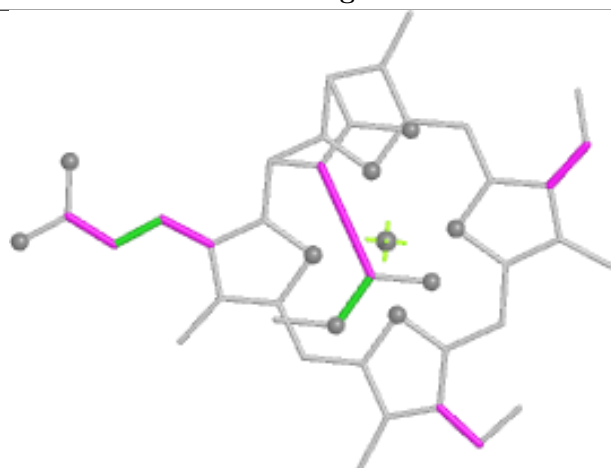
Ligand KC2 F 310



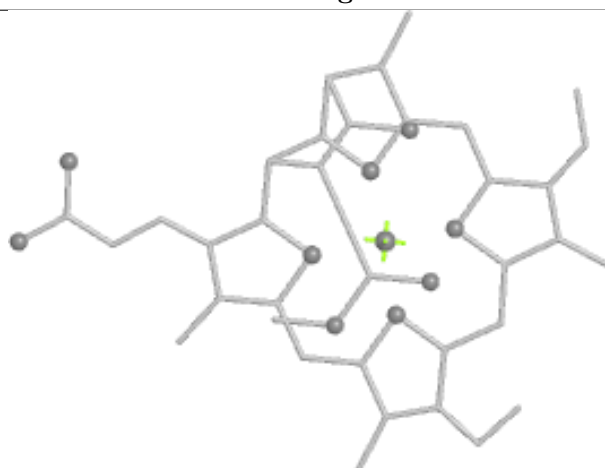
Bond lengths



Bond angles



Torsions



Rings

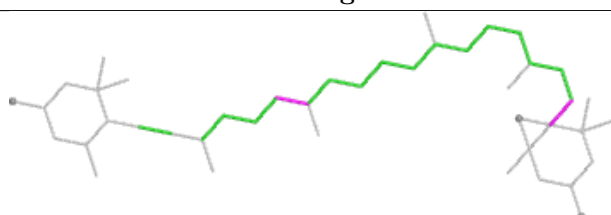
Ligand DD6 F 316



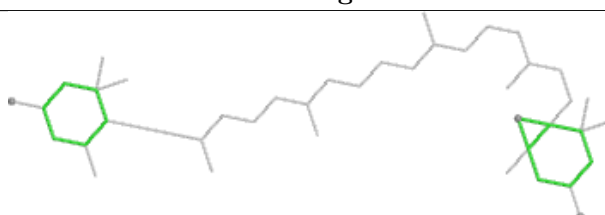
Bond lengths



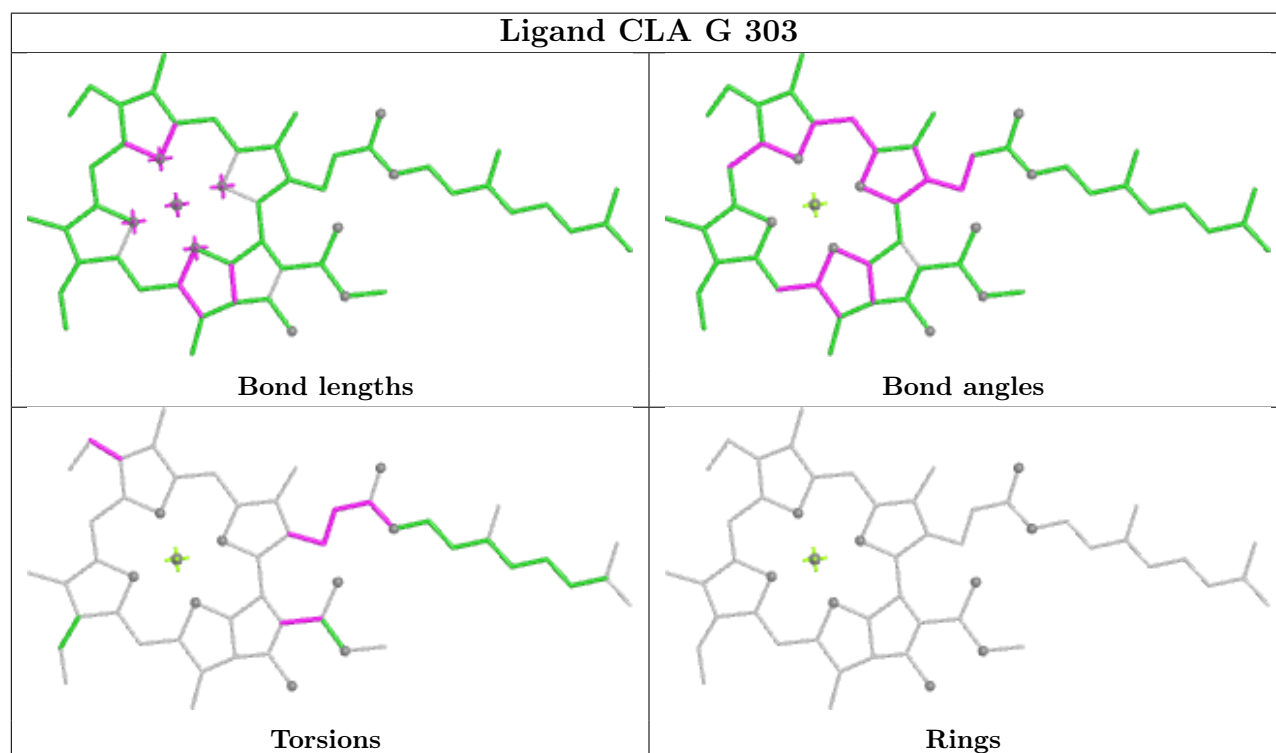
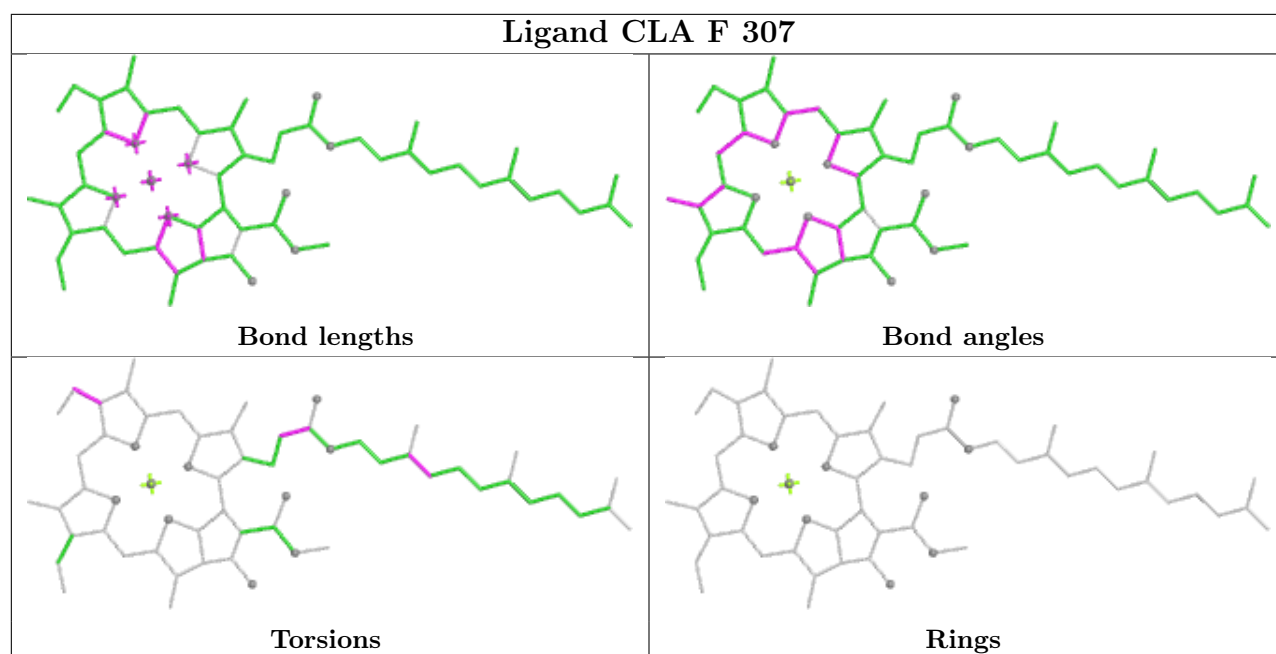
Bond angles

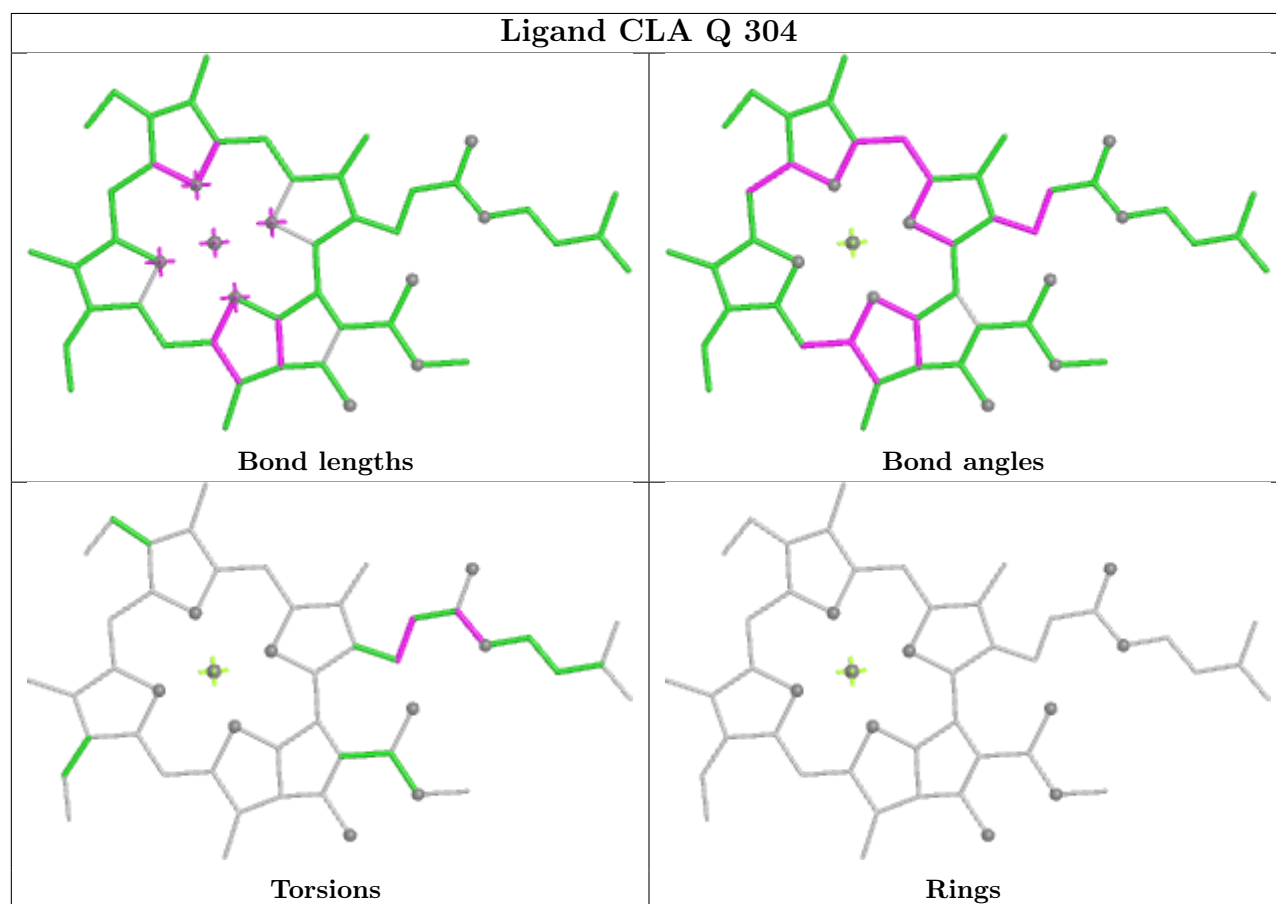
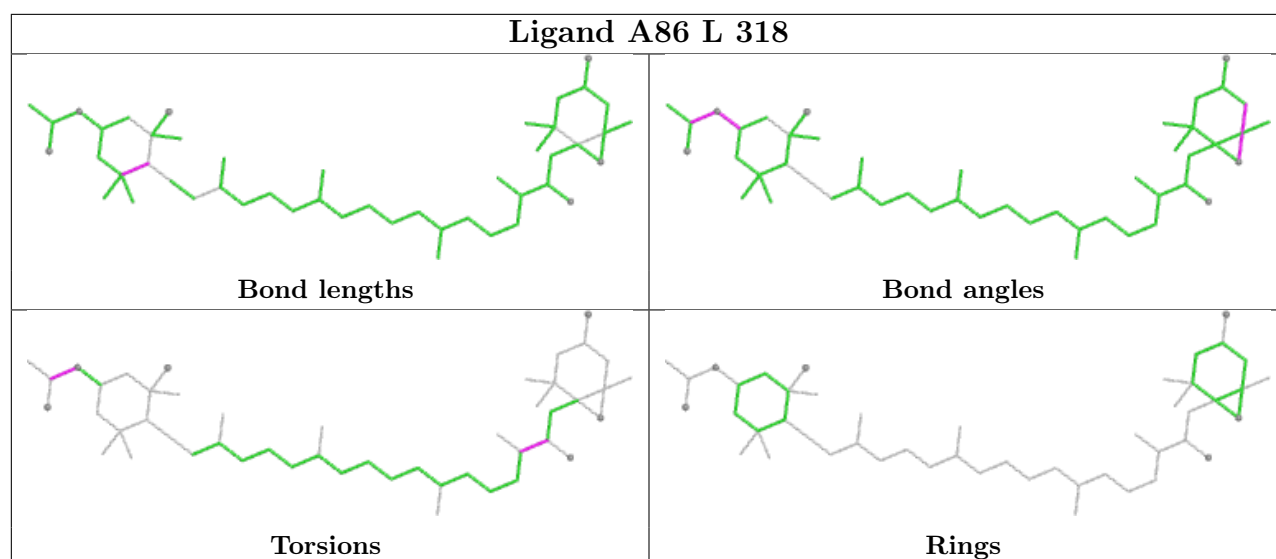


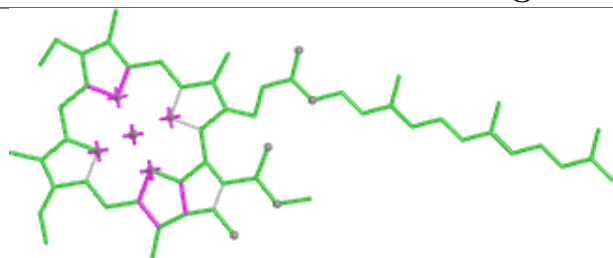
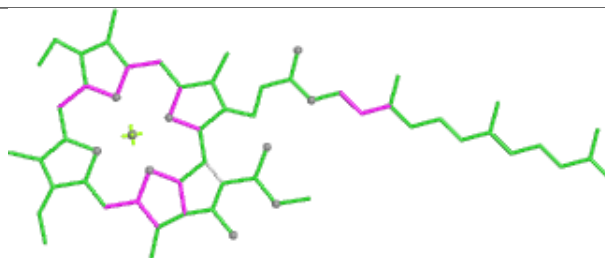
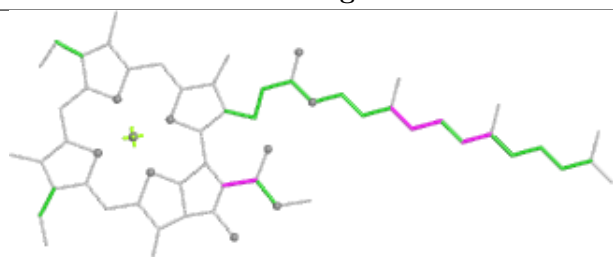
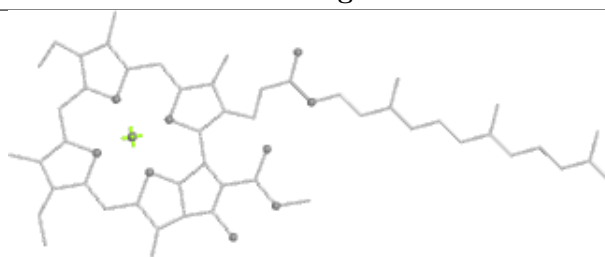
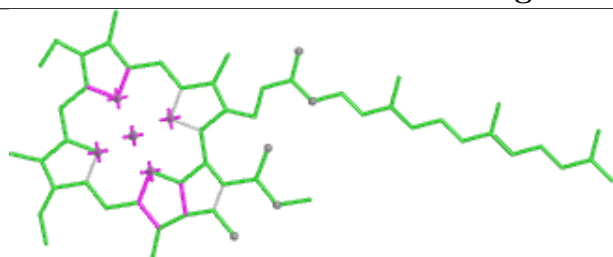
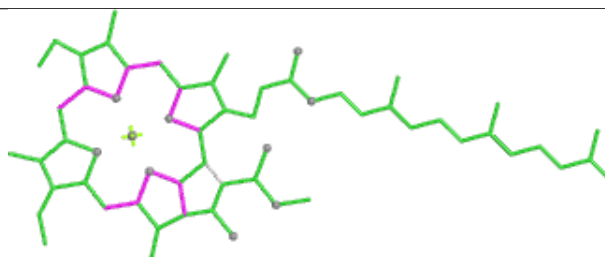
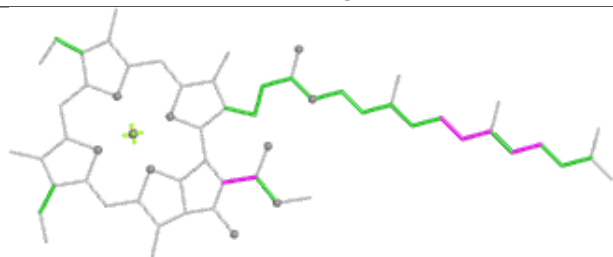
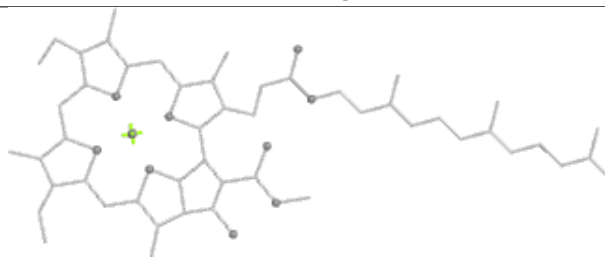
Torsions

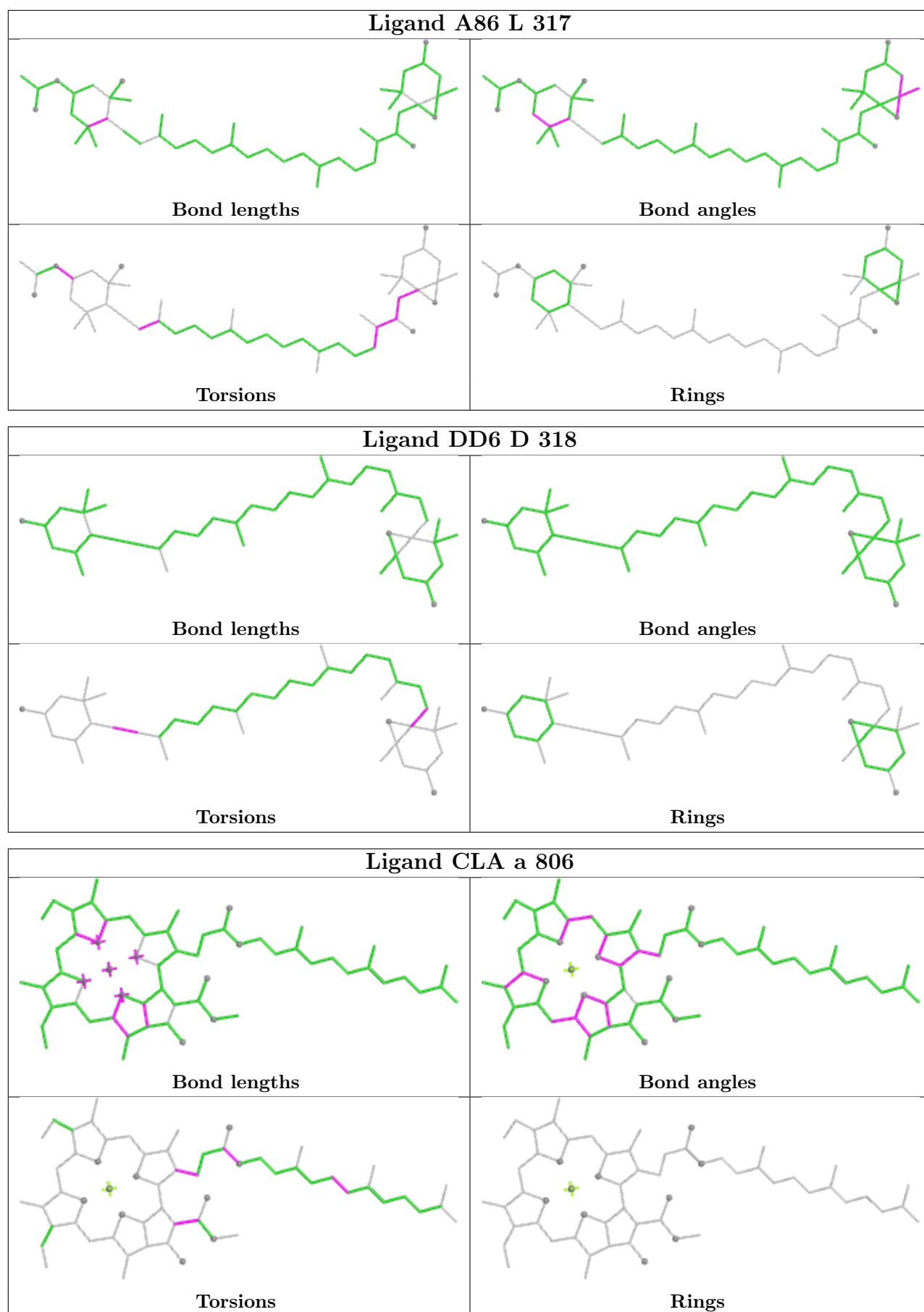


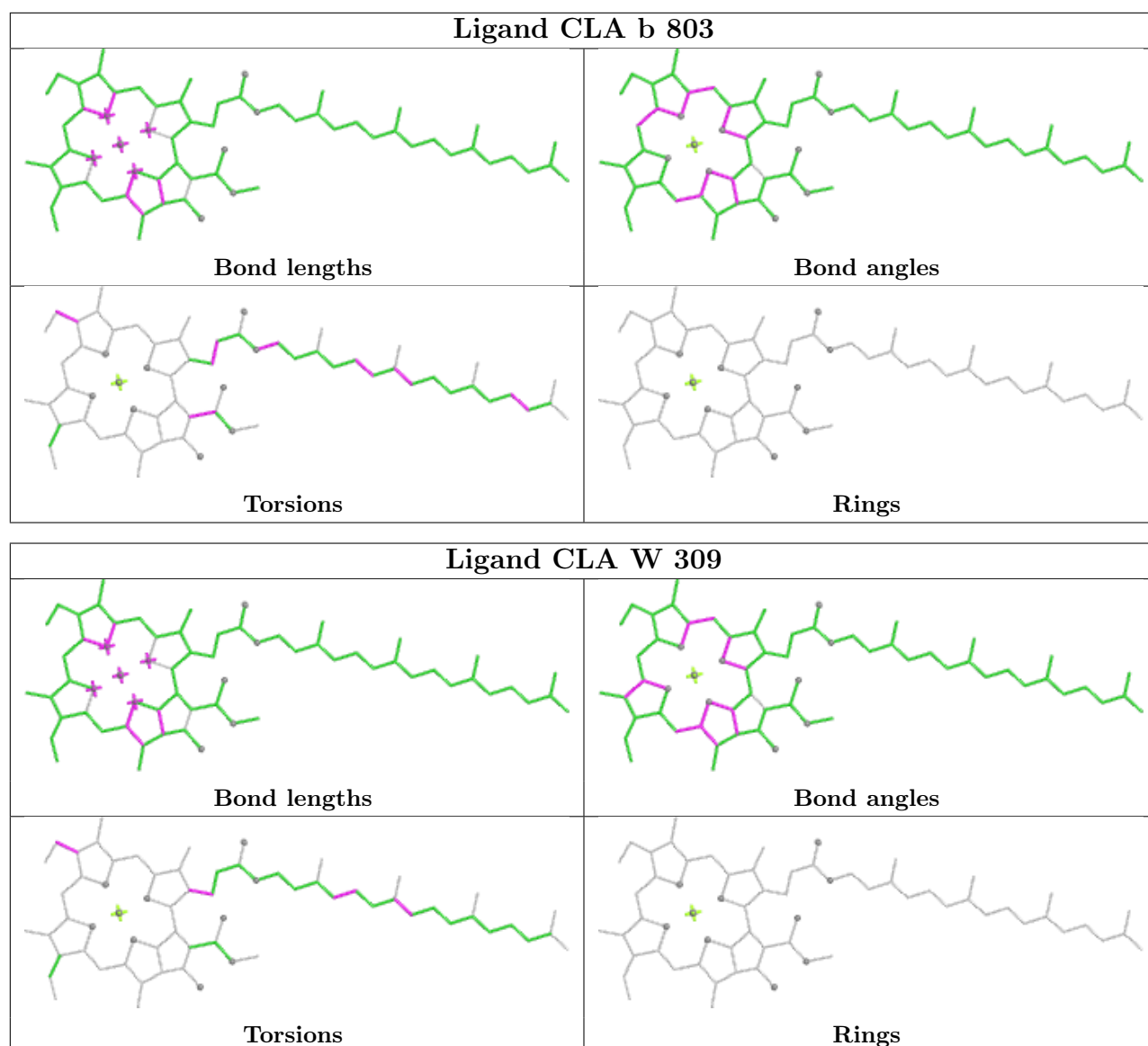
Rings



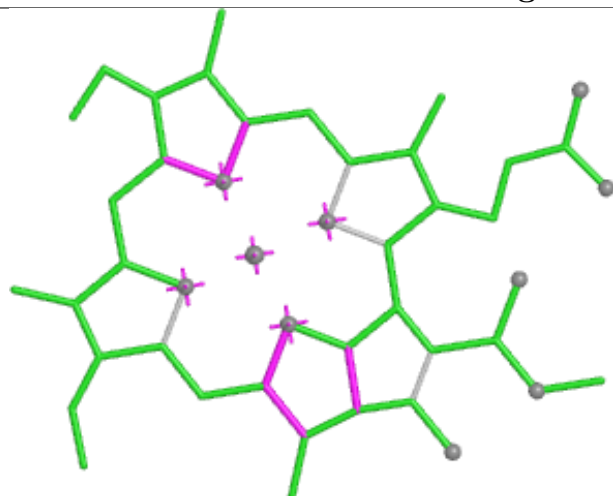


Ligand CLA N 313**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA T 306****Bond lengths****Bond angles****Torsions****Rings**

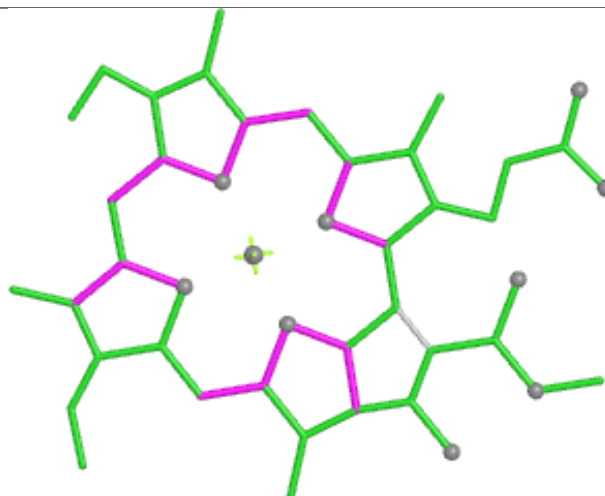




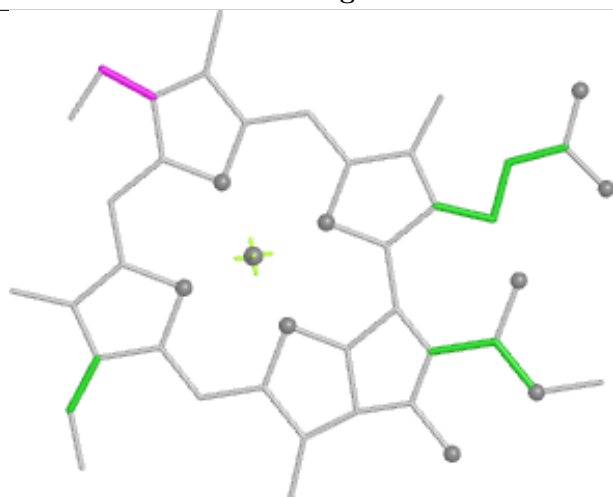
Ligand CLA J 302



Bond lengths



Bond angles

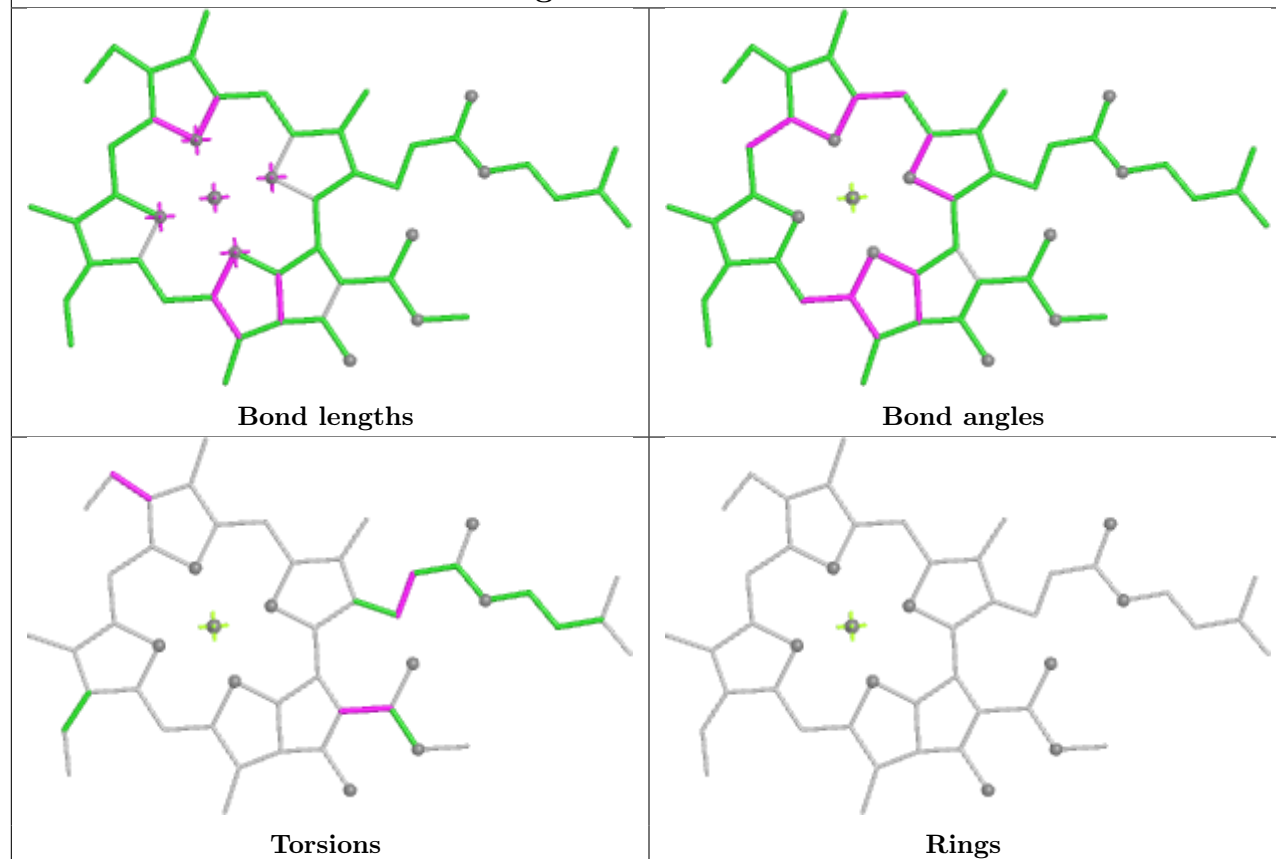


Torsions

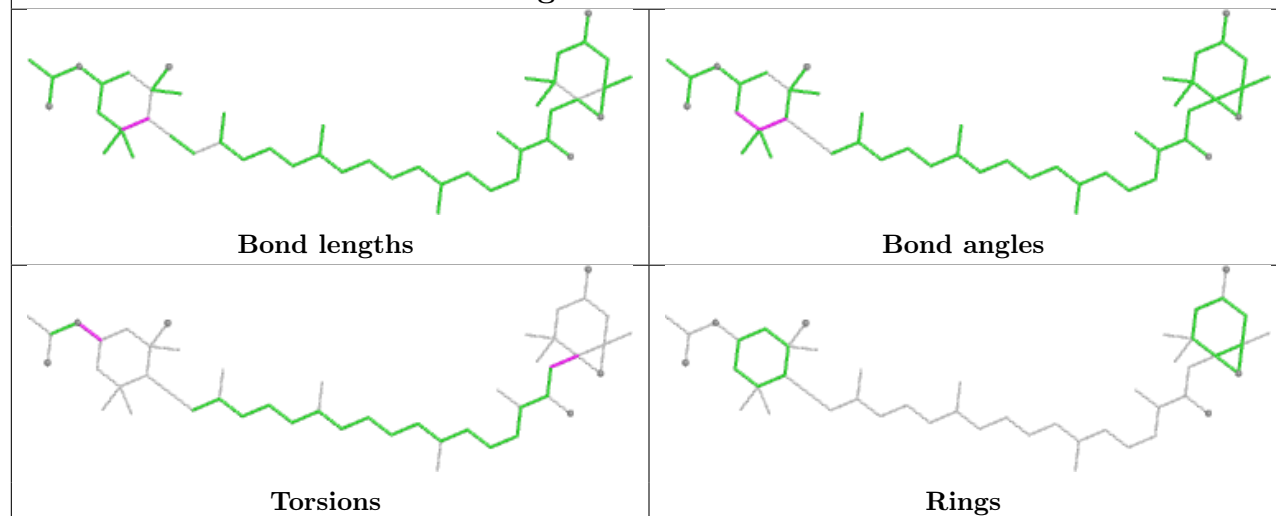


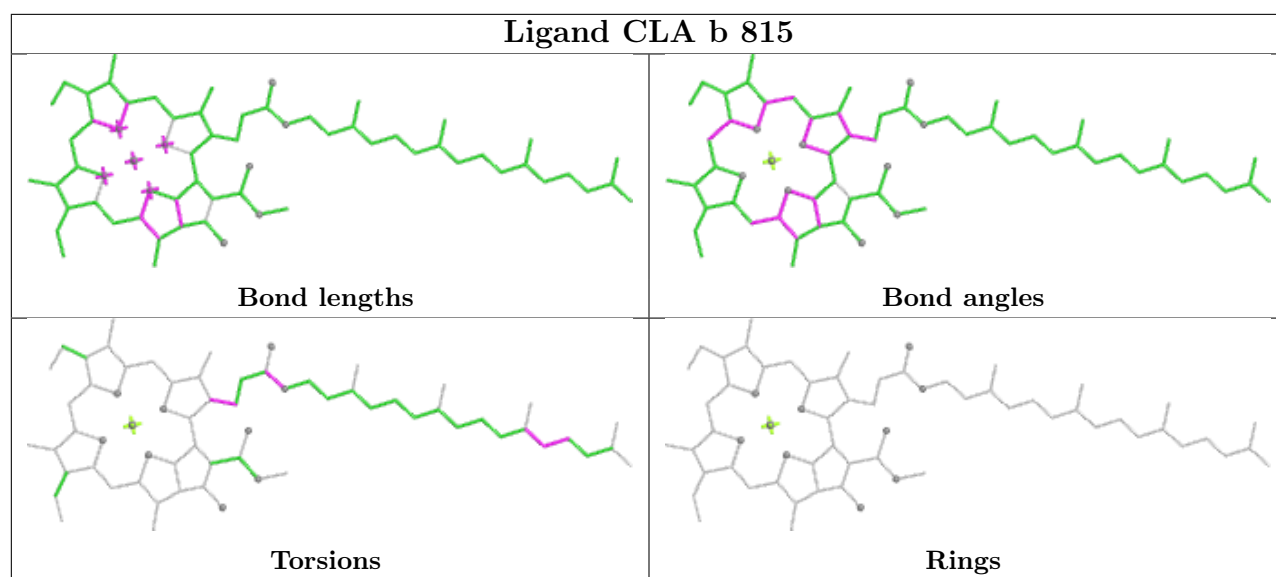
Rings

Ligand CLA b 827

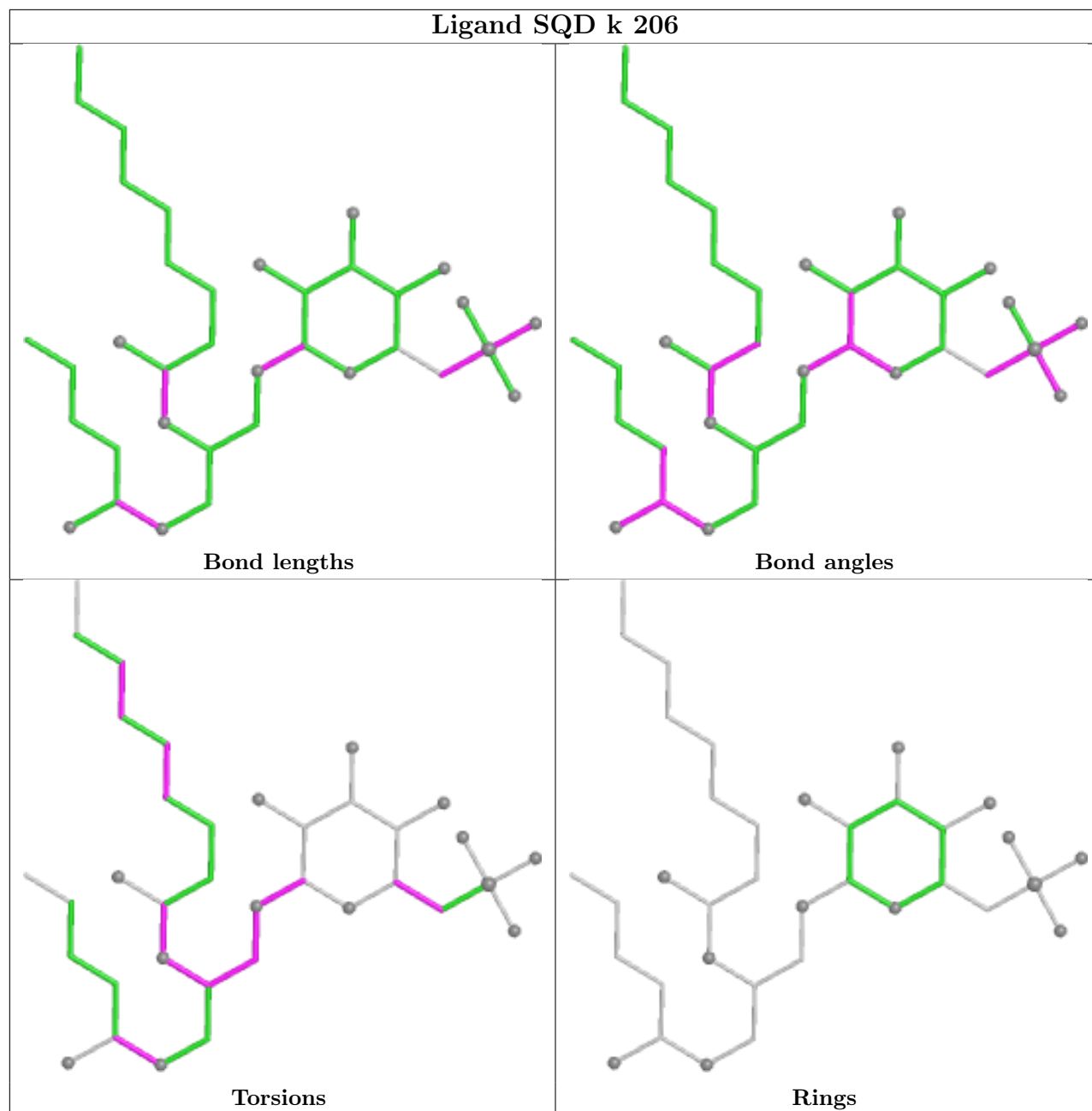


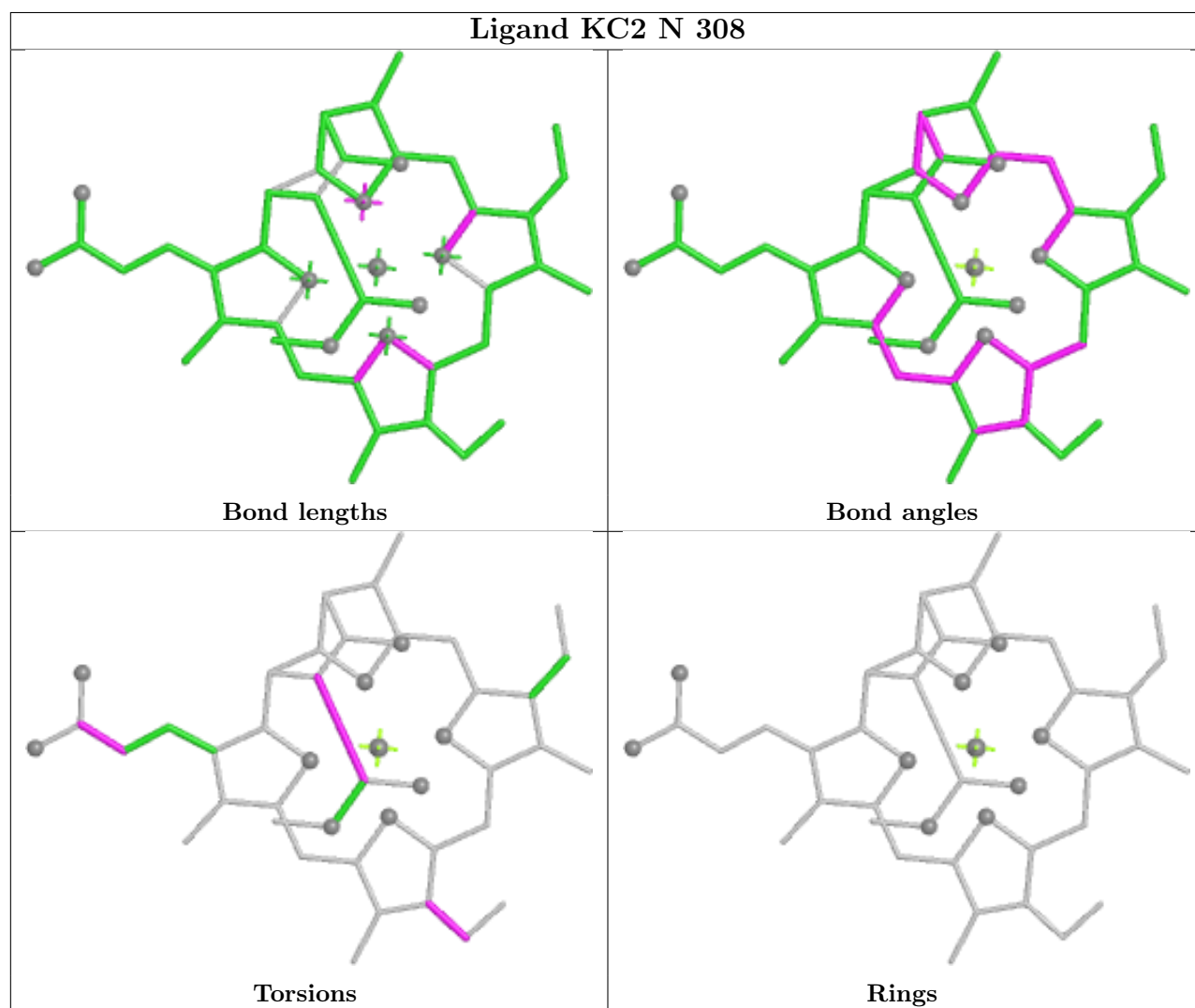
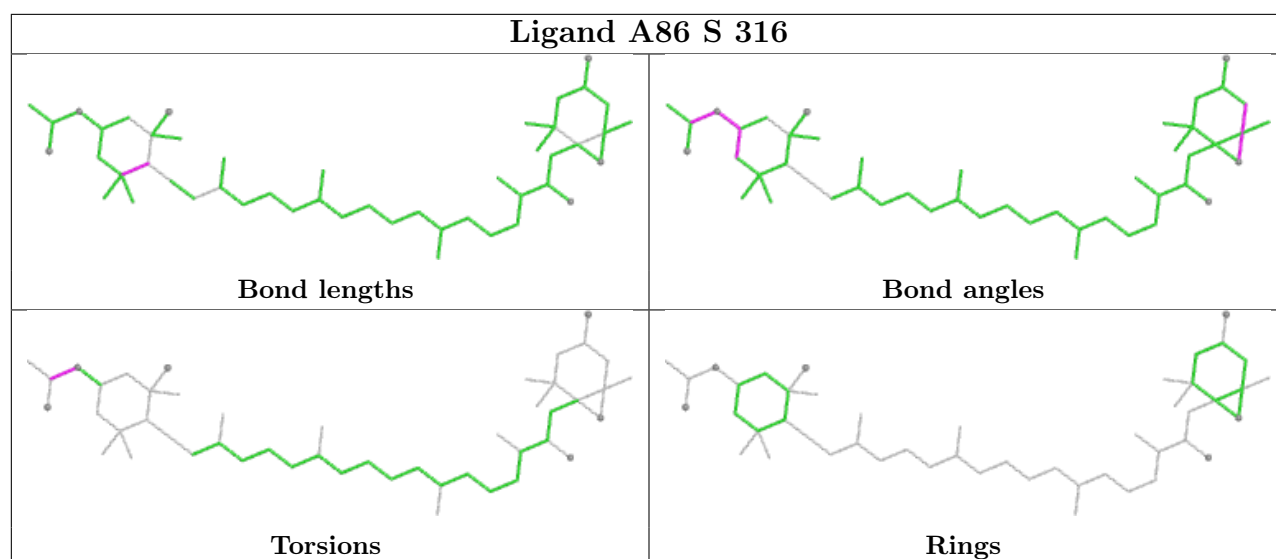
Ligand A86 R 312

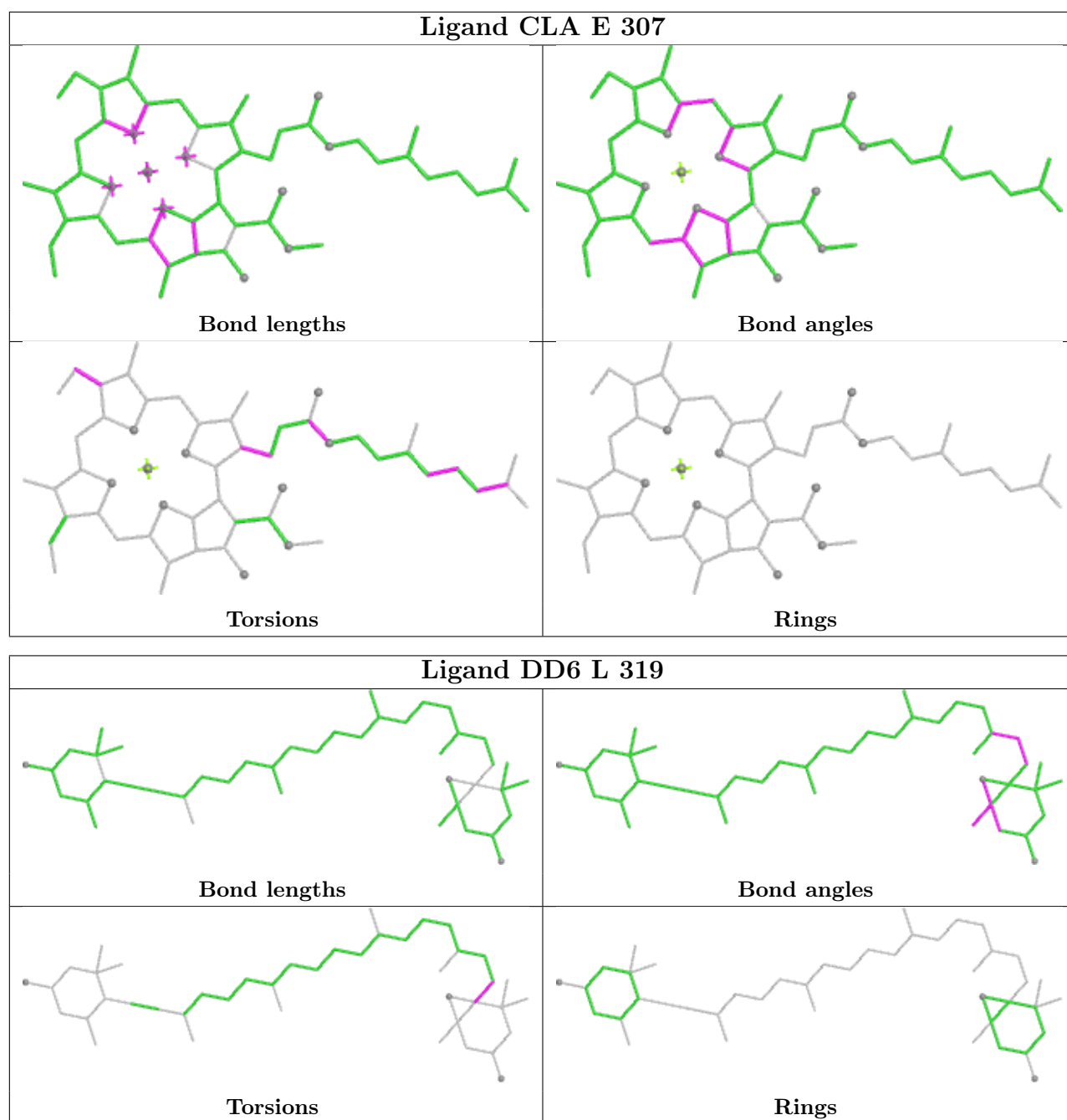




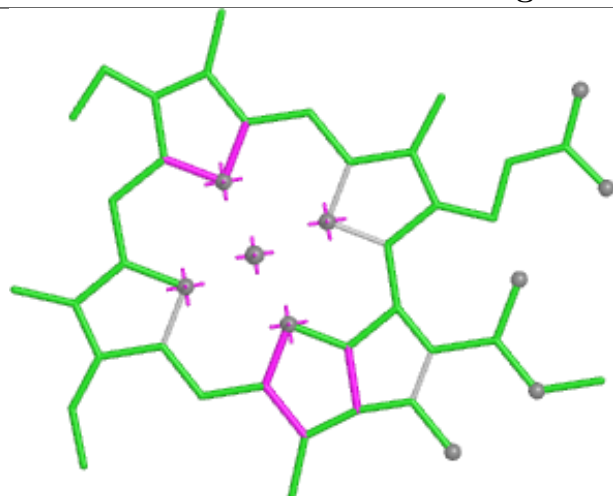
Ligand SQD k 206



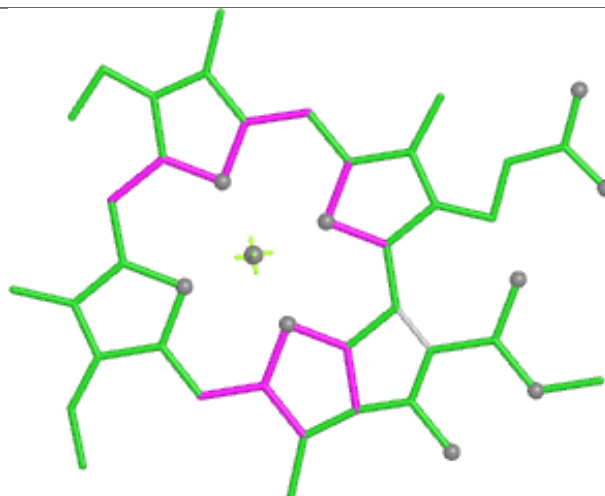




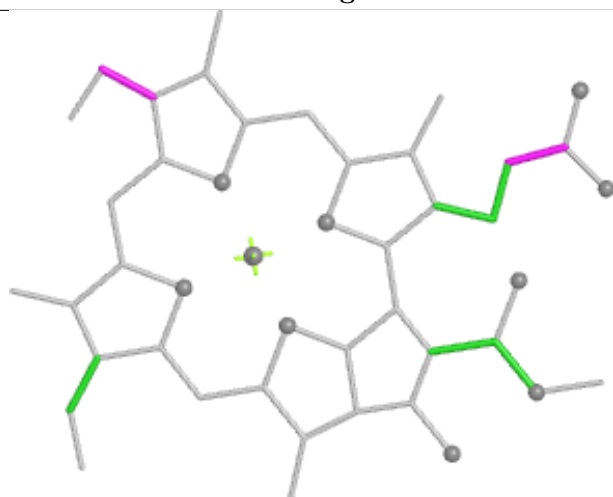
Ligand CLA L 308



Bond lengths



Bond angles

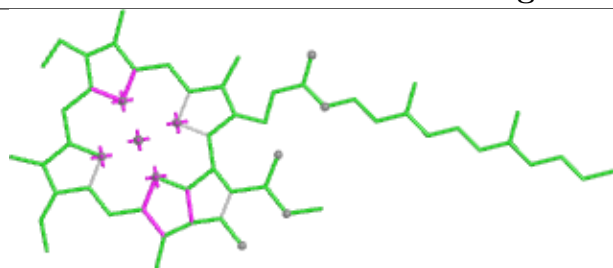


Torsions

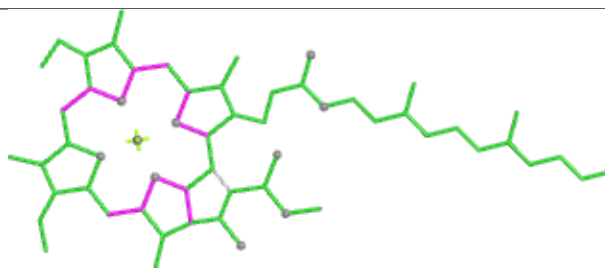


Rings

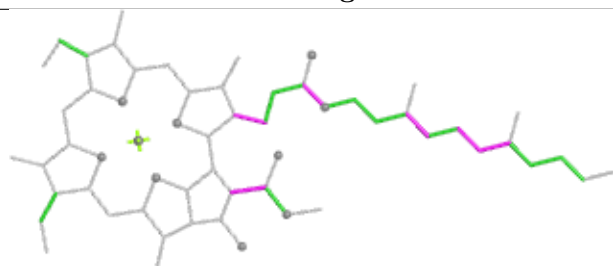
Ligand CLA b 824



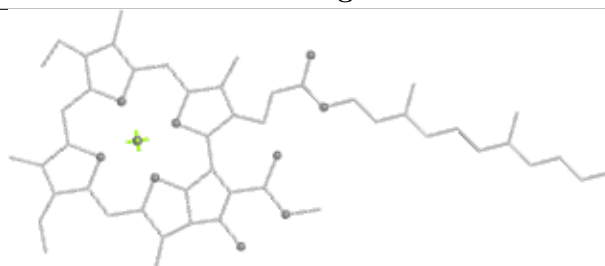
Bond lengths



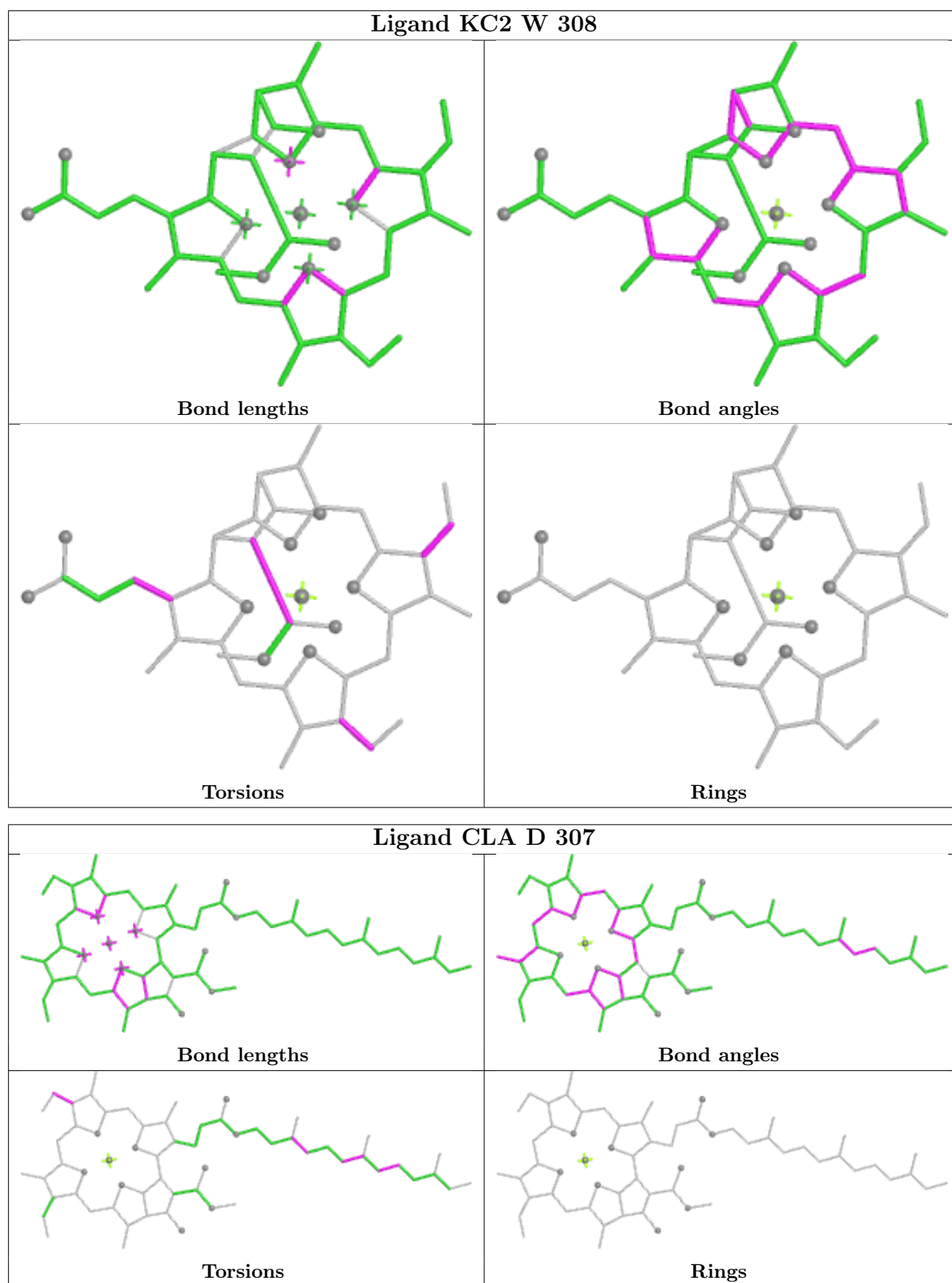
Bond angles



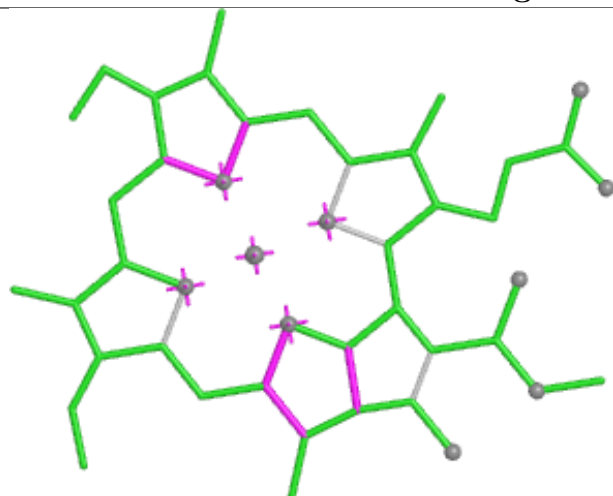
Torsions



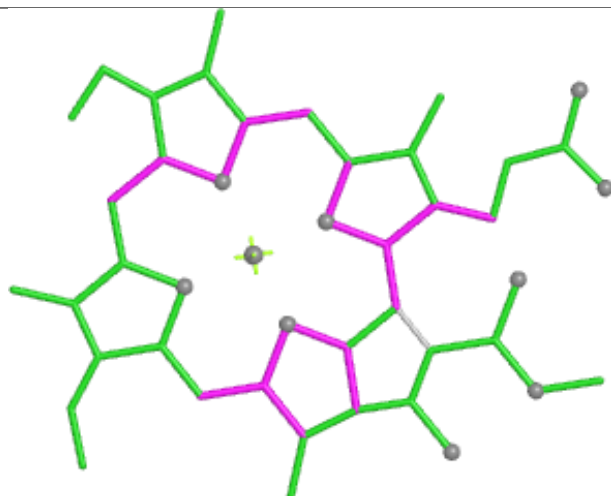
Rings



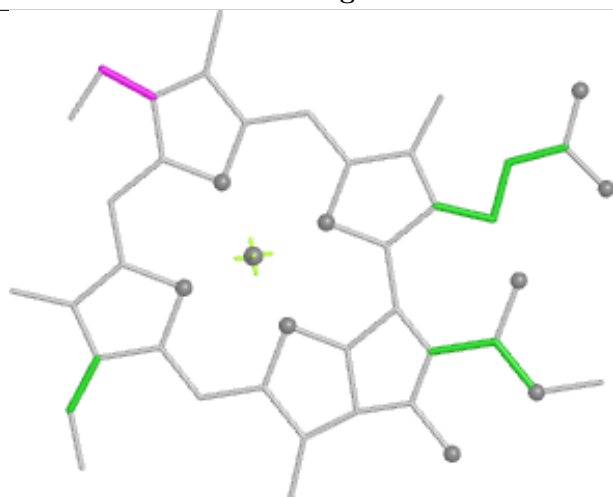
Ligand CLA O 304



Bond lengths



Bond angles

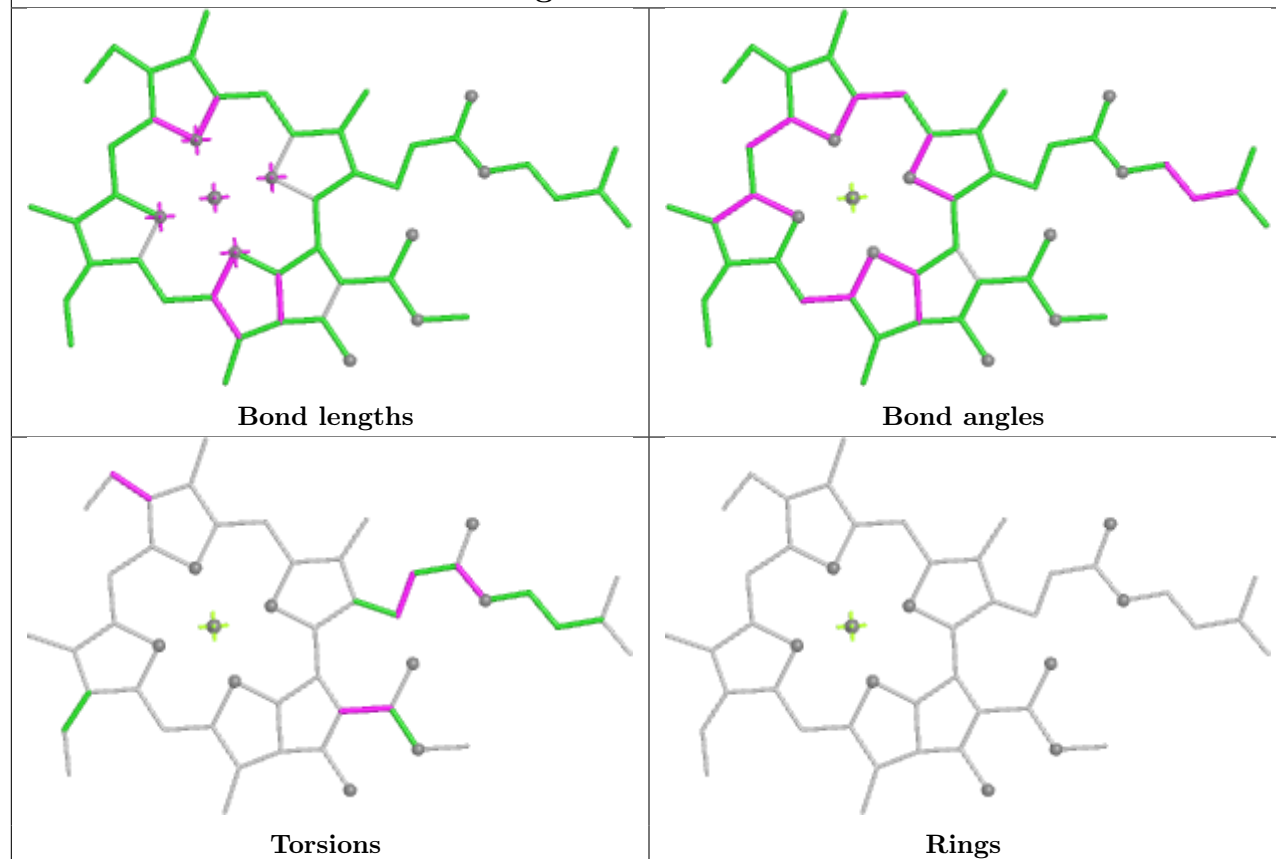


Torsions

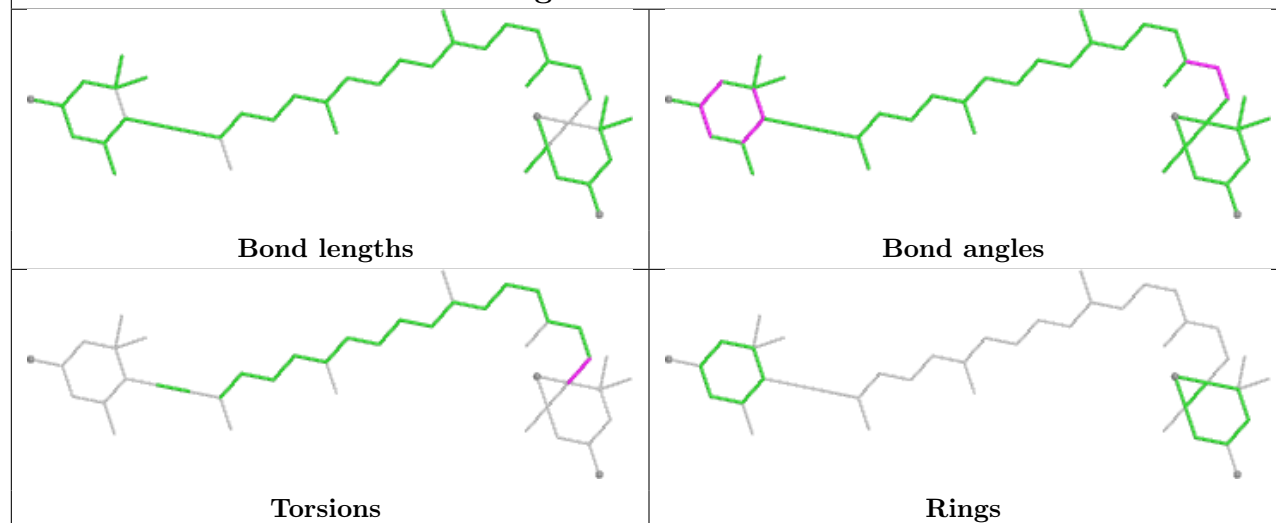


Rings

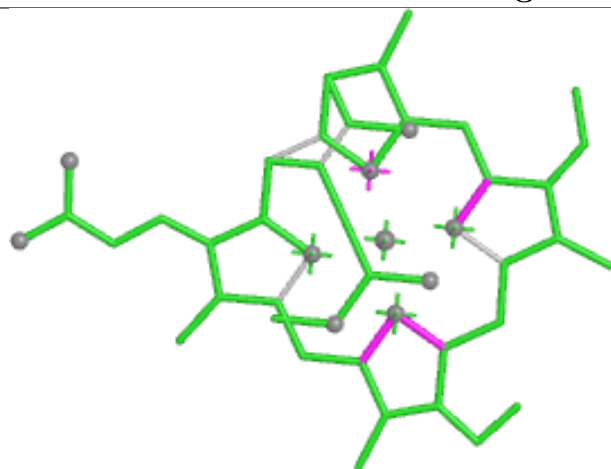
Ligand CLA b 811



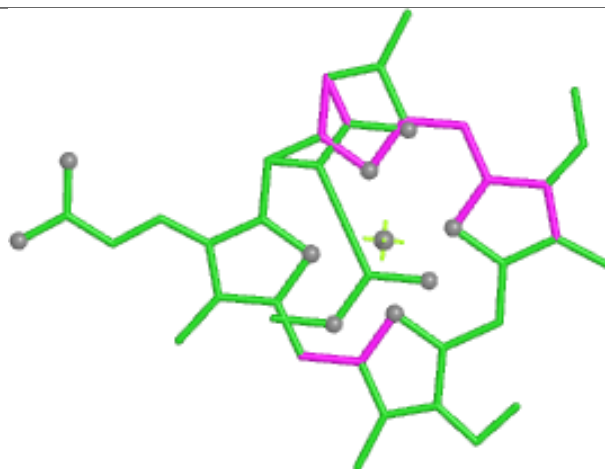
Ligand DD6 F 314



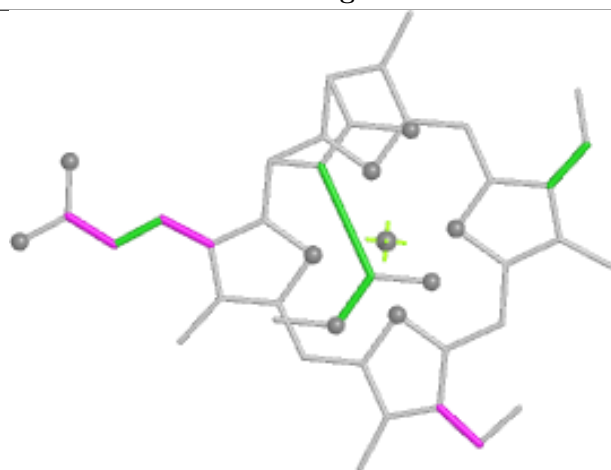
Ligand KC2 R 305



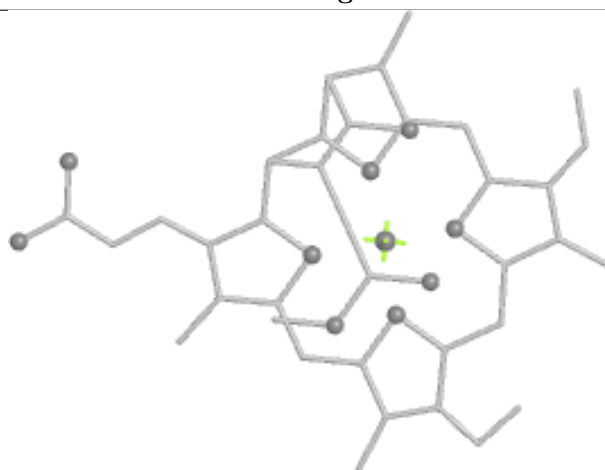
Bond lengths



Bond angles

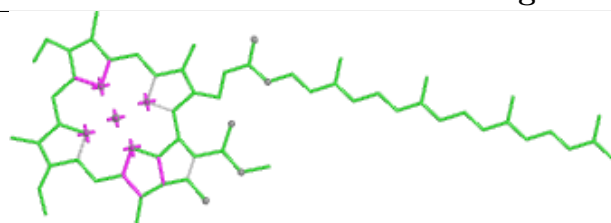


Torsions

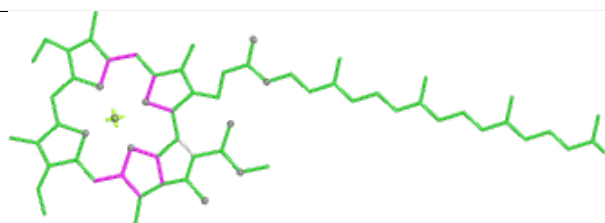


Rings

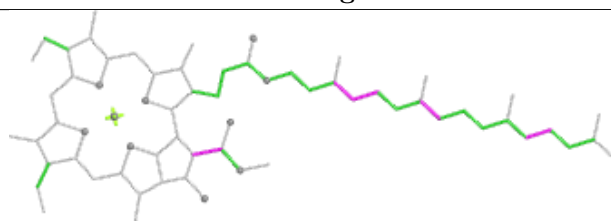
Ligand CLA a 834



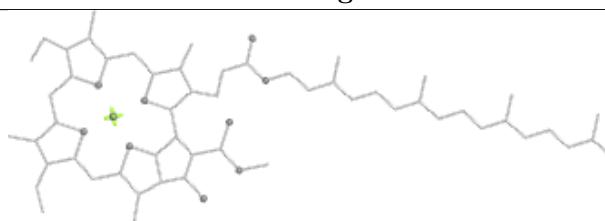
Bond lengths



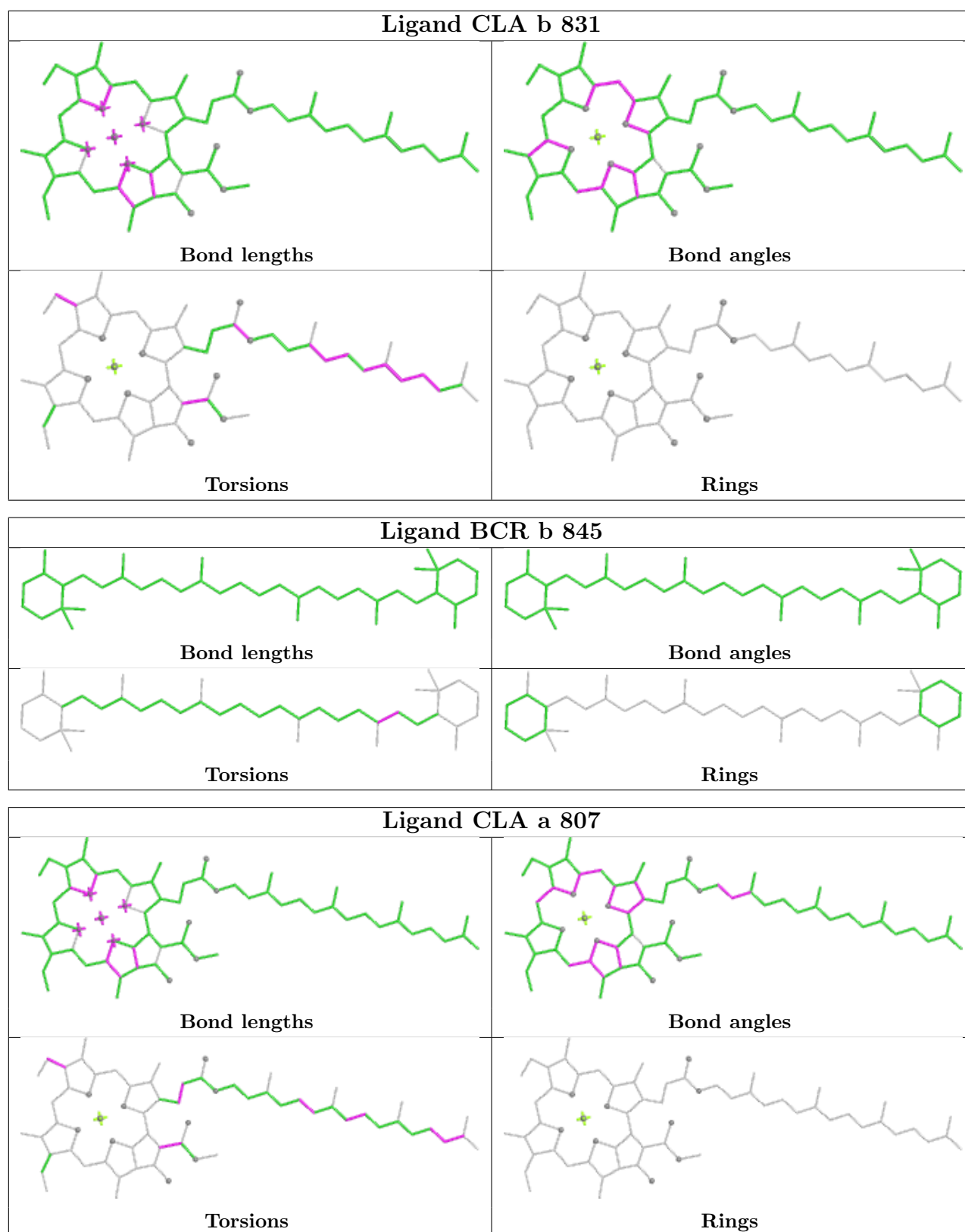
Bond angles



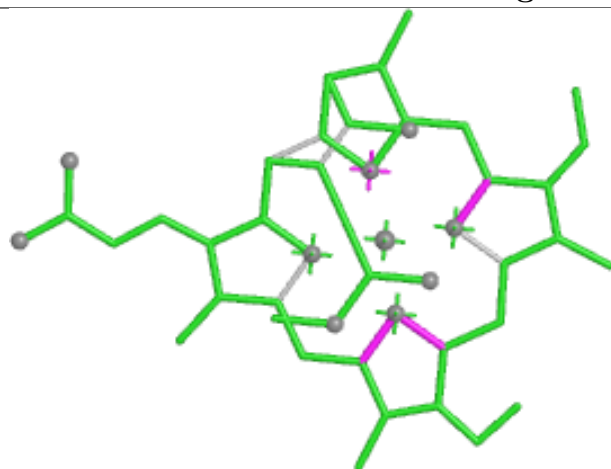
Torsions



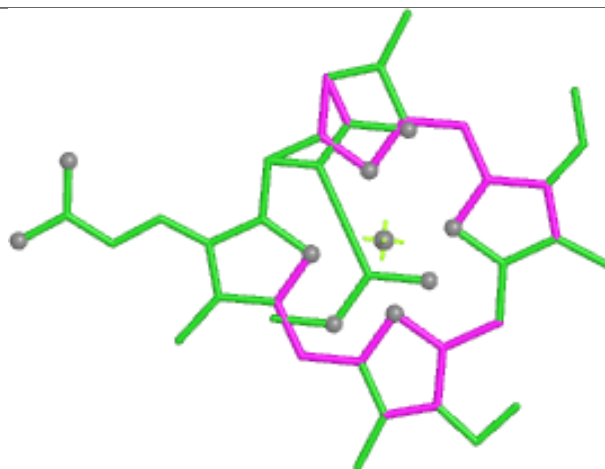
Rings



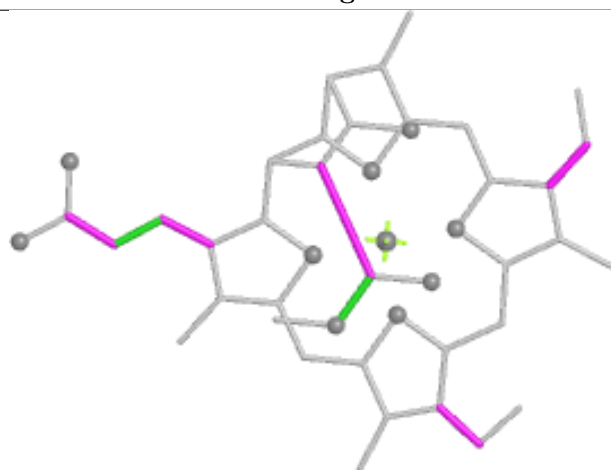
Ligand KC2 P 302



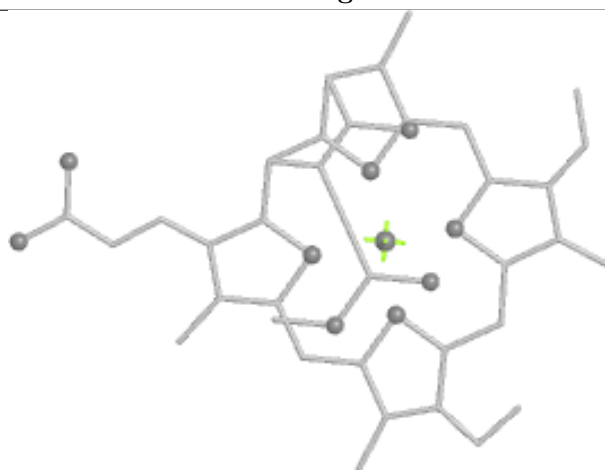
Bond lengths



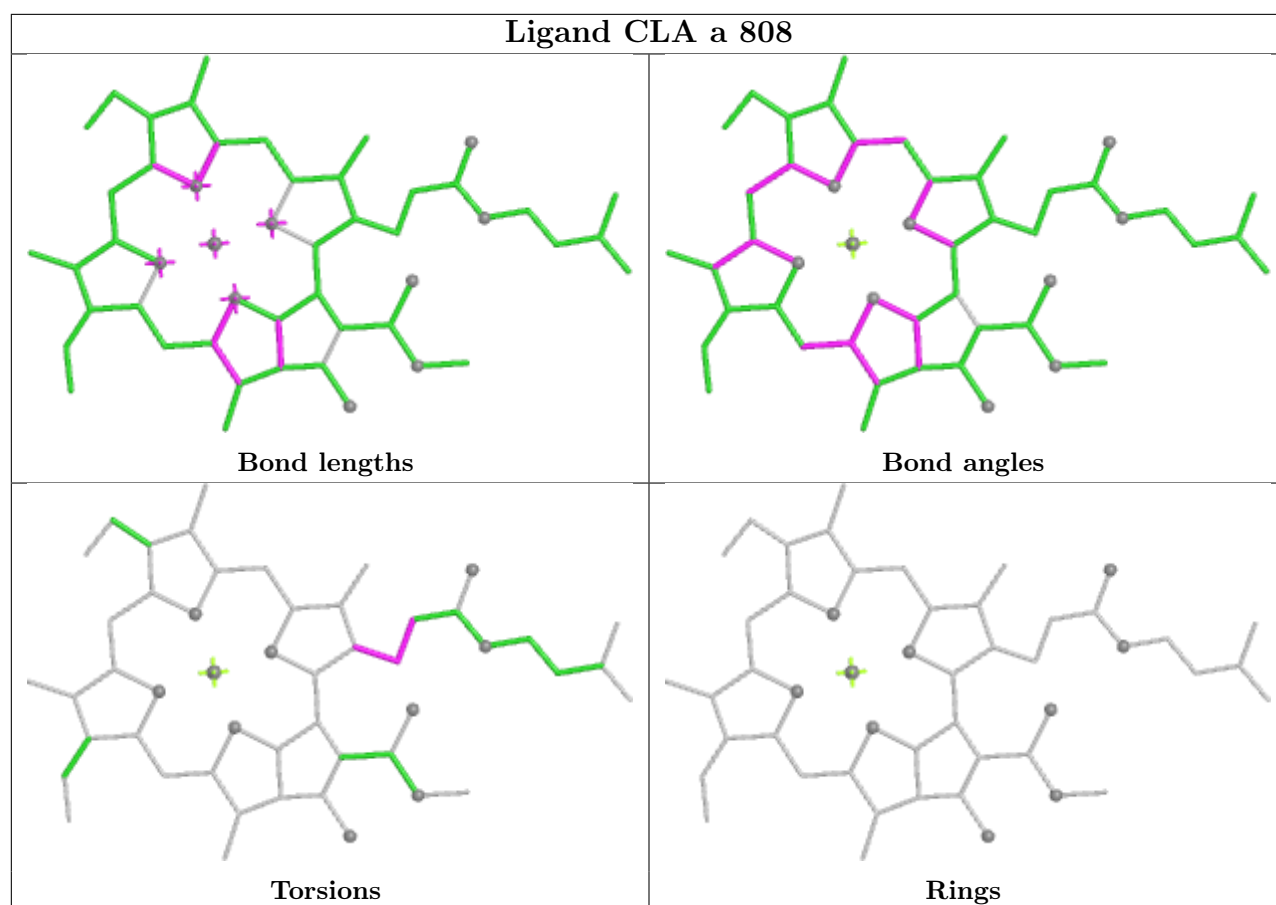
Bond angles



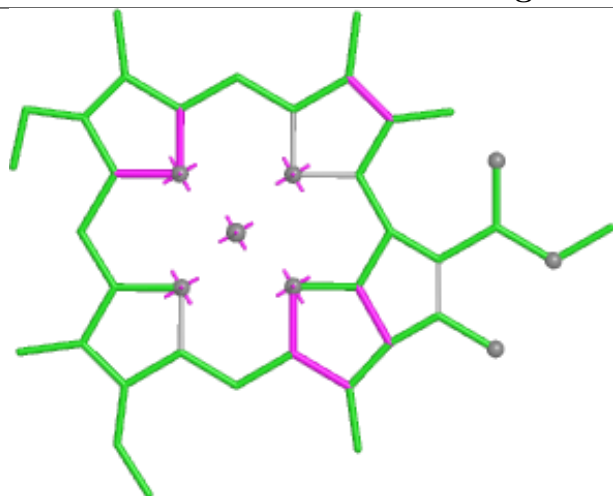
Torsions



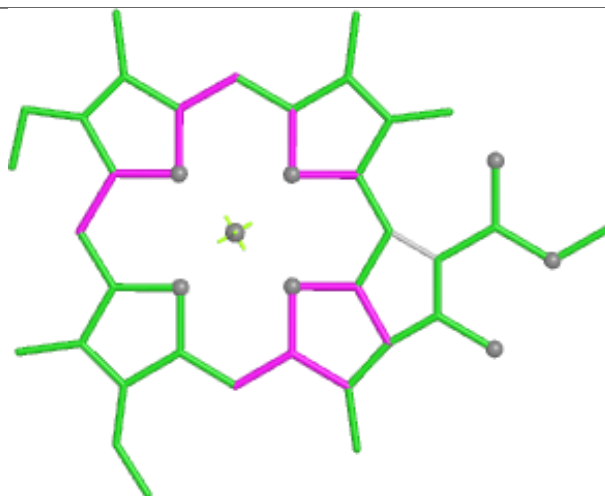
Rings



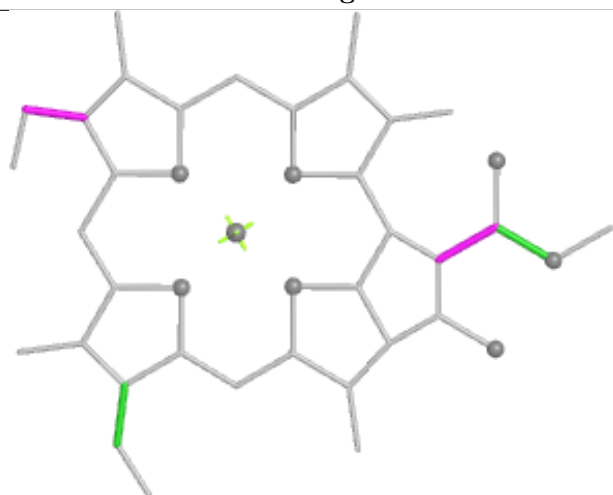
Ligand CLA P 310



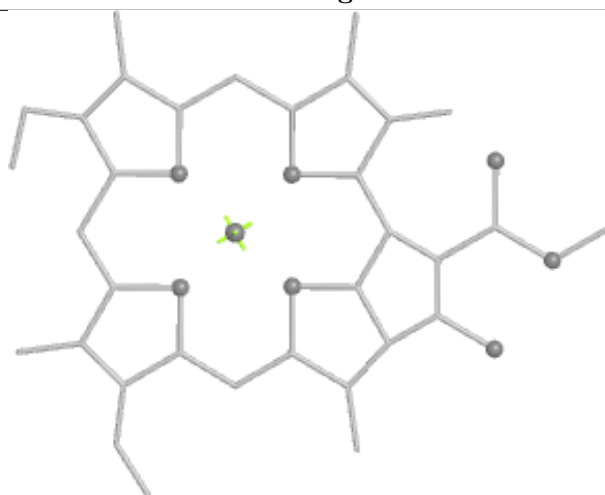
Bond lengths



Bond angles

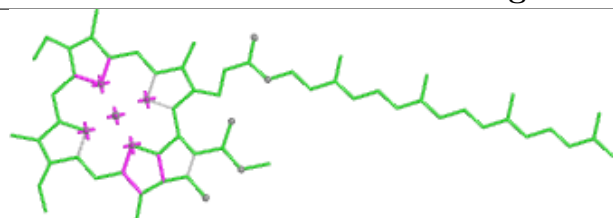


Torsions

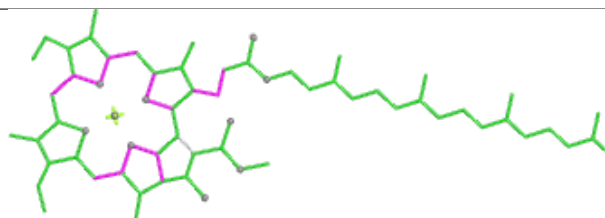


Rings

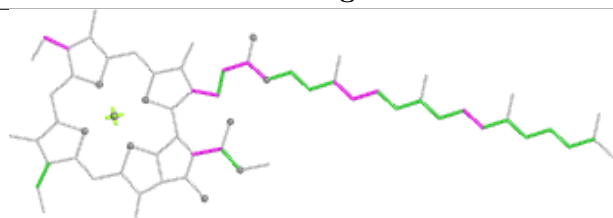
Ligand CLA W 311



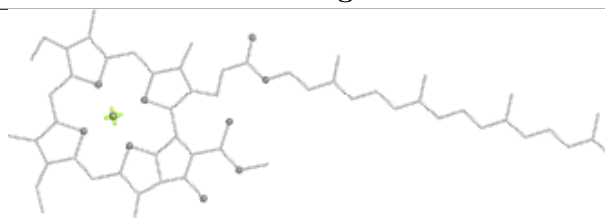
Bond lengths



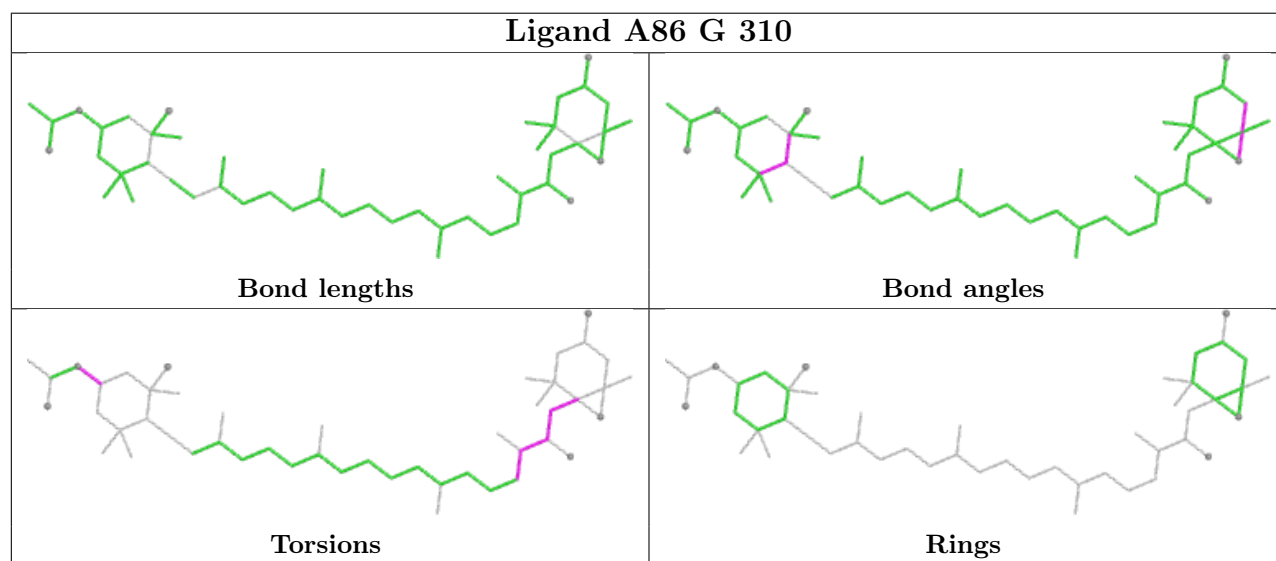
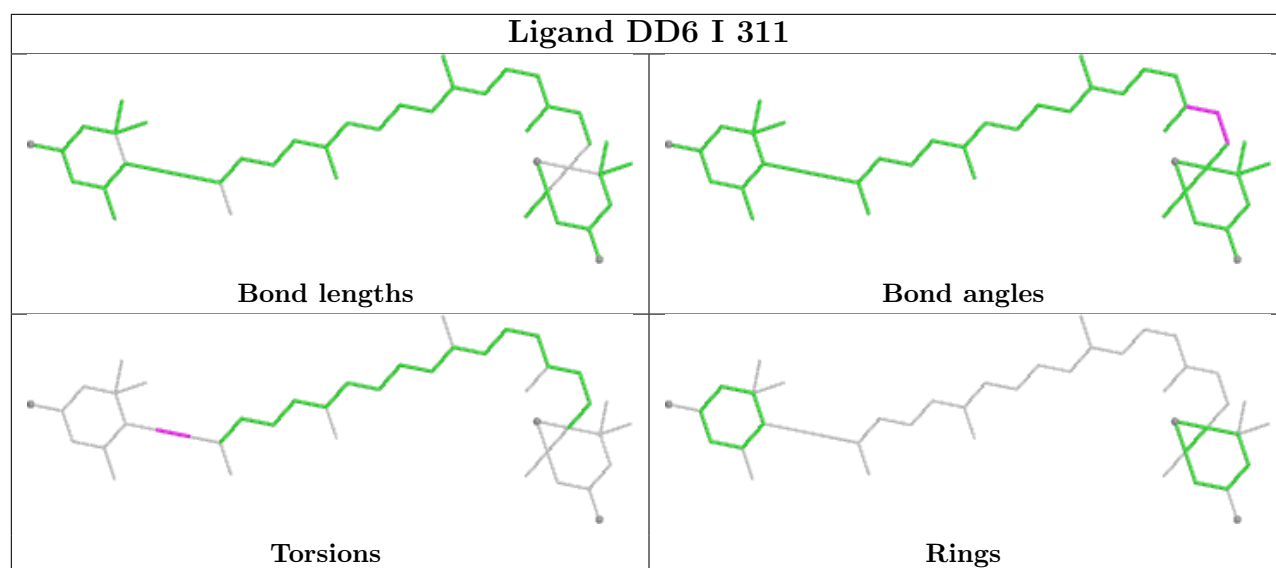
Bond angles

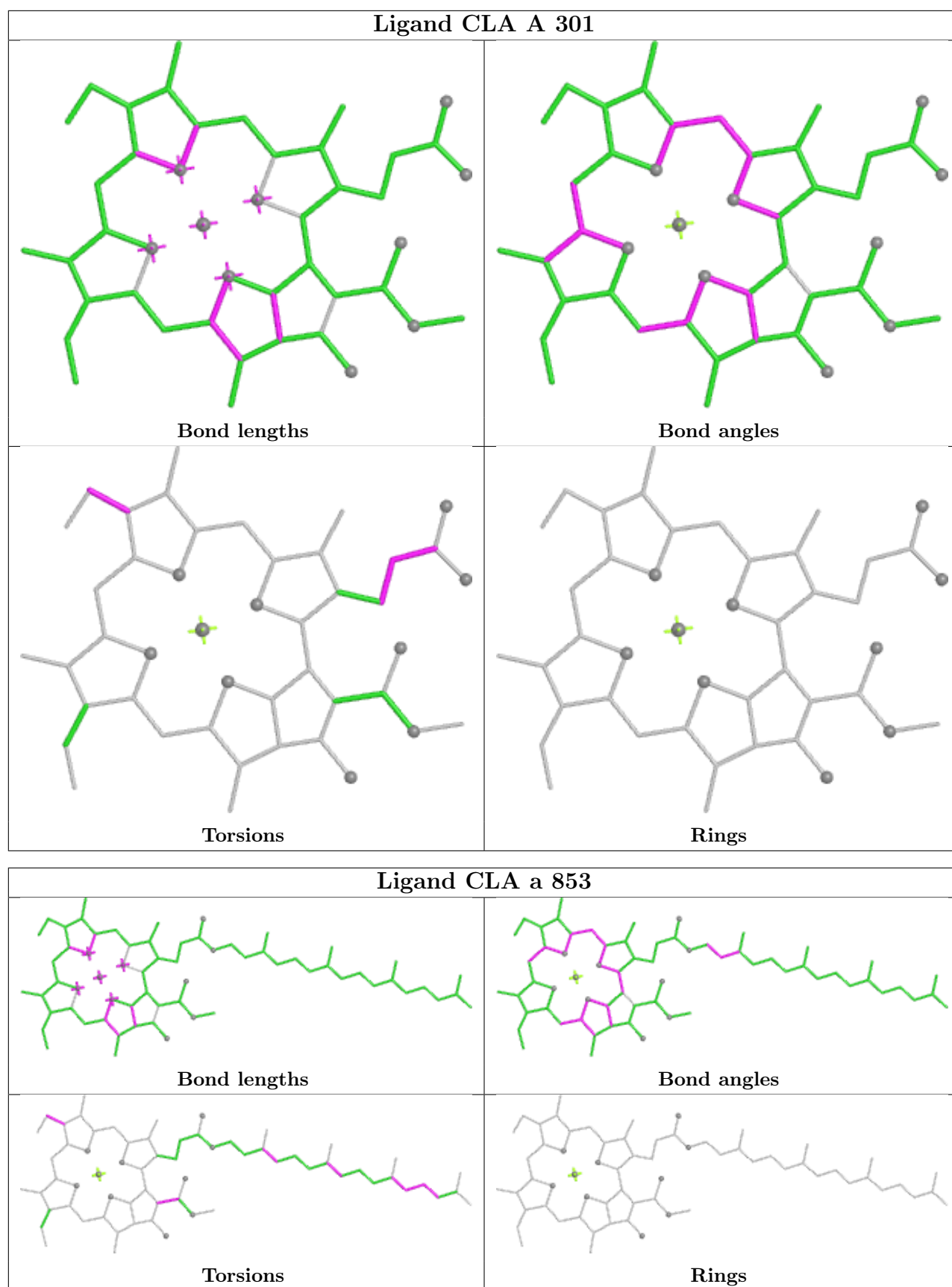


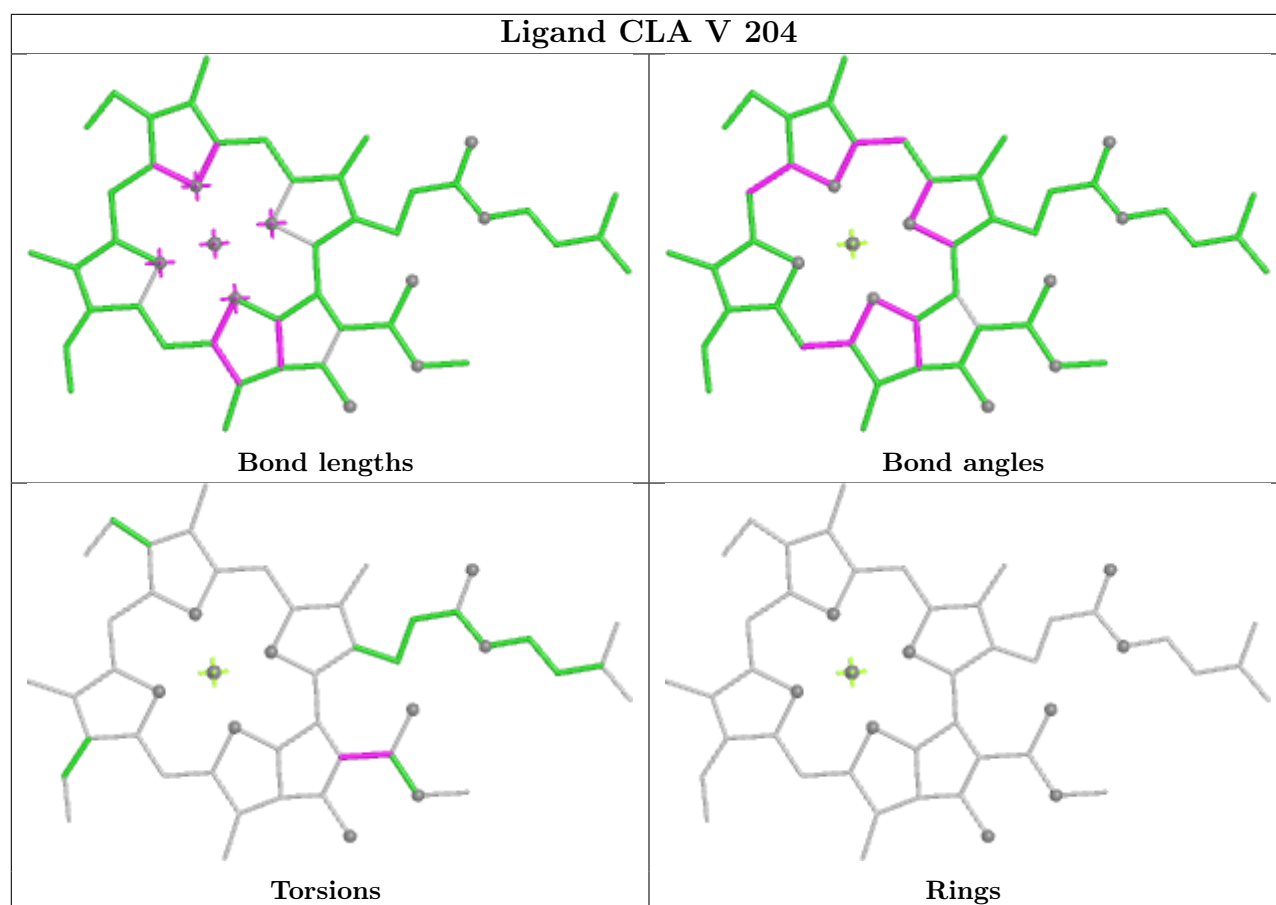
Torsions



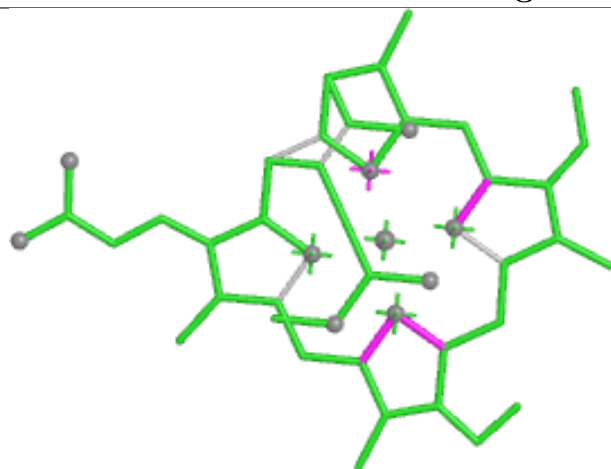
Rings



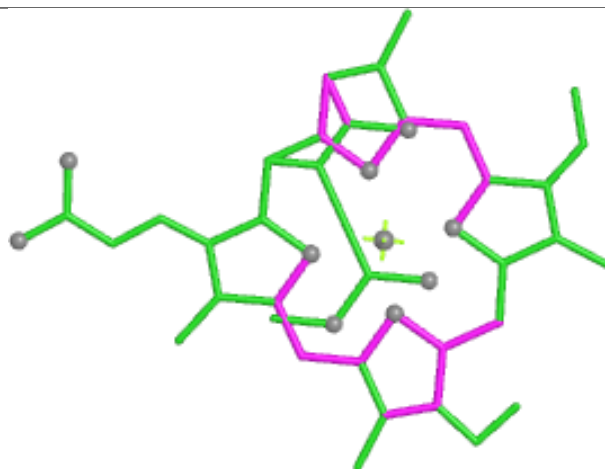




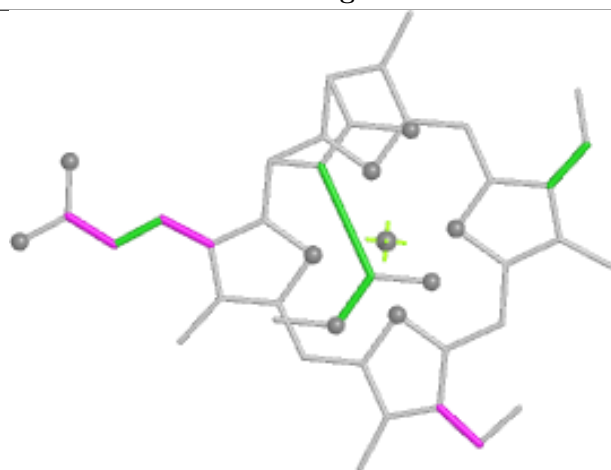
Ligand KC2 O 303



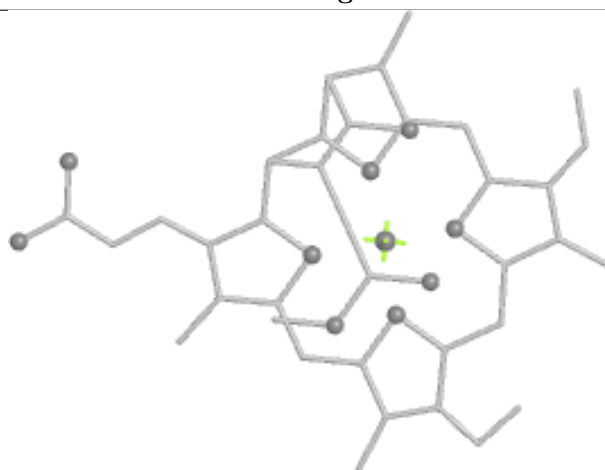
Bond lengths



Bond angles



Torsions

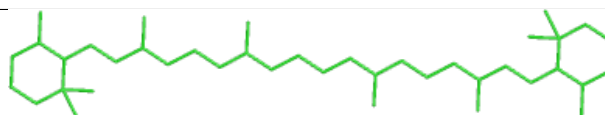


Rings

Ligand BCR b 843



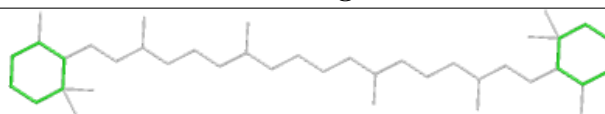
Bond lengths



Bond angles

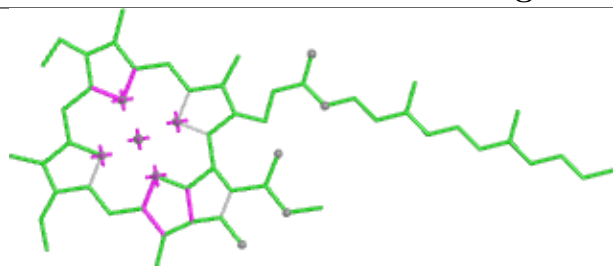


Torsions

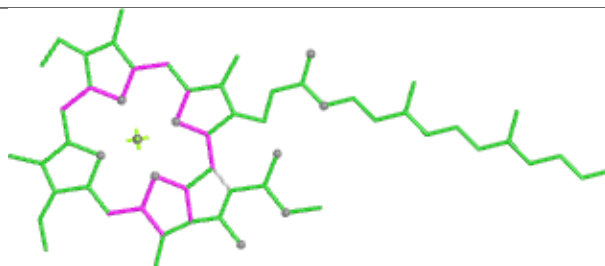


Rings

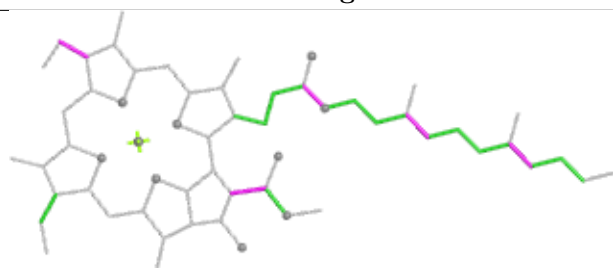
Ligand CLA E 309



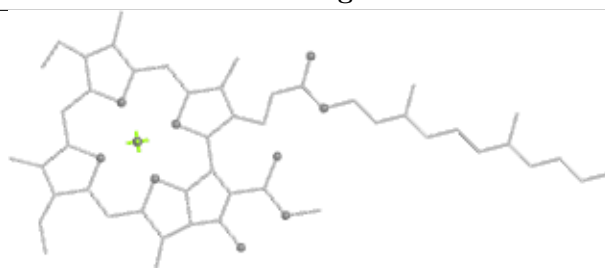
Bond lengths



Bond angles

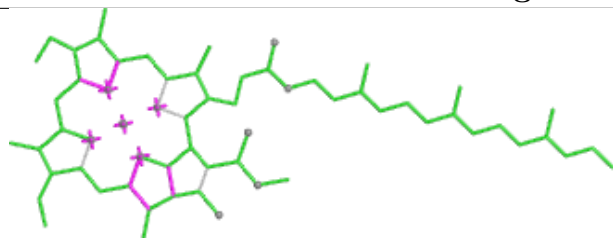


Torsions

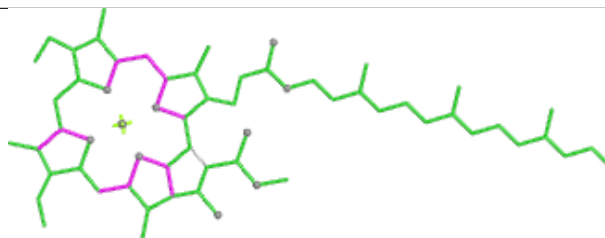


Rings

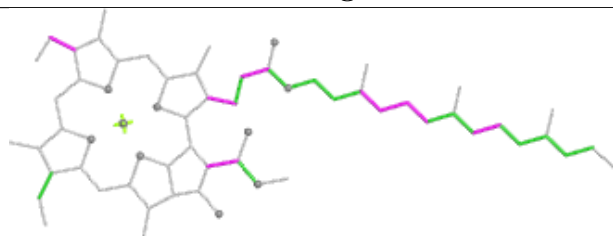
Ligand CLA A 303



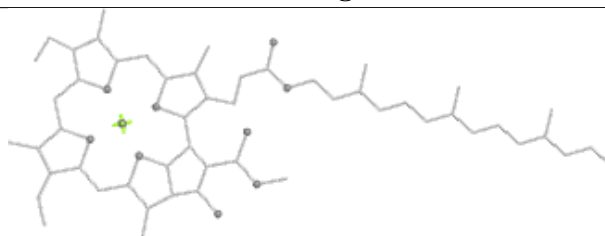
Bond lengths



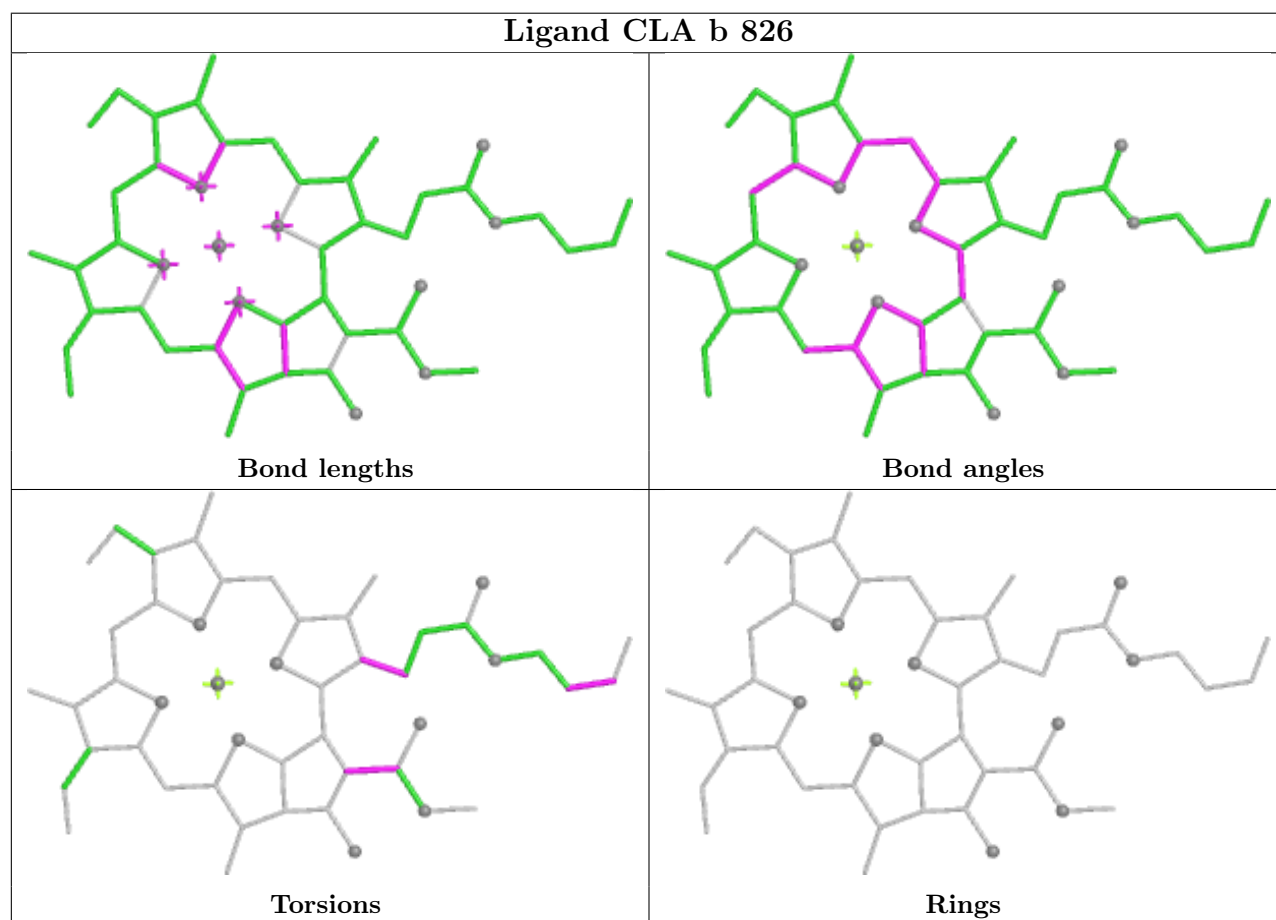
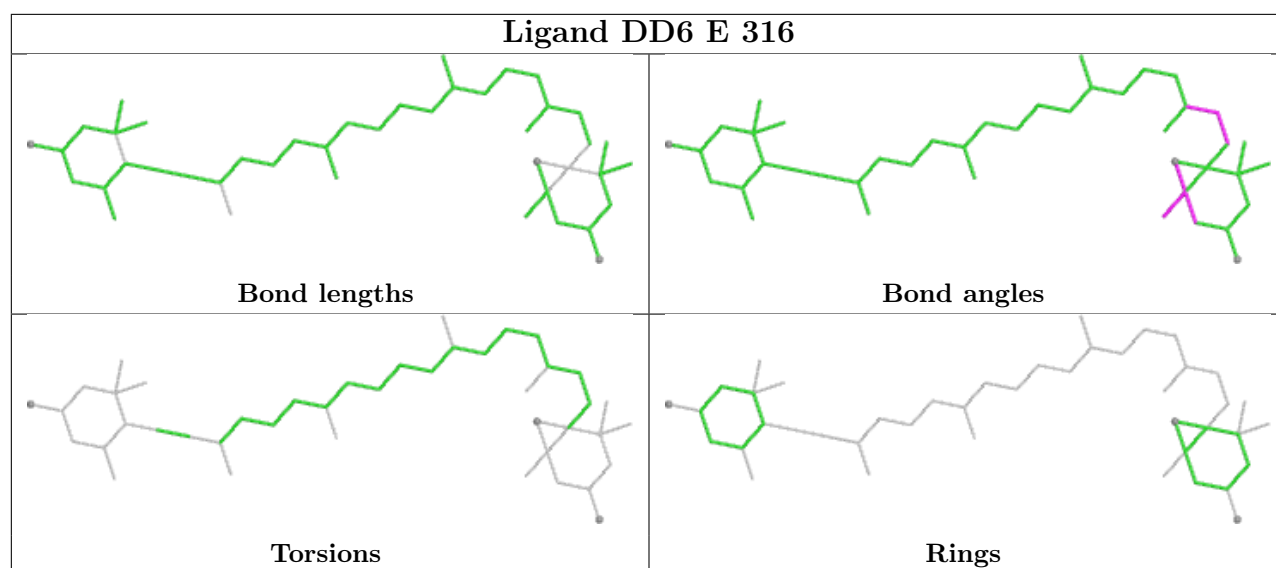
Bond angles

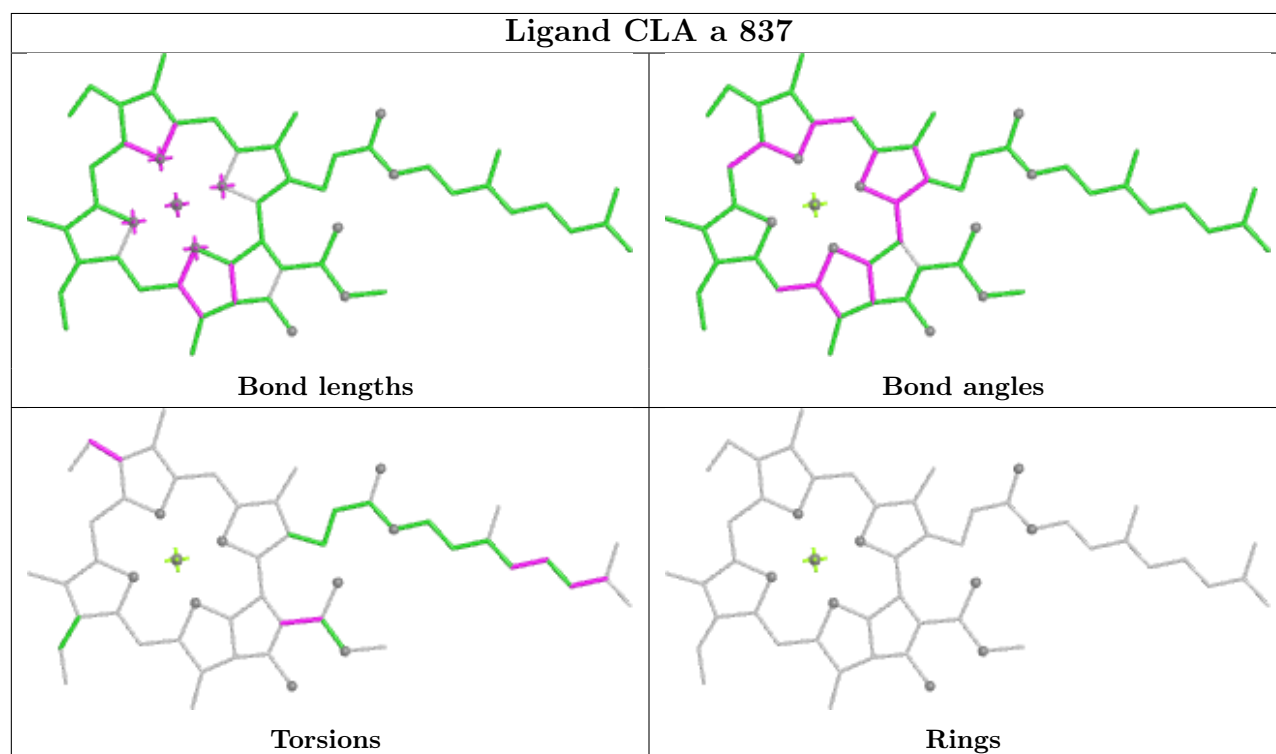
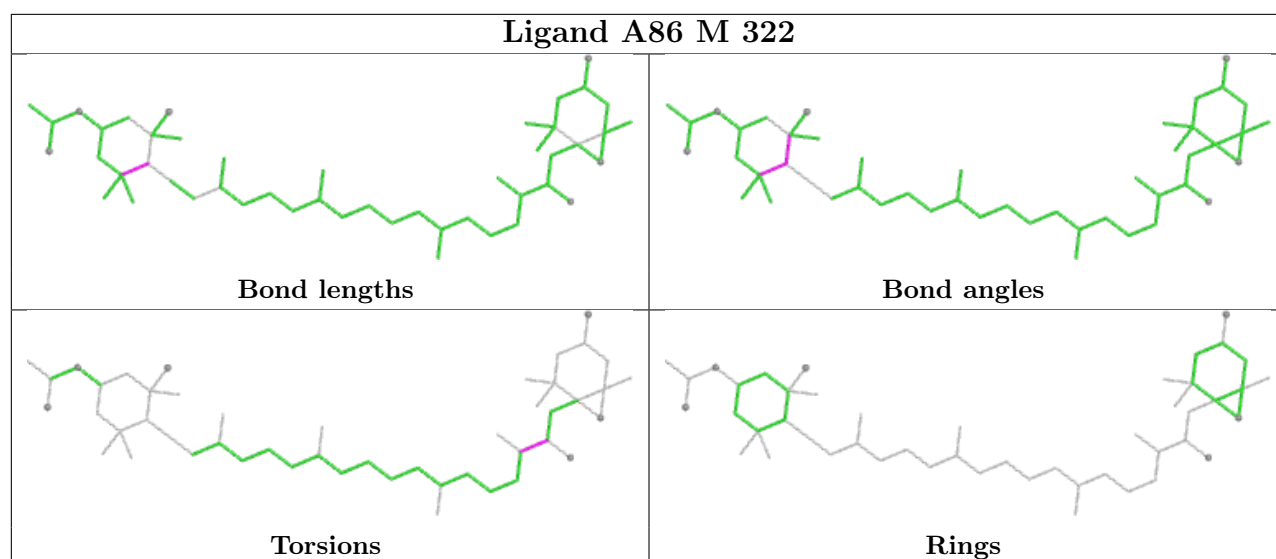


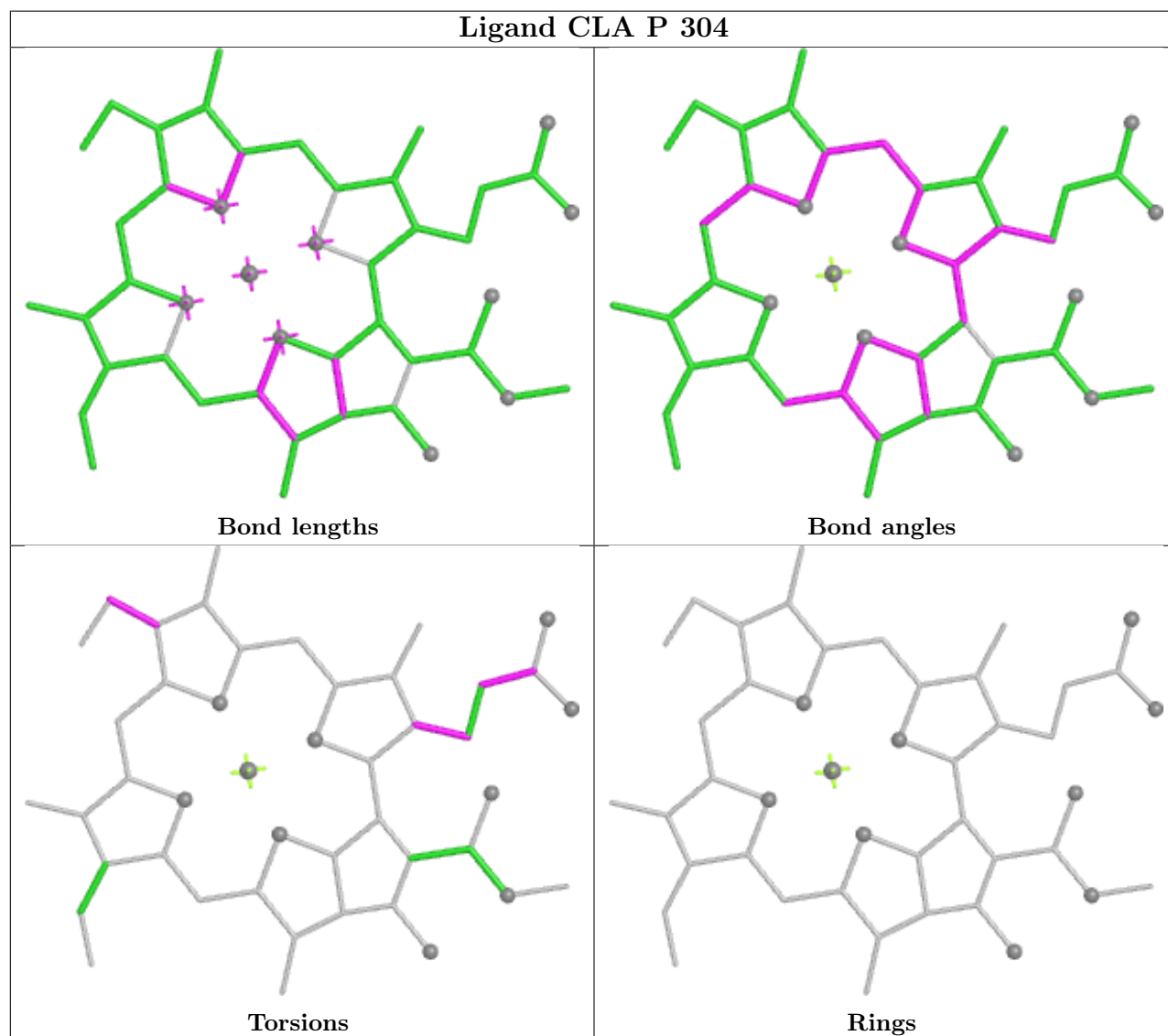
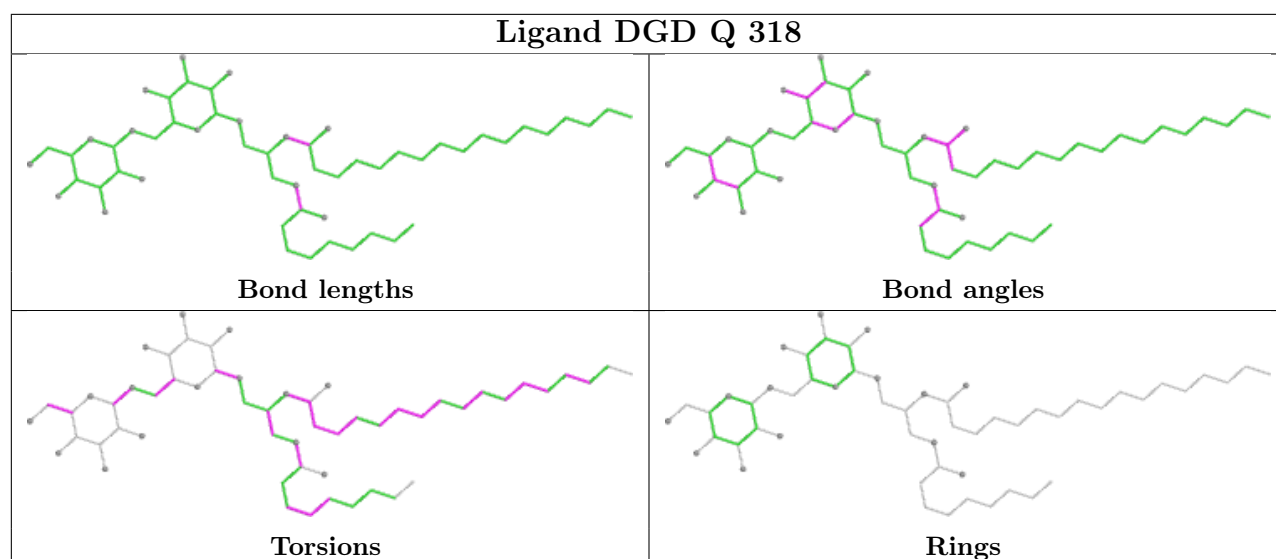
Torsions



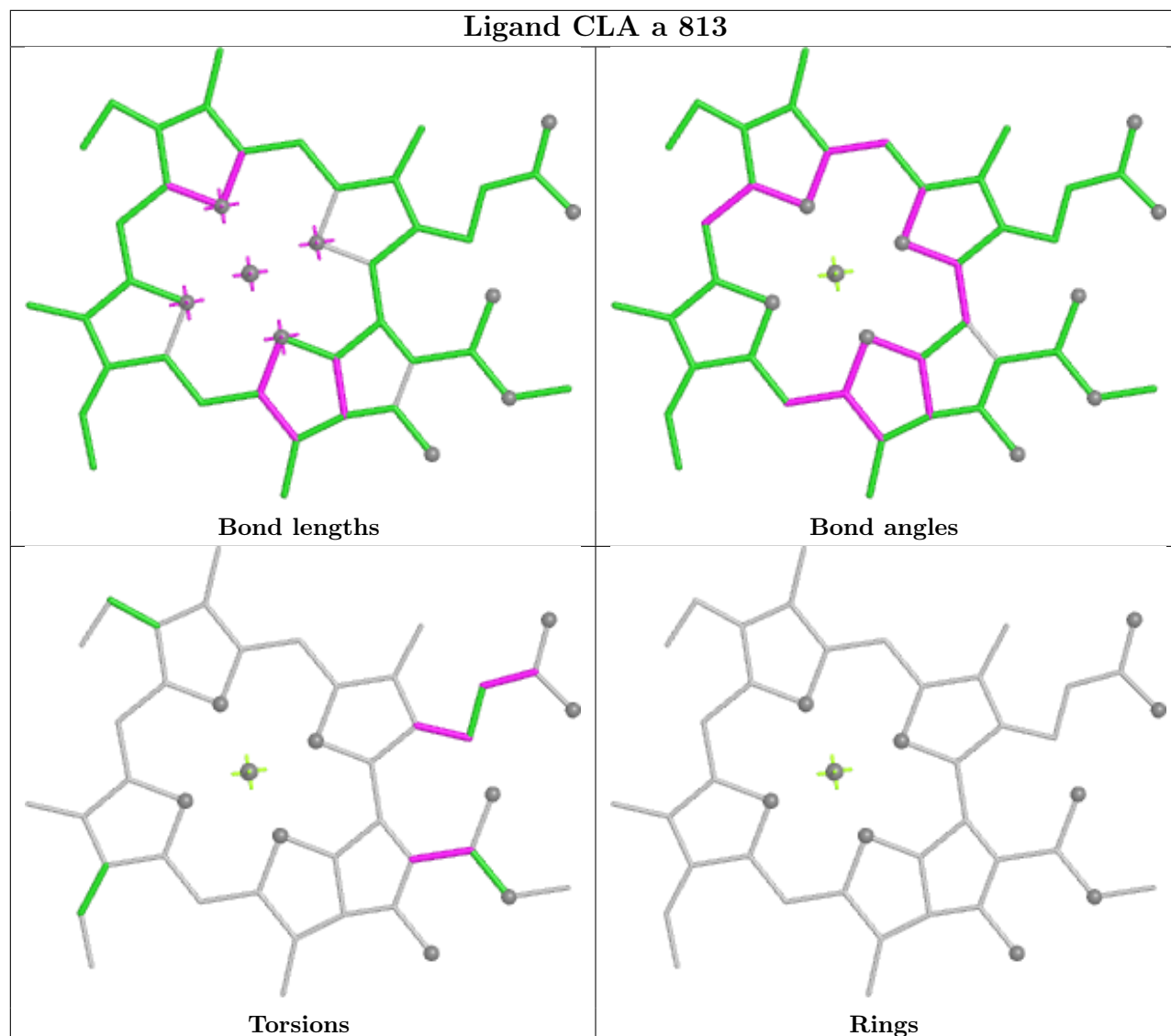
Rings



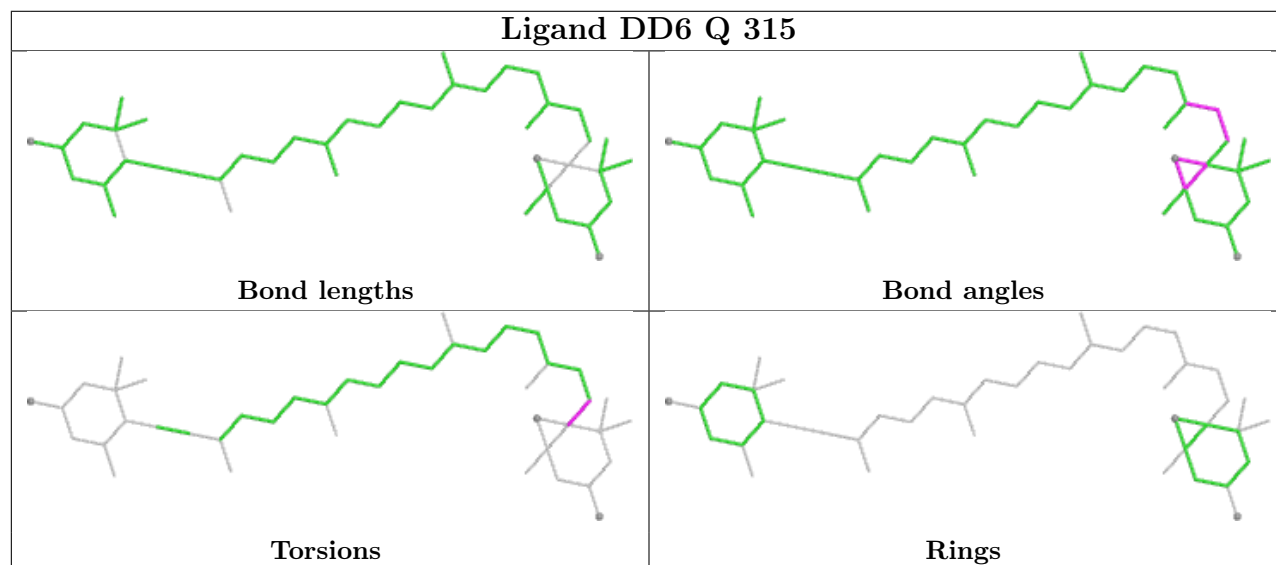


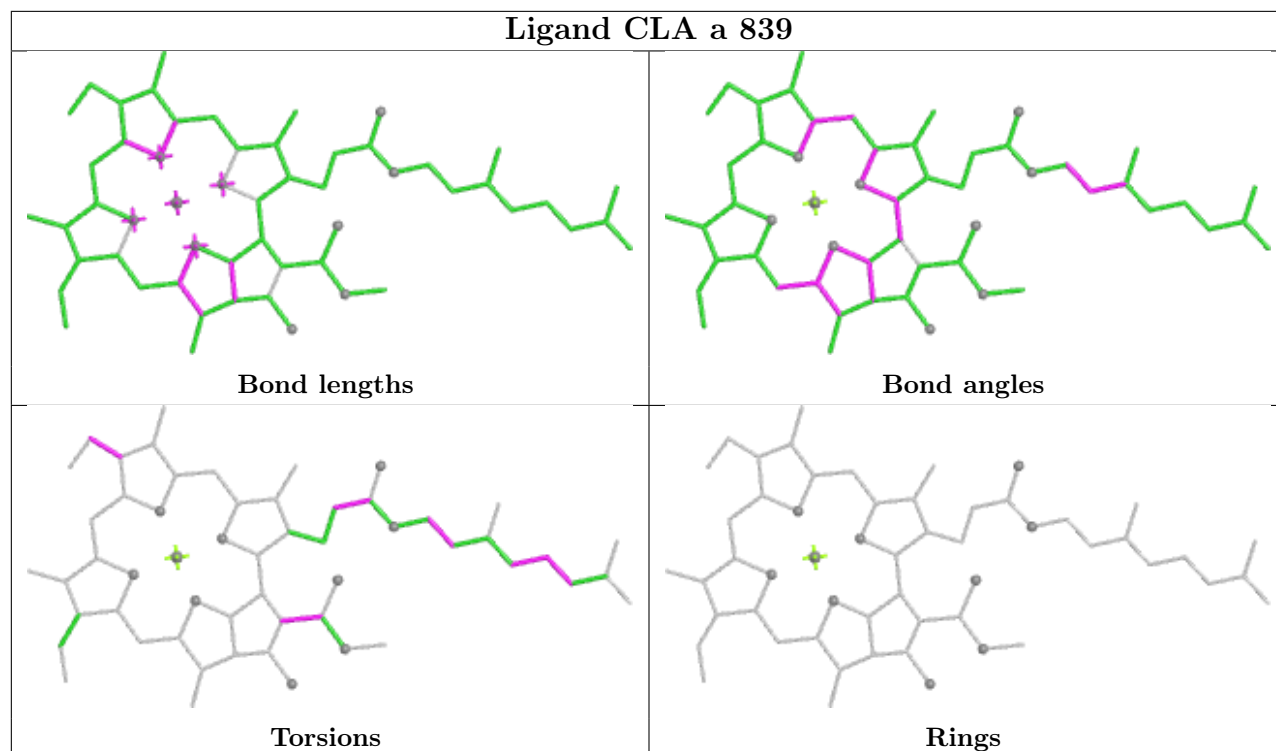
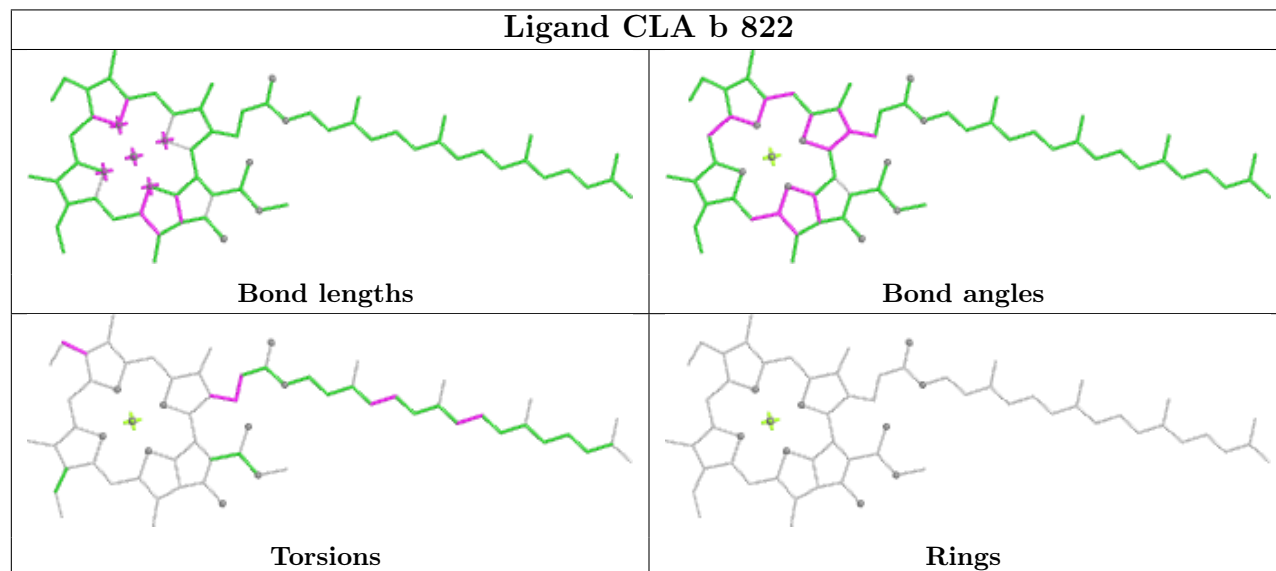


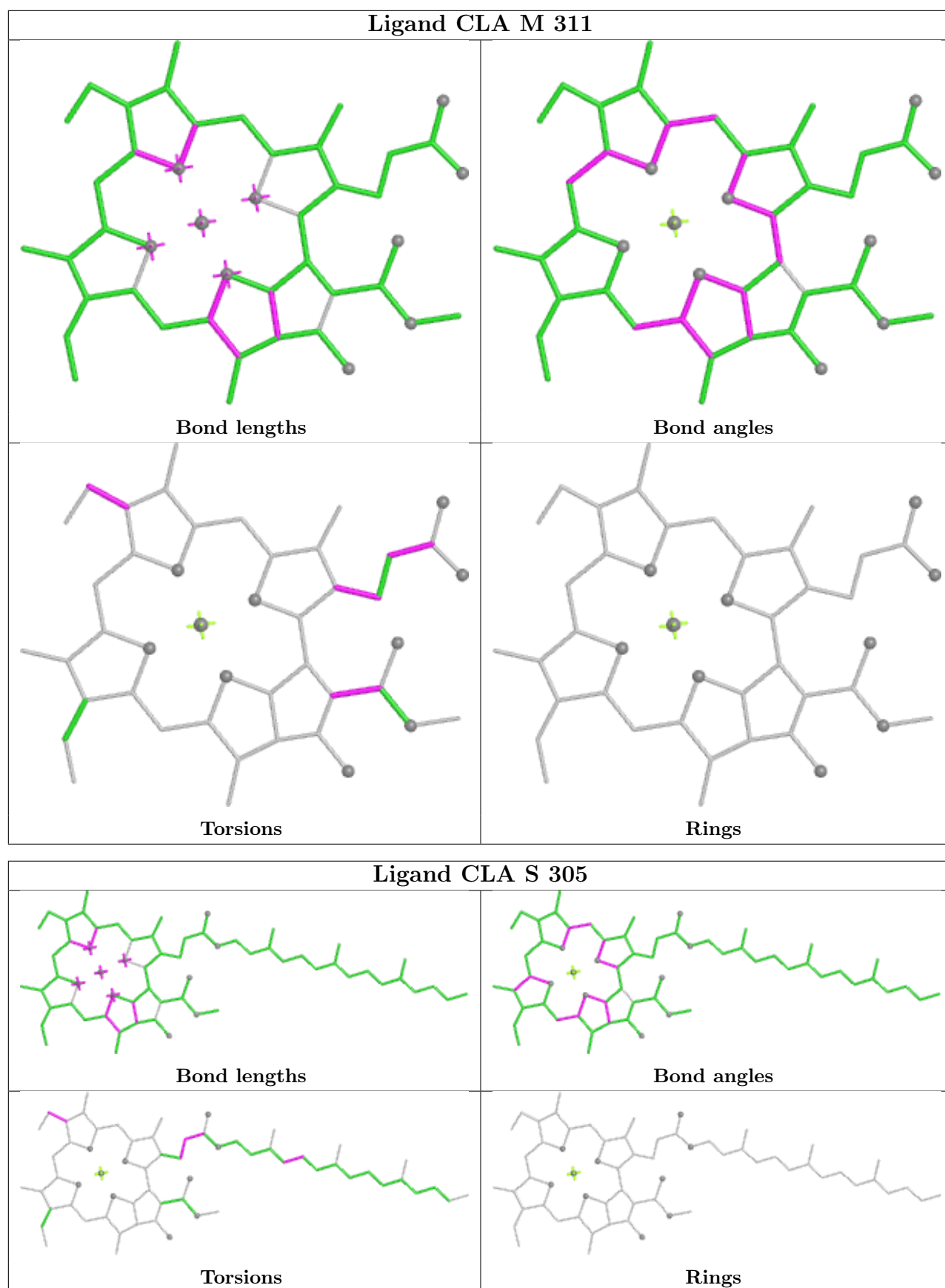
Ligand CLA a 813



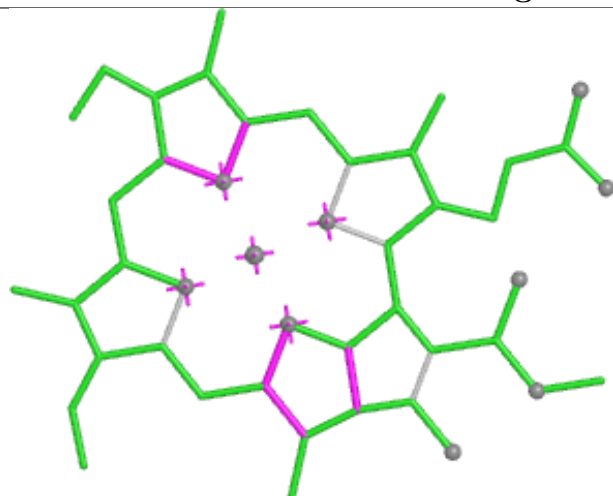
Ligand DD6 Q 315



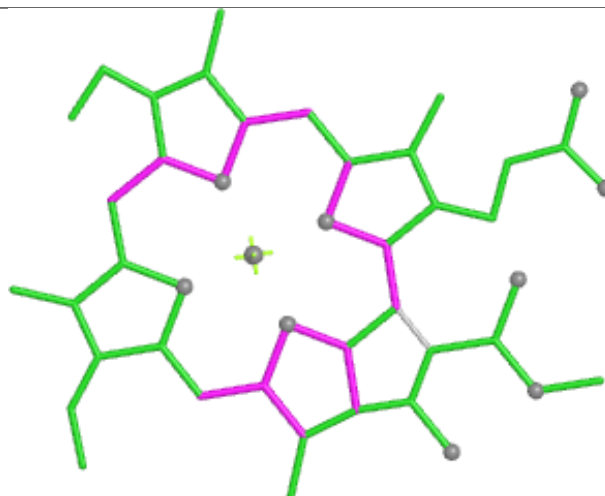
Ligand CLA a 839**Ligand CLA b 822**



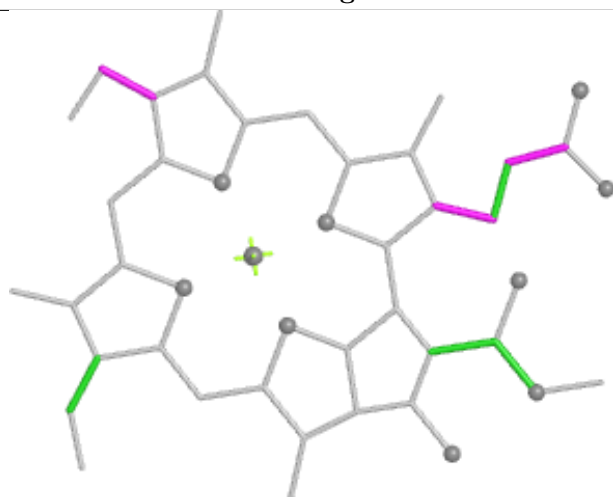
Ligand CLA T 302



Bond lengths



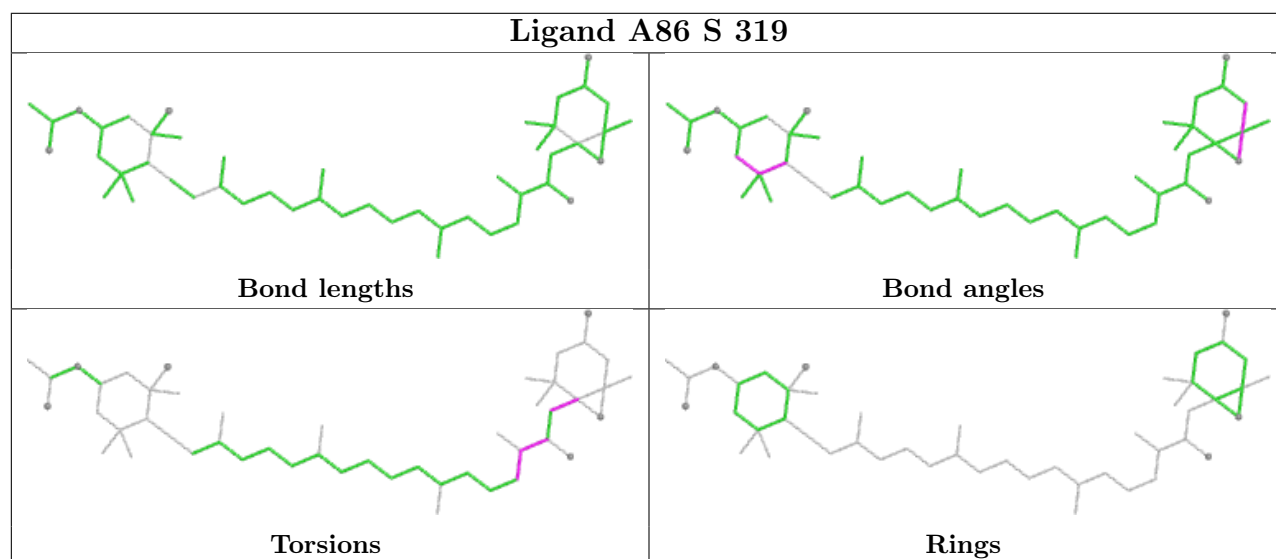
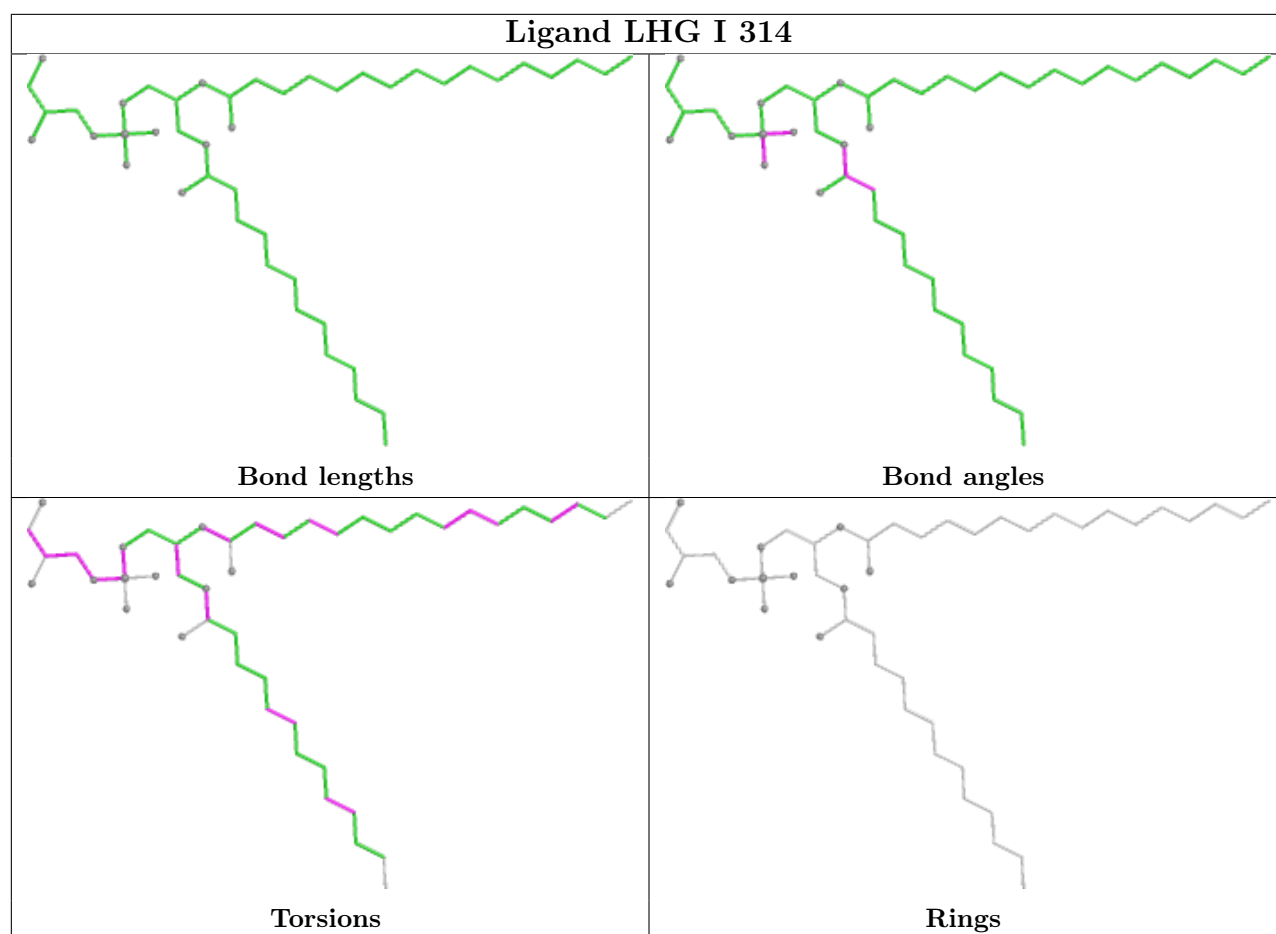
Bond angles

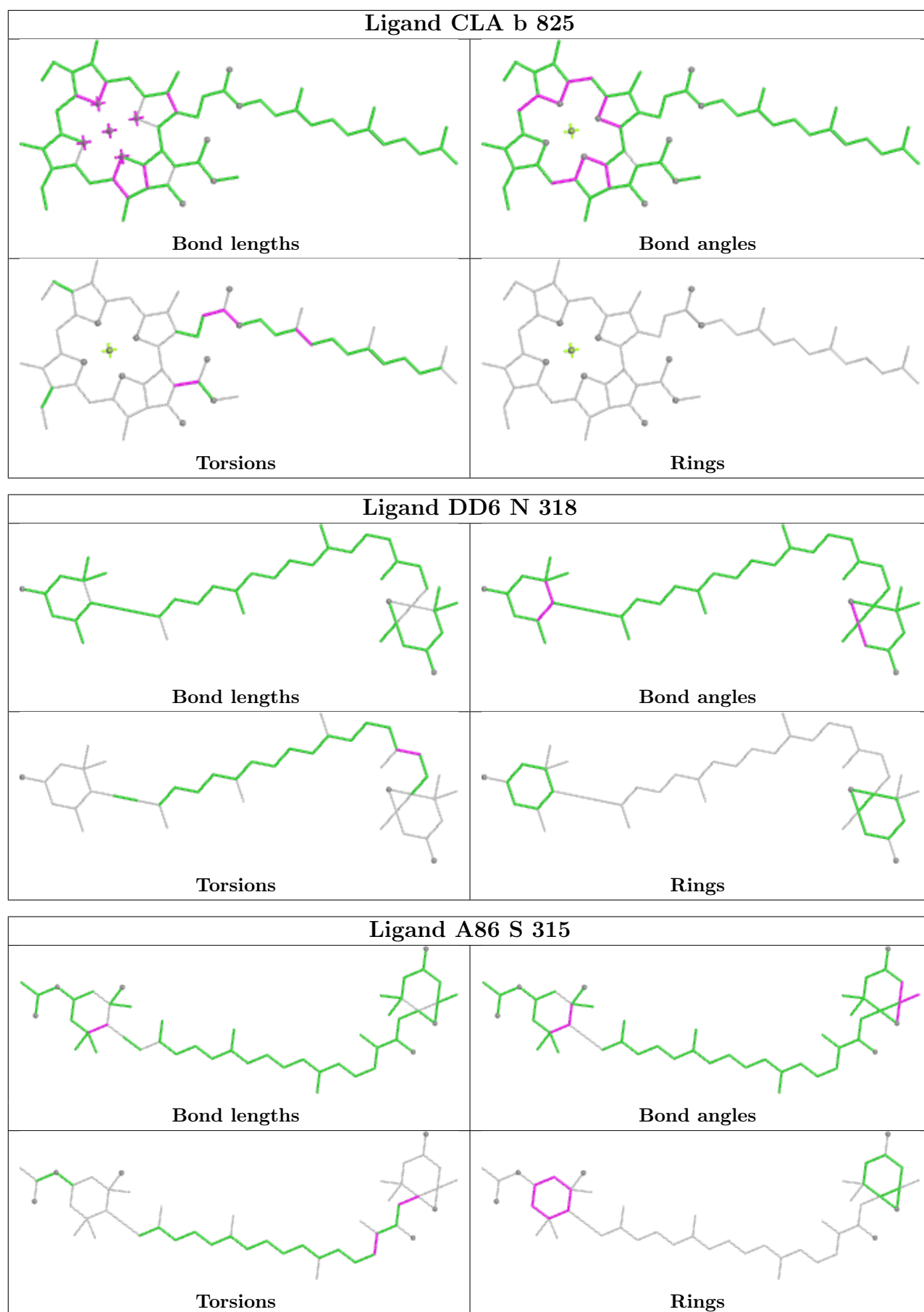


Torsions

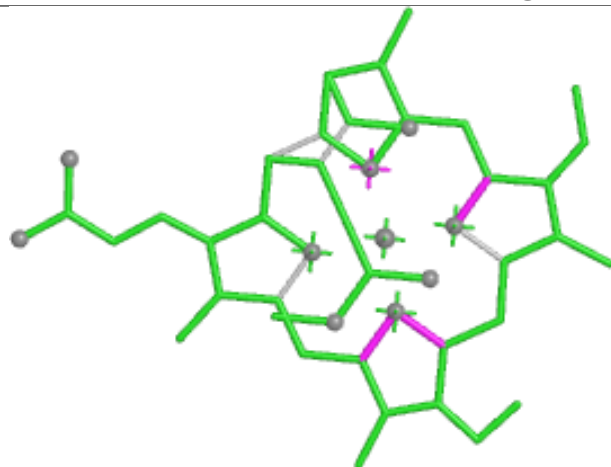


Rings

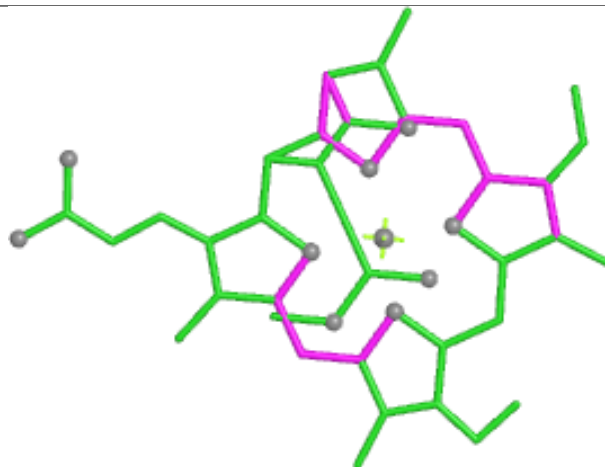




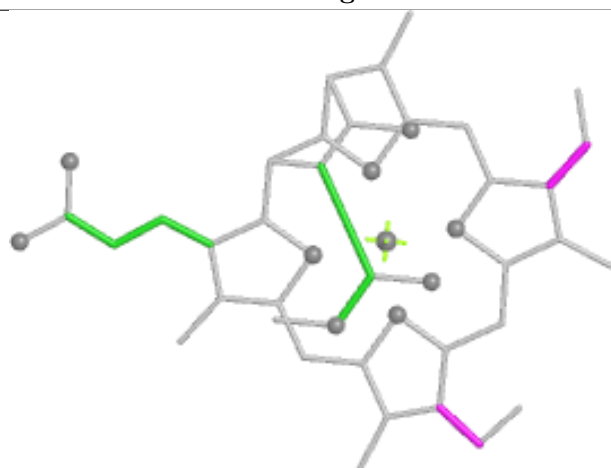
Ligand KC2 S 312



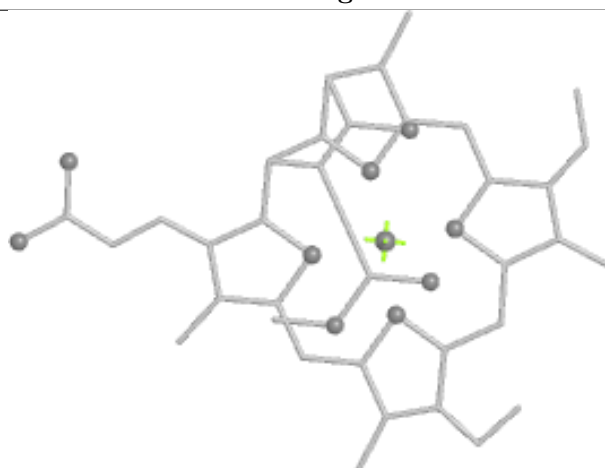
Bond lengths



Bond angles

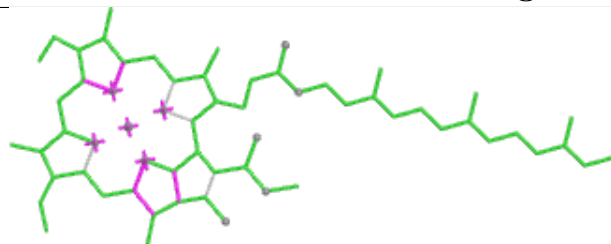


Torsions

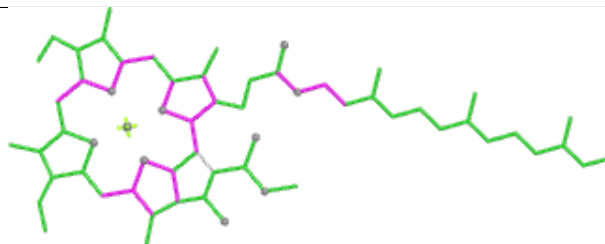


Rings

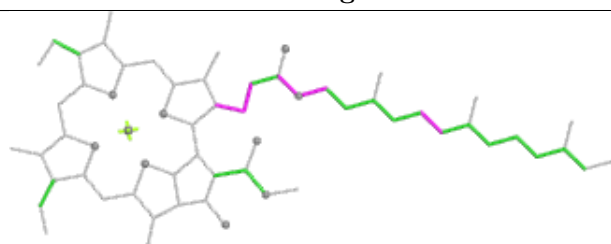
Ligand CLA b 830



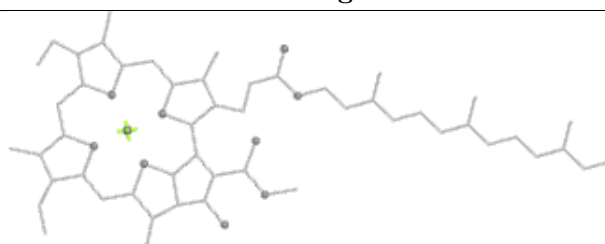
Bond lengths



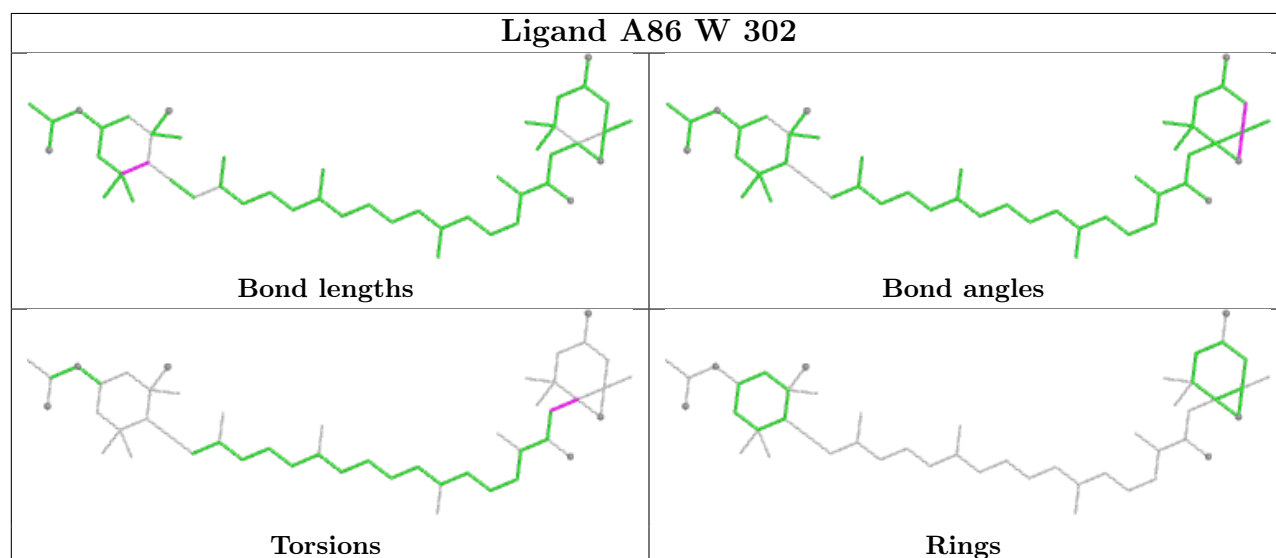
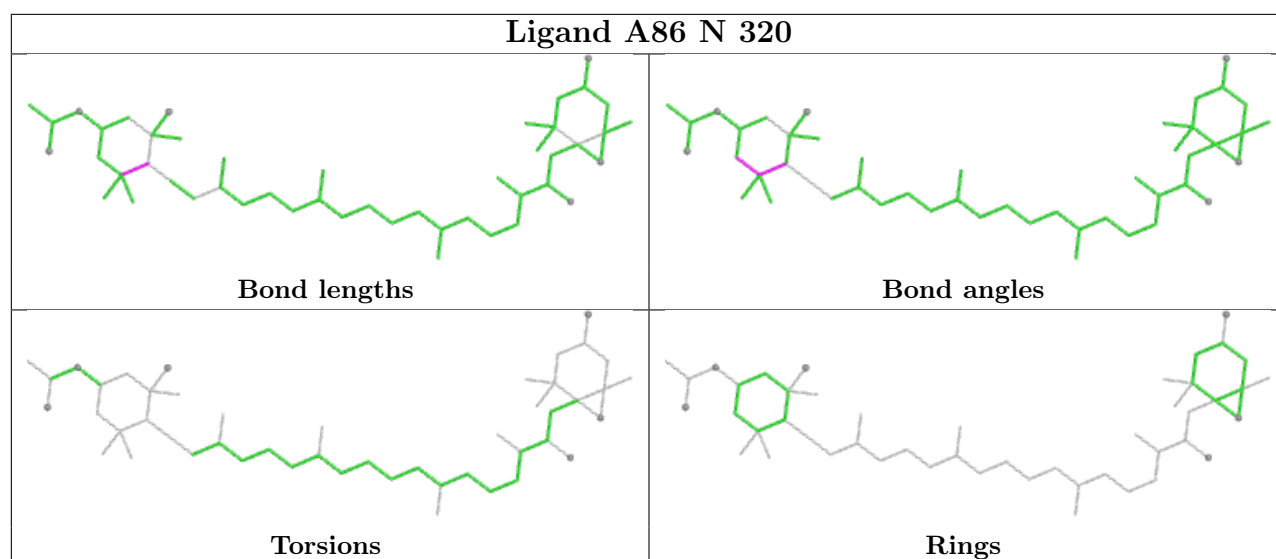
Bond angles



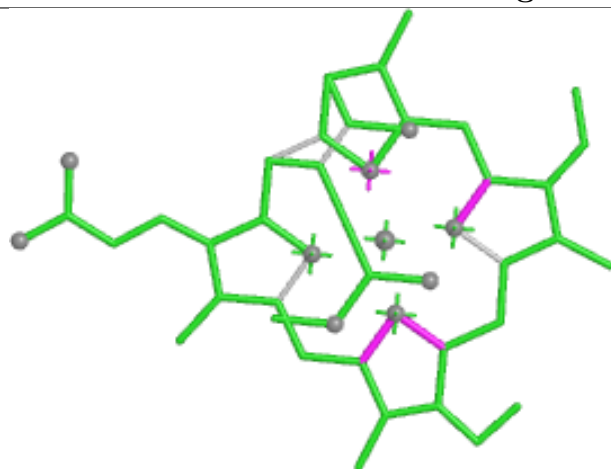
Torsions



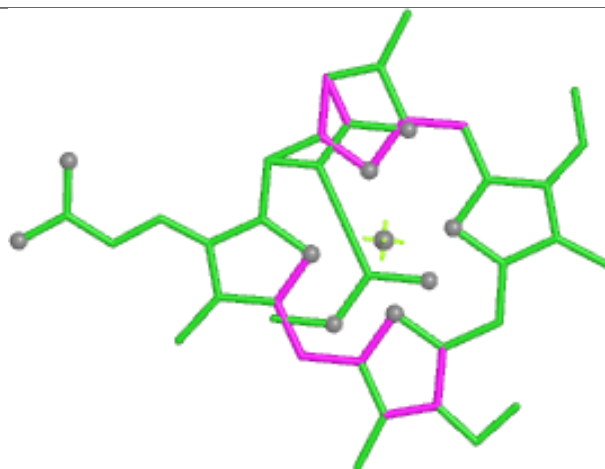
Rings



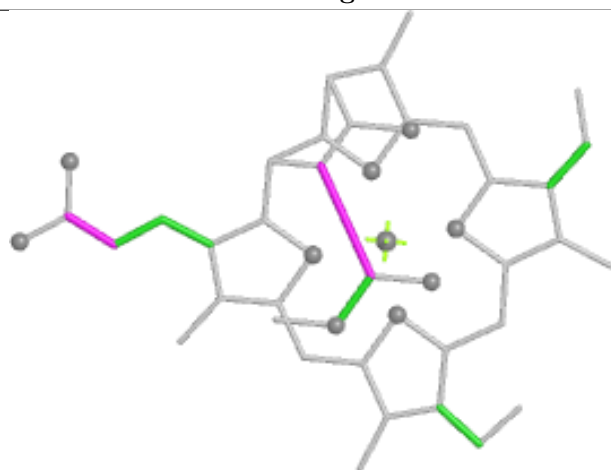
Ligand KC2 P 303



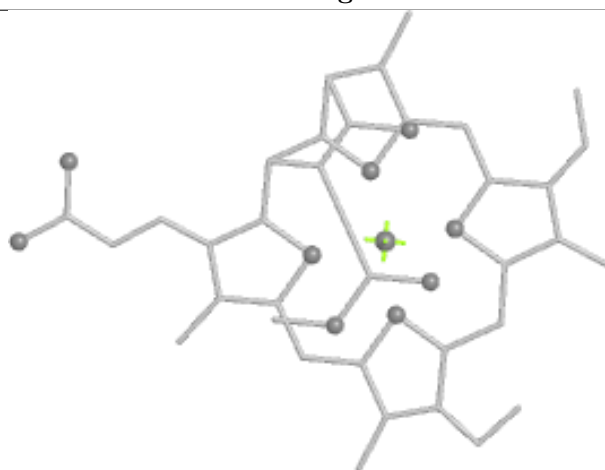
Bond lengths



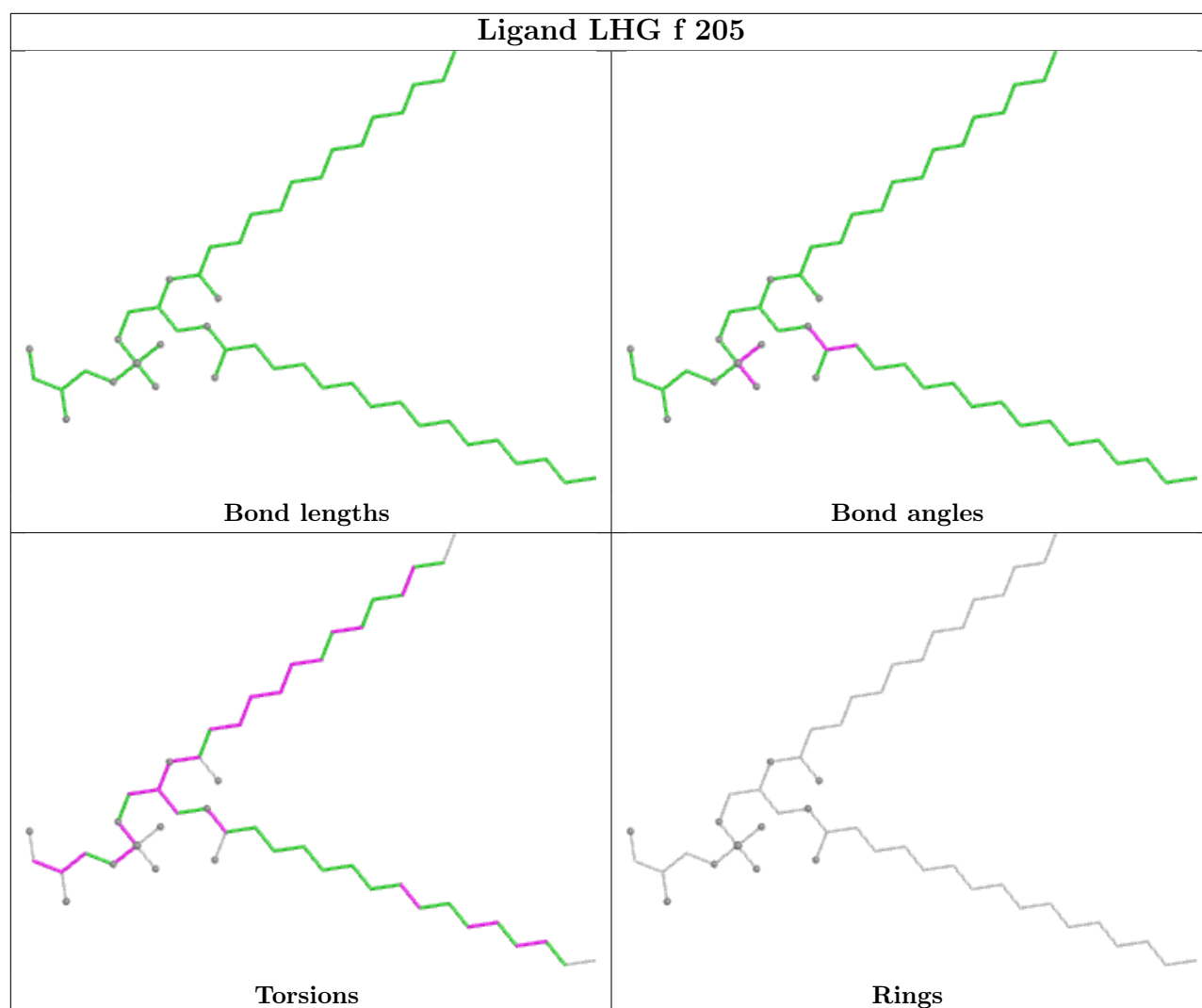
Bond angles



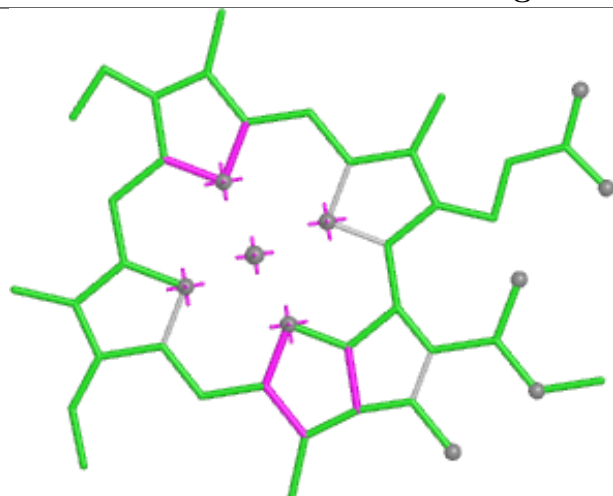
Torsions



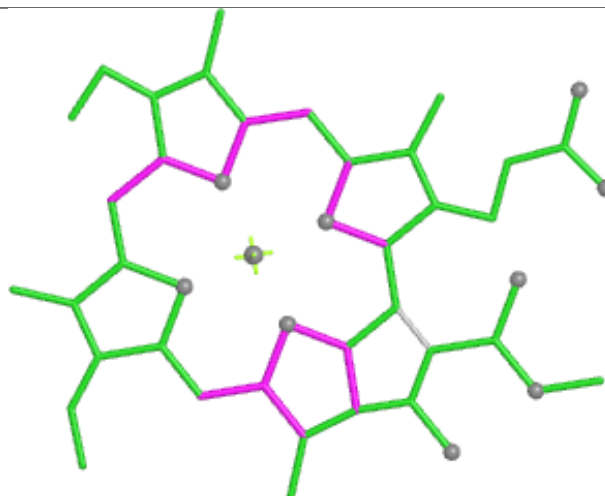
Rings



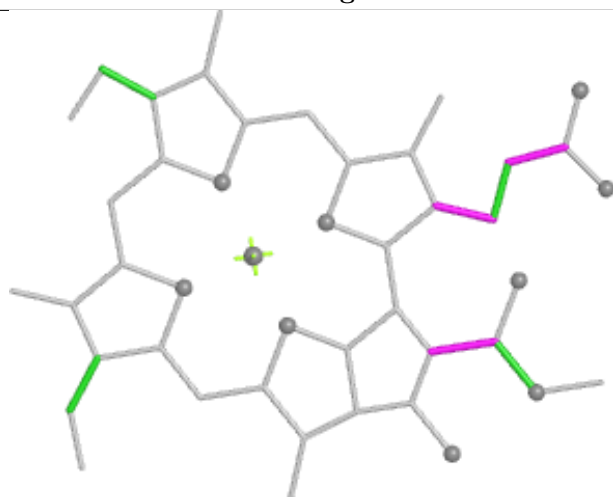
Ligand CLA R 306



Bond lengths



Bond angles

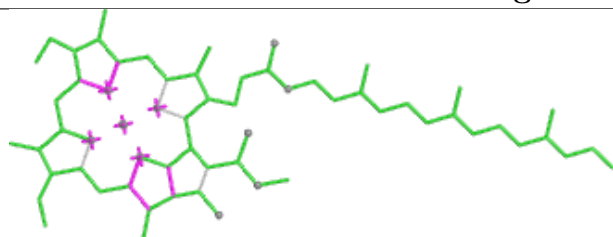


Torsions

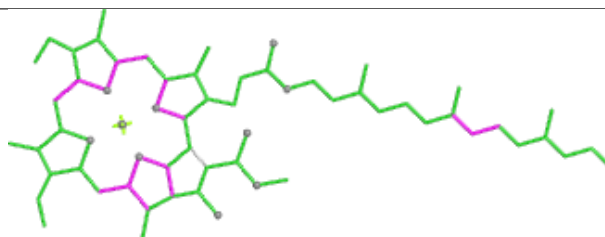


Rings

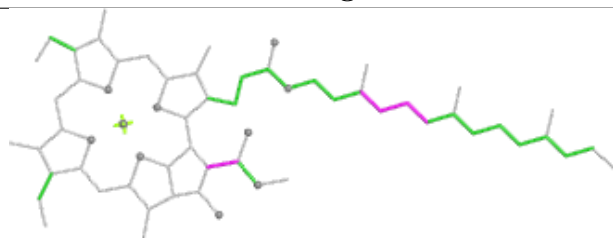
Ligand CLA O 309



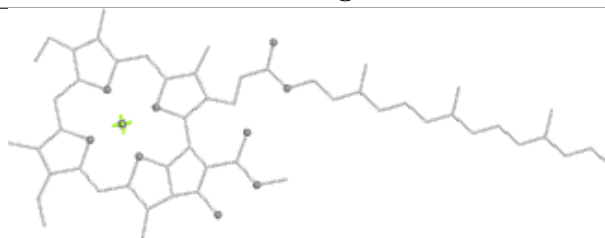
Bond lengths



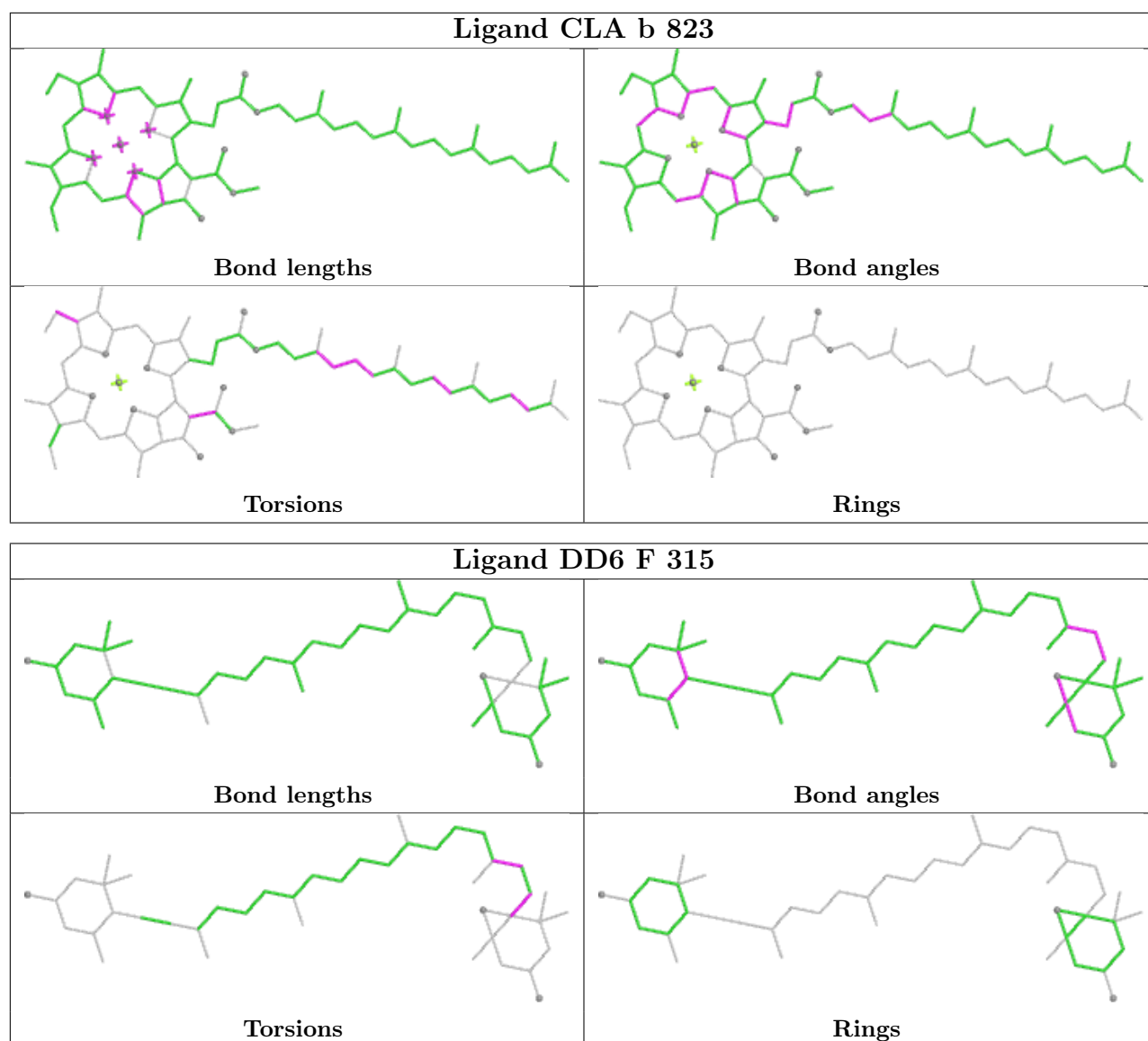
Bond angles



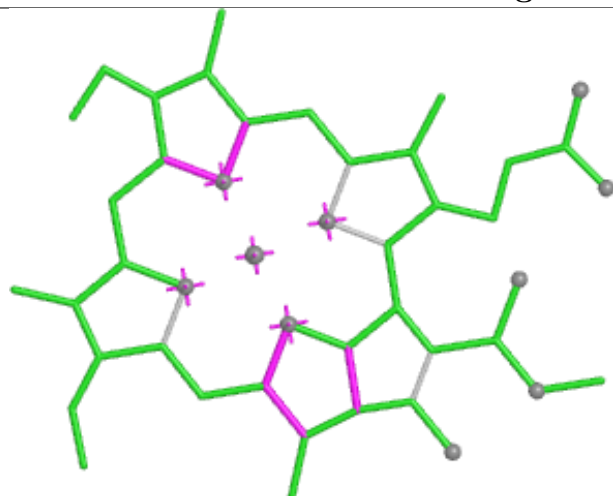
Torsions



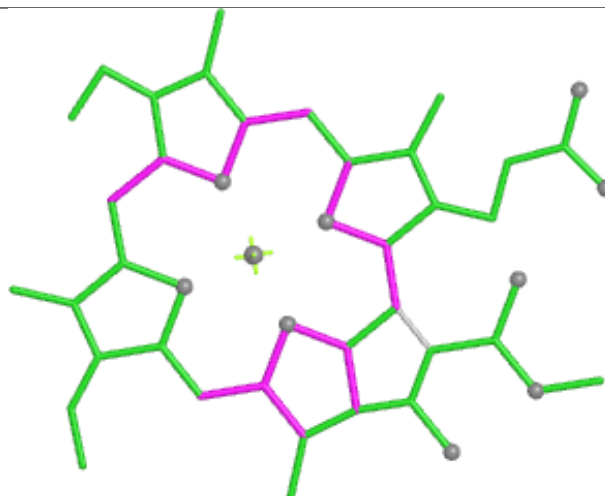
Rings



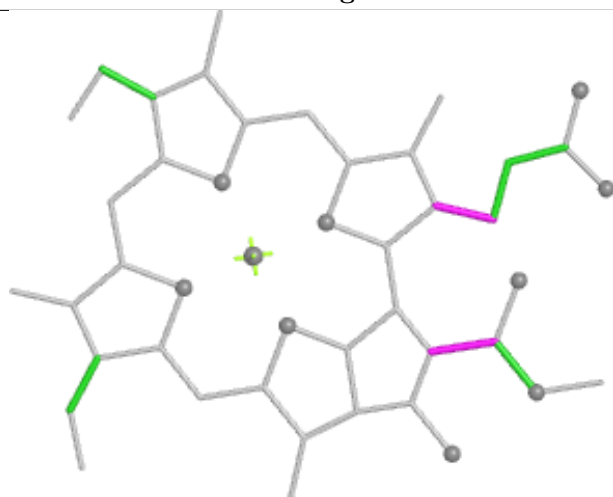
Ligand CLA E 311



Bond lengths



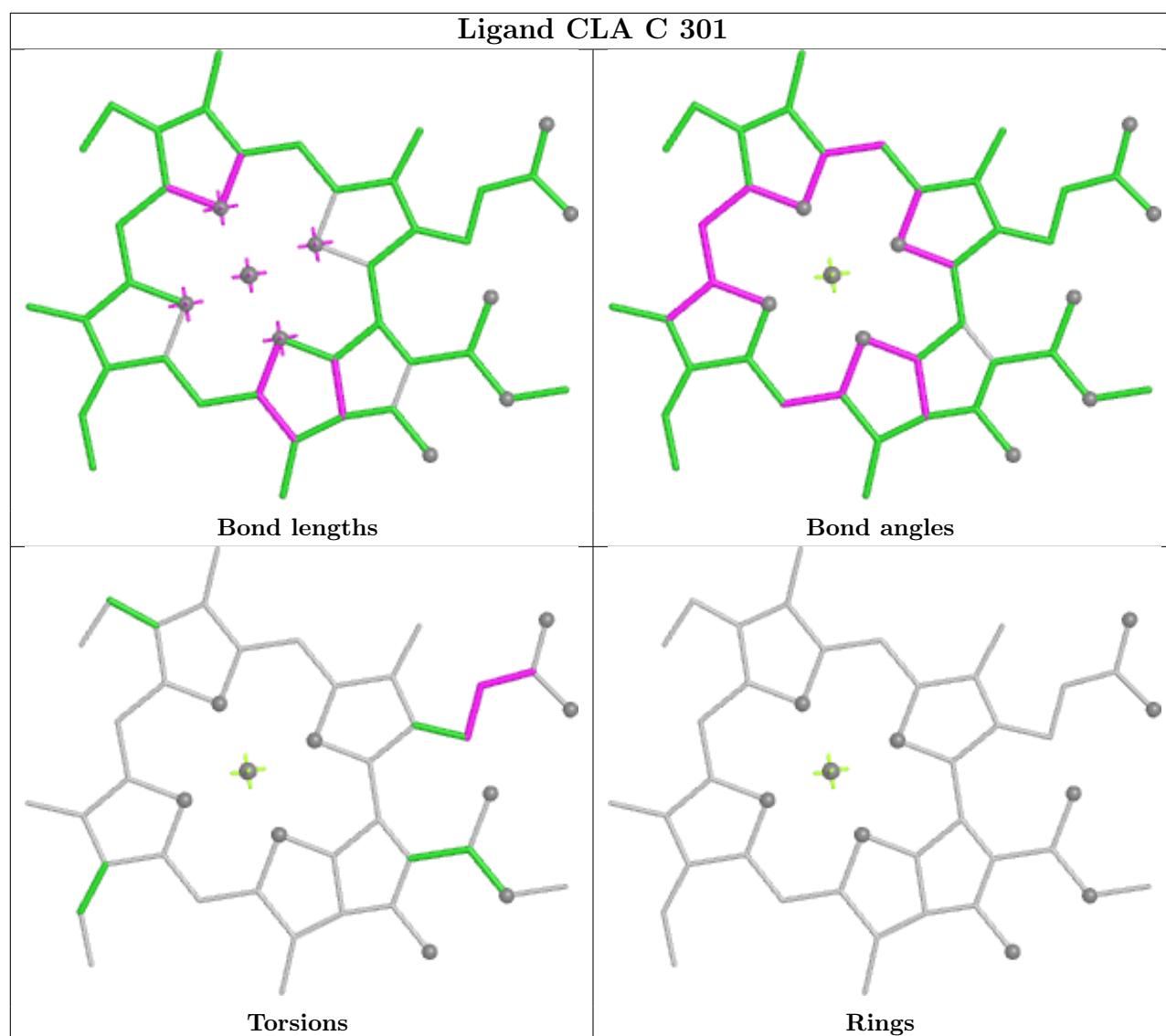
Bond angles

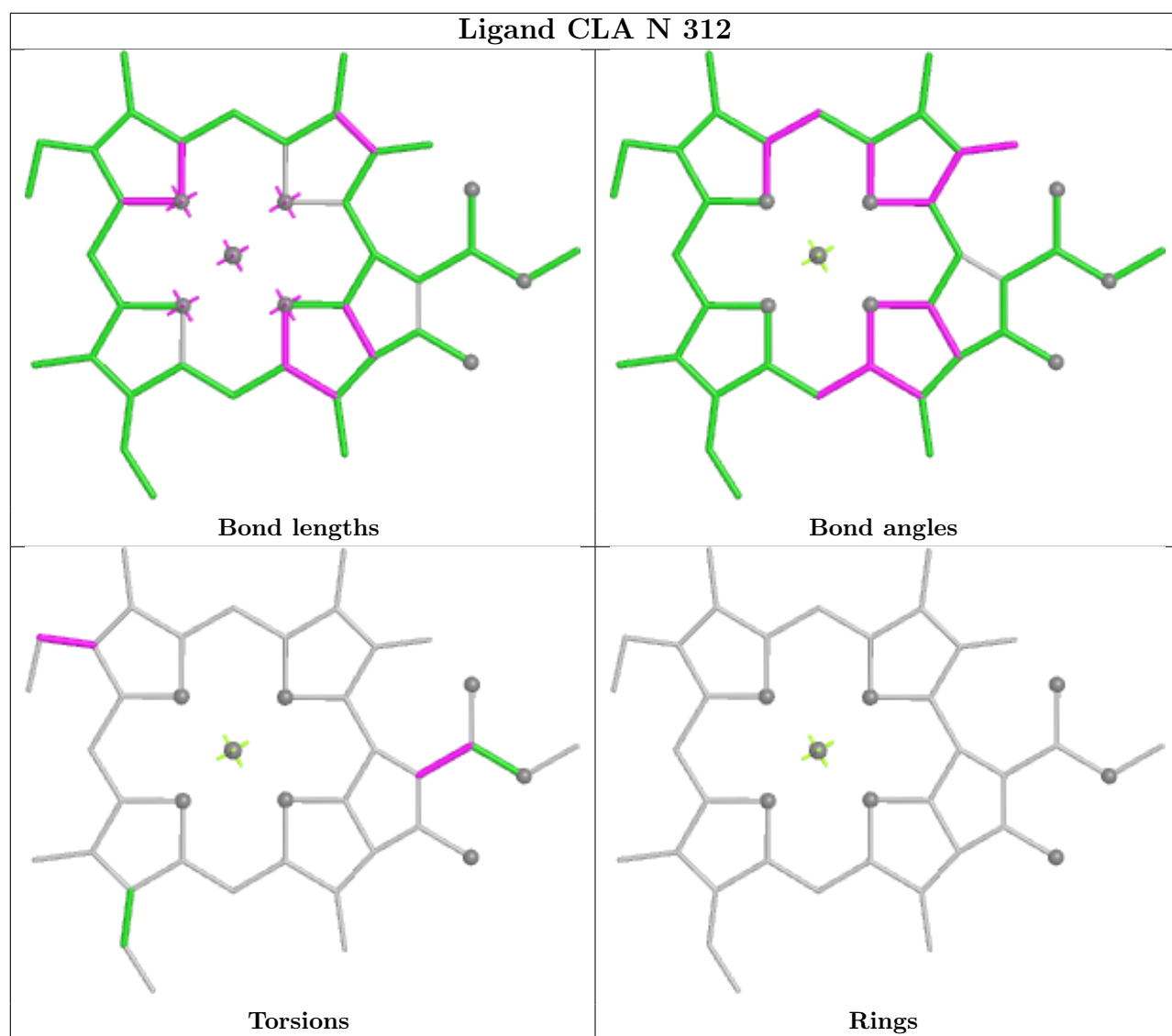


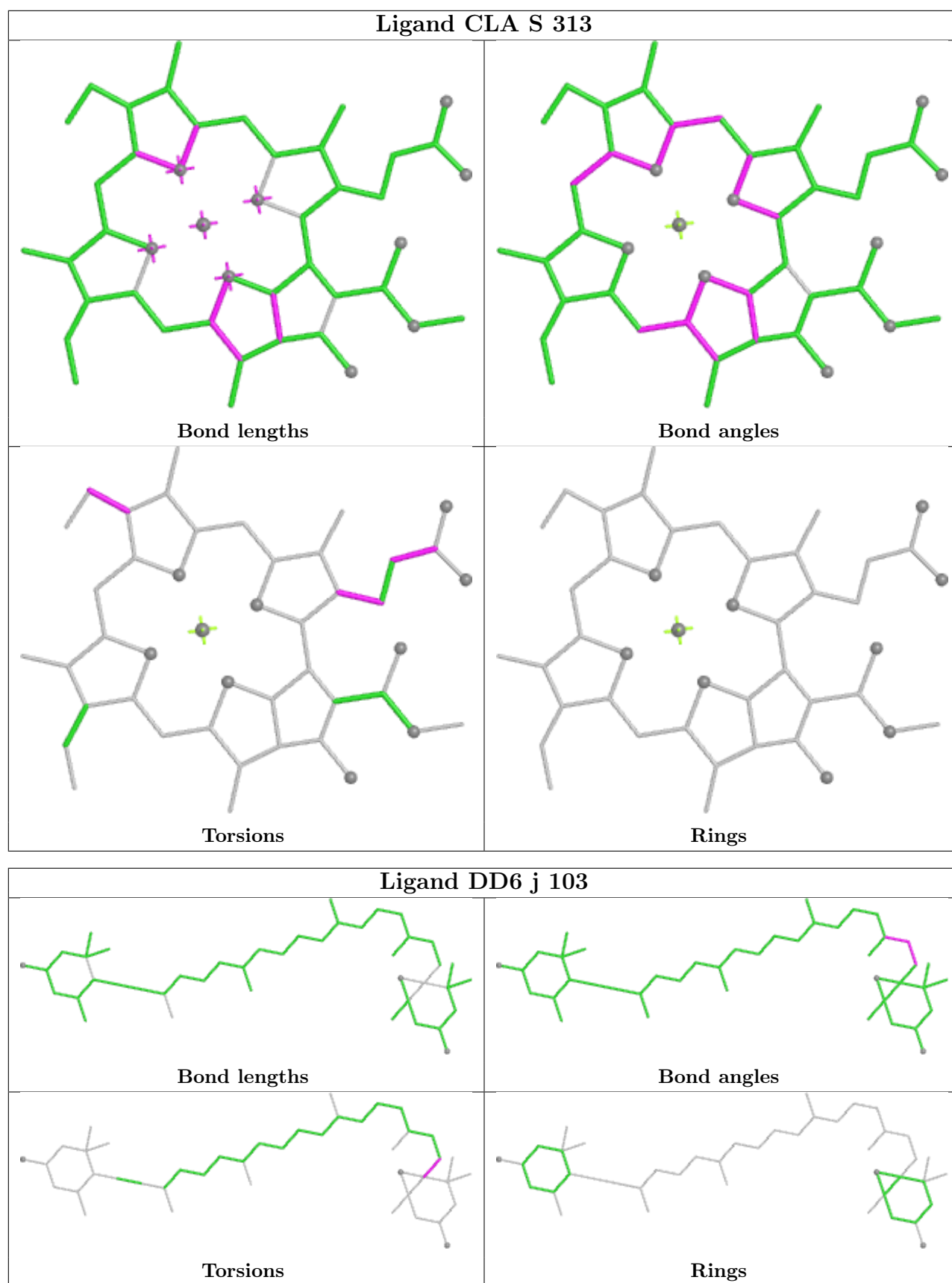
Torsions



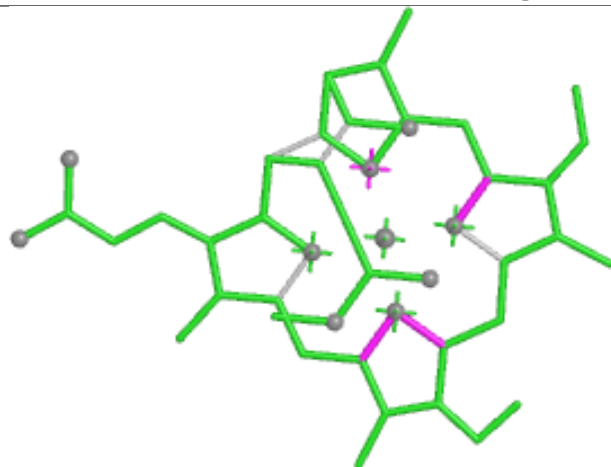
Rings



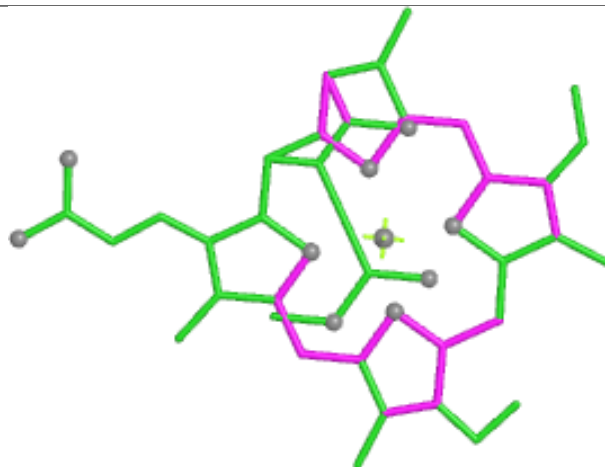




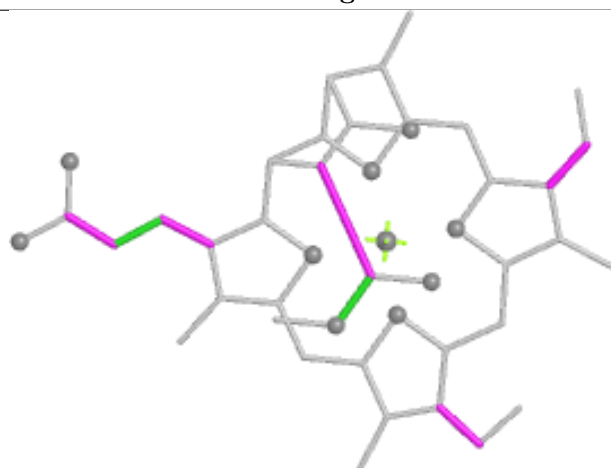
Ligand KC2 T 303



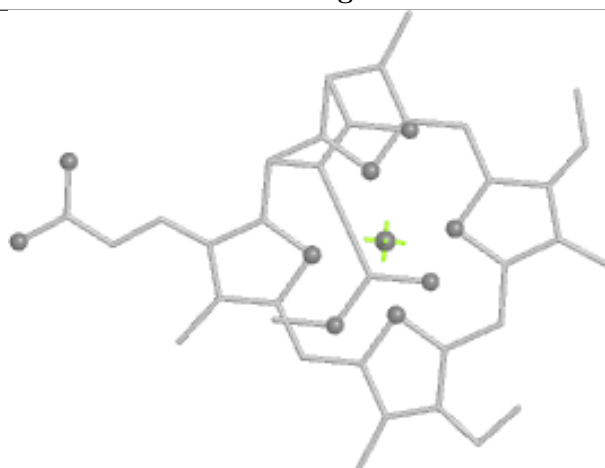
Bond lengths



Bond angles

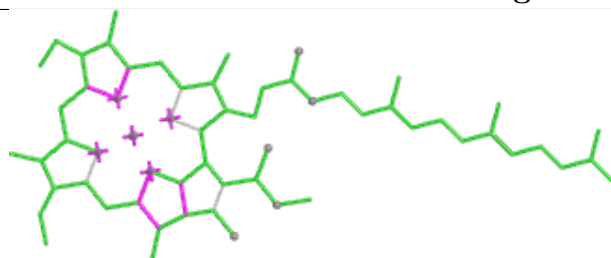


Torsions

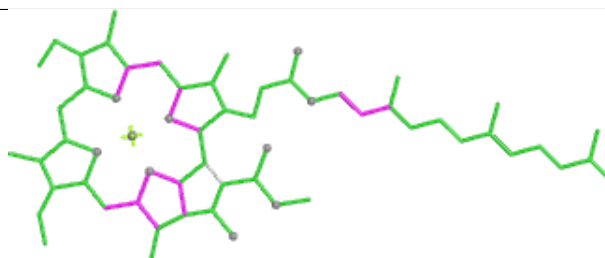


Rings

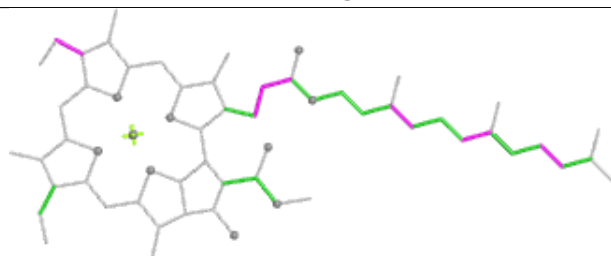
Ligand CLA D 304



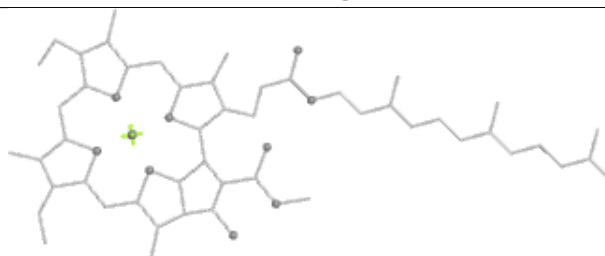
Bond lengths



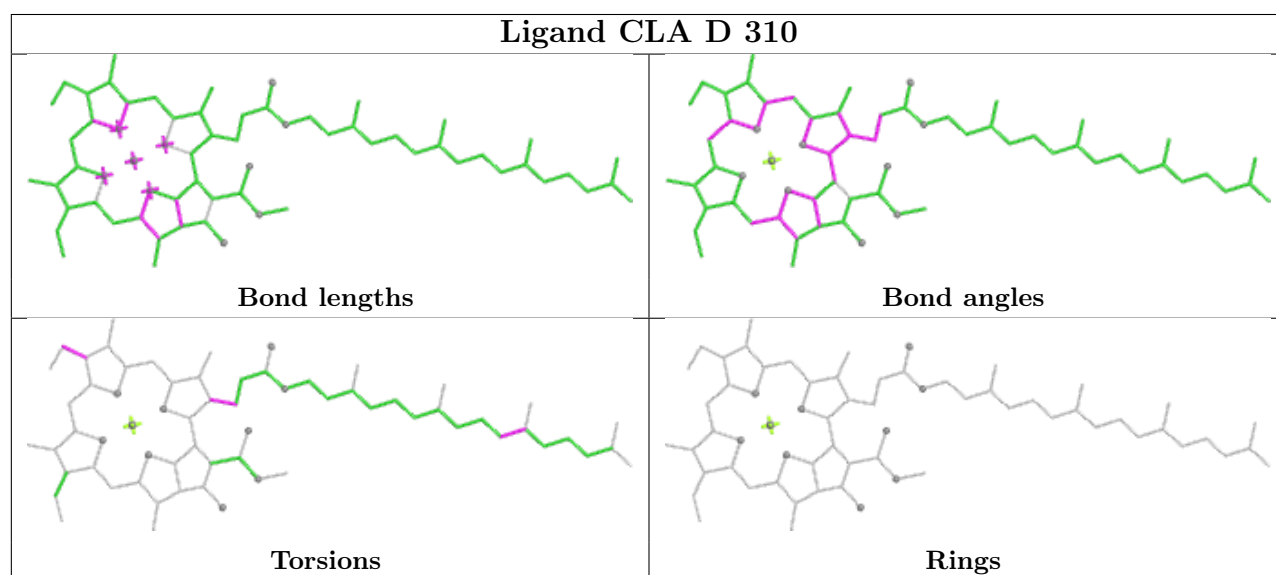
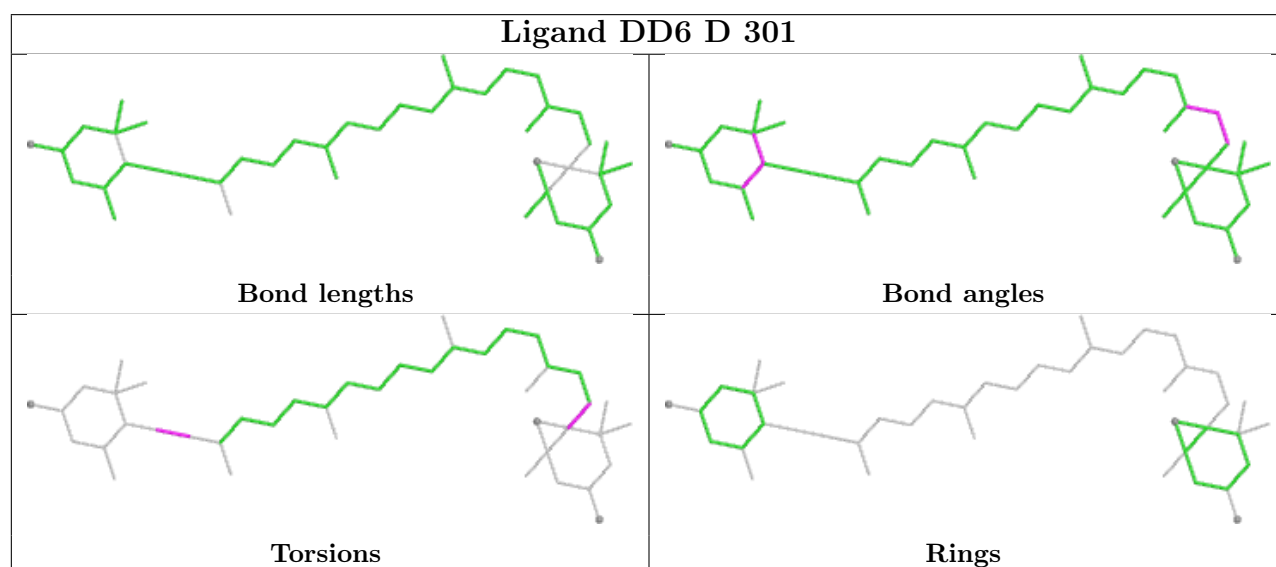
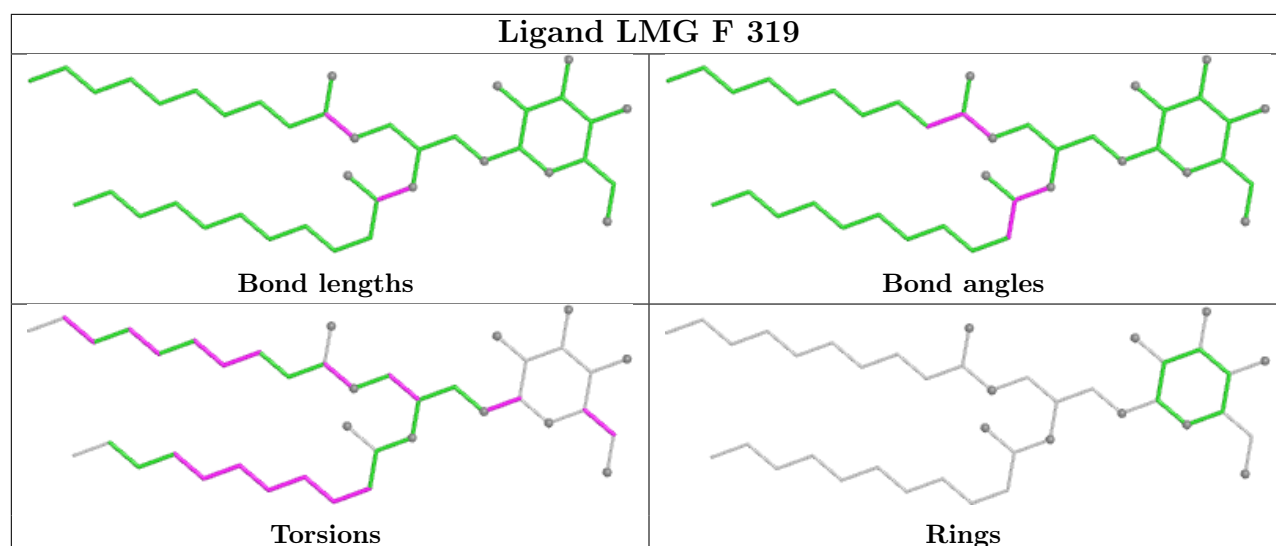
Bond angles



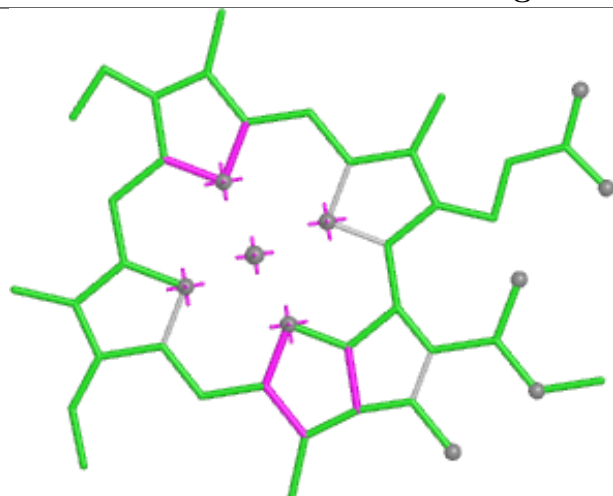
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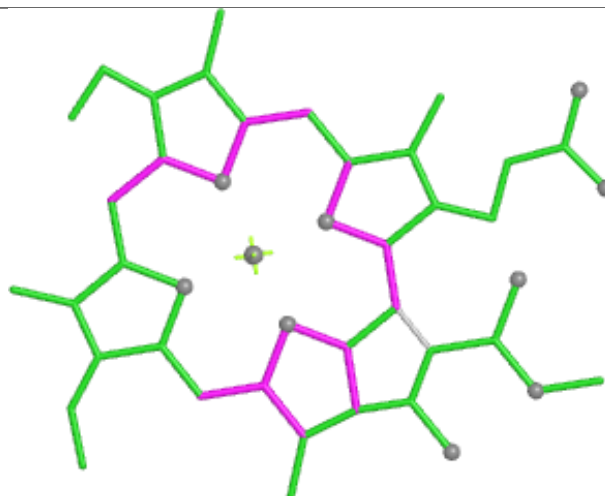
Rings



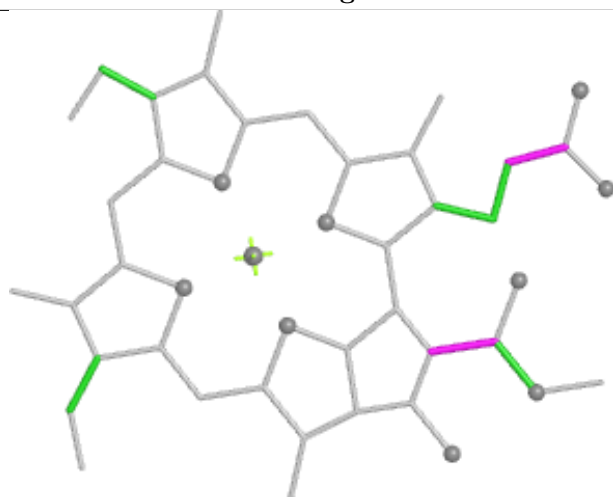
Ligand CLA O 306



Bond lengths



Bond angles

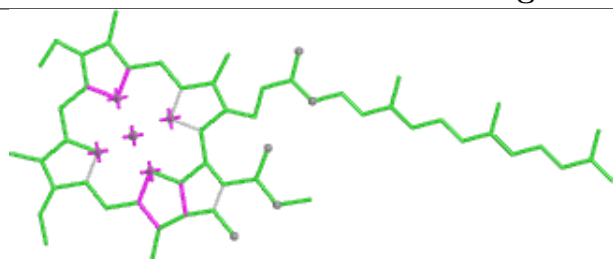


Torsions

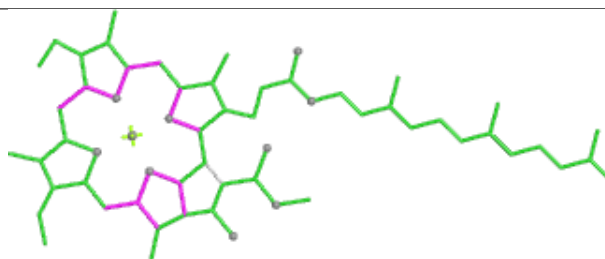


Rings

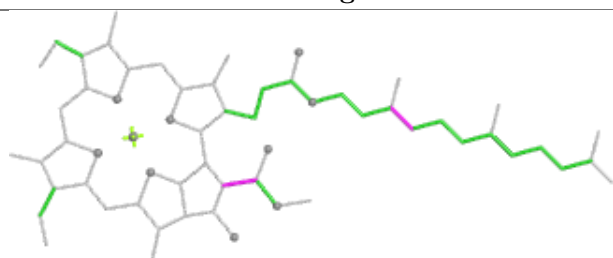
Ligand CLA b 834



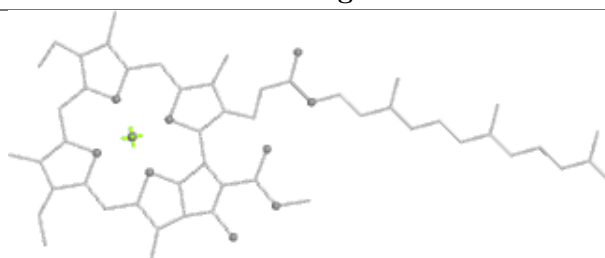
Bond lengths



Bond angles

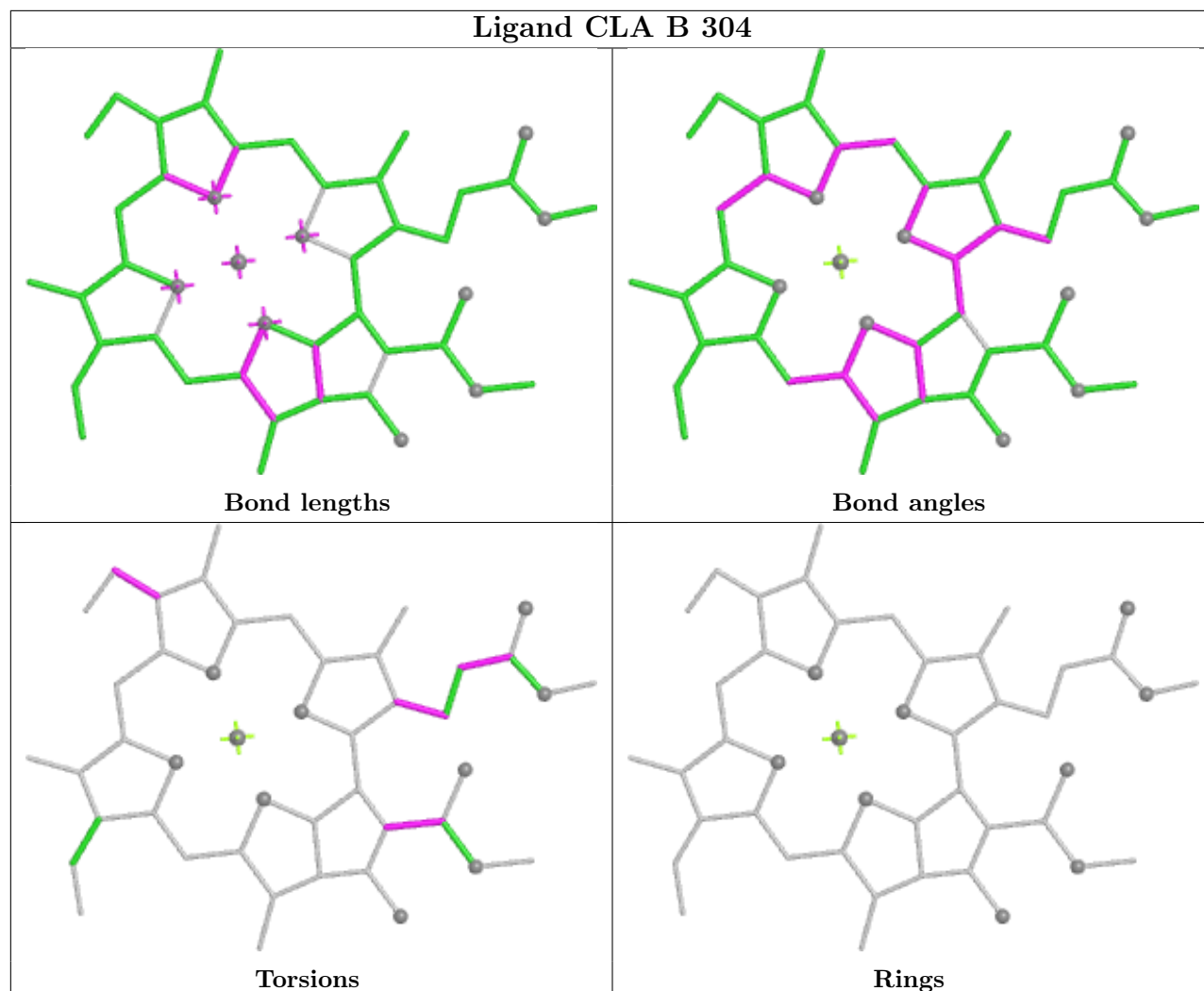


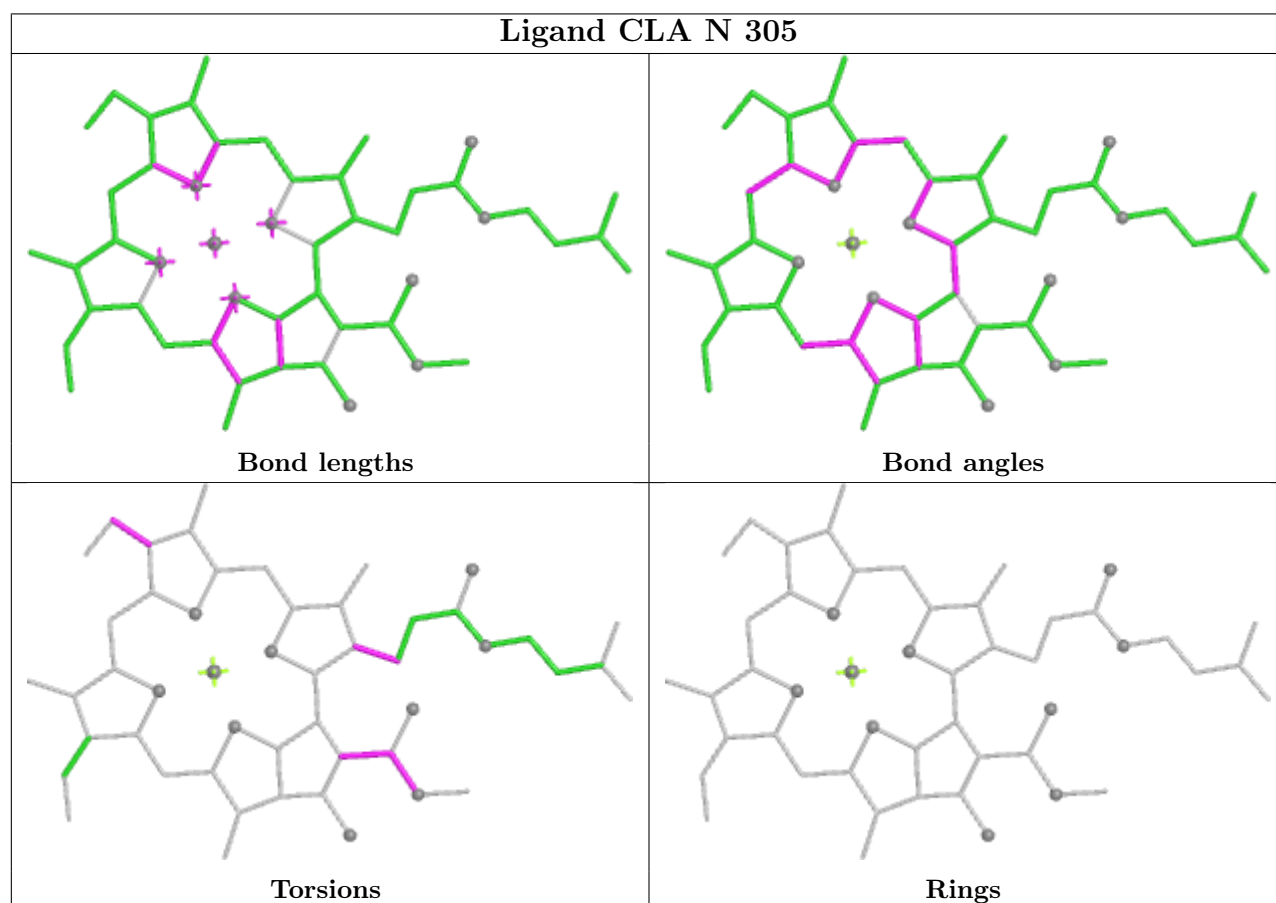
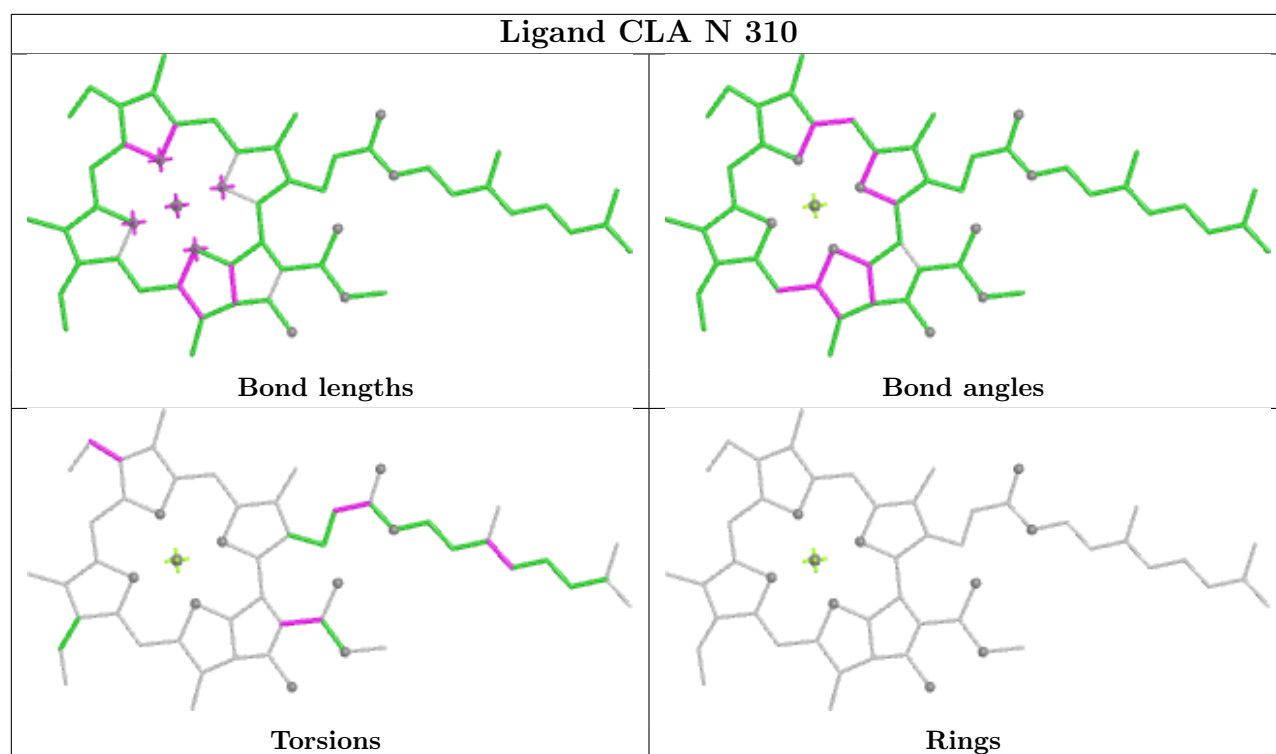
Torsions

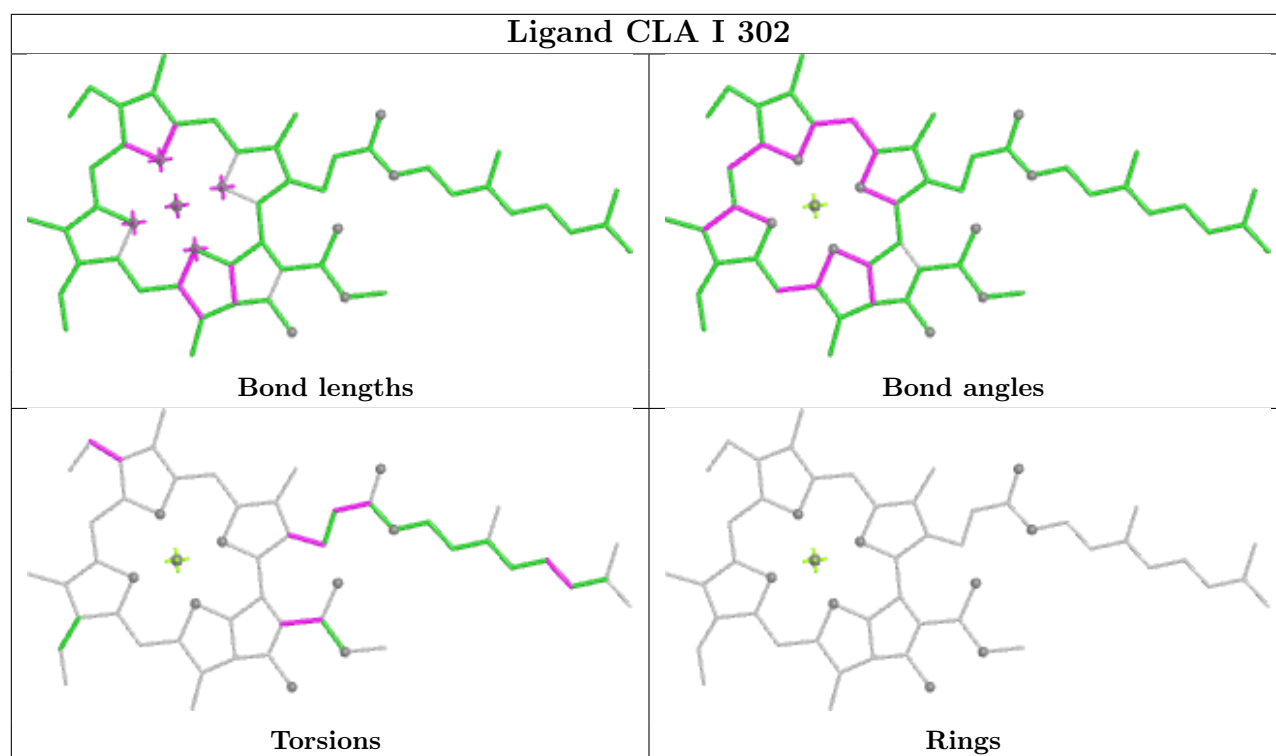


Rings

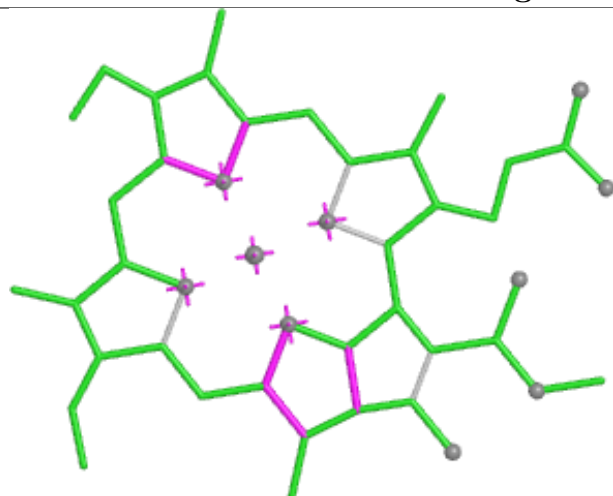
Ligand CLA B 304



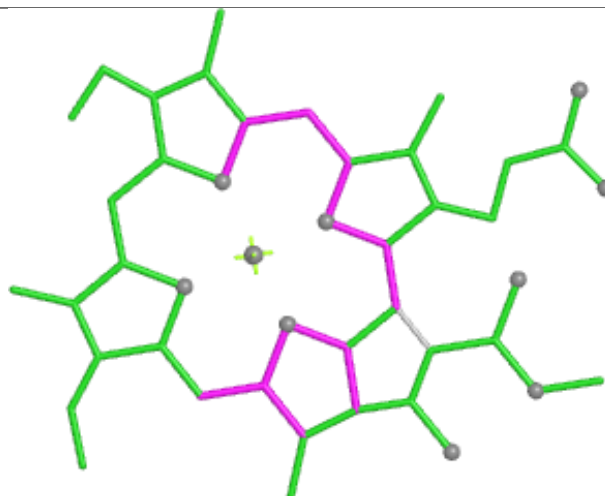




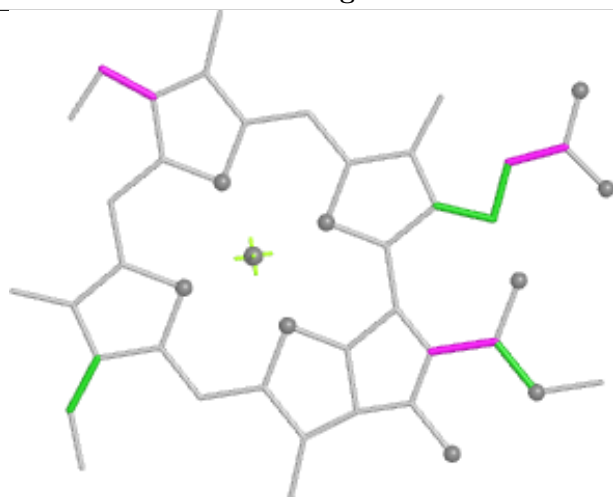
Ligand CLA B 302



Bond lengths



Bond angles

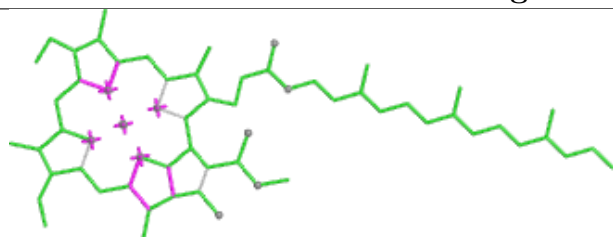


Torsions

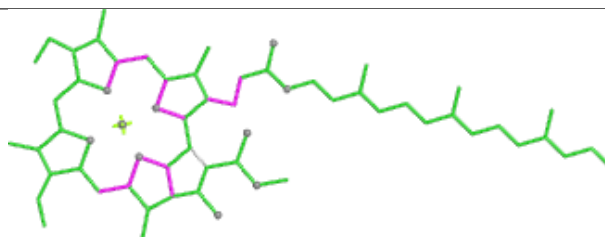


Rings

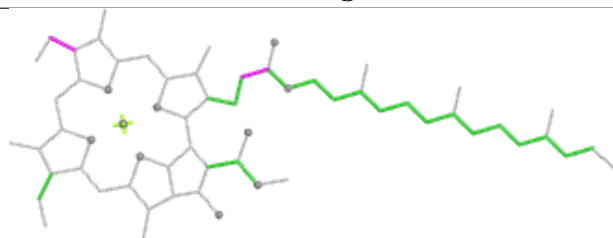
Ligand CLA M 310



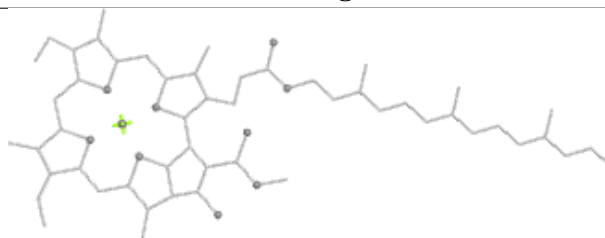
Bond lengths



Bond angles

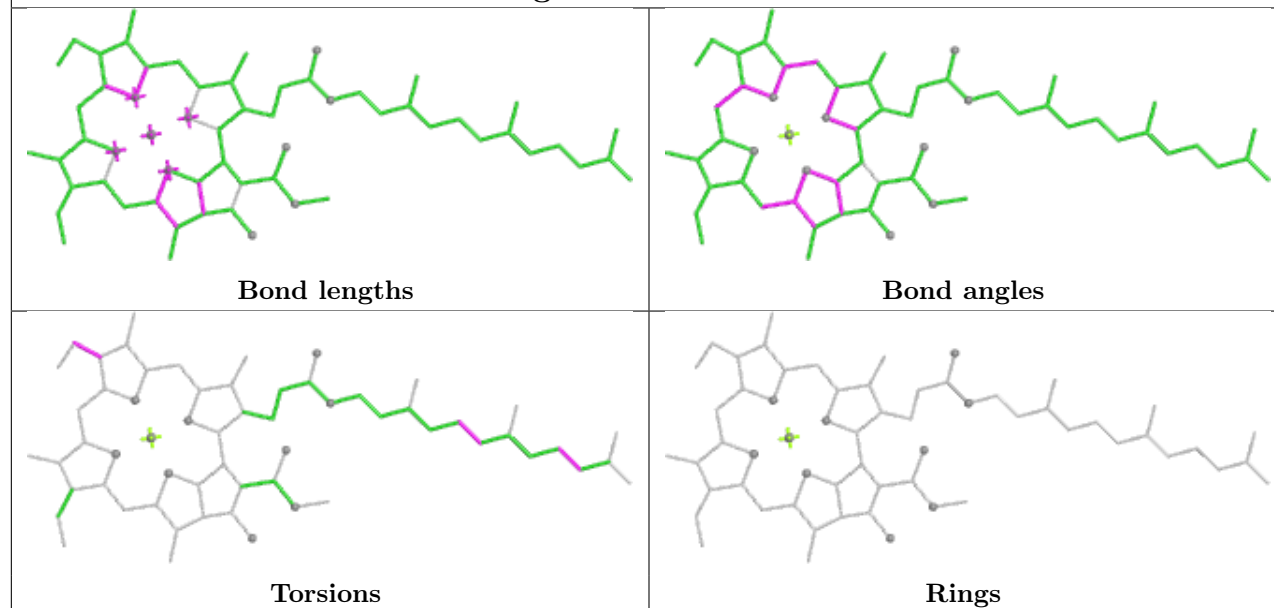


Torsions

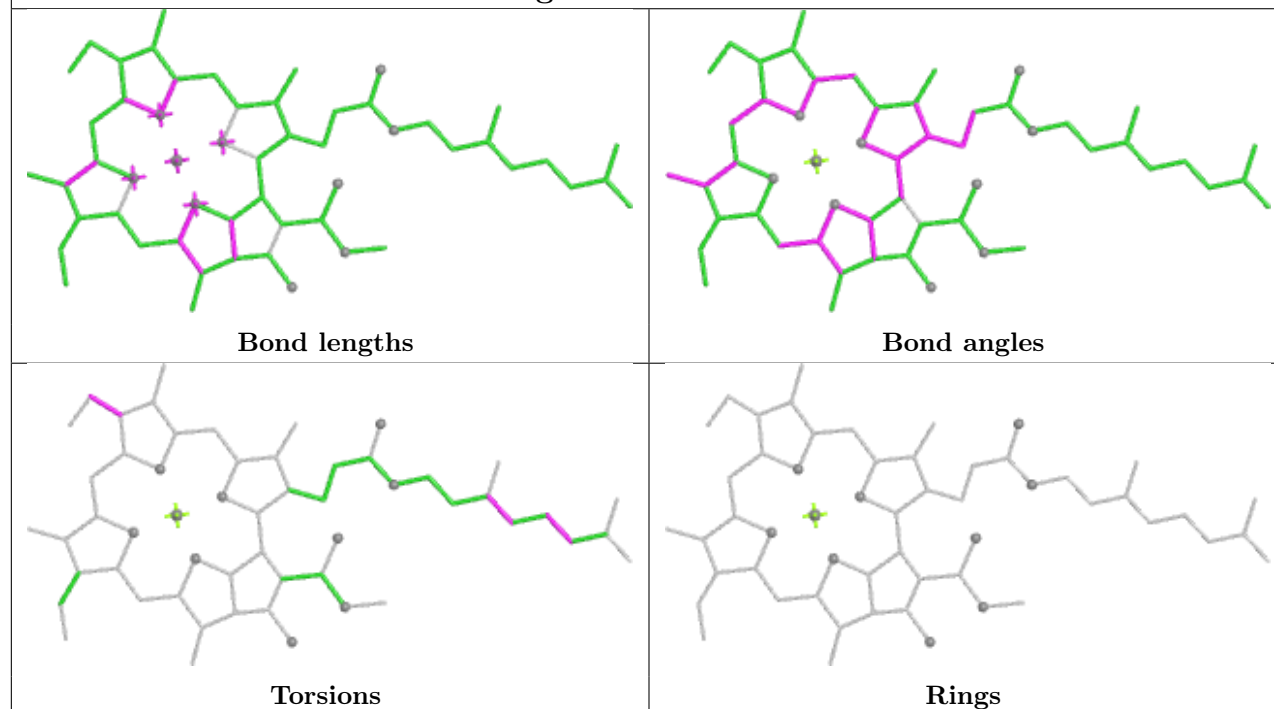


Rings

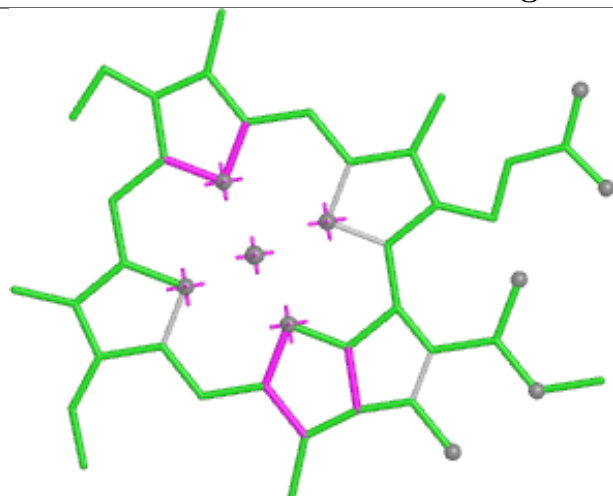
Ligand CLA E 304



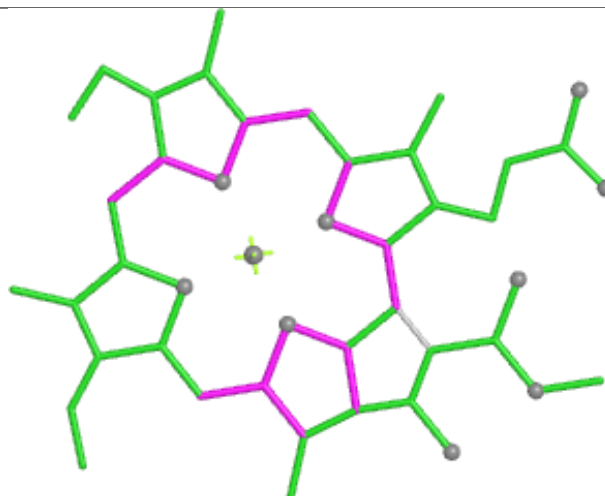
Ligand CLA J 304



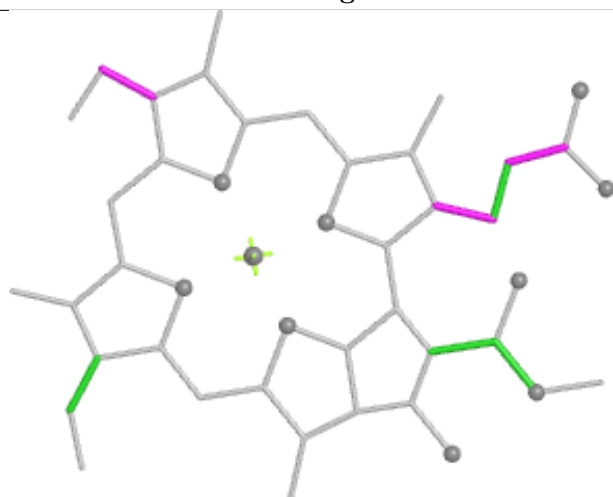
Ligand CLA I 304



Bond lengths



Bond angles

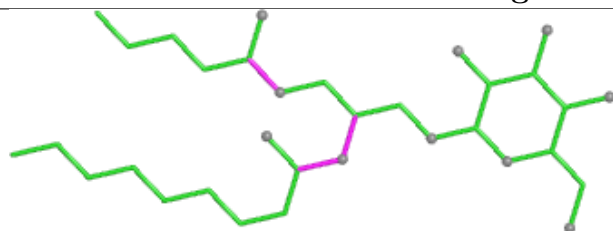


Torsions

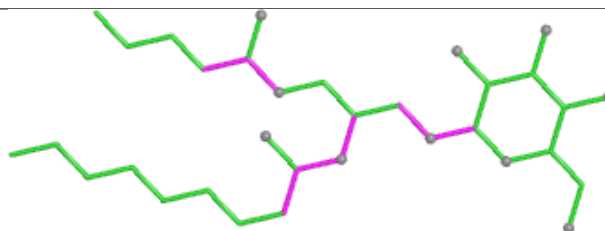


Rings

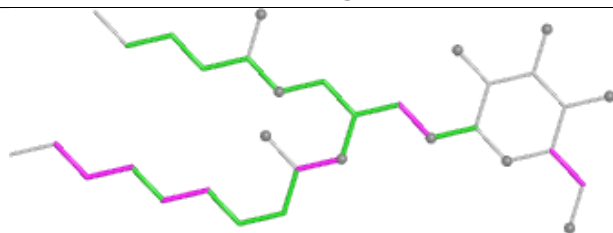
Ligand LMG F 320



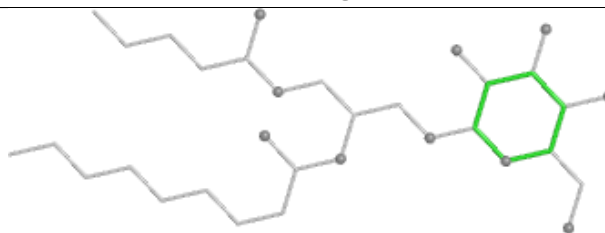
Bond lengths



Bond angles

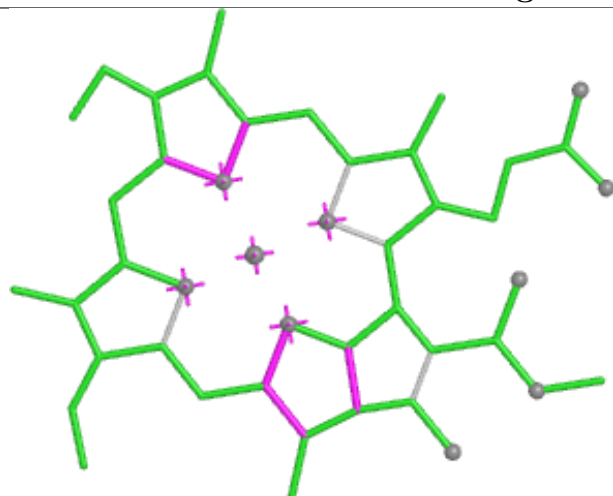


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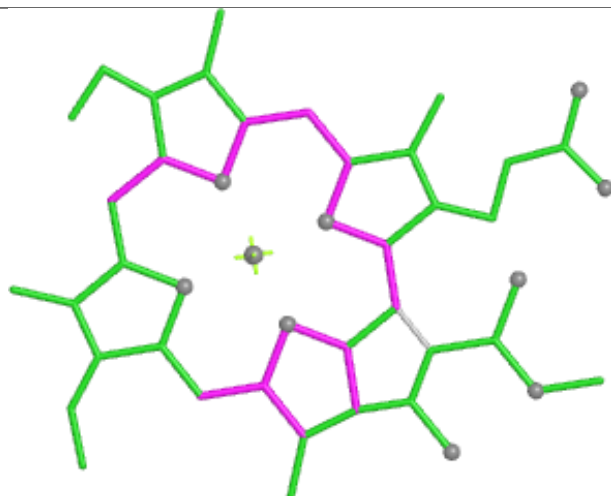


Rings

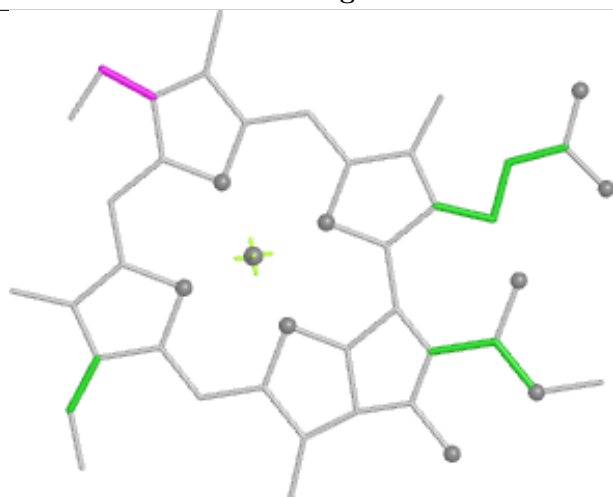
Ligand CLA L 304



Bond lengths



Bond angles

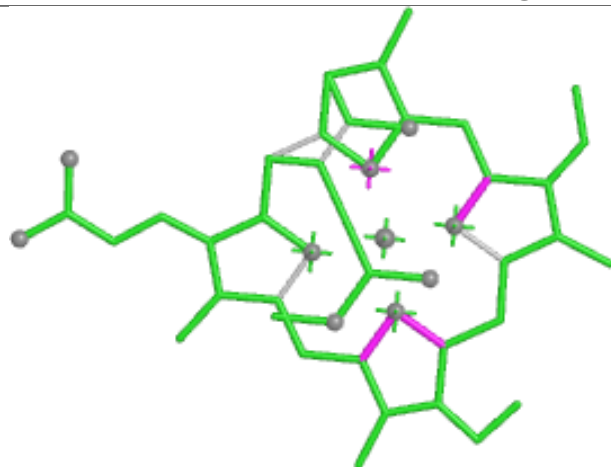


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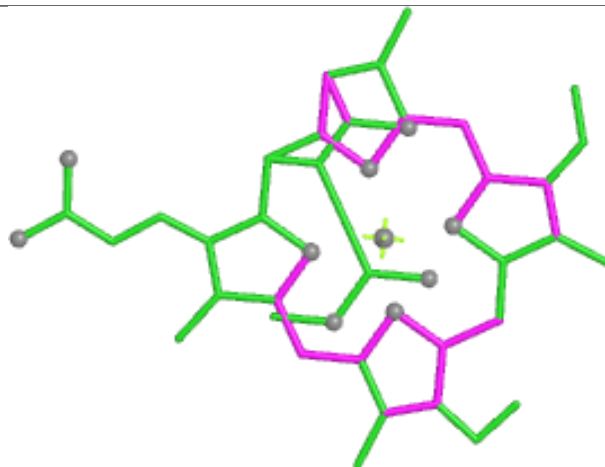


Rings

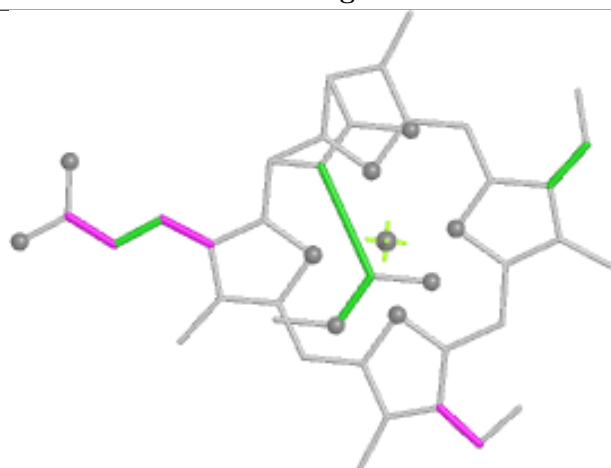
Ligand KC2 O 310



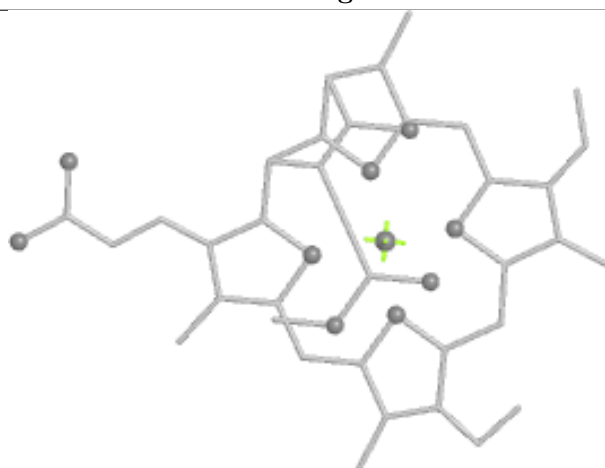
Bond lengths



Bond angles

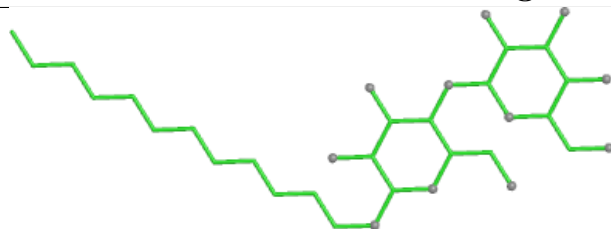


Torsions



Rings

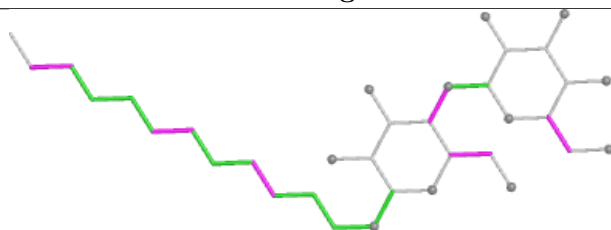
Ligand LMU I 315



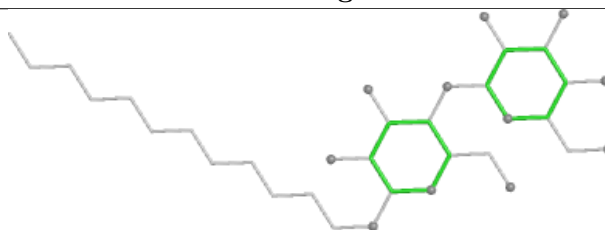
Bond lengths



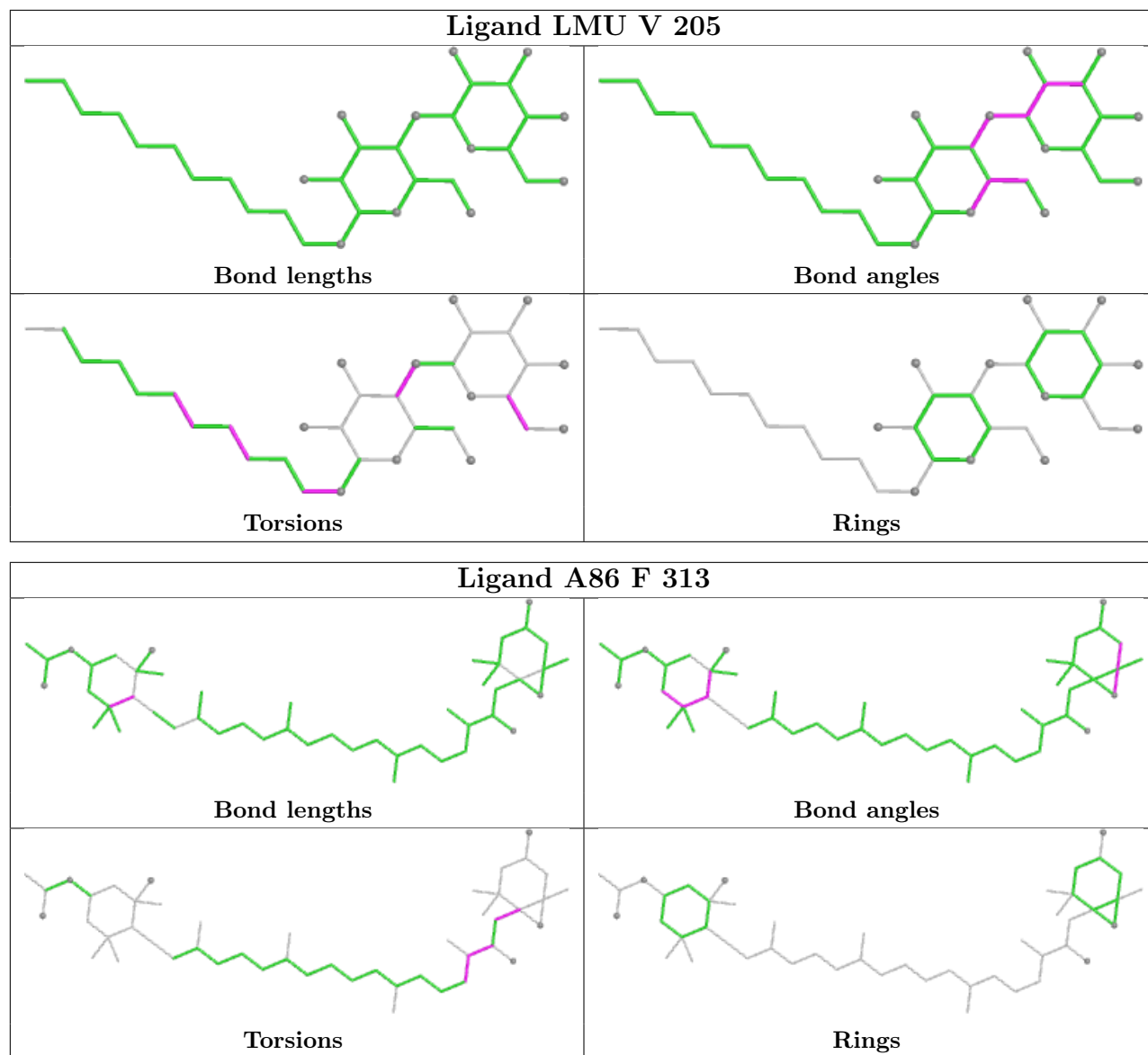
Bond angles

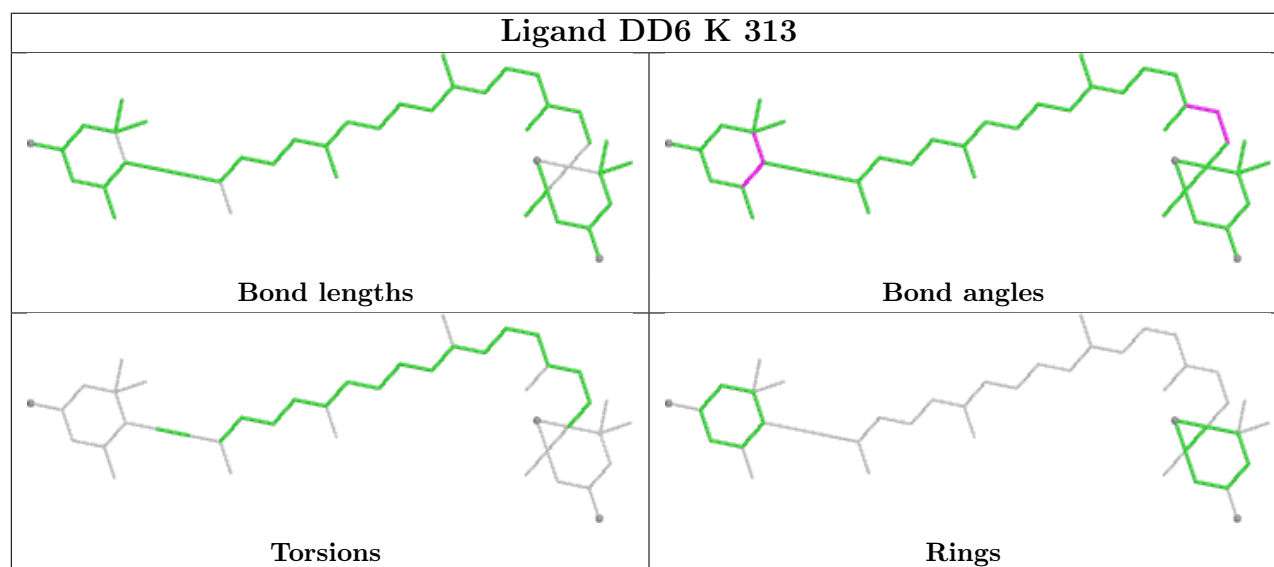
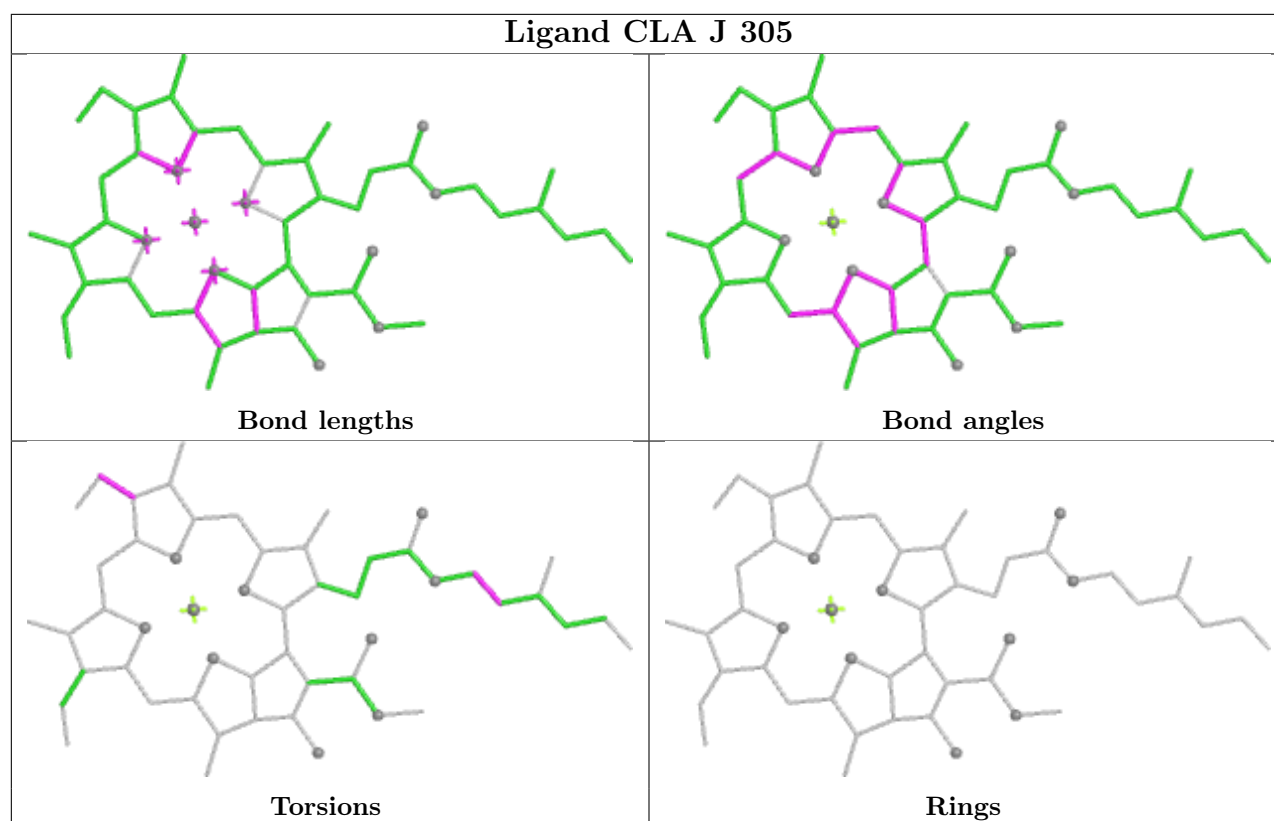


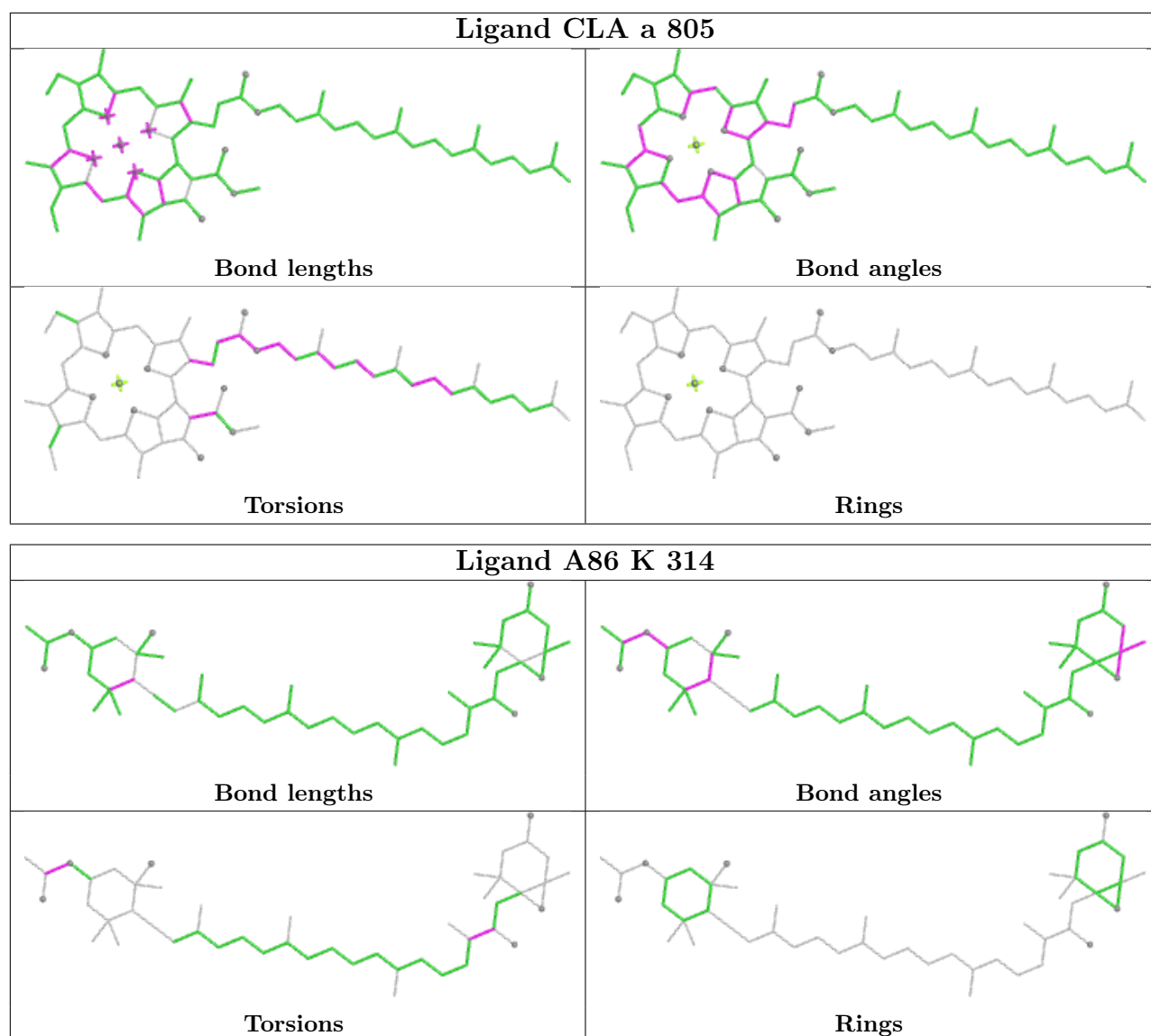
Torsions

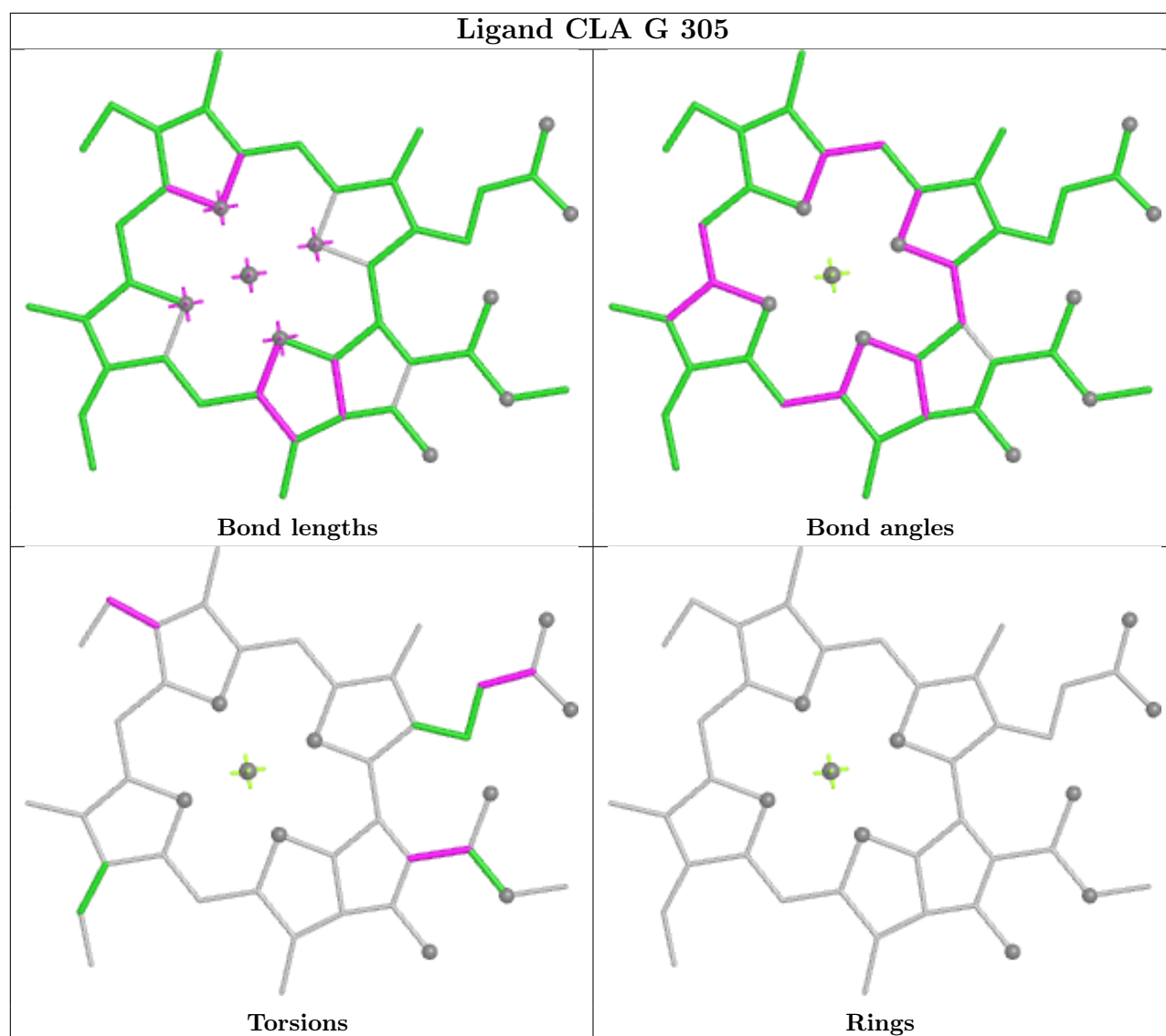


Rings

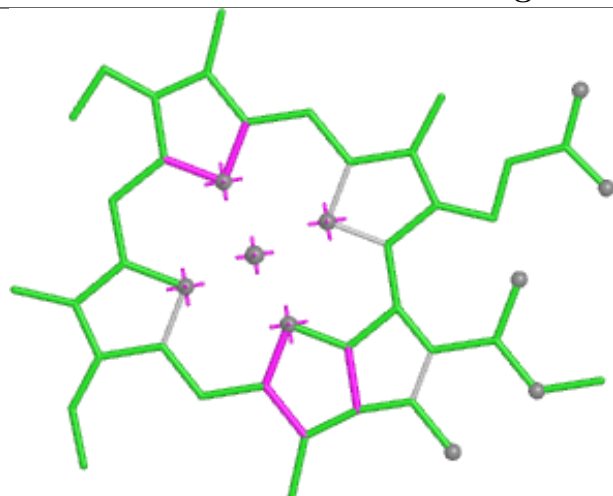




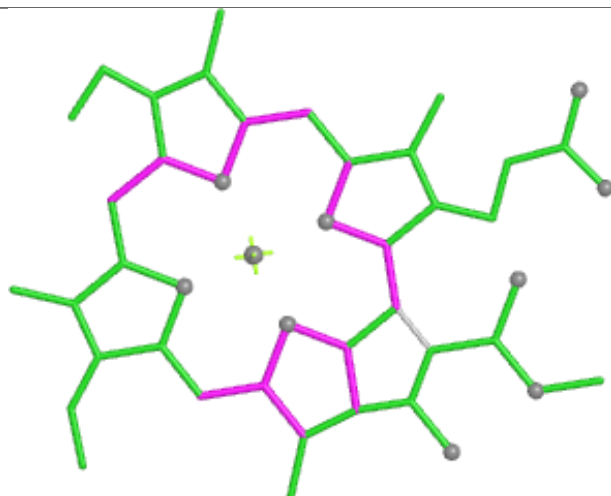




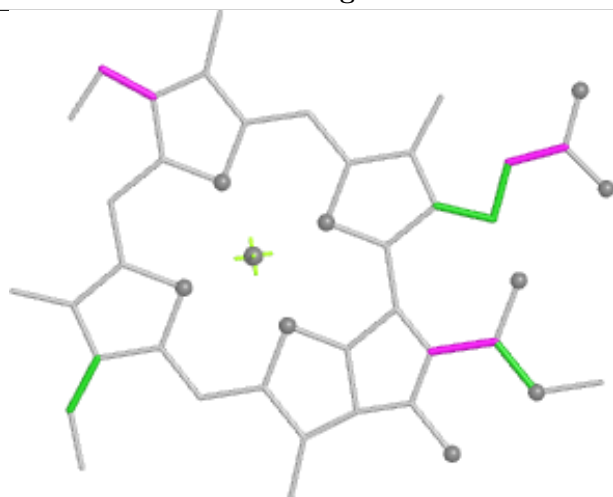
Ligand CLA B 305



Bond lengths



Bond angles

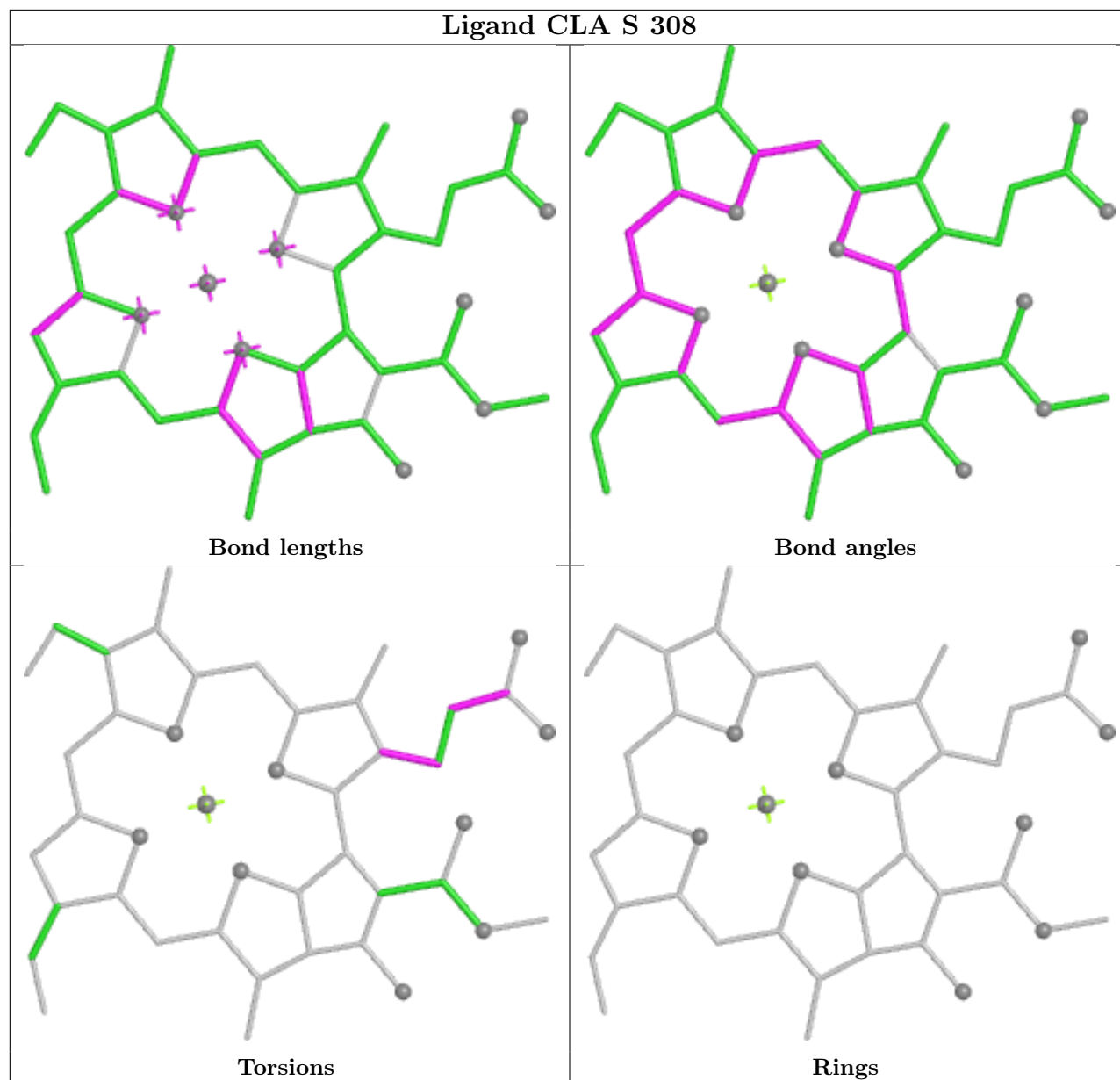


Torsions

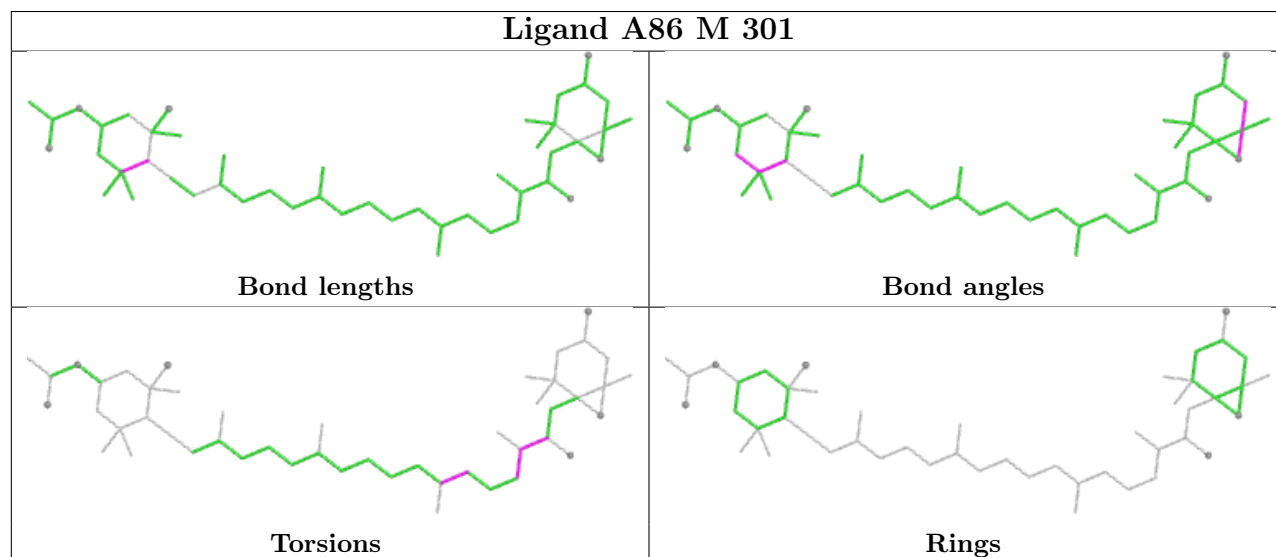


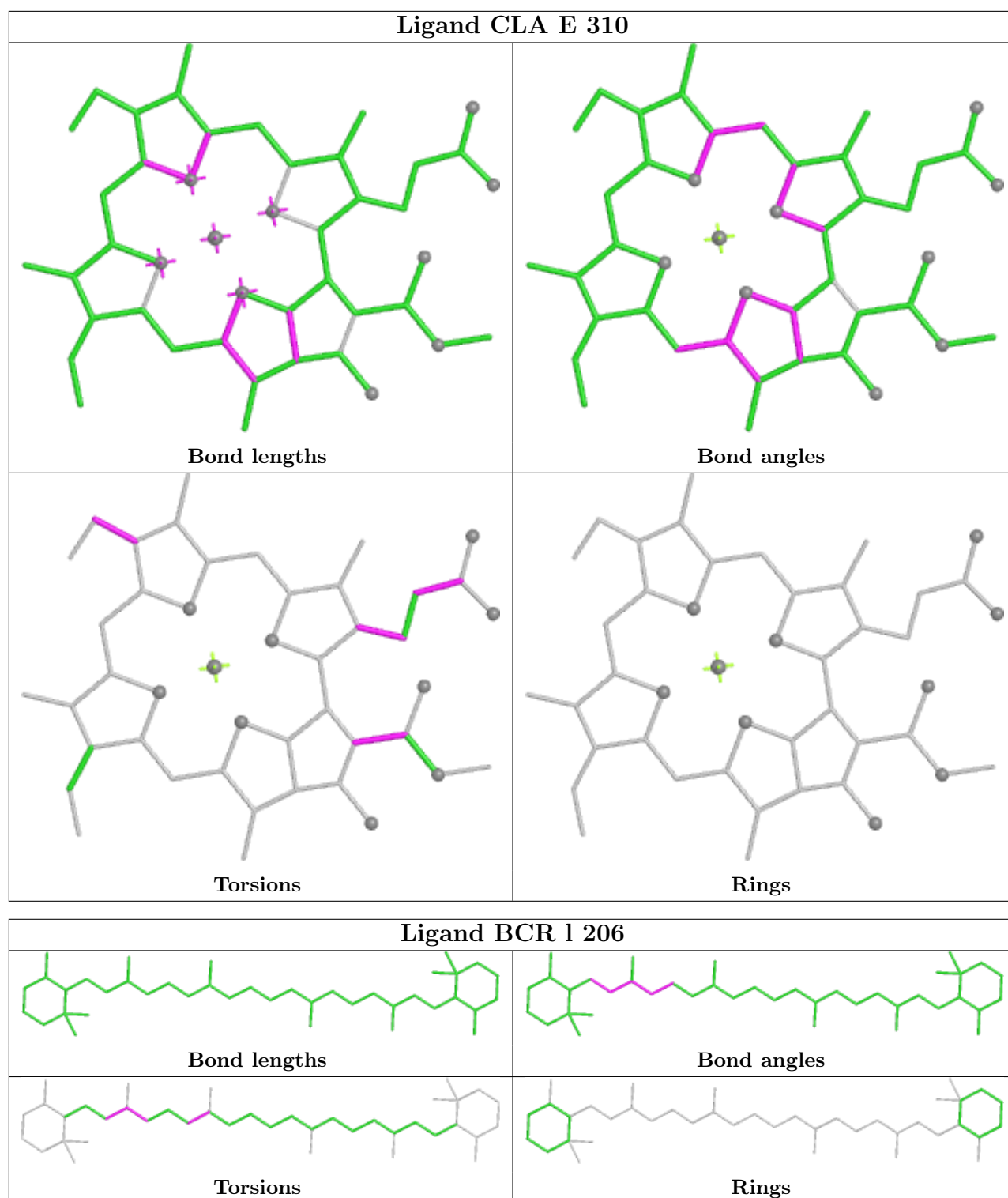
Rings

Ligand CLA S 308

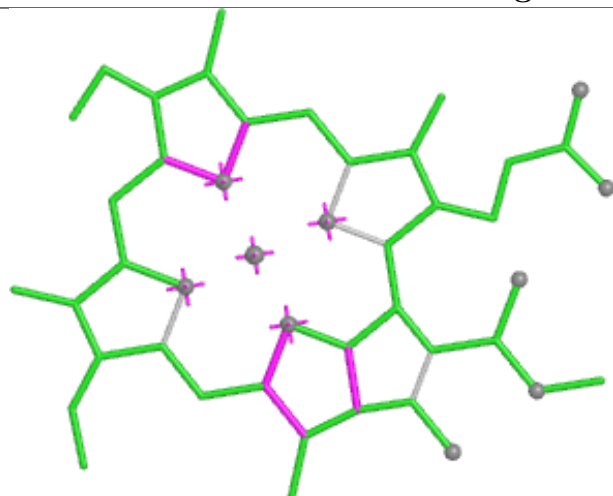


Ligand A86 M 301

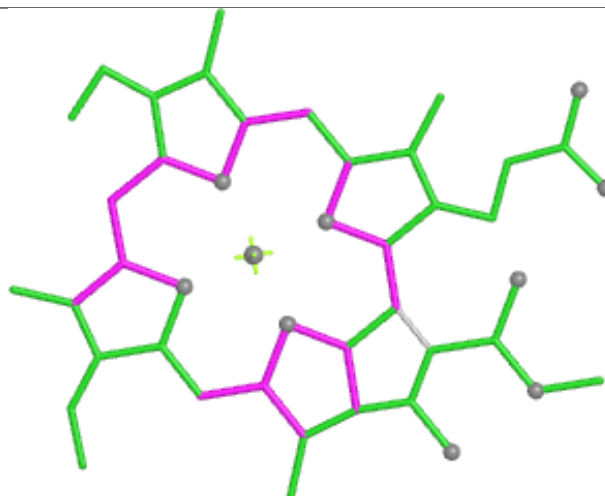




Ligand CLA C 308



Bond lengths



Bond angles

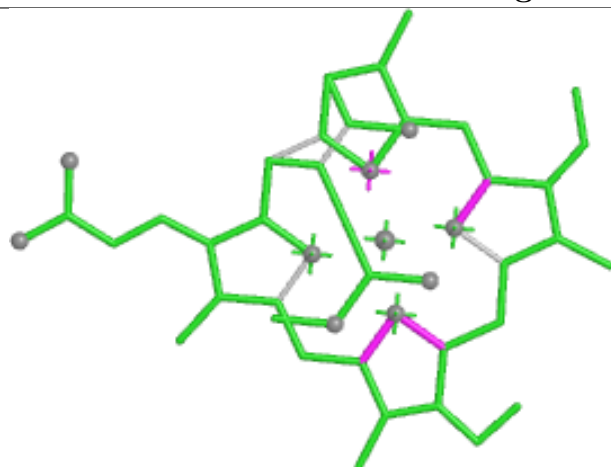


Torsions

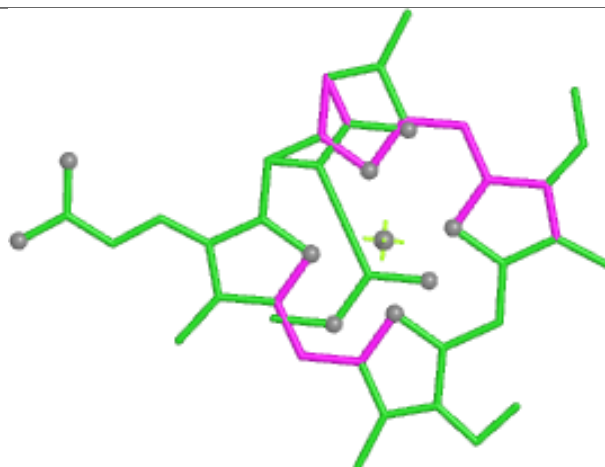


Rings

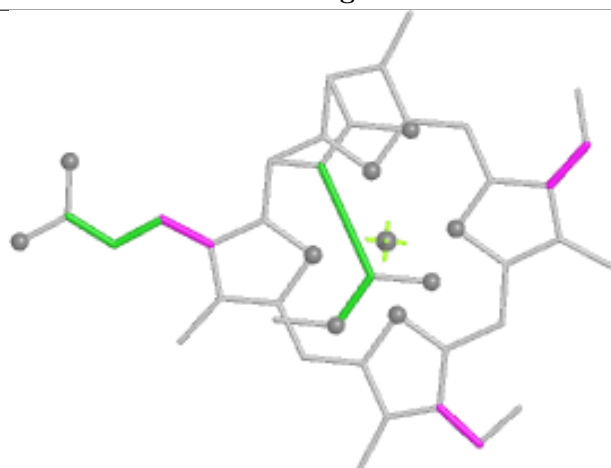
Ligand KC2 K 305



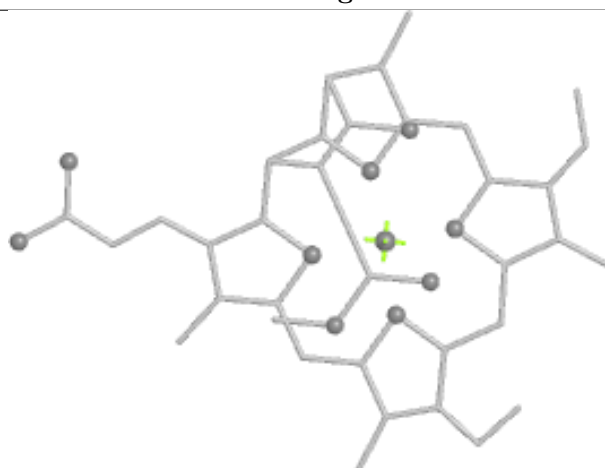
Bond lengths



Bond angles

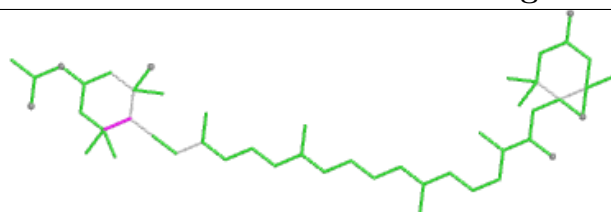


Torsions

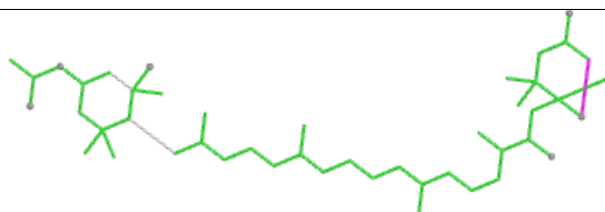


Rings

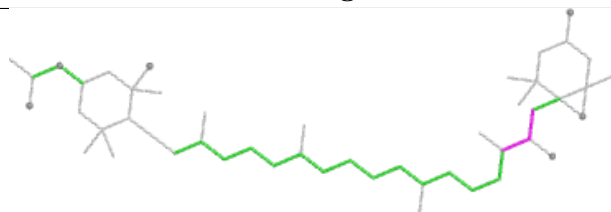
Ligand A86 T 315



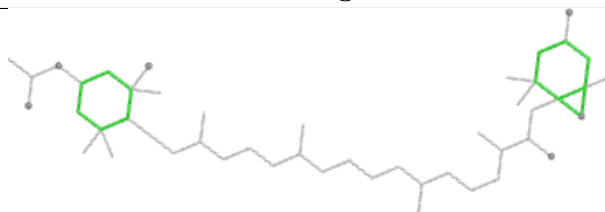
Bond lengths



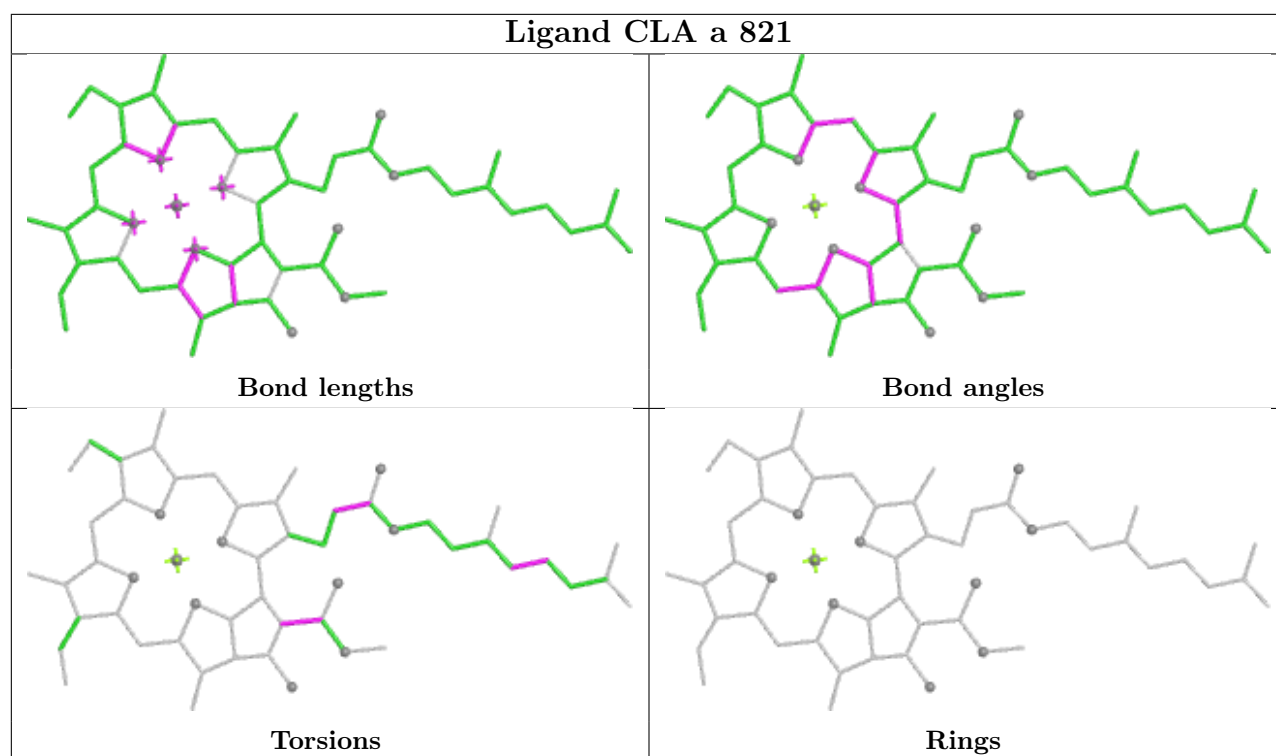
Bond angles



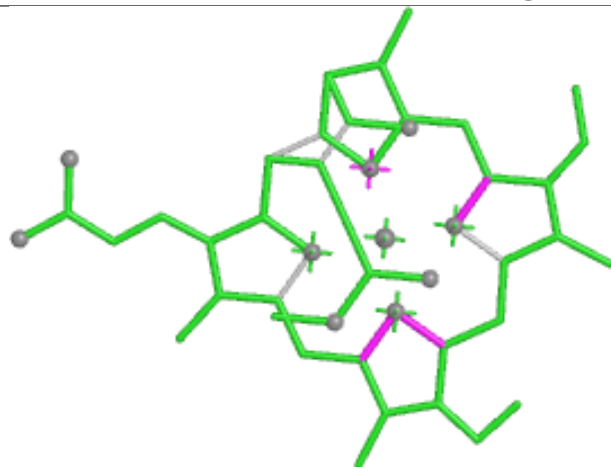
Torsions



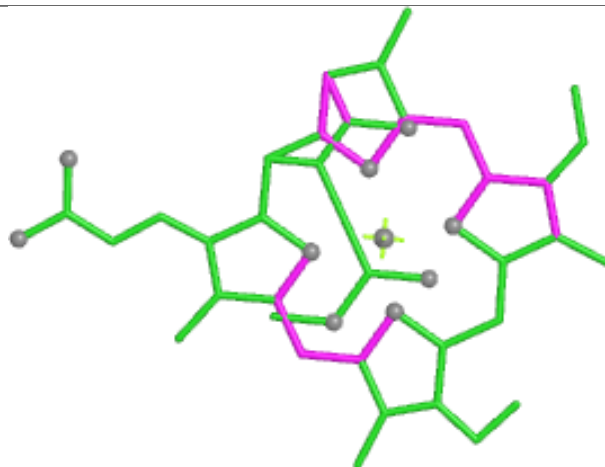
Rings



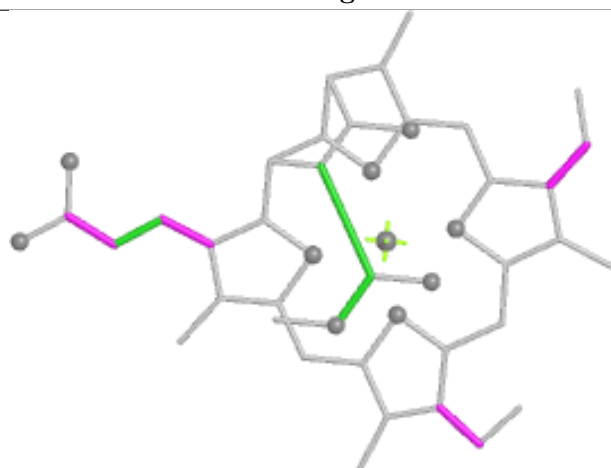
Ligand KC2 J 303



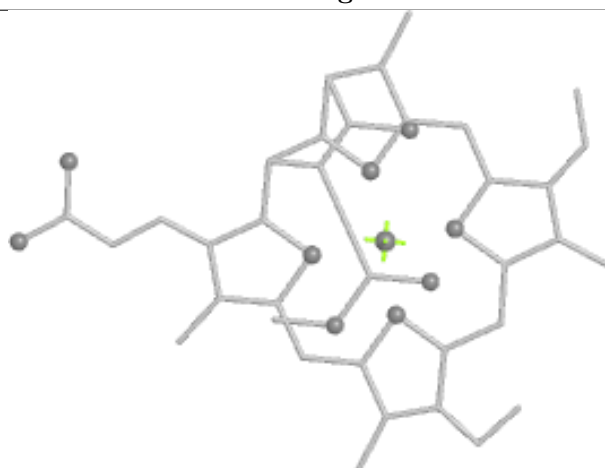
Bond lengths



Bond angles

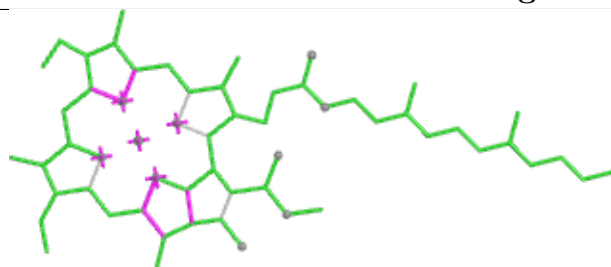


Torsions

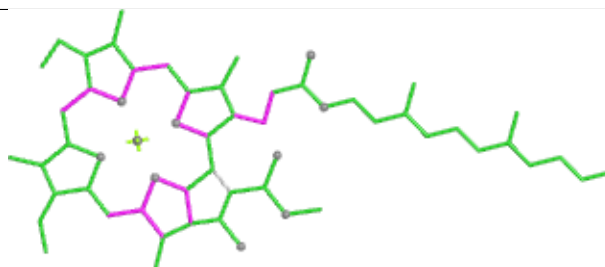


Rings

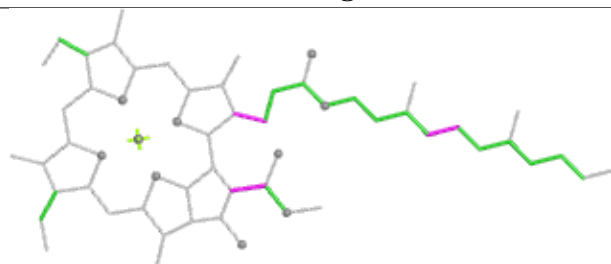
Ligand CLA a 804



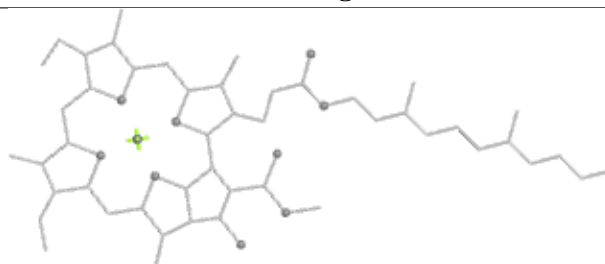
Bond lengths



Bond angles

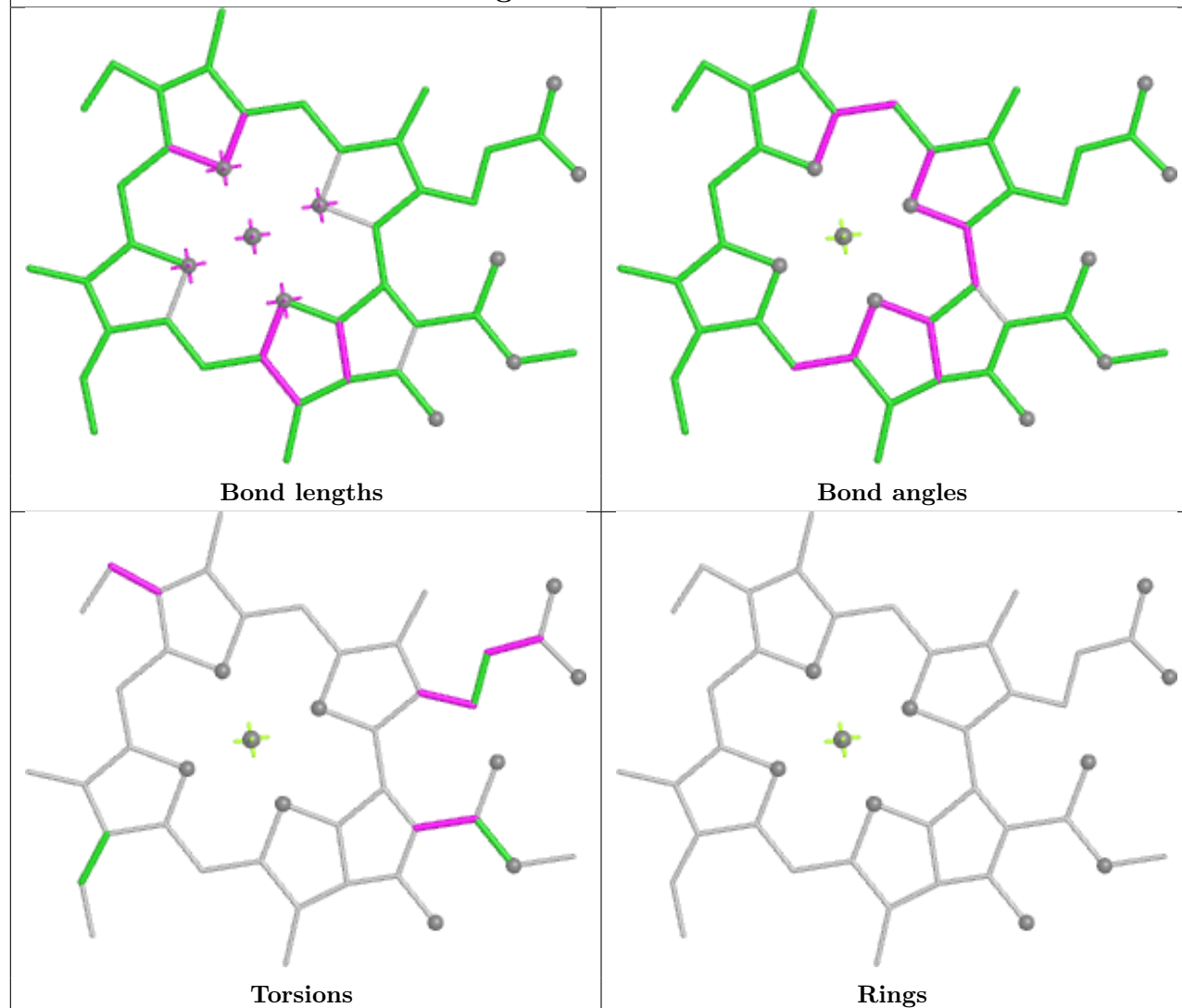


Torsions

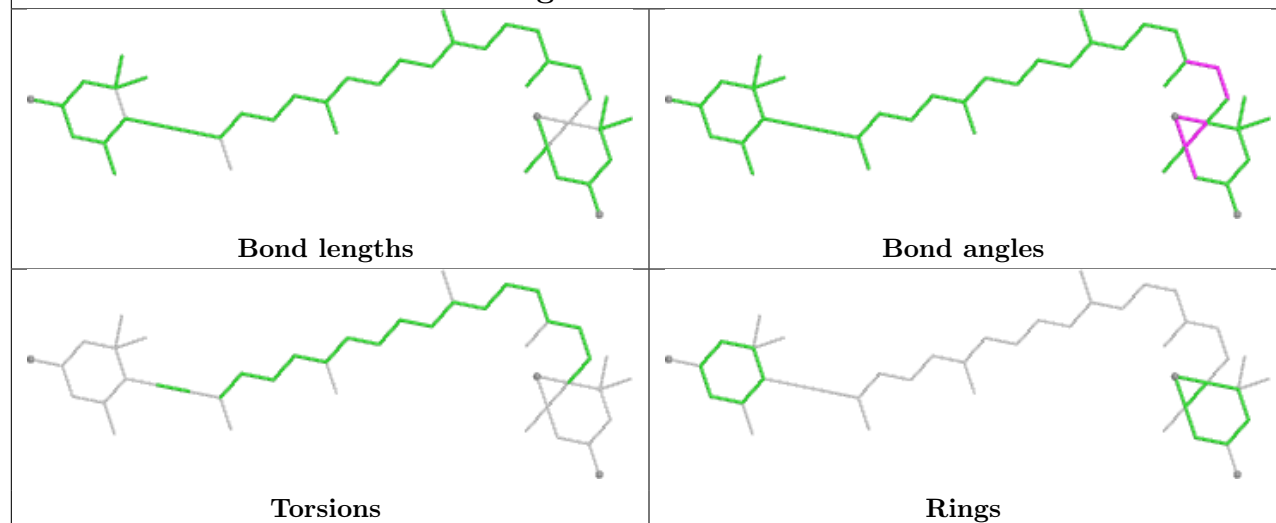


Rings

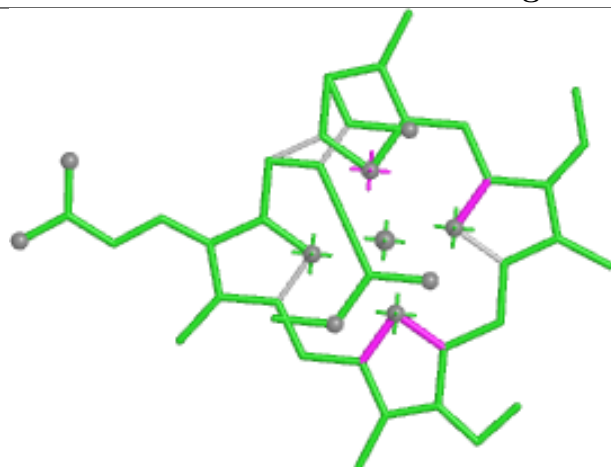
Ligand CLA b 809



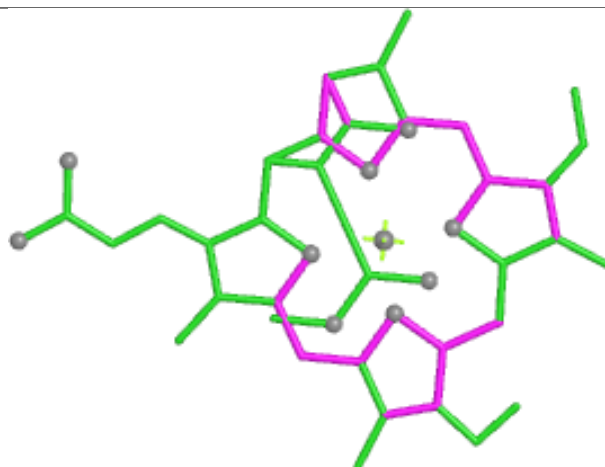
Ligand DD6 J 317



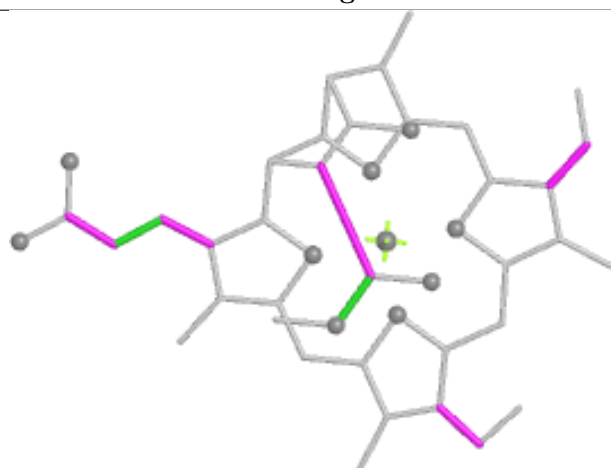
Ligand KC2 I 316



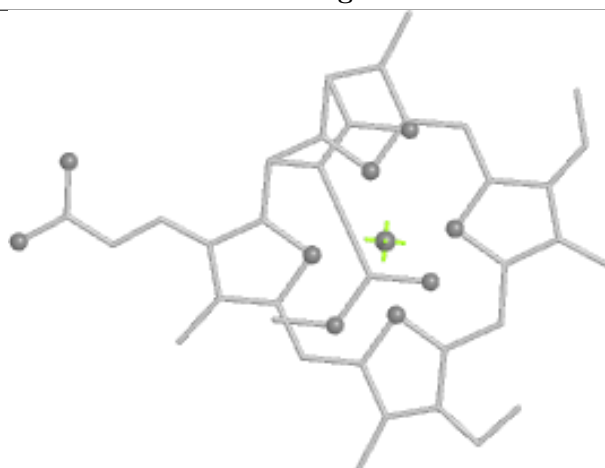
Bond lengths



Bond angles



Torsions



Rings

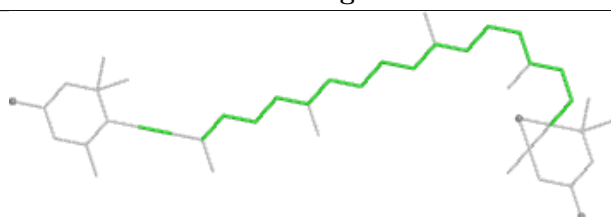
Ligand DD6 A 312



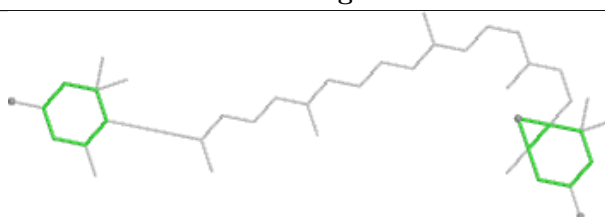
Bond lengths



Bond angles

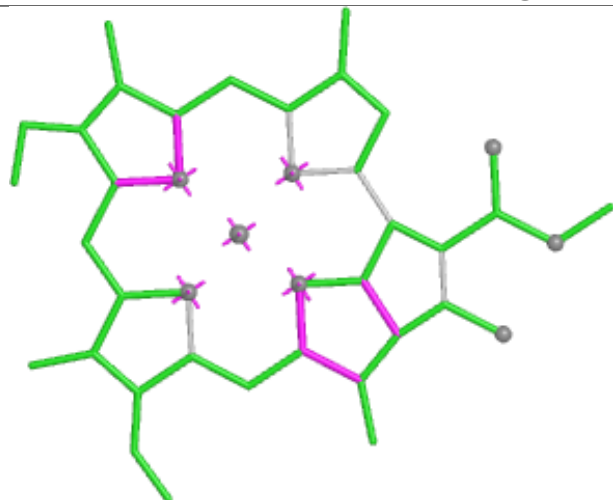


Torsions

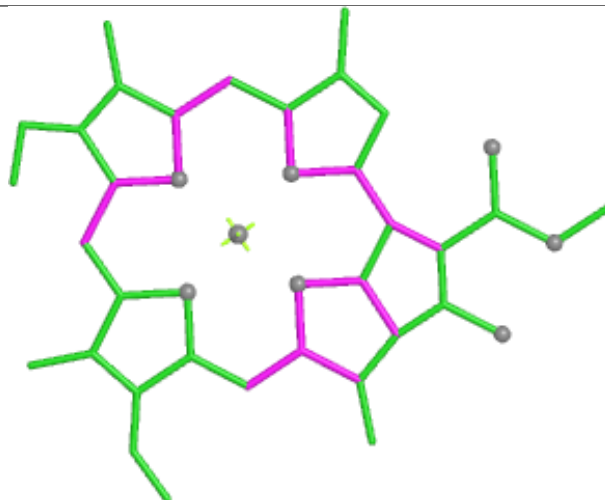


Rings

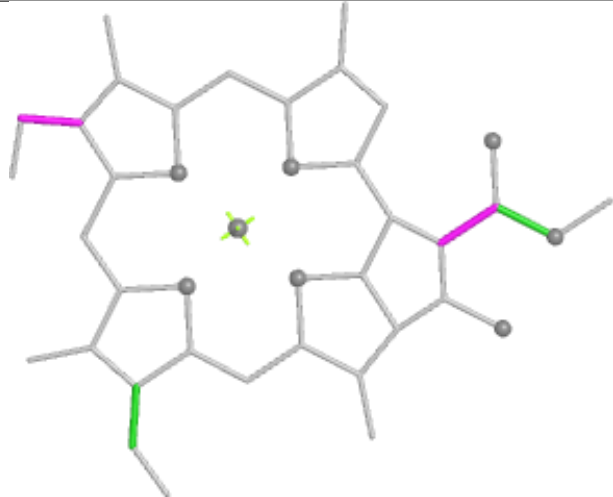
Ligand CLA L 310



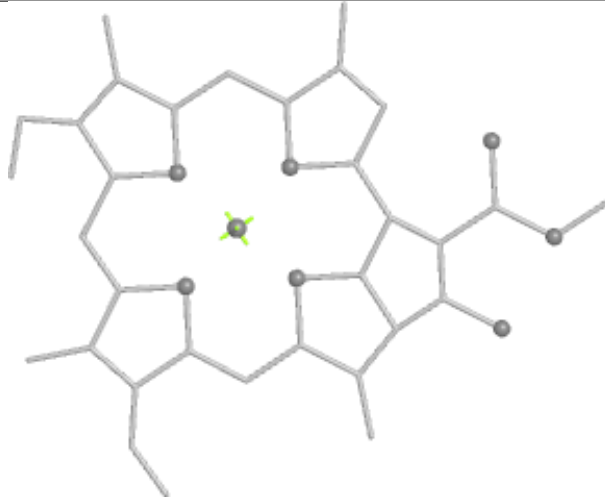
Bond lengths



Bond angles

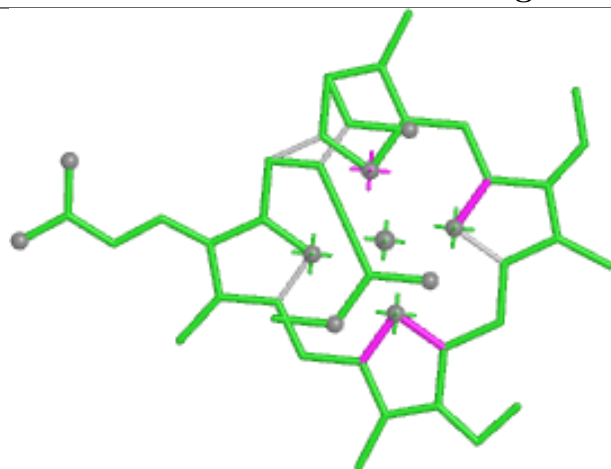


Torsions

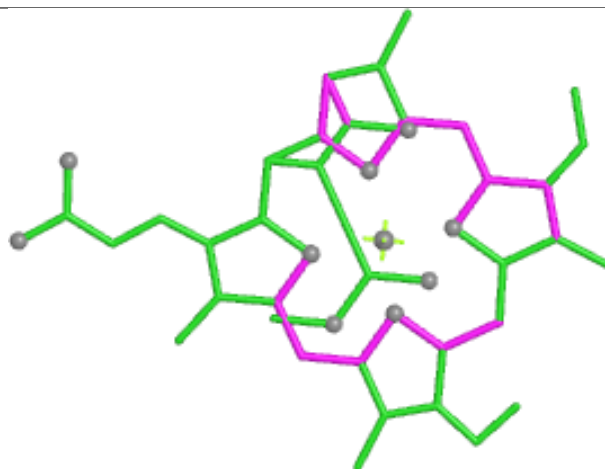


Rings

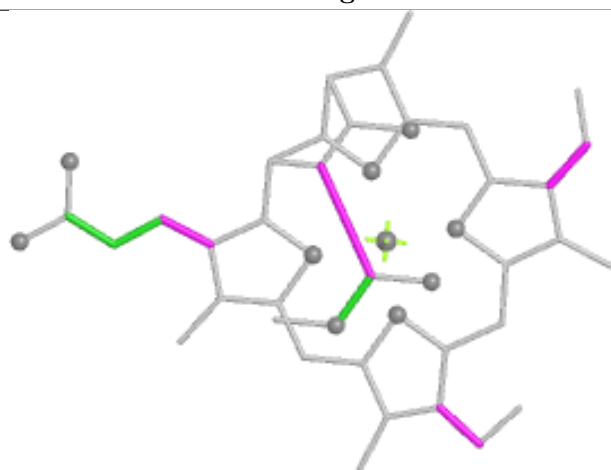
Ligand KC2 N 314



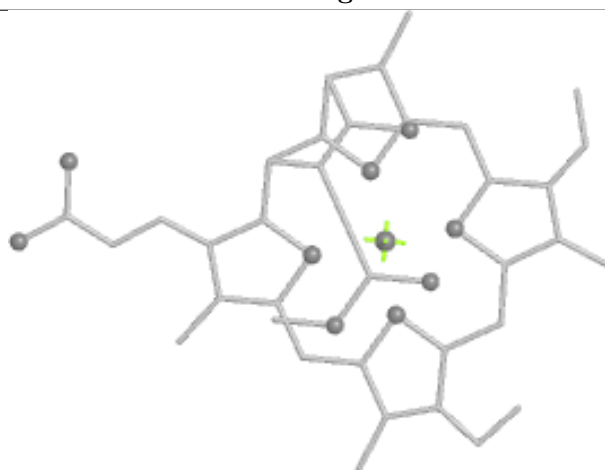
Bond lengths



Bond angles

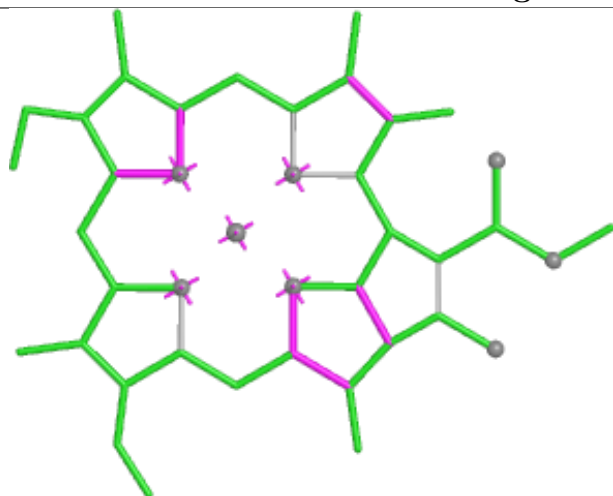


Torsions



Rings

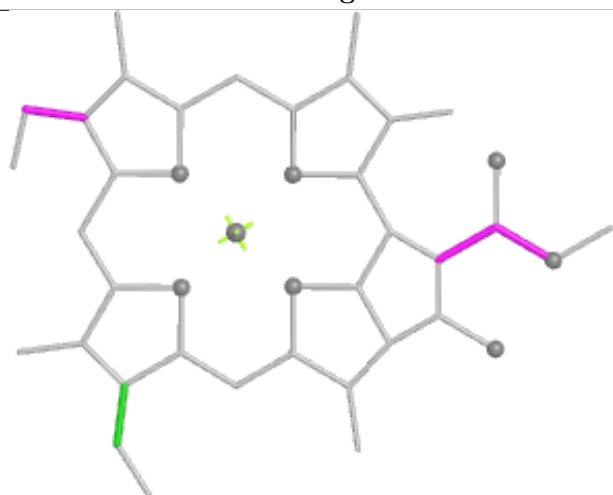
Ligand CLA H 302



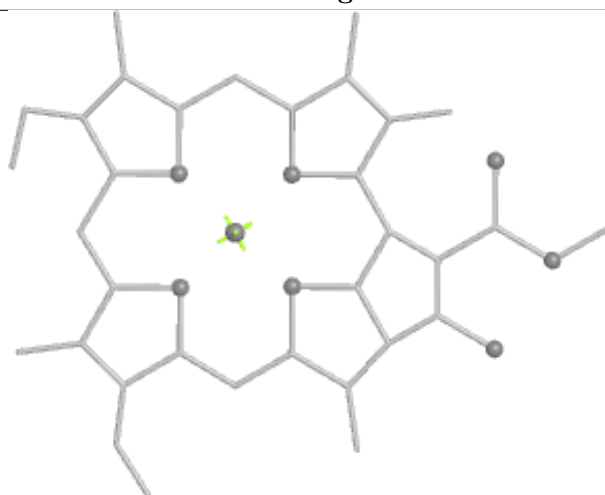
Bond lengths



Bond angles

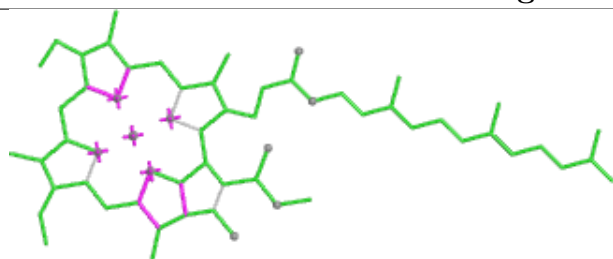


Torsions

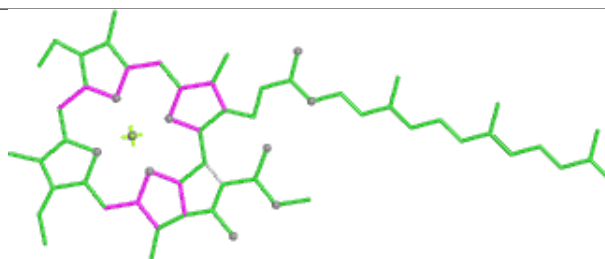


Rings

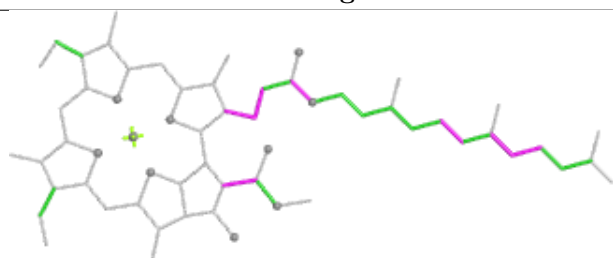
Ligand CLA b 807



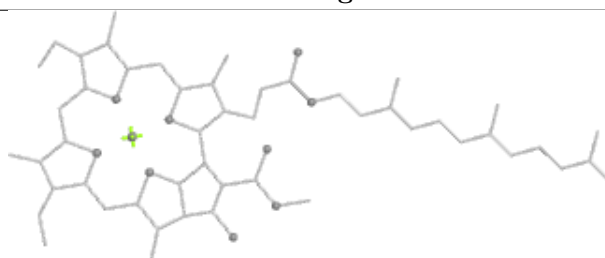
Bond lengths



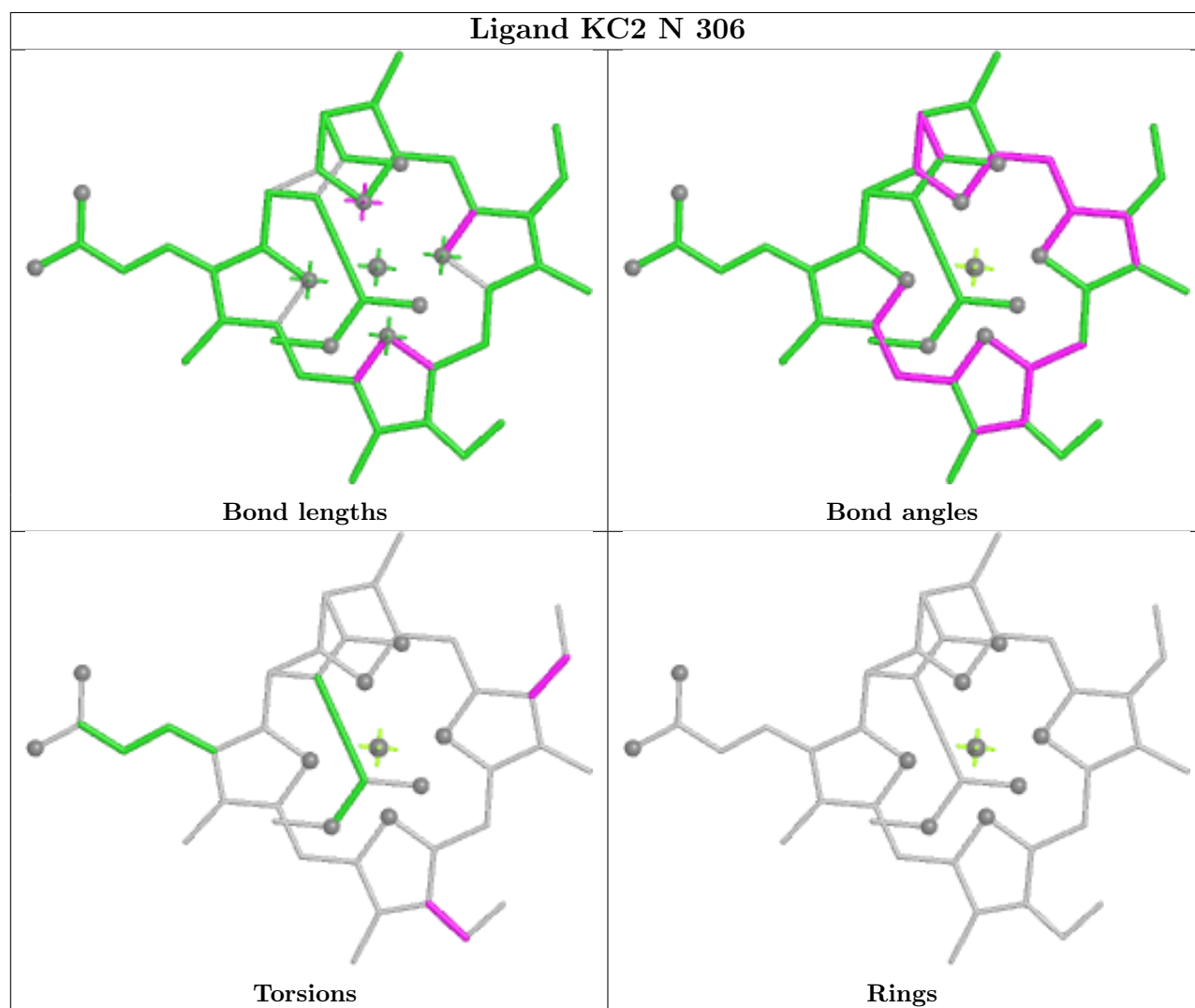
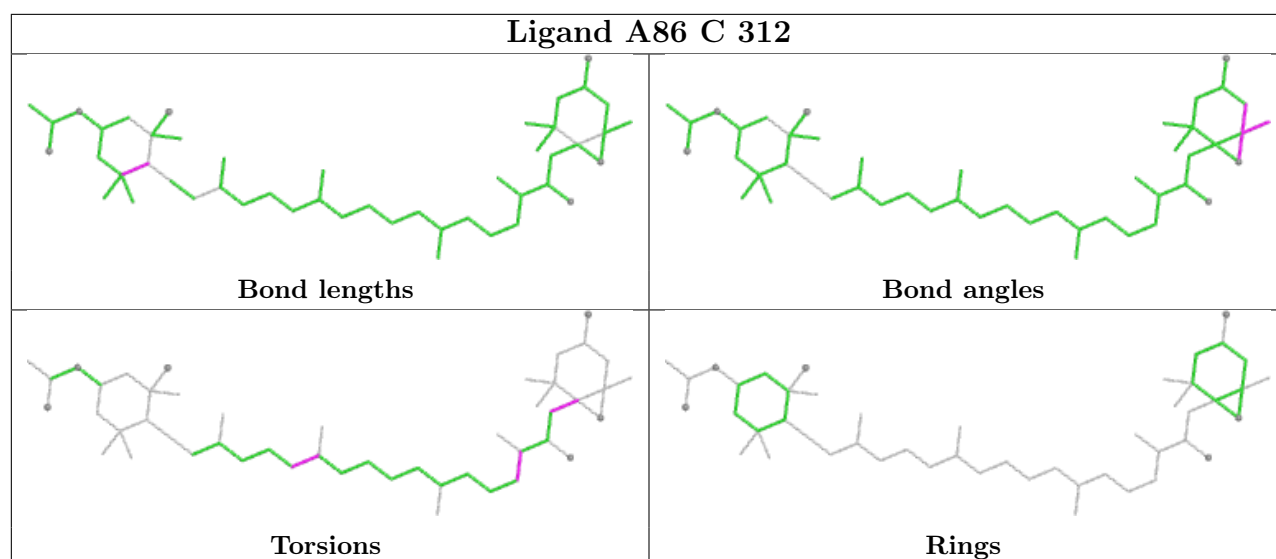
Bond angles



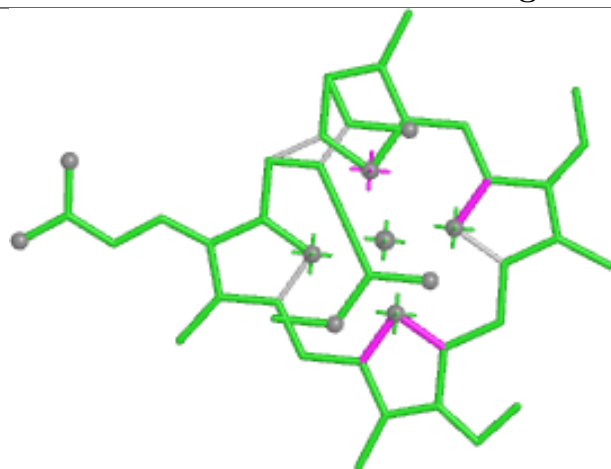
Torsions



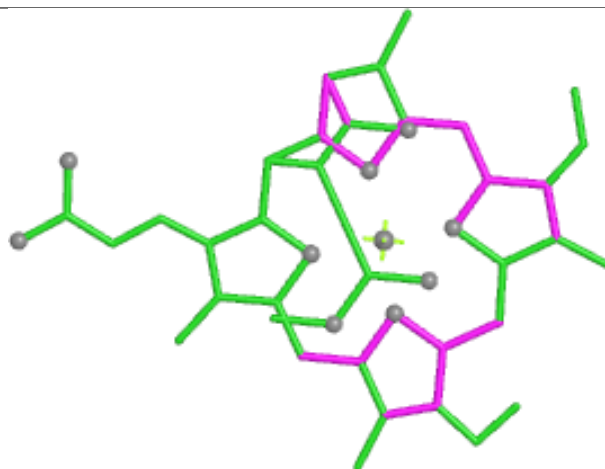
Rings



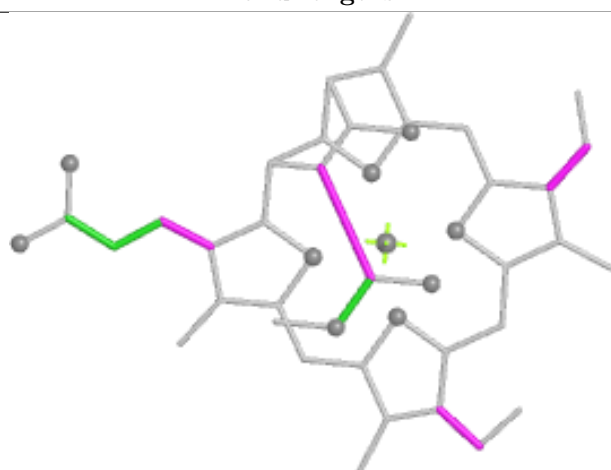
Ligand KC2 S 306



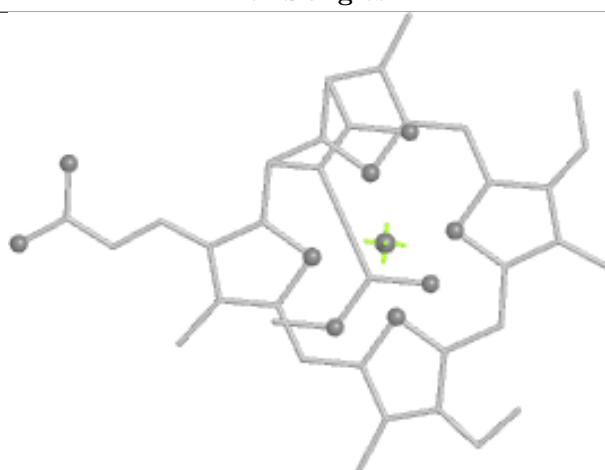
Bond lengths



Bond angles

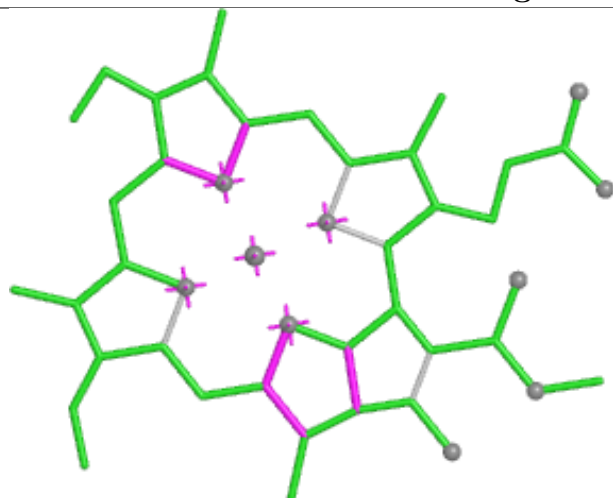


Torsions

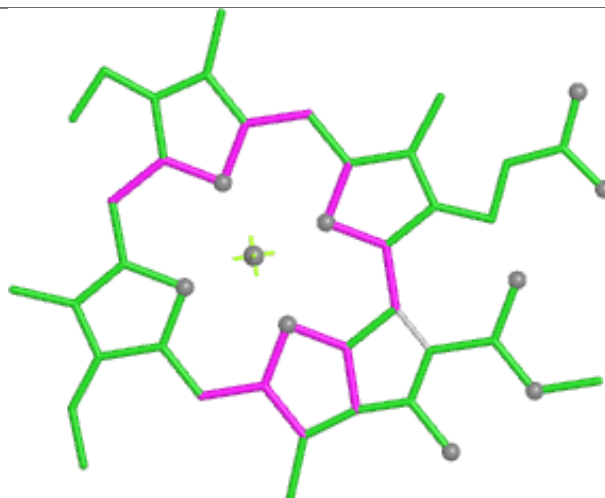


Rings

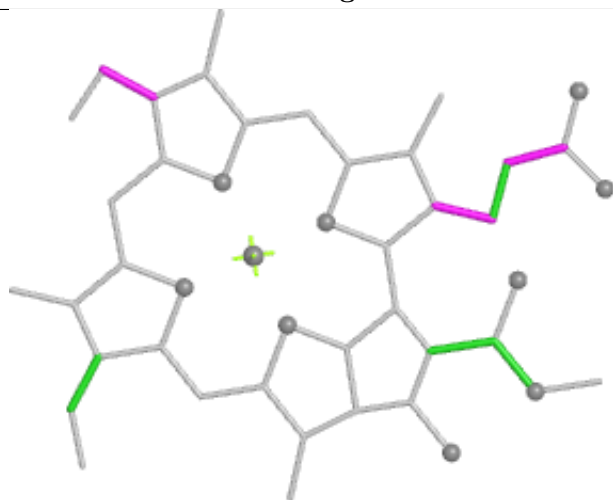
Ligand CLA O 301



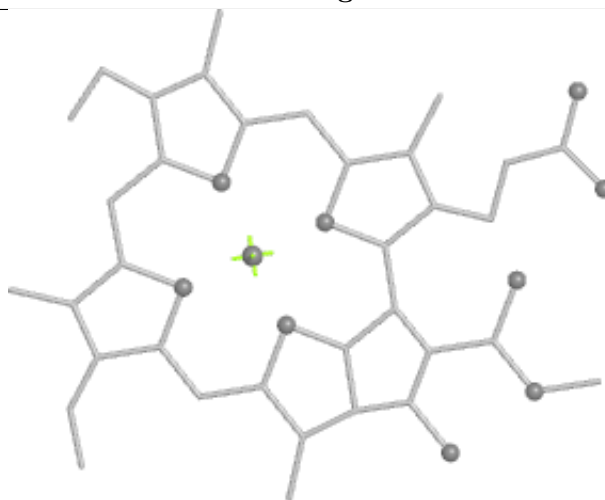
Bond lengths



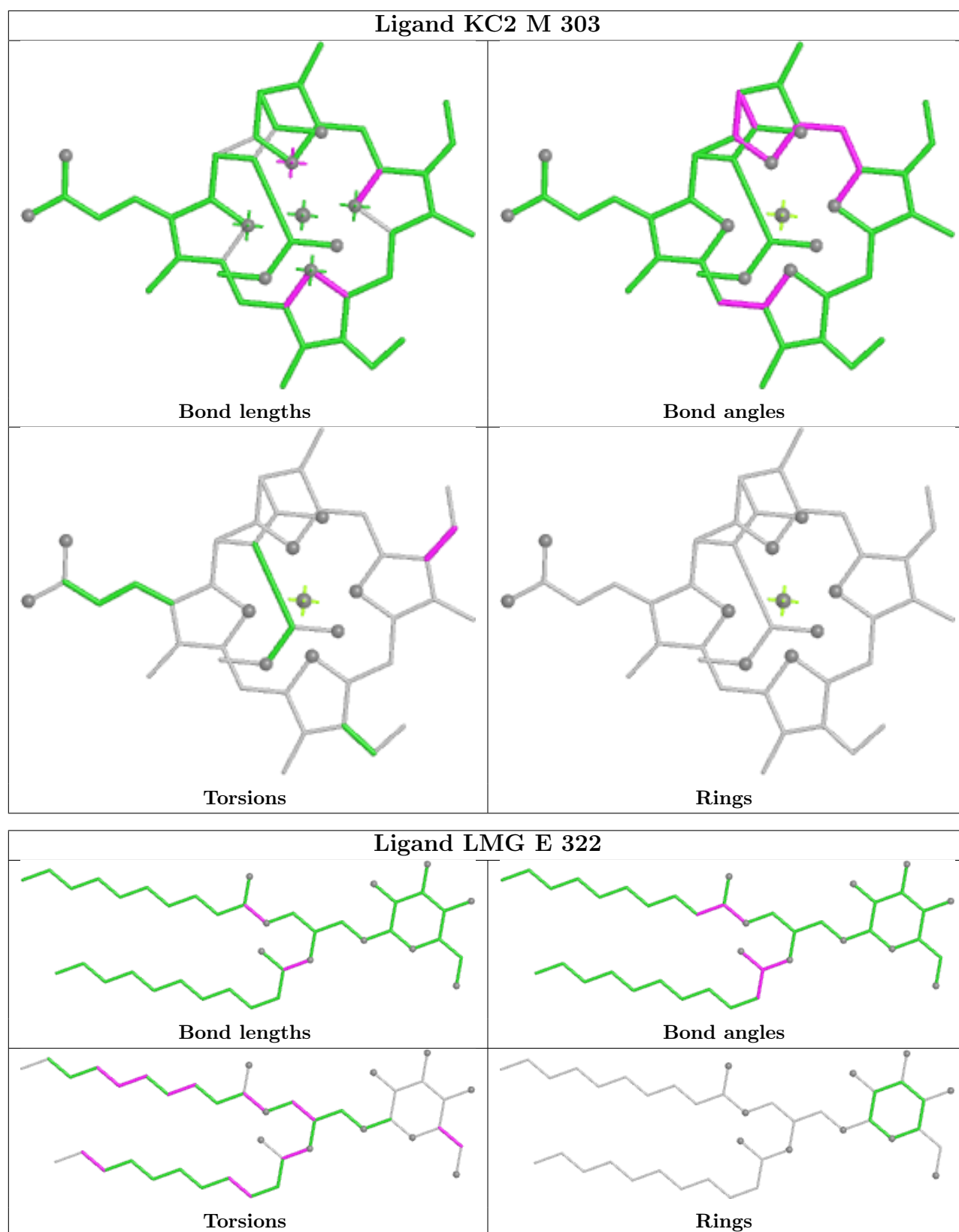
Bond angles

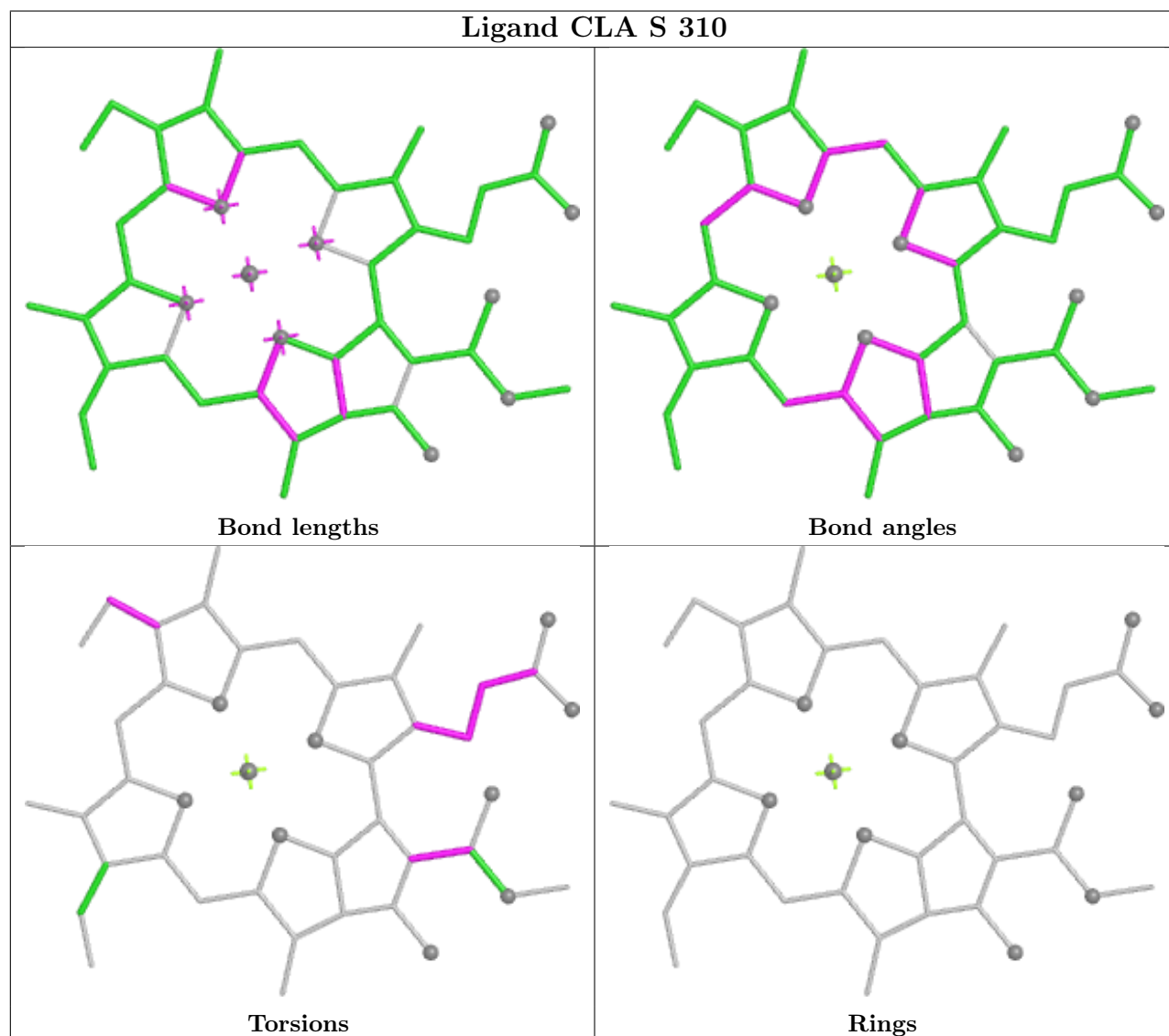
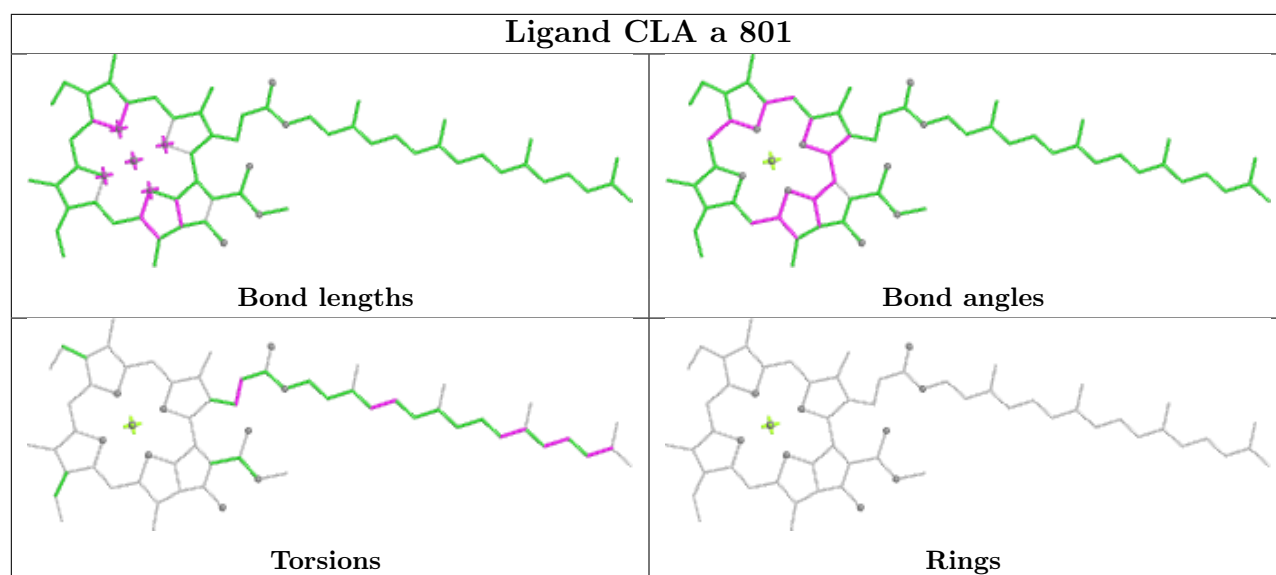


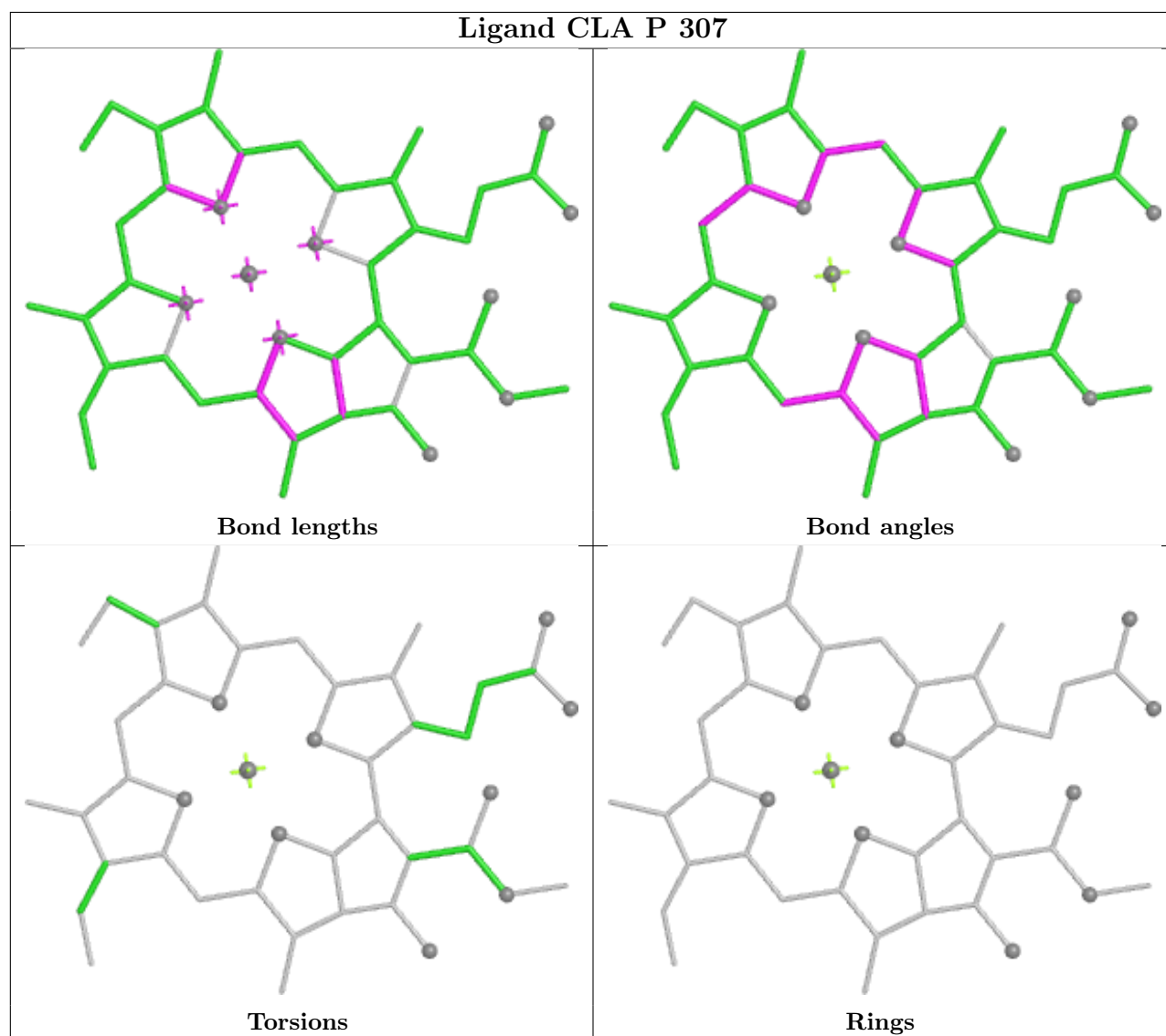
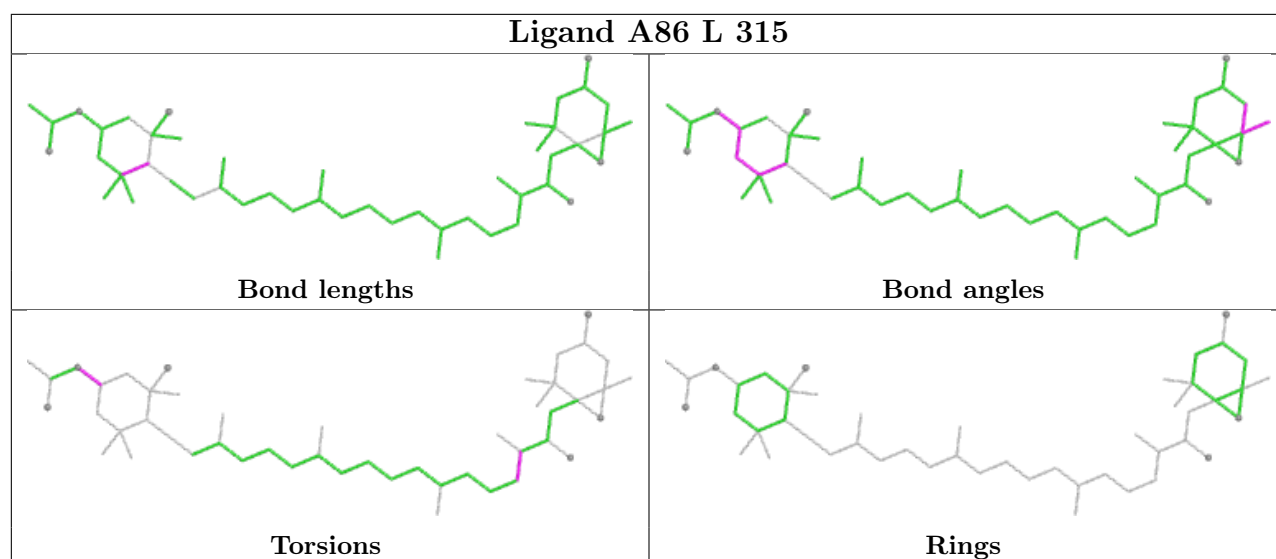
Torsions

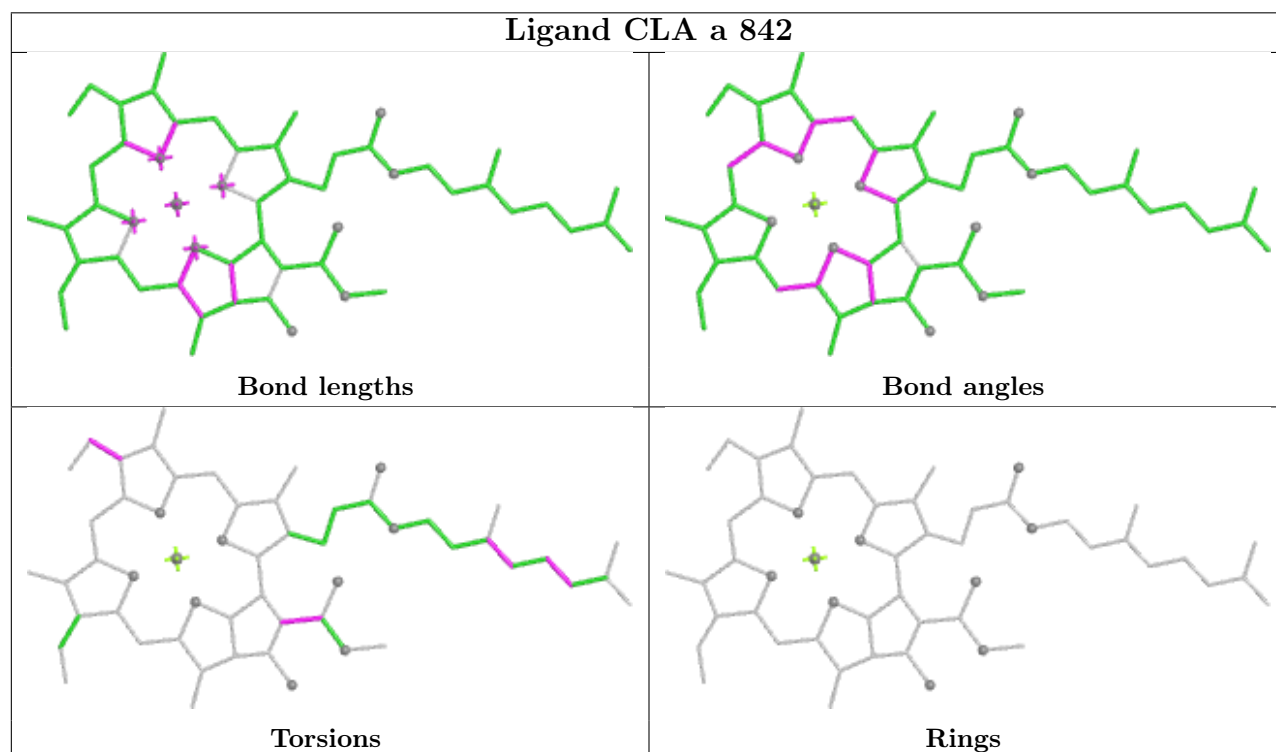
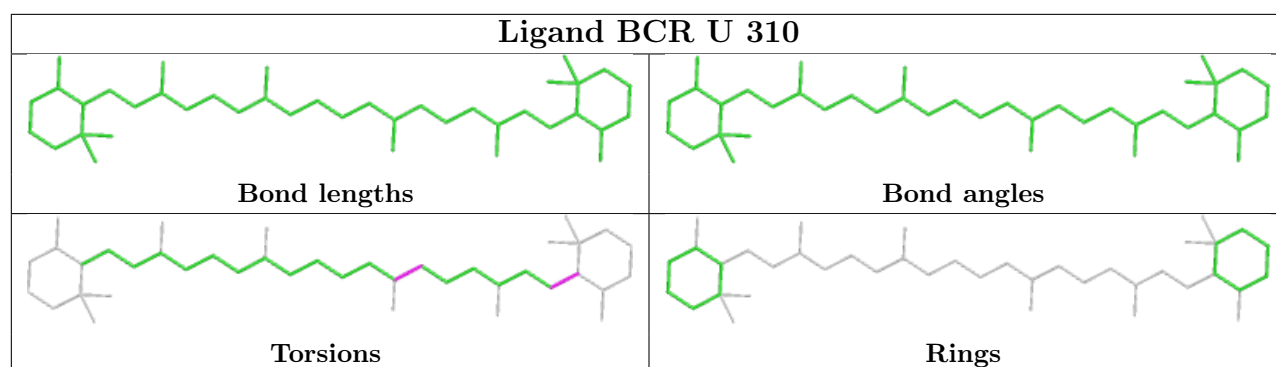


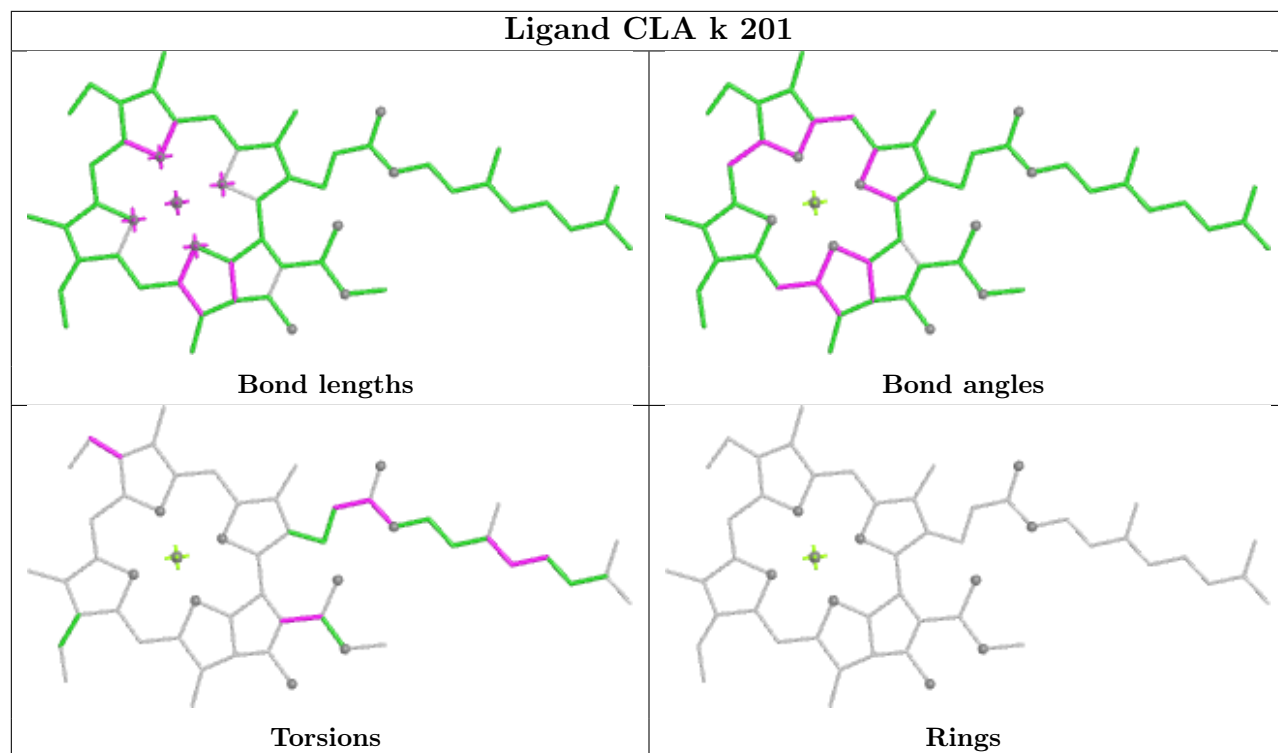
Rings

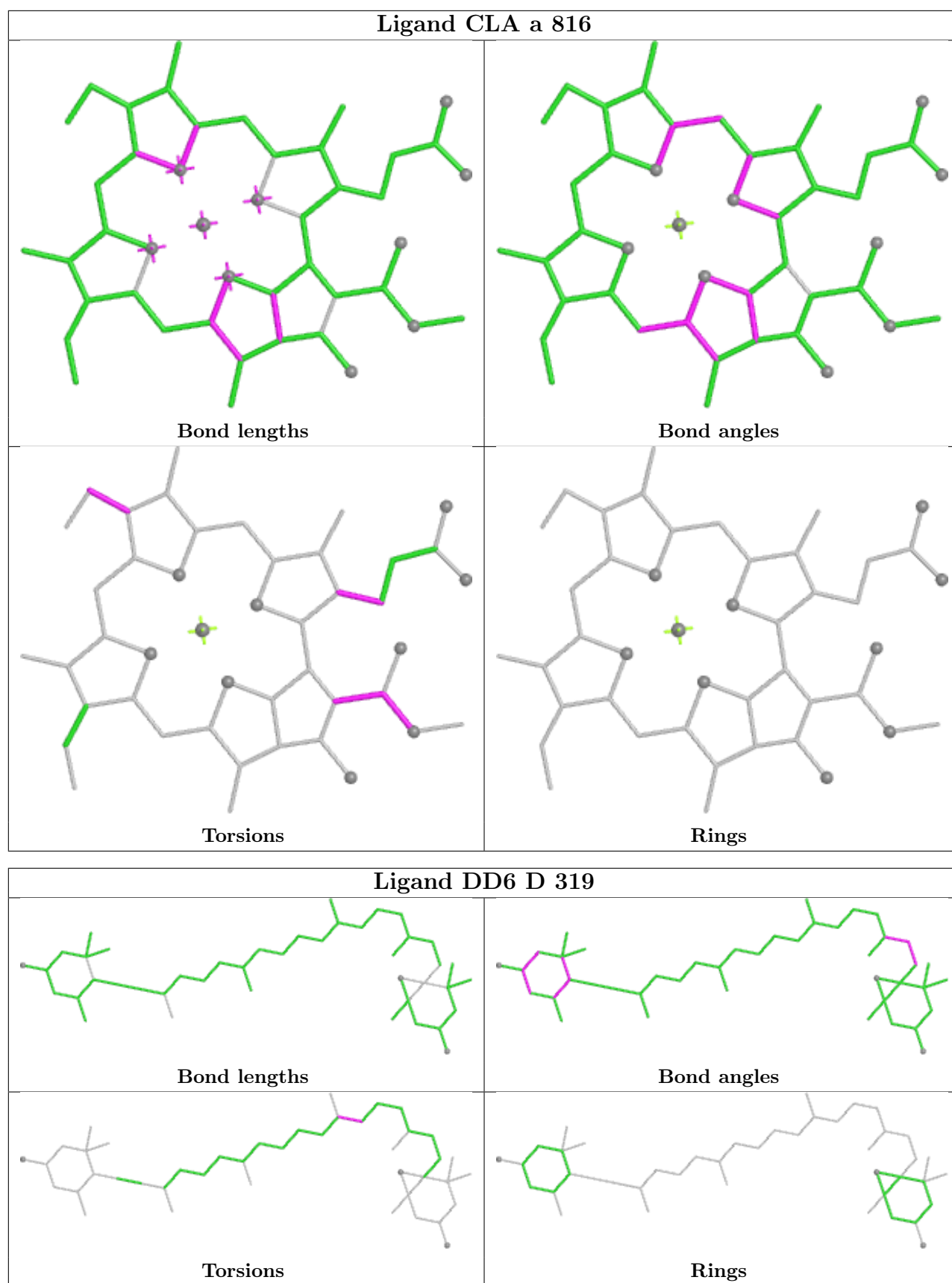




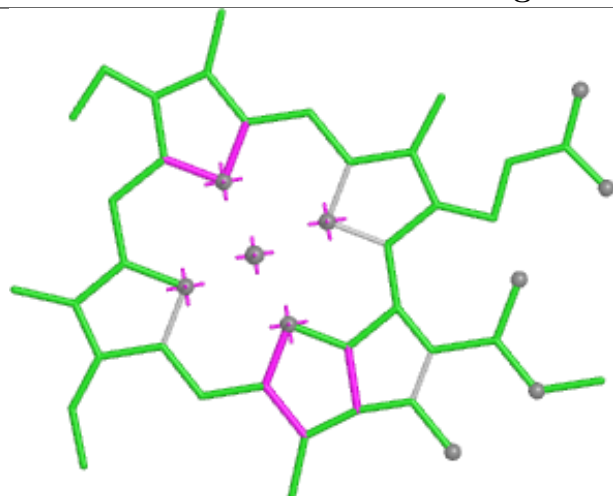




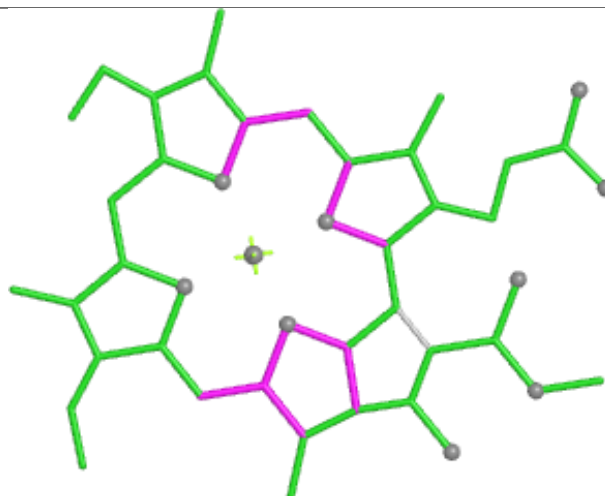




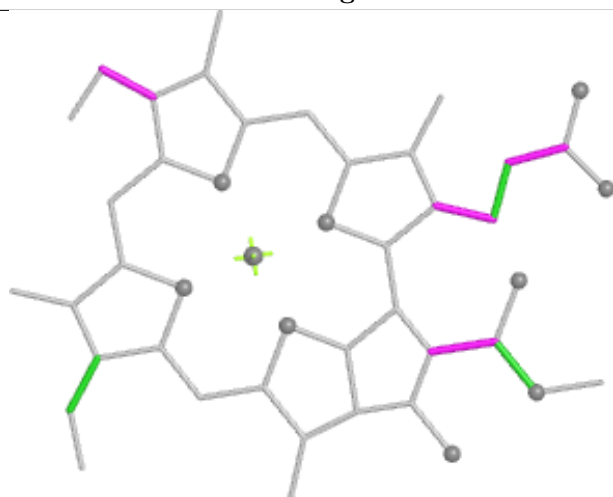
Ligand CLA A 311



Bond lengths



Bond angles

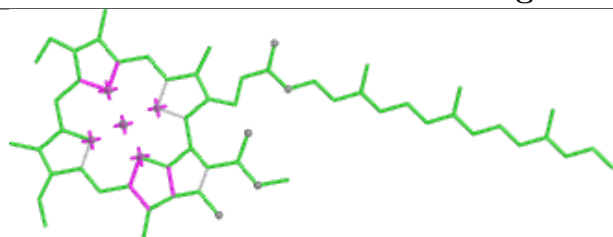


Torsions

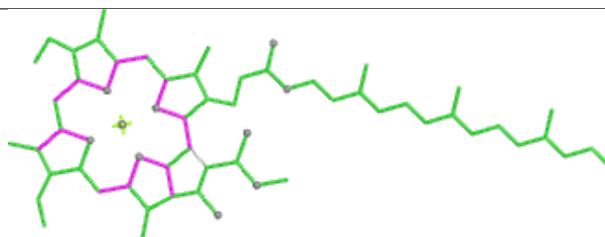


Rings

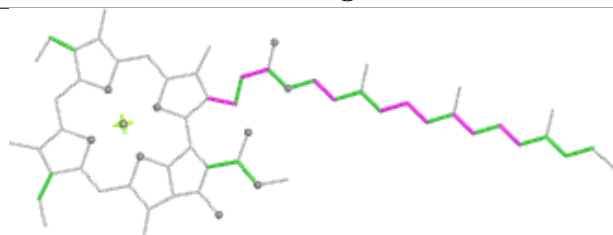
Ligand CLA F 303



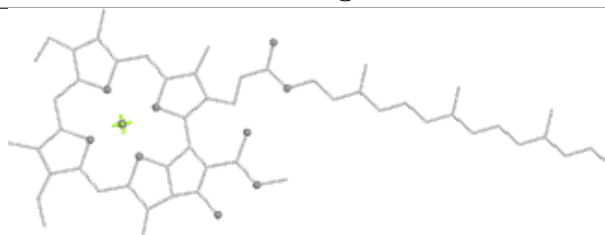
Bond lengths



Bond angles

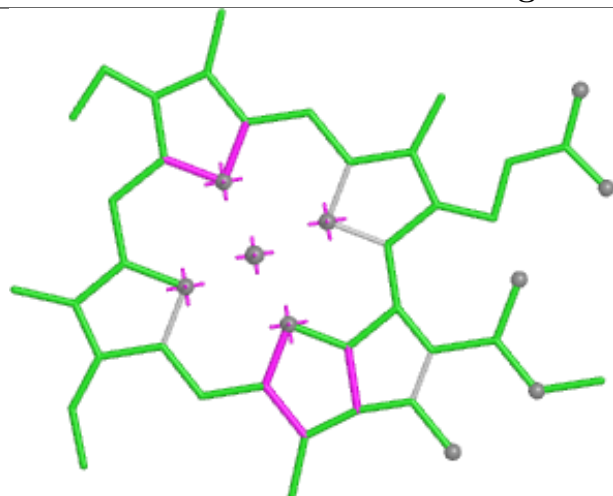


Torsions

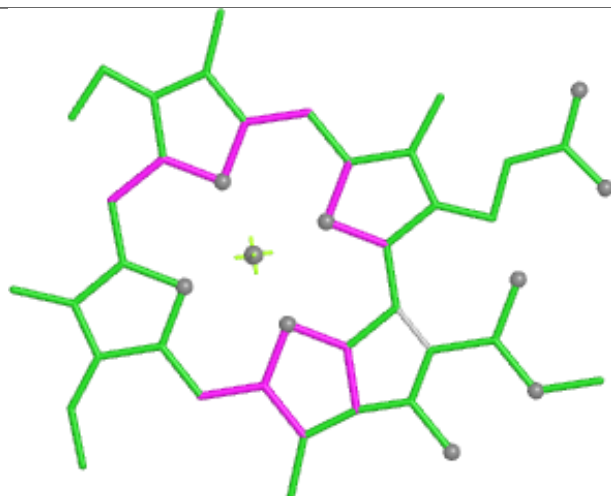


Rings

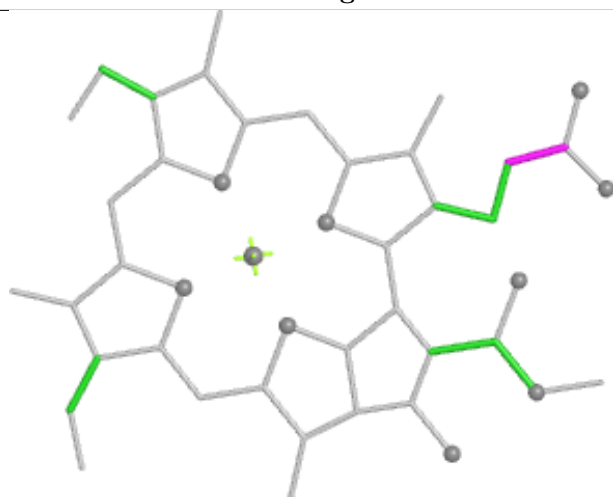
Ligand CLA J 311



Bond lengths



Bond angles

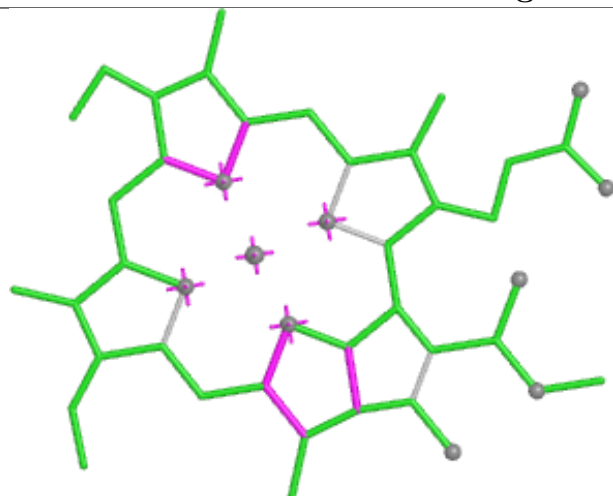


Torsions

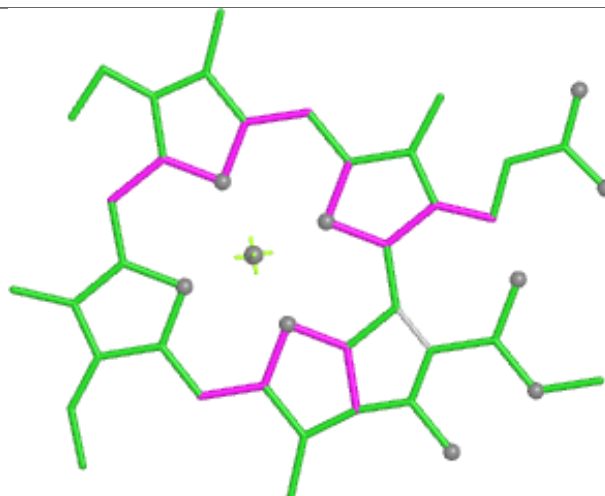


Rings

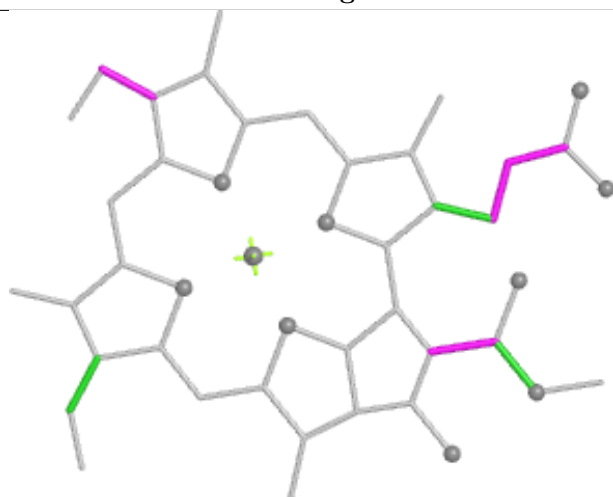
Ligand CLA L 301



Bond lengths



Bond angles

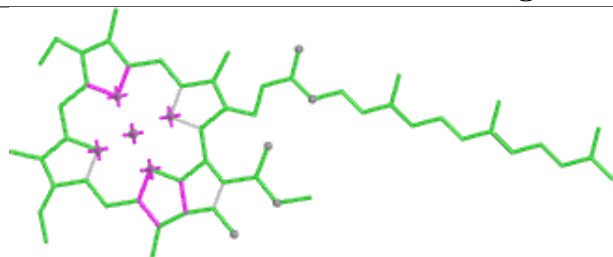


Torsions

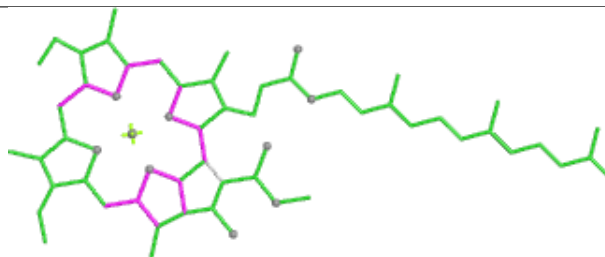


Rings

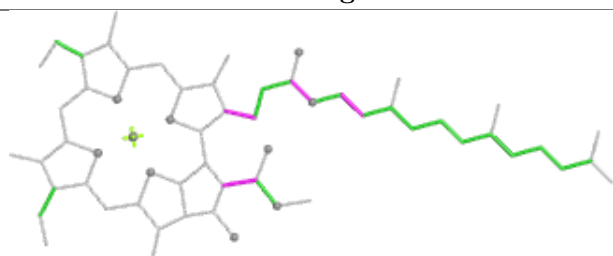
Ligand CLA b 801



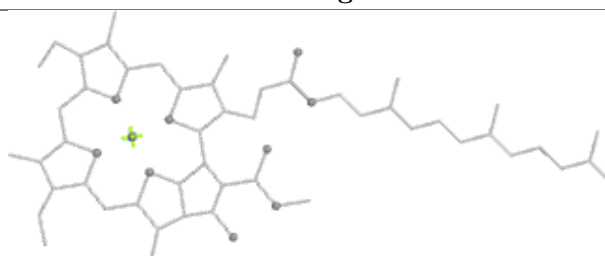
Bond lengths



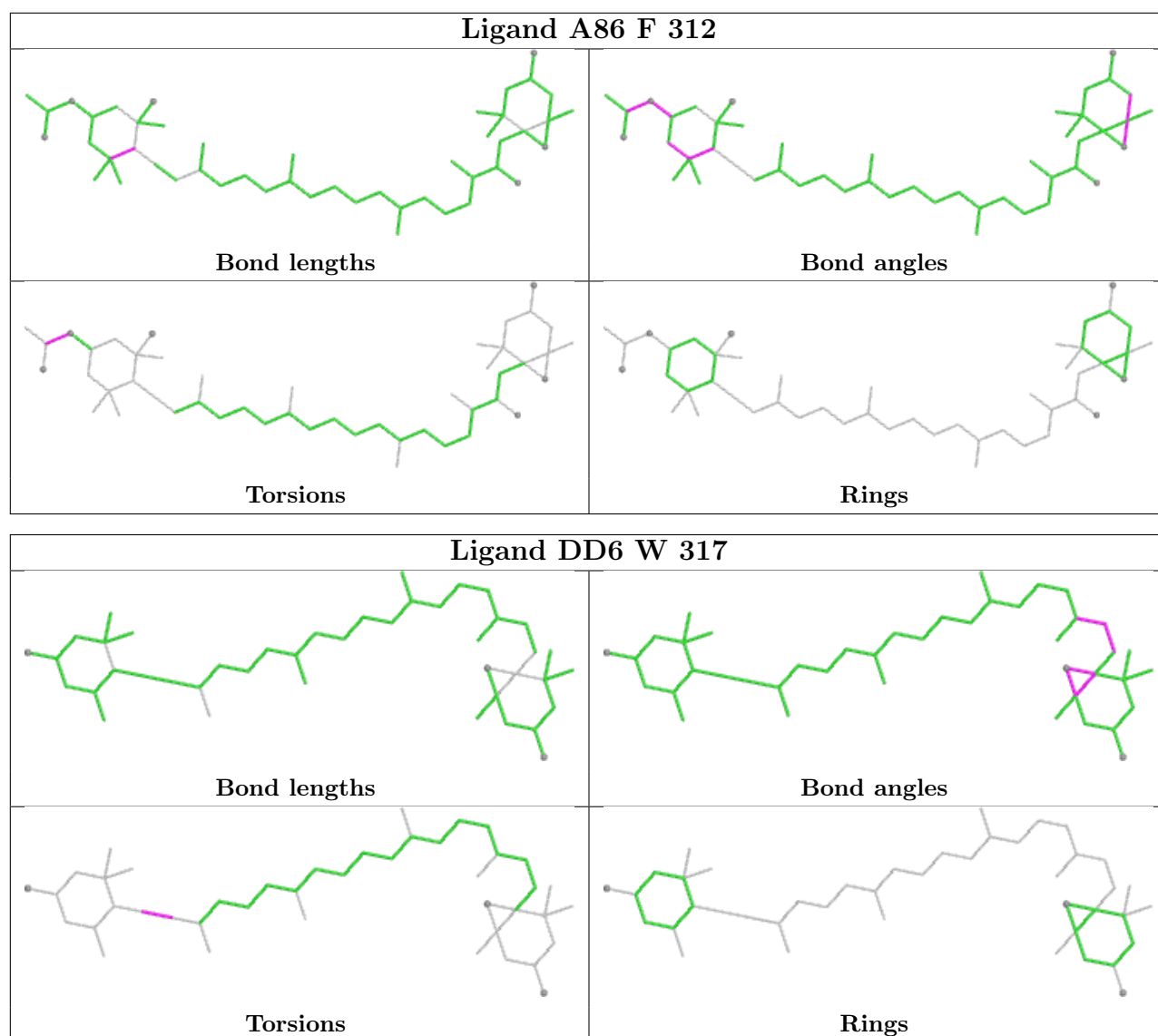
Bond angles

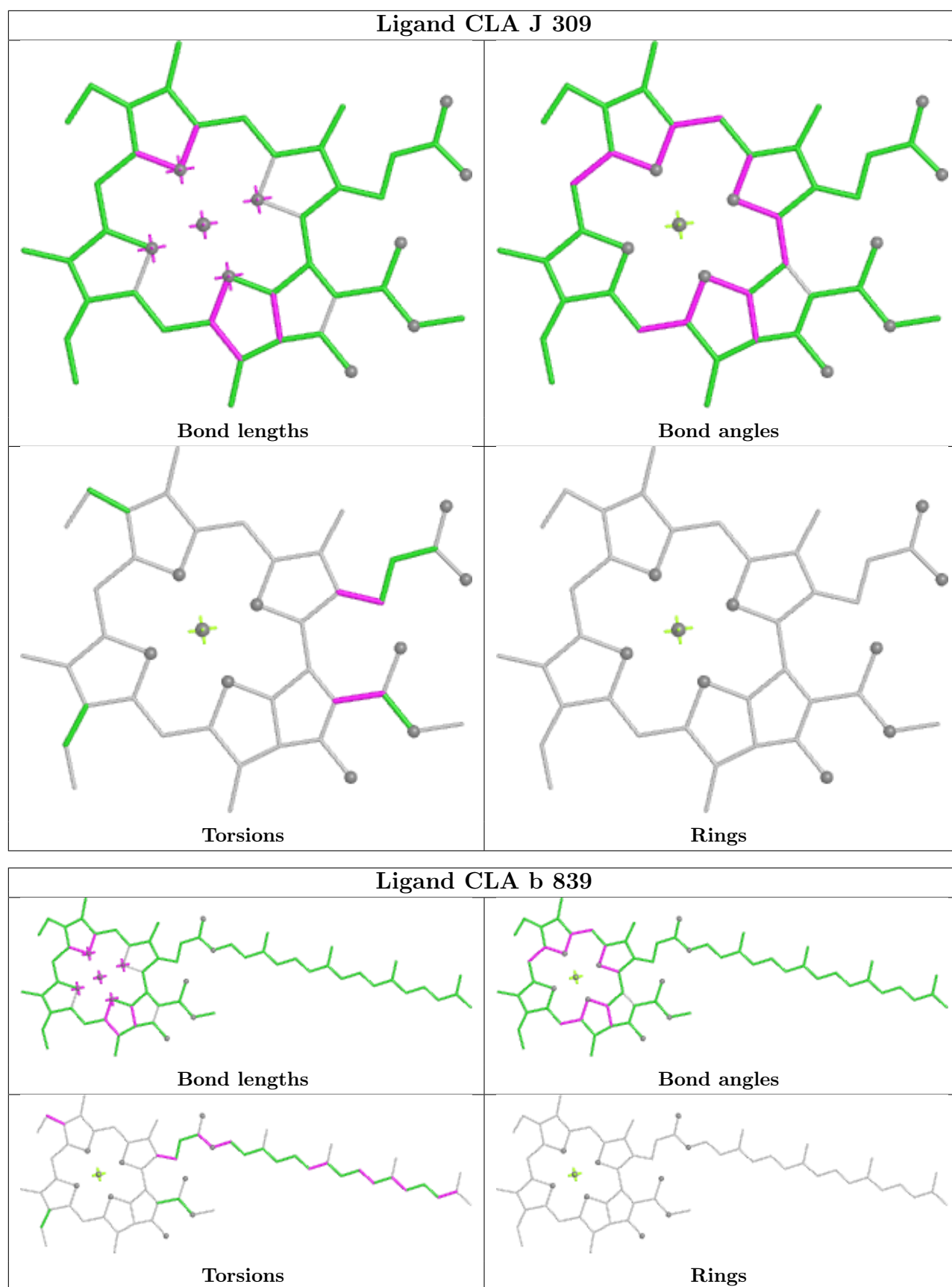


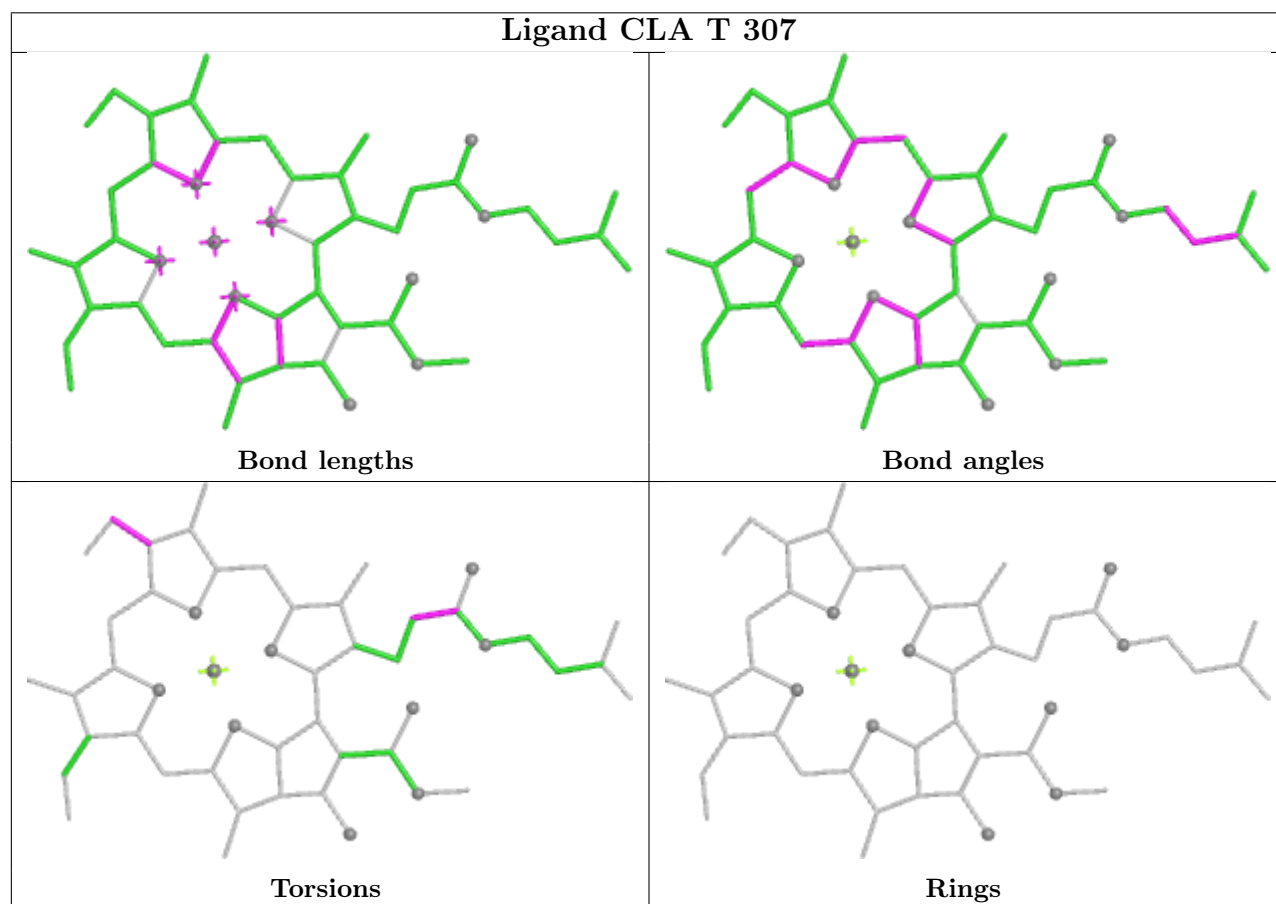
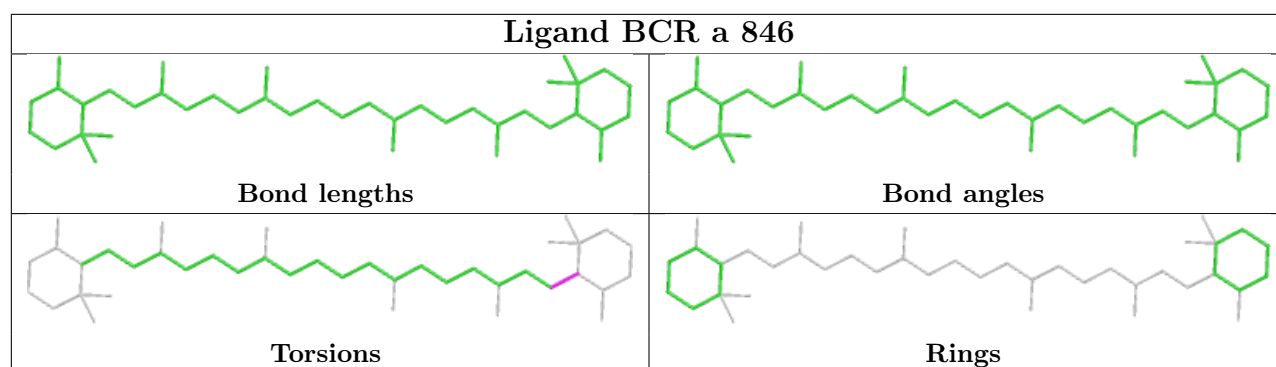
Torsions

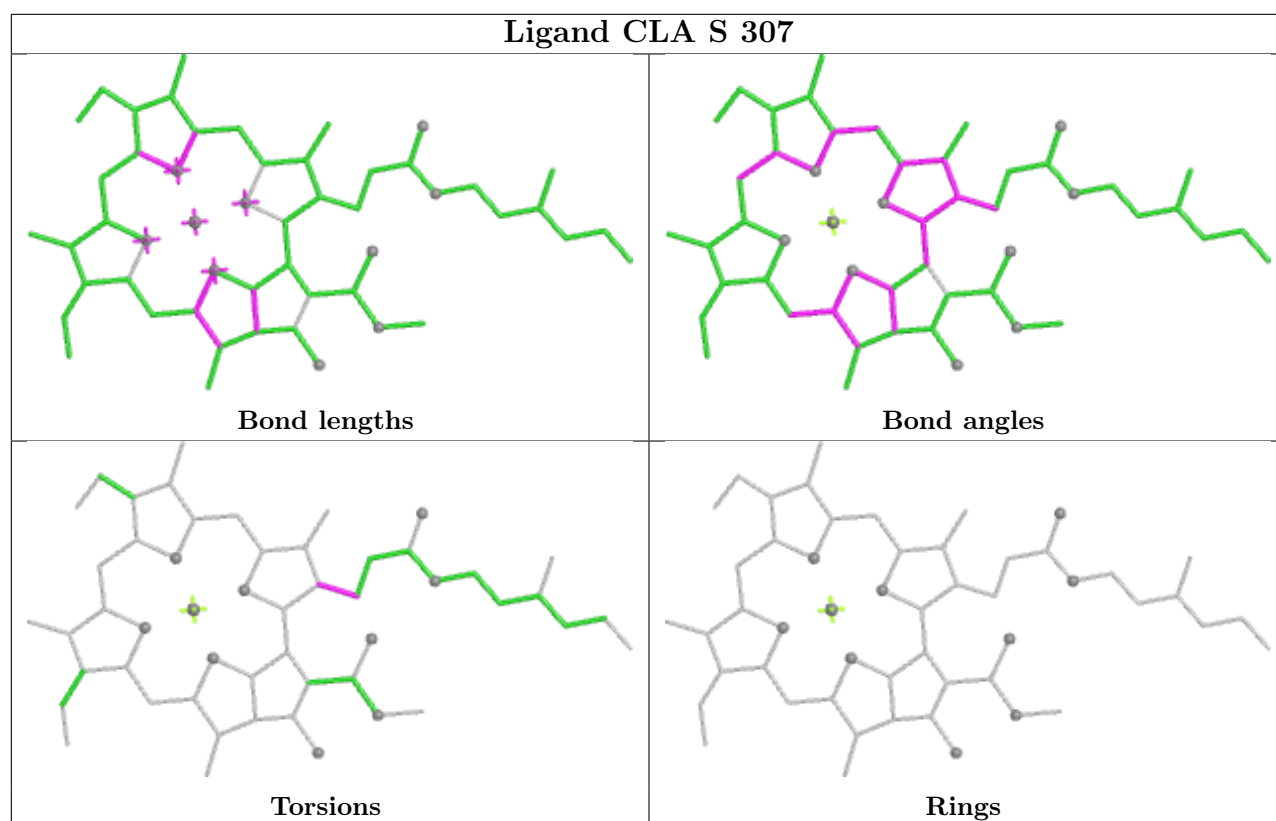


Rings

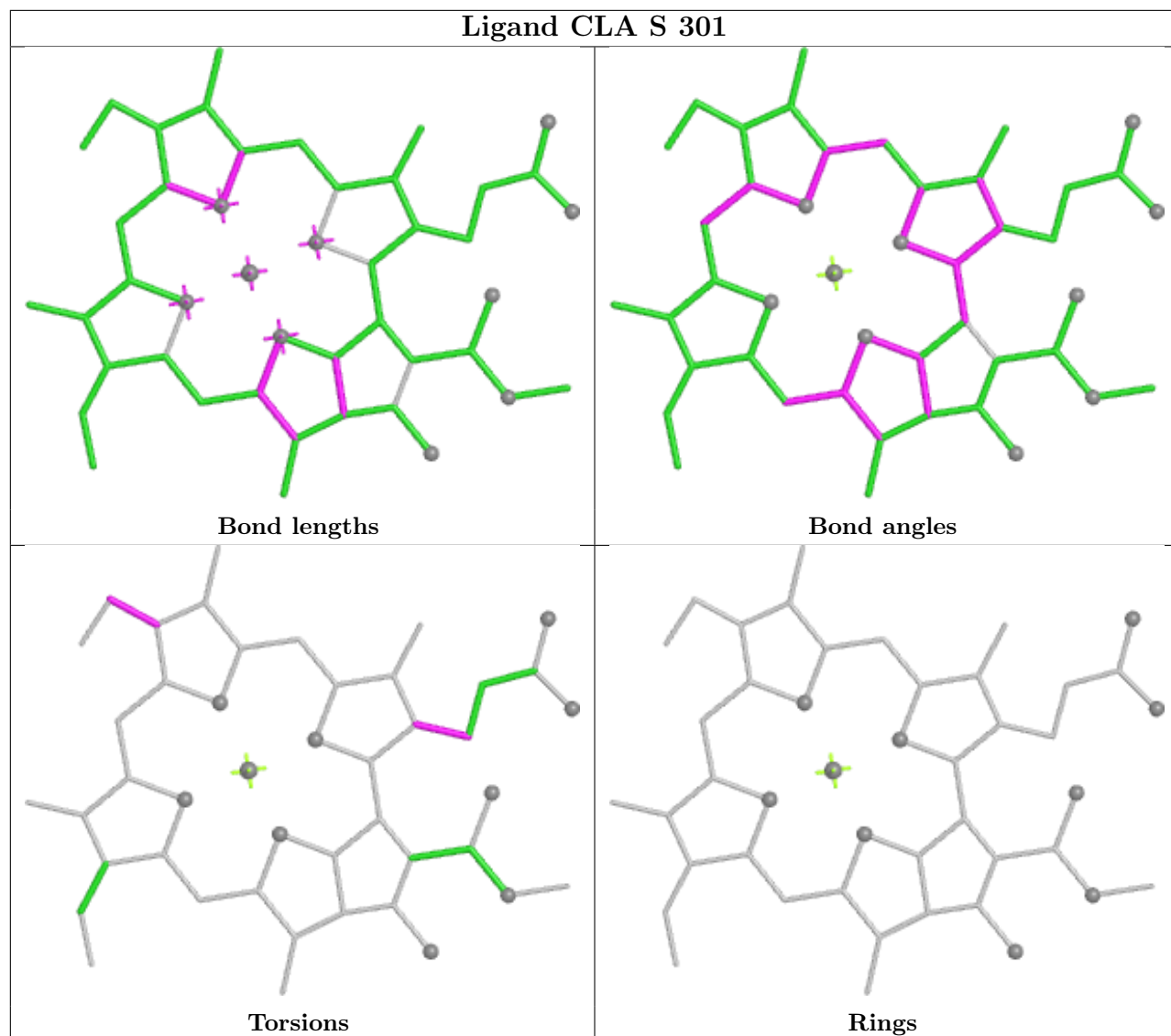




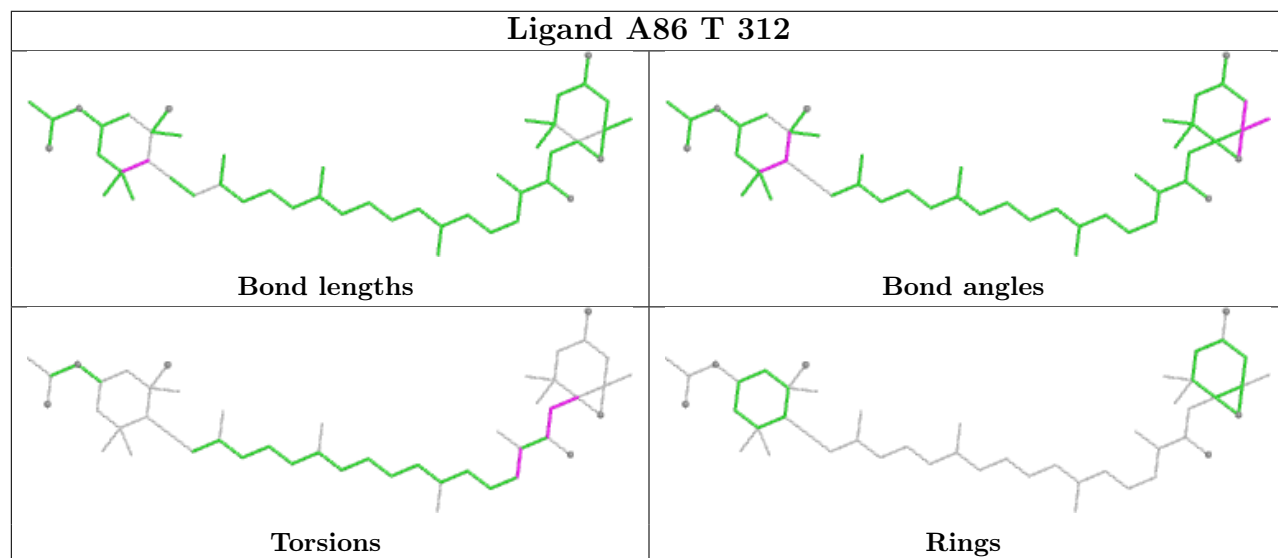


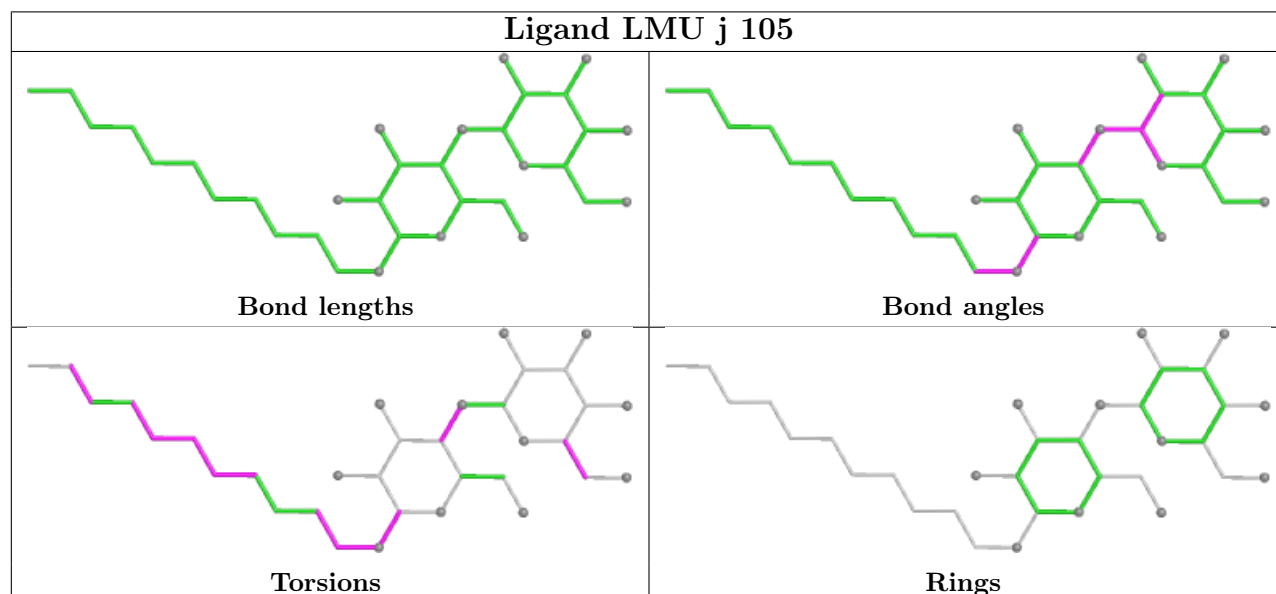
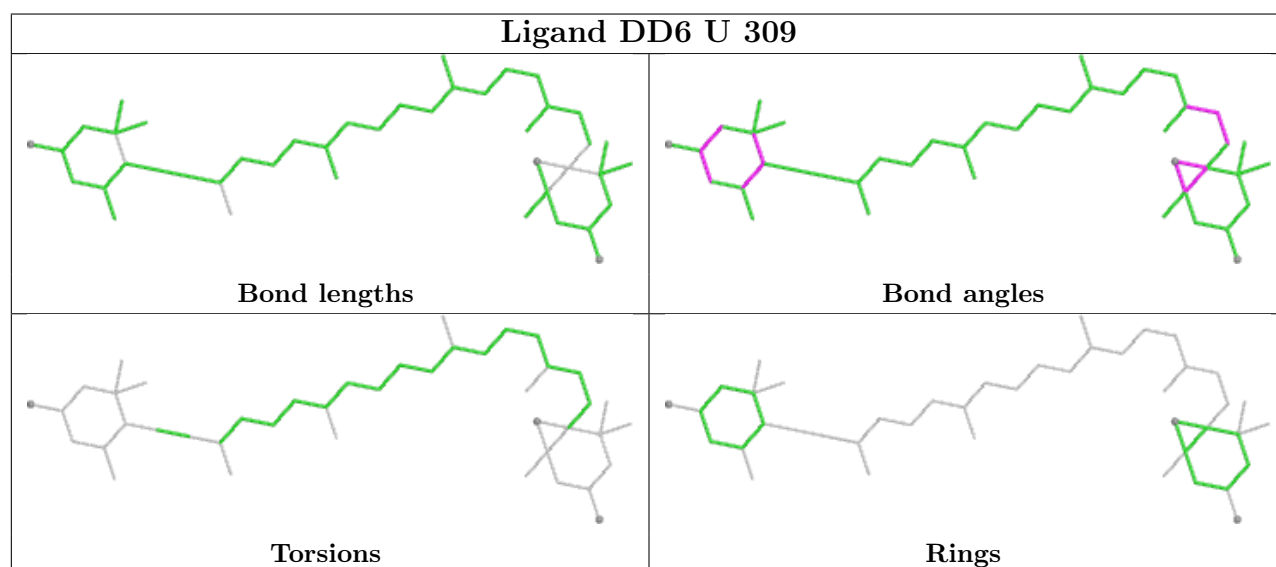
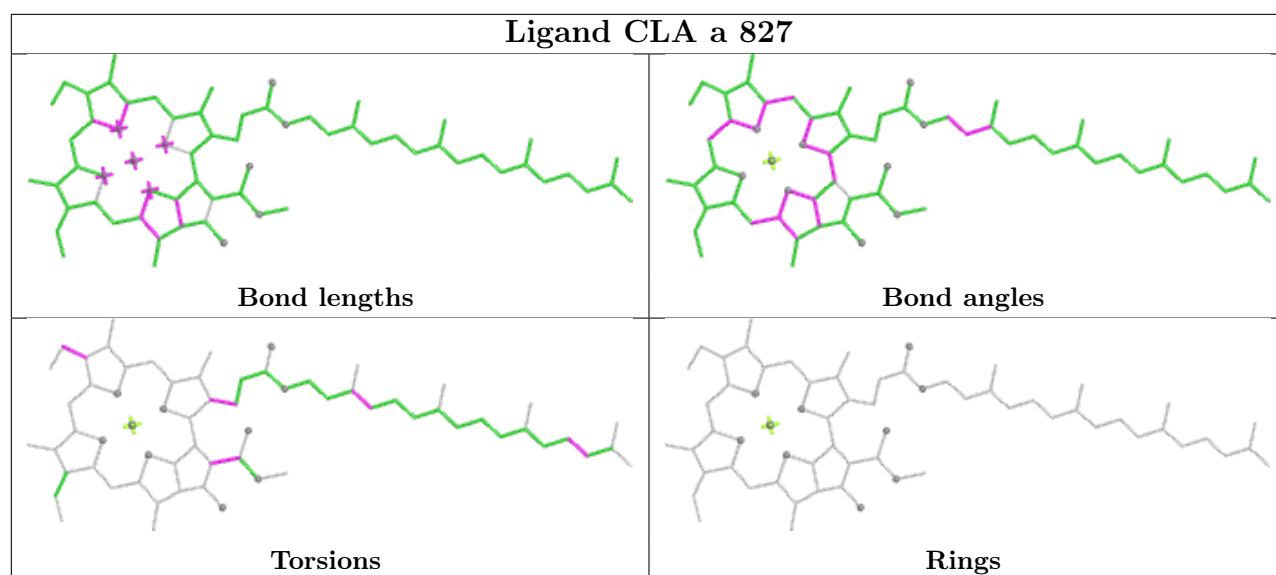


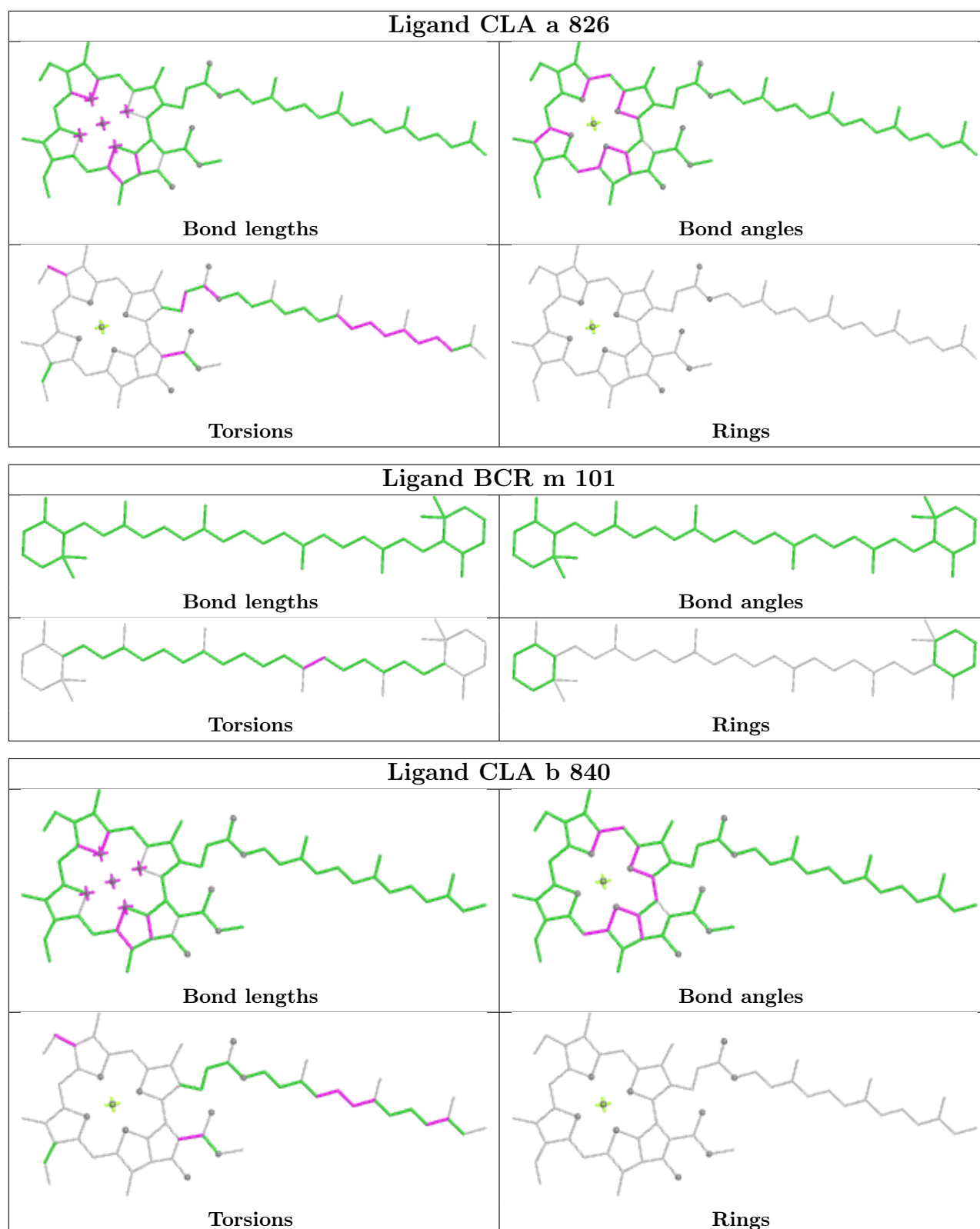
Ligand CLA S 301



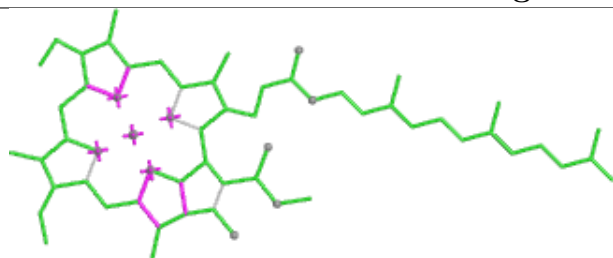
Ligand A86 T 312



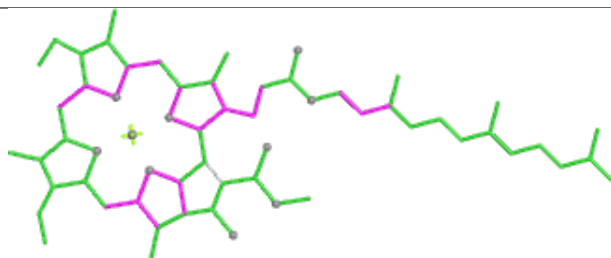




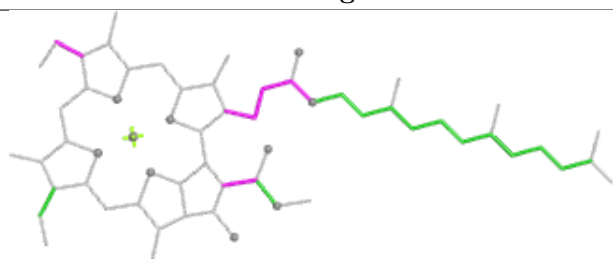
Ligand CLA K 306



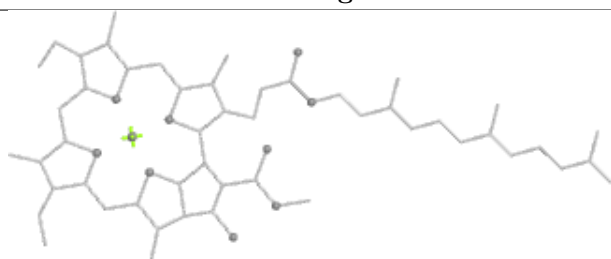
Bond lengths



Bond angles

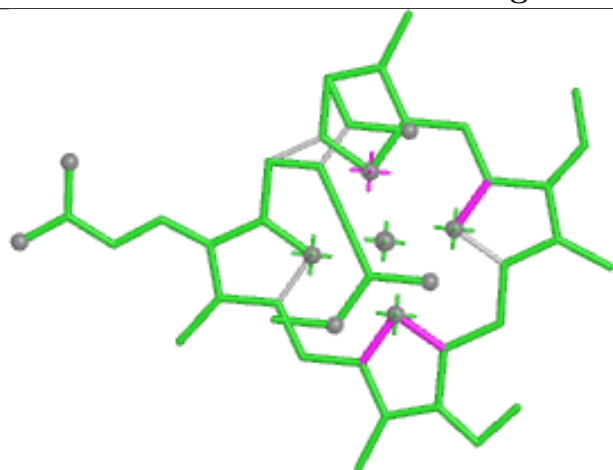


Torsions

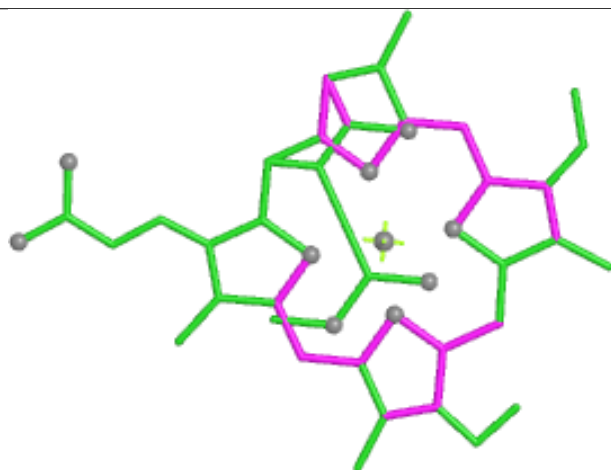


Rings

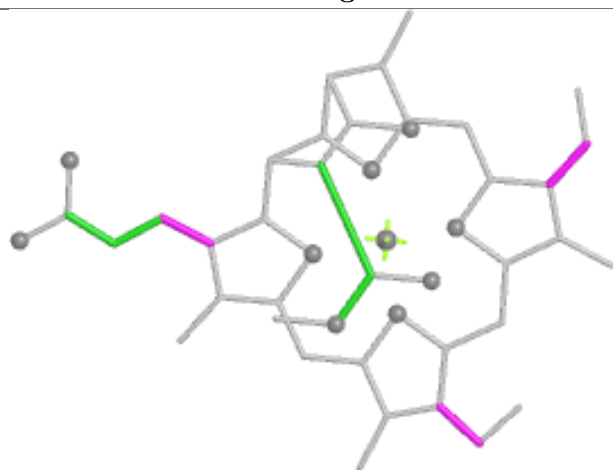
Ligand KC2 W 301



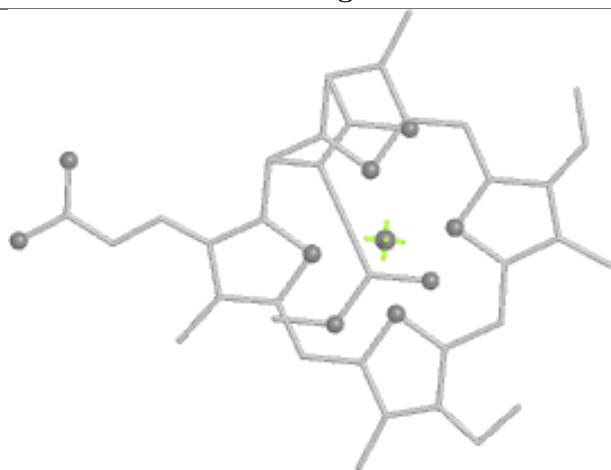
Bond lengths



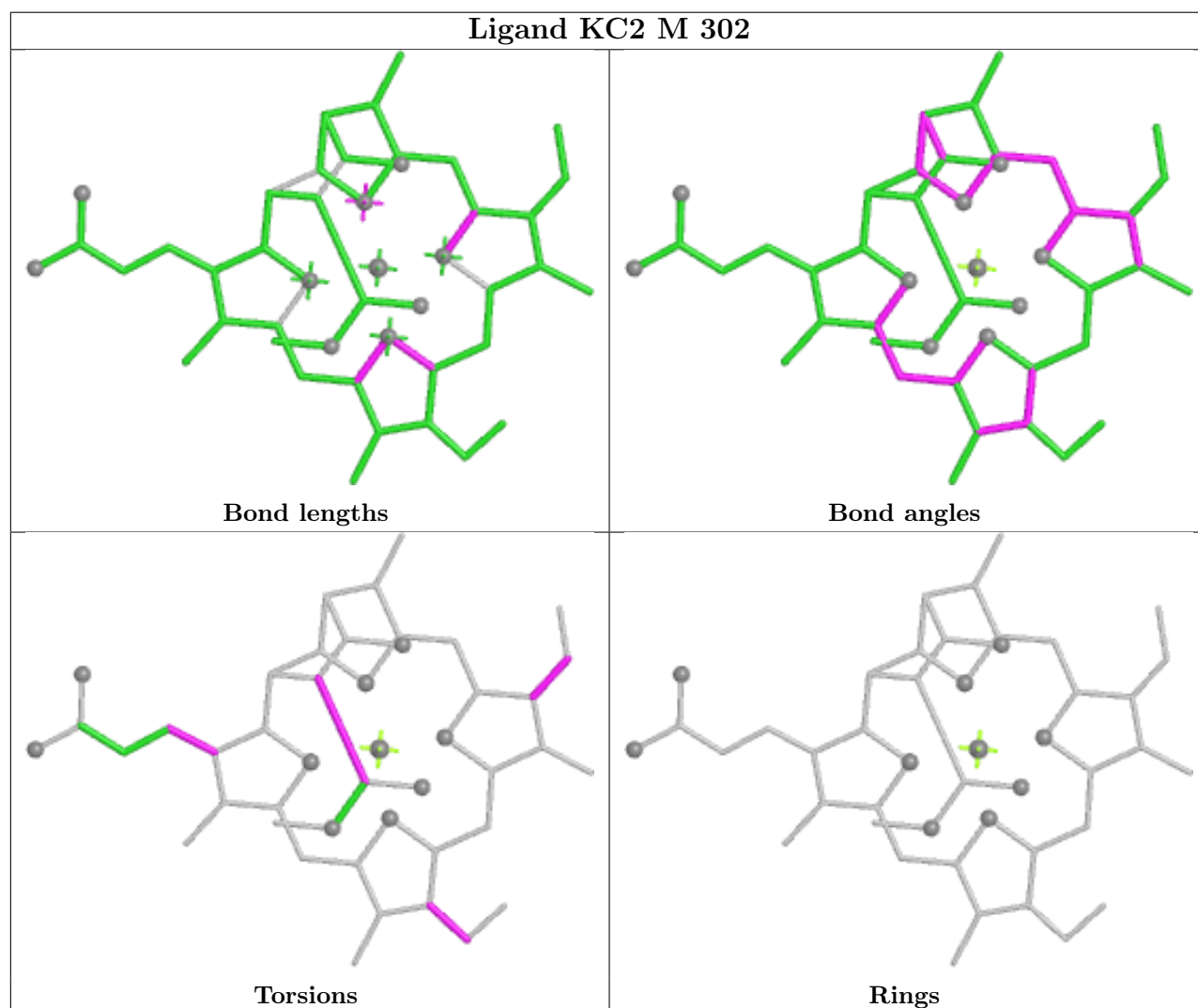
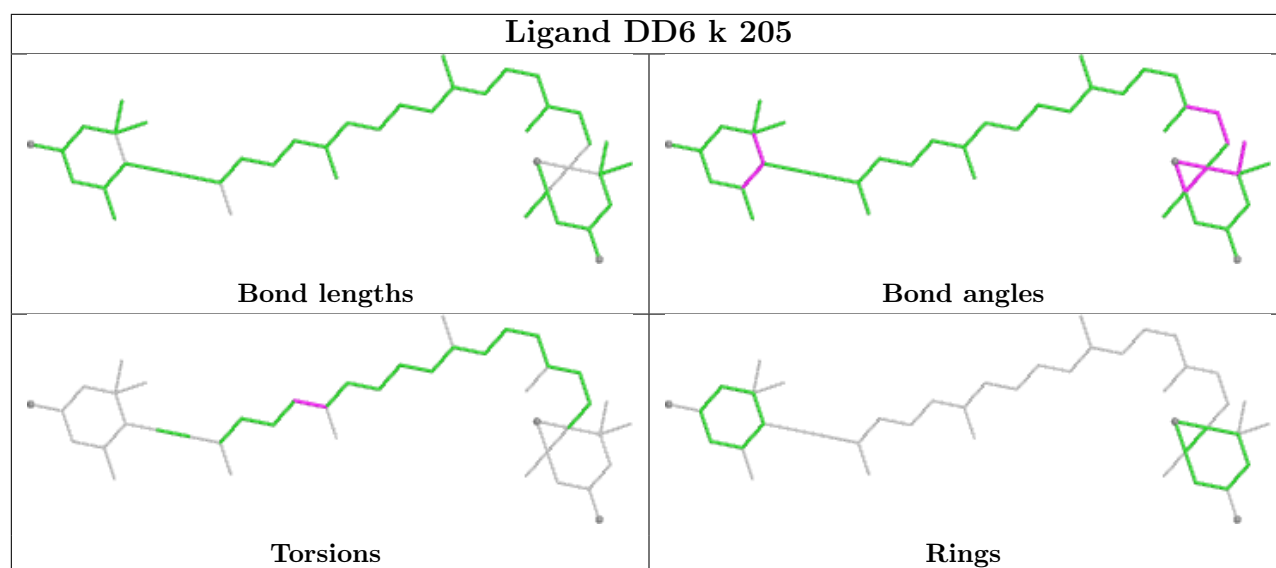
Bond angles



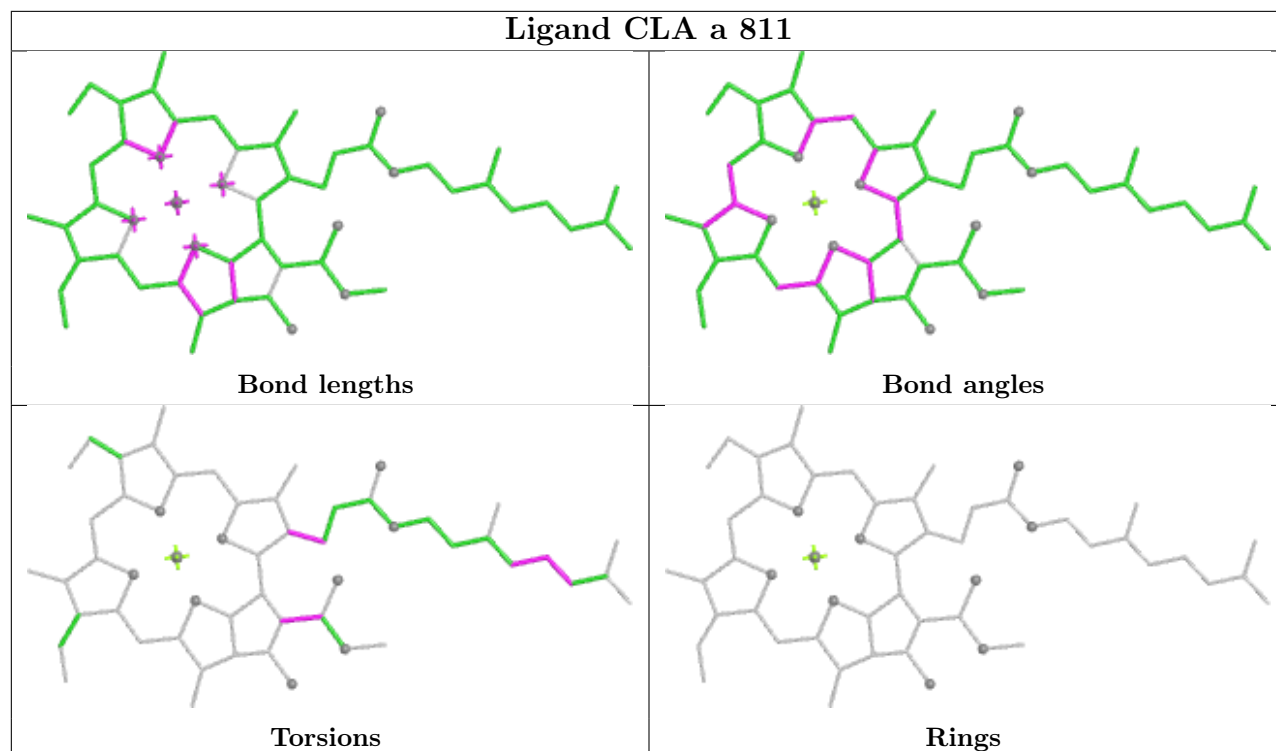
Torsions



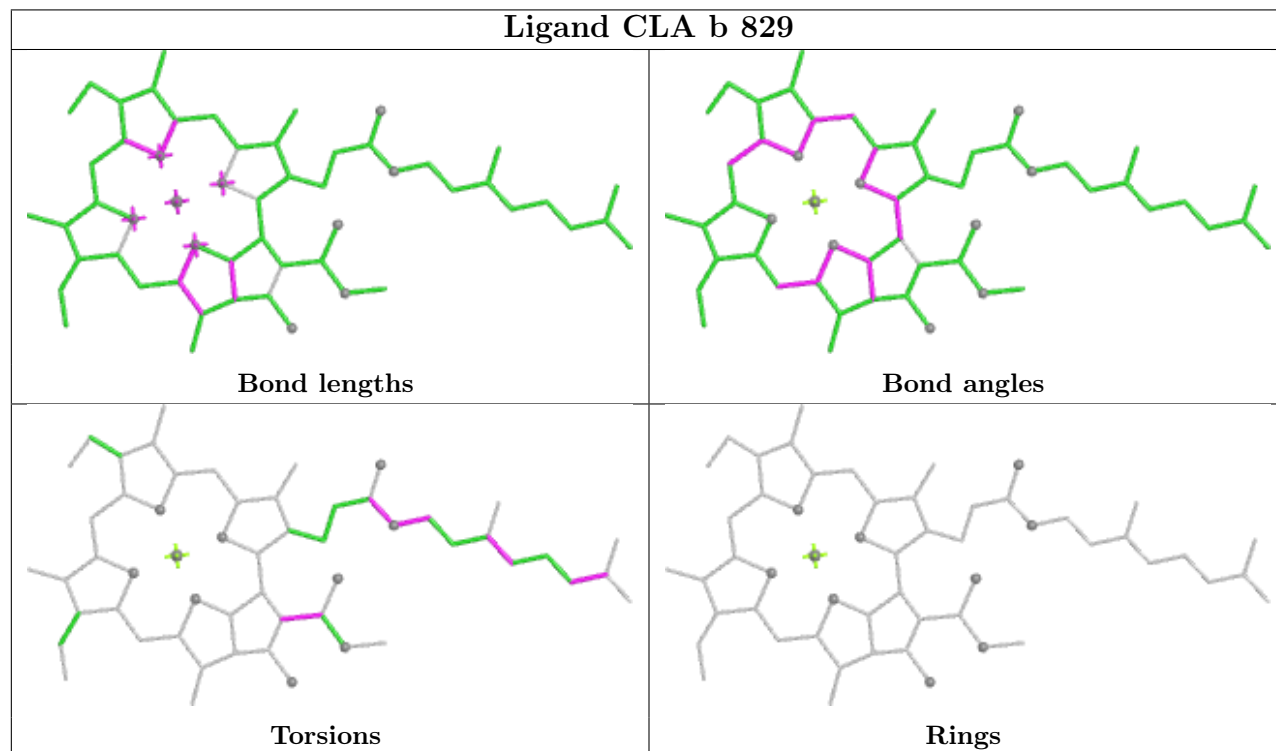
Rings

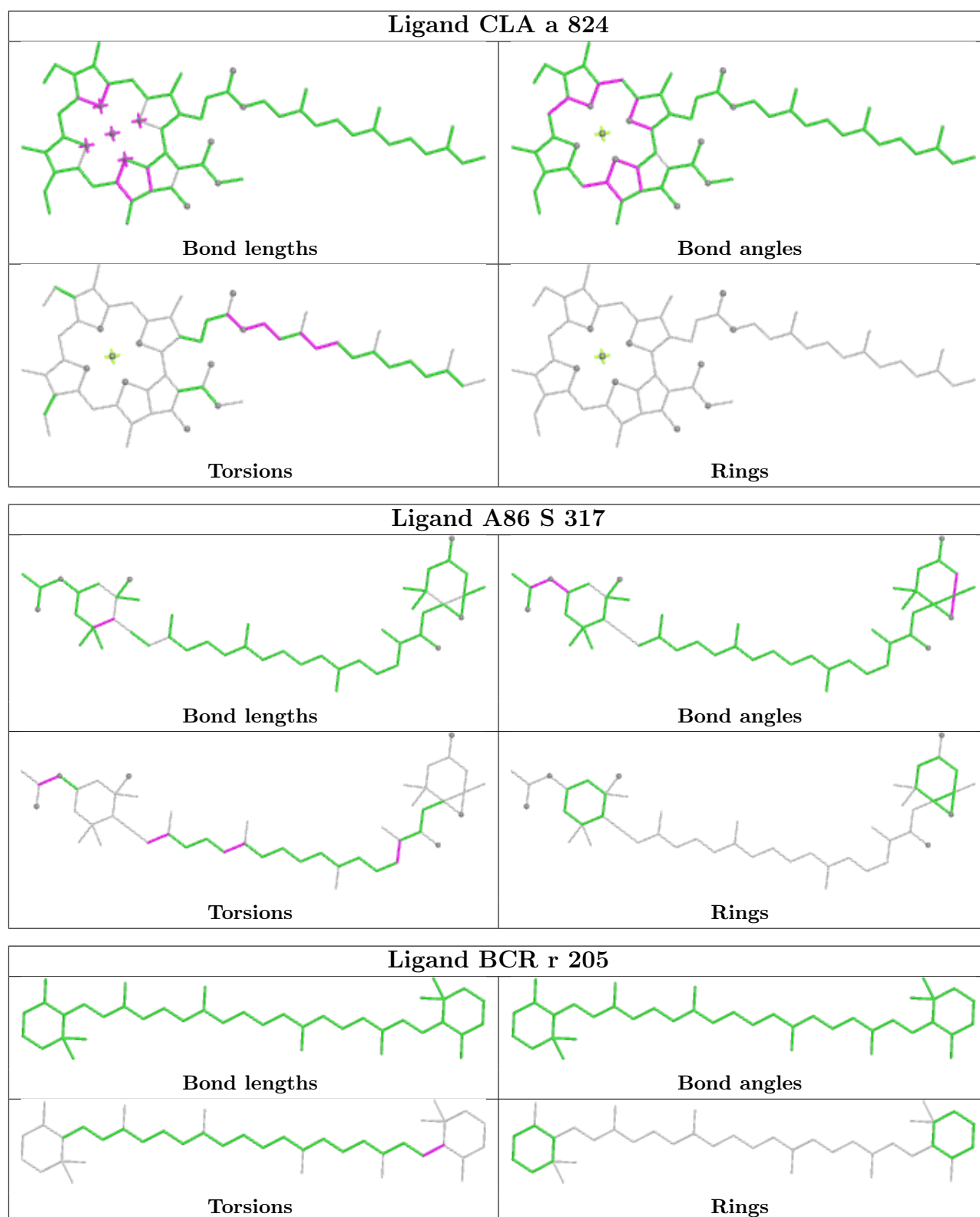


Ligand CLA a 811

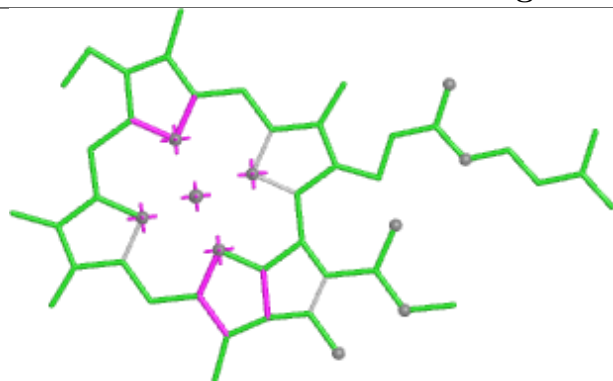


Ligand CLA b 829

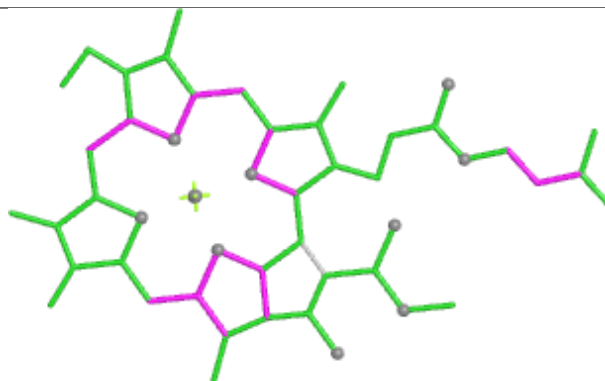




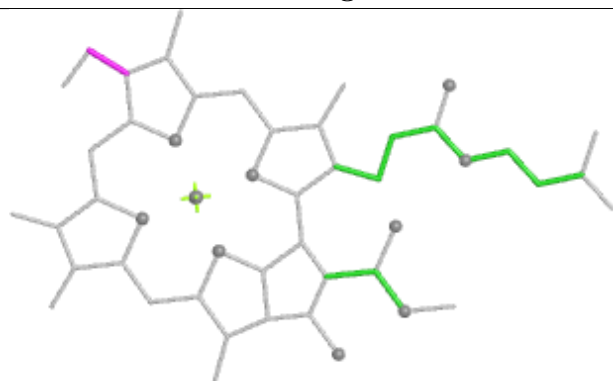
Ligand CLA F 305



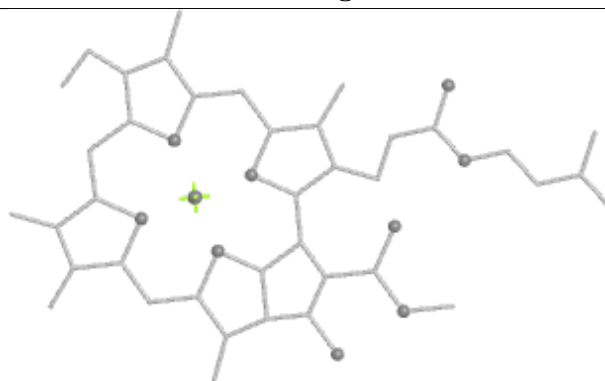
Bond lengths



Bond angles

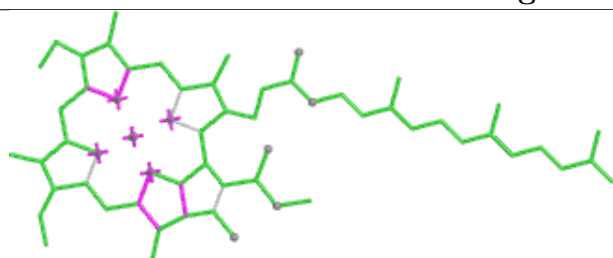


Torsions

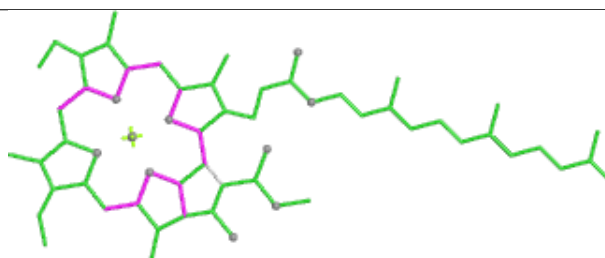


Rings

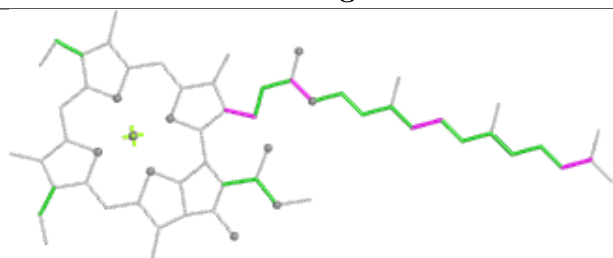
Ligand CLA a 829



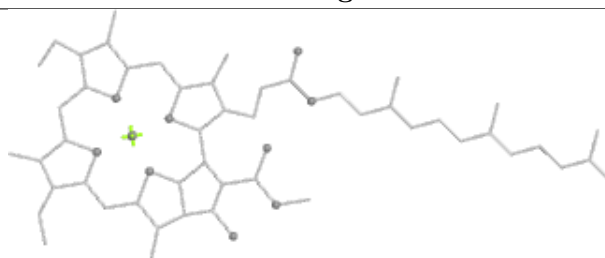
Bond lengths



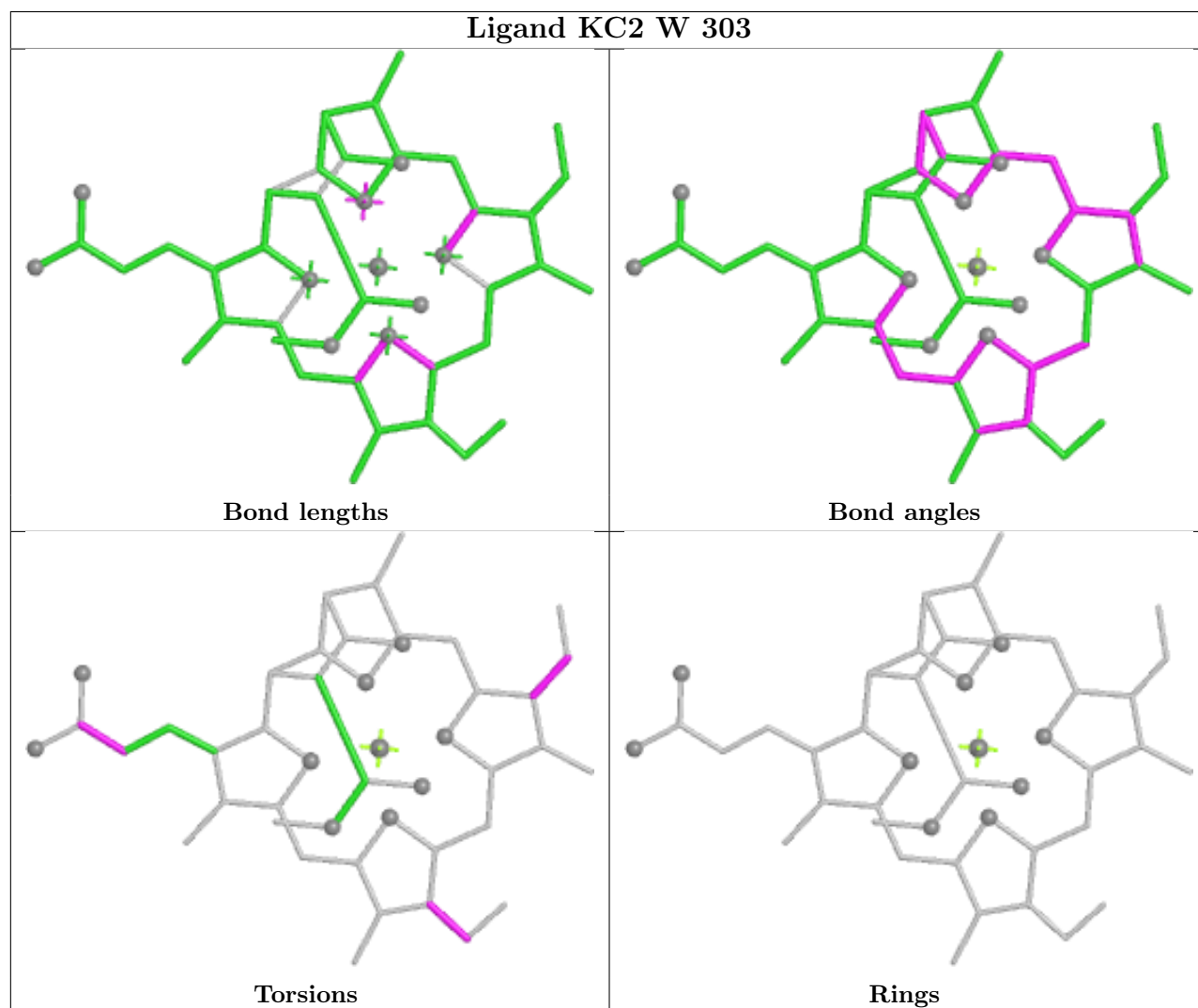
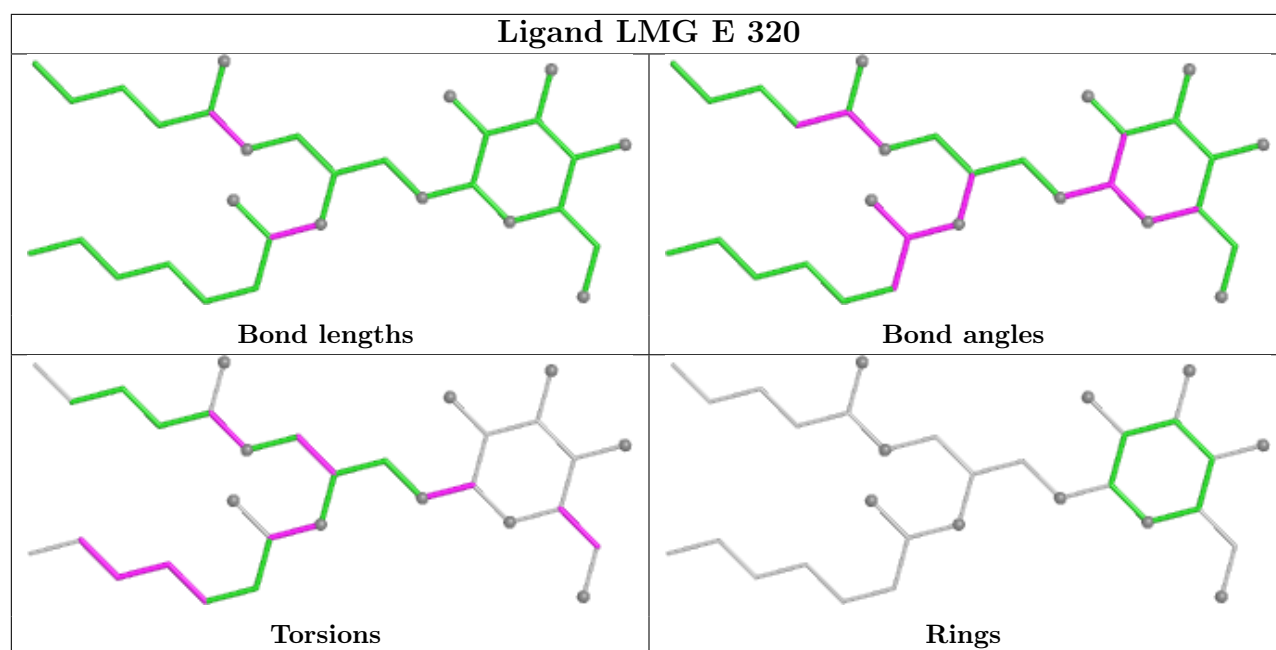
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

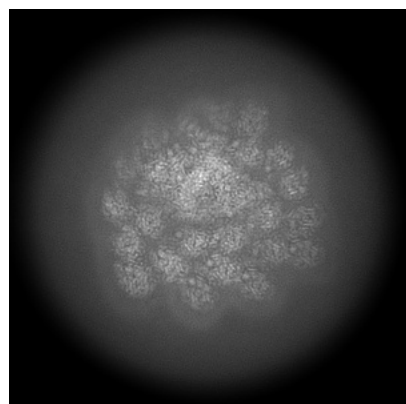
6 Map visualisation [i](#)

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

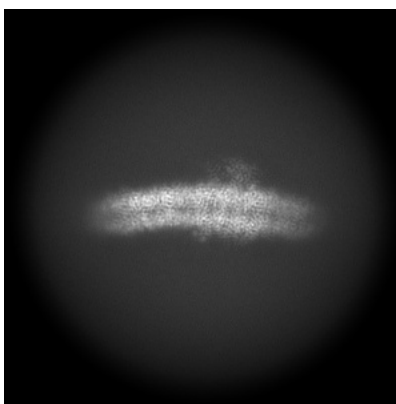
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

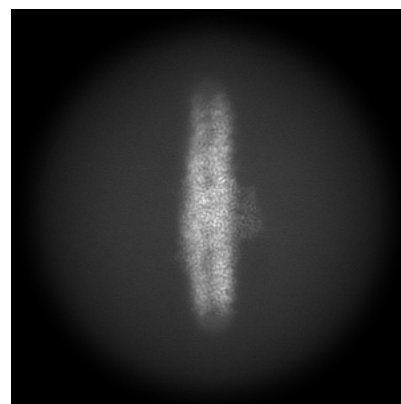
6.1.1 Primary map



X

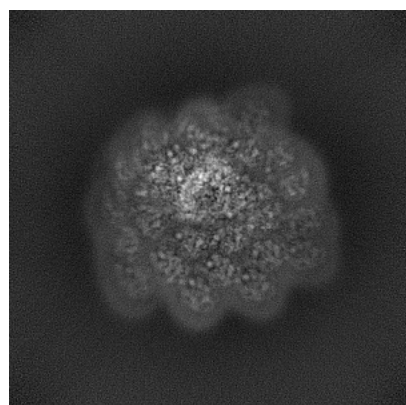


Y

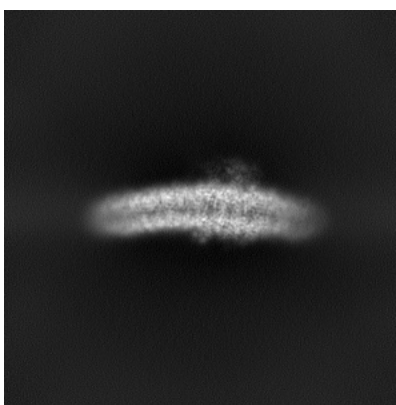


Z

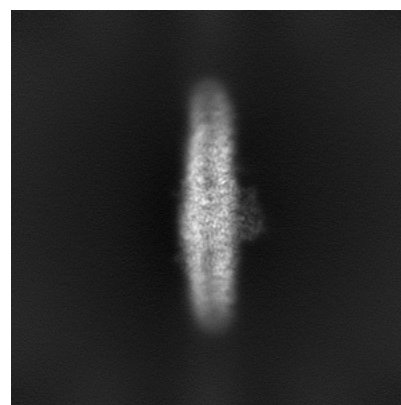
6.1.2 Raw map



X



Y

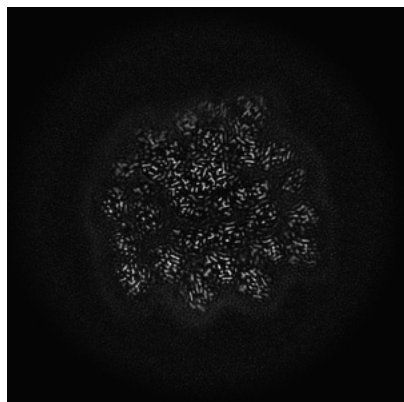


Z

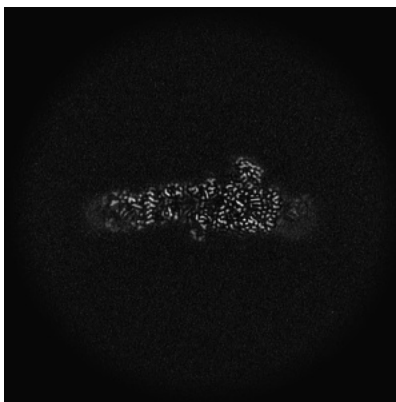
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

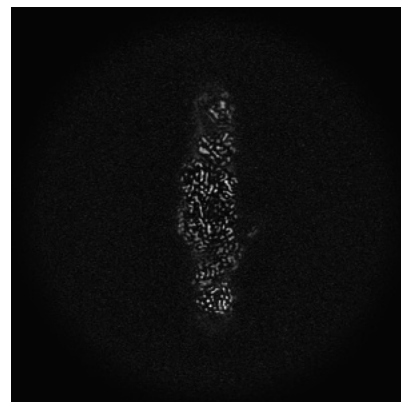
6.2.1 Primary map



X Index: 200

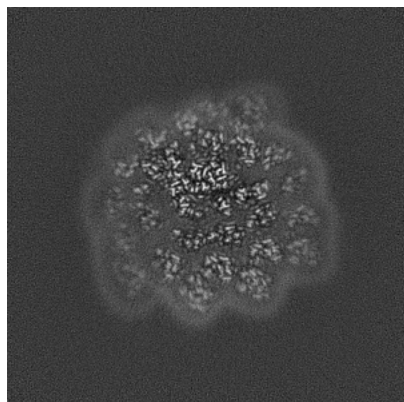


Y Index: 200

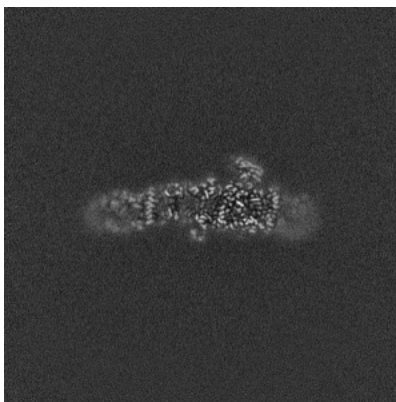


Z Index: 200

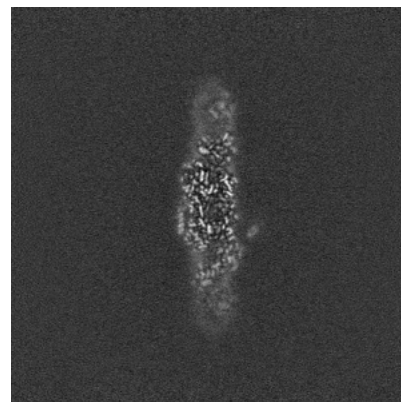
6.2.2 Raw map



X Index: 200



Y Index: 200

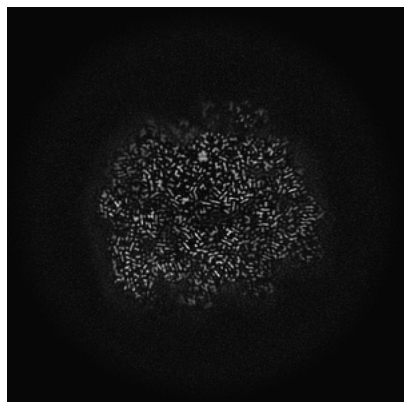


Z Index: 200

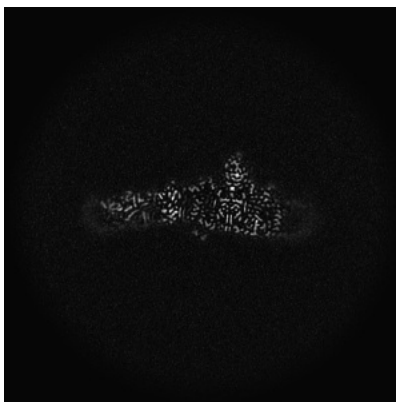
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

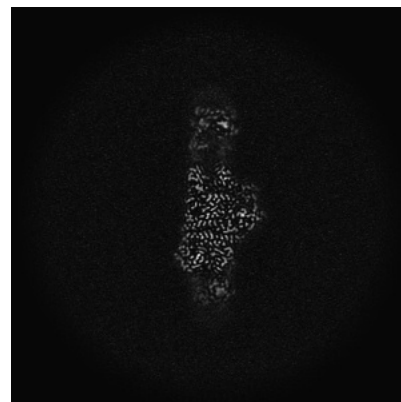
6.3.1 Primary map



X Index: 210

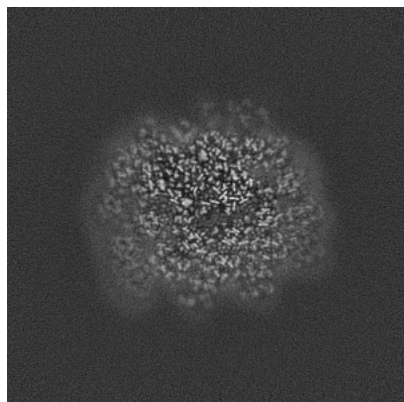


Y Index: 191

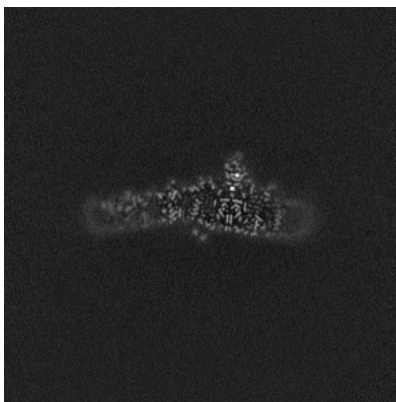


Z Index: 232

6.3.2 Raw map



X Index: 211



Y Index: 191

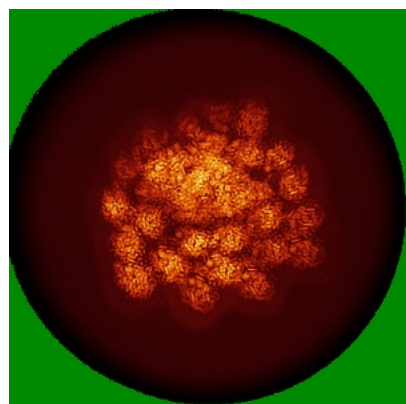


Z Index: 232

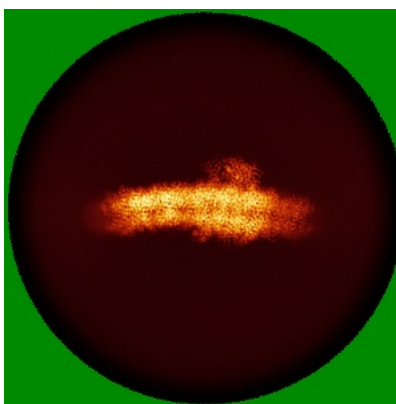
The images above show the largest variance slices of the map in three orthogonal directions.

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

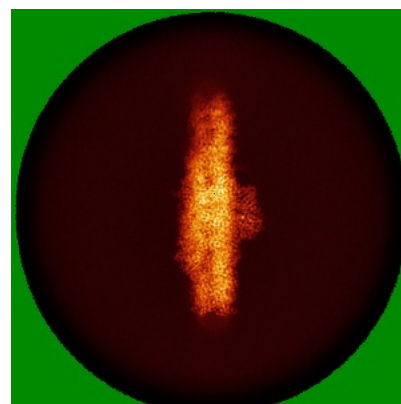
6.4.1 Primary map



X

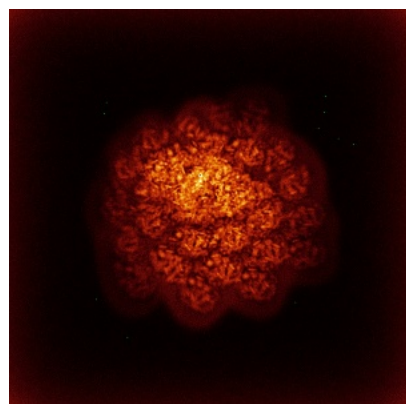


Y

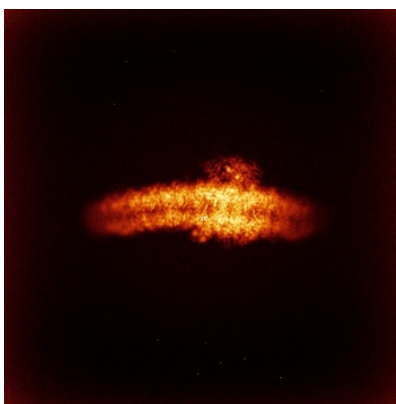


Z

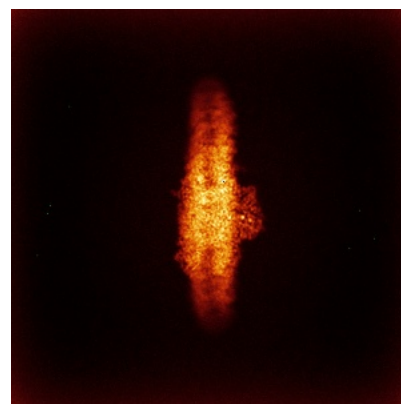
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



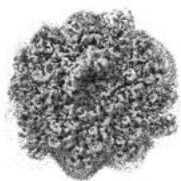
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

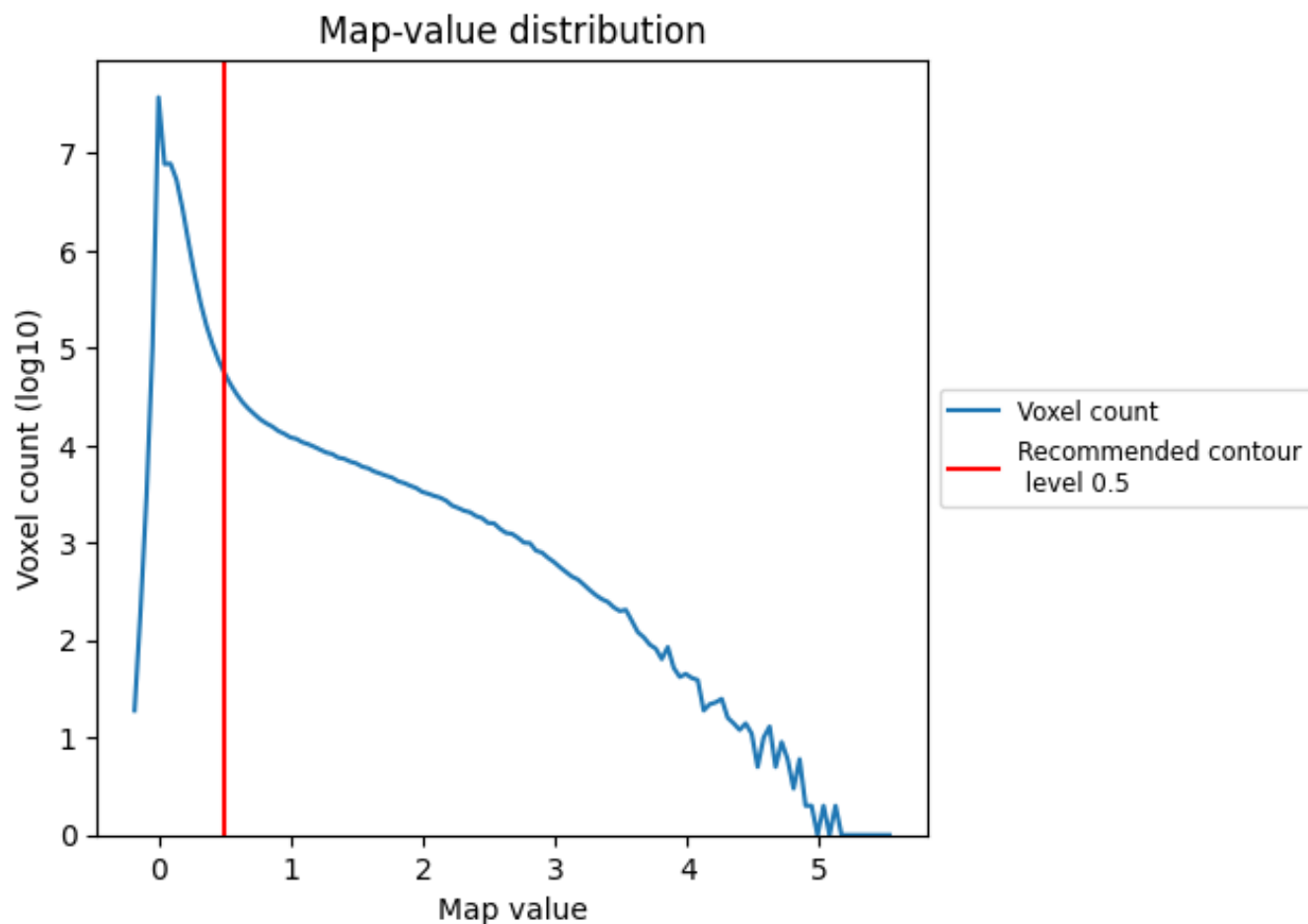
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

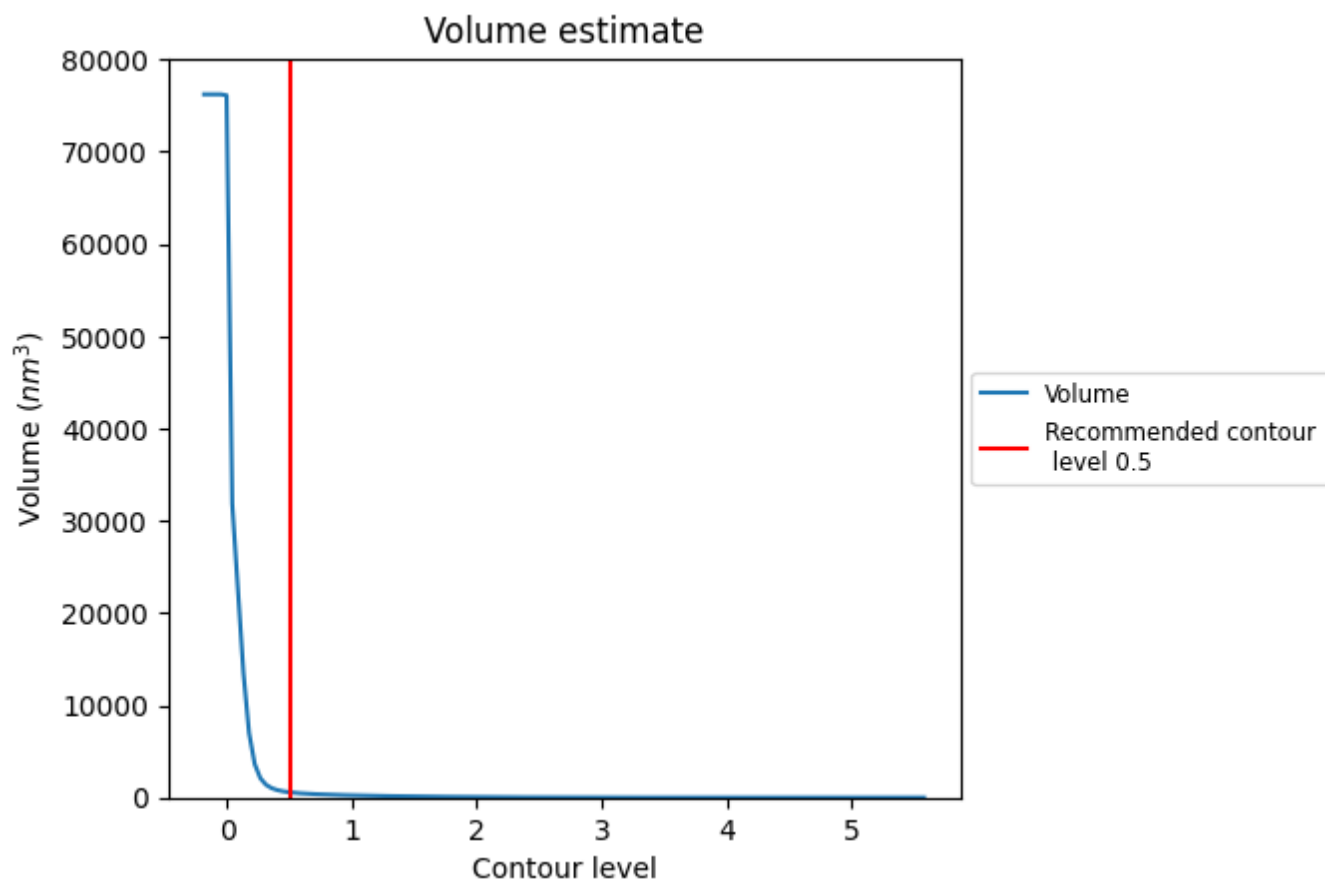
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

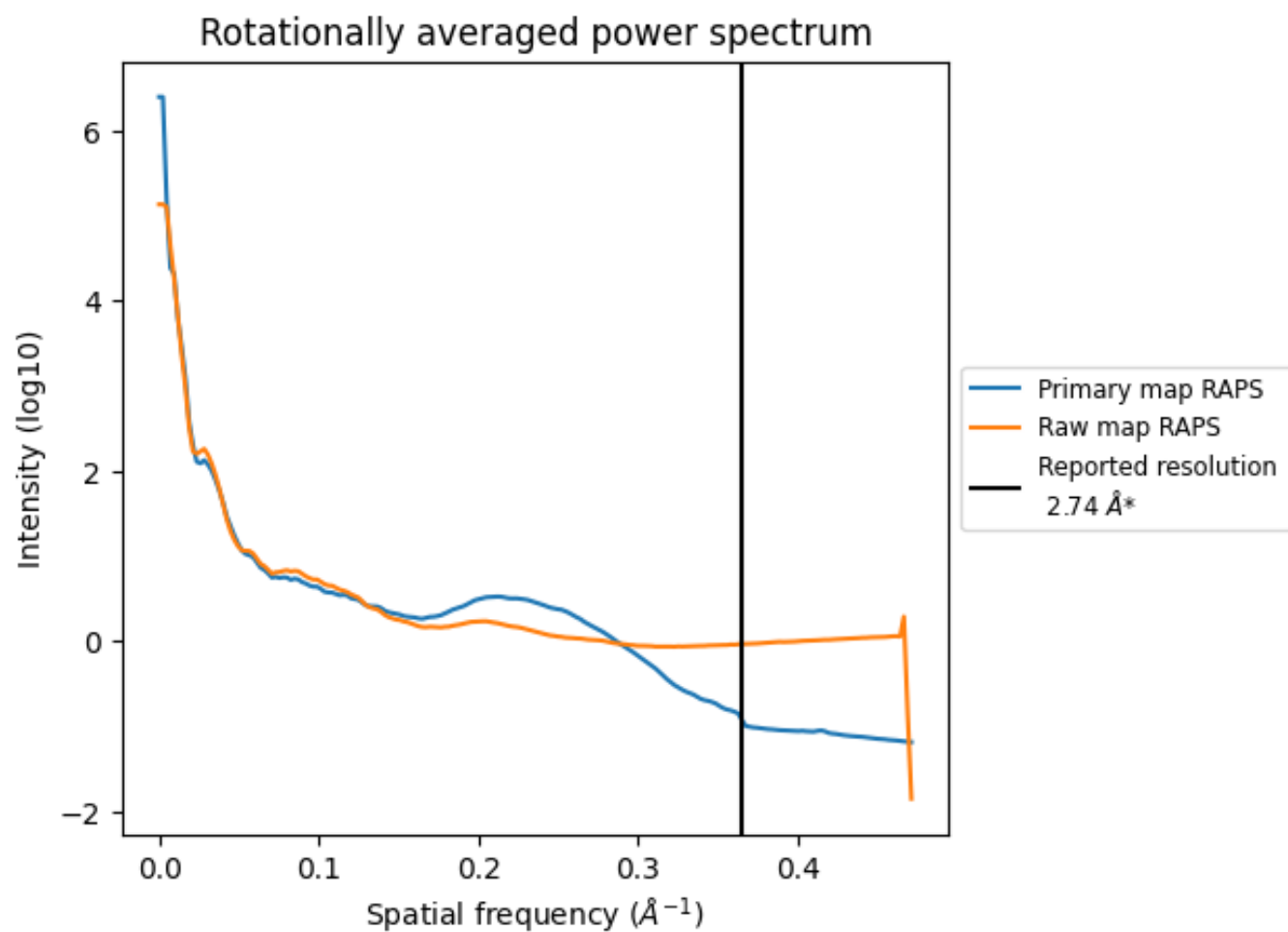
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

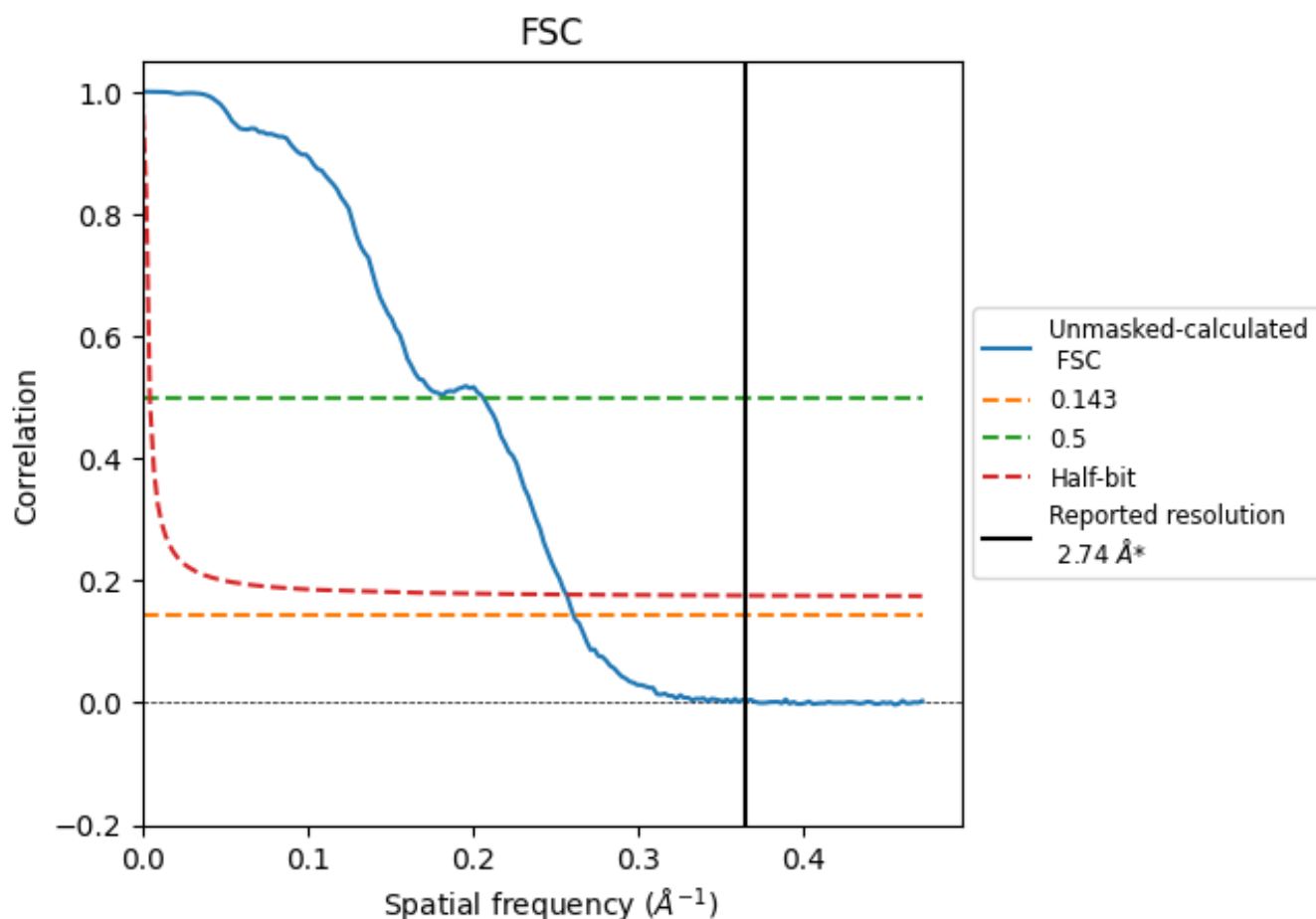


*Reported resolution corresponds to spatial frequency of $0.365 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

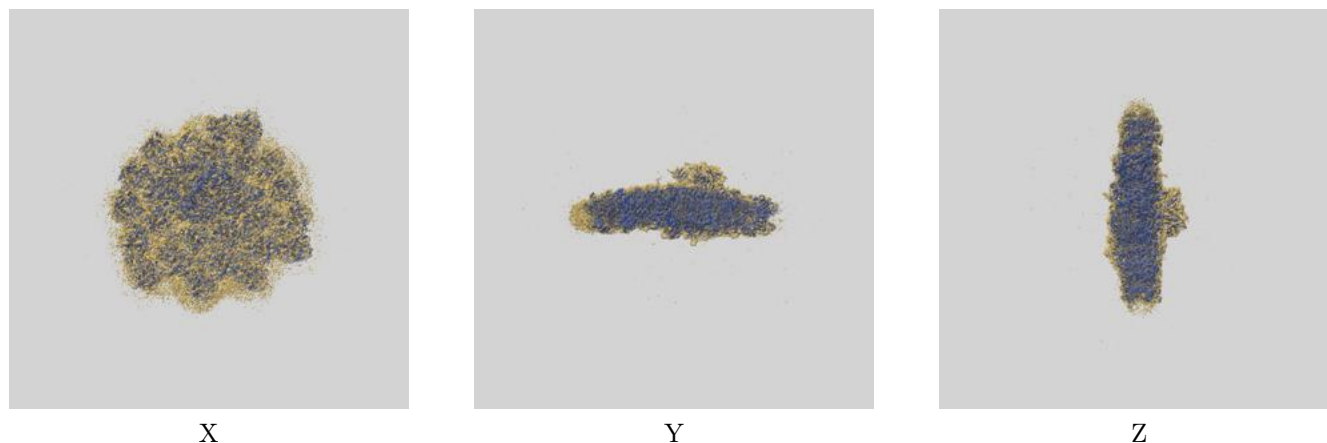
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.85	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

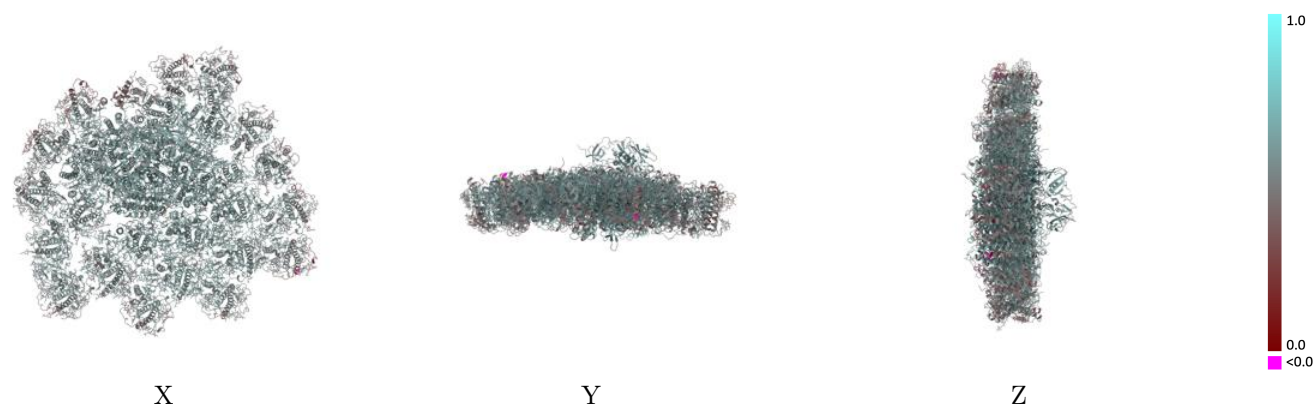
This section contains information regarding the fit between EMDB map EMD-39717 and PDB model 8Z11. Per-residue inclusion information can be found in [section 3](#) on [page 41](#).

9.1 Map-model overlay [i](#)



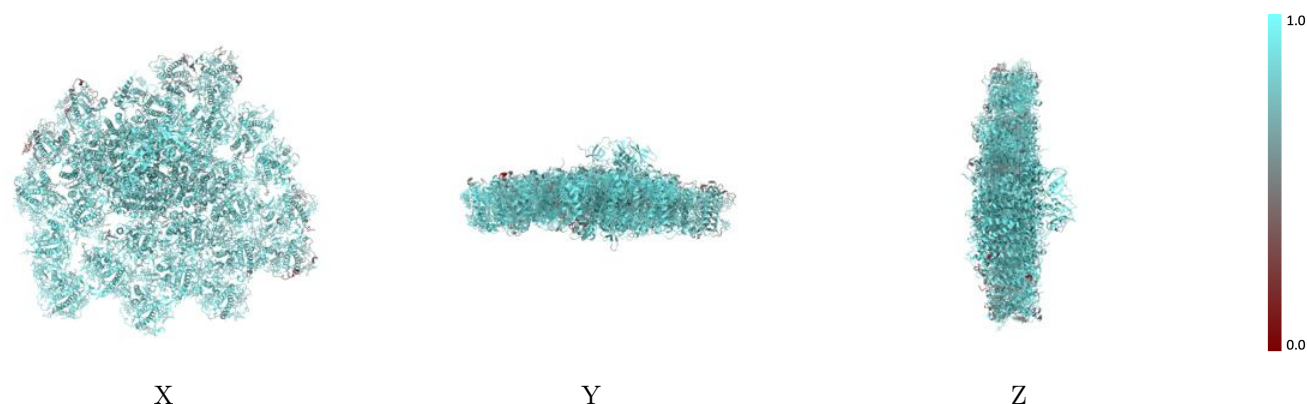
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



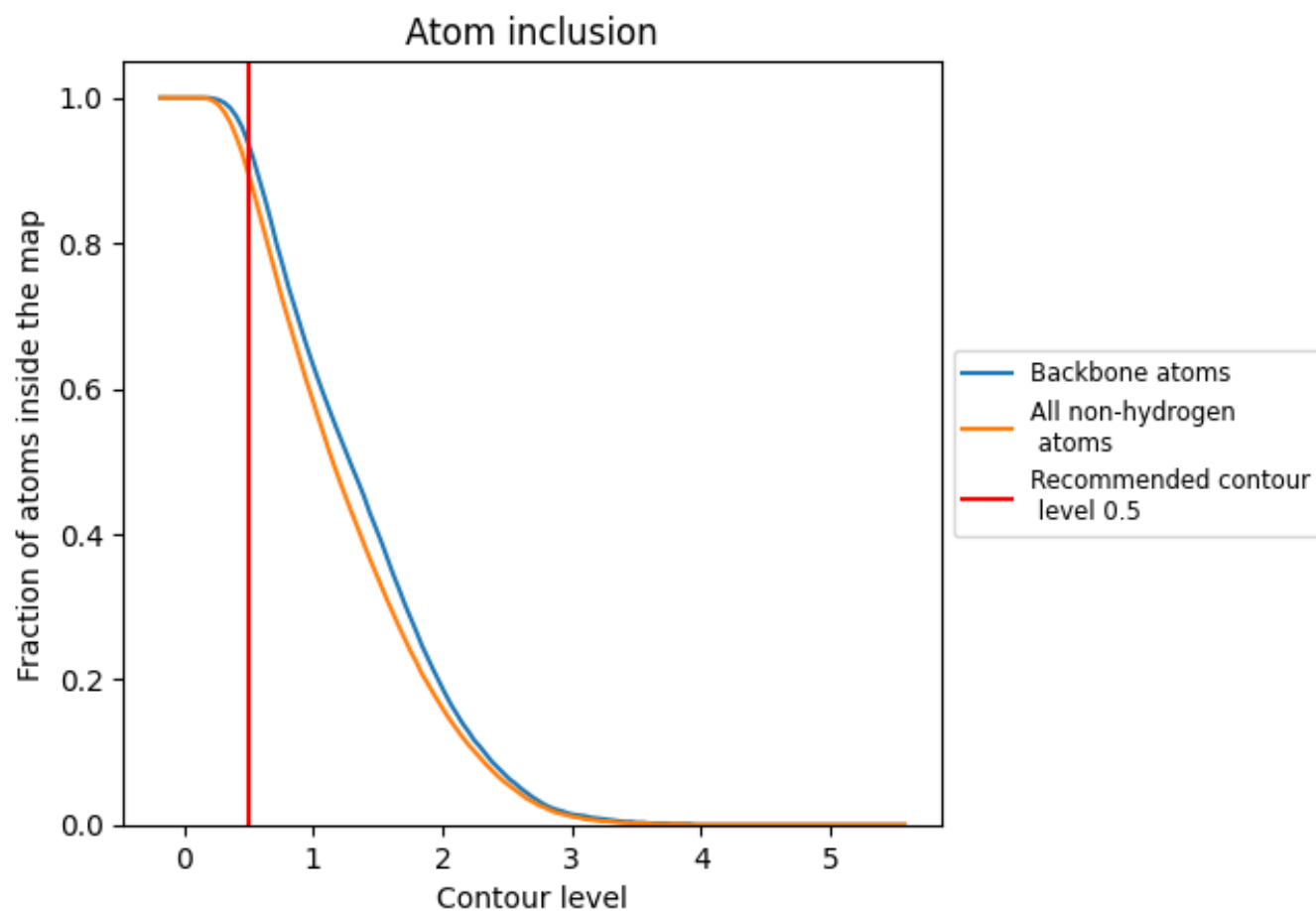
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

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

