



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 07:52 AM JST

PDB ID : 9JJ8 / pdb_00009jj8
EMDB ID : EMD-61519
Title : Structural insights into the PSI-FCPI supercomplex from the coccolithophore
Emiliana huxleyi
Authors : Shen, L.L.; Li, Z.H.; Wang, W.D.
Deposited on : 2024-09-13
Resolution : 2.79 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

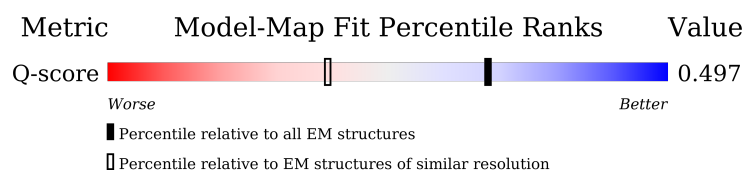
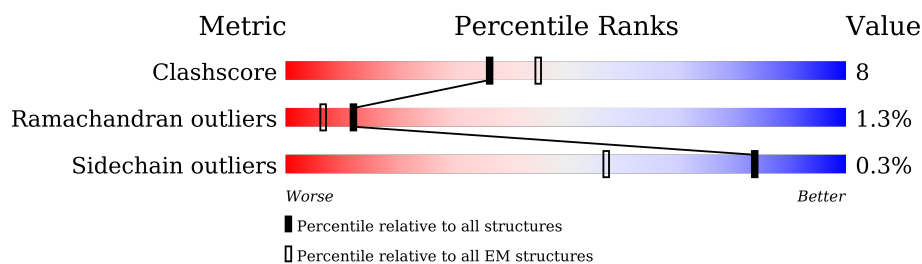
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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.



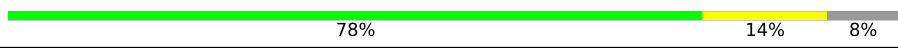
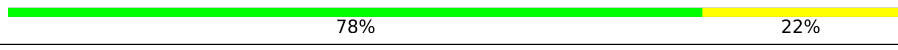
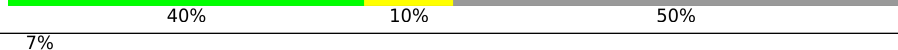
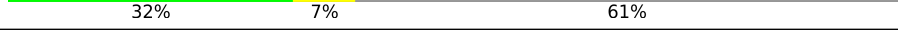
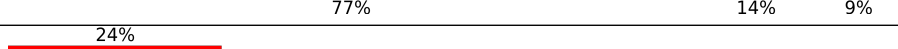
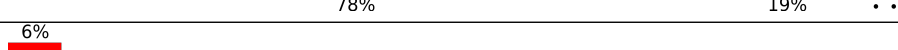
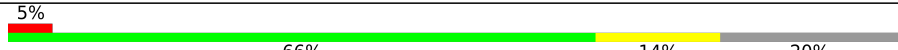
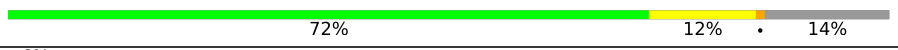
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	752	
2	b	734	
3	c	81	
4	d	142	

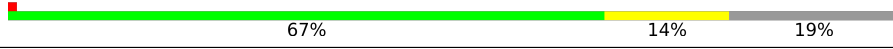
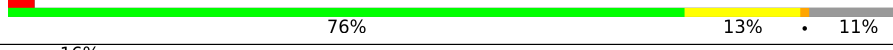
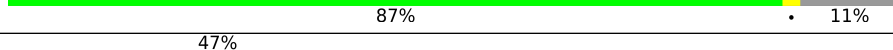
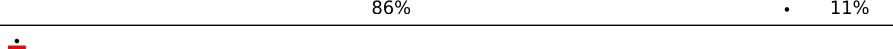
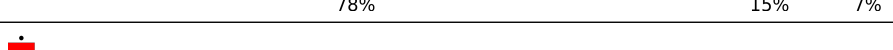
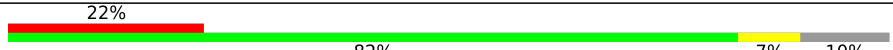
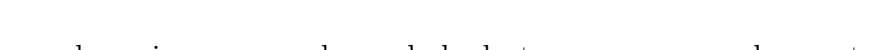
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Mol	Chain	Length	Quality of chain
5	e	131	
6	f	184	
7	i	36	
8	j	40	
9	l	145	
10	m	30	
11	k	145	
12	o	123	
13	A	201	
14	B	177	
15	C	233	
16	D	231	
17	E	217	
18	F	239	
19	G	204	
20	H	210	
21	J	251	
22	K	198	
23	L	244	
24	M	224	
24	P	224	
24	W	224	
25	O	219	
26	Q	257	
27	5	219	

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Mol	Chain	Length	Quality of chain
27	R	219	
27	V	219	
27	X	219	
28	4	255	
28	7	255	
28	S	255	
28	x	255	
28	y	255	
28	z	255	
29	T	211	
30	U	198	
31	0	254	
32	1	253	
33	3	268	
34	6	250	
34	8	250	
35	9	245	
36	I	209	
37	h	133	
38	2	260	
38	Y	260	
38	Z	260	

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
46	LMG	4	326	-	-	X	-
48	A86	Q	304	-	-	X	-
49	KC2	5	313	-	-	X	-
51	A1ECV	0	321	X	-	-	-
51	A1ECV	1	318	X	-	-	-
51	A1ECV	2	311	X	-	-	-
51	A1ECV	4	315	X	-	-	-
51	A1ECV	4	321	X	-	-	-
51	A1ECV	5	309	X	-	-	-
51	A1ECV	5	312	X	-	-	-
51	A1ECV	6	320	X	-	-	-
51	A1ECV	7	317	X	-	-	-
51	A1ECV	7	323	X	-	-	-
51	A1ECV	9	314	X	-	-	-
51	A1ECV	9	317	X	-	-	-
51	A1ECV	E	311	X	-	-	-
51	A1ECV	G	316	X	-	-	-
51	A1ECV	L	318	X	-	-	-
51	A1ECV	M	316	X	-	-	-
51	A1ECV	O	315	X	-	-	-
51	A1ECV	P	315	X	-	-	-
51	A1ECV	Q	316	X	-	-	-
51	A1ECV	Q	319	X	-	-	-
51	A1ECV	R	310	X	-	-	-
51	A1ECV	R	313	X	-	-	-
51	A1ECV	S	312	X	-	-	-
51	A1ECV	S	318	X	-	-	-
51	A1ECV	T	317	X	-	-	-
51	A1ECV	V	317	X	-	-	-
51	A1ECV	W	317	X	-	-	-
51	A1ECV	X	310	X	-	-	-
51	A1ECV	X	313	X	-	-	-
51	A1ECV	Y	306	X	-	-	-
51	A1ECV	Y	312	X	-	-	-
51	A1ECV	Z	308	X	-	-	-
51	A1ECV	Z	314	X	-	-	-
51	A1ECV	x	310	X	-	-	-
51	A1ECV	x	316	X	-	-	-
51	A1ECV	y	311	X	-	-	-
51	A1ECV	y	317	X	-	-	-
51	A1ECV	z	310	X	-	-	-
51	A1ECV	z	316	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 114135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	741	Total	C	N	O	S	0	0
			5835	3817	993	995	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	733	Total	C	N	O	S	0	0
			5818	3828	982	987	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	80	Total	C	N	O	S	0	0
			598	365	105	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	140	Total	C	N	O	S	0	0
			1103	710	184	206	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	63	Total	C	N	O	S	0	0
			491	314	86	90	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	161	Total	C	N	O	S	0	0
			1232	797	207	224	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	33	Total	C	N	O	S	0	0
			254	176	34	43	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			318	211	47	57	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	143	Total	C	N	O	S	0	0
			1084	716	172	195	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	30	Total	C	N	O	S	0	0
			224	149	35	38	2		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	73	Total	C	N	O	S	0	0
			533	347	87	93	6		

- Molecule 12 is a protein called Linker-protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	48	Total	C	N	O	S	0	0
			360	231	61	66	2		

- Molecule 13 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	183	Total	C	N	O	S	0	0
			1419	916	229	264	10		

- Molecule 14 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	172	Total	C	N	O	S	0	0
			1255	805	212	231	7		

- Molecule 15 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	176	Total	C	N	O	S	0	0
			1329	857	221	242	9		

- Molecule 16 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	189	Total	C	N	O	S	0	0
			1424	921	226	271	6		

- Molecule 17 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	187	Total	C	N	O	S	0	0
			1384	896	222	258	8		

- Molecule 18 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	188	Total	C	N	O	S	0	0
			1411	907	244	251	9		

- Molecule 19 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	171	Total	C	N	O	S	0	0
			1340	875	226	232	7		

- Molecule 20 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	168	Total	C	N	O	S	0	0
			1263	810	206	235	12		

- Molecule 21 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	171	Total	C	N	O	S	0	0
			1270	810	223	230	7		

- Molecule 22 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	168	Total	C	N	O	S	0	0
			1251	806	206	231	8		

- Molecule 23 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	210	Total	C	N	O	S	0	0
			1626	1064	273	281	8		

- Molecule 24 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	P	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		
24	W	193	Total	C	N	O	S	0	0
			1455	940	247	263	5		

- Molecule 25 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	155	Total	C	N	O	S	0	0
			1133	717	200	209	7		

- Molecule 26 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	215	Total	C	N	O	S	0	0
			1666	1094	273	294	5		

- Molecule 27 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	188	Total	C	N	O	S	0	0
			1353	872	227	248	6		
27	X	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		
27	5	177	Total	C	N	O	S	0	0
			1311	848	219	238	6		

- Molecule 28 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	4	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	7	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
28	x	228	Total	C	N	O		0	0
			1113	657	228	228			
28	y	228	Total	C	N	O		0	0
			1113	657	228	228			
28	z	228	Total	C	N	O		0	0
			1113	657	228	228			

- Molecule 29 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	197	Total	C	N	O	S	0	0
			1482	973	246	257	6		

- Molecule 30 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	158	Total	C	N	O	S	0	0
			1240	801	207	226	6		

- Molecule 31 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	0	218	Total	C	N	O	S	0	0
			1706	1114	278	309	5		

- Molecule 32 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1	201	Total	C	N	O	S	0	0
			1255	794	223	237	1		

- Molecule 33 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3	236	Total	C	N	O	S	0	0
			1775	1155	294	318	8		

- Molecule 34 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	224	Total	C	N	O	S	0	0
			1415	892	255	261	7		
34	6	224	Total	C	N	O	S	0	0
			1326	825	249	250	2		

- Molecule 35 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	209	Total	C	N	O	S	0	0
			1490	970	246	267	7		

- Molecule 36 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	I	156	Total	C	N	O	S	0	0
			1203	780	201	213	9		

- Molecule 37 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	87	Total	C	N	O	S	0	0
			650	425	104	120	1		

- Molecule 38 is a protein called Light harvesting protein.

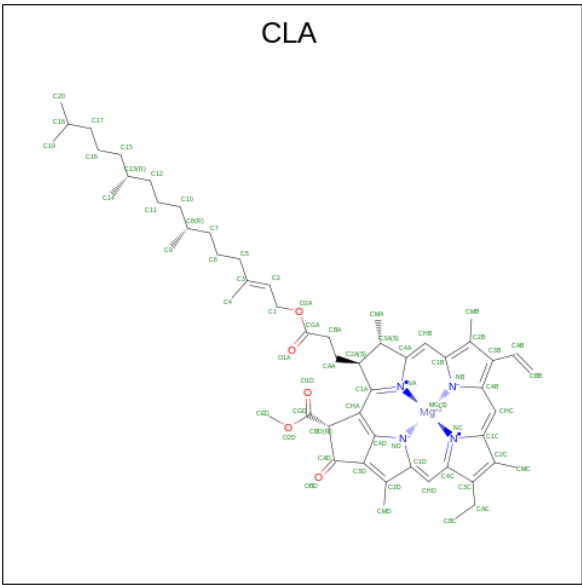
Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	225	Total	C	N	O		0	0
			1099	649	225	225			
38	Z	225	Total	C	N	O		0	0
			1099	649	225	225			

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Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	224	Total	C	N	O	S	0	0
			1383	858	256	263	6		

- Molecule 39 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
39	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
39	b	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
39	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	l	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	k	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	o	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	o	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	o	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	o	1	Total 58	C 48	Mg 1	N 4	O 5	0
39	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
39	C	1	Total 43	C 35	Mg 1	N 4	O 3	0
39	C	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	D	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	E	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	E	1	Total 53	C 43	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	F	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	G	1	Total 58	C 48	Mg 1	N 4	O 5	0
39	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	H	1	Total 48	C 38	Mg 1	N 4	O 5	0
39	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	H	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	H	1	Total 57	C 47	Mg 1	N 4	O 5	0
39	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	J	1	Total 49	C 39	Mg 1	N 4	O 5	0
39	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	J	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	K	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	K	1	Total 59	C 49	Mg 1	N 4	O 5	0
39	K	1	Total 62	C 52	Mg 1	N 4	O 5	0
39	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	L	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	L	1	Total 54	C 44	Mg 1	N 4	O 5	0
39	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	L	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	M	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	M	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	O	1	Total 38	C 32	Mg 1	N 4	O 1	0
39	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	O	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	O	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	P	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	Q	1	Total 54	C 44	Mg 1	N 4	O 5	0
39	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	Q	1	Total 53	C 43	Mg 1	N 4	O 5	0
39	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	S	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	S	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	T	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
39	U	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
39	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	V	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	W	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	W	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	W	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	X	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	0	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	0	1	Total 53	C 43	Mg 1	N 4	O 5	0
39	0	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	0	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	0	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
39	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	0	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	3	1	Total 53	C 43	Mg 1	N 4	O 5	0
39	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
39	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
39	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	5	1	Total 47	C 37	Mg 1	N 4	O 5	0
39	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	7	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
39	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	7	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
39	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
39	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
39	I	1	Total 52	C 42	Mg 1	N 4	O 5	0
39	I	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
39	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	x	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	y	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	y	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	y	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
39	y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	z	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	z	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Y	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0

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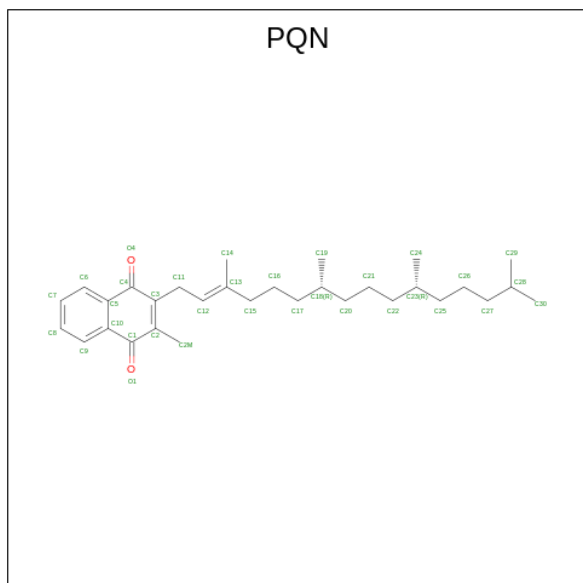
Mol	Chain	Residues	Atoms					AltConf
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	Z	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
39	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
39	6	1	Total 52	C 44	Mg 1	N 4	O 3	0
39	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
39	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
39	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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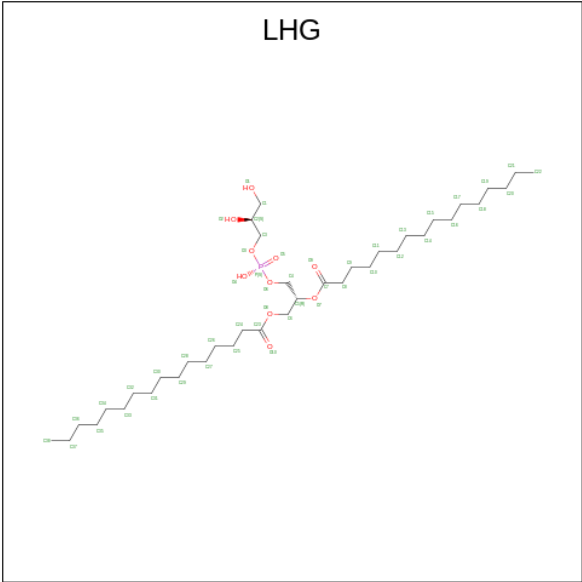
Mol	Chain	Residues	Atoms					AltConf
39	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
39	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 40 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



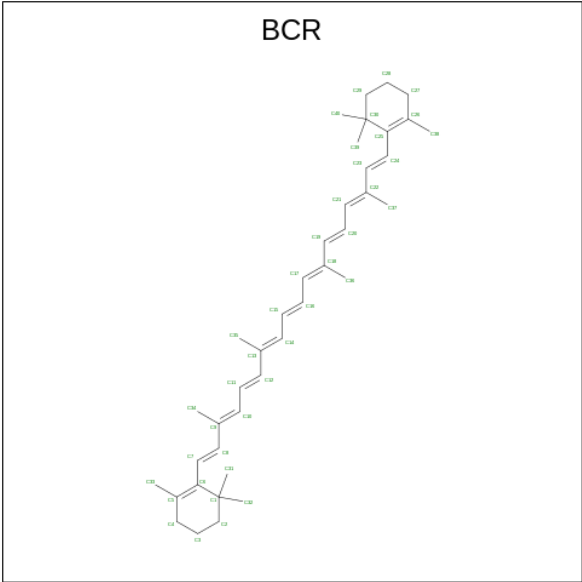
Mol	Chain	Residues	Atoms			AltConf
40	a	1	Total	C	O	0
			33	31	2	
40	b	1	Total	C	O	0
			33	31	2	

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
41	a	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			27	16	10	1	
41	j	1	Total	C	O	P	0
			30	19	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	D	1	Total	C	O	P	0
			35	24	10	1	
41	H	1	Total	C	O	P	0
			35	24	10	1	
41	X	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 42 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



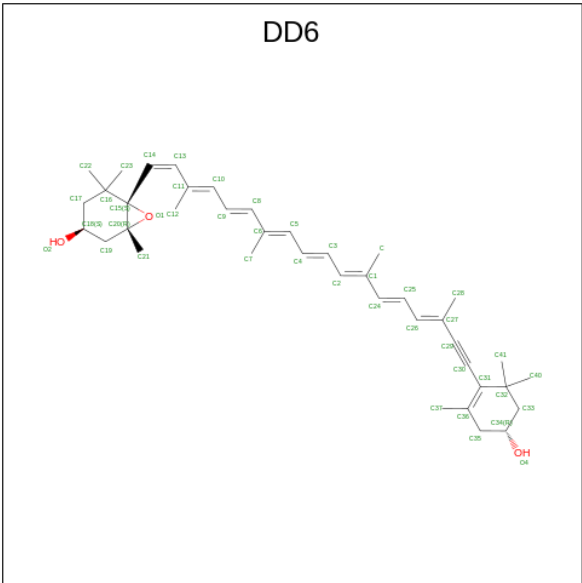
Mol	Chain	Residues	Atoms		AltConf
42	a	1	Total	C	0
			40	40	
42	a	1	Total	C	0
			40	40	
42	a	1	Total	C	0
			40	40	
42	a	1	Total	C	0
			40	40	
42	b	1	Total	C	0
			40	40	
42	b	1	Total	C	0
			40	40	
42	b	1	Total	C	0
			40	40	
42	b	1	Total	C	0
			40	40	
42	b	1	Total	C	0
			40	40	
42	f	1	Total	C	0
			40	40	
42	f	1	Total	C	0
			40	40	
42	i	1	Total	C	0
			40	40	
42	j	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	l	1	Total C 40 40	0
42	m	1	Total C 40 40	0
42	k	1	Total C 40 40	0
42	h	1	Total C 40 40	0

- Molecule 43 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
43	a	1	Total C O 43 40 3	0
43	j	1	Total C O 43 40 3	0
43	o	1	Total C O 43 40 3	0
43	A	1	Total C O 43 40 3	0

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Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total 43	C 40	O 3	0
43	A	1	Total 43	C 40	O 3	0
43	A	1	Total 43	C 40	O 3	0
43	B	1	Total 43	C 40	O 3	0
43	C	1	Total 43	C 40	O 3	0
43	D	1	Total 43	C 40	O 3	0
43	D	1	Total 43	C 40	O 3	0
43	D	1	Total 43	C 40	O 3	0
43	E	1	Total 43	C 40	O 3	0
43	E	1	Total 43	C 40	O 3	0
43	E	1	Total 43	C 40	O 3	0
43	F	1	Total 43	C 40	O 3	0
43	F	1	Total 43	C 40	O 3	0
43	G	1	Total 43	C 40	O 3	0
43	G	1	Total 43	C 40	O 3	0
43	H	1	Total 43	C 40	O 3	0
43	H	1	Total 43	C 40	O 3	0
43	J	1	Total 43	C 40	O 3	0
43	J	1	Total 43	C 40	O 3	0
43	J	1	Total 43	C 40	O 3	0
43	K	1	Total 43	C 40	O 3	0

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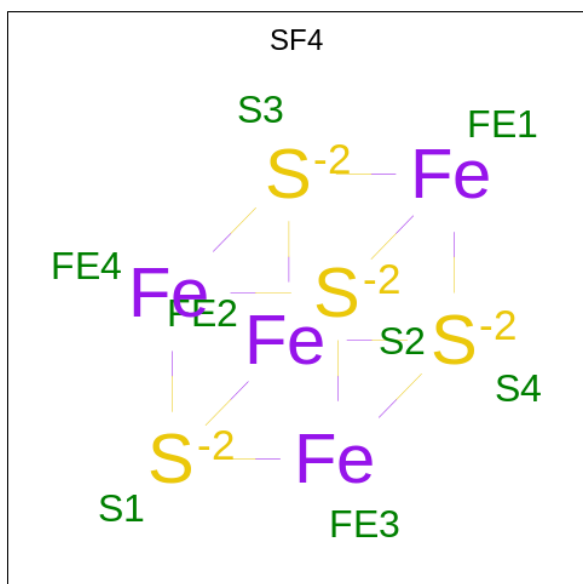
Mol	Chain	Residues	Atoms			AltConf
43	M	1	Total 43	C 40	O 3	0
43	O	1	Total 43	C 40	O 3	0
43	O	1	Total 43	C 40	O 3	0
43	O	1	Total 43	C 40	O 3	0
43	P	1	Total 43	C 40	O 3	0
43	Q	1	Total 43	C 40	O 3	0
43	Q	1	Total 43	C 40	O 3	0
43	R	1	Total 43	C 40	O 3	0
43	S	1	Total 43	C 40	O 3	0
43	T	1	Total 43	C 40	O 3	0
43	U	1	Total 43	C 40	O 3	0
43	V	1	Total 43	C 40	O 3	0
43	W	1	Total 43	C 40	O 3	0
43	X	1	Total 43	C 40	O 3	0
43	1	1	Total 43	C 40	O 3	0
43	3	1	Total 43	C 40	O 3	0
43	3	1	Total 43	C 40	O 3	0
43	4	1	Total 43	C 40	O 3	0
43	4	1	Total 43	C 40	O 3	0
43	5	1	Total 43	C 40	O 3	0
43	7	1	Total 43	C 40	O 3	0

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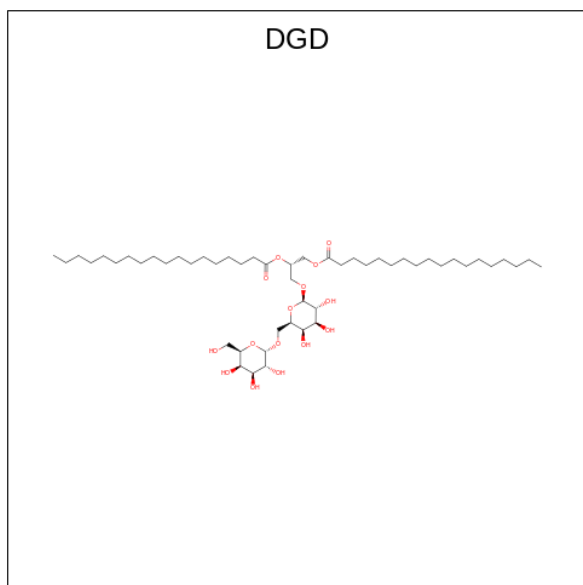
Mol	Chain	Residues	Atoms			AltConf
43	7	1	Total	C	O	0
			43	40	3	
43	I	1	Total	C	O	0
			43	40	3	
43	I	1	Total	C	O	0
			43	40	3	
43	I	1	Total	C	O	0
			43	40	3	
43	x	1	Total	C	O	0
			43	40	3	
43	x	1	Total	C	O	0
			43	40	3	
43	y	1	Total	C	O	0
			43	40	3	
43	y	1	Total	C	O	0
			43	40	3	
43	z	1	Total	C	O	0
			43	40	3	
43	z	1	Total	C	O	0
			43	40	3	
43	Z	1	Total	C	O	0
			43	40	3	
43	2	1	Total	C	O	0
			43	40	3	

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



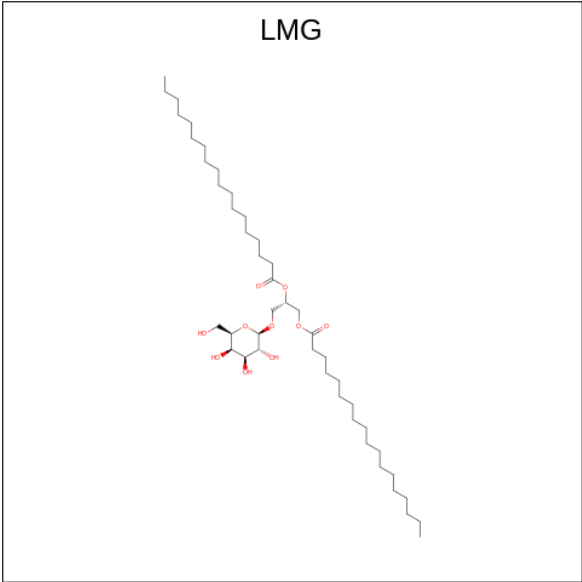
Mol	Chain	Residues	Atoms			AltConf
44	b	1	Total	Fe	S	0
			8	4	4	
44	c	1	Total	Fe	S	0
			8	4	4	
44	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
45	b	1	Total	C	O	0
			60	45	15	
45	C	1	Total	C	O	0
			40	25	15	

- Molecule 46 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



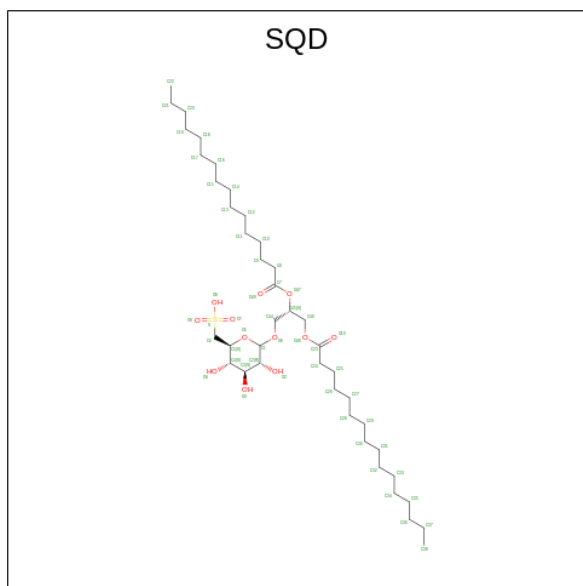
Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	C	O	0
			39	29	10	
46	A	1	Total	C	O	0
			29	19	10	
46	D	1	Total	C	O	0
			37	27	10	
46	F	1	Total	C	O	0
			39	29	10	
46	F	1	Total	C	O	0
			34	24	10	
46	M	1	Total	C	O	0
			39	29	10	
46	M	1	Total	C	O	0
			33	23	10	
46	P	1	Total	C	O	0
			39	29	10	
46	Q	1	Total	C	O	0
			28	18	10	
46	S	1	Total	C	O	0
			32	22	10	
46	S	1	Total	C	O	0
			46	36	10	
46	W	1	Total	C	O	0
			39	29	10	
46	W	1	Total	C	O	0
			33	23	10	
46	0	1	Total	C	O	0
			27	17	10	

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Mol	Chain	Residues	Atoms			AltConf
46	4	1	Total	C	O	0
			32	22	10	
46	4	1	Total	C	O	0
			46	36	10	
46	7	1	Total	C	O	0
			46	36	10	
46	7	1	Total	C	O	0
			32	22	10	
46	9	1	Total	C	O	0
			36	26	10	
46	I	1	Total	C	O	0
			42	32	10	

- Molecule 47 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



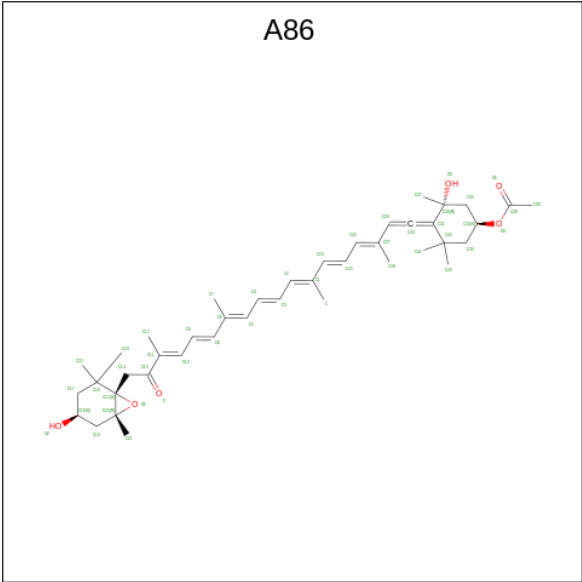
Mol	Chain	Residues	Atoms				AltConf
47	k	1	Total	C	O	S	0
			38	25	12	1	
47	D	1	Total	C	O	S	0
			38	25	12	1	
47	D	1	Total	C	O	S	0
			37	24	12	1	
47	D	1	Total	C	O	S	0
			39	26	12	1	

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Mol	Chain	Residues	Atoms				AltConf
47	E	1	Total	C	O	S	0
			35	22	12	1	
47	F	1	Total	C	O	S	0
			42	29	12	1	
47	F	1	Total	C	O	S	0
			37	24	12	1	
47	H	1	Total	C	O	S	0
			38	25	12	1	
47	M	1	Total	C	O	S	0
			39	26	12	1	
47	P	1	Total	C	O	S	0
			38	25	12	1	
47	S	1	Total	C	O	S	0
			39	26	12	1	
47	T	1	Total	C	O	S	0
			36	23	12	1	
47	W	1	Total	C	O	S	0
			28	15	12	1	
47	4	1	Total	C	O	S	0
			39	26	12	1	
47	7	1	Total	C	O	S	0
			39	26	12	1	
47	9	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 48 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
48	k	1	Total	C	O	0
			48	42	6	
48	B	1	Total	C	O	0
			48	42	6	
48	C	1	Total	C	O	0
			48	42	6	
48	D	1	Total	C	O	0
			48	42	6	
48	E	1	Total	C	O	0
			48	42	6	
48	F	1	Total	C	O	0
			48	42	6	
48	F	1	Total	C	O	0
			48	42	6	
48	G	1	Total	C	O	0
			48	42	6	
48	G	1	Total	C	O	0
			48	42	6	
48	H	1	Total	C	O	0
			48	42	6	
48	J	1	Total	C	O	0
			48	42	6	
48	J	1	Total	C	O	0
			48	42	6	
48	K	1	Total	C	O	0
			48	42	6	
48	L	1	Total	C	O	0
			48	42	6	

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

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Mol	Chain	Residues	Atoms			AltConf
48	S	1	Total	C	O	0
			48	42	6	
48	S	1	Total	C	O	0
			48	42	6	
48	S	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	T	1	Total	C	O	0
			48	42	6	
48	U	1	Total	C	O	0
			48	42	6	
48	U	1	Total	C	O	0
			48	42	6	
48	V	1	Total	C	O	0
			48	42	6	
48	V	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	W	1	Total	C	O	0
			48	42	6	
48	X	1	Total	C	O	0
			48	42	6	
48	X	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	0	1	Total	C	O	0
			48	42	6	
48	1	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
48	1	1	Total	C	O	0
			48	42	6	
48	1	1	Total	C	O	0
			48	42	6	
48	1	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	3	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	4	1	Total	C	O	0
			48	42	6	
48	5	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	7	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
48	8	1	Total	C	O	0
			48	42	6	
48	8	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	9	1	Total	C	O	0
			48	42	6	
48	I	1	Total	C	O	0
			48	42	6	
48	x	1	Total	C	O	0
			48	42	6	
48	y	1	Total	C	O	0
			48	42	6	
48	y	1	Total	C	O	0
			48	42	6	
48	z	1	Total	C	O	0
			48	42	6	
48	Y	1	Total	C	O	0
			48	42	6	
48	Z	1	Total	C	O	0
			48	42	6	
48	Z	1	Total	C	O	0
			48	42	6	
48	2	1	Total	C	O	0
			48	42	6	
48	2	1	Total	C	O	0
			48	42	6	
48	2	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
48	6	1	Total	C	O	0
			48	42	6	
48	6	1	Total	C	O	0
			48	42	6	

Mol	Chain	Residues	Atoms					AltConf
49	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	F	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	G	1	Total 45	C 35	Mg 1	N 4	O 5	0



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PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					AltConf
49	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	M	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	O	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	P	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
49	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Q	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	R	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	V	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
49	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	W	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	0	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	5	1	Total 44	C 35	Mg 1	N 4	O 4	0
49	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	I	1	Total 44	C 35	Mg 1	N 4	O 4	0

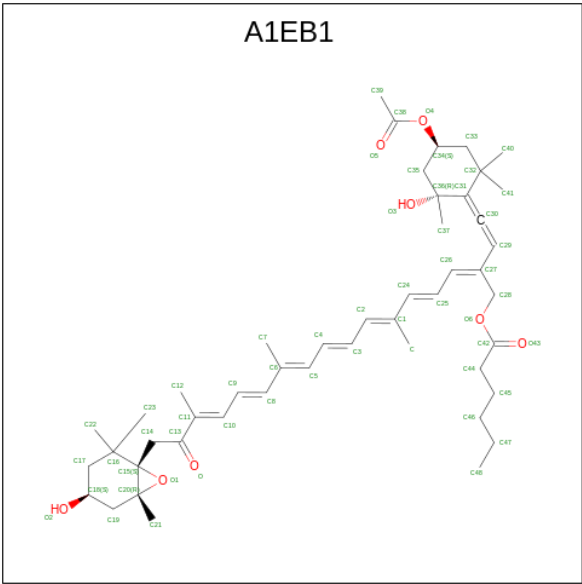
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Mol	Chain	Residues	Atoms					AltConf
49	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	z	1	Total 44	C 34	Mg 1	N 4	O 5	0
49	z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
49	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
49	6	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 50 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-2-[2-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]ethenyl]-6,11,15-trimethyl-16-oxidanylidene-17-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]heptadec

a-2,4,6,8,10,12,14-heptaenyl] hexanoate (CCD ID: A1EB1) (formula: C₄₈H₆₈O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			56	48	8	
50	D	1	Total	C	O	0
			56	48	8	
50	E	1	Total	C	O	0
			56	48	8	
50	F	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	G	1	Total	C	O	0
			56	48	8	
50	H	1	Total	C	O	0
			56	48	8	
50	H	1	Total	C	O	0
			56	48	8	
50	J	1	Total	C	O	0
			56	48	8	
50	K	1	Total	C	O	0
			56	48	8	

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Mol	Chain	Residues	Atoms			AltConf
50	K	1	Total	C	O	0
			56	48	8	
50	K	1	Total	C	O	0
			56	48	8	
50	L	1	Total	C	O	0
			56	48	8	
50	O	1	Total	C	O	0
			56	48	8	
50	Q	1	Total	C	O	0
			56	48	8	
50	Q	1	Total	C	O	0
			56	48	8	
50	R	1	Total	C	O	0
			56	48	8	
50	S	1	Total	C	O	0
			56	48	8	
50	S	1	Total	C	O	0
			56	48	8	
50	T	1	Total	C	O	0
			56	48	8	
50	T	1	Total	C	O	0
			56	48	8	
50	U	1	Total	C	O	0
			56	48	8	
50	U	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	V	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	
50	0	1	Total	C	O	0
			56	48	8	

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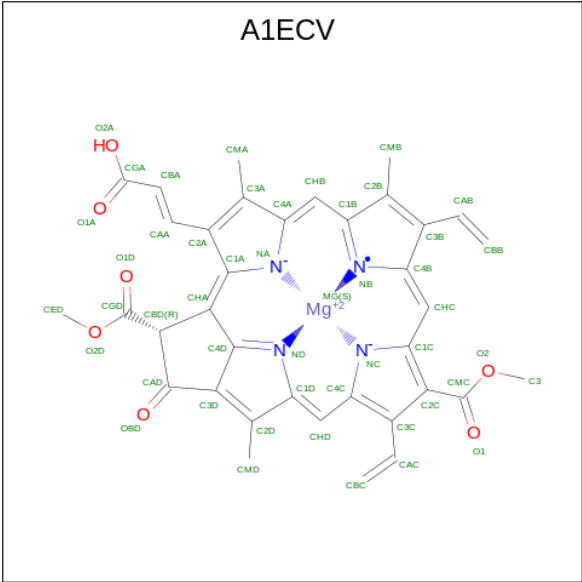
Mol	Chain	Residues	Atoms			AltConf
50	1	1	Total	C	O	0
			56	48	8	
50	1	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	3	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	4	1	Total	C	O	0
			56	48	8	
50	5	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	7	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	8	1	Total	C	O	0
			56	48	8	
50	9	1	Total	C	O	0
			56	48	8	

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Mol	Chain	Residues	Atoms			AltConf
50	h	1	Total	C	O	0
			56	48	8	
50	x	1	Total	C	O	0
			56	48	8	
50	x	1	Total	C	O	0
			56	48	8	
50	y	1	Total	C	O	0
			56	48	8	
50	y	1	Total	C	O	0
			56	48	8	
50	z	1	Total	C	O	0
			48	42	6	
50	z	1	Total	C	O	0
			56	48	8	
50	2	1	Total	C	O	0
			56	48	8	
50	2	1	Total	C	O	0
			56	48	8	
50	6	1	Total	C	O	0
			56	48	8	
50	6	1	Total	C	O	0
			53	45	8	
50	6	1	Total	C	O	0
			48	42	6	
50	6	1	Total	C	O	0
			56	48	8	

- Molecule 51 is Chlorophyll C3 (CCD ID: A1ECV) (formula: $C_{36}H_{28}MgN_4O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
51	E	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	G	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	L	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	M	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	O	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	P	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Q	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	R	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	S	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	T	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	V	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

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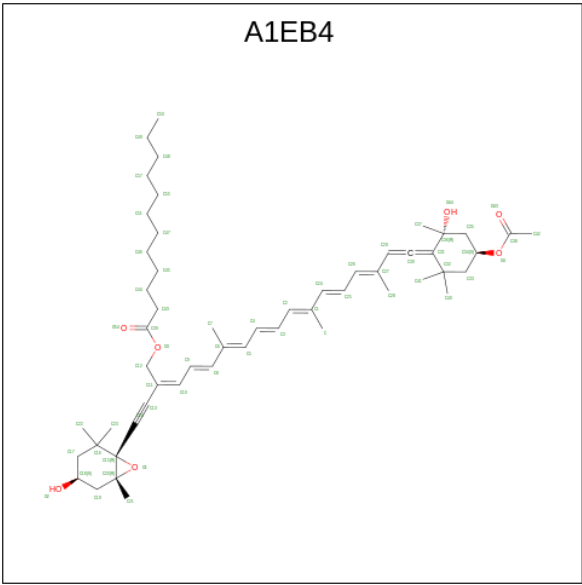
Mol	Chain	Residues	Atoms					AltConf
51	W	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	X	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	X	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	0	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	1	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	4	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	4	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	5	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	5	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	7	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	7	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	9	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	9	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	x	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	x	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	y	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	y	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	z	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	z	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	Y	1	Total 48	C 36	Mg 1	N 4	O 7	0
51	Y	1	Total 48	C 36	Mg 1	N 4	O 7	0

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Mol	Chain	Residues	Atoms					AltConf
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	Z	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	2	1	Total	C	Mg	N	O	0
			48	36	1	4	7	
51	6	1	Total	C	Mg	N	O	0
			48	36	1	4	7	

- Molecule 52 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyl oxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[2-[(1 {R},4 {S},6 {R}) -2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethynyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] dodecanoate (CCD ID: A1EB4) (formula: C₅₄H₇₈O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	C	O	0
			58	51	7	
52	M	1	Total	C	O	0
			57	50	7	
52	P	1	Total	C	O	0
			56	49	7	
52	P	1	Total	C	O	0
			54	47	7	
52	P	1	Total	C	O	0
			57	50	7	

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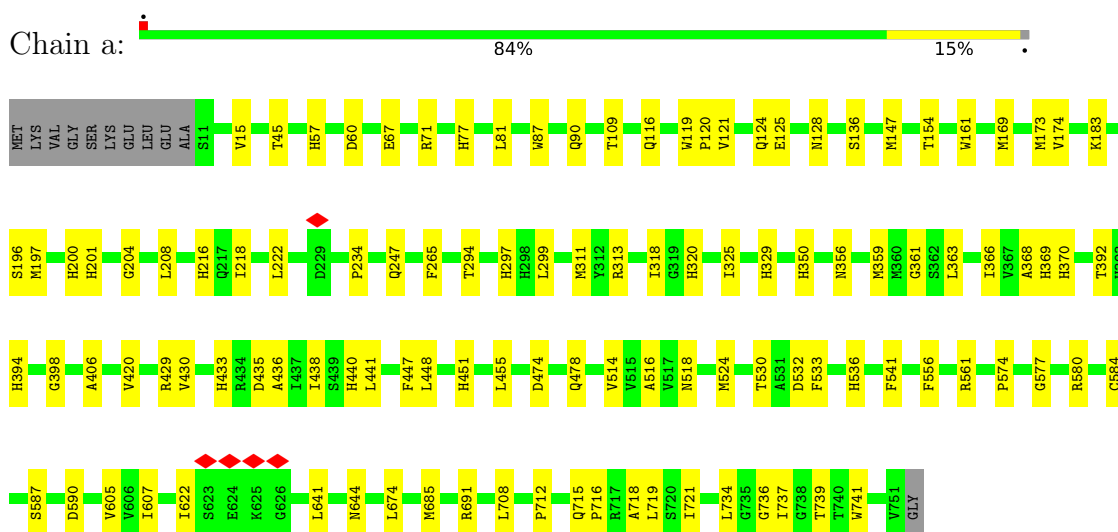
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Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			57	50	7	
52	T	1	Total	C	O	0
			55	48	7	
52	W	1	Total	C	O	0
			56	49	7	
52	W	1	Total	C	O	0
			57	50	7	
52	X	1	Total	C	O	0
			57	50	7	
52	5	1	Total	C	O	0
			57	50	7	

3 Residue-property plots

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

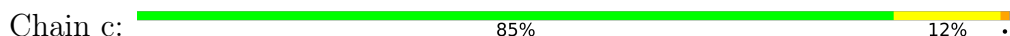
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

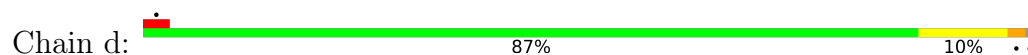


- Molecule 3: Photosystem I iron-sulfur center

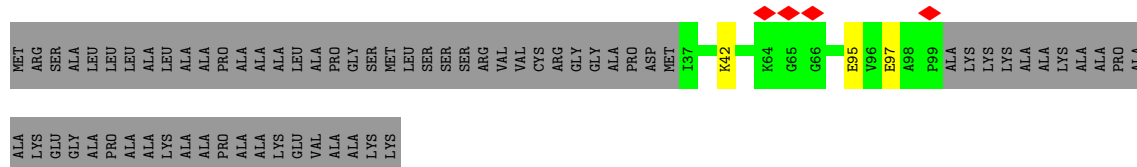




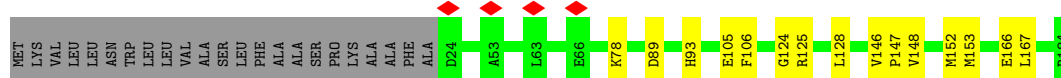
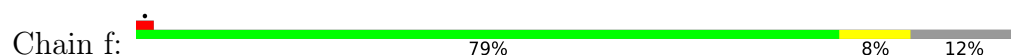
- Molecule 4: Photosystem I reaction center subunit II



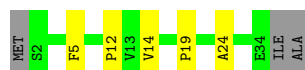
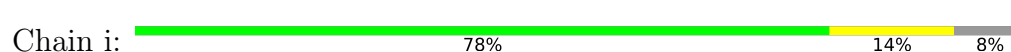
- Molecule 5: Photosystem I reaction center subunit IV



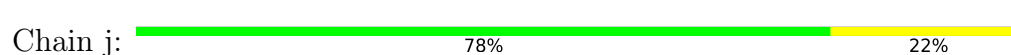
- Molecule 6: Photosystem I reaction center subunit III



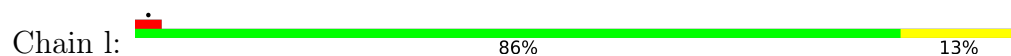
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XII

Chain m:  80% 20%



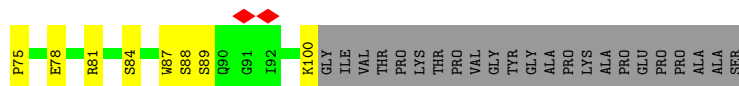
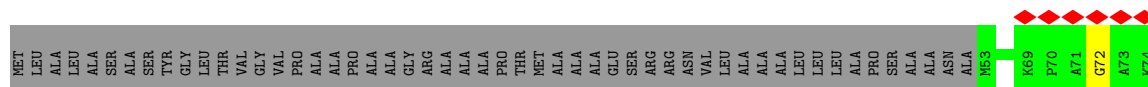
- Molecule 11: PSI-K

Chain k:  40% 10% 50%



- Molecule 12: Linker-protein

Chain o:  7% 32% 7% 61%



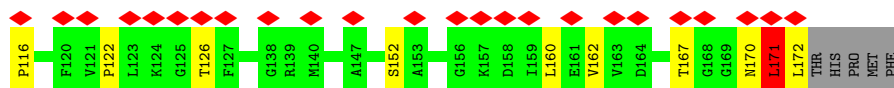
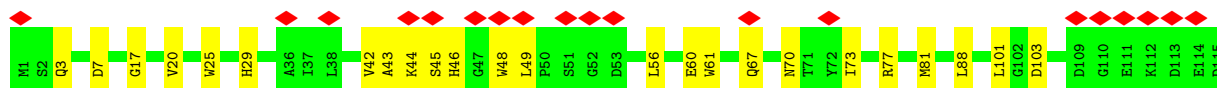
- Molecule 13: Light harvesting protein

Chain A:  77% 14% 9%

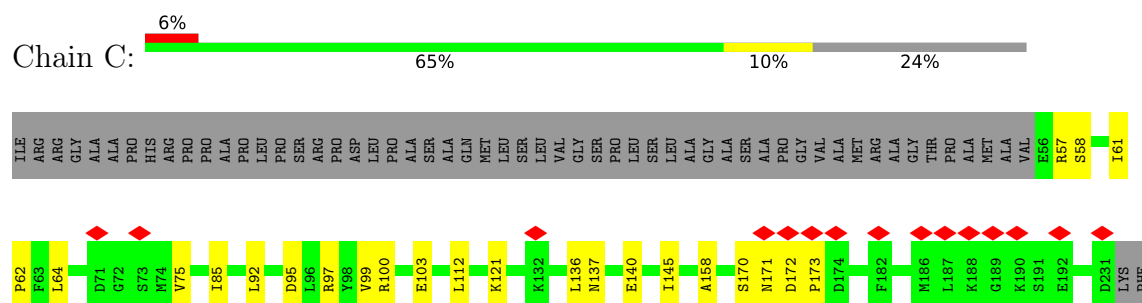


- Molecule 14: Light harvesting protein

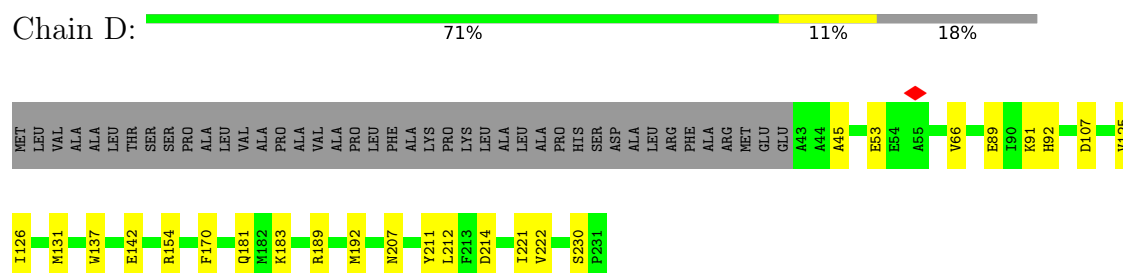
Chain B:  24% 78% 19% ..



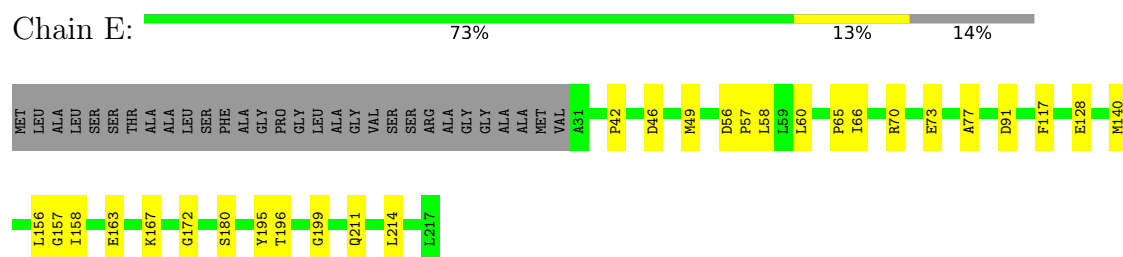
- Molecule 15: Light harvesting protein



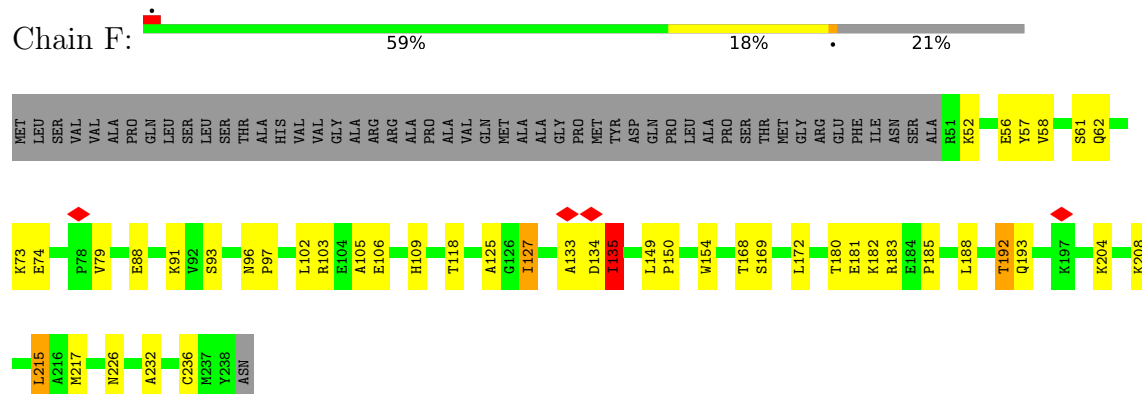
- Molecule 16: Light harvesting protein



- Molecule 17: Light harvesting protein

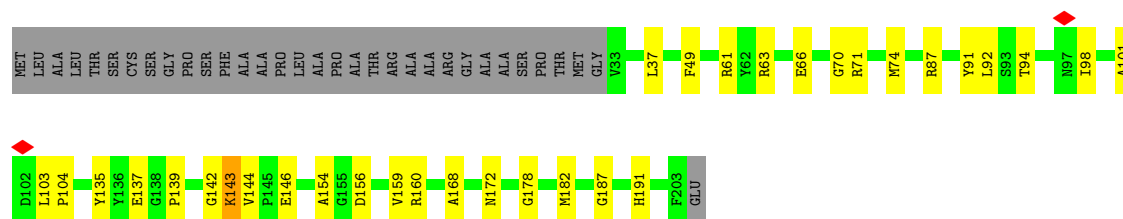


- Molecule 18: Light harvesting protein

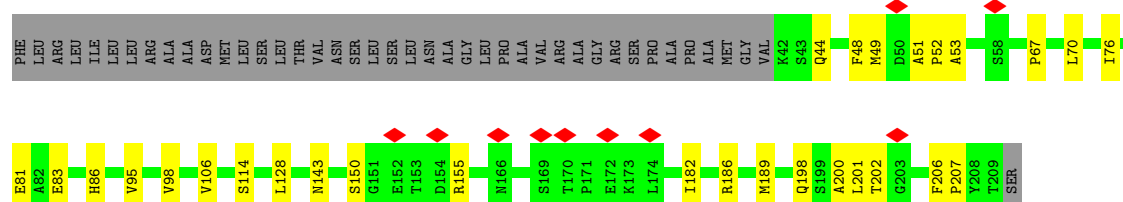


- Molecule 19: Light harvesting protein

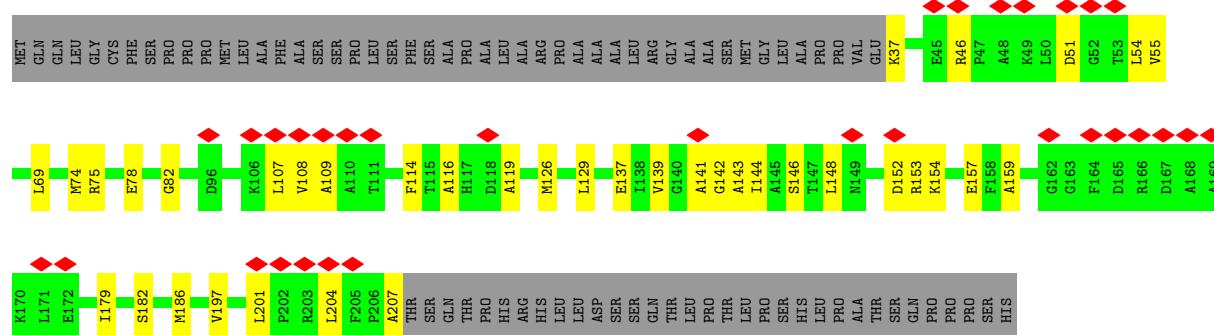




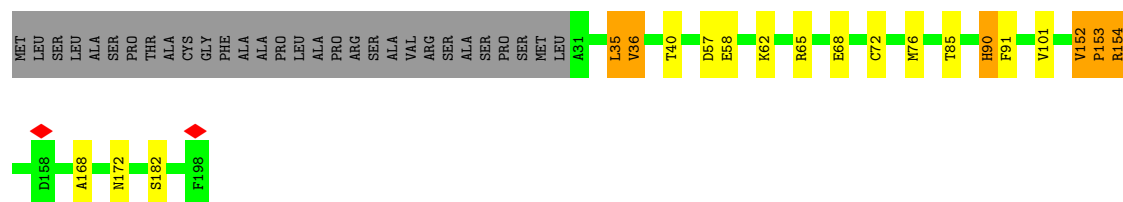
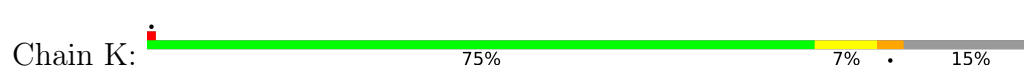
- Molecule 20: Light harvesting protein



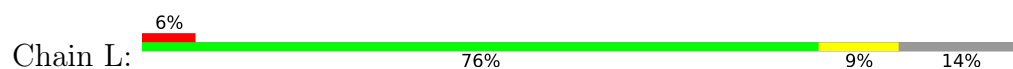
- Molecule 21: Light harvesting protein

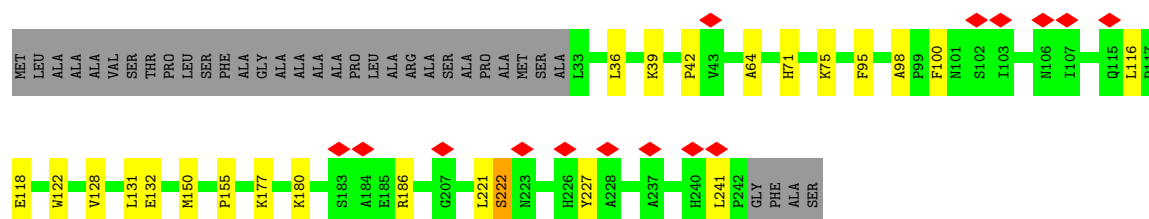


- Molecule 22: Light harvesting protein



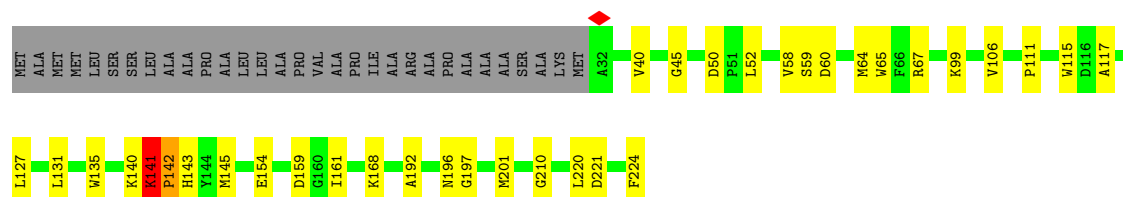
- Molecule 23: Light harvesting protein





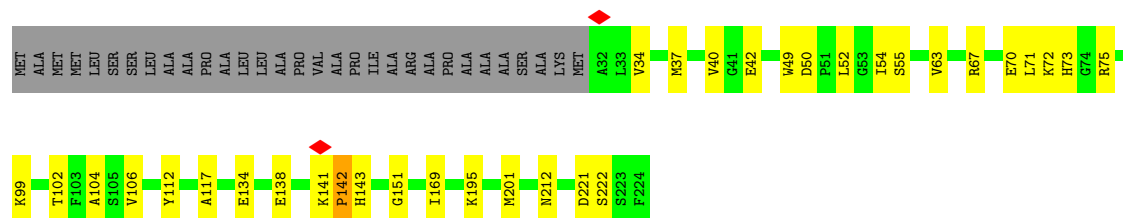
- Molecule 24: Light harvesting protein

Chain M: 71% 15% 14%



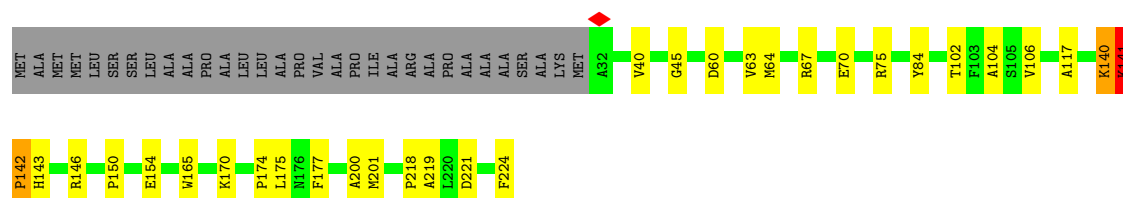
- Molecule 24: Light harvesting protein

Chain P: 71% 15% 14%



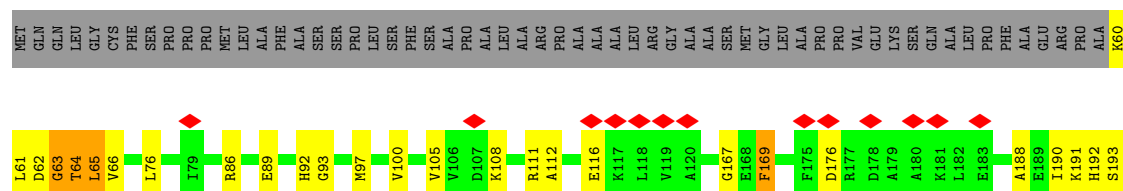
- Molecule 24: Light harvesting protein

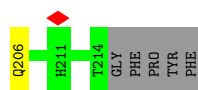
Chain W: 72% 12% 14%



- Molecule 25: Light harvesting protein

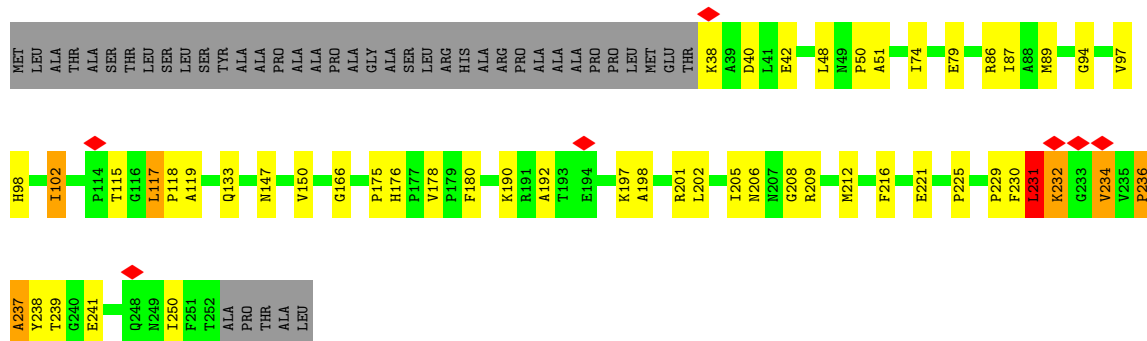
Chain O: 6% 57% 12% 29%





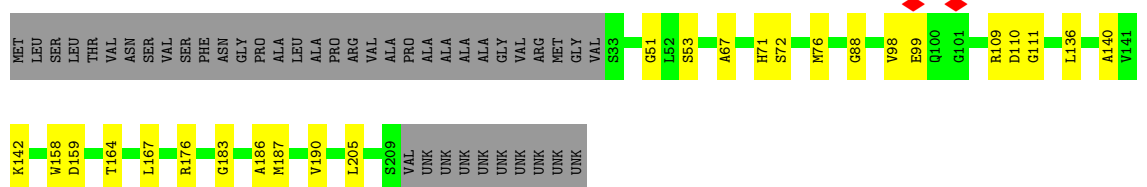
- Molecule 26: Light harvesting protein

Chain Q: 63% 18% 16%



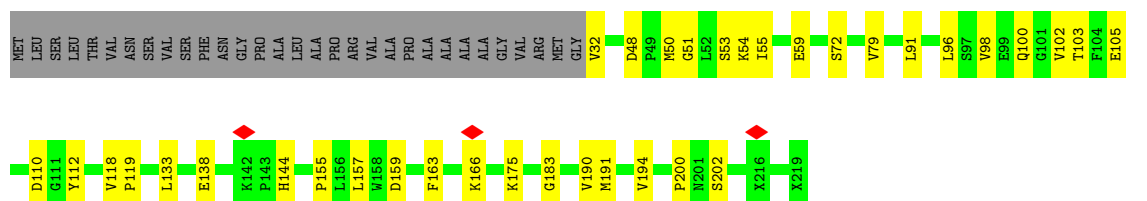
- Molecule 27: Light harvesting protein

Chain R: 69% 11% 19%



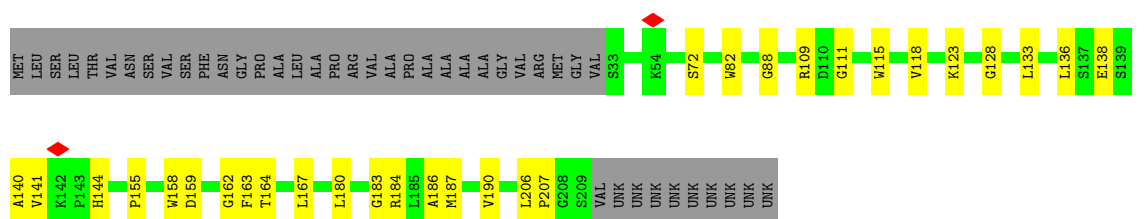
- Molecule 27: Light harvesting protein

Chain V: 69% 16% 14%

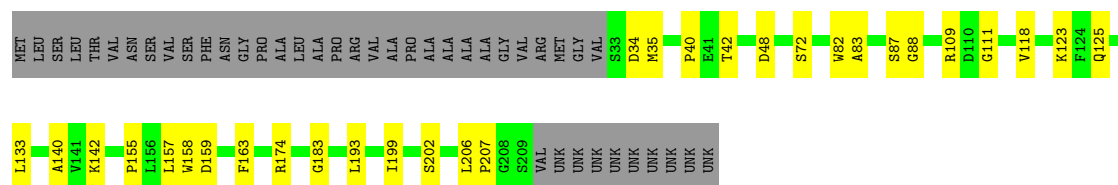


- Molecule 27: Light harvesting protein

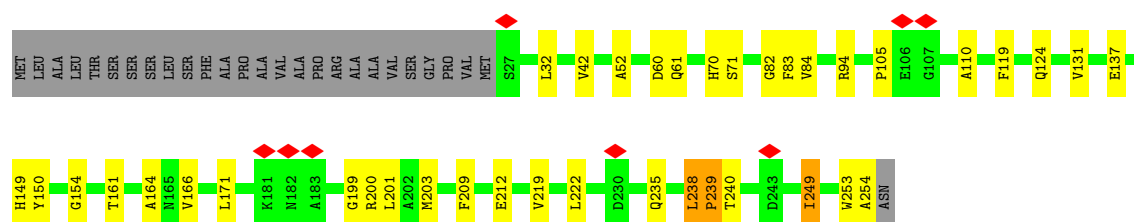
Chain X: 67% 14% 19%



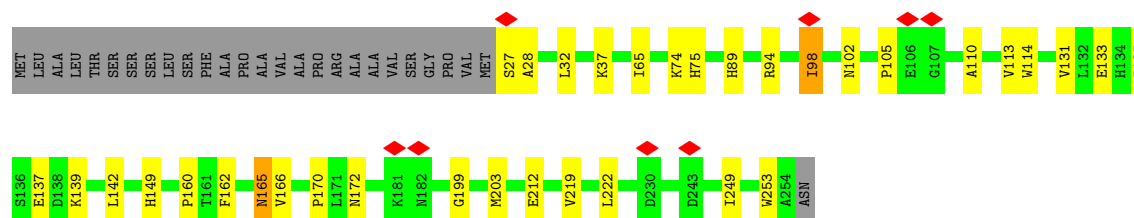
Chain 5: 67% 14% 19%



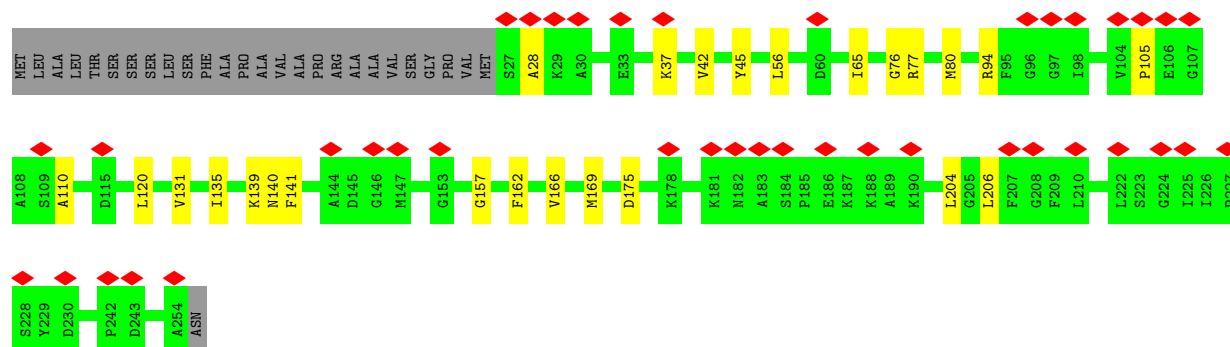
Chain S: 74% 14% 11%



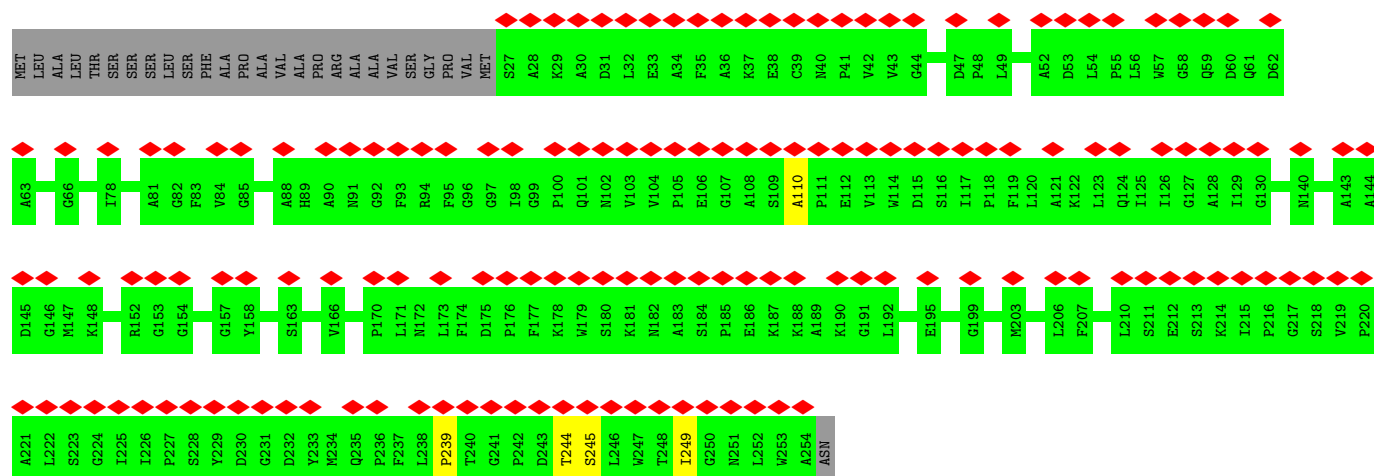
Chain 4: 76% 13% 11%



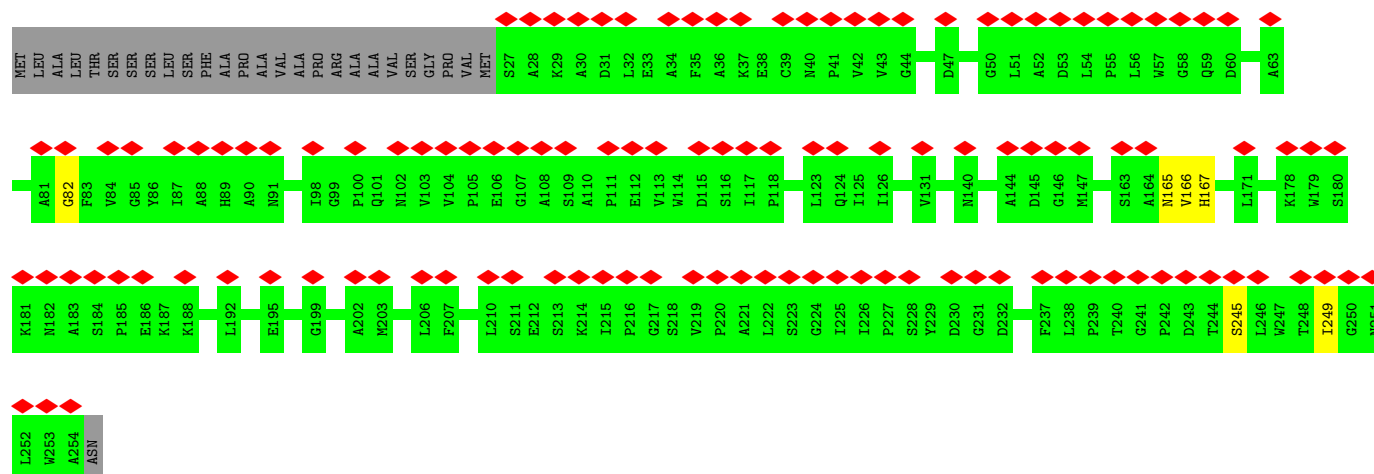
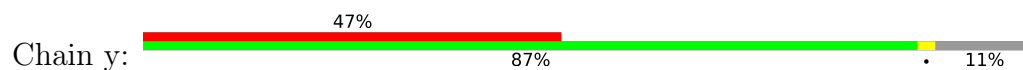
Chain 7:



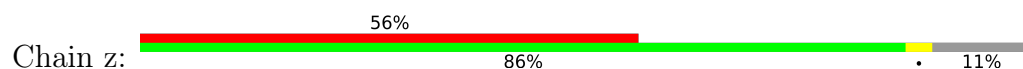
Chain x: 60% 87% 11%

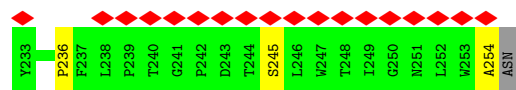


• Molecule 28: Light harvesting protein



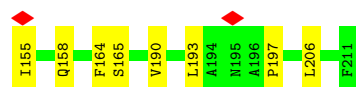
• Molecule 28: Light harvesting protein





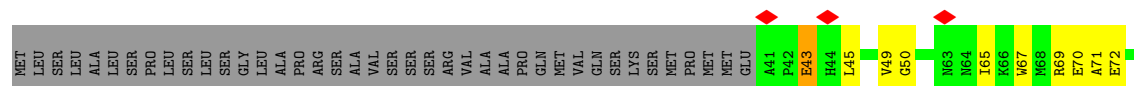
- Molecule 29: Light harvesting protein

Chain T: 78% 15% 7%



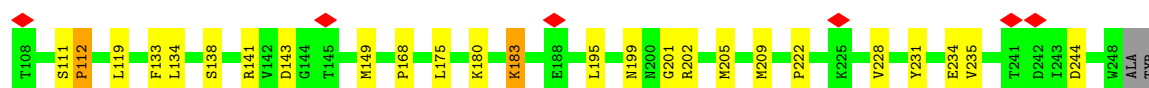
- Molecule 30: Light harvesting protein

Chain U: 63% 16% 20%



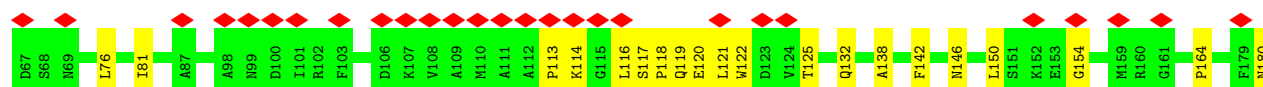
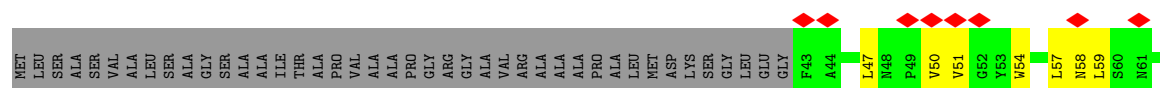
- Molecule 31: Light harvesting protein

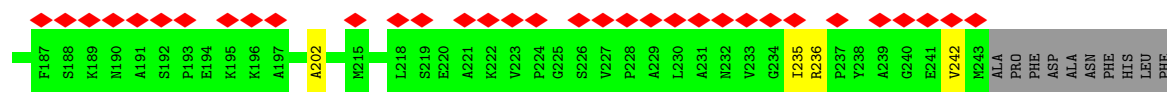
Chain 0: 70% 15% 14%



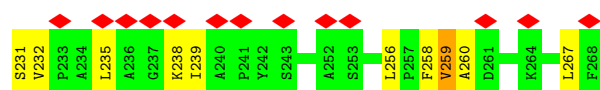
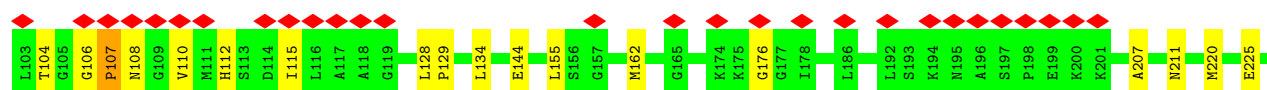
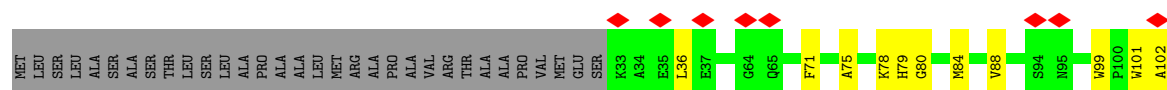
- Molecule 32: Light harvesting protein

Chain 1: 27% 67% 12% 21%

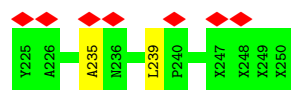
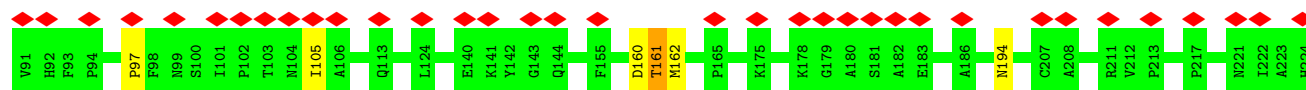
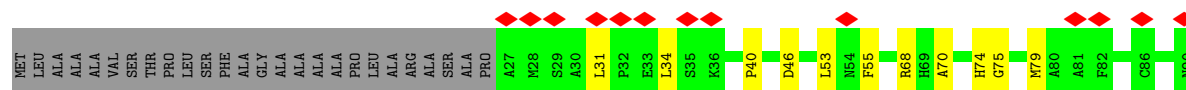
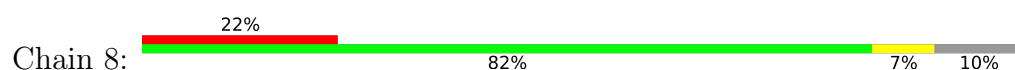




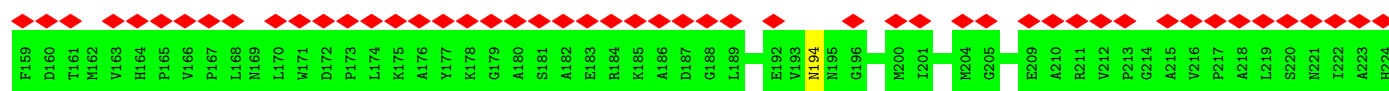
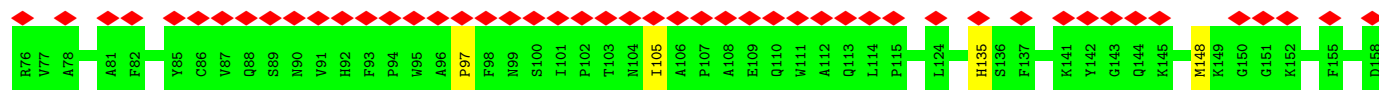
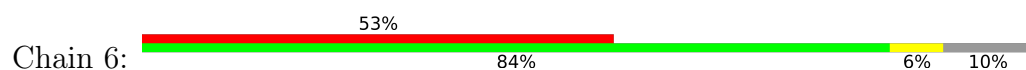
• Molecule 33: Light harvesting protein

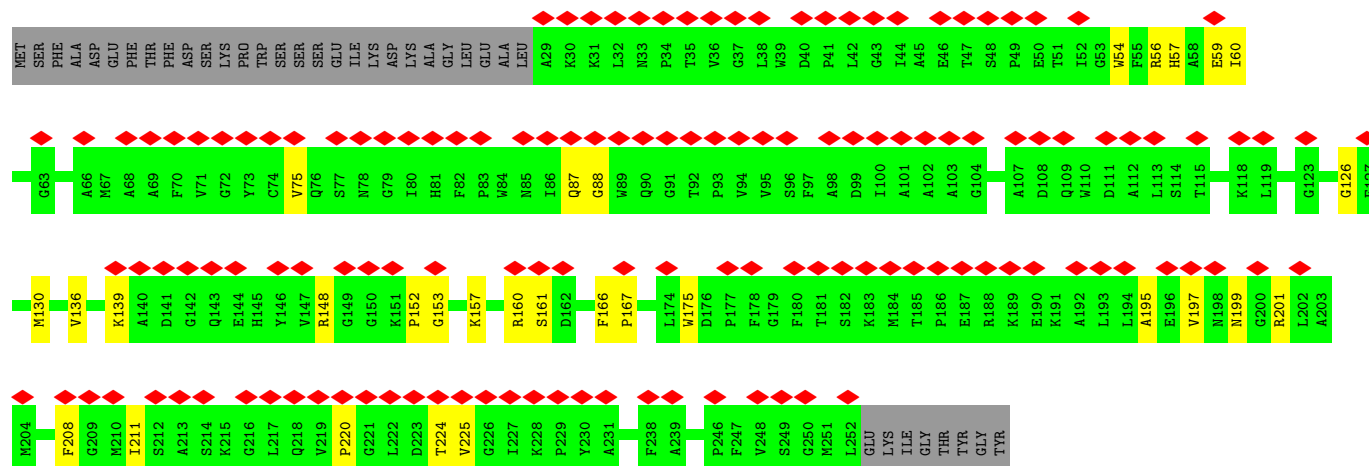


• Molecule 34: Light harvesting protein



• Molecule 34: Light harvesting protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.066	Depositor
Map size ($\text{\AA}$)	533.28, 533.28, 533.28	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A86, DD6, LMG, CLA, A1EB4, LHG, DGD, KC2, SF4, A1EB1, BCR, PQN, A1ECV, SQD

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	0.18	0/6028	0.40	0/8207
2	b	0.22	0/6028	0.46	1/8222 (0.0%)
3	c	0.16	0/608	0.54	0/824
4	d	0.18	0/1128	0.47	0/1525
5	e	0.24	0/503	0.45	0/683
6	f	0.18	0/1263	0.45	0/1714
7	i	0.30	0/261	0.56	0/357
8	j	0.14	0/325	0.33	0/438
9	l	0.19	0/1113	0.41	0/1513
10	m	0.21	0/226	0.62	0/306
11	k	0.19	0/545	0.43	0/737
12	o	0.21	0/371	0.59	0/503
13	A	0.18	0/1458	0.43	0/1979
14	B	0.20	0/1285	0.49	0/1750
15	C	0.21	0/1357	0.48	0/1836
16	D	0.19	0/1462	0.47	0/1988
17	E	0.22	0/1417	0.51	0/1933
18	F	0.28	0/1449	0.64	3/1967 (0.2%)
19	G	0.22	0/1386	0.55	2/1885 (0.1%)
20	H	0.25	0/1296	0.54	0/1757
21	J	0.23	0/1294	0.54	0/1749
22	K	0.24	0/1281	0.56	1/1744 (0.1%)
23	L	0.20	0/1684	0.49	0/2298
24	M	0.21	0/1491	0.42	0/2020
24	P	0.18	0/1491	0.42	0/2020
24	W	0.21	0/1491	0.45	0/2020
25	O	0.25	0/1152	0.60	0/1555
26	Q	0.26	0/1719	0.60	0/2340
27	5	0.24	0/1346	0.60	0/1830
27	R	0.22	0/1346	0.57	0/1830
27	V	0.23	0/1339	0.57	0/1820
27	X	0.23	0/1346	0.54	0/1830

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	4	0.21	0/1801	0.51	2/2451 (0.1%)
28	7	0.20	0/1801	0.48	0/2451
28	S	0.21	0/1801	0.49	0/2451
28	x	0.17	0/1112	0.43	0/1539
28	y	0.16	0/1112	0.38	0/1539
28	z	0.15	0/1112	0.41	0/1539
29	T	0.24	0/1534	0.55	1/2091 (0.0%)
30	U	0.21	0/1274	0.48	0/1726
31	0	0.24	0/1764	0.59	2/2410 (0.1%)
32	1	0.26	0/1284	0.56	0/1770
33	3	0.21	0/1828	0.54	3/2483 (0.1%)
34	6	0.16	0/1317	0.42	0/1813
34	8	0.20	0/1413	0.48	0/1941
35	9	0.25	0/1537	0.57	0/2106
36	I	0.23	0/1233	0.50	0/1666
37	h	0.17	0/669	0.37	0/915
38	2	0.23	0/1401	0.64	0/1911
38	Y	0.19	0/1098	0.59	1/1520 (0.1%)
38	Z	0.18	0/1098	0.58	0/1520
All	All	0.21	0/72678	0.50	16/99022 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	668	ARG	N-CA-C	10.45	123.65	111.11
22	K	36	VAL	N-CA-C	-6.07	107.94	113.71
28	4	165	ASN	CA-C-N	5.99	132.74	121.97
28	4	165	ASN	C-N-CA	5.99	132.74	121.97
33	3	231	SER	CA-C-N	5.66	132.60	122.13

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	5835	0	5733	90	0
2	b	5818	0	5640	71	0
3	c	598	0	581	7	0
4	d	1103	0	1113	20	0
5	e	491	0	480	1	0
6	f	1232	0	1231	13	0
7	i	254	0	262	5	0
8	j	318	0	333	7	0
9	l	1084	0	1090	15	0
10	m	224	0	243	7	0
11	k	533	0	547	11	0
12	o	360	0	363	6	0
13	A	1419	0	1408	20	0
14	B	1255	0	1223	28	0
15	C	1329	0	1352	16	0
16	D	1424	0	1361	20	0
17	E	1384	0	1399	22	0
18	F	1411	0	1407	41	0
19	G	1340	0	1303	17	0
20	H	1263	0	1232	23	0
21	J	1270	0	1295	33	0
22	K	1251	0	1249	16	0
23	L	1626	0	1560	19	0
24	M	1455	0	1468	40	0
24	P	1455	0	1468	26	0
24	W	1455	0	1468	29	0
25	O	1133	0	1141	28	0
26	Q	1666	0	1649	69	0
27	5	1311	0	1326	19	0
27	R	1311	0	1326	18	0
27	V	1353	0	1332	22	0
27	X	1311	0	1326	20	0
28	4	1744	0	1703	23	0
28	7	1744	0	1703	19	0
28	S	1744	0	1703	34	0
28	x	1113	0	529	2	0
28	y	1113	0	529	3	0
28	z	1113	0	529	4	0
29	T	1482	0	1457	22	0
30	U	1240	0	1212	22	0
31	0	1706	0	1662	24	0
32	1	1255	0	932	19	0
33	3	1775	0	1765	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	6	1326	0	910	8	0
34	8	1415	0	1126	9	0
35	9	1490	0	1326	17	0
36	I	1203	0	1215	15	0
37	h	650	0	636	1	0
38	2	1383	0	1078	18	0
38	Y	1099	0	529	4	0
38	Z	1099	0	529	2	0
39	0	457	0	379	18	0
39	1	384	0	279	6	0
39	2	385	0	275	5	0
39	3	477	0	425	12	0
39	4	460	0	454	14	0
39	5	339	0	320	7	0
39	6	345	0	258	3	0
39	7	410	0	353	19	0
39	8	353	0	266	7	0
39	9	347	0	258	10	0
39	A	531	0	527	12	0
39	B	287	0	228	7	0
39	C	470	0	474	13	0
39	D	685	0	725	25	0
39	E	728	0	683	20	0
39	F	551	0	512	13	0
39	G	280	0	257	3	0
39	H	479	0	430	13	0
39	I	520	0	512	12	0
39	J	576	0	506	15	0
39	K	418	0	427	13	0
39	L	420	0	364	7	0
39	M	444	0	424	11	0
39	O	423	0	332	8	0
39	P	352	0	358	8	0
39	Q	437	0	399	13	0
39	R	339	0	320	7	0
39	S	456	0	452	18	0
39	T	406	0	330	15	0
39	U	498	0	410	8	0
39	V	357	0	357	22	0
39	W	398	0	391	13	0
39	X	339	0	320	11	0
39	Y	374	0	265	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Z	374	0	265	3	0
39	a	2327	0	2356	90	0
39	b	2553	0	2635	106	0
39	f	120	0	121	2	0
39	h	55	0	49	0	0
39	i	130	0	144	10	0
39	j	65	0	72	5	0
39	k	162	0	141	3	0
39	l	229	0	222	13	0
39	o	258	0	219	6	0
39	x	337	0	240	5	0
39	y	339	0	244	2	0
39	z	335	0	240	2	0
40	a	33	0	46	4	0
40	b	33	0	46	3	0
41	D	70	0	80	3	0
41	H	35	0	40	3	0
41	X	41	0	55	2	0
41	a	76	0	98	3	0
41	j	30	0	30	1	0
42	a	160	0	224	16	0
42	b	240	0	336	23	0
42	f	80	0	112	6	0
42	h	40	0	56	4	0
42	i	40	0	56	6	0
42	j	40	0	56	1	0
42	k	40	0	56	2	0
42	l	120	0	168	10	0
42	m	40	0	56	5	0
43	1	43	0	0	2	0
43	2	43	0	0	1	0
43	3	86	0	0	3	0
43	4	86	0	0	1	0
43	5	43	0	0	1	0
43	7	86	0	0	5	0
43	A	172	0	0	1	0
43	B	43	0	0	0	0
43	C	43	0	0	0	0
43	D	129	0	0	1	0
43	E	129	0	0	1	0
43	F	86	0	0	7	0
43	G	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	H	86	0	0	1	0
43	I	129	0	0	1	0
43	J	129	0	0	1	0
43	K	43	0	0	0	0
43	M	43	0	0	2	0
43	O	129	0	0	2	0
43	P	43	0	0	2	0
43	Q	86	0	0	5	0
43	R	43	0	0	0	0
43	S	43	0	0	1	0
43	T	43	0	0	0	0
43	U	43	0	0	1	0
43	V	43	0	0	0	0
43	W	43	0	0	0	0
43	X	43	0	0	0	0
43	Z	43	0	0	0	0
43	a	43	0	0	0	0
43	j	43	0	0	0	0
43	o	43	0	0	0	0
43	x	86	0	0	0	0
43	y	86	0	0	0	0
43	z	86	0	0	1	0
44	b	8	0	0	0	0
44	c	16	0	0	0	0
45	C	40	0	38	0	0
45	b	60	0	81	3	0
46	0	27	0	23	4	0
46	4	78	0	93	35	0
46	7	78	0	93	22	0
46	9	36	0	42	0	0
46	A	29	0	28	1	0
46	D	37	0	44	1	0
46	F	73	0	84	22	0
46	I	42	0	54	1	0
46	M	72	0	82	10	0
46	P	39	0	46	5	0
46	Q	28	0	25	2	0
46	S	78	0	93	23	0
46	W	72	0	82	14	0
46	l	39	0	47	4	0
47	4	39	0	42	1	0
47	7	39	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	9	36	0	36	1	0
47	D	114	0	119	6	0
47	E	35	0	34	0	0
47	F	79	0	86	1	0
47	H	38	0	40	3	0
47	M	39	0	42	3	0
47	P	38	0	40	1	0
47	S	39	0	42	4	0
47	T	36	0	35	1	0
47	W	28	0	20	1	0
47	k	38	0	40	2	0
48	0	240	0	0	1	0
48	1	192	0	0	1	0
48	2	144	0	0	1	0
48	3	192	0	0	0	0
48	4	240	0	0	0	0
48	5	48	0	0	2	0
48	6	240	0	0	0	0
48	7	192	0	0	1	0
48	8	288	0	0	0	0
48	9	240	0	0	1	0
48	B	48	0	0	0	0
48	C	48	0	0	0	0
48	D	48	0	0	1	0
48	E	48	0	0	1	0
48	F	96	0	0	9	0
48	G	96	0	0	0	0
48	H	48	0	0	0	0
48	I	48	0	0	1	0
48	J	96	0	0	0	0
48	K	48	0	0	0	0
48	L	288	0	0	4	0
48	M	144	0	0	0	0
48	O	144	0	0	0	0
48	P	96	0	0	0	0
48	Q	240	0	0	31	0
48	R	144	0	0	2	0
48	S	144	0	0	0	0
48	T	144	0	0	0	0
48	U	96	0	0	1	0
48	V	96	0	0	0	0
48	W	144	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	X	96	0	0	0	0
48	Y	48	0	0	0	0
48	Z	96	0	0	1	0
48	k	48	0	0	0	0
48	x	48	0	0	0	0
48	y	96	0	0	0	0
48	z	48	0	0	0	0
49	0	179	0	0	2	0
49	1	135	0	0	0	0
49	2	134	0	0	1	0
49	3	180	0	0	1	0
49	4	180	0	0	1	0
49	5	179	0	0	27	0
49	6	180	0	0	1	0
49	7	135	0	0	1	0
49	8	225	0	0	1	0
49	9	180	0	0	0	0
49	A	90	0	0	0	0
49	B	45	0	0	0	0
49	C	90	0	0	0	0
49	F	89	0	0	9	0
49	G	180	0	0	0	0
49	H	90	0	0	0	0
49	I	89	0	0	0	0
49	J	45	0	0	0	0
49	K	90	0	0	0	0
49	L	225	0	0	1	0
49	M	179	0	0	1	0
49	O	44	0	0	1	0
49	P	224	0	0	3	0
49	Q	134	0	0	1	0
49	R	179	0	0	16	0
49	S	135	0	0	0	0
49	T	180	0	0	2	0
49	V	270	0	0	1	0
49	W	179	0	0	3	0
49	X	224	0	0	20	0
49	Y	90	0	0	1	0
49	Z	90	0	0	0	0
49	x	135	0	0	1	0
49	y	135	0	0	0	0
49	z	134	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	0	224	0	0	4	0
50	1	112	0	0	0	0
50	2	112	0	0	1	0
50	3	280	0	0	0	0
50	4	224	0	0	1	0
50	5	56	0	0	0	0
50	6	213	0	0	0	0
50	7	224	0	0	1	0
50	8	224	0	0	0	0
50	9	56	0	0	1	0
50	C	56	0	0	0	0
50	D	56	0	0	0	0
50	E	56	0	0	0	0
50	F	56	0	0	4	0
50	G	224	0	0	0	0
50	H	112	0	0	1	0
50	J	56	0	0	0	0
50	K	168	0	0	0	0
50	L	56	0	0	0	0
50	O	56	0	0	0	0
50	Q	112	0	0	0	0
50	R	56	0	0	0	0
50	S	112	0	0	1	0
50	T	112	0	0	0	0
50	U	112	0	0	0	0
50	V	224	0	0	0	0
50	h	56	0	0	0	0
50	x	112	0	0	2	0
50	y	112	0	0	0	0
50	z	104	0	0	1	0
51	0	48	0	0	2	0
51	1	48	0	0	1	0
51	2	48	0	0	1	0
51	4	96	0	0	0	0
51	5	96	0	0	0	0
51	6	48	0	0	0	0
51	7	96	0	0	6	0
51	9	96	0	0	2	0
51	E	48	0	0	0	0
51	G	48	0	0	0	0
51	L	48	0	0	0	0
51	M	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	O	48	0	0	0	0
51	P	48	0	0	0	0
51	Q	96	0	0	0	0
51	R	96	0	0	0	0
51	S	96	0	0	0	0
51	T	48	0	0	1	0
51	V	48	0	0	0	0
51	W	48	0	0	0	0
51	X	96	0	0	0	0
51	Y	96	0	0	1	0
51	Z	96	0	0	0	0
51	x	96	0	0	1	0
51	y	96	0	0	1	0
51	z	96	0	0	1	0
52	5	57	0	0	1	0
52	M	115	0	0	0	0
52	P	167	0	0	5	0
52	R	57	0	0	1	0
52	T	55	0	0	0	0
52	W	113	0	0	5	0
52	X	57	0	0	0	0
All	All	114135	0	89288	1557	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 8.

The worst 5 of 1557 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)
46:4:326:LMG:H311	49:5:313:KC2:C3A	1.15	1.56
49:X:314:KC2:C3A	46:7:301:LMG:H311	1.26	1.55
46:4:326:LMG:C31	49:5:313:KC2:C3A	2.03	1.35
46:4:326:LMG:C32	49:5:313:KC2:C4A	2.09	1.30
46:4:326:LMG:C31	49:5:313:KC2:C4A	2.12	1.27

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	739/752 (98%)	706 (96%)	33 (4%)	0	100	100
2	b	731/734 (100%)	698 (96%)	32 (4%)	1 (0%)	48	77
3	c	78/81 (96%)	74 (95%)	3 (4%)	1 (1%)	9	31
4	d	138/142 (97%)	125 (91%)	12 (9%)	1 (1%)	18	47
5	e	61/131 (47%)	58 (95%)	2 (3%)	1 (2%)	7	27
6	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
7	i	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	l	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
10	m	28/30 (93%)	27 (96%)	0	1 (4%)	2	10
11	k	71/145 (49%)	69 (97%)	1 (1%)	1 (1%)	9	30
12	o	46/123 (37%)	36 (78%)	9 (20%)	1 (2%)	5	19
13	A	181/201 (90%)	167 (92%)	13 (7%)	1 (1%)	21	51
14	B	170/177 (96%)	153 (90%)	15 (9%)	2 (1%)	10	34
15	C	174/233 (75%)	164 (94%)	9 (5%)	1 (1%)	21	51
16	D	187/231 (81%)	172 (92%)	14 (8%)	1 (0%)	24	55
17	E	185/217 (85%)	169 (91%)	16 (9%)	0	100	100
18	F	186/239 (78%)	157 (84%)	23 (12%)	6 (3%)	3	11
19	G	169/204 (83%)	148 (88%)	16 (10%)	5 (3%)	3	12
20	H	166/210 (79%)	147 (89%)	18 (11%)	1 (1%)	21	51
21	J	169/251 (67%)	150 (89%)	18 (11%)	1 (1%)	21	51
22	K	166/198 (84%)	149 (90%)	12 (7%)	5 (3%)	3	12
23	L	208/244 (85%)	182 (88%)	24 (12%)	2 (1%)	12	38
24	M	191/224 (85%)	170 (89%)	18 (9%)	3 (2%)	7	27
24	P	191/224 (85%)	175 (92%)	14 (7%)	2 (1%)	12	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	W	191/224 (85%)	176 (92%)	12 (6%)	3 (2%)	7	27
25	O	153/219 (70%)	135 (88%)	13 (8%)	5 (3%)	3	11
26	Q	213/257 (83%)	178 (84%)	24 (11%)	11 (5%)	1	5
27	5	175/219 (80%)	153 (87%)	22 (13%)	0	100	100
27	R	175/219 (80%)	151 (86%)	24 (14%)	0	100	100
27	V	178/219 (81%)	147 (83%)	24 (14%)	7 (4%)	2	8
27	X	175/219 (80%)	157 (90%)	18 (10%)	0	100	100
28	4	226/255 (89%)	202 (89%)	21 (9%)	3 (1%)	9	31
28	7	226/255 (89%)	201 (89%)	24 (11%)	1 (0%)	30	60
28	S	226/255 (89%)	204 (90%)	18 (8%)	4 (2%)	6	23
28	x	226/255 (89%)	203 (90%)	20 (9%)	3 (1%)	9	31
28	y	226/255 (89%)	211 (93%)	13 (6%)	2 (1%)	14	41
28	z	226/255 (89%)	203 (90%)	19 (8%)	4 (2%)	6	23
29	T	195/211 (92%)	169 (87%)	23 (12%)	3 (2%)	8	28
30	U	156/198 (79%)	138 (88%)	16 (10%)	2 (1%)	9	31
31	0	216/254 (85%)	186 (86%)	25 (12%)	5 (2%)	5	18
32	1	199/253 (79%)	163 (82%)	29 (15%)	7 (4%)	3	10
33	3	234/268 (87%)	204 (87%)	26 (11%)	4 (2%)	7	25
34	6	217/250 (87%)	182 (84%)	31 (14%)	4 (2%)	6	23
34	8	217/250 (87%)	186 (86%)	25 (12%)	6 (3%)	4	14
35	9	207/245 (84%)	173 (84%)	32 (16%)	2 (1%)	12	38
36	I	154/209 (74%)	142 (92%)	12 (8%)	0	100	100
37	h	85/133 (64%)	83 (98%)	2 (2%)	0	100	100
38	2	222/260 (85%)	186 (84%)	31 (14%)	5 (2%)	5	18
38	Y	223/260 (86%)	186 (83%)	31 (14%)	6 (3%)	4	15
38	Z	223/260 (86%)	191 (86%)	26 (12%)	6 (3%)	4	15
All	All	9768/11553 (84%)	8765 (90%)	873 (9%)	130 (1%)	12	31

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	101	PRO
13	A	200	SER

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Mol	Chain	Res	Type
15	C	171	ASN
18	F	135	ILE
18	F	181	GLU

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	608/616 (99%)	608 (100%)	0	100	100
2	b	591/592 (100%)	591 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	d	120/122 (98%)	118 (98%)	2 (2%)	53	83
5	e	51/91 (56%)	51 (100%)	0	100	100
6	f	126/144 (88%)	126 (100%)	0	100	100
7	i	29/32 (91%)	29 (100%)	0	100	100
8	j	36/36 (100%)	36 (100%)	0	100	100
9	l	114/115 (99%)	114 (100%)	0	100	100
10	m	23/23 (100%)	23 (100%)	0	100	100
11	k	56/107 (52%)	56 (100%)	0	100	100
12	o	40/85 (47%)	40 (100%)	0	100	100
13	A	155/170 (91%)	155 (100%)	0	100	100
14	B	120/131 (92%)	119 (99%)	1 (1%)	73	90
15	C	140/181 (77%)	140 (100%)	0	100	100
16	D	140/171 (82%)	140 (100%)	0	100	100
17	E	146/163 (90%)	146 (100%)	0	100	100
18	F	140/180 (78%)	138 (99%)	2 (1%)	59	85
19	G	132/153 (86%)	132 (100%)	0	100	100
20	H	131/163 (80%)	131 (100%)	0	100	100
21	J	128/194 (66%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	K	127/149 (85%)	126 (99%)	1 (1%)	73	90
23	L	161/183 (88%)	160 (99%)	1 (1%)	78	92
24	M	146/165 (88%)	145 (99%)	1 (1%)	76	91
24	P	146/165 (88%)	146 (100%)	0	100	100
24	W	146/165 (88%)	144 (99%)	2 (1%)	59	85
25	O	112/160 (70%)	111 (99%)	1 (1%)	70	89
26	Q	171/199 (86%)	167 (98%)	4 (2%)	44	78
27	5	134/157 (85%)	134 (100%)	0	100	100
27	R	134/157 (85%)	134 (100%)	0	100	100
27	V	132/157 (84%)	132 (100%)	0	100	100
27	X	134/157 (85%)	134 (100%)	0	100	100
28	4	179/199 (90%)	179 (100%)	0	100	100
28	7	179/199 (90%)	179 (100%)	0	100	100
28	S	179/199 (90%)	177 (99%)	2 (1%)	65	87
29	T	150/161 (93%)	150 (100%)	0	100	100
30	U	128/162 (79%)	128 (100%)	0	100	100
31	0	177/198 (89%)	177 (100%)	0	100	100
32	1	74/194 (38%)	74 (100%)	0	100	100
33	3	181/204 (89%)	181 (100%)	0	100	100
34	6	58/183 (32%)	58 (100%)	0	100	100
34	8	91/183 (50%)	89 (98%)	2 (2%)	45	78
35	9	126/188 (67%)	126 (100%)	0	100	100
36	I	126/163 (77%)	126 (100%)	0	100	100
37	h	67/94 (71%)	67 (100%)	0	100	100
38	2	82/204 (40%)	82 (100%)	0	100	100
All	All	6434/7883 (82%)	6415 (100%)	19 (0%)	84	95

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	S	240	THR
34	8	160	ASP
34	8	161	THR

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Mol	Chain	Res	Type
24	W	141	LYS
25	O	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
33	3	54	ASN
34	6	195	ASN
33	3	210	ASN
28	7	140	ASN
13	A	82	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

869 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	$\# Z > 2$
48	A86	2	305	-	44,50,50	1.12	2 (4%)	51,76,76	2.43	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	b	816	-	64,68,73	1.31	8 (12%)	77,107,113	1.31	6 (7%)
50	A1EB1	V	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.09	17 (28%)
39	CLA	U	214	-	50,54,73	1.47	7 (14%)	60,90,113	1.42	4 (6%)
39	CLA	G	314	19	62,66,73	1.31	7 (11%)	74,104,113	1.45	6 (8%)
39	CLA	0	323	-	50,54,73	1.43	8 (16%)	60,90,113	1.48	5 (8%)
39	CLA	x	318	-	45,49,73	1.54	8 (17%)	54,84,113	1.57	8 (14%)
49	KC2	W	315	-	49,53,53	1.81	9 (18%)	62,89,89	2.05	14 (22%)
49	KC2	9	311	-	49,53,53	1.79	10 (20%)	62,89,89	2.10	15 (24%)
39	CLA	Z	313	-	45,49,73	1.55	8 (17%)	54,84,113	1.89	10 (18%)
49	KC2	C	312	-	49,53,53	1.76	10 (20%)	62,89,89	2.14	17 (27%)
48	A86	0	304	-	44,50,50	1.20	2 (4%)	51,76,76	1.94	15 (29%)
39	CLA	D	316	-	69,73,73	1.25	7 (10%)	83,113,113	1.26	5 (6%)
39	CLA	S	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.49	6 (11%)
47	SQD	D	304	-	37,38,54	1.14	5 (13%)	46,49,65	1.74	10 (21%)
49	KC2	Q	315	-	49,53,53	1.75	10 (20%)	62,89,89	2.13	18 (29%)
42	BCR	f	804	-	41,41,41	0.68	0	56,56,56	1.98	14 (25%)
48	A86	G	301	-	44,50,50	1.18	2 (4%)	51,76,76	2.46	19 (37%)
43	DD6	x	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.96	16 (30%)
39	CLA	A	311	-	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
48	A86	x	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.26	17 (33%)
48	A86	2	301	-	44,50,50	1.18	3 (6%)	51,76,76	2.31	17 (33%)
49	KC2	0	316	-	49,53,53	1.75	10 (20%)	62,89,89	2.13	19 (30%)
39	CLA	S	310	-	46,50,73	1.51	7 (15%)	55,85,113	1.59	6 (10%)
43	DD6	O	304	-	39,45,45	2.10	4 (10%)	52,67,67	1.91	15 (28%)
48	A86	8	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.24	19 (37%)
39	CLA	L	309	-	57,62,73	1.37	9 (15%)	68,100,113	1.41	7 (10%)
39	CLA	Q	314	-	58,62,73	1.36	9 (15%)	69,99,113	1.37	5 (7%)
39	CLA	V	316	-	54,58,73	1.42	7 (12%)	65,95,113	1.44	9 (13%)
39	CLA	7	314	-	60,64,73	1.36	7 (11%)	72,102,113	1.47	10 (13%)
39	CLA	y	315	-	45,49,73	1.52	7 (15%)	54,84,113	1.57	5 (9%)
48	A86	P	302	-	44,50,50	1.23	2 (4%)	51,76,76	2.31	17 (33%)
49	KC2	2	313	-	48,52,53	1.80	10 (20%)	62,88,89	2.19	19 (30%)
43	DD6	3	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	13 (25%)
49	KC2	M	314	-	49,53,53	1.78	9 (18%)	62,89,89	2.11	19 (30%)
39	CLA	L	320	-	50,54,73	1.47	6 (12%)	60,90,113	1.56	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	R	316	-	56,60,73	1.41	9 (16%)	67,97,113	1.45	5 (7%)
39	CLA	b	839	-	51,55,73	1.45	8 (15%)	61,91,113	1.37	6 (9%)
39	CLA	A	305	13	53,57,73	1.44	8 (15%)	62,93,113	1.41	5 (8%)
39	CLA	M	321	24	50,54,73	1.46	7 (14%)	60,90,113	1.47	5 (8%)
39	CLA	T	309	-	60,64,73	1.37	7 (11%)	72,102,113	1.34	9 (12%)
43	DD6	z	305	-	39,45,45	2.02	2 (5%)	52,67,67	1.89	16 (30%)
39	CLA	9	310	-	45,49,73	1.51	8 (17%)	54,84,113	1.57	8 (14%)
43	DD6	Z	302	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
49	KC2	V	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.25	18 (29%)
48	A86	0	309	-	44,50,50	1.20	2 (4%)	51,76,76	2.35	18 (35%)
39	CLA	X	317	-	56,60,73	1.40	9 (16%)	67,97,113	1.45	6 (8%)
39	CLA	P	316	-	55,59,73	1.41	8 (14%)	66,96,113	1.43	5 (7%)
48	A86	J	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.28	18 (35%)
51	A1ECV	4	315	-	54,56,56	2.65	20 (37%)	61,93,93	4.12	31 (50%)
49	KC2	L	314	-	49,53,53	1.75	9 (18%)	62,89,89	2.17	19 (30%)
49	KC2	1	312	-	49,53,53	1.83	11 (22%)	62,89,89	2.02	15 (24%)
47	SQD	M	301	-	38,39,54	1.11	5 (13%)	47,50,65	1.69	13 (27%)
49	KC2	Q	313	46	48,52,53	1.81	11 (22%)	59,87,89	2.24	17 (28%)
43	DD6	5	303	-	39,45,45	1.90	3 (7%)	52,67,67	1.73	12 (23%)
39	CLA	O	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.58	5 (9%)
39	CLA	a	833	1	49,53,73	1.48	7 (14%)	59,89,113	1.49	5 (8%)
39	CLA	C	307	-	69,73,73	1.24	8 (11%)	83,113,113	1.32	6 (7%)
39	CLA	5	316	-	56,60,73	1.41	9 (16%)	67,97,113	1.42	5 (7%)
39	CLA	P	308	24	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
39	CLA	9	307	-	45,49,73	1.54	8 (17%)	54,84,113	1.51	6 (11%)
39	CLA	b	824	-	64,68,73	1.30	8 (12%)	77,107,113	1.33	4 (5%)
39	CLA	E	319	17	53,57,73	1.43	7 (13%)	62,93,113	1.40	5 (8%)
39	CLA	b	840	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
39	CLA	Y	305	-	45,49,73	1.53	6 (13%)	54,84,113	1.54	5 (9%)
46	LMG	S	322	49	46,46,55	0.95	2 (4%)	54,54,63	1.32	5 (9%)
39	CLA	a	811	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	5 (6%)
39	CLA	U	215	-	45,49,73	1.55	7 (15%)	54,84,113	1.56	6 (11%)
46	LMG	9	321	-	36,36,55	0.91	0	44,44,63	1.20	3 (6%)
49	KC2	L	317	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	18 (29%)
49	KC2	V	308	27	49,53,53	1.77	10 (20%)	62,89,89	2.20	18 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	KC2	X	312	-	49,53,53	1.76	9 (18%)	62,89,89	2.20	19 (30%)
49	KC2	z	313	-	46,50,53	1.98	11 (23%)	49,80,89	2.25	12 (24%)
39	CLA	y	309	-	50,54,73	1.47	7 (14%)	60,90,113	1.43	5 (8%)
48	A86	Z	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.18	19 (37%)
39	CLA	E	318	17	50,54,73	1.46	8 (16%)	60,90,113	1.42	5 (8%)
50	A1EB1	x	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.07	19 (31%)
39	CLA	a	809	-	66,70,73	1.27	7 (10%)	79,109,113	1.32	5 (6%)
39	CLA	a	837	-	69,73,73	1.27	7 (10%)	83,113,113	1.26	5 (6%)
39	CLA	x	317	-	45,49,73	1.53	6 (13%)	54,84,113	1.53	6 (11%)
39	CLA	0	312	31	57,61,73	1.36	9 (15%)	68,98,113	1.41	7 (10%)
39	CLA	M	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.35	6 (7%)
39	CLA	I	308	-	65,69,73	1.27	7 (10%)	78,108,113	1.29	7 (8%)
43	DD6	z	304	-	39,45,45	2.05	4 (10%)	52,67,67	1.88	14 (26%)
49	KC2	3	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.16	19 (30%)
50	A1EB1	8	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	16 (26%)
49	KC2	8	316	-	49,53,53	1.77	10 (20%)	62,89,89	2.20	16 (25%)
39	CLA	b	821	-	69,73,73	1.27	8 (11%)	83,113,113	1.31	7 (8%)
39	CLA	8	313	-	45,49,73	1.51	7 (15%)	54,84,113	1.51	6 (11%)
39	CLA	x	306	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	4 (6%)
46	LMG	M	320	-	33,33,55	0.94	0	41,41,63	1.19	4 (9%)
41	LHG	j	104	-	29,29,48	0.74	1 (3%)	32,35,54	1.23	3 (9%)
39	CLA	8	315	-	47,51,73	1.49	8 (17%)	56,86,113	1.43	4 (7%)
42	BCR	l	207	-	41,41,41	0.69	0	56,56,56	1.81	11 (19%)
50	A1EB1	0	307	-	51,58,58	1.25	3 (5%)	60,85,85	2.24	17 (28%)
42	BCR	l	206	-	41,41,41	0.69	0	56,56,56	1.76	13 (23%)
39	CLA	E	314	-	60,64,73	1.35	9 (15%)	72,102,113	1.36	4 (5%)
49	KC2	8	319	34	49,53,53	1.79	10 (20%)	62,89,89	2.14	17 (27%)
49	KC2	R	306	-	49,53,53	1.81	10 (20%)	62,89,89	2.08	14 (22%)
39	CLA	E	315	-	50,54,73	1.48	8 (16%)	60,90,113	1.45	4 (6%)
39	CLA	H	307	-	49,53,73	1.50	6 (12%)	59,89,113	1.48	4 (6%)
39	CLA	3	322	-	55,59,73	1.40	8 (14%)	66,96,113	1.45	6 (9%)
39	CLA	9	315	-	45,49,73	1.53	8 (17%)	54,84,113	1.53	5 (9%)
39	CLA	D	311	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
50	A1EB1	G	308	-	51,58,58	1.22	3 (5%)	60,85,85	2.28	16 (26%)
50	A1EB1	z	301	-	44,50,58	1.15	2 (4%)	51,76,85	1.70	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	A1EB1	h	203	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	19 (31%)
39	CLA	6	313	-	46,50,73	1.50	6 (13%)	55,85,113	1.48	4 (7%)
48	A86	T	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.22	19 (37%)
39	CLA	b	810	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	5 (6%)
49	KC2	T	314	-	49,53,53	1.75	10 (20%)	62,89,89	2.18	18 (29%)
39	CLA	V	310	-	64,68,73	1.31	8 (12%)	77,107,113	1.43	12 (15%)
49	KC2	z	312	-	49,53,53	1.78	10 (20%)	62,89,89	2.04	15 (24%)
48	A86	7	308	-	44,50,50	1.19	2 (4%)	51,76,76	2.06	16 (31%)
39	CLA	J	317	-	46,50,73	1.53	8 (17%)	55,85,113	1.48	4 (7%)
39	CLA	2	316	-	45,49,73	1.52	7 (15%)	54,84,113	1.58	5 (9%)
39	CLA	b	830	-	69,73,73	1.27	8 (11%)	83,113,113	1.40	7 (8%)
43	DD6	M	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.71	12 (23%)
39	CLA	6	322	-	50,54,73	1.47	6 (12%)	60,90,113	1.46	4 (6%)
46	LMG	Q	322	49	28,28,55	1.26	2 (7%)	36,36,63	1.44	6 (16%)
49	KC2	7	322	-	49,53,53	1.78	10 (20%)	62,89,89	2.11	17 (27%)
50	A1EB1	7	303	-	51,58,58	1.33	3 (5%)	60,85,85	2.01	20 (33%)
39	CLA	8	321	-	46,50,73	1.51	7 (15%)	55,85,113	1.46	4 (7%)
39	CLA	o	206	-	62,66,73	1.32	6 (9%)	74,104,113	1.36	5 (6%)
46	LMG	F	317	-	39,39,55	1.05	2 (5%)	47,47,63	1.23	6 (12%)
50	A1EB1	8	308	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	18 (30%)
46	LMG	7	326	-	32,32,55	0.93	1 (3%)	40,40,63	1.23	3 (7%)
48	A86	L	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.32	18 (35%)
43	DD6	O	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	13 (25%)
48	A86	Q	308	-	44,50,50	1.15	2 (4%)	51,76,76	2.25	15 (29%)
49	KC2	Y	309	-	49,53,53	1.77	9 (18%)	62,89,89	2.11	17 (27%)
52	A1EB4	P	305	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)
39	CLA	k	201	-	56,60,73	1.37	9 (16%)	67,97,113	1.39	5 (7%)
39	CLA	C	305	-	65,69,73	1.30	6 (9%)	78,108,113	1.29	5 (6%)
49	KC2	6	319	-	49,53,53	1.82	11 (22%)	62,89,89	2.05	13 (20%)
39	CLA	b	813	-	58,62,73	1.41	10 (17%)	73,100,113	1.42	6 (8%)
39	CLA	4	322	-	56,60,73	1.40	9 (16%)	67,97,113	1.44	7 (10%)
48	A86	T	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.33	17 (33%)
39	CLA	b	820	-	64,68,73	1.31	9 (14%)	77,107,113	1.29	4 (5%)
49	KC2	3	315	-	49,53,53	1.81	10 (20%)	62,89,89	2.14	15 (24%)
39	CLA	V	311	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	4	319	-	45,49,73	1.53	7 (15%)	54,84,113	1.56	5 (9%)
46	LMG	W	320	-	33,33,55	0.94	1 (3%)	41,41,63	1.21	4 (9%)
49	KC2	V	318	-	49,53,53	1.78	9 (18%)	62,89,89	2.15	17 (27%)
39	CLA	5	308	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
39	CLA	7	324	-	45,49,73	1.53	8 (17%)	54,84,113	1.64	8 (14%)
49	KC2	8	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.12	17 (27%)
50	A1EB1	8	304	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	17 (28%)
51	A1ECV	X	310	-	54,56,56	2.64	20 (37%)	61,93,93	4.12	29 (47%)
50	A1EB1	6	308	-	51,58,58	1.29	4 (7%)	60,85,85	2.25	19 (31%)
39	CLA	Y	304	-	50,54,73	1.46	6 (12%)	60,90,113	1.47	4 (6%)
39	CLA	z	307	-	46,50,73	1.51	6 (13%)	55,85,113	1.50	6 (10%)
39	CLA	F	313	-	61,65,73	1.34	9 (14%)	73,103,113	1.35	6 (8%)
39	CLA	b	814	-	59,63,73	1.36	8 (13%)	71,101,113	1.36	6 (8%)
49	KC2	A	313	-	49,53,53	1.79	10 (20%)	62,89,89	2.14	19 (30%)
48	A86	1	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.29	18 (35%)
49	KC2	I	312	46	48,52,53	1.73	9 (18%)	59,87,89	2.31	19 (32%)
43	DD6	A	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.88	12 (23%)
39	CLA	F	315	18	45,49,73	1.52	6 (13%)	54,84,113	1.66	6 (11%)
39	CLA	A	307	-	64,68,73	1.32	8 (12%)	77,107,113	1.30	6 (7%)
39	CLA	J	316	-	50,54,73	1.46	7 (14%)	60,90,113	1.49	4 (6%)
50	A1EB1	7	305	-	51,58,58	1.29	4 (7%)	60,85,85	2.22	18 (30%)
39	CLA	O	312	-	50,54,73	1.47	8 (16%)	60,90,113	1.45	4 (6%)
39	CLA	x	314	-	45,49,73	1.52	7 (15%)	54,84,113	1.56	5 (9%)
39	CLA	2	318	-	45,49,73	1.53	7 (15%)	54,84,113	1.53	5 (9%)
49	KC2	R	312	-	49,53,53	1.75	11 (22%)	62,89,89	2.18	19 (30%)
39	CLA	i	103	-	69,73,73	1.27	9 (13%)	83,113,113	1.38	10 (12%)
39	CLA	x	309	-	45,49,73	1.53	8 (17%)	54,84,113	1.55	6 (11%)
39	CLA	C	308	-	64,68,73	1.30	8 (12%)	77,107,113	1.35	6 (7%)
50	A1EB1	0	302	-	51,58,58	1.22	3 (5%)	60,85,85	2.11	19 (31%)
39	CLA	b	802	-	69,73,73	1.26	8 (11%)	83,113,113	1.25	5 (6%)
48	A86	L	307	-	44,50,50	1.18	3 (6%)	51,76,76	2.52	20 (39%)
49	KC2	5	311	-	49,53,53	1.78	10 (20%)	62,89,89	2.25	19 (30%)
48	A86	3	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.40	20 (39%)
43	DD6	Q	303	-	39,45,45	2.12	3 (7%)	52,67,67	2.59	17 (32%)
48	A86	0	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.25	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	a	821	-	59,63,73	1.35	8 (13%)	71,101,113	1.40	5 (7%)
39	CLA	2	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.58	5 (9%)
49	KC2	R	314	46	48,52,53	1.74	9 (18%)	59,87,89	2.20	16 (27%)
48	A86	9	304	-	44,50,50	1.16	3 (6%)	51,76,76	2.06	16 (31%)
39	CLA	Y	311	-	45,49,73	1.52	6 (13%)	54,84,113	1.57	6 (11%)
39	CLA	D	312	16	59,63,73	1.35	8 (13%)	71,101,113	1.39	8 (11%)
48	A86	9	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.01	14 (27%)
39	CLA	Z	309	-	45,49,73	1.53	6 (13%)	54,84,113	1.46	4 (7%)
39	CLA	1	310	-	49,53,73	1.50	7 (14%)	59,89,113	1.48	4 (6%)
39	CLA	a	829	-	60,64,73	1.35	6 (10%)	72,102,113	1.39	6 (8%)
48	A86	Q	302	-	44,50,50	1.21	3 (6%)	51,76,76	2.27	18 (35%)
49	KC2	L	312	-	49,53,53	1.81	10 (20%)	62,89,89	1.99	14 (22%)
39	CLA	b	823	-	50,54,73	1.46	6 (12%)	60,90,113	1.46	5 (8%)
51	A1ECV	T	317	-	54,56,56	2.62	20 (37%)	61,93,93	3.84	31 (50%)
39	CLA	J	312	-	50,54,73	1.48	8 (16%)	60,90,113	1.47	4 (6%)
50	A1EB1	V	306	-	51,58,58	1.25	3 (5%)	60,85,85	1.97	19 (31%)
50	A1EB1	V	302	-	51,58,58	1.27	4 (7%)	60,85,85	2.00	20 (33%)
39	CLA	6	321	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	5 (9%)
46	LMG	4	325	-	32,32,55	0.90	0	40,40,63	1.25	4 (10%)
49	KC2	7	320	-	49,53,53	1.79	9 (18%)	62,89,89	2.06	15 (24%)
43	DD6	H	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	10 (19%)
39	CLA	O	310	-	64,68,73	1.32	9 (14%)	77,107,113	1.39	10 (12%)
49	KC2	V	314	-	49,53,53	1.77	9 (18%)	62,89,89	2.14	19 (30%)
39	CLA	O	308	-	41,46,73	1.60	7 (17%)	51,80,113	2.03	11 (21%)
48	A86	P	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.25	18 (35%)
50	A1EB1	3	324	-	51,58,58	1.29	3 (5%)	60,85,85	2.03	18 (30%)
48	A86	3	308	-	44,50,50	1.25	3 (6%)	51,76,76	2.33	18 (35%)
51	A1ECV	5	309	27	54,56,56	2.63	20 (37%)	61,93,93	4.06	30 (49%)
50	A1EB1	1	301	-	51,58,58	1.22	3 (5%)	60,85,85	1.92	17 (28%)
39	CLA	U	211	-	64,68,73	1.31	7 (10%)	77,107,113	1.36	8 (10%)
43	DD6	A	304	-	39,45,45	2.00	2 (5%)	52,67,67	1.75	13 (25%)
39	CLA	b	834	-	62,66,73	1.33	7 (11%)	74,104,113	1.37	6 (8%)
39	CLA	B	206	-	46,50,73	1.51	8 (17%)	55,85,113	1.47	6 (10%)
39	CLA	T	320	-	56,60,73	1.39	8 (14%)	67,97,113	1.36	5 (7%)
39	CLA	b	831	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	KC2	W	312	24,46	48,52,53	1.72	9 (18%)	59,87,89	2.21	18 (30%)
49	KC2	X	315	-	49,53,53	1.77	10 (20%)	62,89,89	2.15	17 (27%)
39	CLA	D	319	16	69,73,73	1.26	6 (8%)	83,113,113	1.31	7 (8%)
39	CLA	0	313	-	59,63,73	1.36	7 (11%)	71,101,113	1.38	6 (8%)
39	CLA	D	318	-	69,73,73	1.26	6 (8%)	83,113,113	1.31	5 (6%)
39	CLA	a	802	-	59,63,73	1.35	7 (11%)	71,101,113	1.39	8 (11%)
49	KC2	B	208	-	49,53,53	1.77	10 (20%)	62,89,89	2.24	19 (30%)
39	CLA	b	812	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
49	KC2	6	317	-	49,53,53	1.76	9 (18%)	62,89,89	2.13	18 (29%)
50	A1EB1	6	304	-	48,55,58	1.32	3 (6%)	57,82,85	2.32	19 (33%)
39	CLA	J	308	-	54,58,73	1.42	6 (11%)	65,95,113	1.41	6 (9%)
39	CLA	b	829	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
39	CLA	Y	314	-	45,49,73	1.53	6 (13%)	54,84,113	1.61	6 (11%)
39	CLA	1	311	-	45,49,73	1.53	7 (15%)	54,84,113	1.47	5 (9%)
39	CLA	b	841	2	69,73,73	1.28	6 (8%)	83,113,113	1.29	6 (7%)
39	CLA	Q	317	-	50,54,73	1.48	7 (14%)	60,90,113	1.40	5 (8%)
39	CLA	b	805	-	69,73,73	1.25	7 (10%)	83,113,113	1.21	6 (7%)
48	A86	7	312	-	44,50,50	1.21	2 (4%)	51,76,76	2.29	18 (35%)
49	KC2	1	314	-	49,53,53	1.78	10 (20%)	62,89,89	2.09	16 (25%)
49	KC2	4	317	-	49,53,53	1.78	9 (18%)	62,89,89	2.12	17 (27%)
43	DD6	C	301	-	39,45,45	2.32	4 (10%)	52,67,67	2.51	14 (26%)
43	DD6	D	303	-	39,45,45	2.10	2 (5%)	52,67,67	2.77	15 (28%)
48	A86	L	302	-	44,50,50	1.13	3 (6%)	51,76,76	2.99	22 (43%)
39	CLA	C	311	-	69,73,73	1.25	6 (8%)	83,113,113	1.29	4 (4%)
46	LMG	4	326	49	46,46,55	0.96	2 (4%)	54,54,63	1.28	6 (11%)
39	CLA	3	314	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
39	CLA	8	318	-	45,49,73	1.53	6 (13%)	54,84,113	1.52	6 (11%)
39	CLA	a	835	-	69,73,73	1.26	8 (11%)	83,113,113	1.32	8 (9%)
43	DD6	3	304	-	39,45,45	2.05	3 (7%)	52,67,67	3.25	19 (36%)
39	CLA	a	801	-	69,73,73	1.27	9 (13%)	83,113,113	1.35	7 (8%)
39	CLA	9	312	35	46,50,73	1.49	8 (17%)	55,85,113	1.53	6 (10%)
39	CLA	6	318	-	45,49,73	1.52	8 (17%)	54,84,113	1.55	5 (9%)
49	KC2	L	321	-	49,53,53	1.80	11 (22%)	62,89,89	2.06	15 (24%)
50	A1EB1	O	301	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	18 (30%)
50	A1EB1	G	304	-	51,58,58	1.31	4 (7%)	60,85,85	2.04	20 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SQD	D	321	-	38,39,54	1.10	5 (13%)	47,50,65	1.70	11 (23%)
39	CLA	X	307	-	69,73,73	1.26	6 (8%)	83,113,113	1.27	6 (7%)
39	CLA	G	318	-	53,57,73	1.43	8 (15%)	62,93,113	1.36	5 (8%)
51	A1ECV	Q	319	-	54,56,56	2.60	21 (38%)	61,93,93	4.04	31 (50%)
39	CLA	i	101	-	69,73,73	1.25	7 (10%)	83,113,113	1.25	5 (6%)
39	CLA	2	308	-	50,54,73	1.48	8 (16%)	60,90,113	1.46	6 (10%)
51	A1ECV	S	318	-	54,56,56	2.67	20 (37%)	61,93,93	3.90	31 (50%)
49	KC2	3	321	-	49,53,53	1.74	9 (18%)	62,89,89	2.12	18 (29%)
50	A1EB1	D	308	-	51,58,58	1.28	3 (5%)	60,85,85	2.34	20 (33%)
48	A86	4	328	-	44,50,50	1.14	2 (4%)	51,76,76	2.28	15 (29%)
49	KC2	9	318	-	49,53,53	1.82	9 (18%)	62,89,89	2.03	14 (22%)
50	A1EB1	K	302	-	51,58,58	1.29	4 (7%)	60,85,85	2.12	21 (35%)
39	CLA	L	310	23	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
39	CLA	O	318	-	50,54,73	1.47	7 (14%)	60,90,113	1.50	7 (11%)
39	CLA	b	809	-	69,73,73	1.24	6 (8%)	83,113,113	1.28	7 (8%)
49	KC2	K	313	22	49,53,53	1.79	10 (20%)	62,89,89	2.19	18 (29%)
39	CLA	H	313	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
43	DD6	4	308	-	39,45,45	2.06	3 (7%)	52,67,67	2.04	14 (26%)
48	A86	k	206	-	44,50,50	1.18	3 (6%)	51,76,76	2.00	13 (25%)
39	CLA	X	316	-	51,55,73	1.45	8 (15%)	61,91,113	1.48	6 (9%)
39	CLA	1	319	-	55,59,73	1.41	9 (16%)	66,96,113	1.43	5 (7%)
39	CLA	8	310	-	49,53,73	1.51	6 (12%)	59,89,113	1.51	7 (11%)
48	A86	9	305	-	44,50,50	1.19	3 (6%)	51,76,76	1.91	17 (33%)
39	CLA	6	312	-	55,59,73	1.39	8 (14%)	65,95,113	1.39	5 (7%)
50	A1EB1	3	310	-	51,58,58	1.27	4 (7%)	60,85,85	2.05	17 (28%)
43	DD6	G	306	-	39,45,45	2.02	3 (7%)	52,67,67	2.07	12 (23%)
39	CLA	D	313	-	69,73,73	1.24	7 (10%)	83,113,113	1.29	8 (9%)
43	DD6	7	309	-	39,45,45	1.99	3 (7%)	52,67,67	1.87	15 (28%)
39	CLA	H	308	-	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
39	CLA	b	836	-	49,53,73	1.50	8 (16%)	59,89,113	1.51	8 (13%)
42	BCR	a	842	-	41,41,41	0.67	0	56,56,56	1.82	14 (25%)
48	A86	7	311	-	44,50,50	1.19	3 (6%)	51,76,76	2.16	16 (31%)
43	DD6	a	846	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	12 (23%)
48	A86	M	302	-	44,50,50	1.18	2 (4%)	51,76,76	2.19	17 (33%)
48	A86	W	303	-	44,50,50	1.19	2 (4%)	51,76,76	2.16	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	b	808	-	49,53,73	1.48	7 (14%)	59,89,113	1.51	6 (10%)
39	CLA	E	306	17	53,57,73	1.42	8 (15%)	62,93,113	1.43	5 (8%)
39	CLA	E	317	-	56,60,73	1.39	6 (10%)	67,97,113	1.43	6 (8%)
39	CLA	G	312	-	56,60,73	1.39	6 (10%)	67,97,113	1.47	6 (8%)
49	KC2	M	311	46	48,52,53	1.72	9 (18%)	59,87,89	2.20	17 (28%)
39	CLA	J	314	-	69,73,73	1.27	7 (10%)	83,113,113	1.22	6 (7%)
49	KC2	L	315	-	49,53,53	1.78	10 (20%)	62,89,89	2.18	15 (24%)
39	CLA	I	310	-	58,62,73	1.36	8 (13%)	69,99,113	1.39	5 (7%)
49	KC2	0	319	-	49,53,53	1.91	11 (22%)	62,89,89	2.01	15 (24%)
49	KC2	4	318	28	49,53,53	1.79	10 (20%)	62,89,89	2.14	16 (25%)
39	CLA	a	805	-	69,73,73	1.24	8 (11%)	83,113,113	1.34	9 (10%)
44	SF4	c	102	-	0,12,12	-	-	-	-	-
49	KC2	T	312	-	49,53,53	1.81	10 (20%)	62,89,89	2.19	17 (27%)
39	CLA	C	306	-	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
43	DD6	O	305	-	39,45,45	1.99	2 (5%)	52,67,67	1.62	12 (23%)
39	CLA	4	316	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	5 (6%)
39	CLA	D	315	-	69,73,73	1.25	7 (10%)	83,113,113	1.26	5 (6%)
39	CLA	F	316	-	55,59,73	1.42	8 (14%)	66,96,113	1.40	5 (7%)
39	CLA	M	310	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
39	CLA	a	827	-	69,73,73	1.28	10 (14%)	83,113,113	1.40	8 (9%)
39	CLA	b	851	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
39	CLA	W	311	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	7 (8%)
49	KC2	F	307	-	49,53,53	1.77	10 (20%)	62,89,89	2.19	18 (29%)
39	CLA	z	308	-	50,54,73	1.46	7 (14%)	60,90,113	1.42	4 (6%)
49	KC2	8	314	-	49,53,53	1.79	10 (20%)	62,89,89	2.07	15 (24%)
50	A1EB1	G	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.07	19 (31%)
50	A1EB1	9	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.05	19 (31%)
50	A1EB1	Q	323	-	51,58,58	1.24	3 (5%)	60,85,85	2.08	15 (25%)
39	CLA	6	311	-	43,48,73	1.56	7 (16%)	51,83,113	1.53	7 (13%)
46	LMG	D	322	-	37,37,55	0.91	0	45,45,63	1.21	5 (11%)
39	CLA	a	804	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
39	CLA	F	321	-	69,73,73	1.26	7 (10%)	83,113,113	1.33	8 (9%)
49	KC2	6	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	19 (30%)
39	CLA	E	310	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
39	CLA	7	318	28	50,54,73	1.44	8 (16%)	60,90,113	1.38	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	BCR	k	204	-	41,41,41	0.71	0	56,56,56	1.90	15 (26%)
39	CLA	K	307	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	4 (4%)
48	A86	z	303	-	44,50,50	1.14	2 (4%)	51,76,76	1.90	11 (21%)
39	CLA	3	316	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	6 (9%)
48	A86	0	308	51	44,50,50	1.27	3 (6%)	51,76,76	2.18	19 (37%)
39	CLA	R	307	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
39	CLA	b	842	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	5 (6%)
39	CLA	4	312	-	69,73,73	1.26	8 (11%)	83,113,113	1.37	10 (12%)
51	A1ECV	W	317	-	54,56,56	2.61	19 (35%)	61,93,93	3.90	29 (47%)
48	A86	8	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.04	15 (29%)
49	KC2	X	306	27	49,53,53	1.85	10 (20%)	62,89,89	2.05	15 (24%)
39	CLA	9	308	-	59,63,73	1.34	8 (13%)	71,101,113	1.51	11 (15%)
39	CLA	x	311	-	49,53,73	1.49	6 (12%)	59,89,113	1.46	4 (6%)
39	CLA	l	204	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	8 (9%)
48	A86	X	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.10	18 (35%)
49	KC2	P	313	24	49,53,53	1.82	11 (22%)	62,89,89	2.21	19 (30%)
48	A86	4	309	-	44,50,50	1.21	3 (6%)	51,76,76	2.13	17 (33%)
39	CLA	8	312	-	49,53,73	1.49	7 (14%)	59,89,113	1.49	4 (6%)
51	A1ECV	7	323	-	54,56,56	2.62	20 (37%)	61,93,93	4.02	29 (47%)
39	CLA	W	313	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
39	CLA	a	834	-	55,59,73	1.40	8 (14%)	66,96,113	1.45	8 (12%)
49	KC2	S	317	-	49,53,53	1.75	10 (20%)	62,89,89	2.17	17 (27%)
39	CLA	a	806	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	6 (7%)
49	KC2	M	307	-	49,53,53	1.76	10 (20%)	62,89,89	2.21	19 (30%)
49	KC2	5	313	46	48,52,53	1.74	9 (18%)	59,87,89	2.19	16 (27%)
49	KC2	Z	310	-	49,53,53	1.76	10 (20%)	62,89,89	2.15	18 (29%)
43	DD6	H	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	10 (19%)
51	A1ECV	9	317	-	54,56,56	2.57	20 (37%)	61,93,93	3.89	30 (49%)
39	CLA	a	812	-	49,53,73	1.49	8 (16%)	59,89,113	1.47	8 (13%)
39	CLA	W	309	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	5 (6%)
49	KC2	G	315	-	49,53,53	1.81	10 (20%)	62,89,89	2.19	19 (30%)
39	CLA	A	308	-	55,59,73	1.42	8 (14%)	66,96,113	1.33	5 (7%)
39	CLA	Z	305	-	45,49,73	1.54	7 (15%)	54,84,113	1.53	6 (11%)
39	CLA	U	210	-	64,68,73	1.32	9 (14%)	77,107,113	1.31	7 (9%)
39	CLA	I	309	-	69,73,73	1.27	7 (10%)	83,113,113	1.29	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	Q	309	-	65,69,73	1.29	8 (12%)	78,108,113	1.32	4 (5%)
50	A1EB1	6	306	-	44,50,58	1.15	2 (4%)	51,76,85	1.86	11 (21%)
41	LHG	a	840	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	7 (13%)
39	CLA	X	311	27	54,58,73	1.41	6 (11%)	65,95,113	1.42	7 (10%)
39	CLA	D	317	-	69,73,73	1.25	8 (11%)	83,113,113	1.34	8 (9%)
39	CLA	S	311	-	69,73,73	1.26	8 (11%)	83,113,113	1.26	5 (6%)
49	KC2	X	318	-	49,53,53	1.77	9 (18%)	62,89,89	2.15	16 (25%)
48	A86	U	206	-	44,50,50	1.20	3 (6%)	51,76,76	2.39	19 (37%)
51	A1ECV	V	317	-	54,56,56	2.61	19 (35%)	61,93,93	3.85	30 (49%)
43	DD6	I	307	-	39,45,45	2.01	3 (7%)	52,67,67	1.90	10 (19%)
39	CLA	4	313	-	50,54,73	1.45	7 (14%)	60,90,113	1.41	4 (6%)
39	CLA	U	213	-	45,49,73	1.52	7 (15%)	54,84,113	1.56	5 (9%)
39	CLA	z	318	-	45,49,73	1.52	7 (15%)	54,84,113	1.58	7 (12%)
39	CLA	K	312	-	69,73,73	1.24	8 (11%)	83,113,113	1.34	6 (7%)
46	LMG	F	320	49	34,34,55	1.14	2 (5%)	42,42,63	1.20	6 (14%)
47	SQD	F	319	-	36,37,54	1.14	5 (13%)	45,48,65	1.72	10 (22%)
48	A86	Q	305	-	44,50,50	1.14	3 (6%)	51,76,76	2.03	14 (27%)
39	CLA	3	320	-	49,53,73	1.49	6 (12%)	59,89,113	1.53	6 (10%)
47	SQD	T	321	-	35,36,54	1.15	5 (14%)	44,47,65	1.80	10 (22%)
39	CLA	B	209	-	60,64,73	1.36	8 (13%)	72,102,113	1.29	6 (8%)
39	CLA	a	813	1	54,58,73	1.42	7 (12%)	65,95,113	1.50	6 (9%)
39	CLA	7	313	-	65,69,73	1.31	8 (12%)	78,108,113	1.33	7 (8%)
39	CLA	9	320	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	8 (14%)
39	CLA	1	313	32	45,49,73	1.51	8 (17%)	54,84,113	1.51	5 (9%)
49	KC2	0	317	31	49,53,53	1.79	10 (20%)	62,89,89	2.15	18 (29%)
39	CLA	W	316	24	45,49,73	1.51	8 (17%)	54,84,113	1.57	9 (16%)
49	KC2	M	313	-	49,53,53	1.79	9 (18%)	62,89,89	2.17	17 (27%)
42	BCR	b	850	-	41,41,41	0.68	0	56,56,56	1.86	12 (21%)
39	CLA	E	308	-	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
49	KC2	2	317	-	49,53,53	1.78	11 (22%)	62,89,89	2.24	19 (30%)
39	CLA	U	209	-	56,60,73	1.39	8 (14%)	67,97,113	1.43	7 (10%)
39	CLA	Y	310	-	45,49,73	1.54	6 (13%)	54,84,113	1.55	5 (9%)
39	CLA	S	308	-	65,69,73	1.30	7 (10%)	78,108,113	1.32	6 (7%)
49	KC2	y	313	-	49,53,53	1.76	10 (20%)	62,89,89	2.13	17 (27%)
39	CLA	6	315	-	45,49,73	1.52	8 (17%)	54,84,113	1.57	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	A1EB1	8	306	-	51,58,58	1.28	3 (5%)	60,85,85	2.08	19 (31%)
39	CLA	y	312	-	46,50,73	1.52	7 (15%)	55,85,113	1.46	4 (7%)
39	CLA	F	312	-	69,73,73	1.26	7 (10%)	83,113,113	1.29	5 (6%)
39	CLA	8	311	-	59,63,73	1.35	7 (11%)	71,101,113	1.40	6 (8%)
39	CLA	W	319	-	50,54,73	1.47	6 (12%)	60,90,113	1.44	4 (6%)
41	LHG	X	301	-	40,40,48	0.67	1 (2%)	43,46,54	1.30	6 (13%)
43	DD6	7	310	-	39,45,45	2.06	3 (7%)	52,67,67	2.49	14 (26%)
39	CLA	b	817	-	63,67,73	1.31	6 (9%)	75,105,113	1.36	7 (9%)
39	CLA	0	318	-	45,49,73	1.54	6 (13%)	54,84,113	1.50	5 (9%)
39	CLA	a	822	-	69,73,73	1.25	7 (10%)	83,113,113	1.34	7 (8%)
48	A86	5	301	-	44,50,50	1.21	2 (4%)	51,76,76	2.19	16 (31%)
50	A1EB1	2	306	-	51,58,58	1.24	3 (5%)	60,85,85	2.09	20 (33%)
46	LMG	0	324	49	27,27,55	1.31	2 (7%)	35,35,63	1.47	4 (11%)
42	BCR	a	843	-	41,41,41	0.73	0	56,56,56	1.94	17 (30%)
39	CLA	Z	307	-	45,49,73	1.52	8 (17%)	54,84,113	1.54	6 (11%)
39	CLA	R	308	-	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
49	KC2	T	315	29	49,53,53	1.76	10 (20%)	62,89,89	2.10	19 (30%)
39	CLA	b	801	-	69,73,73	1.23	10 (14%)	83,113,113	1.33	8 (9%)
43	DD6	D	307	-	39,45,45	1.97	3 (7%)	52,67,67	1.79	10 (19%)
39	CLA	I	301	41	56,60,73	1.40	7 (12%)	67,97,113	1.38	7 (10%)
50	A1EB1	S	302	-	51,58,58	1.30	3 (5%)	60,85,85	1.97	17 (28%)
43	DD6	F	303	-	39,45,45	1.93	2 (5%)	52,67,67	1.79	10 (19%)
49	KC2	H	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.13	18 (29%)
49	KC2	P	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.17	19 (30%)
51	A1ECV	L	318	-	54,56,56	2.62	19 (35%)	61,93,93	3.96	30 (49%)
39	CLA	1	316	-	45,49,73	1.53	6 (13%)	54,84,113	1.54	5 (9%)
39	CLA	3	312	-	69,73,73	1.27	7 (10%)	83,113,113	1.36	8 (9%)
47	SQD	P	301	-	37,38,54	1.11	5 (13%)	46,49,65	1.73	12 (26%)
48	A86	S	307	-	44,50,50	1.19	2 (4%)	51,76,76	2.32	18 (35%)
42	BCR	a	845	-	41,41,41	0.75	0	56,56,56	2.14	15 (26%)
39	CLA	B	204	-	50,54,73	1.47	8 (16%)	60,90,113	1.45	6 (10%)
49	KC2	3	318	-	49,53,53	1.80	10 (20%)	62,89,89	2.13	18 (29%)
39	CLA	y	310	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	5 (9%)
42	BCR	b	847	-	41,41,41	0.71	0	56,56,56	2.01	16 (28%)
39	CLA	8	322	-	45,49,73	1.54	7 (15%)	54,84,113	1.63	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	F	308	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
50	A1EB1	R	303	-	51,58,58	1.31	5 (9%)	60,85,85	2.18	19 (31%)
39	CLA	4	323	-	69,73,73	1.29	9 (13%)	83,113,113	1.27	4 (4%)
39	CLA	5	306	-	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
39	CLA	T	313	-	55,59,73	1.44	7 (12%)	66,96,113	1.27	7 (10%)
51	A1ECV	M	316	-	54,56,56	2.61	19 (35%)	61,93,93	3.89	31 (50%)
39	CLA	b	827	-	69,73,73	1.26	7 (10%)	83,113,113	1.31	4 (4%)
51	A1ECV	x	316	-	54,56,56	2.66	19 (35%)	61,93,93	4.13	30 (49%)
39	CLA	b	837	-	64,68,73	1.31	9 (14%)	77,107,113	1.39	8 (10%)
39	CLA	b	825	-	69,73,73	1.27	9 (13%)	83,113,113	1.34	8 (9%)
50	A1EB1	2	304	-	51,58,58	1.26	4 (7%)	60,85,85	2.16	20 (33%)
39	CLA	a	828	1	54,58,73	1.42	9 (16%)	65,95,113	1.40	5 (7%)
39	CLA	a	832	-	54,58,73	1.42	7 (12%)	65,95,113	1.45	6 (9%)
39	CLA	I	311	-	69,73,73	1.24	7 (10%)	83,113,113	1.35	5 (6%)
51	A1ECV	0	321	48	54,56,56	2.59	19 (35%)	61,93,93	3.71	32 (52%)
50	A1EB1	T	307	-	51,58,58	1.24	4 (7%)	60,85,85	1.95	19 (31%)
50	A1EB1	4	302	-	51,58,58	1.24	4 (7%)	60,85,85	2.12	20 (33%)
39	CLA	k	203	-	59,63,73	1.36	7 (11%)	71,101,113	1.37	5 (7%)
49	KC2	O	317	46	48,52,53	1.80	10 (20%)	59,87,89	2.06	13 (22%)
40	PQN	a	839	-	34,34,34	1.60	2 (5%)	42,45,45	1.10	2 (4%)
39	CLA	Z	315	-	45,49,73	1.53	7 (15%)	54,84,113	1.53	5 (9%)
48	A86	0	301	-	44,50,50	1.26	3 (6%)	51,76,76	2.19	19 (37%)
39	CLA	R	311	27	54,58,73	1.40	8 (14%)	65,95,113	1.41	5 (7%)
39	CLA	F	310	-	58,62,73	1.37	6 (10%)	69,99,113	1.39	6 (8%)
49	KC2	x	313	-	49,53,53	1.77	9 (18%)	62,89,89	2.13	17 (27%)
39	CLA	M	317	-	55,59,73	1.40	9 (16%)	66,96,113	1.41	4 (6%)
39	CLA	S	319	-	56,60,73	1.39	9 (16%)	67,97,113	1.53	9 (13%)
39	CLA	f	803	-	59,63,73	1.37	7 (11%)	71,101,113	1.33	6 (8%)
48	A86	C	303	-	44,50,50	1.21	2 (4%)	51,76,76	1.92	14 (27%)
39	CLA	x	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.48	8 (14%)
51	A1ECV	z	310	-	54,56,56	2.65	20 (37%)	61,93,93	4.17	28 (45%)
39	CLA	a	830	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	4 (4%)
48	A86	T	306	-	44,50,50	1.19	2 (4%)	51,76,76	2.35	15 (29%)
39	CLA	A	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
42	BCR	b	845	-	41,41,41	0.72	0	56,56,56	1.96	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	KC2	W	308	-	49,53,53	1.77	10 (20%)	62,89,89	2.21	17 (27%)
42	BCR	h	202	-	41,41,41	0.74	0	56,56,56	1.87	17 (30%)
50	A1EB1	6	301	-	51,58,58	1.28	3 (5%)	60,85,85	2.00	16 (26%)
52	A1EB4	M	322	-	52,59,63	2.81	6 (11%)	61,85,89	2.80	22 (36%)
39	CLA	V	319	-	56,60,73	1.40	8 (14%)	67,97,113	1.36	5 (7%)
39	CLA	P	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
39	CLA	b	835	-	69,73,73	1.26	7 (10%)	83,113,113	1.24	5 (6%)
39	CLA	7	315	-	54,58,73	1.42	8 (14%)	65,95,113	1.43	7 (10%)
50	A1EB1	4	301	-	51,58,58	1.25	3 (5%)	60,85,85	1.93	18 (30%)
43	DD6	X	304	-	39,45,45	1.92	3 (7%)	52,67,67	1.87	16 (30%)
39	CLA	J	318	-	50,54,73	1.45	8 (16%)	60,90,113	1.48	7 (11%)
39	CLA	0	311	-	59,63,73	1.38	9 (15%)	71,101,113	1.39	10 (14%)
50	A1EB1	4	304	-	51,58,58	1.28	3 (5%)	60,85,85	2.17	21 (35%)
39	CLA	L	316	-	45,49,73	1.51	7 (15%)	54,84,113	1.60	6 (11%)
39	CLA	7	316	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
39	CLA	H	315	-	45,49,73	1.51	8 (17%)	54,84,113	1.50	6 (11%)
48	A86	8	305	-	44,50,50	1.20	3 (6%)	51,76,76	2.63	22 (43%)
48	A86	D	305	-	44,50,50	1.21	3 (6%)	51,76,76	2.71	21 (41%)
39	CLA	I	314	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
48	A86	6	307	-	44,50,50	1.15	3 (6%)	51,76,76	2.11	17 (33%)
43	DD6	J	306	-	39,45,45	1.99	3 (7%)	52,67,67	2.16	12 (23%)
39	CLA	J	307	21	53,57,73	1.43	7 (13%)	62,93,113	1.45	5 (8%)
39	CLA	Q	310	-	69,73,73	1.27	8 (11%)	83,113,113	1.27	10 (12%)
48	A86	U	202	-	44,50,50	1.17	3 (6%)	51,76,76	2.30	20 (39%)
49	KC2	T	316	-	49,53,53	1.76	9 (18%)	62,89,89	2.13	16 (25%)
49	KC2	y	316	-	49,53,53	1.75	10 (20%)	62,89,89	2.15	18 (29%)
39	CLA	1	308	-	45,49,73	1.54	7 (15%)	54,84,113	1.57	5 (9%)
39	CLA	b	838	-	69,73,73	1.25	6 (8%)	83,113,113	1.33	8 (9%)
43	DD6	R	304	-	39,45,45	1.95	4 (10%)	52,67,67	1.84	15 (28%)
49	KC2	5	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.16	18 (29%)
49	KC2	Z	311	-	49,53,53	1.75	9 (18%)	62,89,89	2.16	17 (27%)
39	CLA	P	314	-	45,49,73	1.53	8 (17%)	54,84,113	1.56	6 (11%)
47	SQD	S	301	-	38,39,54	1.14	5 (13%)	47,50,65	1.67	10 (21%)
45	DGD	C	314	-	41,41,67	1.10	2 (4%)	55,55,81	1.38	6 (10%)
51	A1ECV	2	311	-	54,56,56	2.67	20 (37%)	61,93,93	4.19	29 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	DD6	x	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.89	16 (30%)
39	CLA	I	316	36	45,49,73	1.51	6 (13%)	54,84,113	1.50	6 (11%)
49	KC2	S	314	-	49,53,53	1.78	9 (18%)	62,89,89	2.11	17 (27%)
48	A86	y	305	-	44,50,50	1.17	3 (6%)	51,76,76	2.00	16 (31%)
39	CLA	a	825	-	66,70,73	1.27	7 (10%)	79,109,113	1.34	8 (10%)
47	SQD	D	320	39	36,37,54	1.16	5 (13%)	45,48,65	1.86	10 (22%)
39	CLA	E	309	-	57,61,73	1.38	8 (14%)	68,98,113	1.37	6 (8%)
39	CLA	a	836	-	69,73,73	1.24	7 (10%)	83,113,113	1.32	4 (4%)
39	CLA	b	826	-	69,73,73	1.28	10 (14%)	83,113,113	1.26	7 (8%)
39	CLA	V	313	27	69,73,73	1.23	9 (13%)	83,113,113	1.27	4 (4%)
46	LMG	l	208	49	39,39,55	1.06	2 (5%)	47,47,63	1.23	5 (10%)
49	KC2	C	313	-	49,53,53	1.75	9 (18%)	62,89,89	2.16	18 (29%)
39	CLA	z	317	-	46,50,73	1.52	6 (13%)	55,85,113	1.48	4 (7%)
39	CLA	a	807	1	69,73,73	1.27	9 (13%)	83,113,113	1.29	5 (6%)
43	DD6	2	303	-	39,45,45	2.09	4 (10%)	52,67,67	3.79	20 (38%)
50	A1EB1	Q	307	-	51,58,58	1.31	5 (9%)	60,85,85	2.01	15 (25%)
51	A1ECV	y	311	-	54,56,56	2.66	20 (37%)	61,93,93	4.16	31 (50%)
39	CLA	Z	306	-	50,54,73	1.46	7 (14%)	60,90,113	1.46	5 (8%)
52	A1EB4	P	318	-	49,56,63	2.77	5 (10%)	58,82,89	2.27	18 (31%)
39	CLA	E	307	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	8 (9%)
52	A1EB4	X	305	-	52,59,63	2.59	4 (7%)	61,85,89	1.90	19 (31%)
39	CLA	0	315	31	54,58,73	1.39	7 (12%)	65,95,113	1.42	9 (13%)
39	CLA	W	318	-	55,59,73	1.41	8 (14%)	66,96,113	1.42	4 (6%)
43	DD6	I	305	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	13 (25%)
39	CLA	D	314	-	69,73,73	1.27	8 (11%)	83,113,113	1.23	7 (8%)
50	A1EB1	3	302	-	51,58,58	1.30	4 (7%)	60,85,85	2.09	18 (30%)
43	DD6	F	305	-	39,45,45	2.14	3 (7%)	52,67,67	2.66	17 (32%)
43	DD6	Q	306	-	39,45,45	2.01	3 (7%)	52,67,67	1.83	14 (26%)
39	CLA	C	304	-	47,51,73	1.50	8 (17%)	56,86,113	1.44	5 (8%)
48	A86	3	306	-	44,50,50	1.14	3 (6%)	51,76,76	2.24	13 (25%)
49	KC2	9	313	-	49,53,53	1.78	12 (24%)	62,89,89	2.11	15 (24%)
48	A86	6	303	-	44,50,50	1.15	3 (6%)	51,76,76	2.21	15 (29%)
39	CLA	b	803	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
50	A1EB1	J	302	-	51,58,58	1.26	4 (7%)	60,85,85	2.25	23 (38%)
49	KC2	0	314	46,31	48,52,53	1.72	9 (18%)	59,87,89	2.23	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	DD6	D	306	-	39,45,45	2.66	4 (10%)	52,67,67	2.39	12 (23%)
39	CLA	T	319	29	50,54,73	1.47	7 (14%)	60,90,113	1.48	5 (8%)
46	LMG	P	317	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
39	CLA	a	847	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	5 (6%)
48	A86	6	302	-	44,50,50	1.16	3 (6%)	51,76,76	2.16	15 (29%)
48	A86	R	317	-	44,50,50	1.17	2 (4%)	51,76,76	2.06	12 (23%)
49	KC2	W	314	-	49,53,53	1.76	9 (18%)	62,89,89	2.14	17 (27%)
39	CLA	o	202	-	46,50,73	1.51	7 (15%)	55,85,113	1.52	6 (10%)
47	SQD	4	327	-	38,39,54	1.14	5 (13%)	47,50,65	1.69	11 (23%)
43	DD6	T	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.87	13 (25%)
51	A1ECV	5	312	27	54,56,56	2.65	20 (37%)	61,93,93	3.93	31 (50%)
49	KC2	1	315	-	49,53,53	1.80	10 (20%)	62,89,89	2.09	15 (24%)
39	CLA	j	101	-	69,73,73	1.24	7 (10%)	83,113,113	1.33	8 (9%)
43	DD6	K	303	-	39,45,45	1.95	3 (7%)	52,67,67	1.73	11 (21%)
50	A1EB1	H	301	-	51,58,58	1.27	3 (5%)	60,85,85	2.10	17 (28%)
39	CLA	b	815	-	69,73,73	1.27	8 (11%)	83,113,113	1.28	7 (8%)
39	CLA	z	306	-	45,49,73	1.54	7 (15%)	54,84,113	1.52	5 (9%)
47	SQD	H	318	-	37,38,54	1.13	5 (13%)	46,49,65	1.64	8 (17%)
42	BCR	b	844	-	41,41,41	0.71	0	56,56,56	1.84	13 (23%)
52	A1EB4	W	321	-	52,59,63	2.65	5 (9%)	61,85,89	2.25	20 (32%)
39	CLA	a	838	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	5 (6%)
43	DD6	B	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.99	12 (23%)
47	SQD	F	318	-	41,42,54	1.07	5 (12%)	50,53,65	1.70	10 (20%)
39	CLA	l	201	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	6 (7%)
50	A1EB1	U	203	-	51,58,58	1.25	3 (5%)	60,85,85	2.17	19 (31%)
39	CLA	A	315	-	54,58,73	1.41	6 (11%)	65,95,113	1.42	6 (9%)
39	CLA	E	312	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	6 (7%)
42	BCR	a	844	-	41,41,41	0.72	0	56,56,56	1.91	17 (30%)
39	CLA	Z	304	-	45,49,73	1.53	8 (17%)	54,84,113	1.56	5 (9%)
39	CLA	Z	312	-	45,49,73	1.52	6 (13%)	54,84,113	1.51	5 (9%)
39	CLA	a	819	-	53,57,73	1.41	7 (13%)	62,93,113	1.44	7 (11%)
39	CLA	4	311	-	65,69,73	1.32	9 (13%)	78,108,113	1.37	8 (10%)
39	CLA	6	310	-	46,50,73	1.53	7 (15%)	55,85,113	1.44	5 (9%)
39	CLA	M	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	4 (4%)
51	A1ECV	Z	308	-	54,56,56	2.68	20 (37%)	61,93,93	4.21	30 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	z	311	-	45,49,73	1.53	7 (15%)	54,84,113	1.49	5 (9%)
49	KC2	7	319	-	49,53,53	1.76	10 (20%)	62,89,89	2.18	17 (27%)
39	CLA	L	311	23	56,60,73	1.39	8 (14%)	67,97,113	1.38	7 (10%)
39	CLA	b	818	-	59,63,73	1.35	7 (11%)	71,101,113	1.39	8 (11%)
49	KC2	x	312	-	49,53,53	1.76	10 (20%)	62,89,89	2.11	17 (27%)
39	CLA	F	309	-	56,60,73	1.39	7 (12%)	67,97,113	1.40	4 (5%)
51	A1ECV	6	320	-	54,56,56	2.65	19 (35%)	61,93,93	4.01	30 (49%)
48	A86	L	306	-	44,50,50	1.16	3 (6%)	51,76,76	2.15	15 (29%)
49	KC2	G	311	19	49,53,53	1.78	10 (20%)	62,89,89	2.17	16 (25%)
48	A86	Y	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	15 (29%)
39	CLA	T	311	-	60,64,73	1.35	7 (11%)	72,102,113	1.35	5 (6%)
39	CLA	2	312	-	45,49,73	1.51	9 (20%)	54,84,113	1.56	6 (11%)
43	DD6	J	304	-	39,45,45	2.23	5 (12%)	52,67,67	2.35	14 (26%)
39	CLA	D	309	16	53,57,73	1.43	8 (15%)	62,93,113	1.53	7 (11%)
39	CLA	H	306	-	52,56,73	1.44	8 (15%)	62,92,113	1.44	5 (8%)
39	CLA	2	315	-	45,49,73	1.53	8 (17%)	54,84,113	1.50	5 (9%)
42	BCR	f	801	-	41,41,41	0.68	0	56,56,56	1.92	14 (25%)
41	LHG	H	317	-	34,34,48	0.71	0	37,40,54	1.19	3 (8%)
39	CLA	Z	316	-	45,49,73	1.52	6 (13%)	54,84,113	1.61	6 (11%)
48	A86	9	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.38	15 (29%)
46	LMG	A	316	-	29,29,55	1.00	0	37,37,63	1.23	4 (10%)
39	CLA	S	320	-	69,73,73	1.28	9 (13%)	83,113,113	1.29	6 (7%)
50	A1EB1	y	301	-	51,58,58	1.23	4 (7%)	60,85,85	2.16	23 (38%)
39	CLA	2	309	-	50,54,73	1.47	9 (18%)	60,90,113	1.42	6 (10%)
51	A1ECV	Z	314	-	54,56,56	2.64	19 (35%)	61,93,93	4.06	29 (47%)
48	A86	M	303	-	44,50,50	1.22	3 (6%)	51,76,76	2.16	19 (37%)
49	KC2	2	314	-	49,53,53	1.77	10 (20%)	62,89,89	2.16	18 (29%)
39	CLA	V	309	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
39	CLA	T	310	29	56,60,73	1.39	9 (16%)	67,97,113	1.39	5 (7%)
39	CLA	T	308	-	50,54,73	1.45	9 (18%)	60,90,113	1.45	6 (10%)
52	A1EB4	R	305	-	52,59,63	2.56	4 (7%)	61,85,89	1.92	21 (34%)
52	A1EB4	5	304	-	52,59,63	2.56	4 (7%)	61,85,89	1.93	19 (31%)
39	CLA	2	319	-	50,54,73	1.46	7 (14%)	60,90,113	1.67	9 (15%)
41	LHG	a	841	39	26,26,48	0.85	1 (3%)	29,32,54	1.33	3 (10%)
43	DD6	1	304	-	39,45,45	2.22	3 (7%)	52,67,67	3.19	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	A1EB1	H	304	-	51,58,58	1.22	3 (5%)	60,85,85	1.63	11 (18%)
50	A1EB1	F	304	-	51,58,58	1.30	4 (7%)	60,85,85	2.12	18 (30%)
39	CLA	h	201	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	6 (8%)
39	CLA	J	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
50	A1EB1	y	302	-	51,58,58	1.25	3 (5%)	60,85,85	2.21	20 (33%)
39	CLA	4	314	-	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
49	KC2	P	310	46	48,52,53	1.72	9 (18%)	59,87,89	2.21	18 (30%)
48	A86	y	306	-	44,50,50	1.16	2 (4%)	51,76,76	2.50	18 (35%)
39	CLA	z	314	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	5 (9%)
43	DD6	E	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.84	11 (21%)
39	CLA	K	311	-	69,73,73	1.24	6 (8%)	83,113,113	1.27	5 (6%)
47	SQD	k	205	-	37,38,54	1.13	5 (13%)	46,49,65	1.66	9 (19%)
39	CLA	y	307	-	45,49,73	1.53	8 (17%)	54,84,113	1.54	5 (9%)
52	A1EB4	P	319	-	52,59,63	2.81	6 (11%)	61,85,89	2.79	21 (34%)
39	CLA	3	323	-	50,54,73	1.46	8 (16%)	60,90,113	1.50	4 (6%)
39	CLA	B	205	-	46,50,73	1.52	6 (13%)	55,85,113	1.51	6 (10%)
39	CLA	T	318	-	51,55,73	1.44	7 (13%)	61,91,113	1.47	5 (8%)
39	CLA	I	315	-	56,60,73	1.39	6 (10%)	67,97,113	1.45	8 (11%)
39	CLA	B	207	-	59,63,73	1.39	8 (13%)	71,101,113	1.42	7 (9%)
49	KC2	5	305	27	49,53,53	1.73	9 (18%)	62,89,89	2.17	16 (25%)
48	A86	M	306	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	17 (33%)
51	A1ECV	Q	316	26	54,56,56	2.66	21 (38%)	61,93,93	4.02	30 (49%)
39	CLA	b	828	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
39	CLA	Y	307	-	45,49,73	1.53	7 (15%)	54,84,113	1.40	5 (9%)
51	A1ECV	R	310	-	54,56,56	2.60	20 (37%)	61,93,93	4.11	31 (50%)
39	CLA	b	819	-	63,67,73	1.32	8 (12%)	75,105,113	1.36	5 (6%)
39	CLA	W	310	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
48	A86	9	301	-	44,50,50	1.20	3 (6%)	51,76,76	2.14	15 (29%)
51	A1ECV	P	315	-	54,56,56	2.62	19 (35%)	61,93,93	4.01	29 (47%)
45	DGD	b	849	-	61,61,67	0.93	2 (3%)	75,75,81	1.37	8 (10%)
39	CLA	C	309	-	50,54,73	1.47	6 (12%)	60,90,113	1.40	4 (6%)
39	CLA	1	317	-	45,49,73	1.53	6 (13%)	54,84,113	1.53	5 (9%)
39	CLA	X	308	-	64,68,73	1.31	8 (12%)	77,107,113	1.36	8 (10%)
50	A1EB1	K	304	-	51,58,58	1.26	4 (7%)	60,85,85	1.95	18 (30%)
39	CLA	x	308	-	45,49,73	1.51	7 (15%)	54,84,113	1.61	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	Q	320	-	51,55,73	1.44	7 (13%)	61,91,113	1.41	4 (6%)
39	CLA	o	201	-	55,59,73	1.40	8 (14%)	66,96,113	1.40	5 (7%)
48	A86	Z	303	-	44,50,50	1.16	3 (6%)	51,76,76	2.27	18 (35%)
39	CLA	o	205	-	56,60,73	1.40	7 (12%)	67,97,113	1.39	5 (7%)
51	A1ECV	4	321	-	54,56,56	2.64	19 (35%)	61,93,93	3.92	31 (50%)
49	KC2	8	320	-	49,53,53	1.77	9 (18%)	62,89,89	2.14	16 (25%)
50	A1EB1	U	205	-	51,58,58	1.23	4 (7%)	60,85,85	1.99	19 (31%)
44	SF4	b	804	-	0,12,12	-	-	-		
39	CLA	K	314	-	45,49,73	1.52	7 (15%)	54,84,113	1.52	7 (12%)
39	CLA	H	310	-	61,65,73	1.32	8 (13%)	73,103,113	1.36	4 (5%)
39	CLA	9	309	-	45,49,73	1.51	8 (17%)	54,84,113	1.58	5 (9%)
51	A1ECV	y	317	-	54,56,56	2.67	19 (35%)	61,93,93	4.13	30 (49%)
49	KC2	H	311	-	49,53,53	1.78	10 (20%)	62,89,89	2.12	15 (24%)
39	CLA	b	832	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
39	CLA	a	815	-	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
43	DD6	W	305	-	39,45,45	1.91	3 (7%)	52,67,67	1.78	12 (23%)
51	A1ECV	X	313	-	54,56,56	2.64	21 (38%)	61,93,93	3.93	31 (50%)
51	A1ECV	Y	312	-	54,56,56	2.62	19 (35%)	61,93,93	4.04	29 (47%)
49	KC2	X	314	46	48,52,53	1.75	9 (18%)	59,87,89	2.20	17 (28%)
48	A86	S	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.02	14 (27%)
50	A1EB1	0	303	-	51,58,58	1.26	3 (5%)	60,85,85	2.23	17 (28%)
52	A1EB4	W	306	-	51,58,63	2.60	4 (7%)	60,84,89	2.09	19 (31%)
39	CLA	O	309	-	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)
43	DD6	o	204	-	39,45,45	1.99	2 (5%)	52,67,67	1.88	12 (23%)
39	CLA	D	310	47	65,69,73	1.31	8 (12%)	78,108,113	1.33	7 (8%)
49	KC2	I	303	-	49,53,53	1.77	10 (20%)	62,89,89	2.33	21 (33%)
39	CLA	S	313	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
39	CLA	9	319	-	49,53,73	1.50	6 (12%)	59,89,113	1.47	5 (8%)
47	SQD	W	301	-	27,28,54	1.22	4 (14%)	36,39,65	1.79	9 (25%)
51	A1ECV	9	314	-	54,56,56	2.65	20 (37%)	61,93,93	4.01	29 (47%)
48	A86	F	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.23	15 (29%)
42	BCR	l	202	-	41,41,41	0.76	0	56,56,56	1.93	13 (23%)
48	A86	4	306	-	44,50,50	1.18	2 (4%)	51,76,76	1.99	15 (29%)
46	LMG	M	319	49	39,39,55	1.08	2 (5%)	47,47,63	1.56	8 (17%)
48	A86	Q	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.35	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A86	6	305	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	16 (31%)
50	A1EB1	S	303	-	51,58,58	1.25	3 (5%)	60,85,85	2.14	21 (35%)
39	CLA	a	831	-	69,73,73	1.25	7 (10%)	83,113,113	1.32	5 (6%)
39	CLA	P	311	-	69,73,73	1.26	6 (8%)	83,113,113	1.28	5 (6%)
39	CLA	A	306	-	65,69,73	1.30	9 (13%)	78,108,113	1.35	6 (7%)
48	A86	Q	304	-	44,50,50	1.19	3 (6%)	51,76,76	2.14	17 (33%)
43	DD6	A	302	-	39,45,45	1.97	3 (7%)	52,67,67	1.84	11 (21%)
41	LHG	D	302	-	34,34,48	0.70	0	37,40,54	1.27	3 (8%)
39	CLA	M	315	-	45,49,73	1.51	7 (15%)	54,84,113	1.55	9 (16%)
43	DD6	4	307	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	15 (28%)
39	CLA	f	802	-	69,73,73	1.27	7 (10%)	83,113,113	1.26	7 (8%)
39	CLA	5	310	27	54,58,73	1.40	6 (11%)	65,95,113	1.46	6 (9%)
48	A86	1	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.20	18 (35%)
50	A1EB1	C	302	-	51,58,58	1.24	3 (5%)	60,85,85	1.81	16 (26%)
49	KC2	G	317	-	49,53,53	1.77	10 (20%)	62,89,89	2.25	19 (30%)
49	KC2	Y	308	-	49,53,53	1.83	9 (18%)	62,89,89	2.02	14 (22%)
39	CLA	H	309	20	56,60,73	1.40	8 (14%)	67,97,113	1.40	6 (8%)
43	DD6	E	305	-	39,45,45	1.99	3 (7%)	52,67,67	1.92	14 (26%)
48	A86	V	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.45	17 (33%)
39	CLA	E	316	-	56,60,73	1.39	9 (16%)	67,97,113	1.43	6 (8%)
39	CLA	F	306	-	50,54,73	1.46	7 (14%)	60,90,113	1.43	5 (8%)
39	CLA	Q	321	-	57,61,73	1.42	7 (12%)	68,98,113	1.33	8 (11%)
43	DD6	V	303	-	39,45,45	1.97	3 (7%)	52,67,67	1.75	10 (19%)
51	A1ECV	O	315	-	54,56,56	2.63	20 (37%)	61,93,93	3.90	30 (49%)
43	DD6	E	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.77	8 (15%)
39	CLA	S	309	-	69,73,73	1.29	9 (13%)	83,113,113	1.36	10 (12%)
42	BCR	b	848	-	41,41,41	0.75	0	56,56,56	1.78	14 (25%)
48	A86	6	309	-	44,50,50	1.18	2 (4%)	51,76,76	2.22	17 (33%)
39	CLA	7	325	-	54,58,73	1.43	7 (12%)	65,95,113	1.44	7 (10%)
49	KC2	Q	318	26	49,53,53	1.75	10 (20%)	62,89,89	2.19	17 (27%)
51	A1ECV	G	316	-	54,56,56	2.62	19 (35%)	61,93,93	4.03	32 (52%)
51	A1ECV	1	318	-	54,56,56	2.65	20 (37%)	61,93,93	4.15	31 (50%)
48	A86	B	201	-	44,50,50	1.19	3 (6%)	51,76,76	2.49	19 (37%)
39	CLA	l	203	-	53,57,73	1.44	8 (15%)	62,93,113	1.45	7 (11%)
39	CLA	L	308	-	65,69,73	1.31	7 (10%)	78,108,113	1.37	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	G	309	-	60,64,73	1.34	9 (15%)	72,102,113	1.40	6 (8%)
42	BCR	i	102	-	41,41,41	0.72	0	56,56,56	2.26	19 (33%)
42	BCR	m	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.34	7 (12%)
49	KC2	F	311	-	48,52,53	1.73	9 (18%)	59,87,89	2.31	19 (32%)
49	KC2	S	315	28	49,53,53	1.81	10 (20%)	62,89,89	2.15	18 (29%)
50	A1EB1	T	302	-	51,58,58	1.27	3 (5%)	60,85,85	2.04	12 (20%)
39	CLA	b	833	-	69,73,73	1.26	8 (11%)	83,113,113	1.31	6 (7%)
42	BCR	j	103	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
39	CLA	K	306	-	65,69,73	1.31	9 (13%)	78,108,113	1.35	7 (8%)
43	DD6	J	305	-	39,45,45	2.05	3 (7%)	52,67,67	2.29	17 (32%)
46	LMG	W	302	49	39,39,55	1.08	2 (5%)	47,47,63	1.23	4 (8%)
39	CLA	a	816	-	69,73,73	1.27	8 (11%)	83,113,113	1.34	10 (12%)
39	CLA	k	202	-	59,63,73	1.36	9 (15%)	71,101,113	1.35	6 (8%)
47	SQD	E	320	-	34,35,54	1.17	5 (14%)	43,46,65	1.98	11 (25%)
49	KC2	G	313	-	49,53,53	1.79	10 (20%)	62,89,89	2.23	20 (32%)
51	A1ECV	7	317	-	54,56,56	2.65	20 (37%)	61,93,93	4.12	31 (50%)
43	DD6	j	102	-	39,45,45	1.96	2 (5%)	52,67,67	1.85	12 (23%)
50	A1EB1	3	303	-	51,58,58	1.28	4 (7%)	60,85,85	2.05	18 (30%)
39	CLA	z	309	-	45,49,73	1.52	7 (15%)	54,84,113	1.54	6 (11%)
50	A1EB1	z	302	-	51,58,58	1.28	3 (5%)	60,85,85	2.12	20 (33%)
46	LMG	I	302	-	42,42,55	0.89	1 (2%)	50,50,63	1.22	4 (8%)
39	CLA	L	319	-	55,59,73	1.41	6 (10%)	66,96,113	1.40	4 (6%)
49	KC2	V	315	-	49,53,53	1.79	11 (22%)	62,89,89	2.14	16 (25%)
39	CLA	3	319	-	45,49,73	1.52	6 (13%)	54,84,113	1.57	7 (12%)
47	SQD	7	302	-	38,39,54	1.13	5 (13%)	47,50,65	1.69	11 (23%)
39	CLA	A	314	-	69,73,73	1.25	6 (8%)	83,113,113	1.35	7 (8%)
48	A86	1	303	-	44,50,50	1.18	3 (6%)	51,76,76	2.18	17 (33%)
39	CLA	a	818	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
39	CLA	A	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	8 (9%)
48	A86	4	305	-	44,50,50	1.16	2 (4%)	51,76,76	1.94	11 (21%)
48	A86	E	304	-	44,50,50	1.26	3 (6%)	51,76,76	2.41	19 (37%)
51	A1ECV	R	313	-	54,56,56	2.65	20 (37%)	61,93,93	3.85	32 (52%)
39	CLA	a	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
39	CLA	0	322	-	55,59,73	1.42	10 (18%)	66,96,113	1.44	5 (7%)
48	A86	J	301	-	44,50,50	1.17	3 (6%)	51,76,76	2.13	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	a	808	-	60,64,73	1.34	8 (13%)	72,102,113	1.39	4 (5%)
48	A86	1	306	-	44,50,50	1.18	2 (4%)	51,76,76	2.05	13 (25%)
39	CLA	5	315	-	51,55,73	1.44	8 (15%)	61,91,113	1.44	6 (9%)
39	CLA	P	307	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	5 (6%)
49	KC2	4	320	-	49,53,53	1.76	10 (20%)	62,89,89	2.17	17 (27%)
39	CLA	a	823	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	10 (12%)
39	CLA	7	321	-	45,49,73	1.52	7 (15%)	54,84,113	1.59	6 (11%)
48	A86	F	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.12	15 (29%)
48	A86	2	302	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	18 (35%)
49	KC2	6	316	-	49,53,53	1.76	9 (18%)	62,89,89	2.14	19 (30%)
50	A1EB1	E	301	-	51,58,58	1.31	4 (7%)	60,85,85	1.91	19 (31%)
39	CLA	G	310	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	6 (7%)
48	A86	R	301	-	44,50,50	1.22	3 (6%)	51,76,76	2.06	16 (31%)
39	CLA	E	313	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	9 (10%)
39	CLA	M	308	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
39	CLA	a	814	-	65,69,73	1.28	8 (12%)	78,108,113	1.35	6 (7%)
39	CLA	O	313	-	54,58,73	1.40	8 (14%)	65,95,113	1.45	5 (7%)
39	CLA	a	820	-	55,59,73	1.43	9 (16%)	66,96,113	1.35	5 (7%)
39	CLA	X	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	5 (6%)
51	A1ECV	z	316	-	54,56,56	2.66	20 (37%)	61,93,93	4.17	30 (49%)
39	CLA	y	319	-	45,49,73	1.54	8 (17%)	54,84,113	1.59	8 (14%)
39	CLA	y	308	-	49,53,73	1.49	8 (16%)	59,89,113	1.51	7 (11%)
52	A1EB4	M	305	-	53,60,63	2.51	4 (7%)	62,86,89	2.08	16 (25%)
39	CLA	J	311	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
50	A1EB1	L	303	-	51,58,58	1.29	3 (5%)	60,85,85	2.24	19 (31%)
39	CLA	b	806	-	69,73,73	1.23	7 (10%)	83,113,113	1.25	7 (8%)
49	KC2	K	310	-	49,53,53	1.77	10 (20%)	62,89,89	2.19	17 (27%)
50	A1EB1	7	304	-	51,58,58	1.23	4 (7%)	60,85,85	2.03	19 (31%)
39	CLA	0	310	-	65,69,73	1.32	8 (12%)	78,108,113	1.33	7 (8%)
43	DD6	S	306	-	39,45,45	2.01	2 (5%)	52,67,67	1.92	16 (30%)
48	A86	R	302	-	44,50,50	1.15	2 (4%)	51,76,76	2.19	13 (25%)
49	KC2	J	315	-	49,53,53	1.79	9 (18%)	62,89,89	2.11	20 (32%)
48	A86	O	306	-	44,50,50	1.18	3 (6%)	51,76,76	2.57	20 (39%)
39	CLA	3	313	-	57,61,73	1.40	8 (14%)	68,98,113	1.35	5 (7%)
48	A86	8	309	-	44,50,50	1.17	3 (6%)	51,76,76	2.32	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	U	207	-	64,68,73	1.30	8 (12%)	77,107,113	1.33	5 (6%)
48	A86	O	307	-	44,50,50	1.17	2 (4%)	51,76,76	2.35	19 (37%)
51	A1ECV	S	312	-	54,56,56	2.65	20 (37%)	61,93,93	4.10	30 (49%)
39	CLA	R	309	-	69,73,73	1.25	6 (8%)	83,113,113	1.32	7 (8%)
50	A1EB1	7	306	-	51,58,58	1.26	3 (5%)	60,85,85	2.11	22 (36%)
39	CLA	J	313	-	50,54,73	1.47	7 (14%)	60,90,113	1.44	4 (6%)
48	A86	S	304	-	44,50,50	1.13	2 (4%)	51,76,76	1.98	11 (21%)
39	CLA	a	817	1	49,53,73	1.50	9 (18%)	59,89,113	1.49	4 (6%)
39	CLA	J	310	-	59,63,73	1.37	8 (13%)	71,101,113	1.36	7 (9%)
39	CLA	2	310	-	46,50,73	1.51	7 (15%)	55,85,113	1.53	5 (9%)
39	CLA	a	810	-	58,62,73	1.37	8 (13%)	69,99,113	1.37	7 (10%)
41	LHG	D	301	-	34,34,48	0.72	0	37,40,54	1.25	3 (8%)
52	A1EB4	T	304	-	50,57,63	2.65	5 (10%)	59,83,89	2.20	19 (32%)
39	CLA	1	320	-	45,49,73	1.53	6 (13%)	54,84,113	1.56	7 (12%)
43	DD6	U	204	-	39,45,45	2.04	4 (10%)	52,67,67	1.72	12 (23%)
50	A1EB1	3	309	-	51,58,58	1.28	4 (7%)	60,85,85	1.97	15 (25%)
39	CLA	I	313	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	6 (7%)
39	CLA	F	314	18	59,63,73	1.36	6 (10%)	71,101,113	1.48	10 (14%)
39	CLA	O	311	-	46,50,73	1.56	7 (15%)	55,85,113	1.48	6 (10%)
49	KC2	x	315	-	49,53,53	1.79	9 (18%)	62,89,89	2.05	15 (24%)
49	KC2	9	316	35	49,53,53	1.79	10 (20%)	62,89,89	2.11	16 (25%)
49	KC2	y	314	-	49,53,53	1.81	9 (18%)	62,89,89	2.05	14 (22%)
39	CLA	Y	302	-	45,49,73	1.53	7 (15%)	54,84,113	1.56	5 (9%)
50	A1EB1	0	305	-	51,58,58	1.27	3 (5%)	60,85,85	2.03	17 (28%)
39	CLA	a	803	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	6 (7%)
48	A86	K	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.15	18 (35%)
48	A86	W	307	-	44,50,50	1.23	4 (9%)	51,76,76	1.94	13 (25%)
44	SF4	c	101	-	0,12,12	-	-	-	-	-
49	KC2	P	306	24	49,53,53	1.82	12 (24%)	62,89,89	2.19	17 (27%)
39	CLA	Q	312	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	4 (4%)
39	CLA	3	311	-	65,69,73	1.30	8 (12%)	78,108,113	1.27	5 (6%)
39	CLA	a	824	-	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
39	CLA	M	318	24	50,54,73	1.47	7 (14%)	60,90,113	1.50	4 (6%)
48	A86	3	305	-	44,50,50	1.19	2 (4%)	51,76,76	1.79	10 (19%)
43	DD6	G	303	-	39,45,45	1.93	3 (7%)	52,67,67	1.82	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A86	G	305	-	44,50,50	1.19	2 (4%)	51,76,76	2.29	16 (31%)
48	A86	L	301	-	44,50,50	1.16	3 (6%)	51,76,76	2.05	14 (27%)
39	CLA	L	313	-	54,58,73	1.40	8 (14%)	65,95,113	1.40	4 (6%)
39	CLA	U	201	-	50,54,73	1.44	9 (18%)	60,90,113	1.49	7 (11%)
43	DD6	I	306	-	39,45,45	1.95	3 (7%)	52,67,67	1.76	11 (21%)
50	A1EB1	V	307	-	51,58,58	1.26	4 (7%)	60,85,85	2.09	21 (35%)
40	PQN	b	843	-	34,34,34	1.53	2 (5%)	42,45,45	1.26	4 (9%)
39	CLA	y	318	-	46,50,73	1.51	6 (13%)	55,85,113	1.48	4 (7%)
48	A86	8	323	-	44,50,50	1.19	3 (6%)	51,76,76	2.21	16 (31%)
48	A86	V	304	-	44,50,50	1.18	3 (6%)	51,76,76	2.02	17 (33%)
46	LMG	S	321	-	32,32,55	0.92	0	40,40,63	1.21	5 (12%)
43	DD6	y	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.93	15 (28%)
39	CLA	R	315	-	51,55,73	1.45	8 (15%)	61,91,113	1.49	8 (13%)
39	CLA	b	811	-	69,73,73	1.23	10 (14%)	83,113,113	1.40	7 (8%)
39	CLA	1	309	-	46,50,73	1.52	9 (19%)	55,85,113	1.46	5 (9%)
48	A86	4	310	-	44,50,50	1.18	2 (4%)	51,76,76	2.34	17 (33%)
49	KC2	R	318	-	49,53,53	1.78	10 (20%)	62,89,89	2.13	17 (27%)
51	A1ECV	E	311	-	54,56,56	2.67	22 (40%)	61,93,93	3.94	26 (42%)
43	DD6	P	304	-	39,45,45	2.10	3 (7%)	52,67,67	2.77	14 (26%)
39	CLA	C	310	-	69,73,73	1.23	8 (11%)	83,113,113	1.33	5 (6%)
42	BCR	b	846	-	41,41,41	0.74	0	56,56,56	2.13	16 (28%)
39	CLA	B	203	-	50,54,73	1.45	7 (14%)	60,90,113	1.44	5 (8%)
43	DD6	y	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.84	14 (26%)
48	A86	O	302	-	44,50,50	1.22	3 (6%)	51,76,76	2.36	20 (39%)
50	A1EB1	K	305	-	51,58,58	1.25	3 (5%)	60,85,85	2.22	18 (30%)
43	DD6	A	303	-	39,45,45	2.03	3 (7%)	52,67,67	2.88	20 (38%)
39	CLA	Y	313	-	45,49,73	1.53	8 (17%)	54,84,113	1.54	5 (9%)
48	A86	7	307	-	44,50,50	1.24	3 (6%)	51,76,76	2.22	17 (33%)
39	CLA	O	314	-	59,63,73	1.37	8 (13%)	71,101,113	1.35	6 (8%)
47	SQD	9	322	-	35,36,54	1.16	5 (14%)	44,47,65	1.65	9 (20%)
51	A1ECV	x	310	-	54,56,56	2.69	21 (38%)	61,93,93	4.17	31 (50%)
49	KC2	V	312	-	49,53,53	1.77	10 (20%)	62,89,89	2.18	18 (29%)
48	A86	8	307	-	44,50,50	1.23	3 (6%)	51,76,76	2.45	23 (45%)
49	KC2	A	310	13	49,53,53	1.81	9 (18%)	62,89,89	2.04	12 (19%)
49	KC2	4	324	-	49,53,53	1.78	10 (20%)	62,89,89	2.23	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CLA	l	205	-	54,58,73	1.41	8 (14%)	65,95,113	1.44	8 (12%)
39	CLA	b	822	2	54,58,73	1.42	8 (14%)	65,95,113	1.42	5 (7%)
48	A86	W	304	-	44,50,50	1.21	3 (6%)	51,76,76	2.29	18 (35%)
39	CLA	H	312	20	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
50	A1EB1	1	305	-	51,58,58	1.25	4 (7%)	60,85,85	2.08	16 (26%)
50	A1EB1	5	302	-	51,58,58	1.26	3 (5%)	60,85,85	2.12	16 (26%)
39	CLA	b	807	-	69,73,73	1.24	8 (11%)	83,113,113	1.43	8 (9%)
39	CLA	Y	303	-	45,49,73	1.53	7 (15%)	54,84,113	1.52	6 (11%)
48	A86	I	304	-	44,50,50	1.13	3 (6%)	51,76,76	2.14	14 (27%)
49	KC2	z	315	-	49,53,53	1.76	10 (20%)	62,89,89	2.20	18 (29%)
39	CLA	U	208	-	50,54,73	1.47	9 (18%)	60,90,113	1.39	5 (8%)
49	KC2	P	312	-	49,53,53	1.79	10 (20%)	62,89,89	2.17	16 (25%)
39	CLA	Q	311	-	50,54,73	1.45	9 (18%)	60,90,113	1.53	6 (10%)
39	CLA	5	307	-	64,68,73	1.32	7 (10%)	77,107,113	1.30	6 (7%)
48	A86	L	305	-	44,50,50	1.22	3 (6%)	51,76,76	2.17	16 (31%)
50	A1EB1	G	307	-	51,58,58	1.29	4 (7%)	60,85,85	1.87	17 (28%)
48	A86	H	302	-	44,50,50	1.15	3 (6%)	51,76,76	2.29	17 (33%)
46	LMG	7	301	49	46,46,55	0.95	2 (4%)	54,54,63	1.28	6 (11%)
39	CLA	o	203	12	59,63,73	1.35	7 (11%)	71,101,113	1.38	5 (7%)
39	CLA	K	308	22	63,67,73	1.32	8 (12%)	75,105,113	1.30	5 (6%)
50	A1EB1	4	303	-	51,58,58	1.27	3 (5%)	60,85,85	1.84	14 (23%)
39	CLA	0	320	-	49,53,73	1.50	6 (12%)	59,89,113	1.45	5 (8%)
39	CLA	K	309	-	66,70,73	1.28	6 (9%)	79,109,113	1.30	5 (6%)
39	CLA	U	212	-	50,54,73	1.48	7 (14%)	60,90,113	1.42	5 (8%)
50	A1EB1	x	301	-	51,58,58	1.26	4 (7%)	60,85,85	1.97	14 (23%)
48	A86	X	302	-	44,50,50	1.17	2 (4%)	51,76,76	2.19	17 (33%)
51	A1ECV	Y	306	-	54,56,56	2.68	20 (37%)	61,93,93	4.18	29 (47%)
39	CLA	H	316	-	50,54,73	1.47	8 (16%)	60,90,113	1.49	4 (6%)

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
48	A86	2	305	-	-	12/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	b	816	-	-	10/33/109/115	-
50	A1EB1	V	305	-	-	12/42/100/100	0/3/3/3
39	CLA	U	214	-	-	4/17/93/115	-
39	CLA	G	314	19	-	8/31/107/115	-
39	CLA	0	323	-	-	11/17/93/115	-
39	CLA	x	318	-	-	8/10/86/115	-
49	KC2	W	315	-	-	8/15/71/71	-
49	KC2	9	311	-	-	7/15/71/71	-
39	CLA	Z	313	-	-	6/10/86/115	-
49	KC2	C	312	-	-	10/15/71/71	-
48	A86	0	304	-	-	12/34/90/90	0/3/3/3
39	CLA	D	316	-	-	16/39/115/115	-
39	CLA	S	316	-	-	6/10/86/115	-
47	SQD	D	304	-	-	8/33/53/69	0/1/1/1
49	KC2	Q	315	-	-	8/15/71/71	-
42	BCR	f	804	-	-	2/29/63/63	0/2/2/2
48	A86	G	301	-	-	11/34/90/90	0/3/3/3
43	DD6	x	303	-	-	1/26/80/80	0/3/3/3
39	CLA	A	311	-	-	13/39/115/115	-
48	A86	x	305	-	-	8/34/90/90	0/3/3/3
48	A86	2	301	-	-	3/34/90/90	0/3/3/3
49	KC2	0	316	-	-	4/15/71/71	-
39	CLA	S	310	-	-	4/12/88/115	-
43	DD6	O	304	-	-	1/26/80/80	0/3/3/3
48	A86	8	302	-	-	8/34/90/90	0/3/3/3
39	CLA	L	309	-	-	11/25/101/115	-
39	CLA	Q	314	-	-	6/26/102/115	-
39	CLA	V	316	-	-	6/21/97/115	-
39	CLA	7	314	-	-	13/29/105/115	-
39	CLA	y	315	-	-	8/10/86/115	-
48	A86	P	302	-	-	12/34/90/90	0/3/3/3
49	KC2	2	313	-	-	6/13/69/71	-
43	DD6	3	301	-	-	2/26/80/80	0/3/3/3
49	KC2	M	314	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	L	320	-	-	10/17/93/115	-
39	CLA	R	316	-	-	10/24/100/115	-
39	CLA	b	839	-	-	4/18/94/115	-
39	CLA	A	305	13	-	6/20/96/115	-
39	CLA	M	321	24	-	5/17/93/115	-
39	CLA	T	309	-	-	11/29/105/115	-
43	DD6	z	305	-	-	1/26/80/80	0/3/3/3
39	CLA	9	310	-	-	3/10/86/115	-
43	DD6	Z	302	-	-	2/26/80/80	0/3/3/3
49	KC2	V	320	-	-	8/15/71/71	-
48	A86	0	309	-	-	7/34/90/90	0/3/3/3
39	CLA	X	317	-	-	10/24/100/115	-
39	CLA	P	316	-	-	7/23/99/115	-
51	A1ECV	4	315	-	3/3/7/14	9/21/77/77	-
48	A86	J	303	-	-	6/34/90/90	0/3/3/3
49	KC2	L	314	-	-	7/15/71/71	-
49	KC2	1	312	-	-	7/15/71/71	-
47	SQD	M	301	-	-	15/34/54/69	0/1/1/1
49	KC2	Q	313	46	-	9/14/70/71	-
43	DD6	5	303	-	-	1/26/80/80	0/3/3/3
39	CLA	O	316	-	-	6/10/86/115	-
39	CLA	a	833	1	-	11/15/91/115	-
39	CLA	C	307	-	-	12/39/115/115	-
39	CLA	5	316	-	-	10/24/100/115	-
39	CLA	P	308	24	-	22/39/115/115	-
39	CLA	9	307	-	-	4/10/86/115	-
39	CLA	b	824	-	-	10/33/109/115	-
39	CLA	E	319	17	-	13/20/96/115	-
39	CLA	b	840	-	-	11/39/115/115	-
39	CLA	Y	305	-	-	2/10/86/115	-
46	LMG	S	322	49	-	28/41/61/70	0/1/1/1
39	CLA	a	811	-	-	17/39/115/115	-
39	CLA	U	215	-	-	7/10/86/115	-
46	LMG	9	321	-	-	16/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	L	317	-	-	11/15/71/71	-
49	KC2	V	308	27	-	8/15/71/71	-
49	KC2	X	312	-	-	7/15/71/71	-
49	KC2	z	313	-	-	6/16/59/71	-
39	CLA	y	309	-	-	6/17/93/115	-
48	A86	Z	301	-	-	11/34/90/90	0/3/3/3
39	CLA	E	318	17	-	10/17/93/115	-
50	A1EB1	x	302	-	-	15/42/100/100	0/3/3/3
39	CLA	a	809	-	-	14/36/112/115	-
39	CLA	a	837	-	-	5/39/115/115	-
39	CLA	x	317	-	-	5/10/86/115	-
39	CLA	0	312	31	-	8/25/101/115	-
39	CLA	M	309	-	-	17/39/115/115	-
39	CLA	I	308	-	-	10/35/111/115	-
43	DD6	z	304	-	-	6/26/80/80	0/3/3/3
49	KC2	3	317	-	-	7/15/71/71	-
50	A1EB1	8	301	-	-	13/42/100/100	0/3/3/3
49	KC2	8	316	-	-	11/15/71/71	-
39	CLA	b	821	-	-	11/39/115/115	-
39	CLA	8	313	-	-	5/10/86/115	-
39	CLA	x	306	-	-	7/15/91/115	-
46	LMG	M	320	-	-	10/28/48/70	0/1/1/1
41	LHG	j	104	-	-	22/34/34/53	-
39	CLA	8	315	-	-	3/13/89/115	-
42	BCR	l	207	-	-	2/29/63/63	0/2/2/2
50	A1EB1	0	307	-	-	11/42/100/100	0/3/3/3
42	BCR	l	206	-	-	6/29/63/63	0/2/2/2
39	CLA	E	314	-	-	12/29/105/115	-
49	KC2	8	319	34	-	12/15/71/71	-
49	KC2	R	306	-	-	8/15/71/71	-
39	CLA	E	315	-	-	12/17/93/115	-
39	CLA	H	307	-	-	4/15/91/115	-
39	CLA	3	322	-	-	12/23/99/115	-
39	CLA	9	315	-	-	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	D	311	-	-	23/39/115/115	-
50	A1EB1	G	308	-	-	10/42/100/100	0/3/3/3
50	A1EB1	z	301	-	-	12/34/90/100	0/3/3/3
50	A1EB1	h	203	-	-	10/42/100/100	0/3/3/3
39	CLA	6	313	-	-	5/12/88/115	-
48	A86	T	305	-	-	6/34/90/90	0/3/3/3
39	CLA	b	810	-	-	15/39/115/115	-
49	KC2	T	314	-	-	7/15/71/71	-
39	CLA	V	310	-	-	10/33/109/115	-
49	KC2	z	312	-	-	7/15/71/71	-
48	A86	7	308	-	-	8/34/90/90	0/3/3/3
39	CLA	J	317	-	-	4/12/88/115	-
39	CLA	2	316	-	-	6/10/86/115	-
39	CLA	b	830	-	-	13/39/115/115	-
43	DD6	M	304	-	-	0/26/80/80	0/3/3/3
39	CLA	6	322	-	-	11/17/93/115	-
46	LMG	Q	322	49	-	13/23/43/70	0/1/1/1
49	KC2	7	322	-	-	12/15/71/71	-
50	A1EB1	7	303	-	-	17/42/100/100	0/3/3/3
39	CLA	8	321	-	-	4/12/88/115	-
39	CLA	o	206	-	-	14/31/107/115	-
46	LMG	F	317	-	-	20/34/54/70	0/1/1/1
50	A1EB1	8	308	-	-	11/42/100/100	0/3/3/3
46	LMG	7	326	-	-	6/27/47/70	0/1/1/1
48	A86	L	304	-	-	12/34/90/90	0/3/3/3
43	DD6	O	303	-	-	3/26/80/80	0/3/3/3
48	A86	Q	308	-	-	8/34/90/90	0/3/3/3
49	KC2	Y	309	-	-	8/15/71/71	-
52	A1EB4	P	305	-	-	10/37/98/103	0/3/3/3
39	CLA	k	201	-	-	7/24/100/115	-
39	CLA	C	305	-	-	17/35/111/115	-
49	KC2	6	319	-	-	11/15/71/71	-
39	CLA	b	813	-	-	3/25/101/115	-
39	CLA	4	322	-	-	7/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	T	301	-	-	2/34/90/90	0/3/3/3
39	CLA	b	820	-	-	16/33/109/115	-
49	KC2	3	315	-	-	8/15/71/71	-
39	CLA	V	311	-	-	17/39/115/115	-
39	CLA	4	319	-	-	4/10/86/115	-
46	LMG	W	320	-	-	15/28/48/70	0/1/1/1
49	KC2	V	318	-	-	7/15/71/71	-
39	CLA	5	308	-	-	14/39/115/115	-
39	CLA	7	324	-	-	5/10/86/115	-
49	KC2	8	317	-	-	8/15/71/71	-
50	A1EB1	8	304	-	-	10/42/100/100	0/3/3/3
51	A1ECV	X	310	-	3/3/7/14	12/21/77/77	-
50	A1EB1	6	308	-	-	15/42/100/100	0/3/3/3
39	CLA	Y	304	-	-	9/17/93/115	-
39	CLA	z	307	-	-	3/12/88/115	-
39	CLA	F	313	-	-	12/30/106/115	-
39	CLA	b	814	-	-	7/27/103/115	-
49	KC2	A	313	-	-	11/15/71/71	-
48	A86	1	302	-	-	5/34/90/90	0/3/3/3
49	KC2	I	312	46	-	7/14/70/71	-
43	DD6	A	301	-	-	0/26/80/80	0/3/3/3
39	CLA	F	315	18	-	4/10/86/115	-
39	CLA	A	307	-	-	8/33/109/115	-
39	CLA	J	316	-	-	7/17/93/115	-
50	A1EB1	7	305	-	-	16/42/100/100	0/3/3/3
39	CLA	O	312	-	-	7/17/93/115	-
39	CLA	x	314	-	-	7/10/86/115	-
39	CLA	2	318	-	-	5/10/86/115	-
49	KC2	R	312	-	-	8/15/71/71	-
39	CLA	i	103	-	-	17/39/115/115	-
39	CLA	x	309	-	-	4/10/86/115	-
39	CLA	C	308	-	-	16/33/109/115	-
50	A1EB1	0	302	-	-	13/42/100/100	0/3/3/3
39	CLA	b	802	-	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	L	307	-	-	3/34/90/90	0/3/3/3
49	KC2	5	311	-	-	6/15/71/71	-
48	A86	3	307	-	-	6/34/90/90	0/3/3/3
43	DD6	Q	303	-	-	4/26/80/80	0/3/3/3
48	A86	0	306	-	-	2/34/90/90	0/3/3/3
39	CLA	a	821	-	-	13/27/103/115	-
39	CLA	2	307	-	-	4/10/86/115	-
49	KC2	R	314	46	-	7/14/70/71	-
48	A86	9	304	-	-	9/34/90/90	0/3/3/3
39	CLA	Y	311	-	-	6/10/86/115	-
39	CLA	D	312	16	-	9/27/103/115	-
48	A86	9	303	-	-	7/34/90/90	0/3/3/3
39	CLA	Z	309	-	-	2/10/86/115	-
39	CLA	1	310	-	-	6/15/91/115	-
39	CLA	a	829	-	-	7/29/105/115	-
48	A86	Q	302	-	-	7/34/90/90	0/3/3/3
49	KC2	L	312	-	-	8/15/71/71	-
39	CLA	b	823	-	-	9/17/93/115	-
51	A1ECV	T	317	-	3/3/7/14	8/21/77/77	-
39	CLA	J	312	-	-	7/17/93/115	-
50	A1EB1	V	306	-	-	7/42/100/100	0/3/3/3
50	A1EB1	V	302	-	-	12/42/100/100	0/3/3/3
39	CLA	6	321	-	-	5/10/86/115	-
46	LMG	4	325	-	-	16/27/47/70	0/1/1/1
49	KC2	7	320	-	-	7/15/71/71	-
43	DD6	H	305	-	-	2/26/80/80	0/3/3/3
39	CLA	O	310	-	-	15/33/109/115	-
49	KC2	V	314	-	-	9/15/71/71	-
39	CLA	O	308	-	-	4/4/80/115	-
48	A86	P	303	-	-	0/34/90/90	0/3/3/3
50	A1EB1	3	324	-	-	20/42/100/100	0/3/3/3
48	A86	3	308	-	-	6/34/90/90	0/3/3/3
51	A1ECV	5	309	27	3/3/7/14	13/21/77/77	-
50	A1EB1	1	301	-	-	11/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	U	211	-	-	9/33/109/115	-
43	DD6	A	304	-	-	3/26/80/80	0/3/3/3
39	CLA	b	834	-	-	7/31/107/115	-
39	CLA	B	206	-	-	6/12/88/115	-
39	CLA	T	320	-	-	10/24/100/115	-
39	CLA	b	831	-	-	7/21/97/115	-
49	KC2	W	312	24,46	-	8/14/70/71	-
49	KC2	X	315	-	-	8/15/71/71	-
39	CLA	D	319	16	-	22/39/115/115	-
39	CLA	0	313	-	-	12/27/103/115	-
39	CLA	D	318	-	-	16/39/115/115	-
39	CLA	a	802	-	-	7/27/103/115	-
49	KC2	B	208	-	-	9/15/71/71	-
39	CLA	b	812	-	-	10/39/115/115	-
49	KC2	6	317	-	-	9/15/71/71	-
50	A1EB1	6	304	-	-	11/39/97/100	0/3/3/3
39	CLA	J	308	-	-	6/21/97/115	-
39	CLA	b	829	-	-	8/39/115/115	-
39	CLA	Y	314	-	-	8/10/86/115	-
39	CLA	1	311	-	-	7/10/86/115	-
39	CLA	b	841	2	-	12/39/115/115	-
39	CLA	Q	317	-	-	7/17/93/115	-
39	CLA	b	805	-	-	9/39/115/115	-
48	A86	7	312	-	-	4/34/90/90	0/3/3/3
49	KC2	1	314	-	-	11/15/71/71	-
49	KC2	4	317	-	-	5/15/71/71	-
43	DD6	C	301	-	-	3/26/80/80	0/3/3/3
43	DD6	D	303	-	-	0/26/80/80	0/3/3/3
48	A86	L	302	-	-	13/34/90/90	0/3/3/3
39	CLA	C	311	-	-	17/39/115/115	-
46	LMG	4	326	49	-	23/41/61/70	0/1/1/1
39	CLA	3	314	-	-	18/39/115/115	-
39	CLA	8	318	-	-	5/10/86/115	-
39	CLA	a	835	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	DD6	3	304	-	-	3/26/80/80	0/3/3/3
39	CLA	a	801	-	-	16/39/115/115	-
39	CLA	9	312	35	-	5/12/88/115	-
39	CLA	6	318	-	-	8/10/86/115	-
49	KC2	L	321	-	-	7/15/71/71	-
50	A1EB1	O	301	-	-	16/42/100/100	0/3/3/3
50	A1EB1	G	304	-	-	8/42/100/100	0/3/3/3
47	SQD	D	321	-	-	16/34/54/69	0/1/1/1
39	CLA	X	307	-	-	10/39/115/115	-
51	A1ECV	Q	319	-	3/3/7/14	13/21/77/77	-
39	CLA	G	318	-	-	13/20/96/115	-
39	CLA	i	101	-	-	10/39/115/115	-
39	CLA	2	308	-	-	11/17/93/115	-
51	A1ECV	S	318	-	3/3/7/14	9/21/77/77	-
49	KC2	3	321	-	-	10/15/71/71	-
50	A1EB1	D	308	-	-	8/42/100/100	0/3/3/3
48	A86	4	328	-	-	15/34/90/90	0/3/3/3
49	KC2	9	318	-	-	10/15/71/71	-
50	A1EB1	K	302	-	-	6/42/100/100	0/3/3/3
39	CLA	L	310	23	-	14/39/115/115	-
39	CLA	O	318	-	-	6/17/93/115	-
39	CLA	b	809	-	-	16/39/115/115	-
49	KC2	K	313	22	-	9/15/71/71	-
39	CLA	H	313	-	-	9/39/115/115	-
43	DD6	4	308	-	-	1/26/80/80	0/3/3/3
48	A86	k	206	-	-	5/34/90/90	0/3/3/3
39	CLA	X	316	-	-	9/18/94/115	-
39	CLA	1	319	-	-	12/23/99/115	-
39	CLA	8	310	-	-	8/15/91/115	-
48	A86	9	305	-	-	6/34/90/90	0/3/3/3
39	CLA	6	312	-	-	8/20/96/115	-
50	A1EB1	3	310	-	-	11/42/100/100	0/3/3/3
43	DD6	G	306	-	-	4/26/80/80	0/3/3/3
39	CLA	D	313	-	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	DD6	7	309	-	-	2/26/80/80	0/3/3/3
39	CLA	H	308	-	-	7/33/109/115	-
39	CLA	b	836	-	-	3/15/91/115	-
42	BCR	a	842	-	-	4/29/63/63	0/2/2/2
48	A86	7	311	-	-	3/34/90/90	0/3/3/3
43	DD6	a	846	-	-	5/26/80/80	0/3/3/3
48	A86	M	302	-	-	8/34/90/90	0/3/3/3
48	A86	W	303	-	-	4/34/90/90	0/3/3/3
39	CLA	b	808	-	-	7/15/91/115	-
39	CLA	E	306	17	-	6/20/96/115	-
39	CLA	E	317	-	-	8/24/100/115	-
39	CLA	G	312	-	-	12/24/100/115	-
49	KC2	M	311	46	-	7/14/70/71	-
39	CLA	J	314	-	-	20/39/115/115	-
49	KC2	L	315	-	-	9/15/71/71	-
39	CLA	I	310	-	-	10/26/102/115	-
49	KC2	0	319	-	-	10/15/71/71	-
49	KC2	4	318	28	-	9/15/71/71	-
39	CLA	a	805	-	-	11/39/115/115	-
44	SF4	c	102	-	-	-	0/6/5/5
49	KC2	T	312	-	-	10/15/71/71	-
39	CLA	C	306	-	-	8/39/115/115	-
43	DD6	O	305	-	-	5/26/80/80	0/3/3/3
39	CLA	4	316	-	-	13/39/115/115	-
39	CLA	D	315	-	-	9/39/115/115	-
39	CLA	F	316	-	-	10/23/99/115	-
39	CLA	M	310	-	-	14/39/115/115	-
39	CLA	a	827	-	-	6/39/115/115	-
39	CLA	b	851	-	-	13/39/115/115	-
39	CLA	W	311	-	-	15/39/115/115	-
49	KC2	F	307	-	-	9/15/71/71	-
39	CLA	z	308	-	-	4/17/93/115	-
49	KC2	8	314	-	-	10/15/71/71	-
50	A1EB1	G	302	-	-	8/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	9	302	-	-	18/42/100/100	0/3/3/3
50	A1EB1	Q	323	-	-	9/42/100/100	0/3/3/3
39	CLA	6	311	-	-	1/8/84/115	-
46	LMG	D	322	-	-	14/32/52/70	0/1/1/1
39	CLA	a	804	-	-	18/39/115/115	-
39	CLA	F	321	-	-	19/39/115/115	-
49	KC2	6	314	-	-	8/15/71/71	-
39	CLA	E	310	-	-	9/39/115/115	-
39	CLA	7	318	28	-	5/17/93/115	-
42	BCR	k	204	-	-	2/29/63/63	0/2/2/2
39	CLA	K	307	-	-	14/39/115/115	-
48	A86	z	303	-	-	9/34/90/90	0/3/3/3
39	CLA	3	316	-	-	7/21/97/115	-
48	A86	0	308	51	-	2/34/90/90	0/3/3/3
39	CLA	R	307	-	-	12/39/115/115	-
39	CLA	b	842	-	-	14/39/115/115	-
39	CLA	4	312	-	-	18/39/115/115	-
51	A1ECV	W	317	-	3/3/7/14	10/21/77/77	-
48	A86	8	303	-	-	6/34/90/90	0/3/3/3
49	KC2	X	306	27	-	10/15/71/71	-
39	CLA	9	308	-	-	17/27/103/115	-
39	CLA	x	311	-	-	2/15/91/115	-
39	CLA	l	204	-	-	11/39/115/115	-
48	A86	X	303	-	-	8/34/90/90	0/3/3/3
49	KC2	P	313	24	-	10/15/71/71	-
48	A86	4	309	-	-	1/34/90/90	0/3/3/3
39	CLA	8	312	-	-	8/15/91/115	-
51	A1ECV	7	323	-	2/2/7/14	10/21/77/77	-
39	CLA	W	313	-	-	10/39/115/115	-
39	CLA	a	834	-	-	6/23/99/115	-
49	KC2	S	317	-	-	7/15/71/71	-
39	CLA	a	806	-	-	17/39/115/115	-
49	KC2	M	307	-	-	7/15/71/71	-
49	KC2	5	313	46	-	7/14/70/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	Z	310	-	-	9/15/71/71	-
43	DD6	H	303	-	-	1/26/80/80	0/3/3/3
51	A1ECV	9	317	-	3/3/7/14	9/21/77/77	-
39	CLA	a	812	-	-	4/15/91/115	-
39	CLA	W	309	-	-	12/39/115/115	-
49	KC2	G	315	-	-	11/15/71/71	-
39	CLA	A	308	-	-	9/23/99/115	-
39	CLA	Z	305	-	-	4/10/86/115	-
39	CLA	U	210	-	-	9/33/109/115	-
39	CLA	I	309	-	-	12/39/115/115	-
39	CLA	Q	309	-	-	9/35/111/115	-
50	A1EB1	6	306	-	-	5/34/90/100	0/3/3/3
41	LHG	a	840	-	-	26/53/53/53	-
39	CLA	X	311	27	-	5/21/97/115	-
39	CLA	D	317	-	-	16/39/115/115	-
39	CLA	S	311	-	-	13/39/115/115	-
51	A1ECV	V	317	-	3/3/7/14	13/21/77/77	-
48	A86	U	206	-	-	3/34/90/90	0/3/3/3
49	KC2	X	318	-	-	7/15/71/71	-
43	DD6	I	307	-	-	1/26/80/80	0/3/3/3
39	CLA	4	313	-	-	3/17/93/115	-
39	CLA	U	213	-	-	6/10/86/115	-
39	CLA	z	318	-	-	6/10/86/115	-
39	CLA	K	312	-	-	17/39/115/115	-
46	LMG	F	320	49	-	14/29/49/70	0/1/1/1
47	SQD	F	319	-	-	13/32/52/69	0/1/1/1
48	A86	Q	305	-	-	16/34/90/90	0/3/3/3
39	CLA	3	320	-	-	5/15/91/115	-
47	SQD	T	321	-	-	13/31/51/69	0/1/1/1
39	CLA	B	209	-	-	12/29/105/115	-
39	CLA	a	813	1	-	4/21/97/115	-
39	CLA	7	313	-	-	21/35/111/115	-
39	CLA	9	320	-	-	4/10/86/115	-
39	CLA	1	313	32	-	5/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	0	317	31	-	3/15/71/71	-
39	CLA	W	316	24	-	3/10/86/115	-
49	KC2	M	313	-	-	6/15/71/71	-
42	BCR	b	850	-	-	6/29/63/63	0/2/2/2
39	CLA	E	308	-	-	11/39/115/115	-
49	KC2	2	317	-	-	7/15/71/71	-
39	CLA	U	209	-	-	8/24/100/115	-
39	CLA	Y	310	-	-	4/10/86/115	-
39	CLA	S	308	-	-	18/35/111/115	-
49	KC2	y	313	-	-	8/15/71/71	-
39	CLA	6	315	-	-	1/10/86/115	-
50	A1EB1	8	306	-	-	13/42/100/100	0/3/3/3
39	CLA	y	312	-	-	5/12/88/115	-
39	CLA	F	312	-	-	8/39/115/115	-
39	CLA	8	311	-	-	11/27/103/115	-
39	CLA	W	319	-	-	8/17/93/115	-
41	LHG	X	301	-	-	25/45/45/53	-
43	DD6	7	310	-	-	4/26/80/80	0/3/3/3
39	CLA	b	817	-	-	7/32/108/115	-
39	CLA	0	318	-	-	3/10/86/115	-
39	CLA	a	822	-	-	9/39/115/115	-
48	A86	5	301	-	-	3/34/90/90	0/3/3/3
50	A1EB1	2	306	-	-	16/42/100/100	0/3/3/3
46	LMG	0	324	49	-	13/21/41/70	0/1/1/1
42	BCR	a	843	-	-	0/29/63/63	0/2/2/2
39	CLA	Z	307	-	-	0/10/86/115	-
39	CLA	R	308	-	-	11/33/109/115	-
49	KC2	T	315	29	-	7/15/71/71	-
39	CLA	b	801	-	-	10/39/115/115	-
43	DD6	D	307	-	-	2/26/80/80	0/3/3/3
39	CLA	I	301	41	-	7/24/100/115	-
50	A1EB1	S	302	-	-	11/42/100/100	0/3/3/3
43	DD6	F	303	-	-	0/26/80/80	0/3/3/3
49	KC2	H	314	-	-	11/15/71/71	-
51	A1ECV	L	318	-	3/3/7/14	12/21/77/77	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	P	320	-	-	9/15/71/71	-
39	CLA	1	316	-	-	5/10/86/115	-
39	CLA	3	312	-	-	22/39/115/115	-
47	SQD	P	301	-	-	12/33/53/69	0/1/1/1
48	A86	S	307	-	-	6/34/90/90	0/3/3/3
42	BCR	a	845	-	-	4/29/63/63	0/2/2/2
39	CLA	B	204	-	-	4/17/93/115	-
49	KC2	3	318	-	-	6/15/71/71	-
39	CLA	y	310	-	-	7/10/86/115	-
42	BCR	b	847	-	-	4/29/63/63	0/2/2/2
39	CLA	8	322	-	-	4/10/86/115	-
39	CLA	F	308	-	-	16/39/115/115	-
50	A1EB1	R	303	-	-	10/42/100/100	0/3/3/3
39	CLA	4	323	-	-	13/39/115/115	-
39	CLA	5	306	-	-	13/39/115/115	-
51	A1ECV	M	316	-	3/3/7/14	10/21/77/77	-
39	CLA	T	313	-	-	6/23/99/115	-
39	CLA	b	827	-	-	10/39/115/115	-
51	A1ECV	x	316	-	3/3/7/14	7/21/77/77	-
39	CLA	b	837	-	-	10/33/109/115	-
39	CLA	b	825	-	-	14/39/115/115	-
50	A1EB1	2	304	-	-	16/42/100/100	0/3/3/3
39	CLA	a	828	1	-	6/21/97/115	-
39	CLA	a	832	-	-	7/21/97/115	-
51	A1ECV	0	321	48	2/2/7/14	10/21/77/77	-
39	CLA	I	311	-	-	15/39/115/115	-
50	A1EB1	T	307	-	-	6/42/100/100	0/3/3/3
50	A1EB1	4	302	-	-	11/42/100/100	0/3/3/3
39	CLA	k	203	-	-	9/27/103/115	-
49	KC2	O	317	46	-	7/14/70/71	-
40	PQN	a	839	-	-	7/23/43/43	0/2/2/2
39	CLA	Z	315	-	-	4/10/86/115	-
48	A86	0	301	-	-	4/34/90/90	0/3/3/3
39	CLA	R	311	27	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	F	310	-	-	7/26/102/115	-
49	KC2	x	313	-	-	6/15/71/71	-
39	CLA	M	317	-	-	6/23/99/115	-
39	CLA	S	319	-	-	10/24/100/115	-
39	CLA	f	803	-	-	11/27/103/115	-
48	A86	C	303	-	-	6/34/90/90	0/3/3/3
39	CLA	x	307	-	-	4/10/86/115	-
51	A1ECV	z	310	-	3/3/7/14	13/21/77/77	-
39	CLA	a	830	-	-	20/39/115/115	-
48	A86	T	306	-	-	6/34/90/90	0/3/3/3
39	CLA	A	312	-	-	15/39/115/115	-
42	BCR	b	845	-	-	1/29/63/63	0/2/2/2
49	KC2	W	308	-	-	6/15/71/71	-
42	BCR	h	202	-	-	6/29/63/63	0/2/2/2
50	A1EB1	6	301	-	-	12/42/100/100	0/3/3/3
52	A1EB4	M	322	-	-	6/38/99/103	0/3/3/3
39	CLA	V	319	-	-	6/24/100/115	-
39	CLA	P	309	-	-	14/39/115/115	-
39	CLA	b	835	-	-	16/39/115/115	-
39	CLA	7	315	-	-	6/21/97/115	-
50	A1EB1	4	301	-	-	12/42/100/100	0/3/3/3
43	DD6	X	304	-	-	0/26/80/80	0/3/3/3
39	CLA	J	318	-	-	7/17/93/115	-
39	CLA	0	311	-	-	11/27/103/115	-
50	A1EB1	4	304	-	-	9/42/100/100	0/3/3/3
39	CLA	L	316	-	-	8/10/86/115	-
39	CLA	7	316	-	-	10/39/115/115	-
39	CLA	H	315	-	-	6/10/86/115	-
48	A86	8	305	-	-	12/34/90/90	0/3/3/3
48	A86	D	305	-	-	8/34/90/90	0/3/3/3
39	CLA	I	314	-	-	14/39/115/115	-
48	A86	6	307	-	-	10/34/90/90	0/3/3/3
43	DD6	J	306	-	-	3/26/80/80	0/3/3/3
39	CLA	J	307	21	-	10/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	Q	310	-	-	20/39/115/115	-
48	A86	U	202	-	-	4/34/90/90	0/3/3/3
49	KC2	T	316	-	-	7/15/71/71	-
49	KC2	y	316	-	-	7/15/71/71	-
39	CLA	l	308	-	-	6/10/86/115	-
39	CLA	b	838	-	-	15/39/115/115	-
43	DD6	R	304	-	-	0/26/80/80	0/3/3/3
49	KC2	5	314	-	-	8/15/71/71	-
49	KC2	Z	311	-	-	10/15/71/71	-
39	CLA	P	314	-	-	4/10/86/115	-
47	SQD	S	301	-	-	13/34/54/69	0/1/1/1
45	DGD	C	314	-	-	15/29/69/95	0/2/2/2
51	A1ECV	2	311	-	3/3/7/14	10/21/77/77	-
43	DD6	x	304	-	-	0/26/80/80	0/3/3/3
39	CLA	I	316	36	-	2/10/86/115	-
49	KC2	S	314	-	-	6/15/71/71	-
48	A86	y	305	-	-	0/34/90/90	0/3/3/3
39	CLA	a	825	-	-	11/36/112/115	-
47	SQD	D	320	39	-	11/32/52/69	0/1/1/1
39	CLA	E	309	-	-	7/25/101/115	-
39	CLA	a	836	-	-	9/39/115/115	-
39	CLA	b	826	-	-	9/39/115/115	-
39	CLA	V	313	27	-	8/39/115/115	-
46	LMG	l	208	49	-	15/34/54/70	0/1/1/1
49	KC2	C	313	-	-	11/15/71/71	-
39	CLA	z	317	-	-	7/12/88/115	-
39	CLA	a	807	1	-	13/39/115/115	-
43	DD6	2	303	-	-	2/26/80/80	0/3/3/3
50	A1EB1	Q	307	-	-	8/42/100/100	0/3/3/3
51	A1ECV	y	311	-	3/3/7/14	12/21/77/77	-
39	CLA	Z	306	-	-	9/17/93/115	-
52	A1EB4	P	318	-	-	9/35/96/103	0/3/3/3
39	CLA	E	307	-	-	21/39/115/115	-
52	A1EB4	X	305	-	-	10/38/99/103	0/3/3/3
39	CLA	0	315	31	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	W	318	-	-	7/23/99/115	-
43	DD6	I	305	-	-	1/26/80/80	0/3/3/3
39	CLA	D	314	-	-	11/39/115/115	-
50	A1EB1	3	302	-	-	15/42/100/100	0/3/3/3
43	DD6	F	305	-	-	1/26/80/80	0/3/3/3
43	DD6	Q	306	-	-	1/26/80/80	0/3/3/3
39	CLA	C	304	-	-	5/13/89/115	-
48	A86	3	306	-	-	8/34/90/90	0/3/3/3
49	KC2	9	313	-	-	6/15/71/71	-
48	A86	6	303	-	-	2/34/90/90	0/3/3/3
39	CLA	b	803	-	-	14/39/115/115	-
50	A1EB1	J	302	-	-	9/42/100/100	0/3/3/3
49	KC2	0	314	46,31	-	8/14/70/71	-
43	DD6	D	306	-	-	0/26/80/80	0/3/3/3
39	CLA	T	319	29	-	10/17/93/115	-
46	LMG	P	317	49	-	18/34/54/70	0/1/1/1
39	CLA	a	847	-	-	20/39/115/115	-
48	A86	6	302	-	-	7/34/90/90	0/3/3/3
48	A86	R	317	-	-	3/34/90/90	0/3/3/3
49	KC2	W	314	-	-	7/15/71/71	-
39	CLA	o	202	-	-	5/12/88/115	-
47	SQD	4	327	-	-	17/34/54/69	0/1/1/1
43	DD6	T	303	-	-	1/26/80/80	0/3/3/3
51	A1ECV	5	312	27	3/3/7/14	13/21/77/77	-
49	KC2	1	315	-	-	11/15/71/71	-
39	CLA	j	101	-	-	19/39/115/115	-
43	DD6	K	303	-	-	0/26/80/80	0/3/3/3
50	A1EB1	H	301	-	-	12/42/100/100	0/3/3/3
39	CLA	b	815	-	-	14/39/115/115	-
39	CLA	z	306	-	-	4/10/86/115	-
47	SQD	H	318	-	-	9/33/53/69	0/1/1/1
42	BCR	b	844	-	-	6/29/63/63	0/2/2/2
52	A1EB4	W	321	-	-	8/38/99/103	0/3/3/3
39	CLA	a	838	-	-	12/39/115/115	-
43	DD6	B	202	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SQD	F	318	-	-	17/37/57/69	0/1/1/1
39	CLA	l	201	-	-	16/39/115/115	-
50	A1EB1	U	203	-	-	9/42/100/100	0/3/3/3
39	CLA	A	315	-	-	8/21/97/115	-
39	CLA	E	312	-	-	23/39/115/115	-
42	BCR	a	844	-	-	0/29/63/63	0/2/2/2
39	CLA	Z	304	-	-	5/10/86/115	-
39	CLA	Z	312	-	-	4/10/86/115	-
39	CLA	a	819	-	-	11/20/96/115	-
51	A1ECV	Z	308	-	3/3/7/14	12/21/77/77	-
39	CLA	4	311	-	-	19/35/111/115	-
39	CLA	M	312	-	-	14/39/115/115	-
39	CLA	6	310	-	-	6/12/88/115	-
39	CLA	z	311	-	-	5/10/86/115	-
49	KC2	7	319	-	-	7/15/71/71	-
39	CLA	L	311	23	-	10/24/100/115	-
39	CLA	b	818	-	-	11/27/103/115	-
49	KC2	x	312	-	-	8/15/71/71	-
39	CLA	F	309	-	-	6/24/100/115	-
51	A1ECV	6	320	-	3/3/7/14	12/21/77/77	-
48	A86	L	306	-	-	12/34/90/90	0/3/3/3
49	KC2	G	311	19	-	9/15/71/71	-
48	A86	Y	301	-	-	5/34/90/90	0/3/3/3
39	CLA	T	311	-	-	5/29/105/115	-
39	CLA	2	312	-	-	7/10/86/115	-
43	DD6	J	304	-	-	3/26/80/80	0/3/3/3
39	CLA	D	309	16	-	8/20/96/115	-
39	CLA	H	306	-	-	10/19/95/115	-
39	CLA	2	315	-	-	5/10/86/115	-
42	BCR	f	801	-	-	4/29/63/63	0/2/2/2
41	LHG	H	317	-	-	18/39/39/53	-
39	CLA	Z	316	-	-	8/10/86/115	-
48	A86	9	306	-	-	6/34/90/90	0/3/3/3
46	LMG	A	316	-	-	13/24/44/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	S	320	-	-	15/39/115/115	-
51	A1ECV	Z	314	-	3/3/7/14	9/21/77/77	-
39	CLA	2	309	-	-	6/17/93/115	-
50	A1EB1	y	301	-	-	11/42/100/100	0/3/3/3
48	A86	M	303	-	-	0/34/90/90	0/3/3/3
49	KC2	2	314	-	-	10/15/71/71	-
39	CLA	V	309	-	-	11/39/115/115	-
39	CLA	T	310	29	-	6/24/100/115	-
39	CLA	T	308	-	-	10/17/93/115	-
52	A1EB4	R	305	-	-	10/38/99/103	0/3/3/3
52	A1EB4	5	304	-	-	5/38/99/103	0/3/3/3
39	CLA	2	319	-	-	13/17/93/115	-
41	LHG	a	841	39	-	13/31/31/53	-
43	DD6	1	304	-	-	4/26/80/80	0/3/3/3
50	A1EB1	H	304	-	-	14/42/100/100	0/3/3/3
50	A1EB1	F	304	-	-	11/42/100/100	0/3/3/3
39	CLA	h	201	-	-	10/27/103/115	-
39	CLA	J	309	-	-	17/39/115/115	-
50	A1EB1	y	302	-	-	10/42/100/100	0/3/3/3
39	CLA	4	314	-	-	10/39/115/115	-
49	KC2	P	310	46	-	8/14/70/71	-
48	A86	y	306	-	-	6/34/90/90	0/3/3/3
39	CLA	z	314	-	-	5/10/86/115	-
43	DD6	E	303	-	-	1/26/80/80	0/3/3/3
39	CLA	K	311	-	-	14/39/115/115	-
47	SQD	k	205	-	-	13/33/53/69	0/1/1/1
39	CLA	y	307	-	-	4/10/86/115	-
52	A1EB4	P	319	-	-	6/38/99/103	0/3/3/3
39	CLA	3	323	-	-	11/17/93/115	-
39	CLA	B	205	-	-	5/12/88/115	-
39	CLA	T	318	-	-	9/18/94/115	-
39	CLA	I	315	-	-	6/24/100/115	-
39	CLA	B	207	-	-	14/27/103/115	-
49	KC2	5	305	27	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	M	306	-	-	2/34/90/90	0/3/3/3
51	A1ECV	Q	316	26	3/3/7/14	9/21/77/77	-
39	CLA	b	828	-	-	15/39/115/115	-
39	CLA	Y	307	-	-	5/10/86/115	-
51	A1ECV	R	310	-	3/3/7/14	11/21/77/77	-
39	CLA	b	819	-	-	11/32/108/115	-
39	CLA	W	310	-	-	16/39/115/115	-
48	A86	9	301	-	-	9/34/90/90	0/3/3/3
51	A1ECV	P	315	-	3/3/7/14	15/21/77/77	-
45	DGD	b	849	-	-	27/49/89/95	0/2/2/2
39	CLA	C	309	-	-	13/17/93/115	-
39	CLA	1	317	-	-	6/10/86/115	-
39	CLA	X	308	-	-	18/33/109/115	-
50	A1EB1	K	304	-	-	8/42/100/100	0/3/3/3
39	CLA	x	308	-	-	2/10/86/115	-
39	CLA	Q	320	-	-	8/18/94/115	-
39	CLA	o	201	-	-	5/23/99/115	-
51	A1ECV	4	321	-	3/3/7/14	10/21/77/77	-
39	CLA	o	205	-	-	12/24/100/115	-
48	A86	Z	303	-	-	8/34/90/90	0/3/3/3
49	KC2	8	320	-	-	8/15/71/71	-
50	A1EB1	U	205	-	-	11/42/100/100	0/3/3/3
44	SF4	b	804	-	-	-	0/6/5/5
39	CLA	K	314	-	-	6/10/86/115	-
39	CLA	H	310	-	-	7/30/106/115	-
39	CLA	9	309	-	-	3/10/86/115	-
51	A1ECV	y	317	-	3/3/7/14	9/21/77/77	-
49	KC2	H	311	-	-	9/15/71/71	-
39	CLA	b	832	-	-	15/39/115/115	-
51	A1ECV	X	313	-	3/3/7/14	9/21/77/77	-
39	CLA	a	815	-	-	16/39/115/115	-
43	DD6	W	305	-	-	1/26/80/80	0/3/3/3
51	A1ECV	Y	312	-	3/3/7/14	9/21/77/77	-
49	KC2	X	314	46	-	7/14/70/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	S	305	-	-	6/34/90/90	0/3/3/3
50	A1EB1	0	303	-	-	10/42/100/100	0/3/3/3
52	A1EB4	W	306	-	-	10/37/98/103	0/3/3/3
39	CLA	O	309	-	-	6/15/91/115	-
43	DD6	o	204	-	-	2/26/80/80	0/3/3/3
39	CLA	D	310	47	-	19/35/111/115	-
49	KC2	I	303	-	-	7/15/71/71	-
39	CLA	S	313	-	-	7/39/115/115	-
39	CLA	9	319	-	-	8/15/91/115	-
47	SQD	W	301	-	-	8/22/42/69	0/1/1/1
51	A1ECV	9	314	-	3/3/7/14	9/21/77/77	-
48	A86	F	301	-	-	4/34/90/90	0/3/3/3
42	BCR	l	202	-	-	4/29/63/63	0/2/2/2
48	A86	4	306	-	-	8/34/90/90	0/3/3/3
46	LMG	M	319	49	-	13/34/54/70	0/1/1/1
48	A86	Q	301	-	-	5/34/90/90	0/3/3/3
48	A86	6	305	-	-	11/34/90/90	0/3/3/3
50	A1EB1	S	303	-	-	14/42/100/100	0/3/3/3
39	CLA	a	831	-	-	12/39/115/115	-
39	CLA	P	311	-	-	10/39/115/115	-
39	CLA	A	306	-	-	11/35/111/115	-
48	A86	Q	304	-	-	2/34/90/90	0/3/3/3
43	DD6	A	302	-	-	0/26/80/80	0/3/3/3
41	LHG	D	302	-	-	21/39/39/53	-
39	CLA	M	315	-	-	4/10/86/115	-
43	DD6	4	307	-	-	1/26/80/80	0/3/3/3
39	CLA	f	802	-	-	11/39/115/115	-
39	CLA	5	310	27	-	6/21/97/115	-
48	A86	1	307	-	-	0/34/90/90	0/3/3/3
50	A1EB1	C	302	-	-	10/42/100/100	0/3/3/3
49	KC2	G	317	-	-	7/15/71/71	-
49	KC2	Y	308	-	-	9/15/71/71	-
39	CLA	H	309	20	-	5/24/100/115	-
43	DD6	E	305	-	-	3/26/80/80	0/3/3/3
48	A86	V	301	-	-	2/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	E	316	-	-	8/24/100/115	-
39	CLA	F	306	-	-	6/17/93/115	-
39	CLA	Q	321	-	-	6/25/101/115	-
51	A1ECV	O	315	-	3/3/7/14	11/21/77/77	-
43	DD6	V	303	-	-	0/26/80/80	0/3/3/3
43	DD6	E	302	-	-	0/26/80/80	0/3/3/3
39	CLA	S	309	-	-	19/39/115/115	-
42	BCR	b	848	-	-	1/29/63/63	0/2/2/2
48	A86	6	309	-	-	13/34/90/90	0/3/3/3
39	CLA	7	325	-	-	9/21/97/115	-
49	KC2	Q	318	26	-	6/15/71/71	-
51	A1ECV	G	316	-	3/3/7/14	15/21/77/77	-
51	A1ECV	1	318	-	3/3/7/14	8/21/77/77	-
48	A86	B	201	-	-	5/34/90/90	0/3/3/3
39	CLA	l	203	-	-	8/20/96/115	-
39	CLA	L	308	-	-	15/35/111/115	-
39	CLA	G	309	-	-	15/29/105/115	-
42	BCR	i	102	-	-	4/29/63/63	0/2/2/2
42	BCR	m	101	-	-	9/29/63/63	0/2/2/2
49	KC2	F	311	-	-	7/14/70/71	-
49	KC2	S	315	28	-	7/15/71/71	-
50	A1EB1	T	302	-	-	14/42/100/100	0/3/3/3
51	A1ECV	7	317	-	3/3/7/14	7/21/77/77	-
39	CLA	b	833	-	-	15/39/115/115	-
39	CLA	K	306	-	-	13/35/111/115	-
42	BCR	j	103	-	-	4/29/63/63	0/2/2/2
43	DD6	J	305	-	-	3/26/80/80	0/3/3/3
39	CLA	a	816	-	-	15/39/115/115	-
39	CLA	k	202	-	-	13/27/103/115	-
46	LMG	W	302	49	-	18/34/54/70	0/1/1/1
47	SQD	E	320	-	-	12/30/50/69	0/1/1/1
49	KC2	G	313	-	-	6/15/71/71	-
43	DD6	j	102	-	-	6/26/80/80	0/3/3/3
50	A1EB1	3	303	-	-	8/42/100/100	0/3/3/3
39	CLA	z	309	-	-	5/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	A1EB1	z	302	-	-	13/42/100/100	0/3/3/3
46	LMG	I	302	-	-	23/37/57/70	0/1/1/1
39	CLA	L	319	-	-	8/23/99/115	-
49	KC2	V	315	-	-	9/15/71/71	-
39	CLA	3	319	-	-	6/10/86/115	-
47	SQD	7	302	-	-	15/34/54/69	0/1/1/1
39	CLA	A	314	-	-	17/39/115/115	-
48	A86	1	303	-	-	2/34/90/90	0/3/3/3
39	CLA	a	818	-	-	11/39/115/115	-
39	CLA	A	309	-	-	13/39/115/115	-
48	A86	4	305	-	-	6/34/90/90	0/3/3/3
48	A86	E	304	-	-	2/34/90/90	0/3/3/3
51	A1ECV	R	313	-	3/3/7/14	11/21/77/77	-
39	CLA	a	826	-	-	18/39/115/115	-
39	CLA	0	322	-	-	14/23/99/115	-
48	A86	J	301	-	-	2/34/90/90	0/3/3/3
39	CLA	a	808	-	-	12/29/105/115	-
48	A86	1	306	-	-	9/34/90/90	0/3/3/3
39	CLA	5	315	-	-	5/18/94/115	-
39	CLA	P	307	-	-	12/39/115/115	-
49	KC2	4	320	-	-	10/15/71/71	-
39	CLA	a	823	-	-	10/39/115/115	-
39	CLA	7	321	-	-	6/10/86/115	-
48	A86	F	302	-	-	2/34/90/90	0/3/3/3
48	A86	2	302	-	-	5/34/90/90	0/3/3/3
49	KC2	6	316	-	-	10/15/71/71	-
50	A1EB1	E	301	-	-	9/42/100/100	0/3/3/3
39	CLA	G	310	-	-	12/39/115/115	-
48	A86	R	301	-	-	2/34/90/90	0/3/3/3
39	CLA	E	313	-	-	13/39/115/115	-
39	CLA	M	308	-	-	12/39/115/115	-
39	CLA	a	814	-	-	15/35/111/115	-
39	CLA	O	313	-	-	4/21/97/115	-
39	CLA	a	820	-	-	10/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	X	309	-	-	14/39/115/115	-
51	A1ECV	z	316	-	3/3/7/14	8/21/77/77	-
39	CLA	y	319	-	-	5/10/86/115	-
39	CLA	y	308	-	-	9/15/91/115	-
52	A1EB4	M	305	-	-	9/39/100/103	0/3/3/3
39	CLA	J	311	-	-	12/39/115/115	-
50	A1EB1	L	303	-	-	15/42/100/100	0/3/3/3
39	CLA	b	806	-	-	15/39/115/115	-
49	KC2	K	310	-	-	7/15/71/71	-
50	A1EB1	7	304	-	-	14/42/100/100	0/3/3/3
39	CLA	0	310	-	-	25/35/111/115	-
43	DD6	S	306	-	-	4/26/80/80	0/3/3/3
48	A86	R	302	-	-	11/34/90/90	0/3/3/3
49	KC2	J	315	-	-	10/15/71/71	-
48	A86	O	306	-	-	6/34/90/90	0/3/3/3
39	CLA	3	313	-	-	5/25/101/115	-
48	A86	8	309	-	-	4/34/90/90	0/3/3/3
39	CLA	U	207	-	-	17/33/109/115	-
48	A86	O	307	-	-	9/34/90/90	0/3/3/3
51	A1ECV	S	312	-	3/3/7/14	9/21/77/77	-
39	CLA	R	309	-	-	13/39/115/115	-
50	A1EB1	7	306	-	-	10/42/100/100	0/3/3/3
39	CLA	J	313	-	-	9/17/93/115	-
48	A86	S	304	-	-	8/34/90/90	0/3/3/3
39	CLA	a	817	1	-	6/15/91/115	-
39	CLA	J	310	-	-	8/27/103/115	-
39	CLA	2	310	-	-	6/12/88/115	-
39	CLA	a	810	-	-	8/26/102/115	-
41	LHG	D	301	-	-	8/39/39/53	-
52	A1EB4	T	304	-	-	9/36/97/103	0/3/3/3
39	CLA	1	320	-	-	6/10/86/115	-
43	DD6	U	204	-	-	1/26/80/80	0/3/3/3
50	A1EB1	3	309	-	-	9/42/100/100	0/3/3/3
39	CLA	I	313	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CLA	F	314	18	-	10/27/103/115	-
39	CLA	O	311	-	-	2/12/88/115	-
49	KC2	x	315	-	-	10/15/71/71	-
49	KC2	9	316	35	-	9/15/71/71	-
49	KC2	y	314	-	-	7/15/71/71	-
39	CLA	Y	302	-	-	4/10/86/115	-
50	A1EB1	0	305	-	-	16/42/100/100	0/3/3/3
39	CLA	a	803	-	-	17/39/115/115	-
48	A86	K	301	-	-	6/34/90/90	0/3/3/3
48	A86	W	307	-	-	2/34/90/90	0/3/3/3
44	SF4	c	101	-	-	-	0/6/5/5
49	KC2	P	306	24	-	7/15/71/71	-
39	CLA	Q	312	-	-	11/39/115/115	-
39	CLA	3	311	-	-	16/35/111/115	-
39	CLA	a	824	-	-	7/39/115/115	-
39	CLA	M	318	24	-	7/17/93/115	-
48	A86	3	305	-	-	12/34/90/90	0/3/3/3
43	DD6	G	303	-	-	1/26/80/80	0/3/3/3
48	A86	G	305	-	-	7/34/90/90	0/3/3/3
48	A86	L	301	-	-	7/34/90/90	0/3/3/3
39	CLA	L	313	-	-	3/21/97/115	-
39	CLA	U	201	-	-	11/17/93/115	-
43	DD6	I	306	-	-	2/26/80/80	0/3/3/3
50	A1EB1	V	307	-	-	12/42/100/100	0/3/3/3
40	PQN	b	843	-	-	3/23/43/43	0/2/2/2
39	CLA	y	318	-	-	7/12/88/115	-
48	A86	8	323	-	-	4/34/90/90	0/3/3/3
48	A86	V	304	-	-	3/34/90/90	0/3/3/3
46	LMG	S	321	-	-	11/27/47/70	0/1/1/1
43	DD6	y	304	-	-	0/26/80/80	0/3/3/3
51	A1ECV	E	311	-	3/3/7/14	8/21/77/77	-
39	CLA	b	811	-	-	10/39/115/115	-
39	CLA	R	315	-	-	7/18/94/115	-
39	CLA	1	309	-	-	6/12/88/115	-
48	A86	4	310	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	KC2	R	318	-	-	7/15/71/71	-
43	DD6	P	304	-	-	2/26/80/80	0/3/3/3
39	CLA	C	310	-	-	18/39/115/115	-
42	BCR	b	846	-	-	3/29/63/63	0/2/2/2
39	CLA	B	203	-	-	5/17/93/115	-
43	DD6	y	303	-	-	1/26/80/80	0/3/3/3
48	A86	O	302	-	-	2/34/90/90	0/3/3/3
50	A1EB1	K	305	-	-	7/42/100/100	0/3/3/3
43	DD6	A	303	-	-	5/26/80/80	0/3/3/3
39	CLA	Y	313	-	-	5/10/86/115	-
48	A86	7	307	-	-	3/34/90/90	0/3/3/3
39	CLA	O	314	-	-	7/27/103/115	-
51	A1ECV	x	310	-	3/3/7/14	7/21/77/77	-
47	SQD	9	322	-	-	10/31/51/69	0/1/1/1
49	KC2	V	312	-	-	6/15/71/71	-
48	A86	8	307	-	-	12/34/90/90	0/3/3/3
49	KC2	A	310	13	-	7/15/71/71	-
49	KC2	4	324	-	-	8/15/71/71	-
39	CLA	l	205	-	-	2/21/97/115	-
39	CLA	b	822	2	-	4/21/97/115	-
48	A86	W	304	-	-	0/34/90/90	0/3/3/3
39	CLA	H	312	20	-	19/39/115/115	-
50	A1EB1	1	305	-	-	10/42/100/100	0/3/3/3
50	A1EB1	5	302	-	-	9/42/100/100	0/3/3/3
39	CLA	b	807	-	-	14/39/115/115	-
39	CLA	Y	303	-	-	4/10/86/115	-
48	A86	I	304	-	-	11/34/90/90	0/3/3/3
49	KC2	z	315	-	-	10/15/71/71	-
39	CLA	U	208	-	-	5/17/93/115	-
49	KC2	P	312	-	-	7/15/71/71	-
39	CLA	Q	311	-	-	5/17/93/115	-
39	CLA	5	307	-	-	5/33/109/115	-
48	A86	L	305	-	-	2/34/90/90	0/3/3/3
50	A1EB1	G	307	-	-	17/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	H	302	-	-	6/34/90/90	0/3/3/3
46	LMG	7	301	49	-	23/41/61/70	0/1/1/1
39	CLA	o	203	12	-	7/27/103/115	-
39	CLA	K	308	22	-	13/32/108/115	-
50	A1EB1	4	303	-	-	12/42/100/100	0/3/3/3
39	CLA	0	320	-	-	8/15/91/115	-
39	CLA	K	309	-	-	9/36/112/115	-
39	CLA	U	212	-	-	7/17/93/115	-
50	A1EB1	x	301	-	-	14/42/100/100	0/3/3/3
48	A86	X	302	-	-	7/34/90/90	0/3/3/3
51	A1ECV	Y	306	-	3/3/7/14	10/21/77/77	-
39	CLA	H	316	-	-	10/17/93/115	-

The worst 5 of 5838 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	M	322	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	319	A1EB4	C13-C11	-17.07	1.25	1.43
52	P	318	A1EB4	C13-C11	-16.98	1.25	1.43
52	W	321	A1EB4	C13-C11	-16.67	1.25	1.43
52	T	304	A1EB4	C13-C11	-16.45	1.25	1.43

The worst 5 of 10020 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2	303	DD6	O1-C20-C21	17.30	135.78	115.06
43	Z	302	DD6	O1-C20-C21	17.29	135.77	115.06
43	F	305	DD6	O1-C20-C21	13.19	130.87	115.06
51	R	310	A1ECV	C3A-C4A-NA	12.90	119.61	110.10
51	Q	316	A1ECV	C3A-C4A-NA	12.89	119.60	110.10

5 of 115 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
51	E	311	A1ECV	NA
51	E	311	A1ECV	ND
51	E	311	A1ECV	NB
51	G	316	A1ECV	NA
51	G	316	A1ECV	ND

5 of 7595 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	a	801	CLA	CBD-CGD-O2D-CED
39	a	802	CLA	C1A-C2A-CAA-CBA
39	a	803	CLA	CHA-CBD-CGD-O1D
39	a	803	CLA	CHA-CBD-CGD-O2D
39	a	803	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

444 monomers are involved in 930 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	2	305	A86	1	0
39	0	323	CLA	2	0
49	W	315	KC2	1	0
39	Z	313	CLA	1	0
48	0	304	A86	1	0
39	D	316	CLA	2	0
47	D	304	SQD	2	0
49	Q	315	KC2	1	0
42	f	804	BCR	3	0
39	A	311	CLA	2	0
43	O	304	DD6	1	0
39	Q	314	CLA	2	0
39	V	316	CLA	10	0
39	7	314	CLA	5	0
49	2	313	KC2	1	0
39	R	316	CLA	2	0
39	b	839	CLA	3	0
39	A	305	CLA	1	0
43	z	305	DD6	1	0
39	X	317	CLA	3	0
39	P	316	CLA	1	0
47	M	301	SQD	3	0
43	5	303	DD6	1	0
39	O	316	CLA	1	0
39	C	307	CLA	2	0
39	5	316	CLA	2	0
39	P	308	CLA	5	0
39	9	307	CLA	1	0
39	b	824	CLA	4	0
39	b	840	CLA	4	0
39	Y	305	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	S	322	LMG	20	0
39	a	811	CLA	5	0
39	U	215	CLA	1	0
49	X	312	KC2	1	0
39	E	318	CLA	1	0
50	x	302	A1EB1	2	0
39	a	809	CLA	3	0
39	a	837	CLA	1	0
39	x	317	CLA	1	0
39	0	312	CLA	8	0
39	M	309	CLA	2	0
39	I	308	CLA	3	0
49	3	317	KC2	1	0
49	8	316	KC2	1	0
39	b	821	CLA	2	0
39	8	313	CLA	1	0
39	x	306	CLA	1	0
41	j	104	LHG	1	0
42	l	207	BCR	4	0
50	0	307	A1EB1	2	0
42	l	206	BCR	1	0
39	E	314	CLA	5	0
39	E	315	CLA	2	0
39	3	322	CLA	2	0
39	D	311	CLA	2	0
39	6	313	CLA	1	0
39	b	810	CLA	3	0
39	V	310	CLA	5	0
39	2	316	CLA	1	0
39	b	830	CLA	3	0
43	M	304	DD6	2	0
46	Q	322	LMG	2	0
39	8	321	CLA	1	0
39	o	206	CLA	2	0
46	F	317	LMG	15	0
46	7	326	LMG	2	0
48	L	304	A86	4	0
39	k	201	CLA	2	0
39	C	305	CLA	1	0
39	b	813	CLA	2	0
39	b	820	CLA	3	0
39	V	311	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	5	308	CLA	2	0
39	7	324	CLA	4	0
39	F	313	CLA	3	0
39	b	814	CLA	2	0
39	2	318	CLA	1	0
49	R	312	KC2	1	0
39	i	103	CLA	6	0
39	C	308	CLA	3	0
39	b	802	CLA	1	0
43	Q	303	DD6	5	0
39	a	821	CLA	2	0
49	R	314	KC2	15	0
39	D	312	CLA	2	0
48	9	303	A86	1	0
39	Z	309	CLA	1	0
39	1	310	CLA	1	0
39	a	829	CLA	2	0
48	Q	302	A86	2	0
39	b	823	CLA	1	0
51	T	317	A1ECV	1	0
39	6	321	CLA	1	0
46	4	325	LMG	2	0
39	O	310	CLA	4	0
39	O	308	CLA	1	0
39	b	834	CLA	2	0
39	B	206	CLA	1	0
39	T	320	CLA	2	0
39	b	831	CLA	2	0
39	D	319	CLA	3	0
39	0	313	CLA	2	0
39	D	318	CLA	5	0
39	a	802	CLA	2	0
39	b	812	CLA	3	0
39	b	829	CLA	2	0
39	b	841	CLA	4	0
39	b	805	CLA	3	0
48	7	312	A86	1	0
39	C	311	CLA	1	0
46	4	326	LMG	33	0
39	3	314	CLA	3	0
39	a	835	CLA	3	0
43	3	304	DD6	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	a	801	CLA	6	0
39	9	312	CLA	4	0
47	D	321	SQD	2	0
39	X	307	CLA	2	0
39	G	318	CLA	1	0
39	i	101	CLA	4	0
39	2	308	CLA	1	0
39	L	310	CLA	2	0
39	b	809	CLA	5	0
39	H	313	CLA	2	0
43	4	308	DD6	1	0
39	8	310	CLA	3	0
39	D	313	CLA	1	0
39	H	308	CLA	2	0
42	a	842	BCR	5	0
39	b	808	CLA	1	0
39	E	317	CLA	3	0
39	J	314	CLA	3	0
49	L	315	KC2	1	0
39	C	306	CLA	2	0
43	O	305	DD6	1	0
39	4	316	CLA	1	0
39	D	315	CLA	1	0
39	F	316	CLA	2	0
39	M	310	CLA	3	0
39	a	827	CLA	2	0
39	b	851	CLA	4	0
39	W	311	CLA	2	0
49	F	307	KC2	1	0
50	9	302	A1EB1	1	0
46	D	322	LMG	1	0
39	a	804	CLA	2	0
39	F	321	CLA	1	0
39	E	310	CLA	4	0
39	7	318	CLA	3	0
42	k	204	BCR	2	0
39	K	307	CLA	1	0
39	R	307	CLA	2	0
39	b	842	CLA	2	0
39	4	312	CLA	2	0
39	9	308	CLA	3	0
39	x	311	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	l	204	CLA	1	0
51	7	323	A1ECV	4	0
39	W	313	CLA	2	0
39	a	806	CLA	1	0
49	5	313	KC2	26	0
43	H	303	DD6	1	0
51	9	317	A1ECV	2	0
39	a	812	CLA	1	0
39	W	309	CLA	2	0
39	I	309	CLA	2	0
39	Q	309	CLA	2	0
41	a	840	LHG	3	0
39	X	311	CLA	1	0
39	D	317	CLA	5	0
39	S	311	CLA	5	0
48	U	206	A86	1	0
39	K	312	CLA	2	0
46	F	320	LMG	7	0
47	F	319	SQD	1	0
39	3	320	CLA	1	0
47	T	321	SQD	1	0
39	B	209	CLA	4	0
39	a	813	CLA	3	0
39	7	313	CLA	2	0
39	1	313	CLA	2	0
49	M	313	KC2	1	0
42	b	850	BCR	5	0
39	E	308	CLA	1	0
39	U	209	CLA	1	0
39	S	308	CLA	2	0
39	F	312	CLA	1	0
39	8	311	CLA	2	0
41	X	301	LHG	2	0
43	7	310	DD6	5	0
39	b	817	CLA	3	0
39	a	822	CLA	5	0
48	5	301	A86	2	0
46	0	324	LMG	4	0
42	a	843	BCR	4	0
39	R	308	CLA	1	0
49	T	315	KC2	2	0
39	b	801	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	I	301	CLA	3	0
43	F	303	DD6	6	0
39	3	312	CLA	4	0
47	P	301	SQD	1	0
42	a	845	BCR	5	0
39	B	204	CLA	1	0
39	y	310	CLA	1	0
42	b	847	BCR	4	0
39	F	308	CLA	3	0
39	4	323	CLA	7	0
39	5	306	CLA	2	0
39	T	313	CLA	2	0
39	b	827	CLA	7	0
39	b	837	CLA	1	0
39	b	825	CLA	2	0
50	2	304	A1EB1	1	0
39	a	832	CLA	1	0
39	I	311	CLA	1	0
51	0	321	A1ECV	2	0
39	k	203	CLA	1	0
49	O	317	KC2	1	0
40	a	839	PQN	4	0
39	R	311	CLA	1	0
39	F	310	CLA	1	0
39	M	317	CLA	2	0
39	S	319	CLA	2	0
39	f	803	CLA	1	0
39	x	307	CLA	2	0
39	a	830	CLA	4	0
39	A	312	CLA	1	0
42	b	845	BCR	3	0
42	h	202	BCR	4	0
39	V	319	CLA	1	0
39	P	309	CLA	1	0
39	b	835	CLA	1	0
39	J	318	CLA	2	0
39	0	311	CLA	3	0
50	4	304	A1EB1	1	0
39	7	316	CLA	4	0
48	D	305	A86	1	0
39	J	307	CLA	1	0
39	Q	310	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	1	308	CLA	2	0
39	b	838	CLA	4	0
47	S	301	SQD	4	0
51	2	311	A1ECV	1	0
39	a	825	CLA	7	0
47	D	320	SQD	2	0
39	a	836	CLA	6	0
39	b	826	CLA	7	0
39	V	313	CLA	5	0
46	l	208	LMG	4	0
39	a	807	CLA	3	0
43	2	303	DD6	1	0
51	y	311	A1ECV	1	0
39	Z	306	CLA	1	0
52	P	318	A1EB4	3	0
39	0	315	CLA	2	0
39	W	318	CLA	1	0
39	D	314	CLA	2	0
43	F	305	DD6	1	0
39	C	304	CLA	1	0
39	b	803	CLA	2	0
49	0	314	KC2	2	0
43	D	306	DD6	1	0
39	T	319	CLA	1	0
46	P	317	LMG	5	0
39	a	847	CLA	2	0
49	W	314	KC2	2	0
47	4	327	SQD	1	0
39	j	101	CLA	5	0
39	b	815	CLA	4	0
39	z	306	CLA	1	0
47	H	318	SQD	3	0
42	b	844	BCR	2	0
52	W	321	A1EB4	1	0
39	a	838	CLA	3	0
39	l	201	CLA	3	0
39	A	315	CLA	2	0
39	E	312	CLA	3	0
42	a	844	BCR	3	0
39	6	310	CLA	1	0
39	M	312	CLA	4	0
39	z	311	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	7	319	KC2	1	0
39	L	311	CLA	2	0
39	b	818	CLA	3	0
49	x	312	KC2	1	0
39	F	309	CLA	1	0
39	T	311	CLA	1	0
39	D	309	CLA	1	0
39	H	306	CLA	3	0
42	f	801	BCR	3	0
41	H	317	LHG	3	0
39	Z	316	CLA	1	0
46	A	316	LMG	1	0
39	S	320	CLA	3	0
39	2	309	CLA	1	0
39	V	309	CLA	2	0
39	T	308	CLA	9	0
52	R	305	A1EB4	1	0
52	5	304	A1EB4	1	0
43	1	304	DD6	2	0
50	H	304	A1EB1	1	0
50	F	304	A1EB1	4	0
39	J	309	CLA	3	0
39	4	314	CLA	4	0
49	P	310	KC2	1	0
43	E	303	DD6	1	0
39	K	311	CLA	1	0
47	k	205	SQD	2	0
39	y	307	CLA	1	0
52	P	319	A1EB4	2	0
39	T	318	CLA	1	0
39	I	315	CLA	1	0
39	B	207	CLA	2	0
49	5	305	KC2	1	0
39	b	828	CLA	6	0
39	b	819	CLA	1	0
39	W	310	CLA	7	0
45	b	849	DGD	3	0
39	X	308	CLA	4	0
39	x	308	CLA	1	0
39	Q	320	CLA	1	0
39	o	201	CLA	2	0
48	Z	303	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	o	205	CLA	2	0
39	K	314	CLA	1	0
39	H	310	CLA	3	0
39	b	832	CLA	5	0
39	a	815	CLA	4	0
49	X	314	KC2	19	0
50	0	303	A1EB1	2	0
52	W	306	A1EB4	4	0
39	O	309	CLA	1	0
39	D	310	CLA	2	0
39	S	313	CLA	4	0
39	9	319	CLA	2	0
47	W	301	SQD	1	0
48	F	301	A86	1	0
42	l	202	BCR	5	0
46	M	319	LMG	10	0
48	Q	301	A86	1	0
50	S	303	A1EB1	1	0
39	a	831	CLA	4	0
39	A	306	CLA	3	0
48	Q	304	A86	28	0
43	A	302	DD6	1	0
41	D	302	LHG	3	0
39	f	802	CLA	1	0
48	l	307	A86	1	0
49	Y	308	KC2	1	0
39	H	309	CLA	2	0
39	E	316	CLA	1	0
39	Q	321	CLA	3	0
39	S	309	CLA	2	0
42	b	848	BCR	5	0
39	7	325	CLA	1	0
51	l	318	A1ECV	1	0
39	l	203	CLA	2	0
39	L	308	CLA	3	0
39	G	309	CLA	1	0
42	i	102	BCR	6	0
42	m	101	BCR	5	0
49	F	311	KC2	8	0
39	b	833	CLA	3	0
42	j	103	BCR	1	0
39	K	306	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	J	305	DD6	1	0
46	W	302	LMG	14	0
39	a	816	CLA	7	0
51	7	317	A1ECV	2	0
50	z	302	A1EB1	1	0
46	I	302	LMG	1	0
49	V	315	KC2	1	0
47	7	302	SQD	1	0
39	A	314	CLA	3	0
39	a	818	CLA	3	0
39	A	309	CLA	1	0
48	E	304	A86	1	0
39	a	826	CLA	3	0
39	a	808	CLA	1	0
39	5	315	CLA	2	0
39	P	307	CLA	3	0
39	a	823	CLA	3	0
39	7	321	CLA	1	0
48	F	302	A86	8	0
49	6	316	KC2	1	0
39	G	310	CLA	1	0
39	E	313	CLA	2	0
39	M	308	CLA	1	0
39	a	814	CLA	2	0
39	O	313	CLA	1	0
39	a	820	CLA	2	0
39	X	309	CLA	2	0
51	z	316	A1ECV	1	0
39	J	311	CLA	4	0
39	b	806	CLA	1	0
39	0	310	CLA	2	0
43	S	306	DD6	1	0
48	R	302	A86	2	0
39	3	313	CLA	1	0
39	U	207	CLA	3	0
39	R	309	CLA	1	0
50	7	306	A1EB1	1	0
39	J	313	CLA	1	0
39	a	817	CLA	2	0
39	J	310	CLA	1	0
39	2	310	CLA	1	0
43	U	204	DD6	1	0

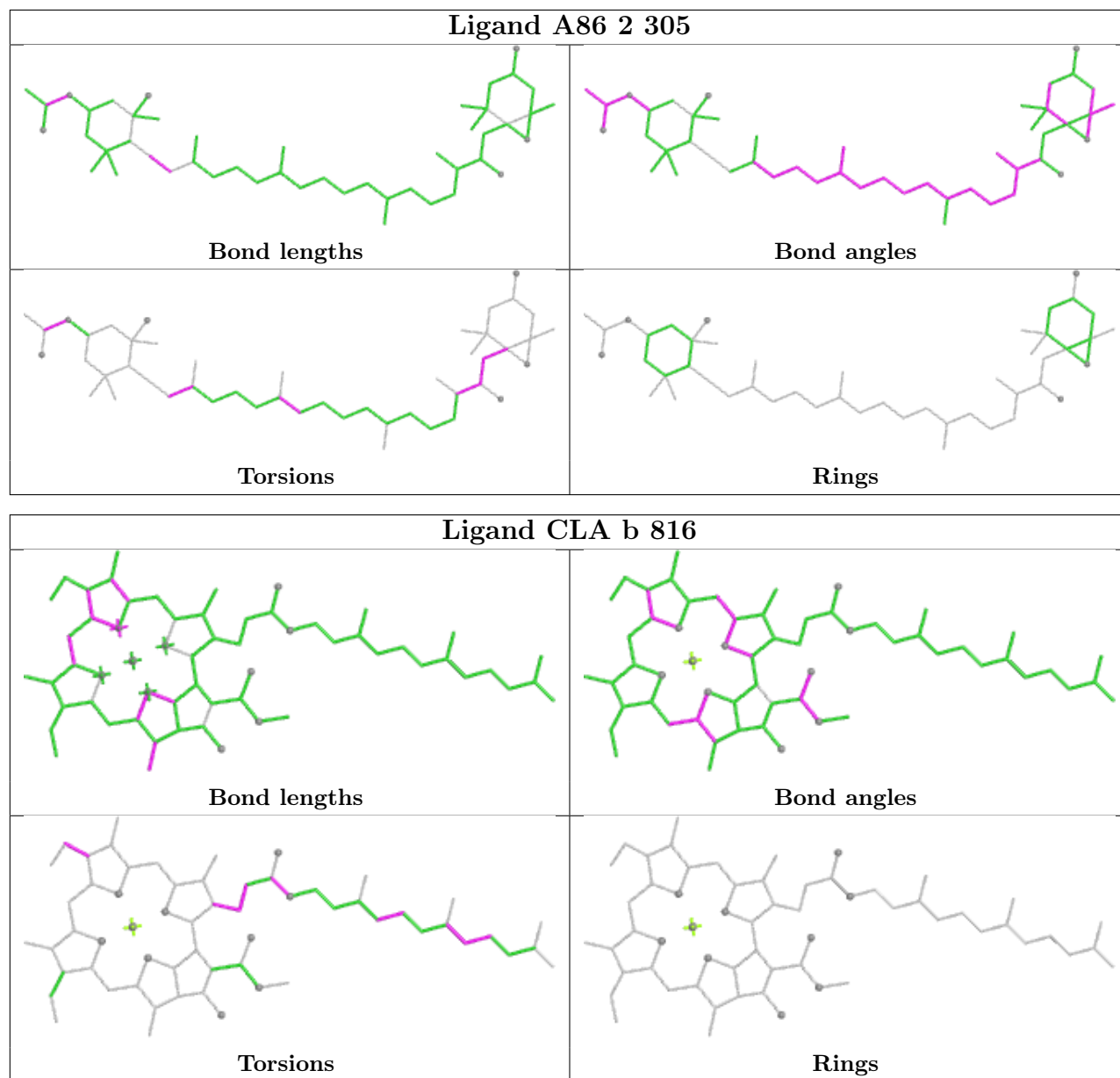
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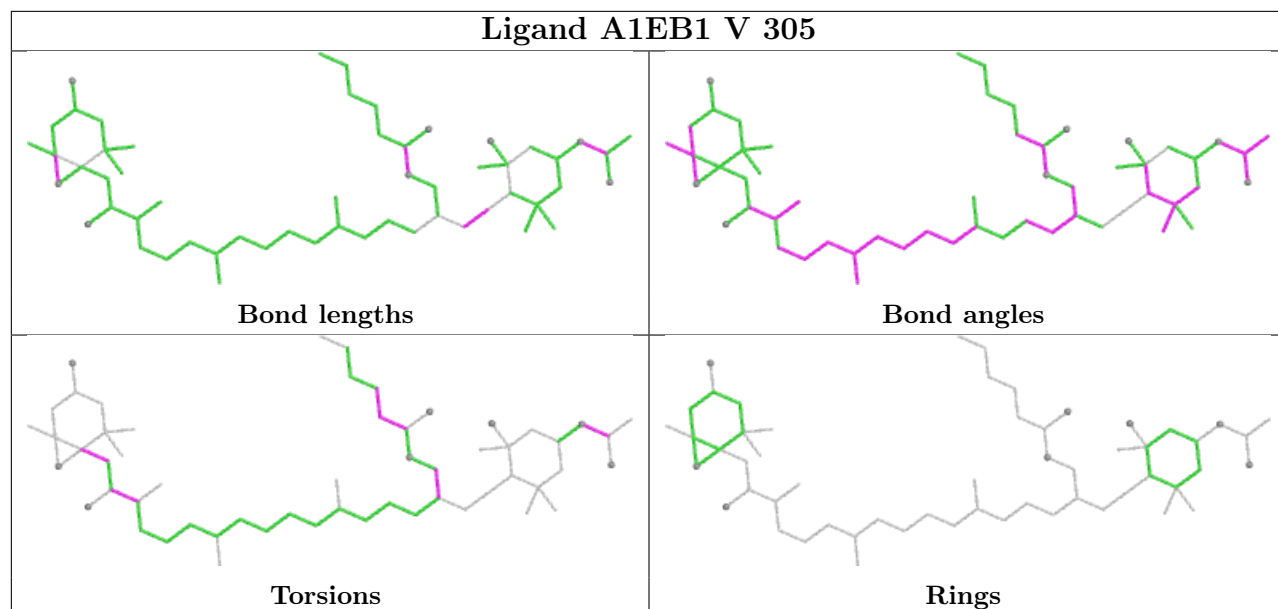
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	I	313	CLA	2	0
39	F	314	CLA	3	0
39	a	803	CLA	3	0
48	W	307	A86	1	0
39	Q	312	CLA	1	0
39	3	311	CLA	2	0
39	a	824	CLA	5	0
39	L	313	CLA	1	0
39	U	201	CLA	1	0
43	I	306	DD6	1	0
40	b	843	PQN	3	0
46	S	321	LMG	3	0
39	b	811	CLA	2	0
39	1	309	CLA	1	0
43	P	304	DD6	2	0
39	C	310	CLA	3	0
42	b	846	BCR	4	0
39	Y	313	CLA	1	0
47	9	322	SQD	1	0
51	x	310	A1ECV	1	0
49	4	324	KC2	1	0
39	l	205	CLA	7	0
39	b	822	CLA	2	0
48	W	304	A86	5	0
39	H	312	CLA	2	0
39	b	807	CLA	3	0
48	I	304	A86	1	0
39	U	208	CLA	2	0
49	P	312	KC2	2	0
39	Q	311	CLA	3	0
46	7	301	LMG	20	0
39	K	308	CLA	1	0
39	K	309	CLA	1	0
51	Y	306	A1ECV	1	0
39	H	316	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

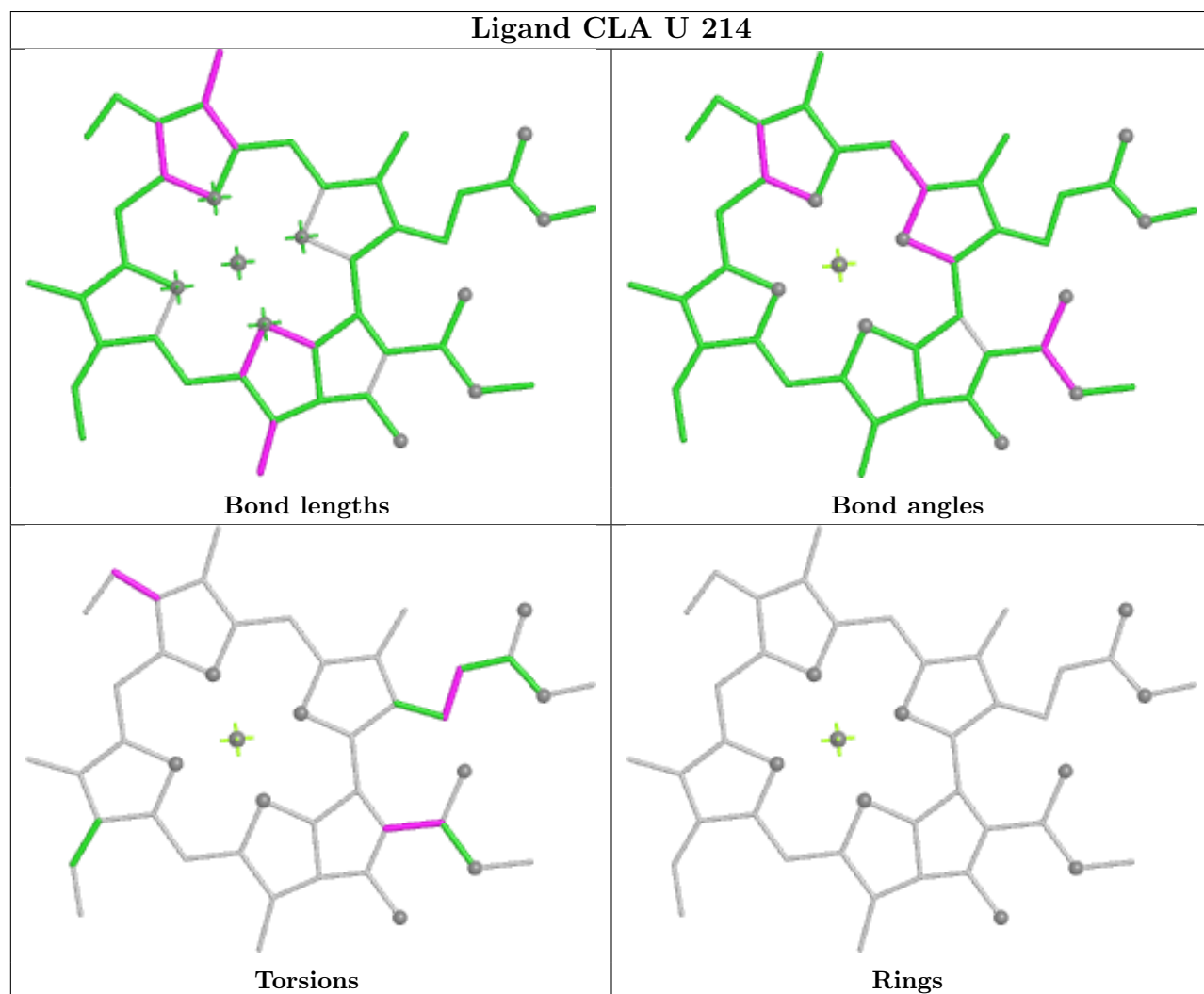
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



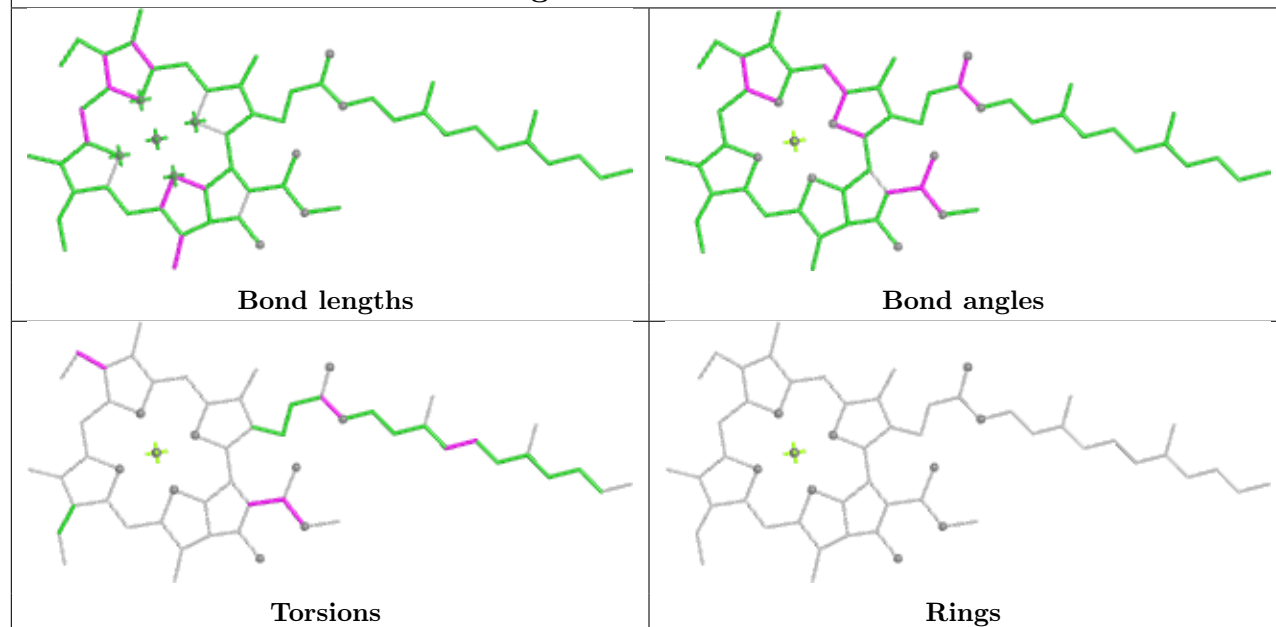
Ligand A1EB1 V 305



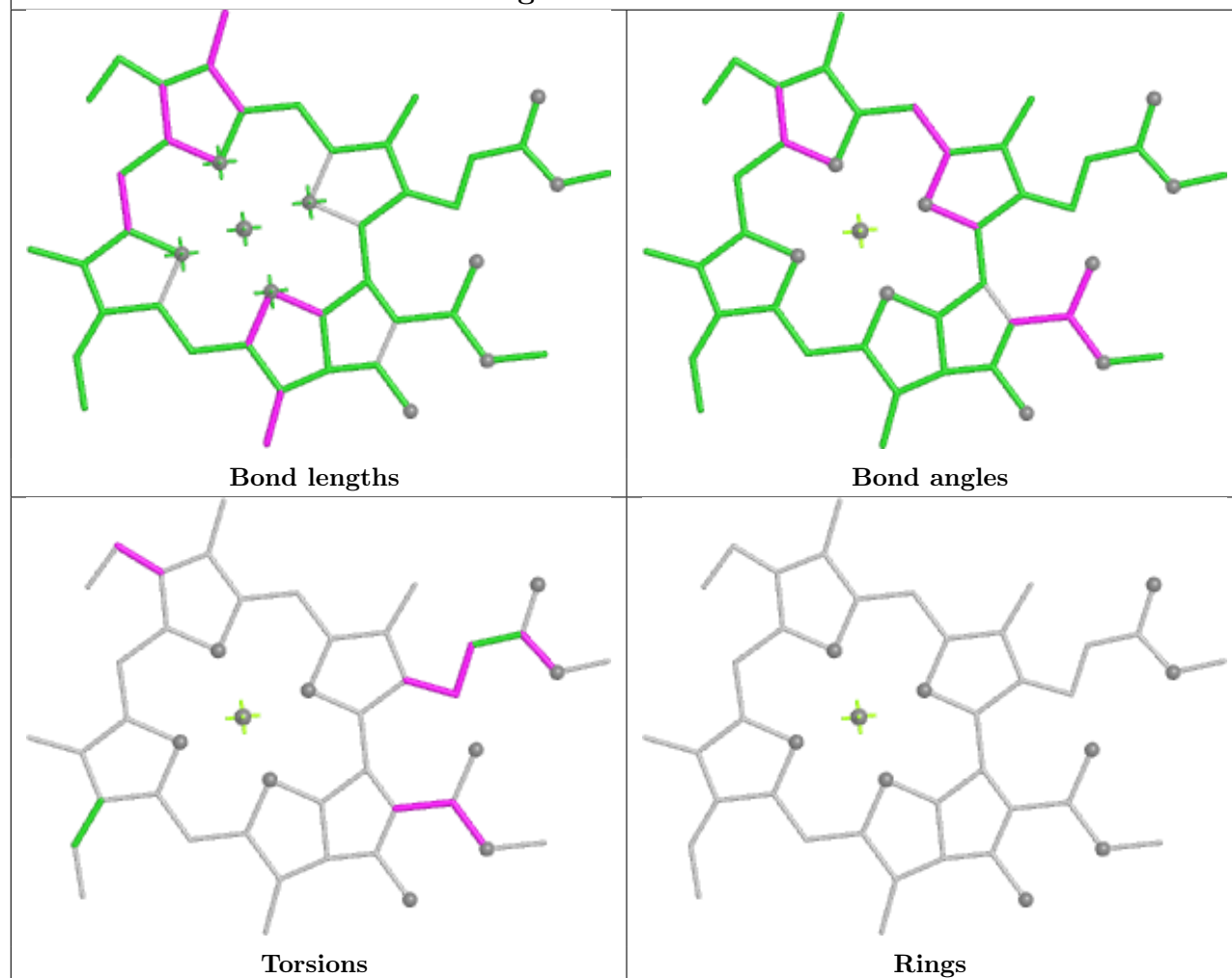
Ligand CLA U 214

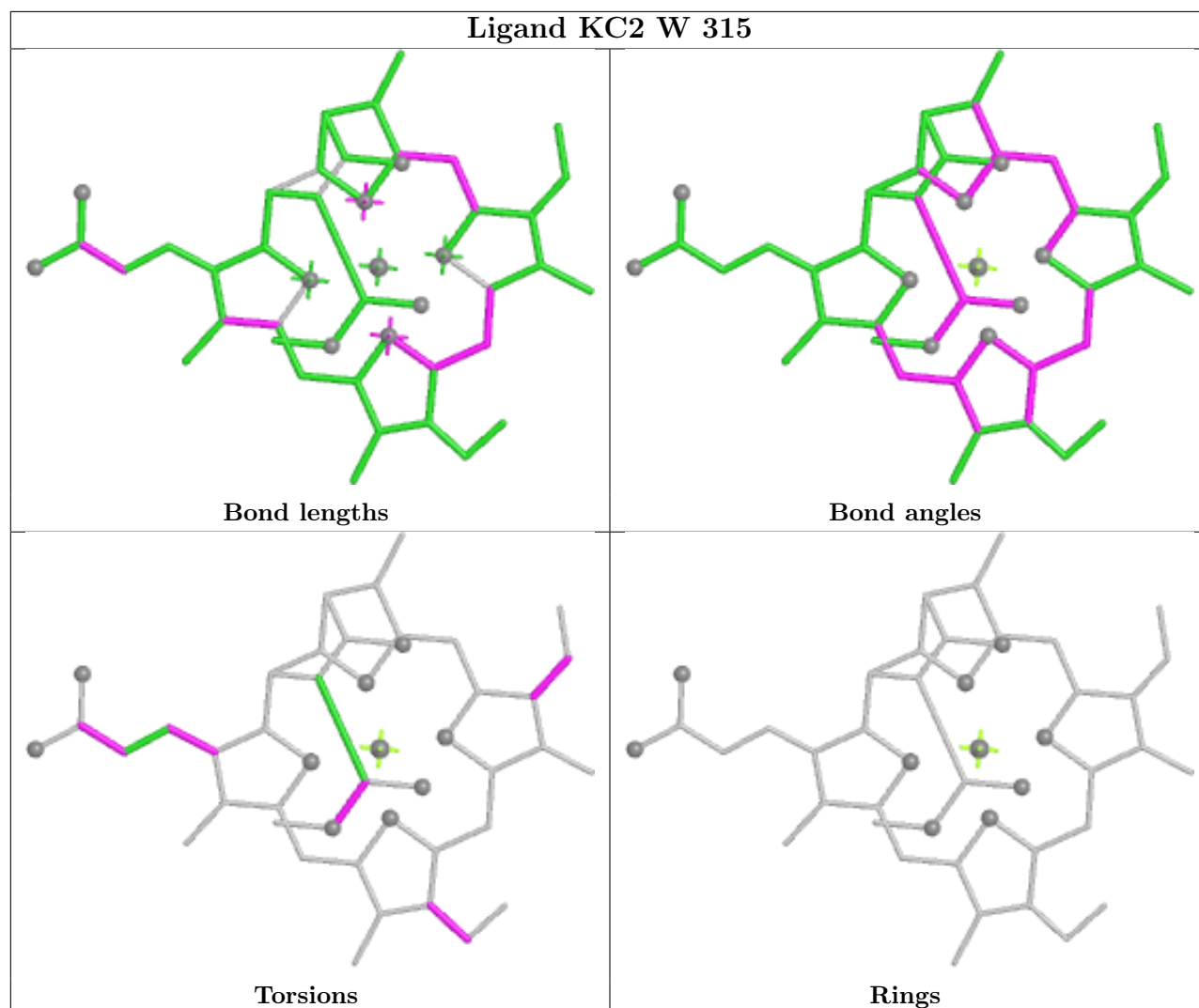
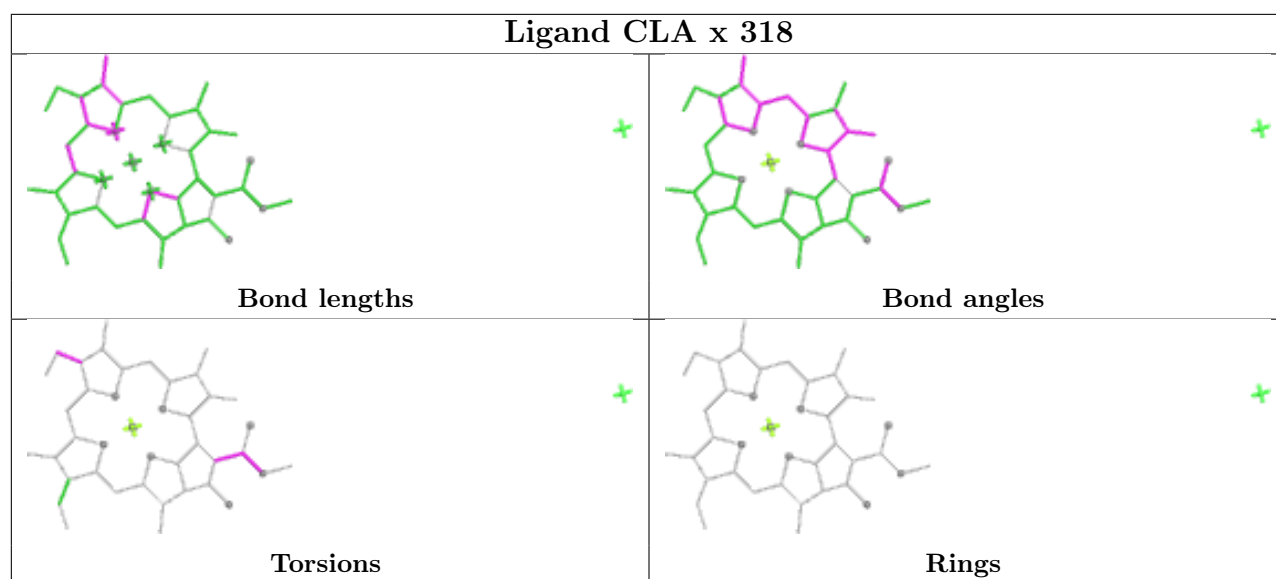


Ligand CLA G 314

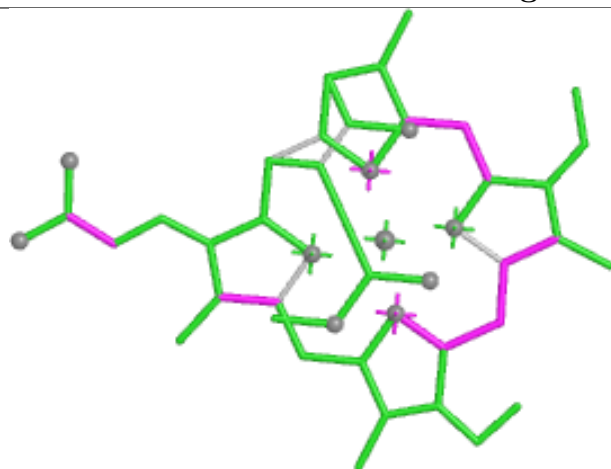


Ligand CLA 0 323

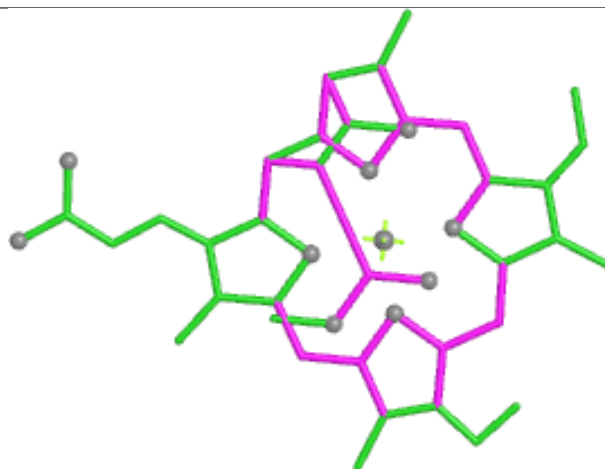




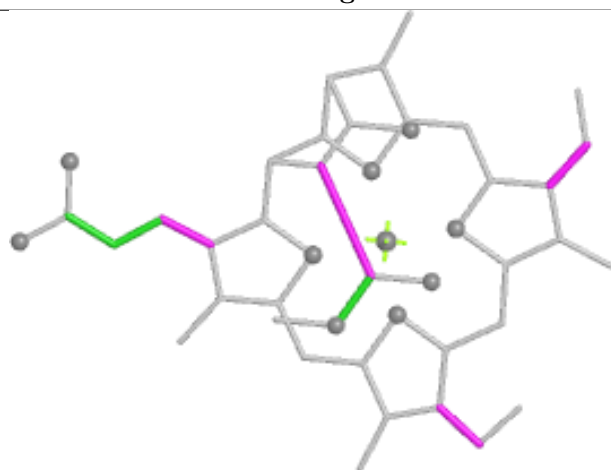
Ligand KC2 9 311



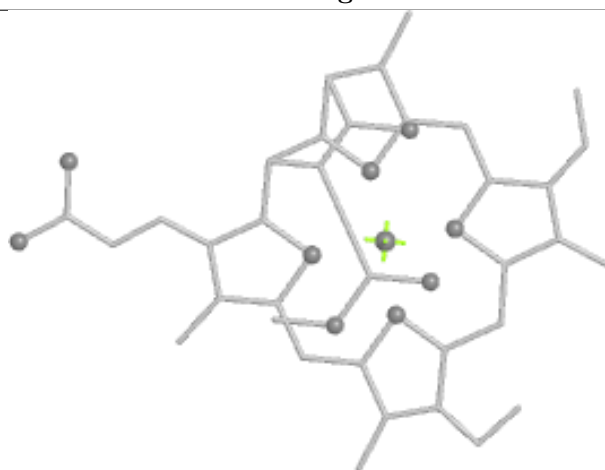
Bond lengths



Bond angles

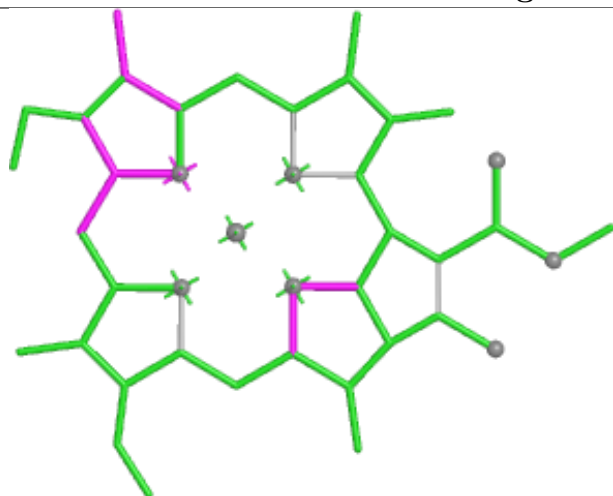


Torsions



Rings

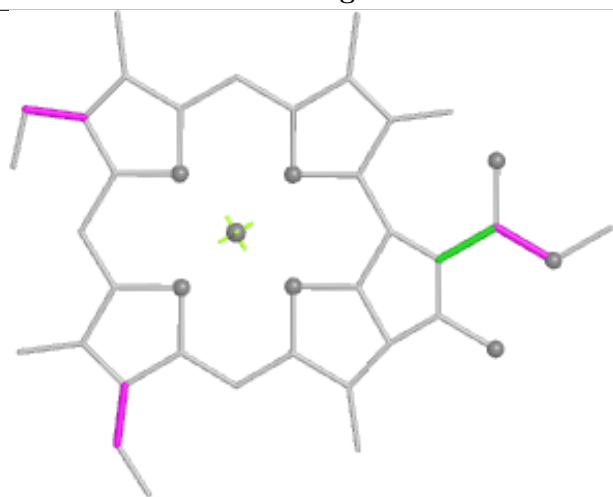
Ligand CLA Z 313



Bond lengths



Bond angles

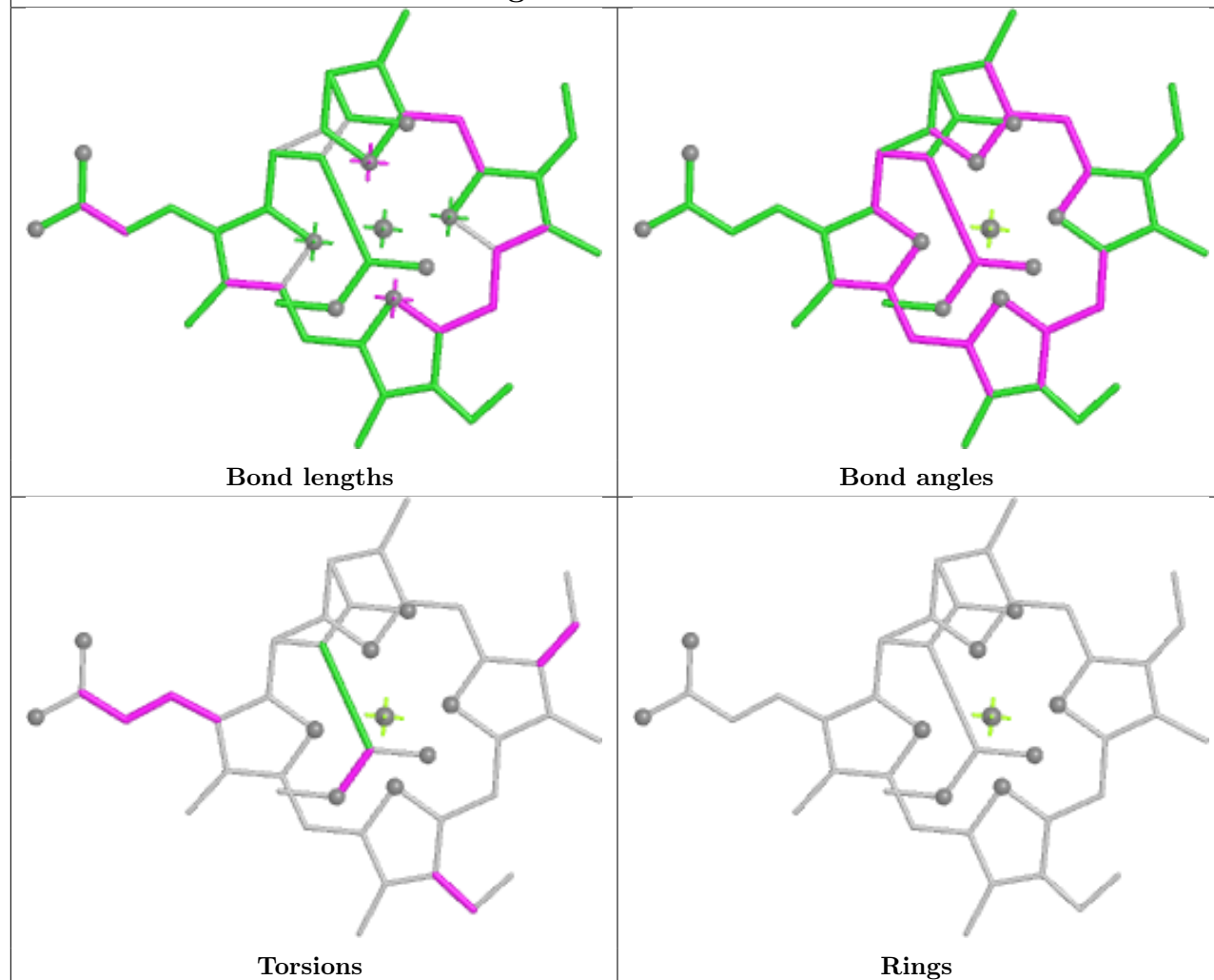


Torsions

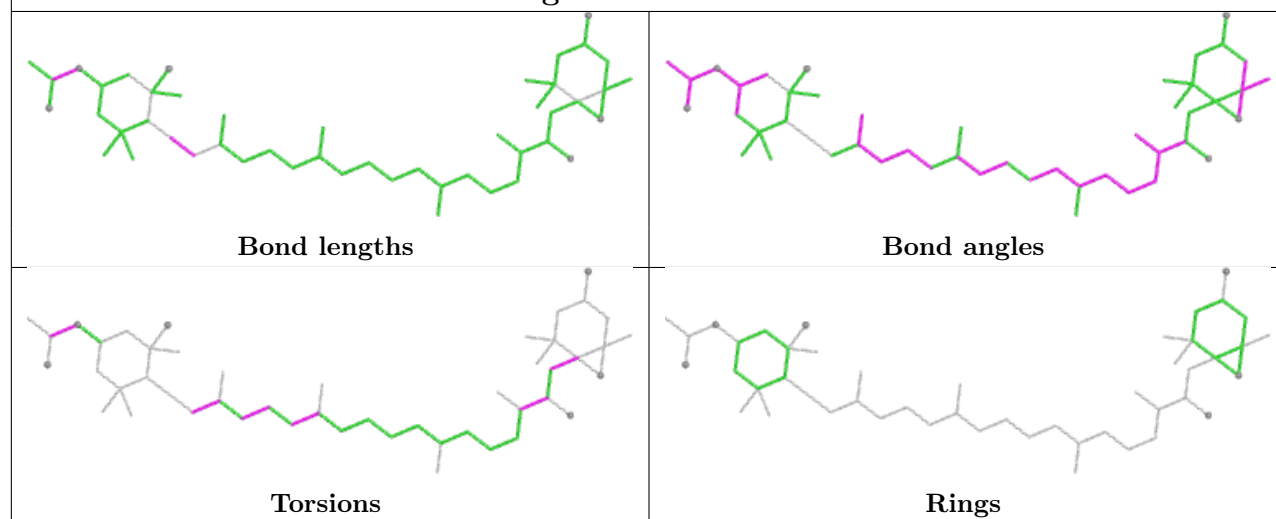


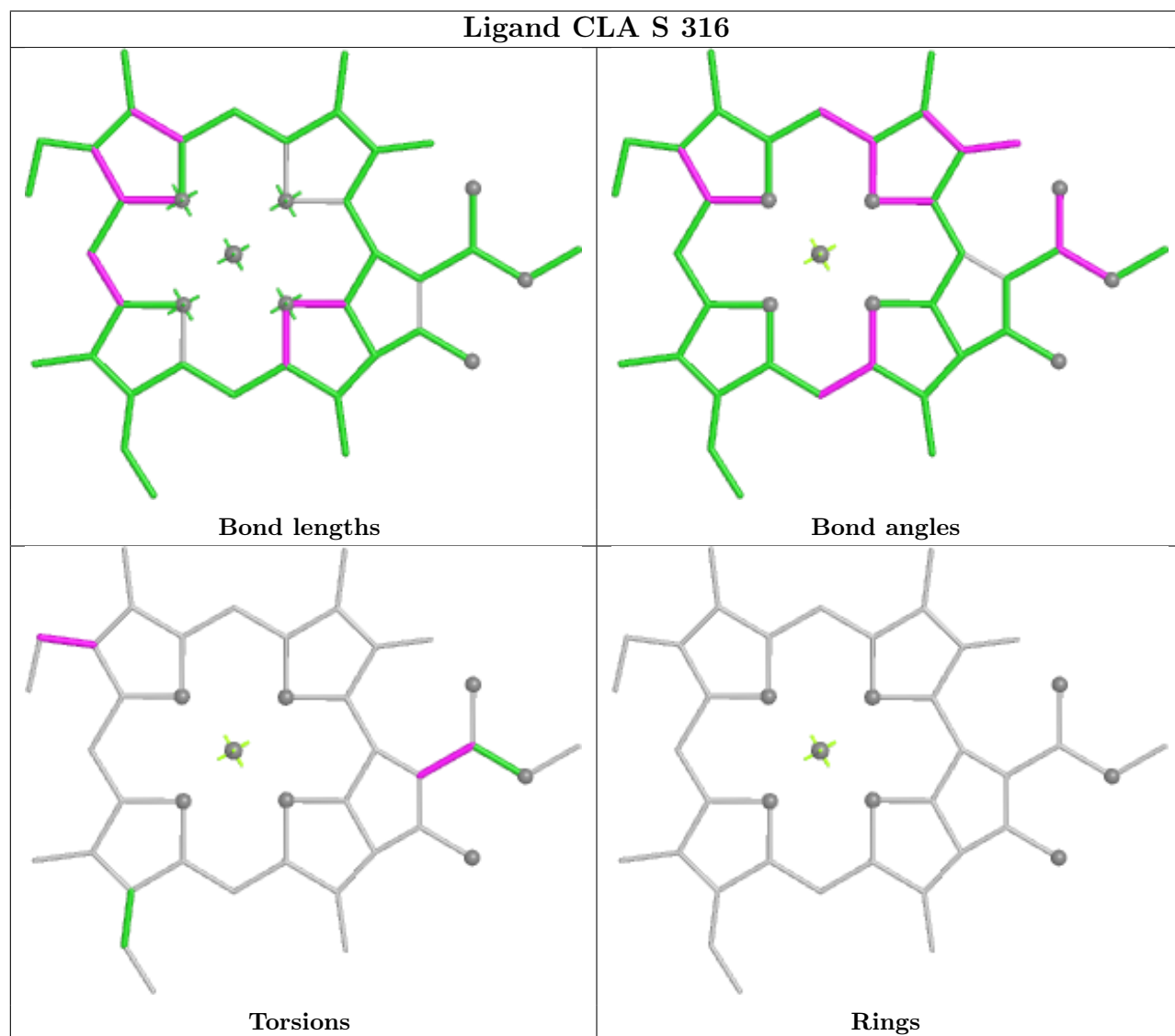
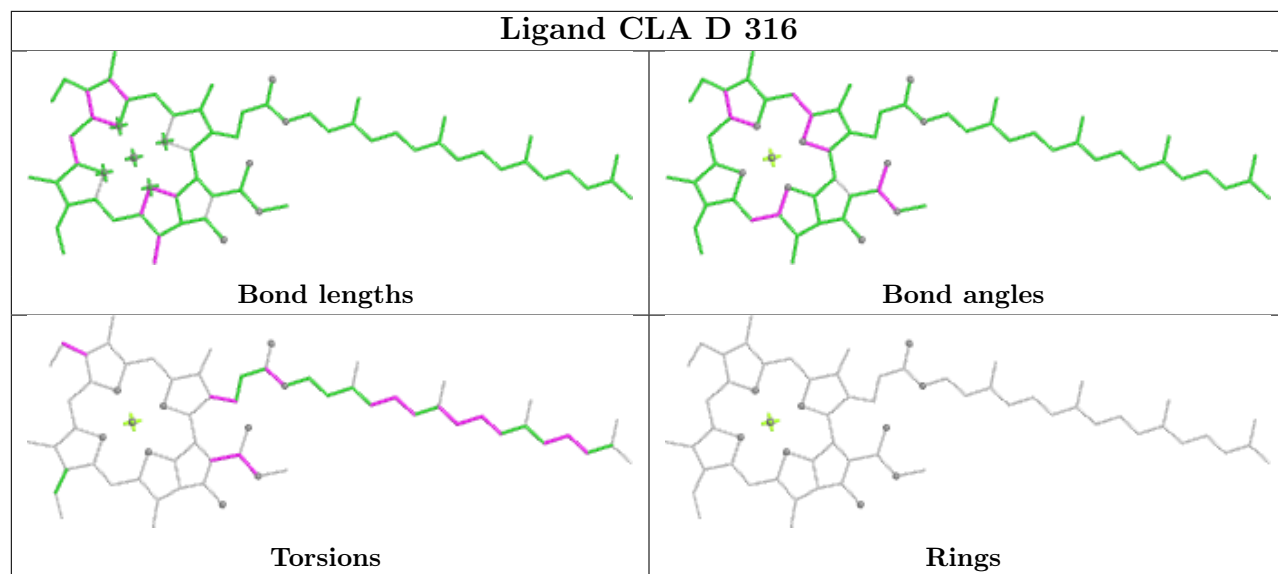
Rings

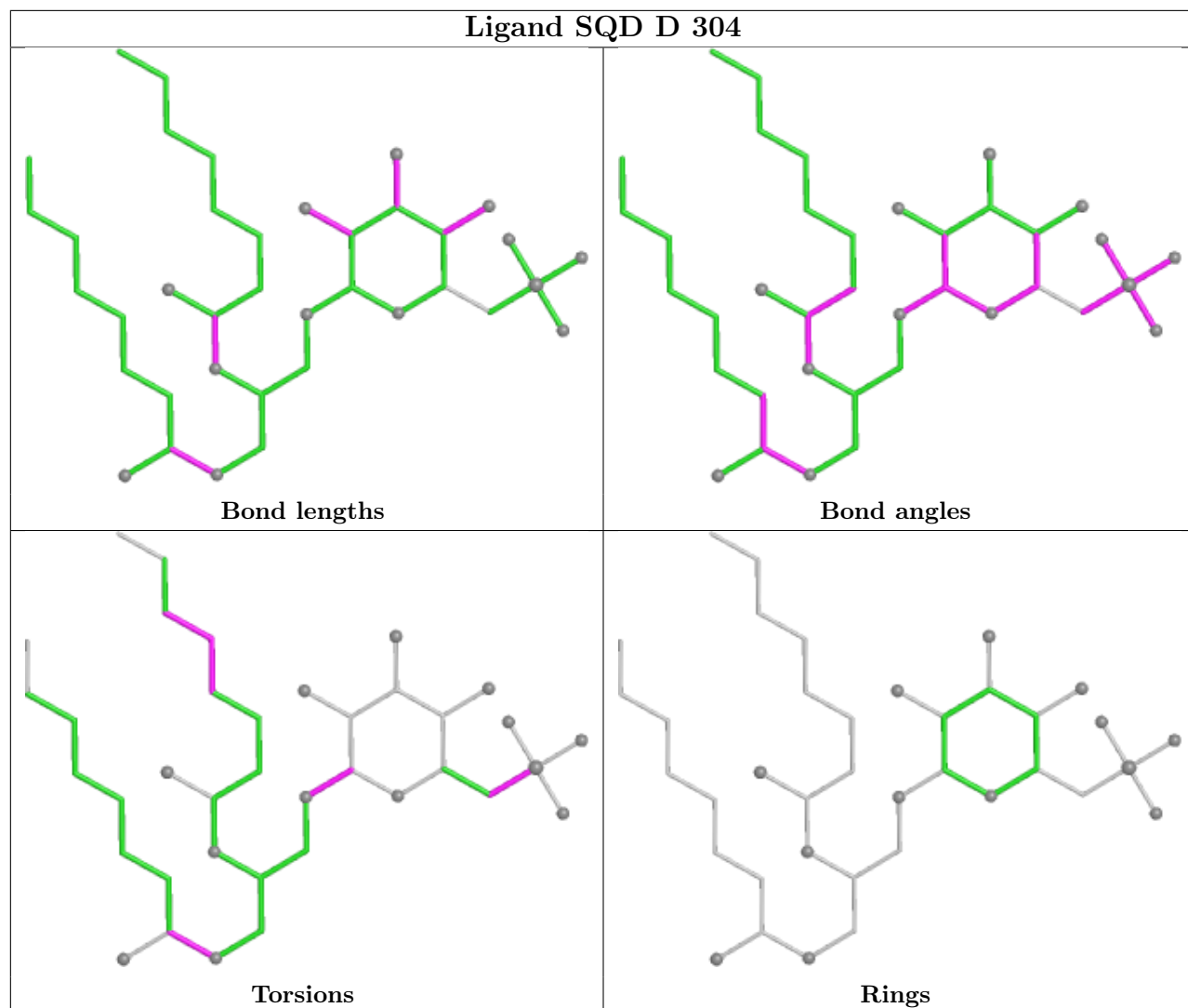
Ligand KC2 C 312

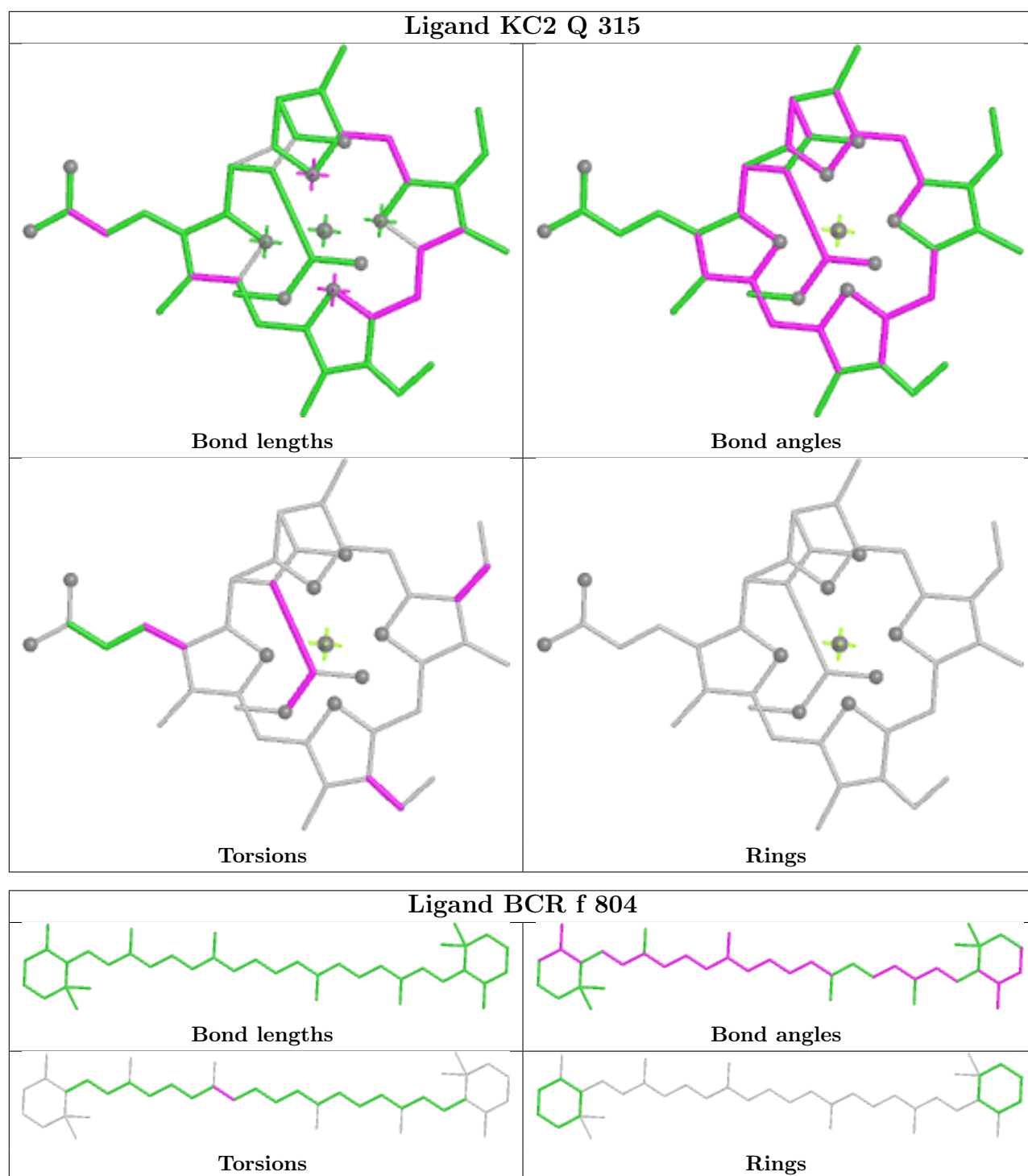


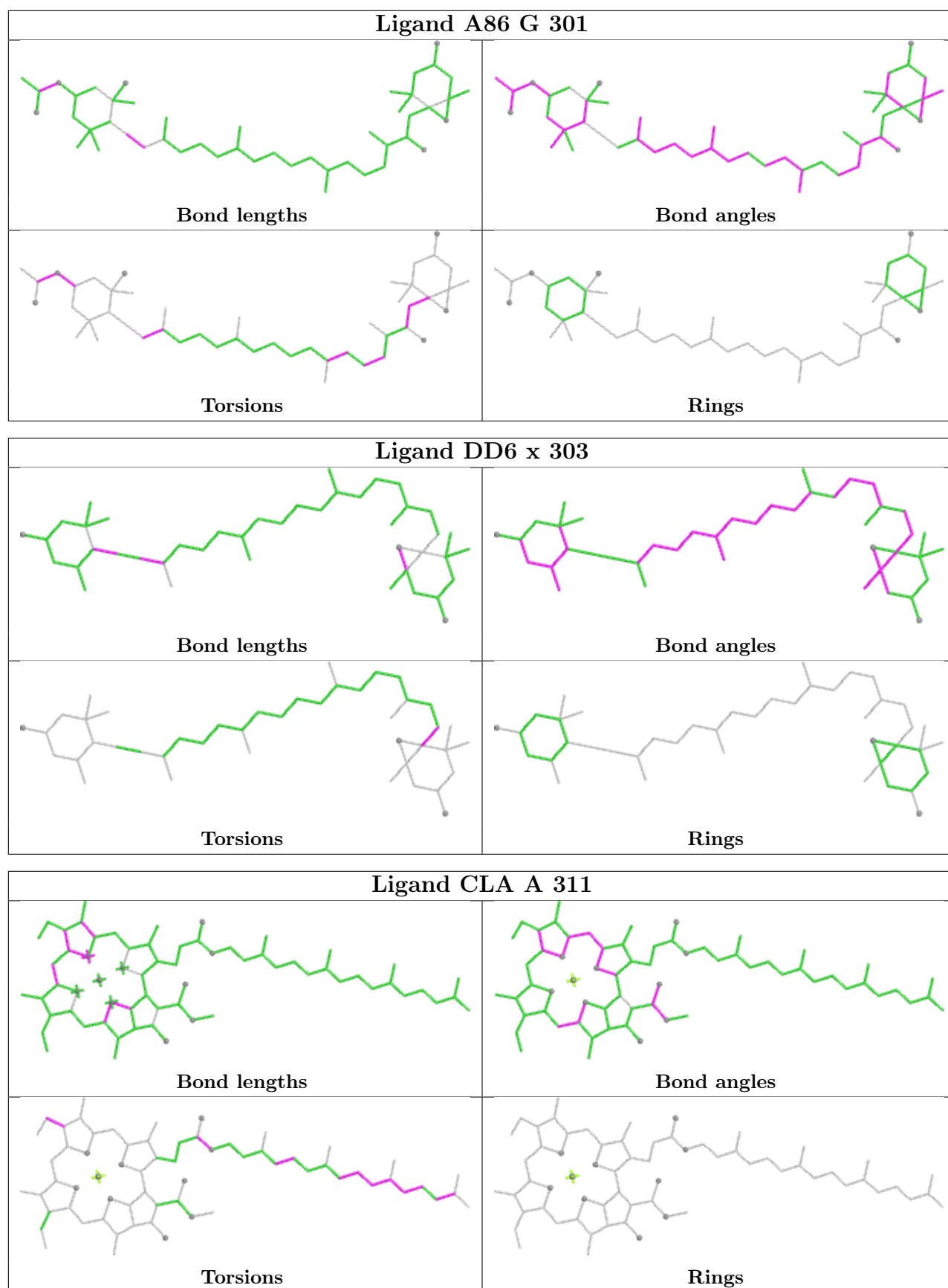
Ligand A86 0 304

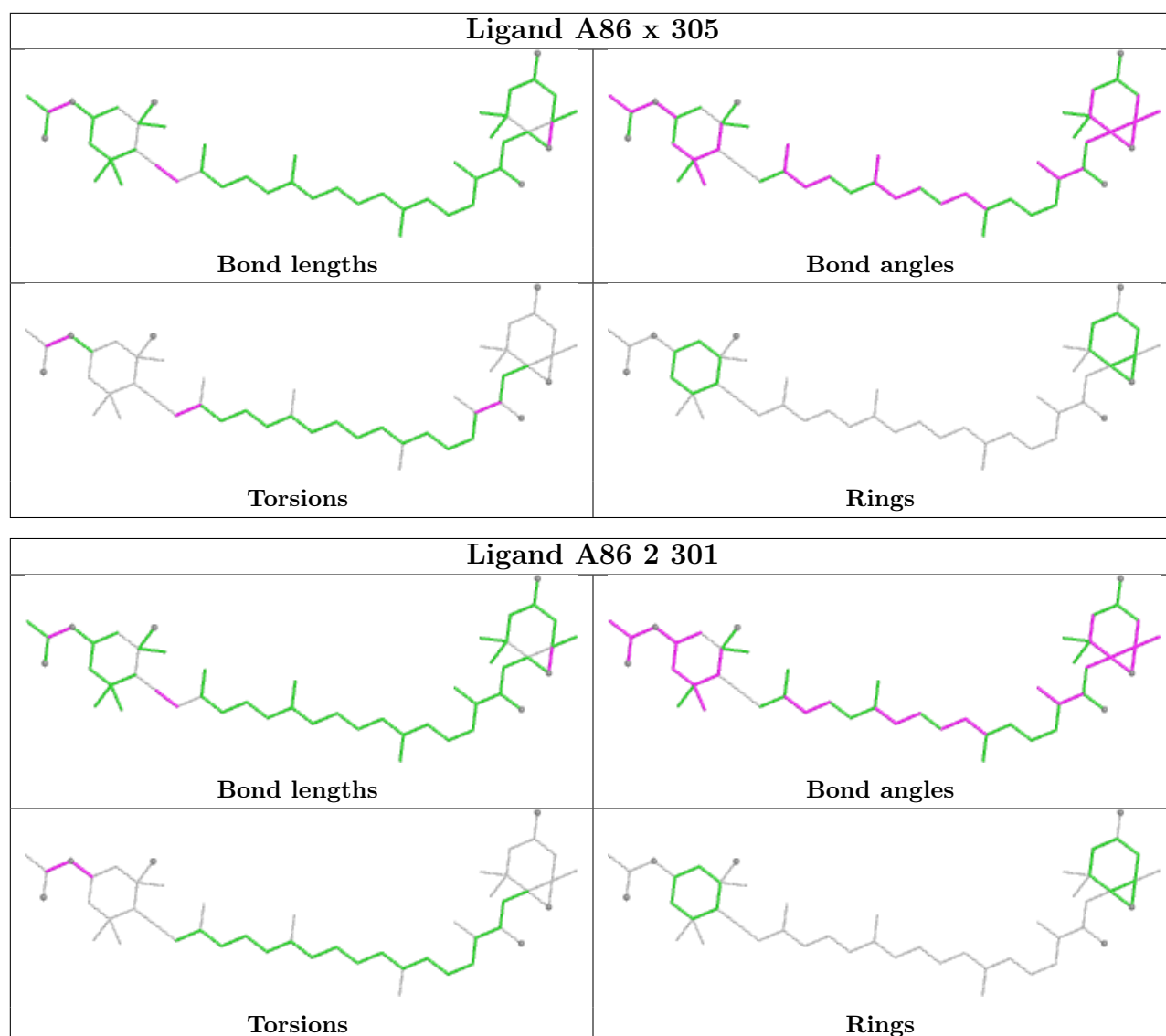




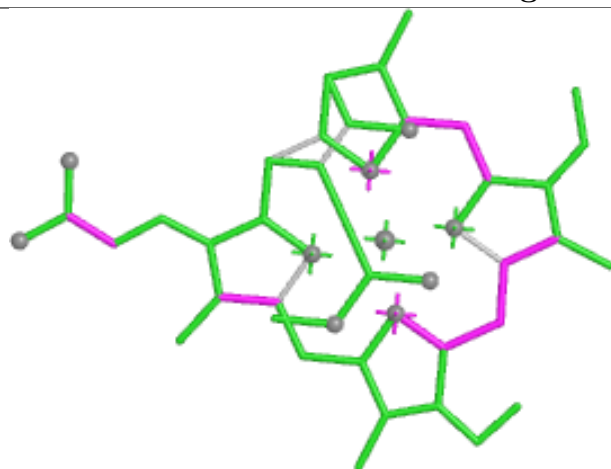




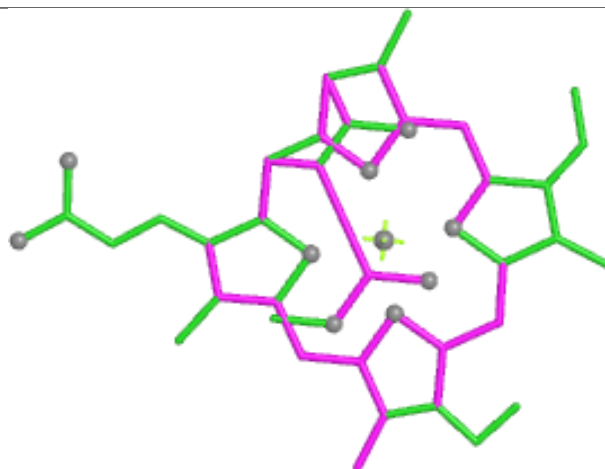




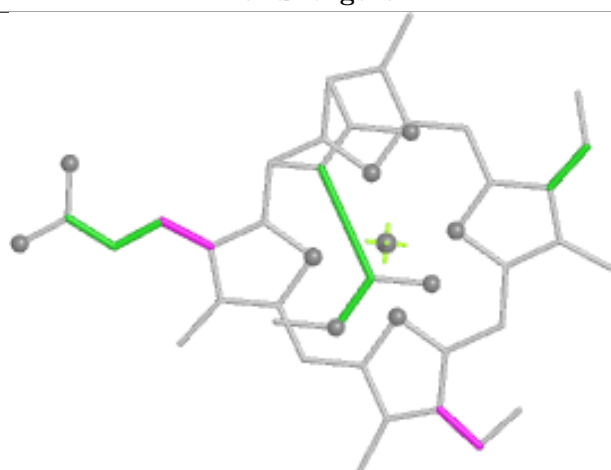
Ligand KC2 0 316



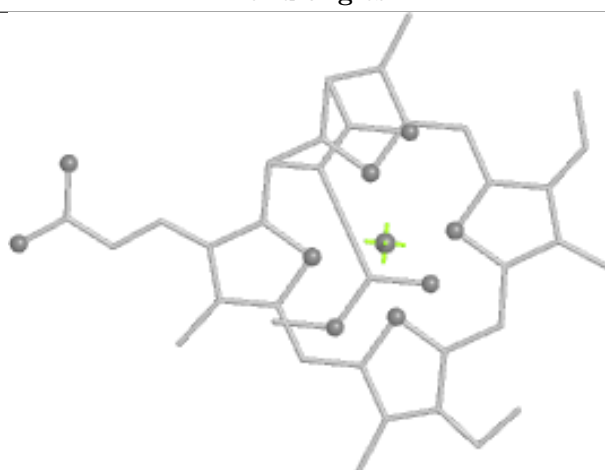
Bond lengths



Bond angles

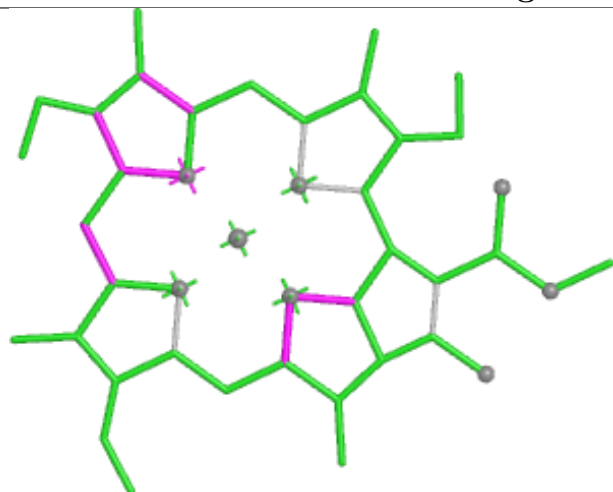


Torsions

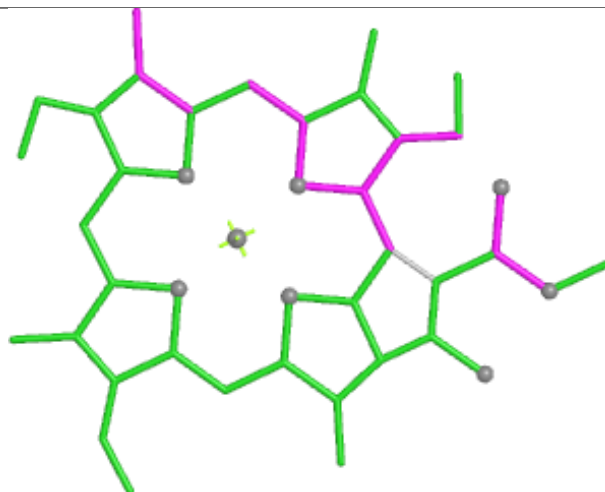


Rings

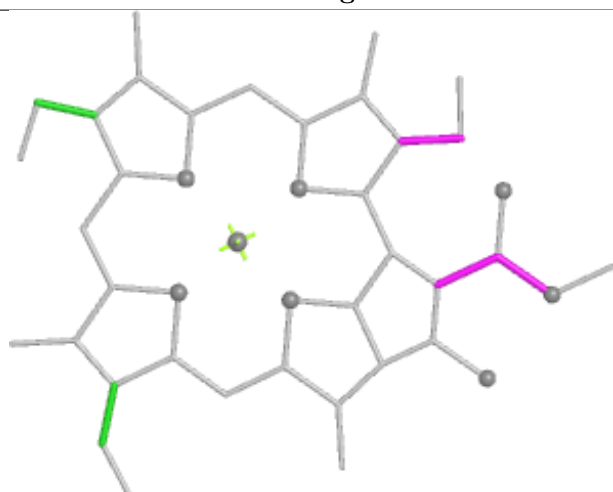
Ligand CLA S 310



Bond lengths



Bond angles

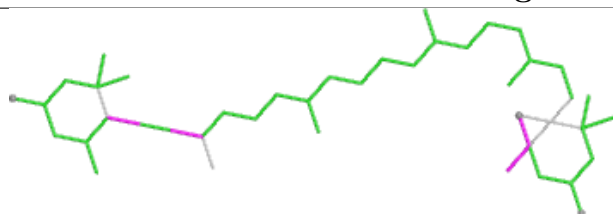


Torsions

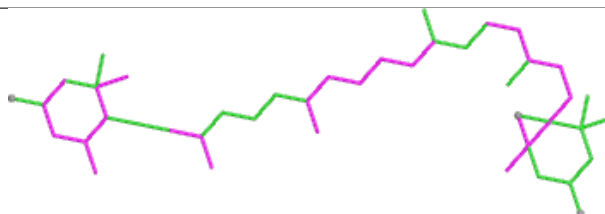


Rings

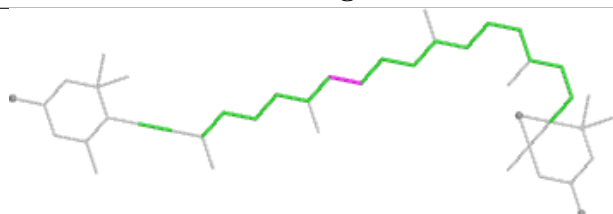
Ligand DD6 O 304



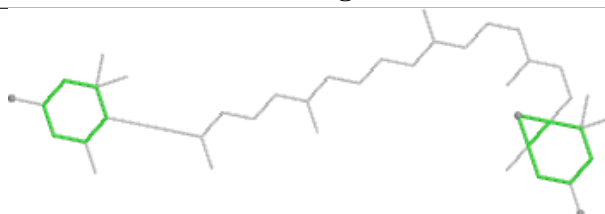
Bond lengths



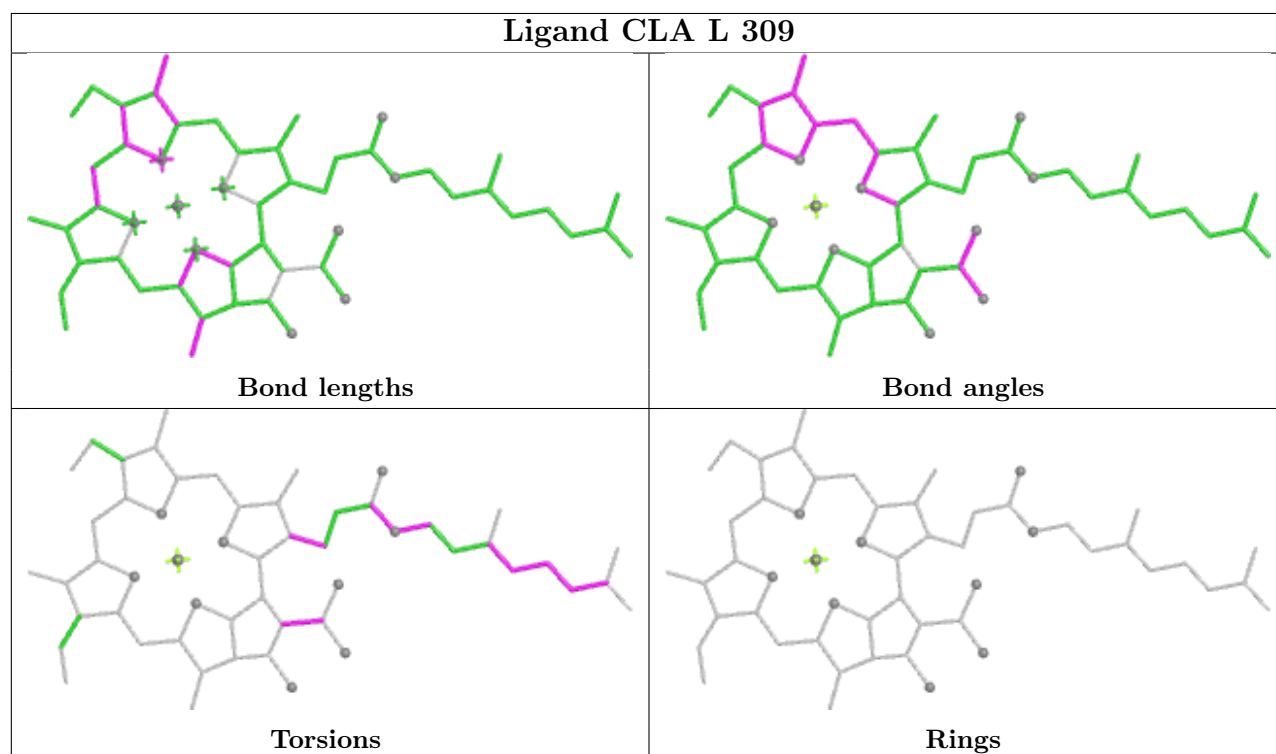
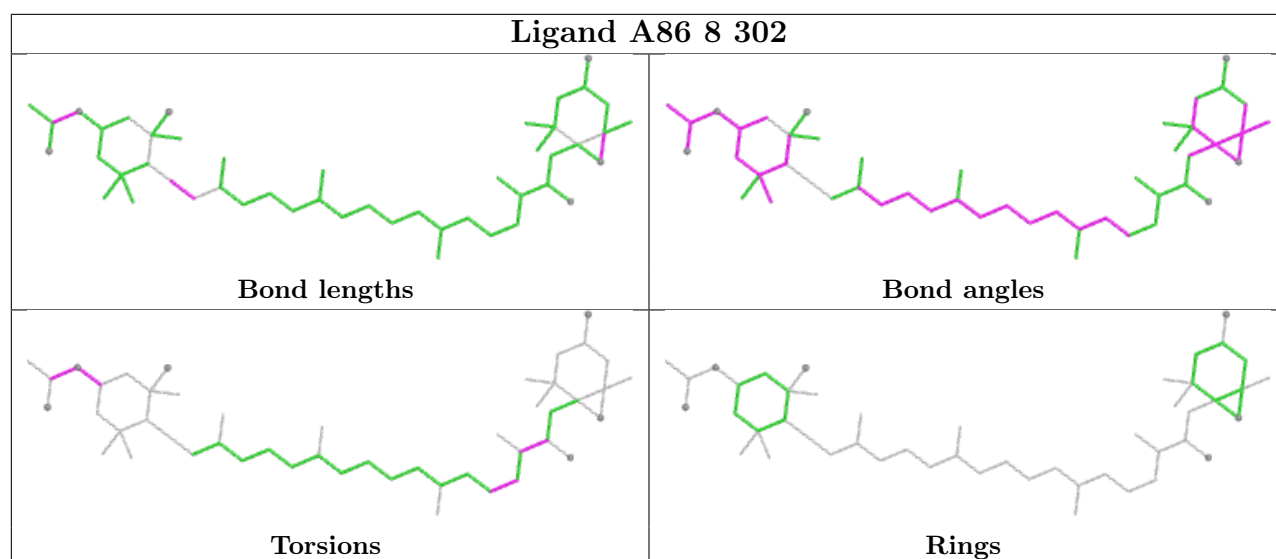
Bond angles

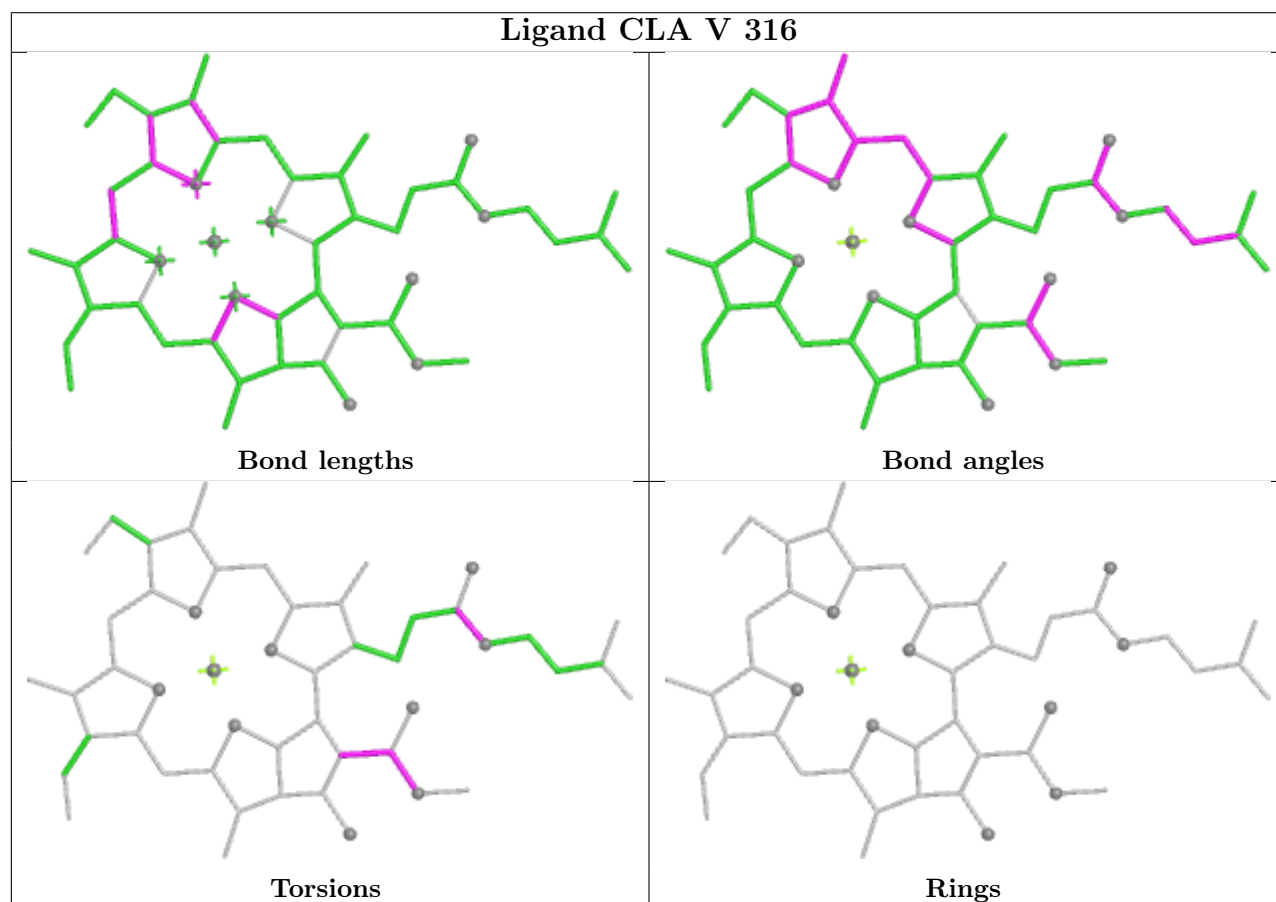
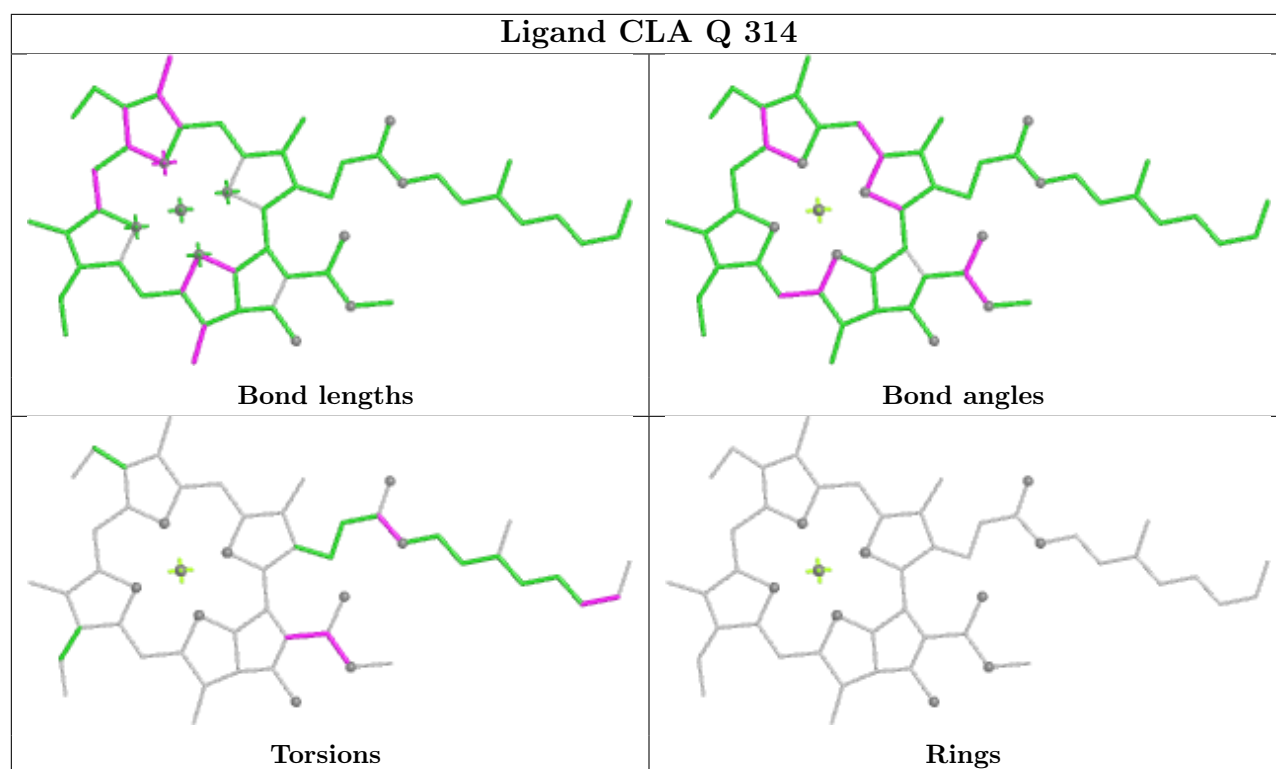


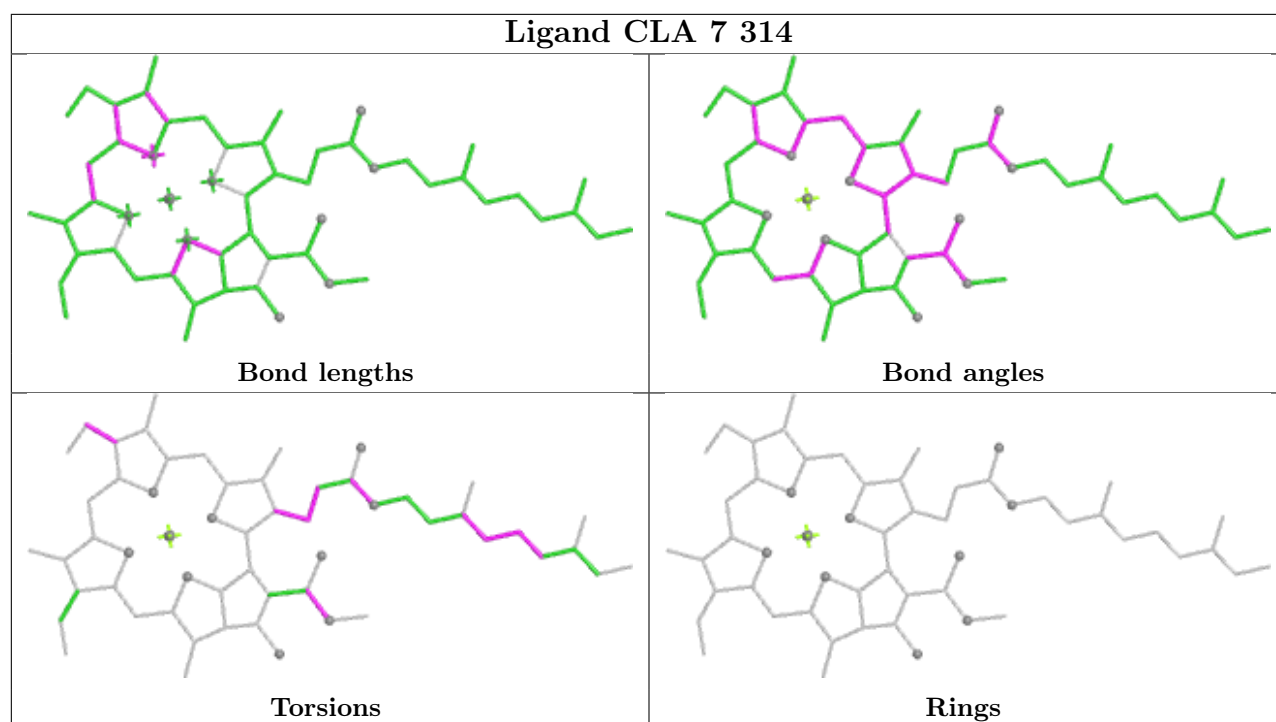
Torsions



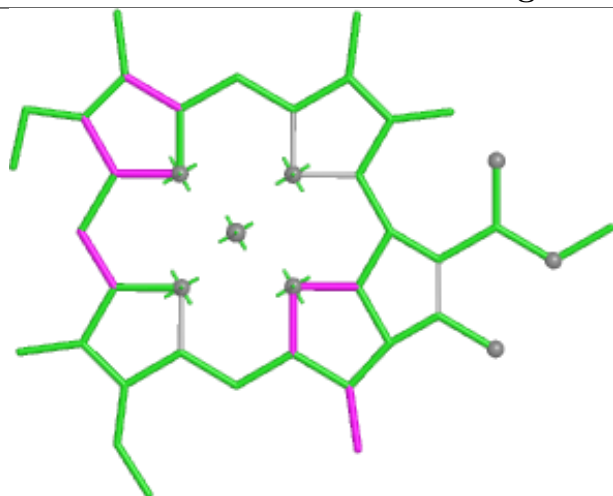
Rings



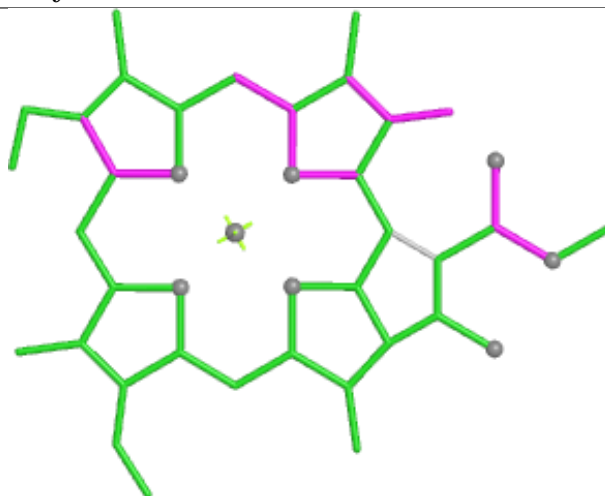




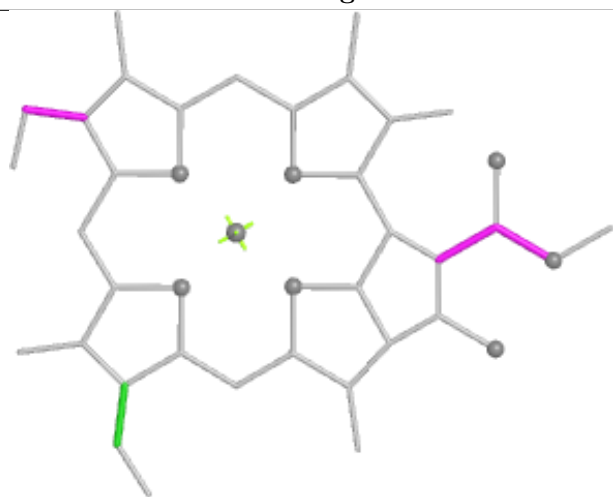
Ligand CLA y 315



Bond lengths



Bond angles

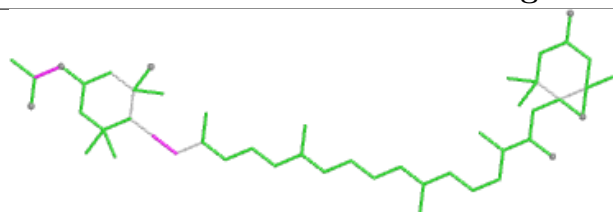


Torsions

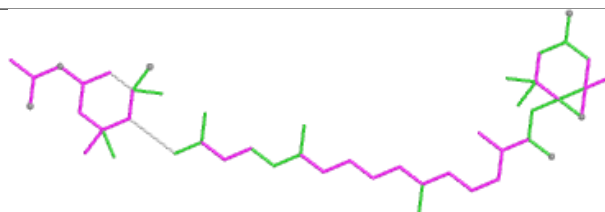


Rings

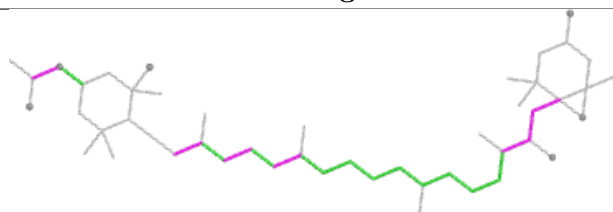
Ligand A86 P 302



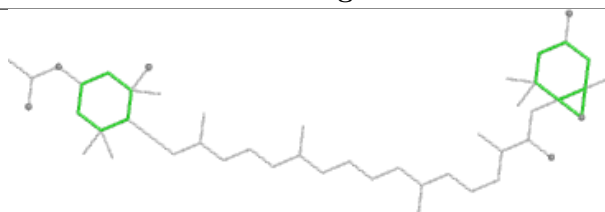
Bond lengths



Bond angles

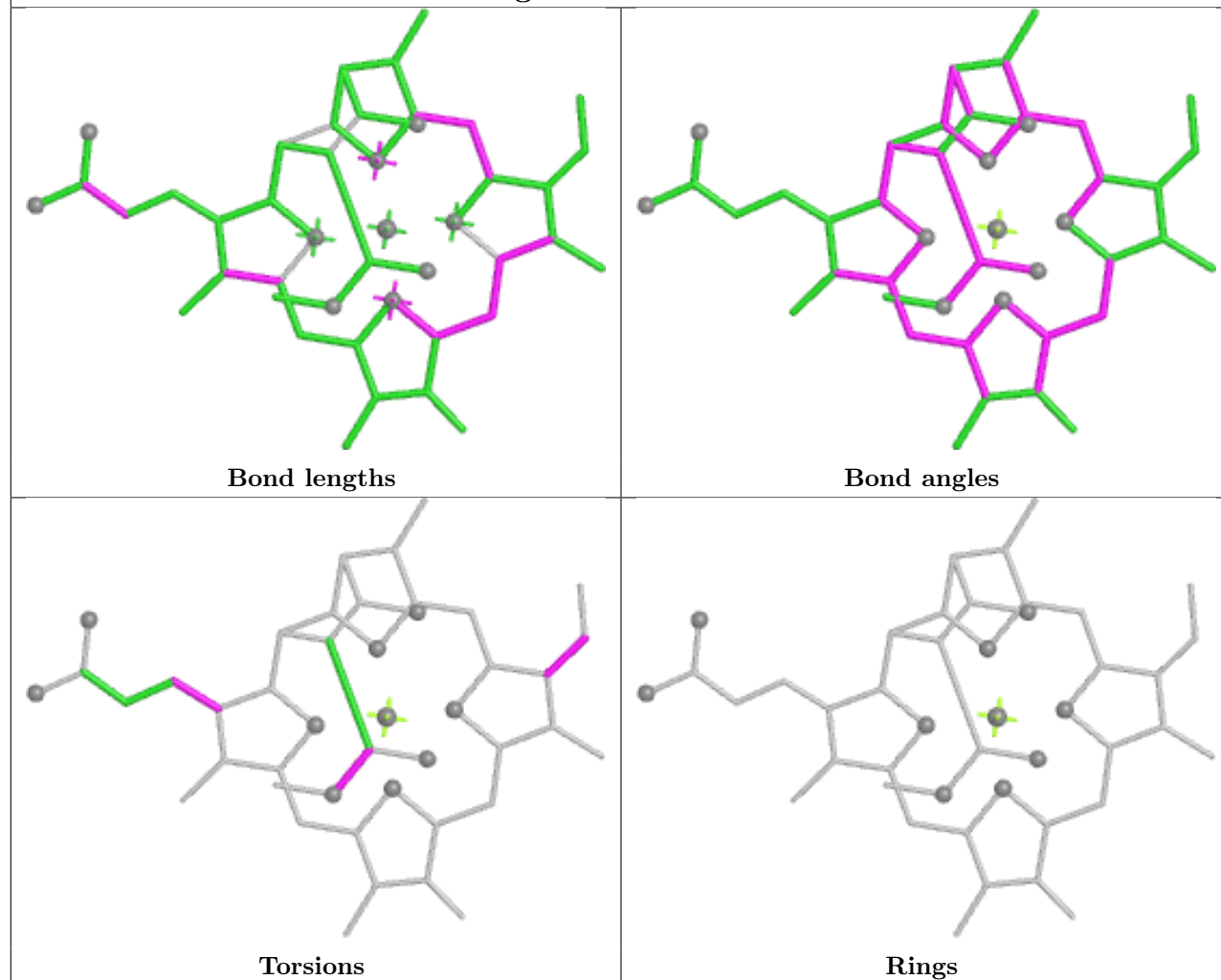


Torsions

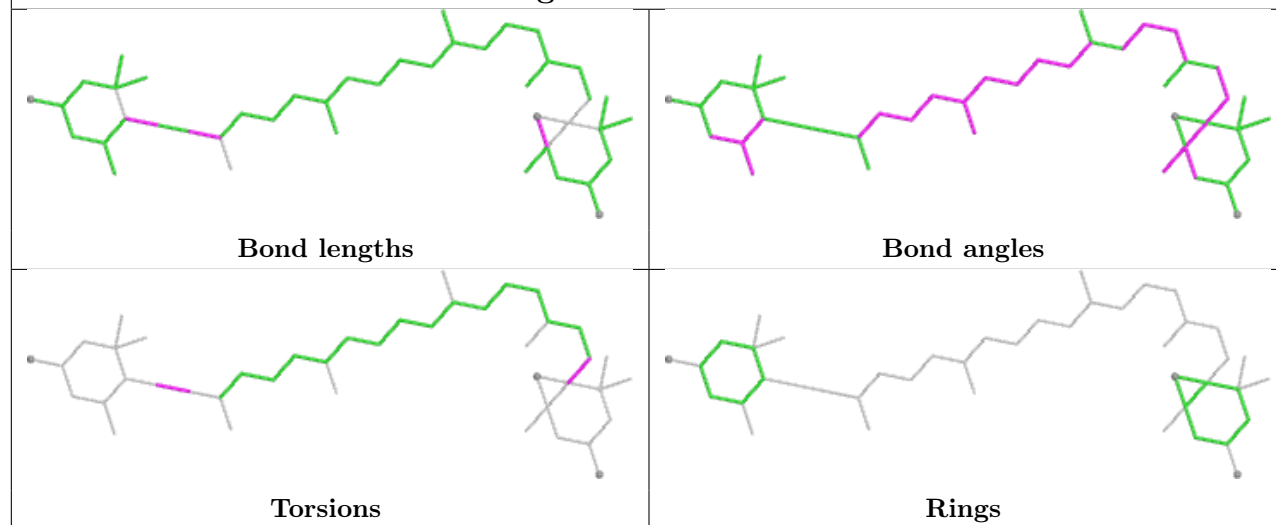


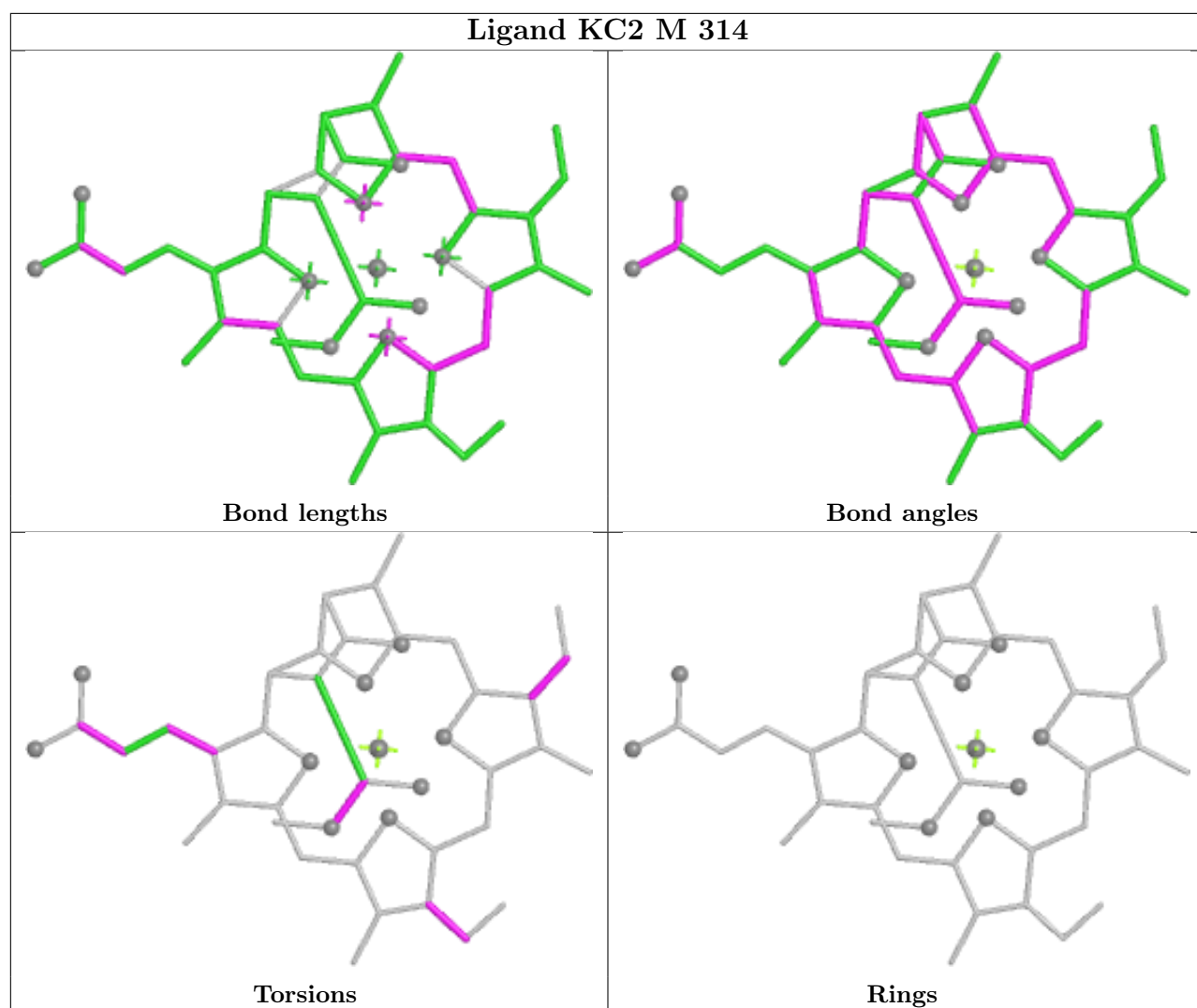
Rings

Ligand KC2 2 313

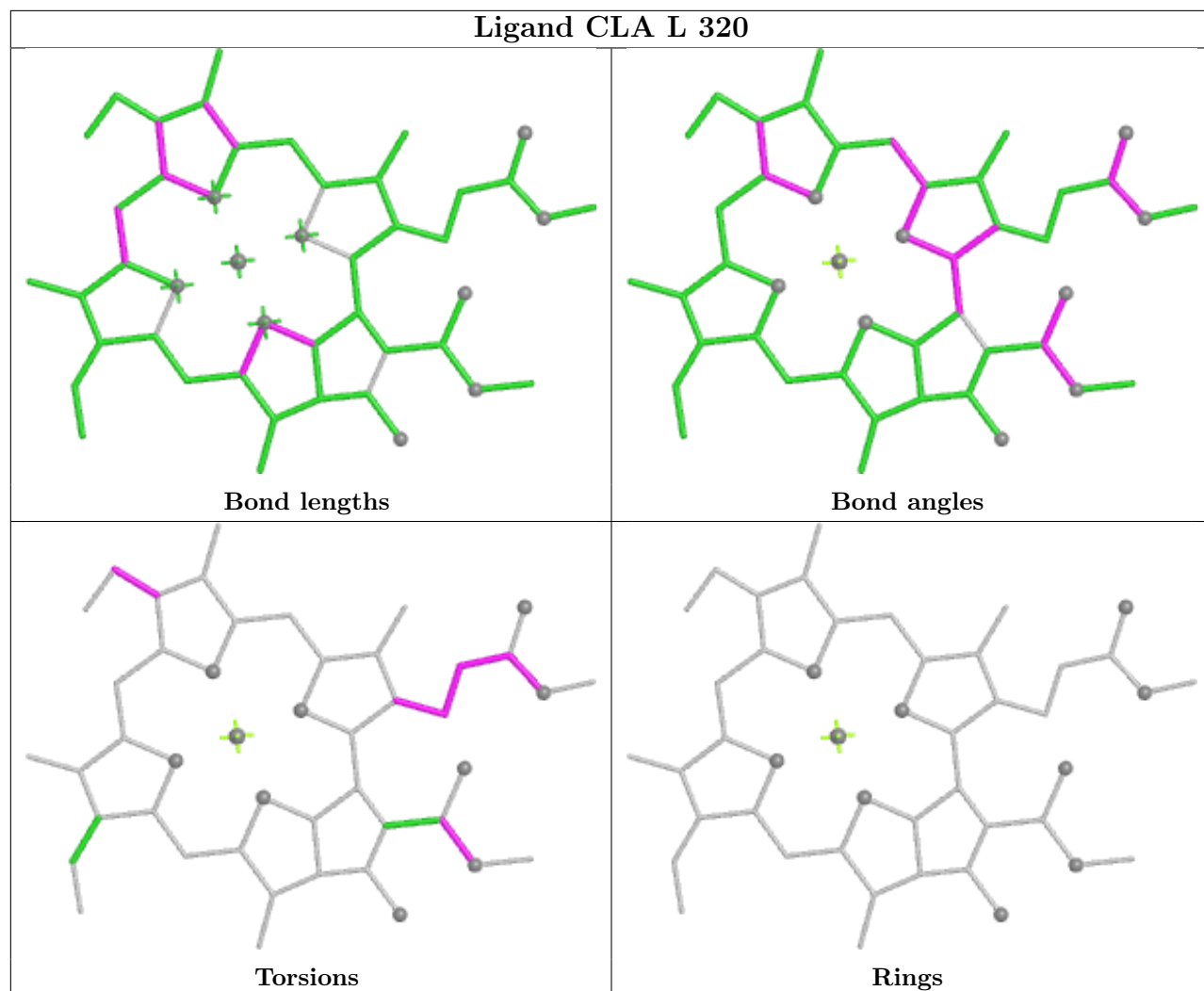


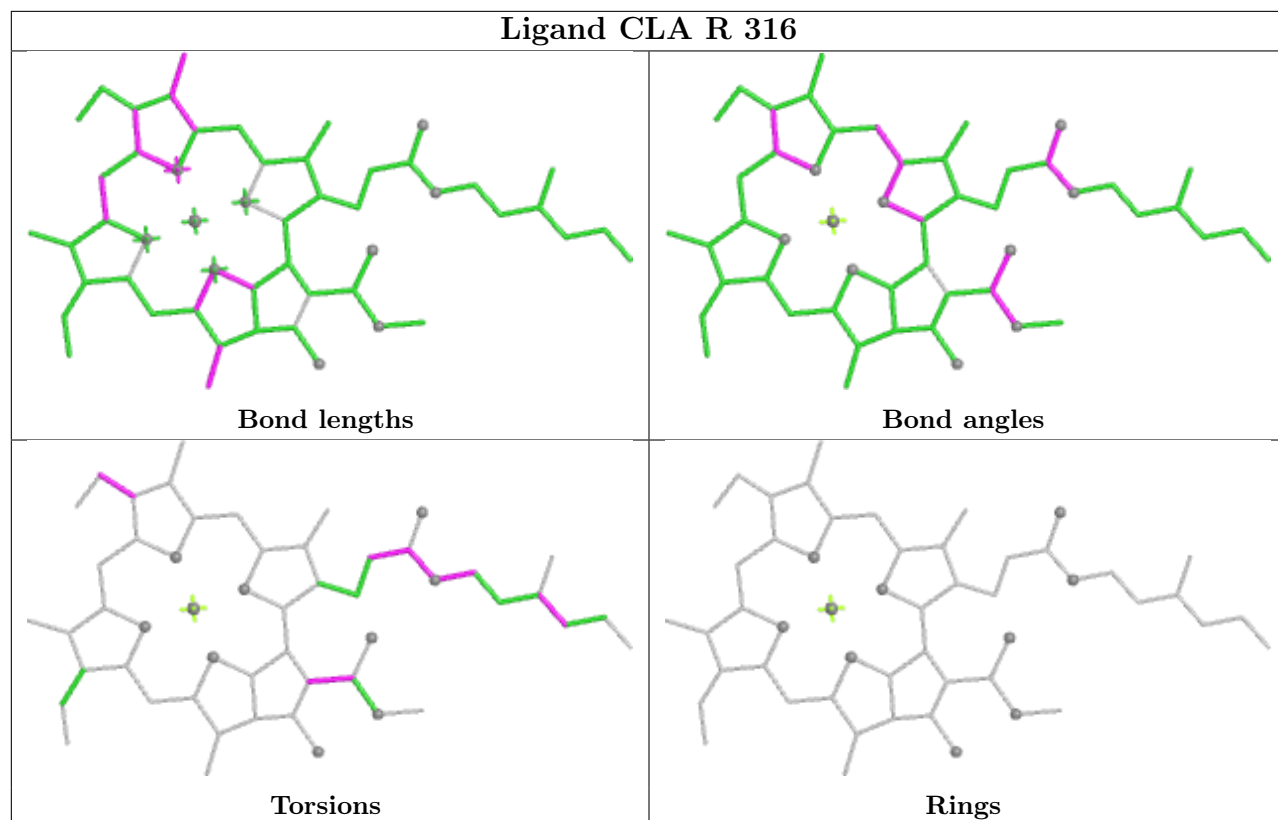
Ligand DD6 3 301



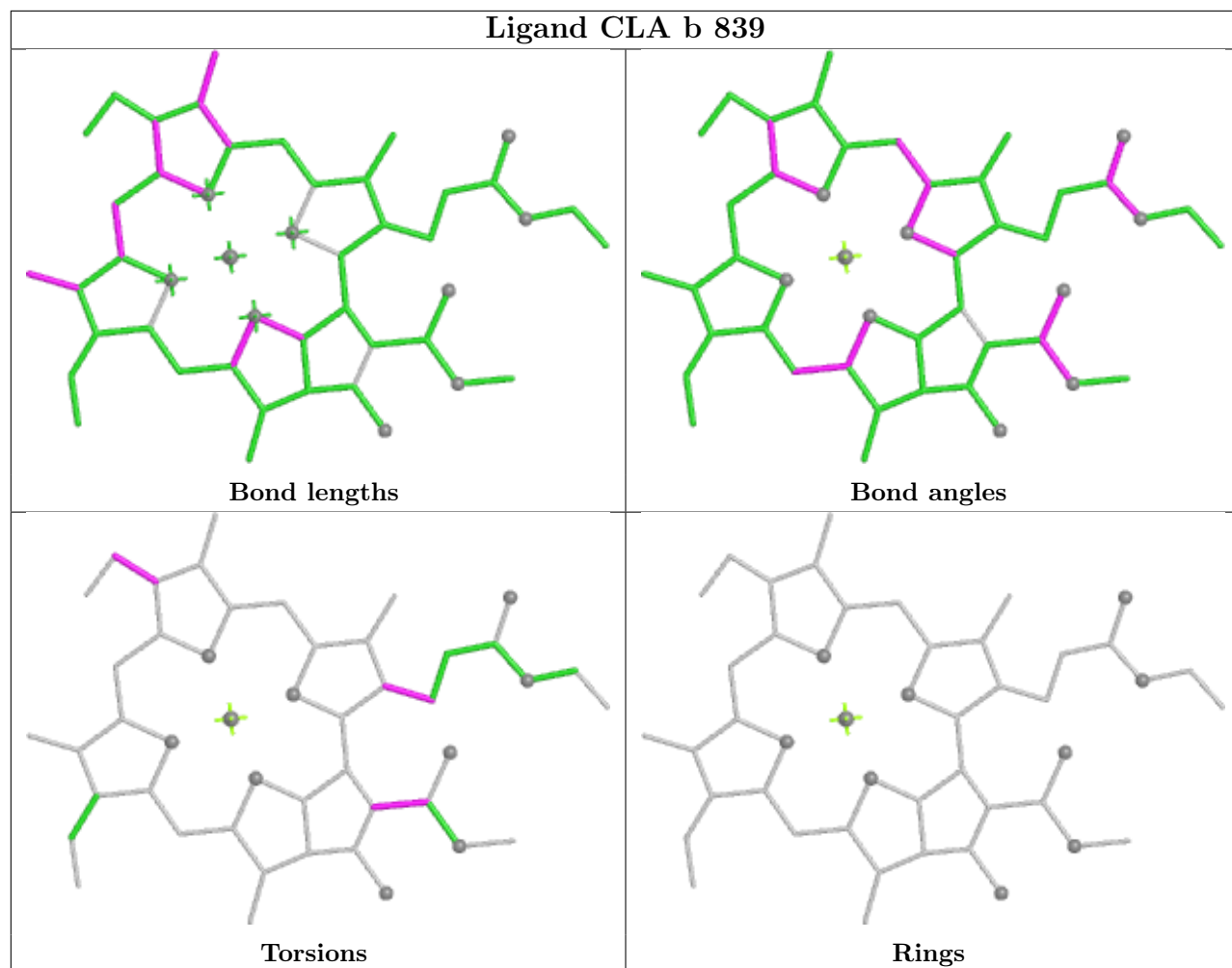


Ligand CLA L 320

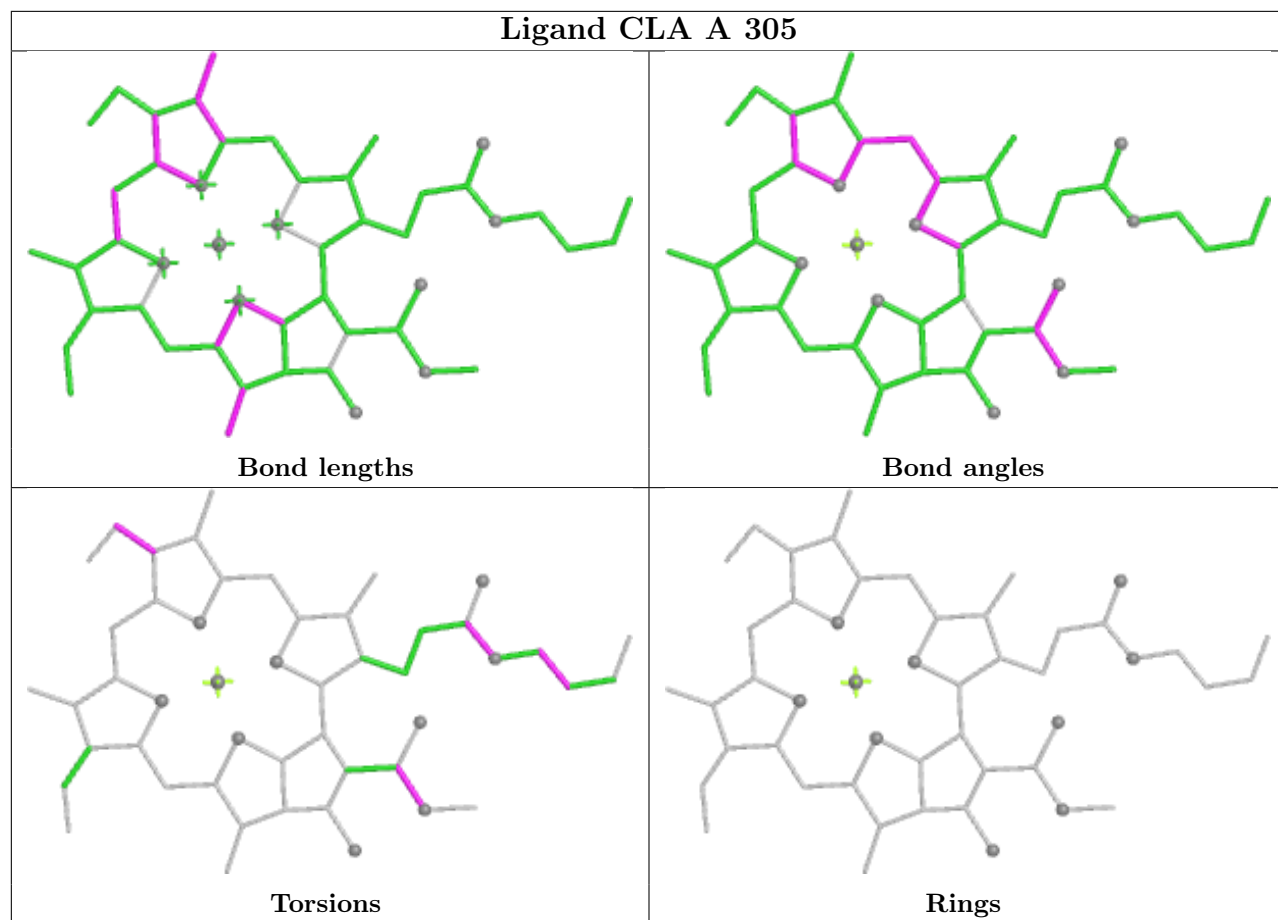


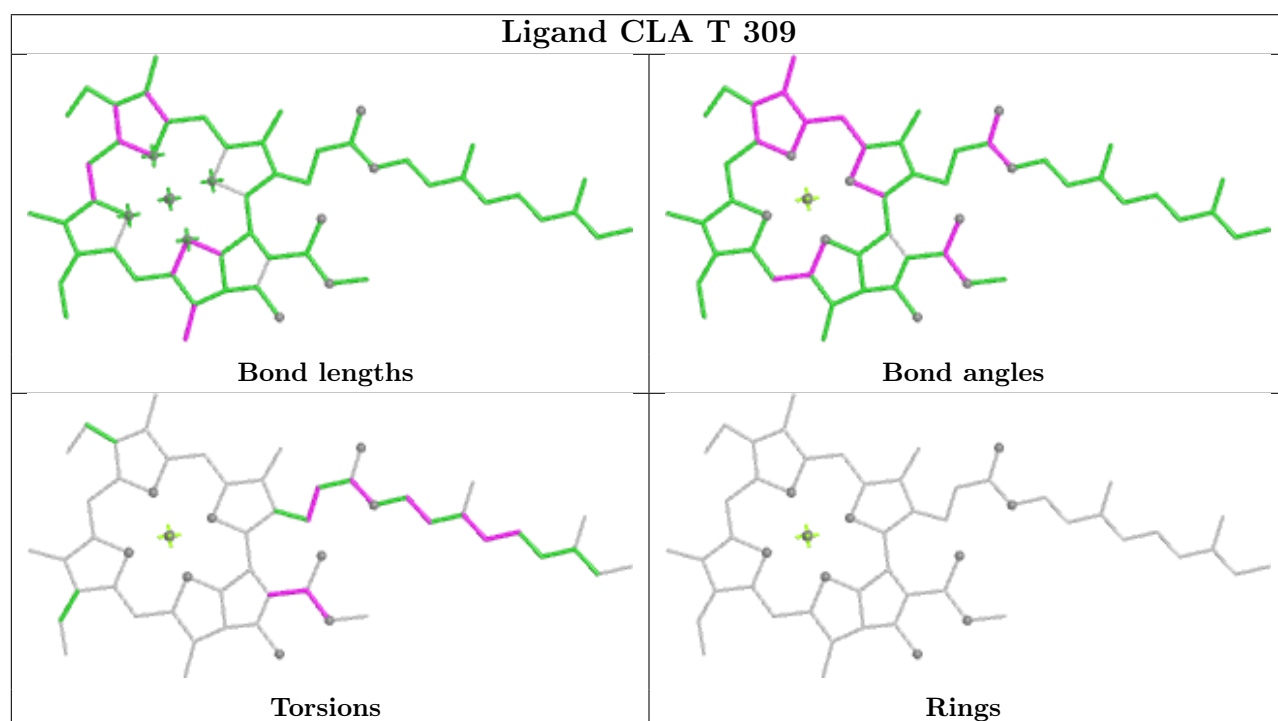
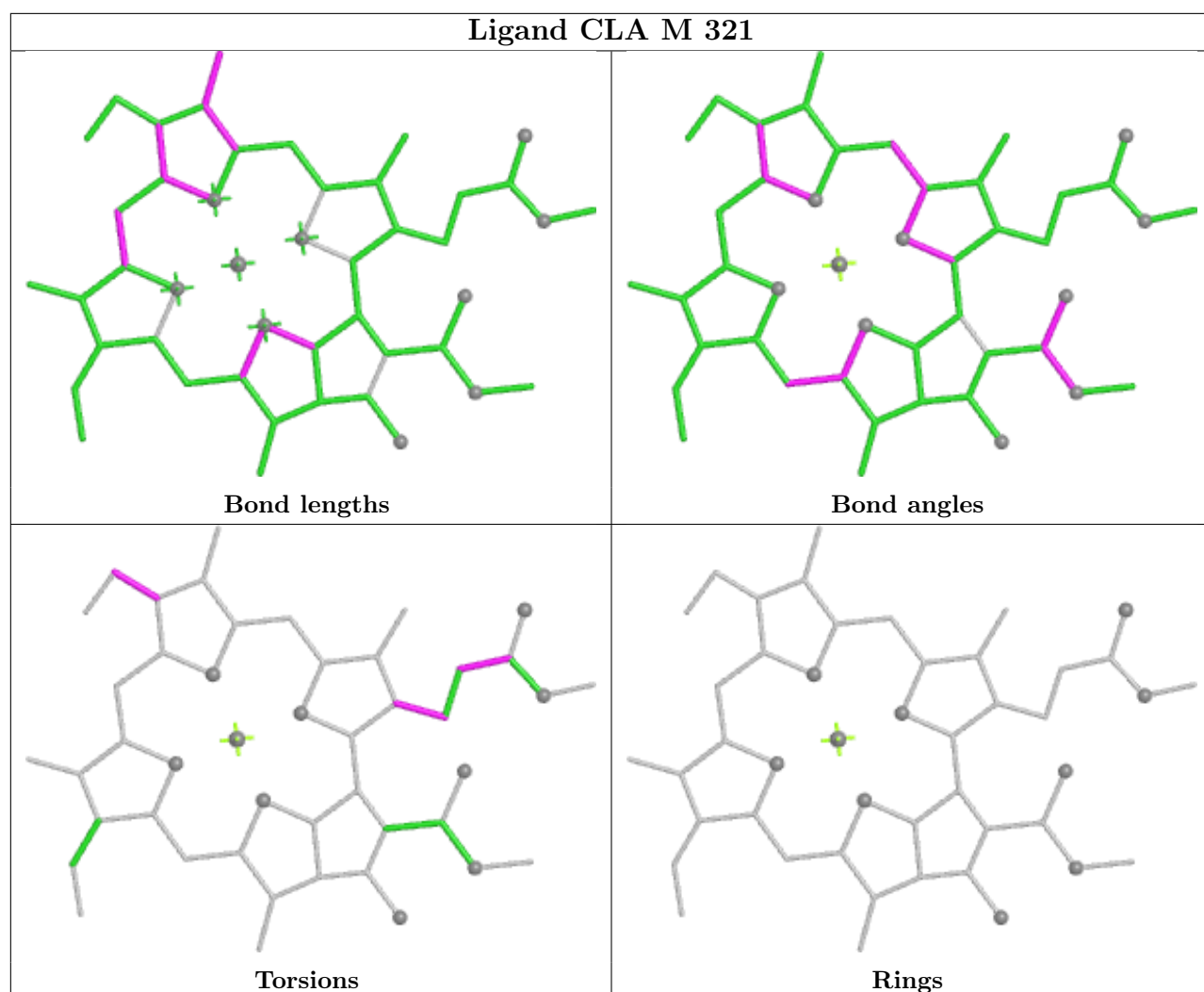


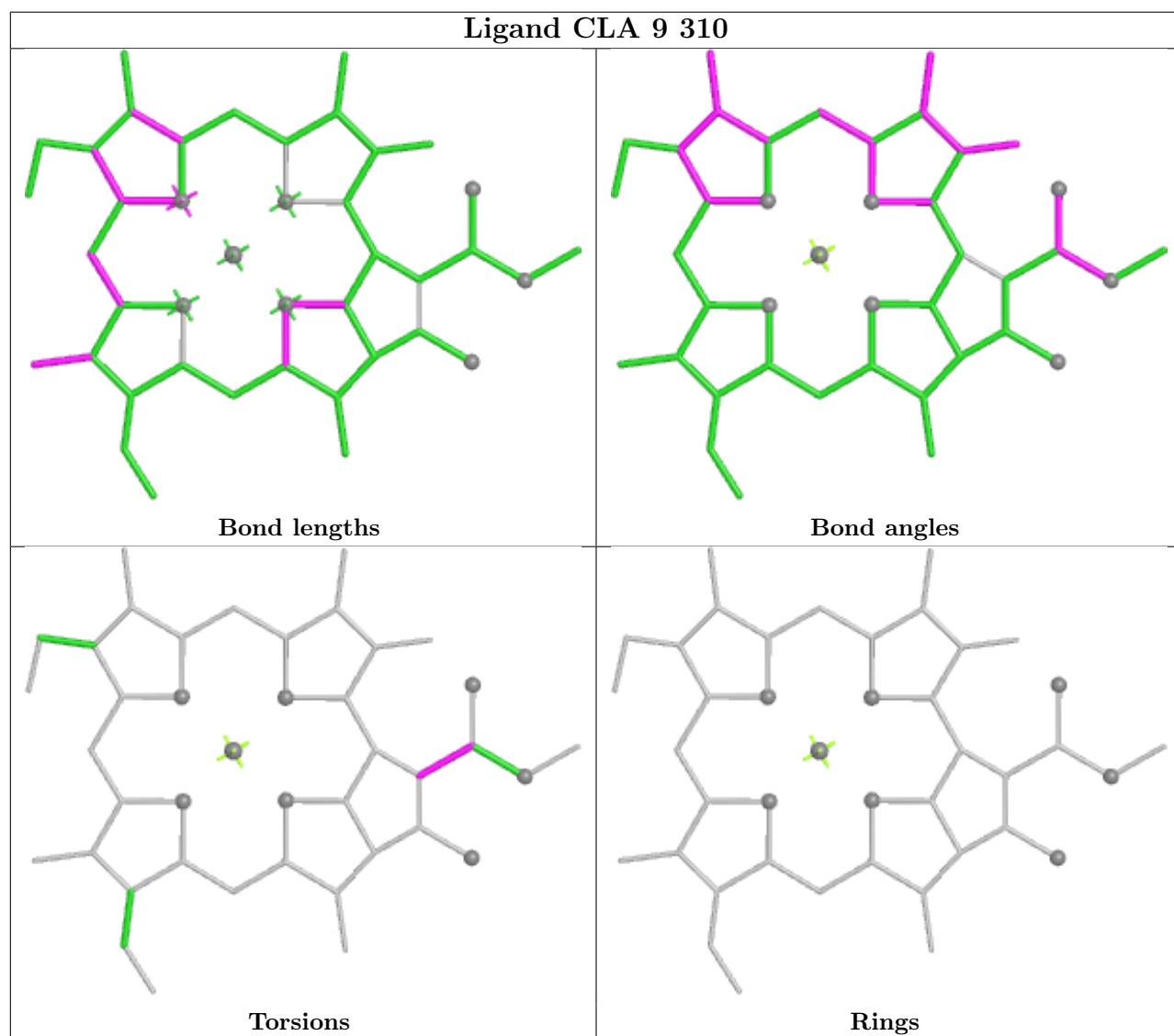
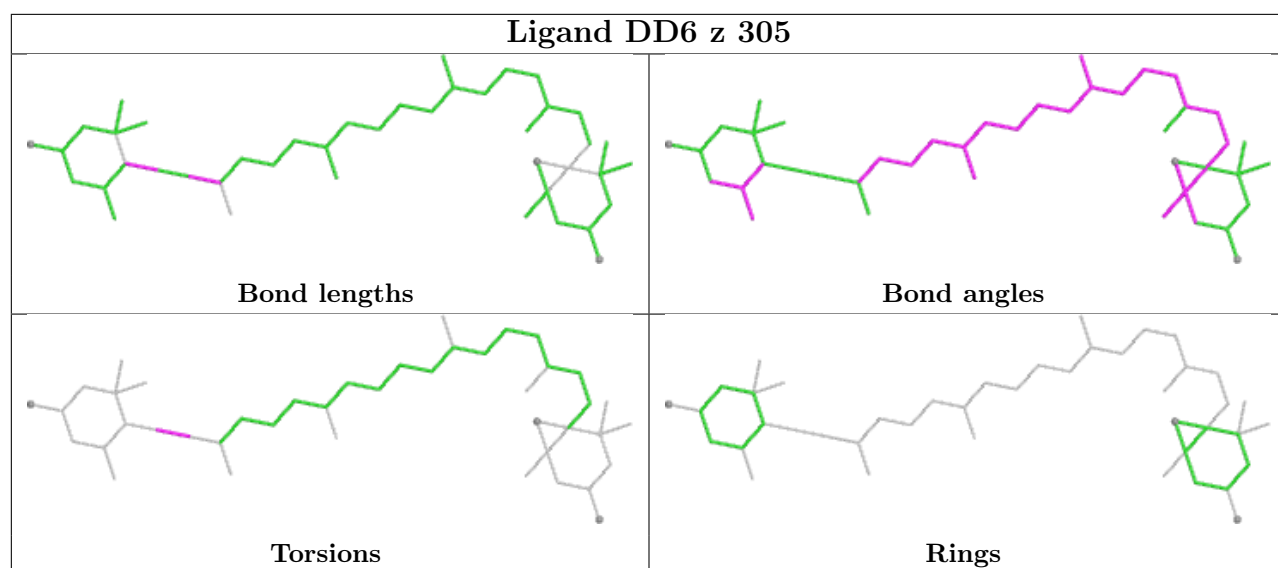
Ligand CLA b 839



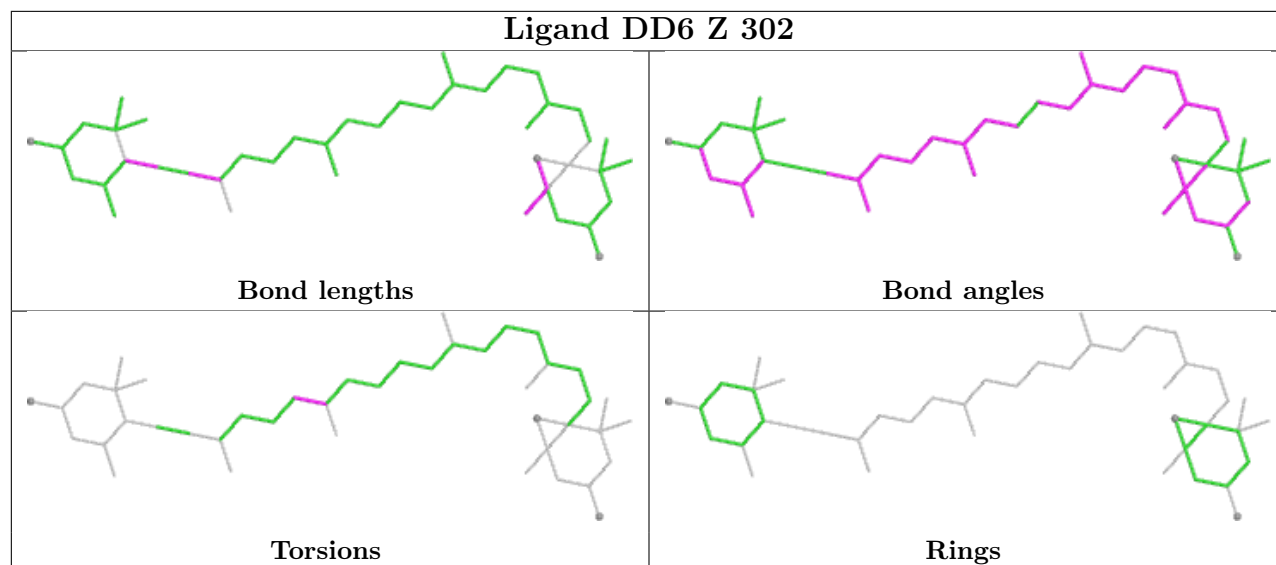
Ligand CLA A 305



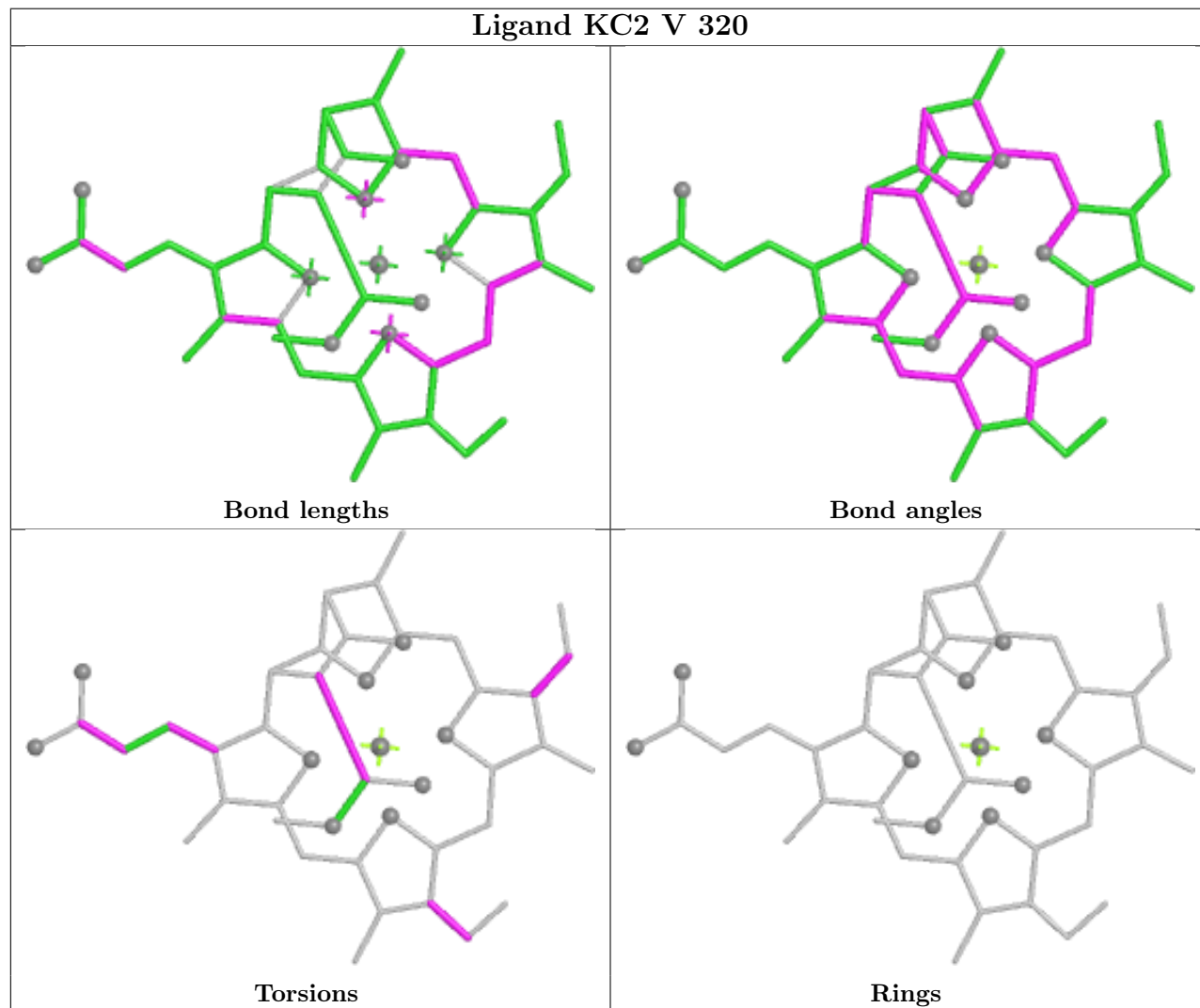


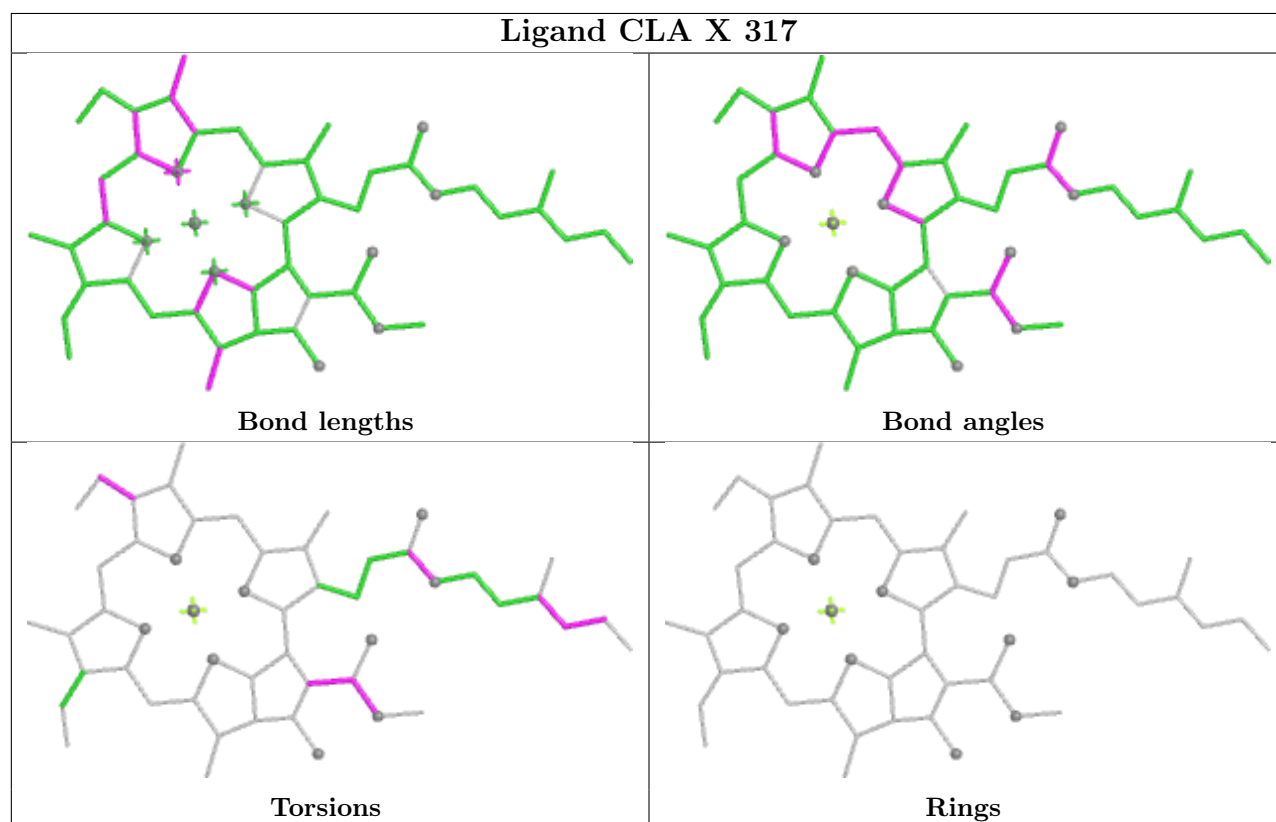
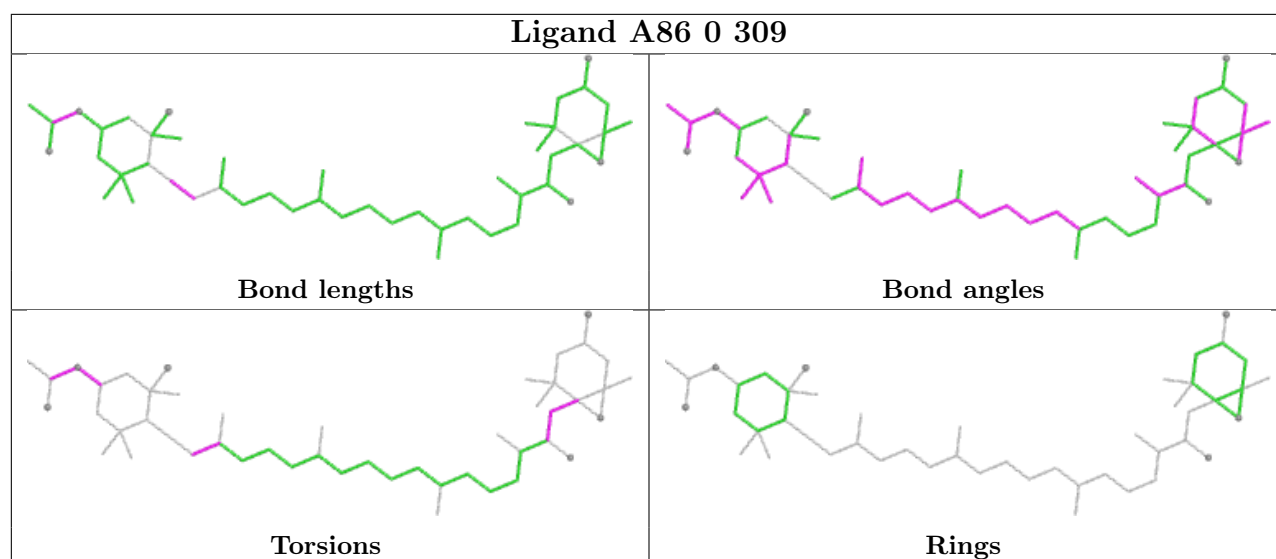


Ligand DD6 Z 302

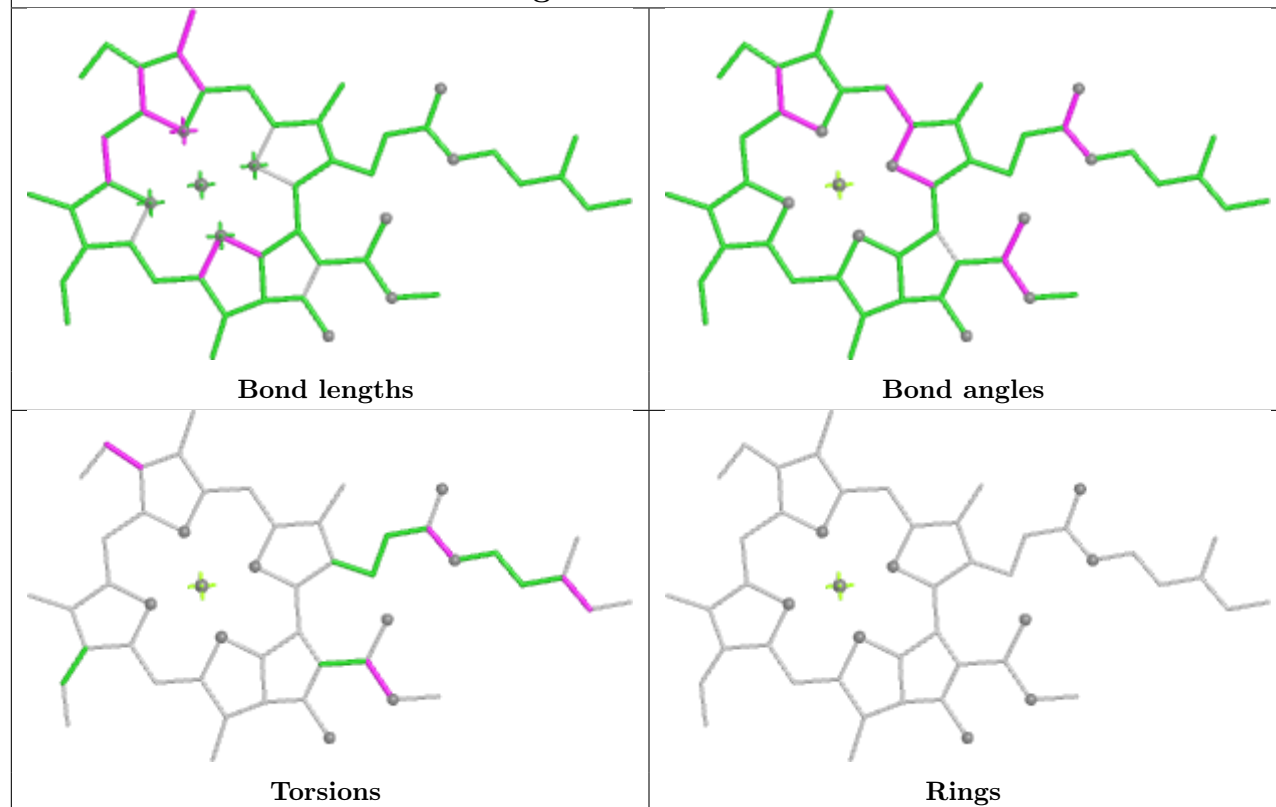


Ligand KC2 V 320

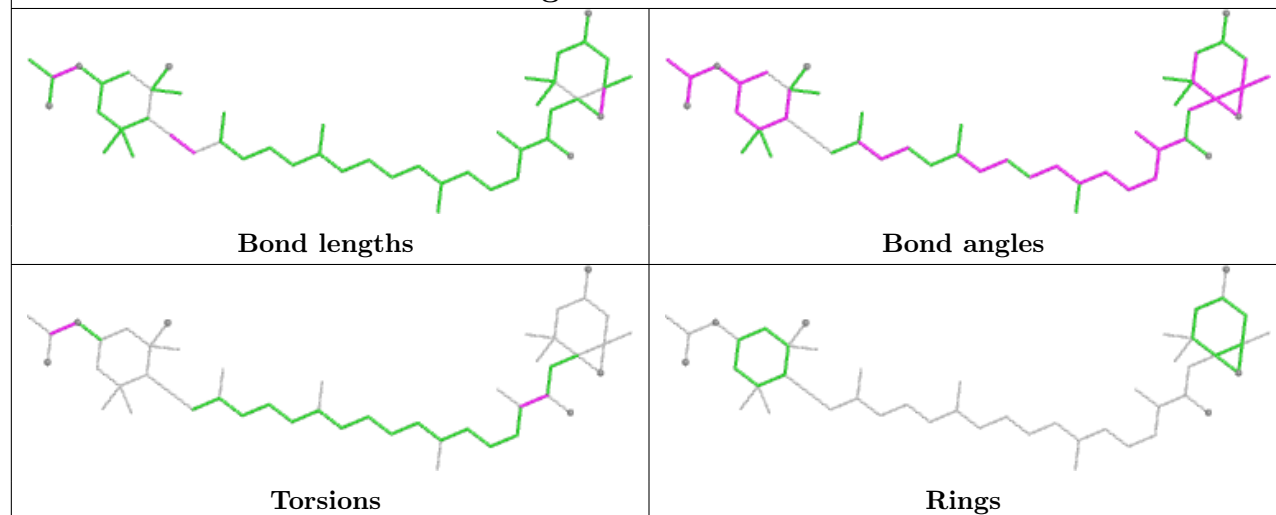




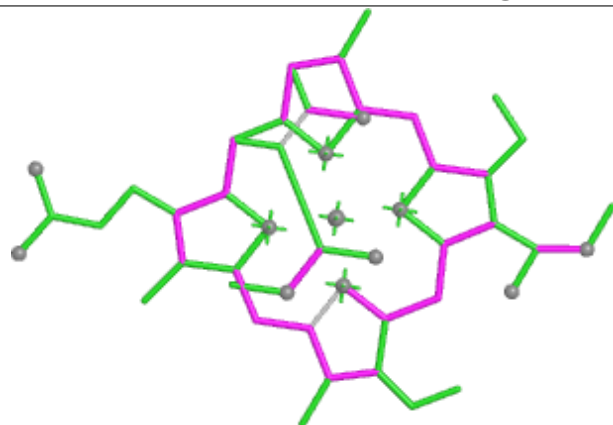
Ligand CLA P 316



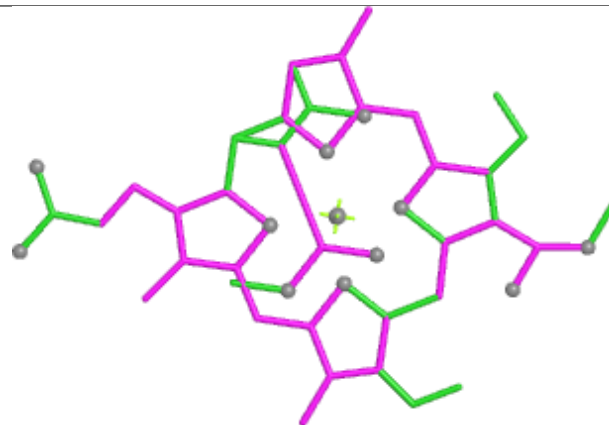
Ligand A86 J 303



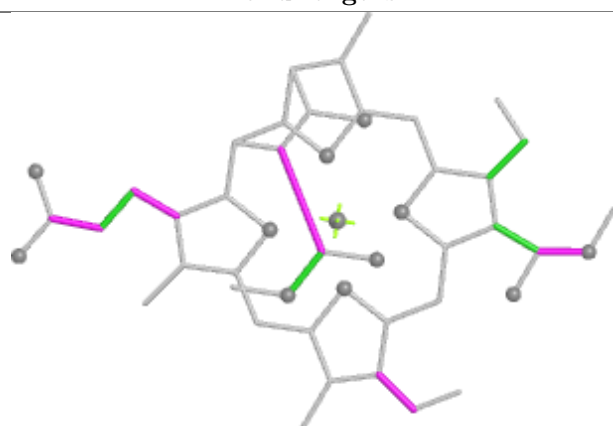
Ligand A1ECV 4 315



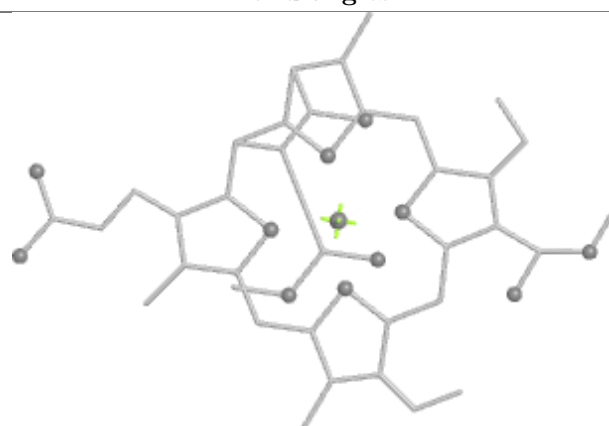
Bond lengths



Bond angles

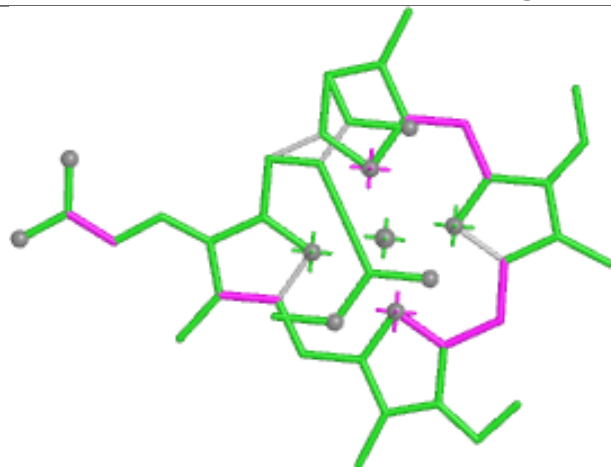


Torsions



Rings

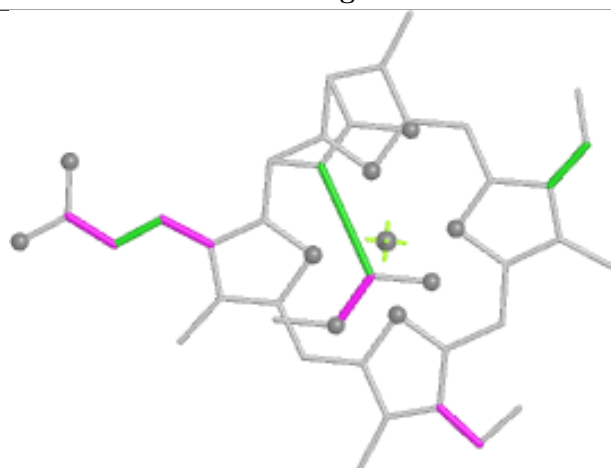
Ligand KC2 L 314



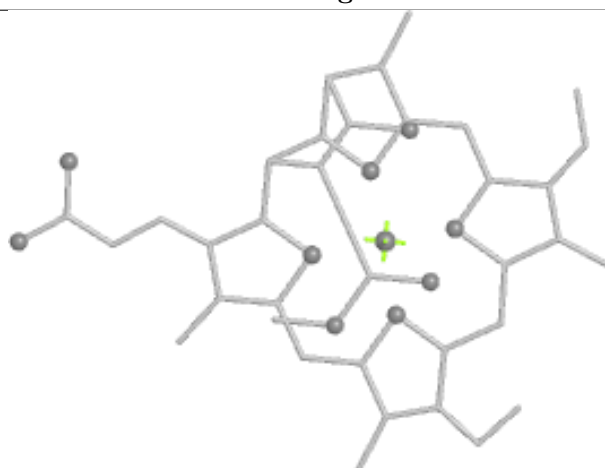
Bond lengths



Bond angles

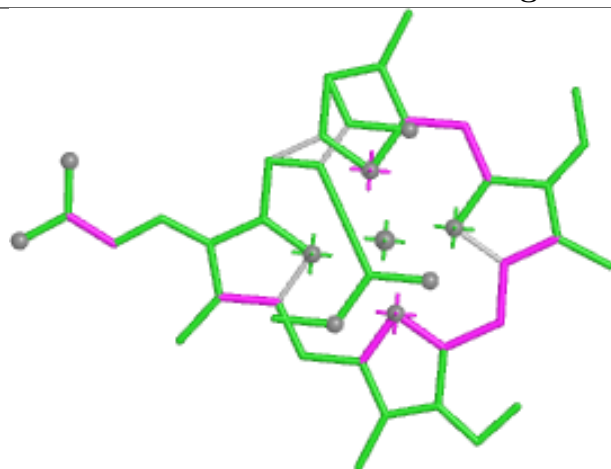


Torsions

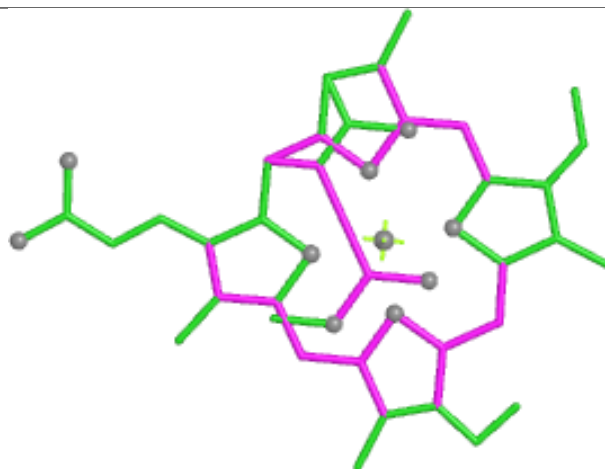


Rings

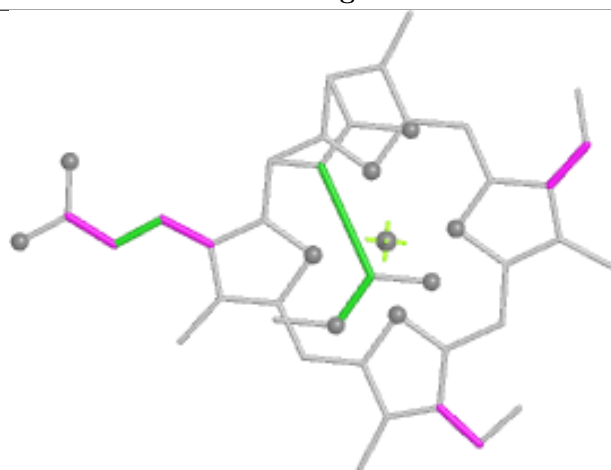
Ligand KC2 1 312



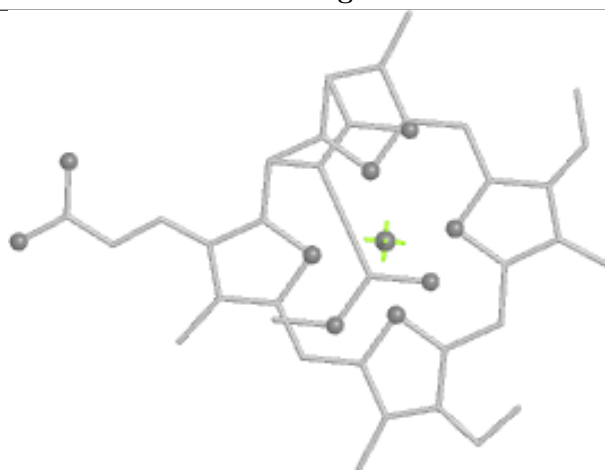
Bond lengths



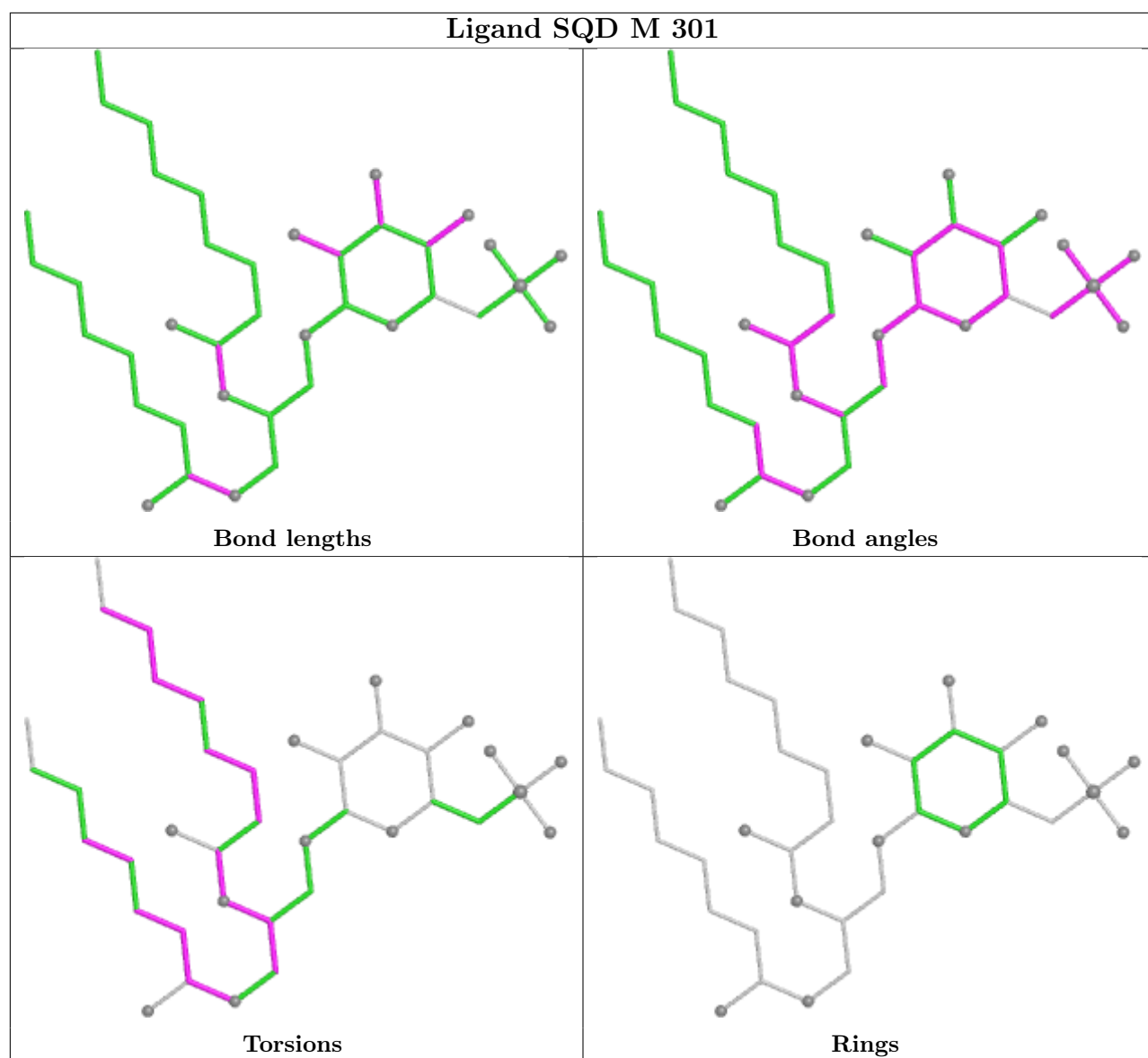
Bond angles



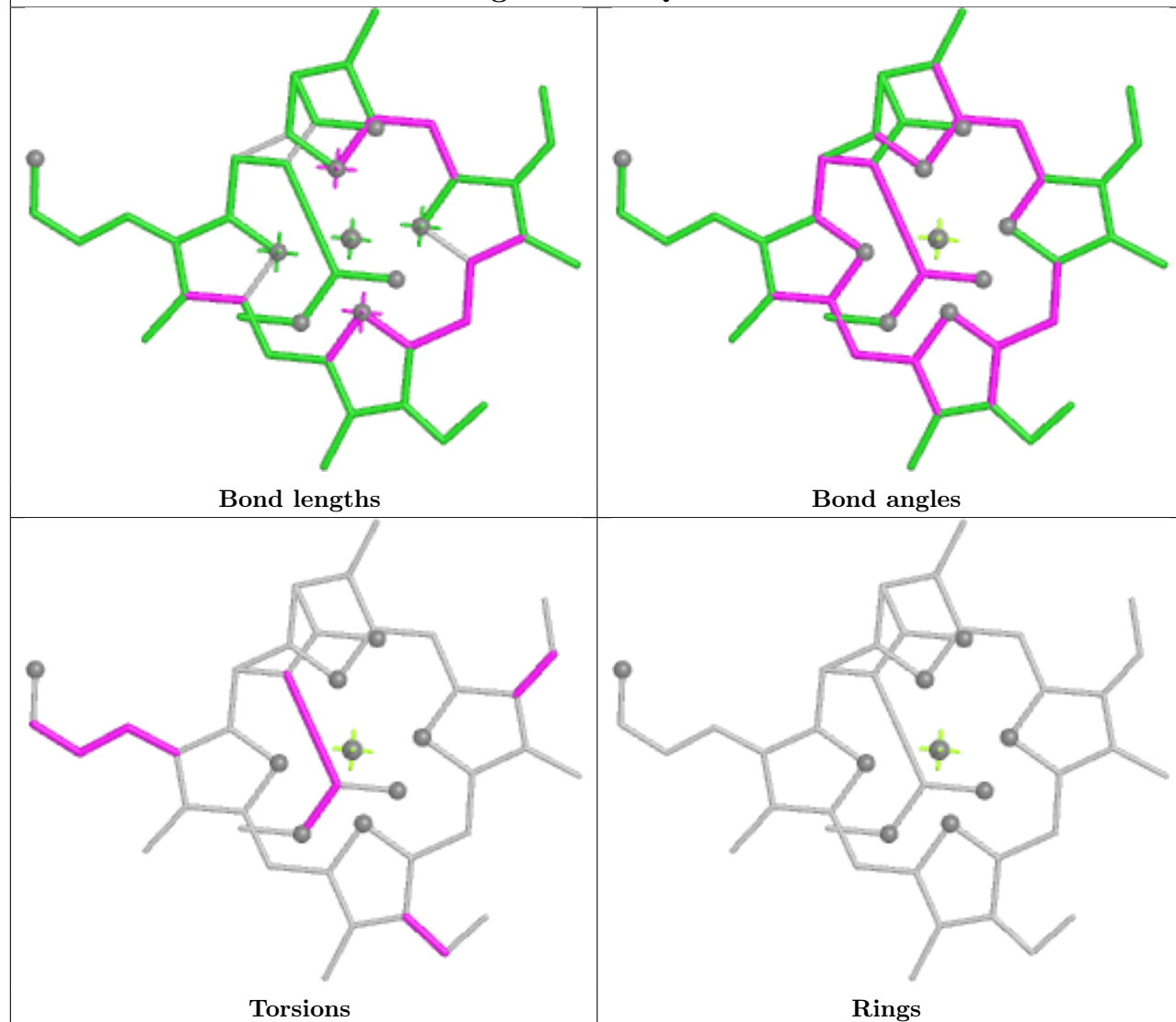
Torsions



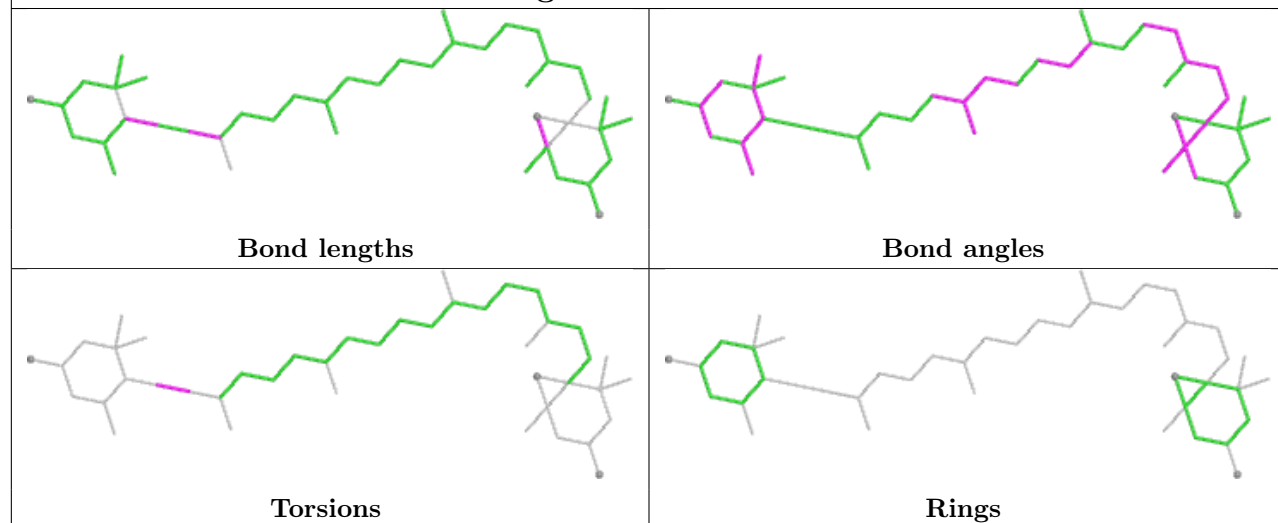
Rings



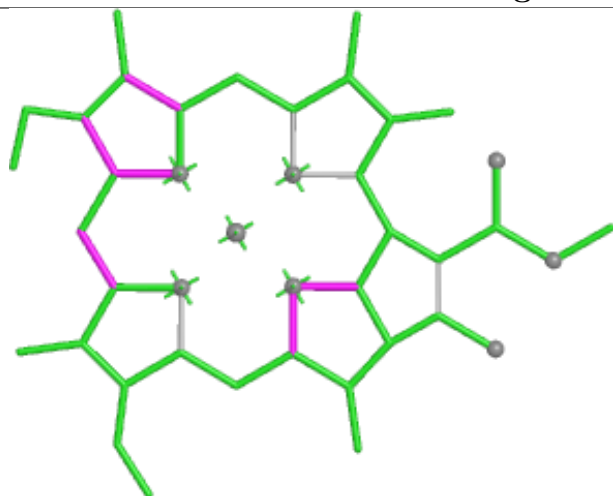
Ligand KC2 Q 313



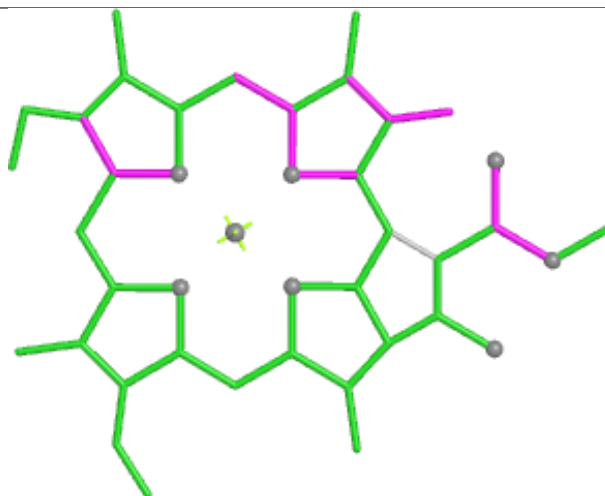
Ligand DD6 5 303



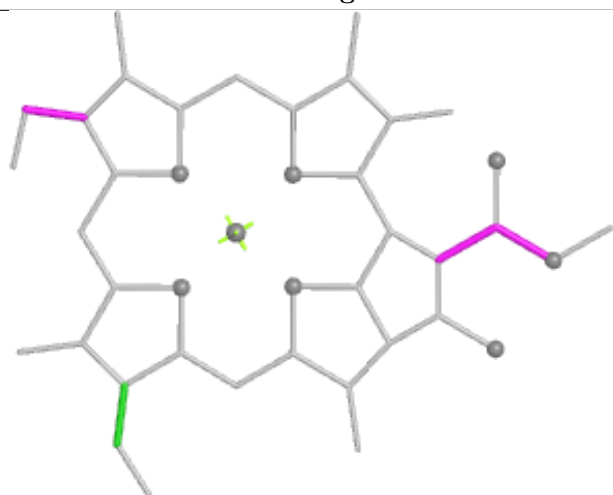
Ligand CLA O 316



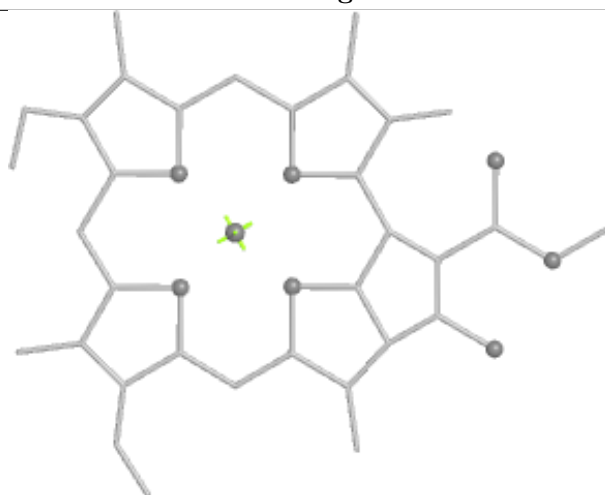
Bond lengths



Bond angles

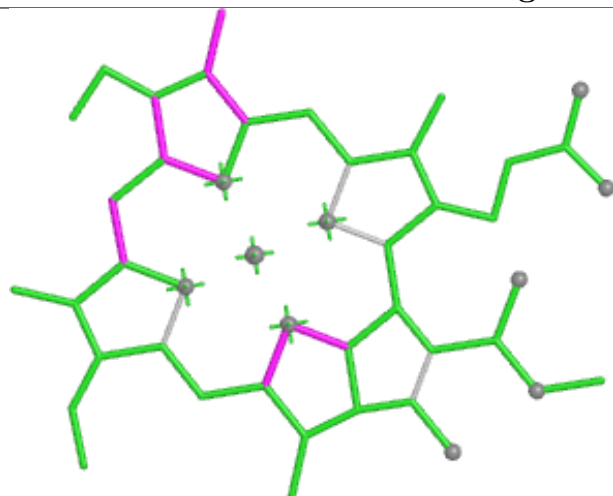


Torsions

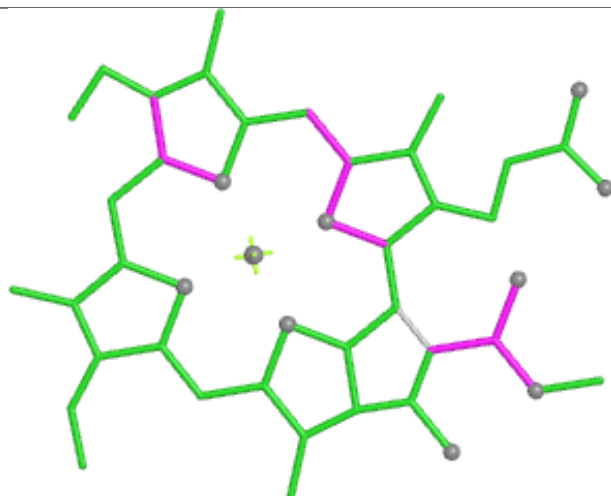


Rings

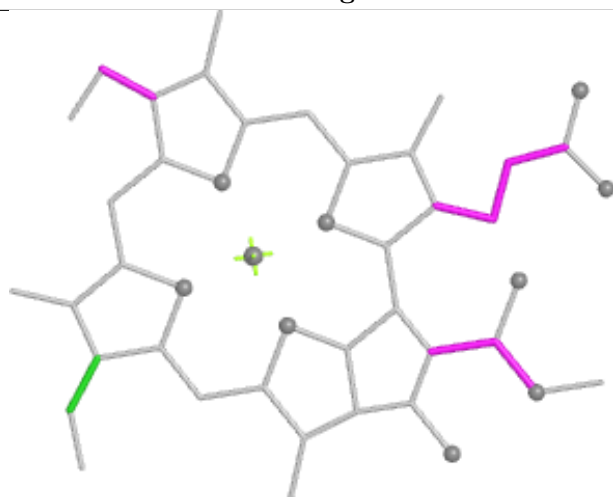
Ligand CLA a 833



Bond lengths



Bond angles

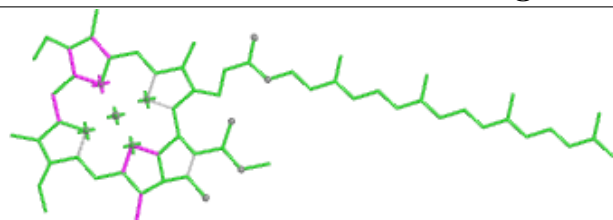


Torsions

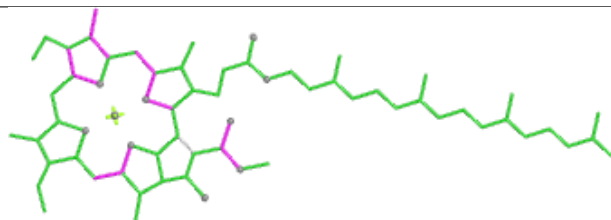


Rings

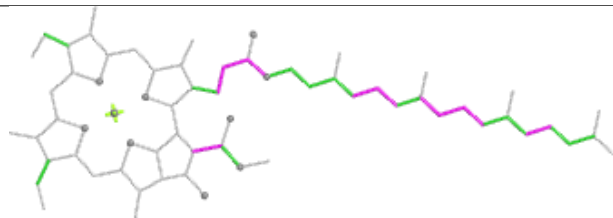
Ligand CLA C 307



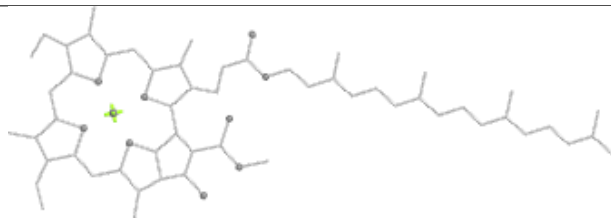
Bond lengths



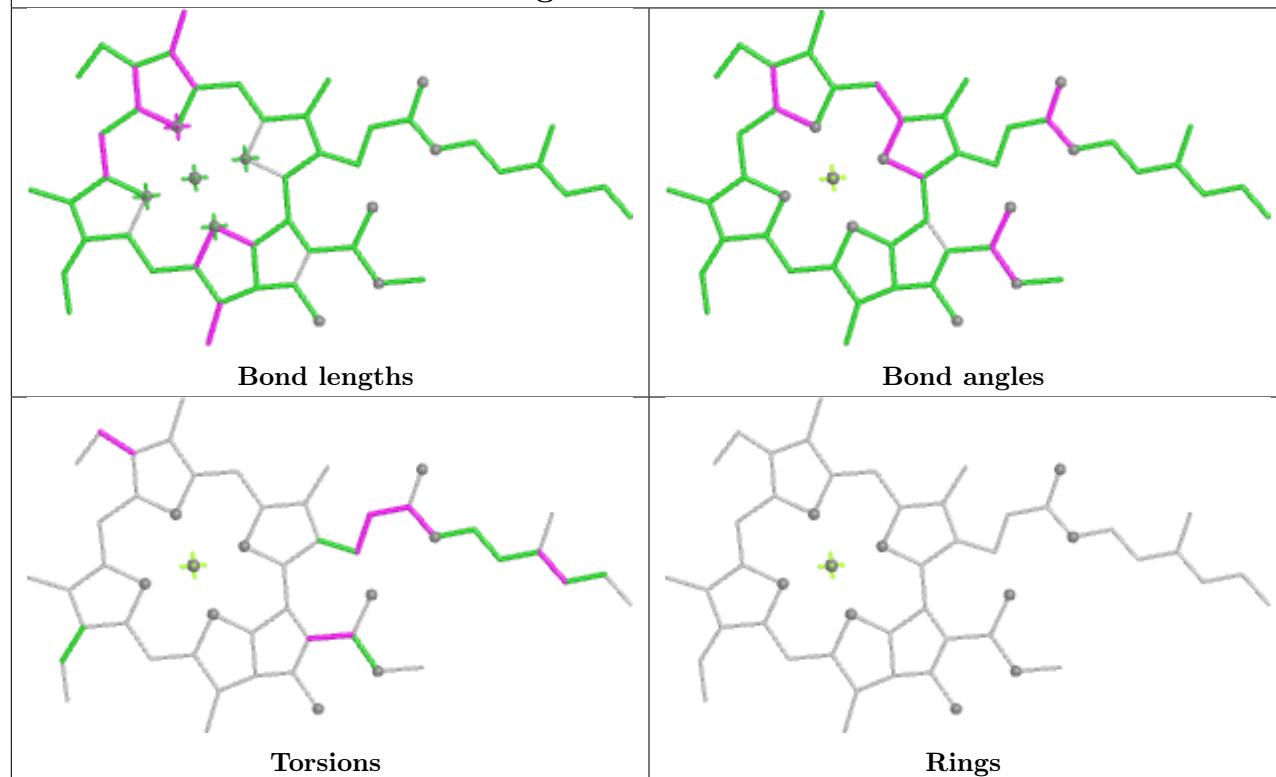
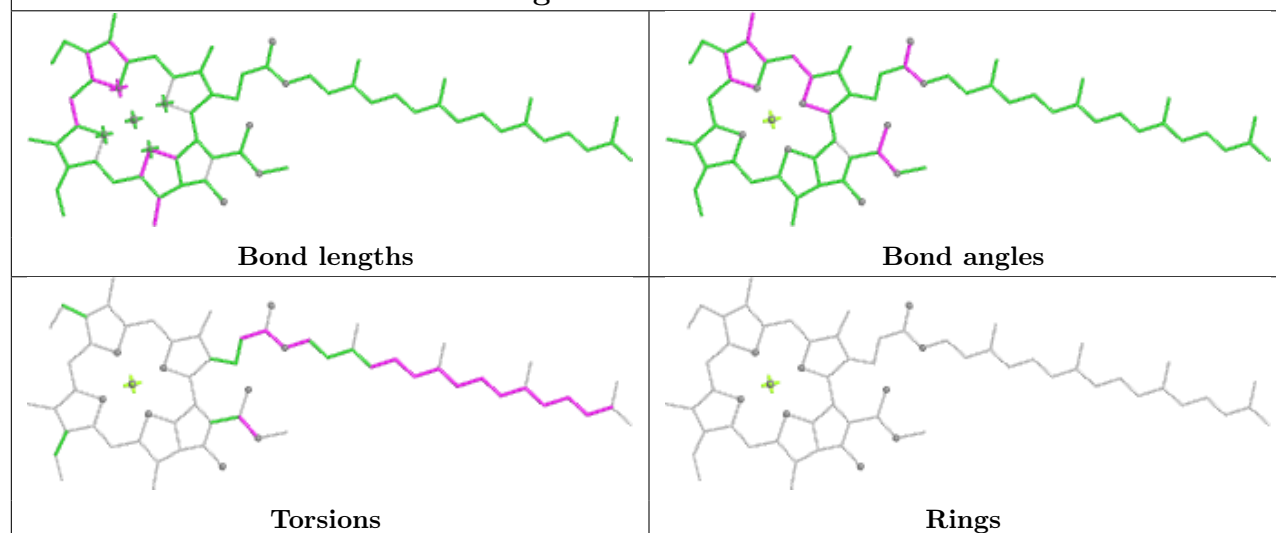
Bond angles



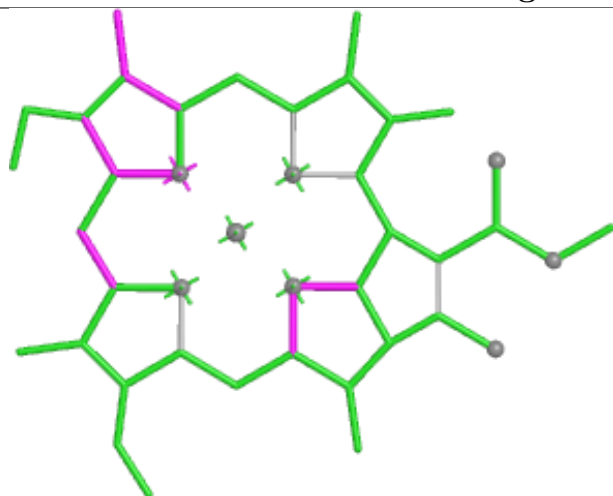
Torsions



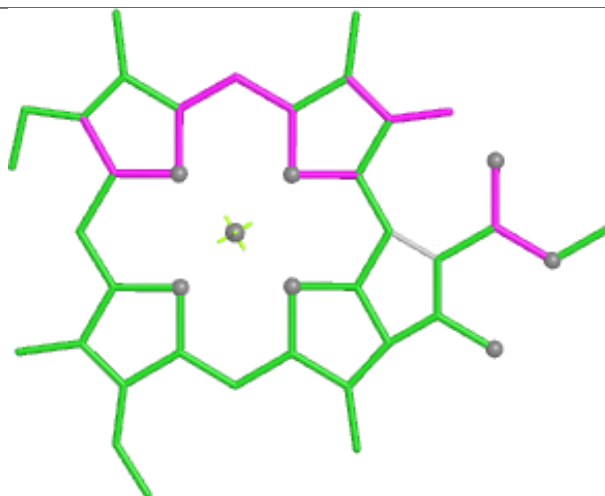
Rings

Ligand CLA 5 316**Ligand CLA P 308**

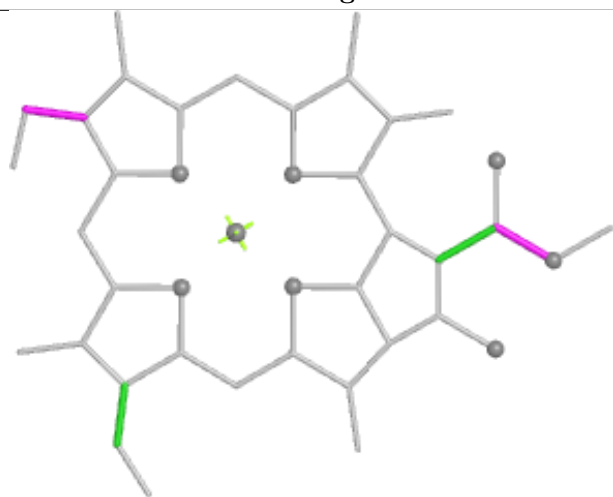
Ligand CLA 9 307



Bond lengths



Bond angles

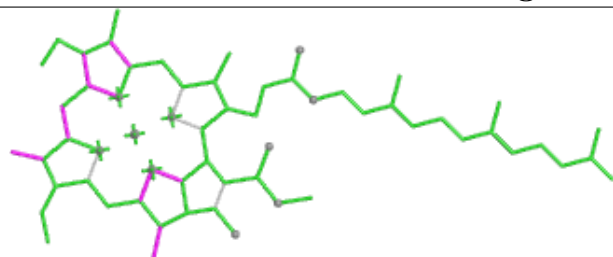


Torsions

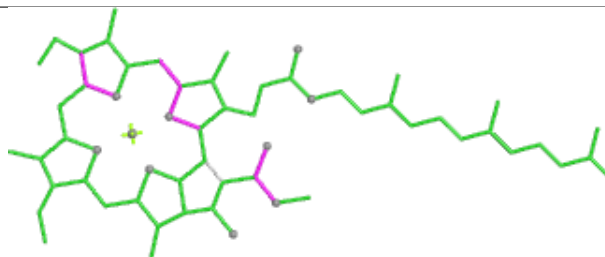


Rings

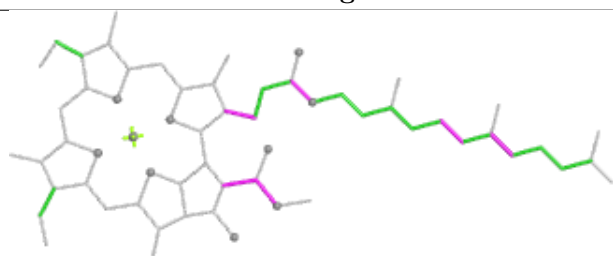
Ligand CLA b 824



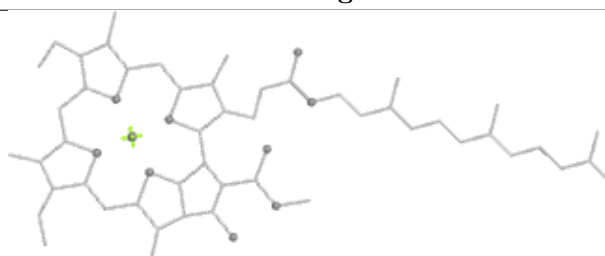
Bond lengths



Bond angles

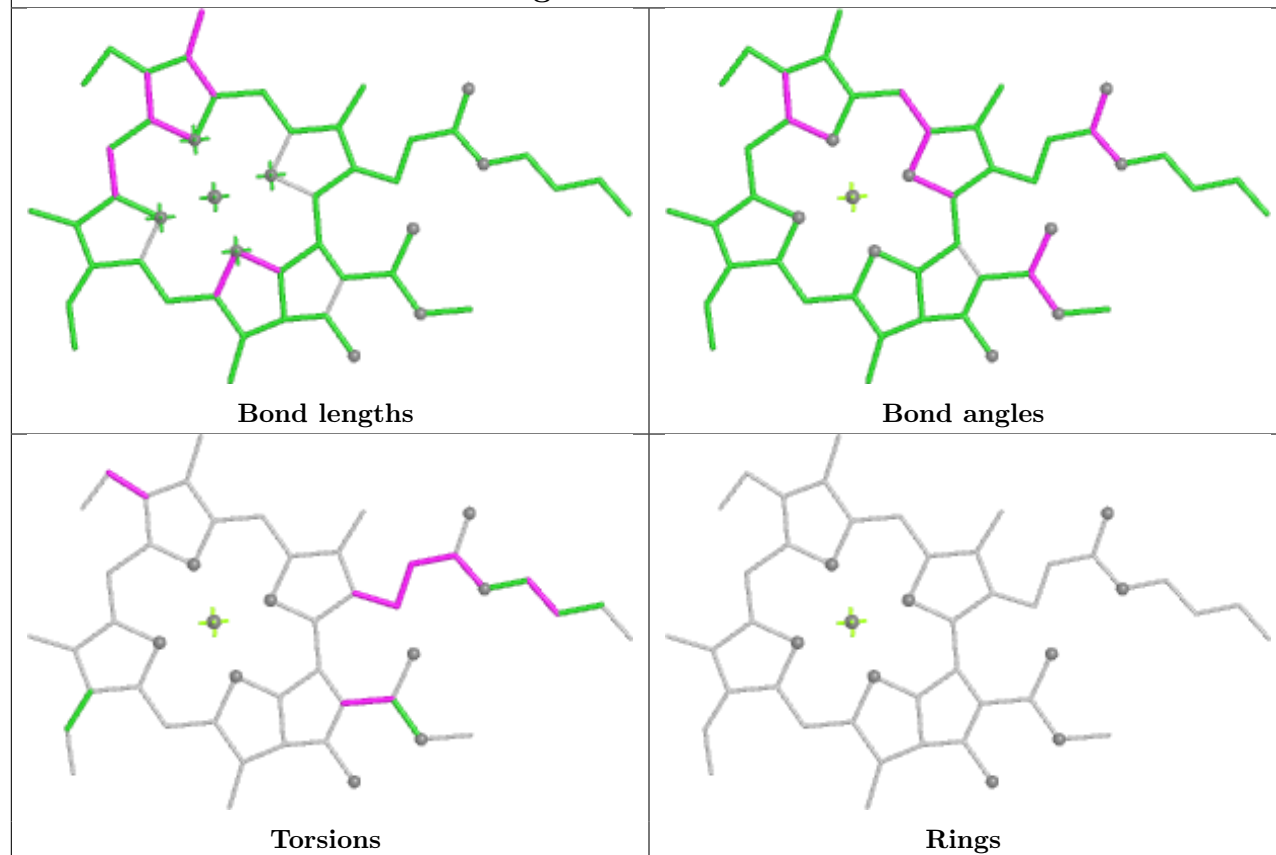


Torsions

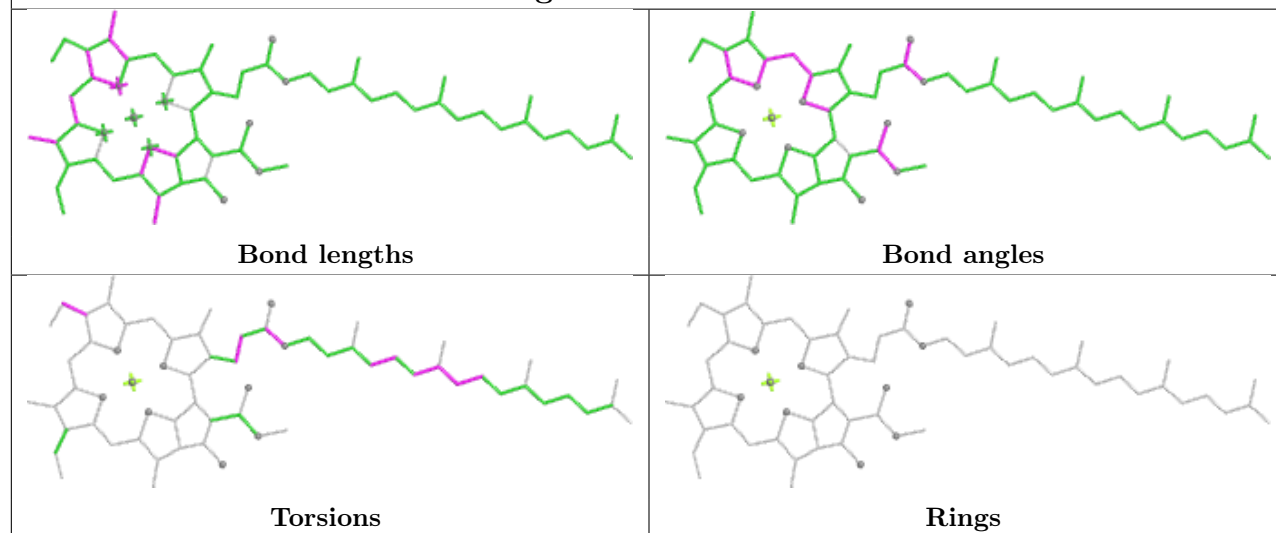


Rings

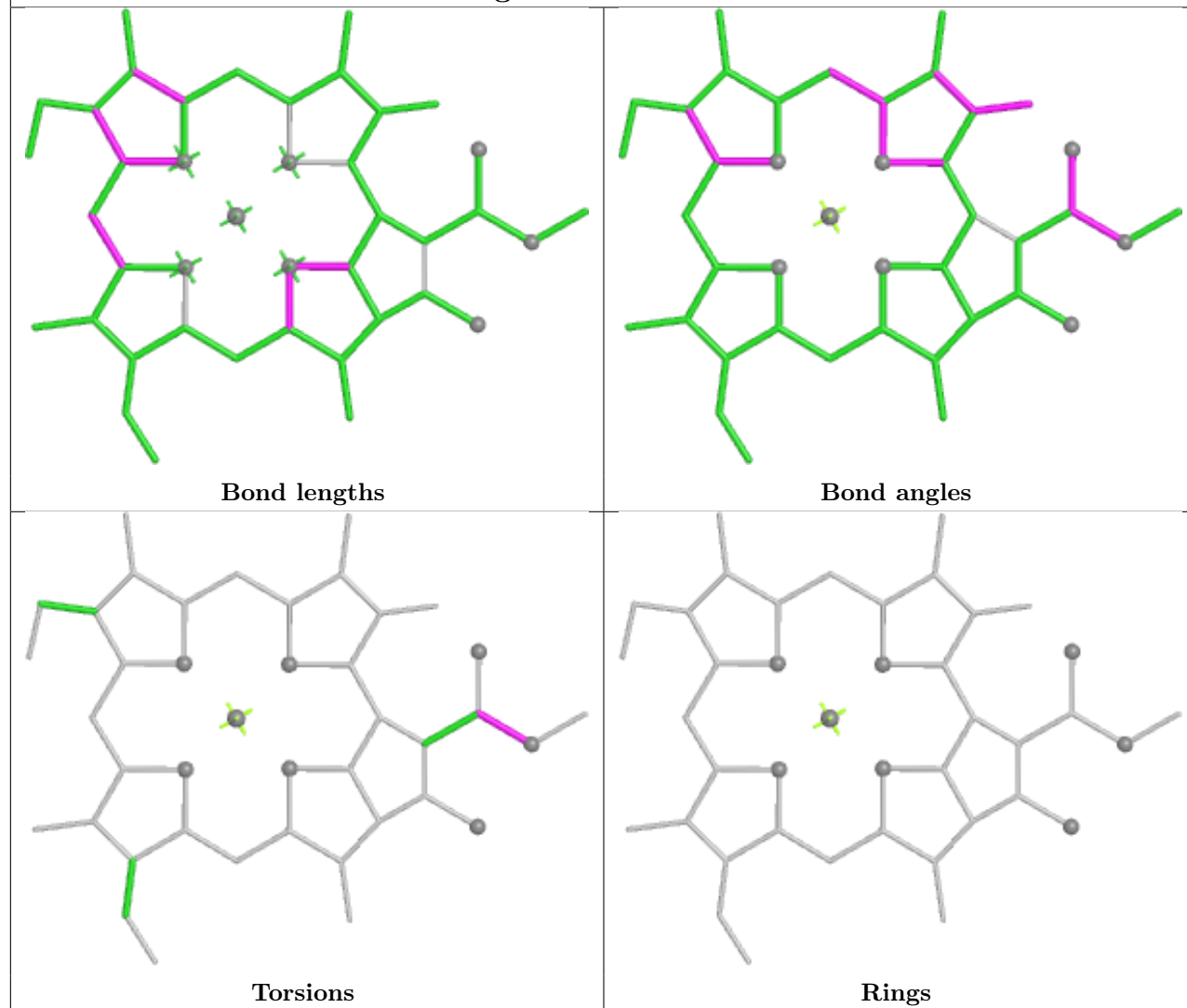
Ligand CLA E 319



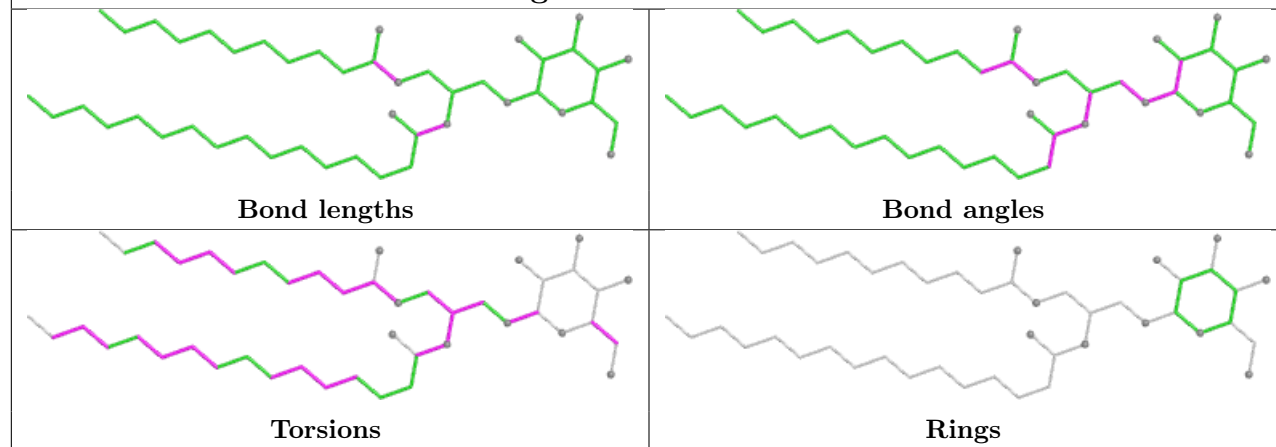
Ligand CLA b 840



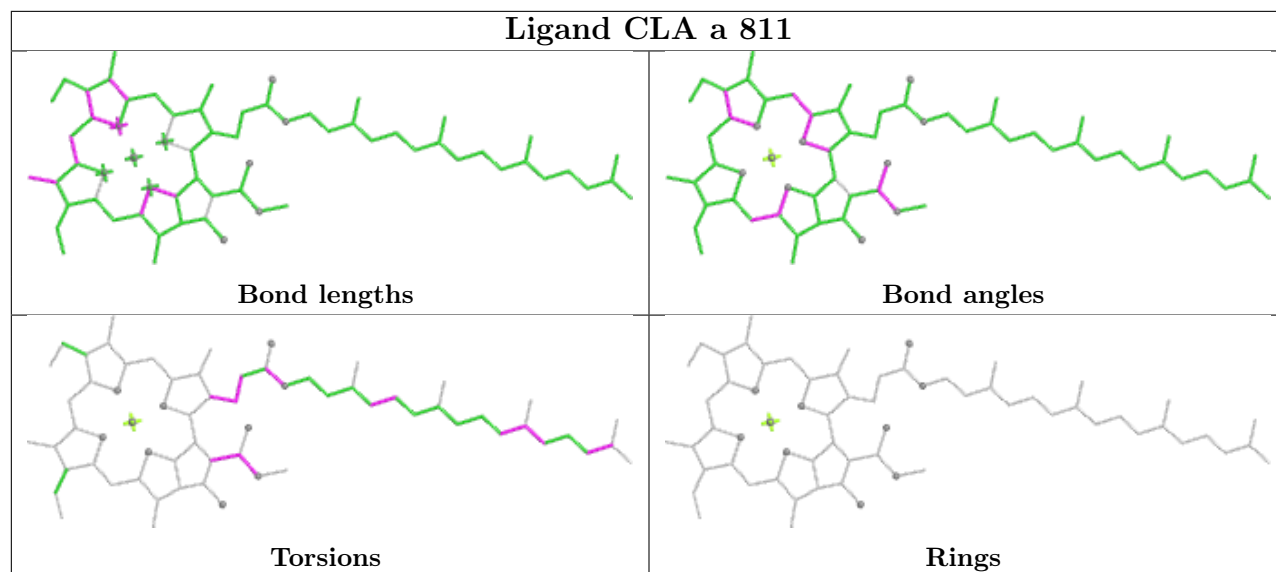
Ligand CLA Y 305



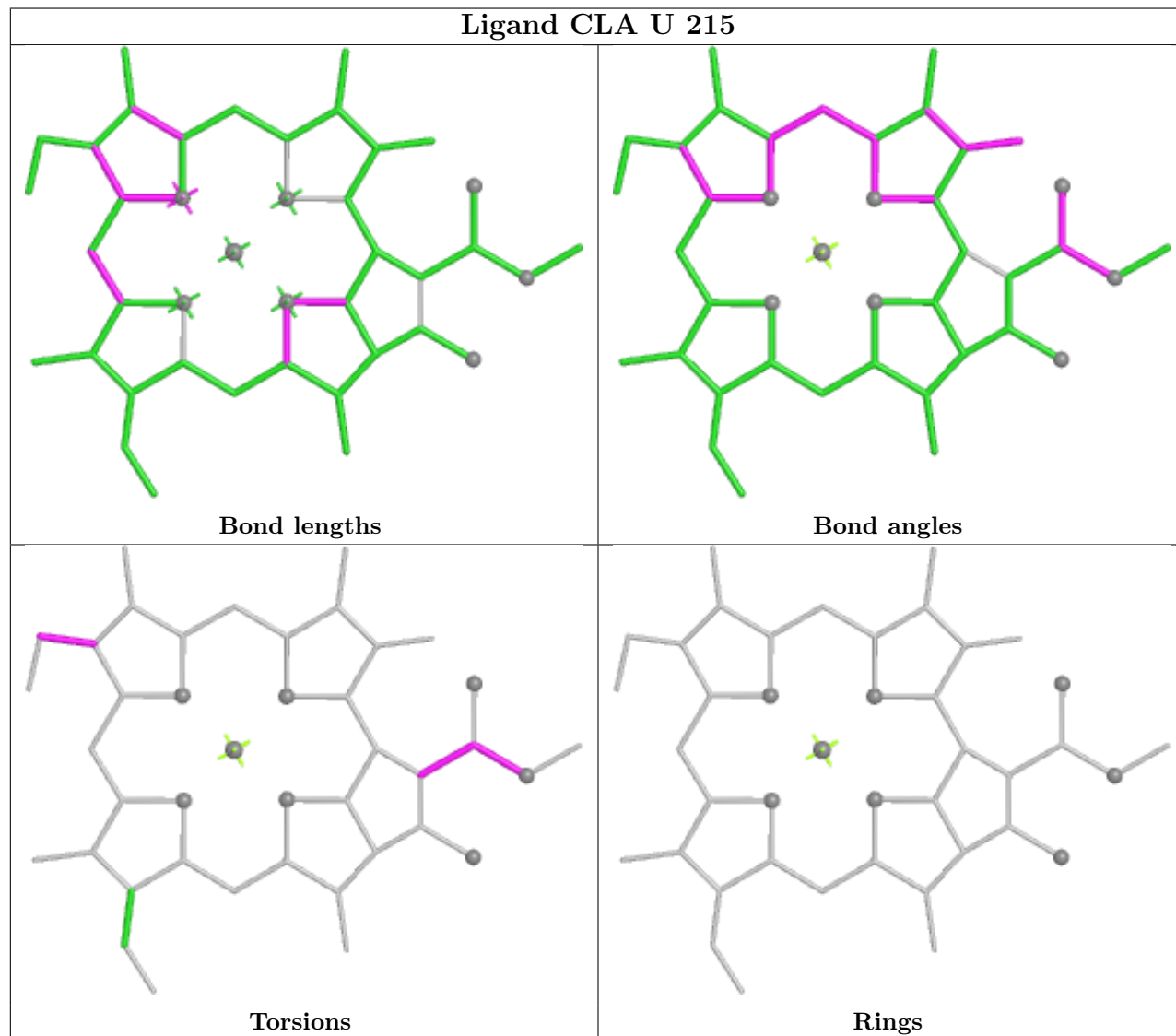
Ligand LMG S 322

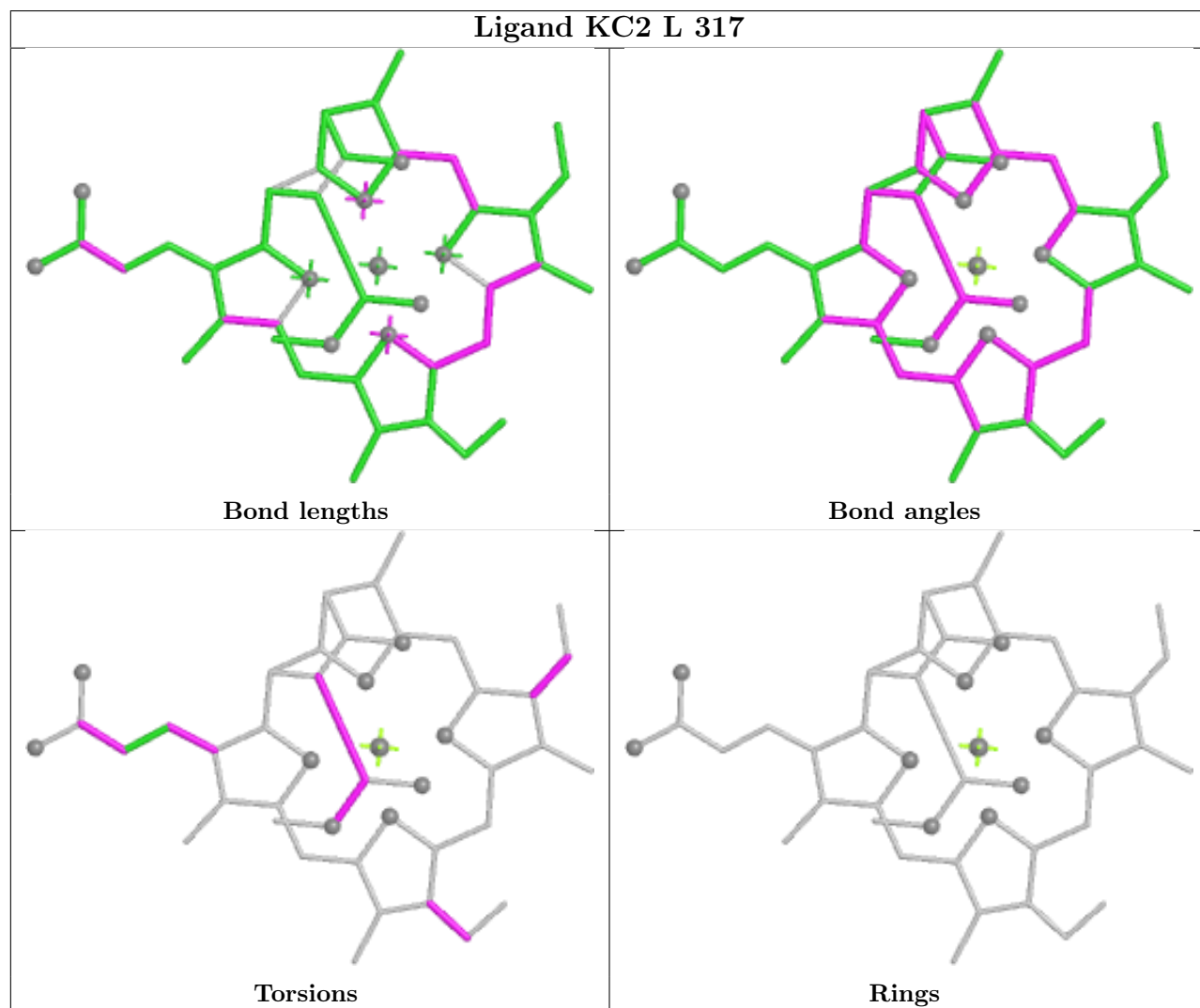
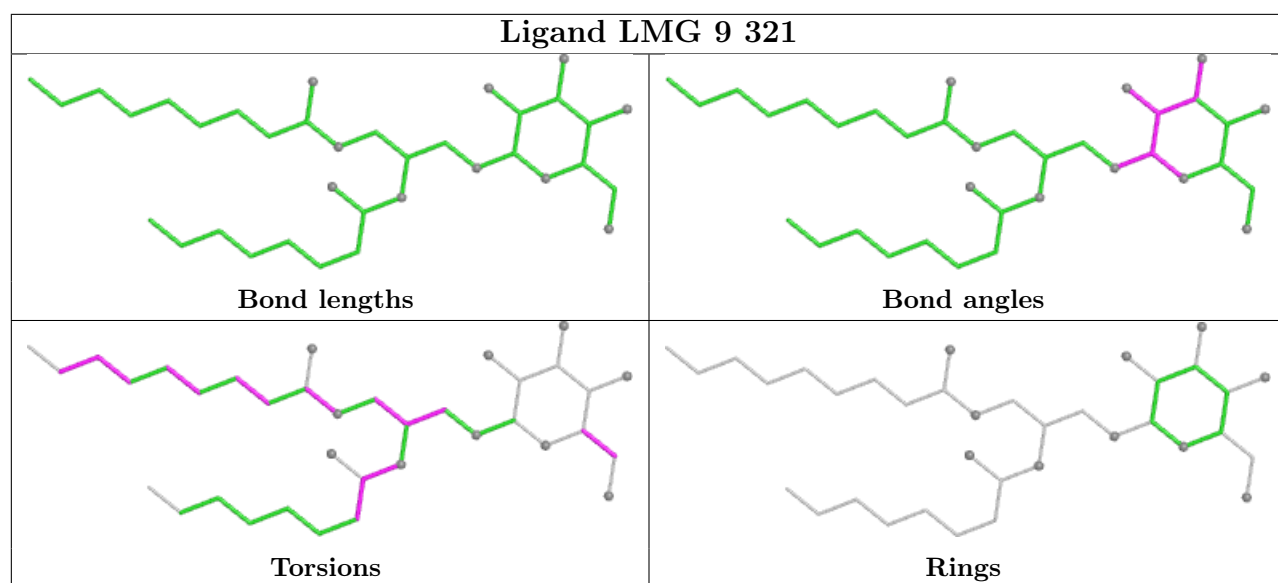


Ligand CLA a 811

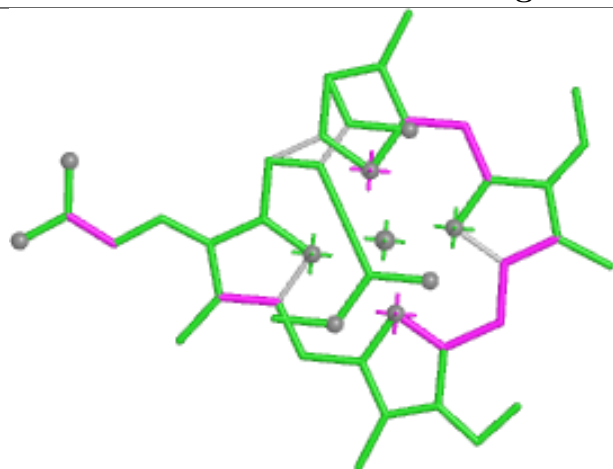


Ligand CLA U 215

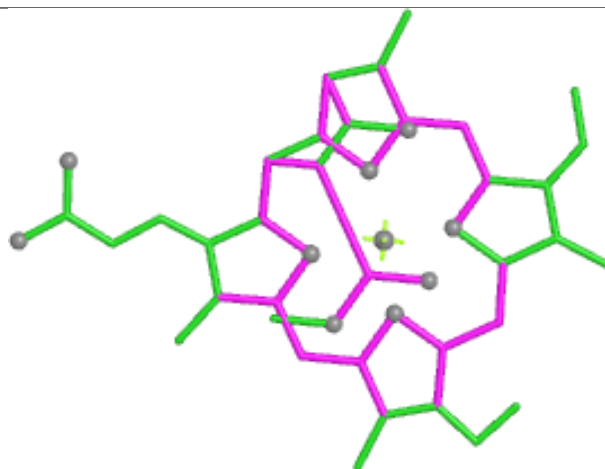




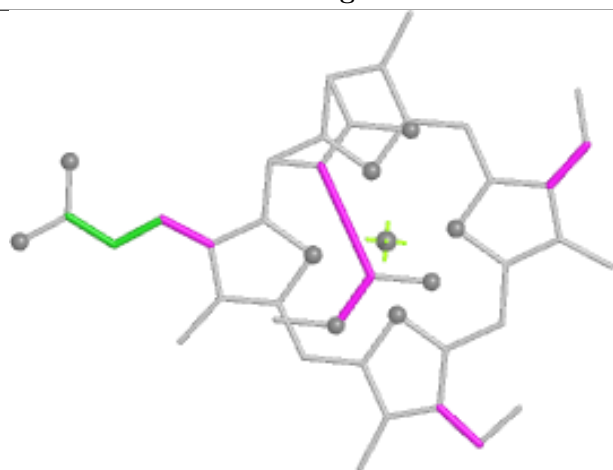
Ligand KC2 V 308



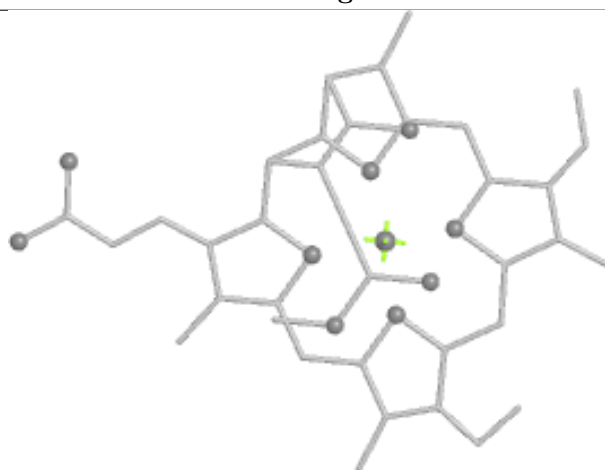
Bond lengths



Bond angles

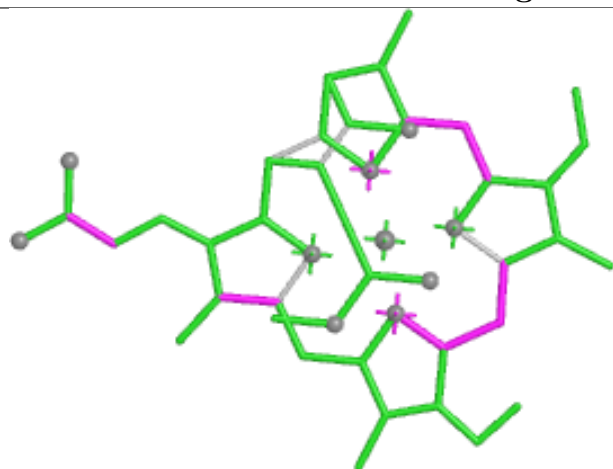


Torsions

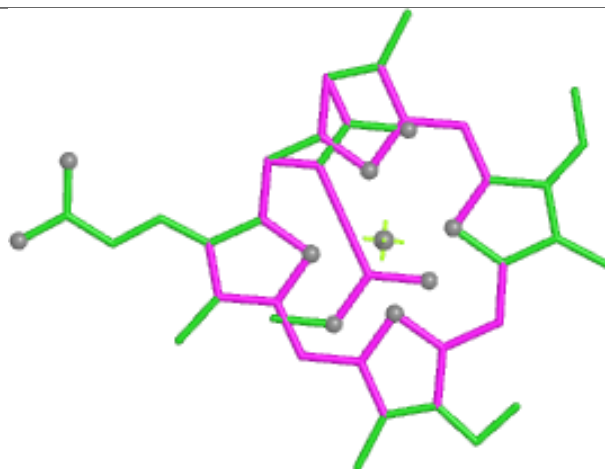


Rings

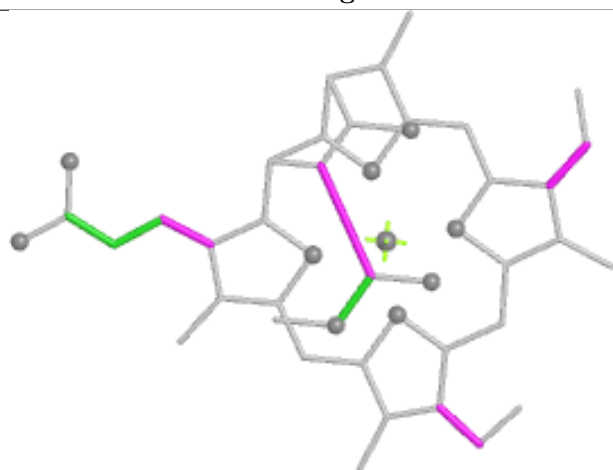
Ligand KC2 X 312



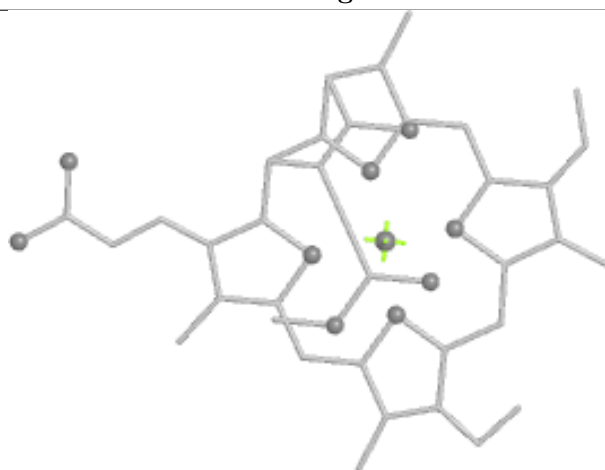
Bond lengths



Bond angles

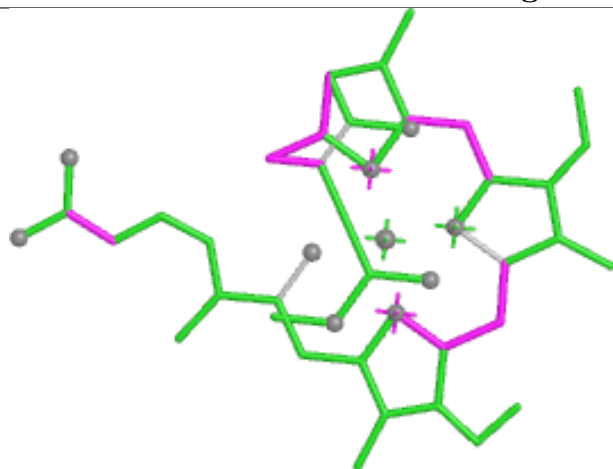


Torsions

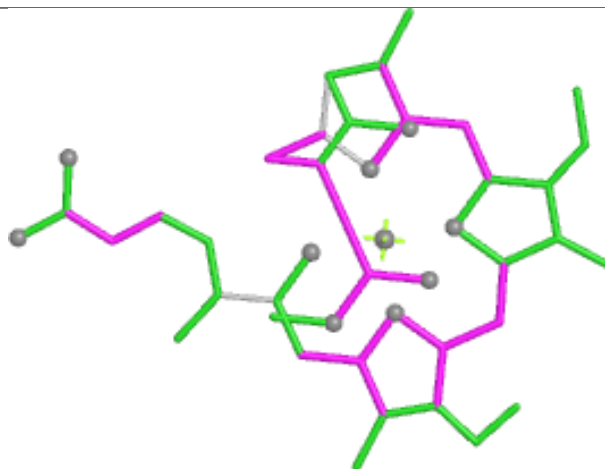


Rings

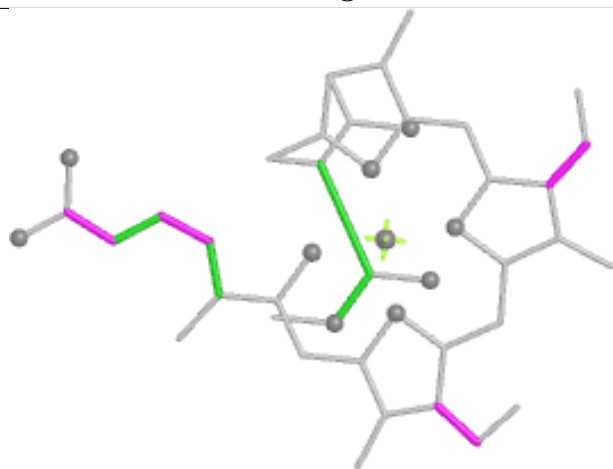
Ligand KC2 z 313



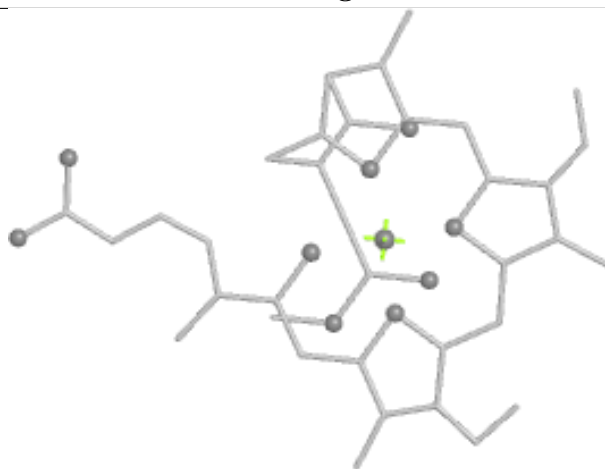
Bond lengths



Bond angles

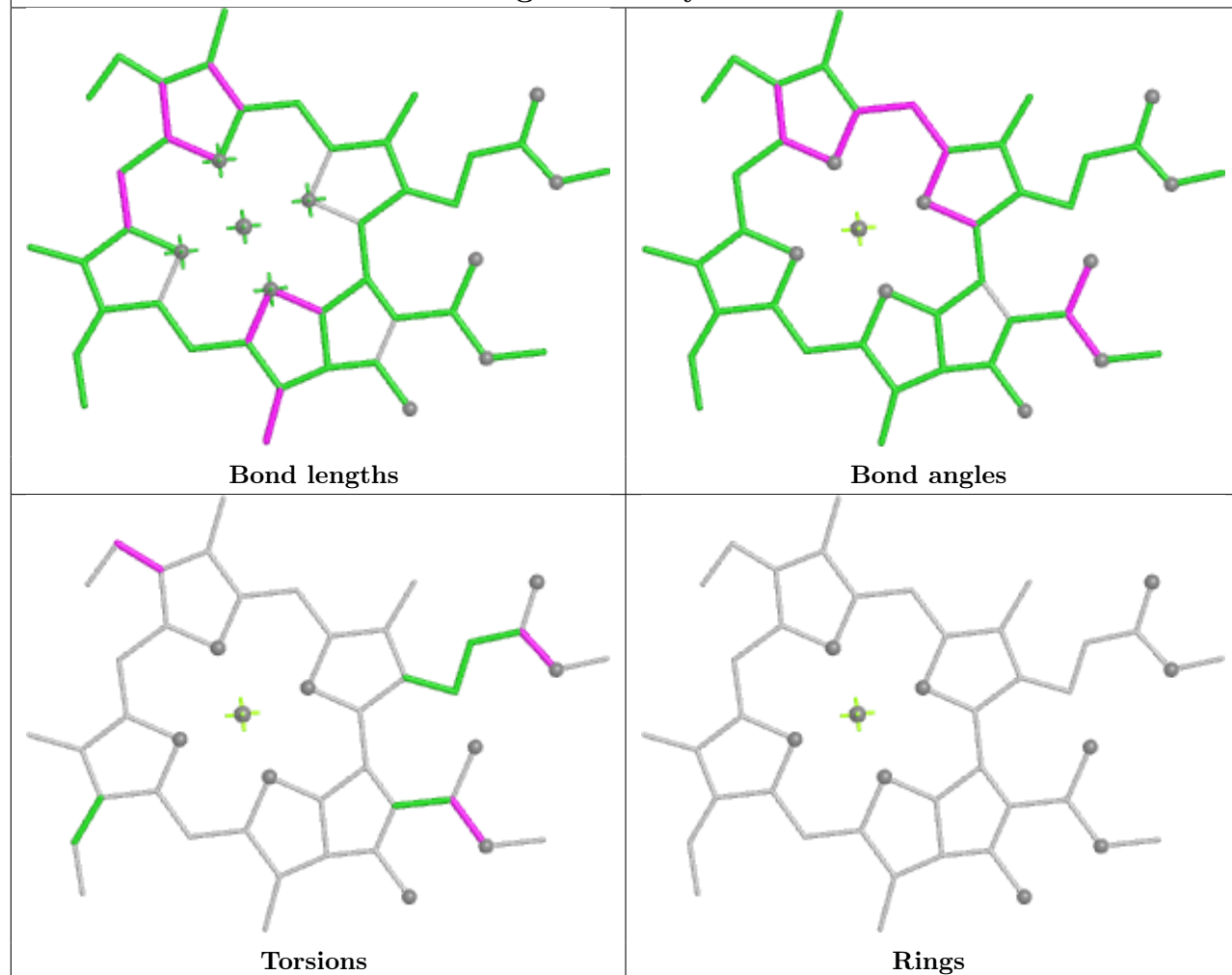


Torsions

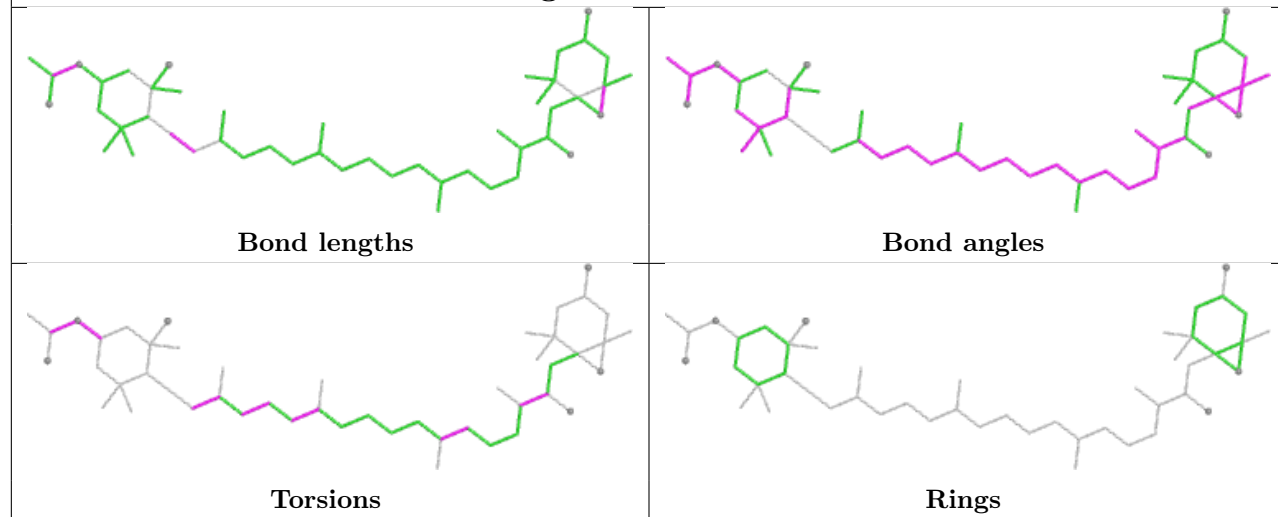


Rings

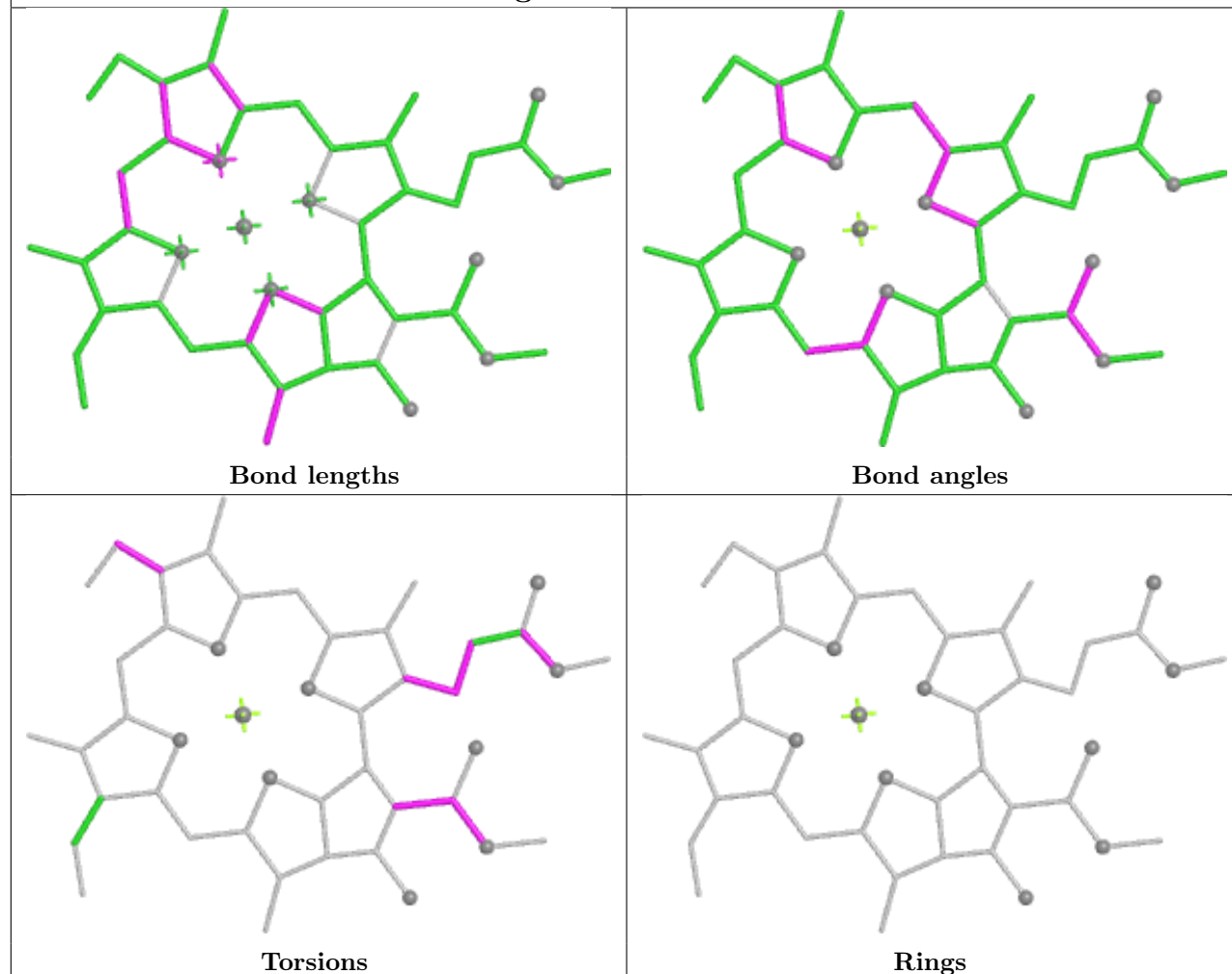
Ligand CLA y 309



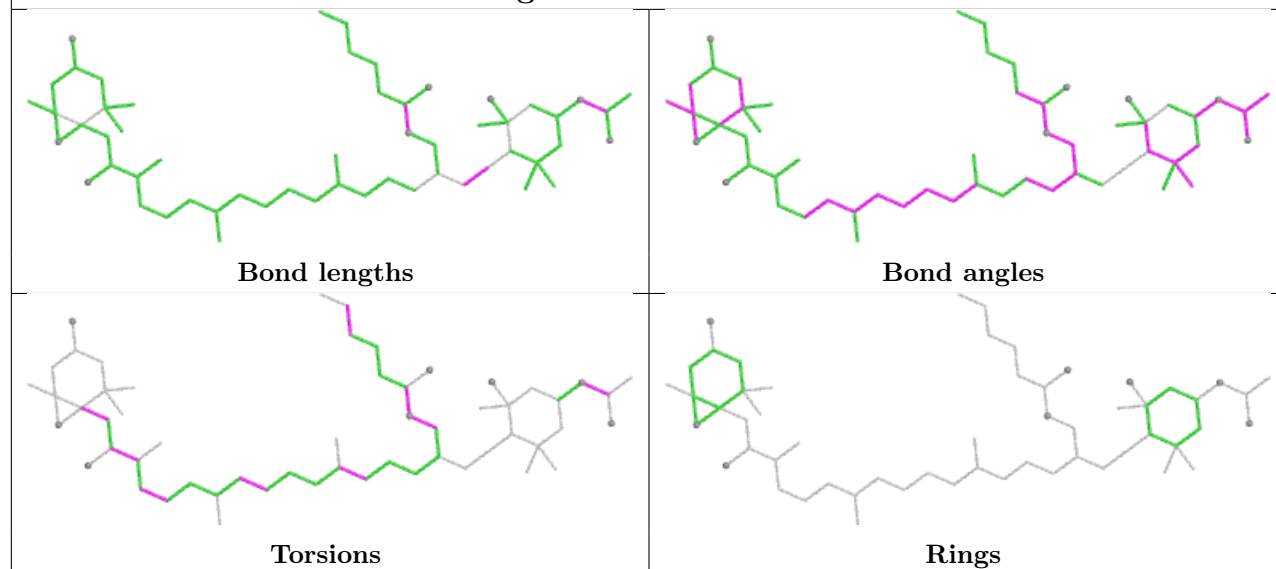
Ligand A86 Z 301

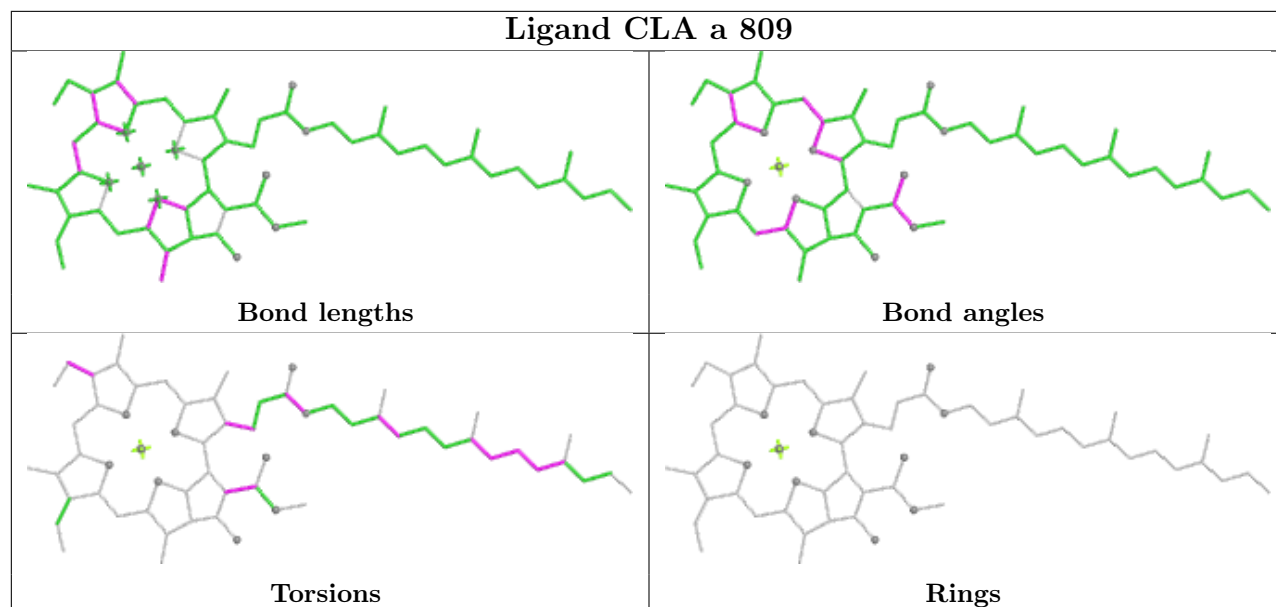
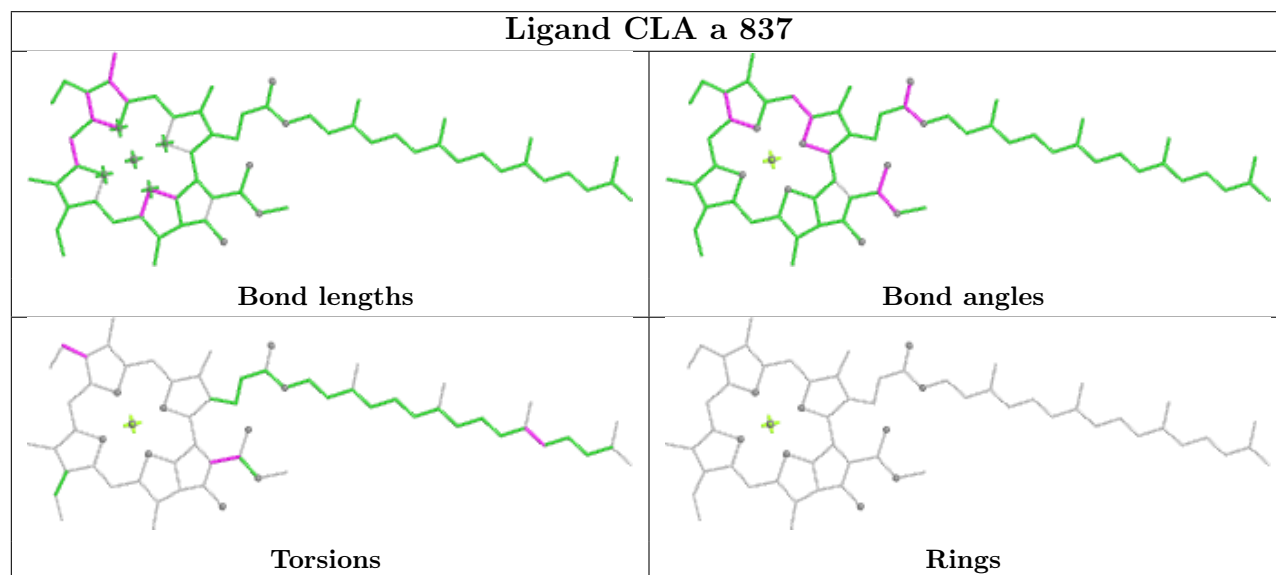


Ligand CLA E 318

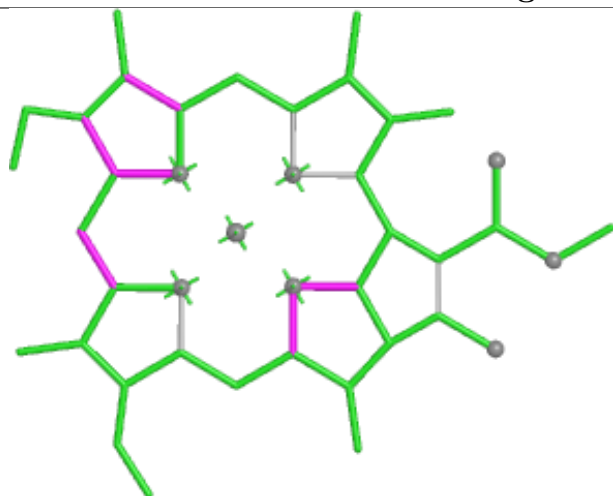


Ligand A1EB1 x 302

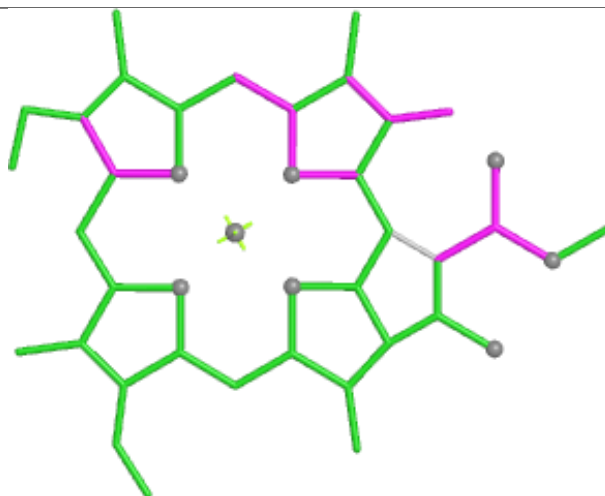


Ligand CLA a 809**Ligand CLA a 837**

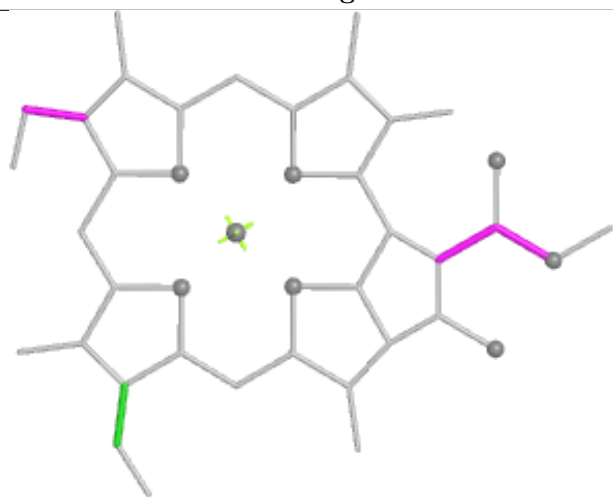
Ligand CLA x 317



Bond lengths



Bond angles

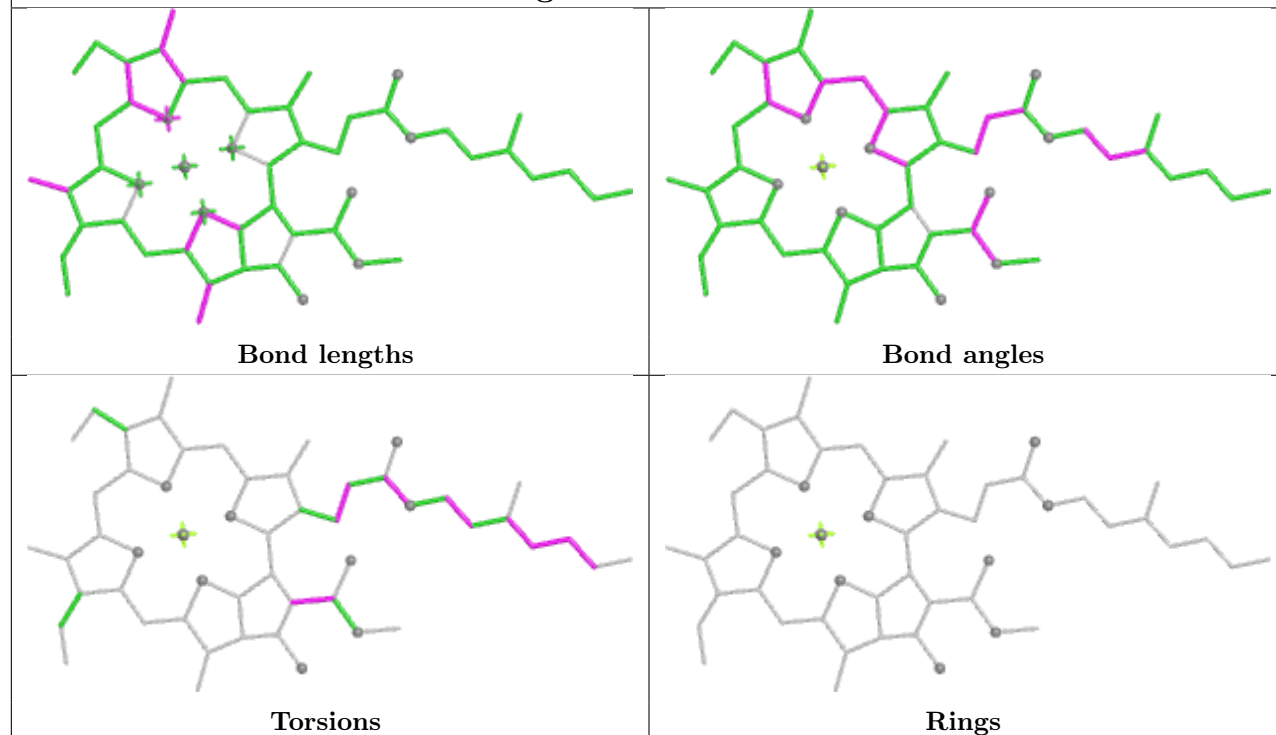


Torsions

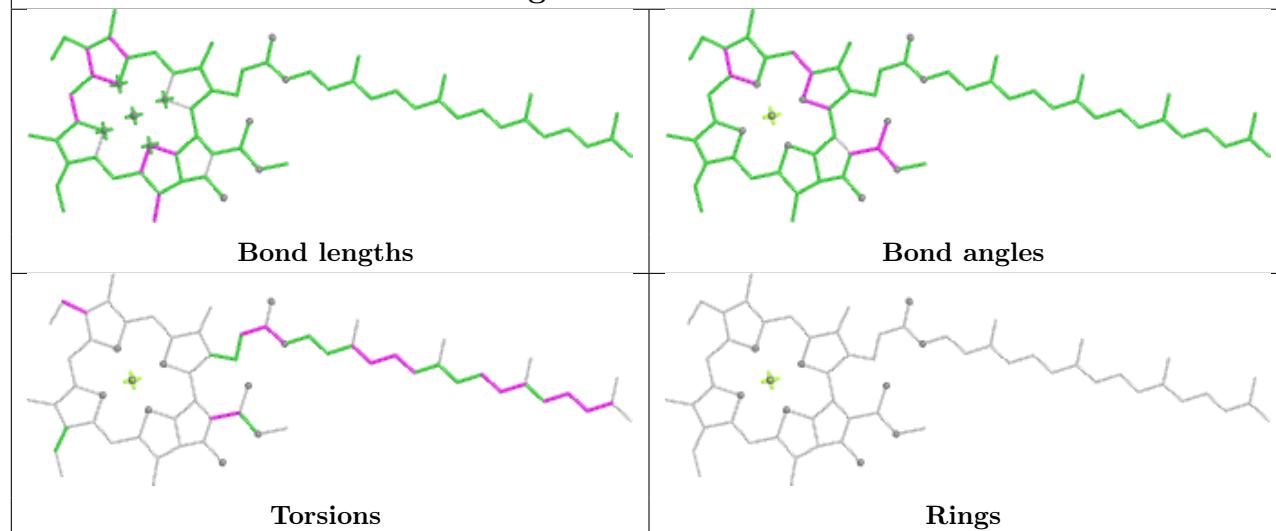


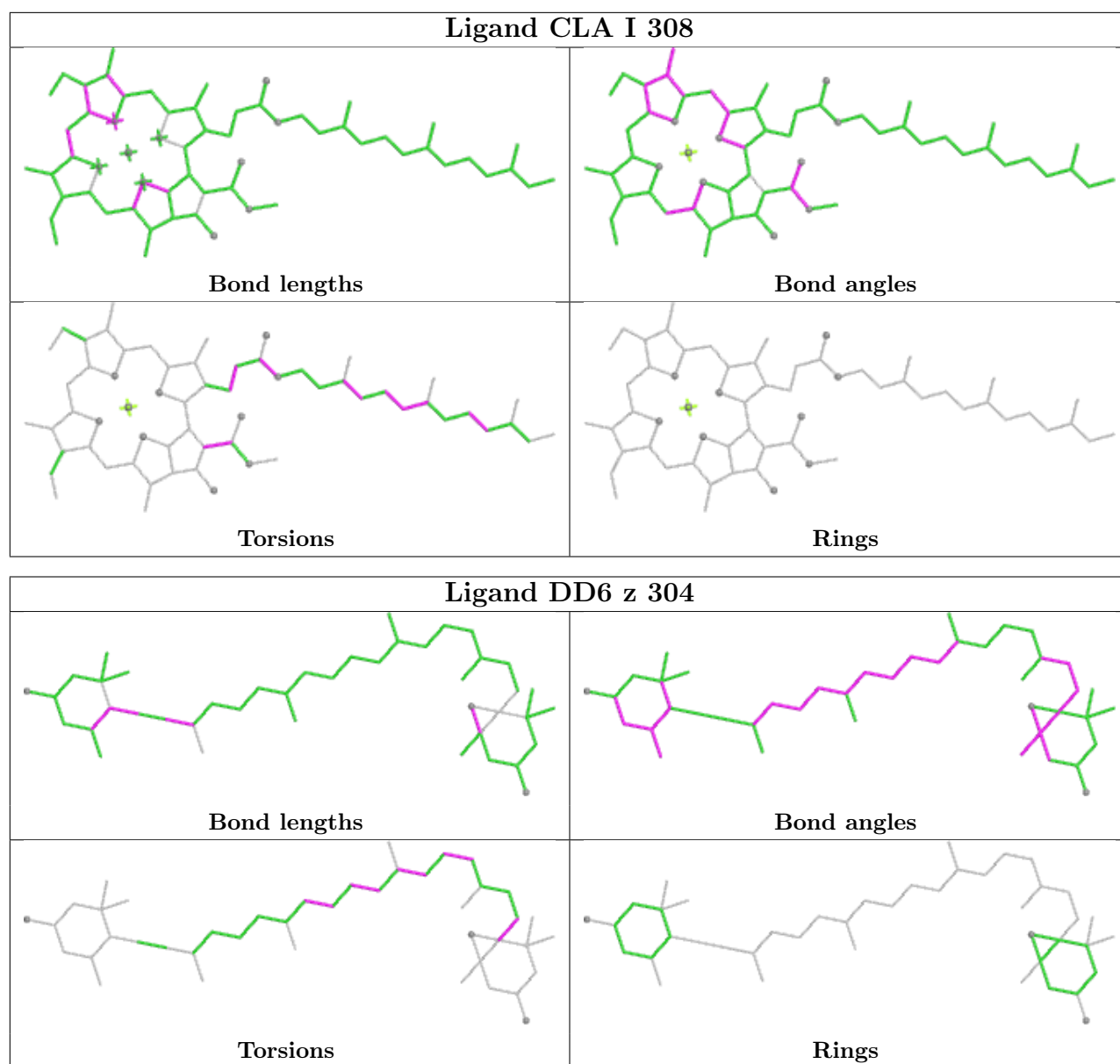
Rings

Ligand CLA 0 312

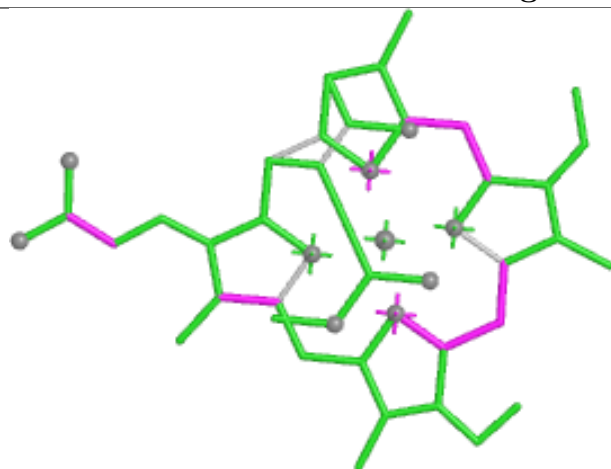


Ligand CLA M 309

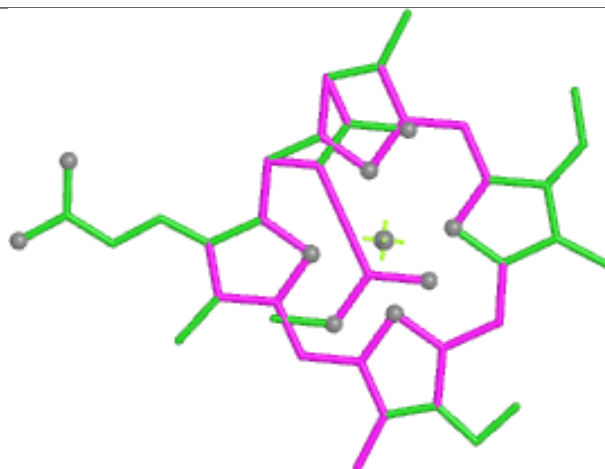




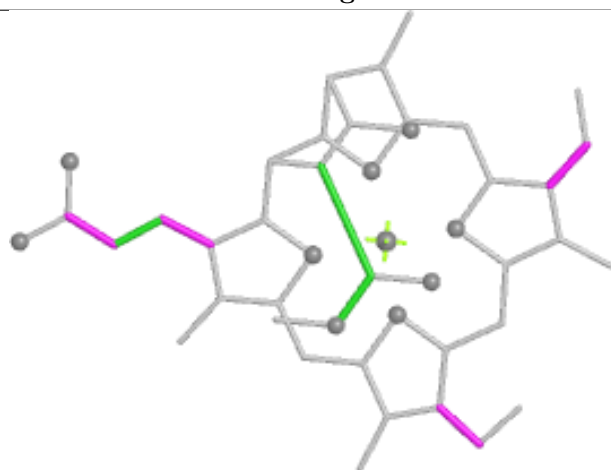
Ligand KC2 3 317



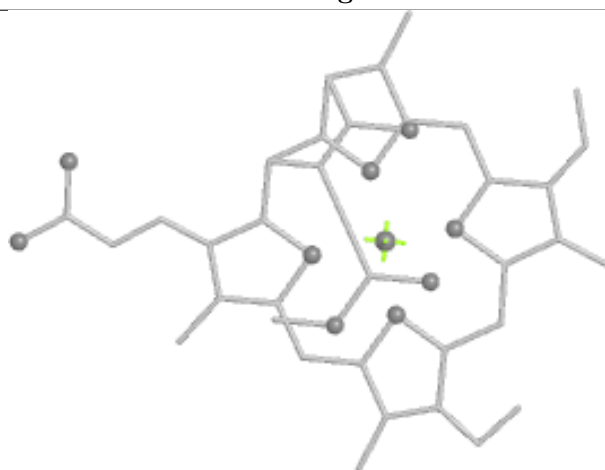
Bond lengths



Bond angles

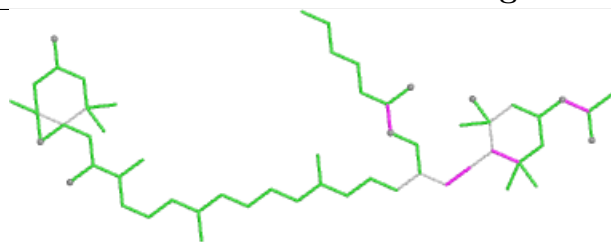


Torsions

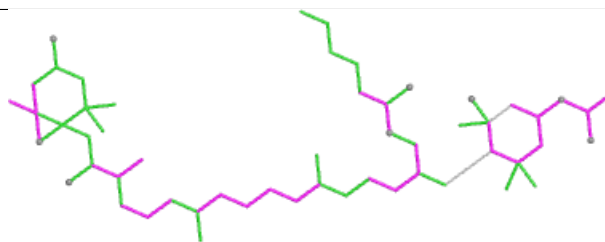


Rings

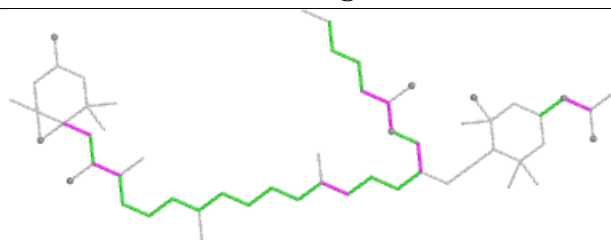
Ligand A1EB1 8 301



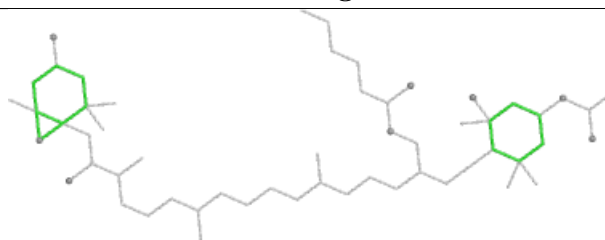
Bond lengths



Bond angles

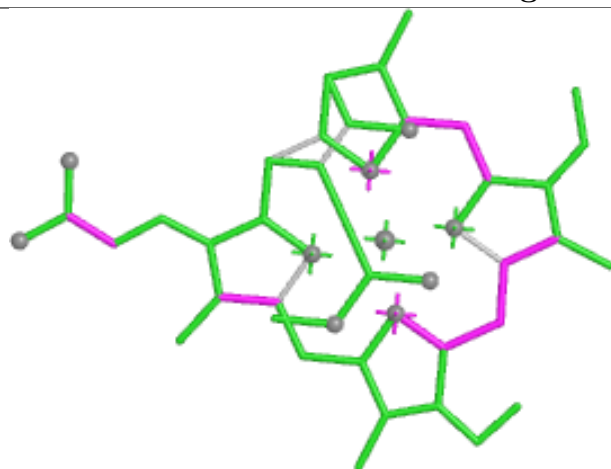


Torsions

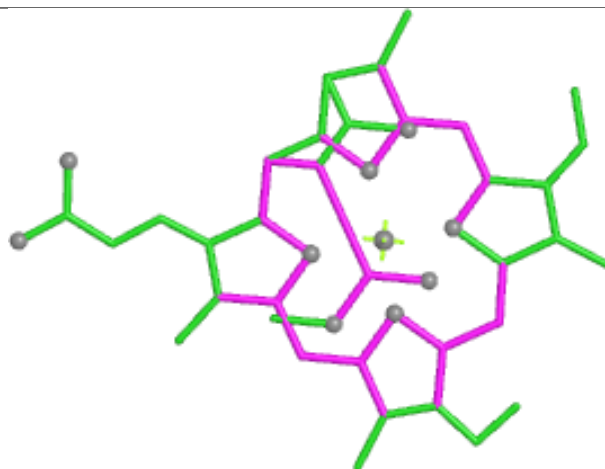


Rings

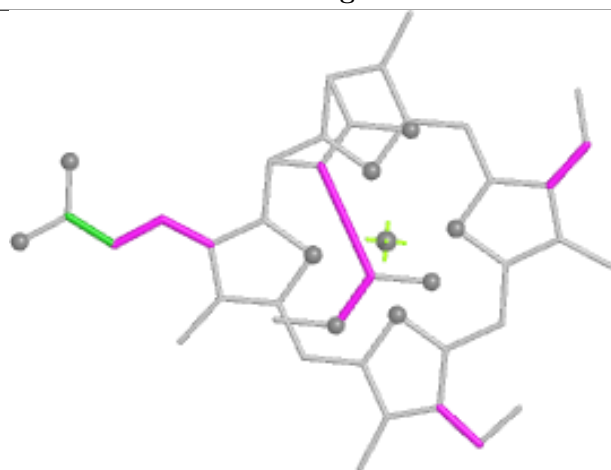
Ligand KC2 8 316



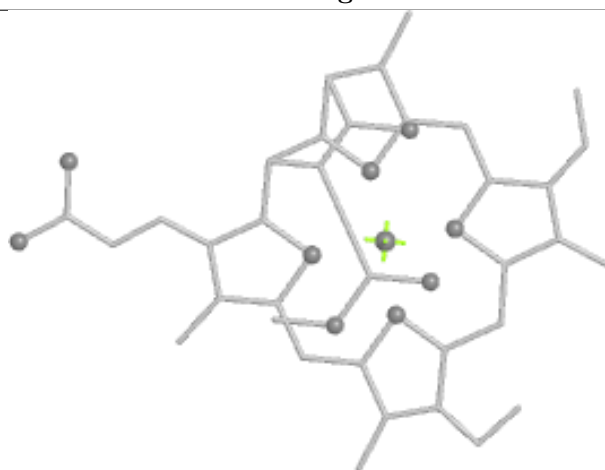
Bond lengths



Bond angles

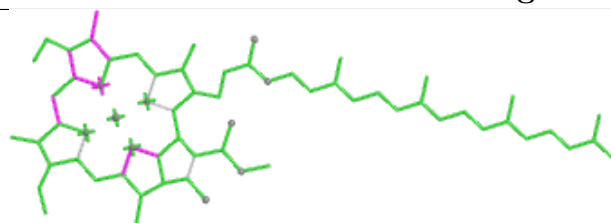


Torsions

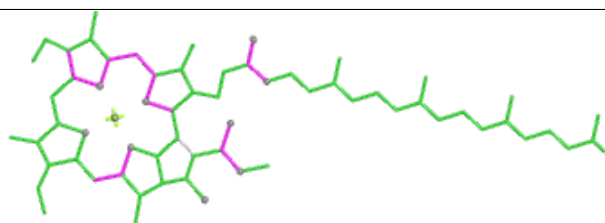


Rings

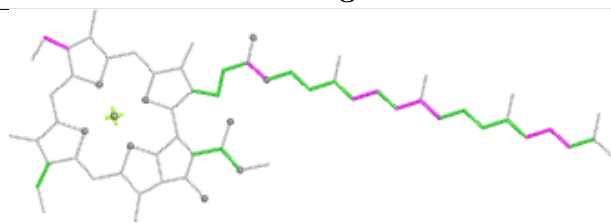
Ligand CLA b 821



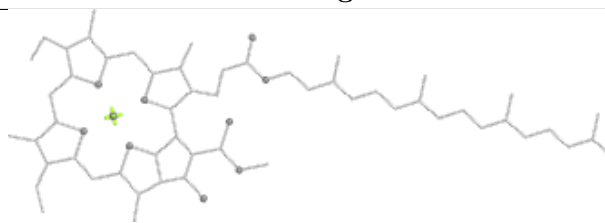
Bond lengths



Bond angles

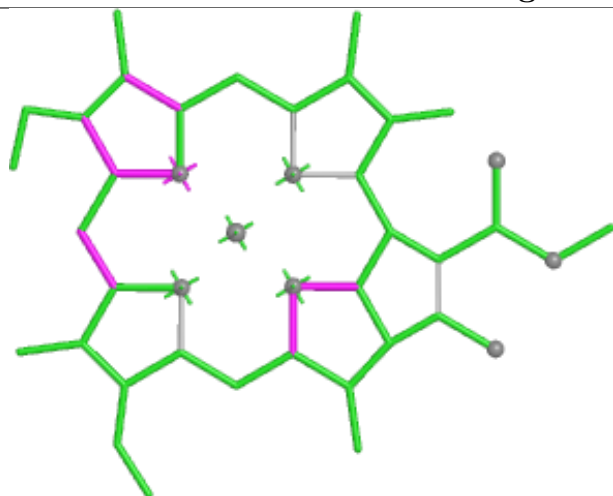


Torsions

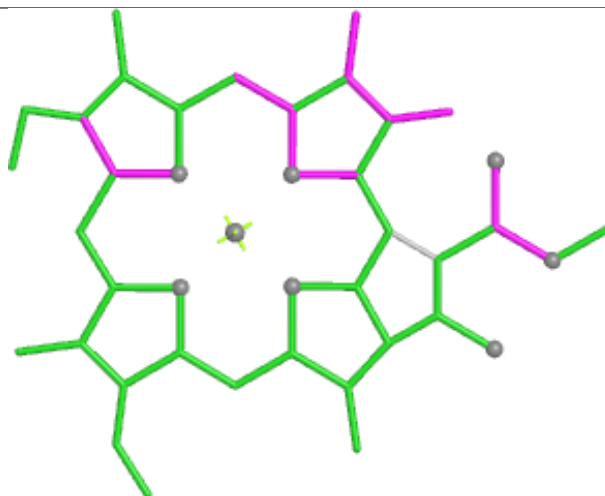


Rings

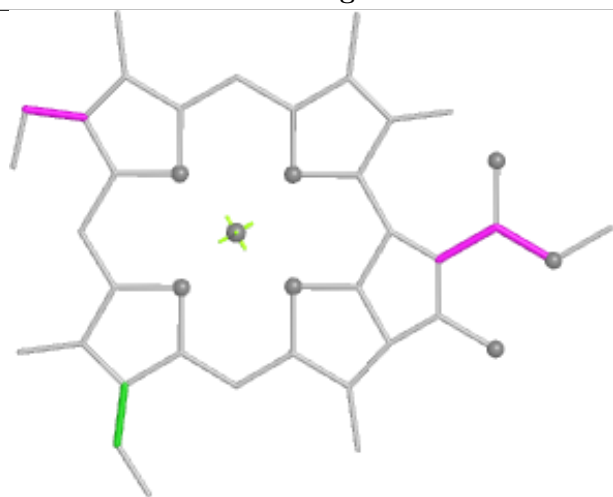
Ligand CLA 8 313



Bond lengths



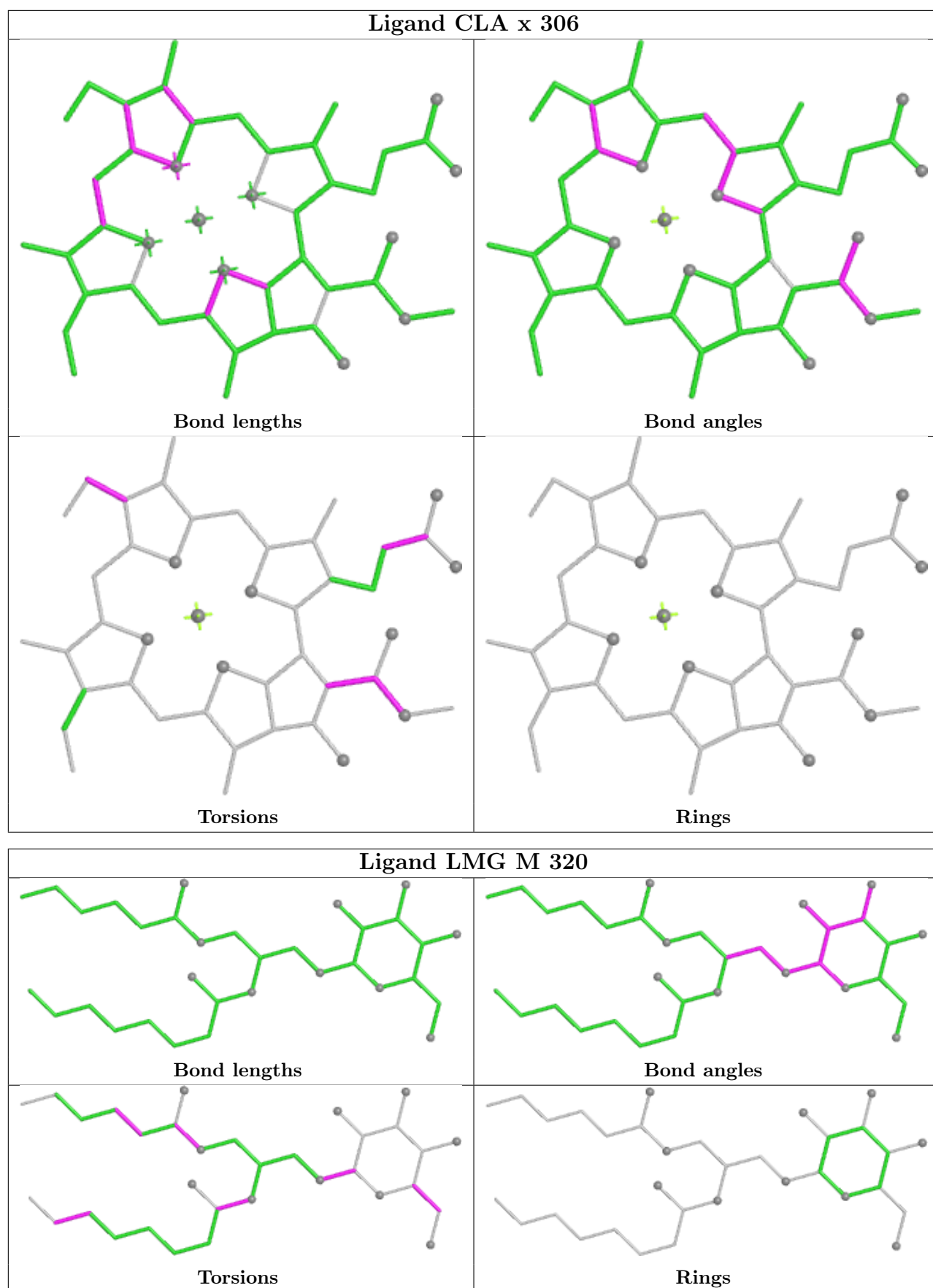
Bond angles

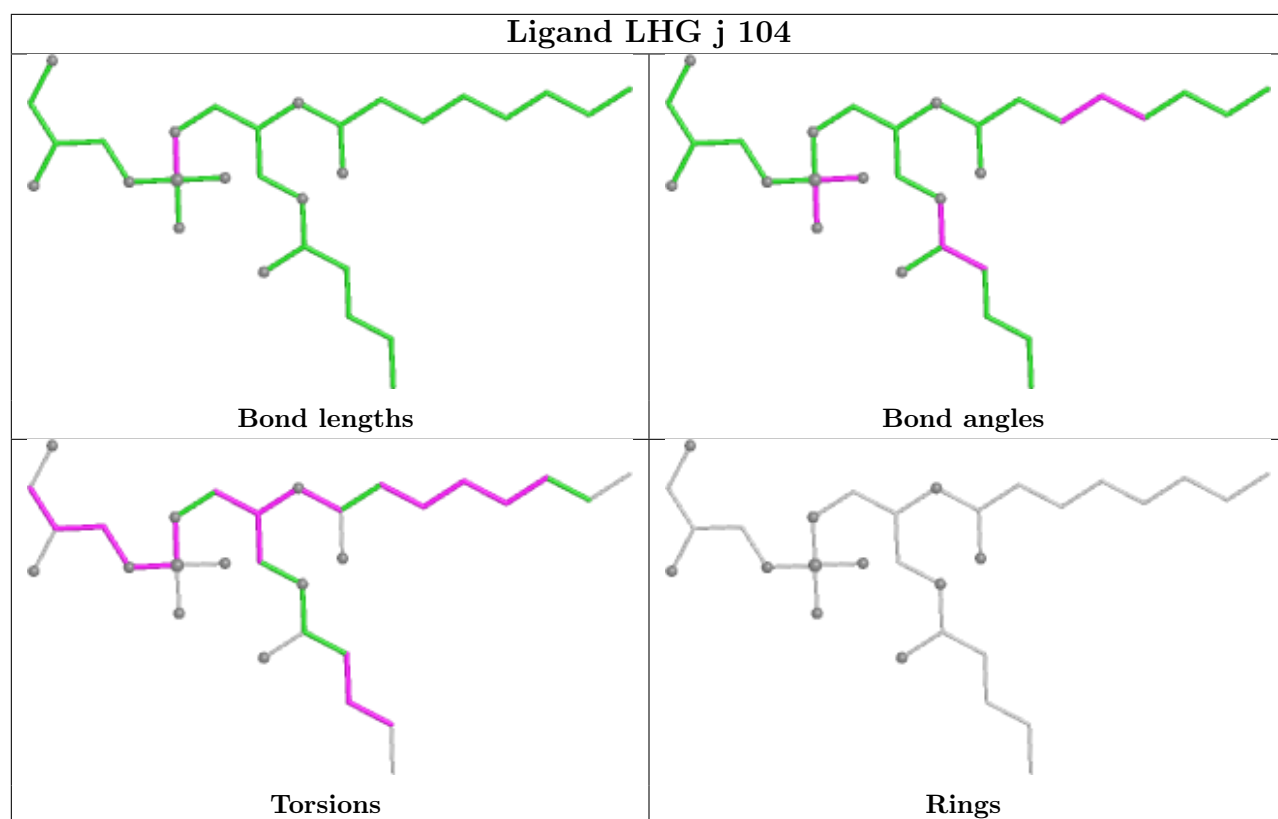


Torsions

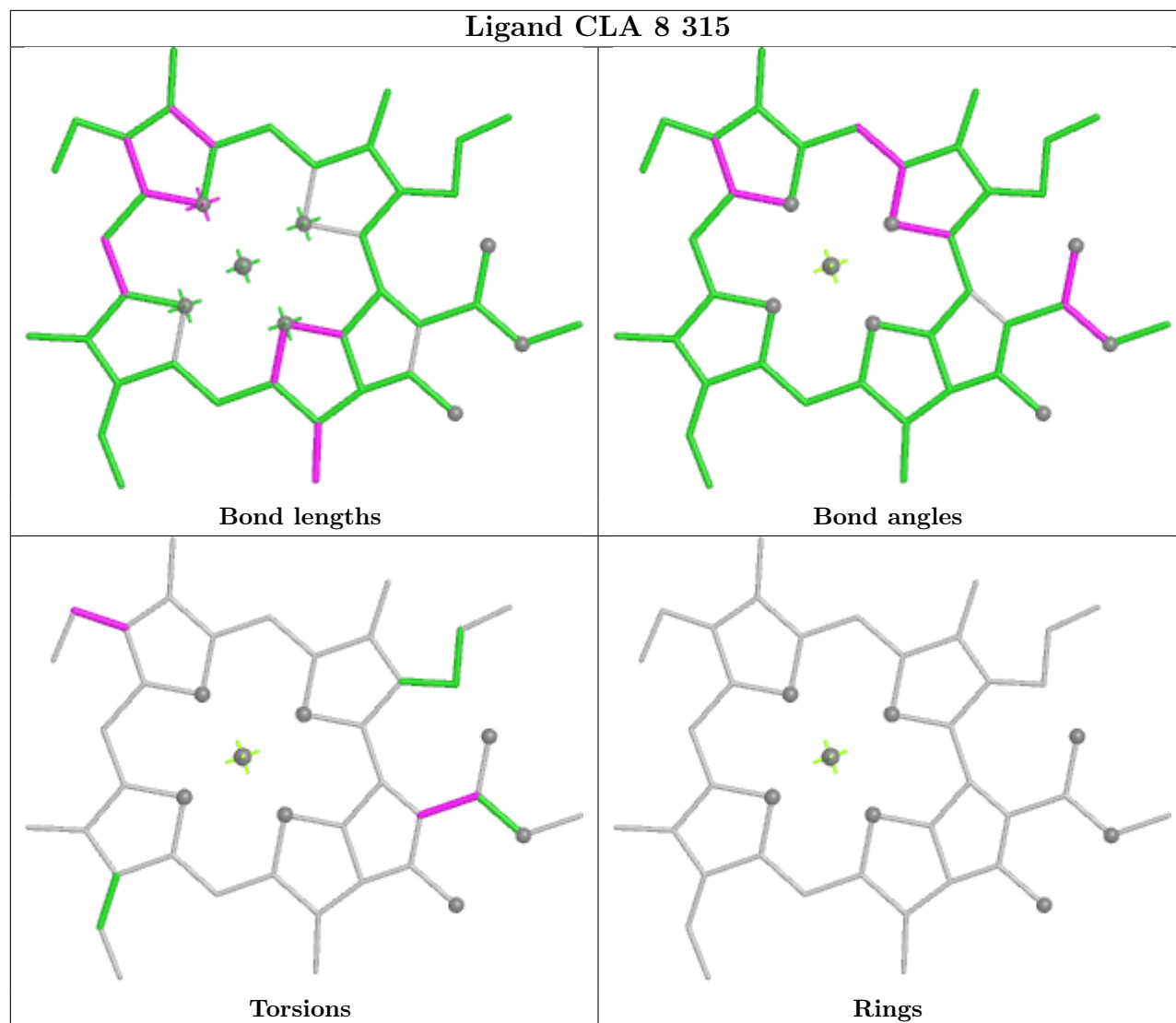


Rings

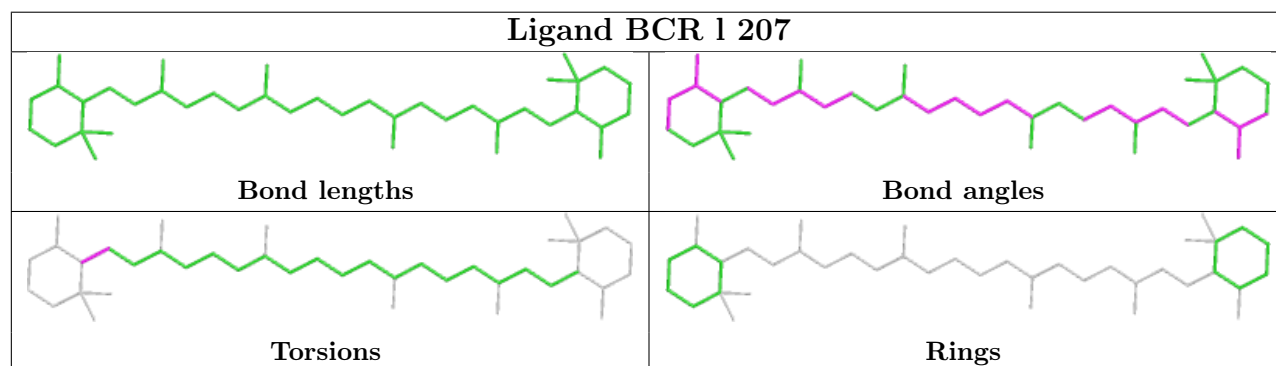


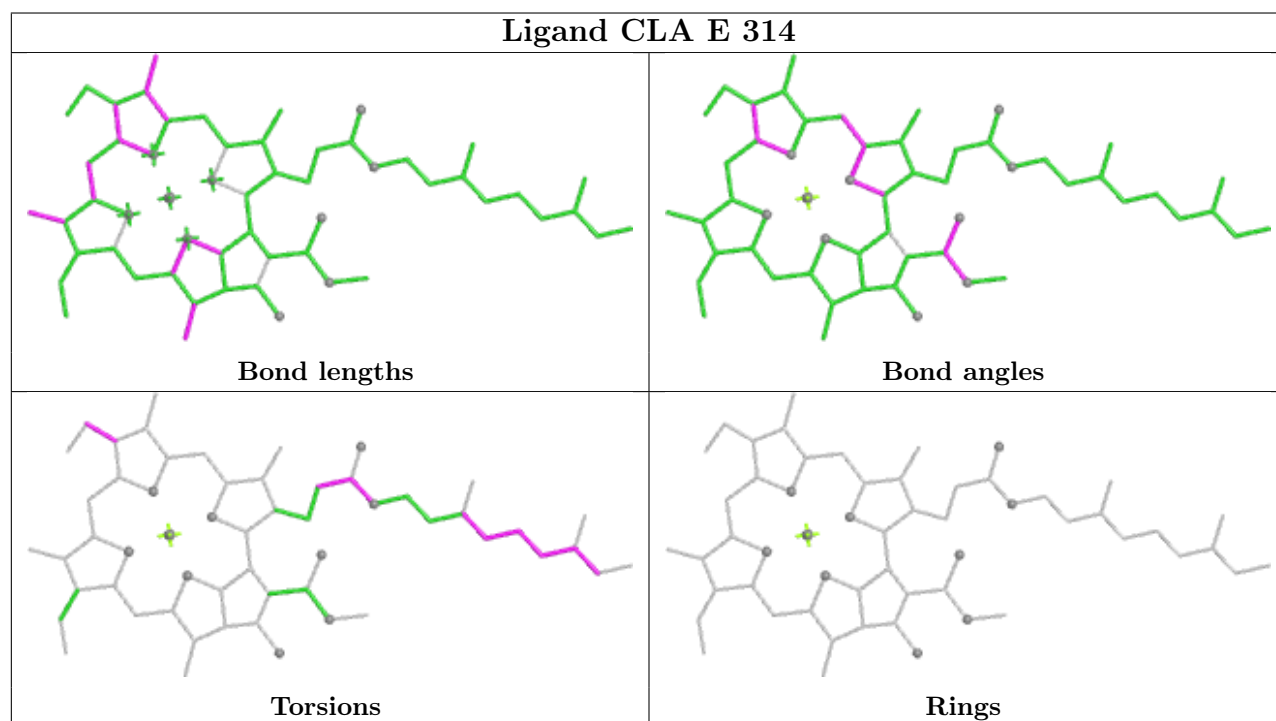
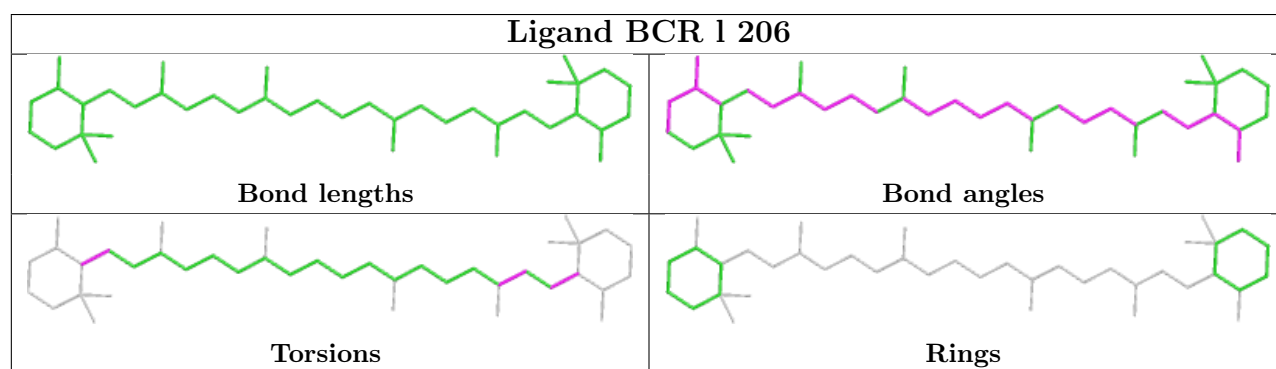
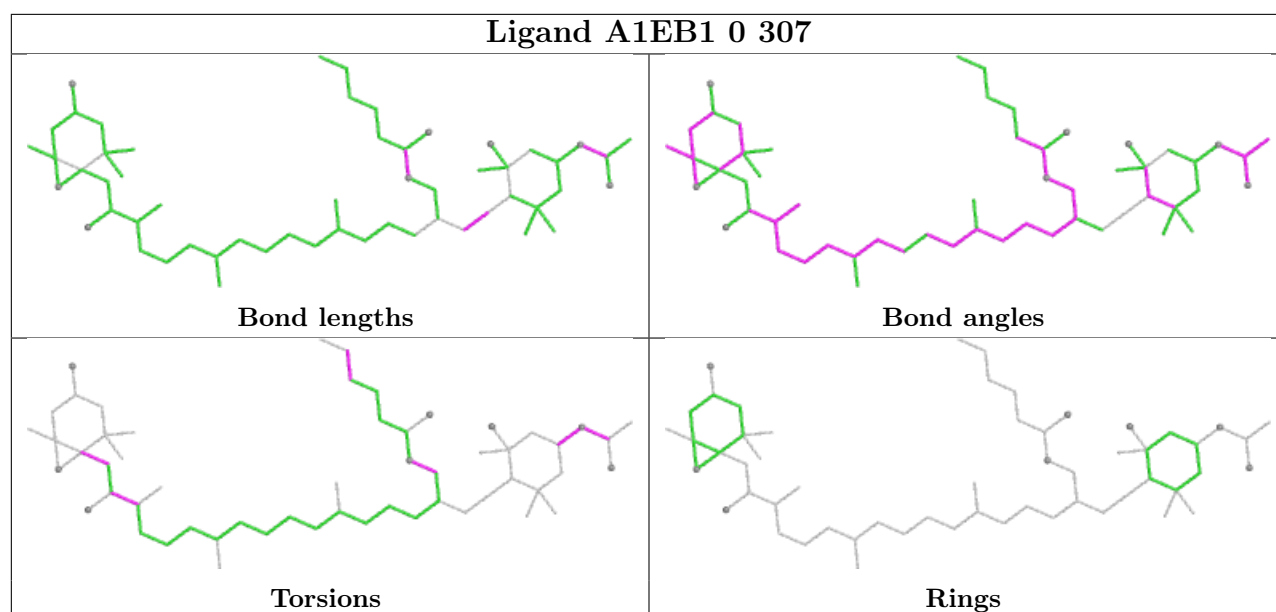


Ligand CLA 8 315

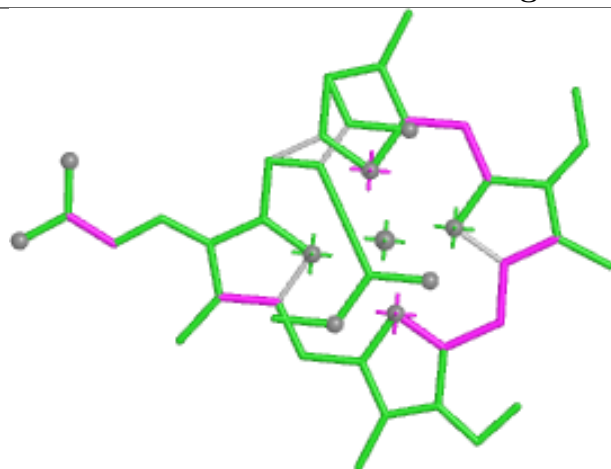


Ligand BCR 1 207

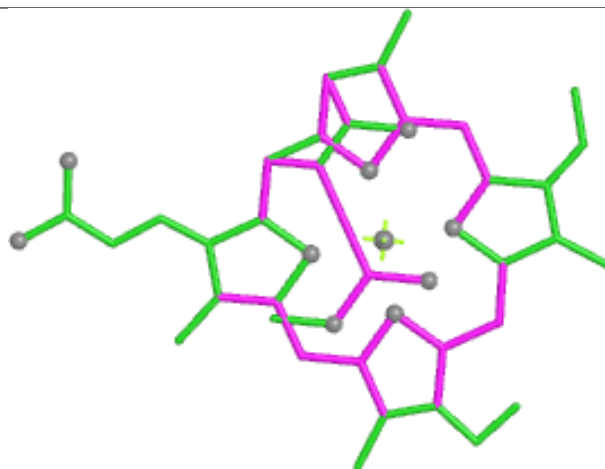




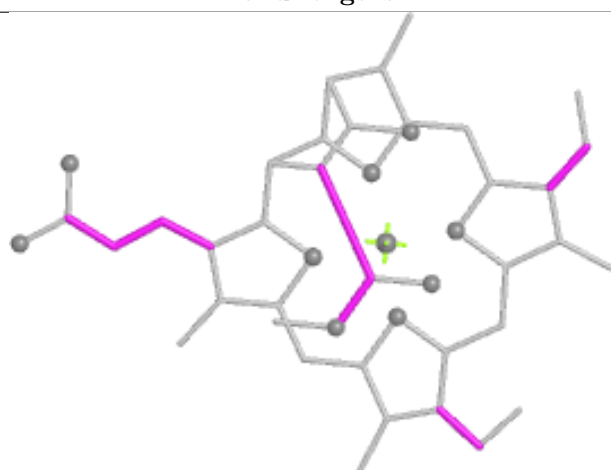
Ligand KC2 8 319



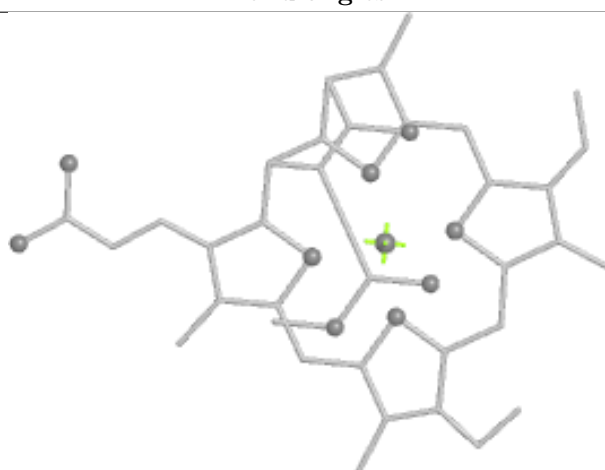
Bond lengths



Bond angles

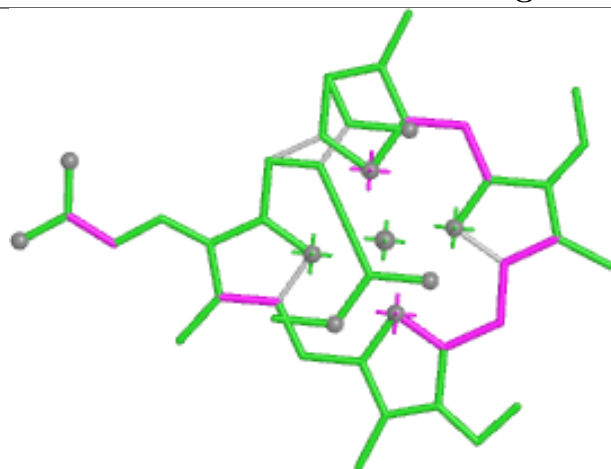


Torsions

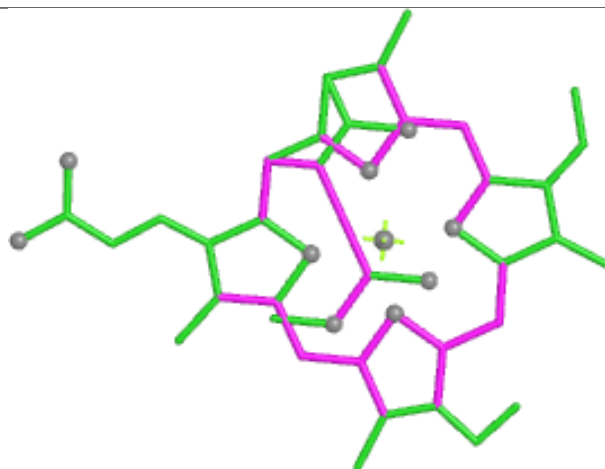


Rings

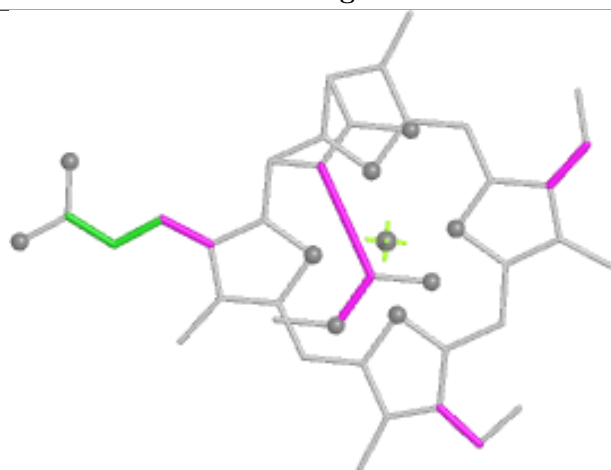
Ligand KC2 R 306



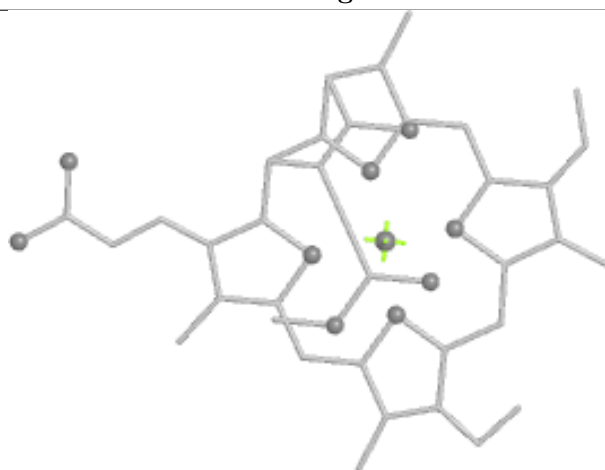
Bond lengths



Bond angles

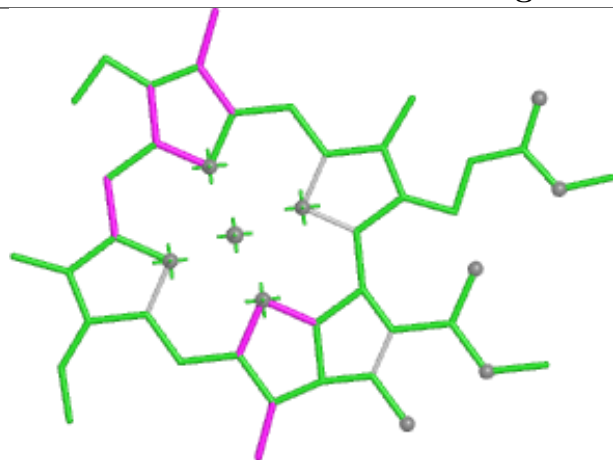


Torsions

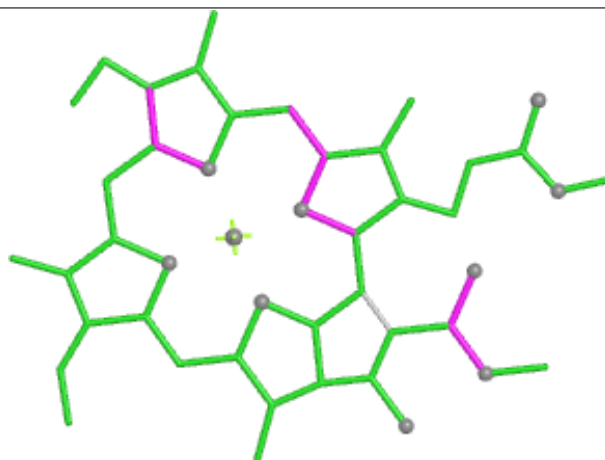


Rings

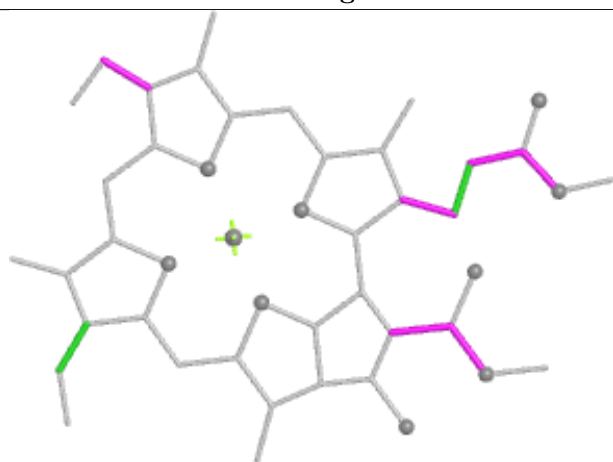
Ligand CLA E 315



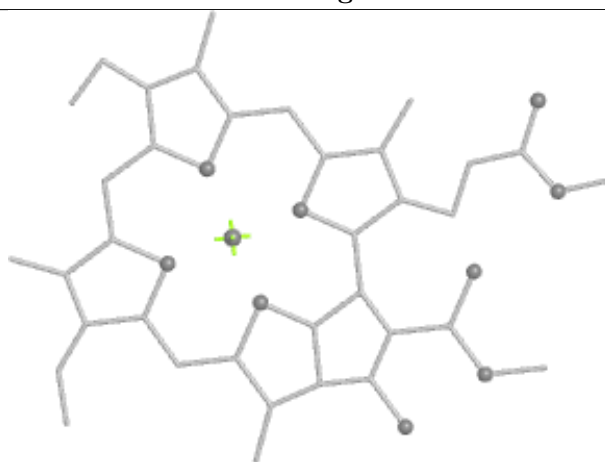
Bond lengths



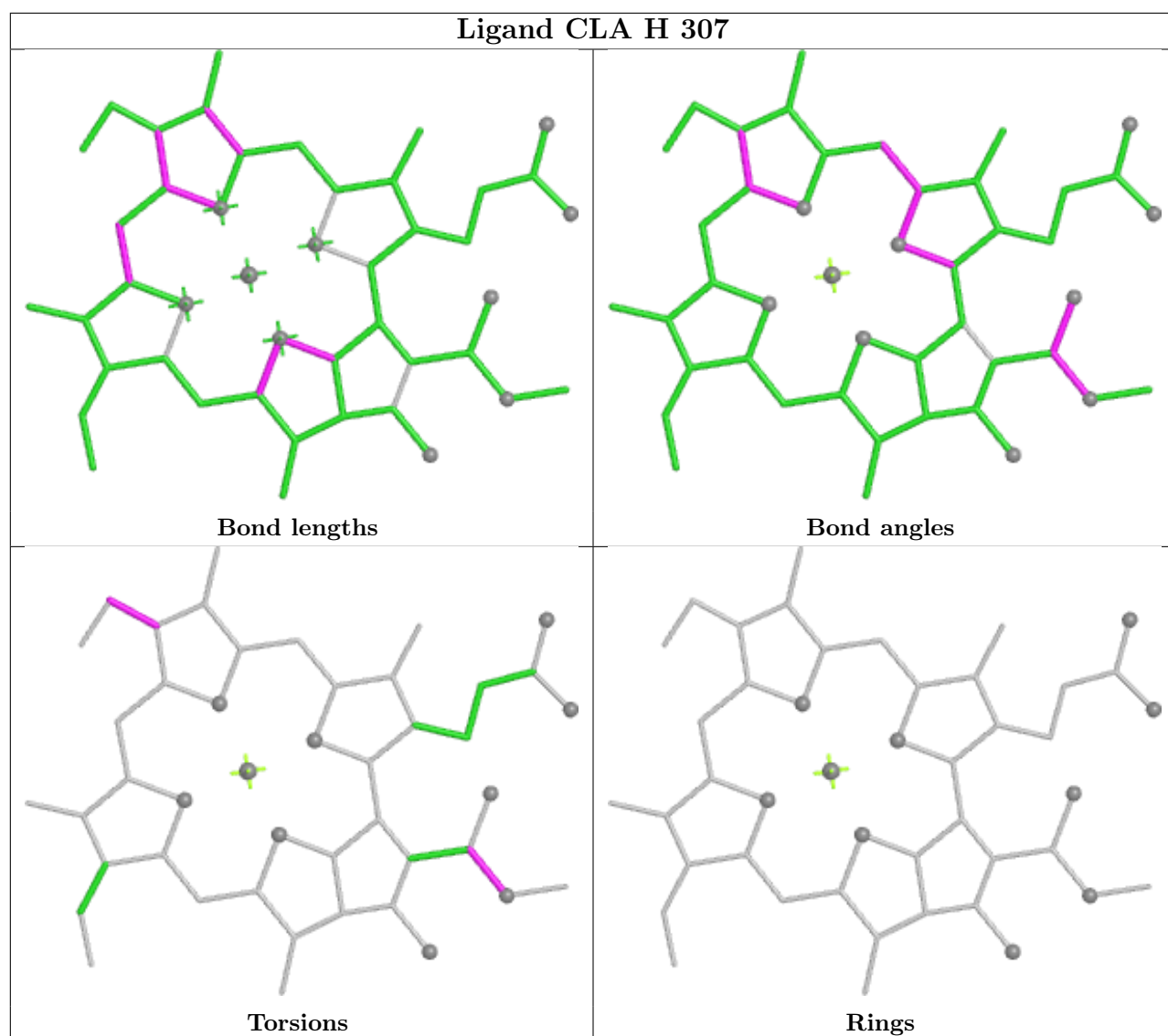
Bond angles

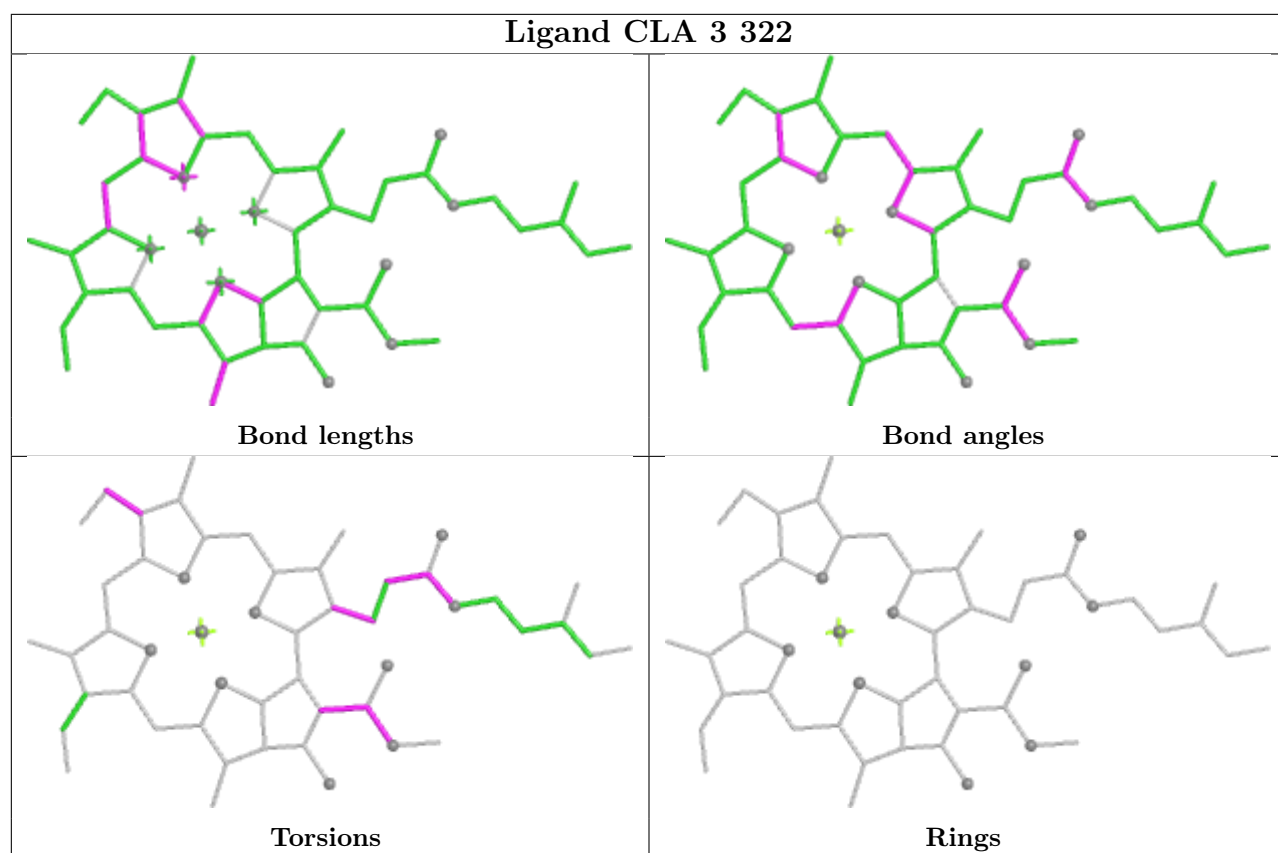


Torsions

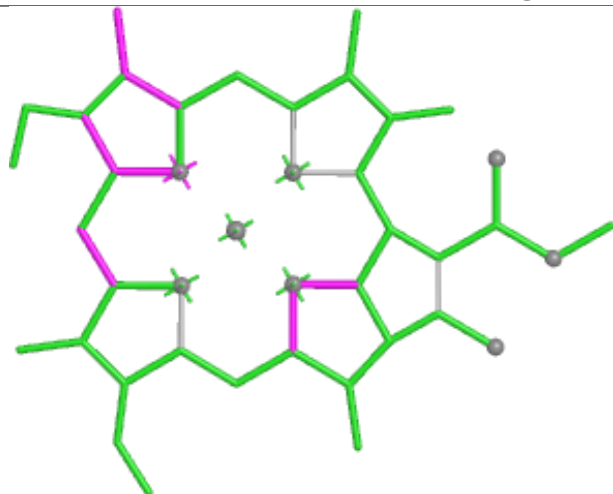


Rings





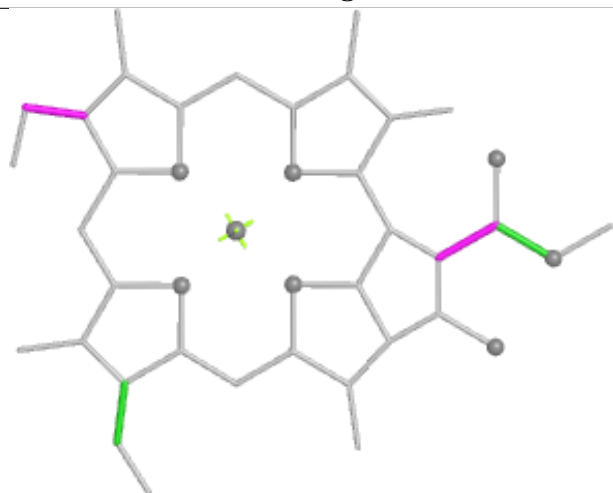
Ligand CLA 9 315



Bond lengths



Bond angles

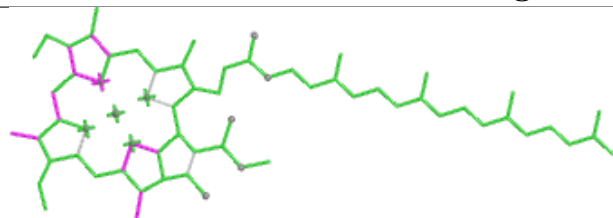


Torsions

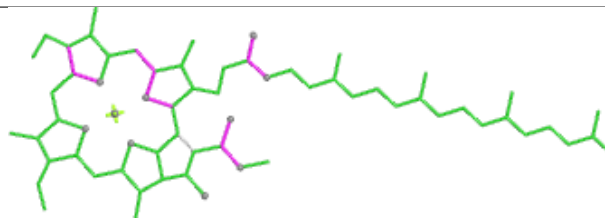


Rings

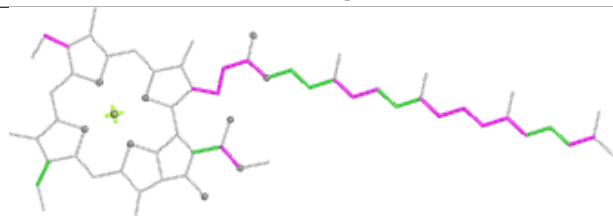
Ligand CLA D 311



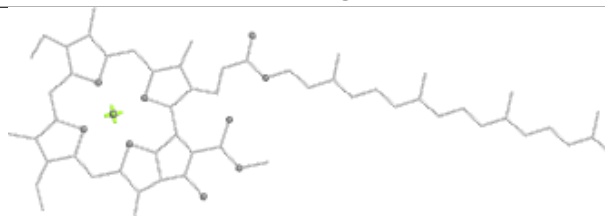
Bond lengths



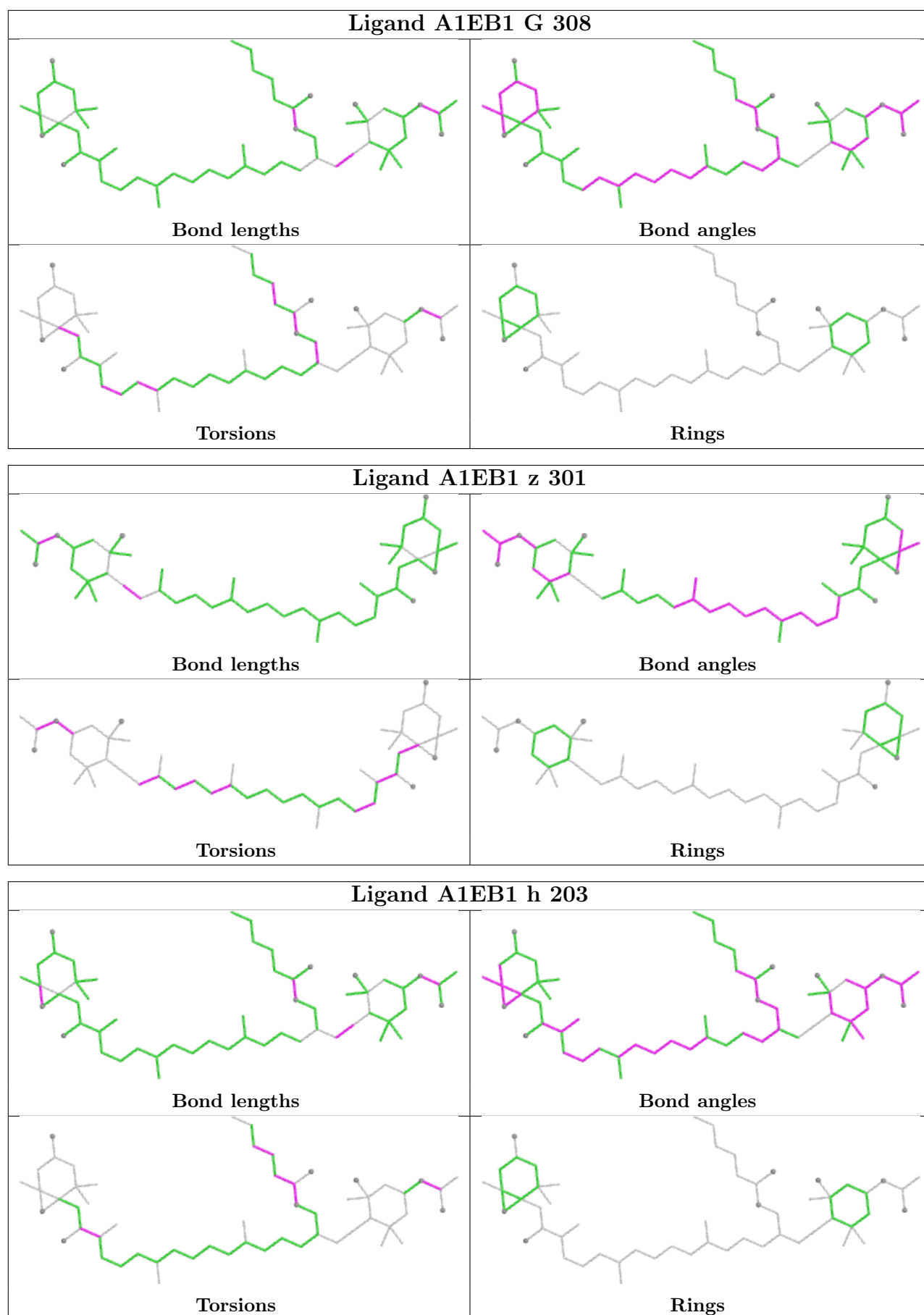
Bond angles



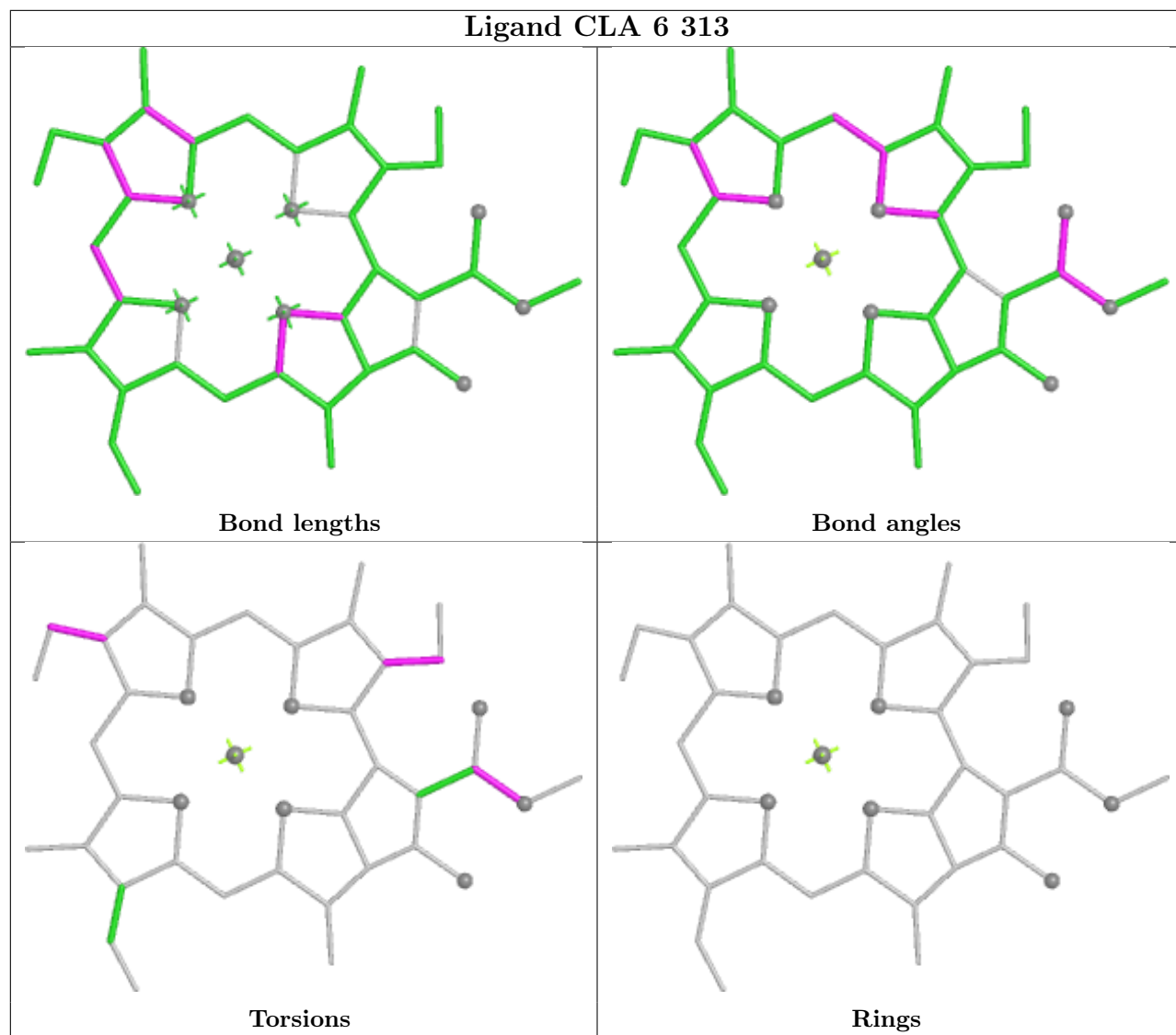
Torsions



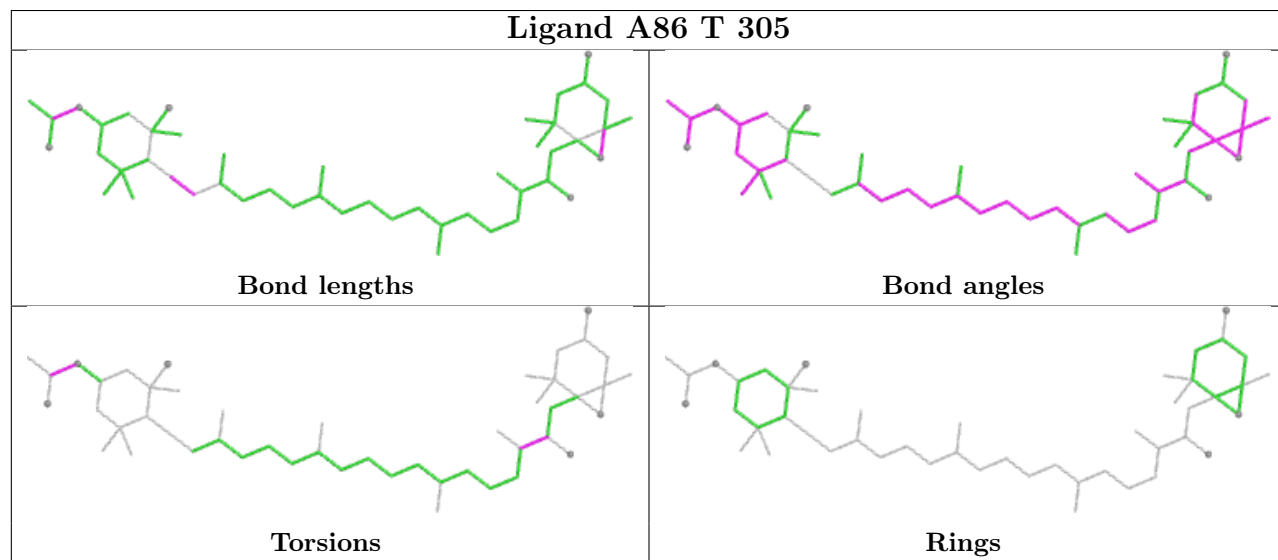
Rings



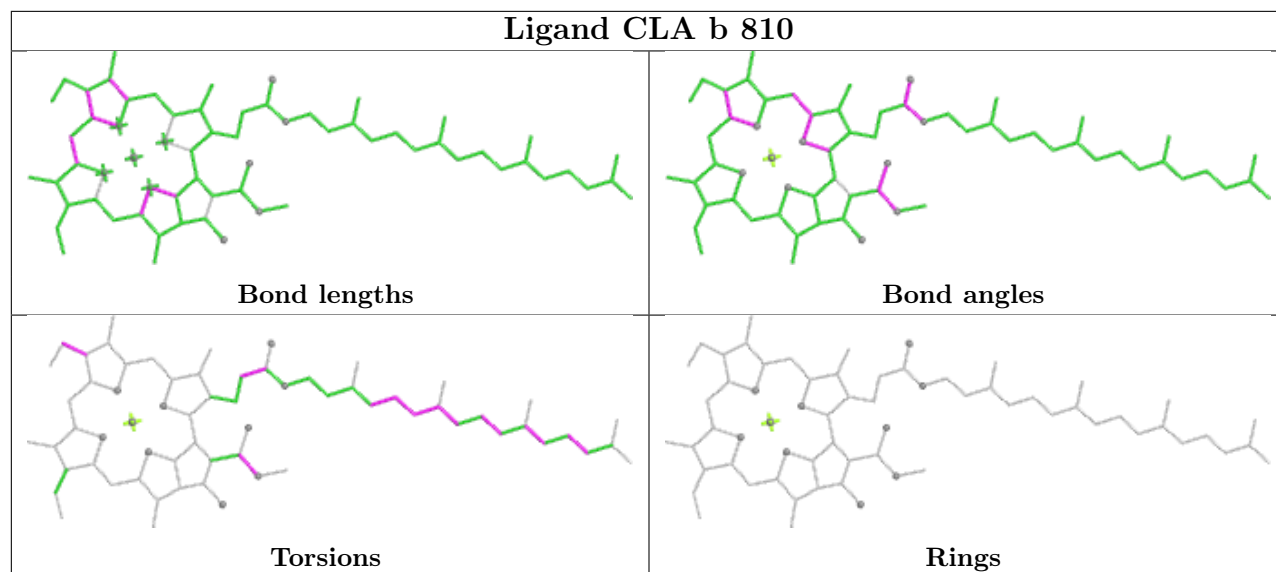
Ligand CLA 6 313



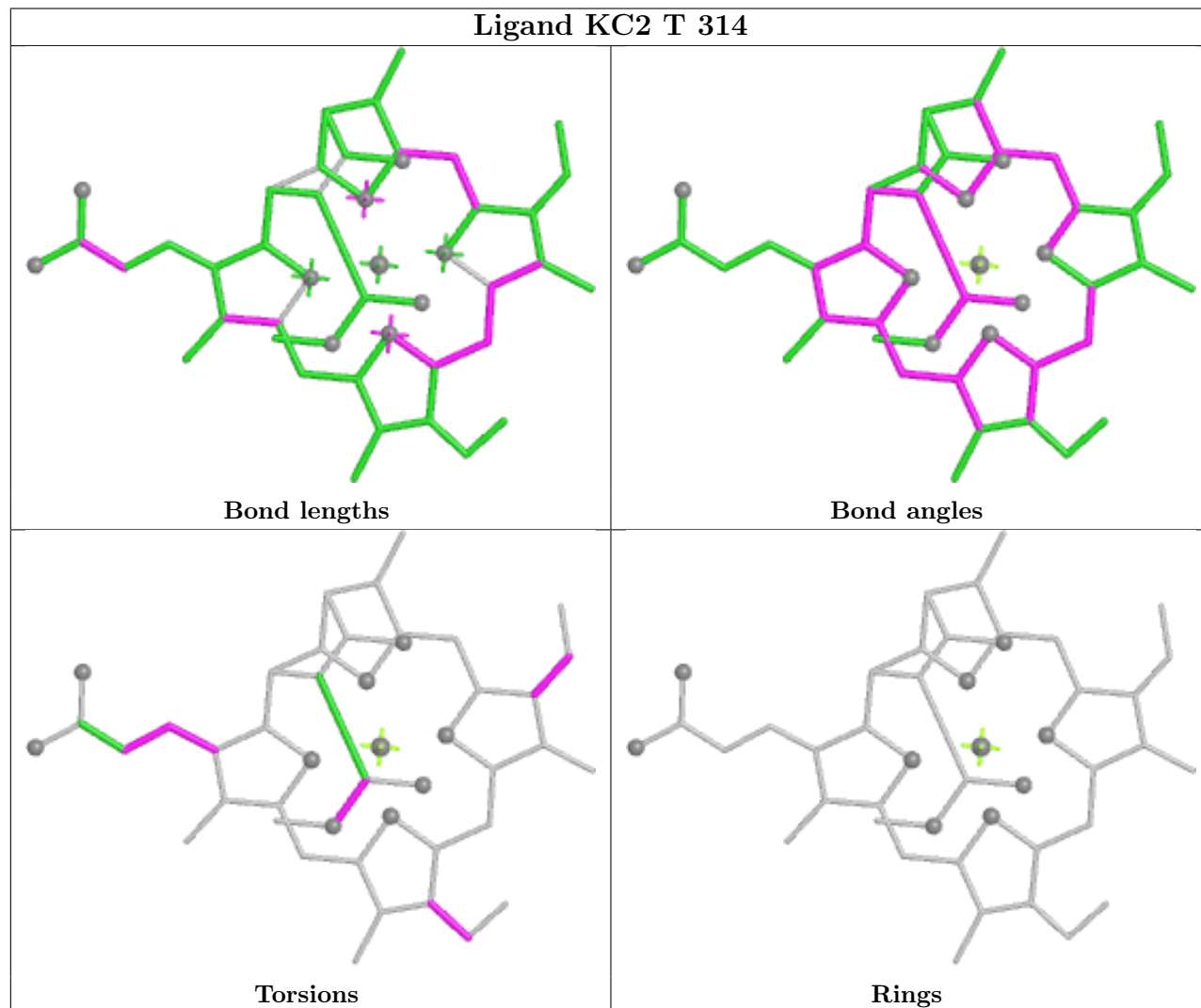
Ligand A86 T 305



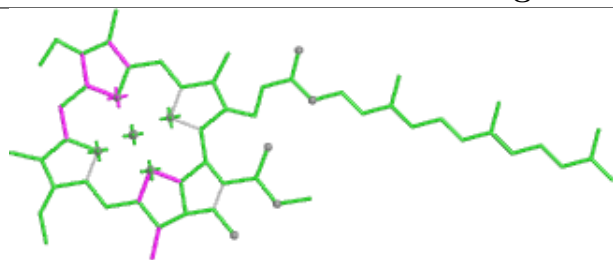
Ligand CLA b 810



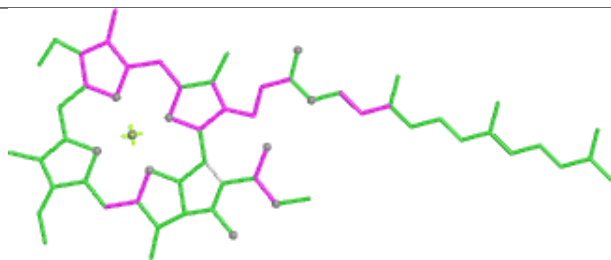
Ligand KC2 T 314



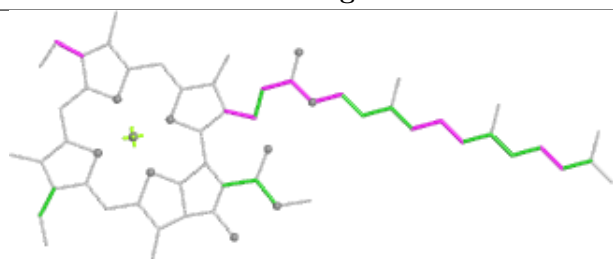
Ligand CLA V 310



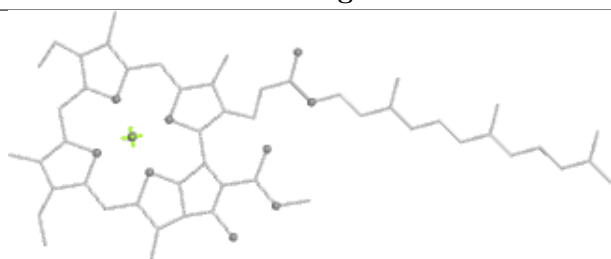
Bond lengths



Bond angles

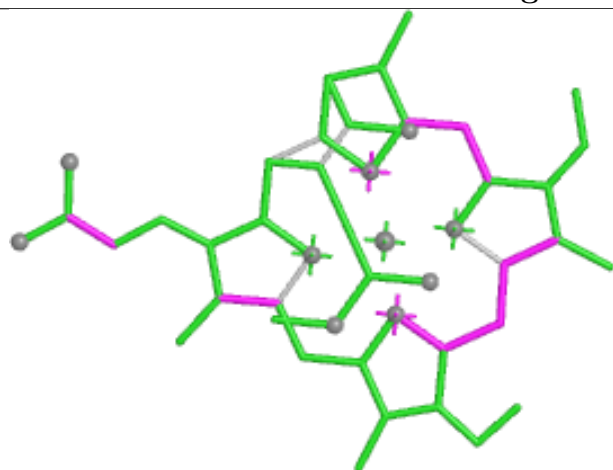


Torsions

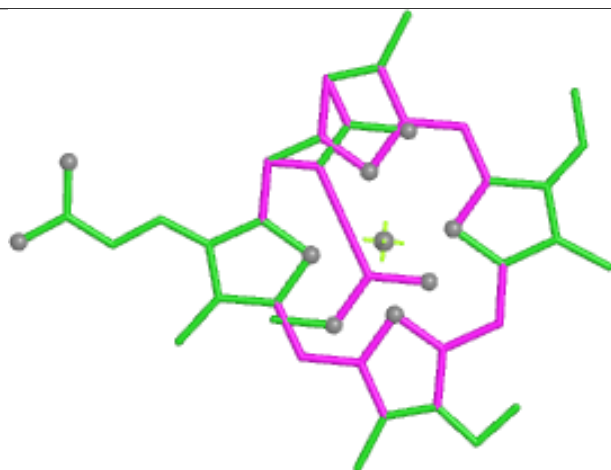


Rings

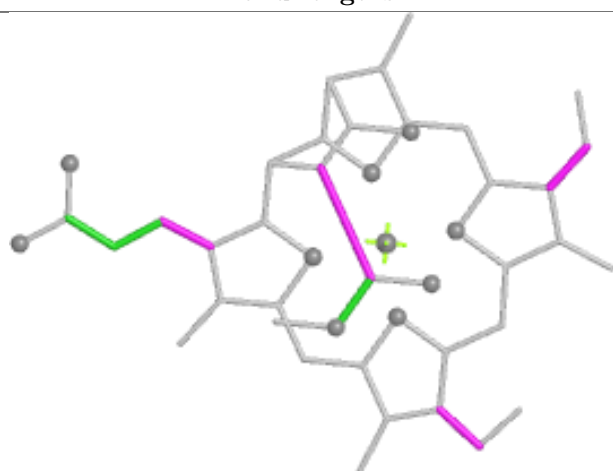
Ligand KC2 z 312



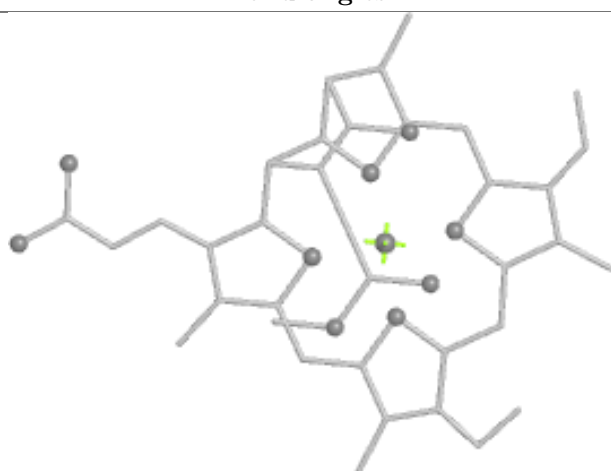
Bond lengths



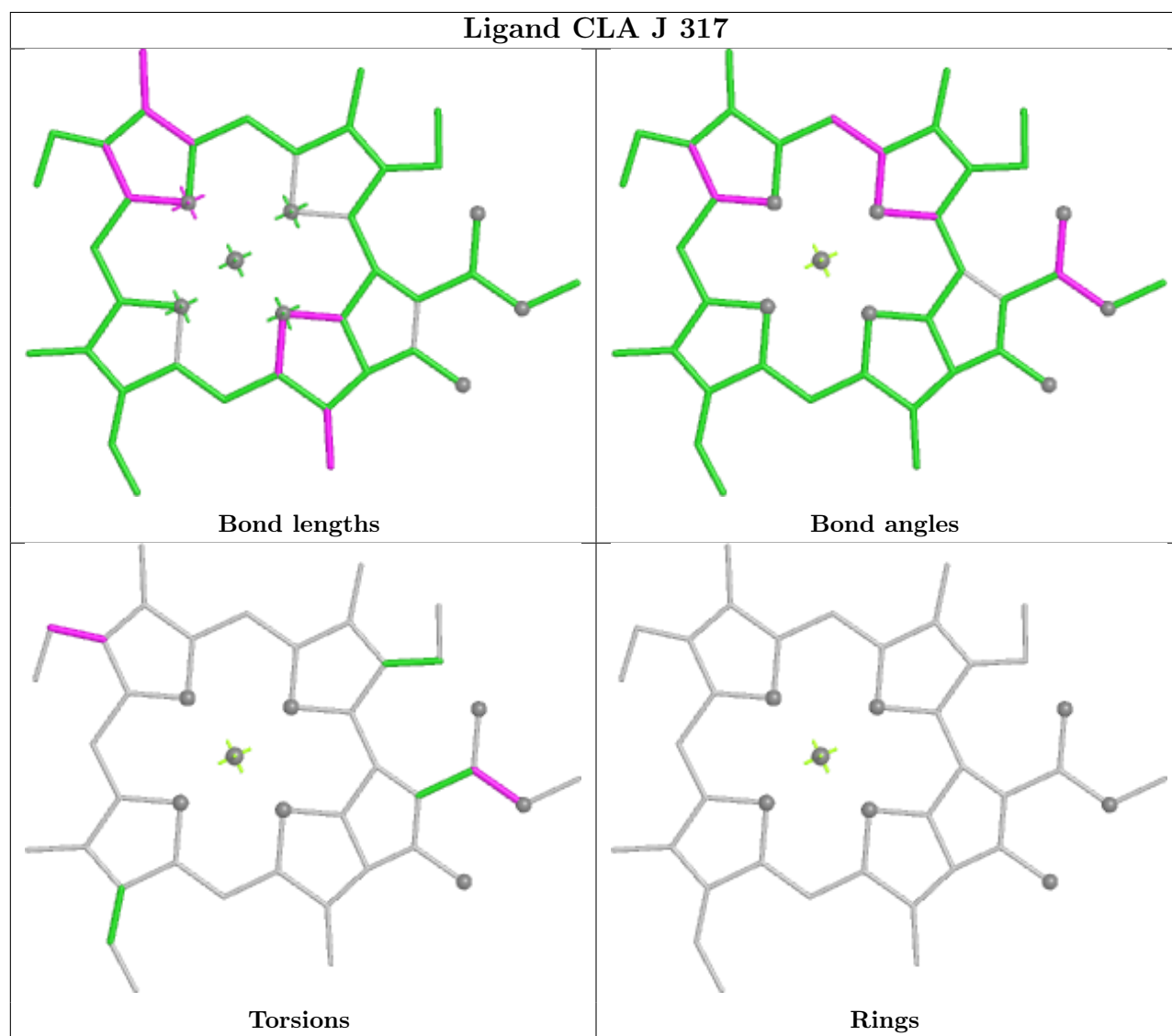
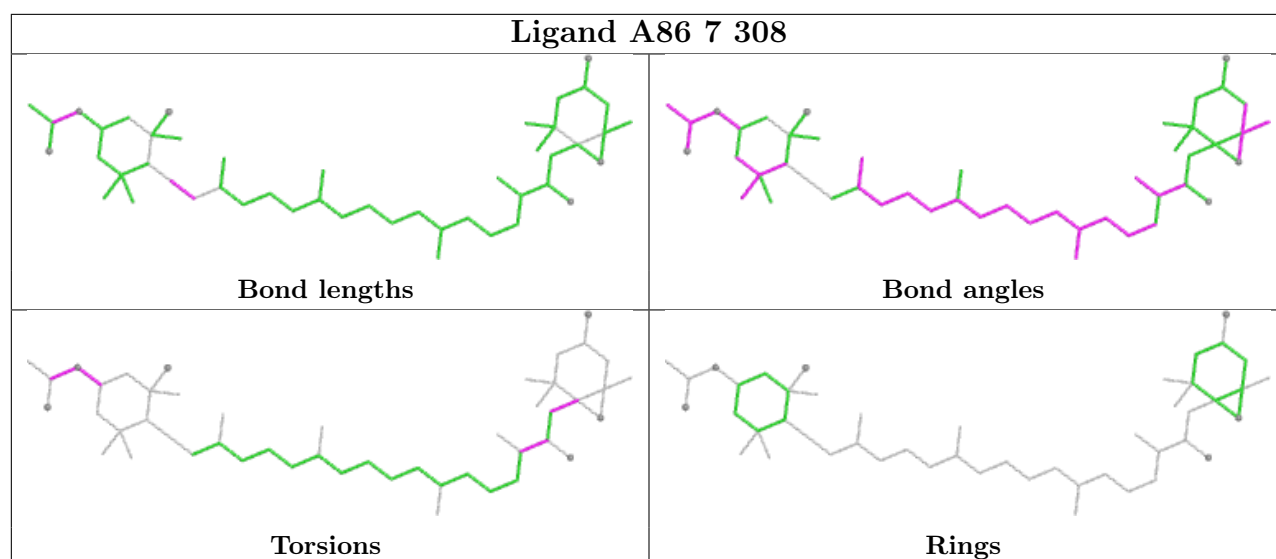
Bond angles



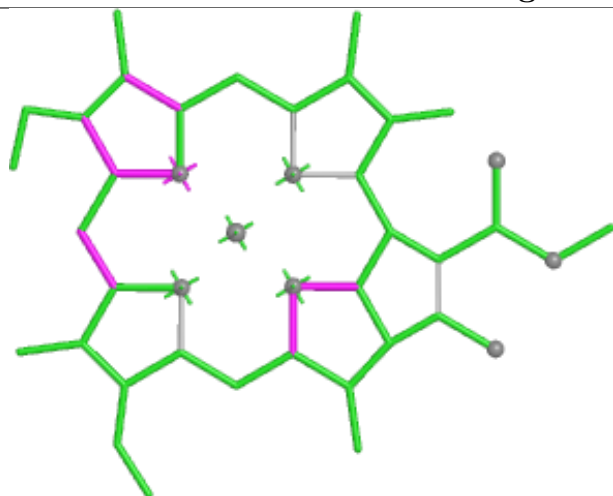
Torsions



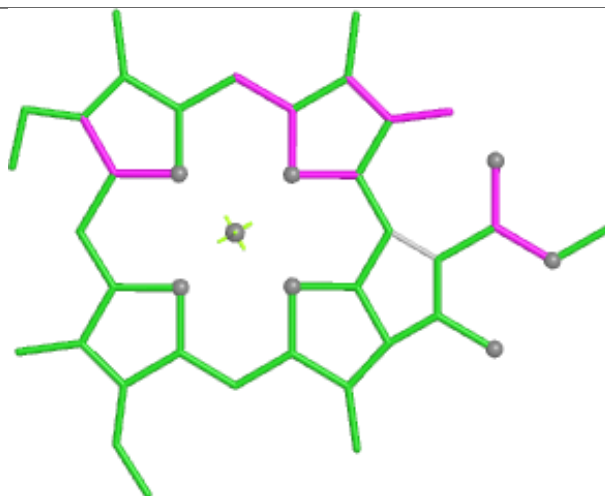
Rings



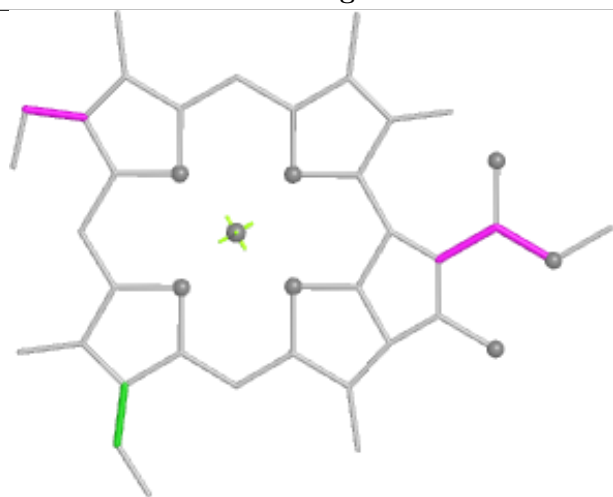
Ligand CLA 2 316



Bond lengths



Bond angles

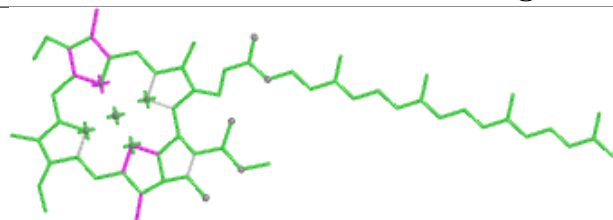


Torsions

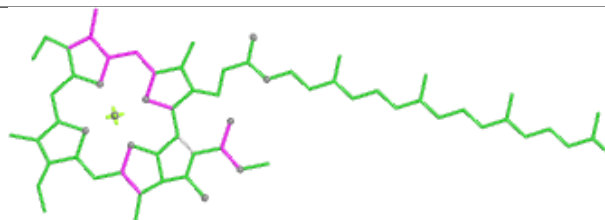


Rings

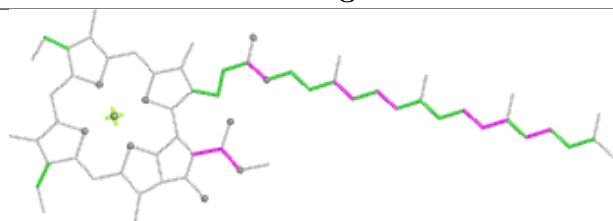
Ligand CLA b 830



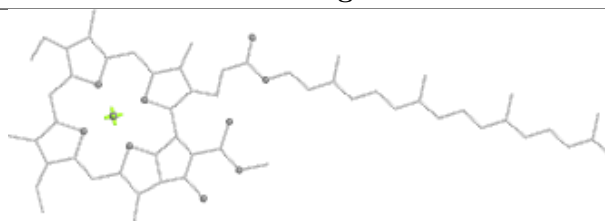
Bond lengths



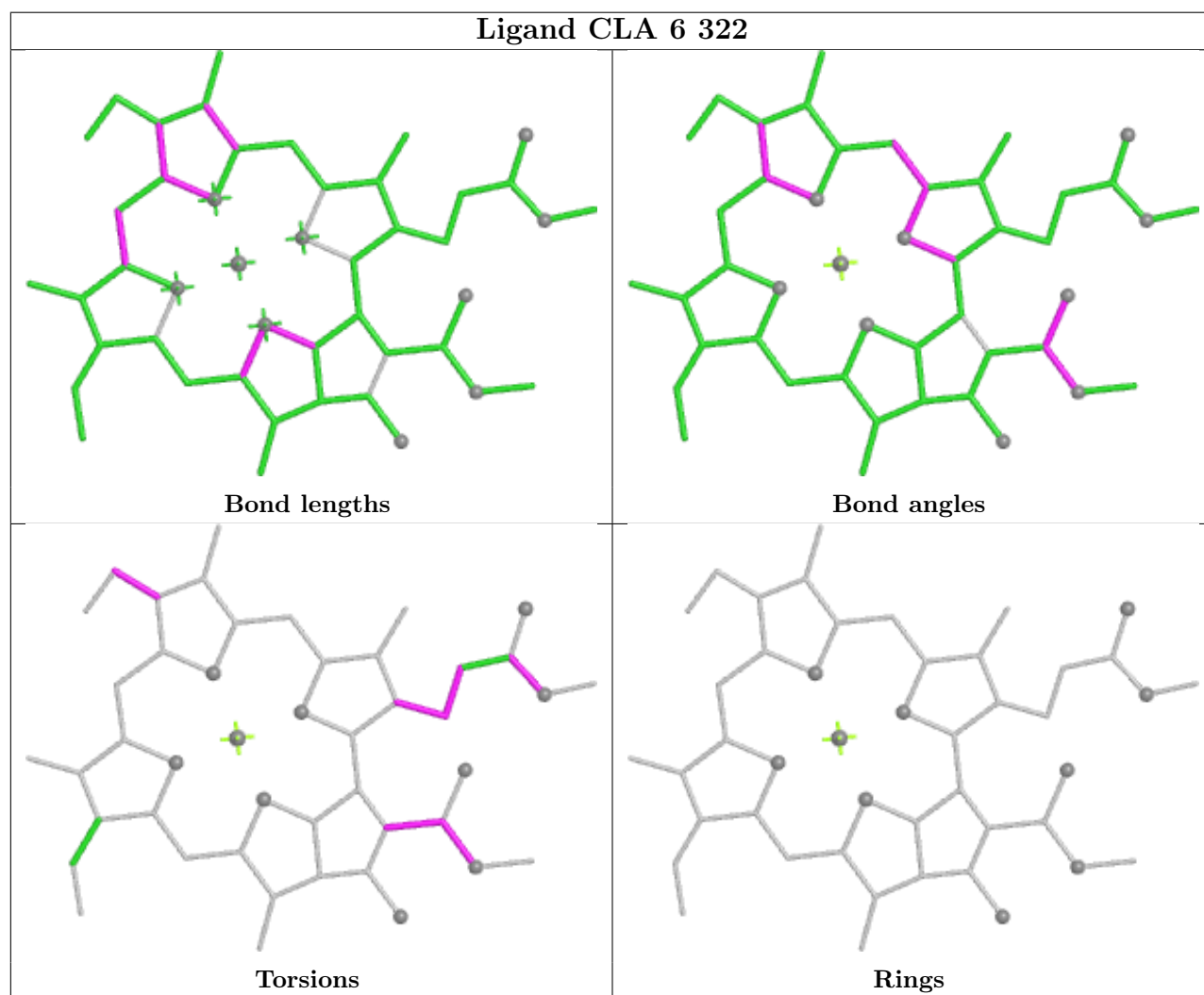
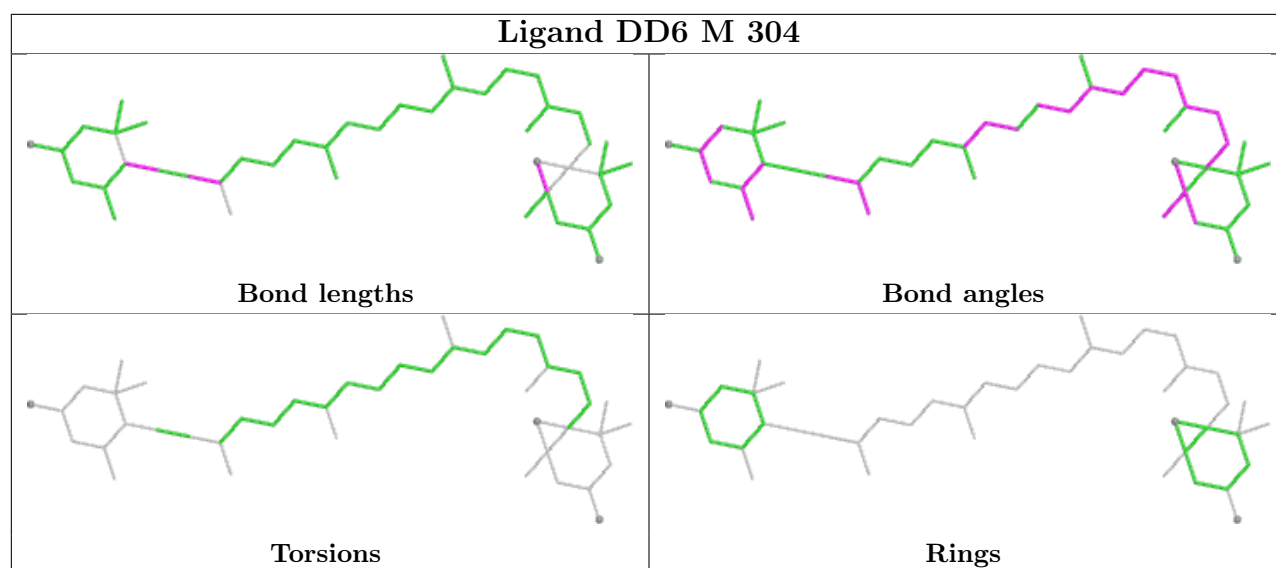
Bond angles

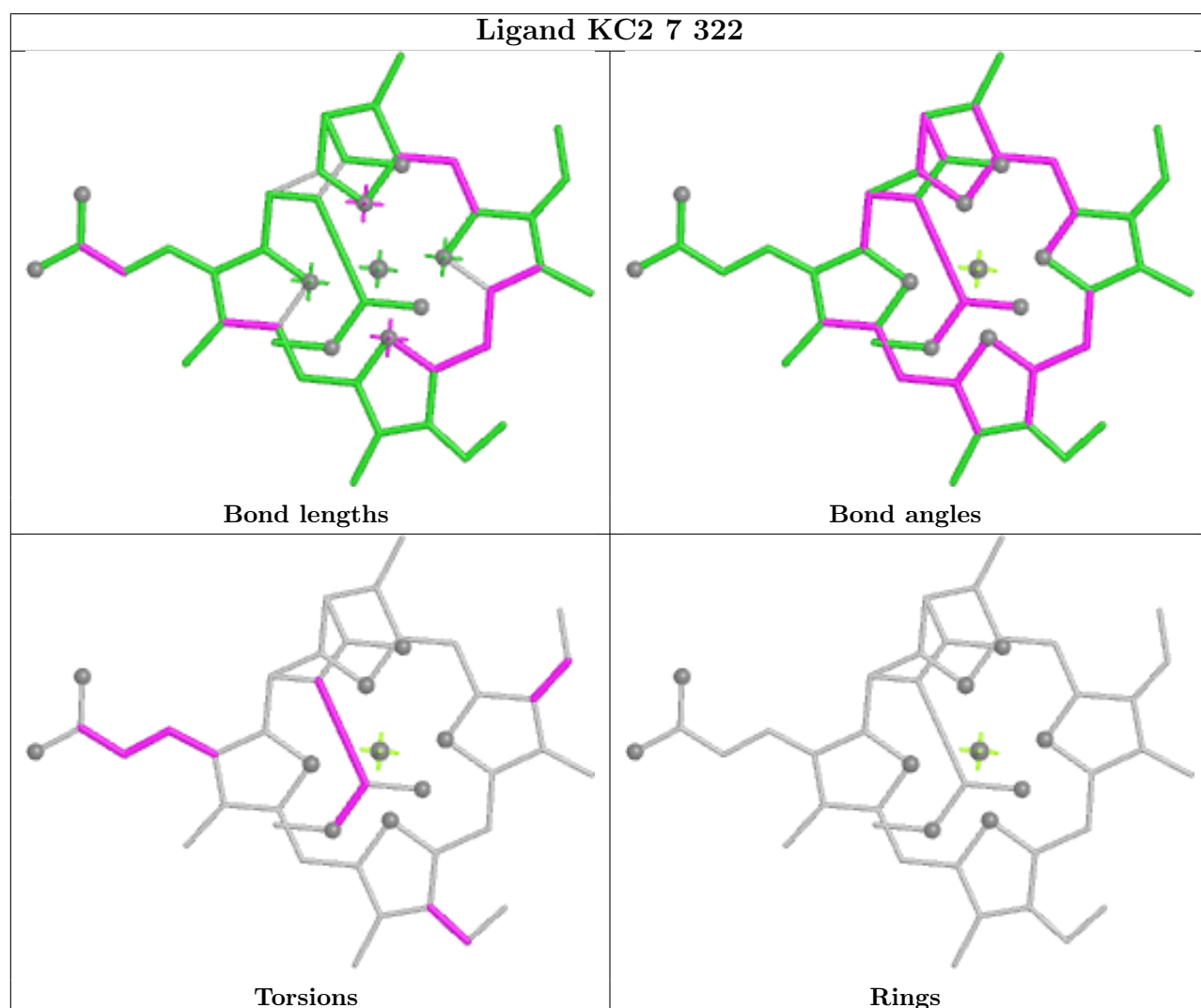
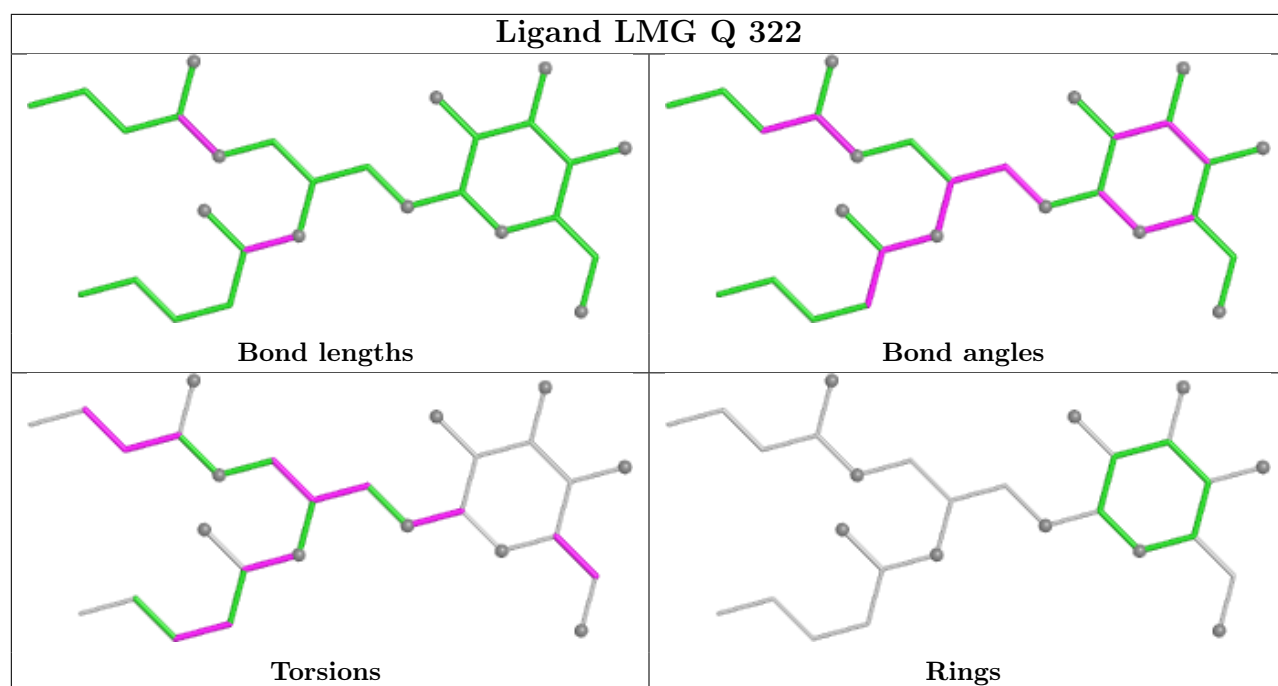


Torsions

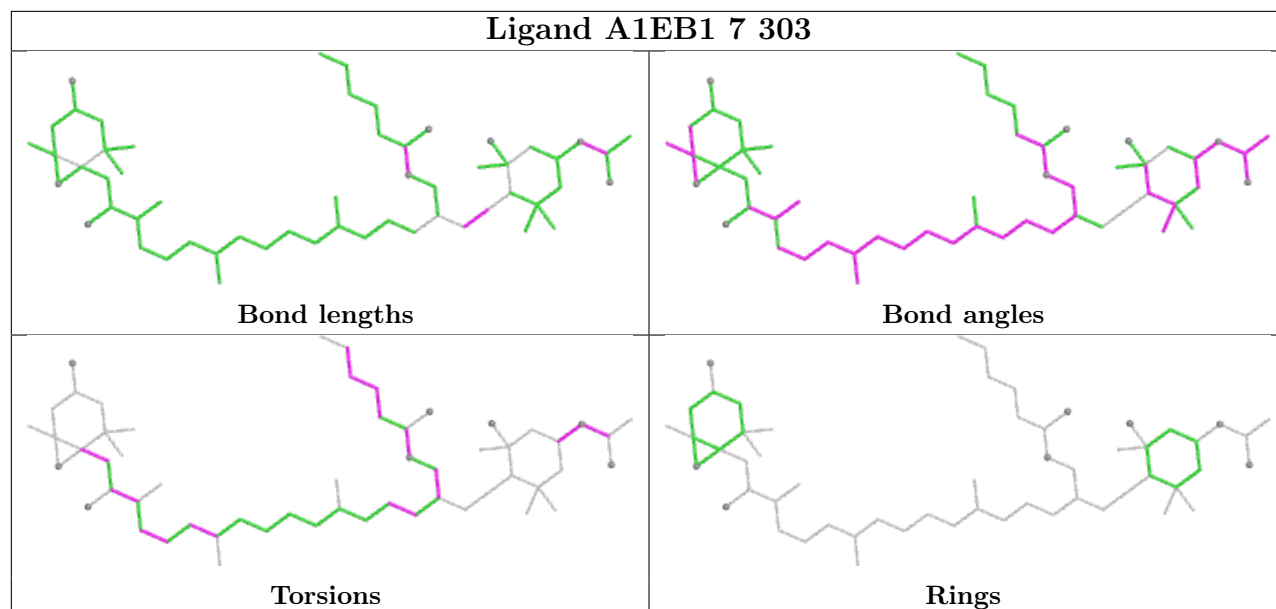


Rings

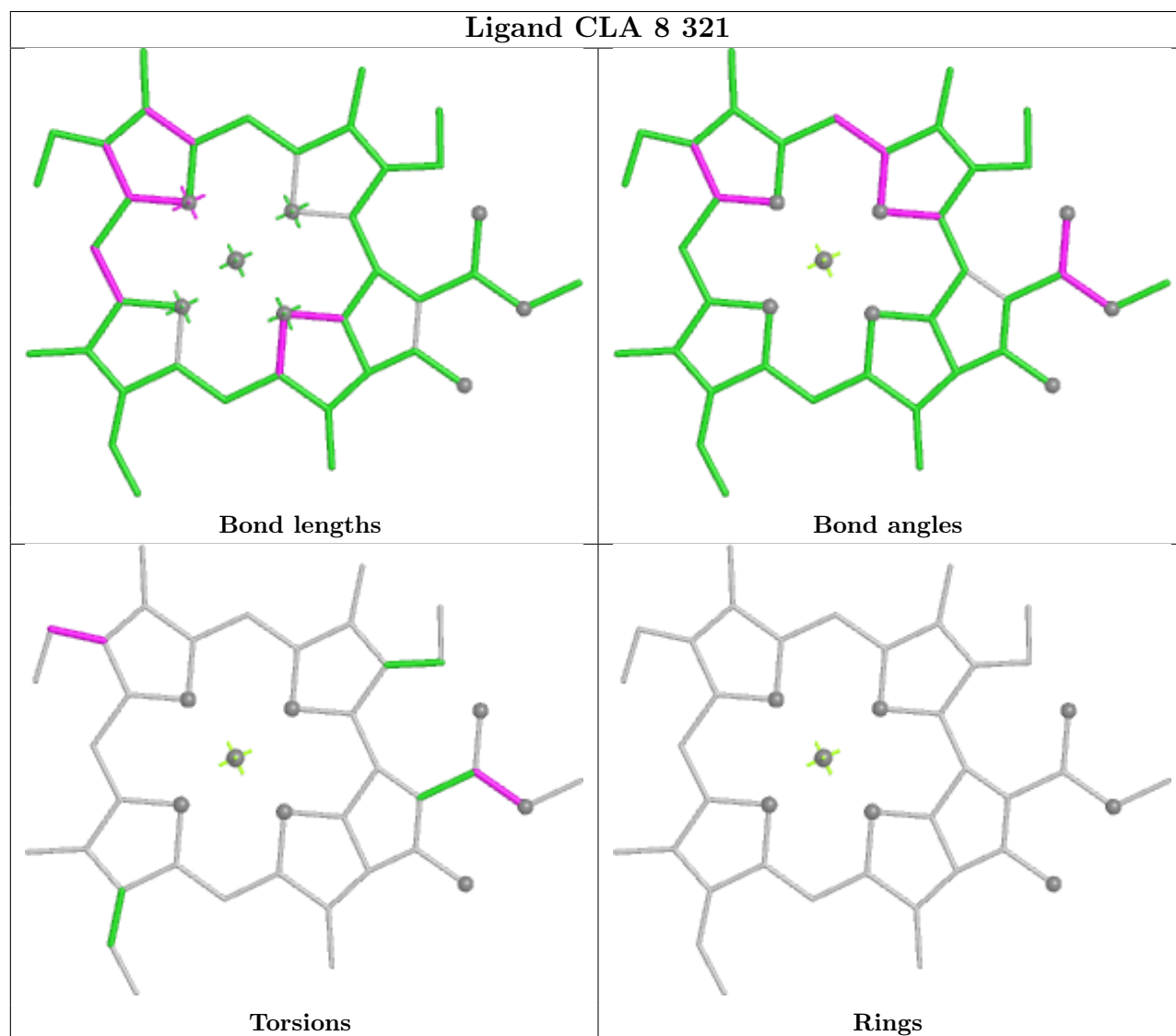




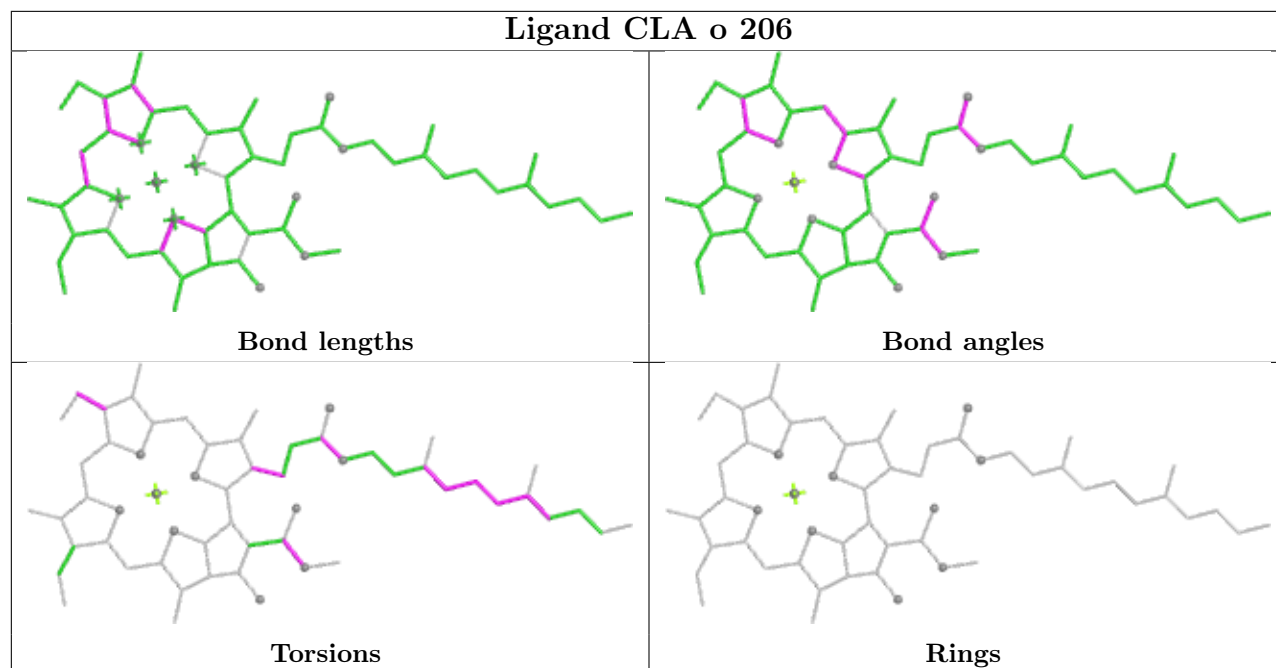
Ligand A1EB1 7 303



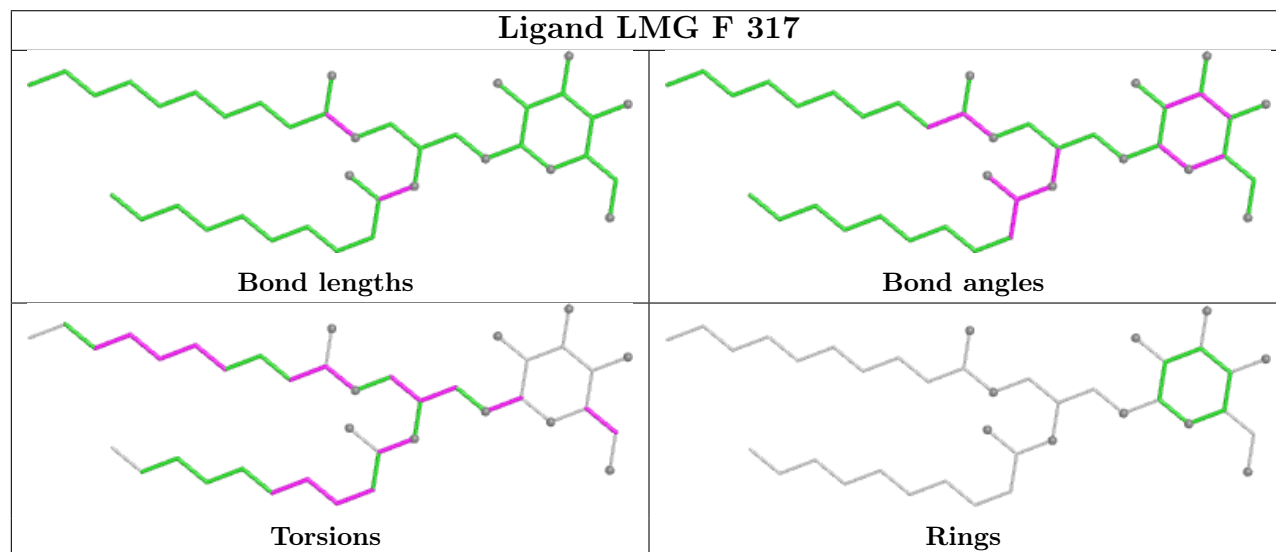
Ligand CLA 8 321

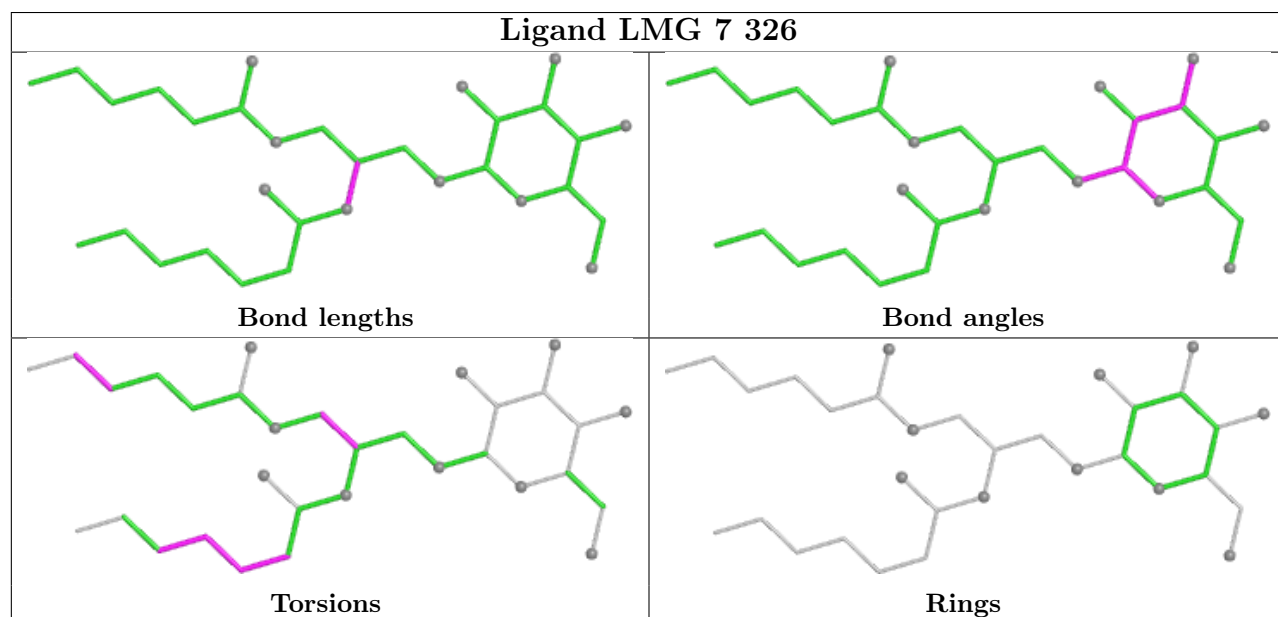
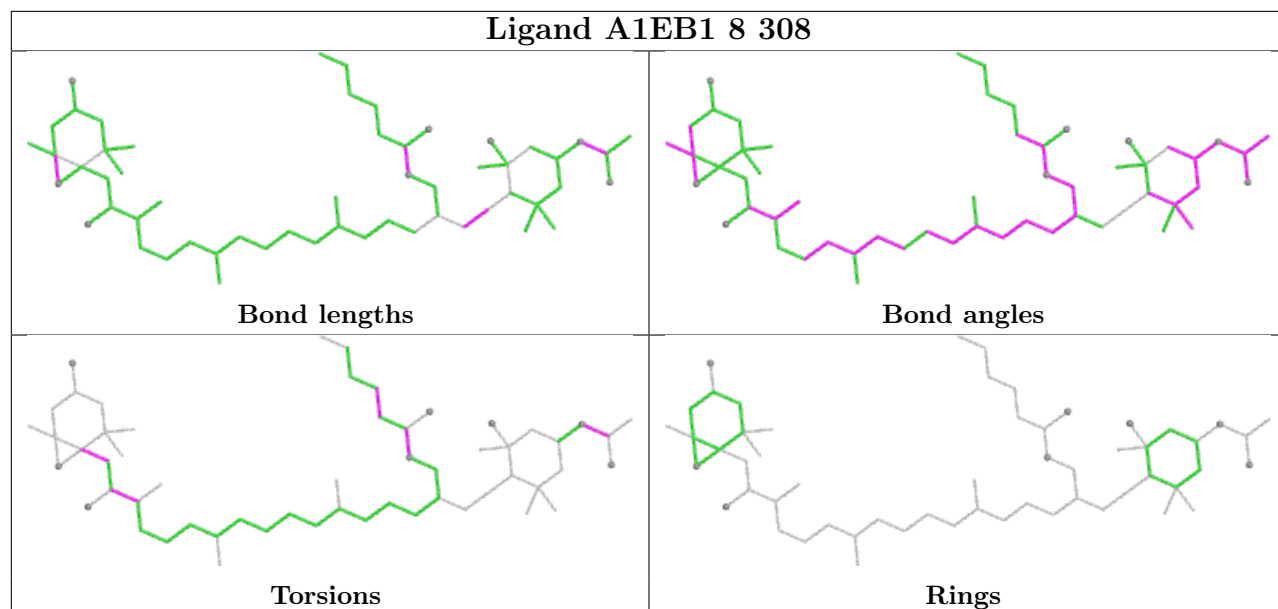


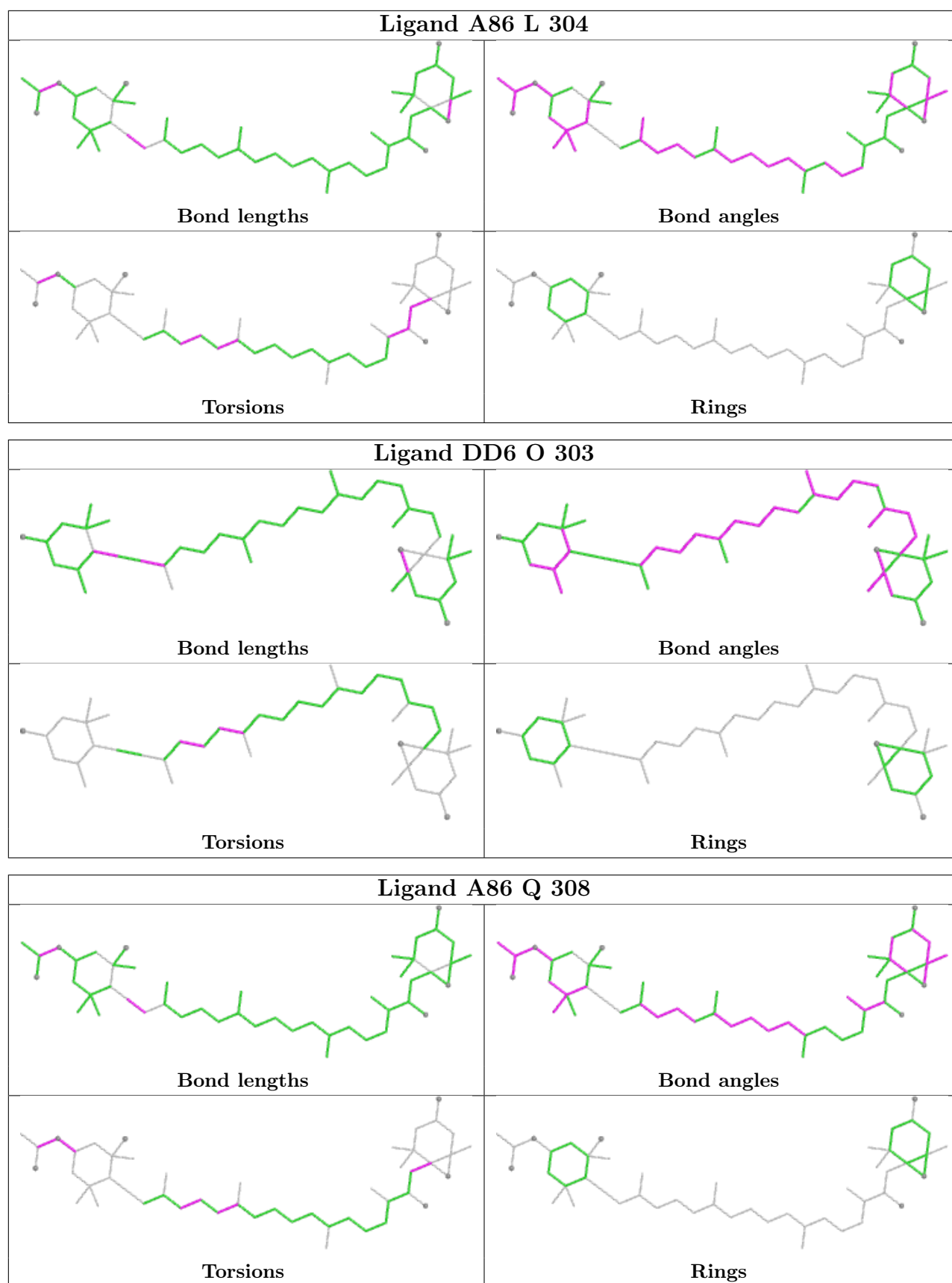
Ligand CLA o 206



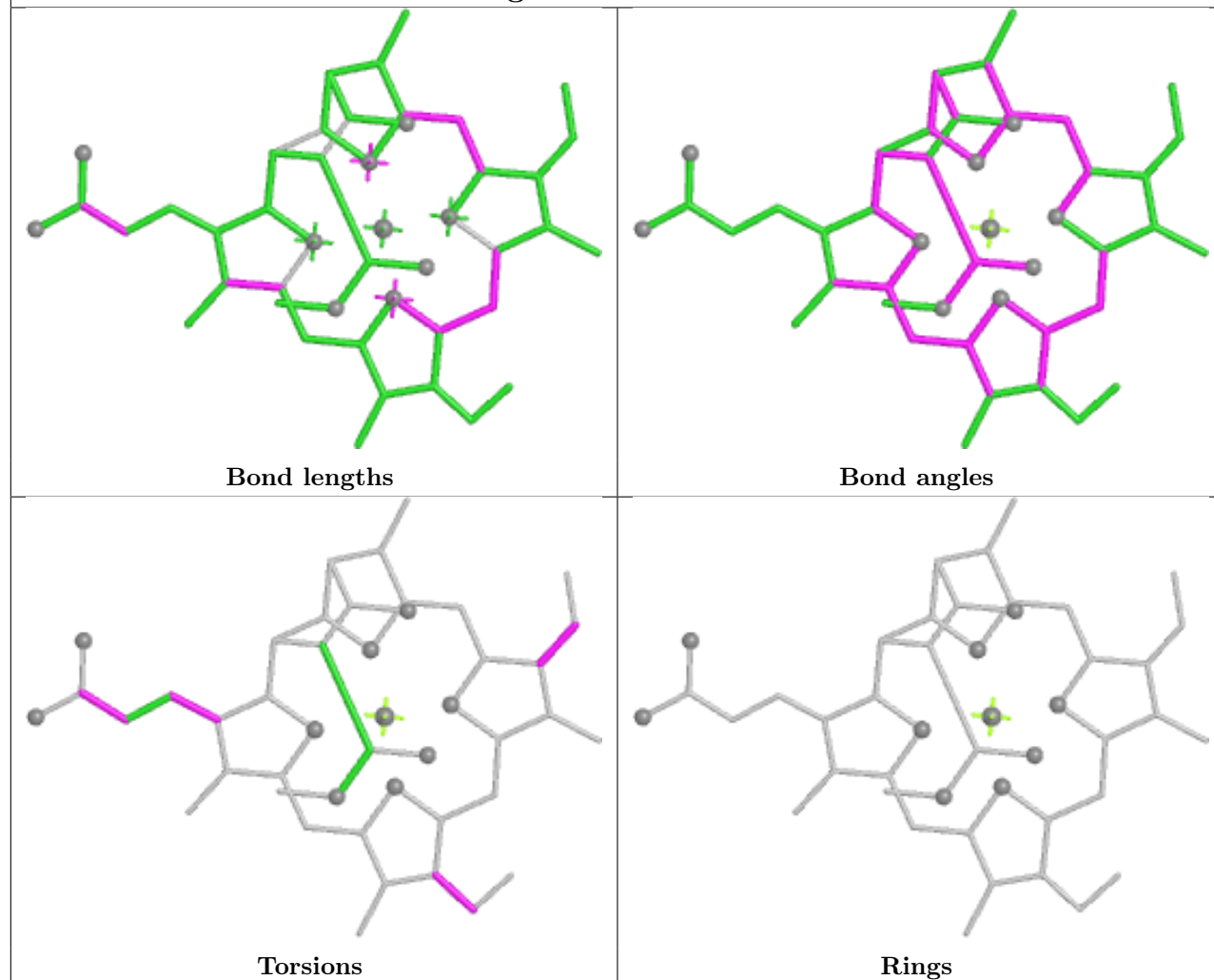
Ligand LMG F 317



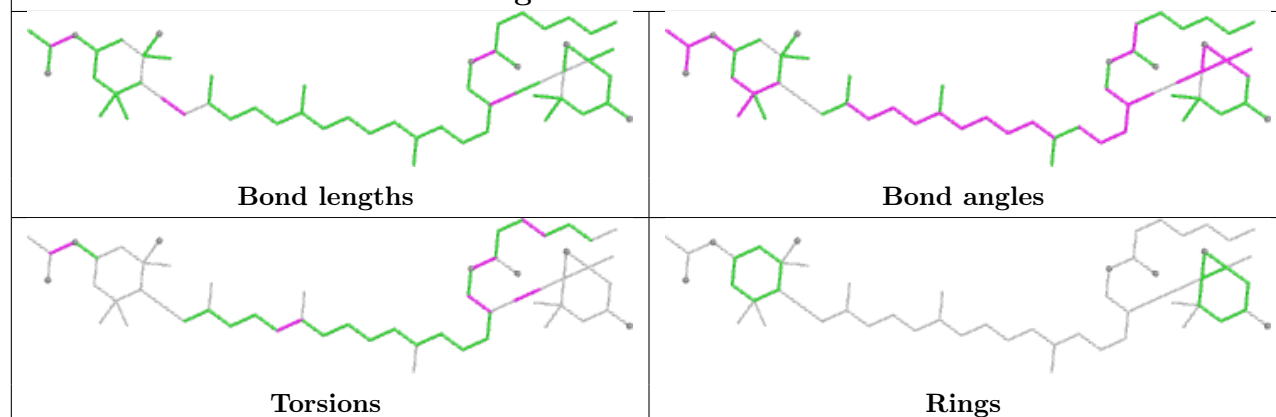




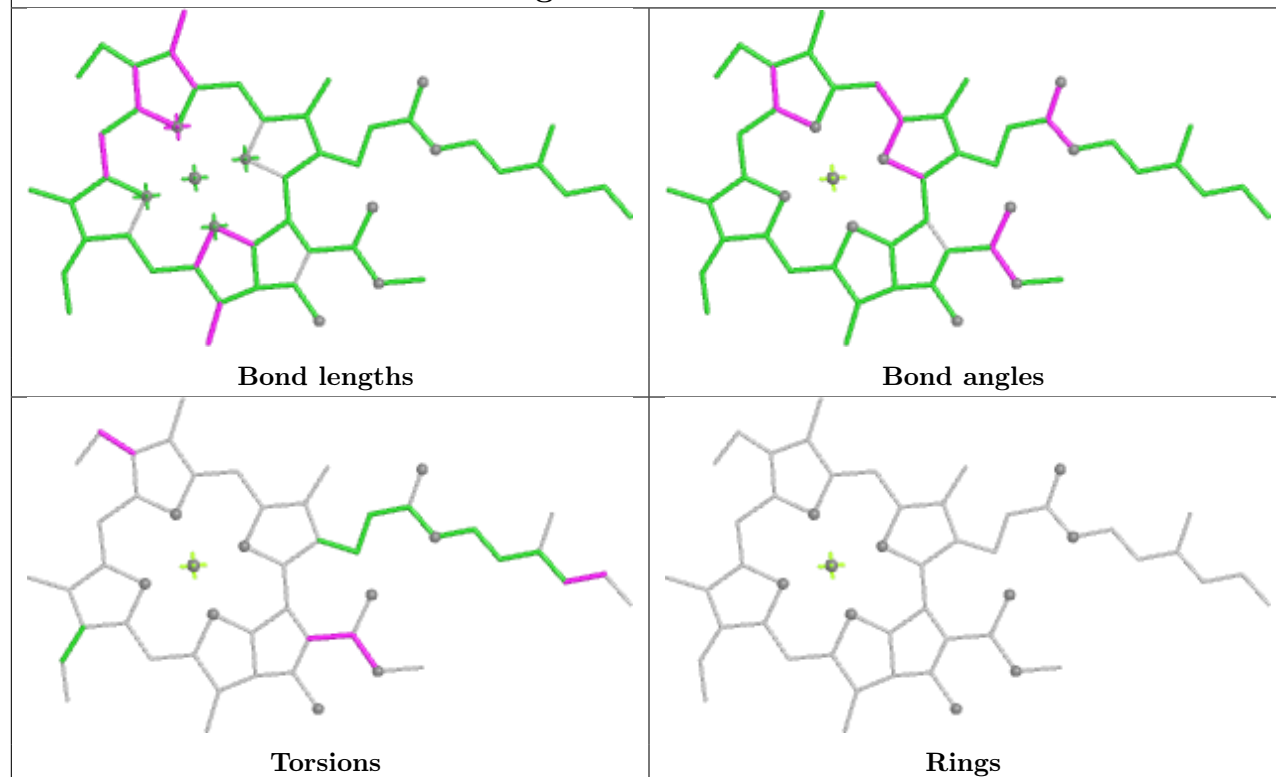
Ligand KC2 Y 309



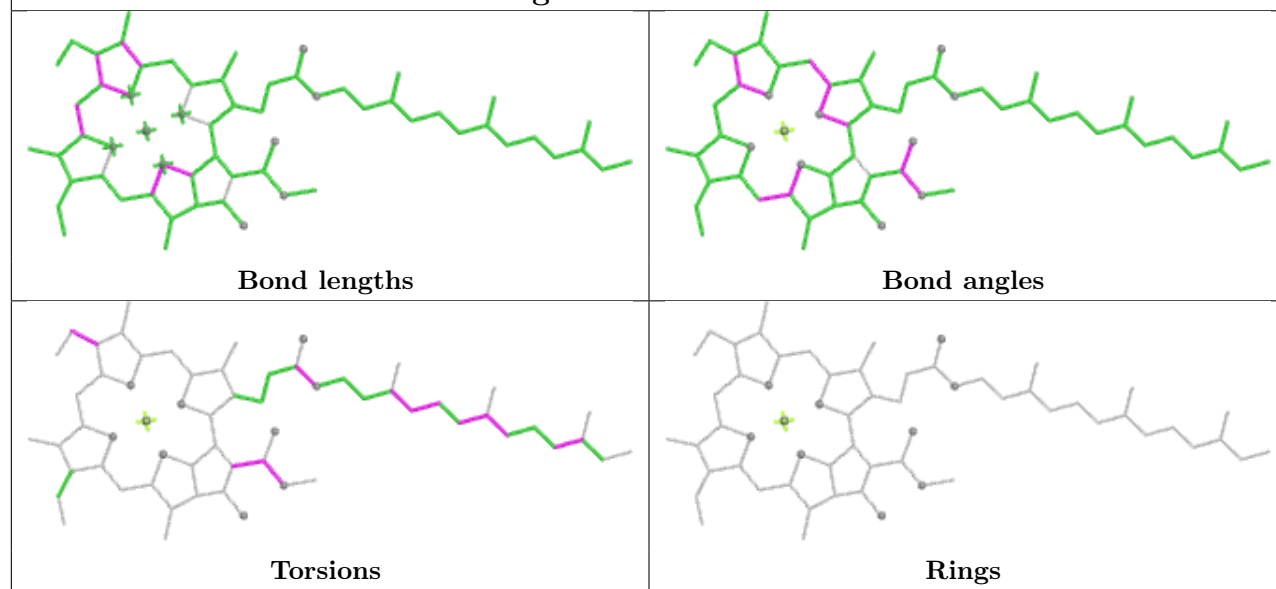
Ligand A1EB4 P 305



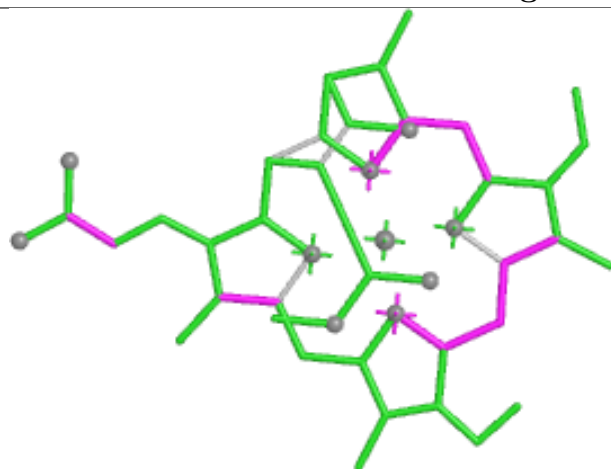
Ligand CLA k 201



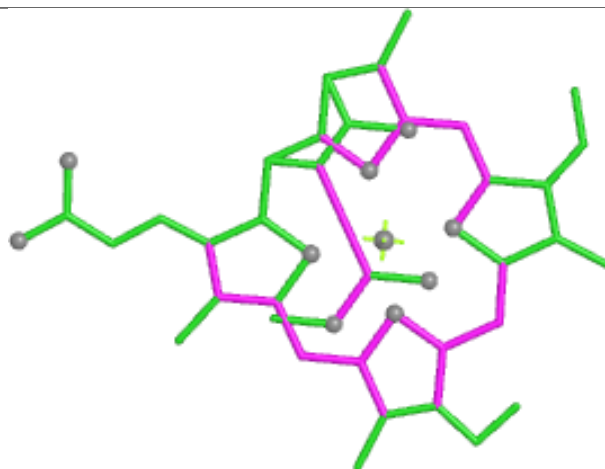
Ligand CLA C 305



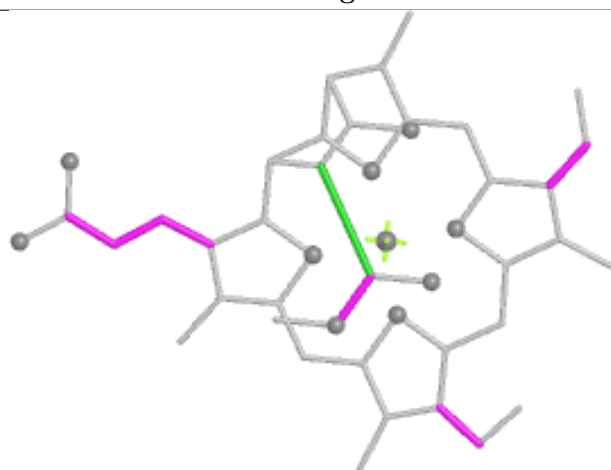
Ligand KC2 6 319



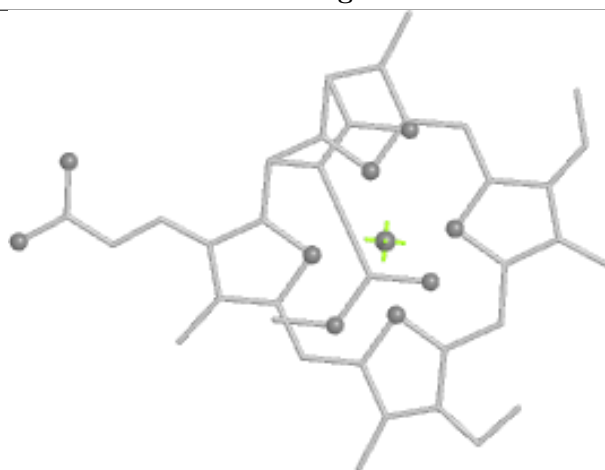
Bond lengths



Bond angles

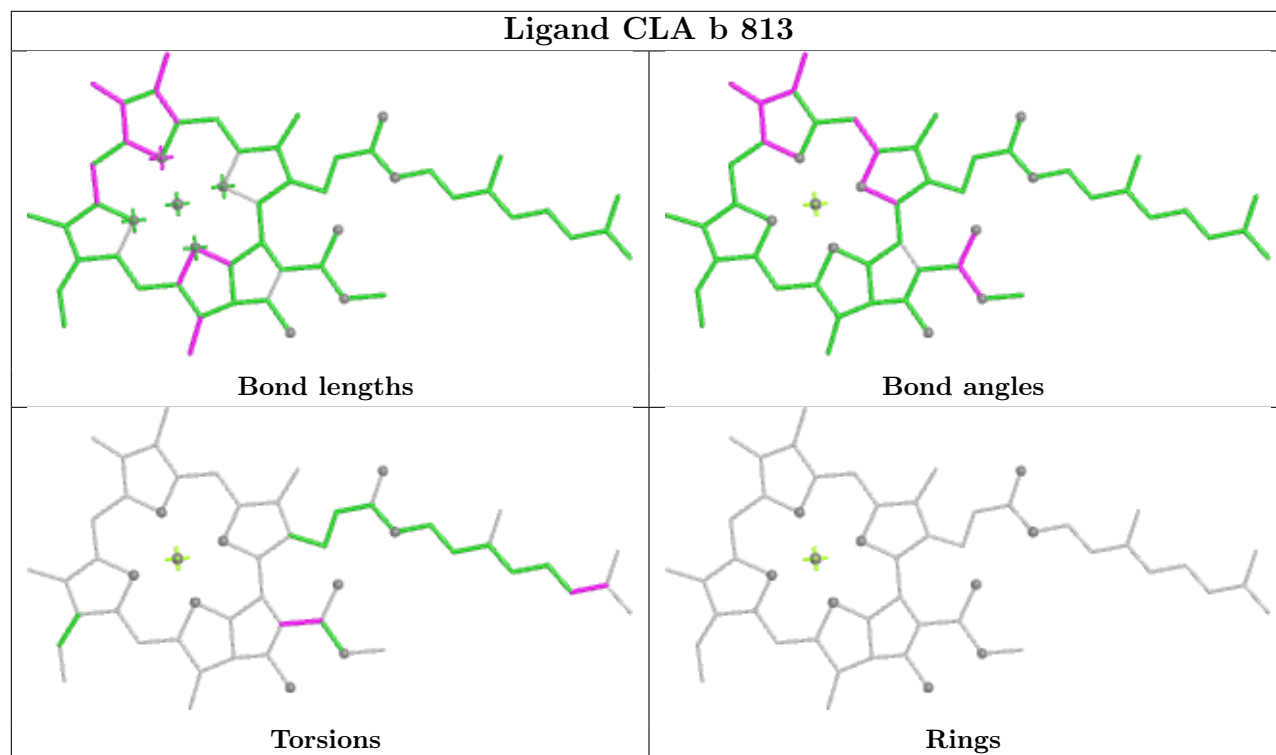


Torsions

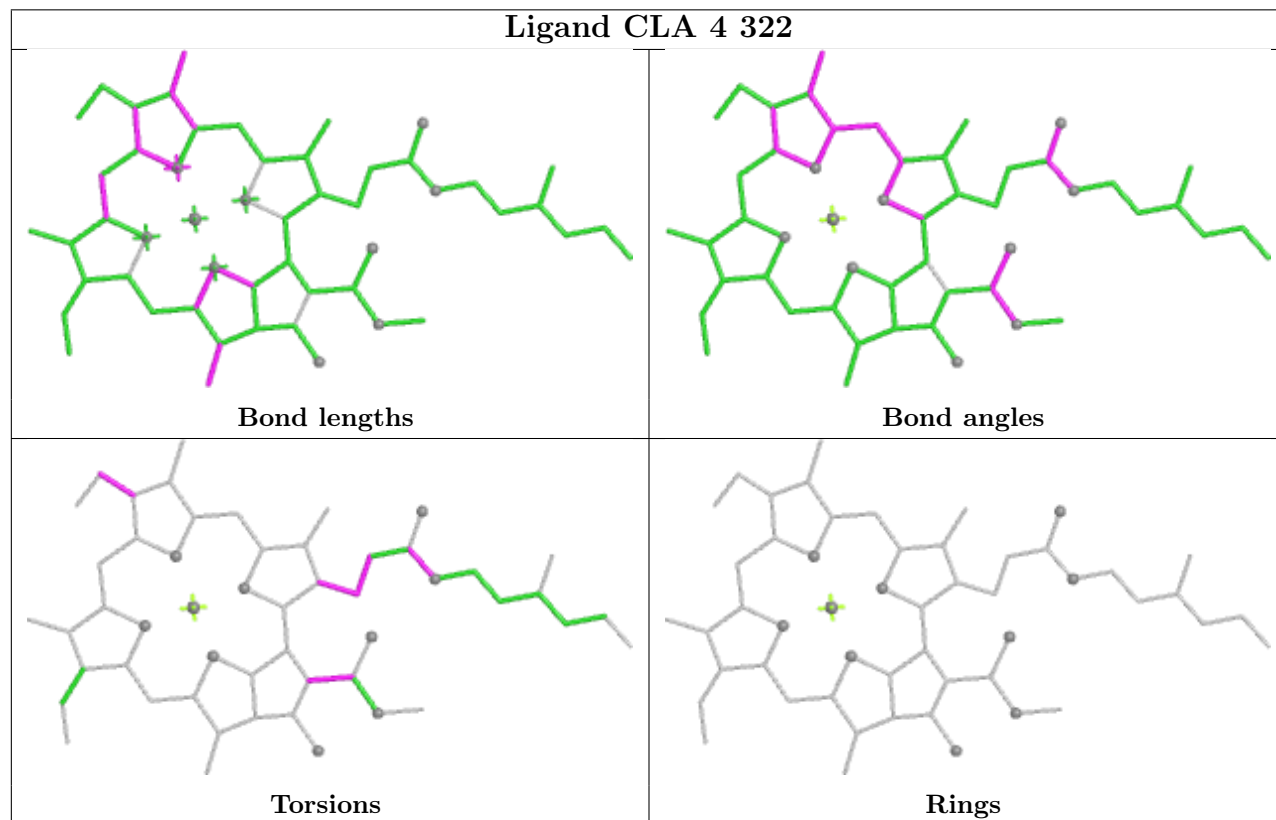


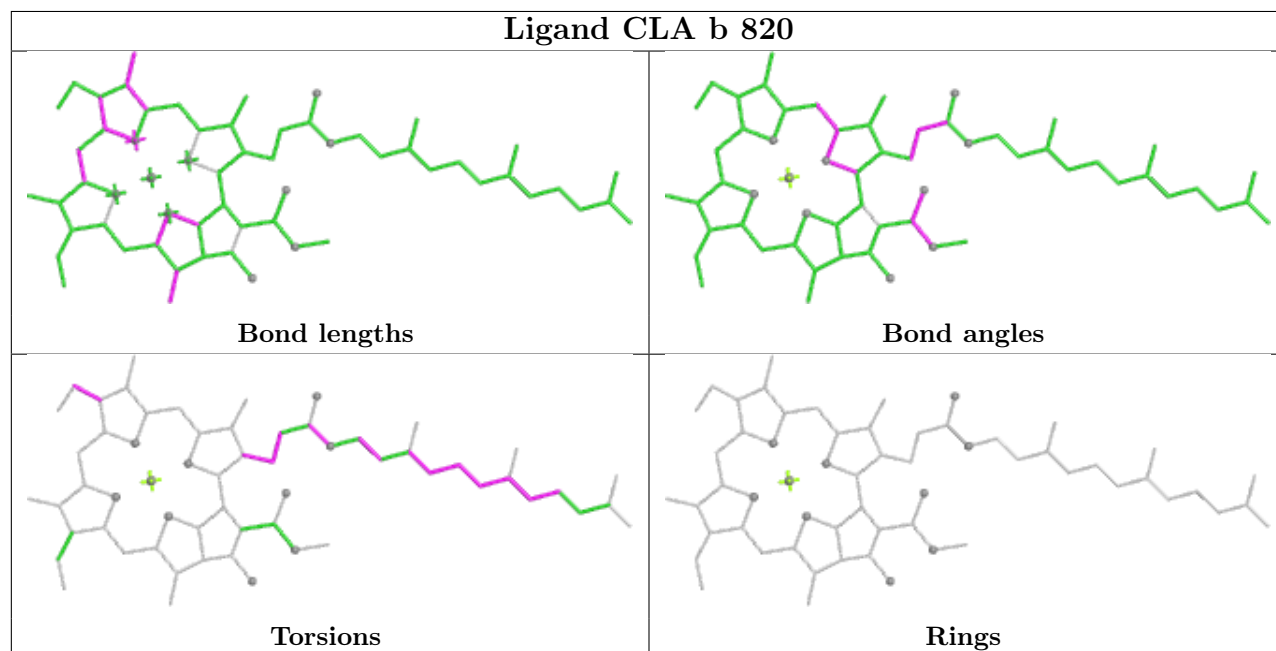
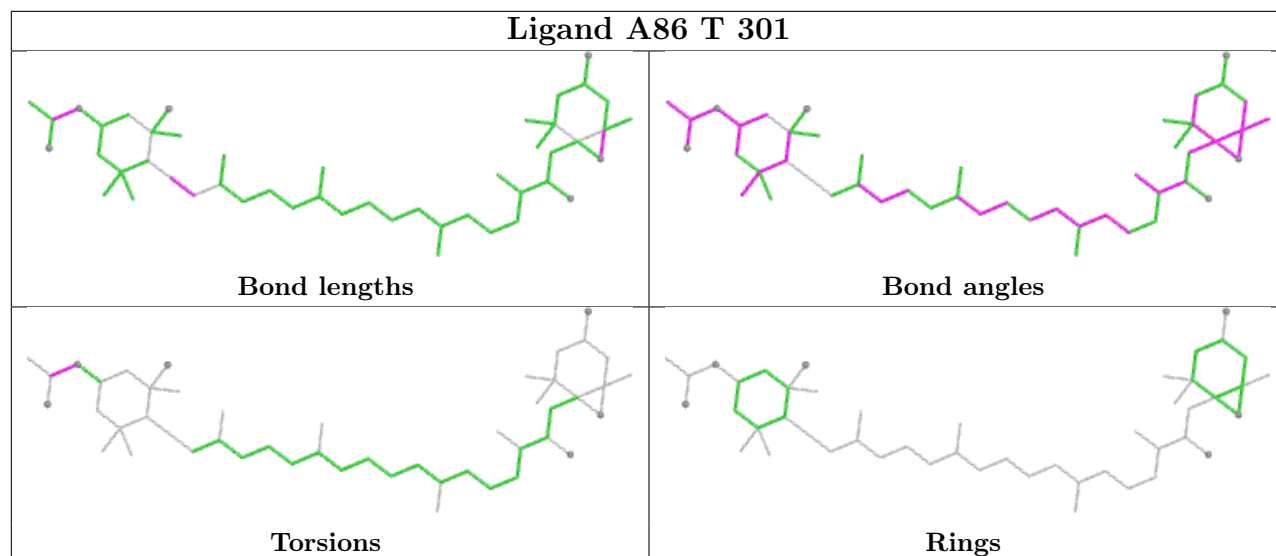
Rings

Ligand CLA b 813

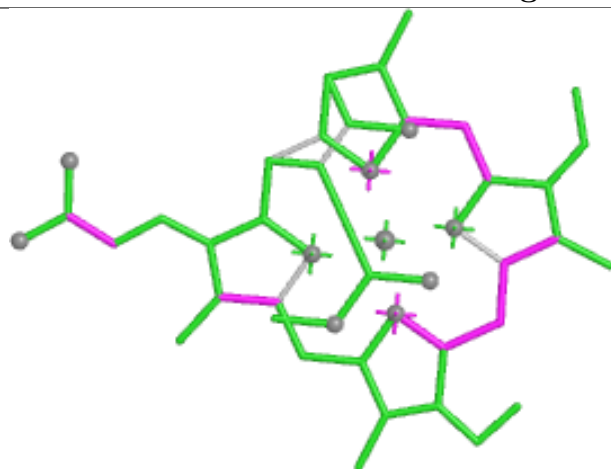


Ligand CLA 4 322

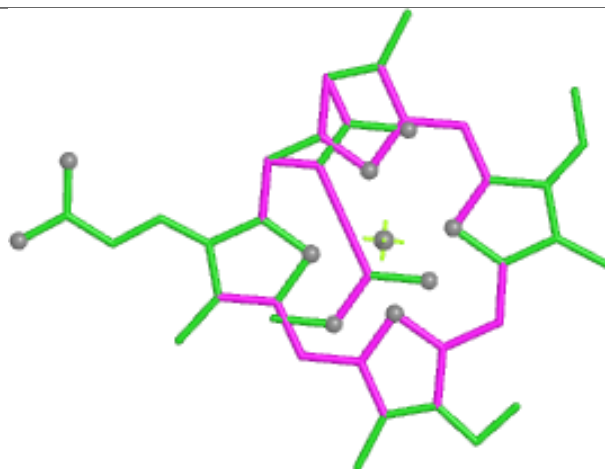




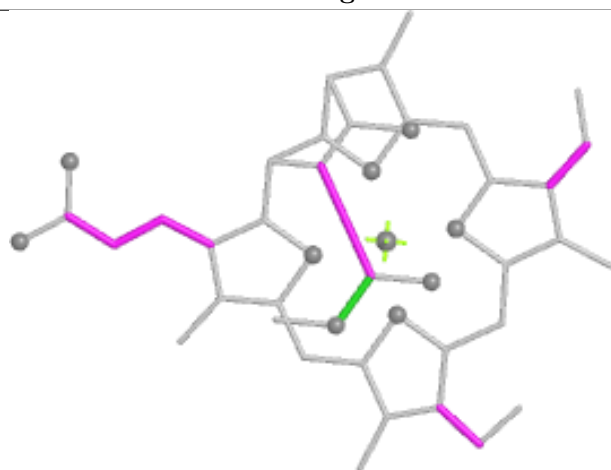
Ligand KC2 3 315



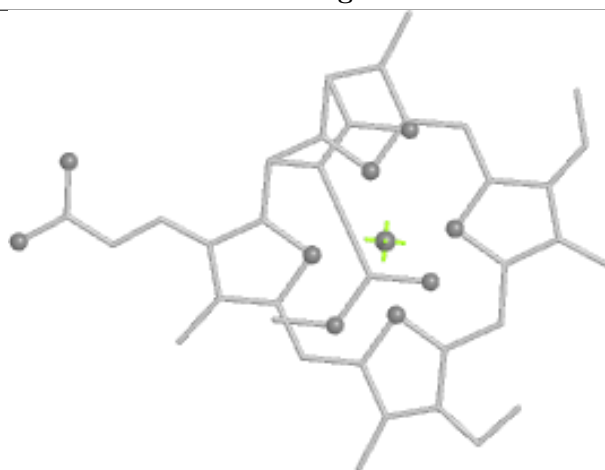
Bond lengths



Bond angles

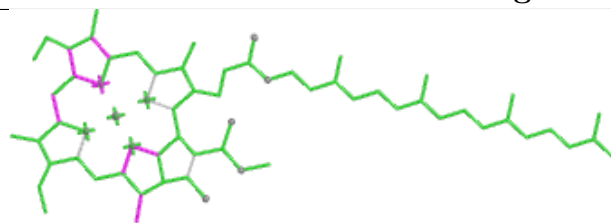


Torsions

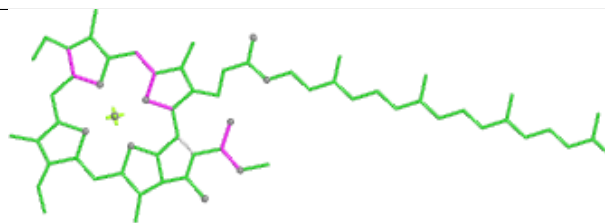


Rings

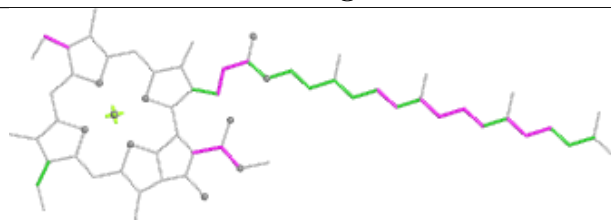
Ligand CLA V 311



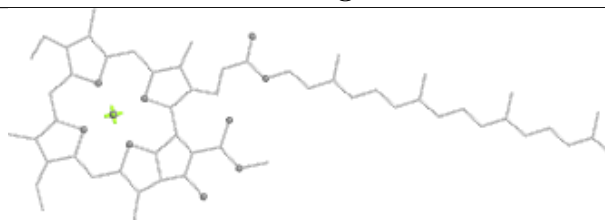
Bond lengths



Bond angles

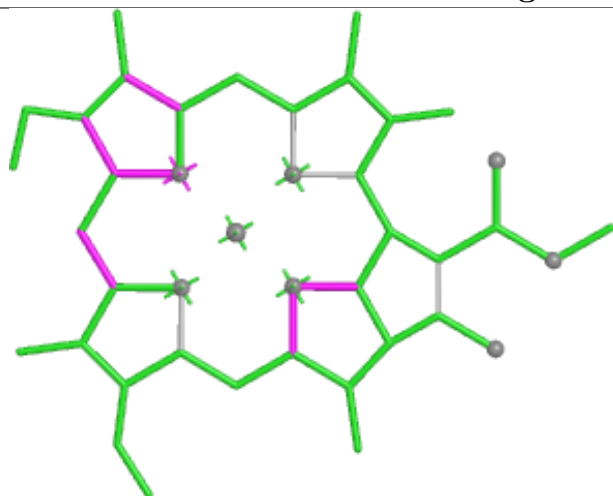


Torsions

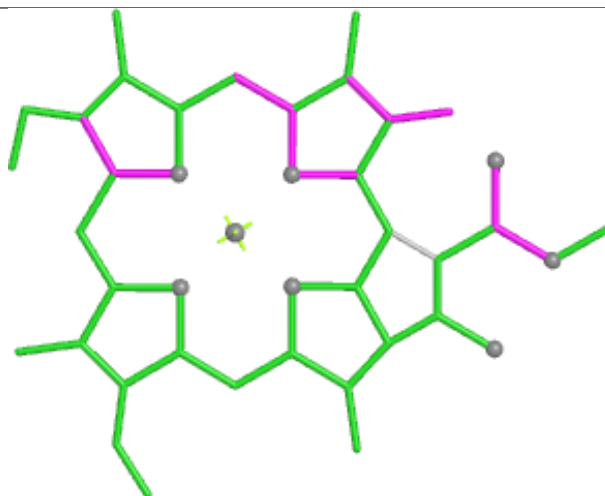


Rings

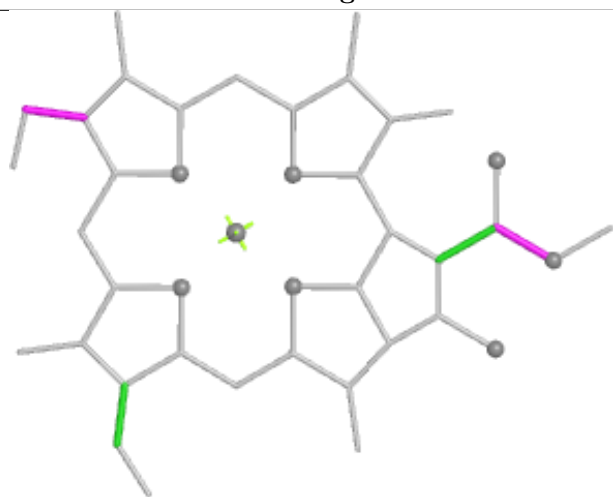
Ligand CLA 4 319



Bond lengths



Bond angles

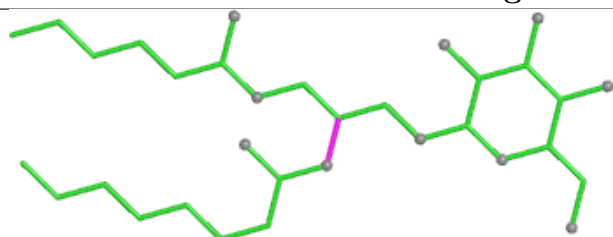


Torsions

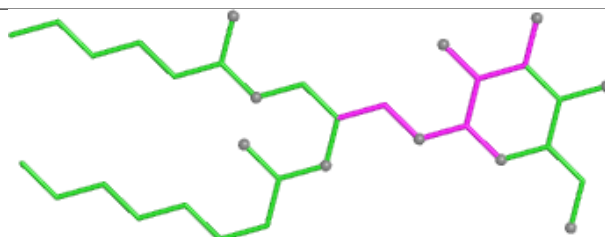


Rings

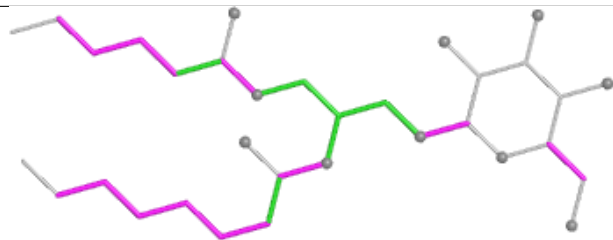
Ligand LMG W 320



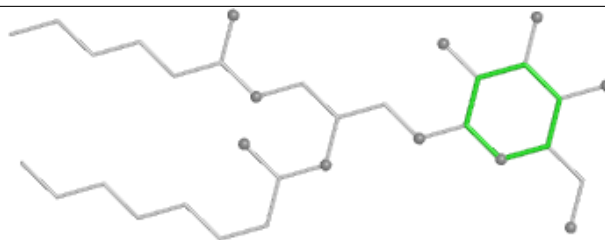
Bond lengths



Bond angles

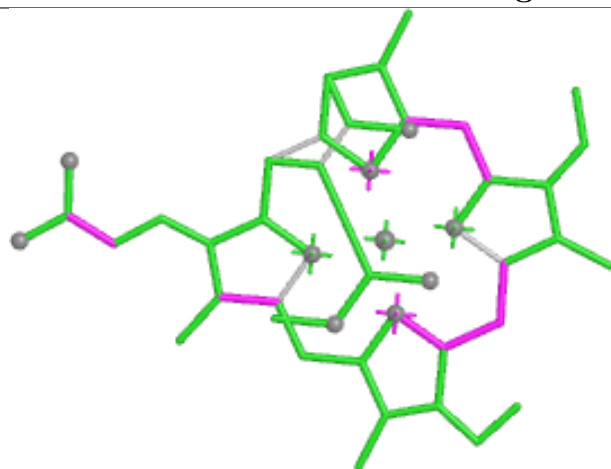


Torsions

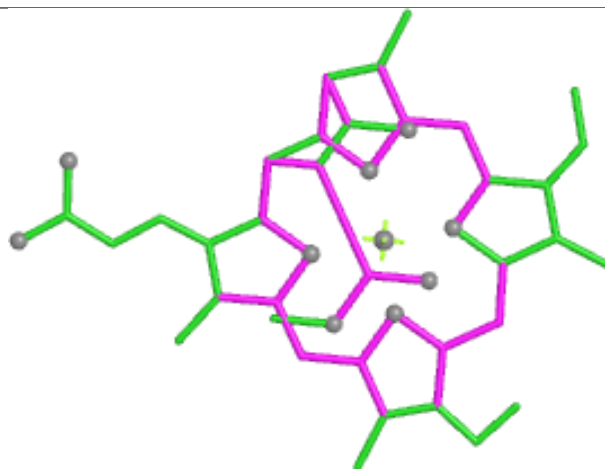


Rings

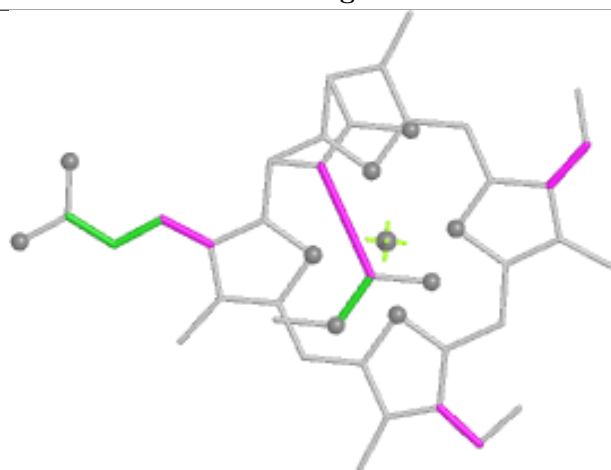
Ligand KC2 V 318



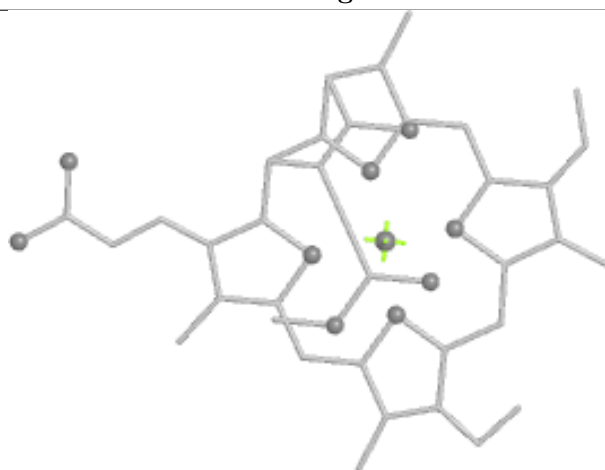
Bond lengths



Bond angles

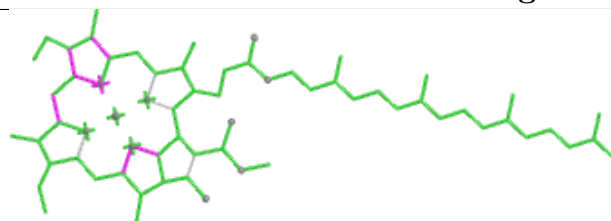


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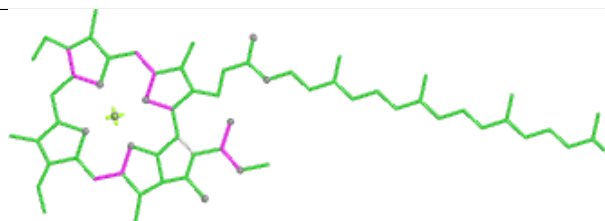


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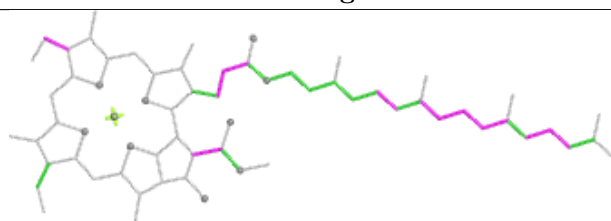
Ligand CLA 5 308



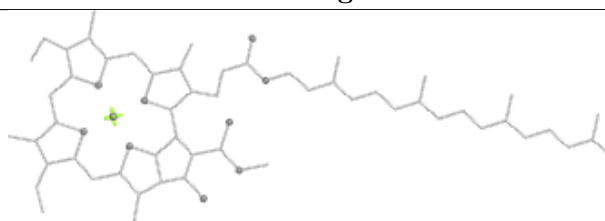
Bond lengths



Bond angles

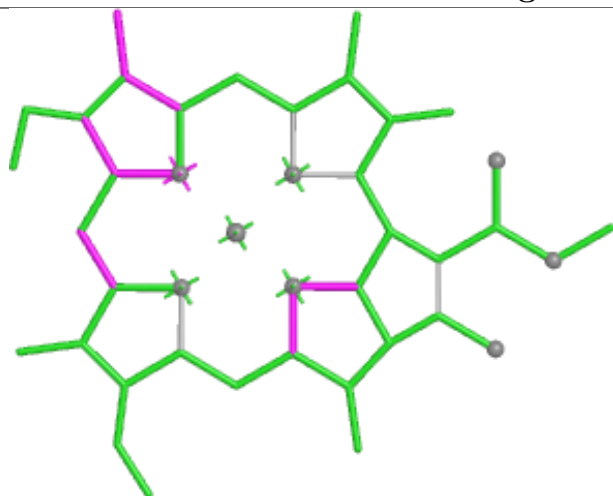


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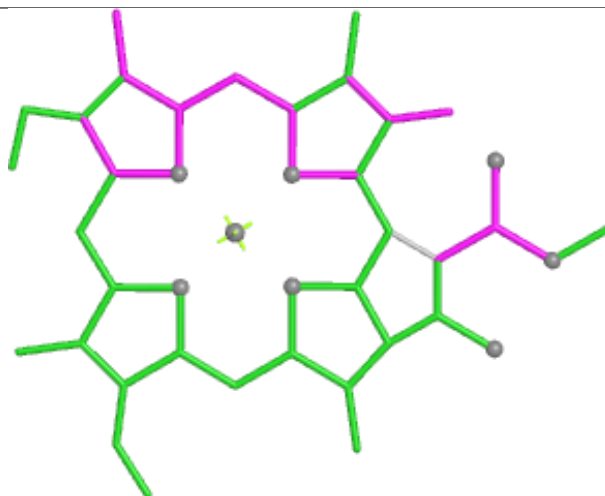


Rings

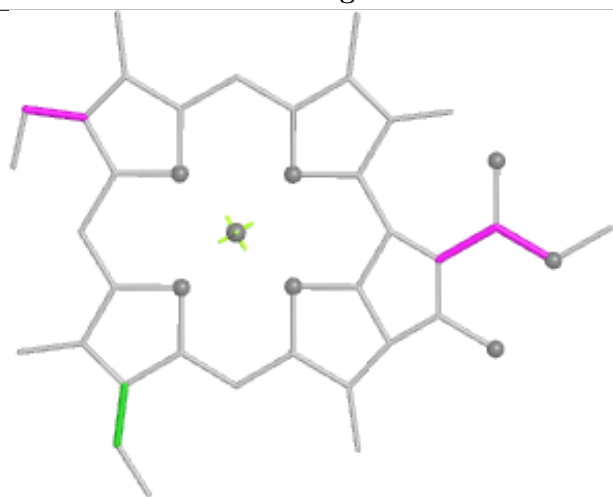
Ligand CLA 7 324



Bond lengths



Bond angles

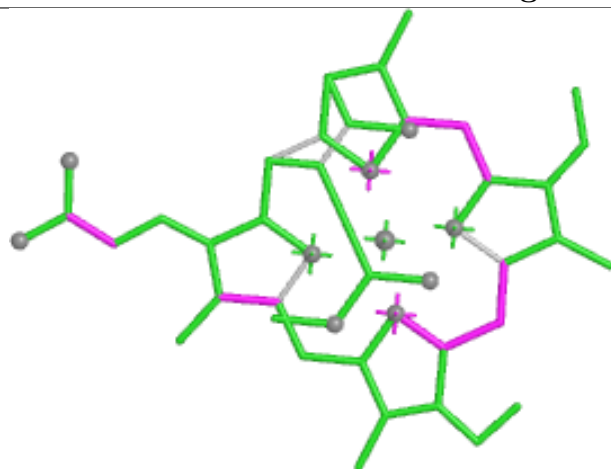


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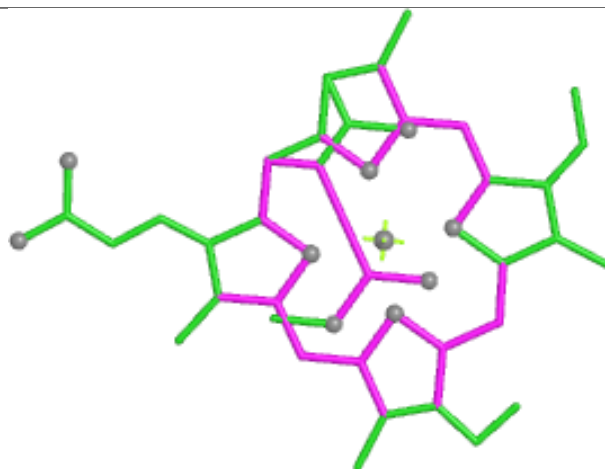


Rings

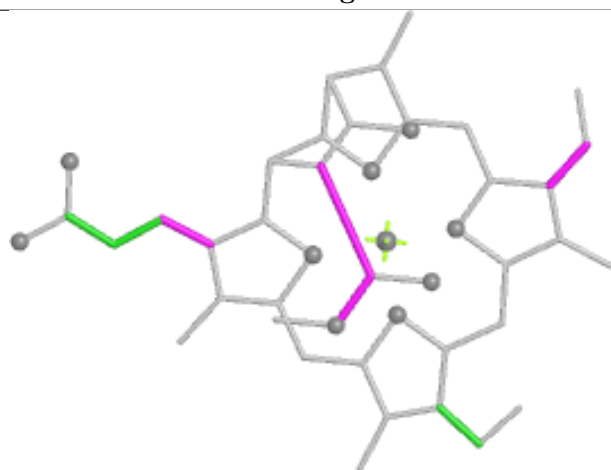
Ligand KC2 8 317



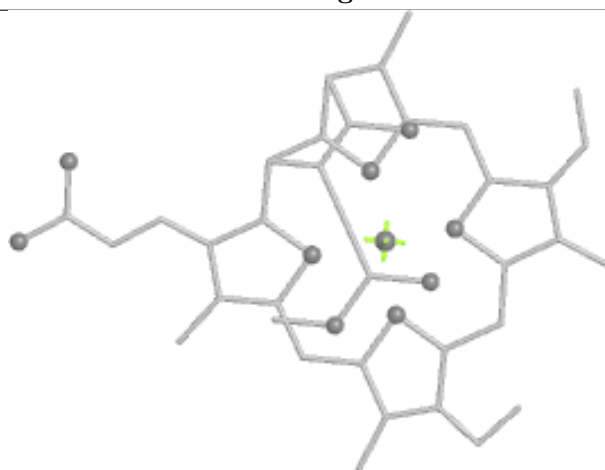
Bond lengths



Bond angles

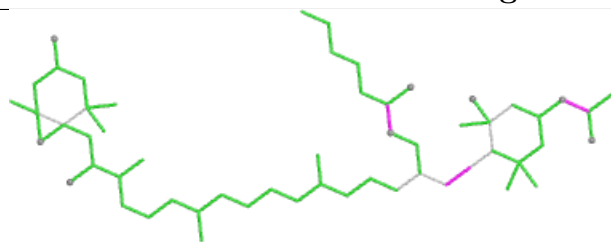


Torsions

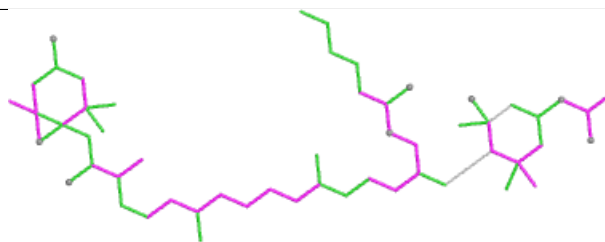


Rings

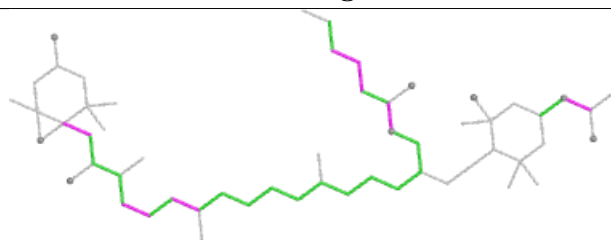
Ligand A1EB1 8 304



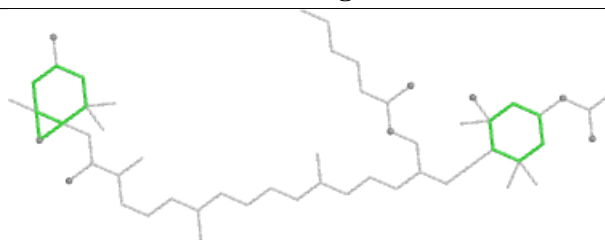
Bond lengths



Bond angles

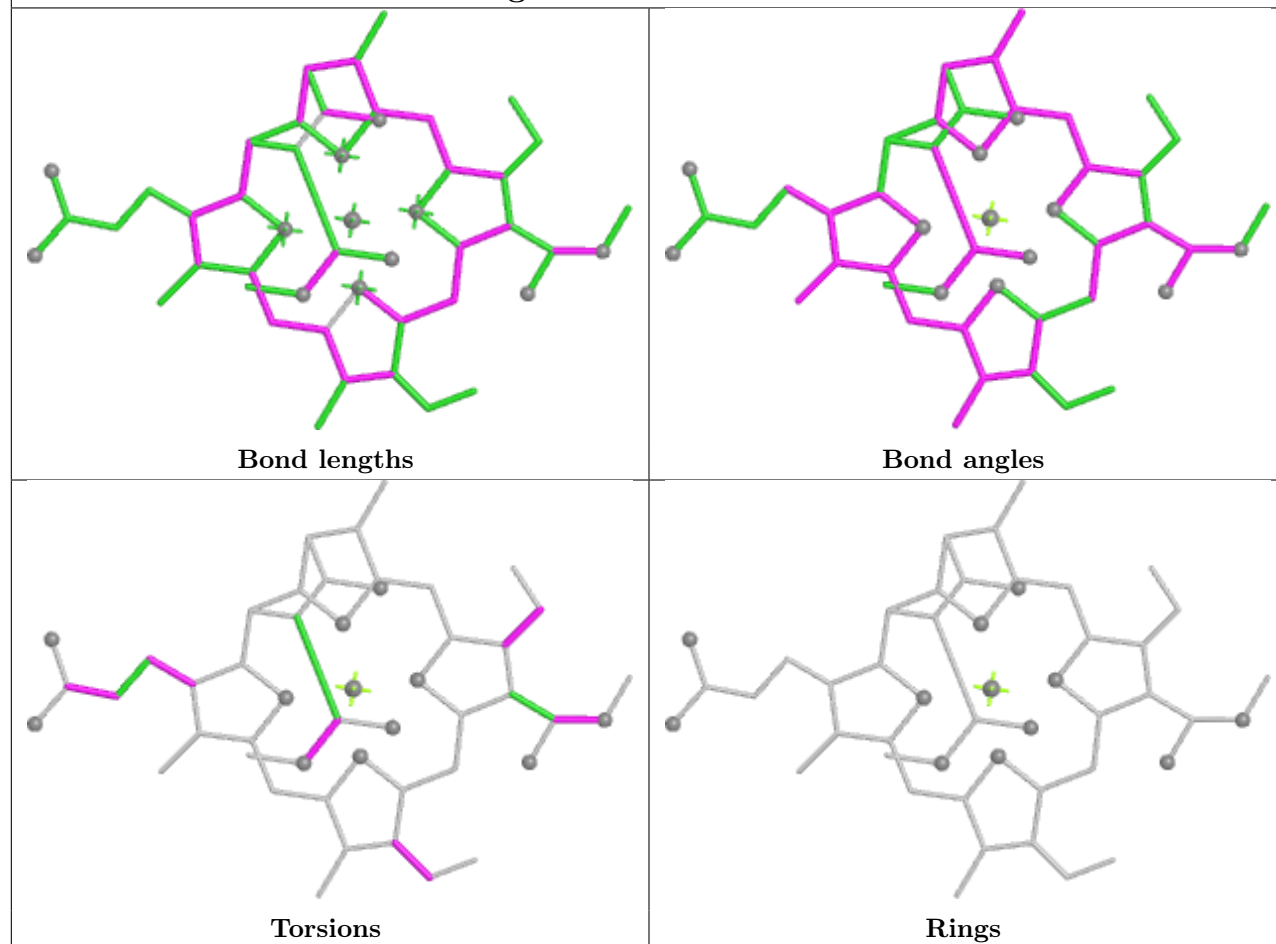


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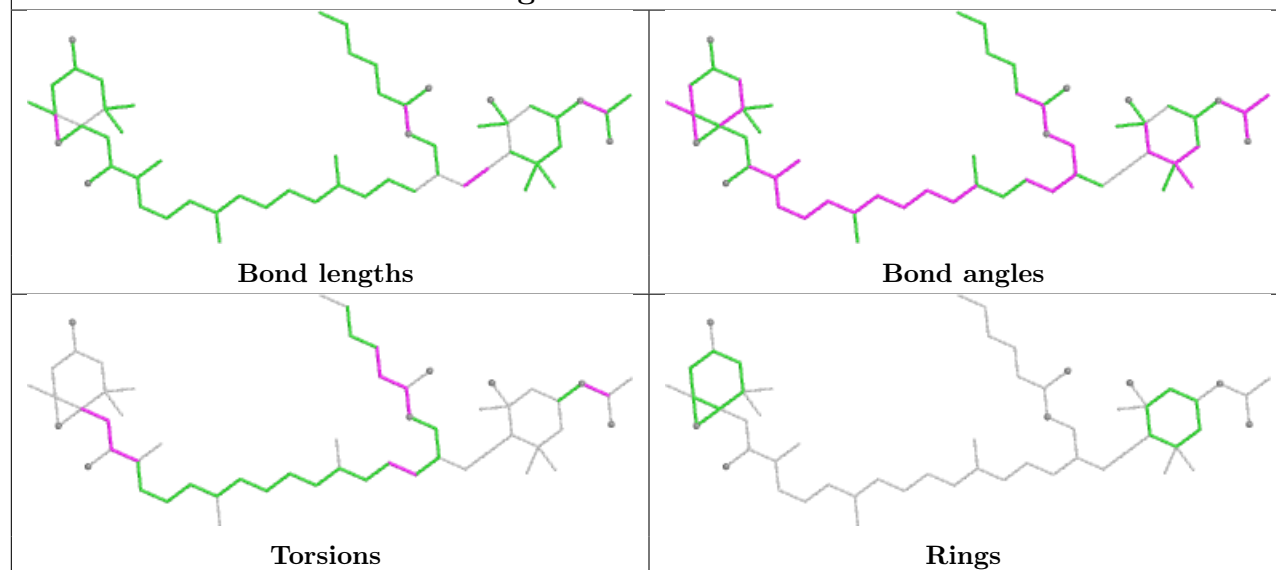


Rings

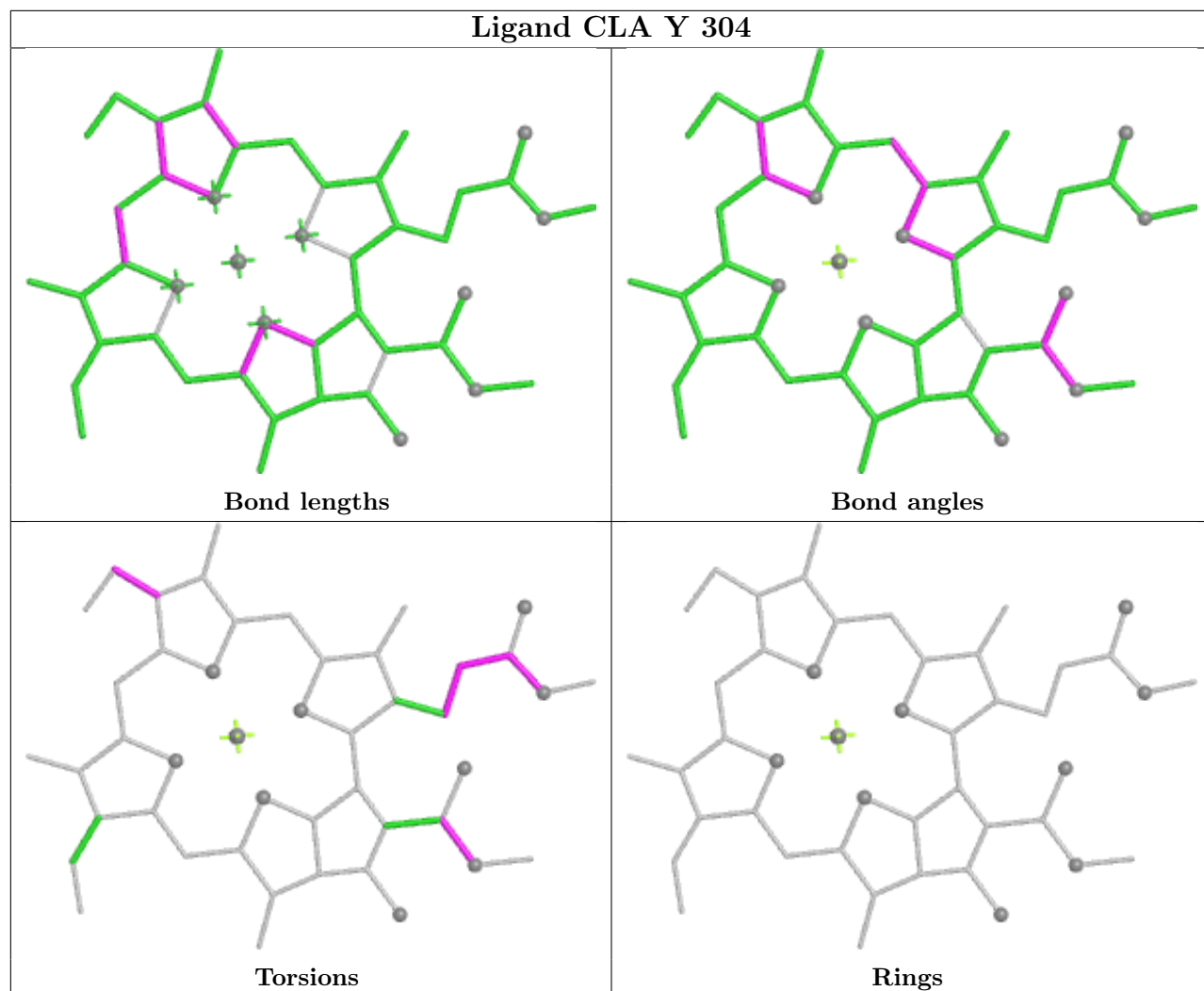
Ligand A1ECV X 310



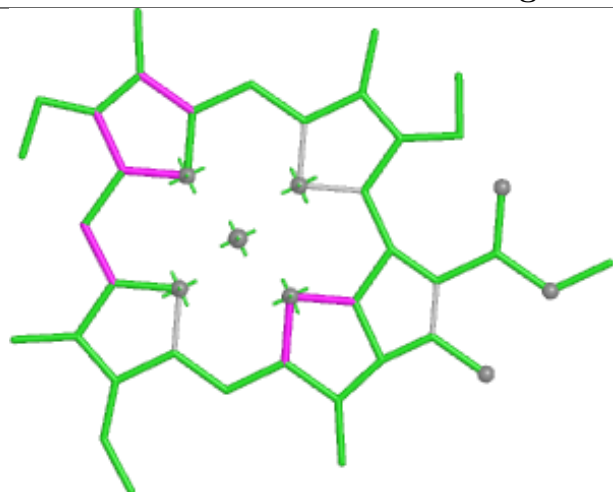
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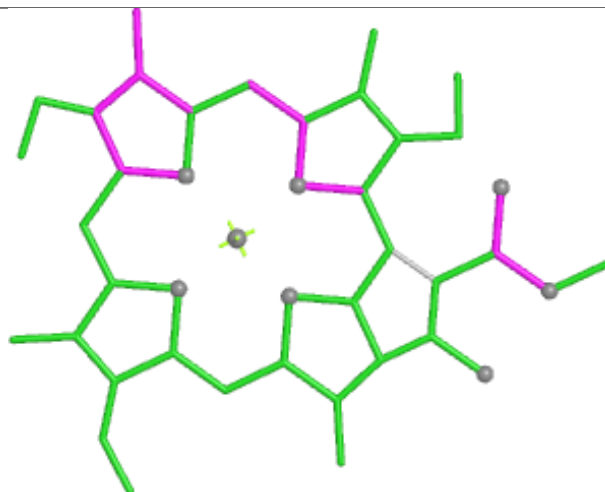
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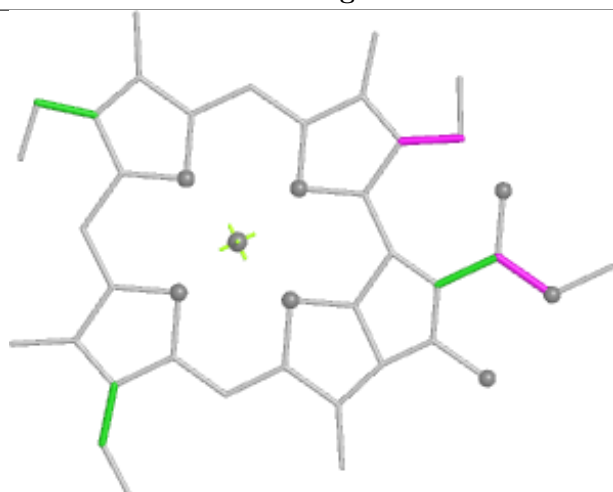
Ligand CLA z 307



Bond lengths



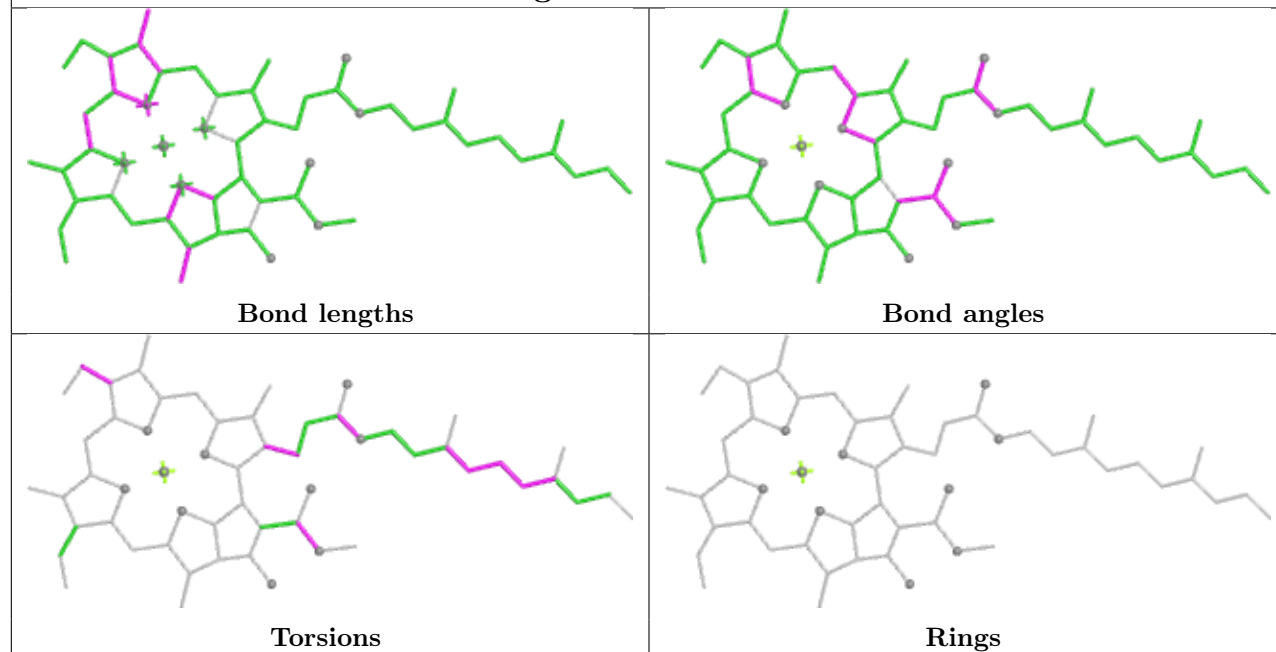
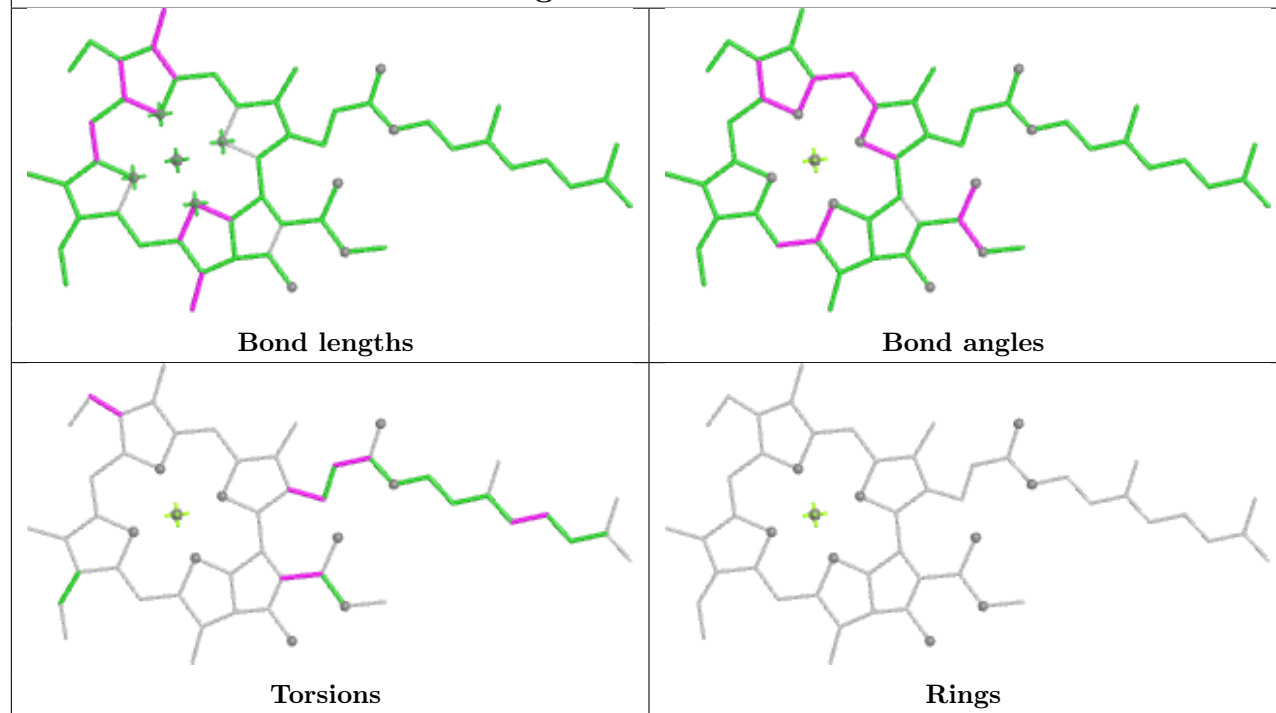
Bond angles



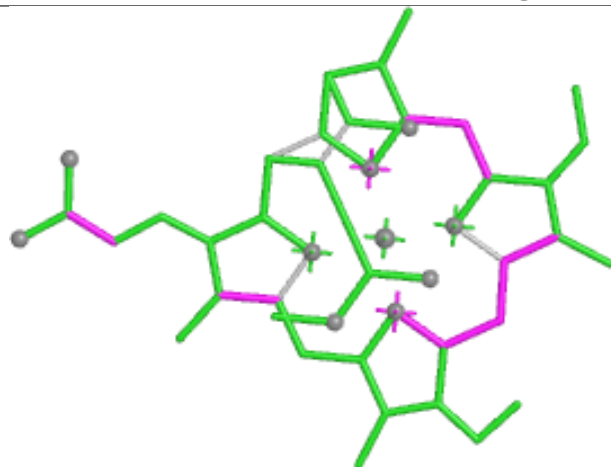
Torsions



Rings

Ligand CLA F 313**Ligand CLA b 814**

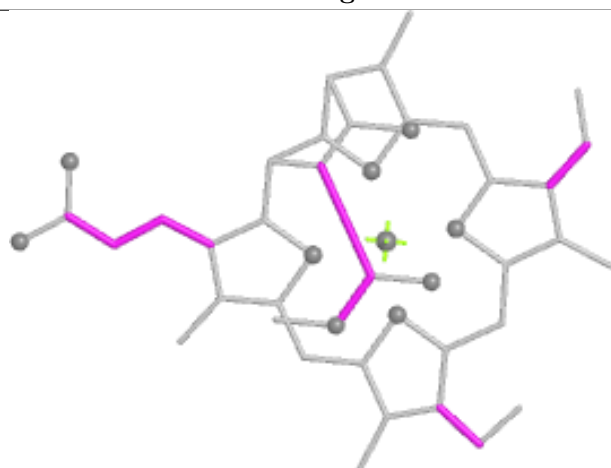
Ligand KC2 A 313



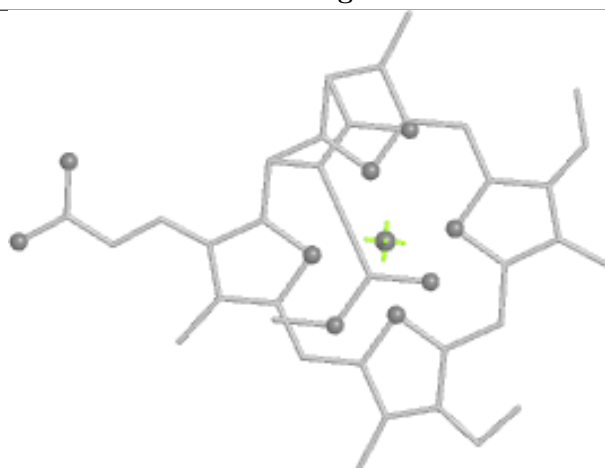
Bond lengths



Bond angles

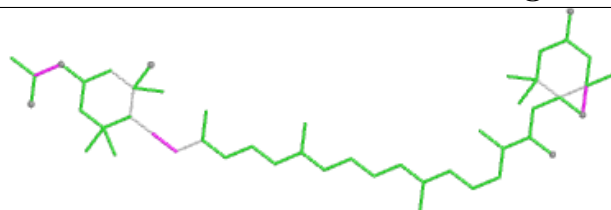


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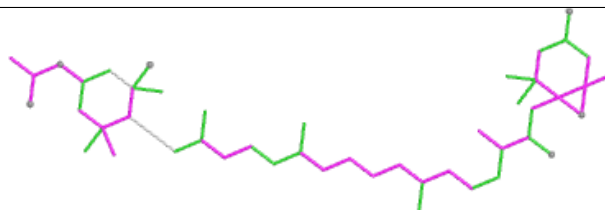


Rings

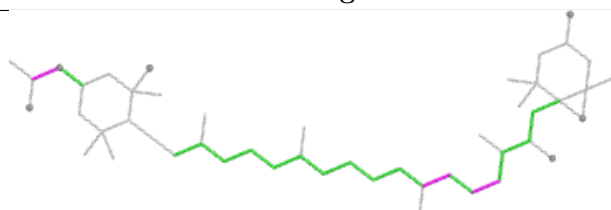
Ligand A86 1 302



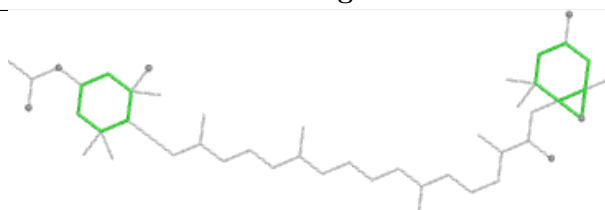
Bond lengths



Bond angles

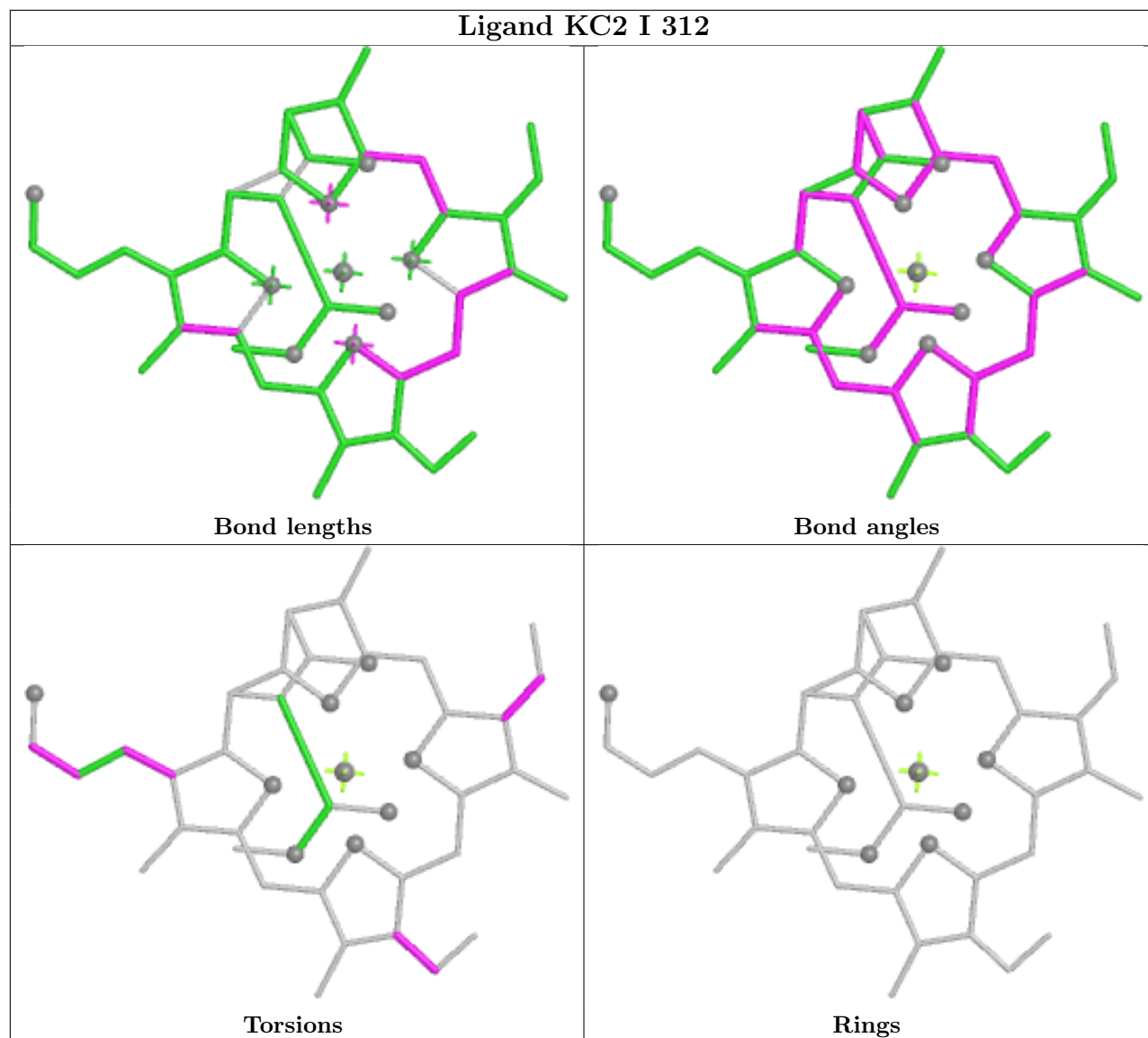


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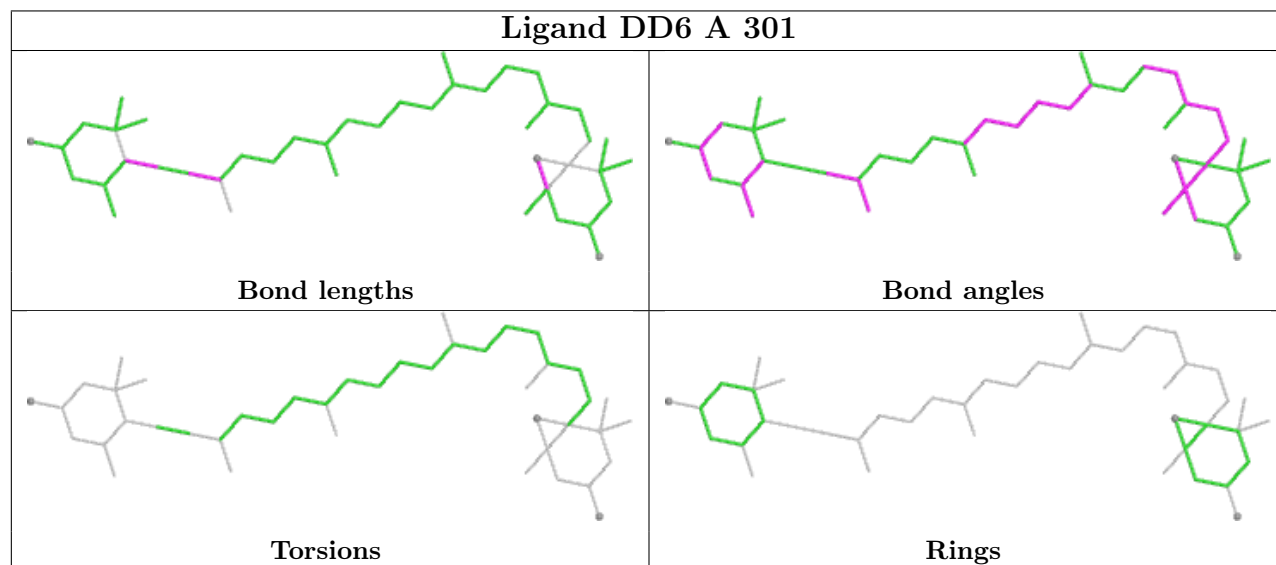


Rings

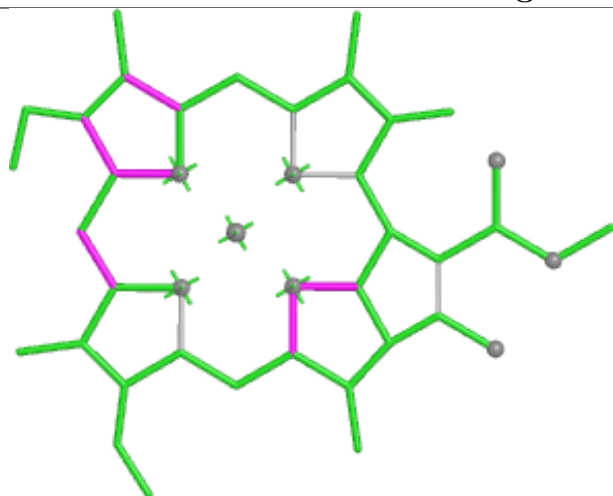
Ligand KC2 I 312



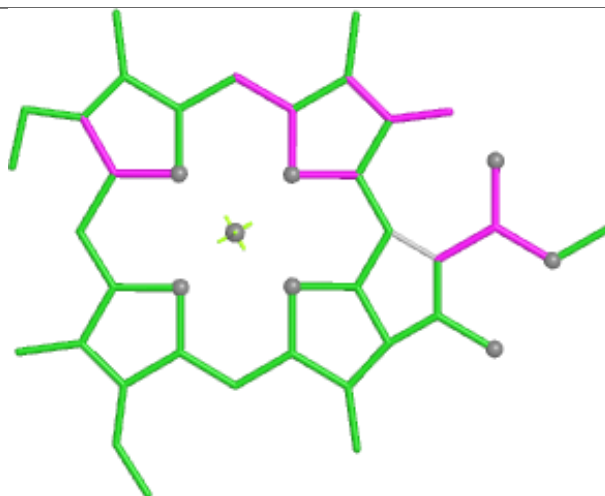
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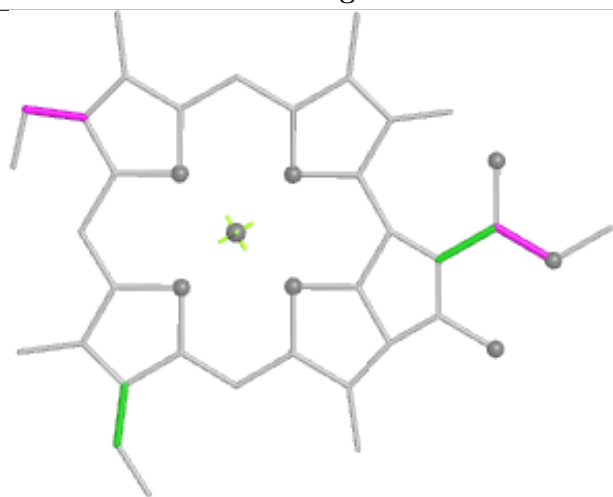
Ligand CLA F 315



Bond lengths



Bond angles

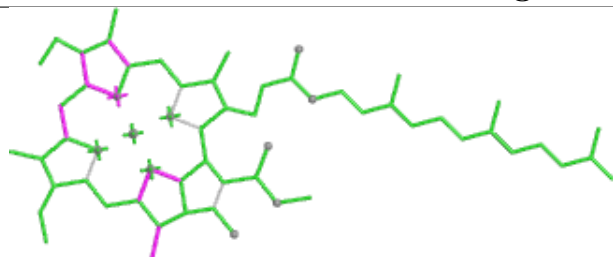


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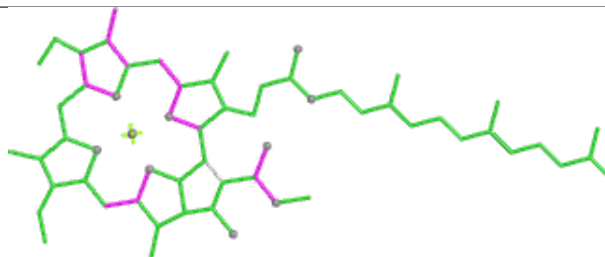


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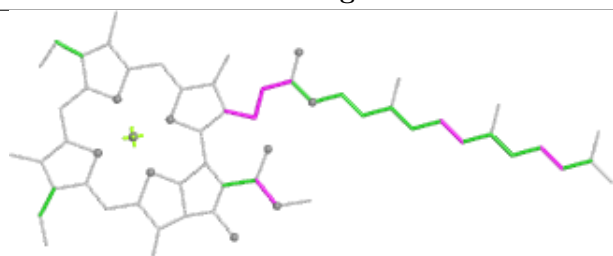
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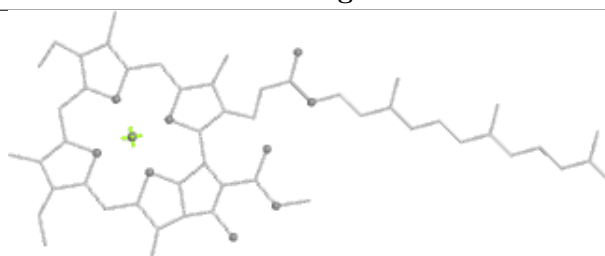
Bond lengths



Bond angles

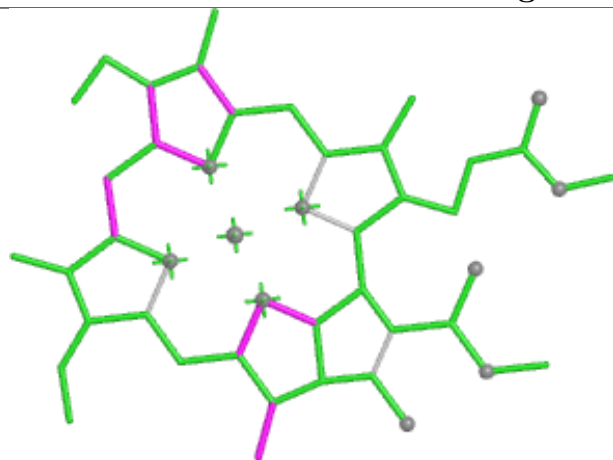


Torsions

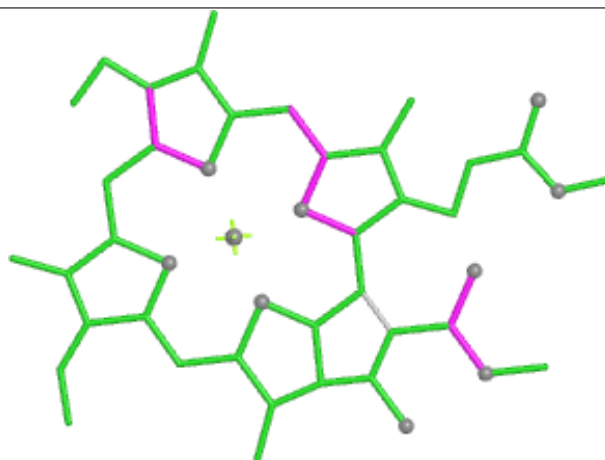


Rings

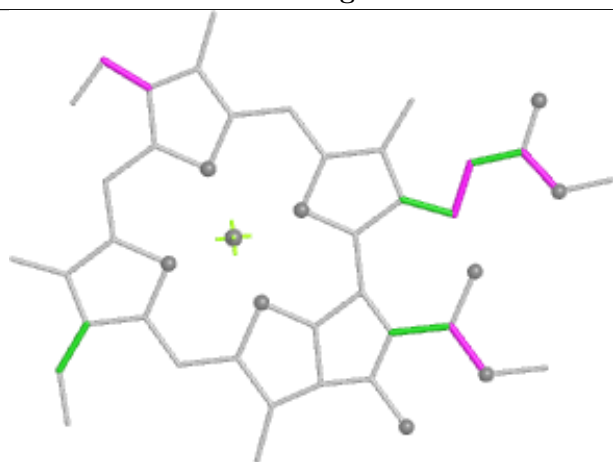
Ligand CLA J 316



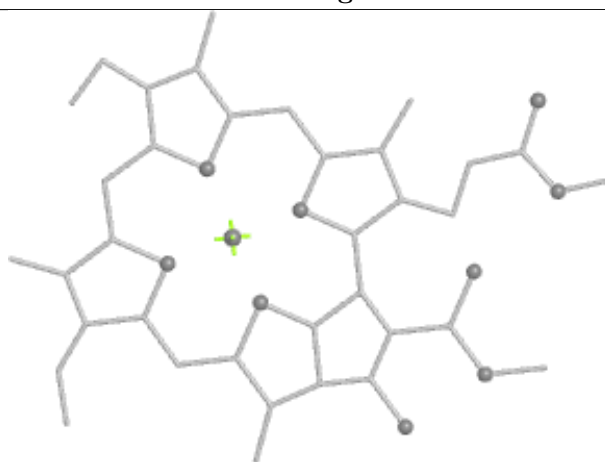
Bond lengths



Bond angles

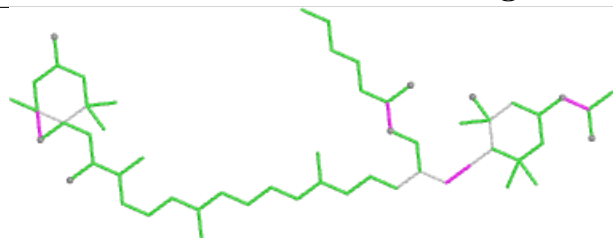


Torsions

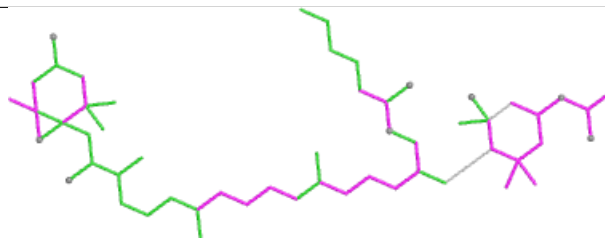


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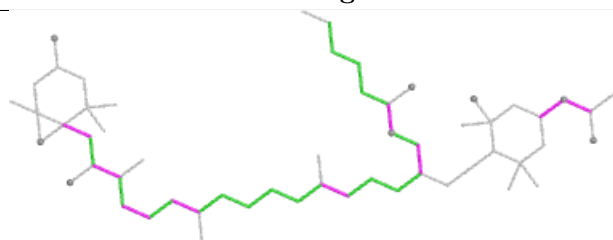
Ligand A1EB1 7 305



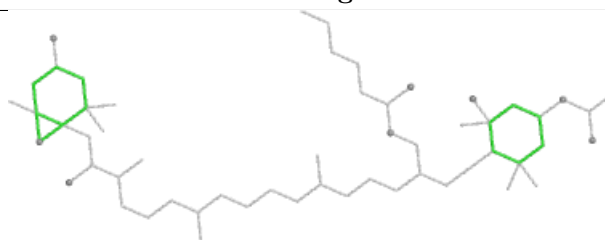
Bond lengths



Bond angles

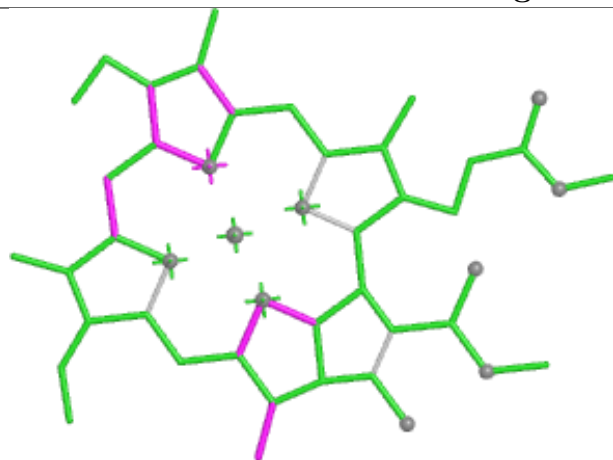


Torsions

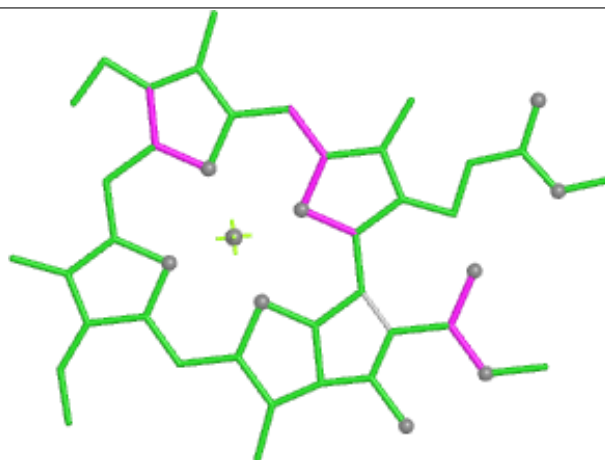


Rings

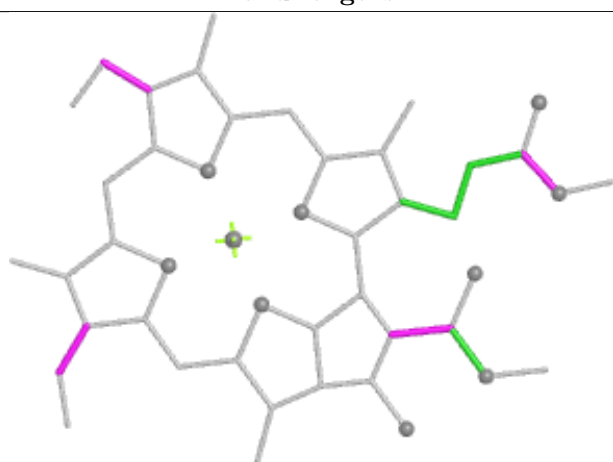
Ligand CLA O 312



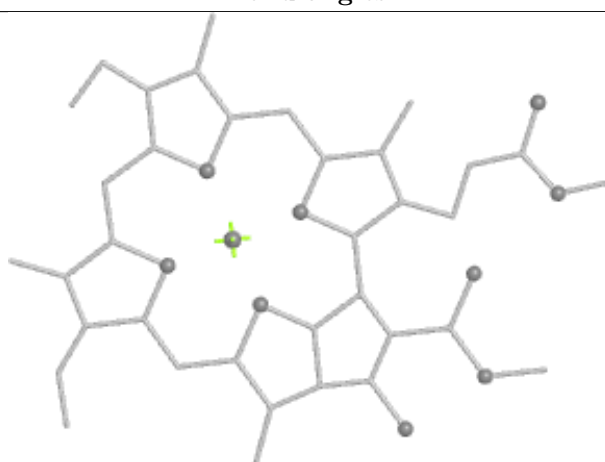
Bond lengths



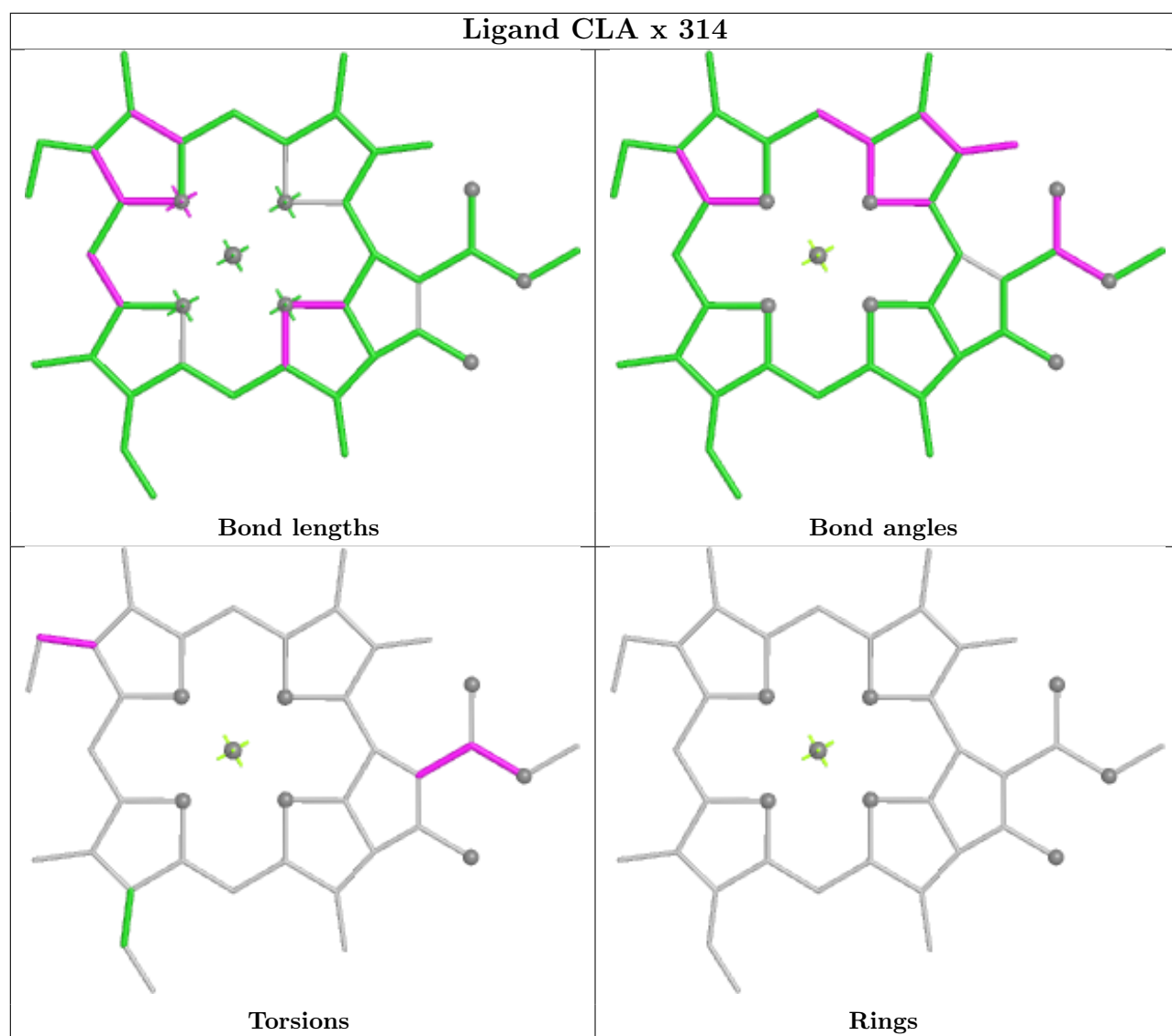
Bond angles



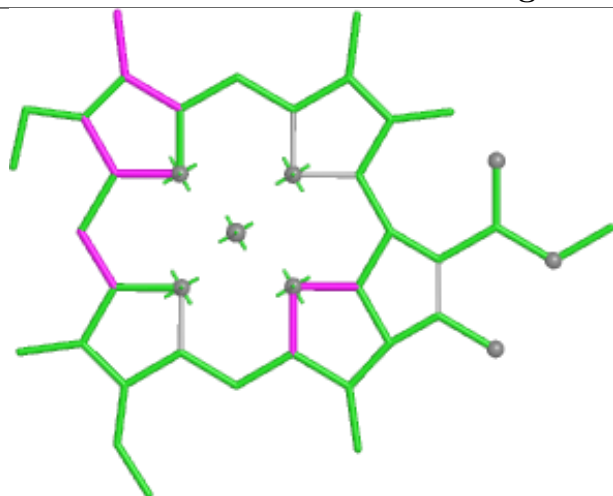
Torsions



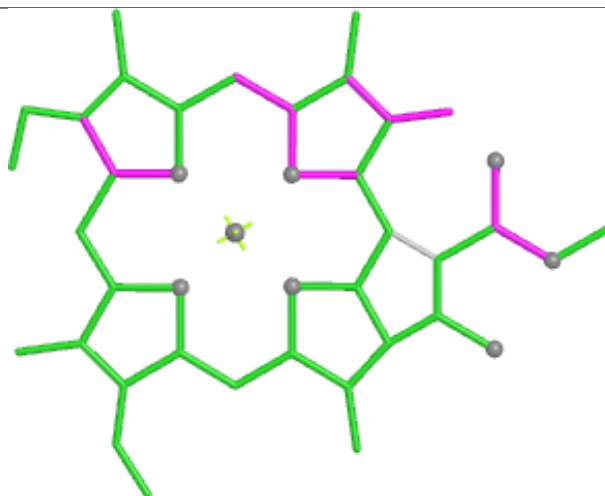
Rings



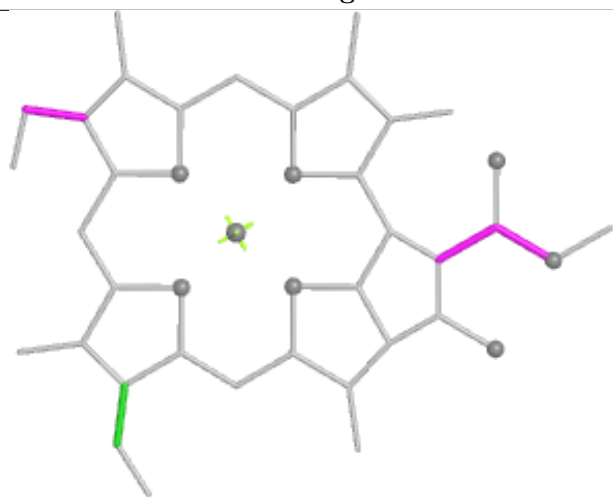
Ligand CLA 2 318



Bond lengths



Bond angles

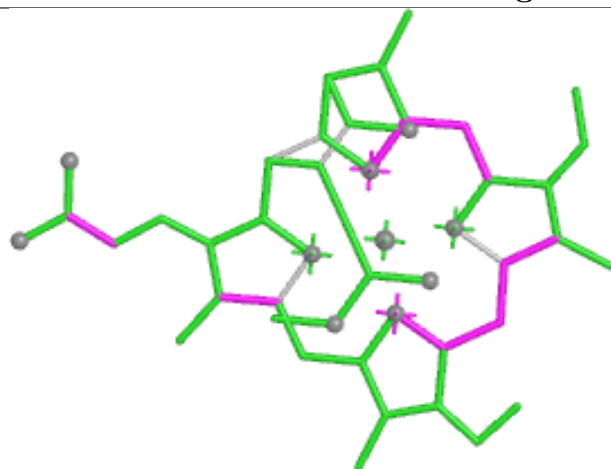


Torsions

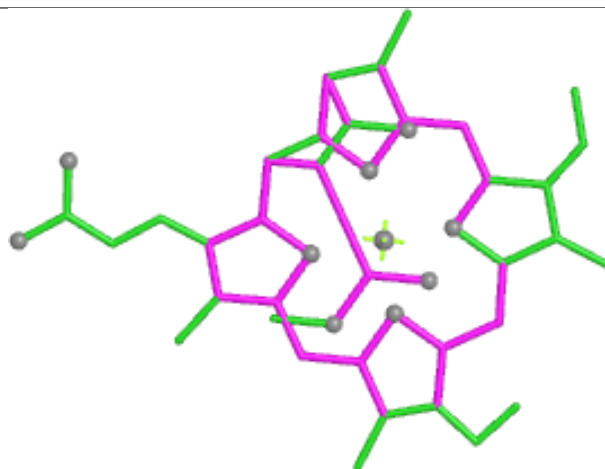


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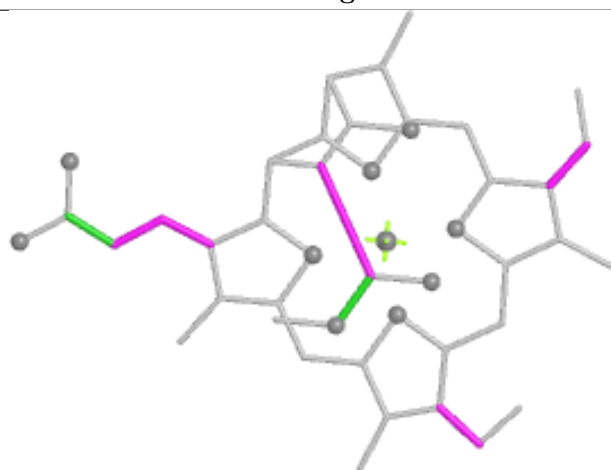
Ligand KC2 R 312



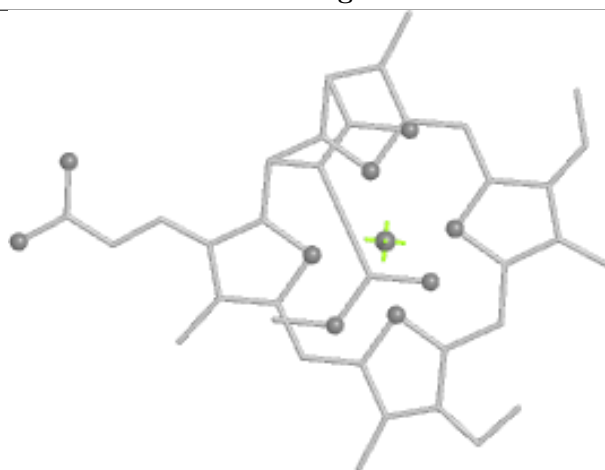
Bond lengths



Bond angles

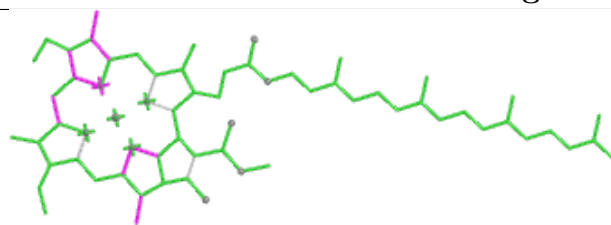


Torsions

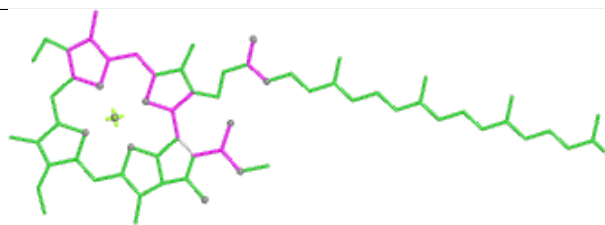


Rings

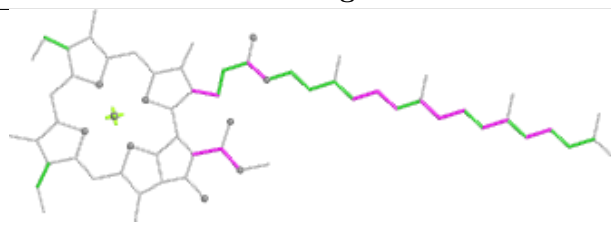
Ligand CLA i 103



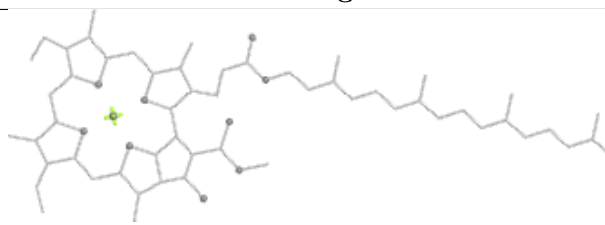
Bond lengths



Bond angles

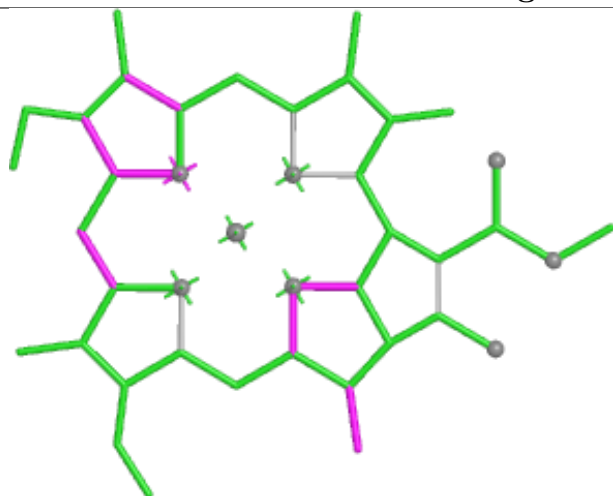


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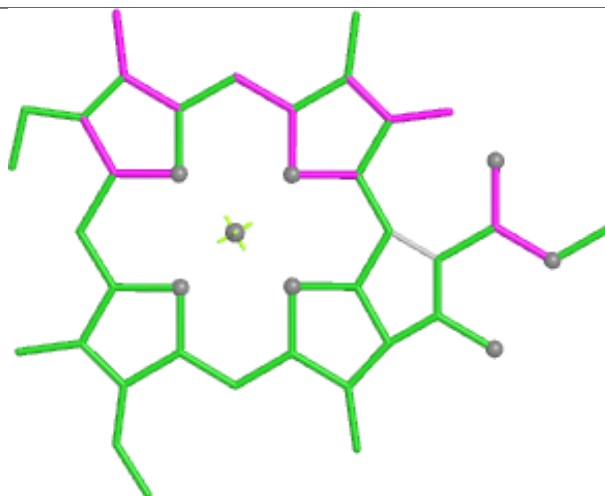


Rings

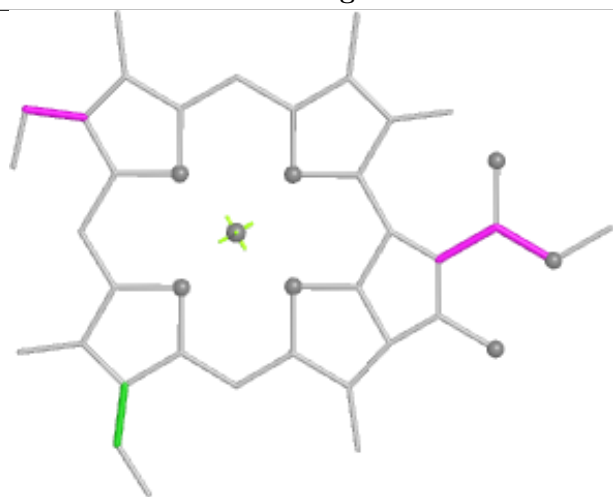
Ligand CLA x 309



Bond lengths



Bond angles

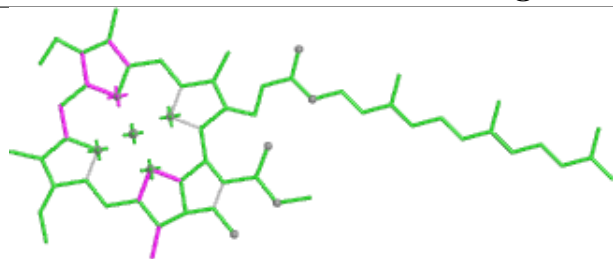


Torsions

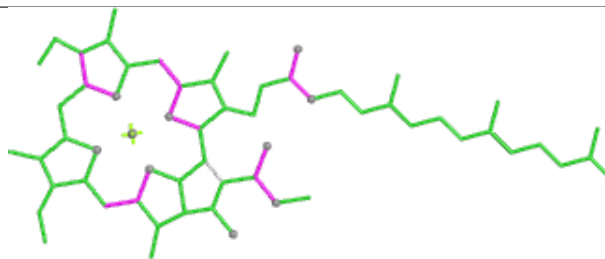


Rings

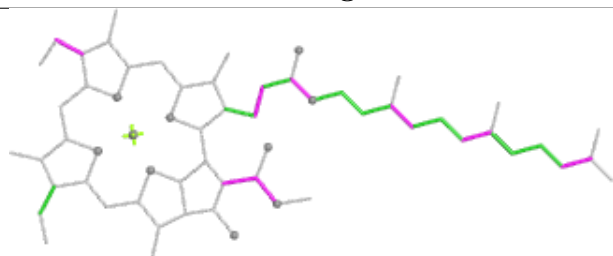
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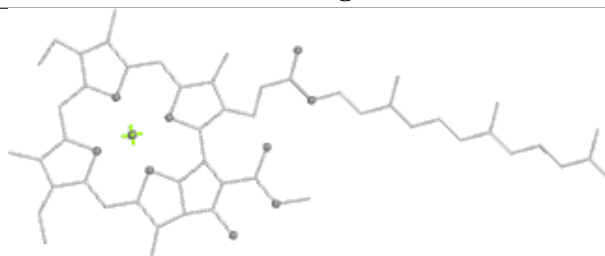
Bond lengths



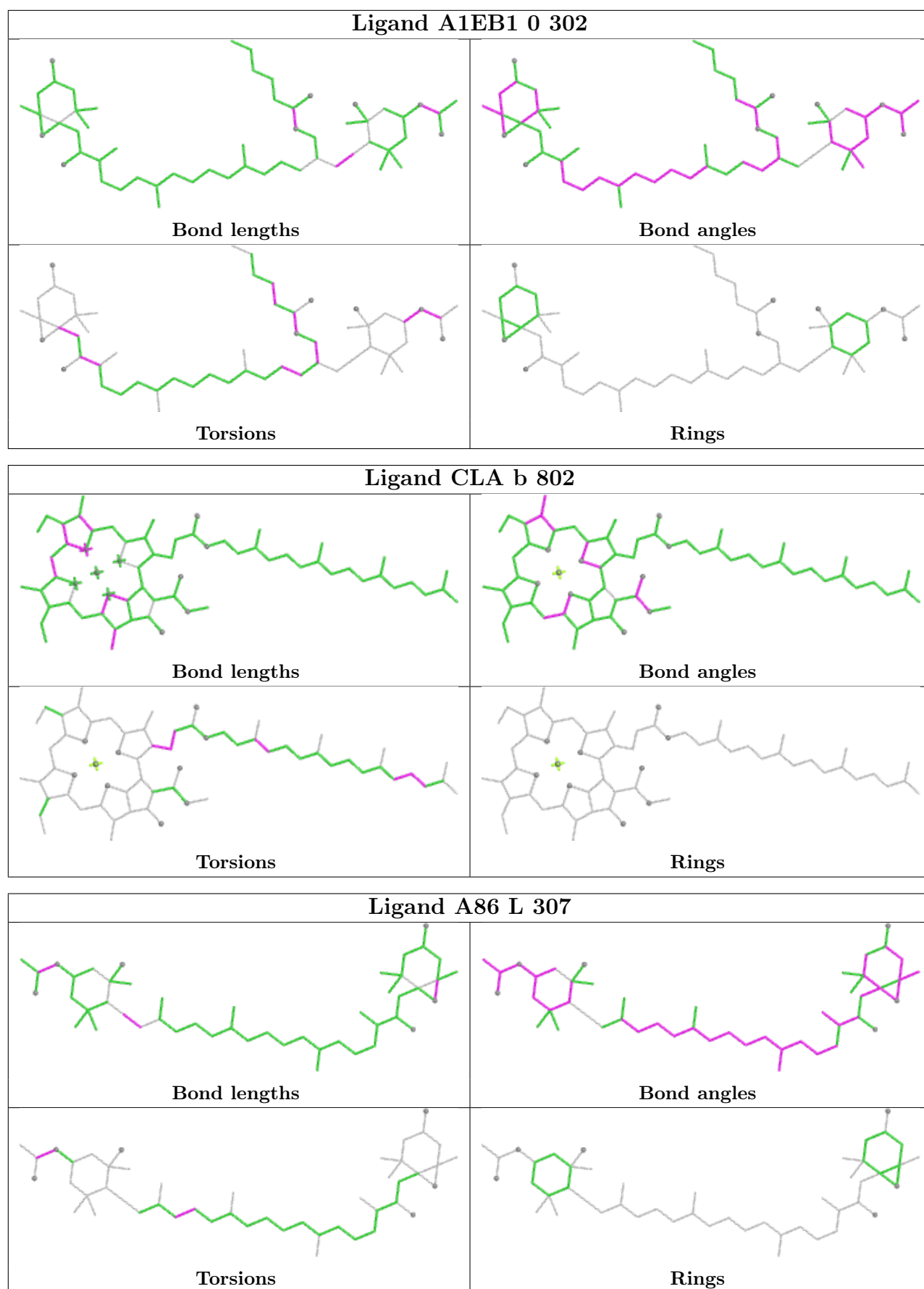
Bond angles



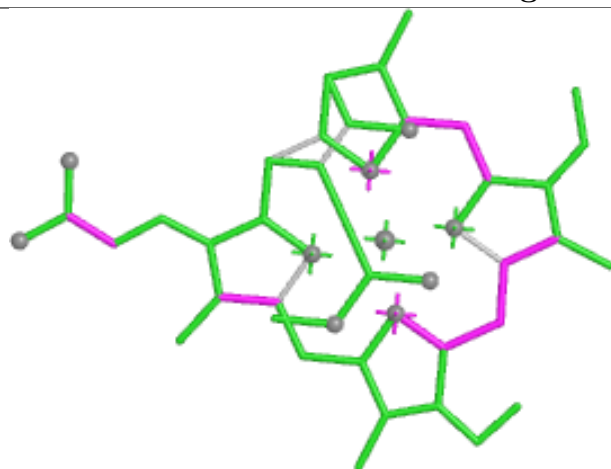
Torsions



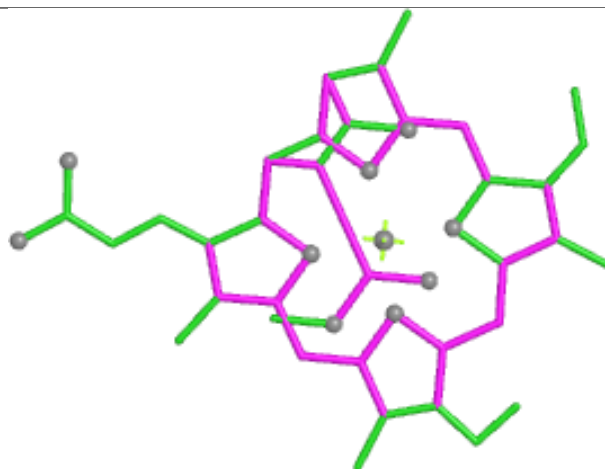
Rings



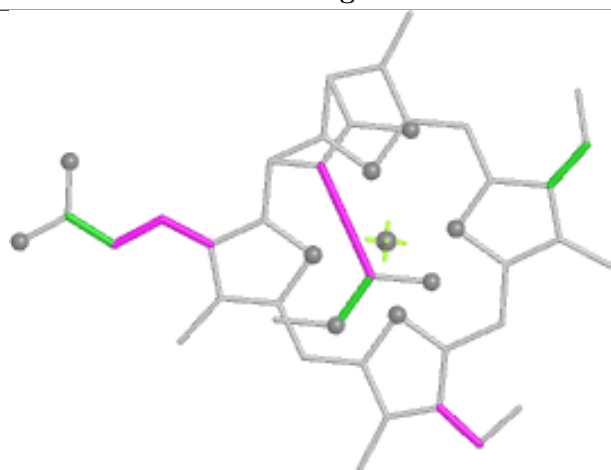
Ligand KC2 5 311



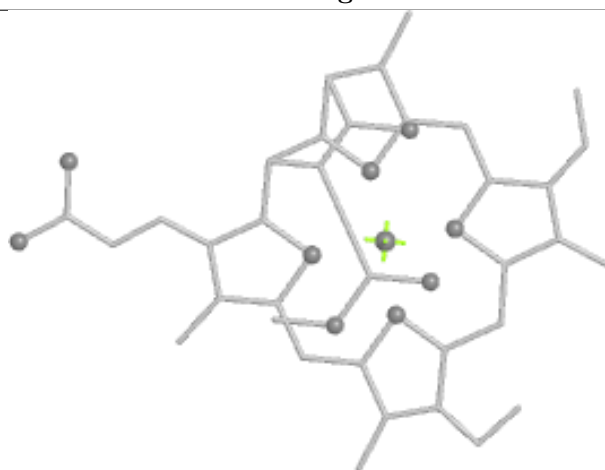
Bond lengths



Bond angles

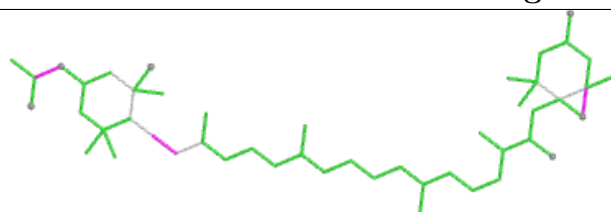


Torsions

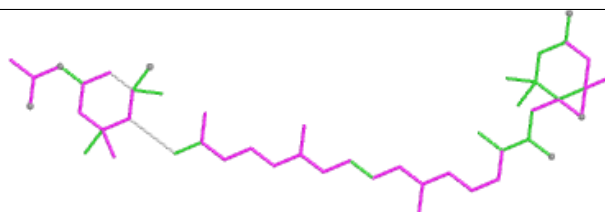


Rings

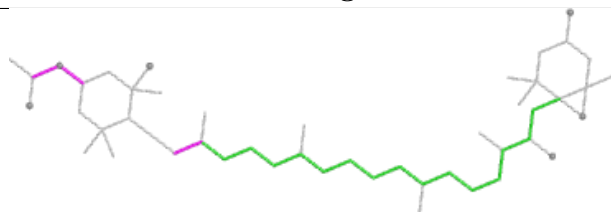
Ligand A86 3 307



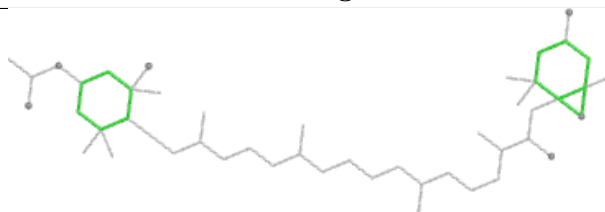
Bond lengths



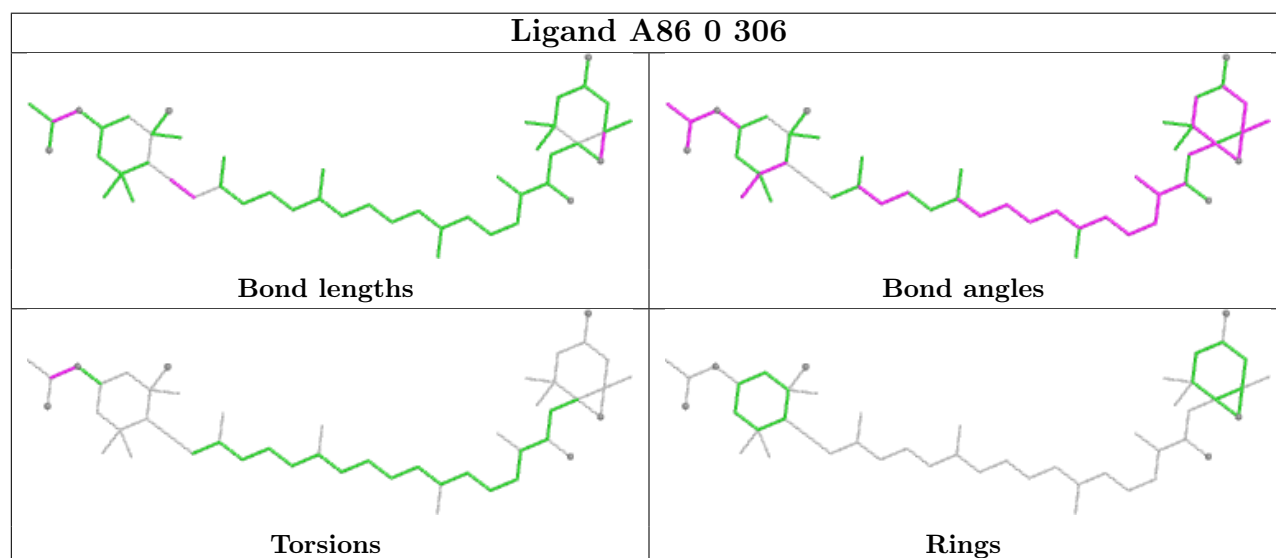
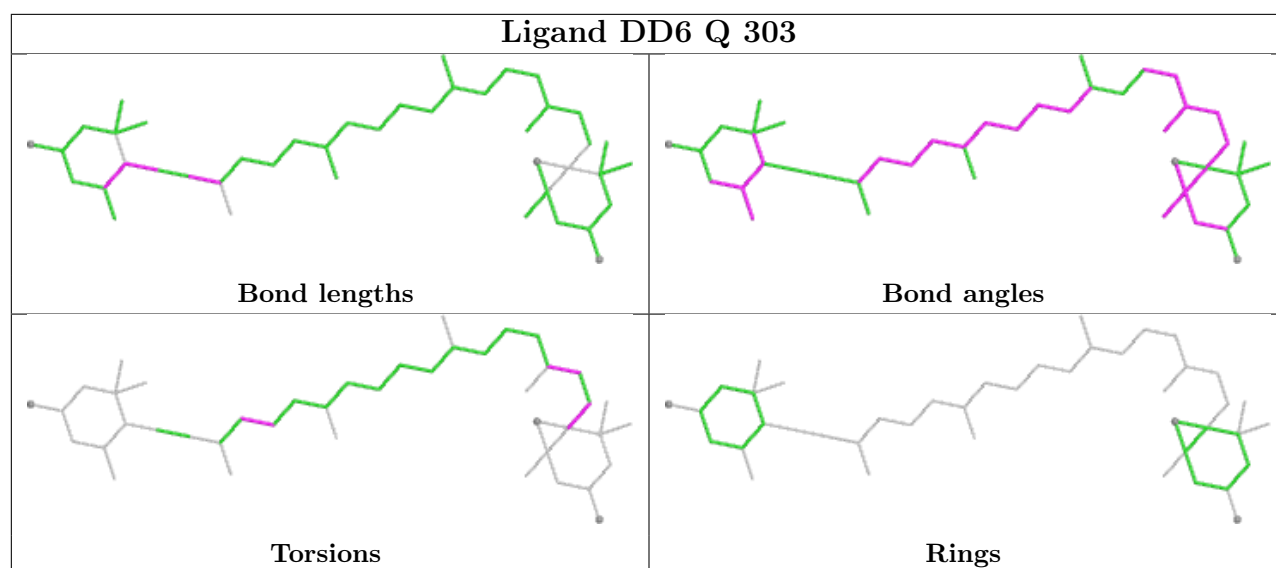
Bond angles

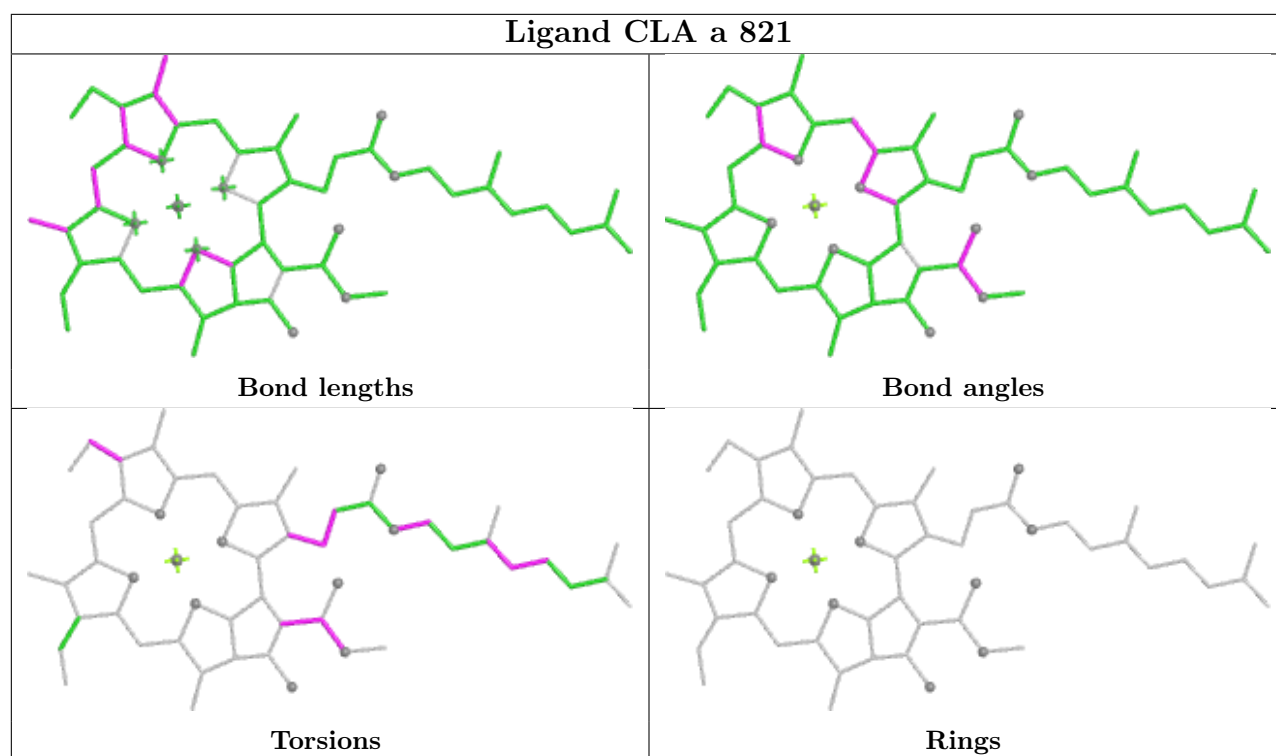


Torsions

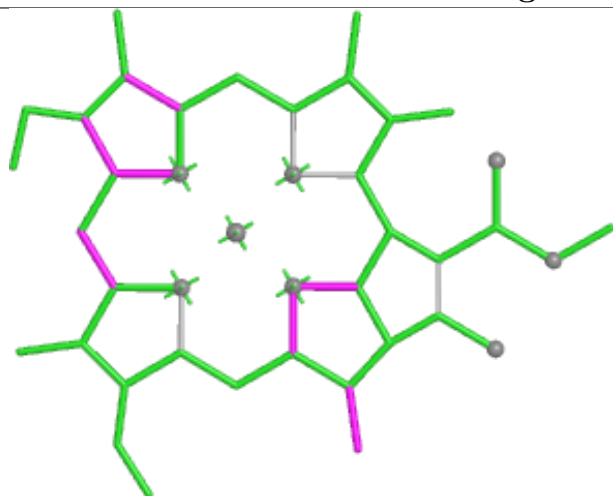


Rings

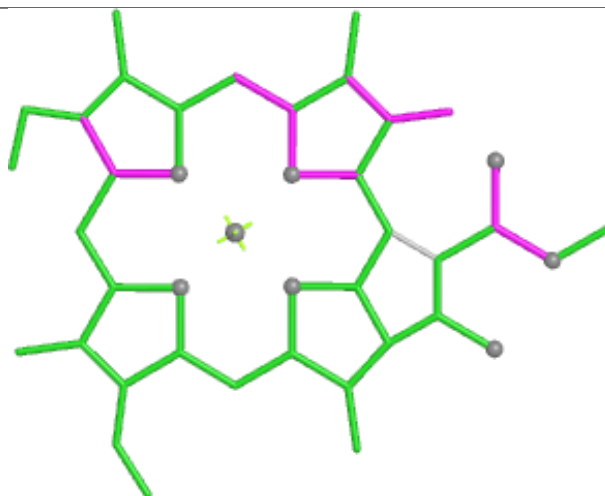




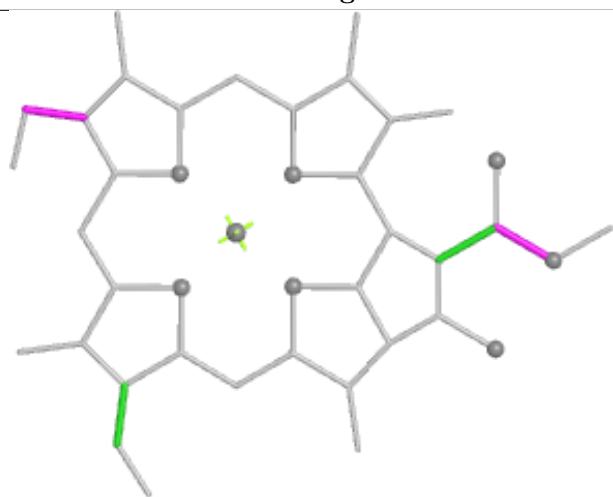
Ligand CLA 2 307



Bond lengths



Bond angles

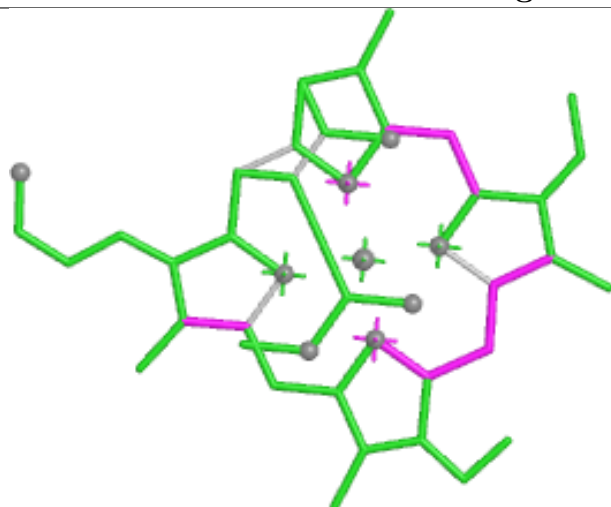


Torsions

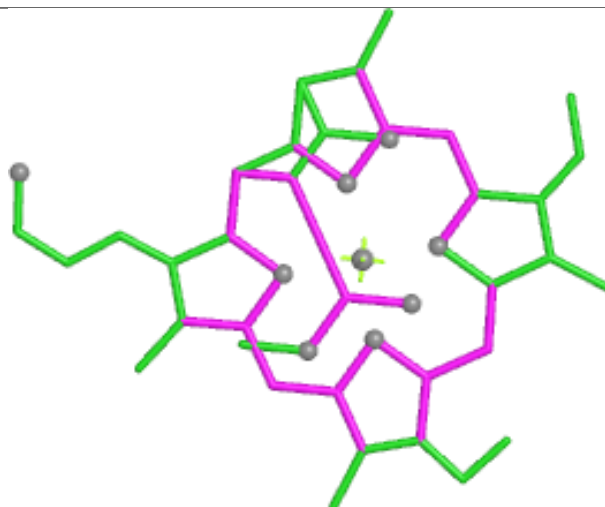


Rings

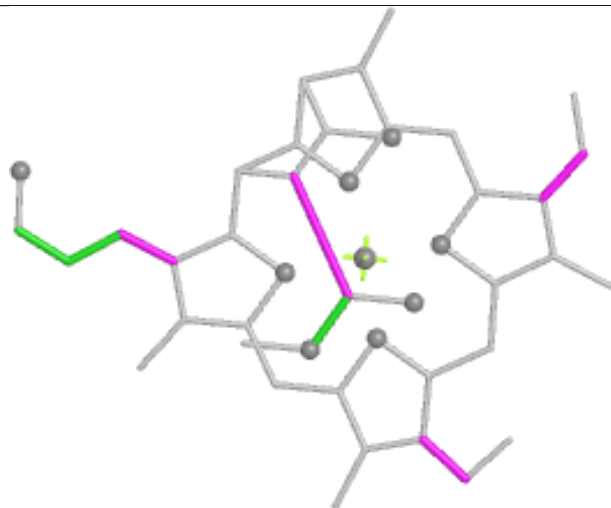
Ligand KC2 R 314



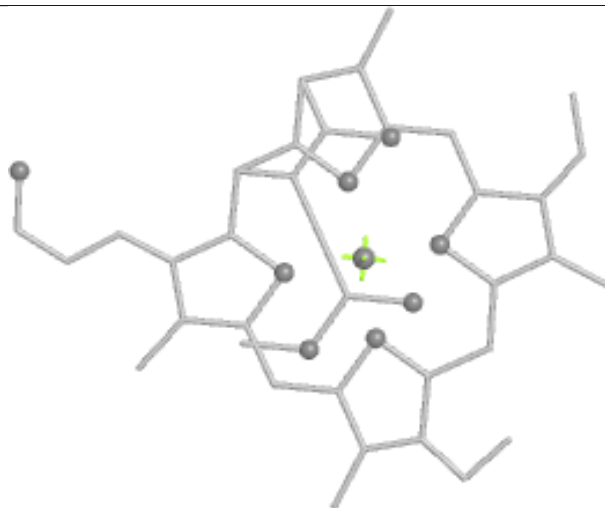
Bond lengths



Bond angles

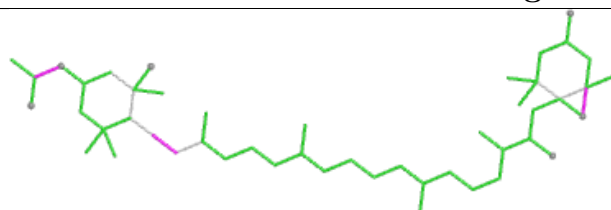


Torsions

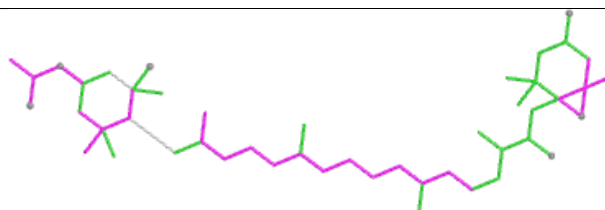


Rings

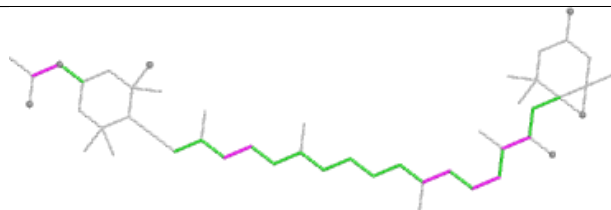
Ligand A86 9 304



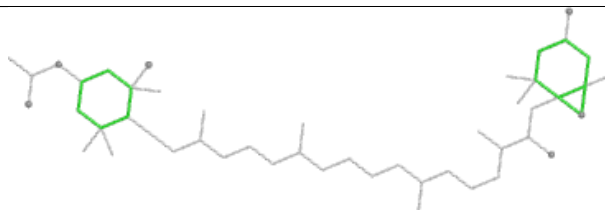
Bond lengths



Bond angles

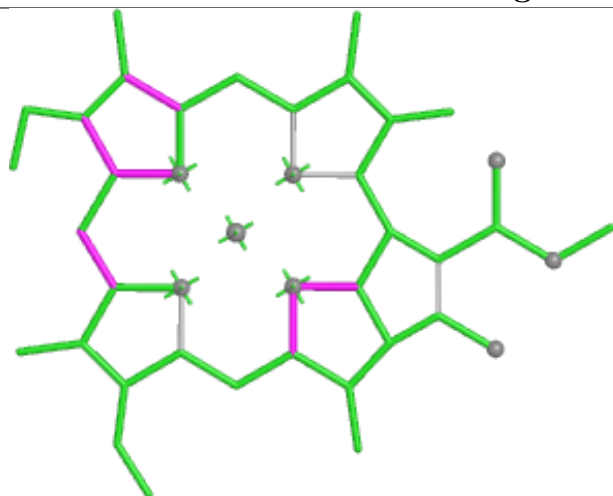


Torsions

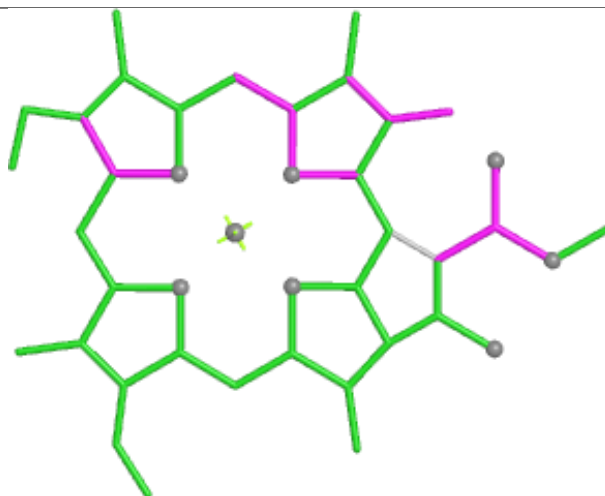


Rings

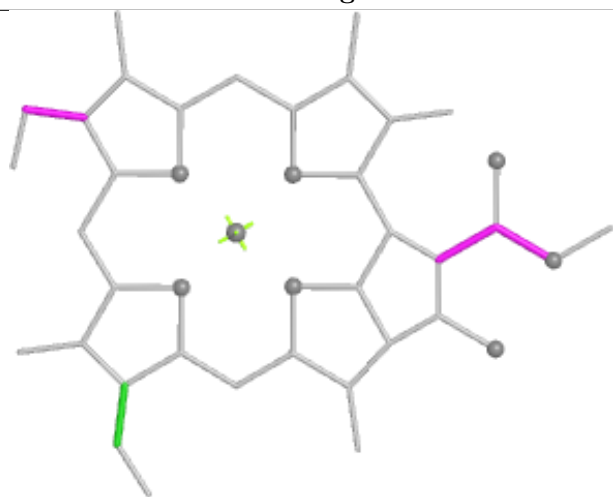
Ligand CLA Y 311



Bond lengths



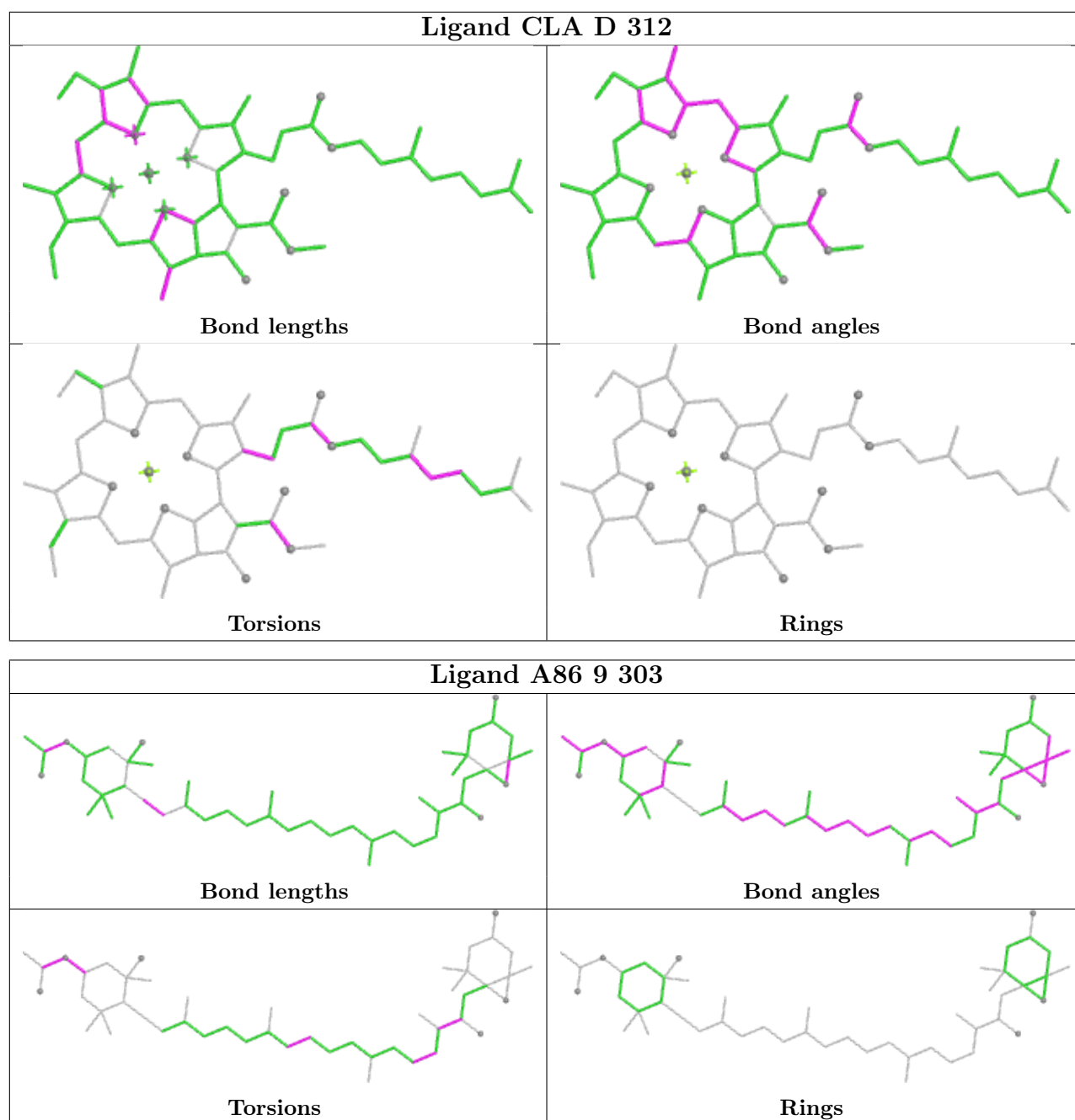
Bond angles



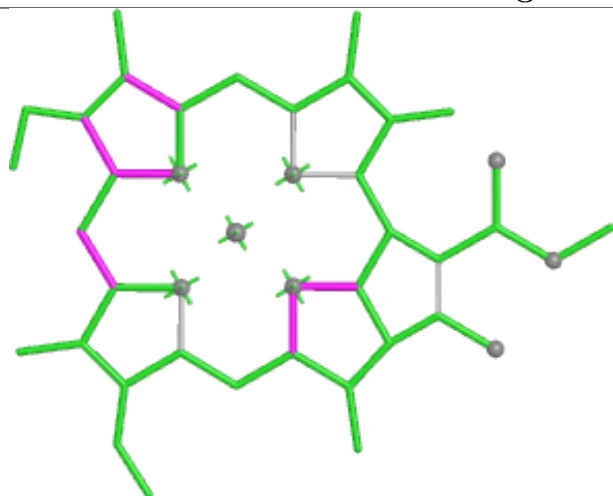
Torsions



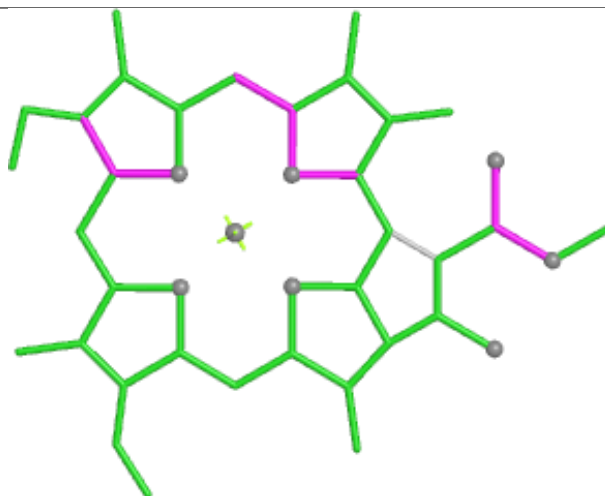
Rings



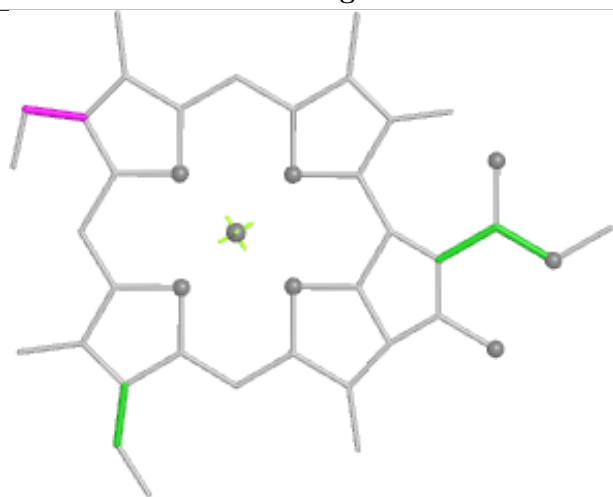
Ligand CLA Z 309



Bond lengths



Bond angles

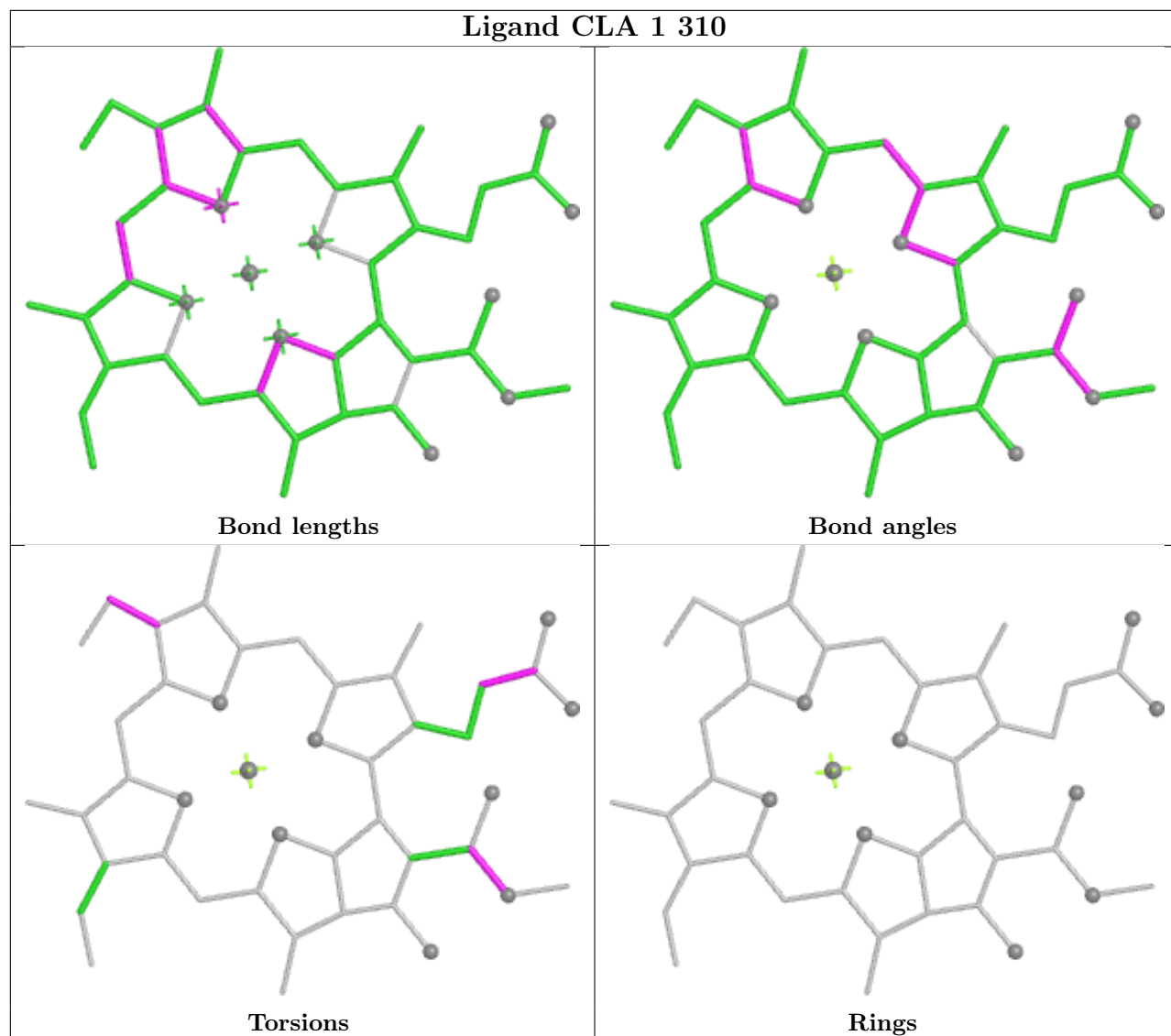


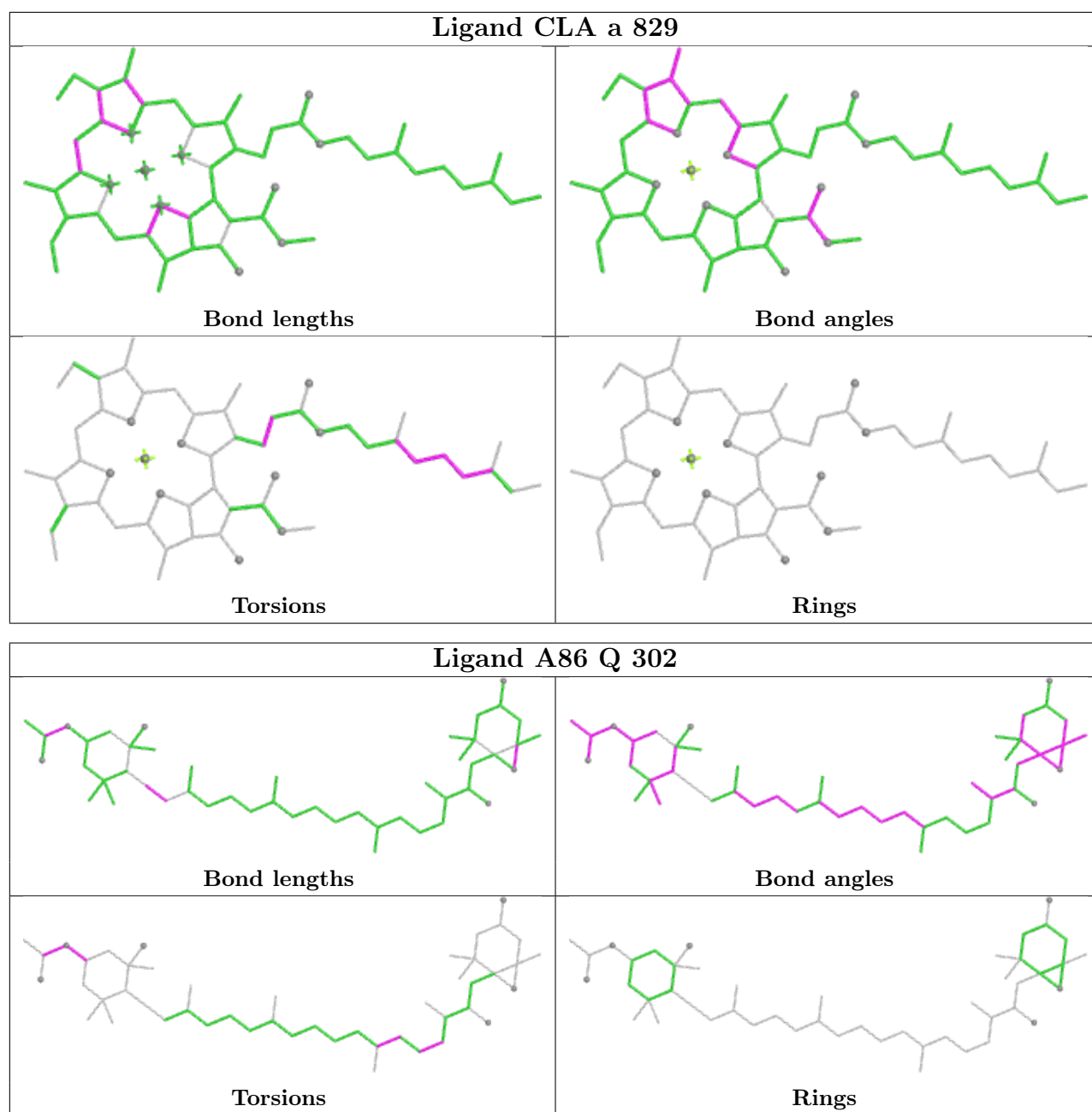
Torsions



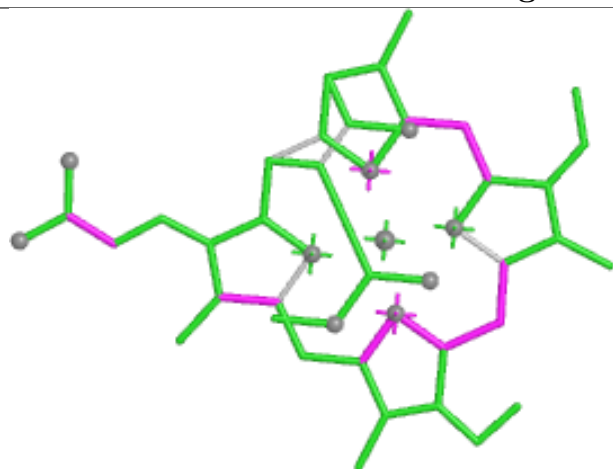
Rings

Ligand CLA 1 310

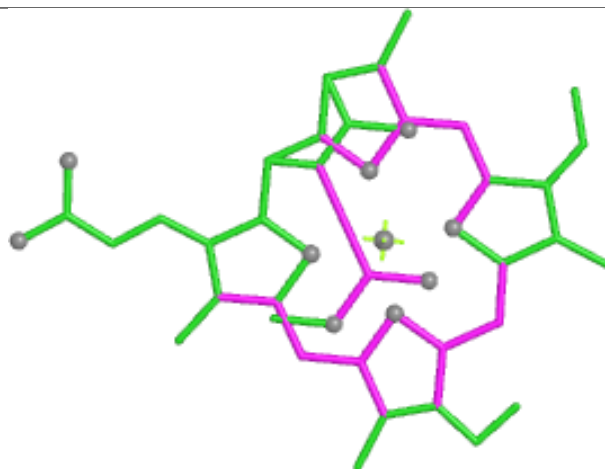




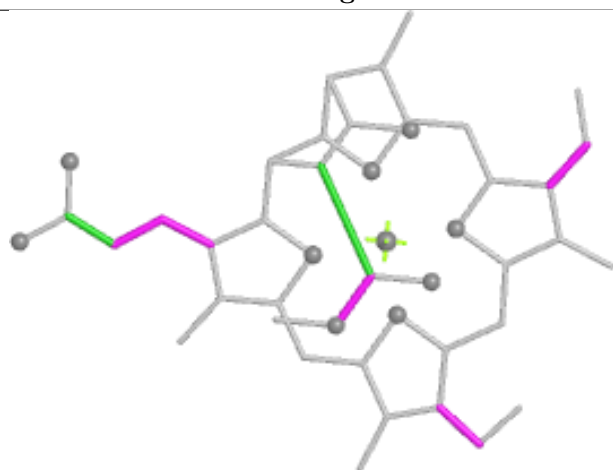
Ligand KC2 L 312



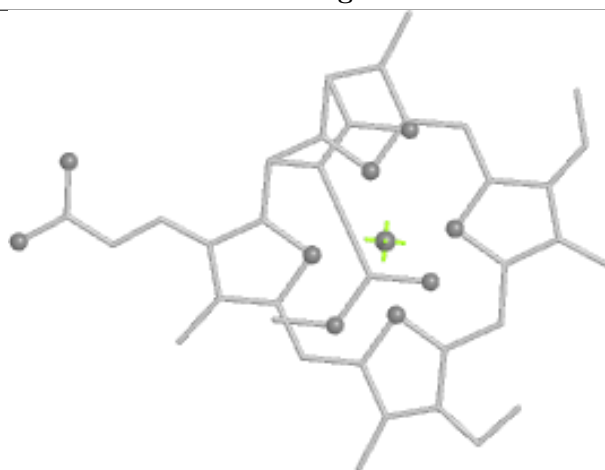
Bond lengths



Bond angles

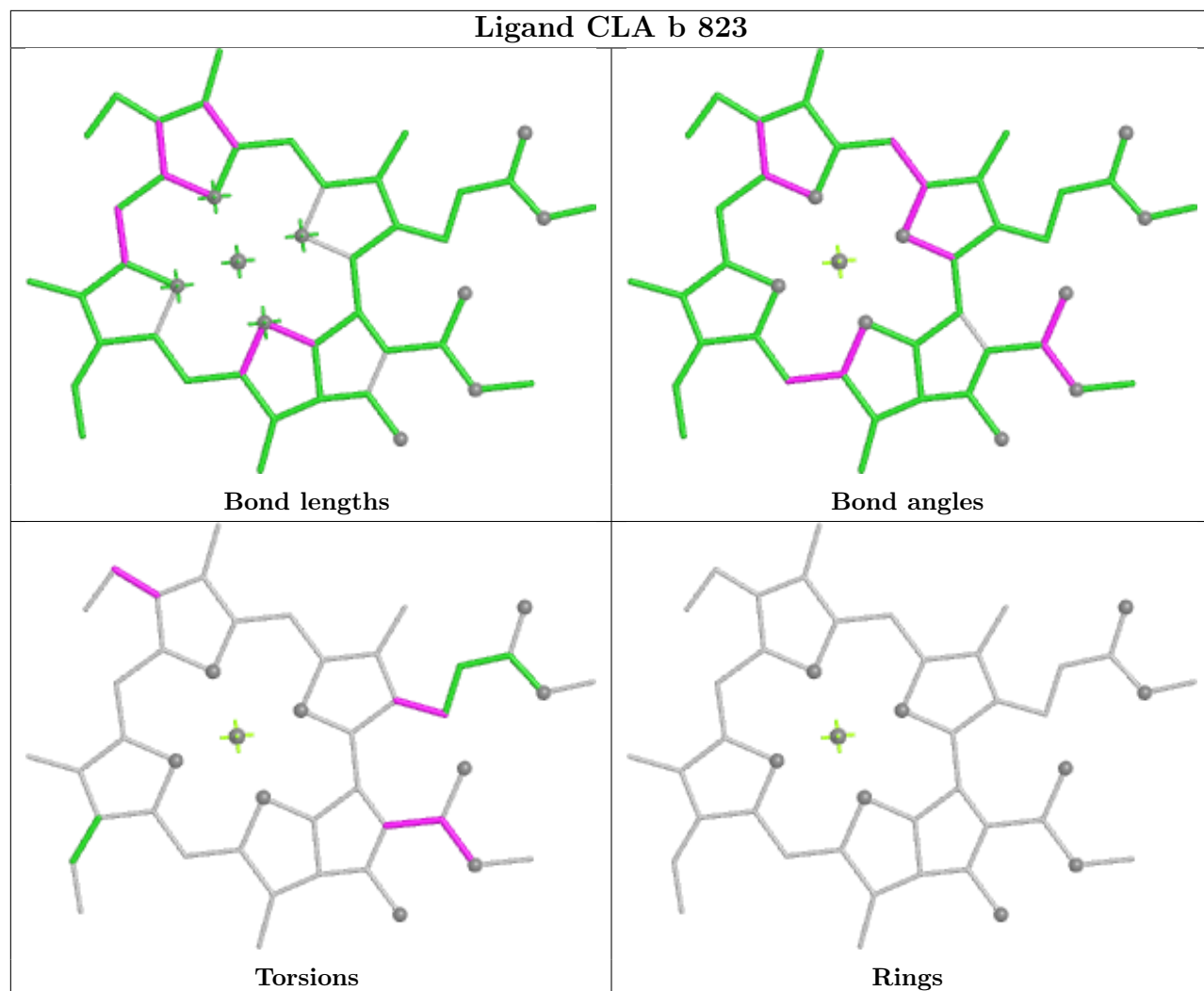


Torsions

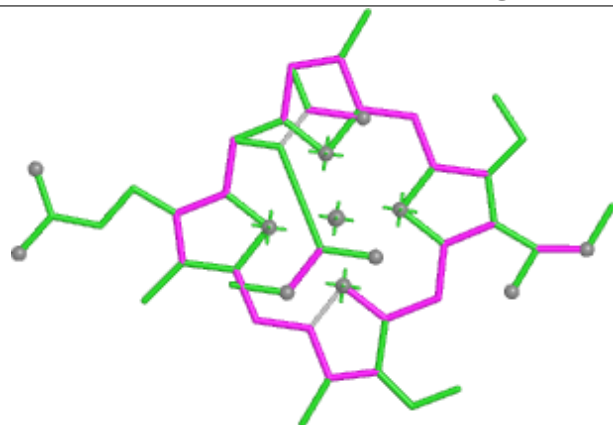


Rings

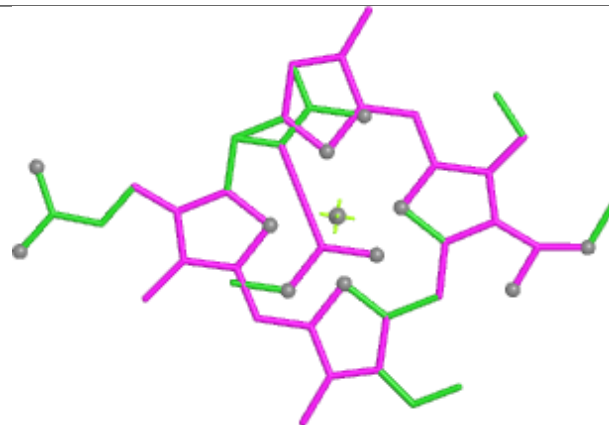
Ligand CLA b 823



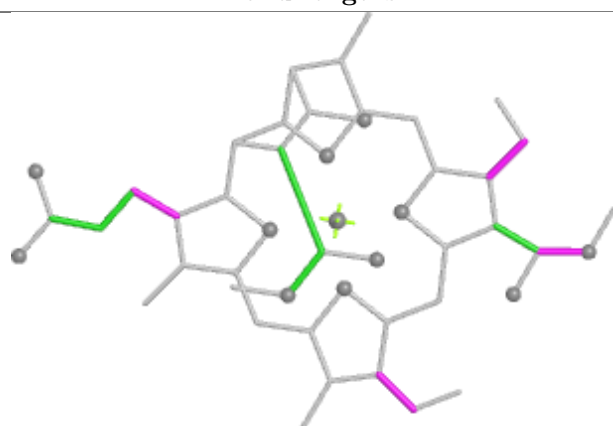
Ligand A1ECV T 317



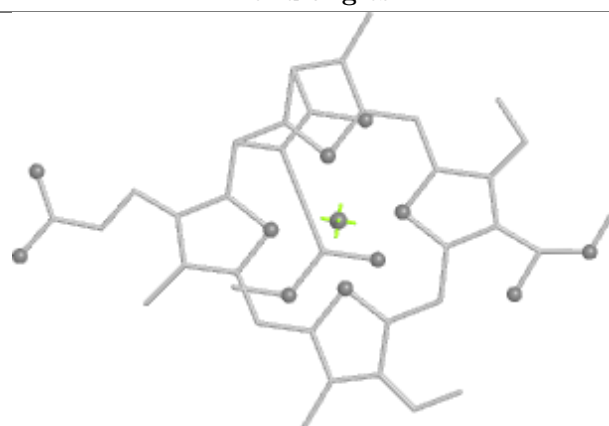
Bond lengths



Bond angles

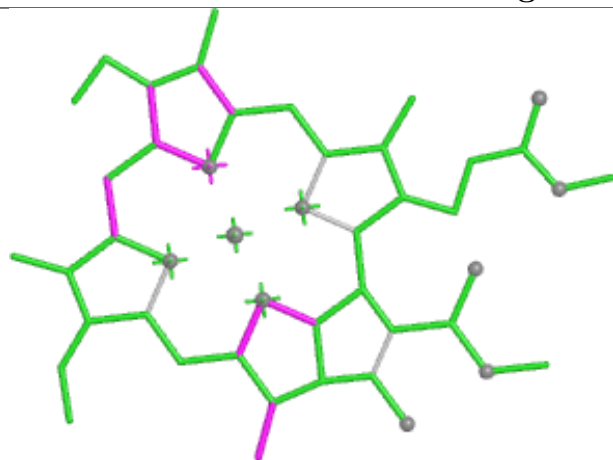


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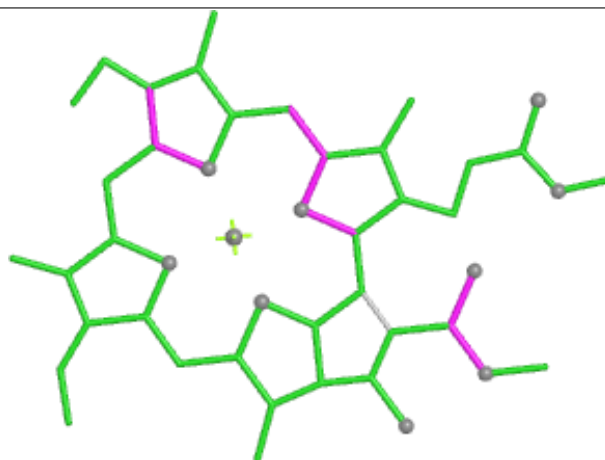


Rings

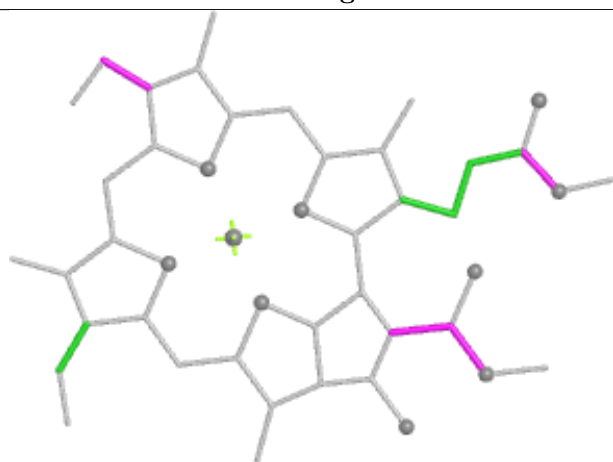
Ligand CLA J 312



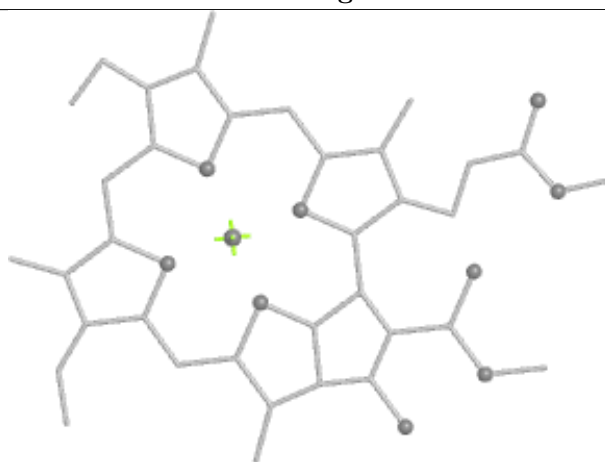
Bond lengths



Bond angles

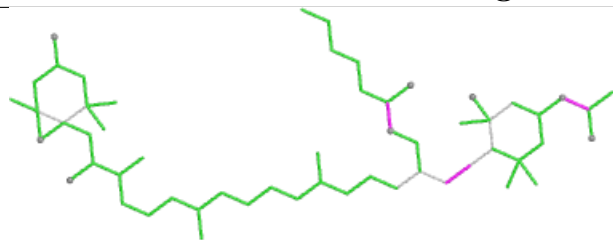


Torsions

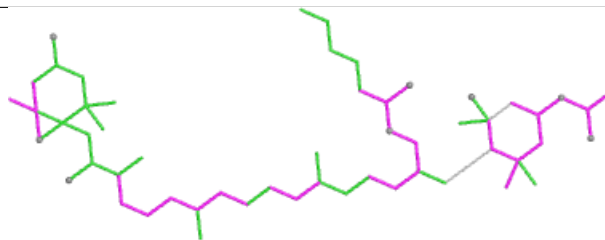


Rings

Ligand A1EB1 V 306



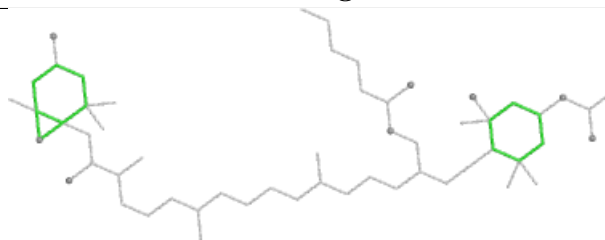
Bond lengths



Bond angles

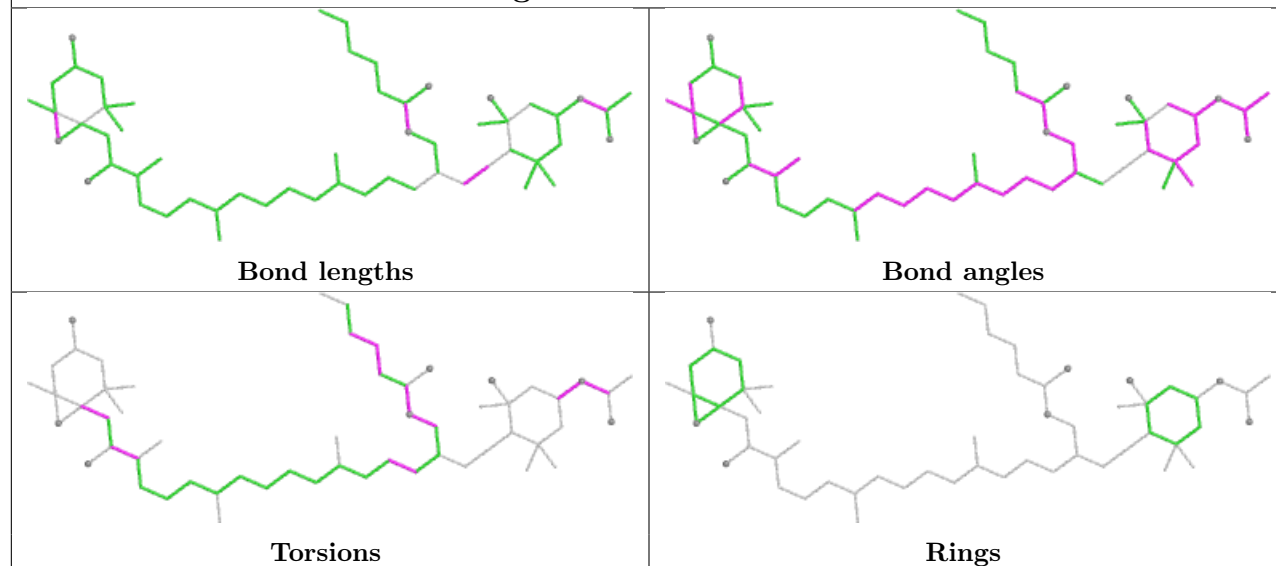


Torsions

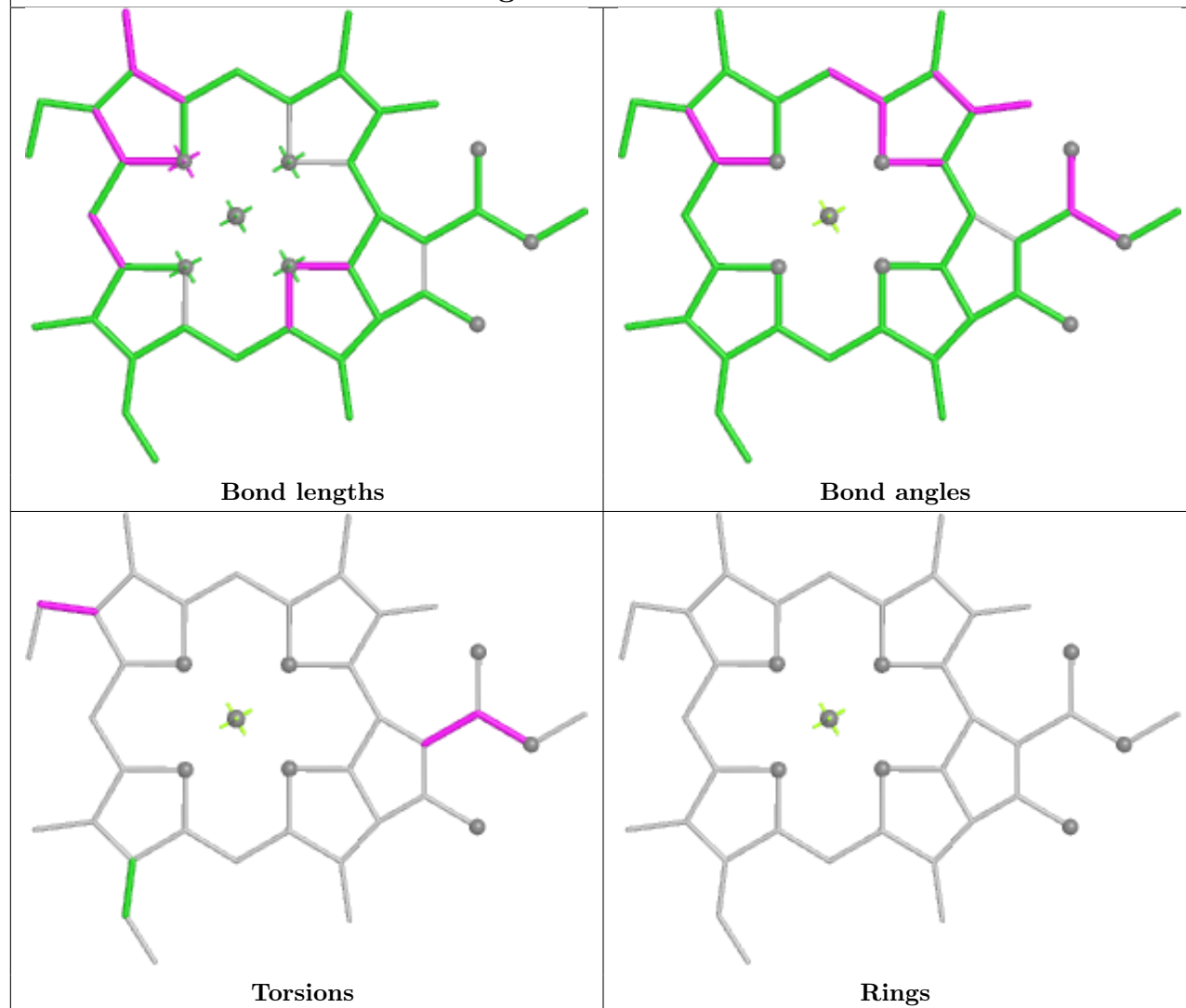


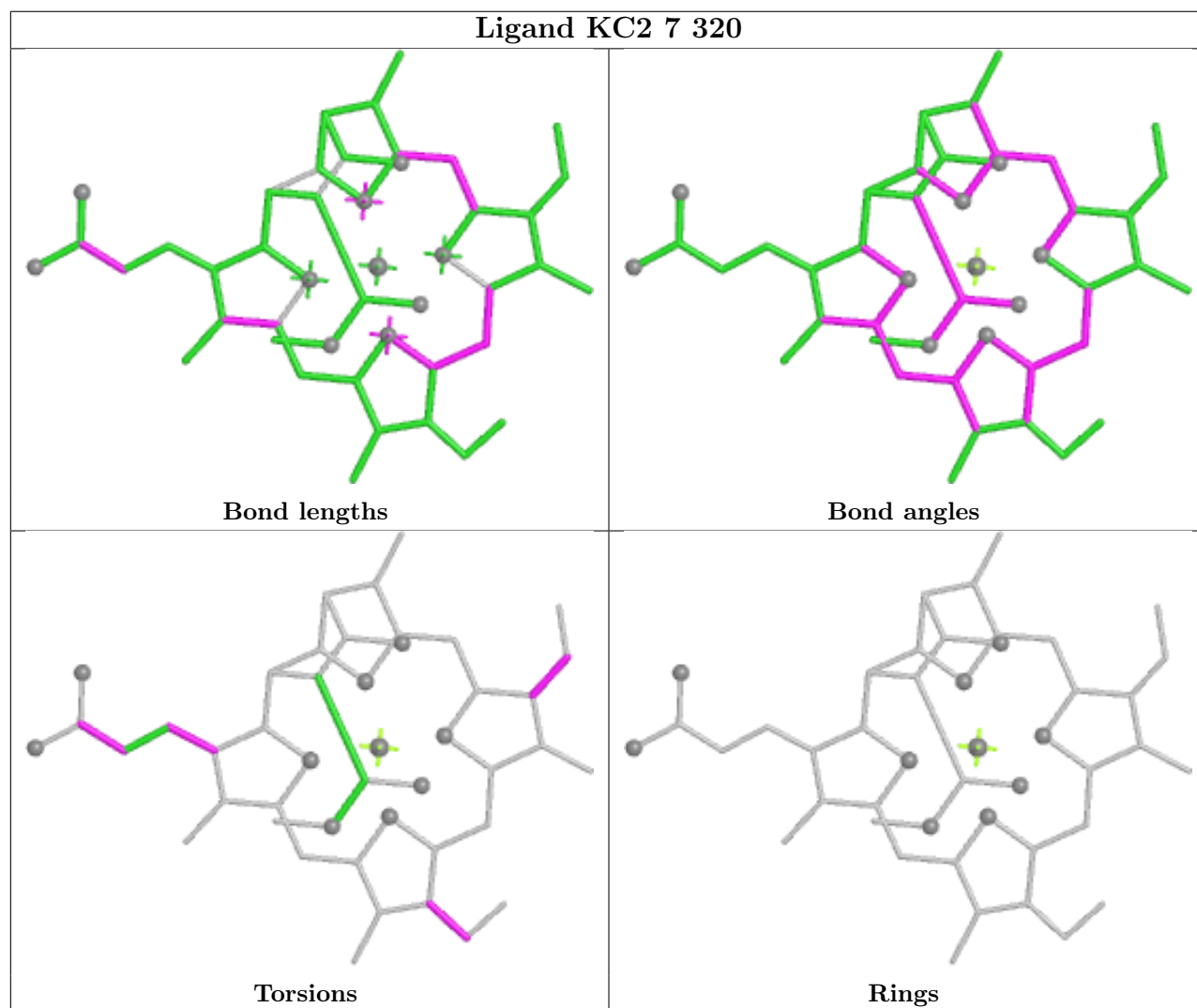
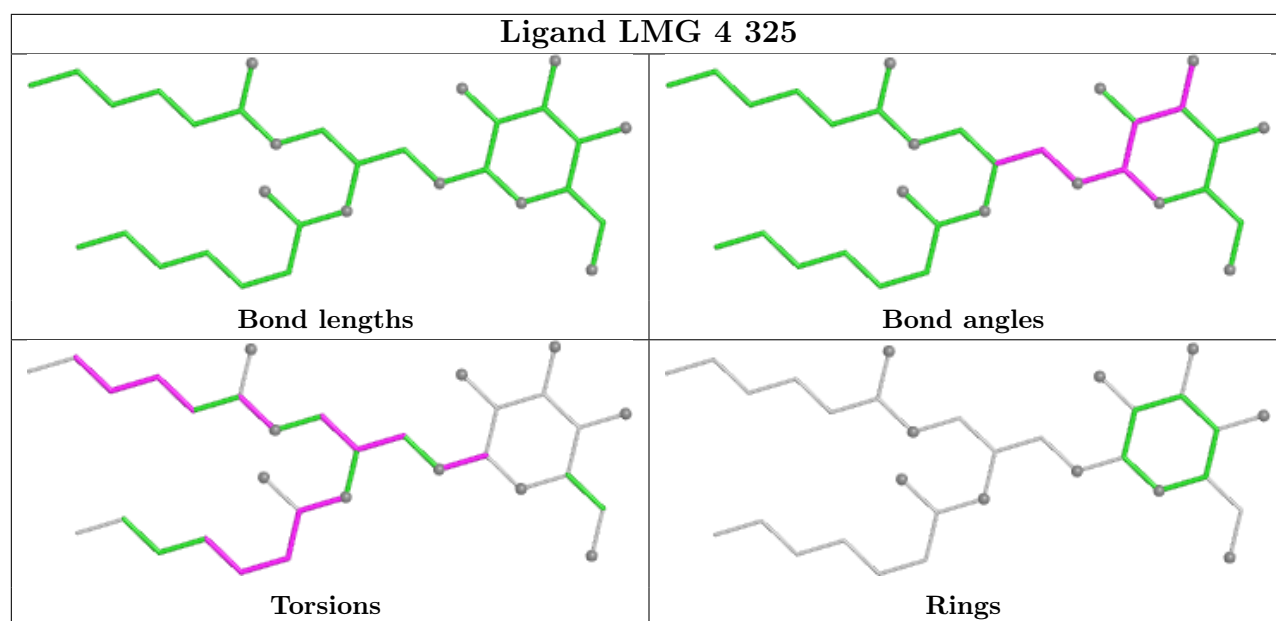
Rings

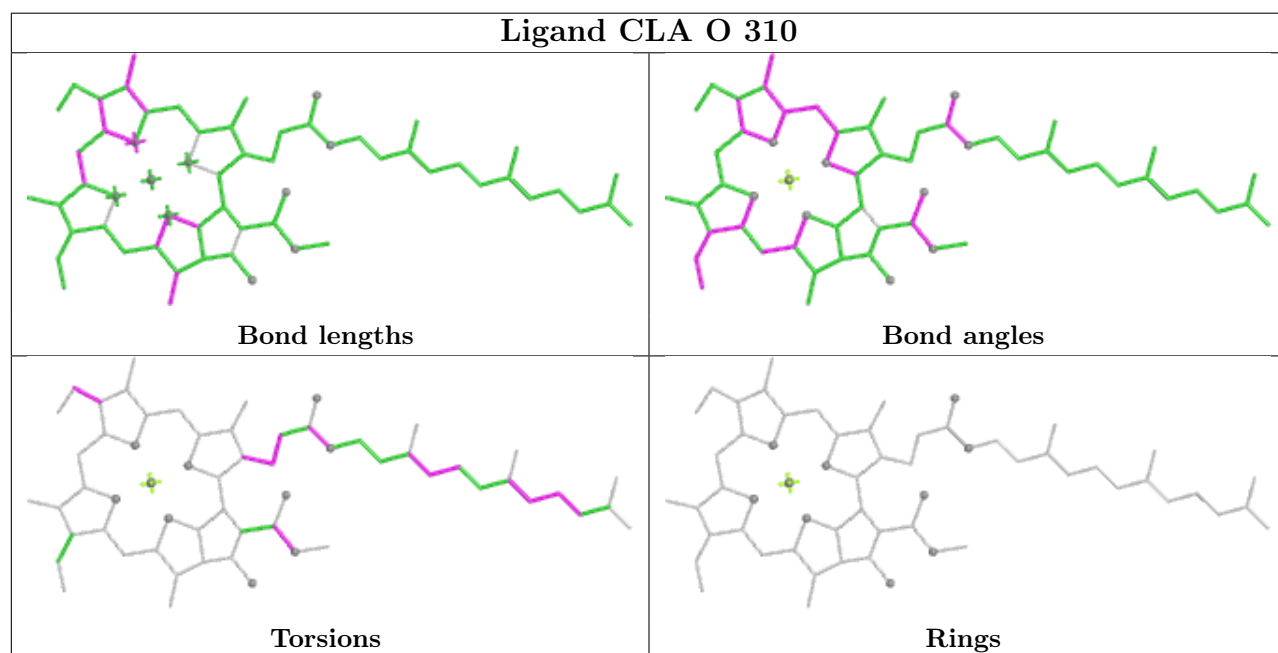
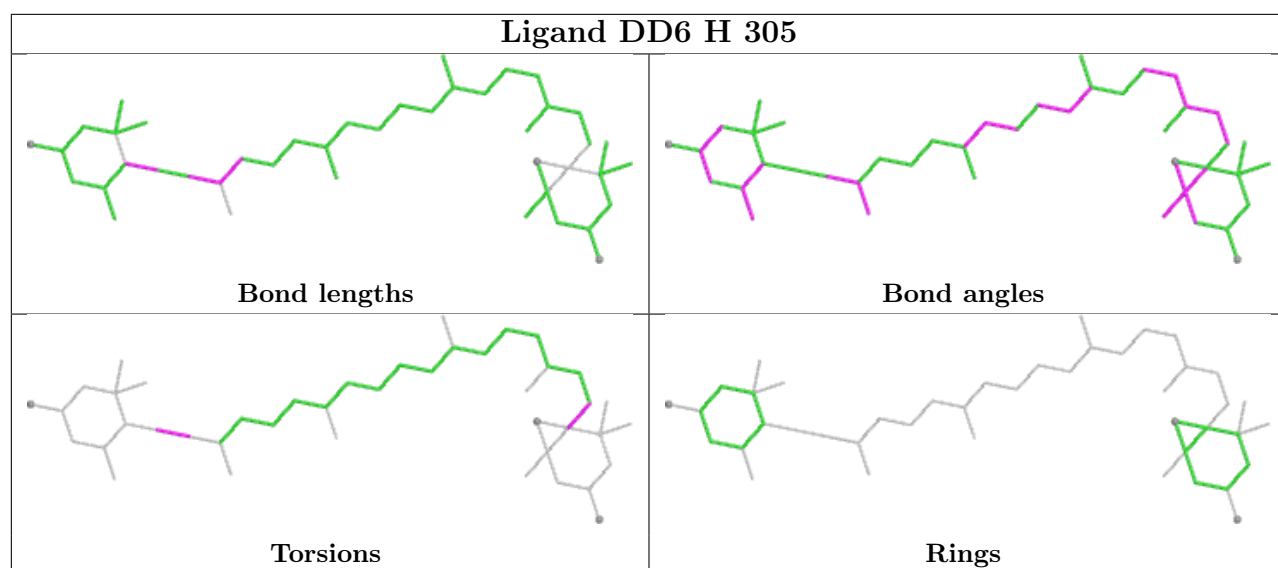
Ligand A1EB1 V 302



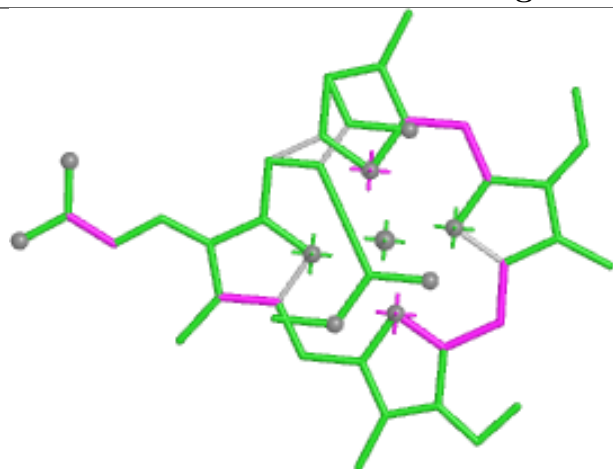
Ligand CLA 6 321



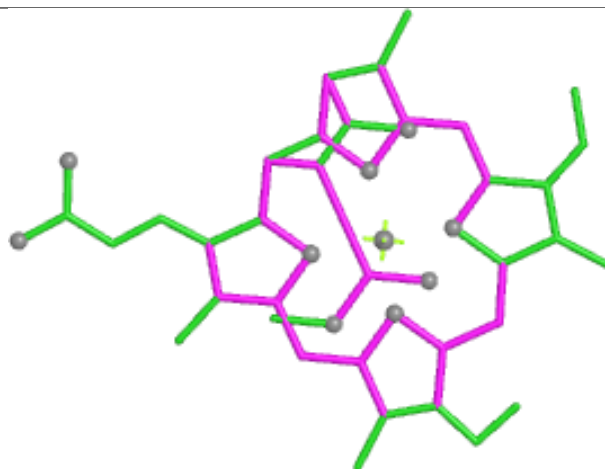




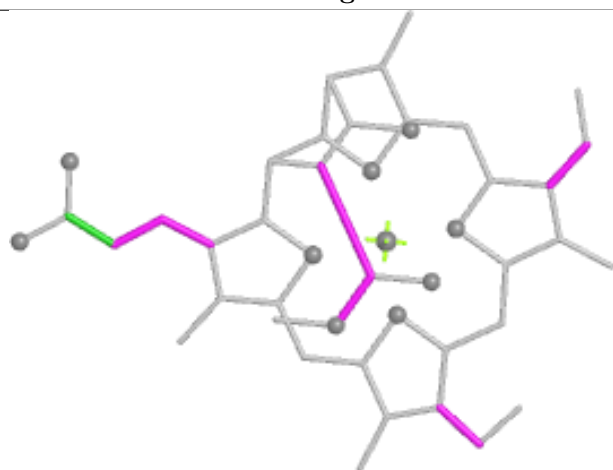
Ligand KC2 V 314



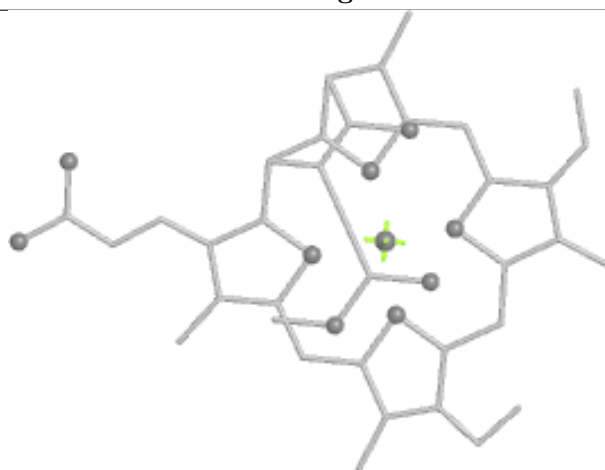
Bond lengths



Bond angles

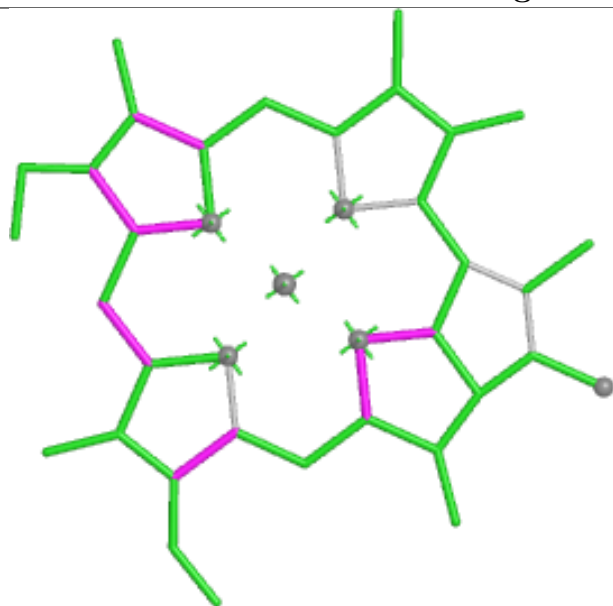


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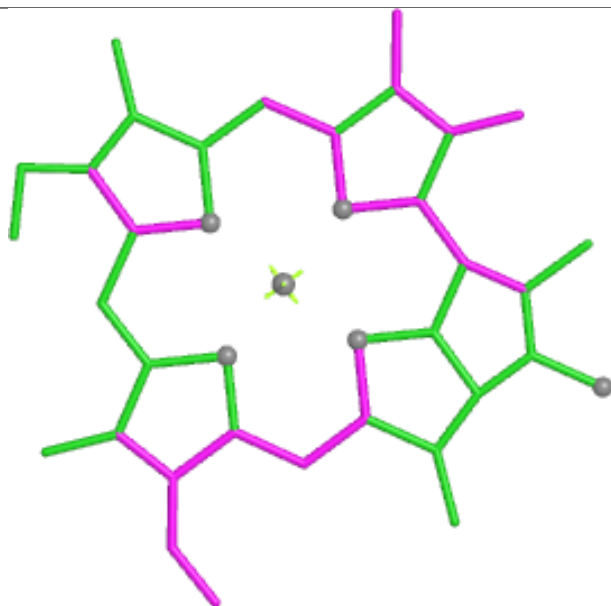


Rings

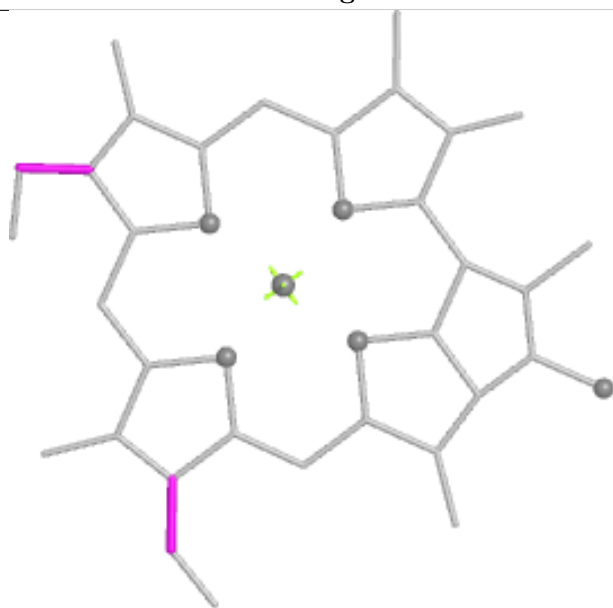
Ligand CLA O 308



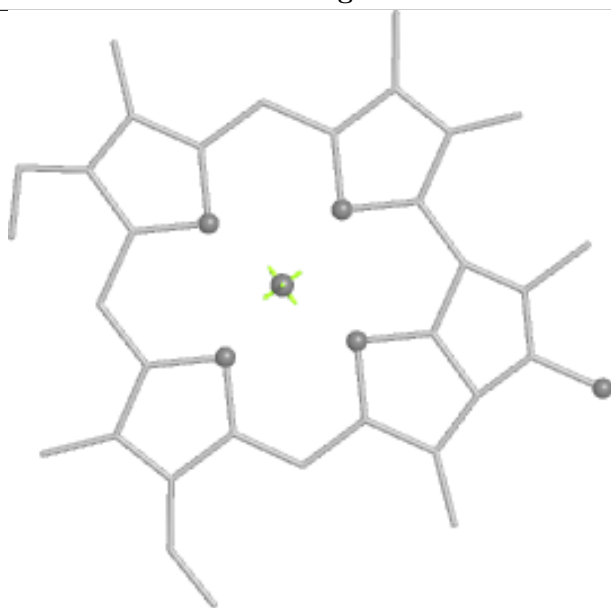
Bond lengths



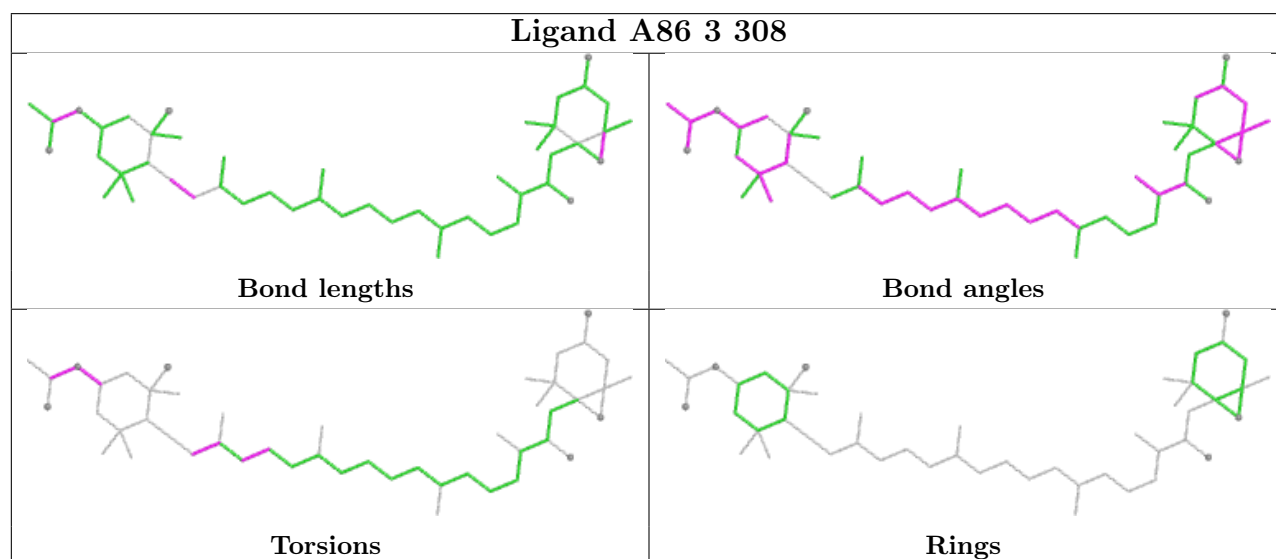
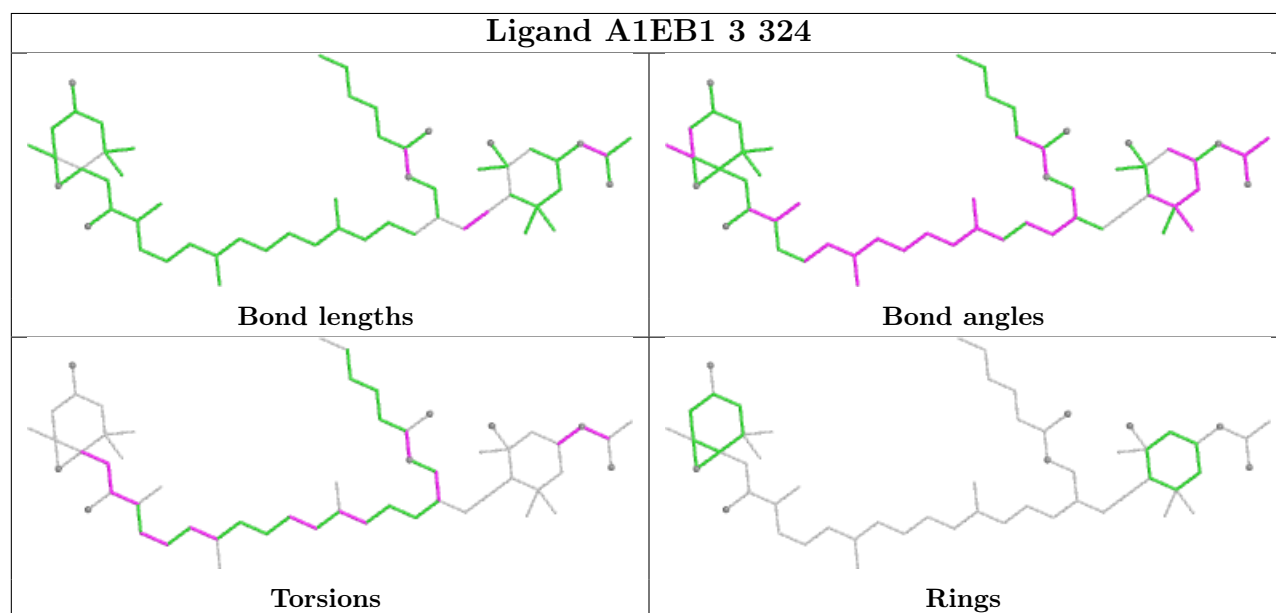
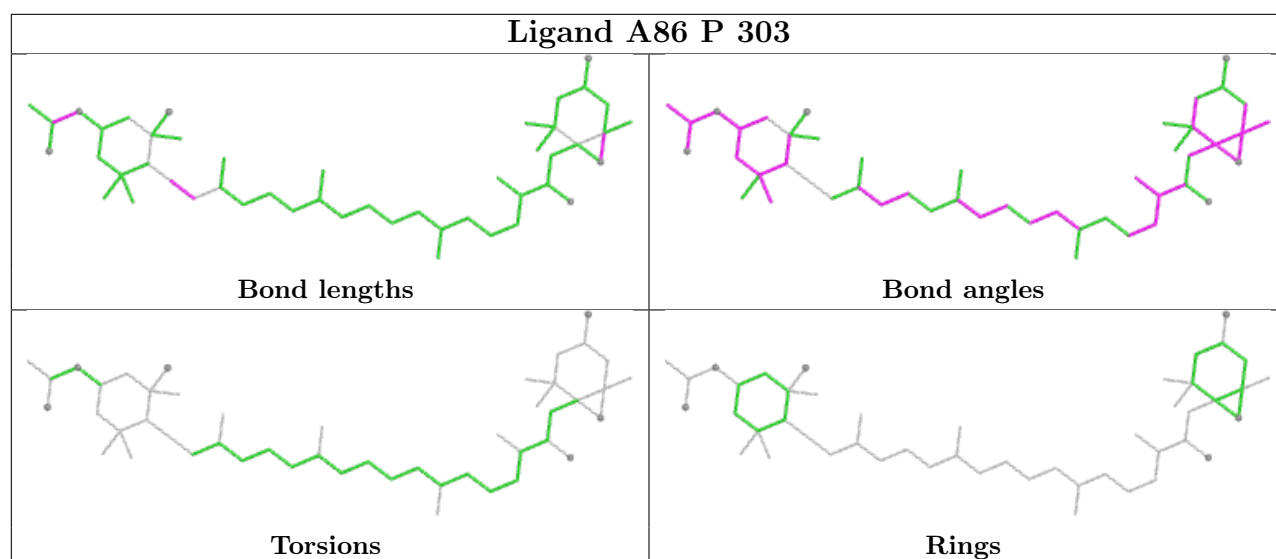
Bond angles



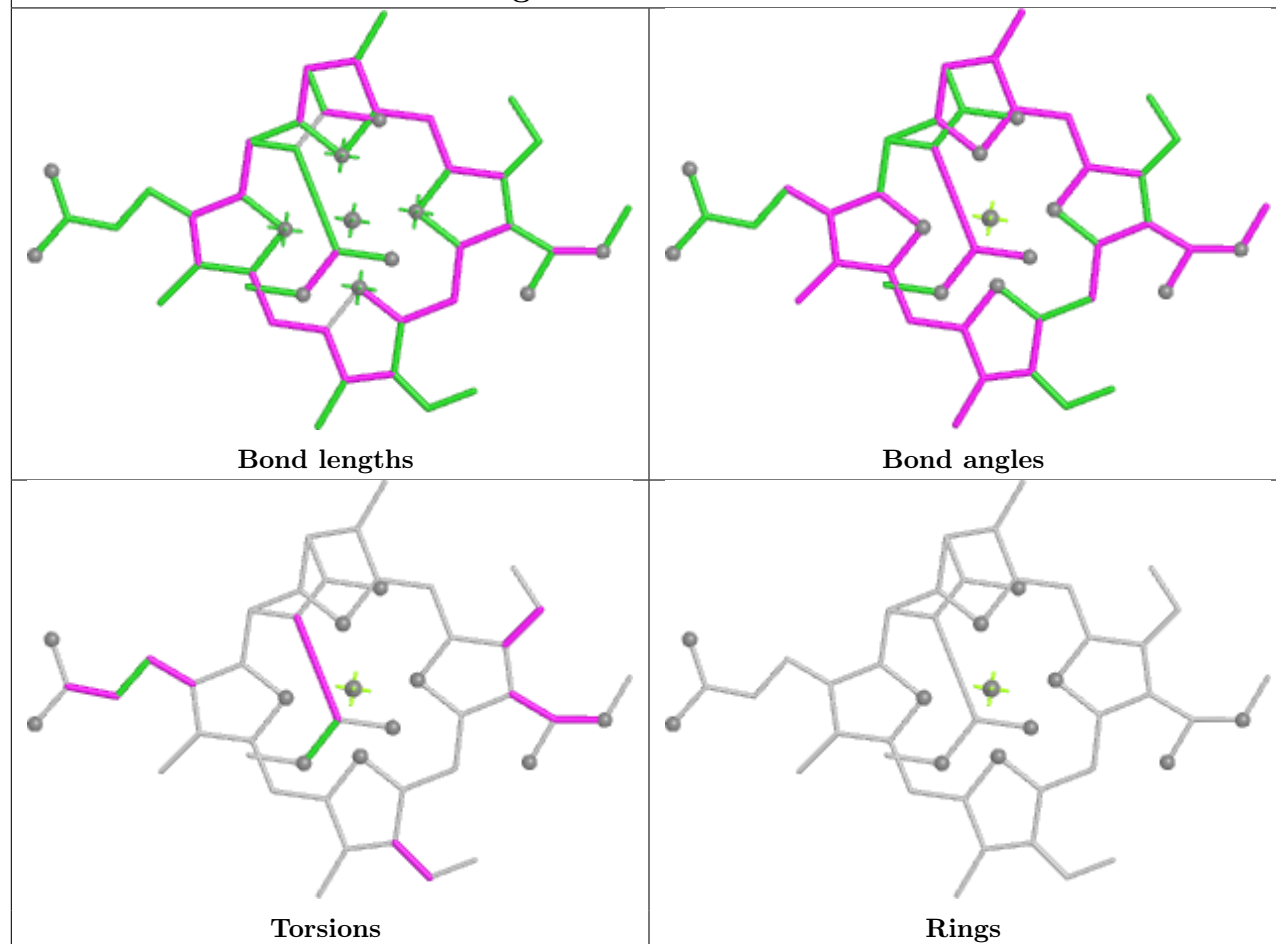
Torsions



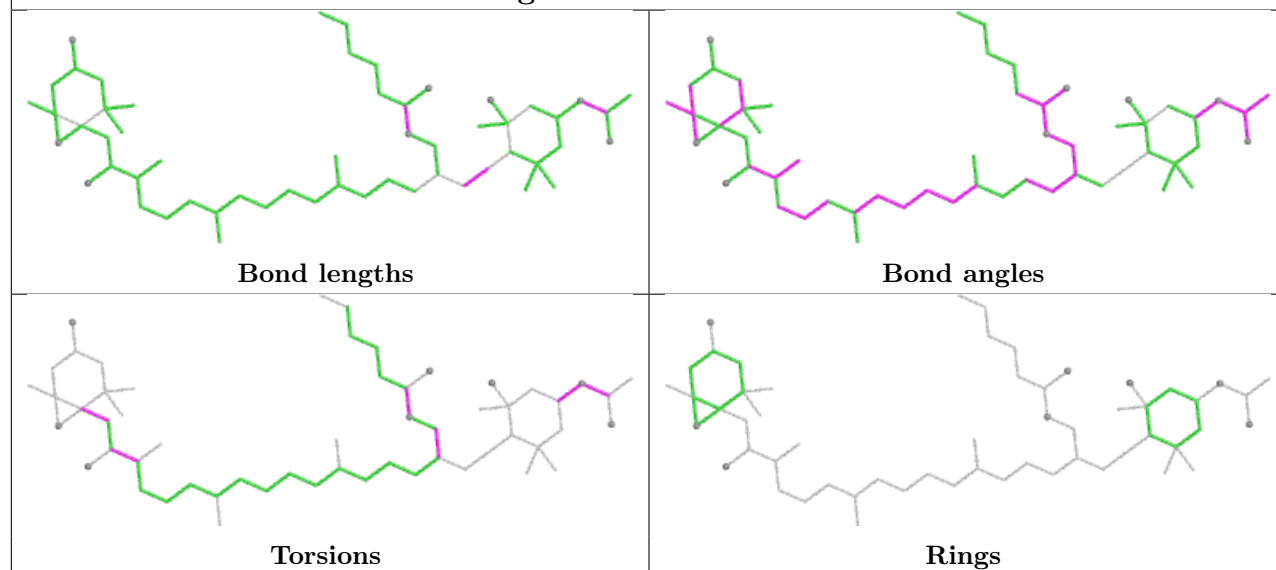
Rings

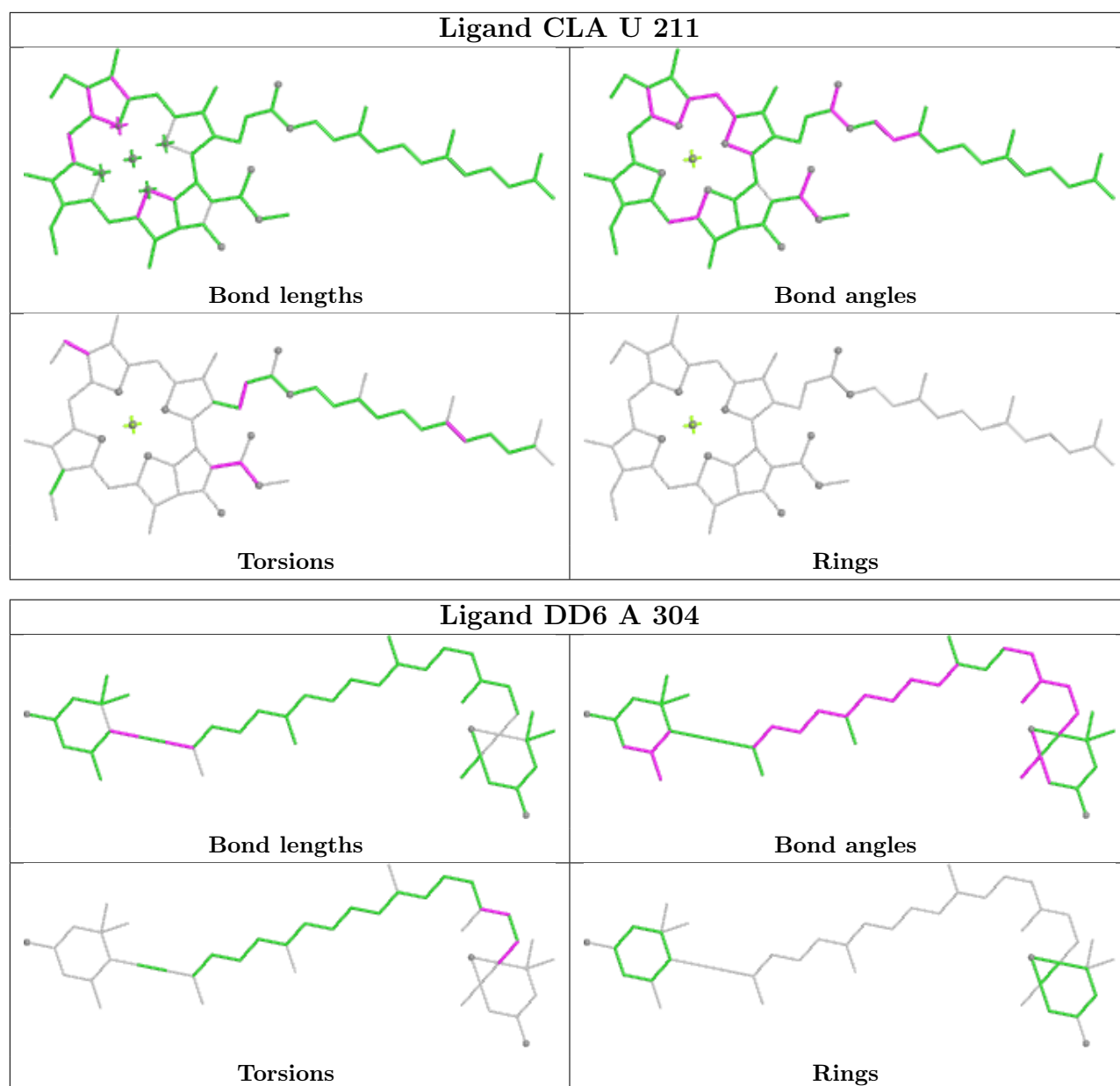


Ligand A1ECV 5 309

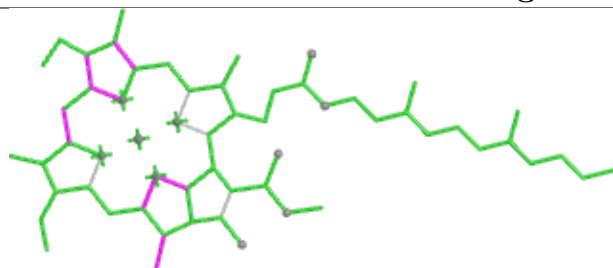


Ligand A1EB1 1 301

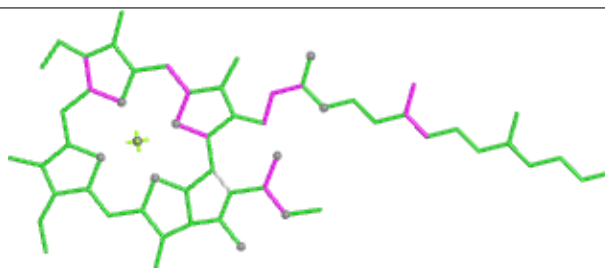




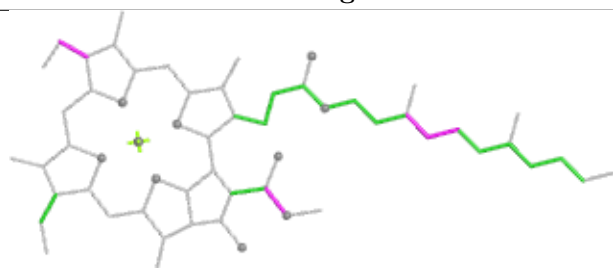
Ligand CLA b 834



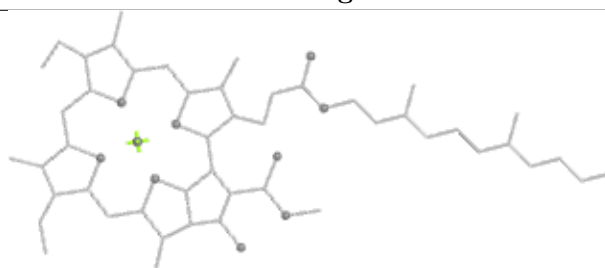
Bond lengths



Bond angles

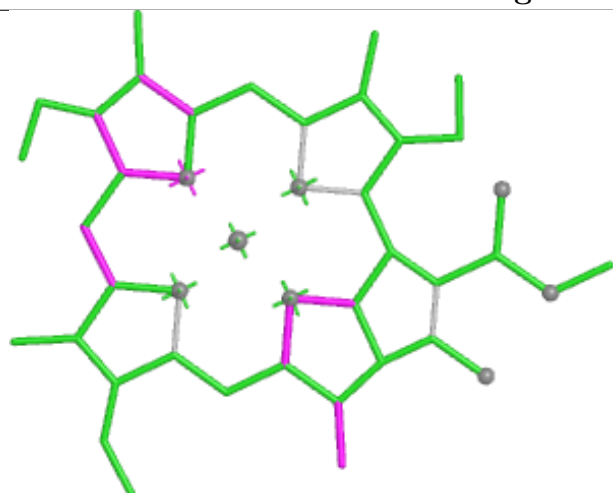


Torsions

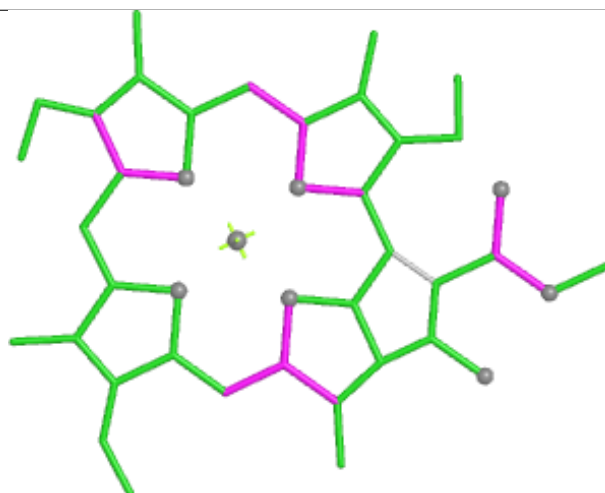


Rings

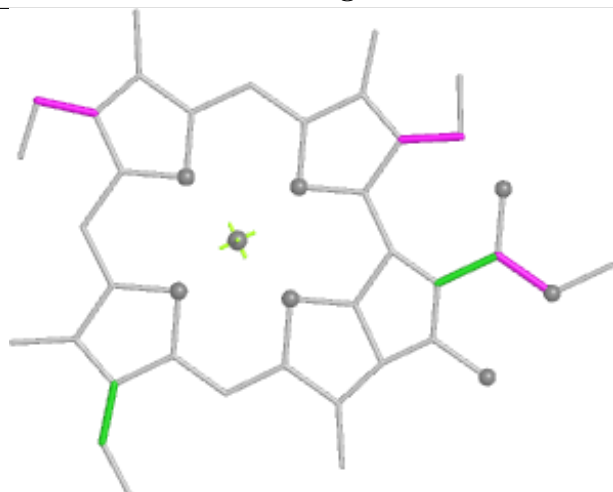
Ligand CLA B 206



Bond lengths



Bond angles

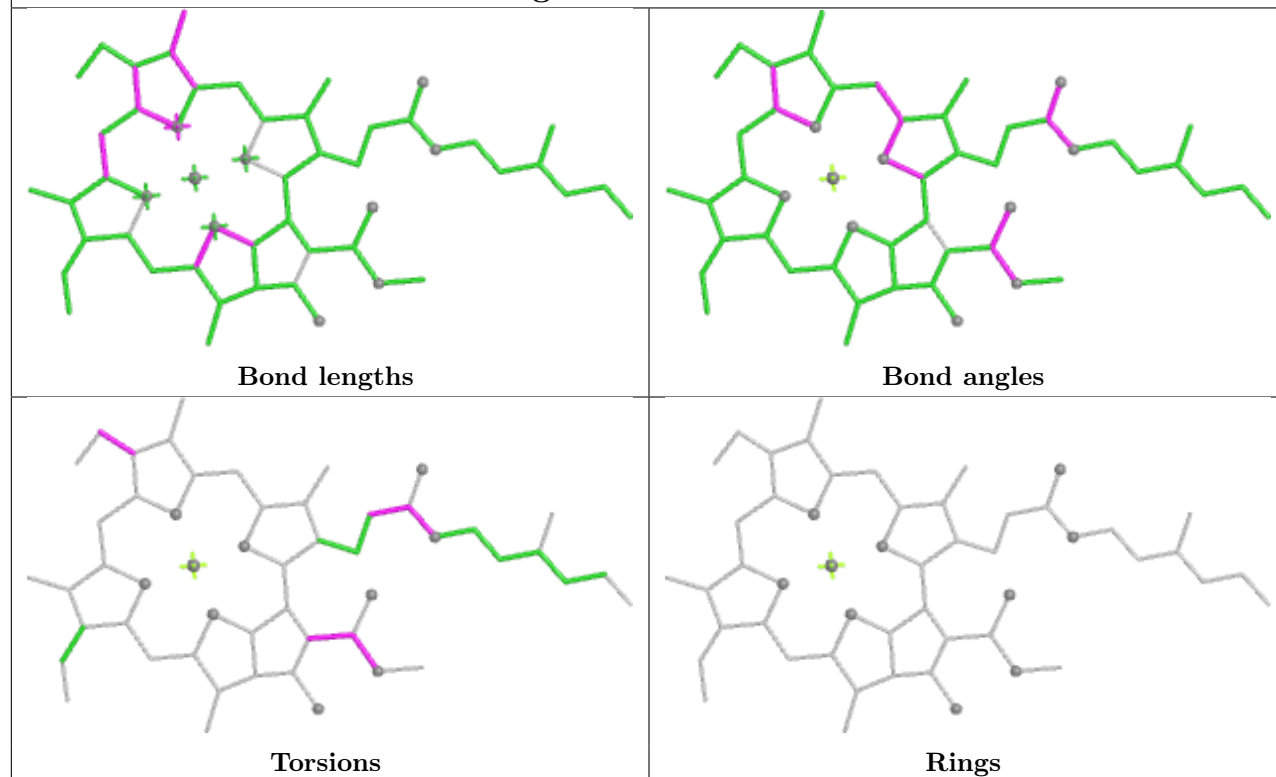


Torsions

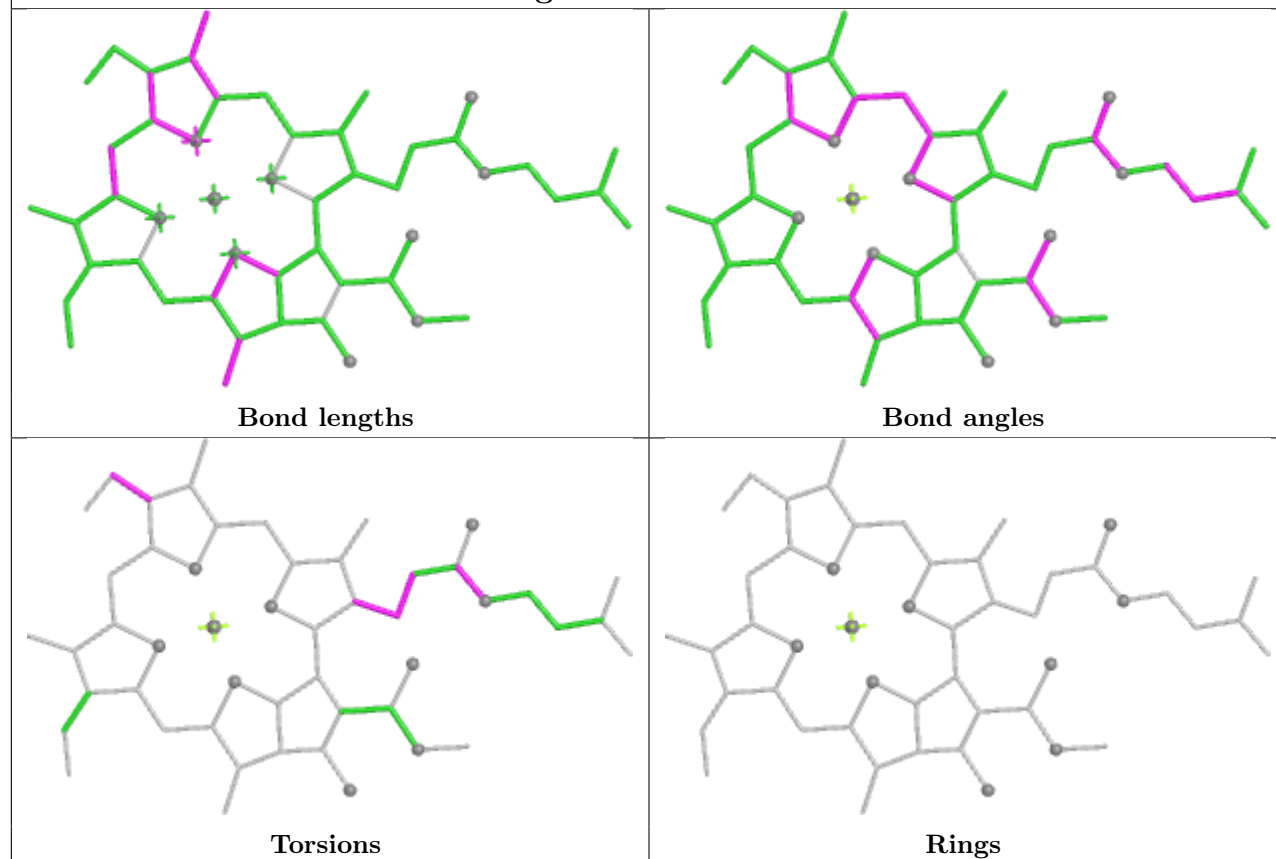


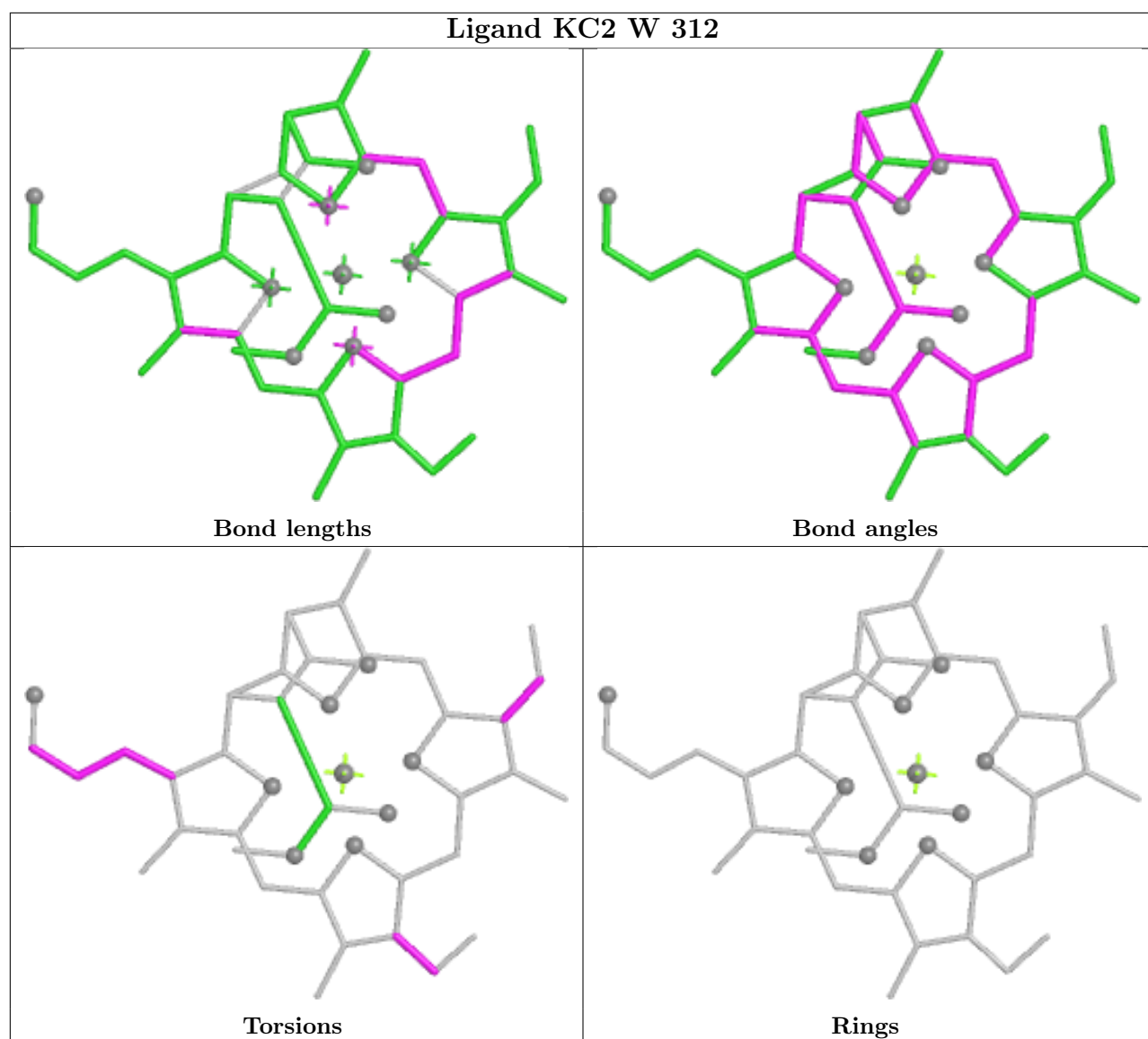
Rings

Ligand CLA T 320

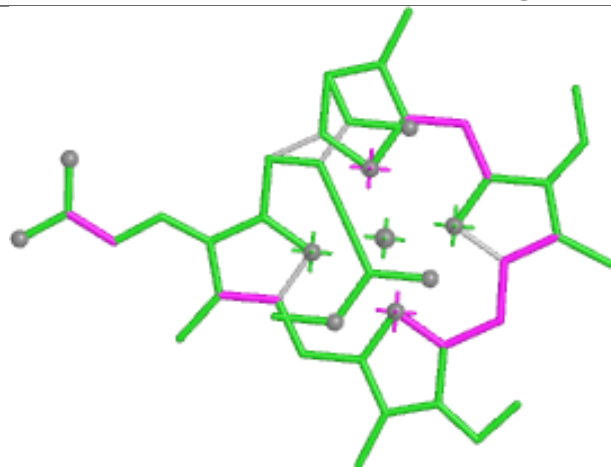


Ligand CLA b 831





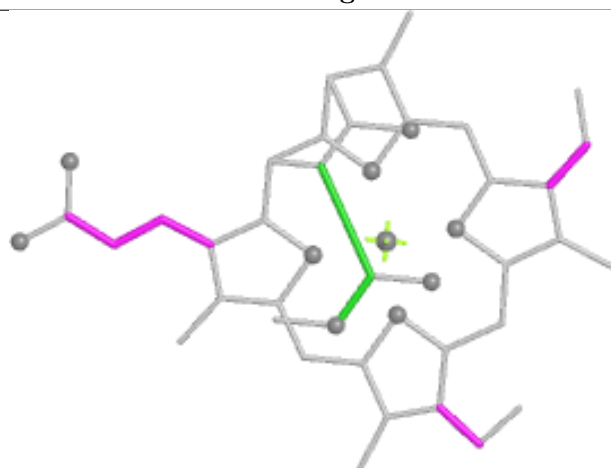
Ligand KC2 X 315



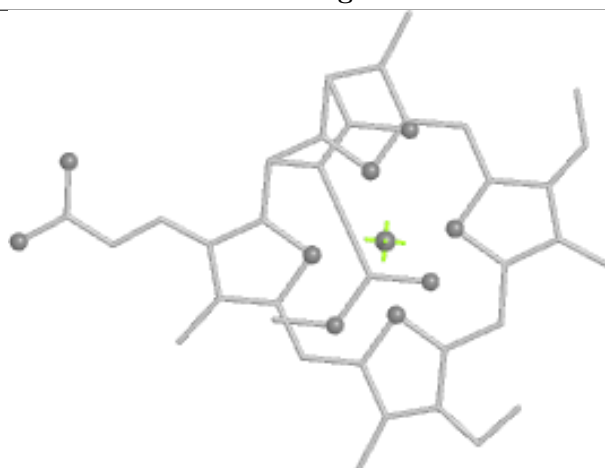
Bond lengths



Bond angles

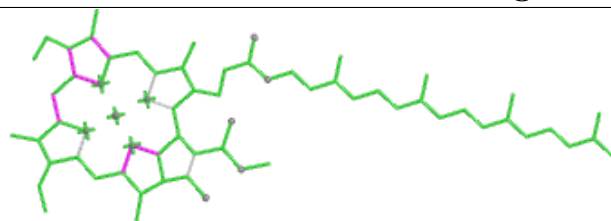


Torsions

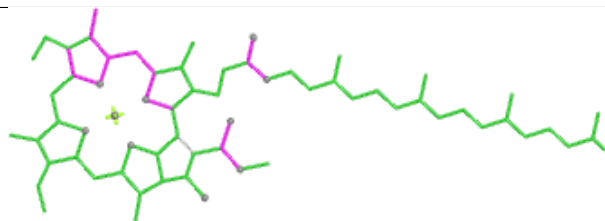


Rings

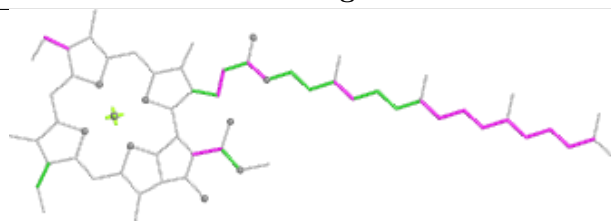
Ligand CLA D 319



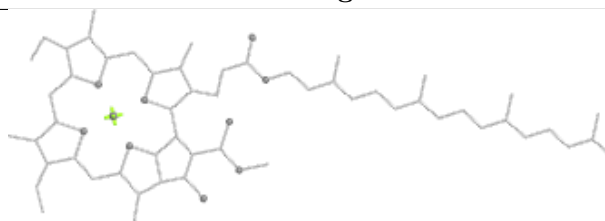
Bond lengths



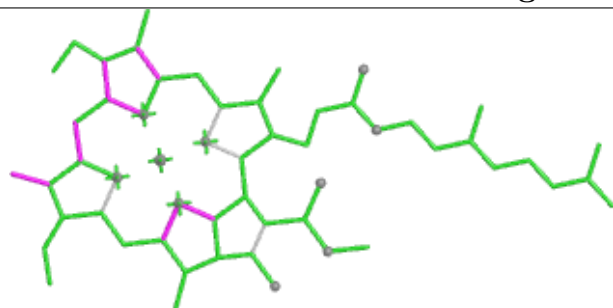
Bond angles



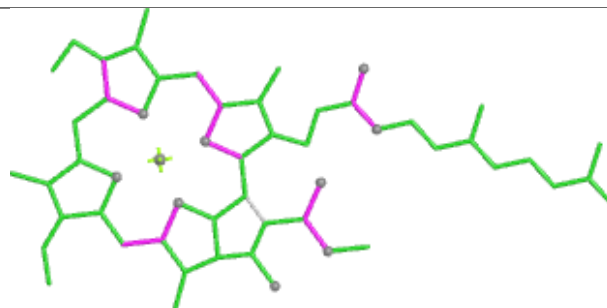
Torsions



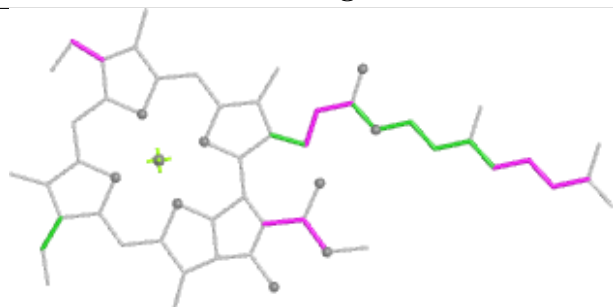
Rings

Ligand CLA 0 313

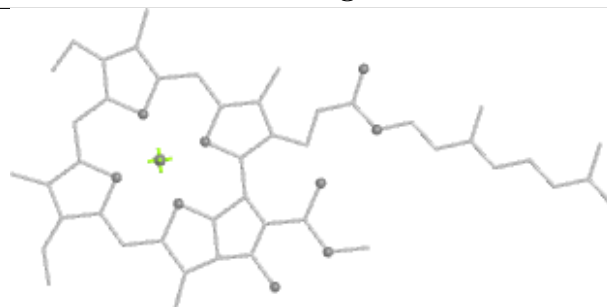
Bond lengths



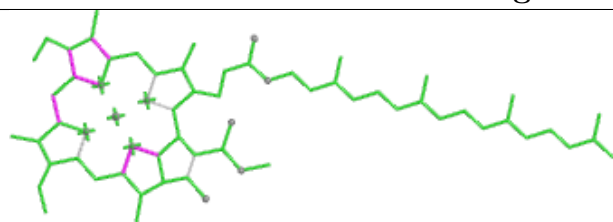
Bond angles



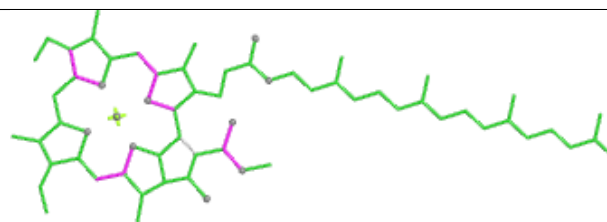
Torsions



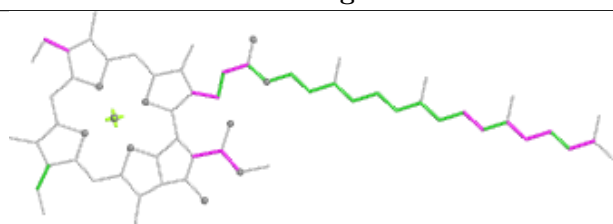
Rings

Ligand CLA D 318

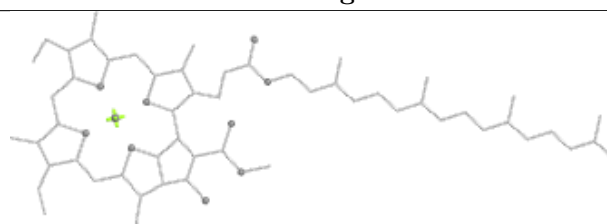
Bond lengths



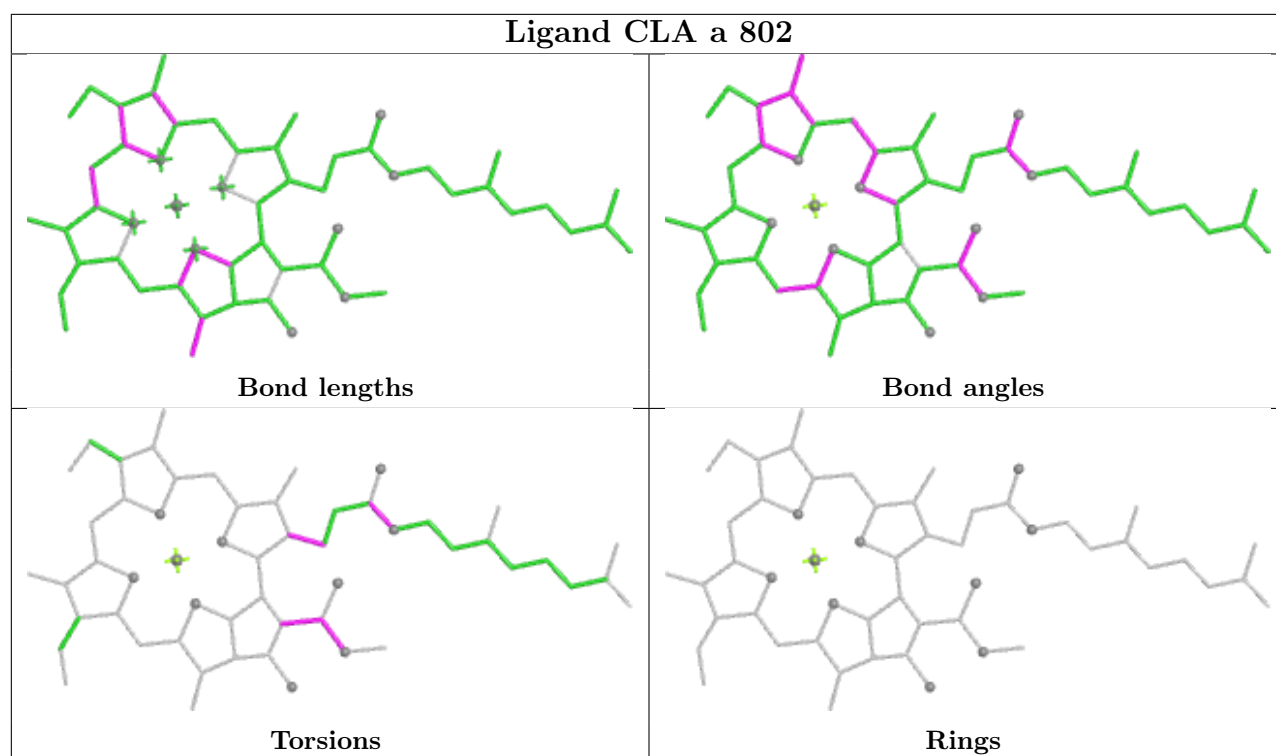
Bond angles



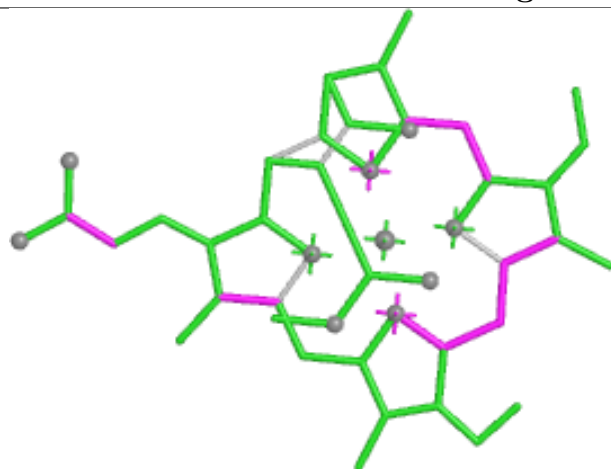
Torsions



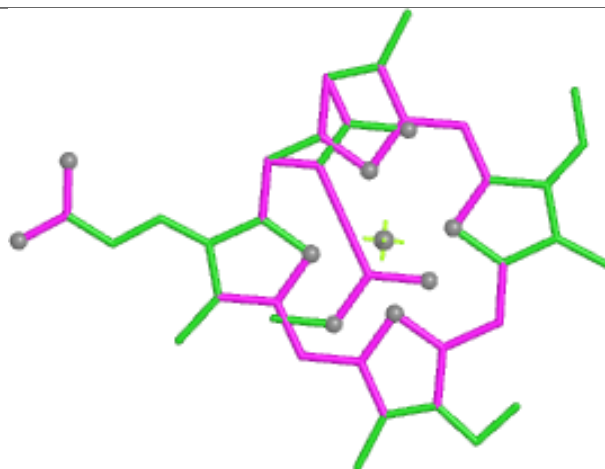
Rings



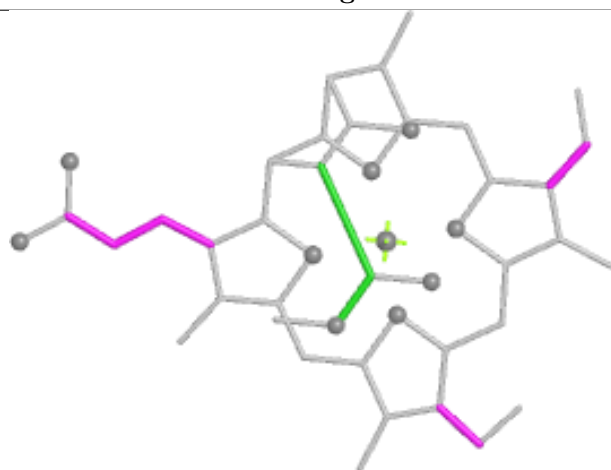
Ligand KC2 B 208



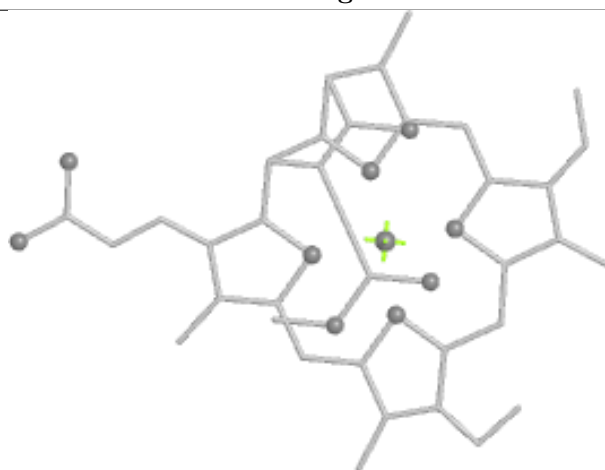
Bond lengths



Bond angles

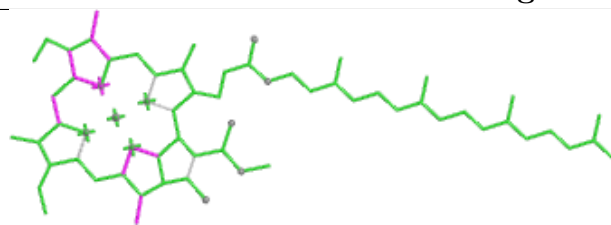


Torsions

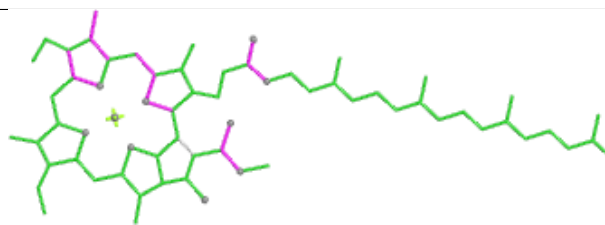


Rings

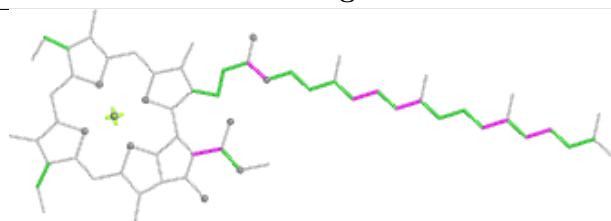
Ligand CLA b 812



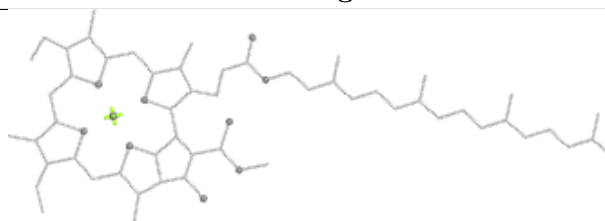
Bond lengths



Bond angles

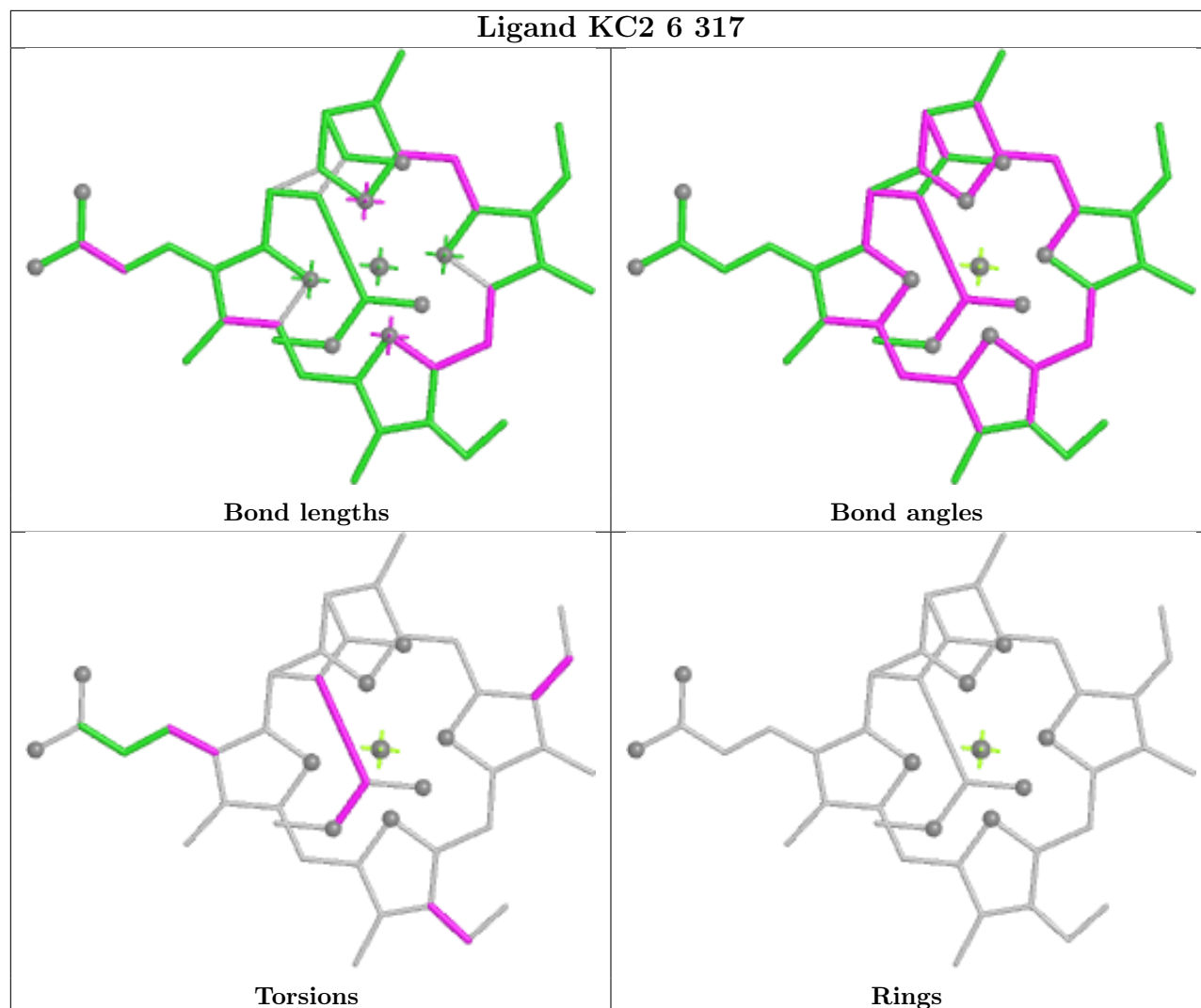


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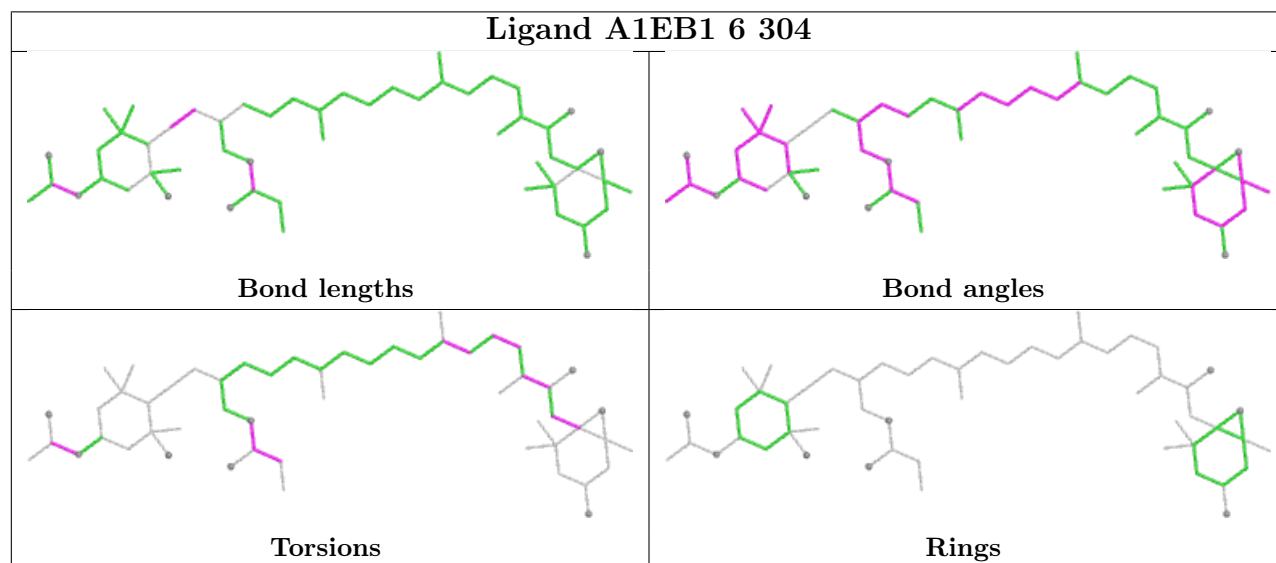


Rings

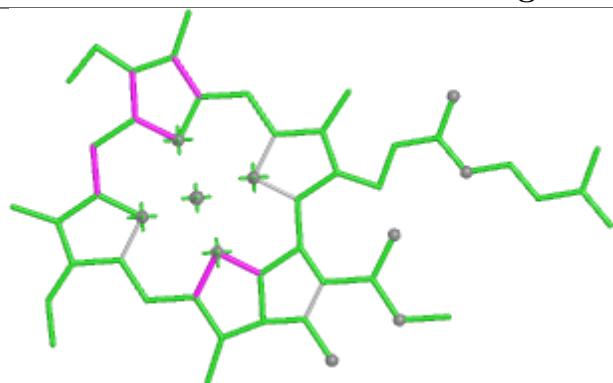
Ligand KC2 6 317



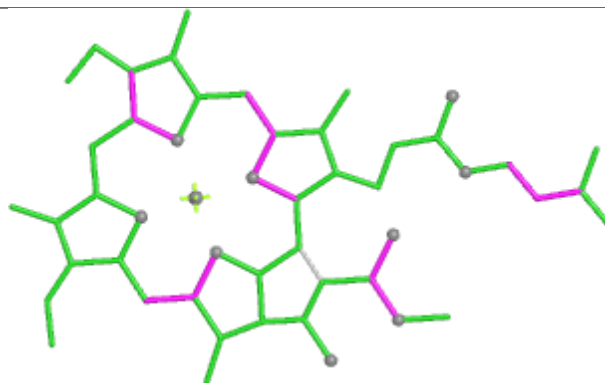
Ligand A1EB1 6 304



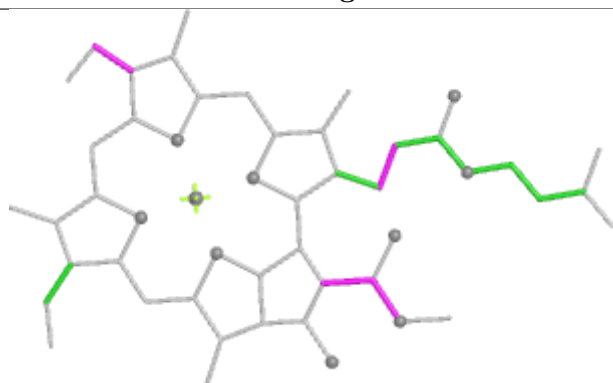
Ligand CLA J 308



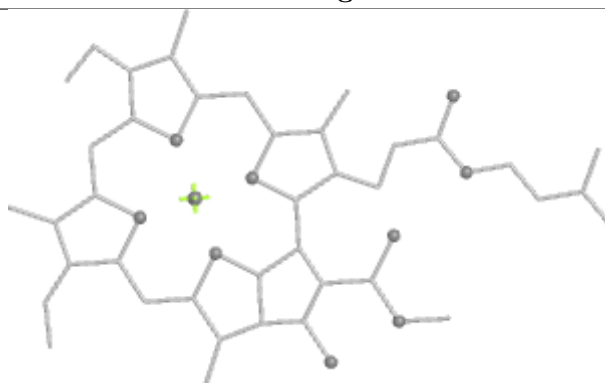
Bond lengths



Bond angles

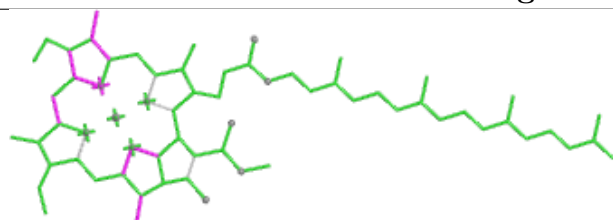


Torsions

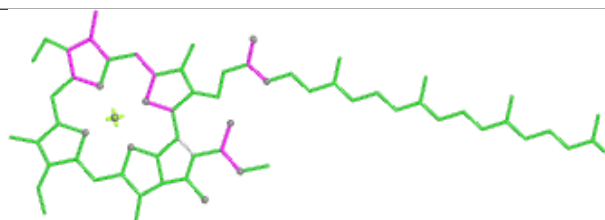


Rings

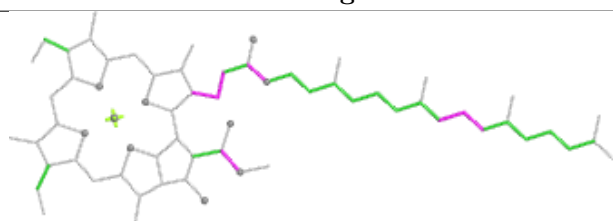
Ligand CLA b 829



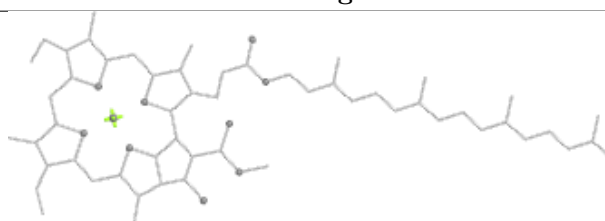
Bond lengths



Bond angles

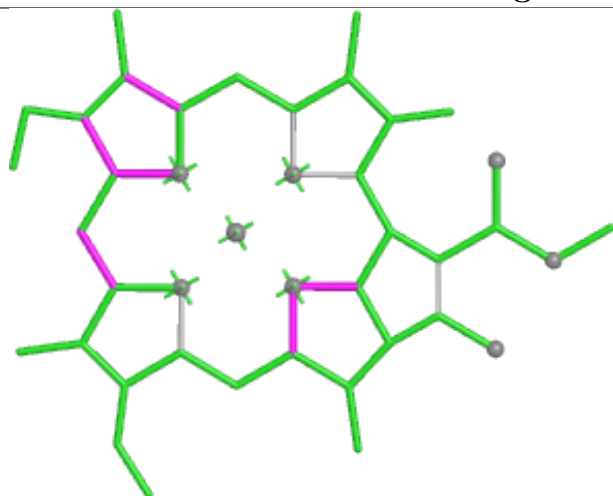


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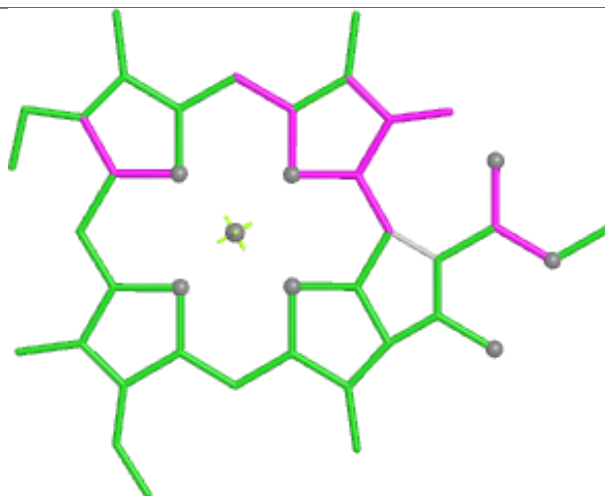


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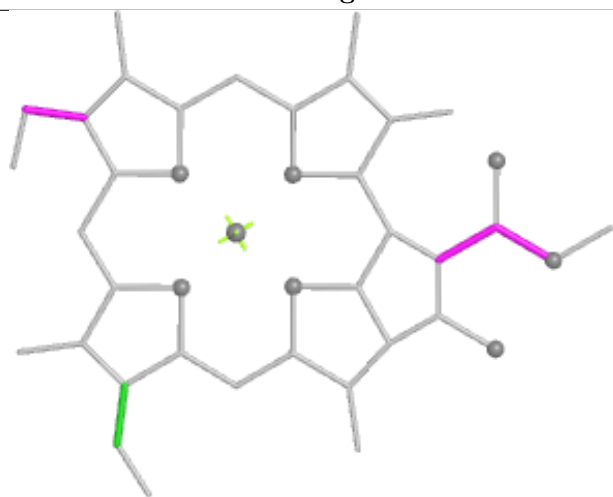
Ligand CLA Y 314



Bond lengths



Bond angles

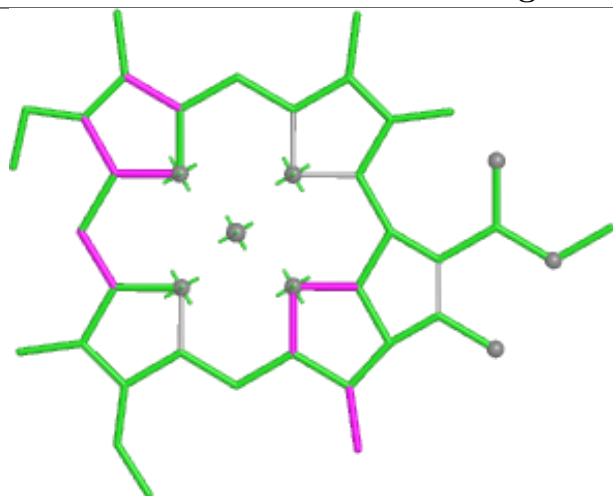


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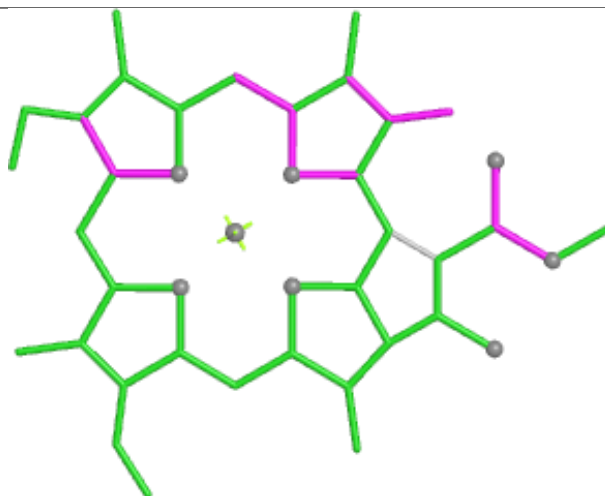


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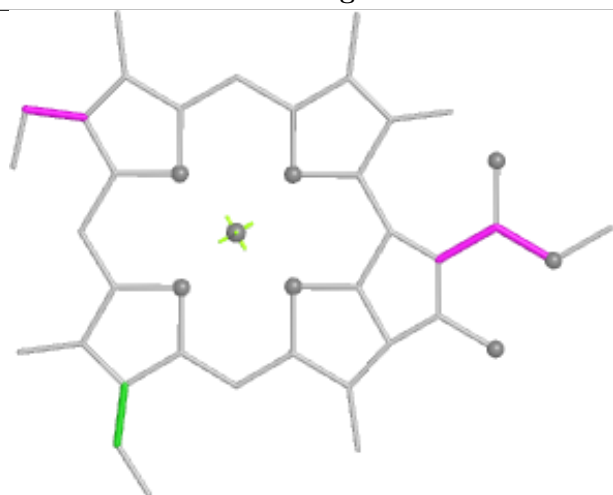
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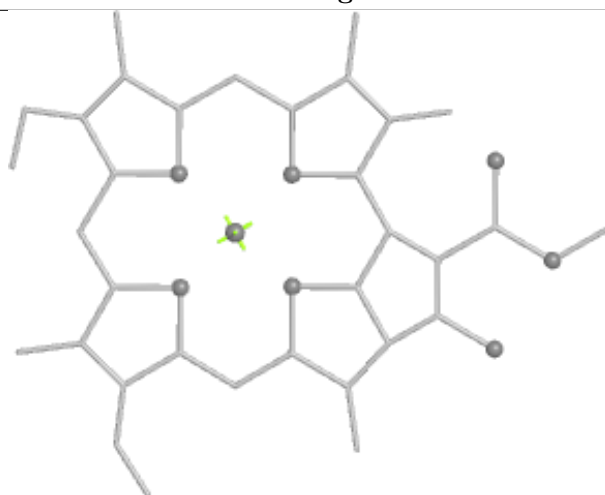
Bond lengths



Bond angles

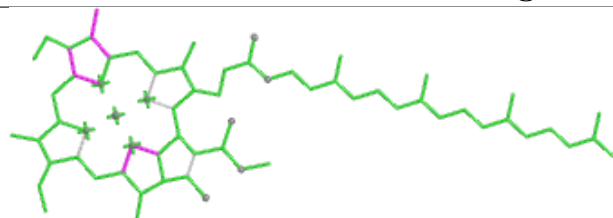


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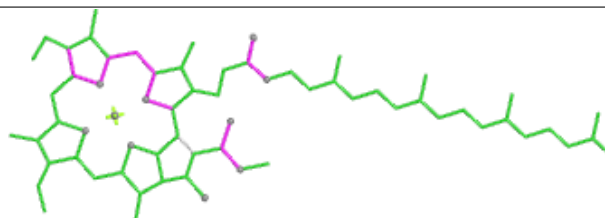


Rings

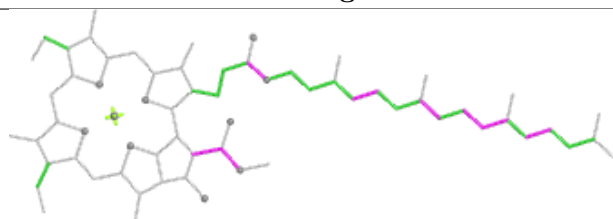
Ligand CLA b 841



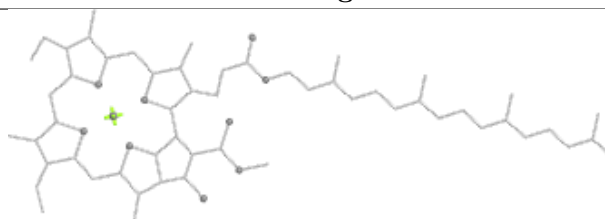
Bond lengths



Bond angles

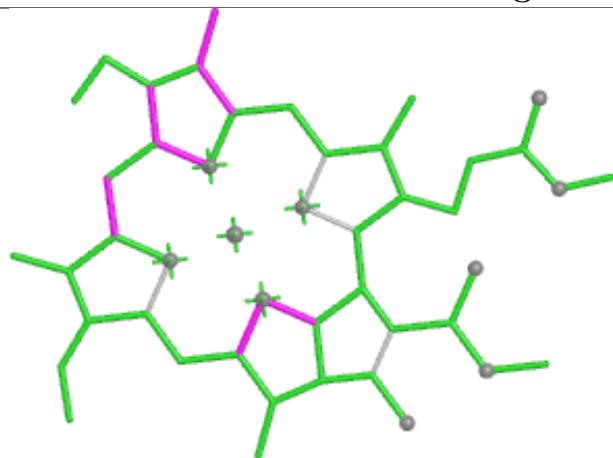


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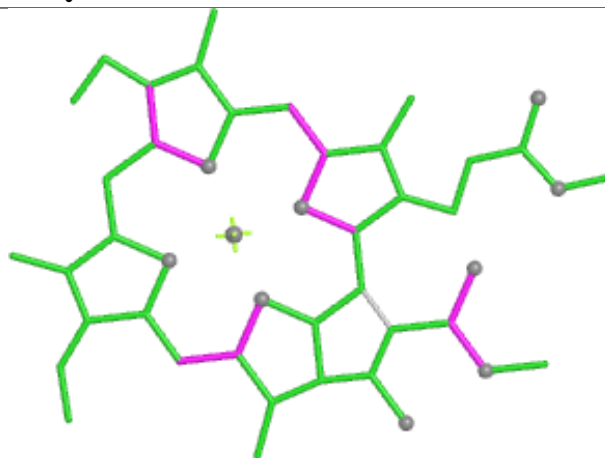


Rings

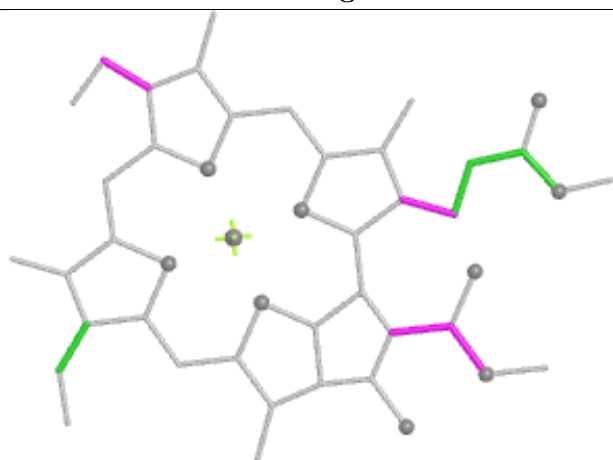
Ligand CLA Q 317



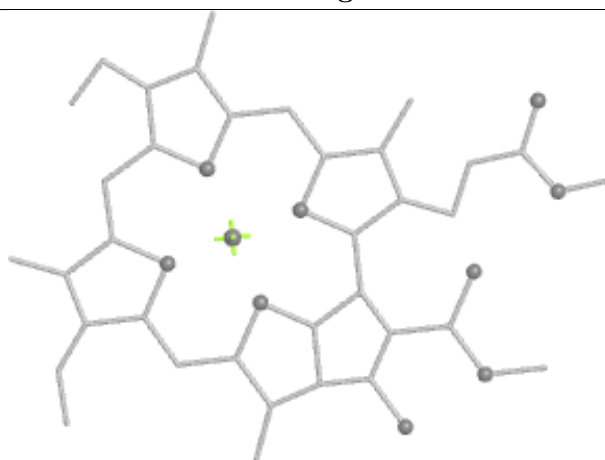
Bond lengths



Bond angles

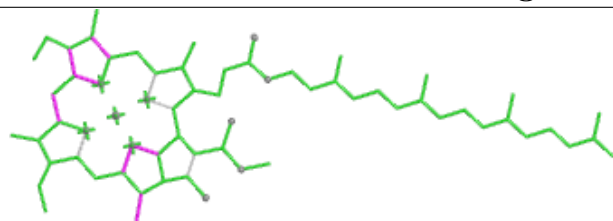


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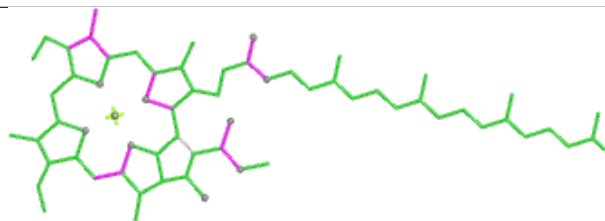


Rings

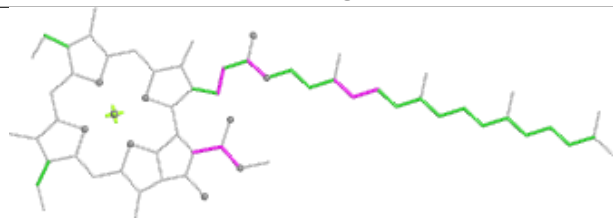
Ligand CLA b 805



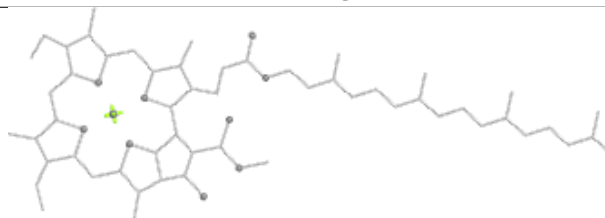
Bond lengths



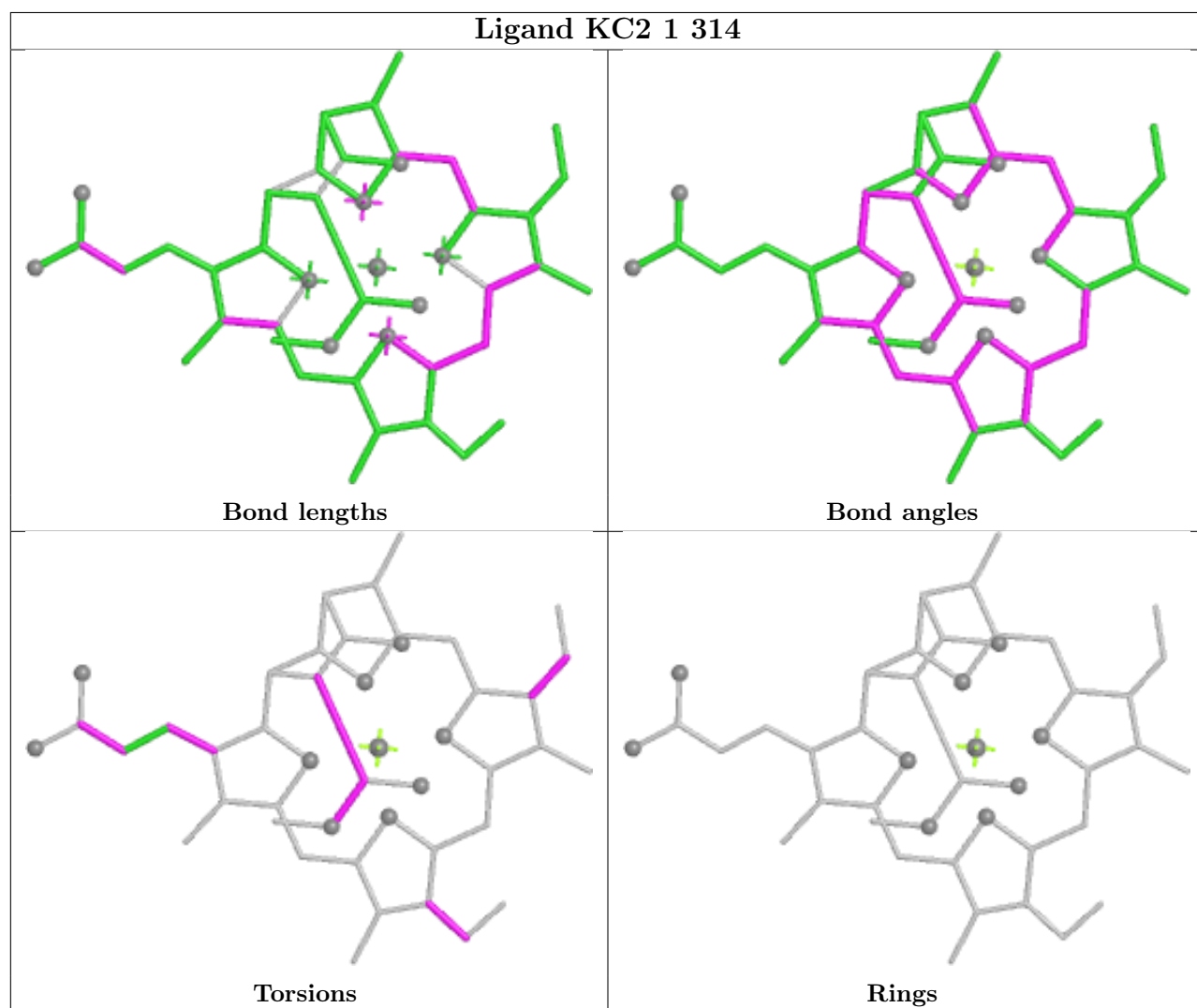
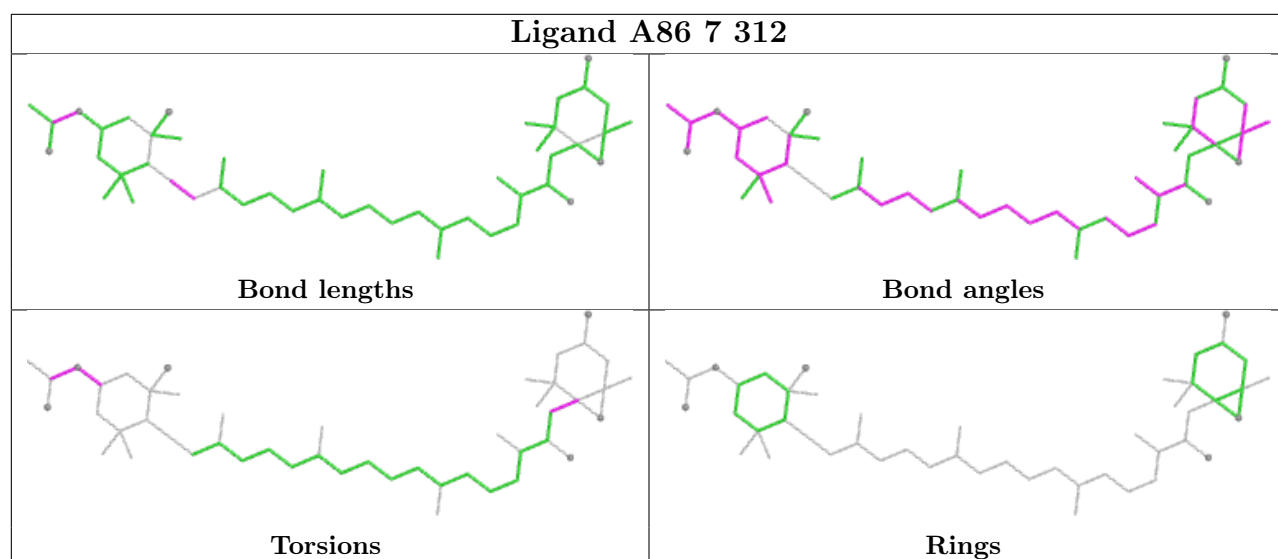
Bond angles



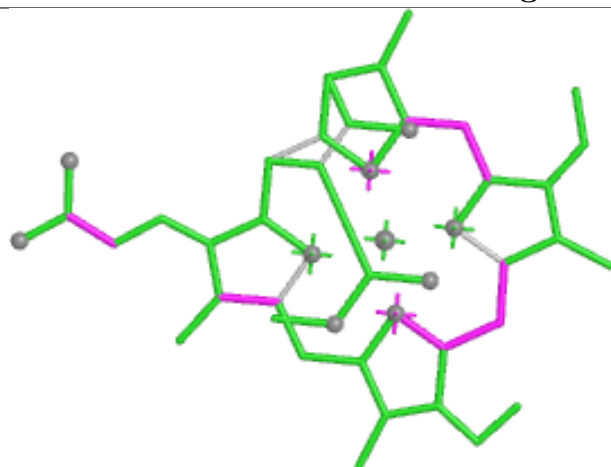
Torsions



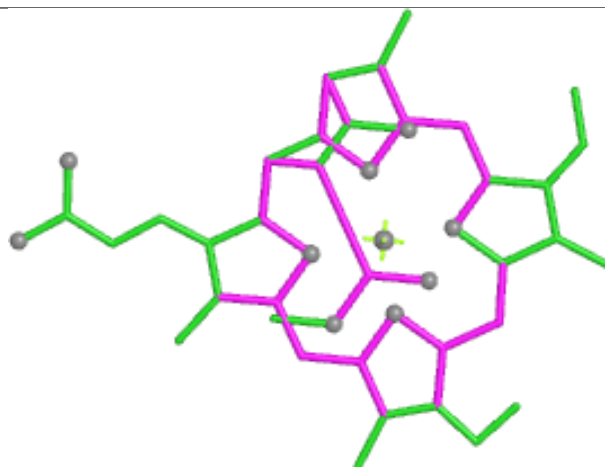
Rings



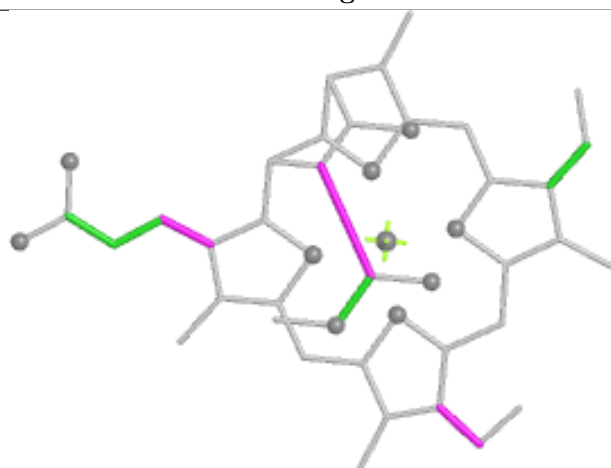
Ligand KC2 4 317



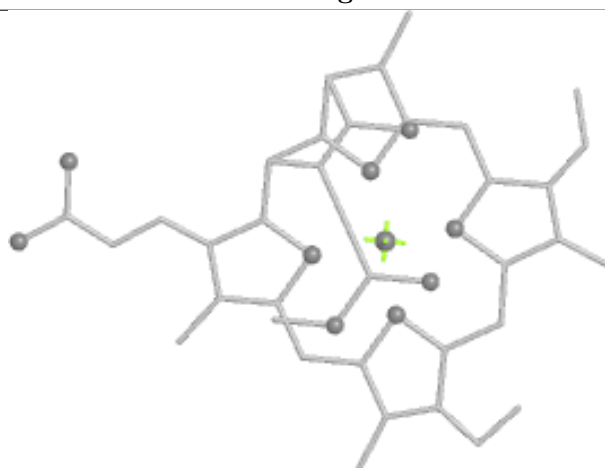
Bond lengths



Bond angles



Torsions

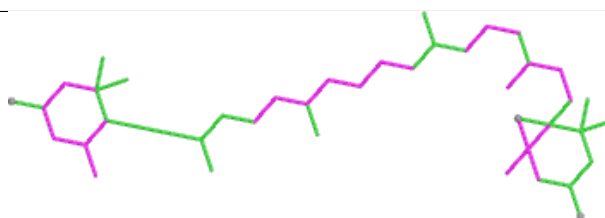


Rings

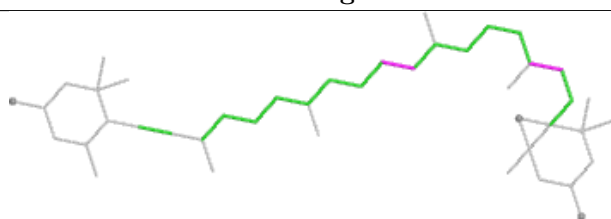
Ligand DD6 C 301



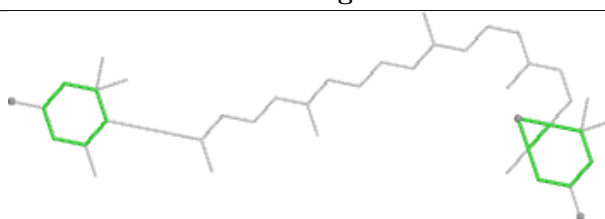
Bond lengths



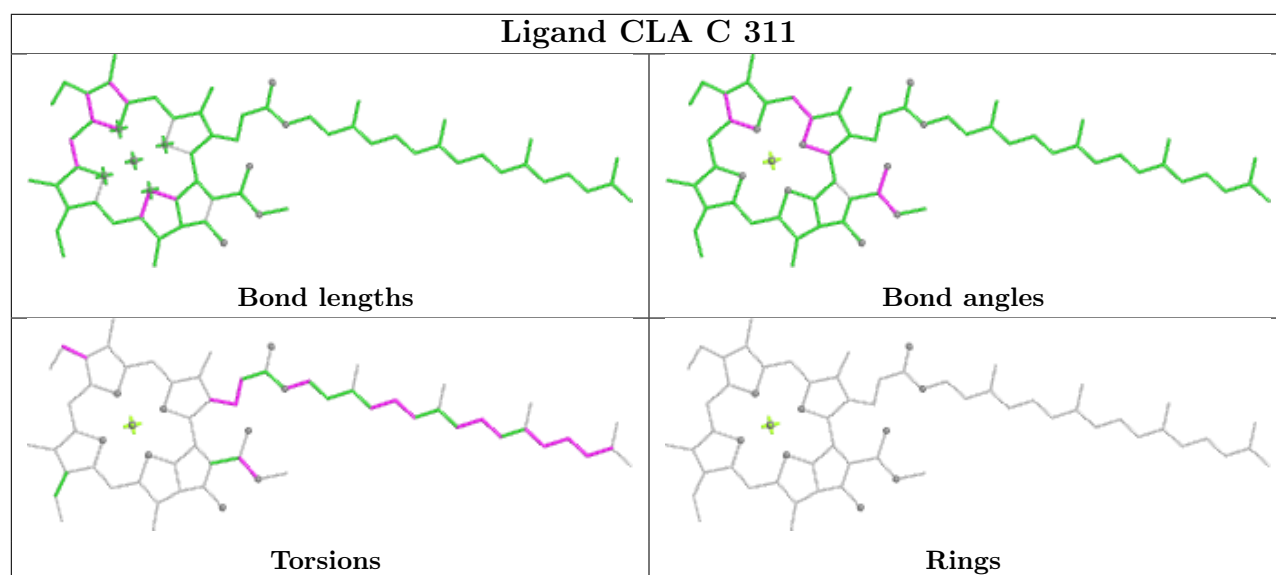
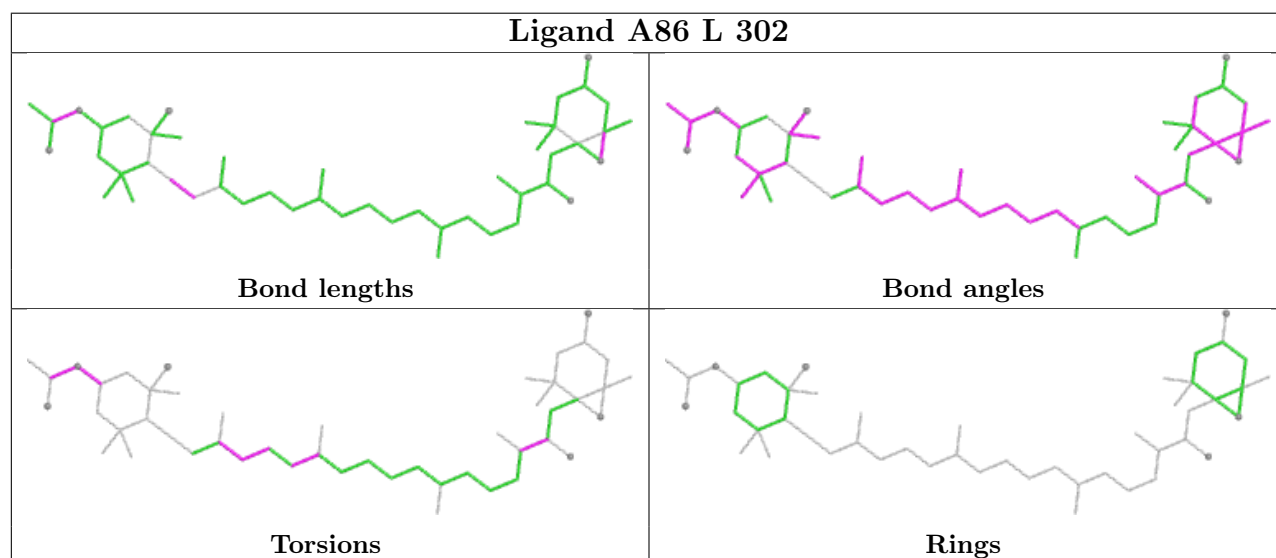
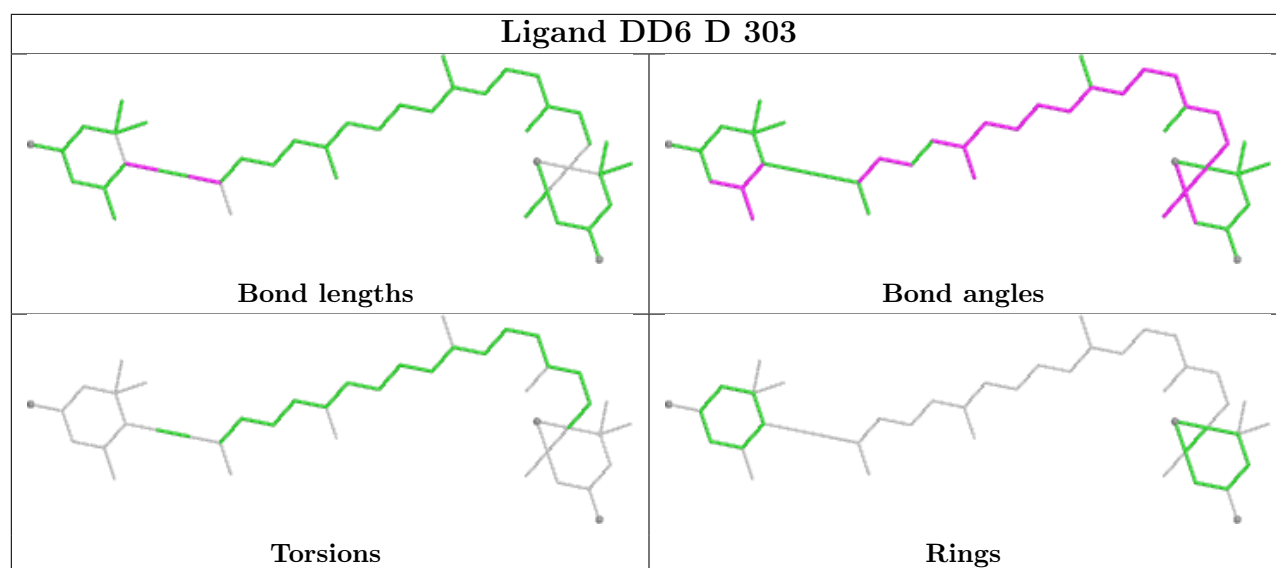
Bond angles

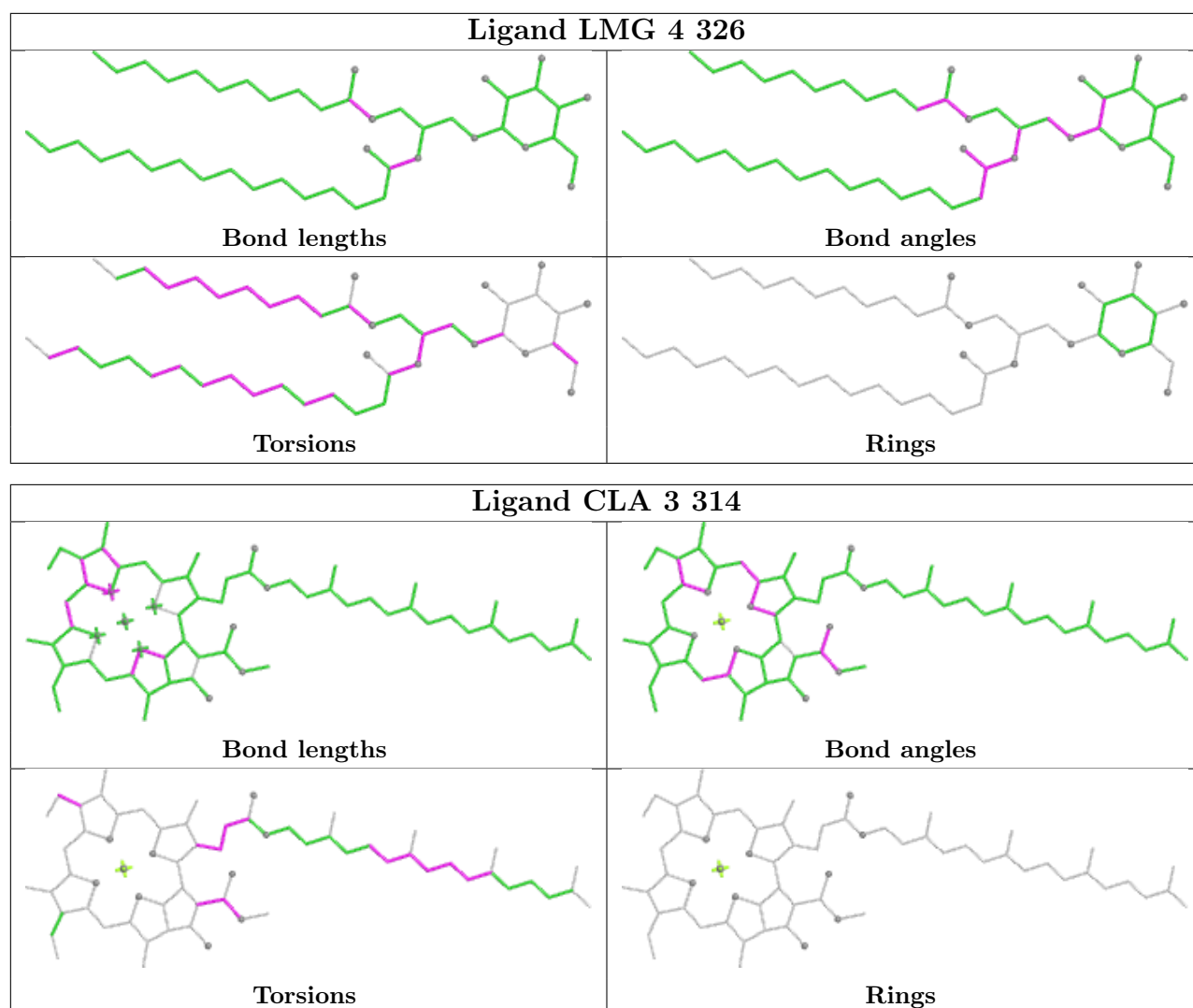


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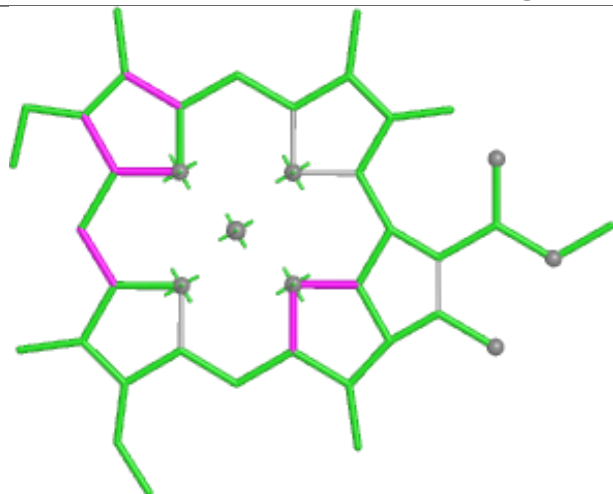


Rings





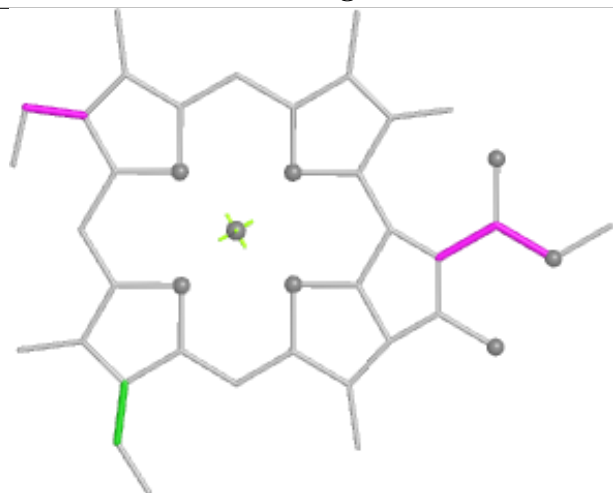
Ligand CLA 8 318



Bond lengths



Bond angles

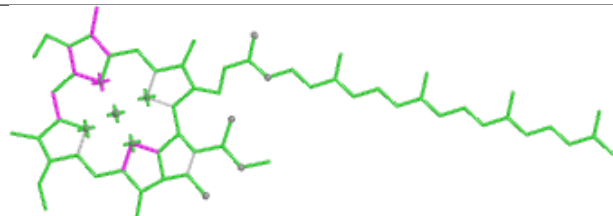


Torsions

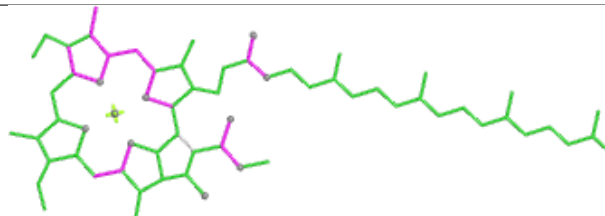


Rings

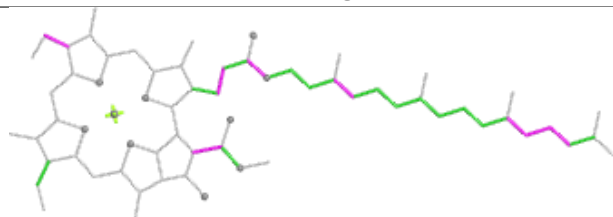
Ligand CLA a 835



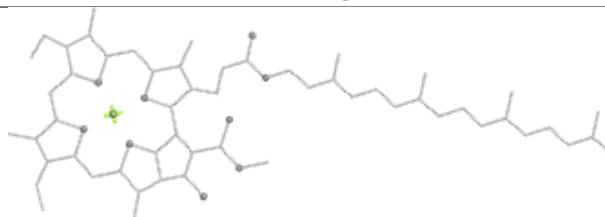
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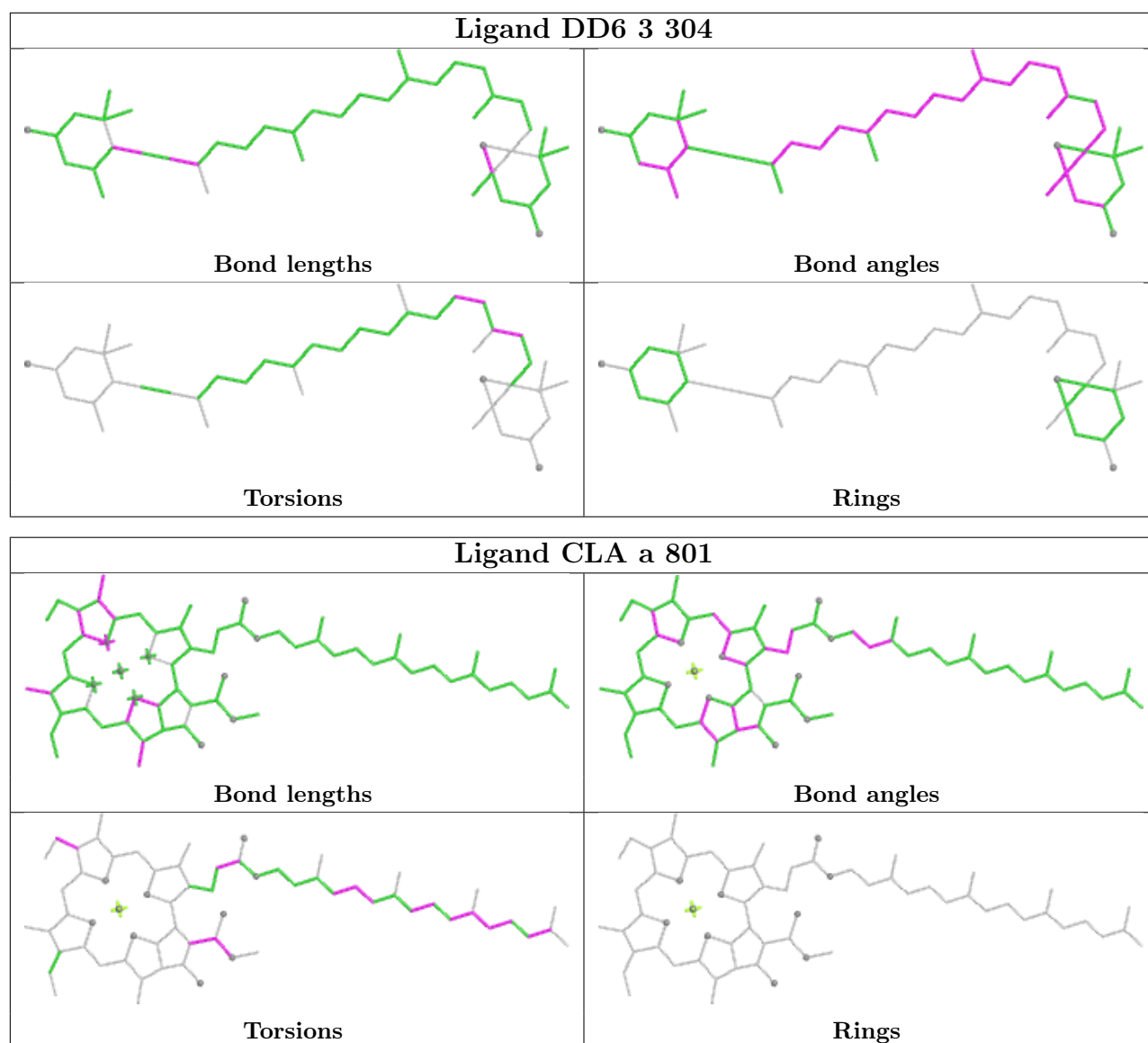
Bond angles



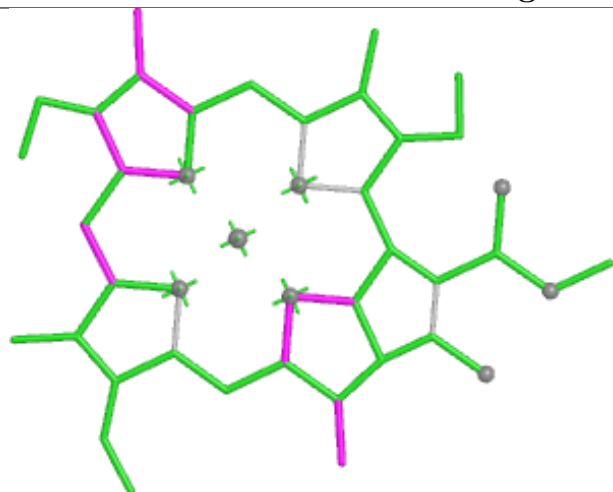
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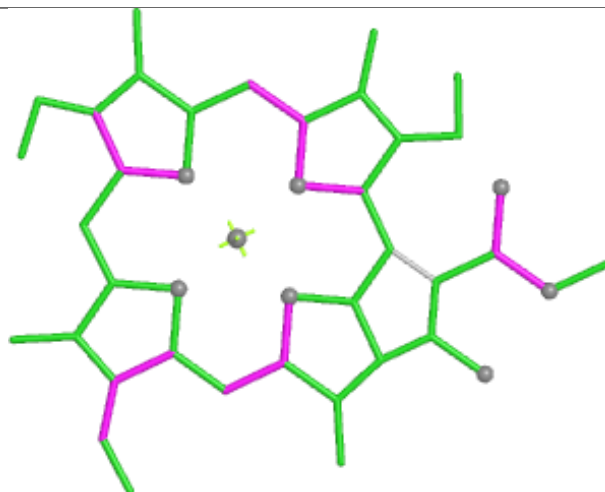
Rings



Ligand CLA 9 312



Bond lengths



Bond angles

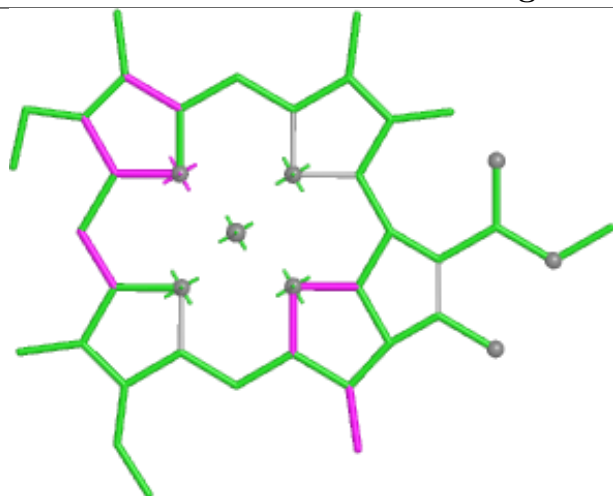


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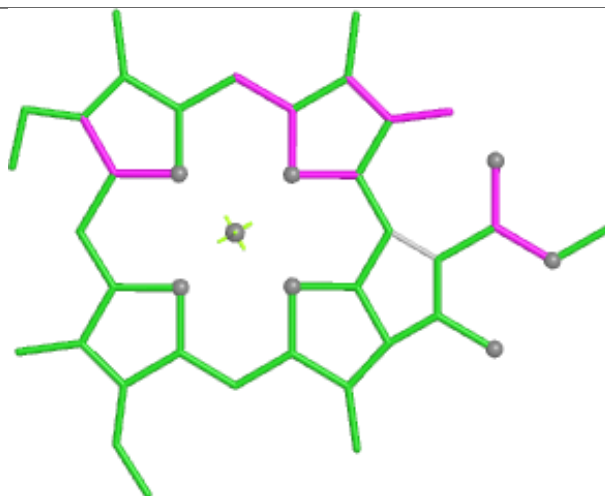


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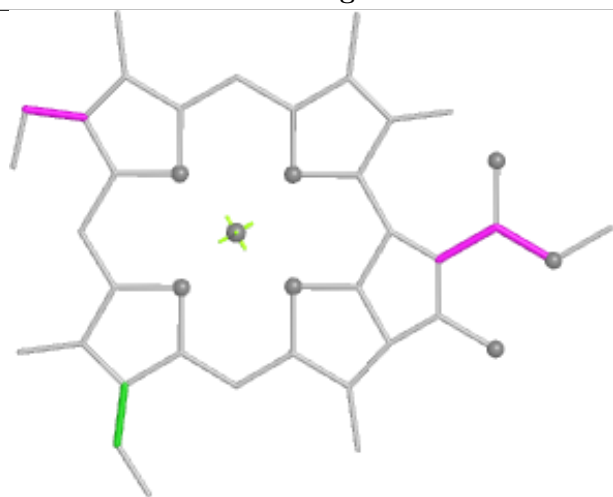
Ligand CLA 6 318



Bond lengths



Bond angles

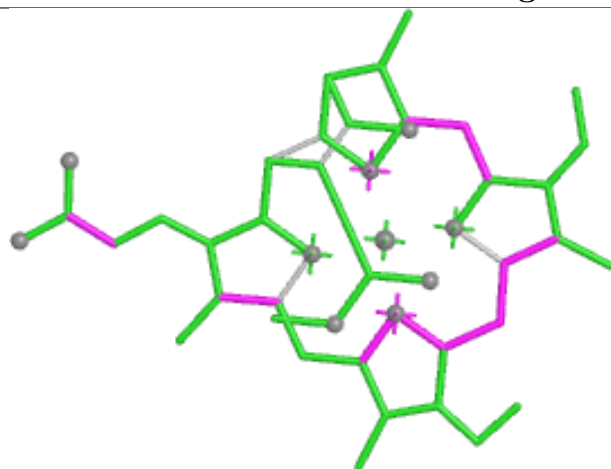


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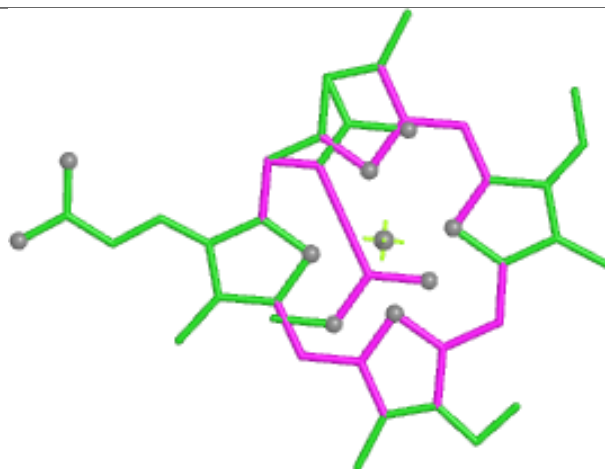


Rings

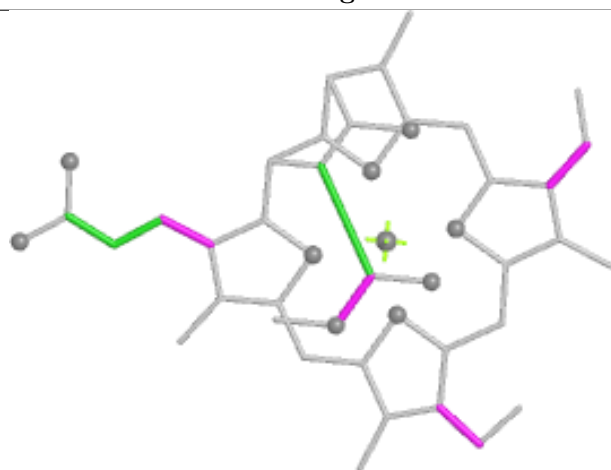
Ligand KC2 L 321



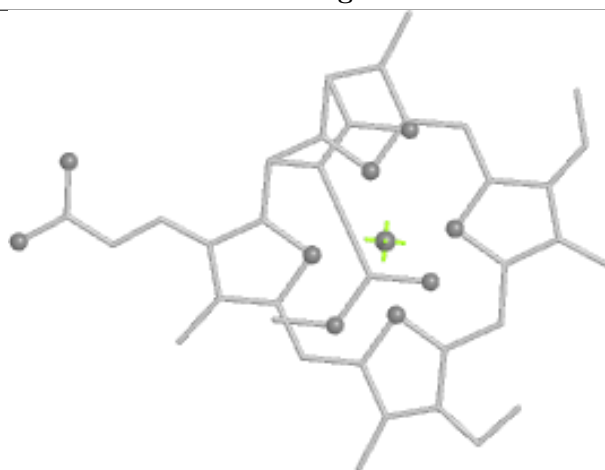
Bond lengths



Bond angles

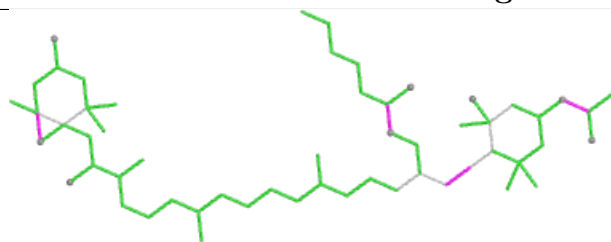


Torsions

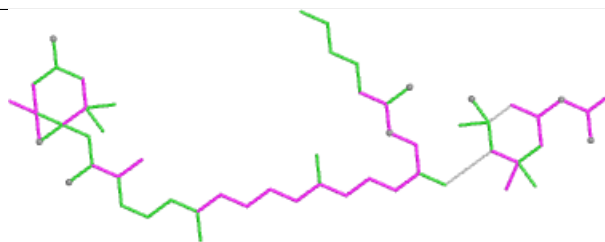


Rings

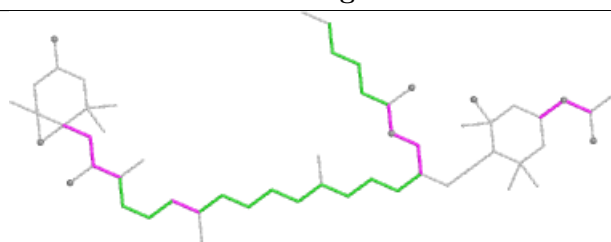
Ligand A1EB1 O 301



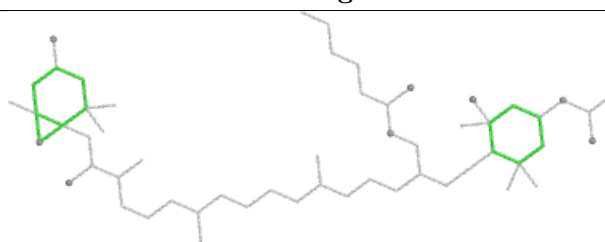
Bond lengths



Bond angles

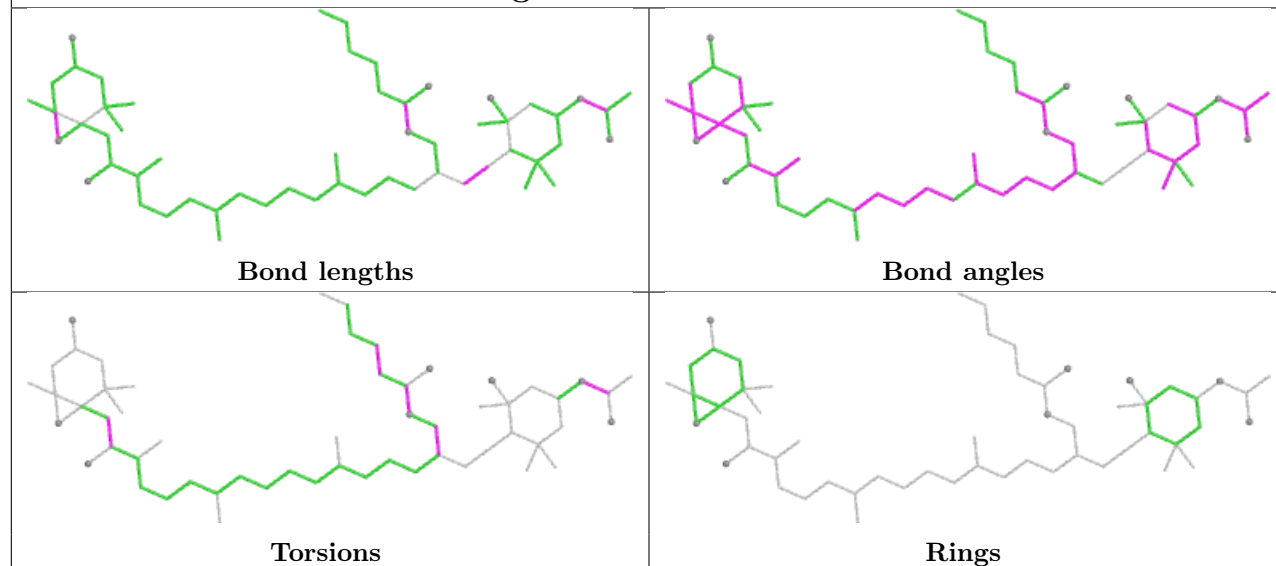


Torsions

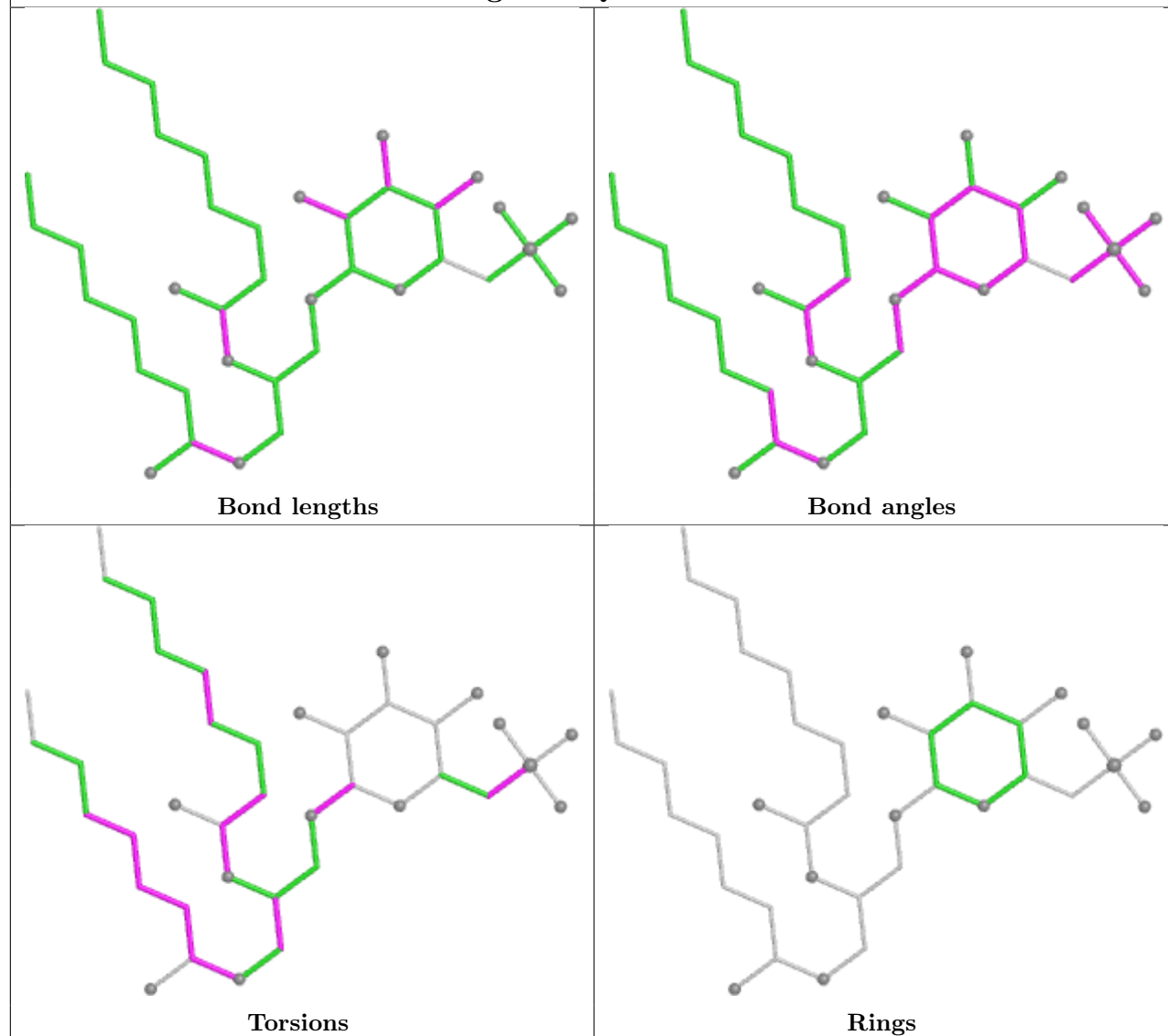


Rings

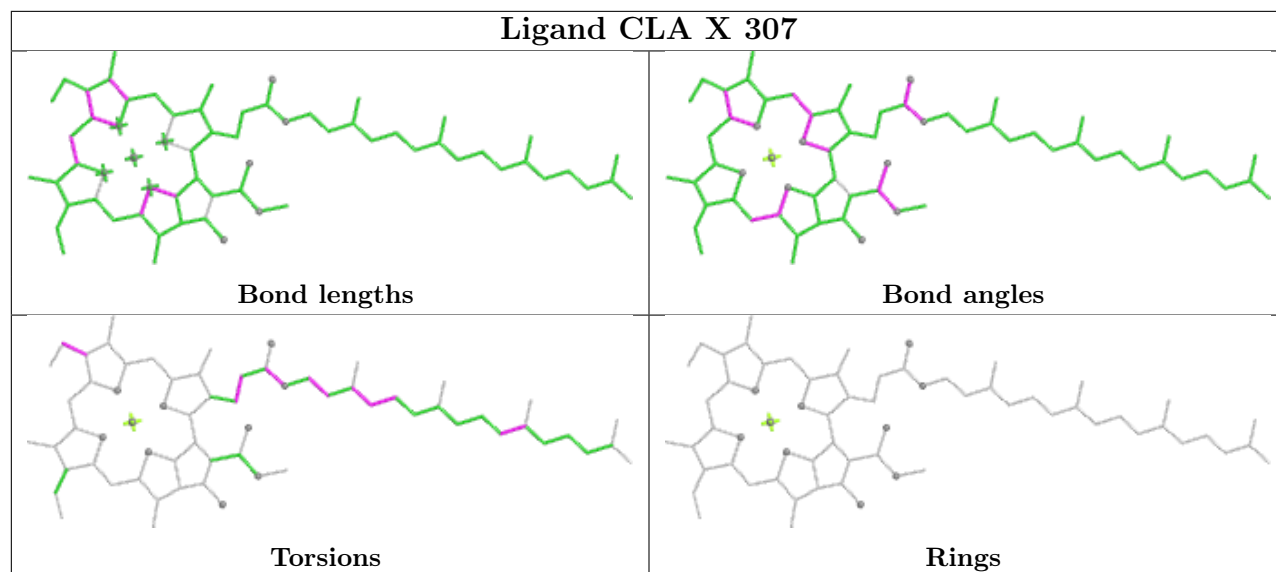
Ligand A1EB1 G 304



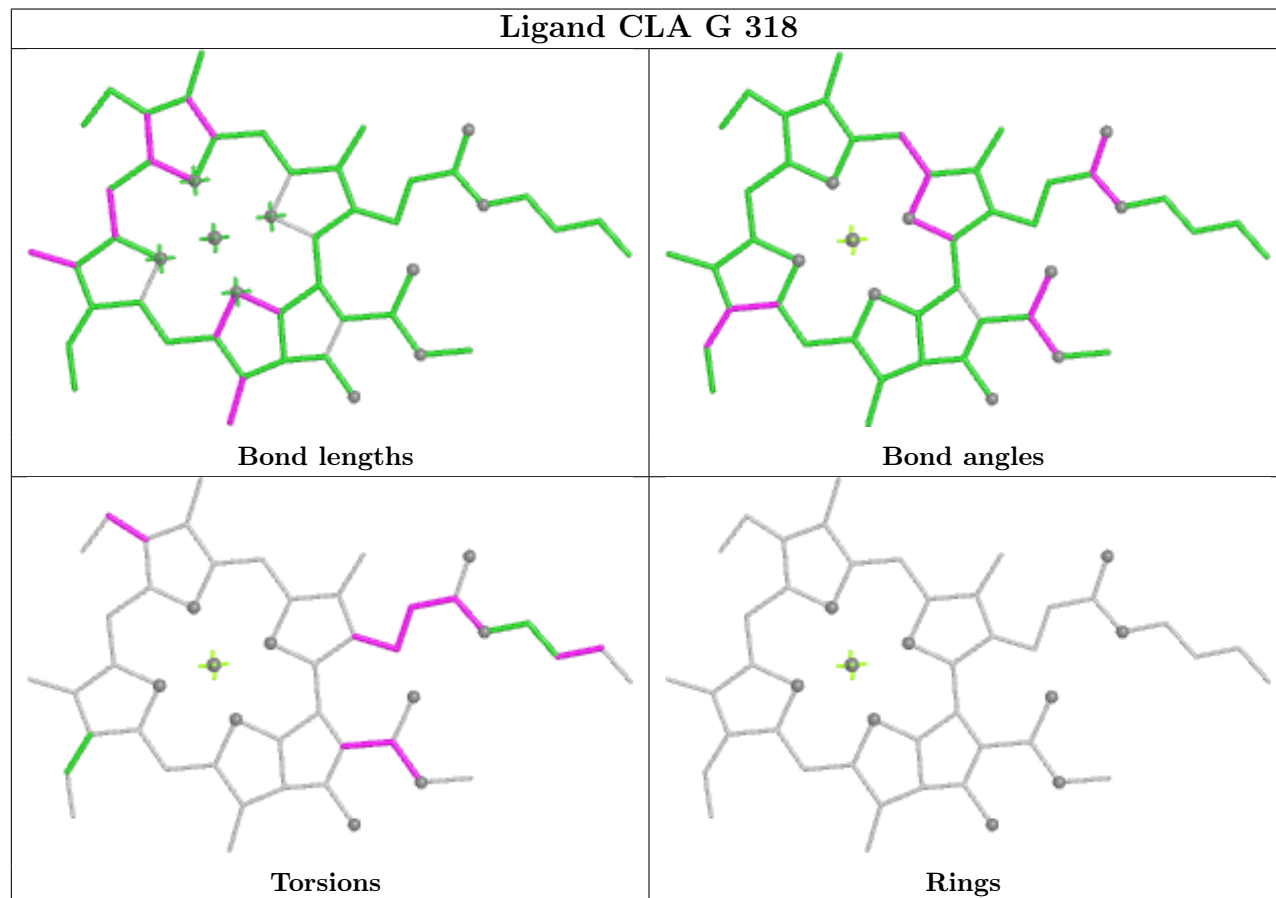
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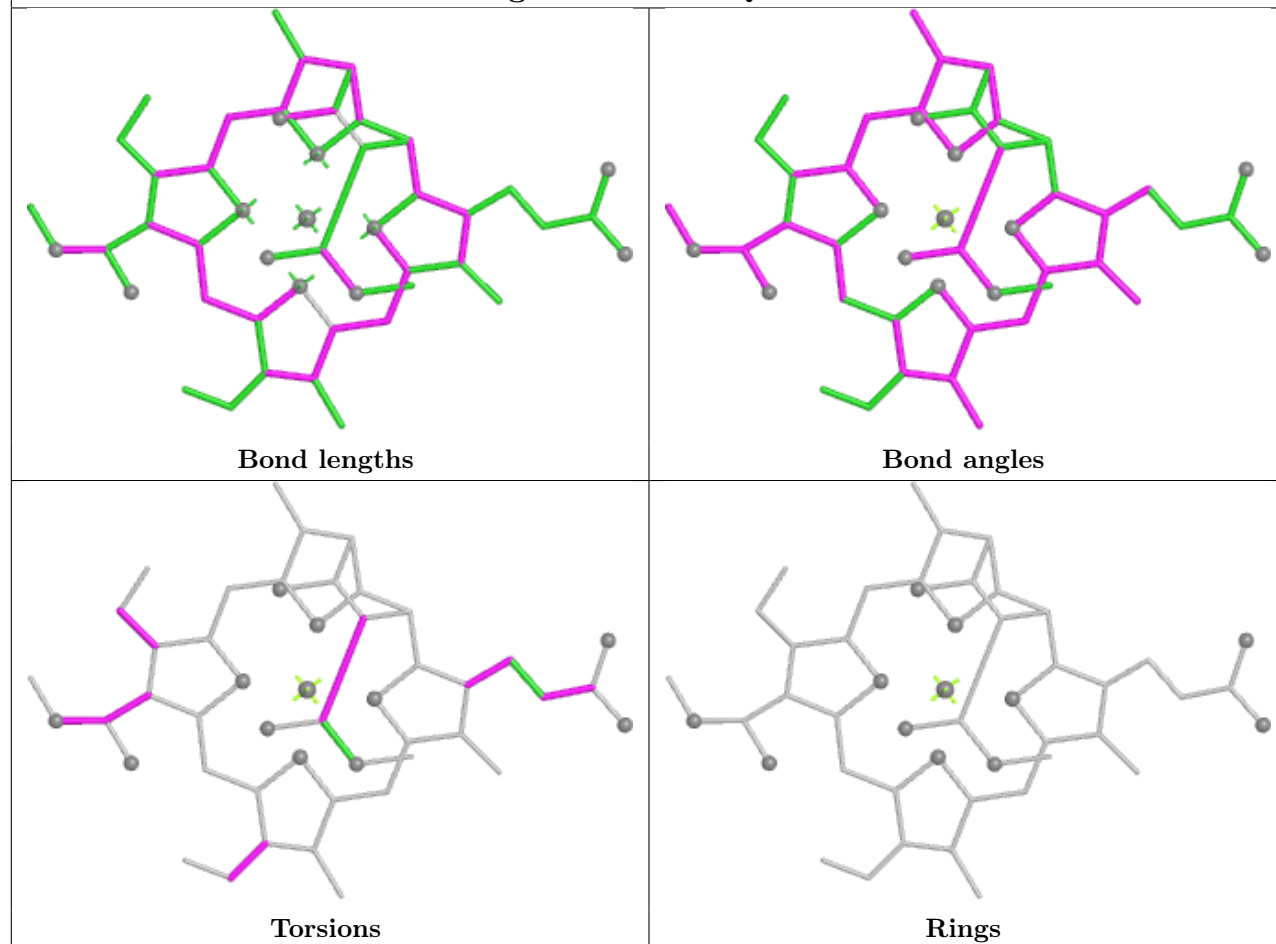
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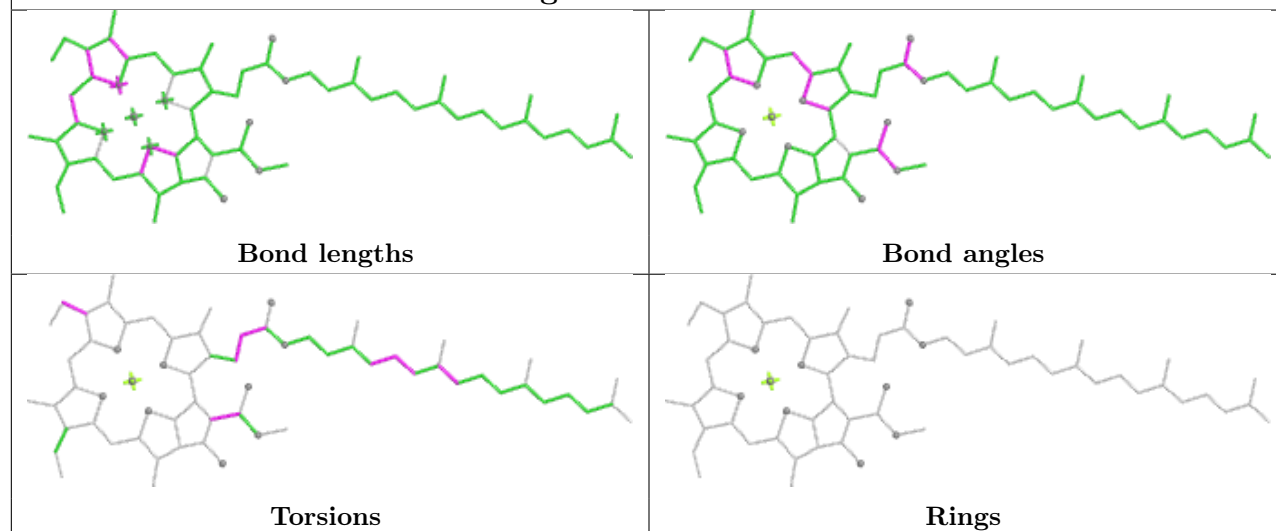
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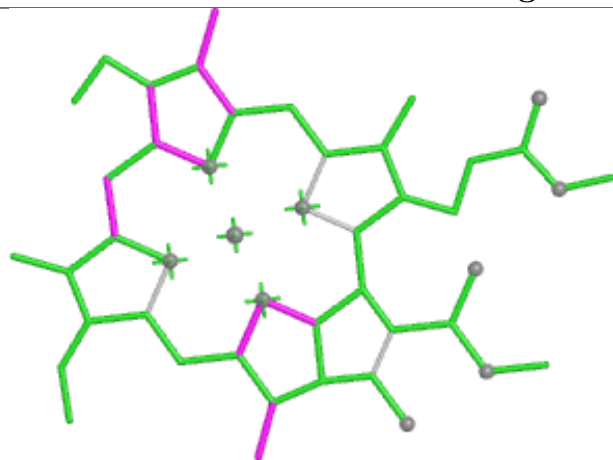
Ligand A1ECV Q 319



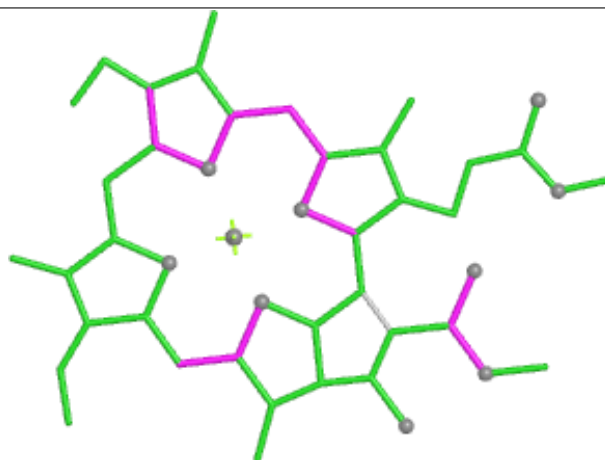
Ligand CLA i 101



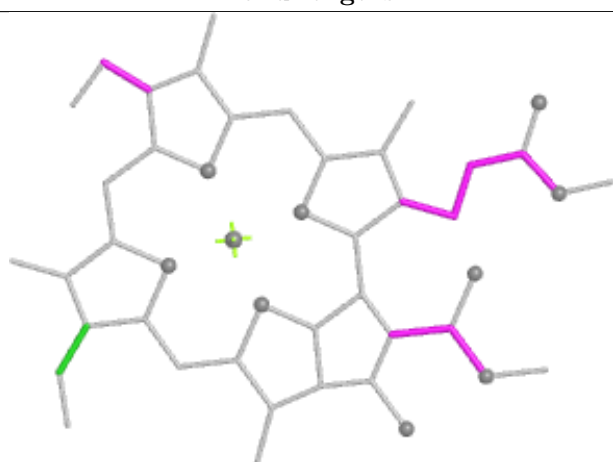
Ligand CLA 2 308



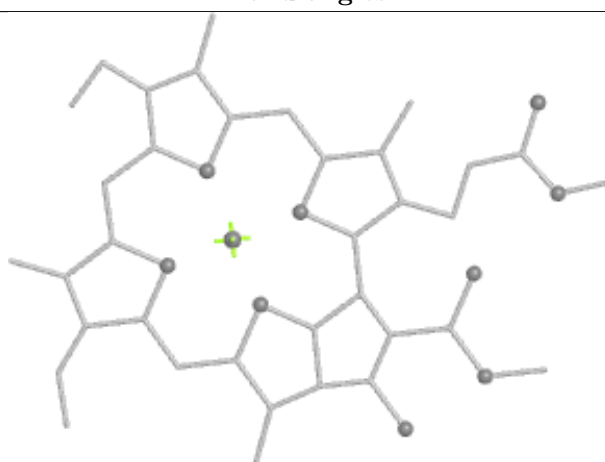
Bond lengths



Bond angles

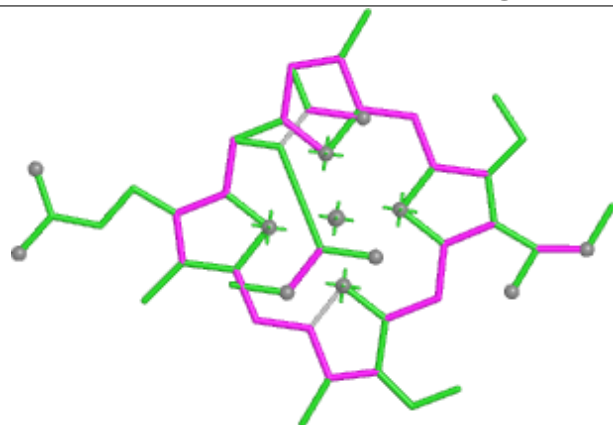


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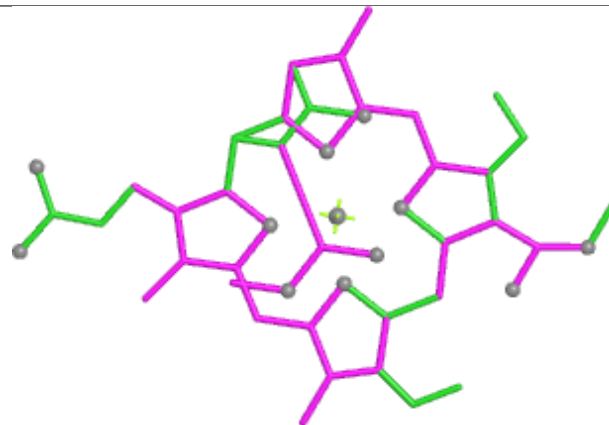


Rings

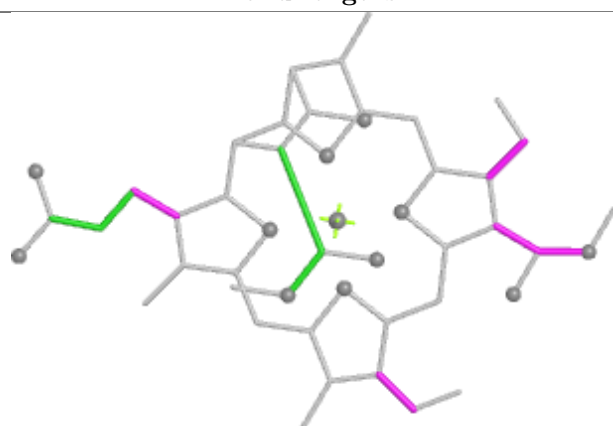
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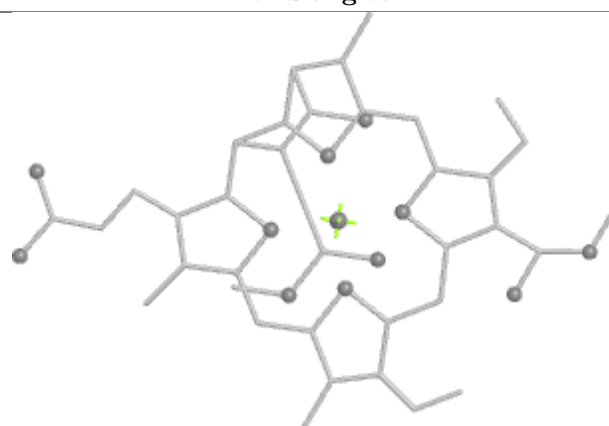
Bond lengths



Bond angles

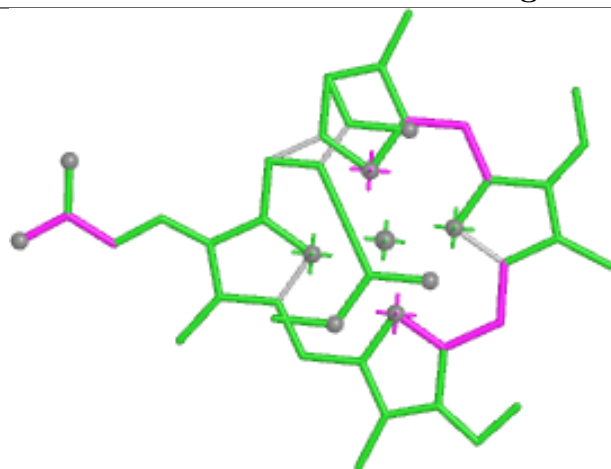


Torsions

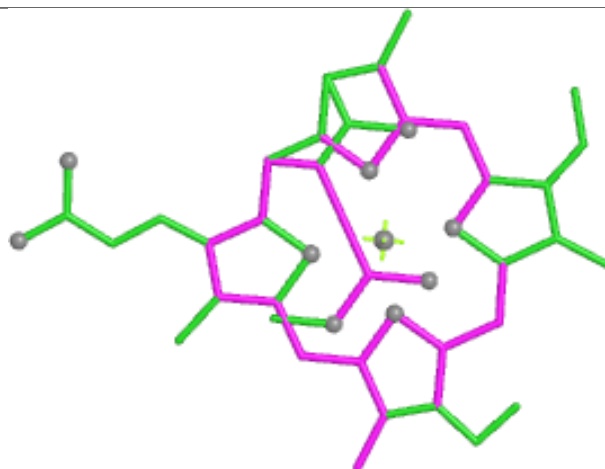


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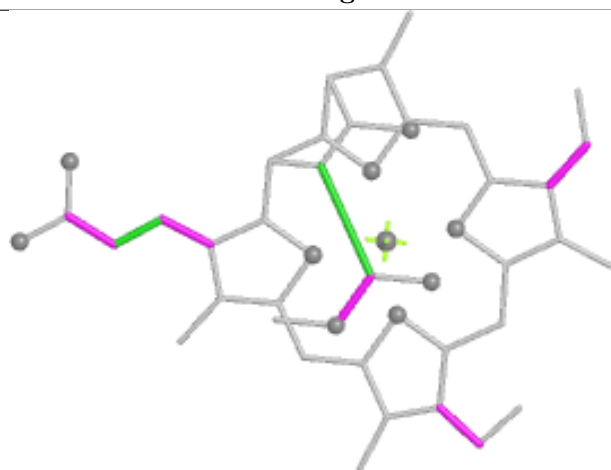
Ligand KC2 3 321



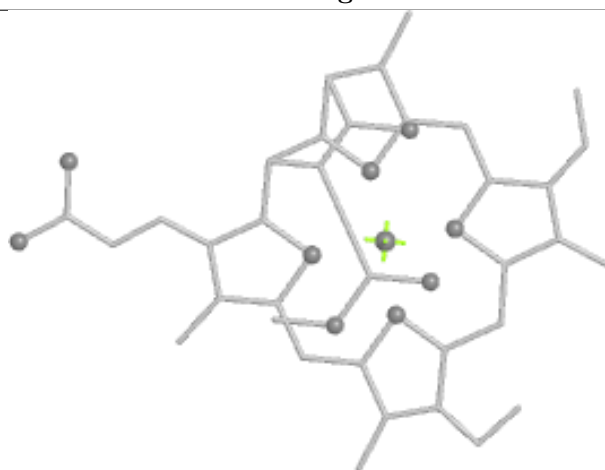
Bond lengths



Bond angles

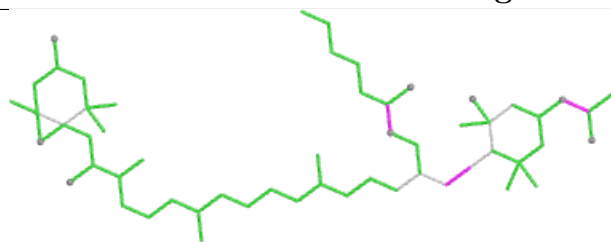


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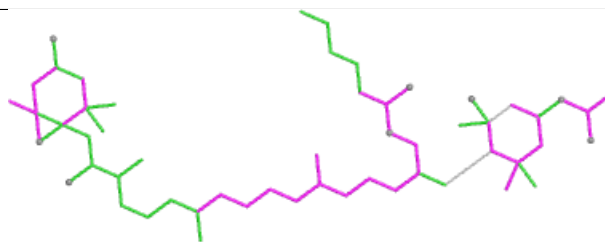


Rings

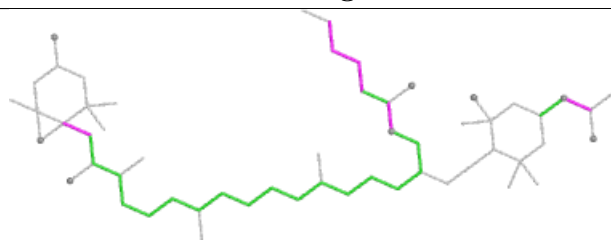
Ligand A1EB1 D 308



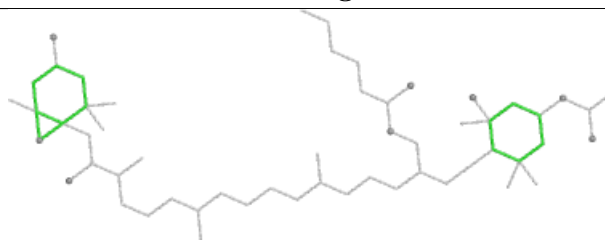
Bond lengths



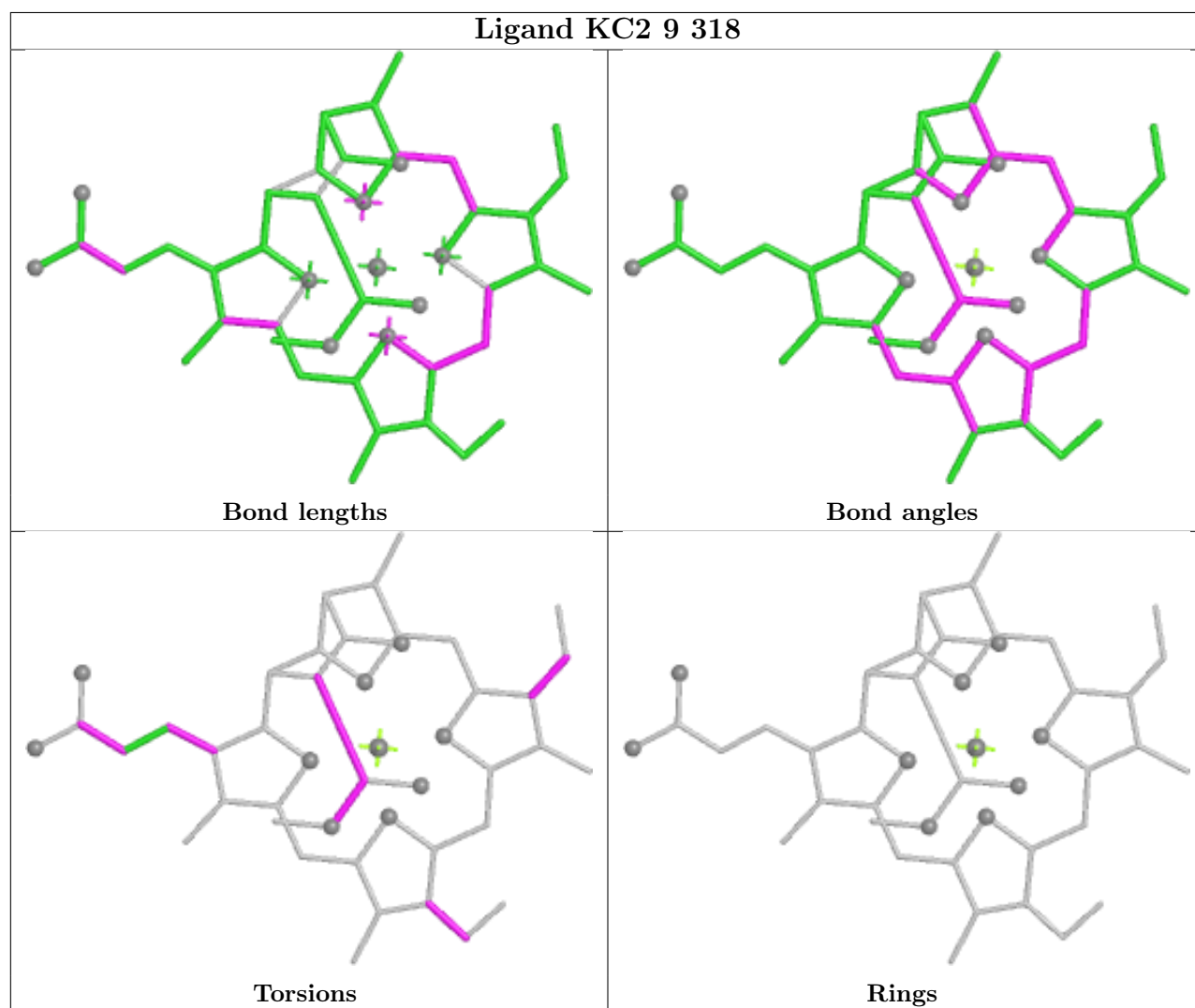
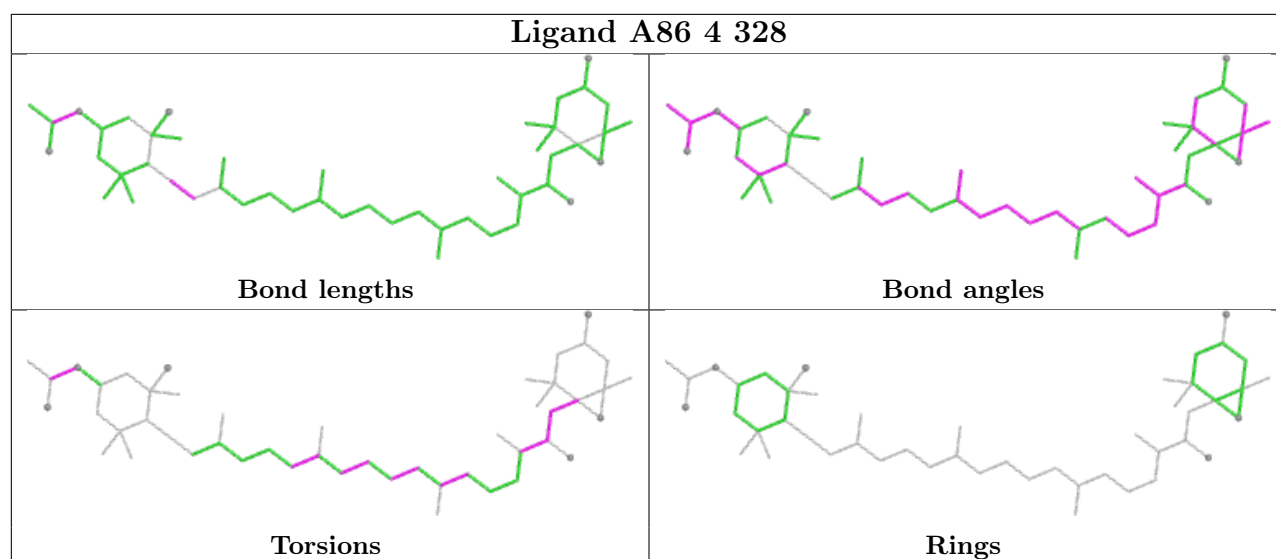
Bond angles

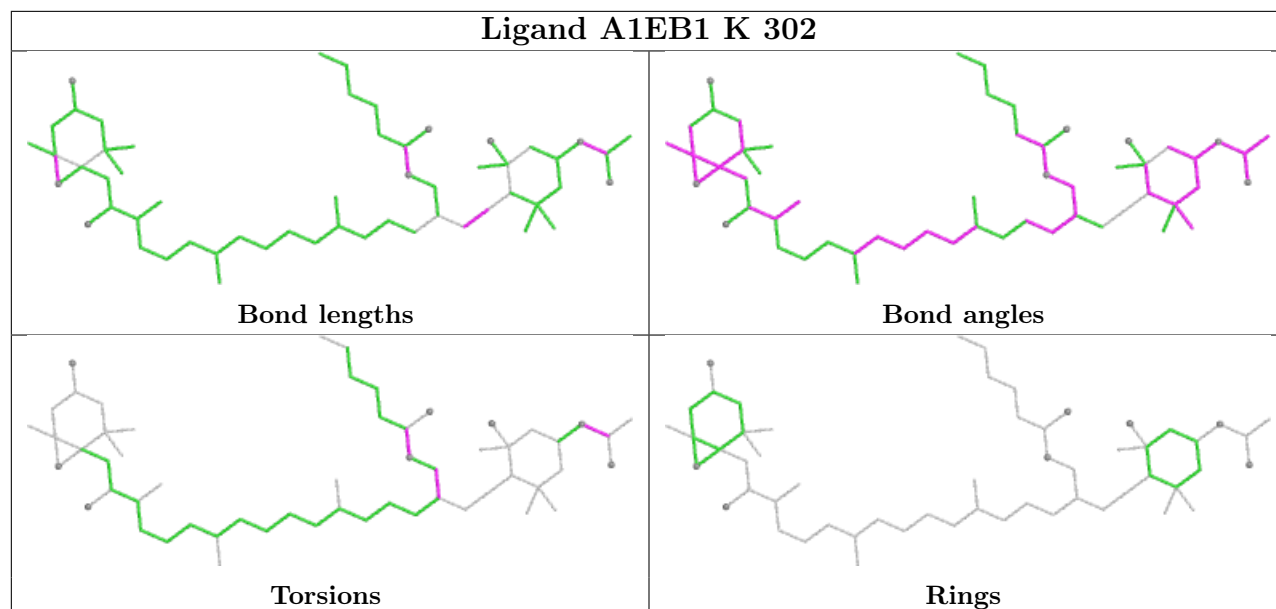
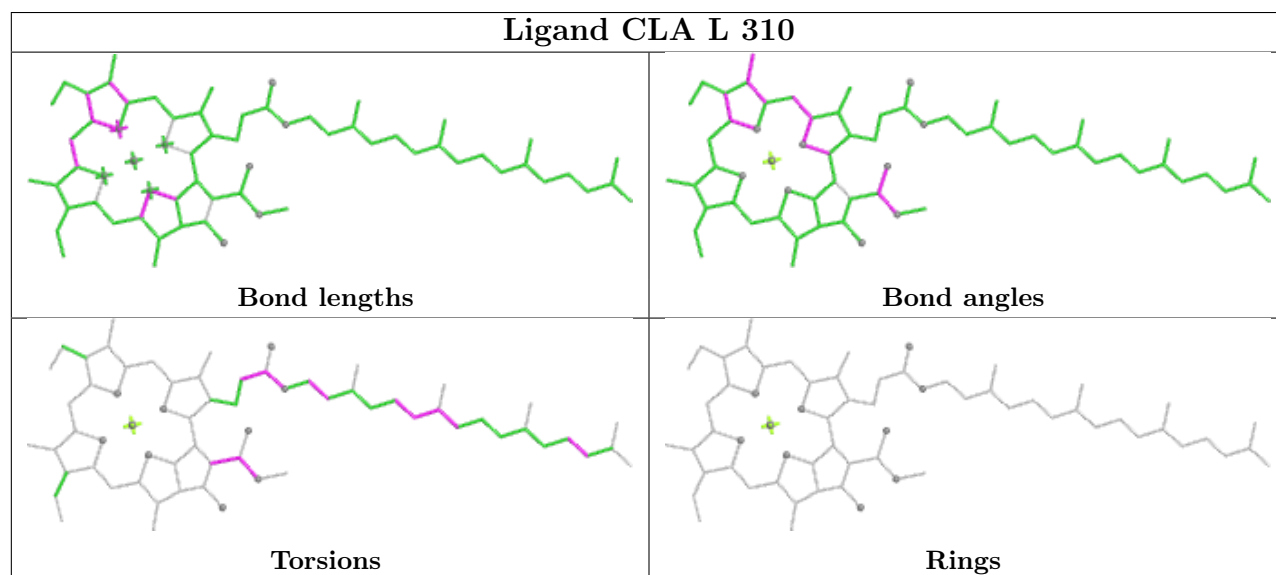


Torsions

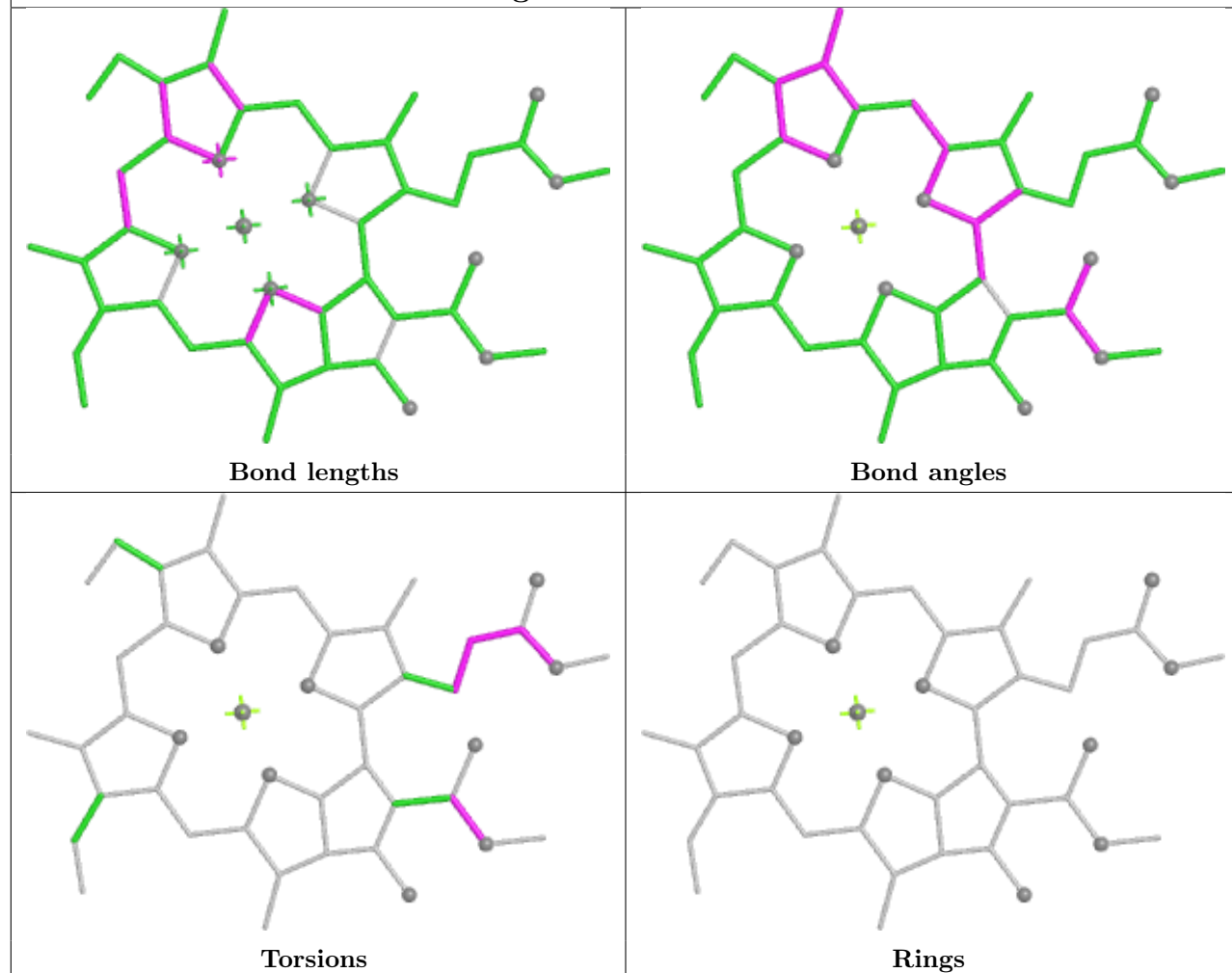


Rings

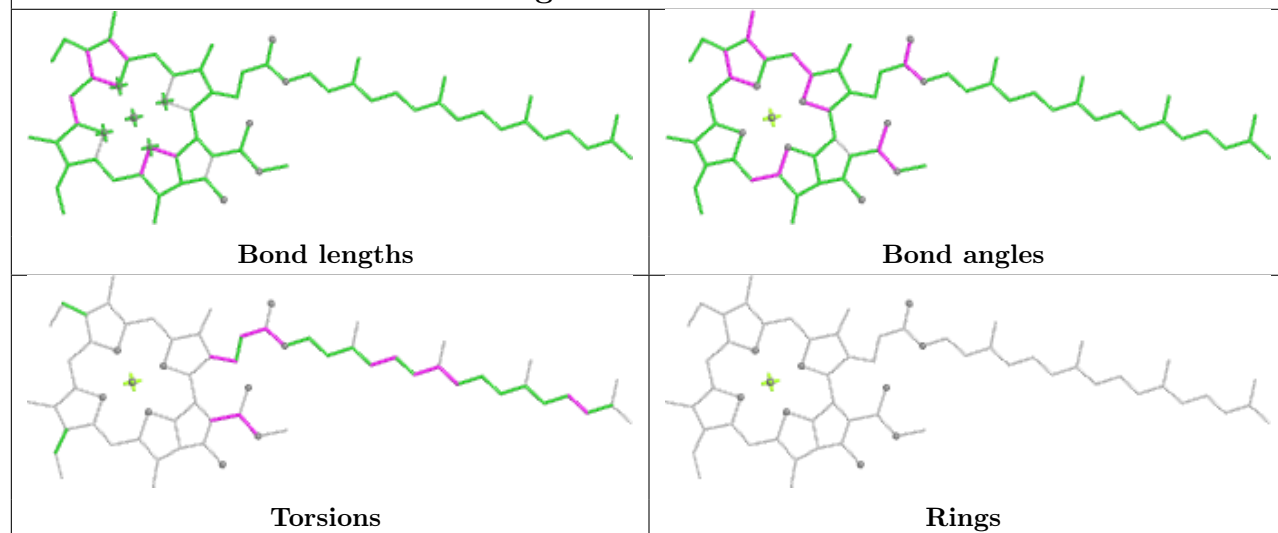


Ligand A1EB1 K 302**Ligand CLA L 310**

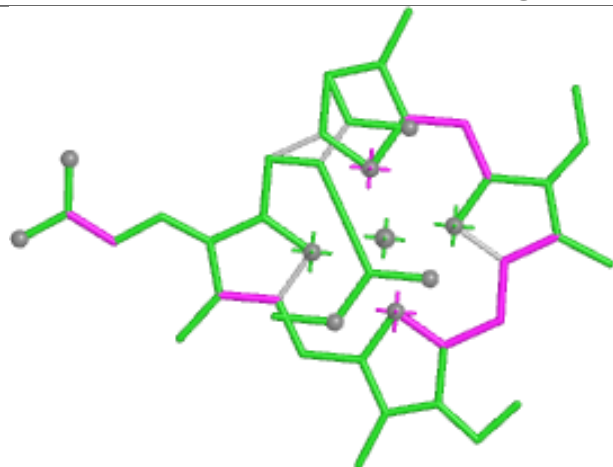
Ligand CLA O 318



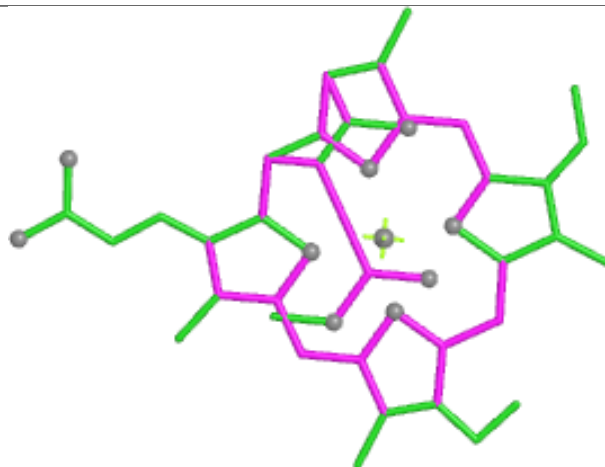
Ligand CLA b 809



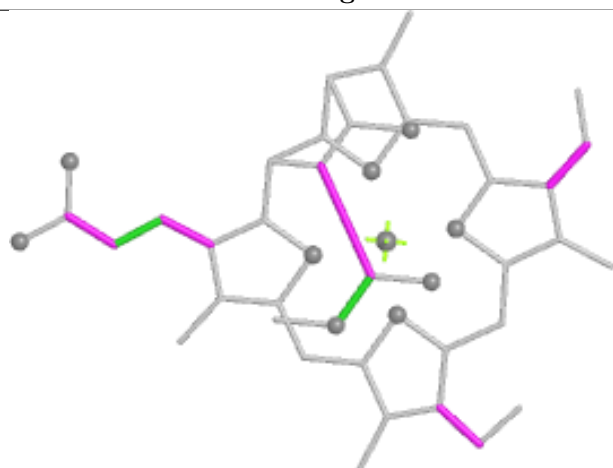
Ligand KC2 K 313



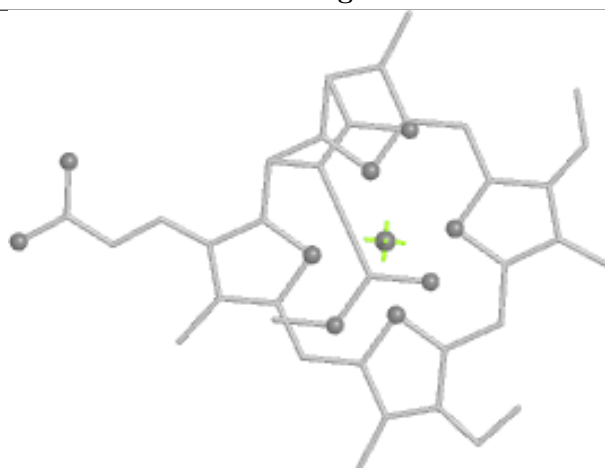
Bond lengths



Bond angles

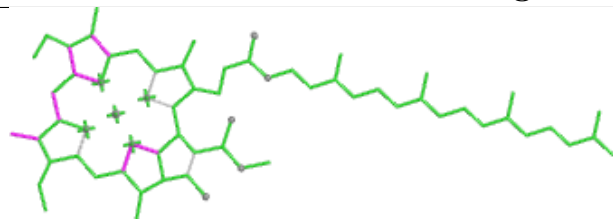


Torsions

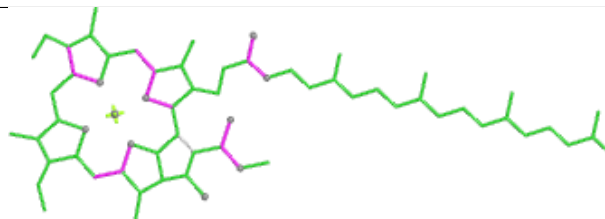


Rings

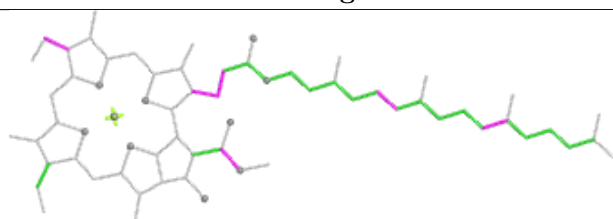
Ligand CLA H 313



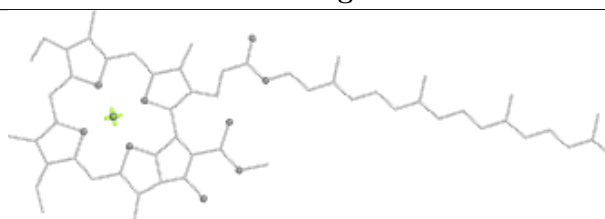
Bond lengths



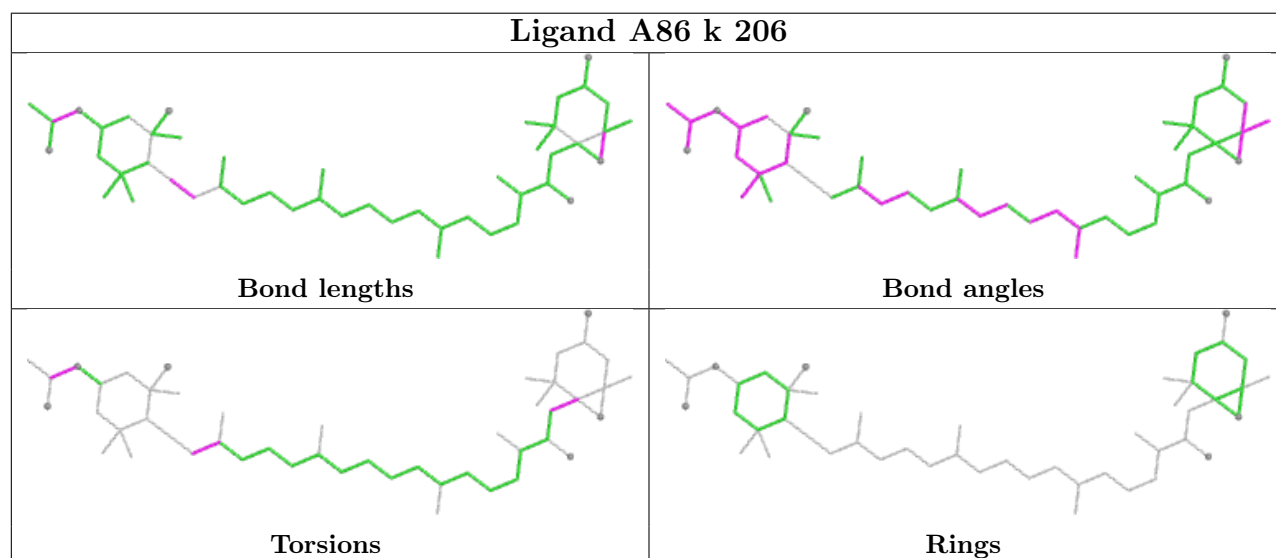
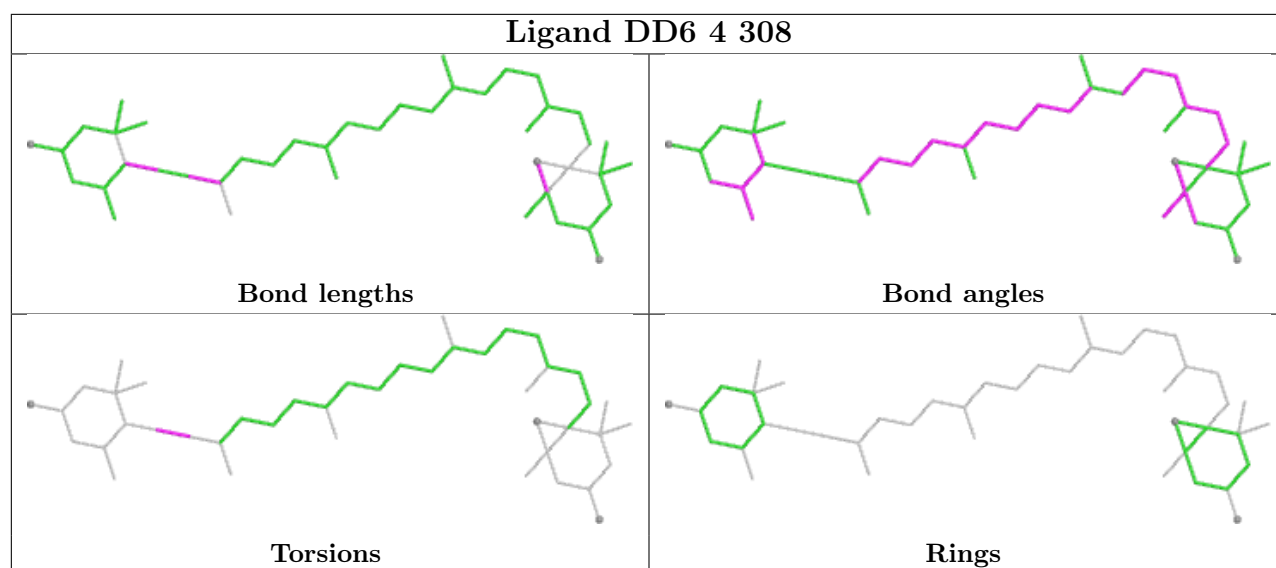
Bond angles



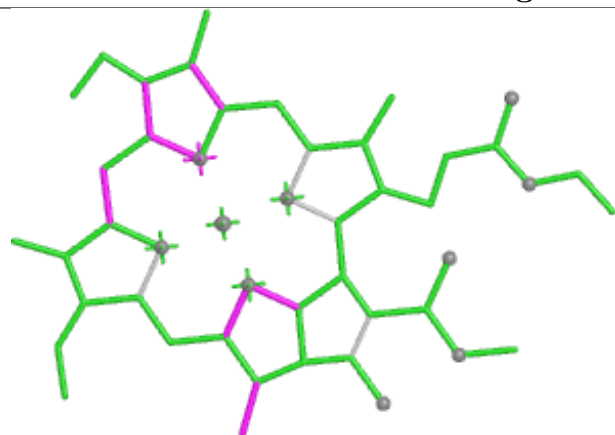
Torsions



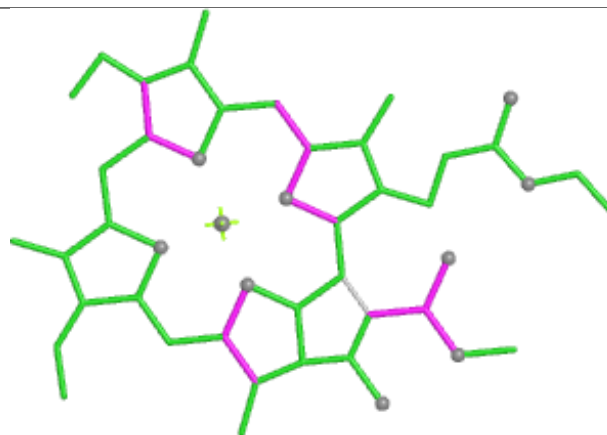
Rings



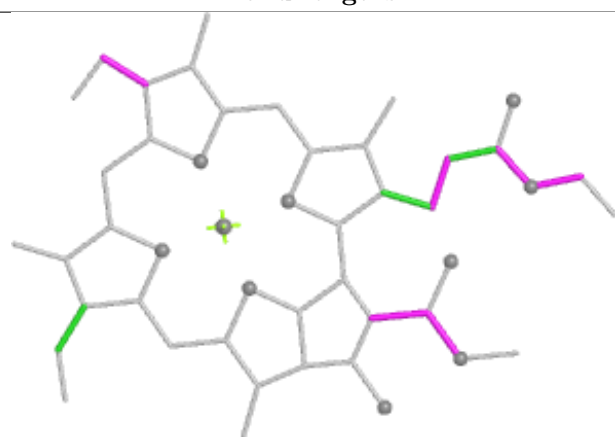
Ligand CLA X 316



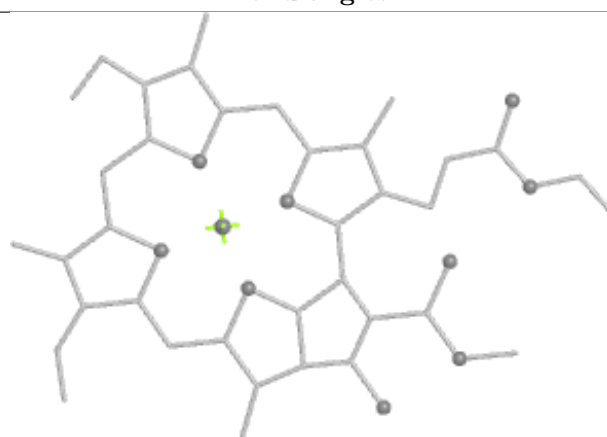
Bond lengths



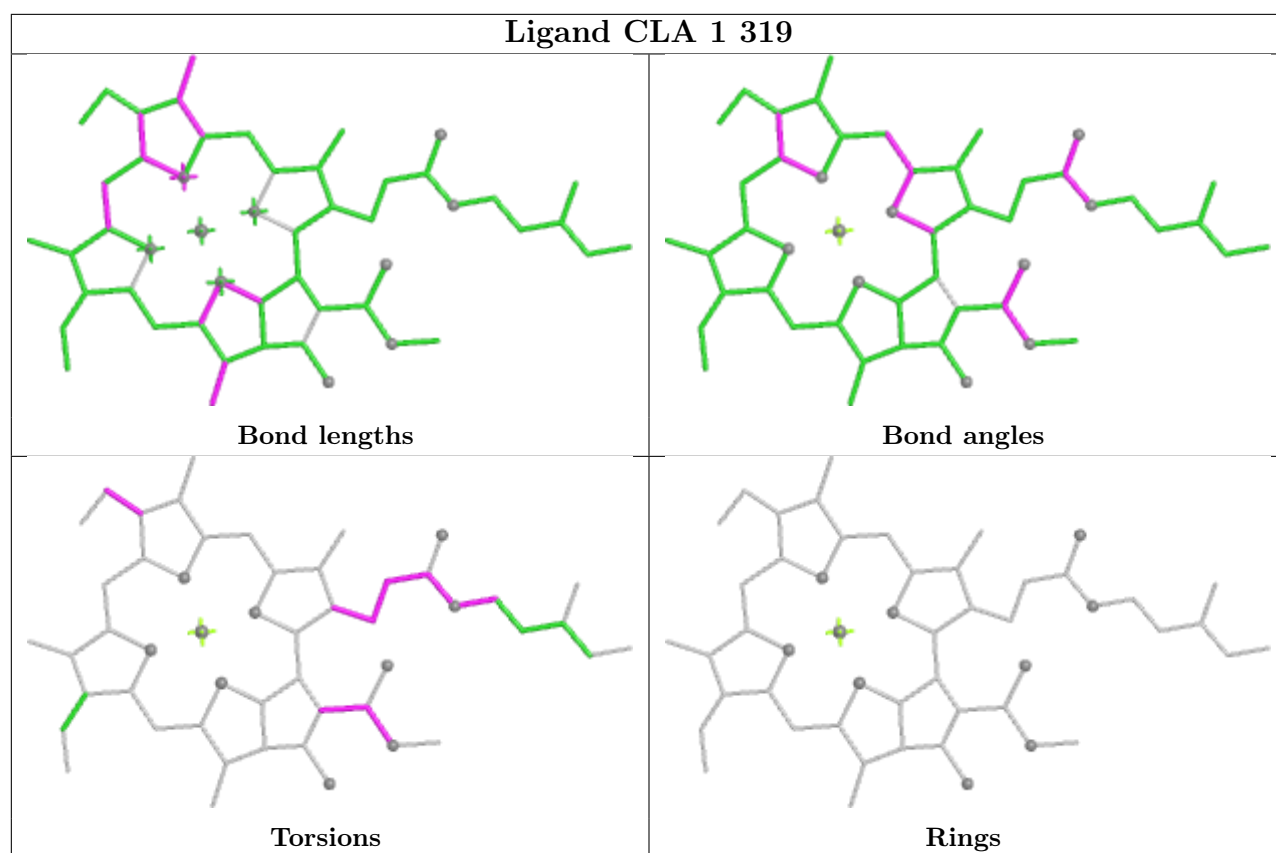
Bond angles



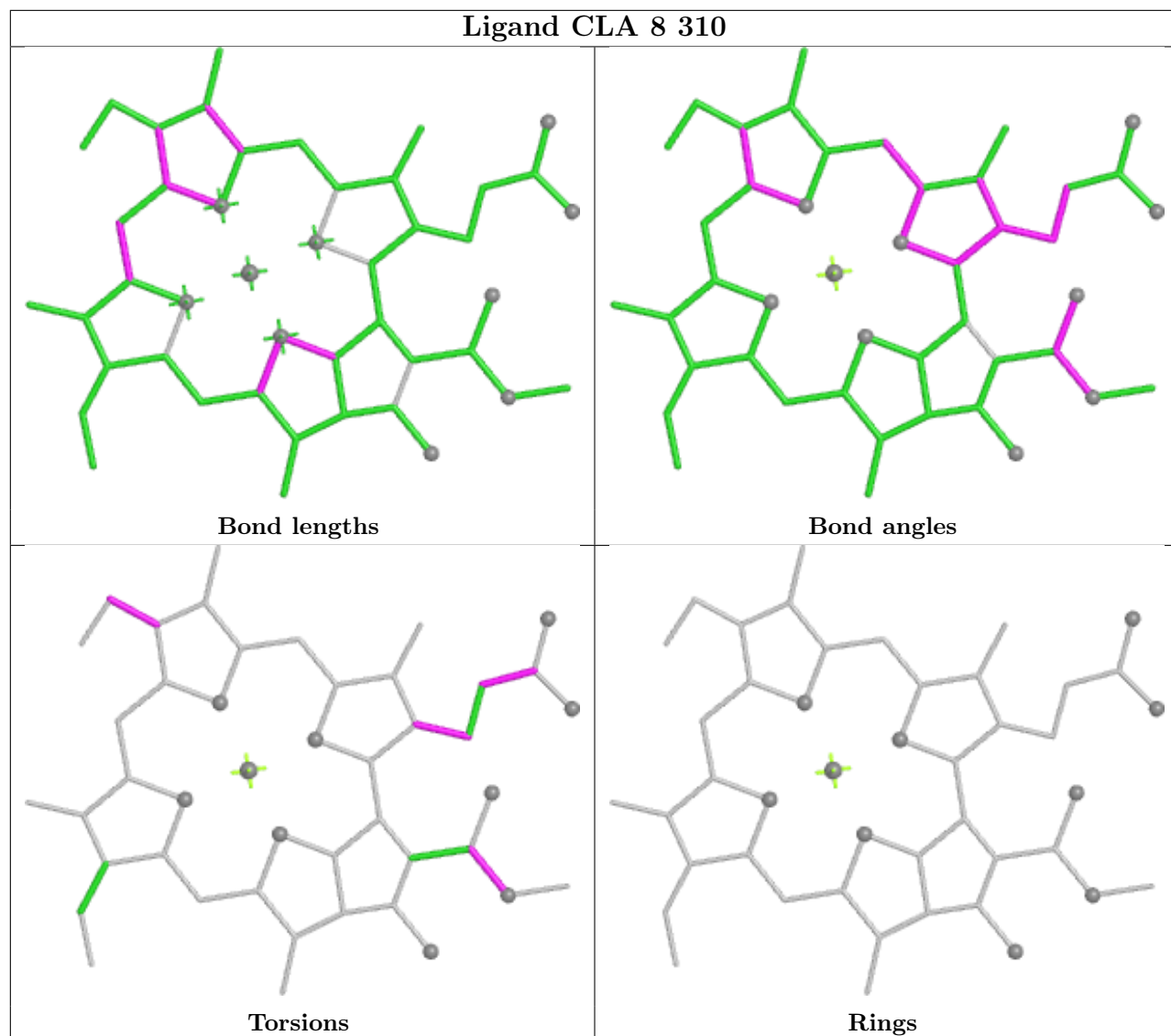
Torsions



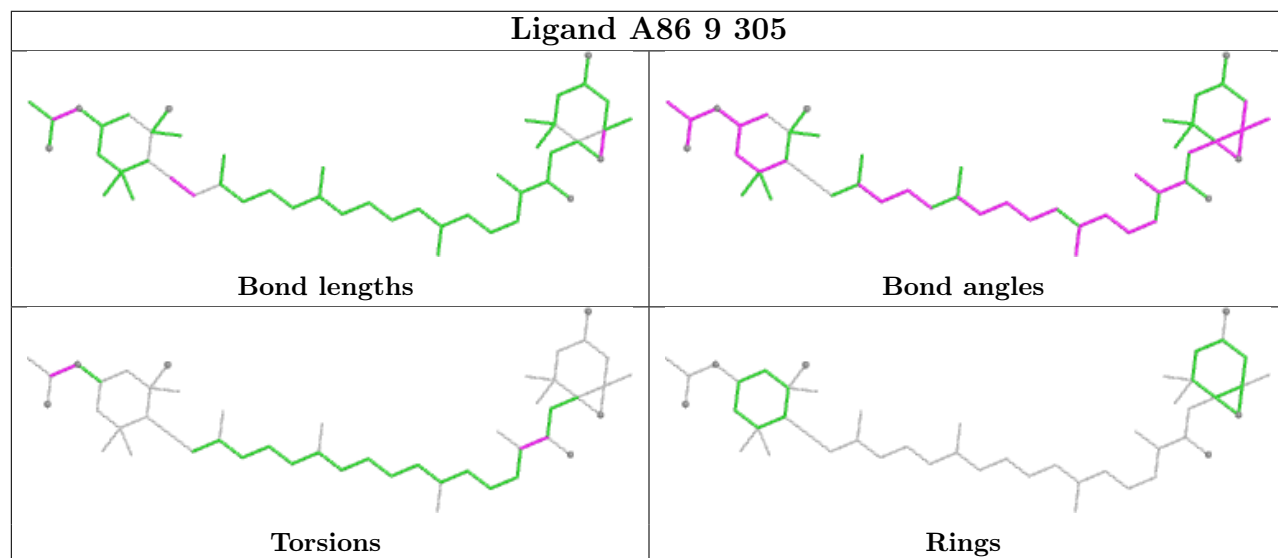
Rings

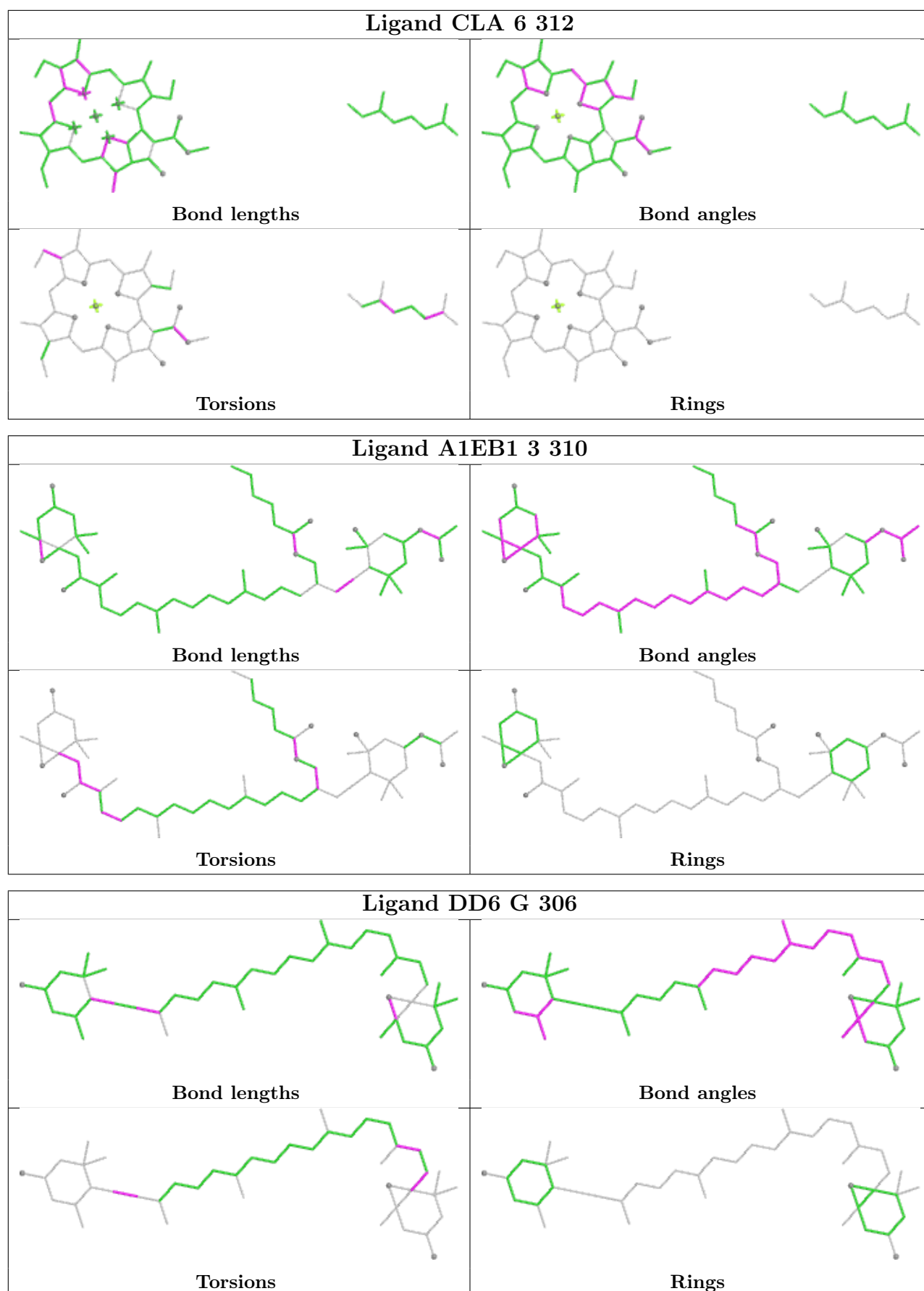


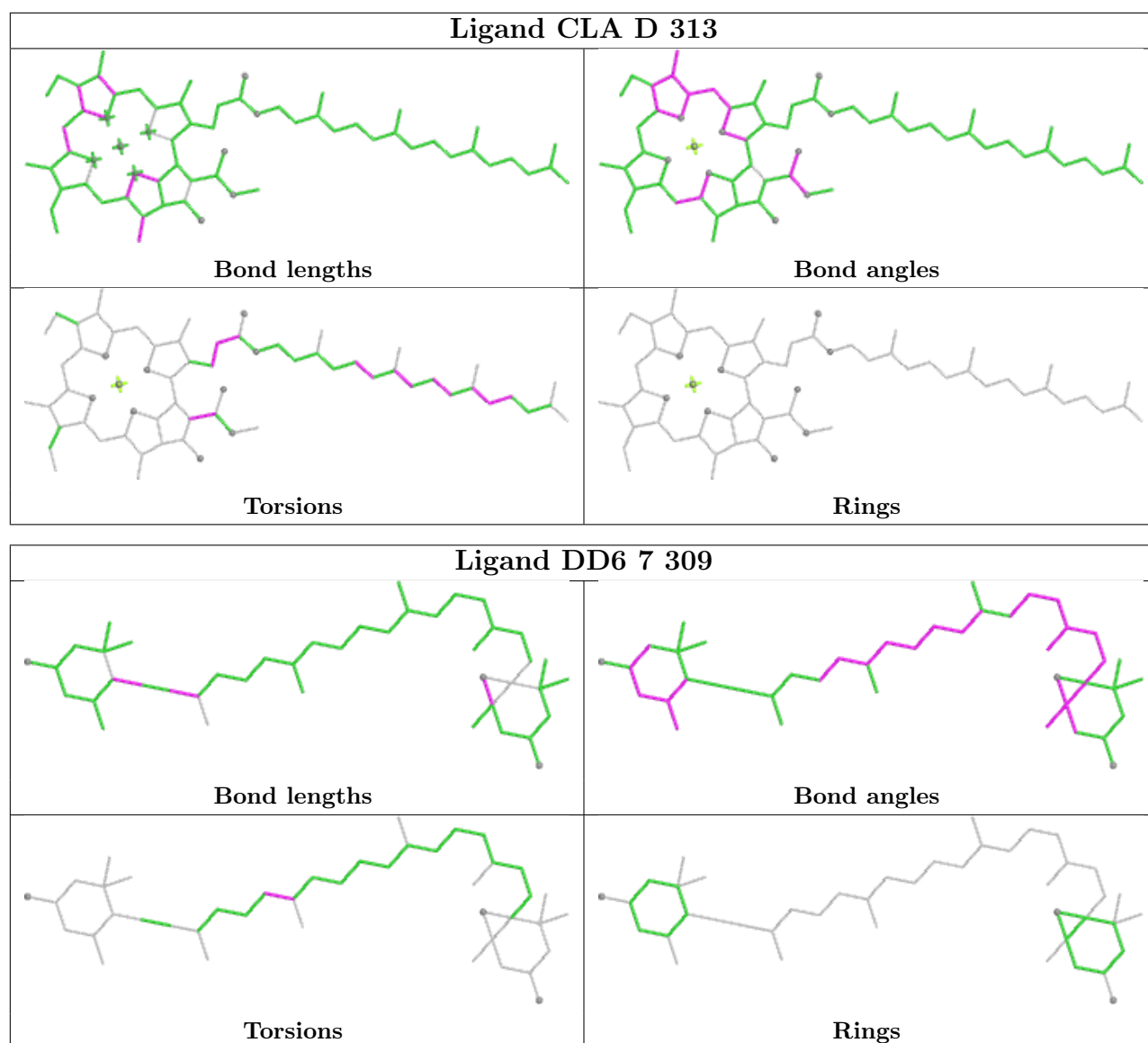
Ligand CLA 8 310

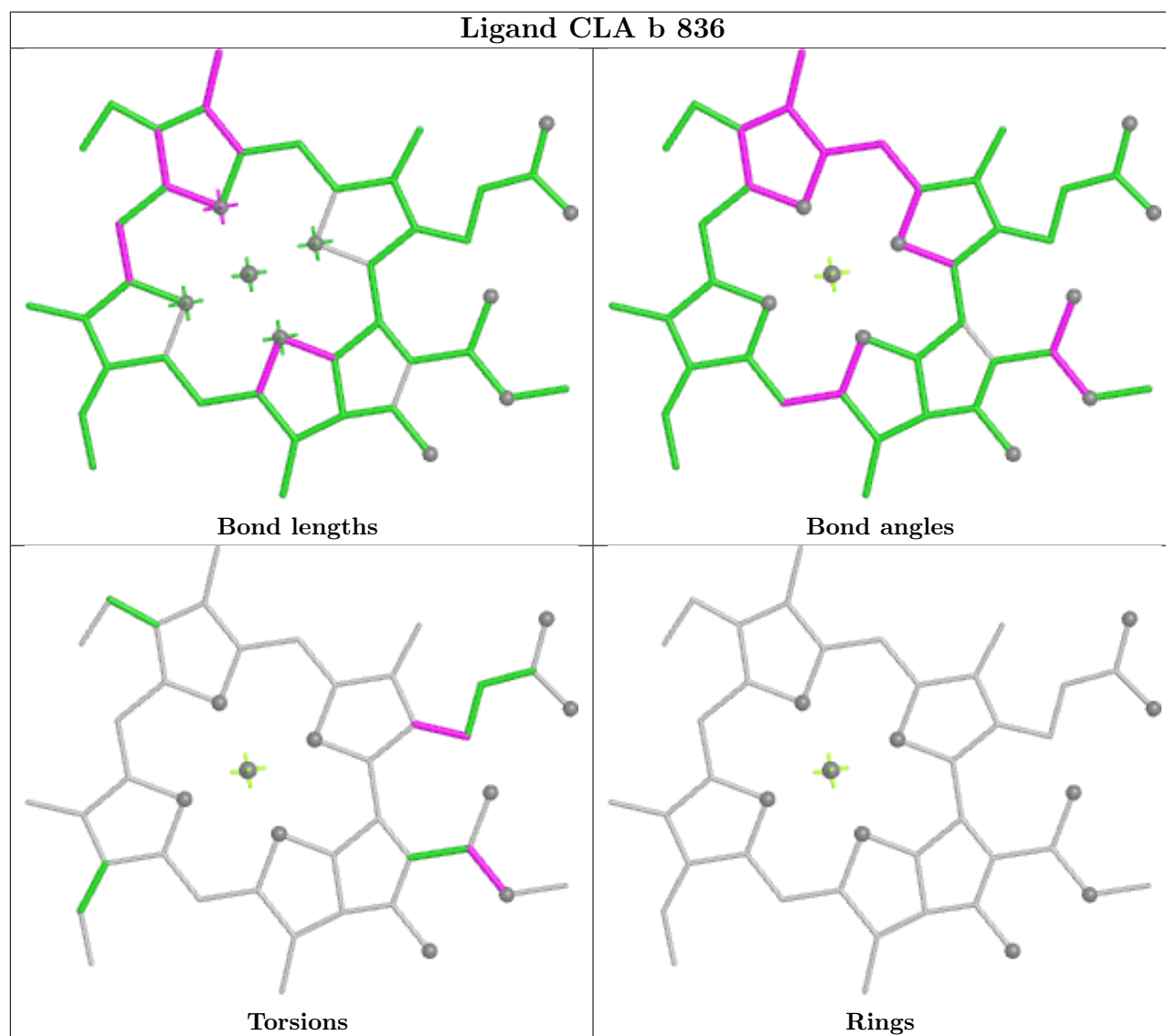
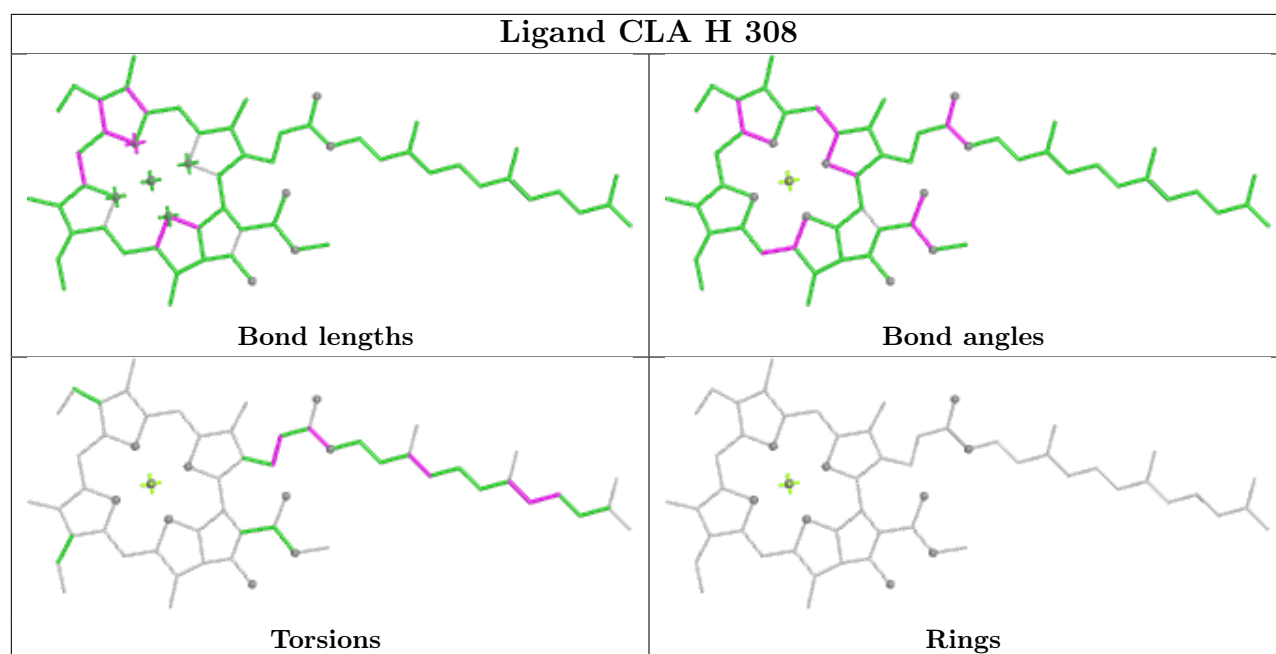


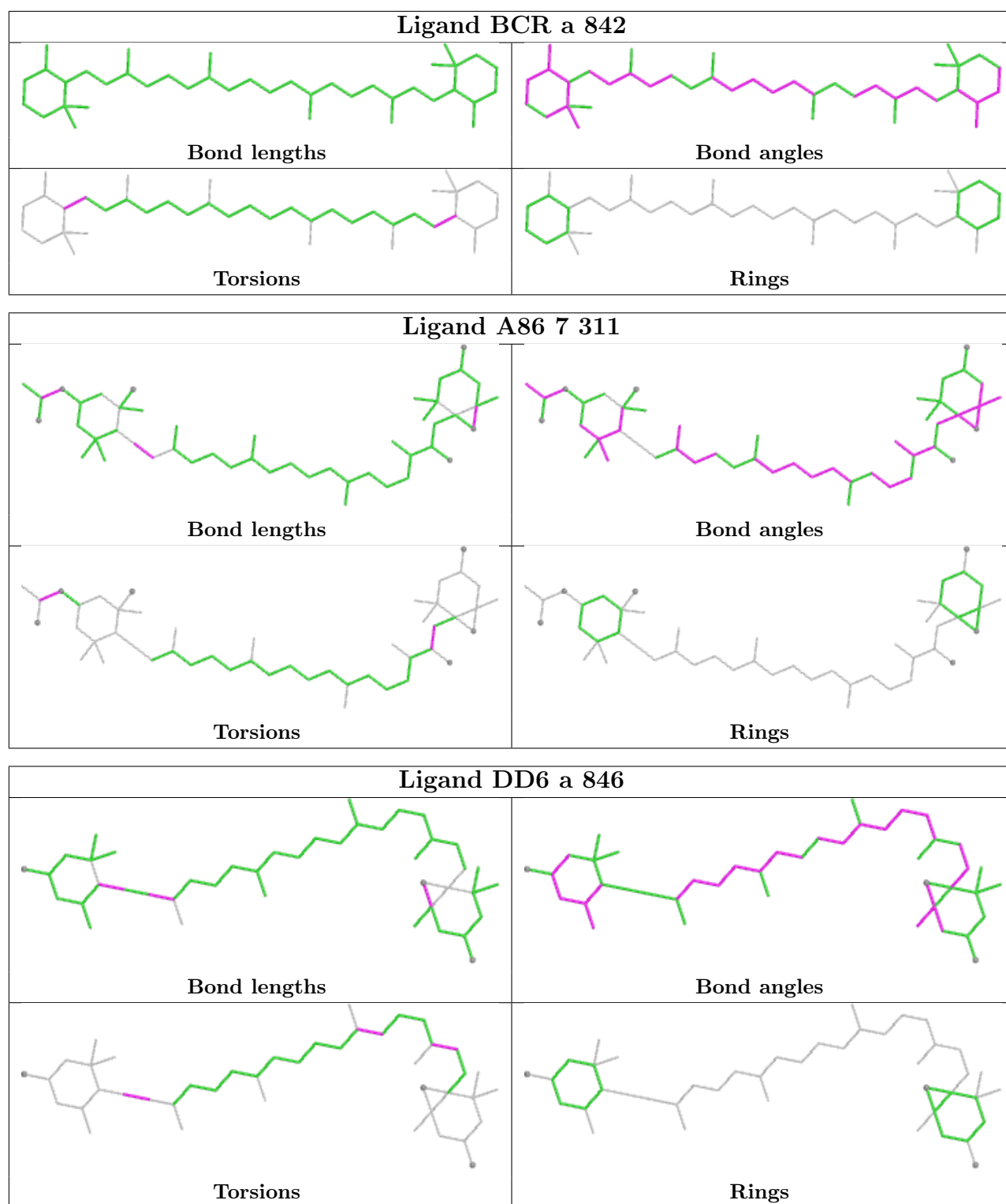
Ligand A86 9 305

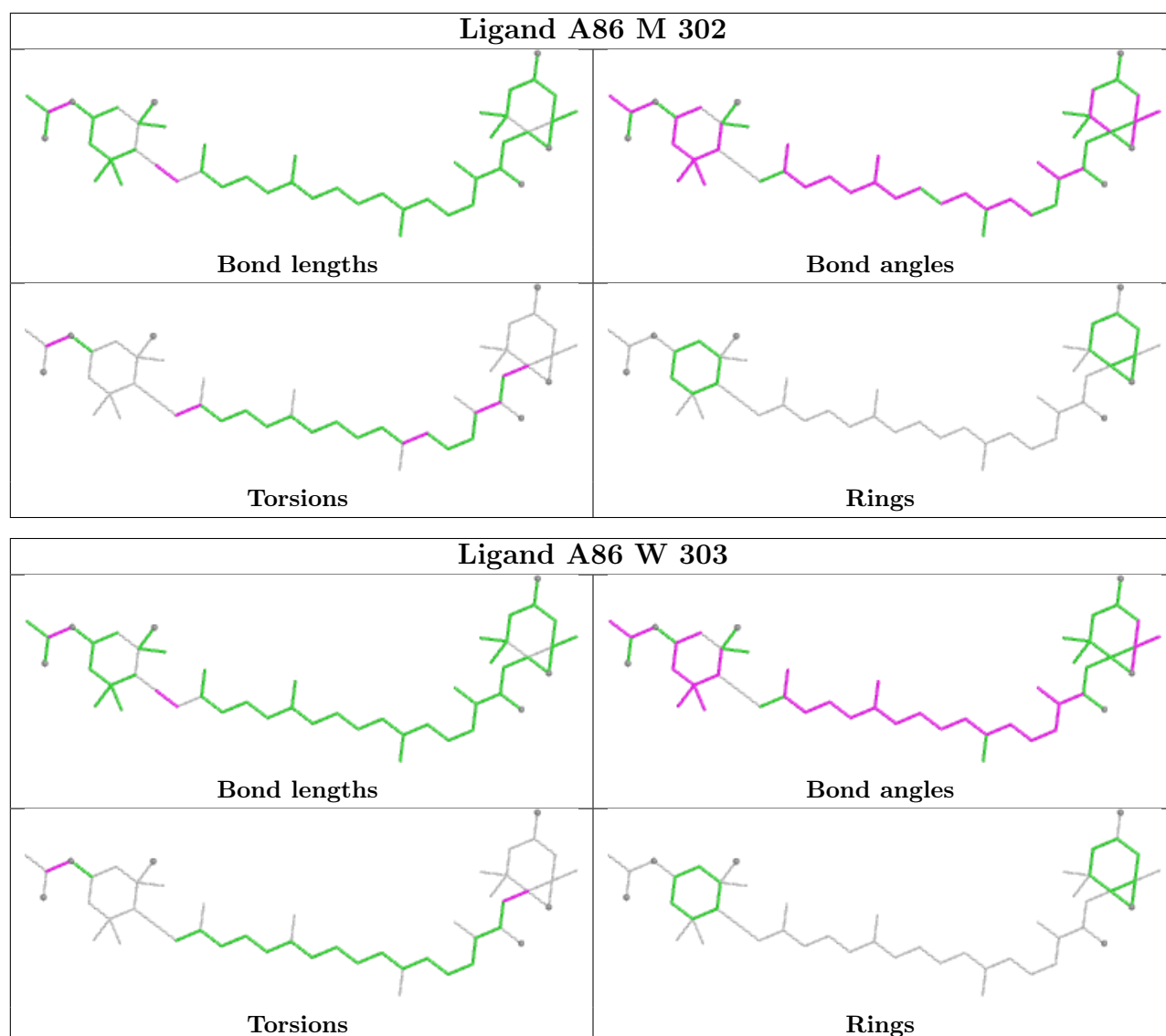




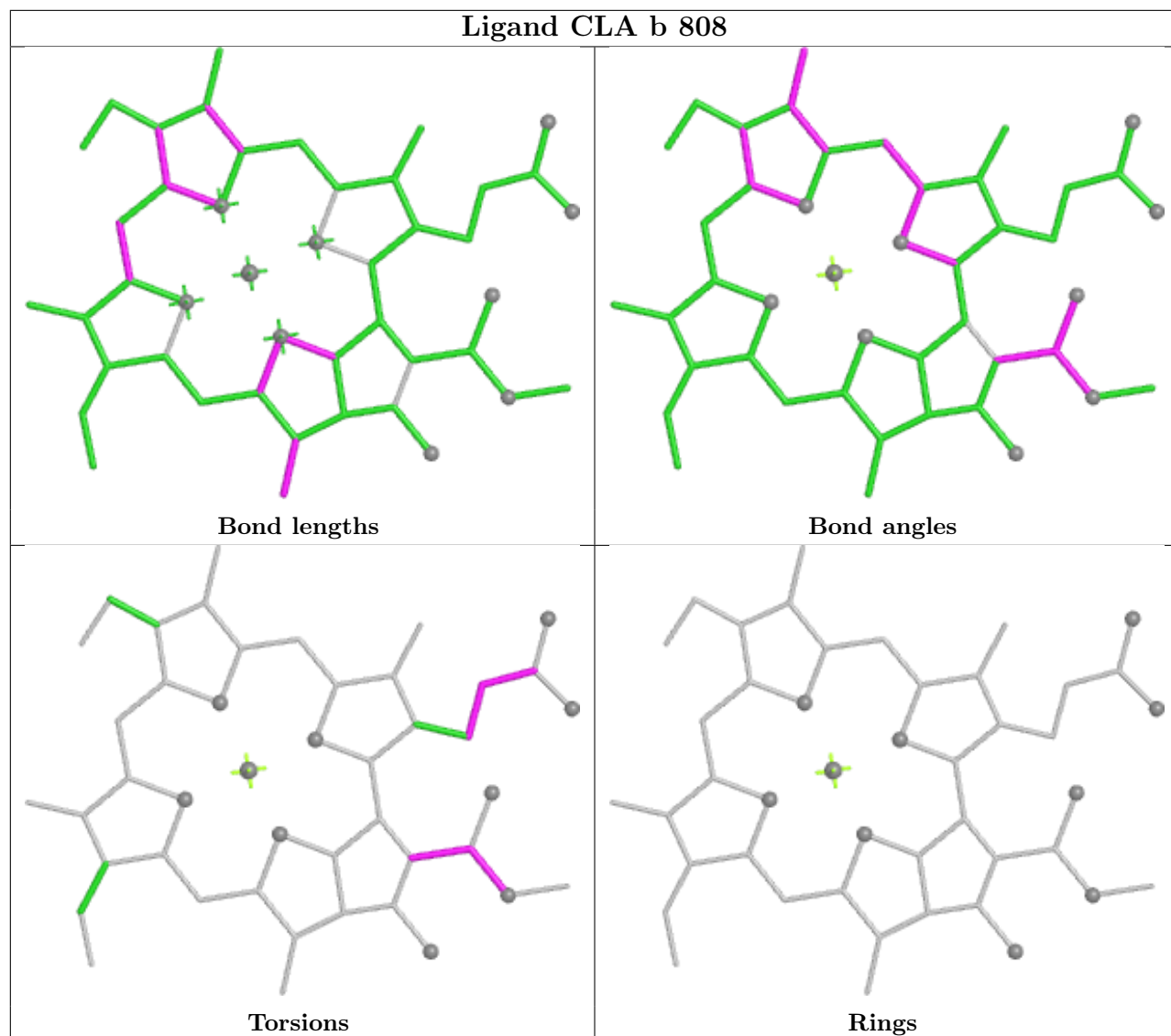




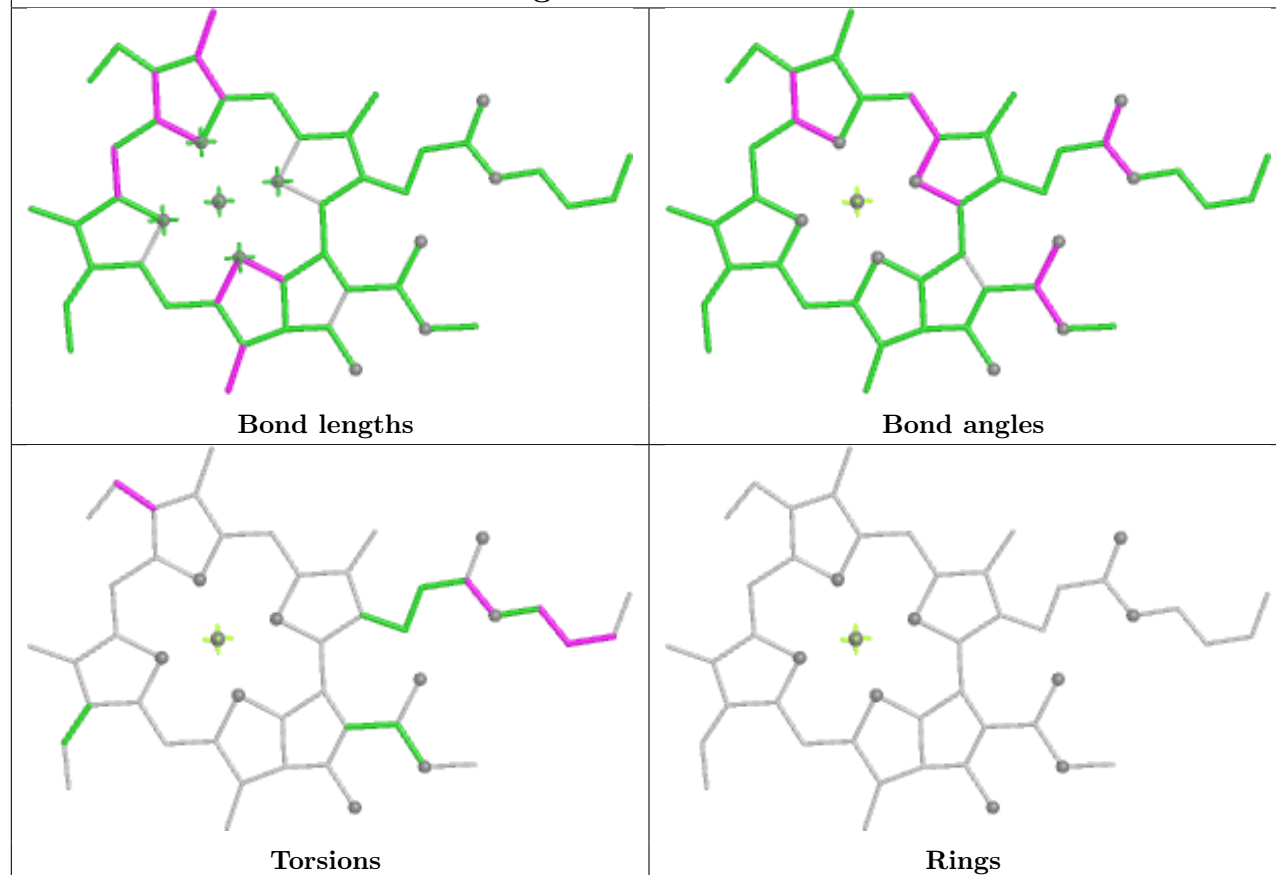




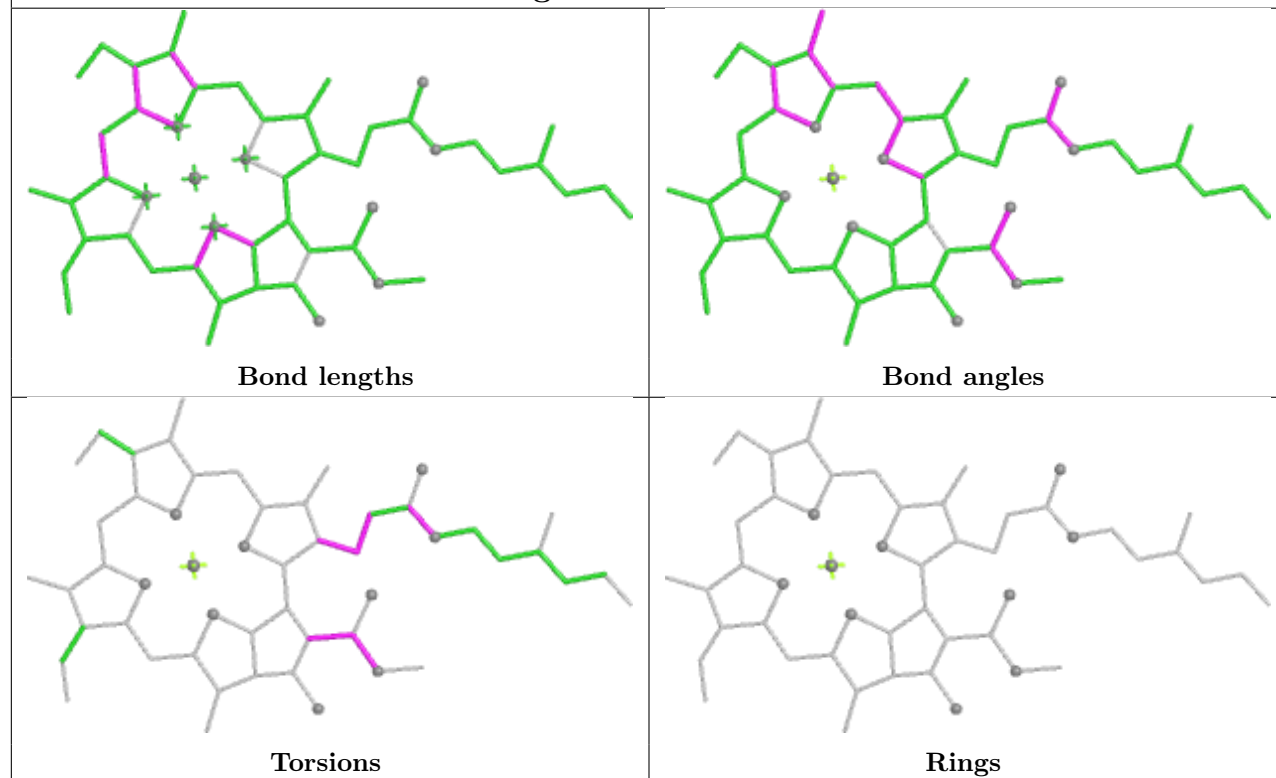
Ligand CLA b 808

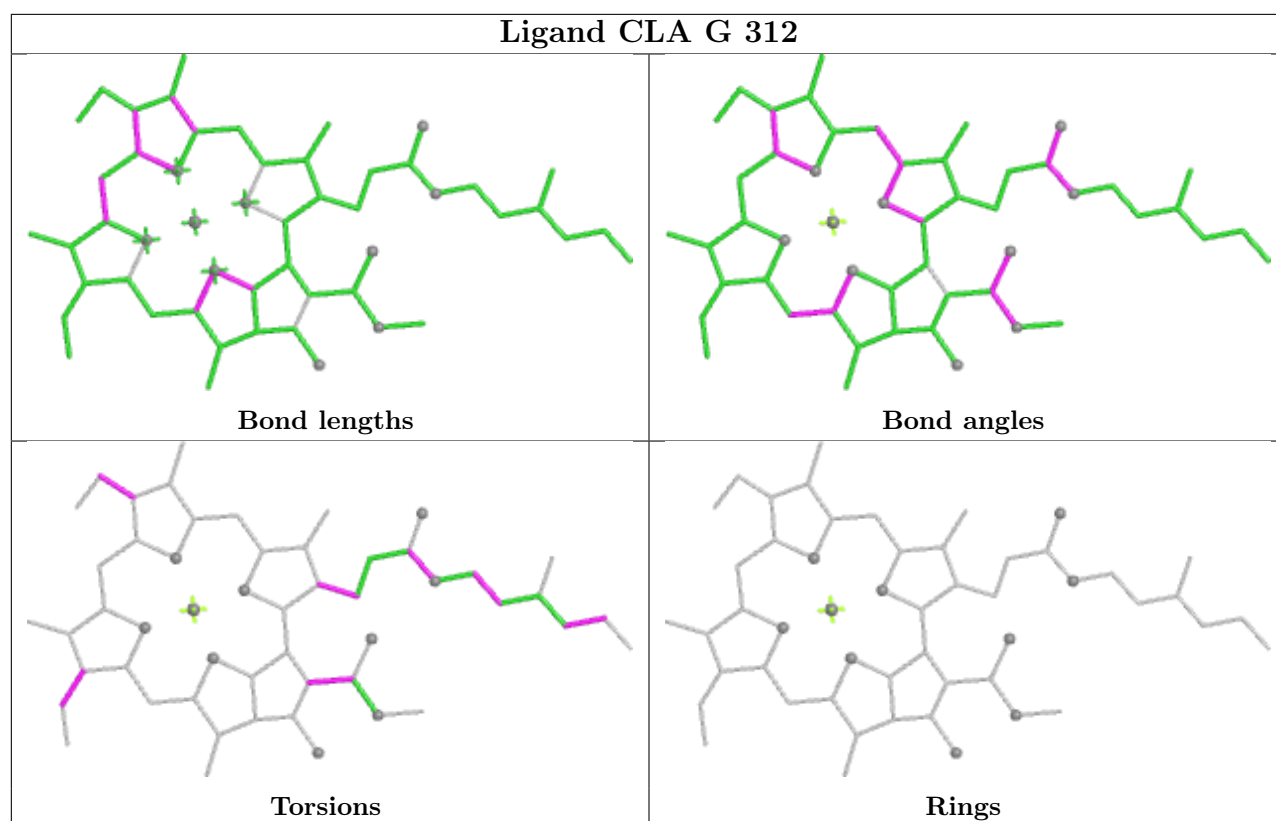


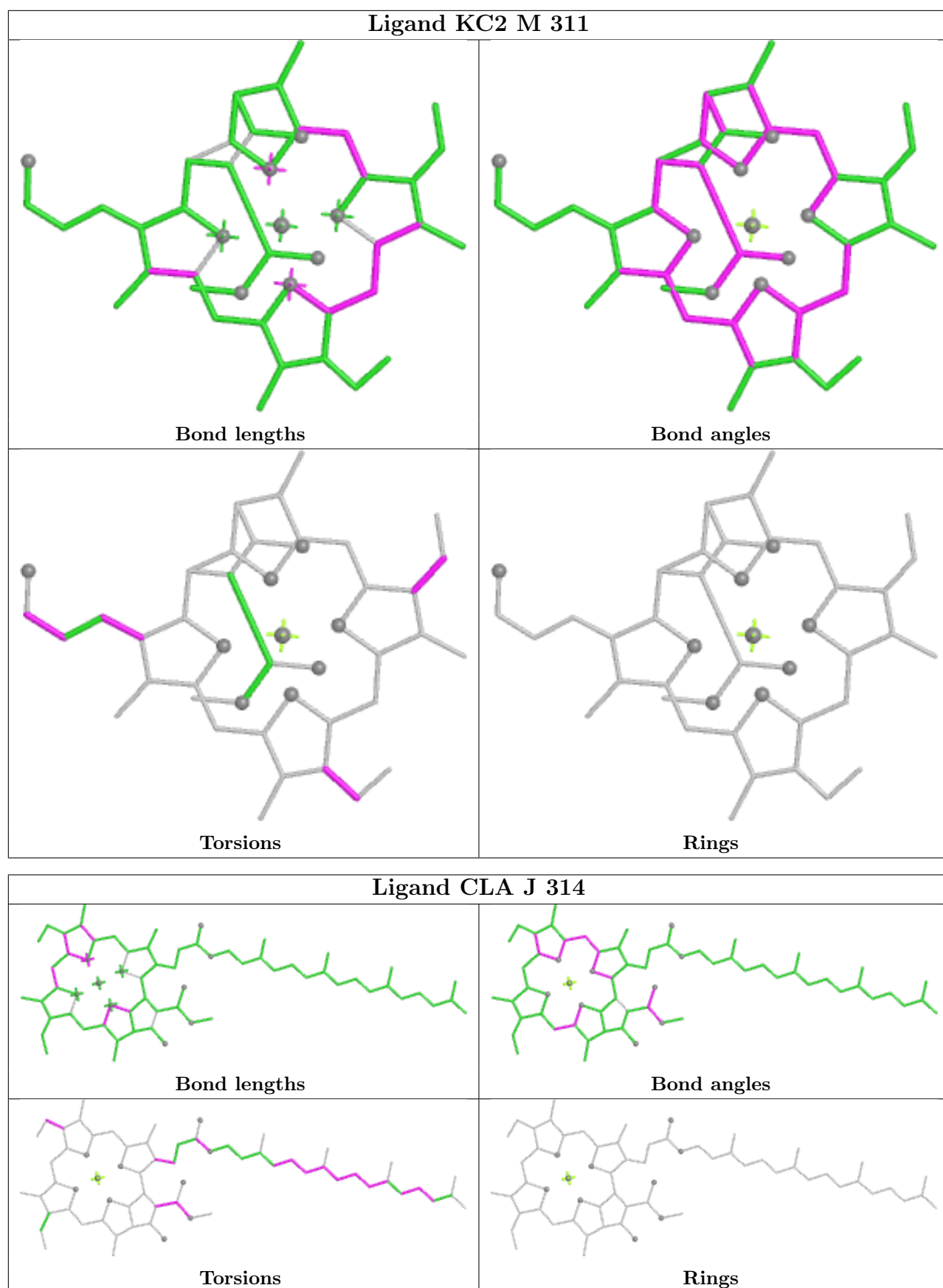
Ligand CLA E 306



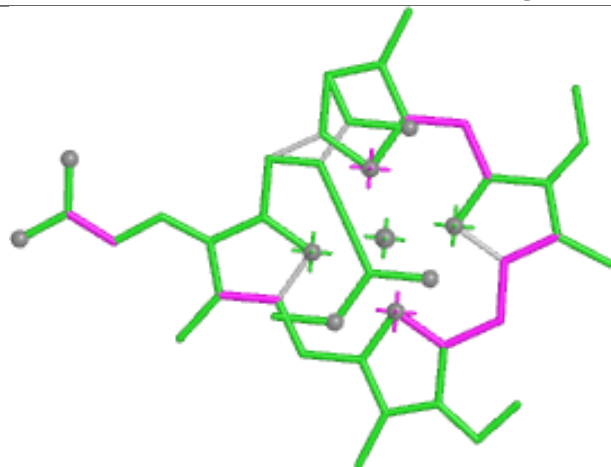
Ligand CLA E 317



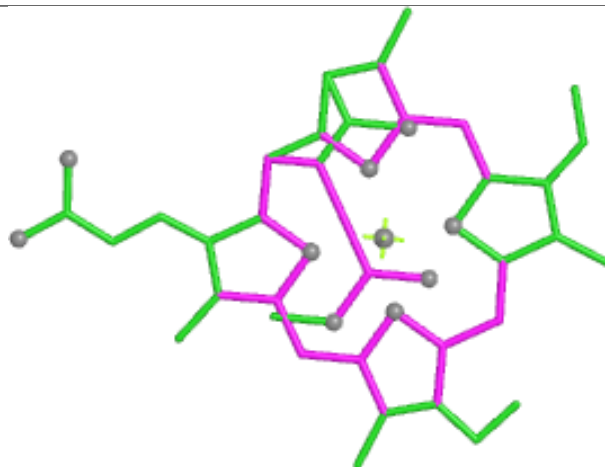




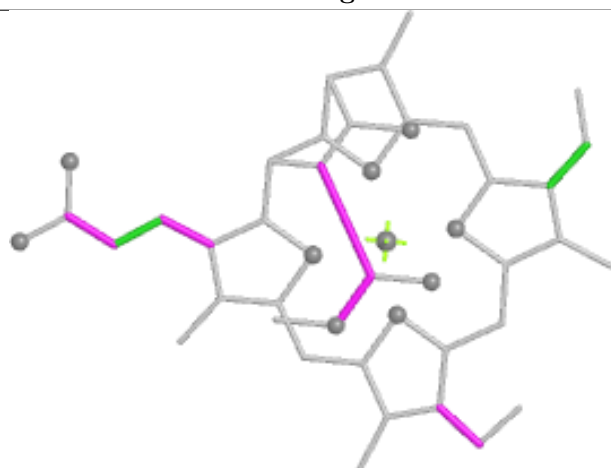
Ligand KC2 L 315



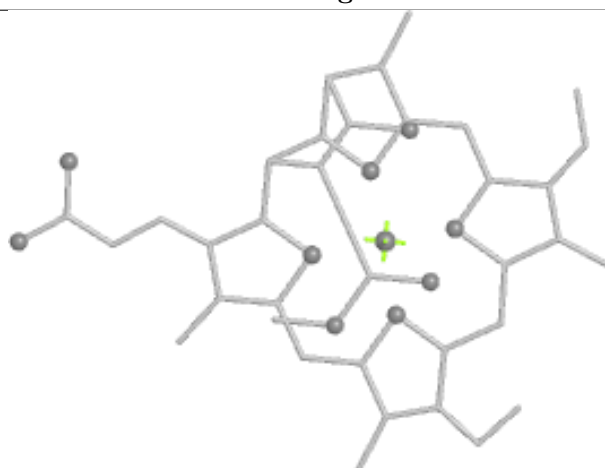
Bond lengths



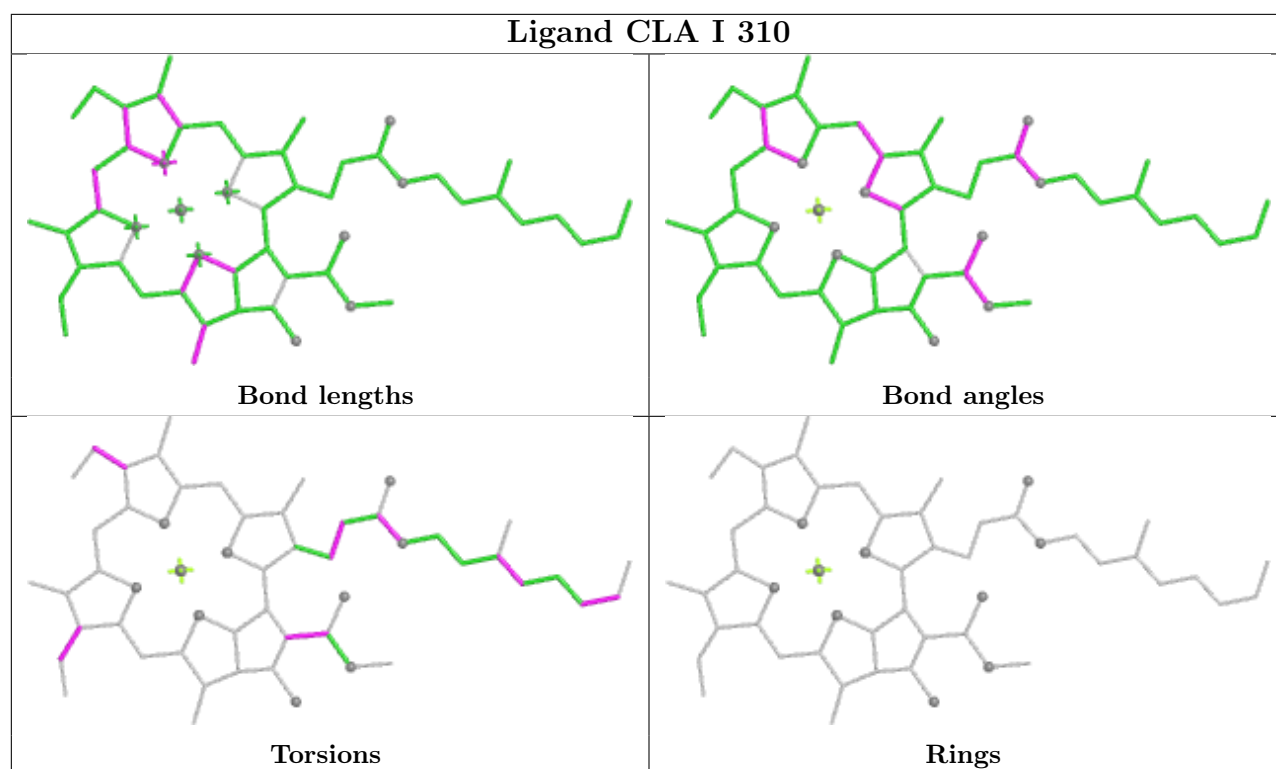
Bond angles



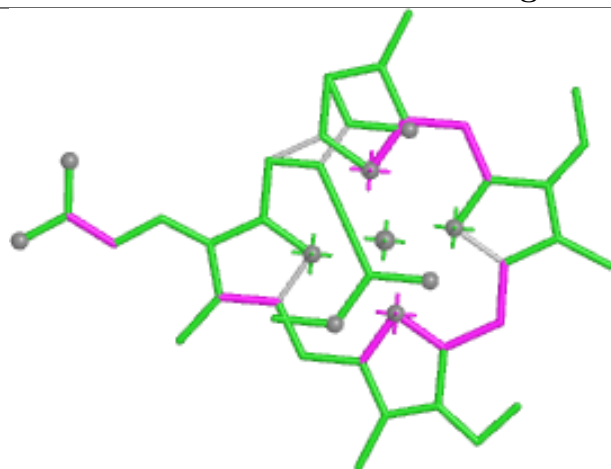
Torsions



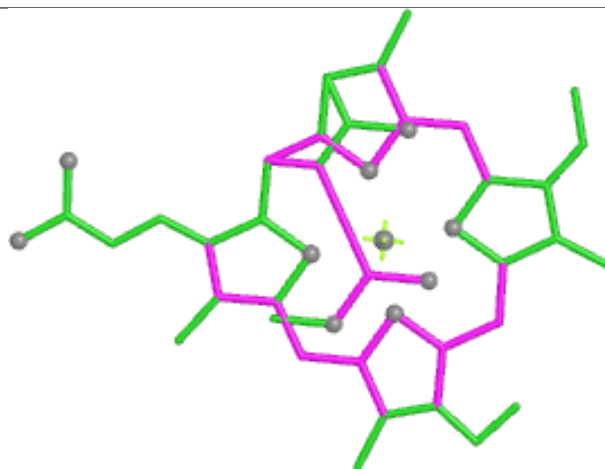
Rings



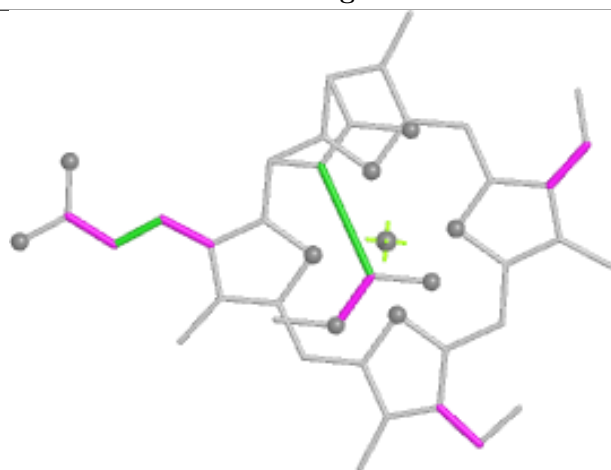
Ligand KC2 0 319



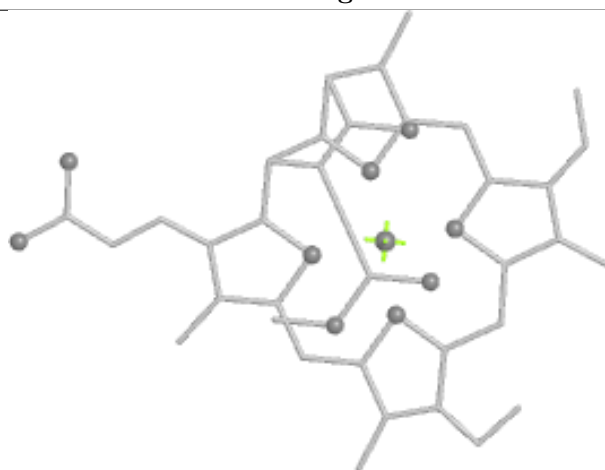
Bond lengths



Bond angles

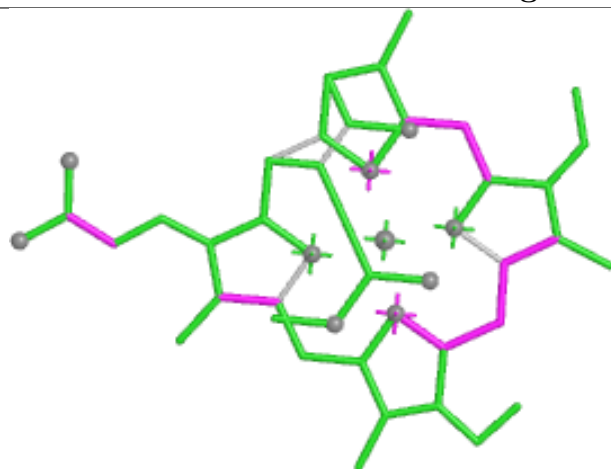


Torsions

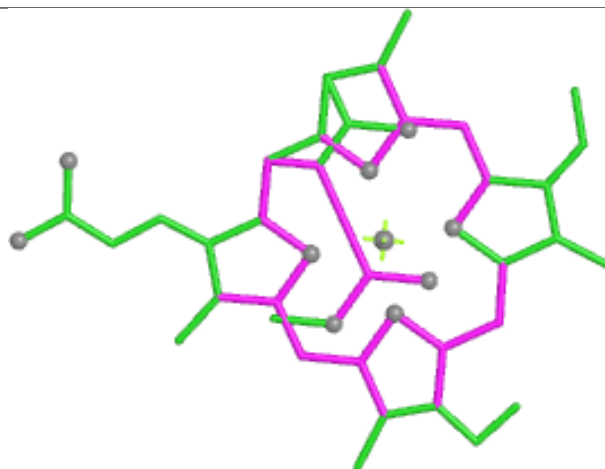


Rings

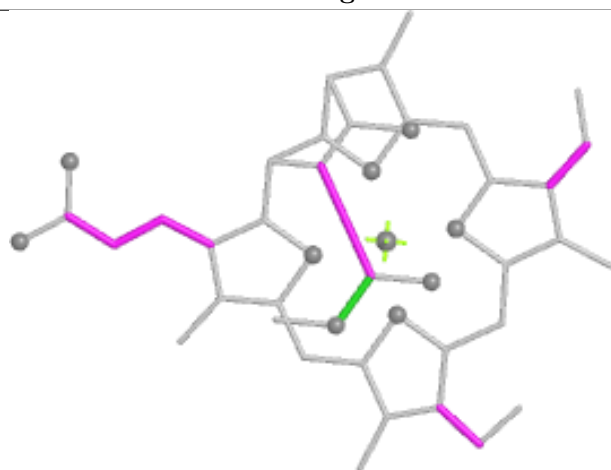
Ligand KC2 4 318



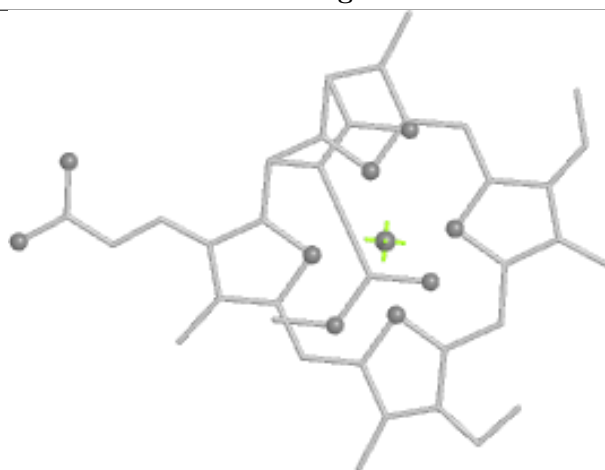
Bond lengths



Bond angles

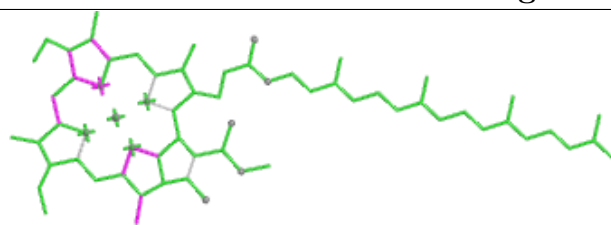


Torsions

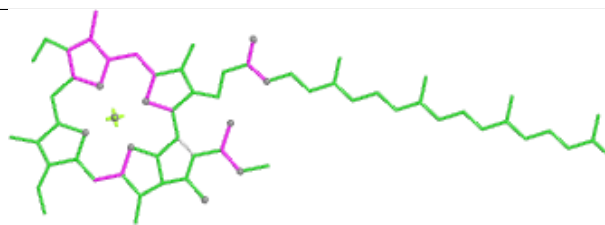


Rings

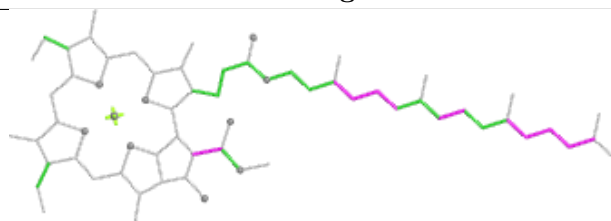
Ligand CLA a 805



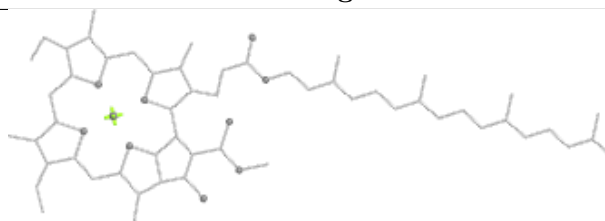
Bond lengths



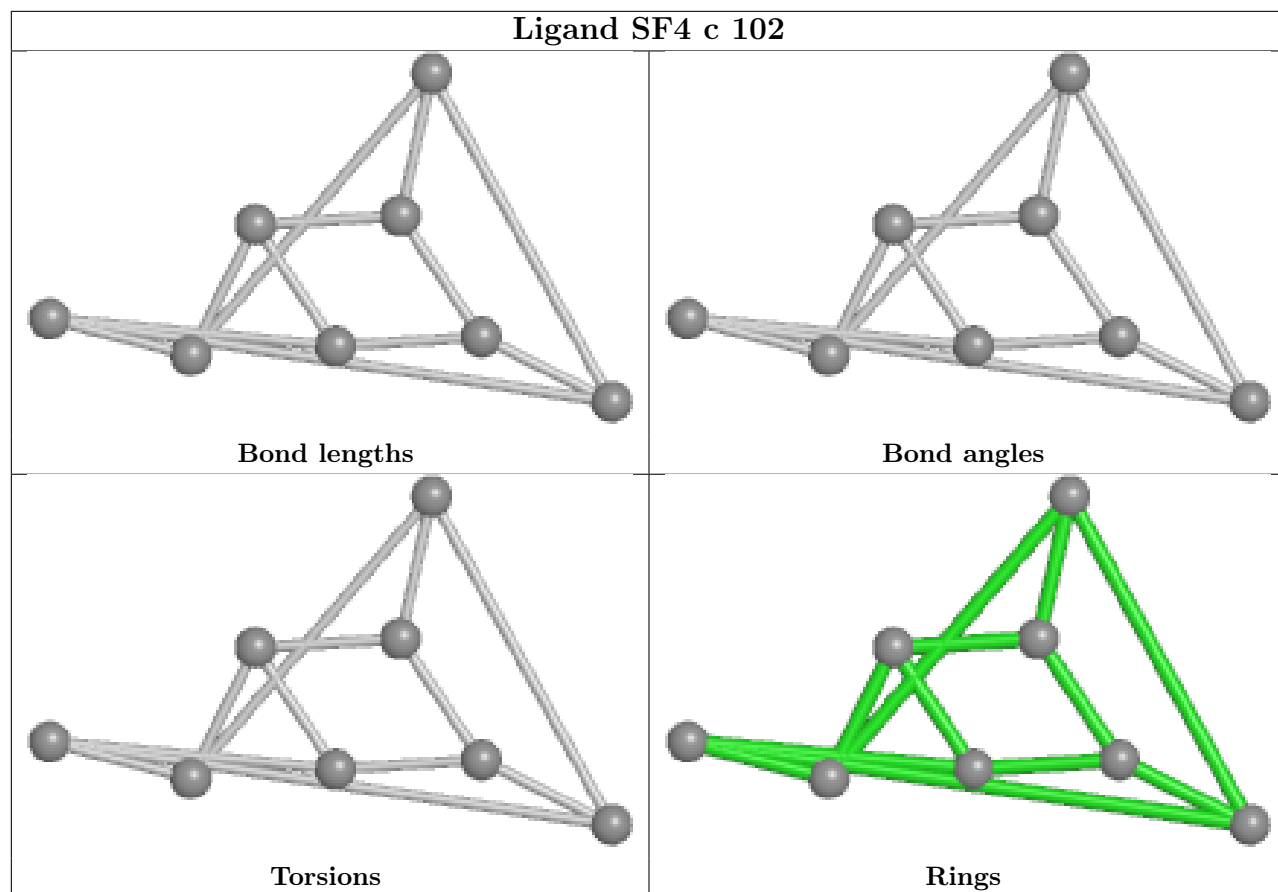
Bond angles



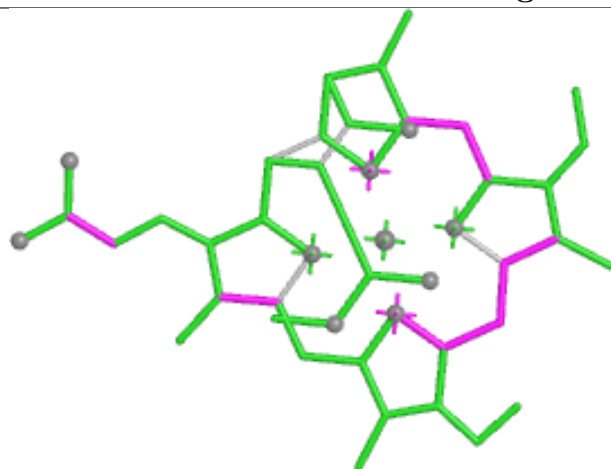
Torsions



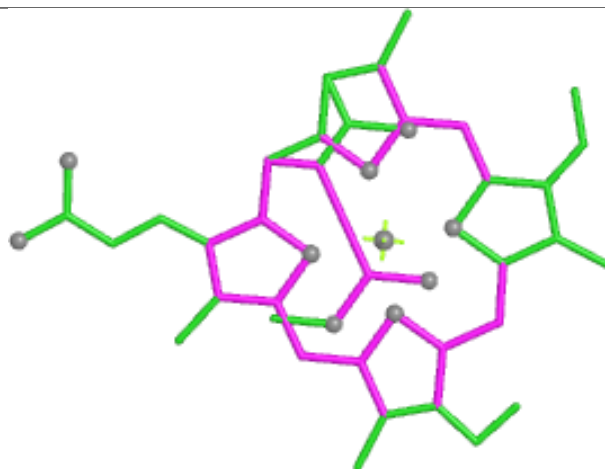
Rings



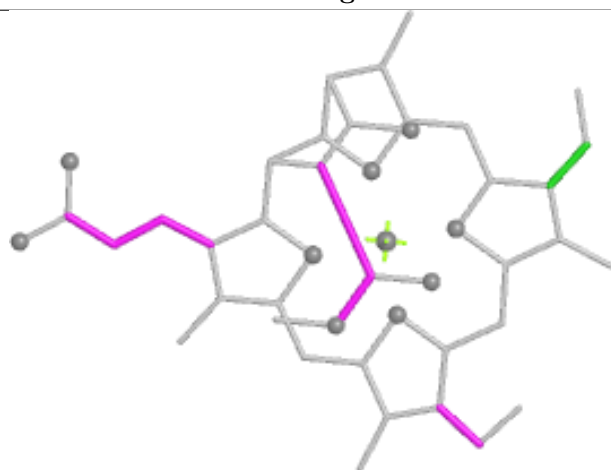
Ligand KC2 T 312



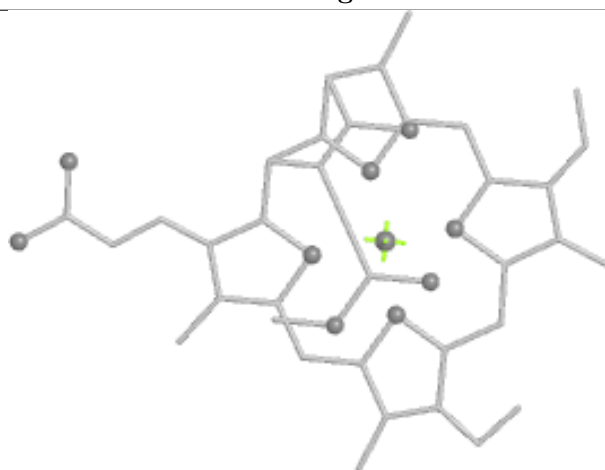
Bond lengths



Bond angles

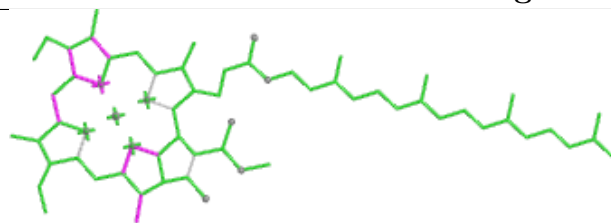


Torsions

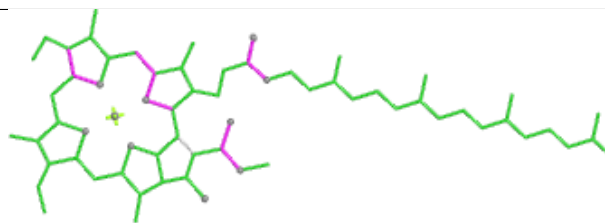


Rings

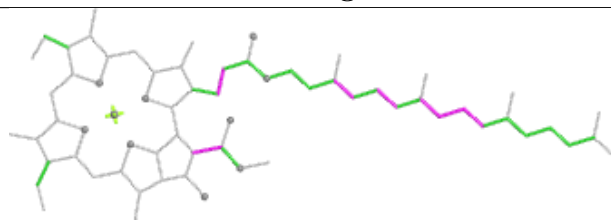
Ligand CLA C 306



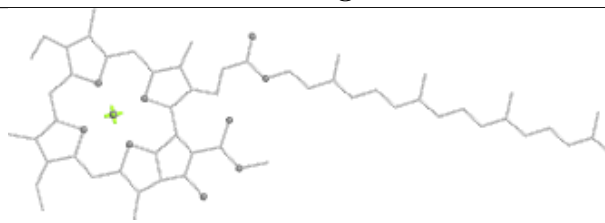
Bond lengths



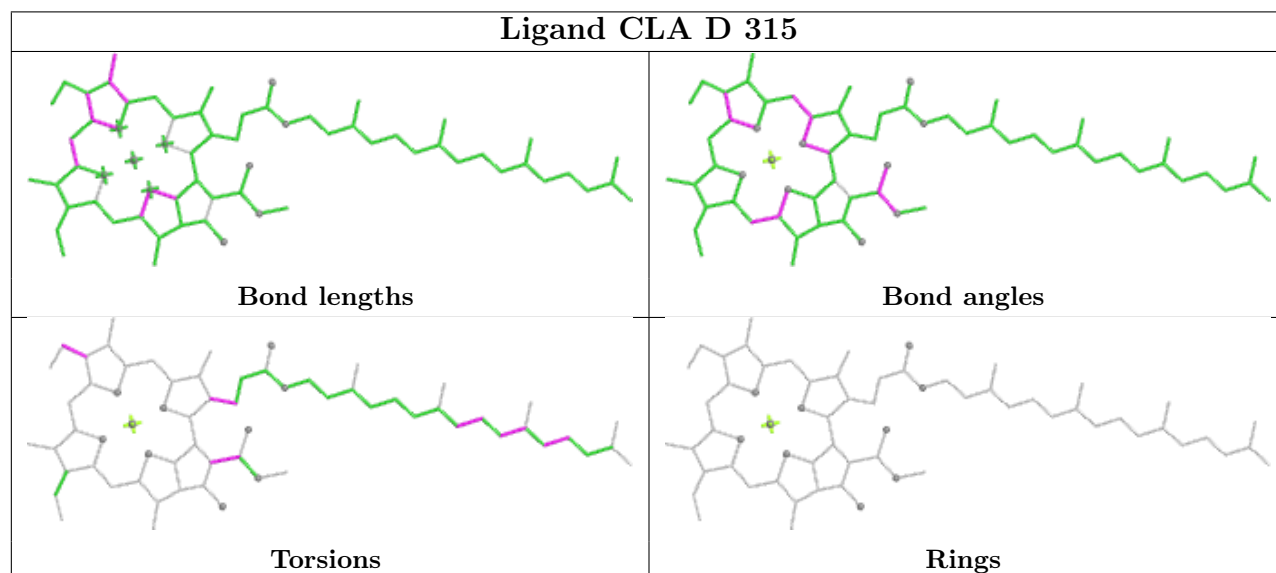
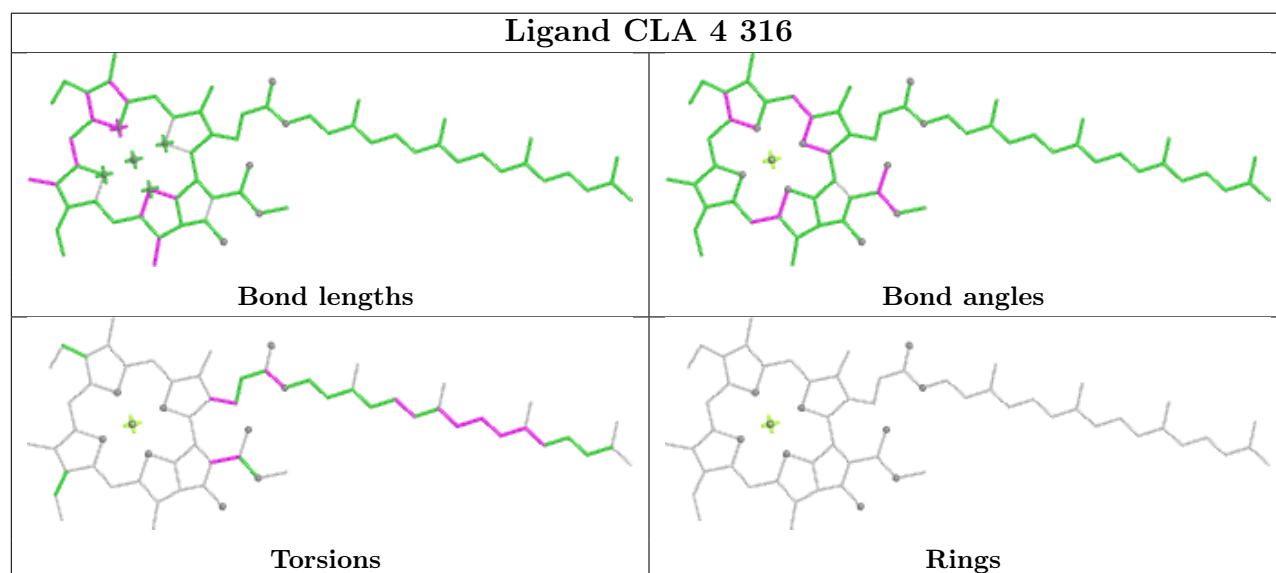
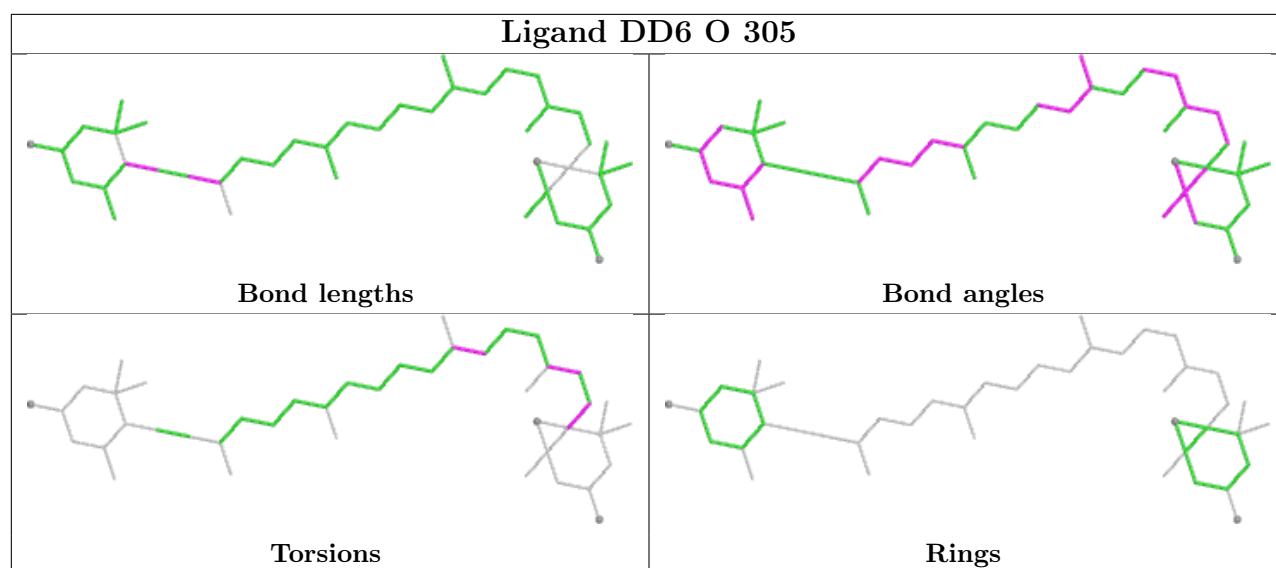
Bond angles



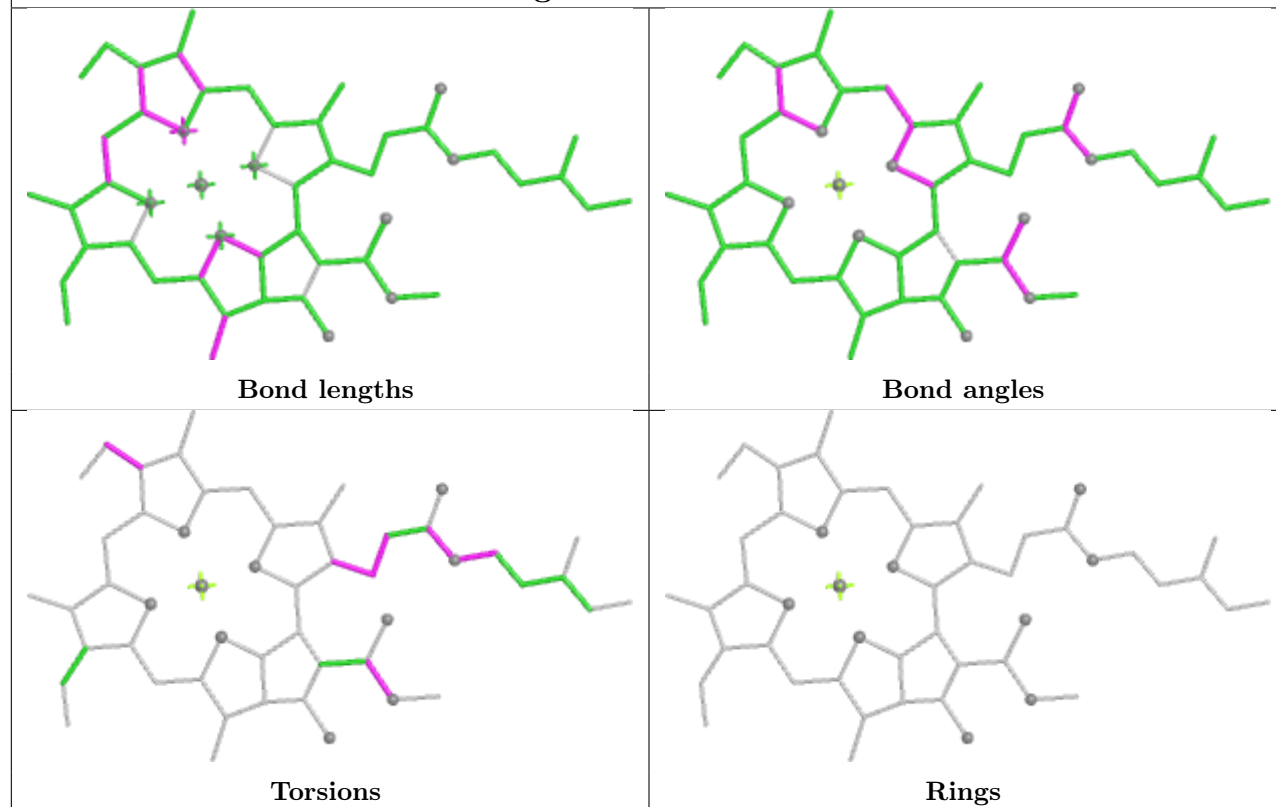
Torsions



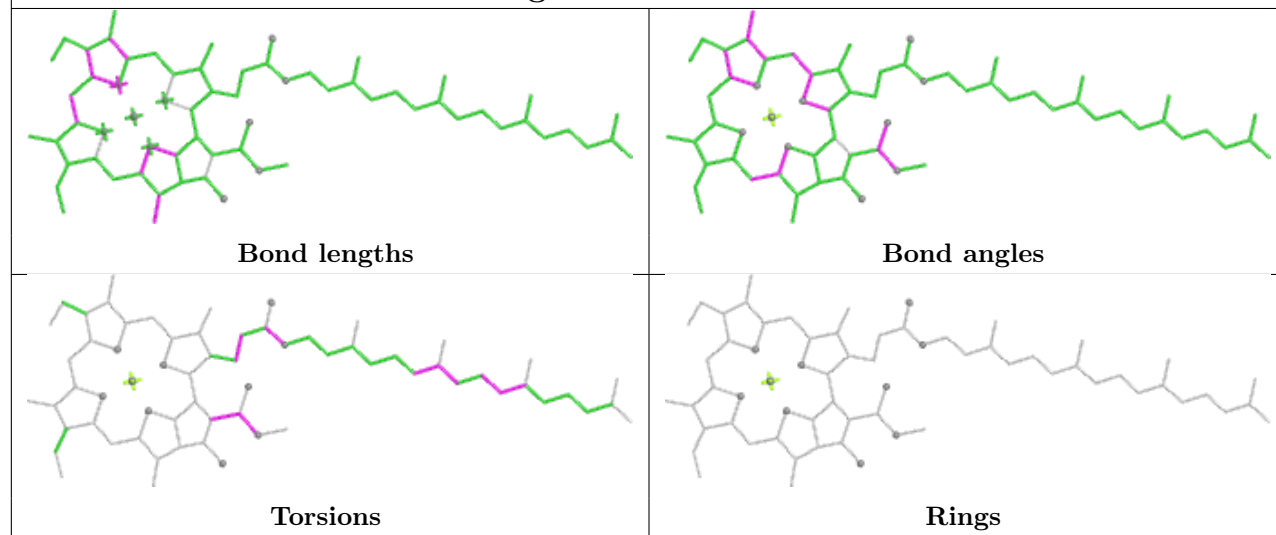
Rings

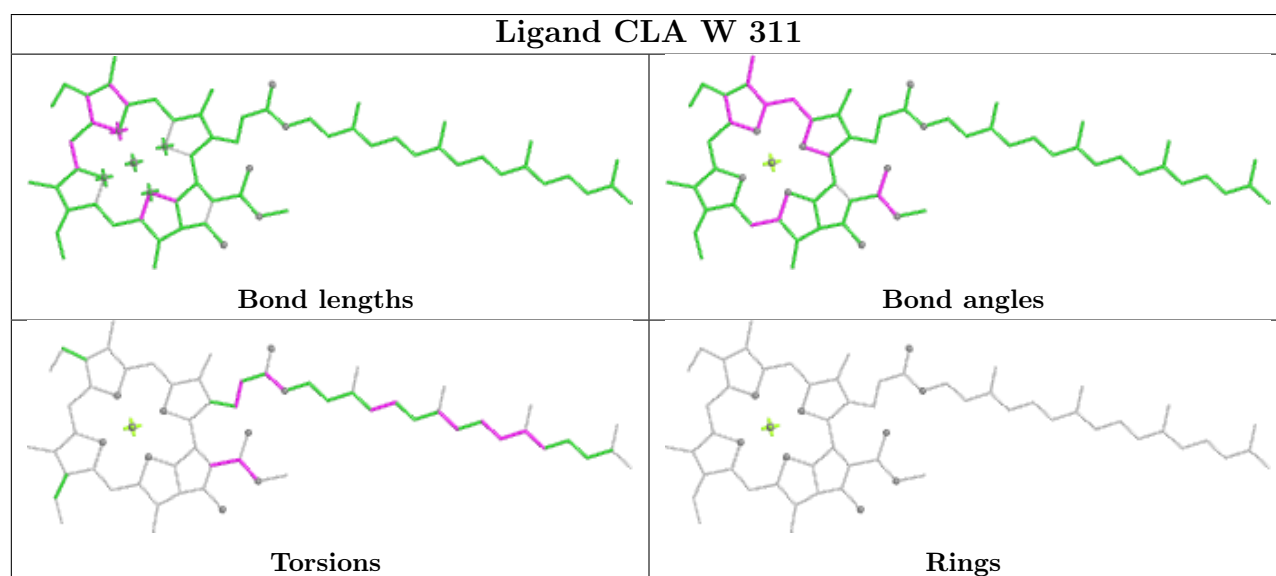
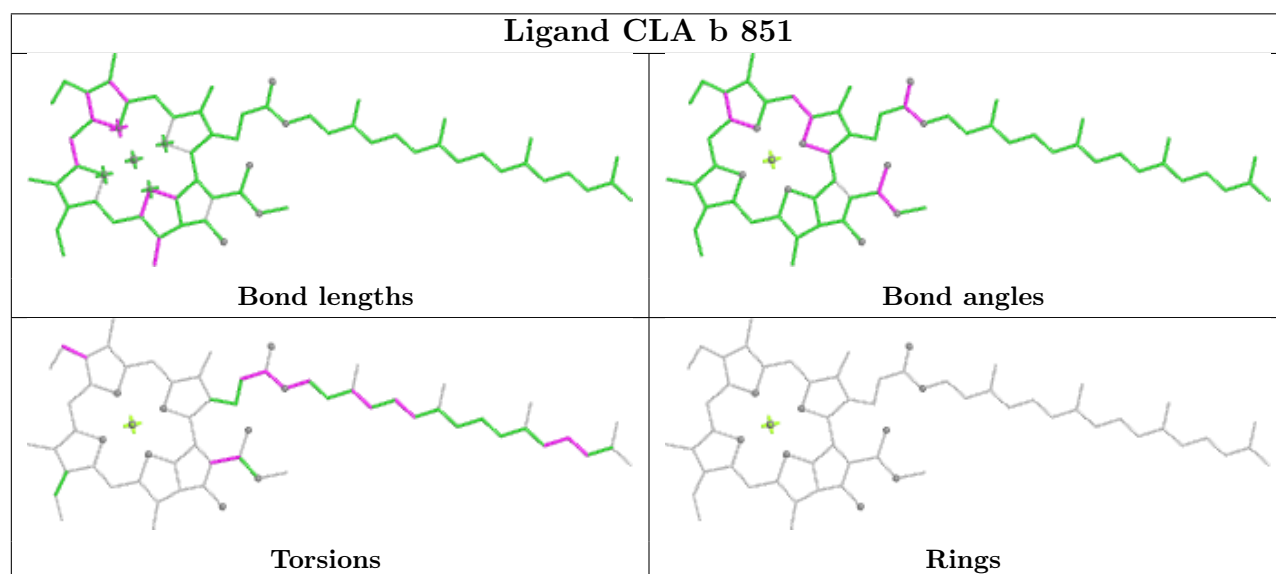
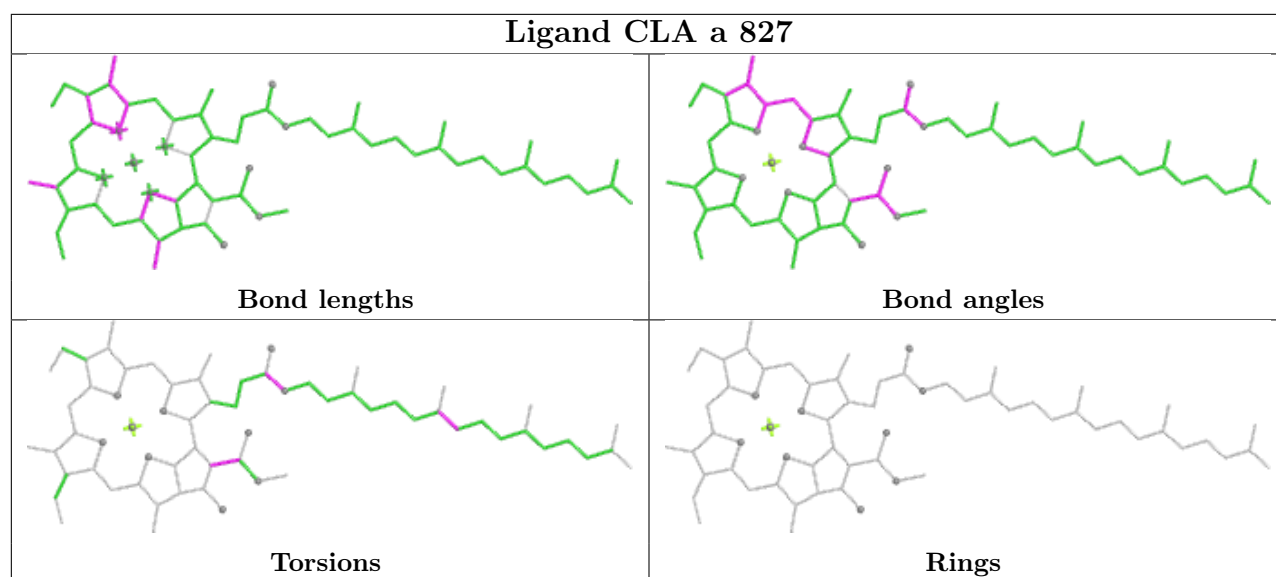


Ligand CLA F 316

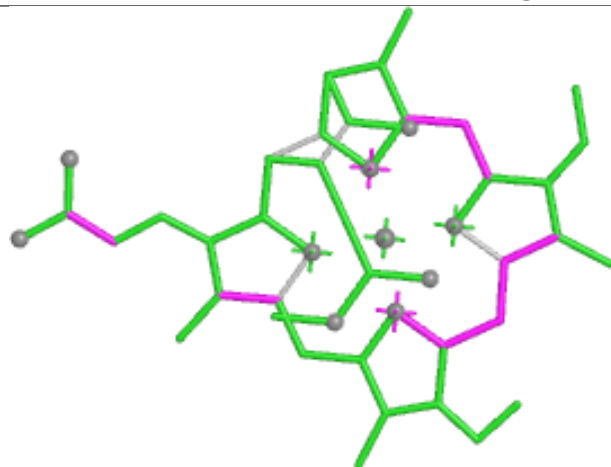


Ligand CLA M 310





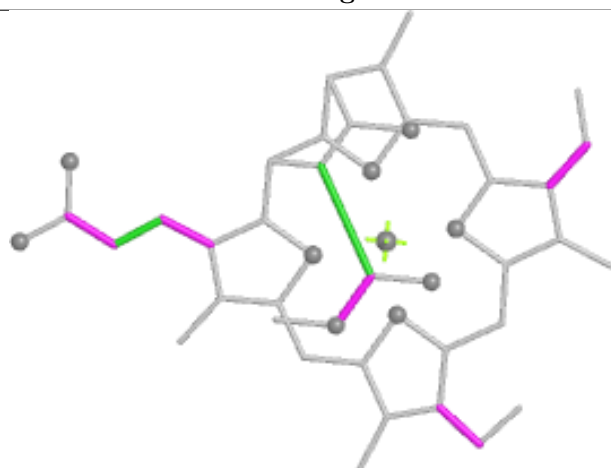
Ligand KC2 F 307



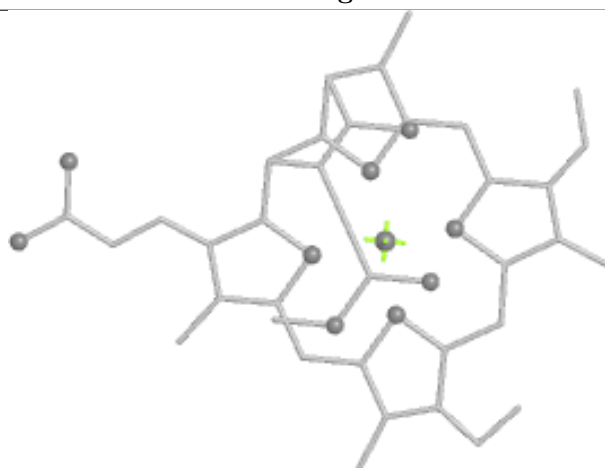
Bond lengths



Bond angles

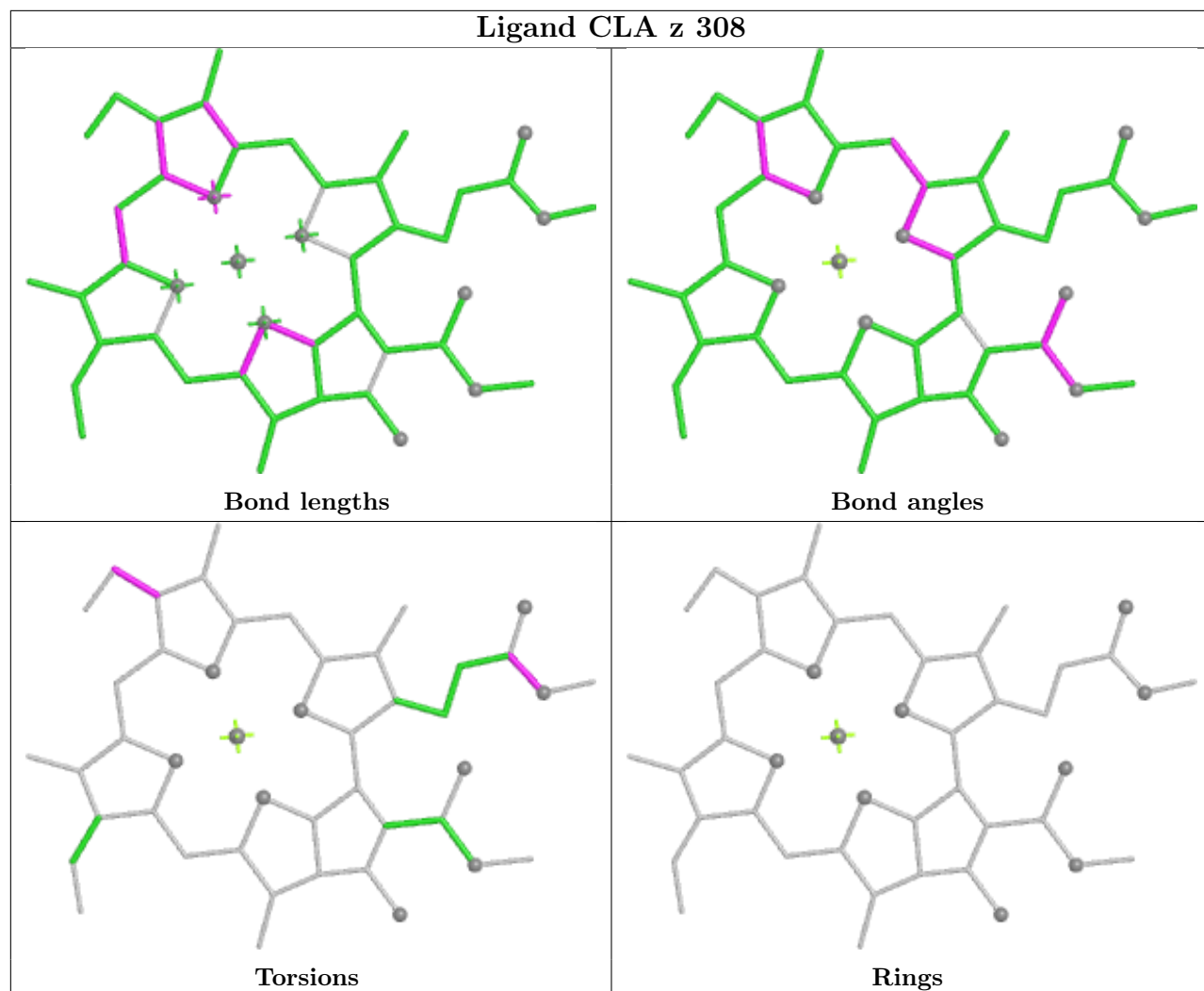


Torsions

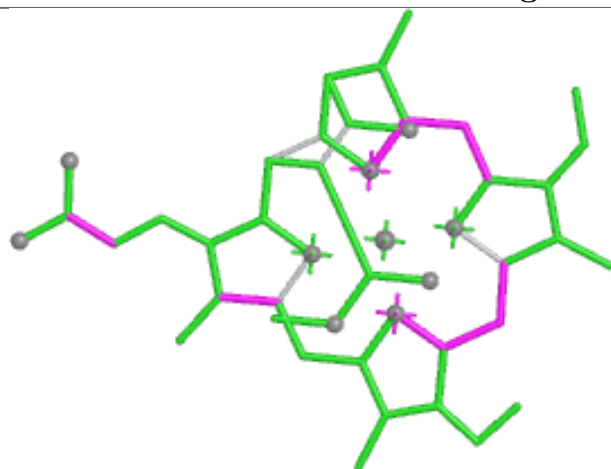


Rings

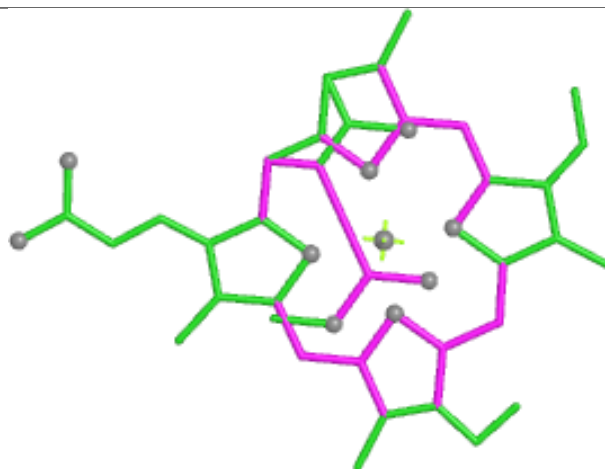
Ligand CLA z 308



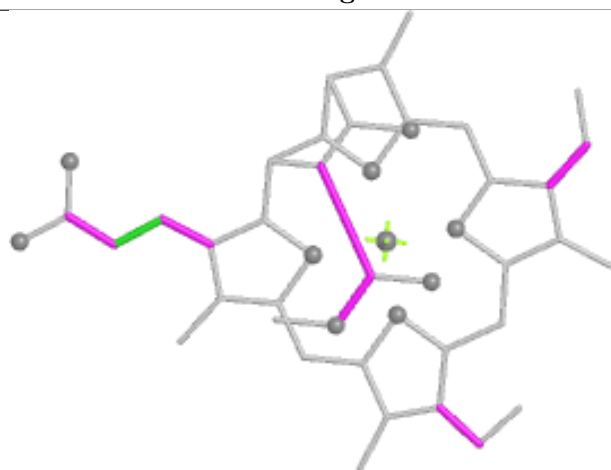
Ligand KC2 8 314



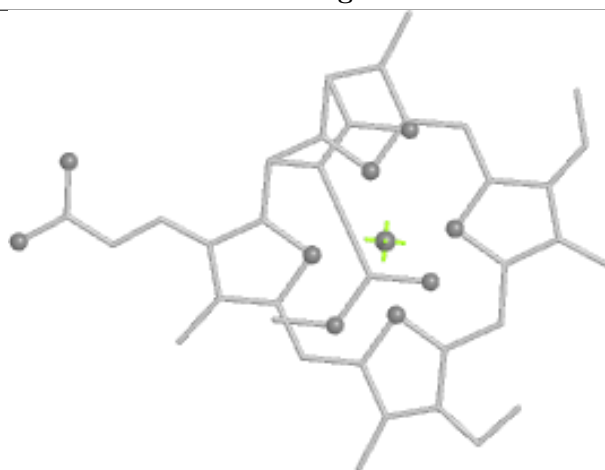
Bond lengths



Bond angles

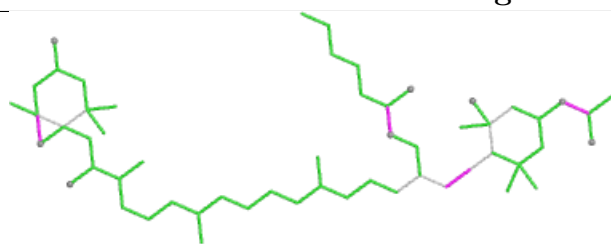


Torsions

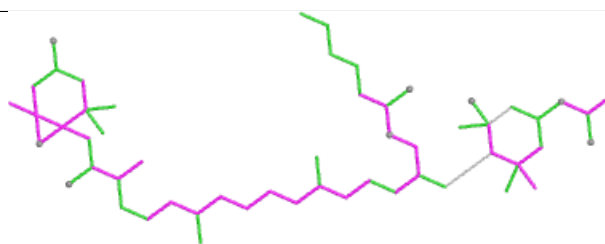


Rings

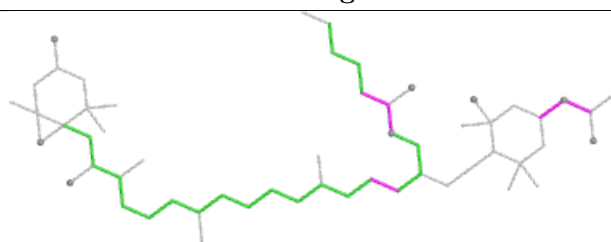
Ligand A1EB1 G 302



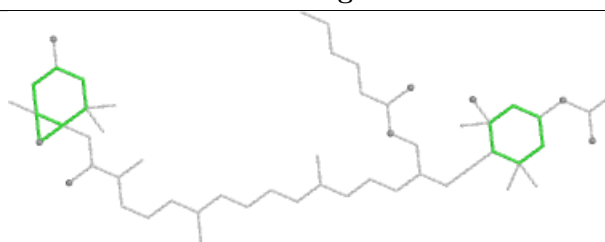
Bond lengths



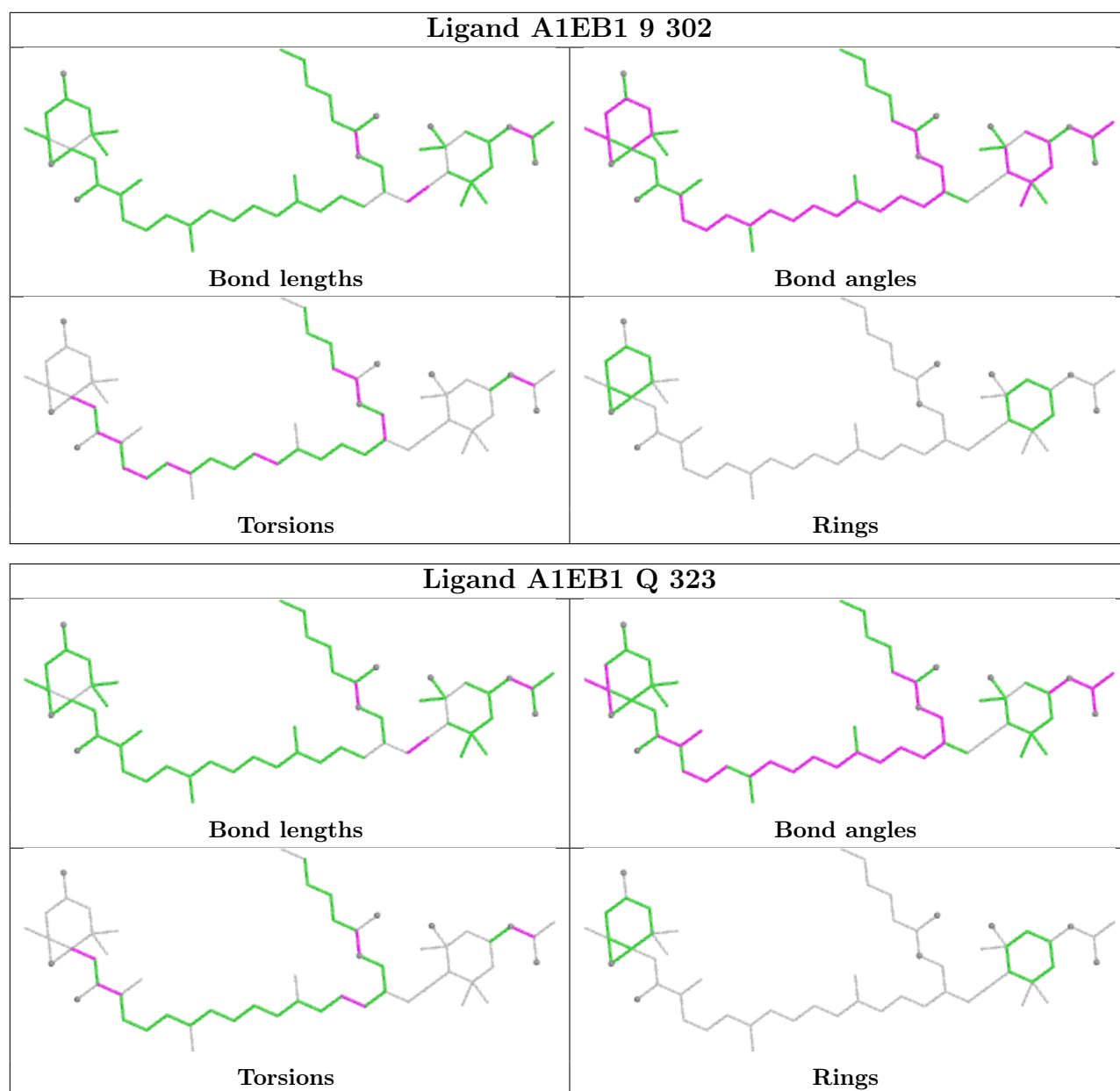
Bond angles



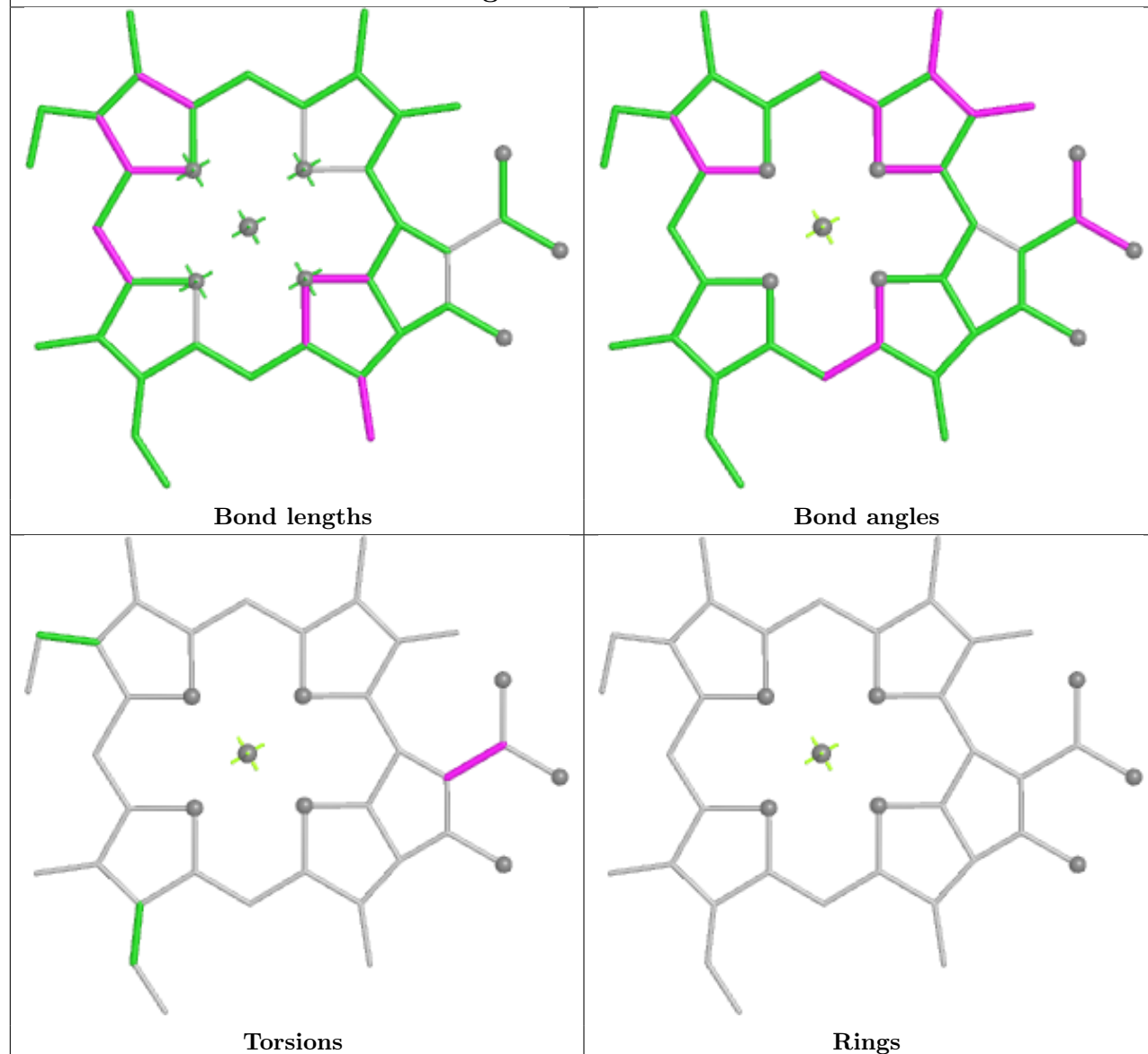
Torsions



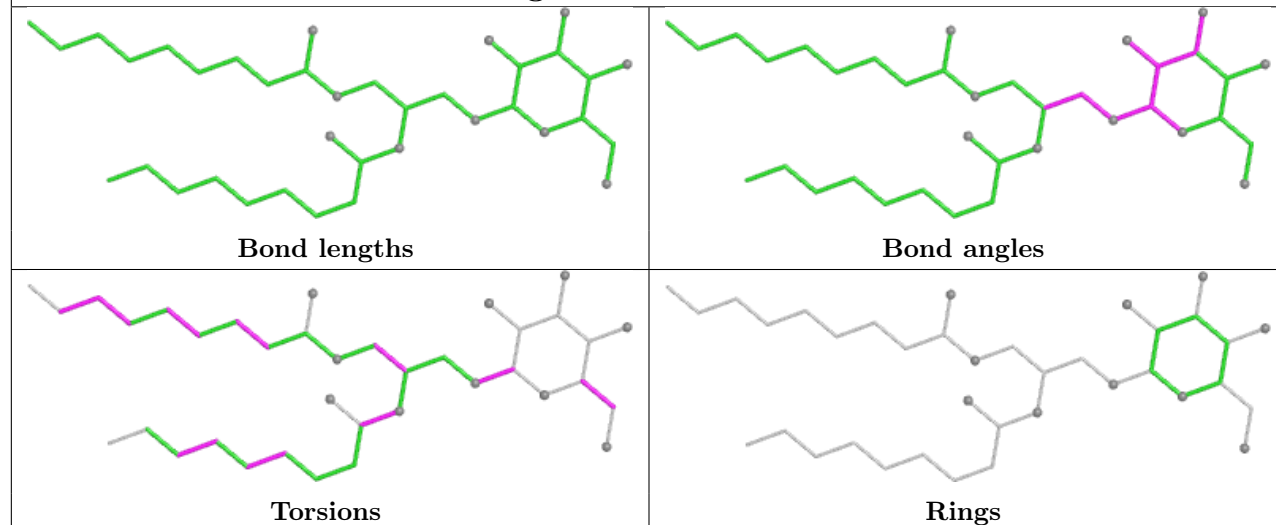
Rings

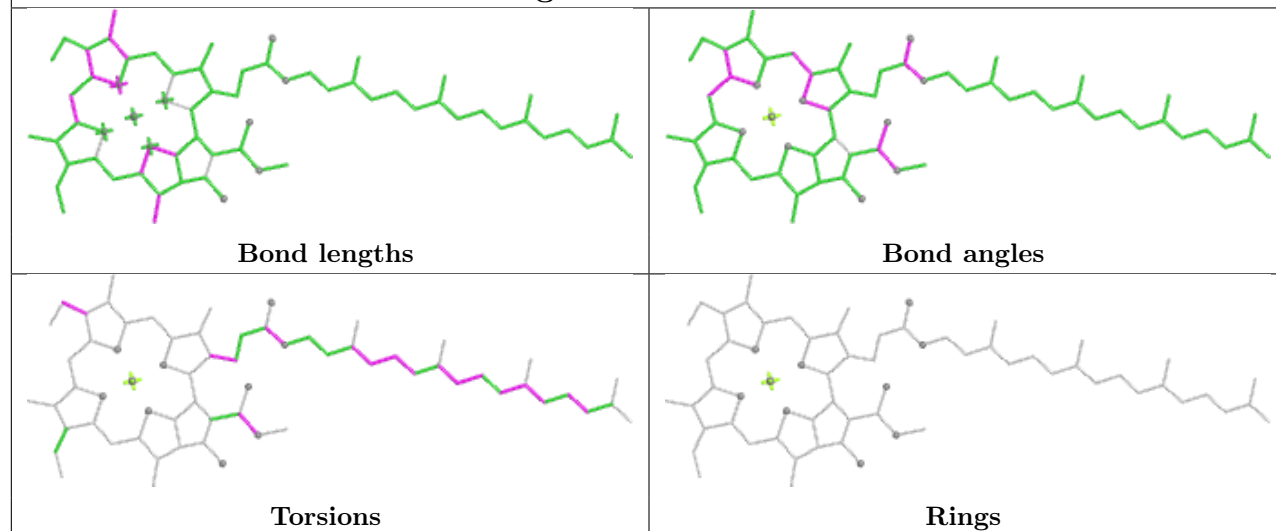
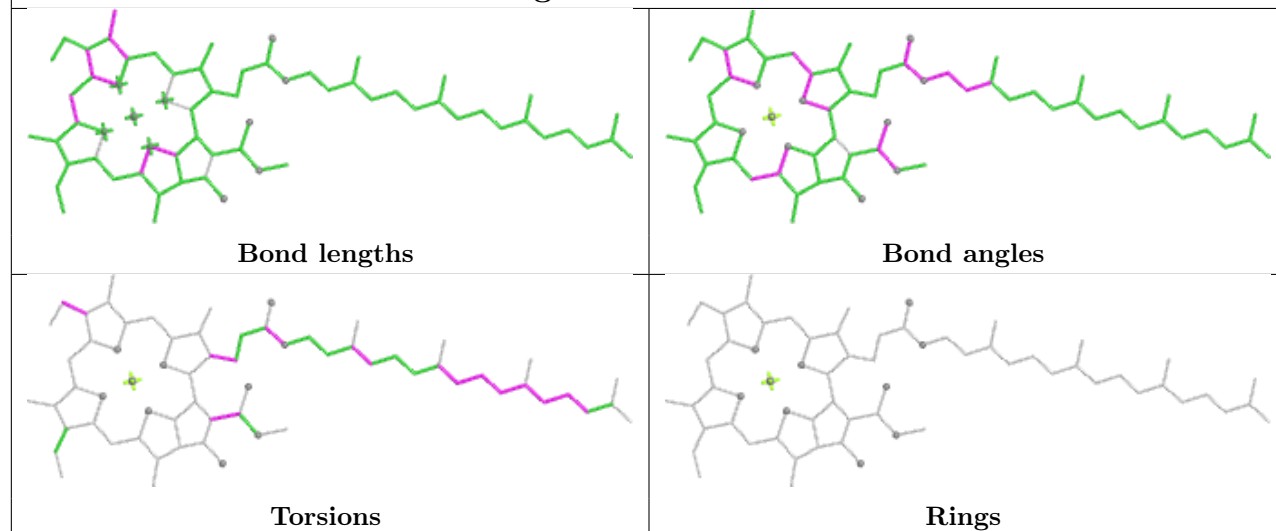


Ligand CLA 6 311

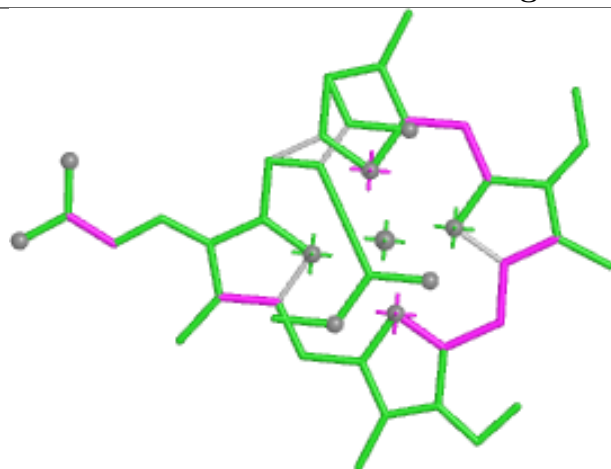


Ligand LMG D 322

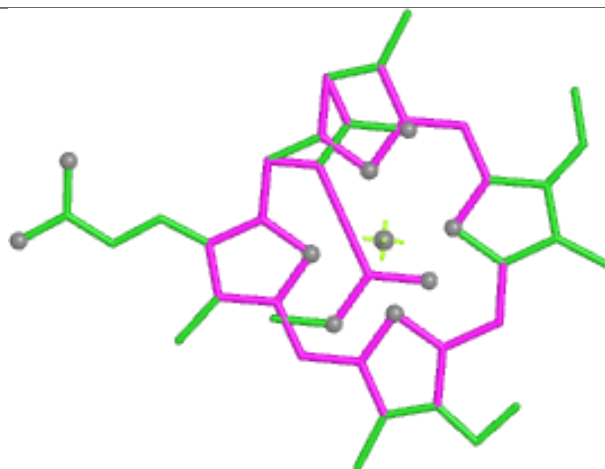


Ligand CLA a 804**Ligand CLA F 321**

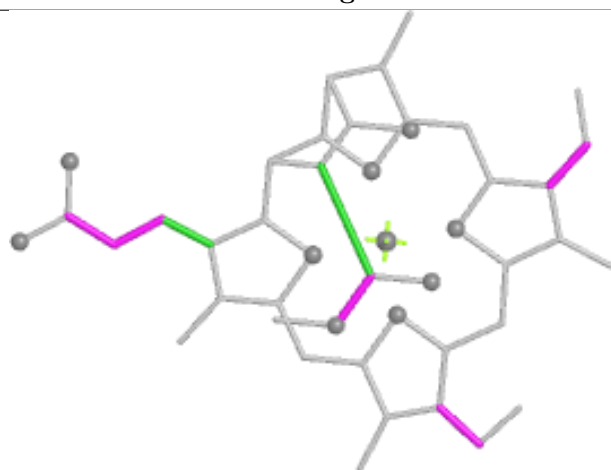
Ligand KC2 6 314



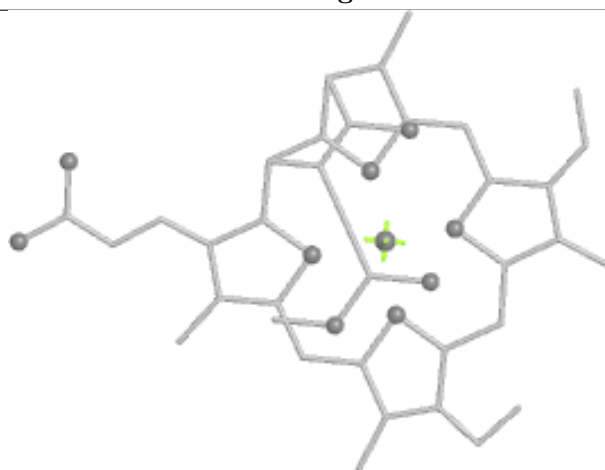
Bond lengths



Bond angles

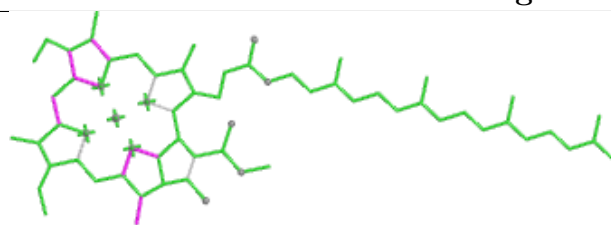


Torsions

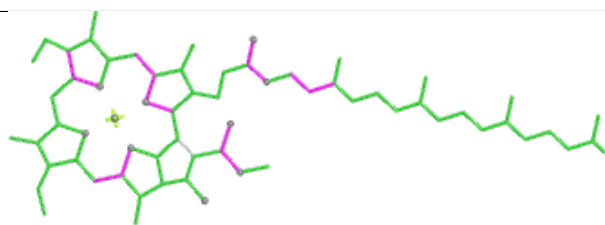


Rings

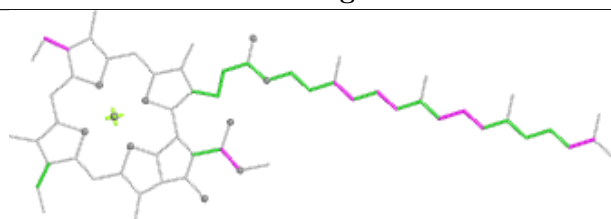
Ligand CLA E 310



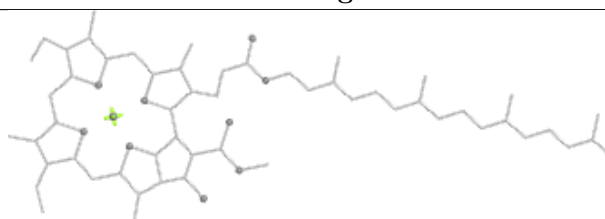
Bond lengths



Bond angles

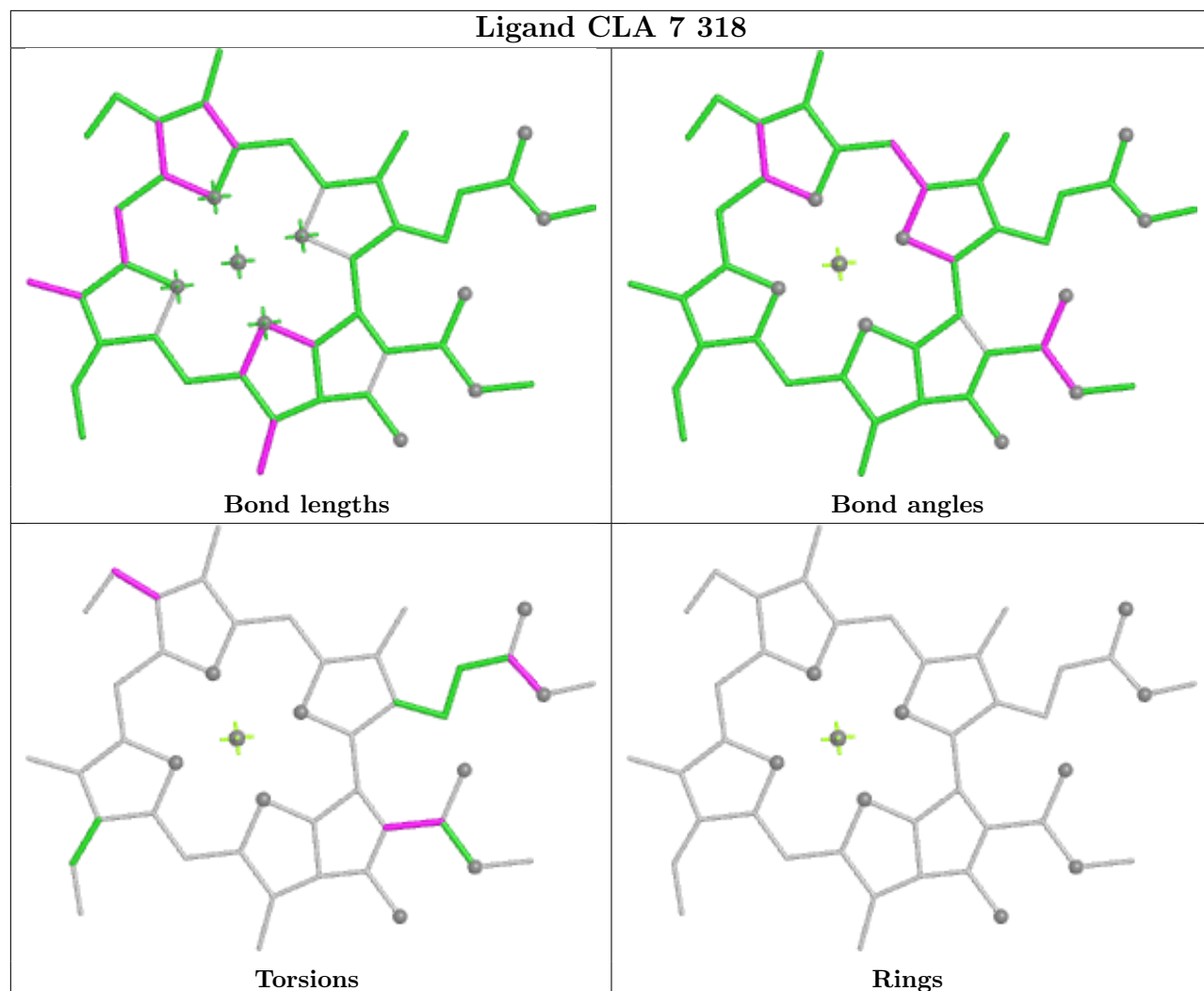


Torsions

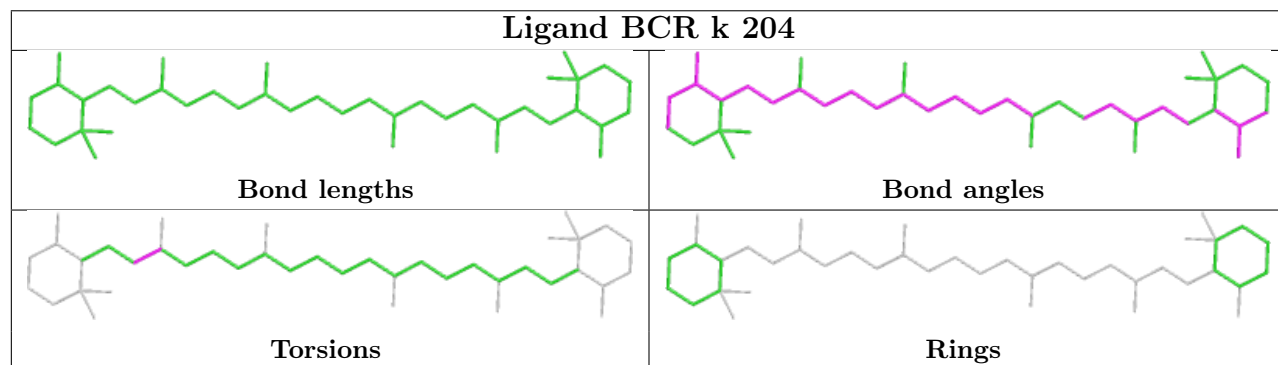


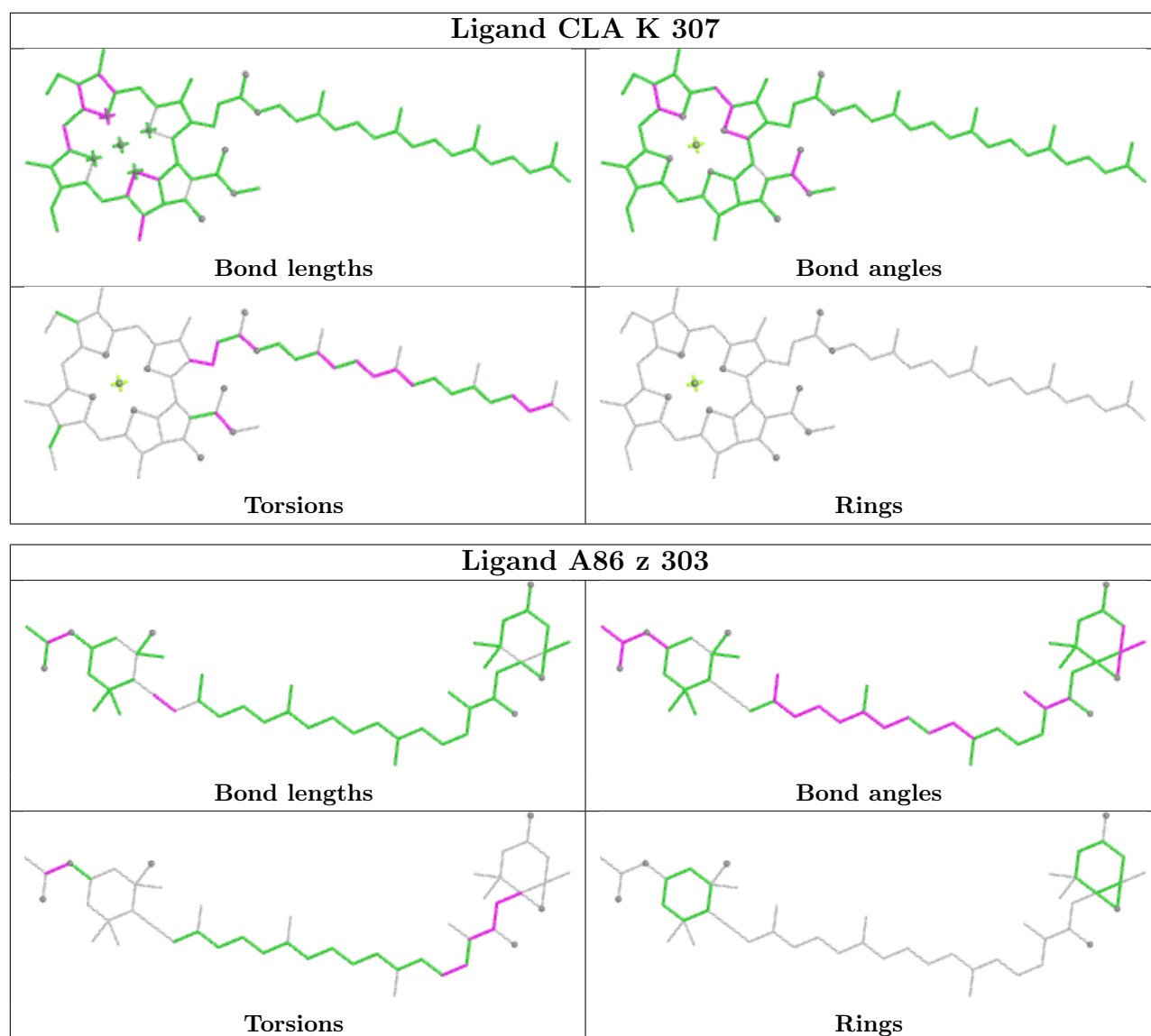
Rings

Ligand CLA 7 318

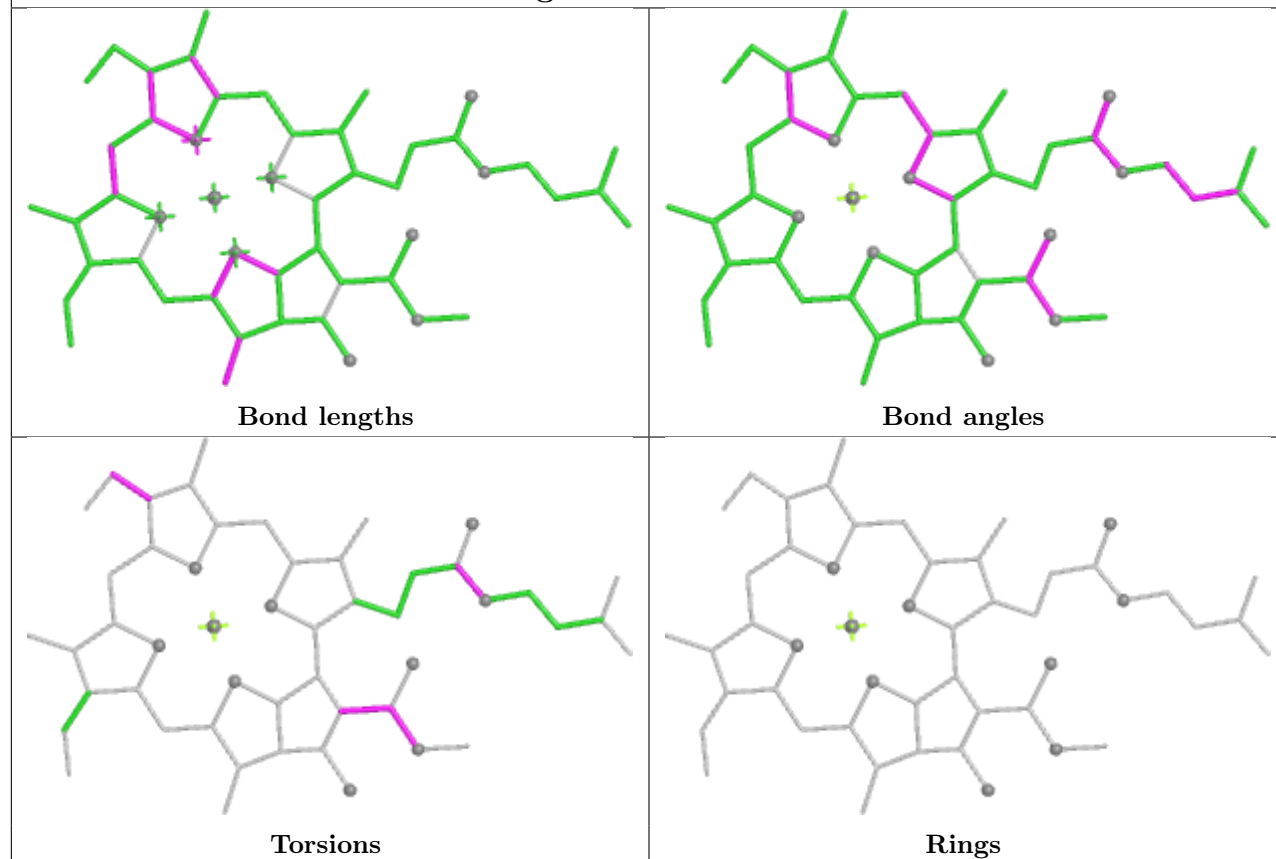


Ligand BCR k 204

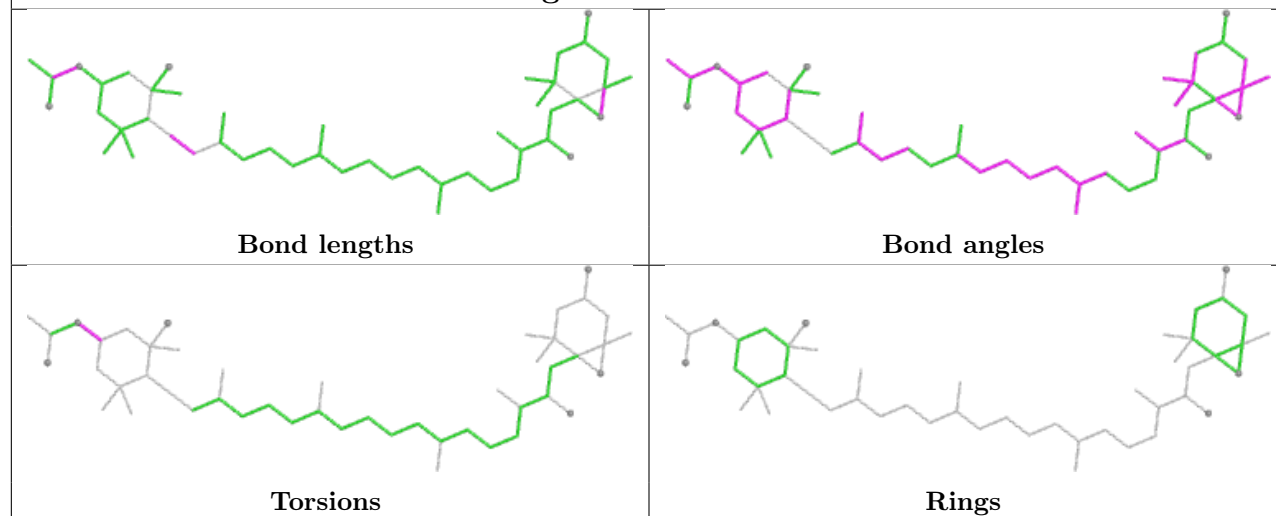


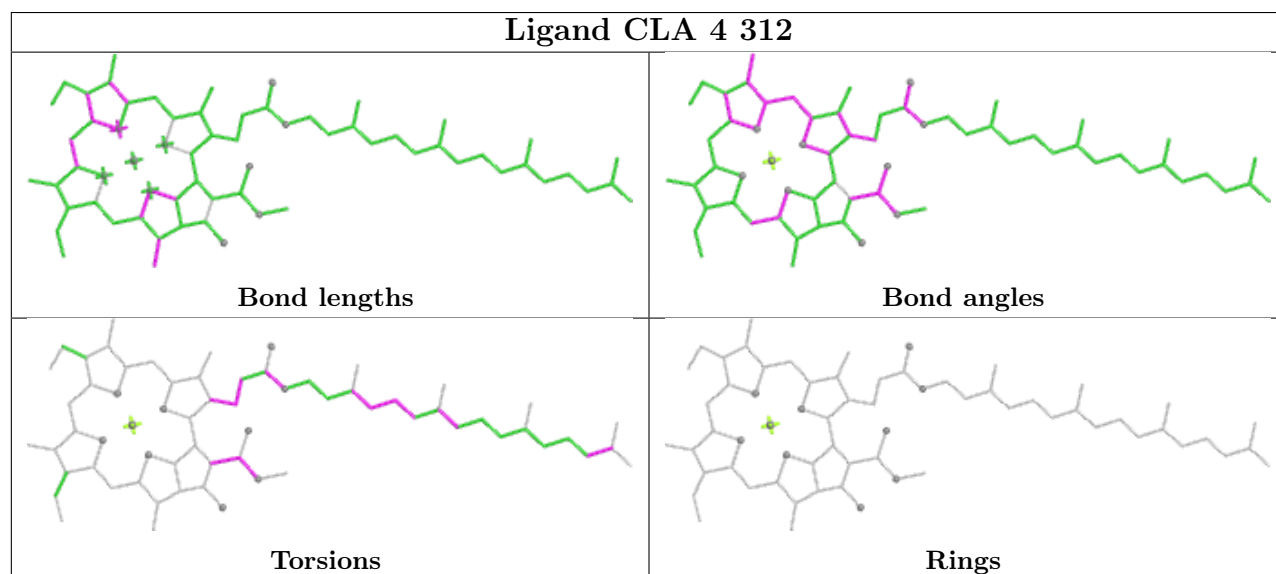
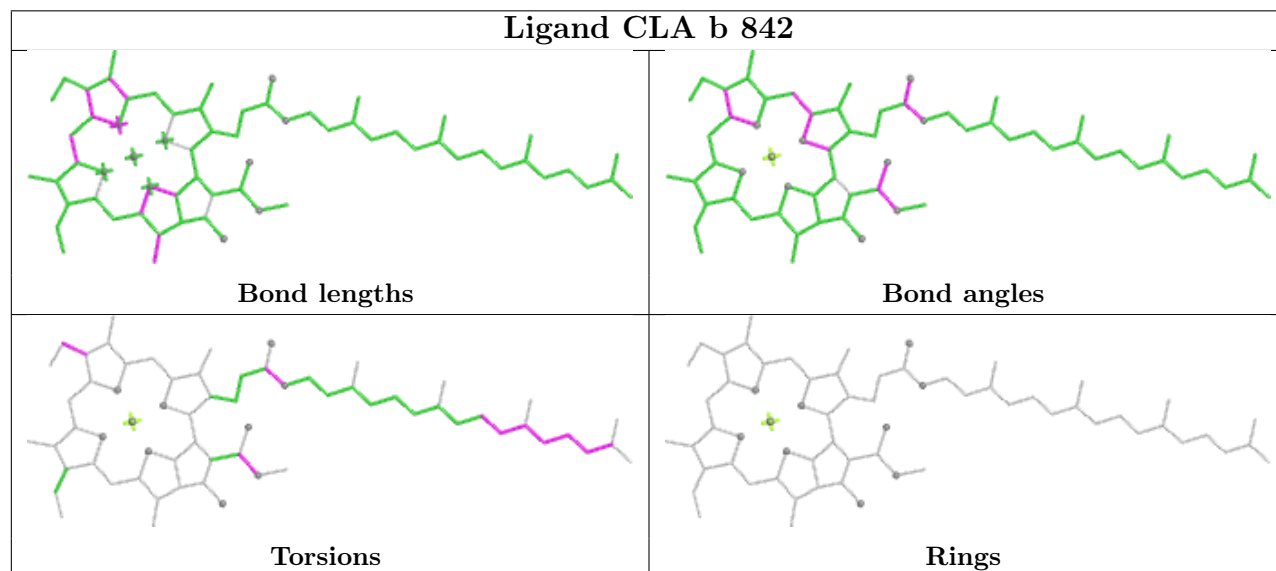
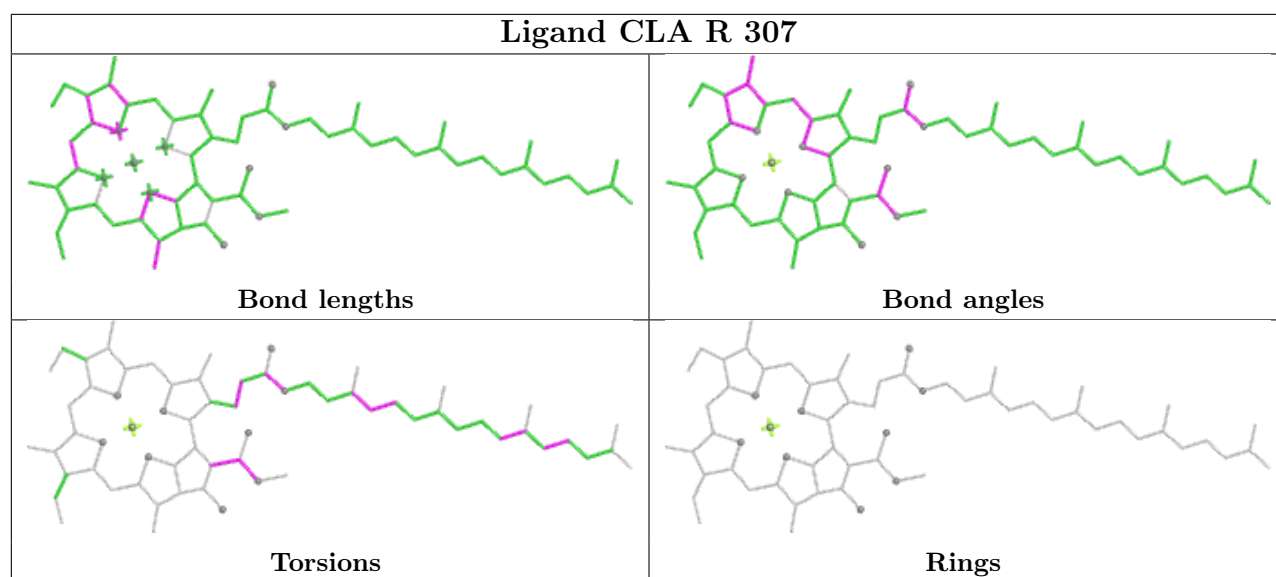


Ligand CLA 3 316

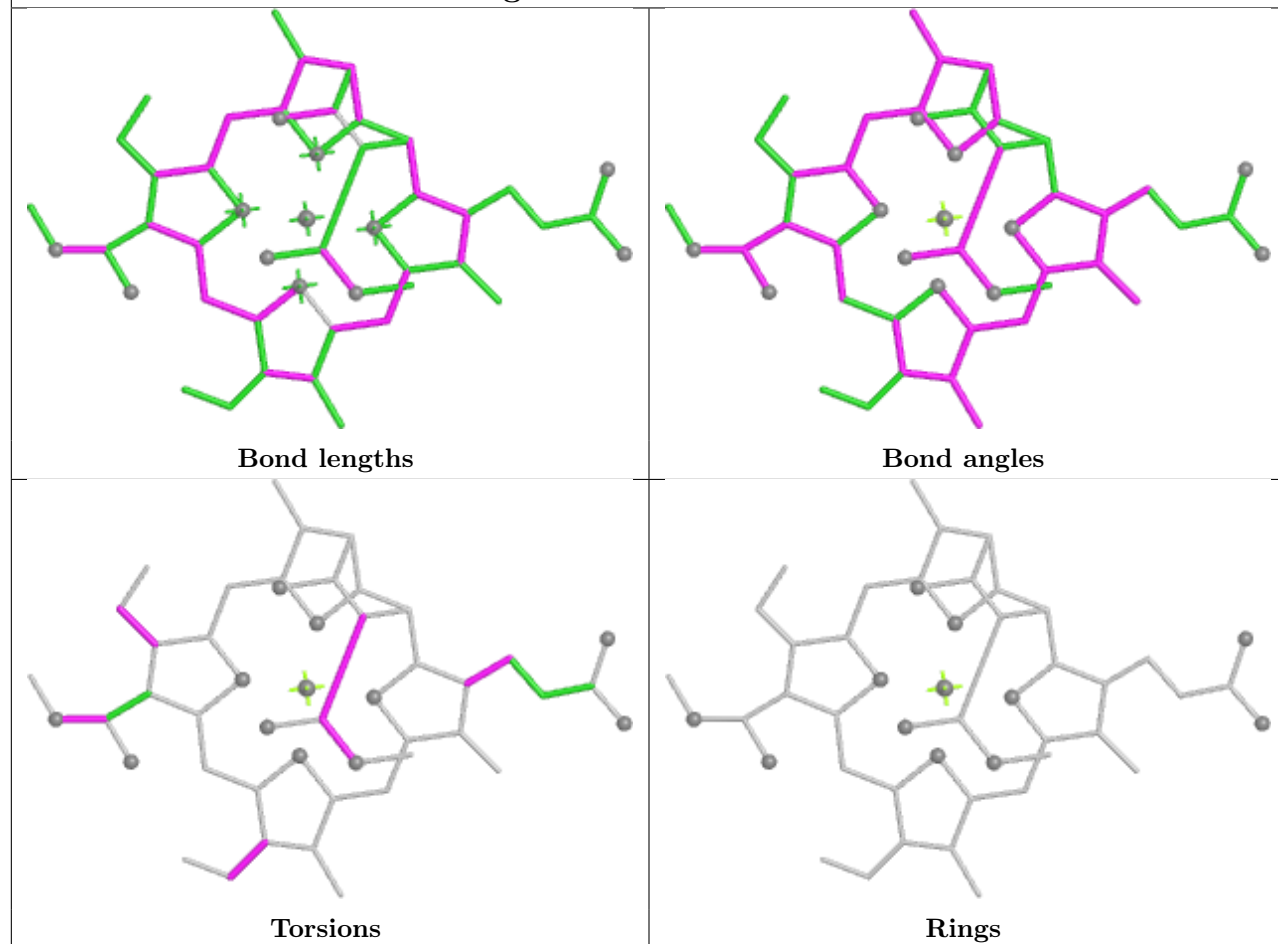


Ligand A86 0 308

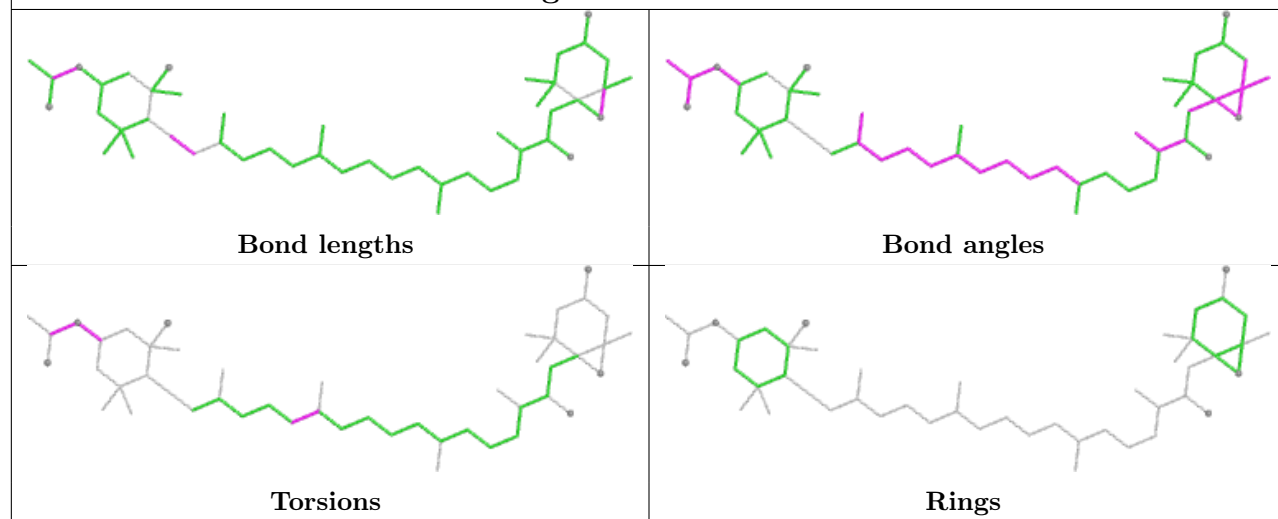




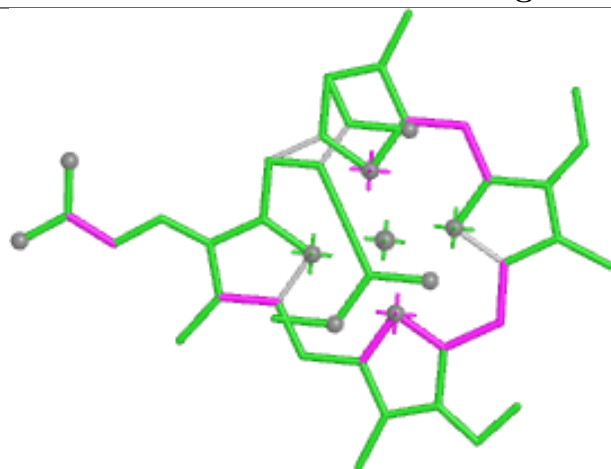
Ligand A1ECV W 317



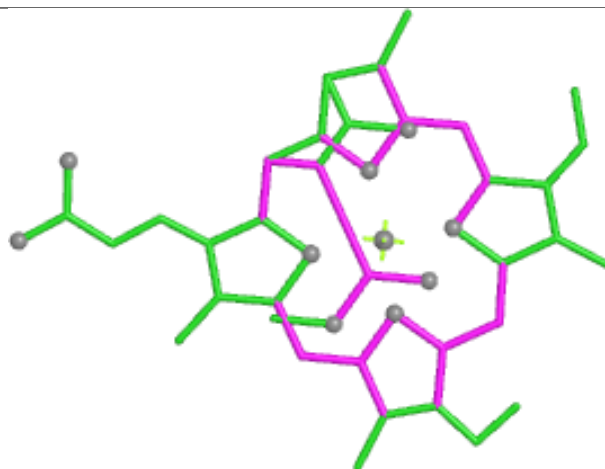
Ligand A86 8 303



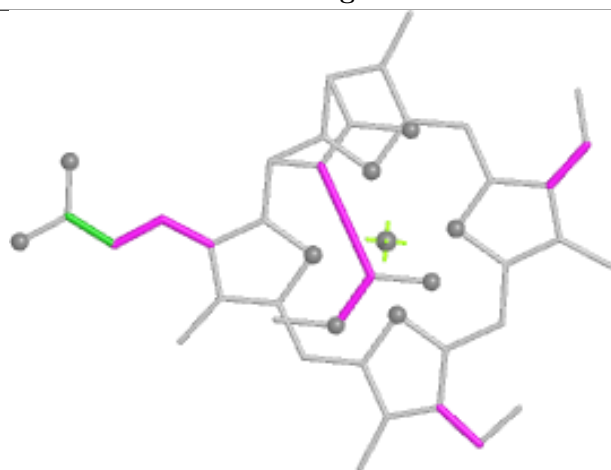
Ligand KC2 X 306



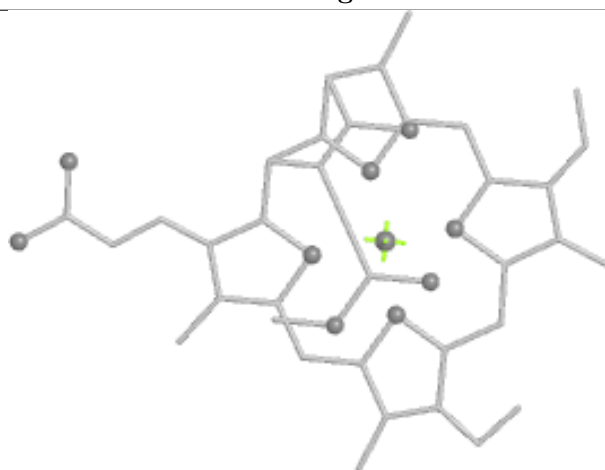
Bond lengths



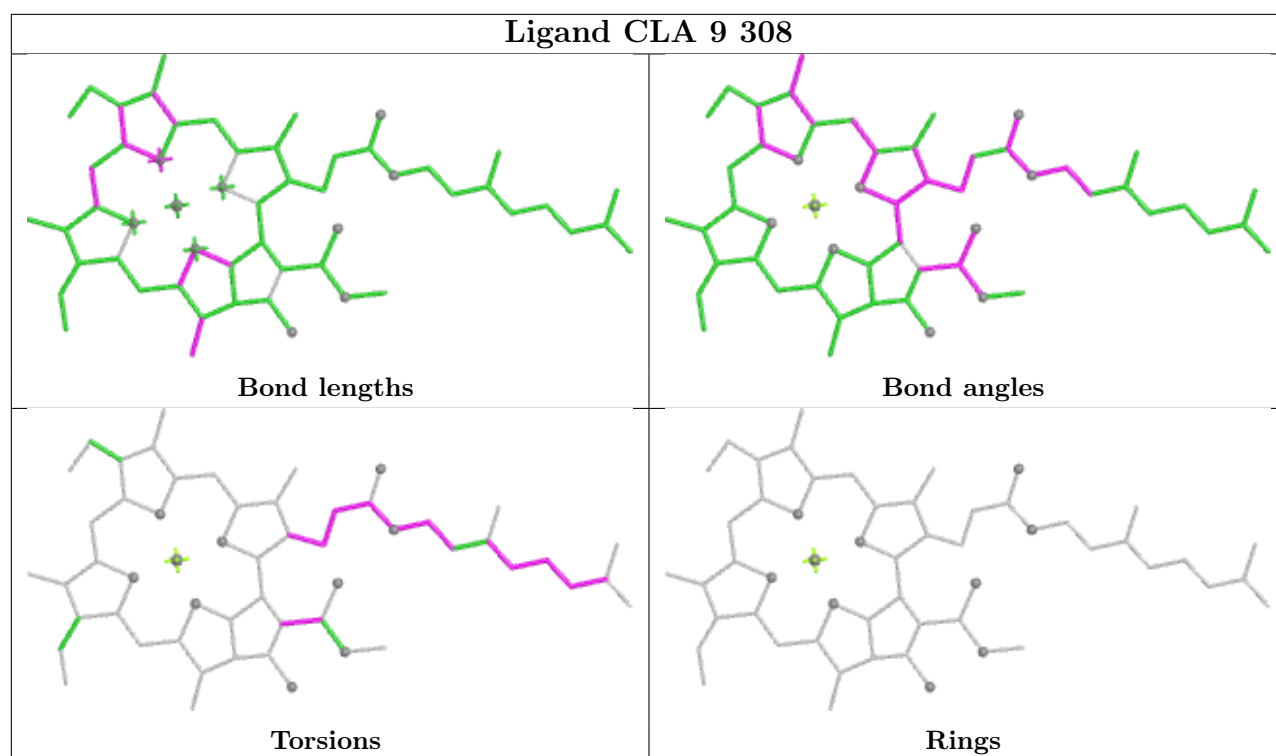
Bond angles

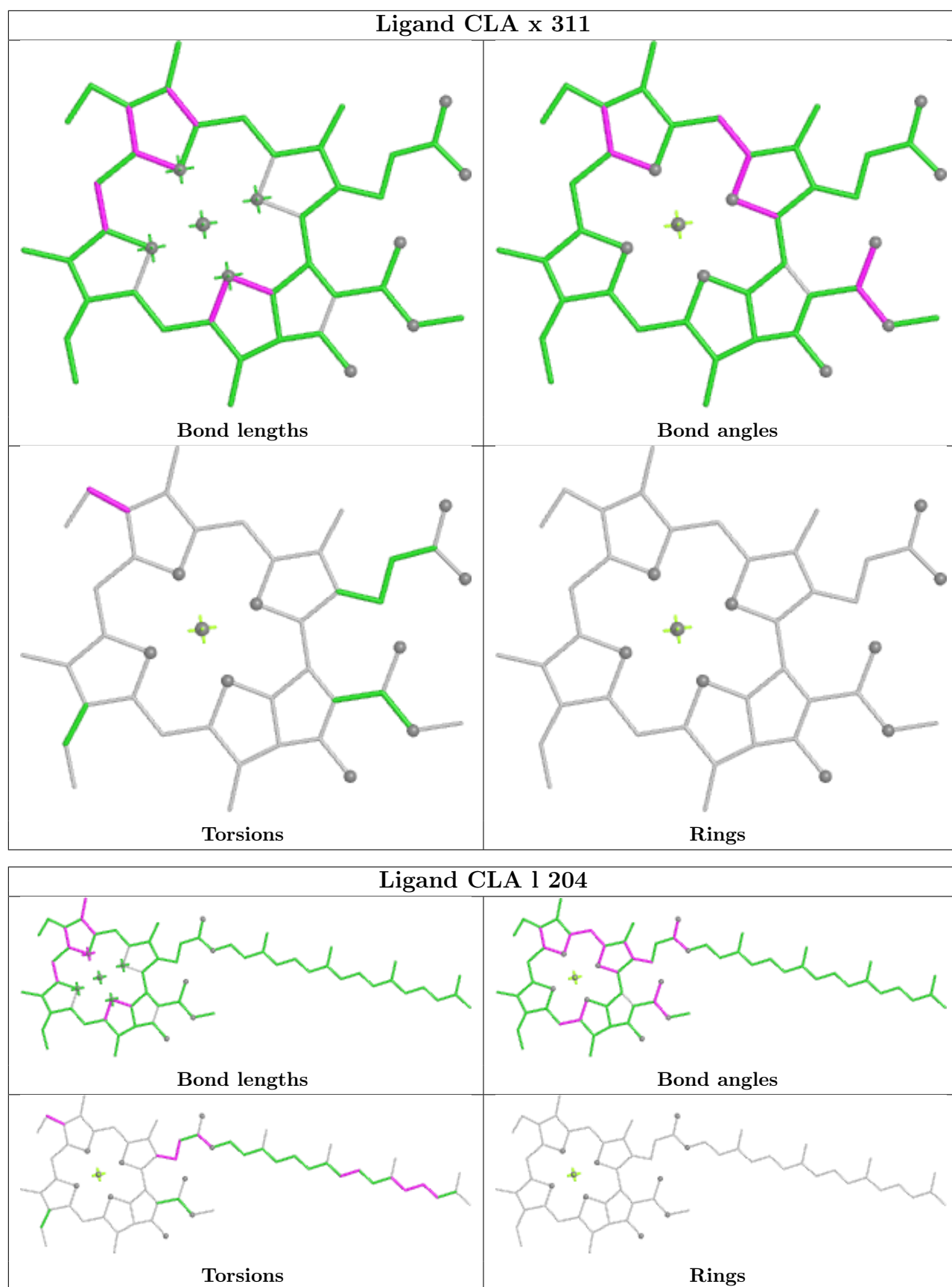


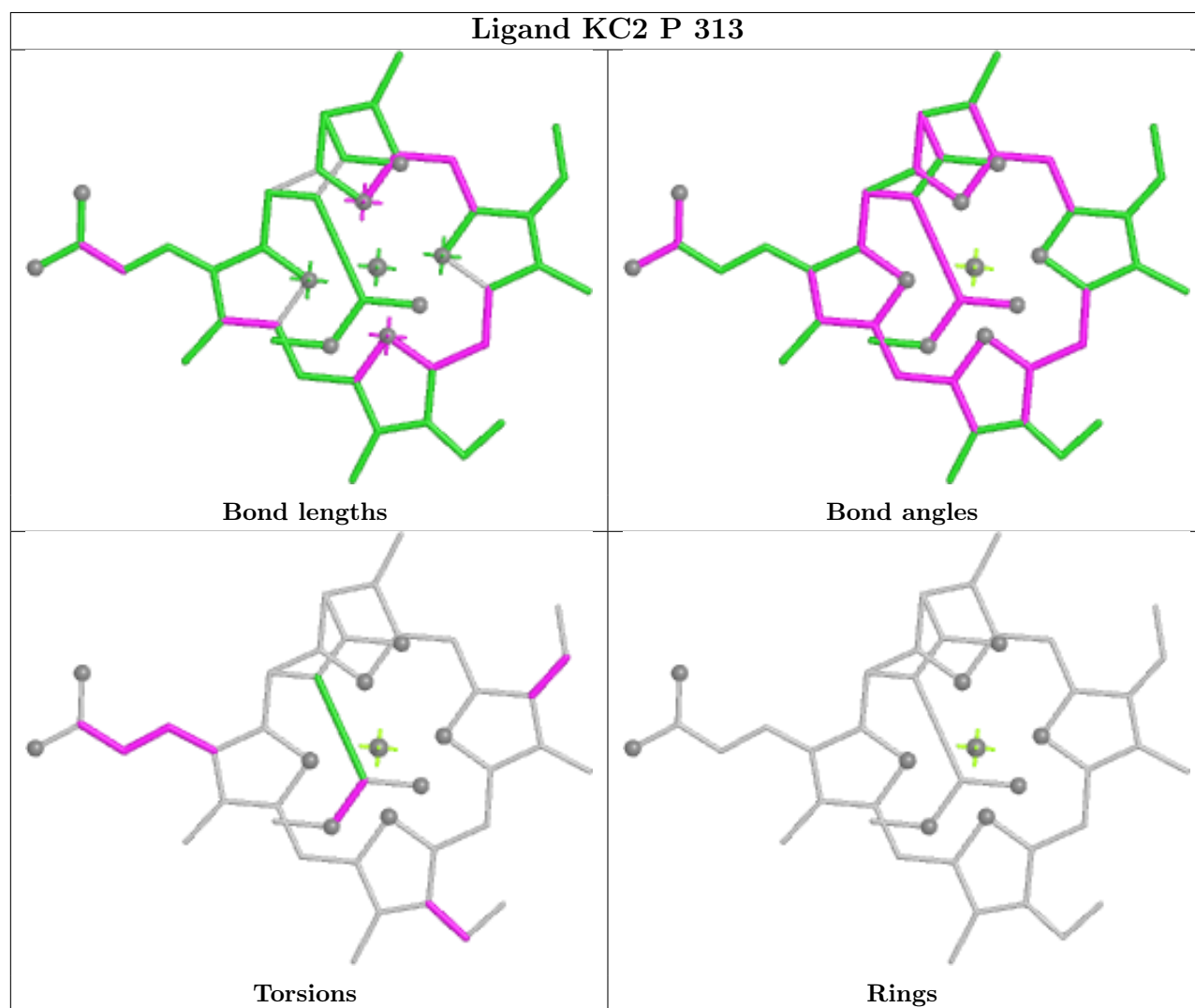
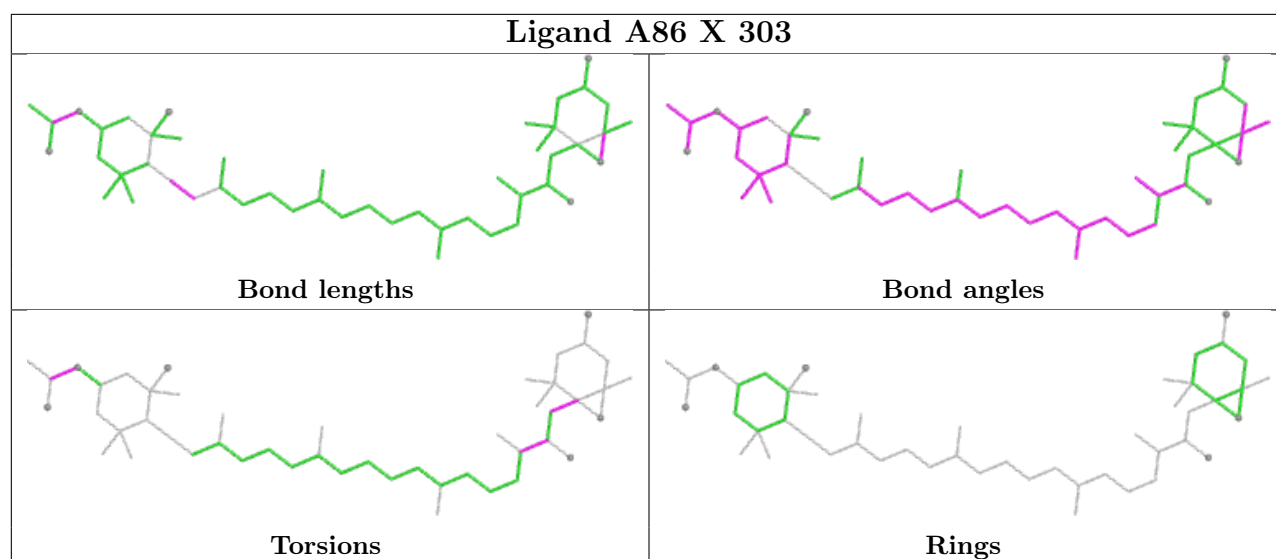
Torsions

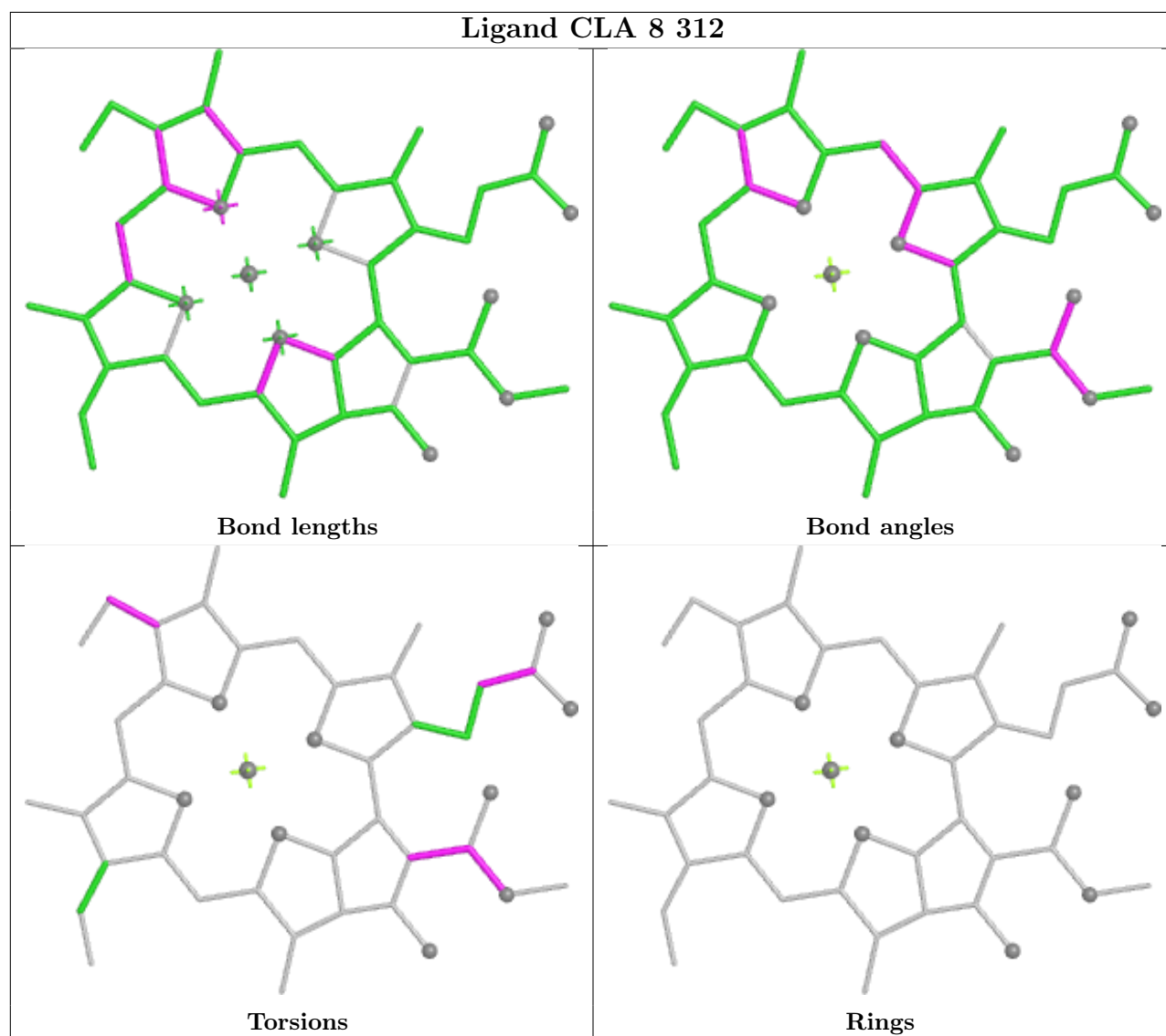
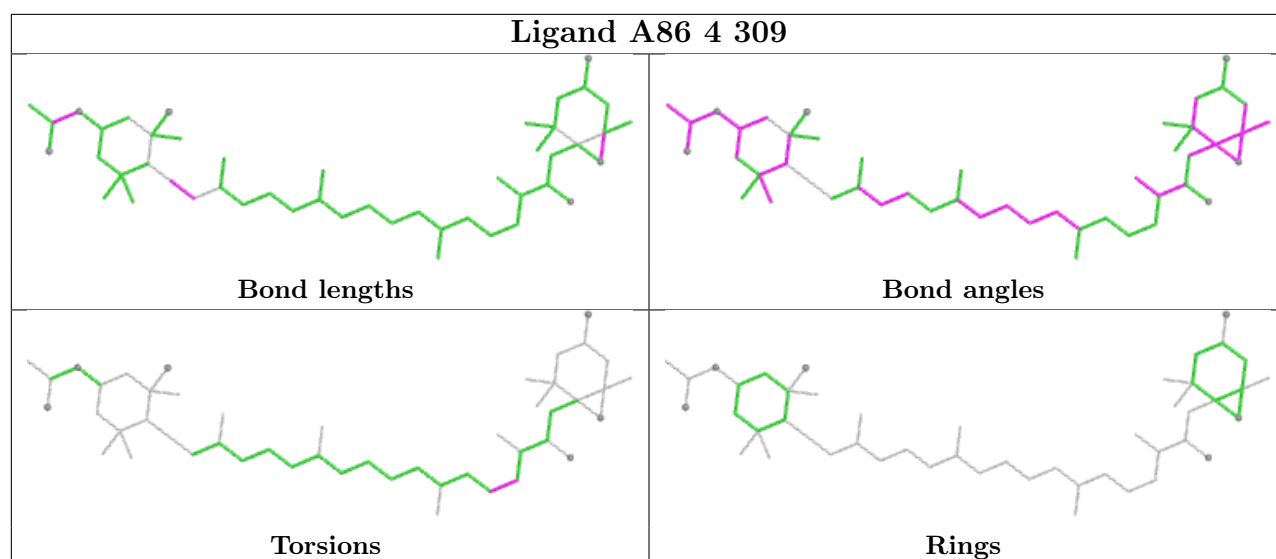


Rings

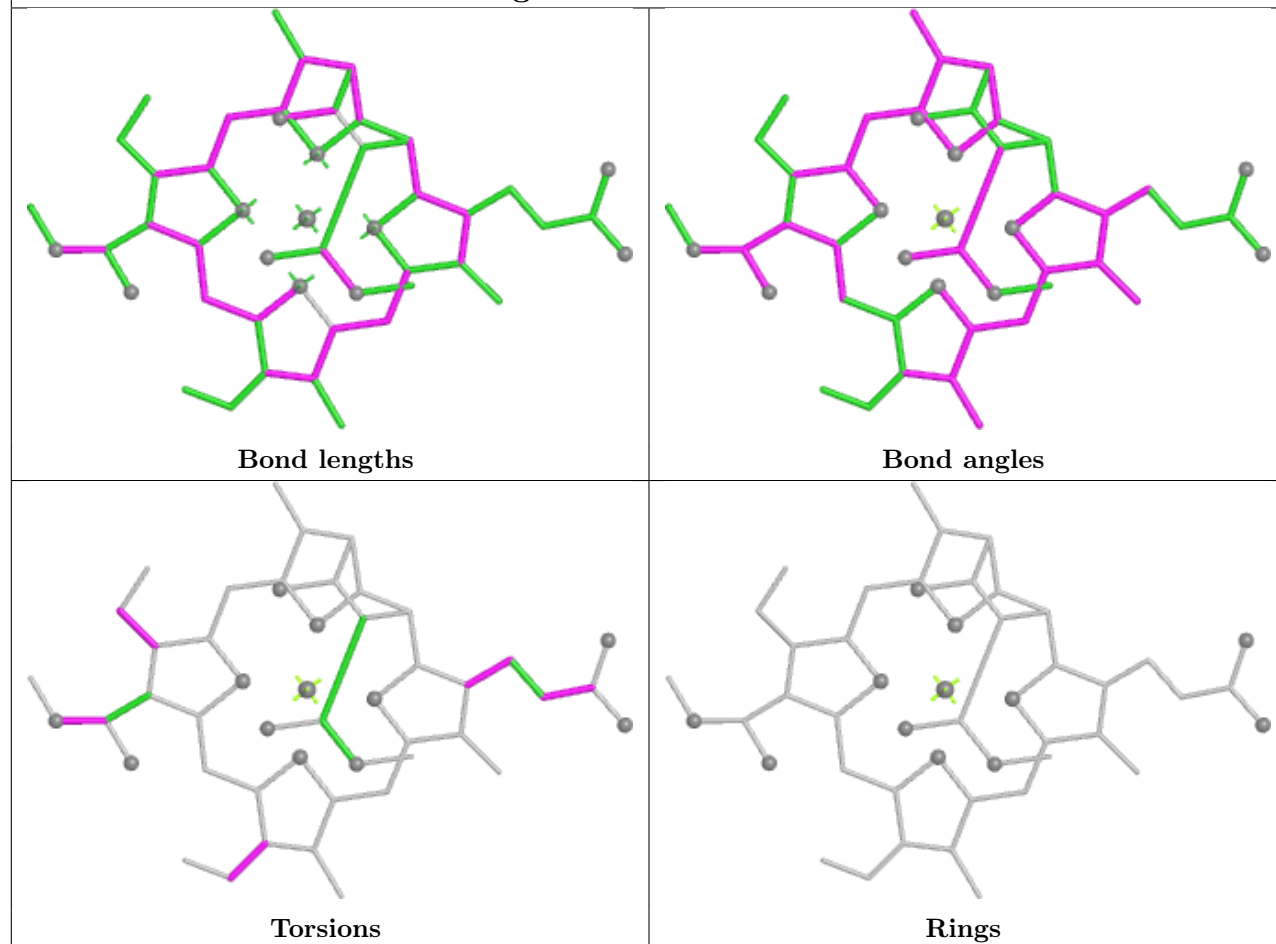




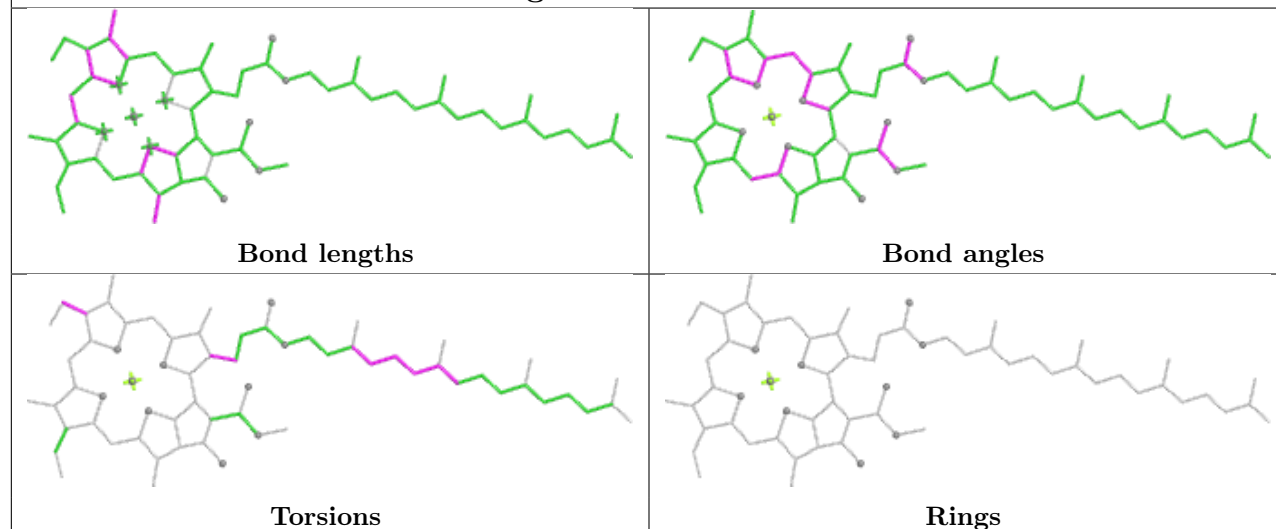


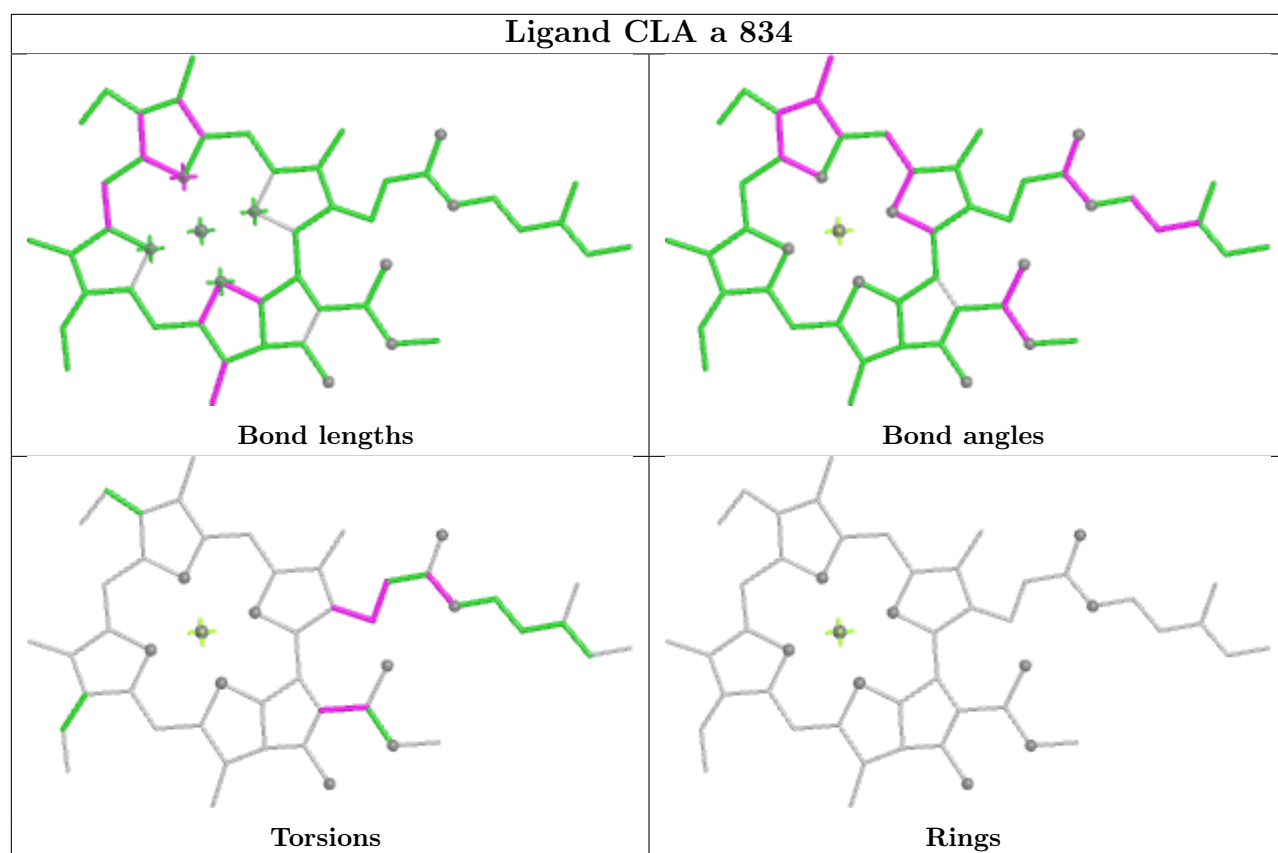


Ligand A1ECV 7 323

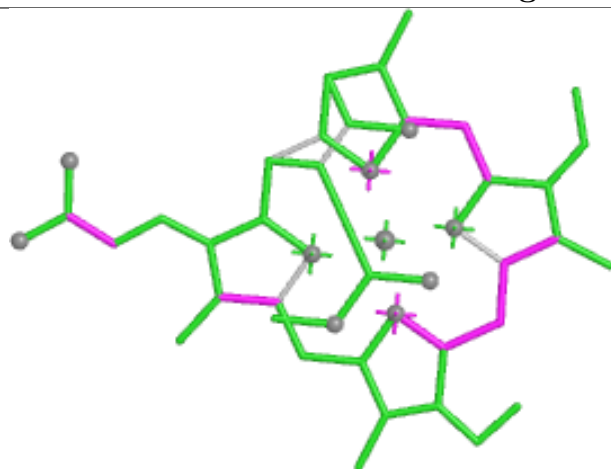


Ligand CLA W 313

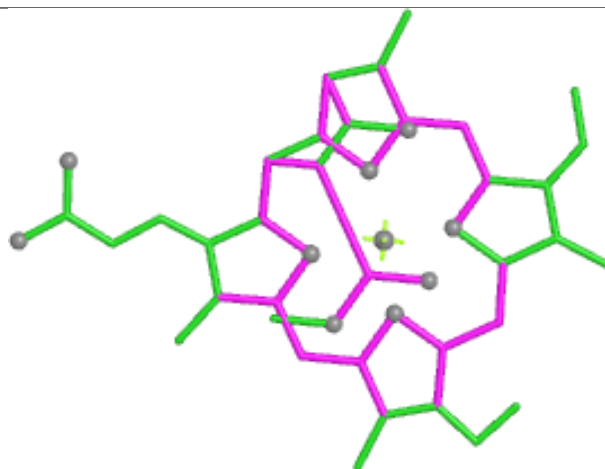




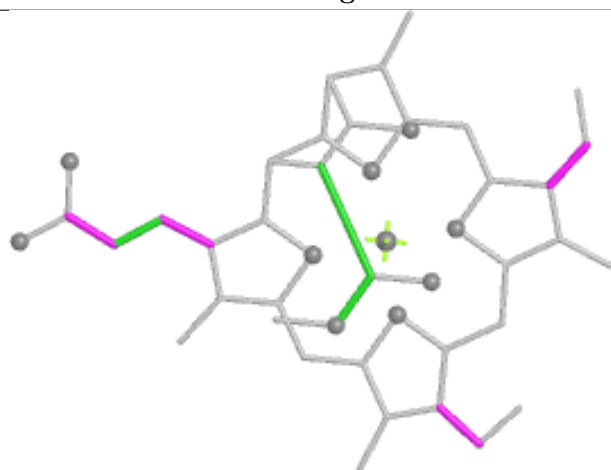
Ligand KC2 S 317



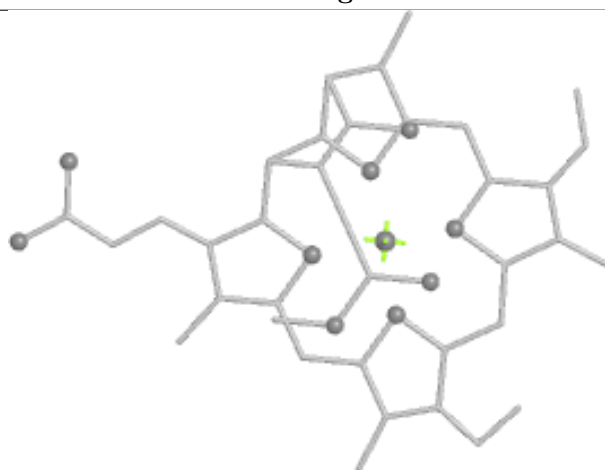
Bond lengths



Bond angles

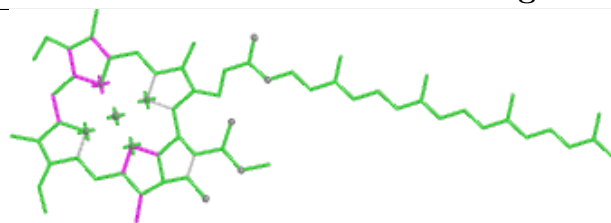


Torsions

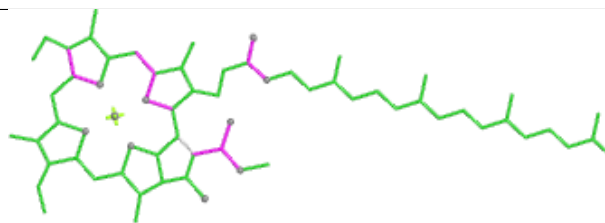


Rings

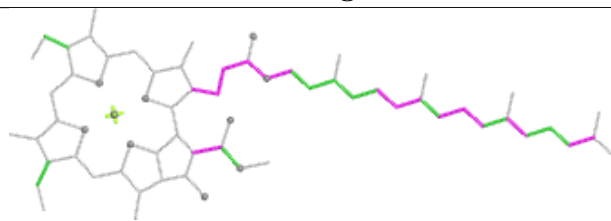
Ligand CLA a 806



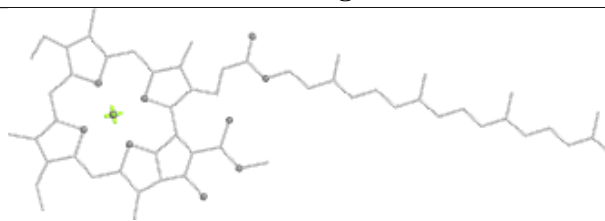
Bond lengths



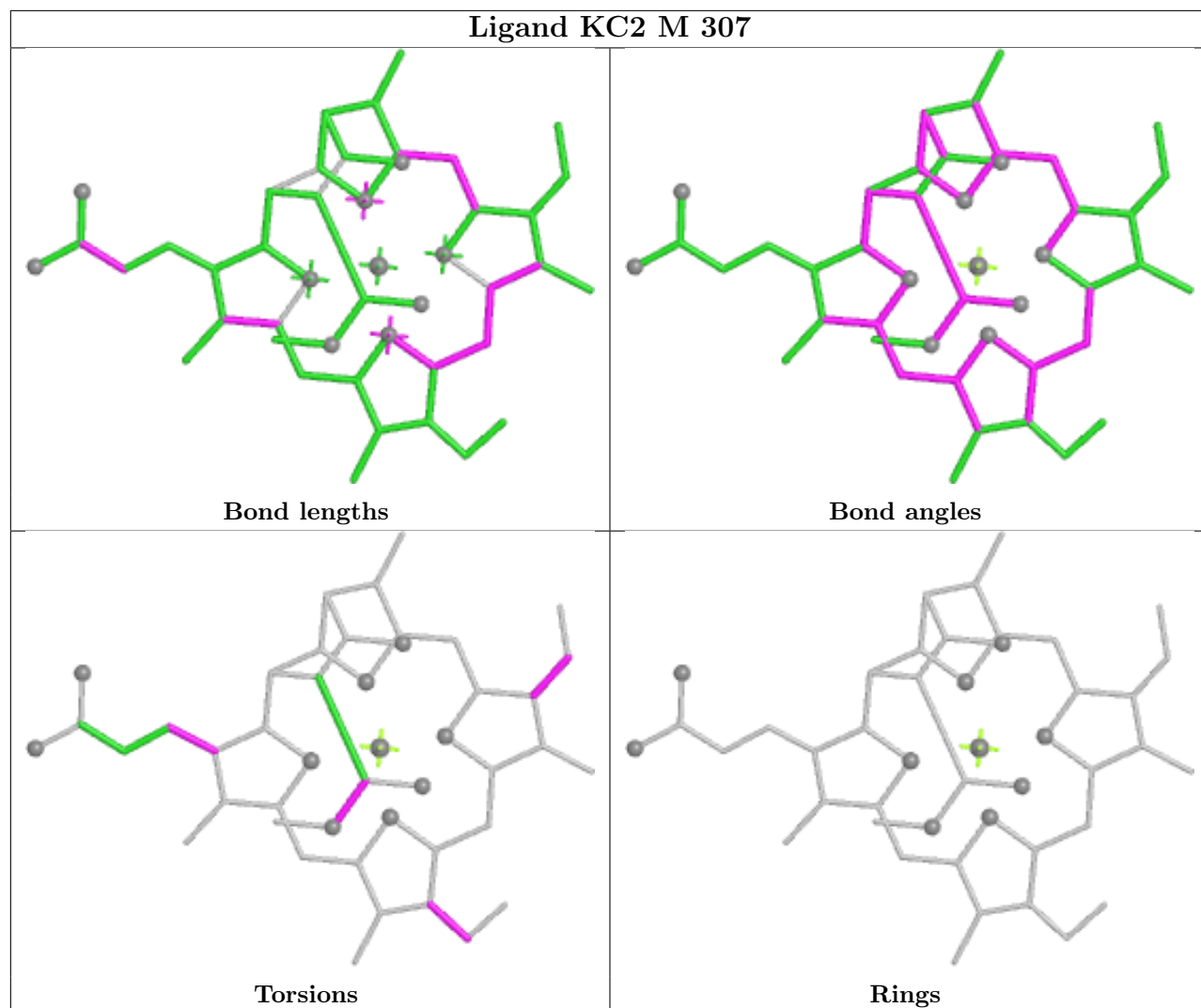
Bond angles



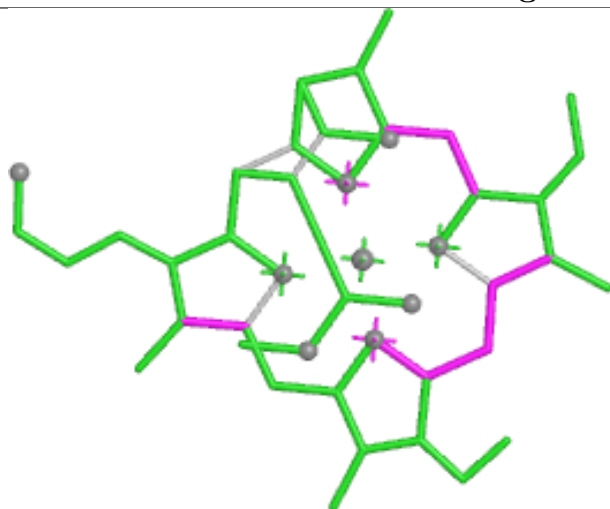
Torsions



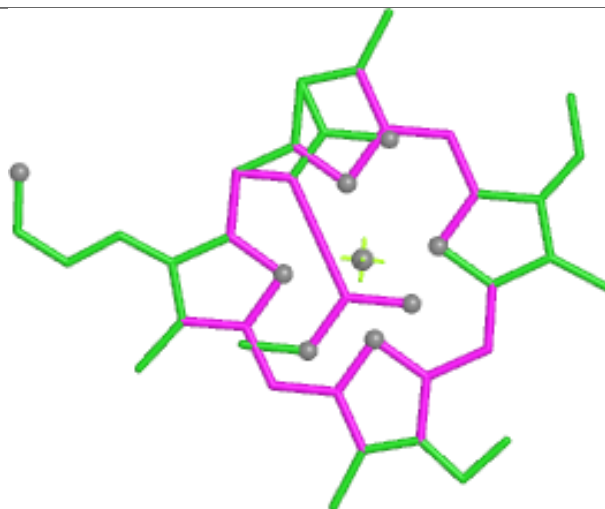
Rings



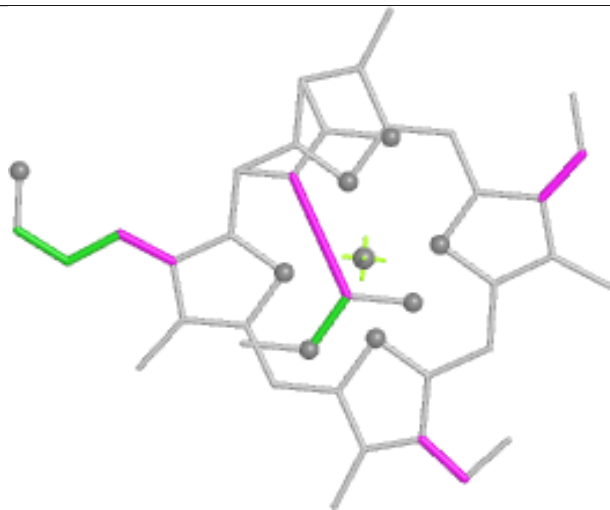
Ligand KC2 5 313



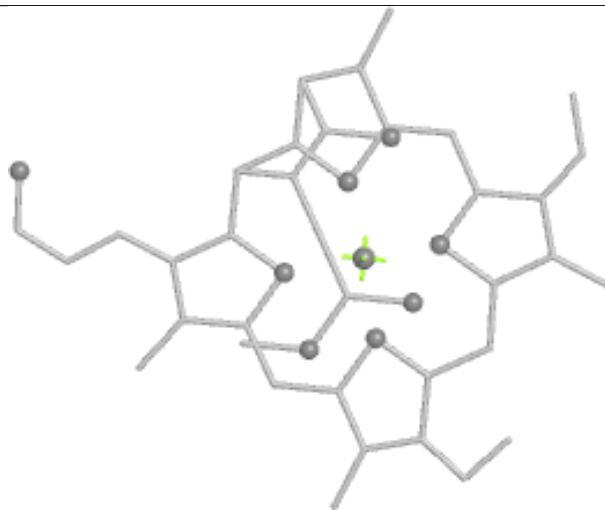
Bond lengths



Bond angles

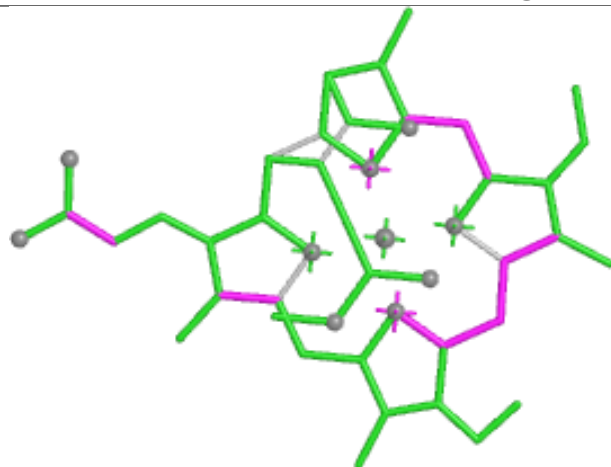


Torsions



Rings

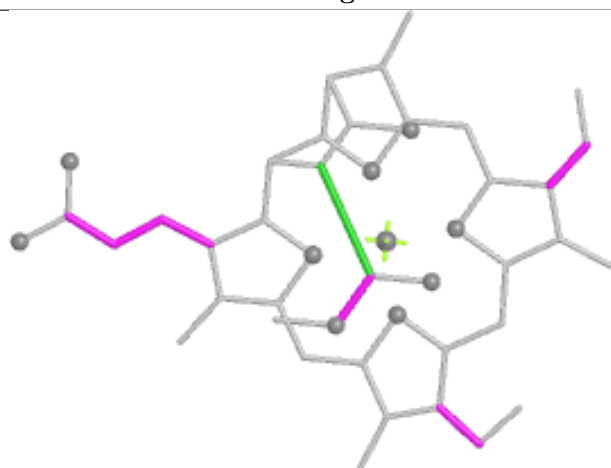
Ligand KC2 Z 310



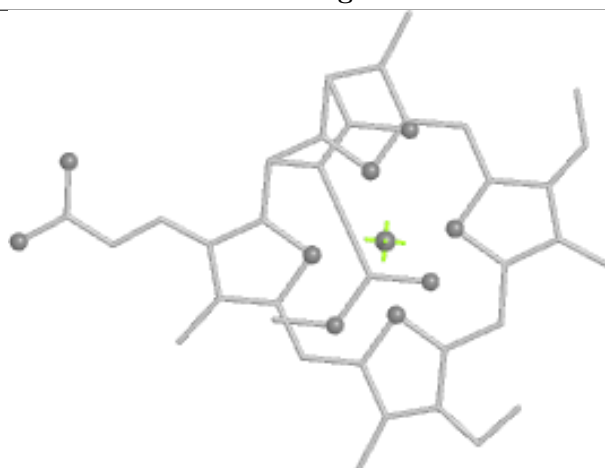
Bond lengths



Bond angles



Torsions

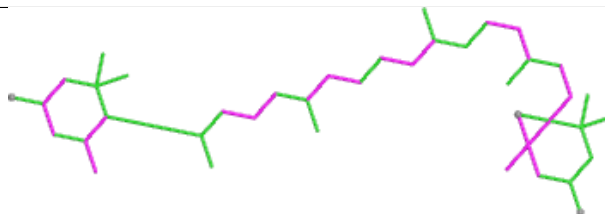


Rings

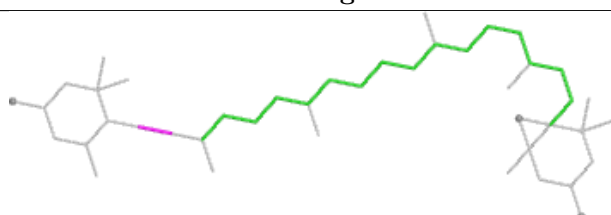
Ligand DD6 H 303



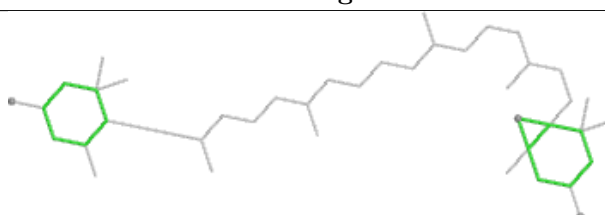
Bond lengths



Bond angles

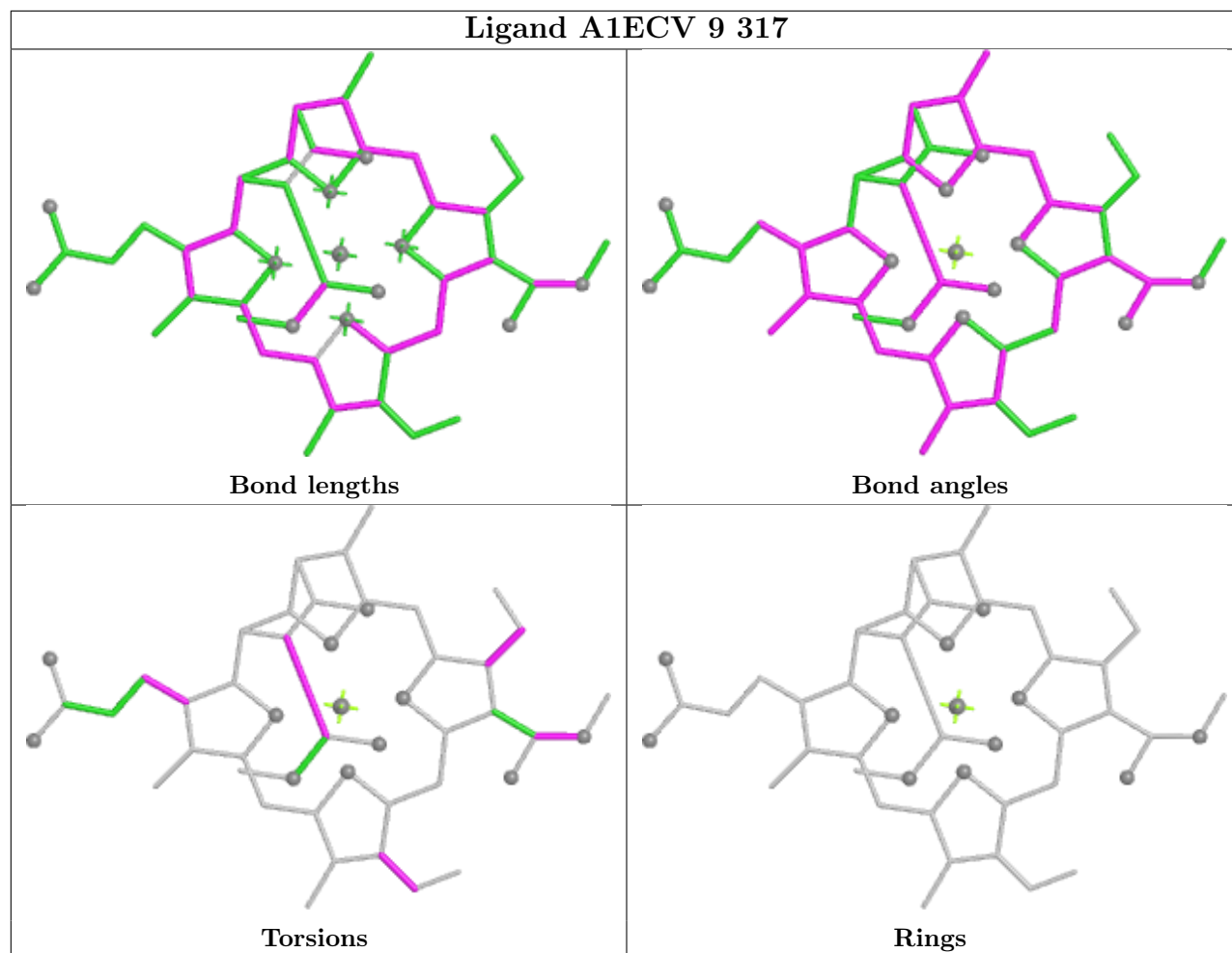


Torsions

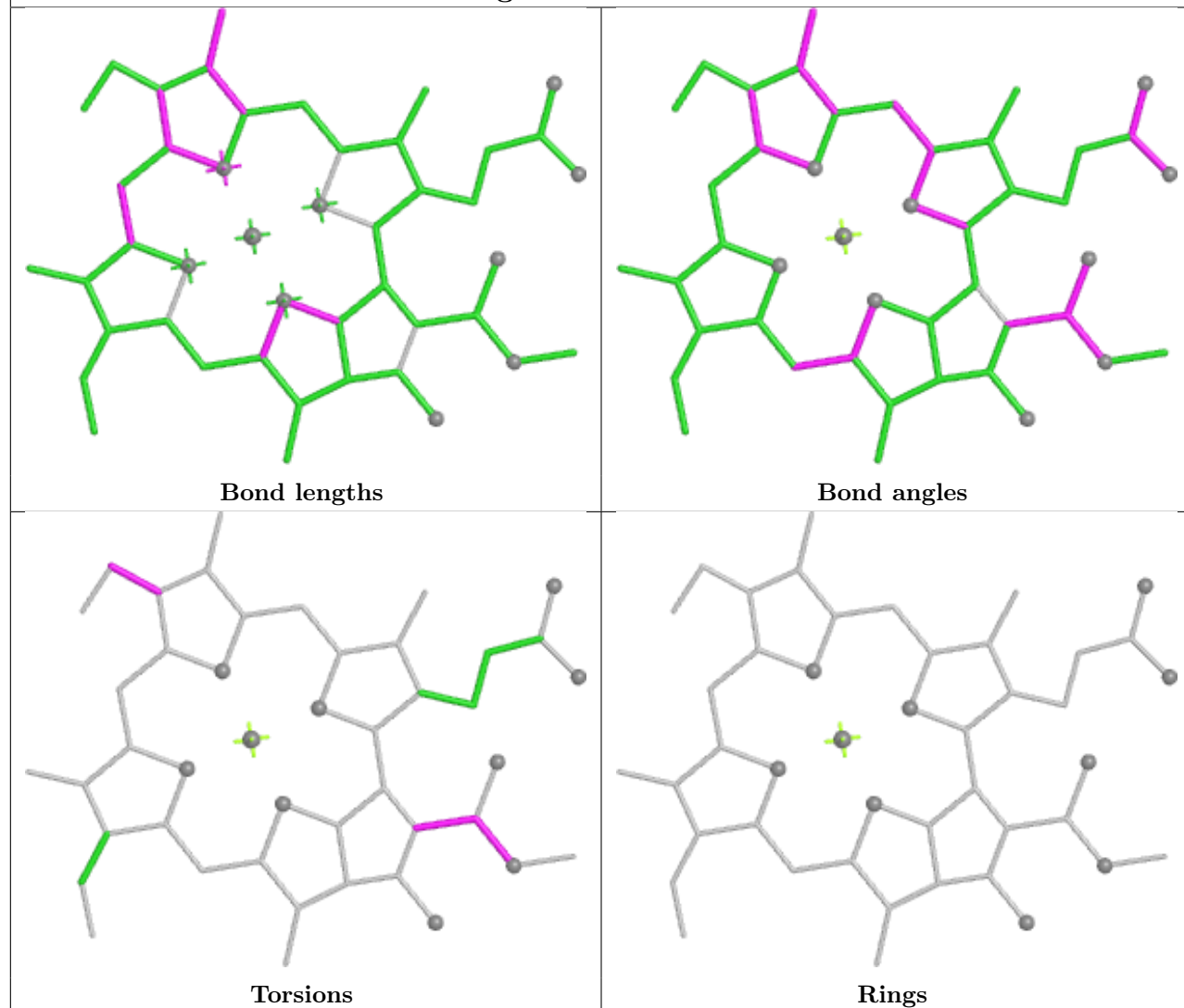


Rings

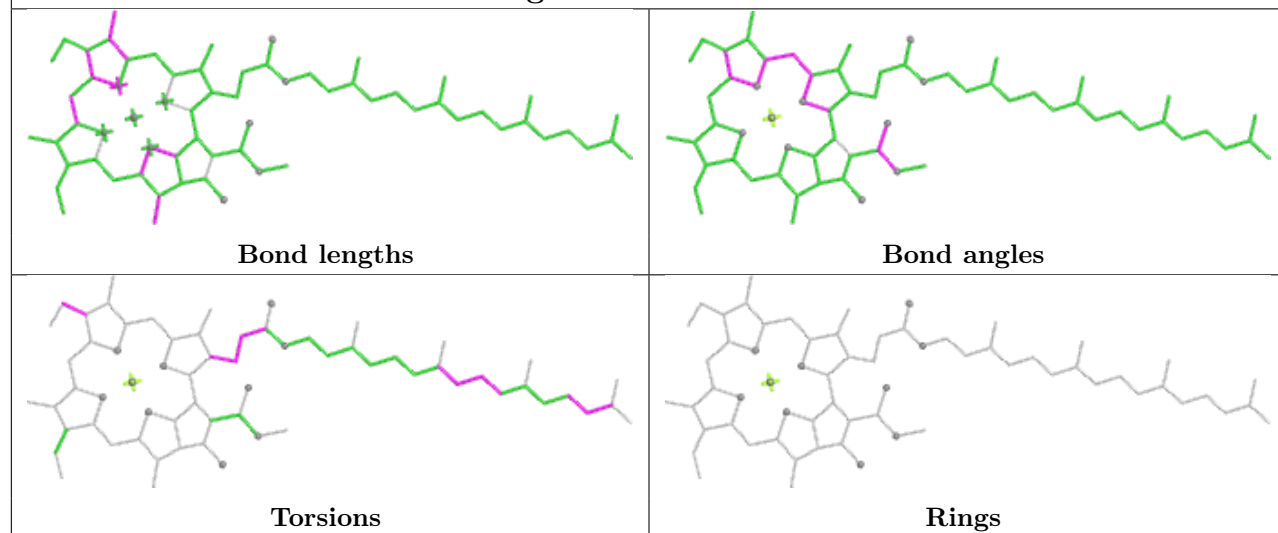
Ligand A1ECV 9 317



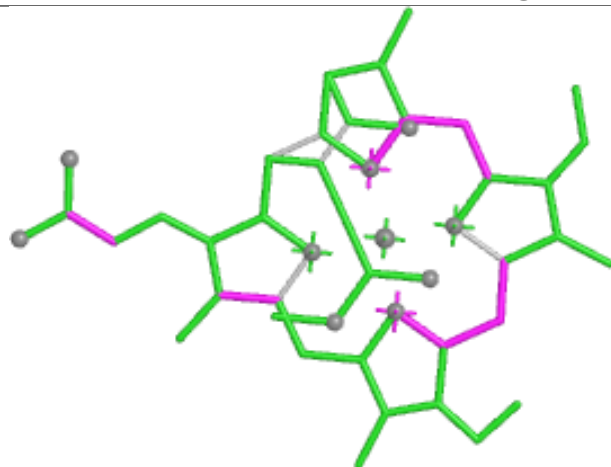
Ligand CLA a 812



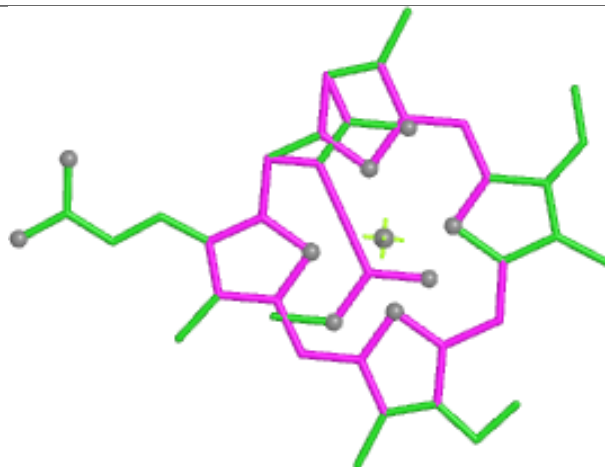
Ligand CLA W 309



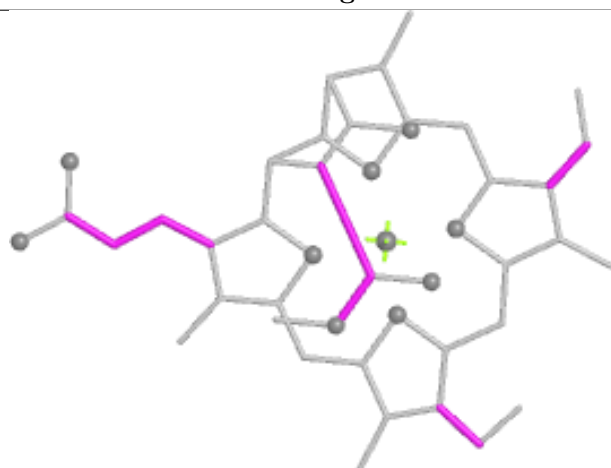
Ligand KC2 G 315



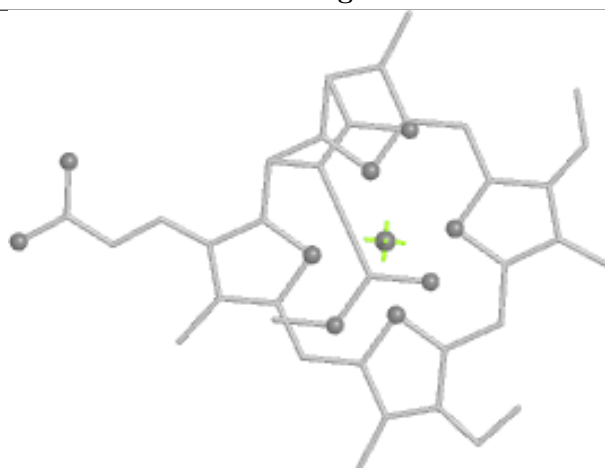
Bond lengths



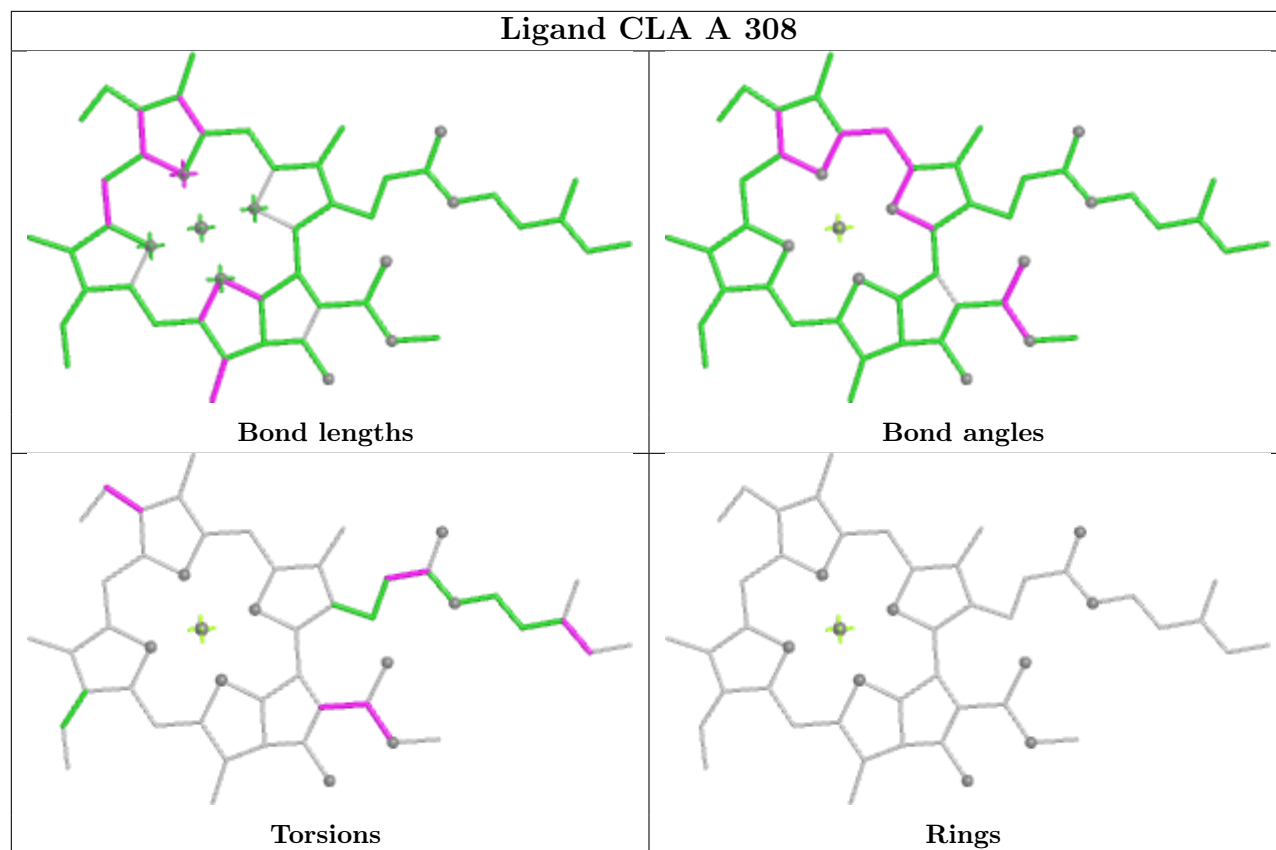
Bond angles



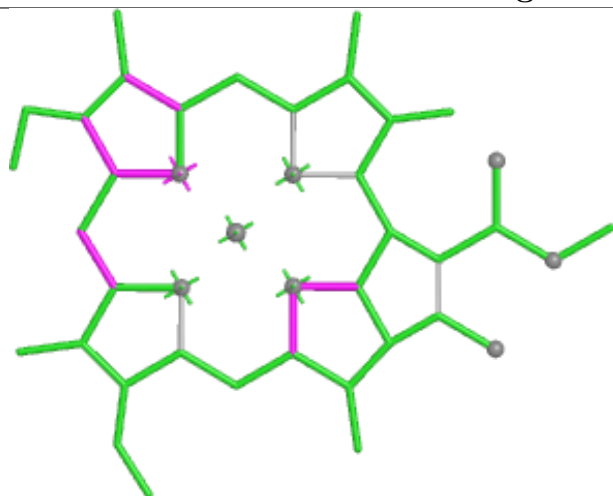
Torsions



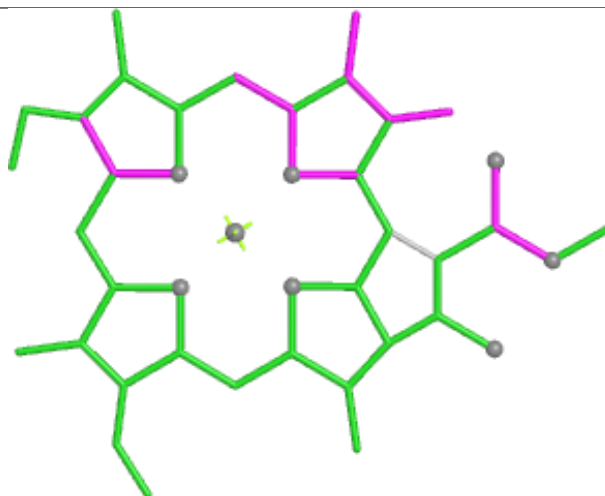
Rings



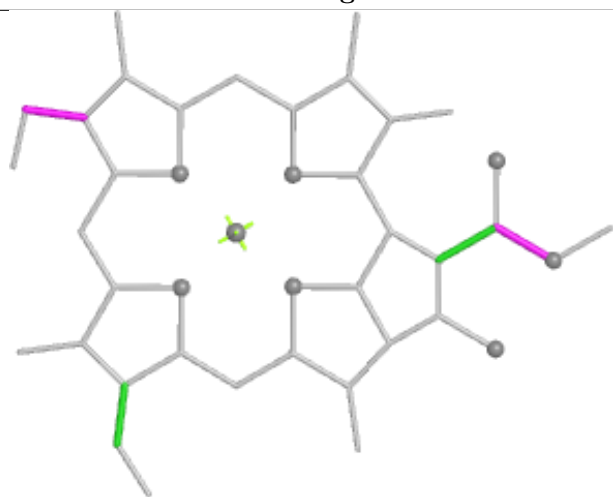
Ligand CLA Z 305



Bond lengths



Bond angles

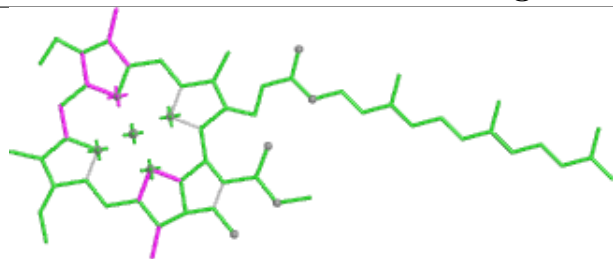


Torsions

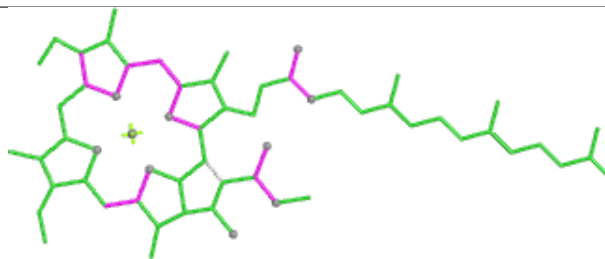


Rings

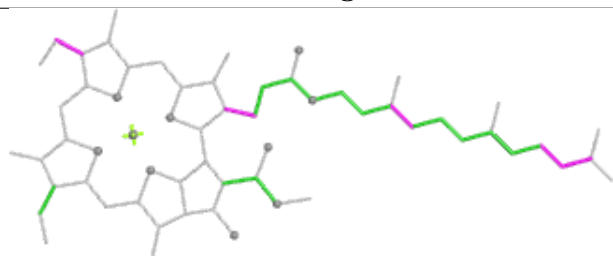
Ligand CLA U 210



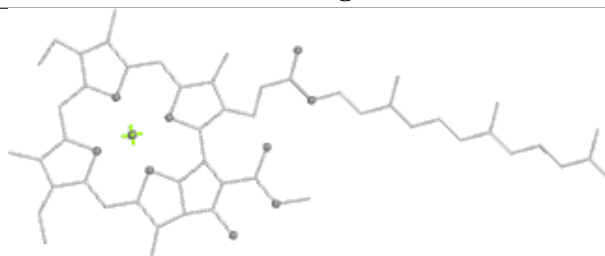
Bond lengths



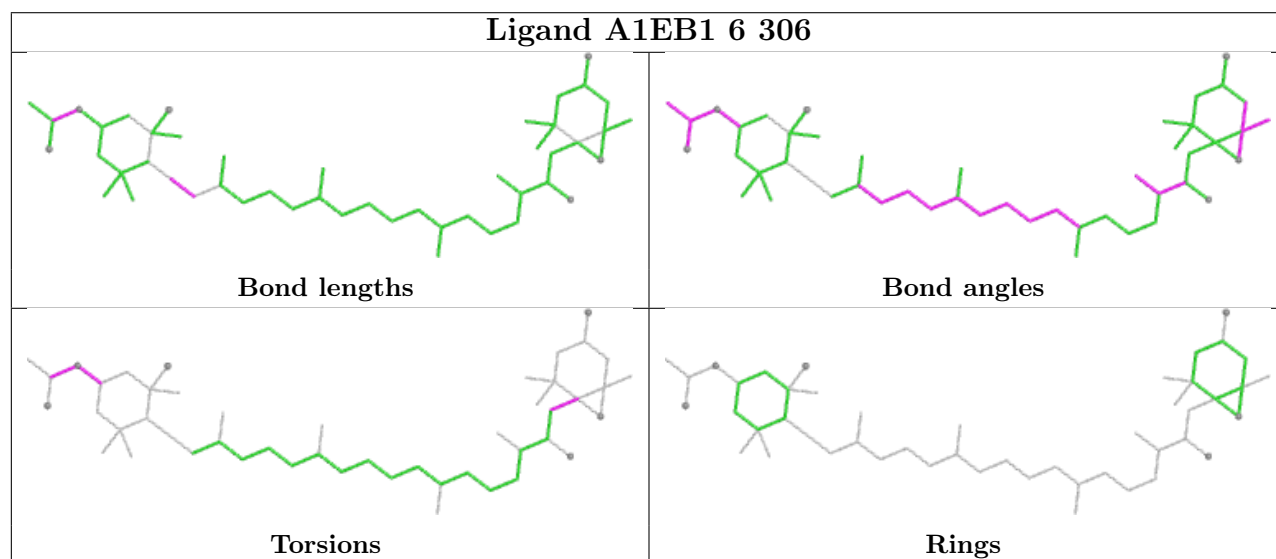
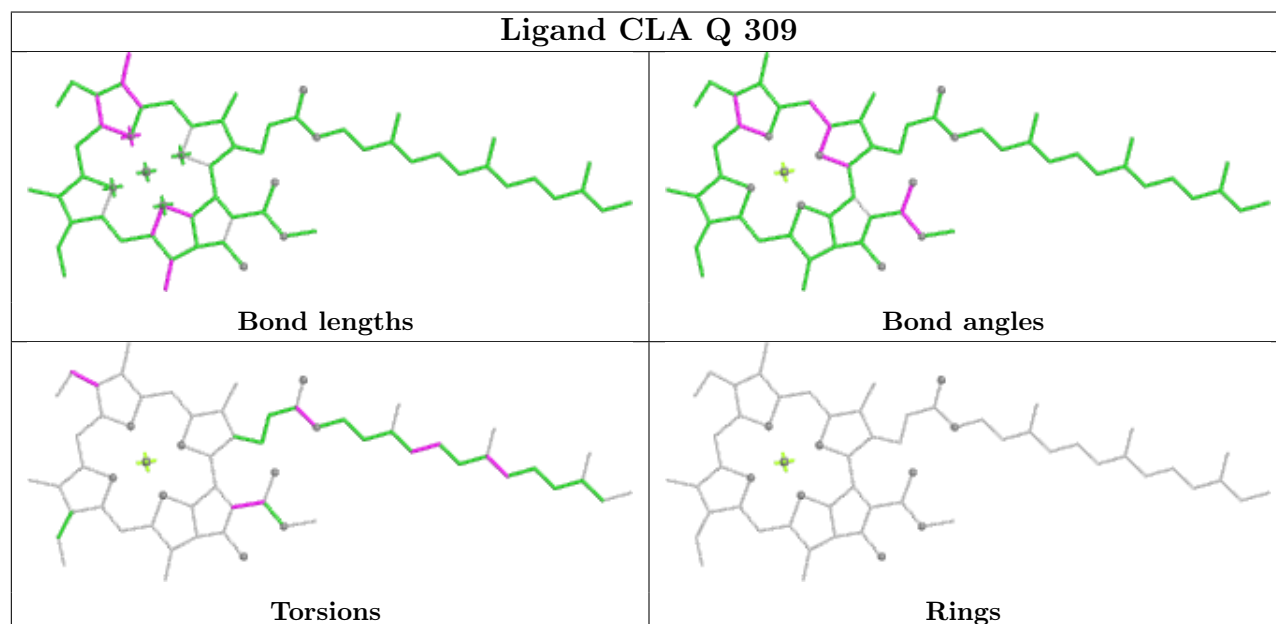
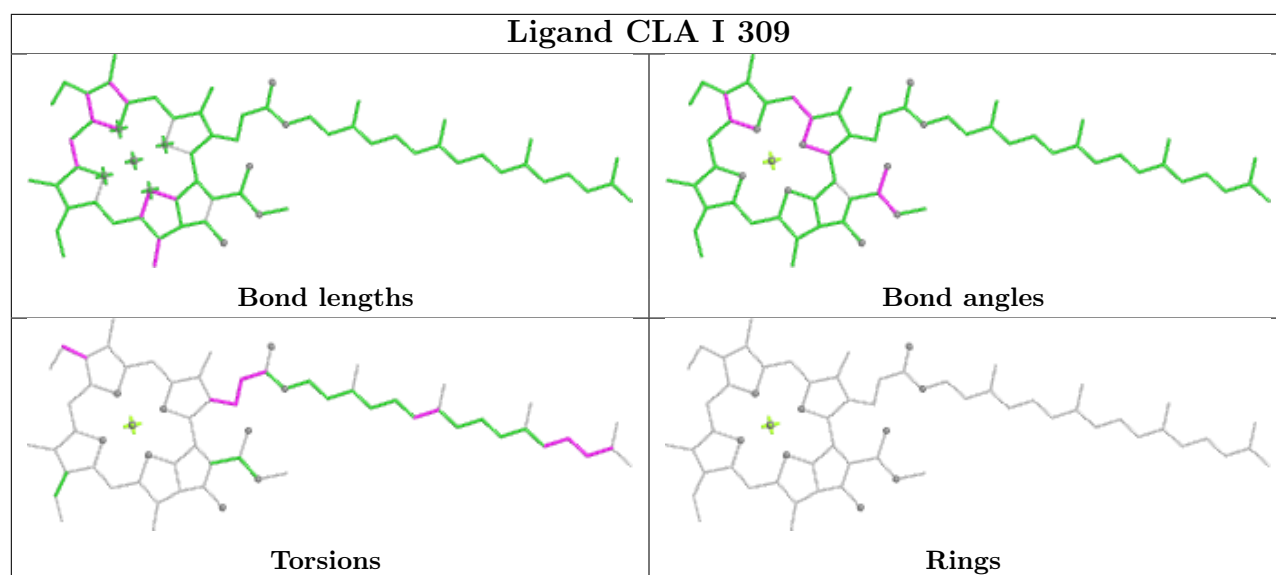
Bond angles

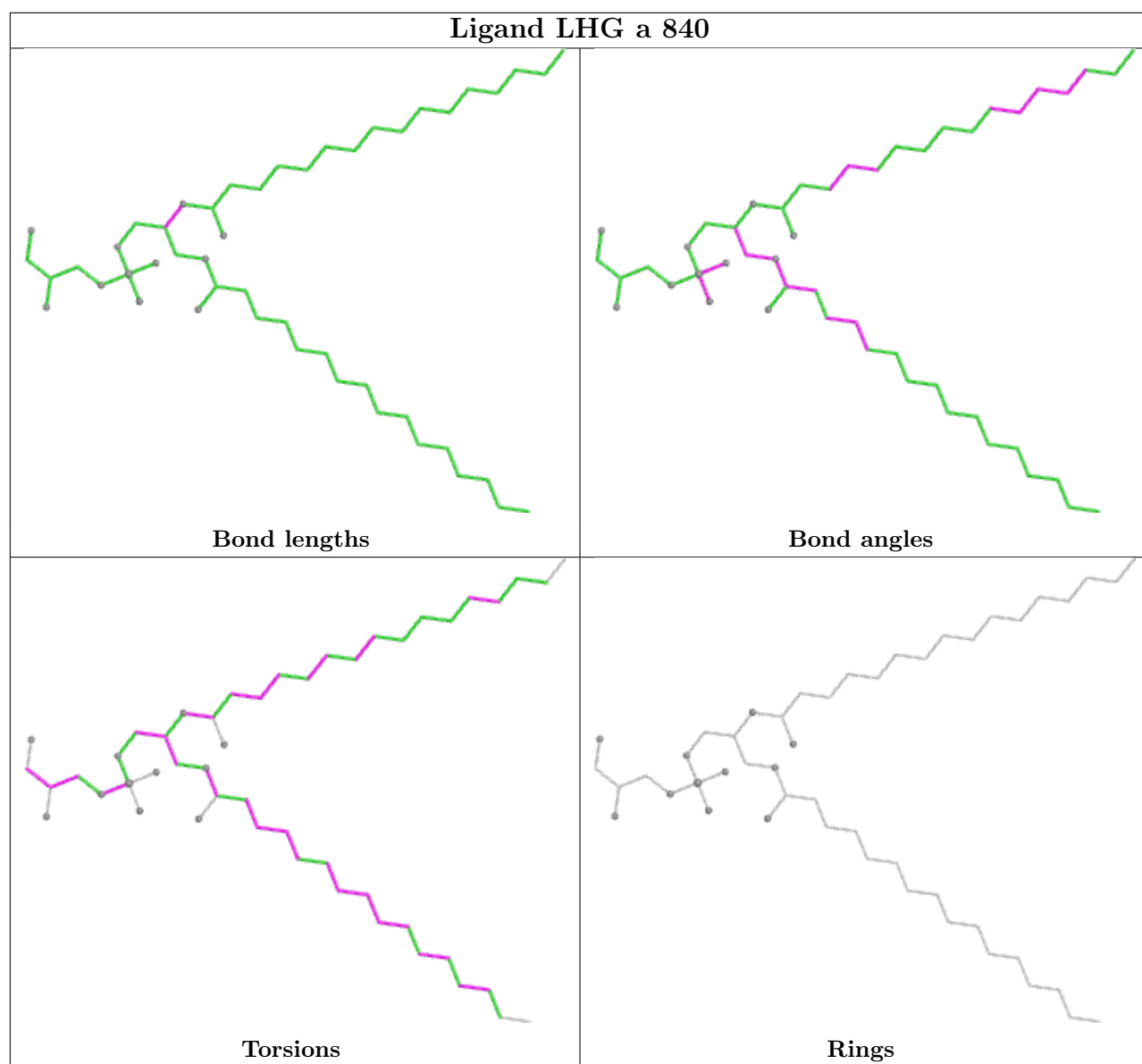


Torsions

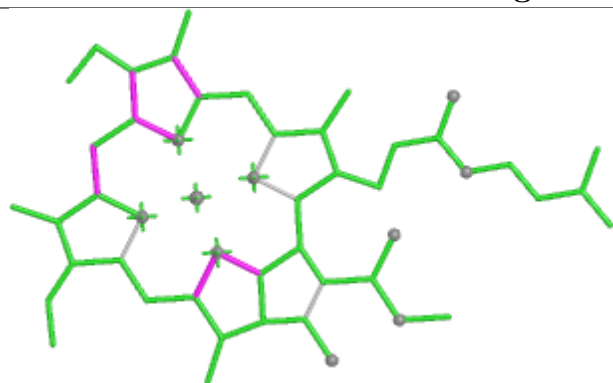


Rings

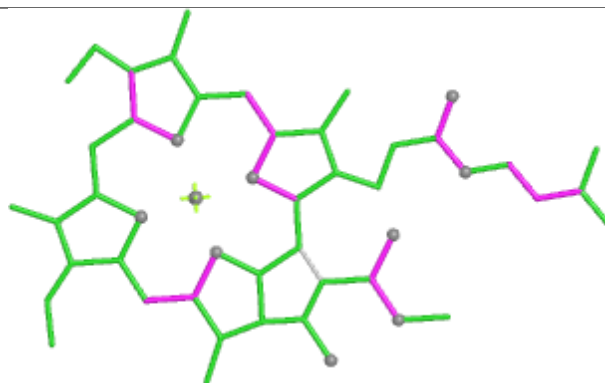




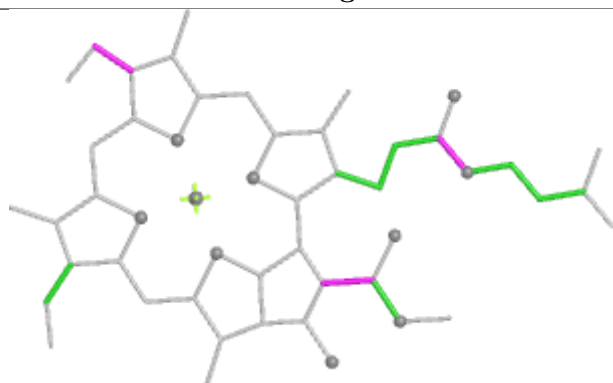
Ligand CLA X 311



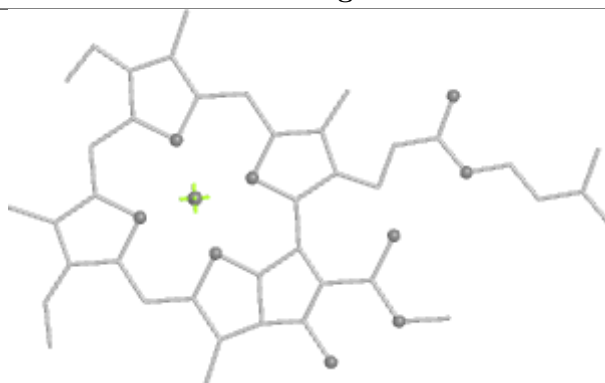
Bond lengths



Bond angles

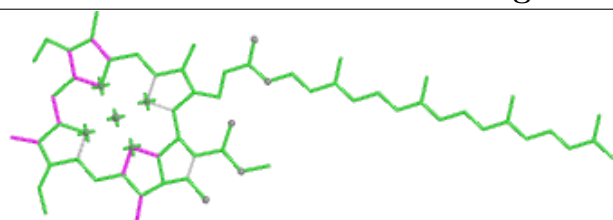


Torsions

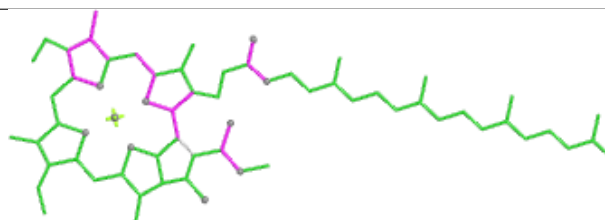


Rings

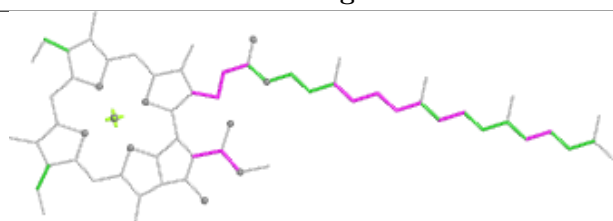
Ligand CLA D 317



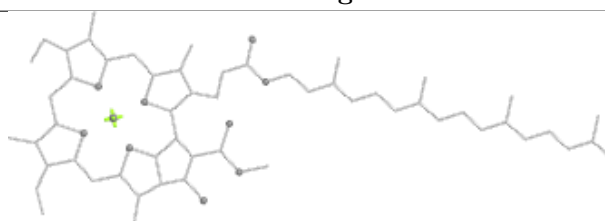
Bond lengths



Bond angles

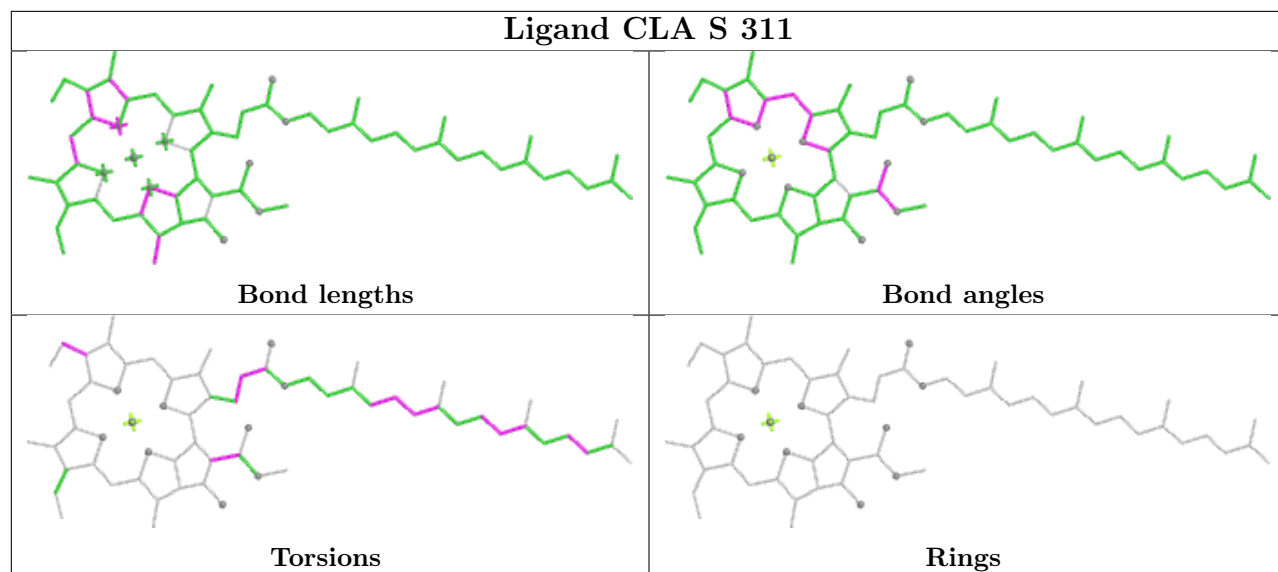


Torsions

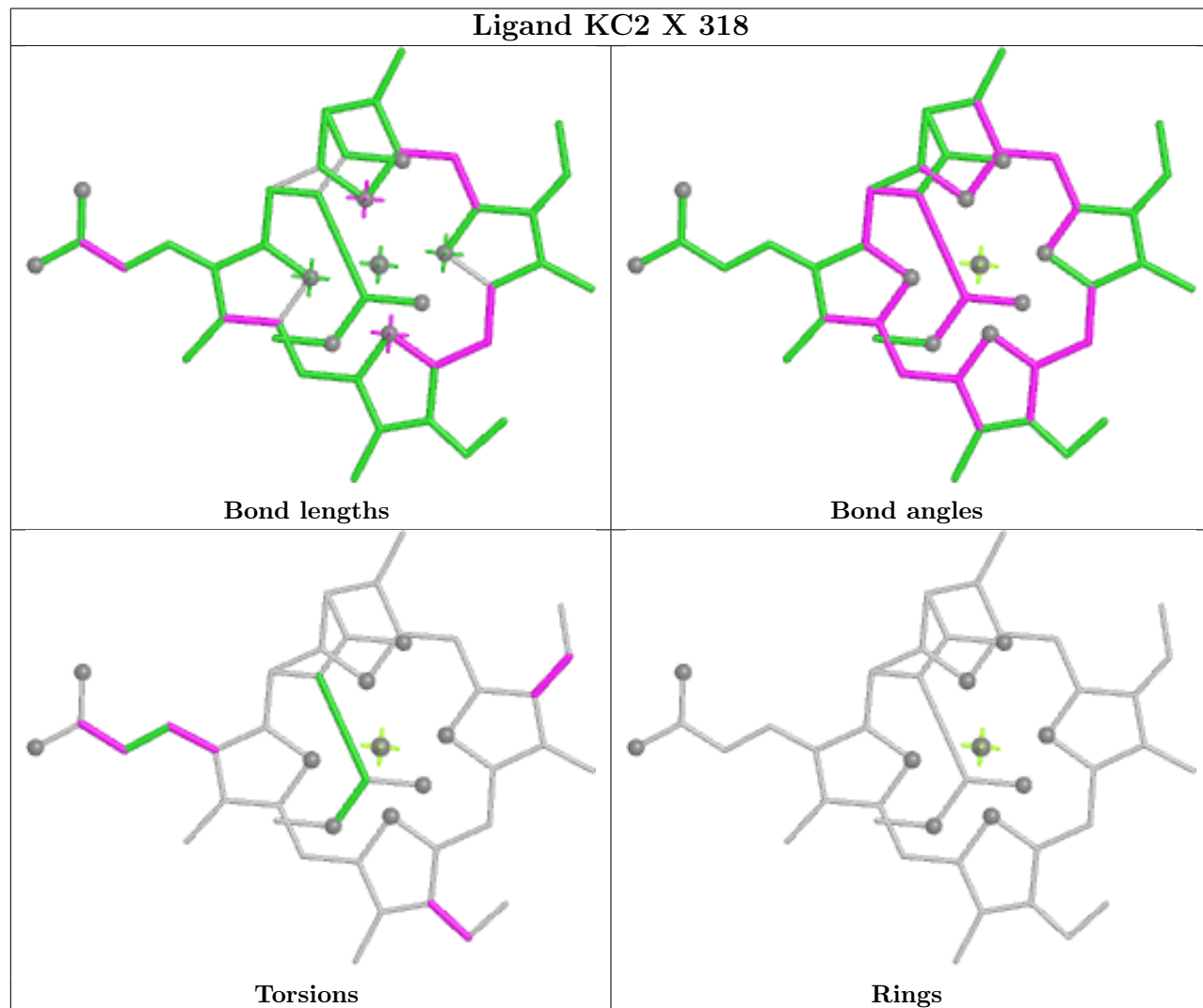


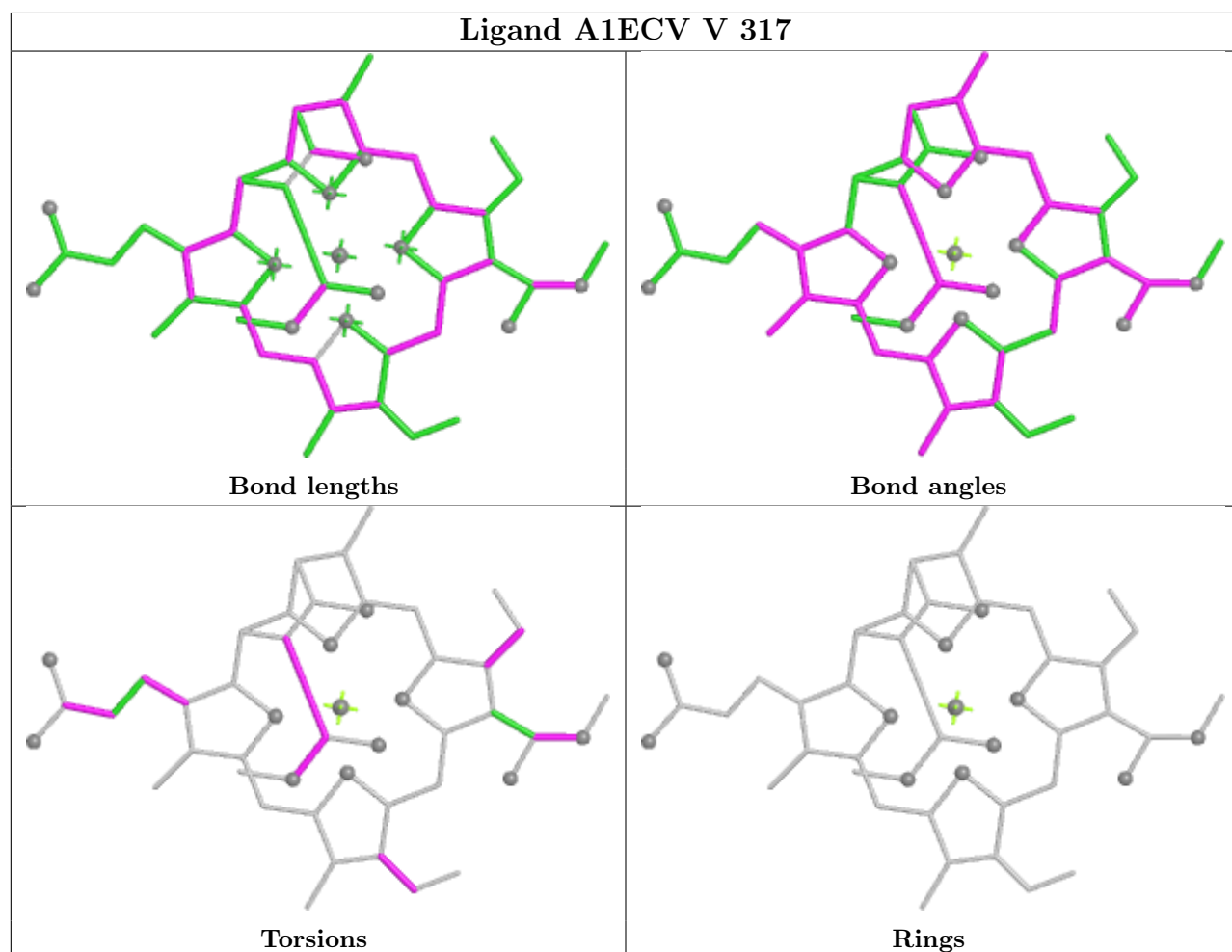
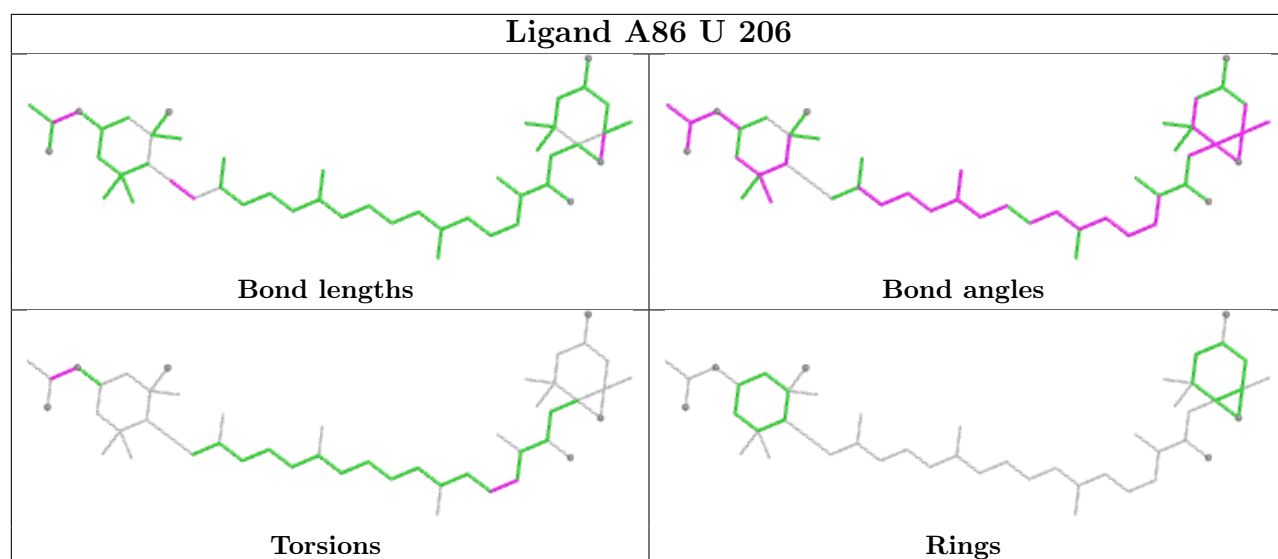
Rings

Ligand CLA S 311

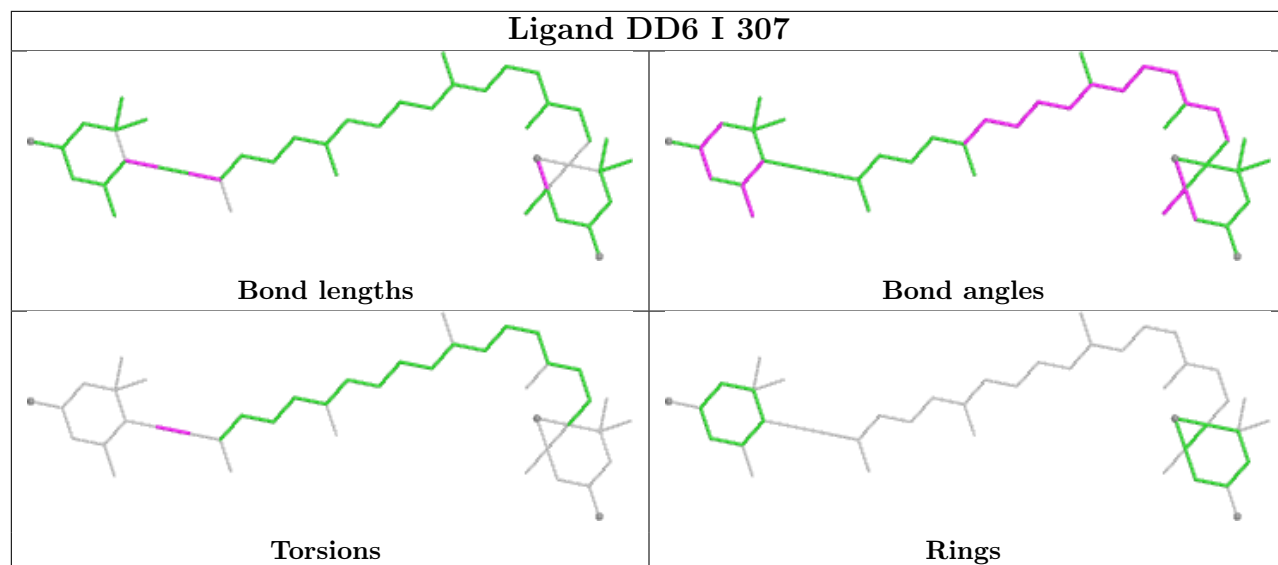


Ligand KC2 X 318

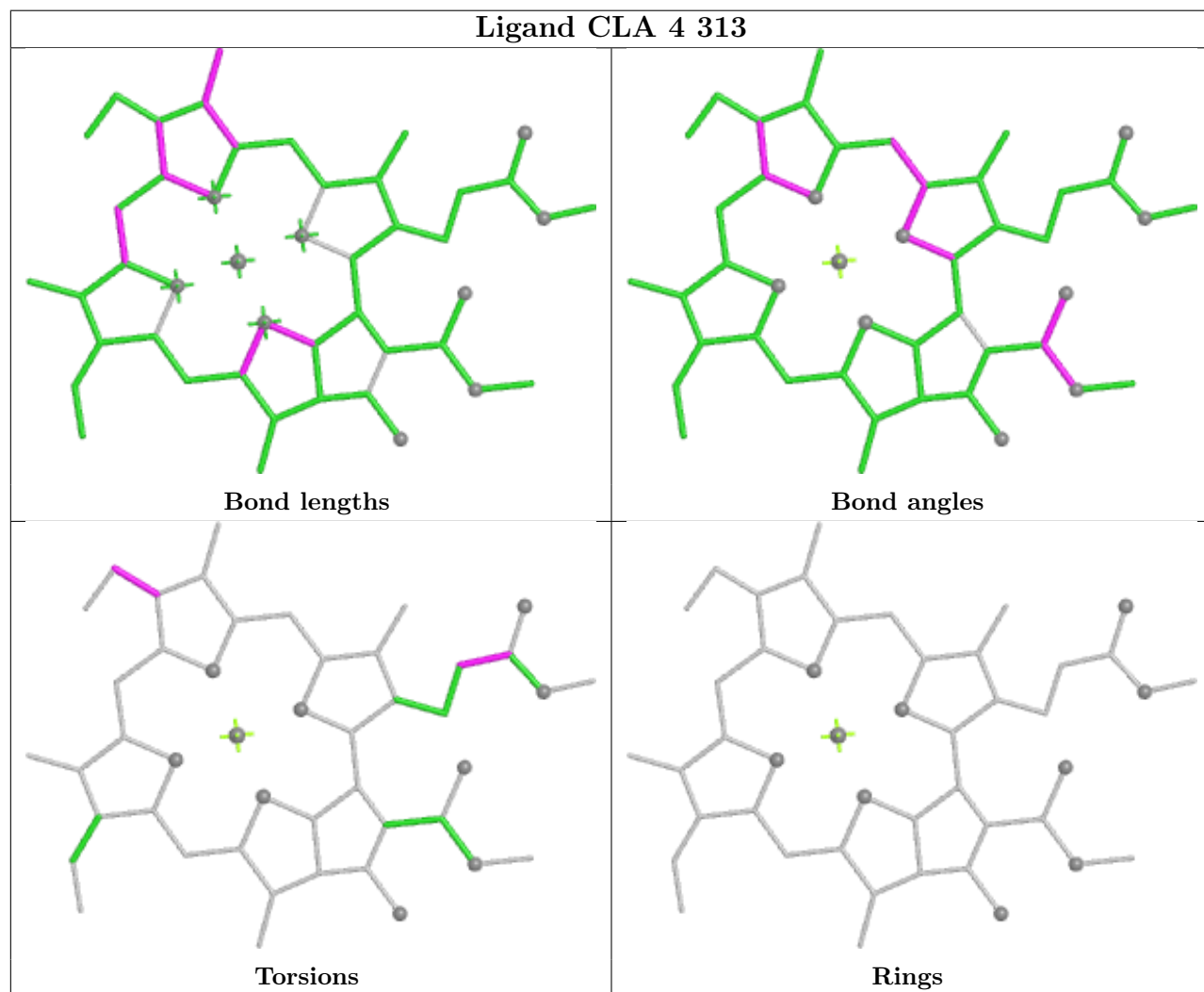




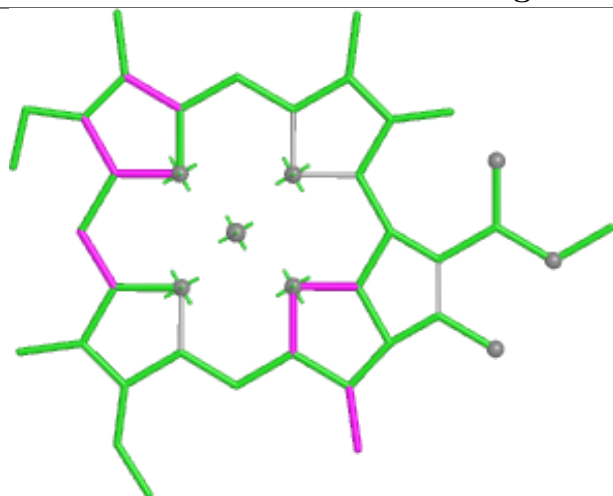
Ligand DD6 I 307



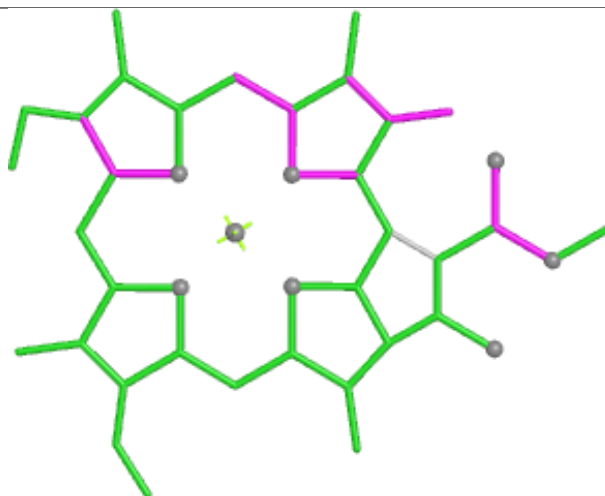
Ligand CLA 4 313



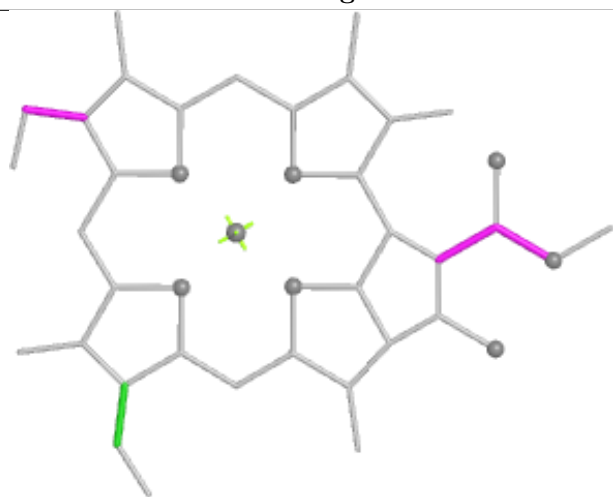
Ligand CLA U 213



Bond lengths



Bond angles

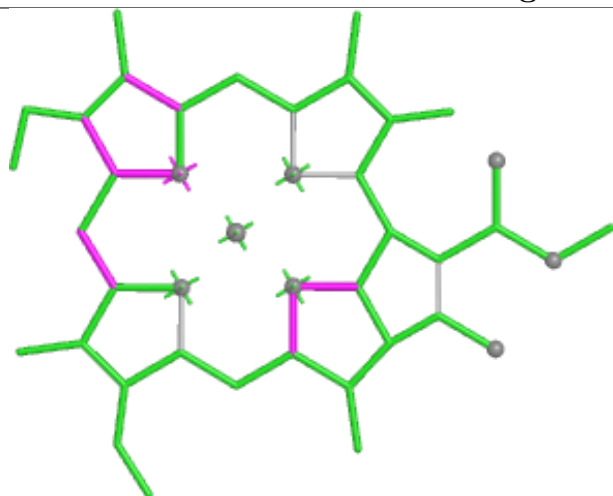


Torsions

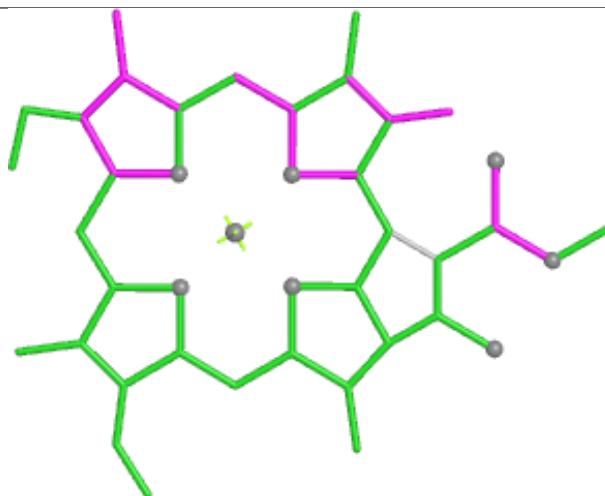


Rings

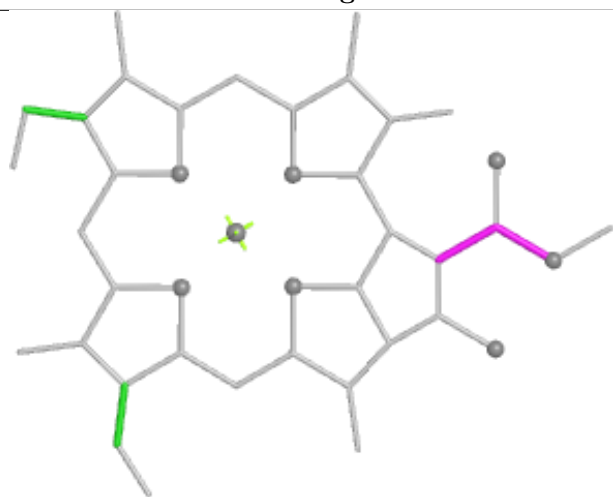
Ligand CLA z 318



Bond lengths



Bond angles

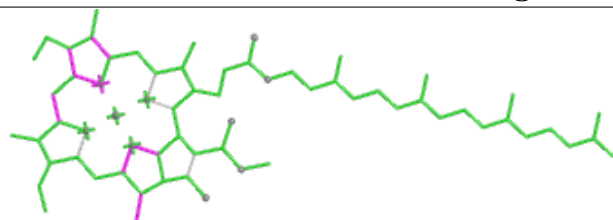


Torsions

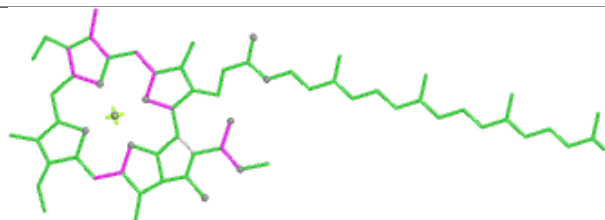


Rings

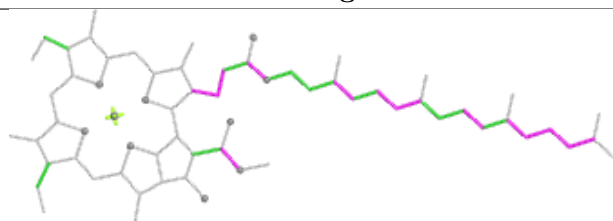
Ligand CLA K 312



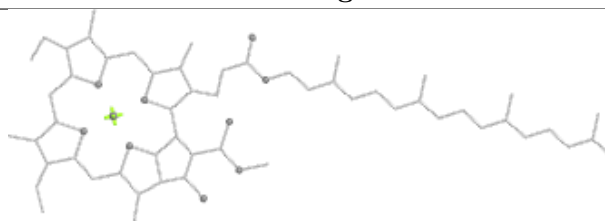
Bond lengths



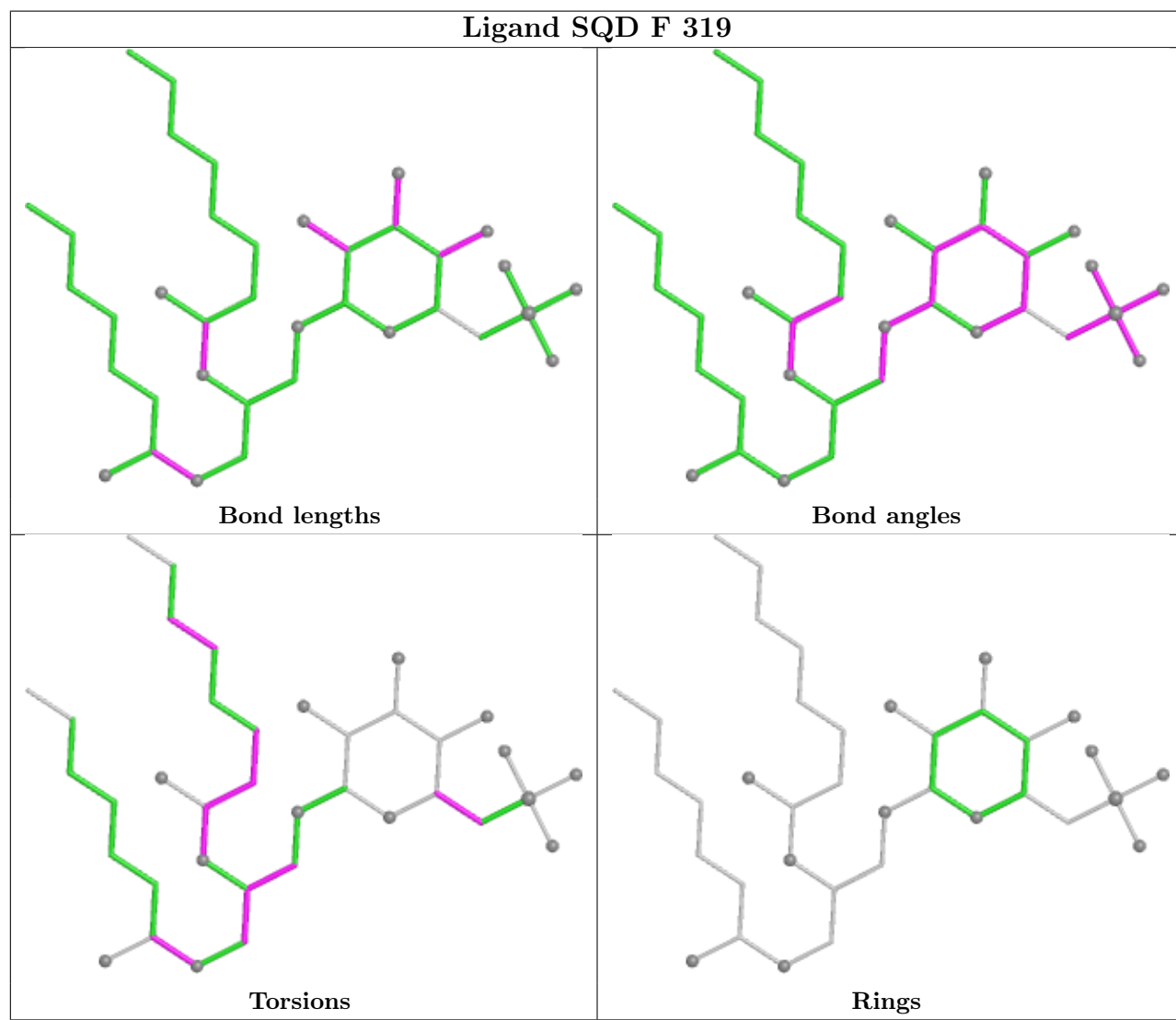
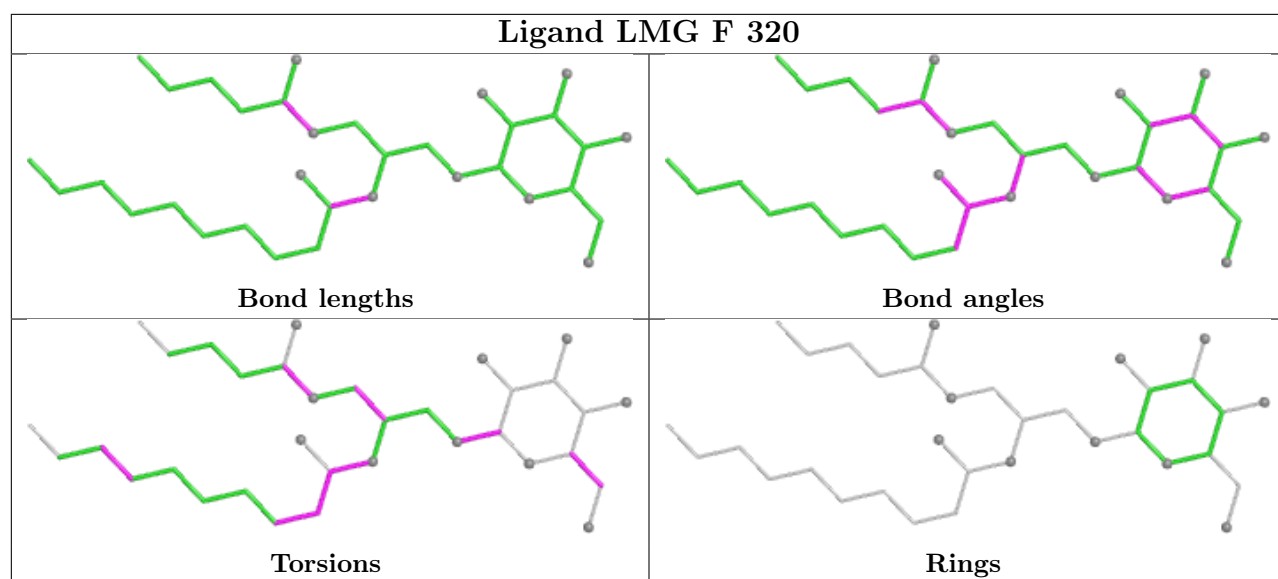
Bond angles

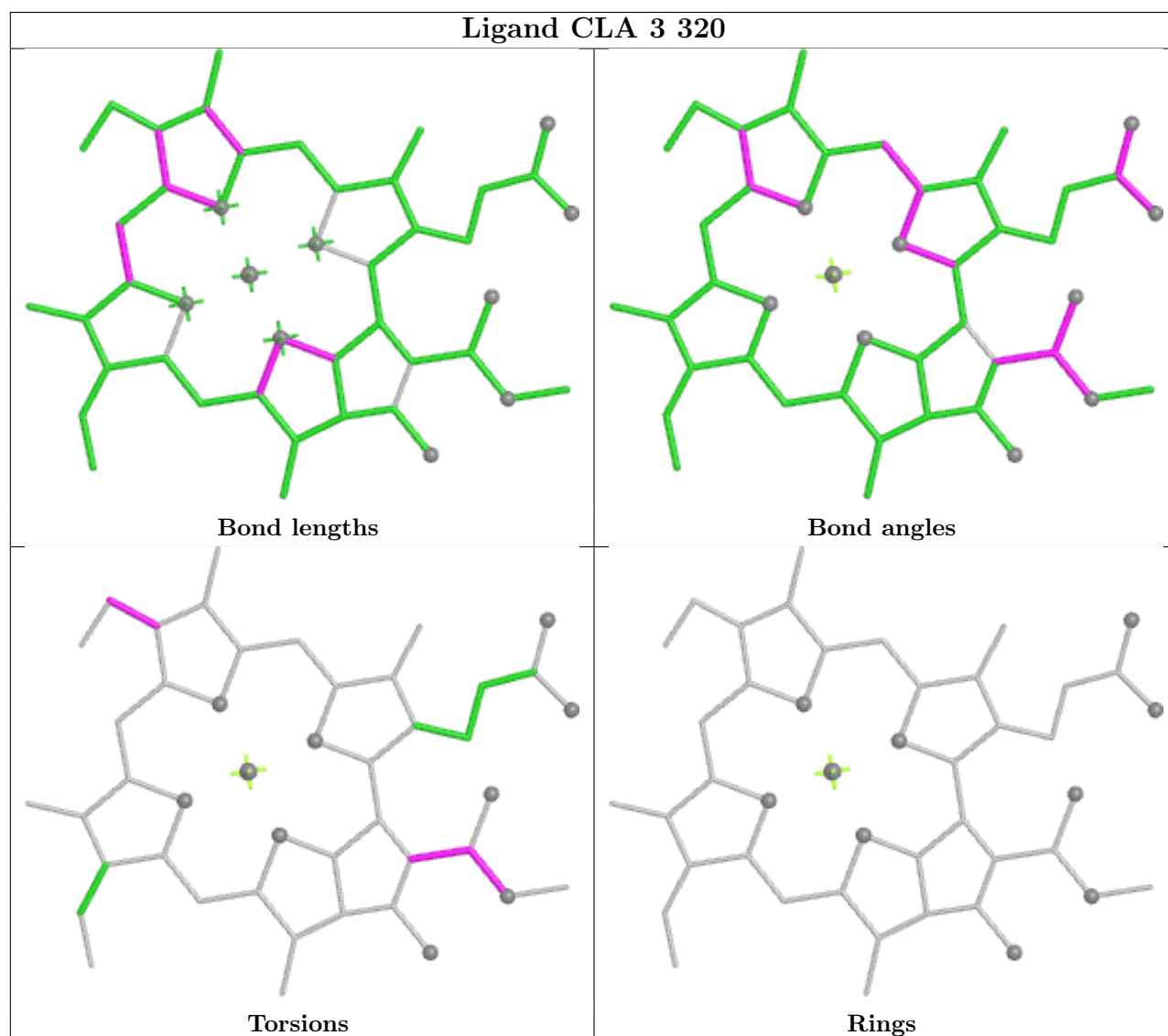
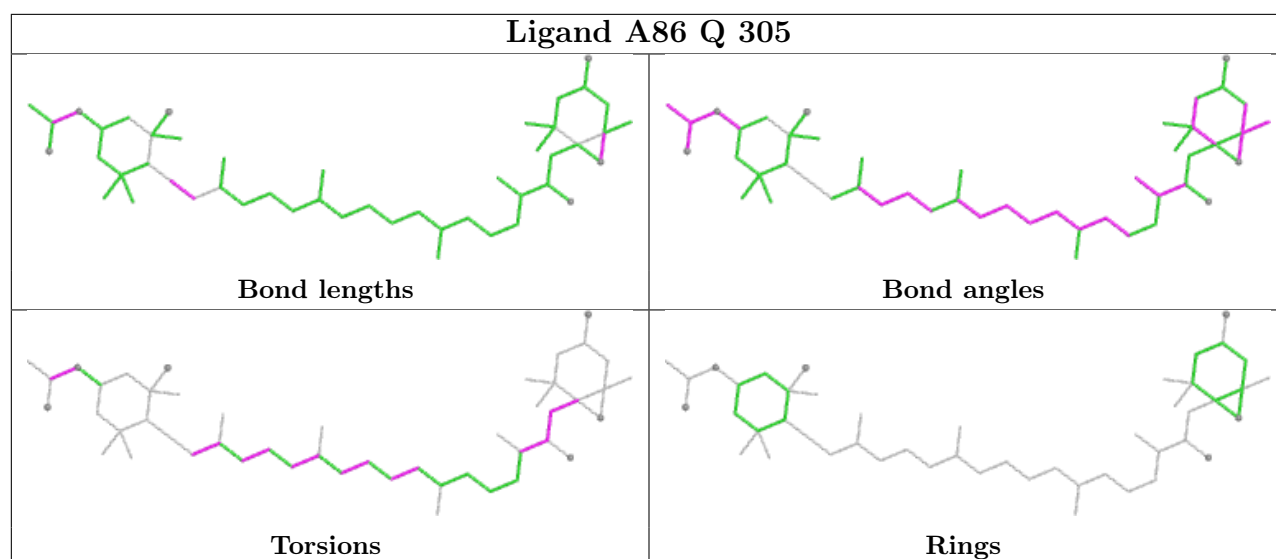


Torsions

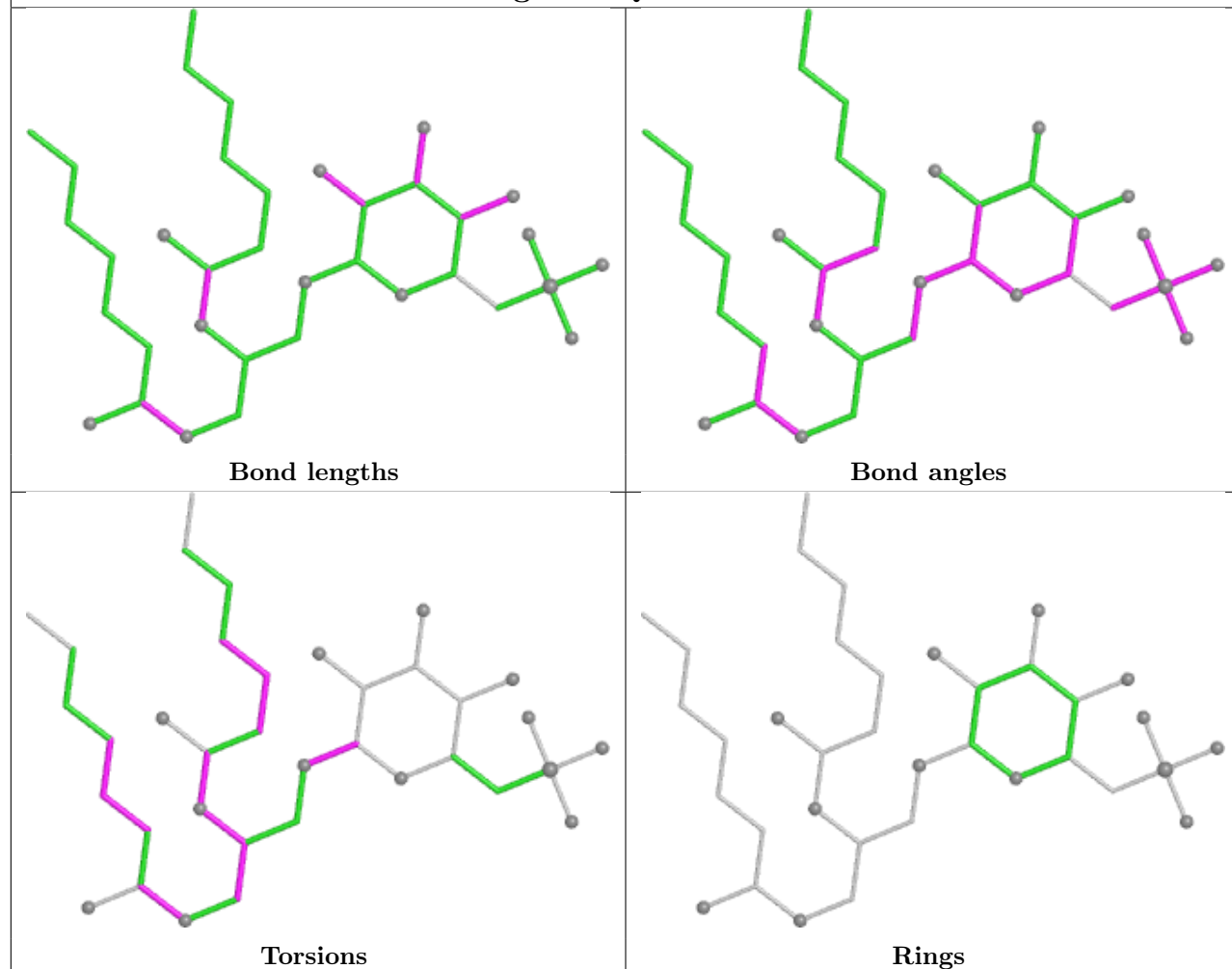


Rings

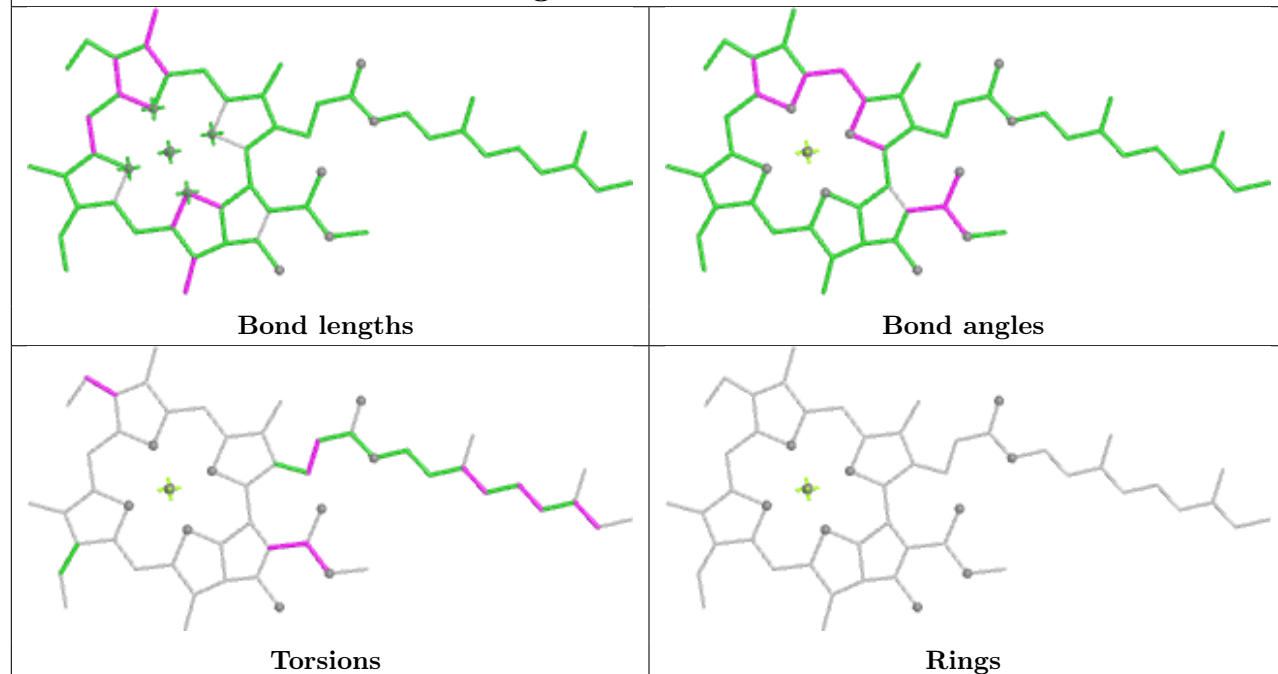




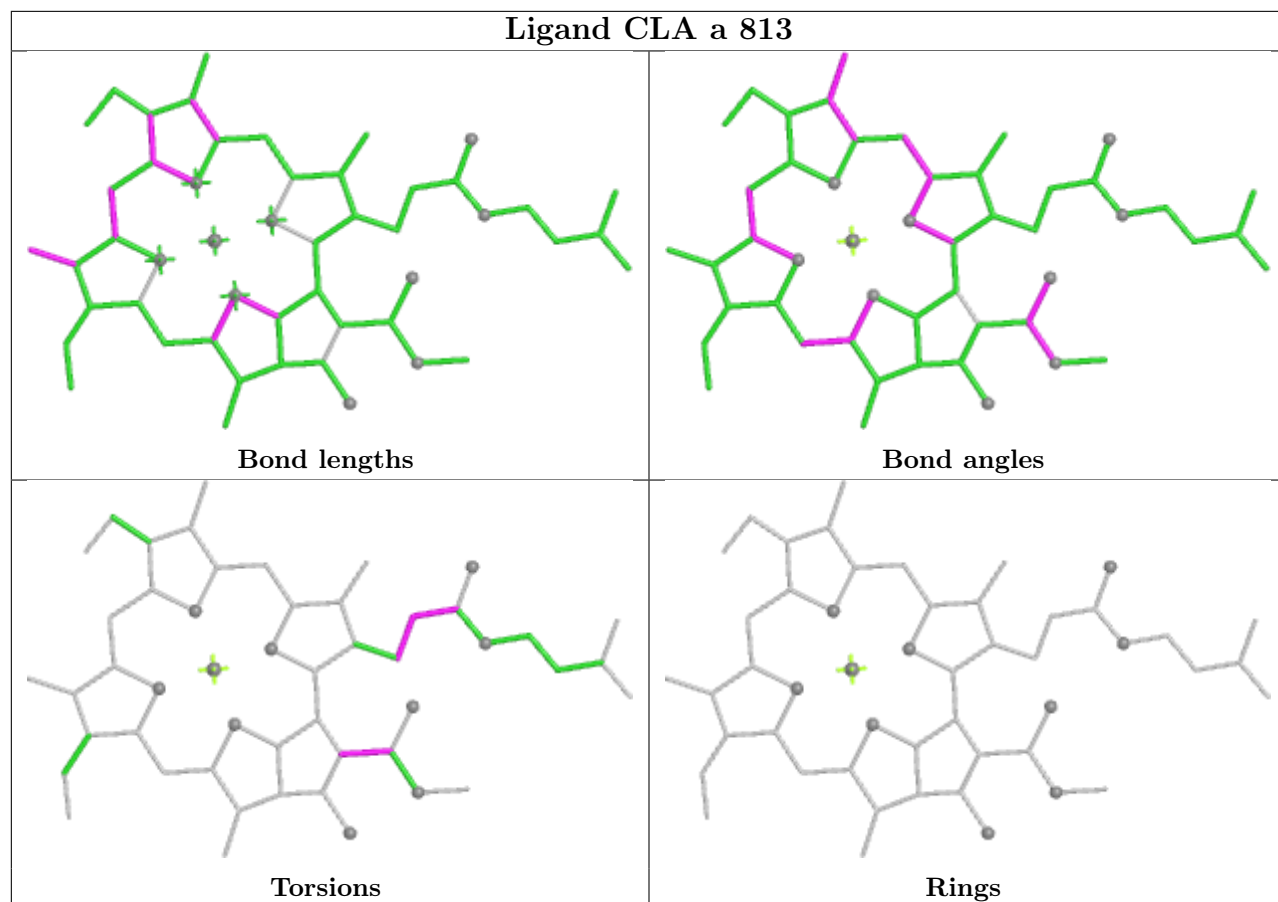
Ligand SQD T 321



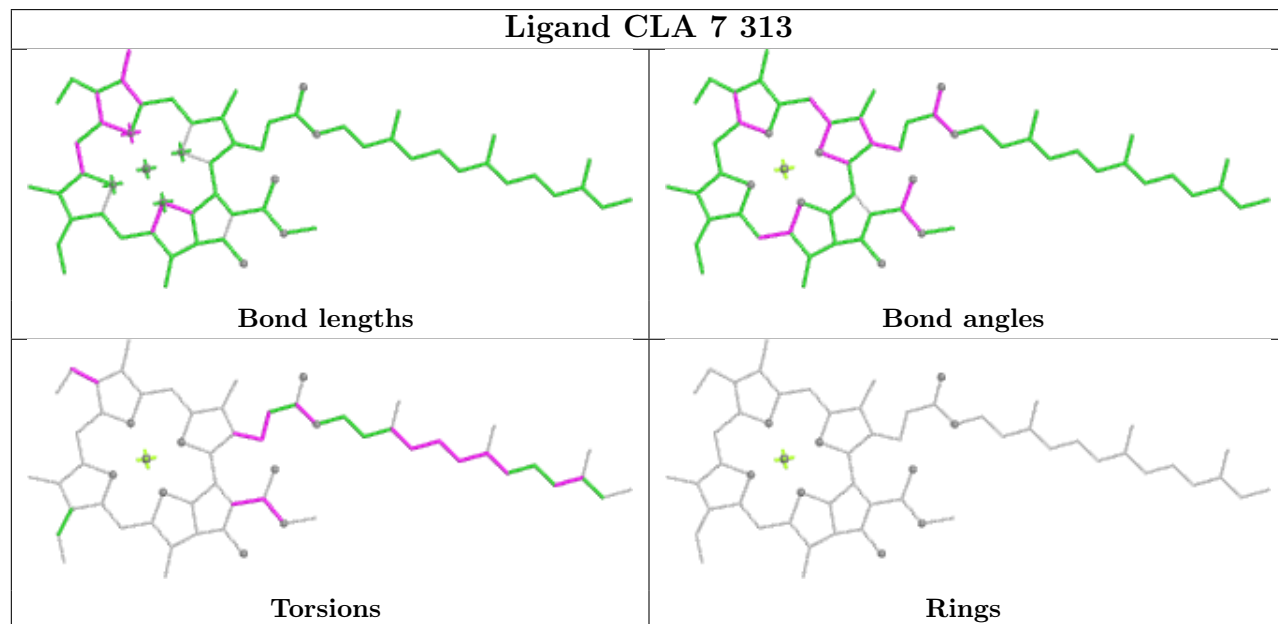
Ligand CLA B 209



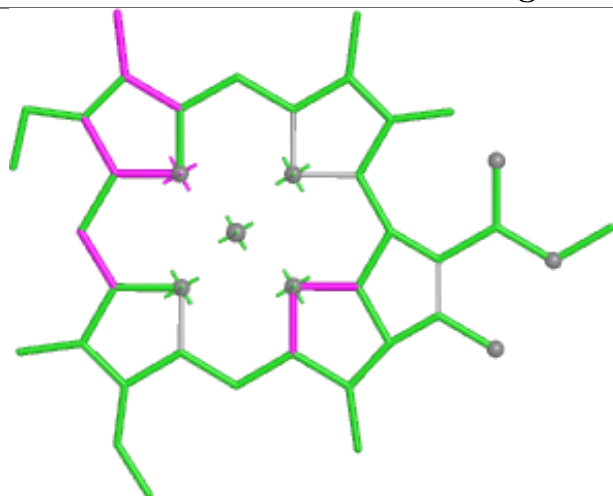
Ligand CLA a 813



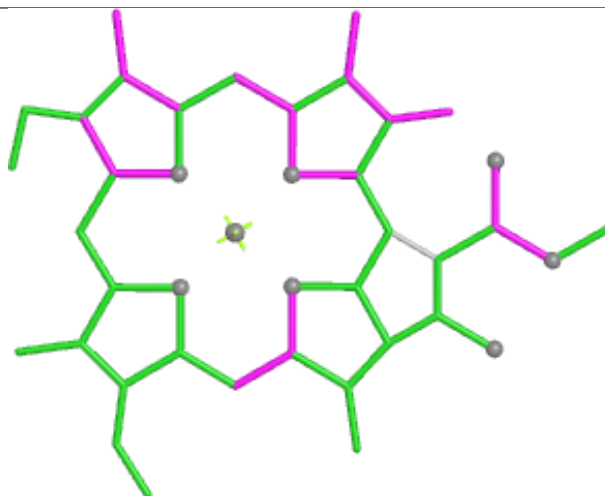
Ligand CLA 7 313



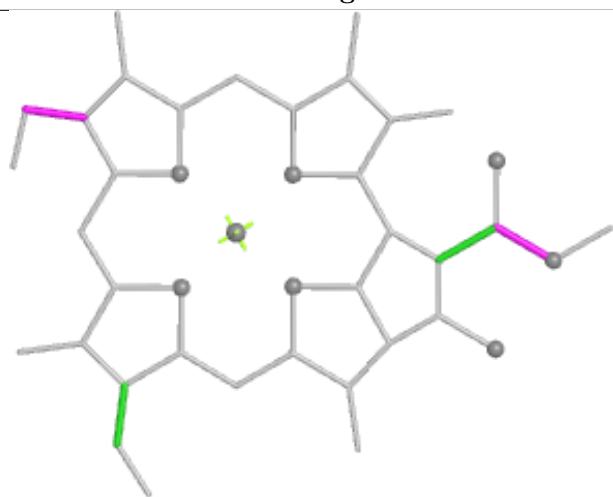
Ligand CLA 9 320



Bond lengths



Bond angles

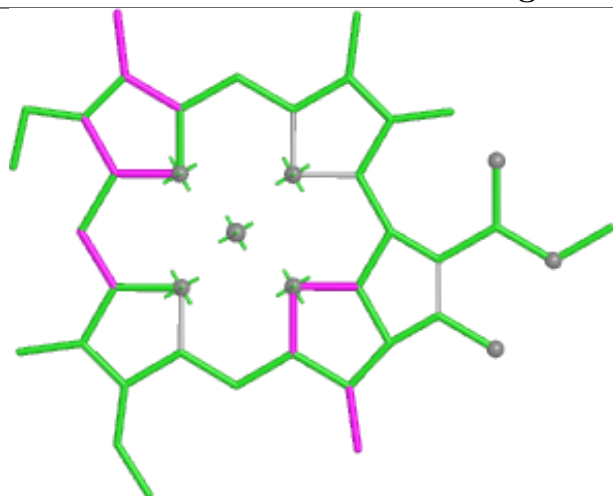


Torsions

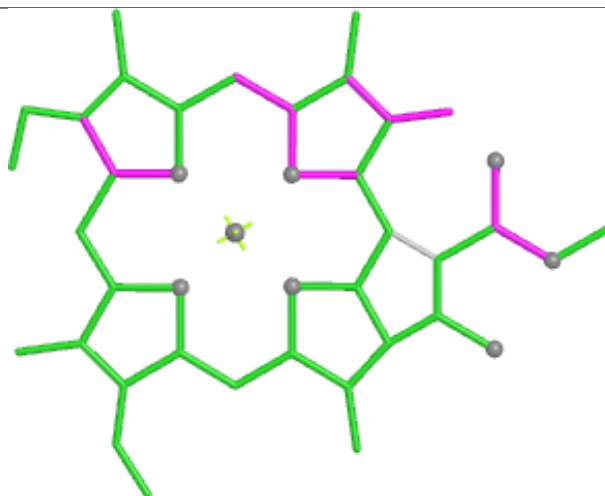


Rings

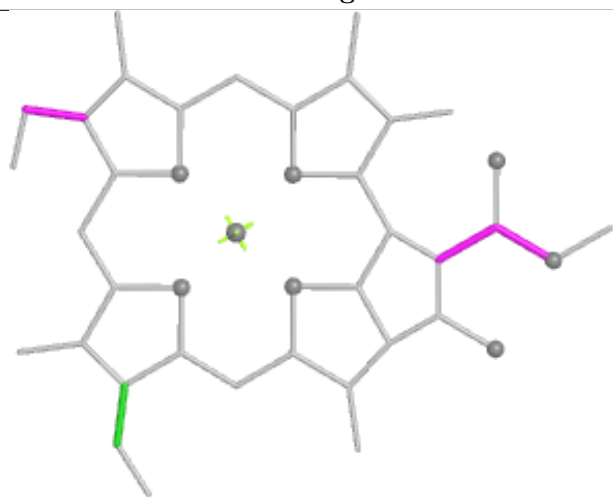
Ligand CLA 1 313



Bond lengths



Bond angles

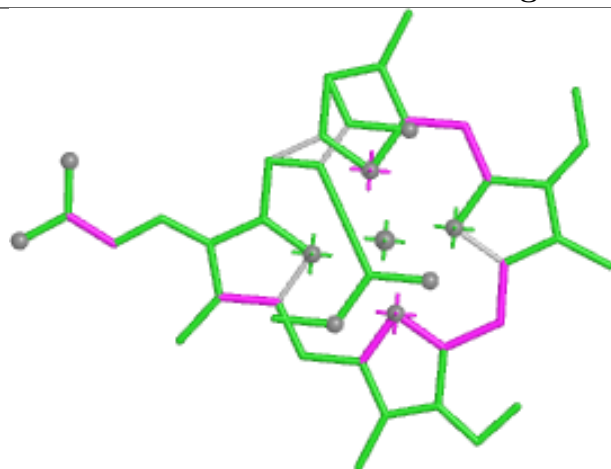


Torsions



Rings

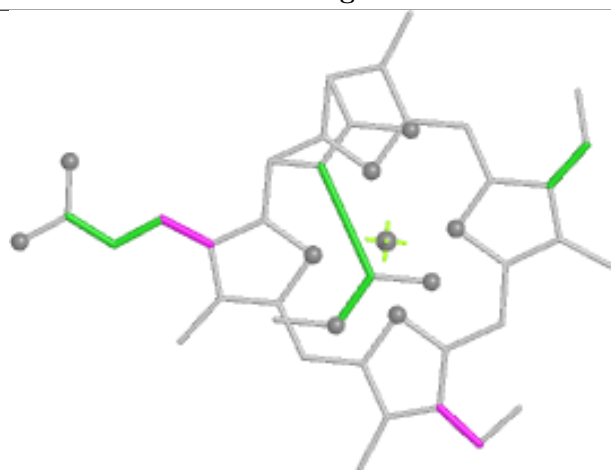
Ligand KC2 0 317



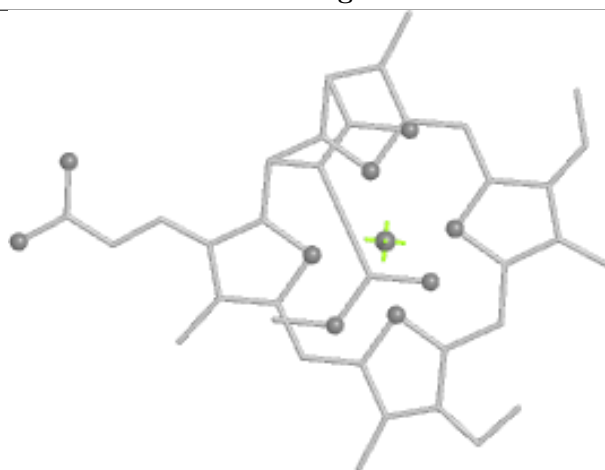
Bond lengths



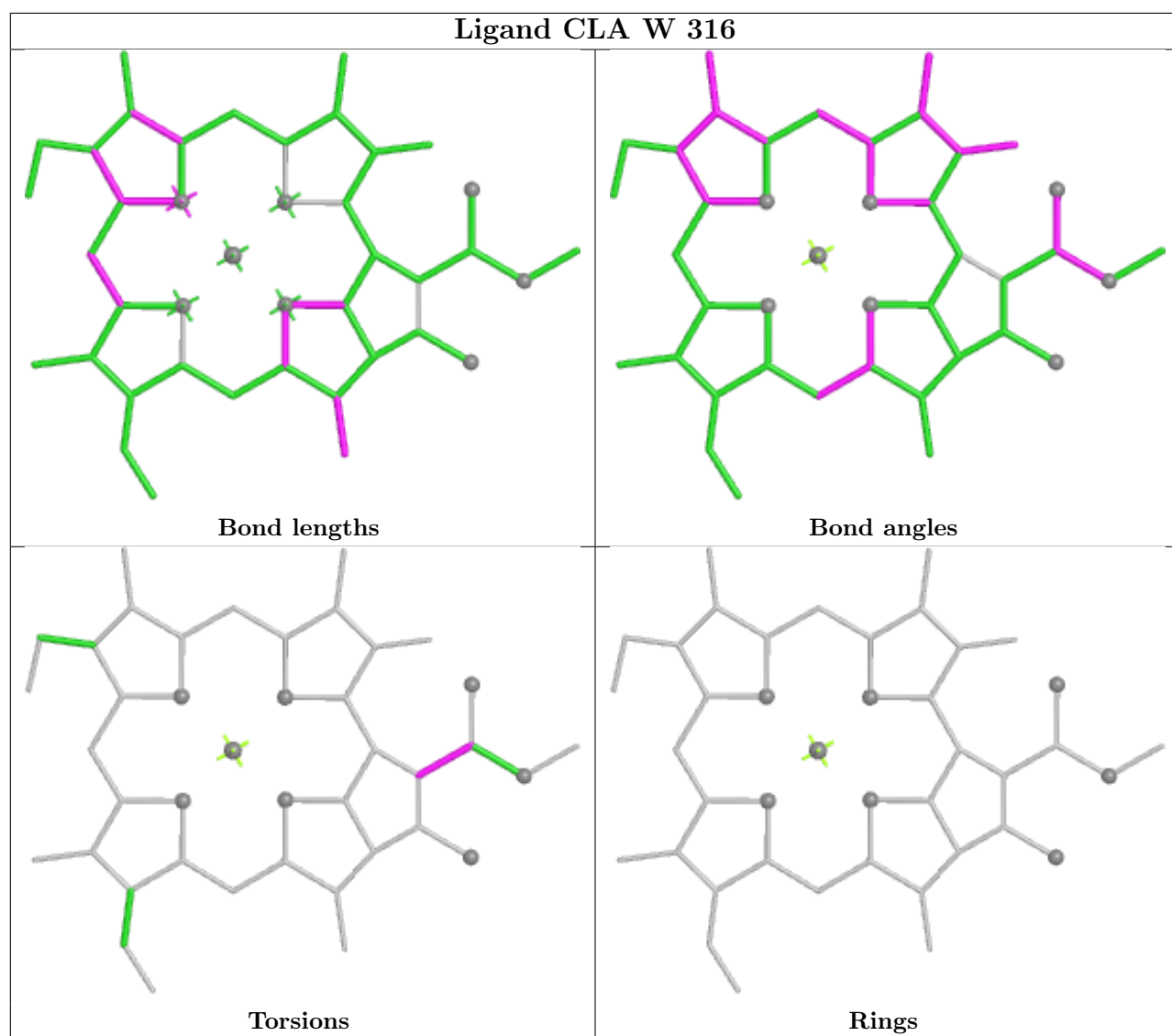
Bond angles

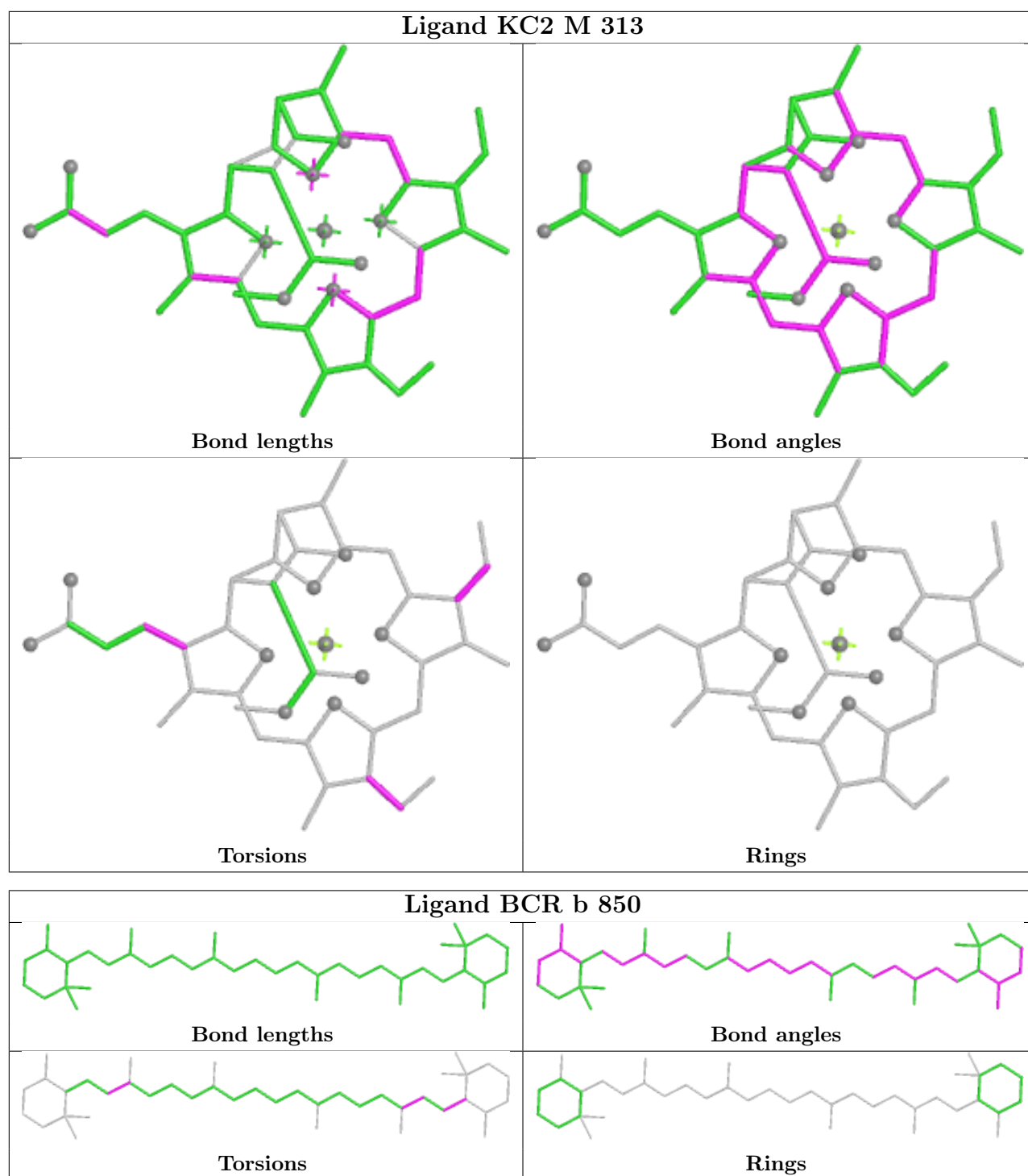


Torsions

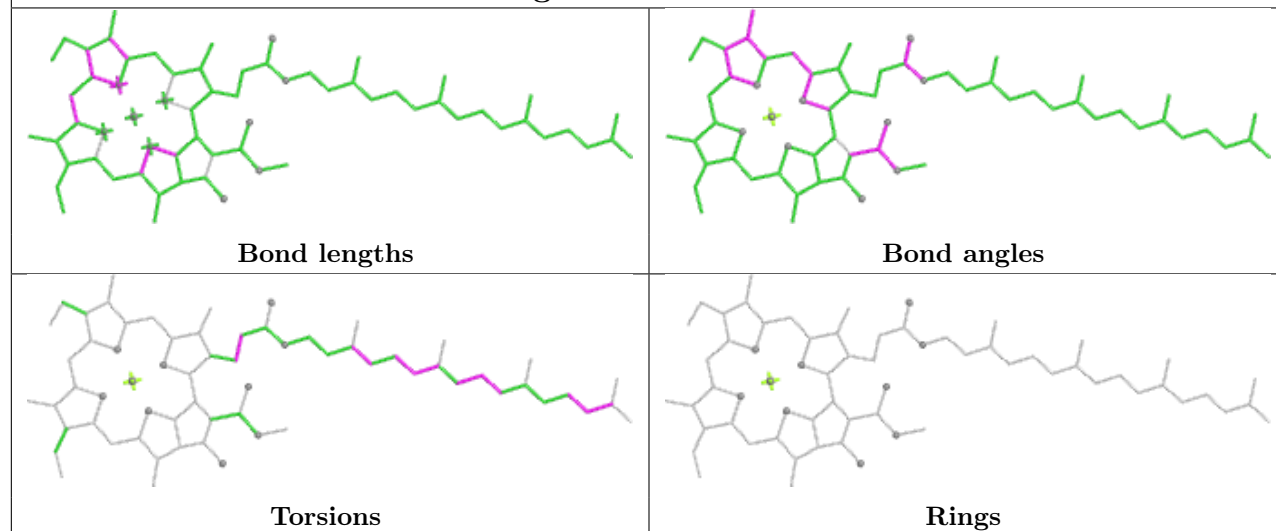


Rings

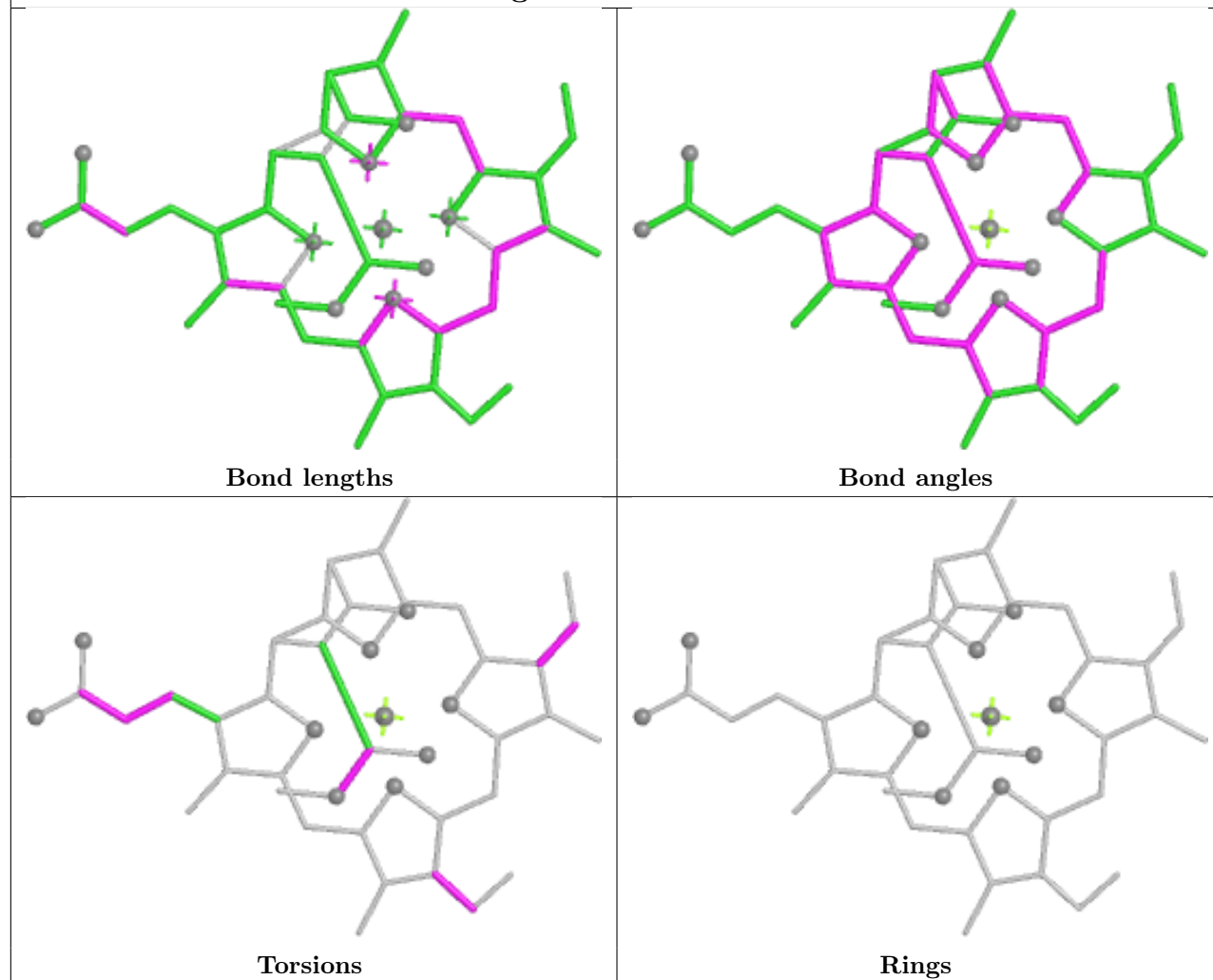


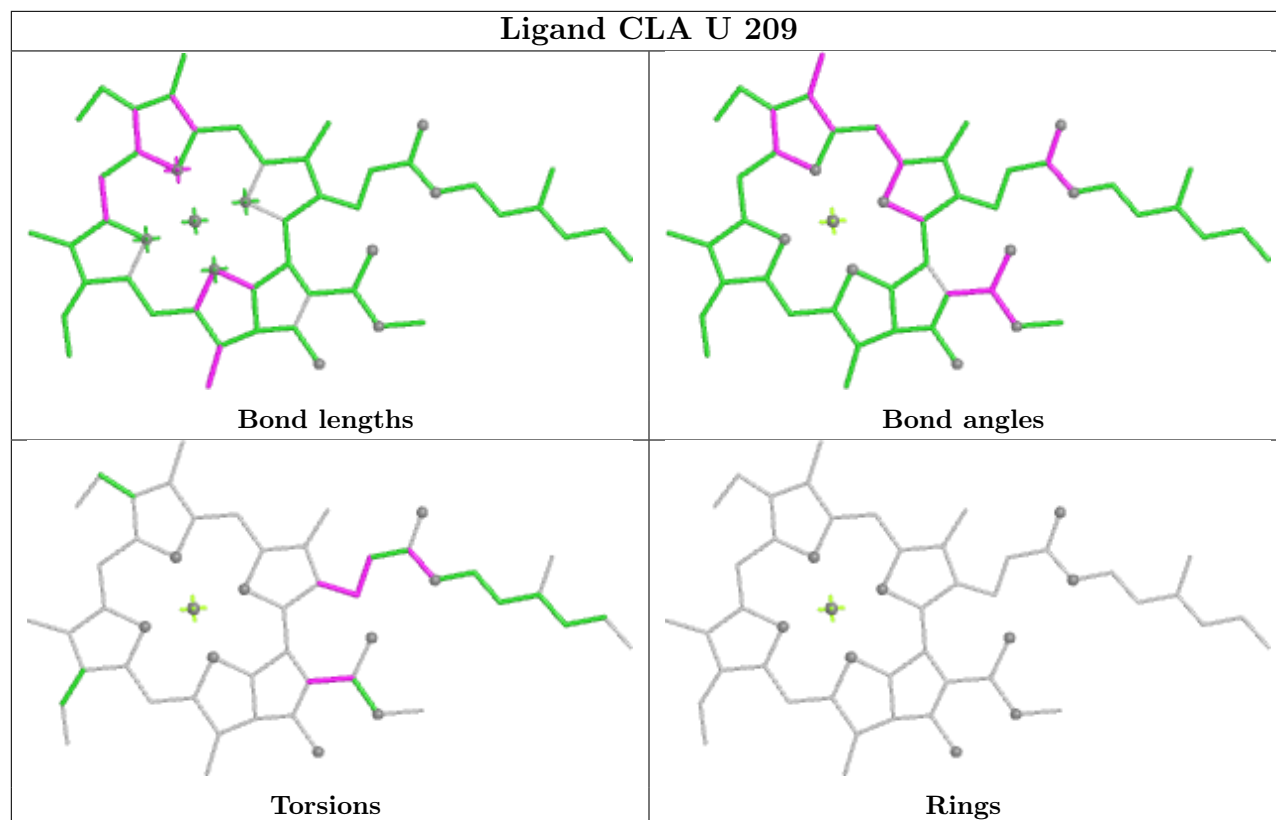


Ligand CLA E 308

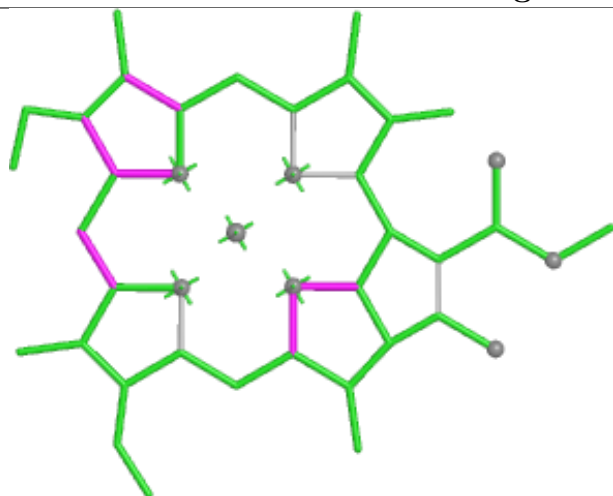


Ligand KC2 2 317

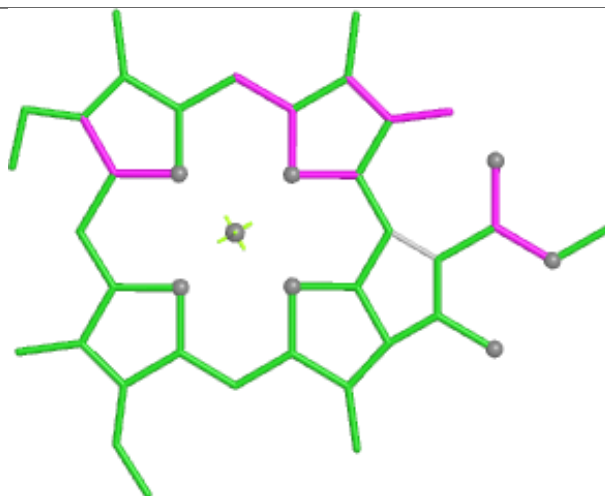




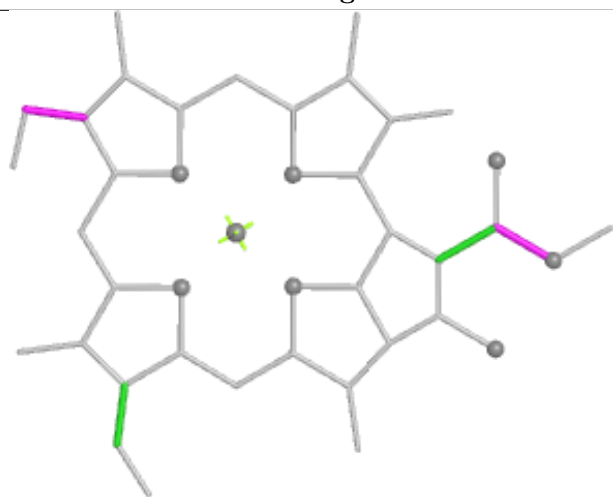
Ligand CLA Y 310



Bond lengths



Bond angles

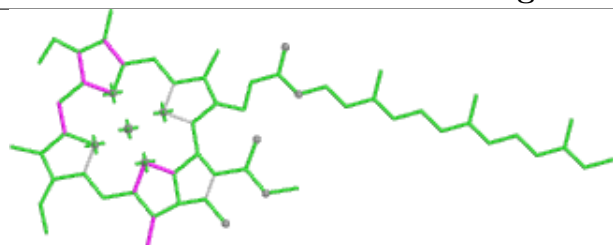


Torsions

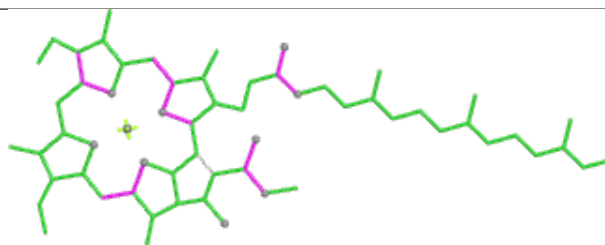


Rings

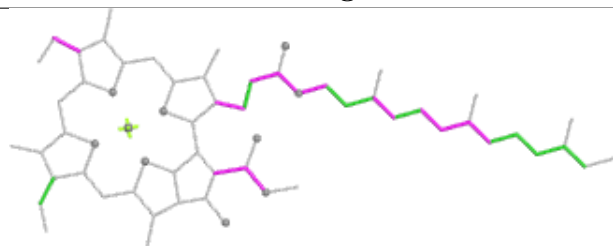
Ligand CLA S 308



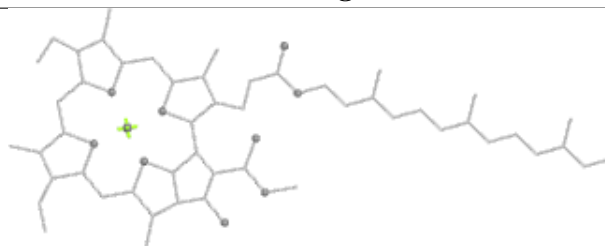
Bond lengths



Bond angles

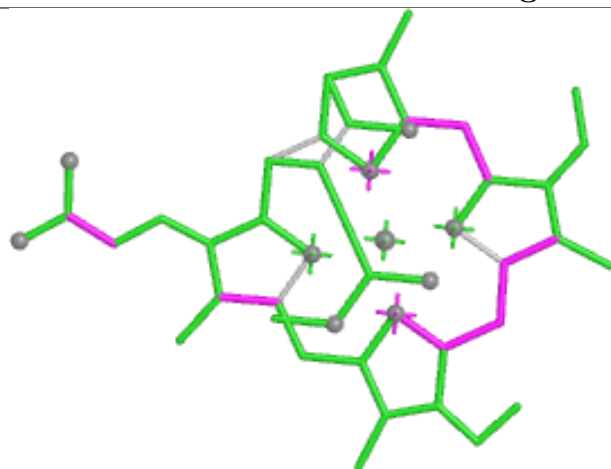


Torsions

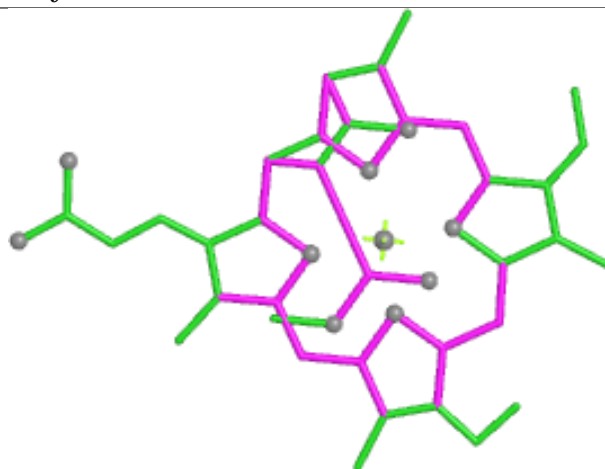


Rings

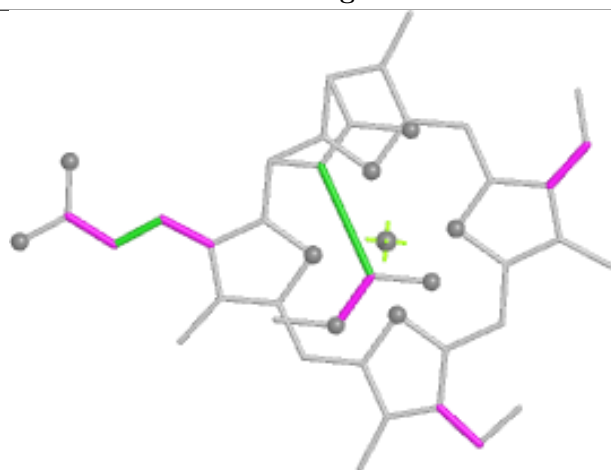
Ligand KC2 y 313



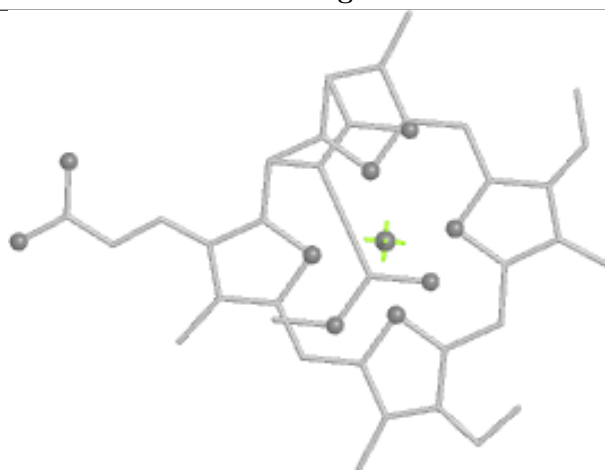
Bond lengths



Bond angles

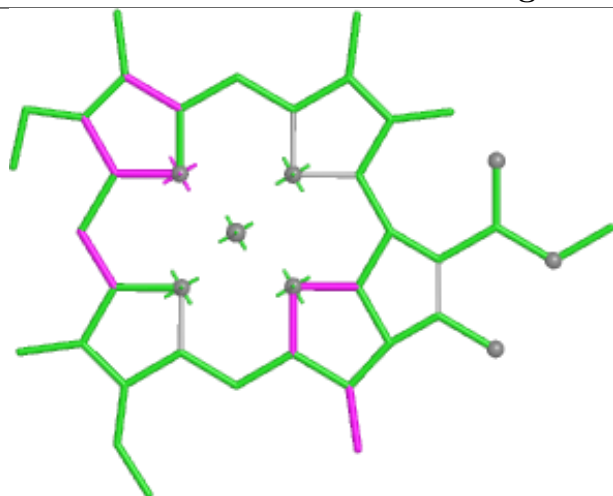


Torsions

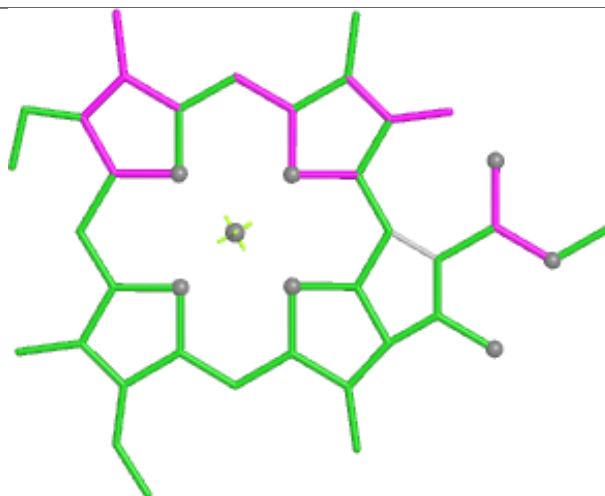


Rings

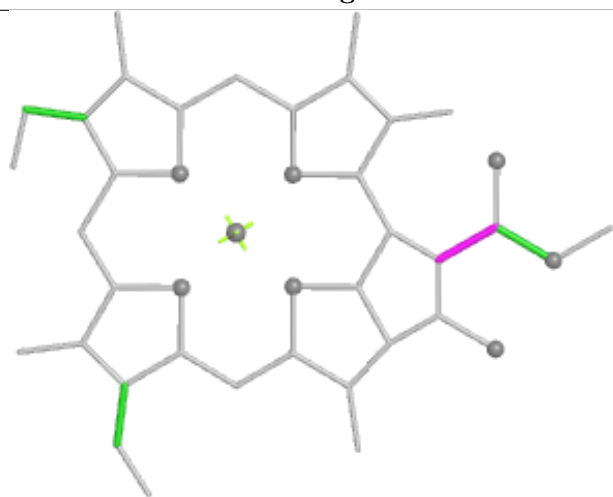
Ligand CLA 6 315



Bond lengths



Bond angles

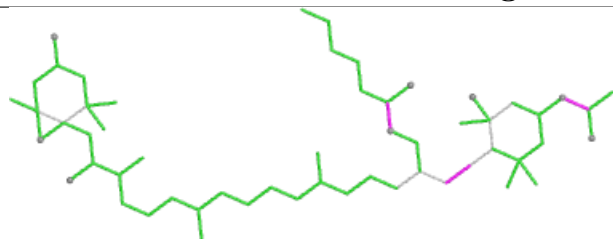


Torsions

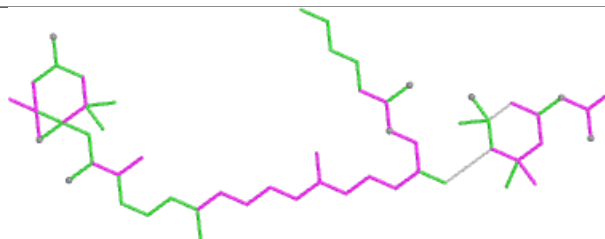


Rings

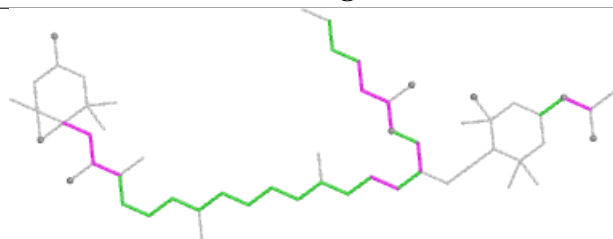
Ligand A1EB1 8 306



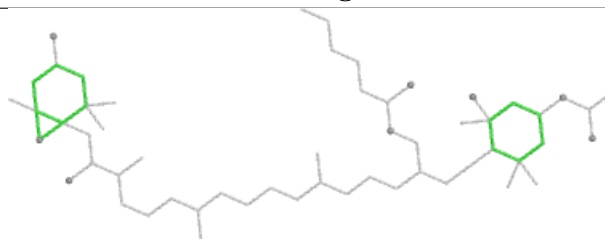
Bond lengths



Bond angles

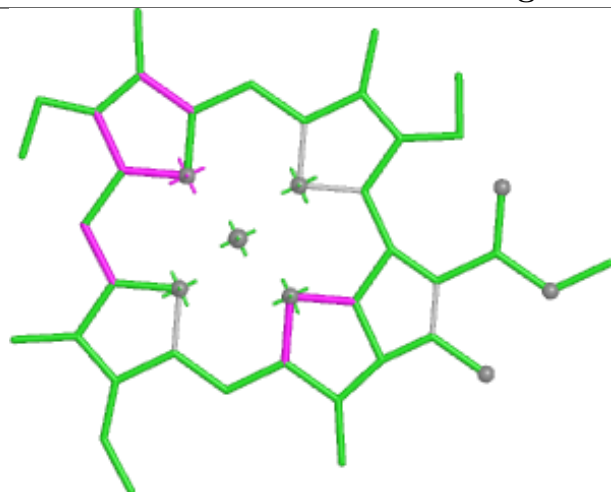


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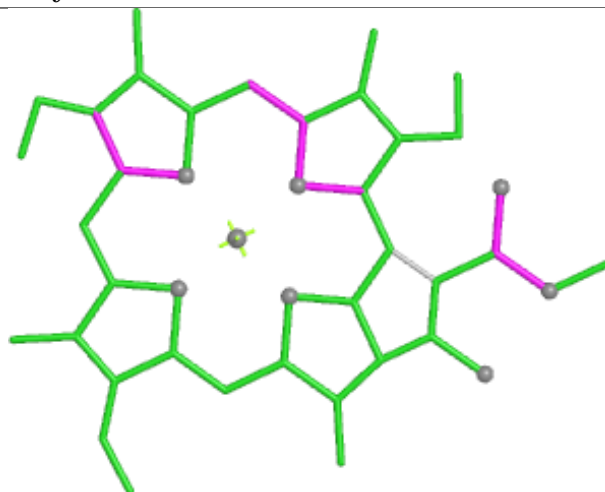


Rings

Ligand CLA y 312



Bond lengths



Bond angles

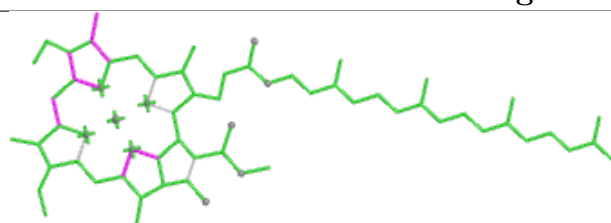


Torsions

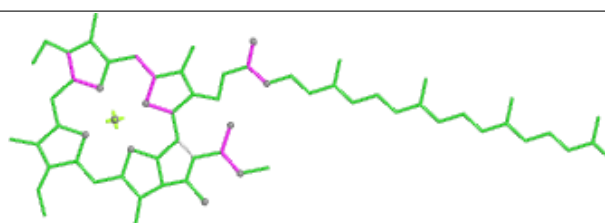


Rings

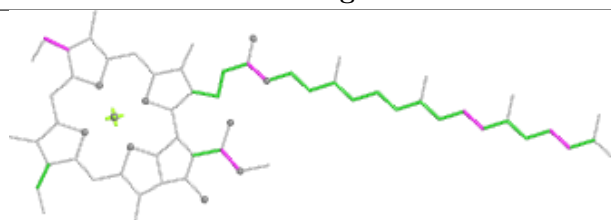
Ligand CLA F 312



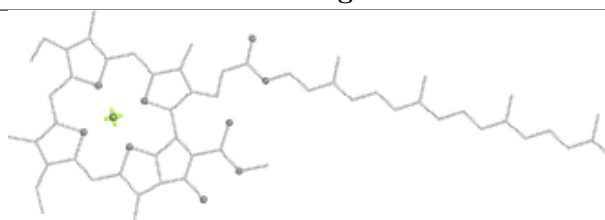
Bond lengths



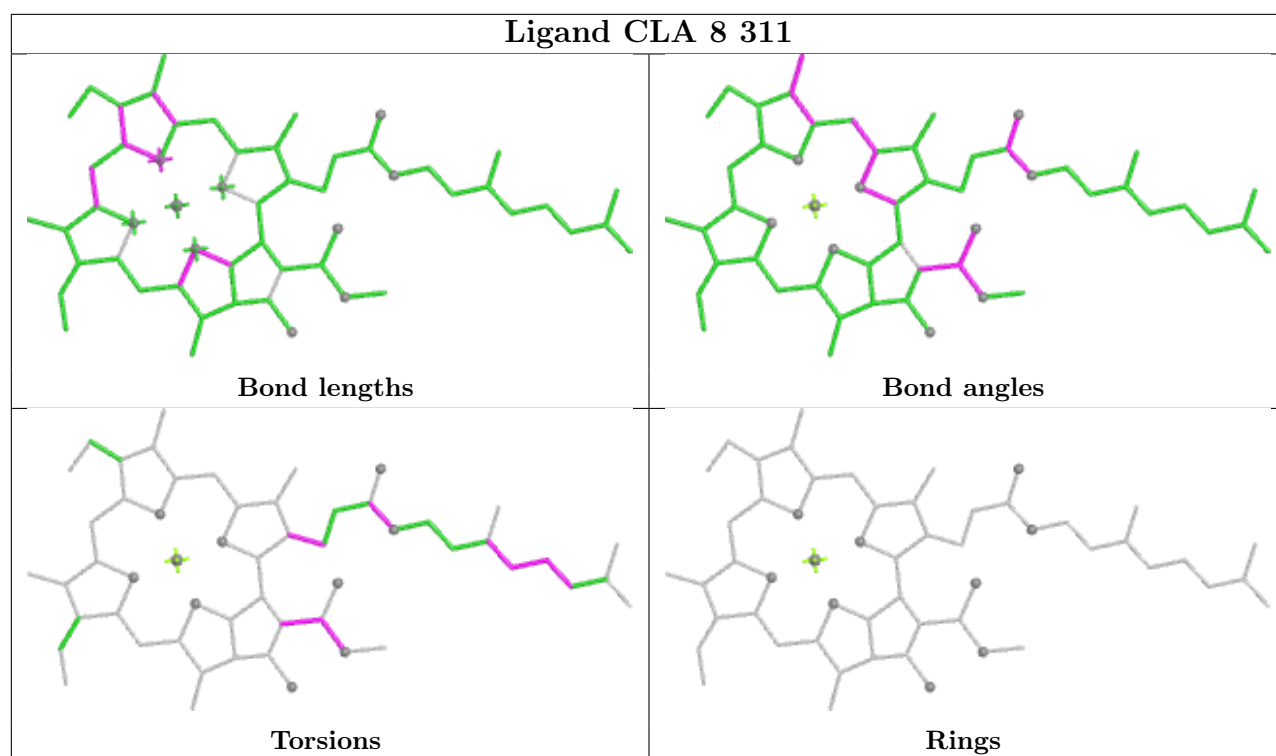
Bond angles



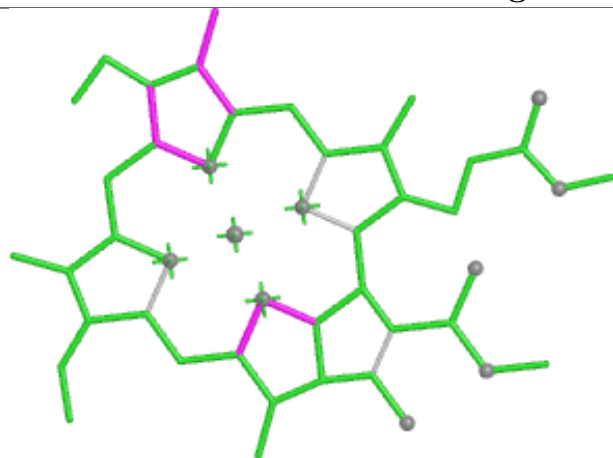
Torsions



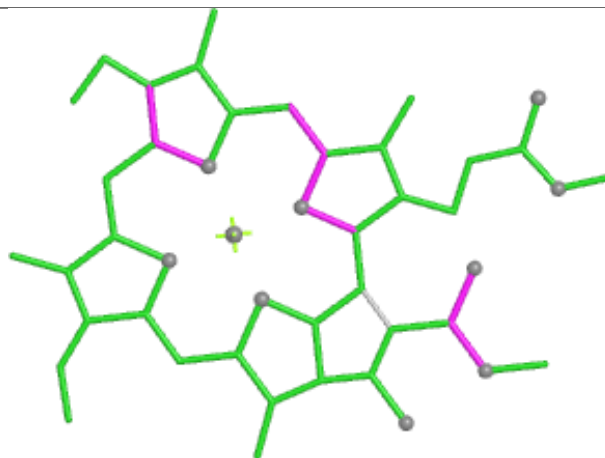
Rings



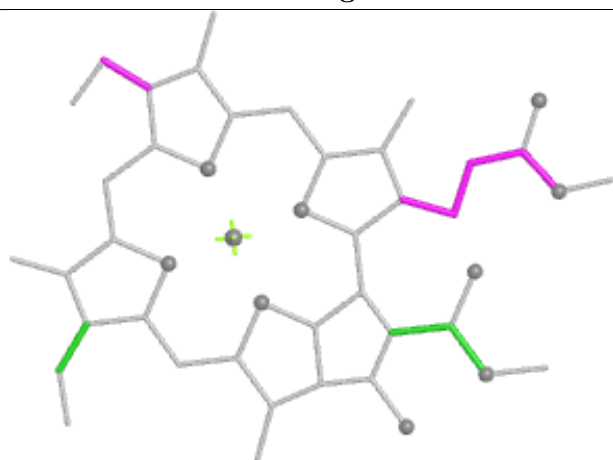
Ligand CLA W 319



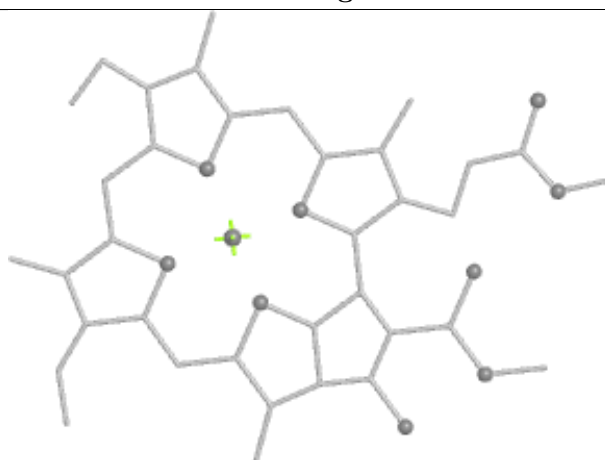
Bond lengths



Bond angles

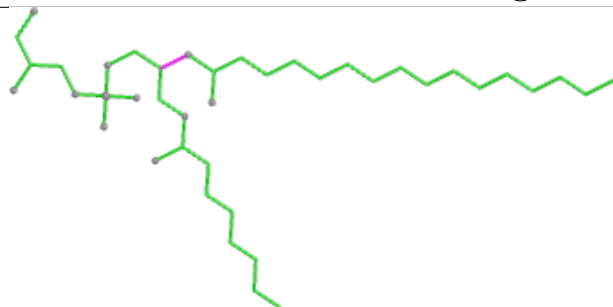


Torsions

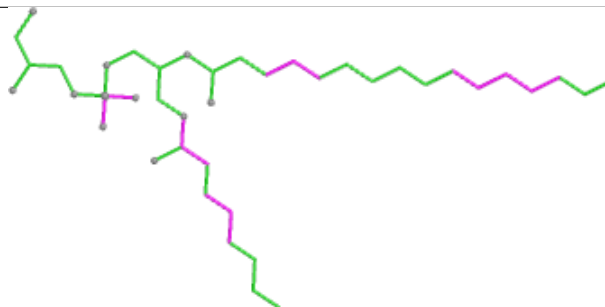


Rings

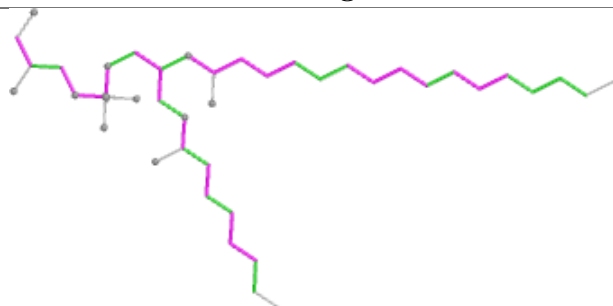
Ligand LHG X 301



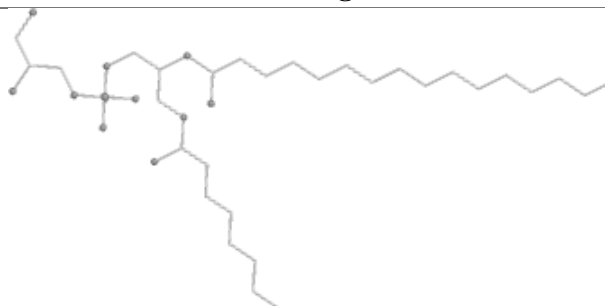
Bond lengths



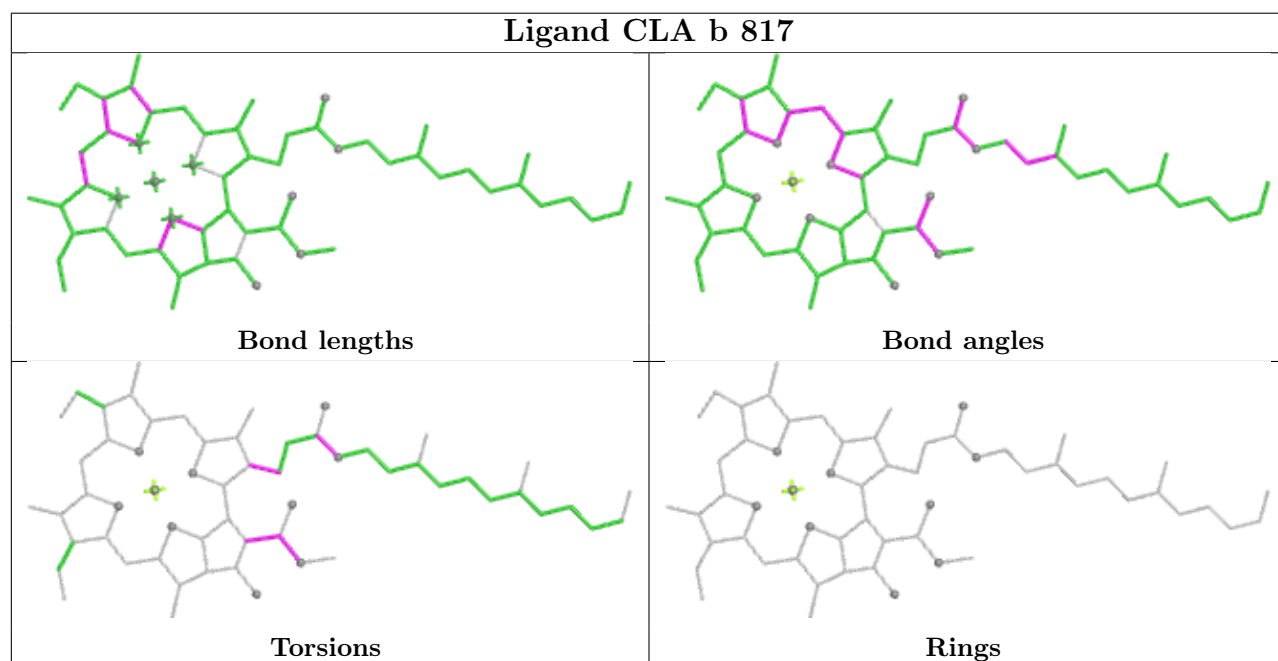
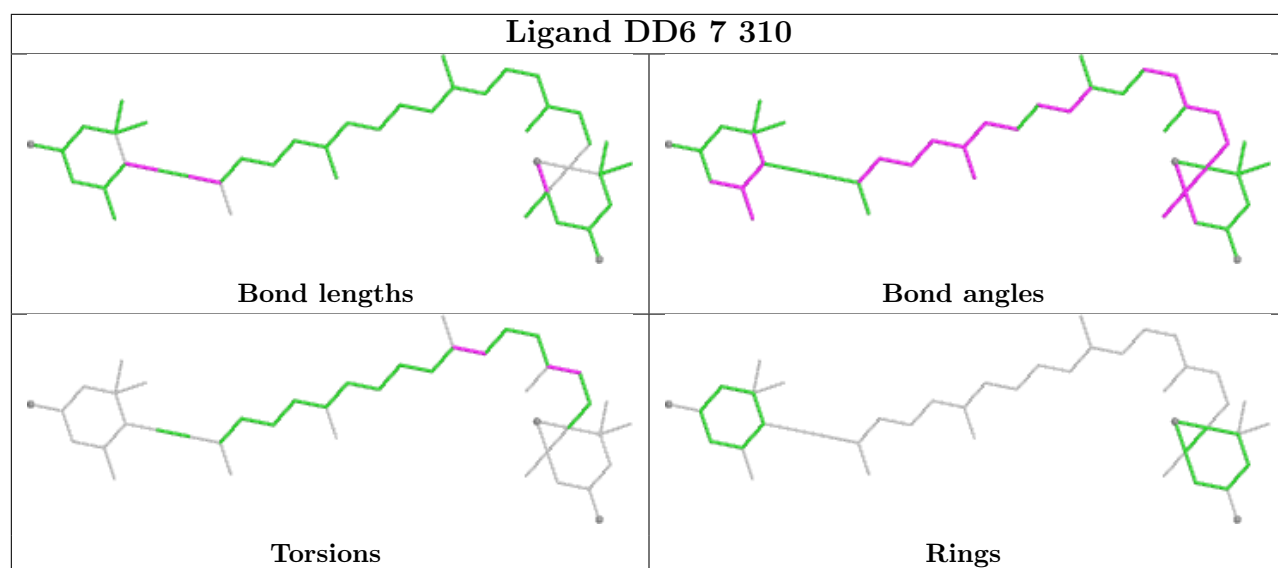
Bond angles



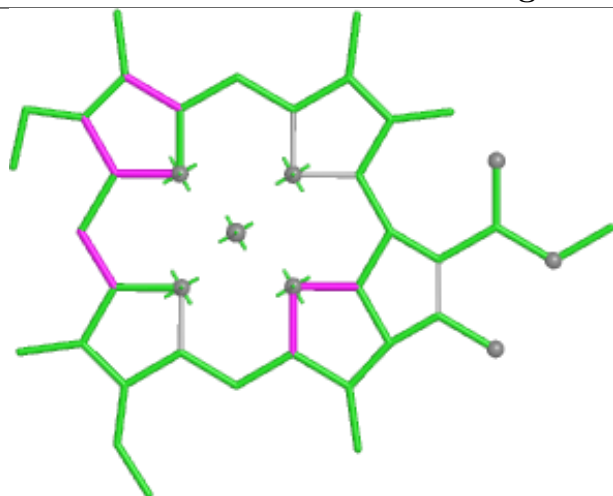
Torsions



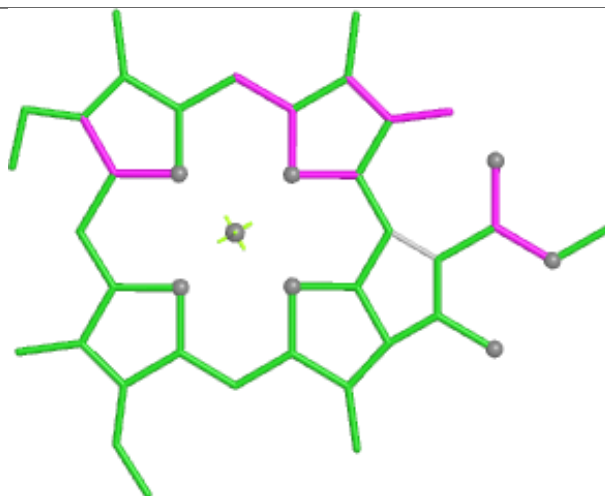
Rings



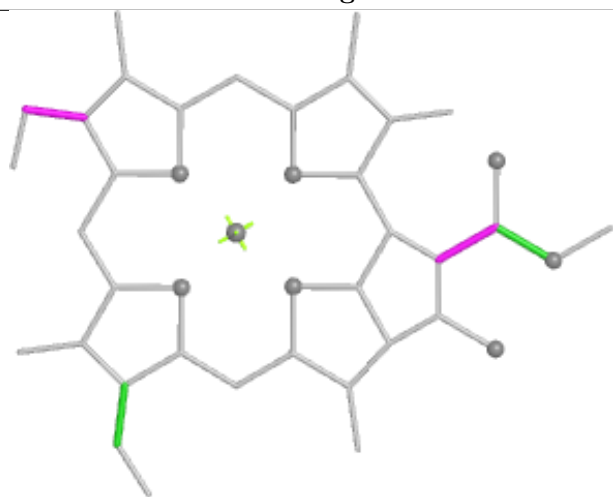
Ligand CLA 0 318



Bond lengths



Bond angles

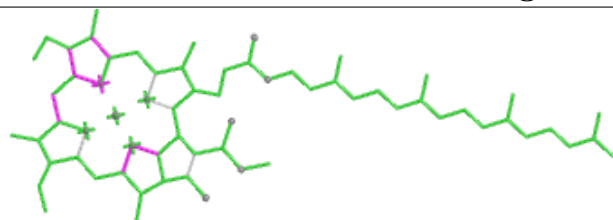


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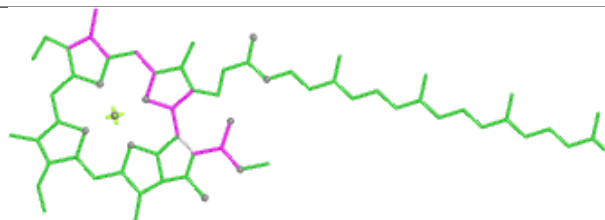


Rings

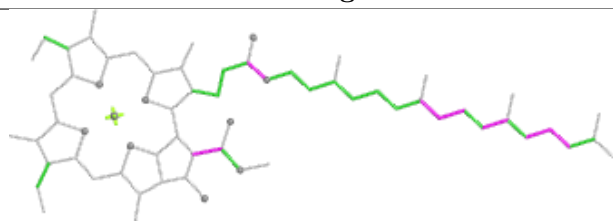
Ligand CLA a 822



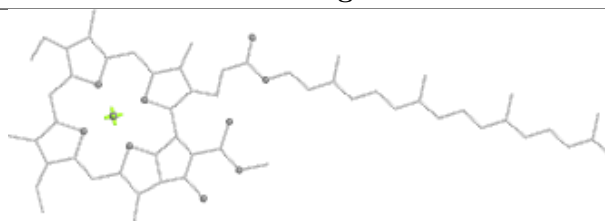
Bond lengths



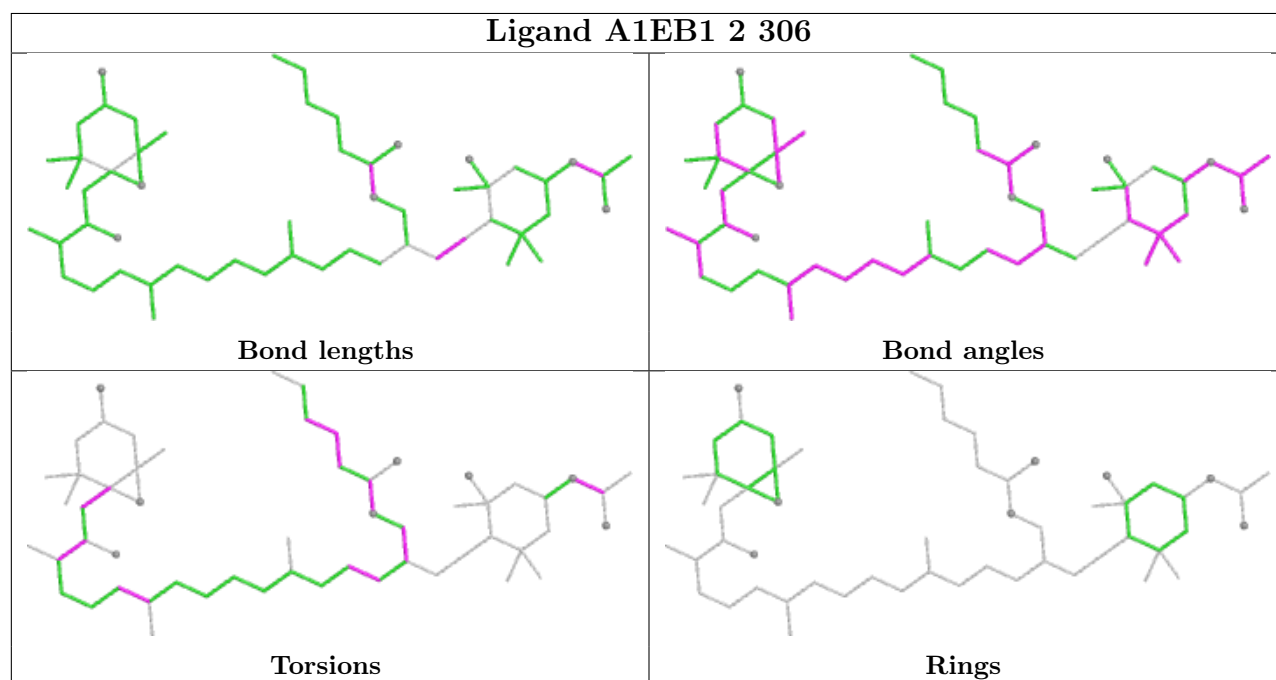
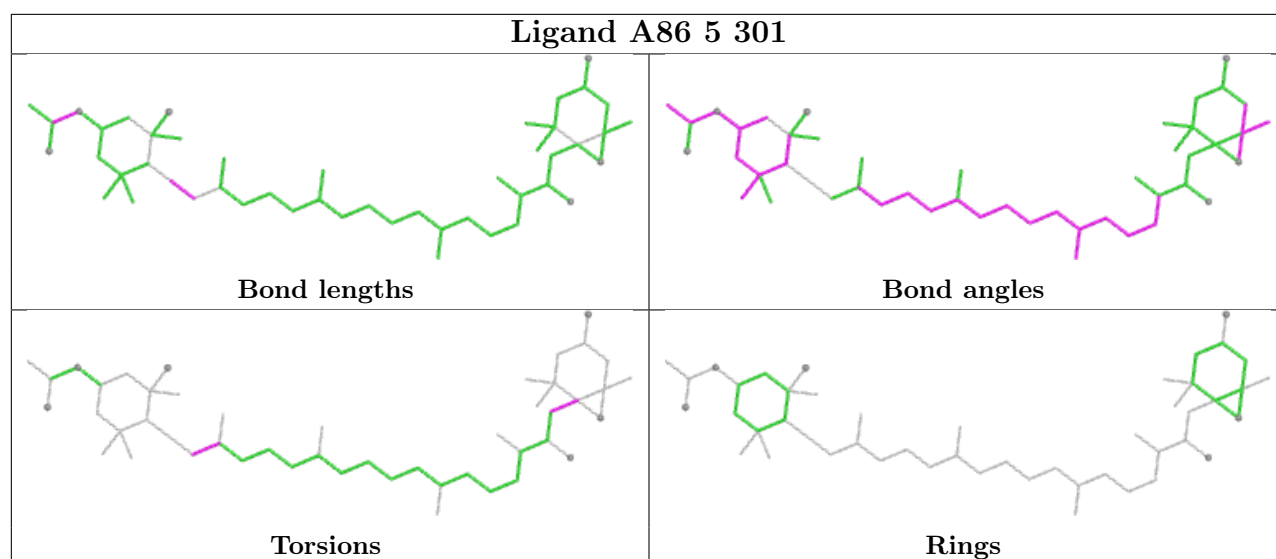
Bond angles

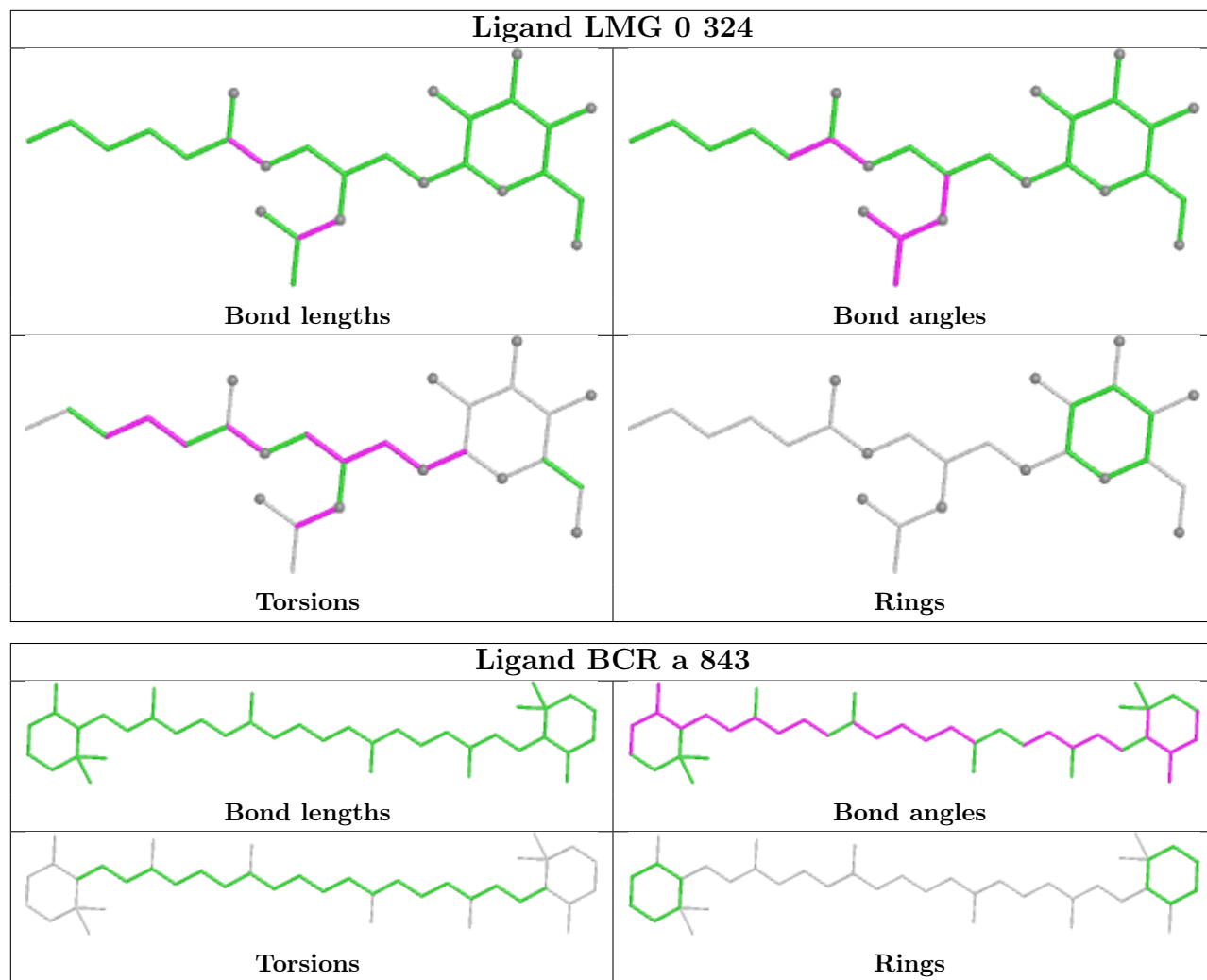


Torsions

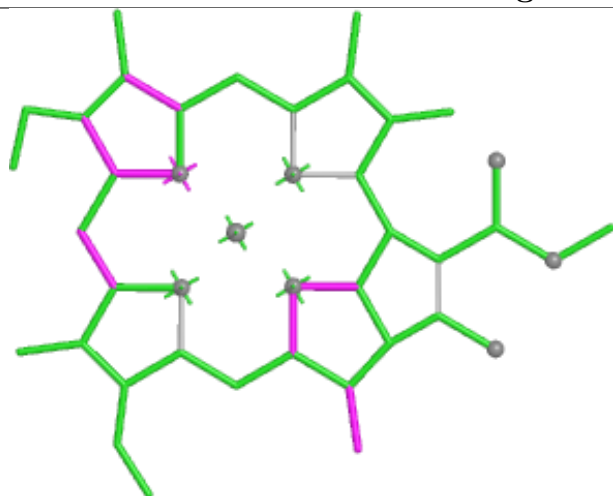


Rings

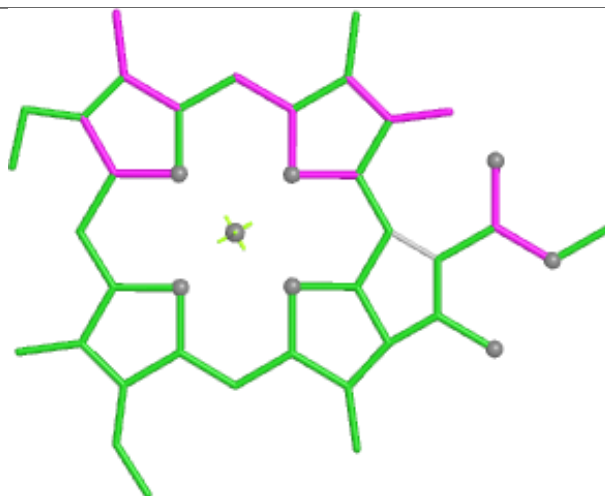




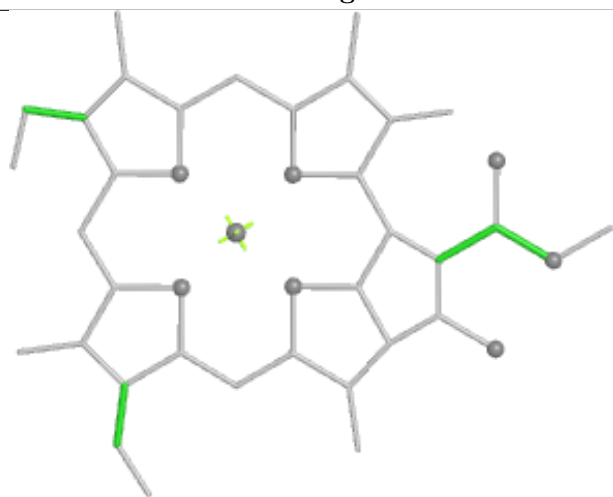
Ligand CLA Z 307



Bond lengths



Bond angles

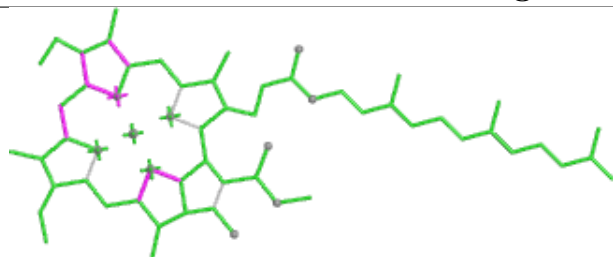


Torsions

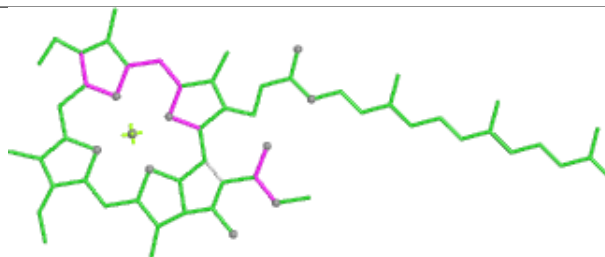


Rings

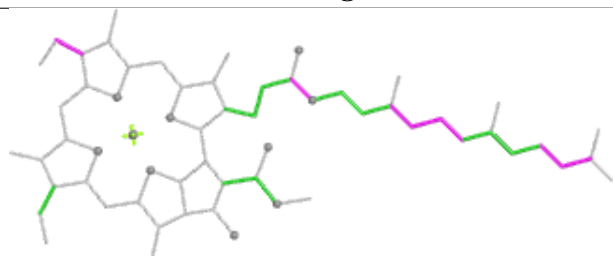
Ligand CLA R 308



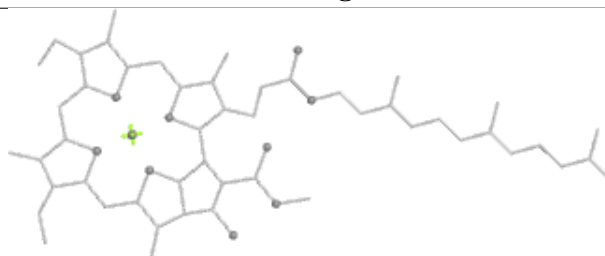
Bond lengths



Bond angles

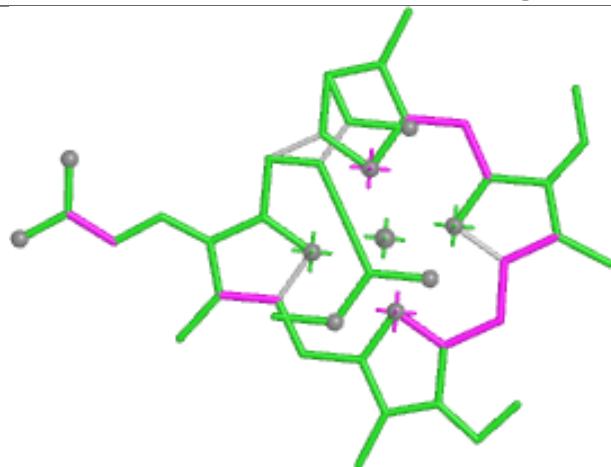


Torsions

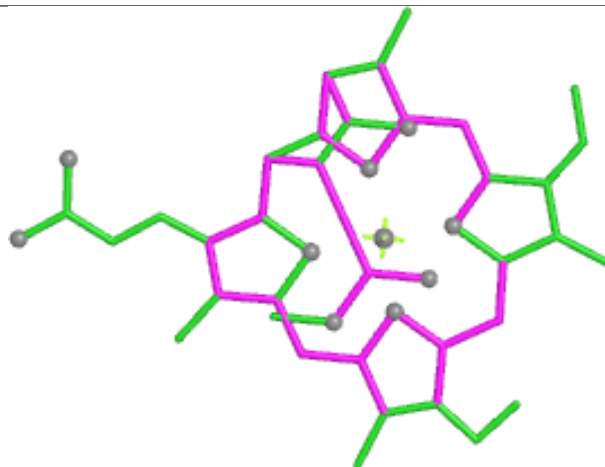


Rings

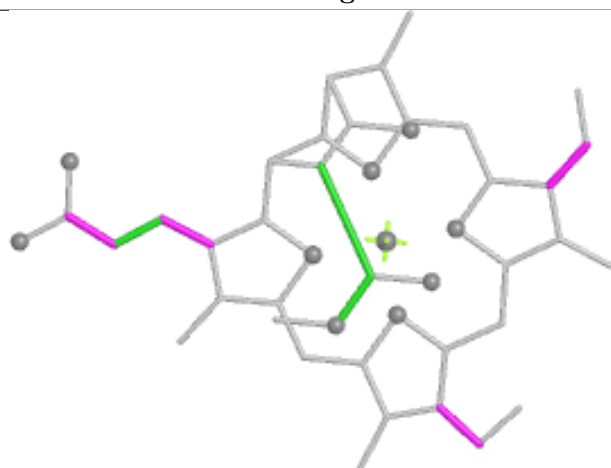
Ligand KC2 T 315



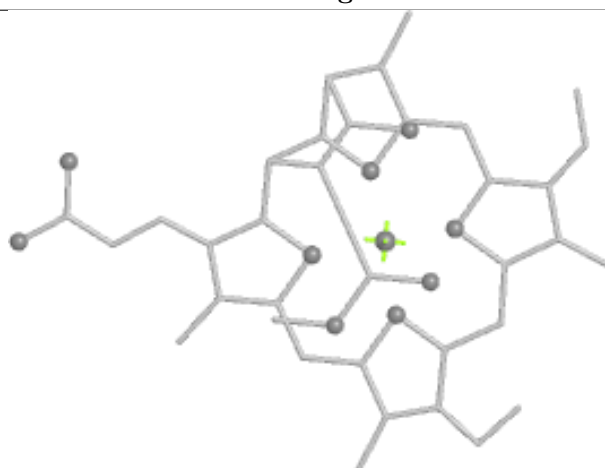
Bond lengths



Bond angles

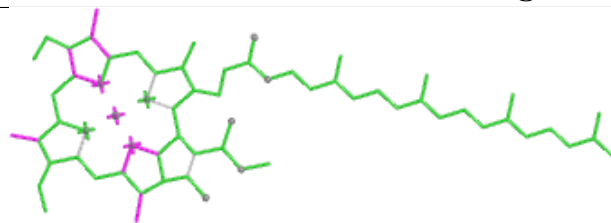


Torsions

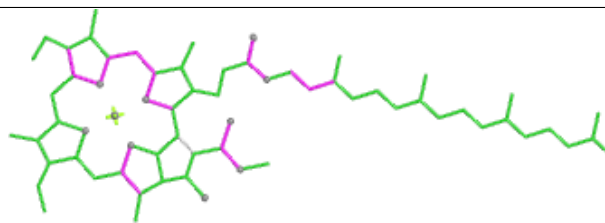


Rings

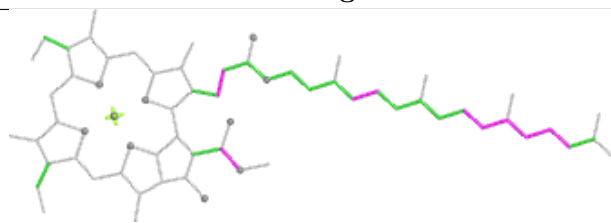
Ligand CLA b 801



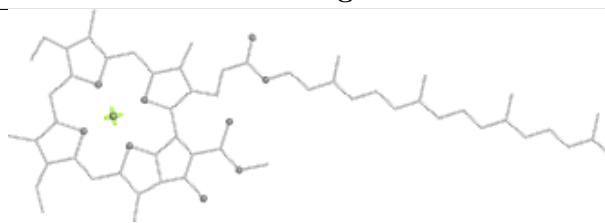
Bond lengths



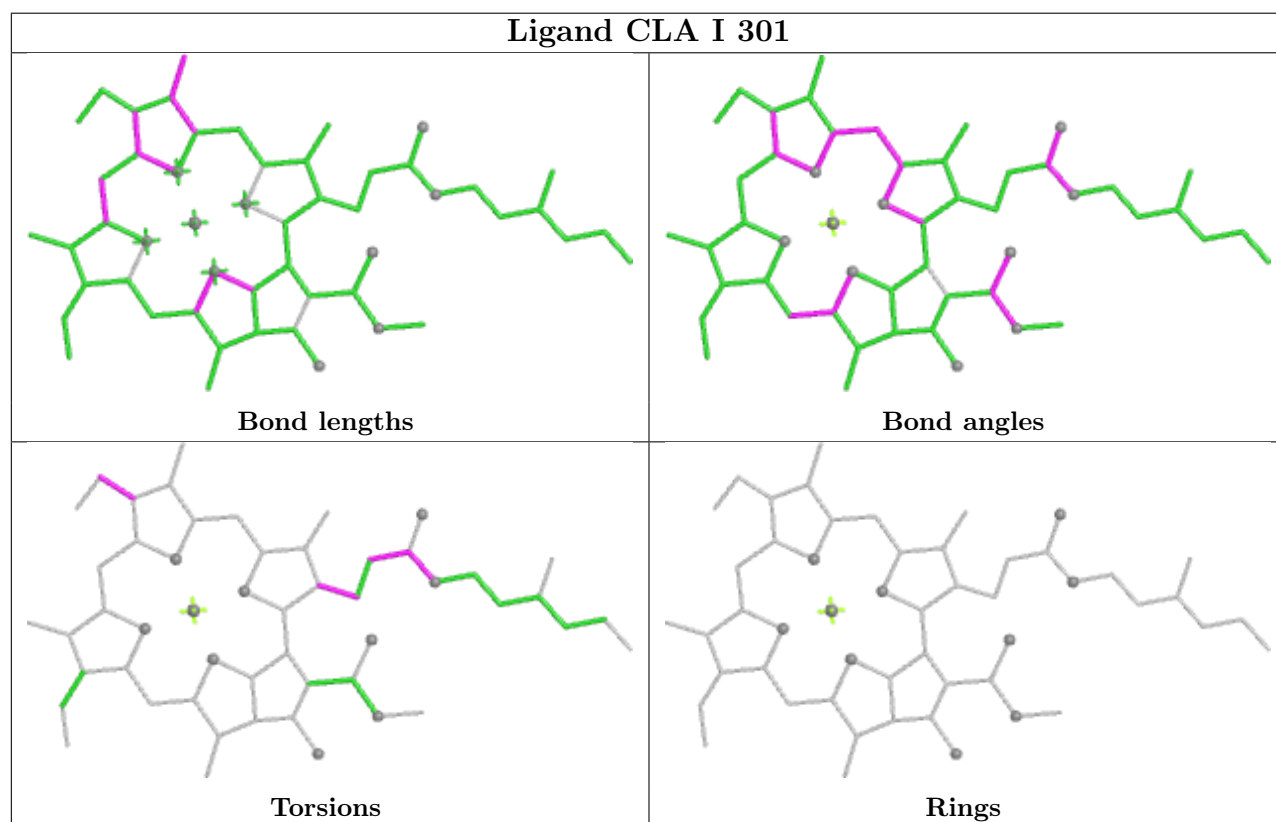
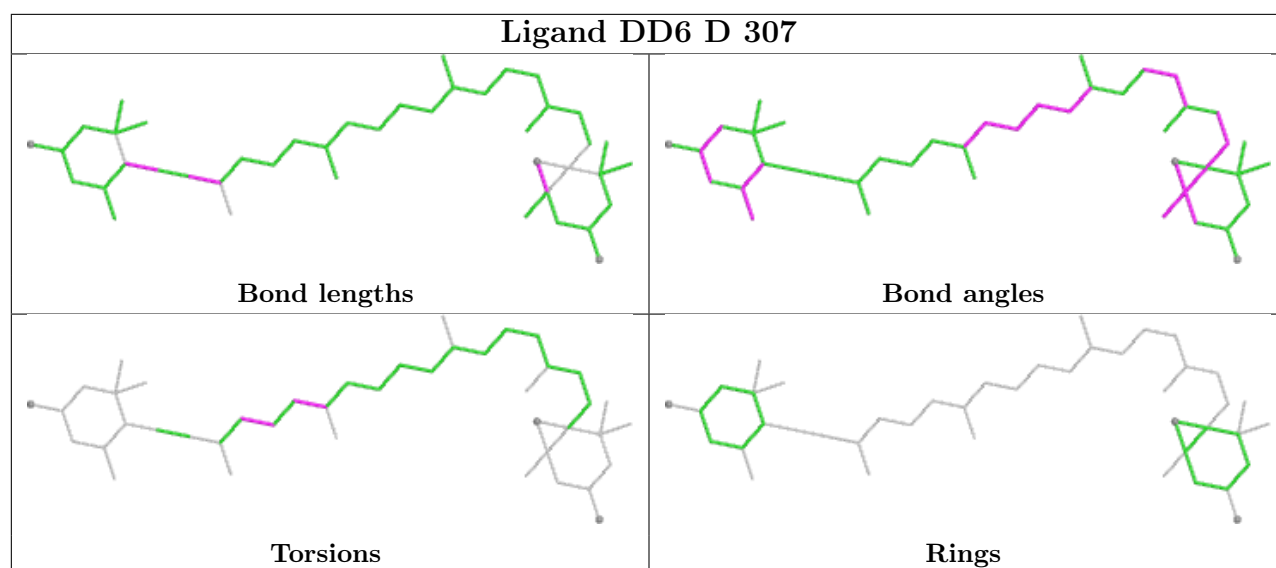
Bond angles

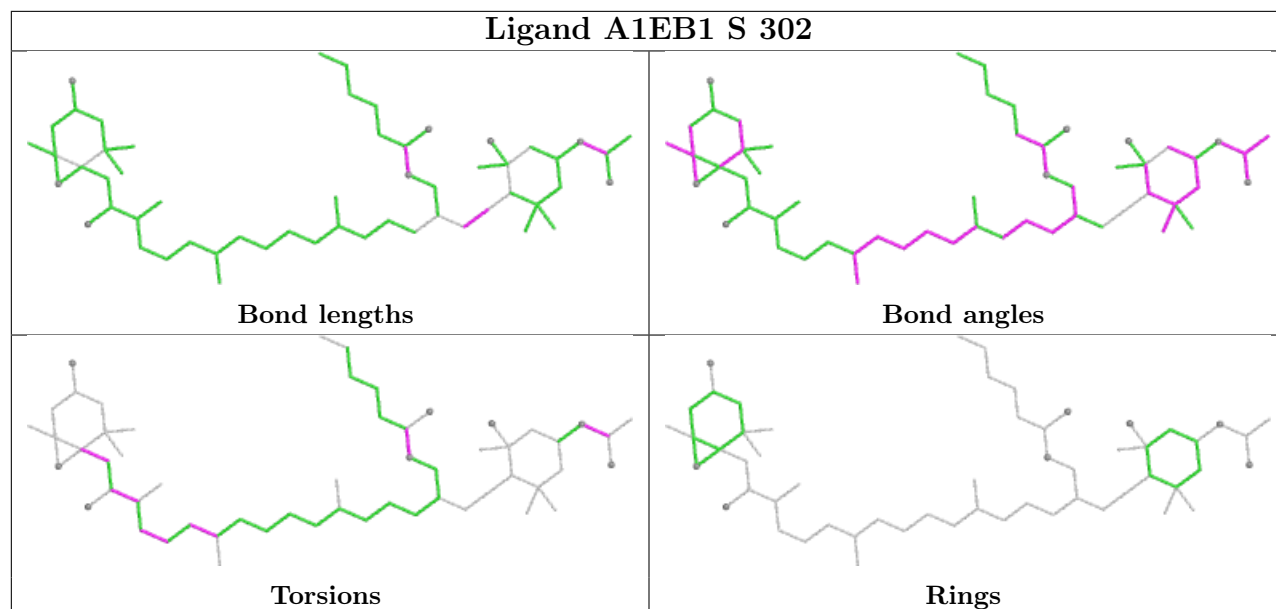
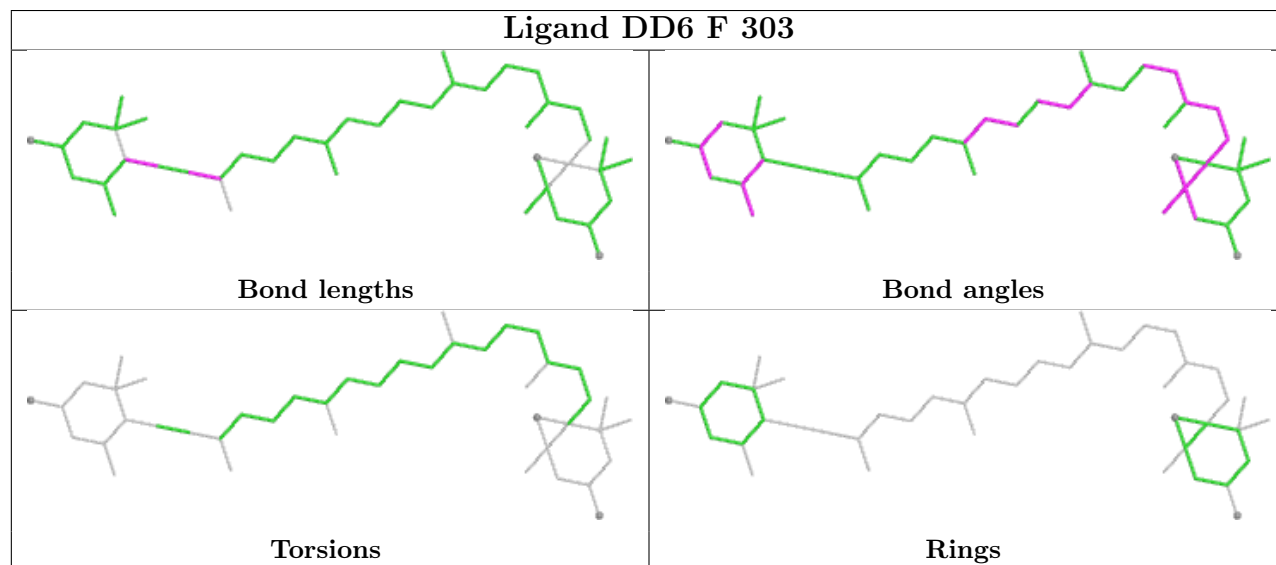


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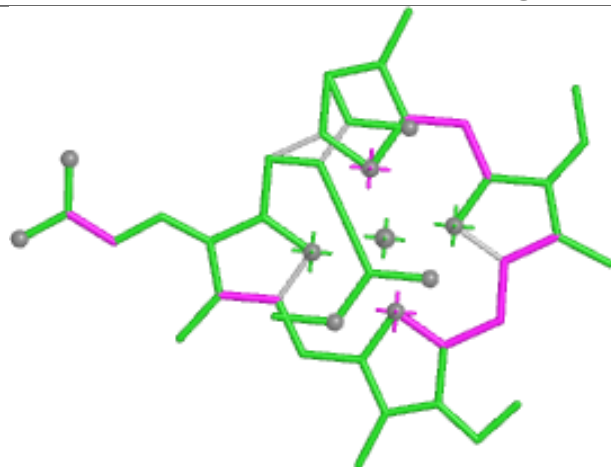


Rings



Ligand A1EB1 S 302**Ligand DD6 F 303**

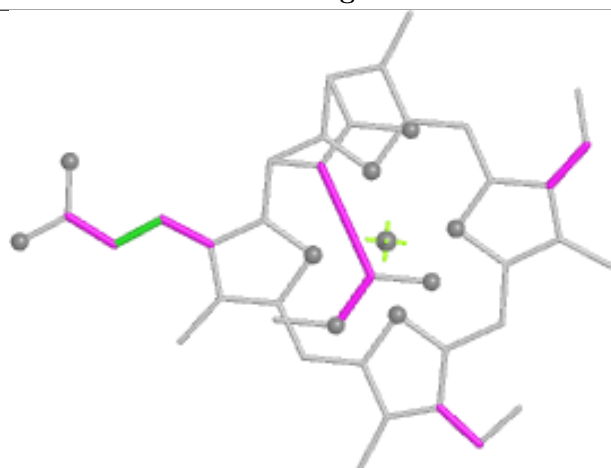
Ligand KC2 H 314



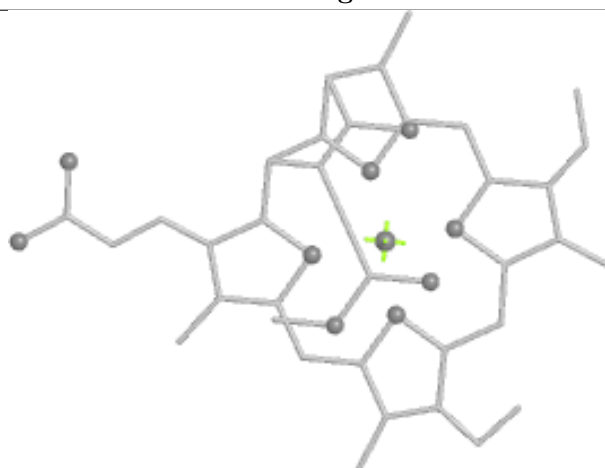
Bond lengths



Bond angles

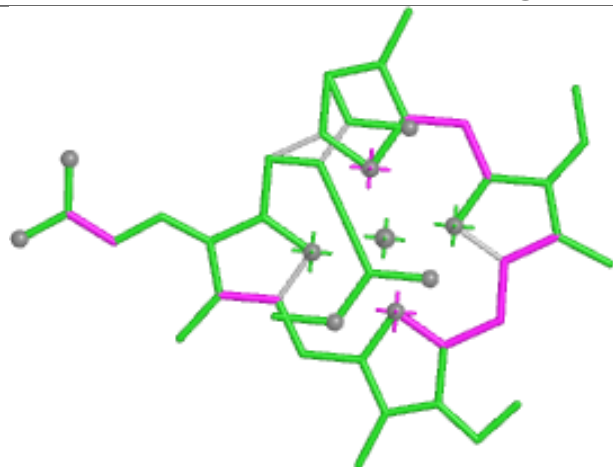


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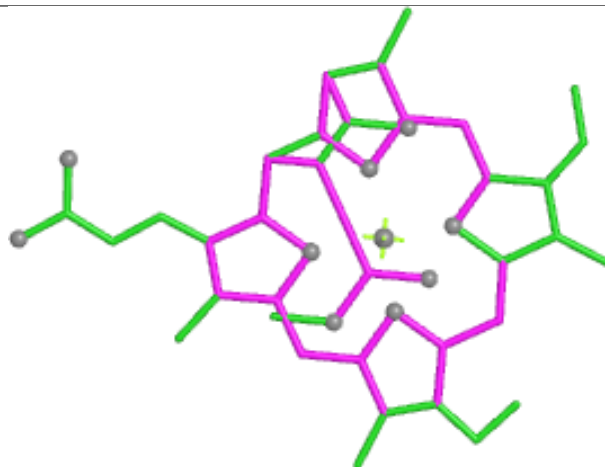


Rings

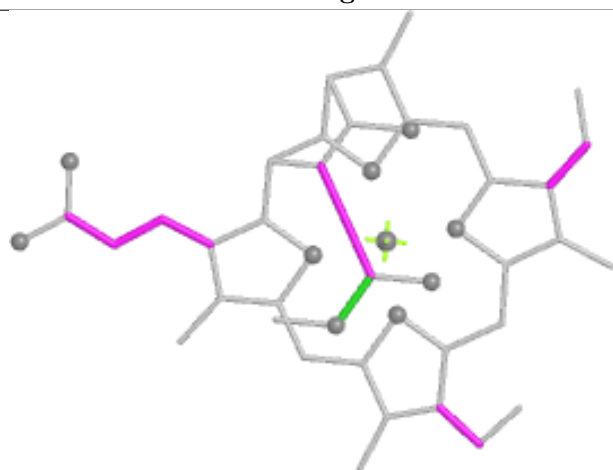
Ligand KC2 P 320



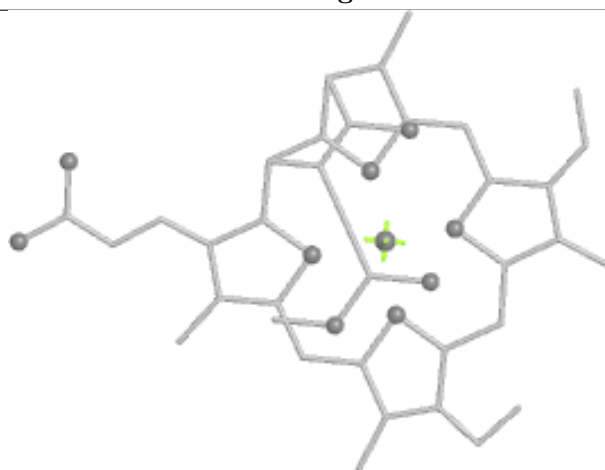
Bond lengths



Bond angles

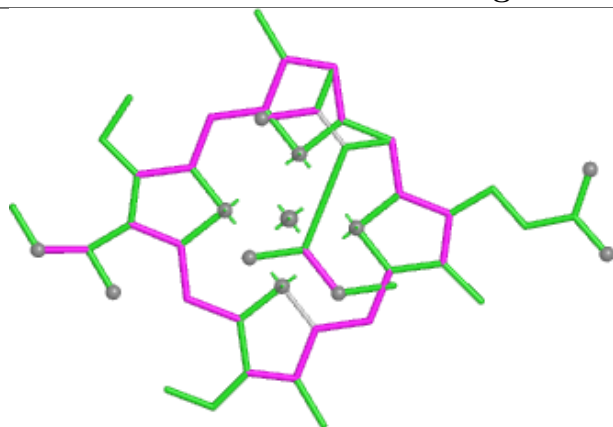


Torsions

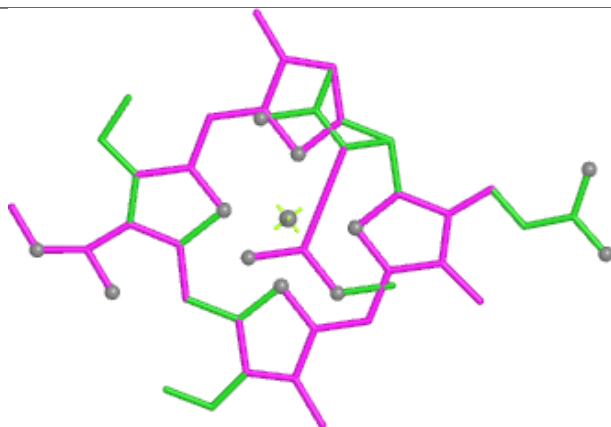


Rings

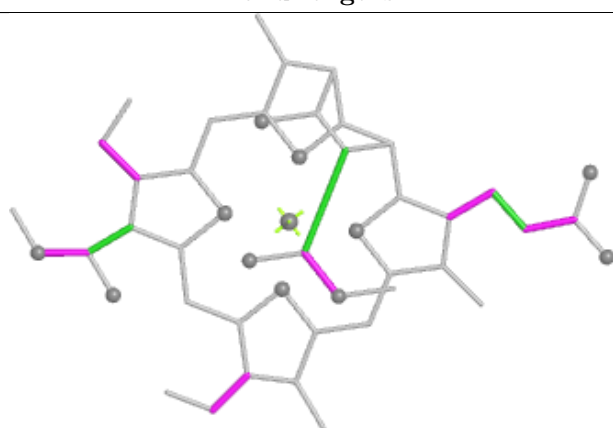
Ligand A1ECV L 318



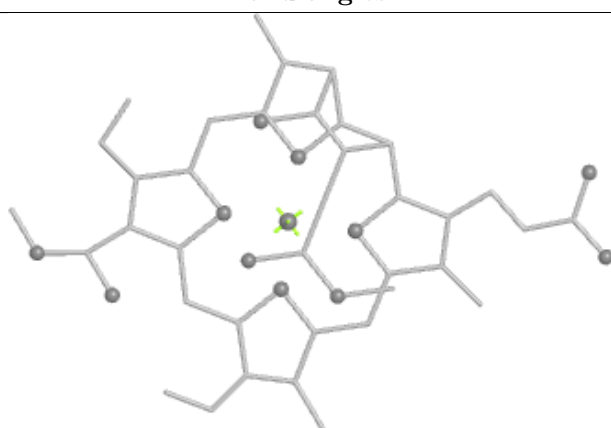
Bond lengths



Bond angles

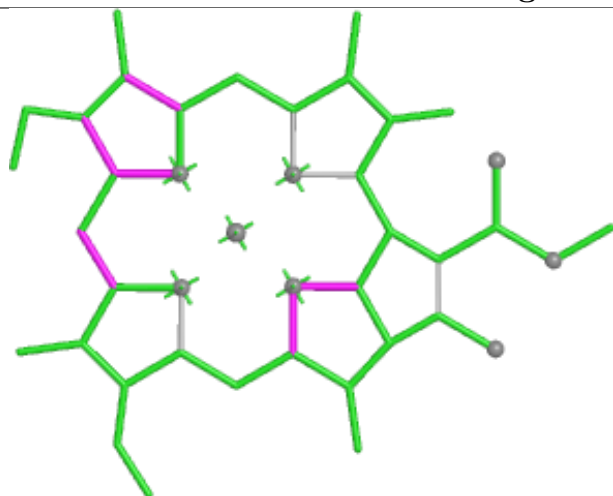


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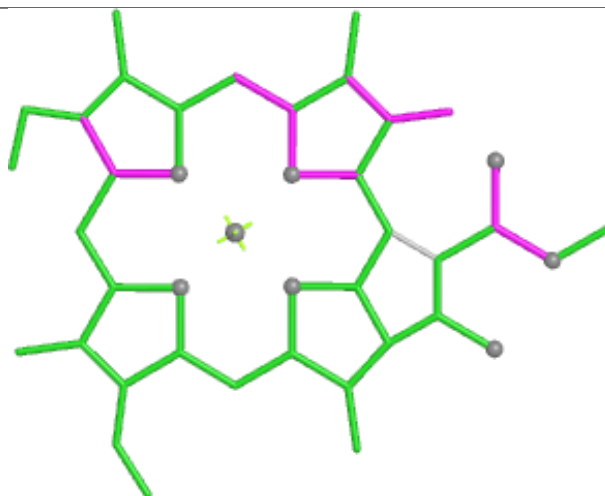


Rings

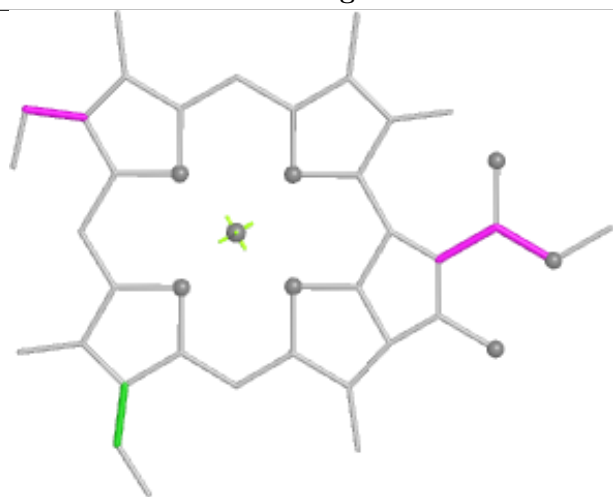
Ligand CLA 1 316



Bond lengths



Bond angles

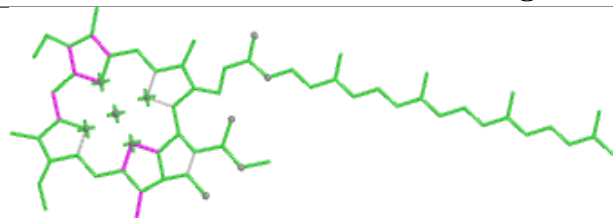


Torsions

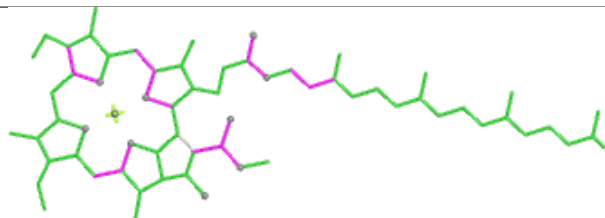


Rings

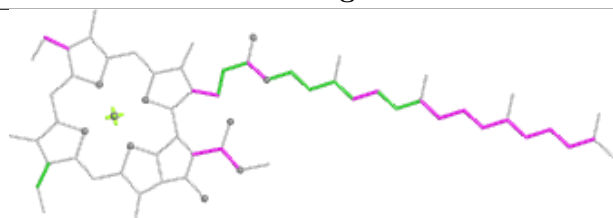
Ligand CLA 3 312



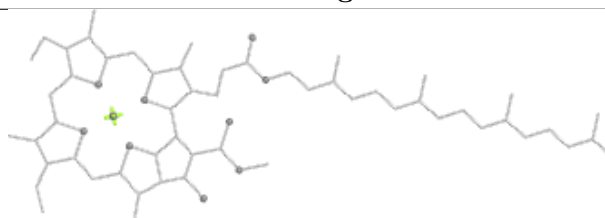
Bond lengths



Bond angles

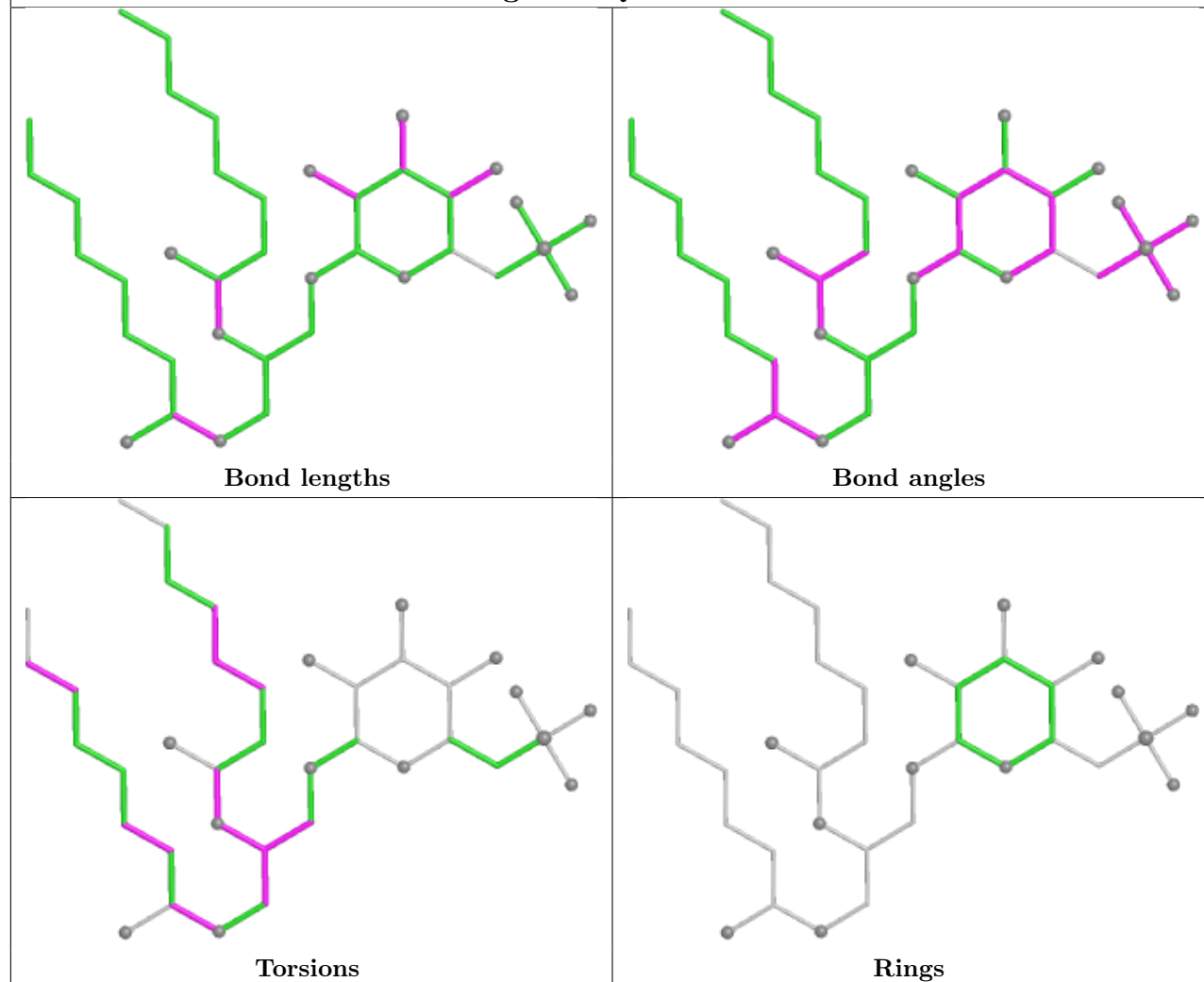


Torsions

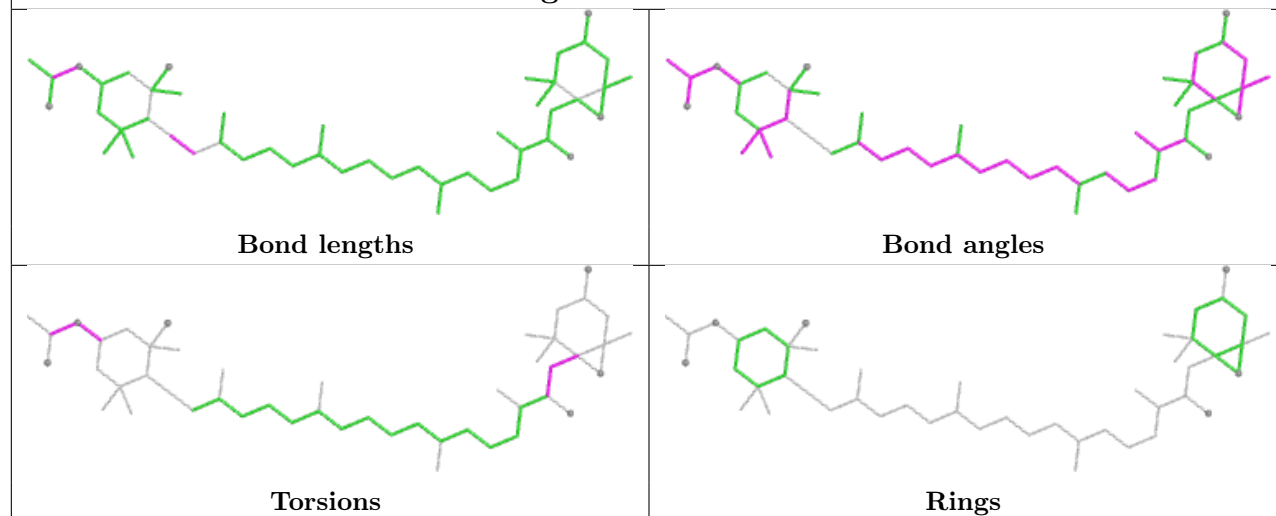


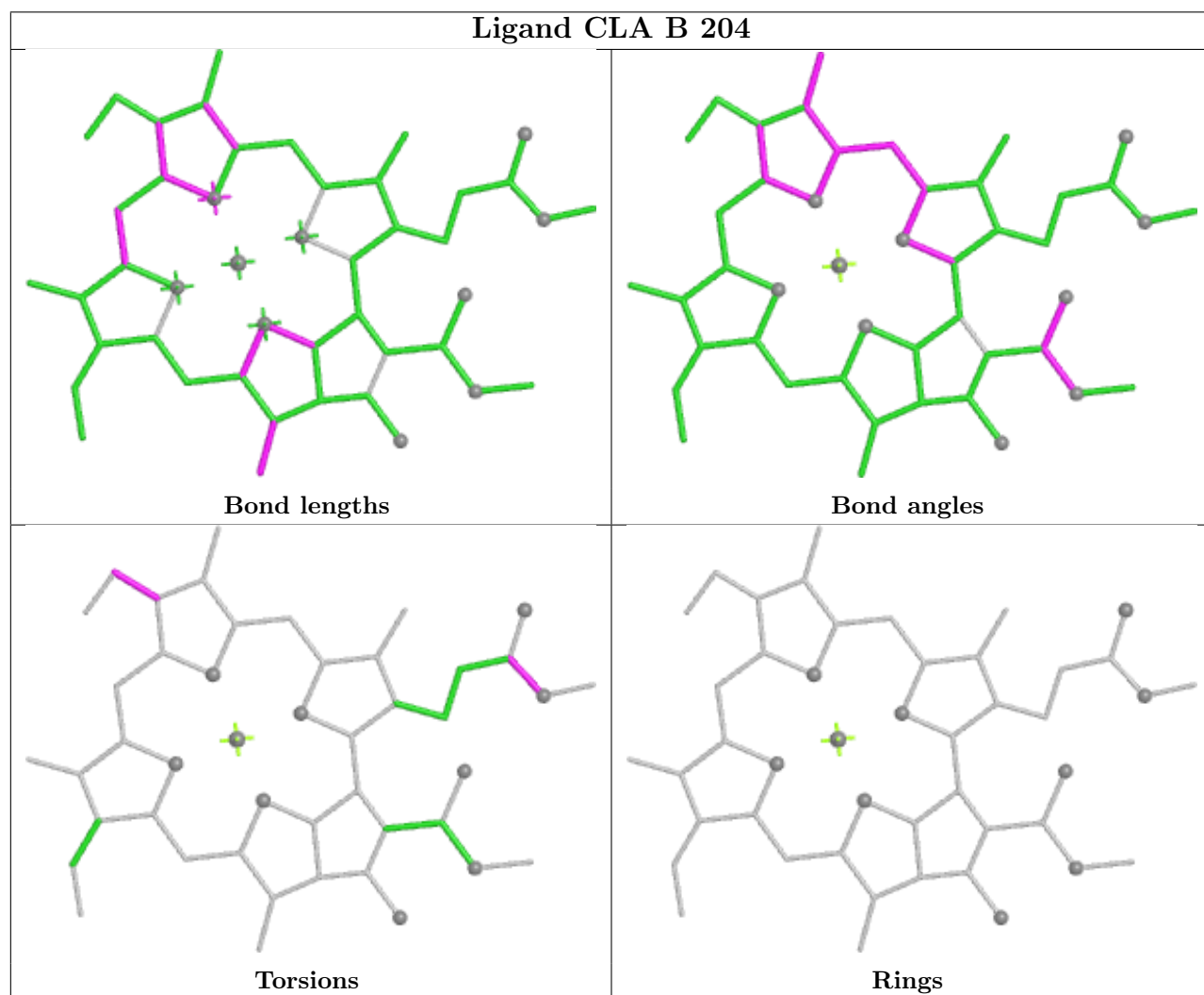
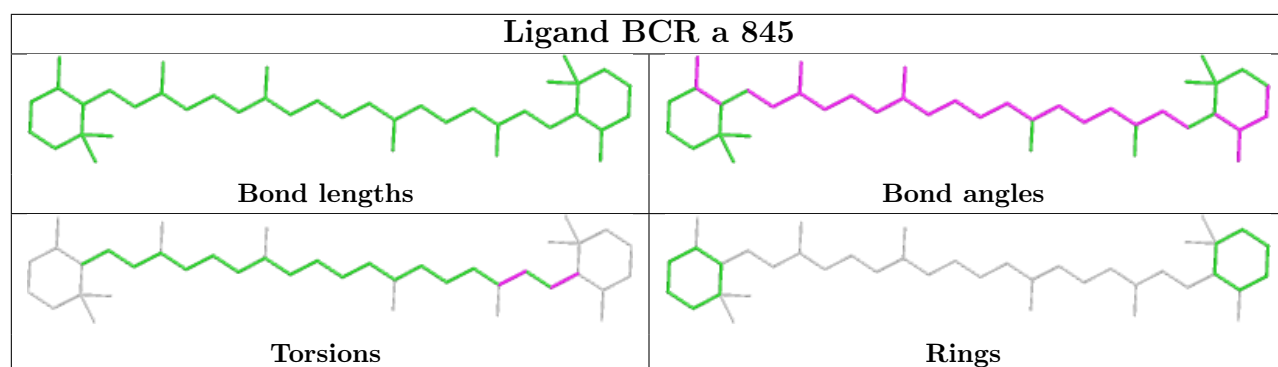
Rings

Ligand SQD P 301

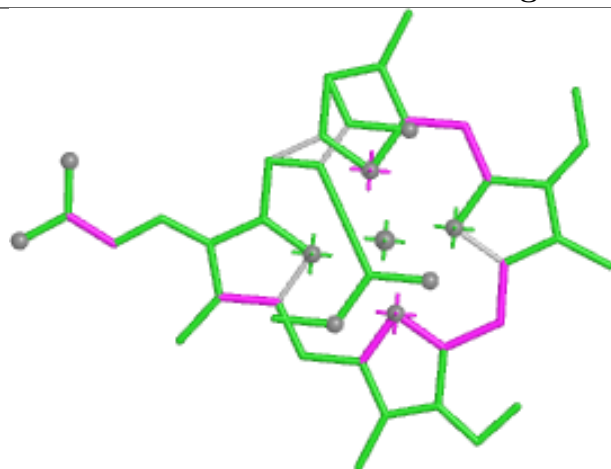


Ligand A86 S 307

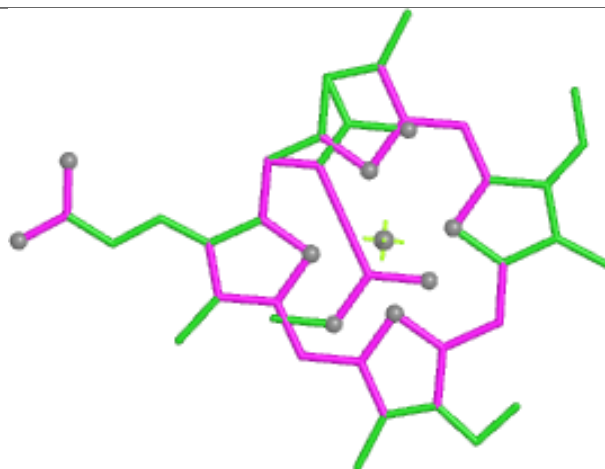




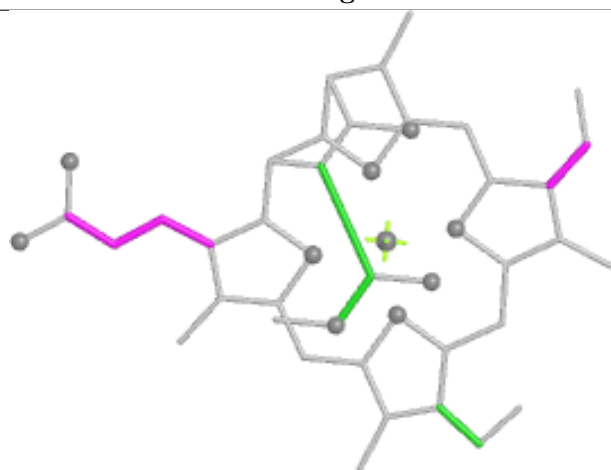
Ligand KC2 3 318



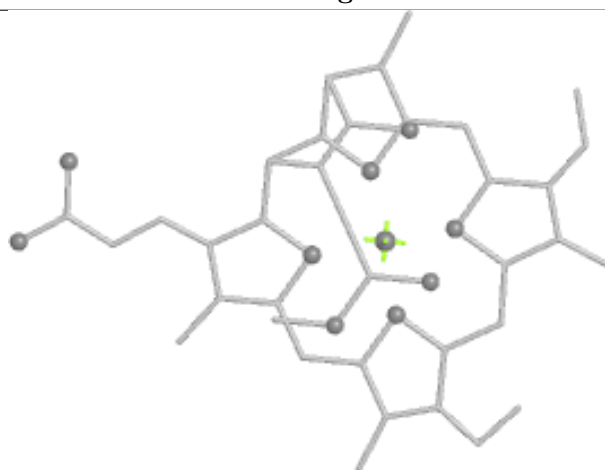
Bond lengths



Bond angles

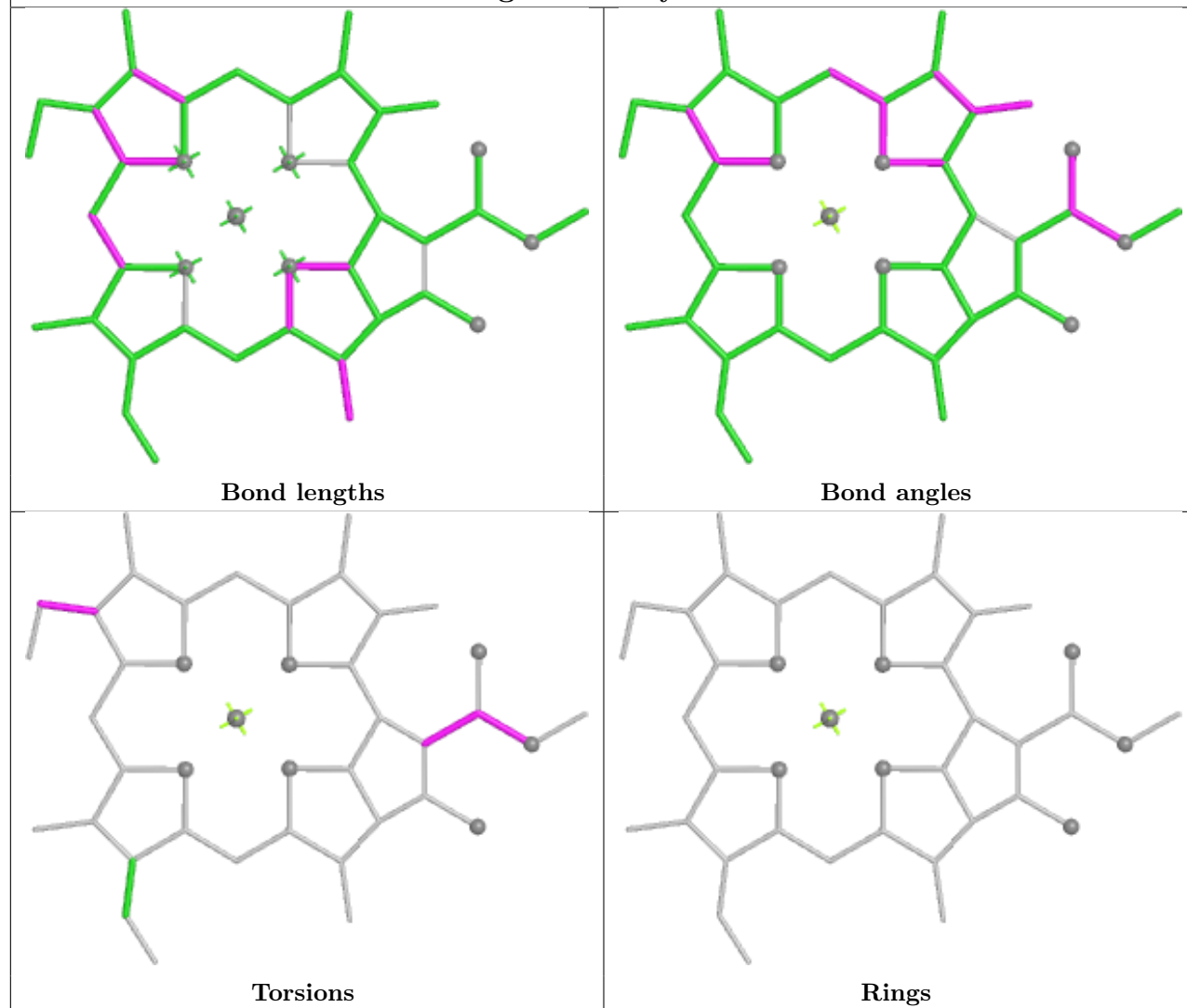


Torsions

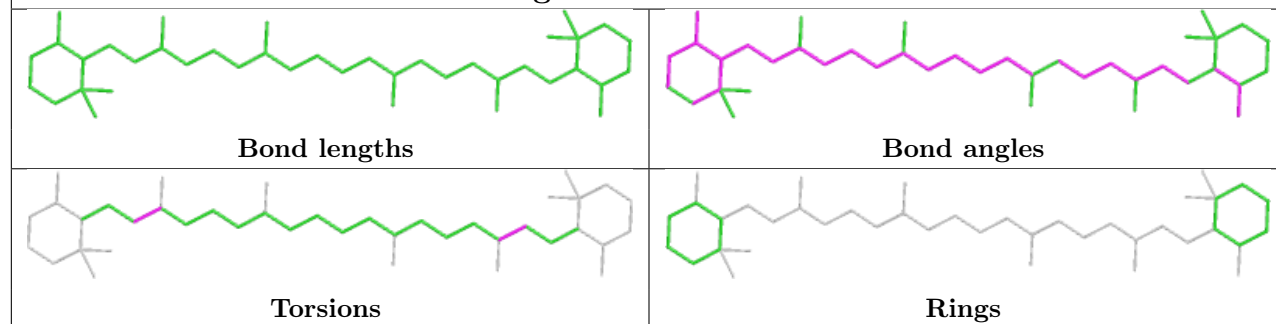


Rings

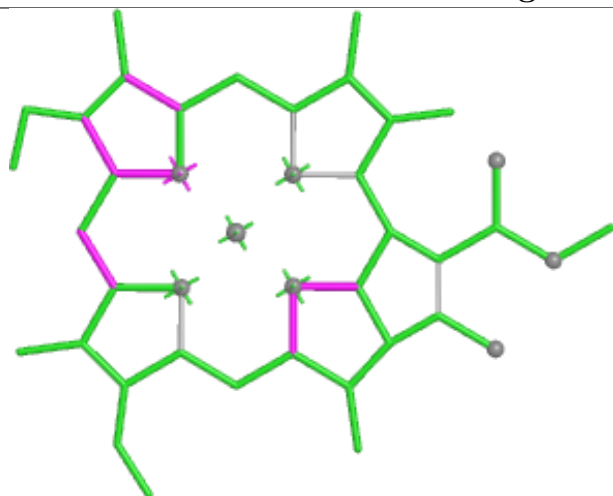
Ligand CLA y 310



Ligand BCR b 847



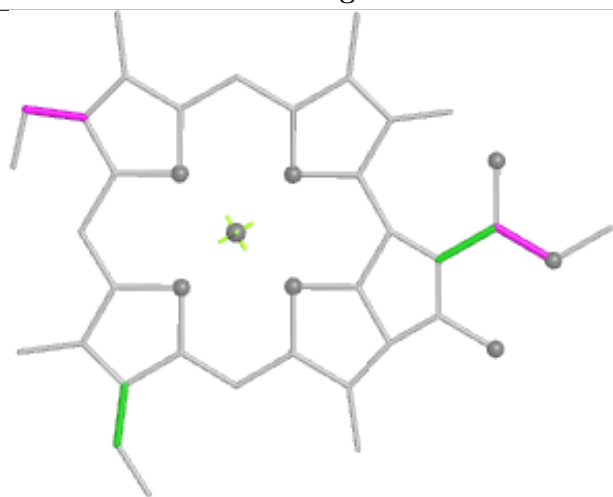
Ligand CLA 8 322



Bond lengths



Bond angles

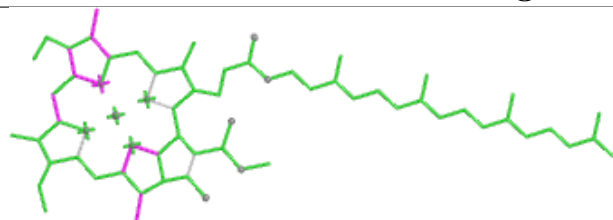


Torsions

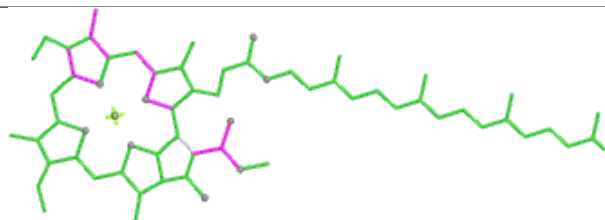


Rings

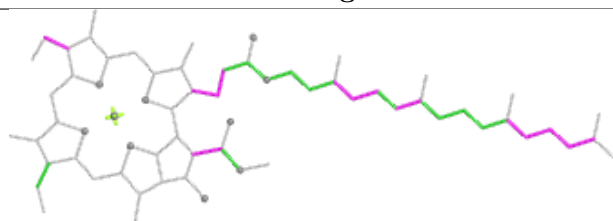
Ligand CLA F 308



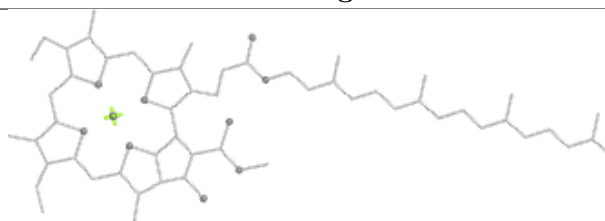
Bond lengths



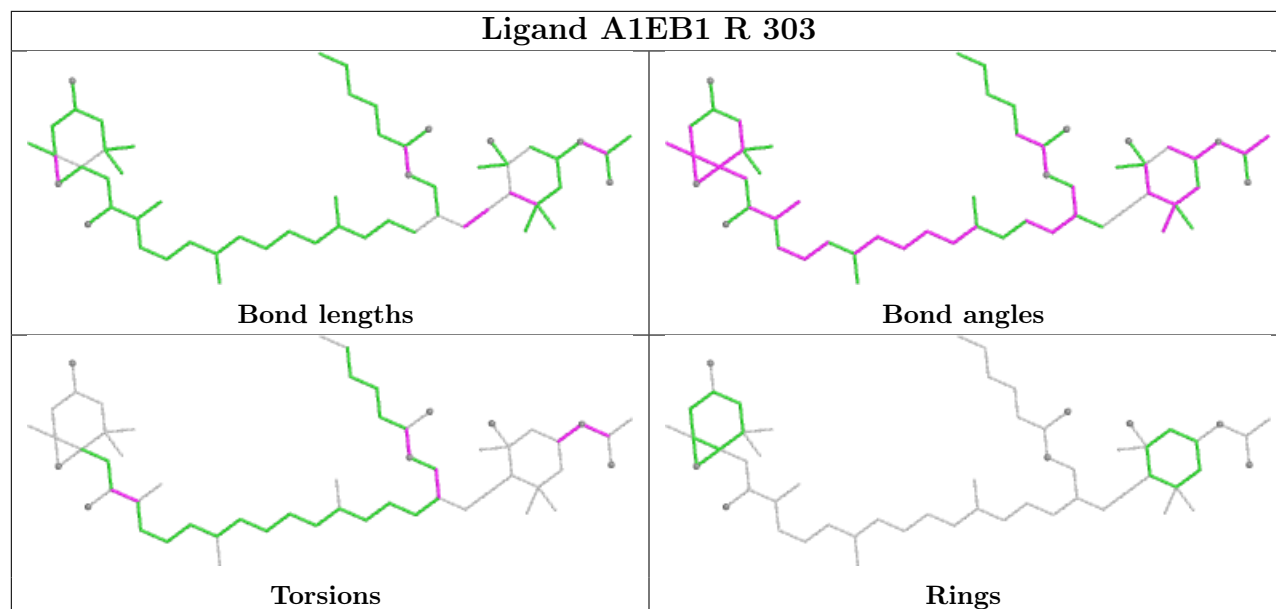
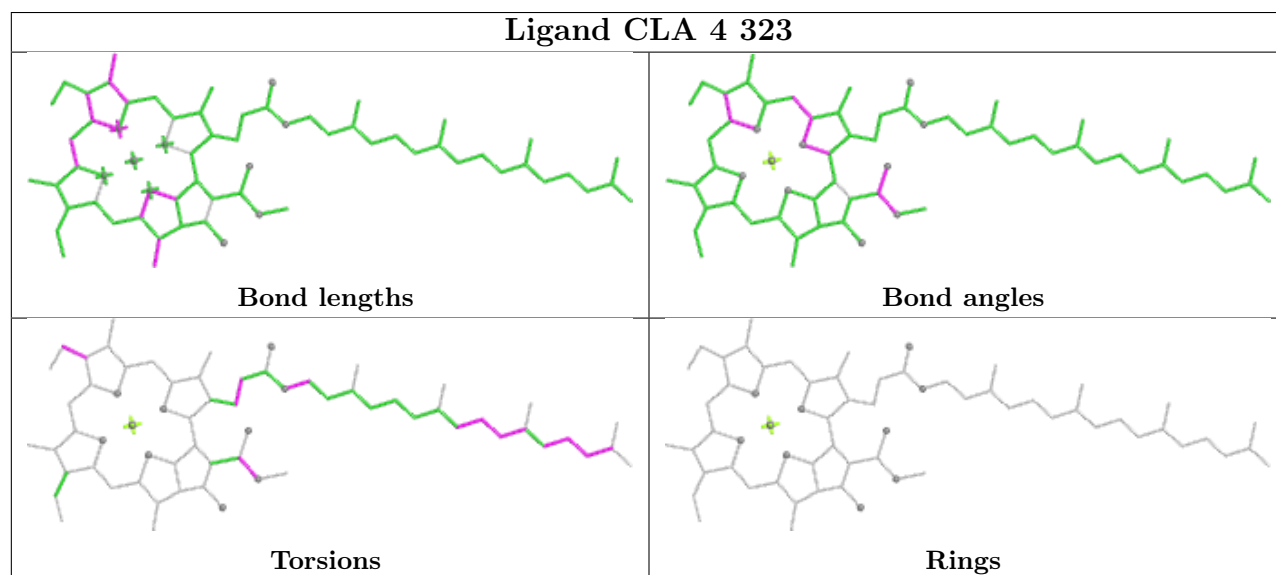
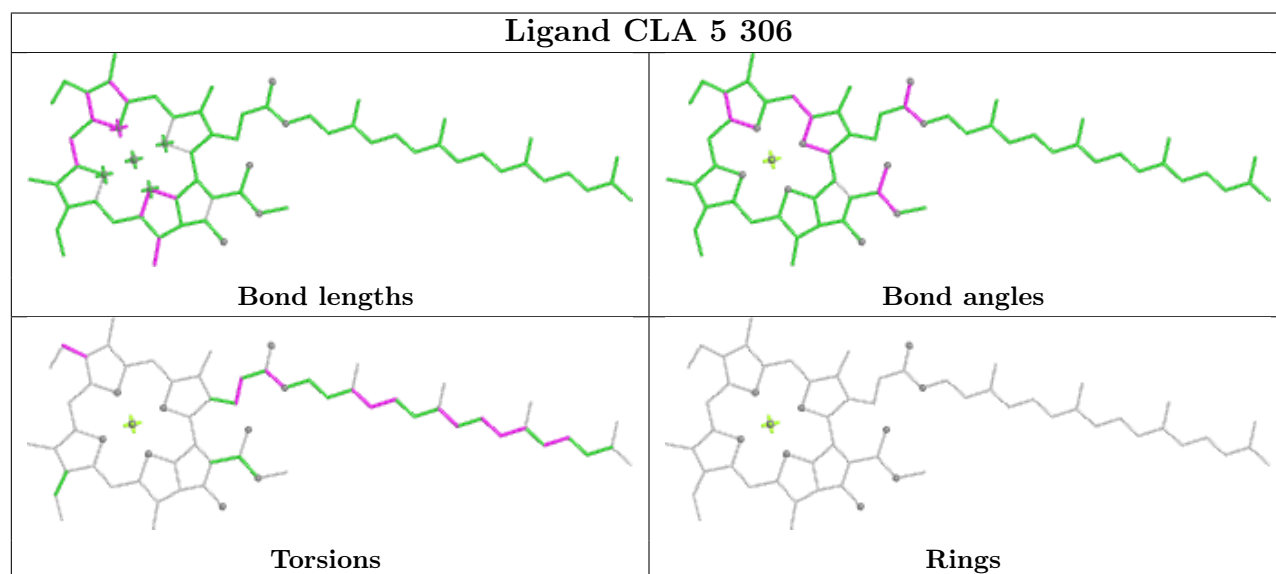
Bond angles

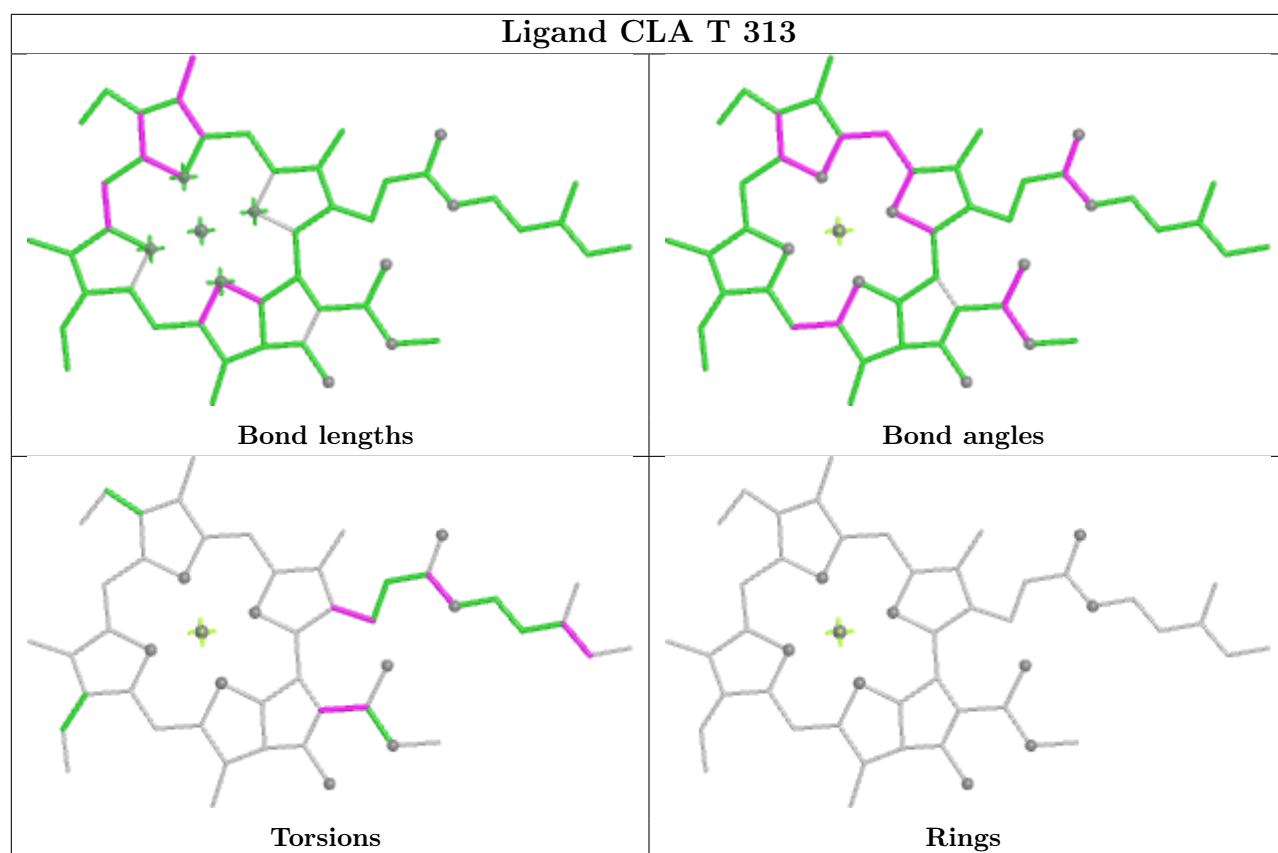


Torsions

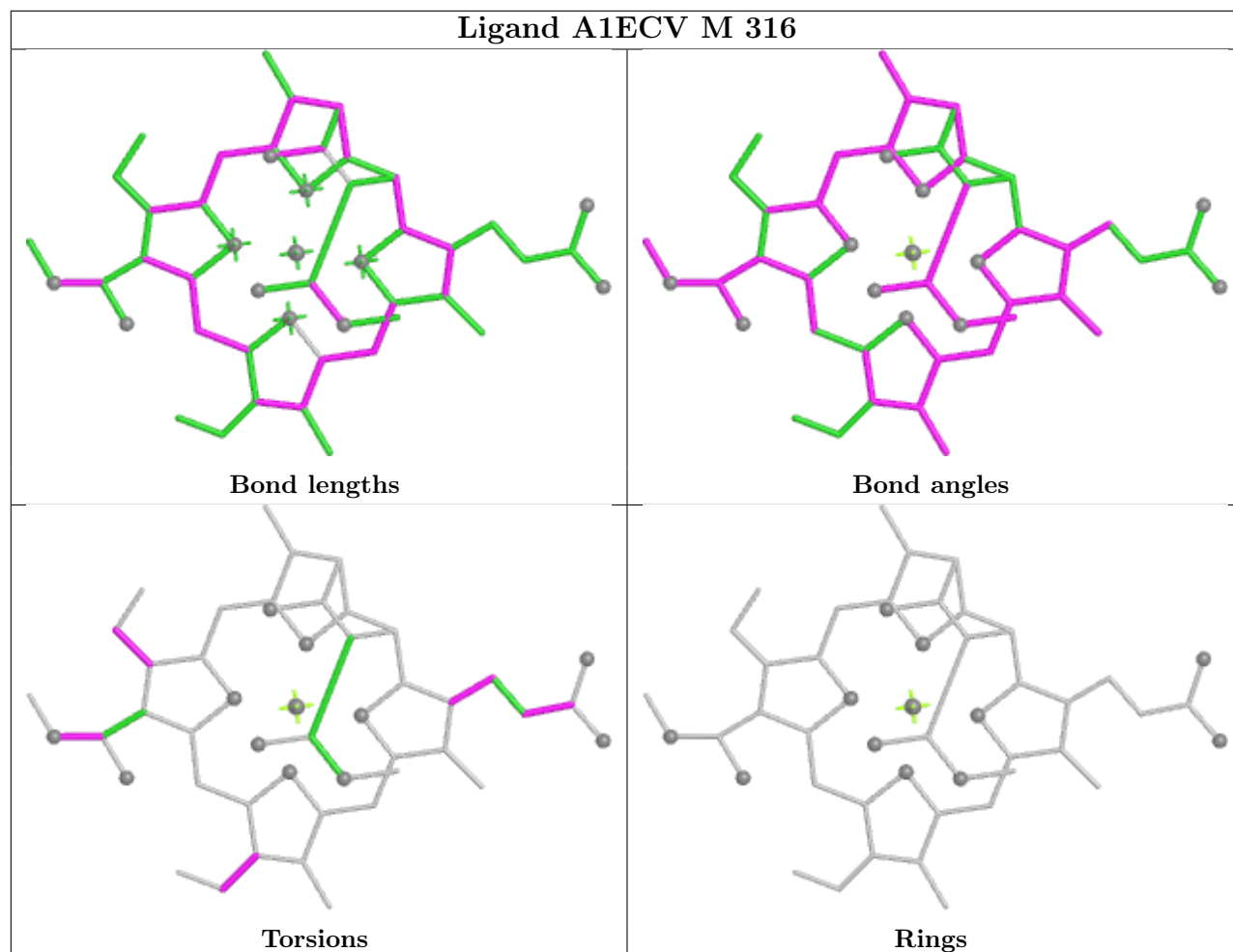


Rings

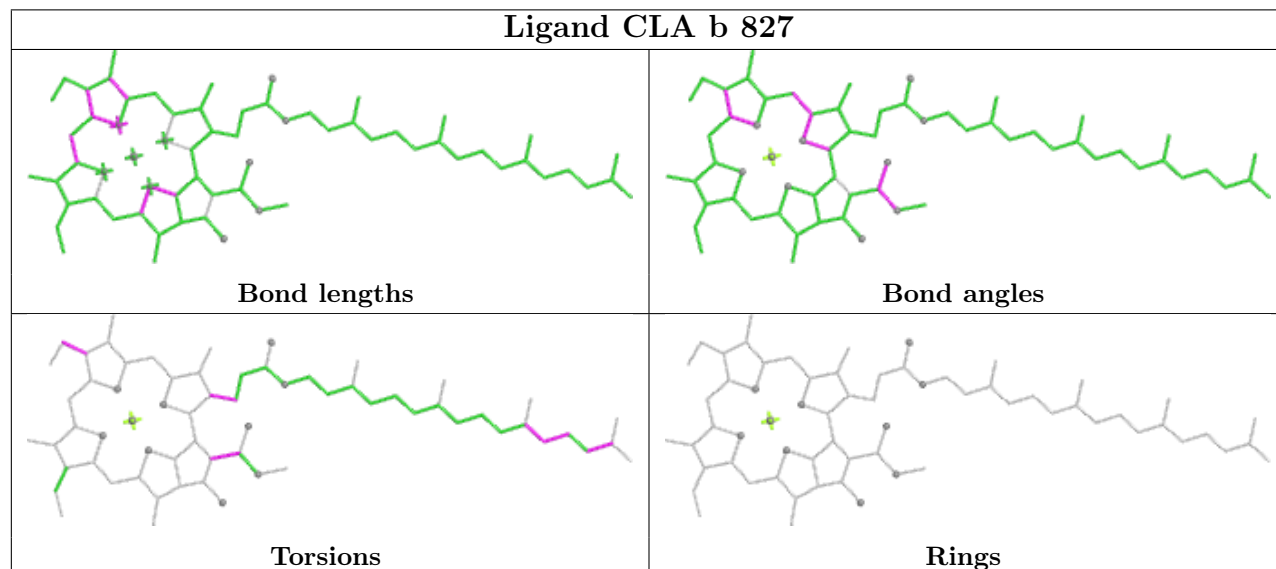
Ligand A1EB1 R 303**Ligand CLA 4 323****Ligand CLA 5 306**



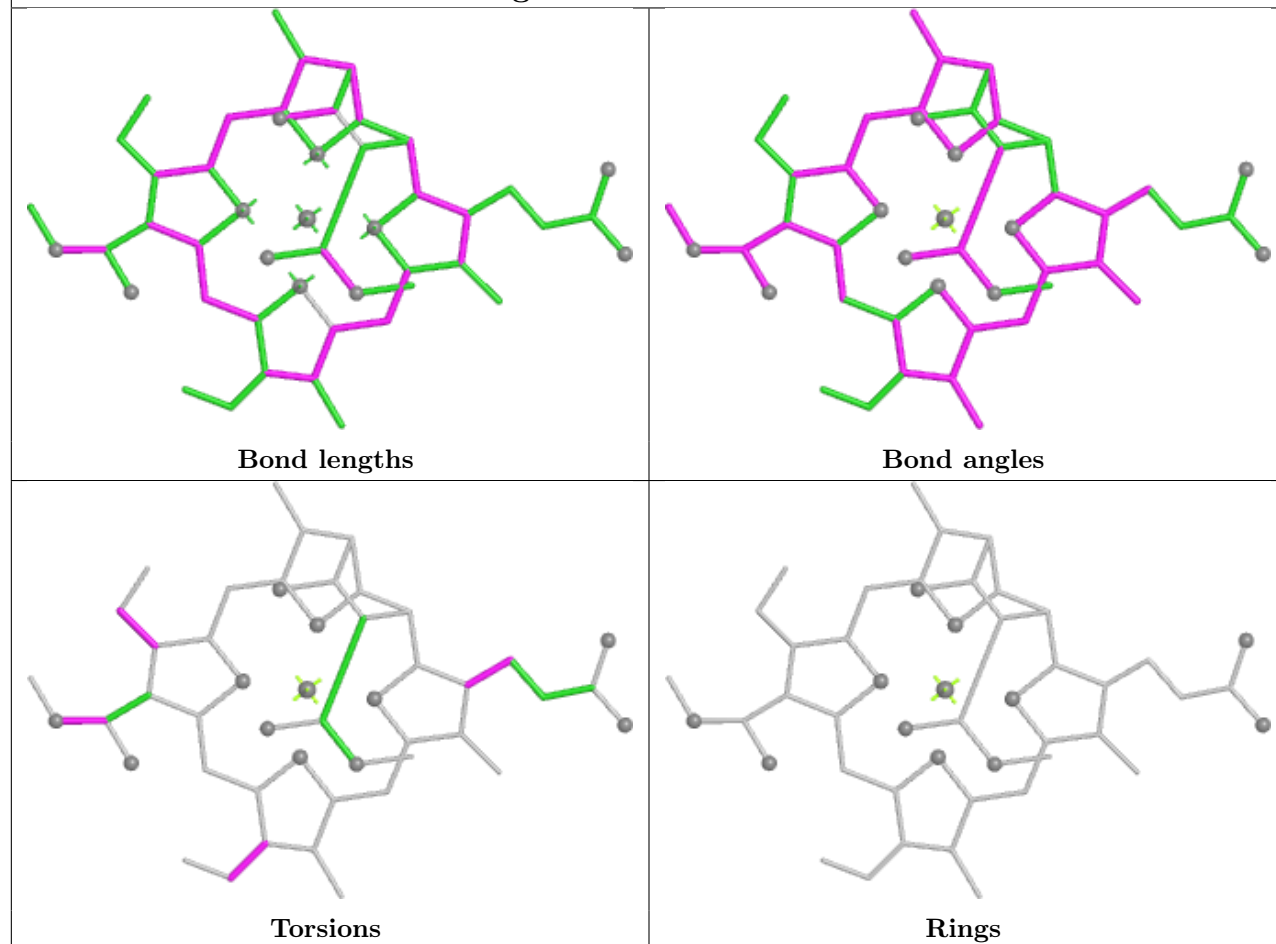
Ligand A1ECV M 316



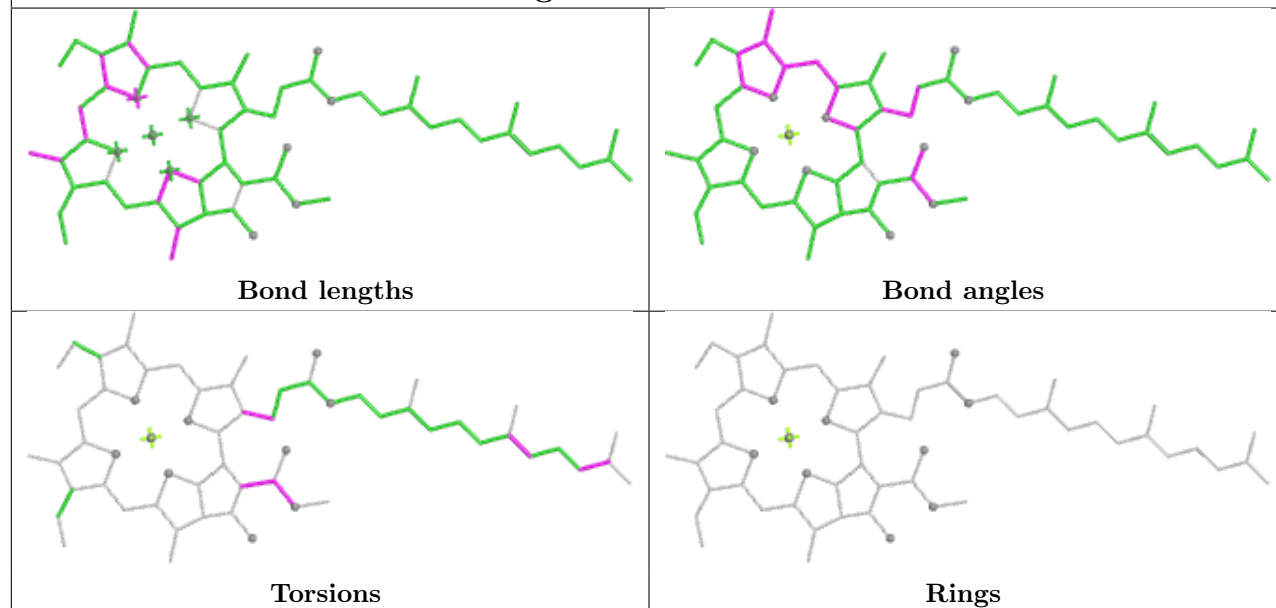
Ligand CLA b 827

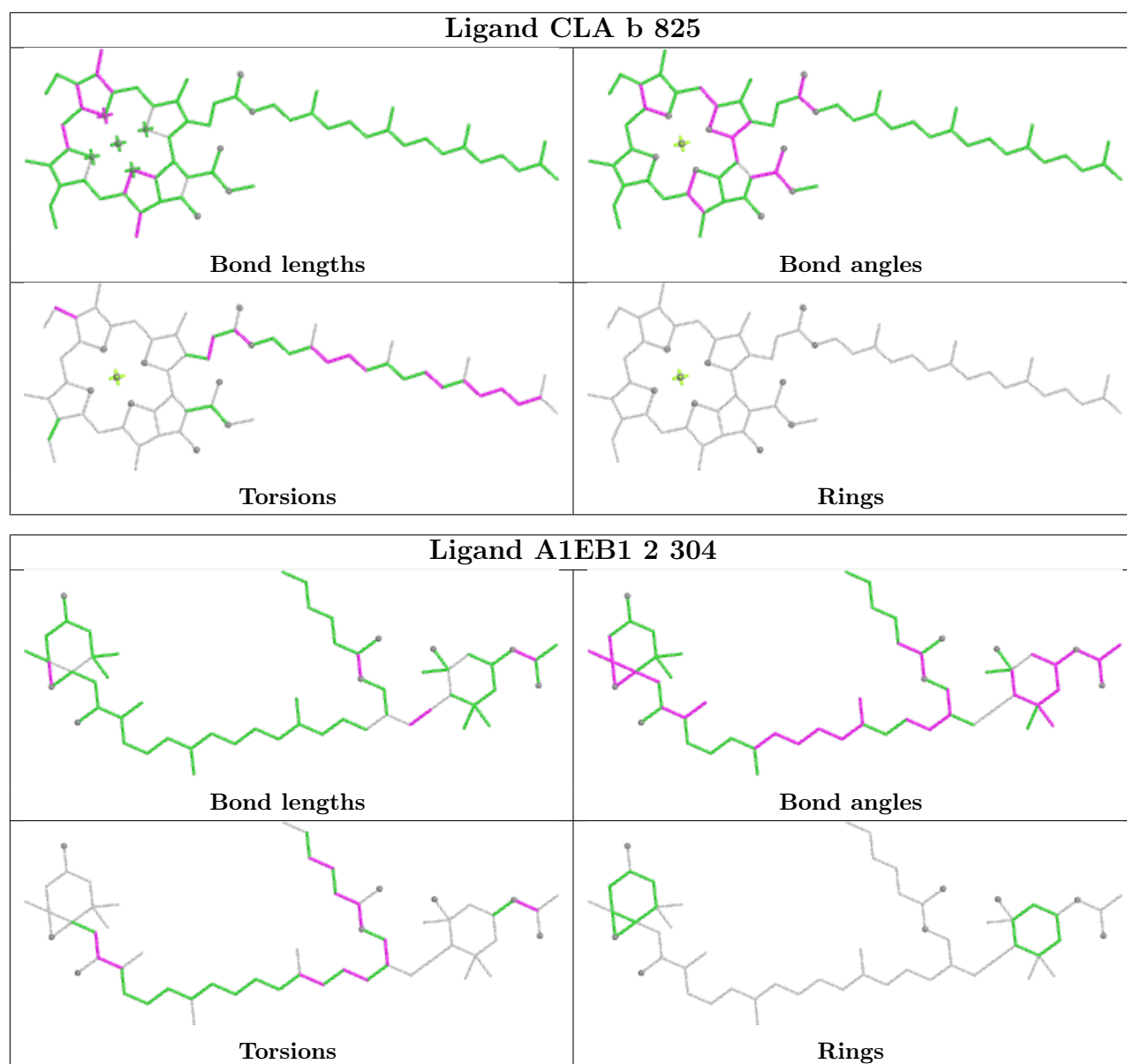


Ligand A1ECV x 316

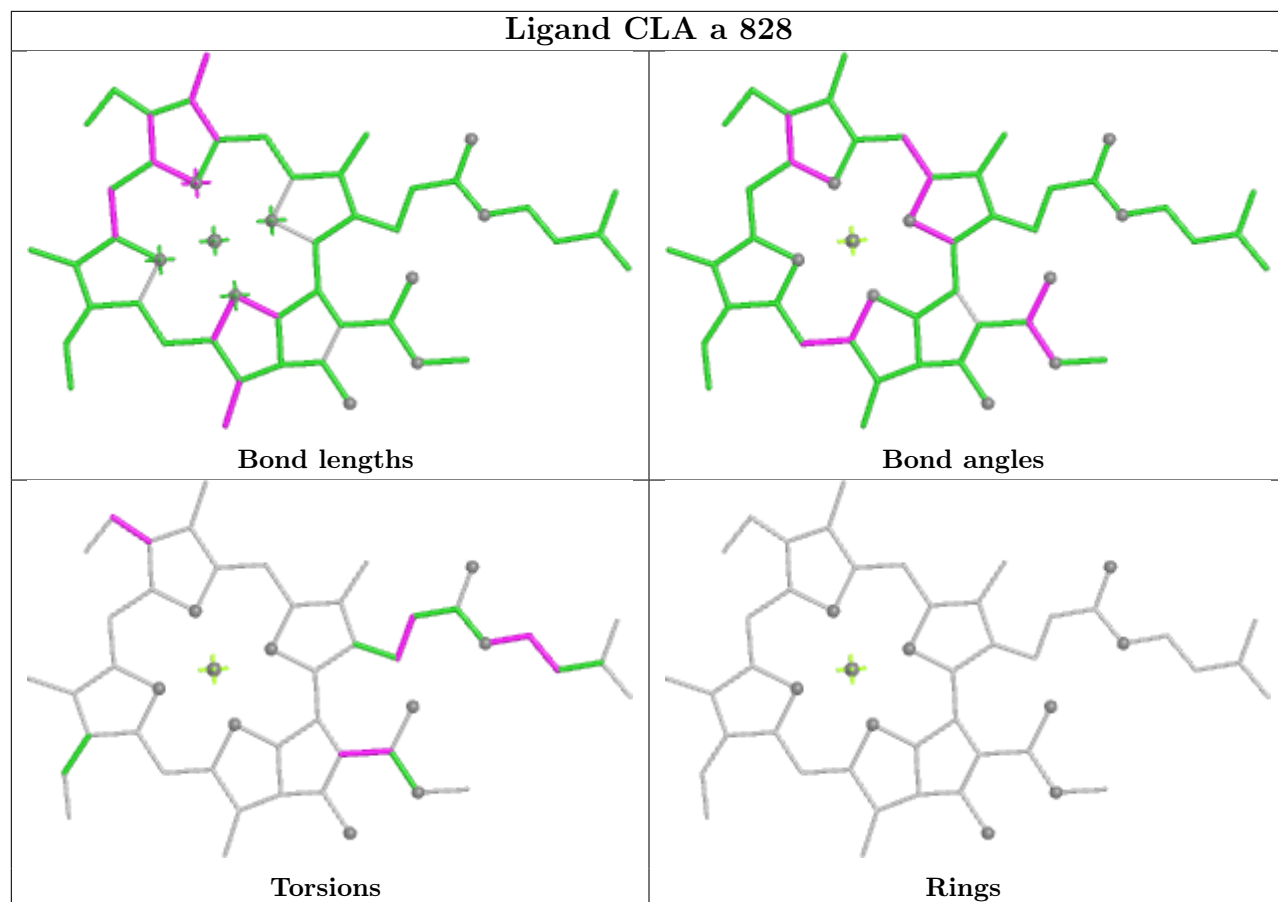


Ligand CLA b 837

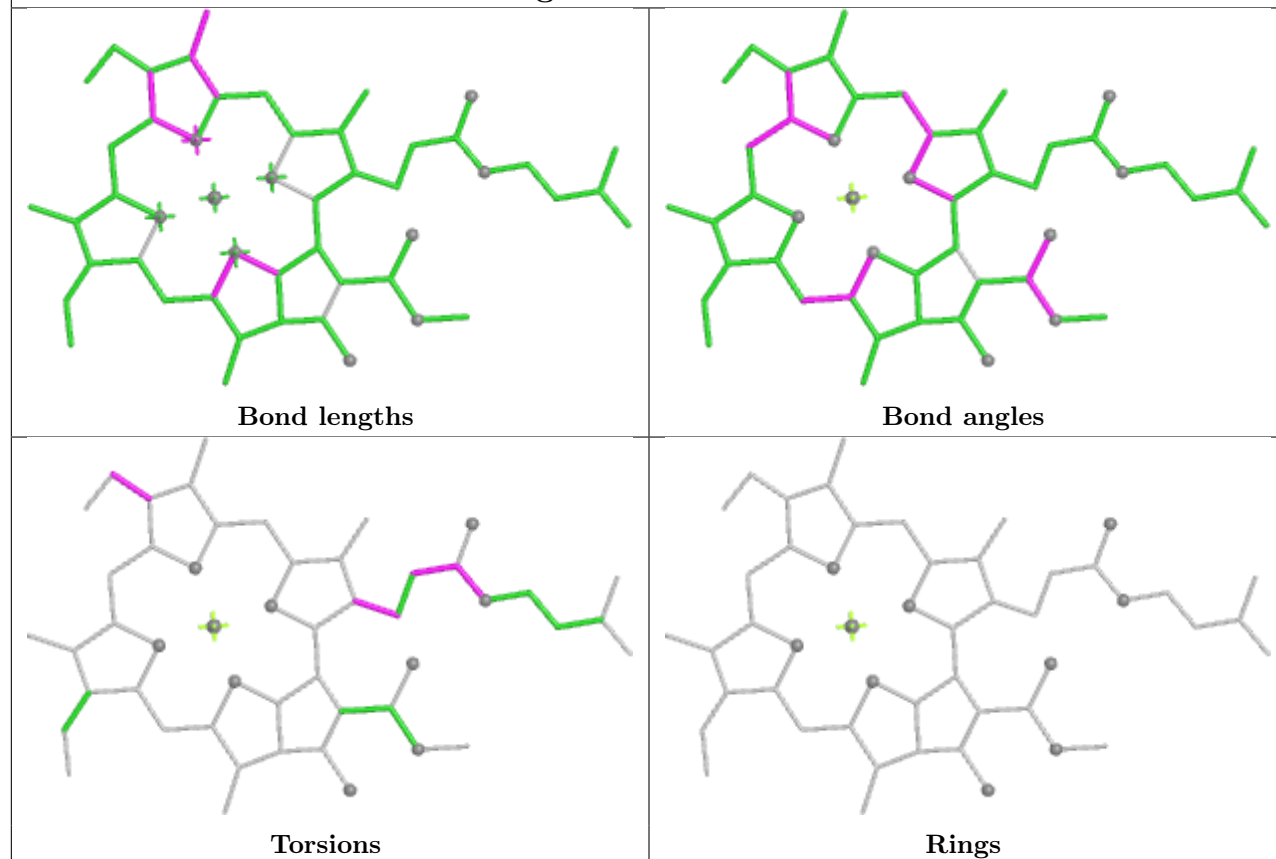




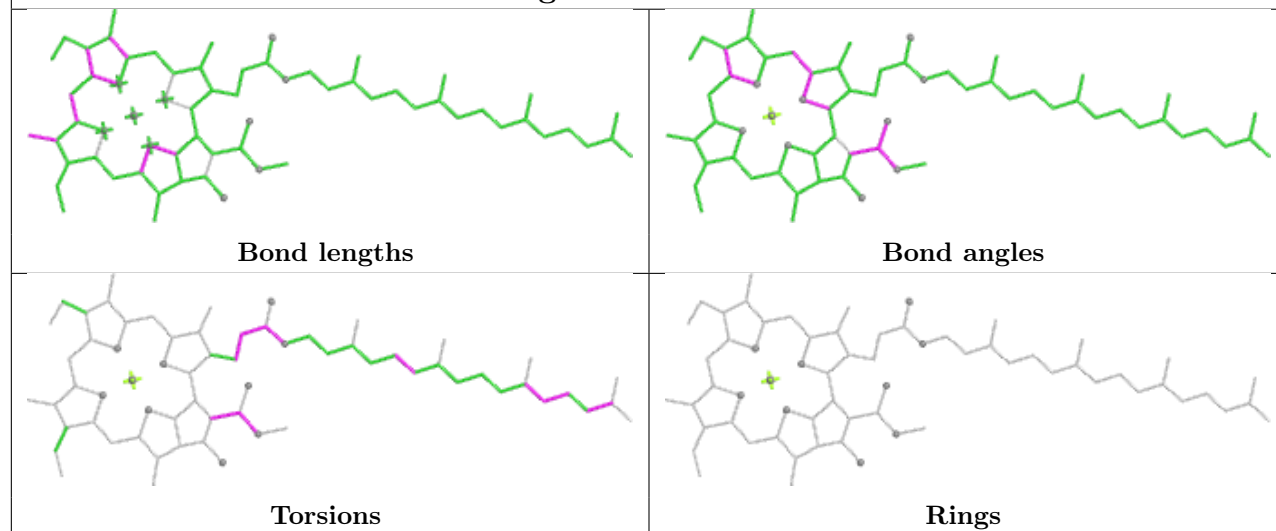
Ligand CLA a 828



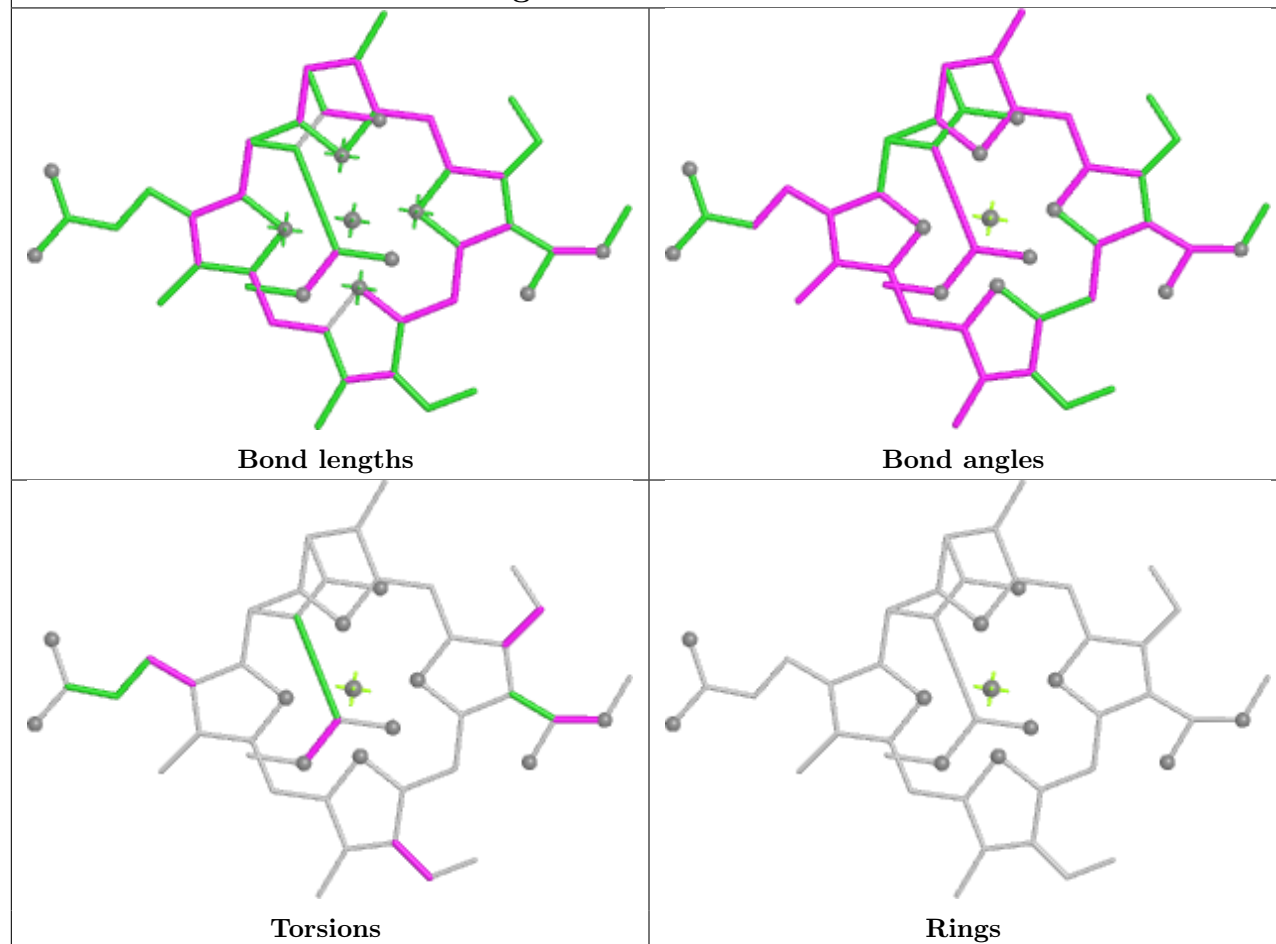
Ligand CLA a 832



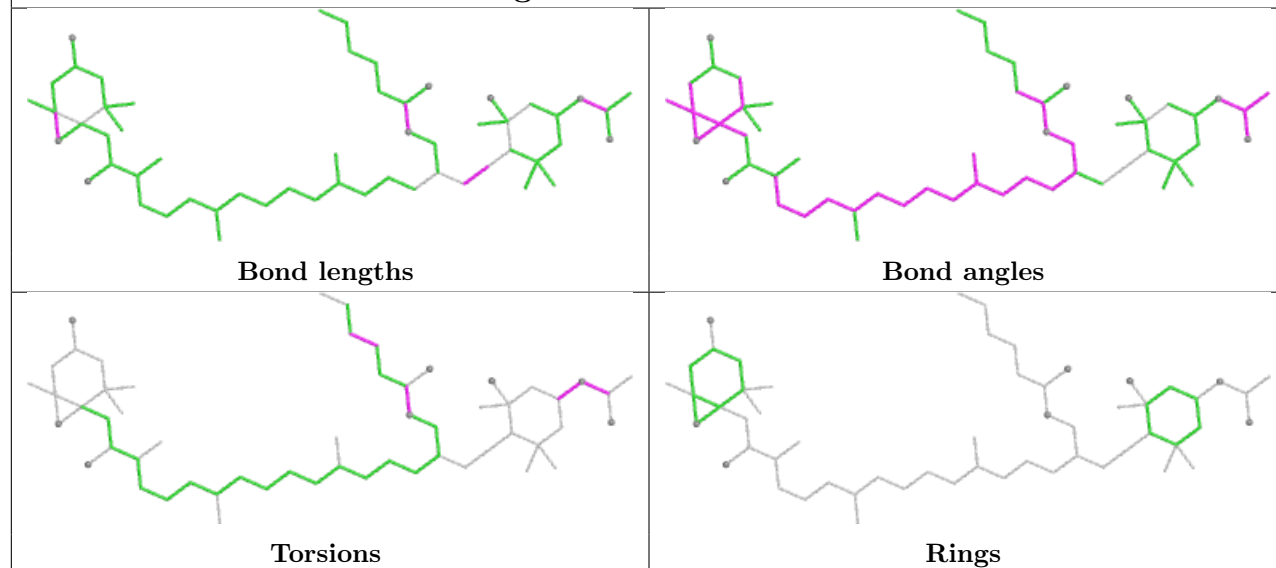
Ligand CLA I 311

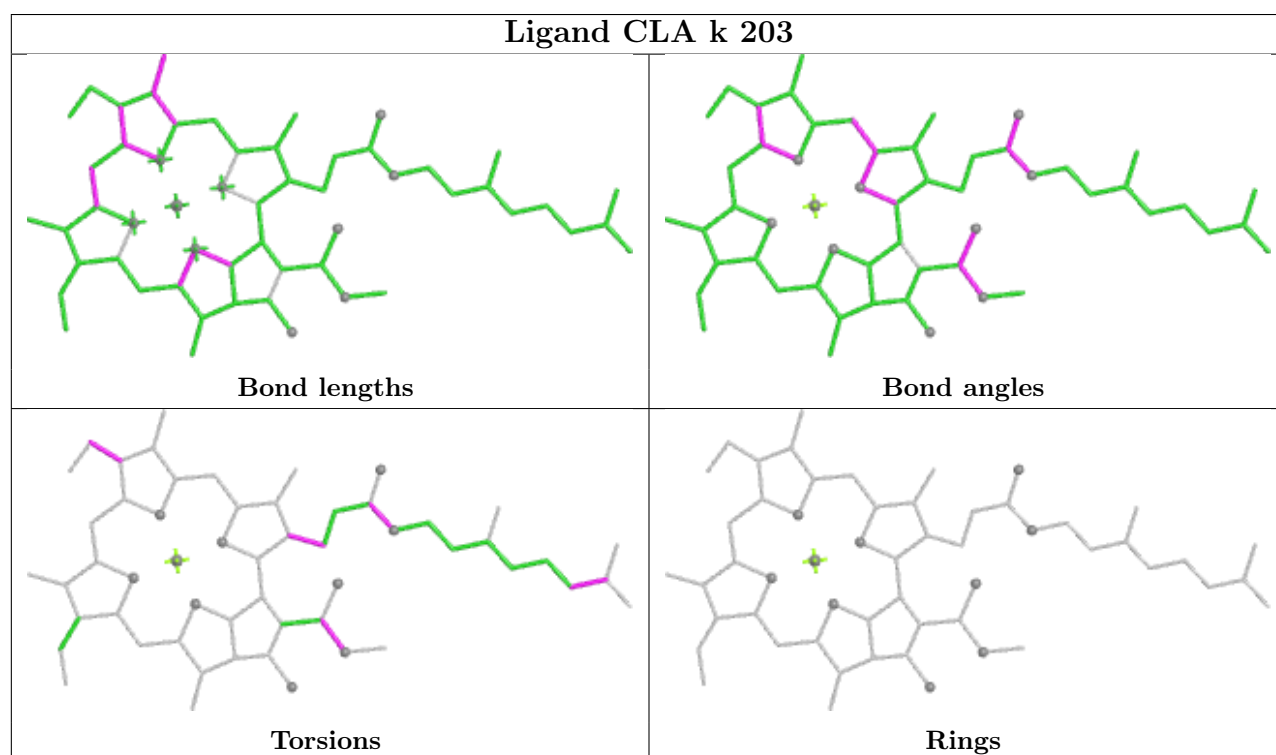
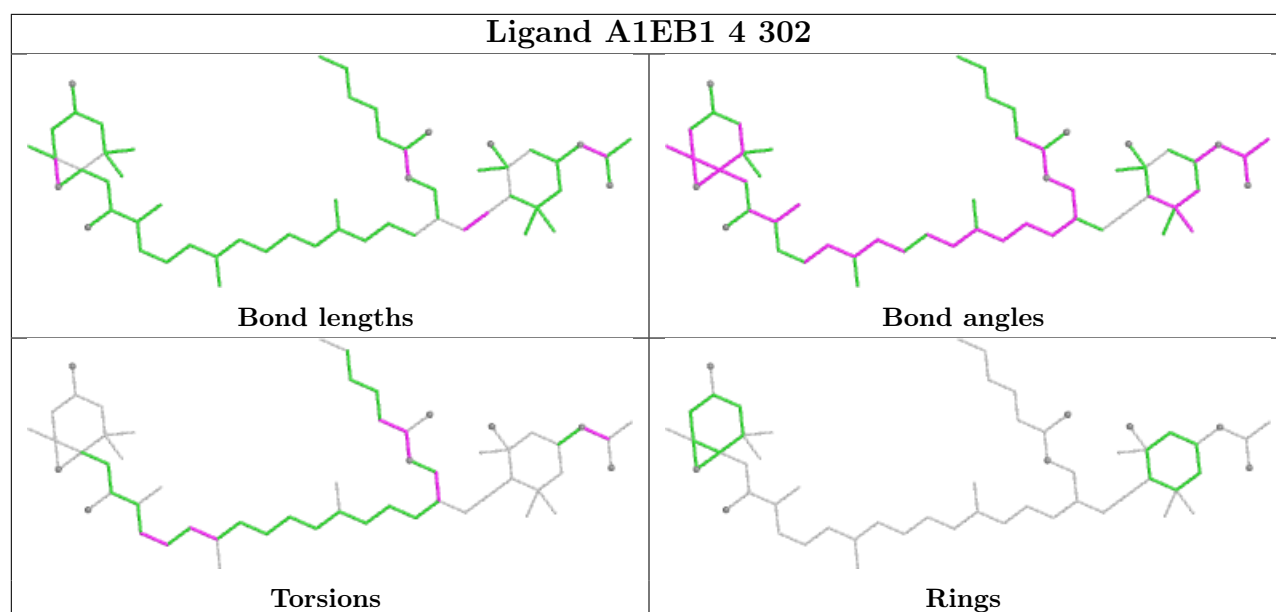


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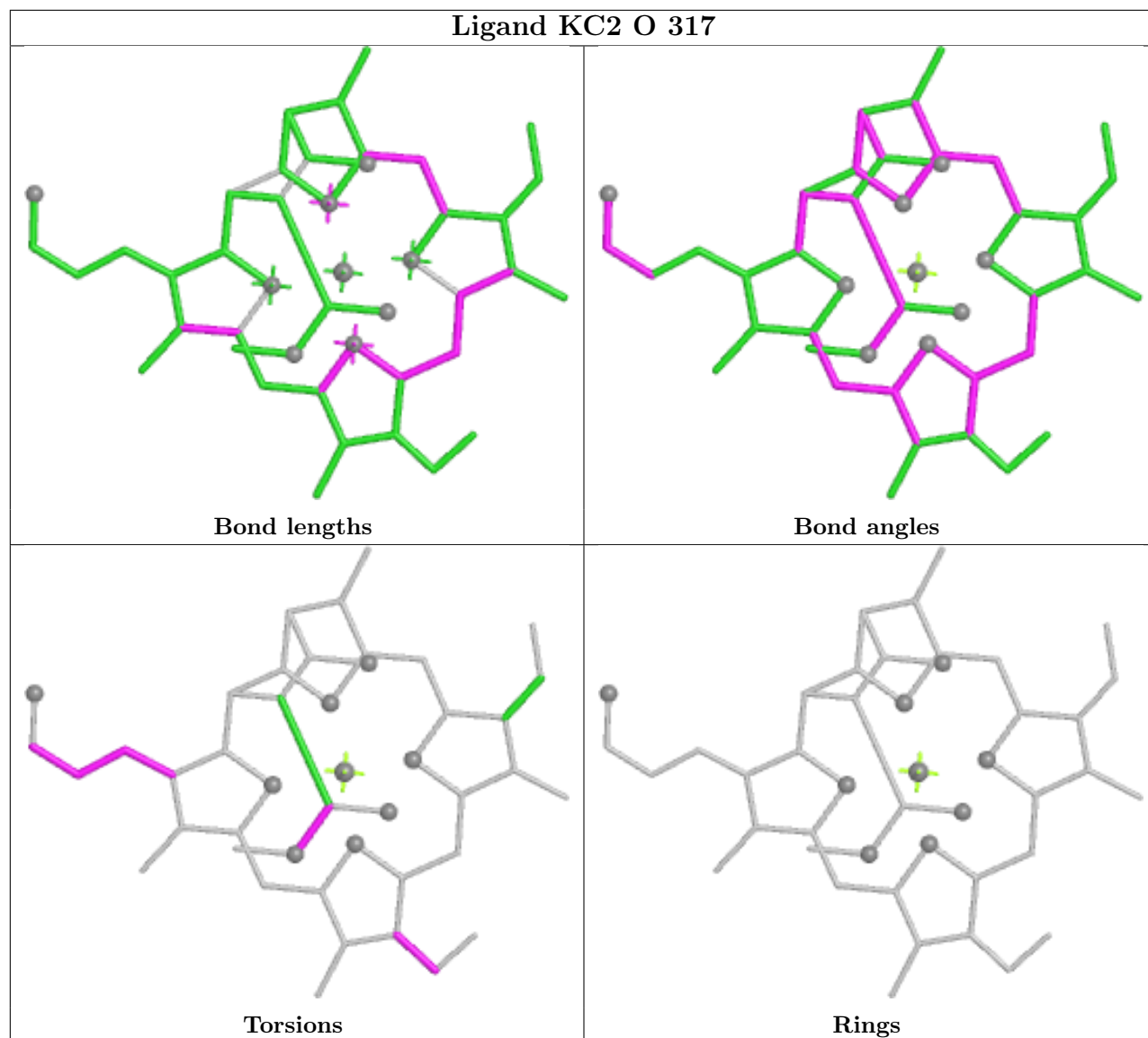


Ligand A1EB1 T 307

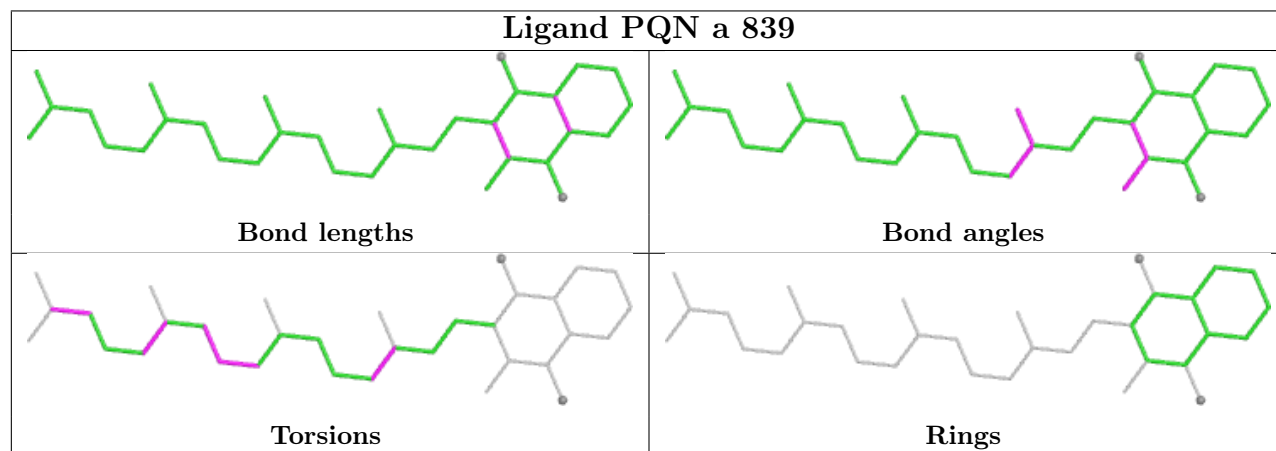




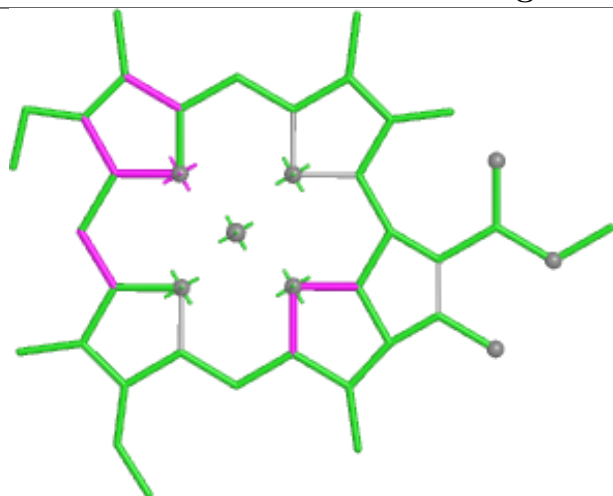
Ligand KC2 O 317



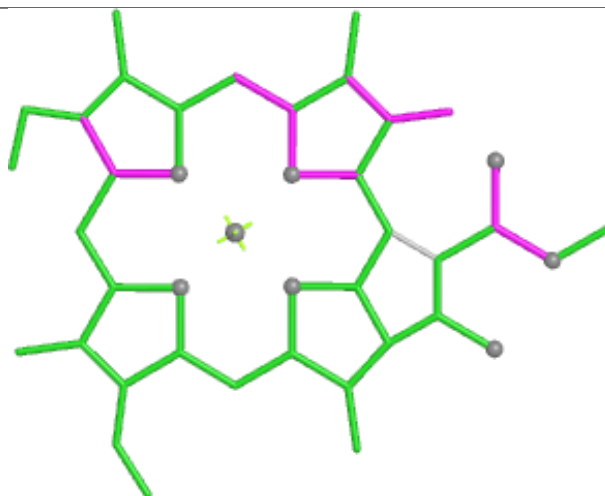
Ligand PQN a 839



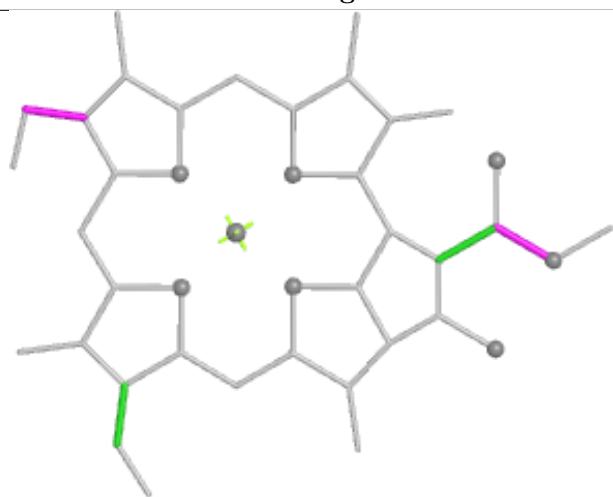
Ligand CLA Z 315



Bond lengths



Bond angles

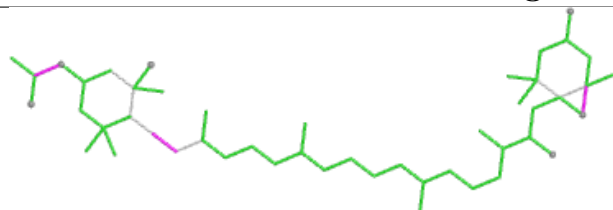


Torsions

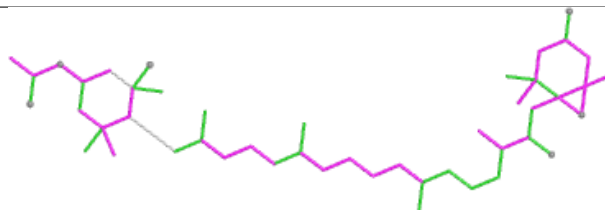


Rings

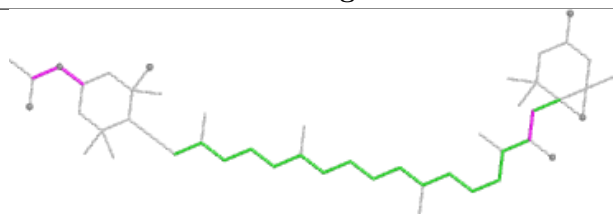
Ligand A86 0 301



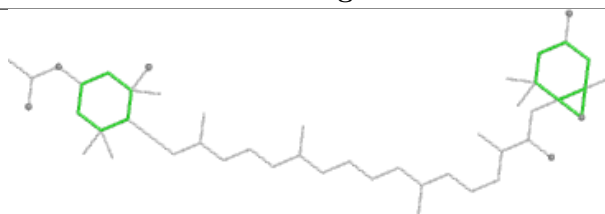
Bond lengths



Bond angles

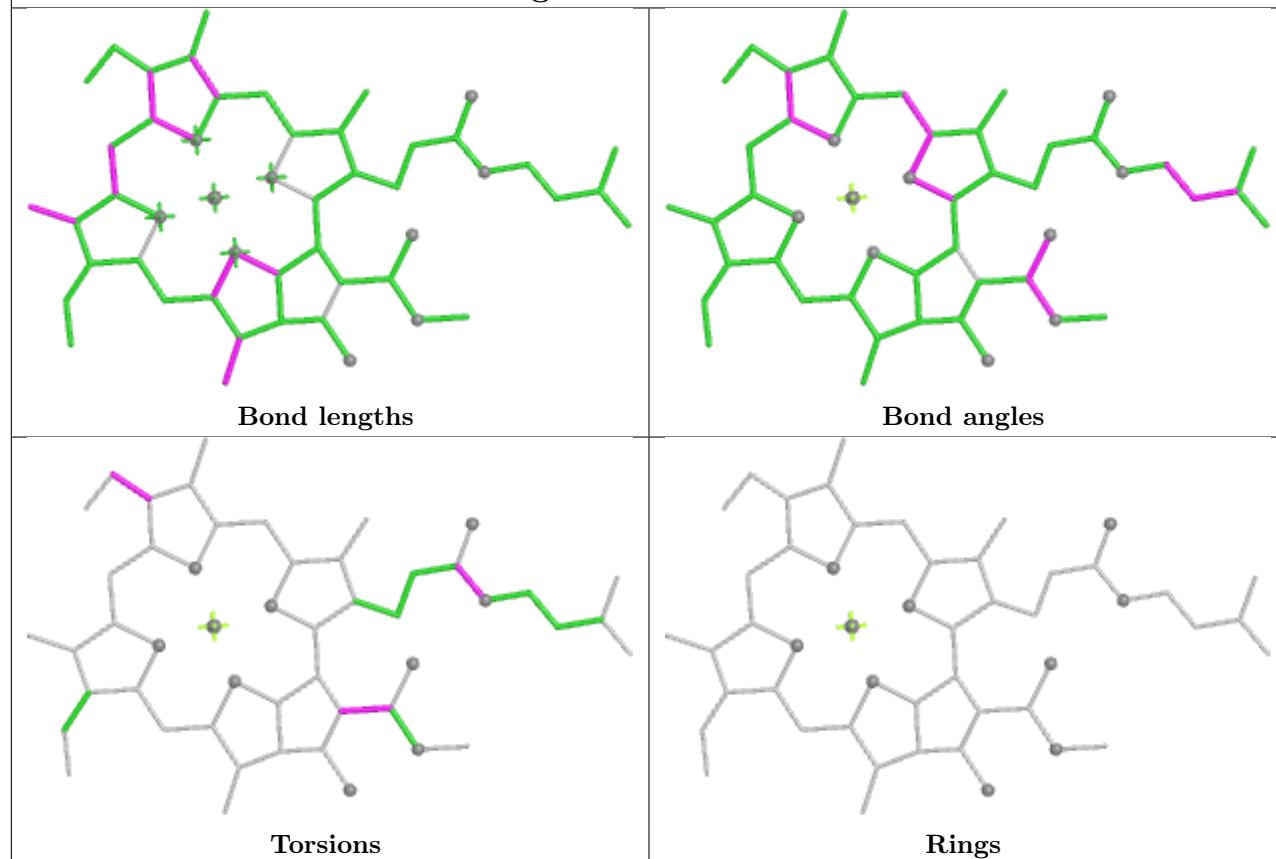


Torsions

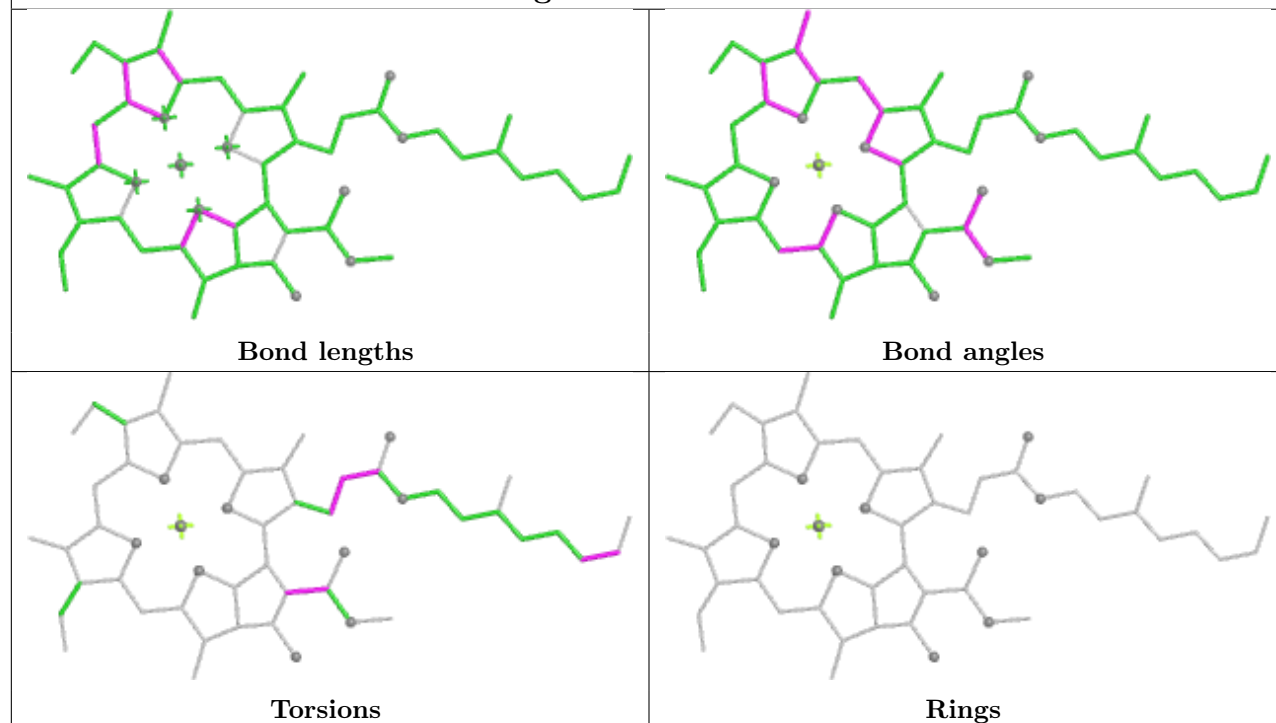


Rings

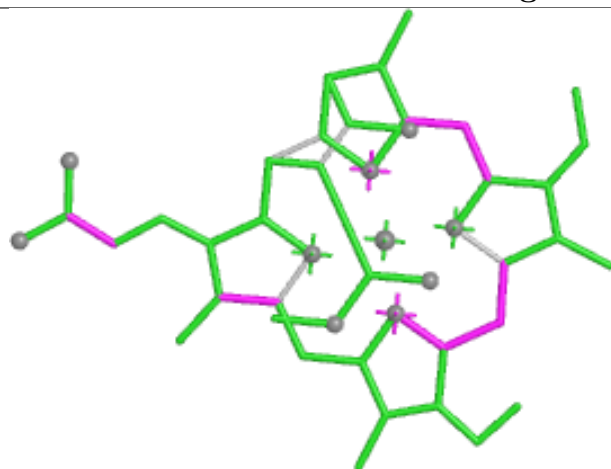
Ligand CLA R 311



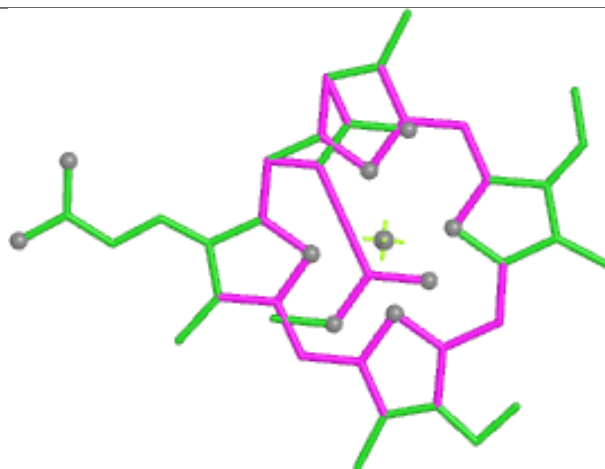
Ligand CLA F 310



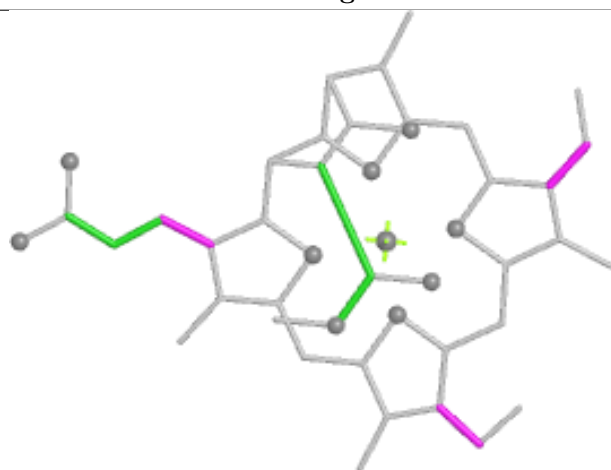
Ligand KC2 x 313



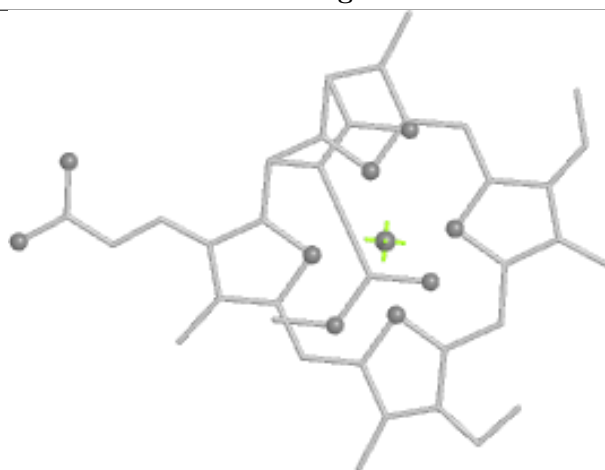
Bond lengths



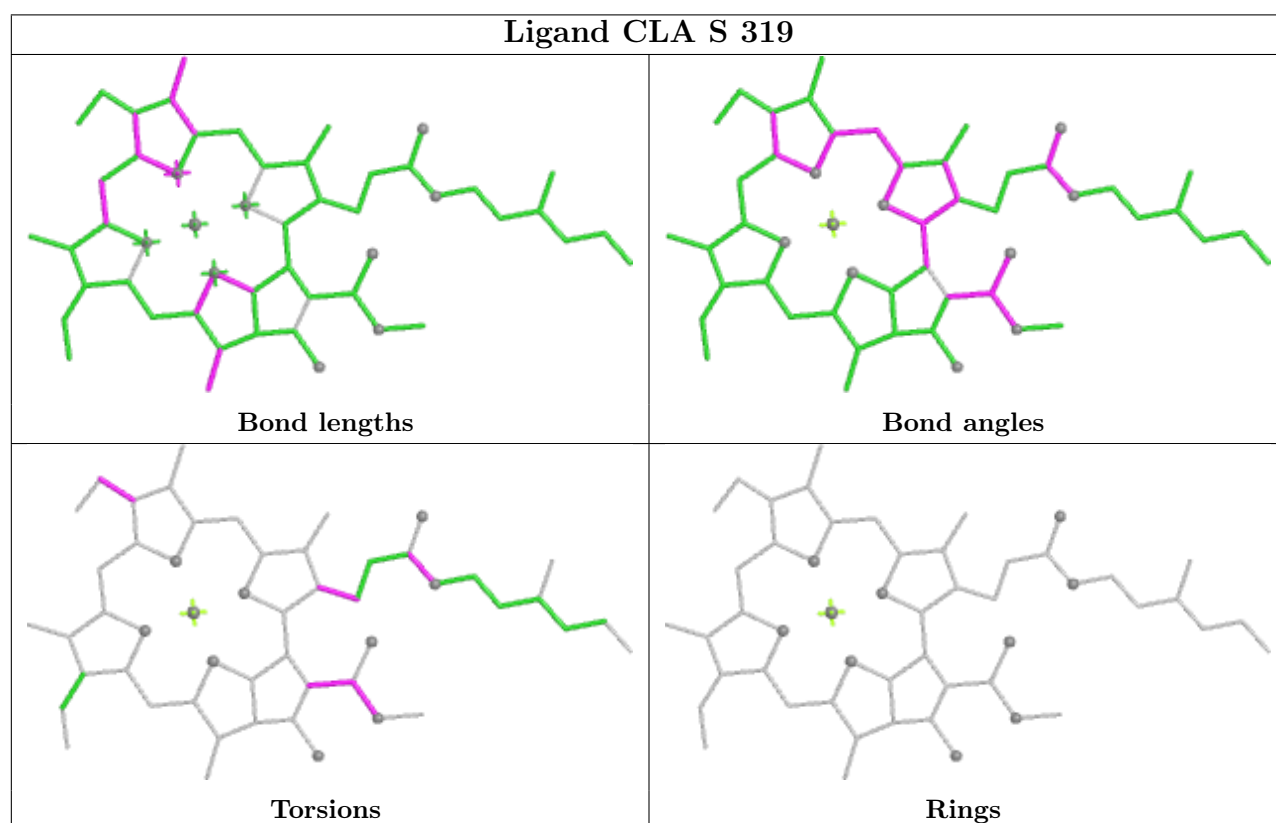
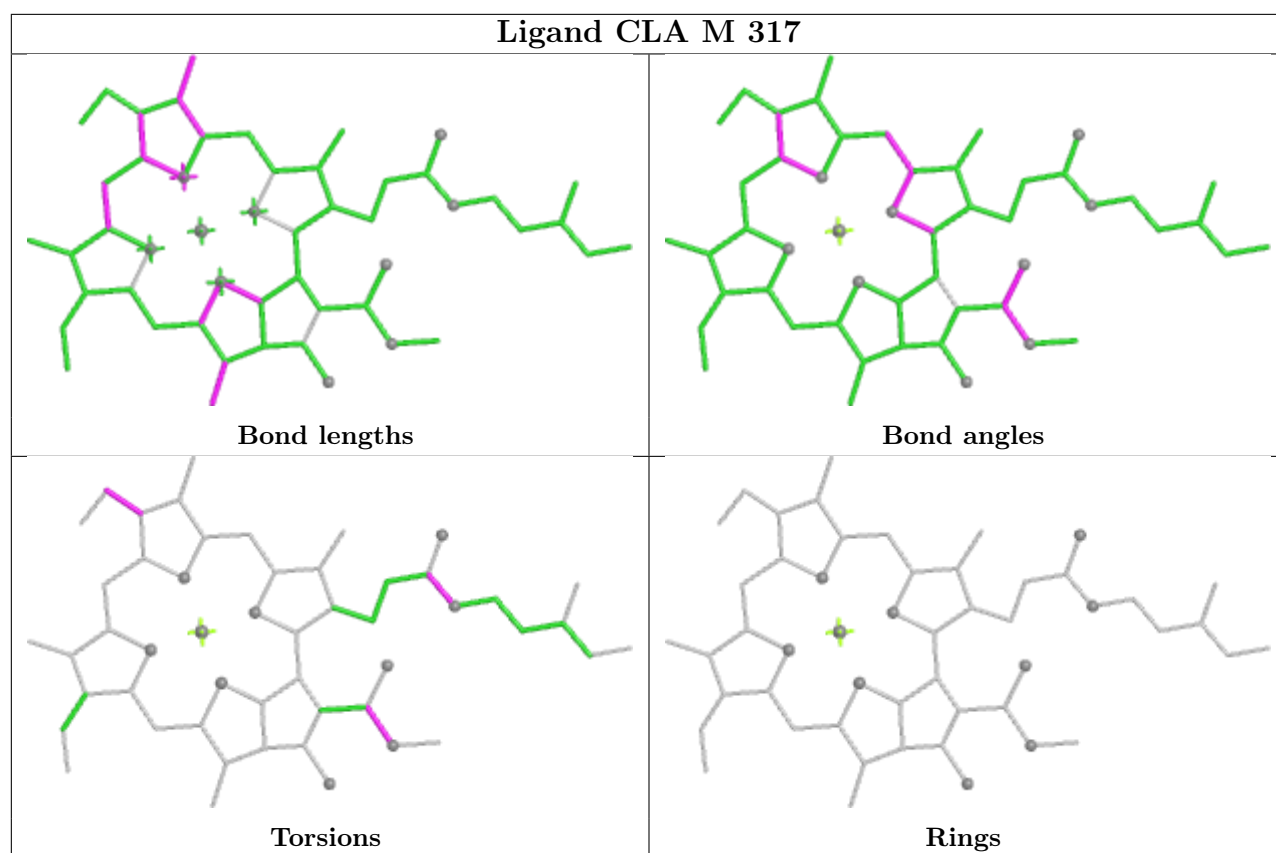
Bond angles

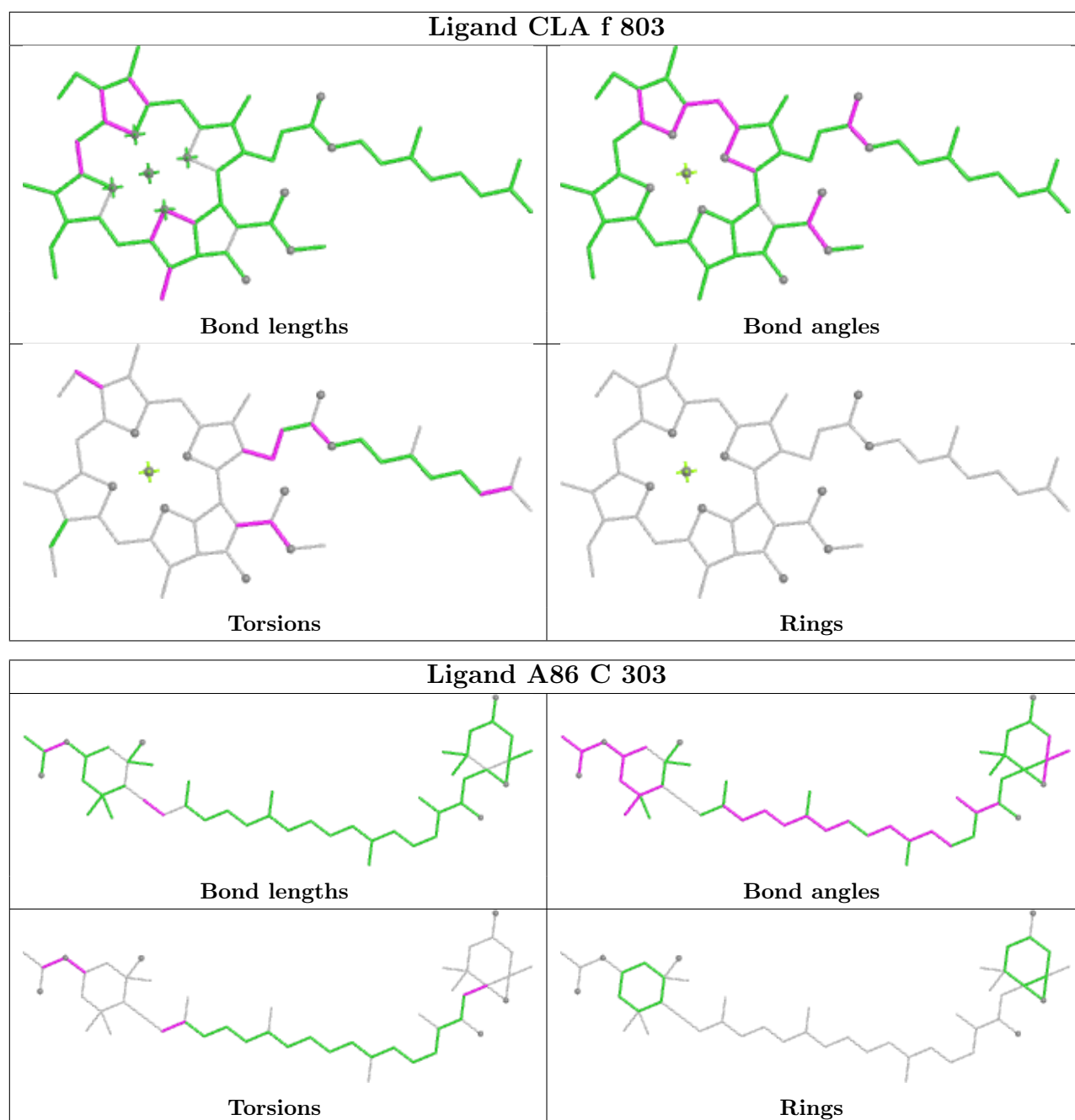


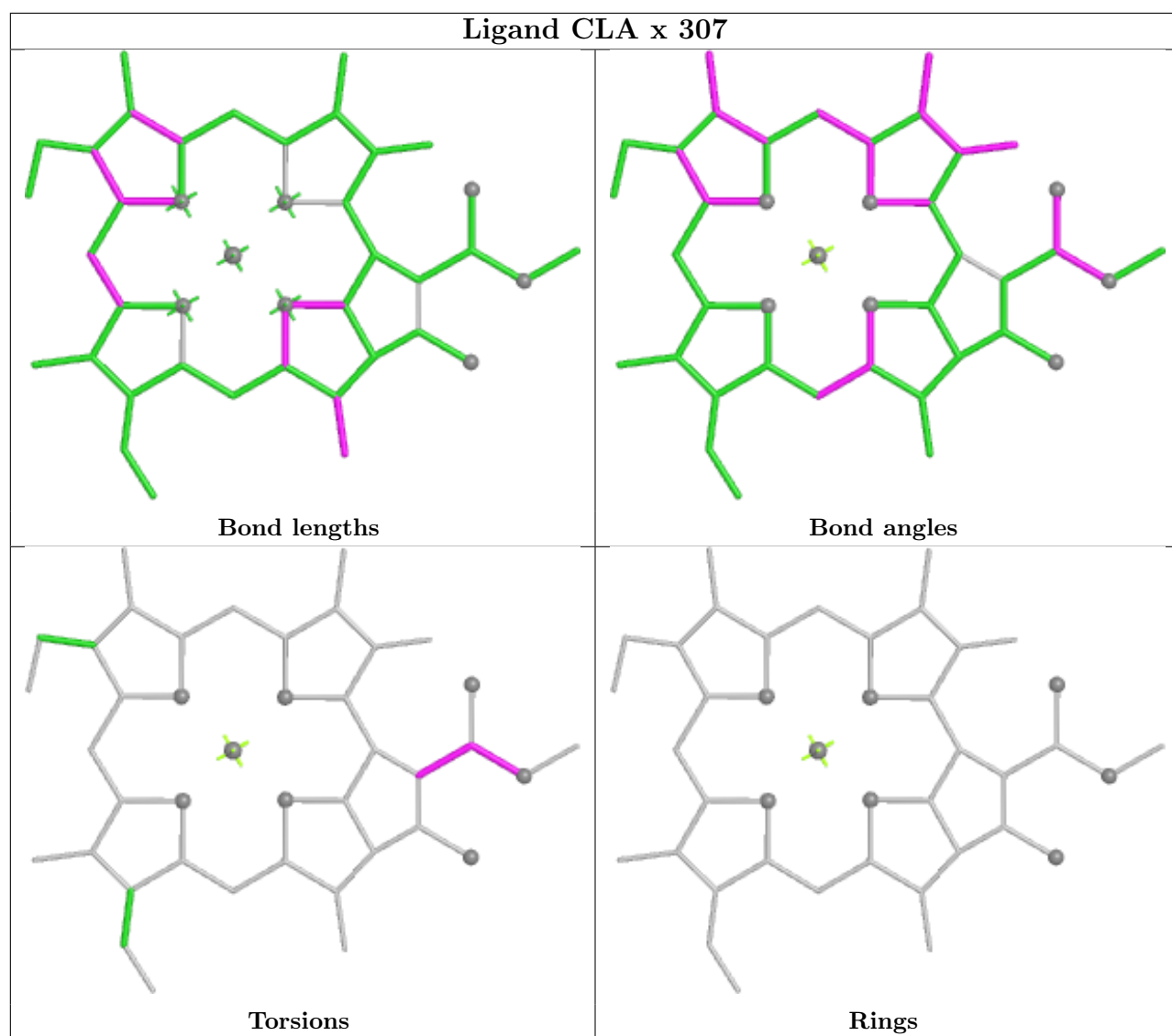
Torsions



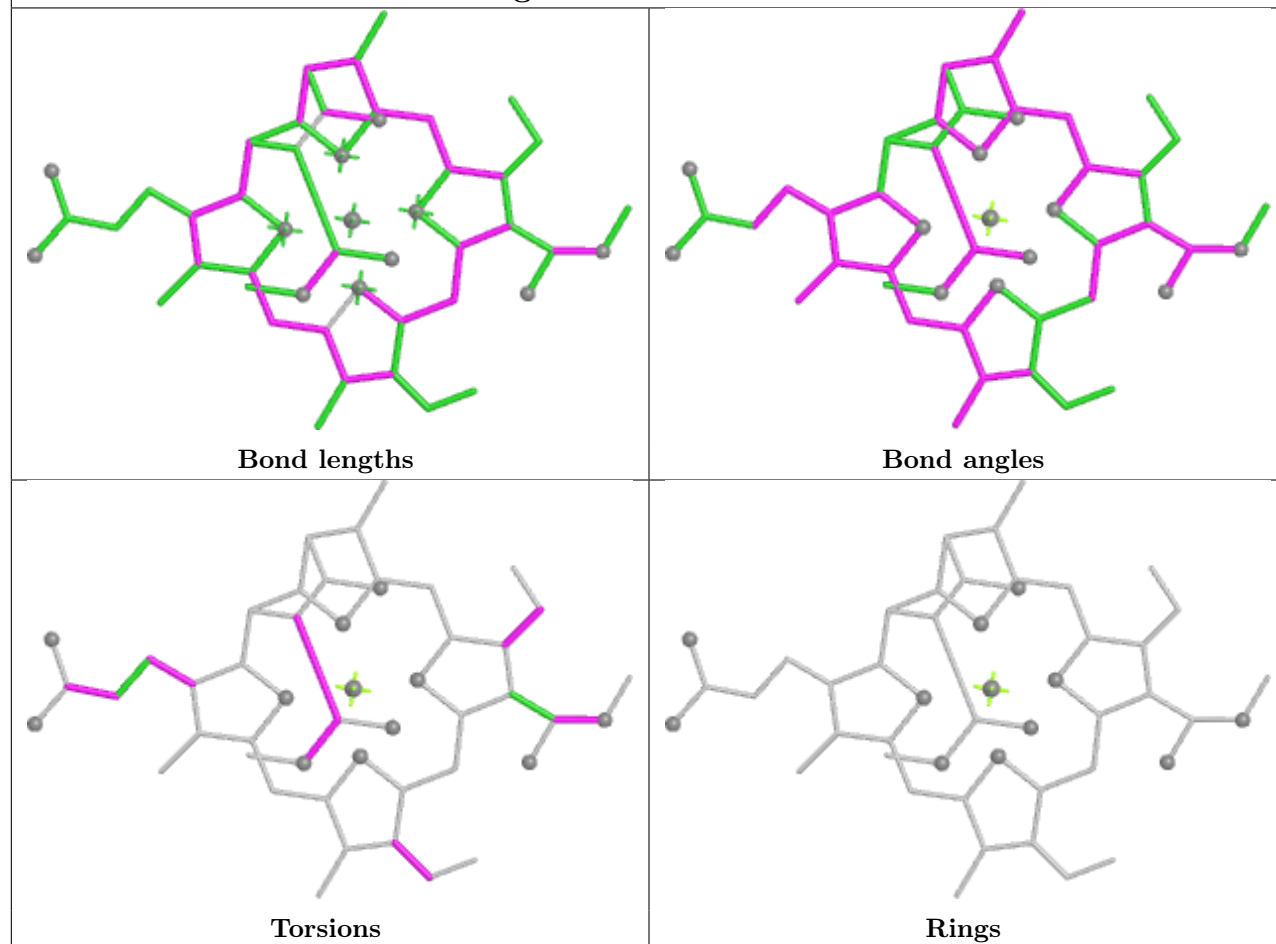
Rings



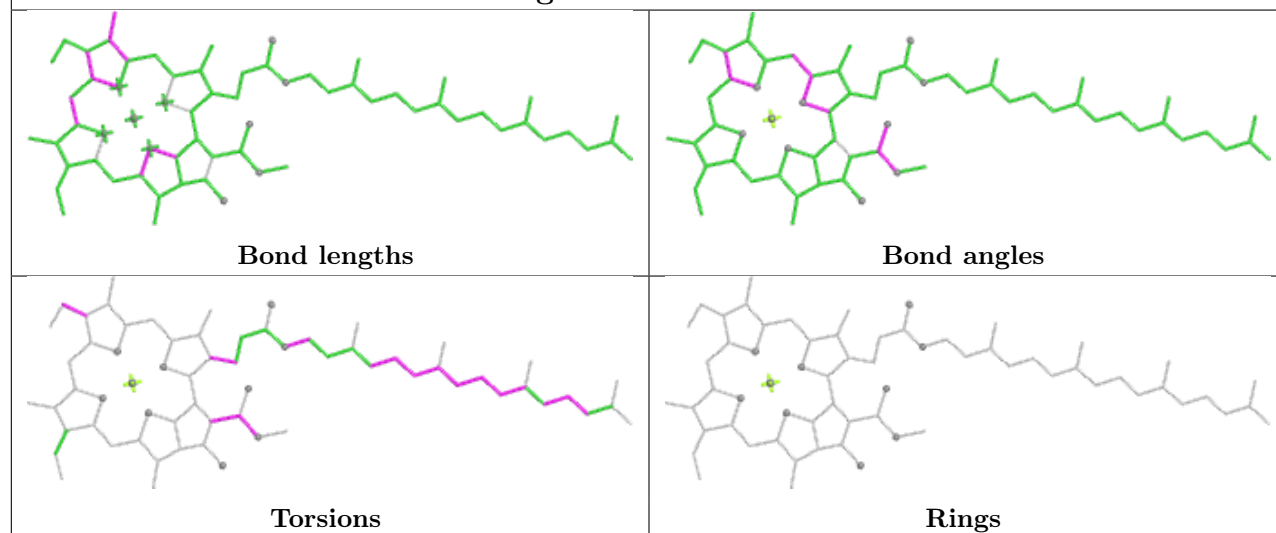


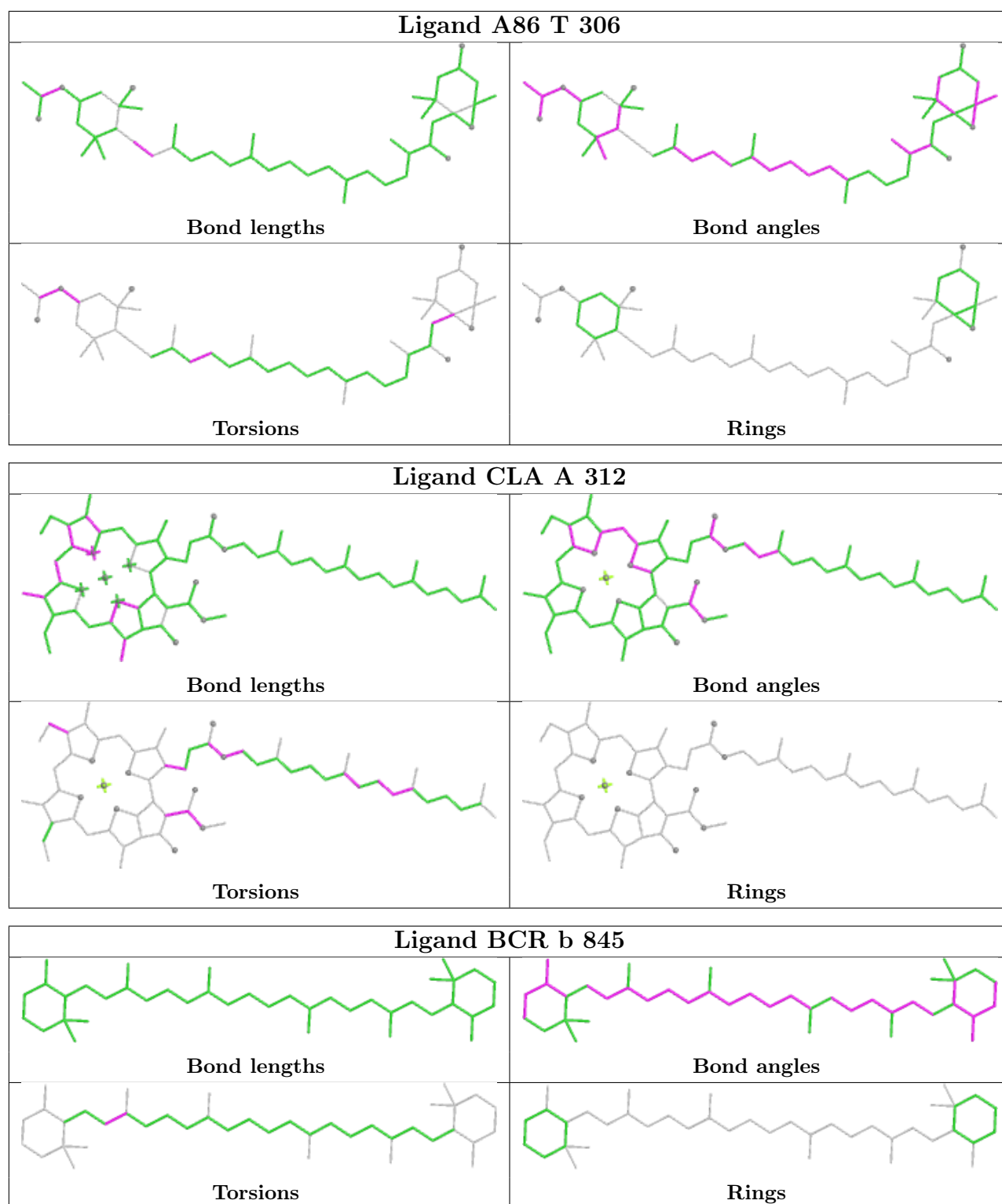


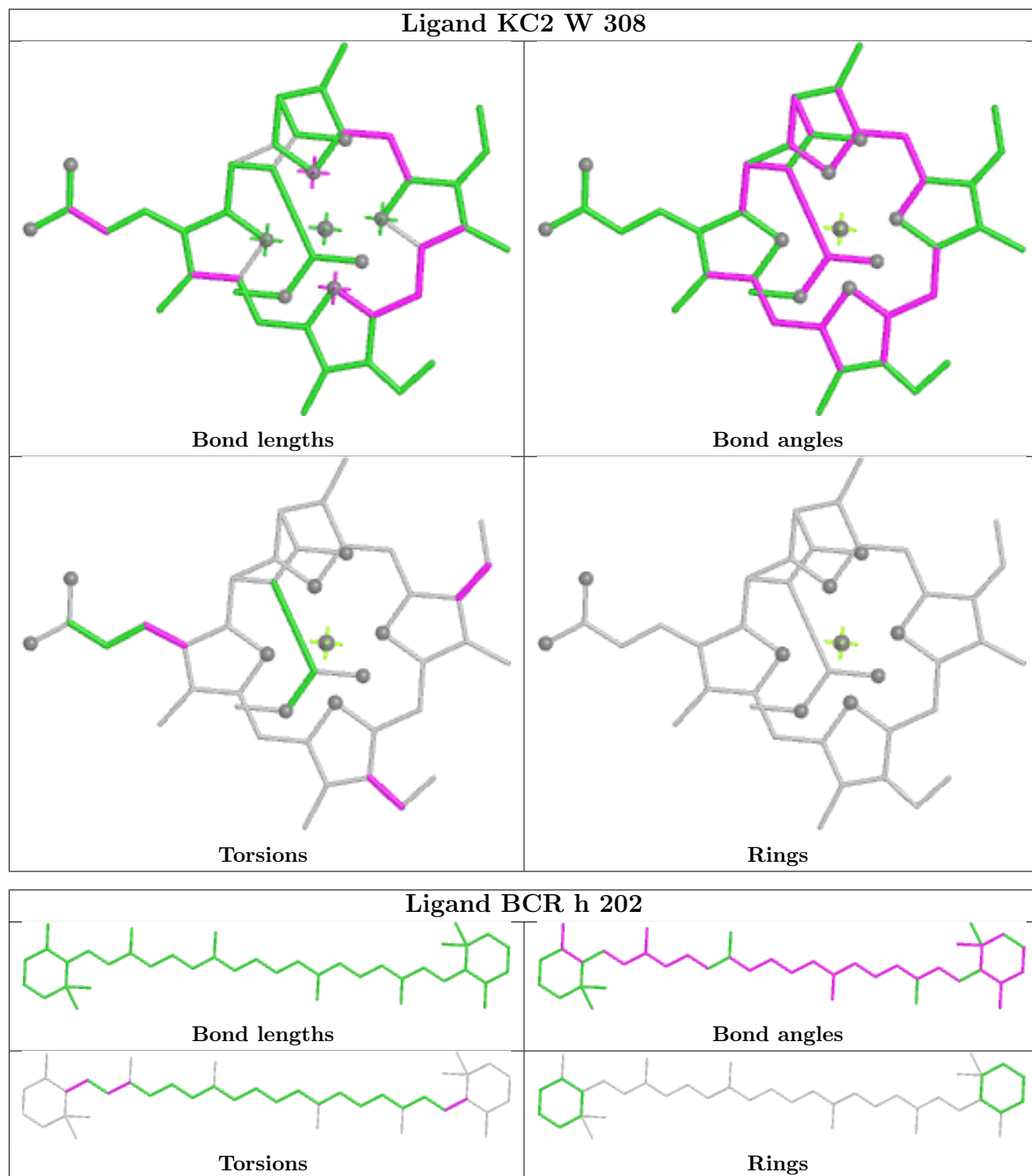
Ligand A1ECV z 310

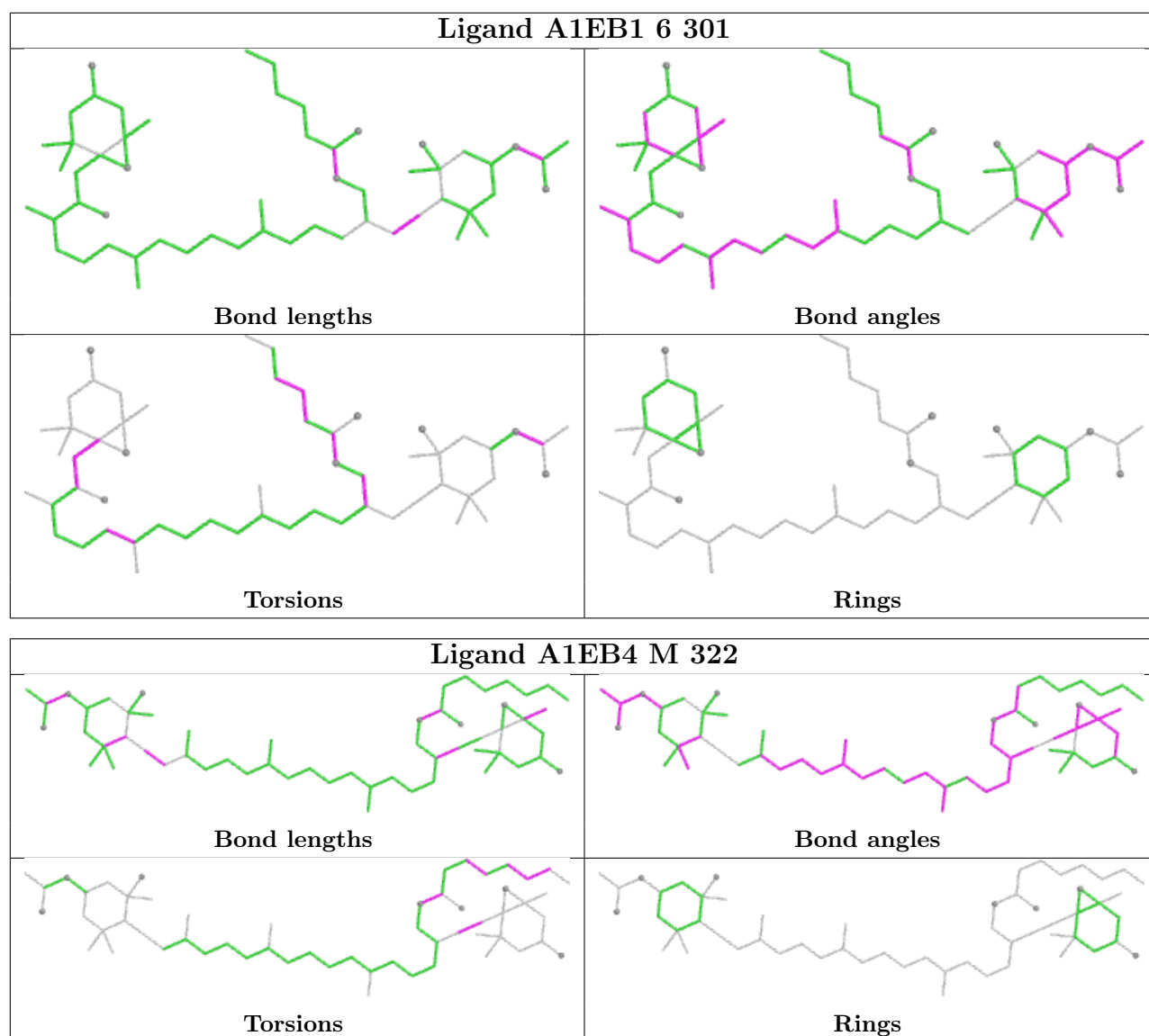


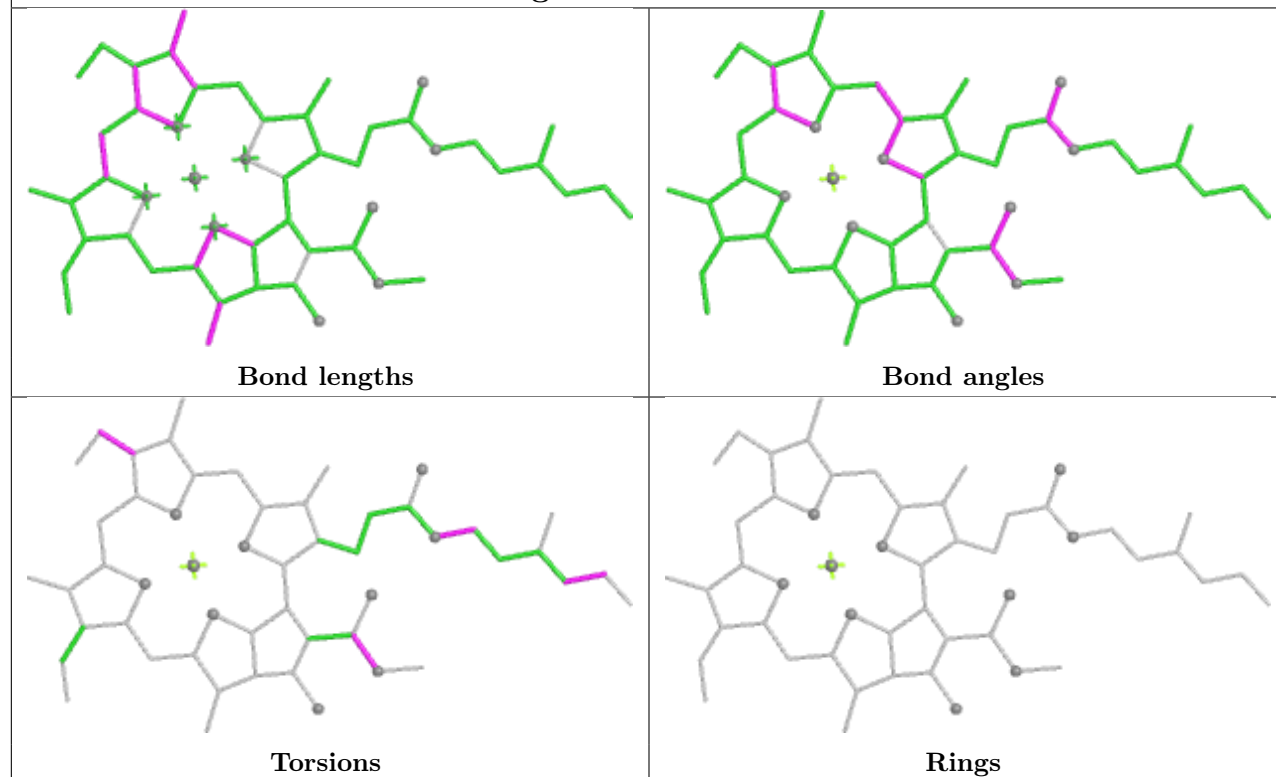
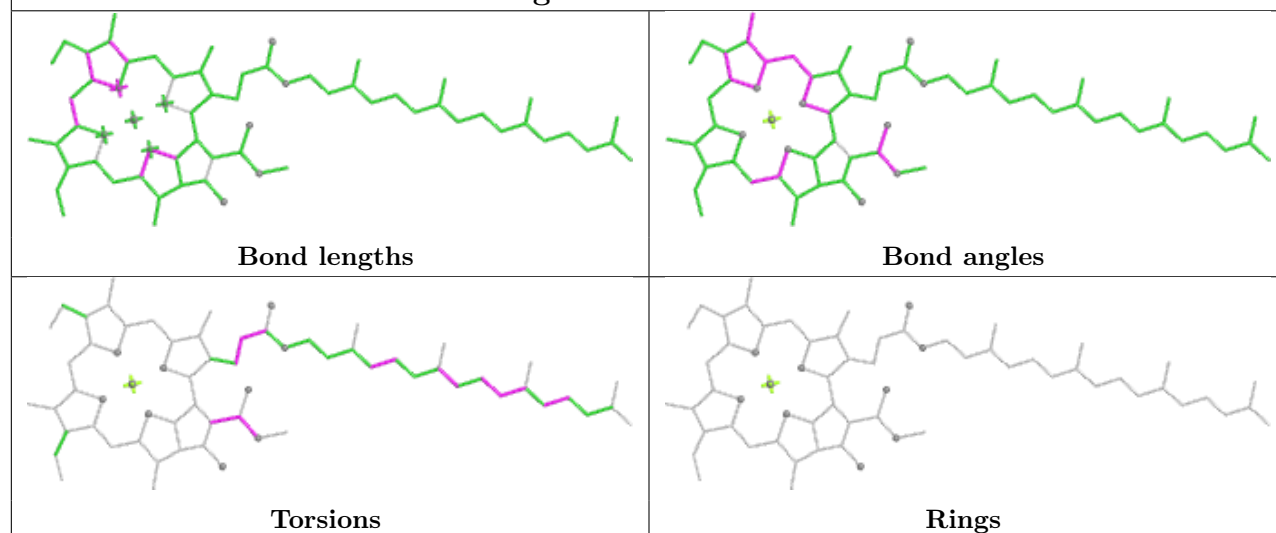
Ligand CLA a 830

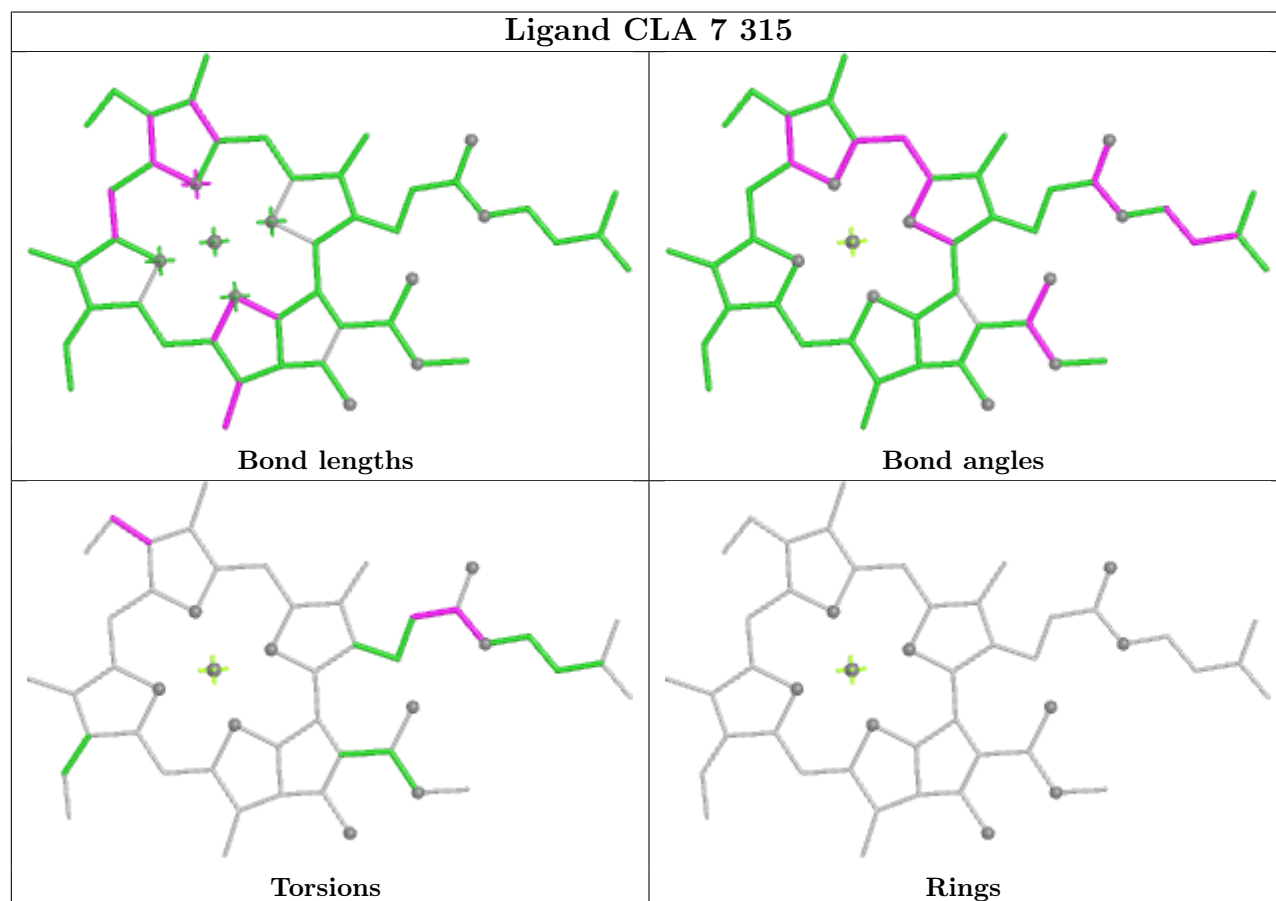
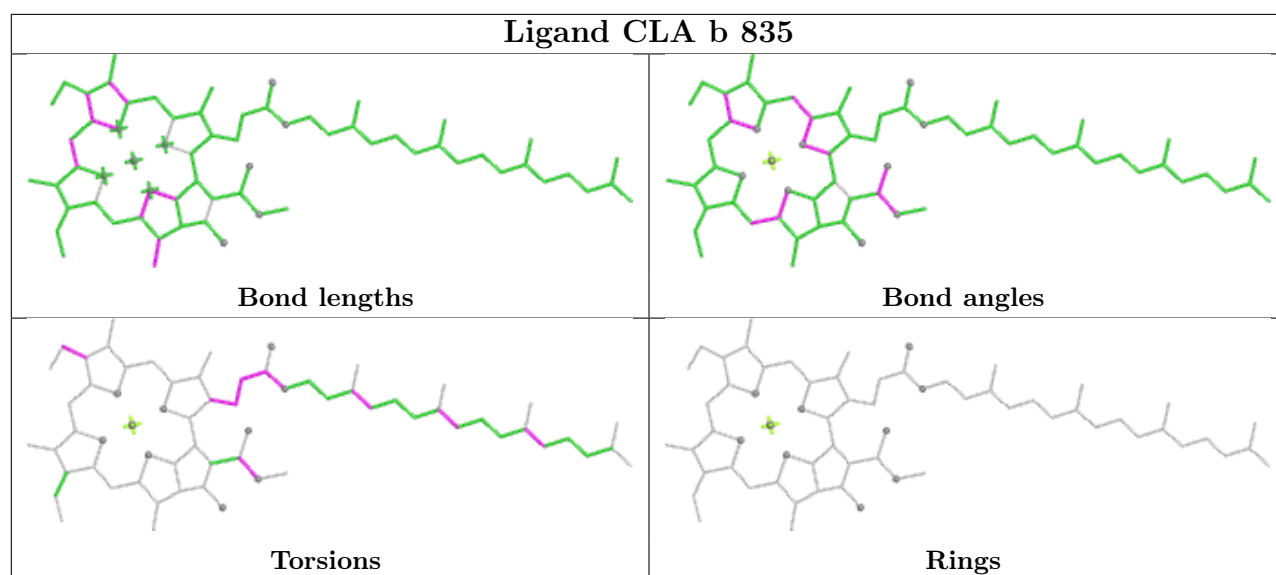


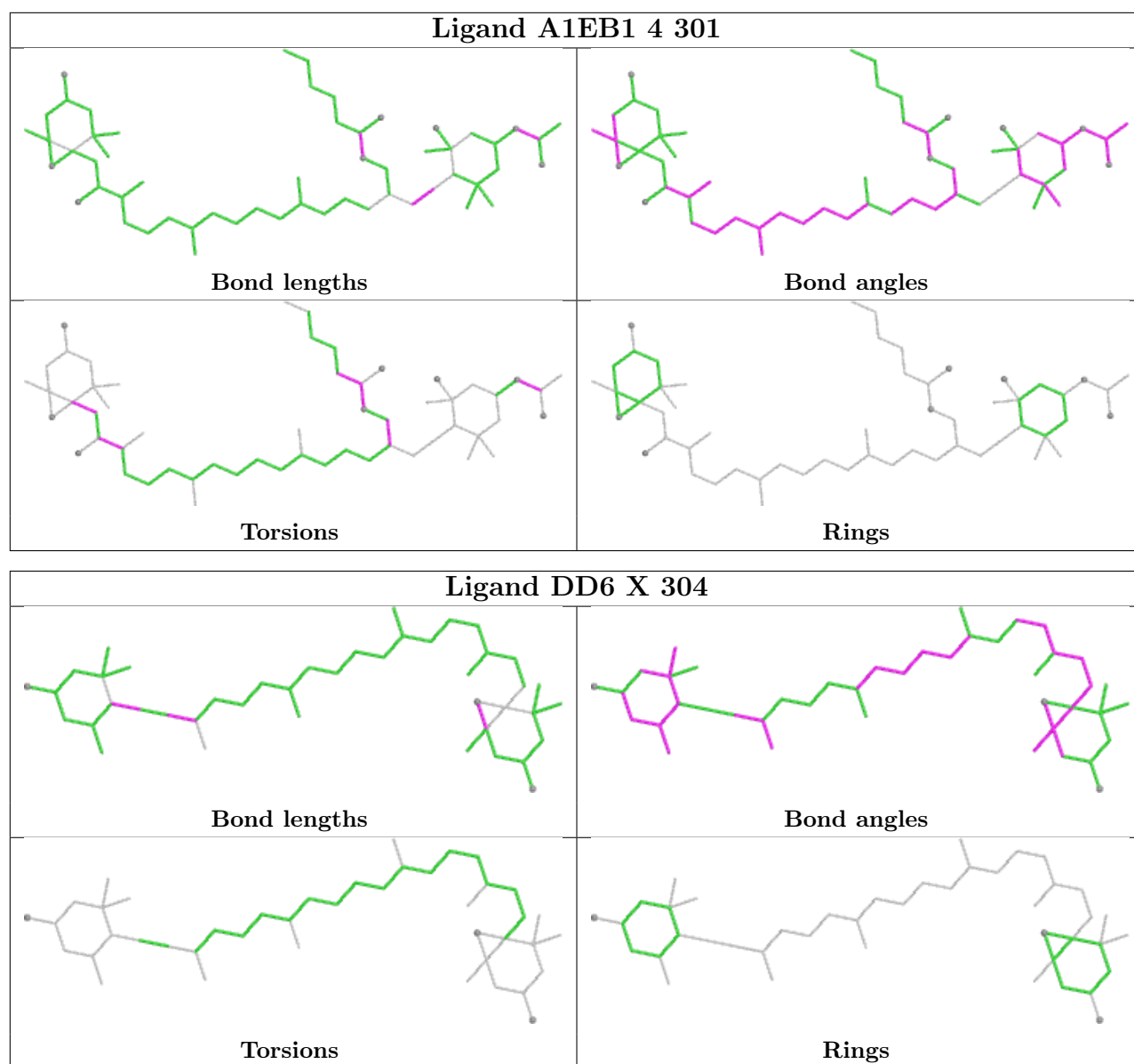




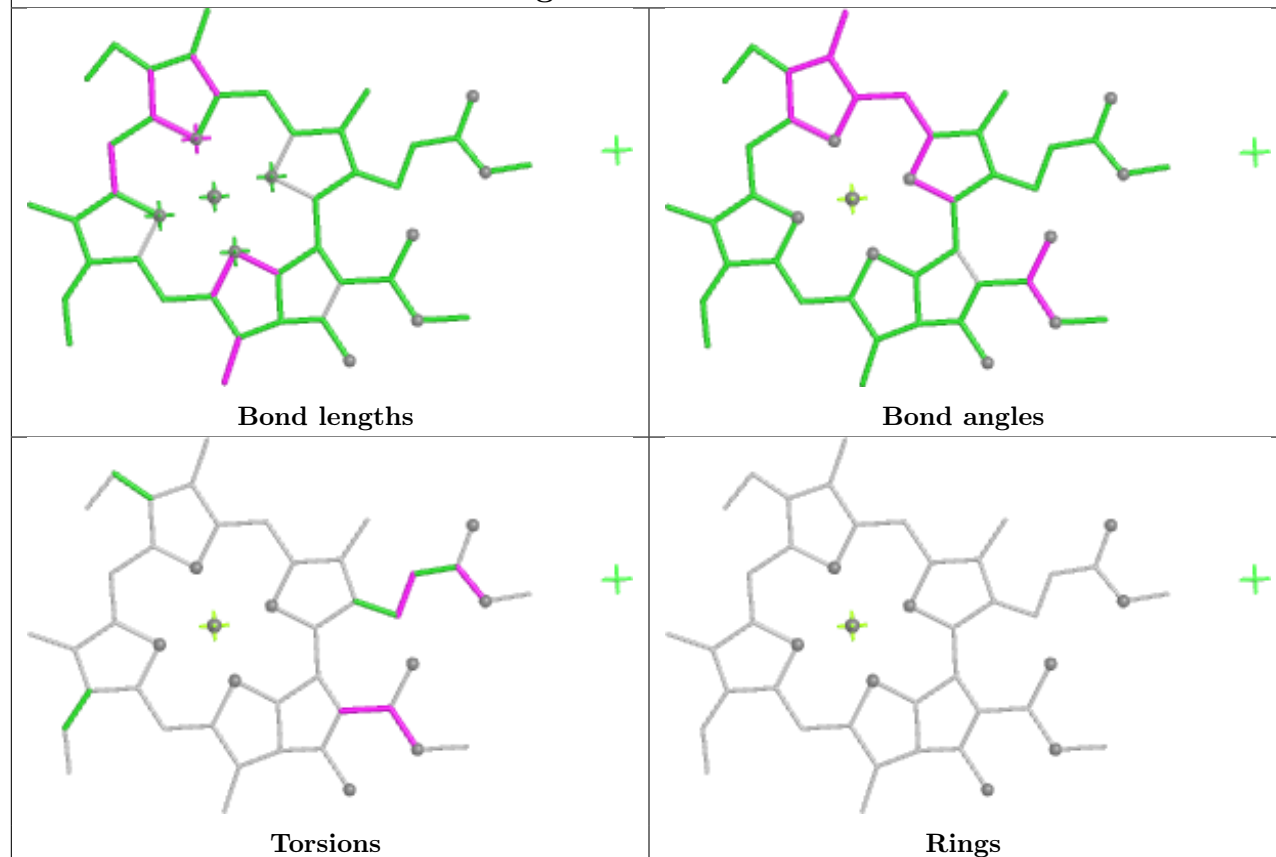


Ligand CLA V 319**Ligand CLA P 309**

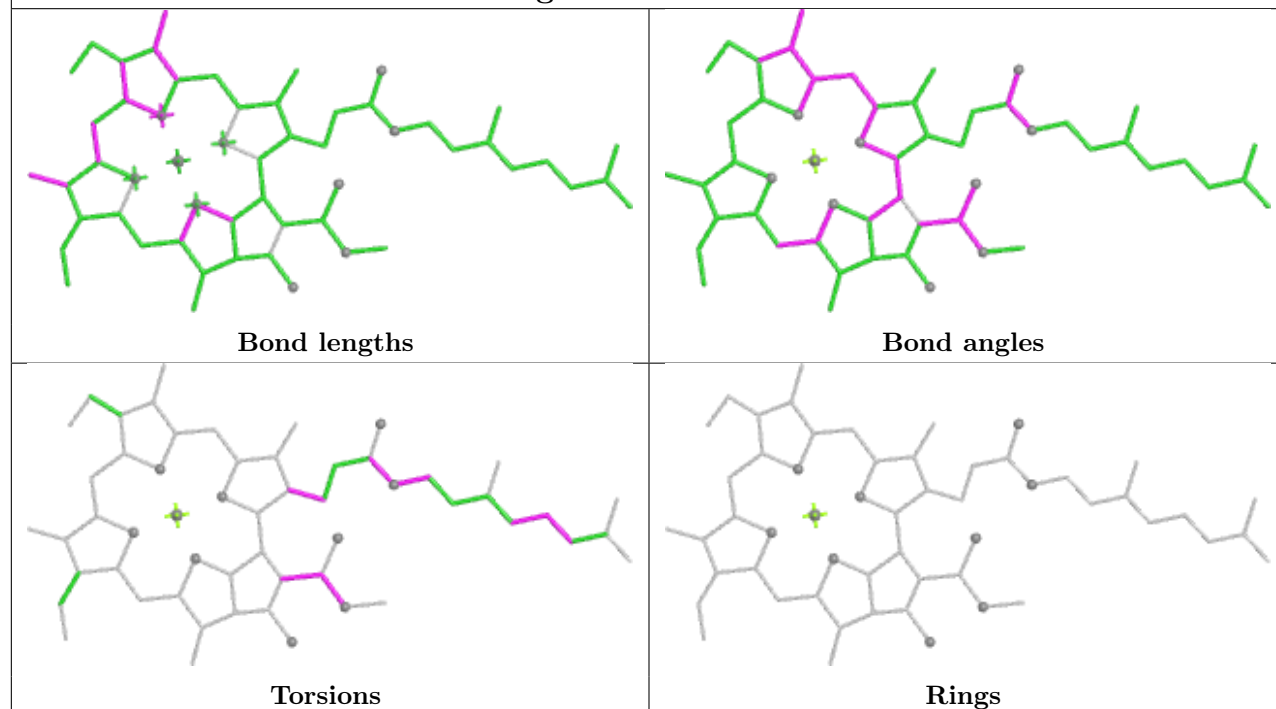




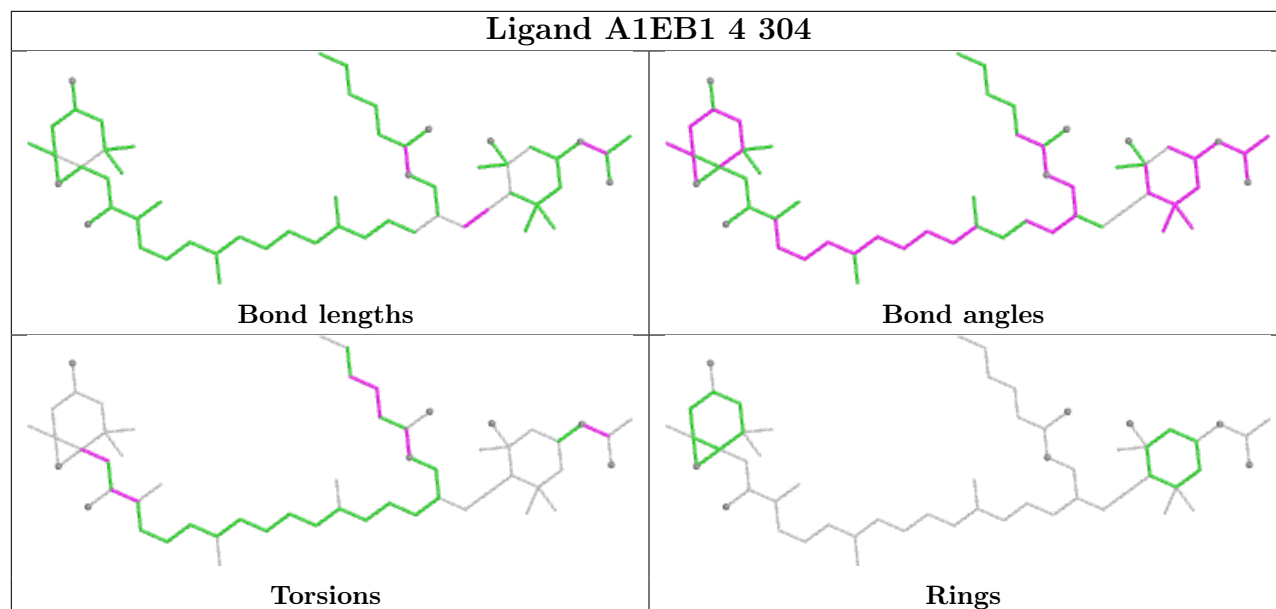
Ligand CLA J 318



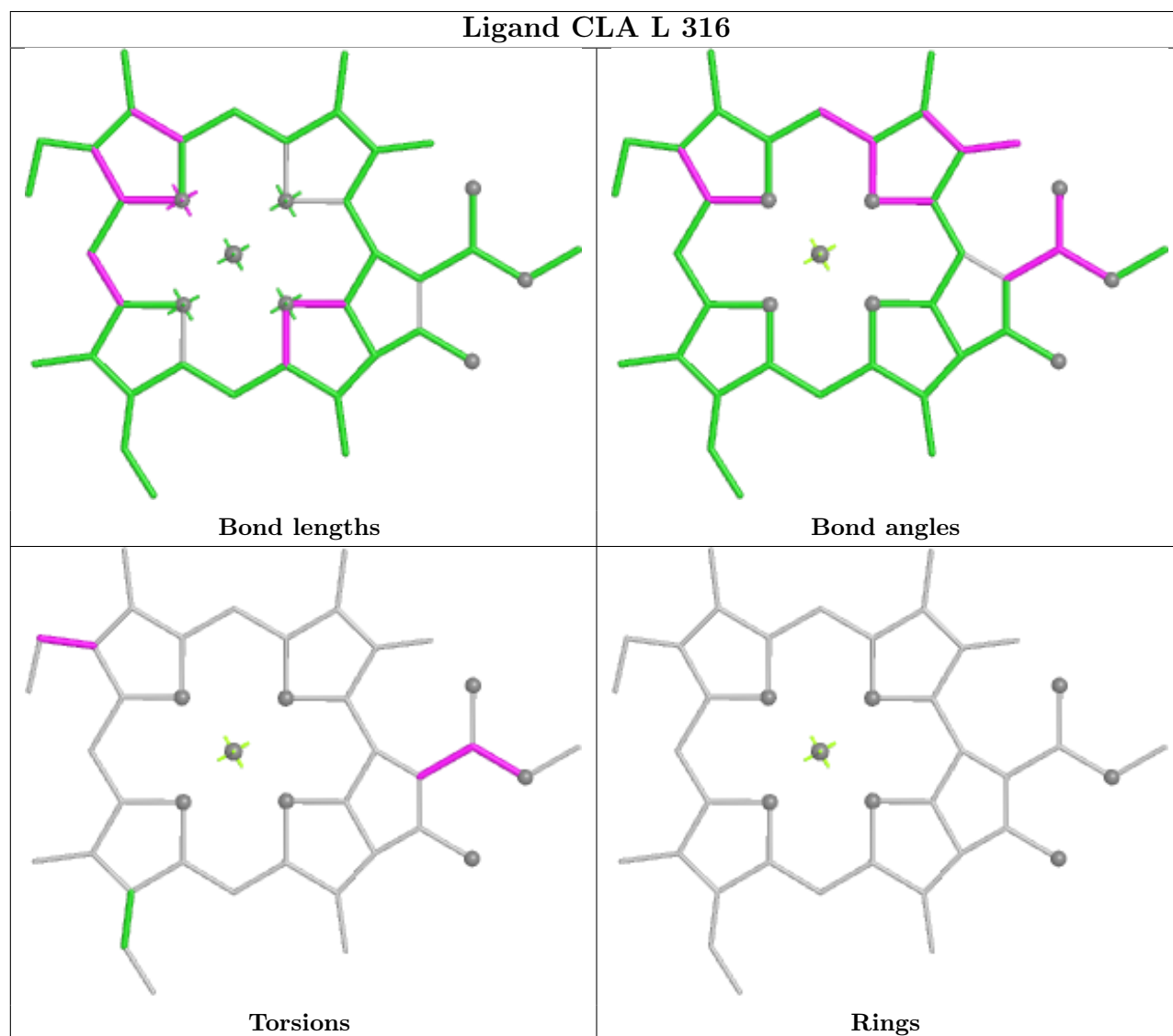
Ligand CLA 0 311



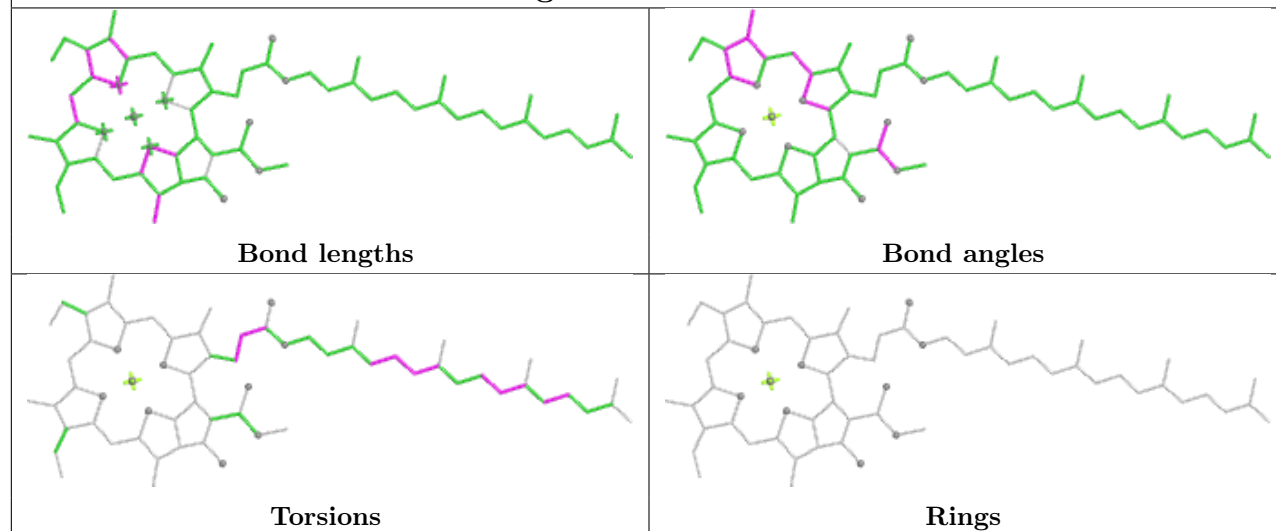
Ligand A1EB1 4 304



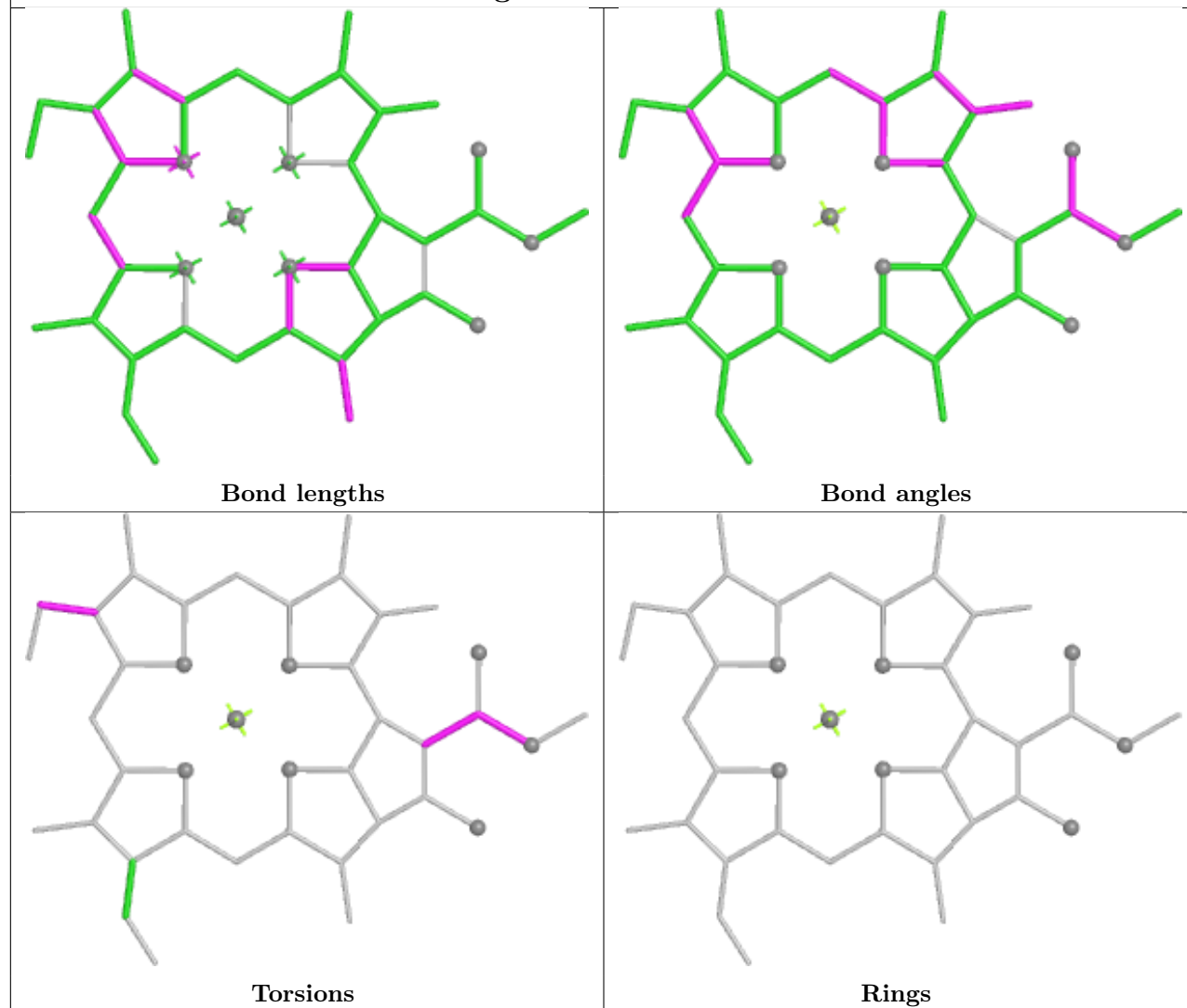
Ligand CLA L 316

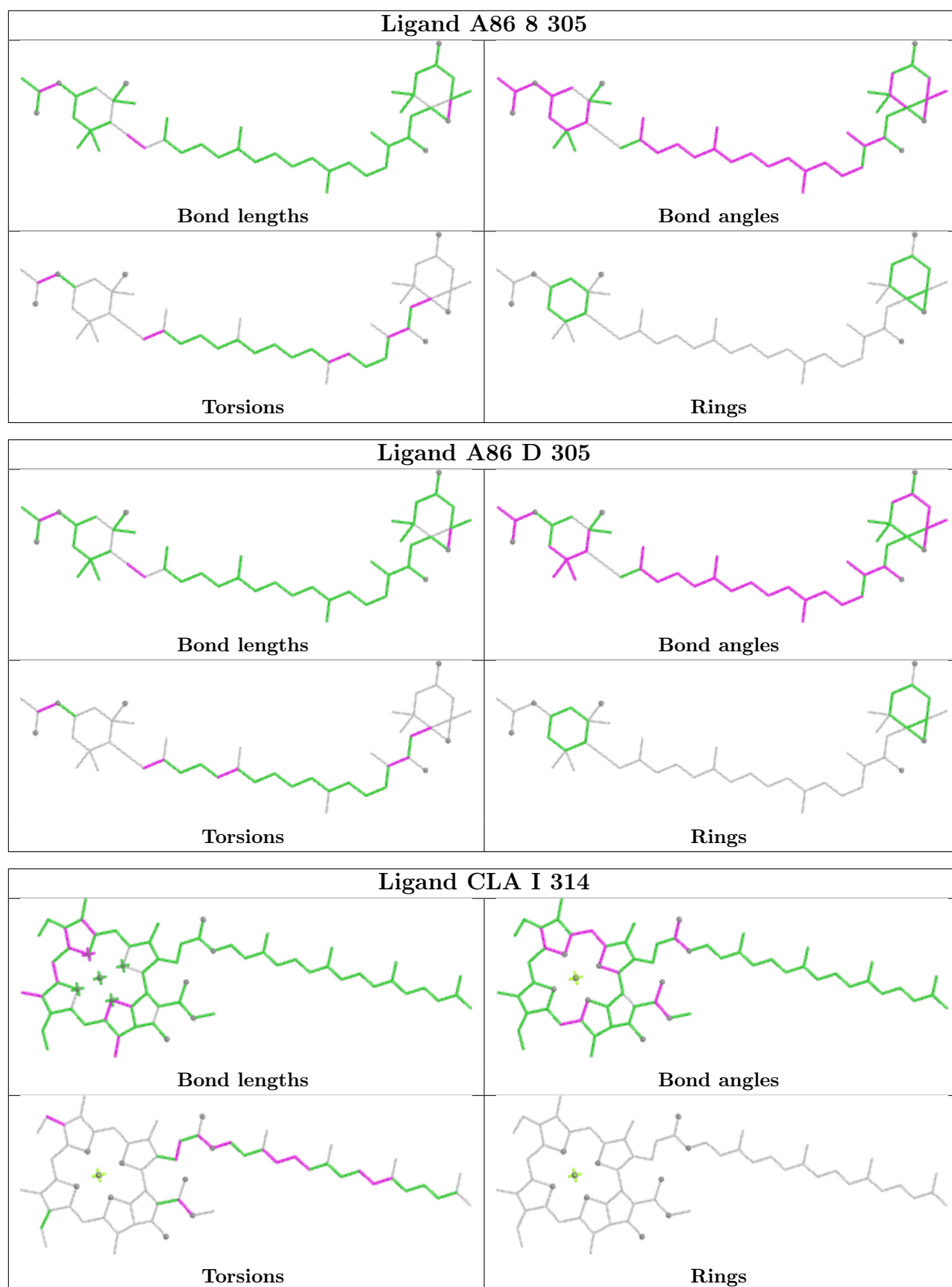


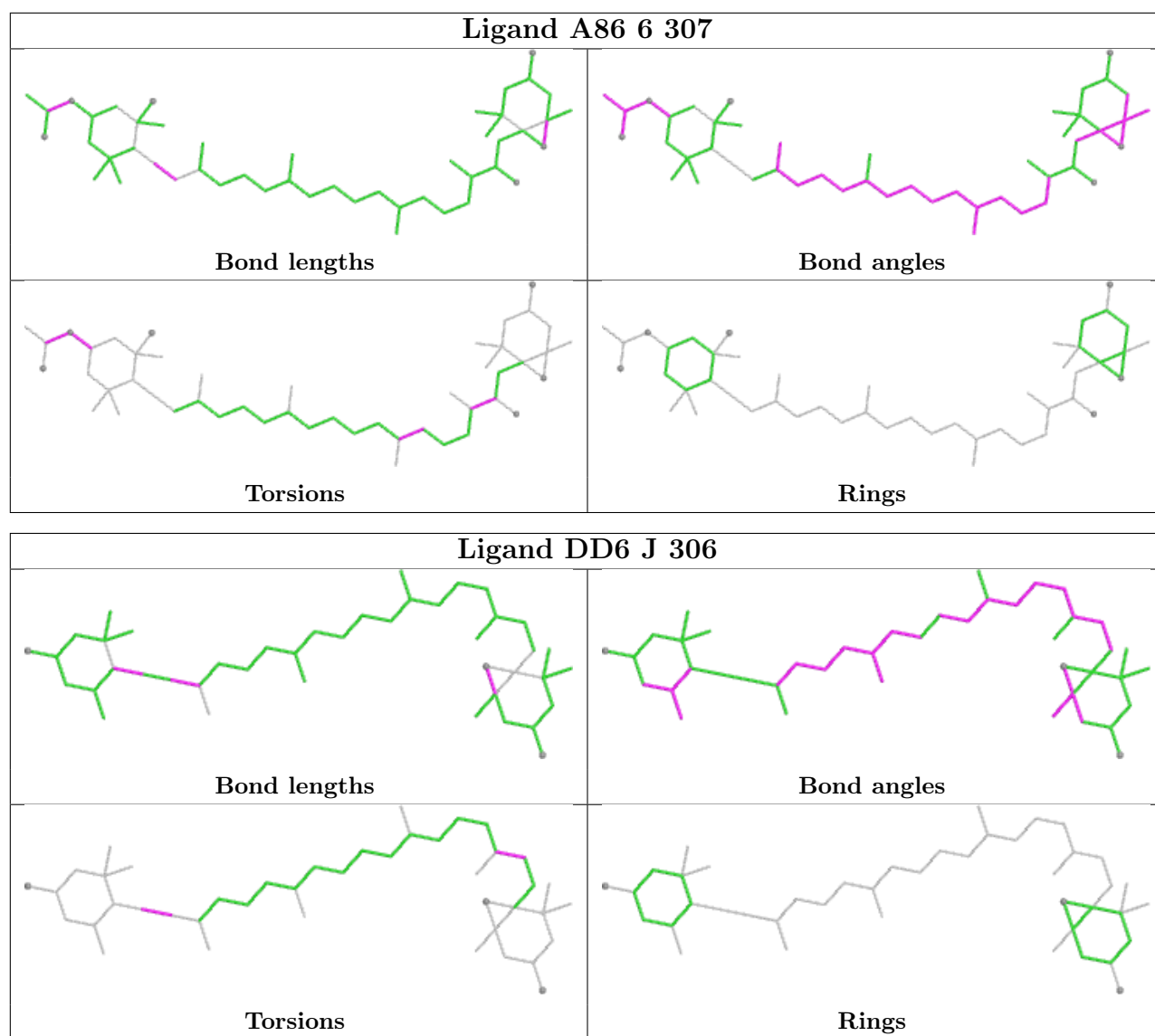
Ligand CLA 7 316



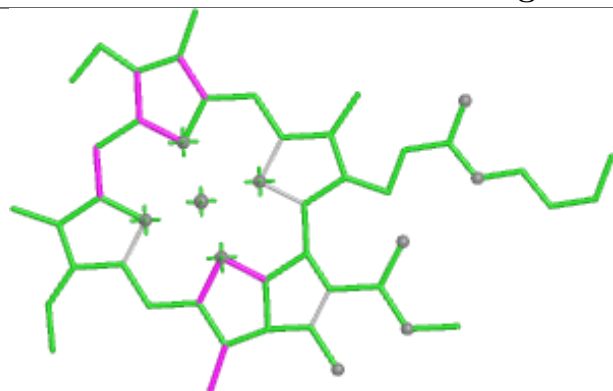
Ligand CLA H 315



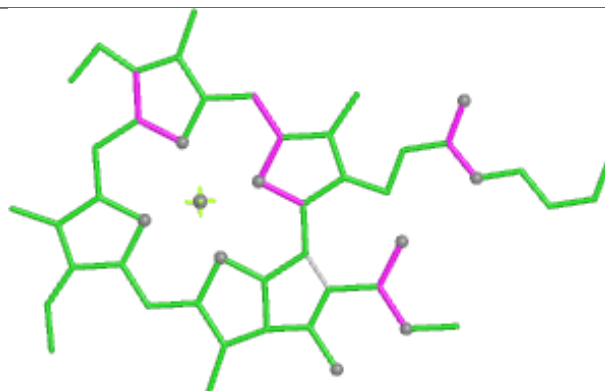




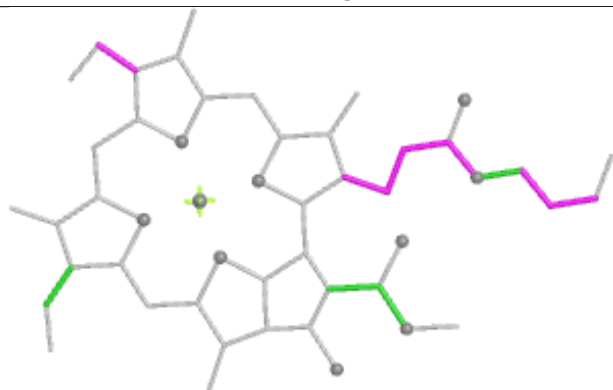
Ligand CLA J 307



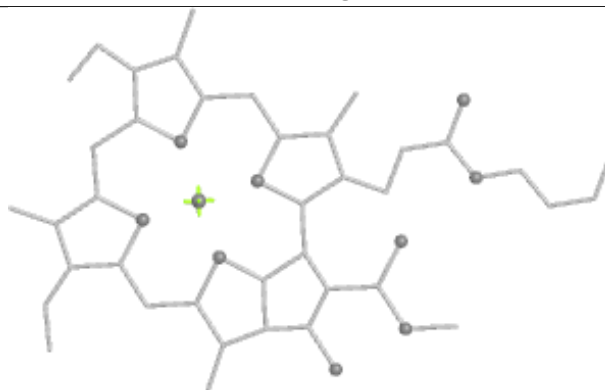
Bond lengths



Bond angles

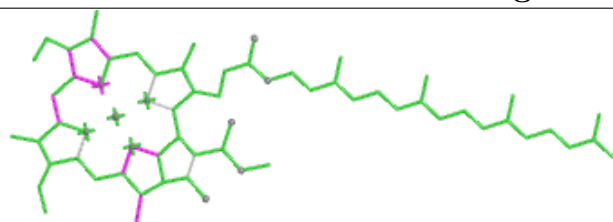


Torsions

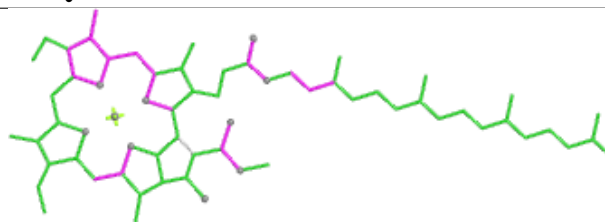


Rings

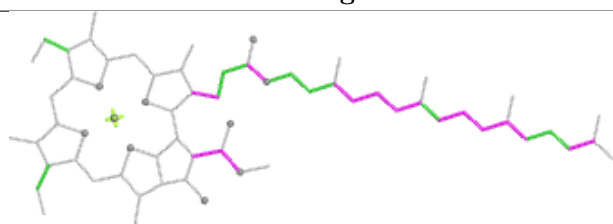
Ligand CLA Q 310



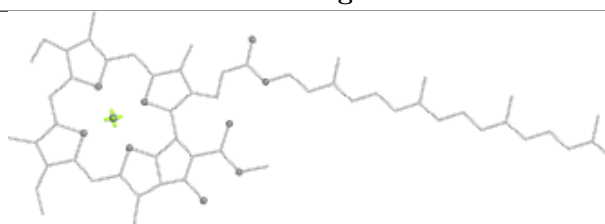
Bond lengths



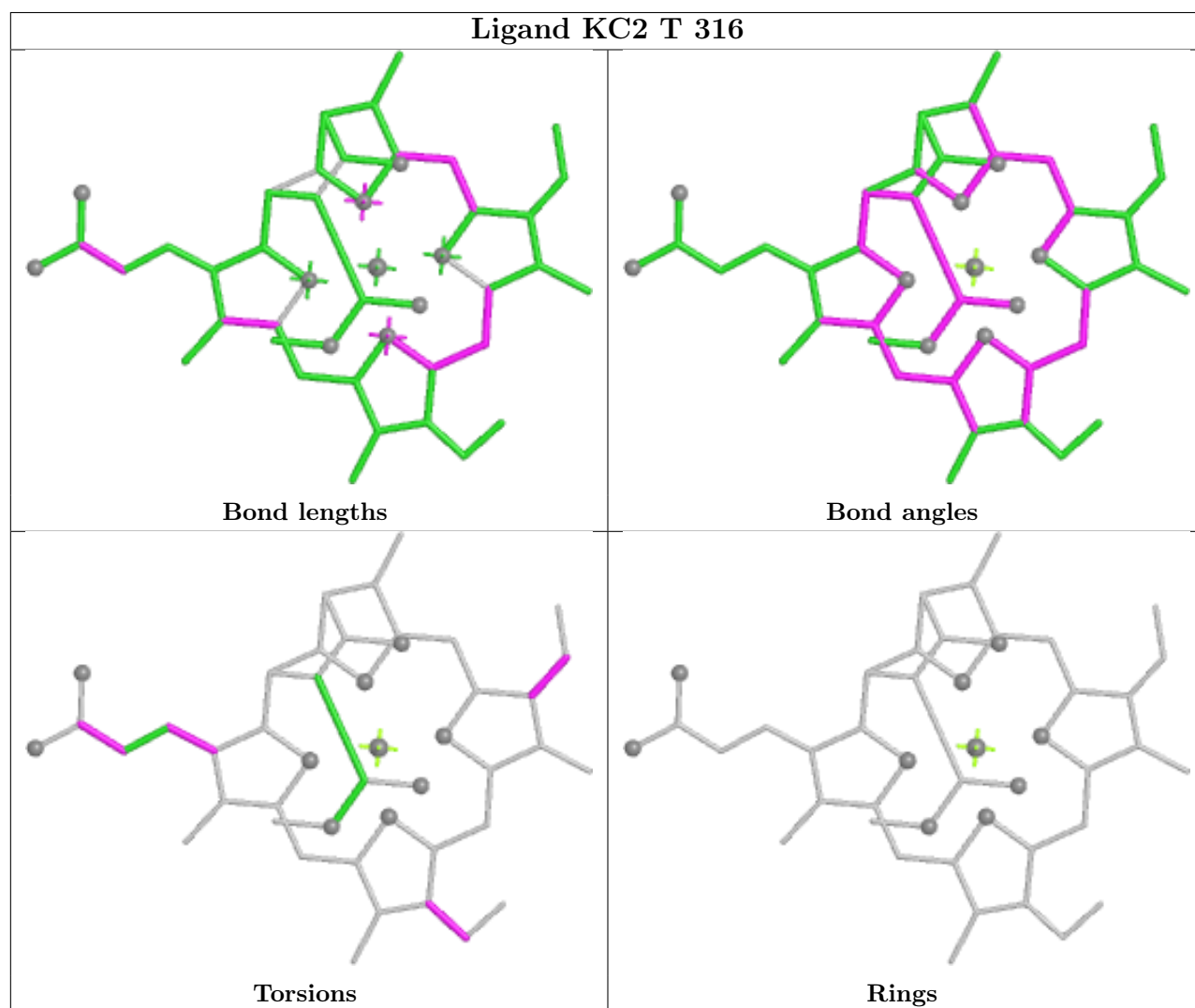
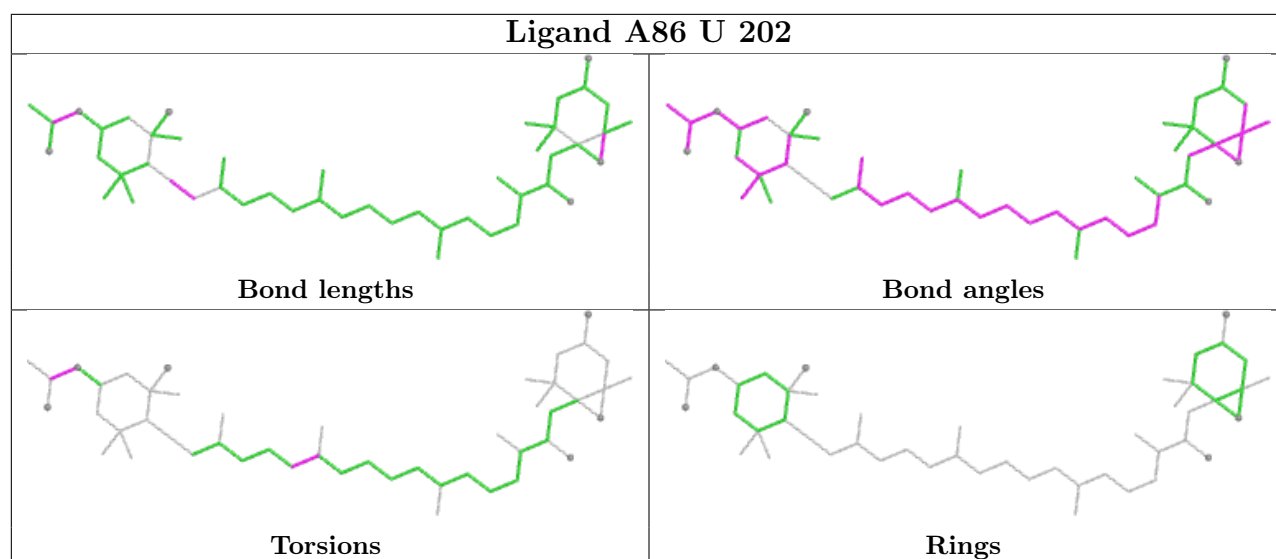
Bond angles



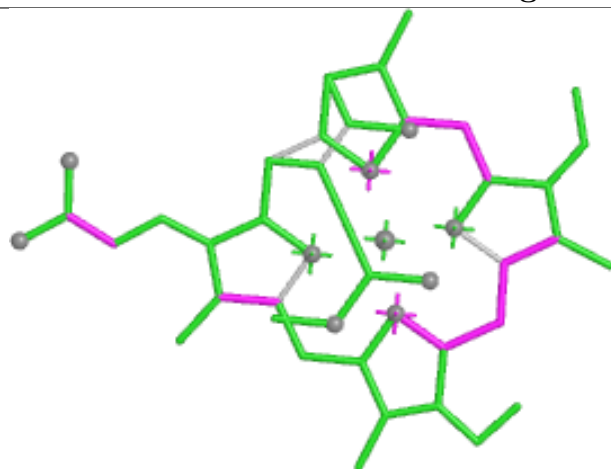
Torsions



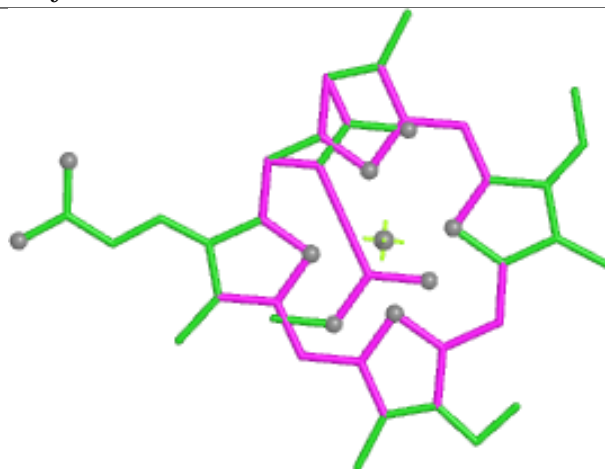
Rings



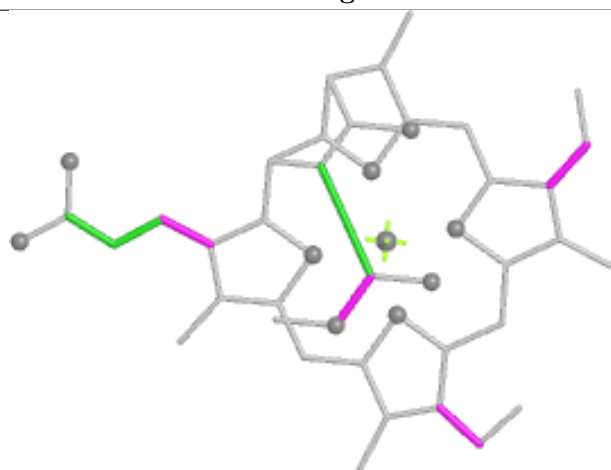
Ligand KC2 y 316



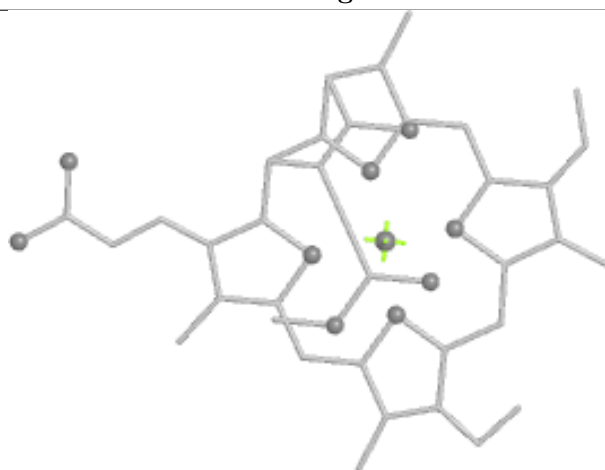
Bond lengths



Bond angles

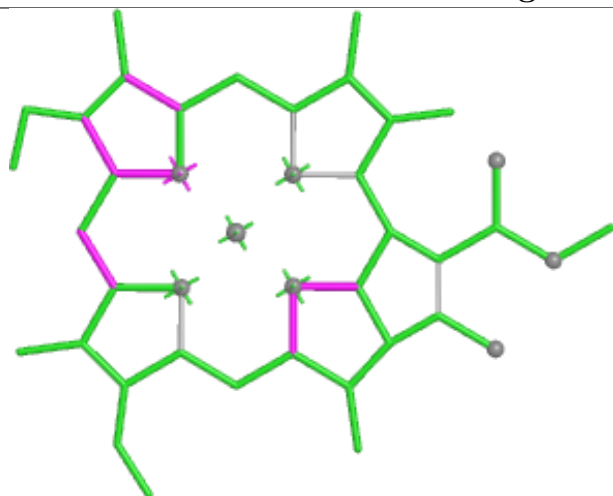


Torsions

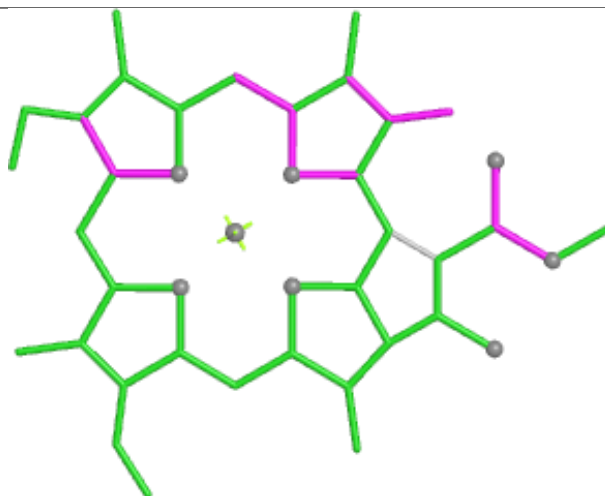


Rings

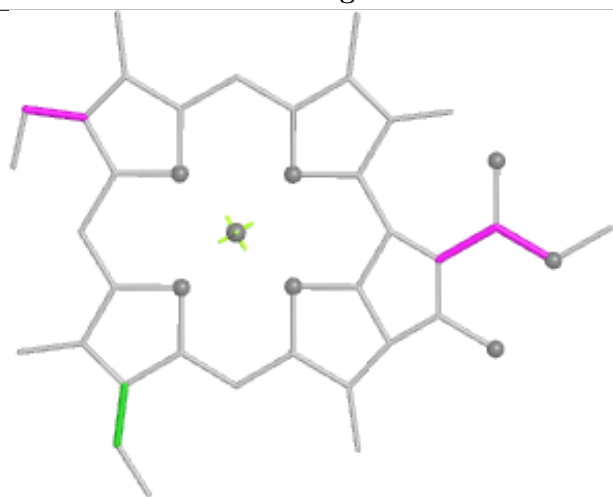
Ligand CLA 1 308



Bond lengths



Bond angles

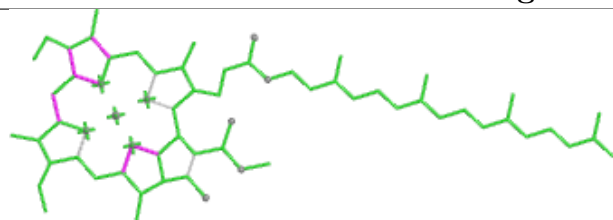


Torsions

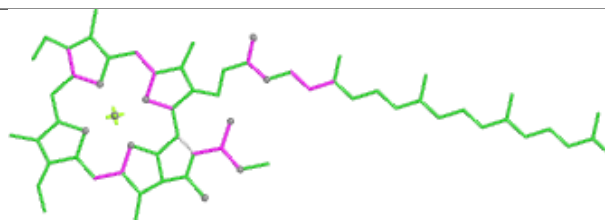


Rings

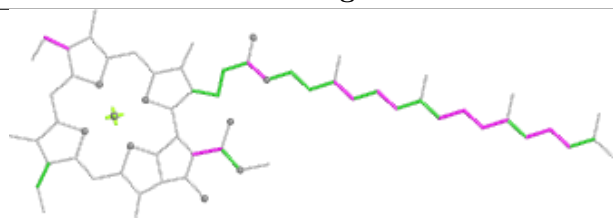
Ligand CLA b 838



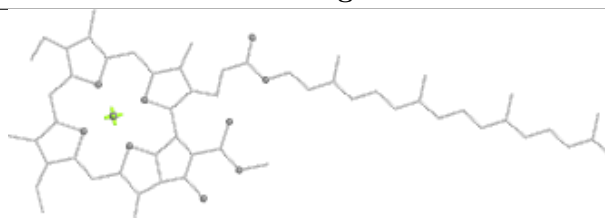
Bond lengths



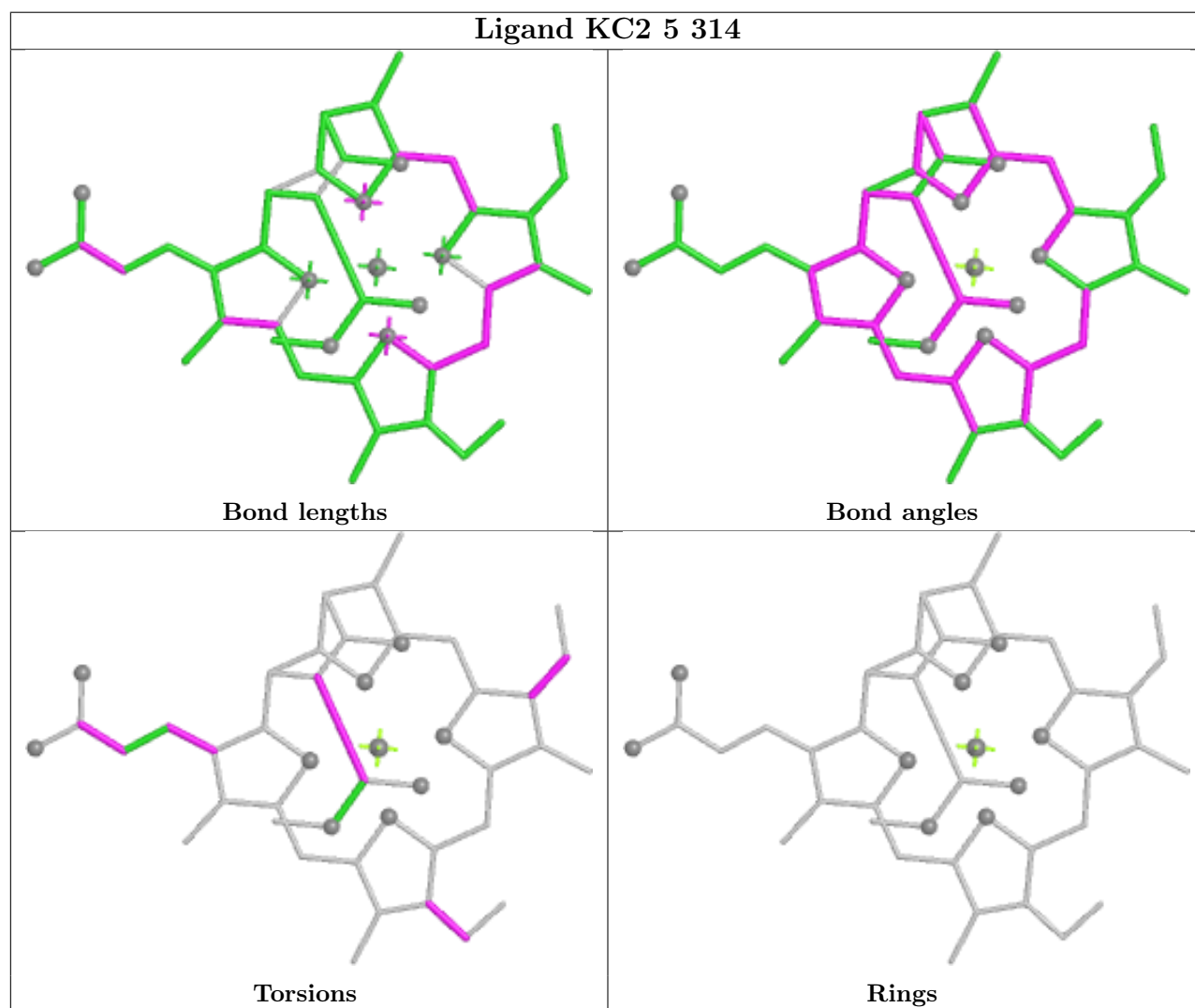
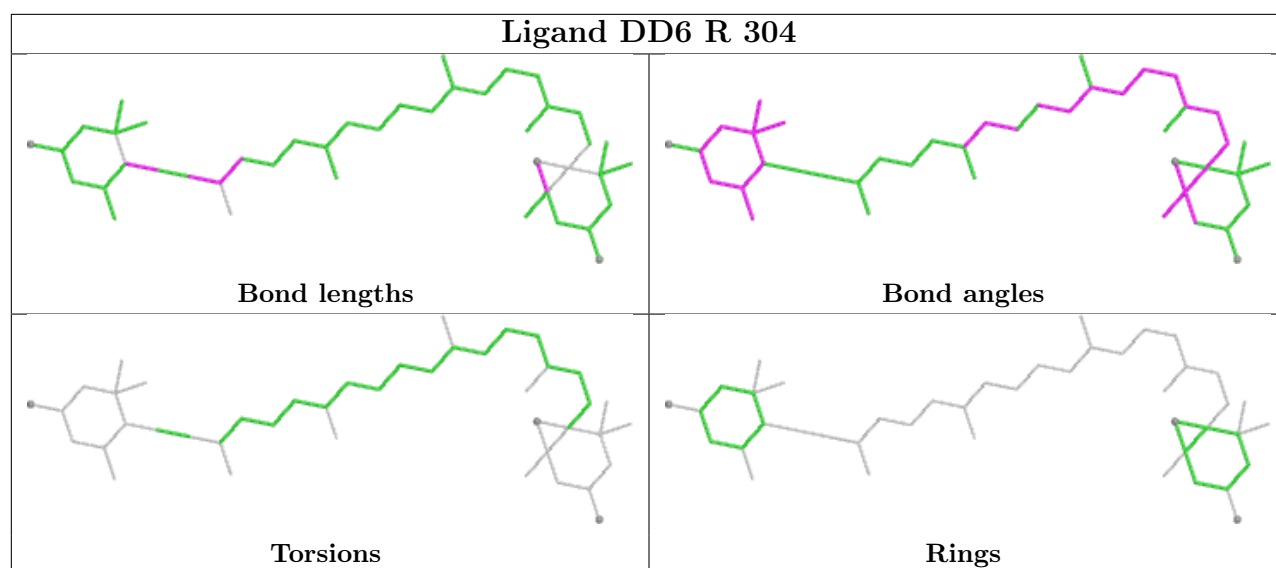
Bond angles



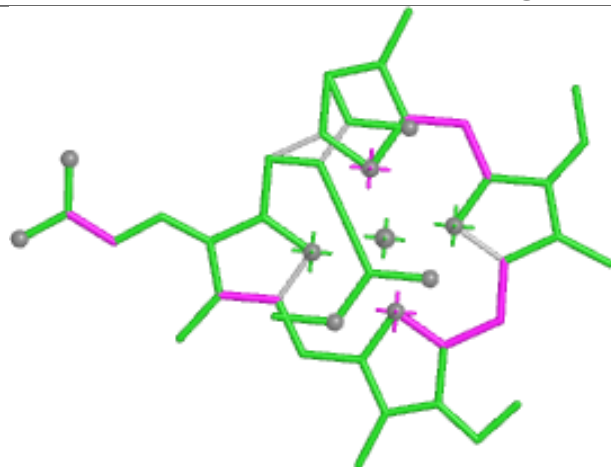
Torsions



Rings



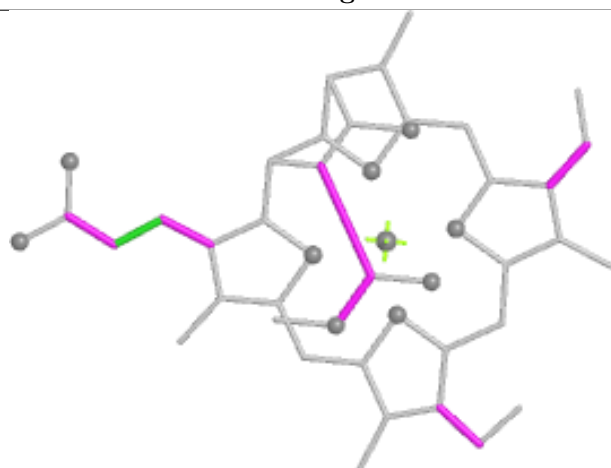
Ligand KC2 Z 311



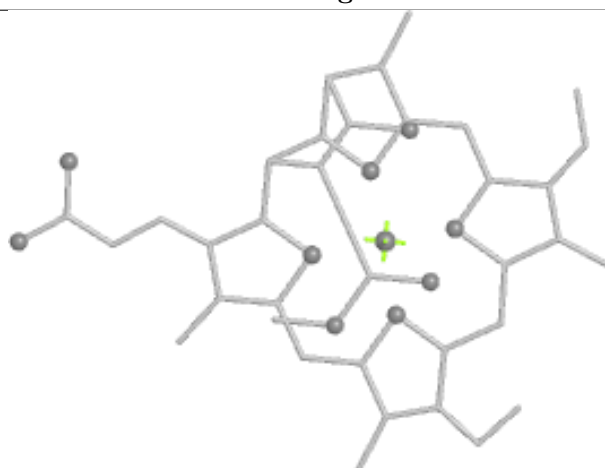
Bond lengths



Bond angles

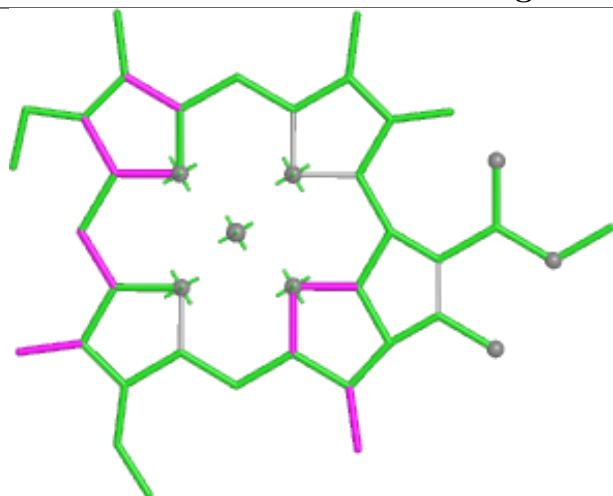


Torsions



Rings

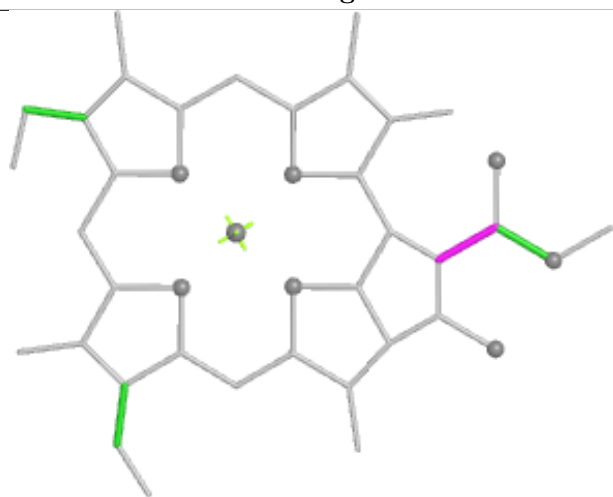
Ligand CLA P 314



Bond lengths



Bond angles

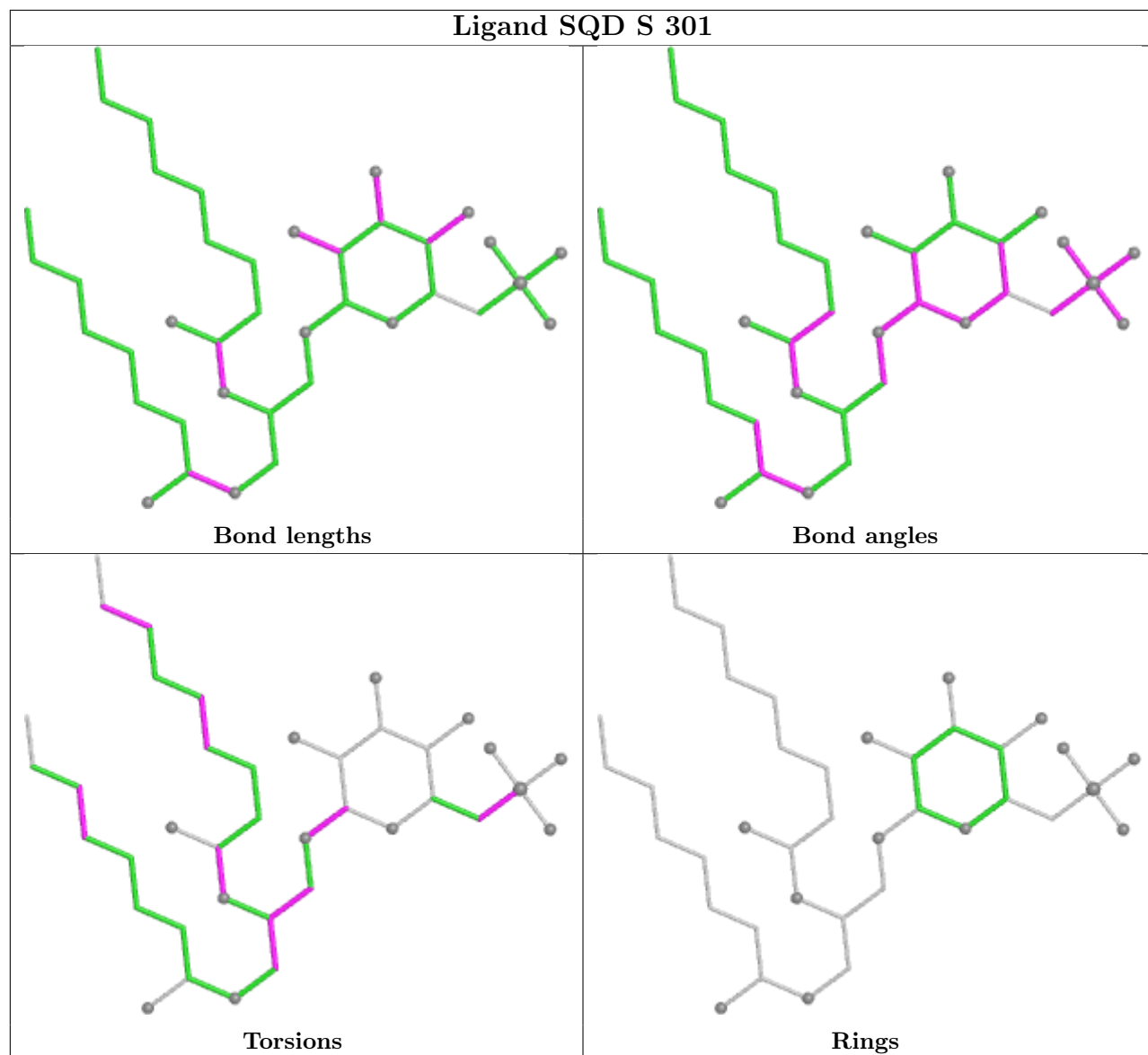


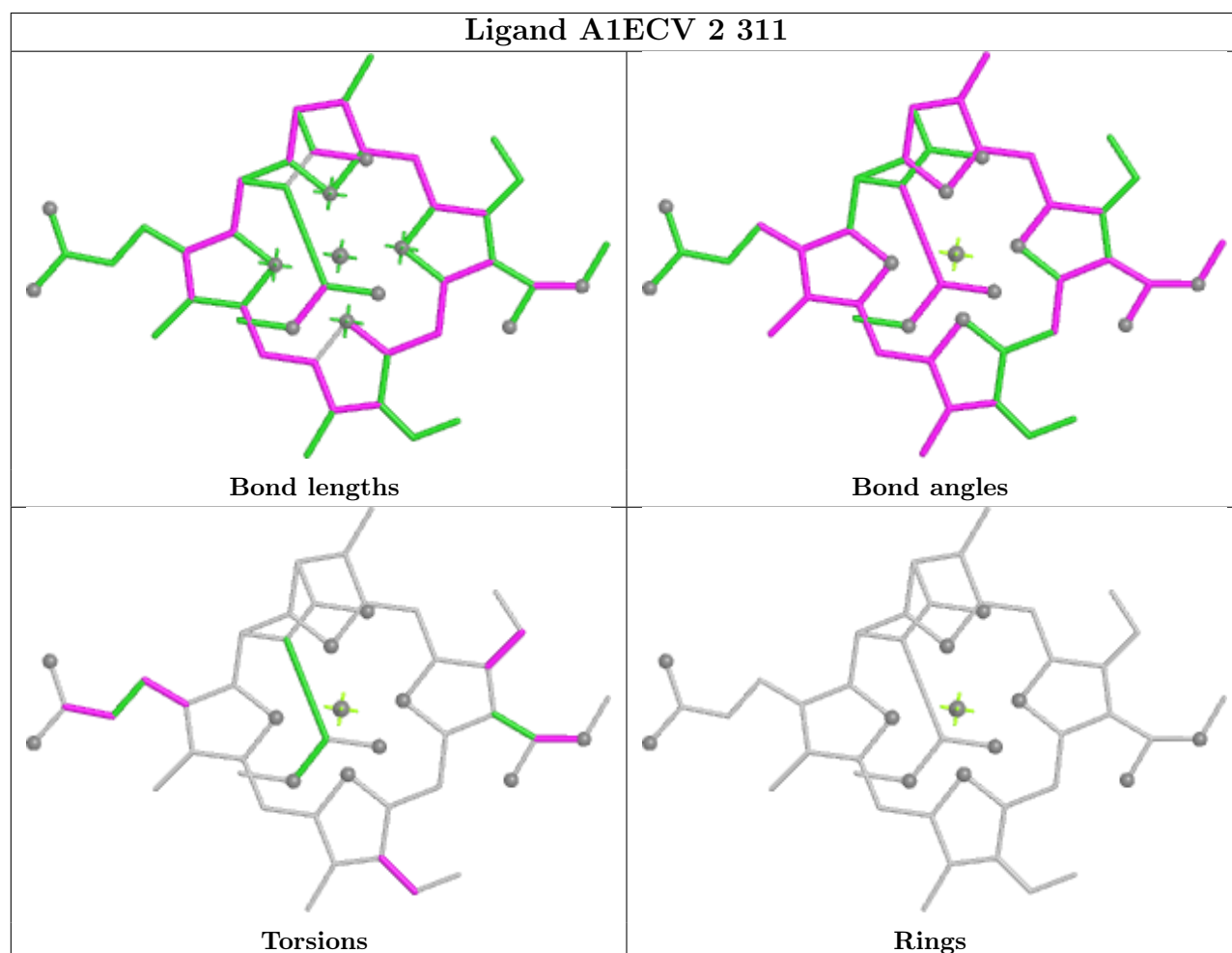
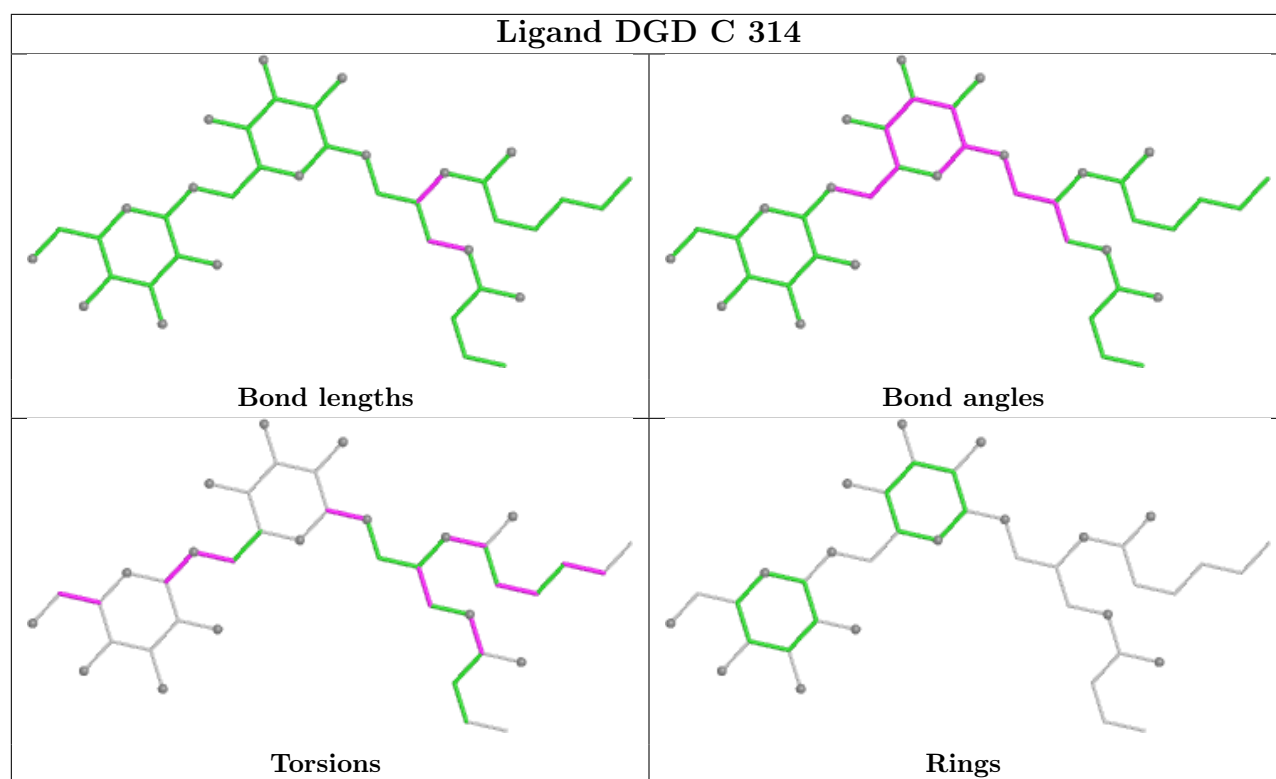
Torsions

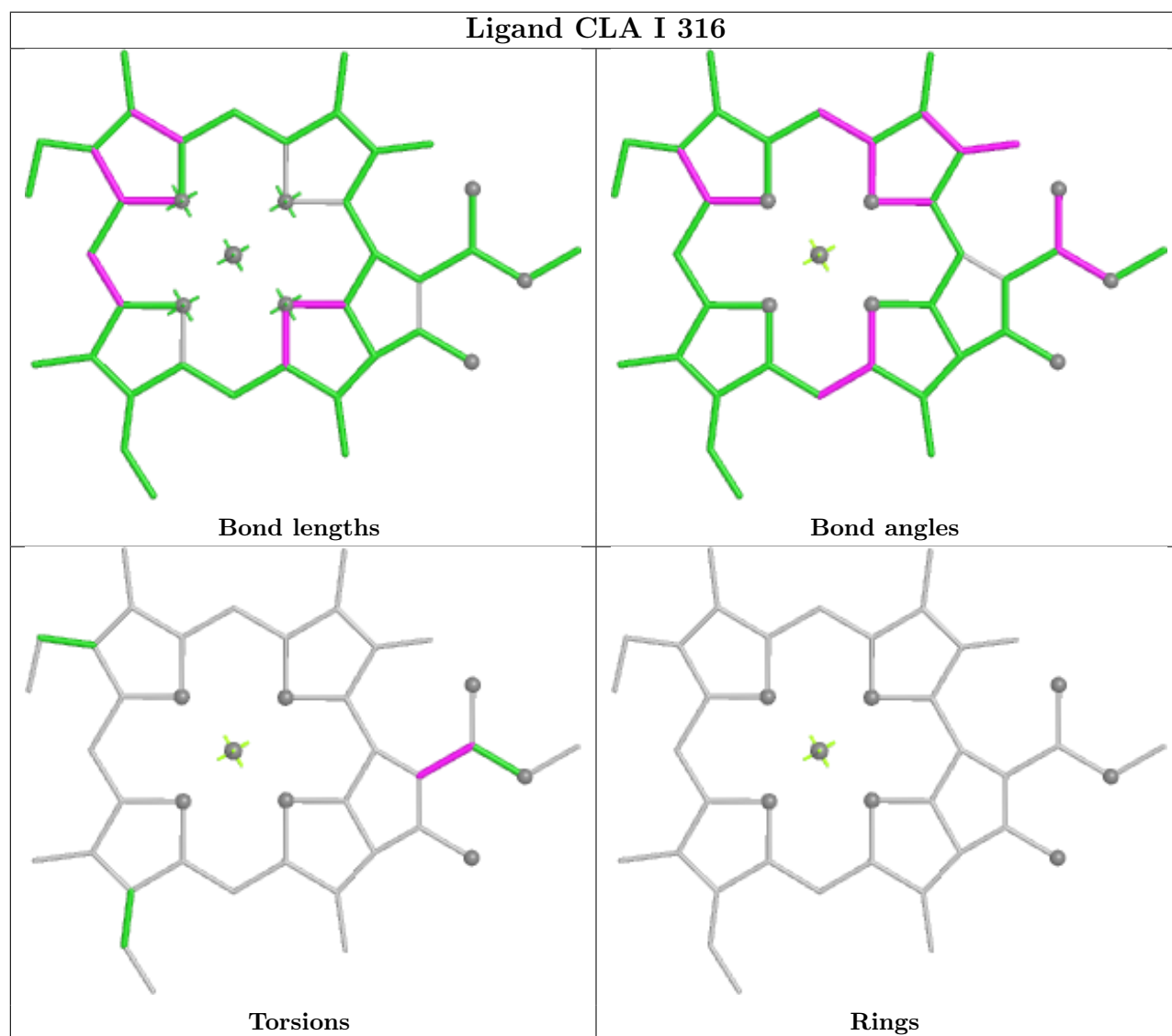
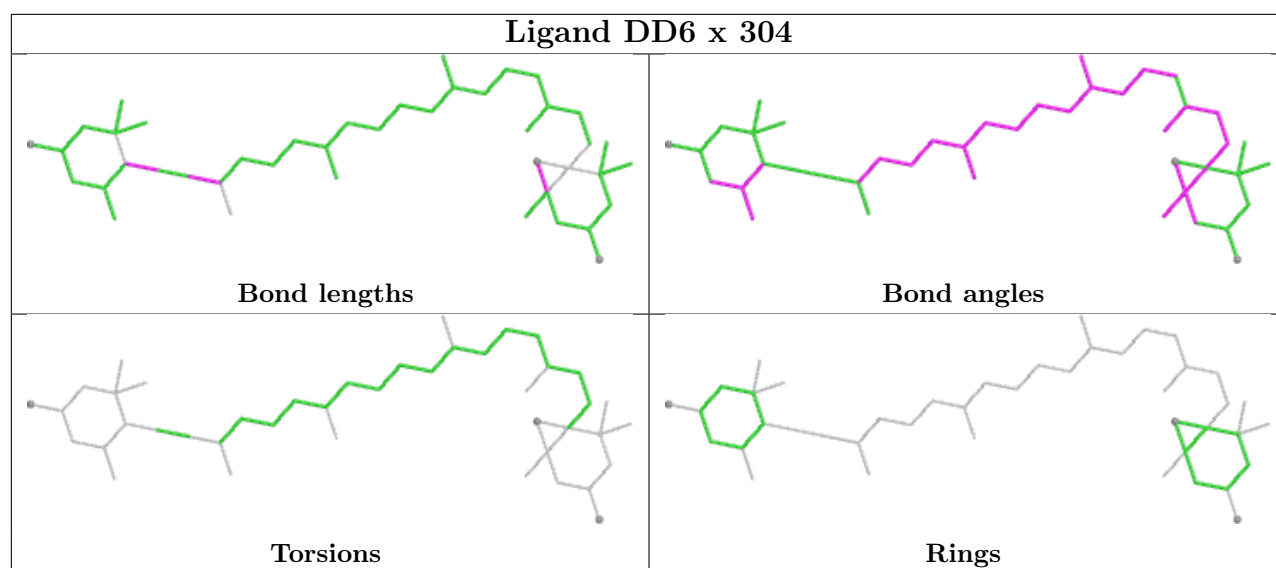


Rings

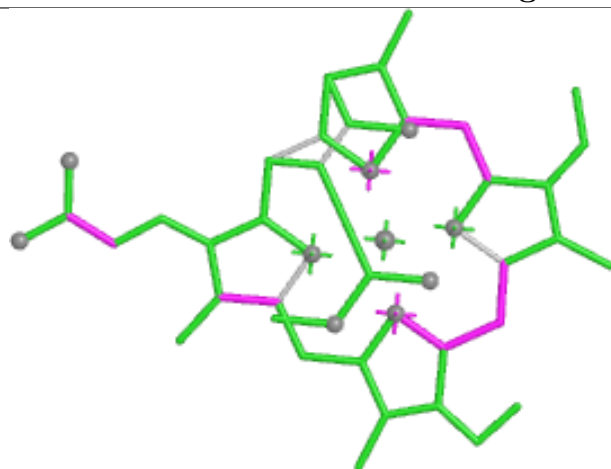
Ligand SQD S 301



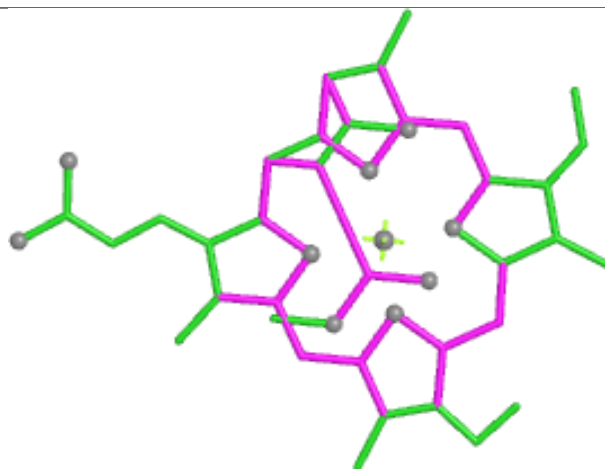




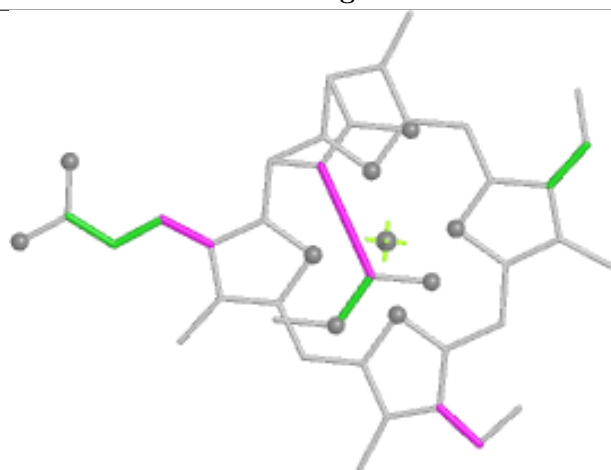
Ligand KC2 S 314



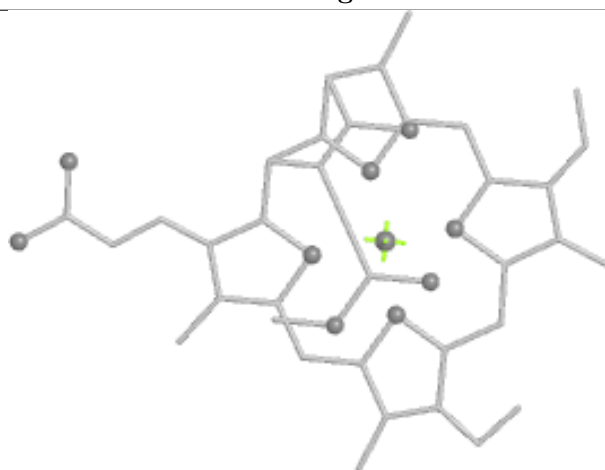
Bond lengths



Bond angles

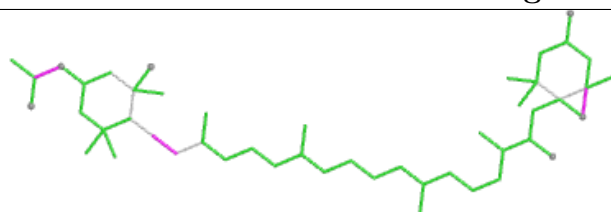


Torsions

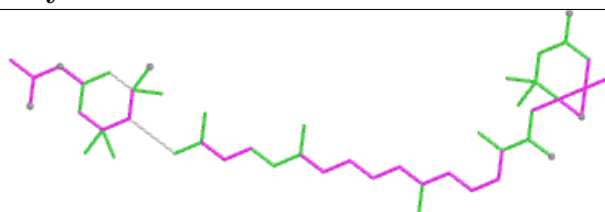


Rings

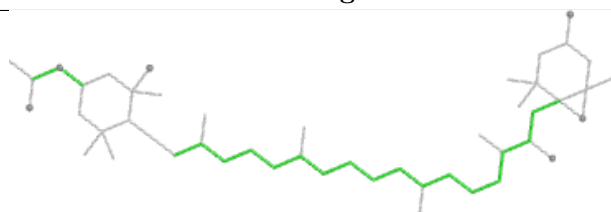
Ligand A86 y 305



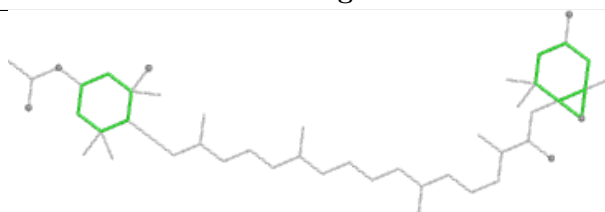
Bond lengths



Bond angles

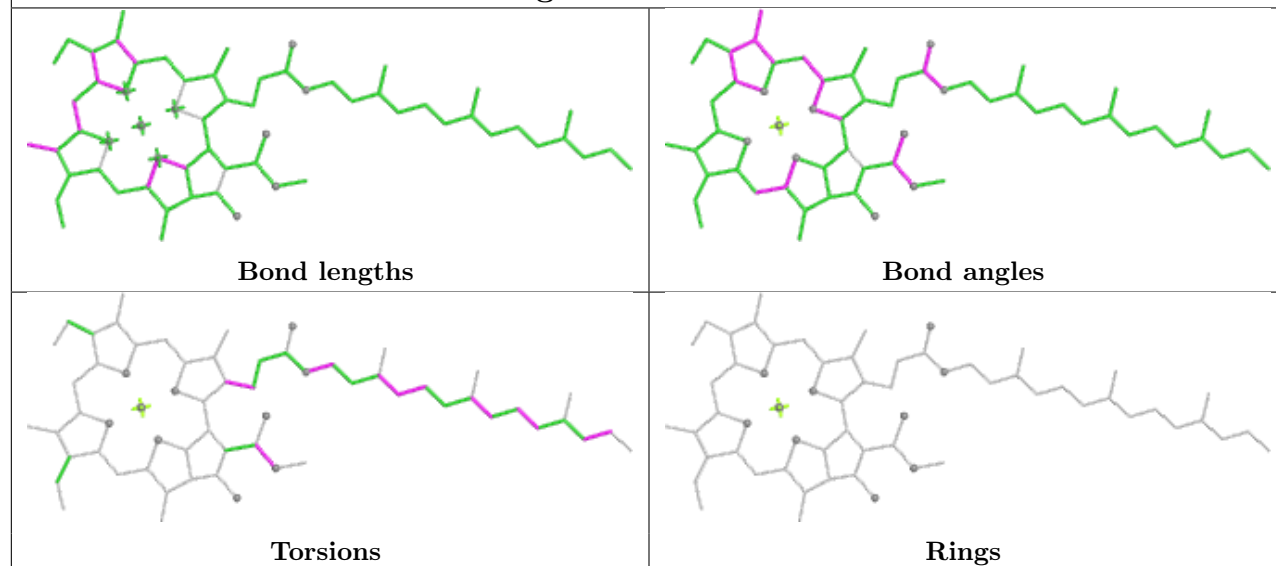


Torsions

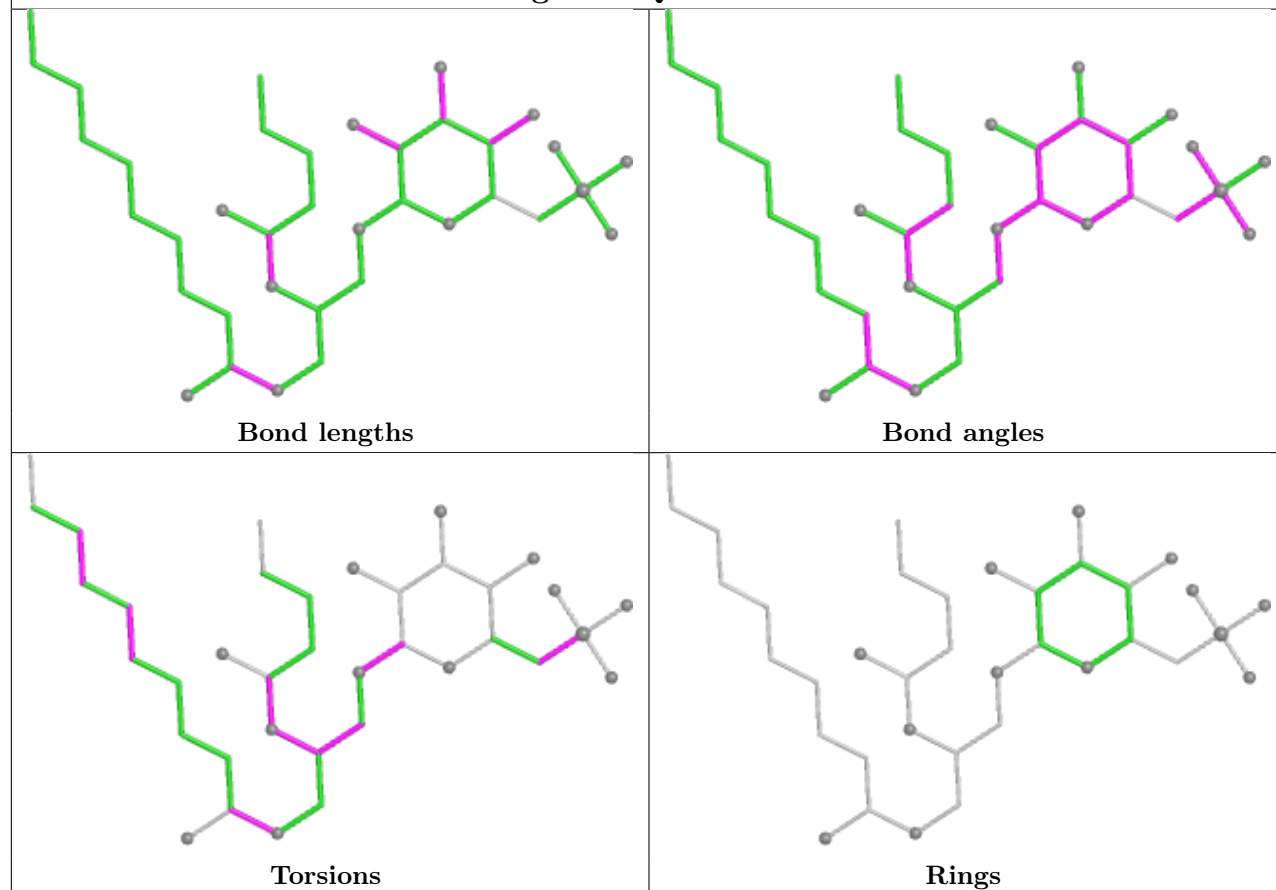


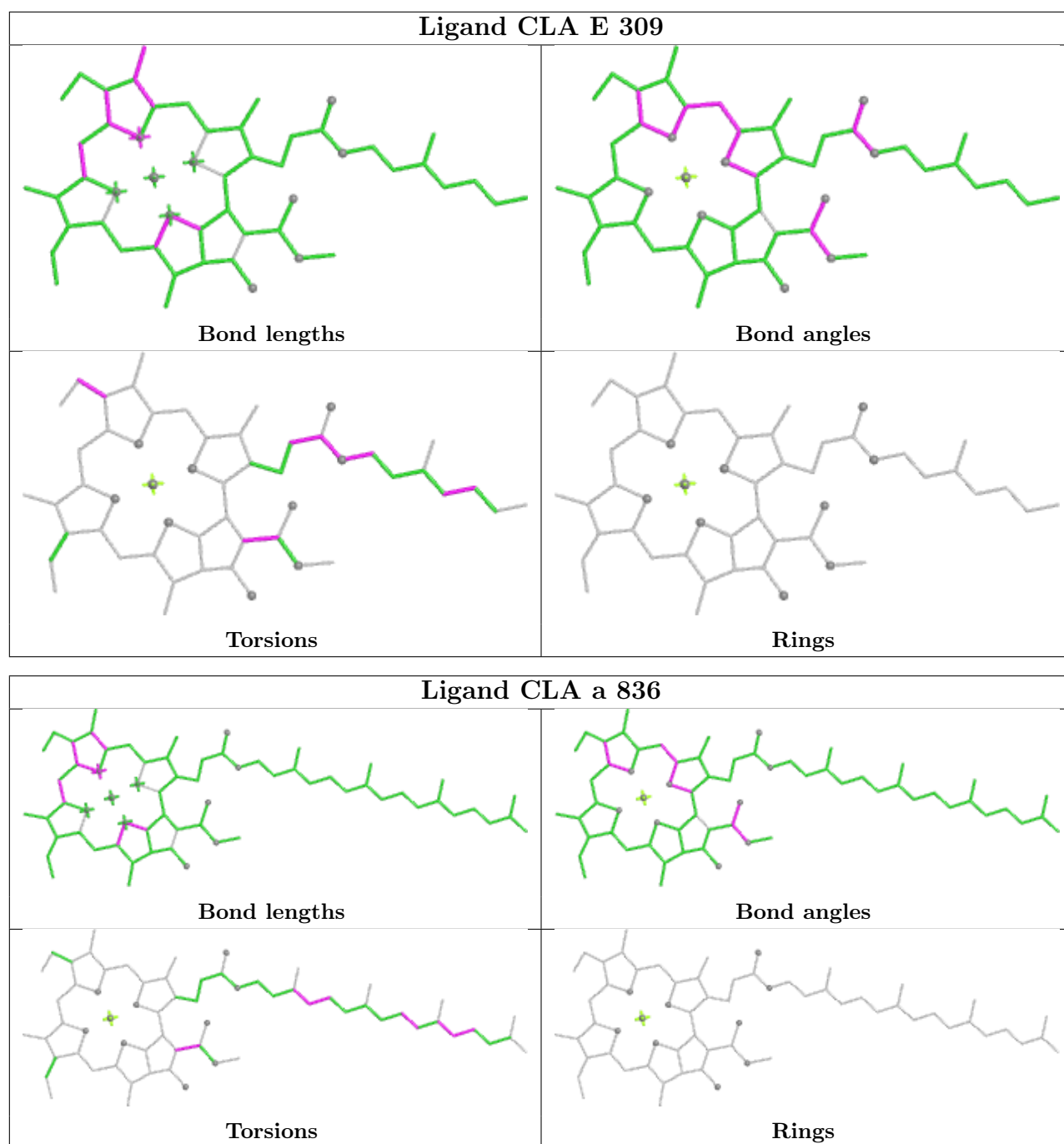
Rings

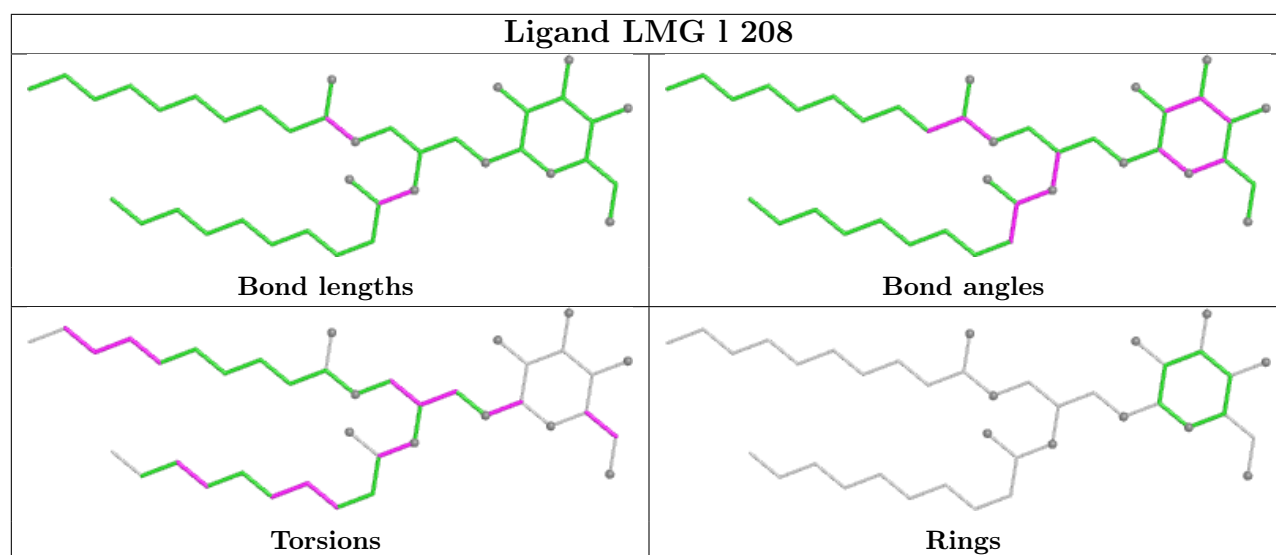
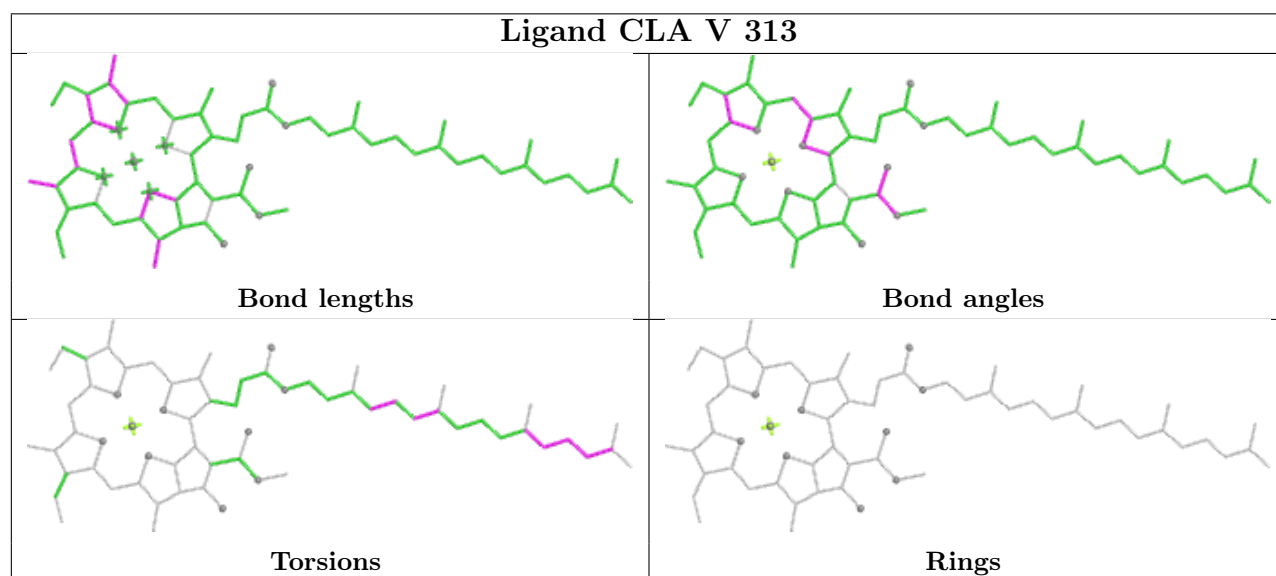
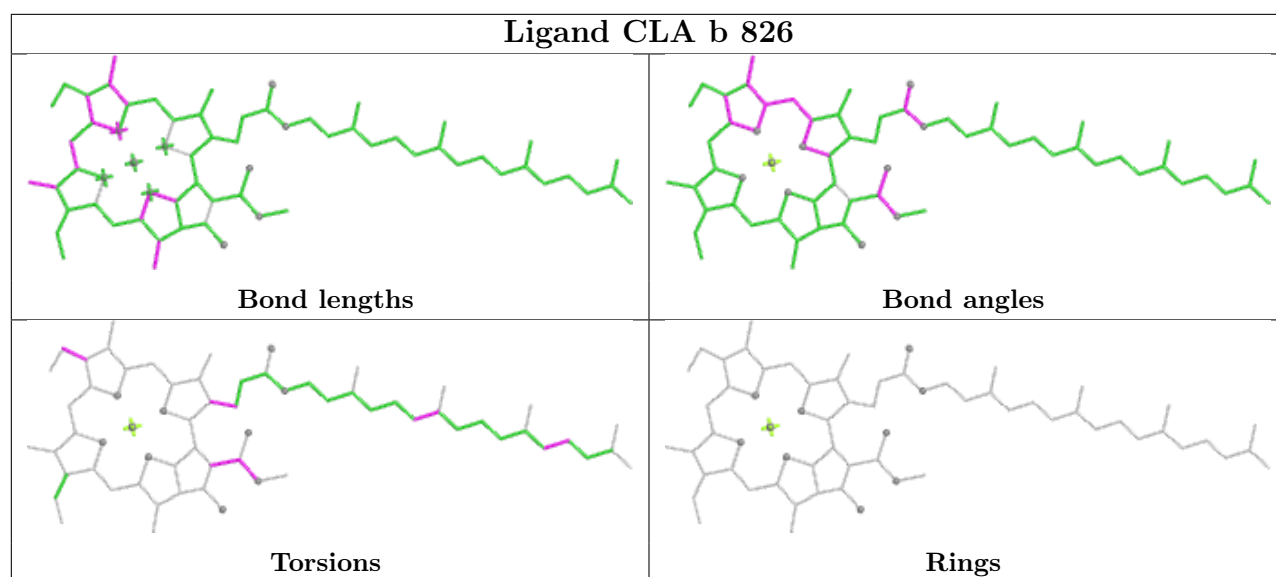
Ligand CLA a 825



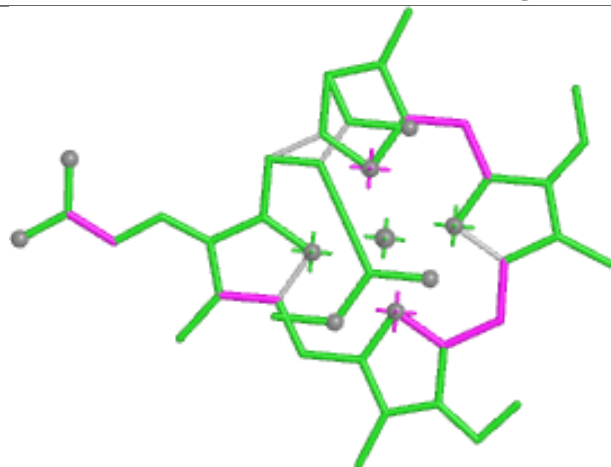
Ligand SQD D 320







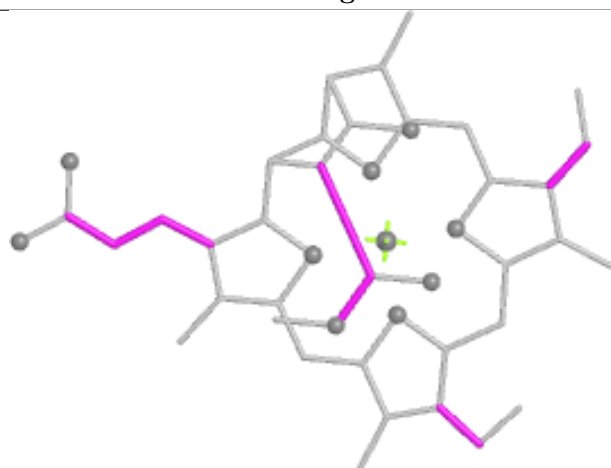
Ligand KC2 C 313



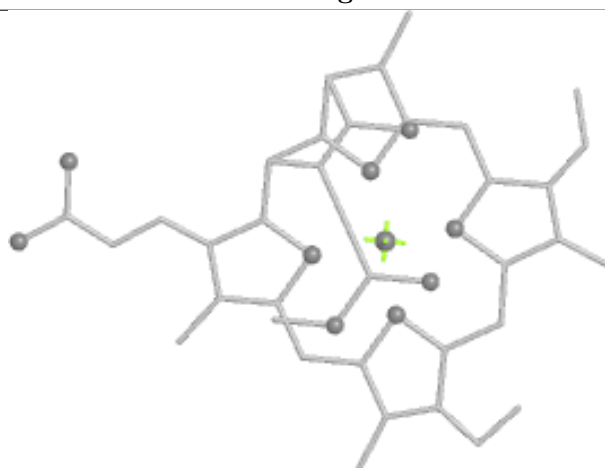
Bond lengths



Bond angles

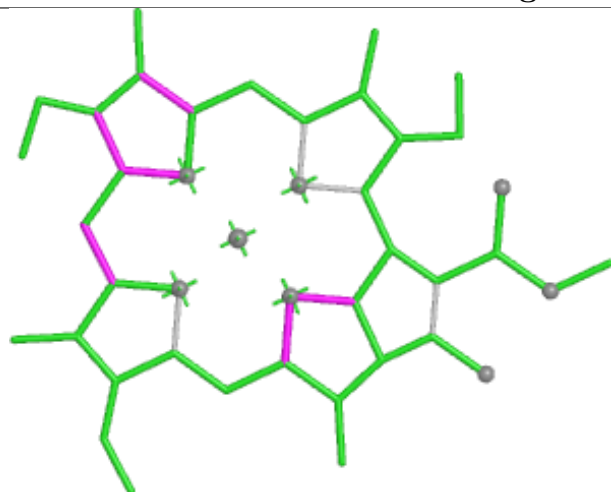


Torsions

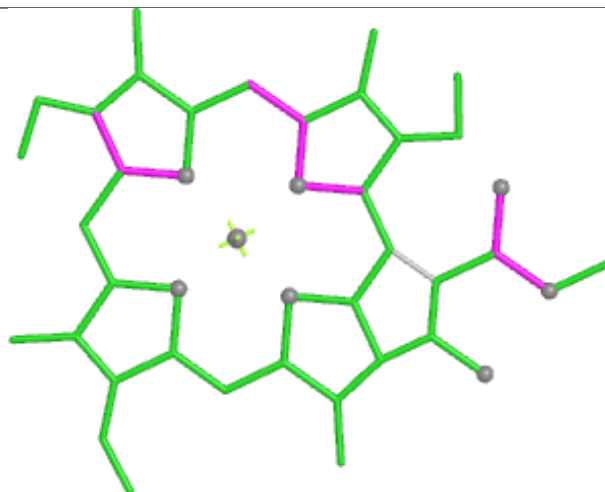


Rings

Ligand CLA z 317



Bond lengths



Bond angles

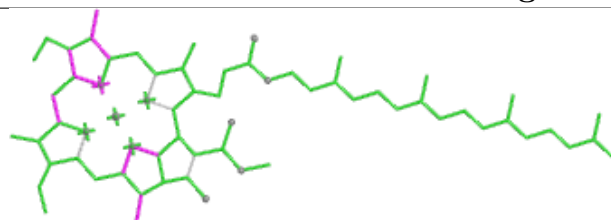


Torsions

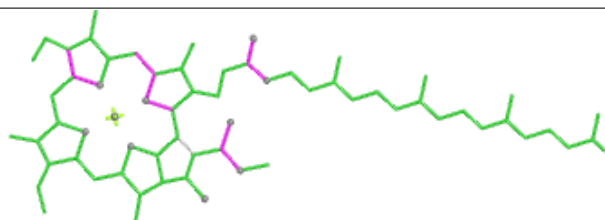


Rings

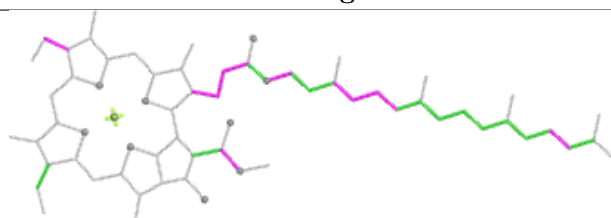
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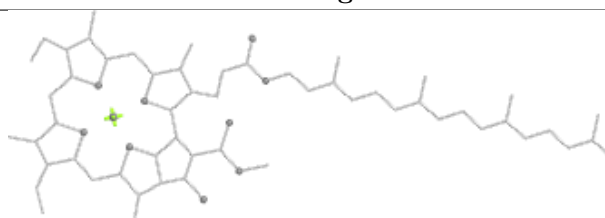
Bond lengths



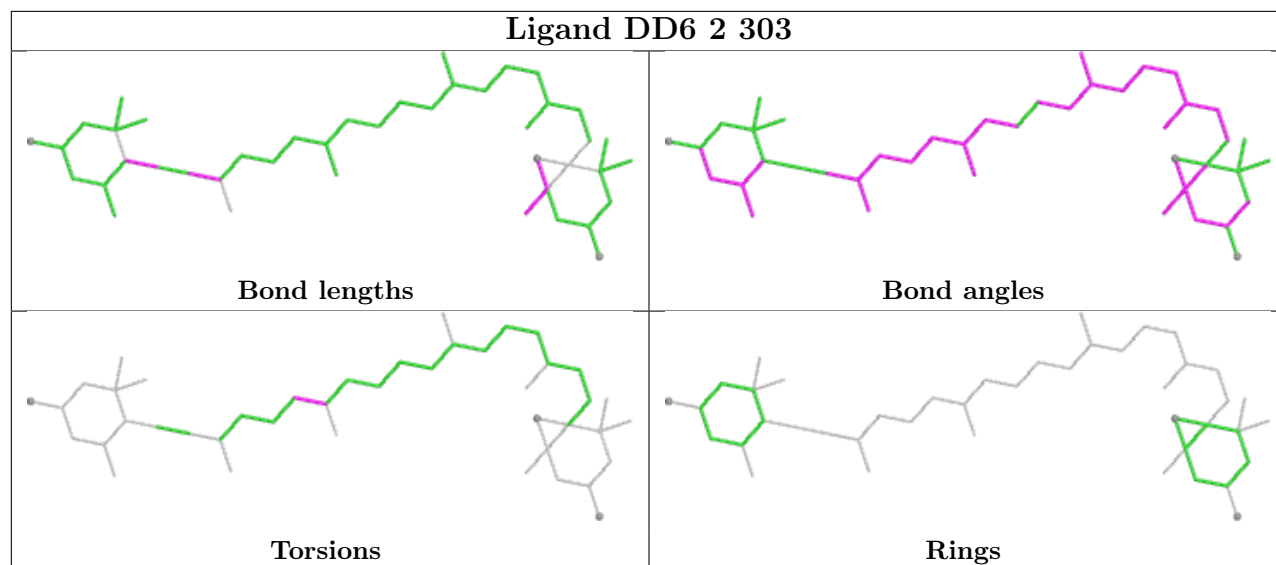
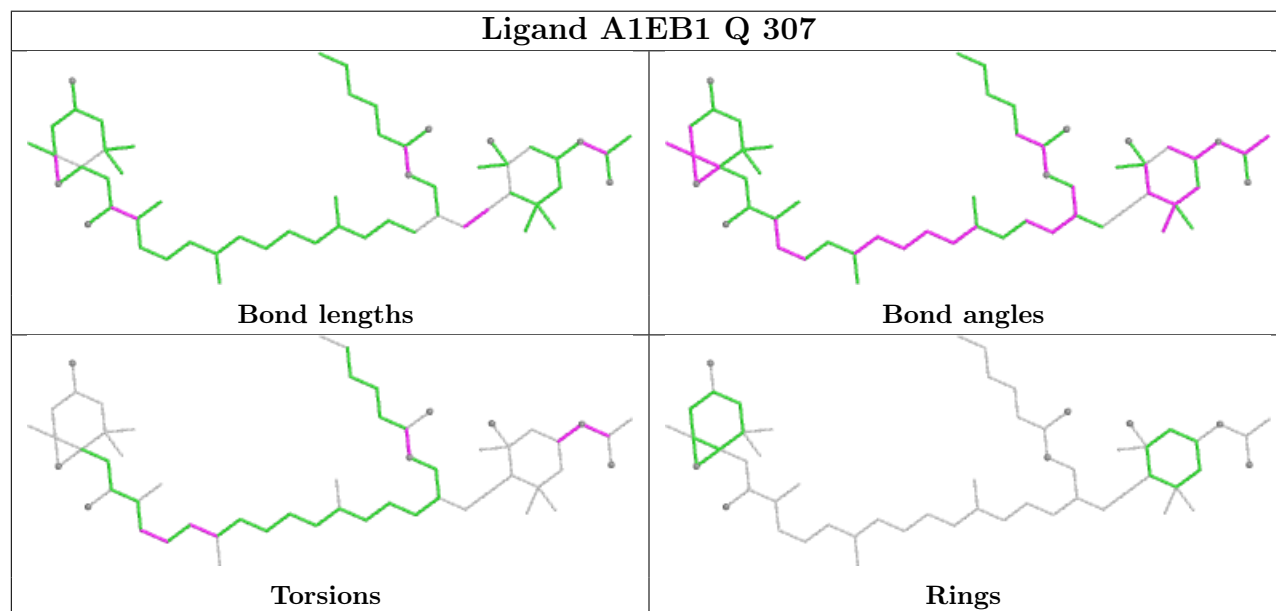
Bond angles



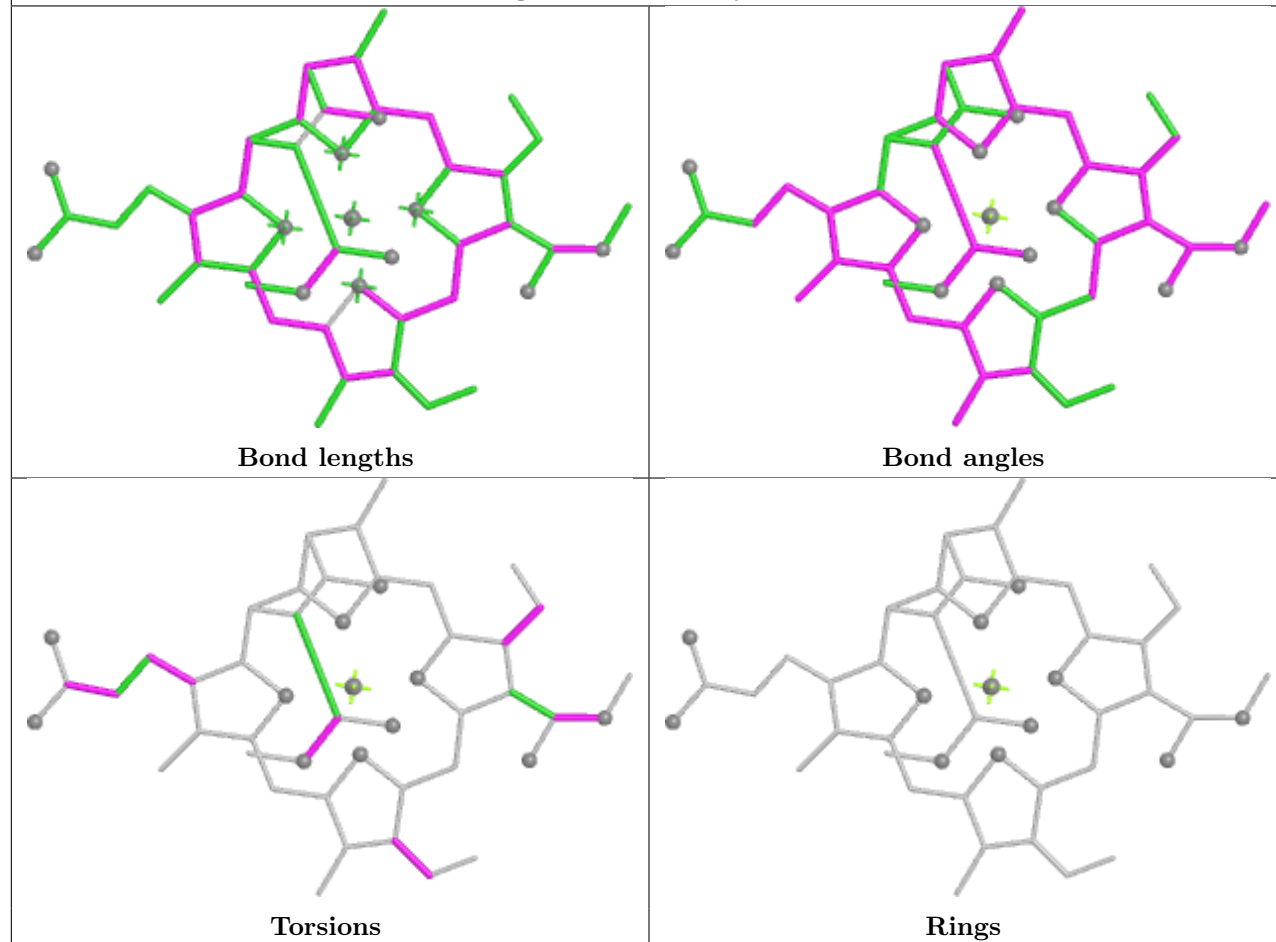
Torsions



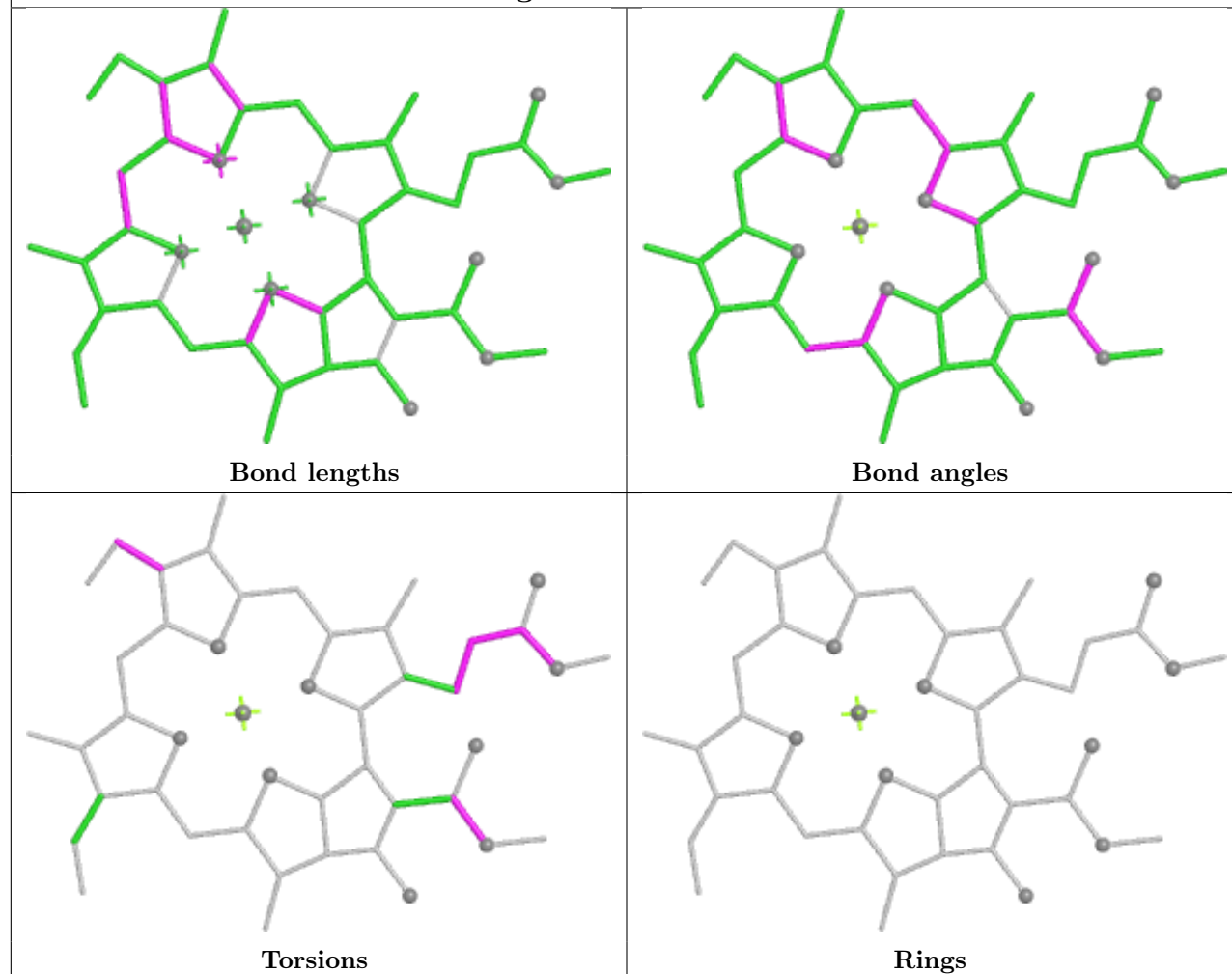
Rings

Ligand DD6 2 303**Ligand A1EB1 Q 307**

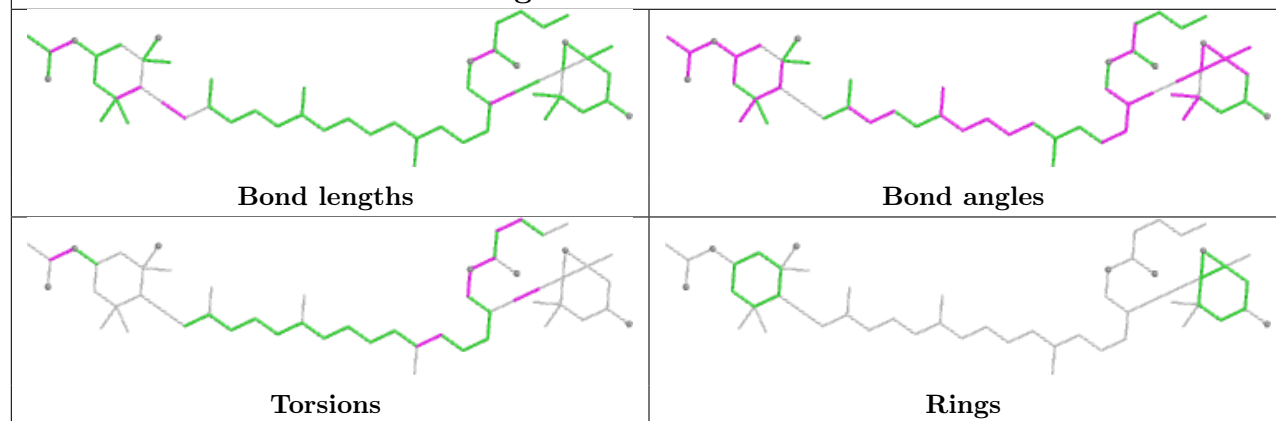
Ligand A1ECV y 311

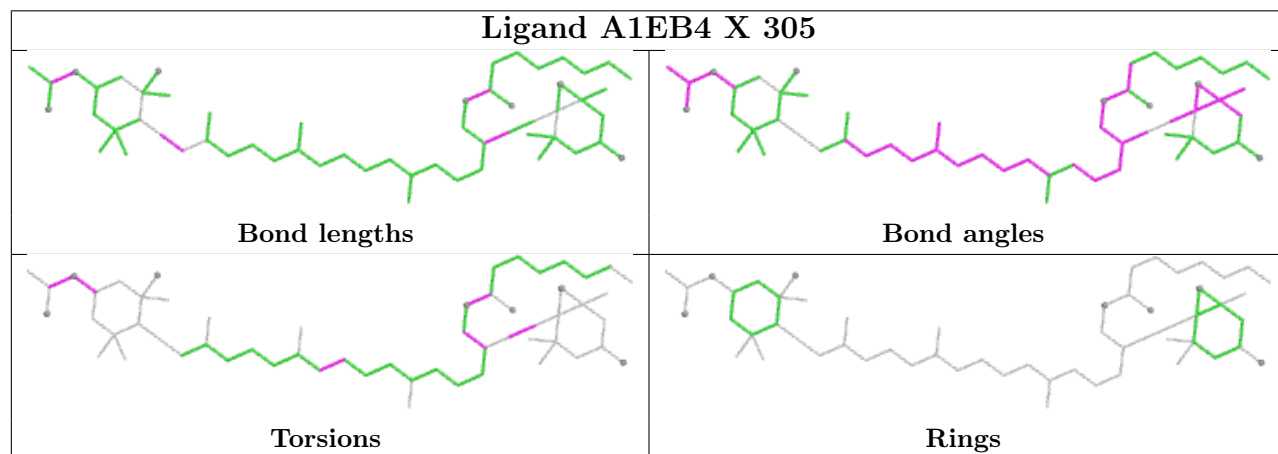
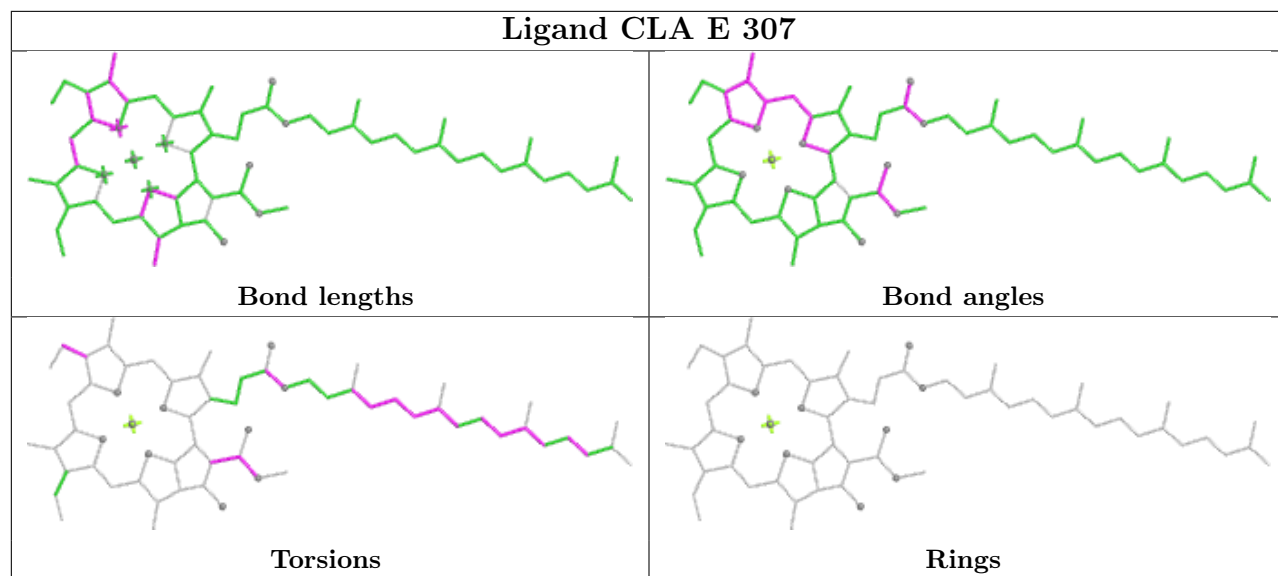


Ligand CLA Z 306

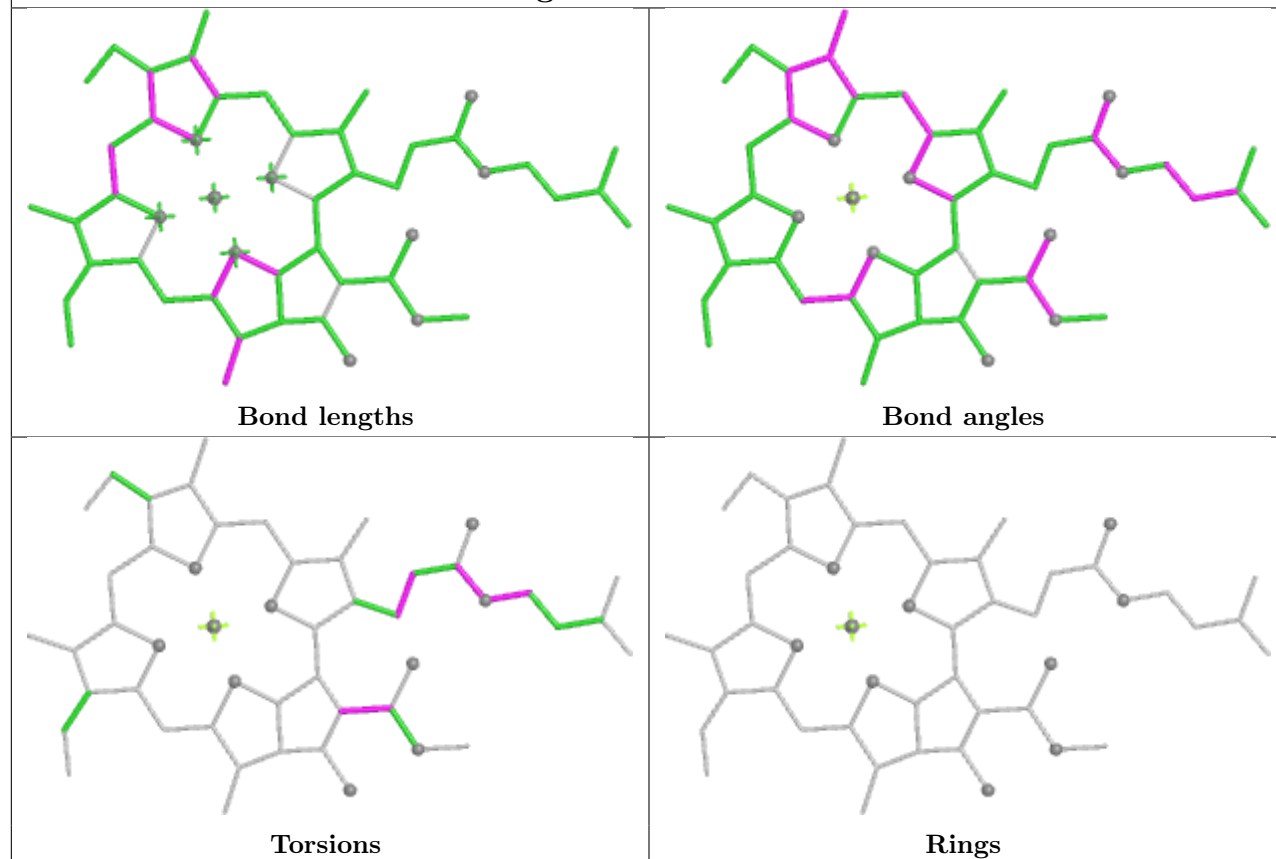


Ligand A1EB4 P 318

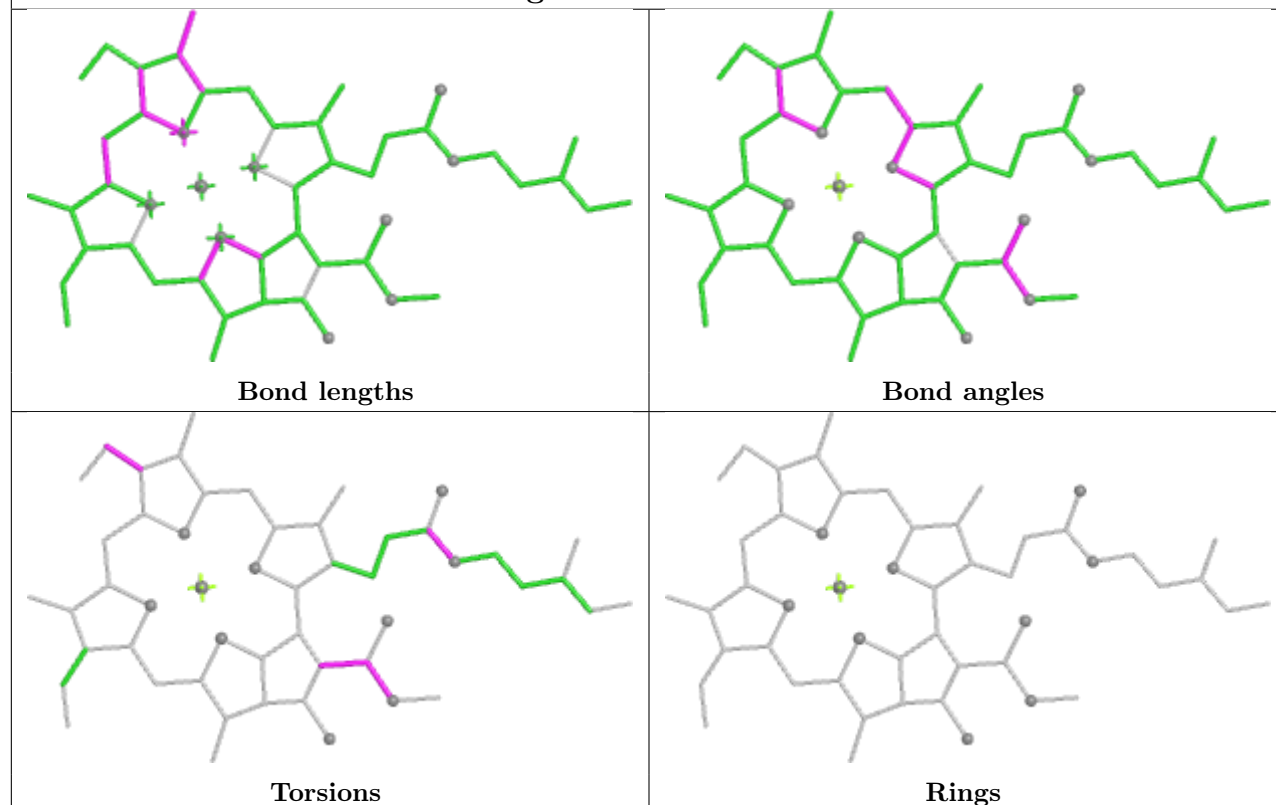


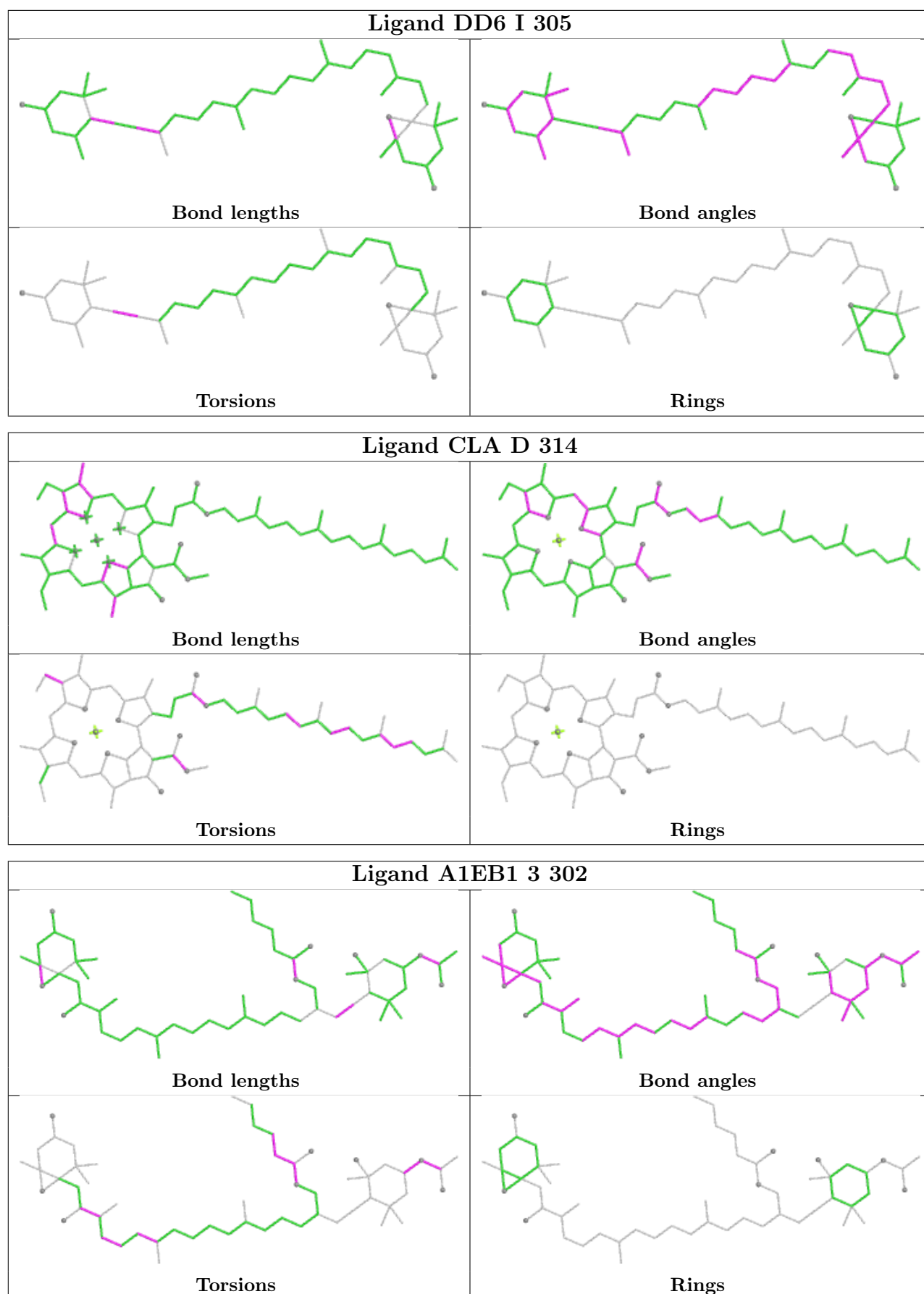


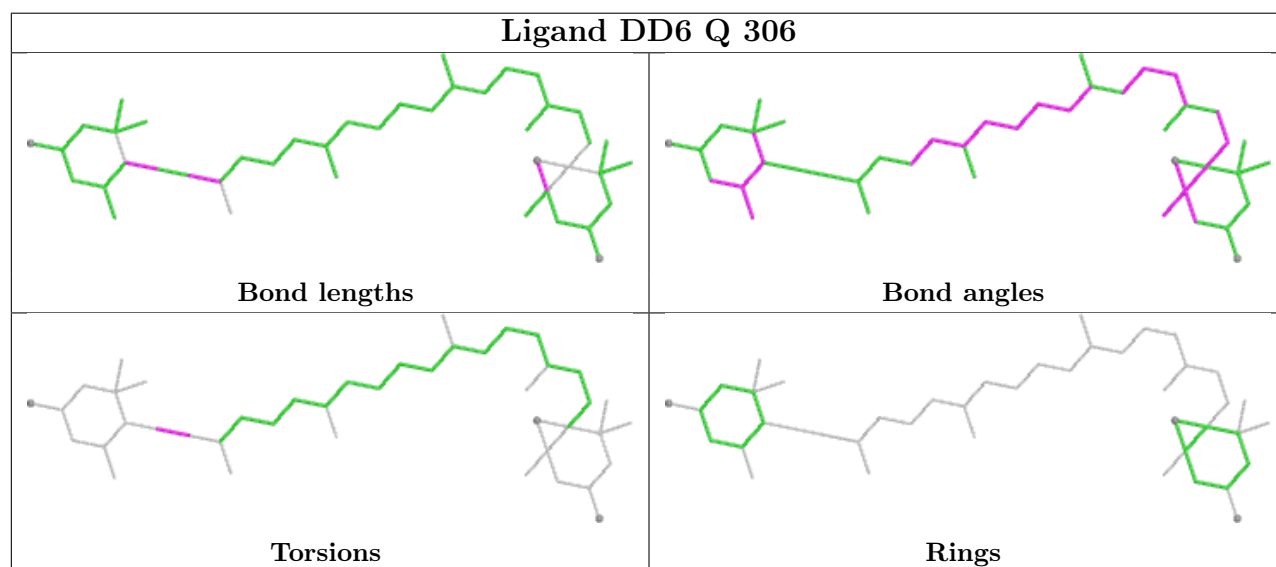
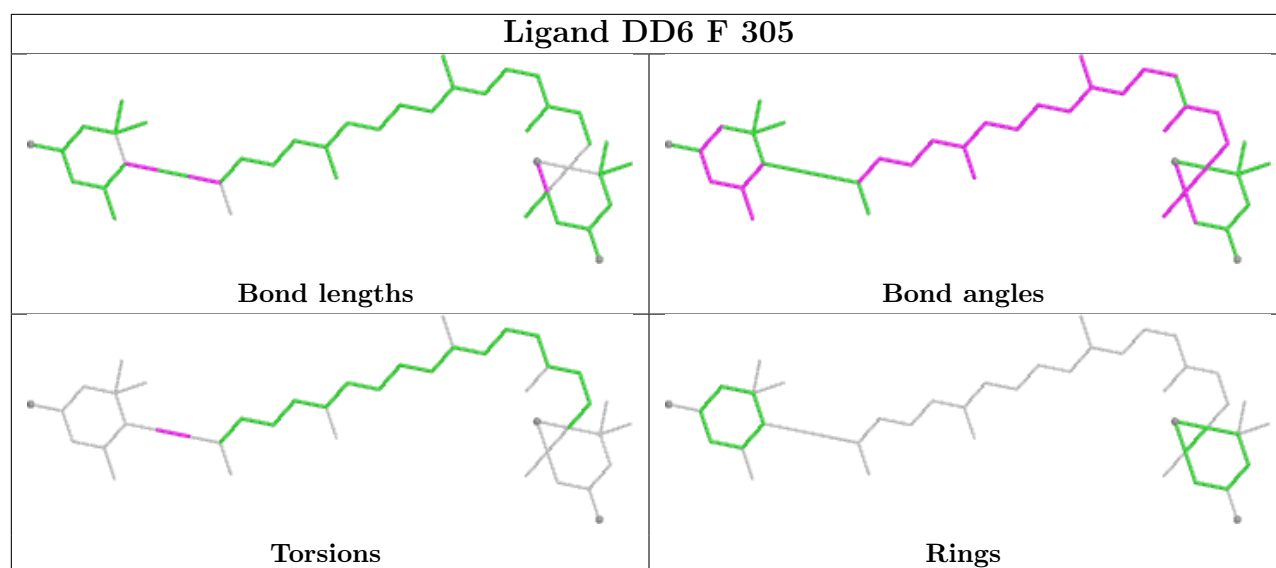
Ligand CLA 0 315

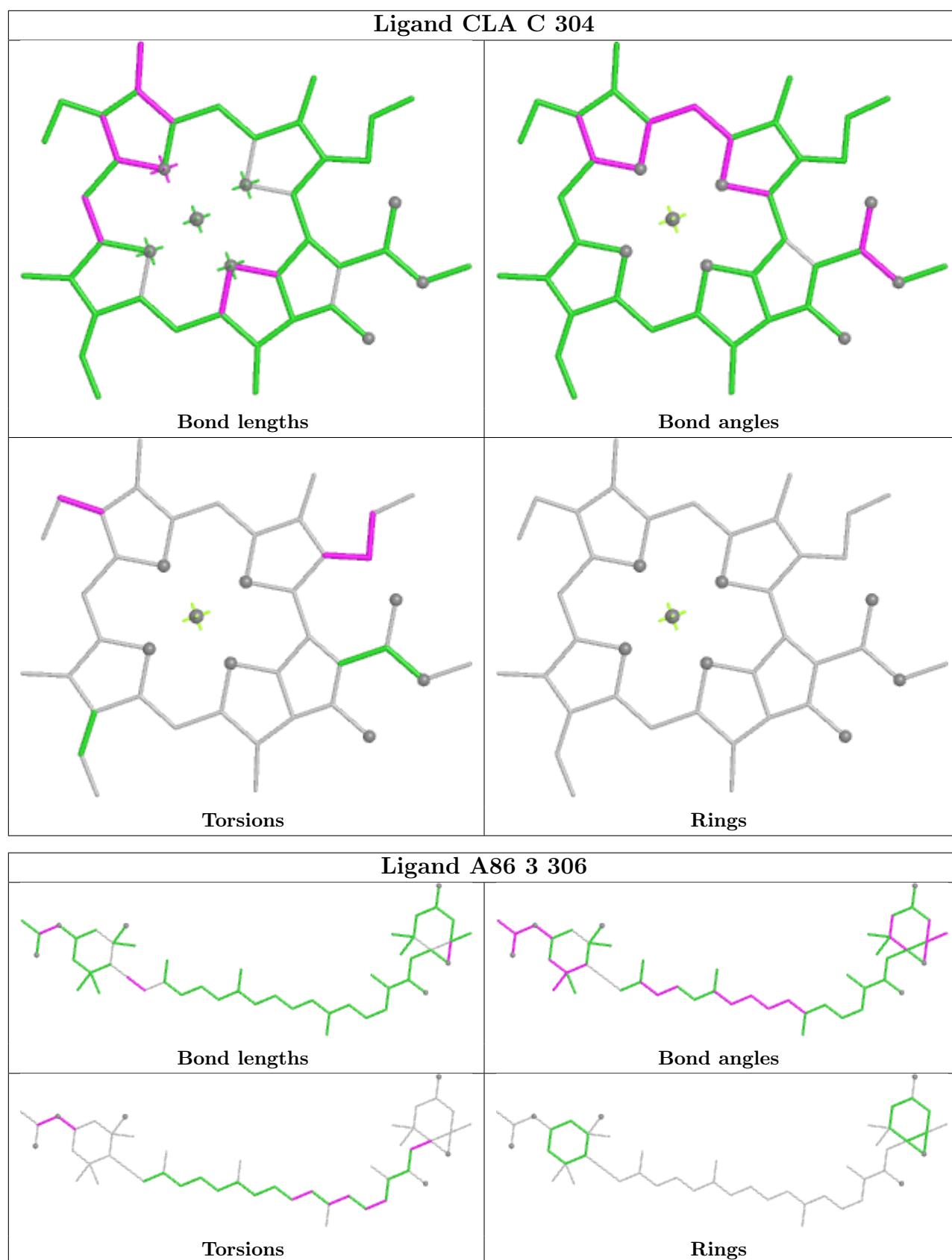


Ligand CLA W 318

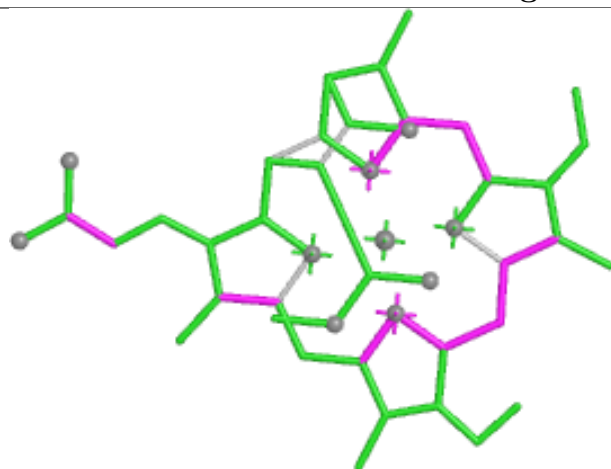




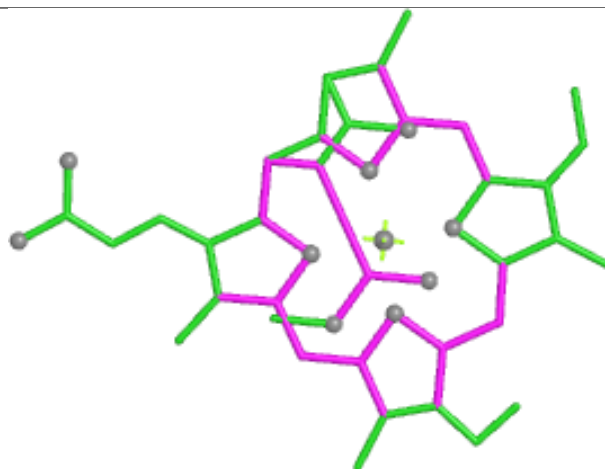




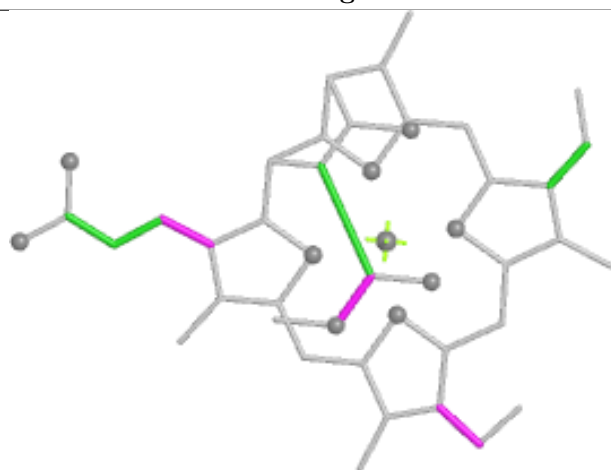
Ligand KC2 9 313



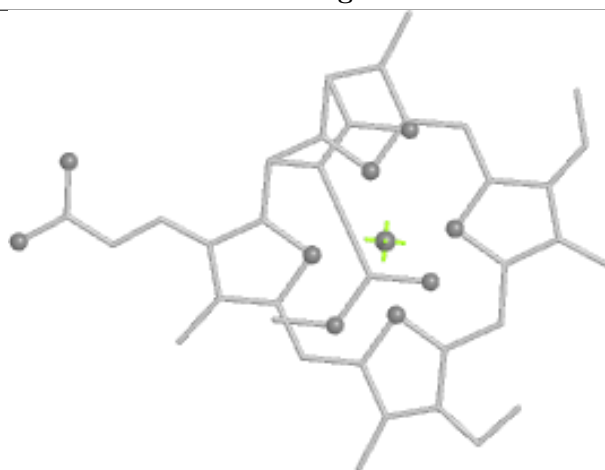
Bond lengths



Bond angles

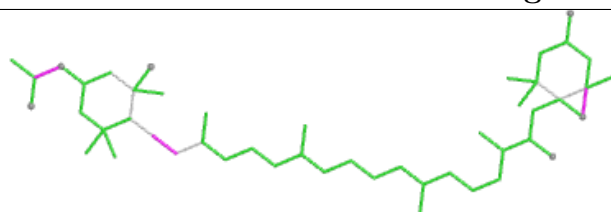


Torsions

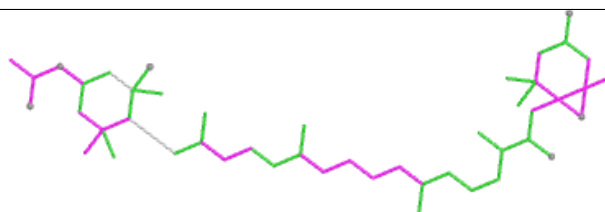


Rings

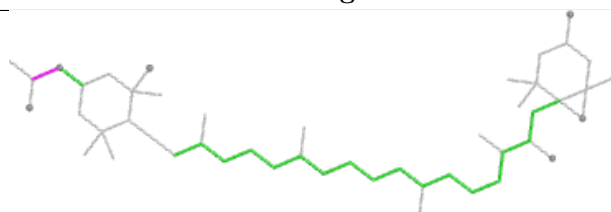
Ligand A86 6 303



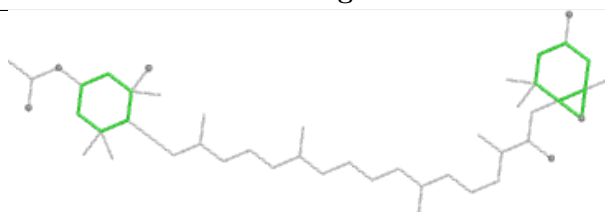
Bond lengths



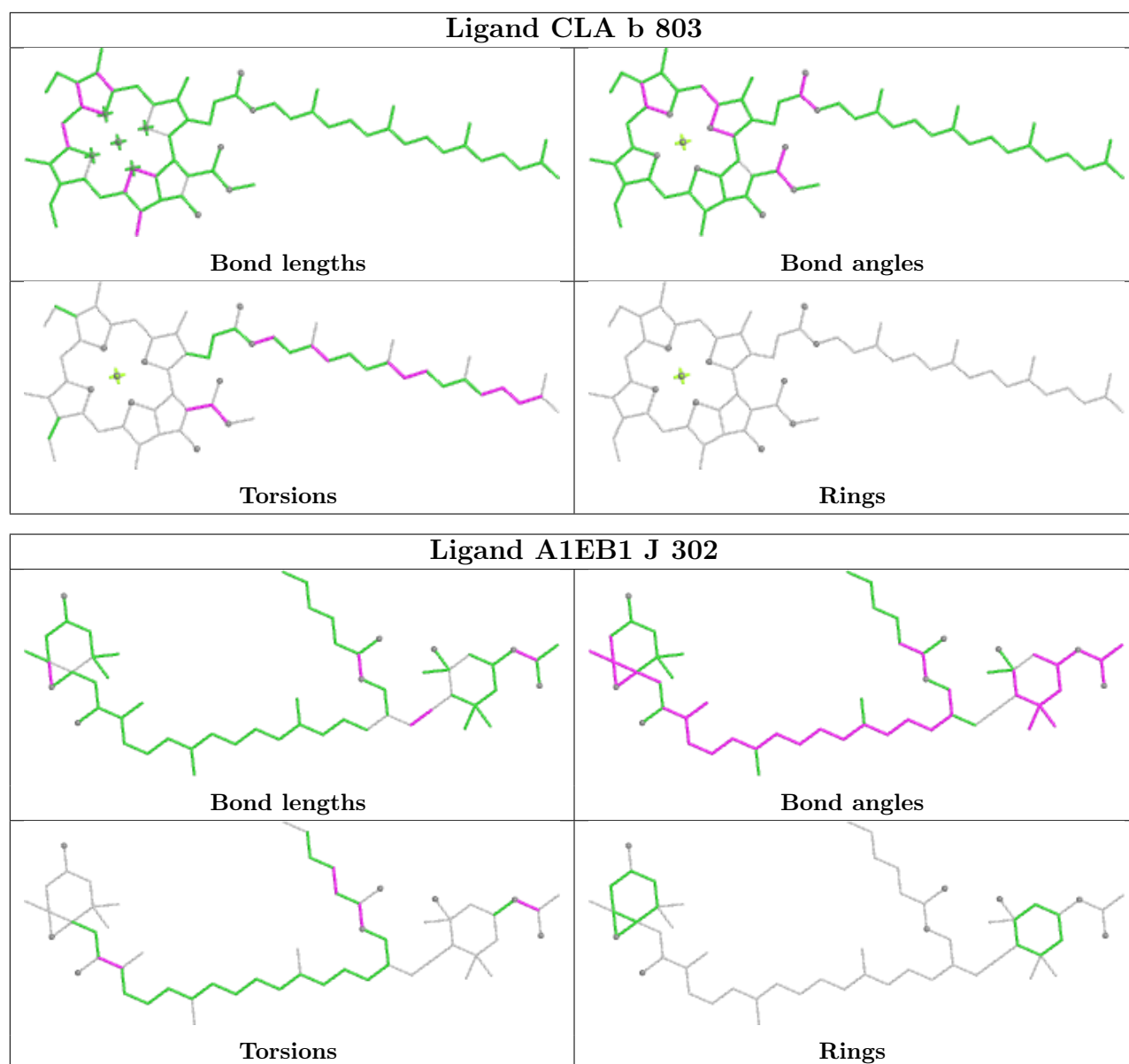
Bond angles



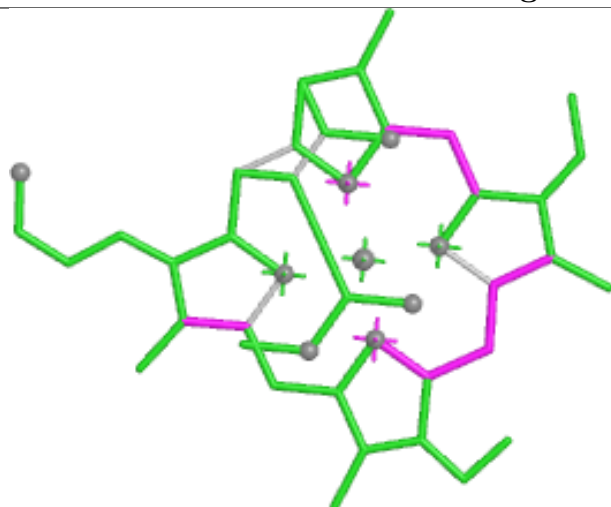
Torsions



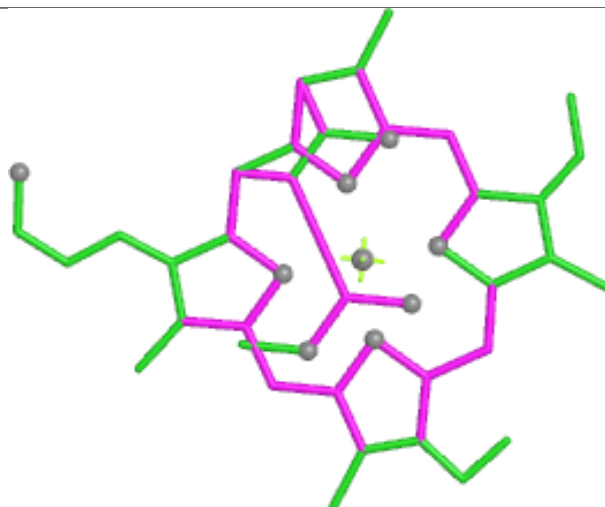
Rings



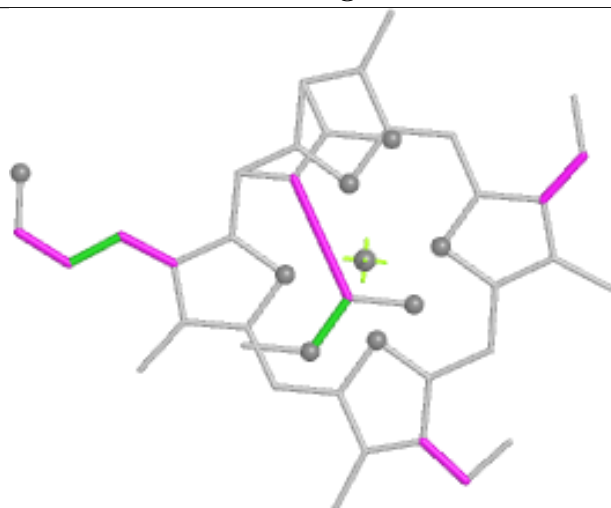
Ligand KC2 O 314



Bond lengths



Bond angles

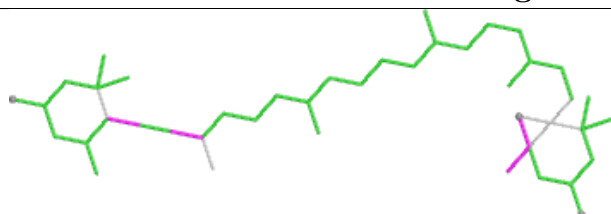


Torsions

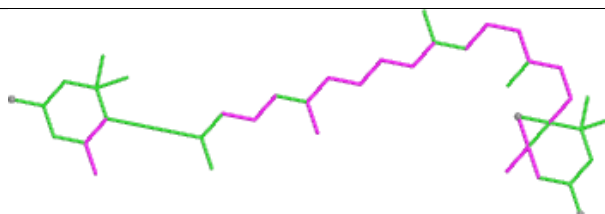


Rings

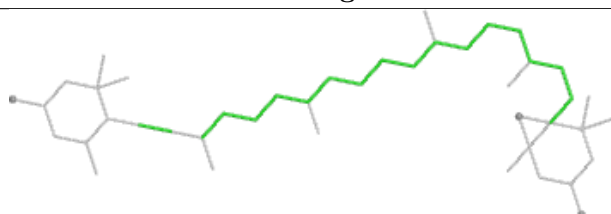
Ligand DD6 D 306



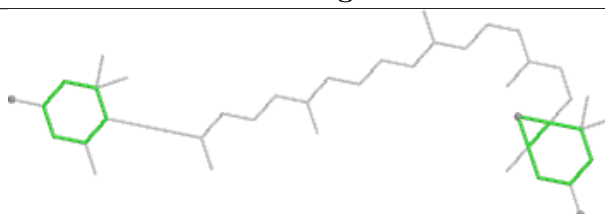
Bond lengths



Bond angles

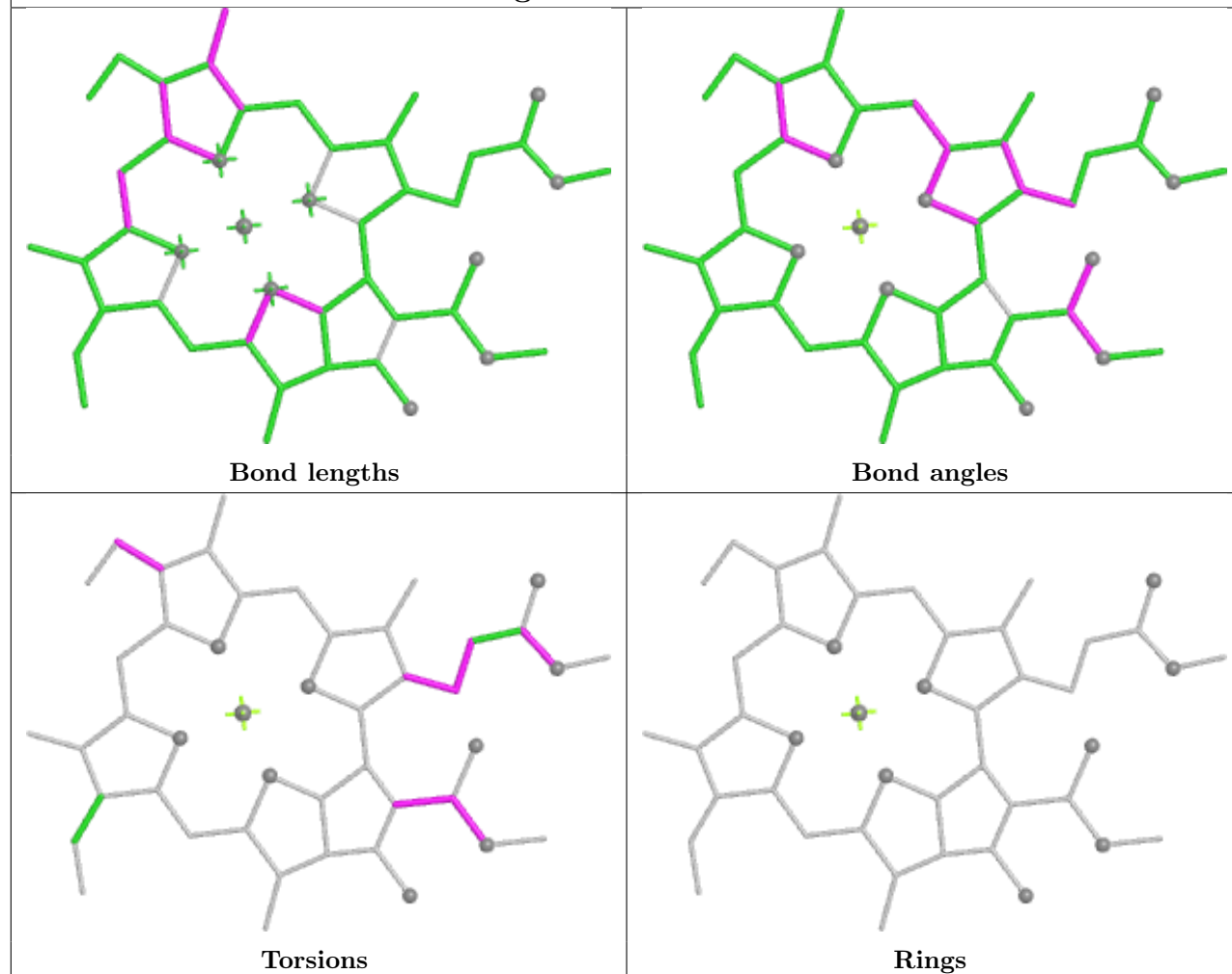


Torsions

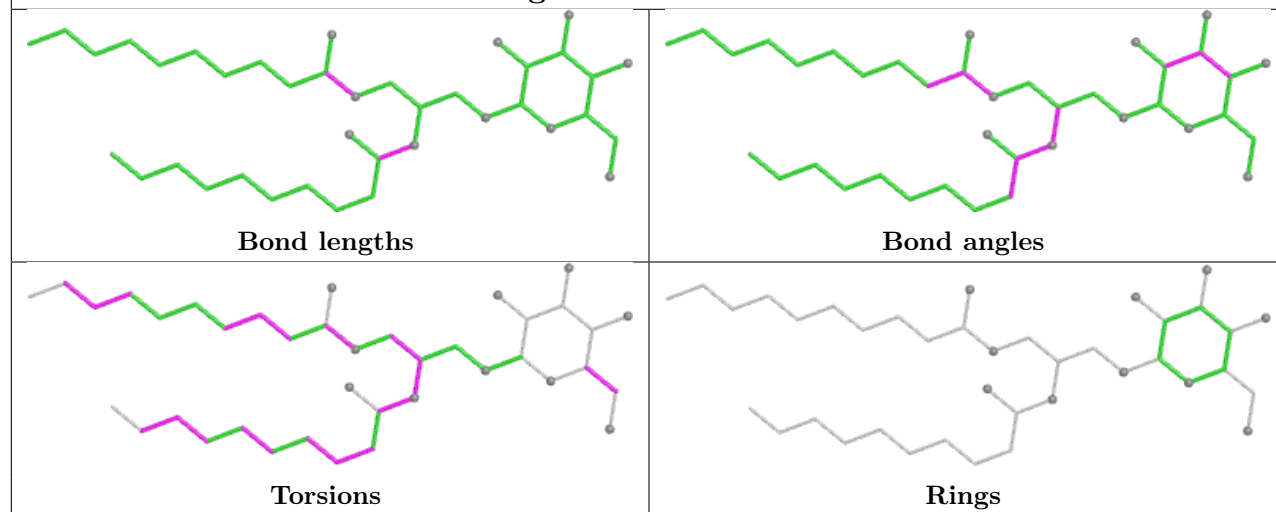


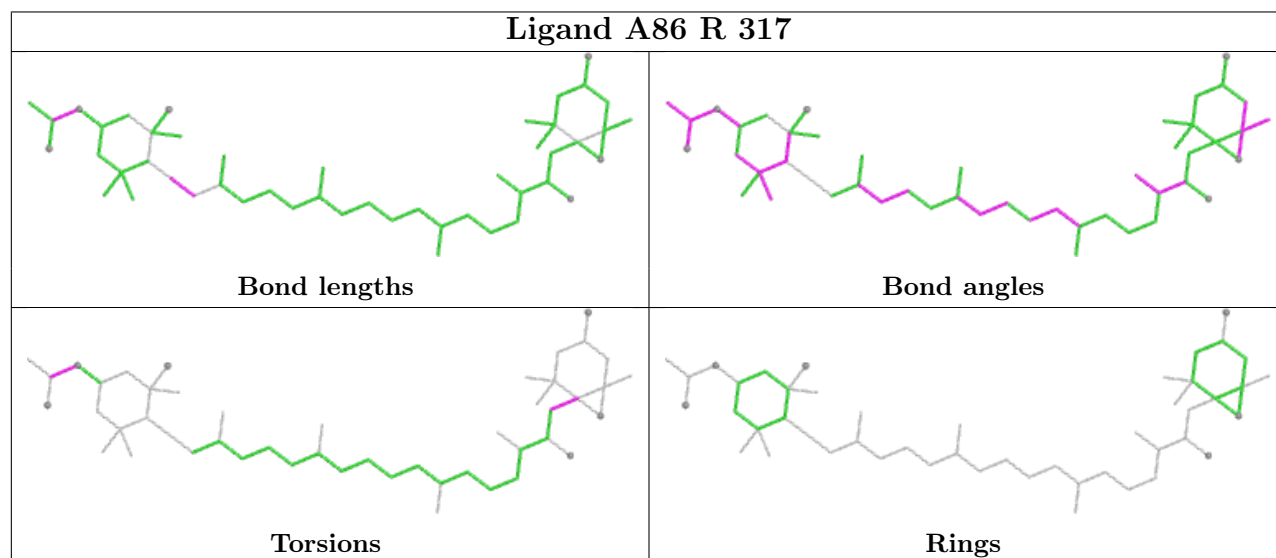
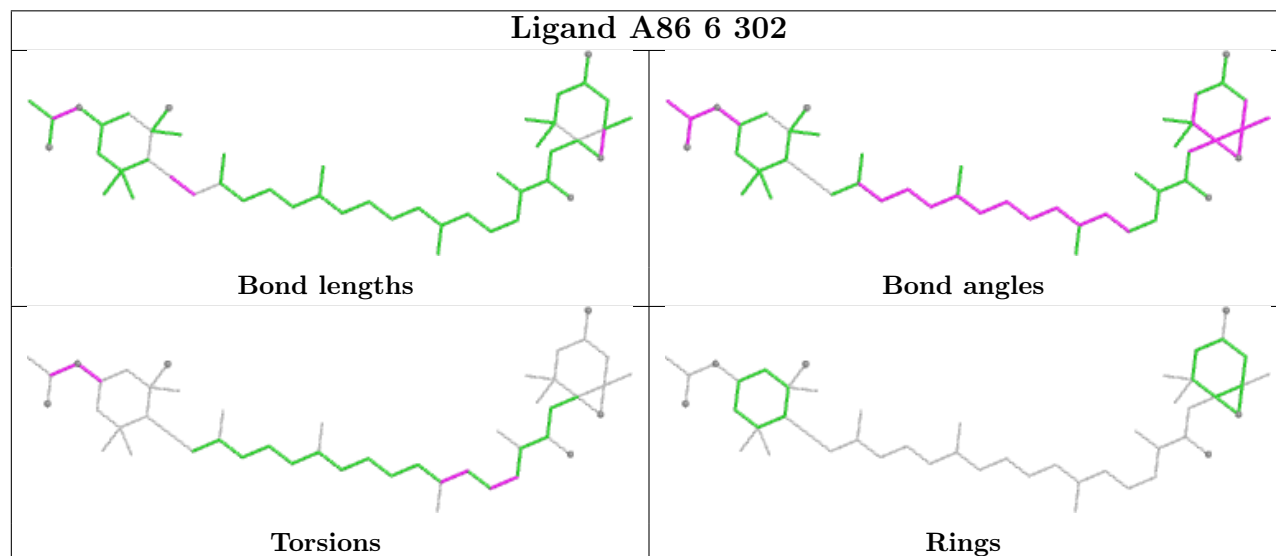
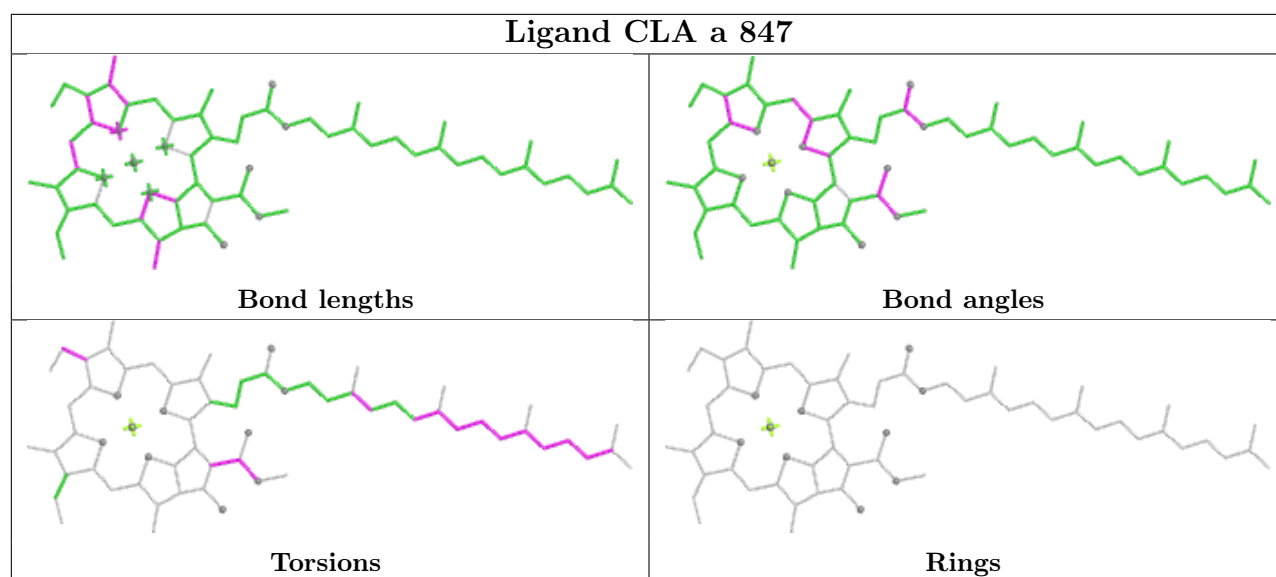
Rings

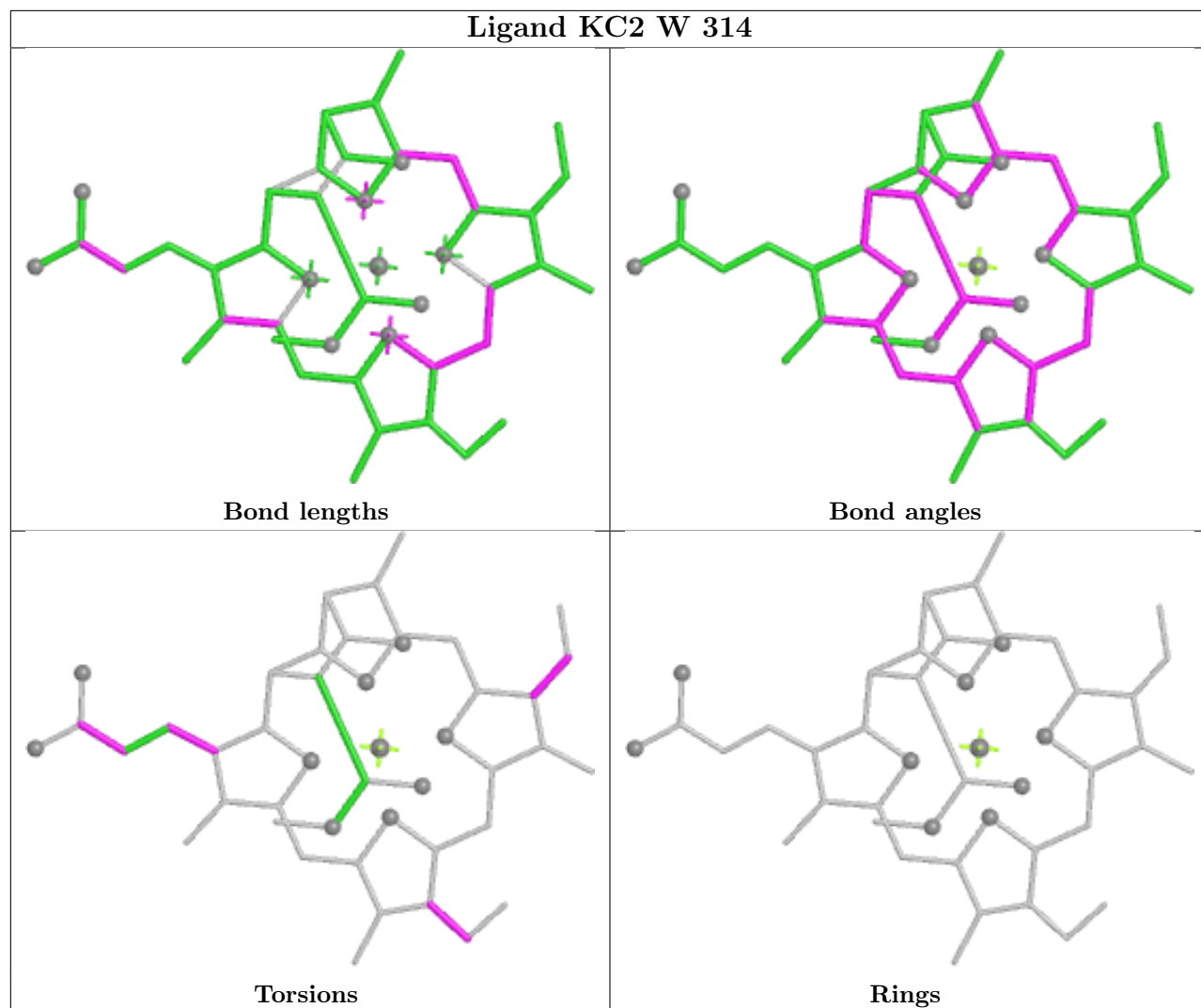
Ligand CLA T 319



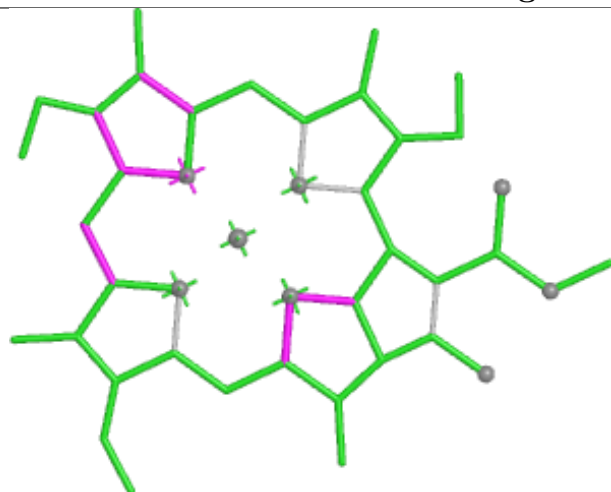
Ligand LMG P 317



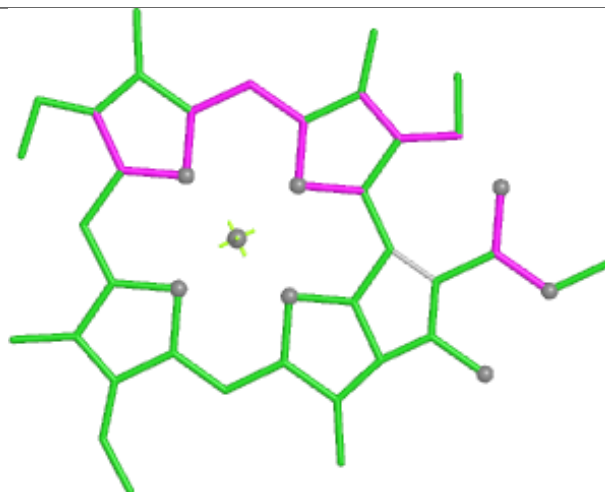




Ligand CLA o 202



Bond lengths



Bond angles

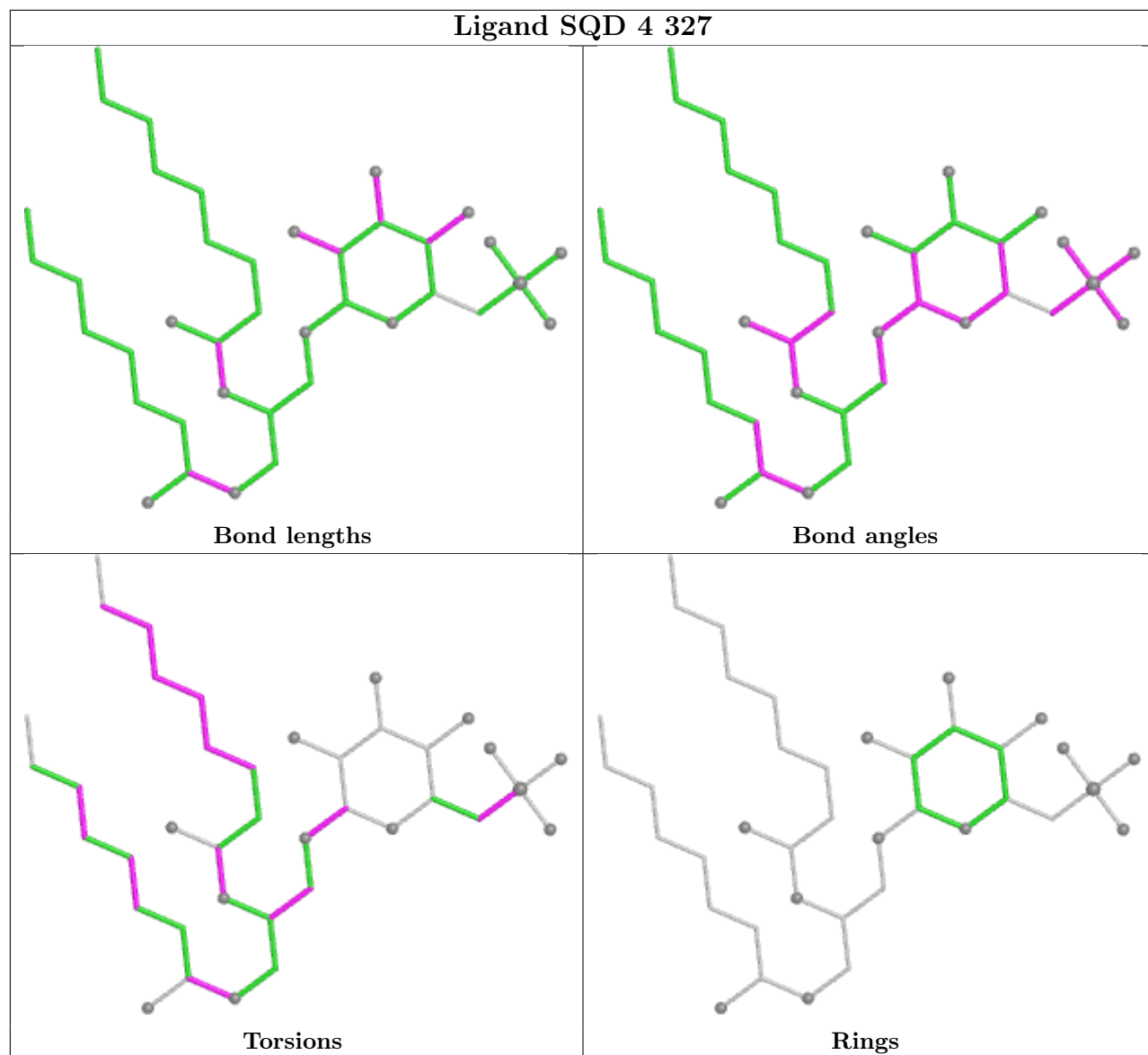


Torsions

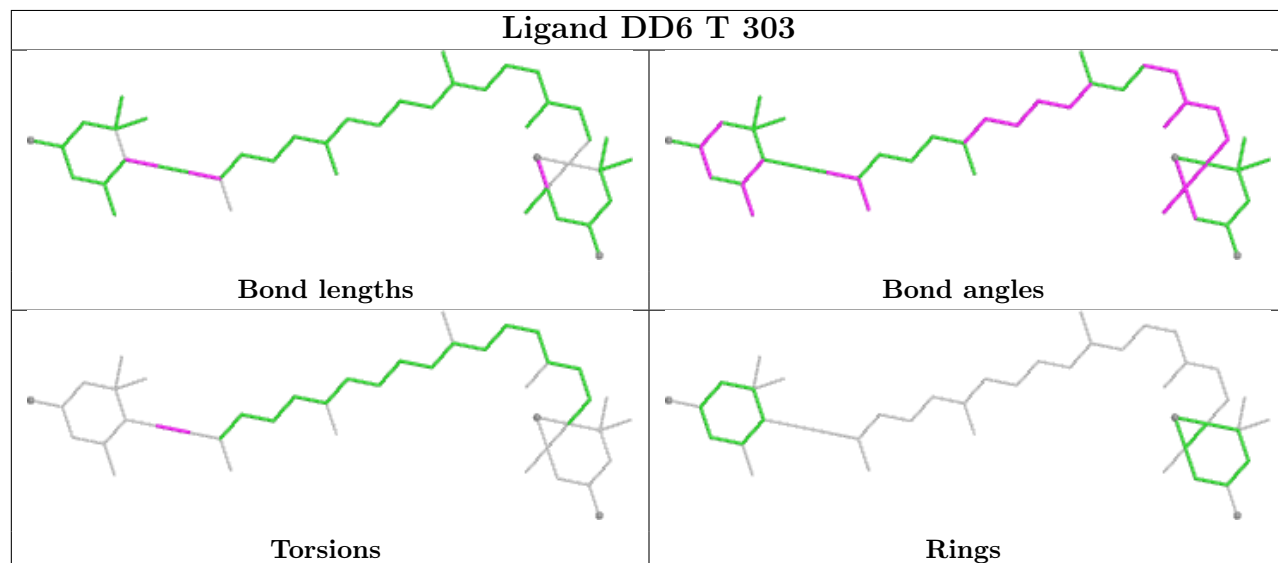


Rings

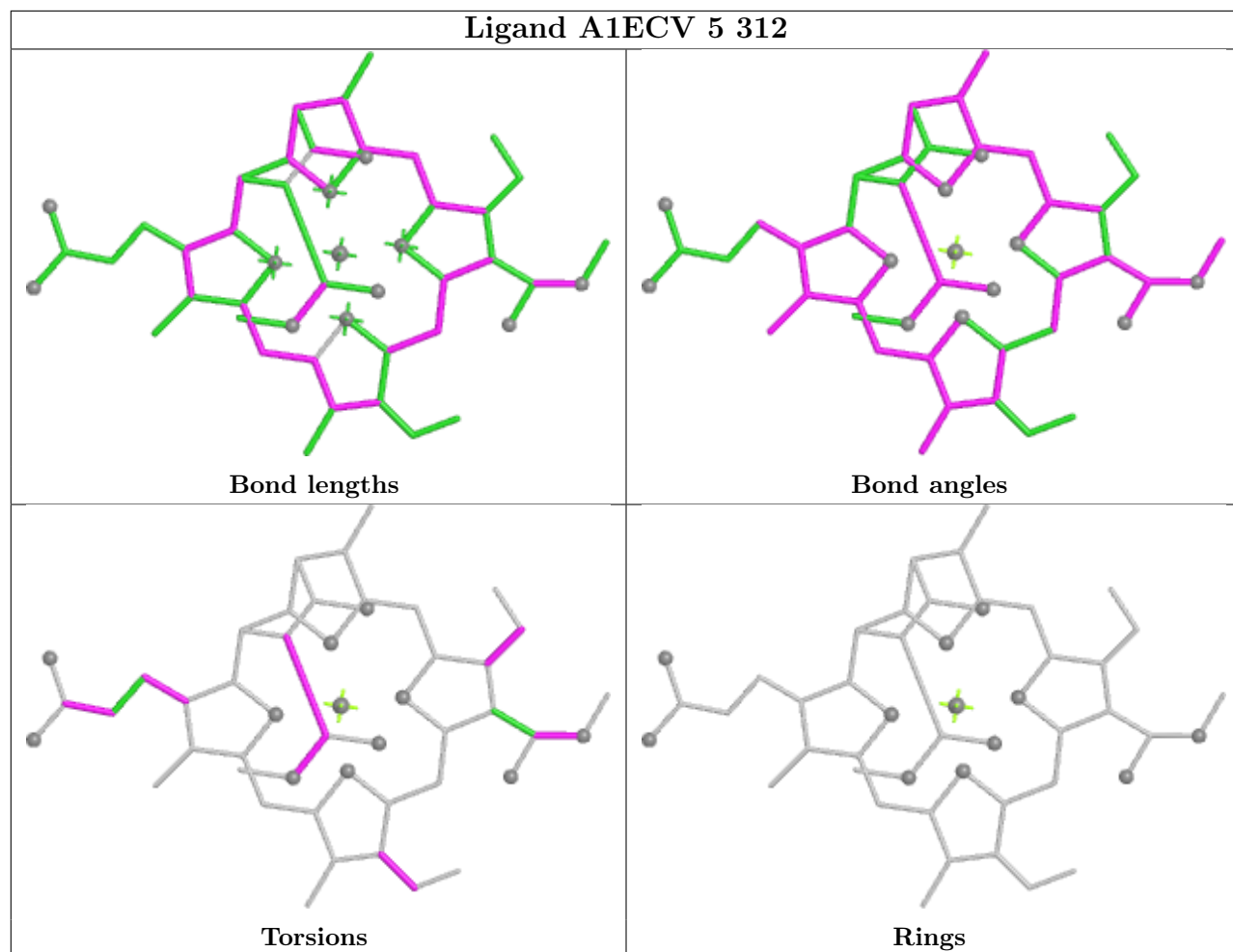
Ligand SQD 4 327



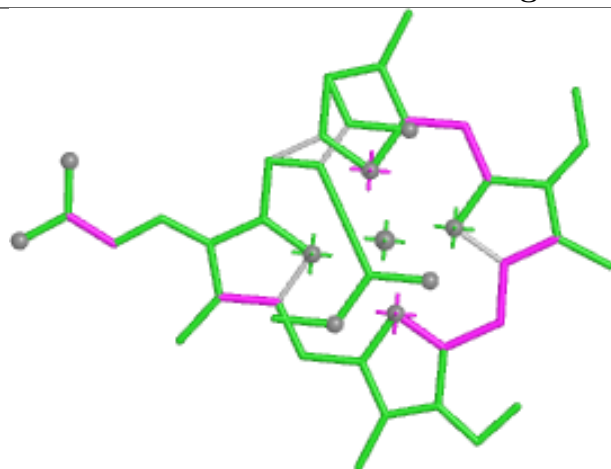
Ligand DD6 T 303



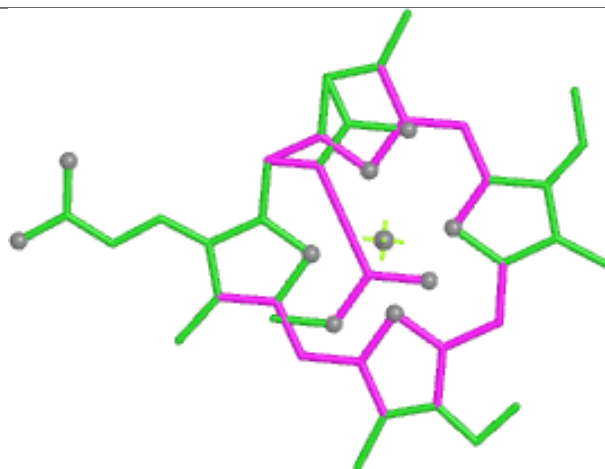
Ligand A1ECV 5 312



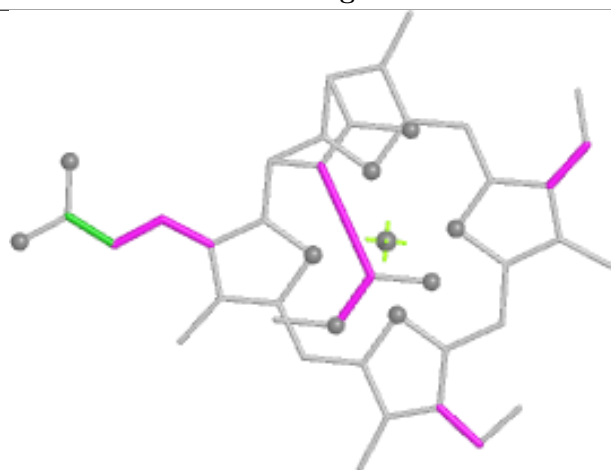
Ligand KC2 1 315



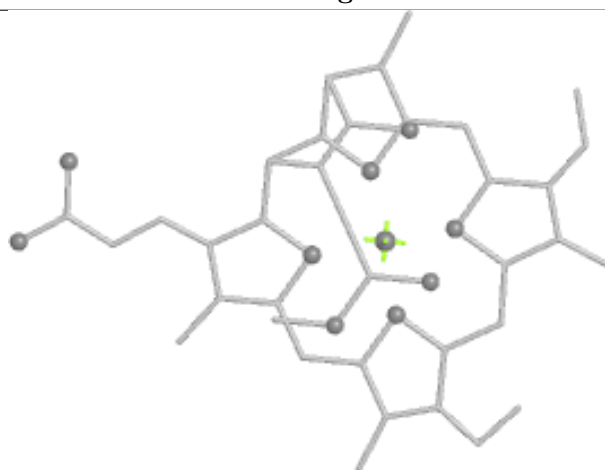
Bond lengths



Bond angles

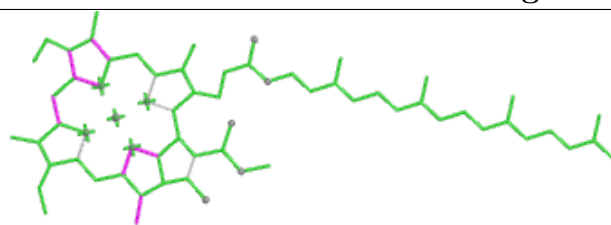


Torsions

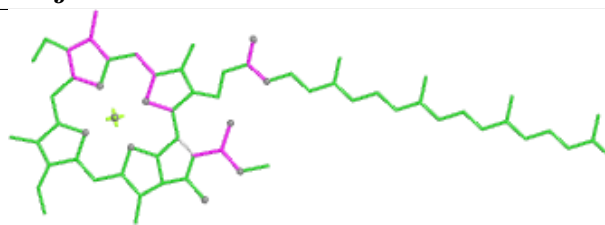


Rings

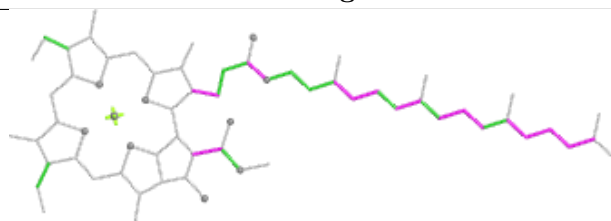
Ligand CLA j 101



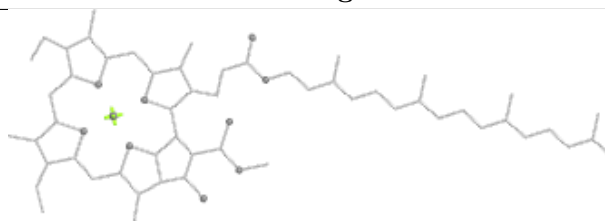
Bond lengths



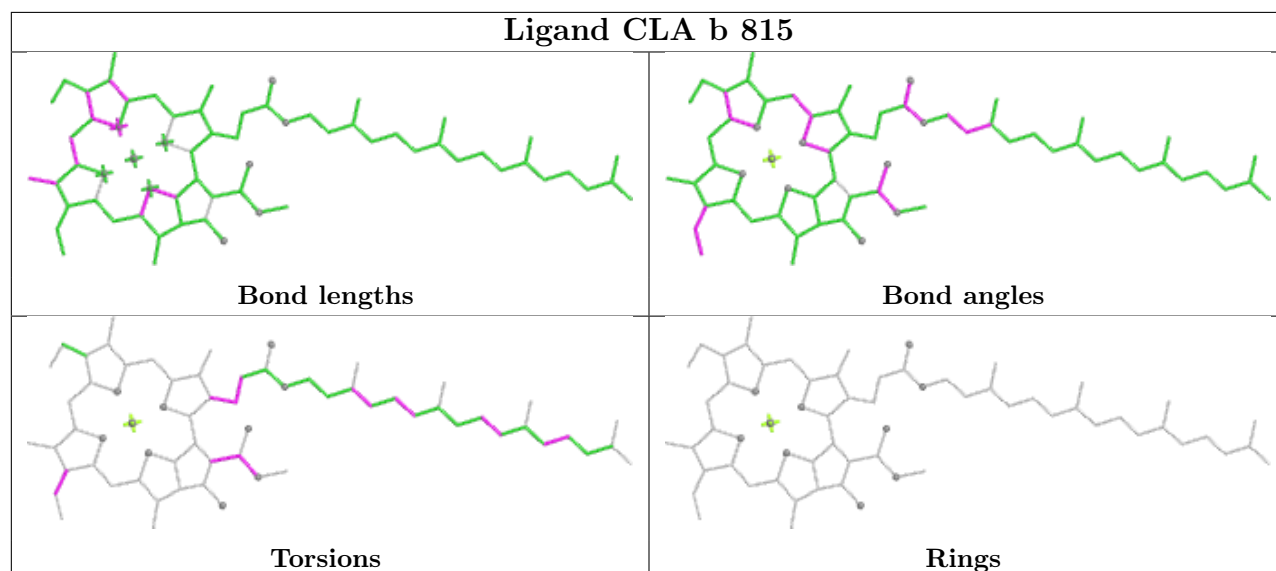
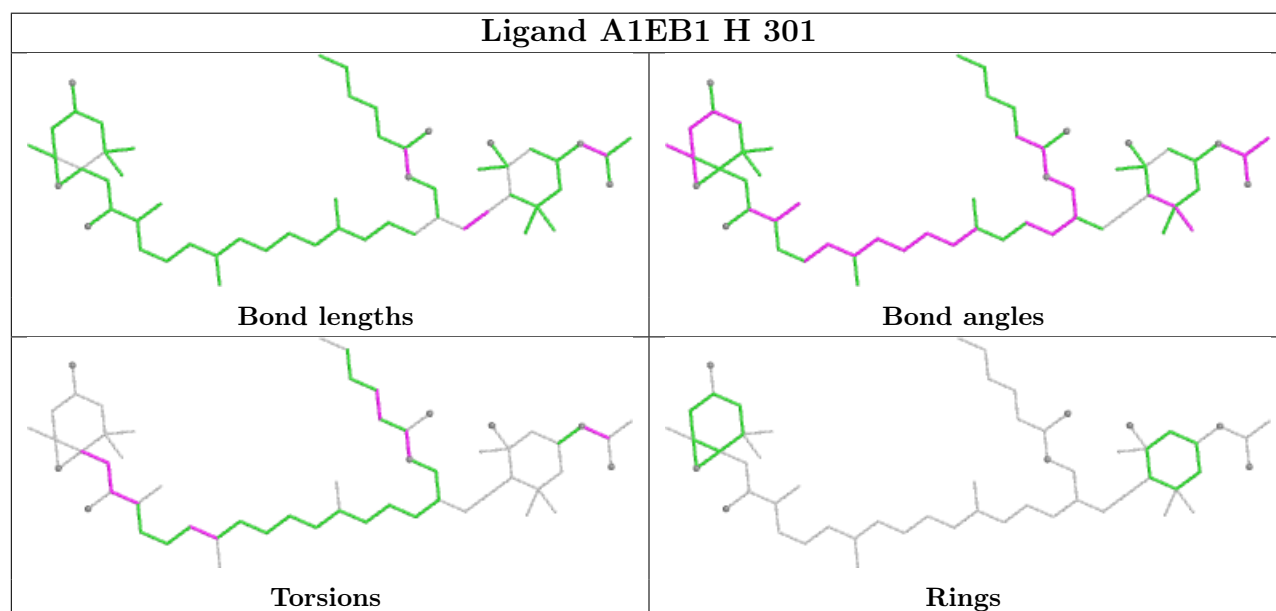
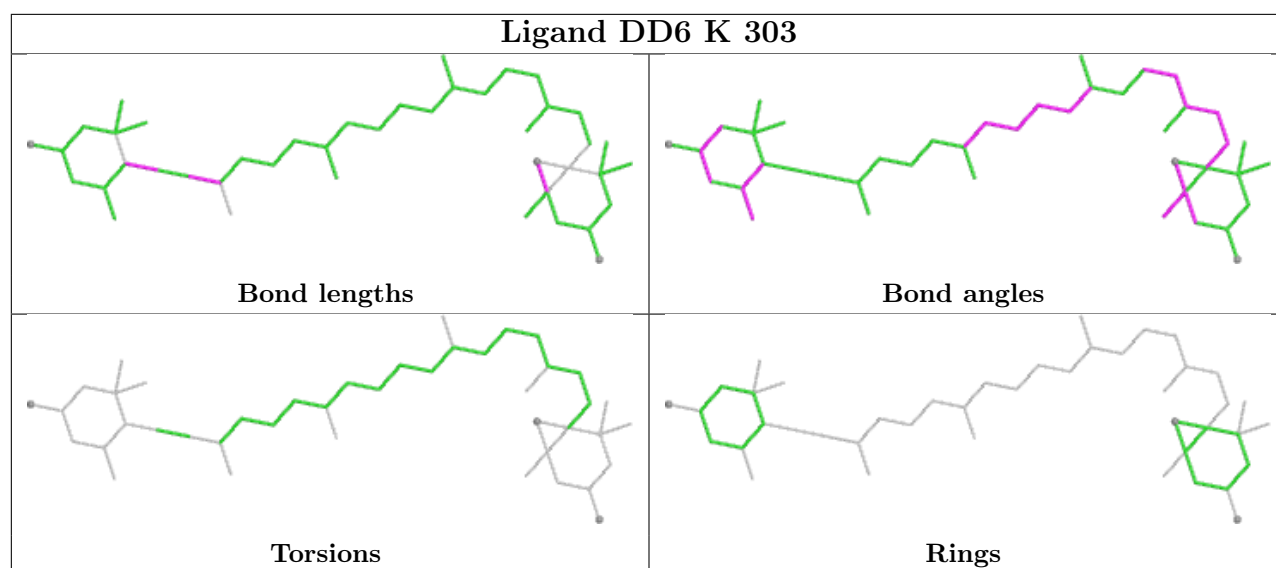
Bond angles



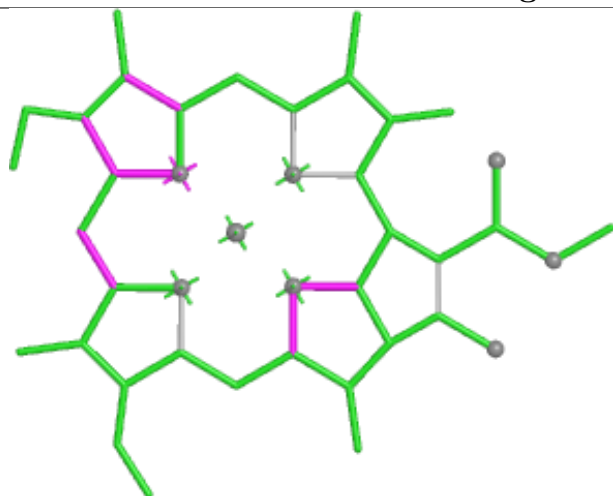
Torsions



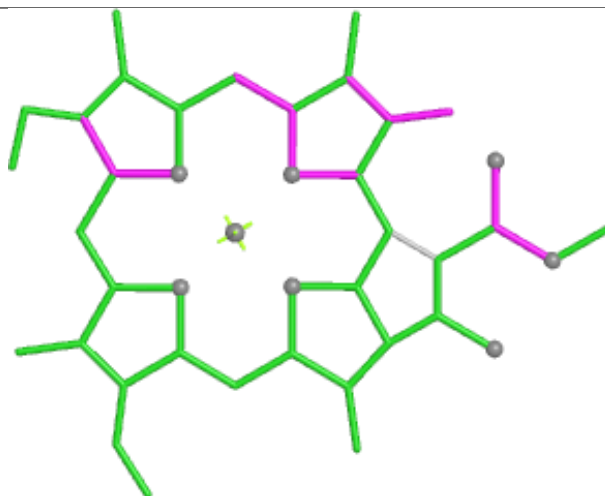
Rings



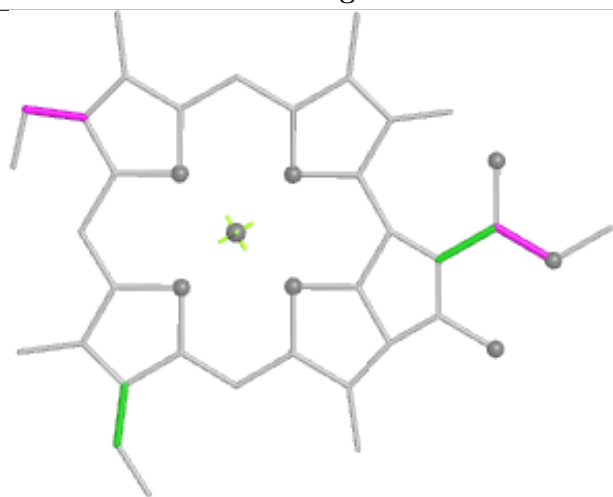
Ligand CLA z 306



Bond lengths



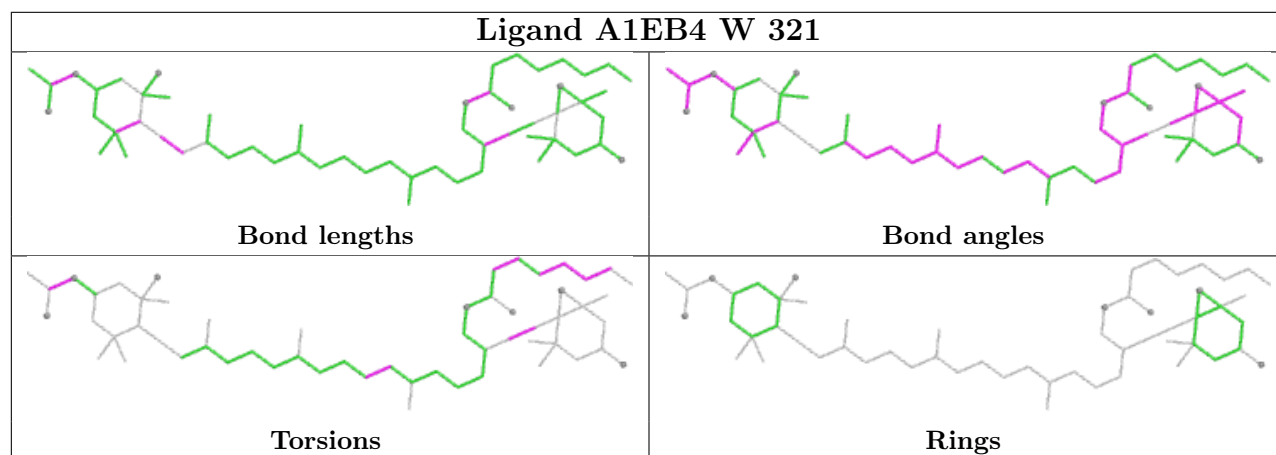
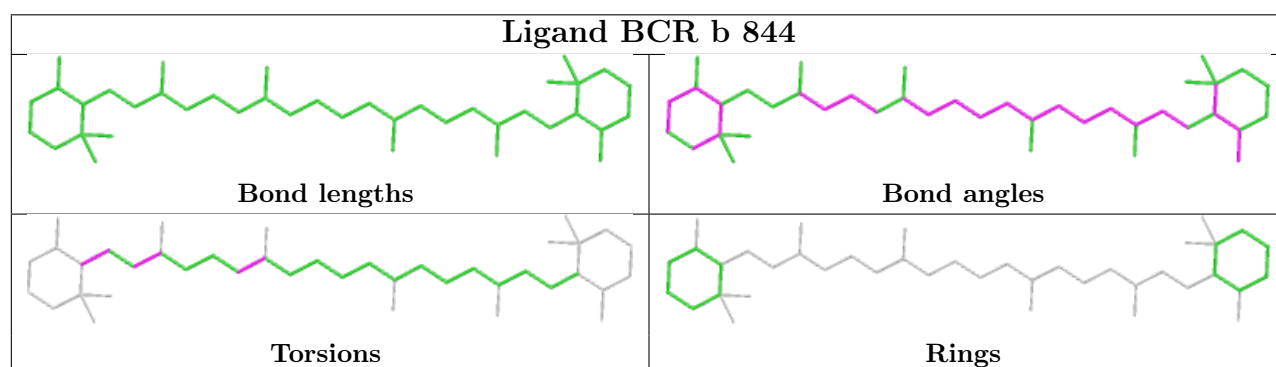
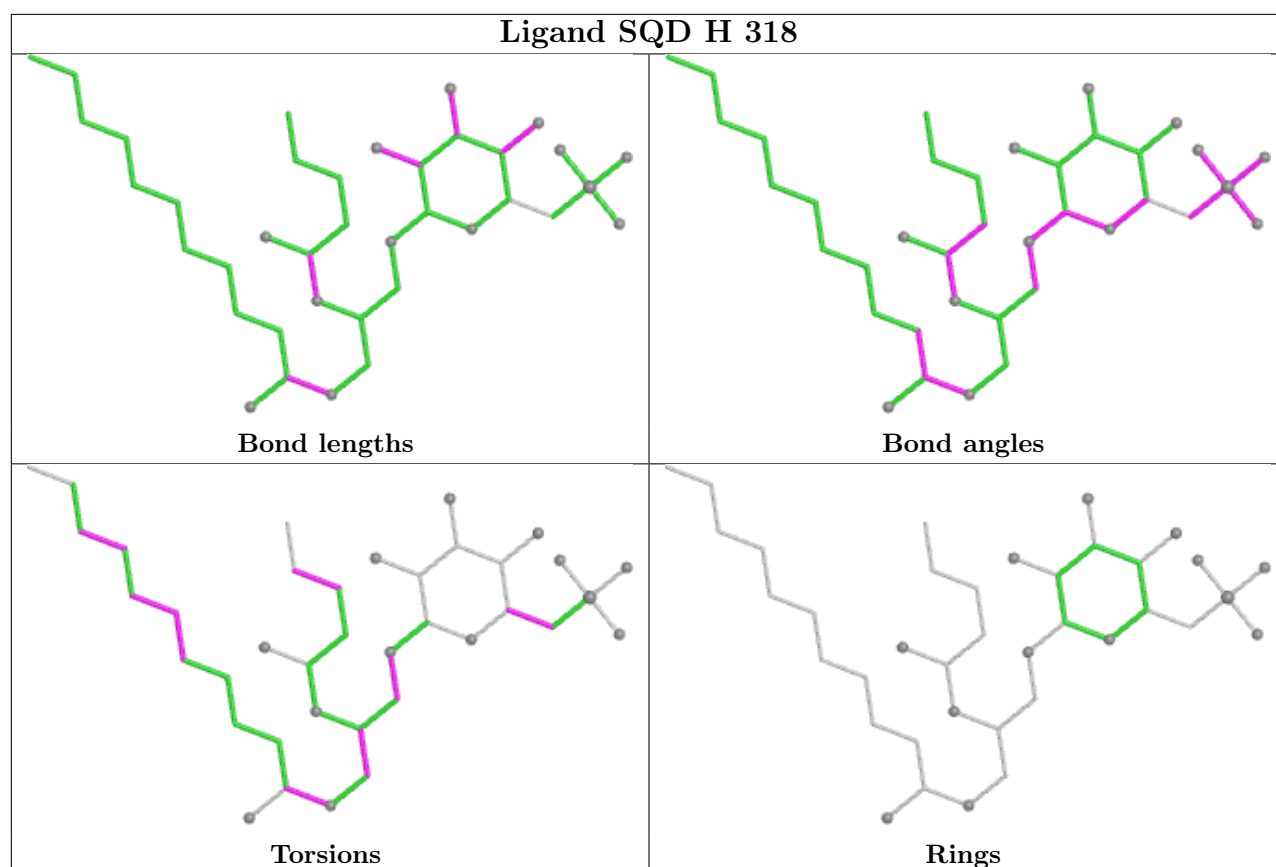
Bond angles

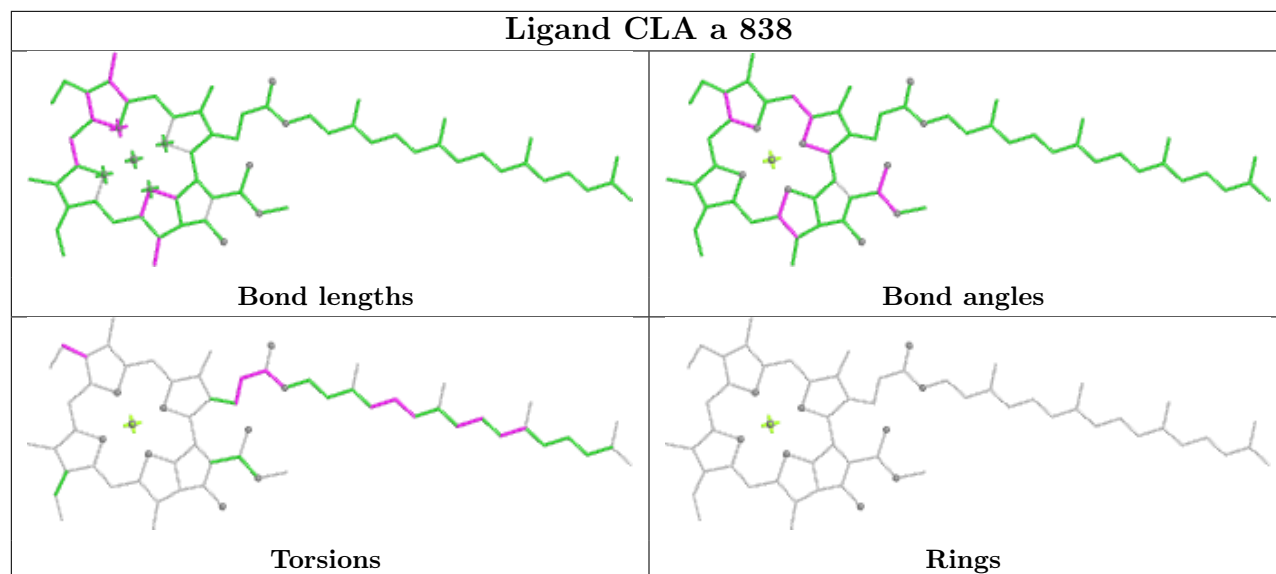
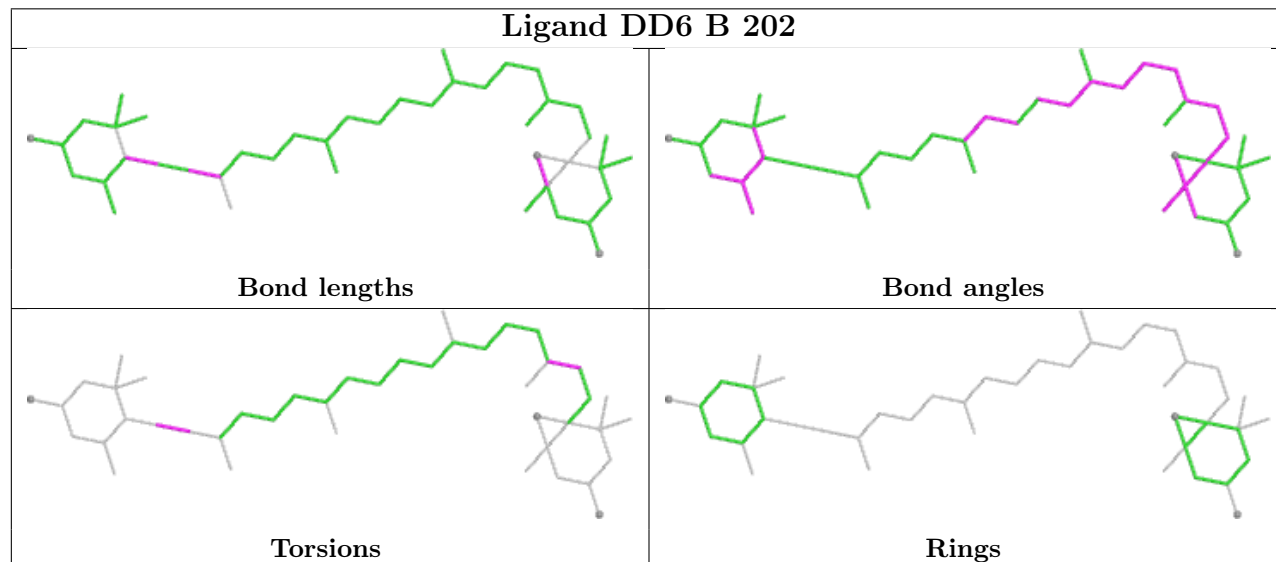


Torsions

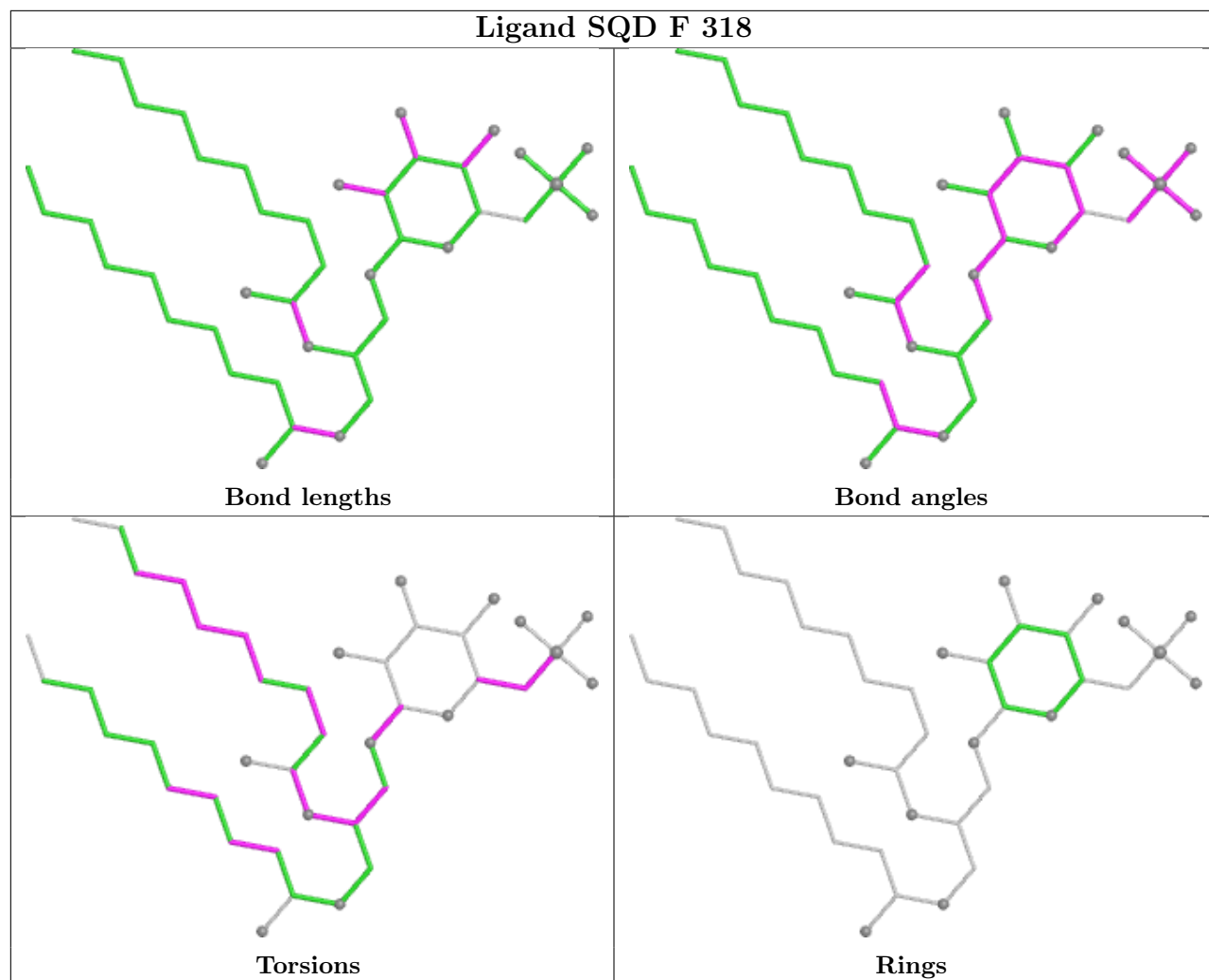


Rings

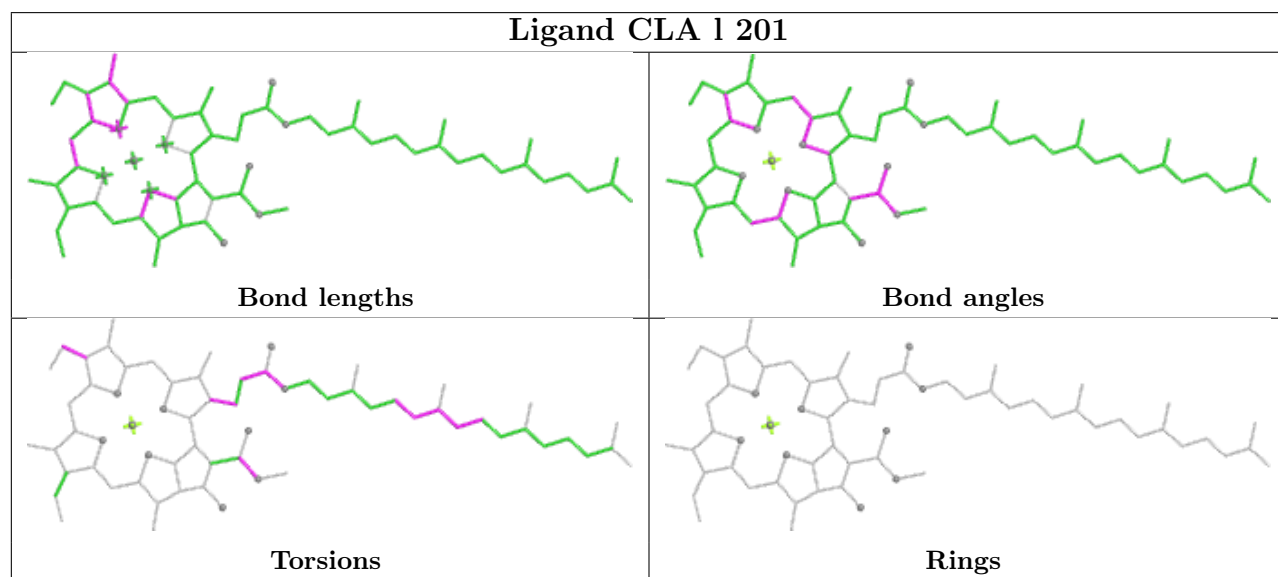


Ligand CLA a 838**Ligand DD6 B 202**

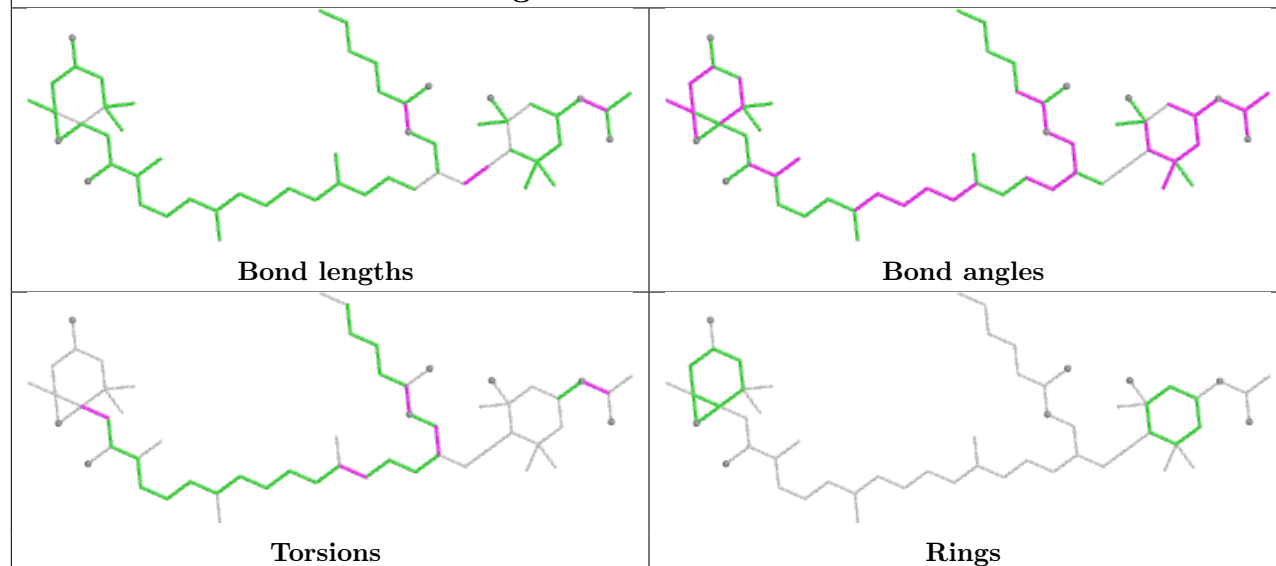
Ligand SQD F 318



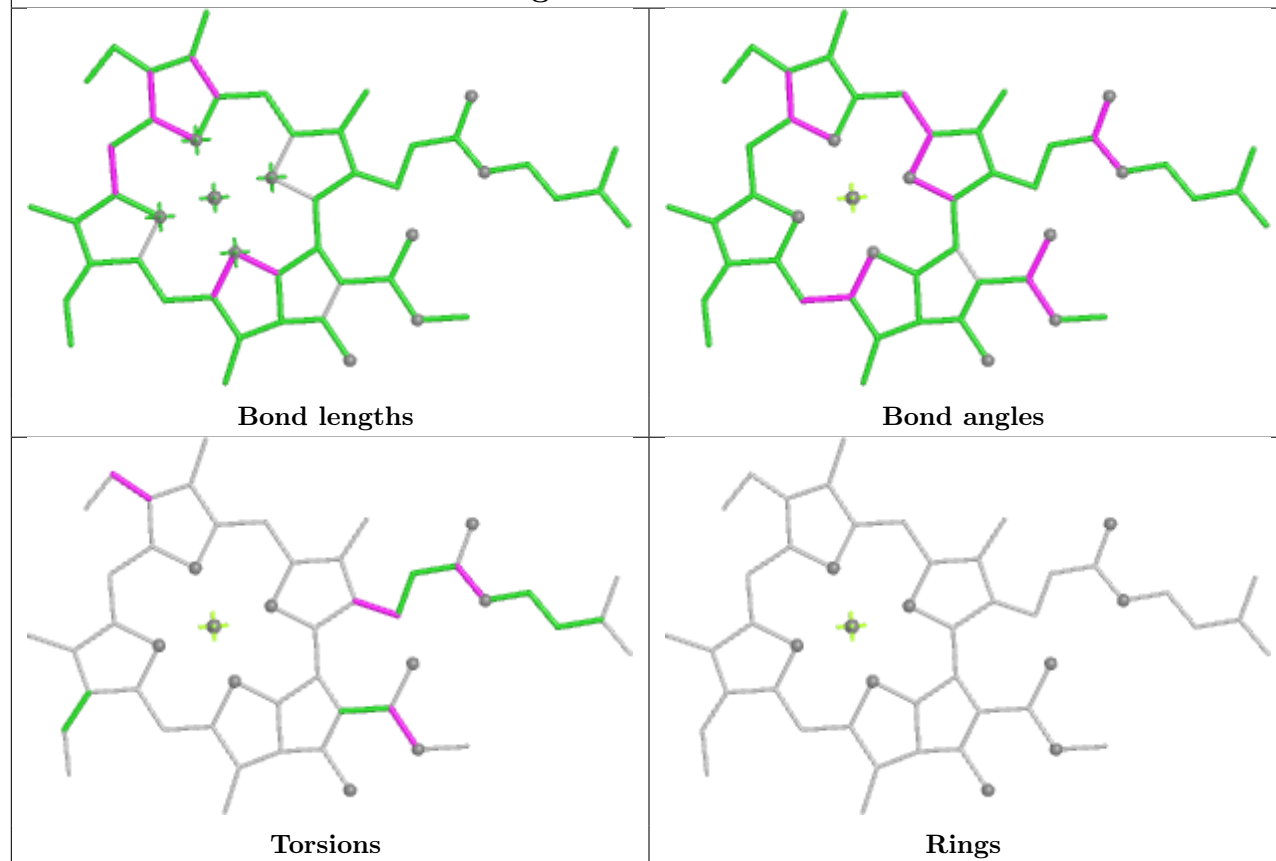
Ligand CLA 1 201

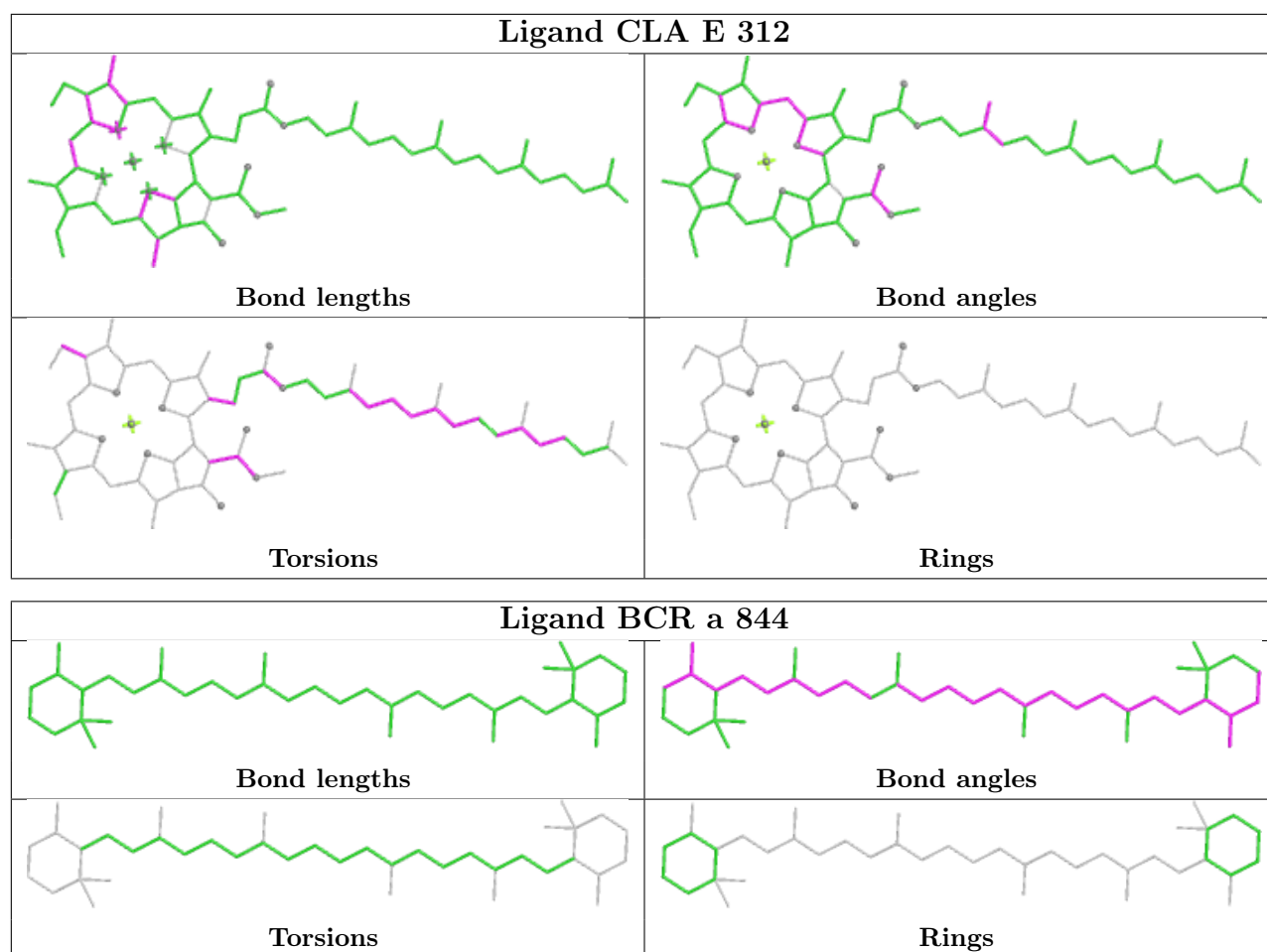


Ligand A1EB1 U 203

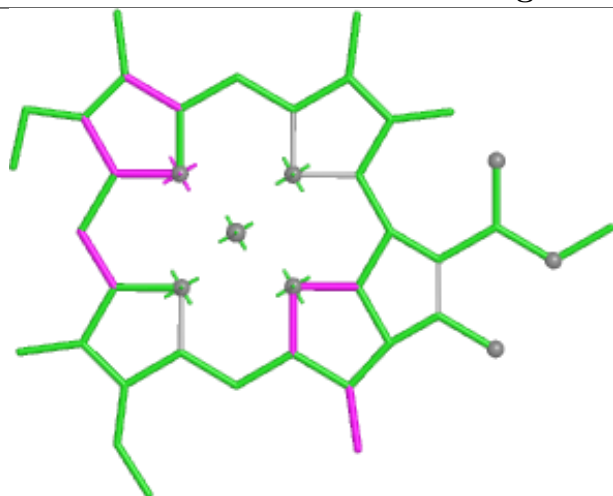


Ligand CLA A 315

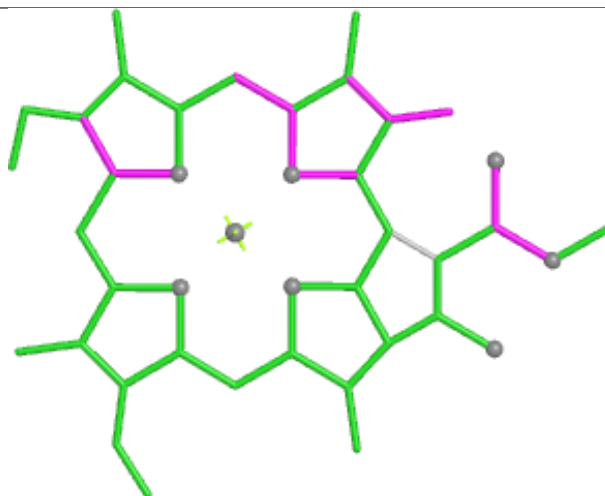




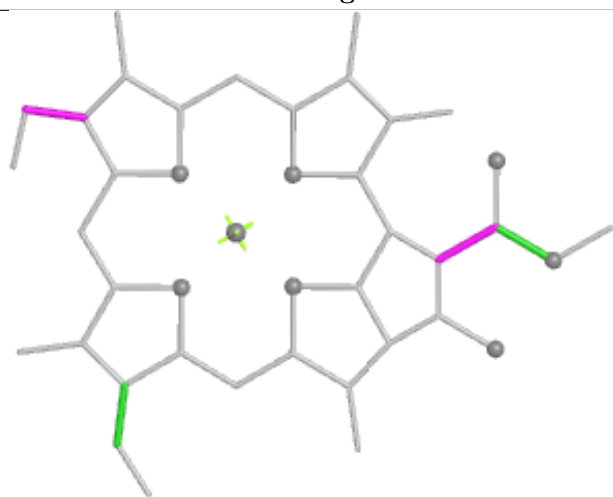
Ligand CLA Z 304



Bond lengths



Bond angles

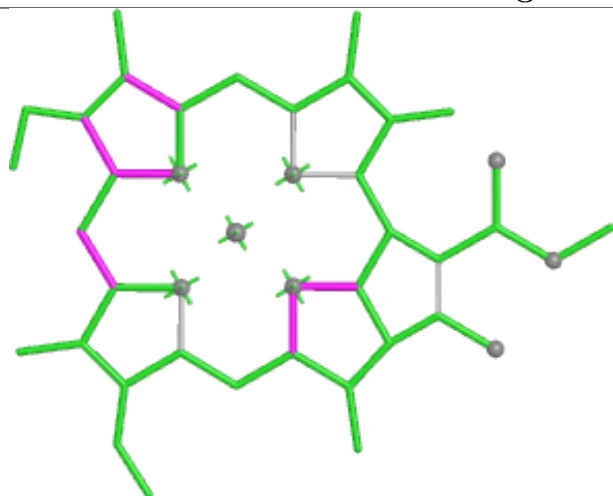


Torsions

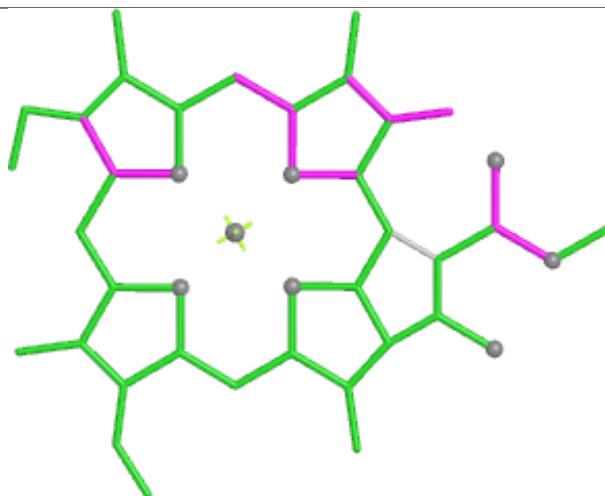


Rings

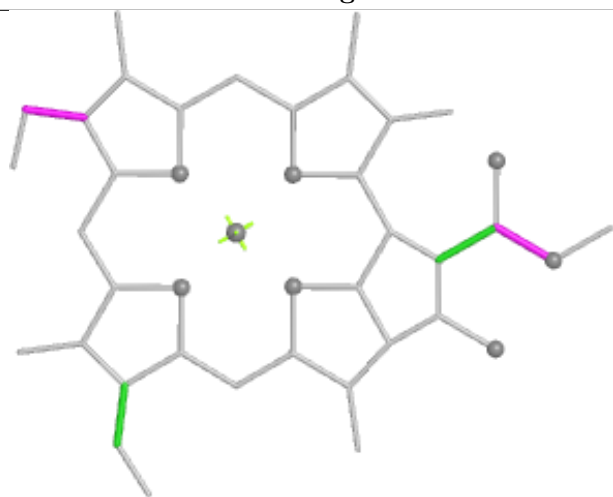
Ligand CLA Z 312



Bond lengths



Bond angles

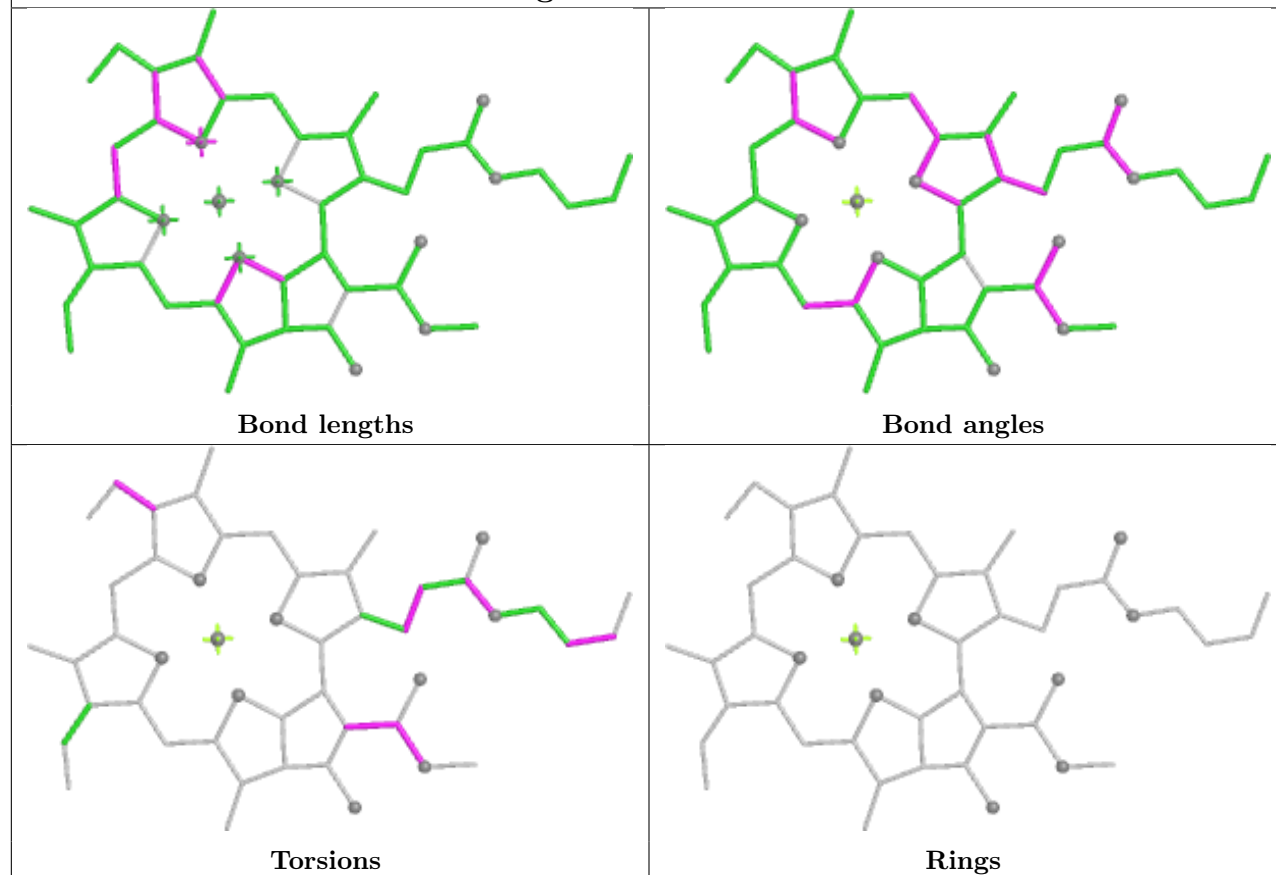


Torsions

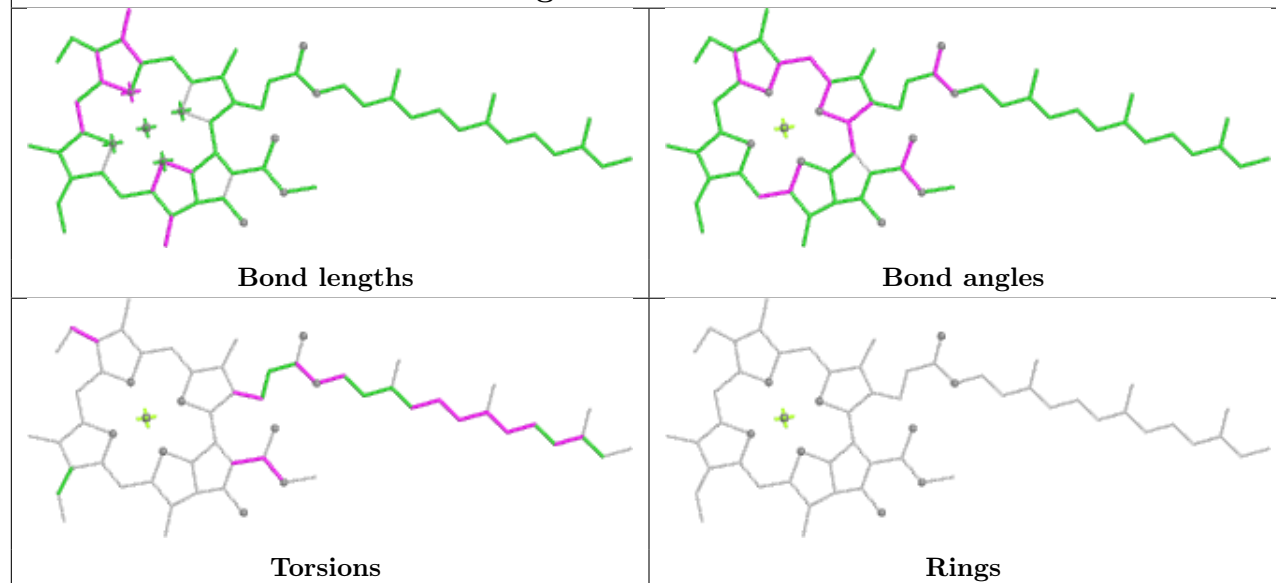


Rings

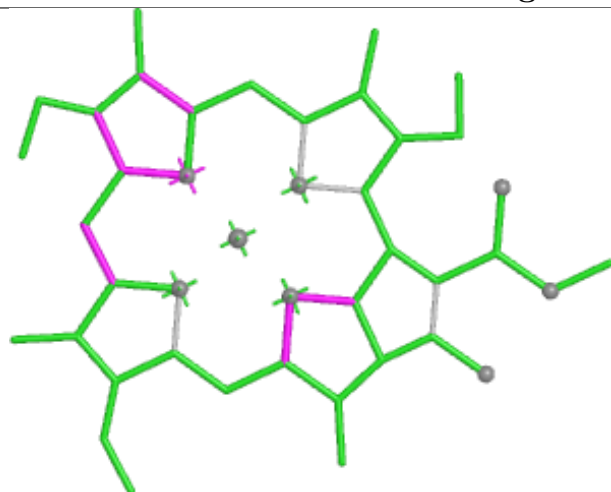
Ligand CLA a 819



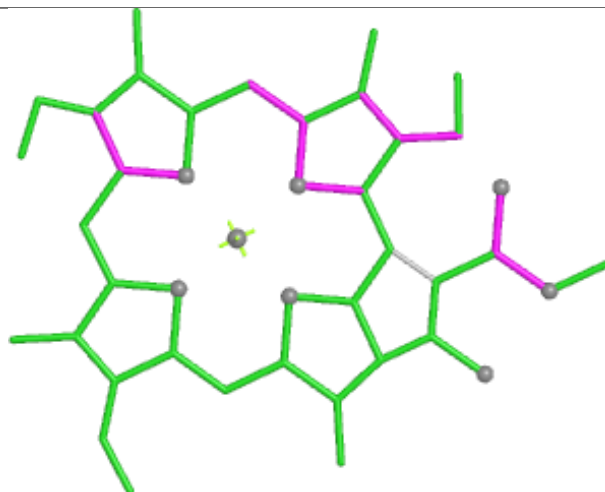
Ligand CLA 4 311



Ligand CLA 6 310



Bond lengths



Bond angles

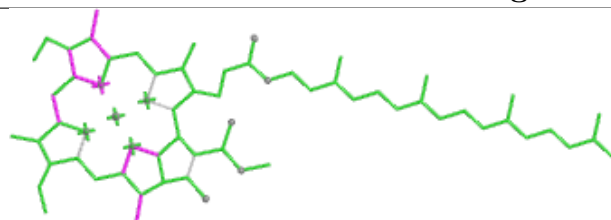


Torsions

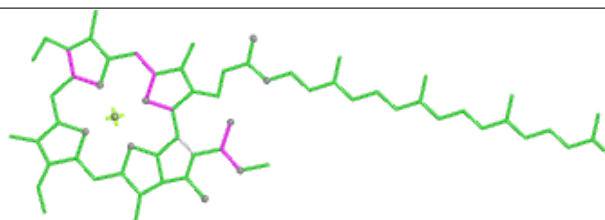


Rings

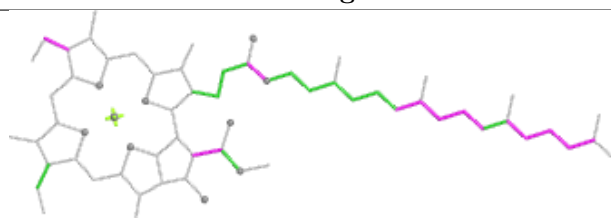
Ligand CLA M 312



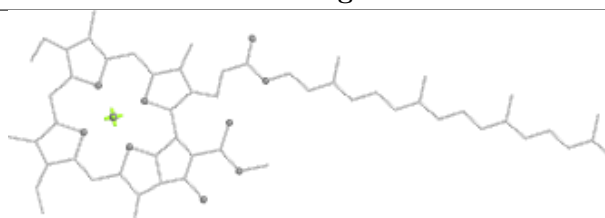
Bond lengths



Bond angles

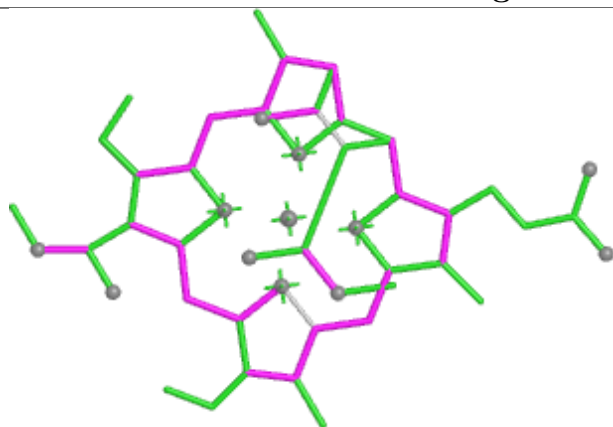


Torsions

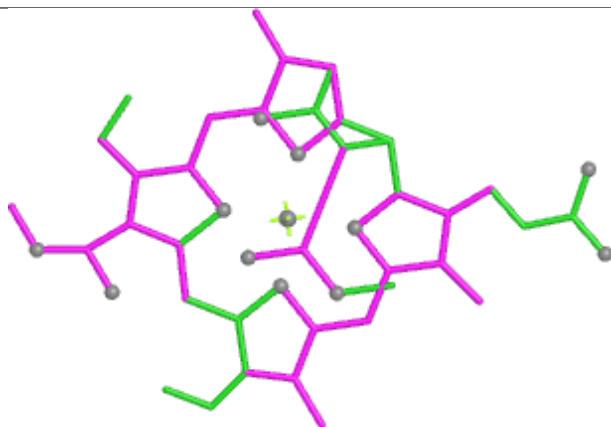


Rings

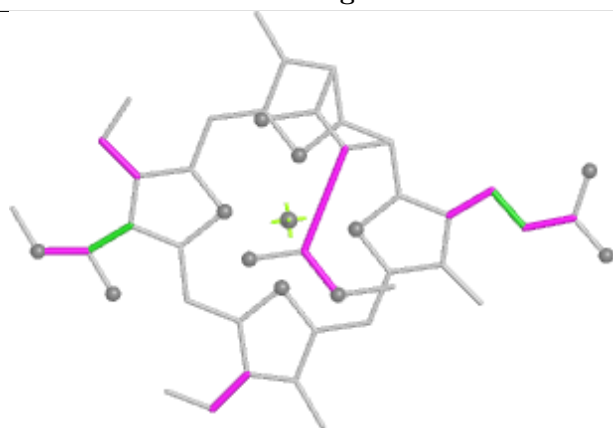
Ligand A1ECV Z 308



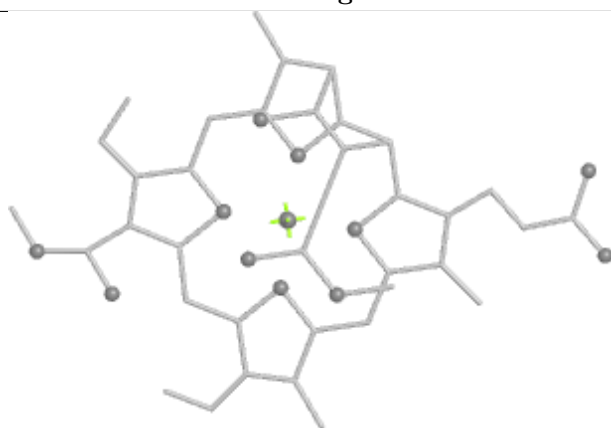
Bond lengths



Bond angles

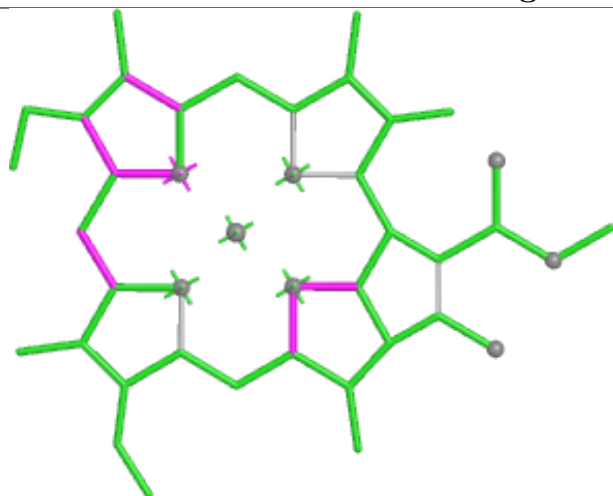


Torsions

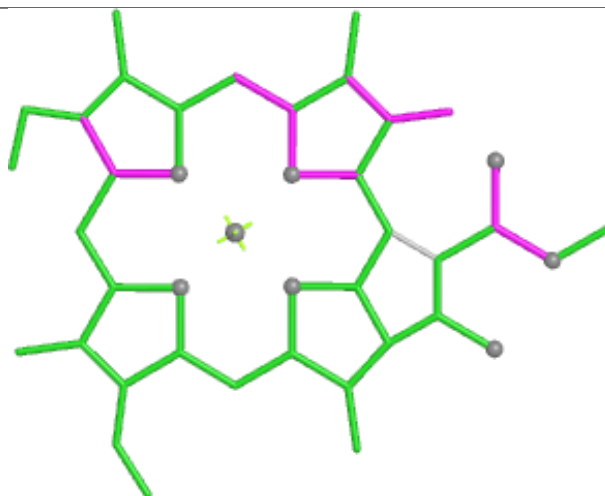


Rings

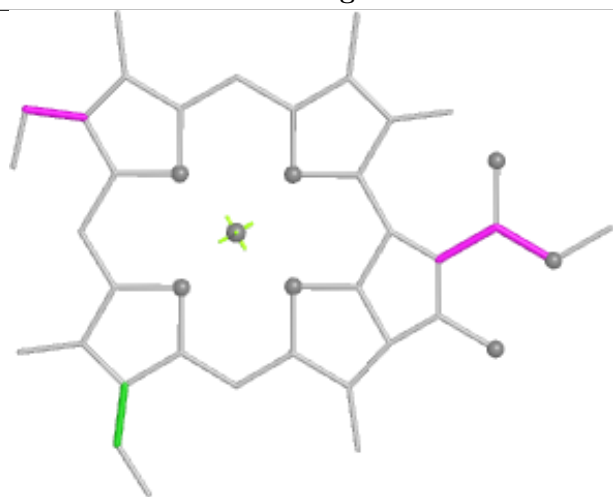
Ligand CLA z 311



Bond lengths



Bond angles

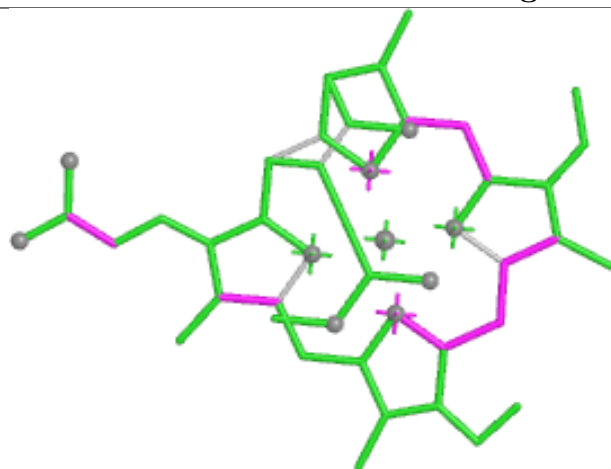


Torsions

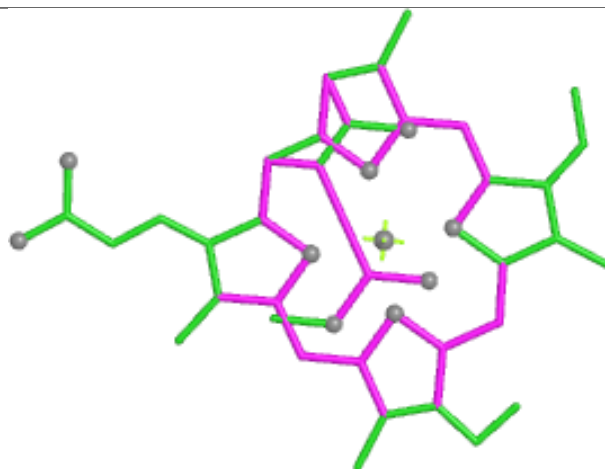


Rings

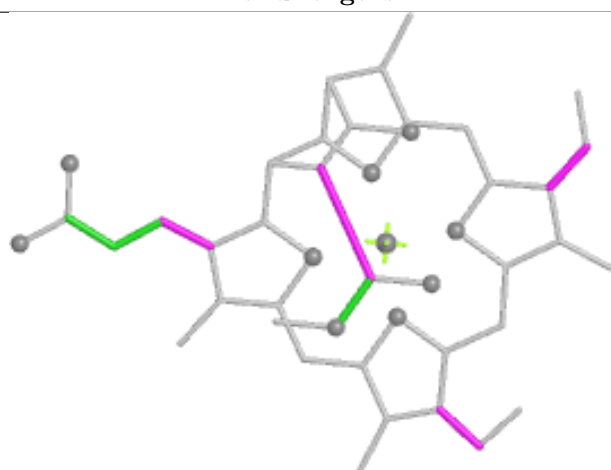
Ligand KC2 7 319



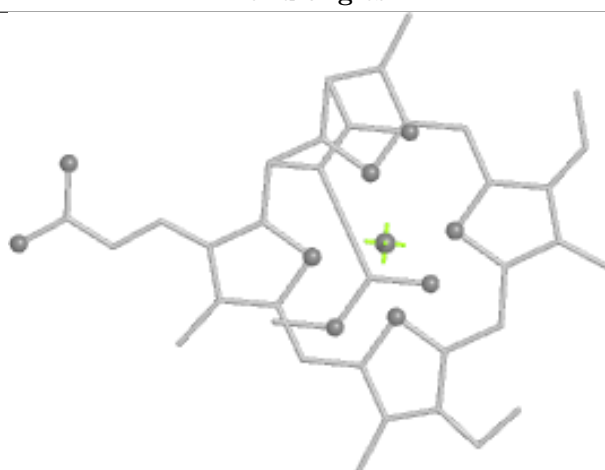
Bond lengths



Bond angles

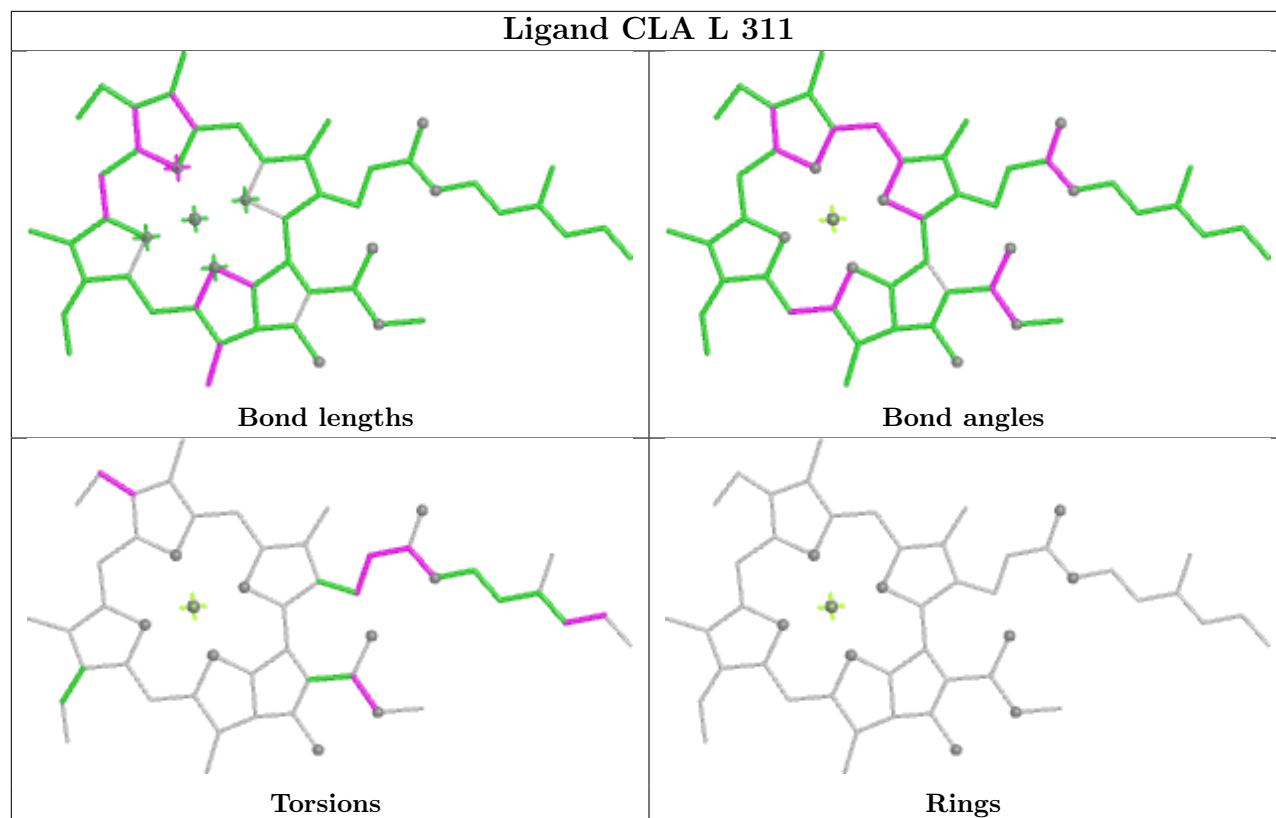


Torsions

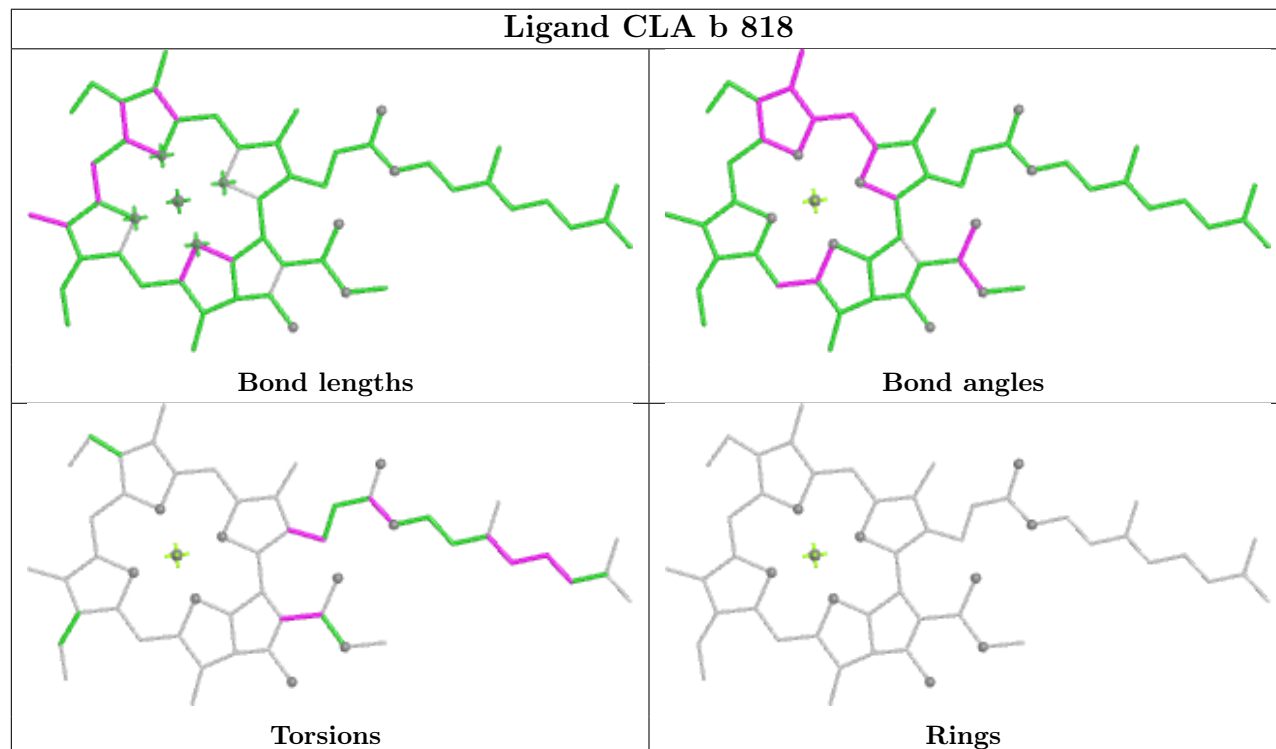


Rings

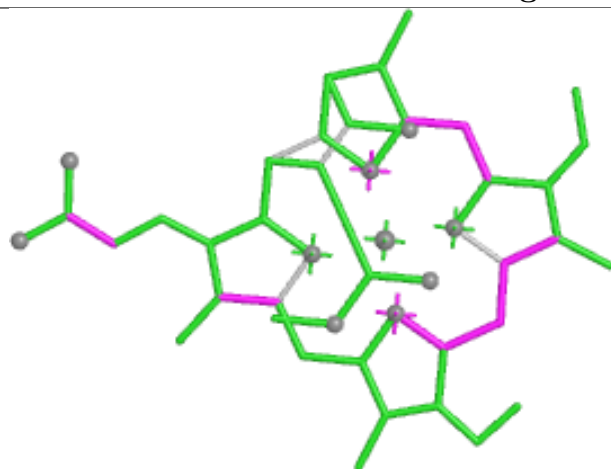
Ligand CLA L 311



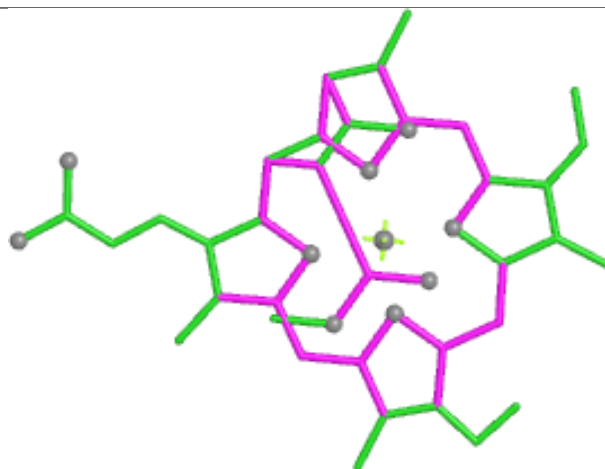
Ligand CLA b 818



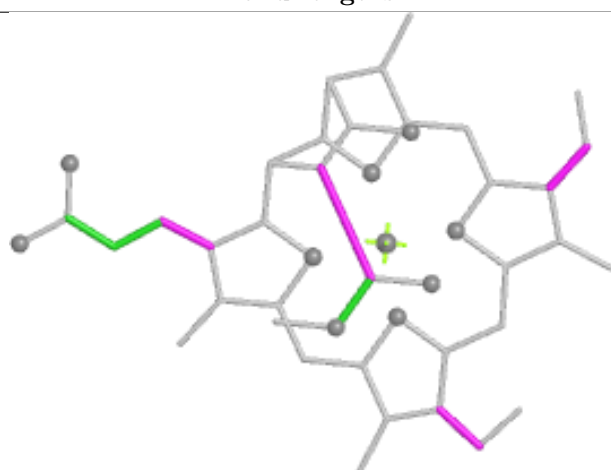
Ligand KC2 x 312



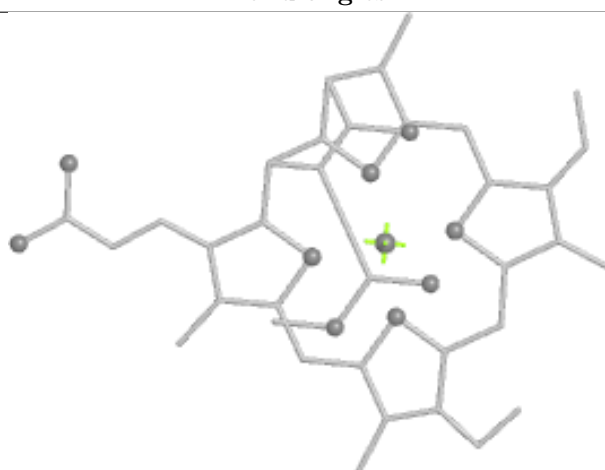
Bond lengths



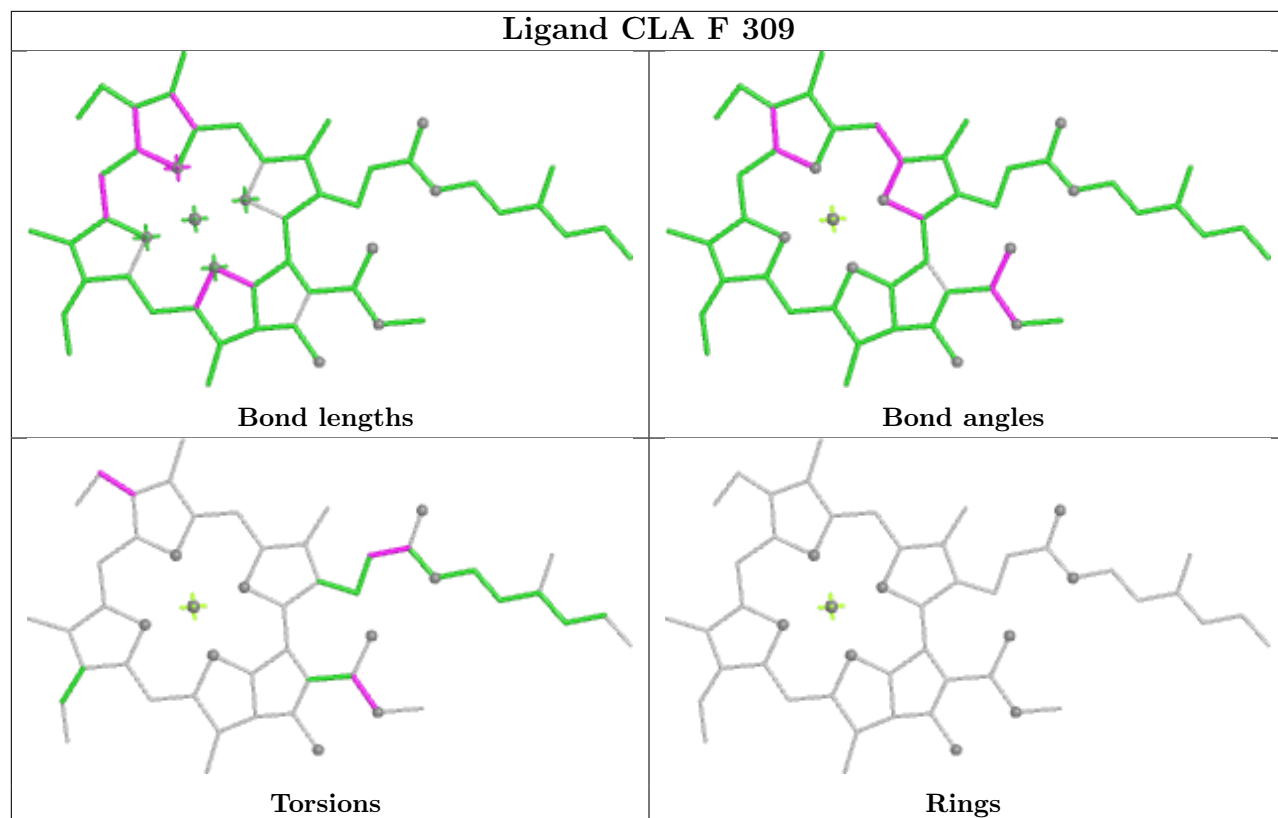
Bond angles



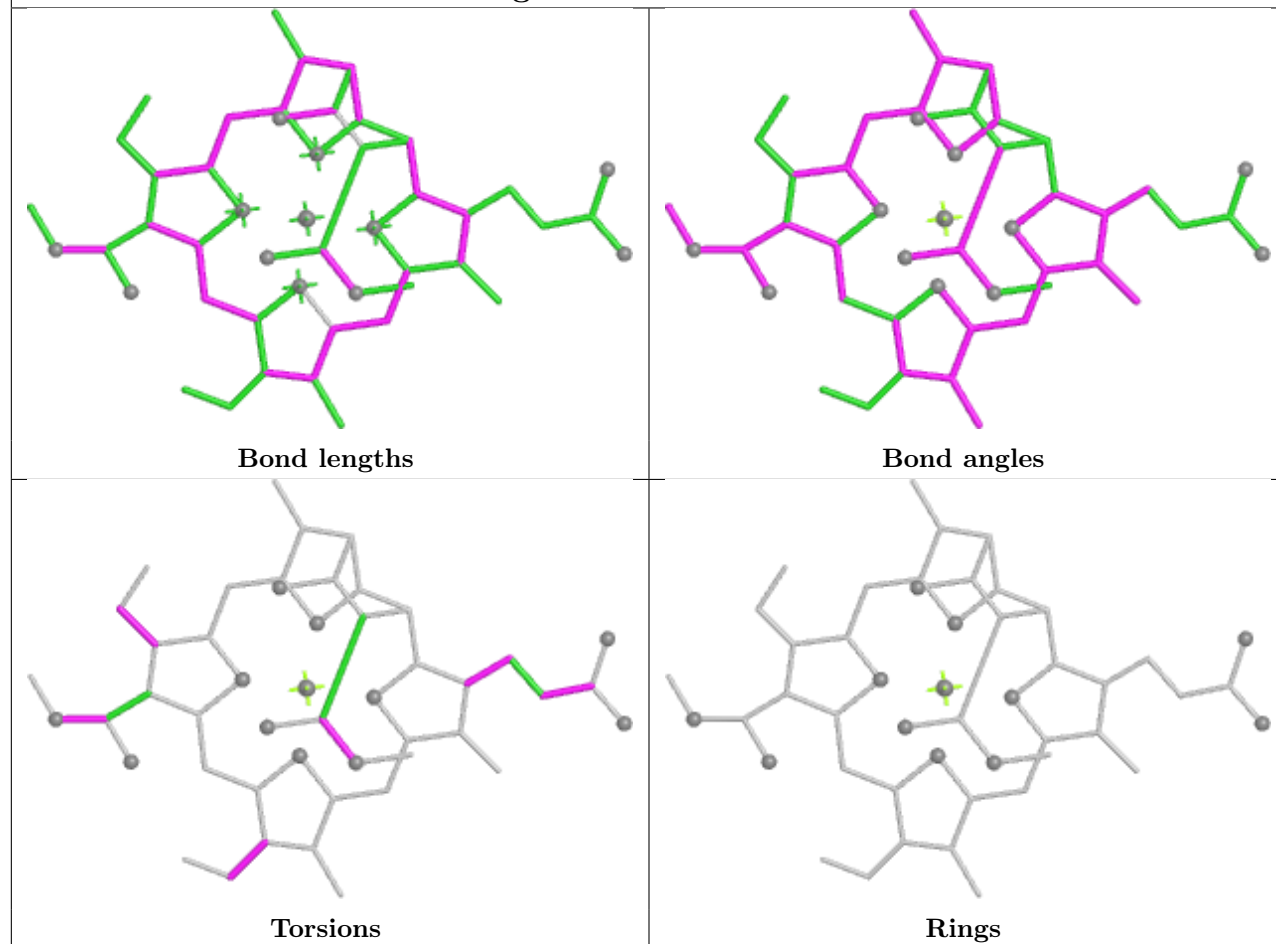
Torsions



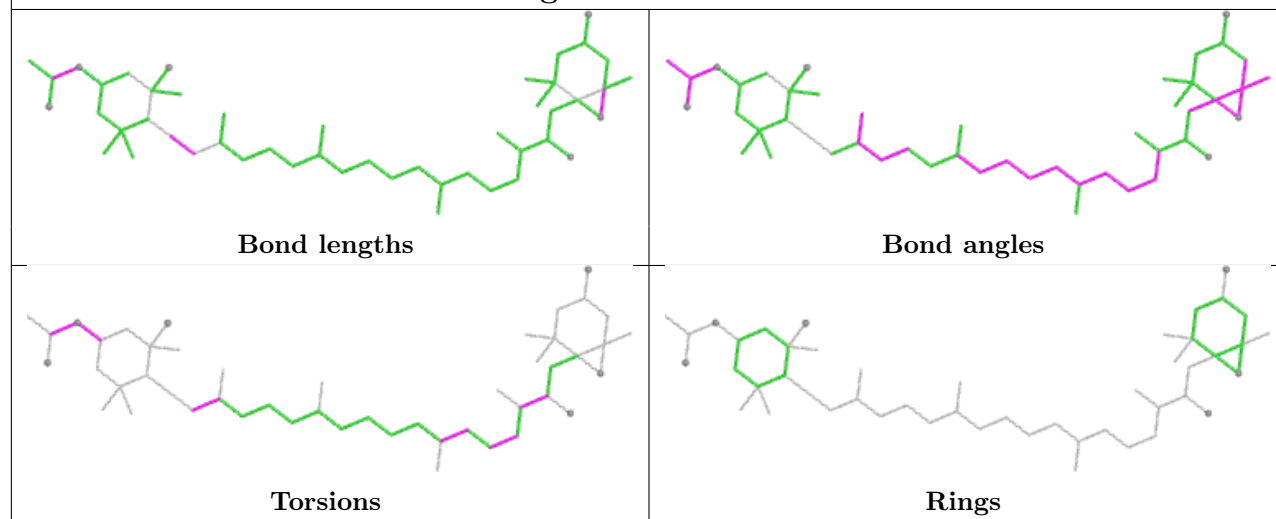
Rings



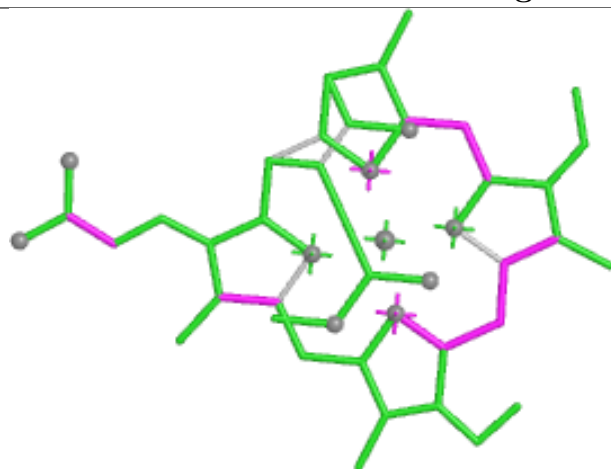
Ligand A1ECV 6 320



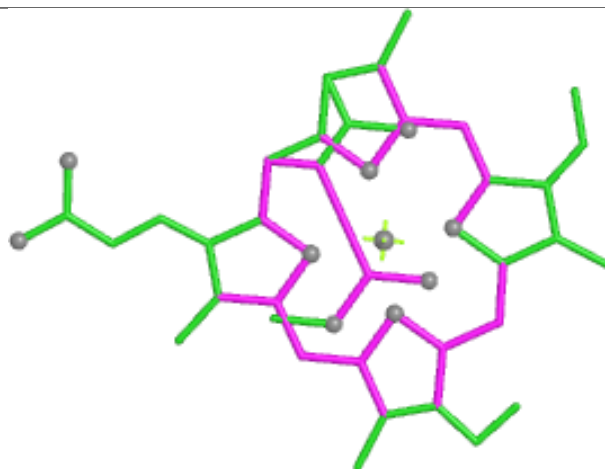
Ligand A86 L 306



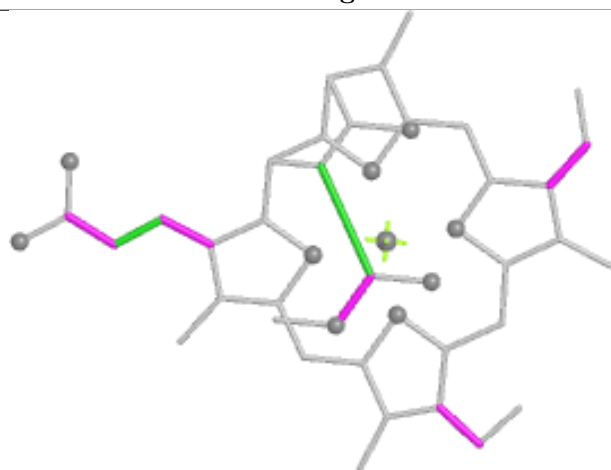
Ligand KC2 G 311



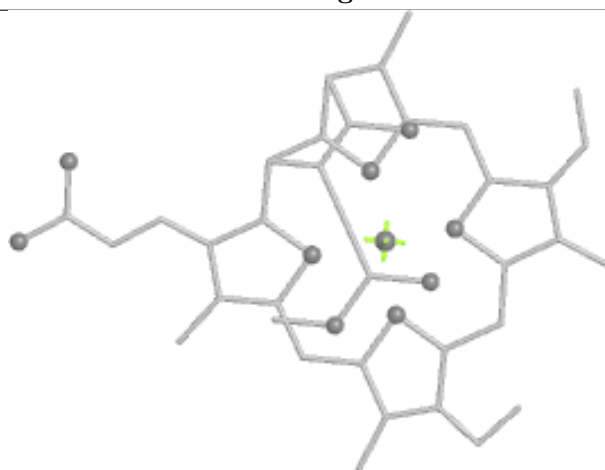
Bond lengths



Bond angles

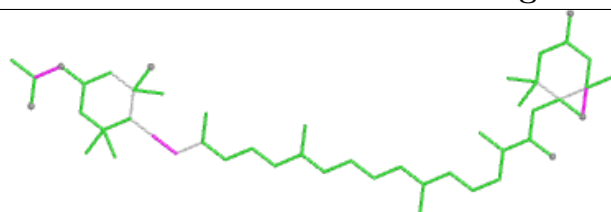


Torsions

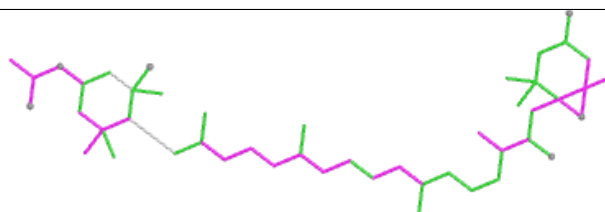


Rings

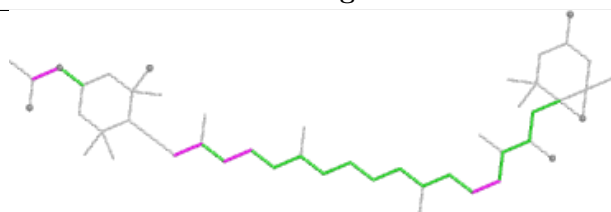
Ligand A86 Y 301



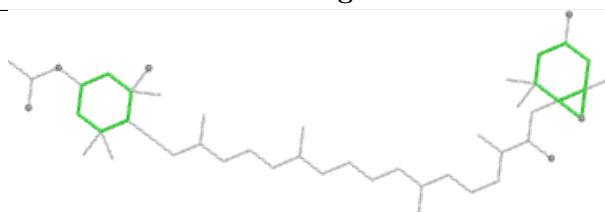
Bond lengths



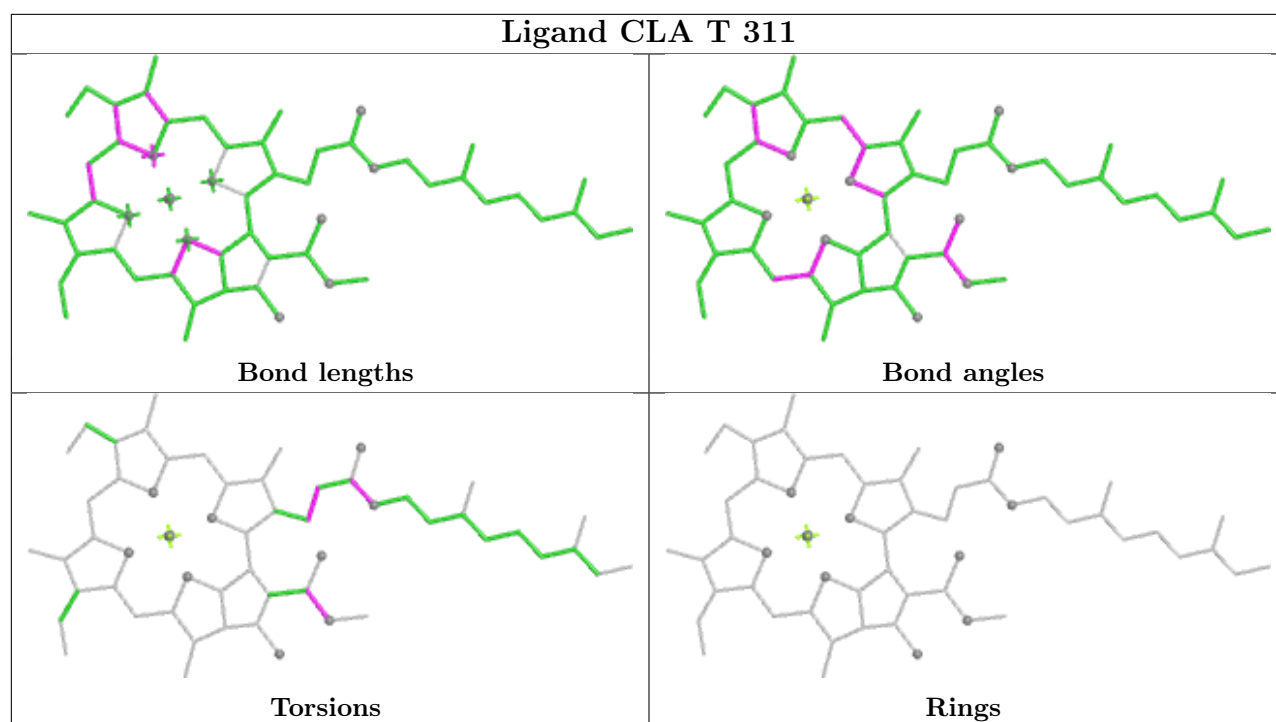
Bond angles



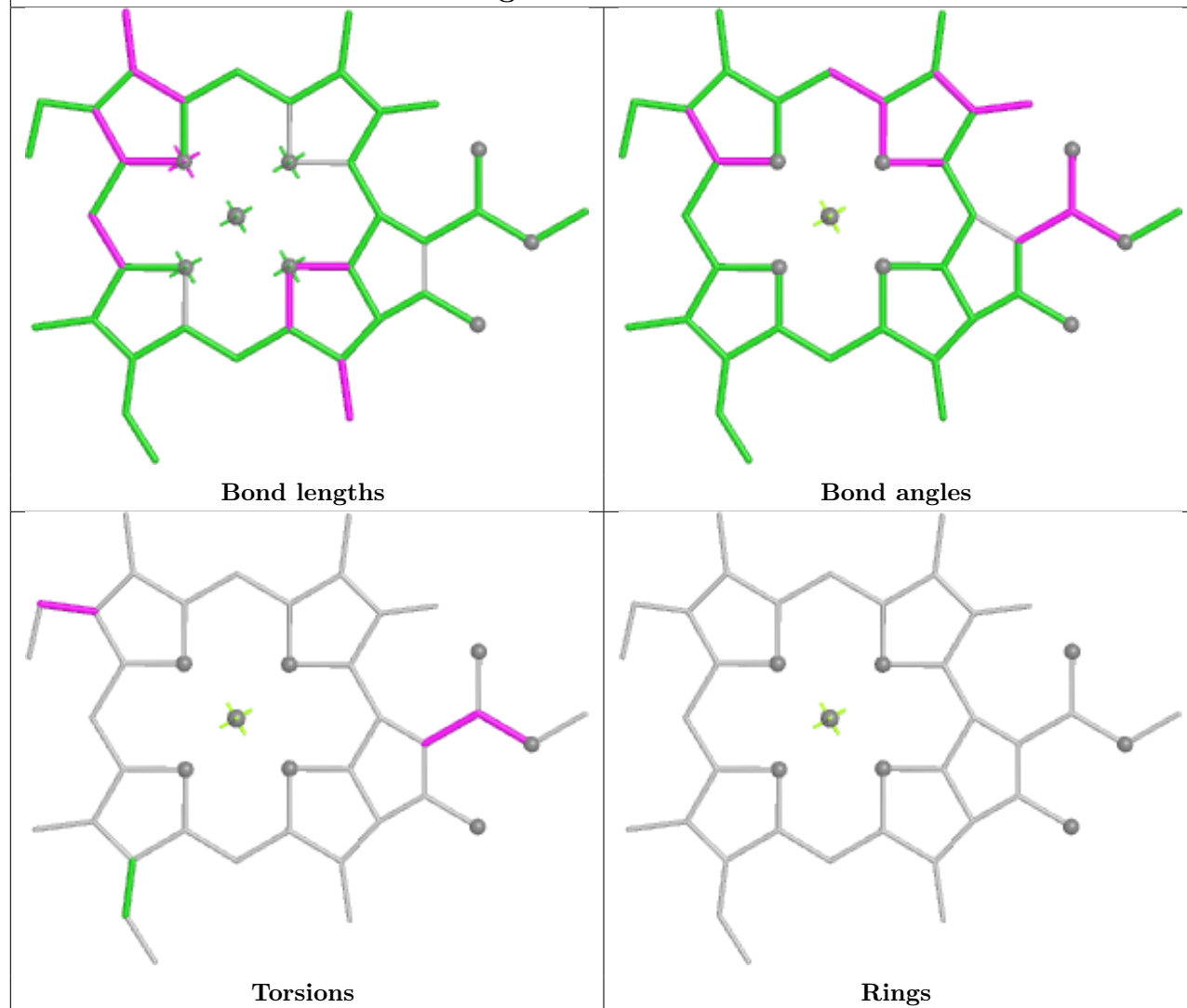
Torsions



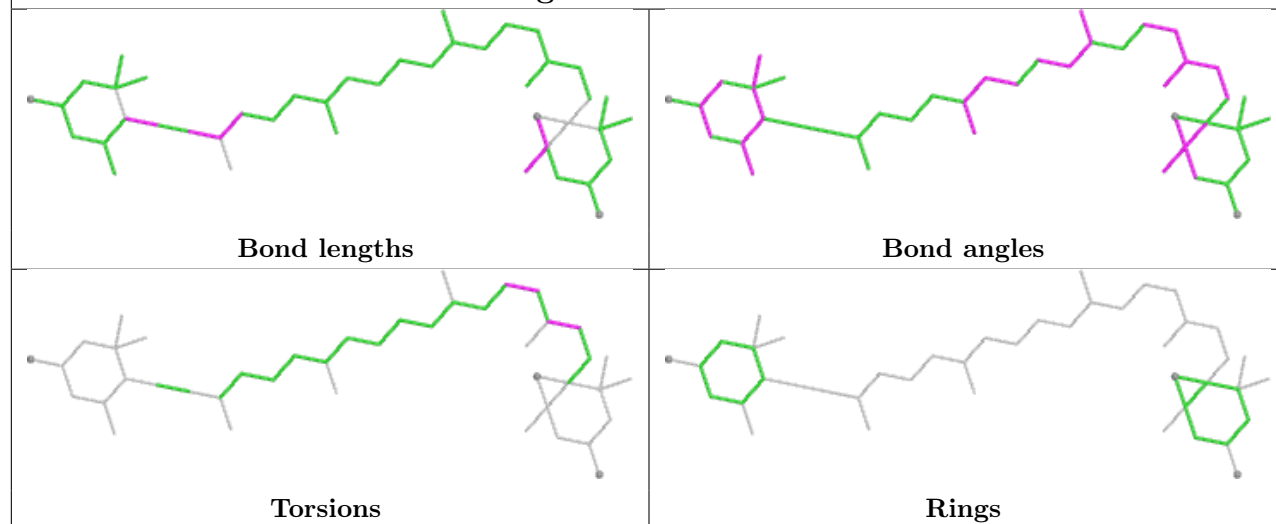
Rings



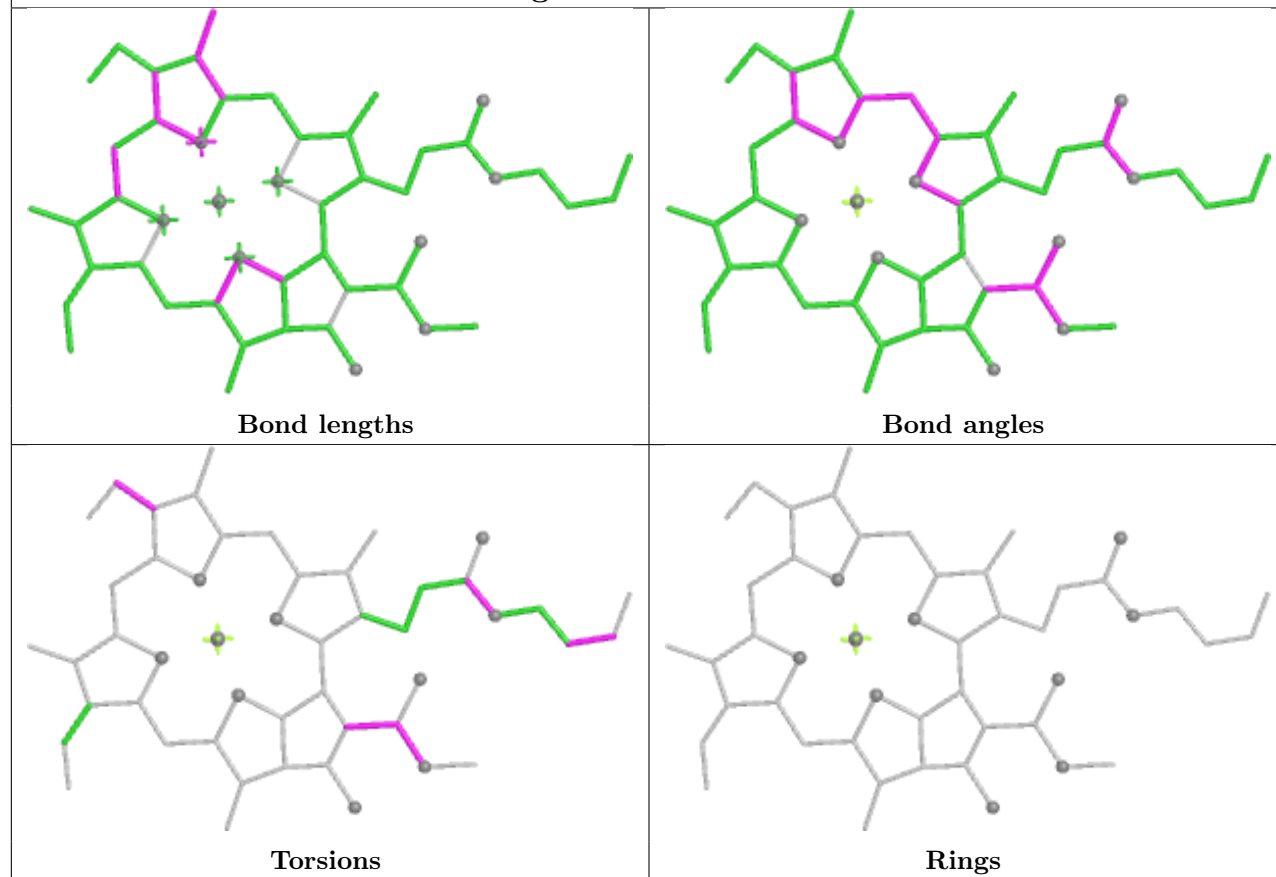
Ligand CLA 2 312

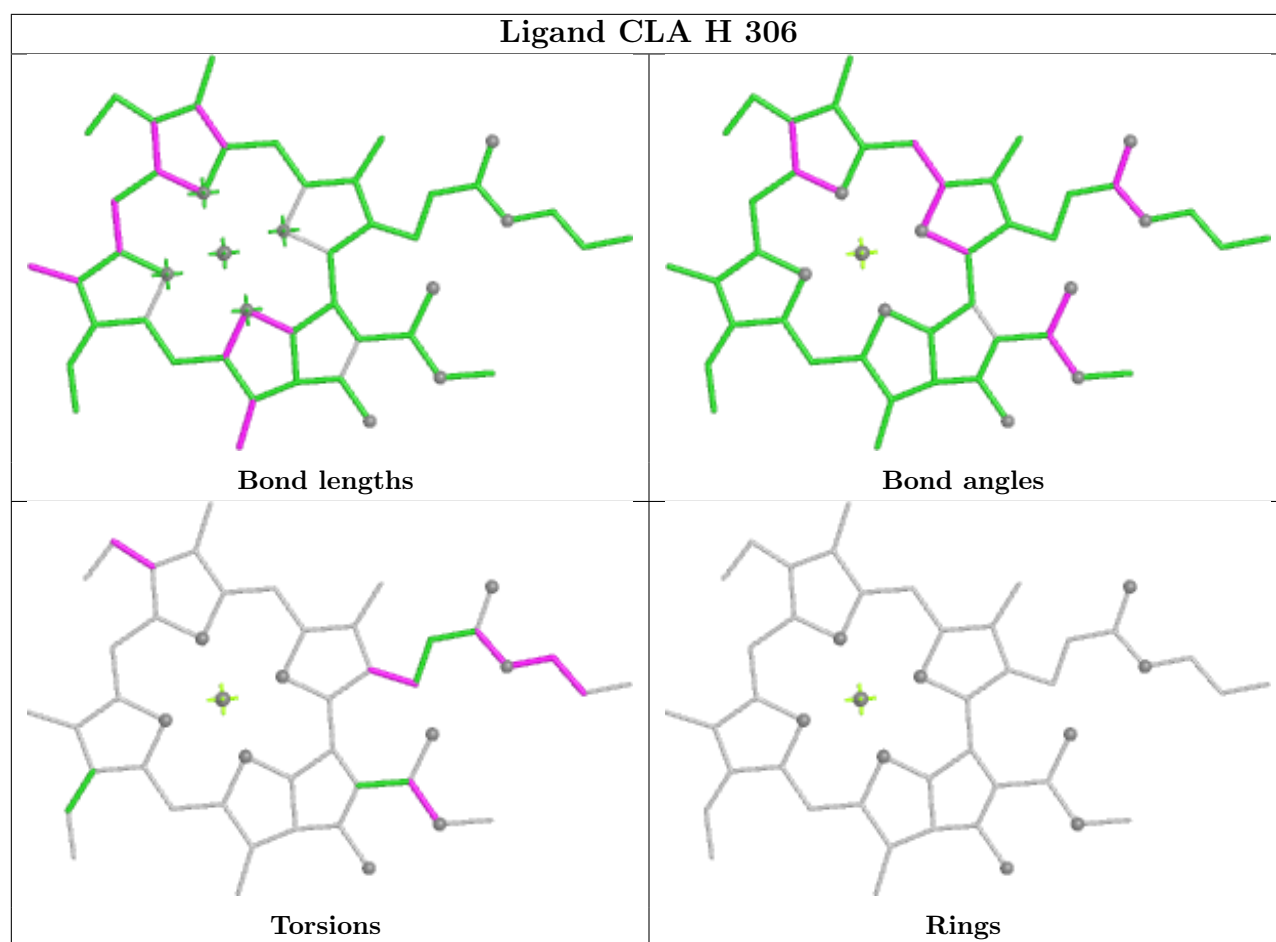


Ligand DD6 J 304

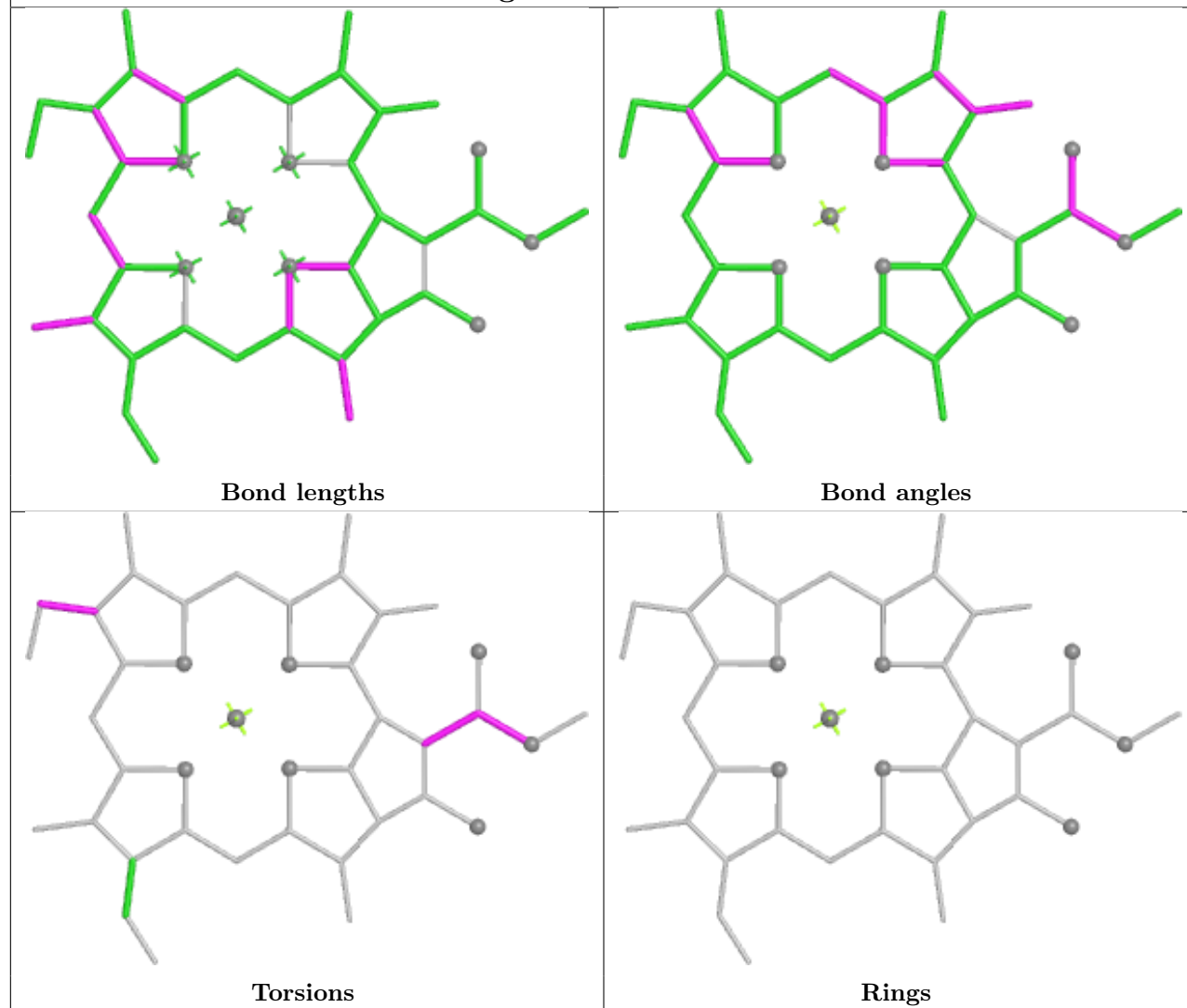


Ligand CLA D 309

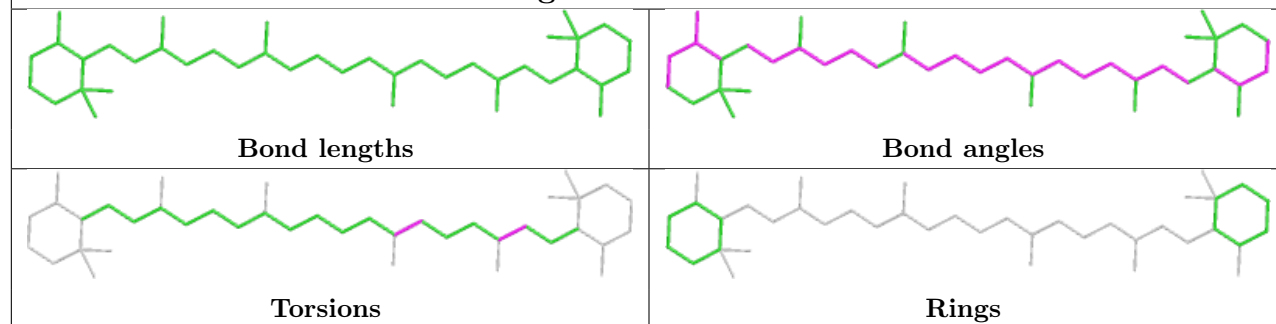


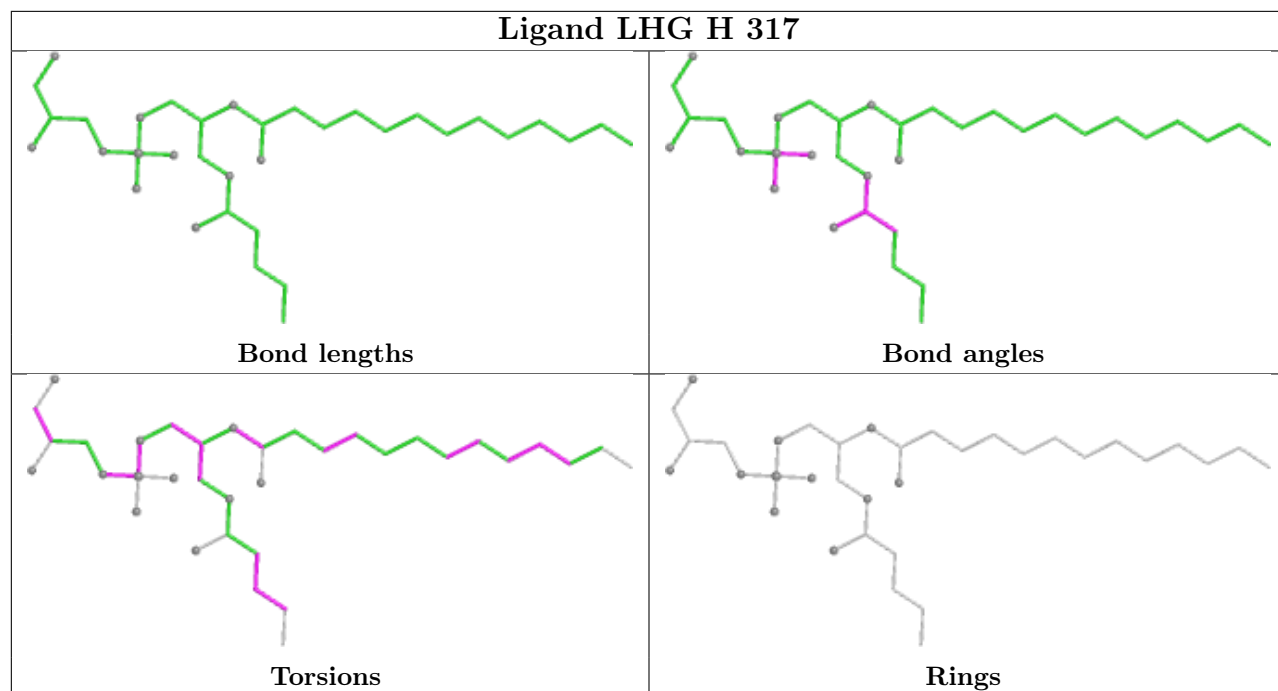


Ligand CLA 2 315

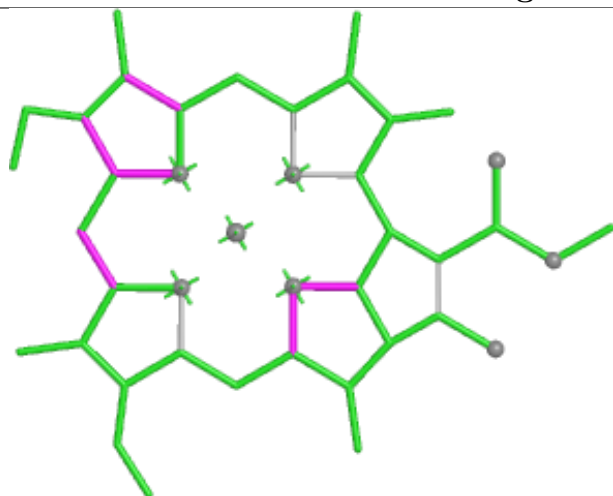


Ligand BCR f 801

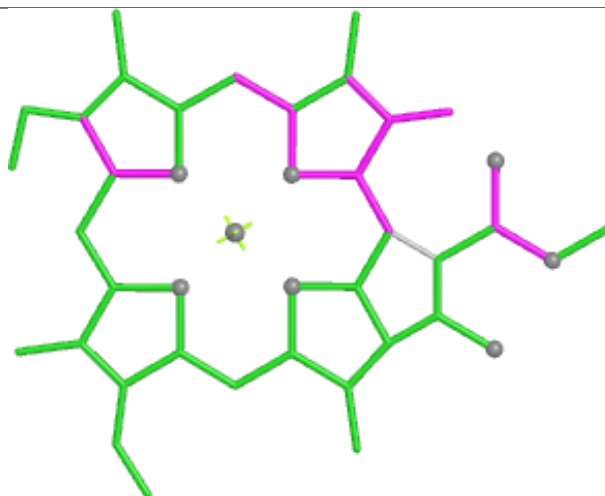




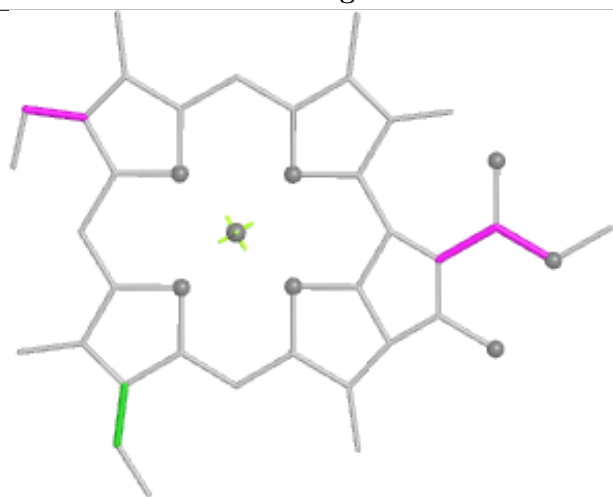
Ligand CLA Z 316



Bond lengths



Bond angles

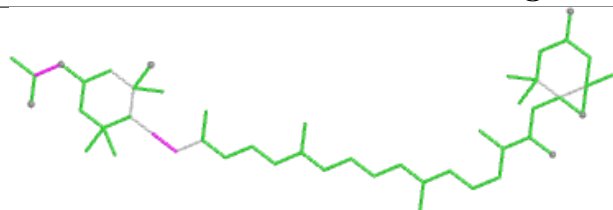


Torsions

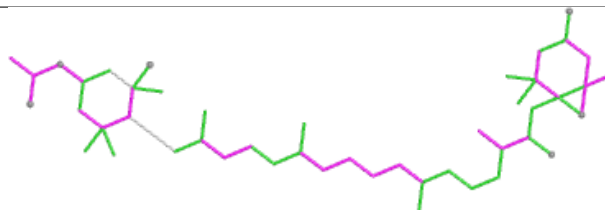


Rings

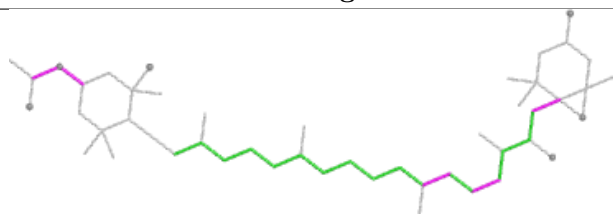
Ligand A86 9 306



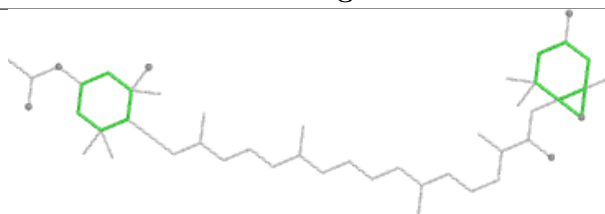
Bond lengths



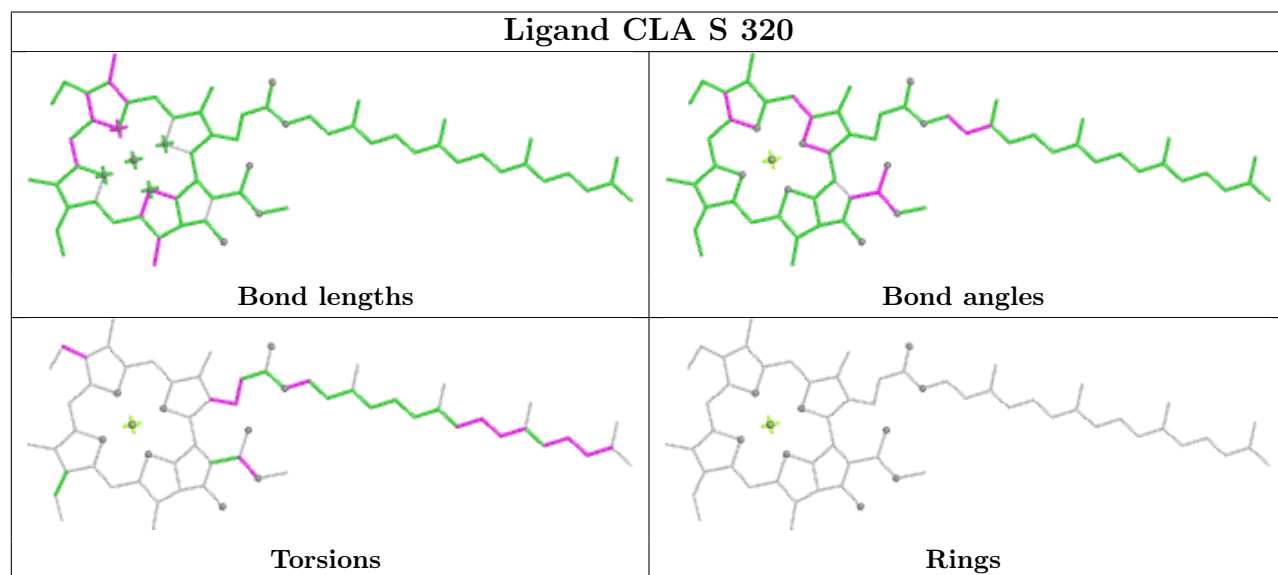
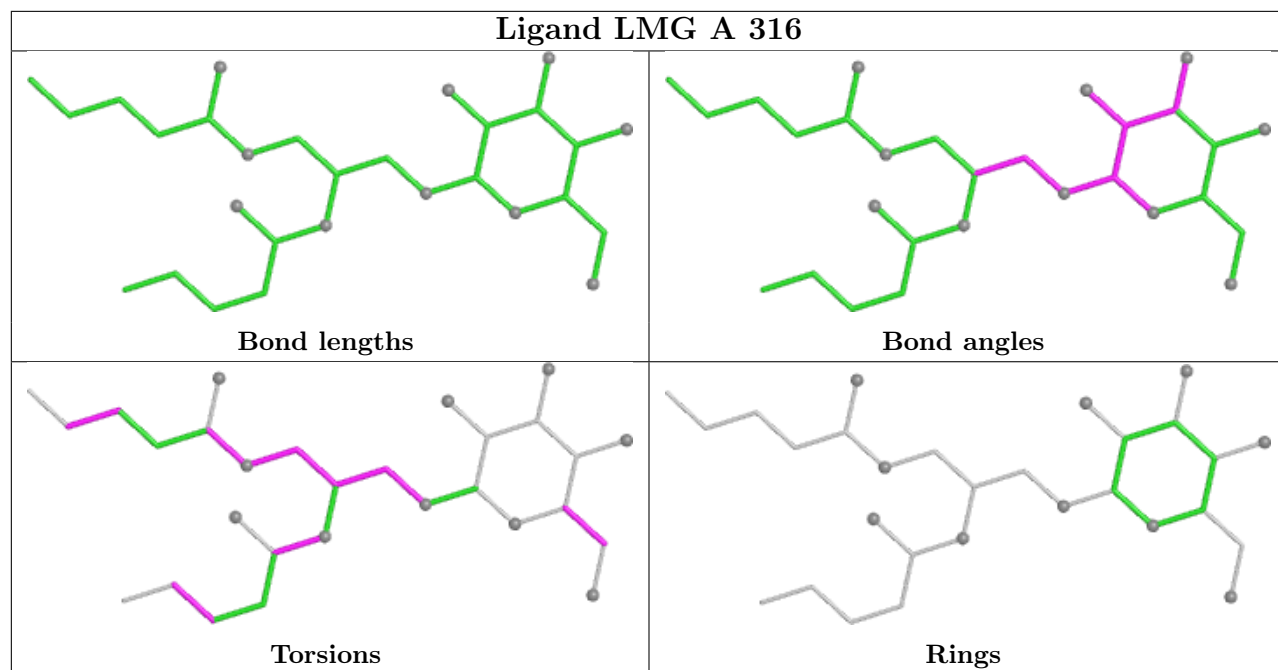
Bond angles

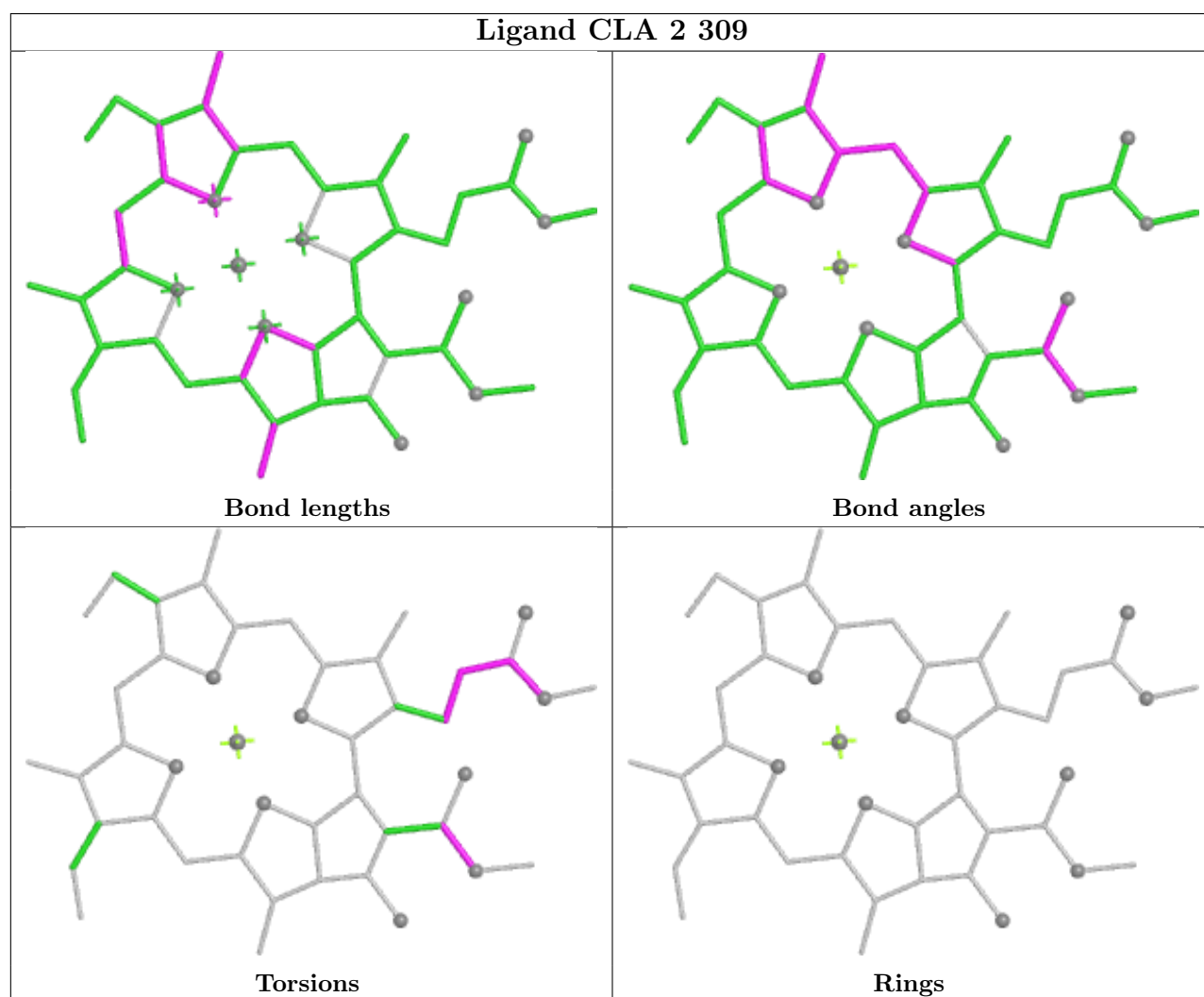
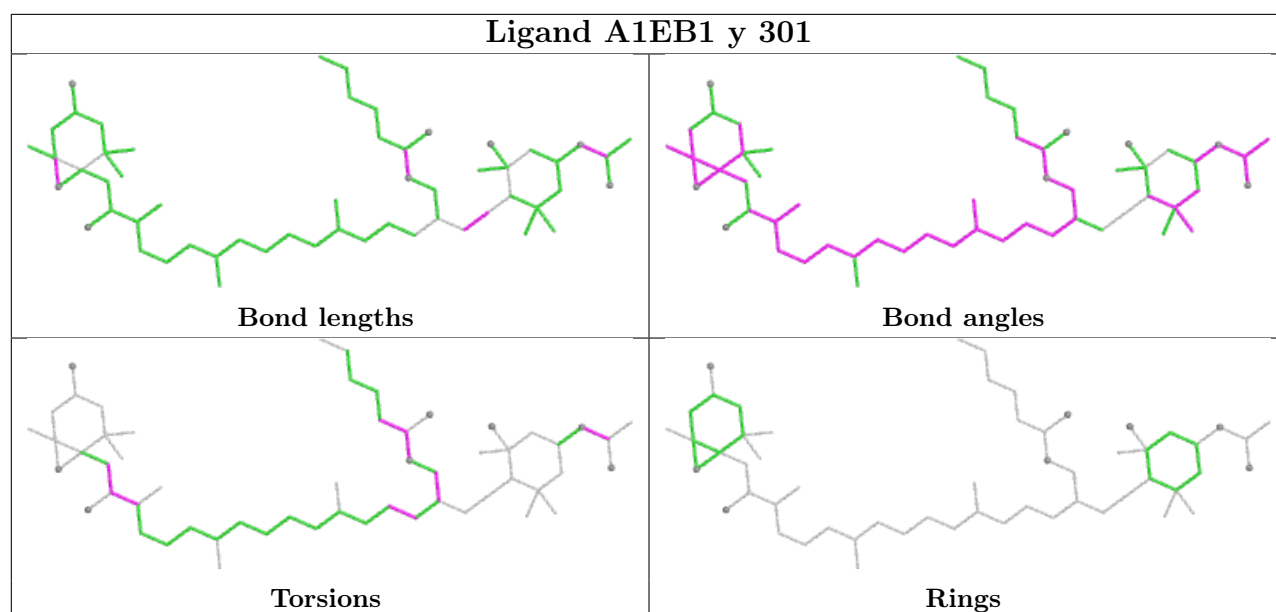


Torsions

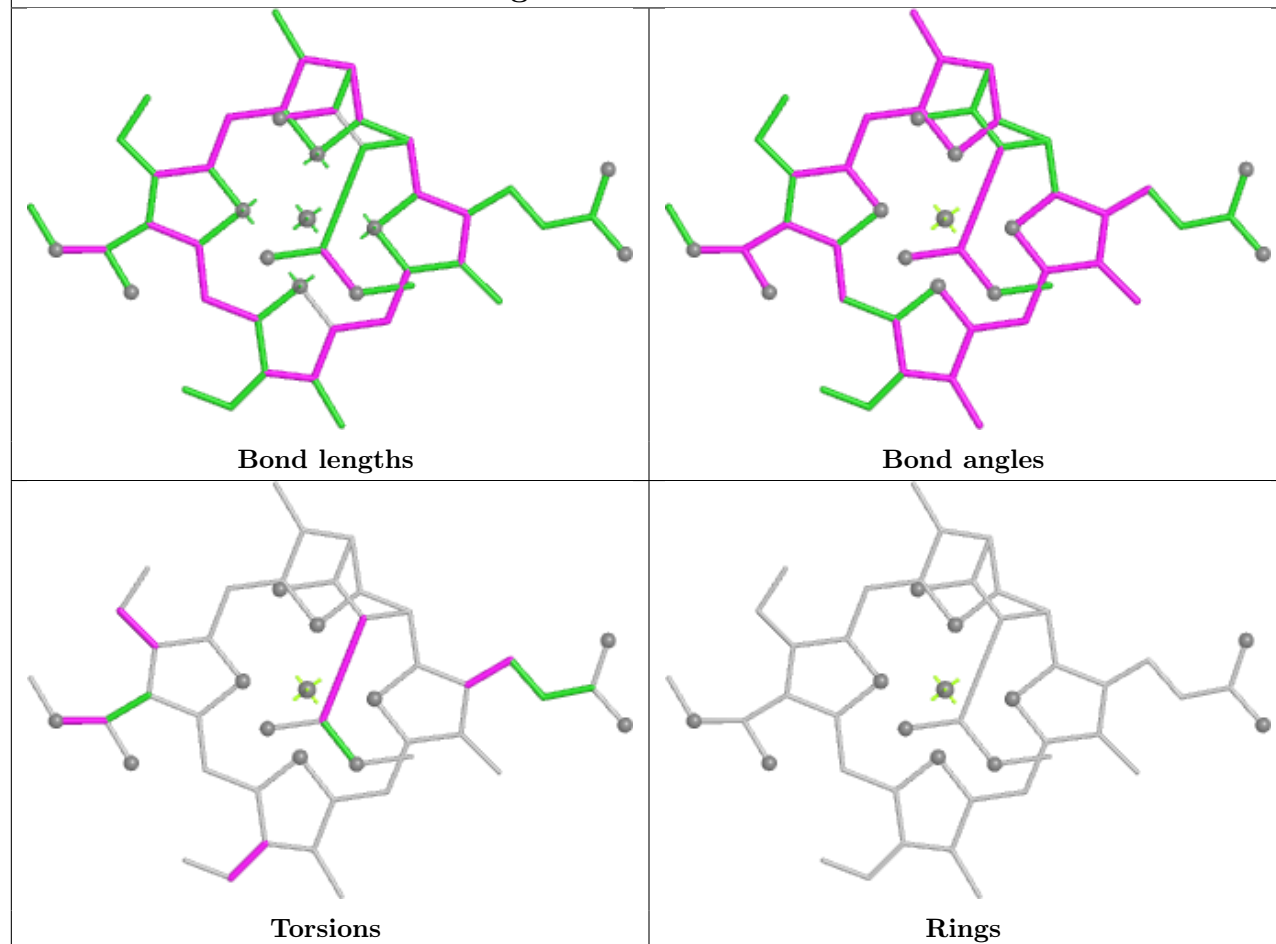


Rings

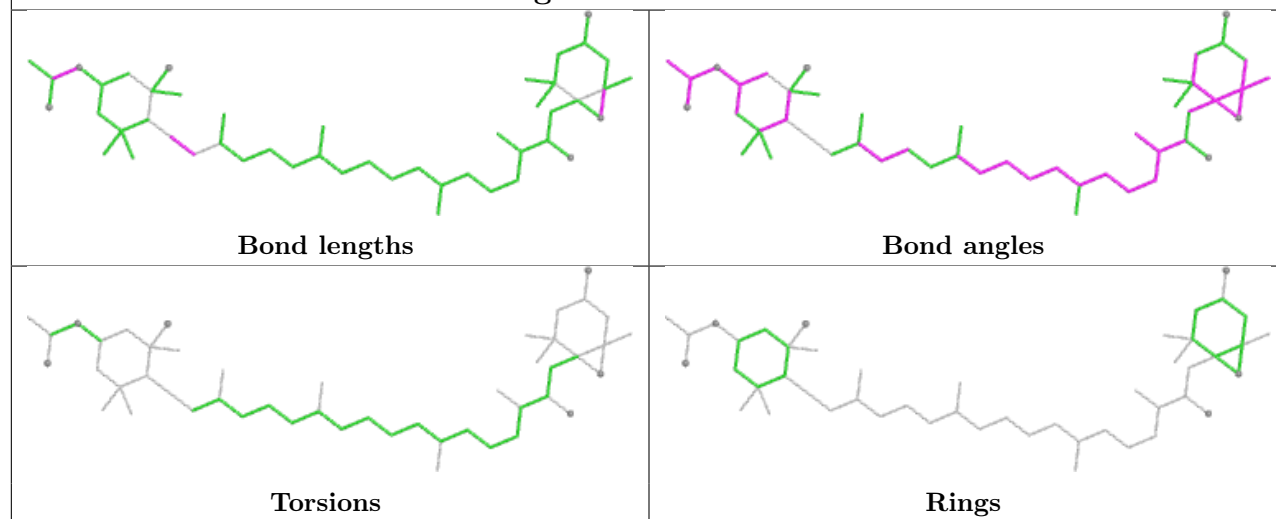




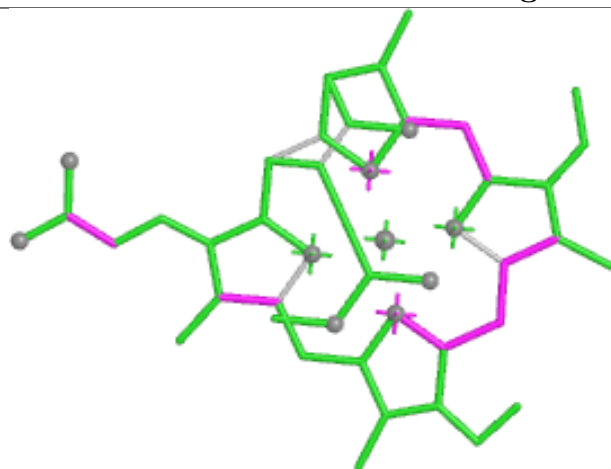
Ligand A1ECV Z 314



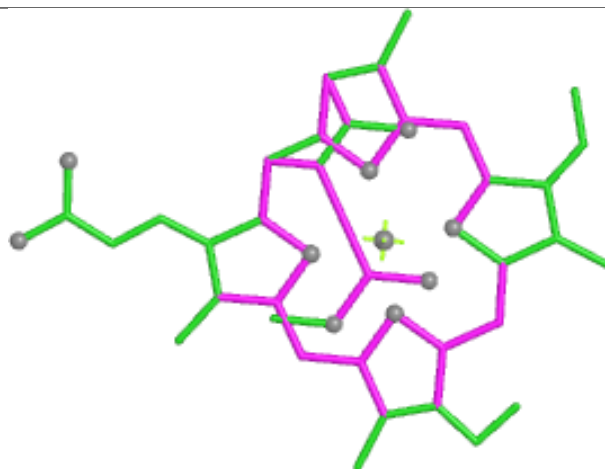
Ligand A86 M 303



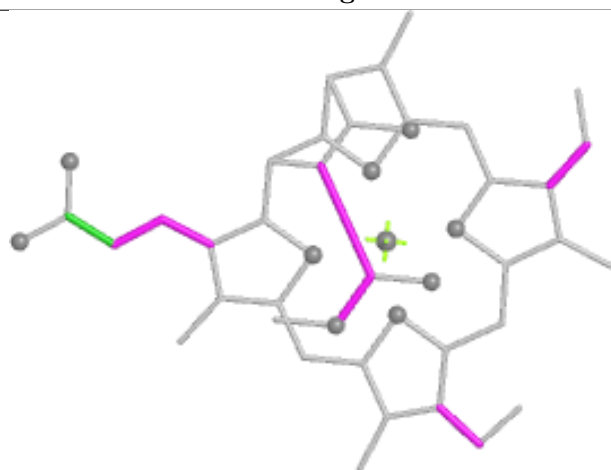
Ligand KC2 2 314



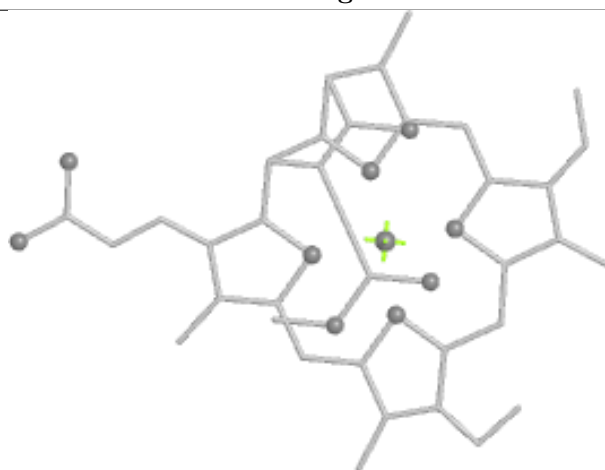
Bond lengths



Bond angles

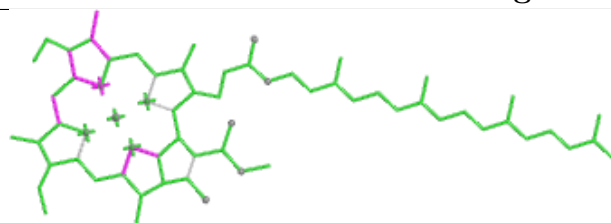


Torsions

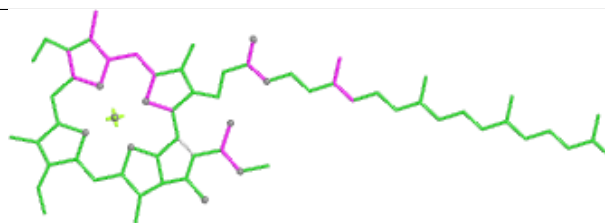


Rings

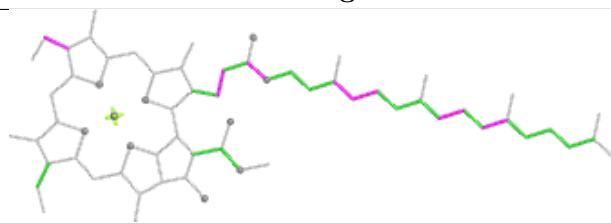
Ligand CLA V 309



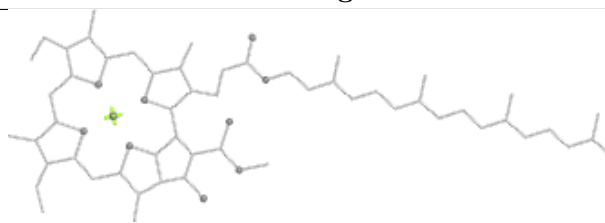
Bond lengths



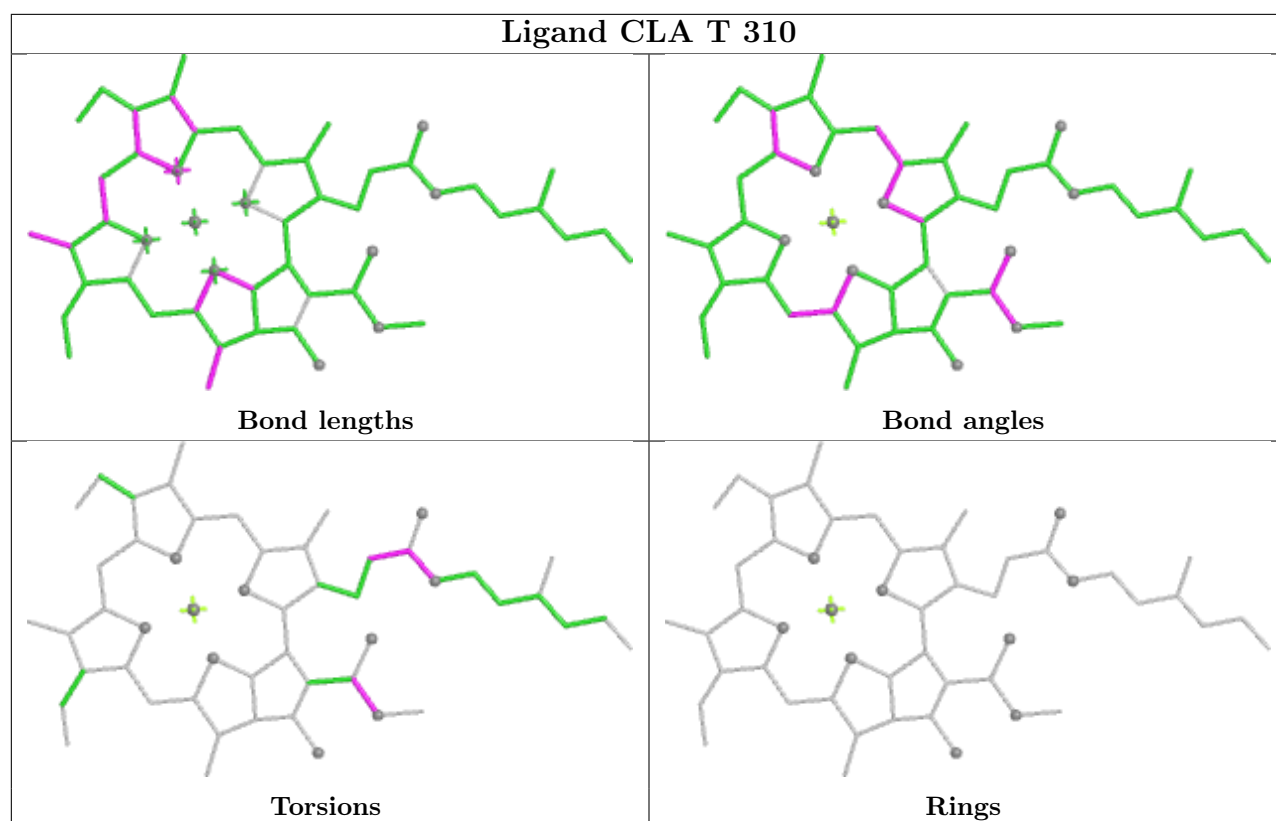
Bond angles



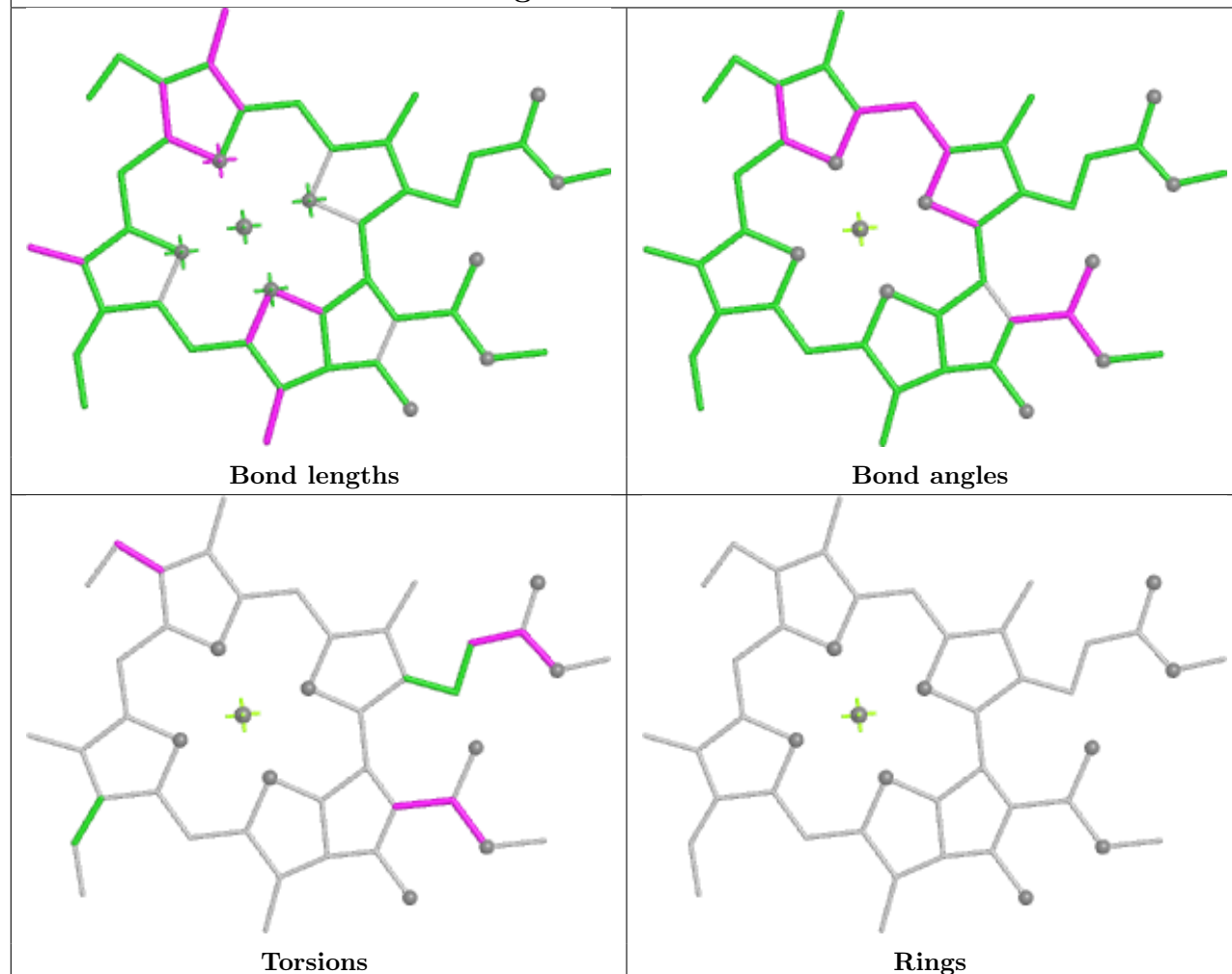
Torsions



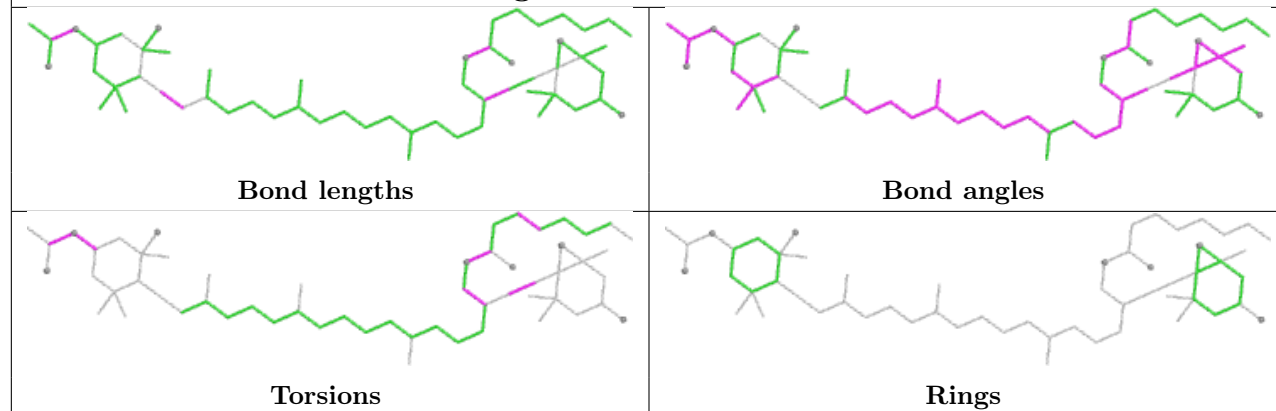
Rings

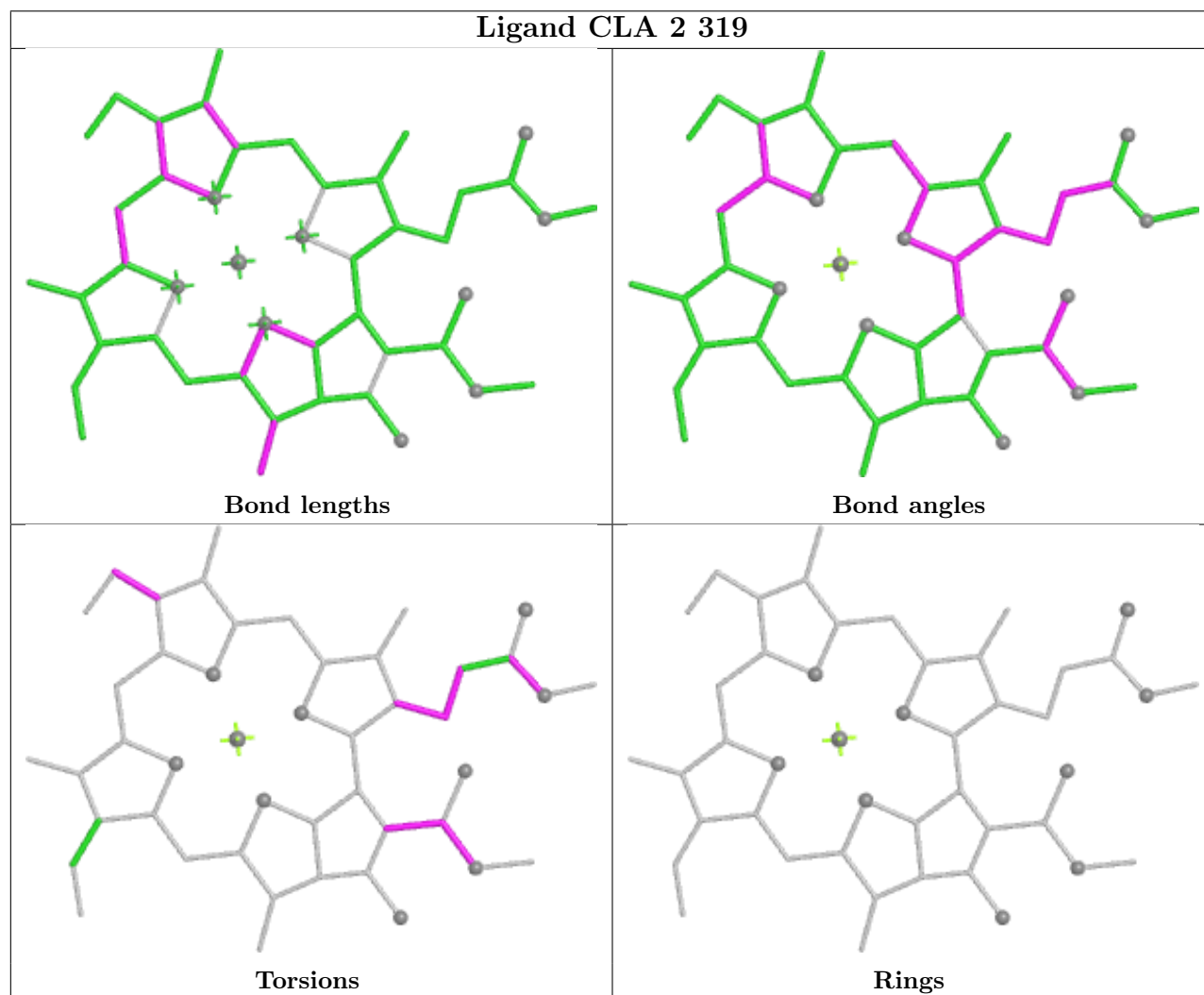
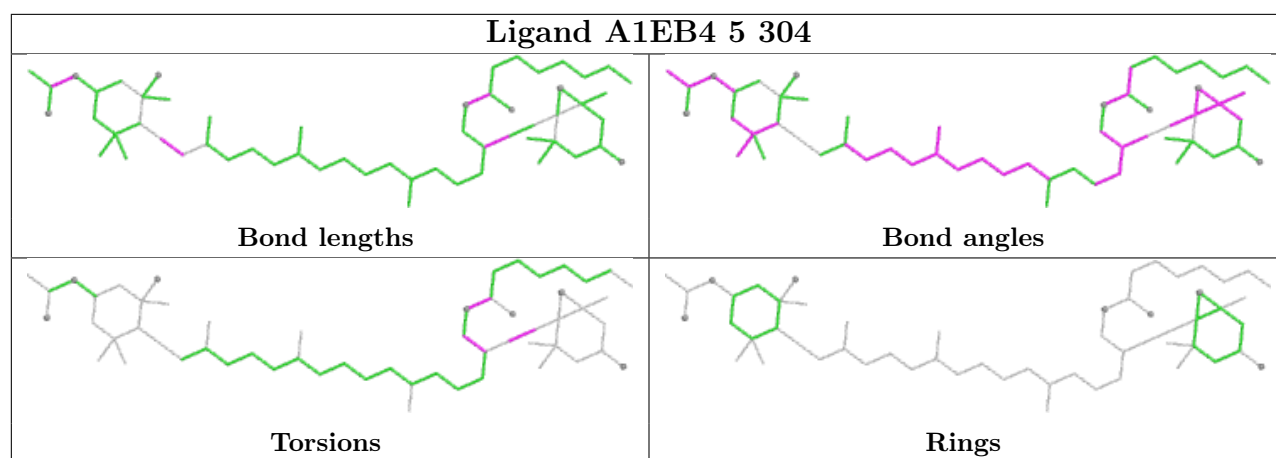


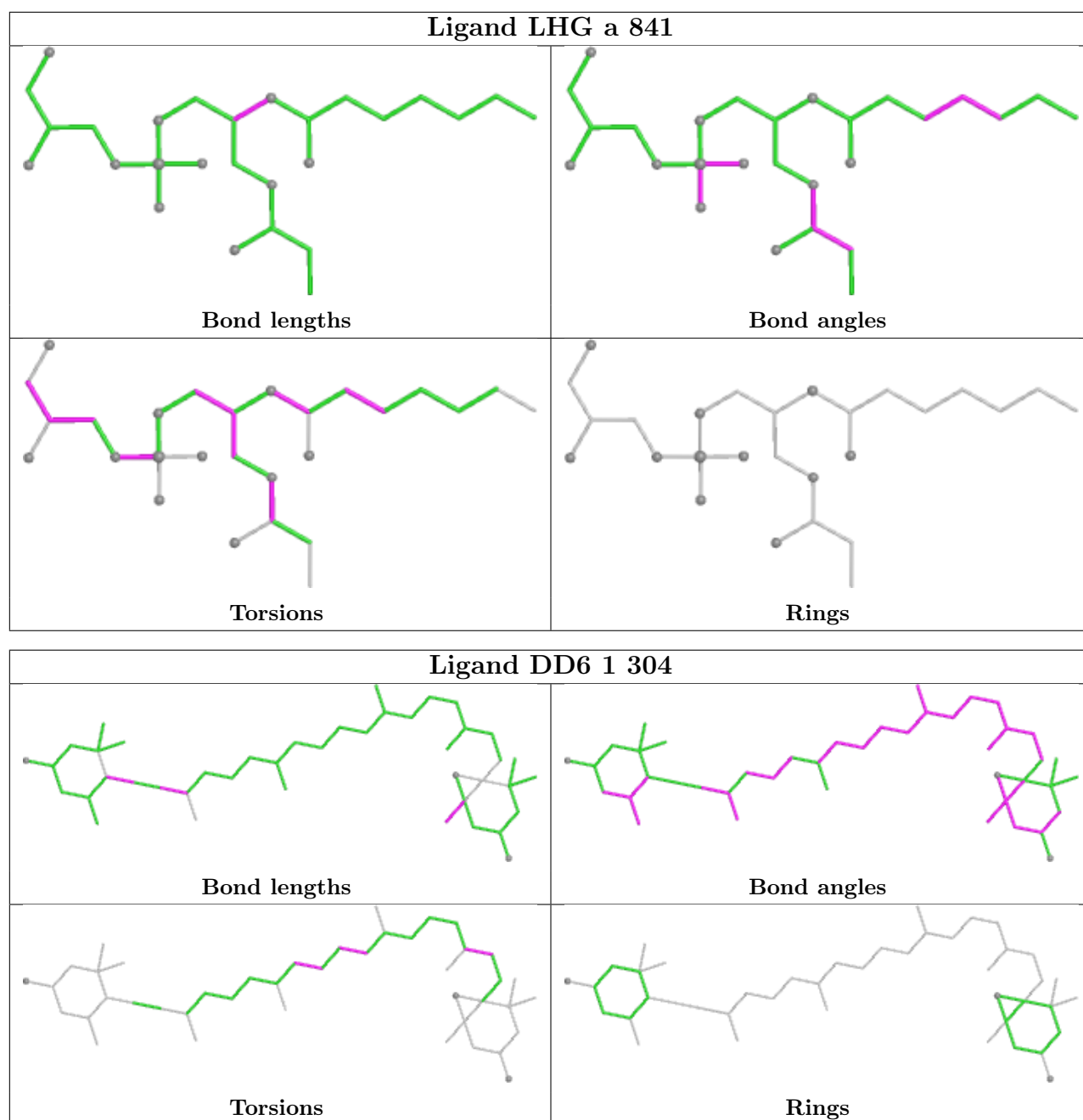
Ligand CLA T 308

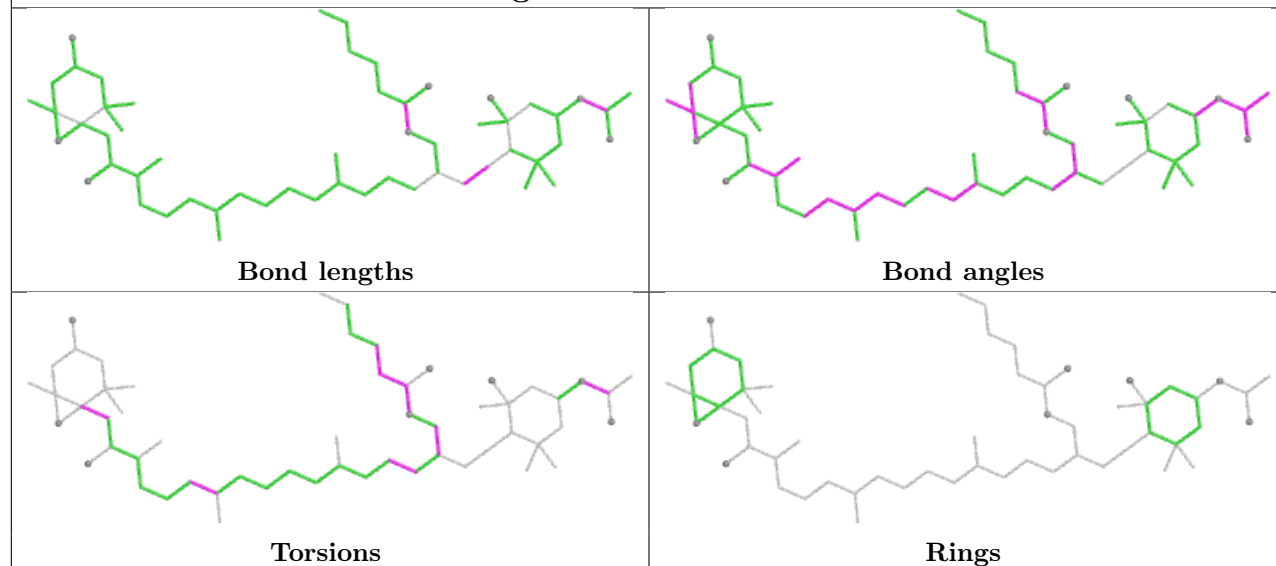
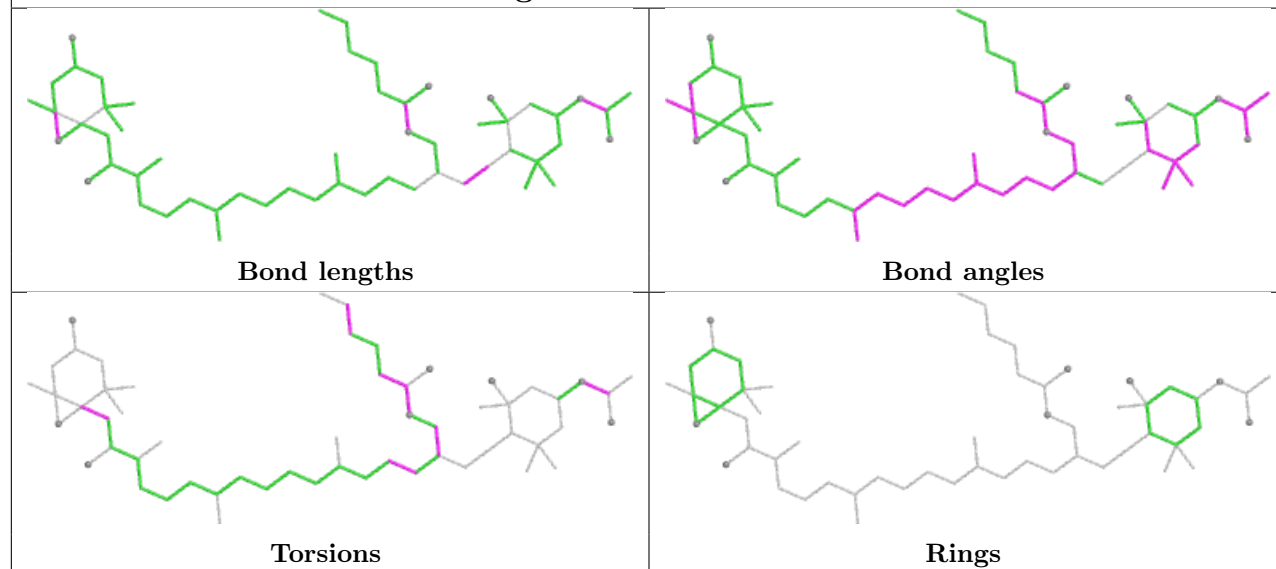


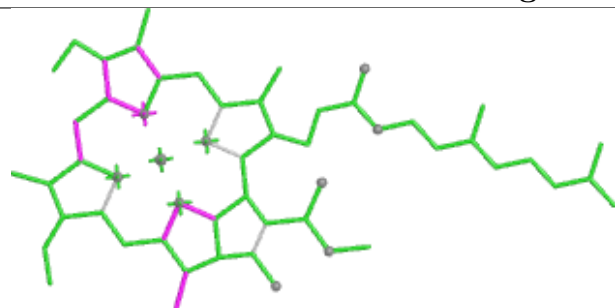
Ligand A1EB4 R 305



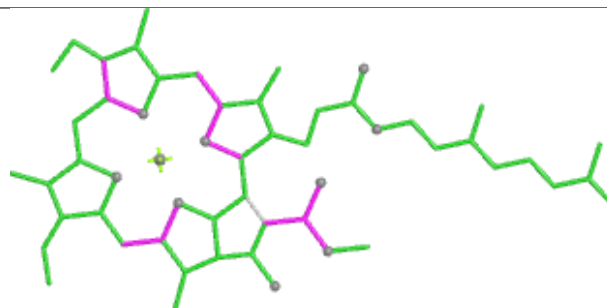




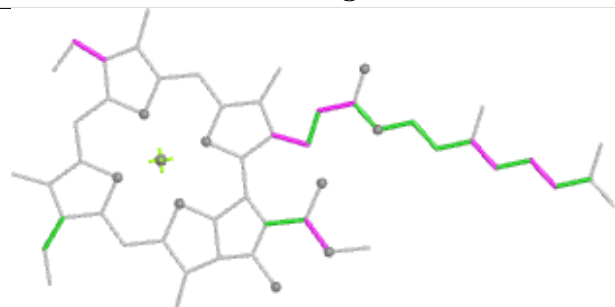
Ligand A1EB1 H 304**Ligand A1EB1 F 304**

Ligand CLA h 201

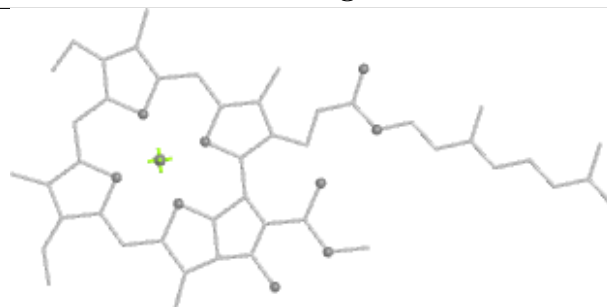
Bond lengths



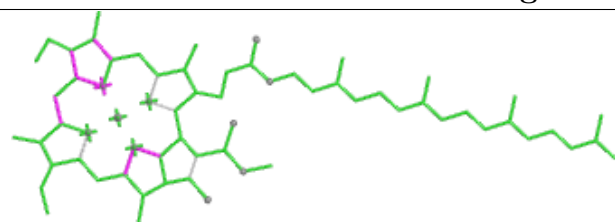
Bond angles



Torsions



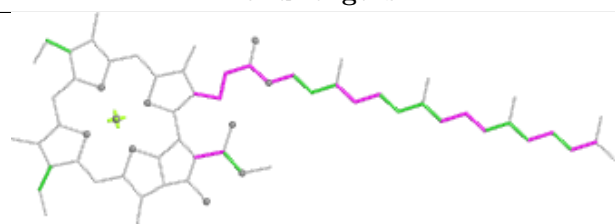
Rings

Ligand CLA J 309

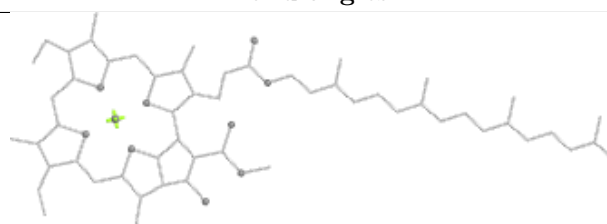
Bond lengths



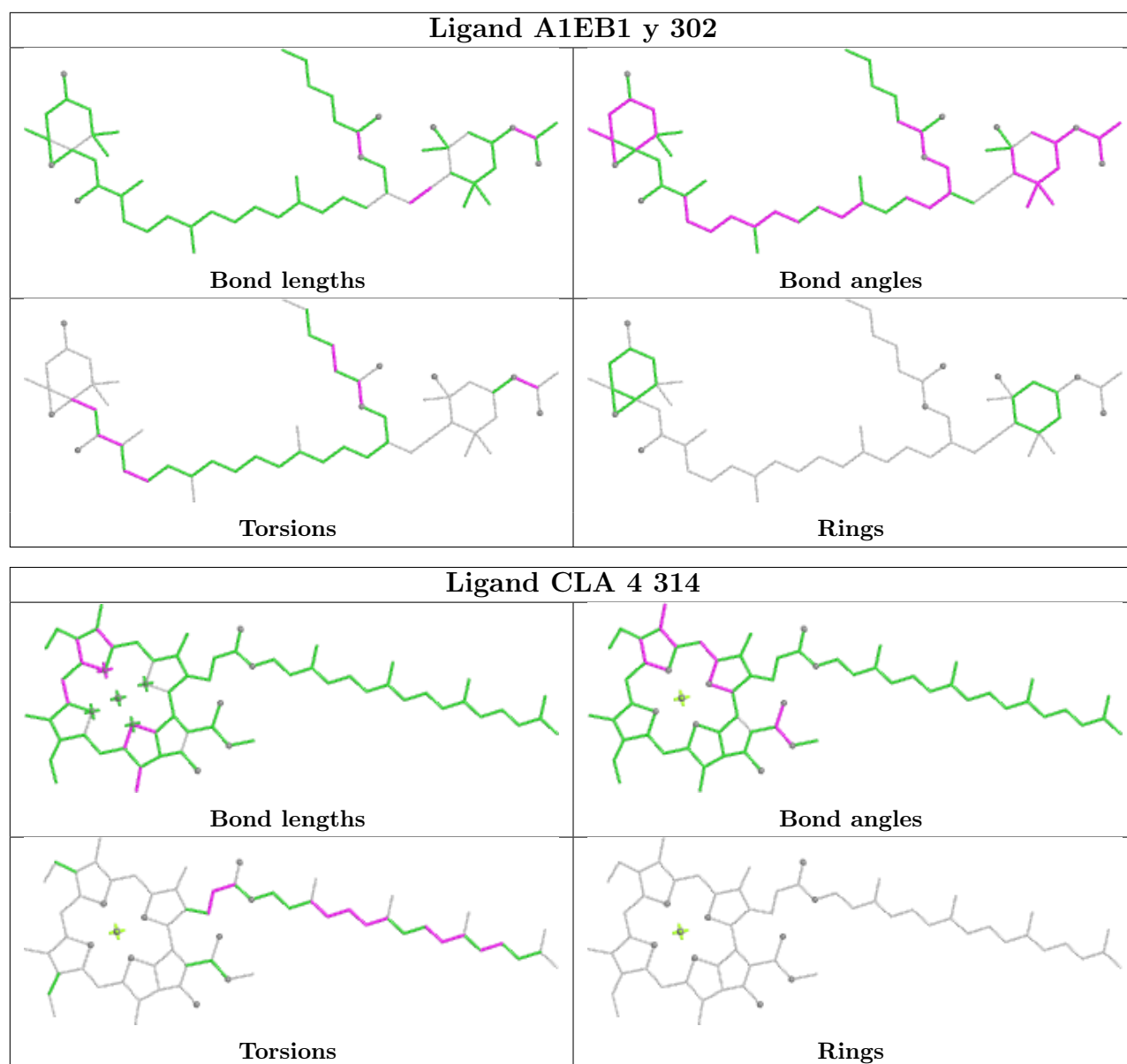
Bond angles



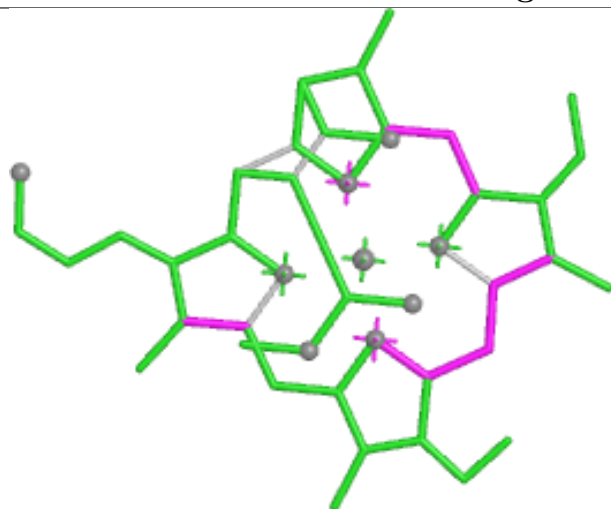
Torsions



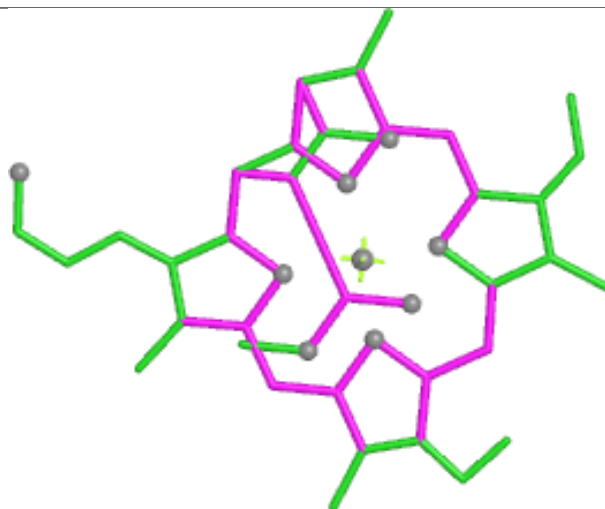
Rings



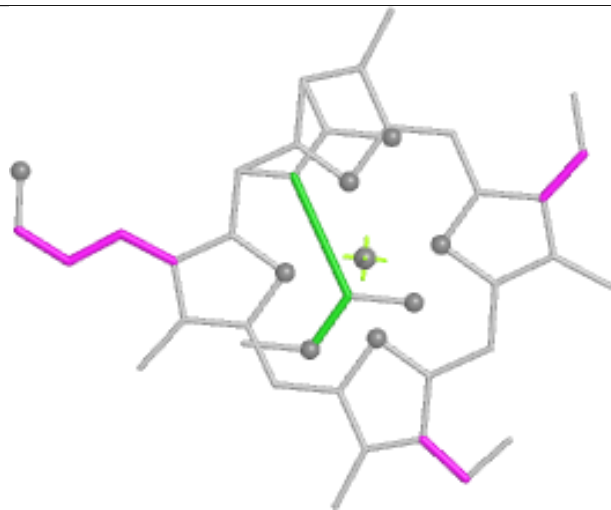
Ligand KC2 P 310



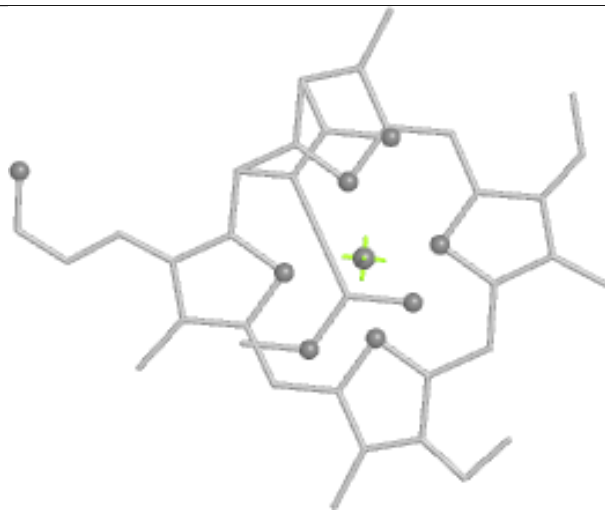
Bond lengths



Bond angles

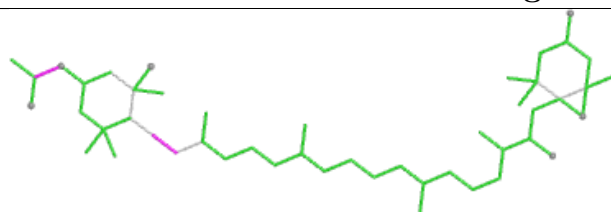


Torsions

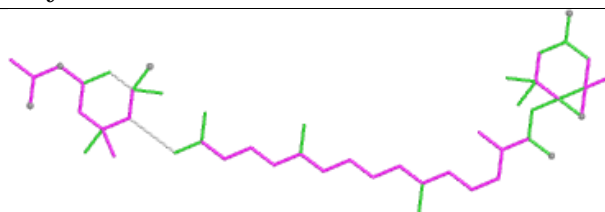


Rings

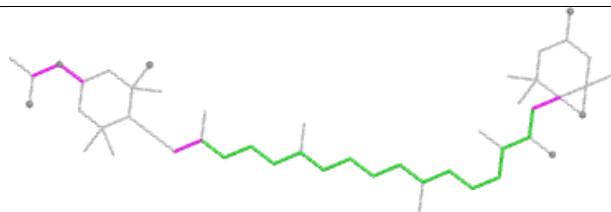
Ligand A86 y 306



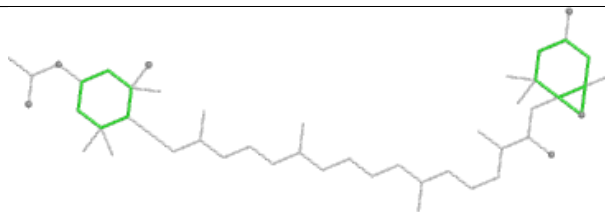
Bond lengths



Bond angles

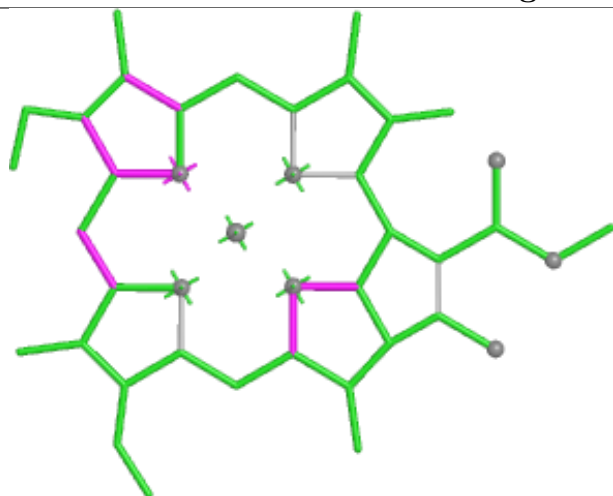


Torsions

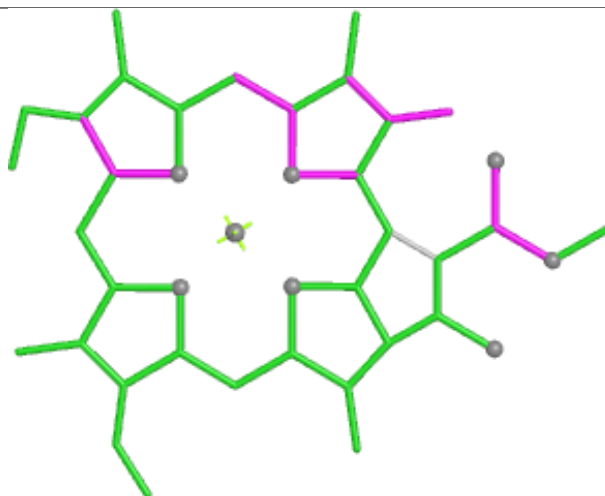


Rings

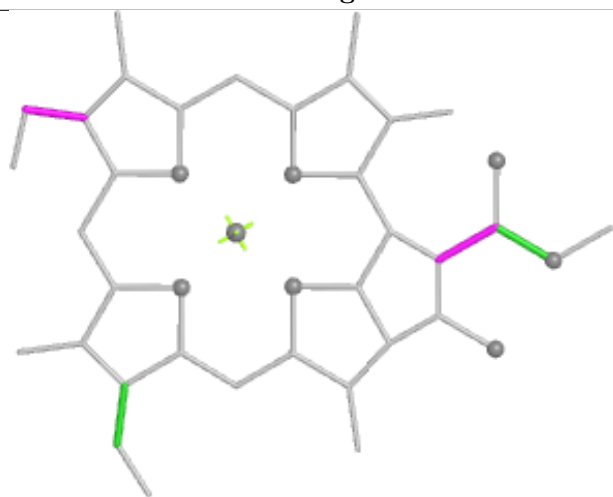
Ligand CLA z 314



Bond lengths



Bond angles

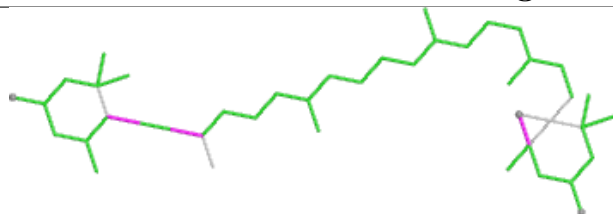


Torsions

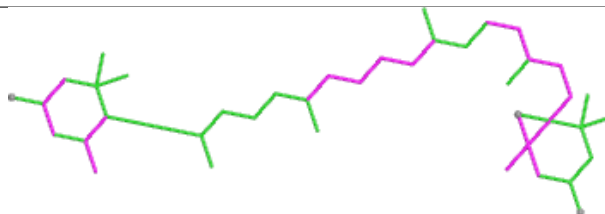


Rings

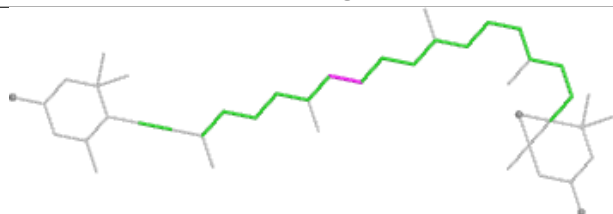
Ligand DD6 E 303



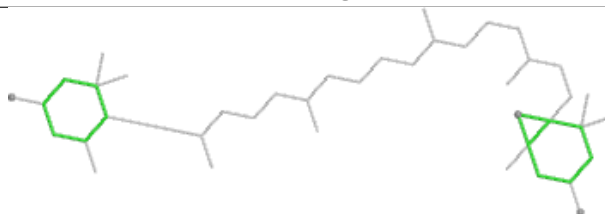
Bond lengths



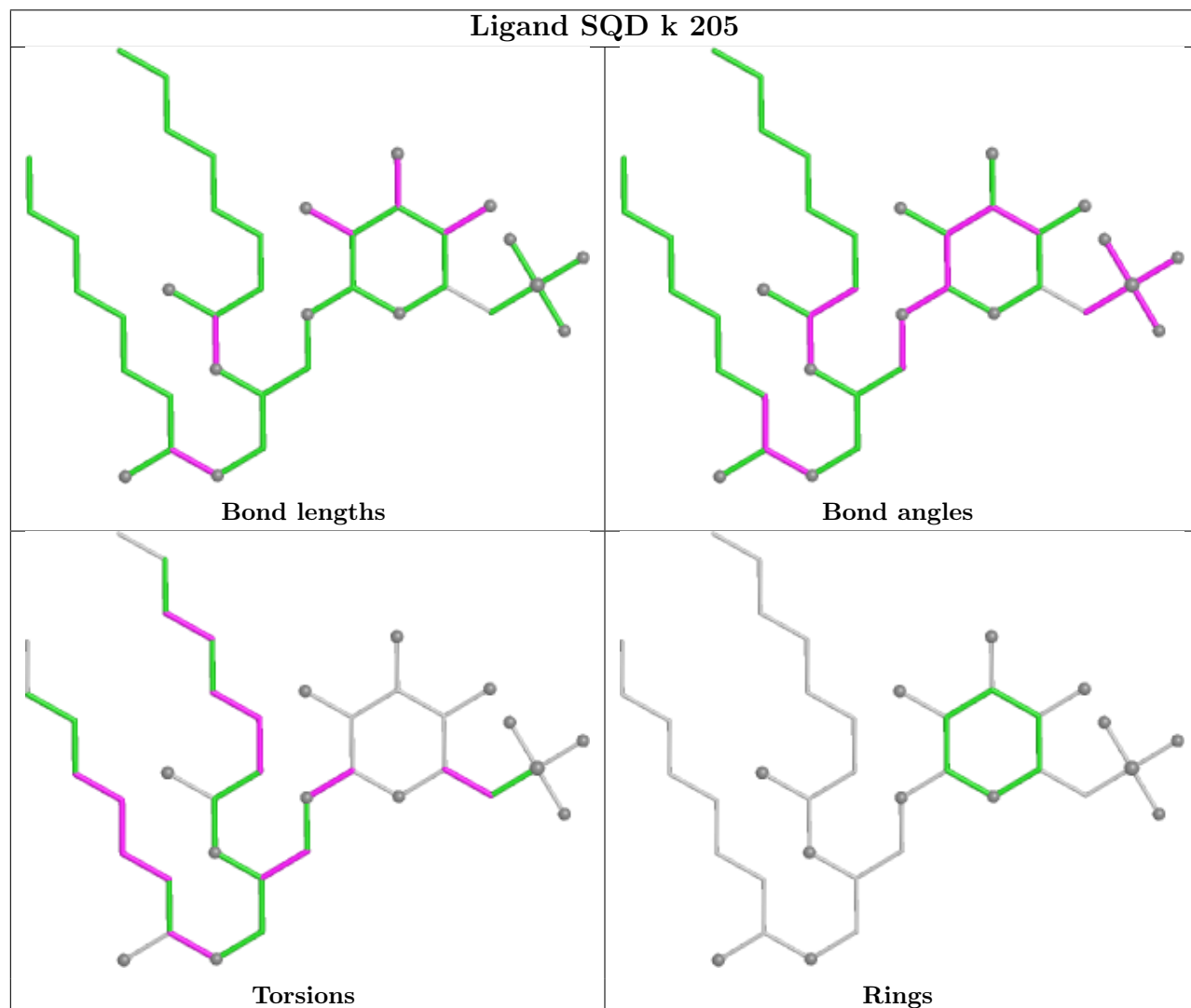
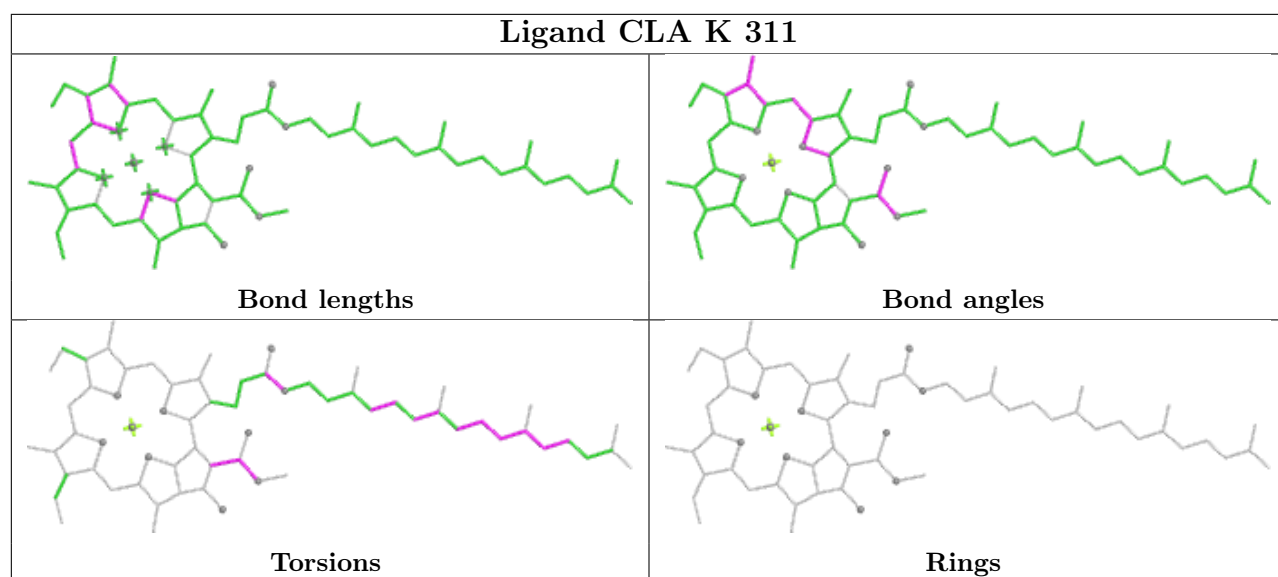
Bond angles



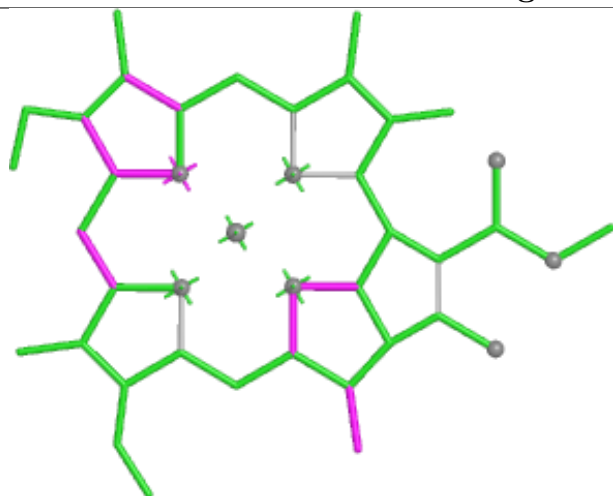
Torsions



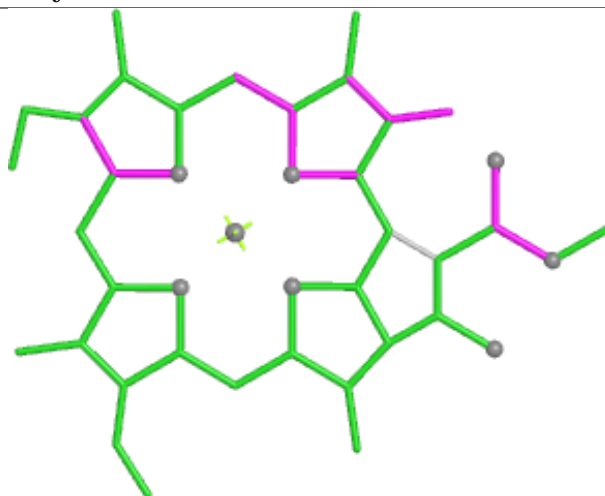
Rings



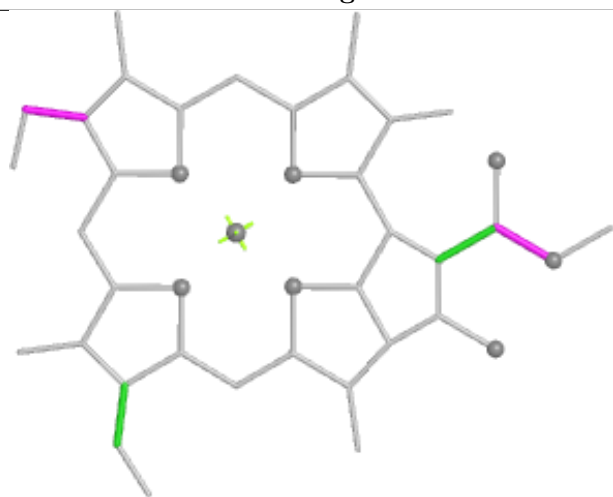
Ligand CLA y 307



Bond lengths



Bond angles

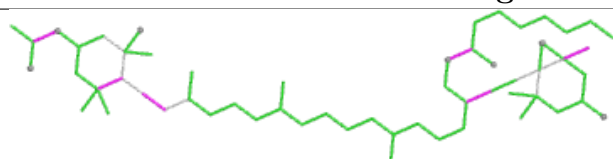


Torsions

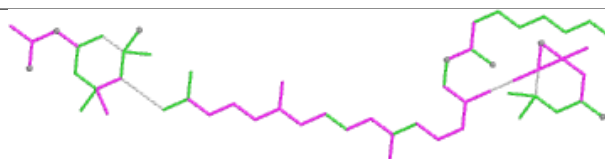


Rings

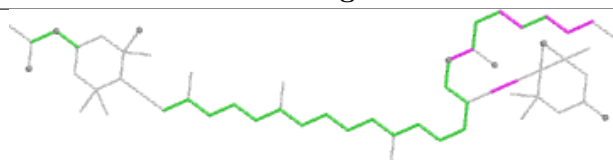
Ligand A1EB4 P 319



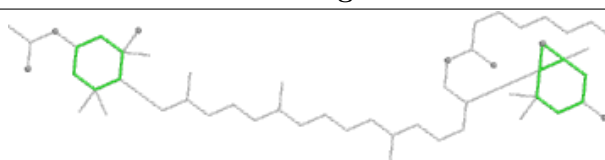
Bond lengths



Bond angles

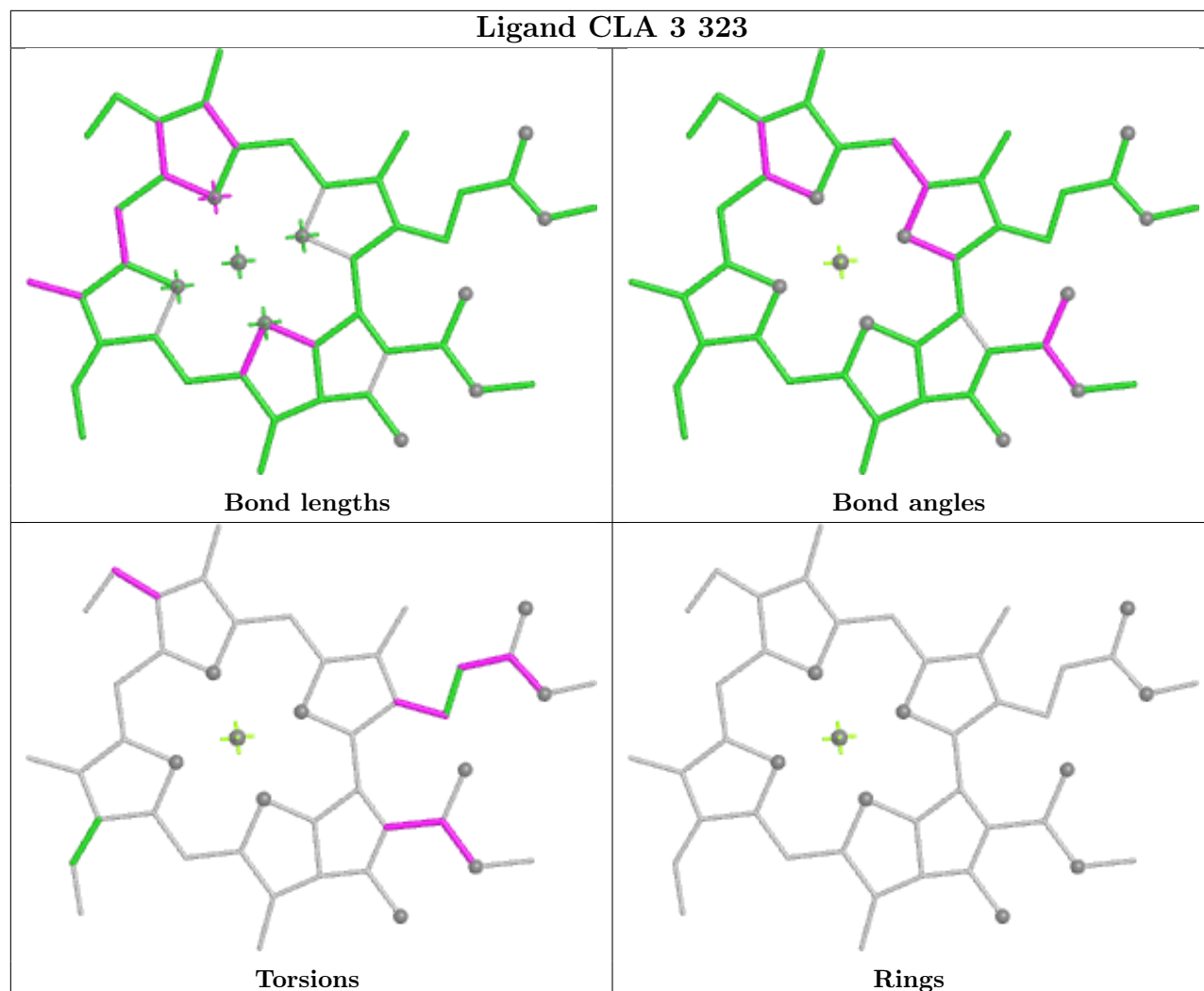


Torsions

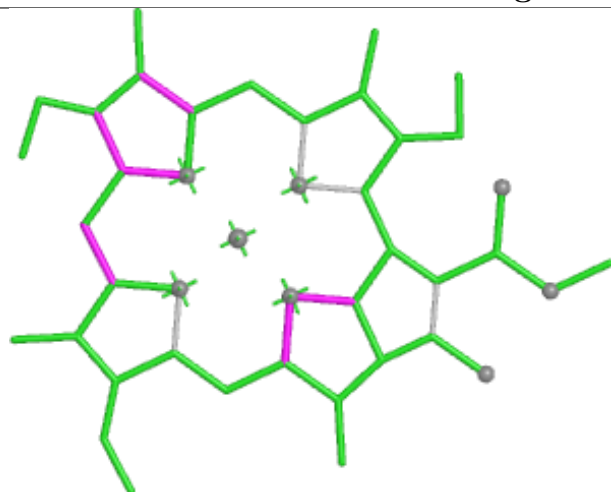


Rings

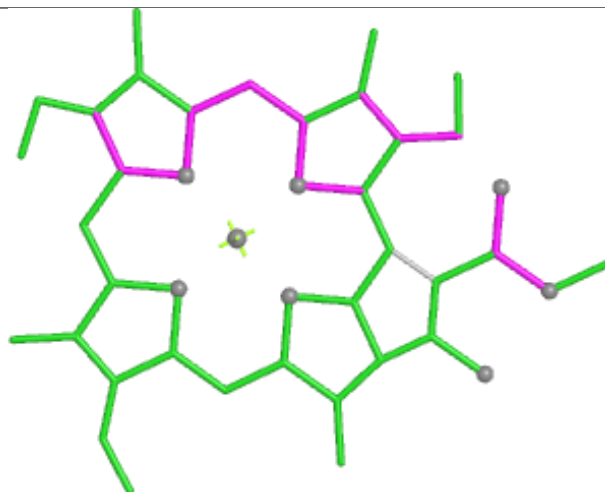
Ligand CLA 3 323



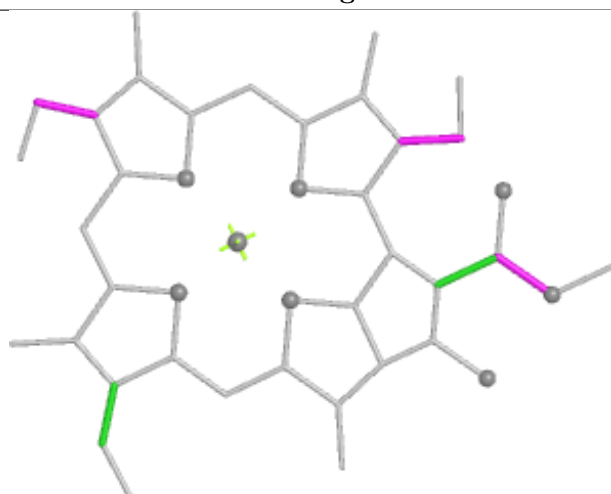
Ligand CLA B 205



Bond lengths



Bond angles

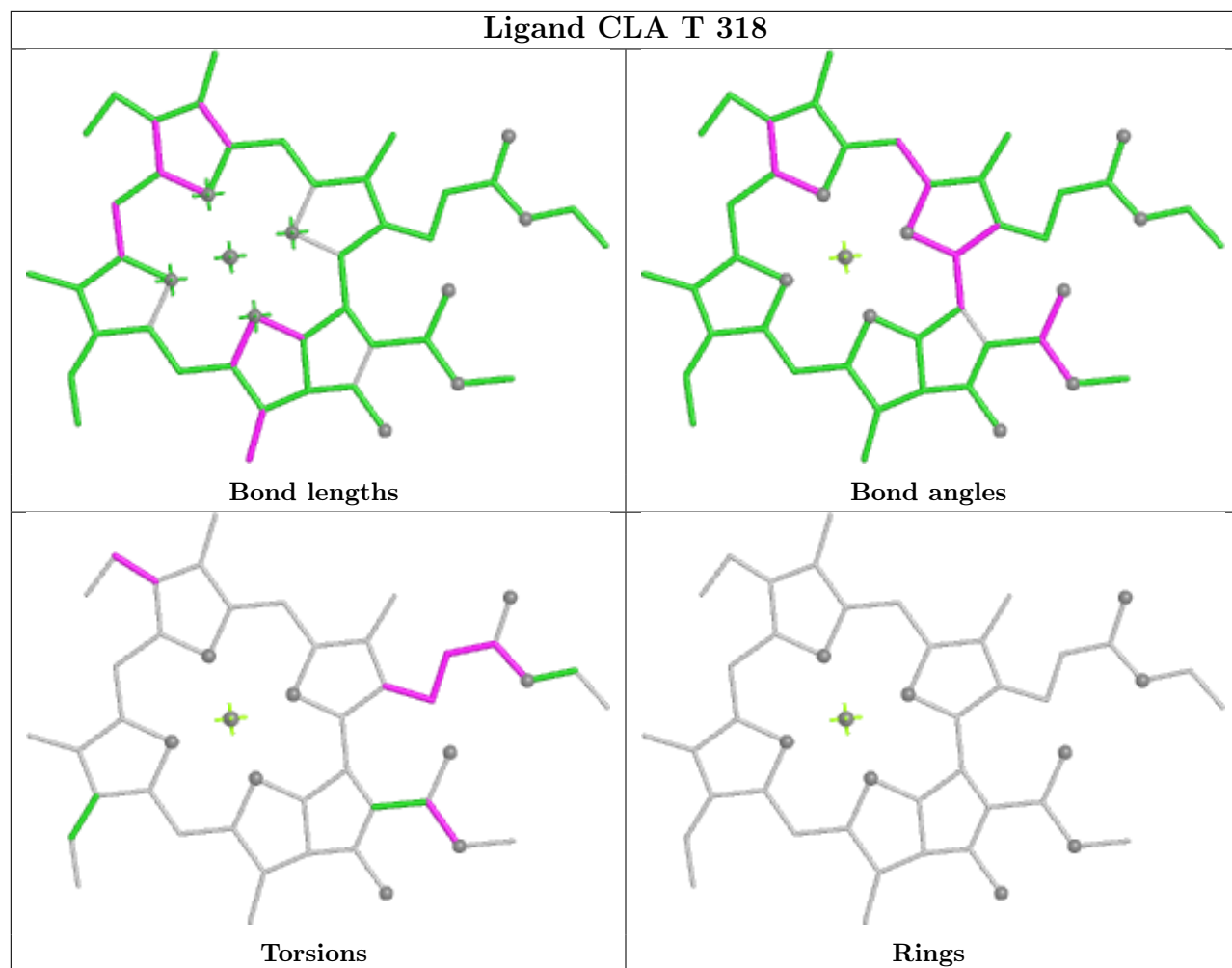


Torsions

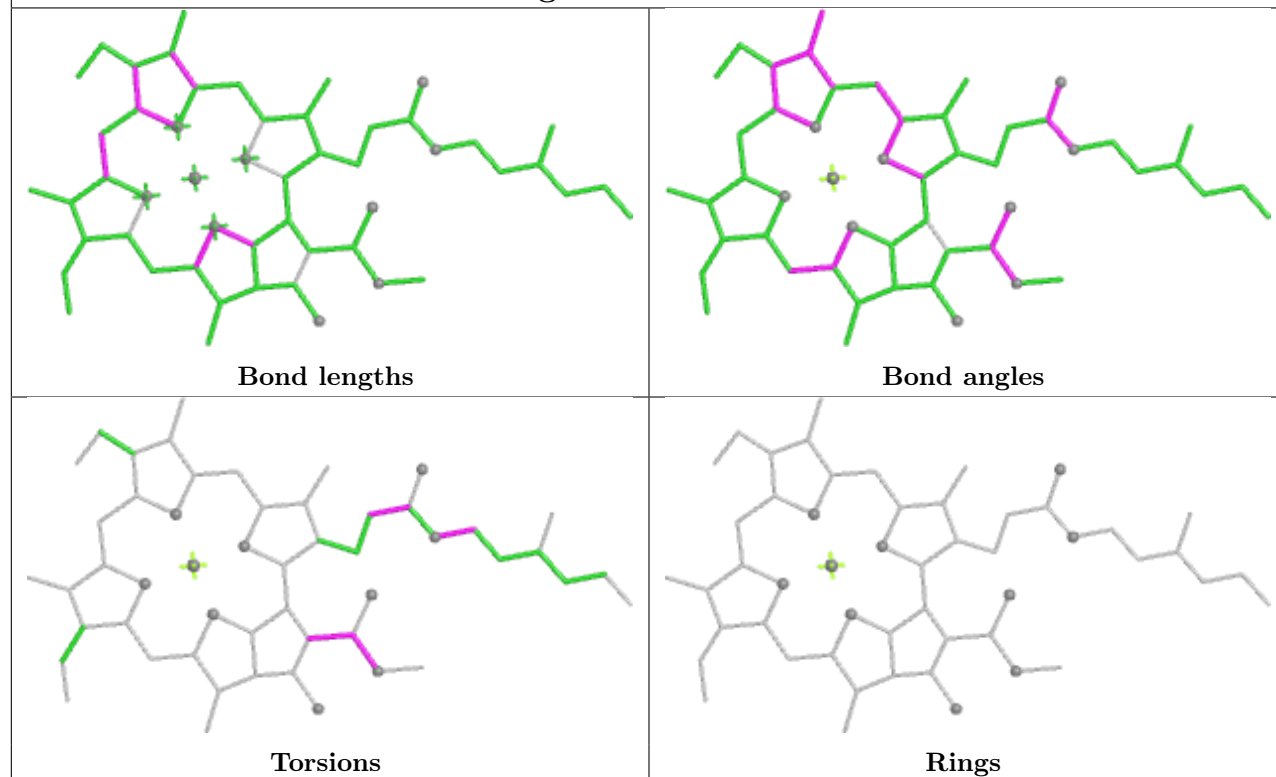


Rings

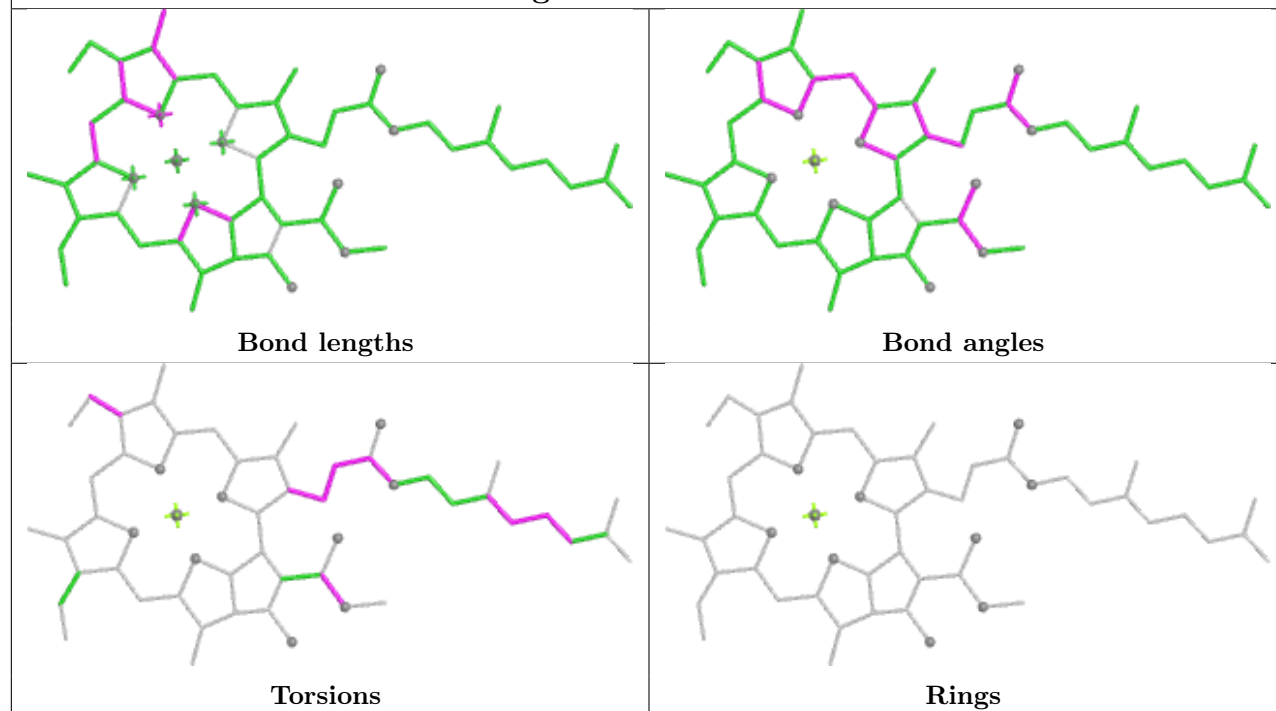
Ligand CLA T 318



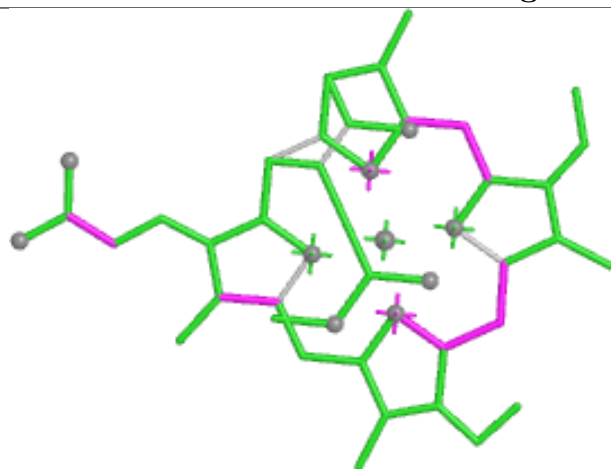
Ligand CLA I 315



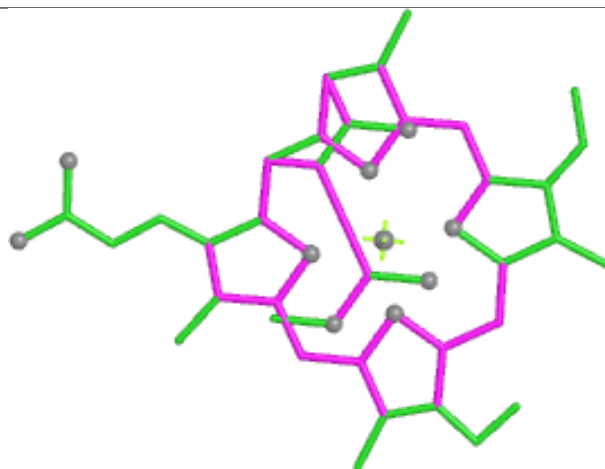
Ligand CLA B 207



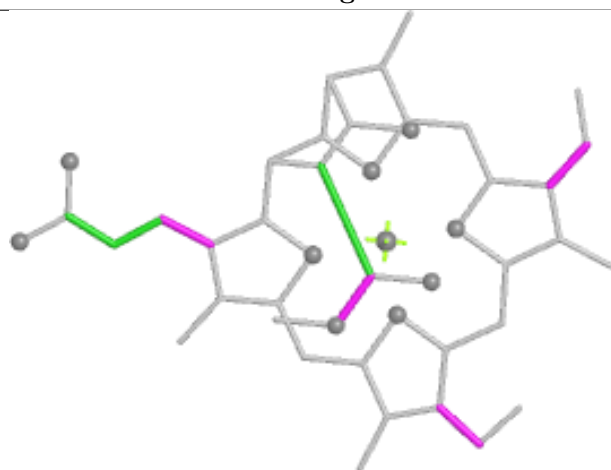
Ligand KC2 5 305



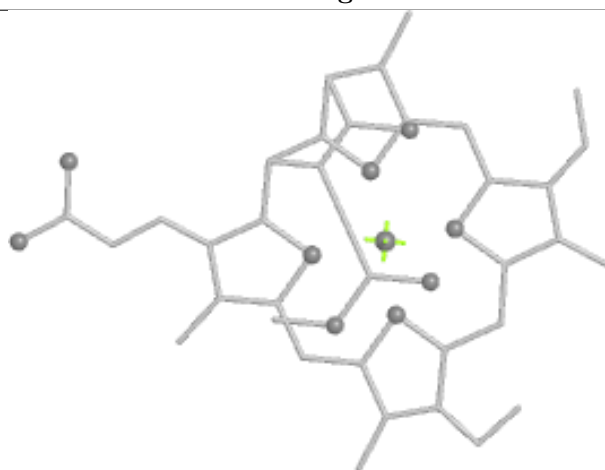
Bond lengths



Bond angles

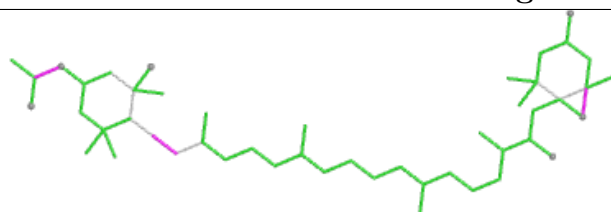


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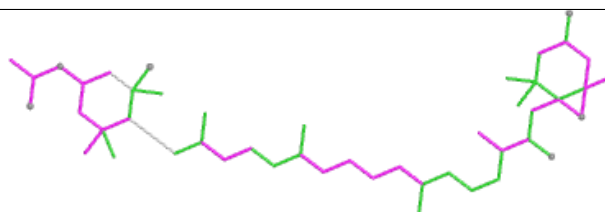


Rings

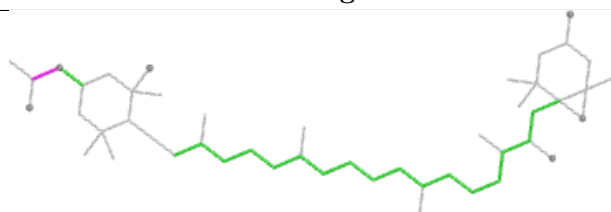
Ligand A86 M 306



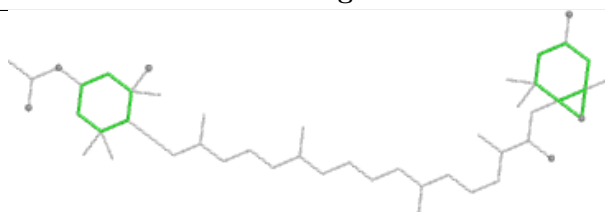
Bond lengths



Bond angles

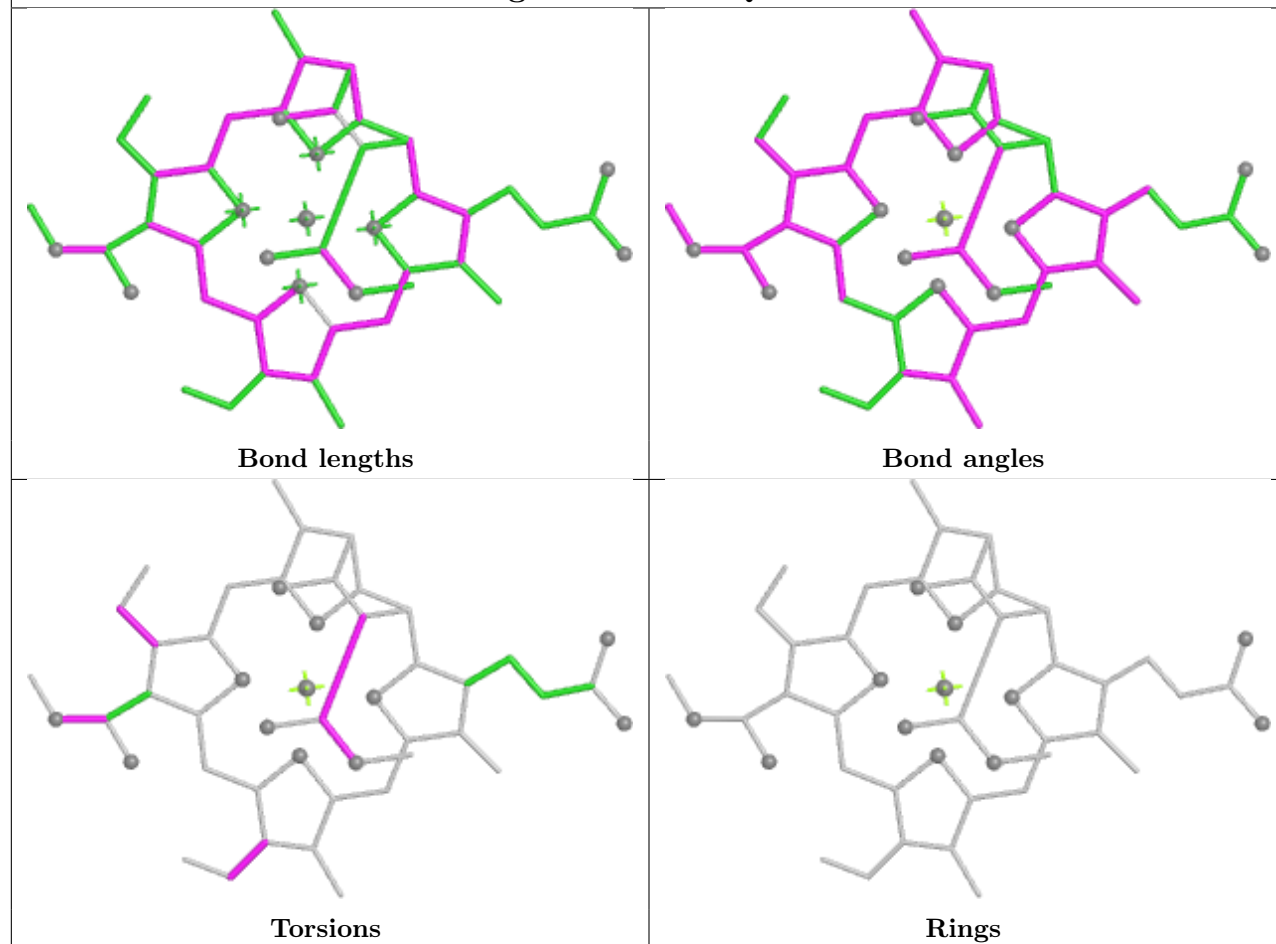


Torsions

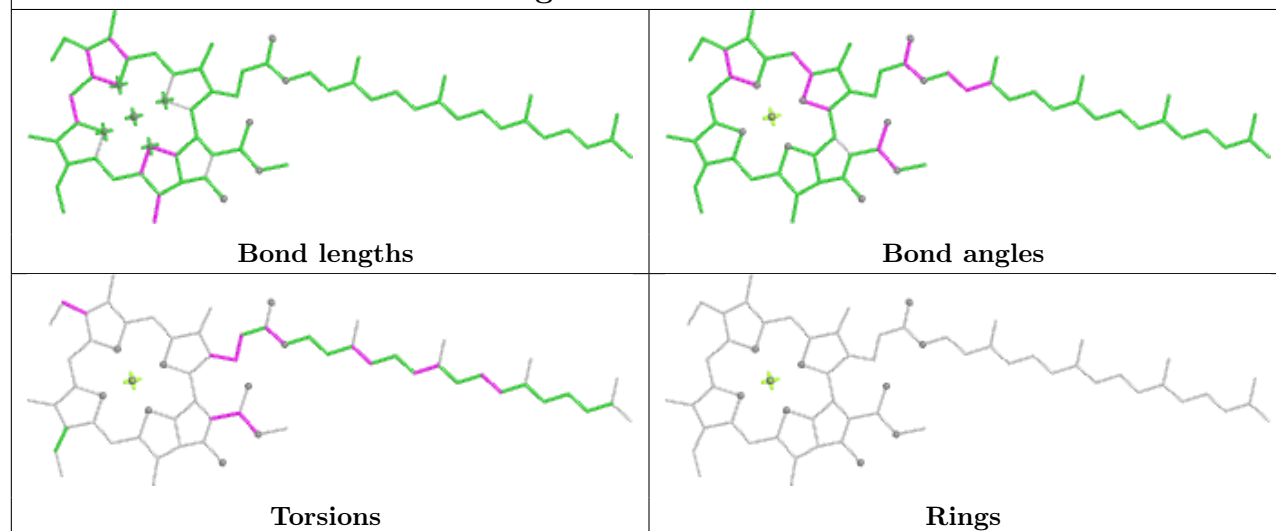


Rings

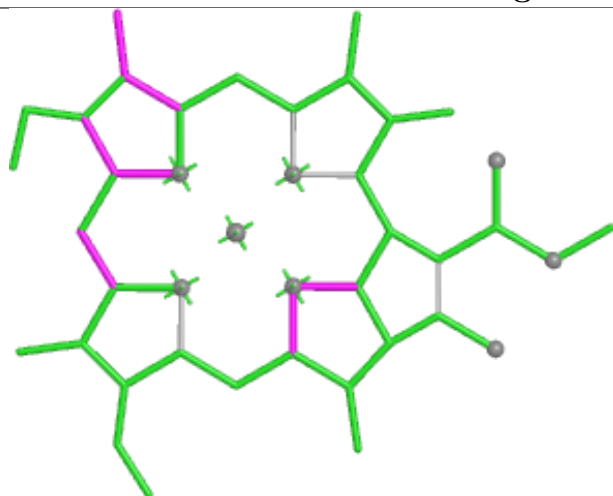
Ligand A1ECV Q 316



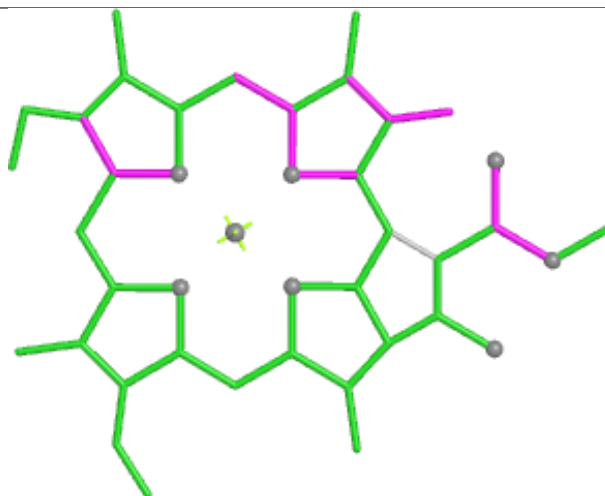
Ligand CLA b 828



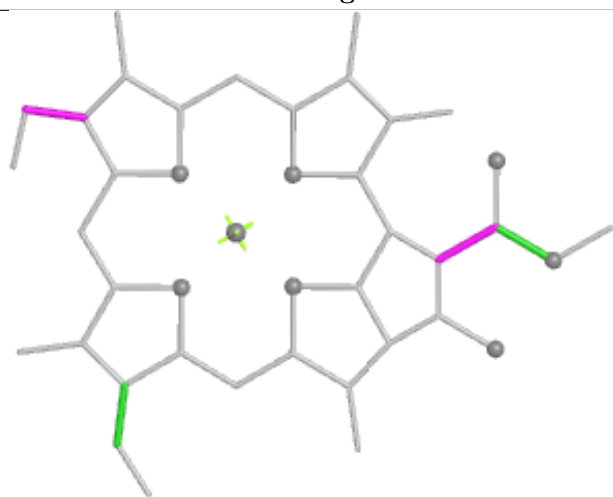
Ligand CLA Y 307



Bond lengths



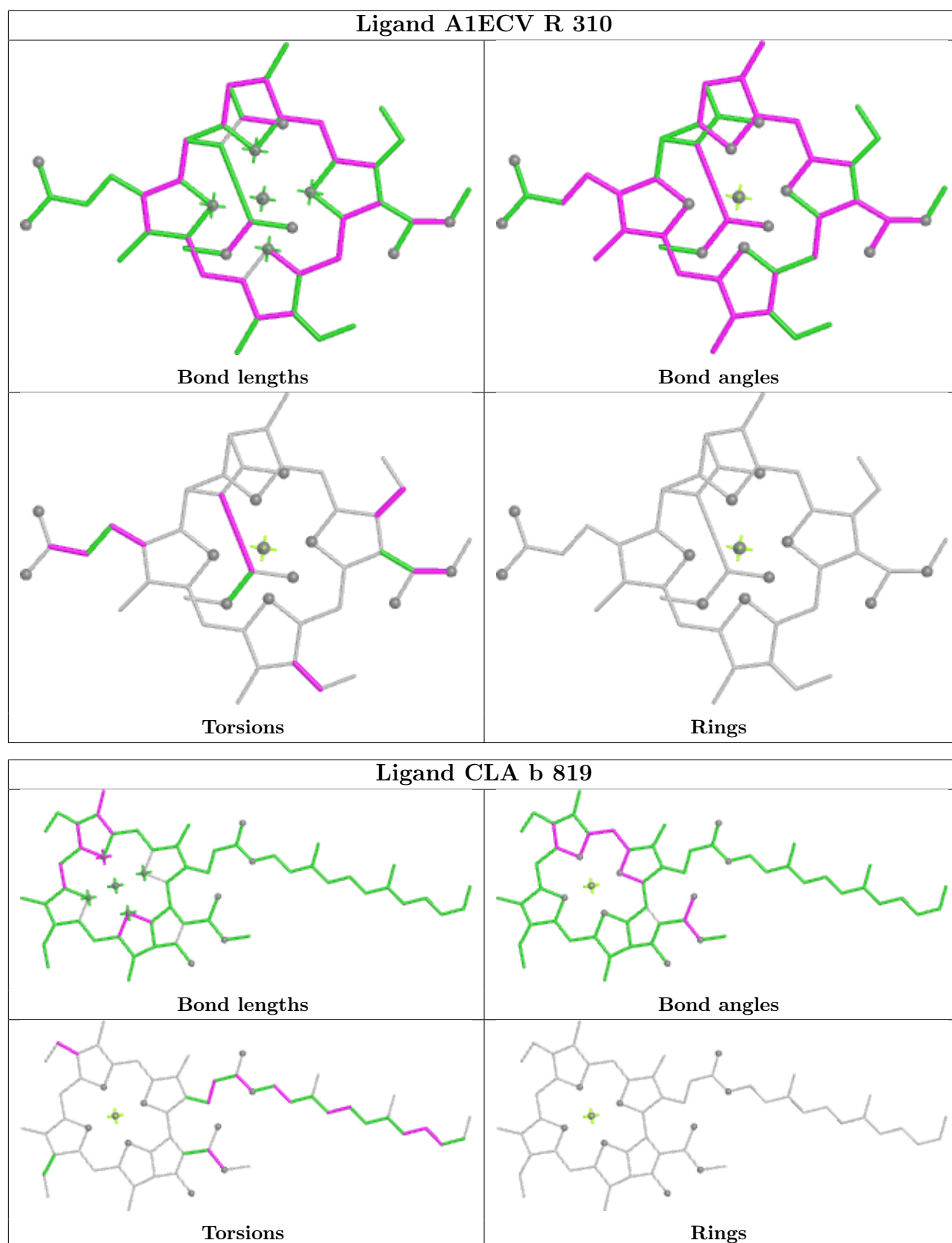
Bond angles

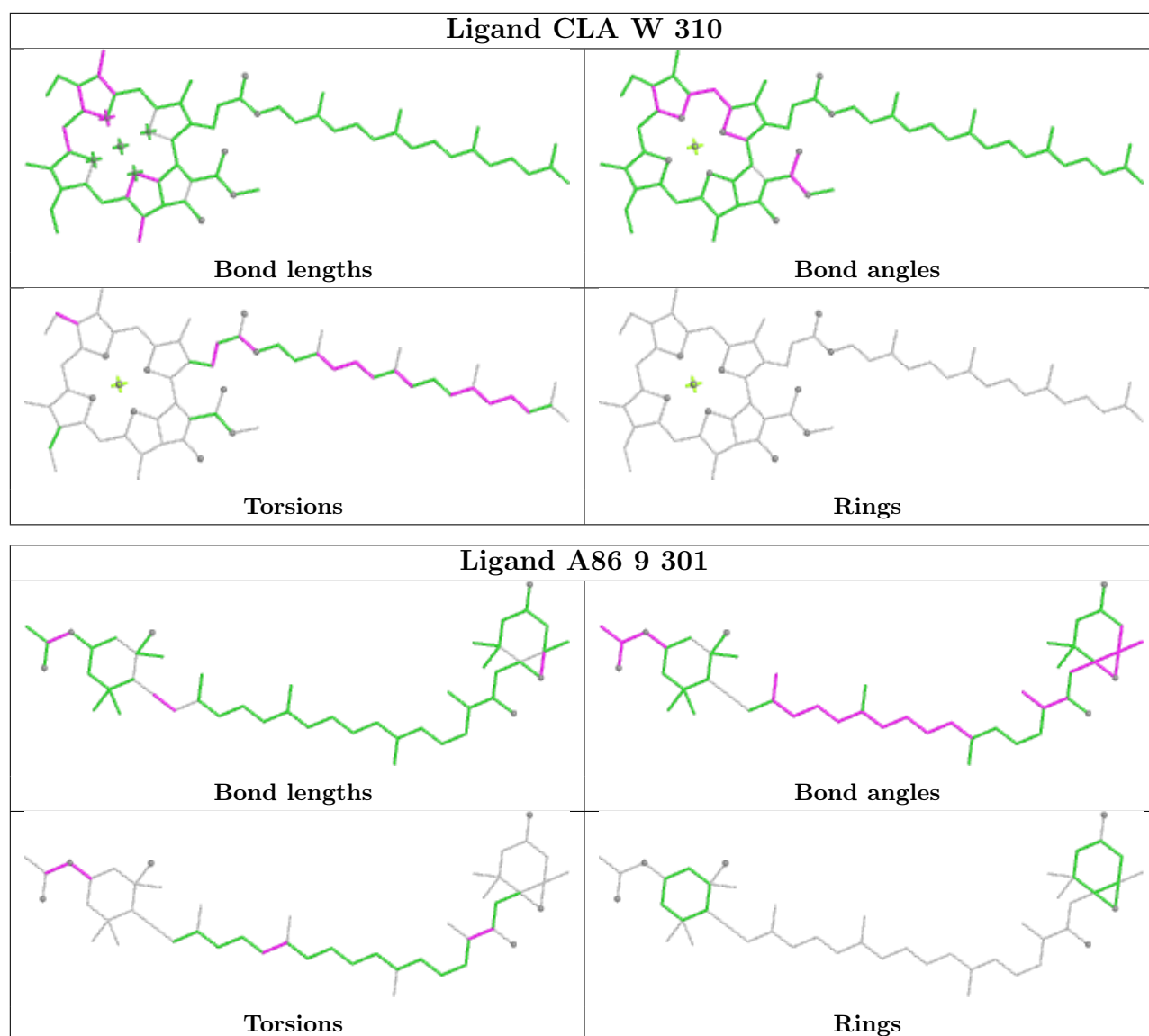


Torsions

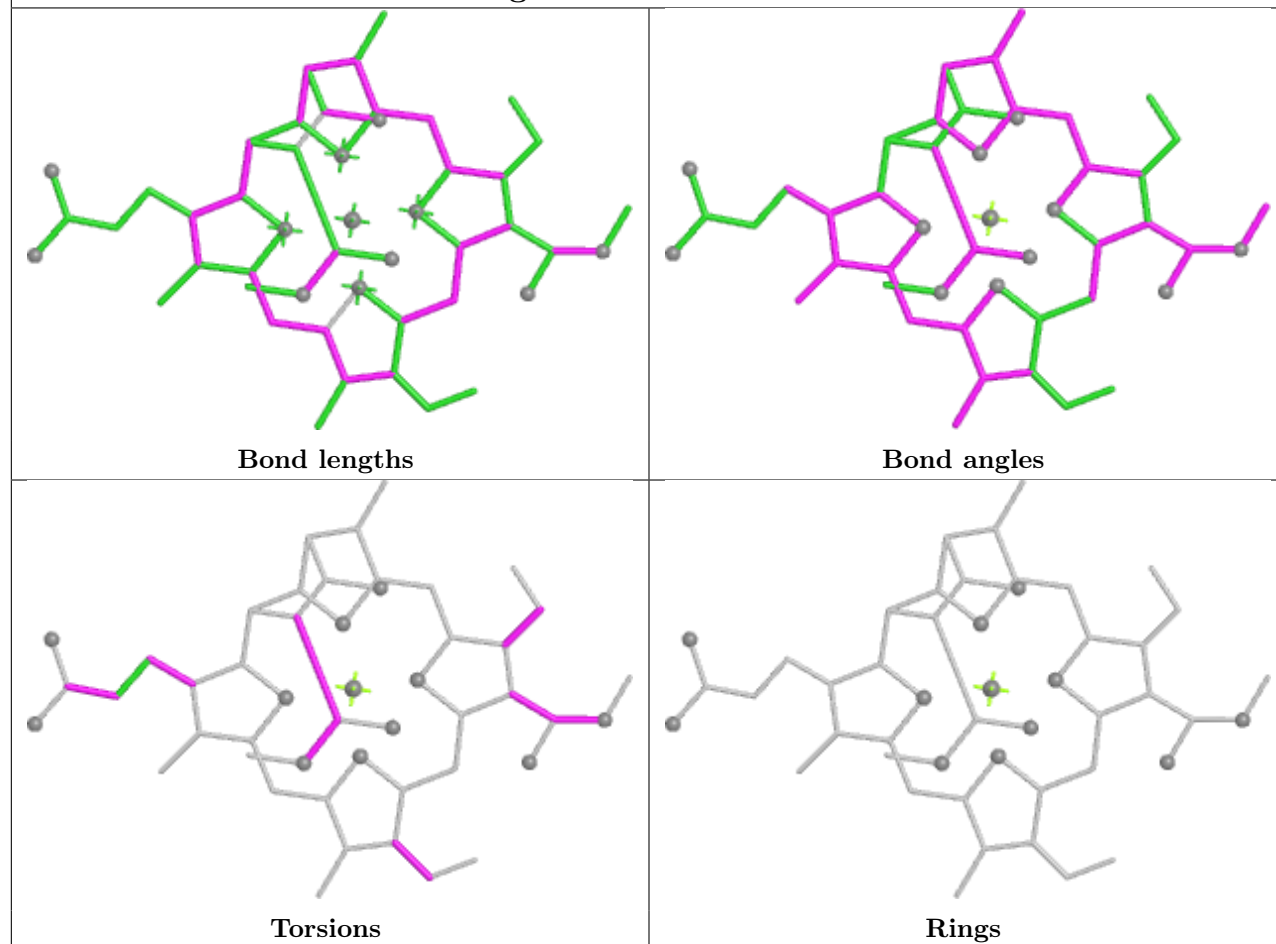


Rings

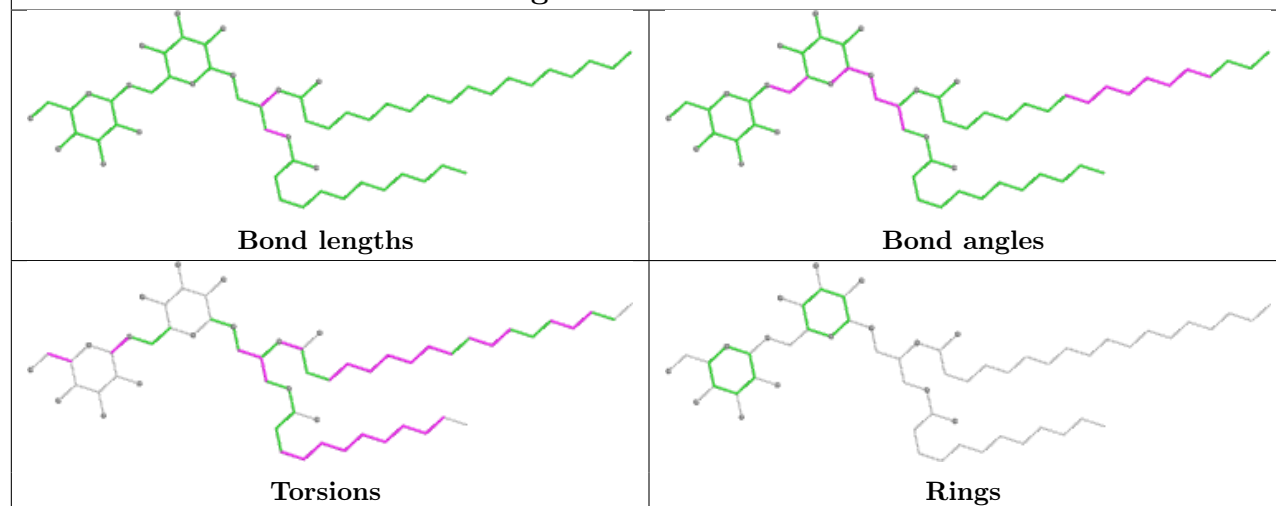


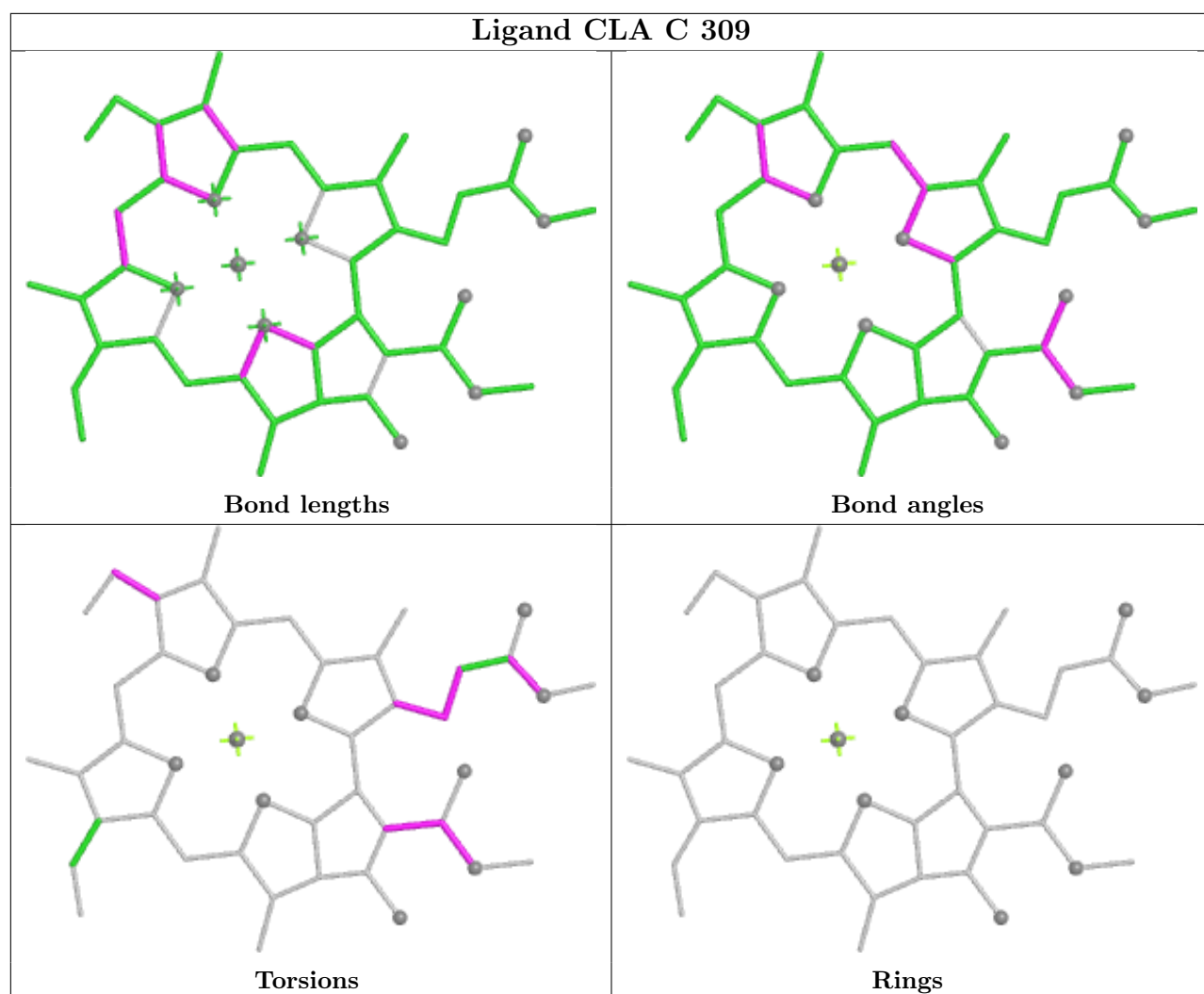


Ligand A1ECV P 315

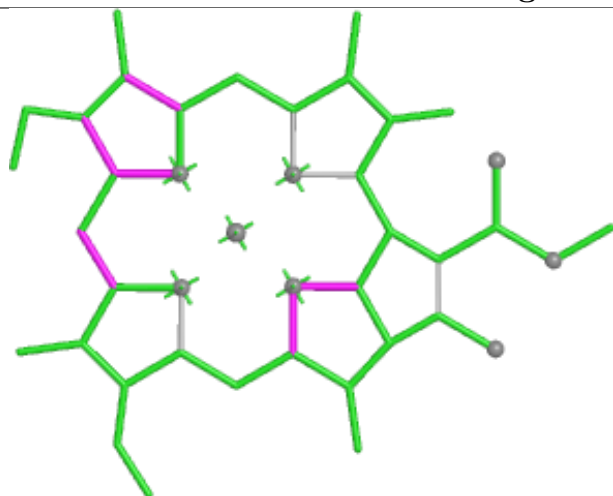


Ligand DGD b 849

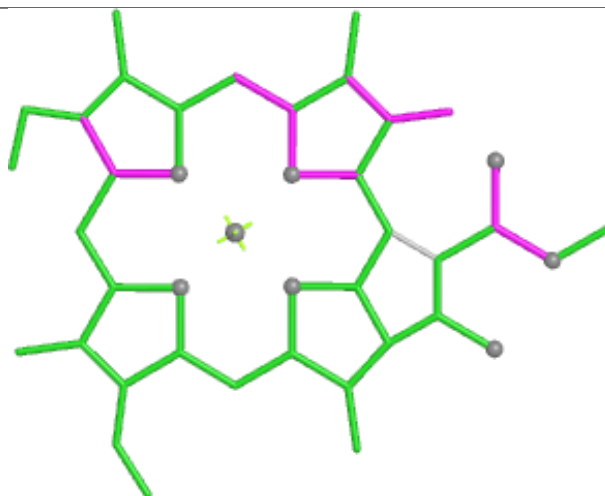




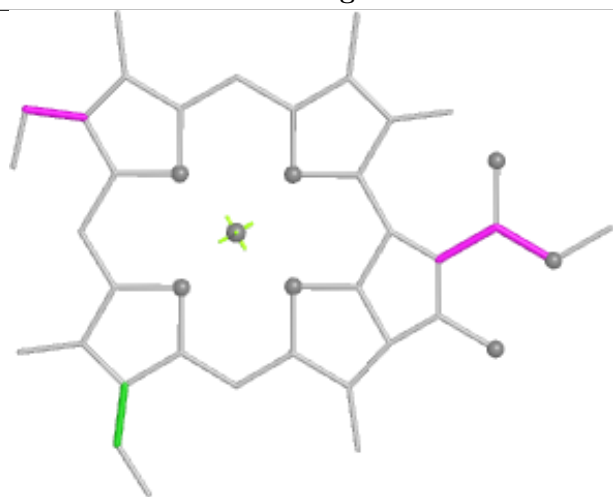
Ligand CLA 1 317



Bond lengths



Bond angles

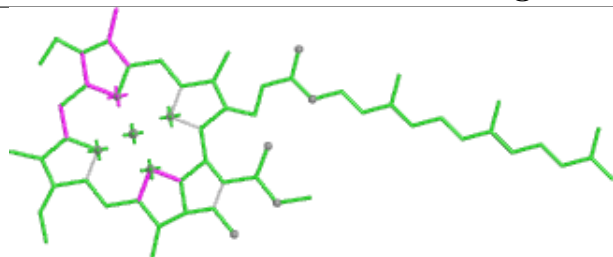


Torsions

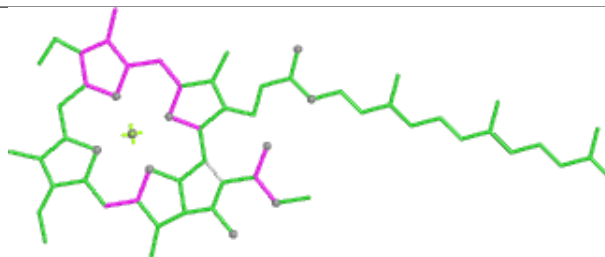


Rings

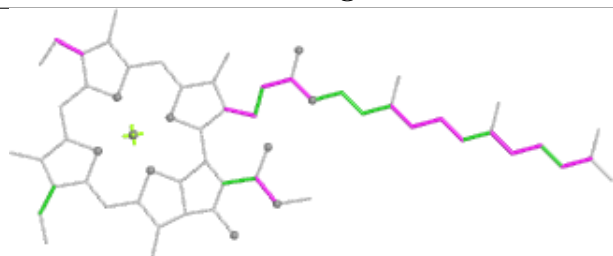
Ligand CLA X 308



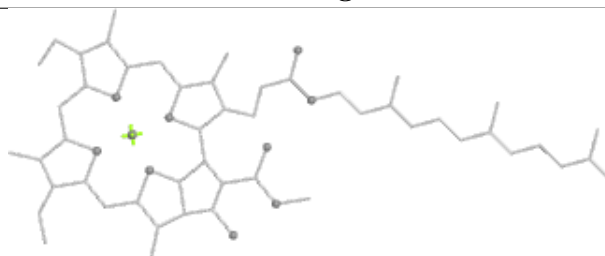
Bond lengths



Bond angles

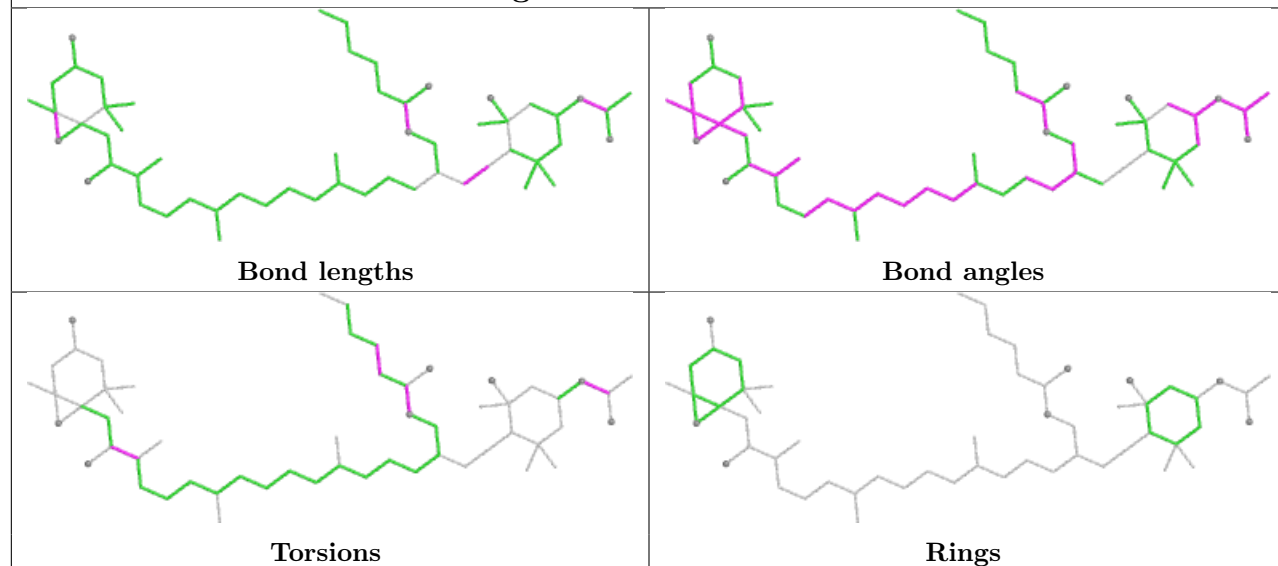


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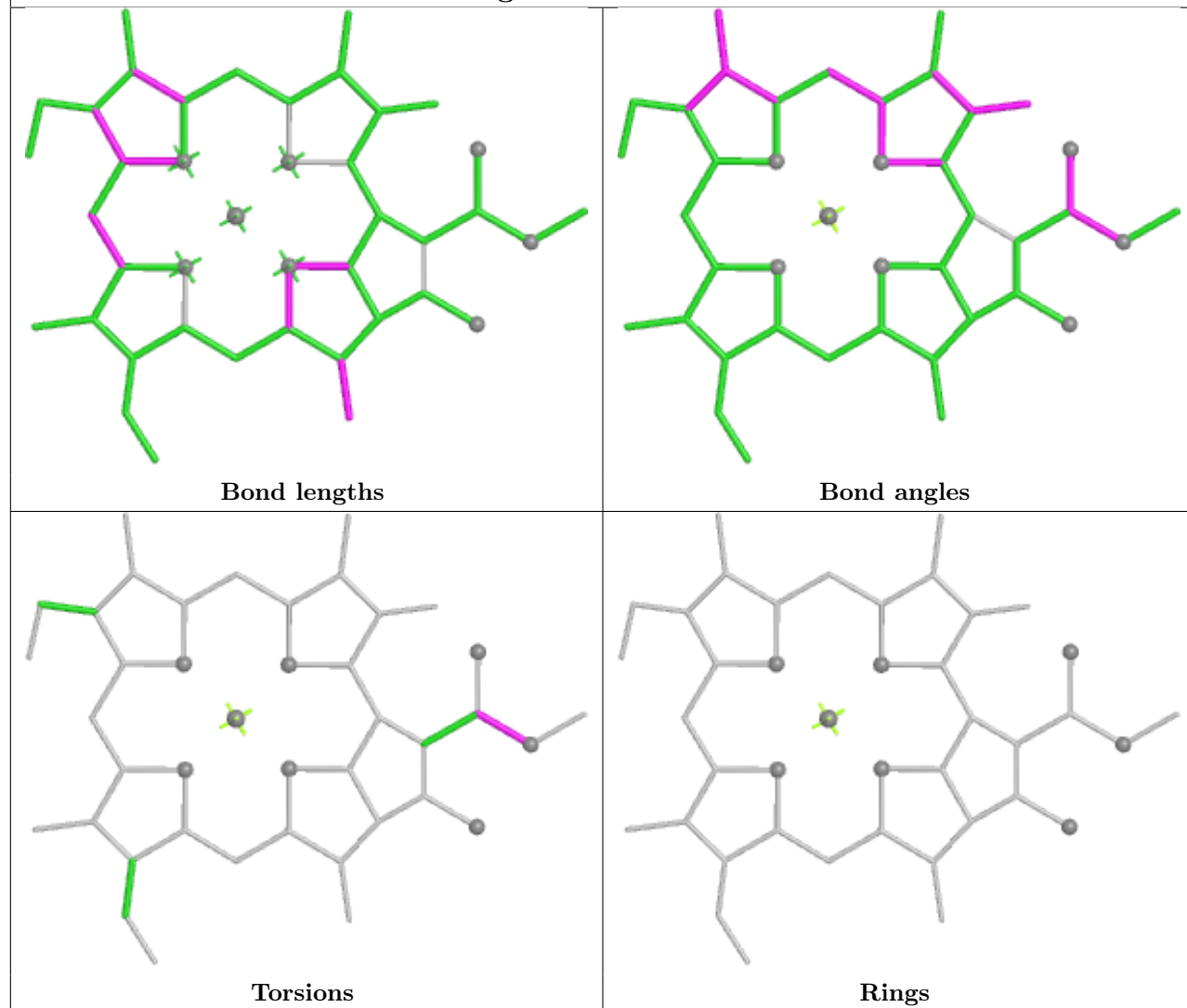


Rings

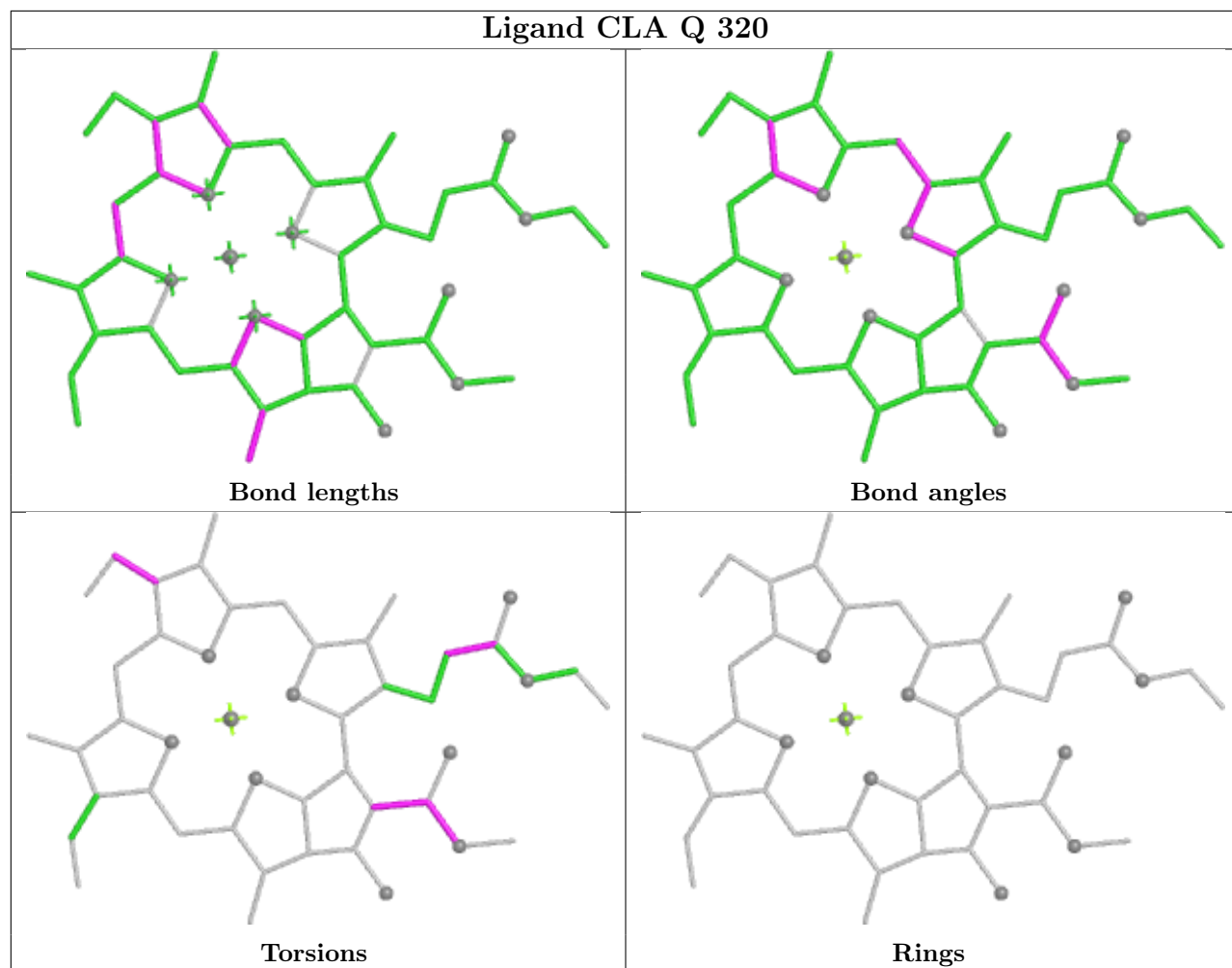
Ligand A1EB1 K 304



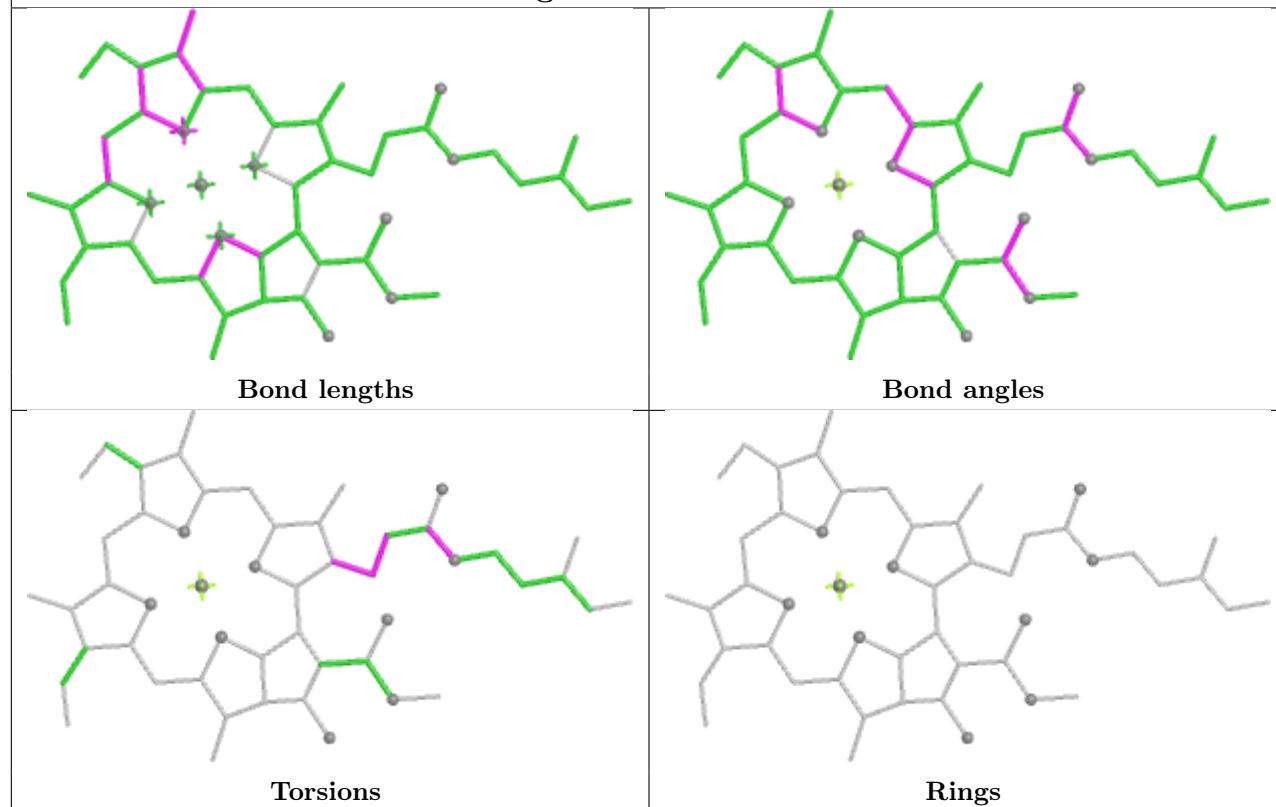
Ligand CLA x 308



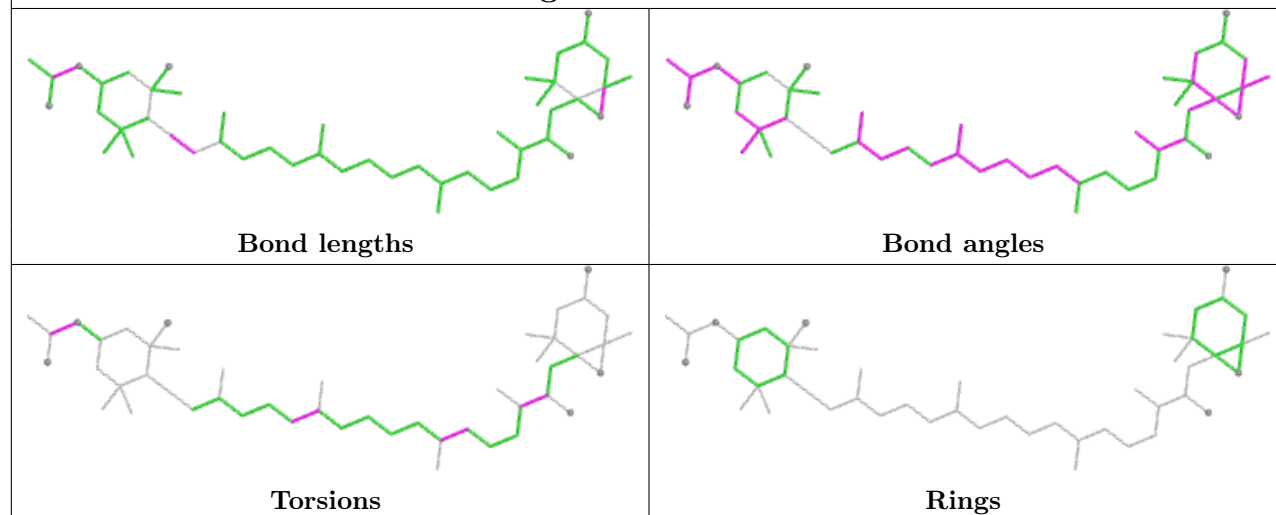
Ligand CLA Q 320

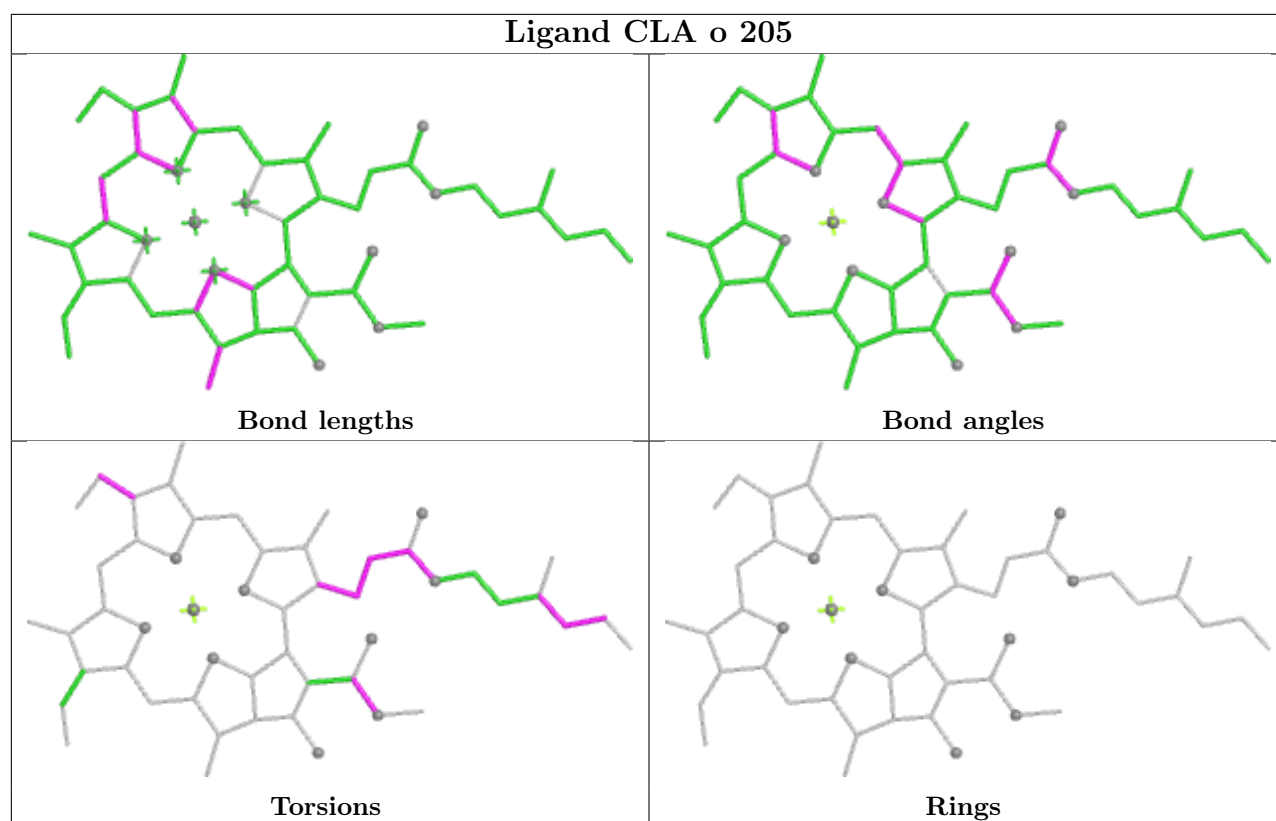


Ligand CLA o 201

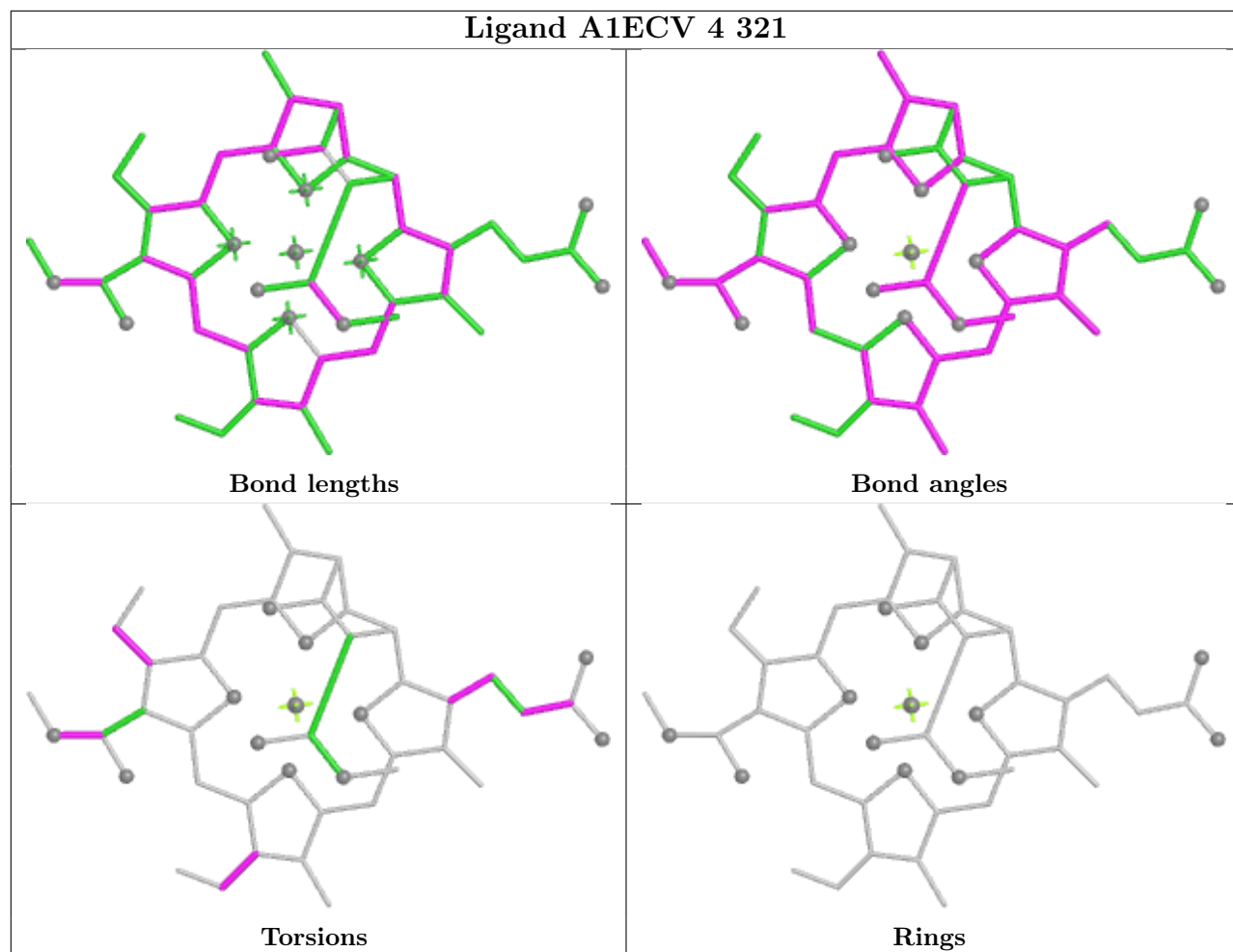


Ligand A86 Z 303

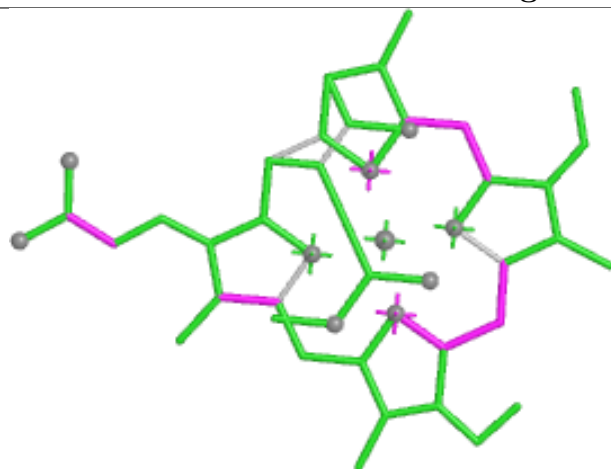




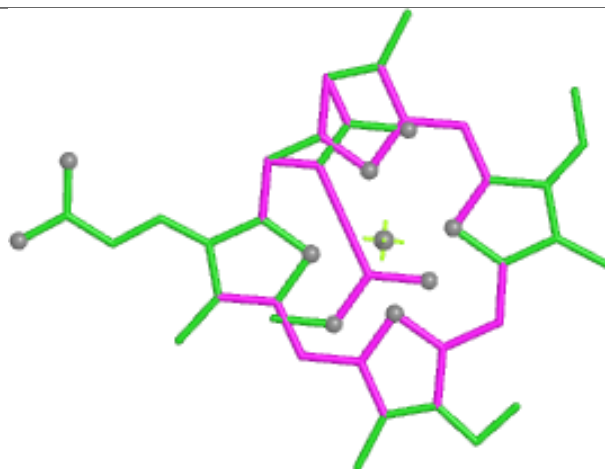
Ligand A1ECV 4 321



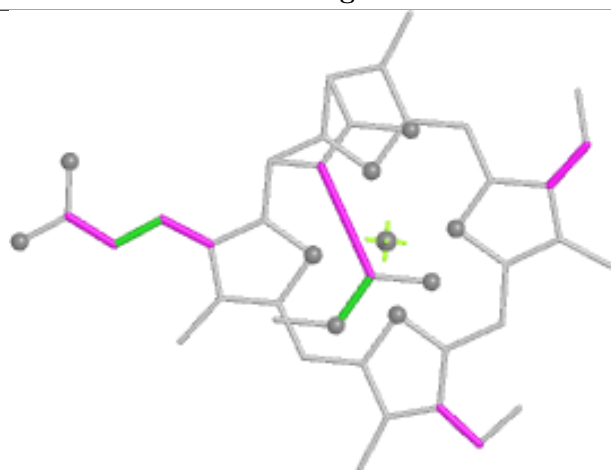
Ligand KC2 8 320



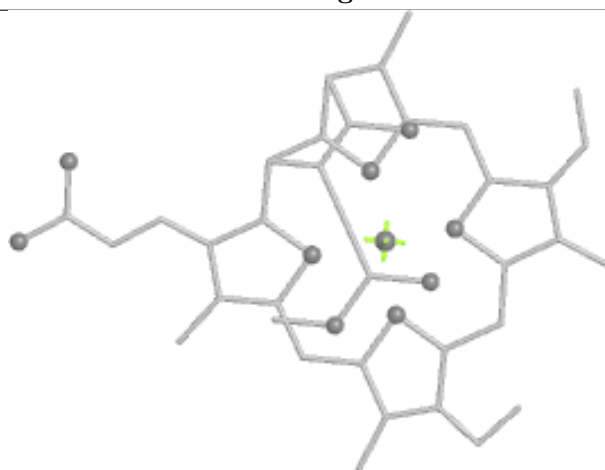
Bond lengths



Bond angles

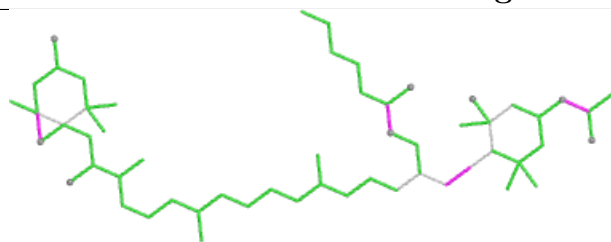


Torsions

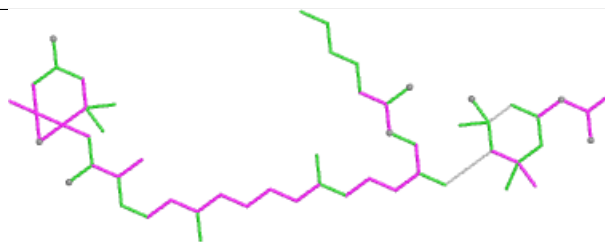


Rings

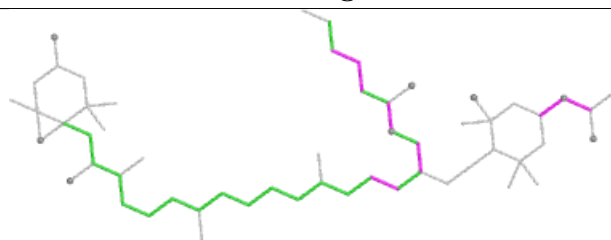
Ligand A1EB1 U 205



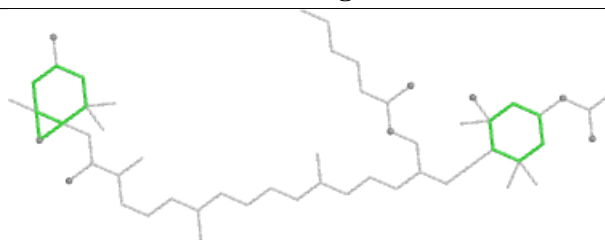
Bond lengths



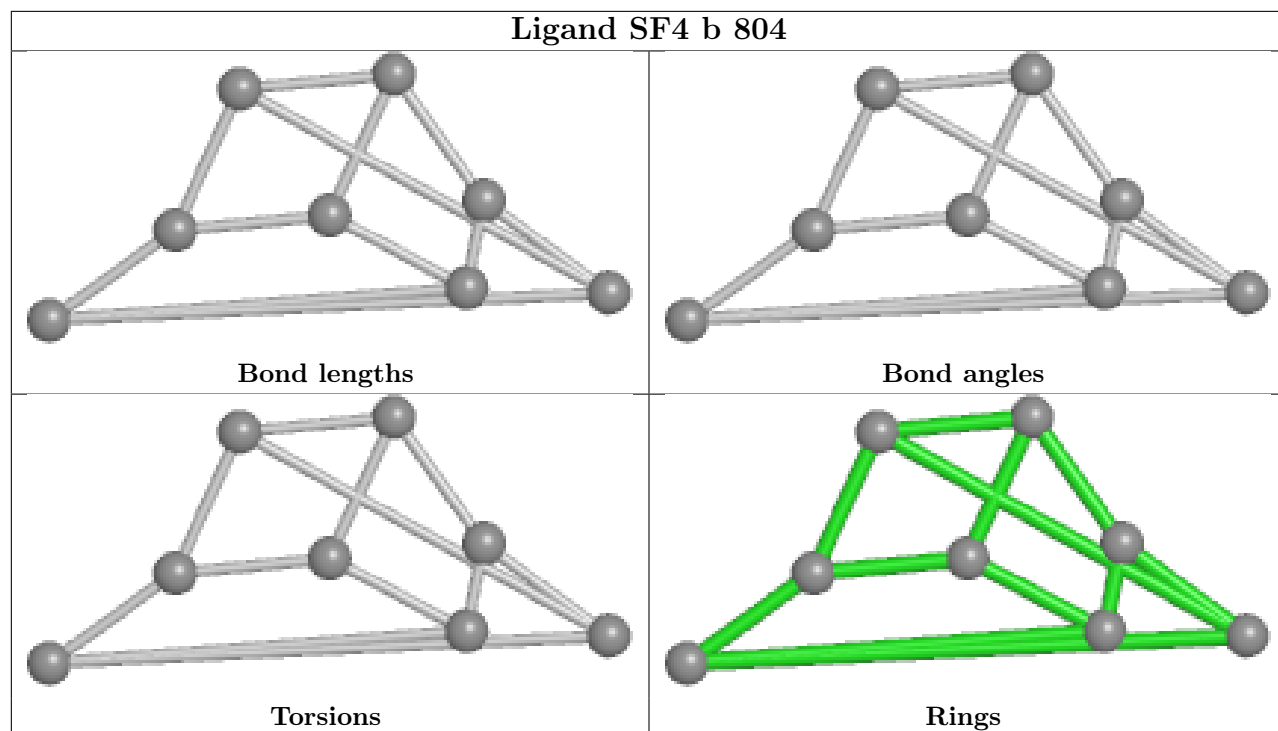
Bond angles



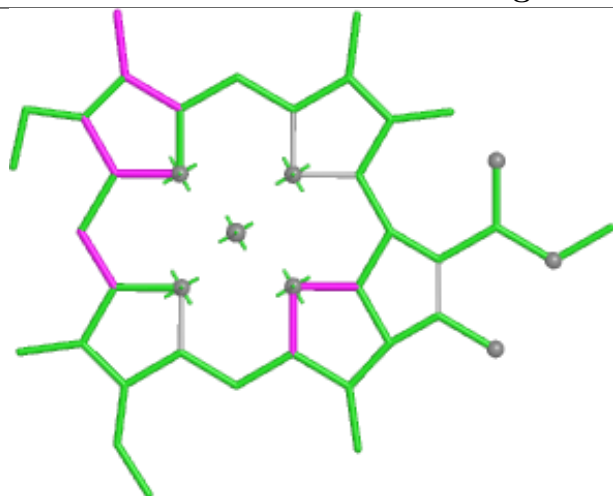
Torsions



Rings



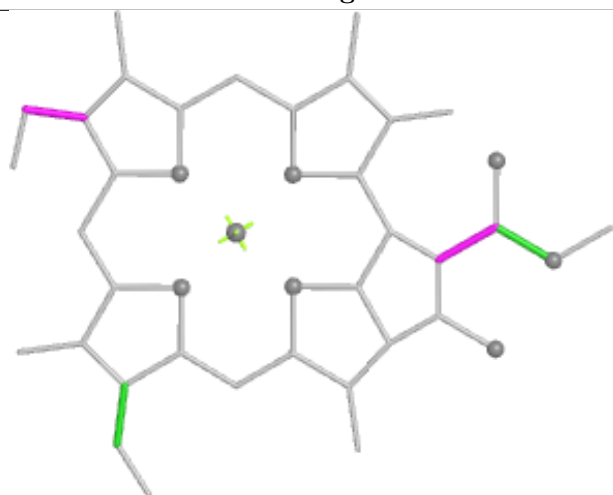
Ligand CLA K 314



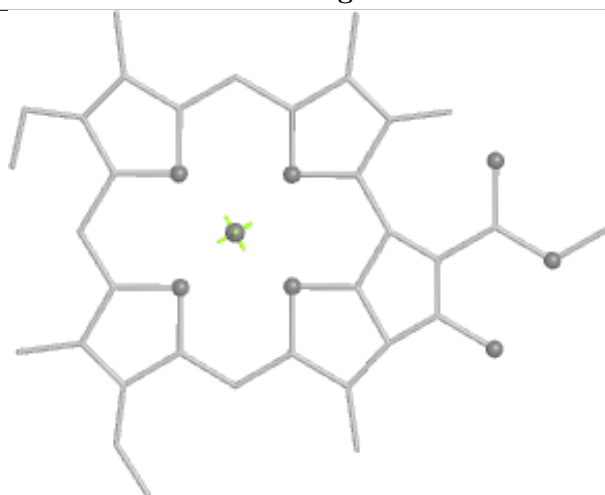
Bond lengths



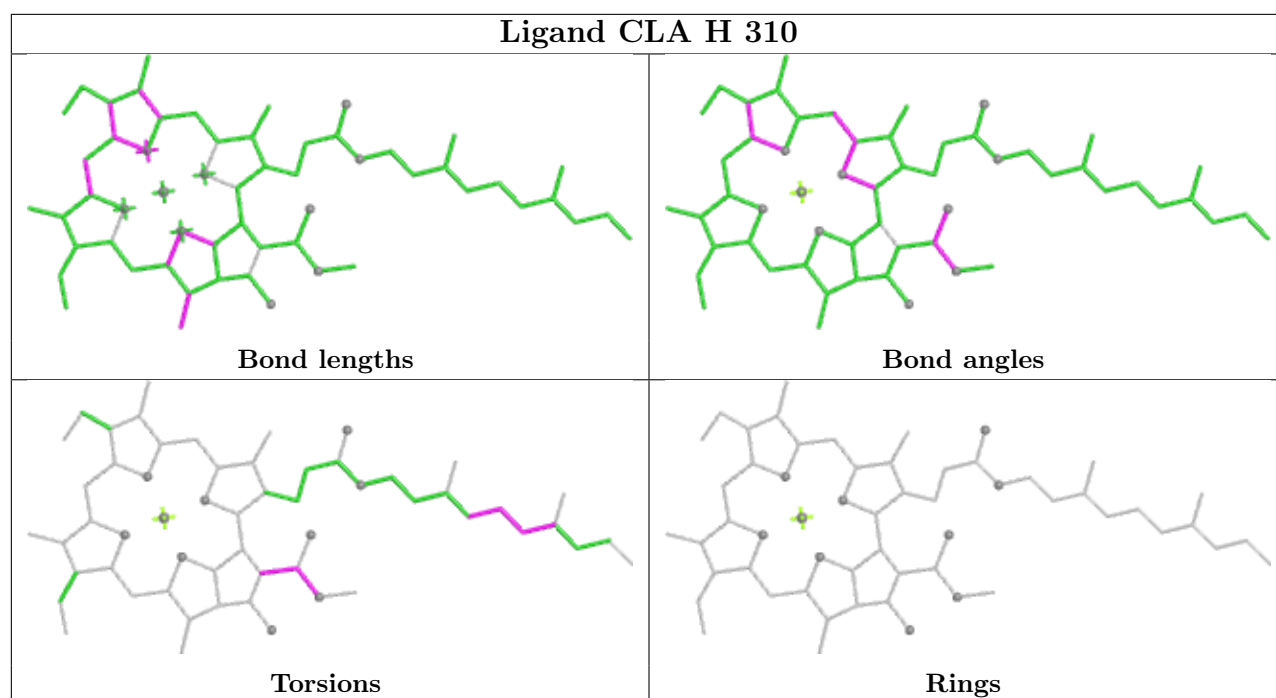
Bond angles



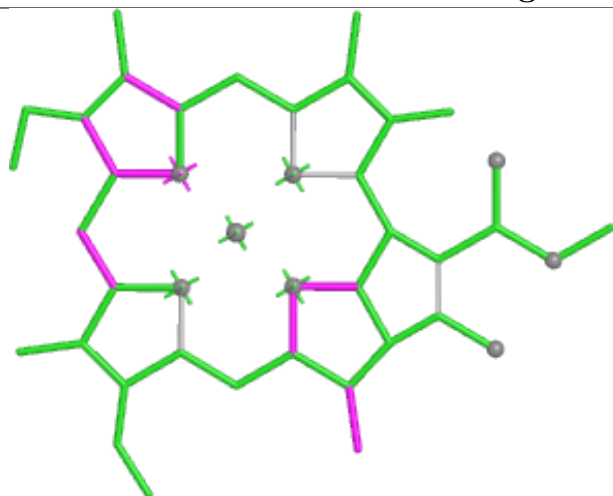
Torsions



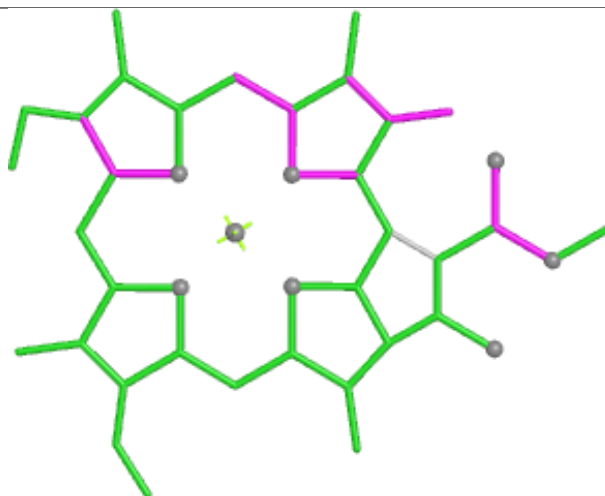
Rings



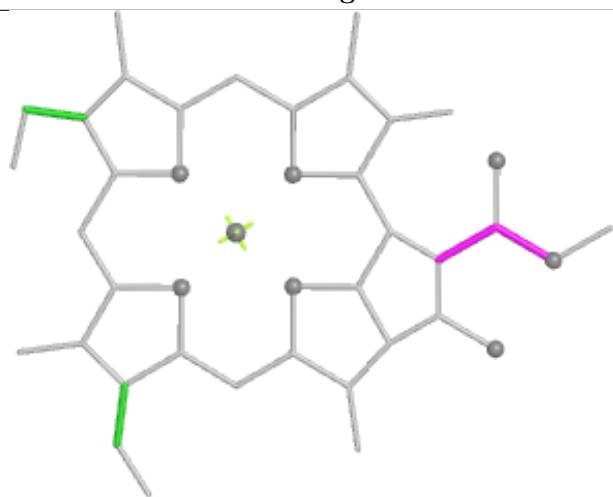
Ligand CLA 9 309



Bond lengths



Bond angles

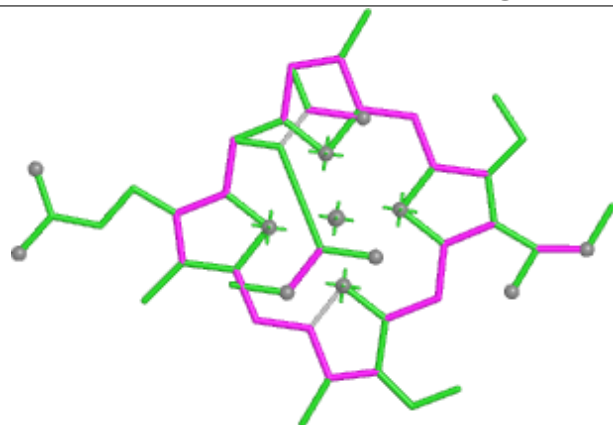


Torsions

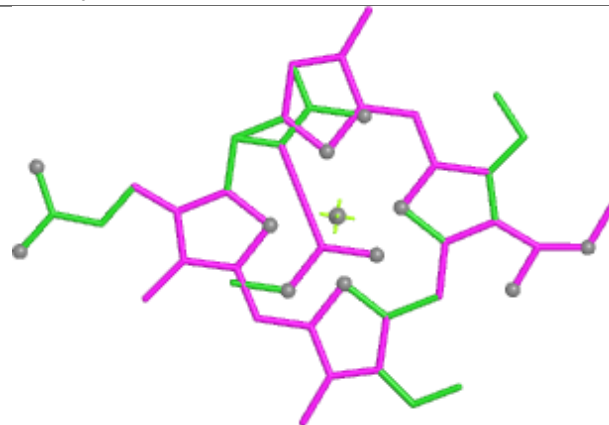


Rings

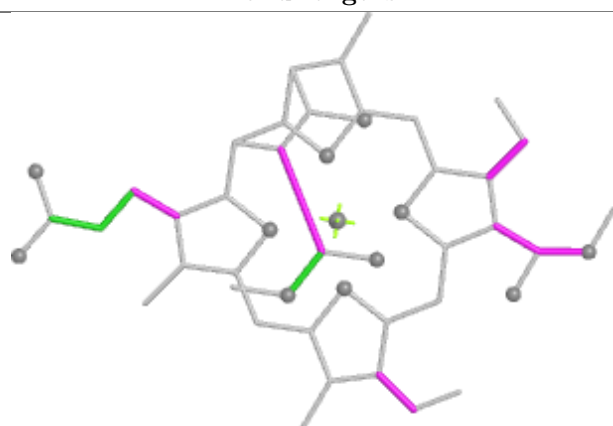
Ligand A1ECV y 317



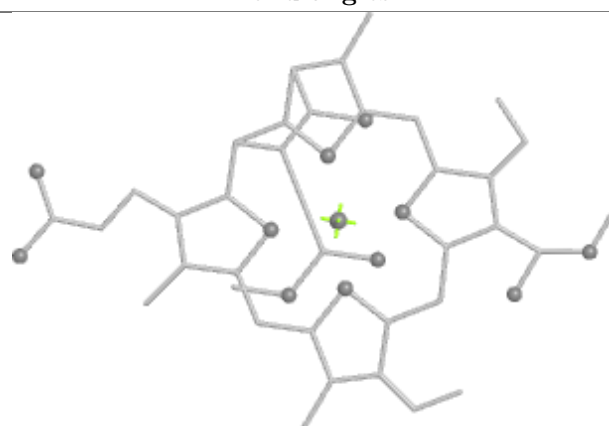
Bond lengths



Bond angles

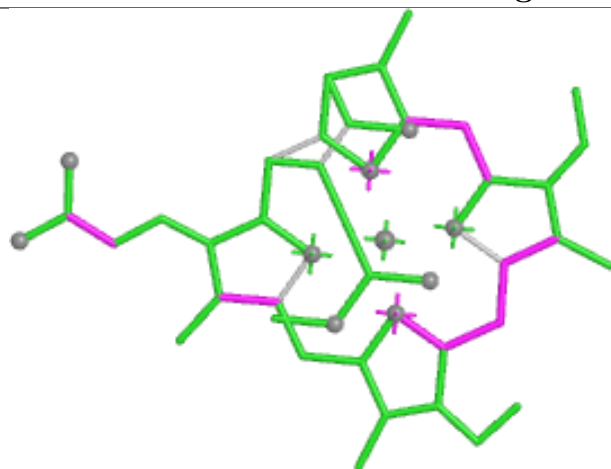


Torsions

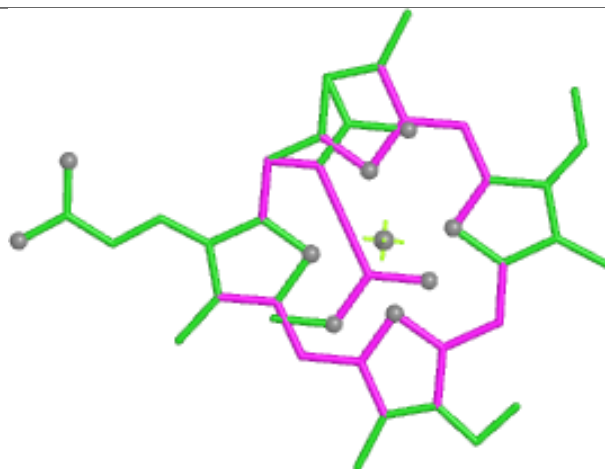


Rings

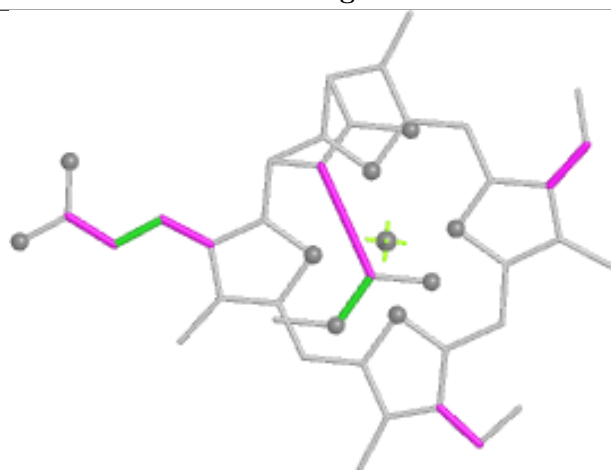
Ligand KC2 H 311



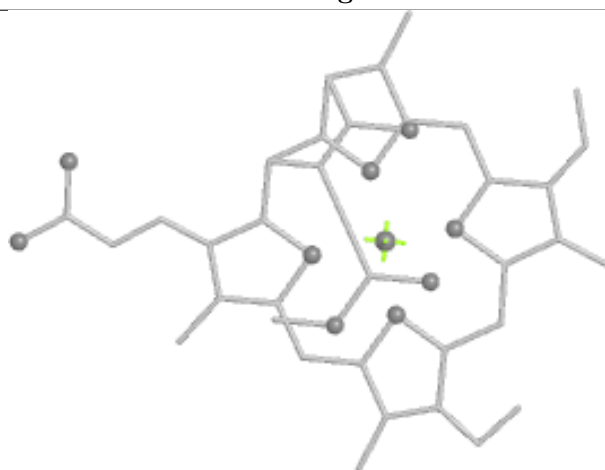
Bond lengths



Bond angles

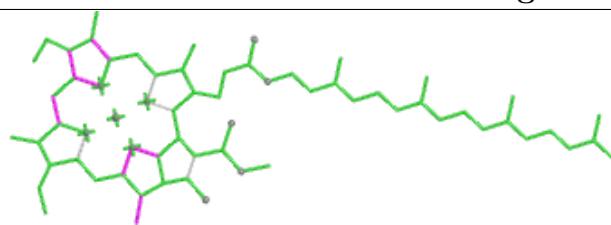


Torsions

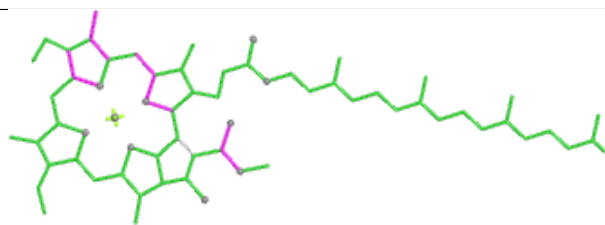


Rings

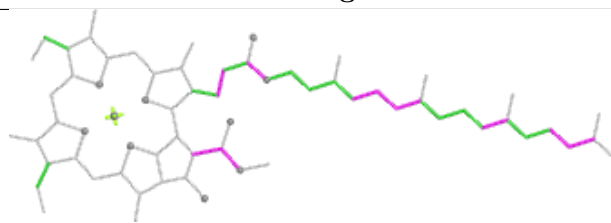
Ligand CLA b 832



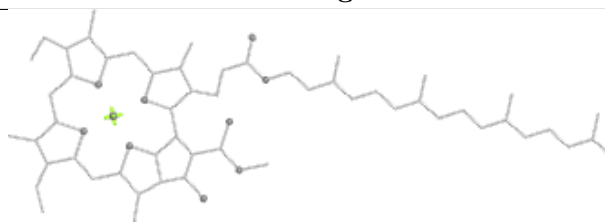
Bond lengths



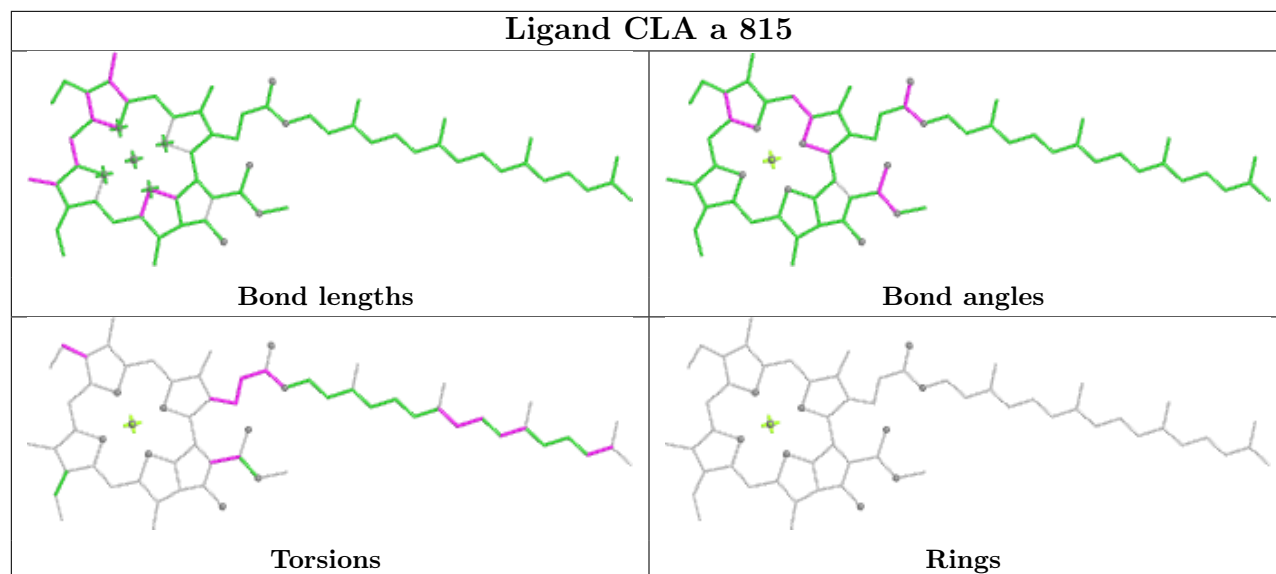
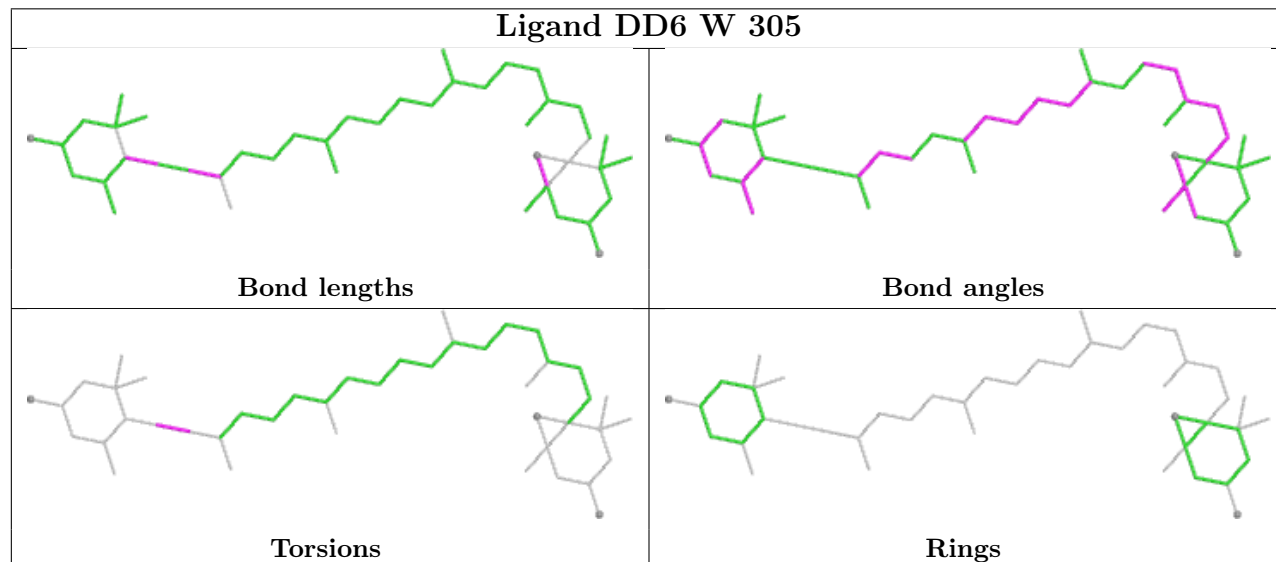
Bond angles



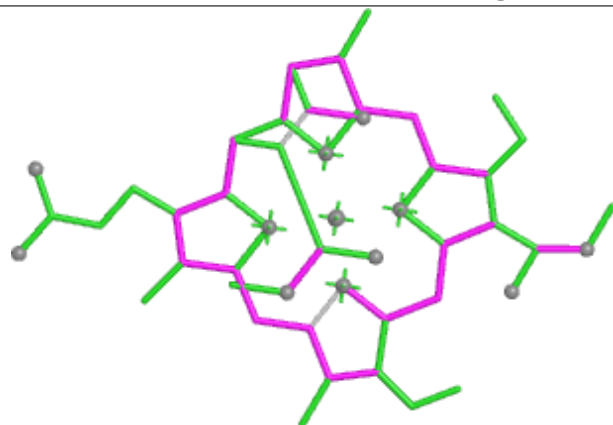
Torsions



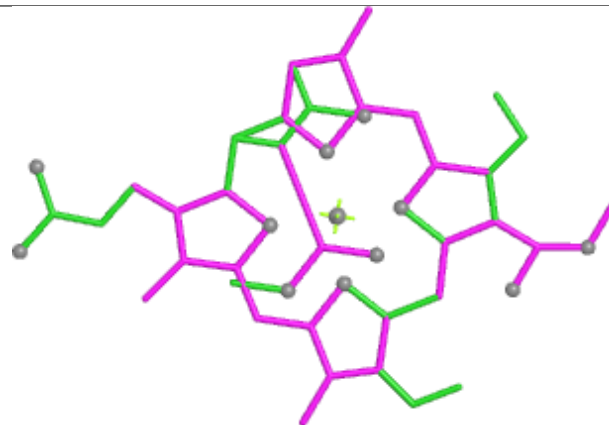
Rings

Ligand CLA a 815**Ligand DD6 W 305**

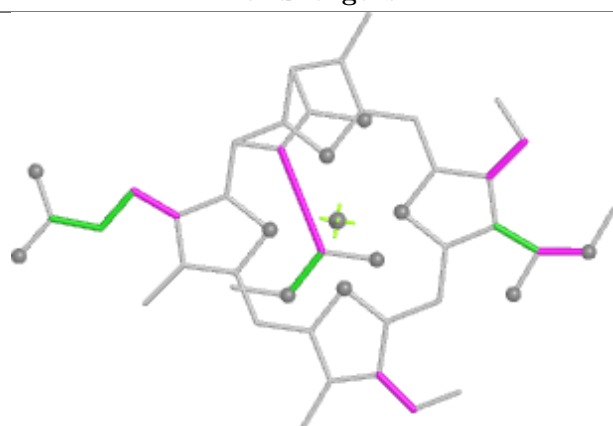
Ligand A1ECV X 313



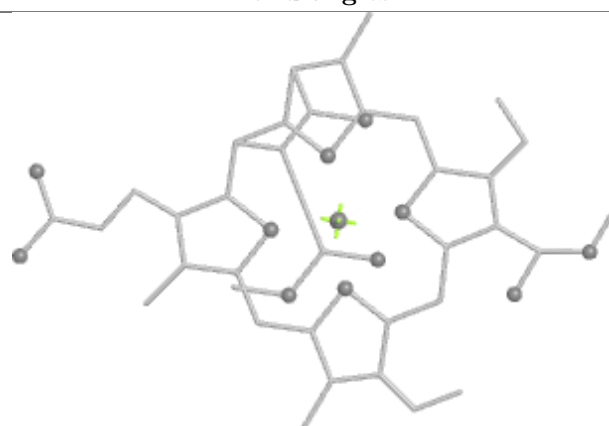
Bond lengths



Bond angles

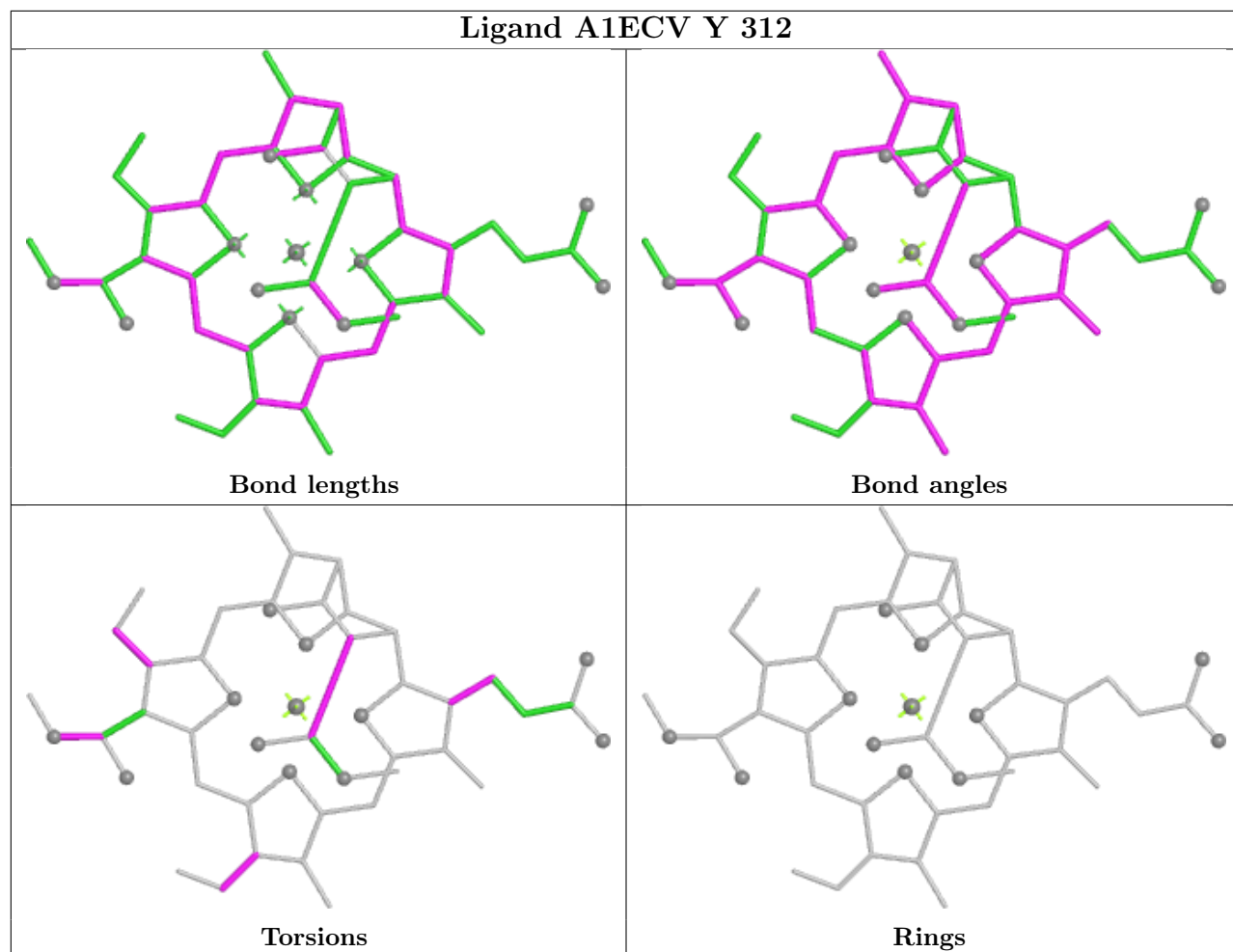


Torsions

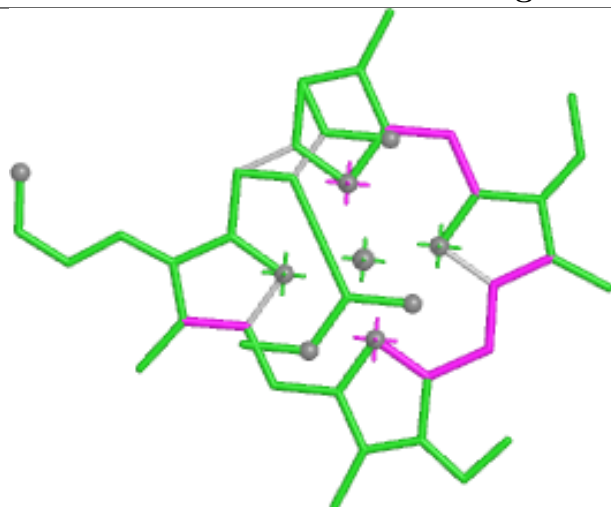


Rings

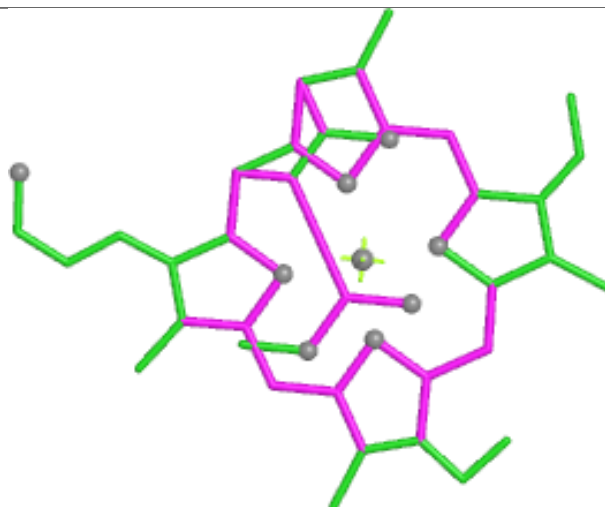
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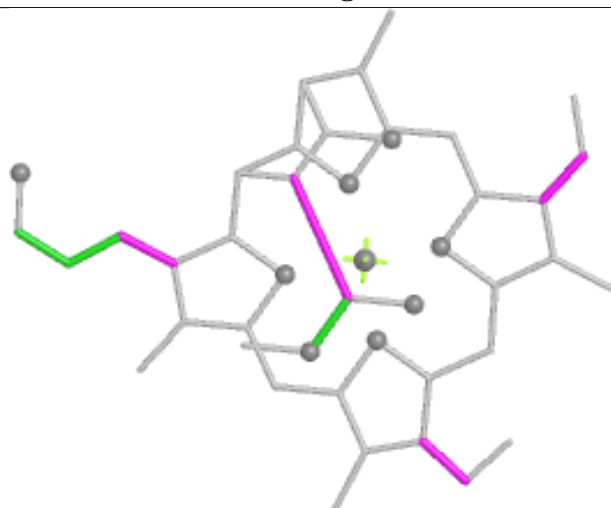
Ligand KC2 X 314



Bond lengths



Bond angles

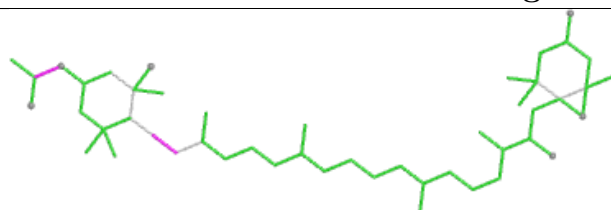


Torsions

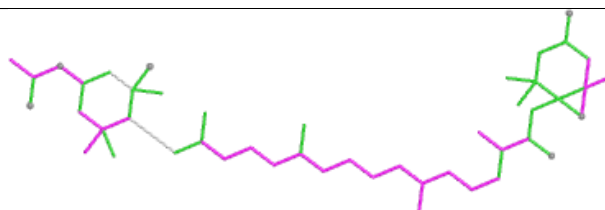


Rings

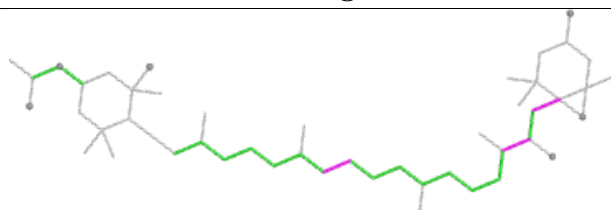
Ligand A86 S 305



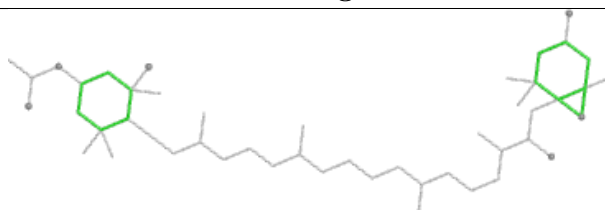
Bond lengths



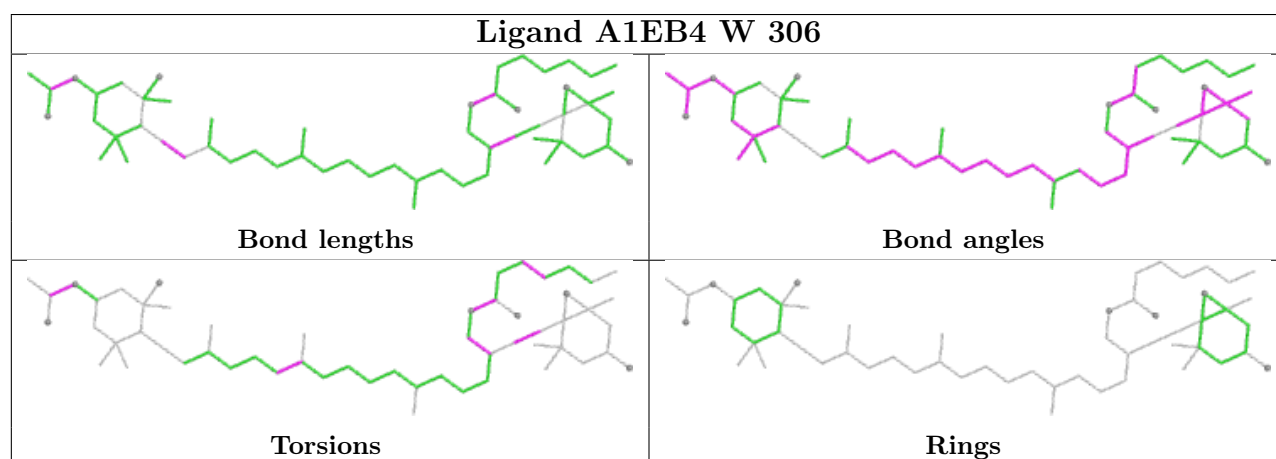
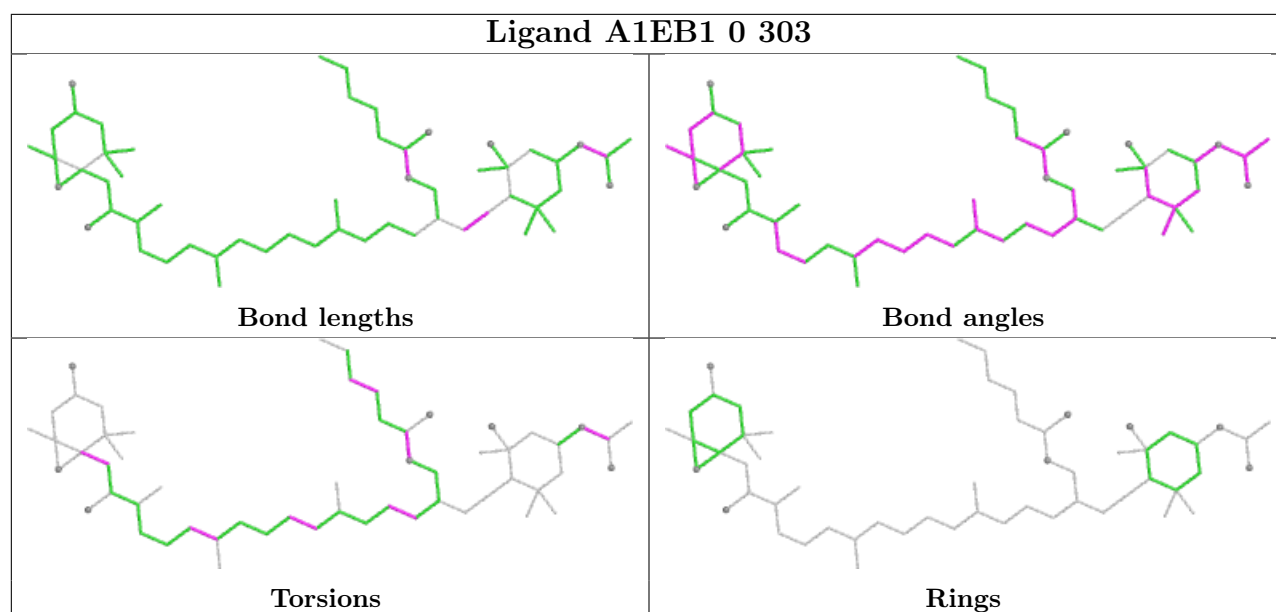
Bond angles

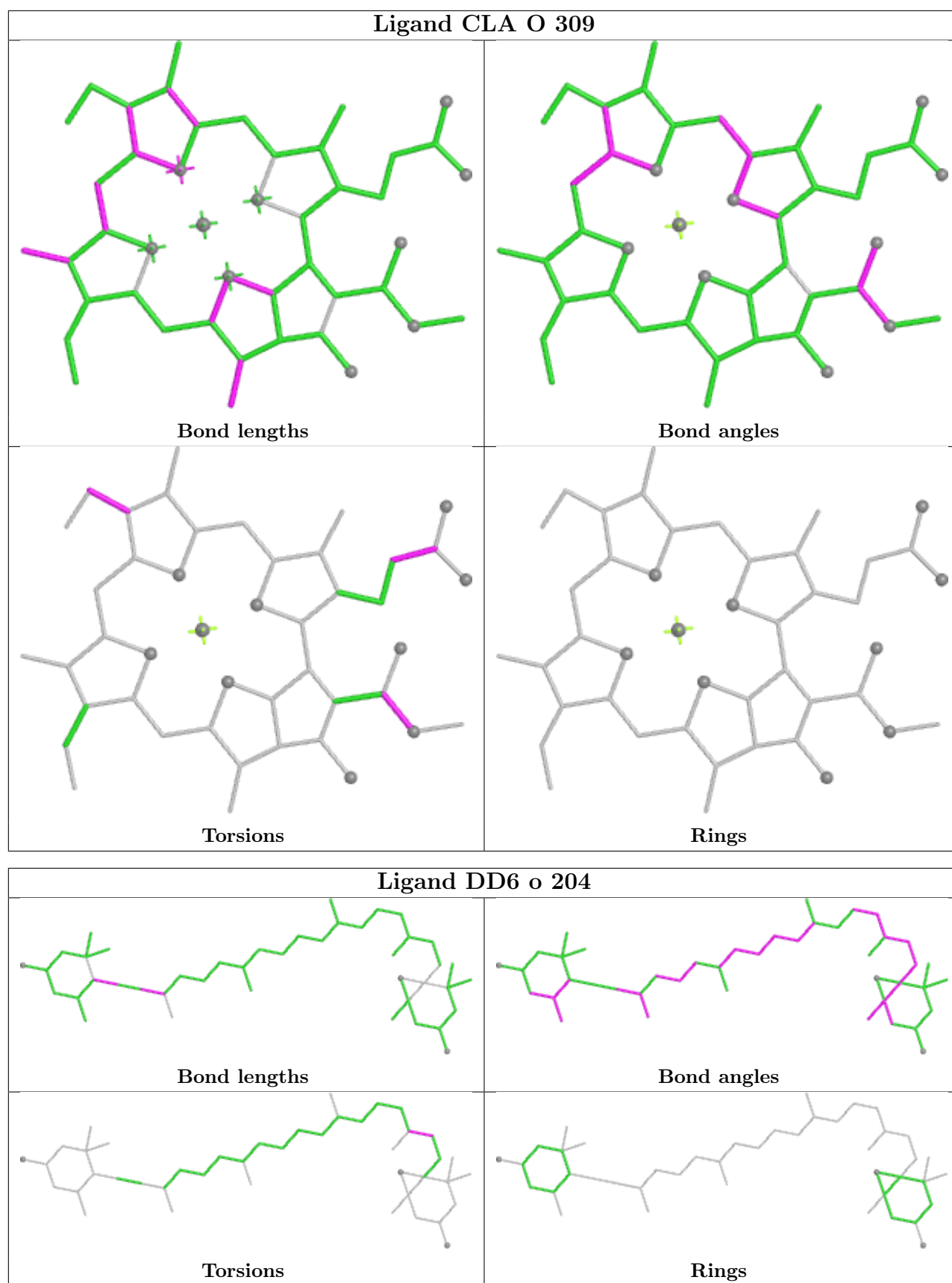


Torsions

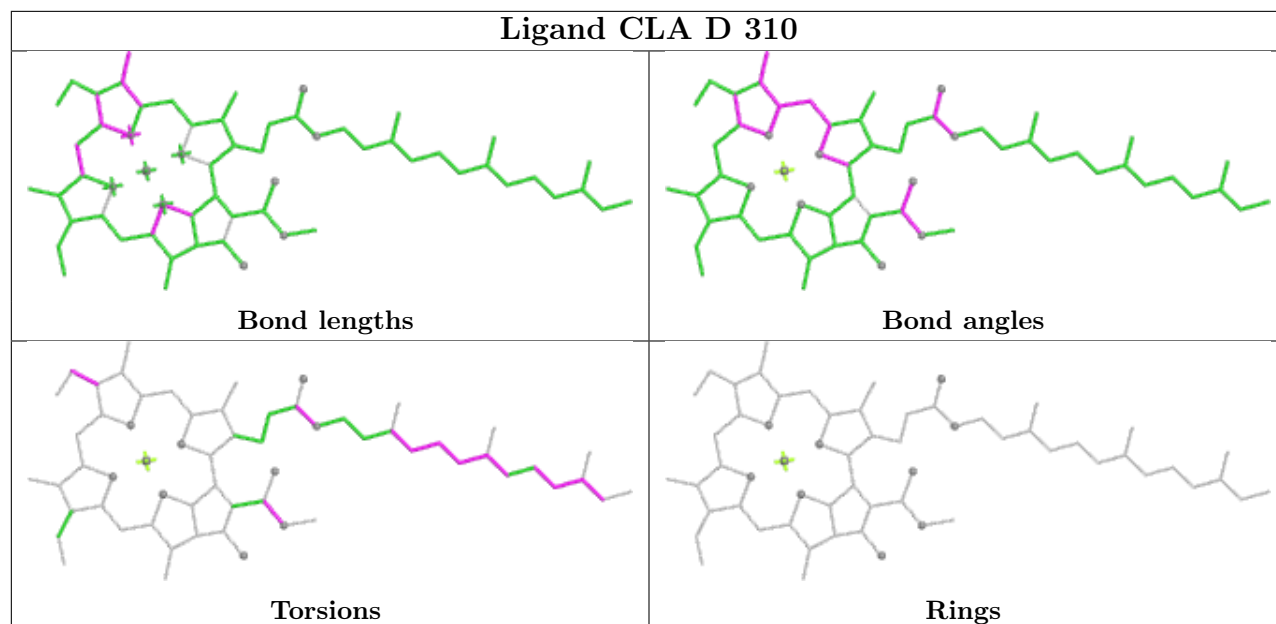


Rings

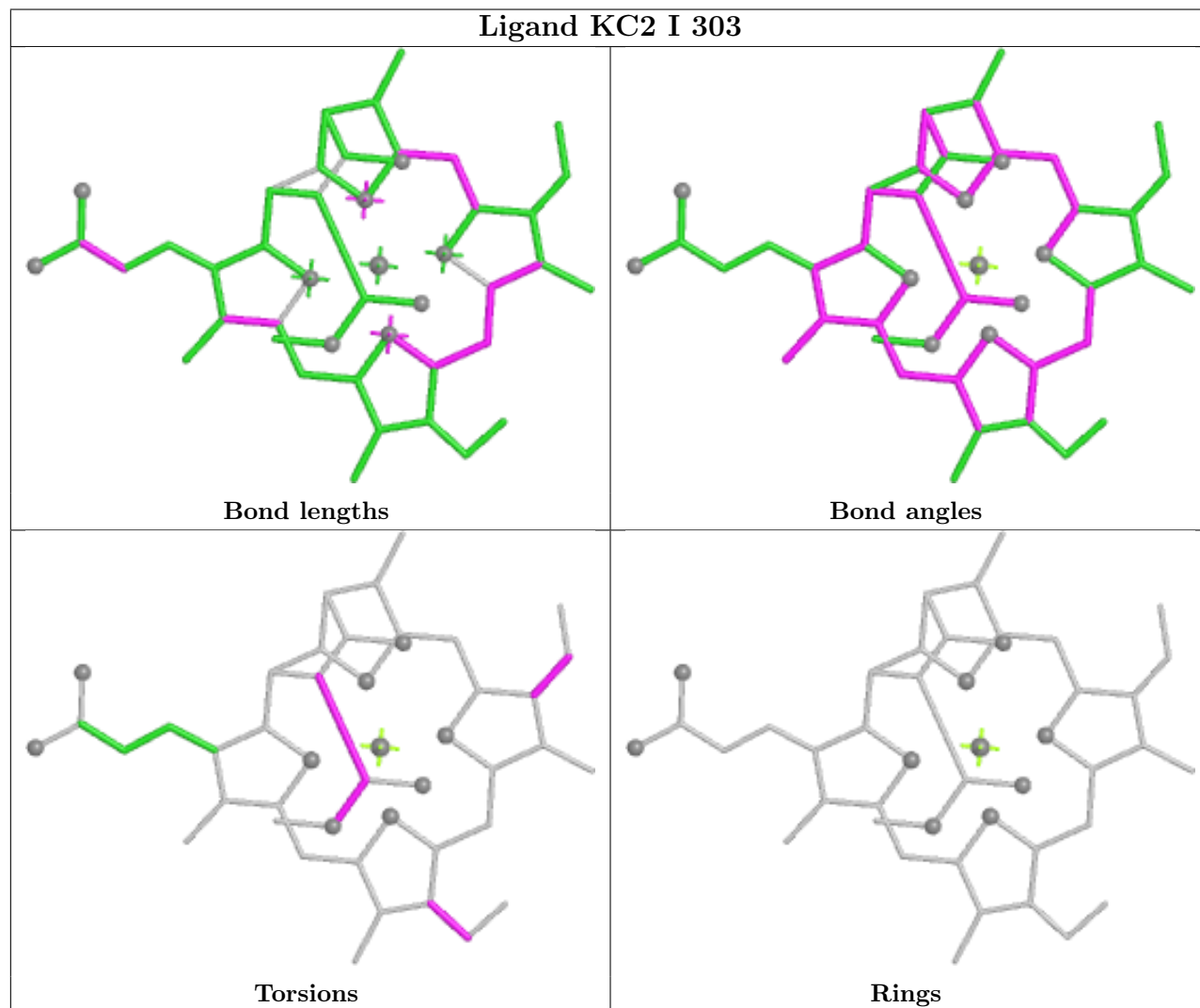




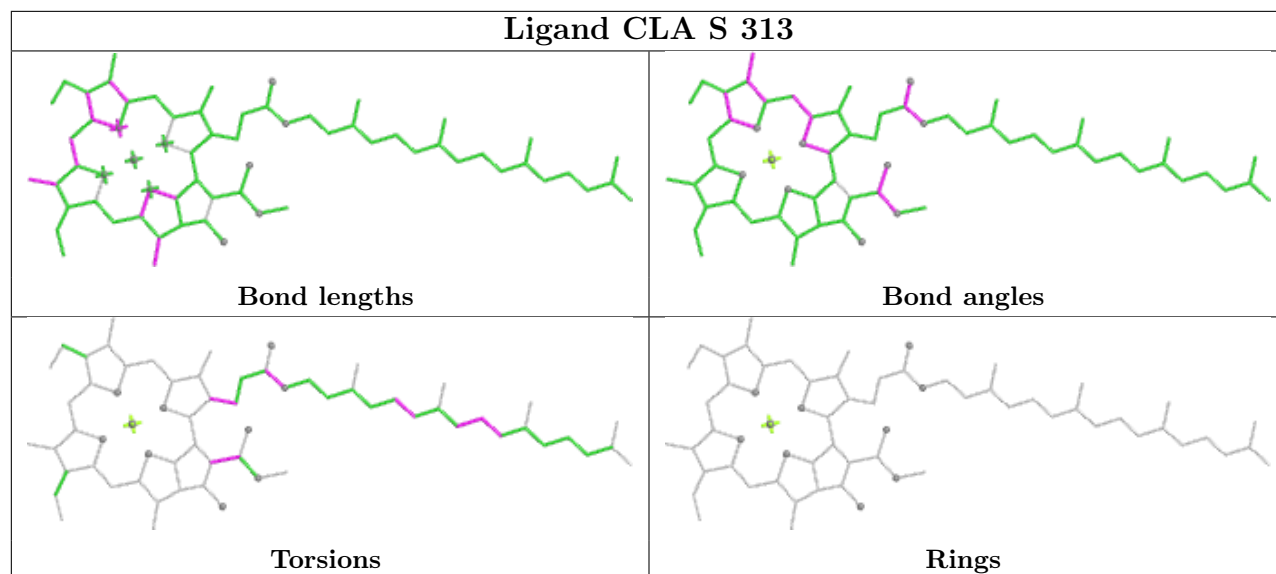
Ligand CLA D 310



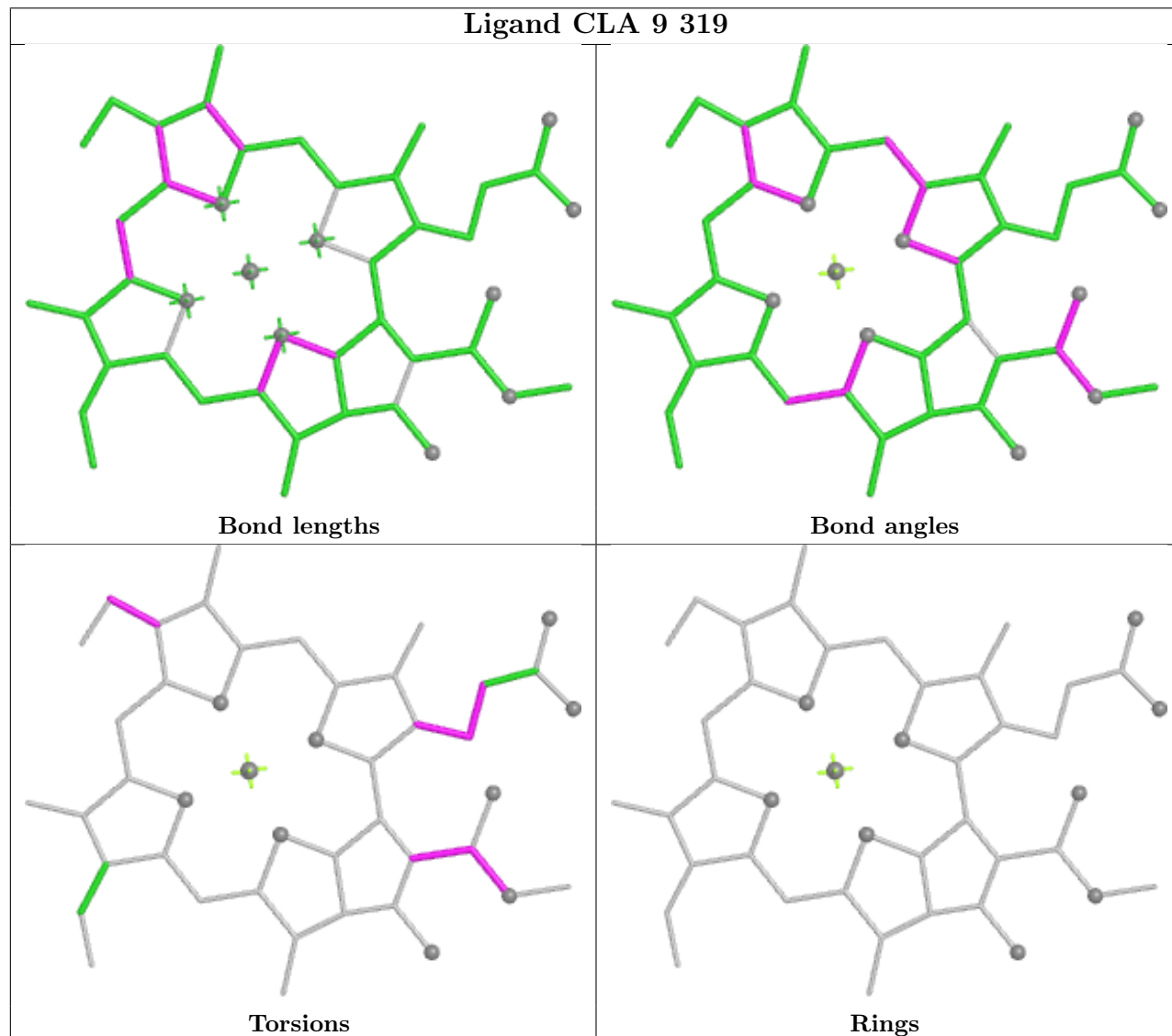
Ligand KC2 I 303

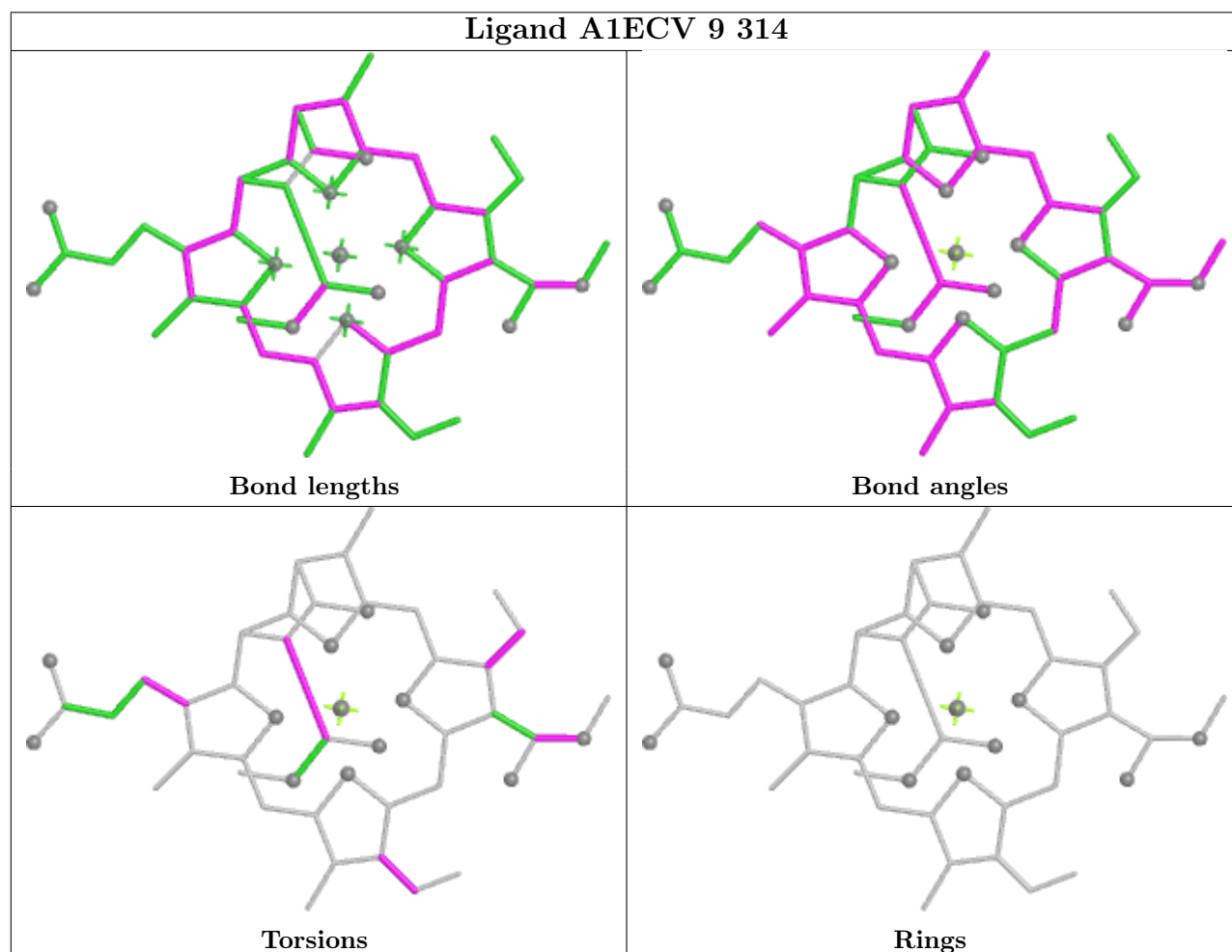
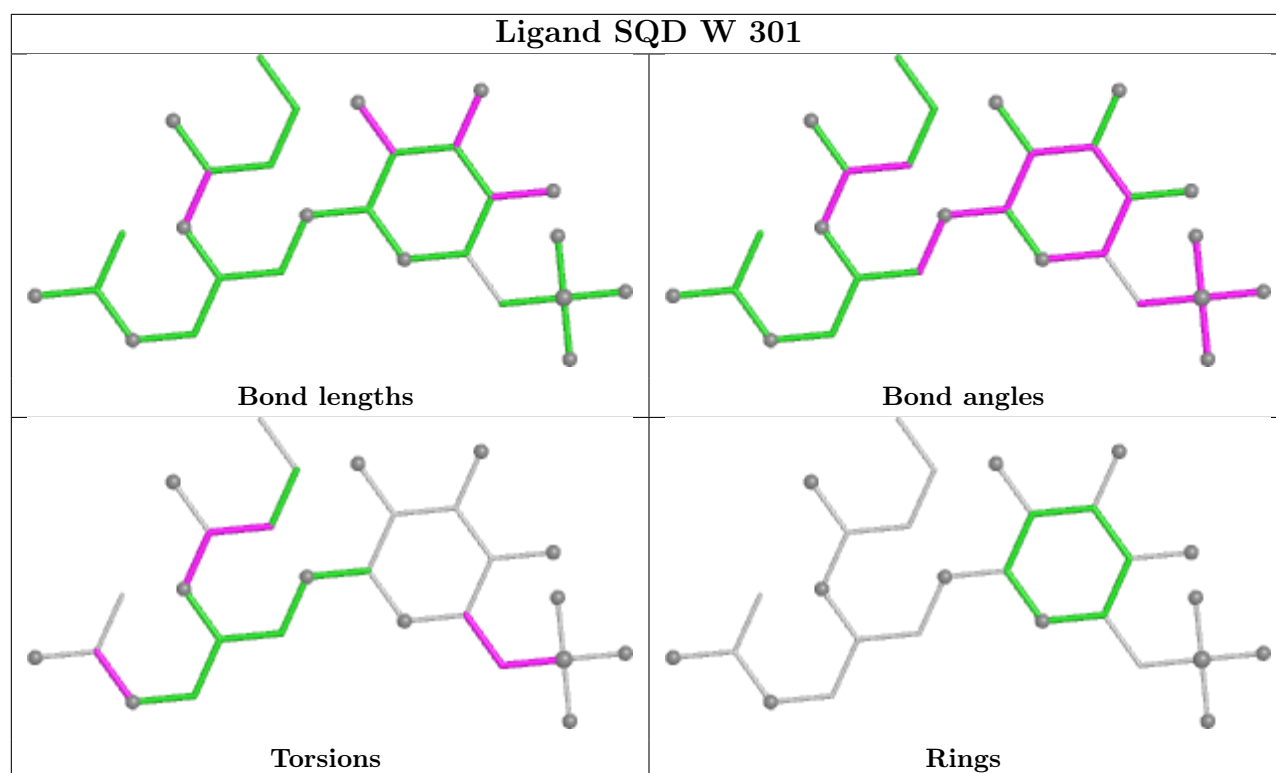


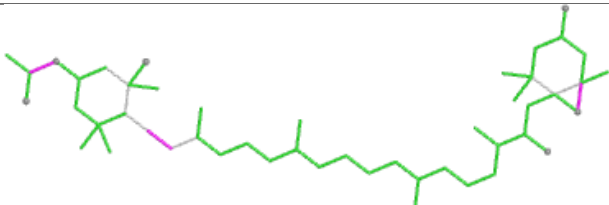
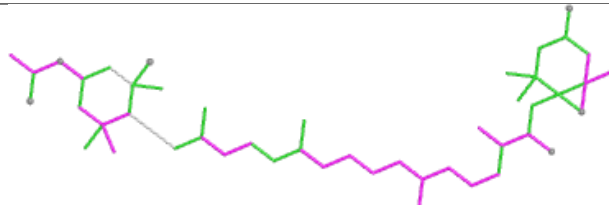
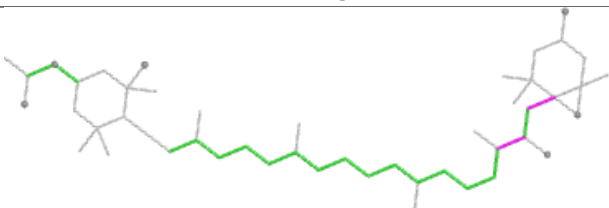
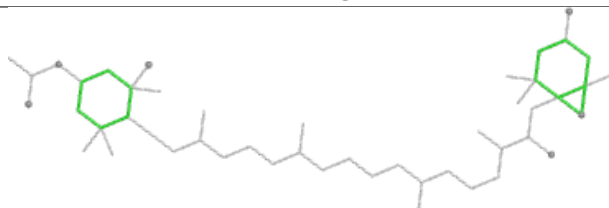
Ligand CLA S 313

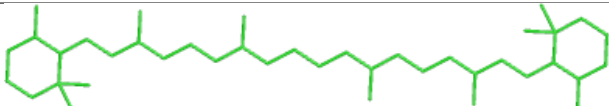
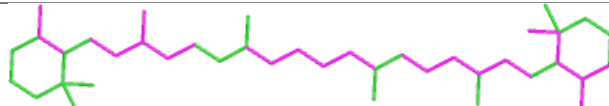
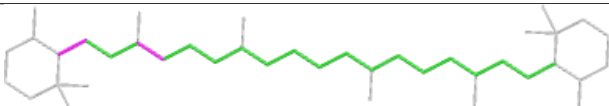
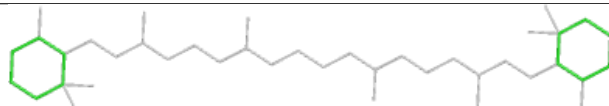


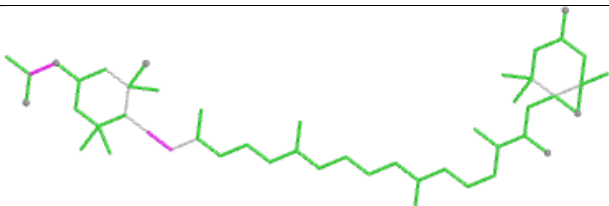
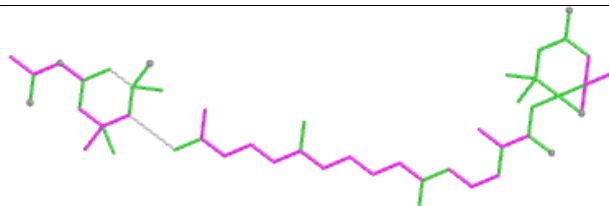
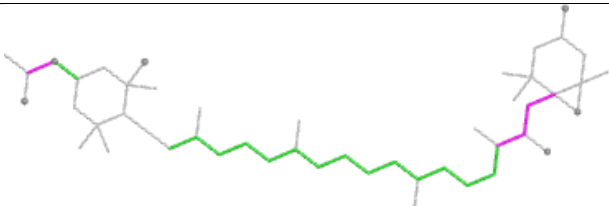
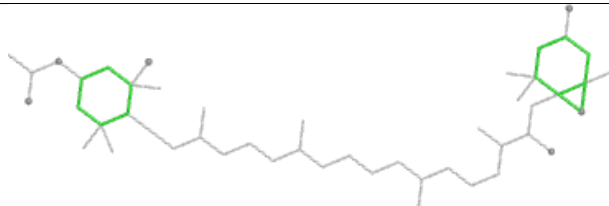
Ligand CLA 9 319

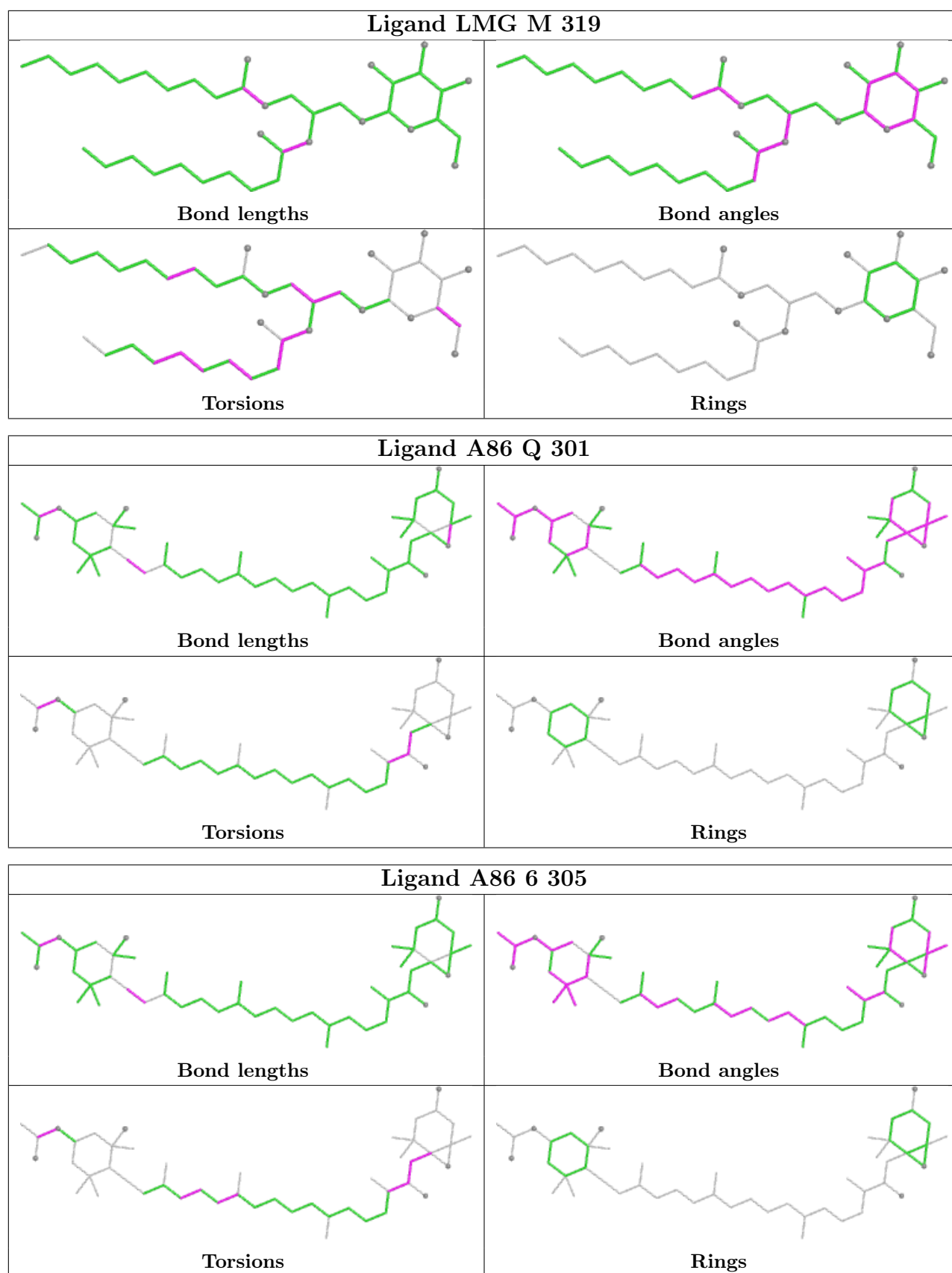


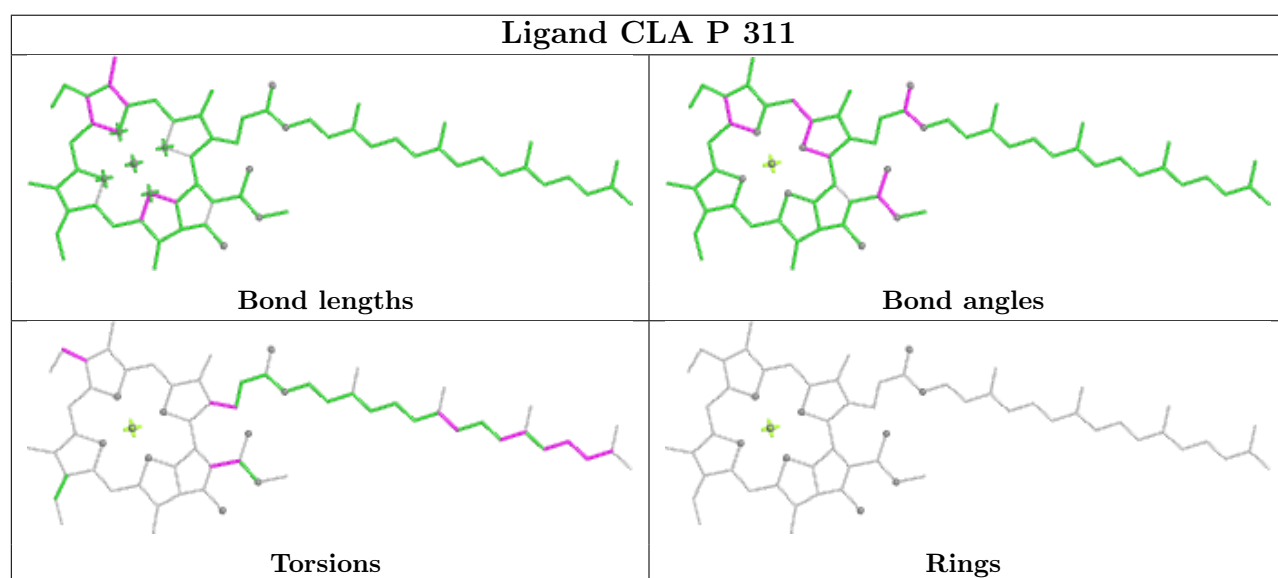
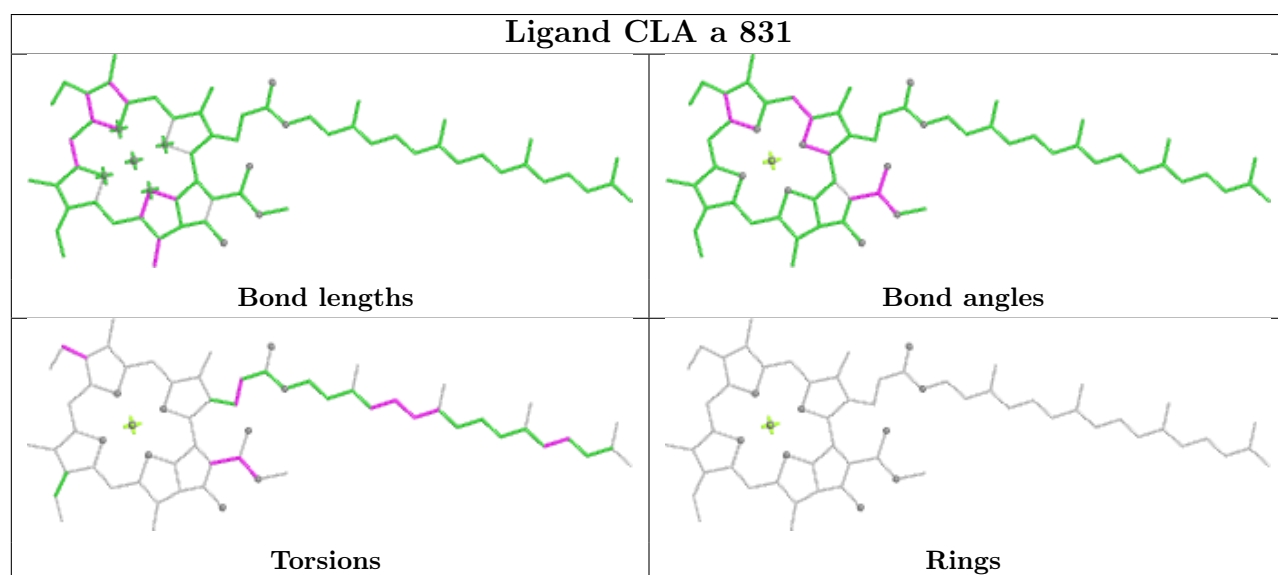
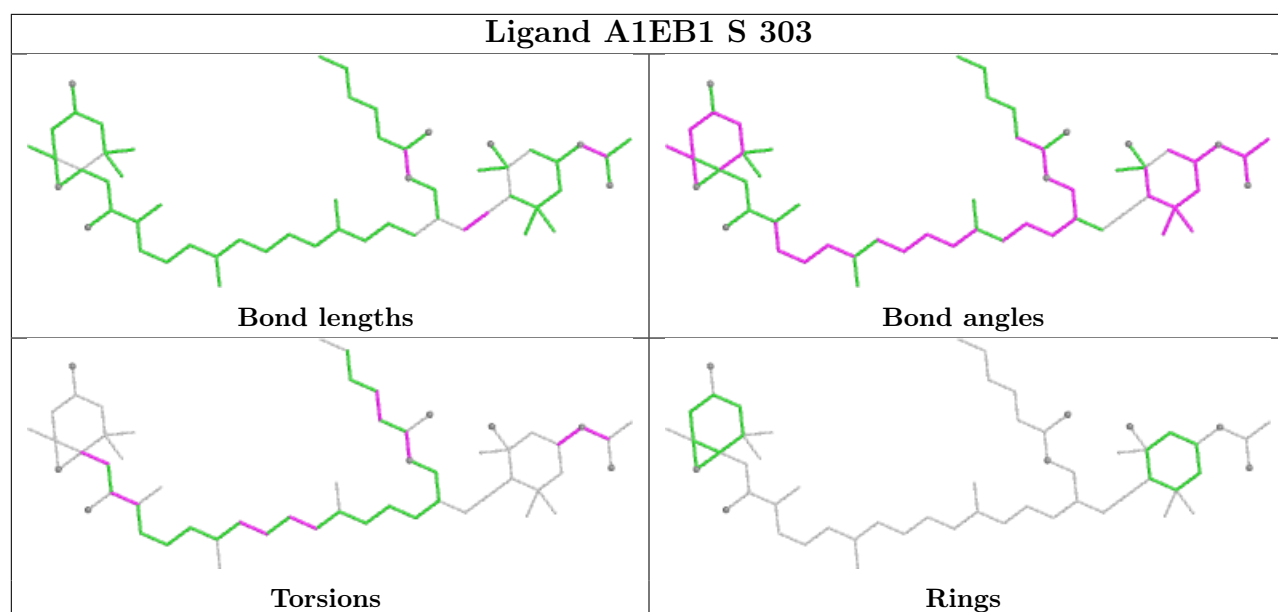


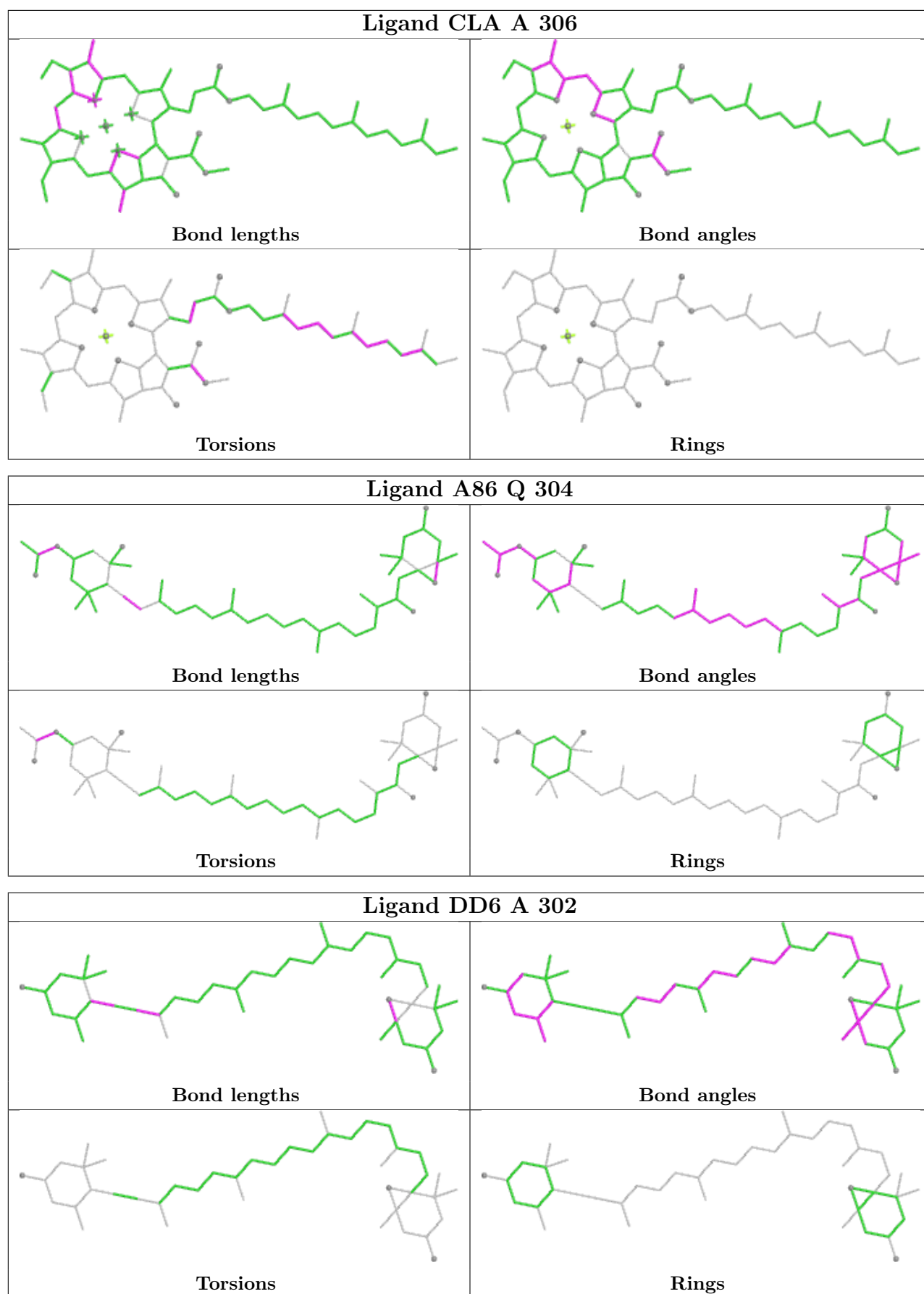
Ligand A86 F 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

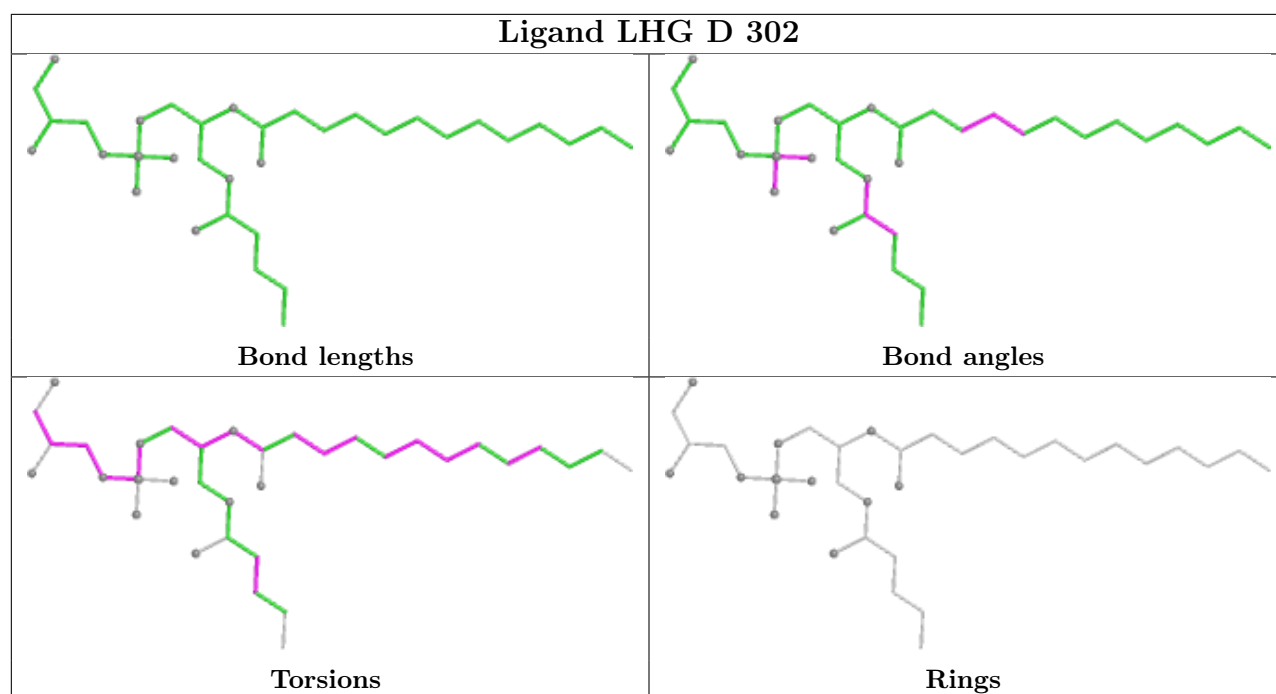
Ligand BCR 1 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

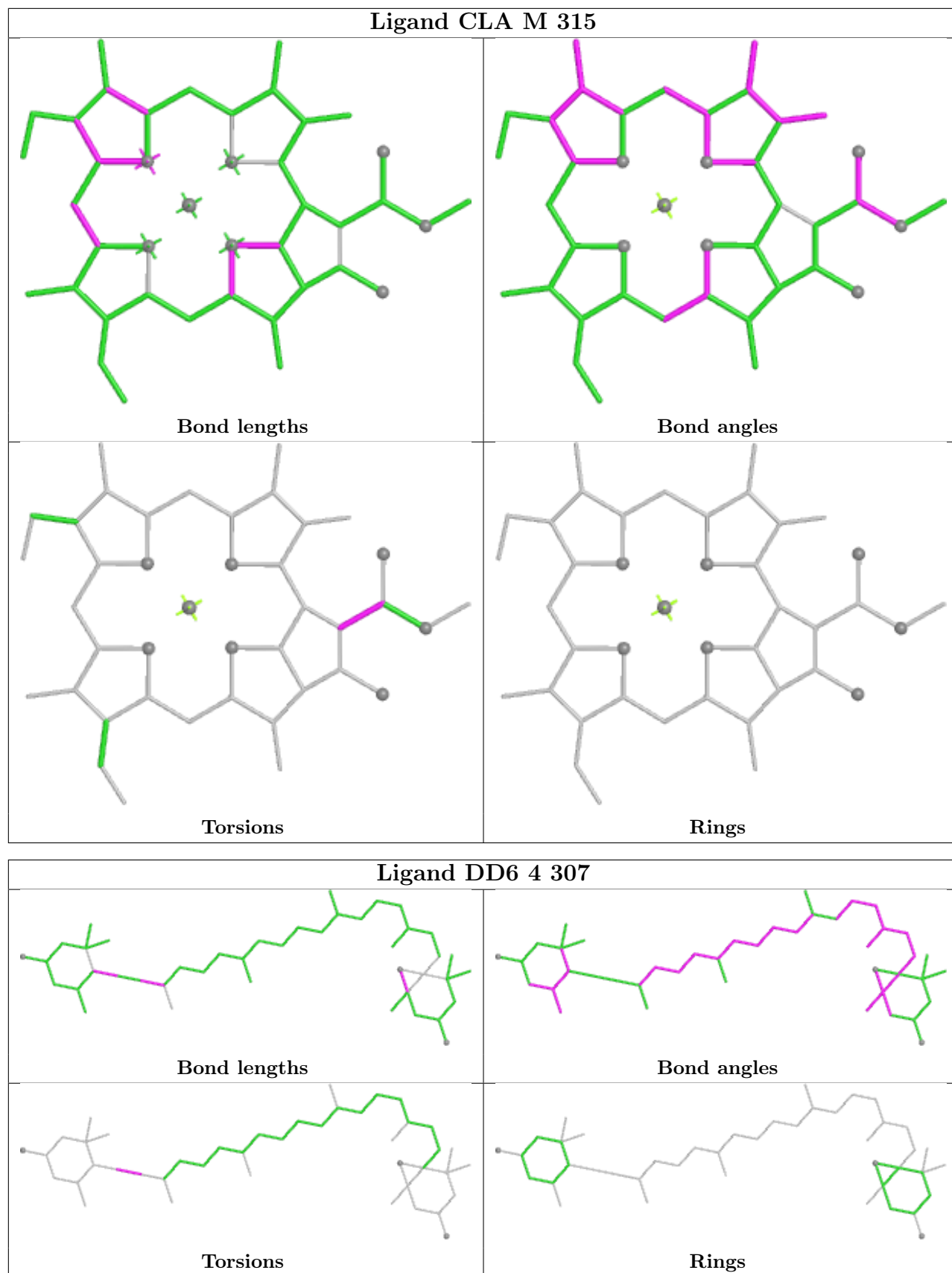
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Bond lengths	Bond angles
	
Torsions	Rings

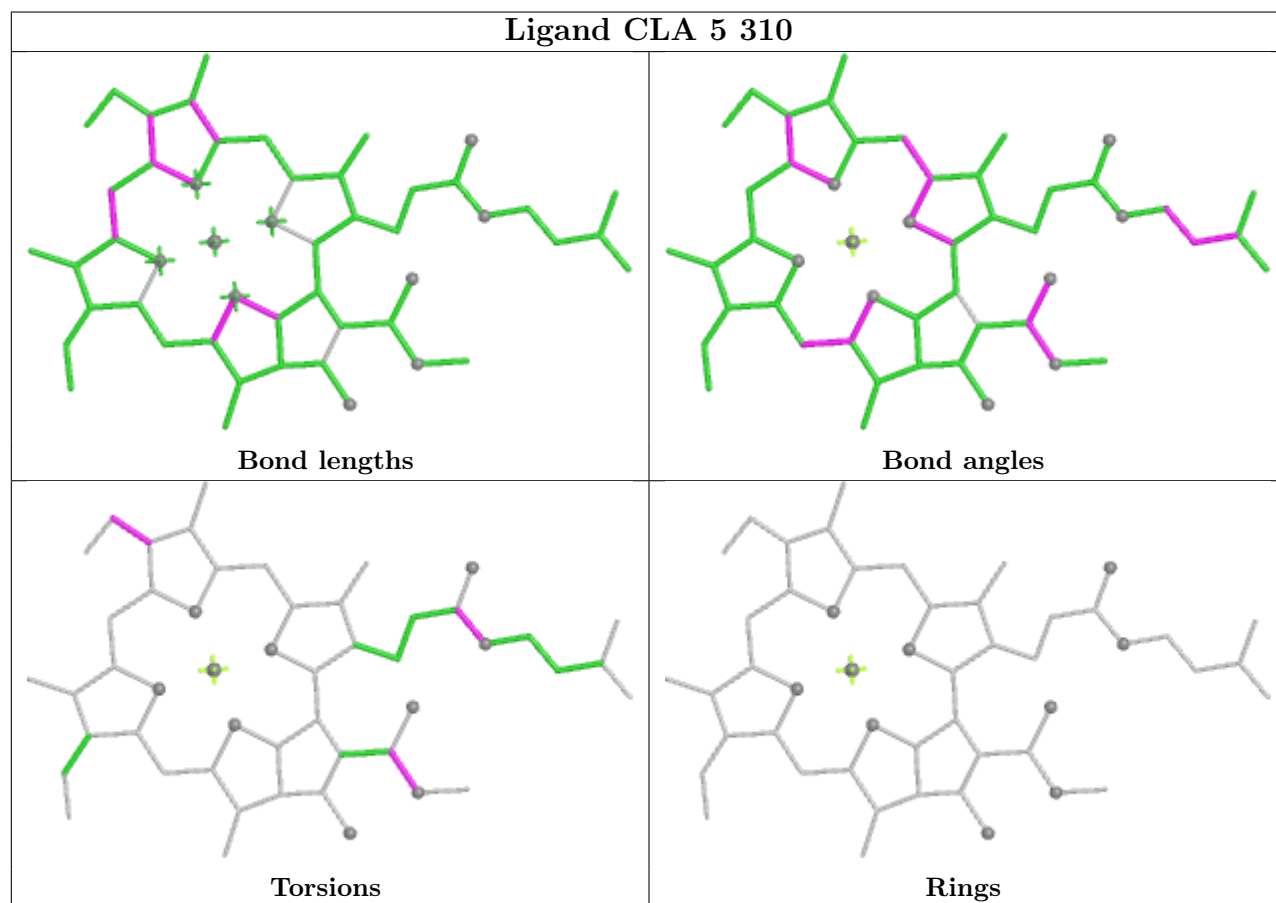
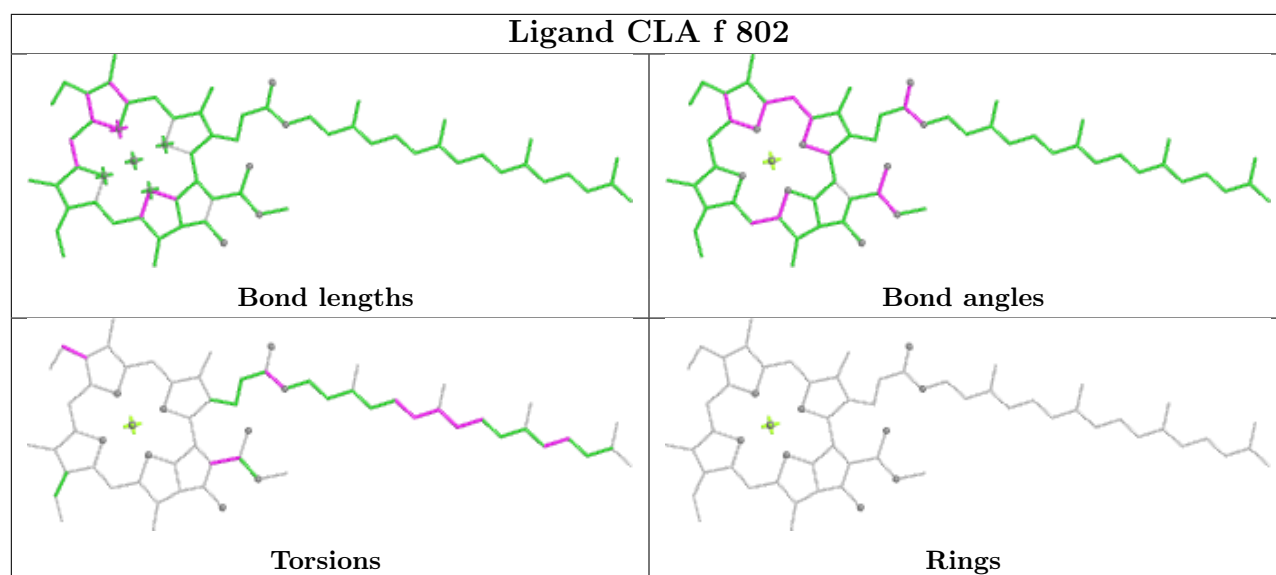


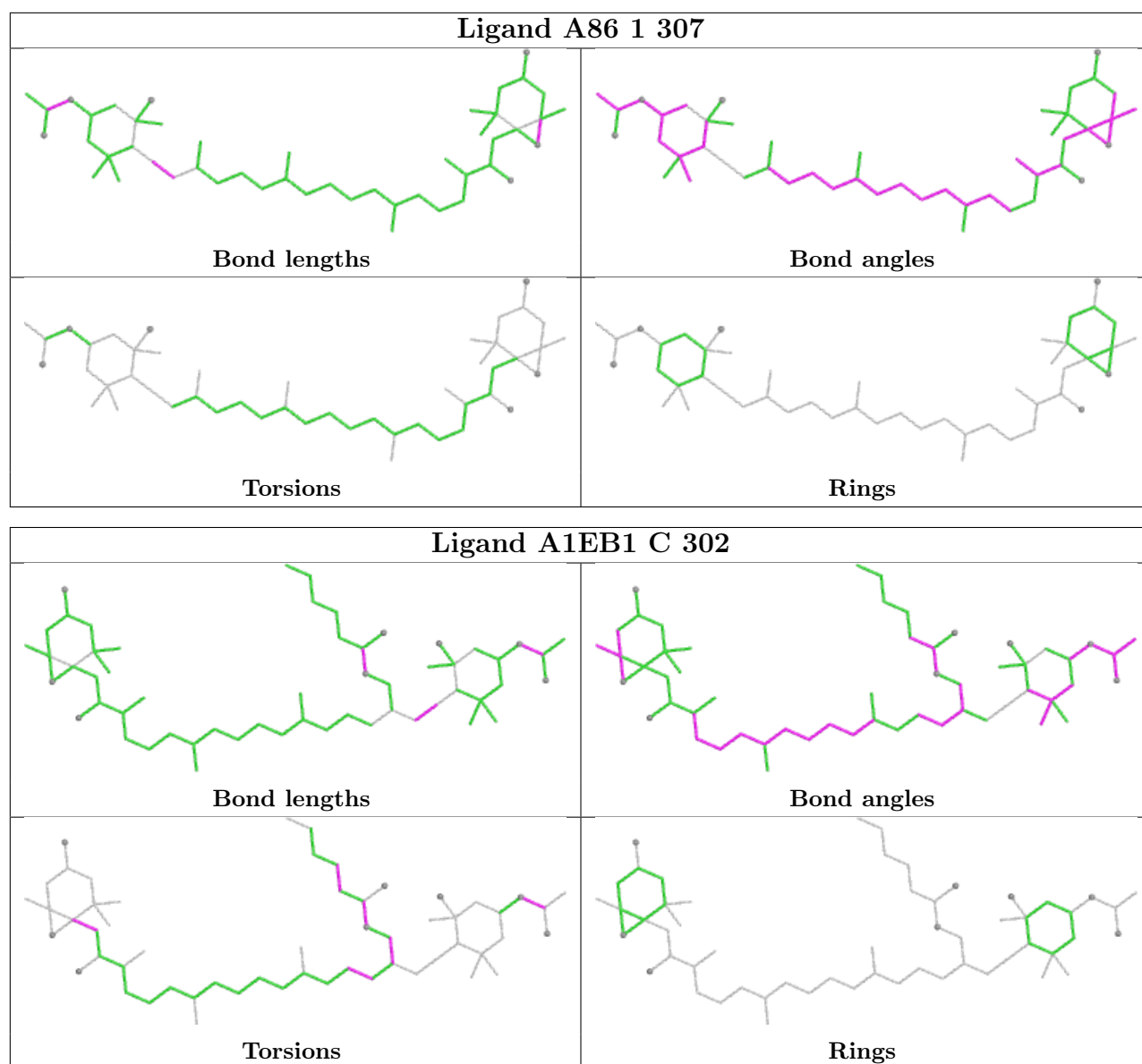




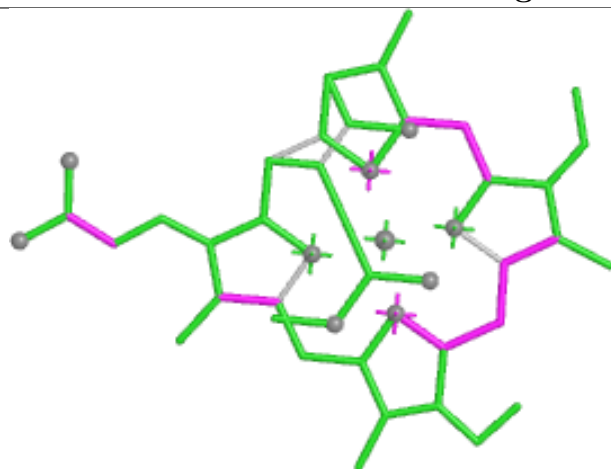




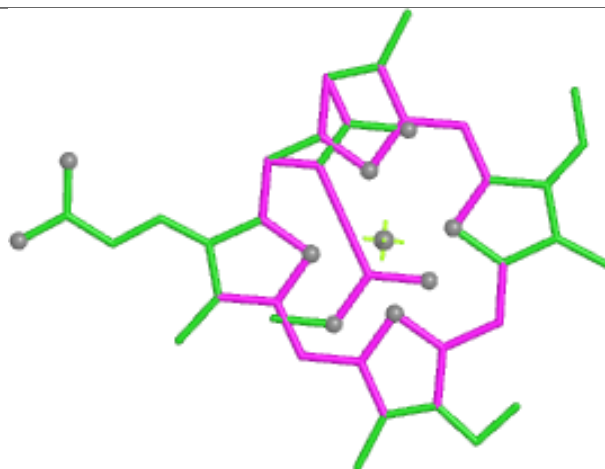




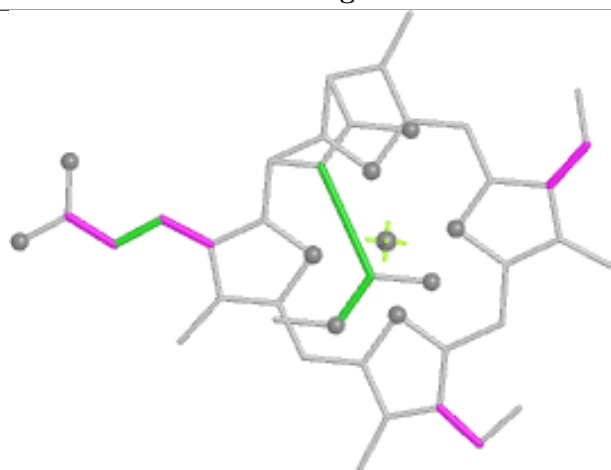
Ligand KC2 G 317



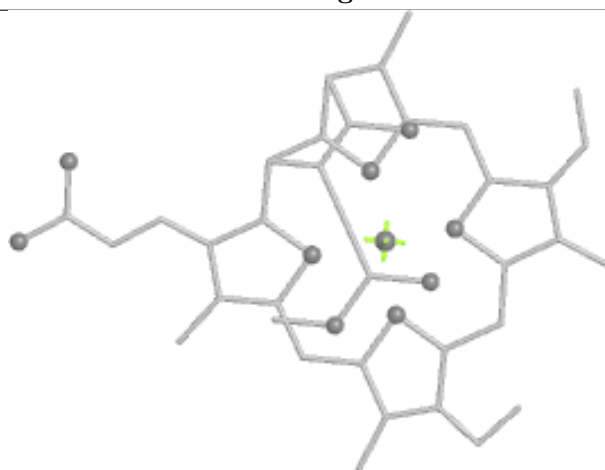
Bond lengths



Bond angles

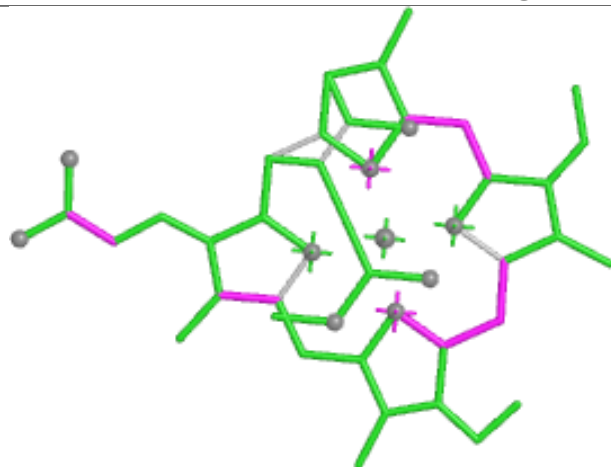


Torsions

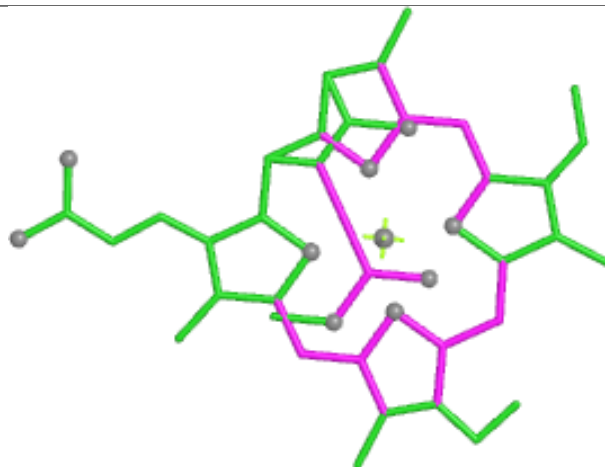


Rings

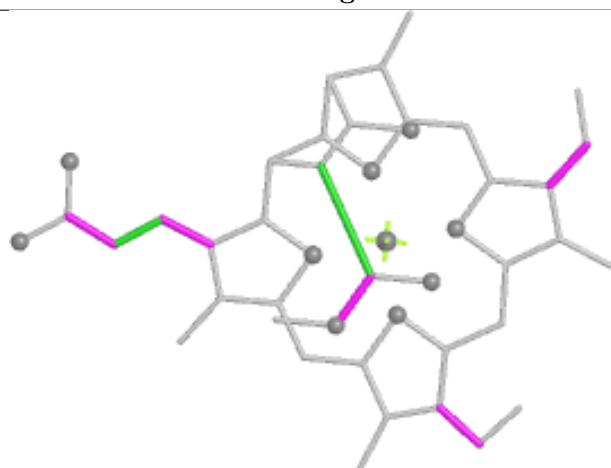
Ligand KC2 Y 308



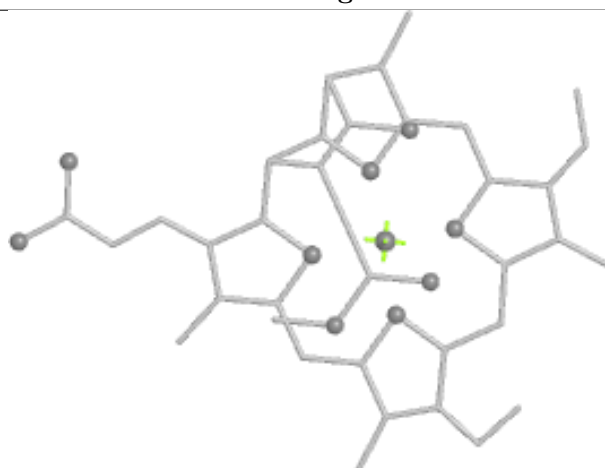
Bond lengths



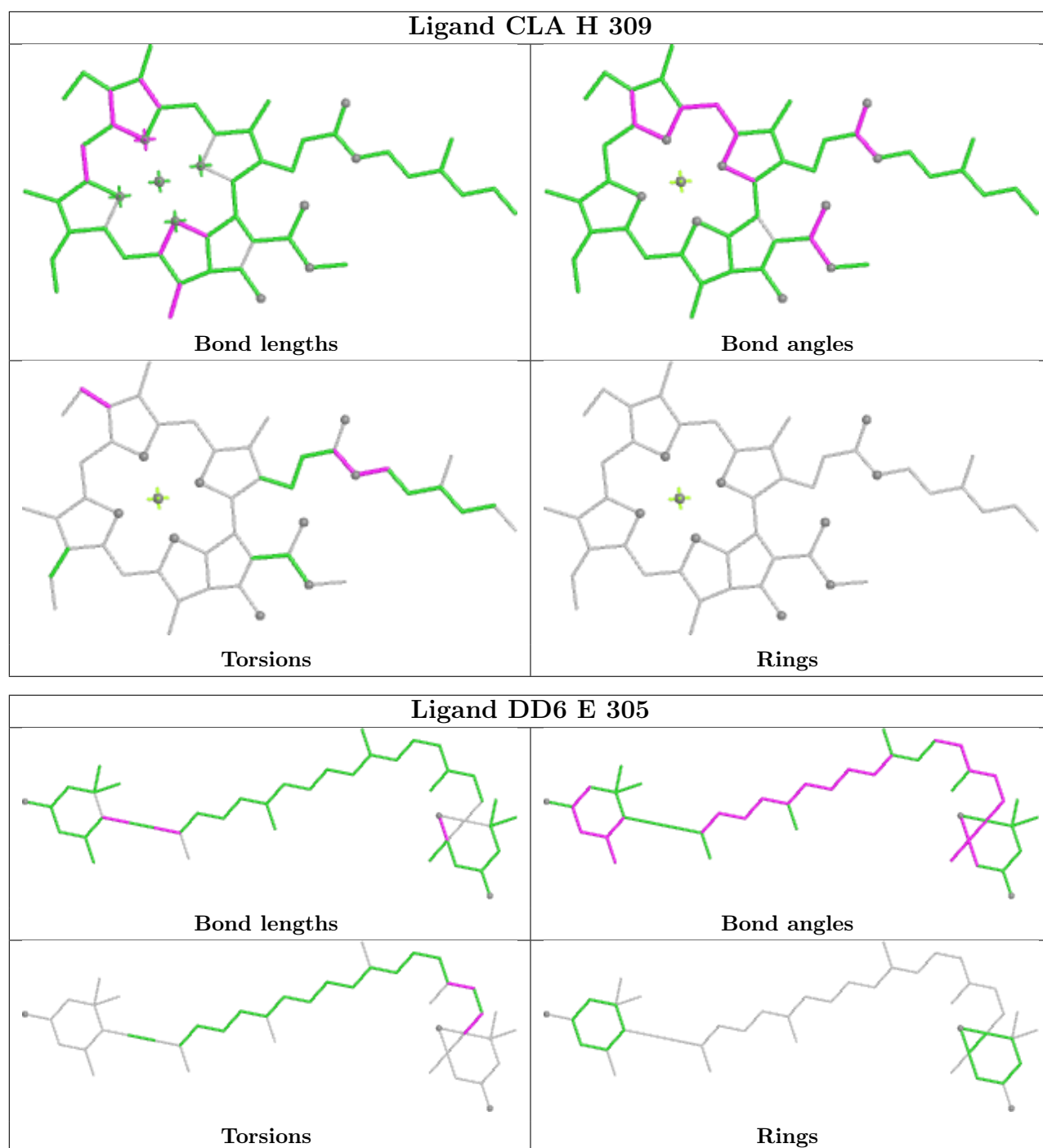
Bond angles

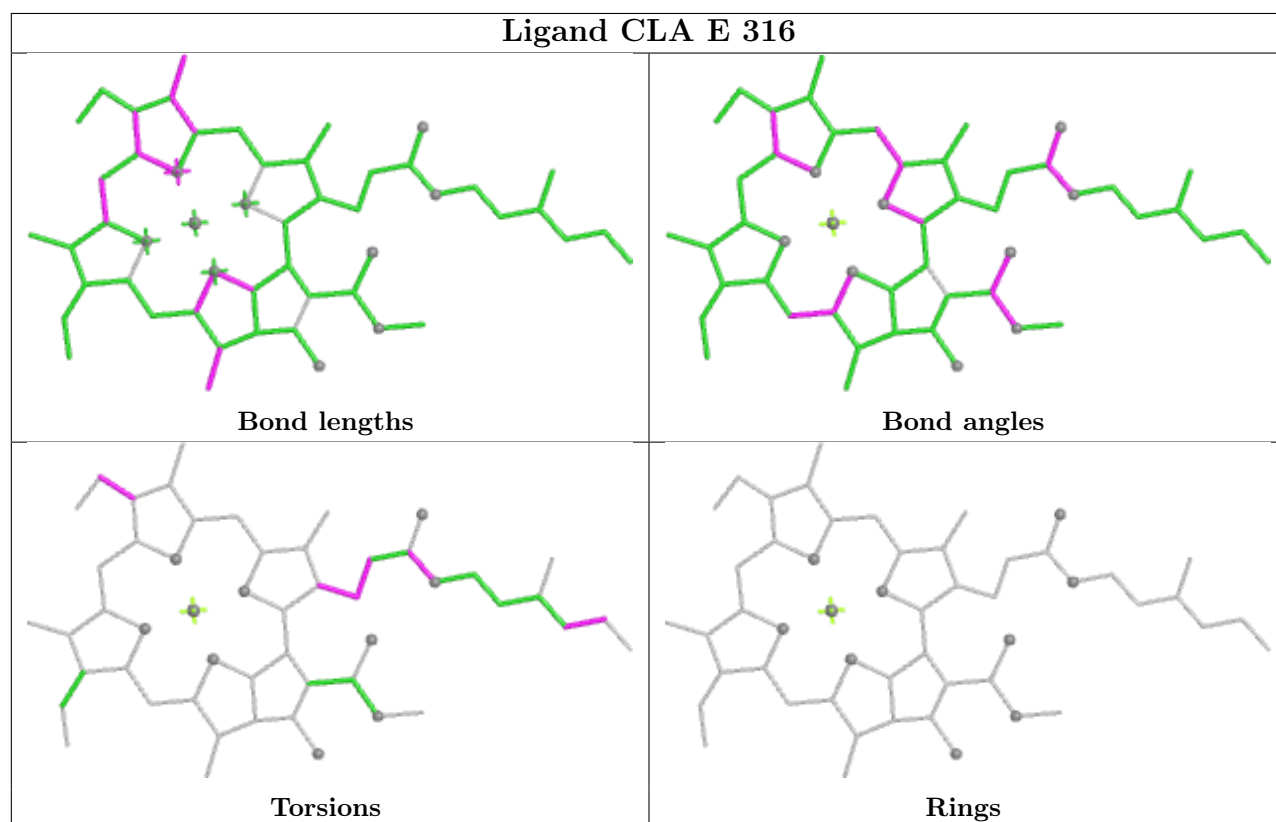
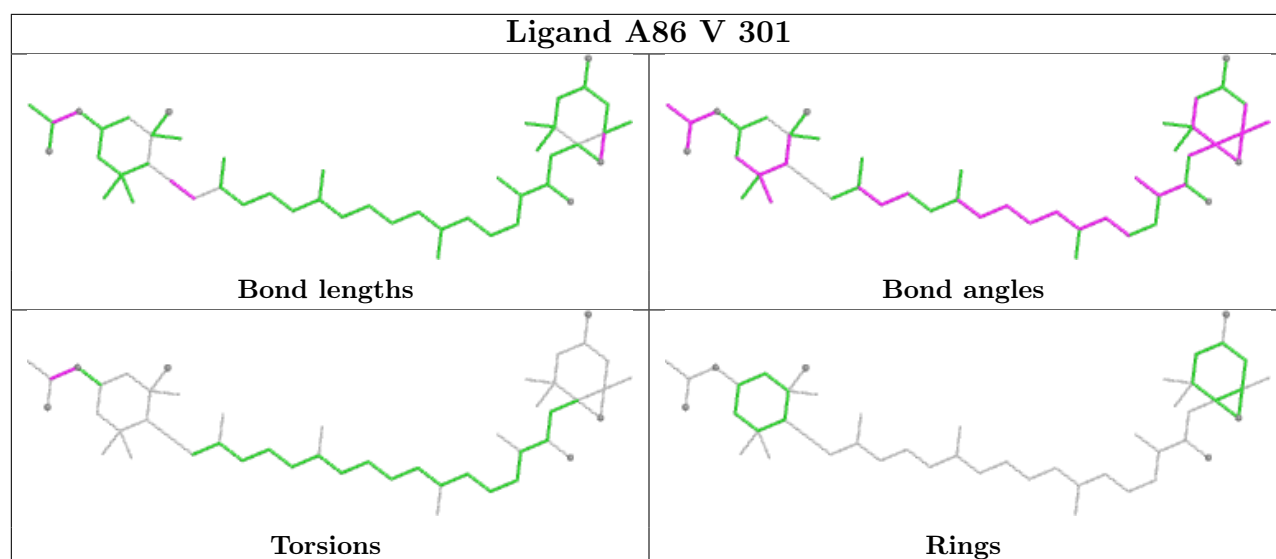


Torsions

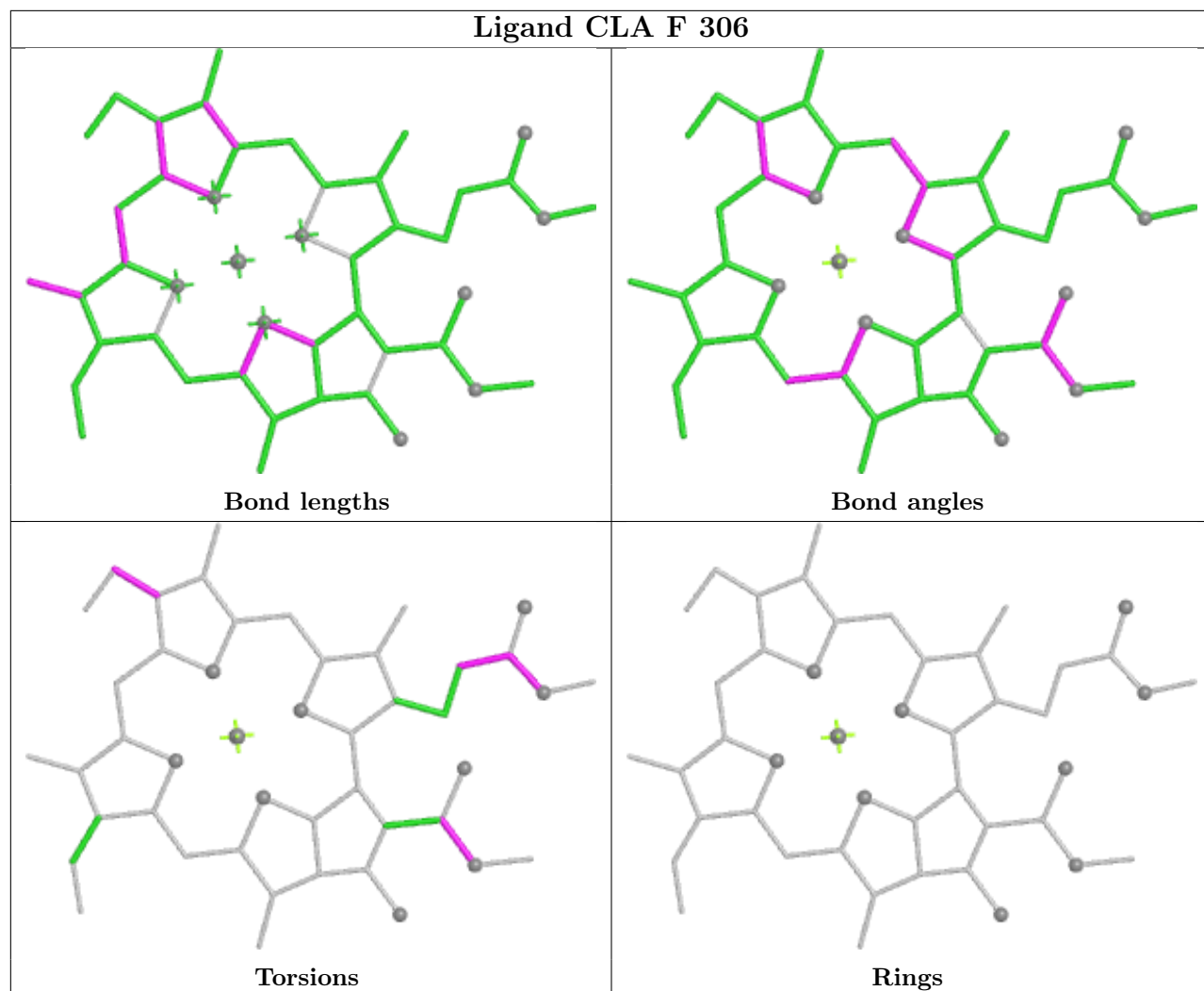


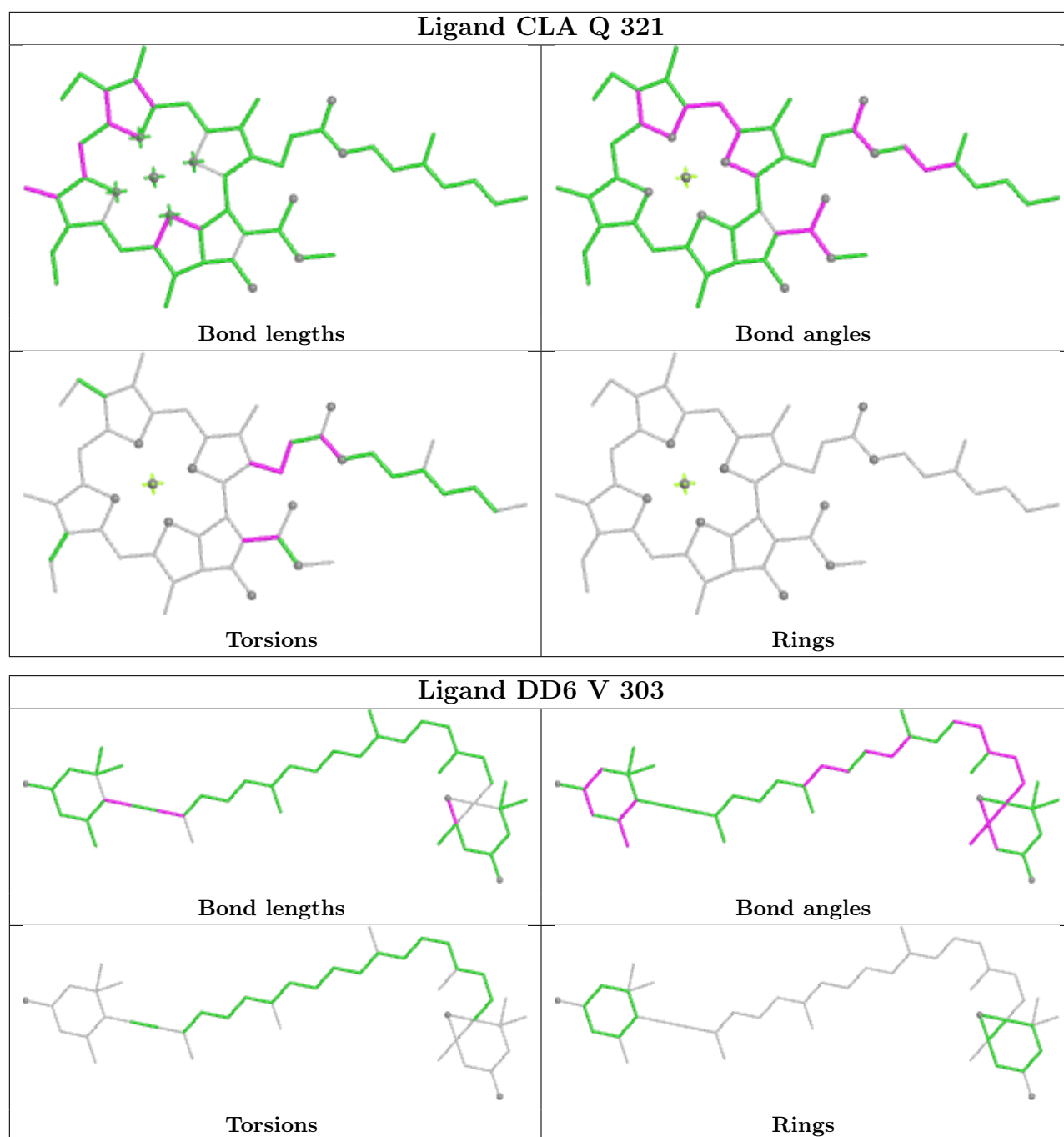
Rings



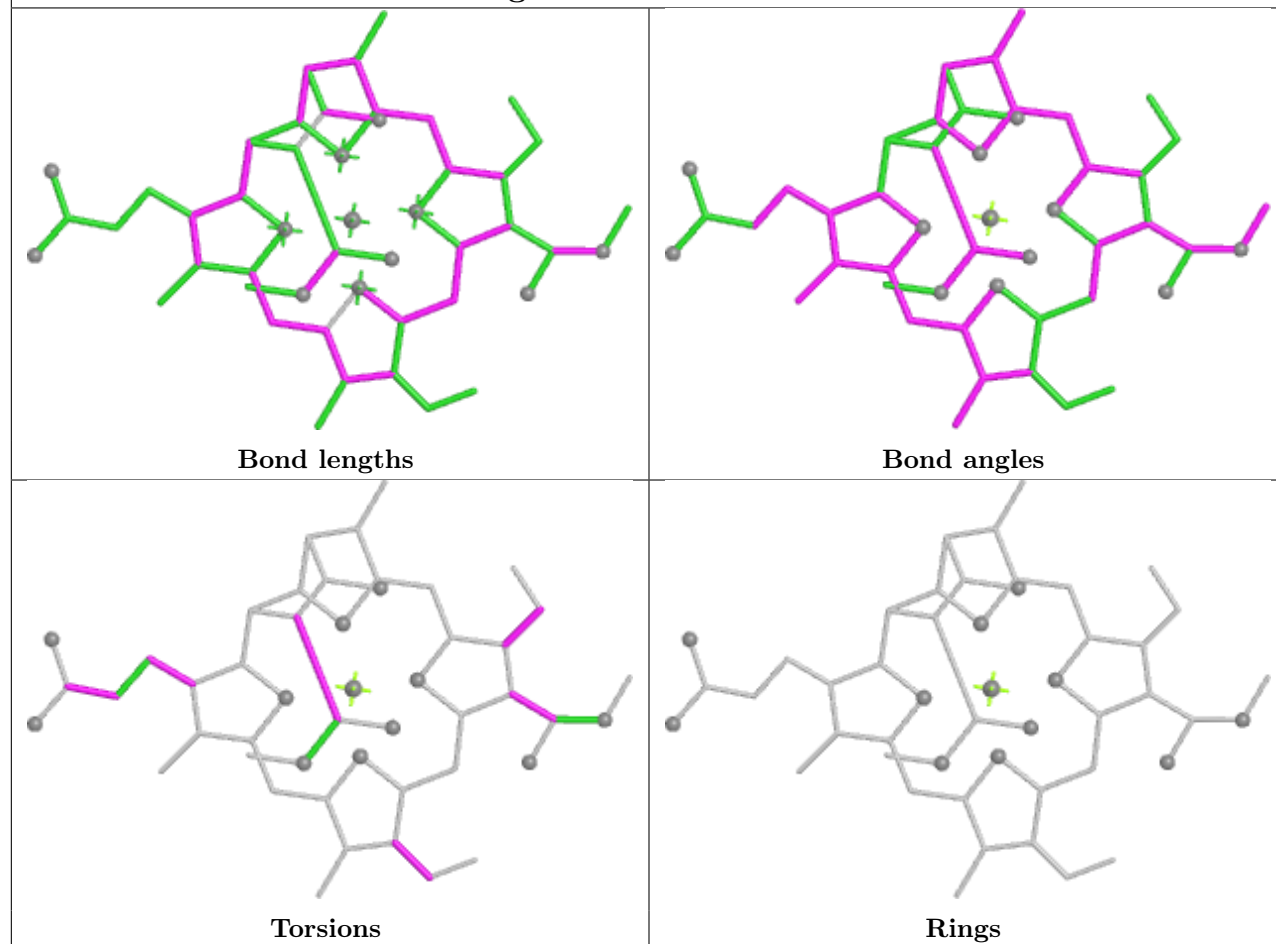


Ligand CLA F 306

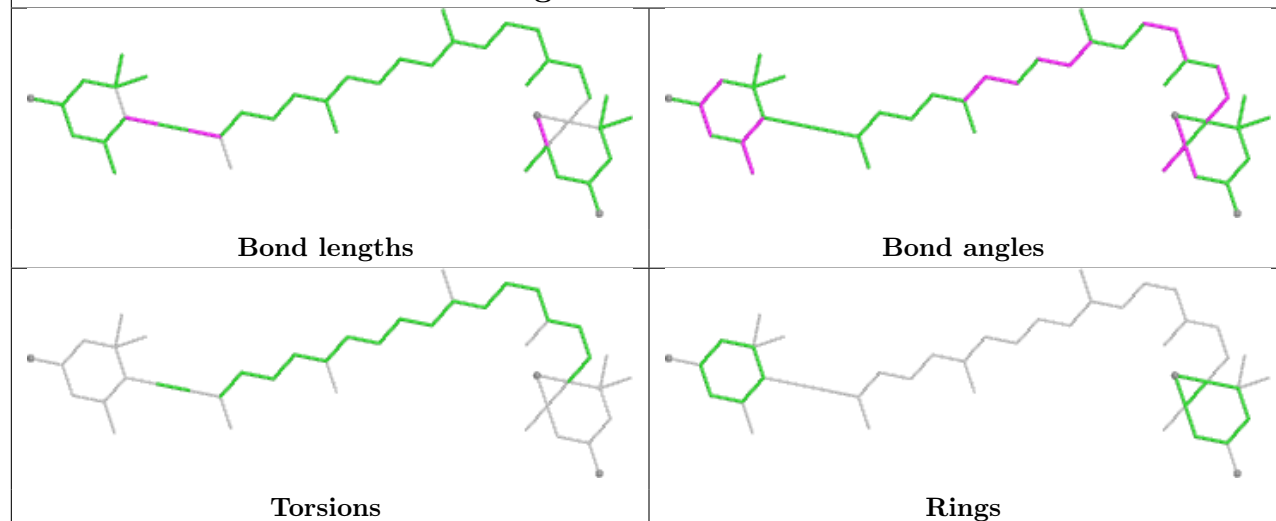


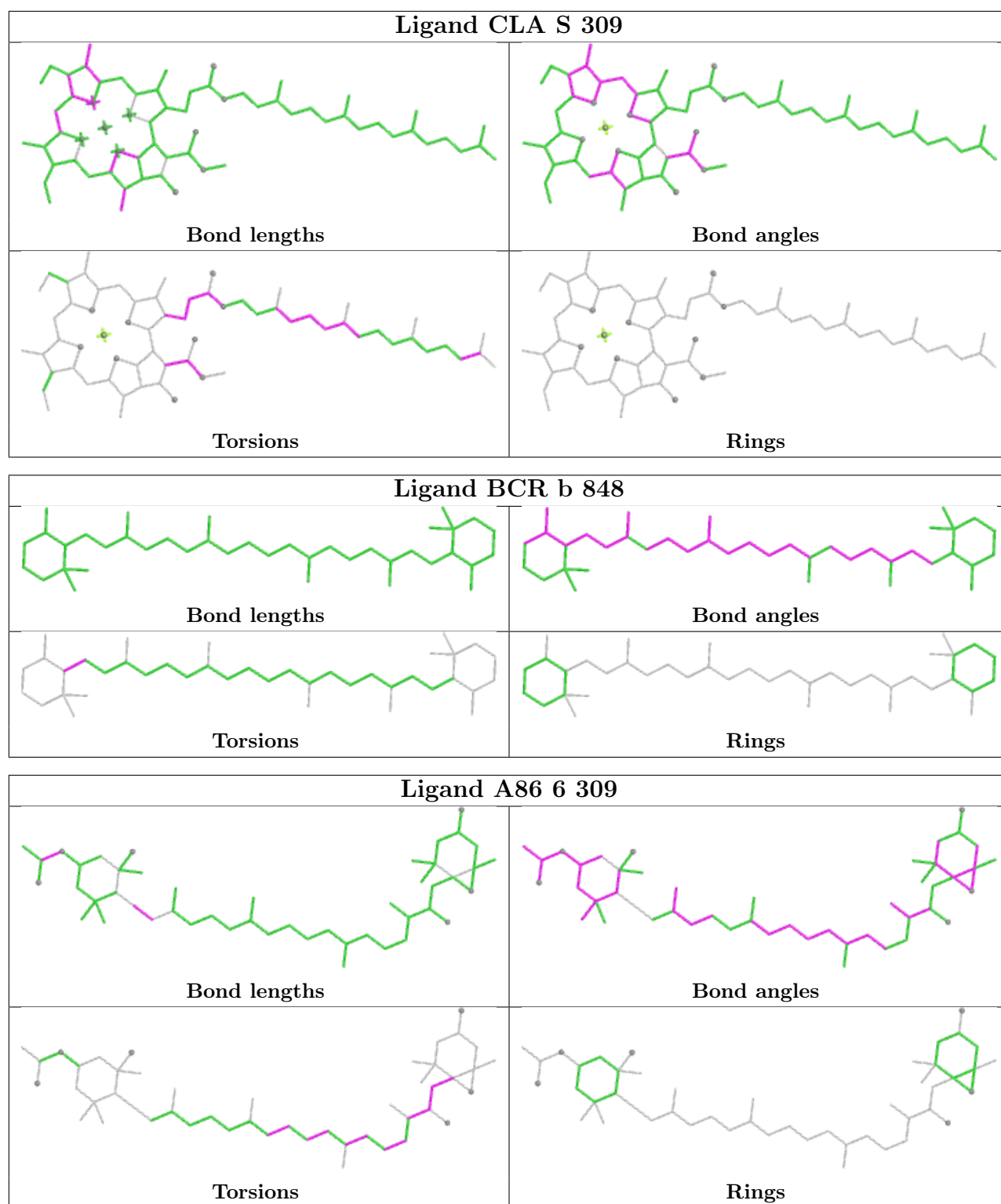


Ligand A1ECV O 315

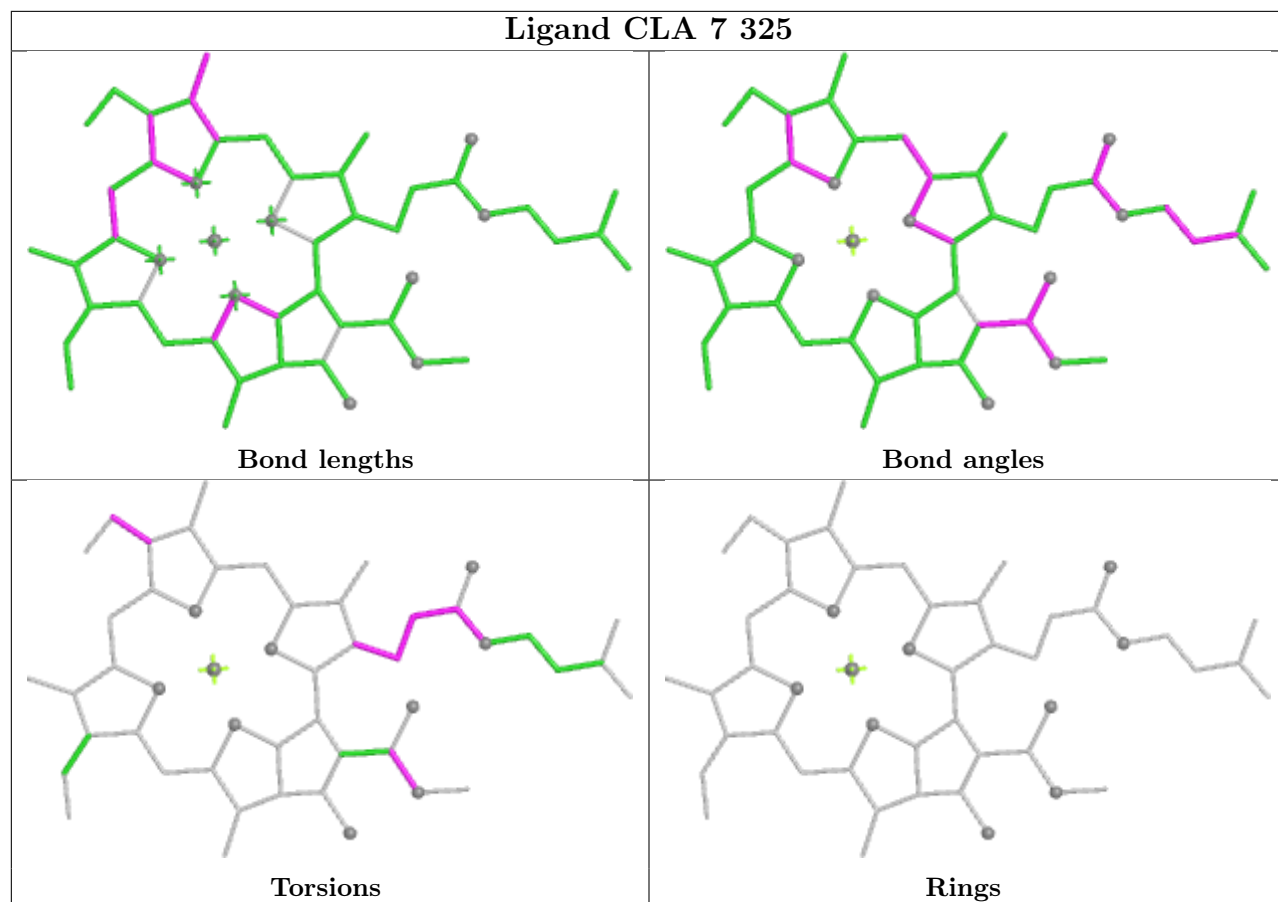


Ligand DD6 E 302

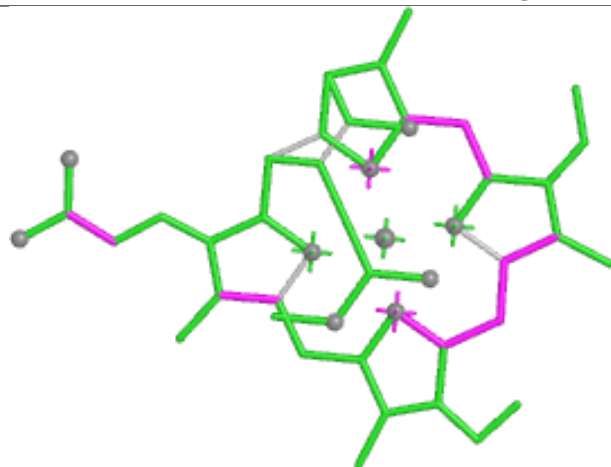




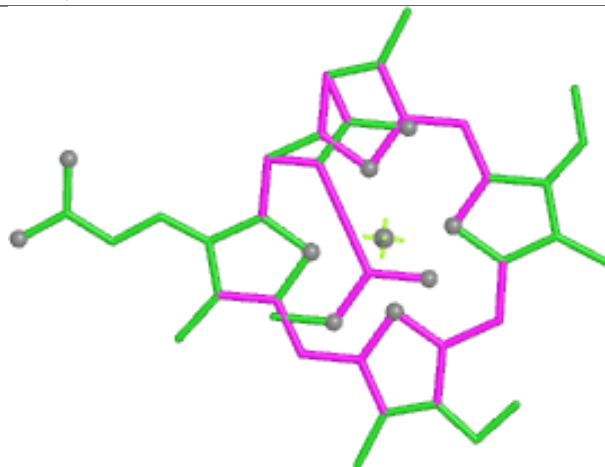
Ligand CLA 7 325



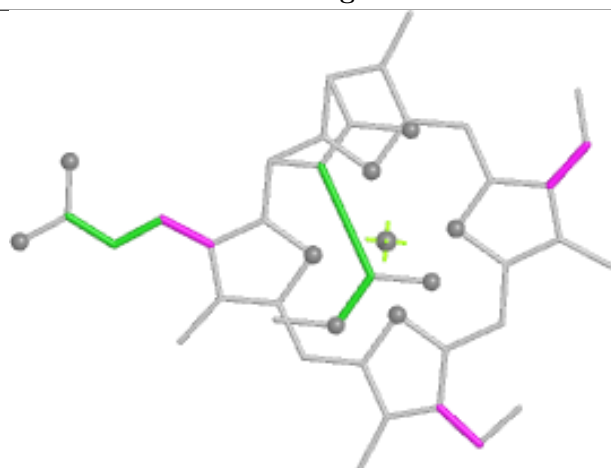
Ligand KC2 Q 318



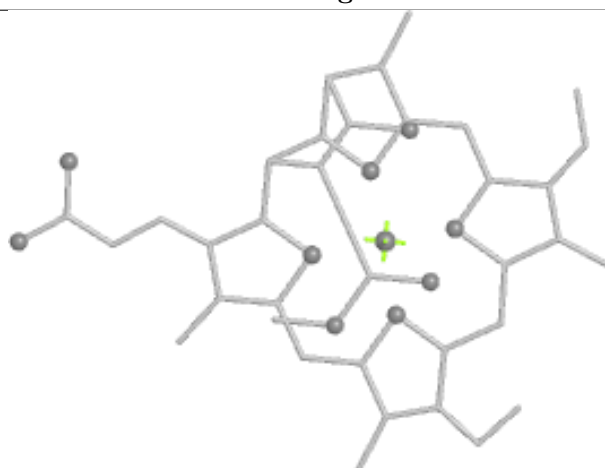
Bond lengths



Bond angles

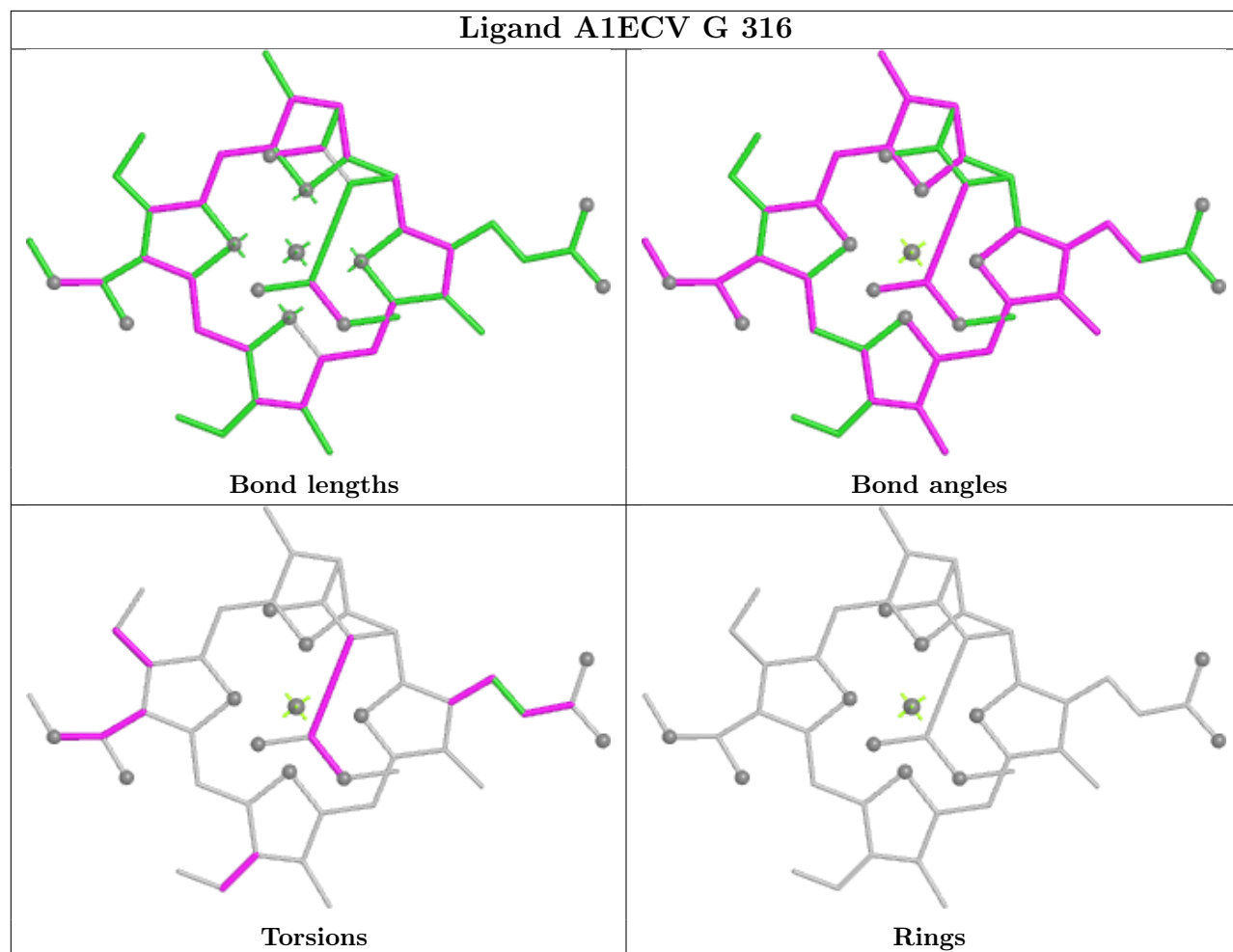


Torsions

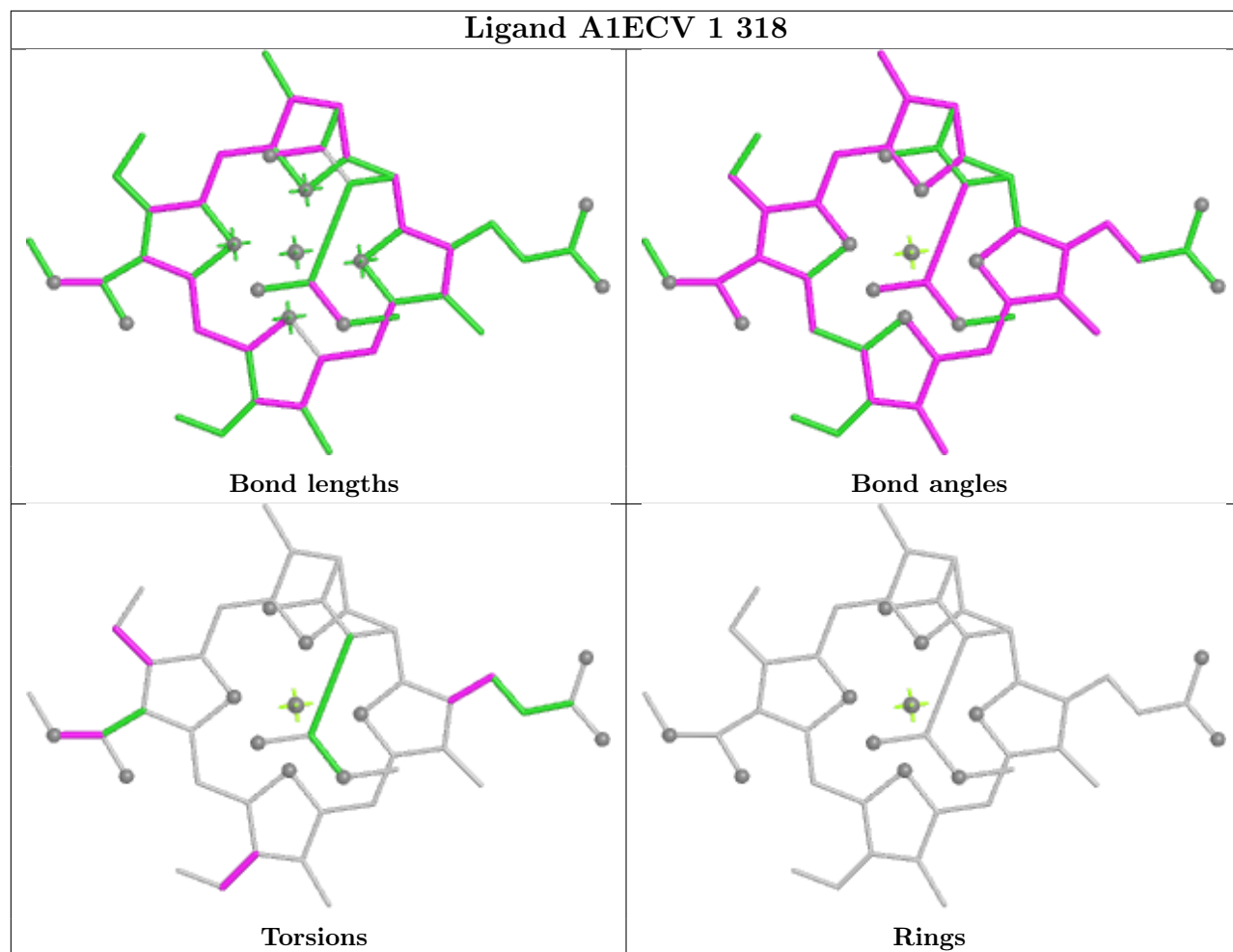


Rings

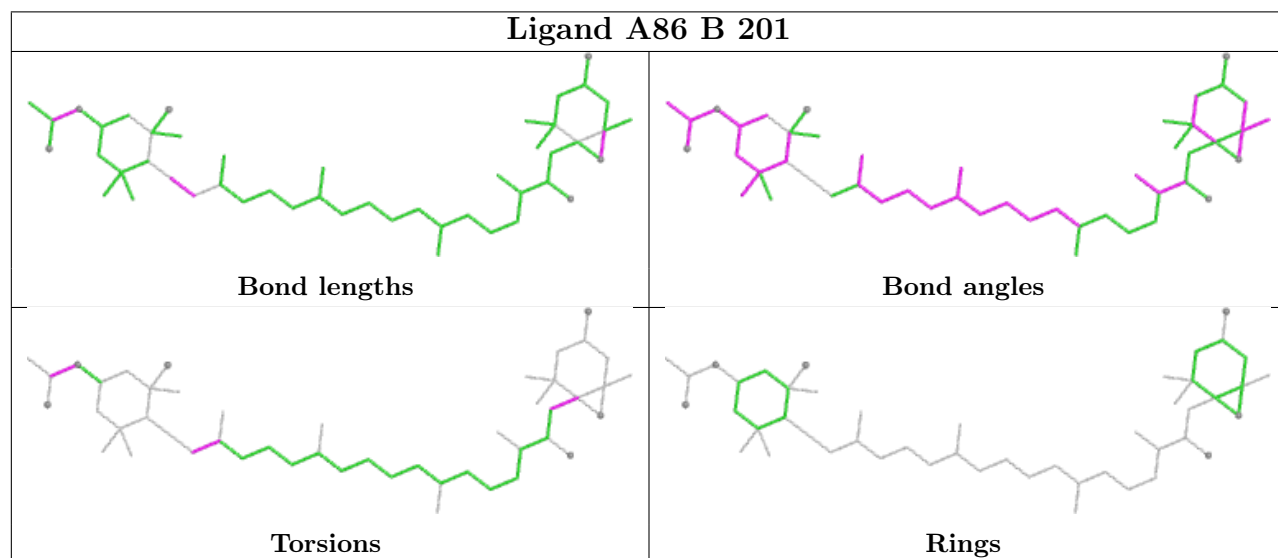
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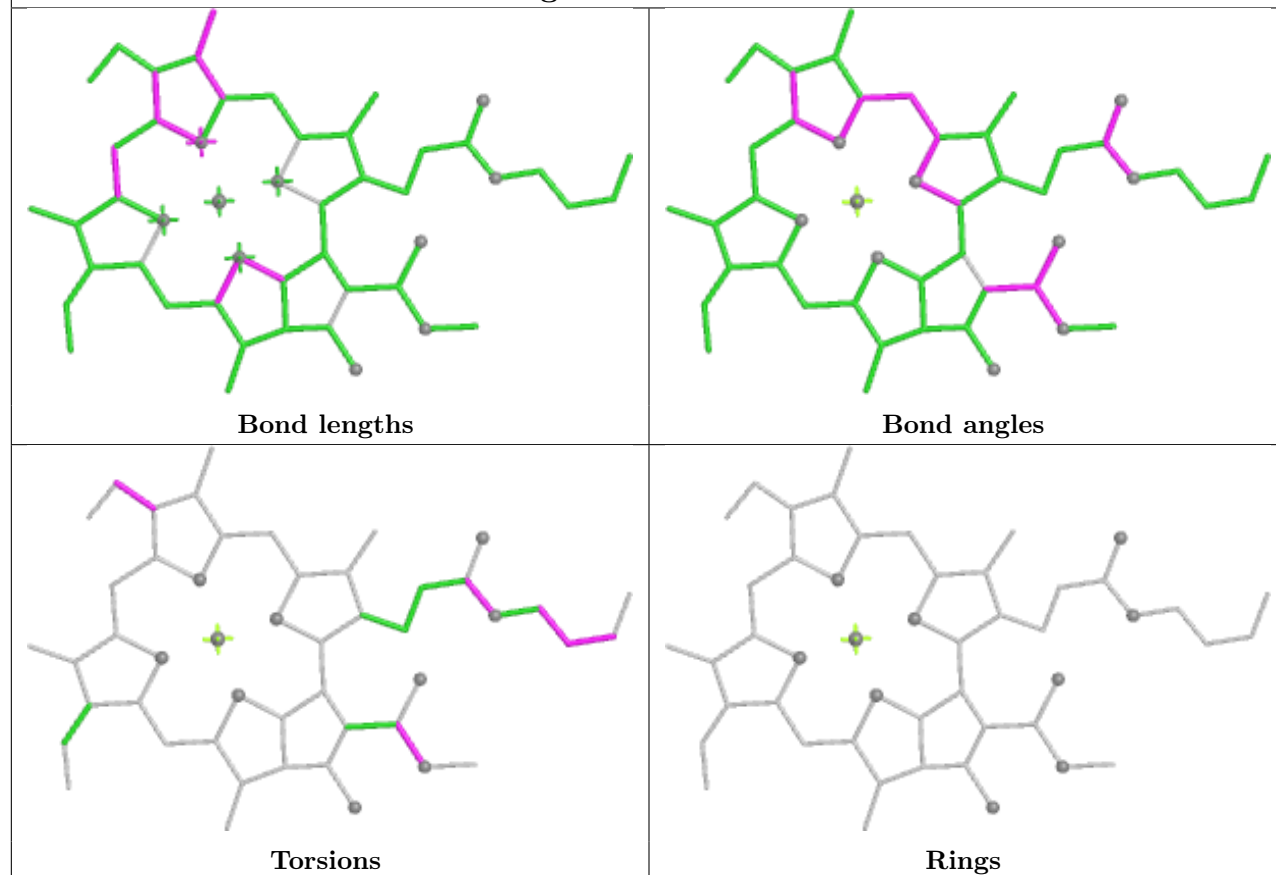
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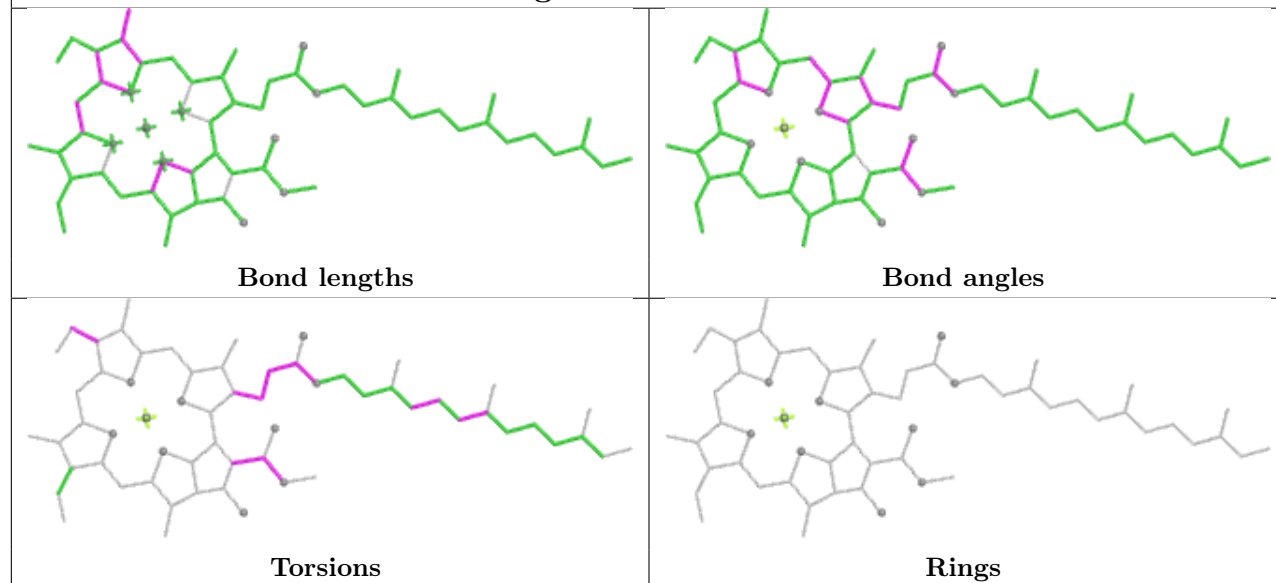
Ligand A86 B 201

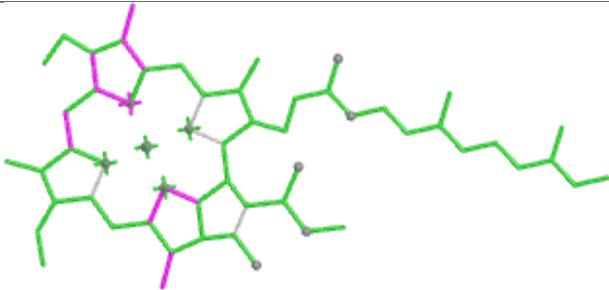
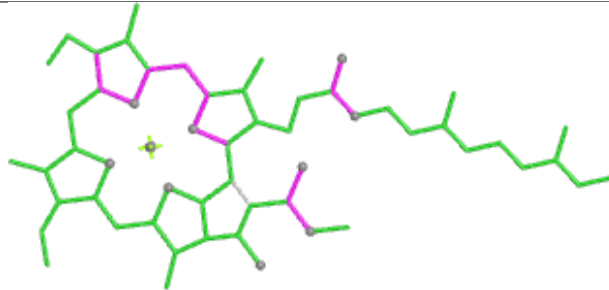
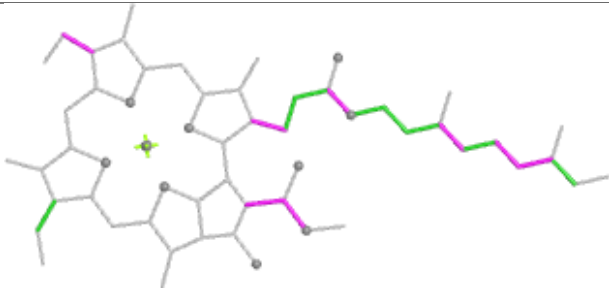
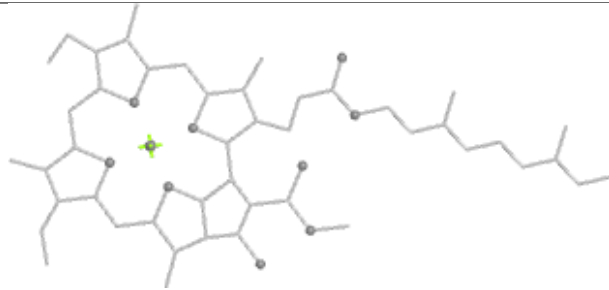


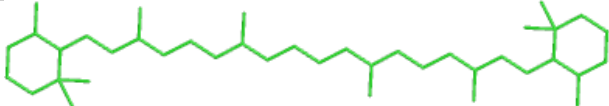
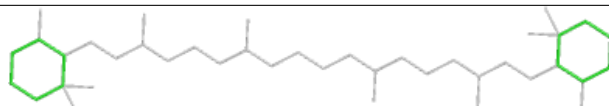
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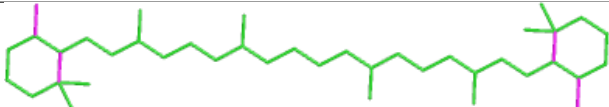
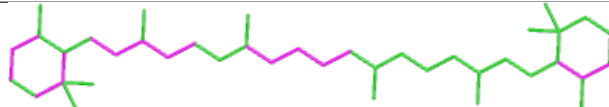
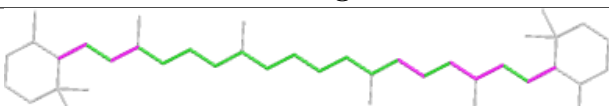
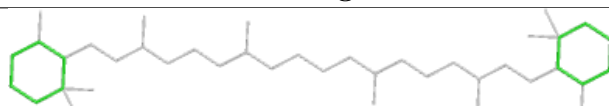


Ligand CLA L 308

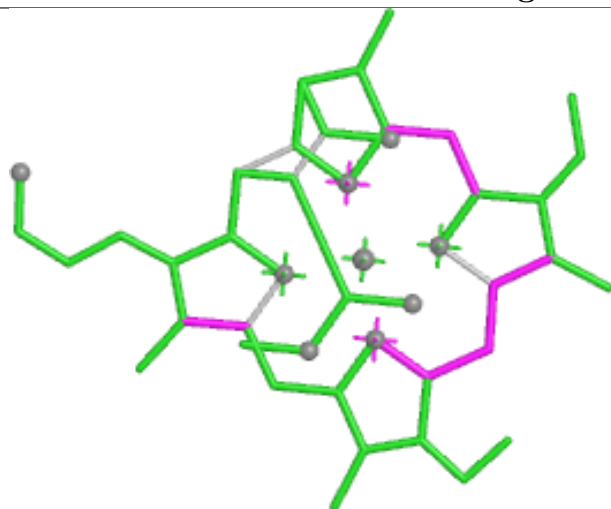


Ligand CLA G 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

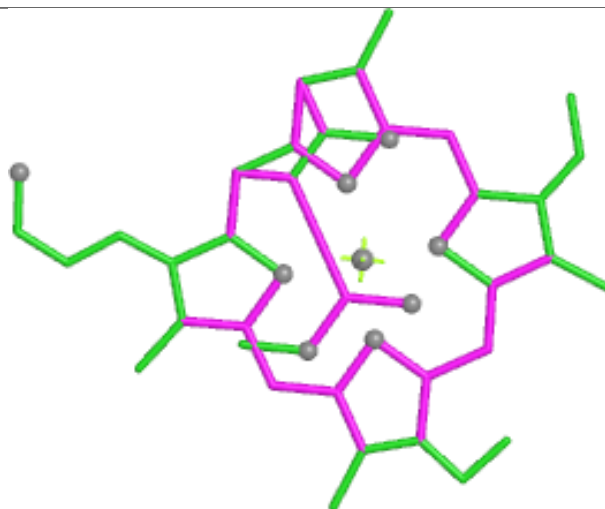
Ligand BCR i 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

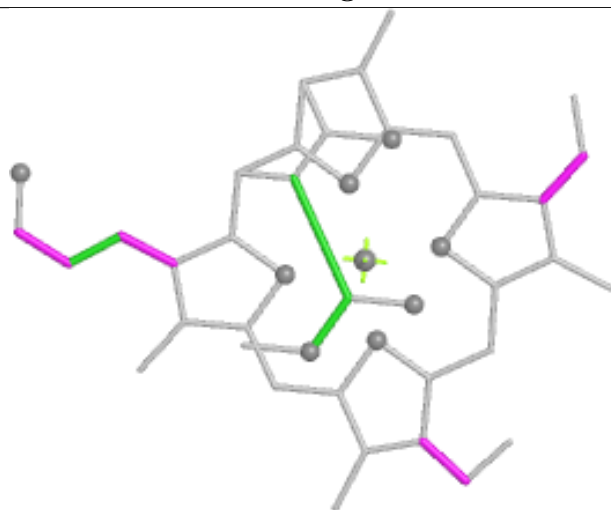
Ligand KC2 F 311



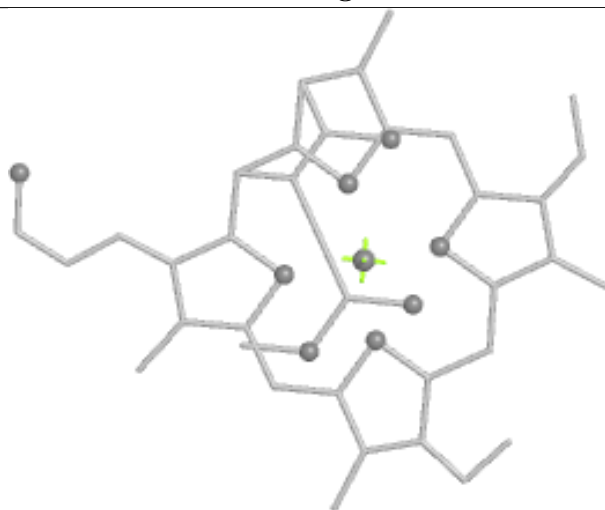
Bond lengths



Bond angles

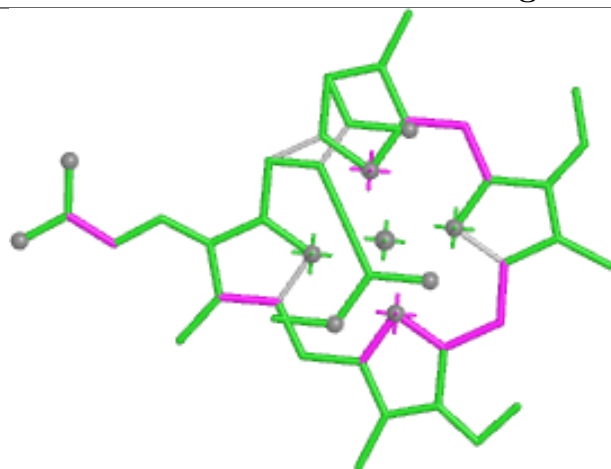


Torsions



Rings

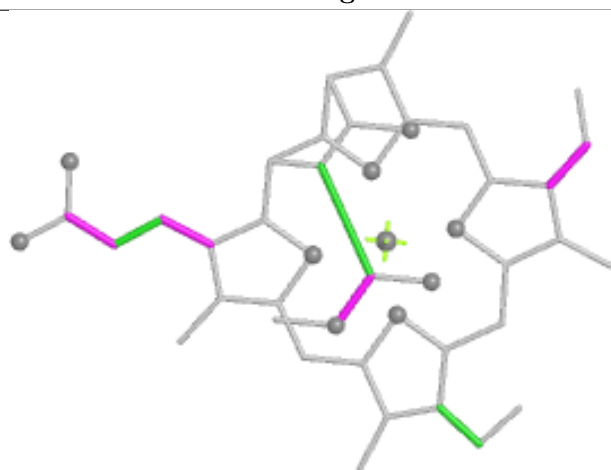
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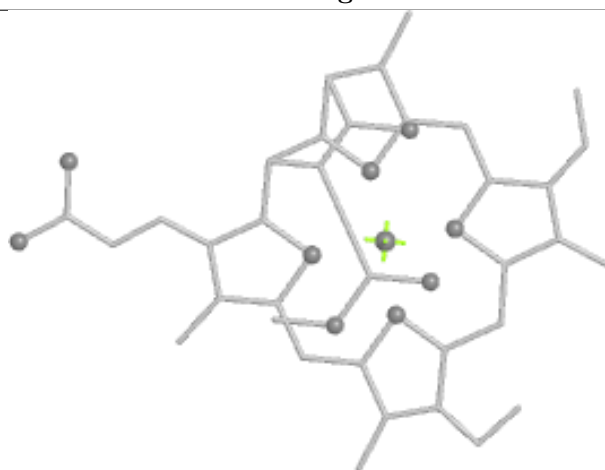
Bond lengths



Bond angles

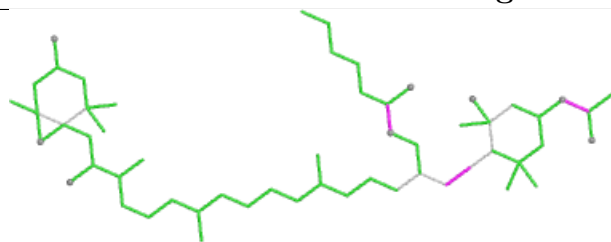


Torsions

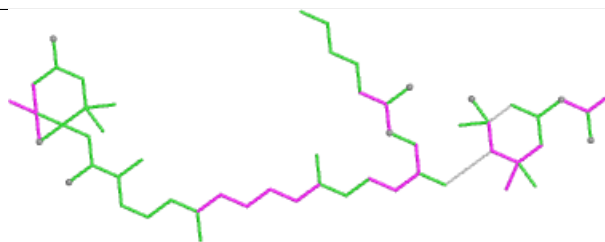


Rings

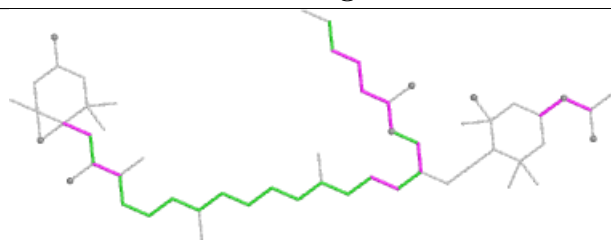
Ligand A1EB1 T 302



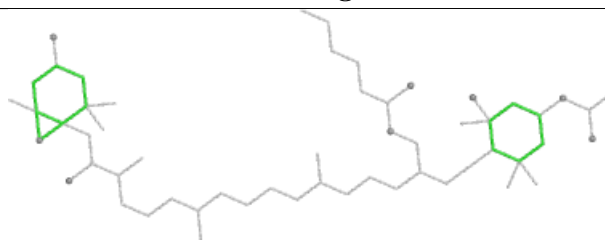
Bond lengths



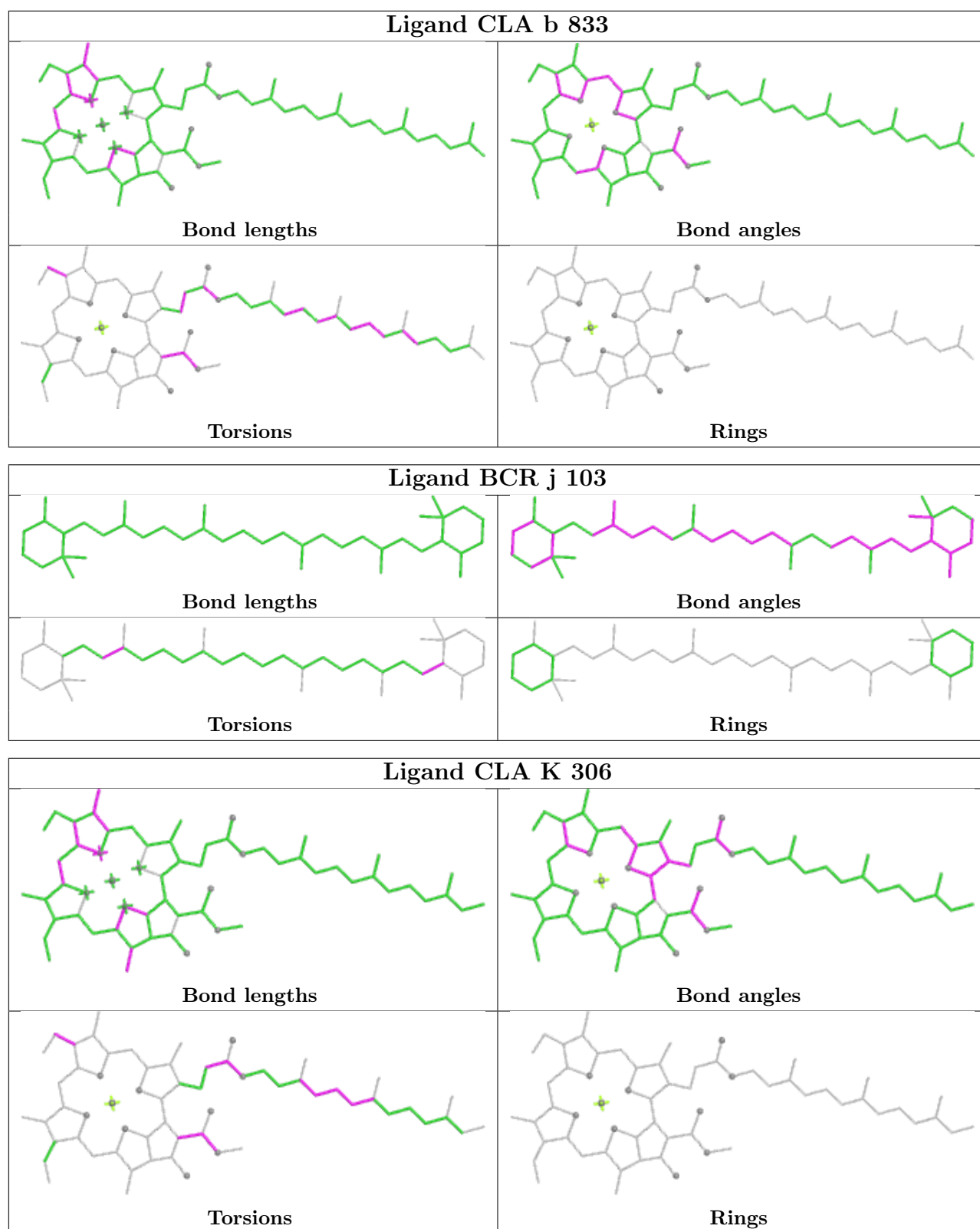
Bond angles

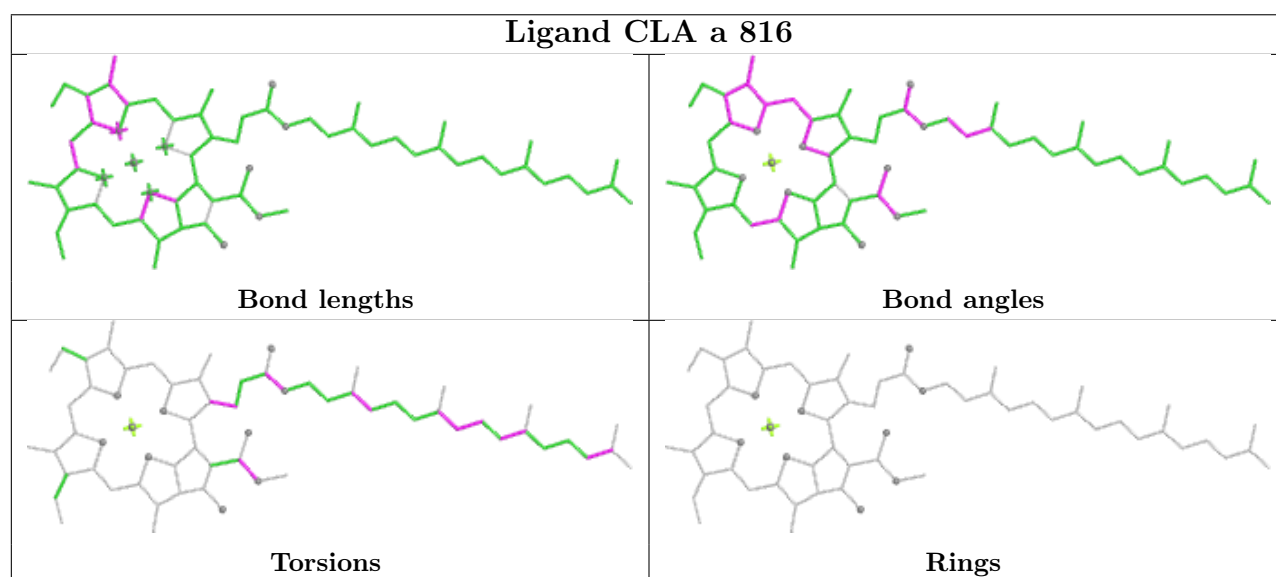
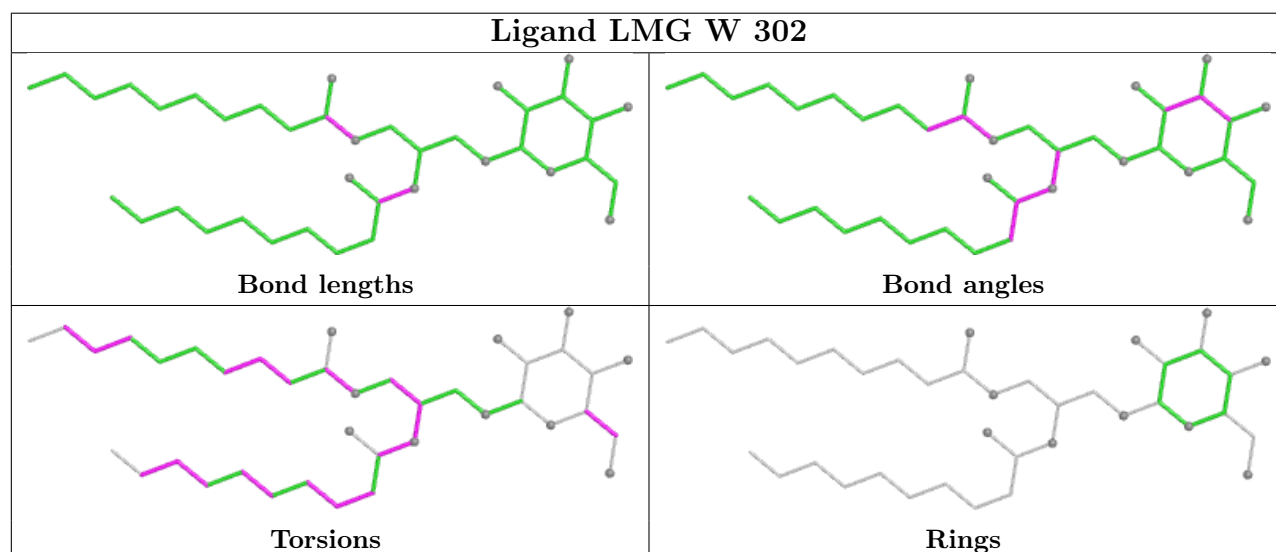
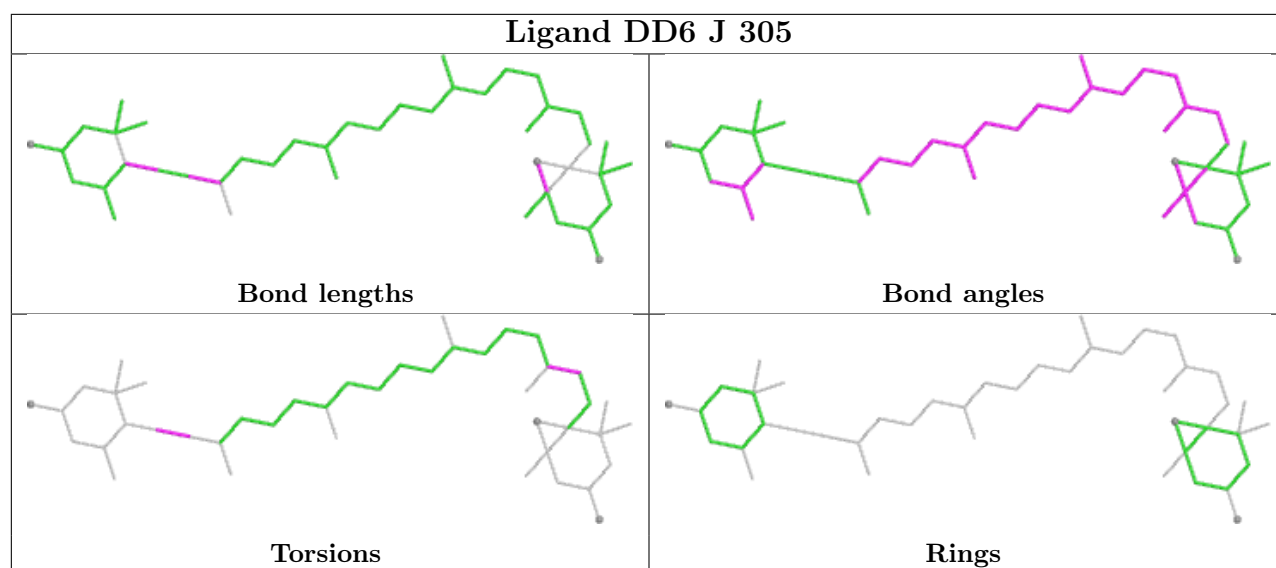


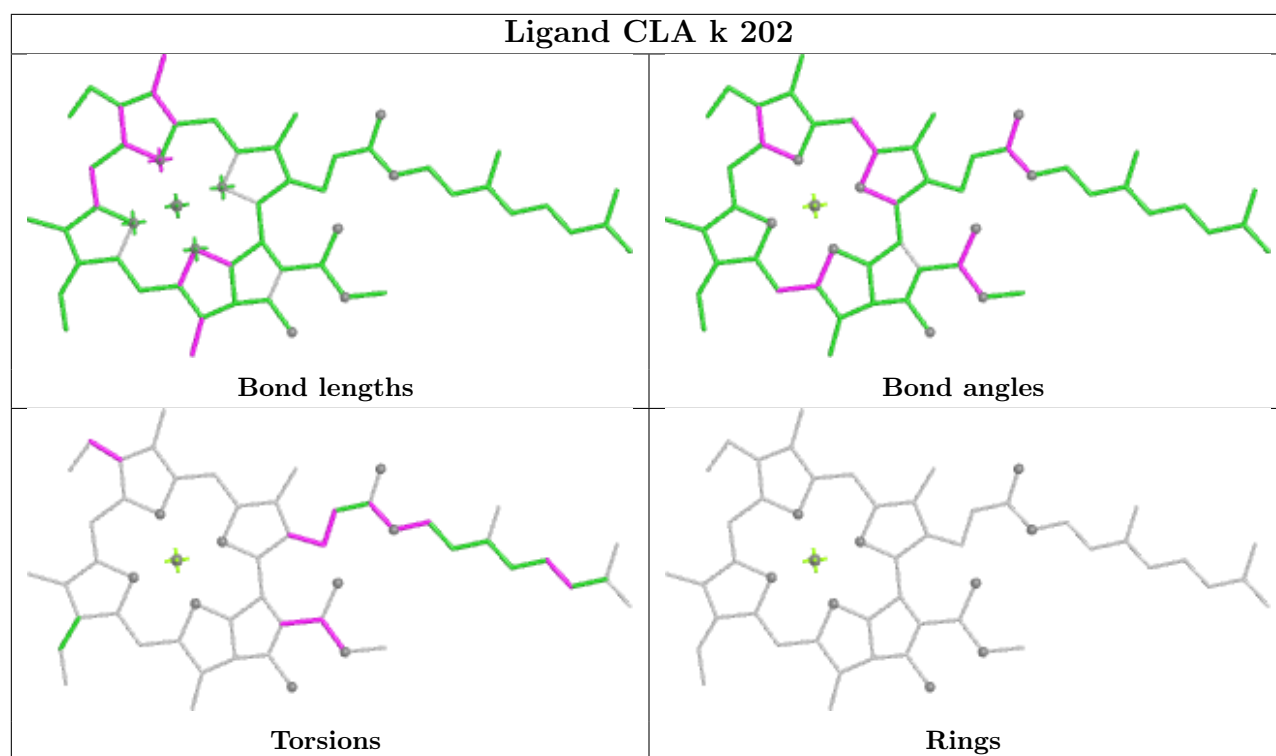
Torsions



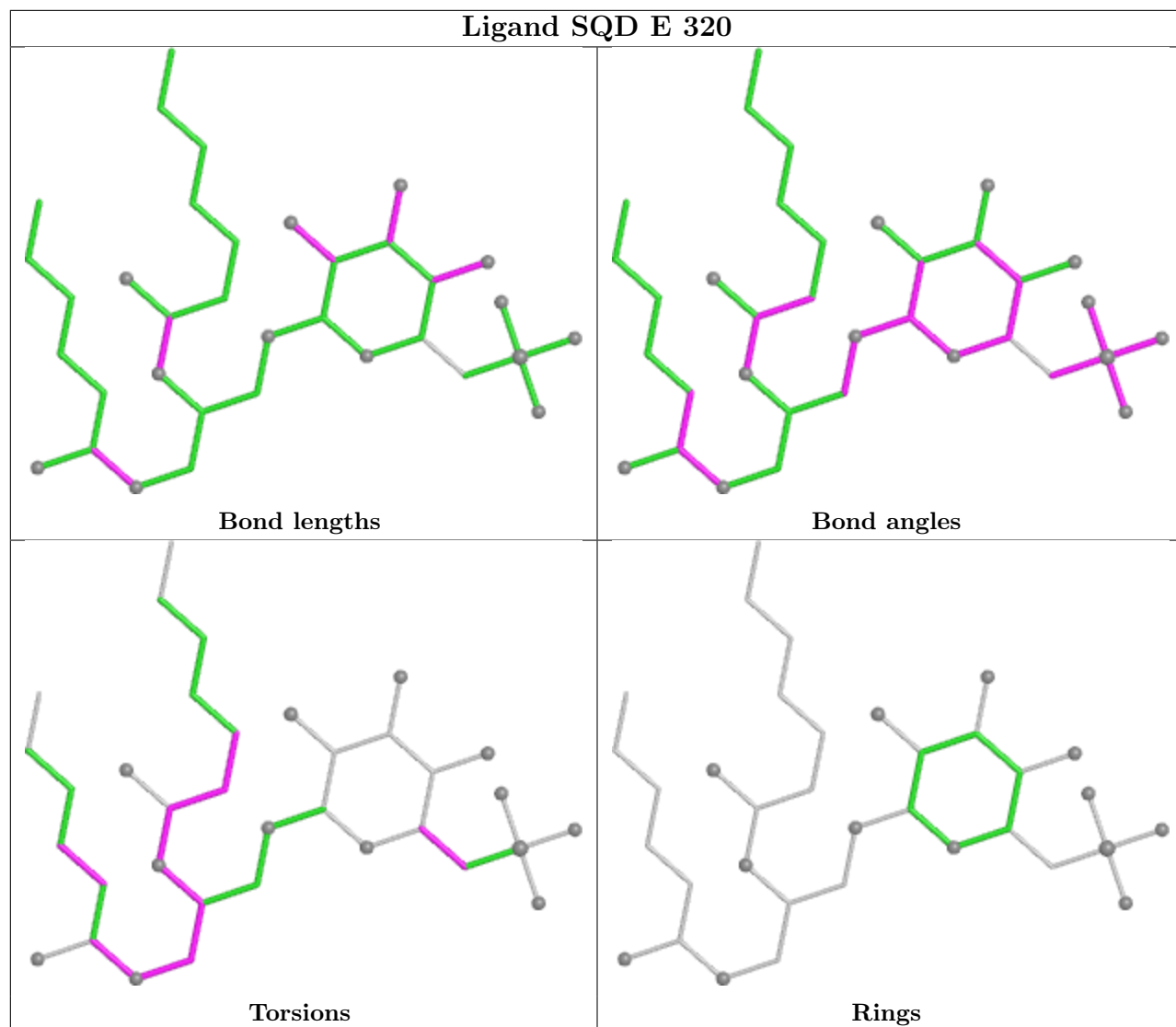
Rings



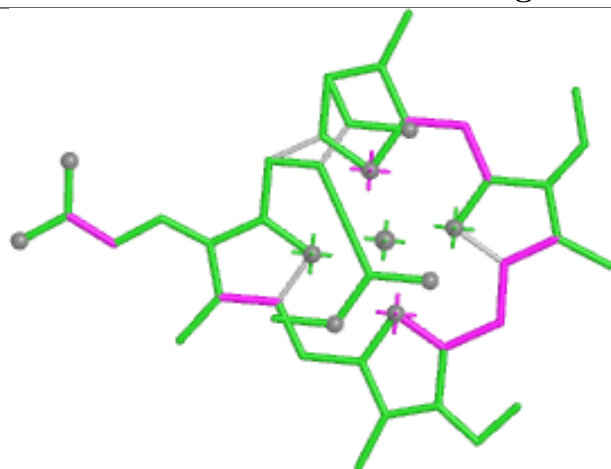




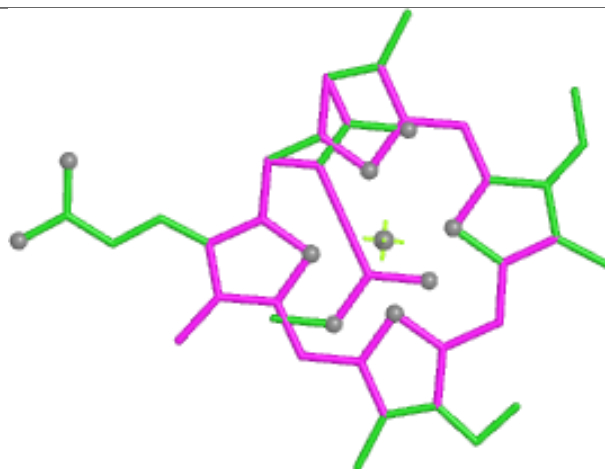
Ligand SQD E 320



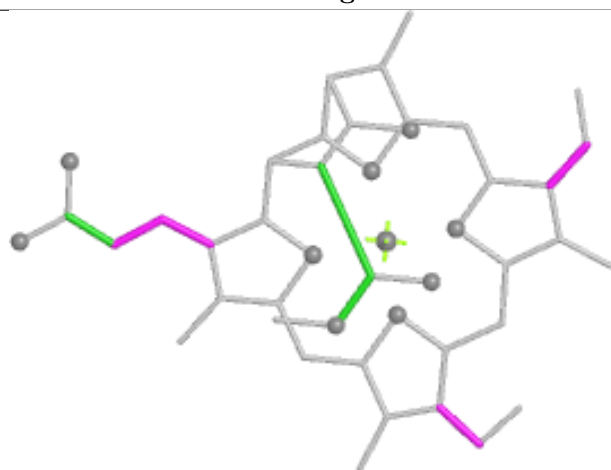
Ligand KC2 G 313



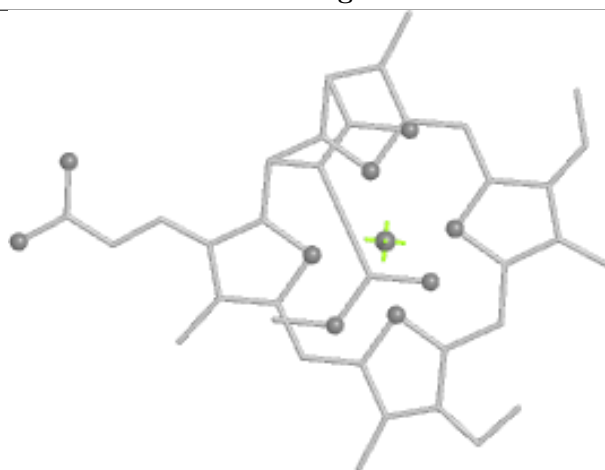
Bond lengths



Bond angles

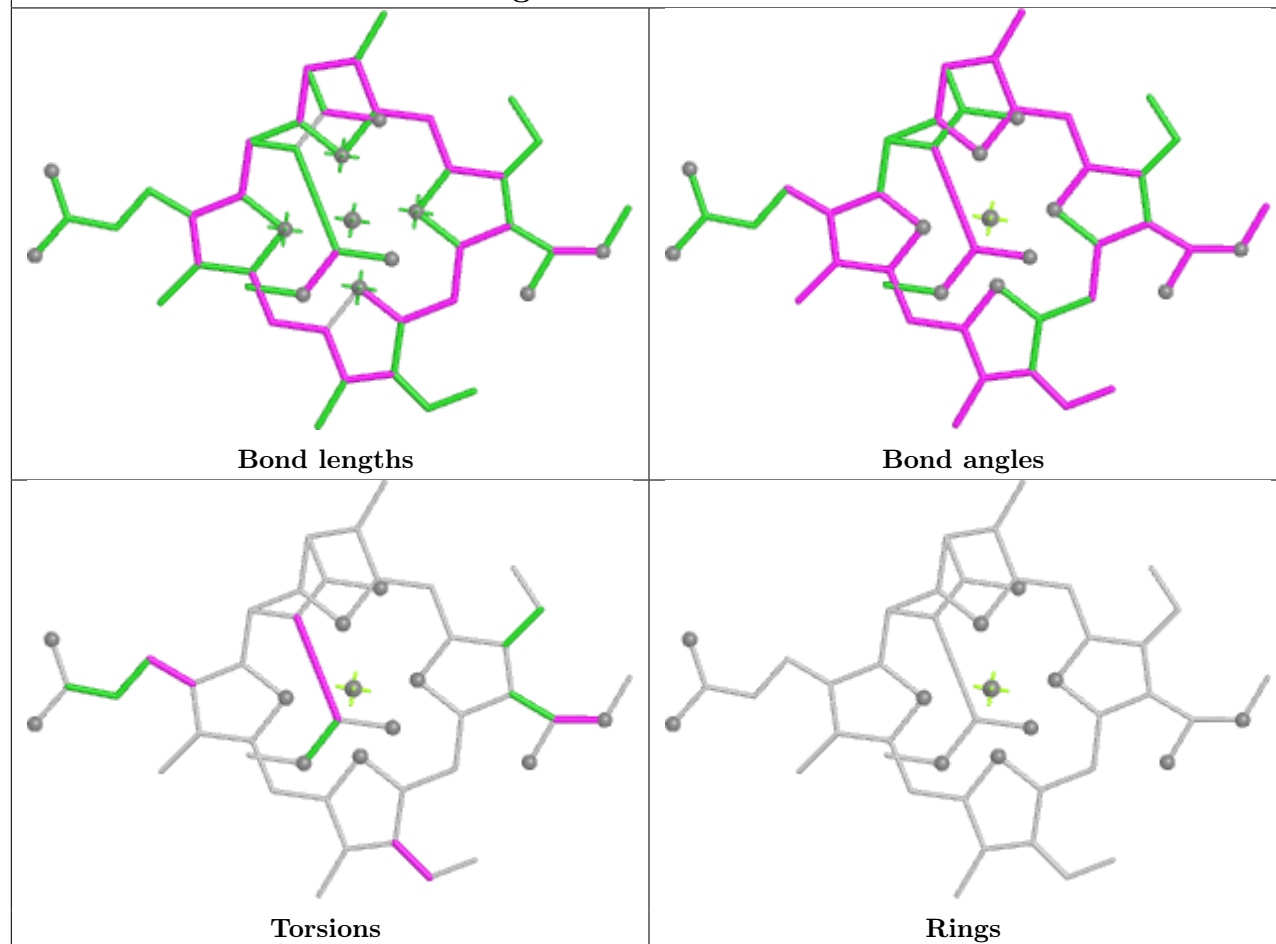


Torsions

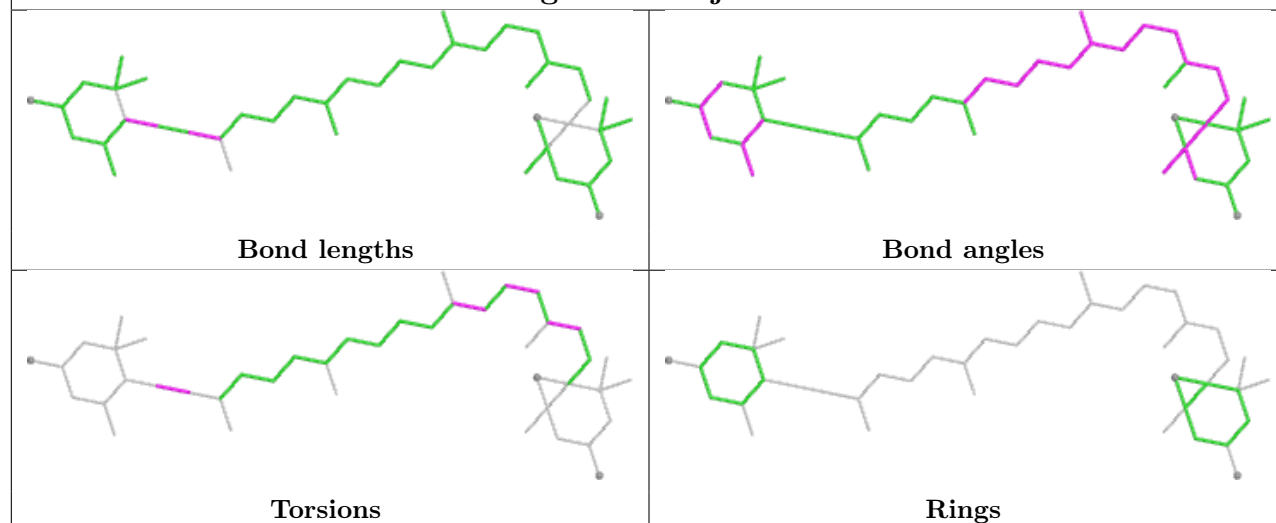


Rings

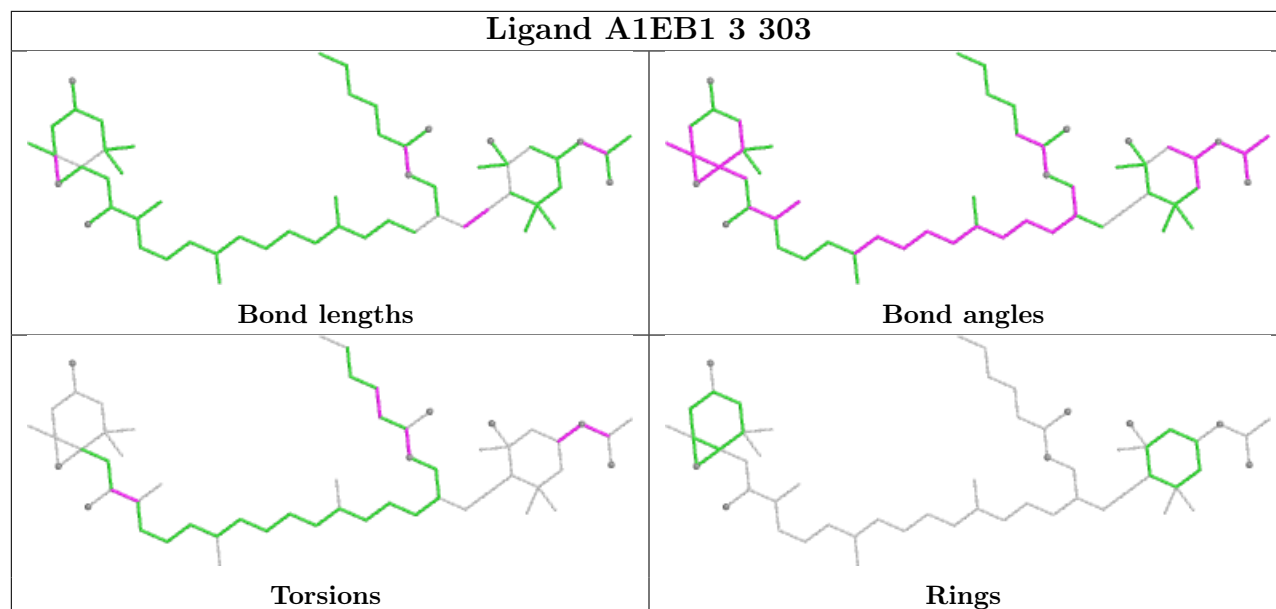
Ligand A1ECV 7 317



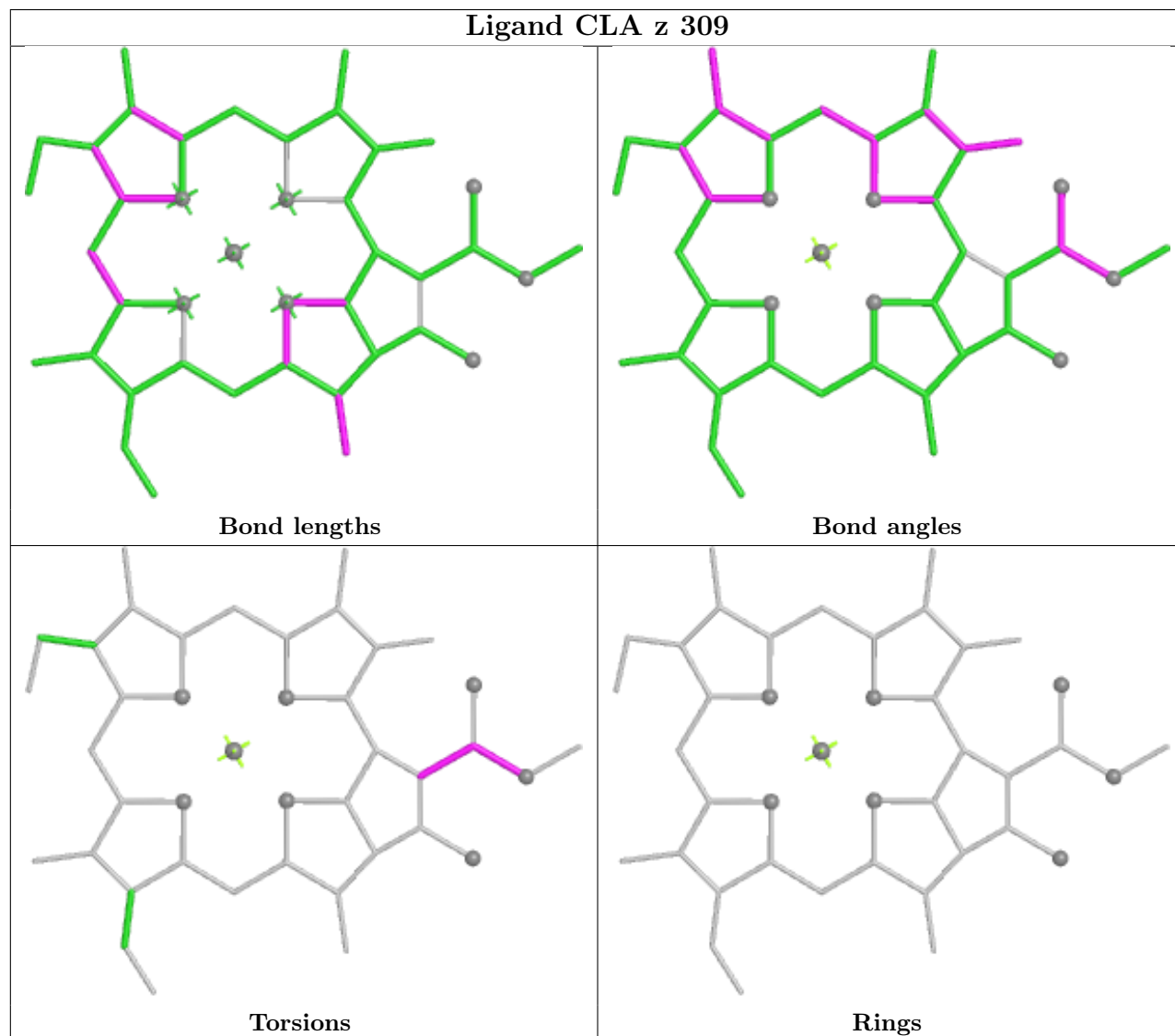
Ligand DD6 j 102

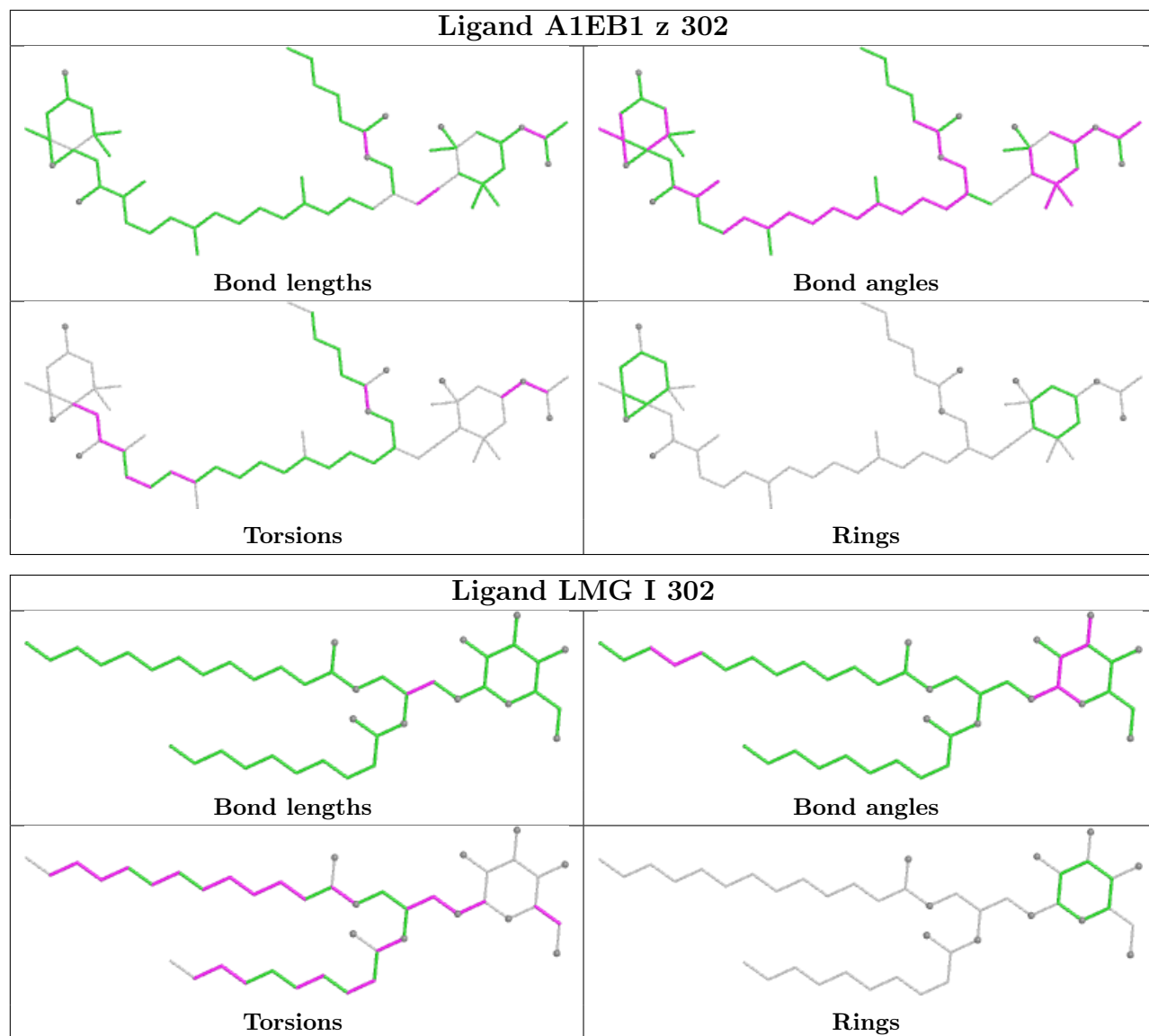


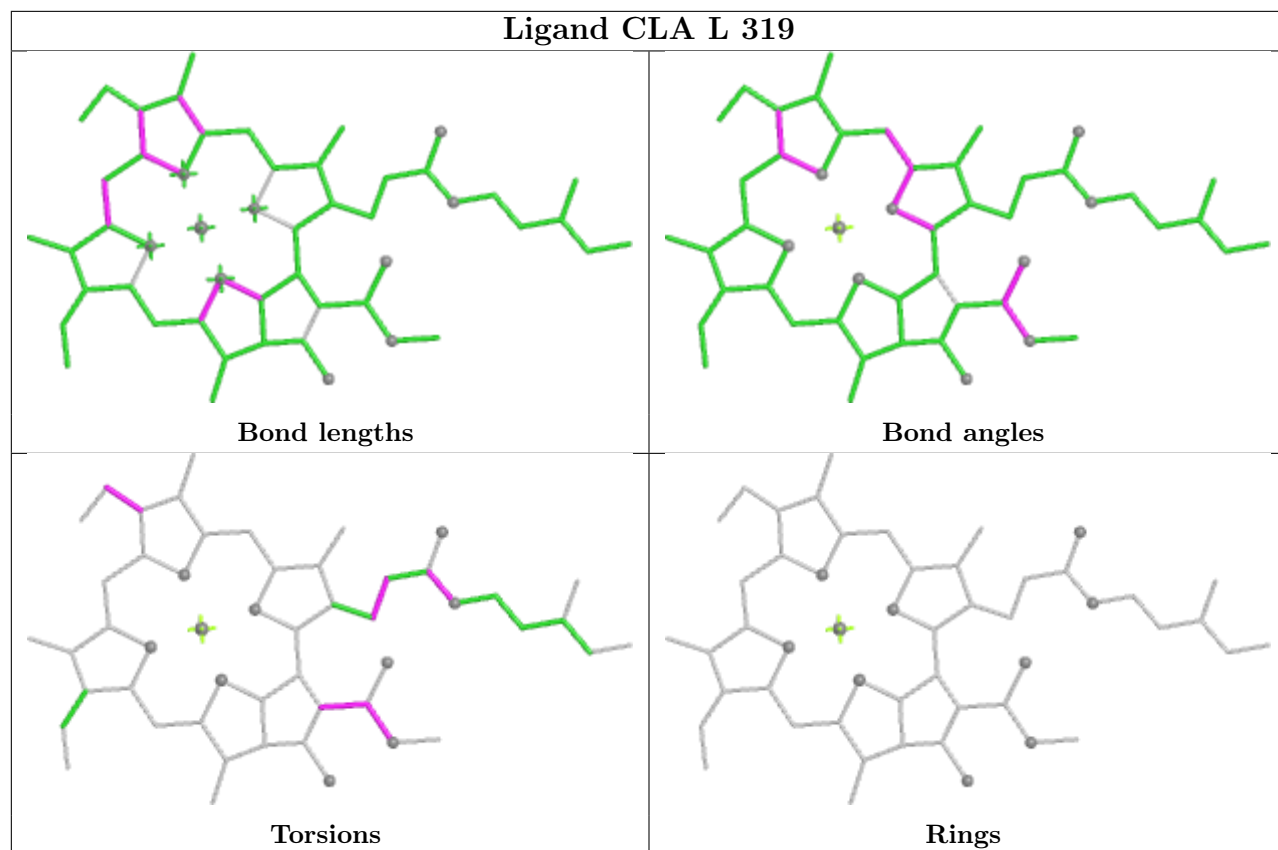
Ligand A1EB1 3 303



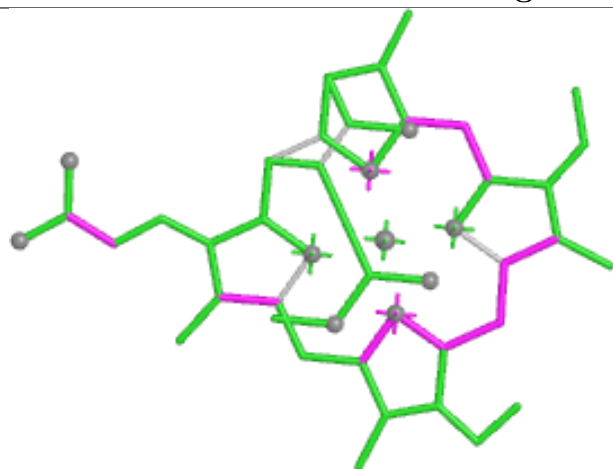
Ligand CLA z 309



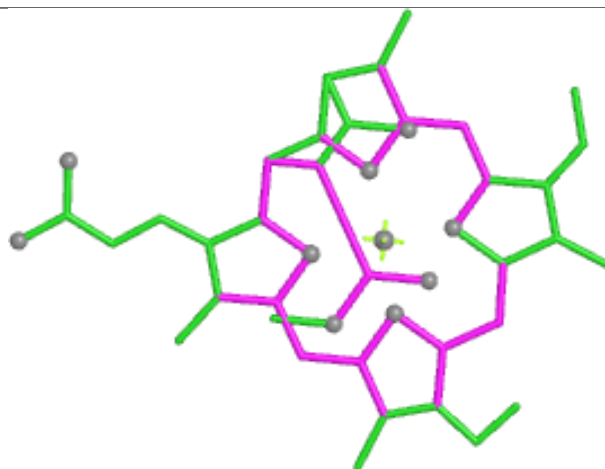




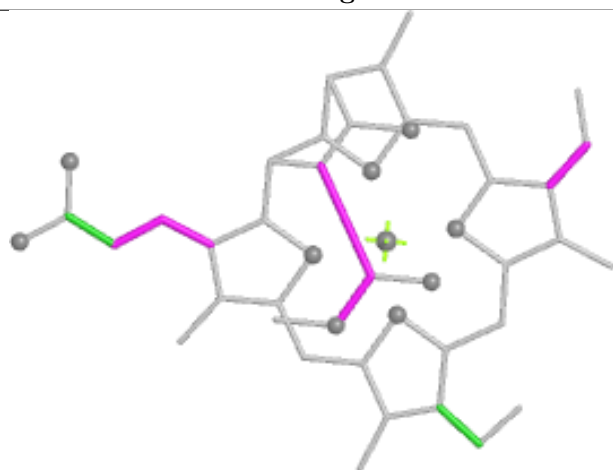
Ligand KC2 V 315



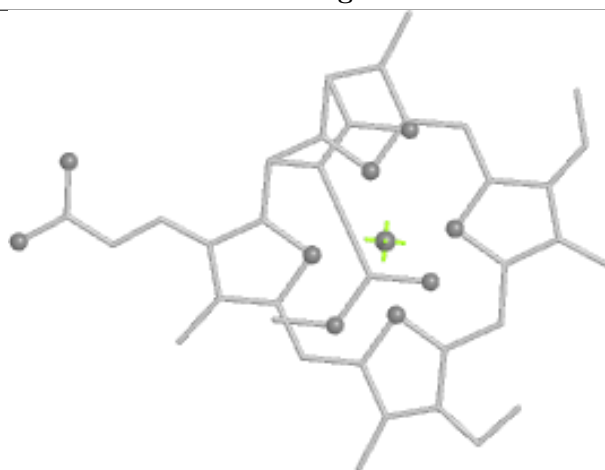
Bond lengths



Bond angles

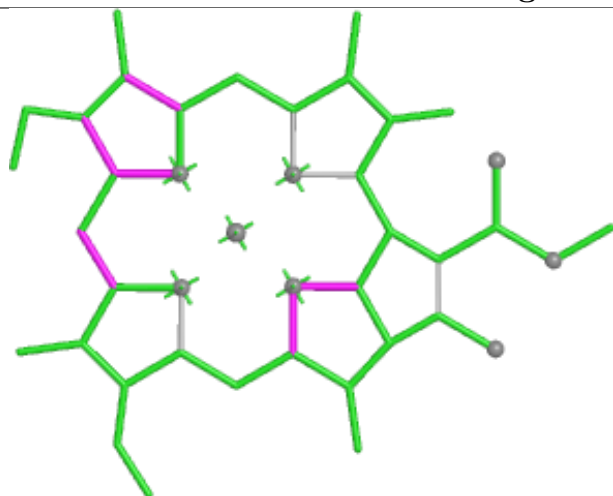


Torsions

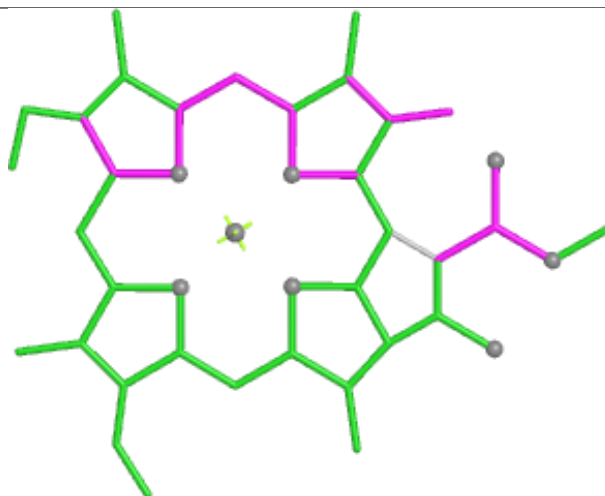


Rings

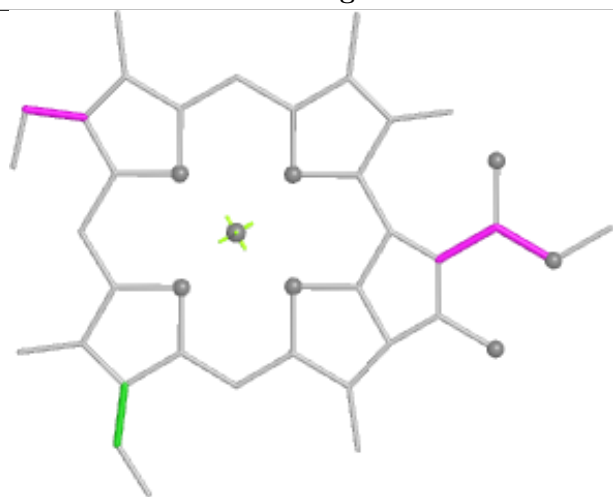
Ligand CLA 3 319



Bond lengths



Bond angles

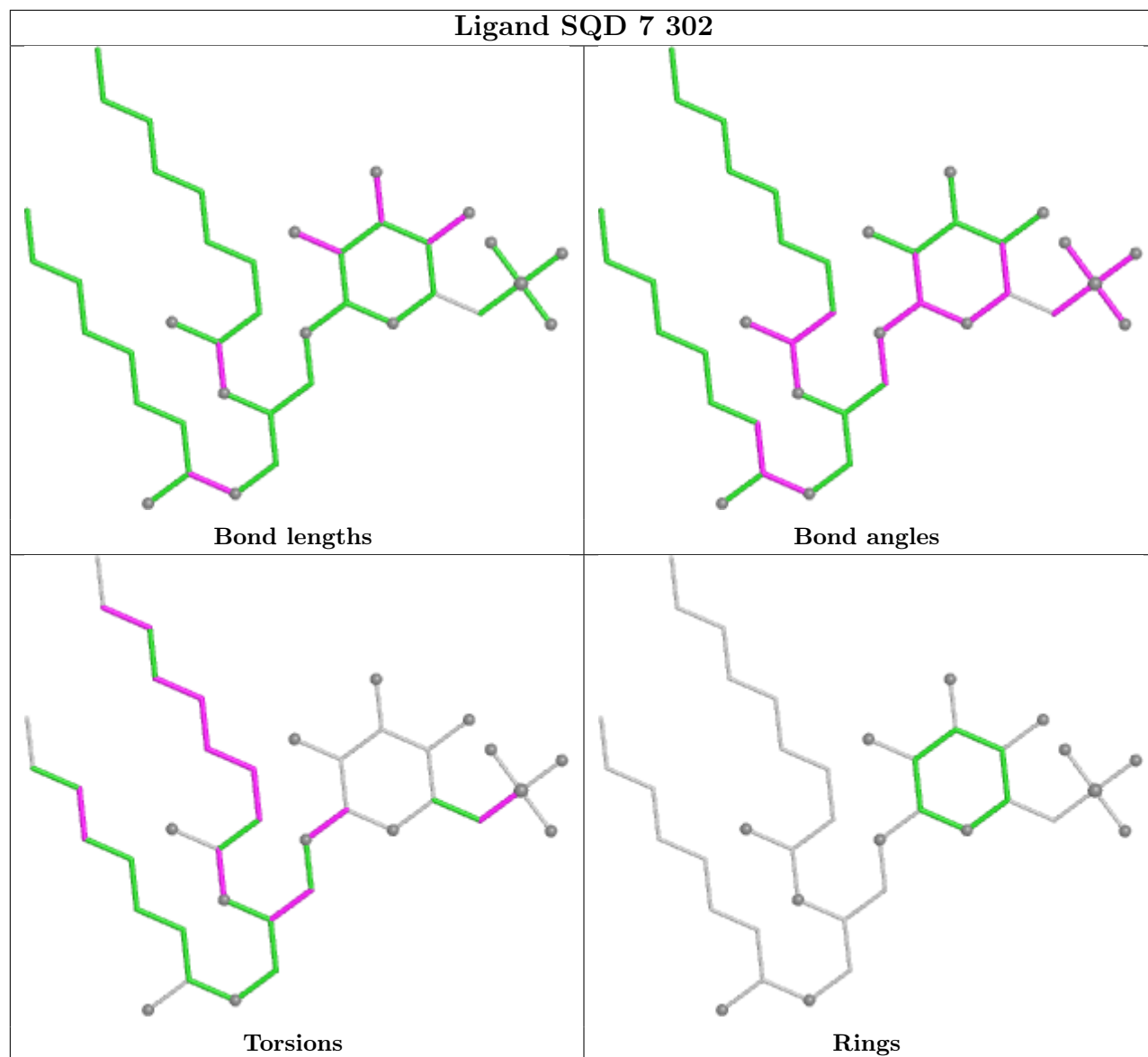


Torsions

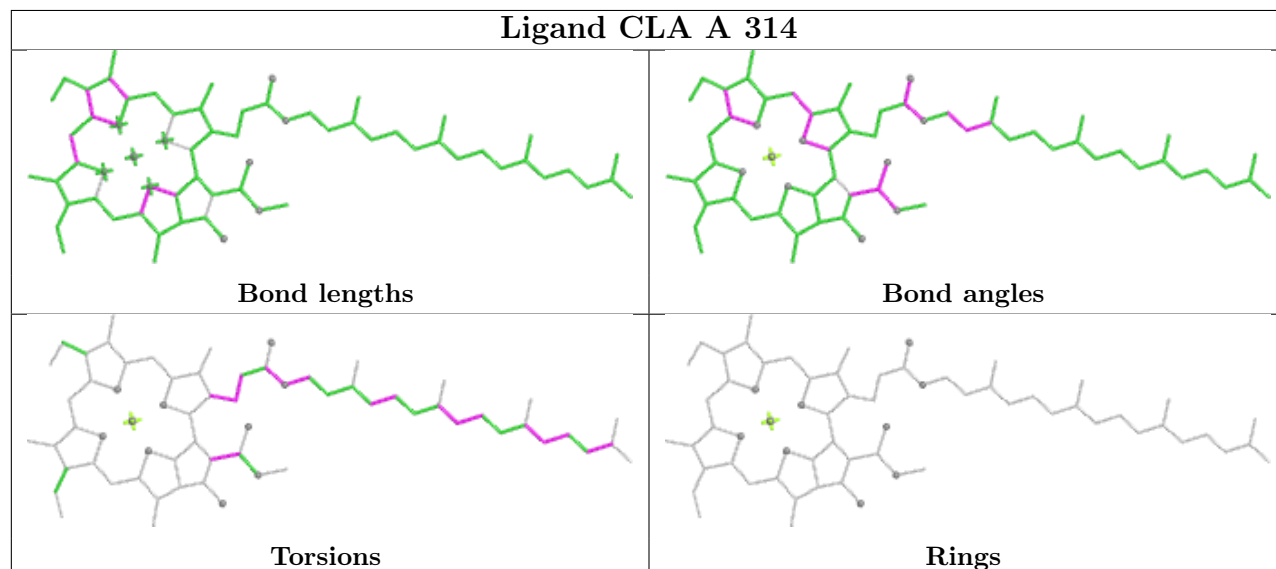


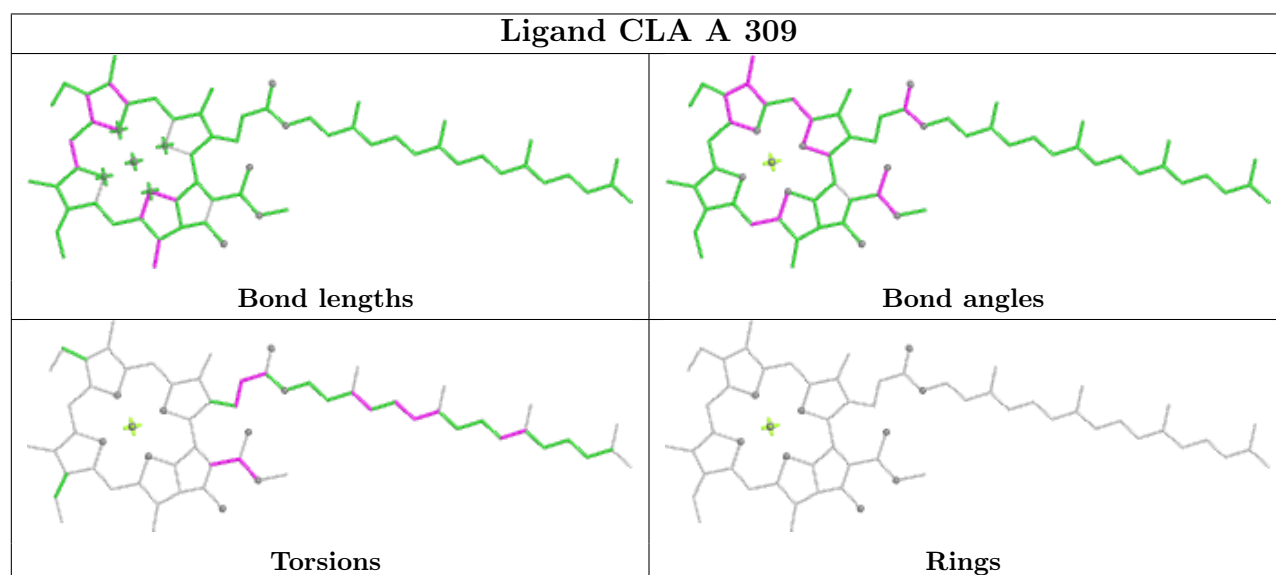
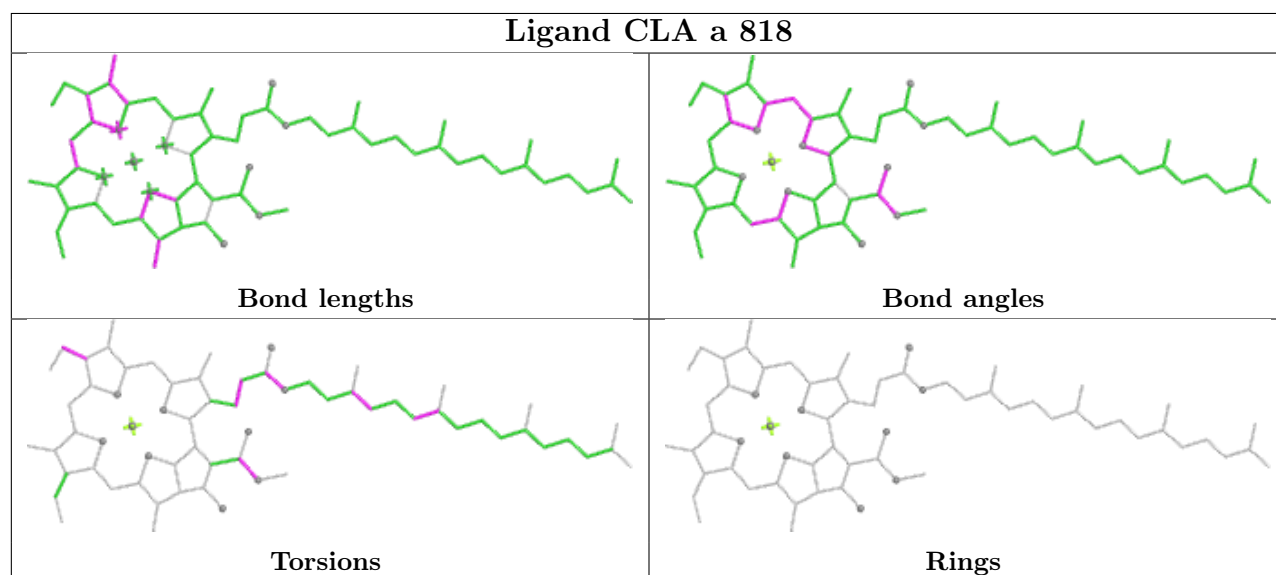
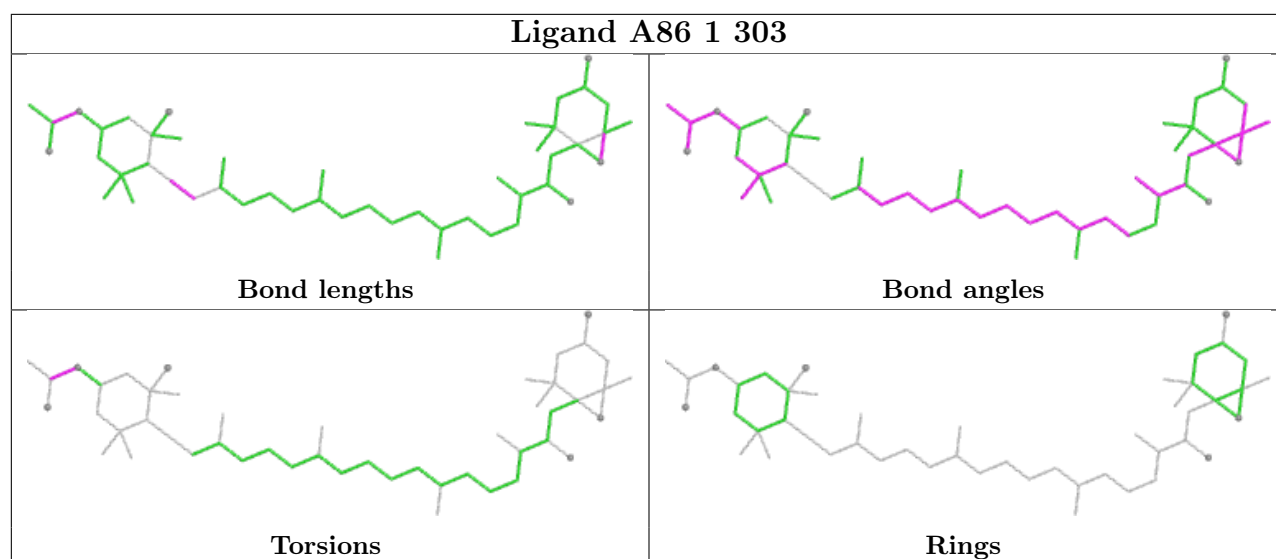
Rings

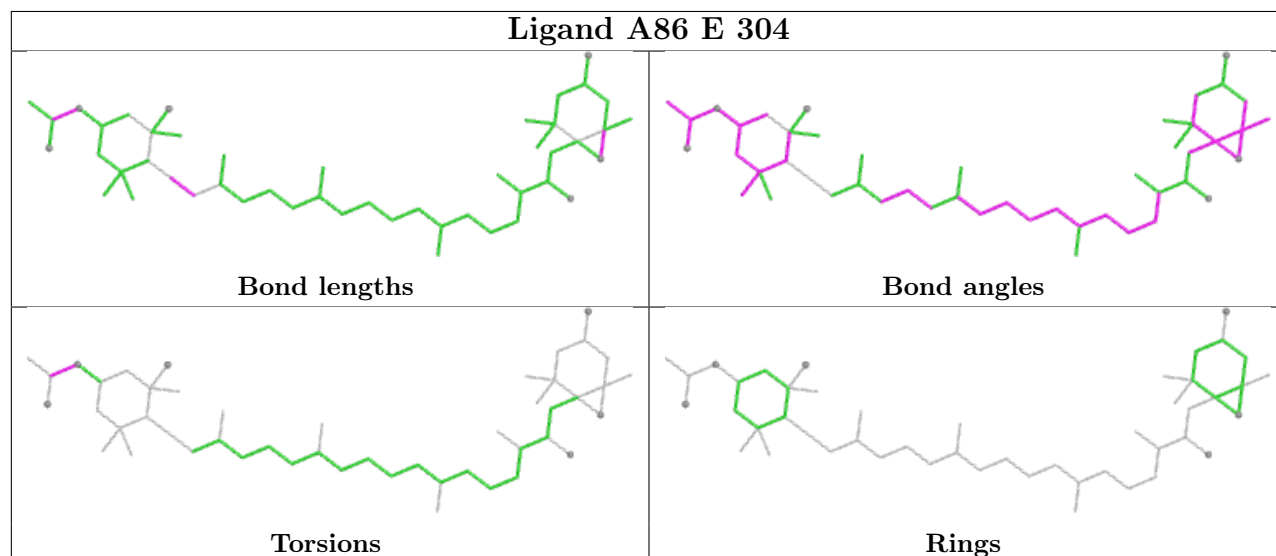
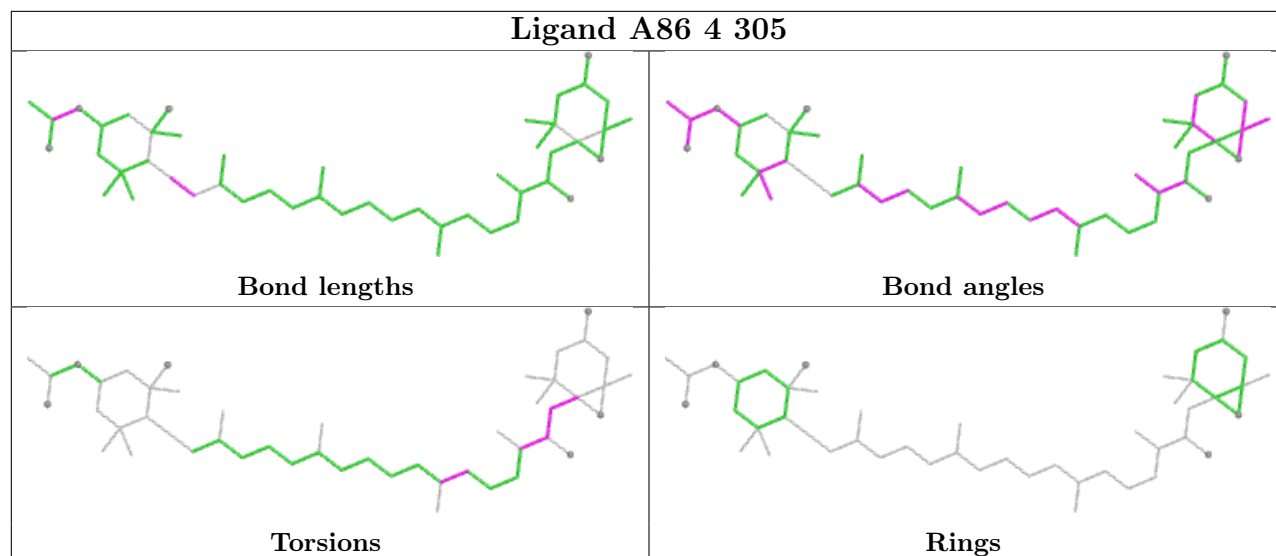
Ligand SQD 7 302

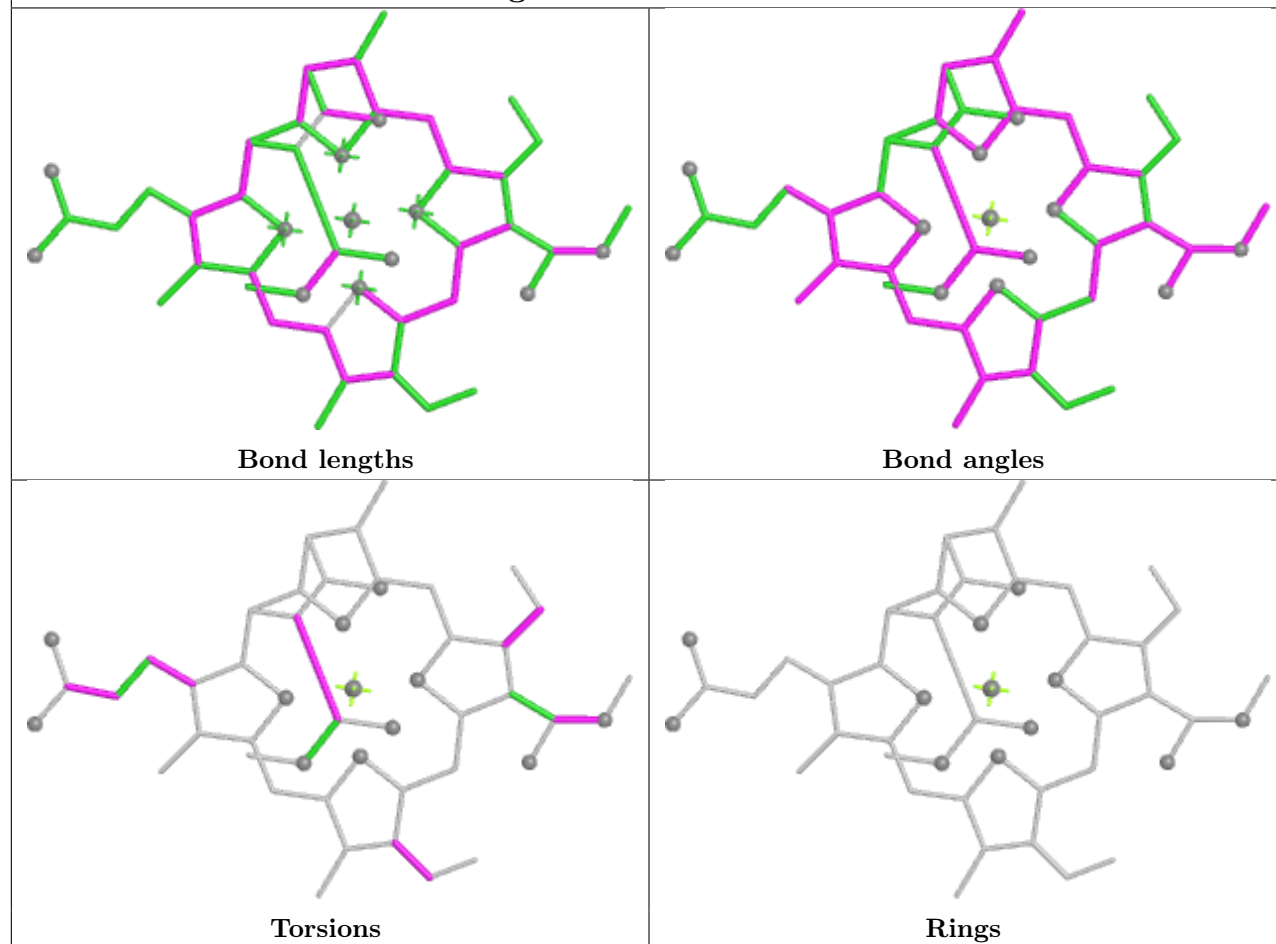
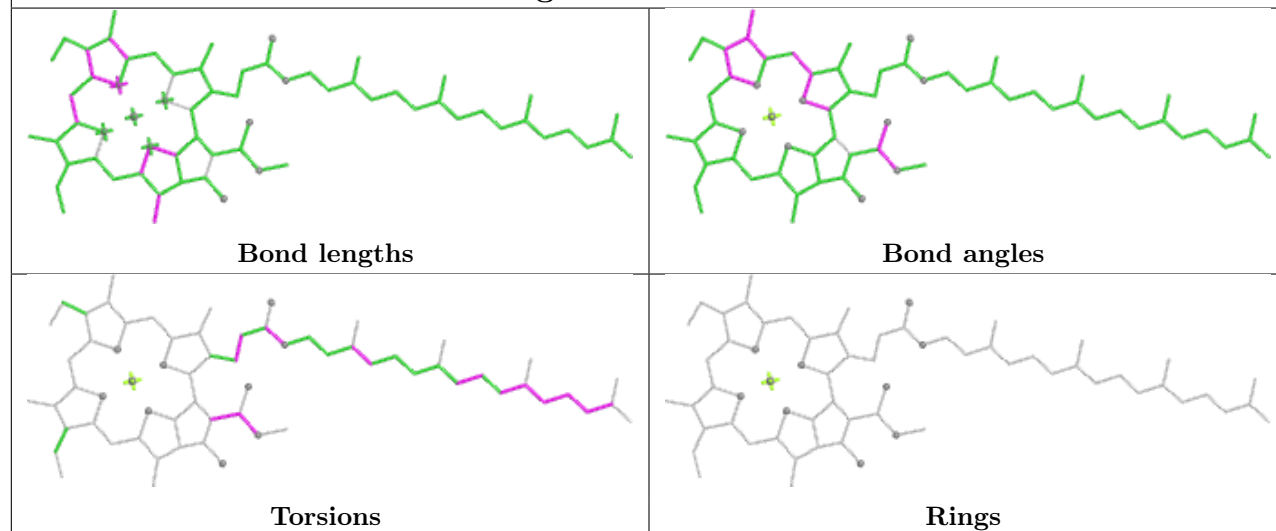


Ligand CLA A 314

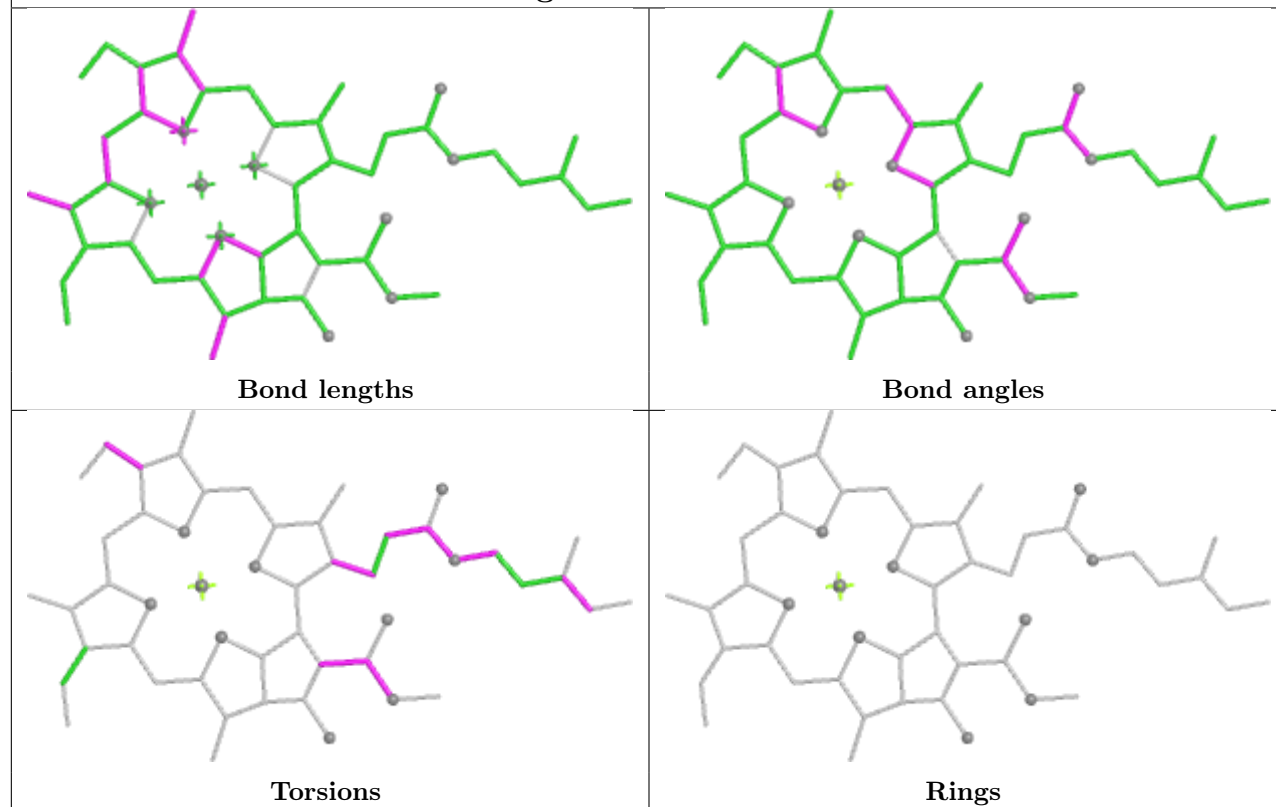




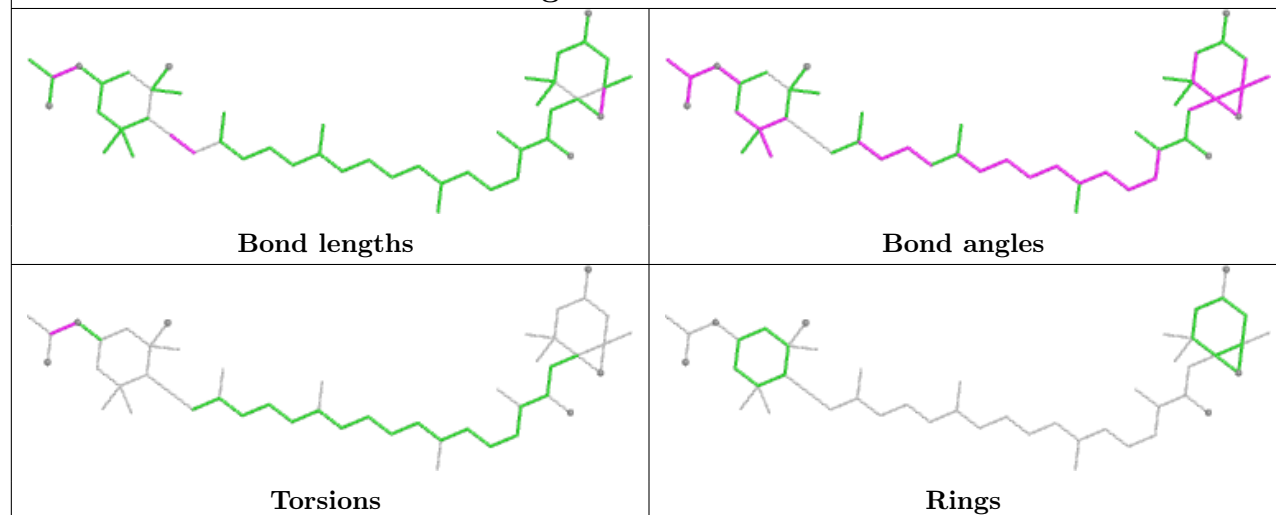


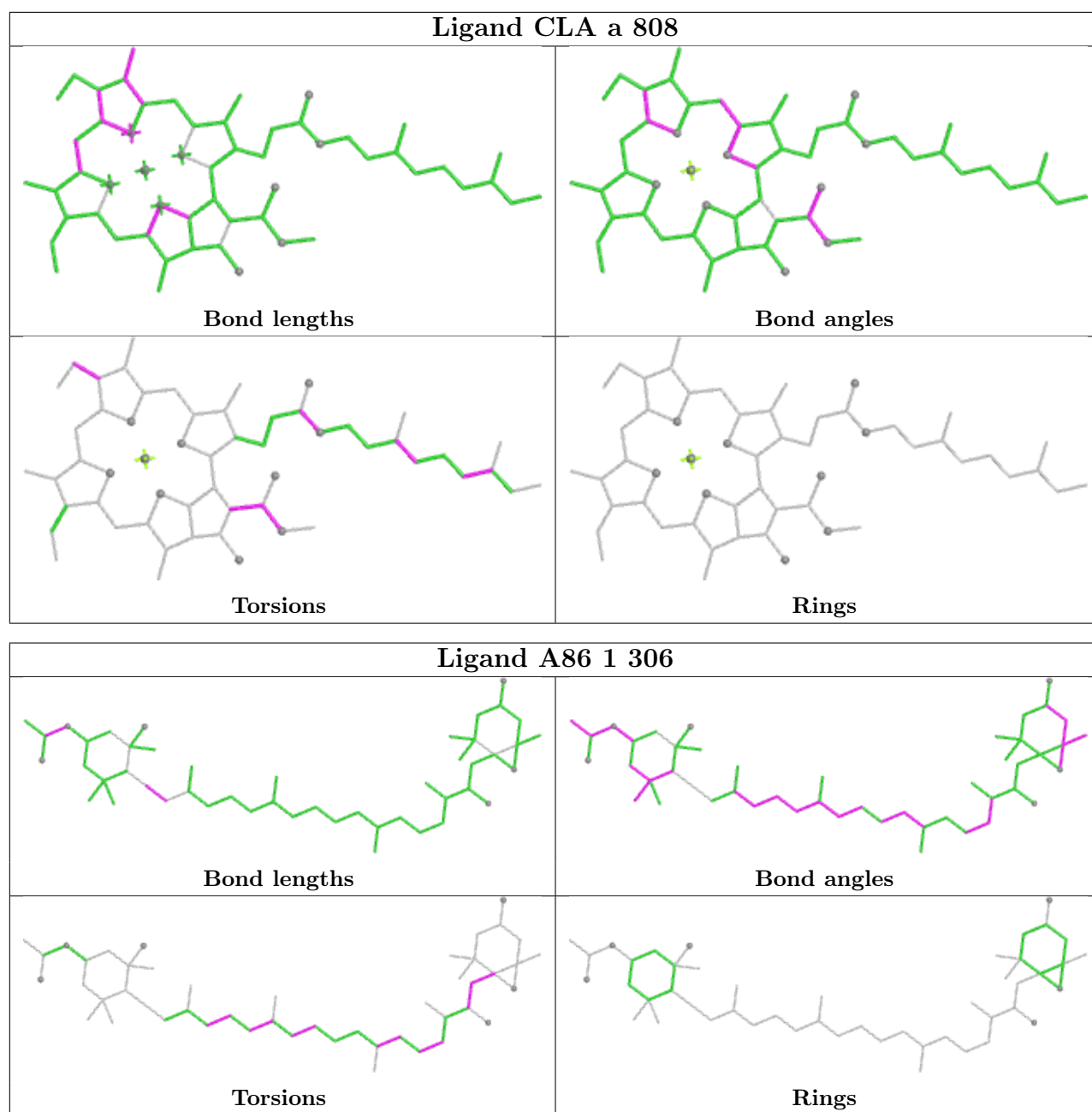
Ligand A1ECV R 313**Ligand CLA a 826**

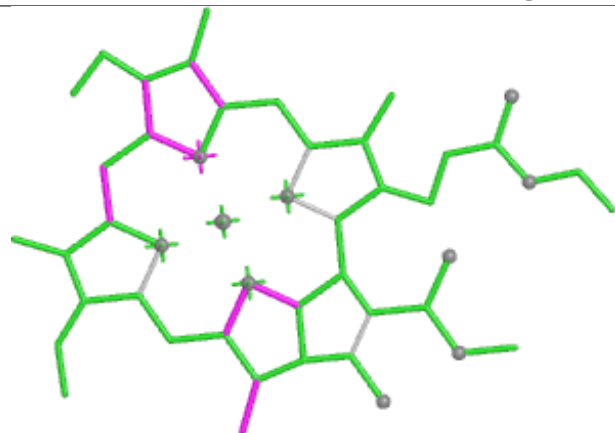
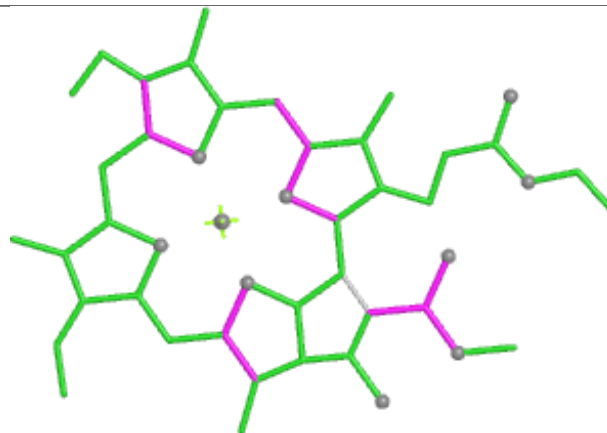
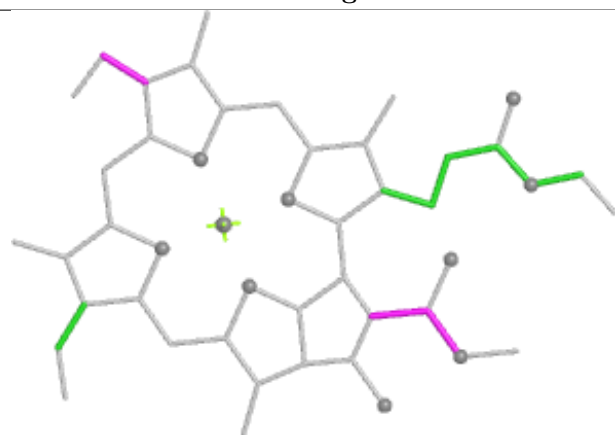
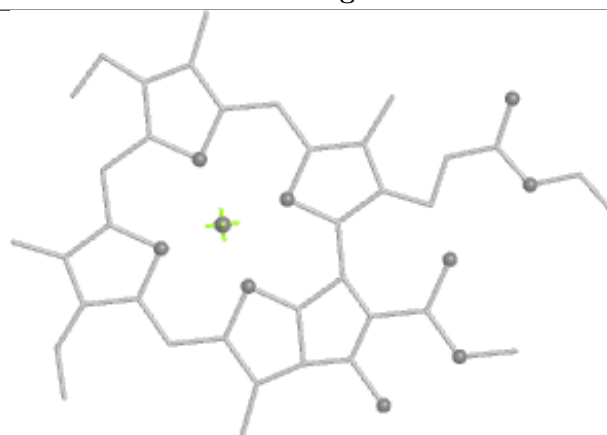
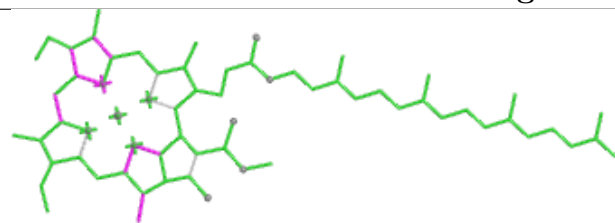
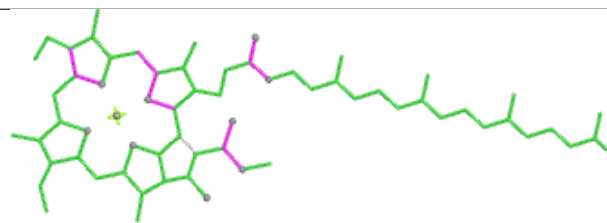
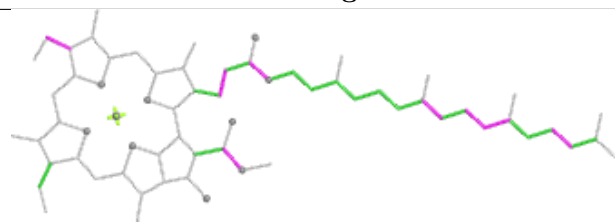
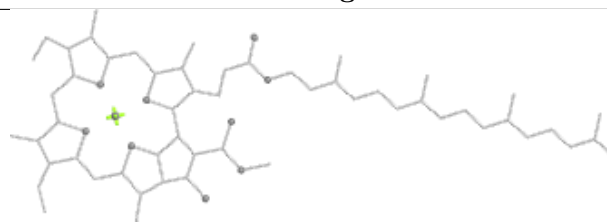
Ligand CLA 0 322



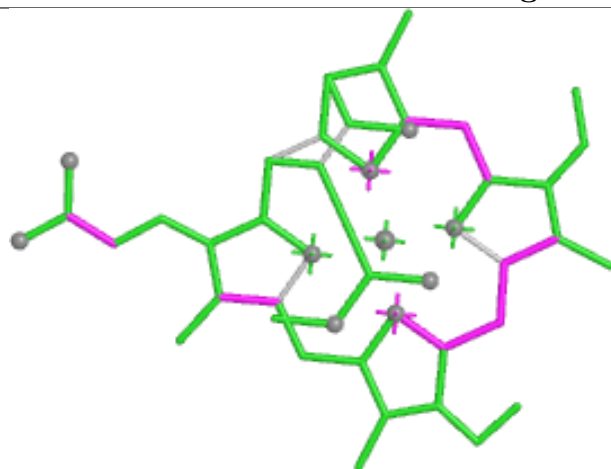
Ligand A86 J 301



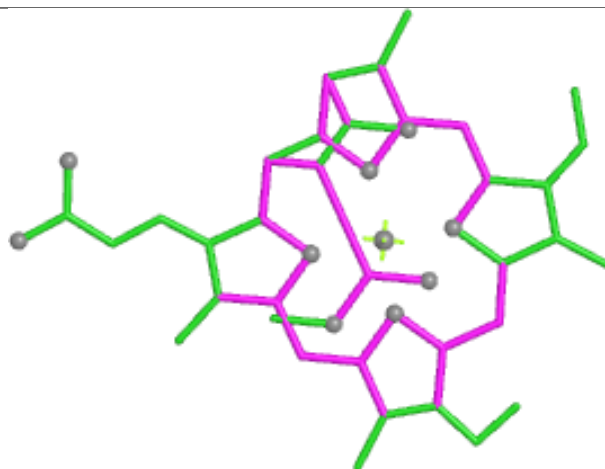


Ligand CLA 5 315**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA P 307****Bond lengths****Bond angles****Torsions****Rings**

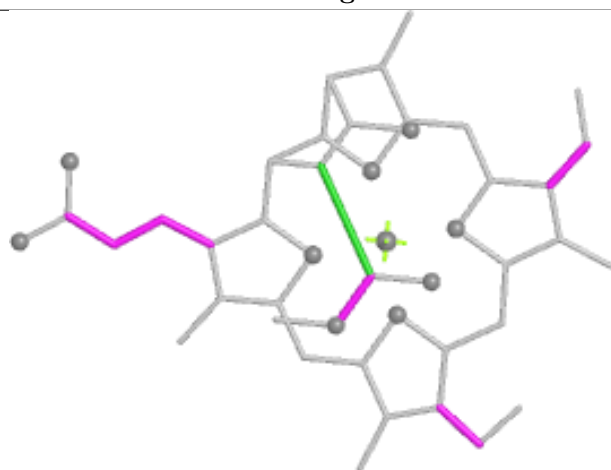
Ligand KC2 4 320



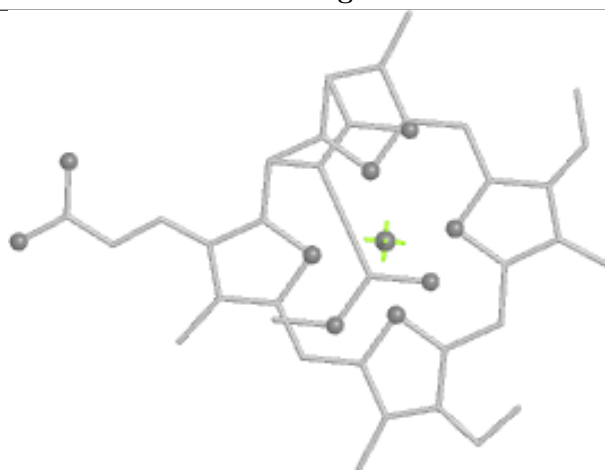
Bond lengths



Bond angles

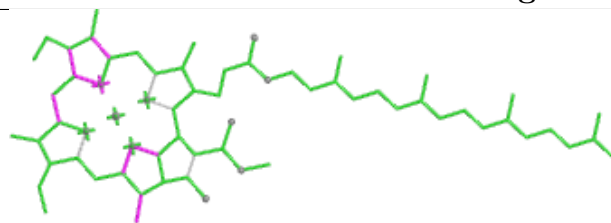


Torsions

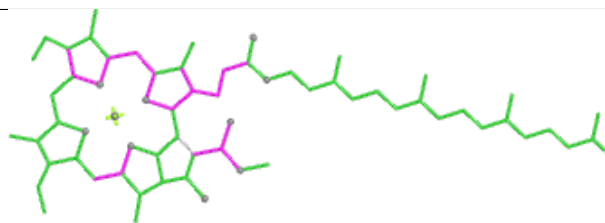


Rings

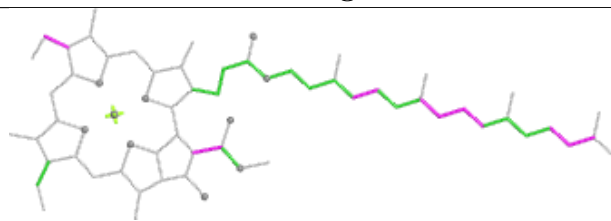
Ligand CLA a 823



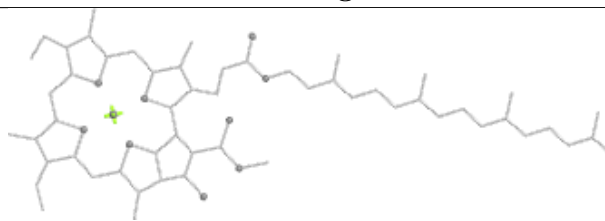
Bond lengths



Bond angles

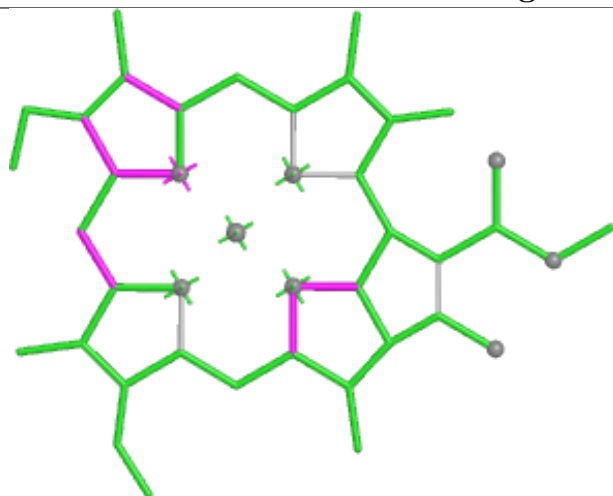


Torsions



Rings

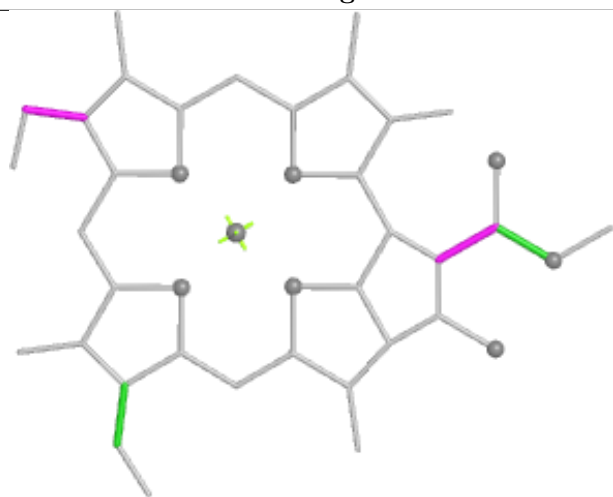
Ligand CLA 7 321



Bond lengths



Bond angles

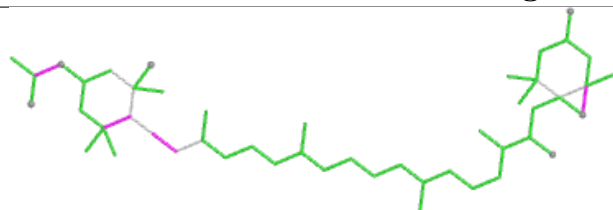


Torsions

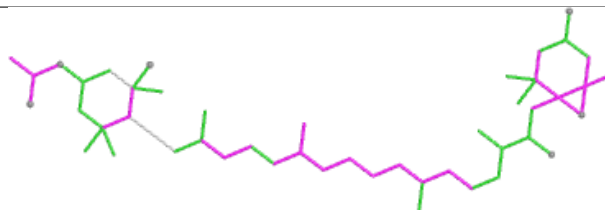


Rings

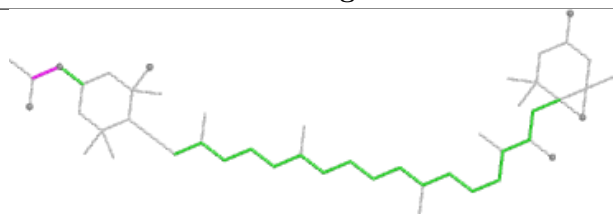
Ligand A86 F 302



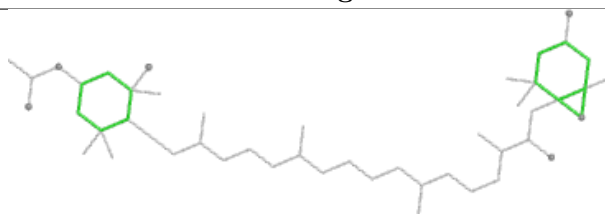
Bond lengths



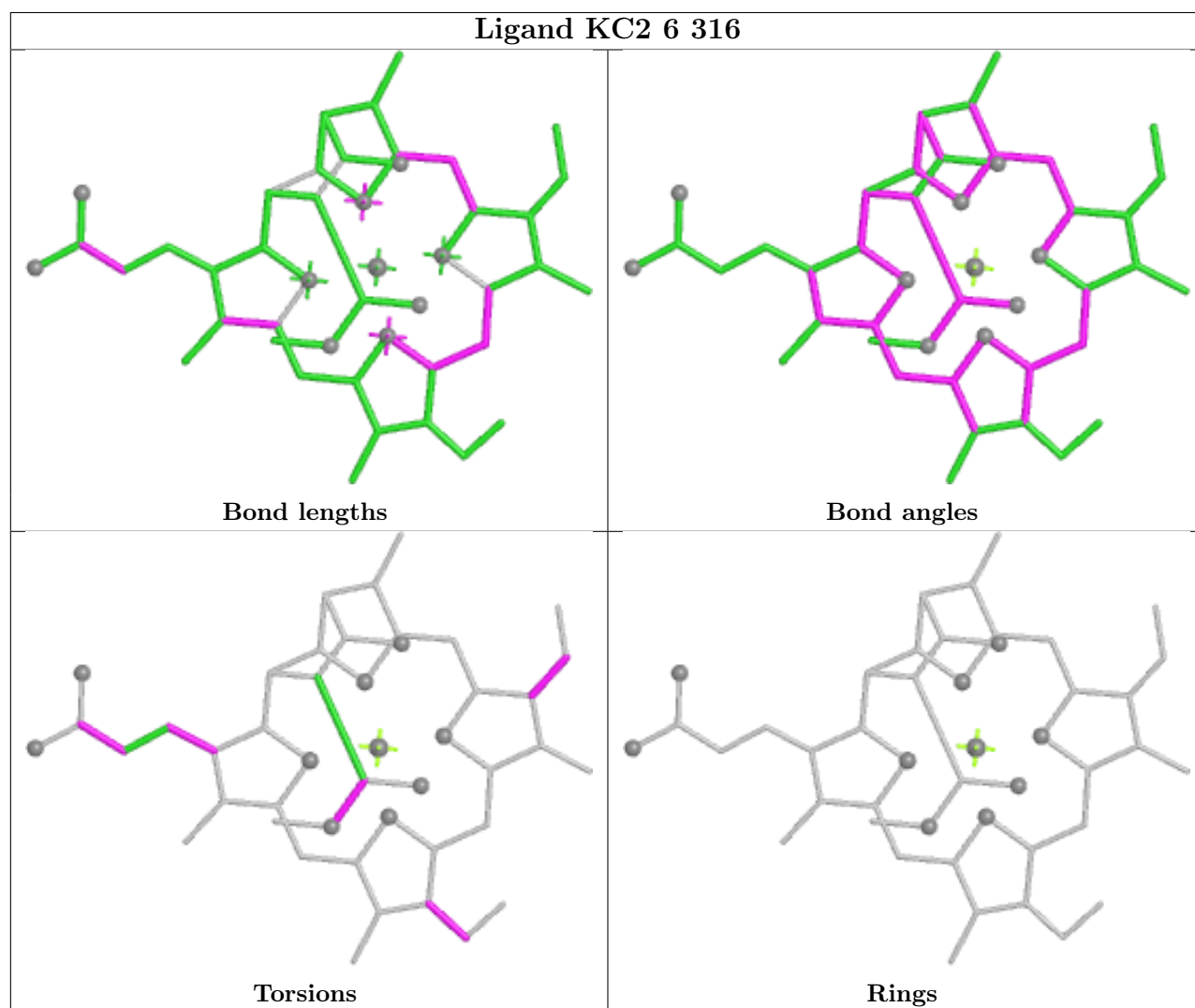
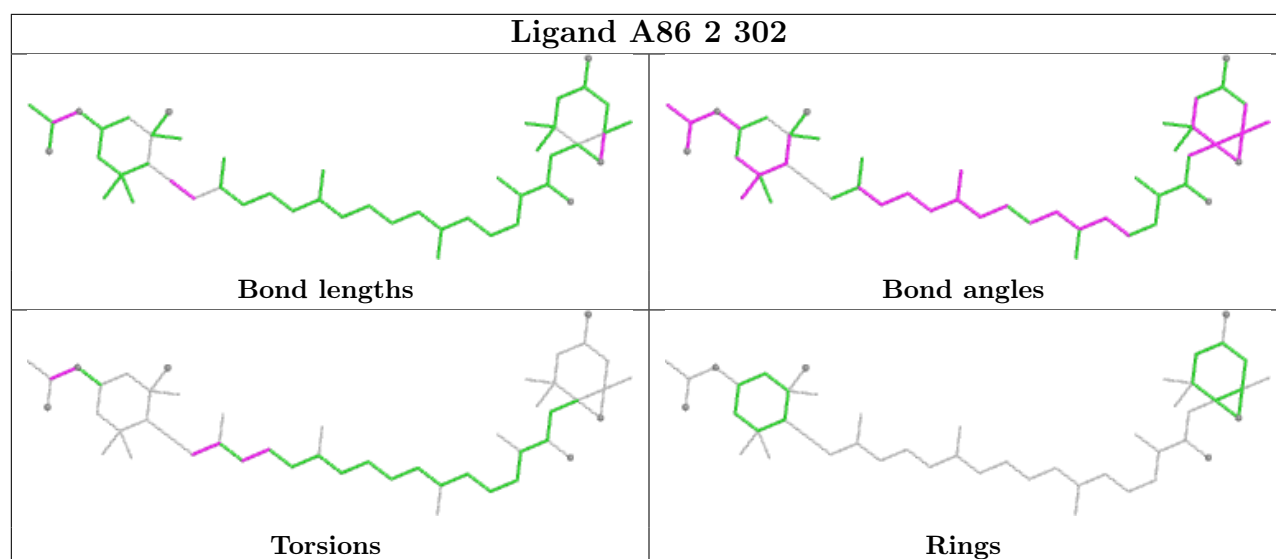
Bond angles

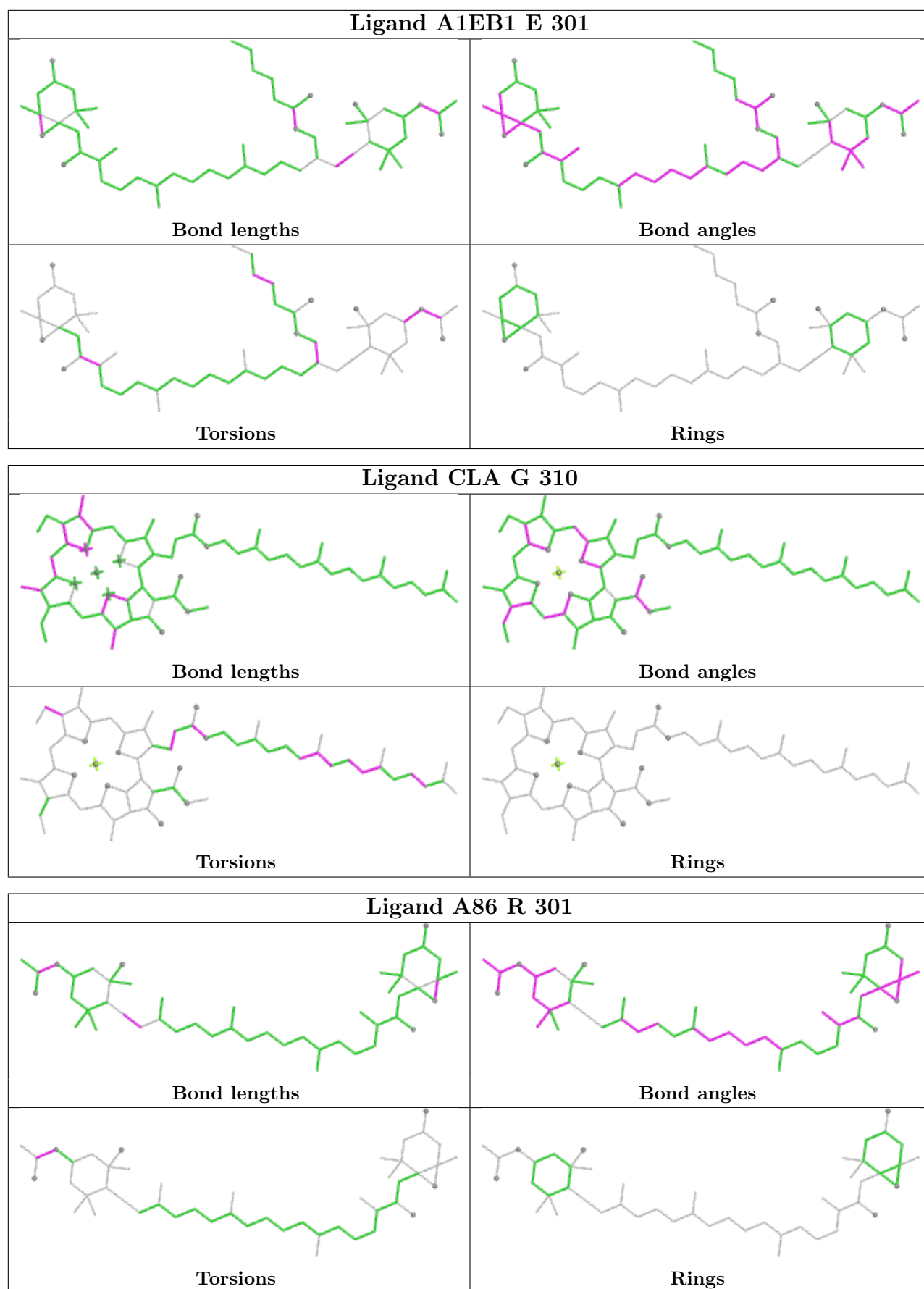


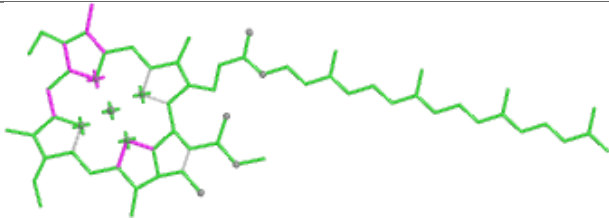
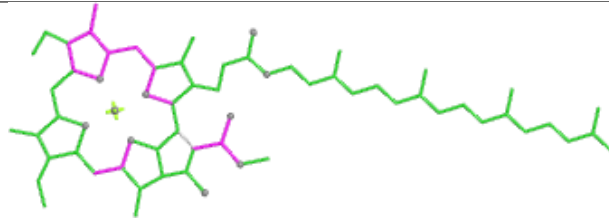
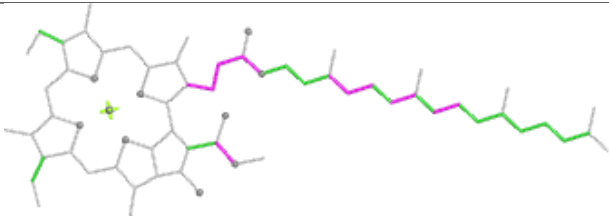
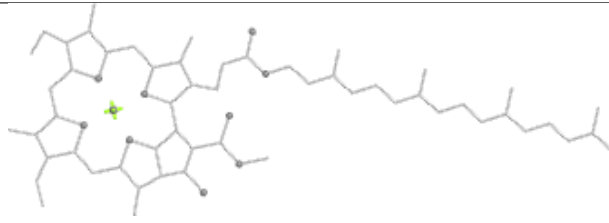
Torsions

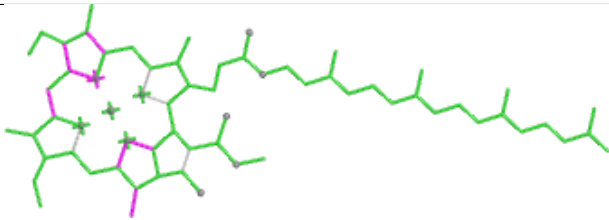
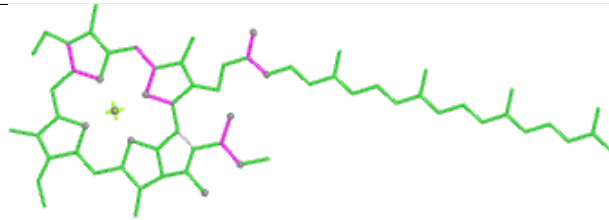
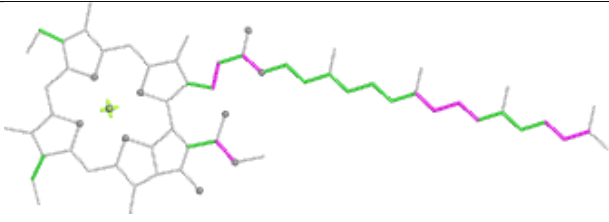
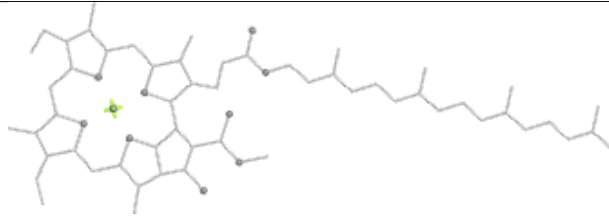


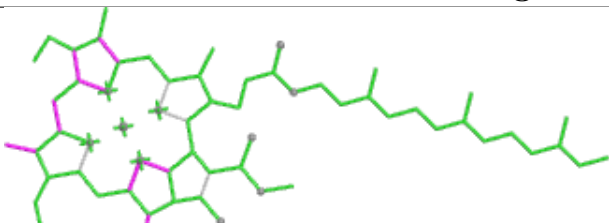
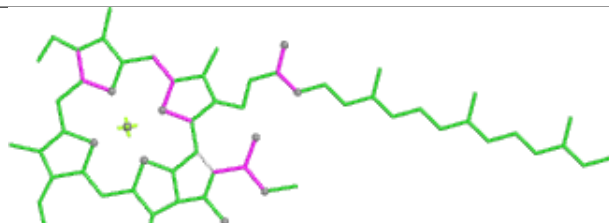
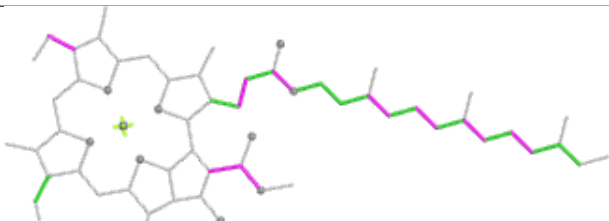
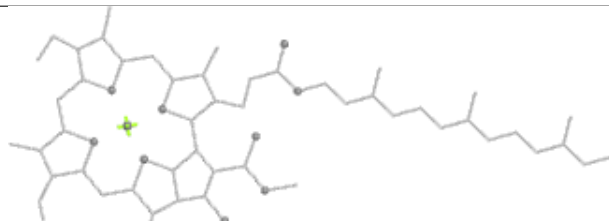
Rings



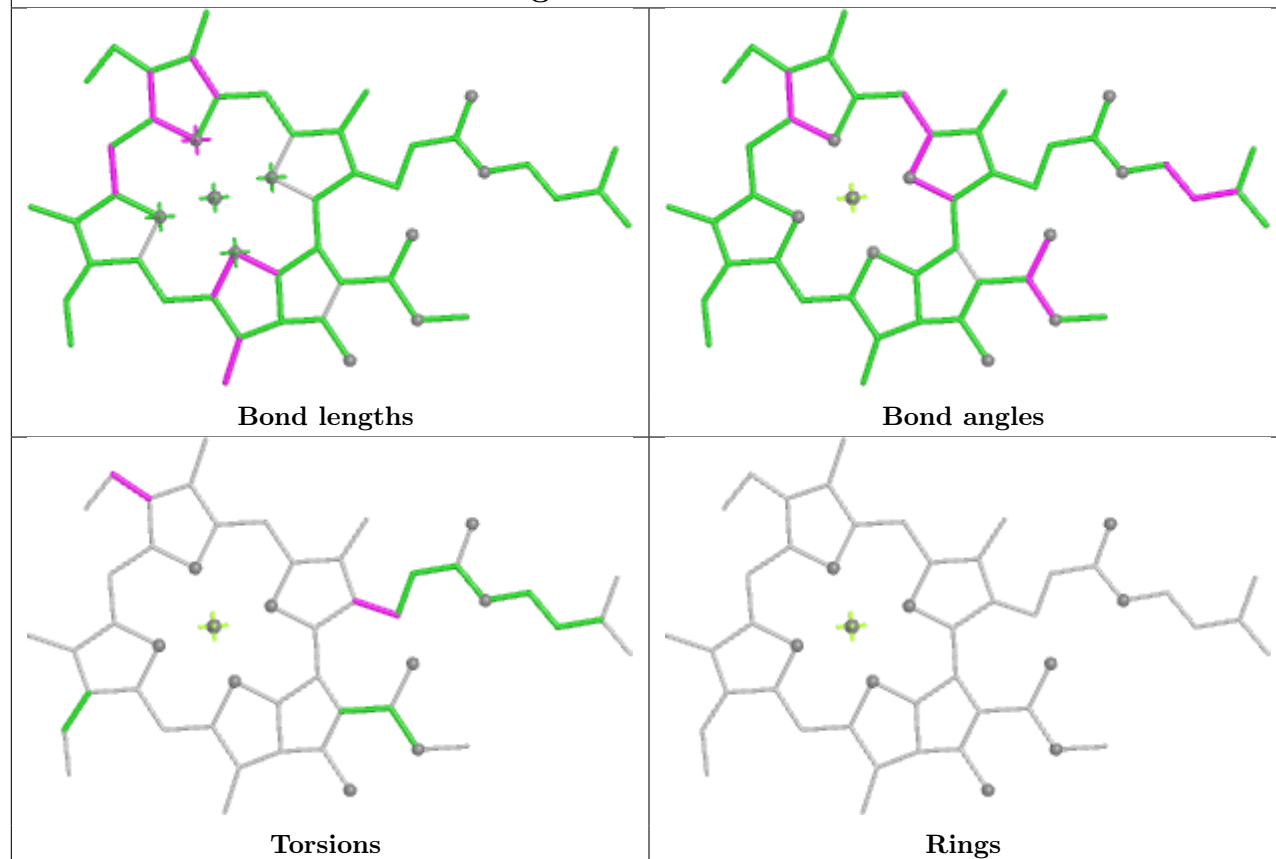


Ligand CLA E 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

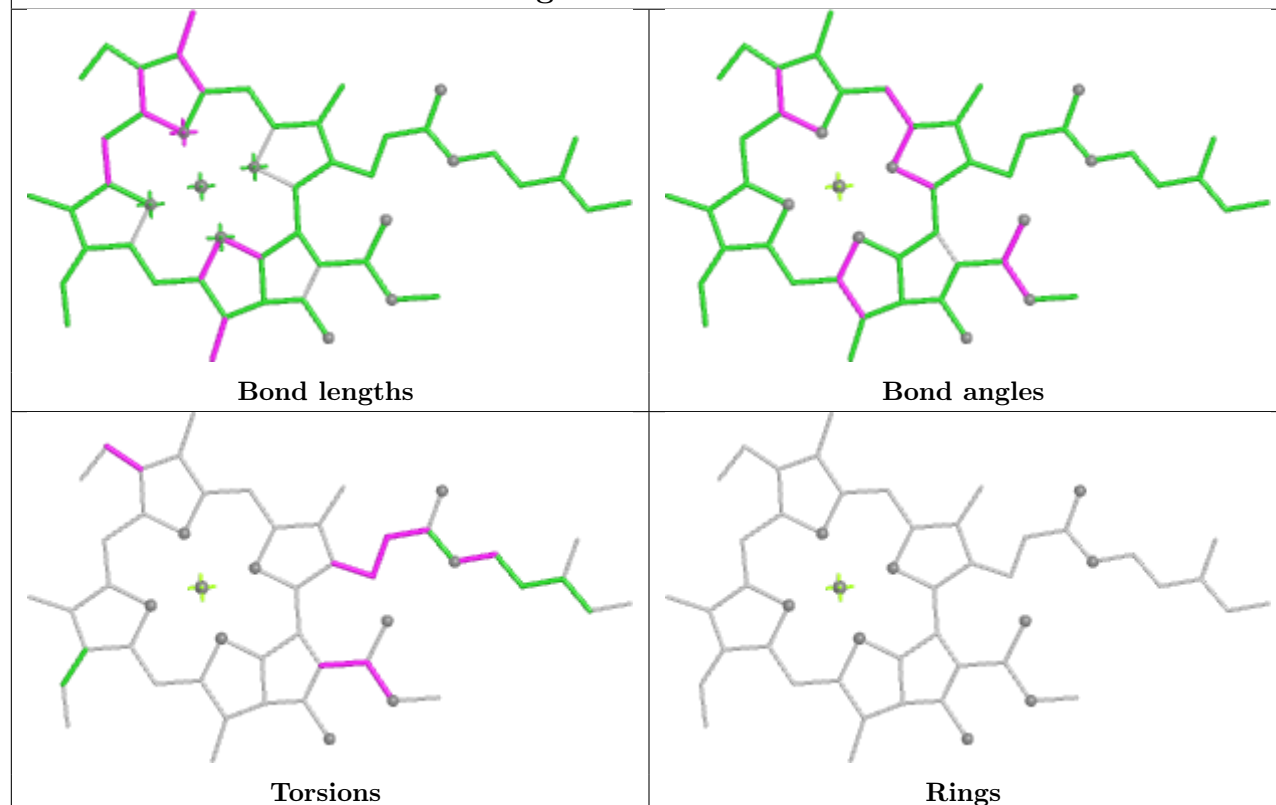
Ligand CLA M 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

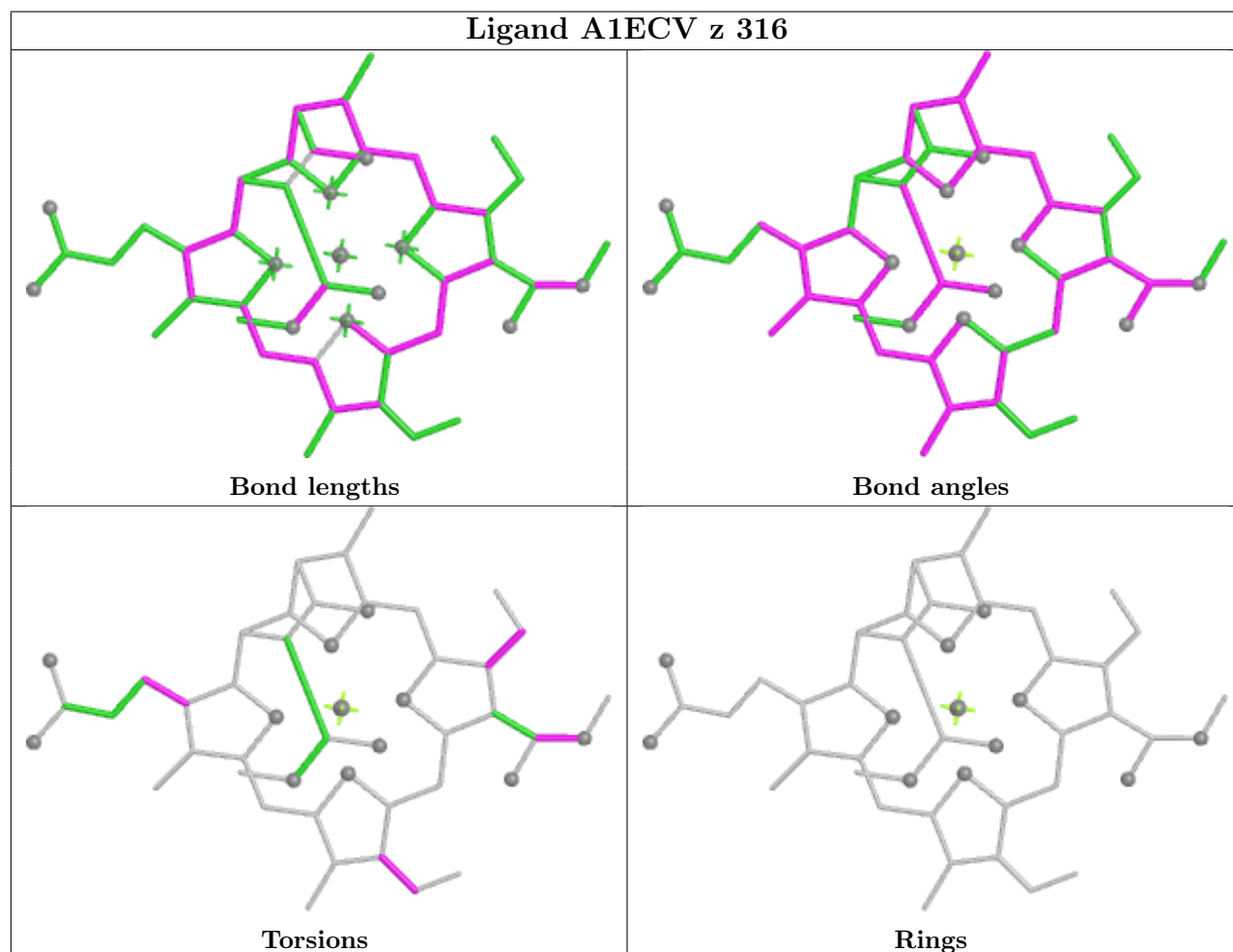
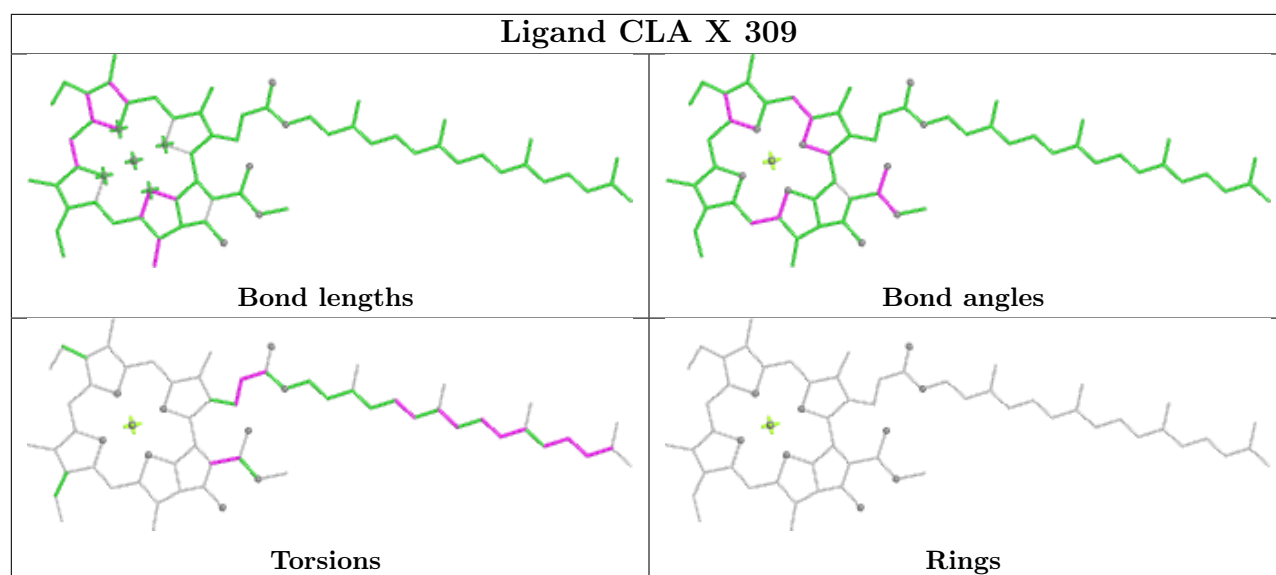
Ligand CLA a 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 313

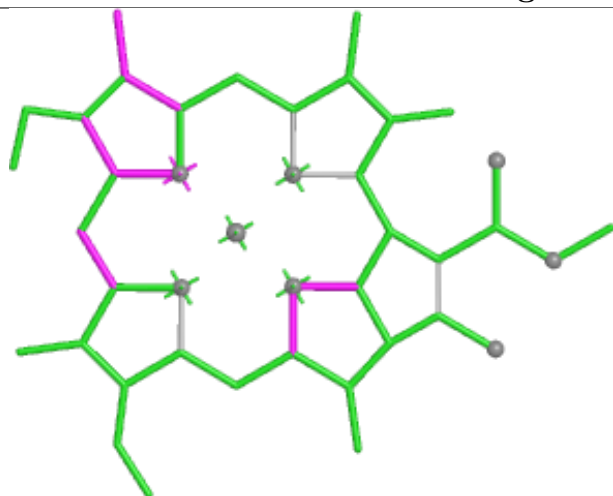


Ligand CLA a 820

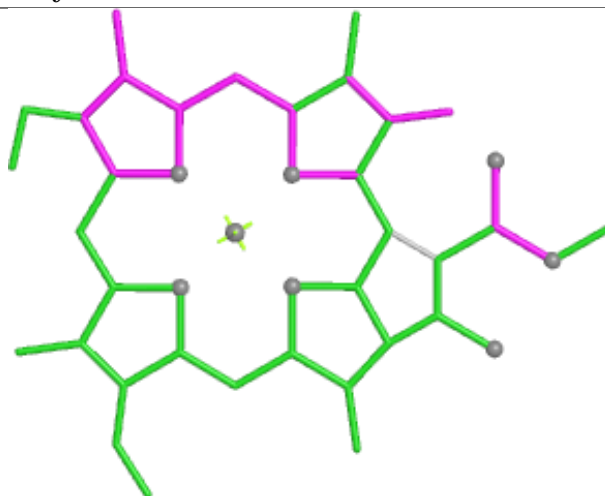




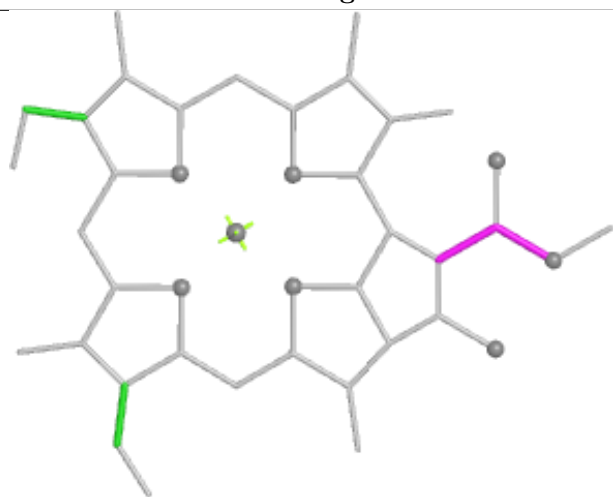
Ligand CLA y 319



Bond lengths



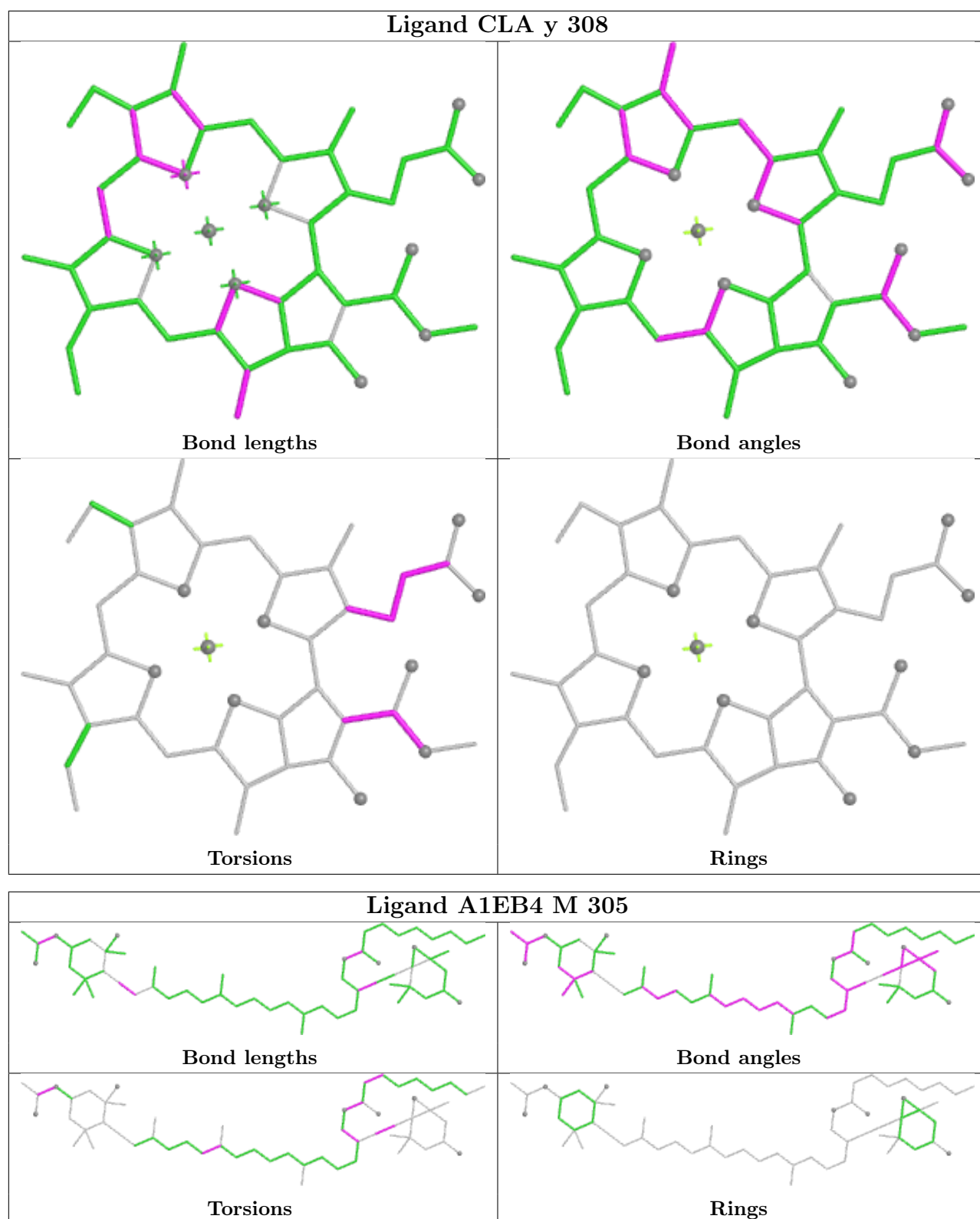
Bond angles



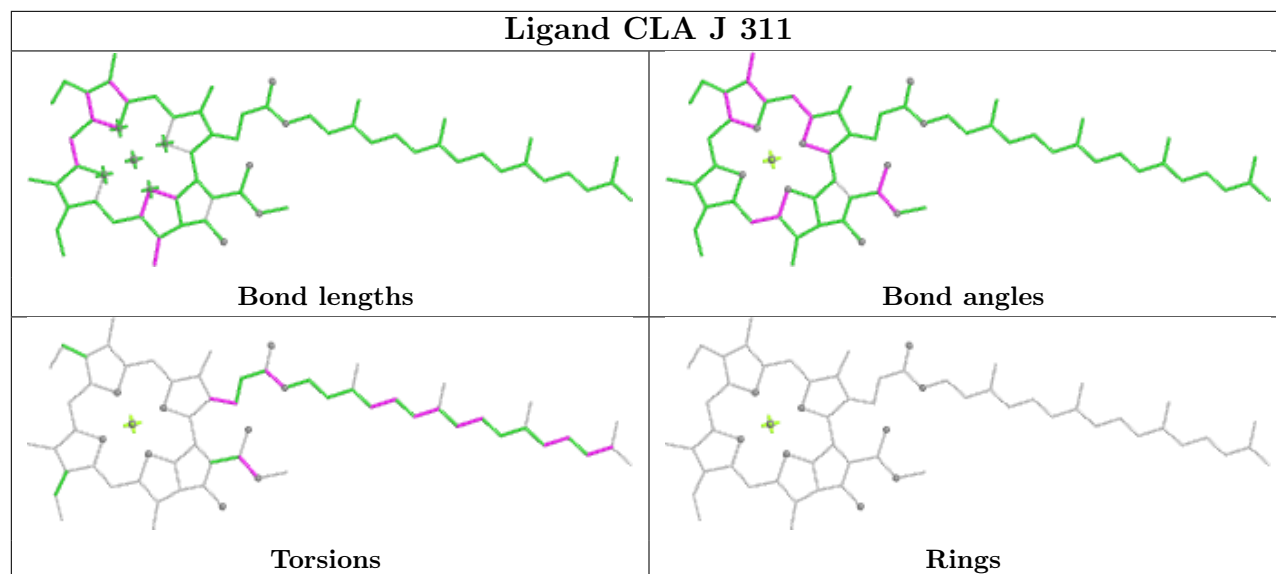
Torsions



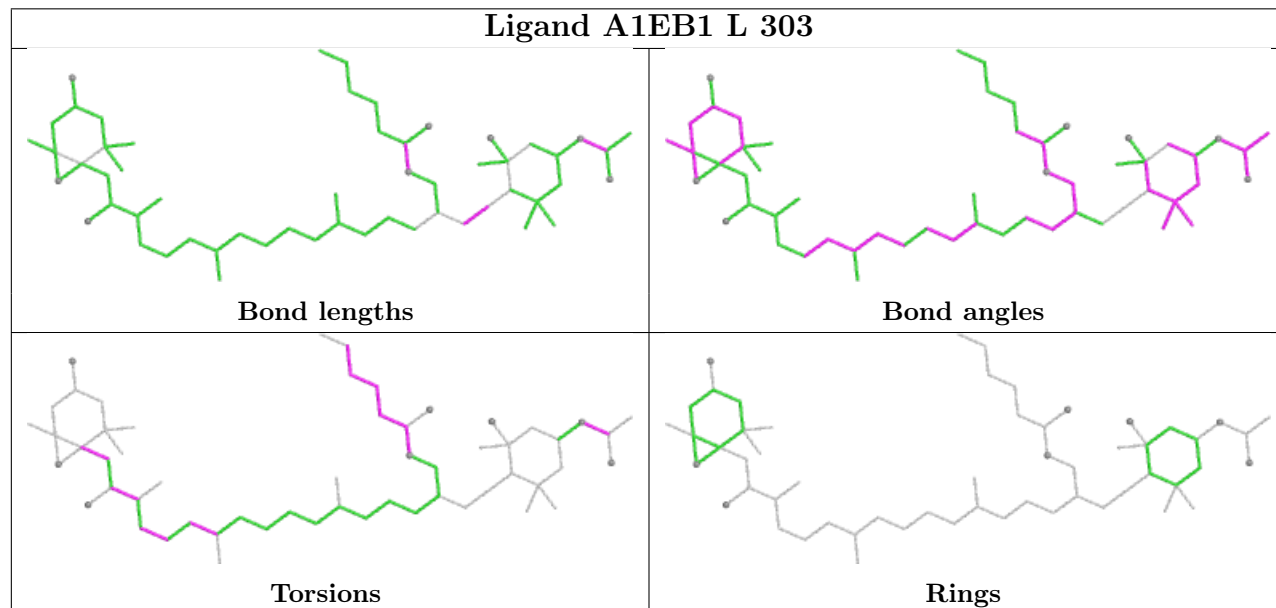
Rings



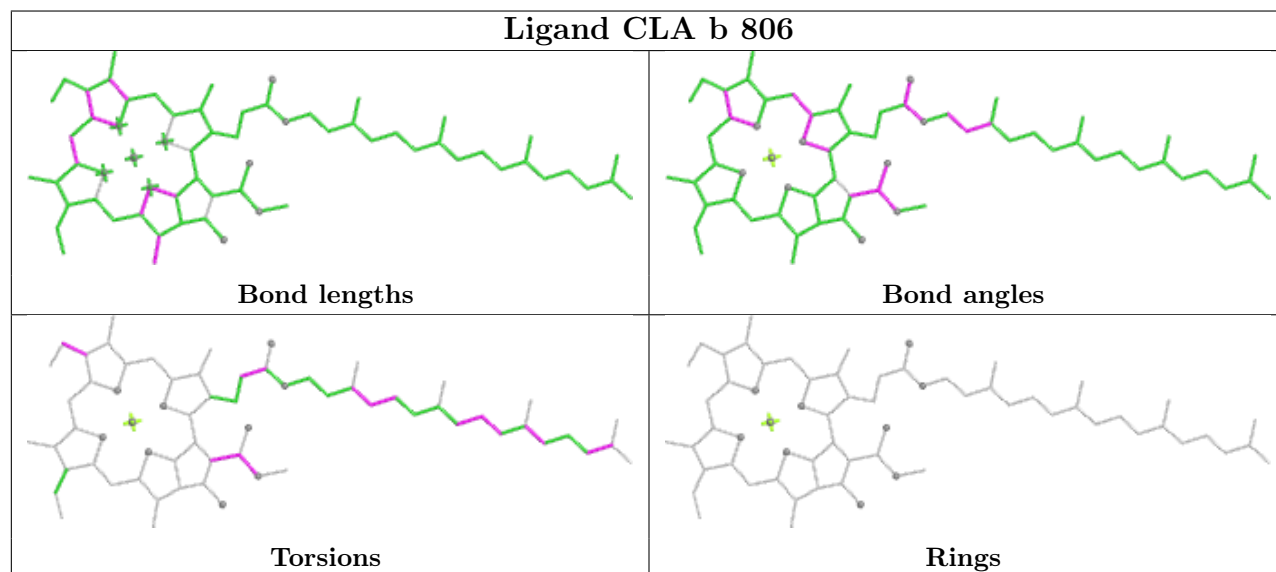
Ligand CLA J 311



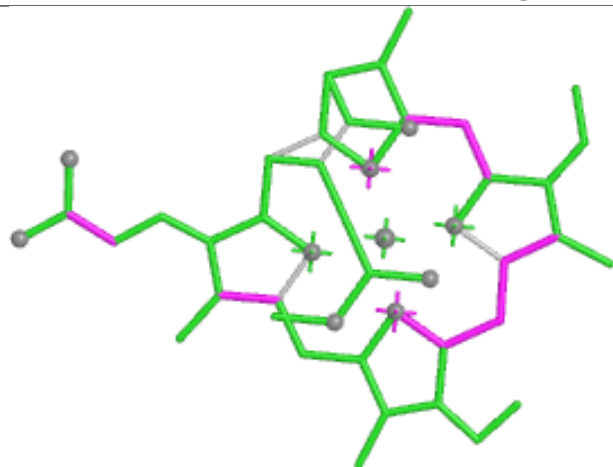
Ligand A1EB1 L 303



Ligand CLA b 806



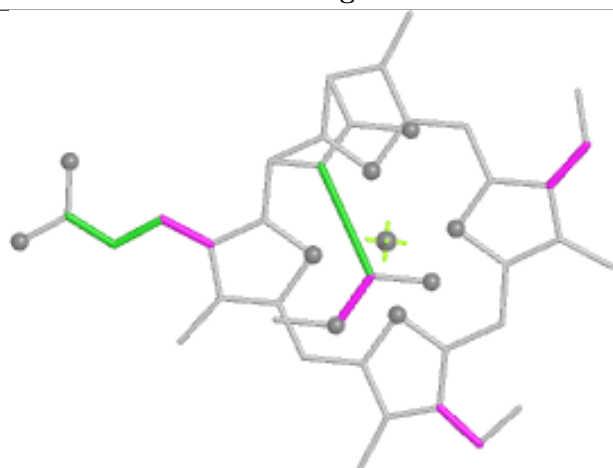
Ligand KC2 K 310



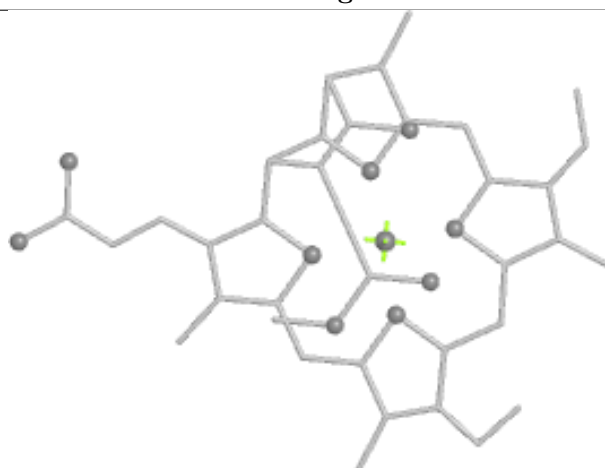
Bond lengths



Bond angles

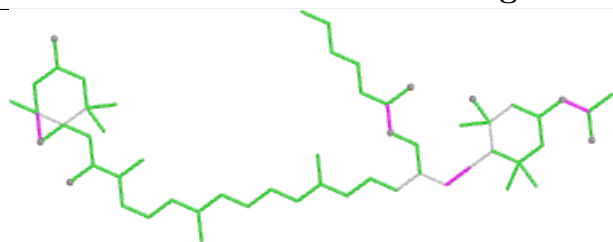


Torsions

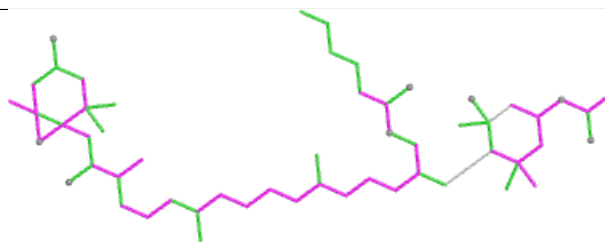


Rings

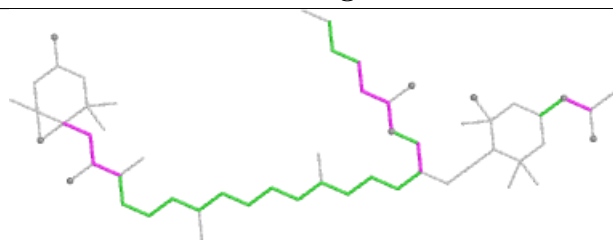
Ligand A1EB1 7 304



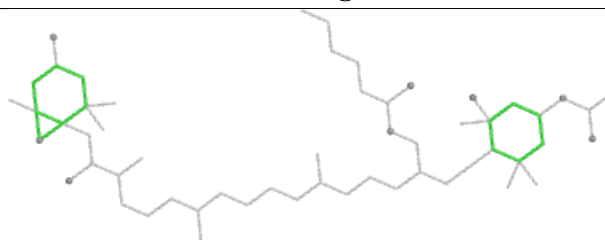
Bond lengths



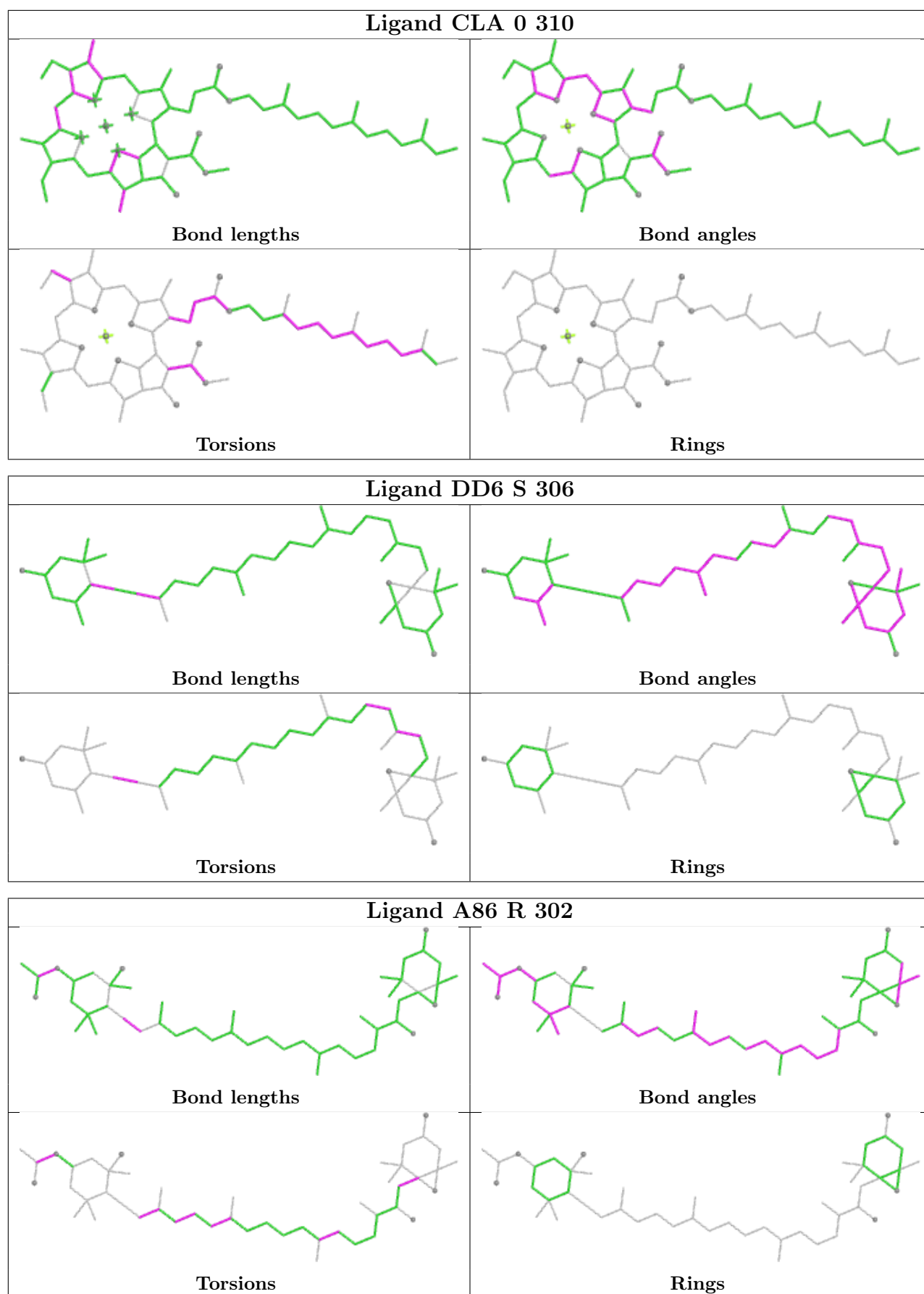
Bond angles



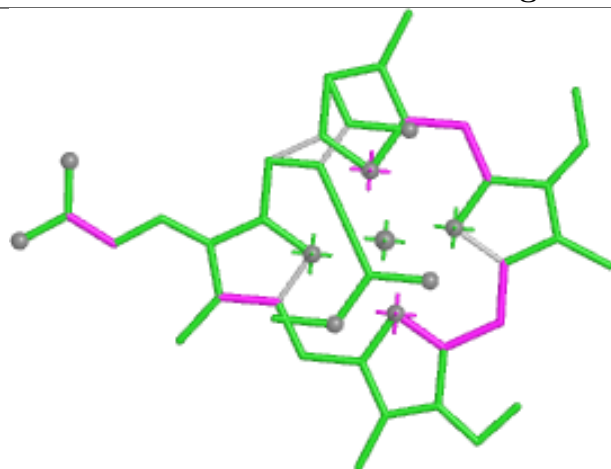
Torsions



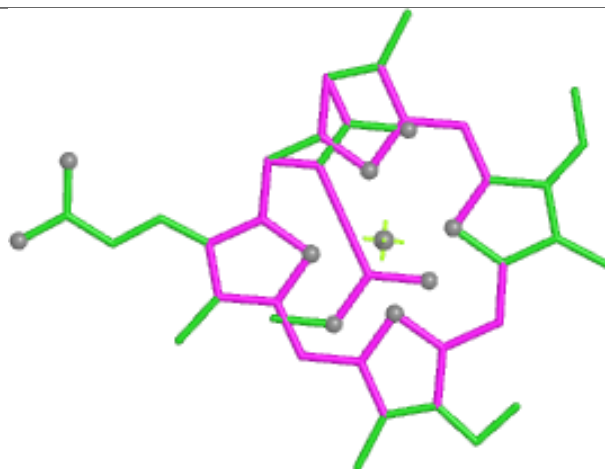
Rings



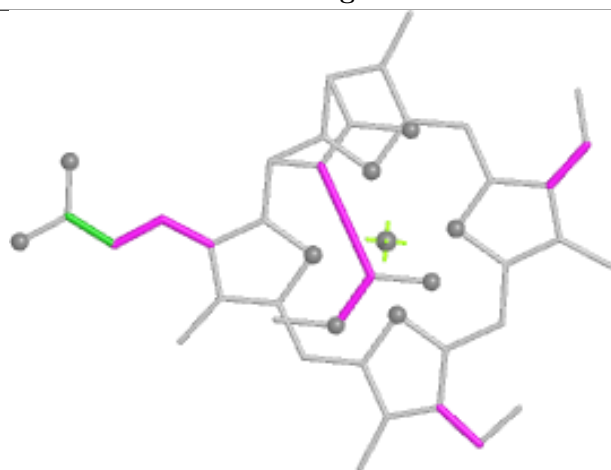
Ligand KC2 J 315



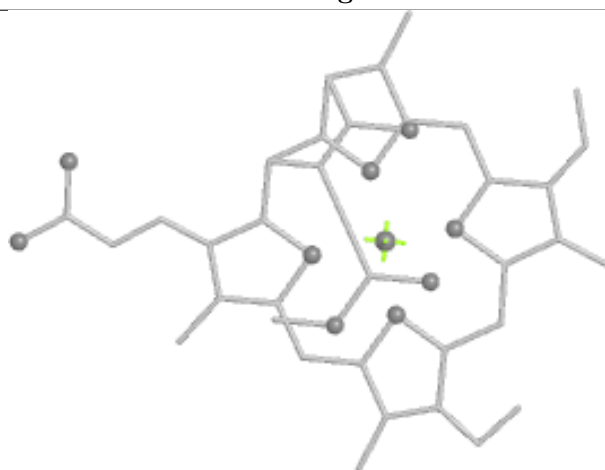
Bond lengths



Bond angles

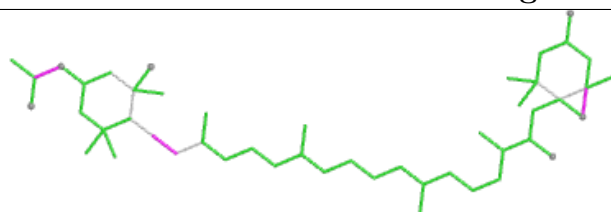


Torsions

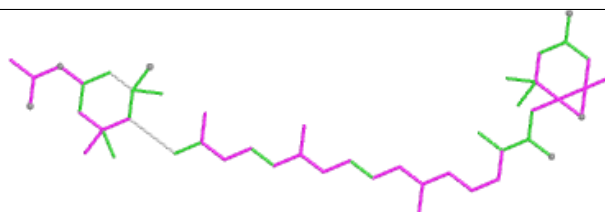


Rings

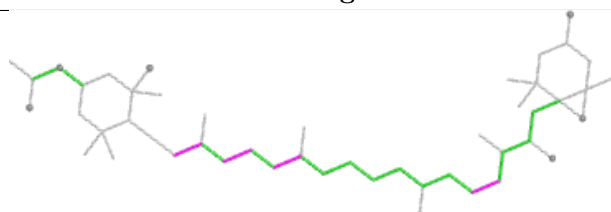
Ligand A86 O 306



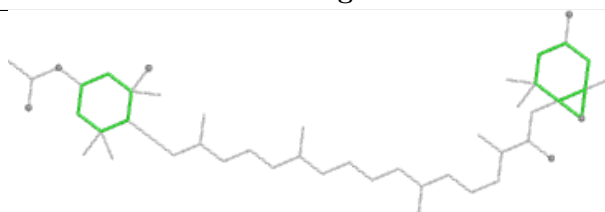
Bond lengths



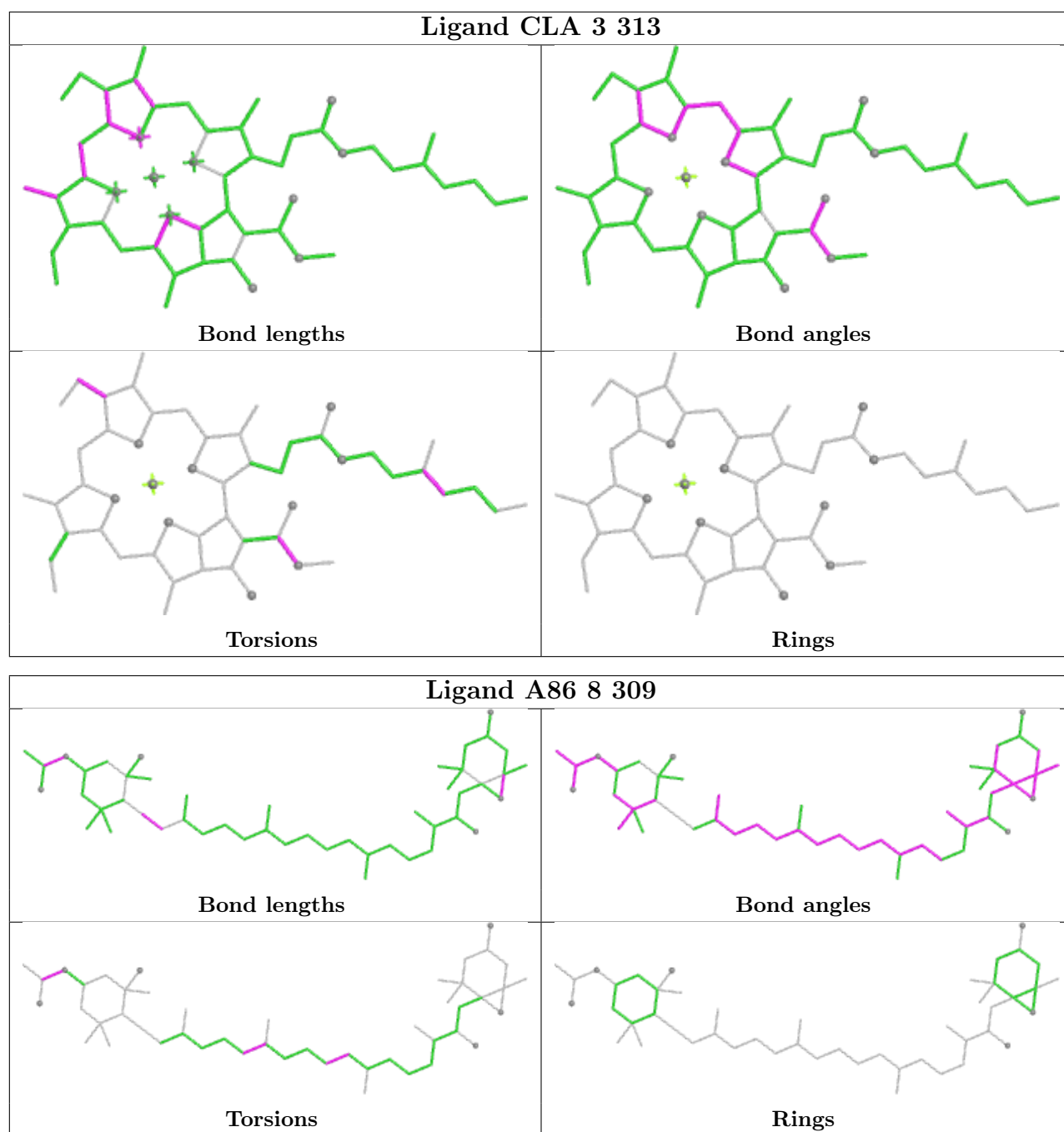
Bond angles

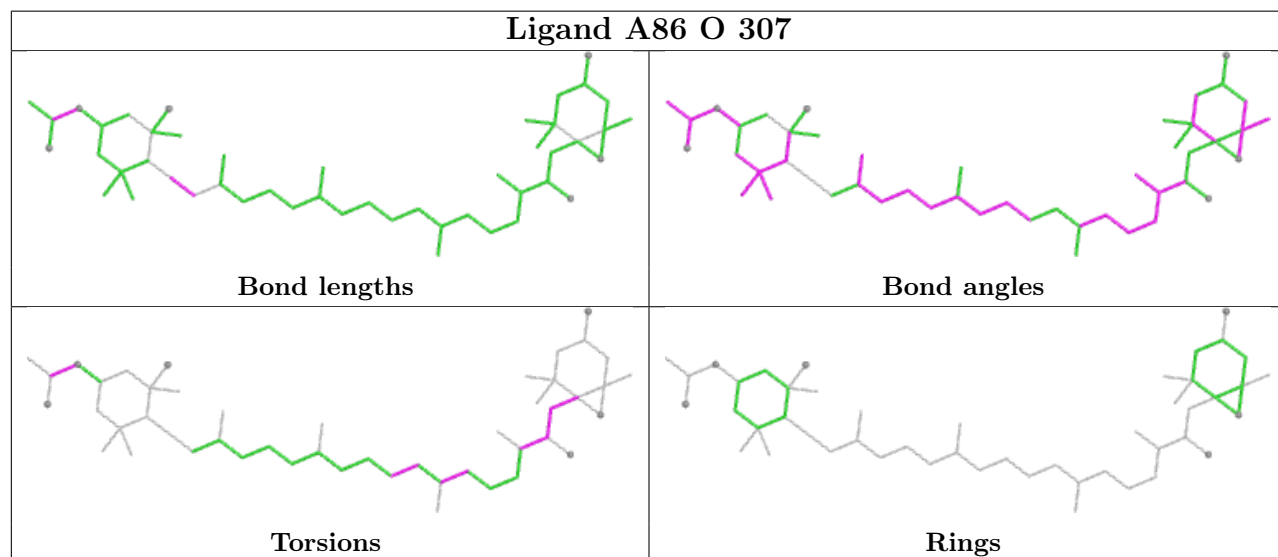
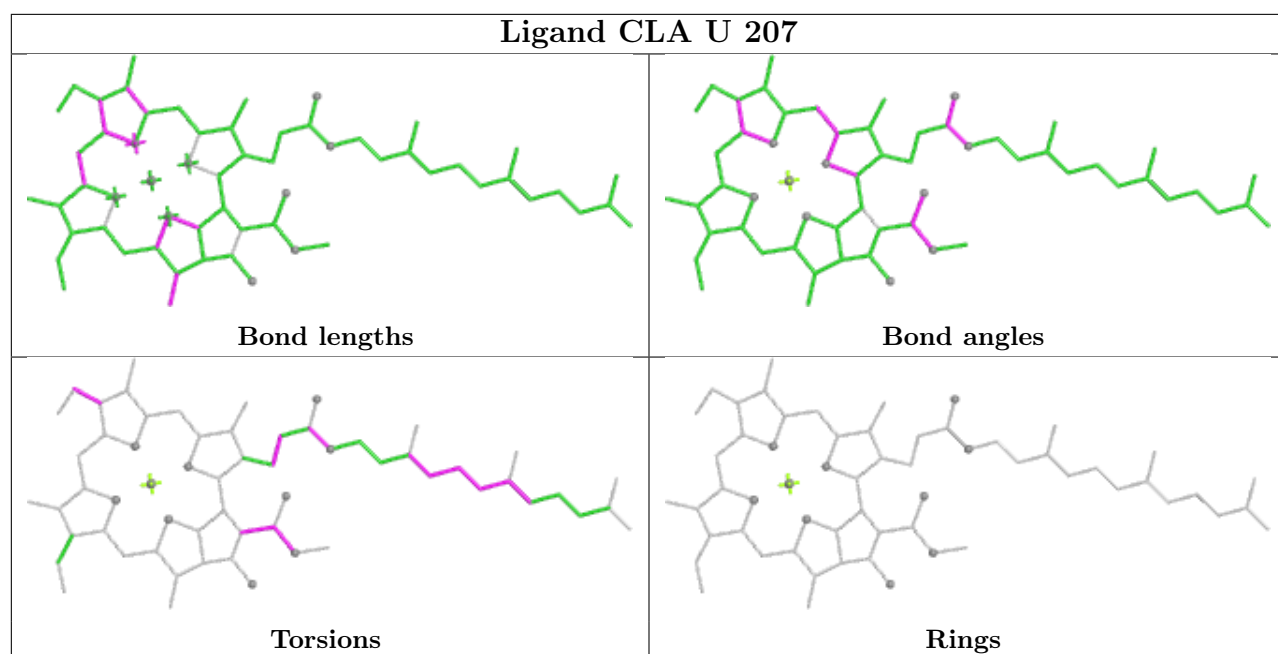


Torsions

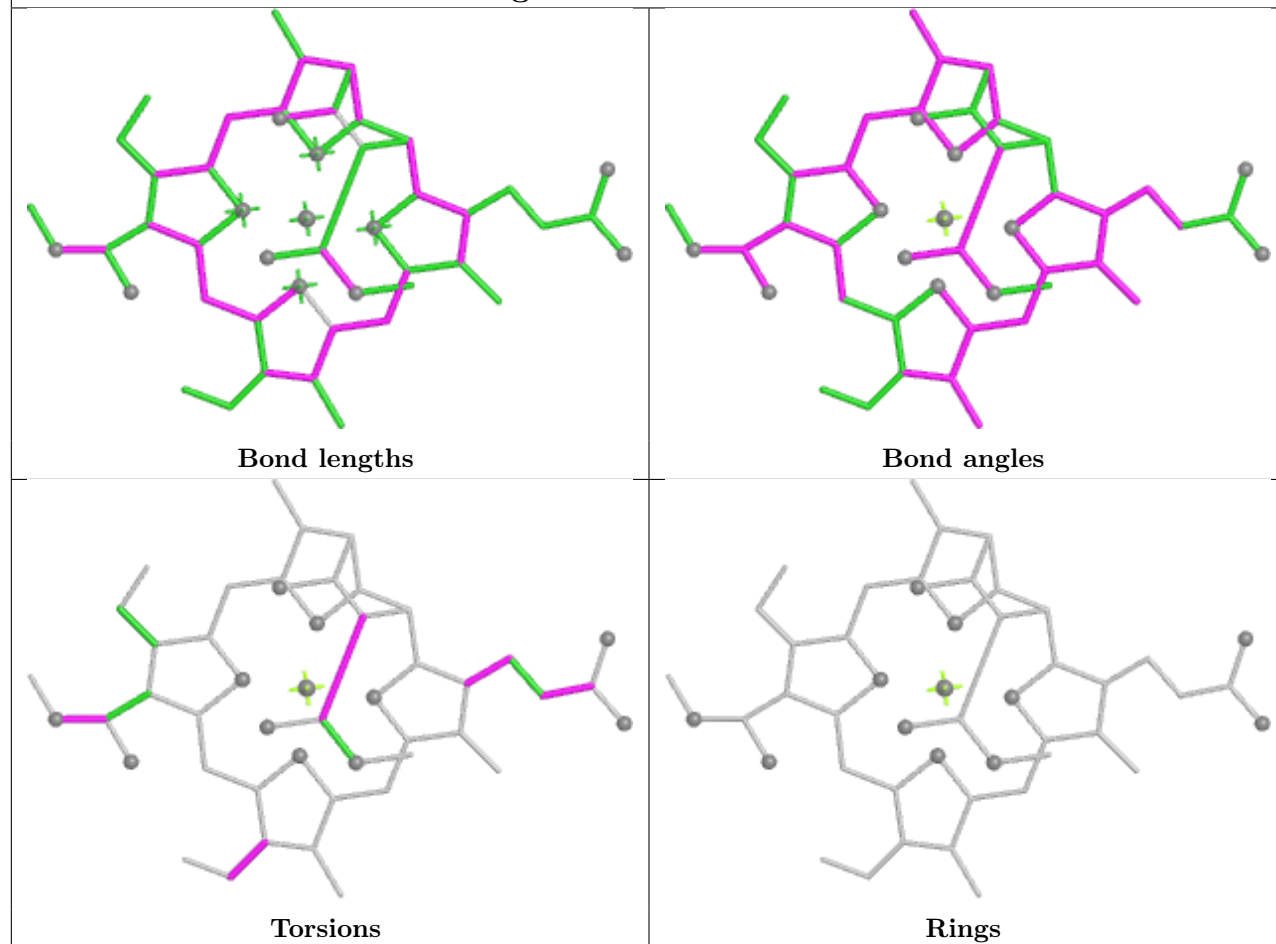


Rings

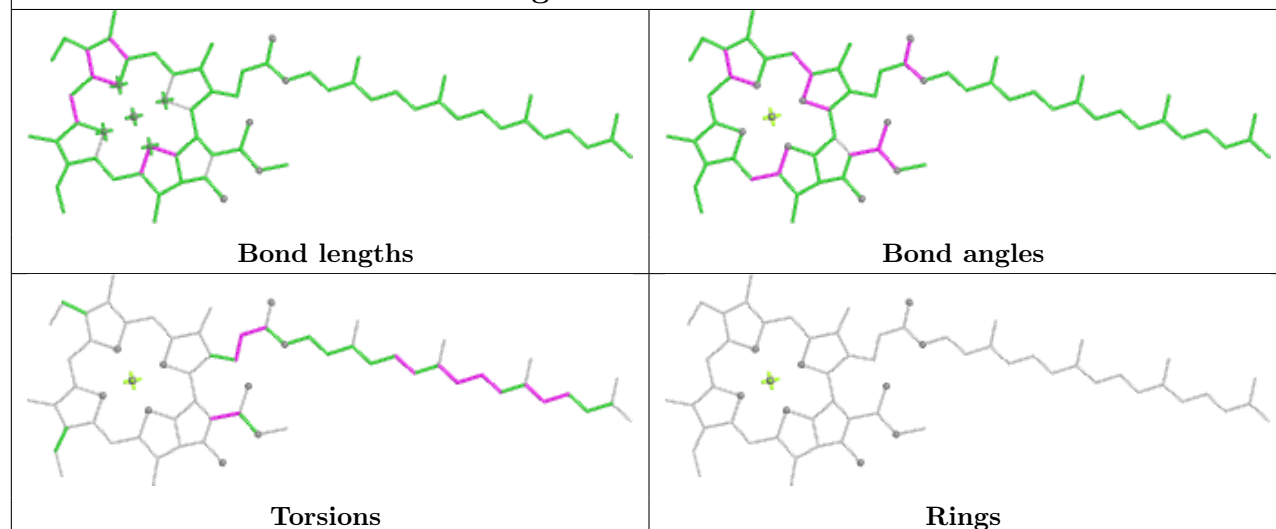




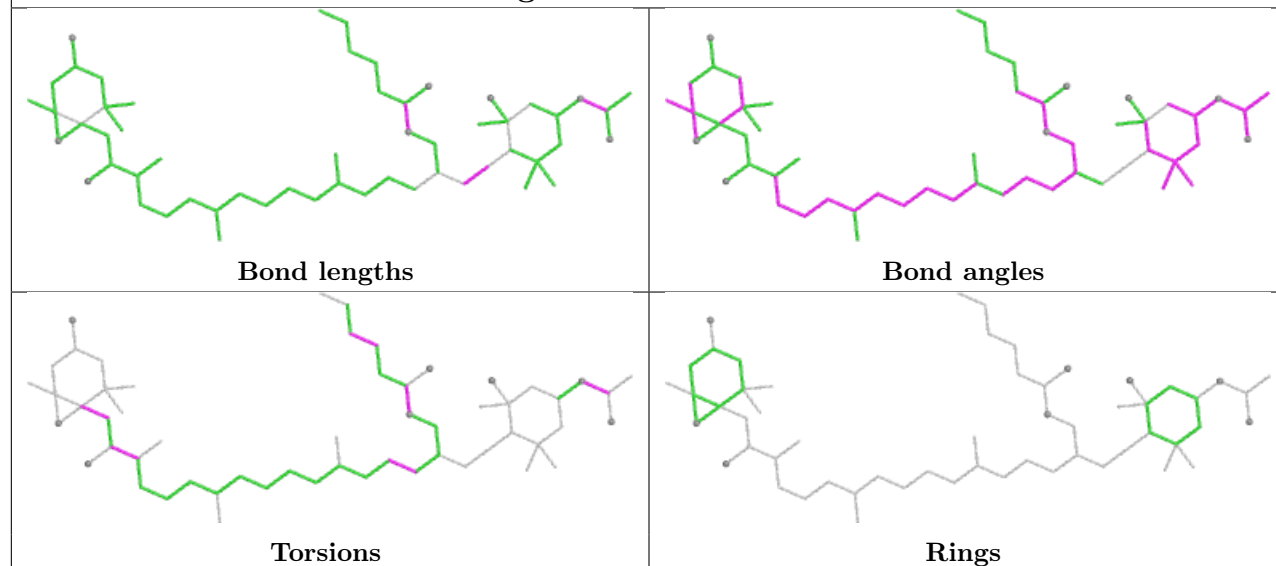
Ligand A1ECV S 312



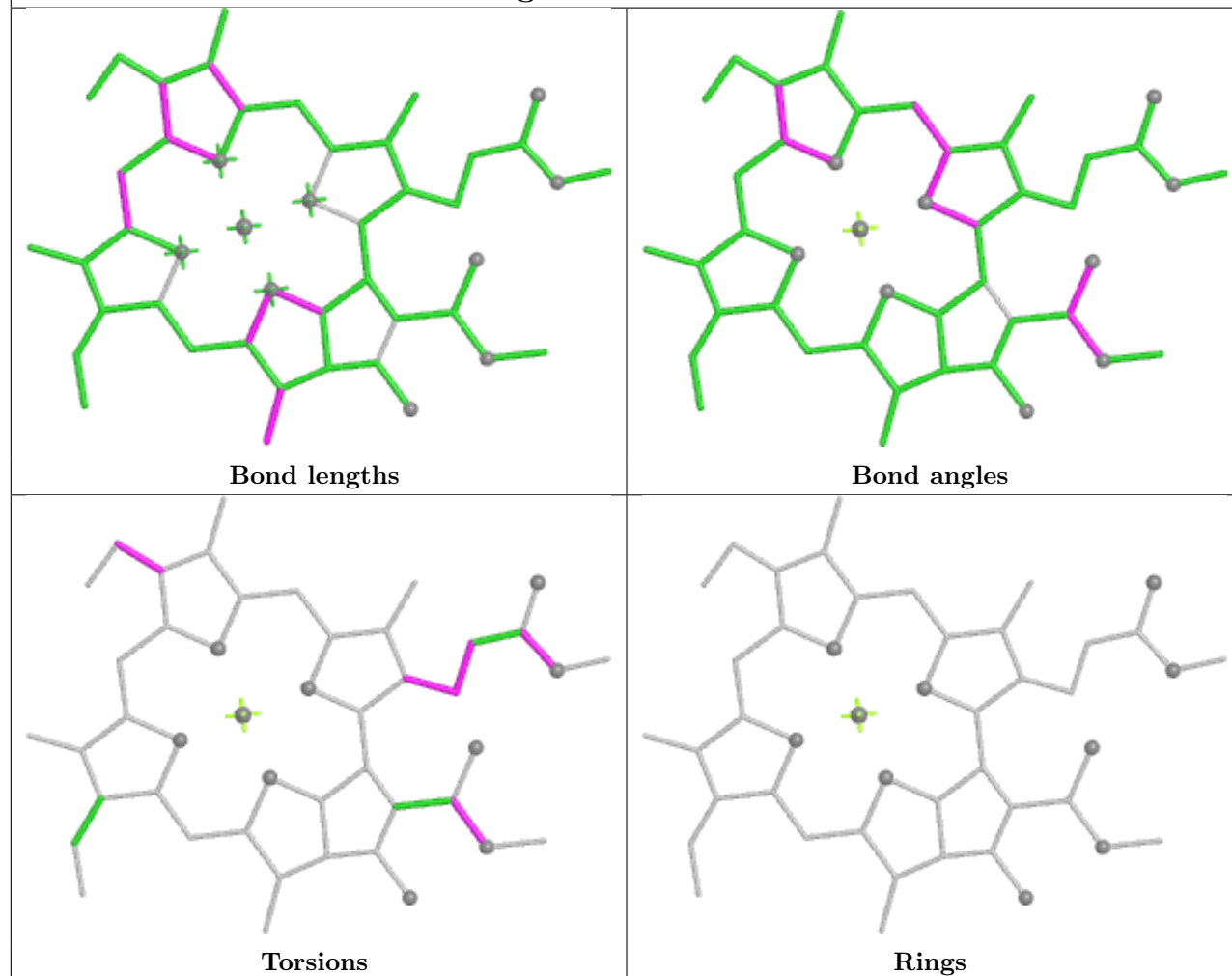
Ligand CLA R 309

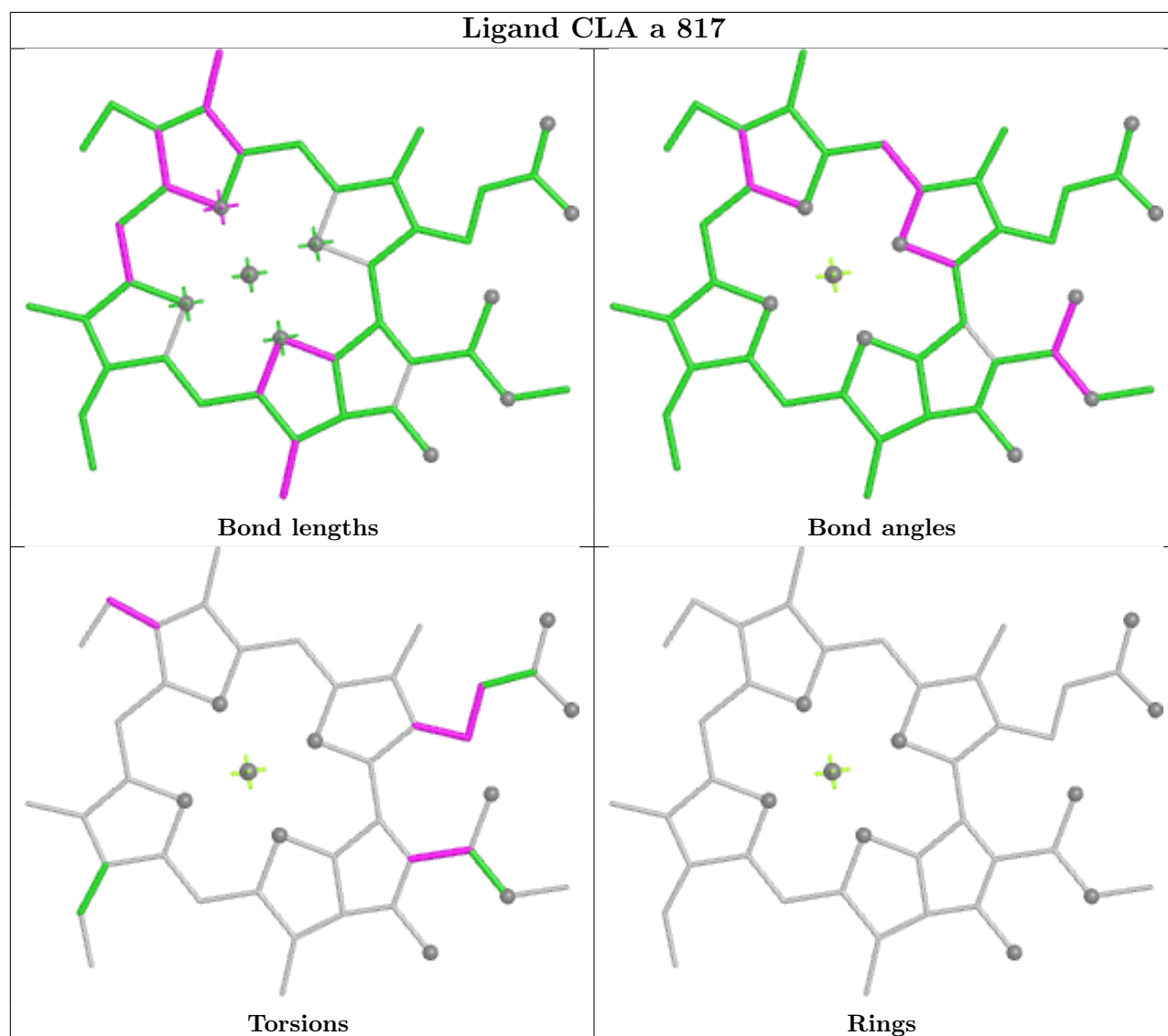
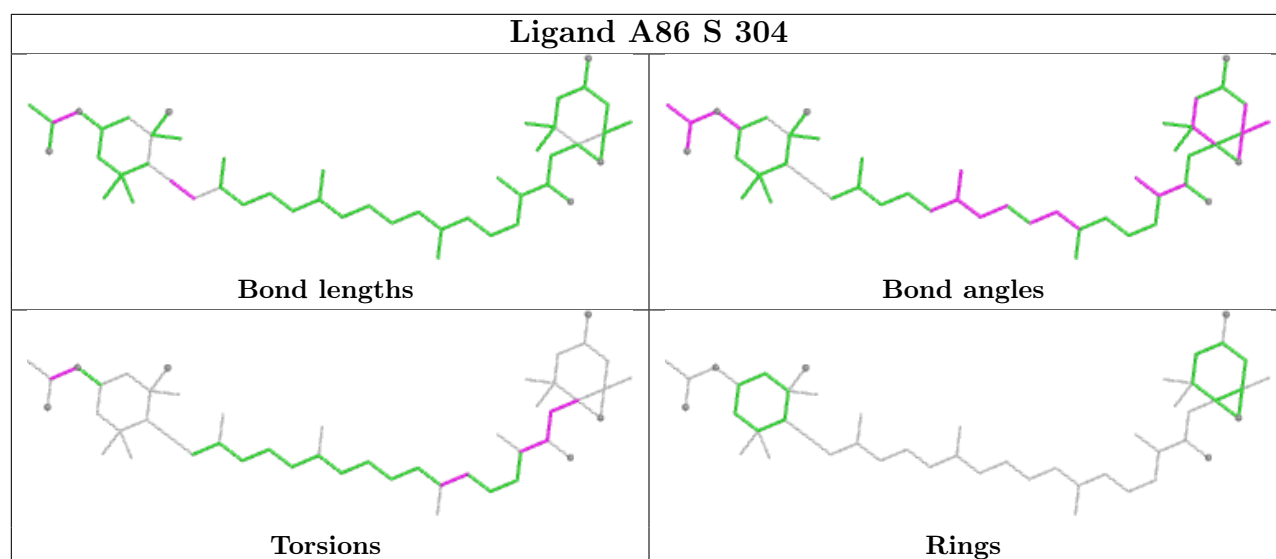


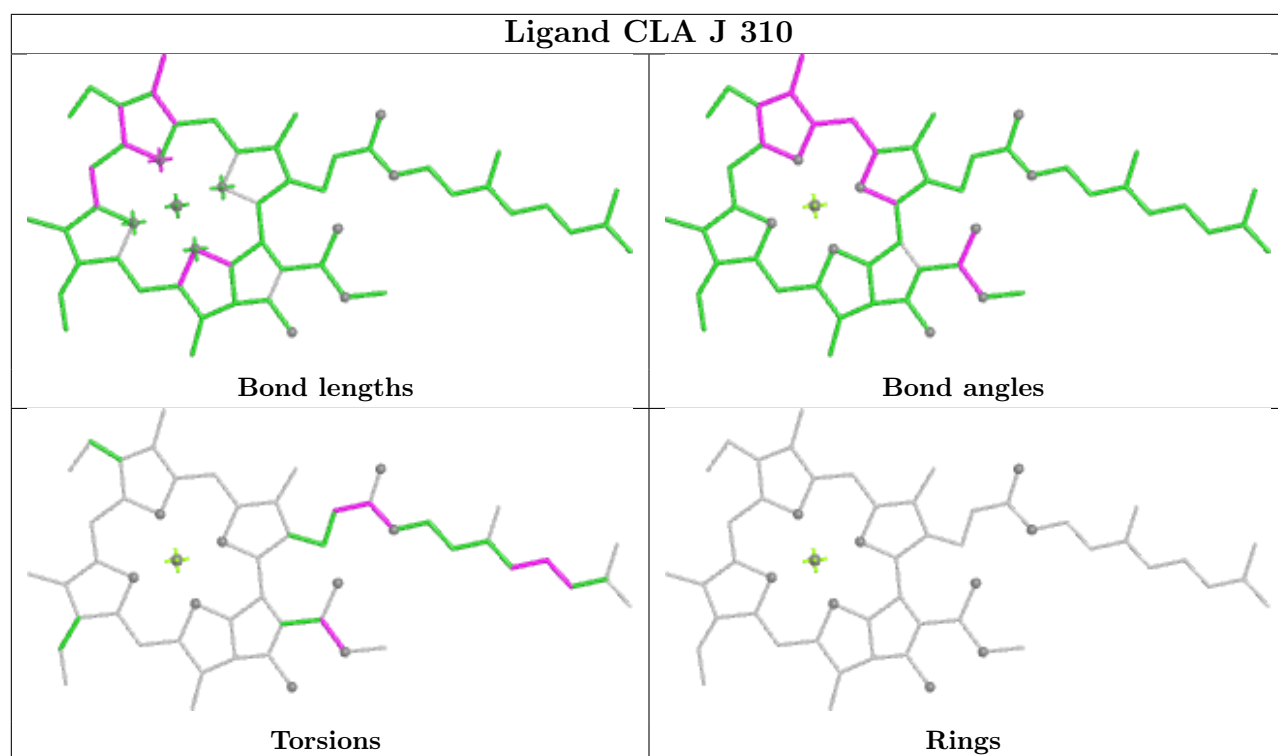
Ligand A1EB1 7 306



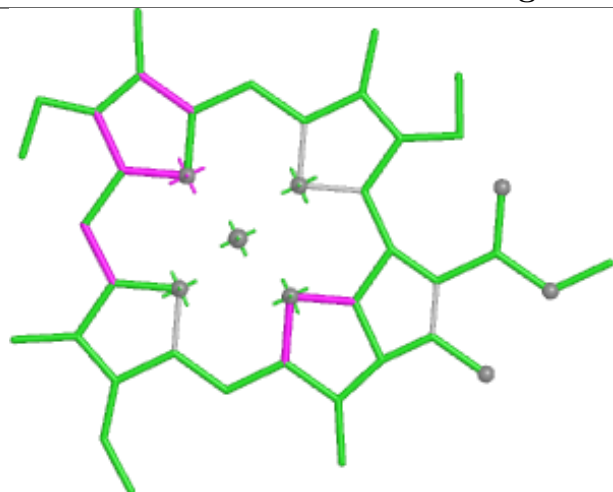
Ligand CLA J 313



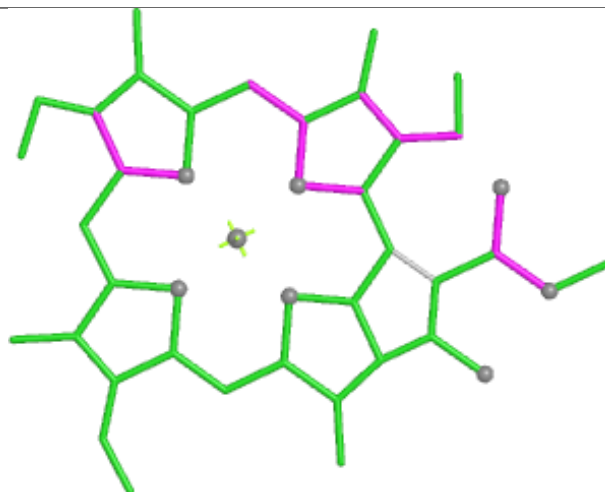




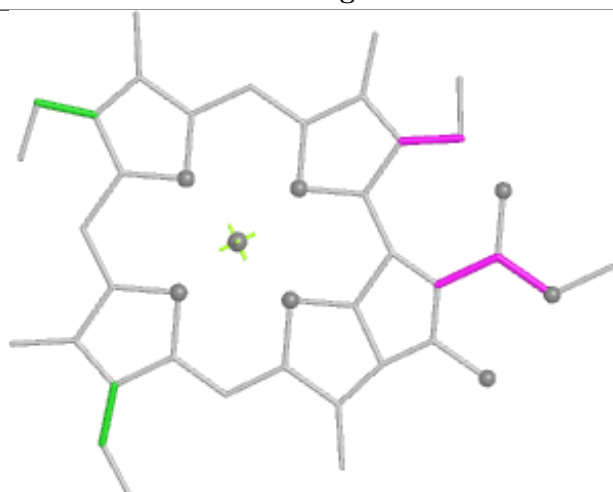
Ligand CLA 2 310



Bond lengths



Bond angles

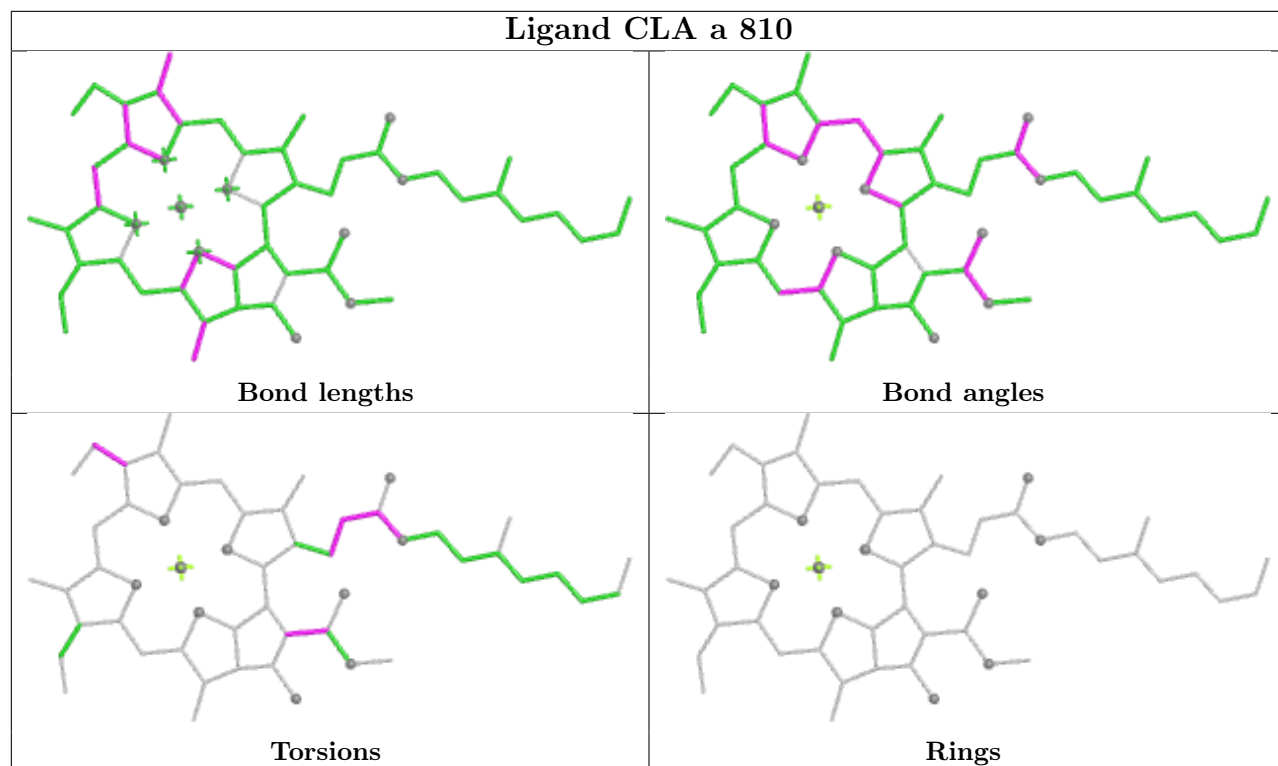


Torsions

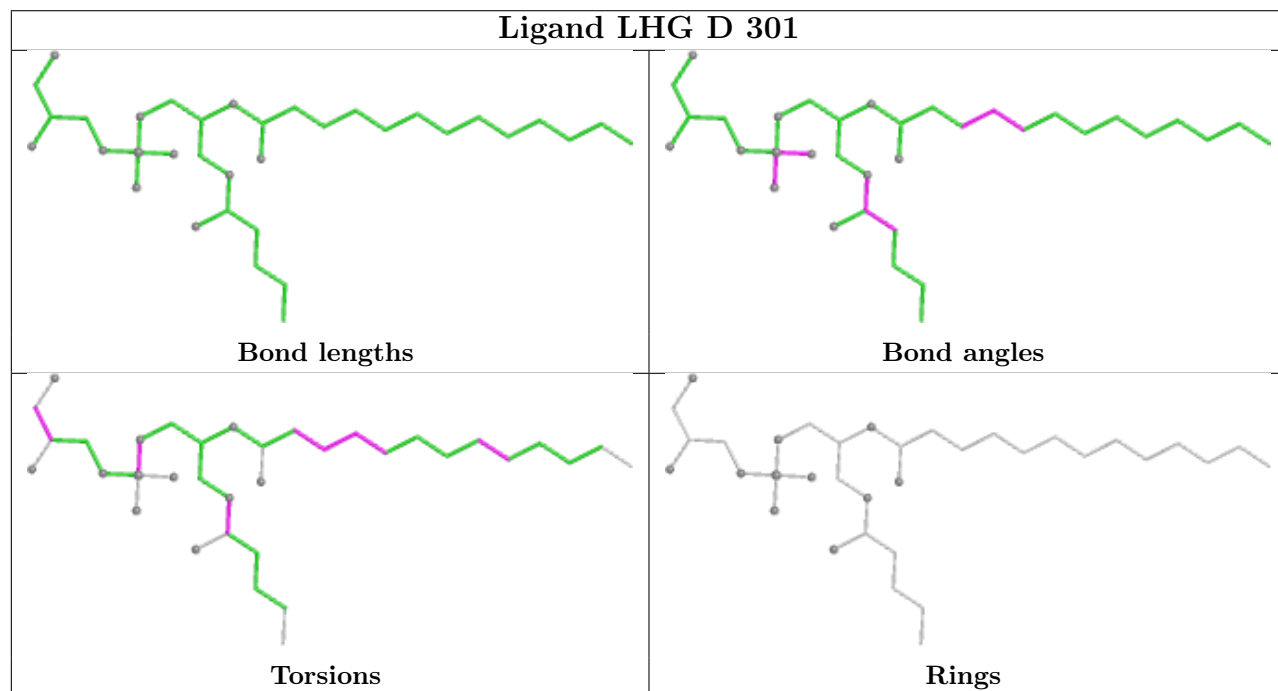


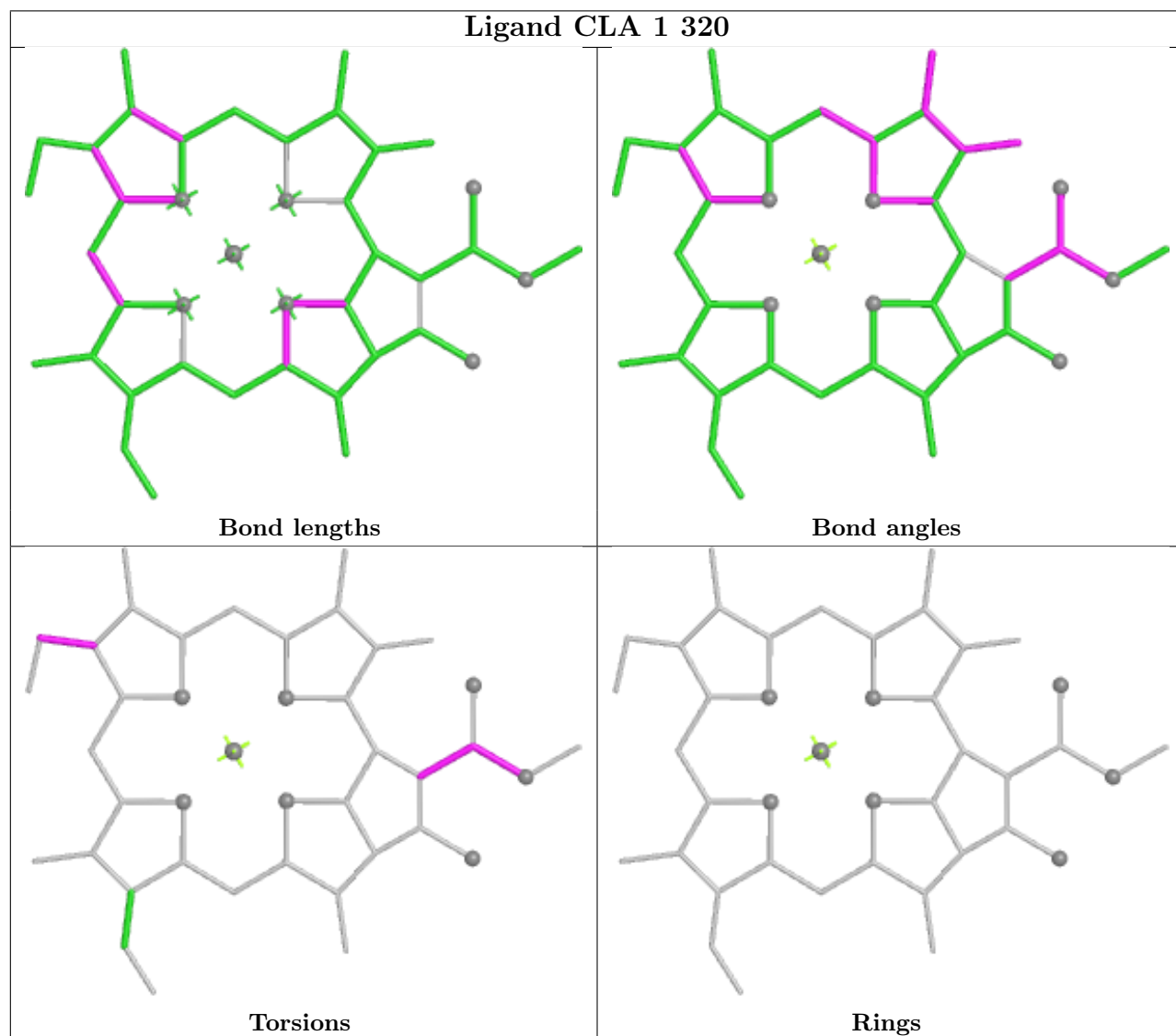
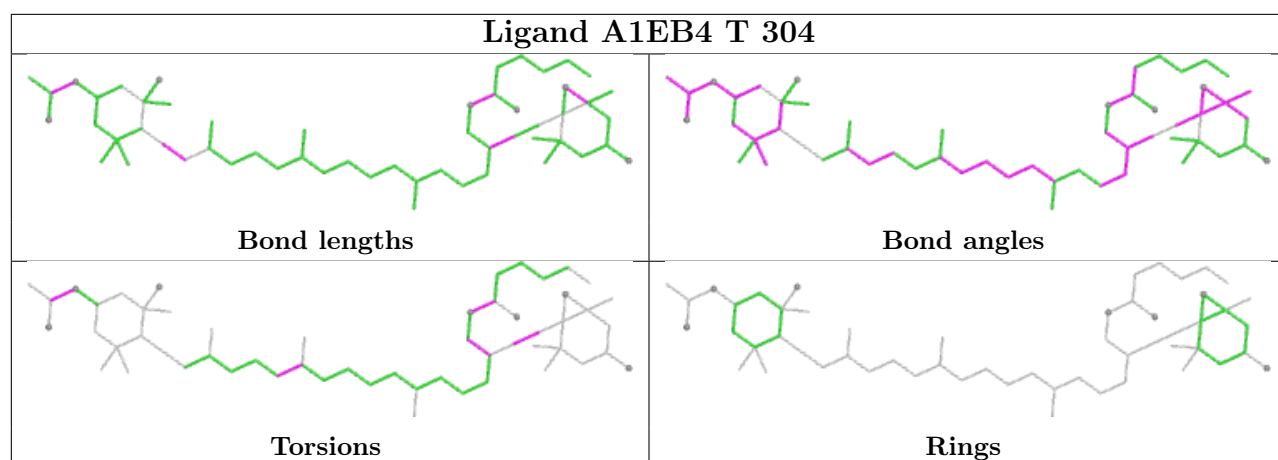
Rings

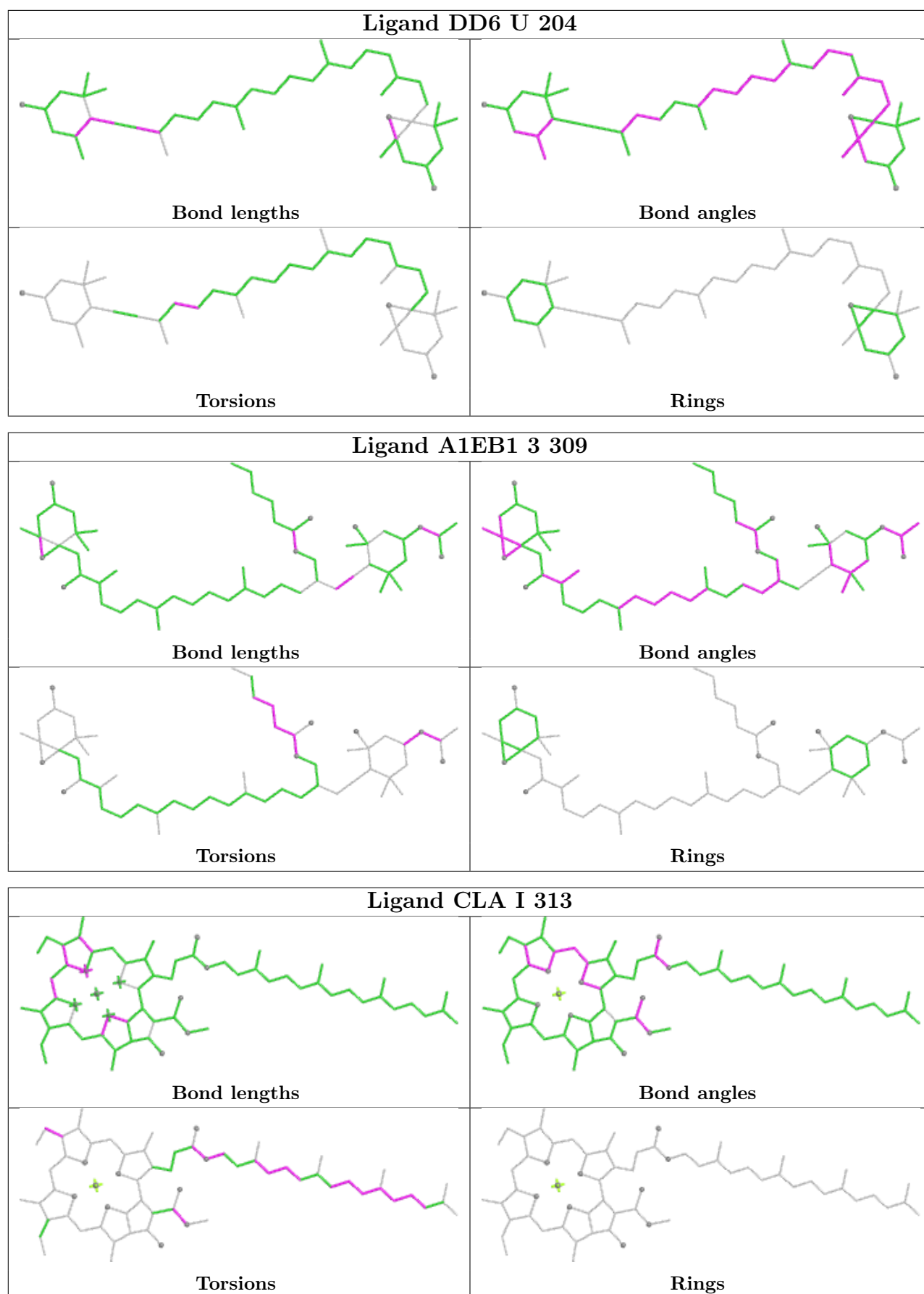
Ligand CLA a 810

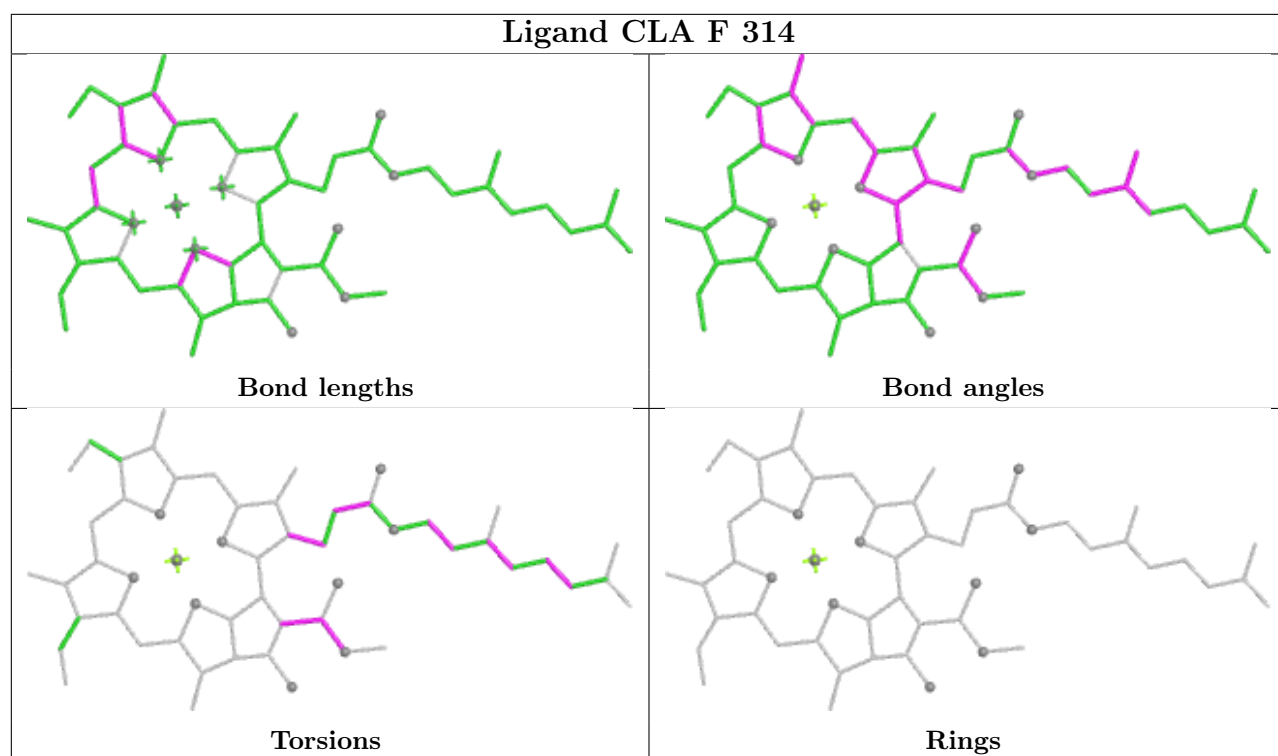


Ligand LHG D 301

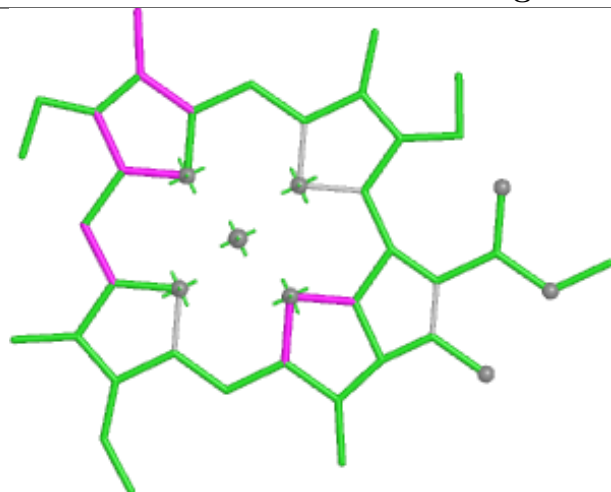




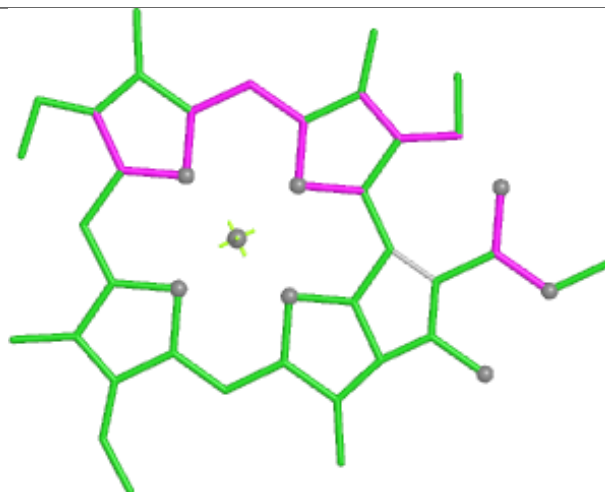




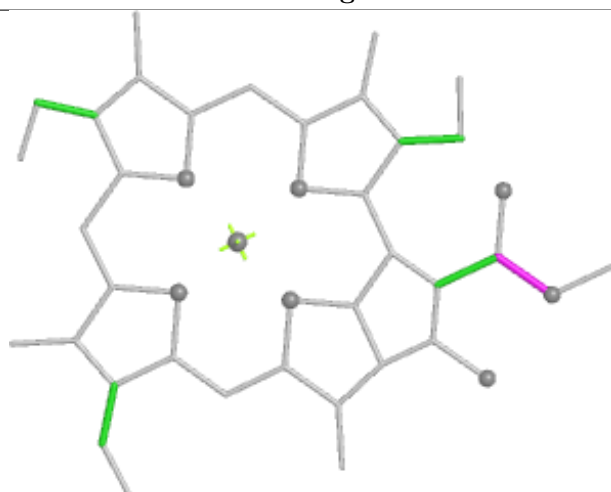
Ligand CLA O 311



Bond lengths



Bond angles

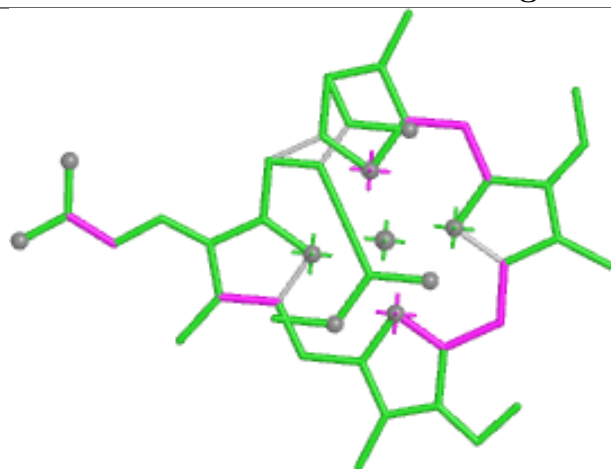


Torsions

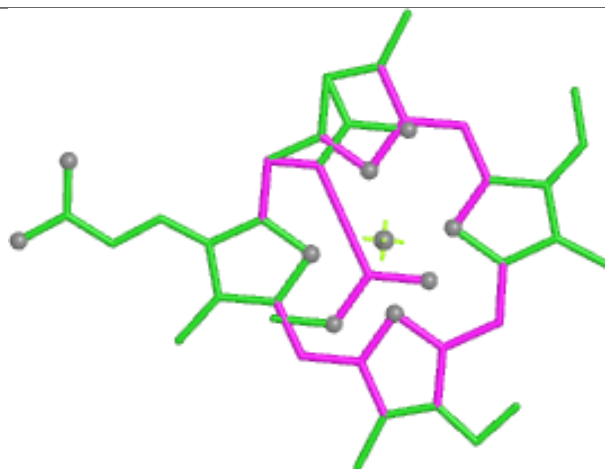


Rings

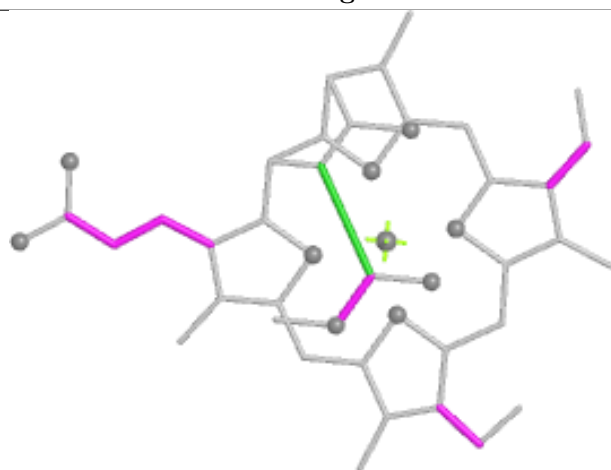
Ligand KC2 x 315



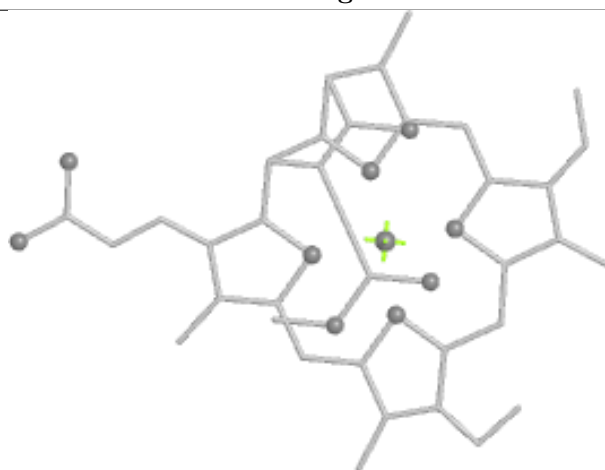
Bond lengths



Bond angles

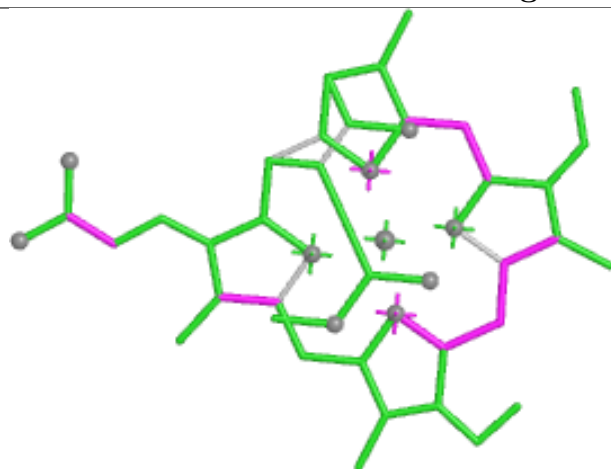


Torsions

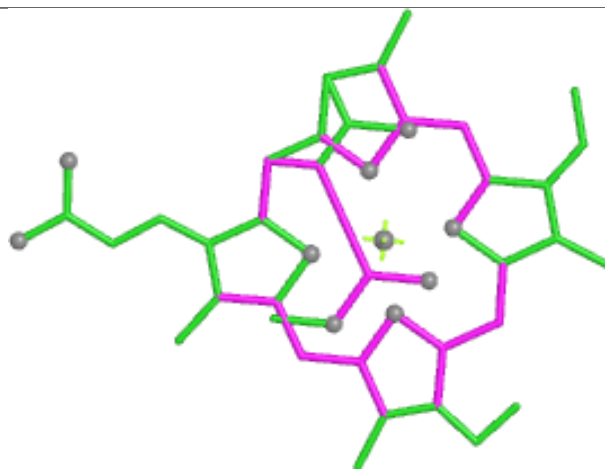


Rings

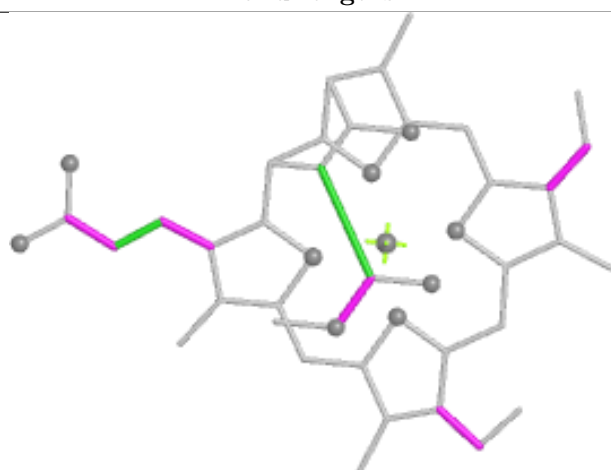
Ligand KC2 9 316



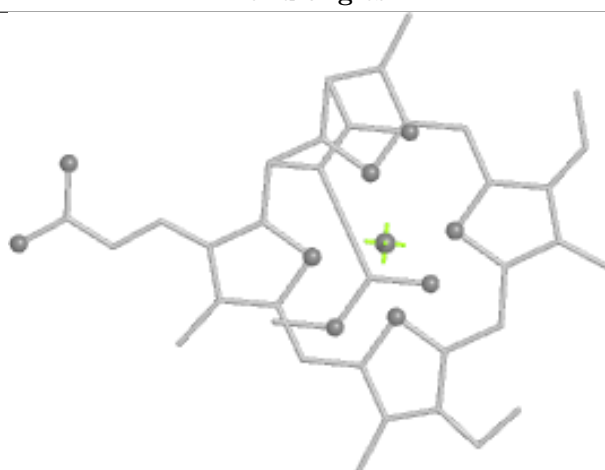
Bond lengths



Bond angles

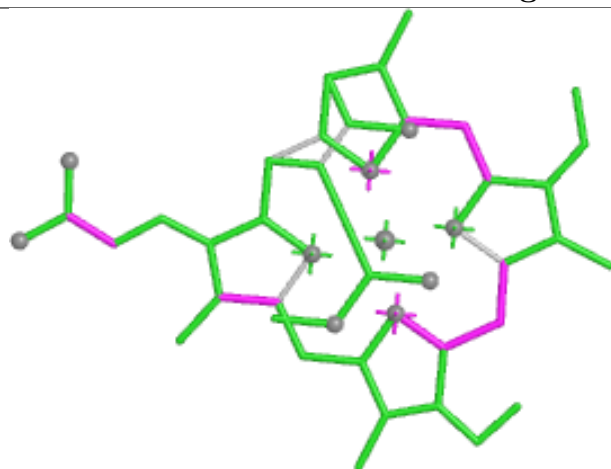


Torsions

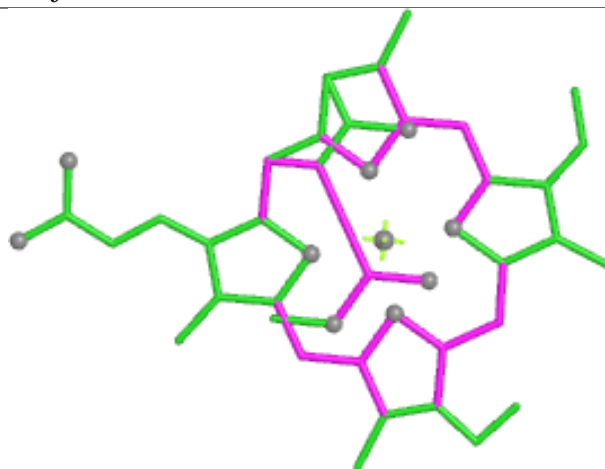


Rings

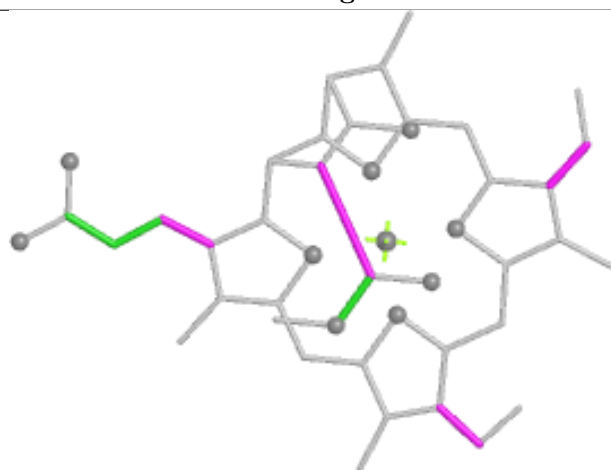
Ligand KC2 y 314



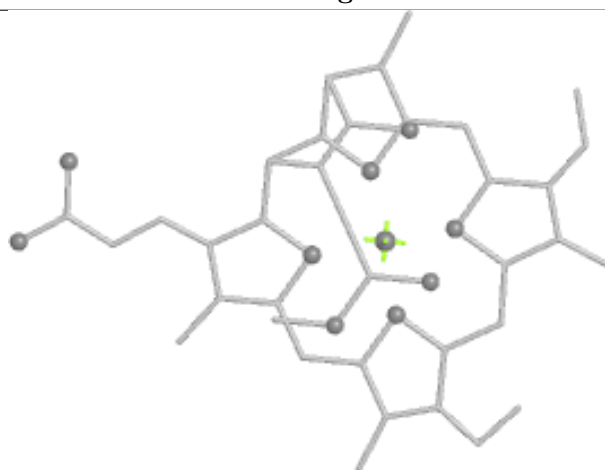
Bond lengths



Bond angles

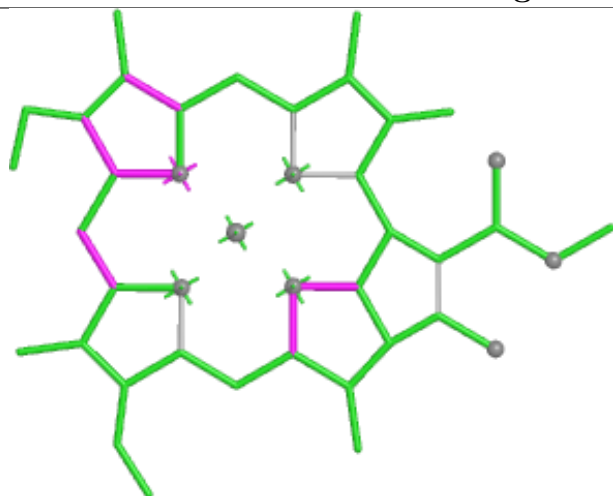


Torsions

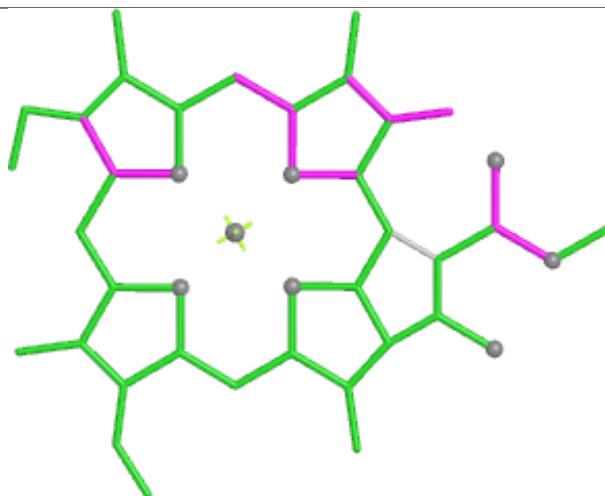


Rings

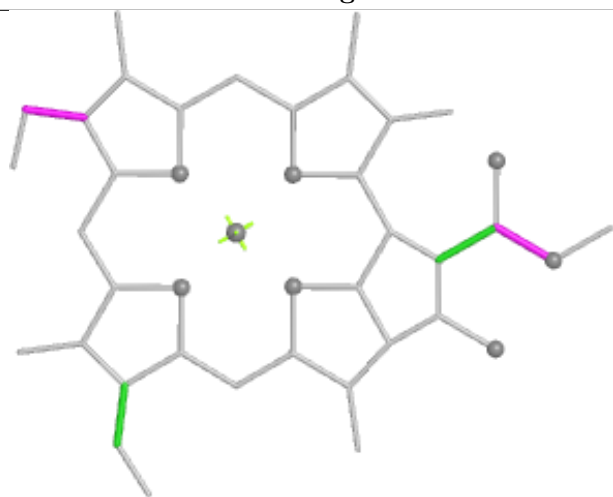
Ligand CLA Y 302



Bond lengths



Bond angles

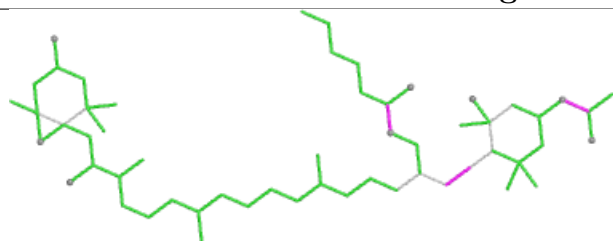


Torsions

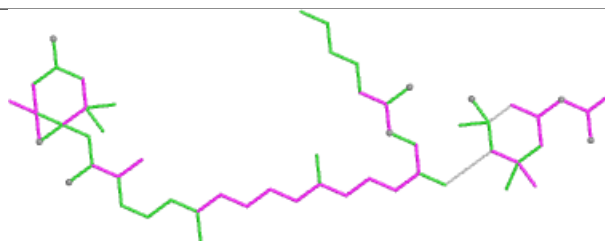


Rings

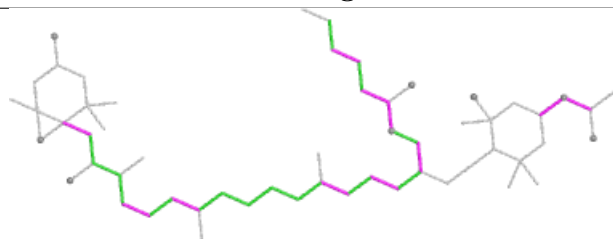
Ligand A1EB1 0 305



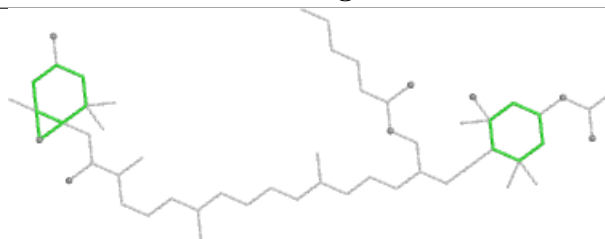
Bond lengths



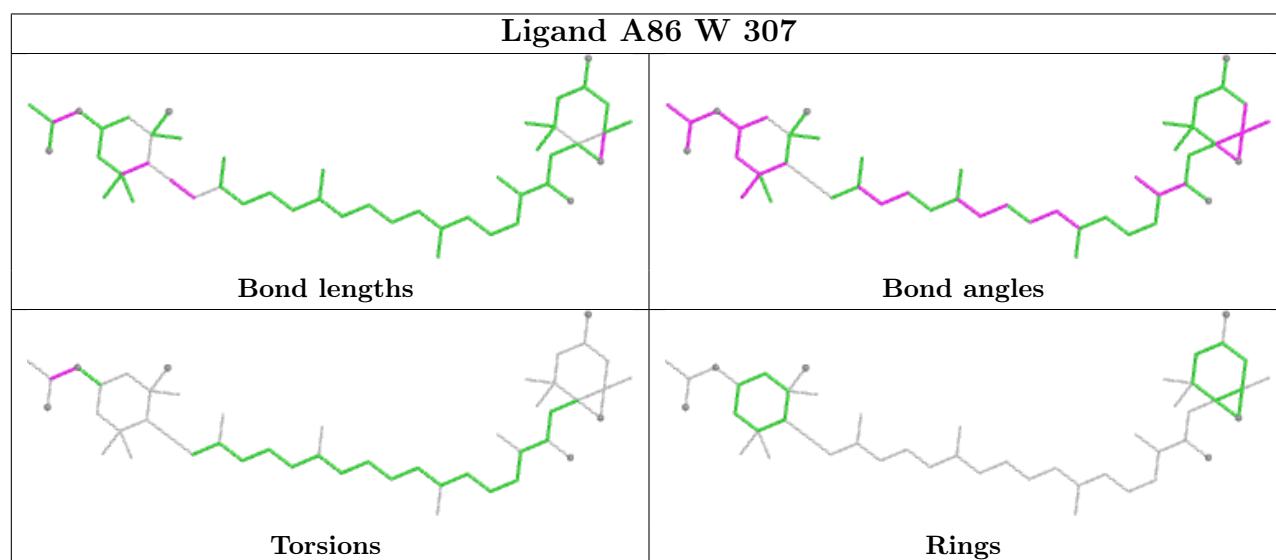
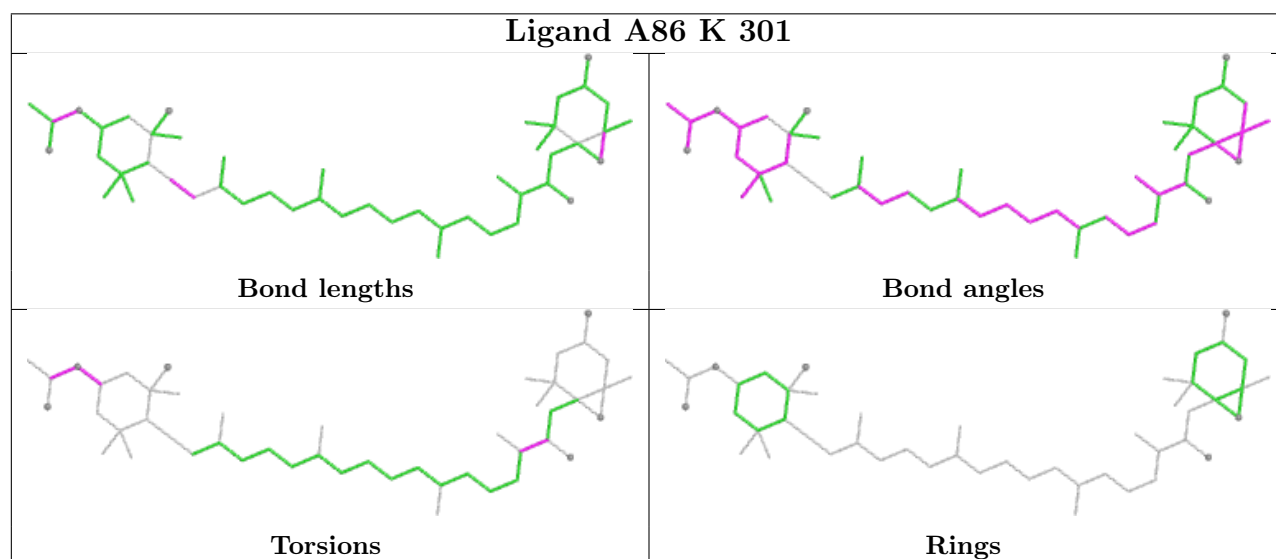
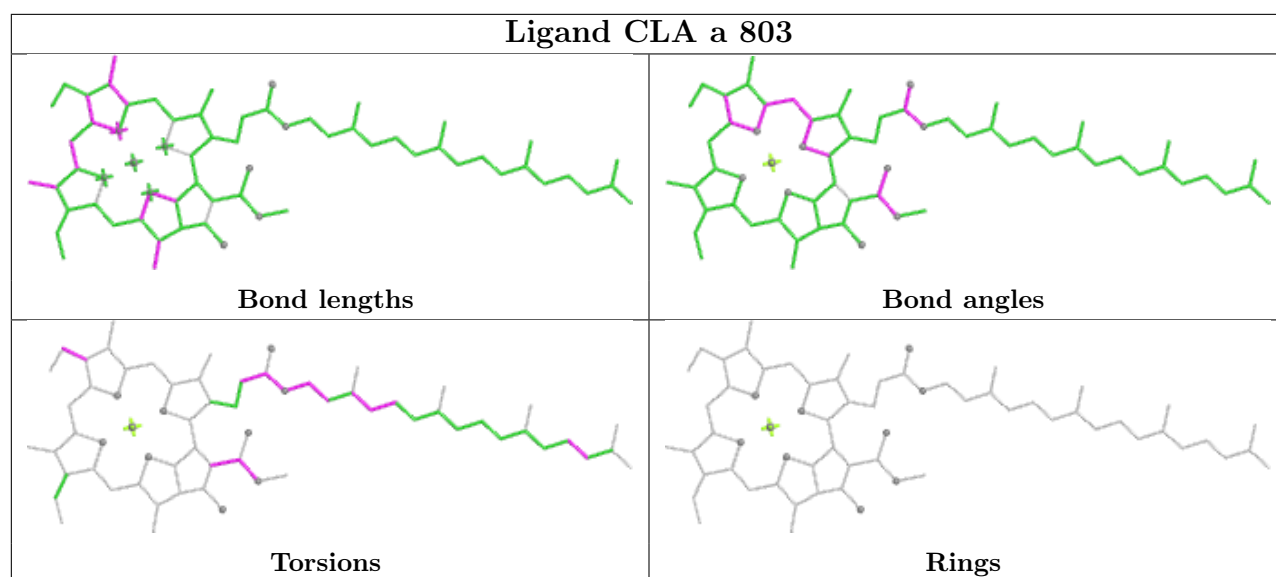
Bond angles

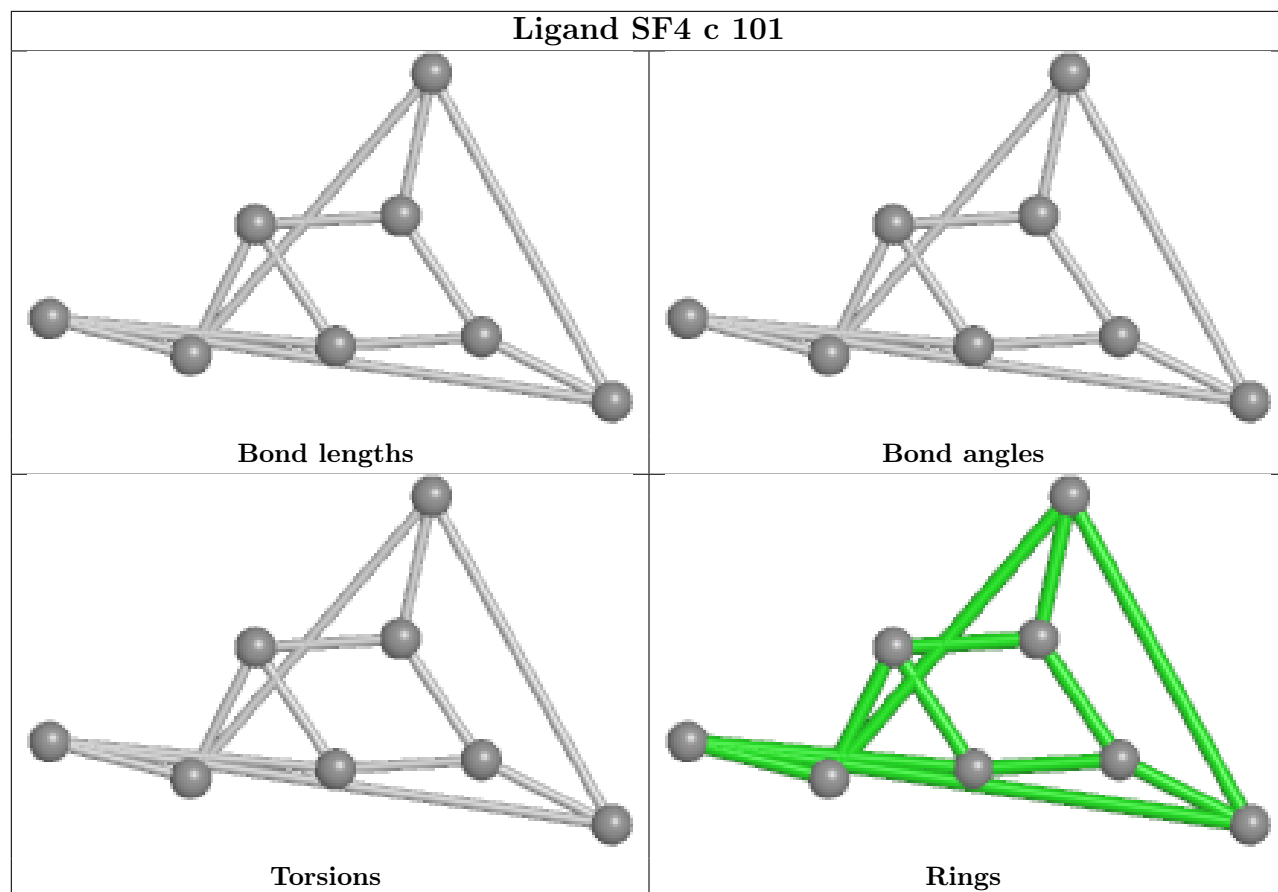


Torsions

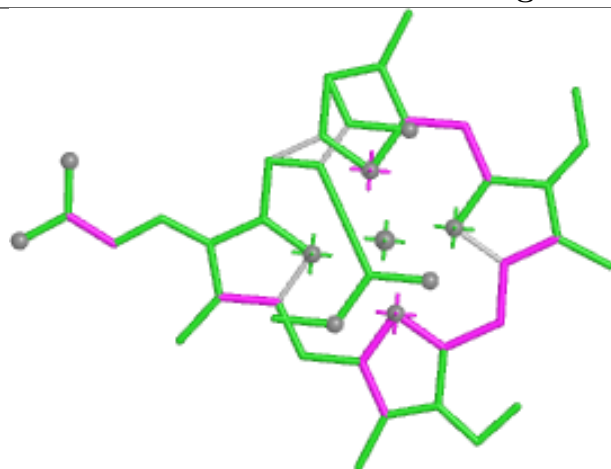


Rings

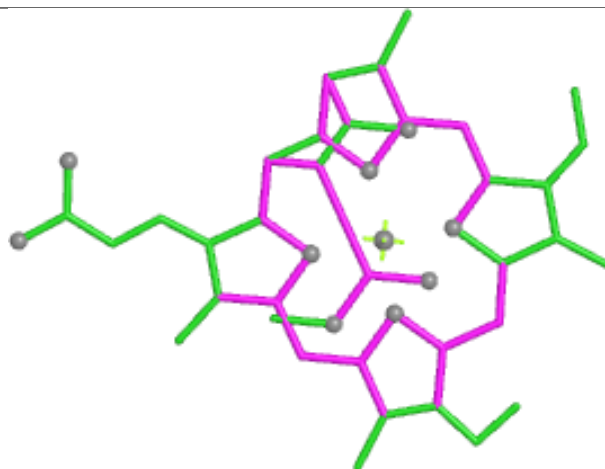




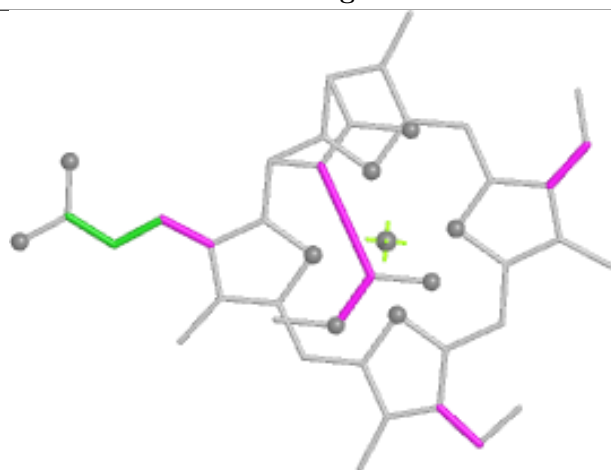
Ligand KC2 P 306



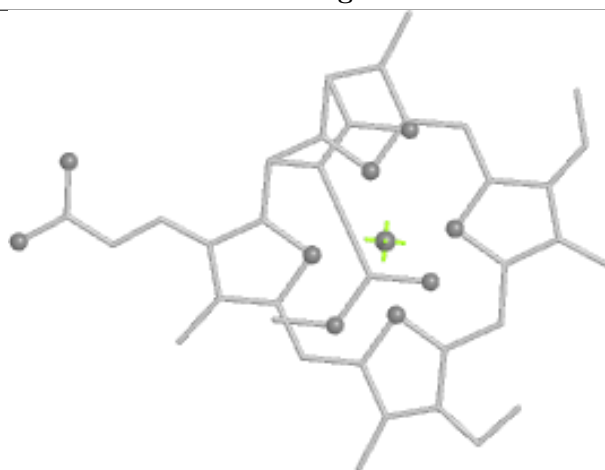
Bond lengths



Bond angles

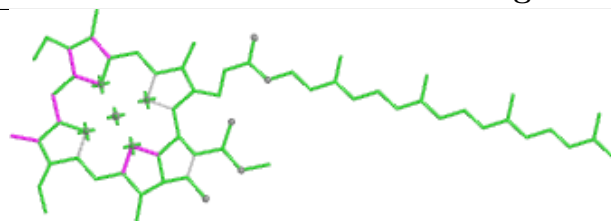


Torsions

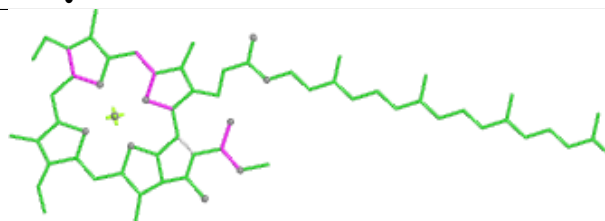


Rings

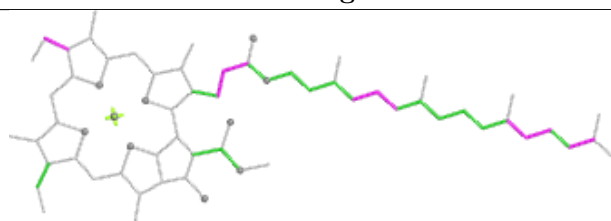
Ligand CLA Q 312



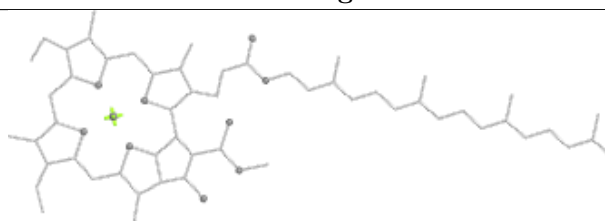
Bond lengths



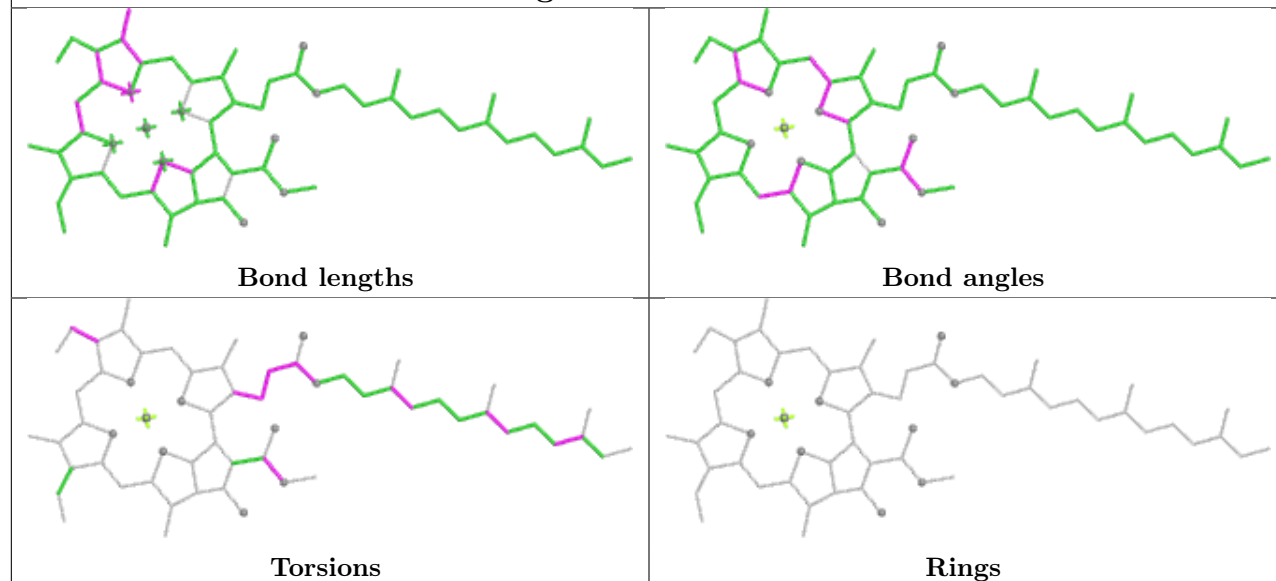
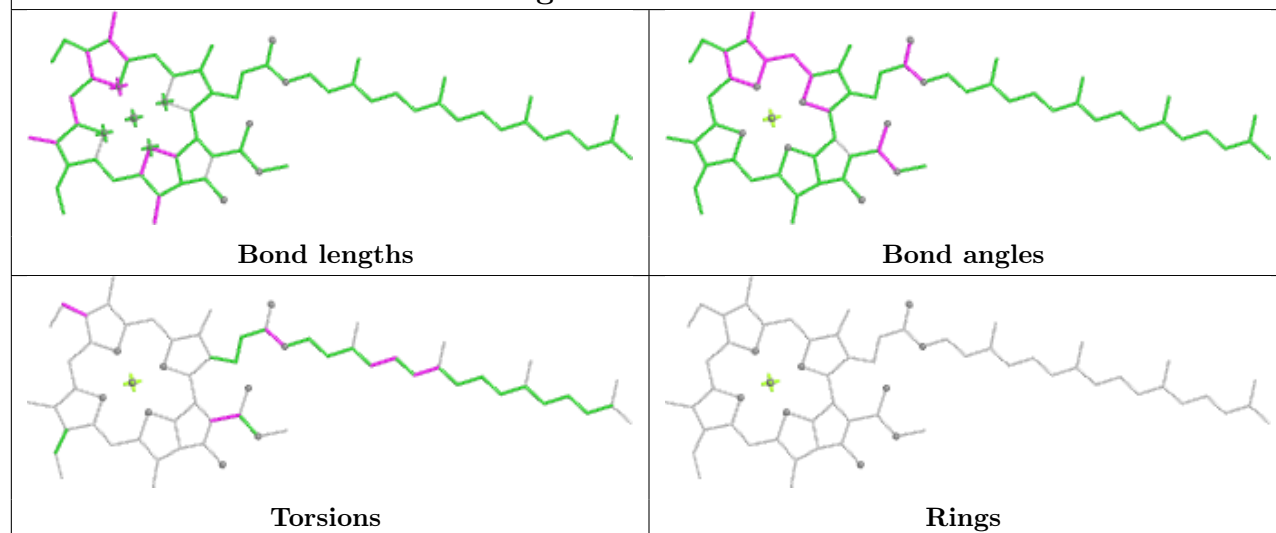
Bond angles

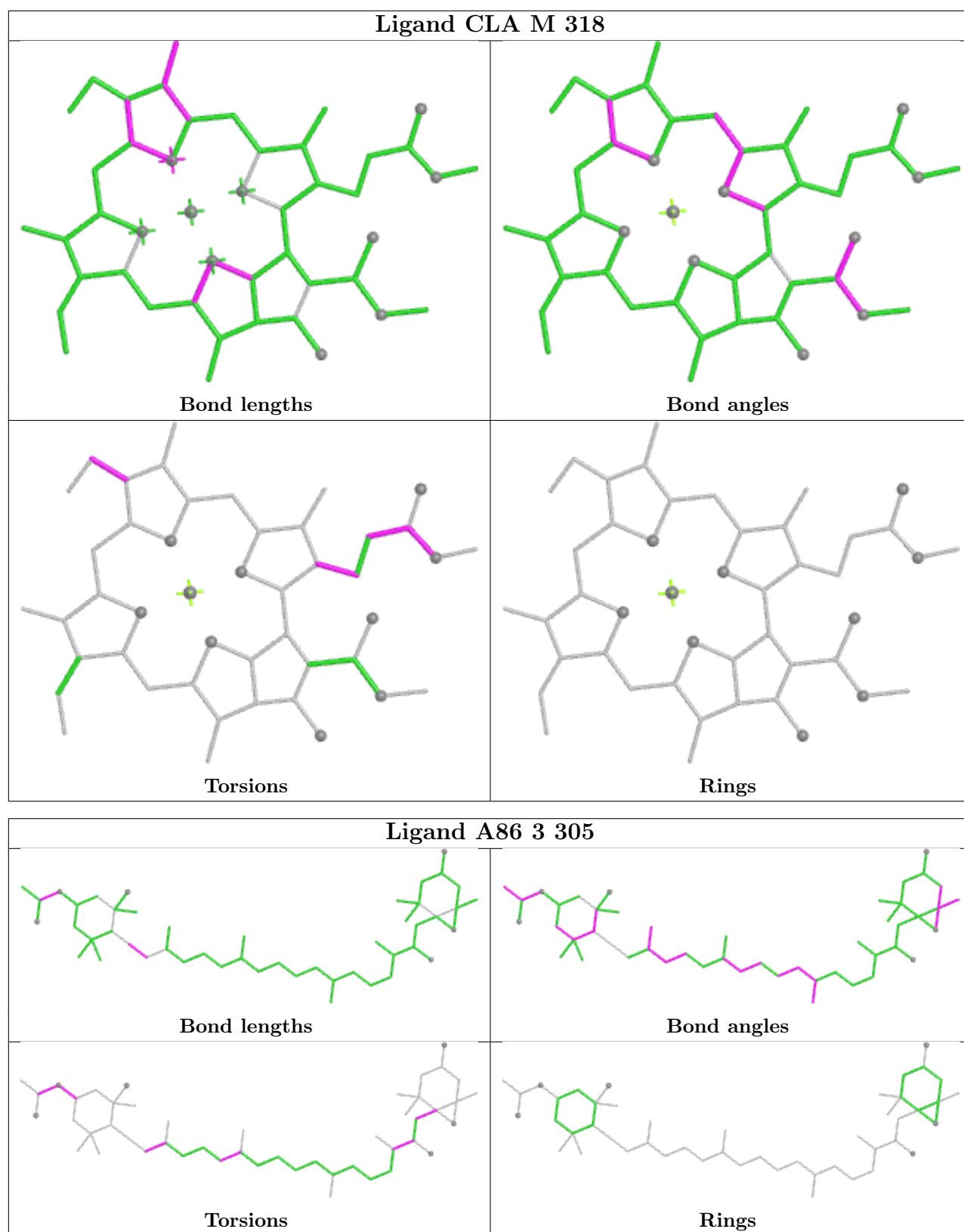


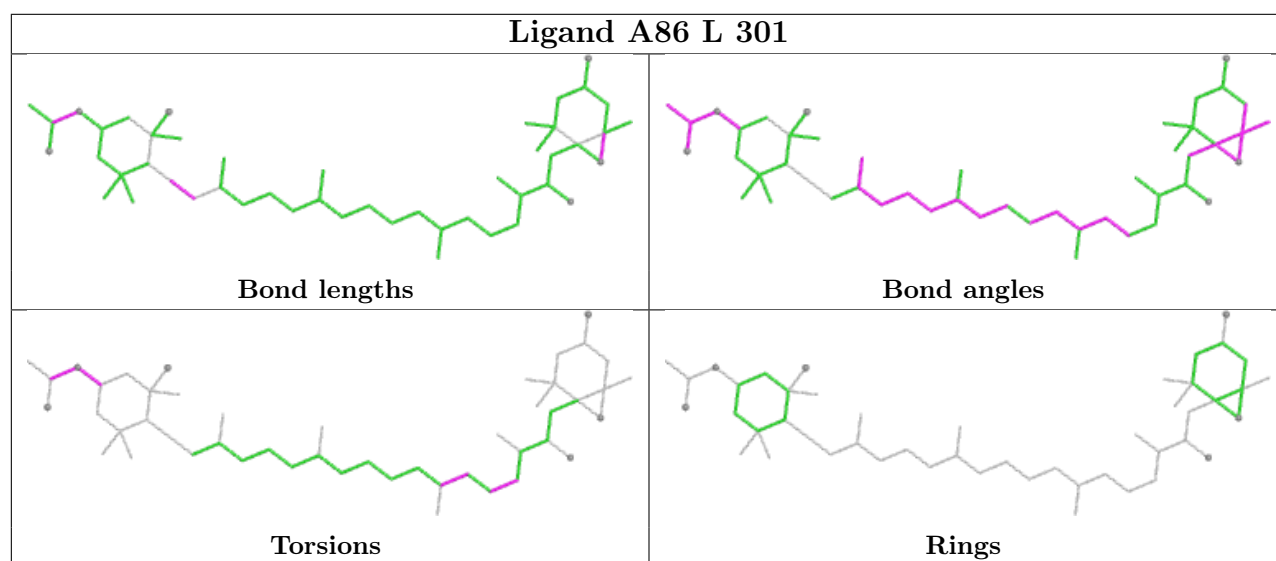
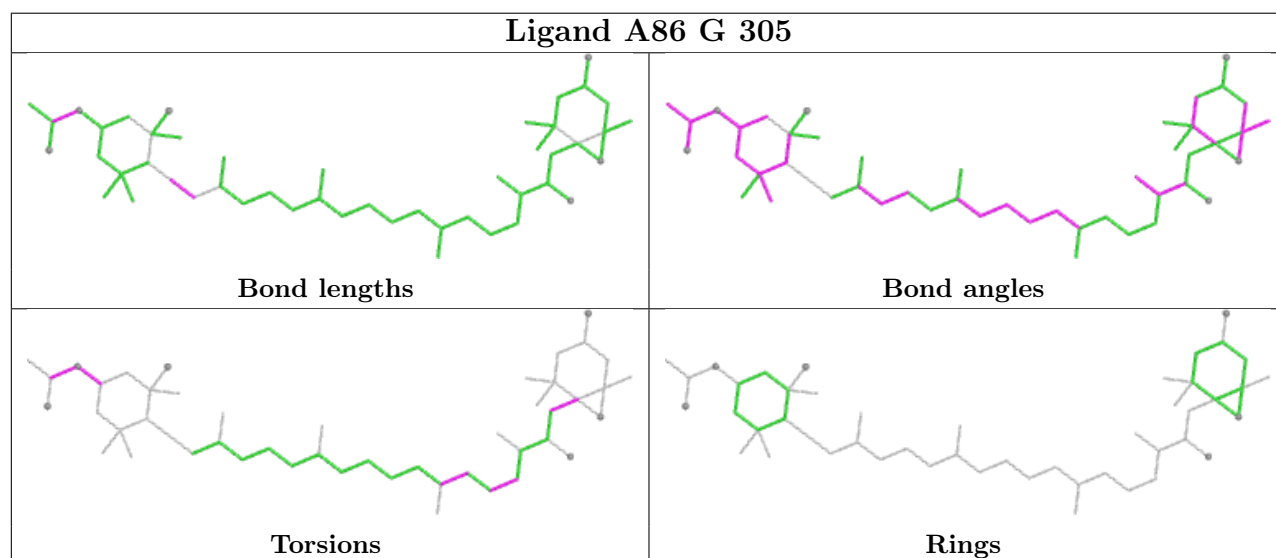
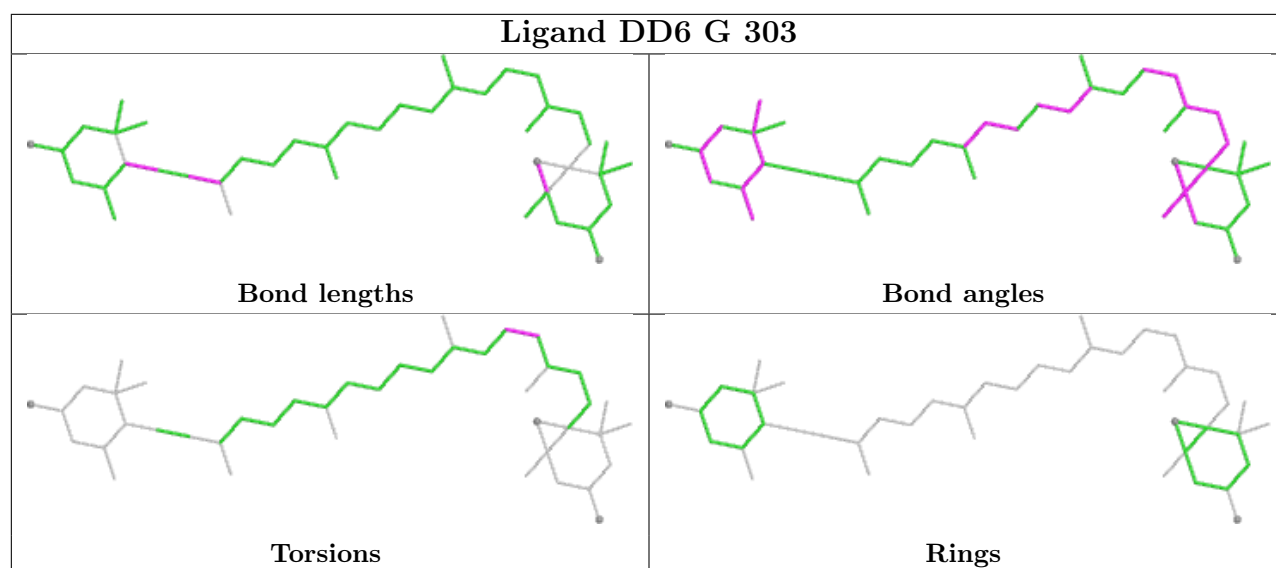
Torsions



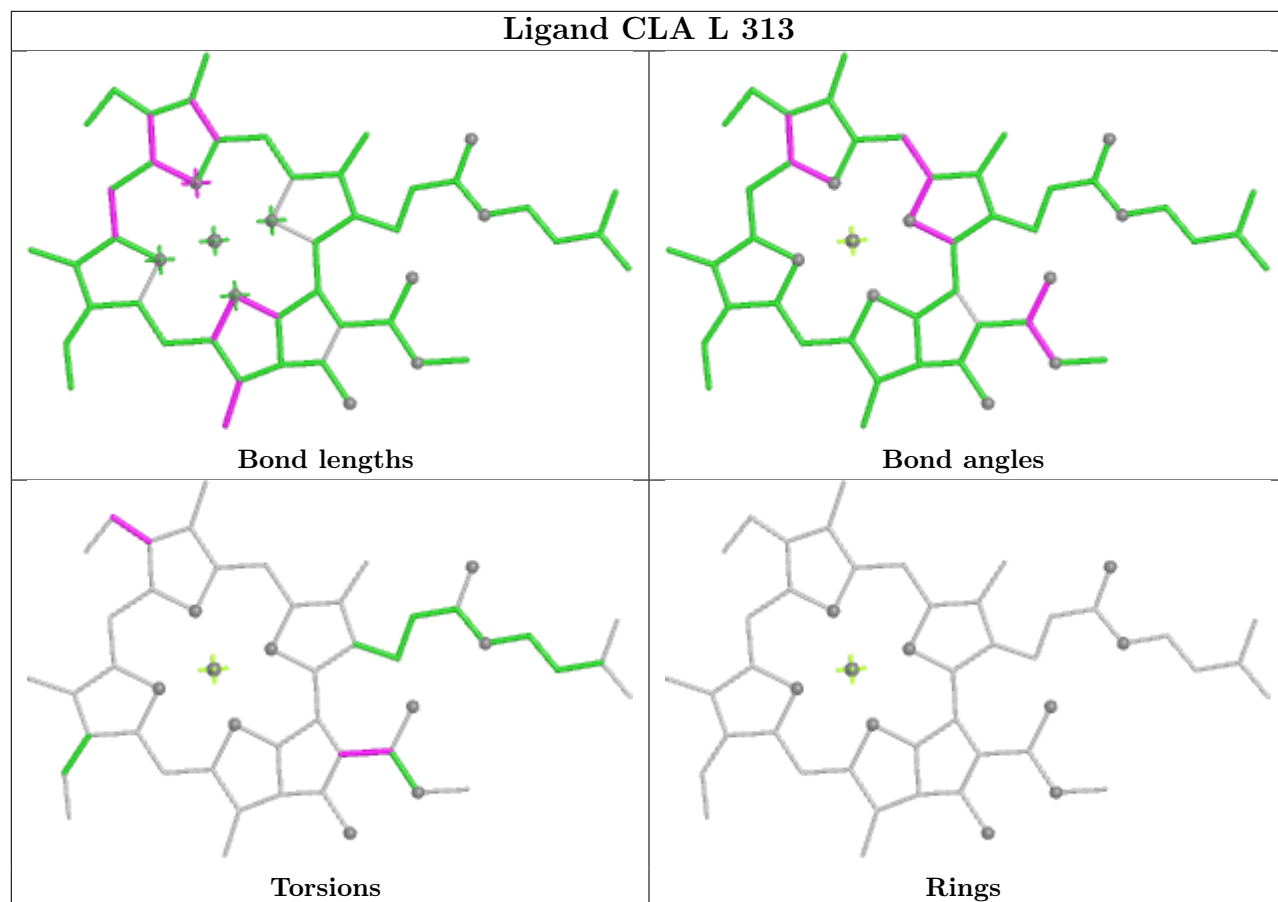
Rings

Ligand CLA 3 311**Ligand CLA a 824**

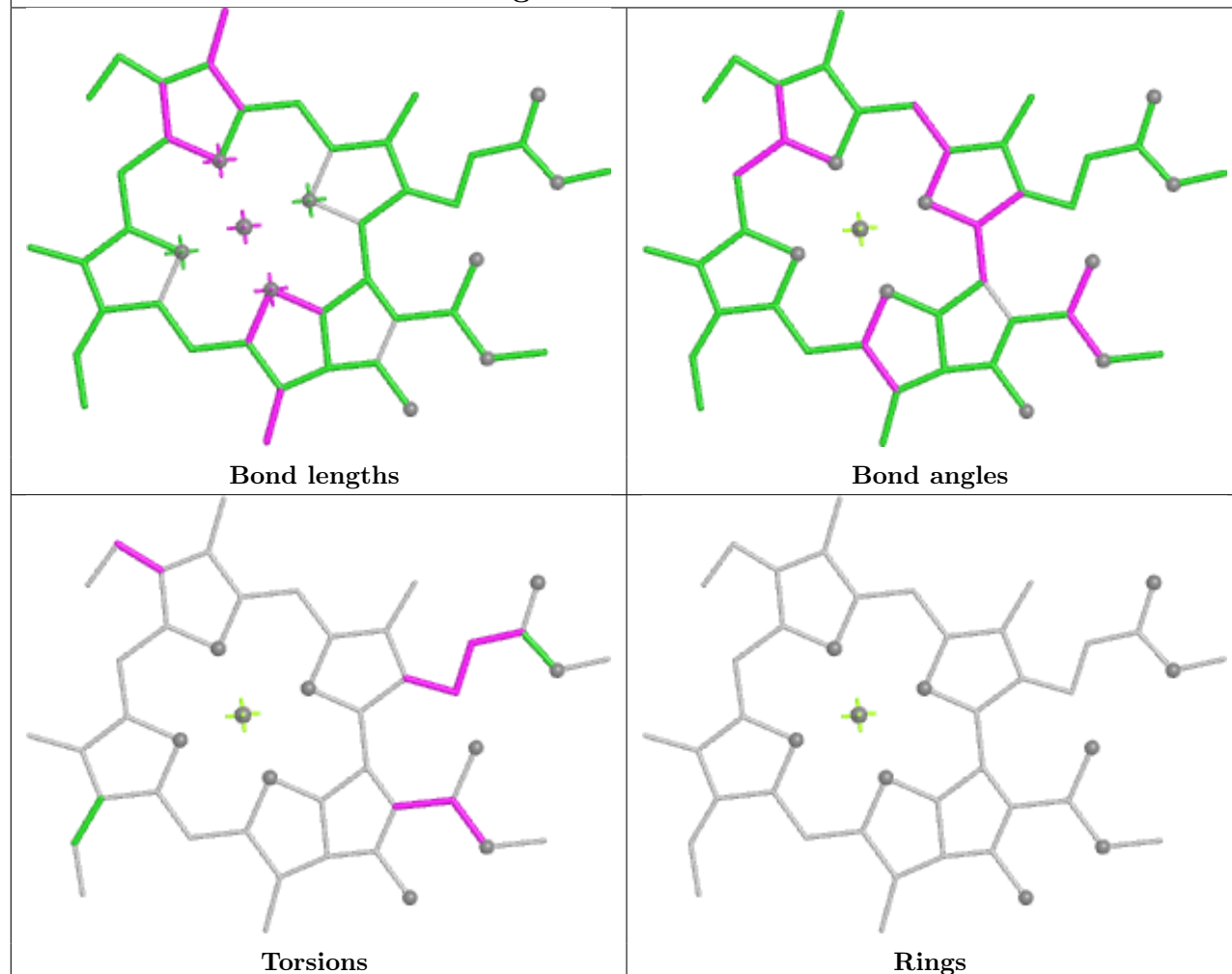




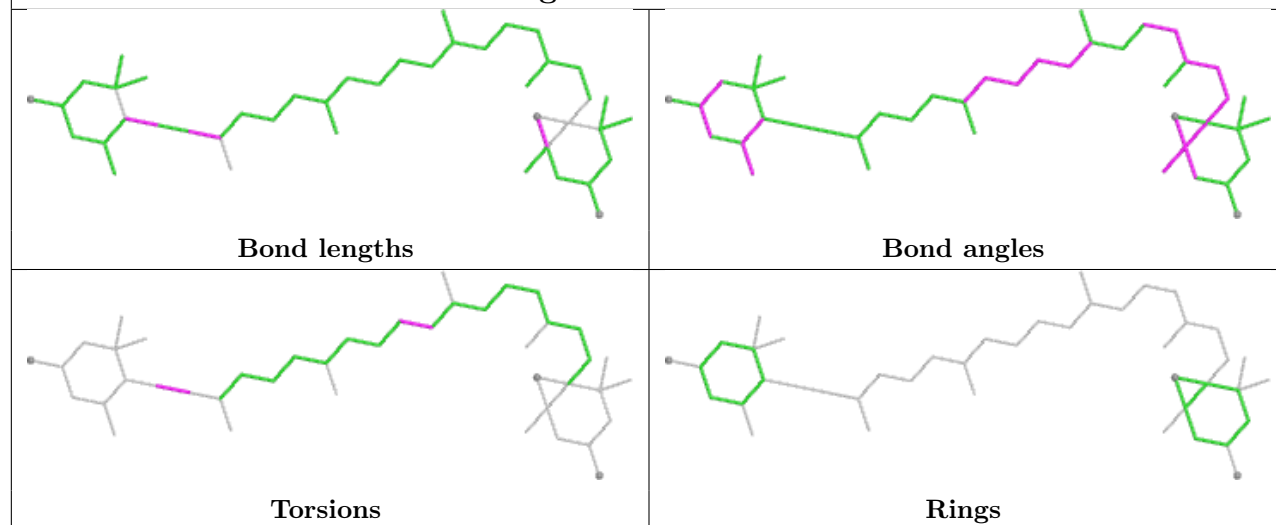
Ligand CLA L 313

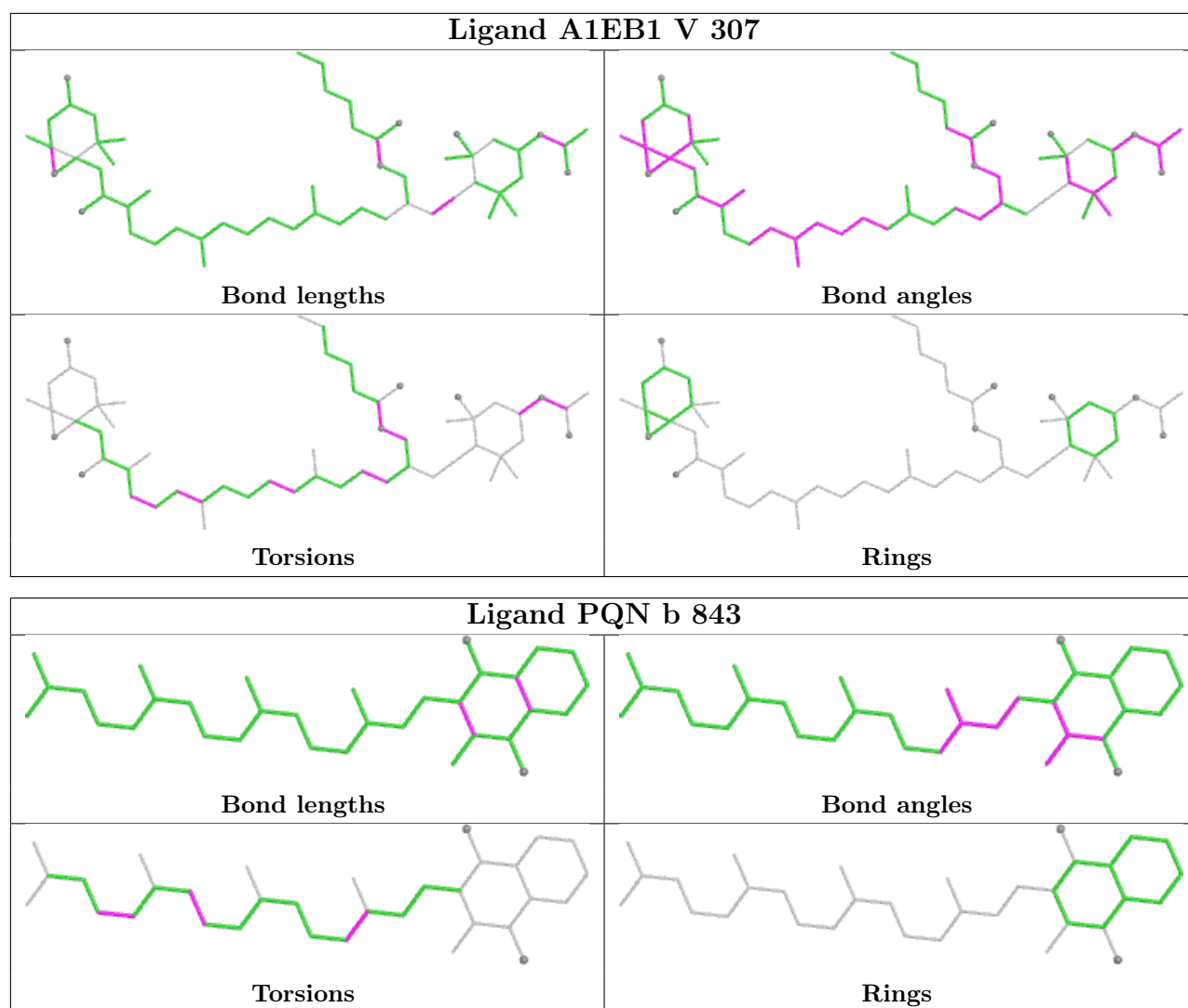


Ligand CLA U 201

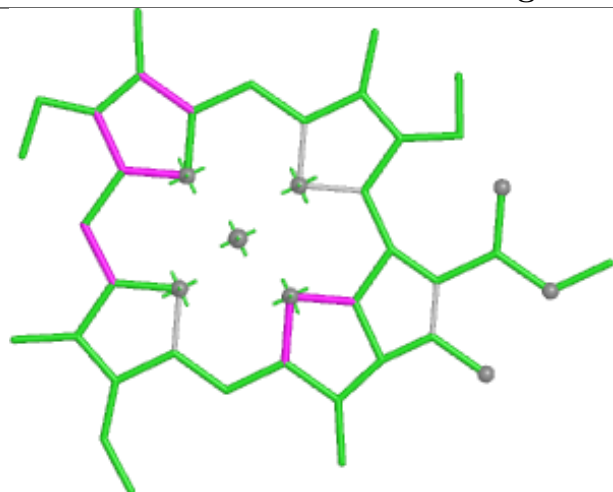


Ligand DD6 I 306

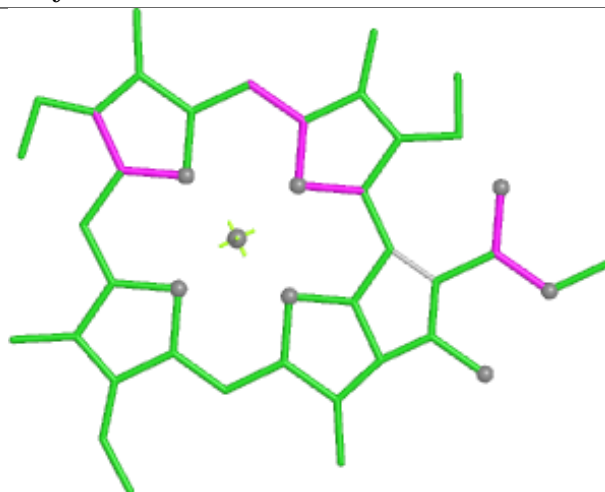




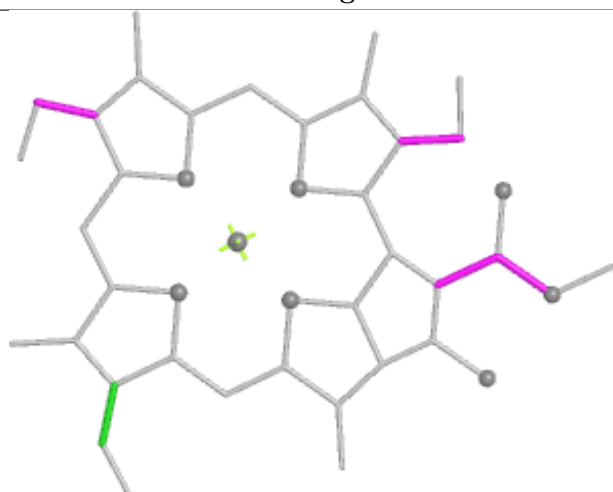
Ligand CLA y 318



Bond lengths



Bond angles

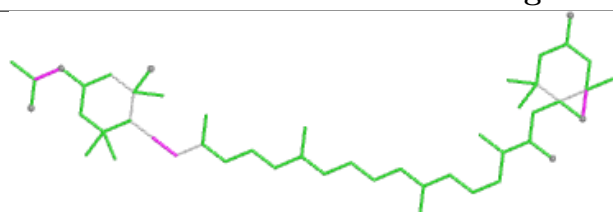


Torsions

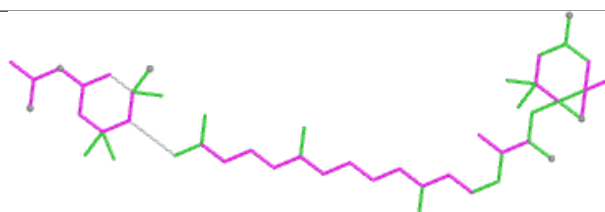


Rings

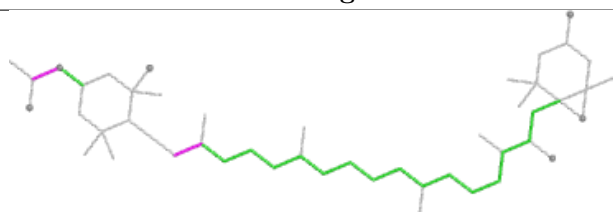
Ligand A86 8 323



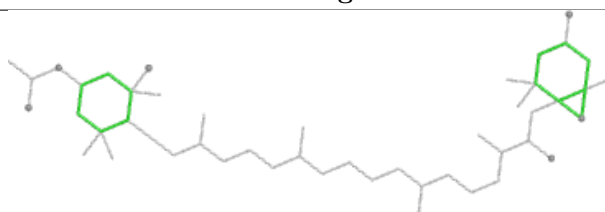
Bond lengths



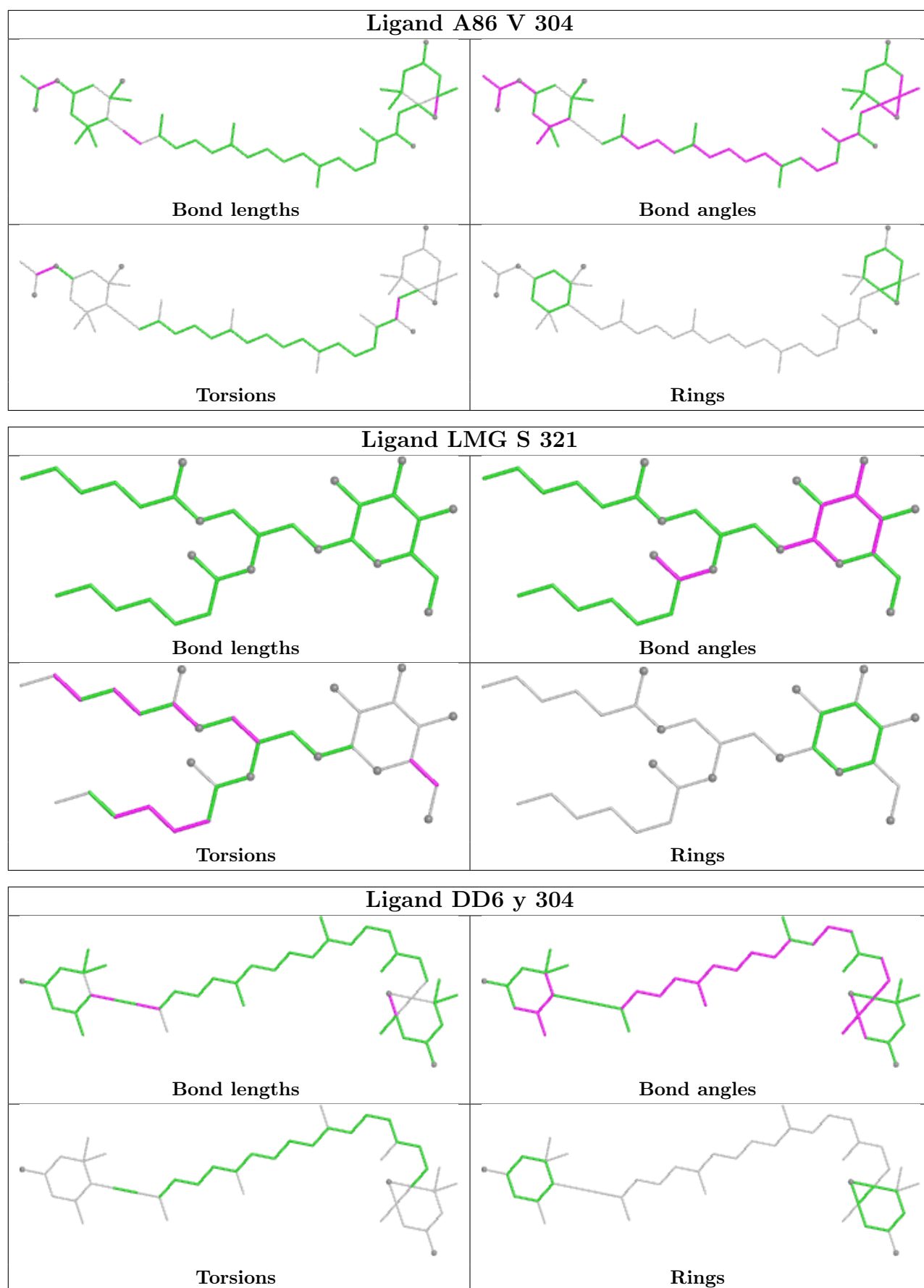
Bond angles



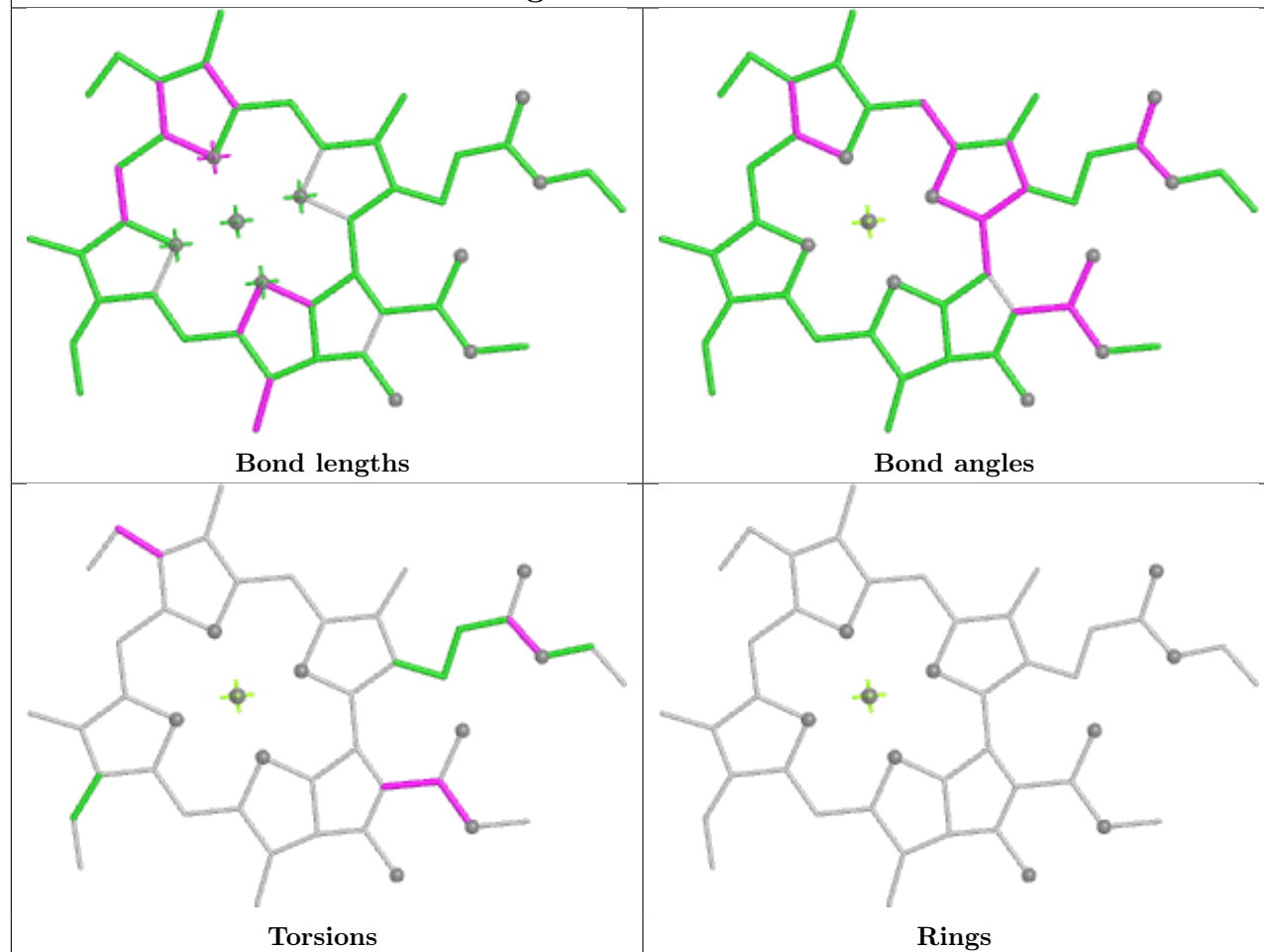
Torsions



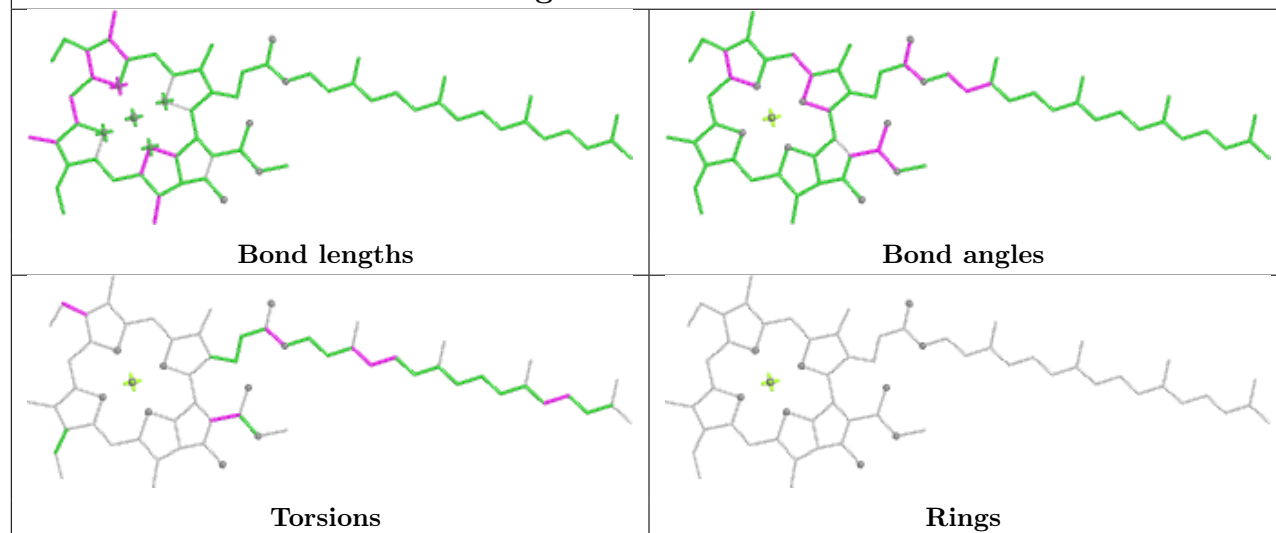
Rings



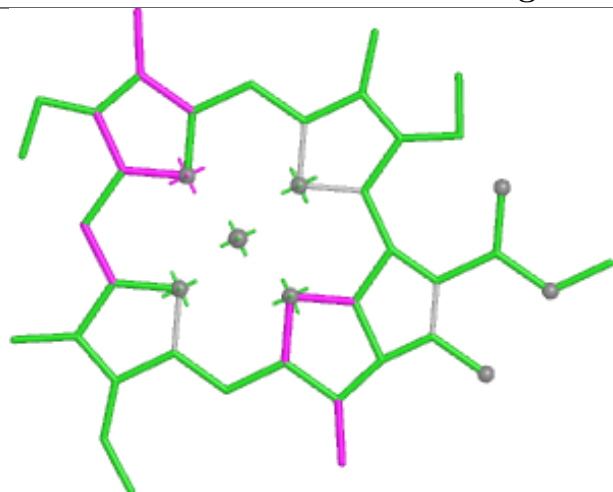
Ligand CLA R 315



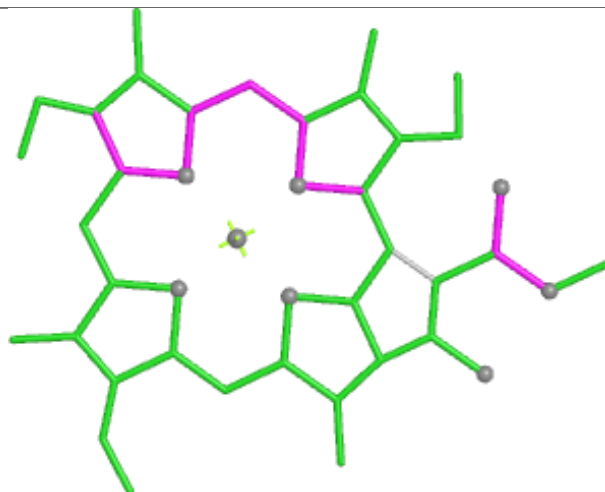
Ligand CLA b 811



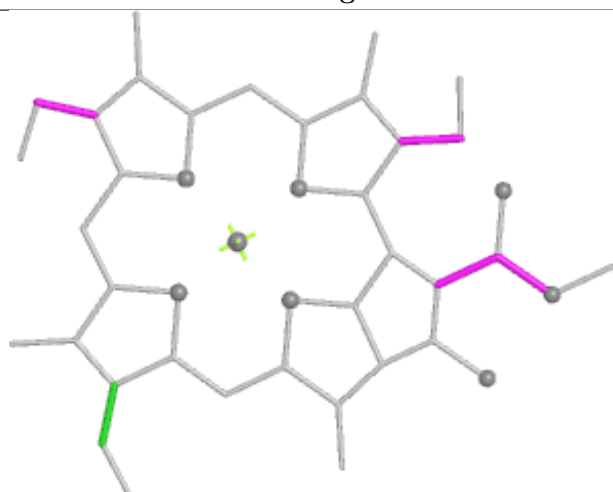
Ligand CLA 1 309



Bond lengths



Bond angles

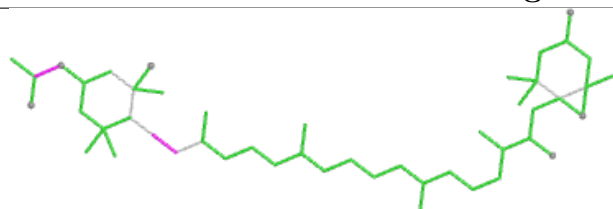


Torsions

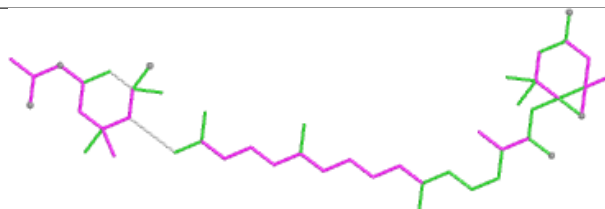


Rings

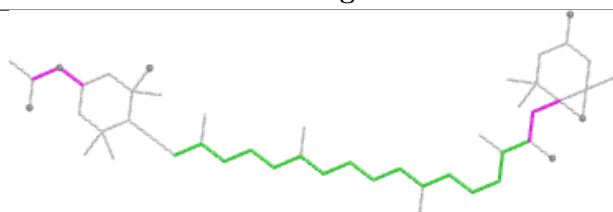
Ligand A86 4 310



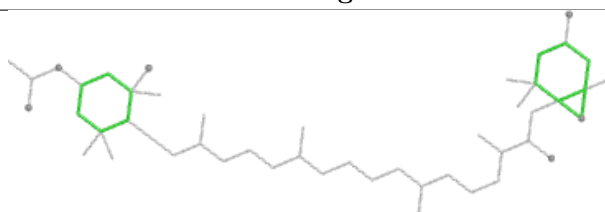
Bond lengths



Bond angles

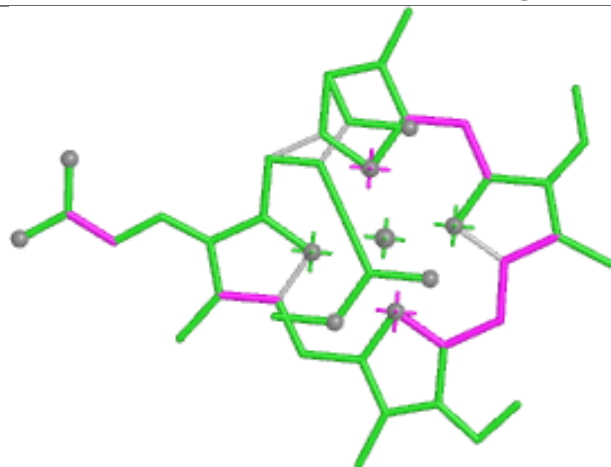


Torsions



Rings

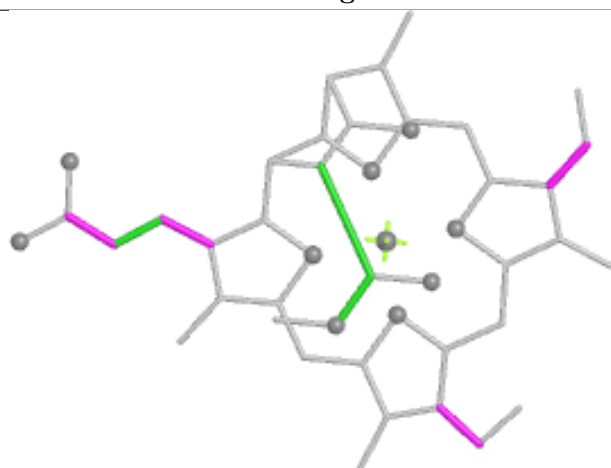
Ligand KC2 R 318



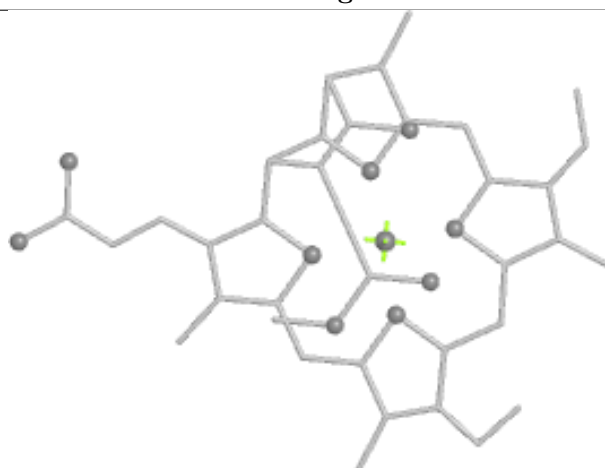
Bond lengths



Bond angles

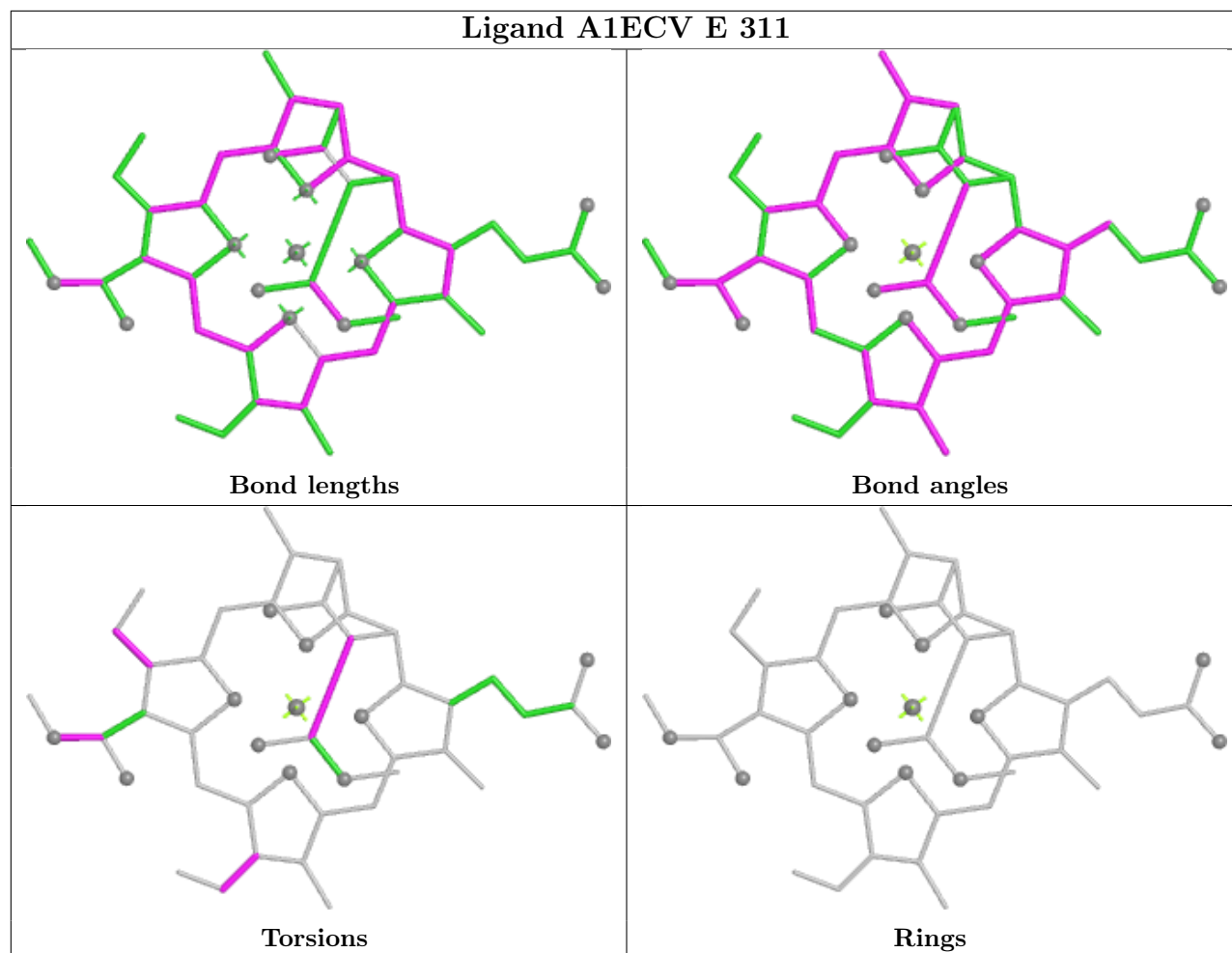


Torsions

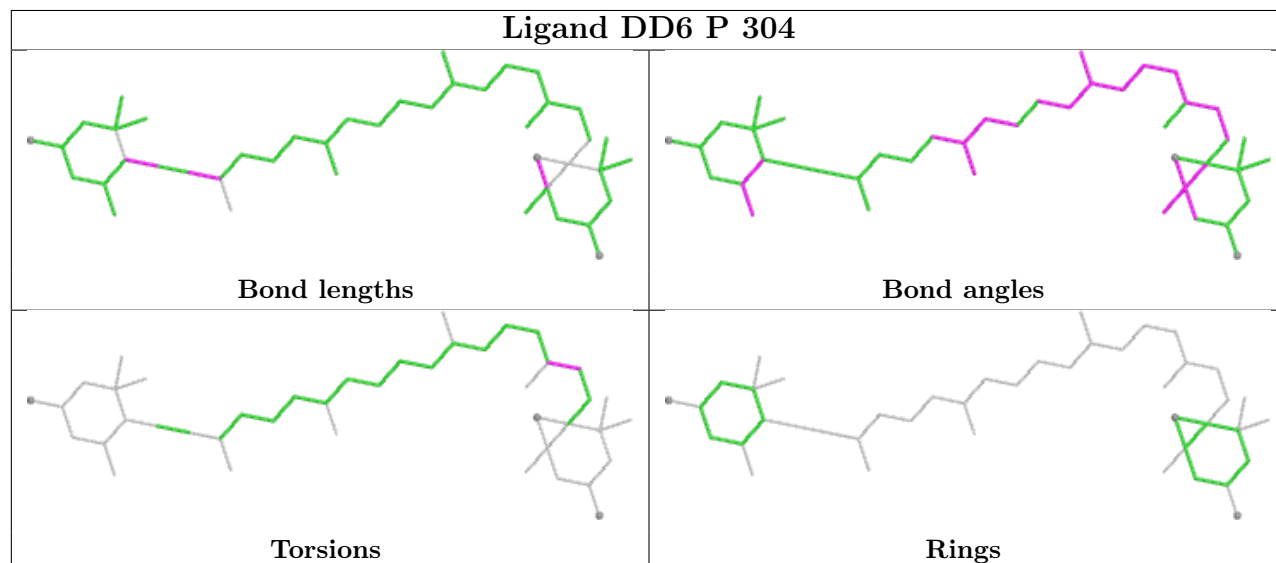


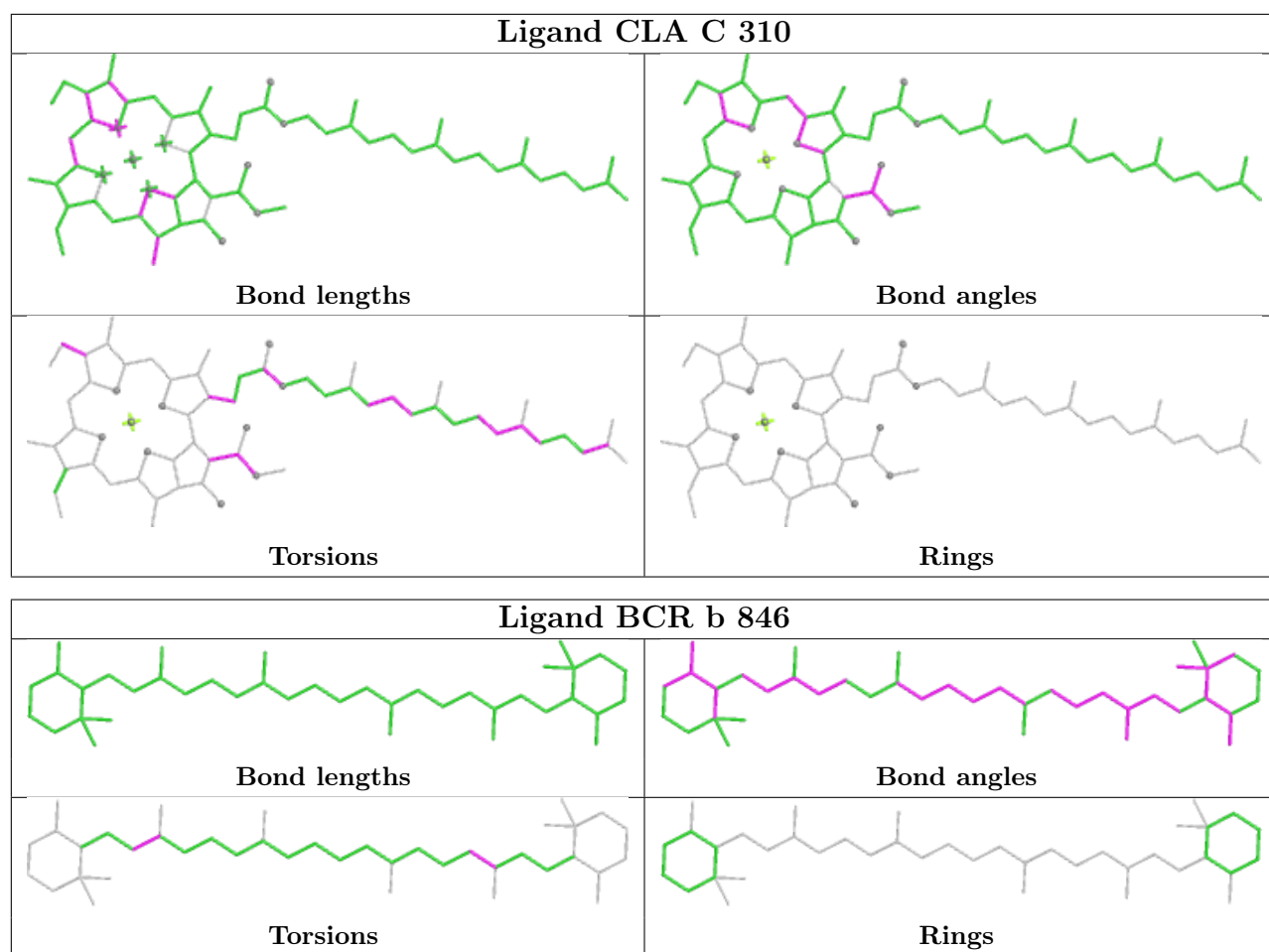
Rings

Ligand A1ECV E 311

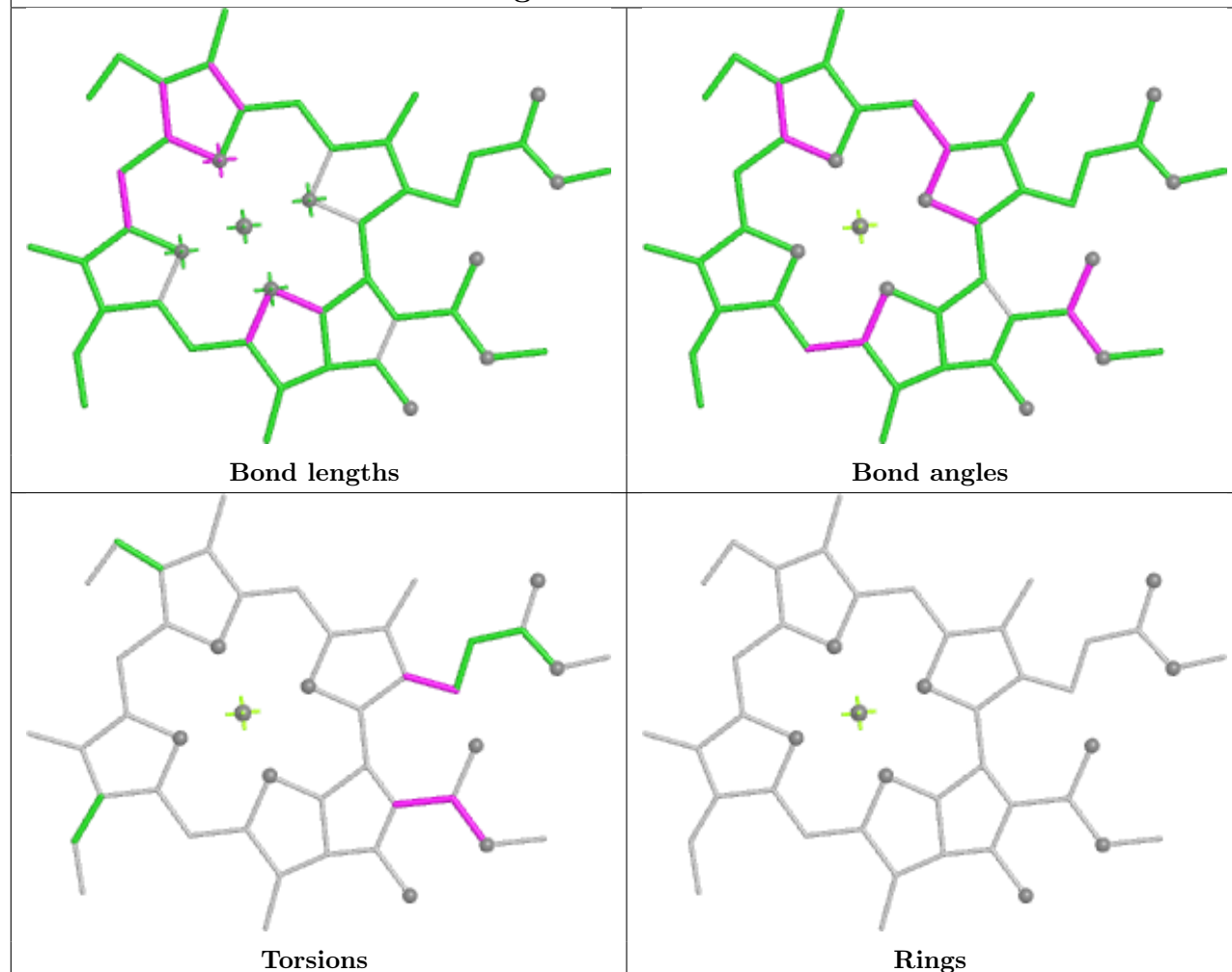


Ligand DD6 P 304

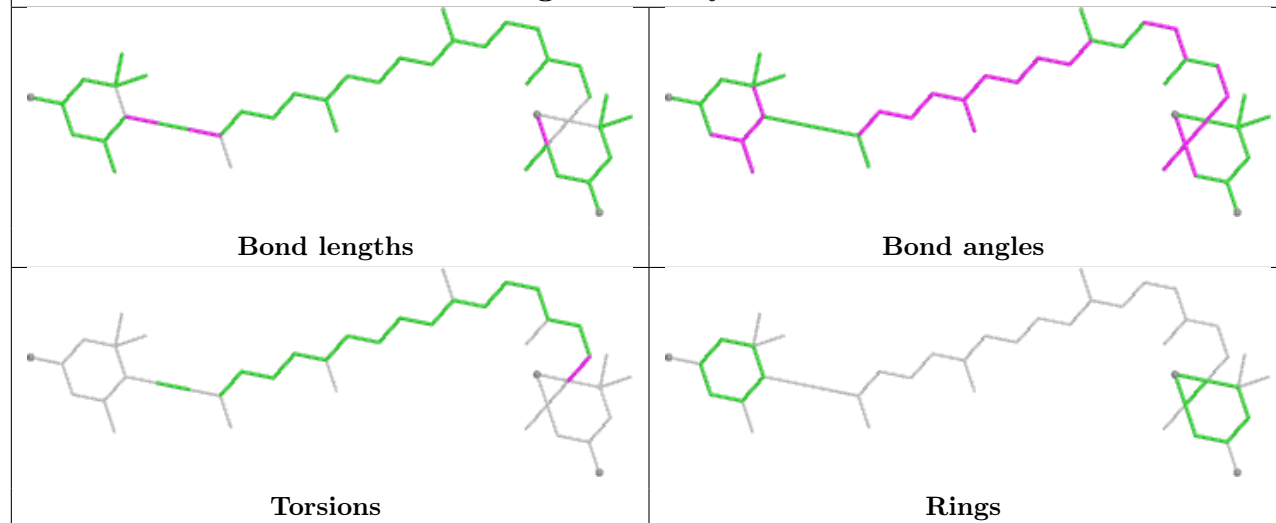


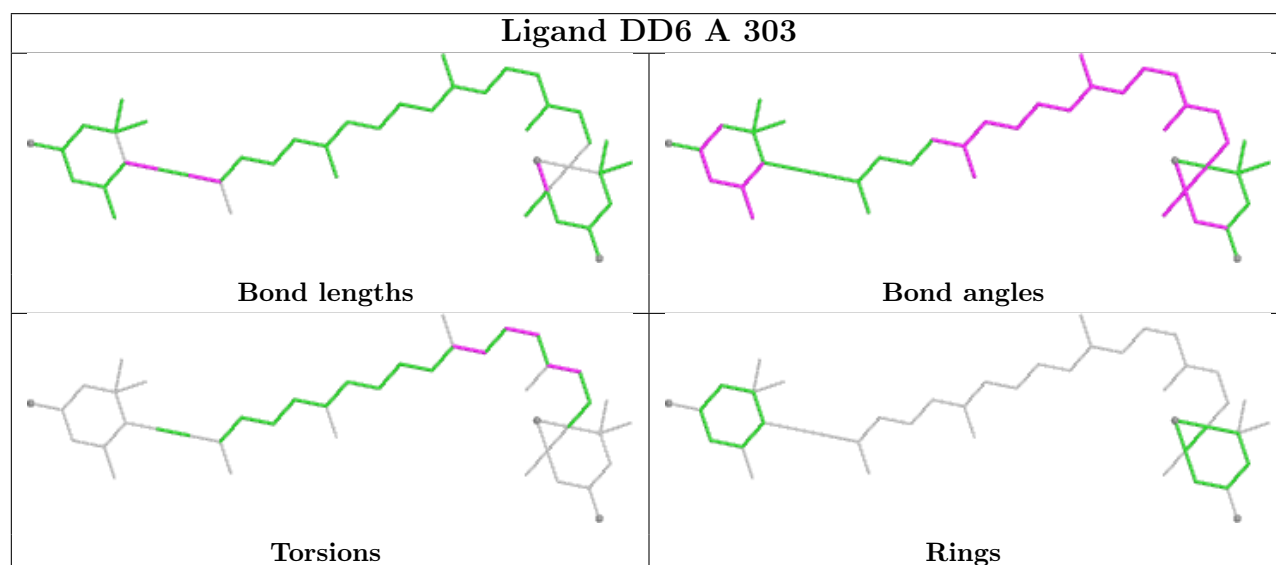
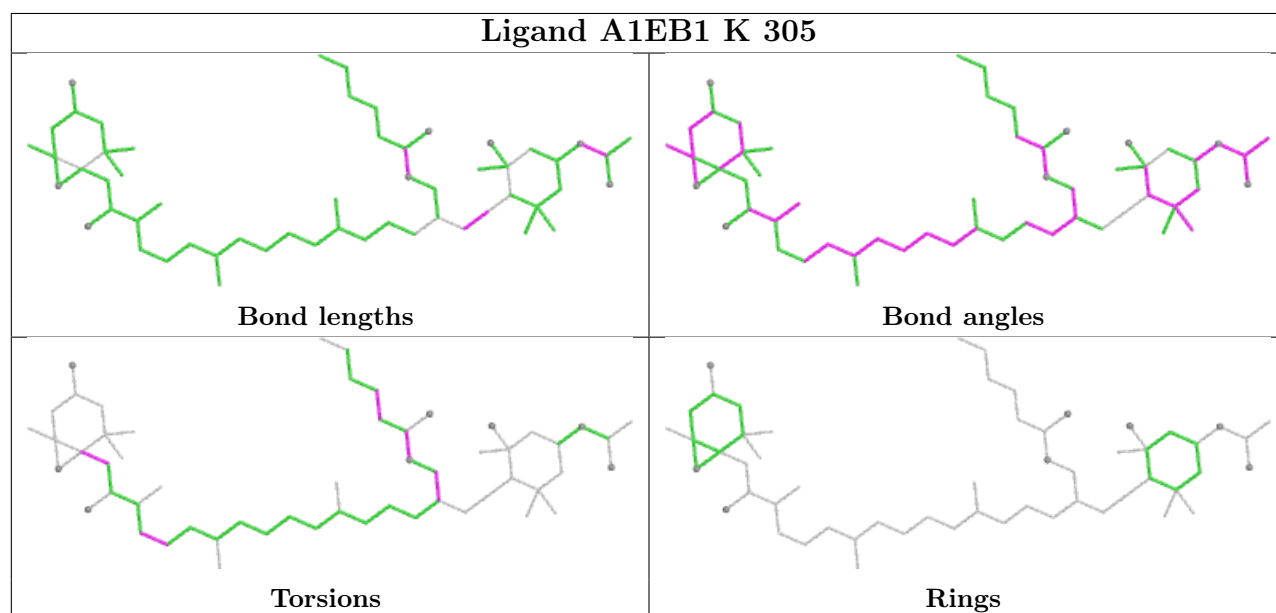
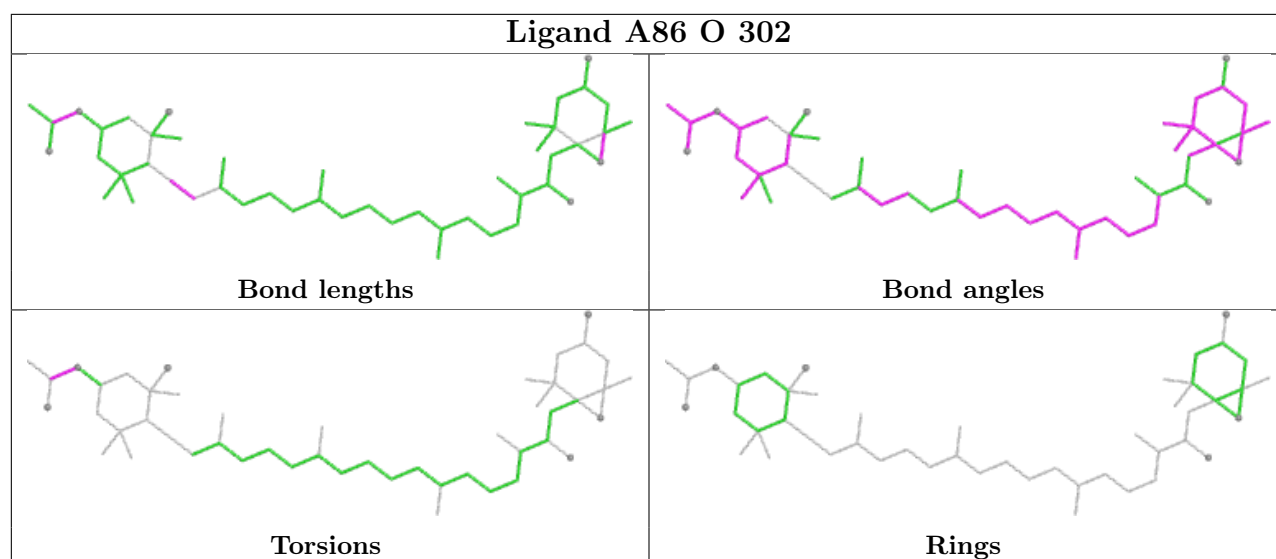


Ligand CLA B 203

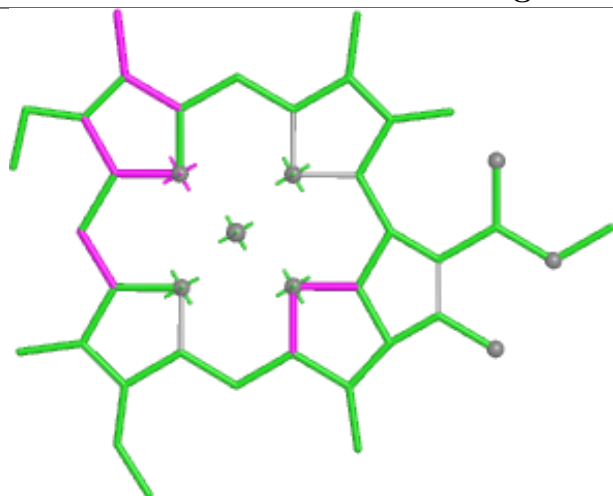


Ligand DD6 y 303

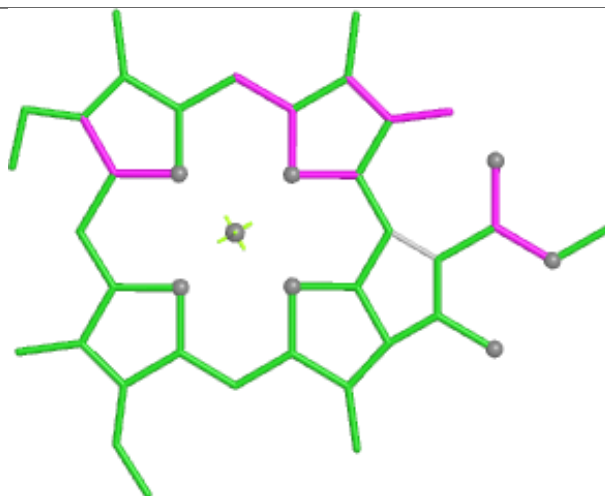




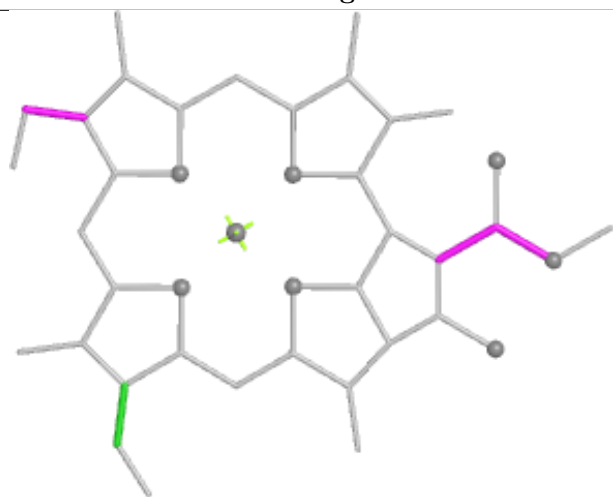
Ligand CLA Y 313



Bond lengths



Bond angles

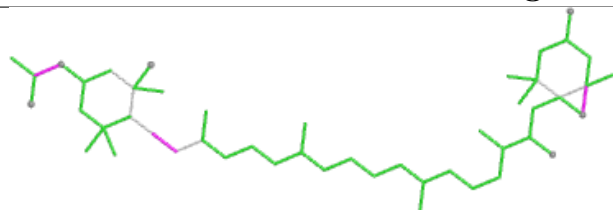


Torsions

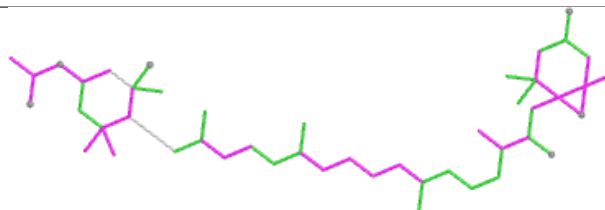


Rings

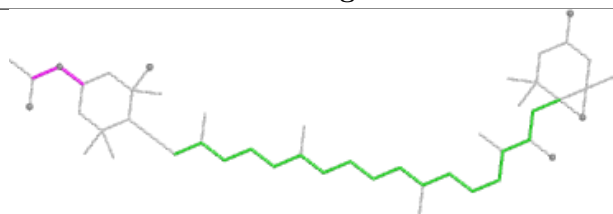
Ligand A86 7 307



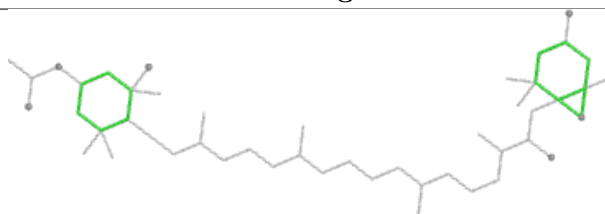
Bond lengths



Bond angles

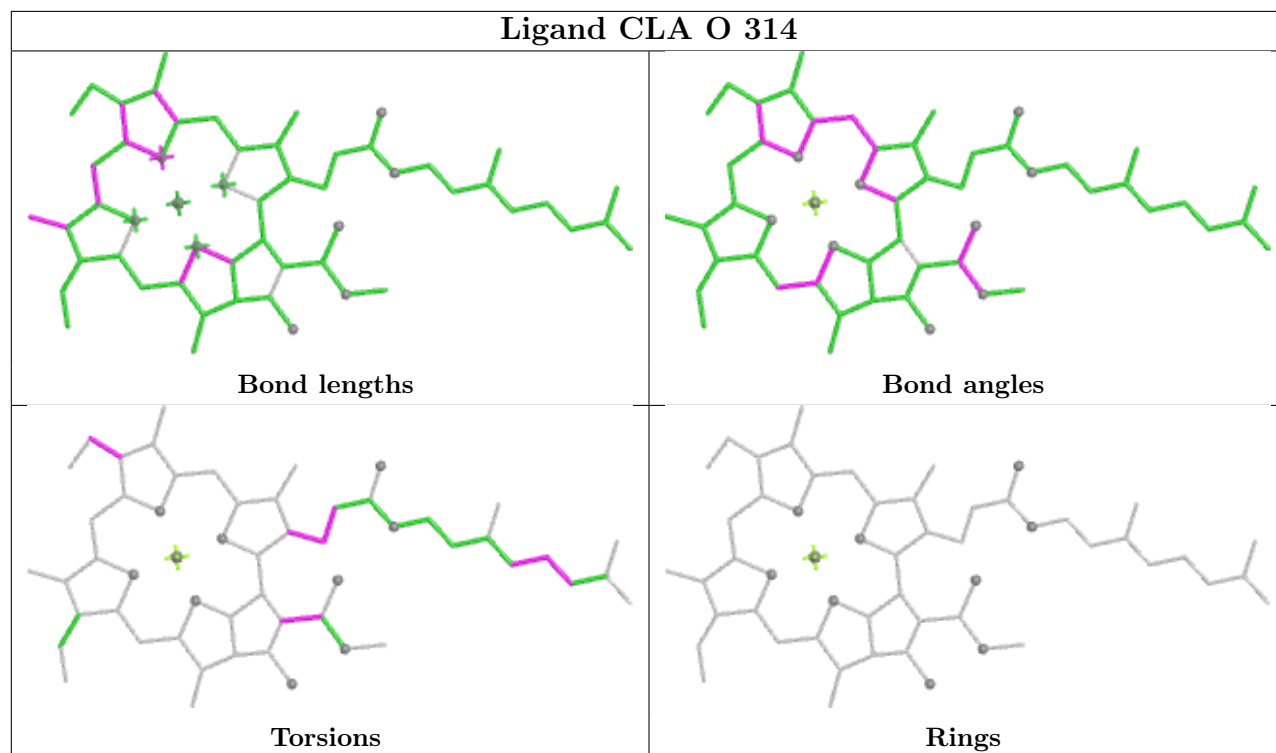


Torsions

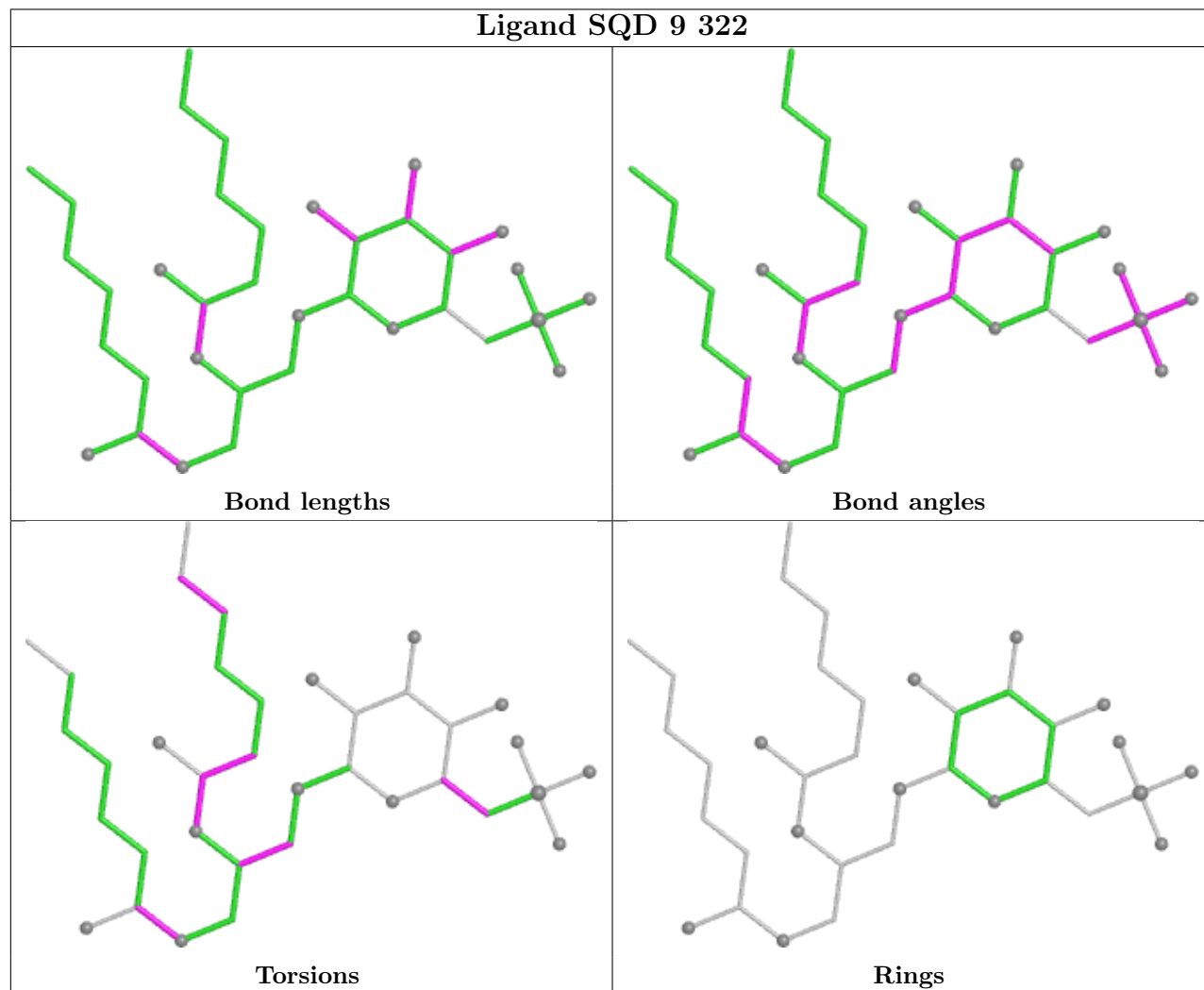


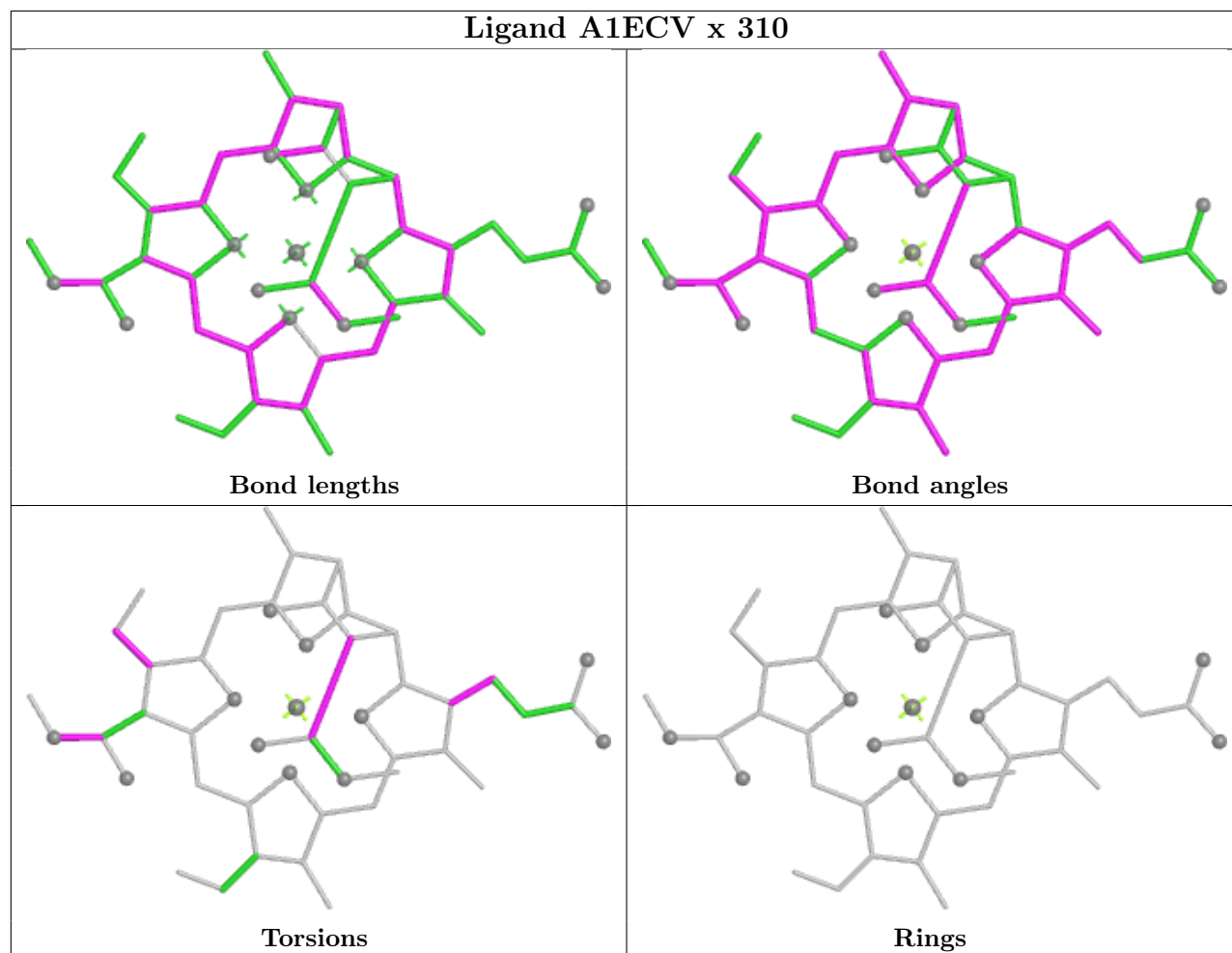
Rings

Ligand CLA O 314

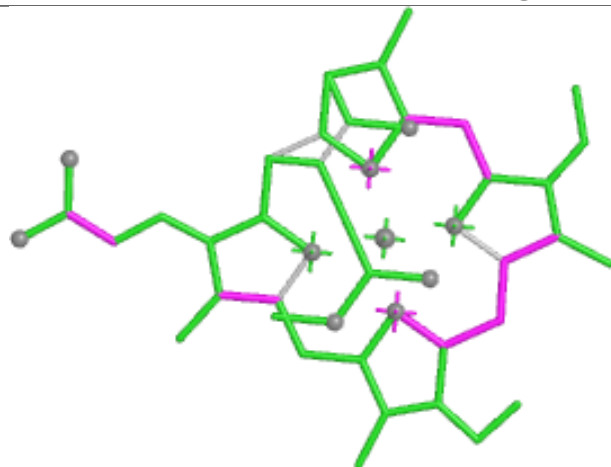


Ligand SQD 9 322

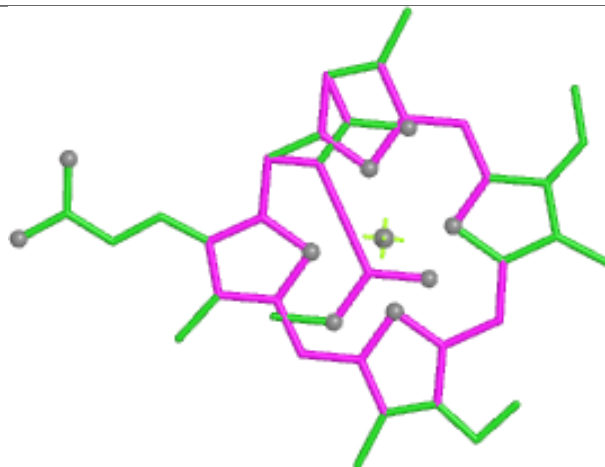




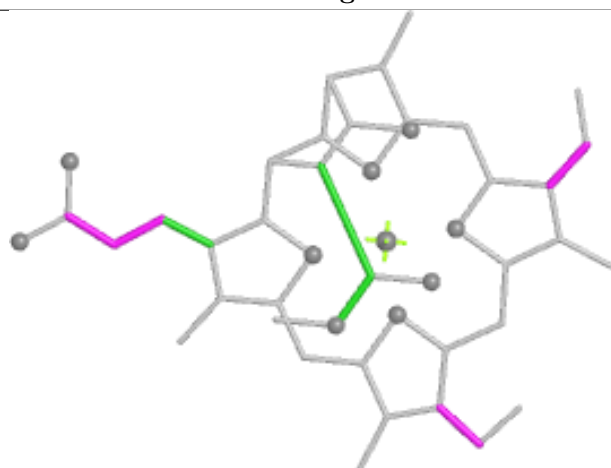
Ligand KC2 V 312



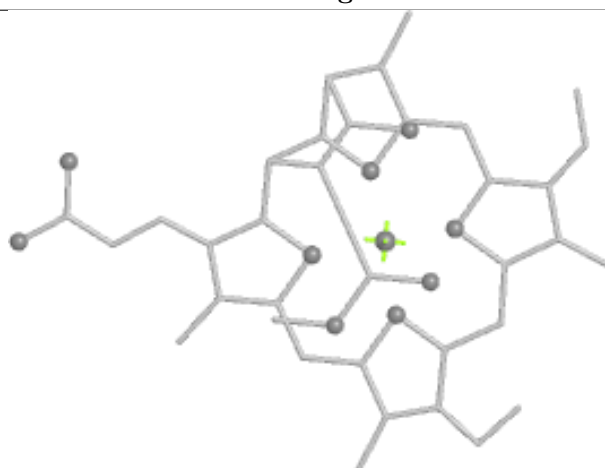
Bond lengths



Bond angles

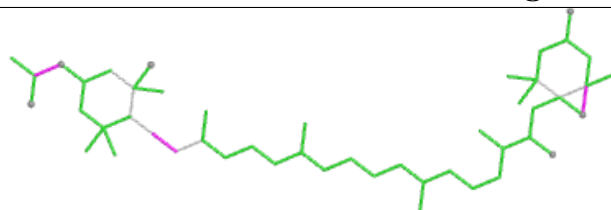


Torsions

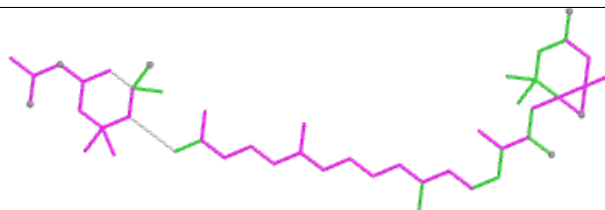


Rings

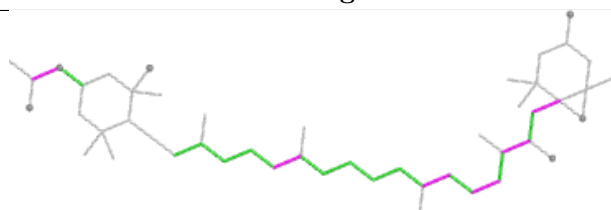
Ligand A86 8 307



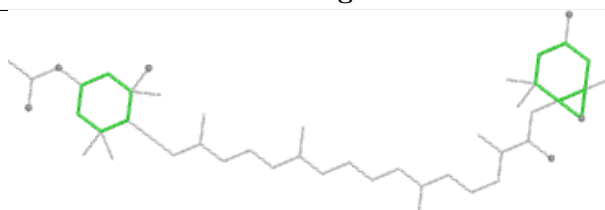
Bond lengths



Bond angles

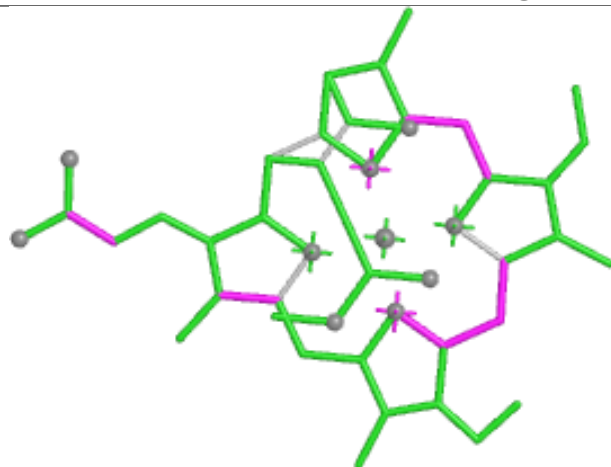


Torsions

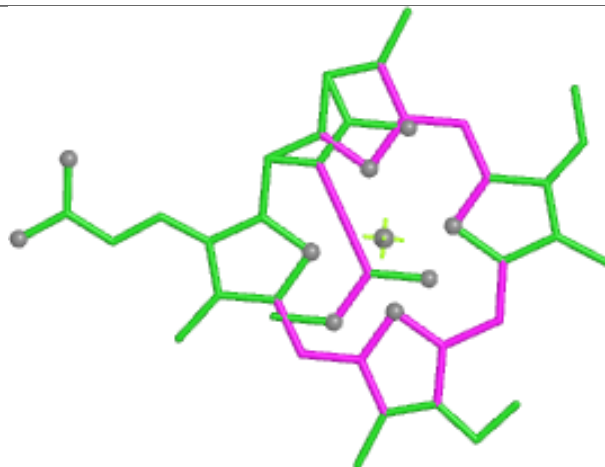


Rings

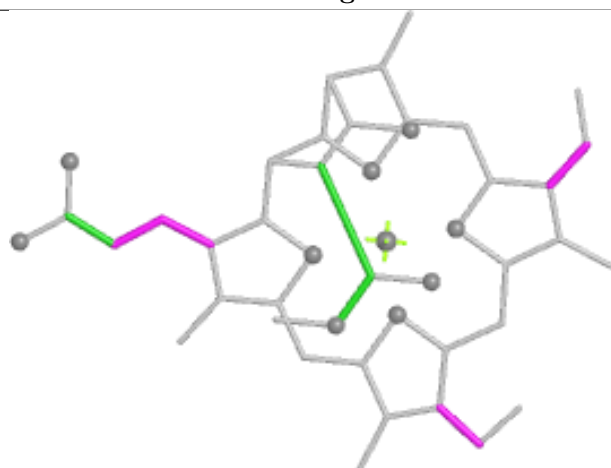
Ligand KC2 A 310



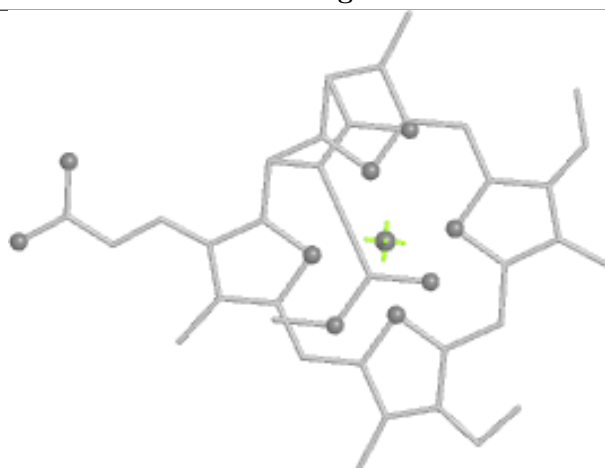
Bond lengths



Bond angles

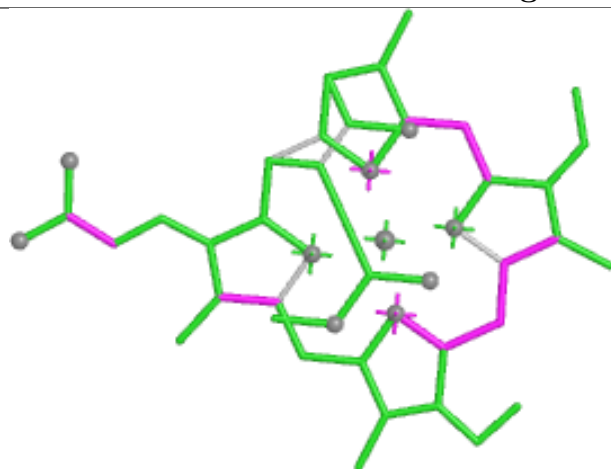


Torsions

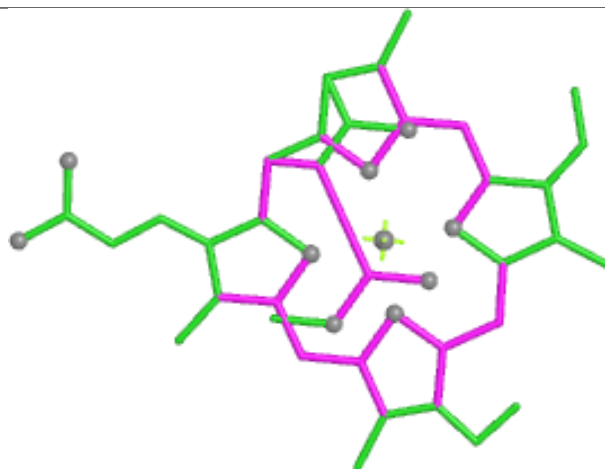


Rings

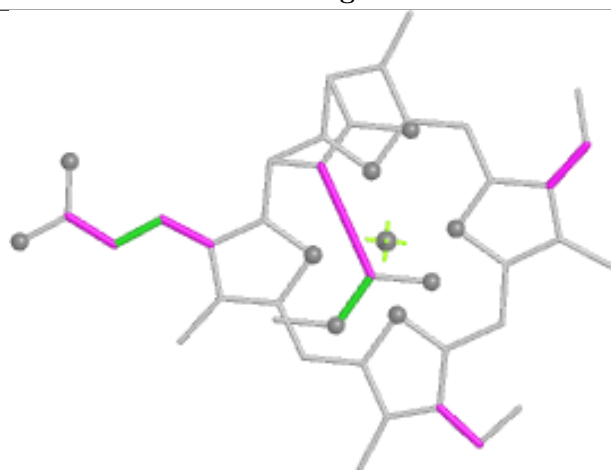
Ligand KC2 4 324



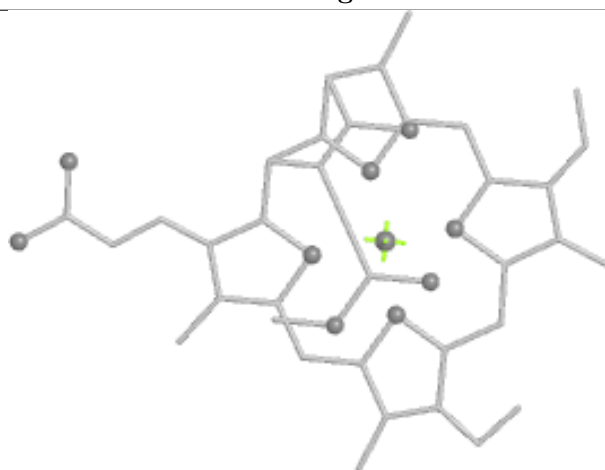
Bond lengths



Bond angles

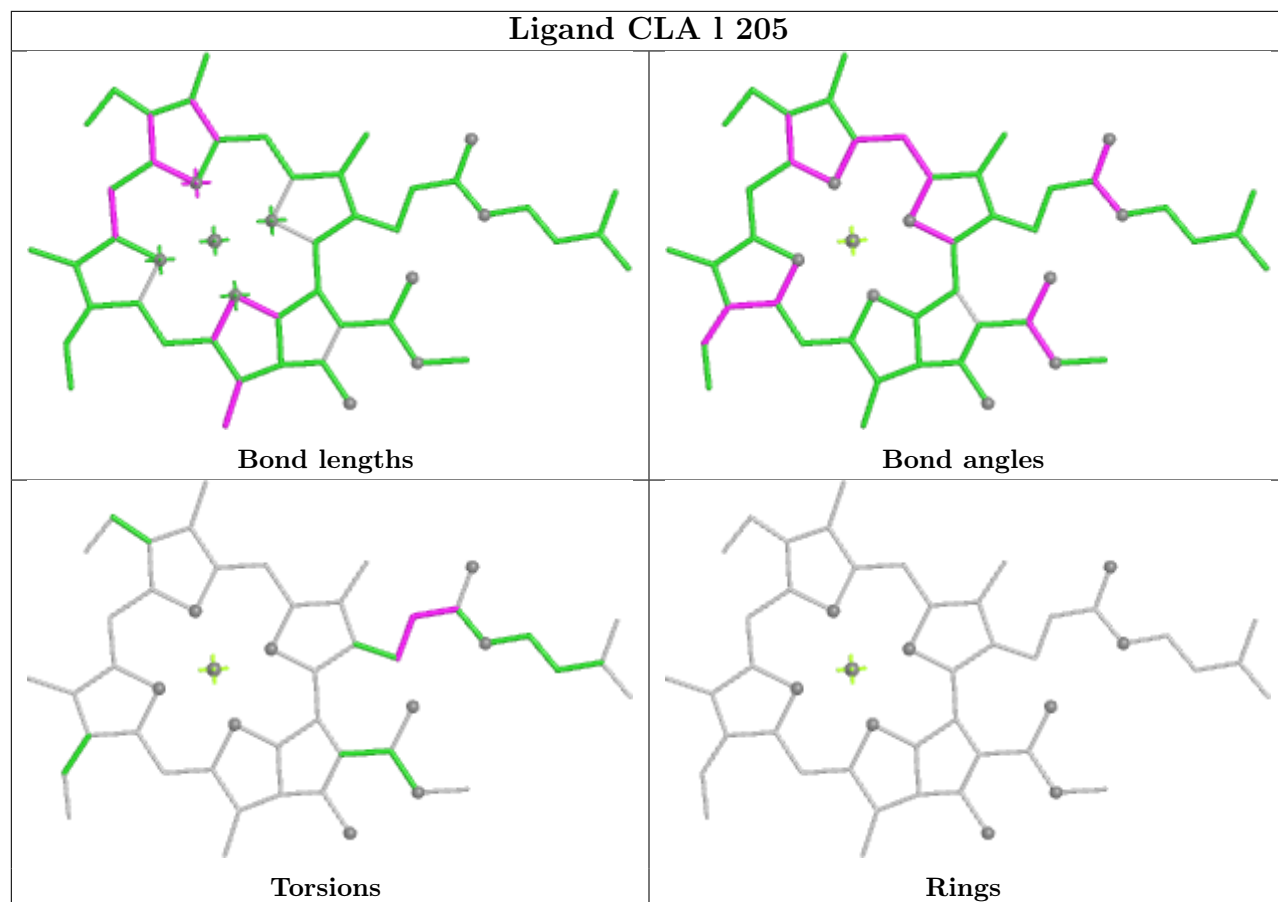


Torsions

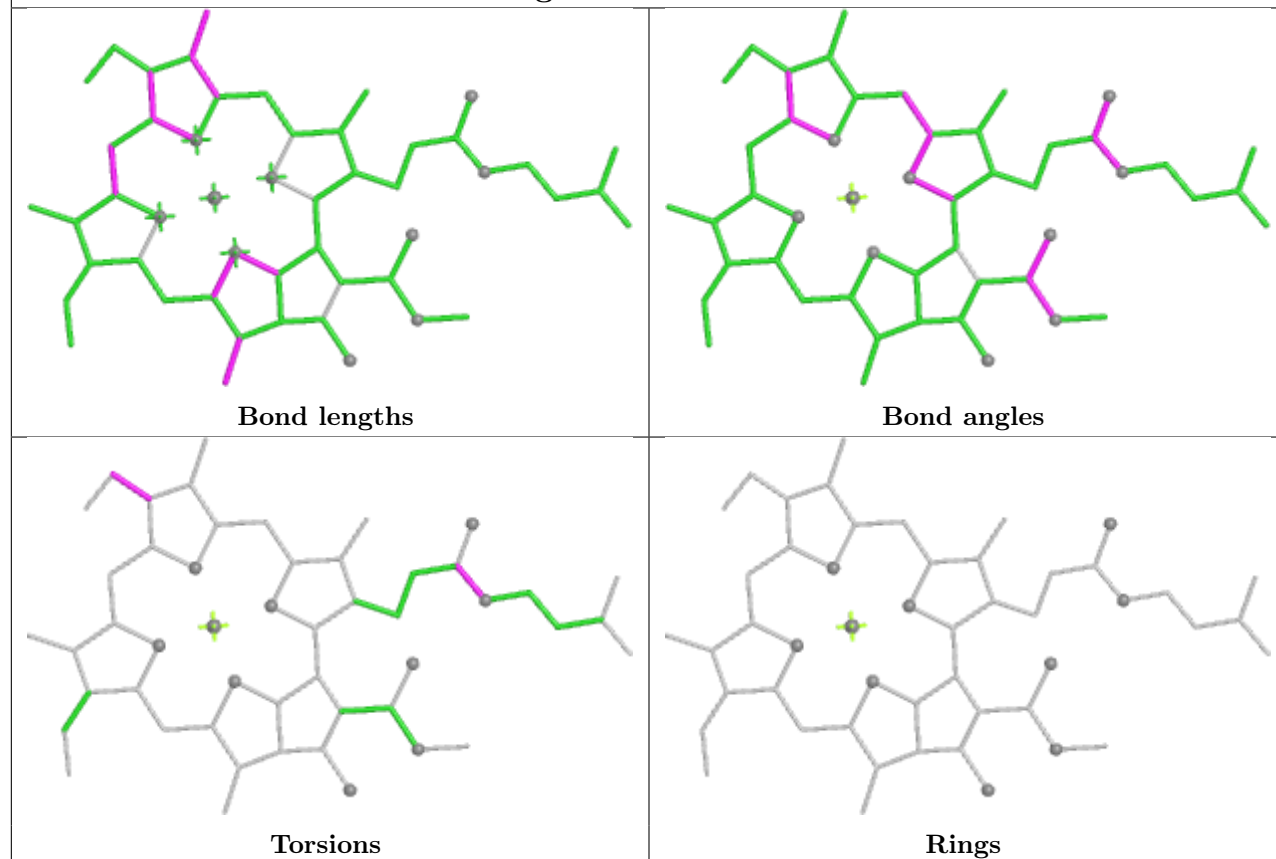


Rings

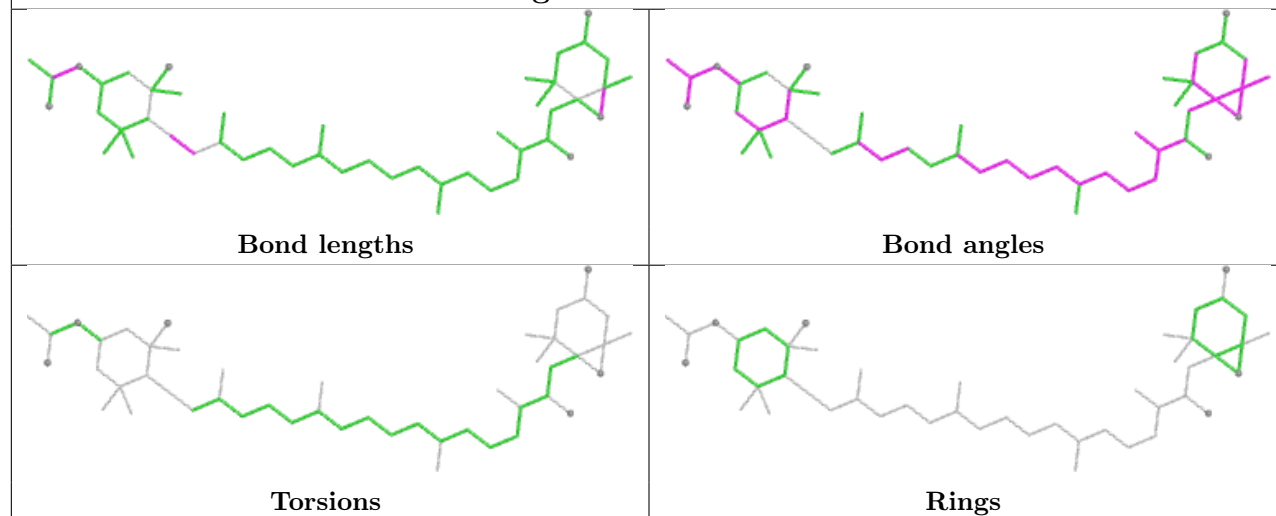
Ligand CLA 1 205

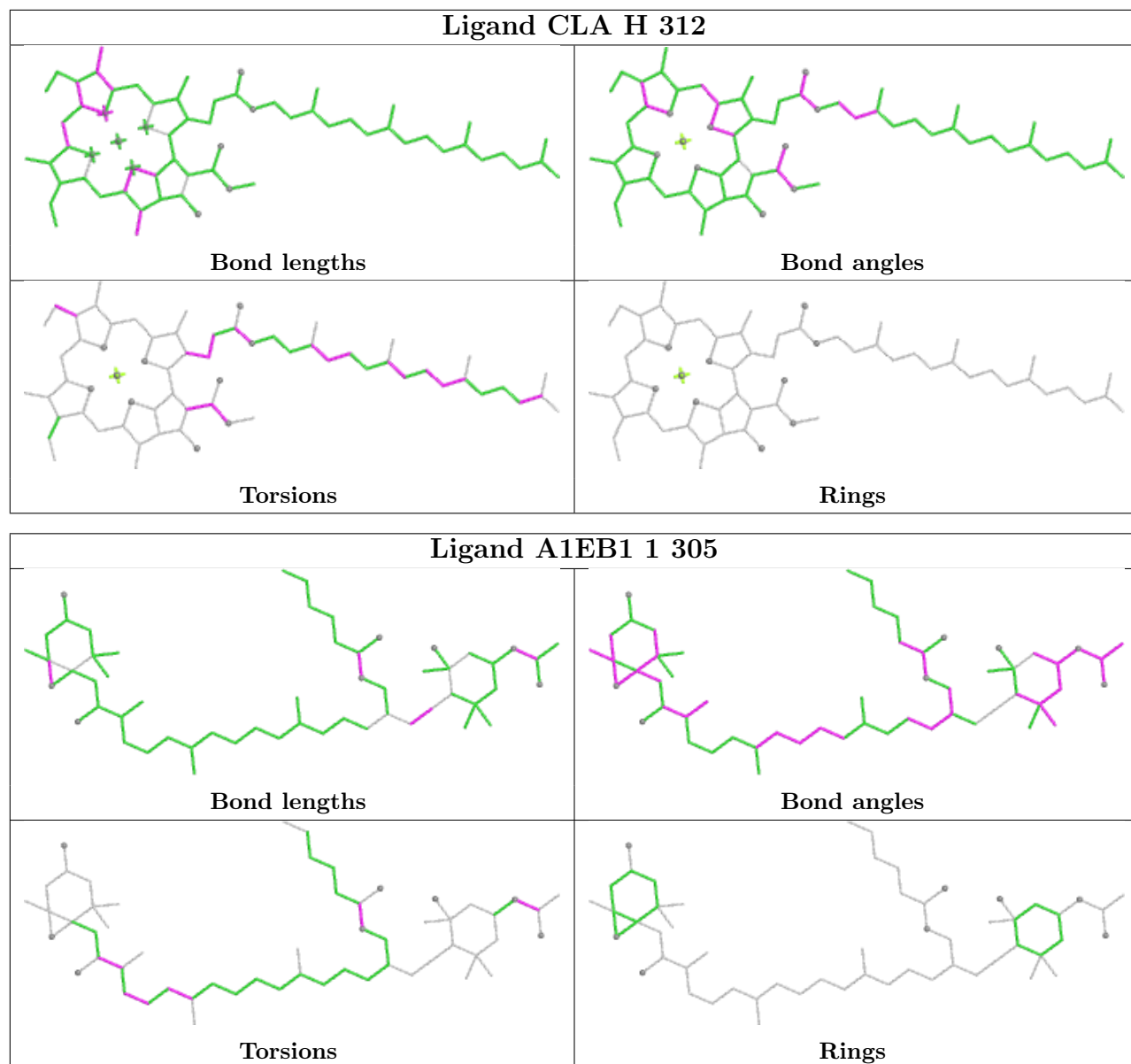


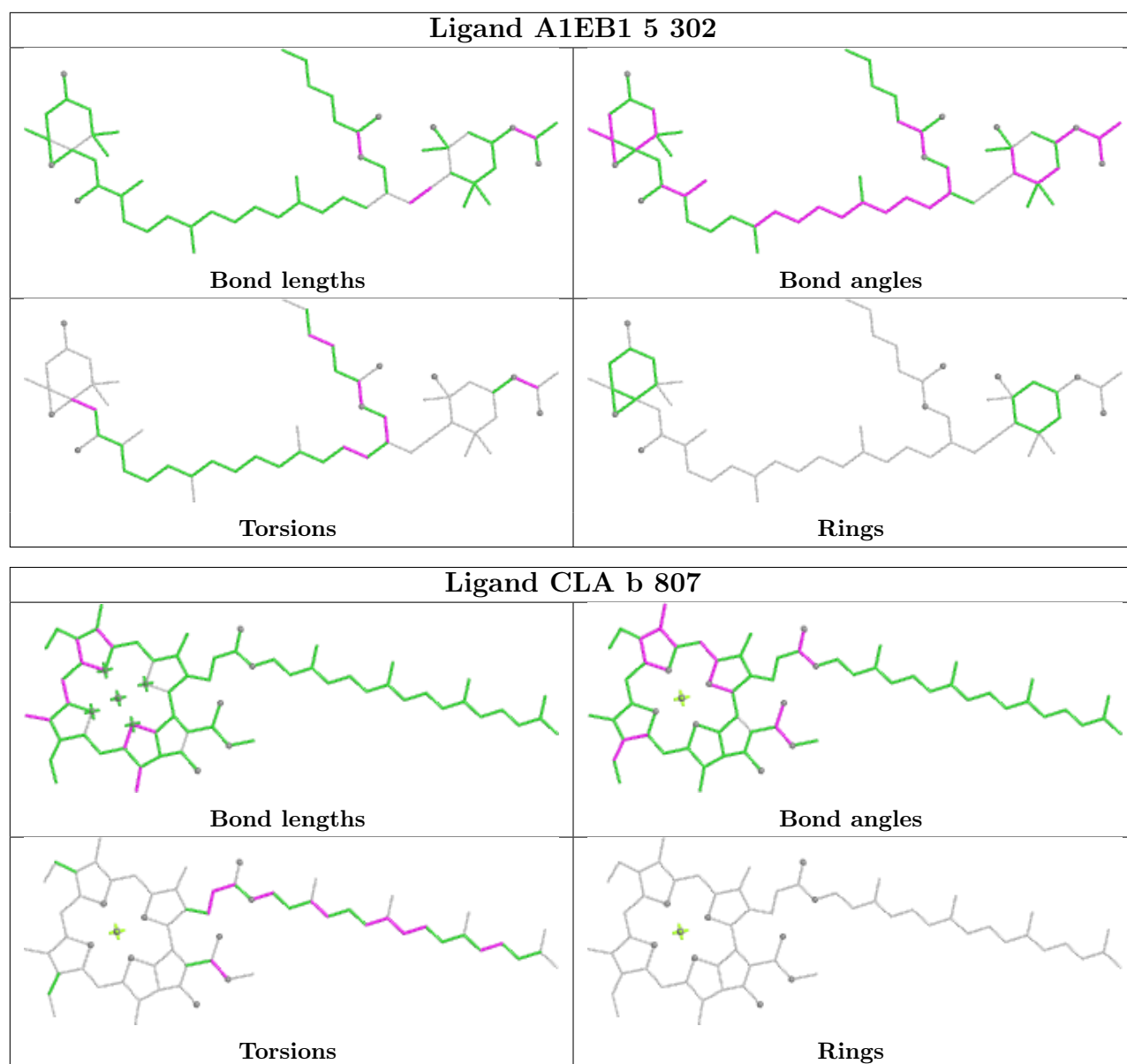
Ligand CLA b 822



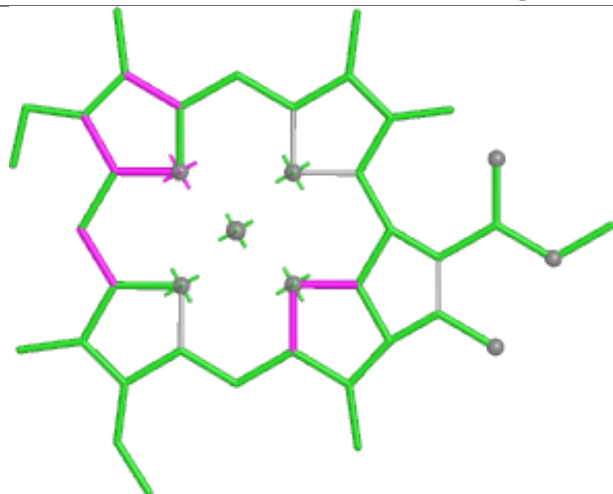
Ligand A86 W 304



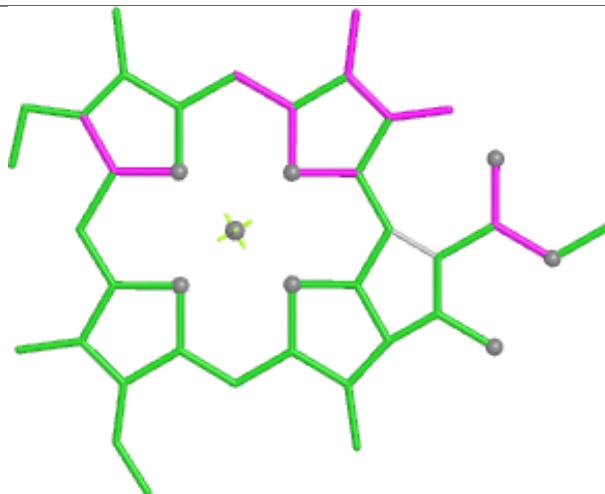




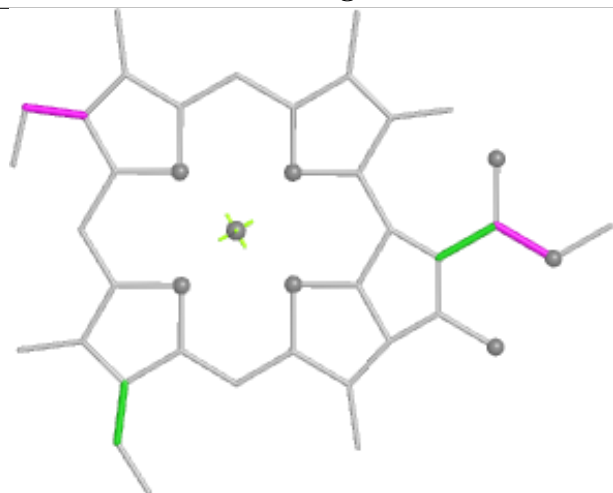
Ligand CLA Y 303



Bond lengths



Bond angles

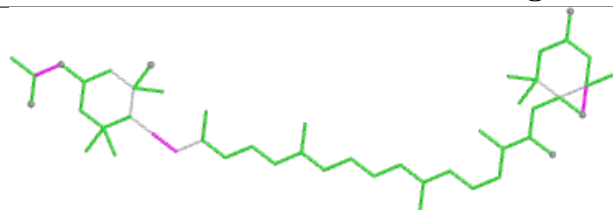


Torsions

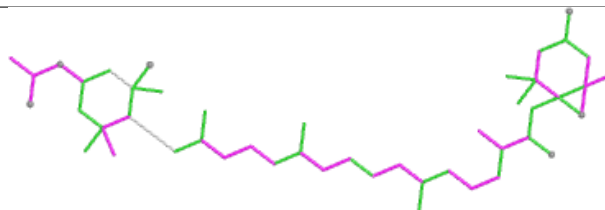


Rings

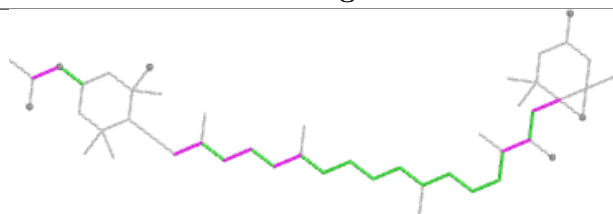
Ligand A86 I 304



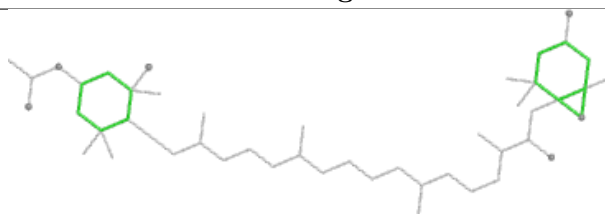
Bond lengths



Bond angles

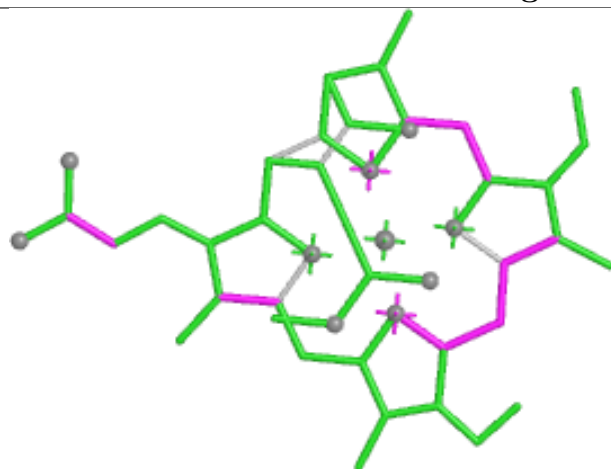


Torsions

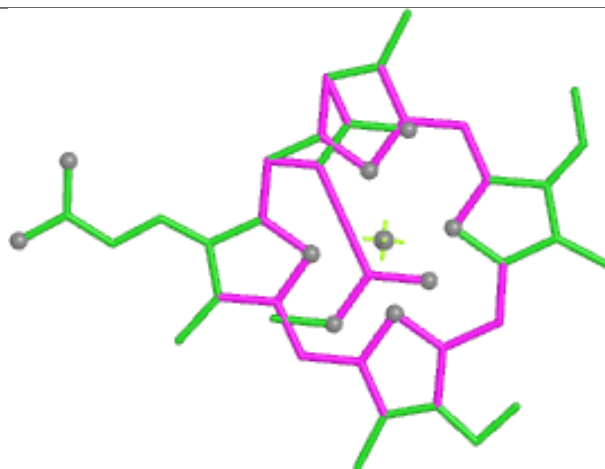


Rings

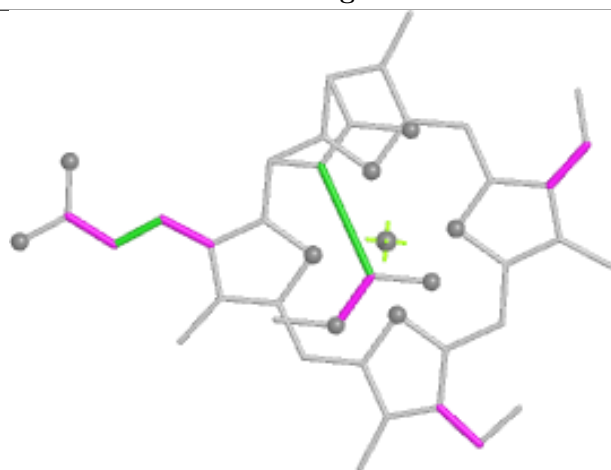
Ligand KC2 z 315



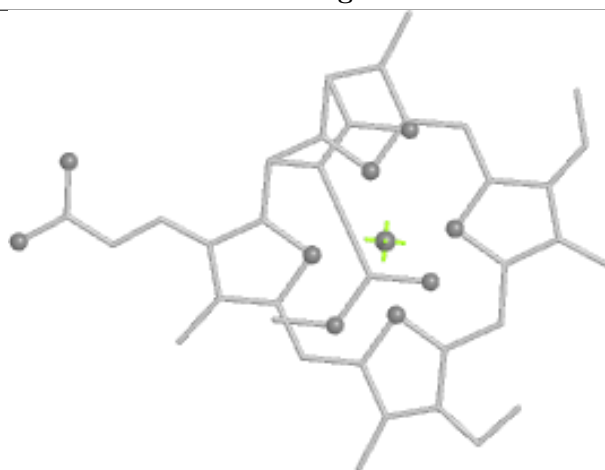
Bond lengths



Bond angles

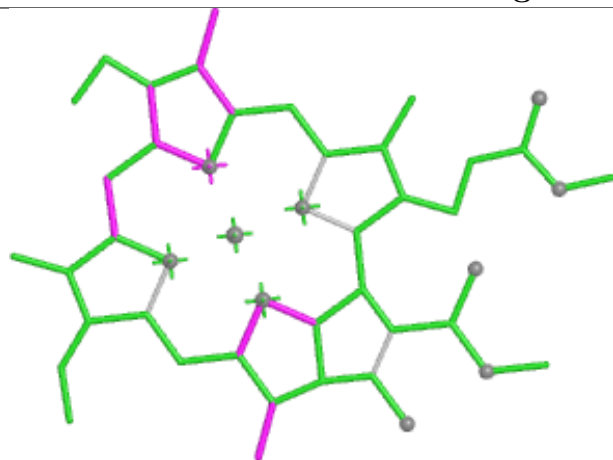


Torsions

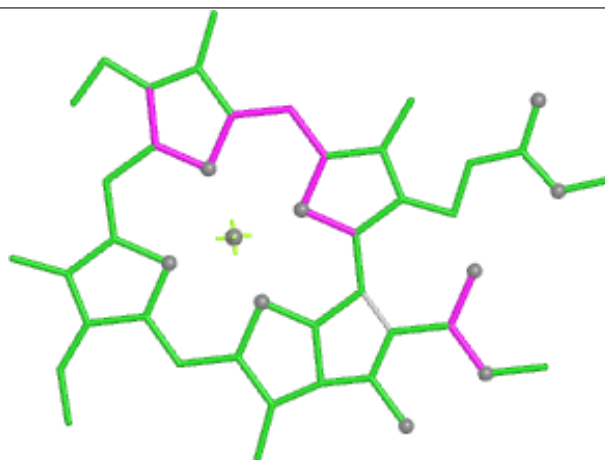


Rings

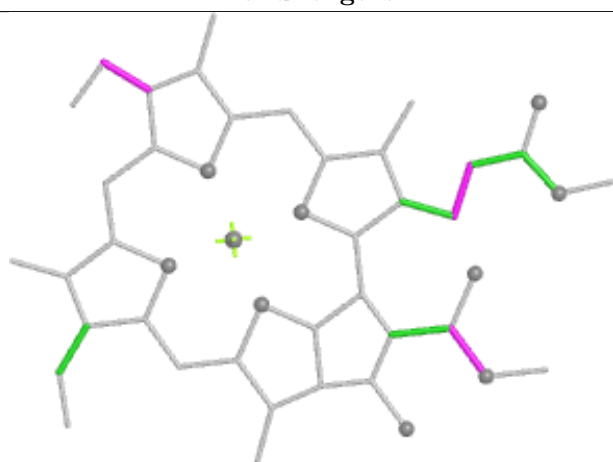
Ligand CLA U 208



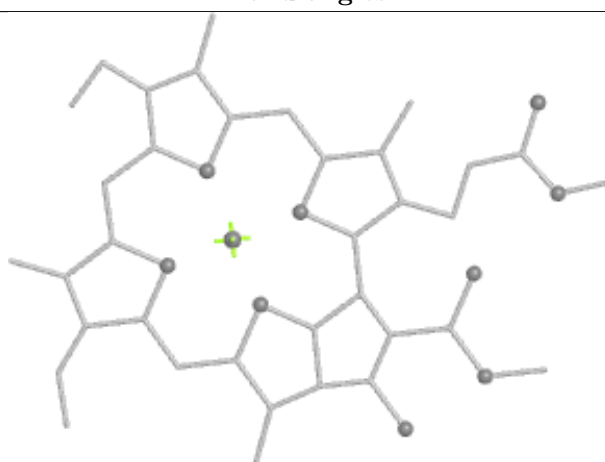
Bond lengths



Bond angles

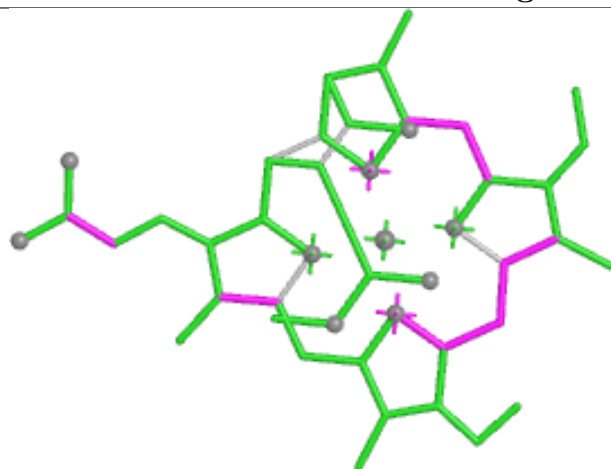


Torsions

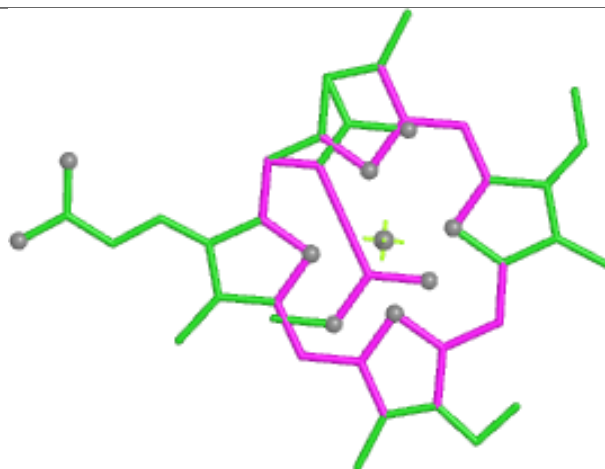


Rings

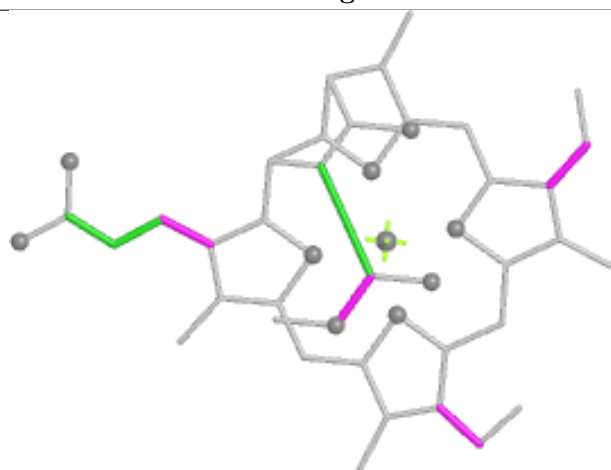
Ligand KC2 P 312



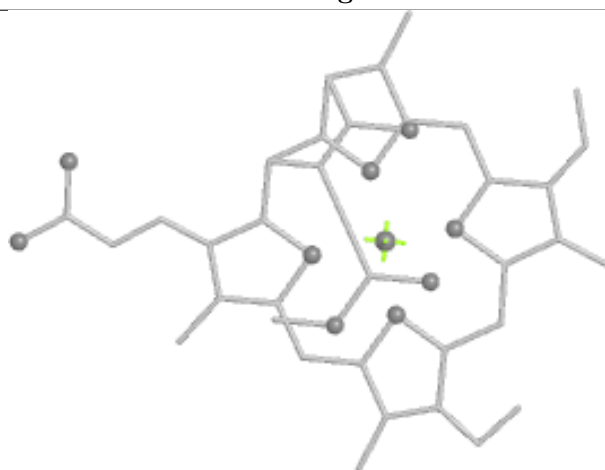
Bond lengths



Bond angles

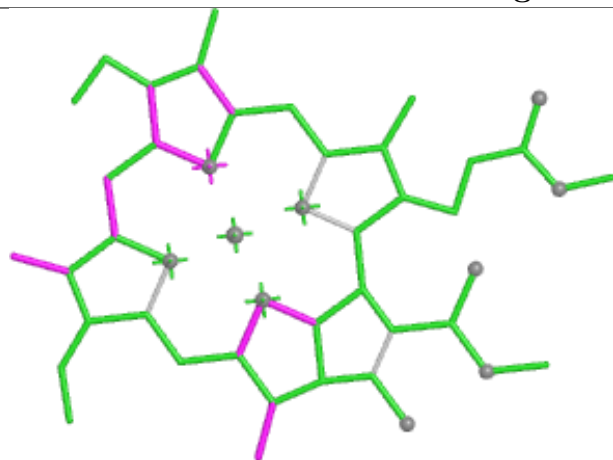


Torsions

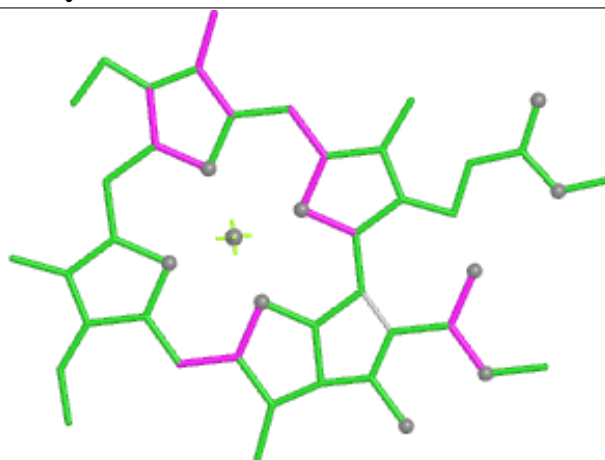


Rings

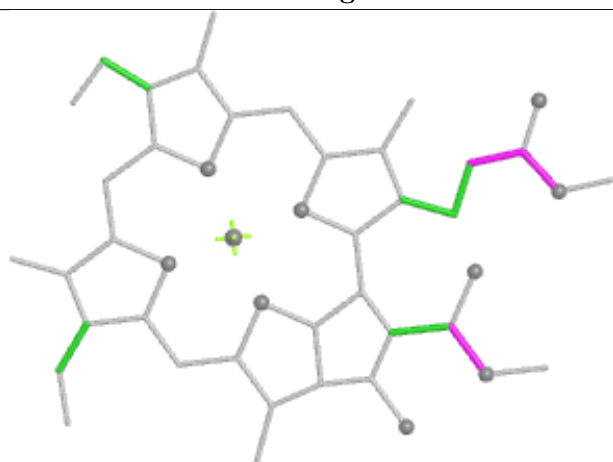
Ligand CLA Q 311



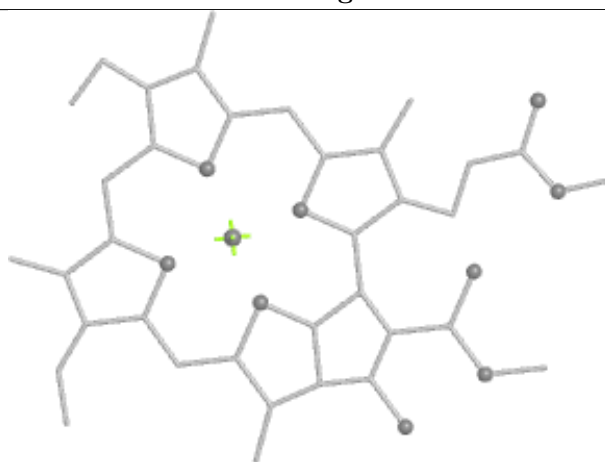
Bond lengths



Bond angles

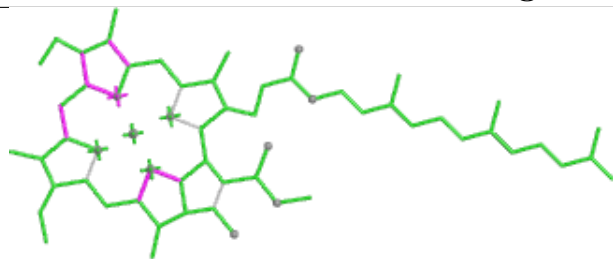


Torsions

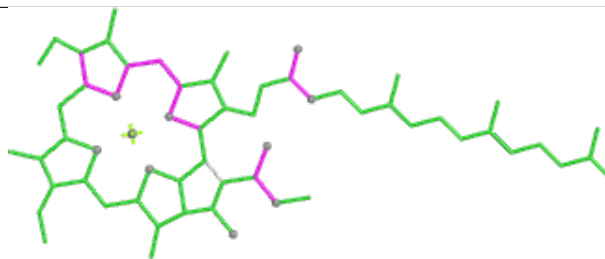


Rings

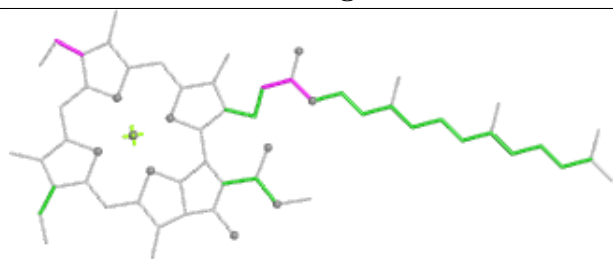
Ligand CLA 5 307



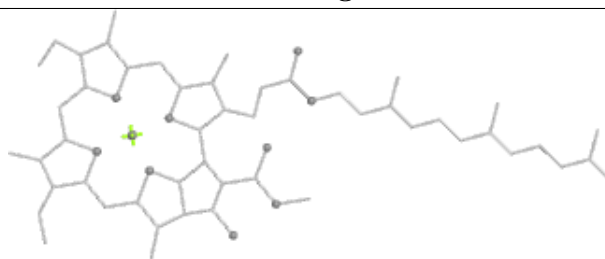
Bond lengths



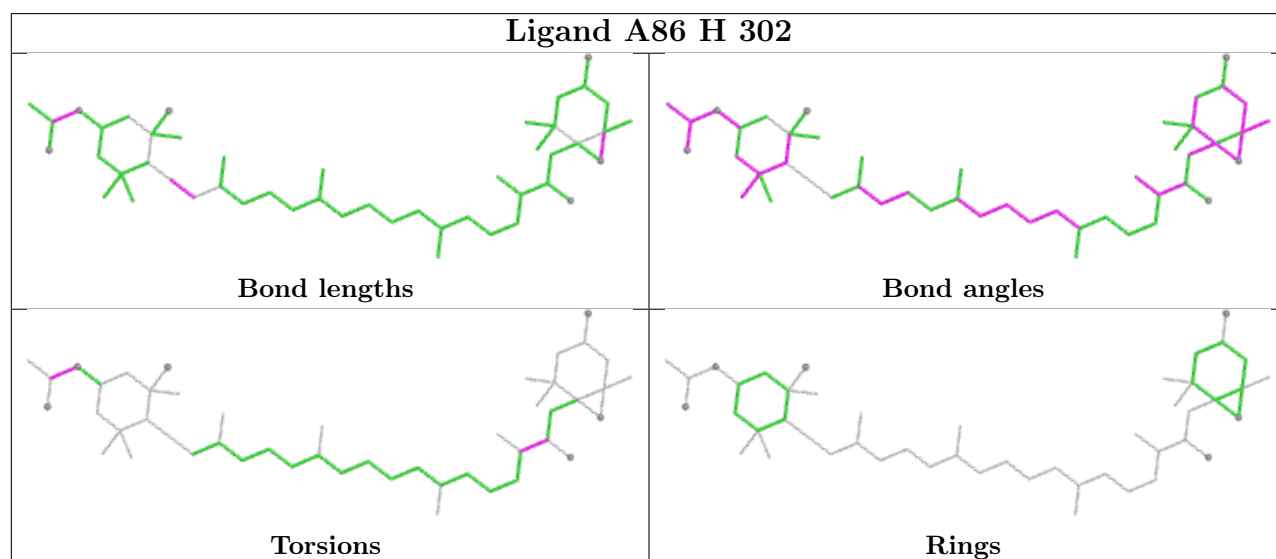
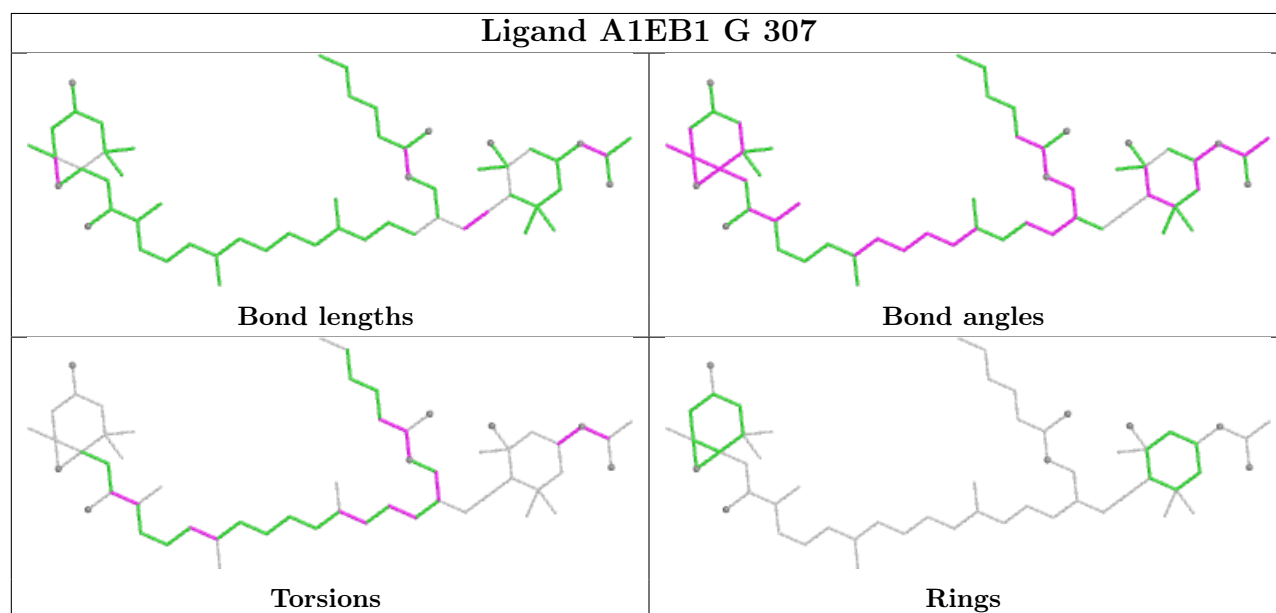
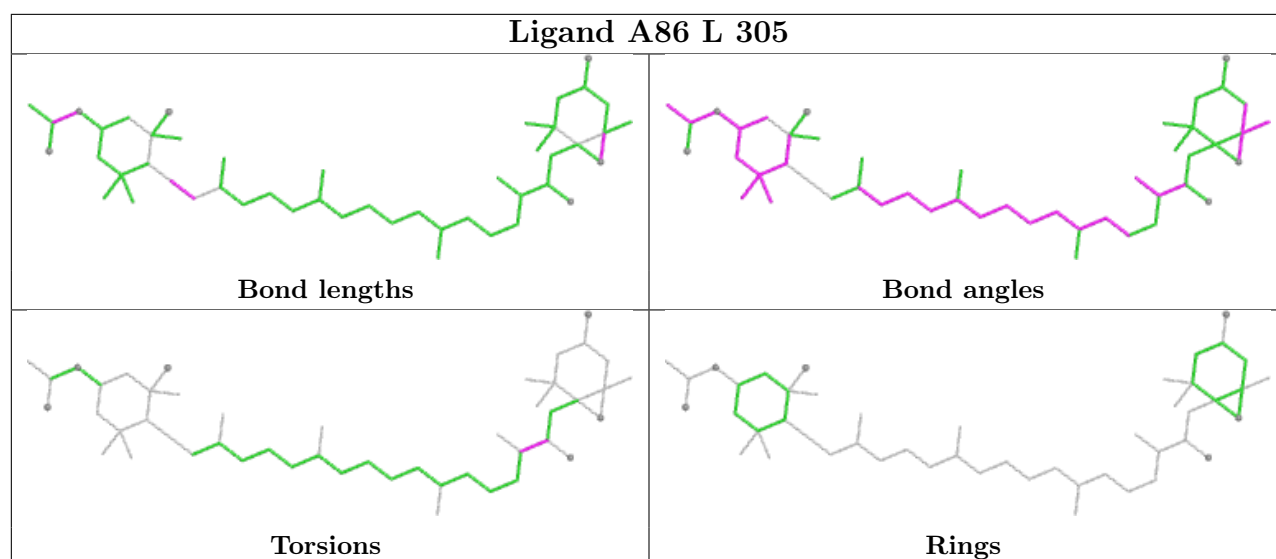
Bond angles

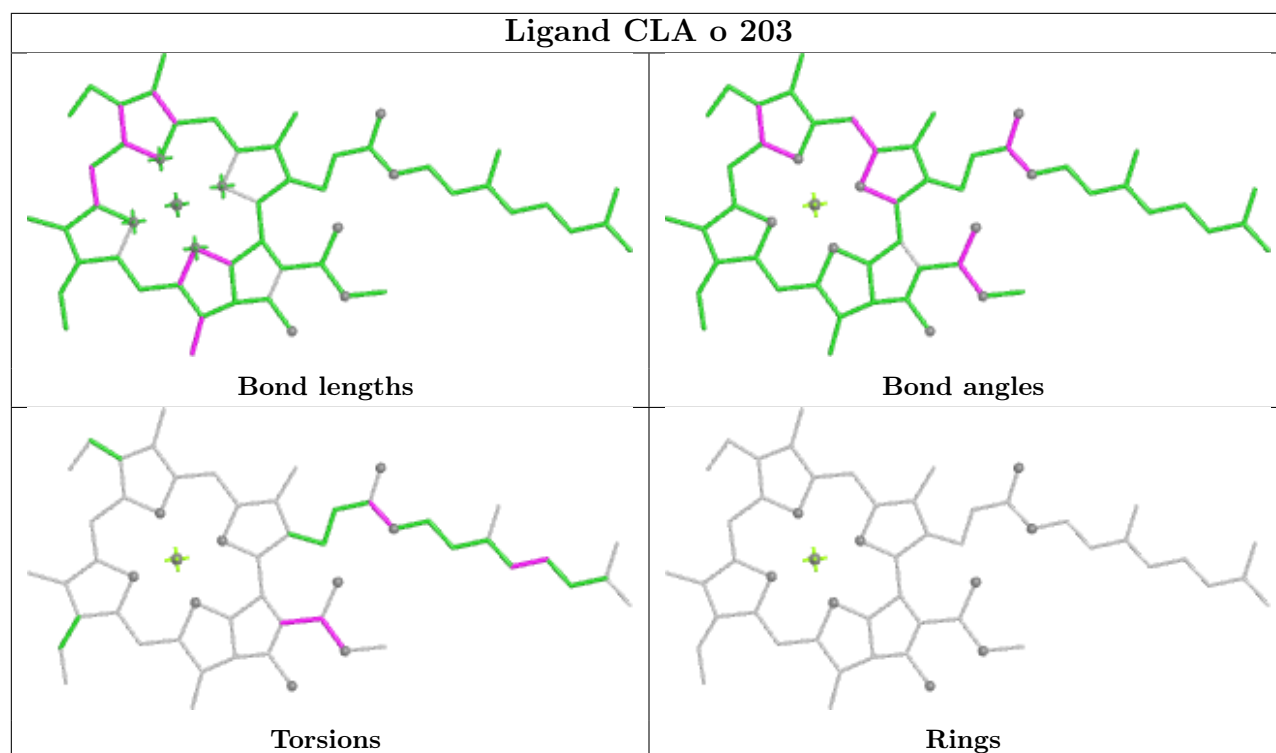
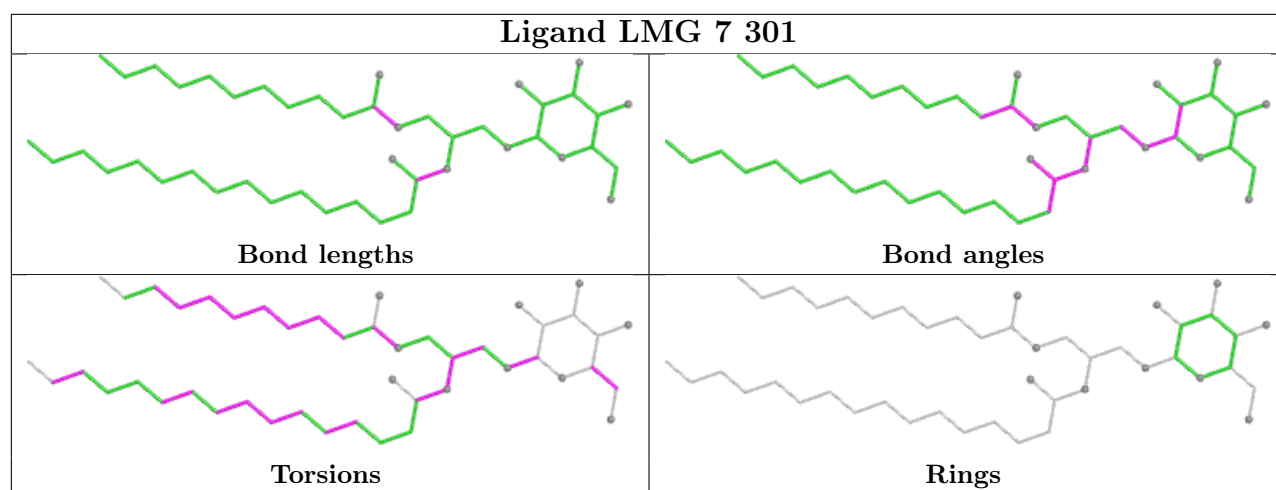


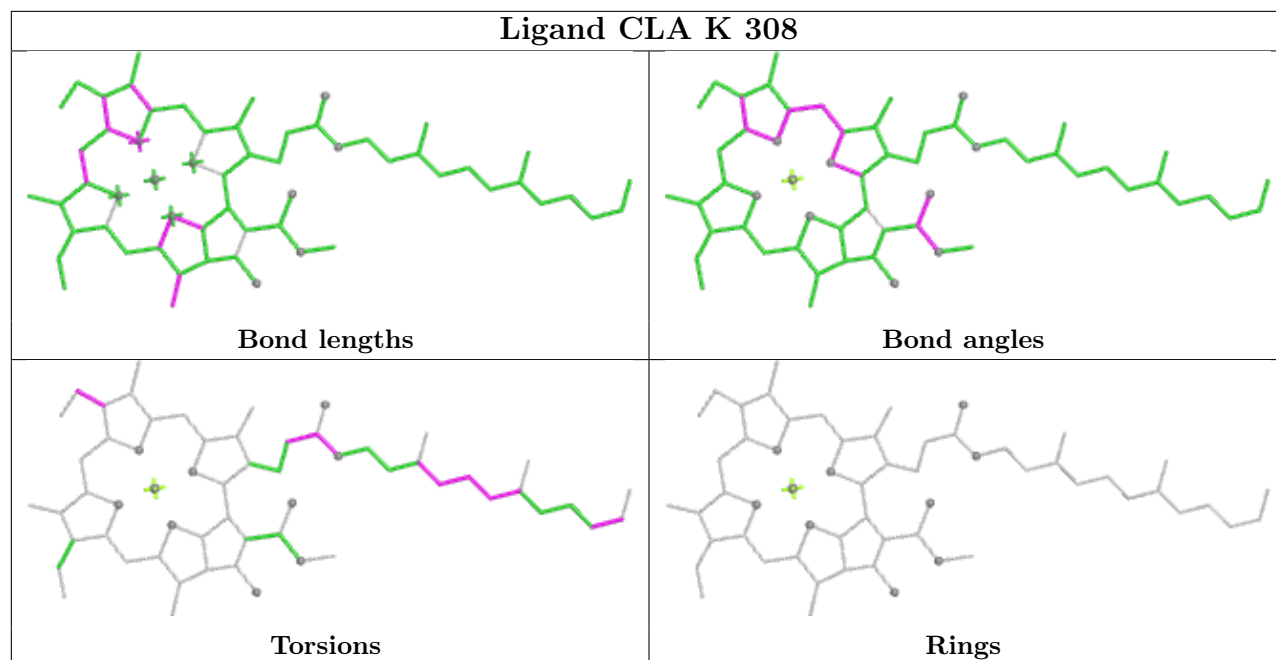
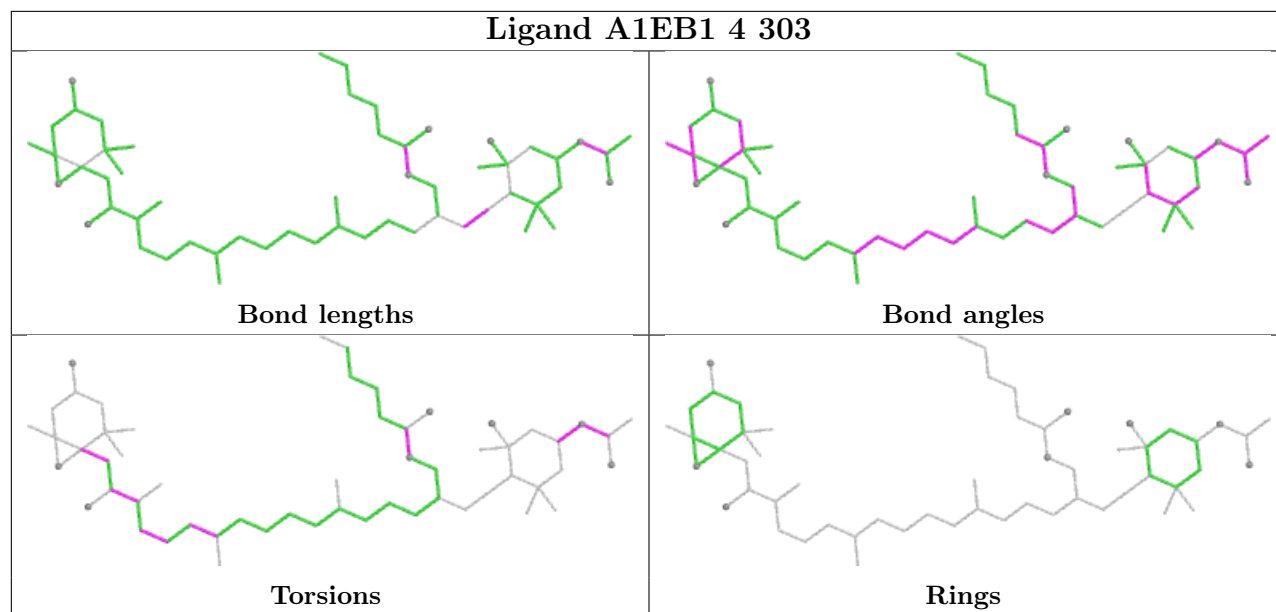
Torsions



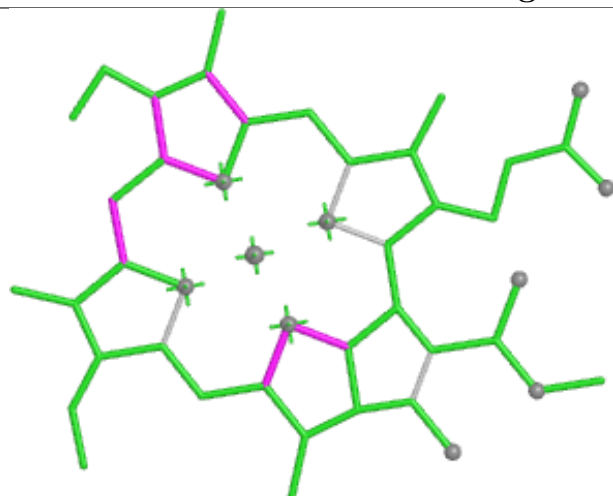
Rings



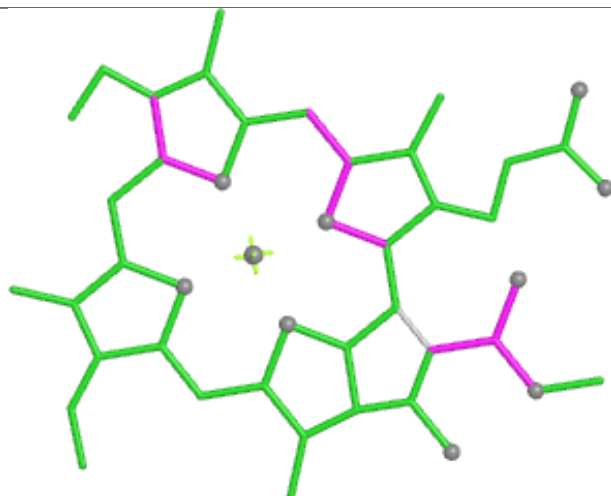


Ligand CLA K 308**Ligand A1EB1 4 303**

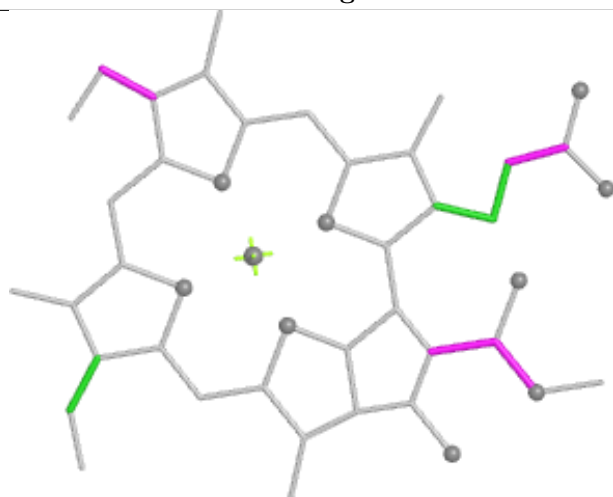
Ligand CLA 0 320



Bond lengths



Bond angles

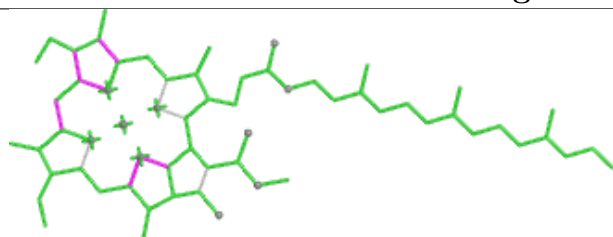


Torsions

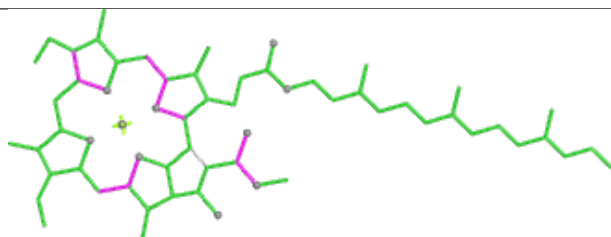


Rings

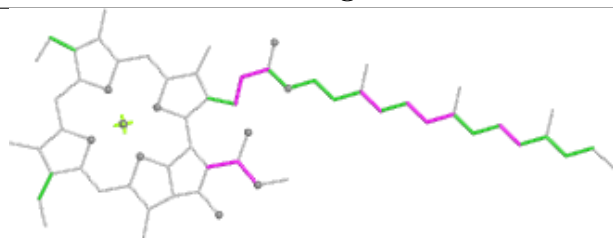
Ligand CLA K 309



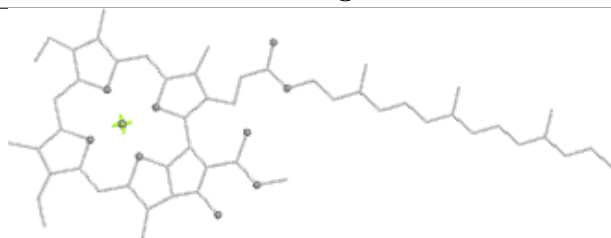
Bond lengths



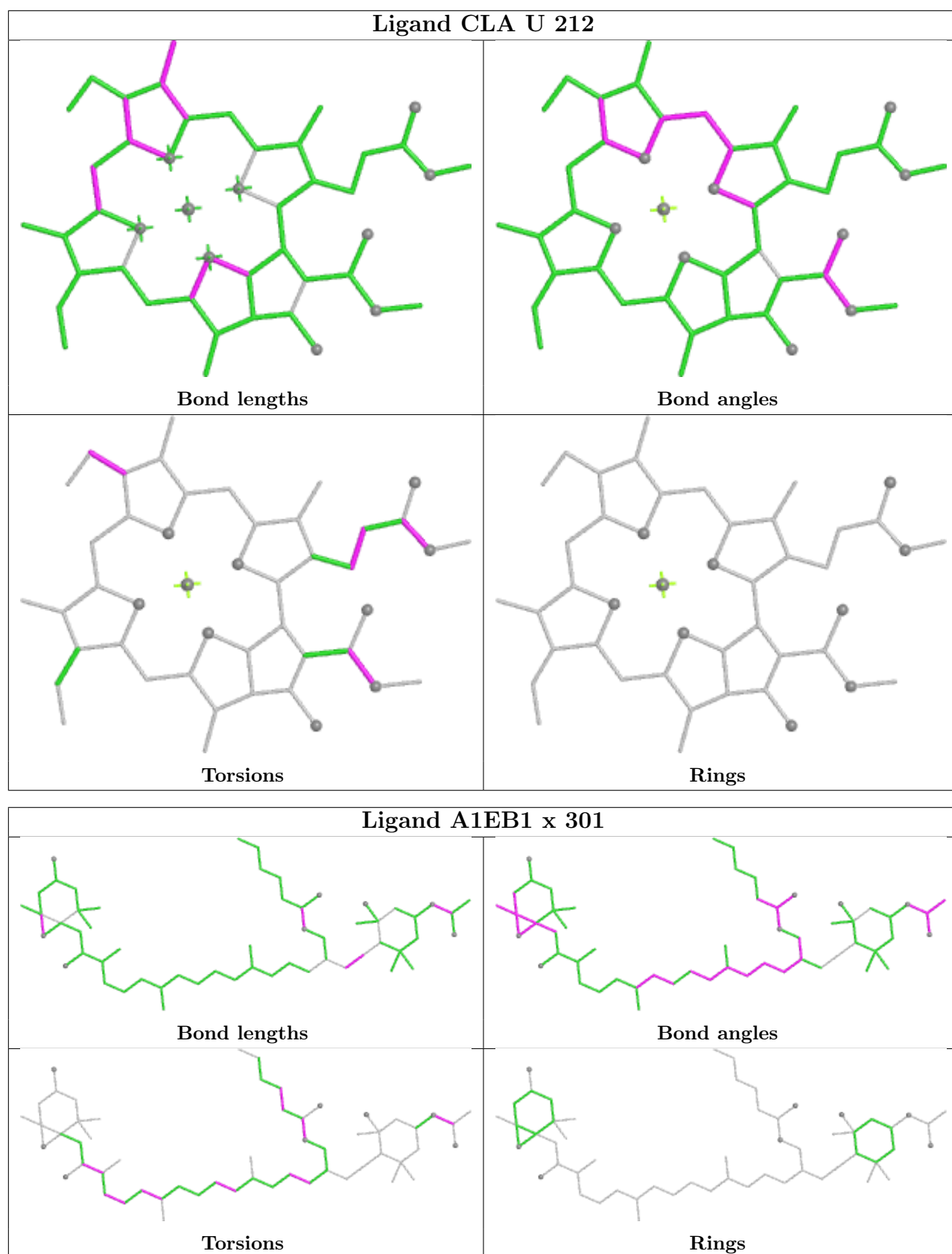
Bond angles

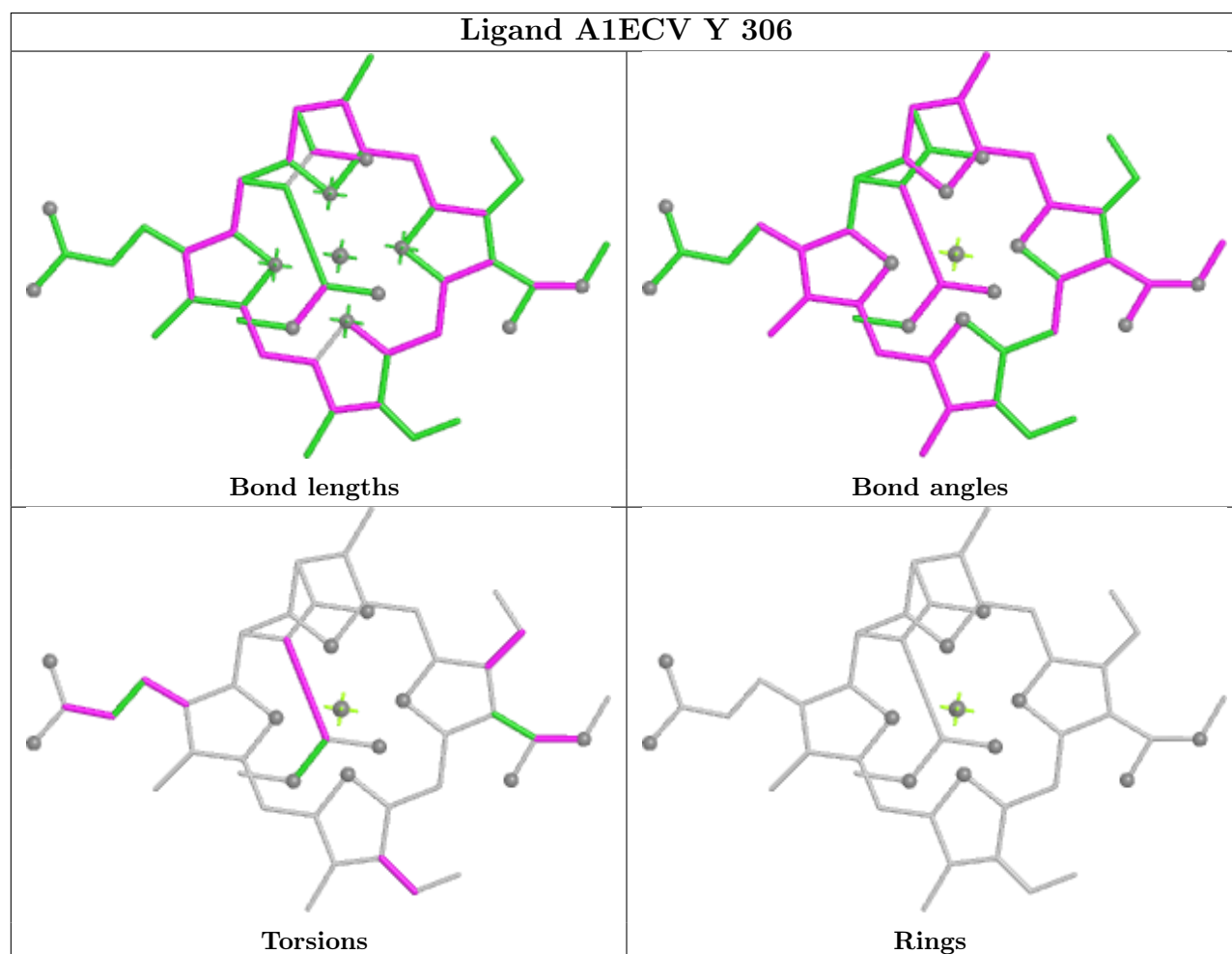
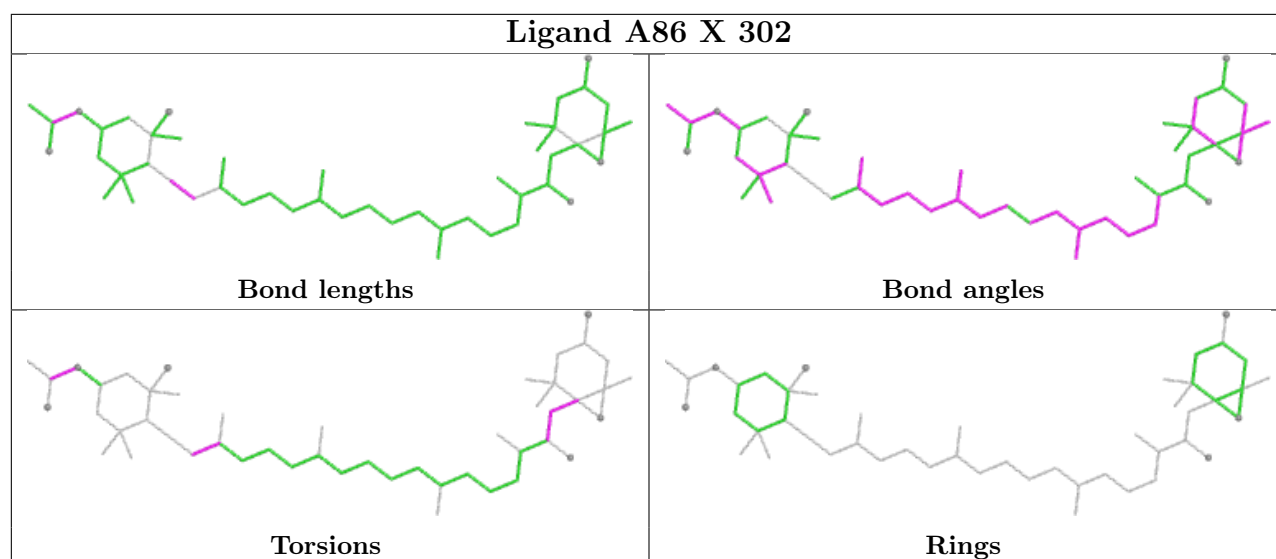


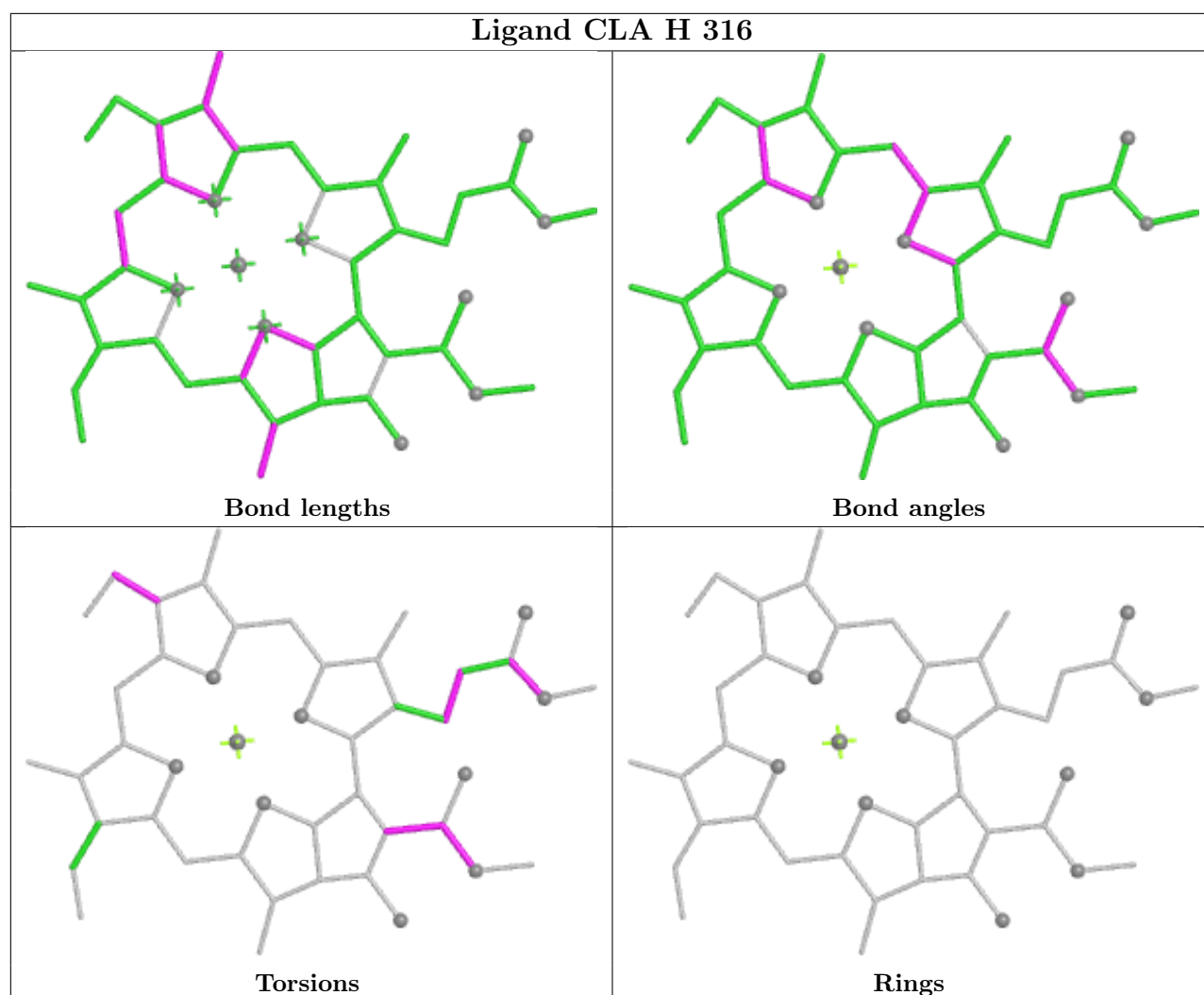
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

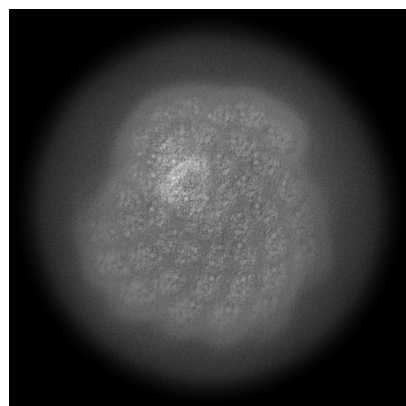
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61519. These allow visual inspection of the internal detail of the map and identification of artifacts.

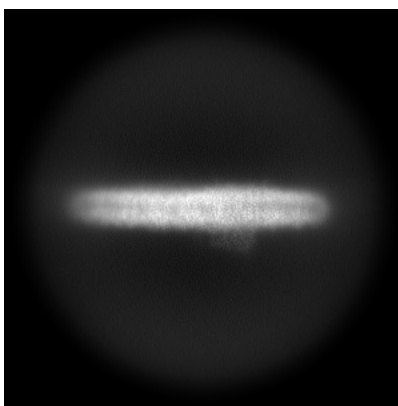
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

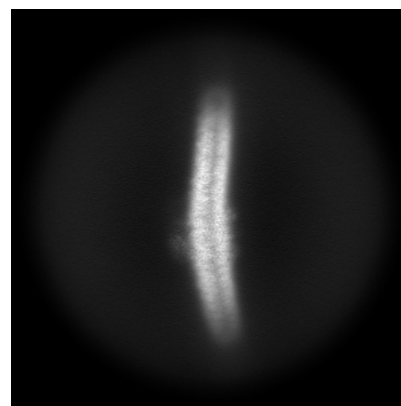
6.1.1 Primary map



X

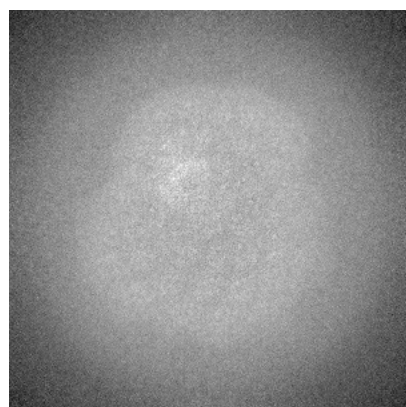


Y

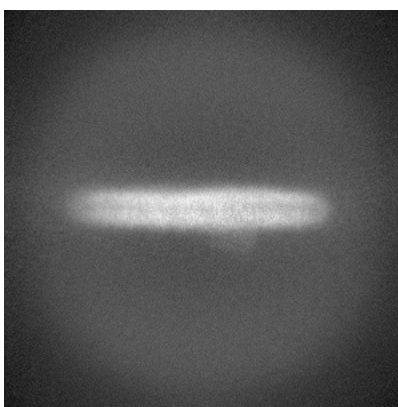


Z

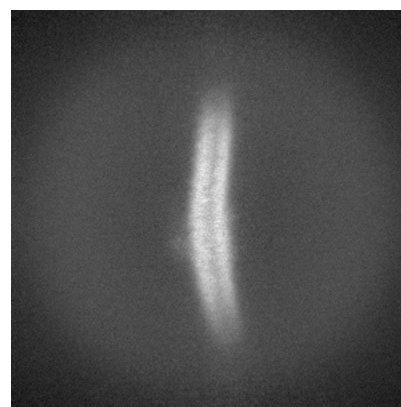
6.1.2 Raw map



X



Y

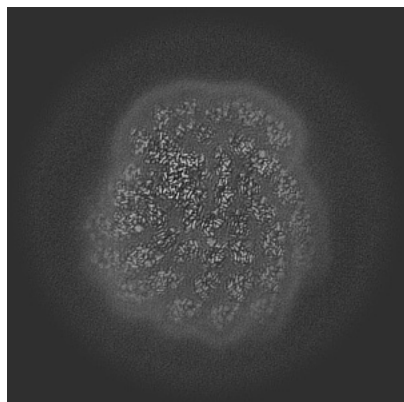


Z

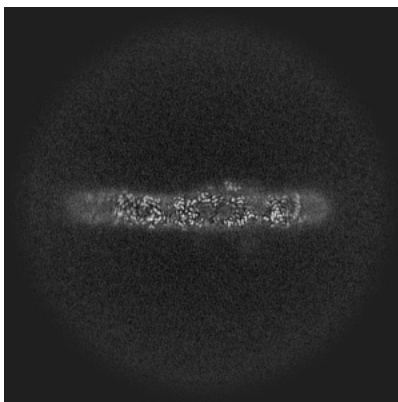
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

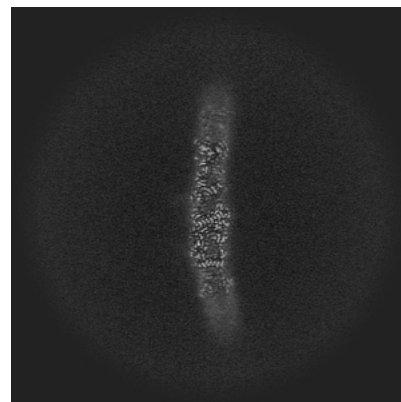
6.2.1 Primary map



X Index: 330

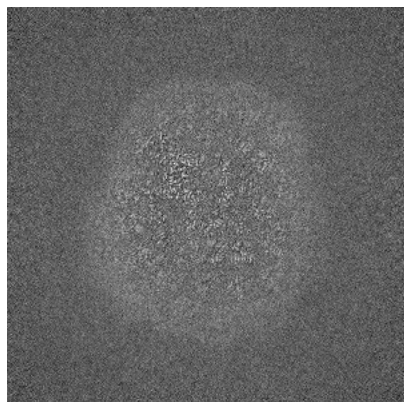


Y Index: 330

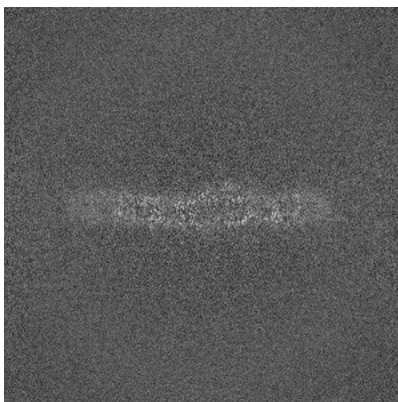


Z Index: 330

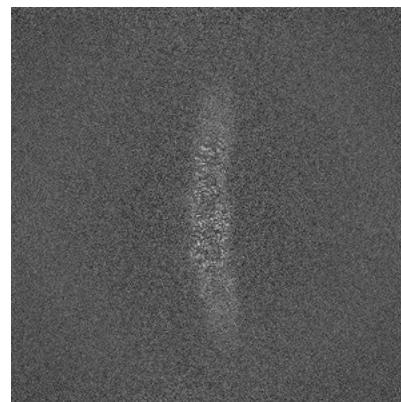
6.2.2 Raw map



X Index: 330



Y Index: 330

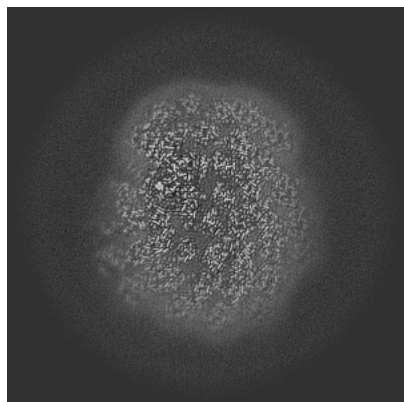


Z Index: 330

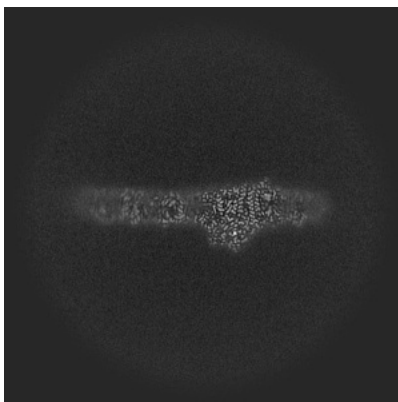
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

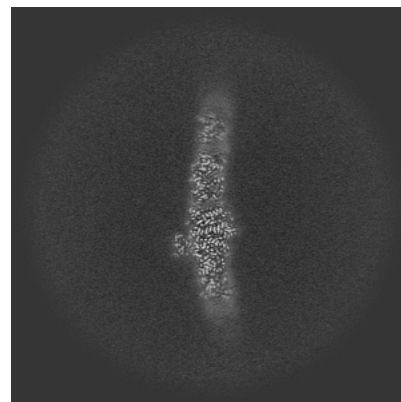
6.3.1 Primary map



X Index: 318

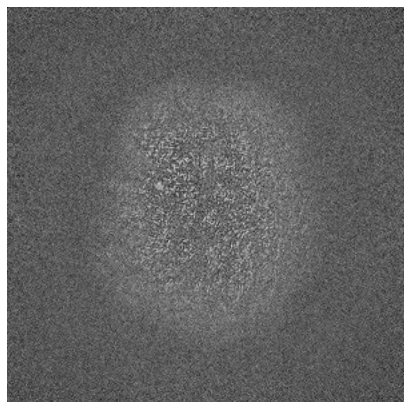


Y Index: 272

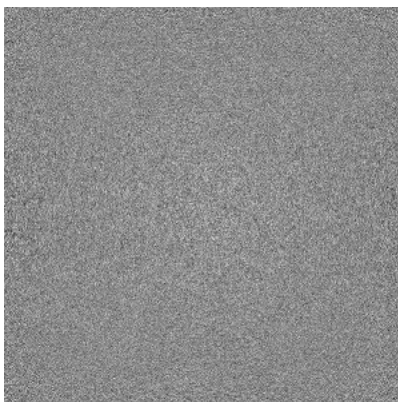


Z Index: 354

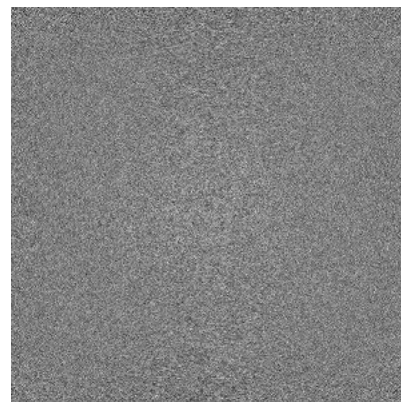
6.3.2 Raw map



X Index: 318



Y Index: 0

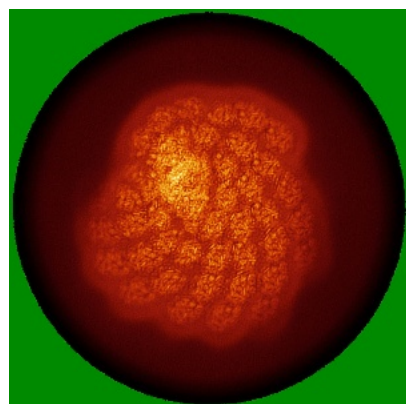


Z Index: 0

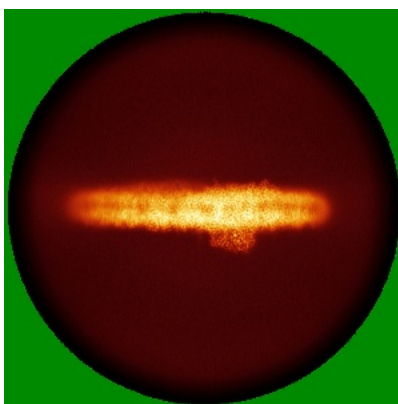
The images above show the largest variance slices of the map in three orthogonal directions.

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

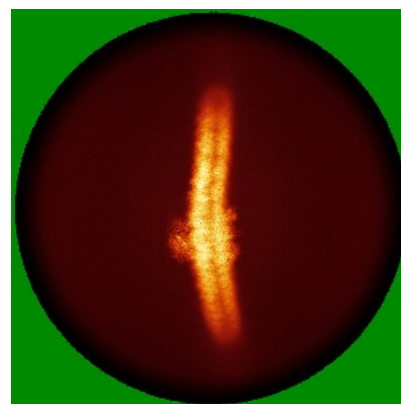
6.4.1 Primary map



X

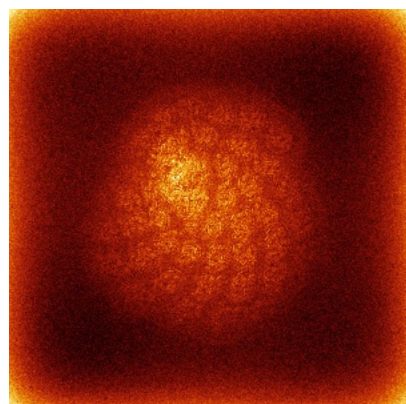


Y

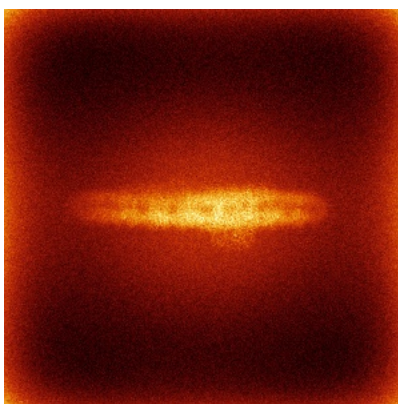


Z

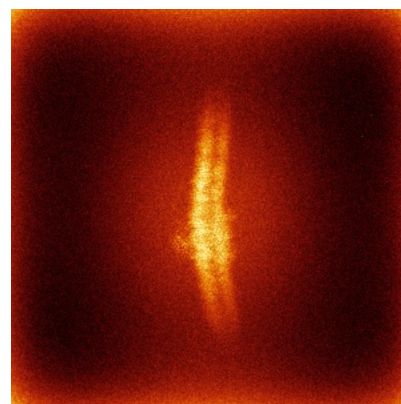
6.4.2 Raw map



X



Y

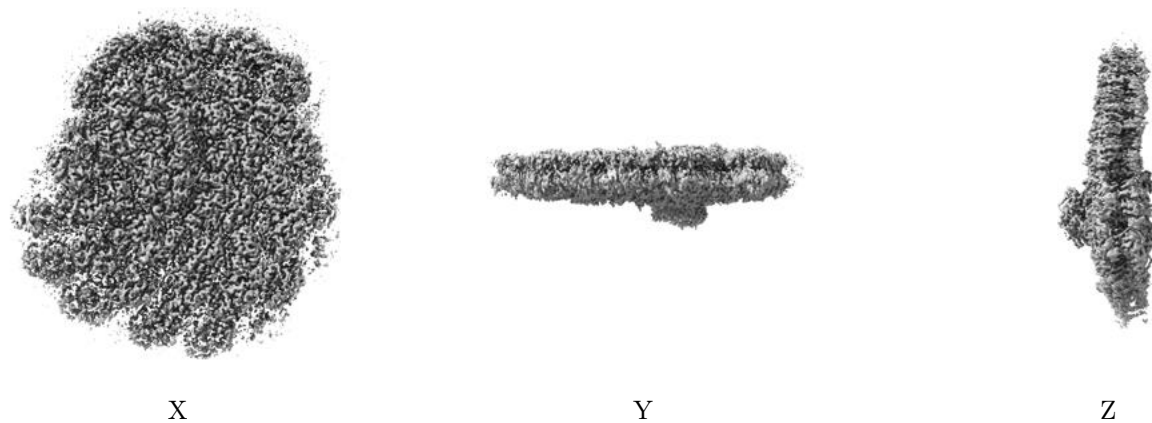


Z

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

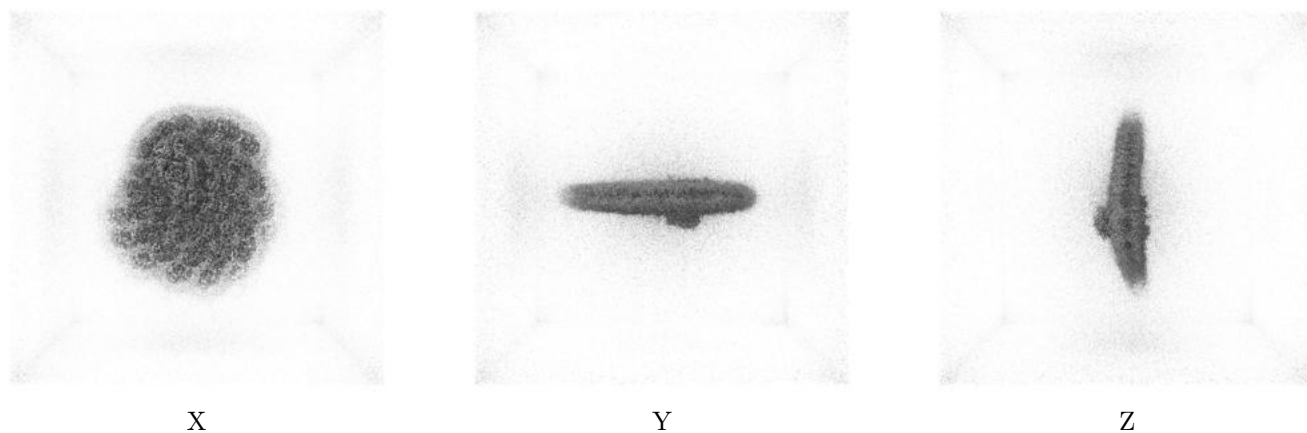
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.066. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

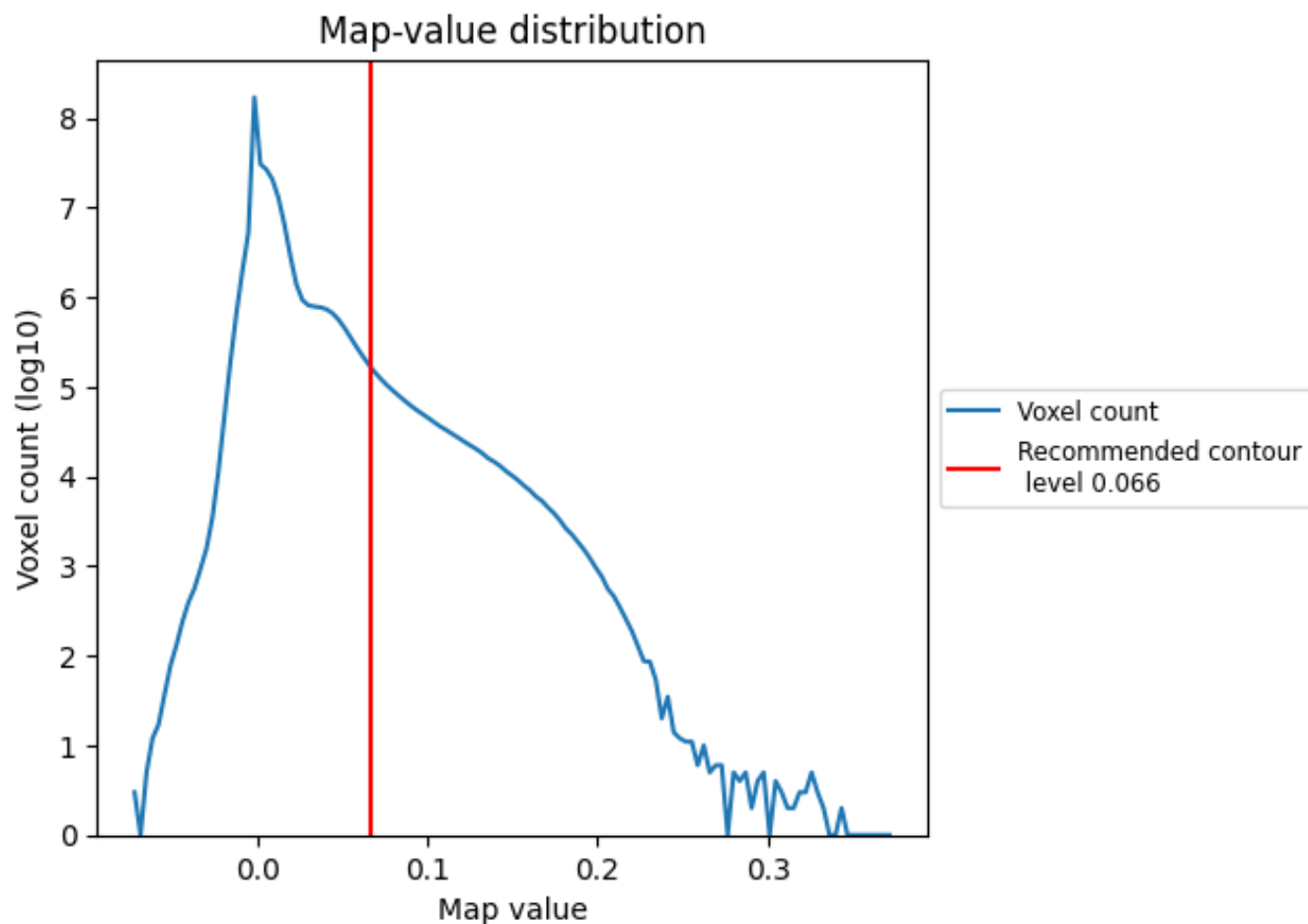
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

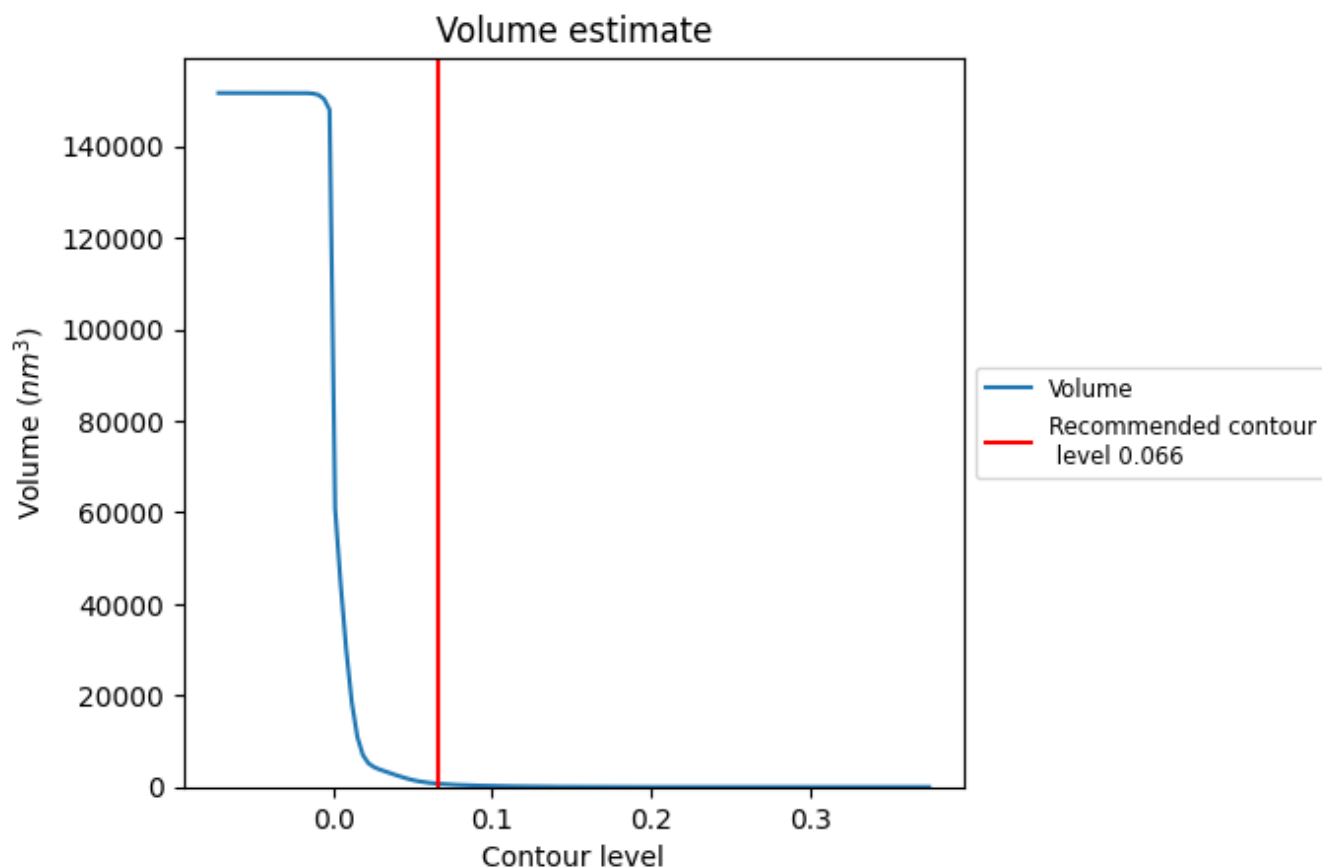
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

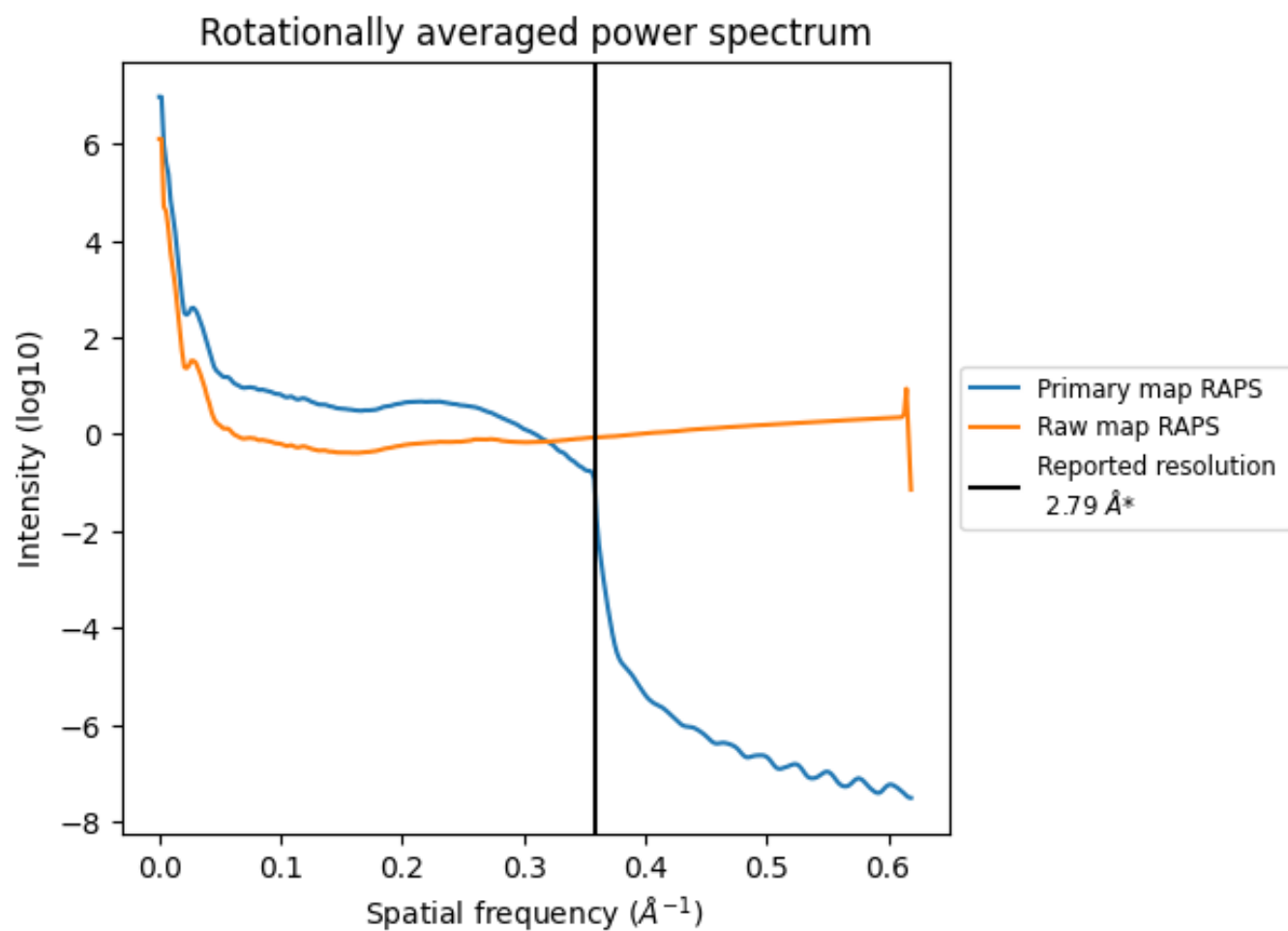
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 712 nm^3 ; this corresponds to an approximate mass of 643 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

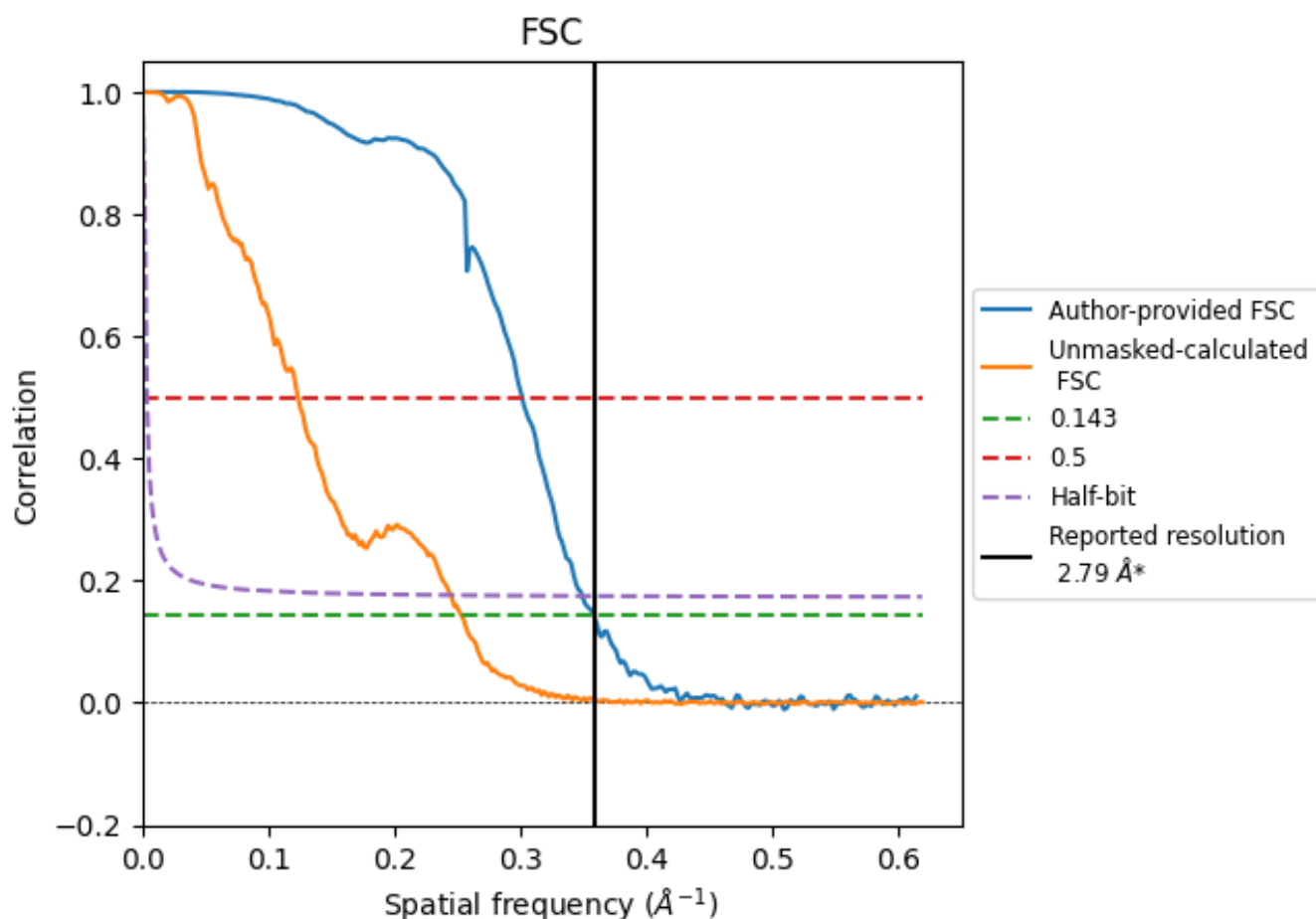


*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

8.2 Resolution estimates [i](#)

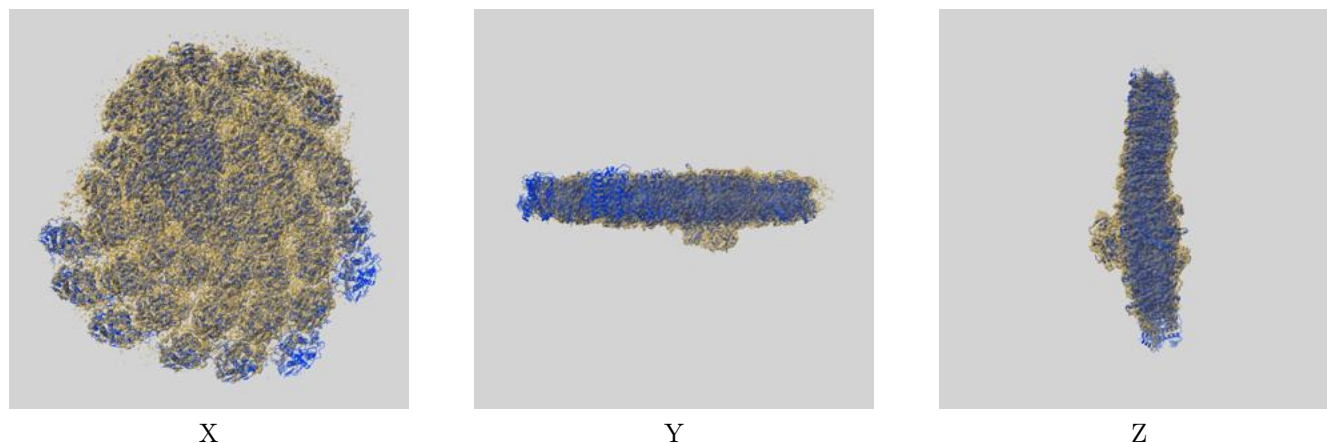
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.32	2.86
Unmasked-calculated*	3.95	8.10	4.08

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

9 Map-model fit [i](#)

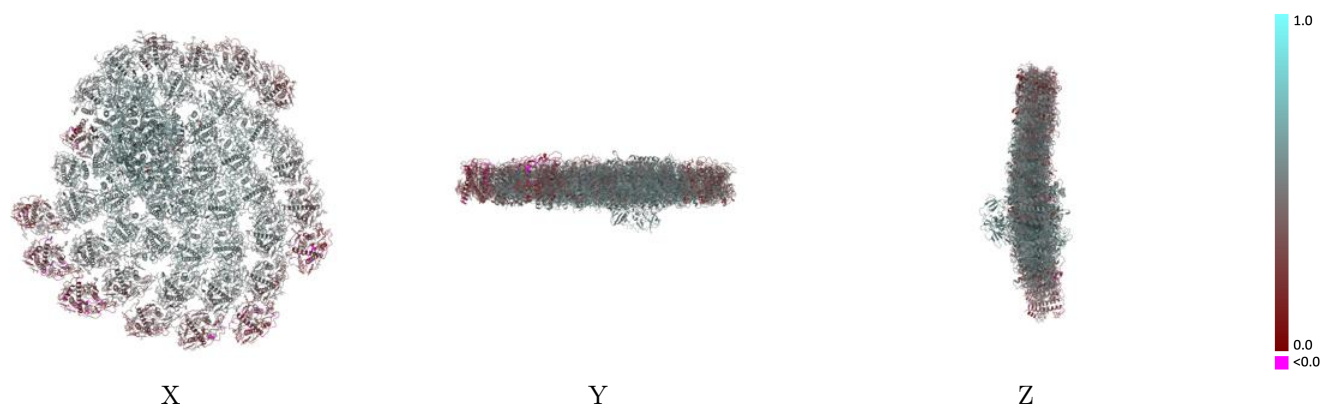
This section contains information regarding the fit between EMDB map EMD-61519 and PDB model 9JJ8. Per-residue inclusion information can be found in section [3](#) on page [62](#).

9.1 Map-model overlay [i](#)



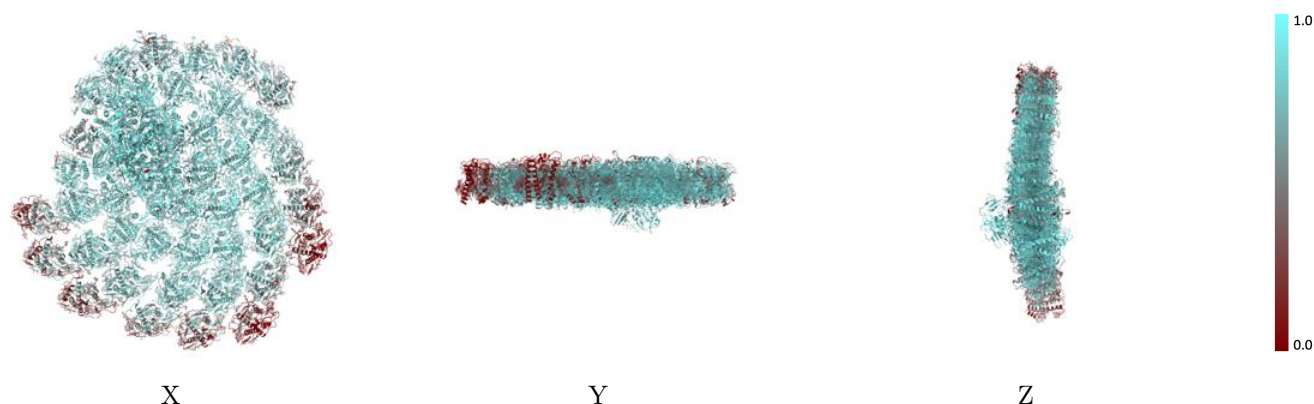
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



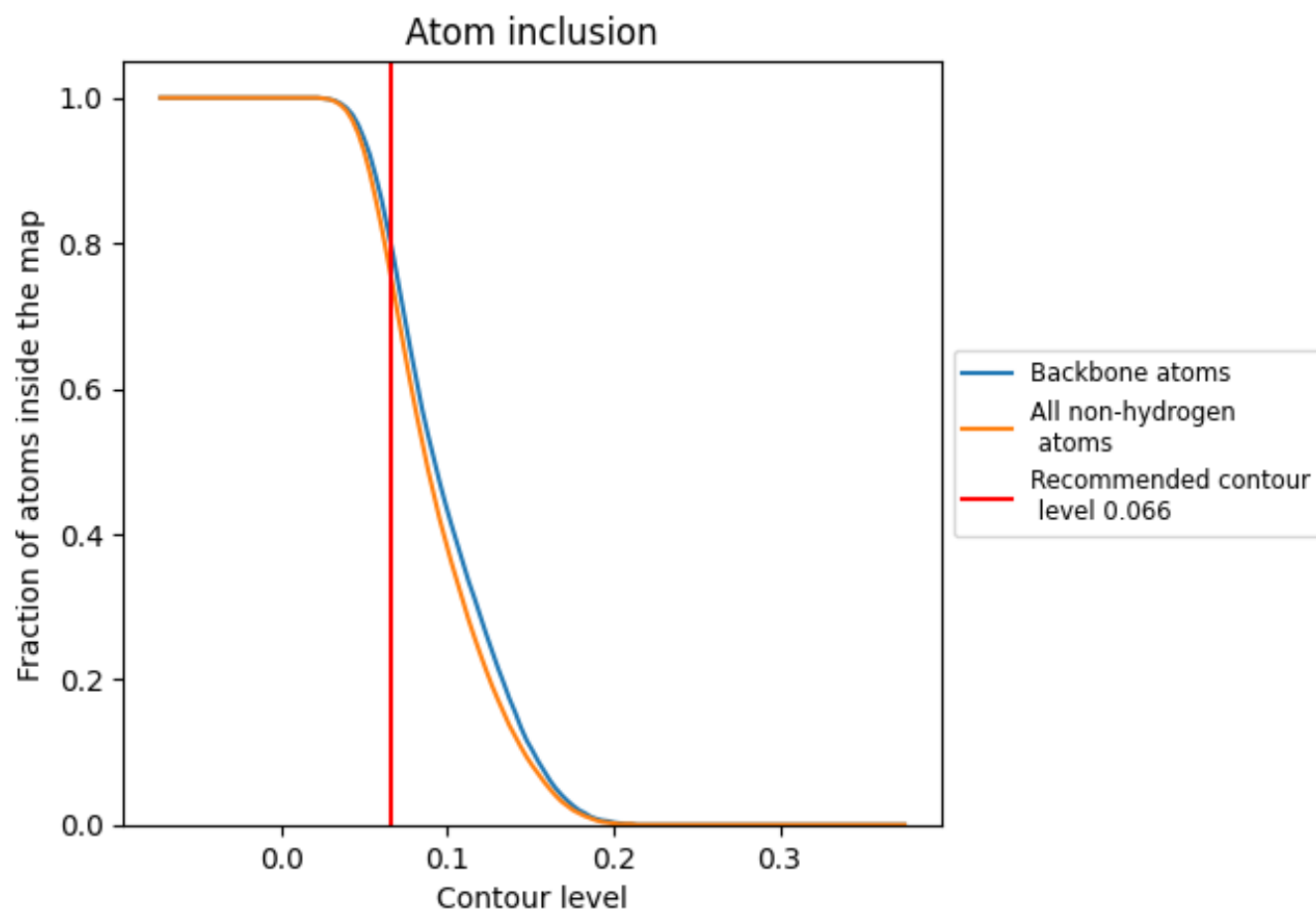
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.066).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.066) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.4970
0	 0.7730	 0.4850
1	 0.5320	 0.3590
2	 0.3860	 0.3210
3	 0.6050	 0.4440
4	 0.7900	 0.5080
5	 0.8680	 0.5370
6	 0.4230	 0.4270
7	 0.6570	 0.4750
8	 0.6230	 0.3800
9	 0.7070	 0.4130
A	 0.8990	 0.5670
B	 0.6160	 0.3650
C	 0.7300	 0.4910
D	 0.9090	 0.5770
E	 0.9140	 0.5810
F	 0.8440	 0.5350
G	 0.8770	 0.5490
H	 0.7460	 0.5100
I	 0.9040	 0.5730
J	 0.6160	 0.4410
K	 0.8850	 0.5630
L	 0.7380	 0.4540
M	 0.9150	 0.5810
O	 0.7290	 0.4320
P	 0.8980	 0.5700
Q	 0.7920	 0.4910
R	 0.8830	 0.5470
S	 0.7930	 0.5050
T	 0.8170	 0.5200
U	 0.7860	 0.5060
V	 0.8500	 0.5200
W	 0.9100	 0.5700
X	 0.8410	 0.5180
Y	 0.0510	 0.2320



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Chain	Atom inclusion	Q-score
Z	 0.0890	 0.2370
a	 0.9340	 0.5960
b	 0.9310	 0.5920
c	 0.9500	 0.5810
d	 0.8370	 0.5680
e	 0.8070	 0.5750
f	 0.8570	 0.5590
h	 0.8640	 0.5510
i	 0.9040	 0.5730
j	 0.9040	 0.5690
k	 0.8880	 0.5540
l	 0.9100	 0.5760
m	 0.8620	 0.5300
o	 0.7770	 0.5290
x	 0.3510	 0.2530
y	 0.4260	 0.2940
z	 0.3600	 0.3220