



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 08:00 AM JST

PDB ID : 9UEN / pdb_00009uen
EMDB ID : EMD-64087
Title : Cryo-EM structure of coccolithophore photosystem I
Authors : Zhao, L.S.; Sun, X.M.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2025-04-08
Resolution : 3.10 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:

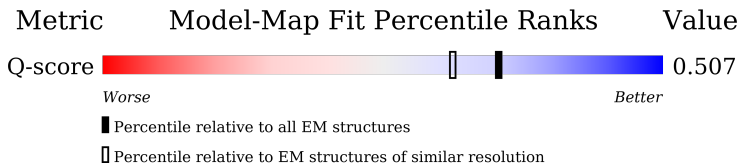
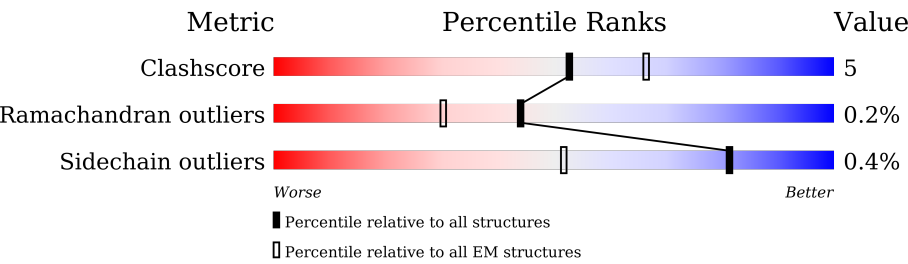
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	201	
2	B	219	
3	C	208	
4	D	255	

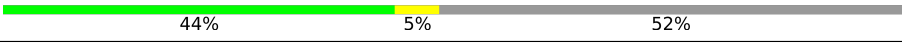
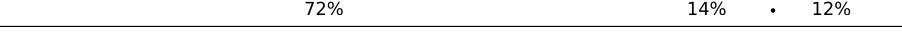
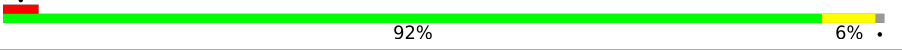
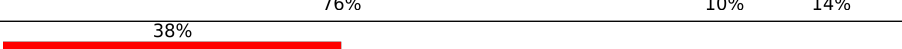
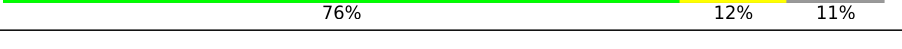
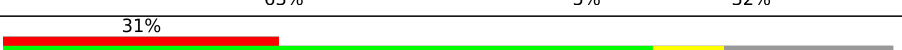
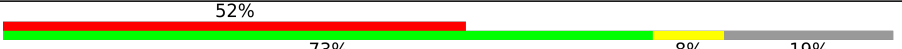
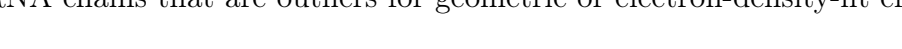
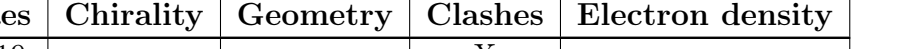
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Mol	Chain	Length	Quality of chain
5	E	217	
6	F	239	
7	G	198	
8	H	199	
9	I	196	
10	J	208	
11	K	204	
12	L	228	
13	M	224	
13	P	224	
13	W	224	
14	N	225	
15	O	210	
15	R	210	
15	T	210	
16	Q	187	
17	S	245	
18	U	198	
19	V	123	
20	X	253	
21	Y	244	
22	Z	254	
23	a	752	
24	b	734	
25	c	81	

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Mol	Chain	Length	Quality of chain
26	d	142	
27	e	131	
28	f	184	
29	i	36	
30	j	40	
31	k	112	
32	l	145	
33	m	30	
34	o	273	
35	p	255	
35	u	255	
35	x	255	
36	q	268	
36	v	268	
37	r	133	
38	t	260	
38	w	260	
38	y	260	
39	z	257	

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
40	CLA	a	819	-	-	X	-
42	DD6	P	315	X	-	-	-
42	DD6	t	312	-	-	X	-
42	DD6	w	312	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 110086 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 Light harvesting protein.

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

- Molecule 2 is a protein called EFCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	148	Total	C	N	O	S	0	0
			1108	711	186	205	6		

- Molecule 3 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	178	Total	C	N	O	S	0	0
			1352	874	225	244	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	103	ALA	VAL	conflict	UNP A0A6V2SE28
C	104	GLU	ASP	conflict	UNP A0A6V2SE28

- Molecule 4 is a protein called EFCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	188	Total	C	N	O	S	1	0
			1446	943	232	265	6		

- Molecule 5 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	187	Total	C	N	O	S	0	0
			1383	896	222	257	8		

- Molecule 6 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	188	Total	C	N	O	S	0	0
			1414	909	244	252	9		

- Molecule 7 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	168	Total	C	N	O	S	0	0
			1248	803	206	231	8		

- Molecule 8 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	S	0	0
			1251	802	205	232	12		

- Molecule 9 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	155	Total	C	N	O	S	0	0
			1195	773	199	214	9		

- Molecule 10 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	166	Total	C	N	O	S	0	0
			1231	783	216	225	7		

- Molecule 11 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	171	Total	C	N	O	S	0	0
			1333	868	226	232	7		

- Molecule 12 is a protein called EFCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	189	Total	C	N	O	S	0	0
			1419	927	236	250	6		

- Molecule 13 is a protein called Light harvesting protein.

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

- Molecule 14 is a protein called EFCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	194	Total	C	N	O	S	0	0
			1454	943	245	257	9		

- Molecule 15 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		
15	R	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		
15	T	179	Total	C	N	O	S	0	0
			1325	858	221	240	6		

- Molecule 16 is a protein called EFCPI-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	156	Total	C	N	O	S	0	0
			1192	763	202	219	8		

- Molecule 17 is a protein called EFCPI-22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	210	Total	C	N	O	S	0	0
			1640	1082	264	288	6		

- Molecule 18 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	144	Total	C	N	O	S	0	0
			1130	728	190	206	6		

- Molecule 19 is a protein called LEFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	47	Total	C	N	O	S	0	0
			351	225	59	65	2		

- Molecule 20 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	211	Total	C	N	O	S	0	0
			1643	1069	273	294	7		

- Molecule 21 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	213	Total	C	N	O	S	0	0
			1660	1090	278	284	8		

- Molecule 22 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	219	Total	C	N	O	S	0	0
			1714	1121	279	309	5		

- Molecule 23 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	741	Total	C	N	O	S	0	0
			5832	3815	993	994	30		

- Molecule 24 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	731	Total	C	N	O	S	0	0
			5807	3822	980	984	21		

- Molecule 25 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	80	Total	C	N	O	S	0	0
			597	365	105	116	11		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	63	Total	C	N	O	S	0	0
			493	313	86	93	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	81	ALA	PRO	conflict	UNP R1EZZ6
e	85	THR	PRO	conflict	UNP R1EZZ6

- Molecule 28 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	161	Total	C	N	O	S	0	0
			1238	800	210	224	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	i	31	Total	C	N	O	S	0	0
			243	170	32	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	40	Total	C	N	O	S	0	0
			317	211	47	56	3		

- Molecule 31 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	70	Total	C	N	O	S	0	0
			510	331	83	90	6		

- Molecule 32 is a protein called Photosystem I reaction center subunit XI.

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

- Molecule 33 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 34 is a protein called EFCPI-30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	236	Total	C	N	O	S	0	0
			1760	1142	290	318	10		

- Molecule 35 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
35	u	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		
35	x	228	Total	C	N	O	S	0	0
			1744	1134	290	313	7		

- Molecule 36 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	238	Total	C	N	O	S	0	0
			1790	1163	296	323	8		
36	v	238	Total	C	N	O	S	0	0
			1790	1163	296	323	8		

- Molecule 37 is a protein called Psar.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	91	Total	C	N	O	S	0	0
			681	443	111	126	1		

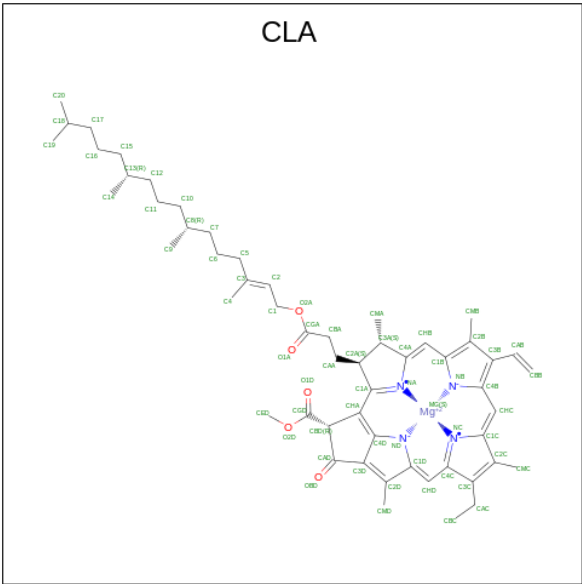
- Molecule 38 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	211	Total	C	N	O	S	0	0
			1631	1057	272	295	7		
38	w	211	Total	C	N	O	S	0	0
			1631	1057	272	295	7		
38	y	201	Total	C	N	O	S	0	0
			1546	1001	261	277	7		

- Molecule 39 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	z	222	Total	C	N	O	S	0	0
			1718	1126	280	307	5		

- Molecule 40 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
40	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	C	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	D	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	D	1	Total 44	C 35	Mg 1	N 4	O 4	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	D	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	E	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	E	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 53	C 43	Mg 1	N 4	O 5	0
40	F	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	F	1	Total 59	C 49	Mg 1	N 4	O 5	0
40	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	G	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	H	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	I	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	I	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	I	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	J	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	K	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	K	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	K	1	Total 59	C 49	Mg 1	N 4	O 5	0
40	K	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	M	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	M	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	M	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	M	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	O	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	O	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	P	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	P	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	P	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Q	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	Q	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	R	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	R	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	S	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	S	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
40	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	U	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	V	1	Total 58	C 48	Mg 1	N 4	O 5	0
40	V	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	X	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	X	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	Z	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	Z	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	Z	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
40	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
40	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
40	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
40	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
40	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	i	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	j	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	k	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	l	1	Total 64	C 54	Mg 1	N 4	O 5	0
40	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	o	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	o	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	o	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	p	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	p	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	q	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	q	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	q	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	q	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	t	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	t	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	t	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	t	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	t	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	t	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	u	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	u	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	u	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	u	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	u	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	u	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	v	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	v	1	Total 52	C 42	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	v	1	Total 63	C 53	Mg 1	N 4	O 5	0
40	v	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	v	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	w	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	w	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	w	1	Total 55	C 45	Mg 1	N 4	O 5	0

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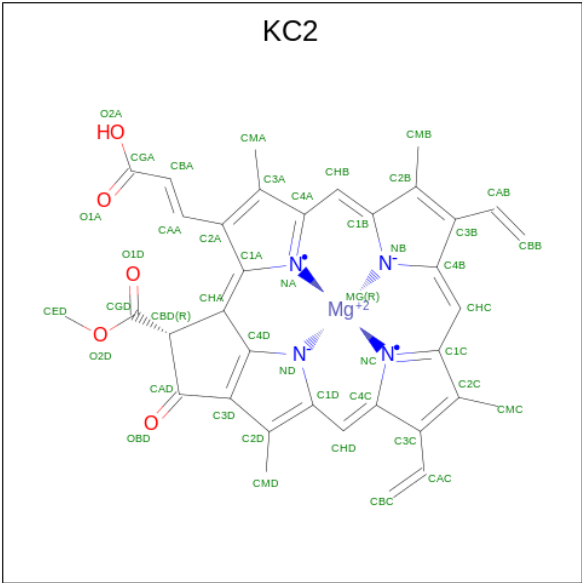
Mol	Chain	Residues	Atoms					AltConf
40	x	1	Total 65	C 55	Mg 1	N 4	O 5	0
40	x	1	Total 51	C 41	Mg 1	N 4	O 5	0
40	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	x	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	x	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	x	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	y	1	Total 49	C 39	Mg 1	N 4	O 5	0
40	y	1	Total 47	C 37	Mg 1	N 4	O 5	0
40	y	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 55	C 45	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 60	C 50	Mg 1	N 4	O 5	0
40	z	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
40	z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
40	z	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 41 is Chlorophyll c2 (CCD ID: KC2) (formula: C₃₅H₂₈MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
41	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
41	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	p	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	q	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	t	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	u	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	v	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	w	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
41	x	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
41	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
41	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 42 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: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



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

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

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Mol	Chain	Residues	Atoms			AltConf
42	H	1	Total 43	C 40	O 3	0
42	H	1	Total 43	C 40	O 3	0
42	H	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	I	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	J	1	Total 43	C 40	O 3	0
42	K	1	Total 43	C 40	O 3	0
42	K	1	Total 43	C 40	O 3	0
42	L	1	Total 43	C 40	O 3	0
42	L	1	Total 43	C 40	O 3	0
42	M	1	Total 43	C 40	O 3	0
42	N	1	Total 43	C 40	O 3	0
42	N	1	Total 43	C 40	O 3	0
42	N	1	Total 43	C 40	O 3	0

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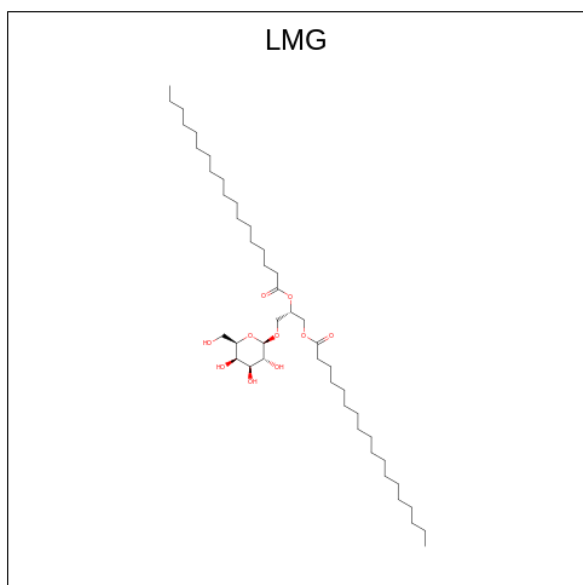
Mol	Chain	Residues	Atoms			AltConf
42	O	1	Total 43	C 40	O 3	0
42	P	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	Q	1	Total 43	C 40	O 3	0
42	R	1	Total 43	C 40	O 3	0
42	T	1	Total 43	C 40	O 3	0
42	U	1	Total 43	C 40	O 3	0
42	U	1	Total 43	C 40	O 3	0
42	W	1	Total 43	C 40	O 3	0
42	X	1	Total 43	C 40	O 3	0
42	Y	1	Total 43	C 40	O 3	0
42	Z	1	Total 43	C 40	O 3	0
42	j	1	Total 43	C 40	O 3	0
42	k	1	Total 43	C 40	O 3	0
42	o	1	Total 43	C 40	O 3	0
42	o	1	Total 43	C 40	O 3	0
42	p	1	Total 43	C 40	O 3	0
42	q	1	Total 43	C 40	O 3	0
42	q	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
42	t	1	Total	C	O	0
			43	40	3	
42	u	1	Total	C	O	0
			43	40	3	
42	v	1	Total	C	O	0
			43	40	3	
42	v	1	Total	C	O	0
			43	40	3	
42	w	1	Total	C	O	0
			43	40	3	
42	x	1	Total	C	O	0
			43	40	3	
42	y	1	Total	C	O	0
			43	40	3	
42	z	1	Total	C	O	0
			43	40	3	
42	z	1	Total	C	O	0
			43	40	3	

- Molecule 43 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



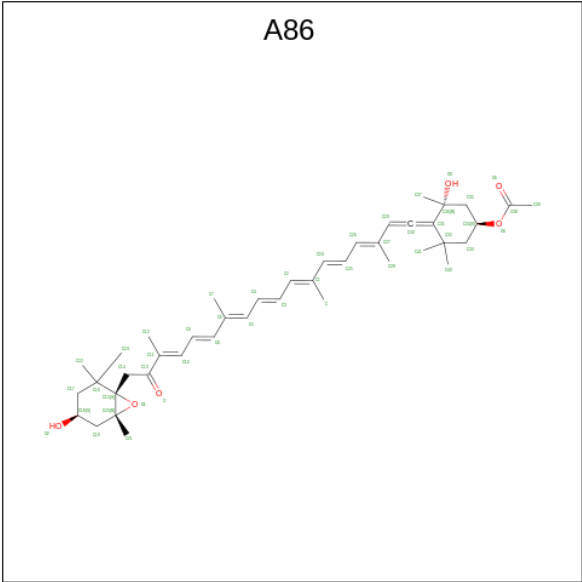
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	C	O	0
			40	30	10	
43	D	1	Total	C	O	0
			40	30	10	

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Mol	Chain	Residues	Atoms			AltConf
43	E	1	Total	C	O	0
			31	21	10	
43	E	1	Total	C	O	0
			31	21	10	
43	E	1	Total	C	O	0
			40	30	10	
43	F	1	Total	C	O	0
			39	29	10	
43	L	1	Total	C	O	0
			37	27	10	
43	M	1	Total	C	O	0
			39	29	10	
43	P	1	Total	C	O	0
			39	29	10	
43	S	1	Total	C	O	0
			39	29	10	
43	T	1	Total	C	O	0
			40	30	10	
43	W	1	Total	C	O	0
			39	29	10	
43	a	1	Total	C	O	0
			35	25	10	
43	a	1	Total	C	O	0
			35	25	10	
43	j	1	Total	C	O	0
			30	20	10	
43	l	1	Total	C	O	0
			39	29	10	
43	p	1	Total	C	O	0
			39	29	10	
43	u	1	Total	C	O	0
			39	29	10	
43	x	1	Total	C	O	0
			39	29	10	

- Molecule 44 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
44	C	1	Total	C	O	0
			48	42	6	
44	D	1	Total	C	O	0
			48	42	6	
44	D	1	Total	C	O	0
			48	42	6	
44	F	1	Total	C	O	0
			48	42	6	
44	F	1	Total	C	O	0
			48	42	6	
44	F	1	Total	C	O	0
			48	42	6	
44	G	1	Total	C	O	0
			48	42	6	
44	G	1	Total	C	O	0
			48	42	6	
44	H	1	Total	C	O	0
			48	42	6	
44	K	1	Total	C	O	0
			48	42	6	
44	L	1	Total	C	O	0
			48	42	6	
44	M	1	Total	C	O	0
			48	42	6	
44	M	1	Total	C	O	0
			48	42	6	
44	M	1	Total	C	O	0
			48	42	6	

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

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

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Mol	Chain	Residues	Atoms			AltConf
44	Y	1	Total	C	O	0
			48	42	6	
44	Y	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	Z	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	o	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	p	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	

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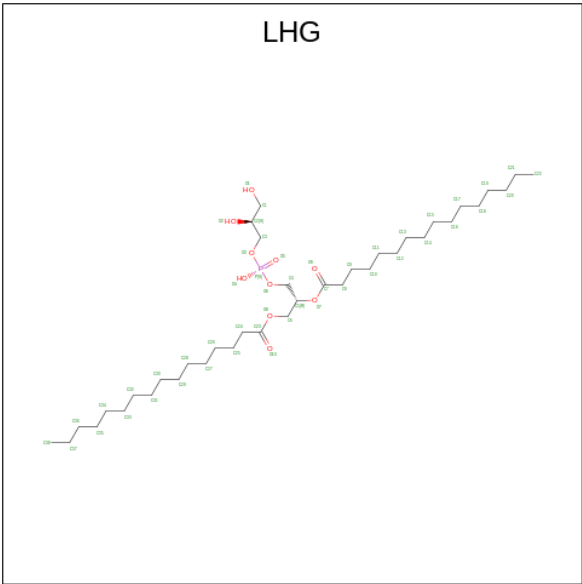
Mol	Chain	Residues	Atoms			AltConf
44	q	1	Total	C	O	0
			48	42	6	
44	q	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	t	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	u	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	v	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	w	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	

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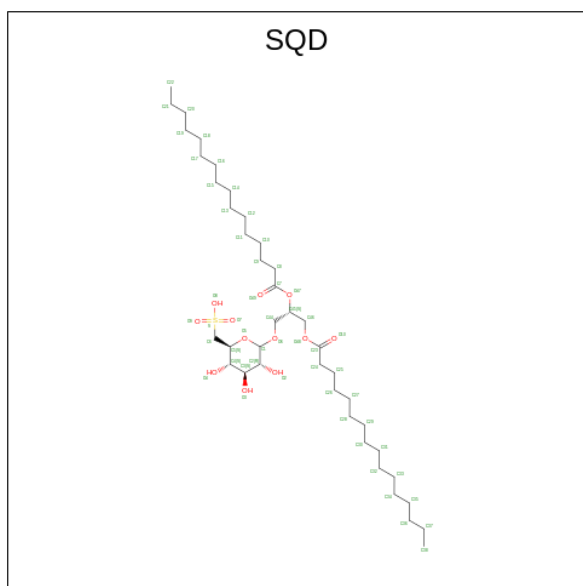
Mol	Chain	Residues	Atoms			AltConf
44	x	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	
44	x	1	Total	C	O	0
			48	42	6	
44	y	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	
44	z	1	Total	C	O	0
			48	42	6	

- Molecule 45 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
45	F	1	Total	C	O	P	0
			40	29	10	1	
45	S	1	Total	C	O	P	0
			40	29	10	1	
45	a	1	Total	C	O	P	0
			48	37	10	1	
45	a	1	Total	C	O	P	0
			30	19	10	1	

- Molecule 46 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
46	F	1	Total	C	O	S	0
			36	23	12	1	
46	I	1	Total	C	O	S	0
			54	41	12	1	
46	M	1	Total	C	O	S	0
			32	19	12	1	
46	P	1	Total	C	O	S	0
			32	19	12	1	
46	W	1	Total	C	O	S	0
			32	19	12	1	
46	k	1	Total	C	O	S	0
			36	23	12	1	

- Molecule 47 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-2-[2-[(4 {S},6 {R})-4-acety

A1EB1

Mol	Chain	Residues	Atoms			AltConf
47	F	1	Total 56	C 48	O 8	0
47	G	1	Total 56	C 48	O 8	0
47	K	1	Total 56	C 48	O 8	0
47	K	1	Total 56	C 48	O 8	0
47	L	1	Total 56	C 48	O 8	0
47	L	1	Total 56	C 48	O 8	0
47	N	1	Total 56	C 48	O 8	0
47	O	1	Total 56	C 48	O 8	0
47	P	1	Total 56	C 48	O 8	0
47	R	1	Total 56	C 48	O 8	0
47	S	1	Total 56	C 48	O 8	0

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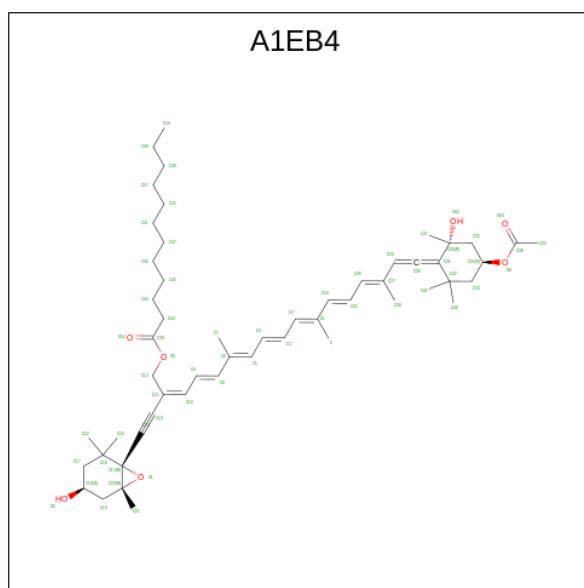
Mol	Chain	Residues	Atoms			AltConf
47	S	1	Total	C	O	0
			56	48	8	
47	T	1	Total	C	O	0
			56	48	8	
47	T	1	Total	C	O	0
			56	48	8	
47	Y	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	Z	1	Total	C	O	0
			56	48	8	
47	o	1	Total	C	O	0
			56	48	8	
47	o	1	Total	C	O	0
			56	48	8	
47	p	1	Total	C	O	0
			56	48	8	
47	p	1	Total	C	O	0
			56	48	8	
47	q	1	Total	C	O	0
			56	48	8	
47	q	1	Total	C	O	0
			56	48	8	
47	q	1	Total	C	O	0
			56	48	8	
47	t	1	Total	C	O	0
			56	48	8	
47	t	1	Total	C	O	0
			56	48	8	
47	t	1	Total	C	O	0
			56	48	8	
47	u	1	Total	C	O	0
			56	48	8	
47	u	1	Total	C	O	0
			56	48	8	
47	v	1	Total	C	O	0
			56	48	8	
47	v	1	Total	C	O	0
			56	48	8	

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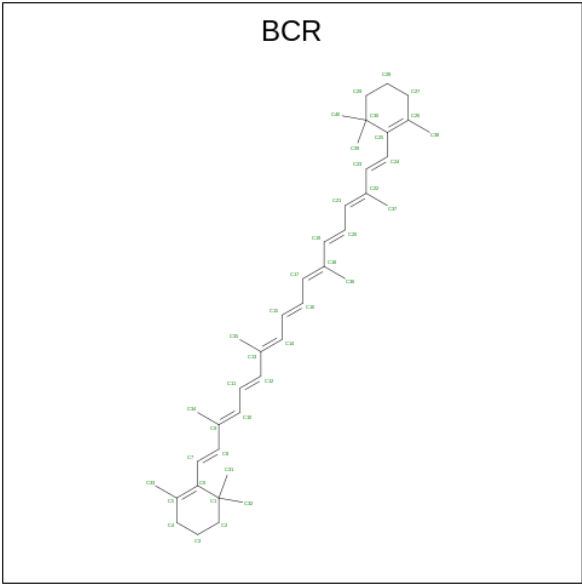
Mol	Chain	Residues	Atoms			AltConf
47	v	1	Total	C	O	0
			56	48	8	
47	v	1	Total	C	O	0
			56	48	8	
47	w	1	Total	C	O	0
			56	48	8	
47	w	1	Total	C	O	0
			56	48	8	
47	x	1	Total	C	O	0
			56	48	8	
47	x	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	y	1	Total	C	O	0
			56	48	8	
47	z	1	Total	C	O	0
			56	48	8	

- Molecule 48 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-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
48	M	1	Total	C	O	0
			56	49	7	
48	P	1	Total	C	O	0
			56	49	7	
48	W	1	Total	C	O	0
			56	49	7	

- Molecule 49 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



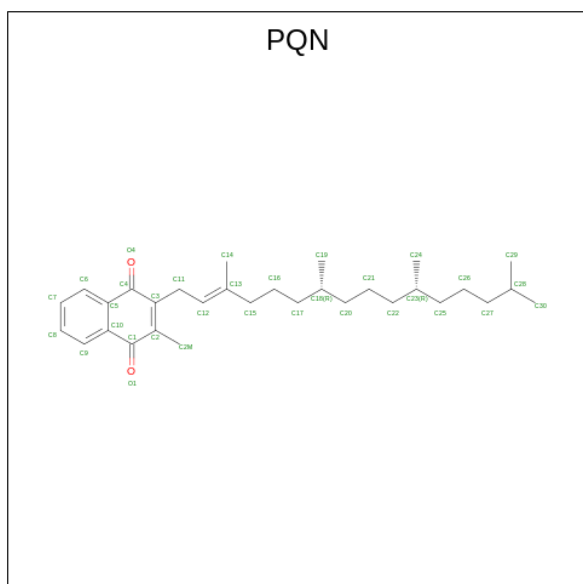
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	a	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	
49	b	1	Total	C	0
			40	40	

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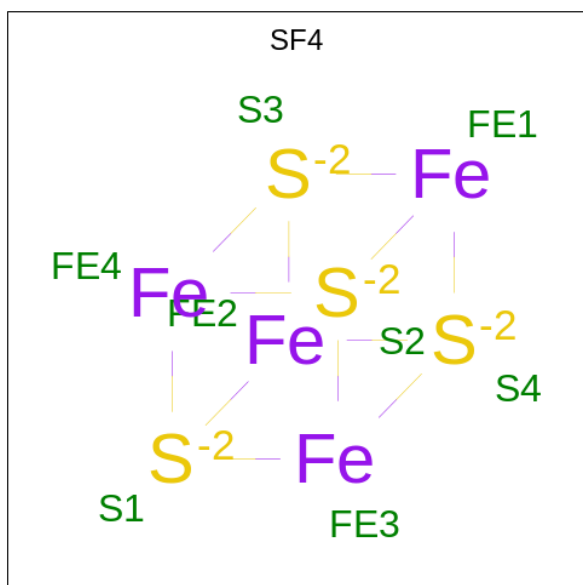
Mol	Chain	Residues	Atoms	AltConf
49	b	1	Total C 40 40	0
49	b	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	f	1	Total C 40 40	0
49	i	1	Total C 40 40	0
49	j	1	Total C 40 40	0
49	k	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	l	1	Total C 40 40	0
49	m	1	Total C 40 40	0
49	r	1	Total C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

- Molecule 50 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



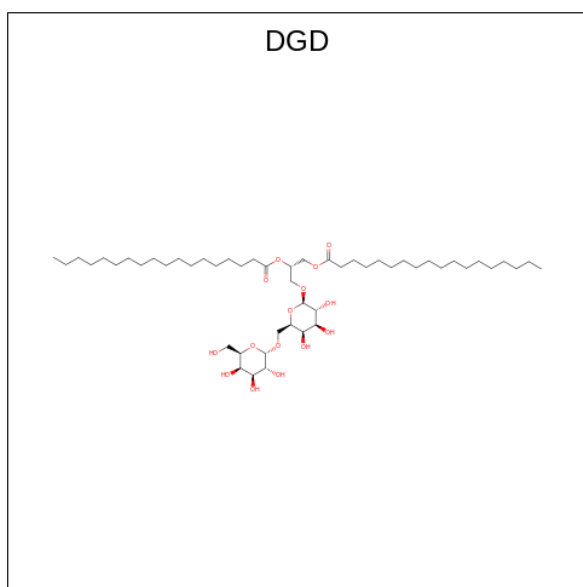
Mol	Chain	Residues	Atoms			AltConf
50	a	1	Total	C	O	0
			28	26	2	
50	b	1	Total	C	O	0
			28	26	2	

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 52 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).



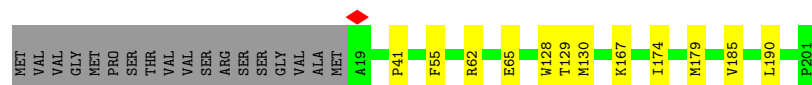
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
52	b	1	56	41	15	0

3 Residue-property plots

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

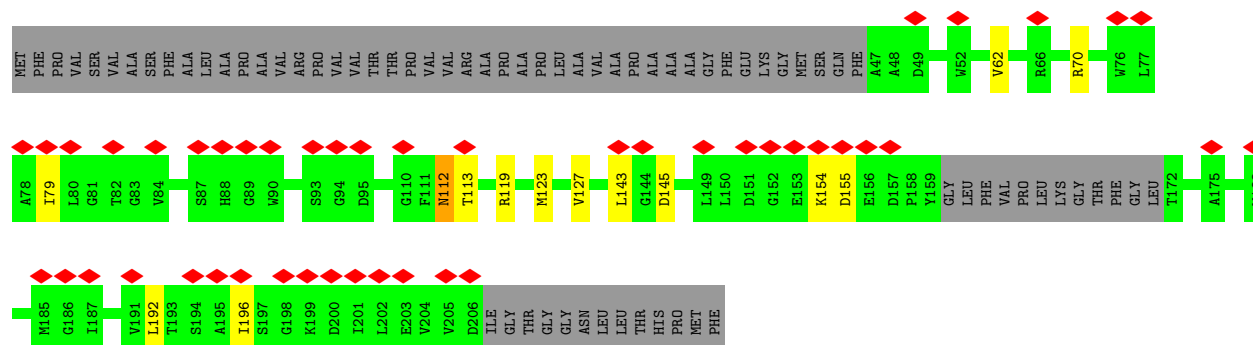
- Molecule 1: Light harvesting protein

Chain A: 



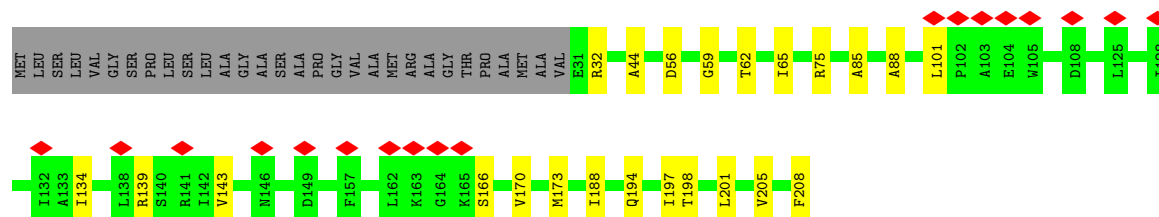
- Molecule 2: EFCPI-1

Chain B: 



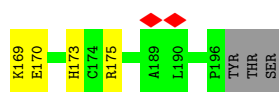
- Molecule 3: Light harvesting protein

Chain C: 

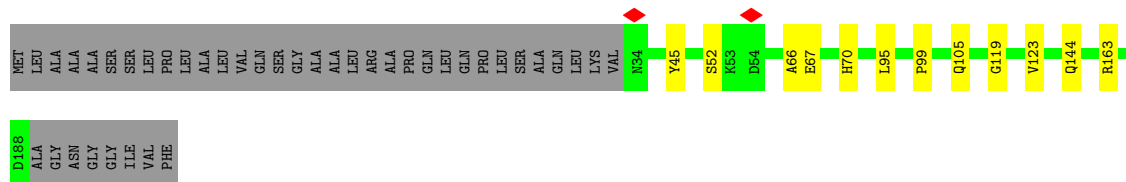


- Molecule 4: EFCPI-6

Chain D: 



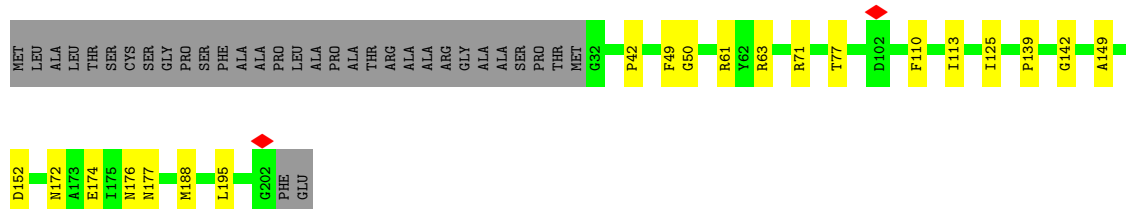
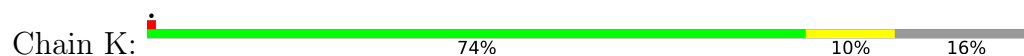
- Molecule 9: Light harvesting protein



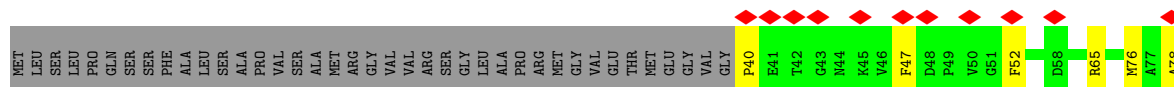
- Molecule 10: Light harvesting protein

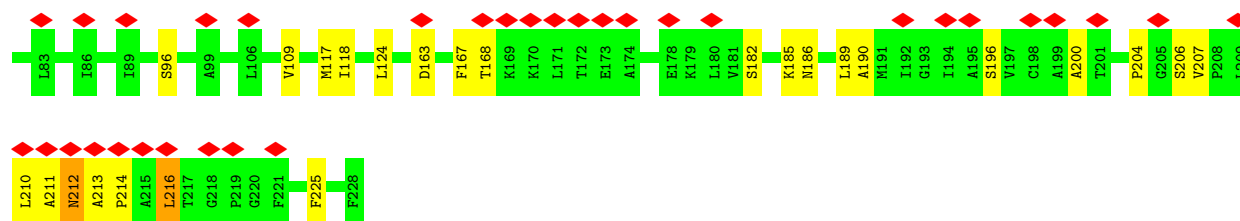


- Molecule 11: Light harvesting protein



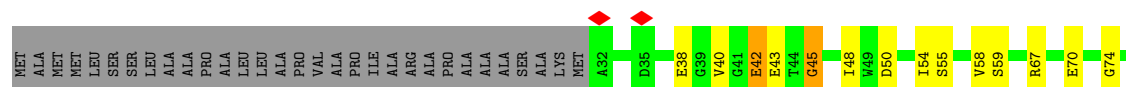
- Molecule 12: EFCPI-12





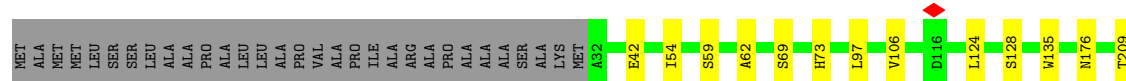
- Molecule 13: Light harvesting protein

Chain M: 74% 12% 14%



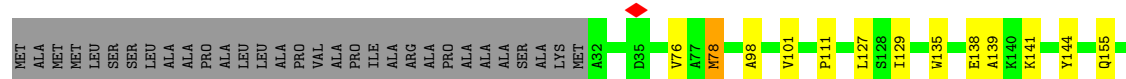
- Molecule 13: Light harvesting protein

Chain P: 79% 7% 14%



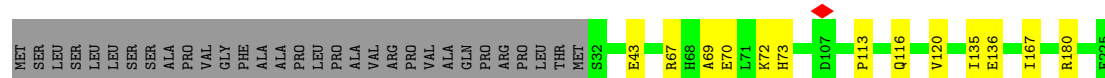
- Molecule 13: Light harvesting protein

Chain W: 76% 9% 14%



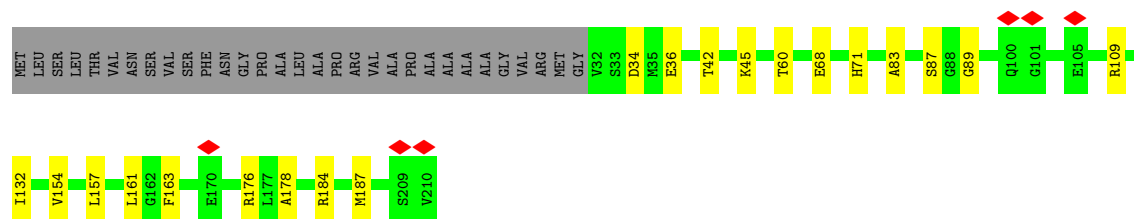
- Molecule 14: EFCPI-17

Chain N: 80% 6% 14%



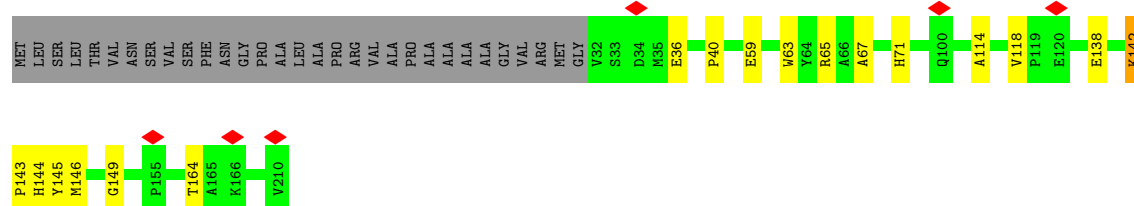
- Molecule 15: Light harvesting protein

Chain O: 76% 10% 15%



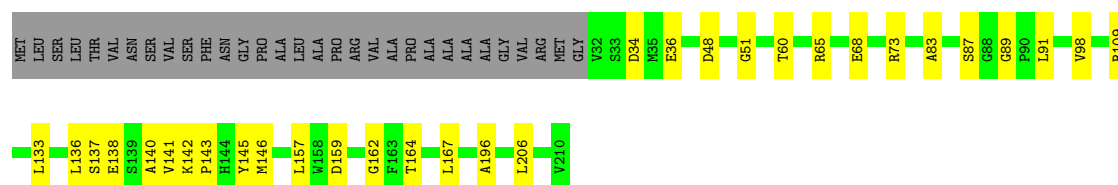
- Molecule 15: Light harvesting protein

Chain R: 77% 8% 15%



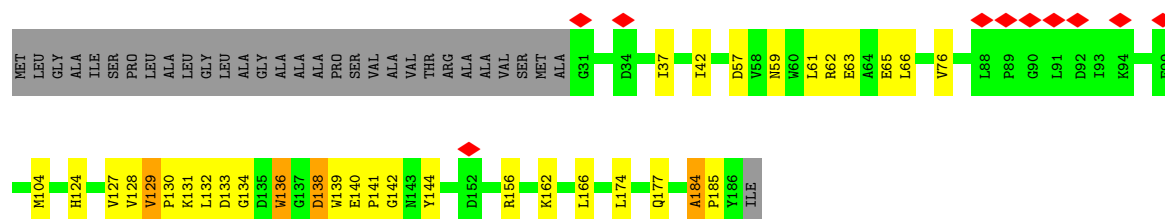
- Molecule 15: Light harvesting protein

Chain T: 70% 15% 15%



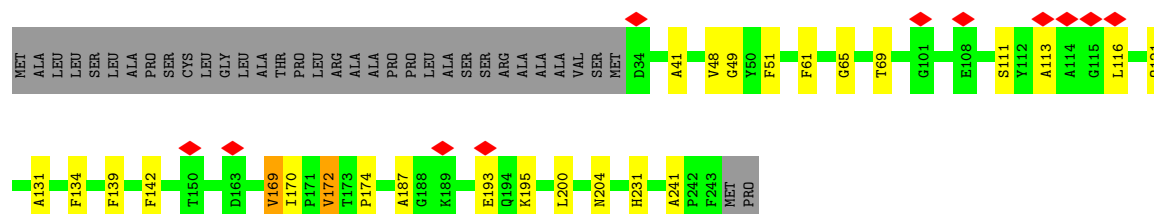
- Molecule 16: EFCPI-18

Chain Q: 5% 65% 16% 17%

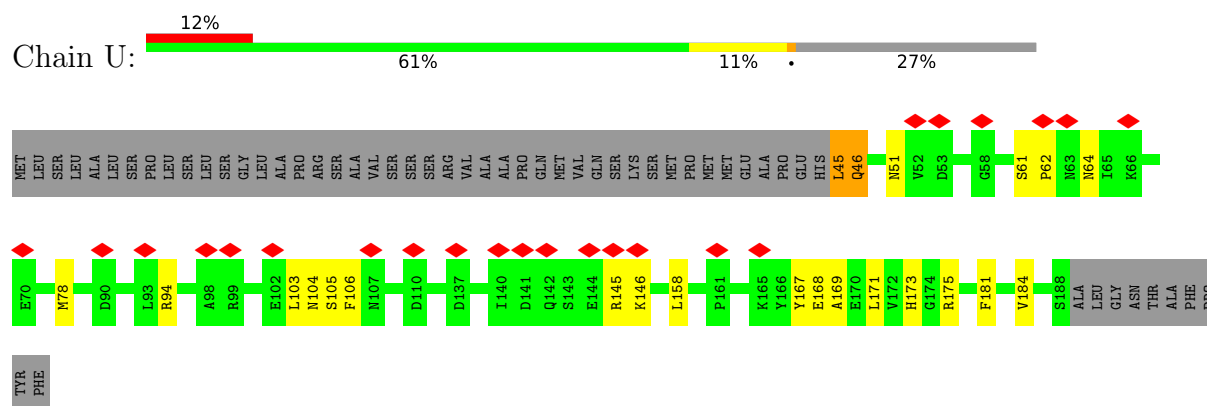


- Molecule 17: EFCPI-22

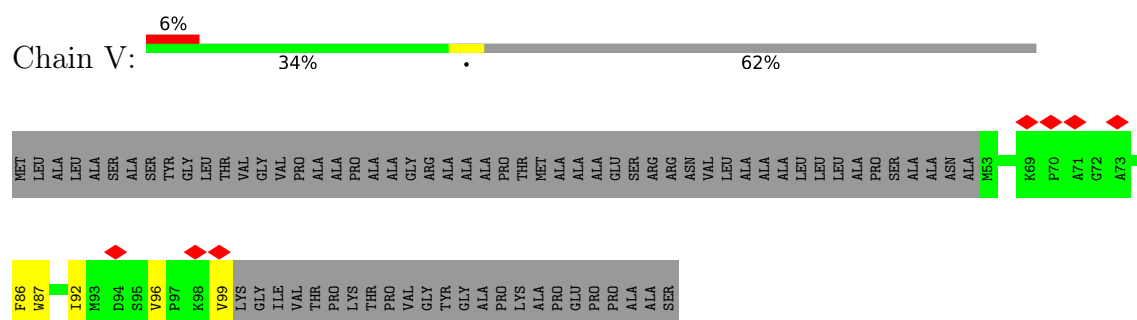
Chain S: 75% 10% 14%



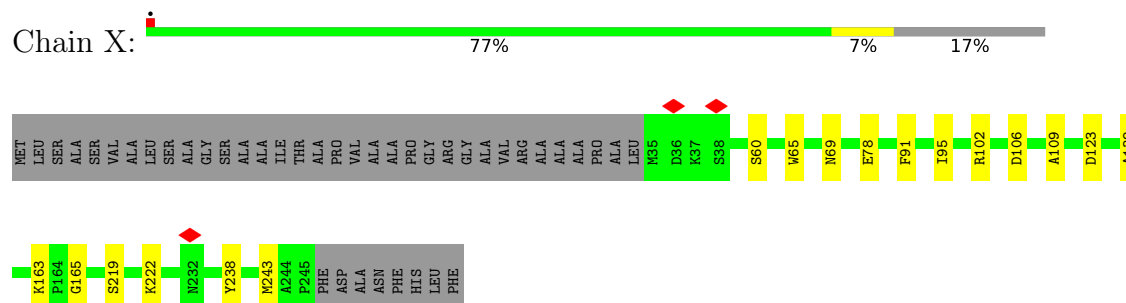
- Molecule 18: Light harvesting protein



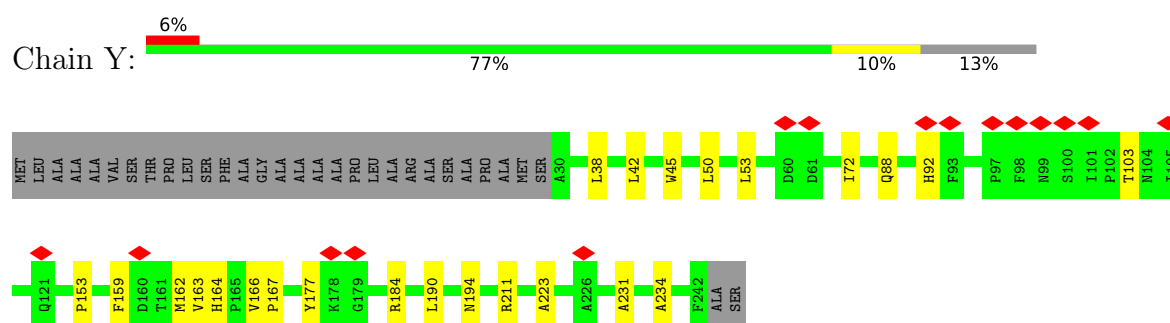
- Molecule 19: LEFP



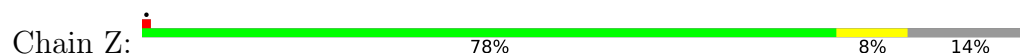
- Molecule 20: Light harvesting protein

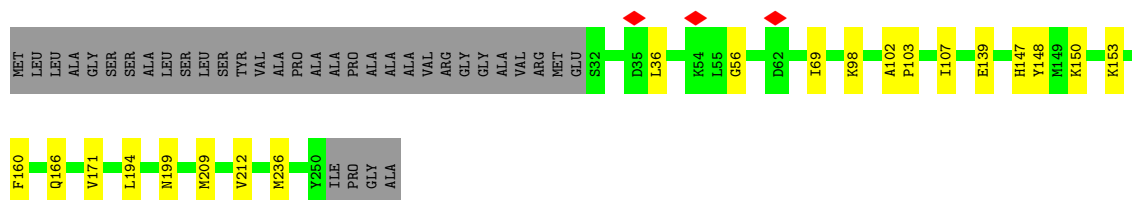


- Molecule 21: Light harvesting protein



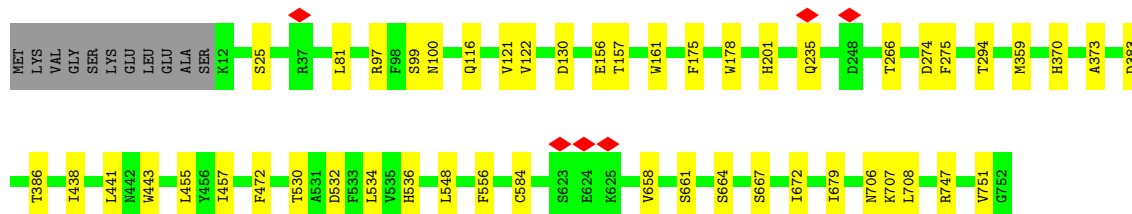
- Molecule 22: Light harvesting protein





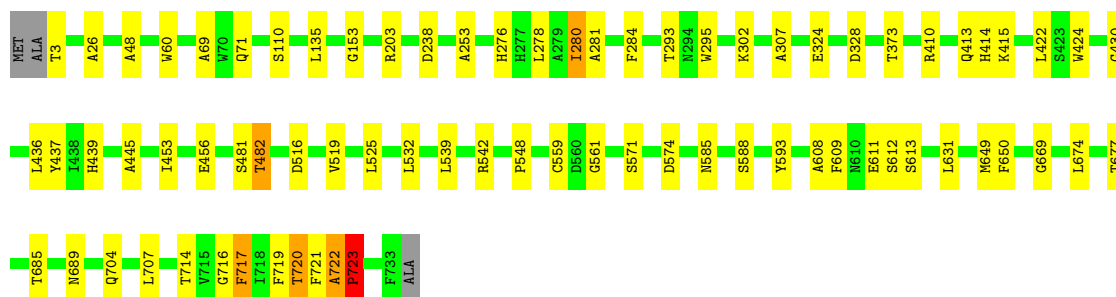
- Molecule 23: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 92% 7% .



- Molecule 24: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 89% 10% .



- Molecule 25: Photosystem I iron-sulfur center

Chain c: 88% 11% .



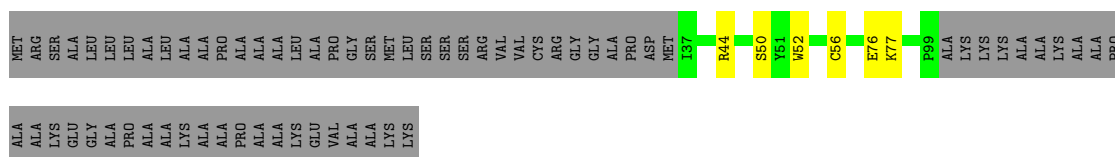
- Molecule 26: Photosystem I reaction center subunit II

Chain d: 91% 7% ..

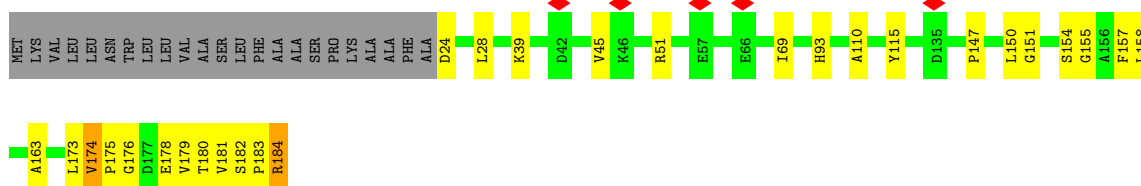


- Molecule 27: Photosystem I reaction center subunit IV

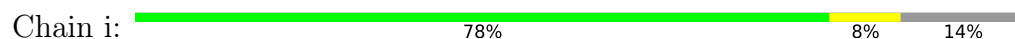
Chain e: 44% 5% 52%



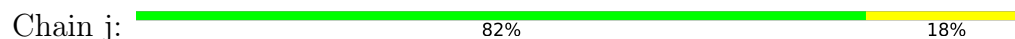
- Molecule 28: Photosystem I reaction center subunit III



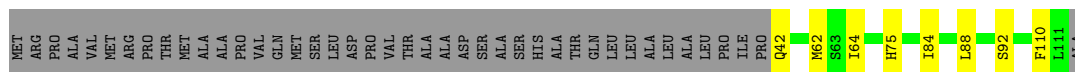
- Molecule 29: Photosystem I reaction center subunit VIII



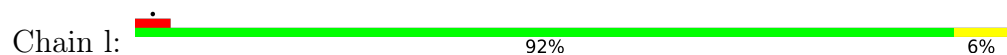
- Molecule 30: Photosystem I reaction center subunit IX



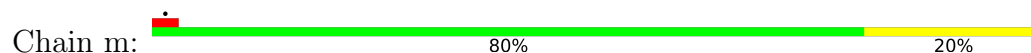
- Molecule 31: PSI-K

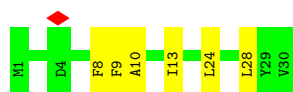


- Molecule 32: Photosystem I reaction center subunit XI

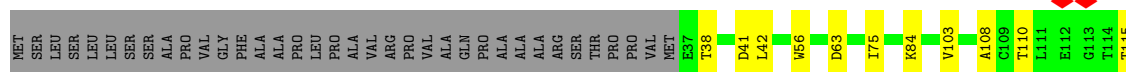
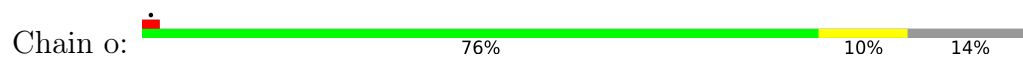


- Molecule 33: Photosystem I reaction center subunit XII

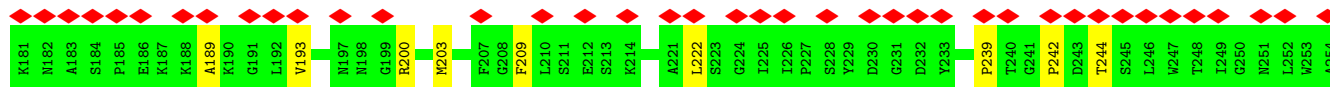
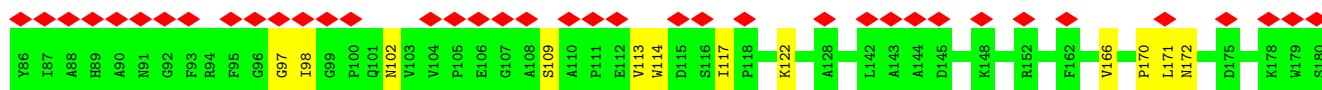
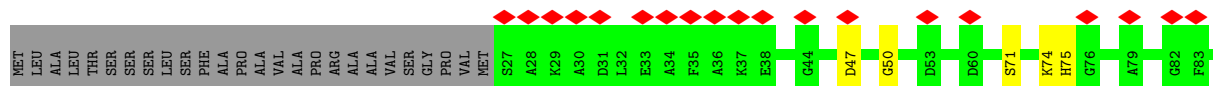
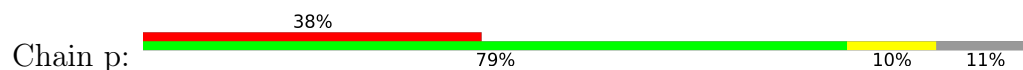




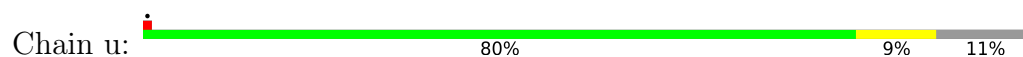
- Molecule 34: EFCPI-30



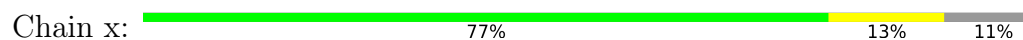
- Molecule 35: Light harvesting protein

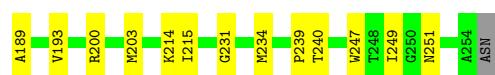


- Molecule 35: Light harvesting protein

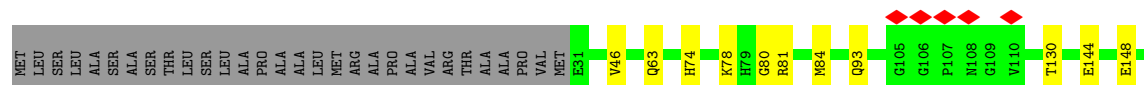
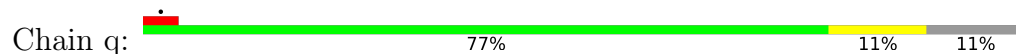


- Molecule 35: Light harvesting protein





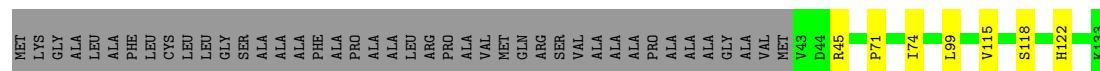
- Molecule 36: Light harvesting protein



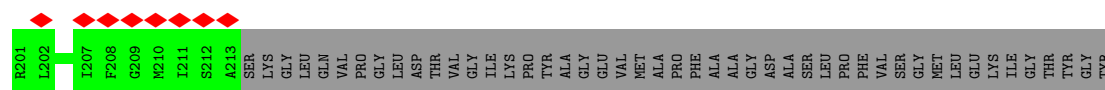
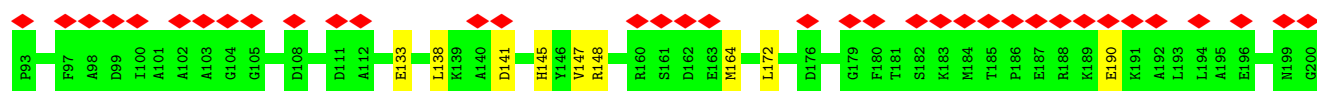
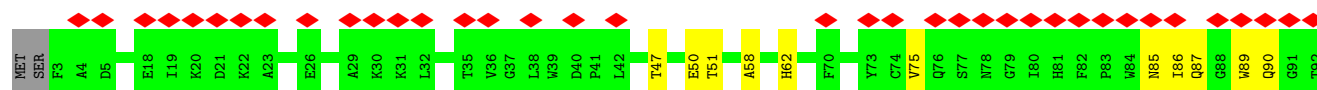
- Molecule 36: Light harvesting protein



- Molecule 37: Psar

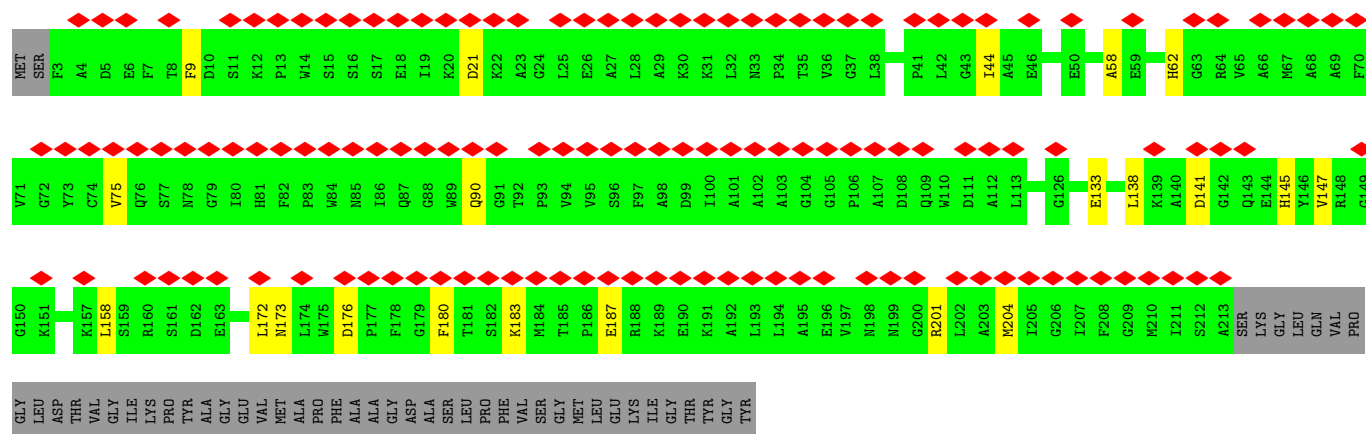


- Molecule 38: Light harvesting protein

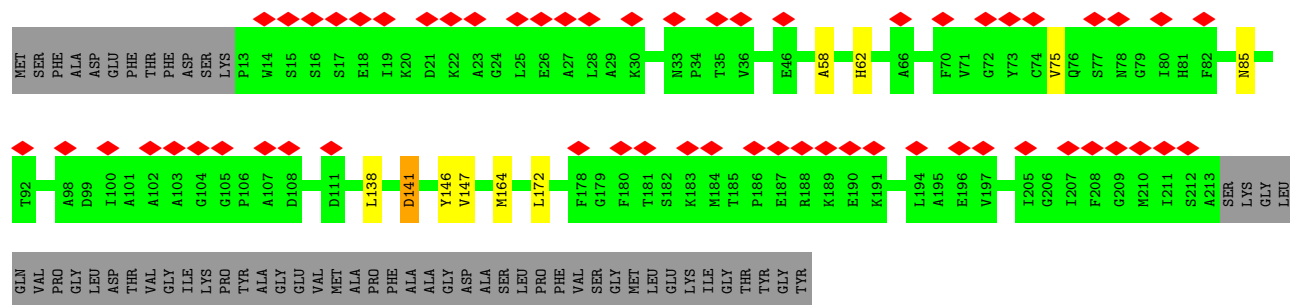
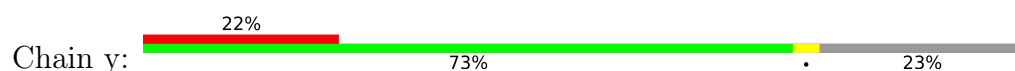


- Molecule 38: Light harvesting protein

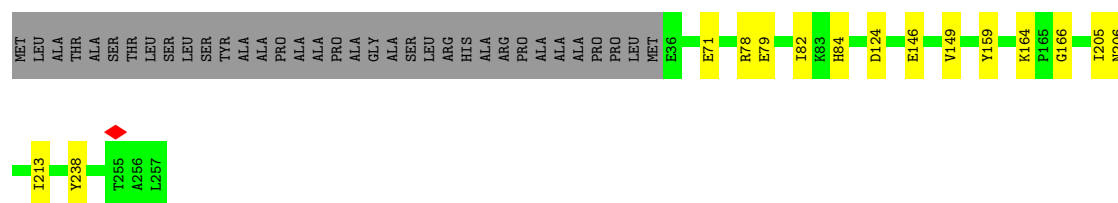
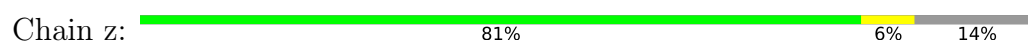




• Molecule 38: Light harvesting protein



• Molecule 39: Light harvesting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.457	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	530.0, 530.0, 530.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.20	0/1458	0.41	0/1979
2	B	0.30	0/1135	0.60	1/1545 (0.1%)
3	C	0.23	0/1381	0.46	0/1865
4	D	0.45	0/1486	0.52	1/2020 (0.0%)
5	E	0.21	0/1416	0.43	0/1933
6	F	0.30	0/1452	0.51	3/1970 (0.2%)
7	G	0.19	0/1277	0.37	0/1739
8	H	0.23	0/1283	0.49	0/1739
9	I	0.20	0/1225	0.40	0/1656
10	J	0.23	0/1254	0.52	0/1692
11	K	0.20	0/1378	0.41	0/1874
12	L	0.28	0/1462	0.55	1/1989 (0.1%)
13	M	0.41	0/1491	0.52	2/2020 (0.1%)
13	P	0.20	0/1491	0.43	0/2020
13	W	0.21	0/1491	0.47	0/2020
14	N	0.19	0/1494	0.43	0/2027
15	O	0.22	0/1360	0.48	0/1850
15	R	0.38	0/1360	0.53	0/1850
15	T	0.23	0/1360	0.51	0/1850
16	Q	0.47	1/1223 (0.1%)	0.64	4/1659 (0.2%)
17	S	0.21	0/1700	0.49	2/2315 (0.1%)
18	U	0.25	0/1158	0.55	1/1567 (0.1%)
19	V	0.22	0/362	0.49	0/492
20	X	0.23	0/1695	0.48	0/2300
21	Y	0.26	0/1719	0.53	0/2342
22	Z	0.24	0/1773	0.50	0/2423
23	a	0.20	0/6024	0.39	0/8200
24	b	0.38	6/6017 (0.1%)	0.46	4/8208 (0.0%)
25	c	0.22	0/607	0.45	0/824
26	d	0.20	0/1128	0.42	0/1525
27	e	0.20	0/503	0.44	0/681
28	f	0.28	0/1269	0.45	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	i	0.23	0/250	0.45	0/342
30	j	0.23	0/324	0.49	0/438
31	k	0.20	0/520	0.40	0/701
32	l	0.19	0/1113	0.37	0/1513
33	m	0.22	0/226	0.35	0/306
34	o	0.26	0/1809	0.54	0/2460
35	p	0.25	0/1801	0.49	0/2451
35	u	0.28	0/1801	0.49	0/2451
35	x	0.24	0/1801	0.48	0/2451
36	q	0.26	0/1843	0.48	0/2503
36	v	0.26	0/1843	0.49	0/2503
37	r	0.23	0/700	0.42	0/958
38	t	0.26	0/1682	0.49	0/2286
38	w	0.24	0/1682	0.51	0/2286
38	y	0.22	0/1594	0.47	0/2167
39	z	0.25	0/1772	0.46	0/2414
All	All	0.27	7/72193 (0.0%)	0.47	19/98125 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	T	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	281	ALA	CA-C	-6.35	1.44	1.52
24	b	284	PHE	C-O	-6.20	1.16	1.24
24	b	281	ALA	C-O	-5.83	1.17	1.24
16	Q	136	TRP	CA-C	-5.79	1.45	1.52
24	b	722	ALA	C-O	-5.38	1.19	1.24

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	722	ALA	CA-C-N	-7.89	109.97	119.84
24	b	722	ALA	C-N-CA	-7.89	109.97	119.84
4	D	93	VAL	N-CA-C	-7.55	103.92	111.77
6	F	152	ALA	N-CA-C	-7.37	103.18	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	129	VAL	O-C-N	6.28	124.44	120.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	T	142	LYS	Peptide
15	T	162	GLY	Peptide

5.2 Too-close contacts [i](#)

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	1419	0	1408	15	0
2	B	1108	0	1082	10	0
3	C	1352	0	1383	15	0
4	D	1446	0	1404	35	0
5	E	1383	0	1399	48	0
6	F	1414	0	1411	21	0
7	G	1248	0	1251	10	0
8	H	1251	0	1225	9	0
9	I	1195	0	1197	8	0
10	J	1231	0	1245	25	0
11	K	1333	0	1297	16	0
12	L	1419	0	1413	37	0
13	M	1455	0	1468	22	0
13	P	1455	0	1468	25	0
13	W	1455	0	1468	24	0
14	N	1454	0	1469	9	0
15	O	1325	0	1344	13	0
15	R	1325	0	1344	16	0
15	T	1325	0	1344	19	0
16	Q	1192	0	1163	39	0
17	S	1640	0	1586	22	0
18	U	1130	0	1116	12	0
19	V	351	0	350	13	0
20	X	1643	0	1607	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Y	1660	0	1617	16	0
22	Z	1714	0	1670	14	0
23	a	5832	0	5730	59	0
24	b	5807	0	5630	63	0
25	c	597	0	581	7	0
26	d	1103	0	1113	8	0
27	e	493	0	482	4	0
28	f	1238	0	1242	40	0
29	i	243	0	255	5	0
30	j	317	0	333	15	0
31	k	510	0	520	9	0
32	l	1084	0	1090	8	0
33	m	224	0	243	5	0
34	o	1760	0	1757	18	0
35	p	1744	0	1703	16	0
35	u	1744	0	1703	16	0
35	x	1744	0	1703	24	0
36	q	1790	0	1776	27	0
36	v	1790	0	1776	26	0
37	r	681	0	667	4	0
38	t	1631	0	1593	29	0
38	w	1631	0	1593	19	0
38	y	1546	0	1523	9	0
39	z	1718	0	1701	13	0
40	A	581	0	562	24	0
40	B	287	0	218	3	0
40	C	429	0	381	4	0
40	D	668	0	613	7	0
40	E	711	0	640	35	0
40	F	544	0	482	12	0
40	G	363	0	303	4	0
40	H	521	0	442	2	0
40	I	445	0	412	0	0
40	J	549	0	441	14	0
40	K	327	0	294	6	0
40	L	394	0	312	10	0
40	M	420	0	413	3	0
40	N	345	0	324	3	0
40	O	328	0	299	0	0
40	P	393	0	364	11	0
40	Q	432	0	375	11	0
40	R	320	0	278	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	S	580	0	496	21	0
40	T	330	0	296	1	0
40	U	345	0	273	1	0
40	V	113	0	104	6	0
40	W	425	0	429	5	0
40	X	484	0	425	2	0
40	Y	478	0	415	0	0
40	Z	507	0	469	2	0
40	a	2596	0	2627	48	0
40	b	2503	0	2570	31	0
40	f	219	0	201	7	0
40	i	55	0	49	4	0
40	j	47	0	35	2	0
40	k	110	0	98	17	0
40	l	259	0	284	4	0
40	o	507	0	469	5	0
40	p	478	0	418	2	0
40	q	508	0	469	2	0
40	t	305	0	249	1	0
40	u	491	0	442	0	0
40	v	508	0	469	4	0
40	w	305	0	249	6	0
40	x	508	0	472	3	0
40	y	305	0	249	7	0
40	z	551	0	498	5	0
41	A	45	0	0	0	0
41	C	45	0	0	1	0
41	E	45	0	0	0	0
41	F	90	0	0	0	0
41	G	90	0	0	0	0
41	H	90	0	0	0	0
41	I	90	0	0	0	0
41	J	45	0	0	0	0
41	K	180	0	0	0	0
41	L	225	0	0	1	0
41	M	225	0	0	2	0
41	N	315	0	0	1	0
41	O	270	0	0	1	0
41	P	225	0	0	1	0
41	Q	90	0	0	10	0
41	R	270	0	0	0	0
41	S	180	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	T	270	0	0	3	0
41	U	45	0	0	0	0
41	W	225	0	0	1	0
41	X	180	0	0	1	0
41	Y	225	0	0	9	0
41	Z	180	0	0	2	0
41	o	180	0	0	1	0
41	p	225	0	0	0	0
41	q	180	0	0	0	0
41	t	135	0	0	15	0
41	u	225	0	0	0	0
41	v	180	0	0	1	0
41	w	135	0	0	13	0
41	x	225	0	0	0	0
41	y	135	0	0	8	0
41	z	180	0	0	1	0
42	A	215	0	0	10	0
42	B	43	0	0	1	0
42	C	129	0	0	1	0
42	D	215	0	0	1	0
42	E	172	0	0	0	0
42	F	129	0	0	1	0
42	G	43	0	0	0	0
42	H	129	0	0	1	0
42	I	172	0	0	2	0
42	J	258	0	0	16	0
42	K	86	0	0	0	0
42	L	86	0	0	32	0
42	M	43	0	0	1	0
42	N	129	0	0	1	0
42	O	43	0	0	1	0
42	P	43	0	0	5	0
42	Q	172	0	0	1	0
42	R	43	0	0	0	0
42	T	43	0	0	0	0
42	U	86	0	0	0	0
42	W	43	0	0	1	0
42	X	43	0	0	0	0
42	Y	43	0	0	9	0
42	Z	43	0	0	0	0
42	j	43	0	0	0	0
42	k	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	o	86	0	0	2	0
42	p	43	0	0	1	0
42	q	86	0	0	7	0
42	t	43	0	0	29	0
42	u	43	0	0	1	0
42	v	86	0	0	5	0
42	w	43	0	0	26	0
42	x	43	0	0	2	0
42	y	43	0	0	17	0
42	z	86	0	0	0	0
43	A	40	0	50	0	0
43	D	40	0	50	1	0
43	E	102	0	114	6	0
43	F	39	0	48	0	0
43	L	37	0	44	0	0
43	M	39	0	48	0	0
43	P	39	0	48	0	0
43	S	39	0	48	0	0
43	T	40	0	50	0	0
43	W	39	0	48	0	0
43	a	70	0	80	3	0
43	j	30	0	30	13	0
43	l	39	0	48	0	0
43	p	39	0	48	0	0
43	u	39	0	48	1	0
43	x	39	0	48	5	0
44	C	48	0	0	0	0
44	D	96	0	0	1	0
44	F	144	0	0	0	0
44	G	96	0	0	3	0
44	H	48	0	0	0	0
44	K	48	0	0	0	0
44	L	48	0	0	1	0
44	M	192	0	0	1	0
44	N	192	0	0	7	0
44	O	144	0	0	0	0
44	P	192	0	0	1	0
44	Q	96	0	0	1	0
44	R	144	0	0	0	0
44	S	192	0	0	0	0
44	T	192	0	0	0	0
44	U	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	W	144	0	0	2	0
44	X	384	0	0	3	0
44	Y	336	0	0	3	0
44	Z	192	0	0	1	0
44	o	240	0	0	1	0
44	p	288	0	0	1	0
44	q	288	0	0	0	0
44	t	144	0	0	1	0
44	u	240	0	0	0	0
44	v	288	0	0	0	0
44	w	192	0	0	1	0
44	x	192	0	0	0	0
44	y	48	0	0	1	0
44	z	336	0	0	1	0
45	F	40	0	50	0	0
45	S	40	0	50	2	0
45	a	78	0	99	0	0
46	F	36	0	36	2	0
46	I	54	0	78	2	0
46	M	32	0	28	1	0
46	P	32	0	28	5	0
46	W	32	0	28	4	0
46	k	36	0	36	3	0
47	F	56	0	0	0	0
47	G	56	0	0	0	0
47	K	112	0	0	1	0
47	L	112	0	0	0	0
47	N	56	0	0	0	0
47	O	56	0	0	0	0
47	P	56	0	0	9	0
47	R	56	0	0	0	0
47	S	112	0	0	0	0
47	T	112	0	0	1	0
47	Y	56	0	0	0	0
47	Z	168	0	0	1	0
47	o	112	0	0	0	0
47	p	112	0	0	2	0
47	q	168	0	0	1	0
47	t	168	0	0	2	0
47	u	112	0	0	2	0
47	v	224	0	0	5	0
47	w	112	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	x	112	0	0	2	0
47	y	168	0	0	4	0
47	z	56	0	0	0	0
48	M	56	0	0	0	0
48	P	56	0	0	4	0
48	W	56	0	0	7	0
49	a	160	0	224	7	0
49	b	240	0	336	2	0
49	f	80	0	112	4	0
49	i	40	0	56	3	0
49	j	40	0	56	0	0
49	k	40	0	56	0	0
49	l	120	0	168	4	0
49	m	40	0	56	4	0
49	r	40	0	56	1	0
50	a	28	0	33	1	0
50	b	28	0	33	2	0
51	b	8	0	0	0	0
51	c	16	0	0	0	0
52	b	56	0	70	7	0
All	All	110086	0	91890	1072	0

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

The worst 5 of 1072 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)
13:P:54:ILE:CG2	47:P:301:A1EB1:O43	1.73	1.36
30:j:1:MET:CE	43:j:101:LMG:H292	1.56	1.34
16:Q:162:LYS:NZ	41:Q:216:KC2:O2A	1.65	1.27
16:Q:42:ILE:HD12	41:Q:216:KC2:CED	1.67	1.23
4:D:103:ILE:CG2	23:a:175:PHE:CZ	2.23	1.20

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	181/201 (90%)	177 (98%)	4 (2%)	0	100	100
2	B	144/219 (66%)	136 (94%)	7 (5%)	1 (1%)	18	49
3	C	176/208 (85%)	166 (94%)	9 (5%)	1 (1%)	21	52
4	D	187/255 (73%)	178 (95%)	8 (4%)	1 (0%)	24	57
5	E	185/217 (85%)	176 (95%)	8 (4%)	1 (0%)	24	57
6	F	186/239 (78%)	175 (94%)	10 (5%)	1 (0%)	24	57
7	G	166/198 (84%)	161 (97%)	5 (3%)	0	100	100
8	H	165/199 (83%)	157 (95%)	8 (5%)	0	100	100
9	I	153/196 (78%)	147 (96%)	6 (4%)	0	100	100
10	J	164/208 (79%)	157 (96%)	6 (4%)	1 (1%)	21	52
11	K	169/204 (83%)	158 (94%)	10 (6%)	1 (1%)	21	52
12	L	187/228 (82%)	173 (92%)	12 (6%)	2 (1%)	11	39
13	M	191/224 (85%)	184 (96%)	7 (4%)	0	100	100
13	P	191/224 (85%)	183 (96%)	8 (4%)	0	100	100
13	W	191/224 (85%)	182 (95%)	9 (5%)	0	100	100
14	N	192/225 (85%)	182 (95%)	10 (5%)	0	100	100
15	O	177/210 (84%)	164 (93%)	13 (7%)	0	100	100
15	R	177/210 (84%)	171 (97%)	6 (3%)	0	100	100
15	T	177/210 (84%)	164 (93%)	12 (7%)	1 (1%)	21	52
16	Q	154/187 (82%)	141 (92%)	10 (6%)	3 (2%)	6	27
17	S	208/245 (85%)	189 (91%)	18 (9%)	1 (0%)	24	57
18	U	142/198 (72%)	128 (90%)	11 (8%)	3 (2%)	5	25
19	V	45/123 (37%)	43 (96%)	2 (4%)	0	100	100
20	X	209/253 (83%)	201 (96%)	8 (4%)	0	100	100
21	Y	211/244 (86%)	199 (94%)	11 (5%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Z	217/254 (85%)	210 (97%)	7 (3%)	0	100	100
23	a	739/752 (98%)	711 (96%)	28 (4%)	0	100	100
24	b	729/734 (99%)	706 (97%)	22 (3%)	1 (0%)	48	78
25	c	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
26	d	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
27	e	61/131 (47%)	59 (97%)	2 (3%)	0	100	100
28	f	159/184 (86%)	154 (97%)	5 (3%)	0	100	100
29	i	29/36 (81%)	27 (93%)	2 (7%)	0	100	100
30	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
31	k	68/112 (61%)	65 (96%)	2 (3%)	1 (2%)	8	32
32	l	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
33	m	28/30 (93%)	28 (100%)	0	0	100	100
34	o	234/273 (86%)	225 (96%)	8 (3%)	1 (0%)	30	61
35	p	226/255 (89%)	223 (99%)	3 (1%)	0	100	100
35	u	226/255 (89%)	221 (98%)	5 (2%)	0	100	100
35	x	226/255 (89%)	220 (97%)	6 (3%)	0	100	100
36	q	236/268 (88%)	229 (97%)	7 (3%)	0	100	100
36	v	236/268 (88%)	224 (95%)	12 (5%)	0	100	100
37	r	89/133 (67%)	88 (99%)	1 (1%)	0	100	100
38	t	209/260 (80%)	200 (96%)	9 (4%)	0	100	100
38	w	209/260 (80%)	202 (97%)	7 (3%)	0	100	100
38	y	199/260 (76%)	194 (98%)	5 (2%)	0	100	100
39	z	220/257 (86%)	215 (98%)	5 (2%)	0	100	100
All	All	9063/10734 (84%)	8676 (96%)	366 (4%)	21 (0%)	44	73

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	81	GLU
5	E	210	VAL
10	J	71	ILE
11	K	139	PRO
12	L	204	PRO

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	155/170 (91%)	155 (100%)	0	100	100
2	B	108/160 (68%)	108 (100%)	0	100	100
3	C	142/161 (88%)	141 (99%)	1 (1%)	76	82
4	D	146/193 (76%)	145 (99%)	1 (1%)	76	82
5	E	146/163 (90%)	146 (100%)	0	100	100
6	F	140/180 (78%)	138 (99%)	2 (1%)	59	76
7	G	127/149 (85%)	127 (100%)	0	100	100
8	H	130/154 (84%)	130 (100%)	0	100	100
9	I	125/153 (82%)	125 (100%)	0	100	100
10	J	123/150 (82%)	123 (100%)	0	100	100
11	K	131/153 (86%)	131 (100%)	0	100	100
12	L	144/174 (83%)	143 (99%)	1 (1%)	76	82
13	M	146/165 (88%)	146 (100%)	0	100	100
13	P	146/165 (88%)	146 (100%)	0	100	100
13	W	146/165 (88%)	144 (99%)	2 (1%)	59	76
14	N	149/174 (86%)	148 (99%)	1 (1%)	76	82
15	O	136/157 (87%)	136 (100%)	0	100	100
15	R	136/157 (87%)	135 (99%)	1 (1%)	76	82
15	T	136/157 (87%)	135 (99%)	1 (1%)	76	82
16	Q	123/141 (87%)	122 (99%)	1 (1%)	73	81
17	S	163/188 (87%)	163 (100%)	0	100	100
18	U	118/162 (73%)	116 (98%)	2 (2%)	53	74
19	V	39/85 (46%)	39 (100%)	0	100	100
20	X	169/194 (87%)	169 (100%)	0	100	100
21	Y	166/183 (91%)	166 (100%)	0	100	100
22	Z	177/198 (89%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	a	607/616 (98%)	607 (100%)	0	100	100
24	b	591/592 (100%)	587 (99%)	4 (1%)	76	82
25	c	68/69 (99%)	68 (100%)	0	100	100
26	d	120/122 (98%)	119 (99%)	1 (1%)	73	81
27	e	51/90 (57%)	51 (100%)	0	100	100
28	f	127/144 (88%)	123 (97%)	4 (3%)	35	64
29	i	28/32 (88%)	28 (100%)	0	100	100
30	j	36/36 (100%)	36 (100%)	0	100	100
31	k	52/85 (61%)	52 (100%)	0	100	100
32	l	114/115 (99%)	114 (100%)	0	100	100
33	m	23/23 (100%)	23 (100%)	0	100	100
34	o	180/208 (86%)	178 (99%)	2 (1%)	65	78
35	p	179/199 (90%)	179 (100%)	0	100	100
35	u	179/199 (90%)	178 (99%)	1 (1%)	78	83
35	x	179/199 (90%)	179 (100%)	0	100	100
36	q	183/204 (90%)	182 (100%)	1 (0%)	81	85
36	v	183/204 (90%)	182 (100%)	1 (0%)	81	85
37	r	71/94 (76%)	70 (99%)	1 (1%)	59	76
38	t	168/204 (82%)	168 (100%)	0	100	100
38	w	168/204 (82%)	167 (99%)	1 (1%)	78	83
38	y	159/204 (78%)	158 (99%)	1 (1%)	78	83
39	z	177/199 (89%)	177 (100%)	0	100	100
All	All	7210/8293 (87%)	7180 (100%)	30 (0%)	81	86

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	b	717	PHE
36	v	84	MET
26	d	38	SER
38	y	141	ASP
36	q	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
36	q	44	ASN
36	q	195	ASN
35	u	140	ASN
16	Q	59	ASN
14	N	110	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](#)

790 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	$\# Z > 2$
40	CLA	u	307	35	59,63,73	1.93	9 (15%)	71,101,113	1.72	9 (12%)
49	BCR	b	847	-	41,41,41	0.19	0	56,56,56	0.58	0
40	CLA	a	831	-	64,68,73	1.85	9 (14%)	77,107,113	1.42	5 (6%)
40	CLA	a	850	-	69,73,73	1.70	9 (13%)	83,113,113	1.53	8 (9%)
41	KC2	o	309	34	49,53,53	1.89	4 (8%)	62,89,89	1.29	7 (11%)
44	A86	G	211	-	44,50,50	0.54	1 (2%)	51,76,76	0.75	1 (1%)
40	CLA	b	838	-	69,73,73	1.75	9 (13%)	83,113,113	1.48	8 (9%)
42	DD6	D	316	-	39,45,45	0.21	0	52,67,67	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	F	321	-	64,68,73	1.84	9 (14%)	77,107,113	1.49	9 (11%)
40	CLA	Y	310	-	59,63,73	1.90	9 (15%)	71,101,113	1.51	7 (9%)
42	DD6	F	314	-	39,45,45	0.30	0	52,67,67	1.03	4 (7%)
40	CLA	Q	205	16	65,69,73	1.87	10 (15%)	78,107,113	1.80	12 (15%)
40	CLA	y	309	-	59,63,73	1.97	9 (15%)	71,101,113	1.68	9 (12%)
40	CLA	b	830	24	65,69,73	1.82	9 (13%)	78,108,113	1.60	9 (11%)
40	CLA	X	312	-	51,55,73	2.13	9 (17%)	61,91,113	1.66	9 (14%)
41	KC2	M	308	13	49,53,53	1.89	4 (8%)	62,89,89	1.44	8 (12%)
41	KC2	A	310	1	49,53,53	1.90	4 (8%)	62,89,89	1.32	8 (12%)
41	KC2	K	305	11	49,53,53	1.87	4 (8%)	62,89,89	1.36	7 (11%)
40	CLA	O	306	15	64,68,73	1.83	10 (15%)	77,107,113	1.56	9 (11%)
52	DGD	b	850	-	57,57,67	0.95	2 (3%)	71,71,81	1.47	9 (12%)
40	CLA	E	303	-	64,68,73	1.88	9 (14%)	77,107,113	1.54	8 (10%)
42	DD6	k	204	-	39,45,45	0.20	0	52,67,67	0.83	4 (7%)
40	CLA	T	305	15	54,58,73	1.98	9 (16%)	65,95,113	1.52	7 (10%)
40	CLA	a	803	-	69,73,73	1.71	9 (13%)	83,113,113	1.37	9 (10%)
41	KC2	Q	201	16	49,53,53	1.91	4 (8%)	62,89,89	1.35	7 (11%)
40	CLA	F	311	-	51,55,73	2.07	9 (17%)	61,91,113	1.60	7 (11%)
41	KC2	F	302	6	49,53,53	1.90	4 (8%)	62,89,89	1.34	9 (14%)
44	A86	u	319	-	44,50,50	0.39	1 (2%)	51,76,76	1.40	4 (7%)
40	CLA	S	319	-	51,55,73	2.03	9 (17%)	61,91,113	1.49	6 (9%)
40	CLA	u	308	35	64,68,73	1.83	9 (14%)	77,107,113	1.52	8 (10%)
48	A1EB4	P	320	-	51,58,63	0.80	1 (1%)	60,84,89	1.23	2 (3%)
41	KC2	T	301	-	49,53,53	1.89	4 (8%)	62,89,89	1.33	7 (11%)
44	A86	x	318	-	44,50,50	0.48	1 (2%)	51,76,76	1.30	2 (3%)
44	A86	p	320	-	44,50,50	0.33	0	51,76,76	1.10	4 (7%)
40	CLA	R	307	-	59,63,73	1.91	9 (15%)	71,101,113	1.54	7 (9%)
44	A86	O	315	-	44,50,50	0.39	1 (2%)	51,76,76	0.73	1 (1%)
46	SQD	M	318	-	31,32,54	1.52	4 (12%)	40,43,65	1.22	5 (12%)
47	A1EB1	Y	323	-	51,58,58	0.39	1 (1%)	60,85,85	0.82	2 (3%)
40	CLA	H	308	8	51,55,73	2.04	9 (17%)	61,91,113	1.56	6 (9%)
42	DD6	o	320	-	39,45,45	0.18	0	52,67,67	0.61	1 (1%)
40	CLA	q	307	36	64,68,73	1.85	10 (15%)	77,107,113	1.62	10 (12%)
44	A86	u	316	-	44,50,50	0.42	1 (2%)	51,76,76	1.29	3 (5%)
47	A1EB1	z	323	-	51,58,58	0.53	1 (1%)	60,85,85	0.94	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	KC2	F	309	6	49,53,53	1.89	4 (8%)	62,89,89	1.34	8 (12%)
40	CLA	b	837	24	64,68,73	1.78	9 (14%)	77,107,113	1.50	7 (9%)
40	CLA	a	816	23	69,73,73	1.73	9 (13%)	83,113,113	1.55	10 (12%)
43	LMG	S	322	-	39,39,55	0.95	2 (5%)	47,47,63	1.22	4 (8%)
44	A86	T	313	-	44,50,50	0.41	1 (2%)	51,76,76	0.91	3 (5%)
40	CLA	o	305	34	59,63,73	1.91	9 (15%)	71,101,113	1.49	9 (12%)
41	KC2	p	304	35	49,53,53	1.89	4 (8%)	62,89,89	1.36	8 (12%)
40	CLA	b	809	24	64,68,73	1.88	9 (14%)	77,107,113	1.63	11 (14%)
40	CLA	q	301	-	59,63,73	1.92	9 (15%)	71,101,113	1.56	7 (9%)
40	CLA	a	836	23	69,73,73	1.73	9 (13%)	83,113,113	1.37	7 (8%)
40	CLA	a	819	23	65,69,73	1.81	9 (13%)	78,108,113	1.53	9 (11%)
44	A86	N	321	-	44,50,50	0.47	1 (2%)	51,76,76	0.89	2 (3%)
40	CLA	B	306	-	56,60,73	2.04	9 (16%)	67,97,113	1.60	9 (13%)
41	KC2	W	309	-	49,53,53	1.90	4 (8%)	62,89,89	1.43	9 (14%)
40	CLA	P	306	13	51,55,73	2.03	9 (17%)	61,91,113	1.54	7 (11%)
40	CLA	E	306	5	59,63,73	1.89	9 (15%)	71,101,113	1.50	7 (9%)
40	CLA	T	304	15	64,68,73	1.83	9 (14%)	77,107,113	1.45	7 (9%)
42	DD6	C	312	-	39,45,45	0.15	0	52,67,67	0.95	1 (1%)
40	CLA	w	309	-	59,63,73	1.96	9 (15%)	71,101,113	1.67	8 (11%)
42	DD6	R	314	-	39,45,45	0.18	0	52,67,67	1.05	3 (5%)
40	CLA	M	307	-	64,68,73	1.81	9 (14%)	77,107,113	1.43	7 (9%)
40	CLA	M	312	13	64,68,73	1.82	9 (14%)	77,107,113	1.49	8 (10%)
41	KC2	R	311	15	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
43	LMG	M	317	-	39,39,55	0.89	2 (5%)	47,47,63	1.33	4 (8%)
40	CLA	O	307	-	66,70,73	1.81	9 (13%)	79,109,113	1.43	7 (8%)
40	CLA	a	808	-	69,73,73	1.80	9 (13%)	83,113,113	1.65	10 (12%)
42	DD6	q	318	-	39,45,45	0.21	0	52,67,67	0.96	3 (5%)
40	CLA	M	306	13	66,70,73	1.76	9 (13%)	79,109,113	1.39	5 (6%)
40	CLA	z	311	-	59,63,73	1.99	9 (15%)	71,101,113	1.86	12 (16%)
42	DD6	Y	322	-	39,45,45	0.17	0	52,67,67	0.78	3 (5%)
41	KC2	M	302	13	49,53,53	1.91	4 (8%)	62,89,89	1.34	5 (8%)
40	CLA	A	311	1	51,55,73	2.03	9 (17%)	61,91,113	1.60	7 (11%)
47	A1EB1	F	322	-	51,58,58	0.53	1 (1%)	60,85,85	0.40	0
47	A1EB1	w	314	-	51,58,58	0.52	1 (1%)	60,85,85	0.65	1 (1%)
44	A86	S	315	-	44,50,50	0.38	1 (2%)	51,76,76	1.25	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A86	N	314	-	44,50,50	0.54	1 (2%)	51,76,76	1.08	4 (7%)
42	DD6	E	317	-	39,45,45	0.18	0	52,67,67	0.68	2 (3%)
47	A1EB1	y	314	-	51,58,58	0.57	1 (1%)	60,85,85	0.40	0
40	CLA	a	826	-	65,69,73	1.76	9 (13%)	78,108,113	1.51	9 (11%)
41	KC2	x	309	-	49,53,53	1.86	4 (8%)	62,89,89	1.42	9 (14%)
40	CLA	I	204	9	51,55,73	2.03	9 (17%)	61,91,113	1.55	7 (11%)
41	KC2	v	309	-	49,53,53	1.88	4 (8%)	62,89,89	1.34	7 (11%)
41	KC2	p	315	-	49,53,53	1.89	4 (8%)	62,89,89	1.42	9 (14%)
41	KC2	z	309	39	49,53,53	1.85	4 (8%)	62,89,89	1.33	6 (9%)
42	DD6	J	313	-	39,45,45	0.20	0	52,67,67	0.74	1 (1%)
41	KC2	O	311	-	49,53,53	1.90	4 (8%)	62,89,89	1.33	8 (12%)
47	A1EB1	T	320	-	51,58,58	0.43	1 (1%)	60,85,85	0.67	1 (1%)
41	KC2	u	304	35	49,53,53	1.87	4 (8%)	62,89,89	1.36	8 (12%)
41	KC2	z	303	39	49,53,53	1.91	4 (8%)	62,89,89	1.32	6 (9%)
46	SQD	k	205	-	35,36,54	1.47	5 (14%)	44,47,65	1.28	5 (11%)
40	CLA	X	311	20	67,71,73	1.83	9 (13%)	80,110,113	1.49	8 (10%)
40	CLA	u	312	-	64,68,73	1.82	9 (14%)	77,107,113	1.41	6 (7%)
40	CLA	W	306	13	64,68,73	1.82	9 (14%)	77,107,113	1.50	9 (11%)
42	DD6	A	316	-	39,45,45	0.16	0	52,67,67	0.63	2 (3%)
40	CLA	b	829	-	51,55,73	2.08	9 (17%)	61,91,113	1.55	9 (14%)
45	LHG	a	849	40	29,29,48	0.78	0	32,35,54	1.19	2 (6%)
41	KC2	S	309	17	49,53,53	1.88	4 (8%)	62,89,89	1.37	9 (14%)
44	A86	u	320	-	44,50,50	0.38	1 (2%)	51,76,76	1.21	2 (3%)
44	A86	Z	315	-	44,50,50	0.49	1 (2%)	51,76,76	1.16	3 (5%)
40	CLA	y	308	-	51,55,73	2.03	9 (17%)	61,91,113	1.54	6 (9%)
40	CLA	o	311	-	67,71,73	1.81	9 (13%)	80,110,113	1.47	8 (10%)
40	CLA	K	307	11	58,62,73	1.91	9 (15%)	69,99,113	1.40	7 (10%)
40	CLA	Y	301	-	64,68,73	1.85	9 (14%)	77,107,113	1.40	6 (7%)
44	A86	W	301	-	44,50,50	0.44	1 (2%)	51,76,76	0.60	1 (1%)
41	KC2	U	201	-	49,53,53	1.90	4 (8%)	62,89,89	1.34	7 (11%)
44	A86	t	310	-	44,50,50	0.51	1 (2%)	51,76,76	0.94	3 (5%)
40	CLA	Q	207	-	51,55,73	2.18	9 (17%)	61,91,113	1.84	11 (18%)
40	CLA	H	311	-	51,55,73	2.10	9 (17%)	61,91,113	1.60	7 (11%)
40	CLA	x	308	35	64,68,73	1.82	9 (14%)	77,107,113	1.50	7 (9%)
40	CLA	P	305	13	64,68,73	1.77	9 (14%)	77,107,113	1.44	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	A86	L	314	-	44,50,50	0.73	1 (2%)	51,76,76	1.17	2 (3%)
40	CLA	Y	313	21	51,55,73	2.16	9 (17%)	61,91,113	1.83	10 (16%)
47	A1EB1	P	301	-	51,58,58	0.54	1 (1%)	60,85,85	0.57	0
40	CLA	Z	304	-	64,68,73	1.83	9 (14%)	77,107,113	1.41	8 (10%)
40	CLA	b	826	24	68,72,73	1.77	9 (13%)	81,111,113	1.39	6 (7%)
40	CLA	A	305	1	65,69,73	1.81	9 (13%)	78,108,113	1.48	7 (8%)
40	CLA	C	309	-	51,55,73	2.12	9 (17%)	61,91,113	1.67	8 (13%)
44	A86	S	318	-	44,50,50	0.42	1 (2%)	51,76,76	1.15	1 (1%)
44	A86	H	315	-	44,50,50	0.49	1 (2%)	51,76,76	1.31	4 (7%)
40	CLA	N	306	-	64,68,73	1.82	9 (14%)	77,107,113	1.39	6 (7%)
41	KC2	z	310	39	49,53,53	1.88	4 (8%)	62,89,89	1.30	7 (11%)
41	KC2	Y	314	-	49,53,53	1.92	4 (8%)	62,89,89	1.38	11 (17%)
40	CLA	a	827	23	69,73,73	1.75	9 (13%)	83,113,113	1.37	6 (7%)
40	CLA	k	201	31	59,63,73	1.90	9 (15%)	71,101,113	1.57	8 (11%)
40	CLA	p	314	35	51,55,73	2.11	9 (17%)	61,91,113	1.71	8 (13%)
43	LMG	l	201	-	39,39,55	0.85	1 (2%)	47,47,63	1.25	4 (8%)
41	KC2	Y	303	21	49,53,53	1.83	4 (8%)	62,89,89	1.31	6 (9%)
40	CLA	A	306	1	64,68,73	1.82	9 (14%)	77,107,113	1.38	7 (9%)
40	CLA	A	303	1	65,69,73	1.78	9 (13%)	78,108,113	1.41	7 (8%)
41	KC2	M	303	13	49,53,53	1.90	4 (8%)	62,89,89	1.32	8 (12%)
40	CLA	a	842	-	69,73,73	1.71	9 (13%)	83,113,113	1.36	8 (9%)
40	CLA	a	804	23	65,69,73	1.86	10 (15%)	78,107,113	1.82	11 (14%)
40	CLA	b	801	-	67,71,73	1.80	10 (14%)	80,110,113	1.54	13 (16%)
41	KC2	N	313	14	49,53,53	1.89	4 (8%)	62,89,89	1.30	7 (11%)
43	LMG	x	301	-	39,39,55	0.88	1 (2%)	47,47,63	1.22	4 (8%)
40	CLA	z	305	39	64,68,73	1.79	9 (14%)	77,107,113	1.53	8 (10%)
41	KC2	S	310	-	49,53,53	1.89	4 (8%)	62,89,89	1.33	8 (12%)
40	CLA	u	305	35	51,55,73	2.04	9 (17%)	61,91,113	1.78	8 (13%)
44	A86	z	318	-	44,50,50	0.57	1 (2%)	51,76,76	0.93	2 (3%)
40	CLA	a	828	23	69,73,73	1.71	9 (13%)	83,113,113	1.37	6 (7%)
47	A1EB1	p	324	-	51,58,58	0.50	1 (1%)	60,85,85	0.41	1 (1%)
47	A1EB1	v	323	-	51,58,58	0.53	1 (1%)	60,85,85	0.59	1 (1%)
40	CLA	X	304	-	51,55,73	2.03	9 (17%)	61,91,113	1.57	7 (11%)
40	CLA	P	312	13	64,68,73	1.81	9 (14%)	77,107,113	1.41	8 (10%)
40	CLA	o	312	-	51,55,73	2.12	9 (17%)	61,91,113	1.71	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	KC2	R	309	15	49,53,53	1.94	4 (8%)	62,89,89	1.38	10 (16%)
42	DD6	D	314	-	39,45,45	0.20	0	52,67,67	0.85	1 (1%)
40	CLA	W	305	13	69,73,73	1.75	9 (13%)	83,113,113	1.38	10 (12%)
44	A86	G	209	-	44,50,50	0.55	1 (2%)	51,76,76	1.18	3 (5%)
41	KC2	Z	308	22	49,53,53	1.87	4 (8%)	62,89,89	1.35	8 (12%)
41	KC2	X	303	20	49,53,53	1.89	4 (8%)	62,89,89	1.33	9 (14%)
41	KC2	P	302	-	49,53,53	1.88	4 (8%)	62,89,89	1.35	8 (12%)
43	LMG	A	317	-	40,40,55	0.84	0	48,48,63	1.22	4 (8%)
40	CLA	K	308	11	63,67,73	1.82	9 (14%)	75,105,113	1.55	10 (13%)
40	CLA	l	203	-	68,72,73	1.74	10 (14%)	81,111,113	1.61	9 (11%)
41	KC2	T	308	15	49,53,53	1.90	4 (8%)	62,89,89	1.37	7 (11%)
44	A86	p	321	-	44,50,50	0.34	0	51,76,76	1.04	3 (5%)
42	DD6	W	315	-	39,45,45	0.20	0	52,67,67	0.74	2 (3%)
40	CLA	W	312	13	64,68,73	1.81	9 (14%)	77,107,113	1.39	9 (11%)
41	KC2	O	309	15	49,53,53	1.88	4 (8%)	62,89,89	1.40	7 (11%)
40	CLA	J	302	10	51,55,73	2.06	9 (17%)	61,91,113	1.54	7 (11%)
40	CLA	T	306	15	64,68,73	1.81	10 (15%)	77,107,113	1.45	8 (10%)
44	A86	N	315	-	44,50,50	0.66	1 (2%)	51,76,76	1.21	3 (5%)
41	KC2	S	304	17	49,53,53	1.88	4 (8%)	62,89,89	1.36	8 (12%)
40	CLA	D	310	4	64,68,73	1.77	9 (14%)	77,107,113	1.43	9 (11%)
40	CLA	t	302	38	51,55,73	2.06	9 (17%)	61,91,113	1.62	7 (11%)
40	CLA	O	304	15	69,73,73	1.74	9 (13%)	83,113,113	1.42	9 (10%)
40	CLA	a	810	-	64,68,73	1.82	9 (14%)	77,107,113	1.51	7 (9%)
40	CLA	f	202	24	69,73,73	1.70	9 (13%)	83,113,113	1.33	7 (8%)
41	KC2	Z	302	-	49,53,53	1.93	4 (8%)	62,89,89	1.30	7 (11%)
43	LMG	a	801	-	35,35,55	0.96	0	43,43,63	1.17	4 (9%)
40	CLA	C	304	3	60,64,73	1.89	10 (16%)	72,102,113	1.55	11 (15%)
41	KC2	q	308	36	49,53,53	1.88	4 (8%)	62,89,89	1.39	8 (12%)
42	DD6	T	314	-	39,45,45	0.21	0	52,67,67	0.72	1 (1%)
44	A86	Z	316	-	44,50,50	0.59	1 (2%)	51,76,76	1.23	3 (5%)
41	KC2	N	302	14	49,53,53	1.89	4 (8%)	62,89,89	1.34	8 (12%)
42	DD6	E	315	-	39,45,45	0.20	0	52,67,67	0.97	3 (5%)
41	KC2	L	308	12	49,53,53	1.91	4 (8%)	62,89,89	1.28	5 (8%)
47	A1EB1	y	312	-	51,58,58	0.44	1 (1%)	60,85,85	0.67	1 (1%)
51	SF4	b	804	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	v	305	-	64,68,73	1.84	9 (14%)	77,107,113	1.52	10 (12%)
41	KC2	q	302	36	49,53,53	1.93	4 (8%)	62,89,89	1.35	8 (12%)
40	CLA	x	311	-	59,63,73	1.99	9 (15%)	71,101,113	1.84	13 (18%)
41	KC2	u	315	-	49,53,53	1.89	4 (8%)	62,89,89	1.41	9 (14%)
40	CLA	q	304	-	56,60,73	1.91	9 (16%)	67,97,113	1.50	9 (13%)
42	DD6	A	315	-	39,45,45	0.17	0	52,67,67	0.74	1 (1%)
41	KC2	o	303	34	49,53,53	1.92	5 (10%)	62,89,89	1.33	8 (12%)
40	CLA	a	814	-	54,58,73	2.00	9 (16%)	65,95,113	1.56	7 (10%)
40	CLA	T	310	-	62,66,73	1.85	9 (14%)	74,104,113	1.52	9 (12%)
44	A86	p	316	-	44,50,50	0.42	0	51,76,76	1.18	3 (5%)
40	CLA	u	306	35	51,55,73	2.03	9 (17%)	61,91,113	1.59	8 (13%)
43	LMG	T	318	-	40,40,55	0.93	3 (7%)	48,48,63	1.25	4 (8%)
40	CLA	a	821	23	69,73,73	1.74	9 (13%)	83,113,113	1.37	7 (8%)
42	DD6	K	311	-	39,45,45	0.17	0	52,67,67	0.80	2 (3%)
40	CLA	l	204	-	69,73,73	1.77	9 (13%)	83,113,113	1.29	6 (7%)
40	CLA	D	304	4	60,64,73	1.90	10 (16%)	72,102,113	1.58	8 (11%)
44	A86	u	317	-	44,50,50	0.56	1 (2%)	51,76,76	1.41	2 (3%)
41	KC2	N	309	-	49,53,53	1.87	4 (8%)	62,89,89	1.31	9 (14%)
40	CLA	R	305	15	64,68,73	1.83	9 (14%)	77,107,113	1.47	6 (7%)
41	KC2	W	302	-	49,53,53	1.89	4 (8%)	62,89,89	1.31	7 (11%)
40	CLA	S	311	-	51,55,73	2.16	9 (17%)	61,91,113	1.86	11 (18%)
51	SF4	c	102	-	0,12,12	-	-	-	-	-
42	DD6	F	315	-	39,45,45	0.21	0	52,67,67	1.02	3 (5%)
41	KC2	I	209	9	49,53,53	1.88	4 (8%)	62,89,89	1.40	9 (14%)
40	CLA	P	311	-	51,55,73	2.07	9 (17%)	61,91,113	1.70	10 (16%)
41	KC2	E	319	-	49,53,53	1.90	4 (8%)	62,89,89	1.37	7 (11%)
42	DD6	y	311	-	39,45,45	0.19	0	52,67,67	1.02	4 (7%)
44	A86	o	318	-	44,50,50	0.60	1 (2%)	51,76,76	0.50	0
42	DD6	Z	318	-	39,45,45	0.21	0	52,67,67	1.05	3 (5%)
40	CLA	E	307	-	69,73,73	1.73	9 (13%)	83,113,113	1.29	6 (7%)
41	KC2	M	309	-	49,53,53	1.93	4 (8%)	62,89,89	1.34	8 (12%)
42	DD6	x	320	-	39,45,45	0.18	0	52,67,67	0.65	0
40	CLA	J	303	-	51,55,73	2.14	8 (15%)	61,91,113	1.67	8 (13%)
40	CLA	Z	311	22	67,71,73	1.82	9 (13%)	80,110,113	1.51	10 (12%)
41	KC2	G	208	-	49,53,53	1.89	4 (8%)	62,89,89	1.29	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	DD6	N	316	-	39,45,45	0.22	0	52,67,67	1.07	3 (5%)
40	CLA	Y	307	21	64,68,73	1.85	9 (14%)	77,107,113	1.56	9 (11%)
40	CLA	v	310	-	55,59,73	1.97	9 (16%)	66,96,113	1.67	10 (15%)
40	CLA	G	205	7	54,58,73	1.97	9 (16%)	65,95,113	1.53	7 (10%)
44	A86	M	320	-	44,50,50	0.37	1 (2%)	51,76,76	0.59	0
40	CLA	b	803	-	69,73,73	1.74	9 (13%)	83,113,113	1.47	9 (10%)
44	A86	O	312	-	44,50,50	0.48	1 (2%)	51,76,76	1.06	2 (3%)
42	DD6	U	209	-	39,45,45	0.27	0	52,67,67	0.80	2 (3%)
47	A1EB1	u	322	-	51,58,58	0.35	0	60,85,85	1.33	6 (10%)
42	DD6	z	322	-	39,45,45	0.22	0	52,67,67	1.05	3 (5%)
42	DD6	Q	212	-	39,45,45	0.20	0	52,67,67	0.73	2 (3%)
44	A86	p	317	-	44,50,50	0.57	1 (2%)	51,76,76	1.31	2 (3%)
44	A86	t	311	-	44,50,50	0.63	1 (2%)	51,76,76	1.29	3 (5%)
40	CLA	b	841	24	69,73,73	1.72	9 (13%)	83,113,113	1.34	8 (9%)
47	A1EB1	Z	319	-	51,58,58	0.51	1 (1%)	60,85,85	0.68	1 (1%)
40	CLA	b	832	24	69,73,73	1.77	9 (13%)	83,113,113	1.55	8 (9%)
40	CLA	a	839	45	69,73,73	1.73	9 (13%)	83,113,113	1.42	7 (8%)
40	CLA	b	840	-	69,73,73	1.79	9 (13%)	83,113,113	1.47	8 (9%)
41	KC2	Z	309	-	49,53,53	1.93	4 (8%)	62,89,89	1.30	6 (9%)
40	CLA	q	311	-	67,71,73	1.85	9 (13%)	80,110,113	1.47	8 (10%)
40	CLA	a	815	23	69,73,73	1.78	9 (13%)	83,113,113	1.45	9 (10%)
40	CLA	W	308	-	64,68,73	1.91	9 (14%)	77,107,113	1.61	11 (14%)
40	CLA	b	815	-	61,65,73	1.87	9 (14%)	73,103,113	1.48	7 (9%)
44	A86	U	210	-	44,50,50	0.43	1 (2%)	51,76,76	1.08	3 (5%)
40	CLA	b	802	-	69,73,73	1.72	9 (13%)	83,113,113	1.38	7 (8%)
41	KC2	L	309	12	49,53,53	1.92	4 (8%)	62,89,89	1.33	7 (11%)
41	KC2	Z	303	22	49,53,53	1.86	4 (8%)	62,89,89	1.32	8 (12%)
40	CLA	T	317	47	51,55,73	2.02	8 (15%)	61,91,113	1.48	7 (11%)
40	CLA	P	313	-	64,68,73	1.81	9 (14%)	77,107,113	1.44	7 (9%)
40	CLA	t	309	-	51,55,73	2.07	9 (17%)	61,91,113	1.62	6 (9%)
42	DD6	E	318	-	39,45,45	0.19	0	52,67,67	0.90	5 (9%)
40	CLA	a	832	23	69,73,73	1.75	9 (13%)	83,113,113	1.36	7 (8%)
40	CLA	p	311	-	59,63,73	2.03	9 (15%)	71,101,113	1.80	12 (16%)
41	KC2	v	303	36	49,53,53	1.90	4 (8%)	62,89,89	1.37	7 (11%)
40	CLA	L	305	12	51,55,73	2.10	9 (17%)	61,91,113	1.61	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	A1EB1	t	314	-	51,58,58	0.62	1 (1%)	60,85,85	0.90	3 (5%)
40	CLA	N	305	14	59,63,73	1.88	9 (15%)	71,101,113	1.51	7 (9%)
40	CLA	a	833	23	64,68,73	1.83	9 (14%)	77,107,113	1.48	8 (10%)
42	DD6	C	310	-	39,45,45	0.19	0	52,67,67	0.94	4 (7%)
44	A86	N	318	-	44,50,50	0.68	1 (2%)	51,76,76	0.46	0
44	A86	w	310	-	44,50,50	0.45	1 (2%)	51,76,76	1.25	2 (3%)
41	KC2	x	303	-	49,53,53	1.94	4 (8%)	62,89,89	1.31	6 (9%)
40	CLA	E	310	-	64,68,73	1.82	9 (14%)	77,107,113	1.49	8 (10%)
40	CLA	R	316	47	51,55,73	2.01	8 (15%)	61,91,113	1.46	8 (13%)
44	A86	Q	210	-	44,50,50	0.41	1 (2%)	51,76,76	0.89	1 (1%)
40	CLA	W	311	-	59,63,73	1.93	9 (15%)	71,101,113	1.60	8 (11%)
40	CLA	G	204	7	59,63,73	1.90	9 (15%)	71,101,113	1.53	8 (11%)
41	KC2	q	309	-	49,53,53	1.88	4 (8%)	62,89,89	1.33	9 (14%)
40	CLA	k	202	-	59,63,73	1.89	9 (15%)	71,101,113	1.48	8 (11%)
44	A86	Y	319	-	44,50,50	0.45	1 (2%)	51,76,76	1.15	4 (7%)
49	BCR	b	844	-	41,41,41	0.26	0	56,56,56	0.59	1 (1%)
50	PQN	b	849	-	29,29,34	0.43	0	36,39,45	0.77	1 (2%)
40	CLA	X	306	20	59,63,73	1.93	9 (15%)	71,101,113	1.62	11 (15%)
40	CLA	a	829	-	69,73,73	1.77	9 (13%)	83,113,113	1.50	9 (10%)
40	CLA	K	301	-	51,55,73	2.03	9 (17%)	61,91,113	1.54	7 (11%)
40	CLA	x	302	-	69,73,73	1.83	9 (13%)	83,113,113	1.53	8 (9%)
40	CLA	z	308	39	64,68,73	1.77	9 (14%)	77,107,113	1.57	10 (12%)
40	CLA	a	837	23	59,63,73	1.92	9 (15%)	71,101,113	1.47	7 (9%)
43	LMG	L	319	-	37,37,55	0.86	0	45,45,63	1.23	4 (8%)
42	DD6	z	321	-	39,45,45	0.22	0	52,67,67	0.91	3 (5%)
40	CLA	b	818	24	66,70,73	1.77	9 (13%)	79,109,113	1.43	7 (8%)
40	CLA	S	306	17	60,64,73	1.88	9 (15%)	72,102,113	1.48	7 (9%)
41	KC2	o	302	-	49,53,53	1.90	4 (8%)	62,89,89	1.37	9 (14%)
41	KC2	Y	308	-	49,53,53	1.88	4 (8%)	62,89,89	1.41	8 (12%)
40	CLA	p	308	-	64,68,73	1.83	9 (14%)	77,107,113	1.55	8 (10%)
49	BCR	a	846	-	41,41,41	0.16	0	56,56,56	0.41	0
44	A86	z	301	-	44,50,50	0.49	1 (2%)	51,76,76	1.08	2 (3%)
40	CLA	G	203	7	57,62,73	1.77	8 (14%)	67,99,113	1.67	12 (17%)
40	CLA	y	302	38	51,55,73	2.14	9 (17%)	61,91,113	1.70	9 (14%)
44	A86	z	319	-	44,50,50	0.54	1 (2%)	51,76,76	1.07	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	BCR	a	844	-	41,41,41	0.17	0	56,56,56	0.47	0
40	CLA	C	302	-	51,55,73	2.09	9 (17%)	61,91,113	1.75	8 (13%)
40	CLA	J	305	10	59,63,73	1.94	10 (16%)	71,101,113	1.52	7 (9%)
40	CLA	L	304	12	61,65,73	1.90	9 (14%)	73,103,113	1.54	8 (10%)
40	CLA	H	306	8	54,58,73	2.00	9 (16%)	65,95,113	1.53	8 (12%)
40	CLA	I	202	9	59,63,73	1.87	9 (15%)	71,101,113	1.46	7 (9%)
40	CLA	F	310	-	51,55,73	2.03	9 (17%)	61,91,113	1.61	11 (18%)
40	CLA	z	307	-	64,68,73	1.86	9 (14%)	77,107,113	1.56	9 (11%)
42	DD6	K	310	-	39,45,45	0.23	0	52,67,67	0.67	2 (3%)
40	CLA	U	206	-	51,55,73	2.07	9 (17%)	61,91,113	1.50	8 (13%)
40	CLA	U	204	18	51,55,73	2.09	9 (17%)	61,91,113	1.60	7 (11%)
44	A86	t	316	-	44,50,50	0.58	1 (2%)	51,76,76	0.50	0
42	DD6	H	313	-	39,45,45	0.24	0	52,67,67	0.98	4 (7%)
40	CLA	U	202	18	59,63,73	1.96	9 (15%)	71,101,113	1.66	10 (14%)
41	KC2	v	302	-	49,53,53	1.93	4 (8%)	62,89,89	1.32	7 (11%)
44	A86	X	321	-	44,50,50	0.81	1 (2%)	51,76,76	1.18	3 (5%)
40	CLA	p	302	-	69,73,73	1.77	9 (13%)	83,113,113	1.46	9 (10%)
40	CLA	q	305	-	64,68,73	1.82	9 (14%)	77,107,113	1.51	9 (11%)
40	CLA	Z	301	-	64,68,73	1.83	9 (14%)	77,107,113	1.39	6 (7%)
43	LMG	E	321	-	40,40,55	0.87	1 (2%)	48,48,63	1.27	7 (14%)
49	BCR	l	207	-	41,41,41	0.26	0	56,56,56	0.92	3 (5%)
43	LMG	W	317	-	39,39,55	0.85	0	47,47,63	1.29	6 (12%)
41	KC2	p	309	-	49,53,53	1.89	4 (8%)	62,89,89	1.40	9 (14%)
40	CLA	A	304	1	69,73,73	1.79	9 (13%)	83,113,113	1.53	11 (13%)
40	CLA	R	306	15	64,68,73	1.84	9 (14%)	77,107,113	1.46	8 (10%)
42	DD6	A	314	-	39,45,45	0.16	0	52,67,67	0.72	1 (1%)
40	CLA	b	823	24	59,63,73	1.87	9 (15%)	71,101,113	1.55	8 (11%)
41	KC2	L	313	12	49,53,53	1.92	4 (8%)	62,89,89	1.34	7 (11%)
40	CLA	l	202	-	69,73,73	1.76	9 (13%)	83,113,113	1.40	9 (10%)
41	KC2	W	304	13	49,53,53	1.88	4 (8%)	62,89,89	1.34	9 (14%)
40	CLA	I	207	9	51,55,73	2.09	9 (17%)	61,91,113	1.72	8 (13%)
41	KC2	t	301	38	49,53,53	1.89	5 (10%)	62,89,89	1.32	8 (12%)
41	KC2	X	308	20	49,53,53	1.89	4 (8%)	62,89,89	1.31	8 (12%)
40	CLA	D	307	4	69,73,73	1.76	9 (13%)	83,113,113	1.46	11 (13%)
44	A86	X	319	-	44,50,50	0.44	1 (2%)	51,76,76	1.46	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	w	304	-	64,68,73	1.83	9 (14%)	77,107,113	1.42	8 (10%)
44	A86	T	319	-	44,50,50	0.62	1 (2%)	51,76,76	0.79	2 (3%)
40	CLA	a	806	23	69,73,73	1.76	9 (13%)	83,113,113	1.55	8 (9%)
40	CLA	F	301	-	57,61,73	1.96	9 (15%)	68,98,113	1.53	7 (10%)
40	CLA	U	203	-	59,63,73	1.98	9 (15%)	71,101,113	1.59	10 (14%)
47	A1EB1	Z	320	-	51,58,58	0.30	0	60,85,85	0.61	0
40	CLA	W	307	13	69,73,73	1.75	9 (13%)	83,113,113	1.37	10 (12%)
40	CLA	P	307	13	63,67,73	1.84	9 (14%)	75,105,113	1.51	8 (10%)
40	CLA	D	303	4	64,68,73	1.78	9 (14%)	77,107,113	1.47	7 (9%)
40	CLA	Y	304	-	51,55,73	2.11	9 (17%)	61,91,113	1.61	8 (13%)
49	BCR	m	101	-	41,41,41	0.17	0	56,56,56	0.34	0
44	A86	K	314	-	44,50,50	0.47	1 (2%)	51,76,76	1.07	3 (5%)
40	CLA	I	203	9	59,63,73	1.96	9 (15%)	71,101,113	1.59	8 (11%)
41	KC2	X	302	-	49,53,53	1.90	4 (8%)	62,89,89	1.33	7 (11%)
42	DD6	Q	214	-	39,45,45	0.18	0	52,67,67	0.77	1 (1%)
40	CLA	o	307	34	64,68,73	1.82	9 (14%)	77,107,113	1.63	11 (14%)
40	CLA	Q	206	-	63,68,73	1.77	9 (14%)	74,105,113	1.83	10 (13%)
40	CLA	O	316	47	51,55,73	2.03	9 (17%)	61,91,113	1.48	7 (11%)
46	SQD	I	215	-	53,54,54	1.20	4 (7%)	62,65,65	1.12	5 (8%)
40	CLA	Q	209	-	51,55,73	2.10	9 (17%)	61,91,113	1.70	9 (14%)
42	DD6	I	213	-	39,45,45	0.26	0	52,67,67	0.99	3 (5%)
42	DD6	t	312	-	39,45,45	0.16	0	52,67,67	0.99	3 (5%)
42	DD6	v	318	-	39,45,45	0.23	0	52,67,67	0.84	3 (5%)
44	A86	z	316	-	44,50,50	0.54	1 (2%)	51,76,76	1.76	3 (5%)
40	CLA	D	302	43	62,66,73	1.88	9 (14%)	74,104,113	1.50	7 (9%)
47	A1EB1	q	321	-	51,58,58	0.53	1 (1%)	60,85,85	0.94	3 (5%)
40	CLA	C	306	3	69,73,73	1.76	9 (13%)	83,113,113	1.37	9 (10%)
42	DD6	H	314	-	39,45,45	0.23	0	52,67,67	0.92	3 (5%)
41	KC2	P	303	13	49,53,53	1.94	4 (8%)	62,89,89	1.40	6 (9%)
44	A86	Y	320	-	44,50,50	0.64	1 (2%)	51,76,76	1.59	3 (5%)
40	CLA	v	307	36	64,68,73	1.85	9 (14%)	77,107,113	1.62	10 (12%)
47	A1EB1	O	317	40	51,58,58	0.56	1 (1%)	60,85,85	0.80	1 (1%)
40	CLA	G	201	7	51,55,73	2.04	9 (17%)	61,91,113	1.54	7 (11%)
40	CLA	F	305	-	51,55,73	2.06	9 (17%)	61,91,113	1.69	8 (13%)
40	CLA	z	324	-	51,55,73	2.10	9 (17%)	61,91,113	1.68	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	BCR	b	843	-	41,41,41	0.13	0	56,56,56	0.43	0
47	A1EB1	o	322	-	51,58,58	0.56	1 (1%)	60,85,85	0.66	1 (1%)
40	CLA	p	307	35	59,63,73	1.98	9 (15%)	71,101,113	1.72	9 (12%)
41	KC2	x	304	35	49,53,53	1.88	4 (8%)	62,89,89	1.32	6 (9%)
44	A86	q	324	-	44,50,50	0.34	0	51,76,76	1.07	3 (5%)
40	CLA	x	312	-	64,68,73	1.82	9 (14%)	77,107,113	1.44	8 (10%)
41	KC2	R	302	15	49,53,53	1.93	5 (10%)	62,89,89	1.34	9 (14%)
40	CLA	u	314	35	51,55,73	2.12	9 (17%)	61,91,113	1.80	9 (14%)
40	CLA	F	306	6	64,68,73	1.82	9 (14%)	77,107,113	1.42	8 (10%)
43	LMG	E	320	-	31,31,55	0.99	1 (3%)	39,39,63	1.17	2 (5%)
42	DD6	J	314	-	39,45,45	0.19	0	52,67,67	0.69	2 (3%)
40	CLA	F	303	6	65,69,73	1.85	10 (15%)	78,107,113	1.79	10 (12%)
44	A86	v	325	-	44,50,50	0.34	0	51,76,76	1.05	2 (3%)
42	DD6	L	317	-	39,45,45	0.15	0	52,67,67	0.71	2 (3%)
44	A86	F	313	-	44,50,50	0.43	1 (2%)	51,76,76	0.78	2 (3%)
40	CLA	M	310	-	60,64,73	1.83	9 (15%)	72,102,113	1.41	9 (12%)
40	CLA	G	207	-	58,62,73	1.93	9 (15%)	69,99,113	1.51	9 (13%)
47	A1EB1	L	318	-	51,58,58	0.58	1 (1%)	60,85,85	0.73	1 (1%)
40	CLA	H	309	-	60,64,73	1.94	9 (15%)	72,102,113	1.74	11 (15%)
44	A86	Z	314	-	44,50,50	0.51	1 (2%)	51,76,76	1.39	3 (5%)
42	DD6	J	301	-	39,45,45	0.22	0	52,67,67	0.75	3 (5%)
40	CLA	W	313	13	64,68,73	1.84	9 (14%)	77,107,113	1.43	7 (9%)
40	CLA	D	306	4	59,63,73	1.91	9 (15%)	71,101,113	1.49	8 (11%)
40	CLA	K	306	-	64,68,73	1.78	9 (14%)	77,107,113	1.48	10 (12%)
44	A86	Y	316	-	44,50,50	0.44	1 (2%)	51,76,76	0.61	1 (1%)
48	A1EB4	W	319	-	51,58,63	0.68	1 (1%)	60,84,89	0.68	1 (1%)
40	CLA	E	302	5	51,55,73	2.08	9 (17%)	61,91,113	1.82	9 (14%)
40	CLA	E	311	-	54,58,73	2.05	9 (16%)	65,95,113	1.62	7 (10%)
43	LMG	F	318	-	39,39,55	0.80	0	47,47,63	1.33	6 (12%)
41	KC2	O	302	15	49,53,53	1.91	5 (10%)	62,89,89	1.40	10 (16%)
40	CLA	J	311	-	51,55,73	2.11	9 (17%)	61,91,113	1.71	7 (11%)
40	CLA	L	306	12	51,55,73	2.15	9 (17%)	61,91,113	1.84	11 (18%)
40	CLA	S	312	-	51,55,73	2.12	9 (17%)	61,91,113	1.76	10 (16%)
41	KC2	W	303	-	49,53,53	1.90	4 (8%)	62,89,89	1.35	9 (14%)
41	KC2	w	301	38	49,53,53	1.89	4 (8%)	62,89,89	1.33	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	Z	312	-	51,55,73	2.15	9 (17%)	61,91,113	1.78	15 (24%)
40	CLA	w	303	38	51,55,73	2.08	9 (17%)	61,91,113	1.62	7 (11%)
44	A86	q	315	-	44,50,50	0.50	1 (2%)	51,76,76	0.90	2 (3%)
40	CLA	a	817	23	54,58,73	1.96	9 (16%)	65,95,113	1.54	7 (10%)
40	CLA	b	824	24	69,73,73	1.70	9 (13%)	83,113,113	1.41	10 (12%)
41	KC2	H	303	-	49,53,53	1.89	4 (8%)	62,89,89	1.33	7 (11%)
41	KC2	K	309	11	49,53,53	1.89	4 (8%)	62,89,89	1.39	8 (12%)
41	KC2	z	304	39	49,53,53	1.87	5 (10%)	62,89,89	1.40	8 (12%)
40	CLA	b	833	24	64,68,73	1.78	9 (14%)	77,107,113	1.47	8 (10%)
40	CLA	z	312	-	64,68,73	1.83	9 (14%)	77,107,113	1.46	9 (11%)
41	KC2	S	303	17	49,53,53	1.91	4 (8%)	62,89,89	1.33	8 (12%)
40	CLA	Z	306	22	64,68,73	1.86	9 (14%)	77,107,113	1.53	9 (11%)
40	CLA	E	313	5	51,55,73	2.04	9 (17%)	61,91,113	1.60	6 (9%)
40	CLA	a	825	-	69,73,73	1.74	9 (13%)	83,113,113	1.38	7 (8%)
49	BCR	b	845	-	41,41,41	0.18	0	56,56,56	0.39	0
41	KC2	L	302	-	49,53,53	1.92	4 (8%)	62,89,89	1.34	9 (14%)
40	CLA	a	824	-	66,70,73	1.79	9 (13%)	79,109,113	1.39	9 (11%)
40	CLA	F	307	6	62,67,73	1.74	9 (14%)	73,105,113	1.59	9 (12%)
40	CLA	b	812	24	64,68,73	1.78	9 (14%)	77,107,113	1.36	6 (7%)
40	CLA	z	313	-	51,55,73	2.12	9 (17%)	61,91,113	1.74	9 (14%)
40	CLA	b	819	24	68,72,73	1.76	9 (13%)	81,111,113	1.40	6 (7%)
42	DD6	E	316	-	39,45,45	0.22	0	52,67,67	0.91	3 (5%)
40	CLA	p	305	35	51,55,73	1.97	9 (17%)	61,91,113	1.68	8 (13%)
40	CLA	A	307	1	64,68,73	1.85	10 (15%)	77,107,113	1.53	8 (10%)
42	DD6	B	305	-	39,45,45	0.19	0	52,67,67	0.78	2 (3%)
40	CLA	t	307	-	59,63,73	1.94	9 (15%)	71,101,113	1.67	9 (12%)
44	A86	p	318	-	44,50,50	0.48	1 (2%)	51,76,76	1.25	3 (5%)
41	KC2	t	306	-	49,53,53	1.88	4 (8%)	62,89,89	1.31	7 (11%)
40	CLA	J	308	10	59,63,73	1.90	10 (16%)	71,101,113	1.49	8 (11%)
40	CLA	N	311	14	64,68,73	1.83	9 (14%)	77,107,113	1.54	8 (10%)
40	CLA	a	805	40,23	58,62,73	1.87	9 (15%)	69,99,113	1.53	7 (10%)
40	CLA	a	840	23	59,63,73	1.88	9 (15%)	71,101,113	1.50	8 (11%)
44	A86	y	310	-	44,50,50	0.53	1 (2%)	51,76,76	1.19	4 (7%)
40	CLA	B	302	2	51,55,73	2.04	9 (17%)	61,91,113	1.51	6 (9%)
44	A86	R	312	-	44,50,50	0.77	1 (2%)	51,76,76	1.28	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	E	308	5	62,66,73	1.84	9 (14%)	74,104,113	1.53	8 (10%)
40	CLA	o	304	34	64,68,73	1.80	9 (14%)	77,107,113	1.44	7 (9%)
44	A86	o	314	-	44,50,50	0.48	1 (2%)	51,76,76	1.40	5 (9%)
40	CLA	q	312	-	64,68,73	1.81	9 (14%)	77,107,113	1.36	6 (7%)
40	CLA	b	808	-	69,73,73	1.77	9 (13%)	83,113,113	1.33	10 (12%)
41	KC2	N	308	14	49,53,53	1.91	4 (8%)	62,89,89	1.36	7 (11%)
41	KC2	O	303	15	49,53,53	1.90	4 (8%)	62,89,89	1.33	8 (12%)
42	DD6	N	319	-	39,45,45	0.15	0	52,67,67	1.04	3 (5%)
40	CLA	b	816	24	51,55,73	2.06	9 (17%)	61,91,113	1.72	9 (14%)
49	BCR	f	203	-	41,41,41	0.22	0	56,56,56	0.40	0
44	A86	R	313	-	44,50,50	0.62	1 (2%)	51,76,76	0.64	0
42	DD6	D	315	-	39,45,45	0.17	0	52,67,67	0.98	3 (5%)
40	CLA	q	306	36	64,68,73	1.83	10 (15%)	77,107,113	1.49	7 (9%)
41	KC2	J	304	-	49,53,53	1.91	4 (8%)	62,89,89	1.41	9 (14%)
44	A86	X	320	-	44,50,50	0.51	1 (2%)	51,76,76	1.01	2 (3%)
46	SQD	P	319	-	31,32,54	1.54	4 (12%)	40,43,65	1.39	8 (20%)
40	CLA	J	312	-	62,66,73	1.84	9 (14%)	74,104,113	1.42	7 (9%)
47	A1EB1	v	321	-	51,58,58	0.51	1 (1%)	60,85,85	0.90	4 (6%)
40	CLA	T	307	-	59,63,73	1.90	9 (15%)	71,101,113	1.56	7 (9%)
42	DD6	P	315	-	39,45,45	0.39	0	52,67,67	1.02	2 (3%)
44	A86	M	316	-	44,50,50	0.49	1 (2%)	51,76,76	0.83	3 (5%)
44	A86	o	316	-	44,50,50	0.56	1 (2%)	51,76,76	1.03	3 (5%)
40	CLA	a	813	23	64,68,73	1.86	9 (14%)	77,107,113	1.48	8 (10%)
40	CLA	R	304	15	55,59,73	1.96	9 (16%)	66,96,113	1.67	11 (16%)
40	CLA	b	813	24	54,58,73	1.94	9 (16%)	65,95,113	1.60	9 (13%)
44	A86	w	311	-	44,50,50	0.55	2 (4%)	51,76,76	1.16	3 (5%)
44	A86	v	319	-	44,50,50	0.36	0	51,76,76	1.30	4 (7%)
40	CLA	E	312	-	51,55,73	2.06	9 (17%)	61,91,113	1.73	7 (11%)
40	CLA	X	301	-	64,68,73	1.82	9 (14%)	77,107,113	1.43	6 (7%)
44	A86	v	317	-	44,50,50	0.46	1 (2%)	51,76,76	0.87	1 (1%)
41	KC2	R	301	15	49,53,53	1.85	4 (8%)	62,89,89	1.34	9 (14%)
40	CLA	x	313	-	59,63,73	1.91	9 (15%)	71,101,113	1.40	7 (9%)
44	A86	x	319	-	44,50,50	0.30	0	51,76,76	1.41	2 (3%)
42	DD6	Q	211	-	39,45,45	0.20	0	52,67,67	0.80	2 (3%)
40	CLA	a	838	23	59,63,73	1.95	9 (15%)	71,101,113	1.65	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	Z	313	22	51,55,73	2.10	9 (17%)	61,91,113	1.82	10 (16%)
40	CLA	O	305	15	51,55,73	2.08	9 (17%)	61,91,113	1.63	8 (13%)
40	CLA	L	311	12	51,55,73	2.13	9 (17%)	61,91,113	1.67	8 (13%)
40	CLA	F	304	6	59,63,73	1.99	9 (15%)	71,101,113	1.61	10 (14%)
40	CLA	R	310	-	51,55,73	2.06	9 (17%)	61,91,113	1.66	8 (13%)
42	DD6	u	321	-	39,45,45	0.21	0	52,67,67	0.62	0
40	CLA	I	206	9	69,73,73	1.76	10 (14%)	83,113,113	1.41	8 (9%)
40	CLA	a	830	-	62,66,73	1.83	9 (14%)	74,104,113	1.52	10 (13%)
40	CLA	D	309	-	62,66,73	1.87	9 (14%)	74,104,113	1.45	7 (9%)
40	CLA	b	805	-	65,69,73	1.81	9 (13%)	78,108,113	1.44	7 (8%)
44	A86	F	317	-	44,50,50	0.42	1 (2%)	51,76,76	0.84	2 (3%)
40	CLA	J	310	-	51,55,73	2.15	9 (17%)	61,91,113	1.78	9 (14%)
40	CLA	p	312	-	51,55,73	2.08	9 (17%)	61,91,113	1.62	8 (13%)
41	KC2	y	306	-	49,53,53	1.89	4 (8%)	62,89,89	1.30	8 (12%)
49	BCR	a	843	-	41,41,41	0.20	0	56,56,56	0.44	0
49	BCR	b	848	-	41,41,41	0.15	0	56,56,56	0.33	0
40	CLA	X	310	-	59,63,73	1.99	8 (13%)	71,101,113	1.82	11 (15%)
40	CLA	B	303	-	51,55,73	2.05	9 (17%)	61,91,113	1.57	7 (11%)
40	CLA	H	310	-	64,68,73	1.83	9 (14%)	77,107,113	1.48	6 (7%)
40	CLA	P	308	-	64,68,73	1.82	9 (14%)	77,107,113	1.41	8 (10%)
40	CLA	a	851	-	69,73,73	1.75	9 (13%)	83,113,113	1.42	8 (9%)
40	CLA	p	306	35	51,55,73	2.07	9 (17%)	61,91,113	1.61	8 (13%)
40	CLA	D	301	4	59,63,73	1.87	9 (15%)	71,101,113	1.46	7 (9%)
40	CLA	q	313	36	51,55,73	2.07	9 (17%)	61,91,113	1.63	8 (13%)
44	A86	q	316	-	44,50,50	0.56	1 (2%)	51,76,76	1.52	1 (1%)
40	CLA	E	314	5	51,55,73	2.13	9 (17%)	61,91,113	2.05	12 (19%)
40	CLA	I	205	9	60,64,73	1.87	9 (15%)	72,102,113	1.46	8 (11%)
41	KC2	N	303	14	49,53,53	1.85	4 (8%)	62,89,89	1.39	9 (14%)
42	DD6	X	322	-	39,45,45	0.18	0	52,67,67	0.73	2 (3%)
44	A86	S	316	-	44,50,50	0.55	1 (2%)	51,76,76	1.13	4 (7%)
44	A86	v	314	-	44,50,50	0.55	1 (2%)	51,76,76	1.65	5 (9%)
40	CLA	A	302	-	64,68,73	1.84	9 (14%)	77,107,113	1.40	7 (9%)
40	CLA	M	305	13	64,68,73	1.80	9 (14%)	77,107,113	1.44	7 (9%)
40	CLA	b	827	24	64,68,73	1.84	9 (14%)	77,107,113	1.56	8 (10%)
40	CLA	w	305	-	53,57,73	2.03	9 (16%)	67,94,113	1.58	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	o	301	-	64,68,73	1.86	9 (14%)	77,107,113	1.40	5 (6%)
45	LHG	F	319	-	39,39,48	0.67	1 (2%)	42,45,54	1.16	2 (4%)
42	DD6	U	211	-	39,45,45	0.20	0	52,67,67	0.82	2 (3%)
47	A1EB1	x	322	-	51,58,58	0.58	1 (1%)	60,85,85	0.58	1 (1%)
40	CLA	Y	306	21	64,68,73	1.85	10 (15%)	77,107,113	1.53	10 (12%)
40	CLA	f	201	-	64,68,73	1.82	9 (14%)	77,107,113	1.37	7 (9%)
44	A86	w	316	-	44,50,50	0.59	1 (2%)	51,76,76	1.15	3 (5%)
47	A1EB1	q	323	-	51,58,58	0.56	1 (1%)	60,85,85	0.50	0
40	CLA	E	309	-	64,68,73	1.82	9 (14%)	77,107,113	1.44	9 (11%)
44	A86	O	313	-	44,50,50	0.30	0	51,76,76	0.82	2 (3%)
44	A86	v	316	-	44,50,50	0.58	1 (2%)	51,76,76	1.51	1 (1%)
49	BCR	b	846	-	41,41,41	0.13	0	56,56,56	0.65	1 (1%)
41	KC2	W	310	13	49,53,53	1.92	4 (8%)	62,89,89	1.36	8 (12%)
42	DD6	D	313	-	39,45,45	0.19	0	52,67,67	0.88	2 (3%)
44	A86	Y	317	41	44,50,50	0.56	1 (2%)	51,76,76	0.97	4 (7%)
42	DD6	I	211	-	39,45,45	0.22	0	52,67,67	1.08	4 (7%)
44	A86	x	316	-	44,50,50	0.45	1 (2%)	51,76,76	1.23	3 (5%)
42	DD6	L	315	-	39,45,45	0.15	0	52,67,67	0.57	2 (3%)
40	CLA	L	312	-	51,55,73	2.10	9 (17%)	61,91,113	1.59	8 (13%)
40	CLA	t	304	-	64,68,73	1.83	10 (15%)	77,107,113	1.44	8 (10%)
44	A86	z	317	-	44,50,50	0.58	1 (2%)	51,76,76	1.72	2 (3%)
40	CLA	V	201	-	62,66,73	1.86	9 (14%)	74,104,113	1.44	6 (8%)
41	KC2	w	307	-	49,53,53	1.89	4 (8%)	62,89,89	1.35	9 (14%)
40	CLA	D	308	4	59,63,73	1.91	9 (15%)	71,101,113	1.50	8 (11%)
48	A1EB4	M	319	-	51,58,63	0.62	1 (1%)	60,84,89	0.61	1 (1%)
40	CLA	b	820	-	69,73,73	1.78	9 (13%)	83,113,113	1.42	9 (10%)
44	A86	C	311	-	44,50,50	0.70	1 (2%)	51,76,76	1.02	3 (5%)
47	A1EB1	y	313	-	51,58,58	0.45	1 (1%)	60,85,85	0.80	2 (3%)
49	BCR	r	201	-	41,41,41	0.19	0	56,56,56	0.39	0
42	DD6	H	312	-	39,45,45	0.22	0	52,67,67	1.12	4 (7%)
41	KC2	O	301	15	49,53,53	1.89	4 (8%)	62,89,89	1.41	8 (12%)
40	CLA	U	205	-	51,55,73	2.09	9 (17%)	61,91,113	1.66	8 (13%)
44	A86	D	319	-	44,50,50	0.46	1 (2%)	51,76,76	1.05	2 (3%)
40	CLA	b	822	-	68,72,73	1.79	9 (13%)	81,111,113	1.52	9 (11%)
49	BCR	a	845	-	41,41,41	0.14	0	56,56,56	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	DD6	I	210	-	39,45,45	0.17	0	52,67,67	0.90	1 (1%)
44	A86	S	317	-	44,50,50	0.46	1 (2%)	51,76,76	0.93	2 (3%)
42	DD6	G	210	-	39,45,45	0.23	0	52,67,67	0.73	2 (3%)
40	CLA	N	304	14	64,68,73	1.82	9 (14%)	77,107,113	1.48	7 (9%)
40	CLA	C	305	3	64,68,73	1.83	9 (14%)	77,107,113	1.52	9 (11%)
41	KC2	N	301	14	49,53,53	1.89	4 (8%)	62,89,89	1.34	7 (11%)
40	CLA	p	313	-	59,63,73	1.93	9 (15%)	71,101,113	1.41	6 (8%)
44	A86	P	316	-	44,50,50	0.39	1 (2%)	51,76,76	1.02	3 (5%)
44	A86	X	317	-	44,50,50	0.49	1 (2%)	51,76,76	1.03	3 (5%)
47	A1EB1	t	313	-	51,58,58	0.42	1 (1%)	60,85,85	0.78	3 (5%)
40	CLA	X	307	20	64,68,73	1.82	9 (14%)	77,107,113	1.49	8 (10%)
41	KC2	G	202	-	49,53,53	1.88	4 (8%)	62,89,89	1.42	10 (16%)
47	A1EB1	G	212	-	51,58,58	0.59	1 (1%)	60,85,85	0.71	1 (1%)
47	A1EB1	p	323	-	51,58,58	0.38	0	60,85,85	1.26	5 (8%)
41	KC2	q	303	36	49,53,53	1.87	4 (8%)	62,89,89	1.32	7 (11%)
45	LHG	S	323	-	39,39,48	0.68	0	42,45,54	1.26	4 (9%)
40	CLA	S	313	-	51,55,73	2.02	9 (17%)	61,91,113	1.54	8 (13%)
40	CLA	l	205	32	69,73,73	1.80	9 (13%)	83,113,113	1.48	9 (10%)
44	A86	x	317	-	44,50,50	0.56	1 (2%)	51,76,76	0.84	2 (3%)
40	CLA	a	811	40,23	65,69,73	1.87	10 (15%)	78,107,113	1.74	10 (12%)
40	CLA	q	310	-	55,59,73	1.97	9 (16%)	66,96,113	1.66	9 (13%)
40	CLA	L	310	-	51,55,73	2.10	9 (17%)	61,91,113	1.73	10 (16%)
40	CLA	S	307	17	64,68,73	1.80	9 (14%)	77,107,113	1.52	7 (9%)
47	A1EB1	u	323	-	51,58,58	0.50	1 (1%)	60,85,85	0.46	0
49	BCR	k	203	-	41,41,41	0.18	0	56,56,56	0.46	1 (1%)
40	CLA	M	311	13	66,70,73	1.82	9 (13%)	79,109,113	1.42	8 (10%)
41	KC2	I	214	-	49,53,53	1.91	4 (8%)	62,89,89	1.34	7 (11%)
40	CLA	v	301	-	59,63,73	1.92	9 (15%)	71,101,113	1.52	7 (9%)
40	CLA	y	304	-	64,68,73	1.85	10 (15%)	77,107,113	1.45	10 (12%)
40	CLA	L	301	-	51,55,73	2.11	8 (15%)	61,91,113	1.61	8 (13%)
40	CLA	A	309	1	69,73,73	1.78	9 (13%)	83,113,113	1.37	6 (7%)
49	BCR	f	206	-	41,41,41	0.21	0	56,56,56	0.53	0
42	DD6	q	320	-	39,45,45	0.19	0	52,67,67	0.79	1 (1%)
40	CLA	Z	307	22	64,68,73	1.84	9 (14%)	77,107,113	1.49	9 (11%)
40	CLA	C	307	3	64,68,73	1.88	9 (14%)	77,107,113	1.61	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	Y	311	-	51,55,73	2.08	9 (17%)	61,91,113	1.56	8 (13%)
44	A86	P	321	-	44,50,50	0.51	1 (2%)	51,76,76	1.31	2 (3%)
40	CLA	z	302	-	64,68,73	1.80	9 (14%)	77,107,113	1.39	6 (7%)
40	CLA	v	313	36	51,55,73	2.09	9 (17%)	61,91,113	1.72	9 (14%)
40	CLA	b	807	-	69,73,73	1.70	9 (13%)	83,113,113	1.34	8 (9%)
42	DD6	I	212	-	39,45,45	0.19	0	52,67,67	0.73	2 (3%)
40	CLA	x	307	-	59,63,73	1.95	9 (15%)	71,101,113	1.74	9 (12%)
40	CLA	j	102	30	51,55,73	2.13	9 (17%)	61,91,113	1.74	11 (18%)
44	A86	P	317	-	44,50,50	0.44	1 (2%)	51,76,76	0.78	2 (3%)
44	A86	X	314	-	44,50,50	0.60	1 (2%)	51,76,76	1.13	4 (7%)
44	A86	w	315	-	44,50,50	0.62	1 (2%)	51,76,76	0.71	2 (3%)
49	BCR	l	206	-	41,41,41	0.14	0	56,56,56	0.41	0
40	CLA	t	305	-	53,57,73	2.05	9 (16%)	67,94,113	1.59	7 (10%)
40	CLA	A	301	1	51,55,73	2.07	9 (17%)	61,91,113	1.62	9 (14%)
40	CLA	i	101	-	59,63,73	1.98	9 (15%)	71,101,113	1.67	9 (12%)
44	A86	R	315	-	44,50,50	0.51	1 (2%)	51,76,76	1.26	3 (5%)
44	A86	F	312	-	44,50,50	0.52	1 (2%)	51,76,76	0.88	2 (3%)
49	BCR	j	103	-	41,41,41	0.23	0	56,56,56	0.53	0
40	CLA	u	311	-	59,63,73	1.99	9 (15%)	71,101,113	1.81	12 (16%)
41	KC2	T	303	-	49,53,53	1.91	4 (8%)	62,89,89	1.40	9 (14%)
40	CLA	J	307	10	51,55,73	2.07	9 (17%)	61,91,113	1.69	11 (18%)
44	A86	Y	315	-	44,50,50	0.59	1 (2%)	51,76,76	1.13	2 (3%)
40	CLA	S	302	-	64,68,73	1.82	9 (14%)	77,107,113	1.41	8 (10%)
40	CLA	D	305	4	47,51,73	1.99	10 (21%)	57,82,113	2.35	10 (17%)
41	KC2	L	303	12	49,53,53	1.89	4 (8%)	62,89,89	1.31	8 (12%)
43	LMG	p	301	-	39,39,55	0.80	0	47,47,63	1.18	3 (6%)
47	A1EB1	L	316	-	51,58,58	0.55	1 (1%)	60,85,85	0.74	1 (1%)
40	CLA	t	303	38	51,55,73	2.06	9 (17%)	61,91,113	1.60	5 (8%)
42	DD6	O	314	-	39,45,45	0.21	0	52,67,67	0.86	3 (5%)
44	A86	M	315	-	44,50,50	0.56	1 (2%)	51,76,76	1.24	3 (5%)
40	CLA	G	206	7	60,64,73	1.85	9 (15%)	72,102,113	1.48	9 (12%)
40	CLA	Q	204	16	54,58,73	2.03	10 (18%)	65,94,113	1.93	11 (16%)
44	A86	Z	317	-	44,50,50	0.59	1 (2%)	51,76,76	0.92	1 (1%)
40	CLA	H	307	-	64,68,73	1.86	9 (14%)	77,107,113	1.59	10 (12%)
45	LHG	a	848	-	47,47,48	0.61	0	50,53,54	1.11	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	Q	202	16	62,66,73	1.89	9 (14%)	74,104,113	1.56	8 (10%)
41	KC2	P	304	13	49,53,53	1.92	4 (8%)	62,89,89	1.36	8 (12%)
42	DD6	D	317	-	39,45,45	0.18	0	52,67,67	0.83	3 (5%)
40	CLA	o	306	34	64,68,73	1.85	10 (15%)	77,107,113	1.49	9 (11%)
40	CLA	a	823	23	59,63,73	1.89	9 (15%)	71,101,113	1.46	7 (9%)
40	CLA	w	302	38	51,55,73	2.02	9 (17%)	61,91,113	1.64	7 (11%)
40	CLA	B	307	-	51,55,73	2.09	9 (17%)	61,91,113	1.81	11 (18%)
42	DD6	Q	213	-	39,45,45	0.22	0	52,67,67	0.73	2 (3%)
40	CLA	I	201	-	69,73,73	1.77	9 (13%)	83,113,113	1.39	7 (8%)
42	DD6	A	313	-	39,45,45	0.16	0	52,67,67	0.66	2 (3%)
46	SQD	F	320	-	35,36,54	1.44	4 (11%)	44,47,65	1.39	8 (18%)
43	LMG	D	318	-	40,40,55	0.81	0	48,48,63	1.23	5 (10%)
40	CLA	J	306	10	56,60,73	1.99	9 (16%)	67,97,113	1.60	9 (13%)
47	A1EB1	N	320	-	51,58,58	0.43	0	60,85,85	1.09	3 (5%)
40	CLA	C	308	-	51,55,73	2.17	9 (17%)	61,91,113	1.79	11 (18%)
40	CLA	A	308	-	59,63,73	1.91	9 (15%)	71,101,113	1.44	6 (8%)
41	KC2	K	302	11	49,53,53	1.90	4 (8%)	62,89,89	1.35	8 (12%)
40	CLA	Q	203	-	53,57,73	2.05	10 (18%)	64,93,113	1.97	10 (15%)
40	CLA	y	305	-	53,57,73	2.05	9 (16%)	67,94,113	1.59	8 (11%)
40	CLA	X	313	20	51,55,73	2.09	9 (17%)	61,91,113	1.78	9 (14%)
47	A1EB1	w	313	-	51,58,58	0.44	1 (1%)	60,85,85	0.62	1 (1%)
41	KC2	H	316	-	49,53,53	1.86	4 (8%)	62,89,89	1.41	10 (16%)
40	CLA	b	821	-	69,73,73	1.71	9 (13%)	83,113,113	1.30	8 (9%)
40	CLA	v	306	36	64,68,73	1.82	9 (14%)	77,107,113	1.44	8 (10%)
41	KC2	Y	309	21,44	49,53,53	1.89	4 (8%)	62,89,89	1.31	7 (11%)
43	LMG	E	301	40	31,31,55	0.92	0	39,39,63	1.23	5 (12%)
46	SQD	W	318	-	31,32,54	1.56	5 (16%)	40,43,65	1.33	5 (12%)
47	A1EB1	K	313	-	51,58,58	0.56	1 (1%)	60,85,85	1.24	2 (3%)
47	A1EB1	x	321	-	51,58,58	0.53	1 (1%)	60,85,85	0.54	1 (1%)
47	A1EB1	q	322	-	51,58,58	0.36	0	60,85,85	0.81	2 (3%)
42	DD6	J	317	-	39,45,45	0.20	0	52,67,67	0.75	1 (1%)
47	A1EB1	t	315	-	51,58,58	0.46	1 (1%)	60,85,85	0.74	2 (3%)
51	SF4	c	101	-	0,12,12	-	-	-	-	-
40	CLA	V	202	19	59,63,73	1.93	9 (15%)	71,101,113	1.55	9 (12%)
41	KC2	O	308	15	49,53,53	1.89	4 (8%)	62,89,89	1.39	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	A1EB1	T	316	40	51,58,58	0.49	1 (1%)	60,85,85	0.75	1 (1%)
40	CLA	U	207	-	51,55,73	2.10	9 (17%)	61,91,113	1.71	7 (11%)
47	A1EB1	o	321	-	51,58,58	0.52	1 (1%)	60,85,85	0.62	0
43	LMG	u	301	-	39,39,55	0.84	0	47,47,63	1.28	4 (8%)
44	A86	W	316	-	44,50,50	0.42	1 (2%)	51,76,76	0.68	1 (1%)
47	A1EB1	R	317	40	51,58,58	0.60	1 (1%)	60,85,85	1.12	2 (3%)
41	KC2	o	308	34	49,53,53	1.87	4 (8%)	62,89,89	1.32	8 (12%)
41	KC2	y	301	38	49,53,53	1.90	4 (8%)	62,89,89	1.36	8 (12%)
41	KC2	p	303	-	49,53,53	1.93	4 (8%)	62,89,89	1.30	6 (9%)
40	CLA	H	302	-	51,55,73	2.10	9 (17%)	61,91,113	1.62	9 (14%)
44	A86	Y	321	-	44,50,50	0.65	1 (2%)	51,76,76	0.76	1 (1%)
47	A1EB1	v	324	-	51,58,58	0.63	1 (1%)	60,85,85	1.16	4 (6%)
47	A1EB1	S	321	-	51,58,58	0.46	1 (1%)	60,85,85	0.75	1 (1%)
42	DD6	J	316	-	39,45,45	0.14	0	52,67,67	0.69	3 (5%)
41	KC2	X	309	-	49,53,53	1.92	4 (8%)	62,89,89	1.38	7 (11%)
44	A86	z	315	-	44,50,50	0.41	0	51,76,76	1.43	5 (9%)
40	CLA	O	310	-	51,55,73	2.11	9 (17%)	61,91,113	1.79	12 (19%)
42	DD6	N	317	-	39,45,45	0.21	0	52,67,67	1.10	3 (5%)
41	KC2	u	303	-	49,53,53	1.93	4 (8%)	62,89,89	1.28	6 (9%)
47	A1EB1	K	315	-	51,58,58	0.57	1 (1%)	60,85,85	0.46	0
40	CLA	K	312	-	51,55,73	2.01	9 (17%)	61,91,113	1.58	7 (11%)
40	CLA	a	835	-	69,73,73	1.72	9 (13%)	83,113,113	1.40	7 (8%)
42	DD6	F	316	-	39,45,45	0.19	0	52,67,67	0.83	2 (3%)
40	CLA	L	307	-	59,63,73	1.90	9 (15%)	71,101,113	1.50	7 (9%)
47	A1EB1	v	322	-	51,58,58	0.37	0	60,85,85	0.82	2 (3%)
40	CLA	b	836	24	64,68,73	1.86	9 (14%)	77,107,113	1.47	8 (10%)
41	KC2	x	310	-	49,53,53	1.89	4 (8%)	62,89,89	1.35	8 (12%)
40	CLA	b	835	24	67,72,73	1.63	8 (11%)	79,111,113	1.54	10 (12%)
41	KC2	u	309	-	49,53,53	1.87	4 (8%)	62,89,89	1.37	9 (14%)
44	A86	q	317	-	44,50,50	0.47	1 (2%)	51,76,76	1.06	1 (1%)
40	CLA	U	208	-	51,55,73	2.00	8 (15%)	61,91,113	1.52	9 (14%)
41	KC2	R	308	15	49,53,53	1.89	4 (8%)	62,89,89	1.34	8 (12%)
42	DD6	v	320	-	39,45,45	0.20	0	52,67,67	0.83	1 (1%)
40	CLA	b	817	24	69,73,73	1.70	9 (13%)	83,113,113	1.38	7 (8%)
40	CLA	J	318	10	51,55,73	2.05	9 (17%)	61,91,113	1.63	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	z	314	-	51,55,73	2.07	9 (17%)	61,91,113	1.82	9 (14%)
40	CLA	a	818	-	51,55,73	2.00	9 (17%)	61,91,113	1.67	8 (13%)
40	CLA	N	310	-	54,58,73	2.01	9 (16%)	65,95,113	1.69	11 (16%)
42	DD6	A	312	-	39,45,45	0.20	0	52,67,67	0.91	2 (3%)
40	CLA	a	822	-	69,73,73	1.74	9 (13%)	83,113,113	1.42	9 (10%)
41	KC2	p	310	-	49,53,53	1.91	4 (8%)	62,89,89	1.33	8 (12%)
50	PQN	a	847	-	29,29,34	0.42	0	36,39,45	0.74	1 (2%)
40	CLA	b	831	24	55,59,73	1.95	9 (16%)	66,96,113	1.53	7 (10%)
40	CLA	N	307	-	64,68,73	1.81	9 (14%)	77,107,113	1.43	7 (9%)
40	CLA	S	314	17	59,63,73	1.93	9 (15%)	71,101,113	1.63	8 (11%)
40	CLA	Y	305	21	59,63,73	1.90	9 (15%)	71,101,113	1.53	7 (9%)
40	CLA	a	807	-	60,64,73	1.87	9 (15%)	72,102,113	1.54	8 (11%)
40	CLA	b	842	-	65,69,73	1.82	9 (13%)	78,108,113	1.43	7 (8%)
41	KC2	v	308	36	49,53,53	1.89	4 (8%)	62,89,89	1.38	7 (11%)
44	A86	Y	318	-	44,50,50	0.66	1 (2%)	51,76,76	0.94	3 (5%)
40	CLA	v	311	-	67,71,73	1.82	9 (13%)	80,110,113	1.46	8 (10%)
40	CLA	H	304	-	51,55,73	2.08	10 (19%)	61,91,113	1.63	10 (16%)
40	CLA	a	820	23	64,68,73	1.86	9 (14%)	77,107,113	1.58	9 (11%)
44	A86	o	315	-	44,50,50	0.55	1 (2%)	51,76,76	1.10	3 (5%)
44	A86	o	317	-	44,50,50	0.47	1 (2%)	51,76,76	1.00	3 (5%)
44	A86	z	320	-	44,50,50	0.59	1 (2%)	51,76,76	0.69	1 (1%)
40	CLA	f	204	28	51,55,73	2.01	9 (17%)	61,91,113	1.59	6 (9%)
44	A86	T	315	-	44,50,50	0.66	1 (2%)	51,76,76	1.16	1 (1%)
40	CLA	u	313	-	59,63,73	1.91	9 (15%)	71,101,113	1.42	7 (9%)
40	CLA	B	304	-	51,55,73	2.10	9 (17%)	61,91,113	1.64	8 (13%)
40	CLA	a	841	23	69,73,73	1.76	9 (13%)	83,113,113	1.43	8 (9%)
40	CLA	a	852	-	59,63,73	1.90	9 (15%)	71,101,113	1.46	6 (8%)
40	CLA	H	305	8	64,68,73	1.81	9 (14%)	77,107,113	1.45	11 (14%)
44	A86	Q	215	-	44,50,50	0.44	1 (2%)	51,76,76	1.39	2 (3%)
40	CLA	S	305	-	56,60,73	2.01	9 (16%)	67,97,113	1.74	12 (17%)
44	A86	v	315	-	44,50,50	0.58	1 (2%)	51,76,76	0.83	2 (3%)
40	CLA	Z	310	-	59,63,73	1.99	9 (15%)	71,101,113	1.81	12 (16%)
40	CLA	J	309	-	51,55,73	2.08	9 (17%)	61,91,113	1.56	8 (13%)
44	A86	u	318	-	44,50,50	0.45	1 (2%)	51,76,76	1.55	3 (5%)
40	CLA	D	312	4	59,63,73	1.95	9 (15%)	71,101,113	1.53	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CLA	X	305	-	54,58,73	2.03	9 (16%)	65,95,113	1.57	8 (12%)
44	A86	X	318	-	44,50,50	0.64	1 (2%)	51,76,76	2.03	4 (7%)
41	KC2	Q	216	-	49,53,53	1.90	4 (8%)	62,89,89	1.36	8 (12%)
41	KC2	R	303	-	49,53,53	1.89	4 (8%)	62,89,89	1.41	10 (16%)
44	A86	X	316	-	44,50,50	0.52	1 (2%)	51,76,76	1.26	2 (3%)
40	CLA	S	301	-	64,68,73	1.87	9 (14%)	77,107,113	1.49	6 (7%)
43	LMG	P	318	-	39,39,55	1.00	3 (7%)	47,47,63	1.32	6 (12%)
42	DD6	J	315	-	39,45,45	0.22	0	52,67,67	0.89	3 (5%)
40	CLA	H	301	-	51,55,73	2.06	9 (17%)	61,91,113	1.59	9 (14%)
41	KC2	w	306	38	49,53,53	1.89	4 (8%)	62,89,89	1.32	9 (14%)
44	A86	q	314	-	44,50,50	0.60	1 (2%)	51,76,76	1.49	5 (9%)
40	CLA	b	811	24	51,55,73	1.98	9 (17%)	61,91,113	1.64	9 (14%)
41	KC2	t	308	-	49,53,53	1.91	4 (8%)	62,89,89	1.38	9 (14%)
40	CLA	u	302	-	69,73,73	1.77	9 (13%)	83,113,113	1.44	8 (9%)
49	BCR	i	102	-	41,41,41	0.37	0	56,56,56	0.68	0
44	A86	q	319	-	44,50,50	0.35	0	51,76,76	1.32	5 (9%)
40	CLA	C	301	3	51,55,73	2.10	9 (17%)	61,91,113	1.65	7 (11%)
41	KC2	K	303	11	49,53,53	1.90	4 (8%)	62,89,89	1.33	8 (12%)
41	KC2	y	307	-	49,53,53	1.90	4 (8%)	62,89,89	1.37	9 (14%)
40	CLA	a	809	-	54,58,73	2.03	9 (16%)	65,95,113	1.57	9 (13%)
40	CLA	v	312	-	64,68,73	1.81	9 (14%)	77,107,113	1.44	6 (7%)
40	CLA	Y	312	-	51,55,73	2.17	9 (17%)	61,91,113	1.88	11 (18%)
49	BCR	l	208	-	41,41,41	0.20	0	56,56,56	0.66	2 (3%)
40	CLA	b	839	24	69,73,73	1.76	9 (13%)	83,113,113	1.50	8 (9%)
40	CLA	D	311	-	51,55,73	2.07	9 (17%)	61,91,113	1.76	9 (14%)
41	KC2	P	309	13	49,53,53	1.87	4 (8%)	62,89,89	1.43	8 (12%)
40	CLA	G	213	-	51,55,73	2.10	9 (17%)	61,91,113	1.75	9 (14%)
42	DD6	j	104	-	39,45,45	0.19	0	52,67,67	0.77	2 (3%)
41	KC2	T	302	-	49,53,53	1.92	5 (10%)	62,89,89	1.34	9 (14%)
41	KC2	T	311	15	49,53,53	1.90	4 (8%)	62,89,89	1.34	8 (12%)
42	DD6	p	322	-	39,45,45	0.17	0	52,67,67	0.70	0
42	DD6	w	312	-	39,45,45	0.18	0	52,67,67	1.06	5 (9%)
40	CLA	a	812	23	59,63,73	1.88	9 (15%)	71,101,113	1.44	9 (12%)
40	CLA	I	208	-	59,63,73	1.96	9 (15%)	71,101,113	1.59	7 (9%)
40	CLA	S	308	-	53,57,73	2.05	9 (16%)	67,94,113	1.65	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	KC2	N	312	14	49,53,53	1.88	4 (8%)	62,89,89	1.35	9 (14%)
44	A86	D	320	-	44,50,50	0.47	1 (2%)	51,76,76	0.89	2 (3%)
44	A86	P	314	-	44,50,50	0.40	0	51,76,76	0.96	3 (5%)
40	CLA	E	304	5	59,63,73	1.89	9 (15%)	71,101,113	1.48	7 (9%)
41	KC2	C	303	-	49,53,53	1.92	4 (8%)	62,89,89	1.37	7 (11%)
44	A86	M	313	-	44,50,50	0.42	1 (2%)	51,76,76	2.18	3 (5%)
41	KC2	P	310	-	49,53,53	1.88	4 (8%)	62,89,89	1.34	7 (11%)
42	DD6	C	313	-	39,45,45	0.19	0	52,67,67	0.65	2 (3%)
41	KC2	T	309	15	49,53,53	1.89	4 (8%)	62,89,89	1.35	6 (9%)
40	CLA	f	205	-	51,55,73	2.03	9 (17%)	61,91,113	1.53	9 (14%)
40	CLA	b	825	-	69,73,73	1.70	9 (13%)	83,113,113	1.39	7 (8%)
44	A86	T	312	-	44,50,50	0.48	1 (2%)	51,76,76	1.17	3 (5%)
40	CLA	o	313	-	51,55,73	2.15	10 (19%)	61,91,113	1.93	9 (14%)
40	CLA	B	301	2	51,55,73	2.13	9 (17%)	61,91,113	1.86	10 (16%)
40	CLA	F	308	-	59,63,73	1.94	9 (15%)	71,101,113	1.54	7 (9%)
40	CLA	Z	305	22	59,63,73	1.89	9 (15%)	71,101,113	1.40	6 (8%)
47	A1EB1	Z	321	-	51,58,58	0.53	1 (1%)	60,85,85	0.35	0
40	CLA	M	304	13	64,68,73	1.79	9 (14%)	77,107,113	1.43	6 (7%)
44	A86	p	319	-	44,50,50	0.41	1 (2%)	51,76,76	1.63	4 (7%)
41	KC2	Y	302	-	49,53,53	1.94	4 (8%)	62,89,89	1.30	7 (11%)
40	CLA	K	304	11	64,68,73	1.78	9 (14%)	77,107,113	1.49	7 (9%)
40	CLA	b	814	24	69,73,73	1.71	9 (13%)	83,113,113	1.41	7 (8%)
40	CLA	x	305	-	55,59,73	1.90	9 (16%)	66,96,113	1.60	7 (10%)
41	KC2	M	301	13	49,53,53	1.89	4 (8%)	62,89,89	1.32	8 (12%)
42	DD6	o	319	-	39,45,45	0.20	0	52,67,67	0.88	4 (7%)
41	KC2	x	315	-	49,53,53	1.90	4 (8%)	62,89,89	1.42	8 (12%)
40	CLA	y	303	-	51,55,73	2.11	9 (17%)	61,91,113	1.77	9 (14%)
40	CLA	E	305	5	64,68,73	1.86	9 (14%)	77,107,113	1.46	8 (10%)
40	CLA	v	304	-	56,60,73	1.91	9 (16%)	67,97,113	1.49	9 (13%)
40	CLA	x	314	35	51,55,73	2.05	9 (17%)	61,91,113	1.64	8 (13%)
40	CLA	z	306	-	59,63,73	1.89	9 (15%)	71,101,113	1.49	8 (11%)
40	CLA	x	306	35	64,68,73	1.78	9 (14%)	77,107,113	1.43	10 (12%)
43	LMG	a	802	-	35,35,55	0.89	1 (2%)	43,43,63	1.30	7 (16%)
42	DD6	M	314	-	39,45,45	0.21	0	52,67,67	0.81	2 (3%)
40	CLA	b	810	24	69,73,73	1.73	9 (13%)	83,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	LMG	j	101	-	30,30,55	0.91	1 (3%)	38,38,63	1.30	3 (7%)
41	KC2	u	310	-	49,53,53	1.87	4 (8%)	62,89,89	1.34	7 (11%)
44	A86	X	315	-	44,50,50	0.49	0	51,76,76	1.68	6 (11%)
40	CLA	b	828	24	59,63,73	1.92	9 (15%)	71,101,113	1.56	9 (12%)
40	CLA	b	806	24	69,73,73	1.73	9 (13%)	83,113,113	1.36	7 (8%)
40	CLA	a	834	-	64,68,73	1.85	9 (14%)	77,107,113	1.53	8 (10%)
47	A1EB1	S	320	-	51,58,58	0.50	1 (1%)	60,85,85	0.81	2 (3%)
40	CLA	b	834	-	69,73,73	1.76	9 (13%)	83,113,113	1.40	5 (6%)
40	CLA	w	308	-	51,55,73	2.04	9 (17%)	61,91,113	1.54	6 (9%)
44	A86	W	314	-	44,50,50	0.66	1 (2%)	51,76,76	0.93	2 (3%)
40	CLA	Q	208	-	64,68,73	1.82	8 (12%)	77,107,113	1.41	10 (12%)
40	CLA	o	310	-	59,63,73	1.99	9 (15%)	71,101,113	1.67	12 (16%)

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
40	CLA	u	307	35	-	8/27/103/115	-
49	BCR	b	847	-	-	4/29/63/63	0/2/2/2
40	CLA	a	831	-	-	9/33/109/115	-
40	CLA	a	850	-	-	4/39/115/115	-
41	KC2	o	309	34	-	10/15/71/71	-
44	A86	G	211	-	-	8/34/90/90	0/3/3/3
40	CLA	b	838	-	-	9/39/115/115	-
42	DD6	D	316	-	-	1/26/80/80	0/3/3/3
40	CLA	F	321	-	-	13/33/109/115	-
40	CLA	Y	310	-	-	10/27/103/115	-
42	DD6	F	314	-	-	1/26/80/80	0/3/3/3
40	CLA	Q	205	16	-	11/36/112/115	-
40	CLA	y	309	-	-	9/27/103/115	-
40	CLA	b	830	24	-	6/35/111/115	-
40	CLA	X	312	-	-	5/18/94/115	-
41	KC2	M	308	13	-	6/15/71/71	-
41	KC2	A	310	1	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	K	305	11	-	5/15/71/71	-
40	CLA	O	306	15	-	10/33/109/115	-
52	DGD	b	850	-	-	19/45/85/95	0/2/2/2
40	CLA	E	303	-	-	5/33/109/115	-
42	DD6	k	204	-	-	1/26/80/80	0/3/3/3
40	CLA	T	305	15	-	3/21/97/115	-
40	CLA	a	803	-	-	7/39/115/115	-
41	KC2	Q	201	16	-	5/15/71/71	-
40	CLA	F	311	-	-	3/18/94/115	-
41	KC2	F	302	6	-	8/15/71/71	-
44	A86	u	319	-	-	11/34/90/90	0/3/3/3
40	CLA	S	319	-	-	7/18/94/115	-
40	CLA	u	308	35	-	7/33/109/115	-
48	A1EB4	P	320	-	-	6/37/98/103	0/3/3/3
41	KC2	T	301	-	-	4/15/71/71	-
44	A86	x	318	-	-	8/34/90/90	0/3/3/3
44	A86	p	320	-	-	7/34/90/90	0/3/3/3
40	CLA	R	307	-	-	6/27/103/115	-
44	A86	O	315	-	-	8/34/90/90	0/3/3/3
46	SQD	M	318	-	-	8/27/47/69	0/1/1/1
47	A1EB1	Y	323	-	-	3/42/100/100	0/3/3/3
40	CLA	H	308	8	-	6/18/94/115	-
42	DD6	o	320	-	-	0/26/80/80	0/3/3/3
40	CLA	q	307	36	-	12/33/109/115	-
44	A86	u	316	-	-	6/34/90/90	0/3/3/3
47	A1EB1	z	323	-	-	8/42/100/100	0/3/3/3
41	KC2	F	309	6	-	6/15/71/71	-
40	CLA	b	837	24	-	10/33/109/115	-
40	CLA	a	816	23	-	6/39/115/115	-
43	LMG	S	322	-	-	9/34/54/70	0/1/1/1
44	A86	T	313	-	-	2/34/90/90	0/3/3/3
40	CLA	o	305	34	-	9/27/103/115	-
41	KC2	p	304	35	-	8/15/71/71	-
40	CLA	b	809	24	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	q	301	-	-	4/27/103/115	-
40	CLA	a	836	23	-	11/39/115/115	-
40	CLA	a	819	23	-	10/35/111/115	-
44	A86	N	321	-	-	8/34/90/90	0/3/3/3
40	CLA	B	306	-	-	9/24/100/115	-
41	KC2	W	309	-	-	6/15/71/71	-
40	CLA	P	306	13	-	1/18/94/115	-
40	CLA	E	306	5	-	9/27/103/115	-
40	CLA	T	304	15	-	6/33/109/115	-
42	DD6	C	312	-	-	2/26/80/80	0/3/3/3
40	CLA	w	309	-	-	9/27/103/115	-
42	DD6	R	314	-	-	0/26/80/80	0/3/3/3
40	CLA	M	307	-	-	9/33/109/115	-
40	CLA	M	312	13	-	15/33/109/115	-
41	KC2	R	311	15	-	10/15/71/71	-
43	LMG	M	317	-	-	9/34/54/70	0/1/1/1
40	CLA	O	307	-	-	10/36/112/115	-
40	CLA	a	808	-	-	7/39/115/115	-
42	DD6	q	318	-	-	0/26/80/80	0/3/3/3
40	CLA	M	306	13	-	5/36/112/115	-
40	CLA	z	311	-	-	9/27/103/115	-
42	DD6	Y	322	-	-	3/26/80/80	0/3/3/3
41	KC2	M	302	13	-	2/15/71/71	-
40	CLA	A	311	1	-	5/18/94/115	-
47	A1EB1	F	322	-	-	9/42/100/100	0/3/3/3
47	A1EB1	w	314	-	-	10/42/100/100	0/3/3/3
44	A86	S	315	-	-	9/34/90/90	0/3/3/3
44	A86	N	314	-	-	2/34/90/90	0/3/3/3
42	DD6	E	317	-	-	1/26/80/80	0/3/3/3
47	A1EB1	y	314	-	-	9/42/100/100	0/3/3/3
40	CLA	a	826	-	-	11/35/111/115	-
41	KC2	x	309	-	-	5/15/71/71	-
40	CLA	I	204	9	-	3/18/94/115	-
41	KC2	v	309	-	-	8/15/71/71	-
41	KC2	p	315	-	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	z	309	39	-	5/15/71/71	-
42	DD6	J	313	-	-	1/26/80/80	0/3/3/3
41	KC2	O	311	-	-	7/15/71/71	-
47	A1EB1	T	320	-	-	11/42/100/100	0/3/3/3
41	KC2	u	304	35	-	8/15/71/71	-
41	KC2	z	303	39	-	6/15/71/71	-
46	SQD	k	205	-	-	3/31/51/69	0/1/1/1
40	CLA	X	311	20	-	11/37/113/115	-
40	CLA	u	312	-	-	8/33/109/115	-
40	CLA	W	306	13	-	12/33/109/115	-
42	DD6	A	316	-	-	1/26/80/80	0/3/3/3
40	CLA	b	829	-	-	3/18/94/115	-
45	LHG	a	849	40	-	17/34/34/53	-
41	KC2	S	309	17	-	10/15/71/71	-
44	A86	u	320	-	-	5/34/90/90	0/3/3/3
44	A86	Z	315	-	-	12/34/90/90	0/3/3/3
40	CLA	y	308	-	-	6/18/94/115	-
40	CLA	o	311	-	-	8/37/113/115	-
40	CLA	K	307	11	-	12/26/102/115	-
40	CLA	Y	301	-	-	10/33/109/115	-
44	A86	W	301	-	-	1/34/90/90	0/3/3/3
41	KC2	U	201	-	-	5/15/71/71	-
44	A86	t	310	-	-	7/34/90/90	0/3/3/3
40	CLA	Q	207	-	-	3/18/94/115	-
40	CLA	H	311	-	-	3/18/94/115	-
40	CLA	x	308	35	-	6/33/109/115	-
40	CLA	P	305	13	-	9/33/109/115	-
44	A86	L	314	-	-	5/34/90/90	0/3/3/3
40	CLA	Y	313	21	-	10/18/94/115	-
47	A1EB1	P	301	-	-	14/42/100/100	0/3/3/3
40	CLA	Z	304	-	-	3/33/109/115	-
40	CLA	b	826	24	-	8/38/114/115	-
40	CLA	A	305	1	-	7/35/111/115	-
40	CLA	C	309	-	-	2/18/94/115	-
44	A86	S	318	-	-	2/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	H	315	-	-	5/34/90/90	0/3/3/3
40	CLA	N	306	-	-	2/33/109/115	-
41	KC2	z	310	39	-	9/15/71/71	-
41	KC2	Y	314	-	-	9/15/71/71	-
40	CLA	a	827	23	-	2/39/115/115	-
40	CLA	k	201	31	-	7/27/103/115	-
40	CLA	p	314	35	-	8/18/94/115	-
43	LMG	l	201	-	-	19/34/54/70	0/1/1/1
41	KC2	Y	303	21	-	7/15/71/71	-
40	CLA	A	306	1	-	10/33/109/115	-
40	CLA	A	303	1	-	11/35/111/115	-
41	KC2	M	303	13	-	4/15/71/71	-
40	CLA	a	842	-	-	15/39/115/115	-
40	CLA	a	804	23	-	10/36/112/115	-
40	CLA	b	801	-	-	7/37/113/115	-
41	KC2	N	313	14	-	4/15/71/71	-
43	LMG	x	301	-	-	15/34/54/70	0/1/1/1
40	CLA	z	305	39	-	14/33/109/115	-
41	KC2	S	310	-	-	8/15/71/71	-
40	CLA	u	305	35	-	1/18/94/115	-
44	A86	z	318	-	-	4/34/90/90	1/3/3/3
40	CLA	a	828	23	-	15/39/115/115	-
47	A1EB1	p	324	-	-	5/42/100/100	0/3/3/3
47	A1EB1	v	323	-	-	13/42/100/100	1/3/3/3
40	CLA	X	304	-	-	7/18/94/115	-
40	CLA	P	312	13	-	14/33/109/115	-
40	CLA	o	312	-	-	6/18/94/115	-
41	KC2	R	309	15	-	7/15/71/71	-
42	DD6	D	314	-	-	3/26/80/80	0/3/3/3
40	CLA	W	305	13	-	7/39/115/115	-
44	A86	G	209	-	-	9/34/90/90	0/3/3/3
41	KC2	Z	308	22	-	4/15/71/71	-
41	KC2	X	303	20	-	1/15/71/71	-
41	KC2	P	302	-	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	LMG	A	317	-	-	22/35/55/70	0/1/1/1
40	CLA	K	308	11	-	10/32/108/115	-
40	CLA	l	203	-	-	14/38/114/115	-
41	KC2	T	308	15	-	8/15/71/71	-
44	A86	p	321	-	-	7/34/90/90	0/3/3/3
42	DD6	W	315	-	-	1/26/80/80	0/3/3/3
40	CLA	W	312	13	-	10/33/109/115	-
41	KC2	O	309	15	-	9/15/71/71	-
40	CLA	J	302	10	-	8/18/94/115	-
40	CLA	T	306	15	-	3/33/109/115	-
44	A86	N	315	-	-	9/34/90/90	0/3/3/3
41	KC2	S	304	17	-	6/15/71/71	-
40	CLA	D	310	4	-	11/33/109/115	-
40	CLA	t	302	38	-	2/18/94/115	-
40	CLA	O	304	15	-	7/39/115/115	-
40	CLA	a	810	-	-	6/33/109/115	-
40	CLA	f	202	24	-	7/39/115/115	-
41	KC2	Z	302	-	-	7/15/71/71	-
43	LMG	a	801	-	-	13/30/50/70	0/1/1/1
40	CLA	C	304	3	-	5/29/105/115	-
41	KC2	q	308	36	-	10/15/71/71	-
42	DD6	T	314	-	-	1/26/80/80	0/3/3/3
44	A86	Z	316	-	-	5/34/90/90	1/3/3/3
41	KC2	N	302	14	-	5/15/71/71	-
42	DD6	E	315	-	-	1/26/80/80	0/3/3/3
41	KC2	L	308	12	-	4/15/71/71	-
47	A1EB1	y	312	-	-	11/42/100/100	0/3/3/3
51	SF4	b	804	-	-	-	0/6/5/5
40	CLA	v	305	-	-	4/33/109/115	-
41	KC2	q	302	36	-	7/15/71/71	-
40	CLA	x	311	-	-	11/27/103/115	-
41	KC2	u	315	-	-	7/15/71/71	-
40	CLA	q	304	-	-	4/24/100/115	-
42	DD6	A	315	-	-	0/26/80/80	0/3/3/3
41	KC2	o	303	34	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	a	814	-	-	3/21/97/115	-
40	CLA	T	310	-	-	8/31/107/115	-
44	A86	p	316	-	-	5/34/90/90	0/3/3/3
40	CLA	u	306	35	-	7/18/94/115	-
43	LMG	T	318	-	-	16/35/55/70	0/1/1/1
40	CLA	a	821	23	-	16/39/115/115	-
42	DD6	K	311	-	-	2/26/80/80	0/3/3/3
40	CLA	l	204	-	-	10/39/115/115	-
40	CLA	D	304	4	-	7/29/105/115	-
44	A86	u	317	-	-	1/34/90/90	0/3/3/3
41	KC2	N	309	-	-	5/15/71/71	-
40	CLA	R	305	15	-	6/33/109/115	-
41	KC2	W	302	-	-	5/15/71/71	-
40	CLA	S	311	-	-	6/18/94/115	-
51	SF4	c	102	-	-	-	0/6/5/5
42	DD6	F	315	-	-	3/26/80/80	0/3/3/3
41	KC2	I	209	9	-	8/15/71/71	-
40	CLA	P	311	-	-	6/18/94/115	-
41	KC2	E	319	-	-	10/15/71/71	-
42	DD6	y	311	-	-	0/26/80/80	0/3/3/3
44	A86	o	318	-	-	3/34/90/90	0/3/3/3
42	DD6	Z	318	-	-	1/26/80/80	0/3/3/3
40	CLA	E	307	-	-	10/39/115/115	-
41	KC2	M	309	-	-	4/15/71/71	-
42	DD6	x	320	-	-	0/26/80/80	0/3/3/3
40	CLA	J	303	-	-	4/18/94/115	-
40	CLA	Z	311	22	-	9/37/113/115	-
41	KC2	G	208	-	-	5/15/71/71	-
42	DD6	N	316	-	-	2/26/80/80	0/3/3/3
40	CLA	Y	307	21	-	9/33/109/115	-
40	CLA	v	310	-	-	12/23/99/115	-
40	CLA	G	205	7	-	1/21/97/115	-
44	A86	M	320	-	-	5/34/90/90	0/3/3/3
40	CLA	b	803	-	-	14/39/115/115	-
44	A86	O	312	-	-	6/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	DD6	U	209	-	-	1/26/80/80	0/3/3/3
47	A1EB1	u	322	-	-	10/42/100/100	0/3/3/3
42	DD6	z	322	-	-	3/26/80/80	0/3/3/3
42	DD6	Q	212	-	-	1/26/80/80	0/3/3/3
44	A86	p	317	-	-	1/34/90/90	0/3/3/3
44	A86	t	311	-	-	12/34/90/90	1/3/3/3
40	CLA	b	841	24	-	6/39/115/115	-
47	A1EB1	Z	319	-	-	7/42/100/100	0/3/3/3
40	CLA	b	832	24	-	6/39/115/115	-
40	CLA	a	839	45	-	10/39/115/115	-
40	CLA	b	840	-	-	13/39/115/115	-
41	KC2	Z	309	-	-	8/15/71/71	-
40	CLA	q	311	-	-	11/37/113/115	-
40	CLA	a	815	23	-	8/39/115/115	-
40	CLA	W	308	-	-	12/33/109/115	-
40	CLA	b	815	-	-	4/30/106/115	-
44	A86	U	210	-	-	2/34/90/90	0/3/3/3
40	CLA	b	802	-	-	13/39/115/115	-
41	KC2	L	309	12	-	7/15/71/71	-
41	KC2	Z	303	22	-	3/15/71/71	-
40	CLA	T	317	47	-	4/18/94/115	-
40	CLA	P	313	-	-	13/33/109/115	-
40	CLA	t	309	-	-	4/18/94/115	-
42	DD6	E	318	-	-	3/26/80/80	0/3/3/3
40	CLA	a	832	23	-	15/39/115/115	-
40	CLA	p	311	-	-	12/27/103/115	-
41	KC2	v	303	36	-	5/15/71/71	-
40	CLA	L	305	12	-	6/18/94/115	-
47	A1EB1	t	314	-	-	17/42/100/100	1/3/3/3
40	CLA	N	305	14	-	6/27/103/115	-
40	CLA	a	833	23	-	8/33/109/115	-
42	DD6	C	310	-	-	1/26/80/80	0/3/3/3
44	A86	N	318	-	-	2/34/90/90	0/3/3/3
44	A86	w	310	-	-	9/34/90/90	0/3/3/3
41	KC2	x	303	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	E	310	-	-	8/33/109/115	-
40	CLA	R	316	47	-	2/18/94/115	-
44	A86	Q	210	-	-	5/34/90/90	0/3/3/3
40	CLA	W	311	-	-	9/27/103/115	-
40	CLA	G	204	7	-	2/27/103/115	-
41	KC2	q	309	-	-	8/15/71/71	-
40	CLA	k	202	-	-	6/27/103/115	-
44	A86	Y	319	-	-	6/34/90/90	0/3/3/3
49	BCR	b	844	-	-	6/29/63/63	0/2/2/2
50	PQN	b	849	-	-	3/17/37/43	0/2/2/2
40	CLA	X	306	20	-	6/27/103/115	-
40	CLA	a	829	-	-	16/39/115/115	-
40	CLA	K	301	-	-	4/18/94/115	-
40	CLA	x	302	-	-	10/39/115/115	-
40	CLA	z	308	39	-	12/33/109/115	-
40	CLA	a	837	23	-	8/27/103/115	-
43	LMG	L	319	-	-	15/32/52/70	0/1/1/1
42	DD6	z	321	-	-	1/26/80/80	0/3/3/3
40	CLA	b	818	24	-	13/36/112/115	-
40	CLA	S	306	17	-	8/29/105/115	-
41	KC2	o	302	-	-	6/15/71/71	-
41	KC2	Y	308	-	-	7/15/71/71	-
40	CLA	p	308	-	-	8/33/109/115	-
49	BCR	a	846	-	-	3/29/63/63	0/2/2/2
44	A86	z	301	-	-	7/34/90/90	0/3/3/3
40	CLA	G	203	7	-	8/26/103/115	-
40	CLA	y	302	38	-	4/18/94/115	-
44	A86	z	319	-	-	8/34/90/90	0/3/3/3
49	BCR	a	844	-	-	2/29/63/63	0/2/2/2
40	CLA	C	302	-	-	7/18/94/115	-
40	CLA	J	305	10	-	9/27/103/115	-
40	CLA	L	304	12	-	2/30/106/115	-
40	CLA	H	306	8	-	0/21/97/115	-
40	CLA	I	202	9	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	F	310	-	-	6/18/94/115	-
40	CLA	z	307	-	-	7/33/109/115	-
42	DD6	K	310	-	-	0/26/80/80	0/3/3/3
40	CLA	U	206	-	-	1/18/94/115	-
40	CLA	U	204	18	-	9/18/94/115	-
44	A86	t	316	-	-	8/34/90/90	0/3/3/3
42	DD6	H	313	-	-	5/26/80/80	0/3/3/3
40	CLA	U	202	18	-	9/27/103/115	-
41	KC2	v	302	-	-	7/15/71/71	-
44	A86	X	321	-	-	5/34/90/90	0/3/3/3
40	CLA	p	302	-	-	7/39/115/115	-
40	CLA	q	305	-	-	4/33/109/115	-
40	CLA	Z	301	-	-	6/33/109/115	-
43	LMG	E	321	-	-	12/35/55/70	0/1/1/1
49	BCR	l	207	-	-	6/29/63/63	0/2/2/2
43	LMG	W	317	-	-	7/34/54/70	0/1/1/1
41	KC2	p	309	-	-	7/15/71/71	-
40	CLA	A	304	1	-	17/39/115/115	-
40	CLA	R	306	15	-	5/33/109/115	-
42	DD6	A	314	-	-	1/26/80/80	0/3/3/3
40	CLA	b	823	24	-	4/27/103/115	-
41	KC2	L	313	12	-	8/15/71/71	-
40	CLA	l	202	-	-	15/39/115/115	-
41	KC2	W	304	13	-	5/15/71/71	-
40	CLA	I	207	9	-	6/18/94/115	-
41	KC2	t	301	38	-	7/15/71/71	-
41	KC2	X	308	20	-	5/15/71/71	-
40	CLA	D	307	4	-	8/39/115/115	-
44	A86	X	319	-	-	8/34/90/90	0/3/3/3
40	CLA	w	304	-	-	9/33/109/115	-
44	A86	T	319	-	-	6/34/90/90	0/3/3/3
40	CLA	a	806	23	-	13/39/115/115	-
40	CLA	F	301	-	-	11/25/101/115	-
40	CLA	U	203	-	-	9/27/103/115	-
47	A1EB1	Z	320	-	-	7/42/100/100	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	W	307	13	-	15/39/115/115	-
40	CLA	P	307	13	-	8/32/108/115	-
40	CLA	D	303	4	-	12/33/109/115	-
40	CLA	Y	304	-	-	2/18/94/115	-
49	BCR	m	101	-	-	0/29/63/63	0/2/2/2
44	A86	K	314	-	-	4/34/90/90	0/3/3/3
40	CLA	I	203	9	-	6/27/103/115	-
41	KC2	X	302	-	-	4/15/71/71	-
42	DD6	Q	214	-	-	1/26/80/80	0/3/3/3
40	CLA	o	307	34	-	16/33/109/115	-
40	CLA	Q	206	-	-	8/35/112/115	-
40	CLA	O	316	47	-	3/18/94/115	-
46	SQD	I	215	-	-	17/49/69/69	0/1/1/1
40	CLA	Q	209	-	-	6/18/94/115	-
42	DD6	I	213	-	-	1/26/80/80	0/3/3/3
42	DD6	t	312	-	-	0/26/80/80	0/3/3/3
42	DD6	v	318	-	-	0/26/80/80	0/3/3/3
44	A86	z	316	-	-	8/34/90/90	1/3/3/3
40	CLA	D	302	43	-	9/31/107/115	-
47	A1EB1	q	321	-	-	16/42/100/100	1/3/3/3
40	CLA	C	306	3	-	16/39/115/115	-
42	DD6	H	314	-	-	2/26/80/80	0/3/3/3
41	KC2	P	303	13	-	3/15/71/71	-
44	A86	Y	320	-	-	10/34/90/90	0/3/3/3
40	CLA	v	307	36	-	13/33/109/115	-
47	A1EB1	O	317	40	-	8/42/100/100	1/3/3/3
40	CLA	G	201	7	-	4/18/94/115	-
40	CLA	F	305	-	-	4/18/94/115	-
40	CLA	z	324	-	-	5/18/94/115	-
49	BCR	b	843	-	-	2/29/63/63	0/2/2/2
47	A1EB1	o	322	-	-	14/42/100/100	0/3/3/3
40	CLA	p	307	35	-	8/27/103/115	-
41	KC2	x	304	35	-	6/15/71/71	-
44	A86	q	324	-	-	7/34/90/90	0/3/3/3
40	CLA	x	312	-	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	R	302	15	-	5/15/71/71	-
40	CLA	u	314	35	-	7/18/94/115	-
40	CLA	F	306	6	-	7/33/109/115	-
43	LMG	E	320	-	-	14/26/46/70	0/1/1/1
42	DD6	J	314	-	-	0/26/80/80	0/3/3/3
40	CLA	F	303	6	-	9/36/112/115	-
44	A86	v	325	-	-	7/34/90/90	0/3/3/3
42	DD6	L	317	-	-	0/26/80/80	0/3/3/3
44	A86	F	313	-	-	7/34/90/90	0/3/3/3
40	CLA	M	310	-	-	6/29/105/115	-
40	CLA	G	207	-	-	6/26/102/115	-
47	A1EB1	L	318	-	-	15/42/100/100	0/3/3/3
40	CLA	H	309	-	-	6/29/105/115	-
44	A86	Z	314	-	-	3/34/90/90	0/3/3/3
42	DD6	J	301	-	-	2/26/80/80	0/3/3/3
40	CLA	W	313	13	-	11/33/109/115	-
40	CLA	D	306	4	-	6/27/103/115	-
40	CLA	K	306	-	-	6/33/109/115	-
44	A86	Y	316	-	-	3/34/90/90	0/3/3/3
48	A1EB4	W	319	-	-	10/37/98/103	0/3/3/3
40	CLA	E	302	5	-	9/18/94/115	-
40	CLA	E	311	-	-	7/21/97/115	-
43	LMG	F	318	-	-	10/34/54/70	0/1/1/1
41	KC2	O	302	15	-	10/15/71/71	-
40	CLA	J	311	-	-	4/18/94/115	-
40	CLA	L	306	12	-	6/18/94/115	-
40	CLA	S	312	-	-	3/18/94/115	-
41	KC2	W	303	-	-	7/15/71/71	-
41	KC2	w	301	38	-	7/15/71/71	-
40	CLA	Z	312	-	-	7/18/94/115	-
40	CLA	w	303	38	-	5/18/94/115	-
44	A86	q	315	-	-	6/34/90/90	0/3/3/3
40	CLA	a	817	23	-	1/21/97/115	-
40	CLA	b	824	24	-	15/39/115/115	-
41	KC2	H	303	-	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	K	309	11	-	8/15/71/71	-
41	KC2	z	304	39	-	3/15/71/71	-
40	CLA	b	833	24	-	14/33/109/115	-
40	CLA	z	312	-	-	11/33/109/115	-
41	KC2	S	303	17	-	5/15/71/71	-
40	CLA	Z	306	22	-	16/33/109/115	-
40	CLA	E	313	5	-	3/18/94/115	-
40	CLA	a	825	-	-	5/39/115/115	-
49	BCR	b	845	-	-	2/29/63/63	0/2/2/2
41	KC2	L	302	-	-	6/15/71/71	-
40	CLA	a	824	-	-	13/36/112/115	-
40	CLA	F	307	6	-	8/32/109/115	-
40	CLA	b	812	24	-	8/33/109/115	-
40	CLA	z	313	-	-	5/18/94/115	-
40	CLA	b	819	24	-	16/38/114/115	-
42	DD6	E	316	-	-	0/26/80/80	0/3/3/3
40	CLA	p	305	35	-	6/18/94/115	-
40	CLA	A	307	1	-	6/33/109/115	-
42	DD6	B	305	-	-	3/26/80/80	0/3/3/3
40	CLA	t	307	-	-	12/27/103/115	-
44	A86	p	318	-	-	10/34/90/90	0/3/3/3
41	KC2	t	306	-	-	9/15/71/71	-
40	CLA	J	308	10	-	10/27/103/115	-
40	CLA	N	311	14	-	13/33/109/115	-
40	CLA	a	805	40,23	-	4/26/102/115	-
40	CLA	a	840	23	-	8/27/103/115	-
44	A86	y	310	-	-	7/34/90/90	0/3/3/3
40	CLA	B	302	2	-	4/18/94/115	-
44	A86	R	312	-	-	5/34/90/90	0/3/3/3
40	CLA	E	308	5	-	8/31/107/115	-
40	CLA	o	304	34	-	6/33/109/115	-
44	A86	o	314	-	-	12/34/90/90	0/3/3/3
40	CLA	q	312	-	-	9/33/109/115	-
40	CLA	b	808	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	N	308	14	-	7/15/71/71	-
41	KC2	O	303	15	-	6/15/71/71	-
42	DD6	N	319	-	-	1/26/80/80	0/3/3/3
40	CLA	b	816	24	-	6/18/94/115	-
49	BCR	f	203	-	-	0/29/63/63	0/2/2/2
44	A86	R	313	-	-	6/34/90/90	0/3/3/3
42	DD6	D	315	-	-	0/26/80/80	0/3/3/3
40	CLA	q	306	36	-	6/33/109/115	-
41	KC2	J	304	-	-	8/15/71/71	-
44	A86	X	320	-	-	6/34/90/90	0/3/3/3
46	SQD	P	319	-	-	8/27/47/69	0/1/1/1
40	CLA	J	312	-	-	12/31/107/115	-
47	A1EB1	v	321	-	-	16/42/100/100	1/3/3/3
40	CLA	T	307	-	-	2/27/103/115	-
42	DD6	P	315	-	1/1/12/24	1/26/80/80	0/3/3/3
44	A86	M	316	-	-	2/34/90/90	0/3/3/3
44	A86	o	316	-	-	11/34/90/90	0/3/3/3
40	CLA	a	813	23	-	6/33/109/115	-
40	CLA	R	304	15	-	9/23/99/115	-
40	CLA	b	813	24	-	8/21/97/115	-
44	A86	w	311	-	-	9/34/90/90	0/3/3/3
44	A86	v	319	-	-	13/34/90/90	0/3/3/3
40	CLA	E	312	-	-	4/18/94/115	-
40	CLA	X	301	-	-	8/33/109/115	-
44	A86	v	317	-	-	1/34/90/90	0/3/3/3
41	KC2	R	301	15	-	5/15/71/71	-
40	CLA	x	313	-	-	4/27/103/115	-
44	A86	x	319	-	-	12/34/90/90	0/3/3/3
42	DD6	Q	211	-	-	2/26/80/80	0/3/3/3
40	CLA	a	838	23	-	9/27/103/115	-
40	CLA	Z	313	22	-	4/18/94/115	-
40	CLA	O	305	15	-	2/18/94/115	-
40	CLA	L	311	12	-	5/18/94/115	-
40	CLA	F	304	6	-	3/27/103/115	-
40	CLA	R	310	-	-	5/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	DD6	u	321	-	-	1/26/80/80	0/3/3/3
40	CLA	I	206	9	-	8/39/115/115	-
40	CLA	a	830	-	-	7/31/107/115	-
40	CLA	D	309	-	-	7/31/107/115	-
40	CLA	b	805	-	-	7/35/111/115	-
44	A86	F	317	-	-	9/34/90/90	0/3/3/3
40	CLA	J	310	-	-	2/18/94/115	-
40	CLA	p	312	-	-	3/18/94/115	-
41	KC2	y	306	-	-	7/15/71/71	-
49	BCR	a	843	-	-	4/29/63/63	0/2/2/2
49	BCR	b	848	-	-	4/29/63/63	0/2/2/2
40	CLA	X	310	-	-	9/27/103/115	-
40	CLA	B	303	-	-	3/18/94/115	-
40	CLA	H	310	-	-	4/33/109/115	-
40	CLA	P	308	-	-	17/33/109/115	-
40	CLA	a	851	-	-	15/39/115/115	-
40	CLA	p	306	35	-	7/18/94/115	-
40	CLA	D	301	4	-	8/27/103/115	-
40	CLA	q	313	36	-	7/18/94/115	-
44	A86	q	316	-	-	3/34/90/90	1/3/3/3
40	CLA	E	314	5	-	13/18/94/115	-
40	CLA	I	205	9	-	8/29/105/115	-
41	KC2	N	303	14	-	4/15/71/71	-
42	DD6	X	322	-	-	0/26/80/80	0/3/3/3
44	A86	S	316	-	-	8/34/90/90	0/3/3/3
44	A86	v	314	-	-	3/34/90/90	0/3/3/3
40	CLA	A	302	-	-	7/33/109/115	-
40	CLA	M	305	13	-	10/33/109/115	-
40	CLA	b	827	24	-	9/33/109/115	-
40	CLA	w	305	-	-	3/19/95/115	-
40	CLA	o	301	-	-	6/33/109/115	-
45	LHG	F	319	-	-	18/44/44/53	-
42	DD6	U	211	-	-	0/26/80/80	0/3/3/3
47	A1EB1	x	322	-	-	4/42/100/100	0/3/3/3
40	CLA	Y	306	21	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	f	201	-	-	8/33/109/115	-
44	A86	w	316	-	-	12/34/90/90	0/3/3/3
47	A1EB1	q	323	-	-	13/42/100/100	0/3/3/3
40	CLA	E	309	-	-	11/33/109/115	-
44	A86	O	313	-	-	3/34/90/90	0/3/3/3
44	A86	v	316	-	-	3/34/90/90	1/3/3/3
49	BCR	b	846	-	-	4/29/63/63	0/2/2/2
41	KC2	W	310	13	-	7/15/71/71	-
42	DD6	D	313	-	-	0/26/80/80	0/3/3/3
44	A86	Y	317	41	-	6/34/90/90	0/3/3/3
42	DD6	I	211	-	-	5/26/80/80	0/3/3/3
44	A86	x	316	-	-	5/34/90/90	0/3/3/3
42	DD6	L	315	-	-	0/26/80/80	0/3/3/3
40	CLA	L	312	-	-	2/18/94/115	-
40	CLA	t	304	-	-	10/33/109/115	-
44	A86	z	317	-	-	6/34/90/90	0/3/3/3
40	CLA	V	201	-	-	8/31/107/115	-
41	KC2	w	307	-	-	4/15/71/71	-
40	CLA	D	308	4	-	3/27/103/115	-
48	A1EB4	M	319	-	-	5/37/98/103	0/3/3/3
40	CLA	b	820	-	-	11/39/115/115	-
44	A86	C	311	-	-	9/34/90/90	1/3/3/3
47	A1EB1	y	313	-	-	13/42/100/100	0/3/3/3
49	BCR	r	201	-	-	2/29/63/63	0/2/2/2
42	DD6	H	312	-	-	0/26/80/80	0/3/3/3
41	KC2	O	301	15	-	8/15/71/71	-
40	CLA	U	205	-	-	5/18/94/115	-
44	A86	D	319	-	-	4/34/90/90	0/3/3/3
40	CLA	b	822	-	-	9/38/114/115	-
49	BCR	a	845	-	-	3/29/63/63	0/2/2/2
42	DD6	I	210	-	-	0/26/80/80	0/3/3/3
44	A86	S	317	-	-	5/34/90/90	0/3/3/3
42	DD6	G	210	-	-	1/26/80/80	0/3/3/3
40	CLA	N	304	14	-	10/33/109/115	-
40	CLA	C	305	3	-	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	N	301	14	-	5/15/71/71	-
40	CLA	p	313	-	-	4/27/103/115	-
44	A86	P	316	-	-	7/34/90/90	0/3/3/3
44	A86	X	317	-	-	6/34/90/90	0/3/3/3
47	A1EB1	t	313	-	-	15/42/100/100	0/3/3/3
40	CLA	X	307	20	-	7/33/109/115	-
41	KC2	G	202	-	-	10/15/71/71	-
47	A1EB1	G	212	-	-	15/42/100/100	0/3/3/3
47	A1EB1	p	323	-	-	10/42/100/100	0/3/3/3
41	KC2	q	303	36	-	6/15/71/71	-
45	LHG	S	323	-	-	23/44/44/53	-
40	CLA	S	313	-	-	5/18/94/115	-
40	CLA	l	205	32	-	13/39/115/115	-
44	A86	x	317	-	-	6/34/90/90	0/3/3/3
40	CLA	a	811	40,23	-	14/36/112/115	-
40	CLA	q	310	-	-	12/23/99/115	-
40	CLA	L	310	-	-	6/18/94/115	-
40	CLA	S	307	17	-	12/33/109/115	-
47	A1EB1	u	323	-	-	4/42/100/100	0/3/3/3
49	BCR	k	203	-	-	4/29/63/63	0/2/2/2
40	CLA	M	311	13	-	13/36/112/115	-
41	KC2	I	214	-	-	6/15/71/71	-
40	CLA	v	301	-	-	6/27/103/115	-
40	CLA	y	304	-	-	8/33/109/115	-
40	CLA	L	301	-	-	2/18/94/115	-
40	CLA	A	309	1	-	13/39/115/115	-
49	BCR	f	206	-	-	4/29/63/63	0/2/2/2
42	DD6	q	320	-	-	6/26/80/80	0/3/3/3
40	CLA	Z	307	22	-	13/33/109/115	-
40	CLA	C	307	3	-	9/33/109/115	-
40	CLA	Y	311	-	-	6/18/94/115	-
44	A86	P	321	-	-	6/34/90/90	0/3/3/3
40	CLA	z	302	-	-	6/33/109/115	-
40	CLA	v	313	36	-	4/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	b	807	-	-	10/39/115/115	-
42	DD6	I	212	-	-	0/26/80/80	0/3/3/3
40	CLA	x	307	-	-	10/27/103/115	-
40	CLA	j	102	30	-	5/18/94/115	-
44	A86	P	317	-	-	3/34/90/90	0/3/3/3
44	A86	X	314	-	-	4/34/90/90	1/3/3/3
44	A86	w	315	-	-	8/34/90/90	1/3/3/3
49	BCR	l	206	-	-	6/29/63/63	0/2/2/2
40	CLA	t	305	-	-	2/19/95/115	-
40	CLA	A	301	1	-	4/18/94/115	-
40	CLA	i	101	-	-	12/27/103/115	-
44	A86	R	315	-	-	7/34/90/90	0/3/3/3
44	A86	F	312	-	-	4/34/90/90	0/3/3/3
49	BCR	j	103	-	-	4/29/63/63	0/2/2/2
40	CLA	u	311	-	-	11/27/103/115	-
41	KC2	T	303	-	-	4/15/71/71	-
40	CLA	J	307	10	-	4/18/94/115	-
44	A86	Y	315	-	-	8/34/90/90	0/3/3/3
40	CLA	S	302	-	-	13/33/109/115	-
40	CLA	D	305	4	-	0/18/82/115	-
41	KC2	L	303	12	-	6/15/71/71	-
43	LMG	p	301	-	-	9/34/54/70	0/1/1/1
47	A1EB1	L	316	-	-	7/42/100/100	0/3/3/3
40	CLA	t	303	38	-	4/18/94/115	-
42	DD6	O	314	-	-	1/26/80/80	0/3/3/3
44	A86	M	315	-	-	5/34/90/90	1/3/3/3
40	CLA	G	206	7	-	11/29/105/115	-
40	CLA	Q	204	16	-	2/23/99/115	-
44	A86	Z	317	-	-	2/34/90/90	1/3/3/3
40	CLA	H	307	-	-	18/33/109/115	-
45	LHG	a	848	-	-	22/52/52/53	-
40	CLA	Q	202	16	-	5/31/107/115	-
41	KC2	P	304	13	-	4/15/71/71	-
42	DD6	D	317	-	-	1/26/80/80	0/3/3/3
40	CLA	o	306	34	-	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	a	823	23	-	7/27/103/115	-
40	CLA	w	302	38	-	0/18/94/115	-
40	CLA	B	307	-	-	8/18/94/115	-
42	DD6	Q	213	-	-	1/26/80/80	0/3/3/3
40	CLA	I	201	-	-	10/39/115/115	-
42	DD6	A	313	-	-	1/26/80/80	0/3/3/3
46	SQD	F	320	-	-	9/31/51/69	0/1/1/1
43	LMG	D	318	-	-	16/35/55/70	0/1/1/1
40	CLA	J	306	10	-	2/24/100/115	-
47	A1EB1	N	320	-	-	7/42/100/100	0/3/3/3
40	CLA	C	308	-	-	7/18/94/115	-
40	CLA	A	308	-	-	2/27/103/115	-
41	KC2	K	302	11	-	6/15/71/71	-
40	CLA	Q	203	-	-	4/21/97/115	-
40	CLA	y	305	-	-	3/19/95/115	-
40	CLA	X	313	20	-	2/18/94/115	-
47	A1EB1	w	313	-	-	13/42/100/100	0/3/3/3
41	KC2	H	316	-	-	5/15/71/71	-
40	CLA	b	821	-	-	7/39/115/115	-
40	CLA	v	306	36	-	10/33/109/115	-
41	KC2	Y	309	21,44	-	8/15/71/71	-
43	LMG	E	301	40	-	14/26/46/70	0/1/1/1
46	SQD	W	318	-	-	7/27/47/69	0/1/1/1
47	A1EB1	K	313	-	-	4/42/100/100	0/3/3/3
47	A1EB1	x	321	-	-	2/42/100/100	0/3/3/3
47	A1EB1	q	322	-	-	8/42/100/100	0/3/3/3
42	DD6	J	317	-	-	1/26/80/80	0/3/3/3
47	A1EB1	t	315	-	-	12/42/100/100	0/3/3/3
51	SF4	c	101	-	-	-	0/6/5/5
40	CLA	V	202	19	-	10/27/103/115	-
41	KC2	O	308	15	-	8/15/71/71	-
47	A1EB1	T	316	40	-	4/42/100/100	0/3/3/3
40	CLA	U	207	-	-	4/18/94/115	-
47	A1EB1	o	321	-	-	8/42/100/100	1/3/3/3
43	LMG	u	301	-	-	15/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	A86	W	316	-	-	5/34/90/90	0/3/3/3
47	A1EB1	R	317	40	-	9/42/100/100	0/3/3/3
41	KC2	o	308	34	-	8/15/71/71	-
41	KC2	y	301	38	-	9/15/71/71	-
41	KC2	p	303	-	-	6/15/71/71	-
40	CLA	H	302	-	-	7/18/94/115	-
44	A86	Y	321	-	-	5/34/90/90	0/3/3/3
47	A1EB1	v	324	-	-	12/42/100/100	0/3/3/3
47	A1EB1	S	321	-	-	9/42/100/100	1/3/3/3
42	DD6	J	316	-	-	0/26/80/80	0/3/3/3
41	KC2	X	309	-	-	6/15/71/71	-
44	A86	z	315	-	-	7/34/90/90	0/3/3/3
40	CLA	O	310	-	-	6/18/94/115	-
42	DD6	N	317	-	-	3/26/80/80	0/3/3/3
41	KC2	u	303	-	-	6/15/71/71	-
47	A1EB1	K	315	-	-	15/42/100/100	1/3/3/3
40	CLA	K	312	-	-	3/18/94/115	-
40	CLA	a	835	-	-	2/39/115/115	-
42	DD6	F	316	-	-	2/26/80/80	0/3/3/3
40	CLA	L	307	-	-	3/27/103/115	-
47	A1EB1	v	322	-	-	7/42/100/100	0/3/3/3
40	CLA	b	836	24	-	6/33/109/115	-
41	KC2	x	310	-	-	6/15/71/71	-
40	CLA	b	835	24	-	13/38/115/115	-
41	KC2	u	309	-	-	6/15/71/71	-
44	A86	q	317	-	-	1/34/90/90	0/3/3/3
40	CLA	U	208	-	-	7/18/94/115	-
41	KC2	R	308	15	-	6/15/71/71	-
42	DD6	v	320	-	-	7/26/80/80	0/3/3/3
40	CLA	b	817	24	-	6/39/115/115	-
40	CLA	J	318	10	-	1/18/94/115	-
40	CLA	z	314	-	-	4/18/94/115	-
40	CLA	a	818	-	-	2/18/94/115	-
40	CLA	N	310	-	-	5/21/97/115	-
42	DD6	A	312	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	a	822	-	-	12/39/115/115	-
41	KC2	p	310	-	-	6/15/71/71	-
50	PQN	a	847	-	-	4/17/37/43	0/2/2/2
40	CLA	b	831	24	-	5/23/99/115	-
40	CLA	N	307	-	-	7/33/109/115	-
40	CLA	S	314	17	-	12/27/103/115	-
40	CLA	Y	305	21	-	7/27/103/115	-
40	CLA	a	807	-	-	9/29/105/115	-
40	CLA	b	842	-	-	10/35/111/115	-
41	KC2	v	308	36	-	10/15/71/71	-
44	A86	Y	318	-	-	9/34/90/90	0/3/3/3
40	CLA	v	311	-	-	10/37/113/115	-
40	CLA	H	304	-	-	5/18/94/115	-
40	CLA	a	820	23	-	13/33/109/115	-
44	A86	o	315	-	-	9/34/90/90	0/3/3/3
44	A86	o	317	-	-	7/34/90/90	0/3/3/3
44	A86	z	320	-	-	1/34/90/90	0/3/3/3
40	CLA	f	204	28	-	2/18/94/115	-
44	A86	T	315	-	-	11/34/90/90	1/3/3/3
40	CLA	u	313	-	-	1/27/103/115	-
40	CLA	B	304	-	-	6/18/94/115	-
40	CLA	a	841	23	-	8/39/115/115	-
40	CLA	a	852	-	-	7/27/103/115	-
40	CLA	H	305	8	-	10/33/109/115	-
44	A86	Q	215	-	-	3/34/90/90	0/3/3/3
40	CLA	S	305	-	-	7/24/100/115	-
44	A86	v	315	-	-	6/34/90/90	0/3/3/3
40	CLA	Z	310	-	-	10/27/103/115	-
40	CLA	J	309	-	-	2/18/94/115	-
44	A86	u	318	-	-	12/34/90/90	0/3/3/3
40	CLA	D	312	4	-	9/27/103/115	-
40	CLA	X	305	-	-	8/21/97/115	-
44	A86	X	318	-	-	5/34/90/90	0/3/3/3
41	KC2	Q	216	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	KC2	R	303	-	-	9/15/71/71	-
44	A86	X	316	-	-	4/34/90/90	0/3/3/3
40	CLA	S	301	-	-	8/33/109/115	-
43	LMG	P	318	-	-	11/34/54/70	0/1/1/1
42	DD6	J	315	-	-	1/26/80/80	0/3/3/3
40	CLA	H	301	-	-	5/18/94/115	-
41	KC2	w	306	38	-	8/15/71/71	-
44	A86	q	314	-	-	3/34/90/90	0/3/3/3
40	CLA	b	811	24	-	5/18/94/115	-
41	KC2	t	308	-	-	6/15/71/71	-
40	CLA	u	302	-	-	7/39/115/115	-
49	BCR	i	102	-	-	4/29/63/63	0/2/2/2
44	A86	q	319	-	-	13/34/90/90	0/3/3/3
40	CLA	C	301	3	-	6/18/94/115	-
41	KC2	K	303	11	-	9/15/71/71	-
41	KC2	y	307	-	-	6/15/71/71	-
40	CLA	a	809	-	-	3/21/97/115	-
40	CLA	v	312	-	-	7/33/109/115	-
40	CLA	Y	312	-	-	4/18/94/115	-
49	BCR	l	208	-	-	5/29/63/63	0/2/2/2
40	CLA	b	839	24	-	13/39/115/115	-
40	CLA	D	311	-	-	4/18/94/115	-
41	KC2	P	309	13	-	4/15/71/71	-
40	CLA	G	213	-	-	8/18/94/115	-
42	DD6	j	104	-	-	1/26/80/80	0/3/3/3
41	KC2	T	302	-	-	3/15/71/71	-
41	KC2	T	311	15	-	8/15/71/71	-
42	DD6	p	322	-	-	3/26/80/80	0/3/3/3
42	DD6	w	312	-	-	1/26/80/80	0/3/3/3
40	CLA	a	812	23	-	1/27/103/115	-
40	CLA	I	208	-	-	8/27/103/115	-
40	CLA	S	308	-	-	5/19/95/115	-
41	KC2	N	312	14	-	8/15/71/71	-
44	A86	D	320	-	-	5/34/90/90	0/3/3/3
44	A86	P	314	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	E	304	5	-	1/27/103/115	-
41	KC2	C	303	-	-	8/15/71/71	-
44	A86	M	313	-	-	3/34/90/90	0/3/3/3
41	KC2	P	310	-	-	7/15/71/71	-
42	DD6	C	313	-	-	2/26/80/80	0/3/3/3
41	KC2	T	309	15	-	5/15/71/71	-
40	CLA	f	205	-	-	3/18/94/115	-
40	CLA	b	825	-	-	9/39/115/115	-
44	A86	T	312	-	-	4/34/90/90	0/3/3/3
40	CLA	o	313	-	-	4/18/94/115	-
40	CLA	B	301	2	-	9/18/94/115	-
40	CLA	F	308	-	-	3/27/103/115	-
40	CLA	Z	305	22	-	8/27/103/115	-
47	A1EB1	Z	321	-	-	9/42/100/100	0/3/3/3
40	CLA	M	304	13	-	10/33/109/115	-
44	A86	p	319	-	-	11/34/90/90	0/3/3/3
41	KC2	Y	302	-	-	5/15/71/71	-
40	CLA	K	304	11	-	7/33/109/115	-
40	CLA	b	814	24	-	13/39/115/115	-
40	CLA	x	305	-	-	2/23/99/115	-
41	KC2	M	301	13	-	7/15/71/71	-
42	DD6	o	319	-	-	1/26/80/80	0/3/3/3
41	KC2	x	315	-	-	7/15/71/71	-
40	CLA	y	303	-	-	4/18/94/115	-
40	CLA	E	305	5	-	5/33/109/115	-
40	CLA	v	304	-	-	4/24/100/115	-
40	CLA	x	314	35	-	5/18/94/115	-
40	CLA	z	306	-	-	5/27/103/115	-
40	CLA	x	306	35	-	14/33/109/115	-
43	LMG	a	802	-	-	12/30/50/70	0/1/1/1
42	DD6	M	314	-	-	1/26/80/80	0/3/3/3
40	CLA	b	810	24	-	14/39/115/115	-
43	LMG	j	101	-	-	10/25/45/70	0/1/1/1
41	KC2	u	310	-	-	6/15/71/71	-
44	A86	X	315	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	CLA	b	828	24	-	2/27/103/115	-
40	CLA	b	806	24	-	15/39/115/115	-
40	CLA	a	834	-	-	6/33/109/115	-
47	A1EB1	S	320	-	-	7/42/100/100	1/3/3/3
40	CLA	b	834	-	-	10/39/115/115	-
40	CLA	w	308	-	-	6/18/94/115	-
44	A86	W	314	-	-	6/34/90/90	0/3/3/3
40	CLA	Q	208	-	-	7/33/109/115	-
40	CLA	o	310	-	-	10/27/103/115	-

The worst 5 of 4171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	309	KC2	MG-ND	-10.40	1.85	2.05
41	Z	309	KC2	MG-ND	-10.36	1.85	2.05
41	v	303	KC2	MG-ND	-10.32	1.85	2.05
41	M	303	KC2	MG-ND	-10.26	1.85	2.05
41	P	304	KC2	MG-ND	-10.26	1.85	2.05

The worst 5 of 4812 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	M	313	A86	O1-C20-C19	-14.27	102.66	113.38
44	X	318	A86	O1-C20-C19	11.95	122.36	113.38
44	z	317	A86	O1-C20-C19	-10.89	105.20	113.38
44	z	316	A86	O1-C20-C19	10.85	121.53	113.38
40	F	303	CLA	C1C-NC-C4C	-10.00	102.21	106.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
42	P	315	DD6	C20

5 of 5342 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	A	303	CLA	C1A-C2A-CAA-CBA
40	A	303	CLA	C3A-C2A-CAA-CBA
40	A	304	CLA	C1A-C2A-CAA-CBA
40	A	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
40	A	304	CLA	C2B-C3B-CAB-CBB

5 of 21 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	t	311	A86	C31-C32-C33-C34-C35-C36
44	X	314	A86	C31-C32-C33-C34-C35-C36
44	C	311	A86	C31-C32-C33-C34-C35-C36
44	Z	317	A86	C31-C32-C33-C34-C35-C36
44	Z	316	A86	C31-C32-C33-C34-C35-C36

264 monomers are involved in 562 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	b	847	BCR	1	0
40	a	850	CLA	1	0
42	F	314	DD6	1	0
52	b	850	DGD	7	0
40	E	303	CLA	4	0
40	T	305	CLA	1	0
41	Q	201	KC2	2	0
40	S	319	CLA	1	0
48	P	320	A1EB4	4	0
41	T	301	KC2	1	0
46	M	318	SQD	1	0
42	o	320	DD6	2	0
40	a	816	CLA	1	0
40	b	809	CLA	3	0
40	a	819	CLA	21	0
40	P	306	CLA	1	0
40	E	306	CLA	8	0
40	M	307	CLA	1	0
40	a	808	CLA	1	0
42	q	318	DD6	6	0
42	Y	322	DD6	9	0
40	A	311	CLA	3	0
47	T	320	A1EB1	1	0
46	k	205	SQD	3	0
40	W	306	CLA	1	0
42	A	316	DD6	10	0
40	b	829	CLA	2	0
40	y	308	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	o	311	CLA	1	0
40	K	307	CLA	1	0
44	W	301	A86	1	0
44	t	310	A86	1	0
40	Q	207	CLA	1	0
40	P	305	CLA	3	0
44	L	314	A86	1	0
47	P	301	A1EB1	9	0
40	b	826	CLA	1	0
40	A	305	CLA	3	0
40	N	306	CLA	1	0
40	k	201	CLA	1	0
40	A	306	CLA	12	0
41	M	303	KC2	1	0
40	a	842	CLA	1	0
43	x	301	LMG	5	0
40	z	305	CLA	3	0
47	p	324	A1EB1	1	0
40	X	304	CLA	2	0
40	o	312	CLA	2	0
40	W	305	CLA	1	0
44	G	209	A86	3	0
41	X	303	KC2	1	0
40	K	308	CLA	2	0
40	l	203	CLA	1	0
41	T	308	KC2	1	0
42	W	315	DD6	1	0
40	W	312	CLA	2	0
44	N	315	A86	7	0
40	f	202	CLA	3	0
43	a	801	LMG	2	0
44	Z	316	A86	1	0
41	N	302	KC2	1	0
40	a	814	CLA	1	0
40	D	304	CLA	1	0
40	R	305	CLA	1	0
42	y	311	DD6	17	0
40	E	307	CLA	12	0
42	x	320	DD6	2	0
42	N	316	DD6	1	0
40	b	803	CLA	1	0
47	u	322	A1EB1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	b	832	CLA	2	0
41	Z	309	KC2	1	0
40	q	311	CLA	2	0
40	a	815	CLA	12	0
40	b	802	CLA	2	0
41	Z	303	KC2	1	0
40	P	313	CLA	1	0
40	a	832	CLA	2	0
40	L	305	CLA	1	0
47	t	314	A1EB1	1	0
40	N	305	CLA	1	0
42	C	310	DD6	1	0
44	Q	210	A86	1	0
40	W	311	CLA	1	0
40	k	202	CLA	16	0
44	Y	319	A86	1	0
50	b	849	PQN	2	0
40	K	301	CLA	2	0
41	Y	308	KC2	9	0
49	a	846	BCR	1	0
40	G	203	CLA	1	0
40	y	302	CLA	1	0
44	z	319	A86	1	0
40	C	302	CLA	1	0
43	E	321	LMG	3	0
49	l	207	BCR	3	0
40	R	306	CLA	1	0
40	l	202	CLA	2	0
40	D	307	CLA	1	0
40	F	301	CLA	7	0
40	U	203	CLA	1	0
40	D	303	CLA	1	0
49	m	101	BCR	4	0
42	Q	214	DD6	1	0
40	o	307	CLA	1	0
40	Q	206	CLA	9	0
46	I	215	SQD	2	0
42	t	312	DD6	29	0
42	v	318	DD6	4	0
40	C	306	CLA	1	0
41	P	303	KC2	1	0
44	Y	320	A86	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	G	201	CLA	1	0
40	F	305	CLA	1	0
40	x	312	CLA	1	0
40	F	306	CLA	1	0
43	E	320	LMG	2	0
42	L	317	DD6	17	0
40	D	306	CLA	1	0
40	K	306	CLA	1	0
48	W	319	A1EB4	7	0
40	E	302	CLA	1	0
40	E	311	CLA	6	0
40	L	306	CLA	7	0
40	S	312	CLA	6	0
40	a	817	CLA	1	0
40	b	824	CLA	2	0
41	z	304	KC2	1	0
40	b	833	CLA	1	0
40	Z	306	CLA	1	0
40	a	824	CLA	1	0
40	F	307	CLA	4	0
40	b	819	CLA	1	0
40	p	305	CLA	1	0
42	B	305	DD6	1	0
44	p	318	A86	1	0
41	t	306	KC2	14	0
44	y	310	A86	1	0
40	E	308	CLA	4	0
46	P	319	SQD	5	0
42	P	315	DD6	5	0
40	b	813	CLA	2	0
42	u	321	DD6	1	0
40	a	830	CLA	1	0
41	y	306	KC2	7	0
49	a	843	BCR	5	0
40	P	308	CLA	6	0
40	p	306	CLA	1	0
40	A	302	CLA	2	0
40	M	305	CLA	1	0
40	b	827	CLA	1	0
40	w	305	CLA	1	0
40	o	301	CLA	1	0
47	x	322	A1EB1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	w	316	A86	1	0
49	b	846	BCR	1	0
41	W	310	KC2	1	0
42	L	315	DD6	15	0
40	L	312	CLA	1	0
40	V	201	CLA	2	0
41	w	307	KC2	1	0
40	b	820	CLA	1	0
47	y	313	A1EB1	4	0
49	r	201	BCR	1	0
42	H	312	DD6	1	0
41	O	301	KC2	1	0
44	D	319	A86	1	0
49	a	845	BCR	1	0
42	I	210	DD6	1	0
40	N	304	CLA	1	0
44	X	317	A86	3	0
47	p	323	A1EB1	1	0
45	S	323	LHG	2	0
40	S	313	CLA	1	0
40	l	205	CLA	1	0
47	u	323	A1EB1	1	0
40	M	311	CLA	1	0
40	v	301	CLA	1	0
49	f	206	BCR	4	0
42	q	320	DD6	1	0
40	C	307	CLA	2	0
40	z	302	CLA	1	0
40	b	807	CLA	1	0
42	I	212	DD6	1	0
40	j	102	CLA	2	0
44	P	317	A86	1	0
40	t	305	CLA	1	0
40	i	101	CLA	4	0
41	T	303	KC2	1	0
44	Y	315	A86	1	0
40	D	305	CLA	1	0
41	L	303	KC2	1	0
42	O	314	DD6	1	0
44	M	315	A86	1	0
40	Q	204	CLA	1	0
40	H	307	CLA	1	0

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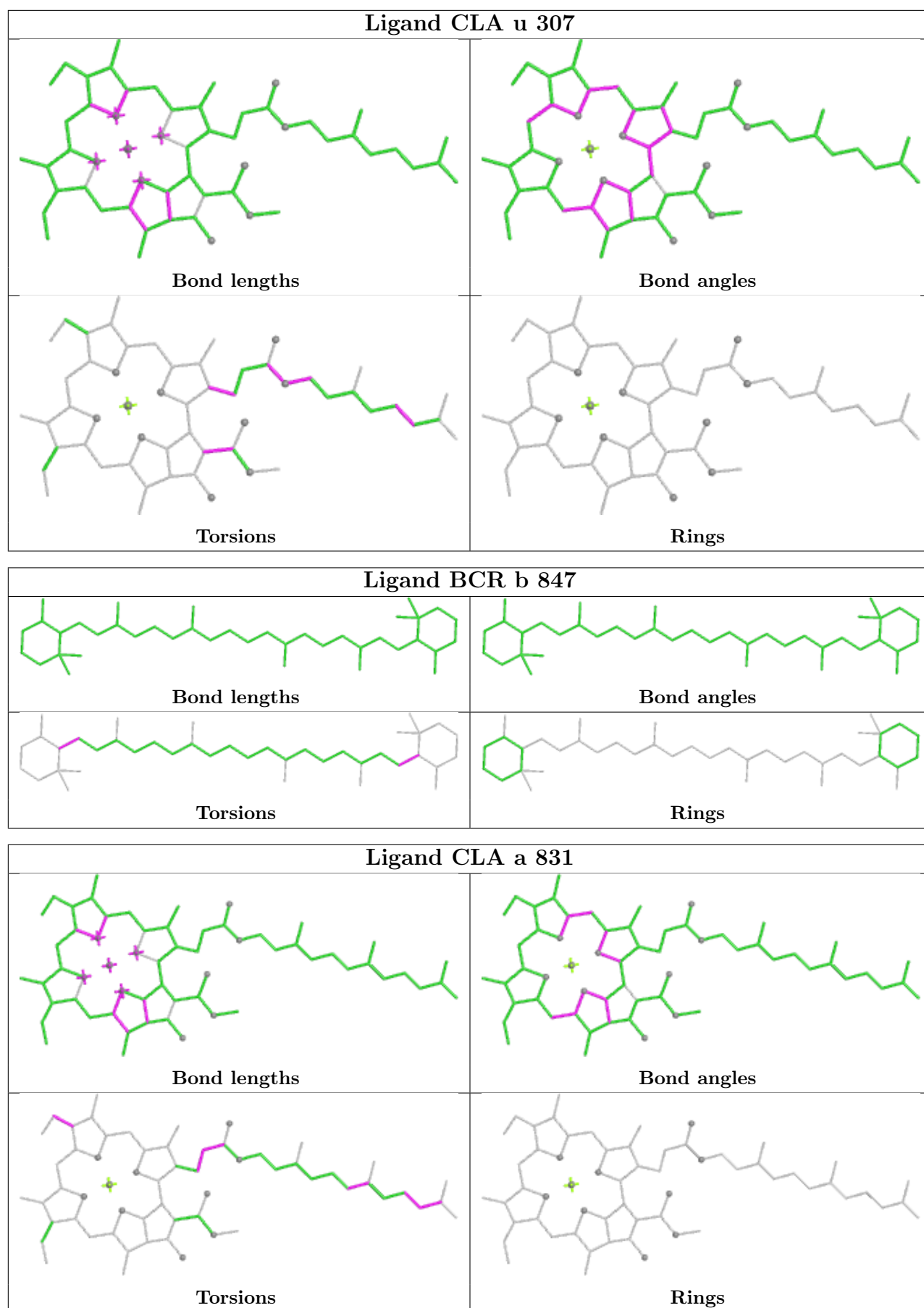
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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40	a	823	CLA	1	0
40	B	307	CLA	3	0
46	F	320	SQD	2	0
43	D	318	LMG	1	0
40	A	308	CLA	4	0
40	y	305	CLA	1	0
43	E	301	LMG	1	0
46	W	318	SQD	4	0
47	x	321	A1EB1	1	0
47	q	322	A1EB1	1	0
47	t	315	A1EB1	1	0
40	V	202	CLA	4	0
43	u	301	LMG	1	0
41	o	308	KC2	1	0
47	v	324	A1EB1	4	0
42	J	316	DD6	15	0
47	K	315	A1EB1	1	0
40	a	835	CLA	1	0
40	L	307	CLA	1	0
47	v	322	A1EB1	1	0
40	b	835	CLA	3	0
42	v	320	DD6	1	0
40	J	318	CLA	2	0
40	N	310	CLA	1	0
50	a	847	PQN	1	0
40	S	314	CLA	1	0
41	v	308	KC2	1	0
40	v	311	CLA	1	0
44	o	315	A86	1	0
40	a	841	CLA	2	0
40	S	305	CLA	5	0
40	J	309	CLA	12	0
41	Q	216	KC2	8	0
40	S	301	CLA	9	0
42	J	315	DD6	1	0
40	H	301	CLA	1	0
41	w	306	KC2	12	0
41	t	308	KC2	1	0
49	i	102	BCR	3	0
41	y	307	KC2	1	0
40	a	809	CLA	1	0

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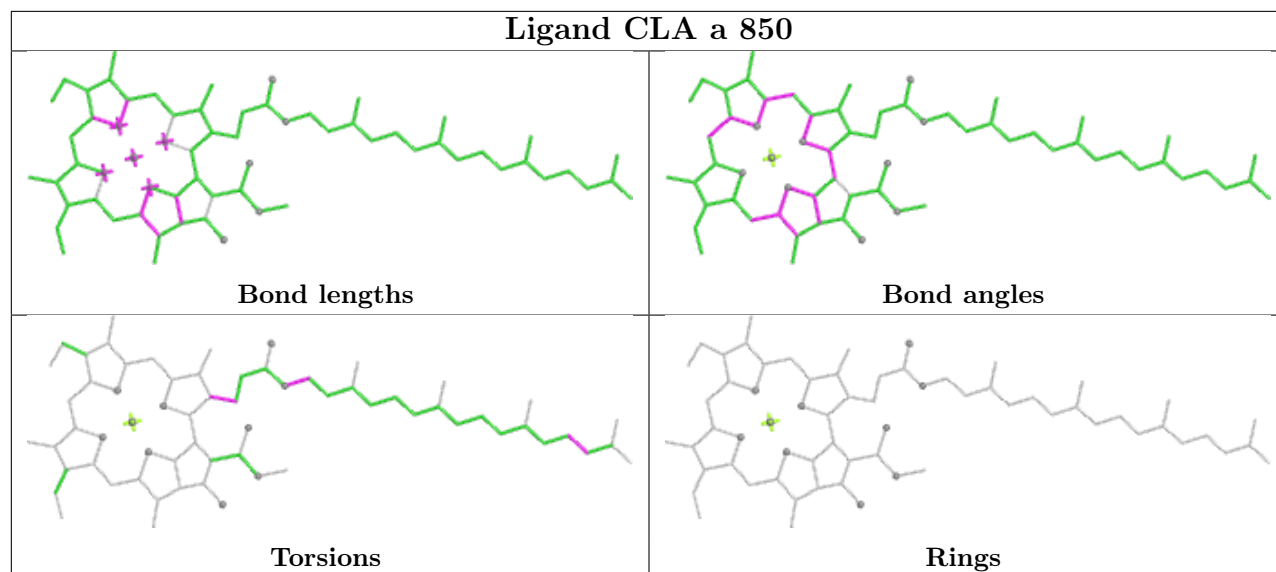
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	v	312	CLA	2	0
49	l	208	BCR	1	0
40	b	839	CLA	1	0
40	D	311	CLA	2	0
40	G	213	CLA	2	0
42	p	322	DD6	1	0
42	w	312	DD6	26	0
40	S	308	CLA	3	0
41	C	303	KC2	1	0
40	f	205	CLA	4	0
40	Z	305	CLA	1	0
47	Z	321	A1EB1	1	0
40	b	814	CLA	3	0
40	x	305	CLA	1	0
41	M	301	KC2	1	0
40	z	306	CLA	1	0
40	x	306	CLA	1	0
43	a	802	LMG	1	0
42	M	314	DD6	1	0
40	b	810	CLA	2	0
43	j	101	LMG	13	0
40	b	828	CLA	1	0
40	b	806	CLA	3	0
40	b	834	CLA	2	0
40	w	308	CLA	5	0
44	W	314	A86	1	0

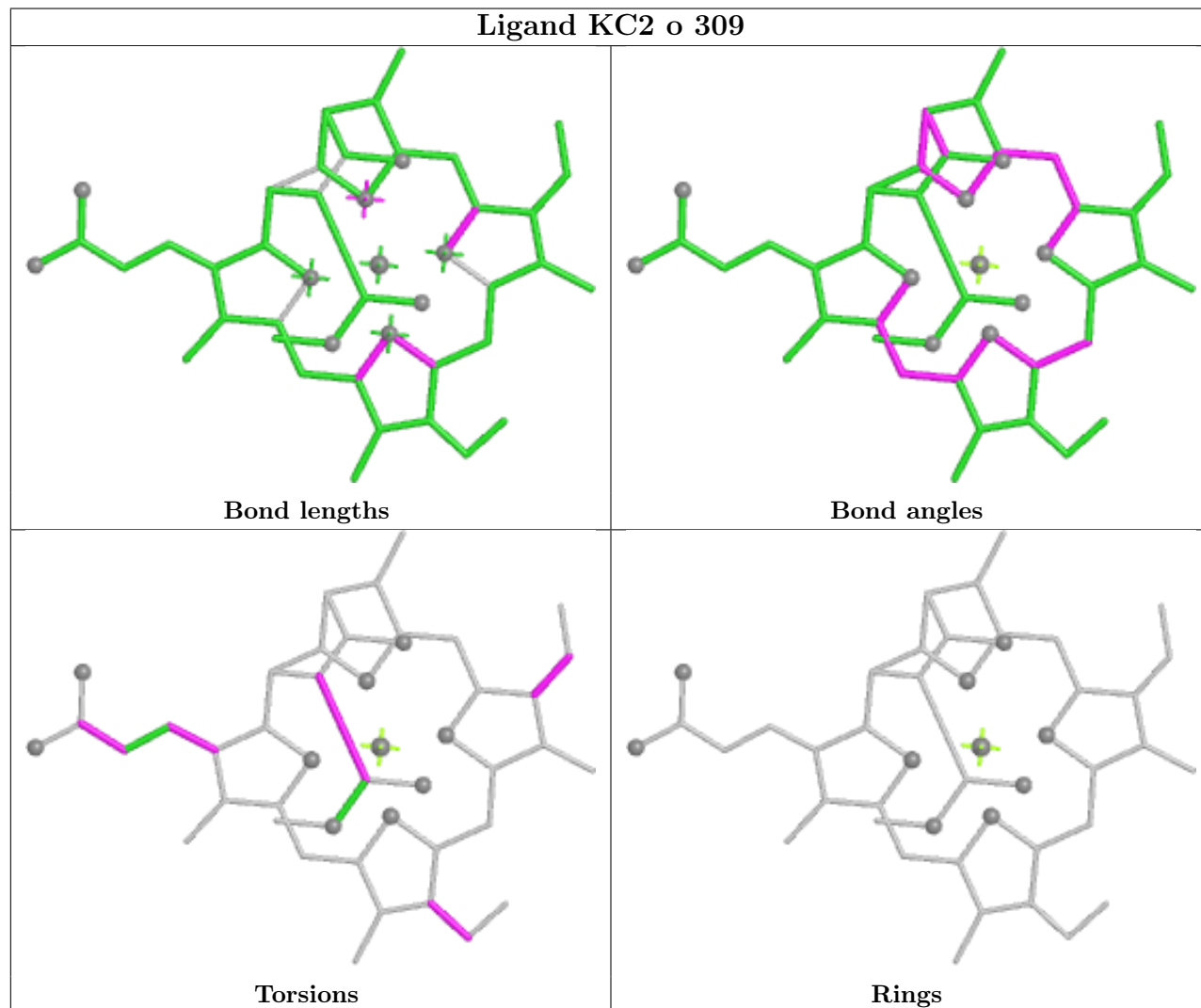
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

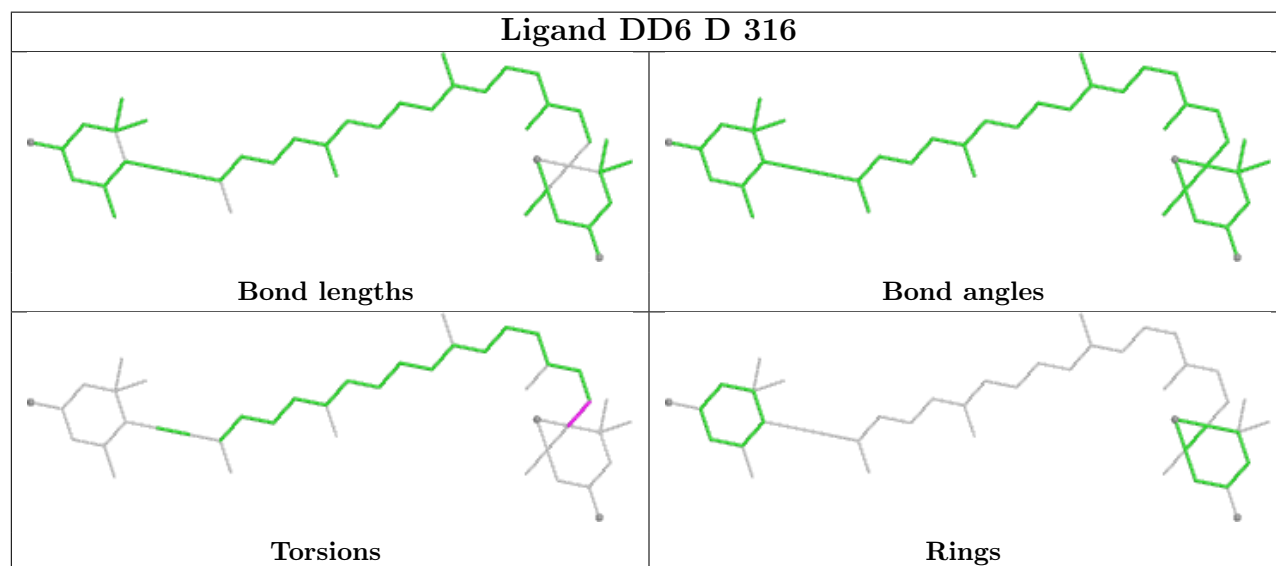
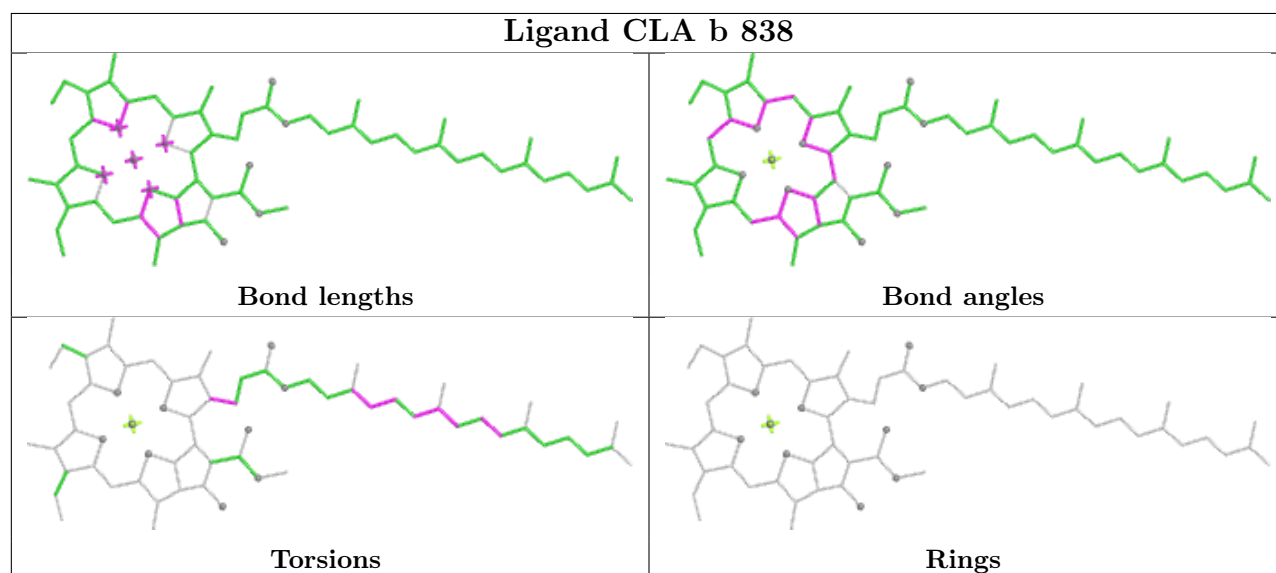
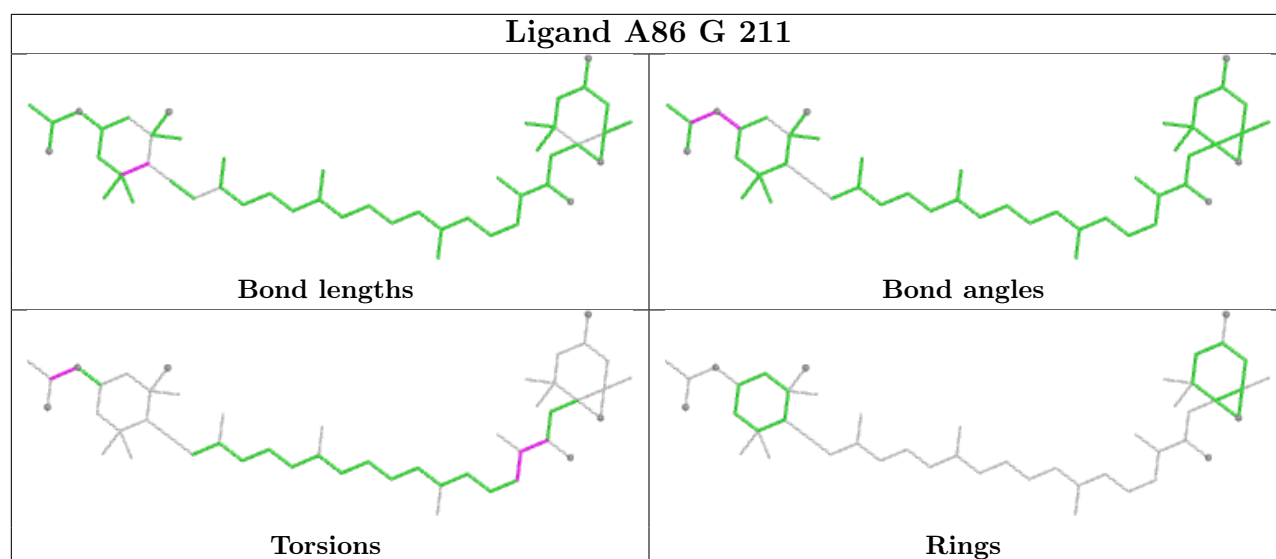


Ligand CLA a 850

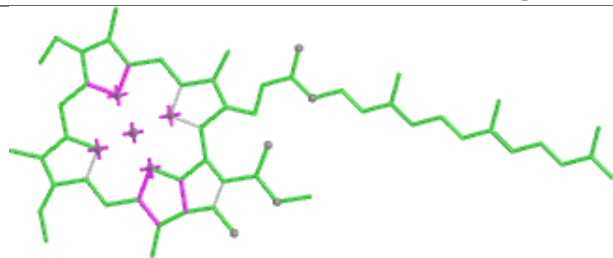


Ligand KC2 o 309

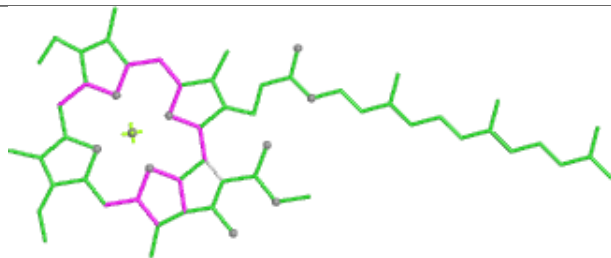




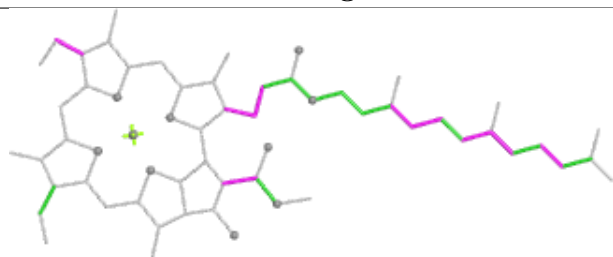
Ligand CLA F 321



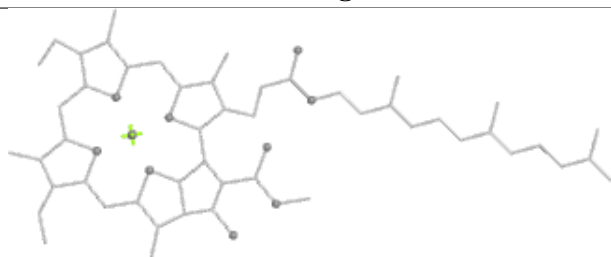
Bond lengths



Bond angles

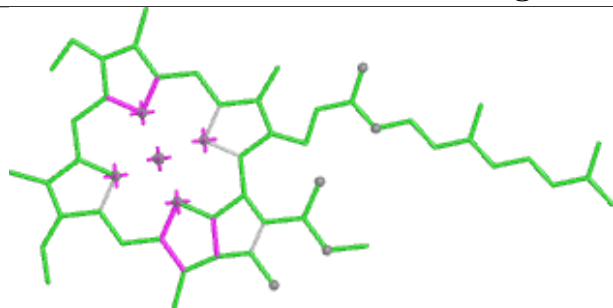


Torsions

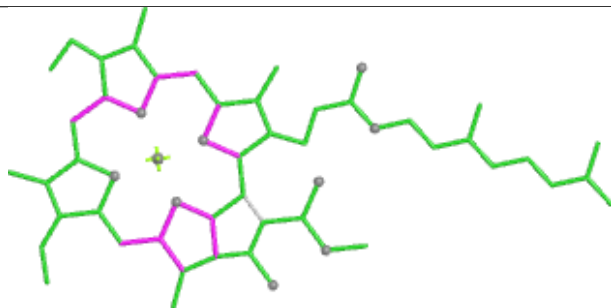


Rings

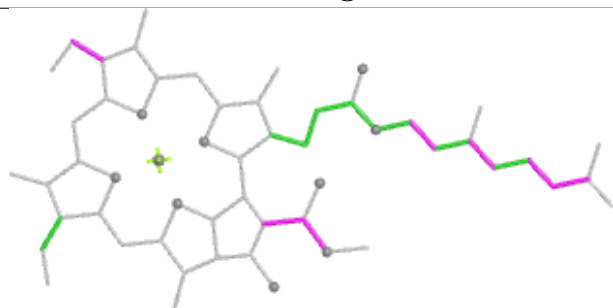
Ligand CLA Y 310



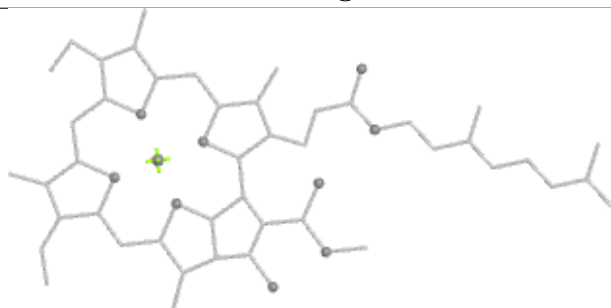
Bond lengths



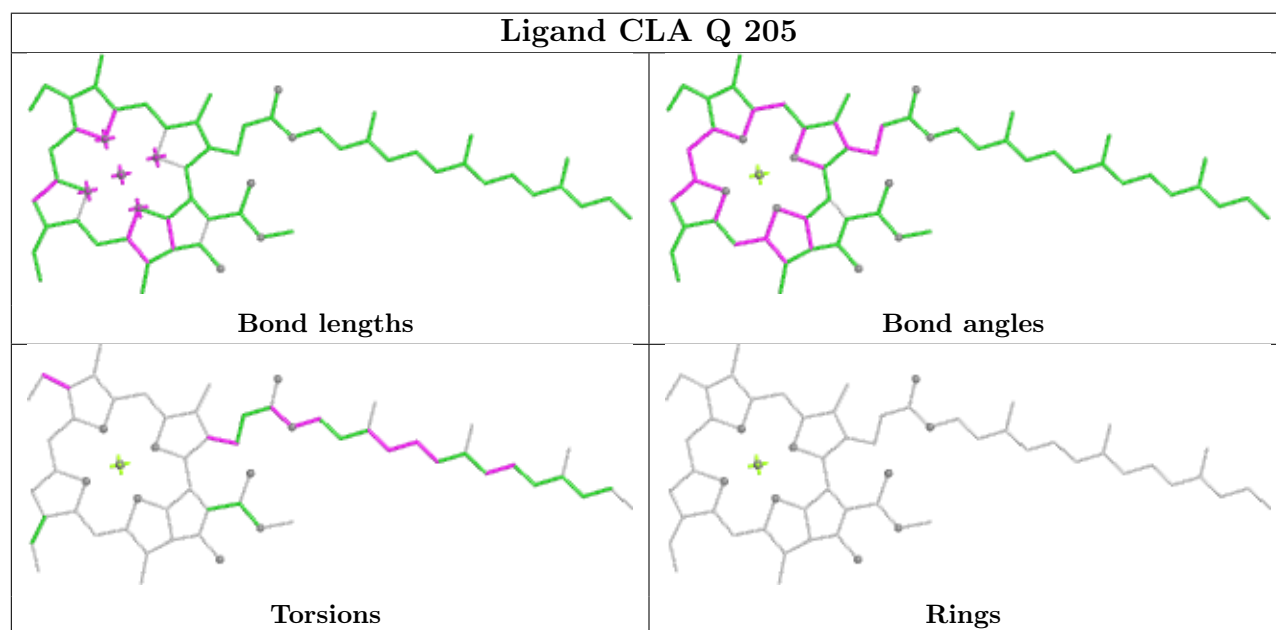
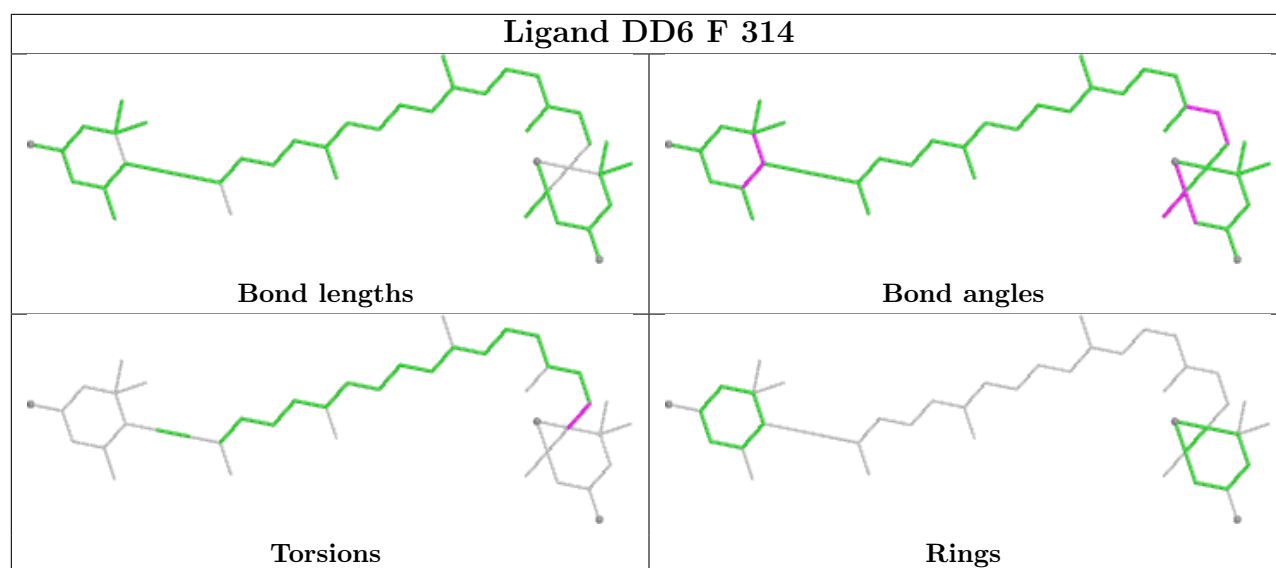
Bond angles

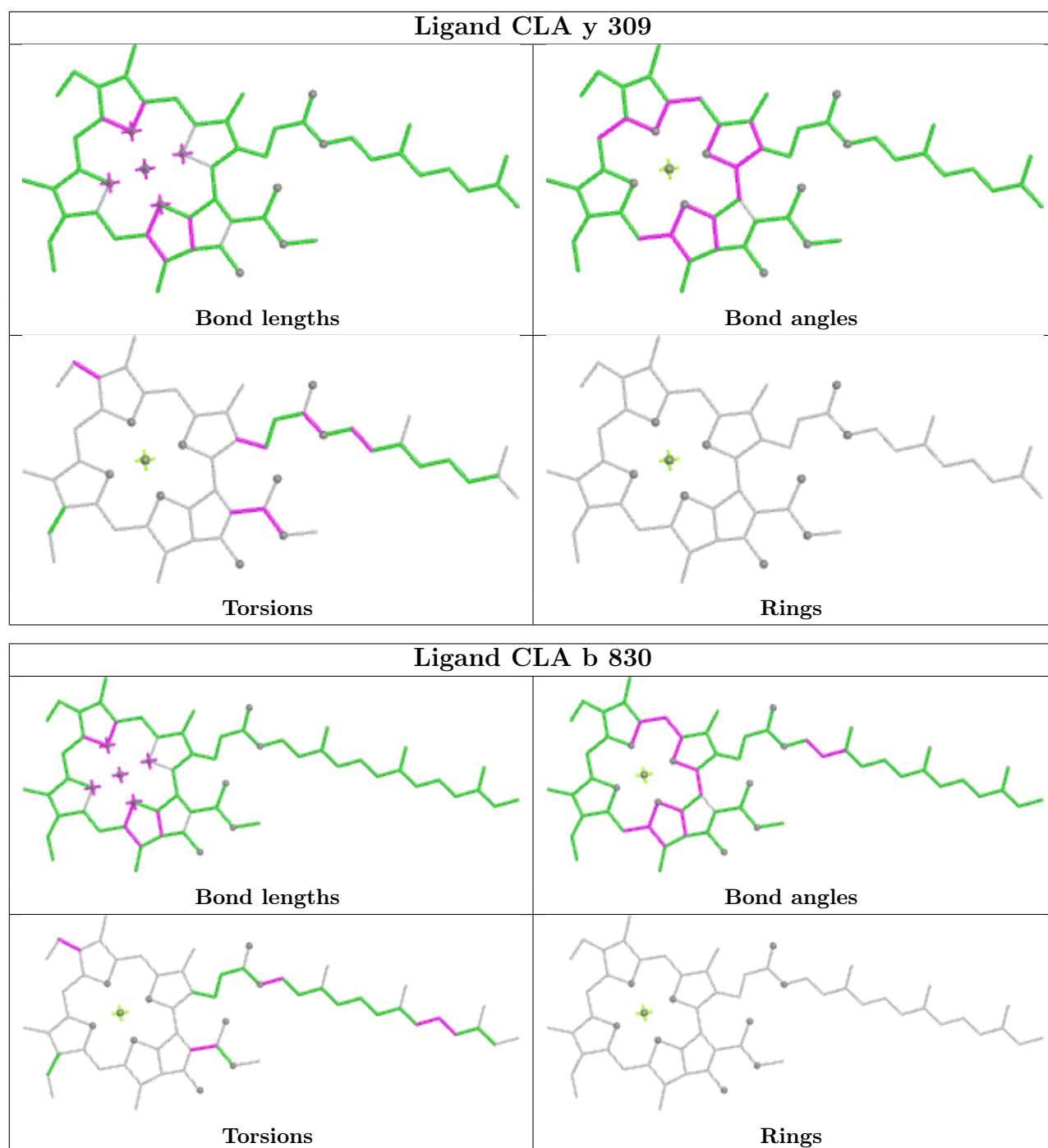


Torsions

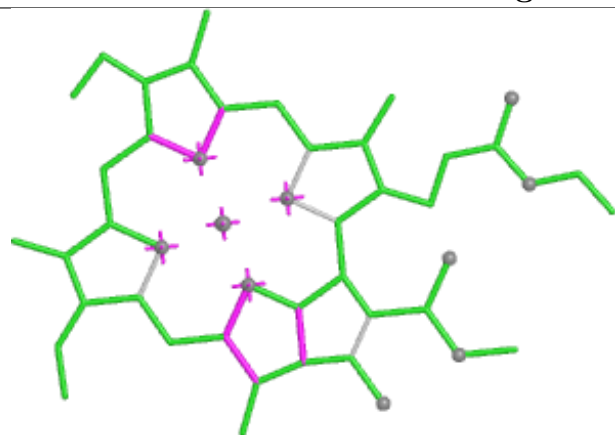


Rings

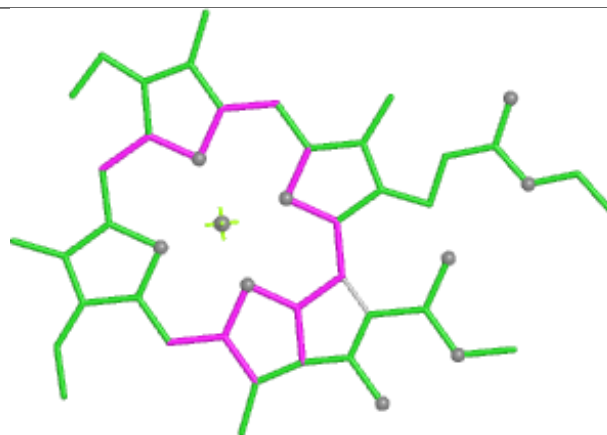




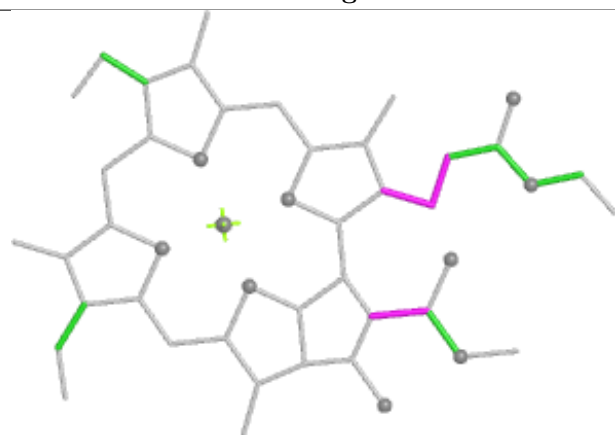
Ligand CLA X 312



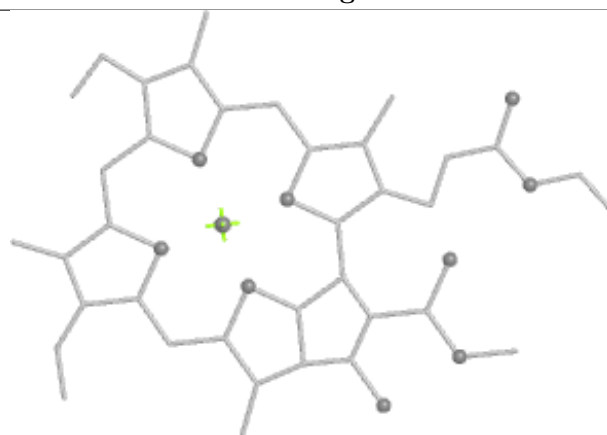
Bond lengths



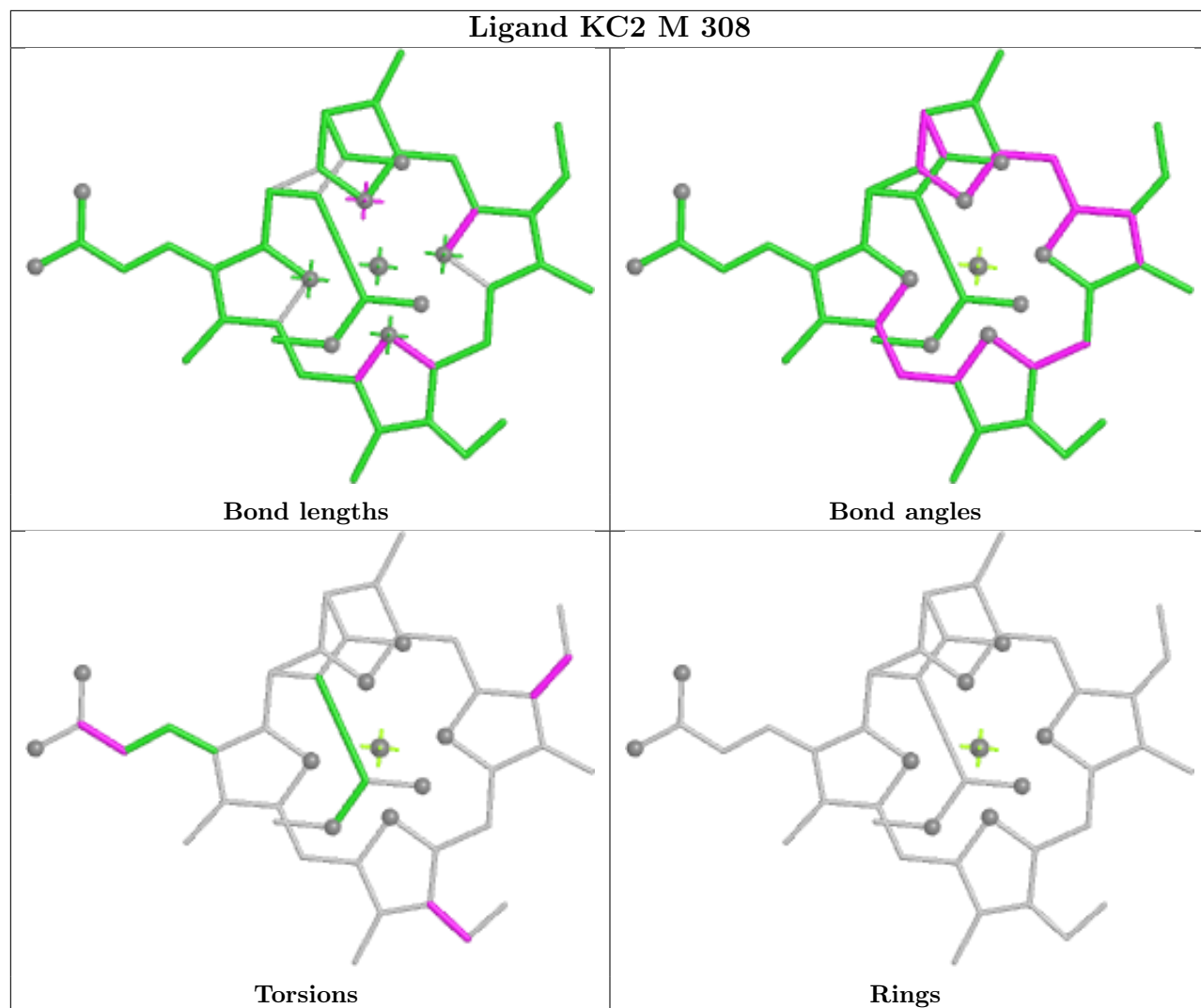
Bond angles



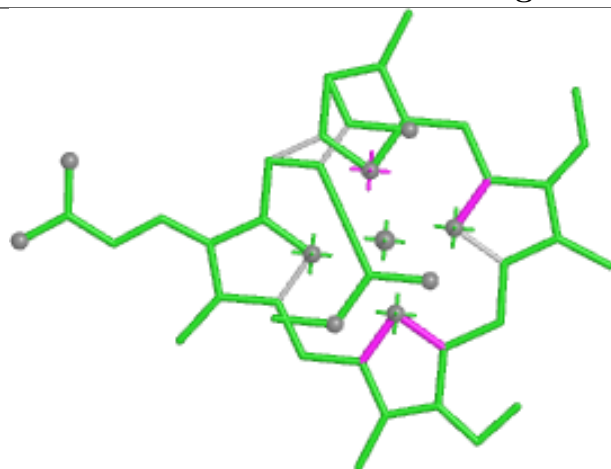
Torsions



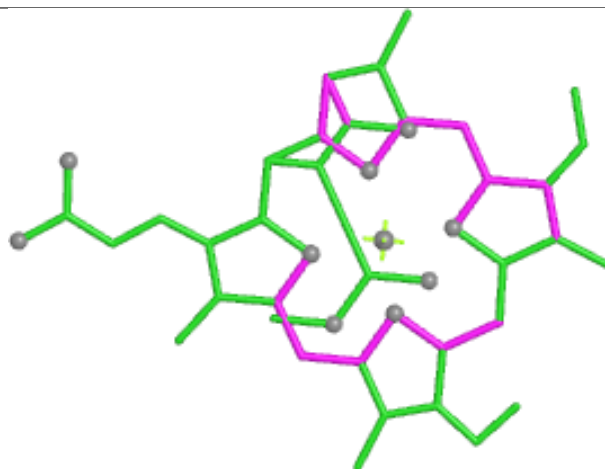
Rings



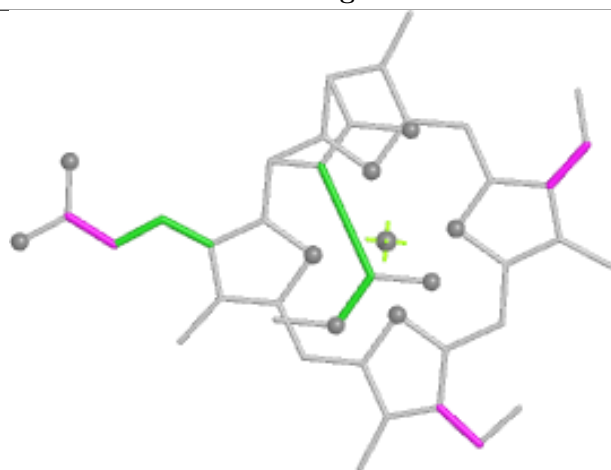
Ligand KC2 A 310



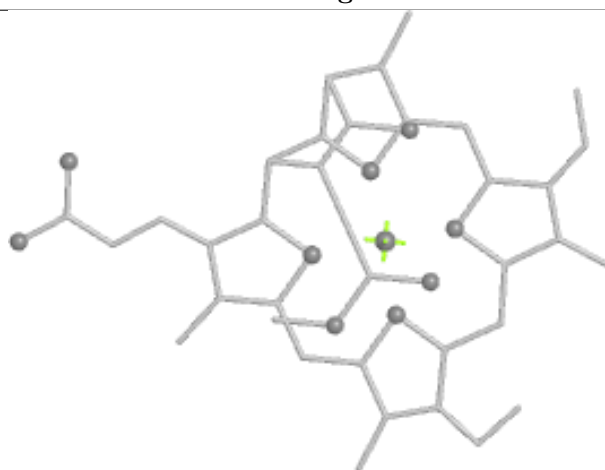
Bond lengths



Bond angles

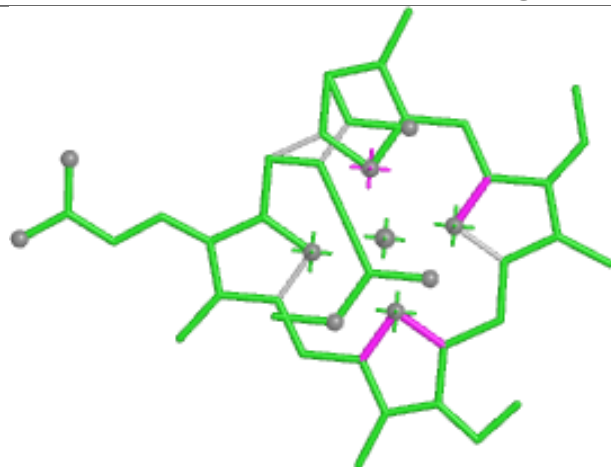


Torsions

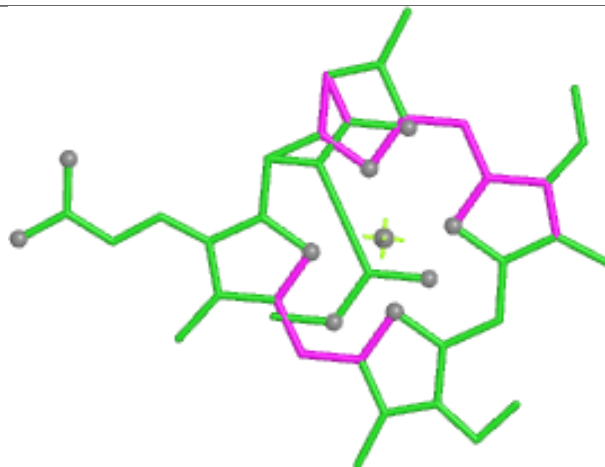


Rings

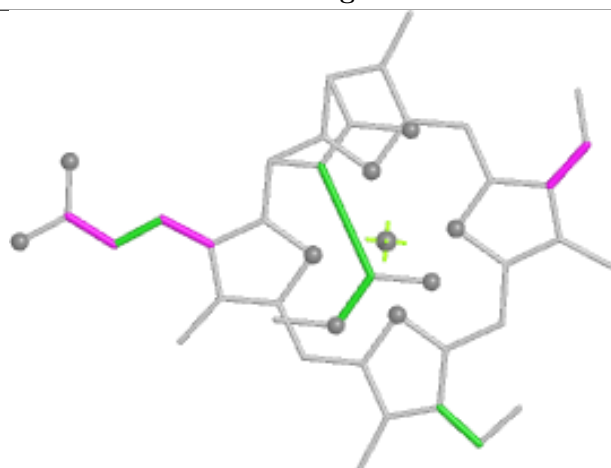
Ligand KC2 K 305



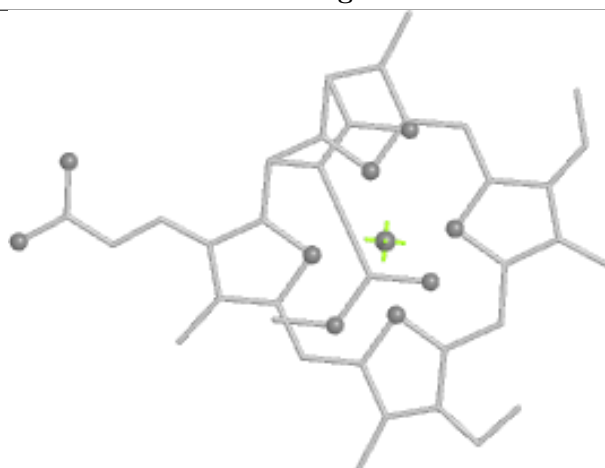
Bond lengths



Bond angles

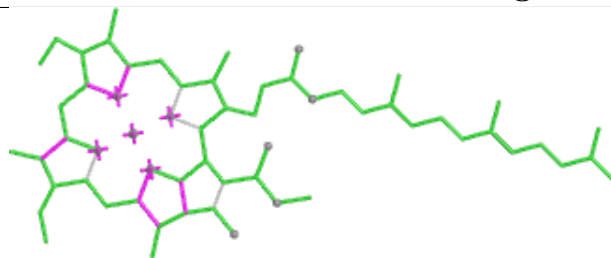


Torsions

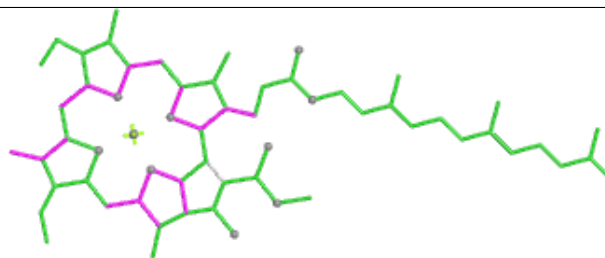


Rings

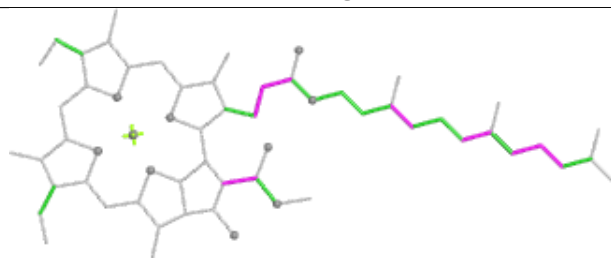
Ligand CLA O 306



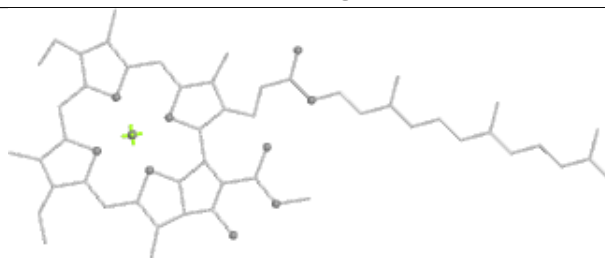
Bond lengths



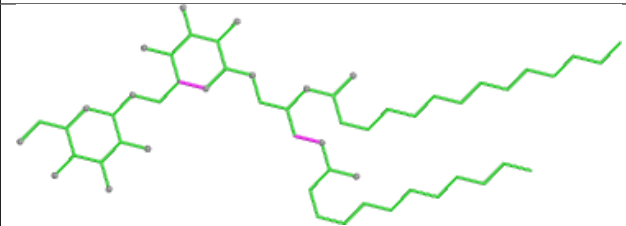
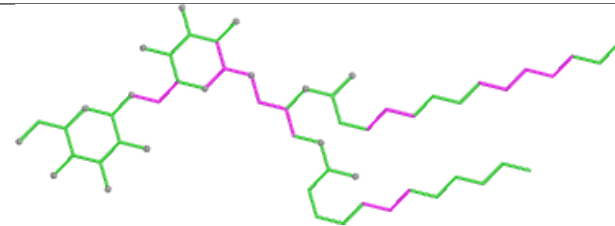
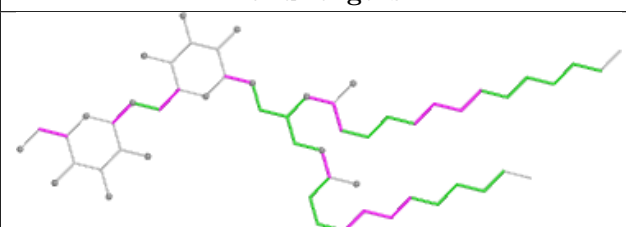
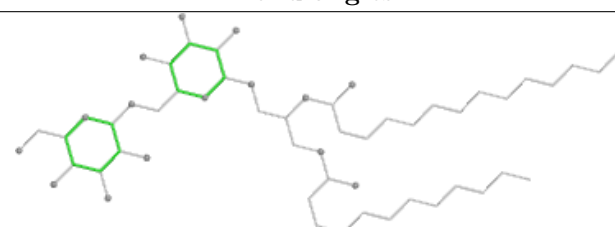
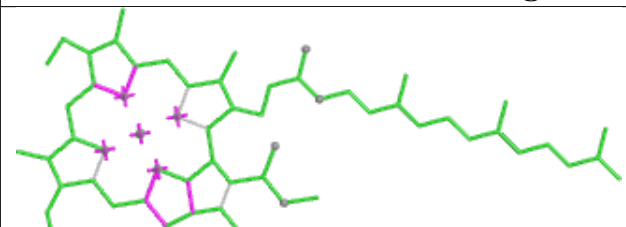
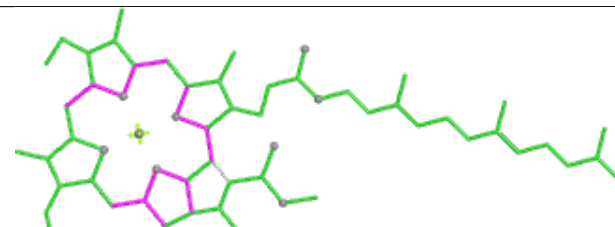
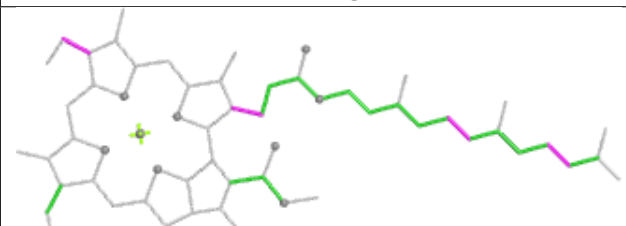
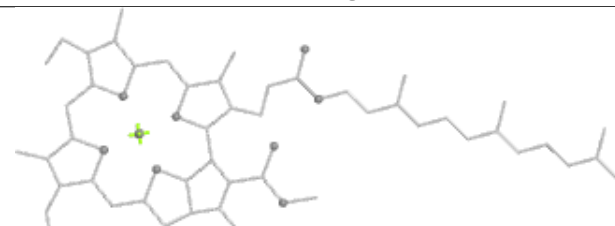
Bond angles

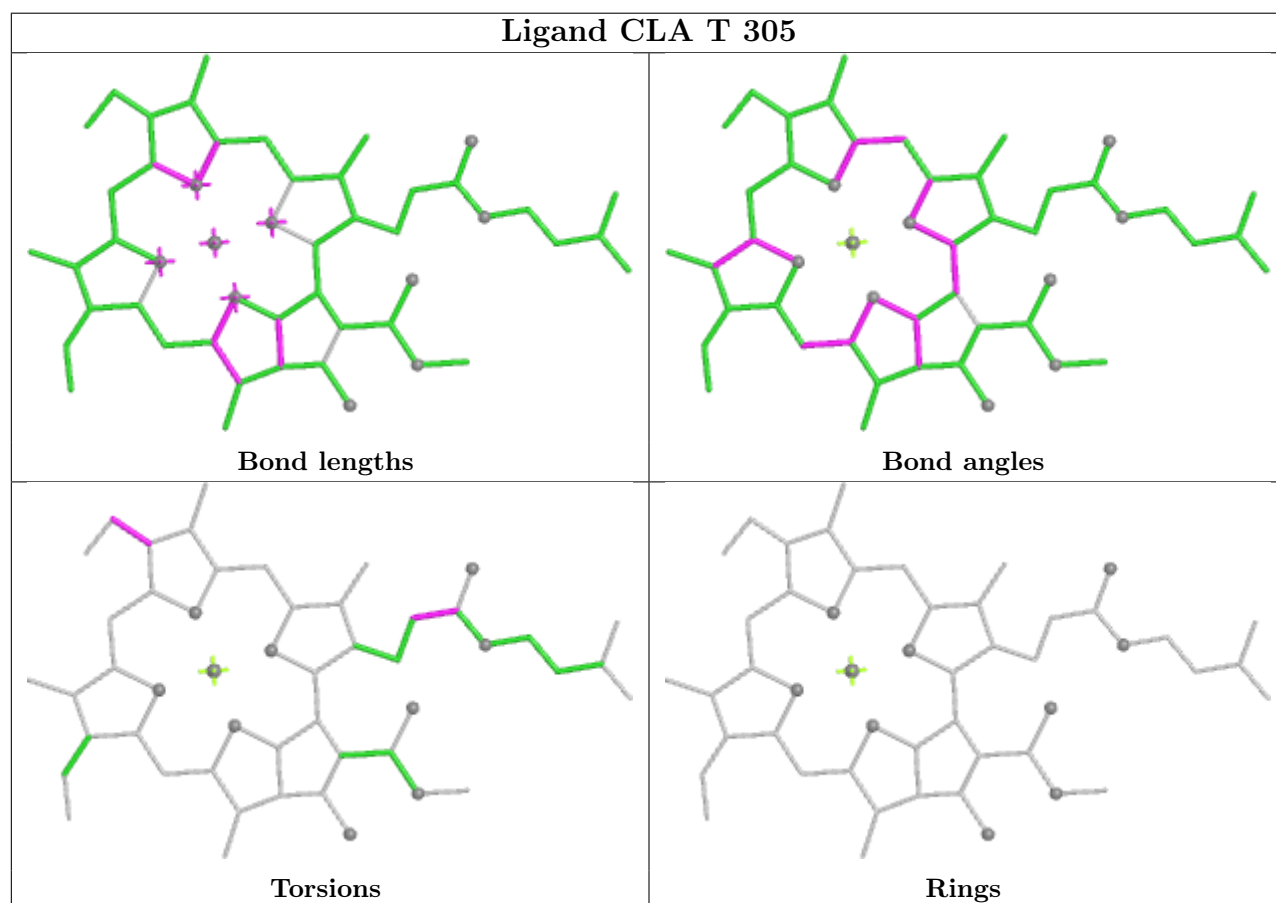
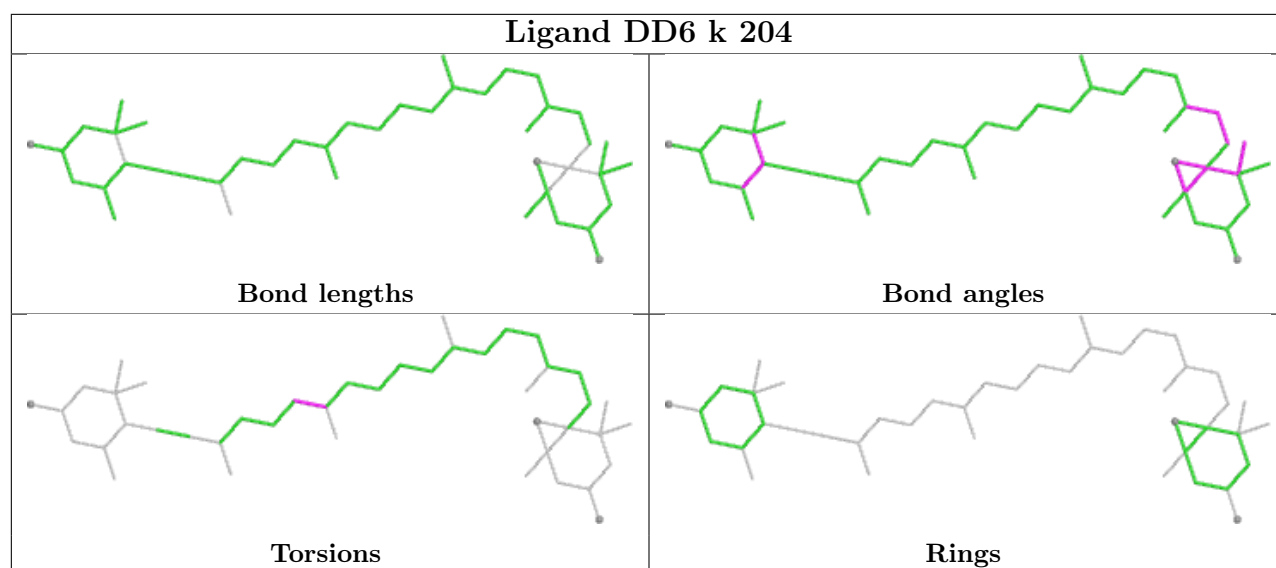


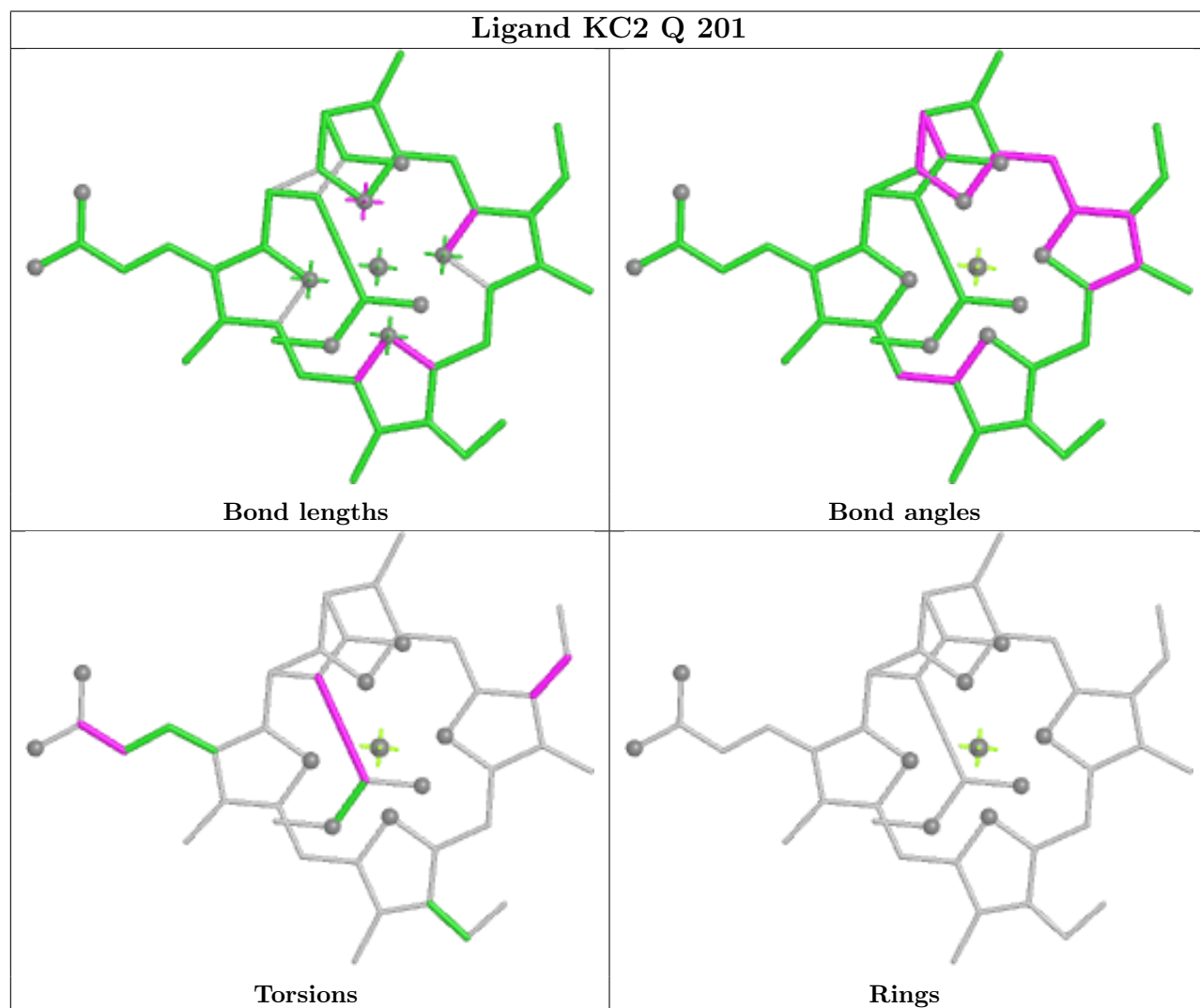
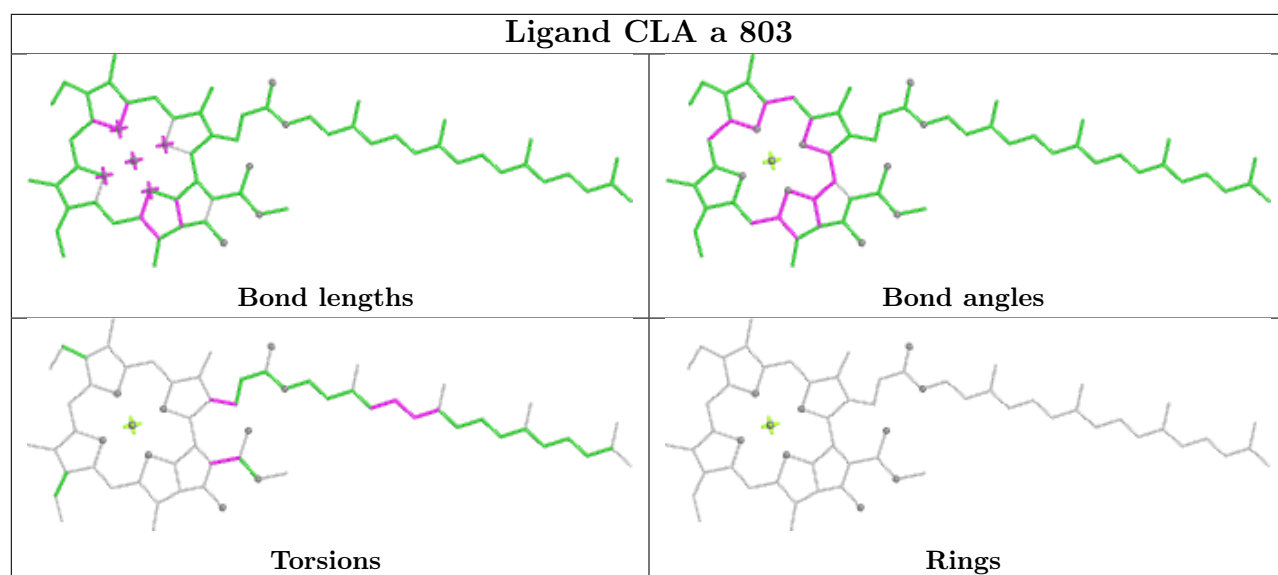
Torsions



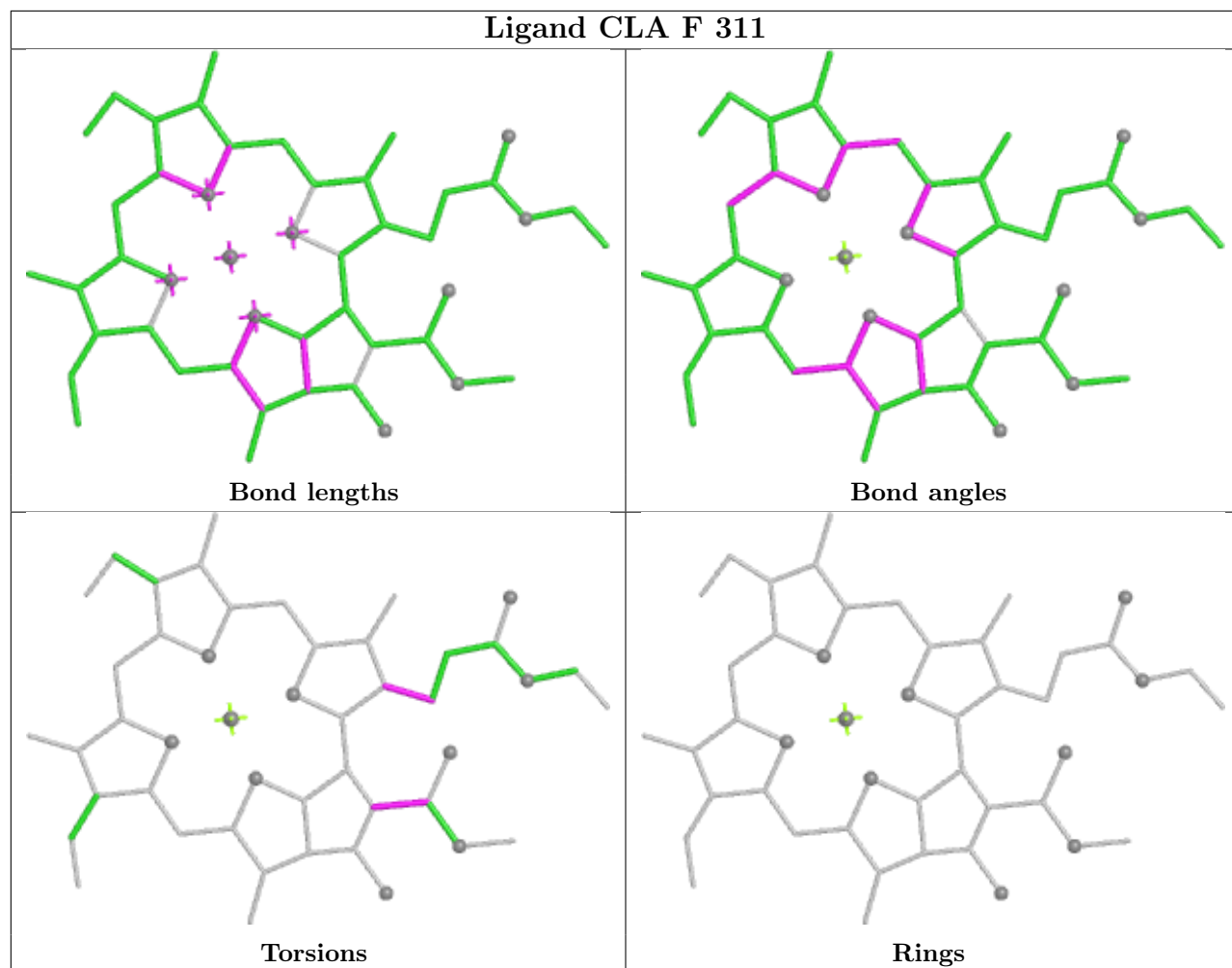
Rings

Ligand DGD b 850	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA E 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

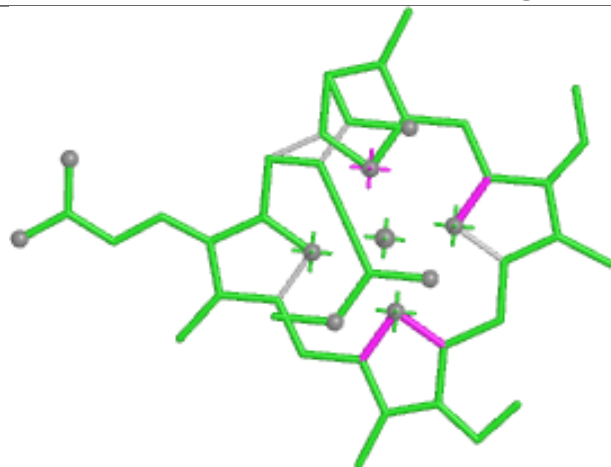




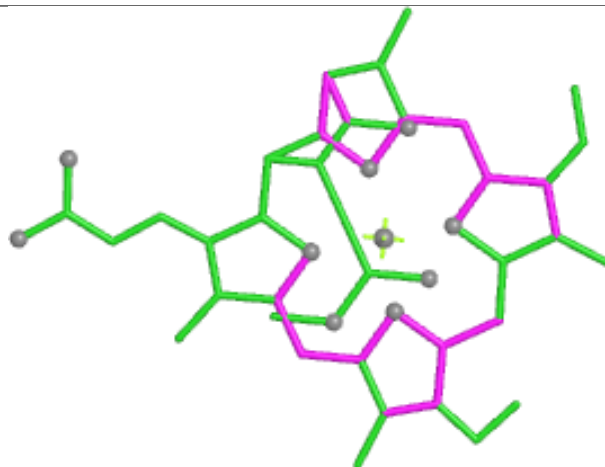
Ligand CLA F 311



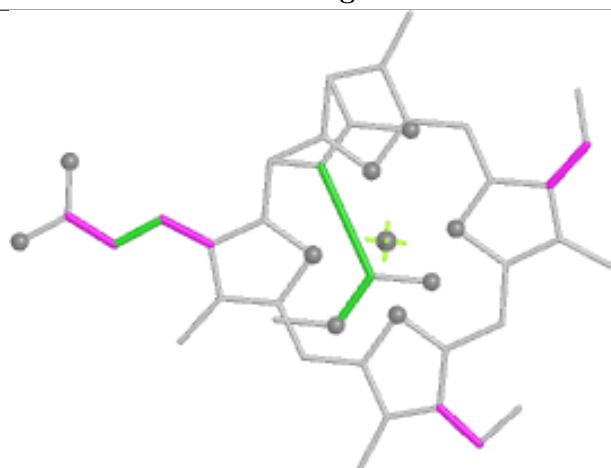
Ligand KC2 F 302



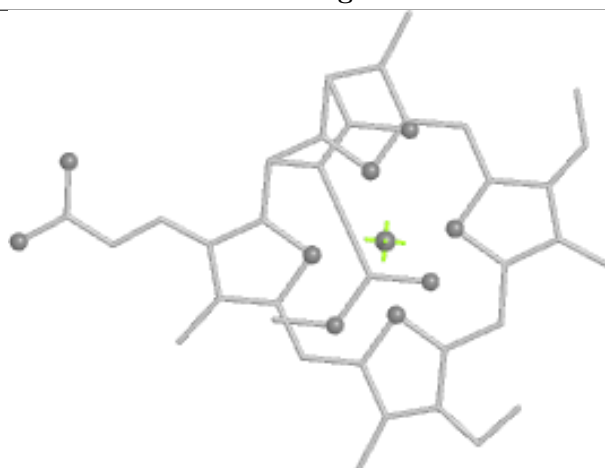
Bond lengths



Bond angles

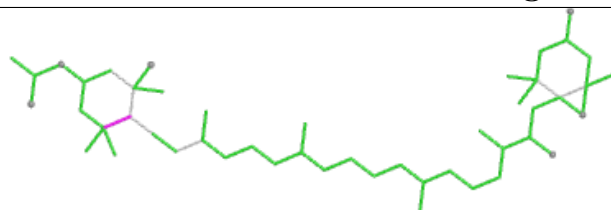


Torsions

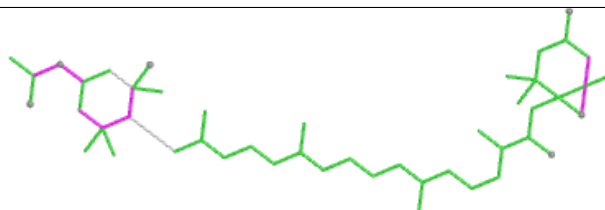


Rings

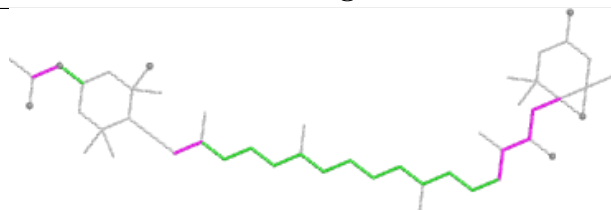
Ligand A86 u 319



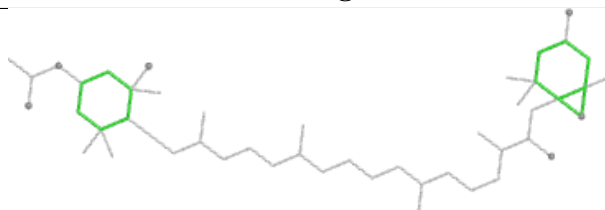
Bond lengths



Bond angles

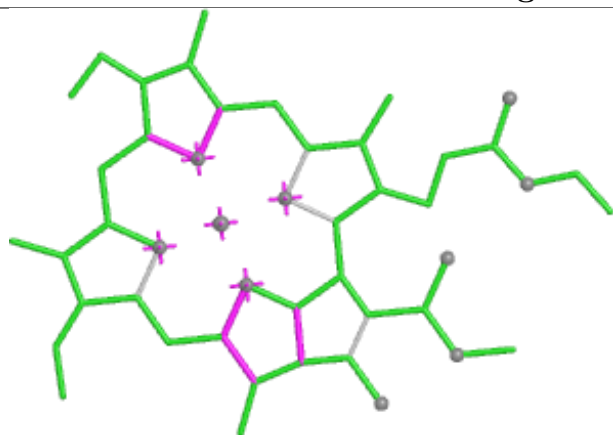


Torsions



Rings

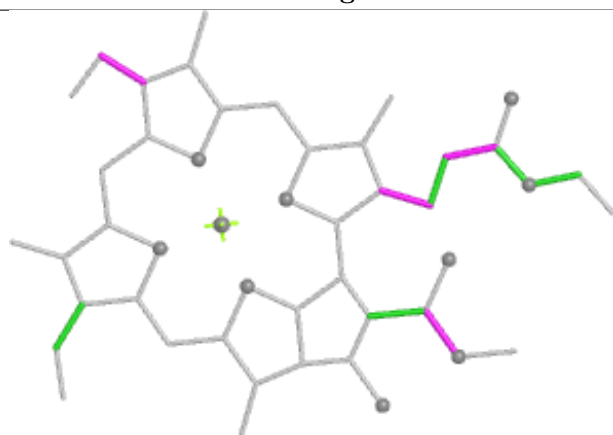
Ligand CLA S 319



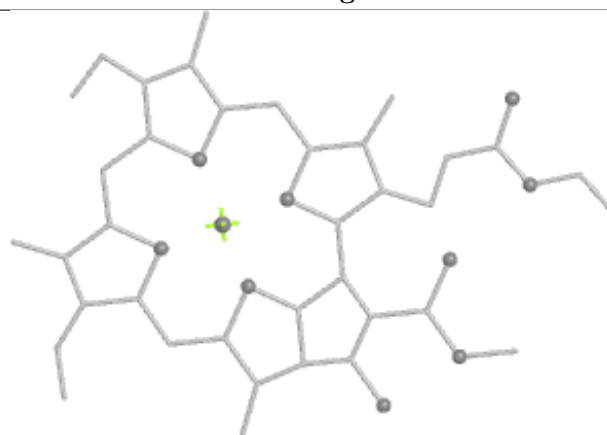
Bond lengths



Bond angles

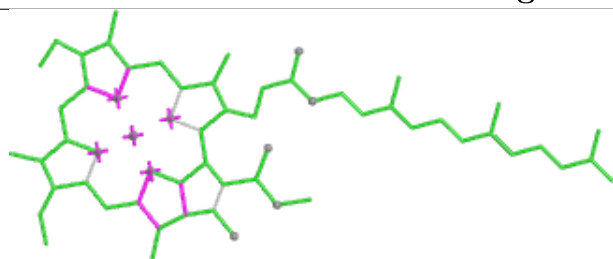


Torsions

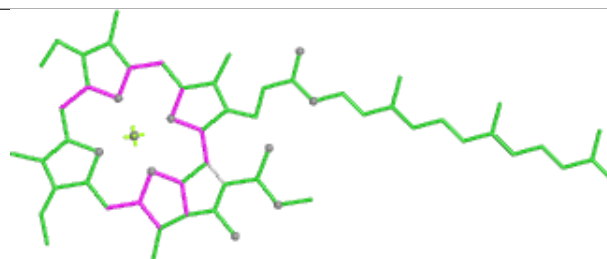


Rings

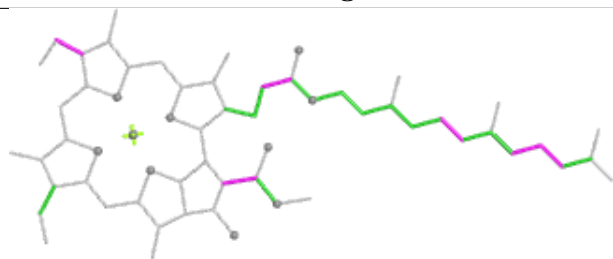
Ligand CLA u 308



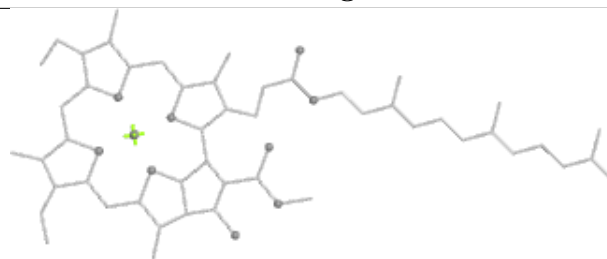
Bond lengths



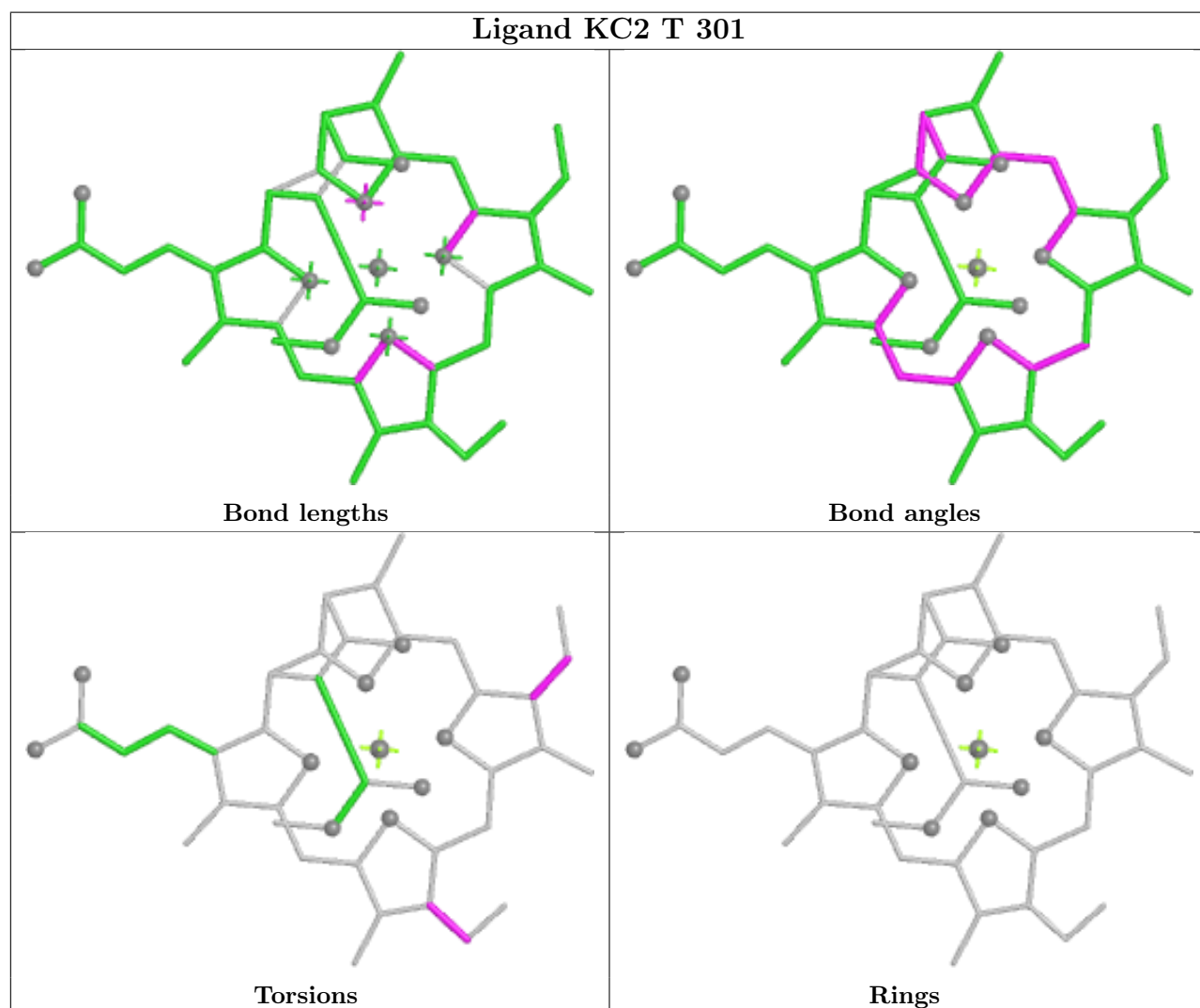
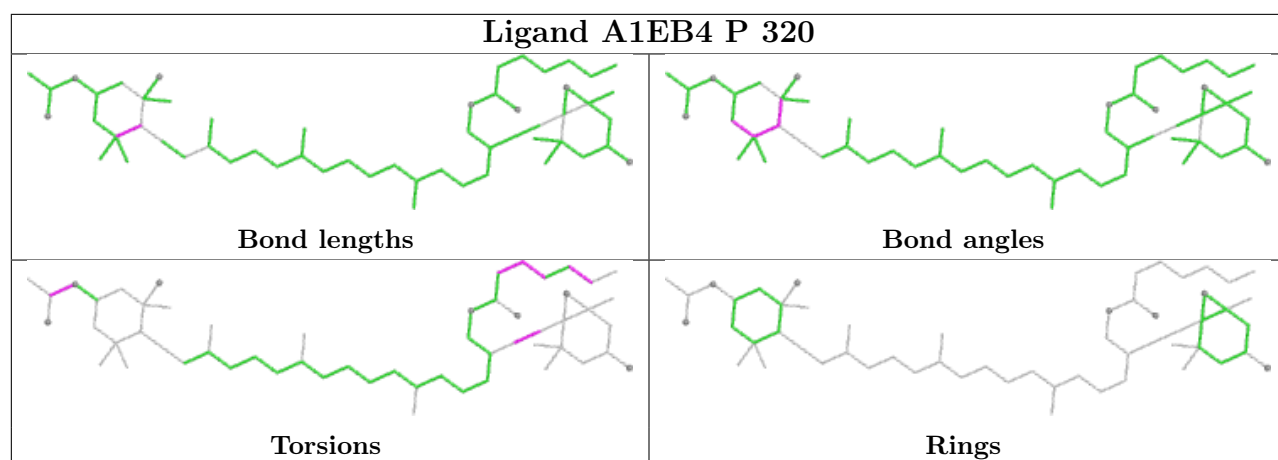
Bond angles

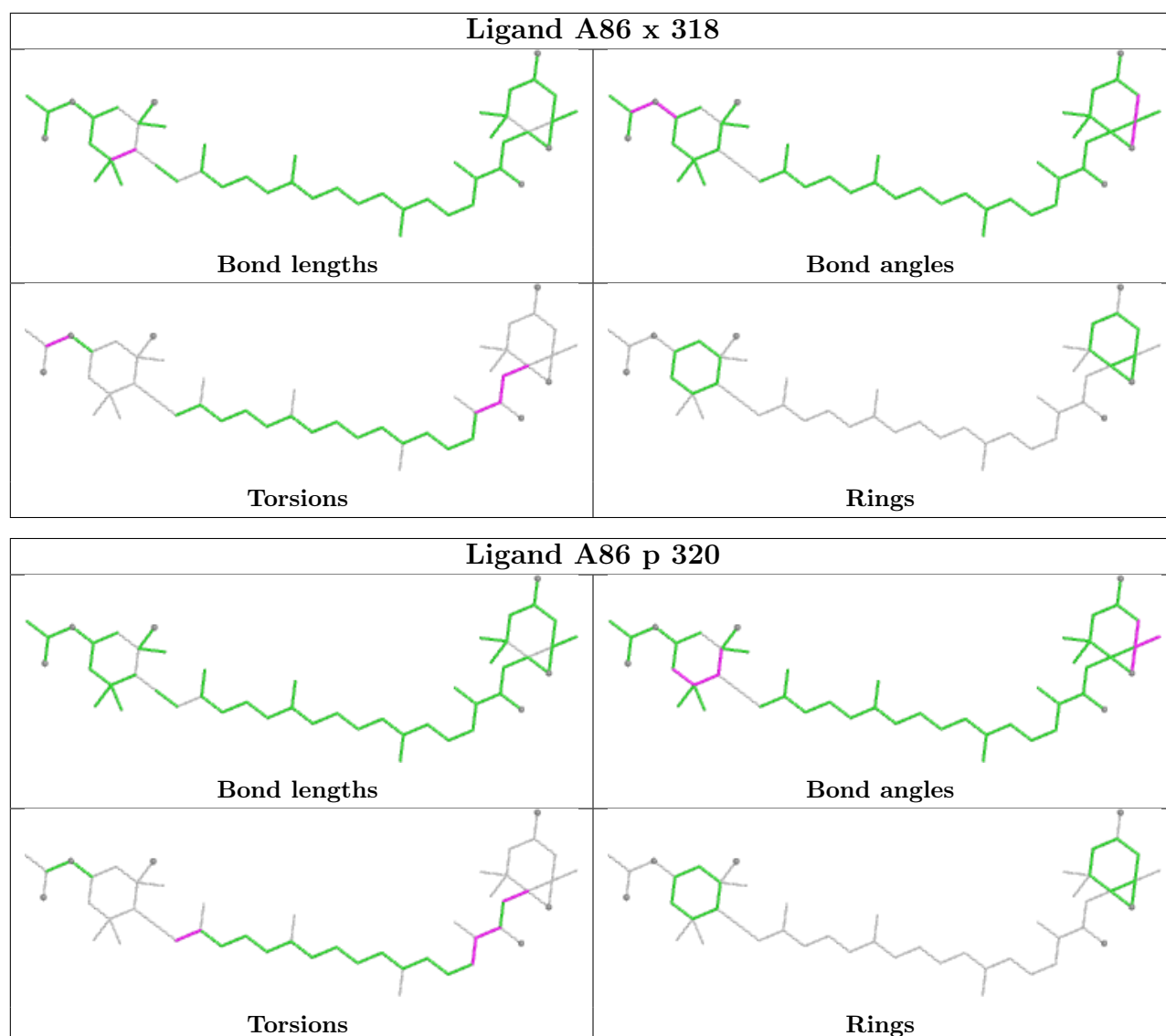


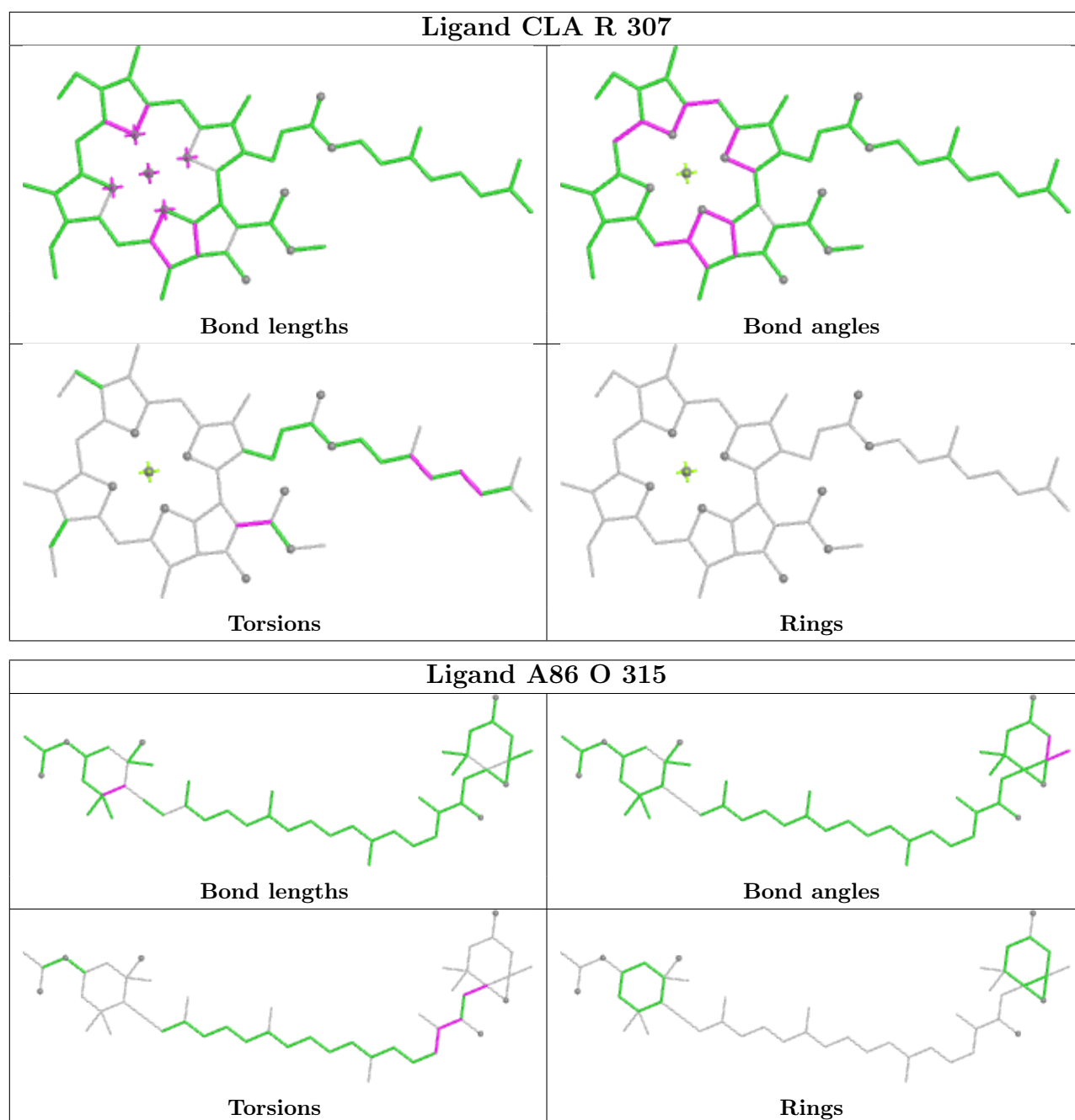
Torsions

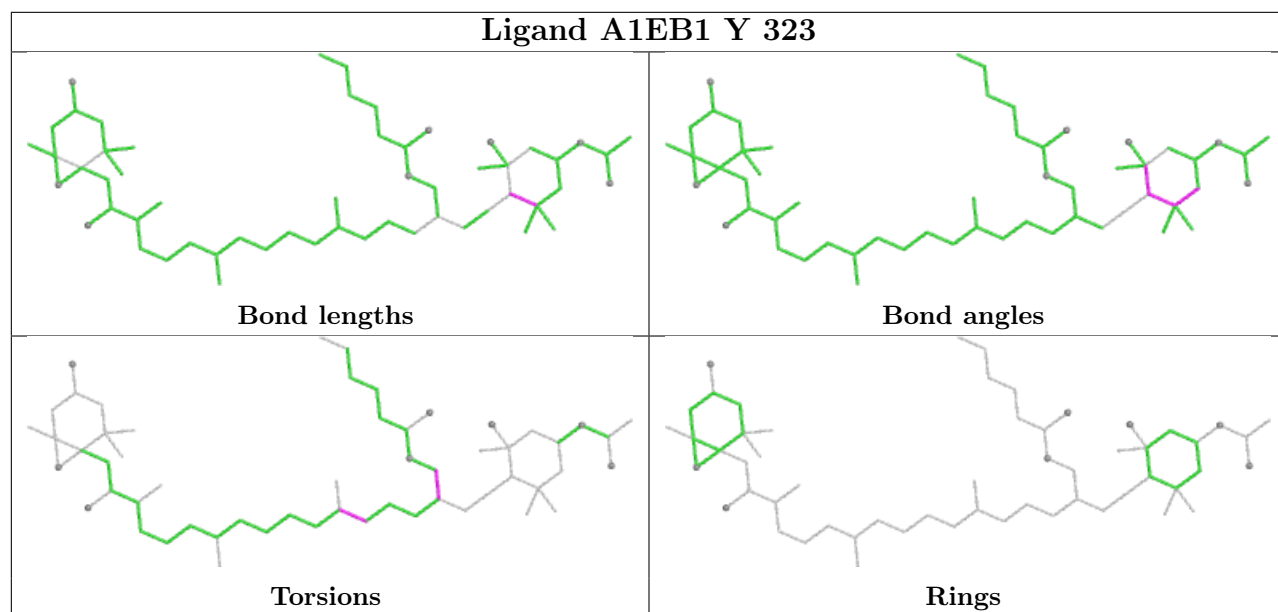
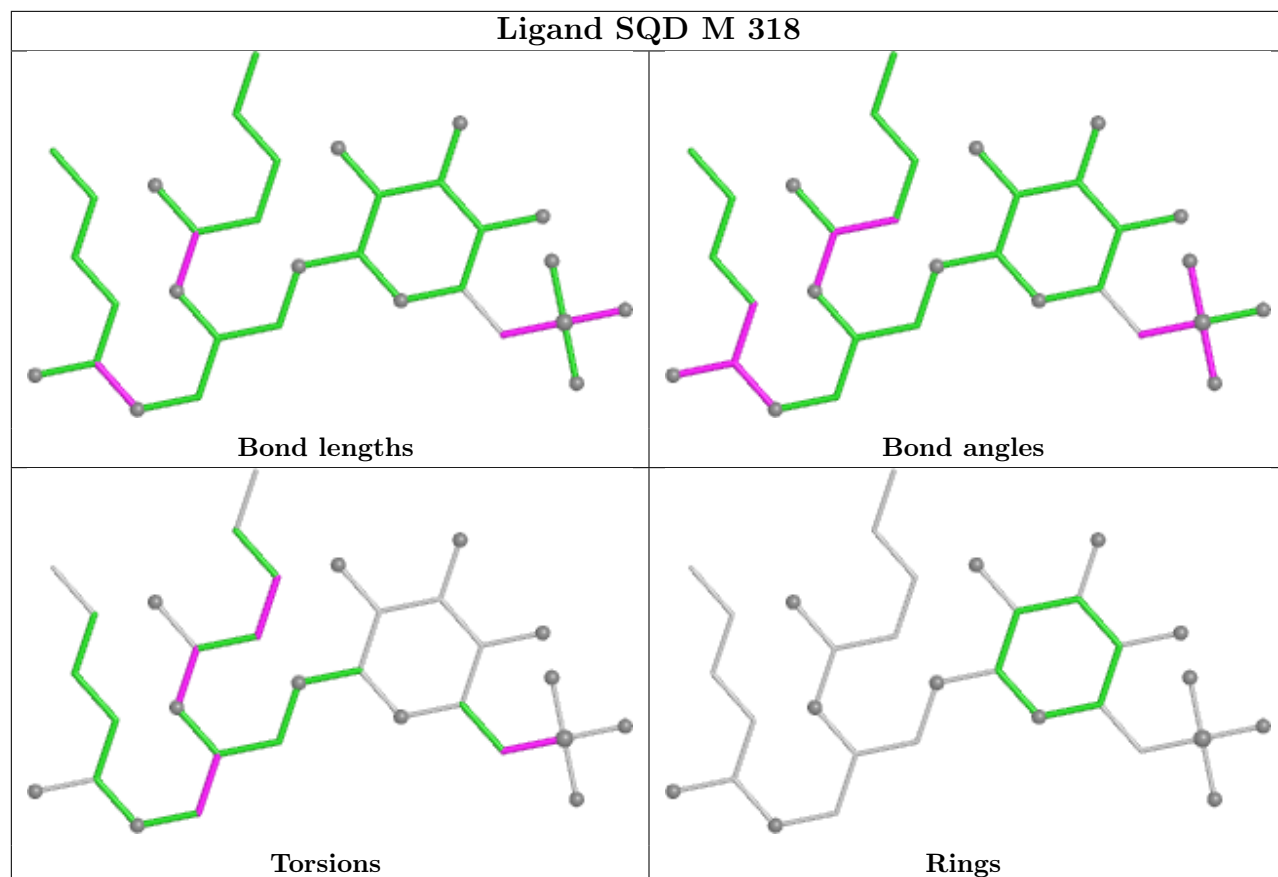


Rings

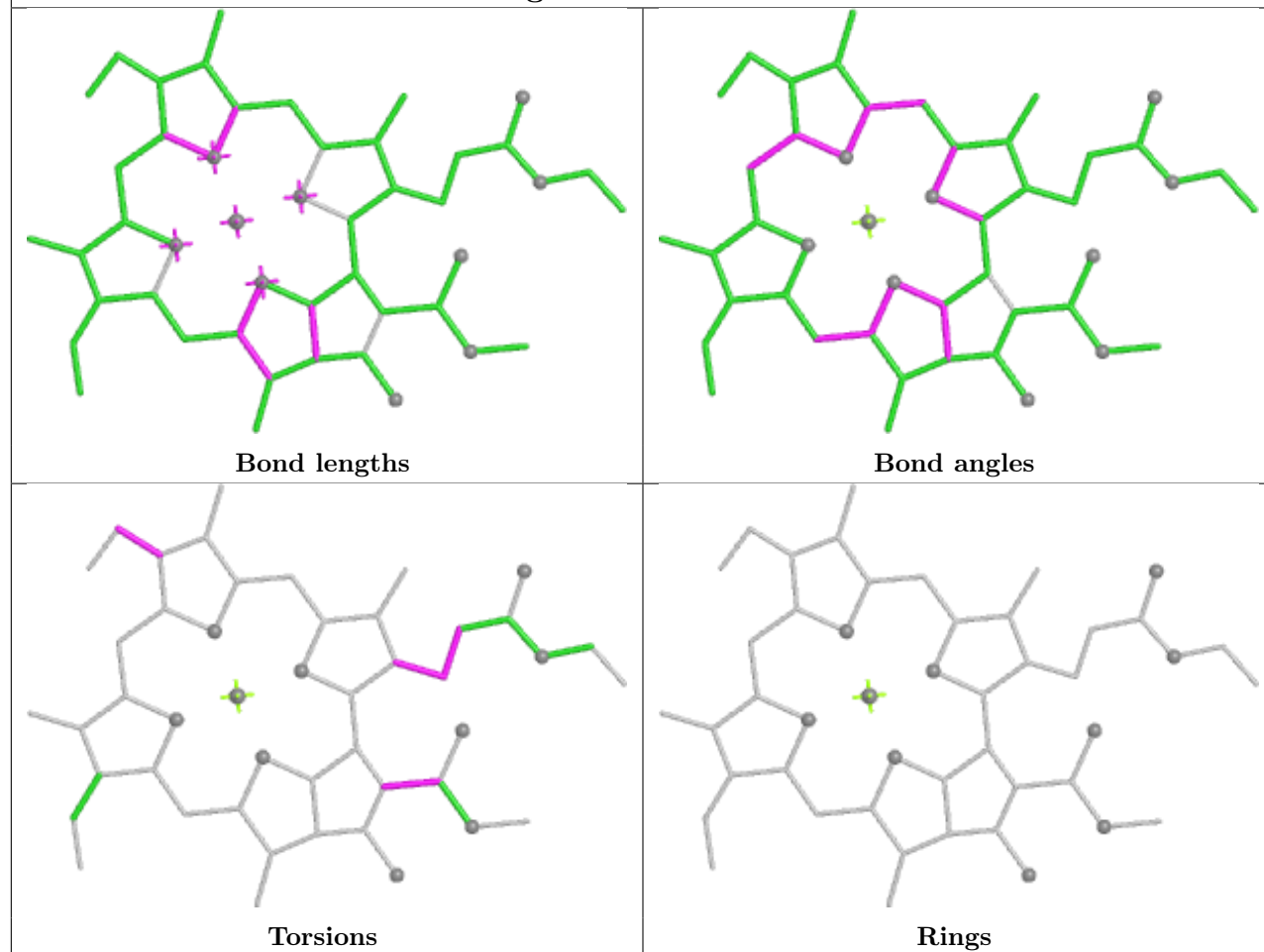




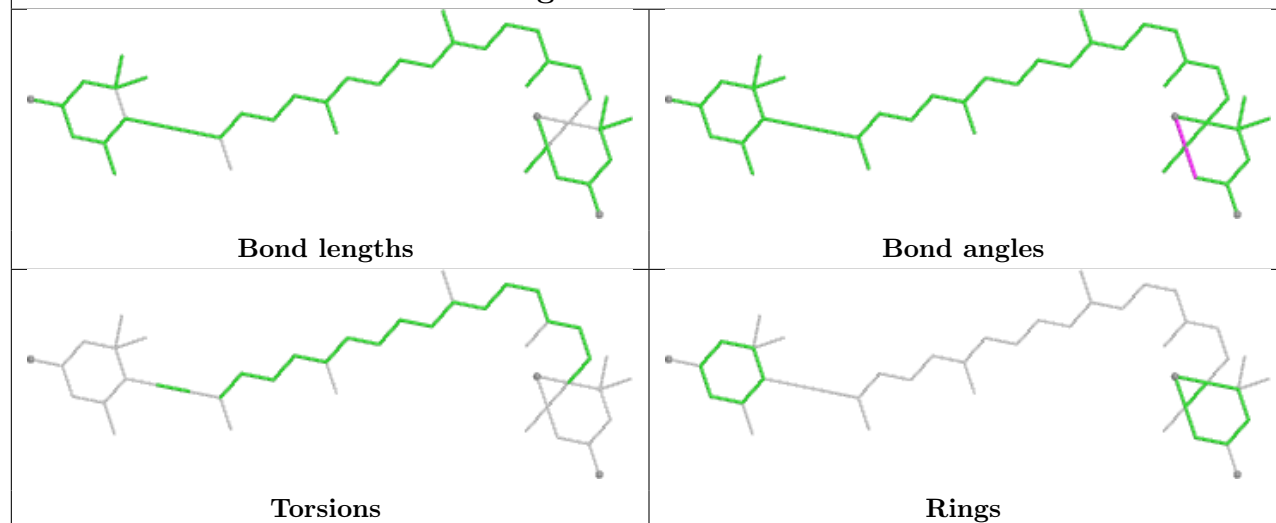


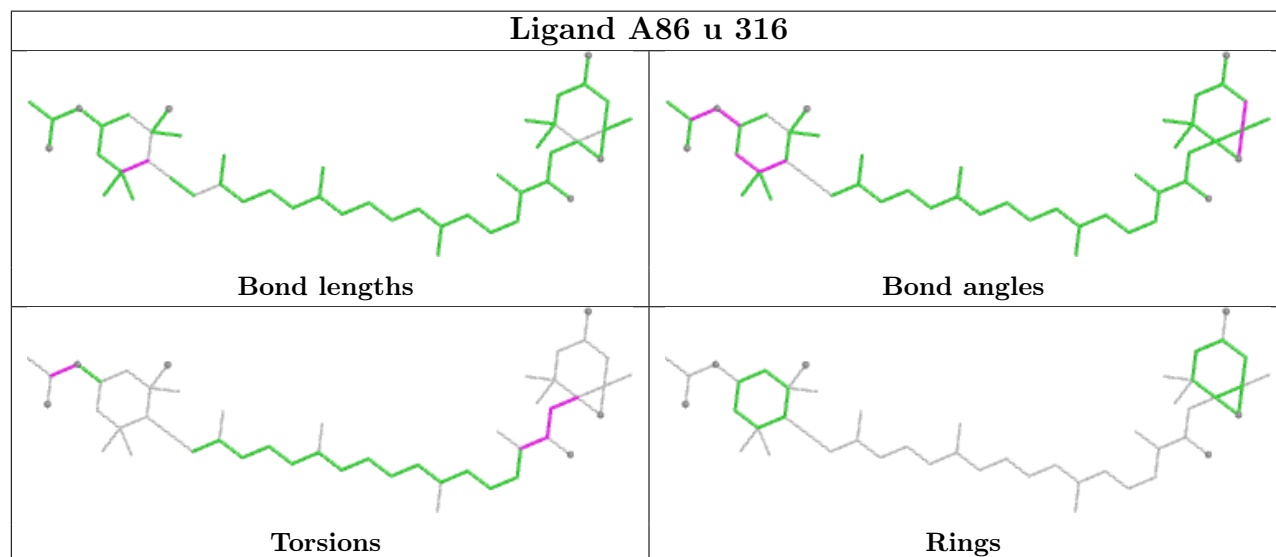
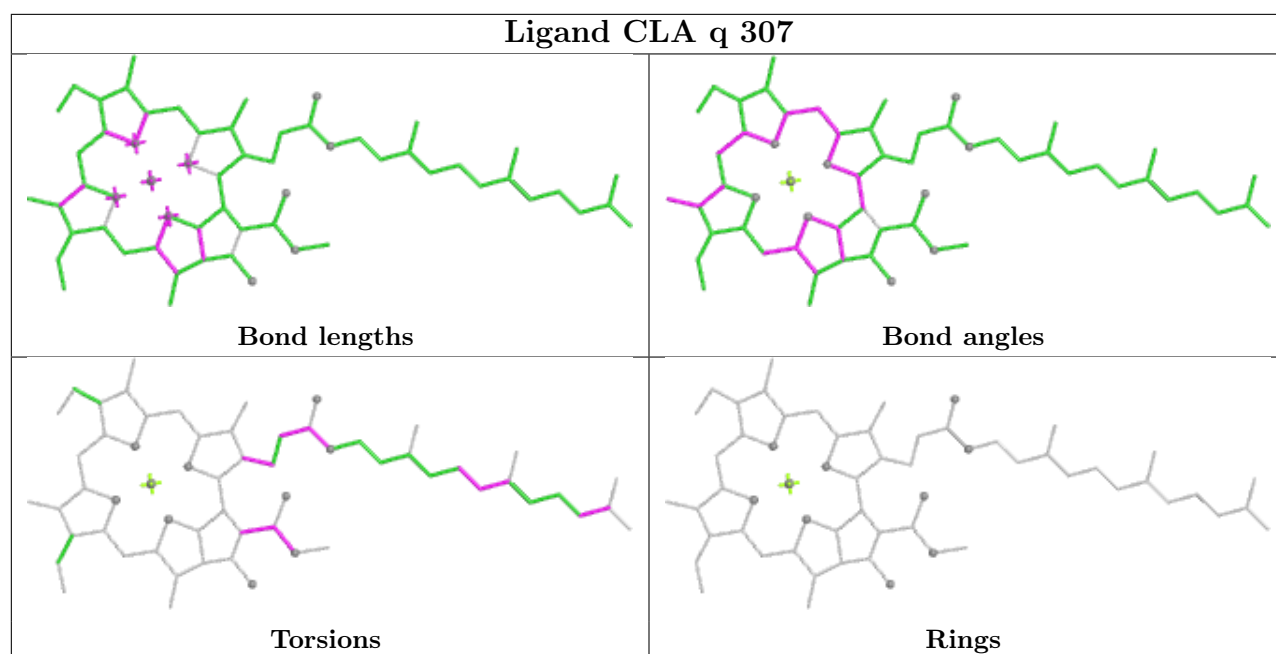


Ligand CLA H 308

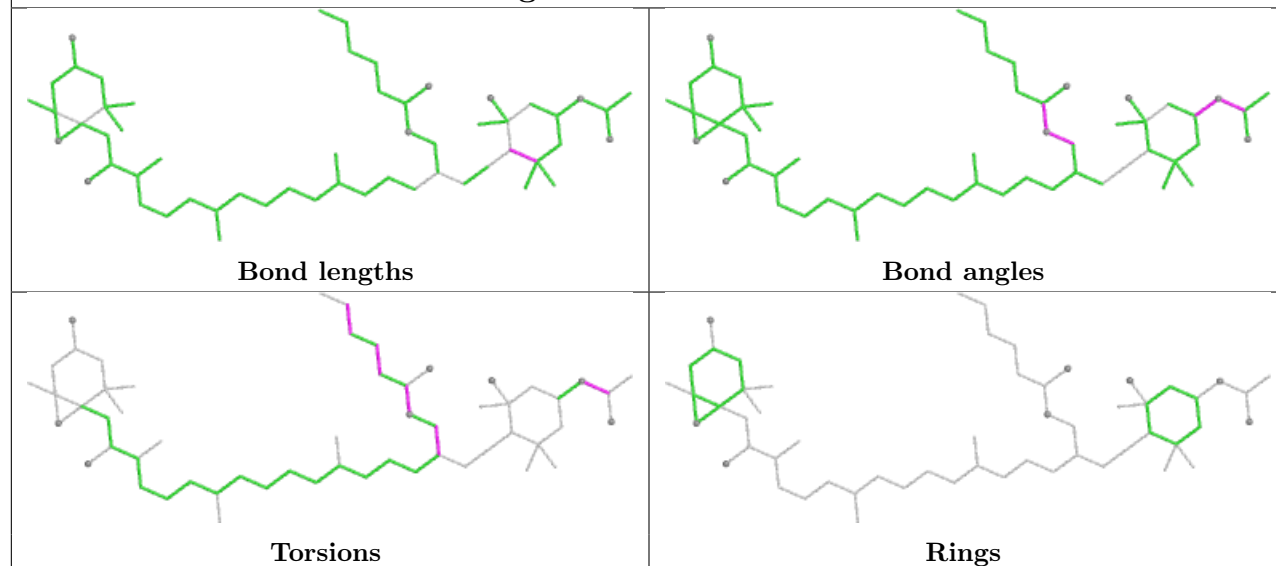


Ligand DD6 o 320

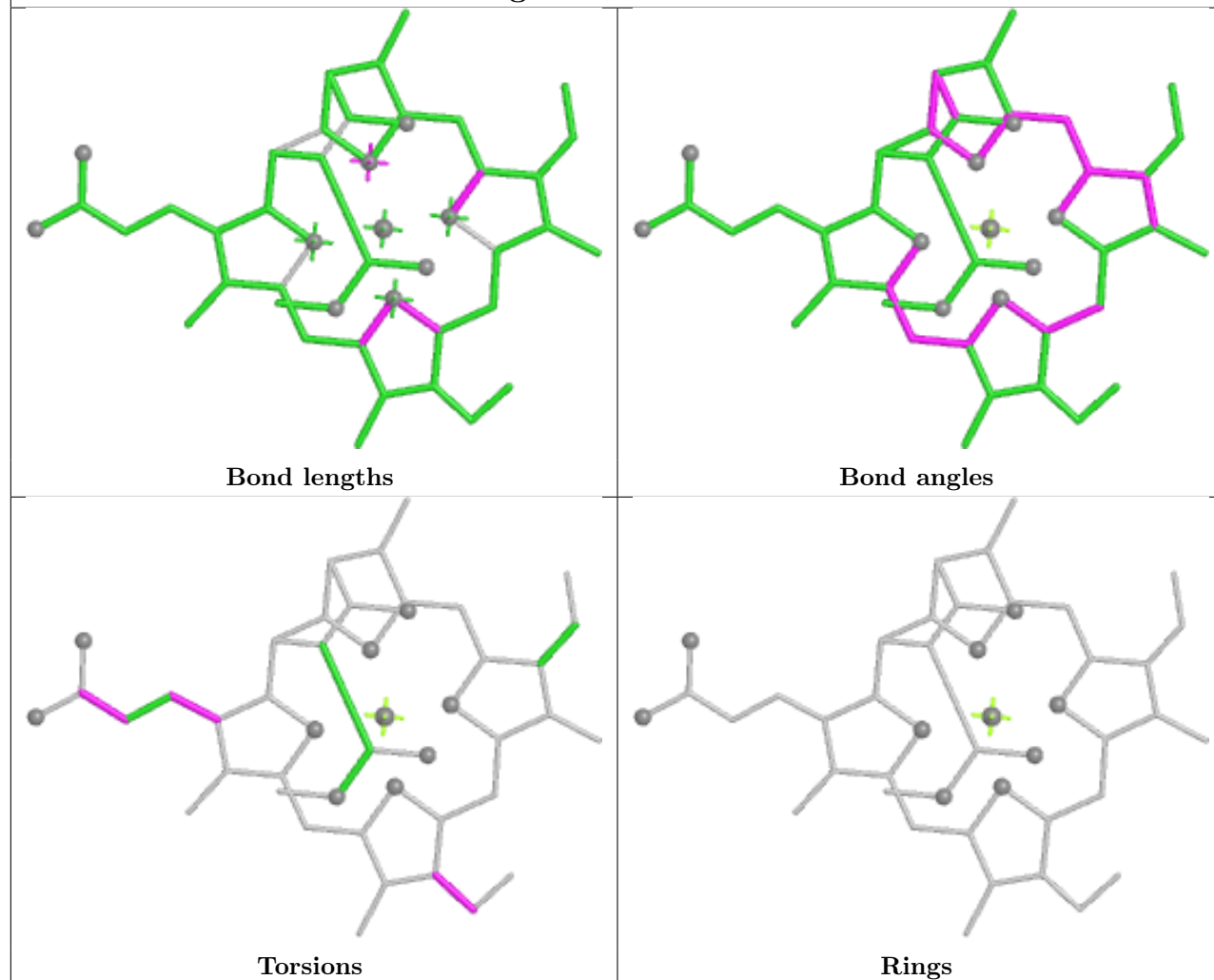


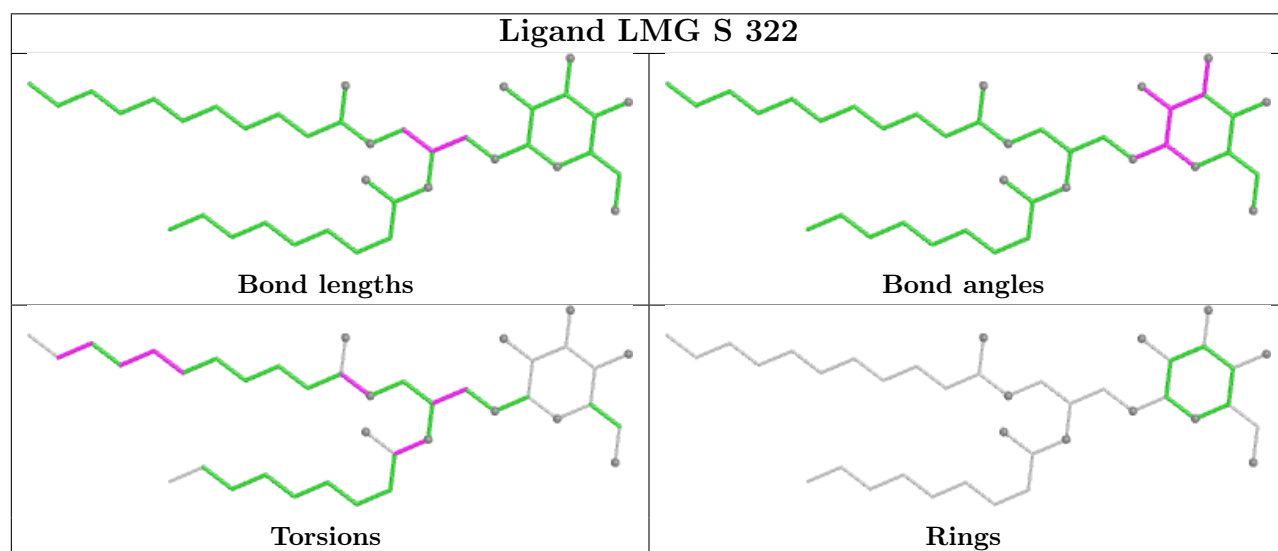
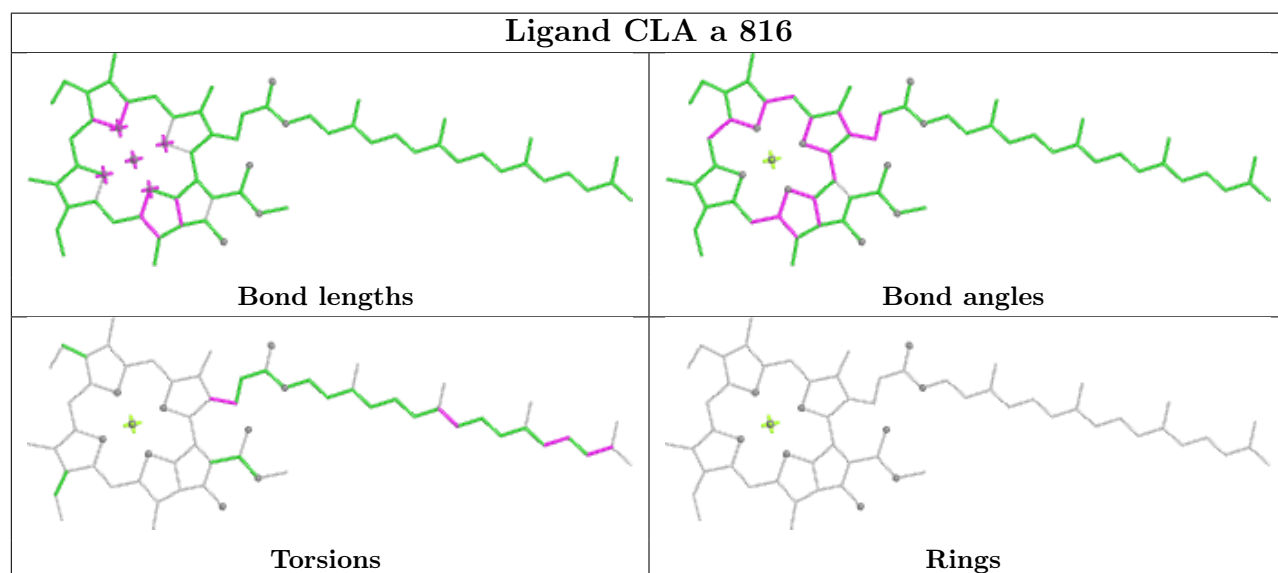
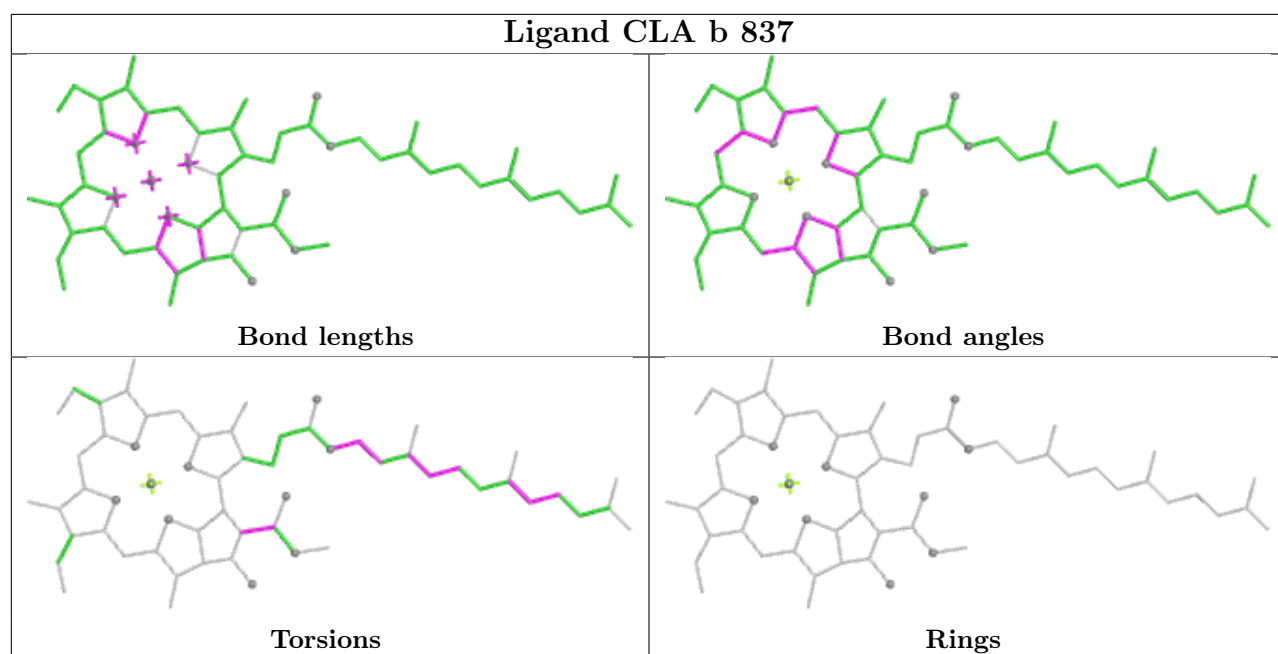


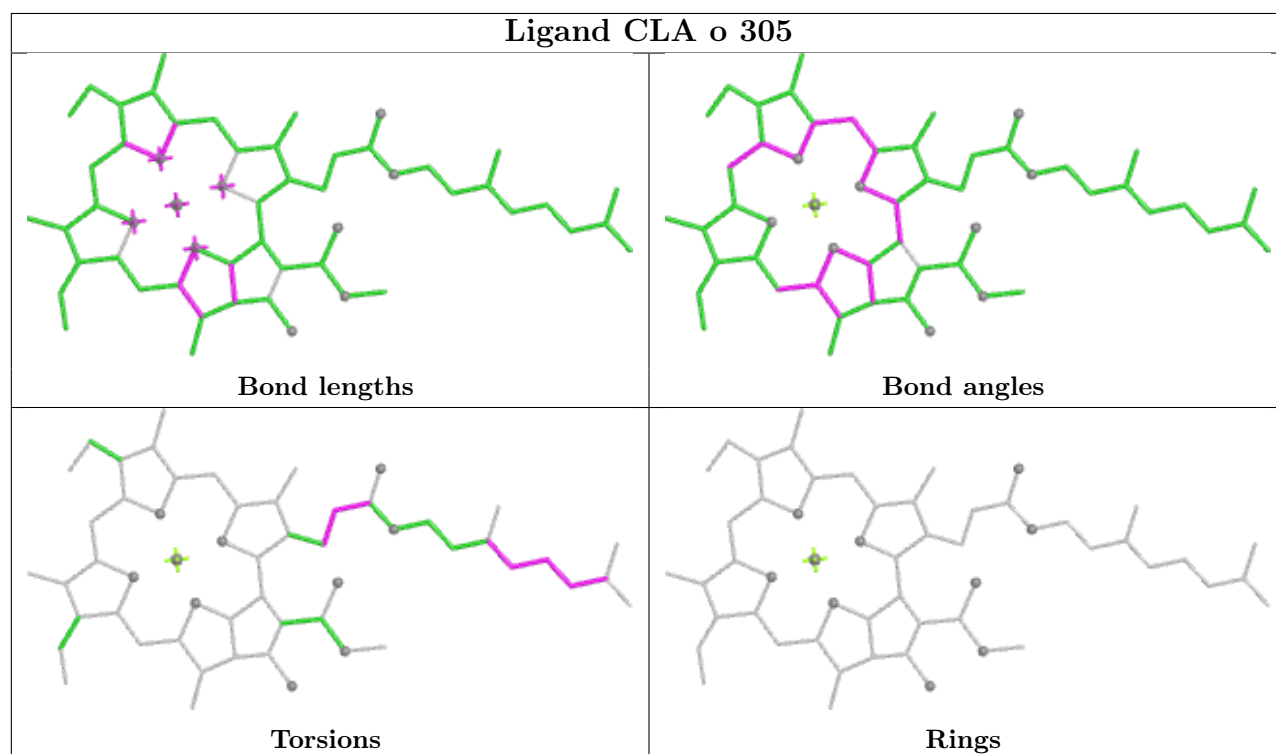
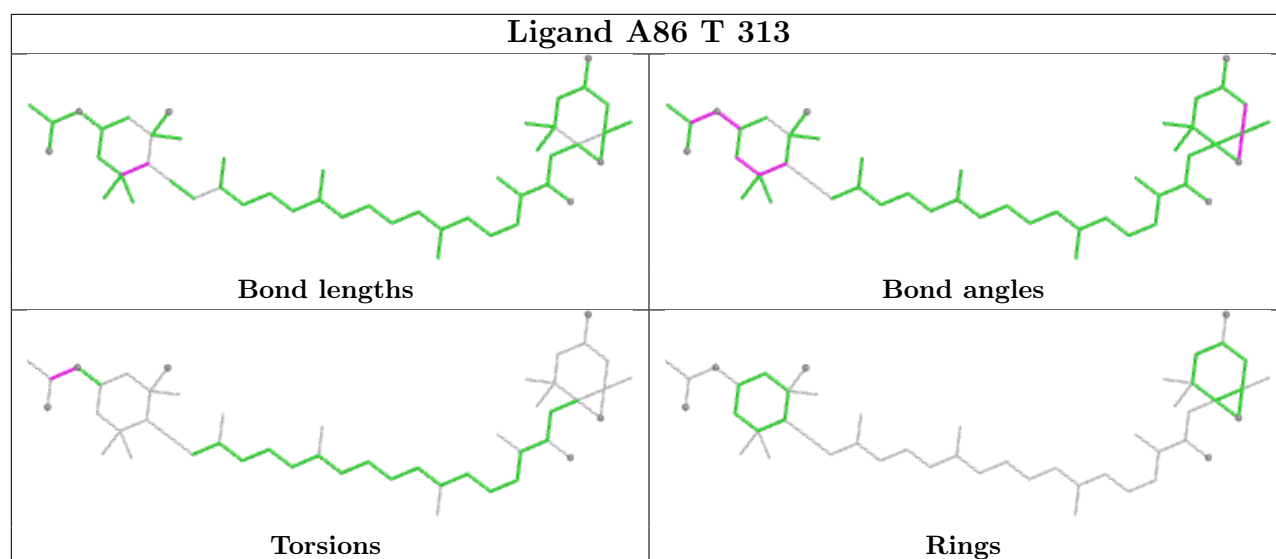
Ligand A1EB1 z 323



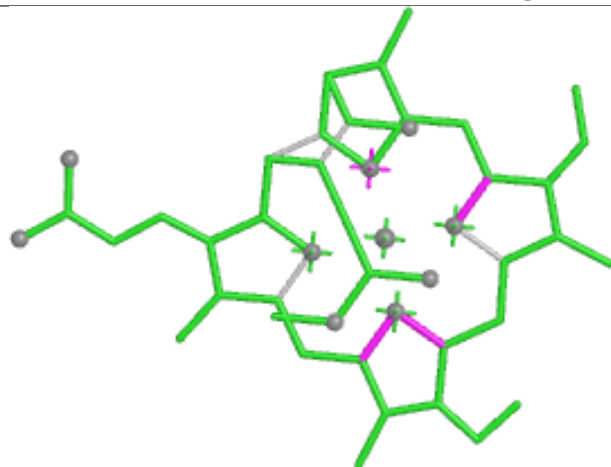
Ligand KC2 F 309



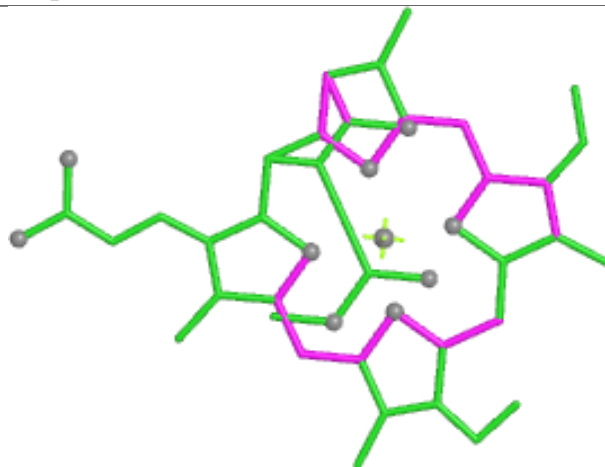




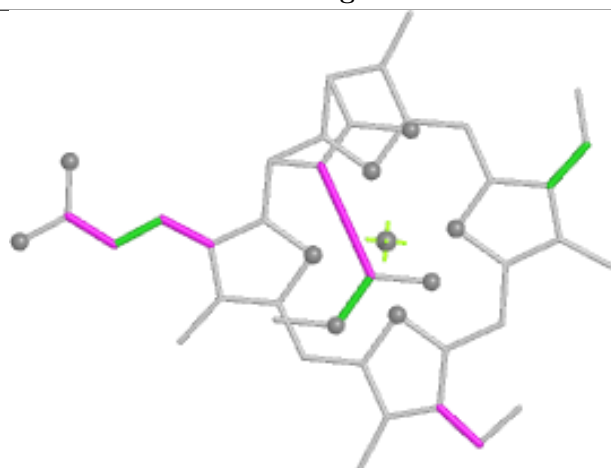
Ligand KC2 p 304



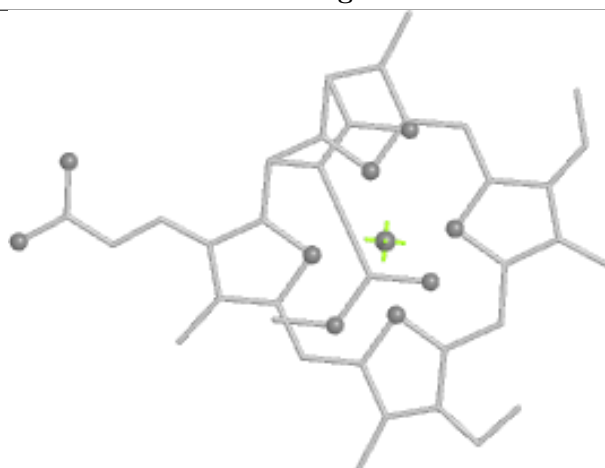
Bond lengths



Bond angles

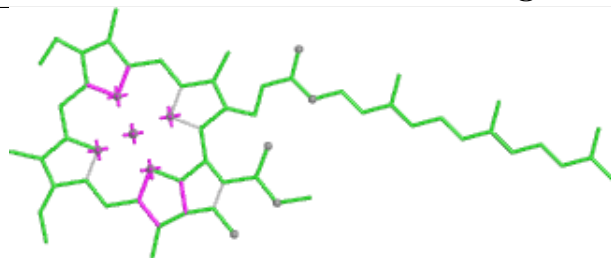


Torsions

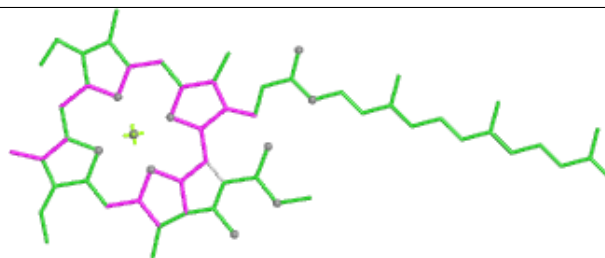


Rings

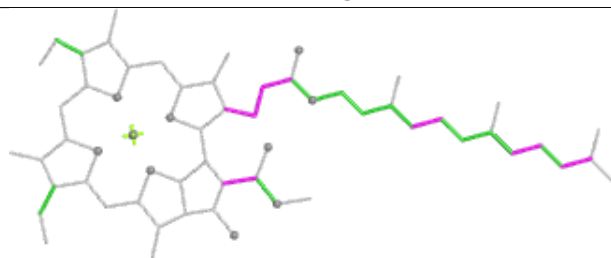
Ligand CLA b 809



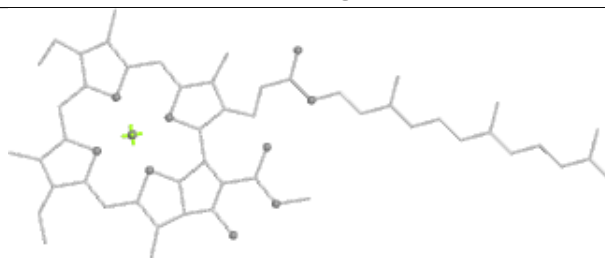
Bond lengths



Bond angles

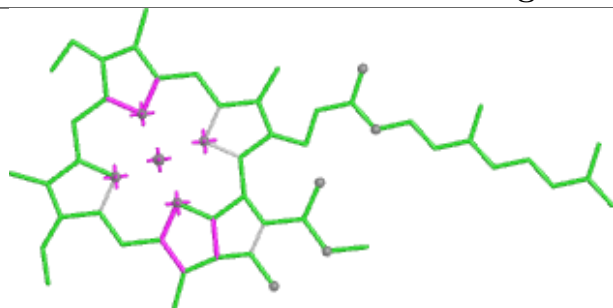


Torsions

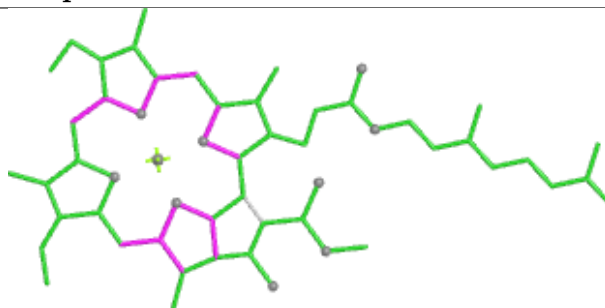


Rings

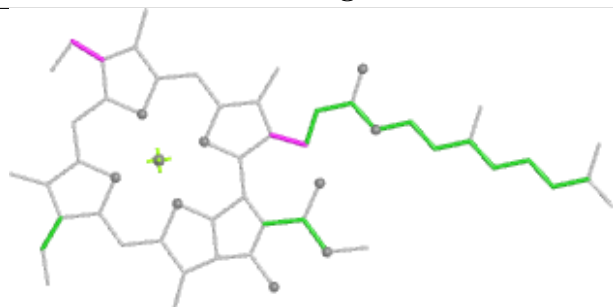
Ligand CLA q 301



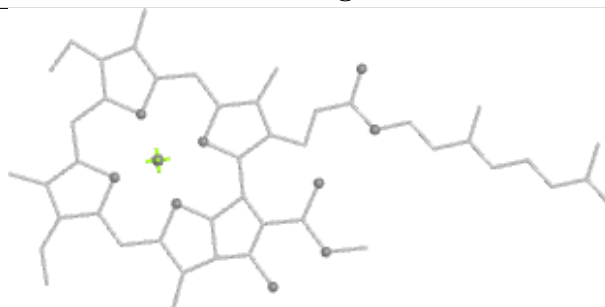
Bond lengths



Bond angles

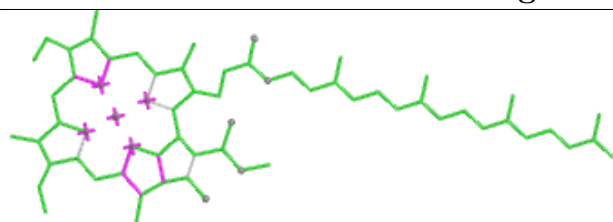


Torsions

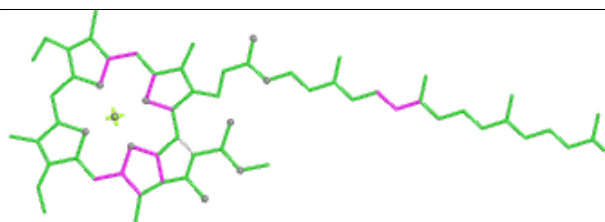


Rings

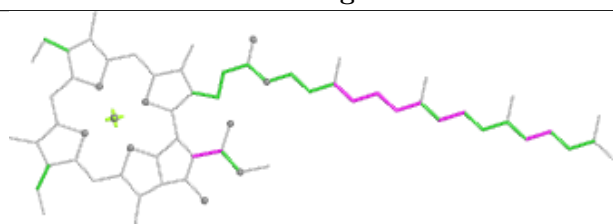
Ligand CLA a 836



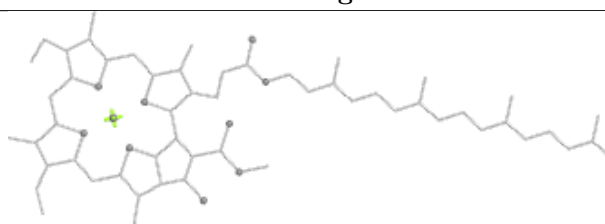
Bond lengths



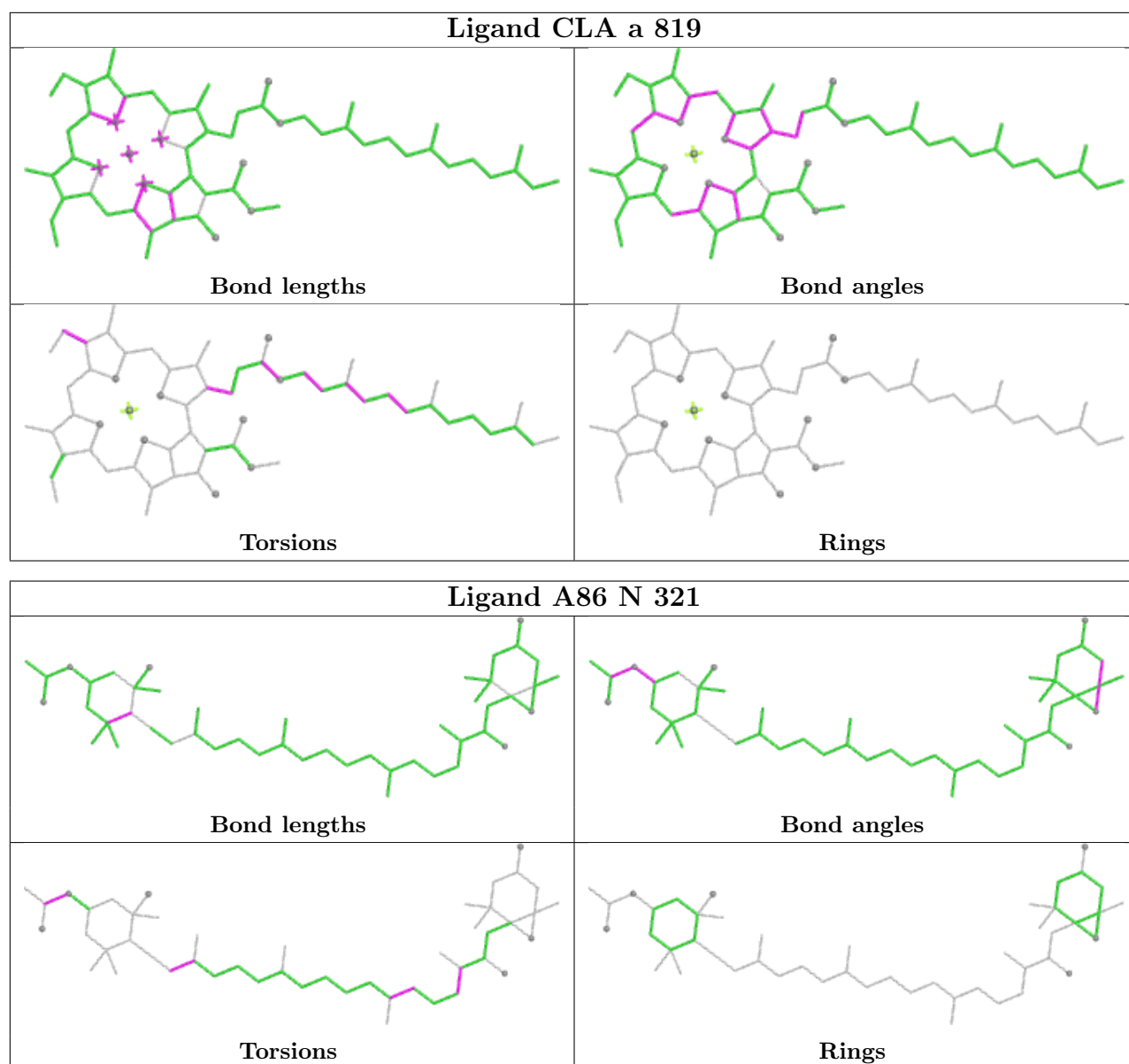
Bond angles

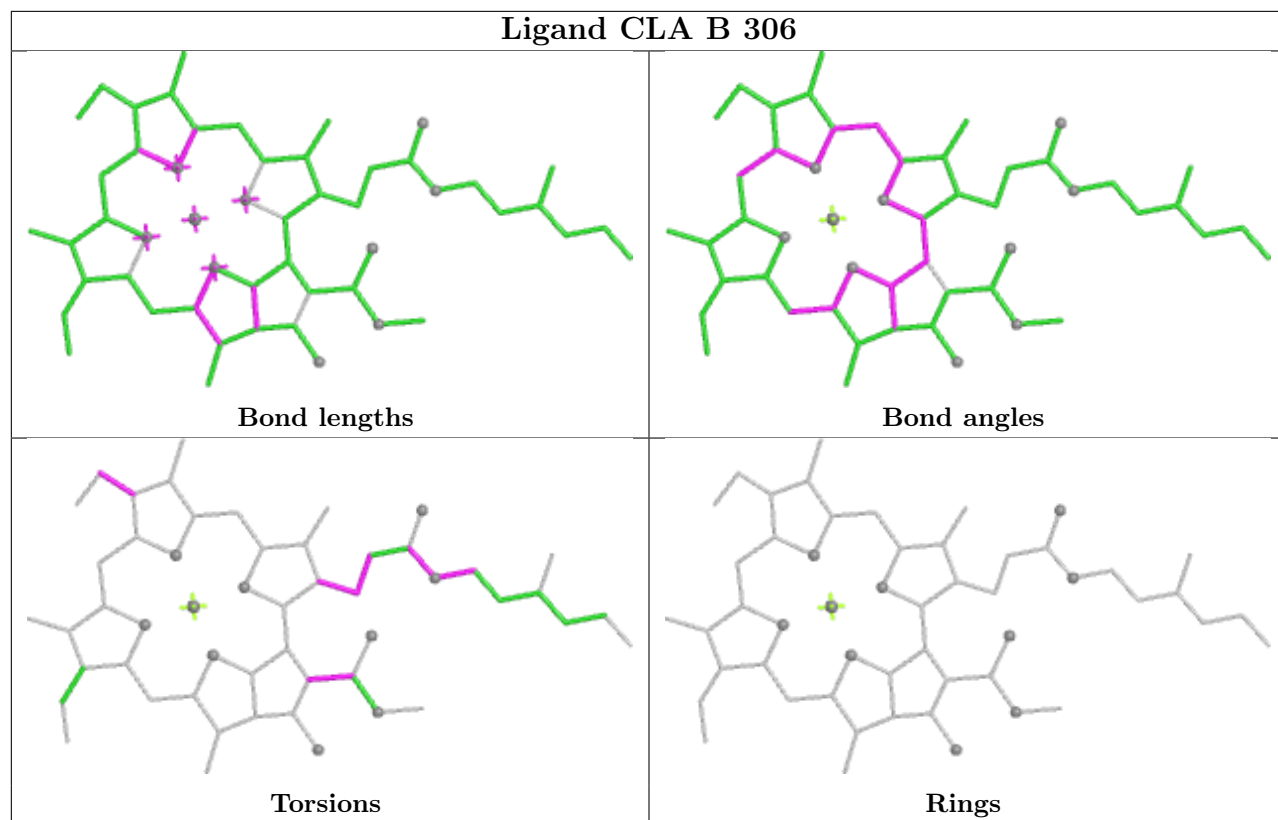


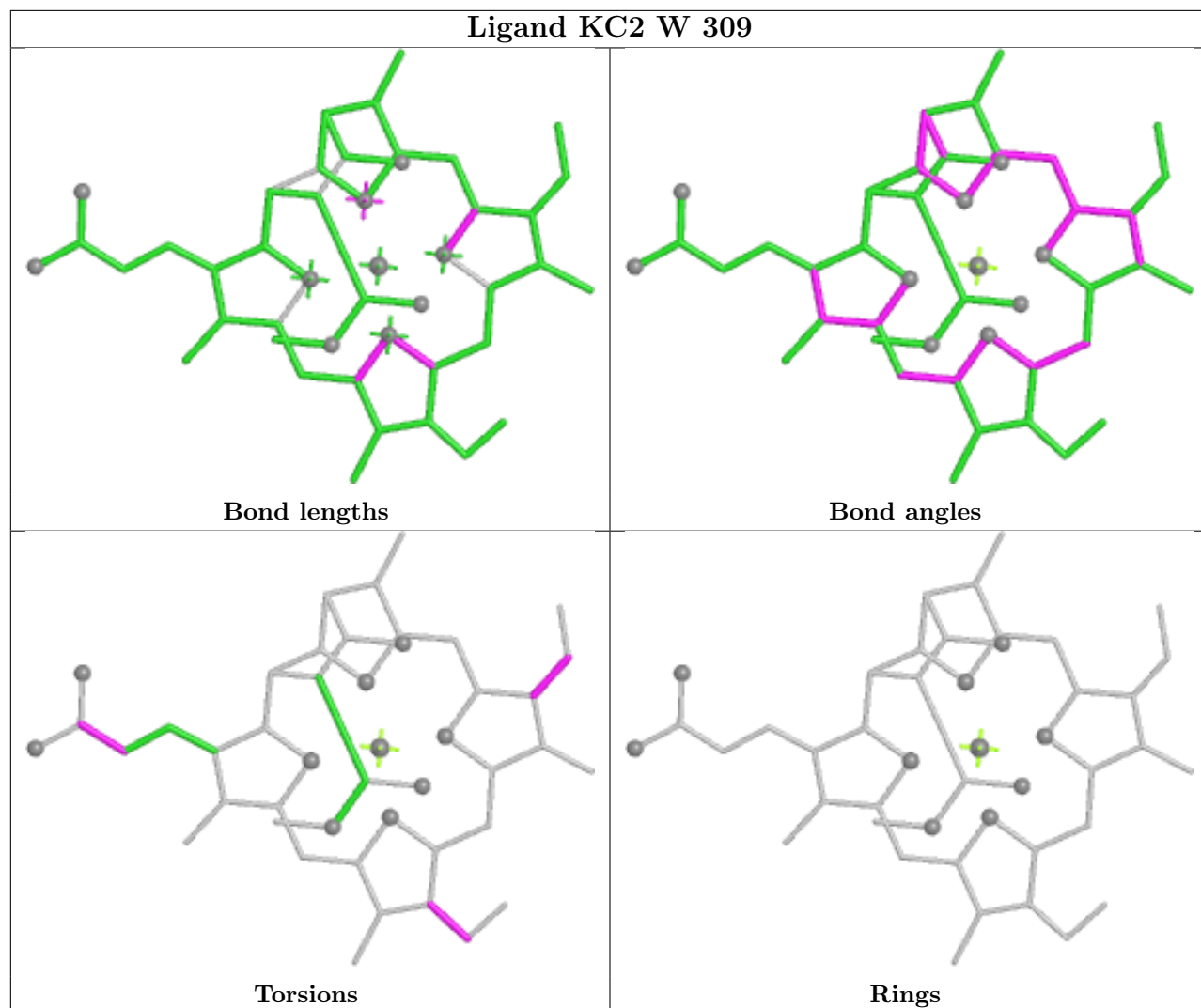
Torsions



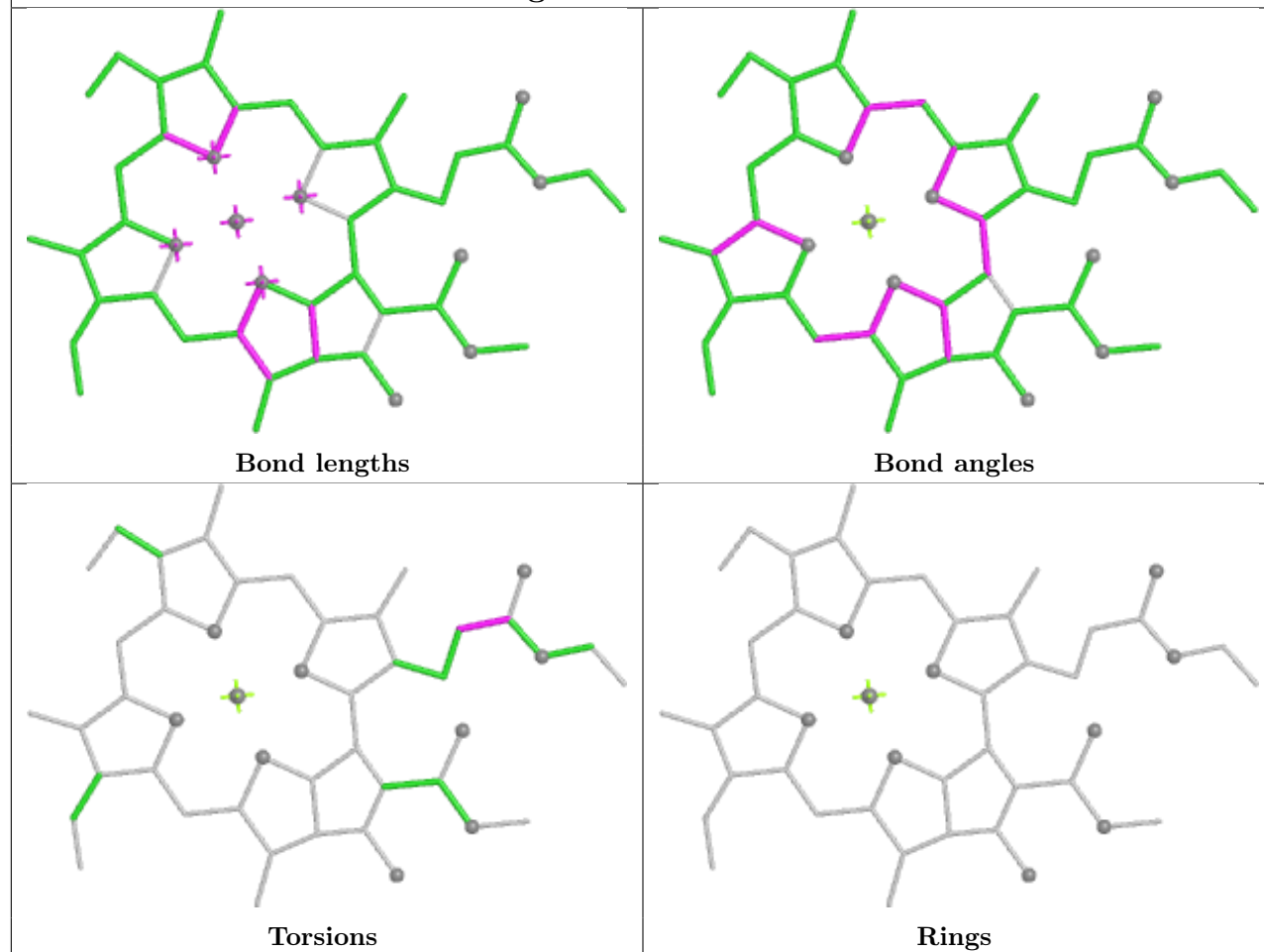
Rings



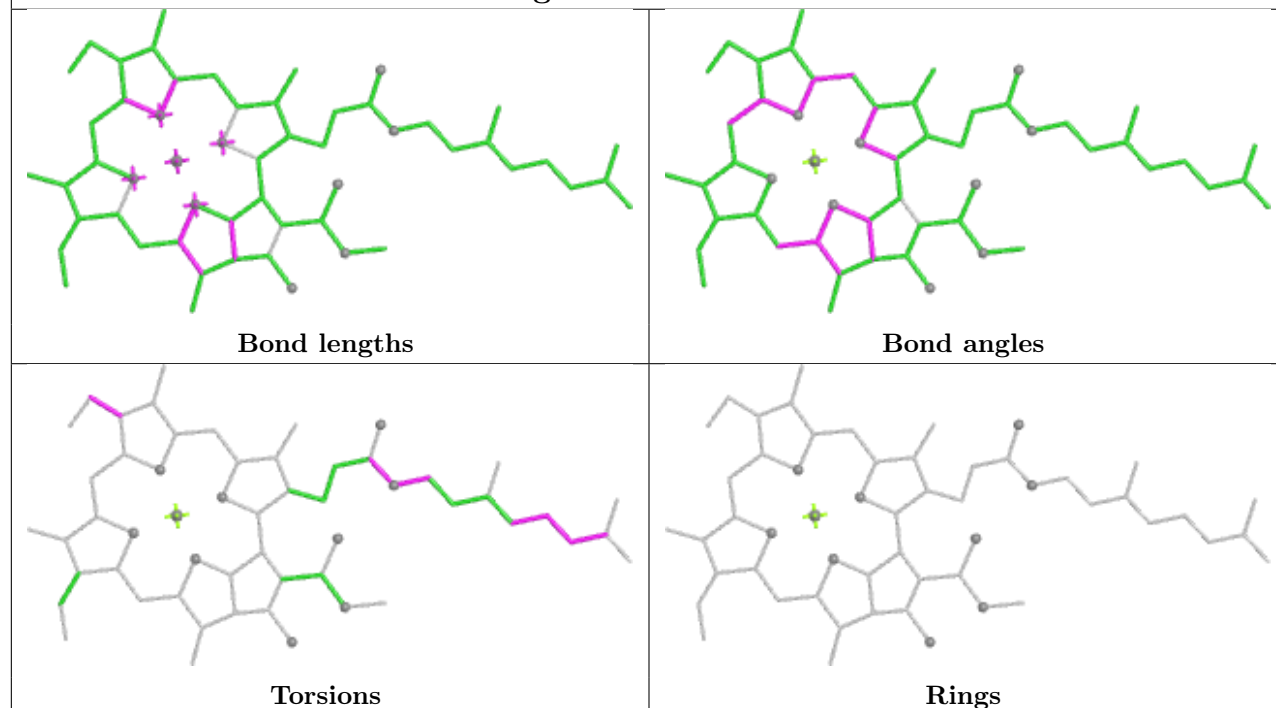


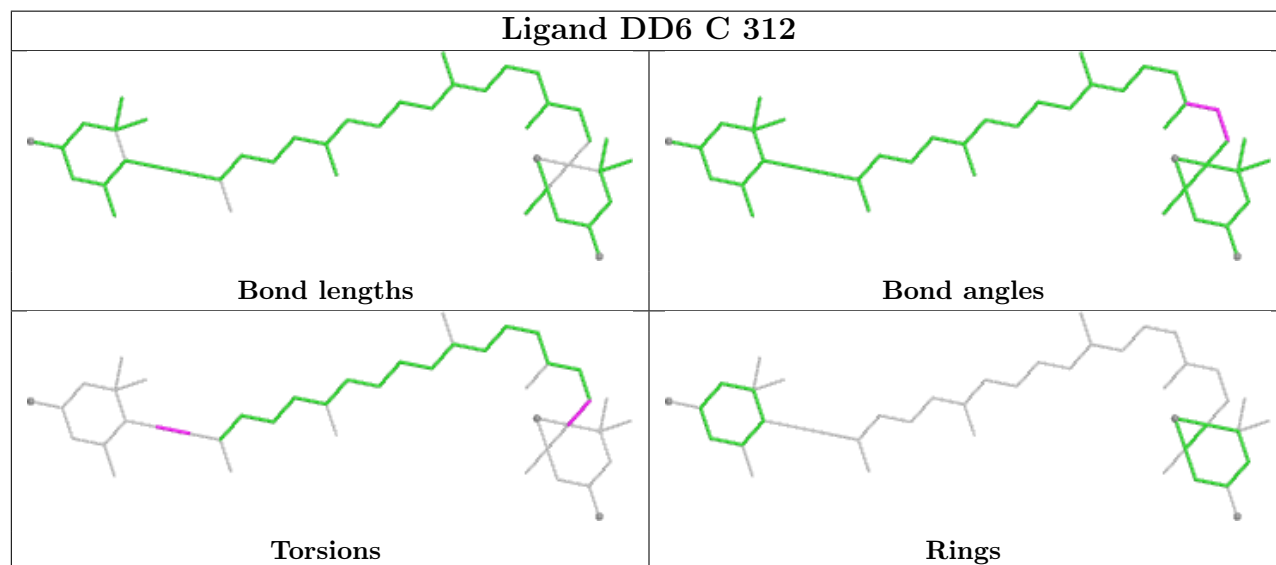
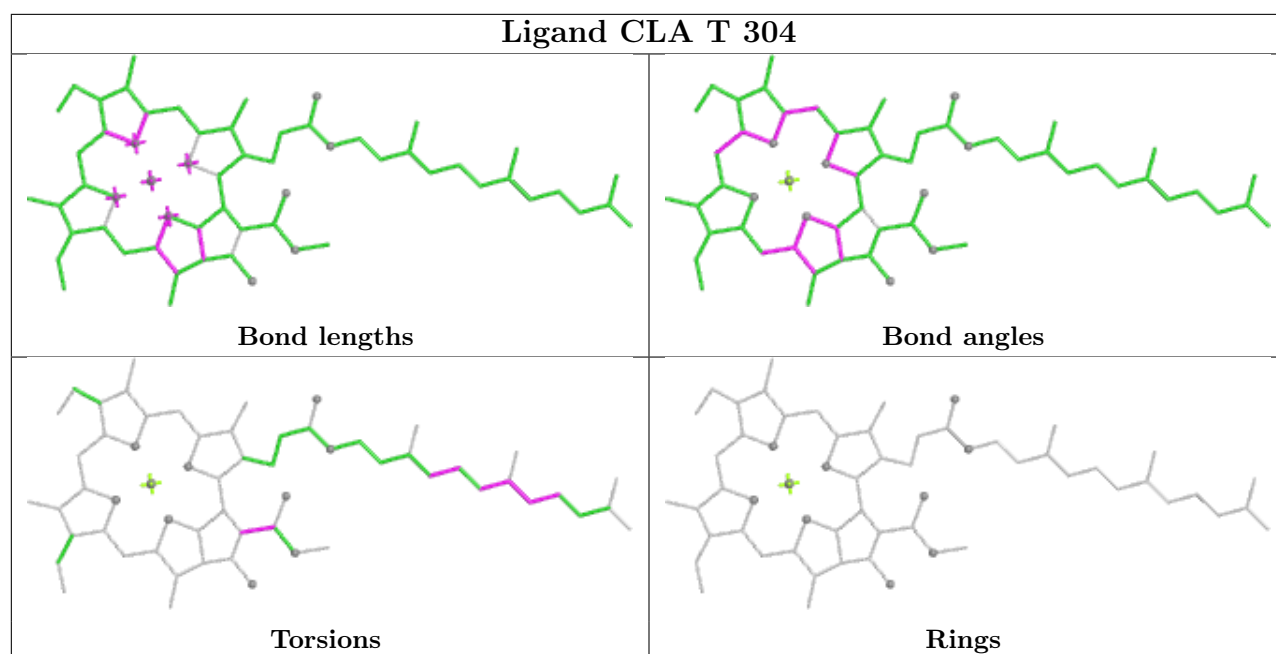


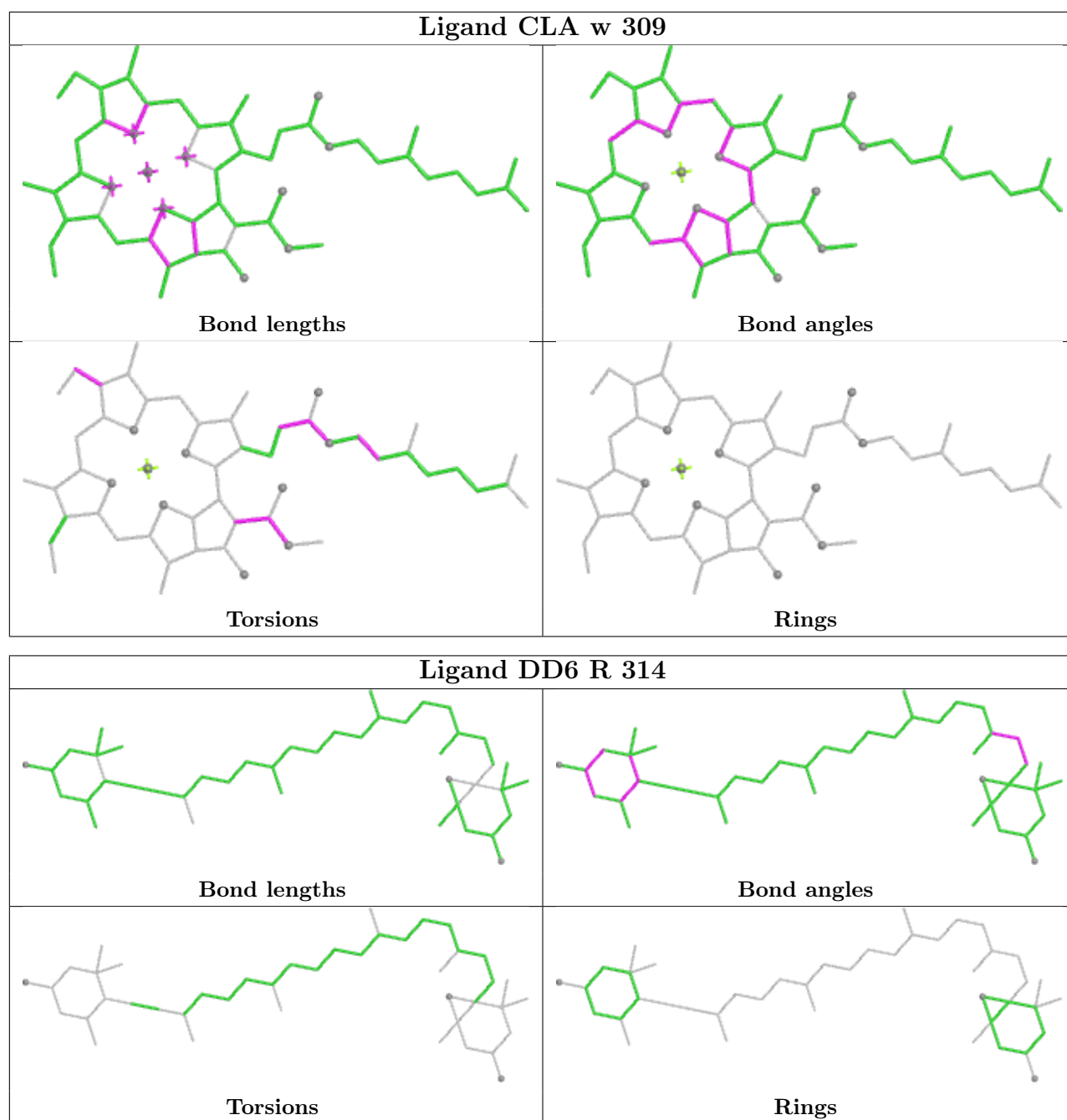
Ligand CLA P 306

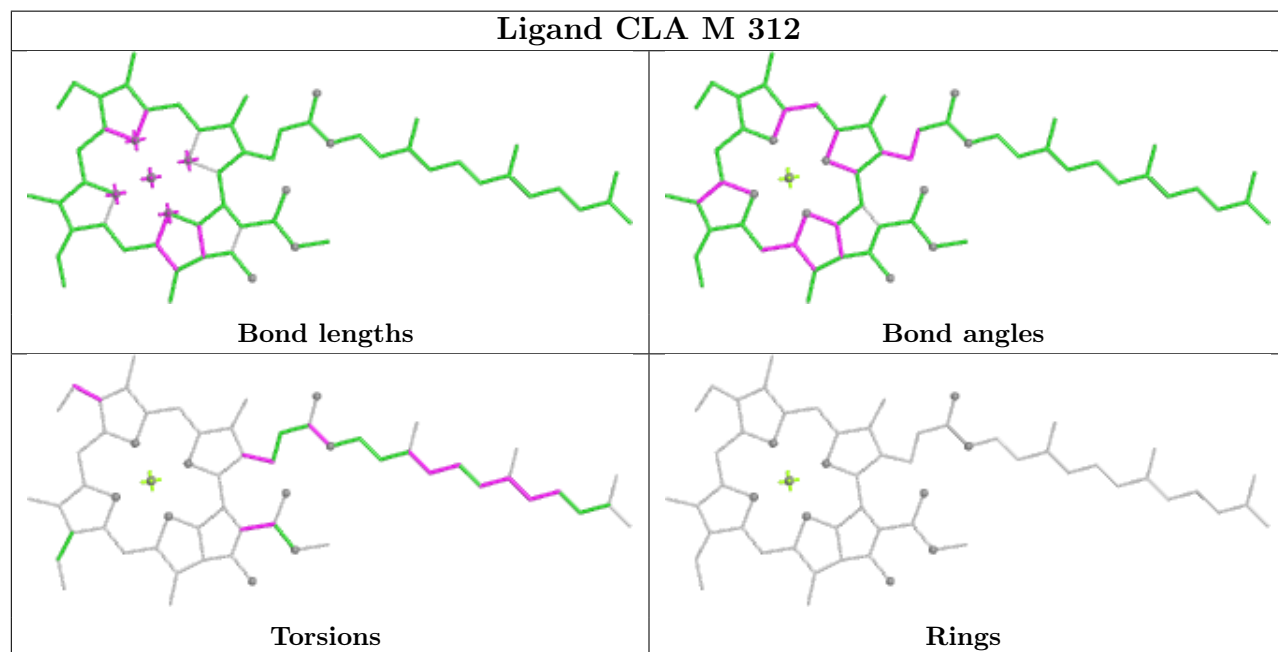
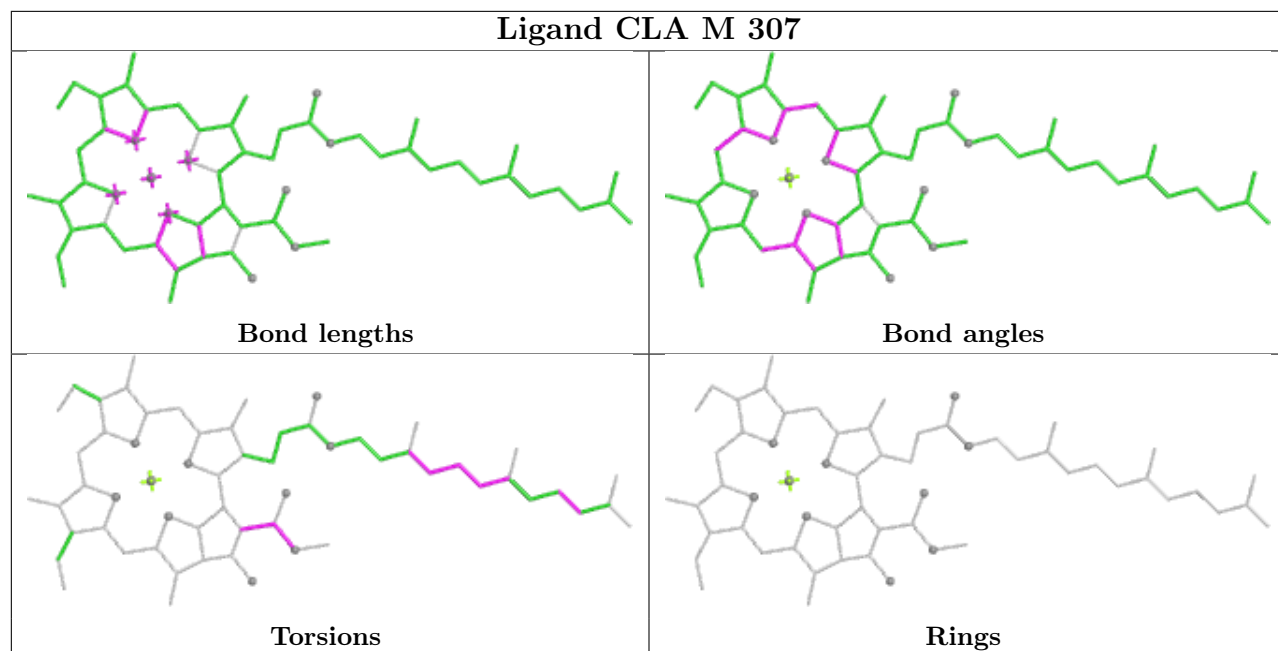


Ligand CLA E 306

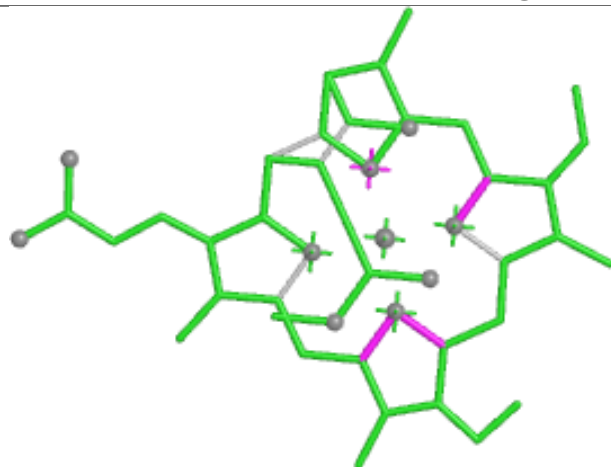




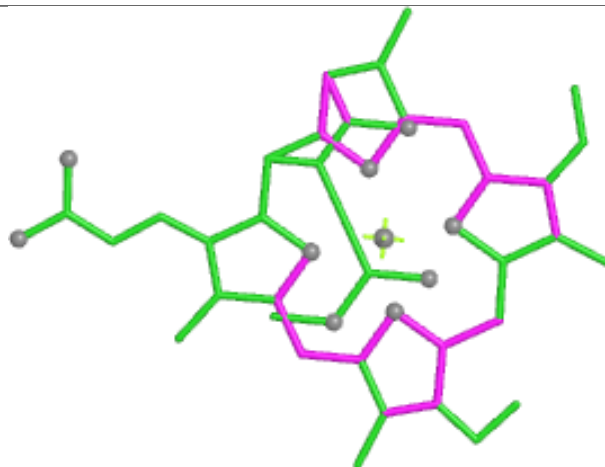




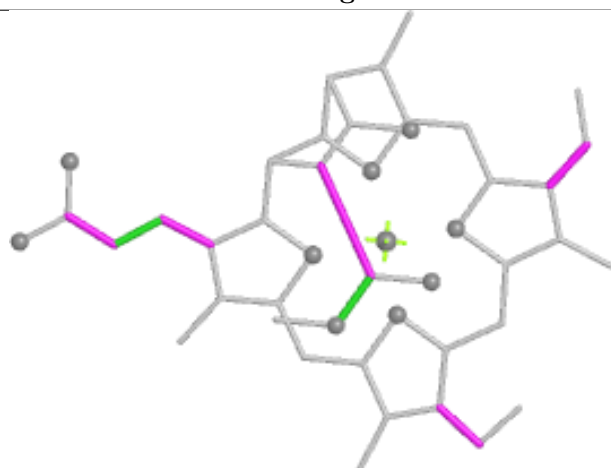
Ligand KC2 R 311



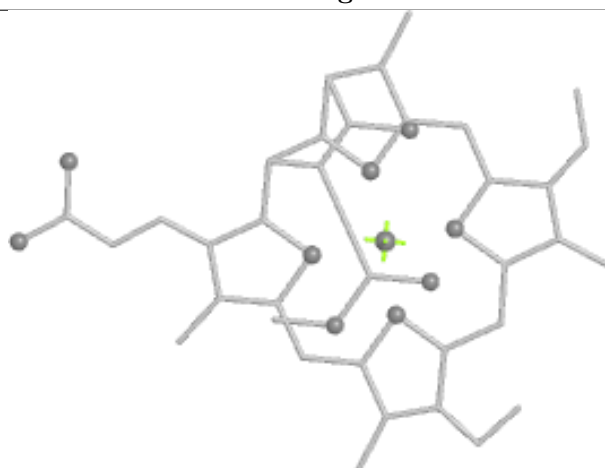
Bond lengths



Bond angles

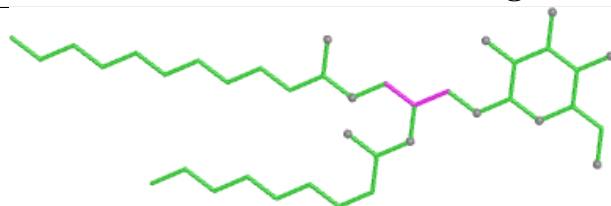


Torsions

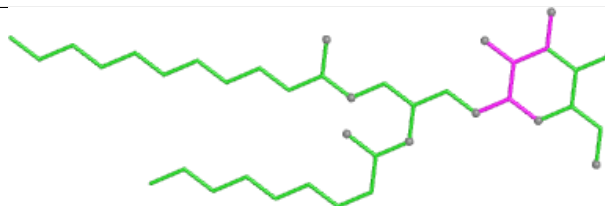


Rings

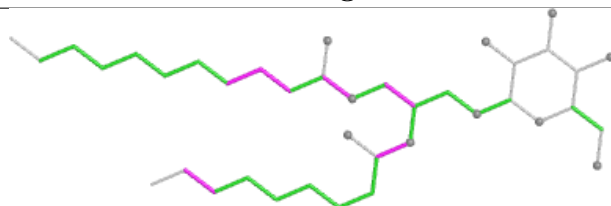
Ligand LMG M 317



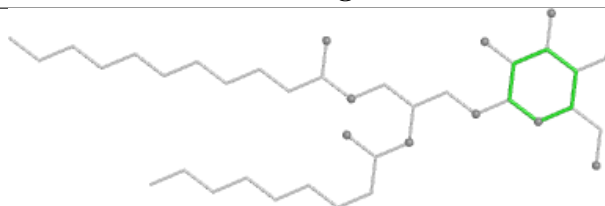
Bond lengths



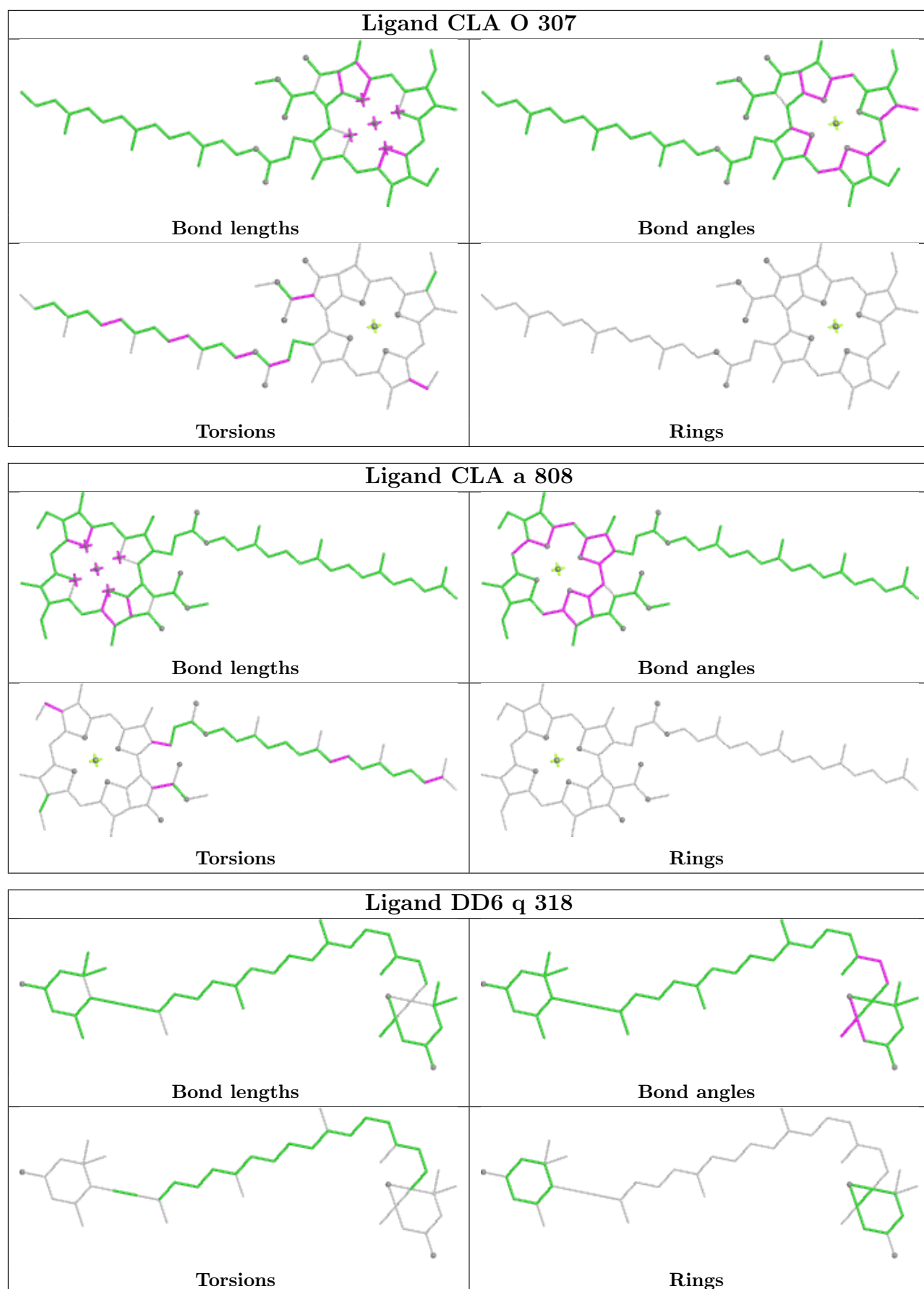
Bond angles

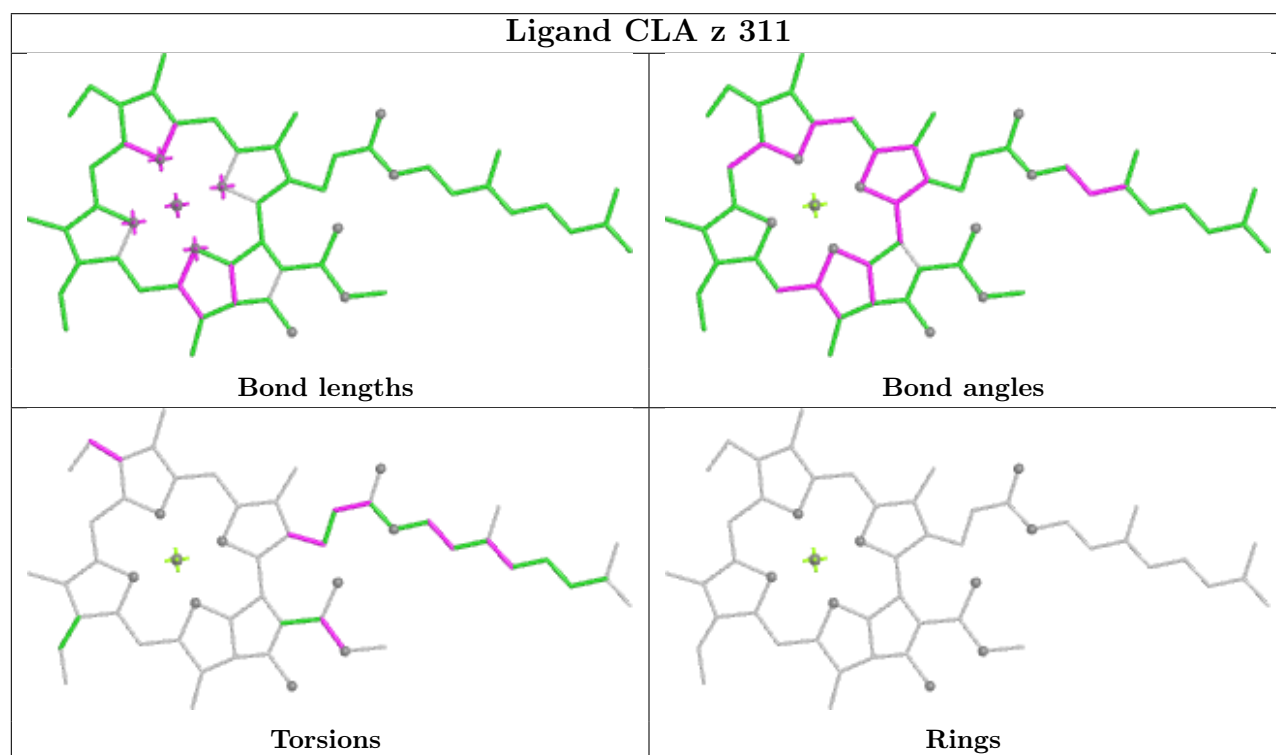
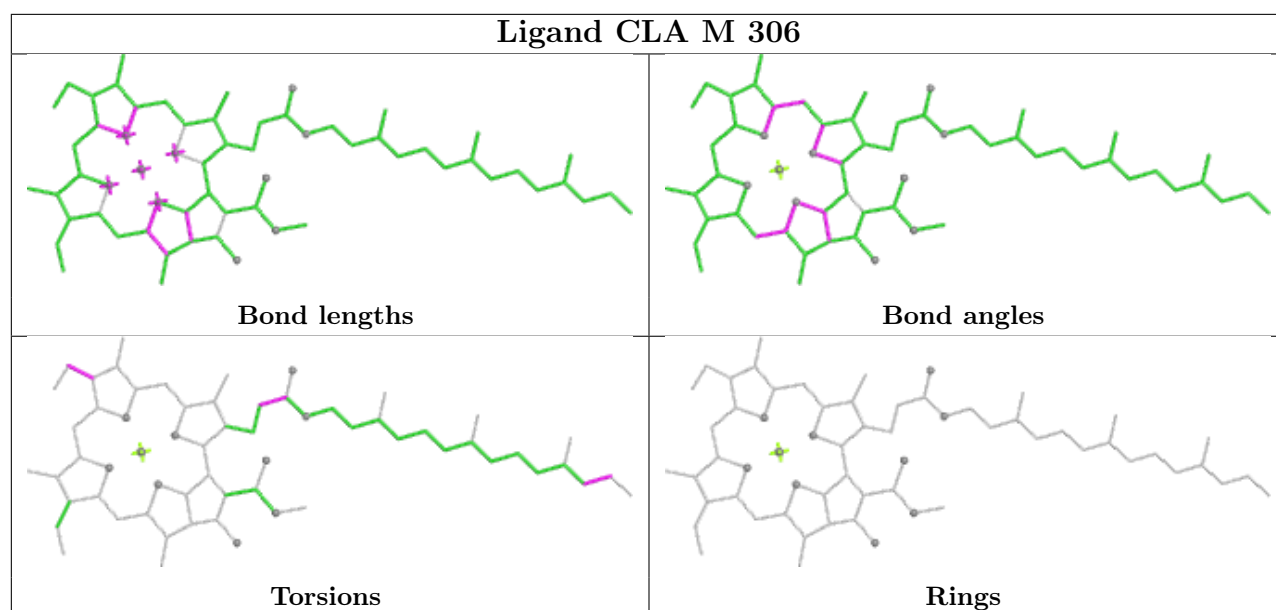


Torsions

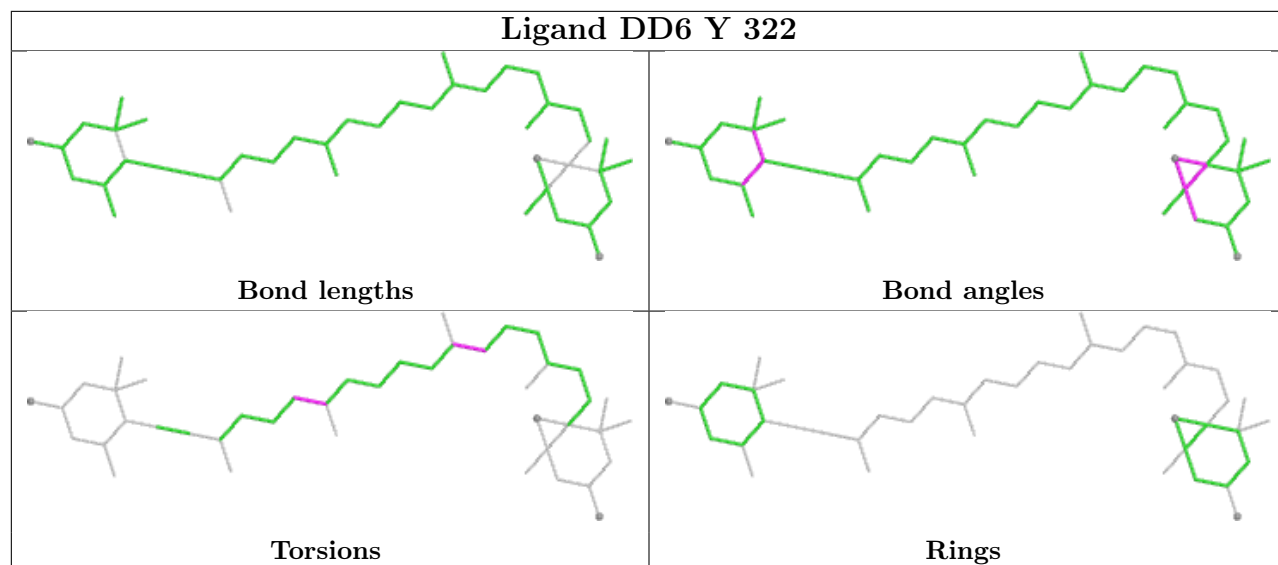


Rings

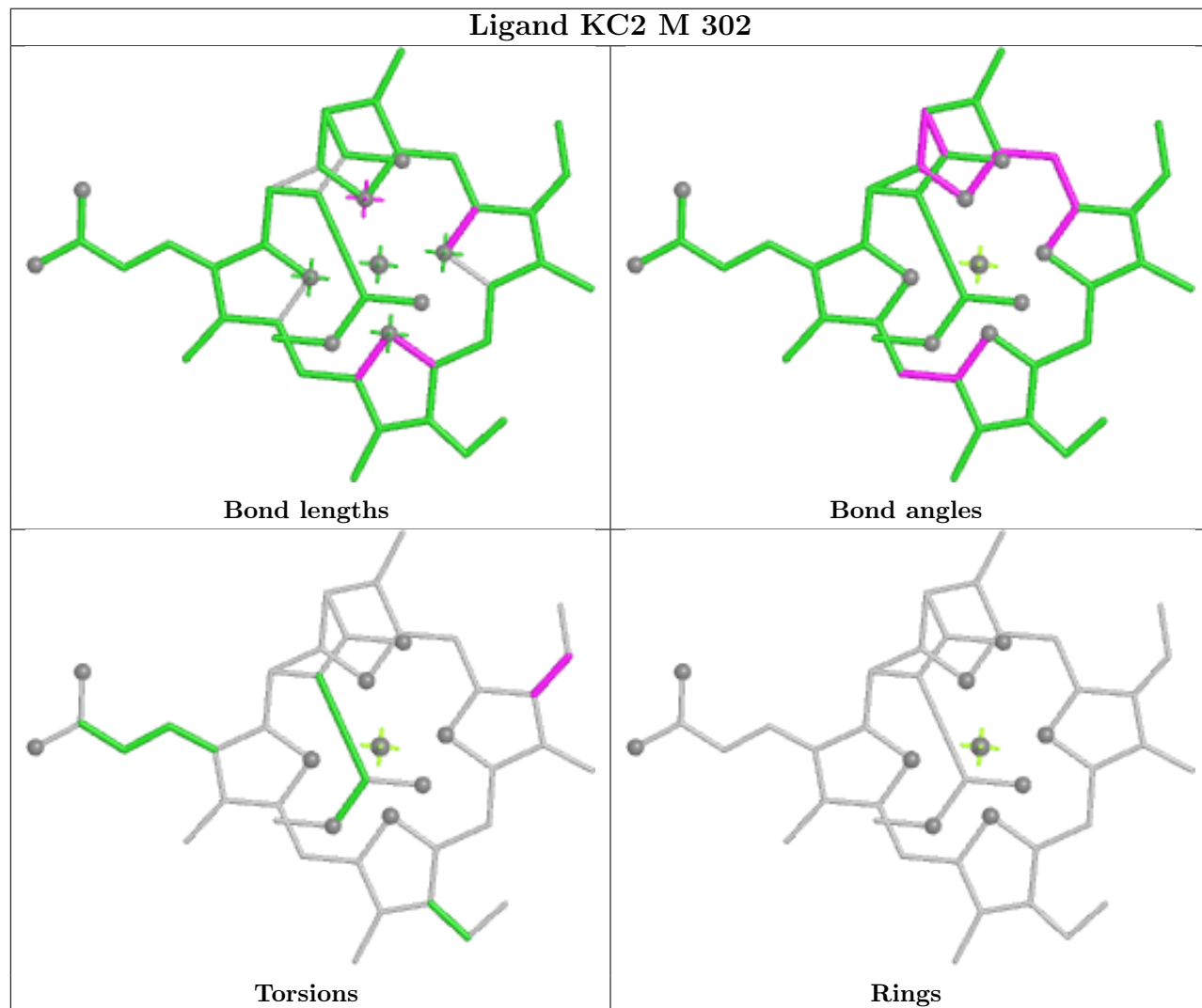




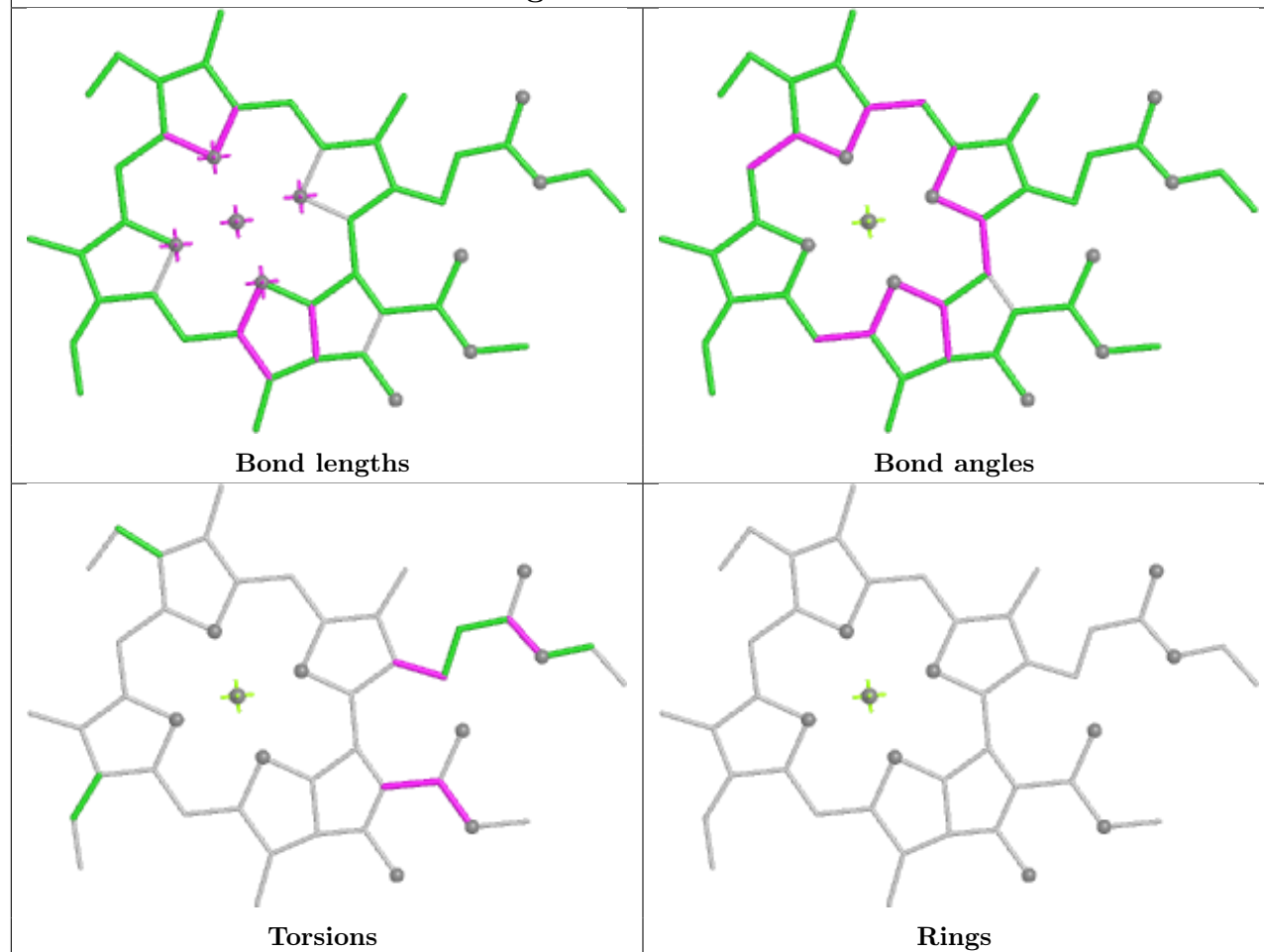
Ligand DD6 Y 322



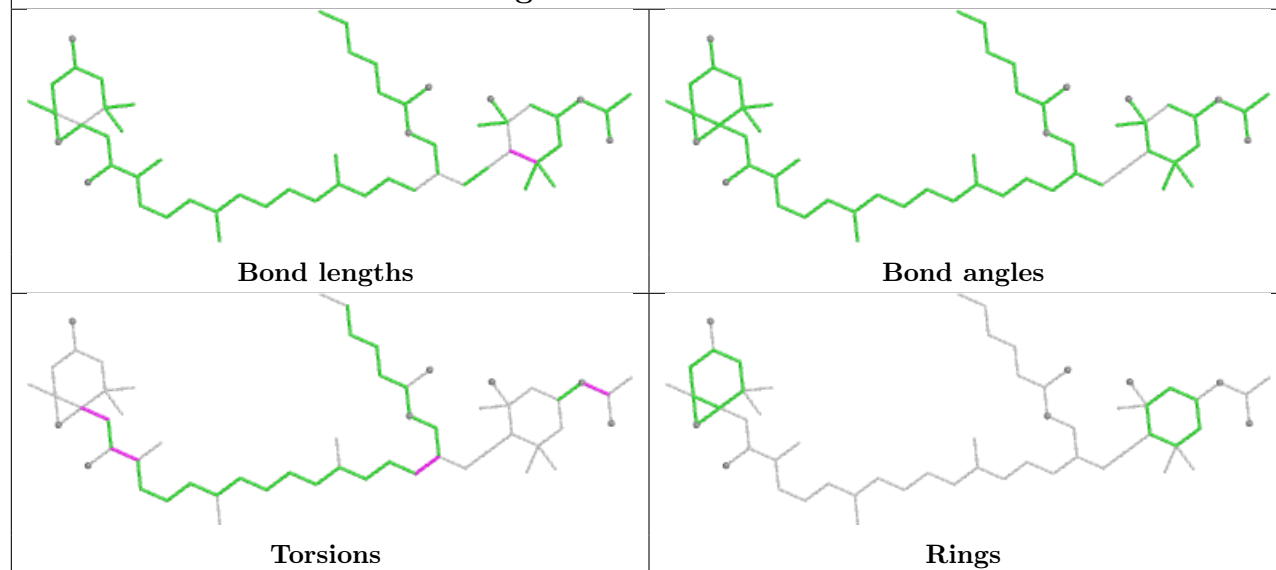
Ligand KC2 M 302

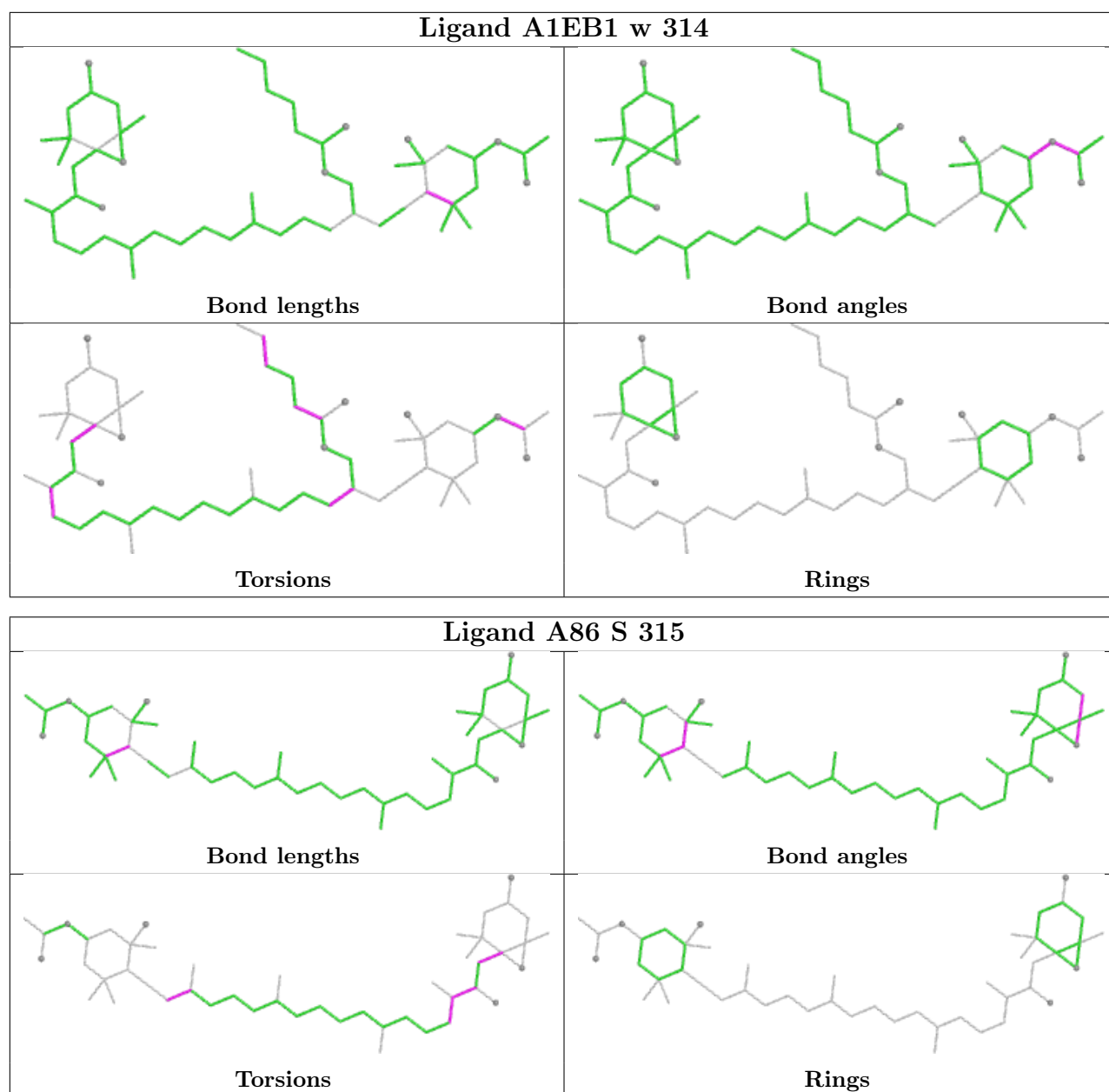


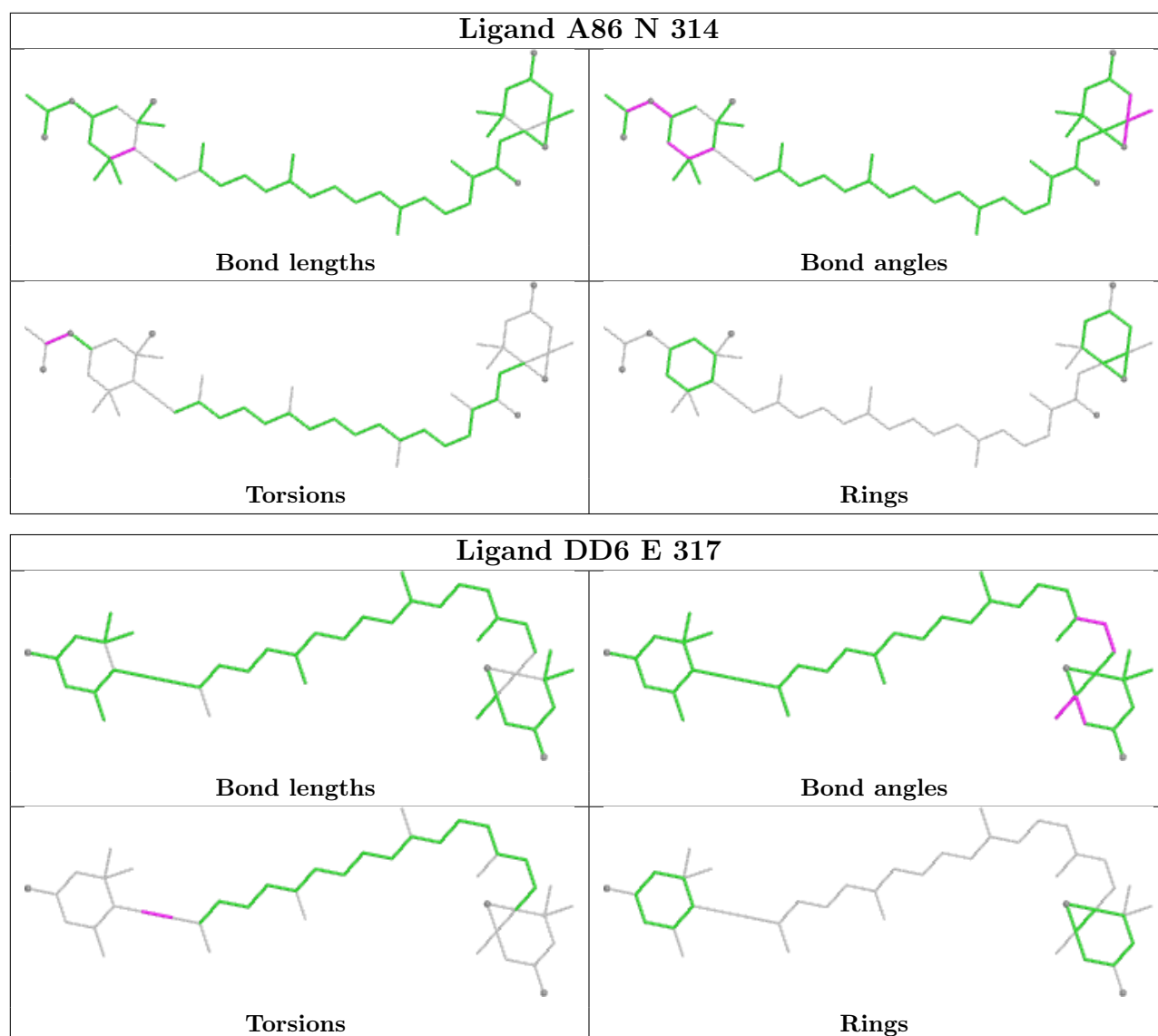
Ligand CLA A 311

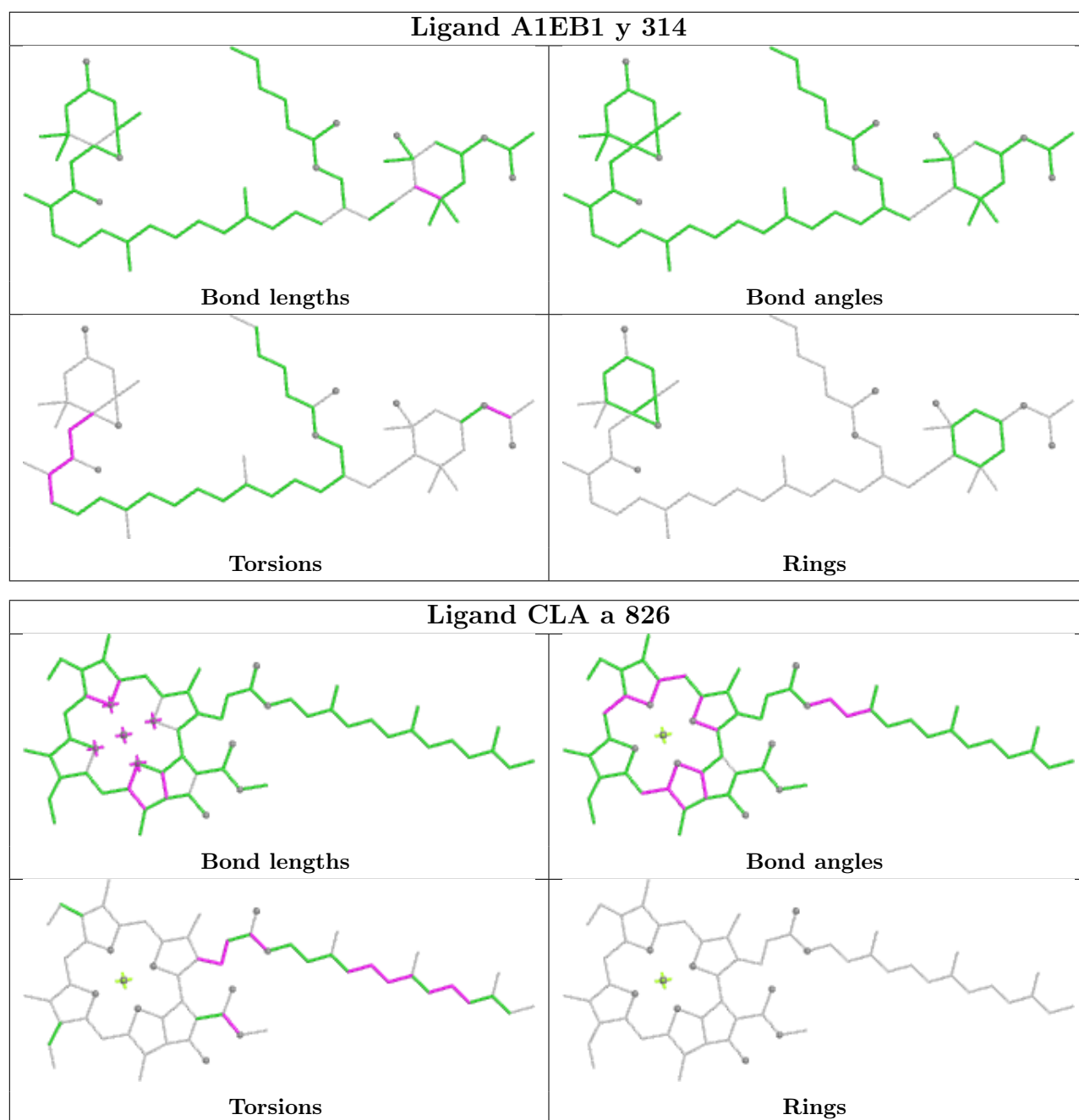


Ligand A1EB1 F 322

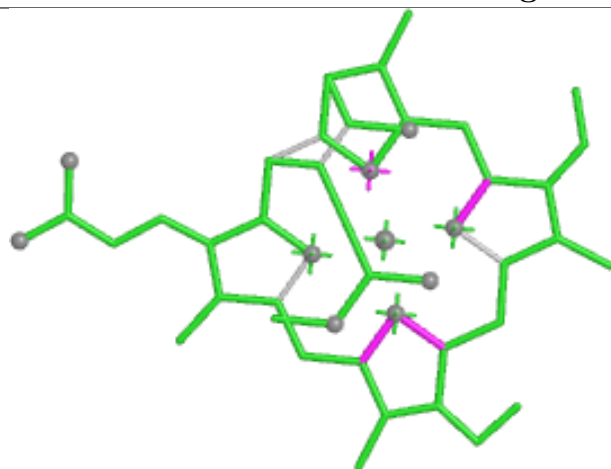




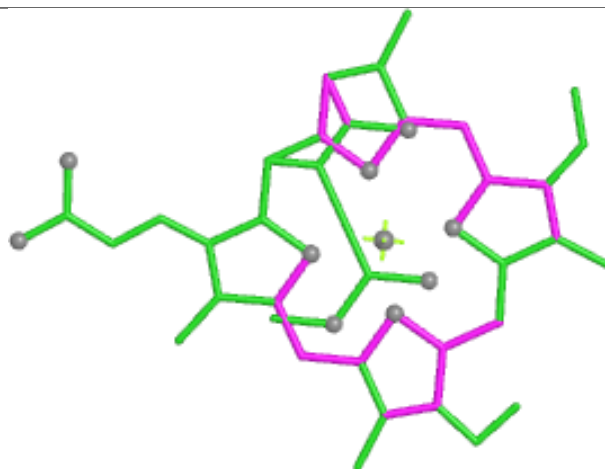




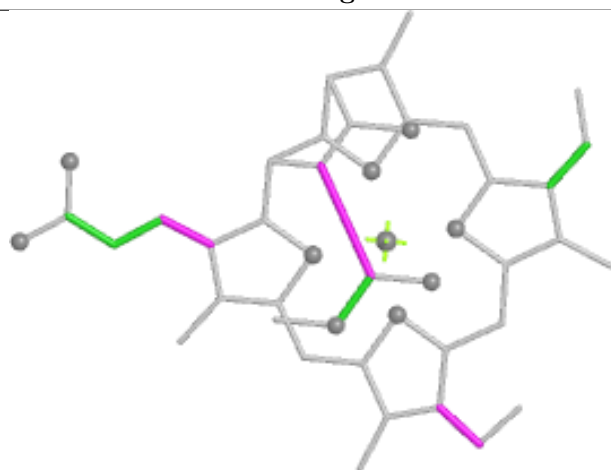
Ligand KC2 x 309



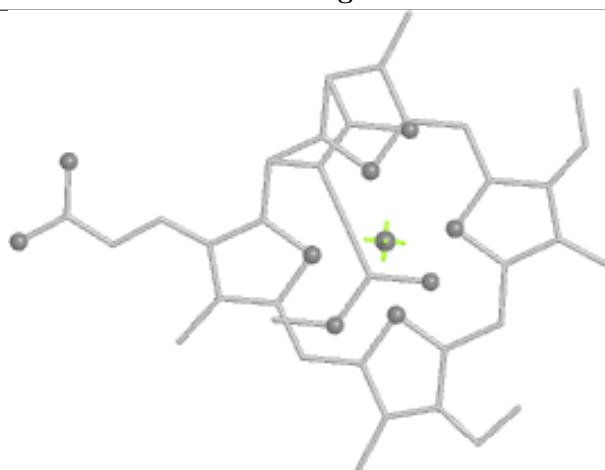
Bond lengths



Bond angles

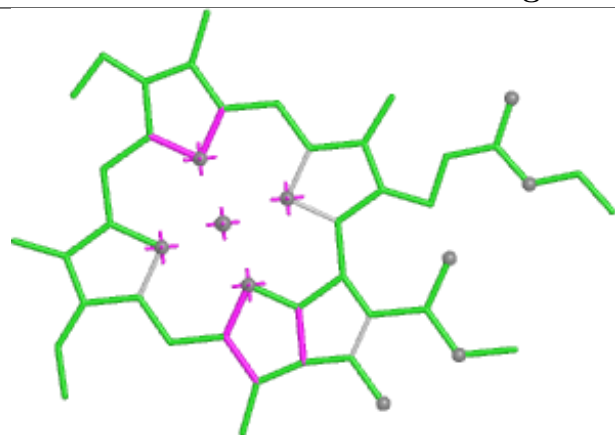


Torsions



Rings

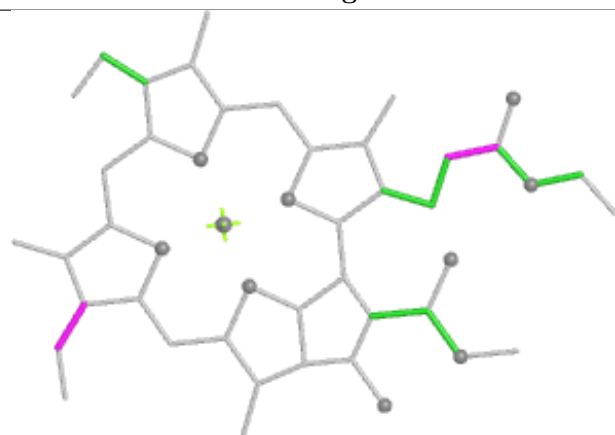
Ligand CLA I 204



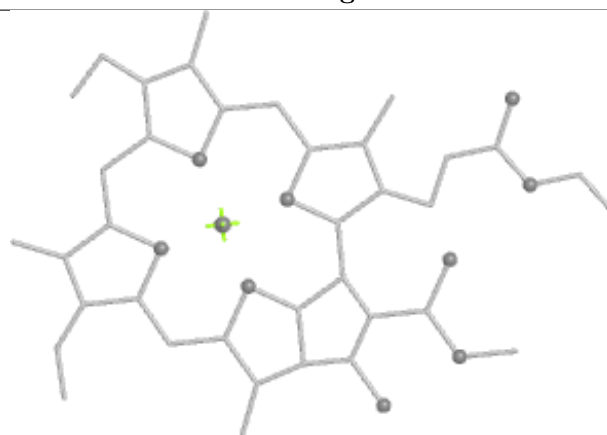
Bond lengths



Bond angles

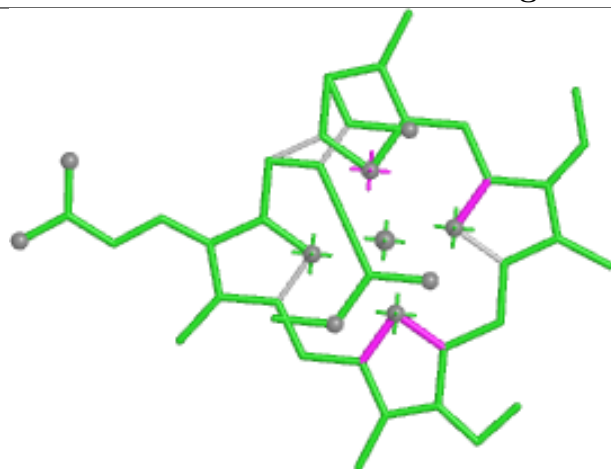


Torsions

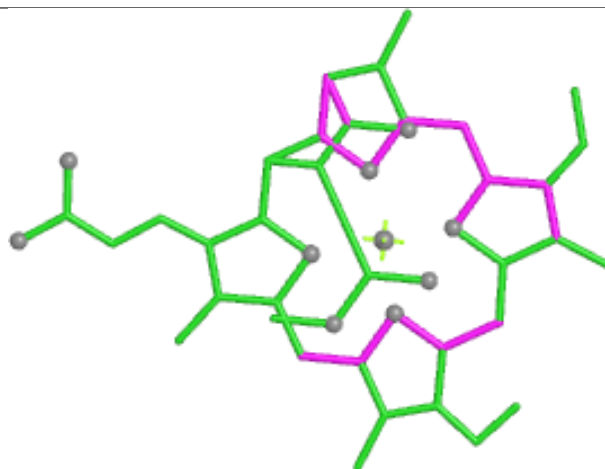


Rings

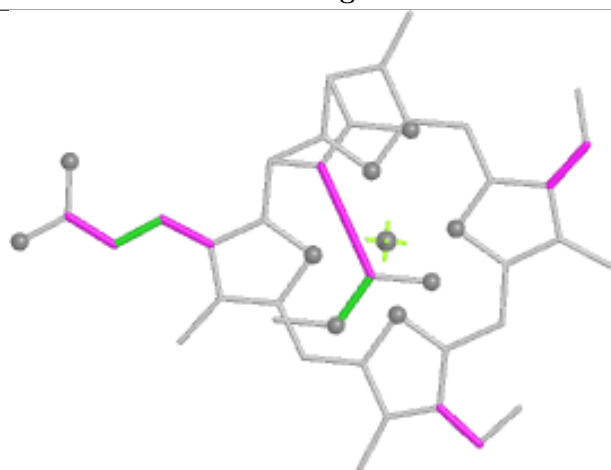
Ligand KC2 v 309



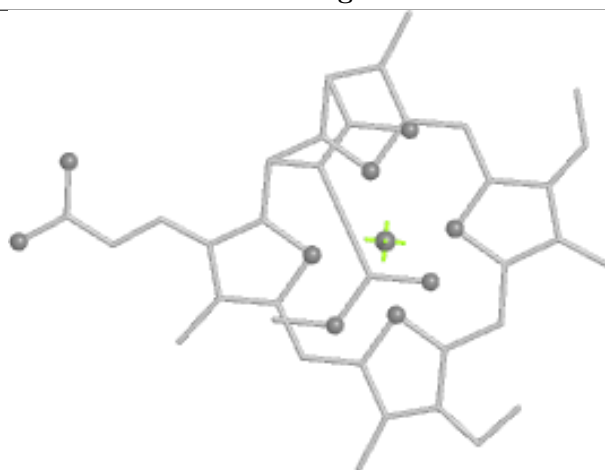
Bond lengths



Bond angles

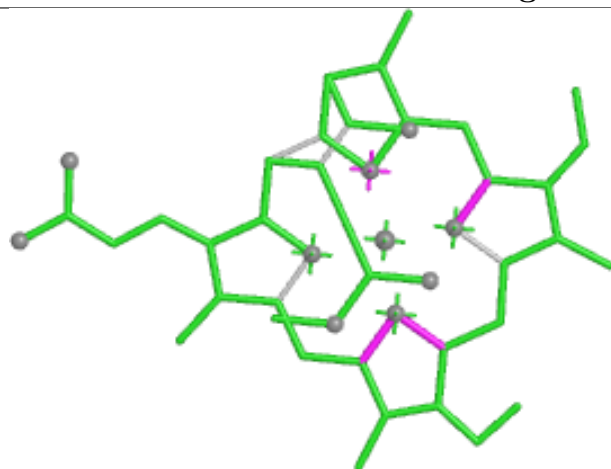


Torsions

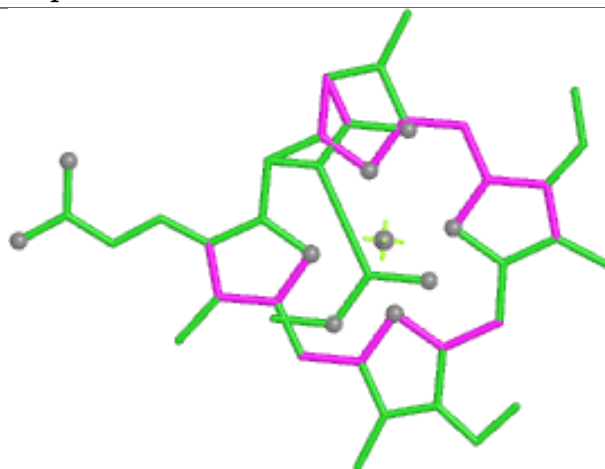


Rings

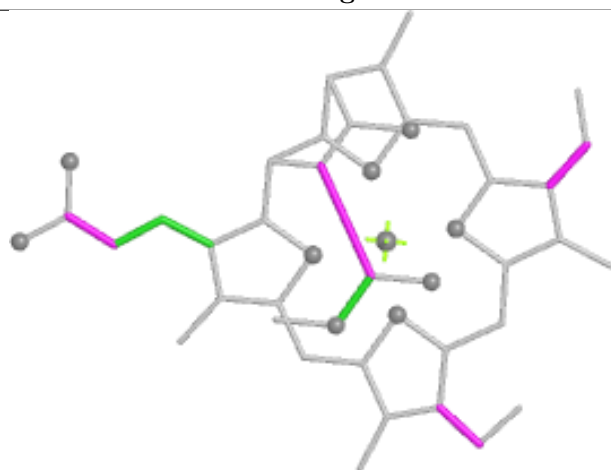
Ligand KC2 p 315



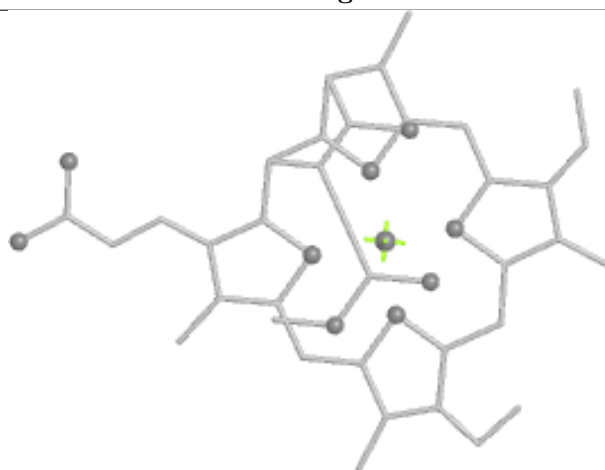
Bond lengths



Bond angles

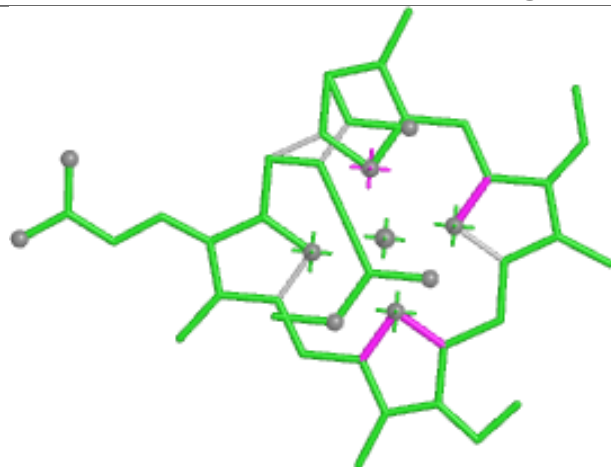


Torsions

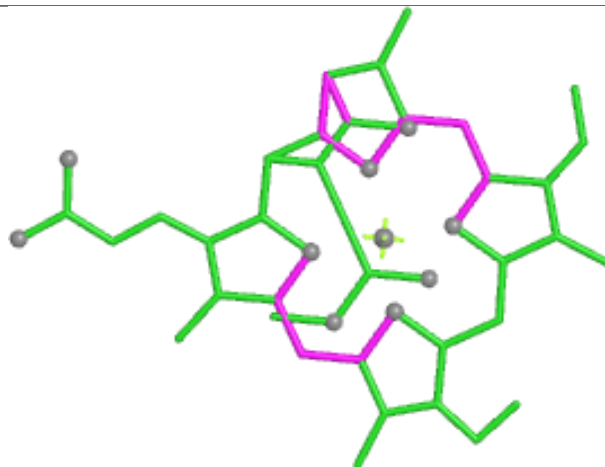


Rings

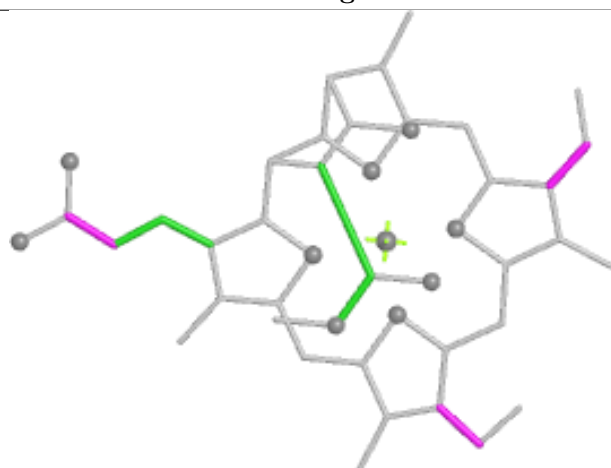
Ligand KC2 z 309



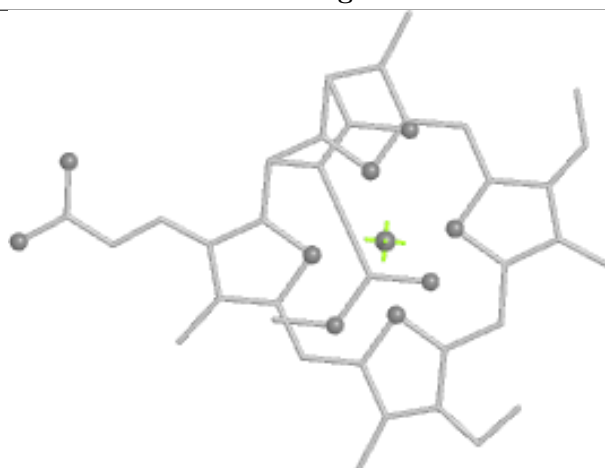
Bond lengths



Bond angles



Torsions



Rings

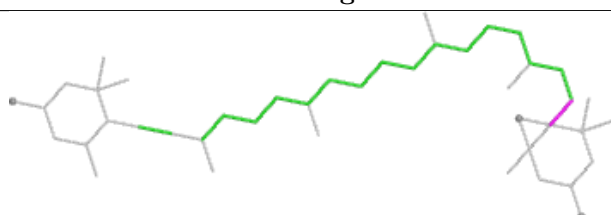
Ligand DD6 J 313



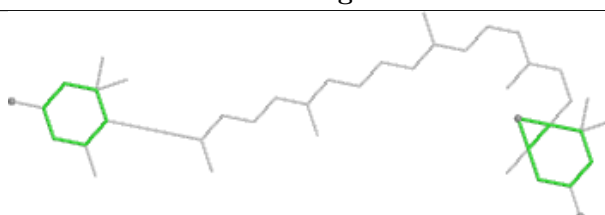
Bond lengths



Bond angles

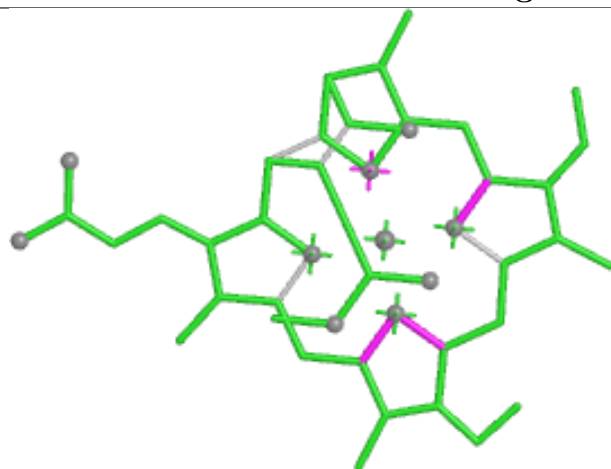


Torsions

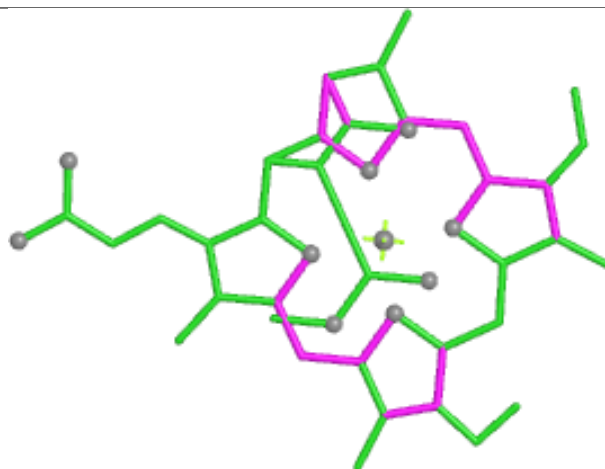


Rings

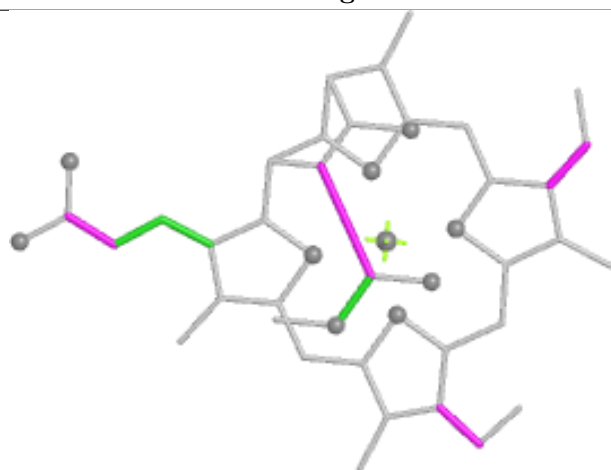
Ligand KC2 O 311



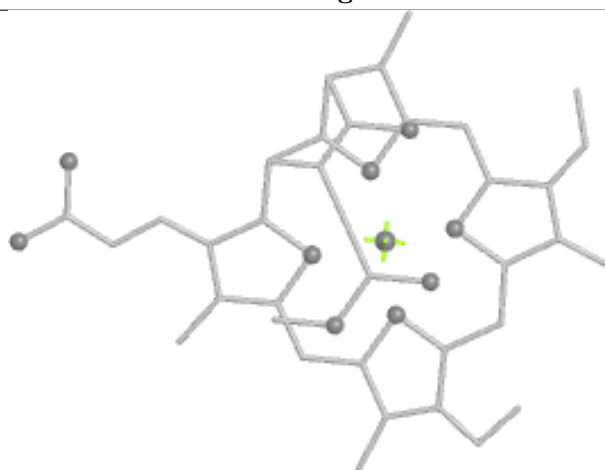
Bond lengths



Bond angles

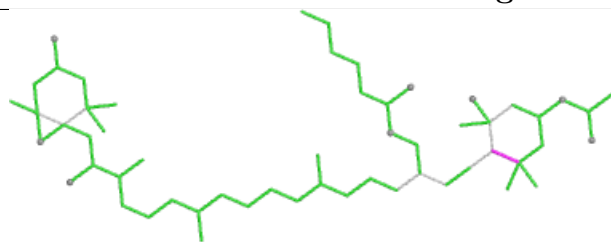


Torsions

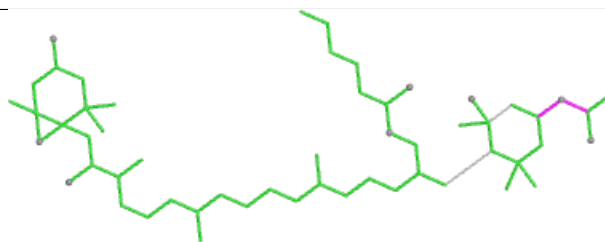


Rings

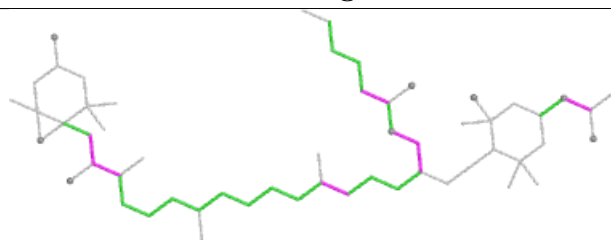
Ligand A1EB1 T 320



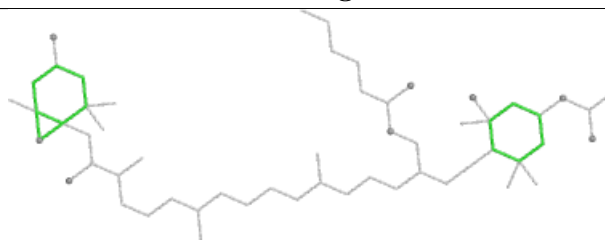
Bond lengths



Bond angles

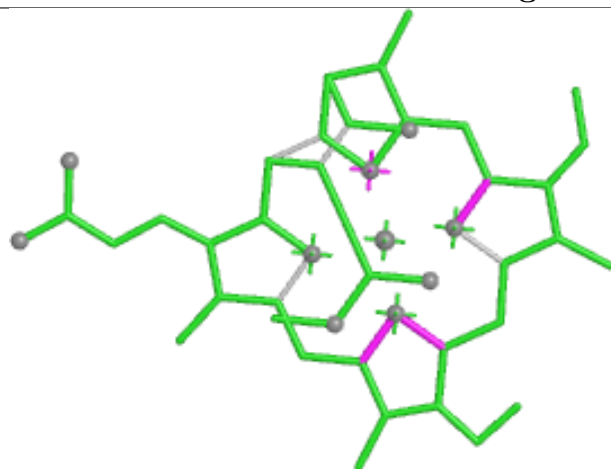


Torsions

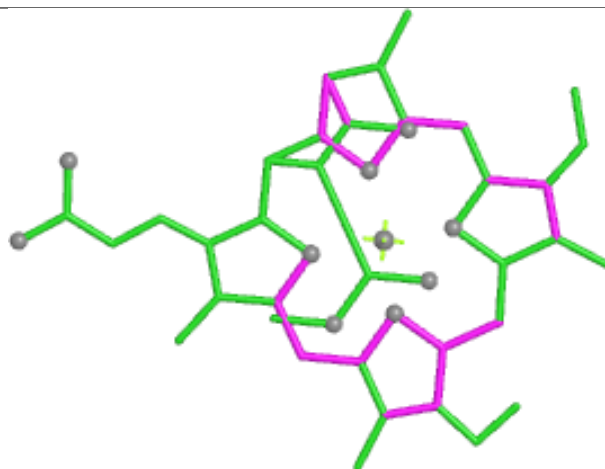


Rings

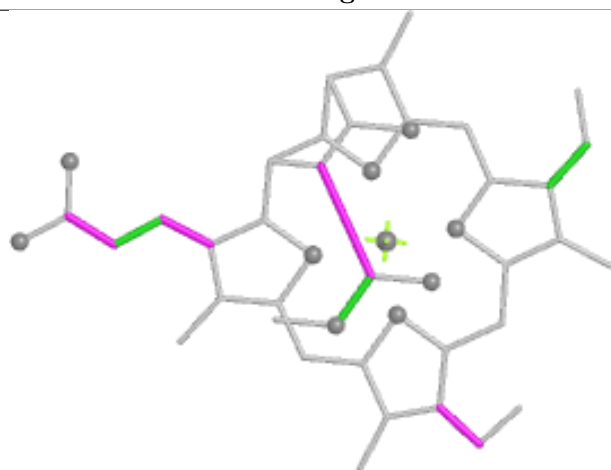
Ligand KC2 u 304



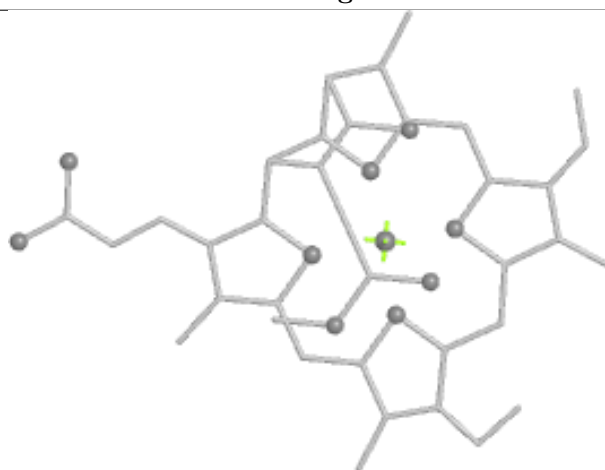
Bond lengths



Bond angles

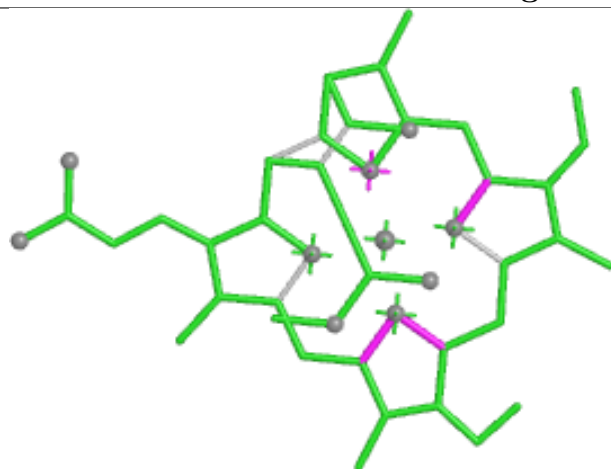


Torsions

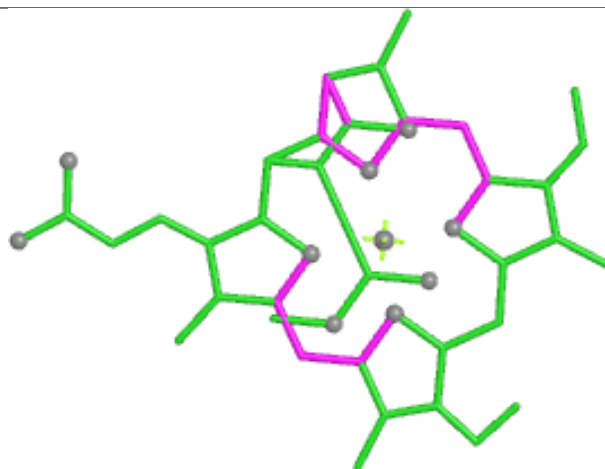


Rings

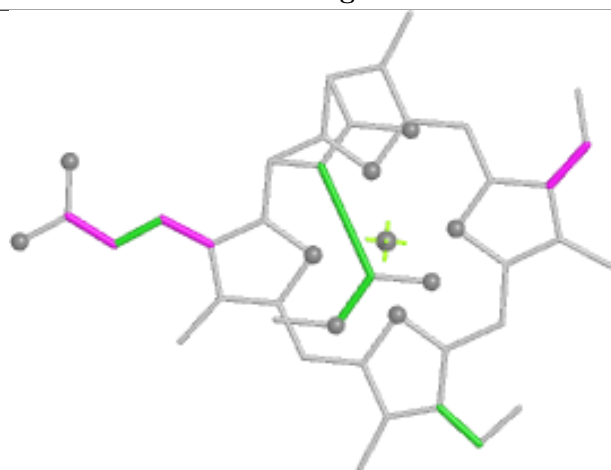
Ligand KC2 z 303



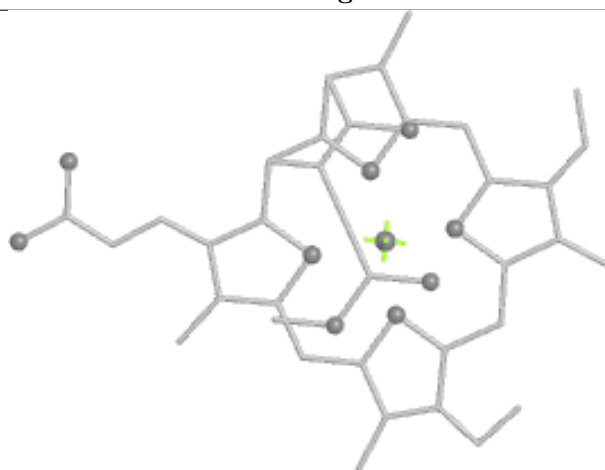
Bond lengths



Bond angles

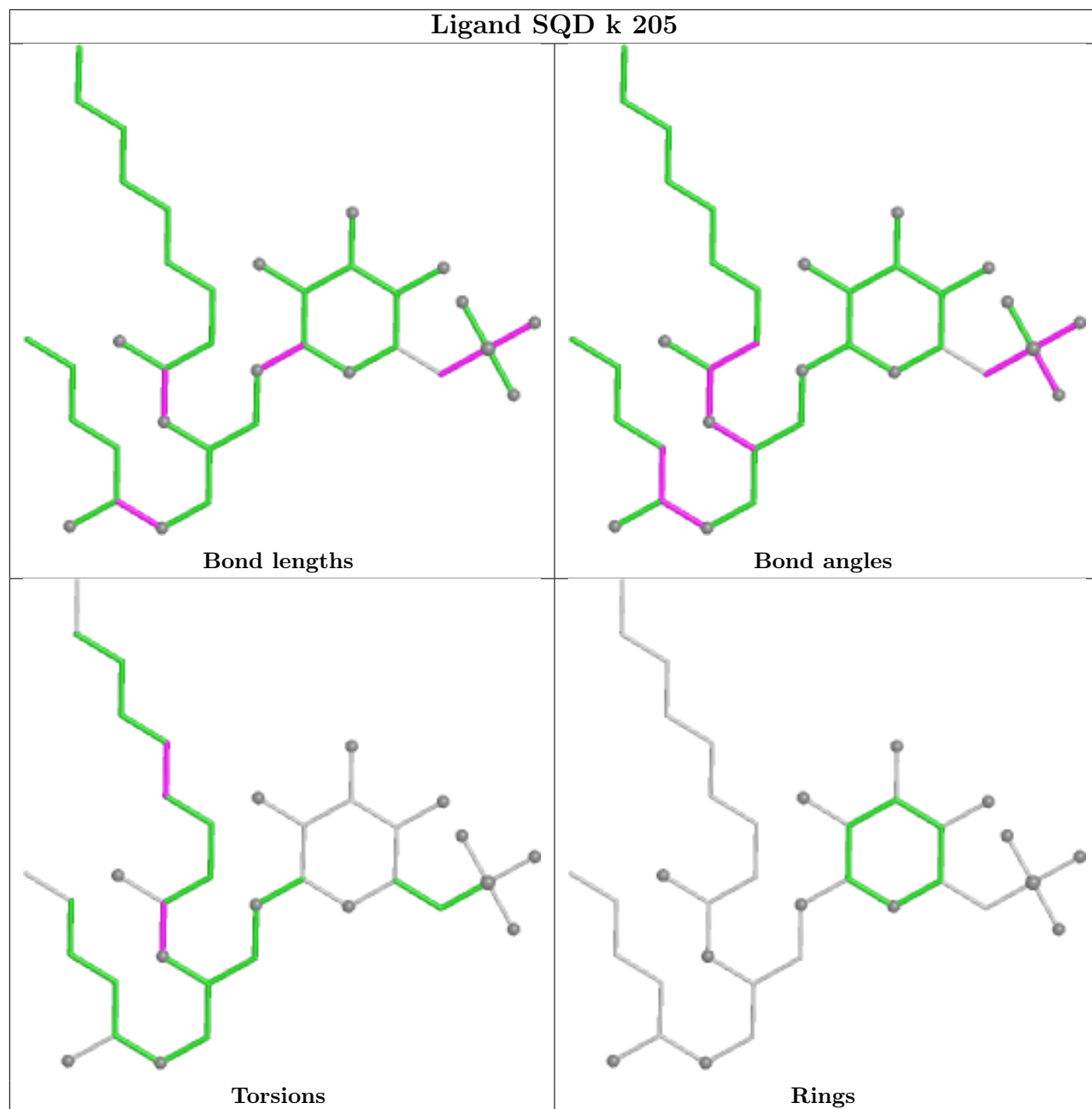


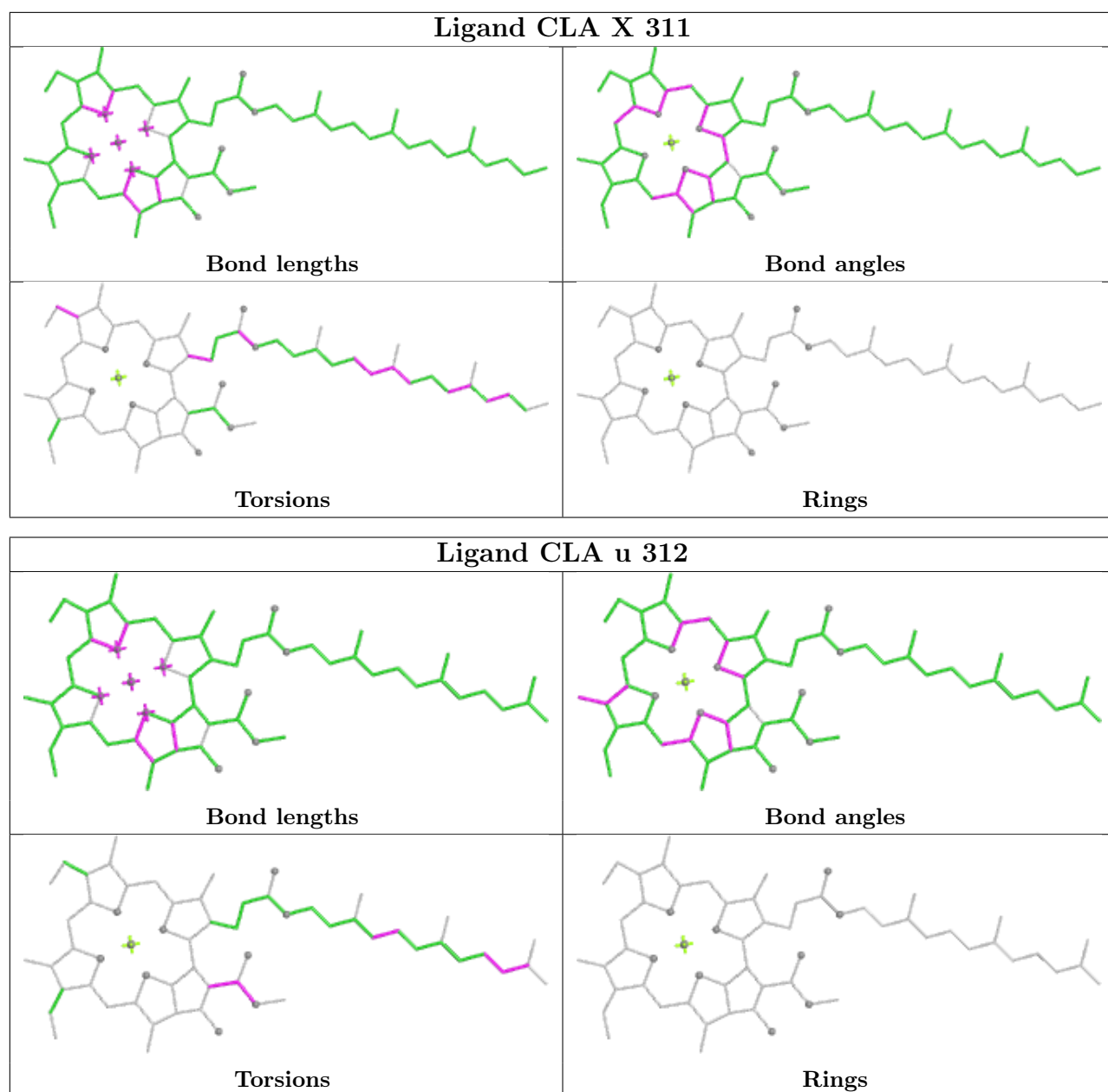
Torsions

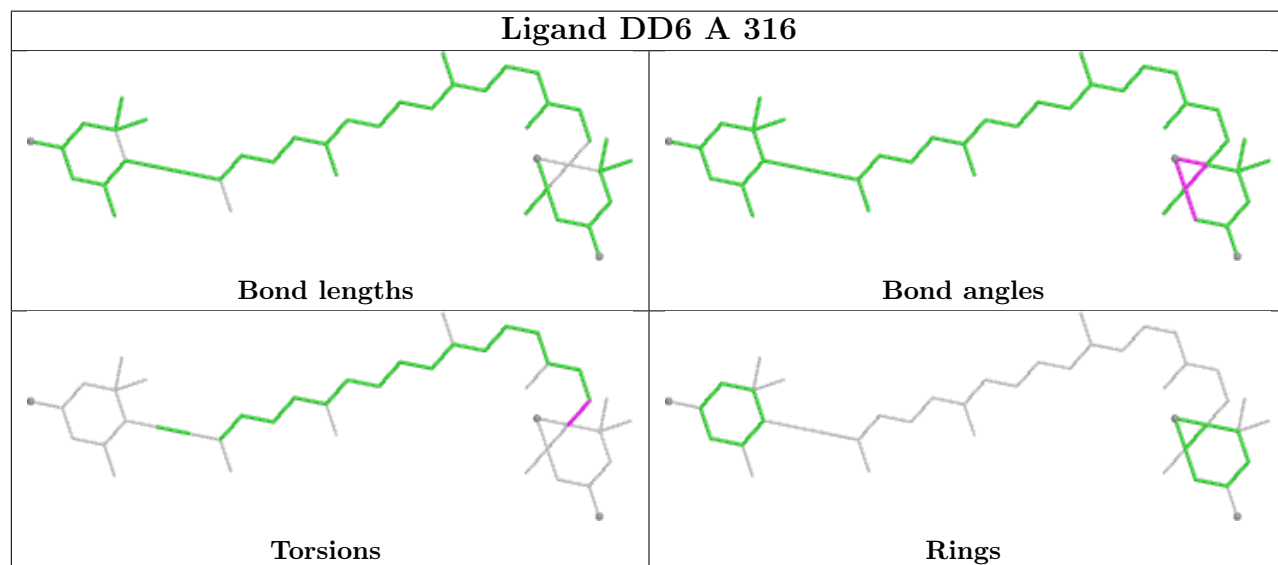
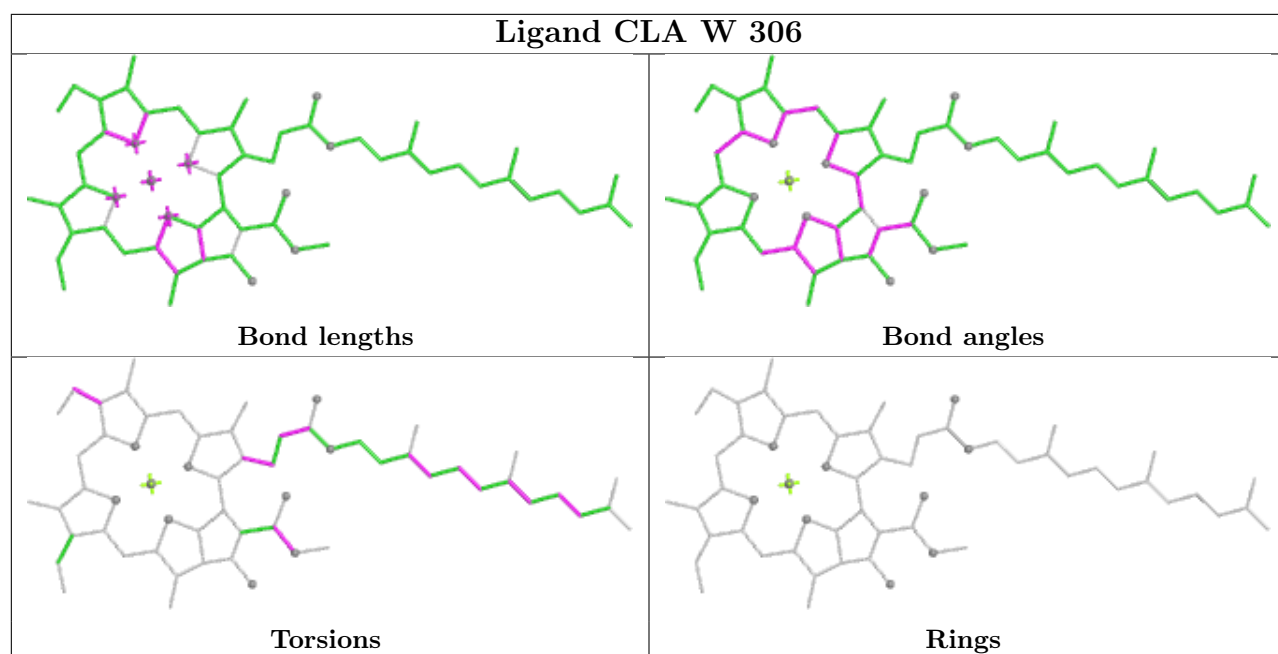


Rings

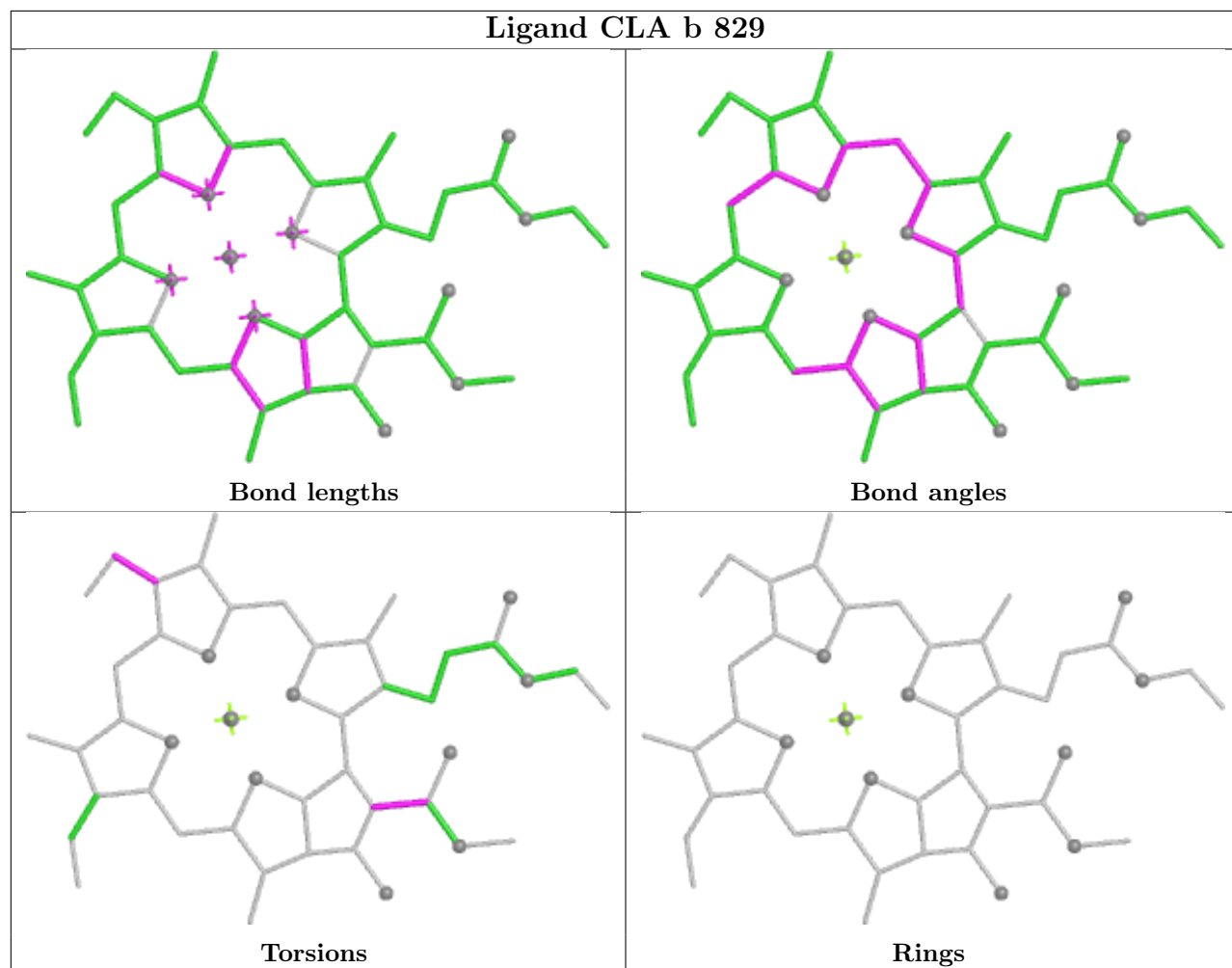
Ligand SQD k 205

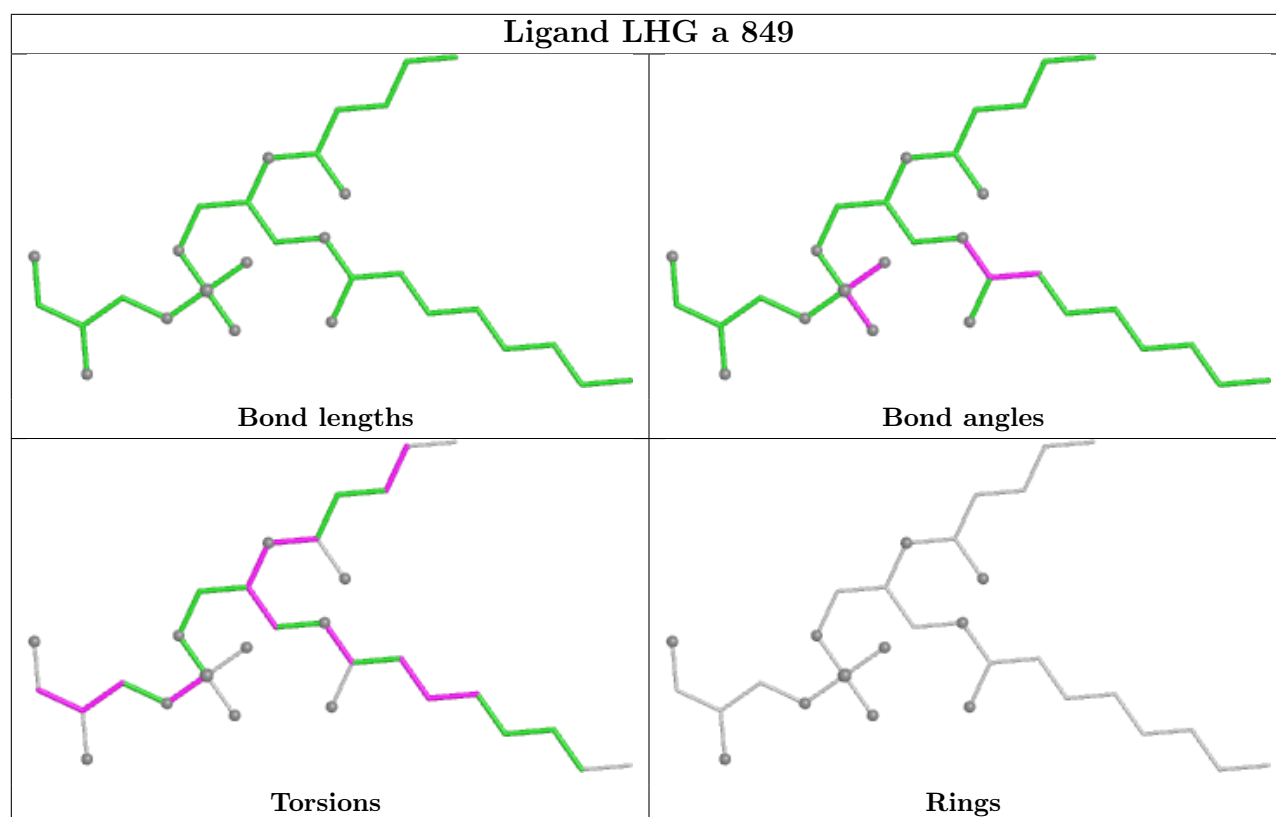




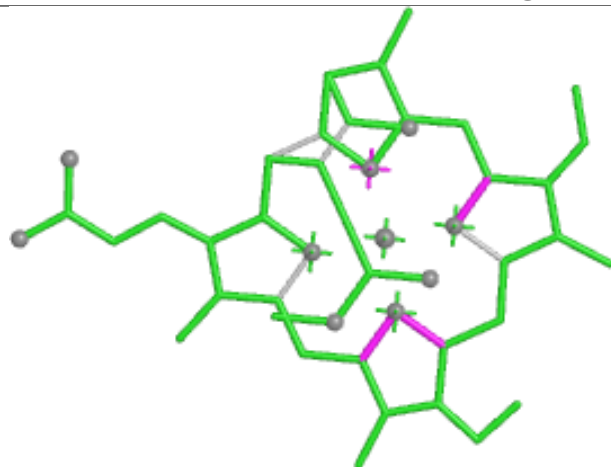


Ligand CLA b 829

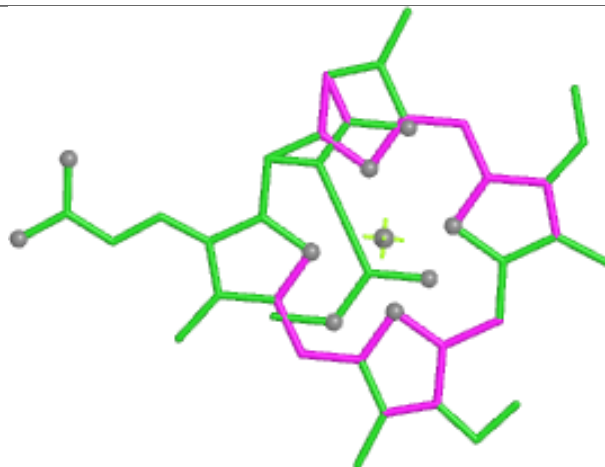




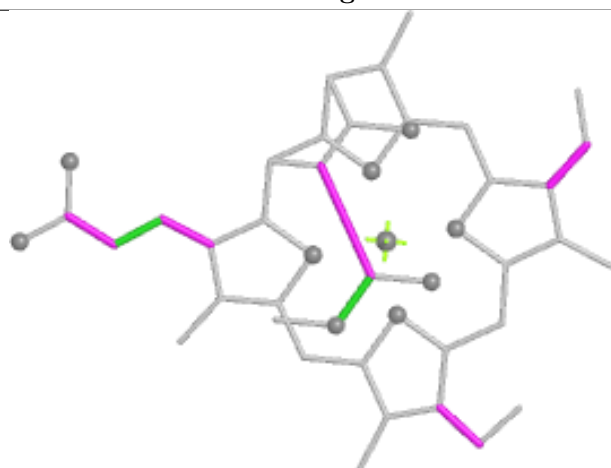
Ligand KC2 S 309



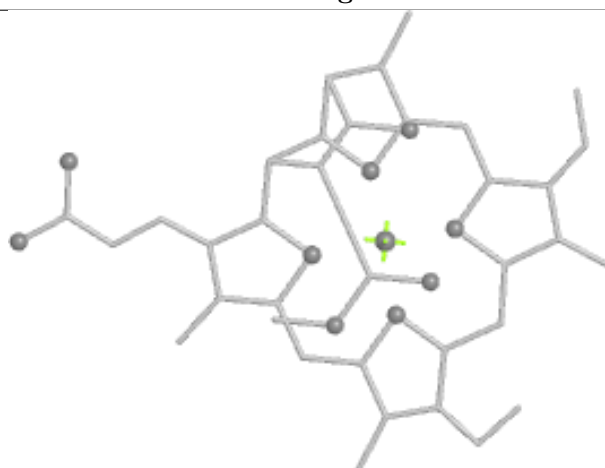
Bond lengths



Bond angles

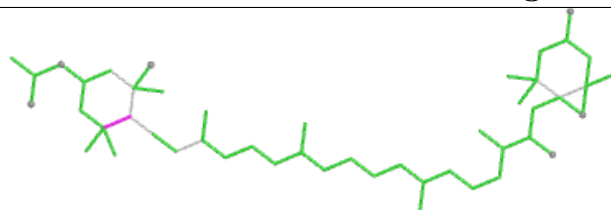


Torsions

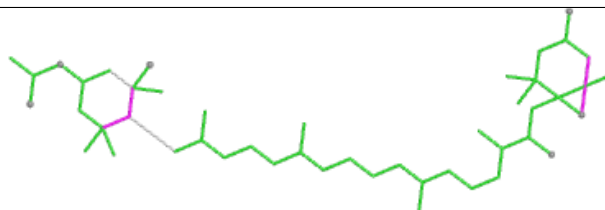


Rings

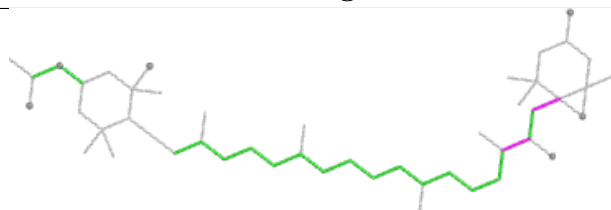
Ligand A86 u 320



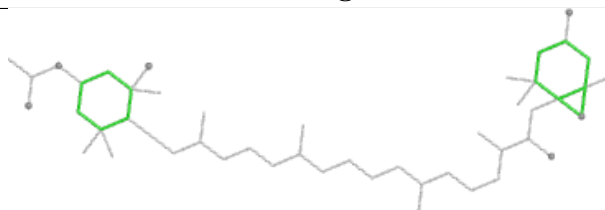
Bond lengths



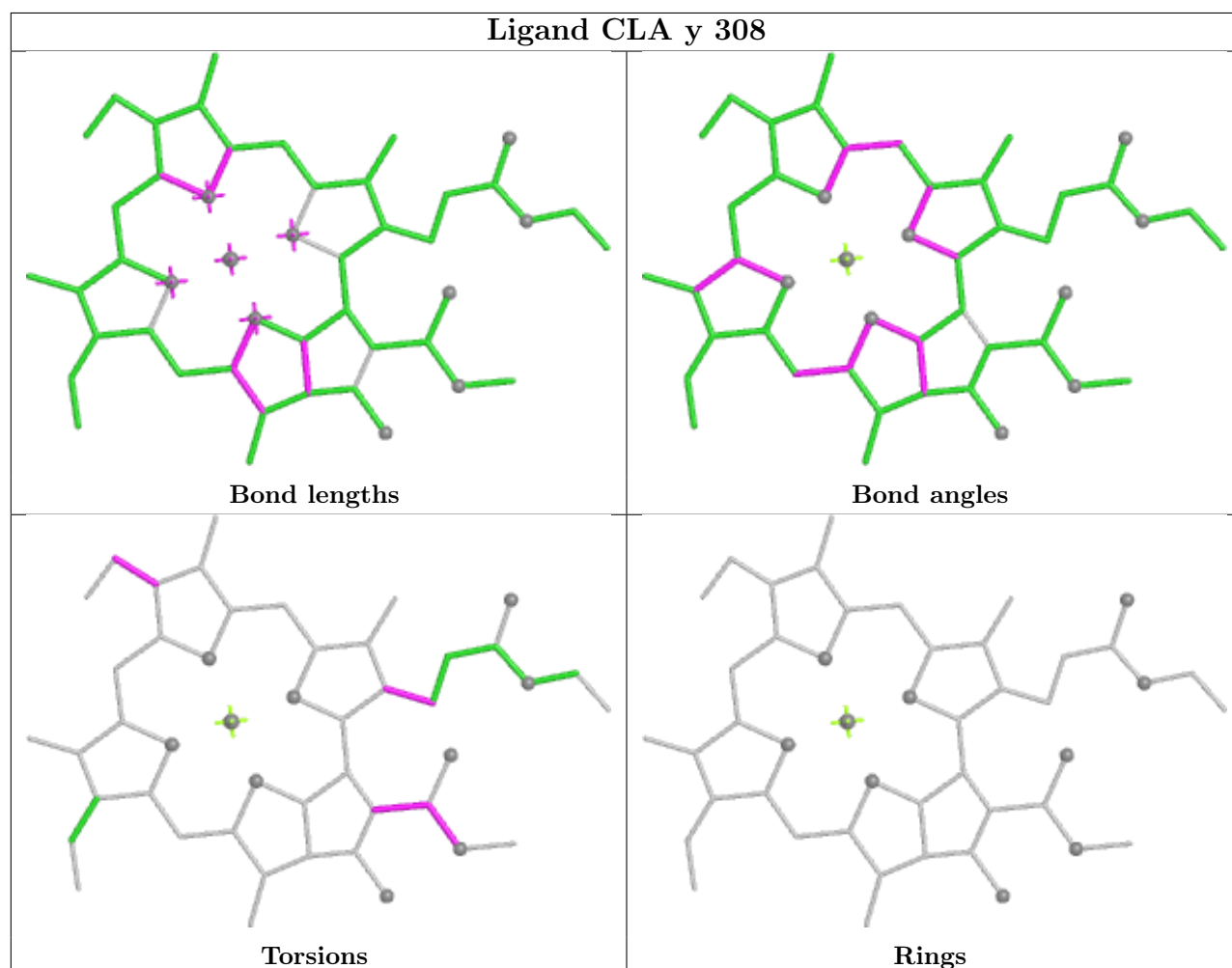
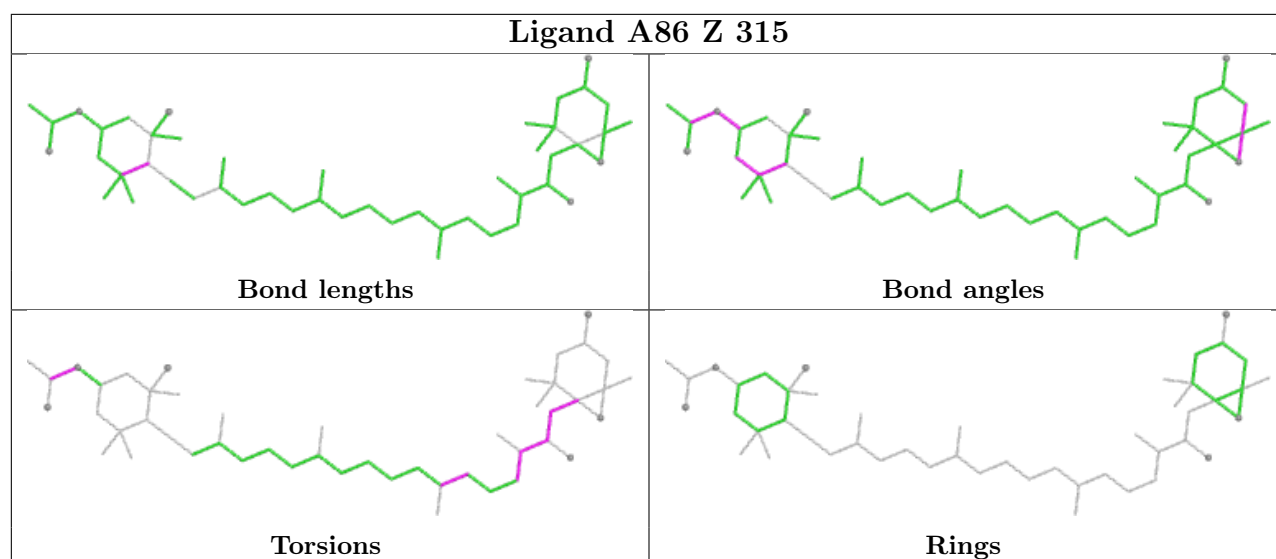
Bond angles

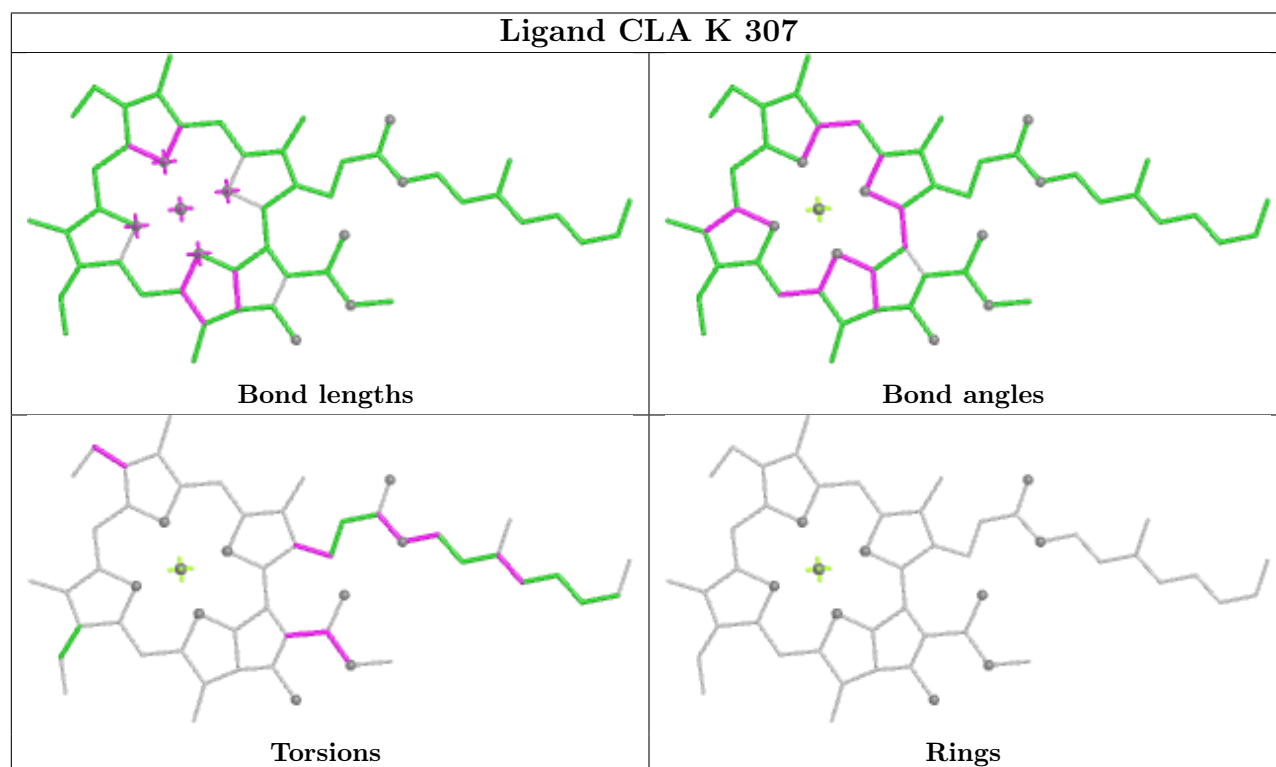
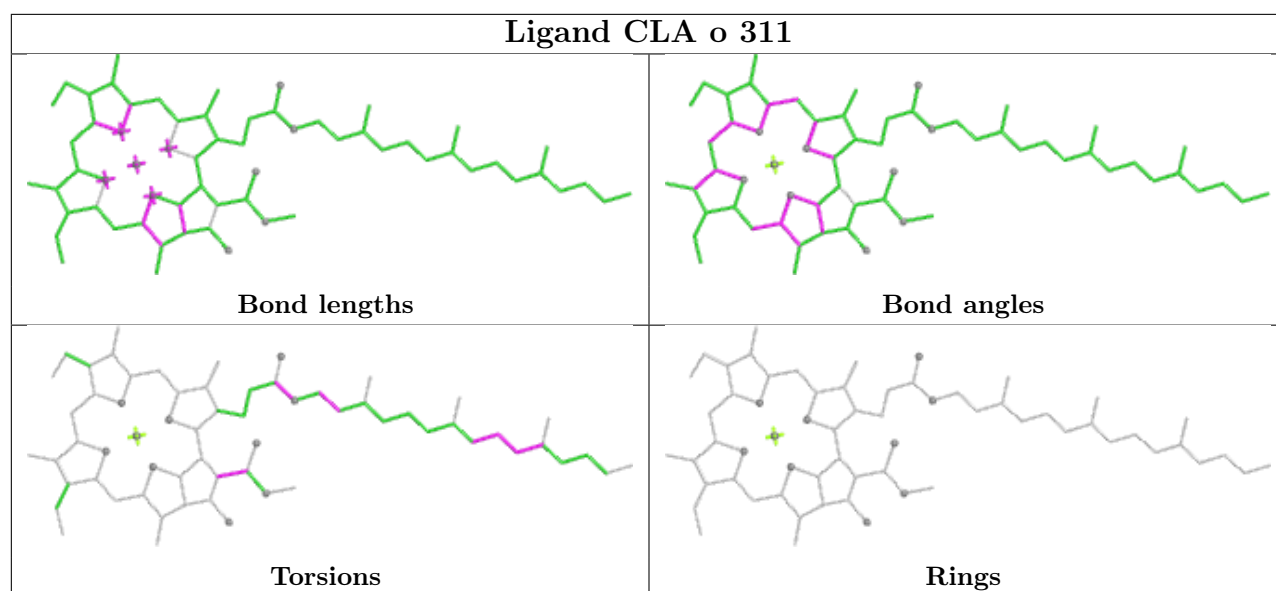


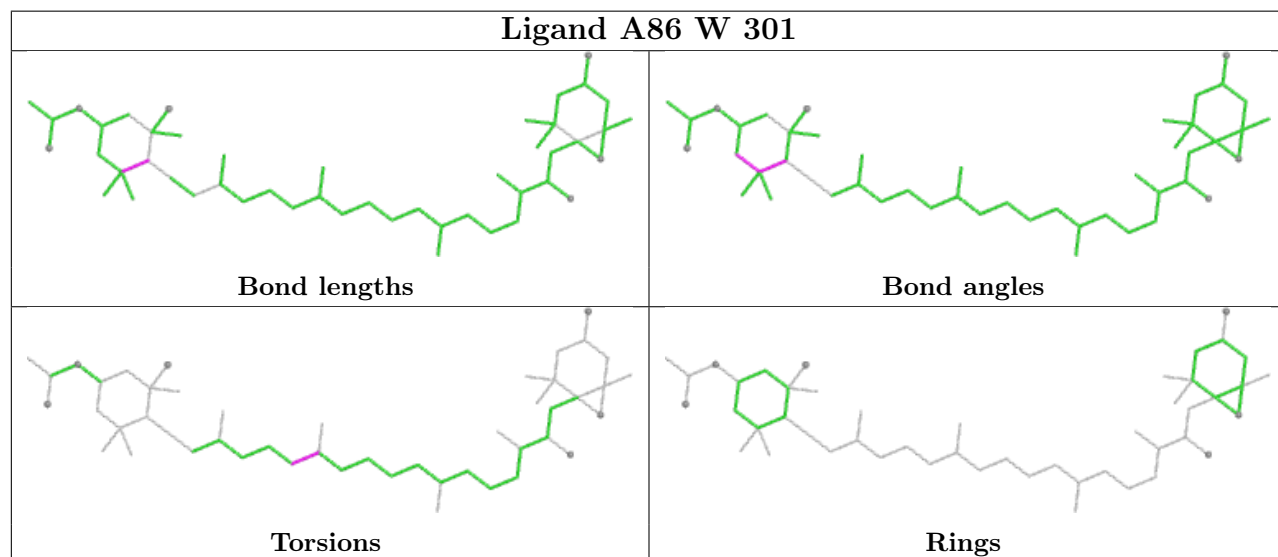
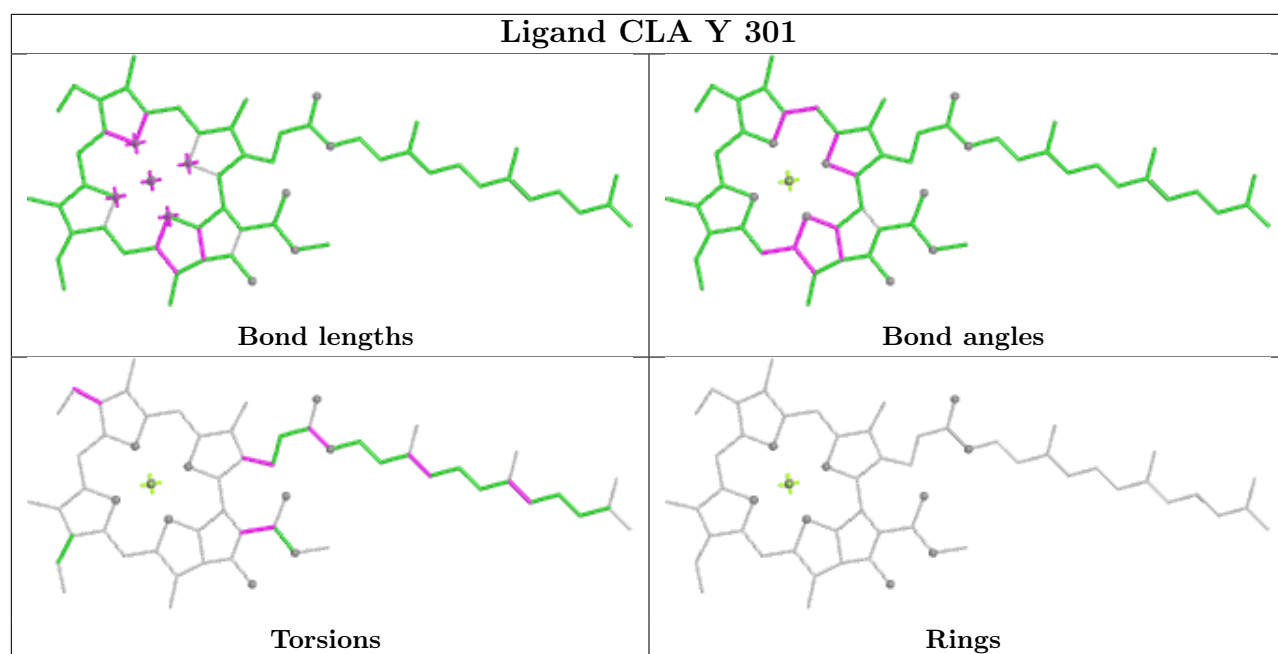
Torsions



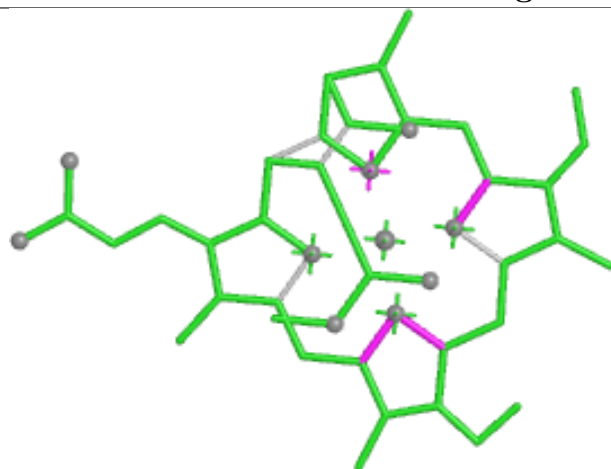
Rings



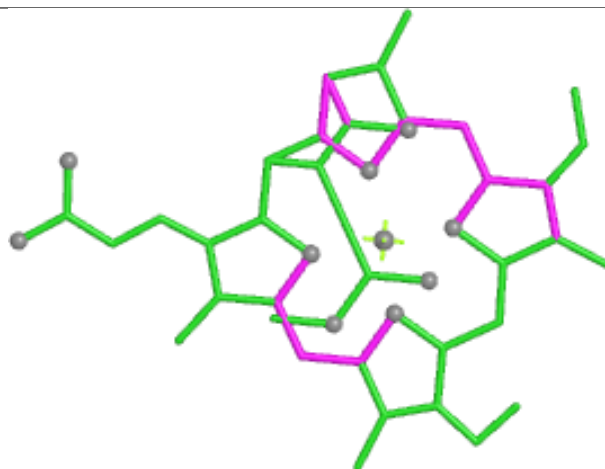




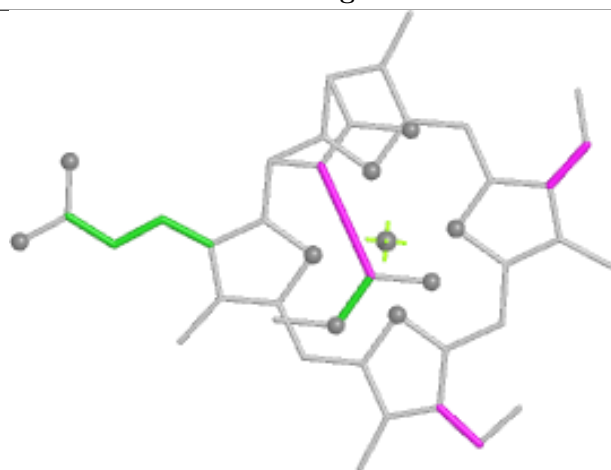
Ligand KC2 U 201



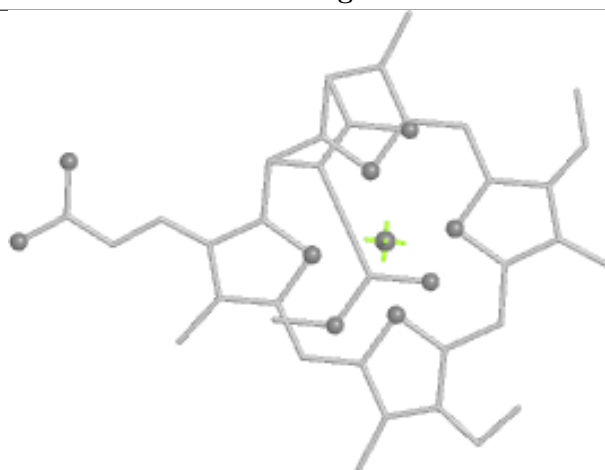
Bond lengths



Bond angles

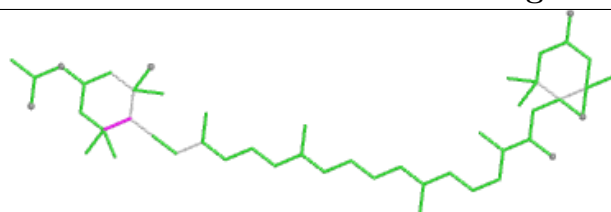


Torsions

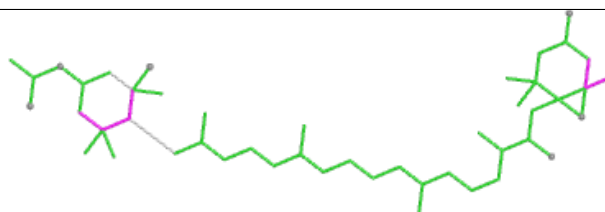


Rings

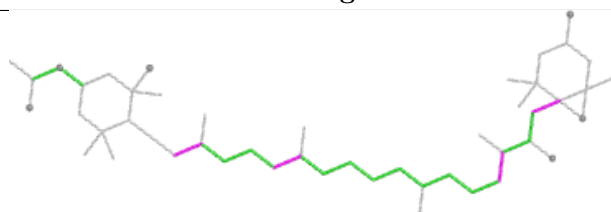
Ligand A86 t 310



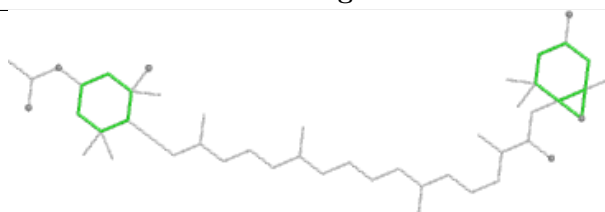
Bond lengths



Bond angles

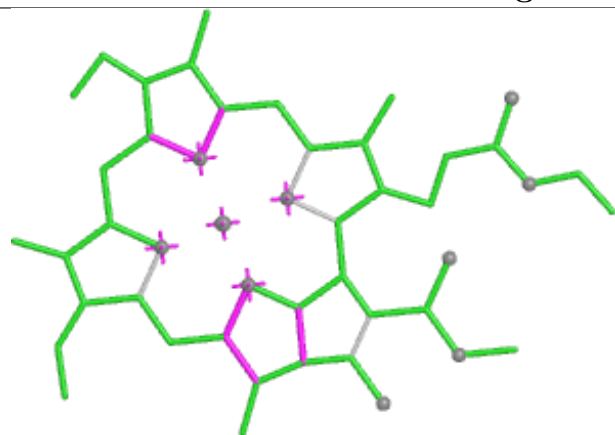


Torsions

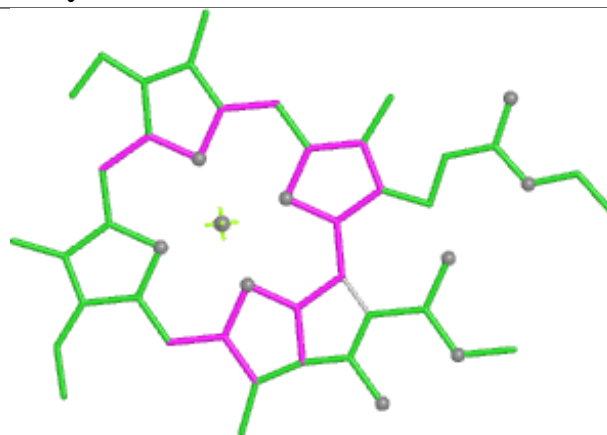


Rings

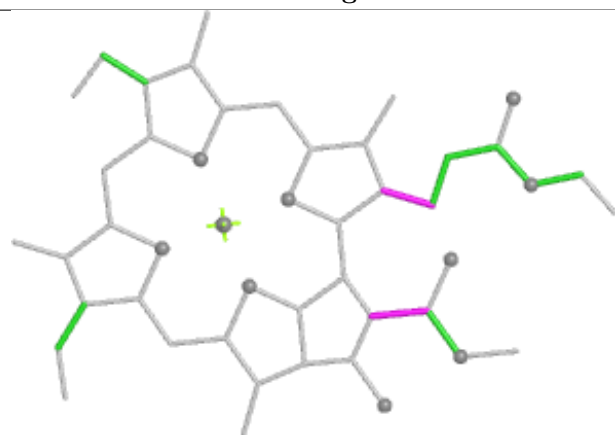
Ligand CLA Q 207



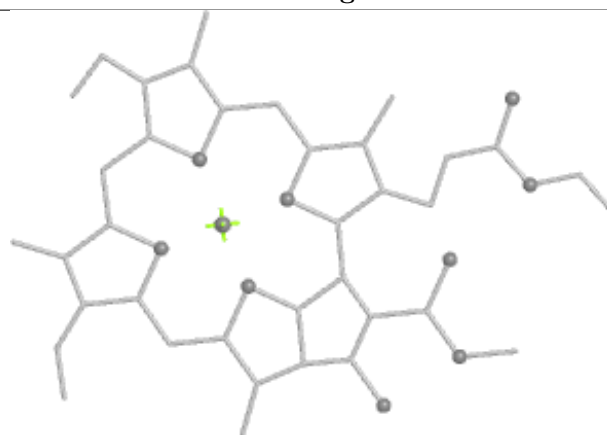
Bond lengths



Bond angles

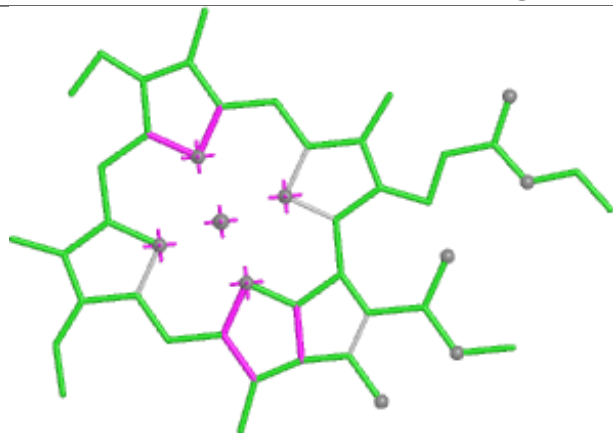


Torsions

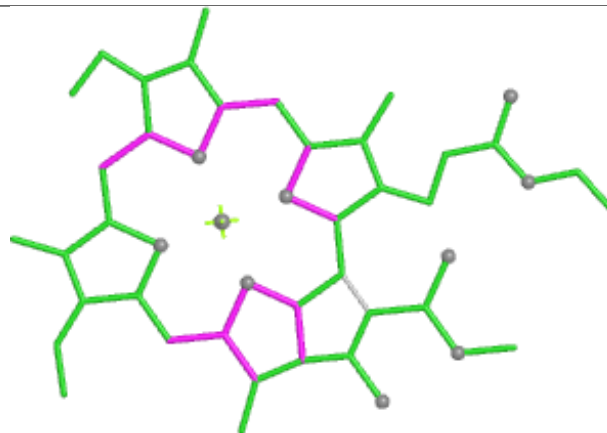


Rings

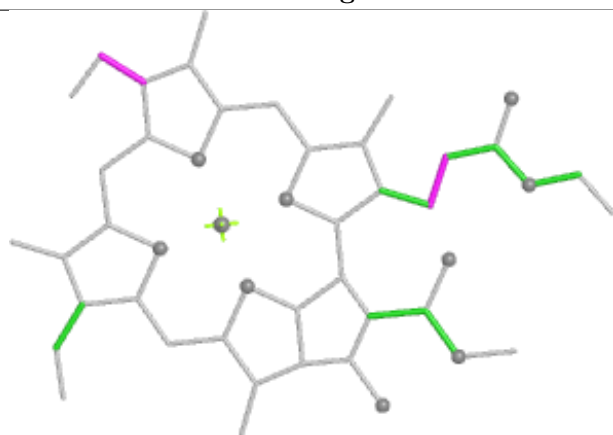
Ligand CLA H 311



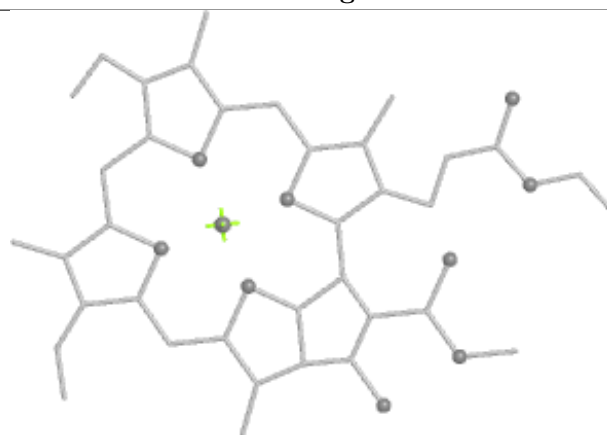
Bond lengths



Bond angles

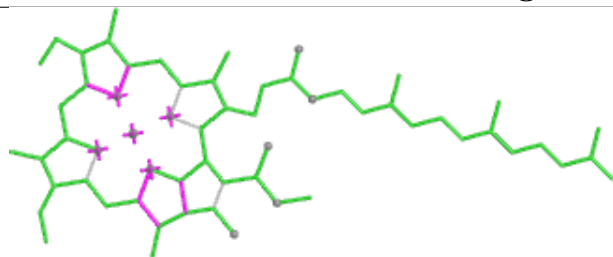


Torsions

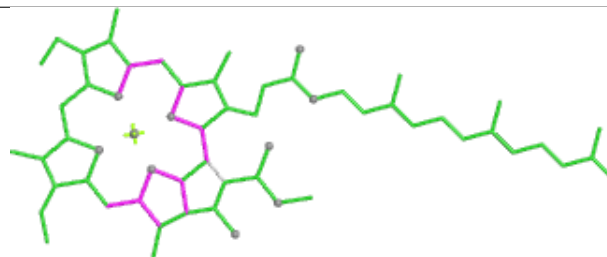


Rings

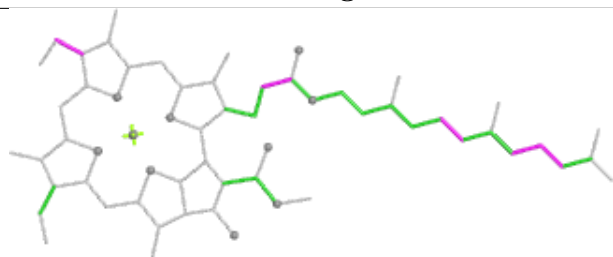
Ligand CLA x 308



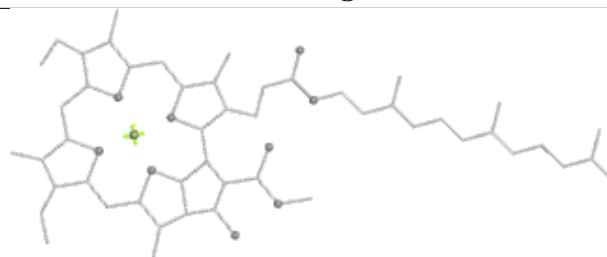
Bond lengths



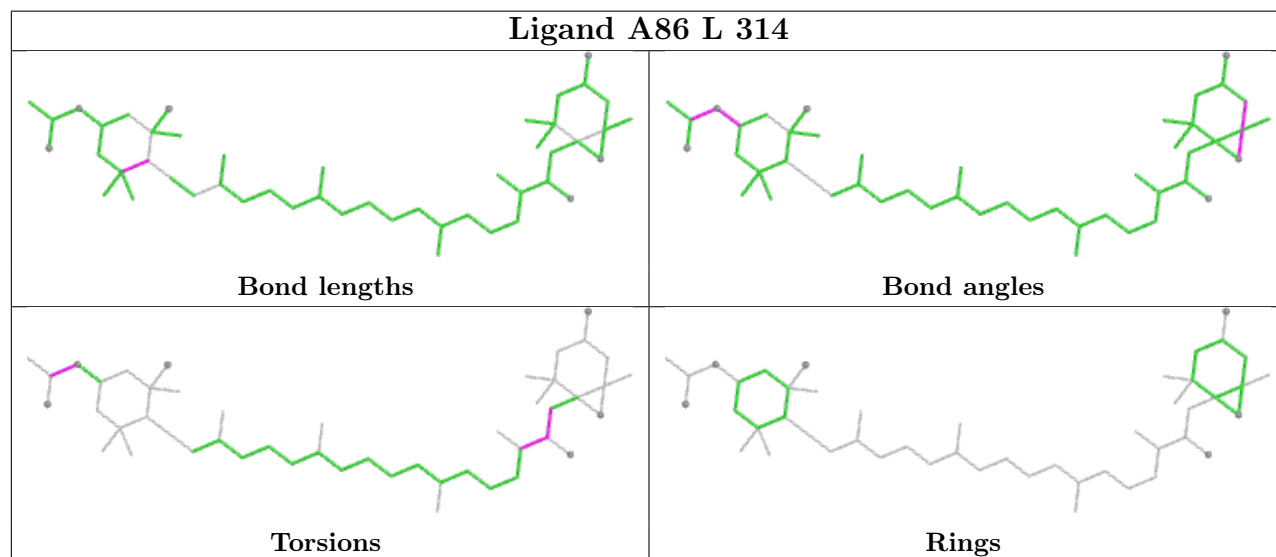
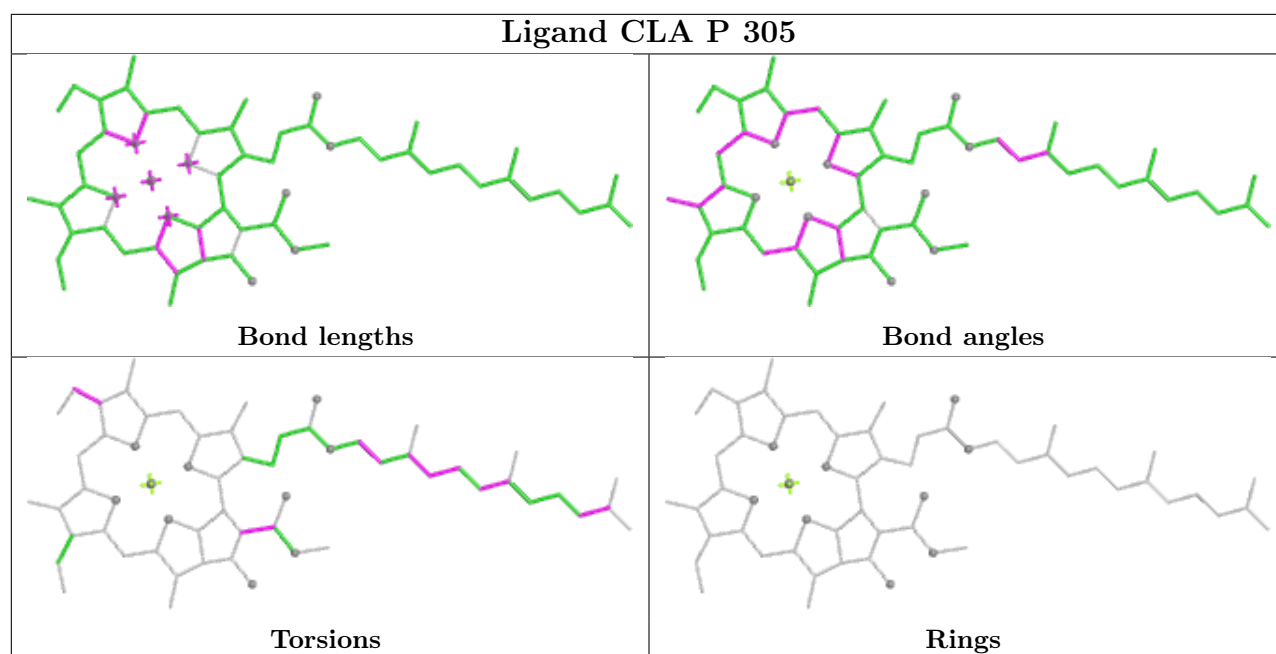
Bond angles



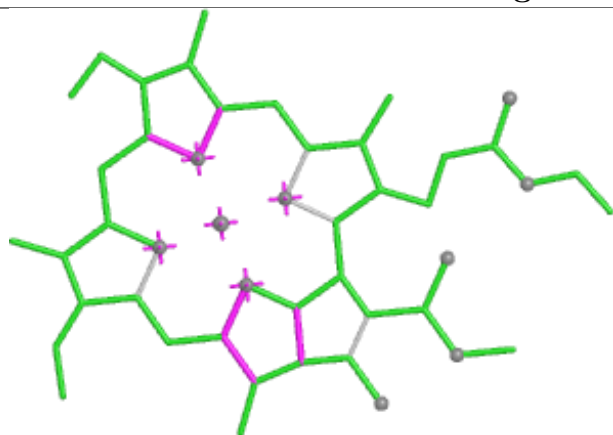
Torsions



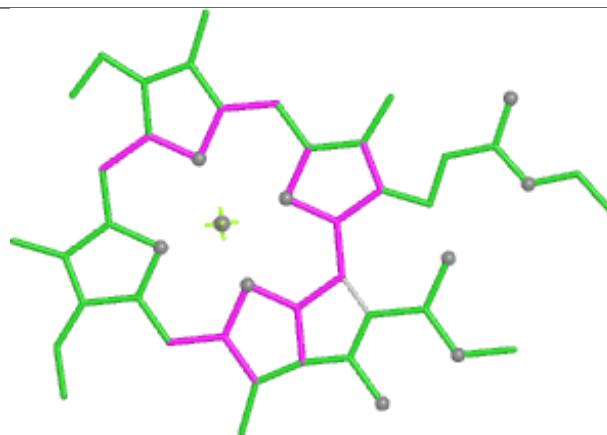
Rings



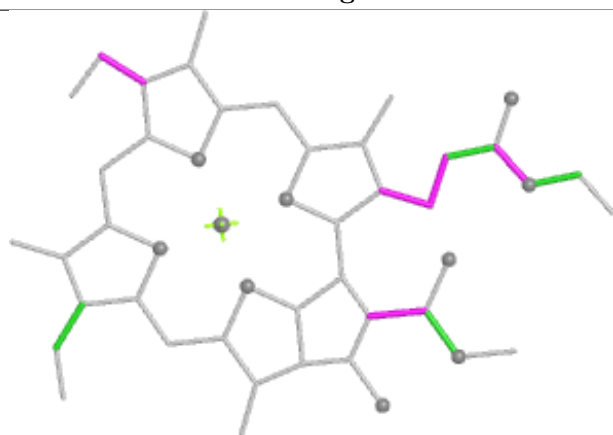
Ligand CLA Y 313



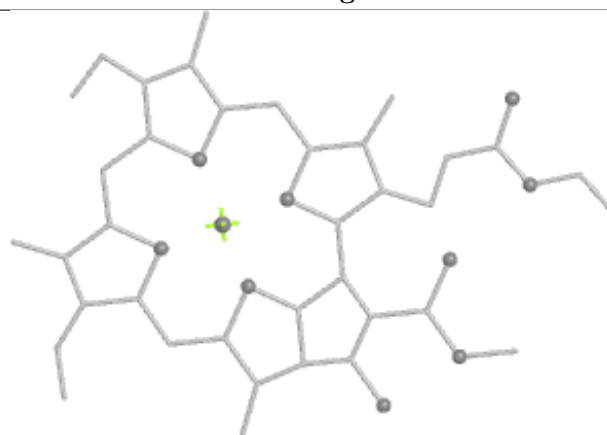
Bond lengths



Bond angles



Torsions

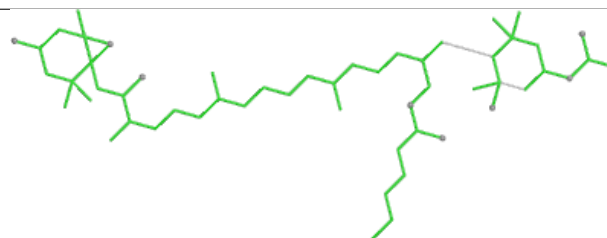


Rings

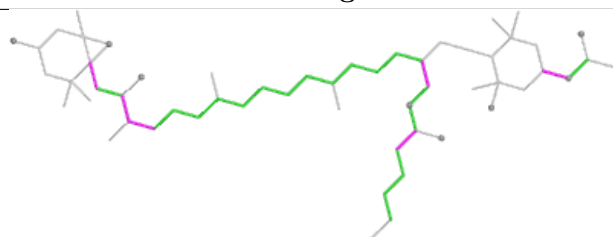
Ligand A1EB1 P 301



Bond lengths



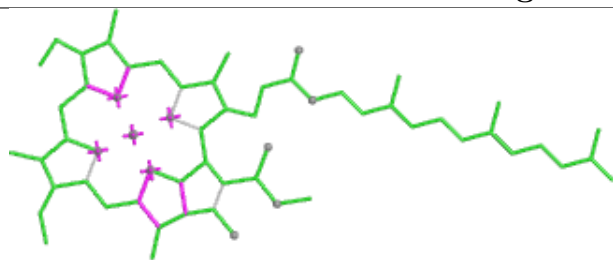
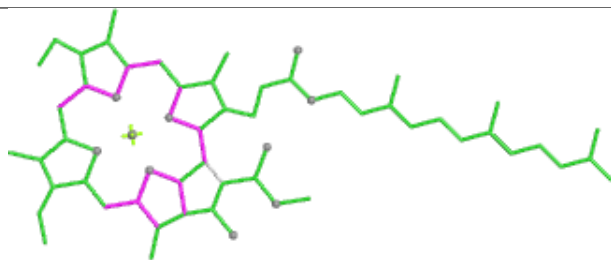
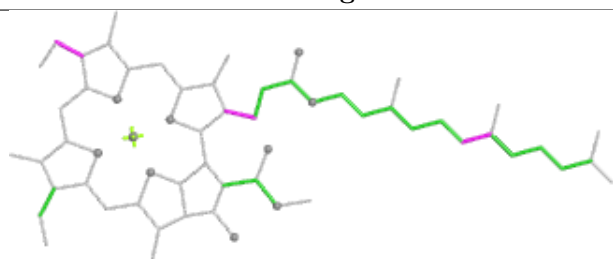
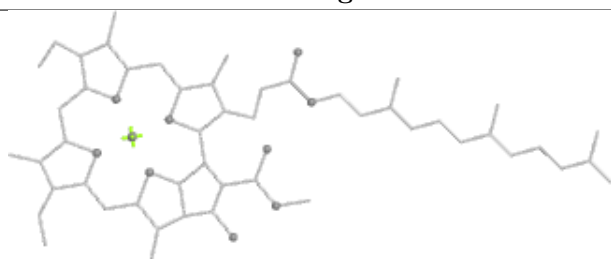
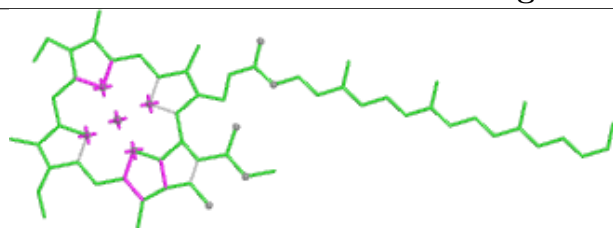
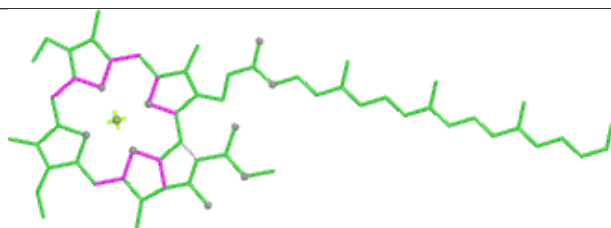
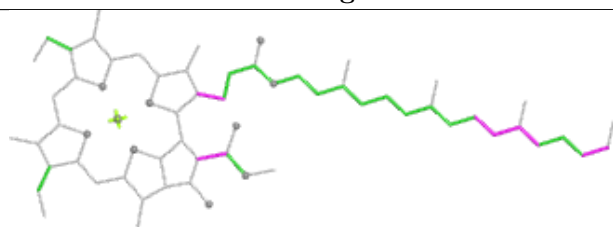
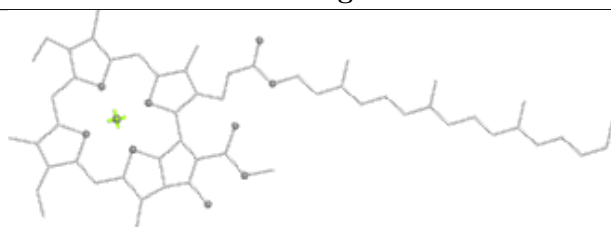
Bond angles

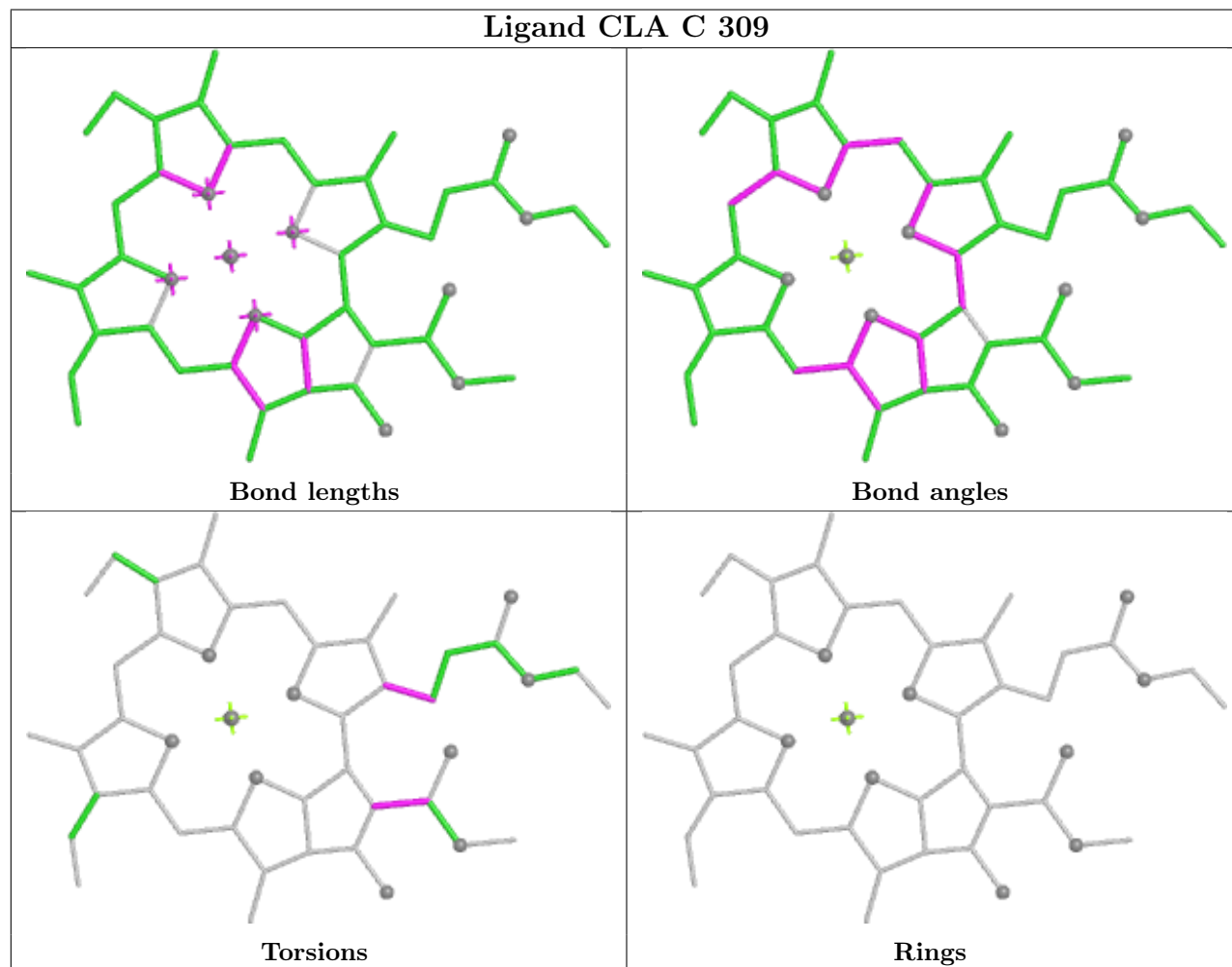
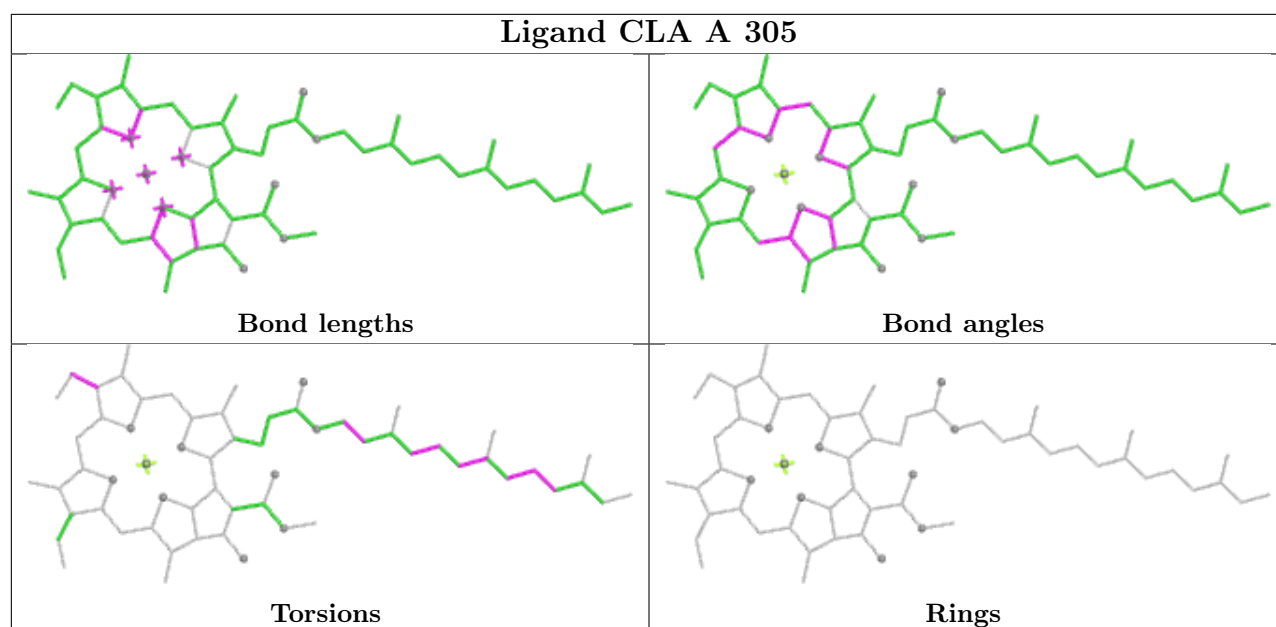


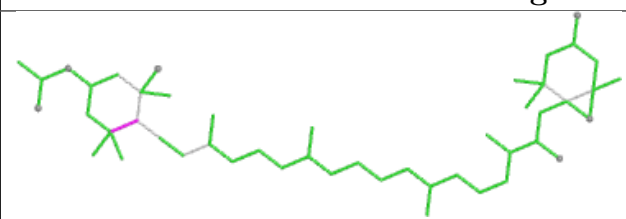
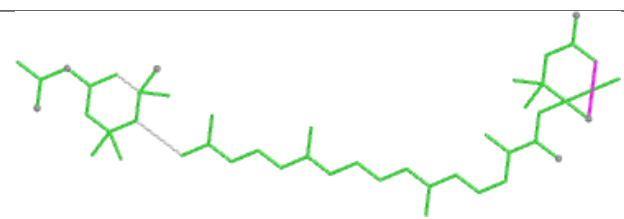
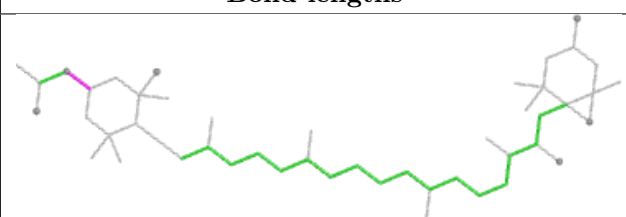
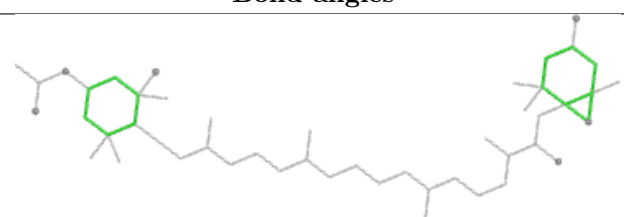
Torsions

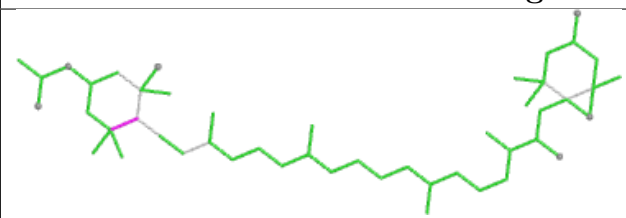
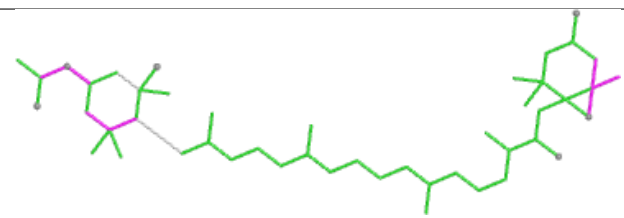
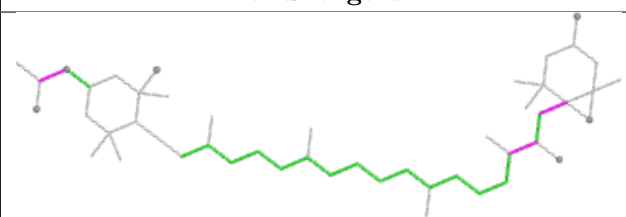
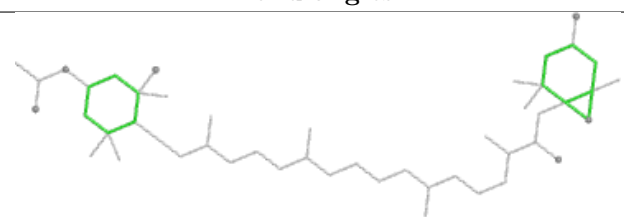


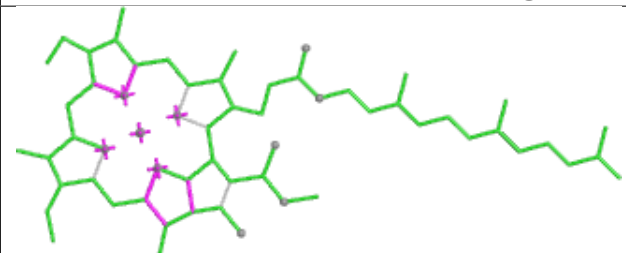
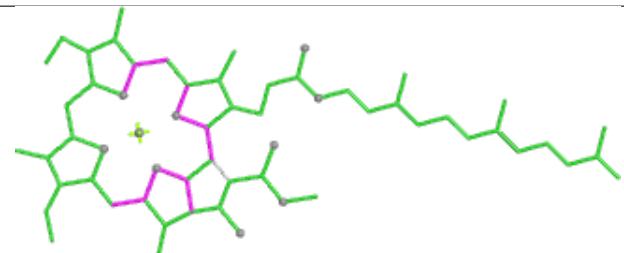
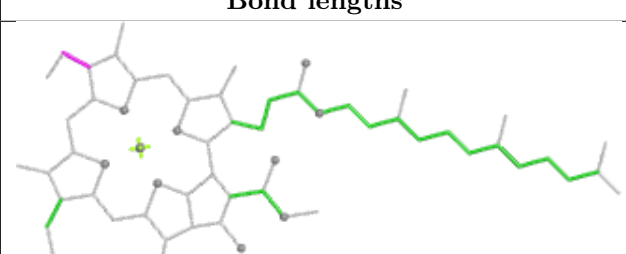
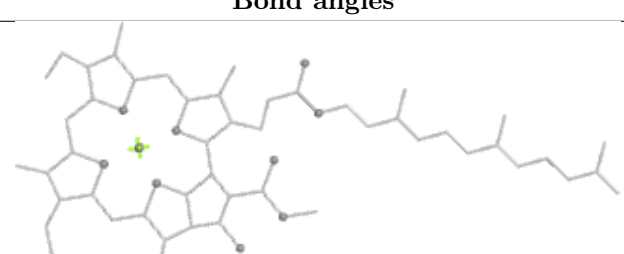
Rings

Ligand CLA Z 304**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA b 826****Bond lengths****Bond angles****Torsions****Rings**

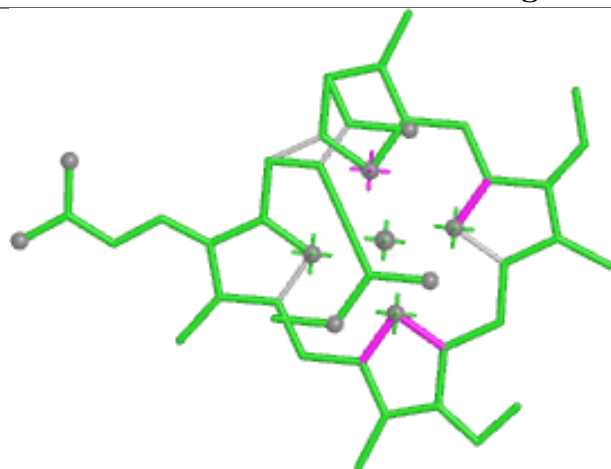


Ligand A86 S 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

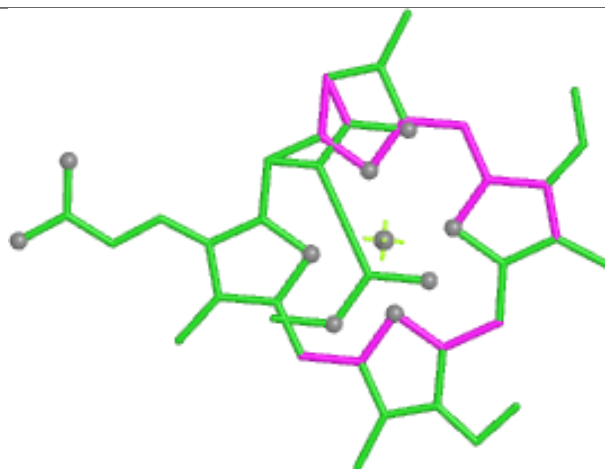
Ligand A86 H 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

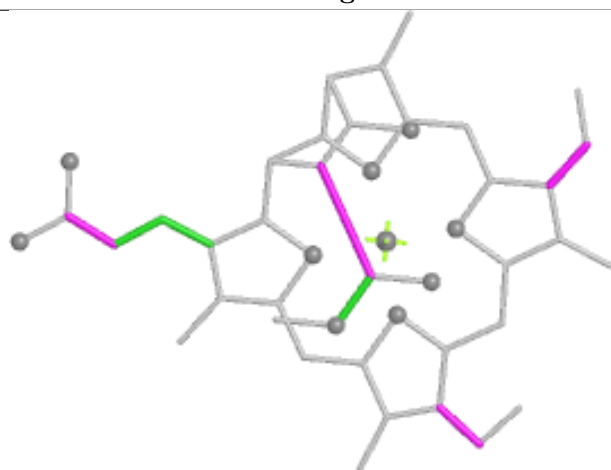
Ligand KC2 z 310



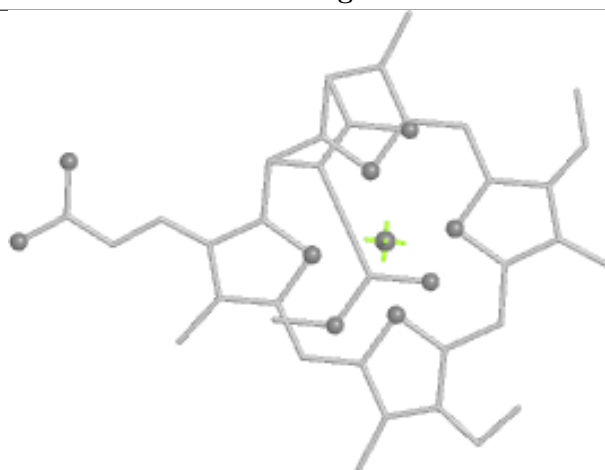
Bond lengths



Bond angles

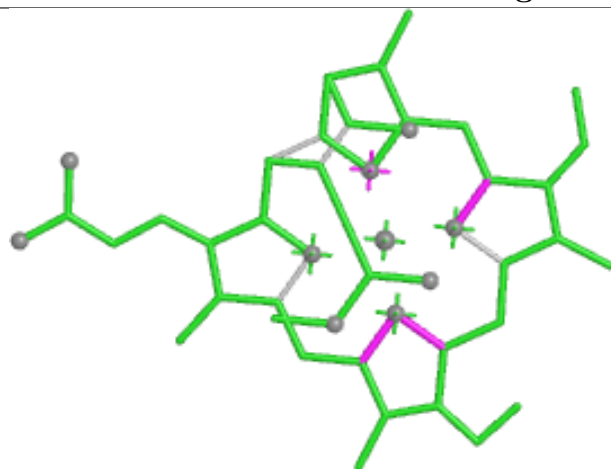


Torsions

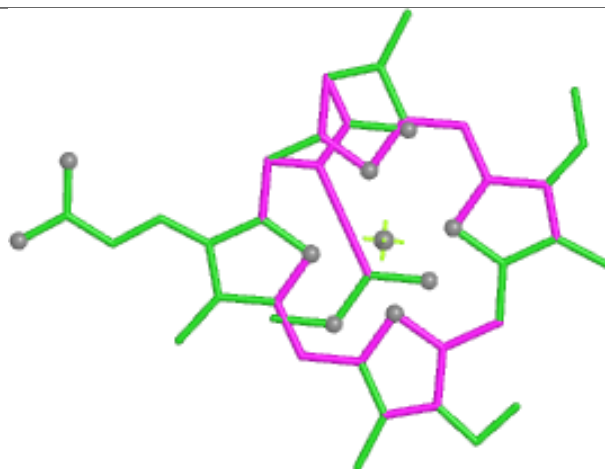


Rings

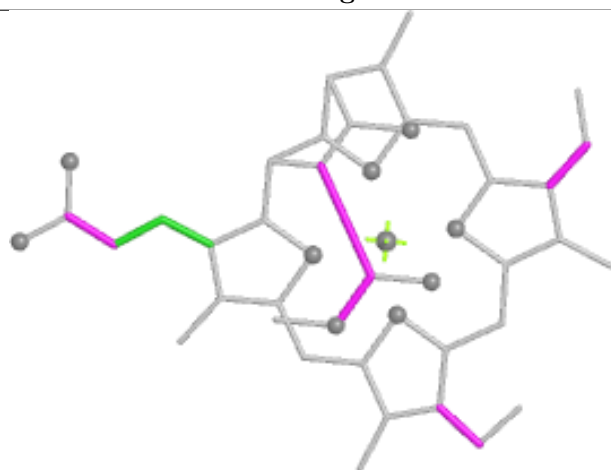
Ligand KC2 Y 314



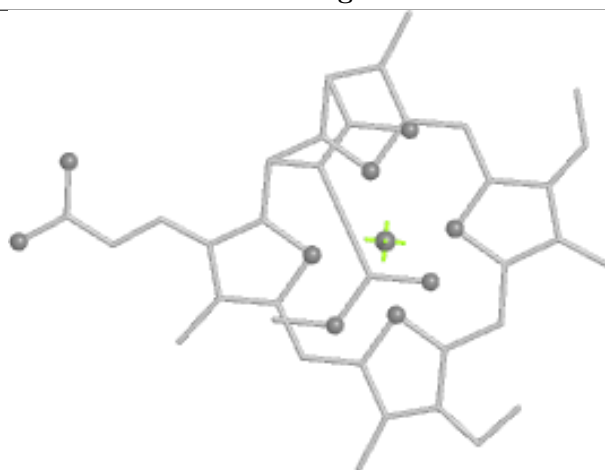
Bond lengths



Bond angles

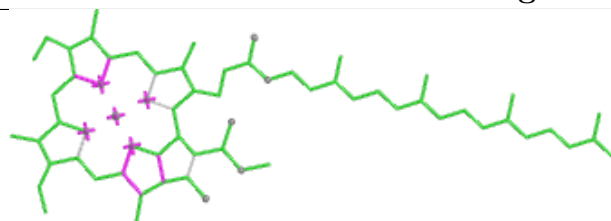


Torsions

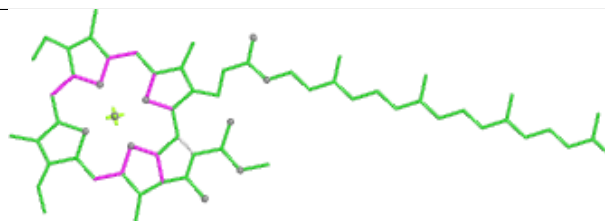


Rings

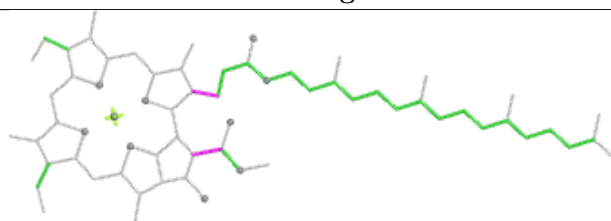
Ligand CLA a 827



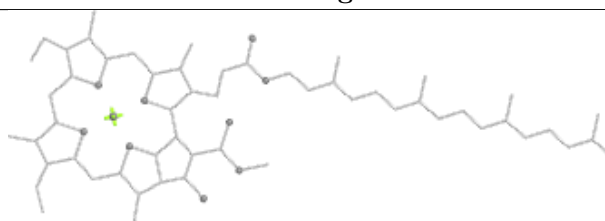
Bond lengths



Bond angles

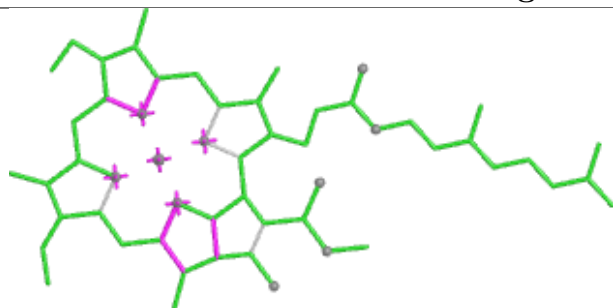


Torsions

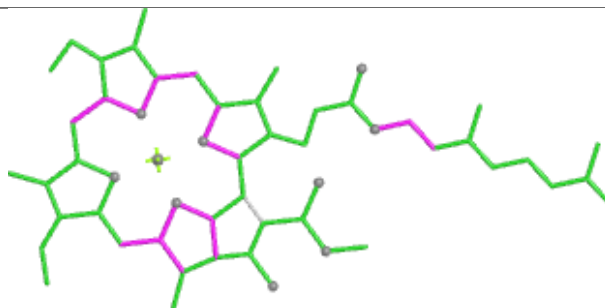


Rings

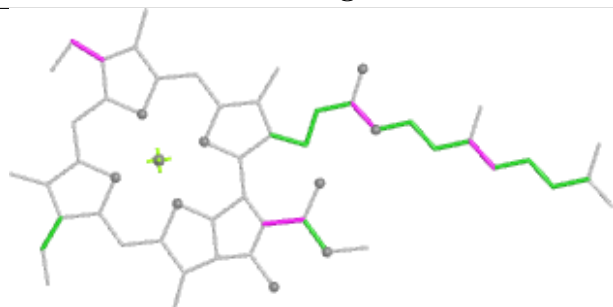
Ligand CLA k 201



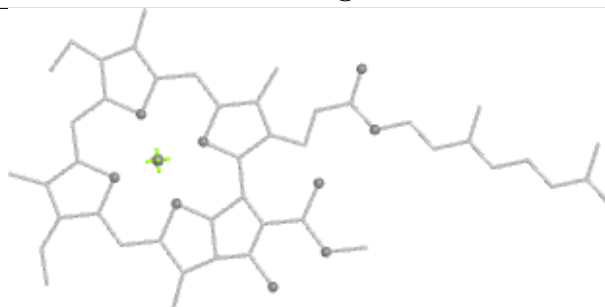
Bond lengths



Bond angles

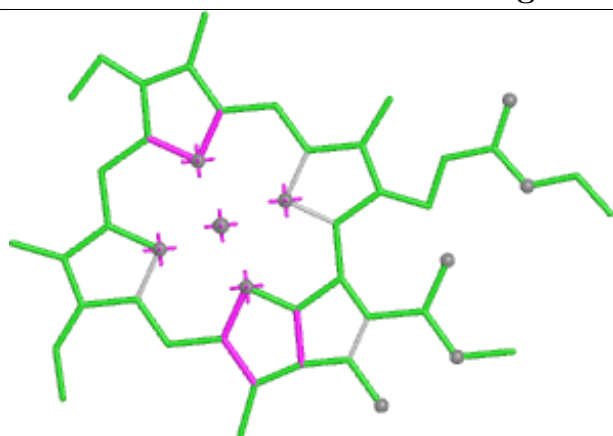


Torsions

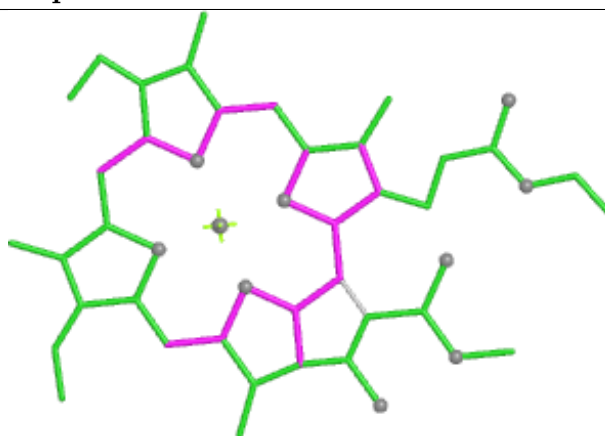


Rings

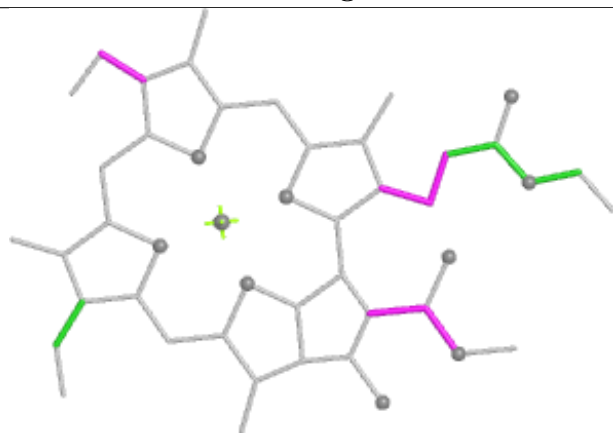
Ligand CLA p 314



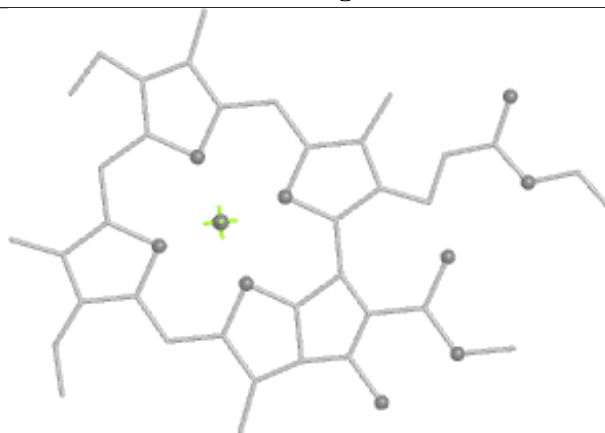
Bond lengths



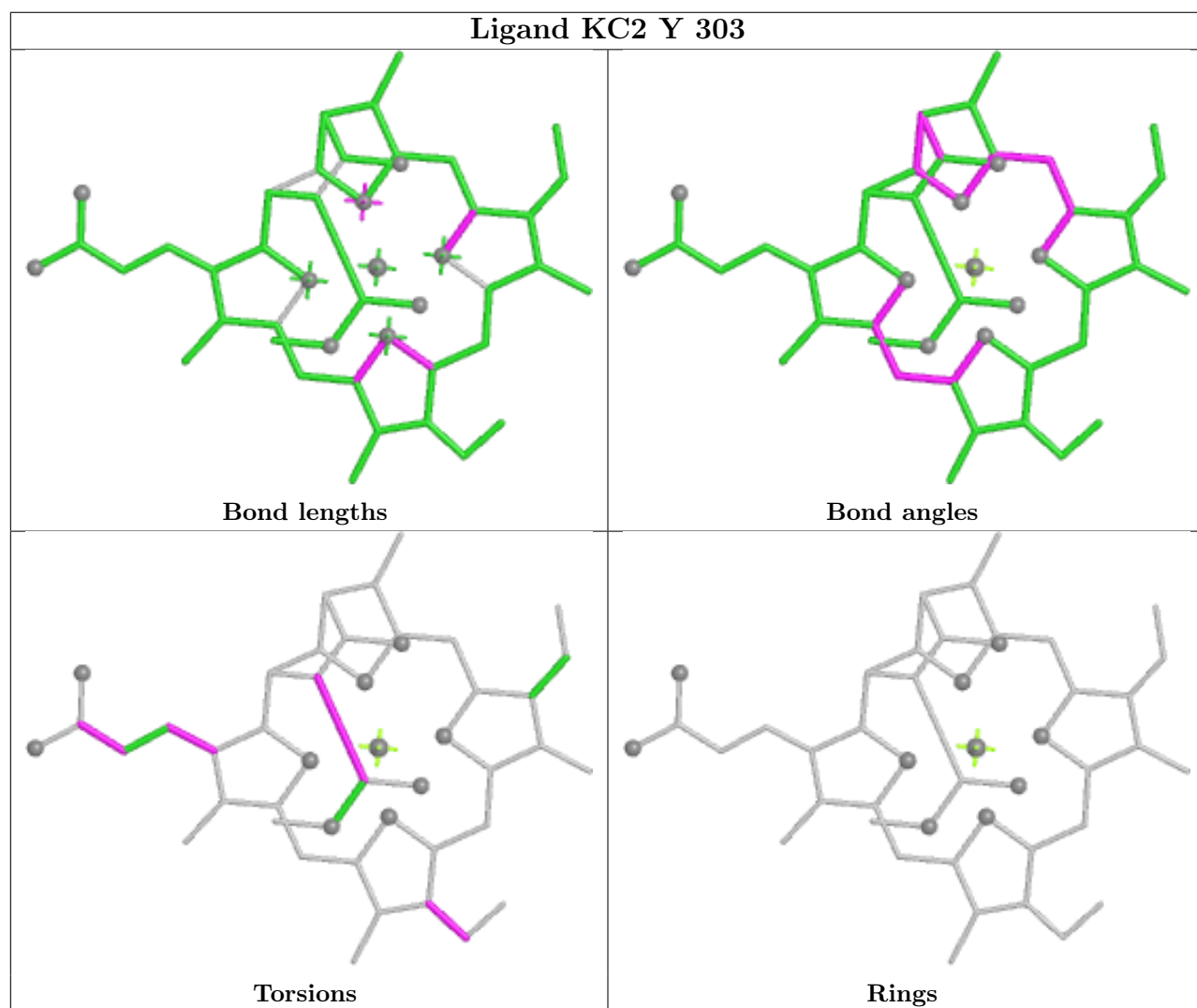
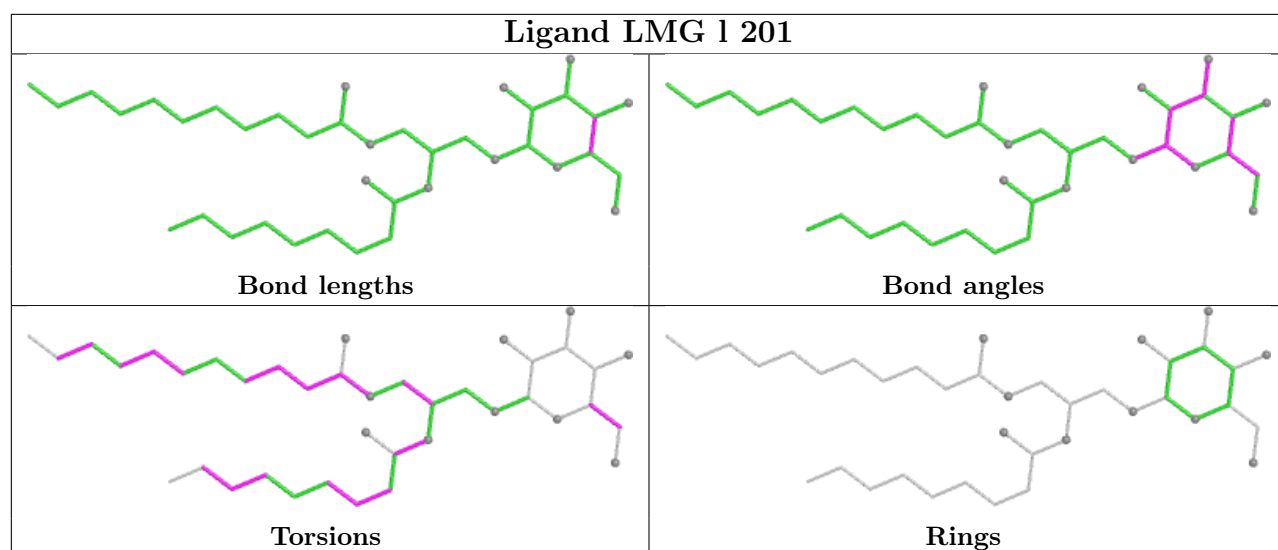
Bond angles

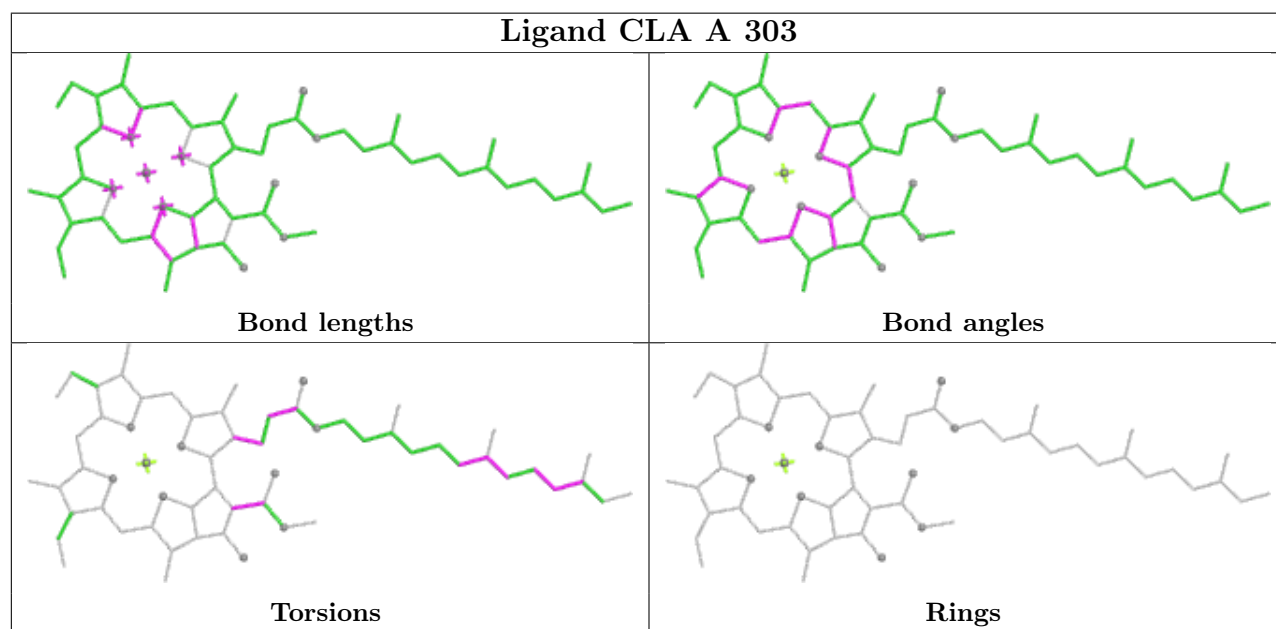
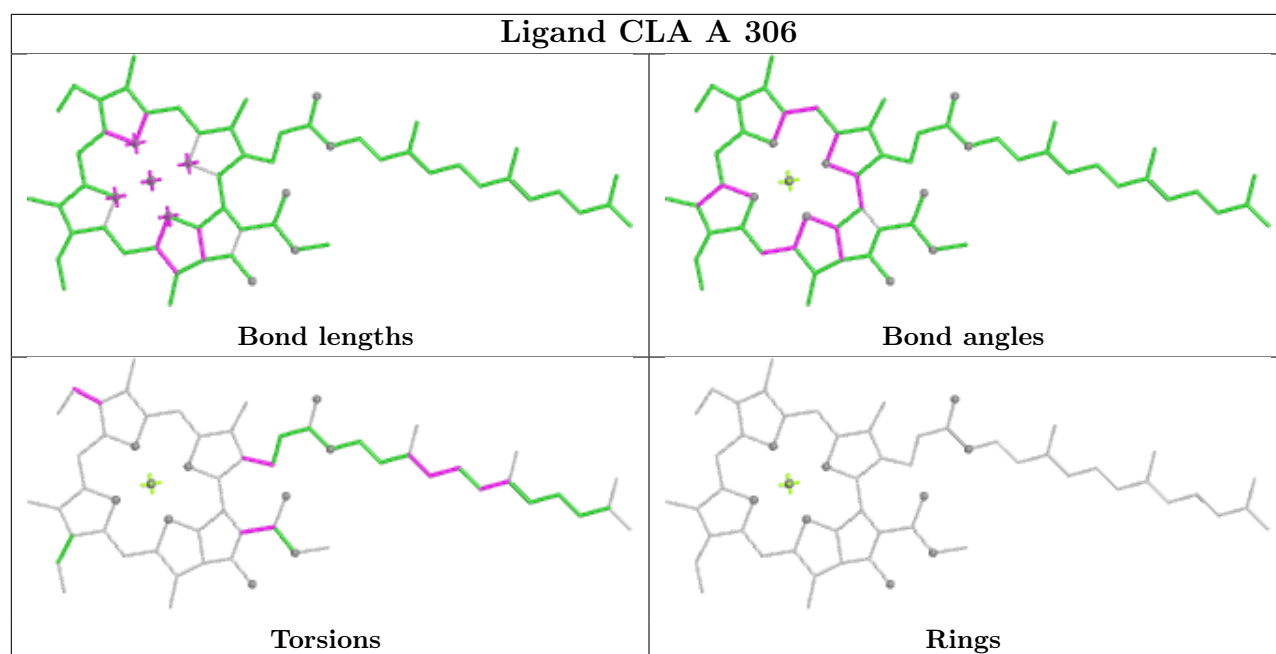


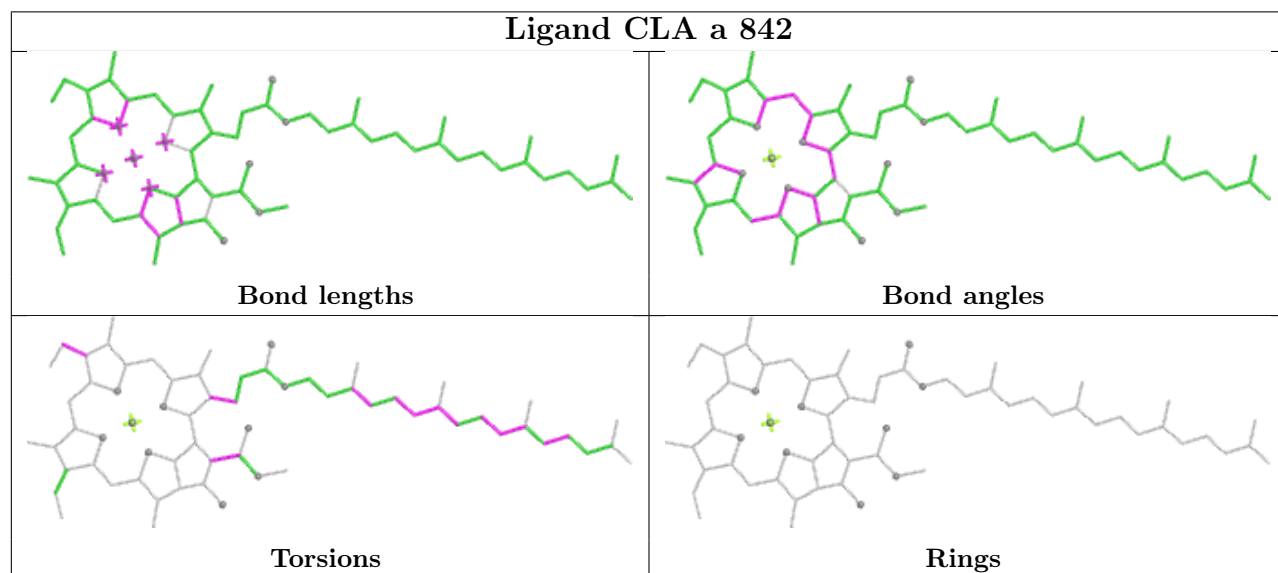
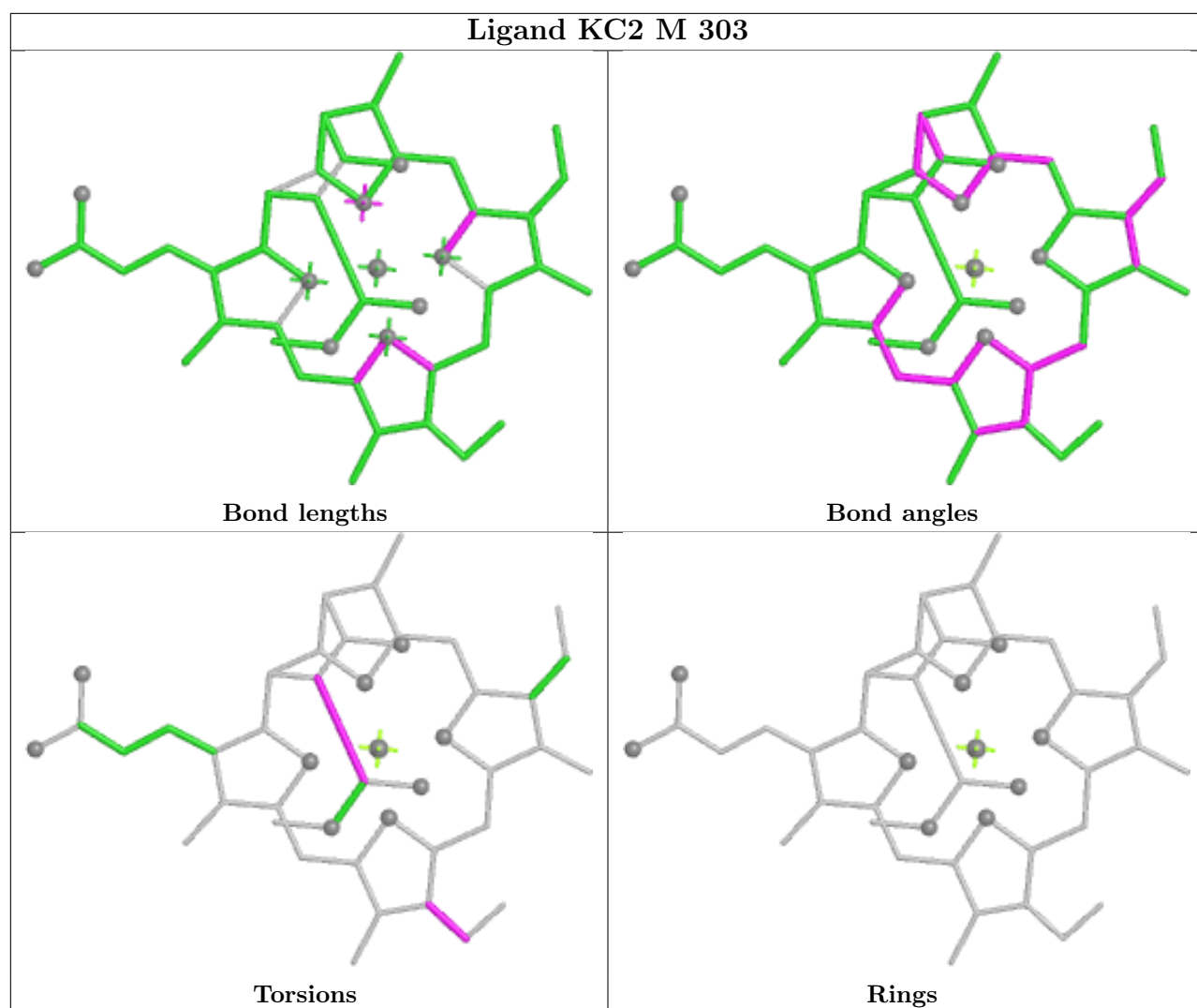
Torsions

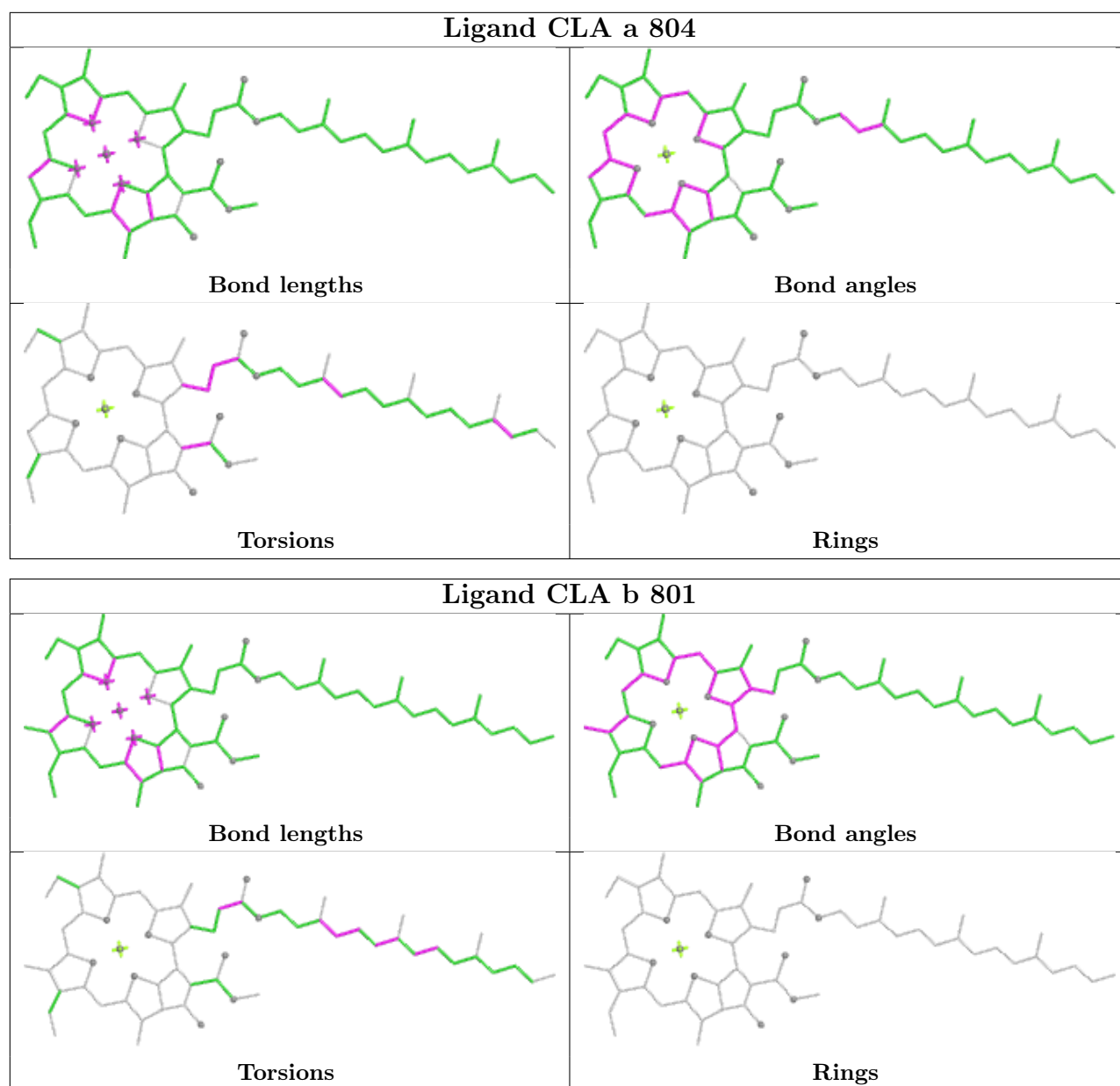


Rings

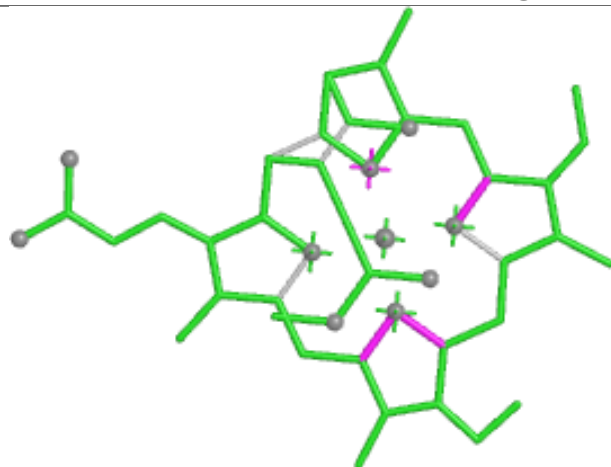




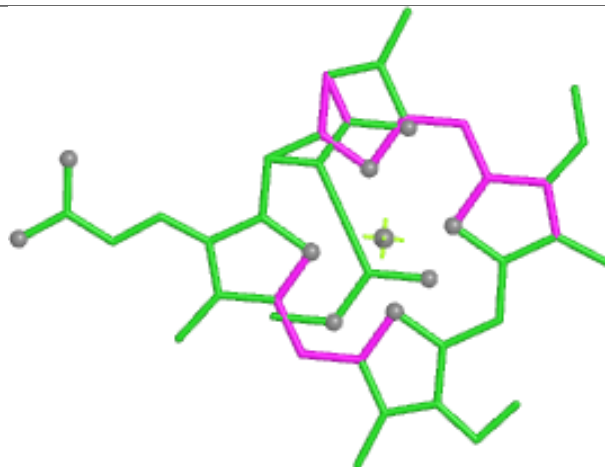




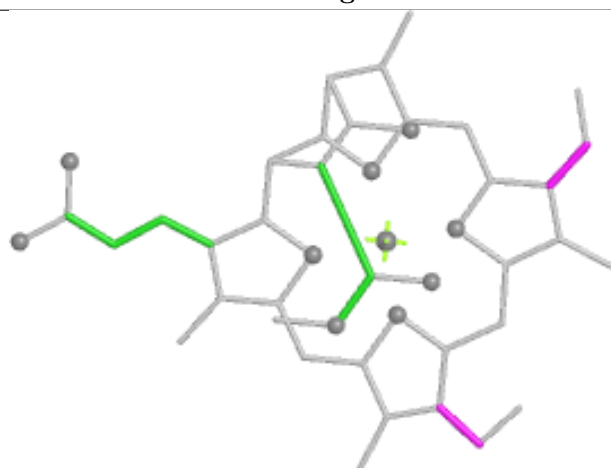
Ligand KC2 N 313



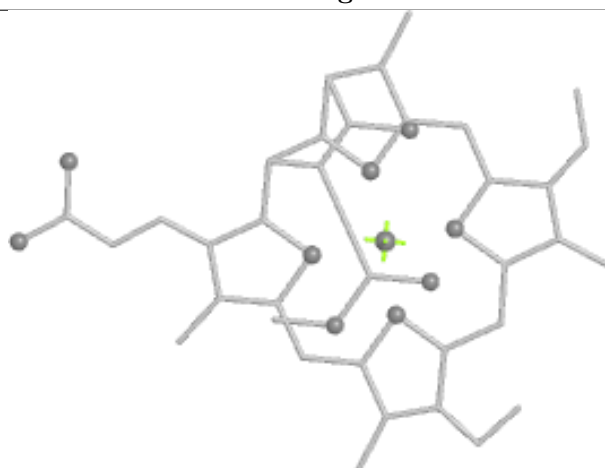
Bond lengths



Bond angles

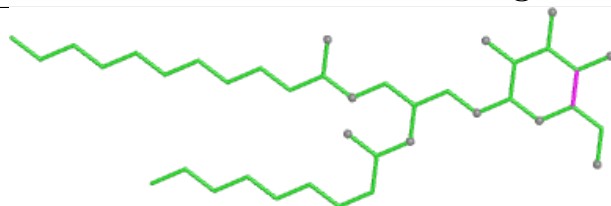


Torsions

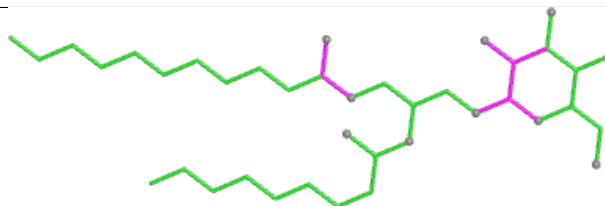


Rings

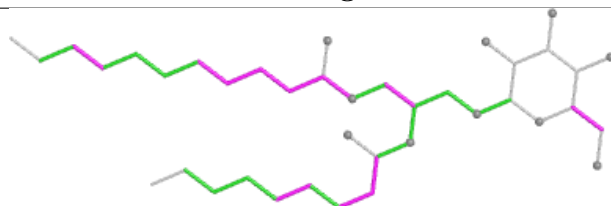
Ligand LMG x 301



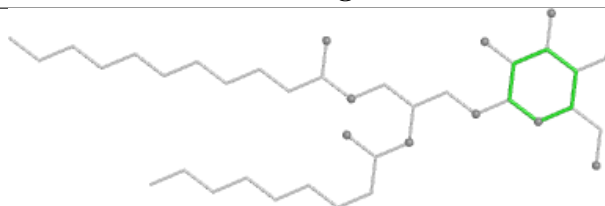
Bond lengths



Bond angles

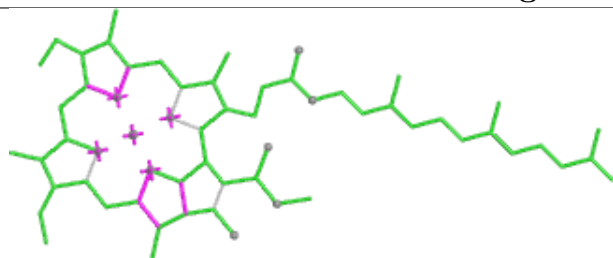


Torsions

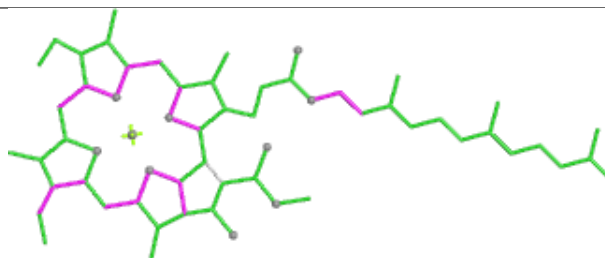


Rings

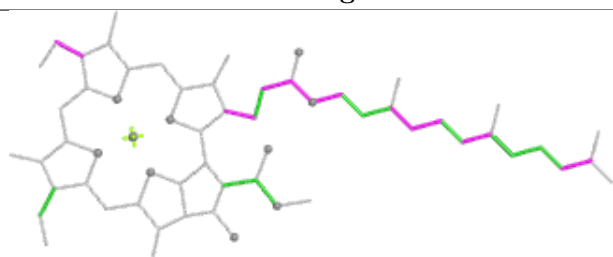
Ligand CLA z 305



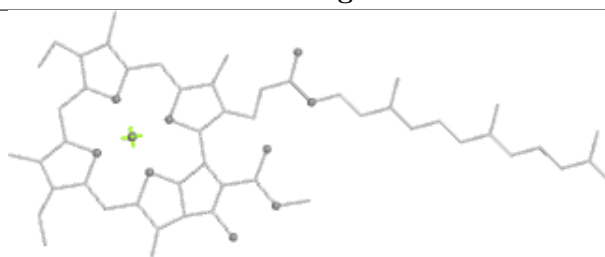
Bond lengths



Bond angles

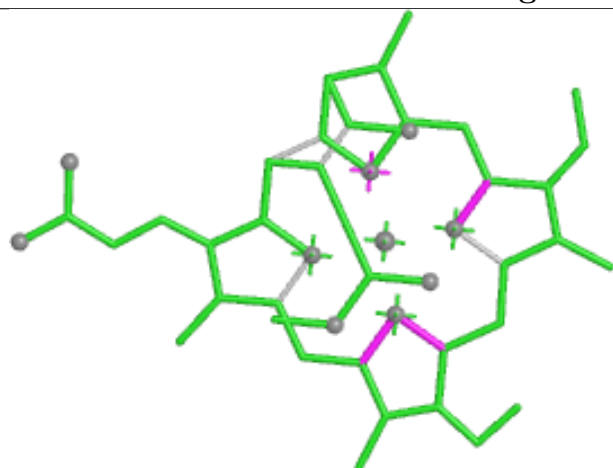


Torsions

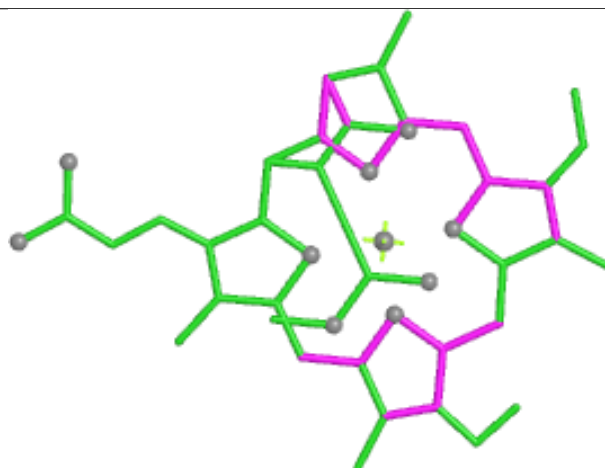


Rings

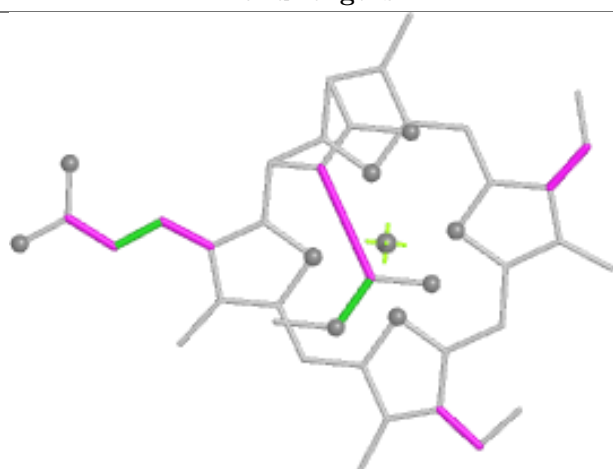
Ligand KC2 S 310



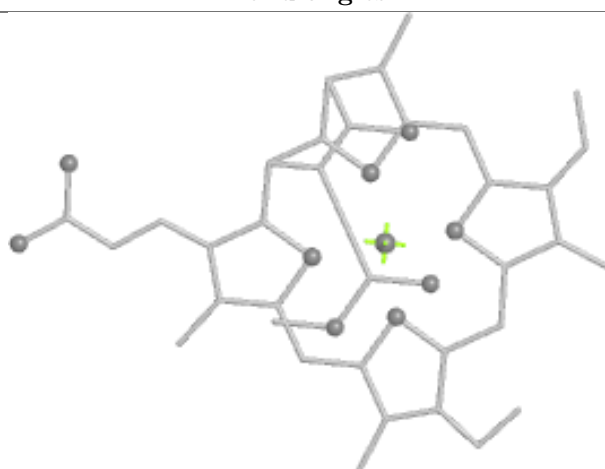
Bond lengths



Bond angles

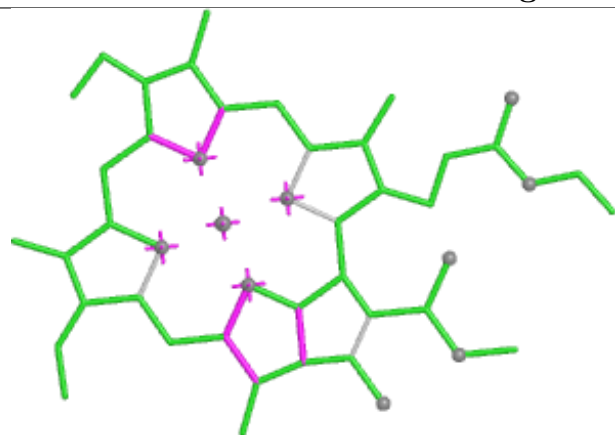


Torsions

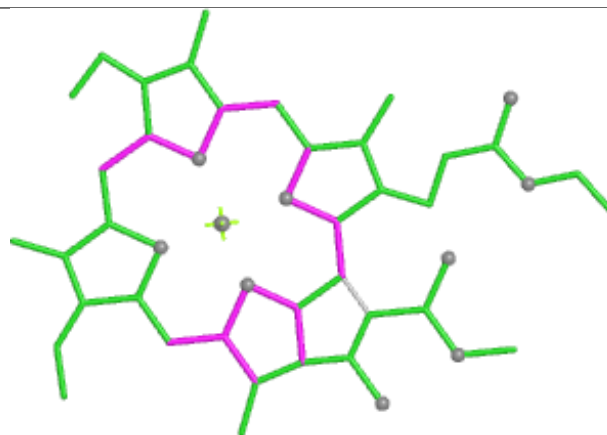


Rings

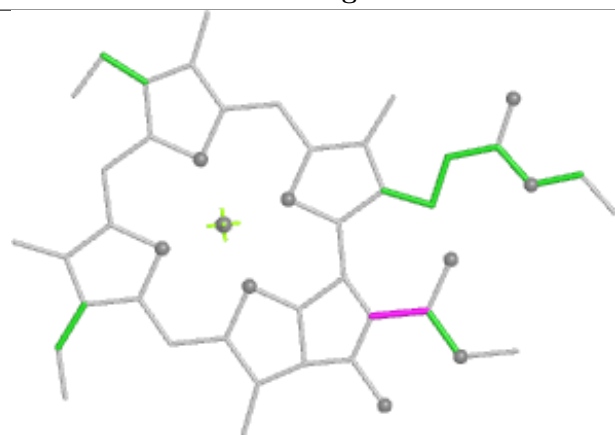
Ligand CLA u 305



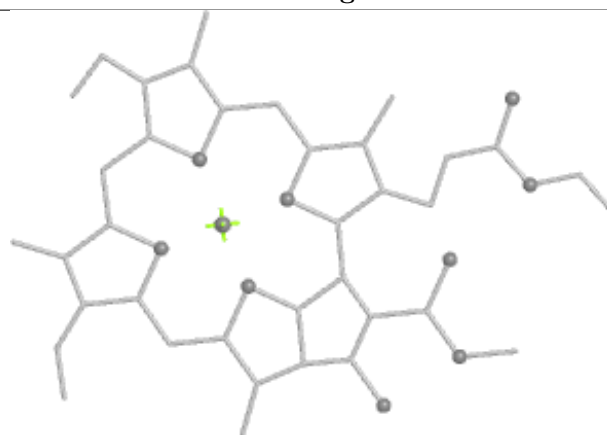
Bond lengths



Bond angles

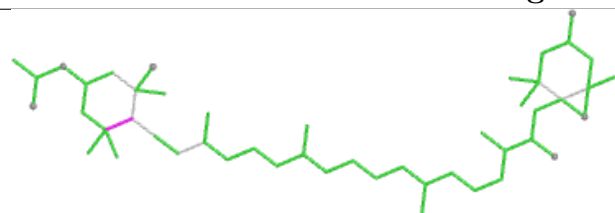


Torsions

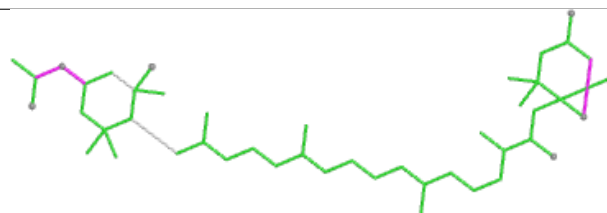


Rings

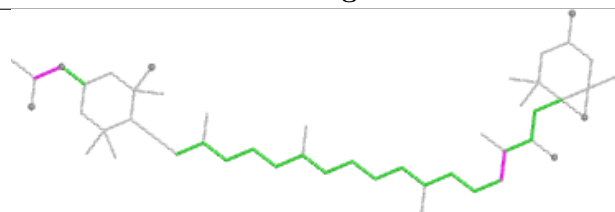
Ligand A86 z 318



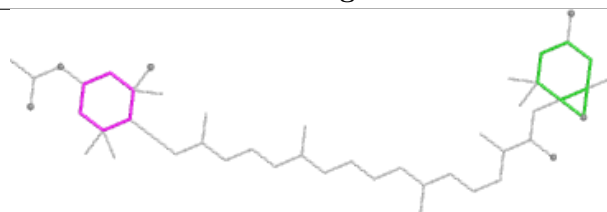
Bond lengths



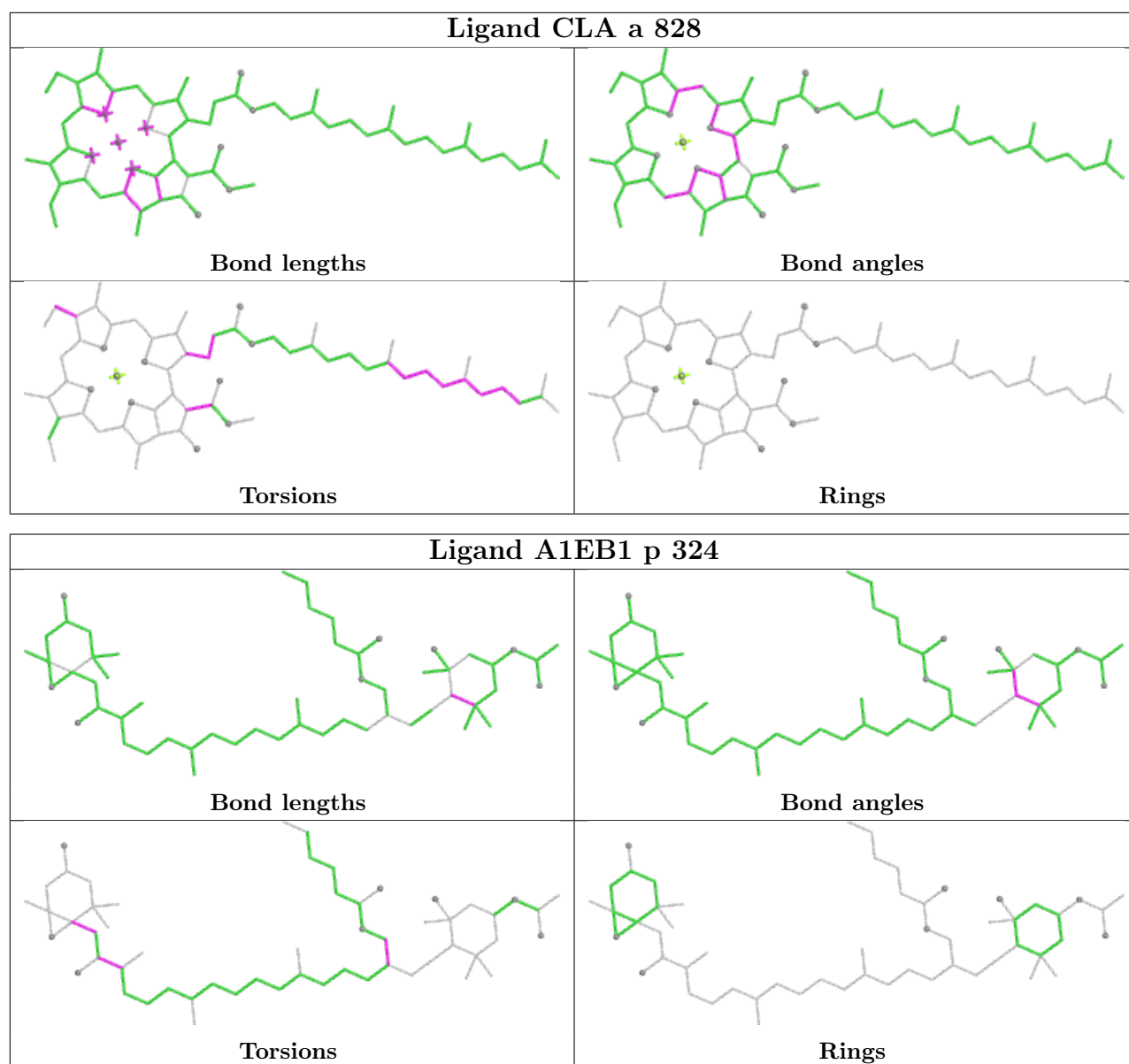
Bond angles

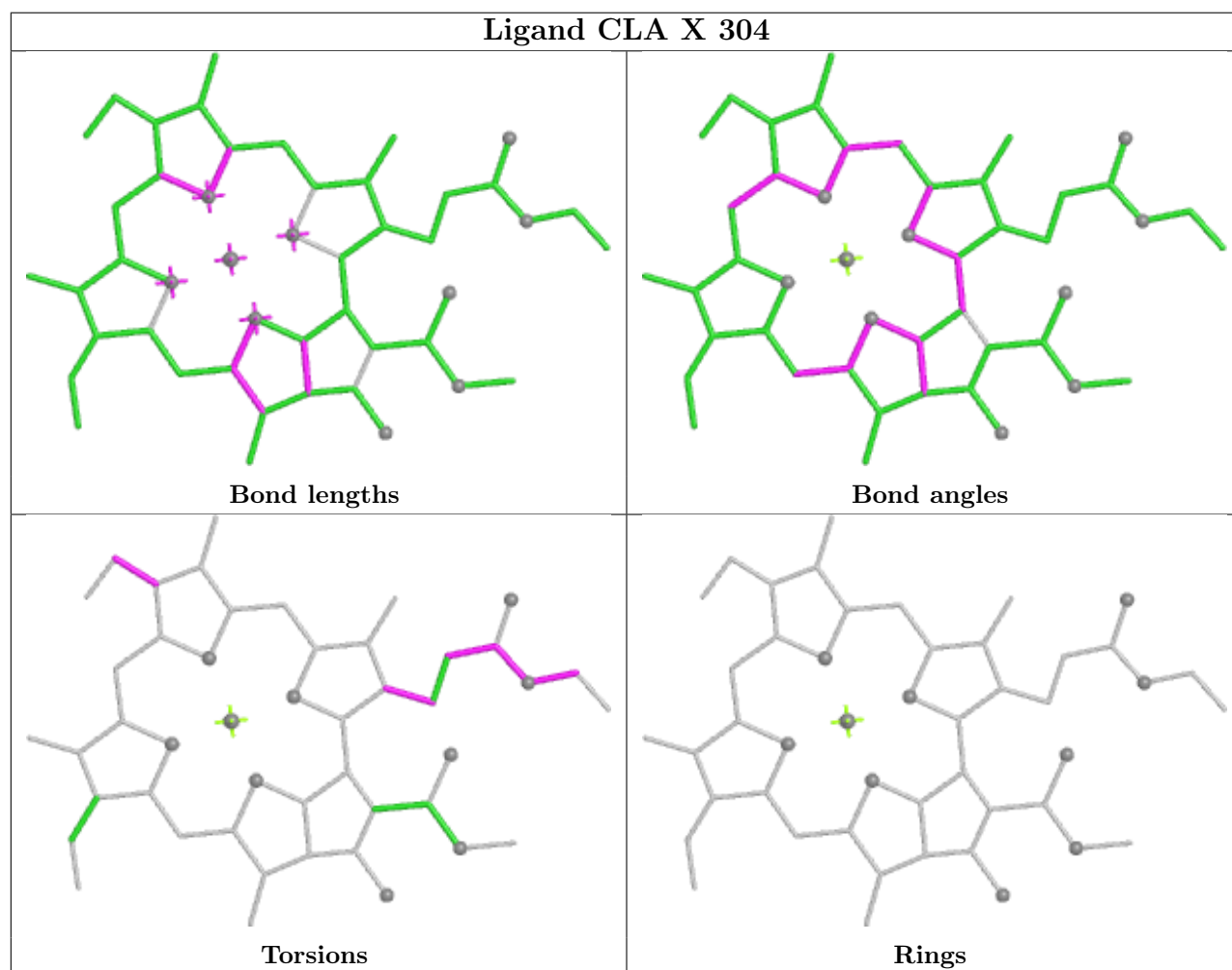
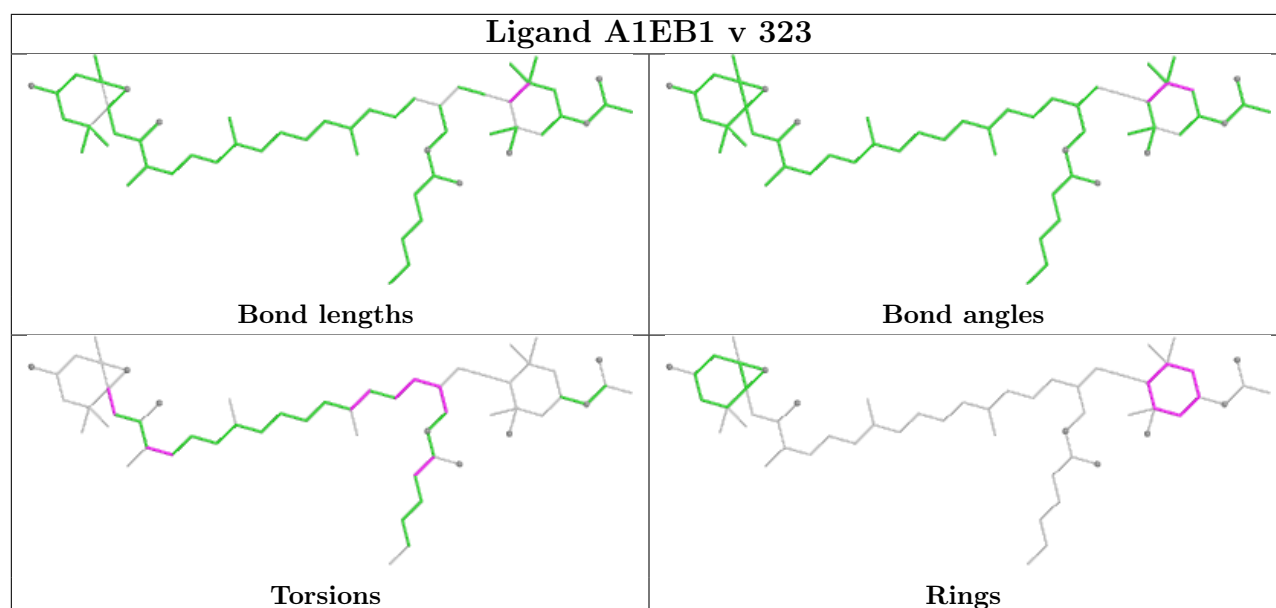


Torsions

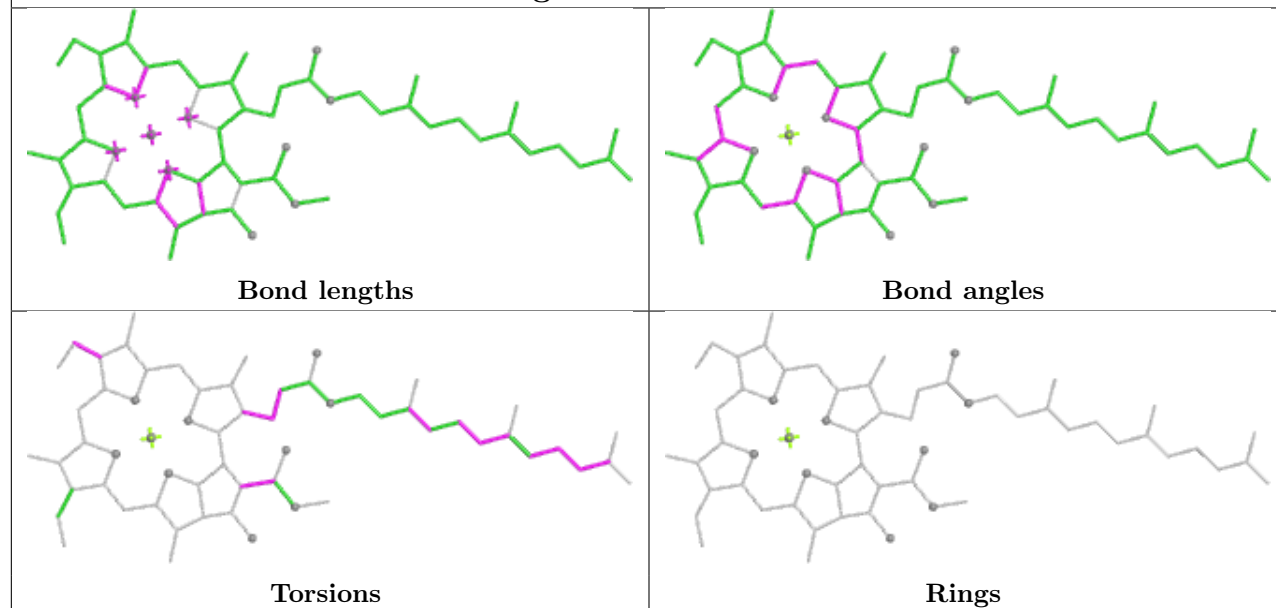


Rings

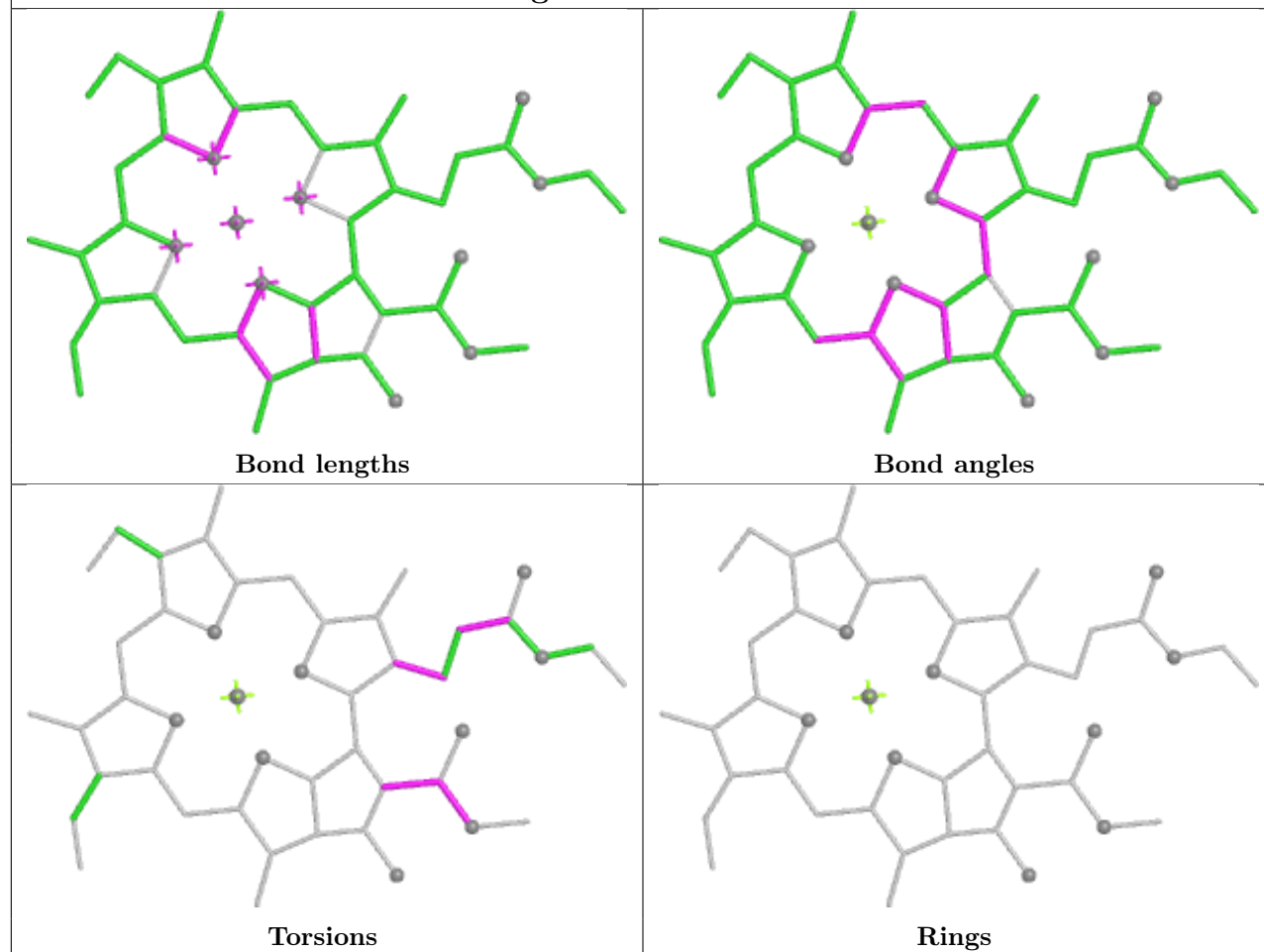




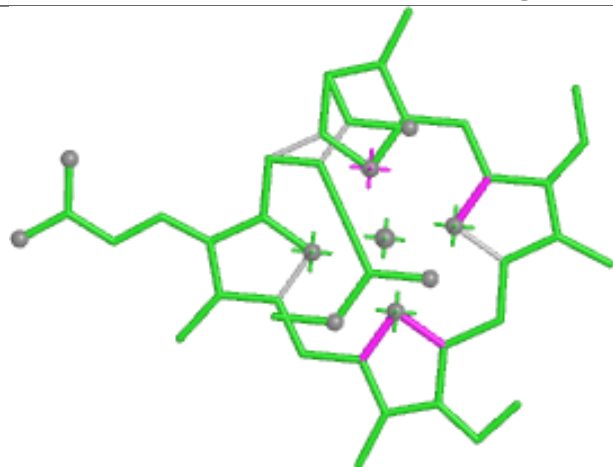
Ligand CLA P 312



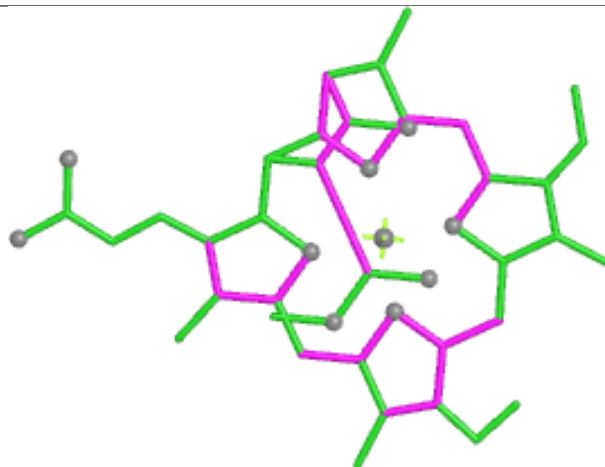
Ligand CLA o 312



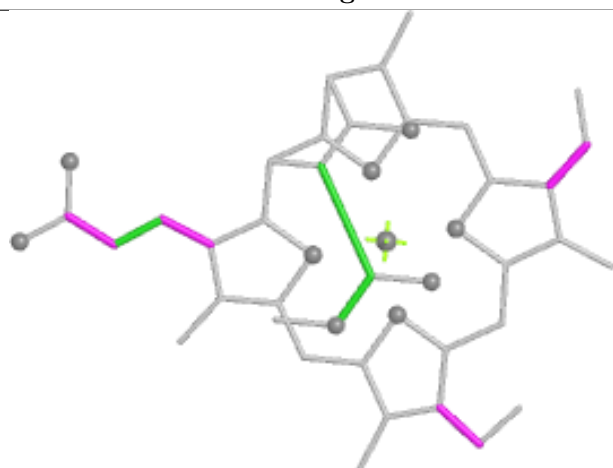
Ligand KC2 R 309



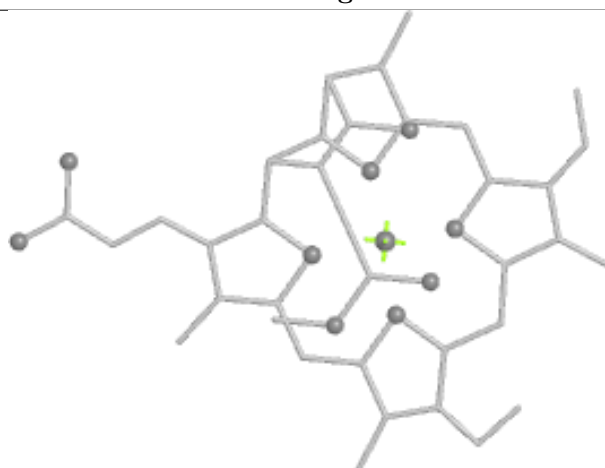
Bond lengths



Bond angles



Torsions



Rings

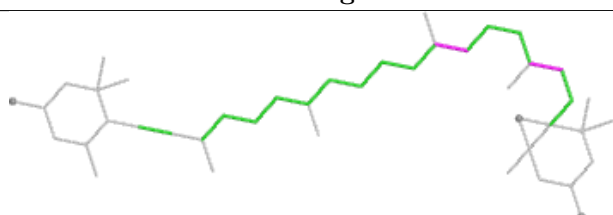
Ligand DD6 D 314



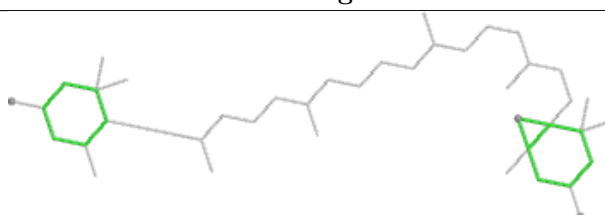
Bond lengths



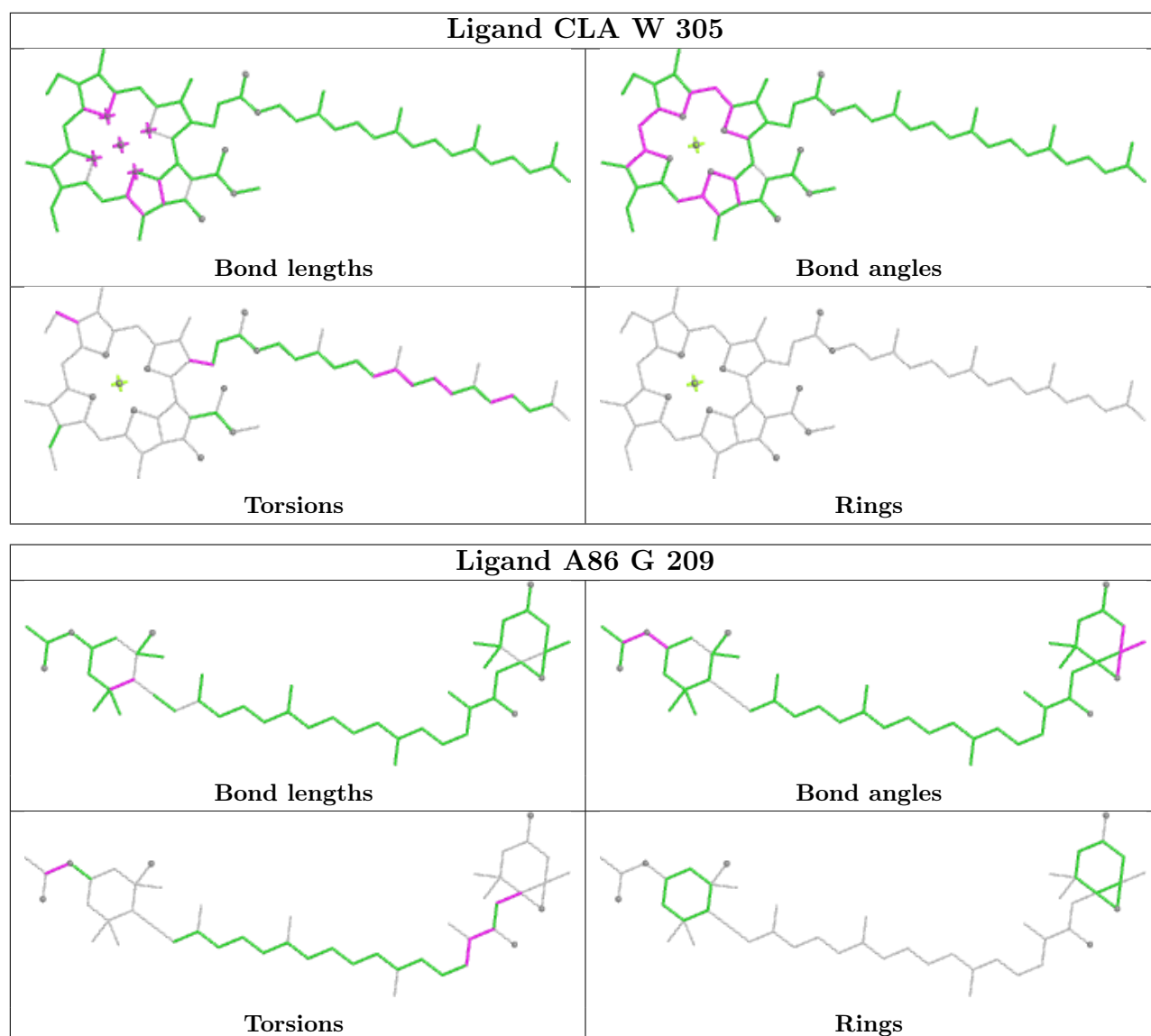
Bond angles



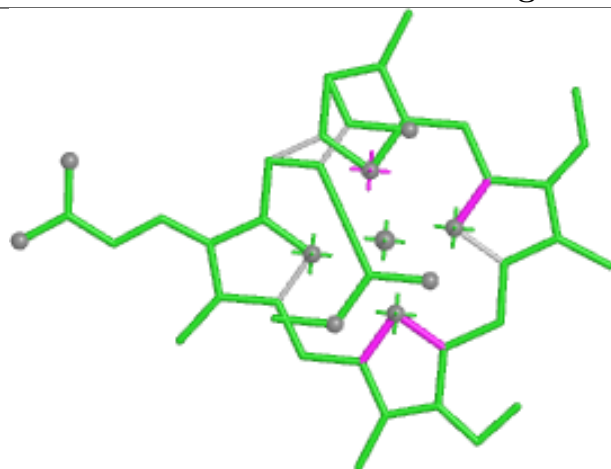
Torsions



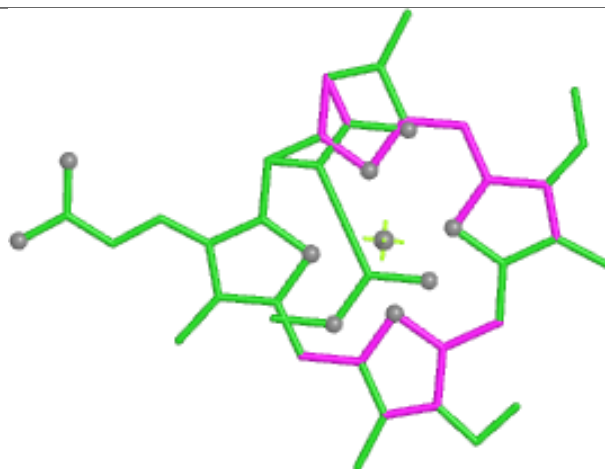
Rings



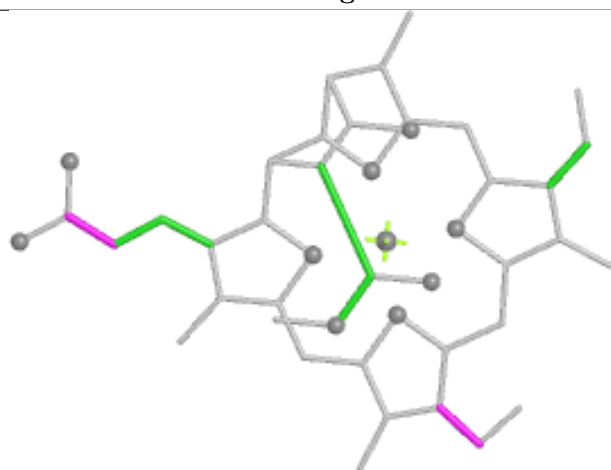
Ligand KC2 Z 308



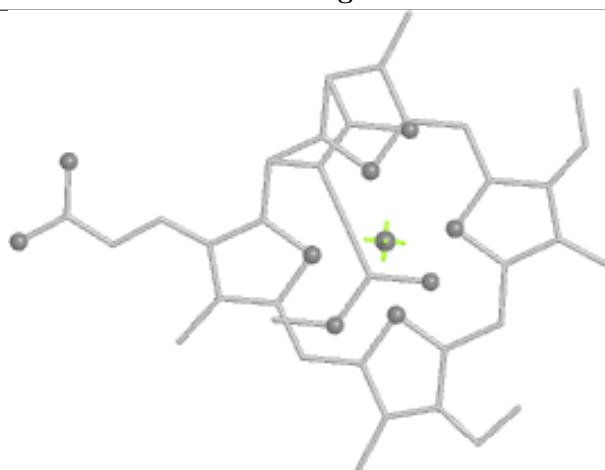
Bond lengths



Bond angles

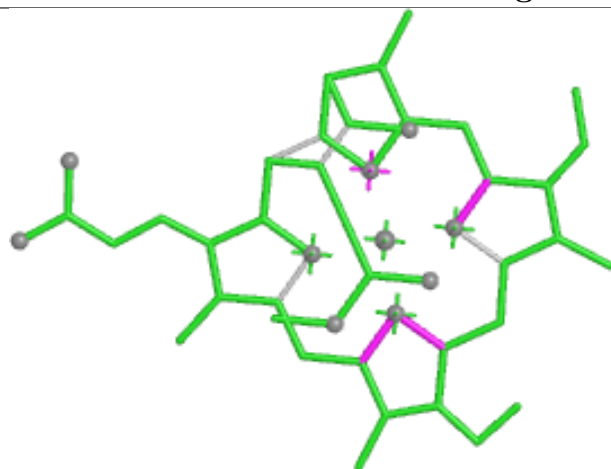


Torsions

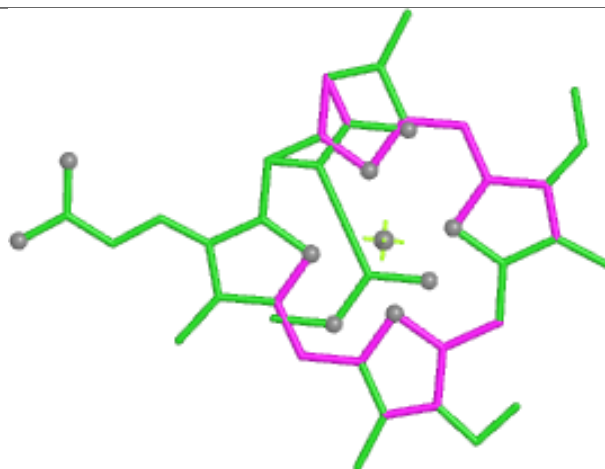


Rings

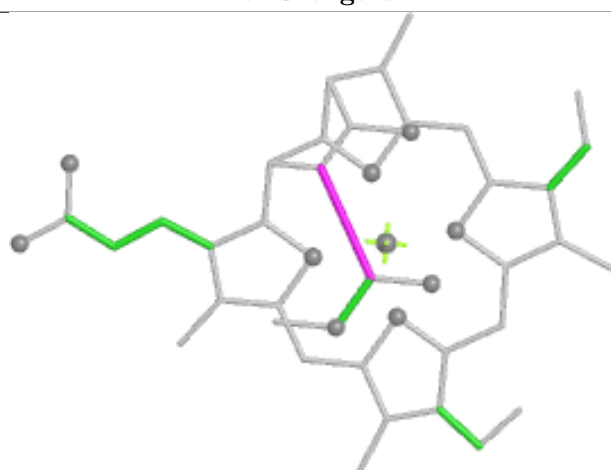
Ligand KC2 X 303



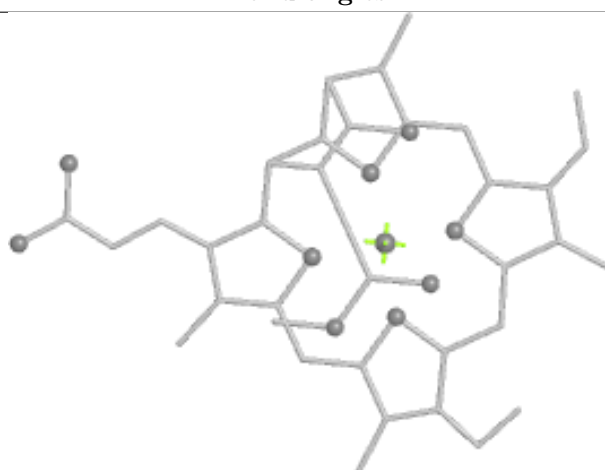
Bond lengths



Bond angles

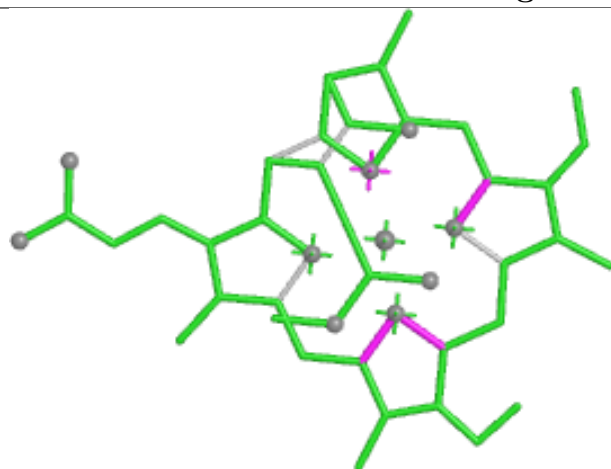


Torsions

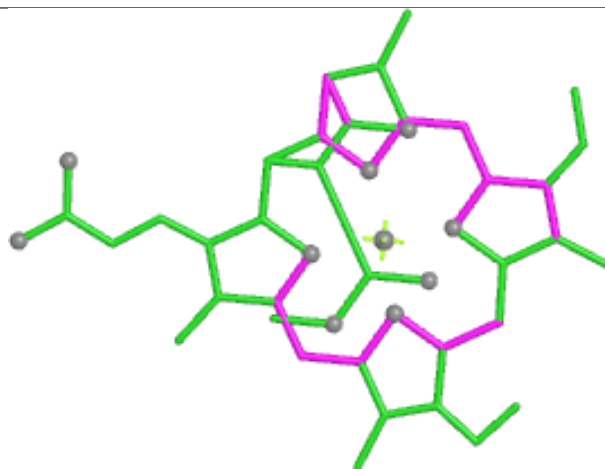


Rings

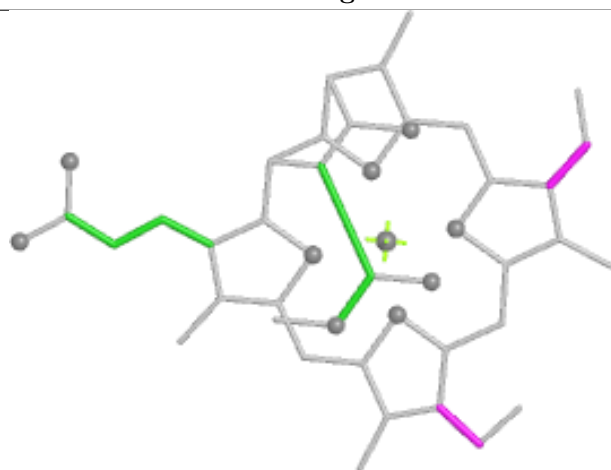
Ligand KC2 P 302



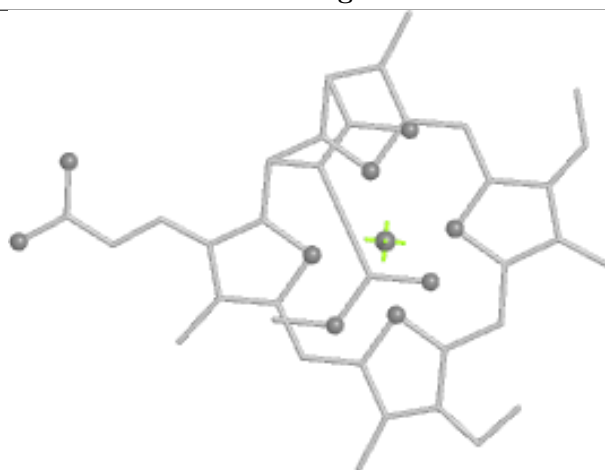
Bond lengths



Bond angles

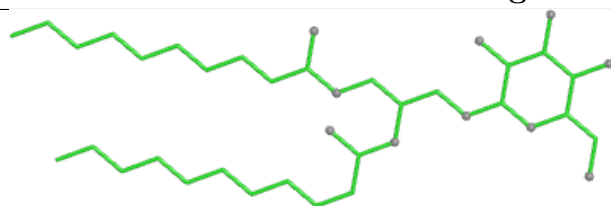


Torsions

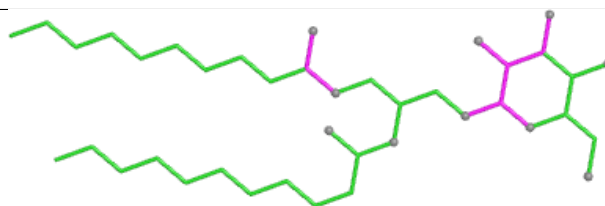


Rings

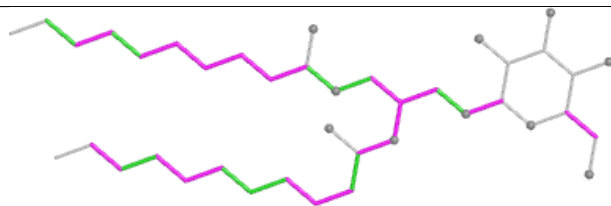
Ligand LMG A 317



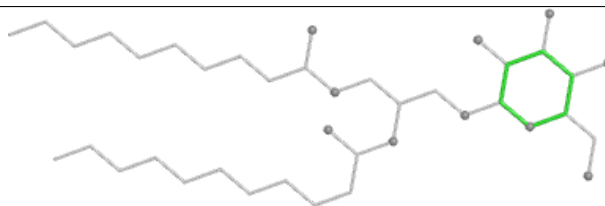
Bond lengths



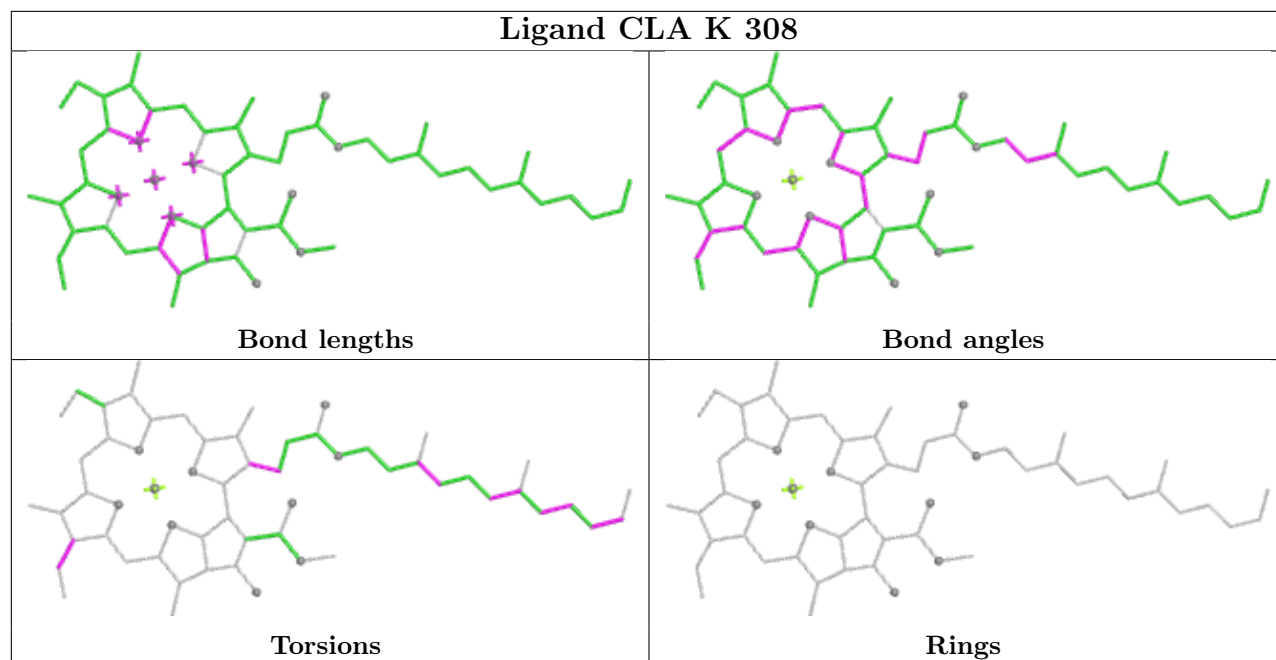
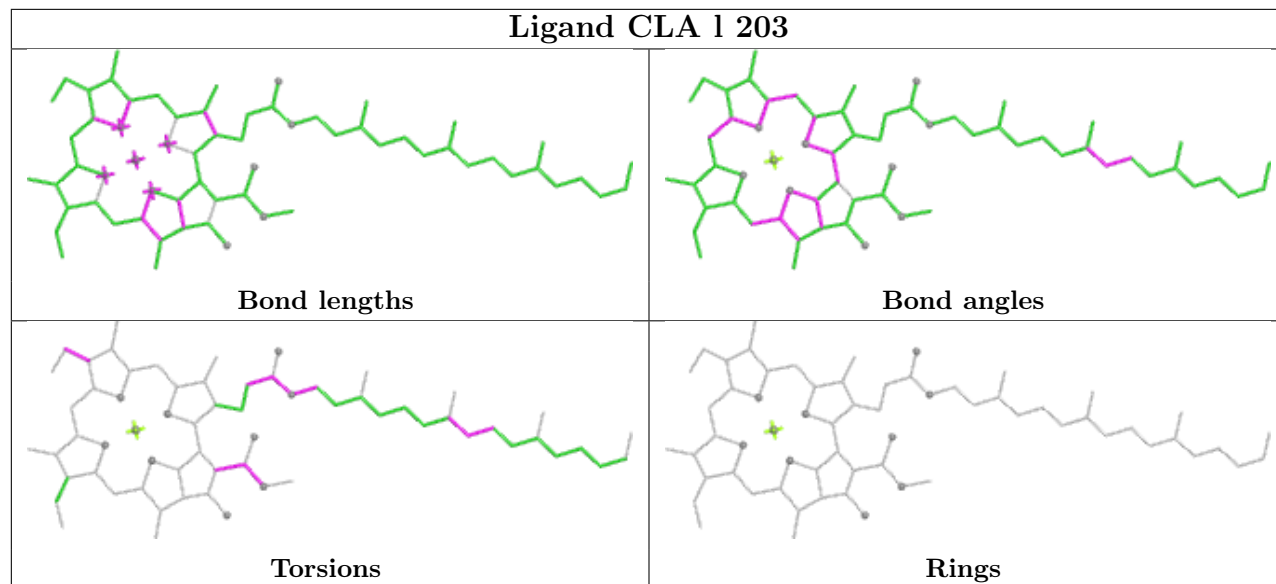
Bond angles



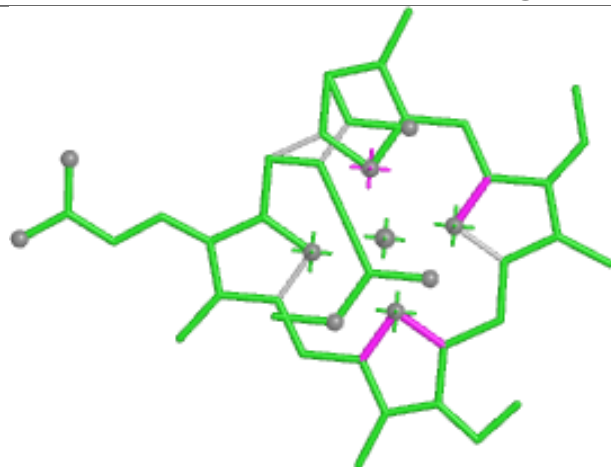
Torsions



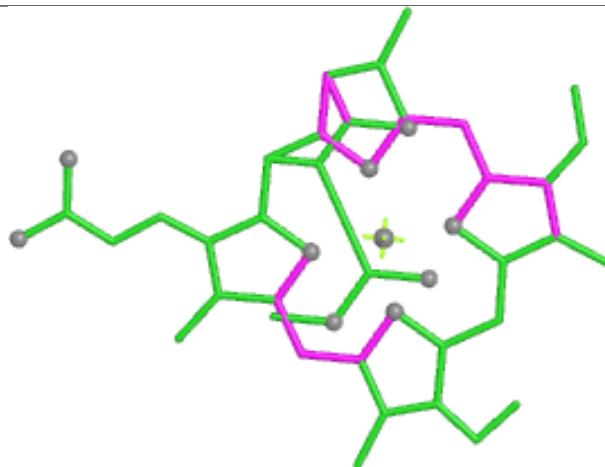
Rings

Ligand CLA K 308**Ligand CLA I 203**

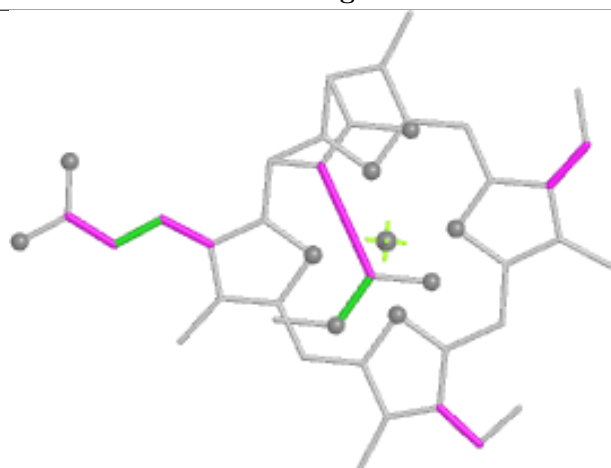
Ligand KC2 T 308



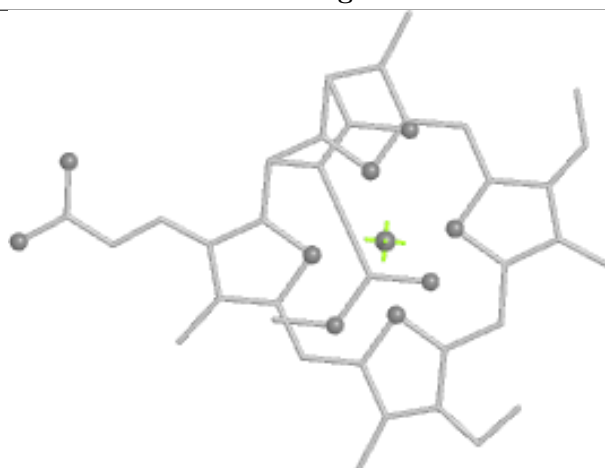
Bond lengths



Bond angles

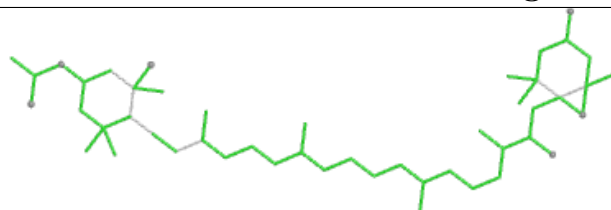


Torsions

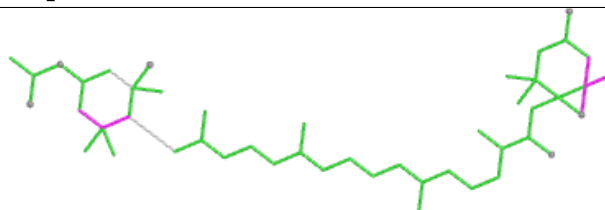


Rings

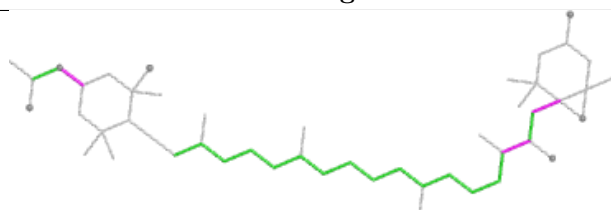
Ligand A86 p 321



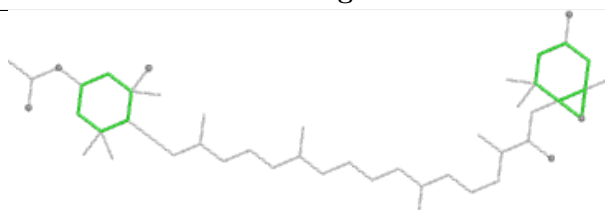
Bond lengths



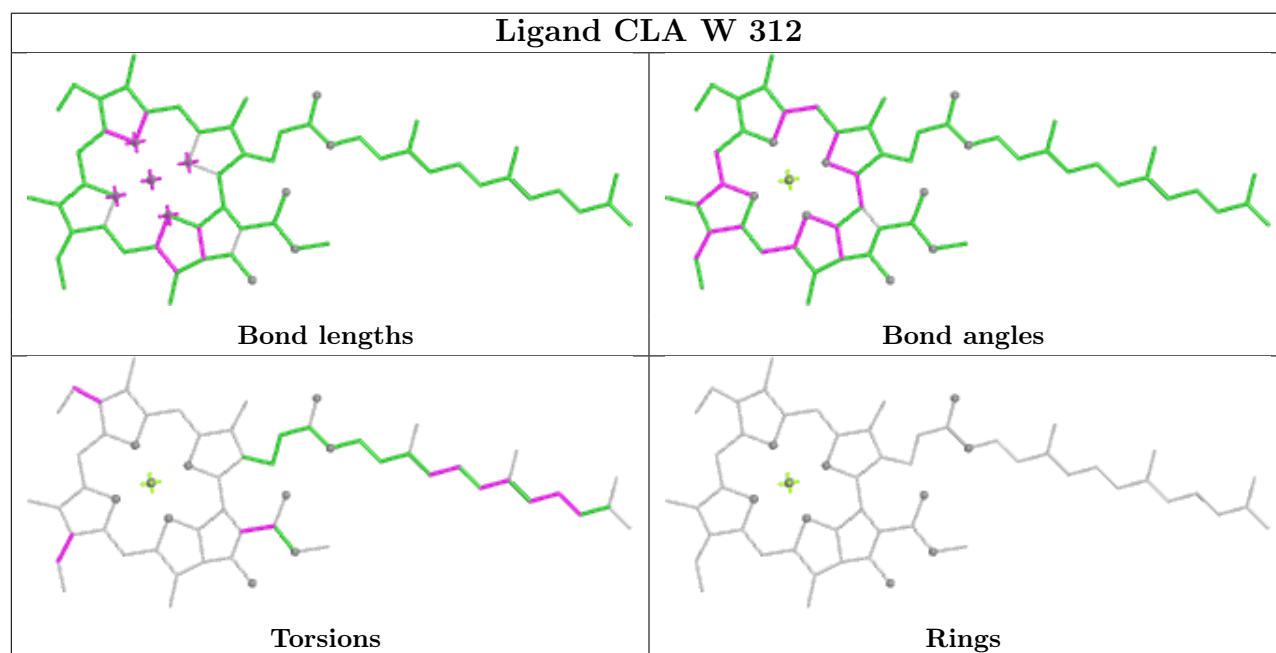
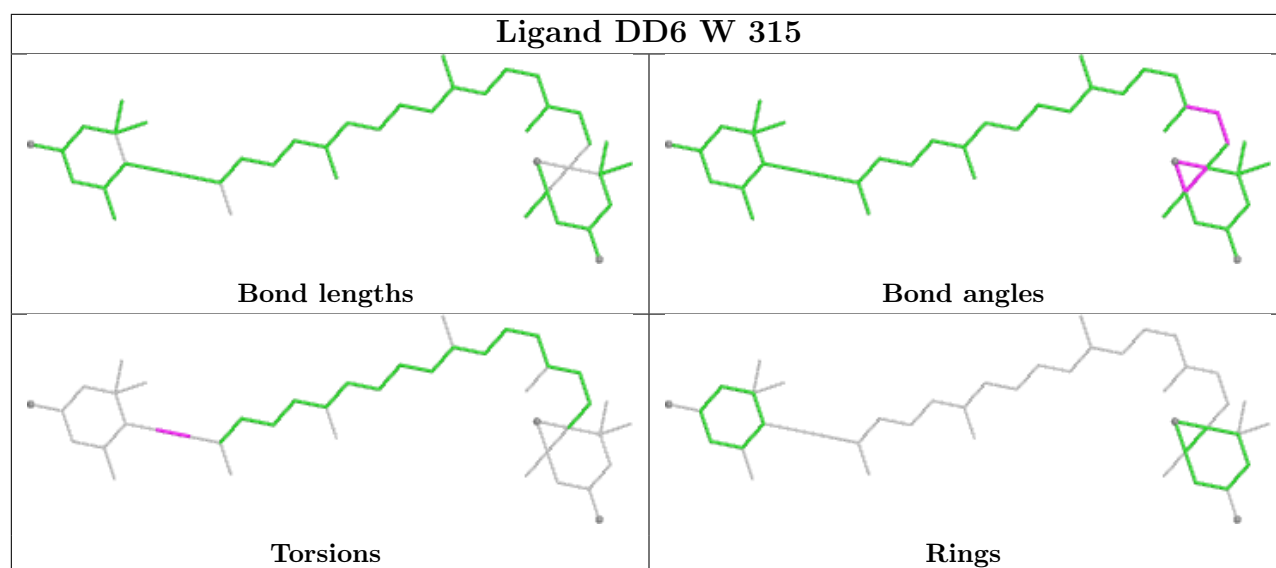
Bond angles



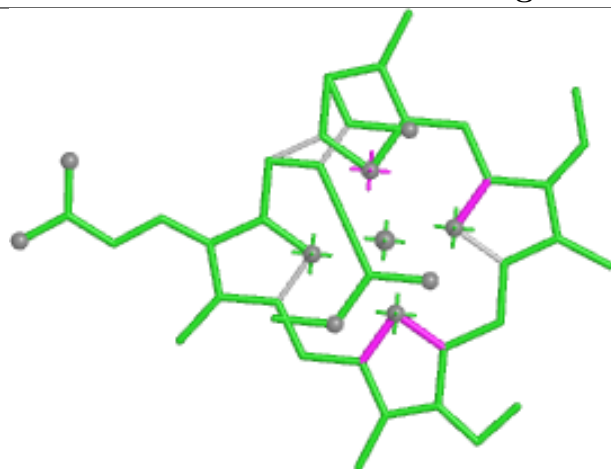
Torsions



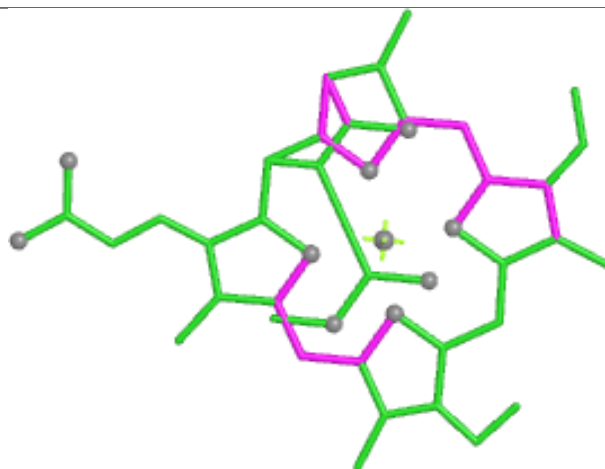
Rings



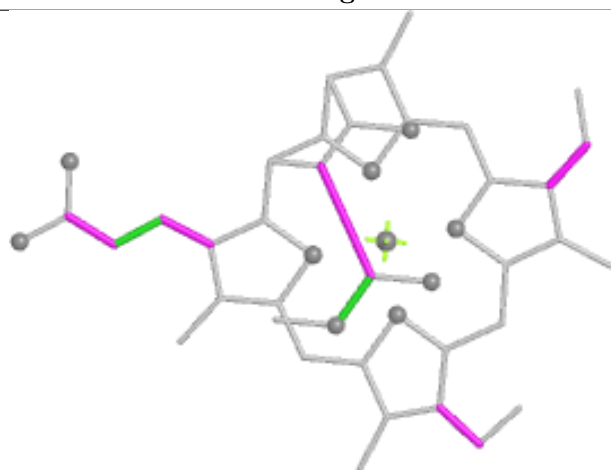
Ligand KC2 O 309



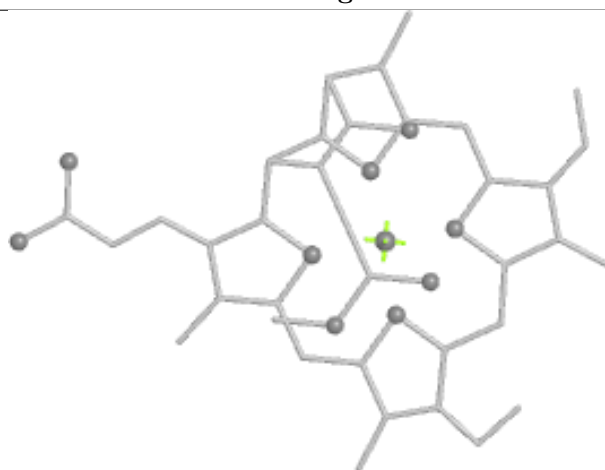
Bond lengths



Bond angles

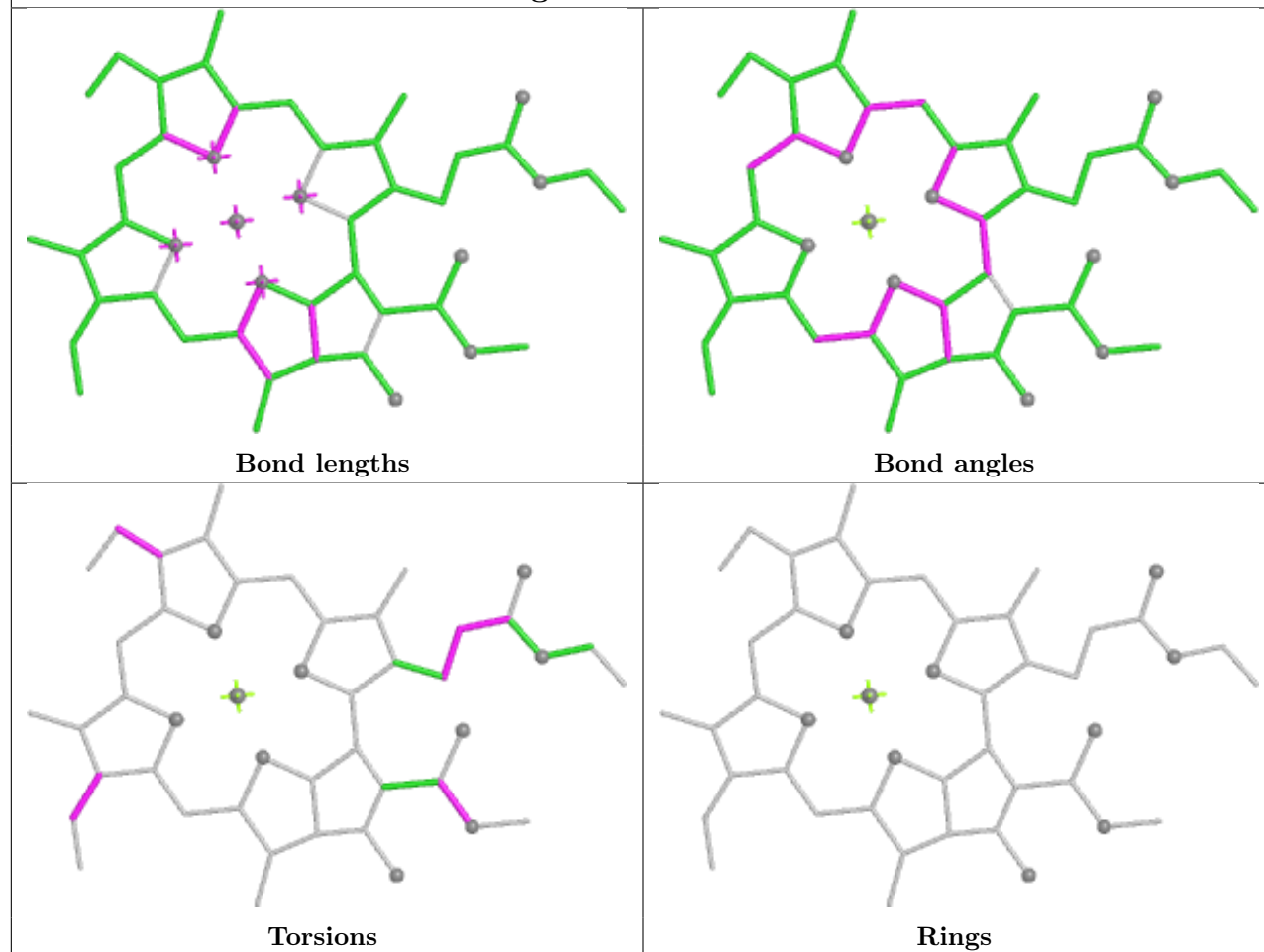


Torsions

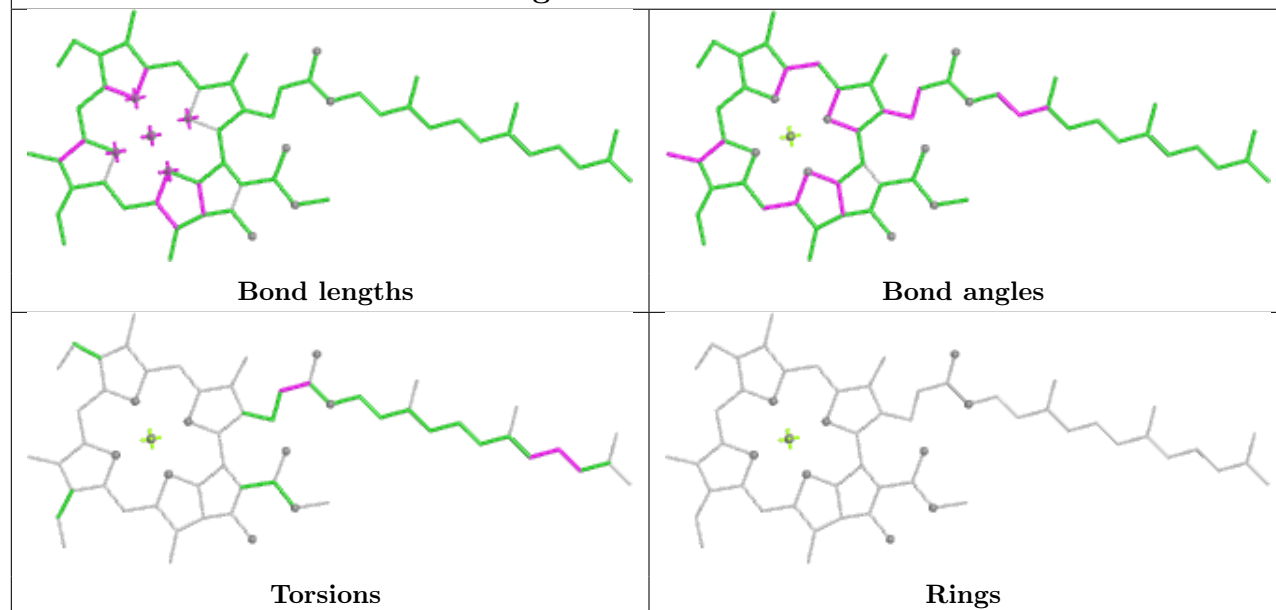


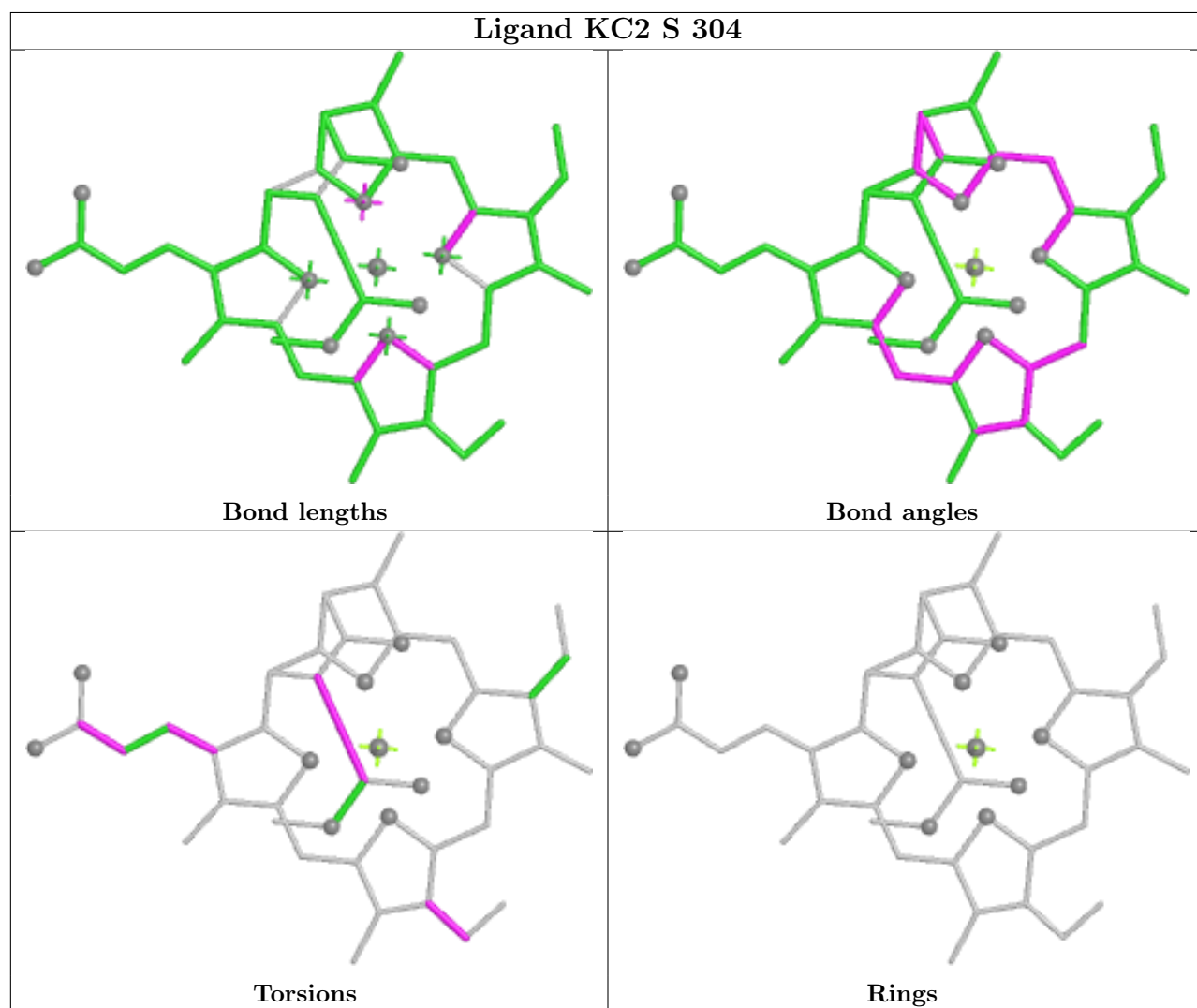
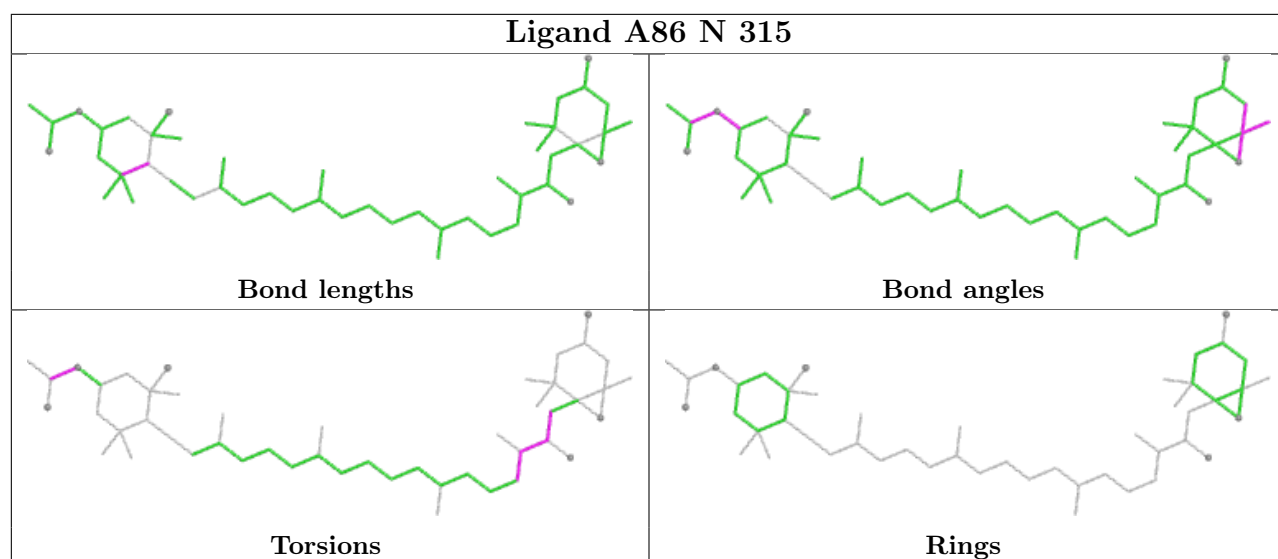
Rings

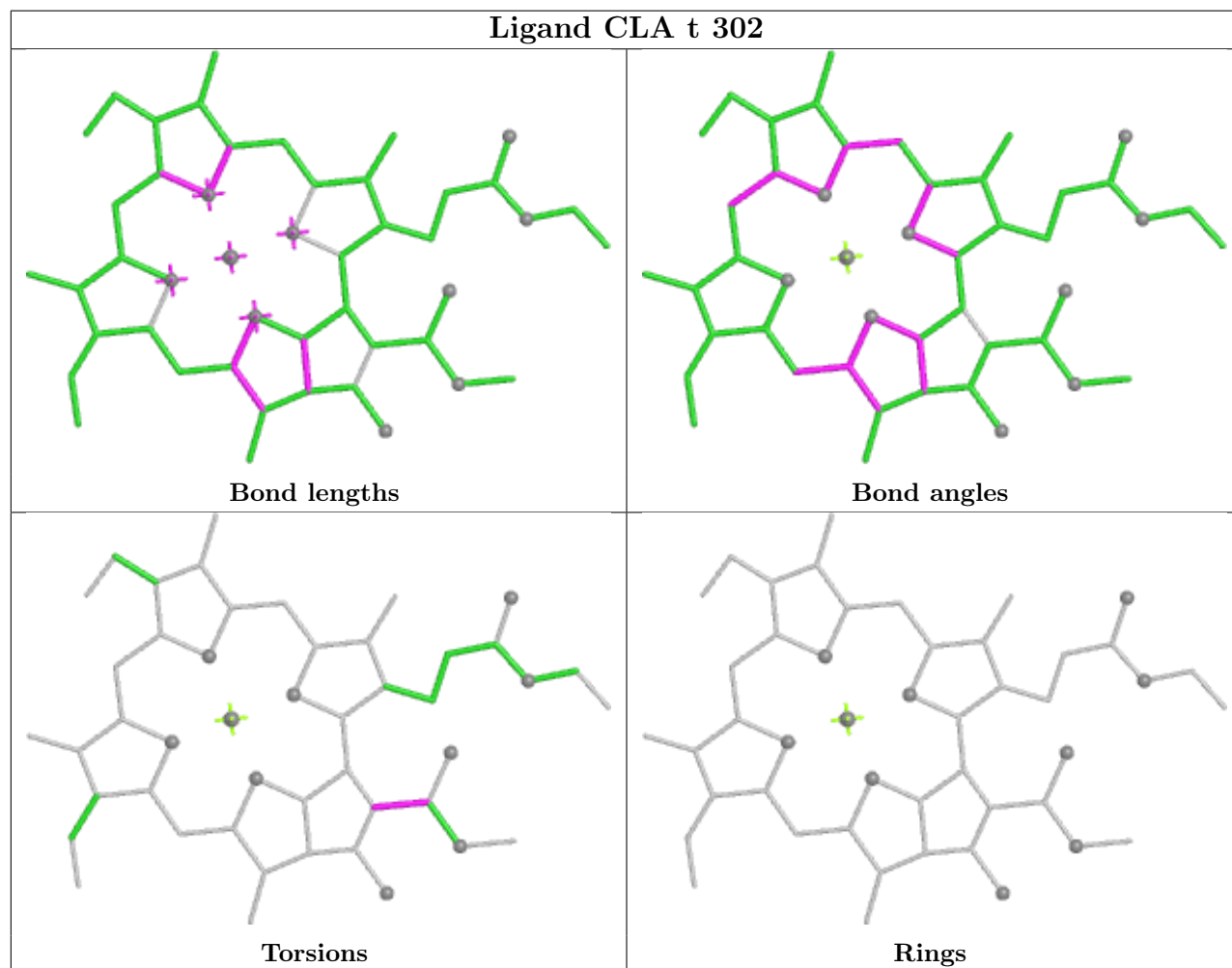
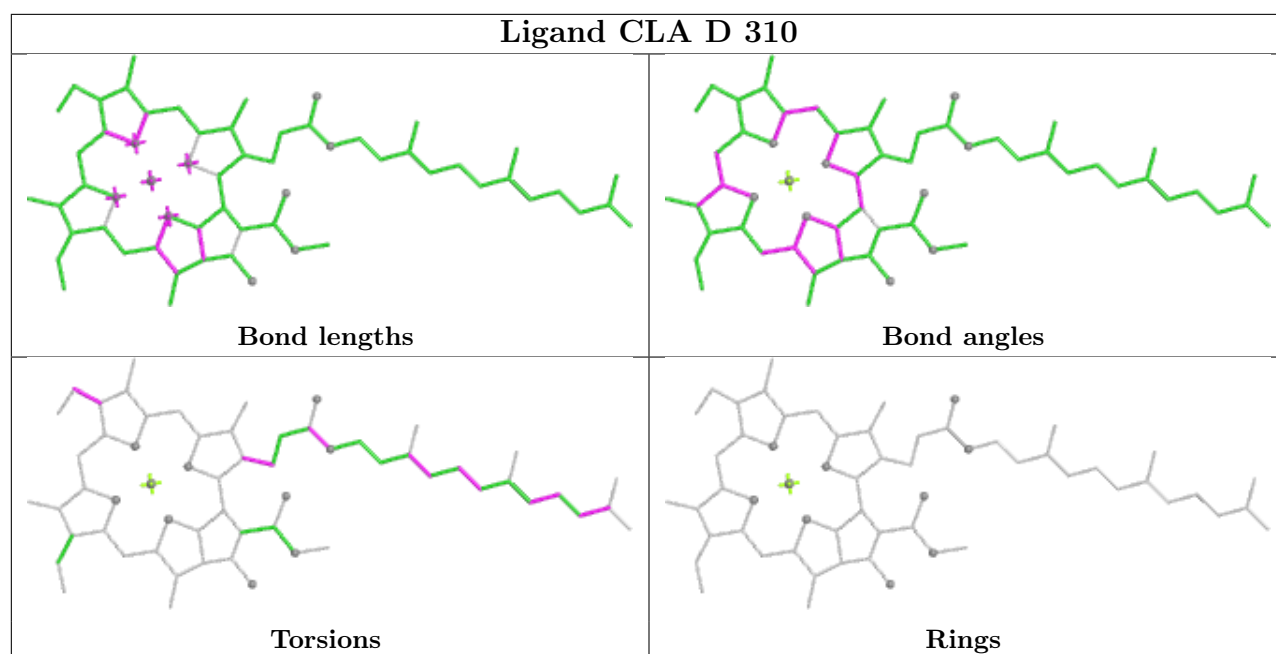
Ligand CLA J 302

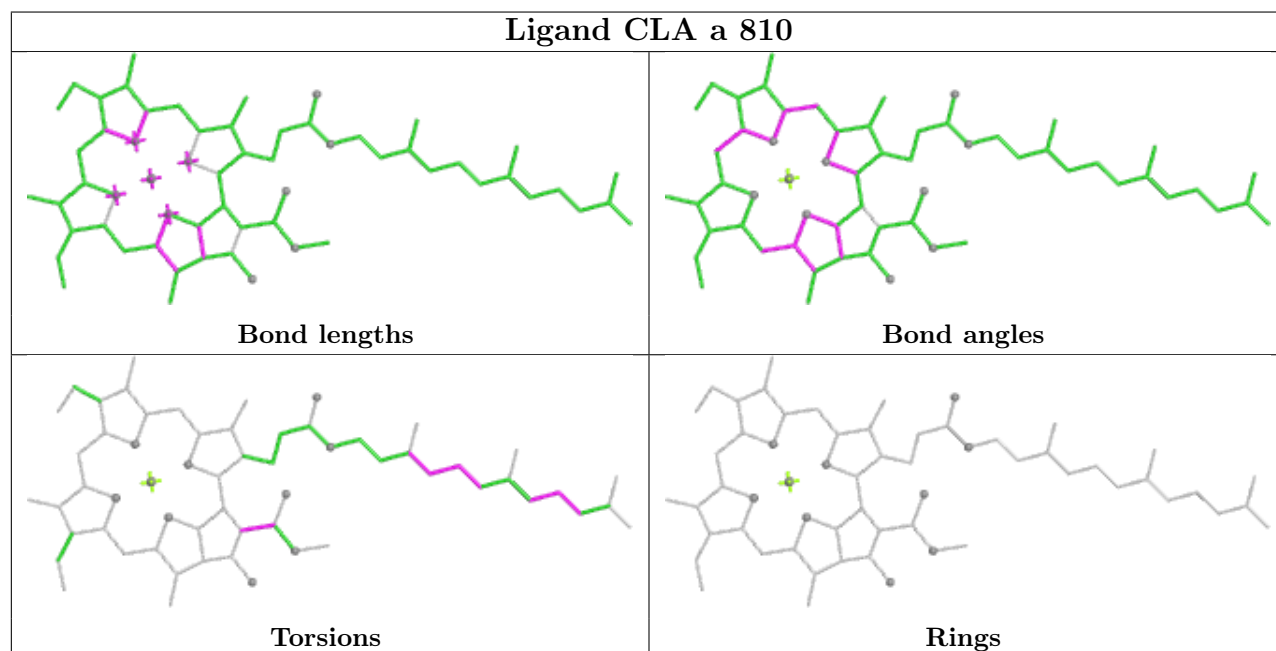
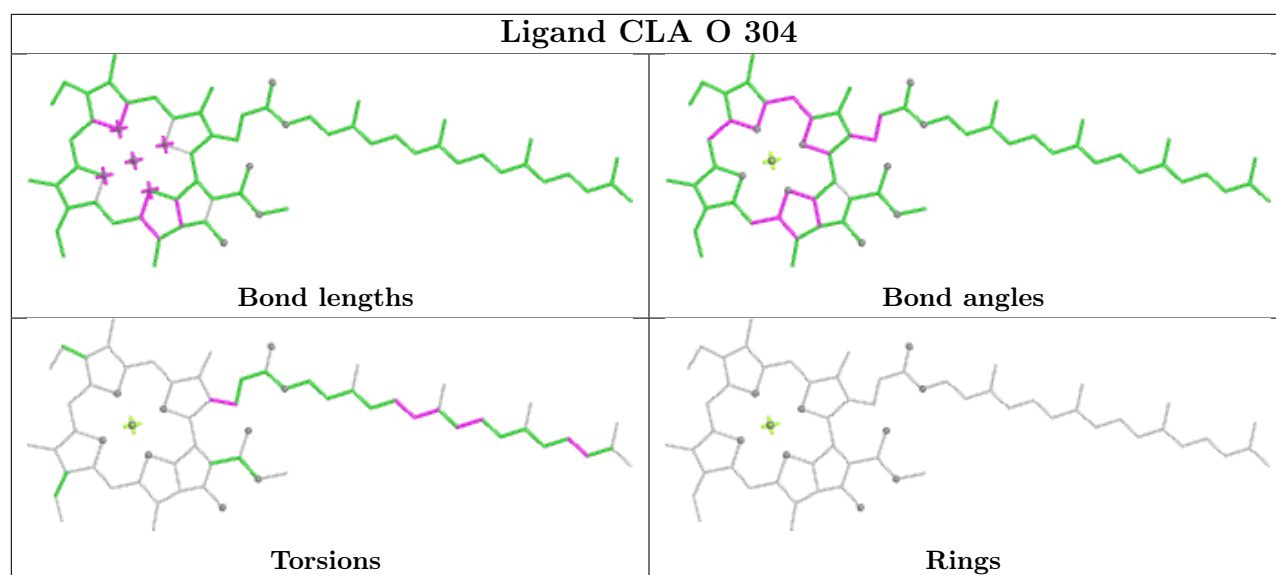


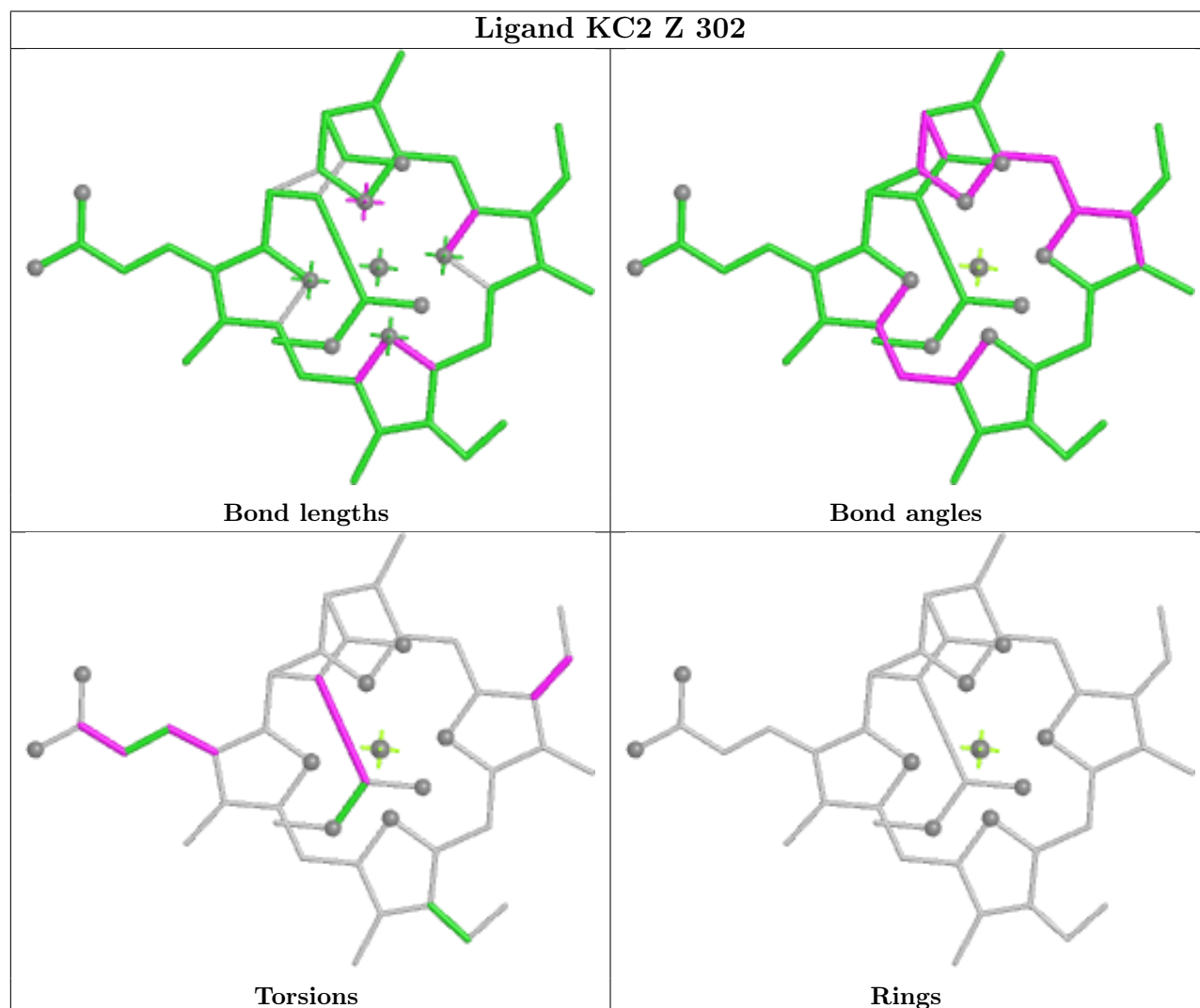
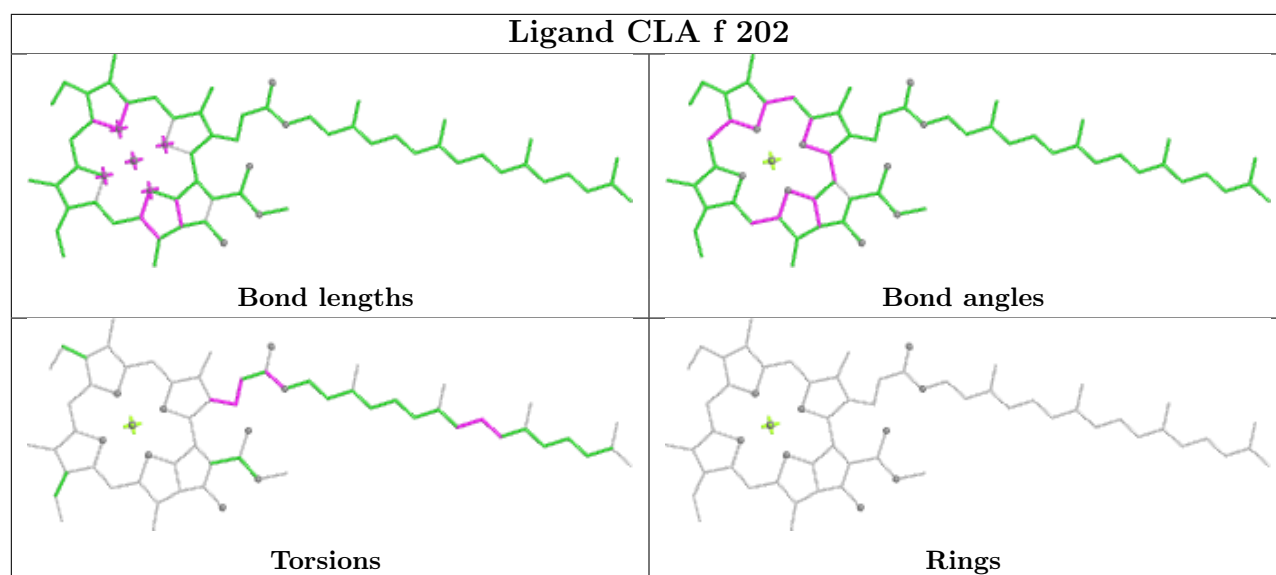
Ligand CLA T 306

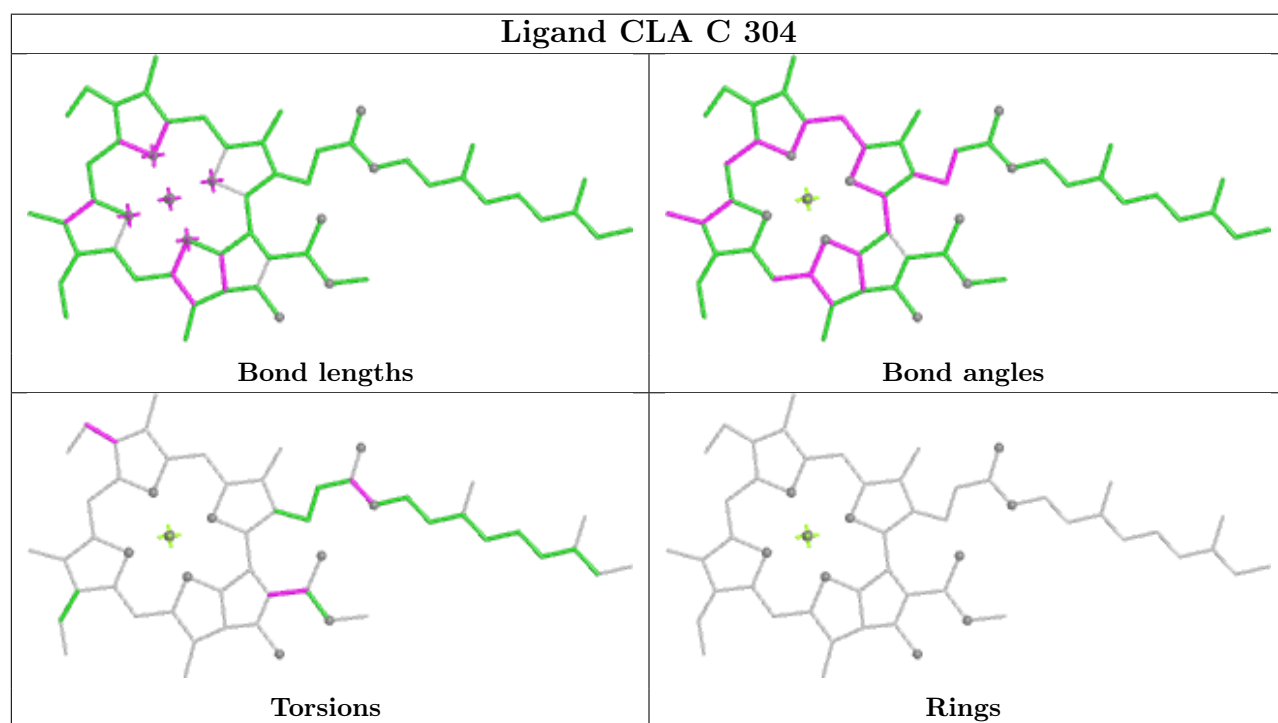
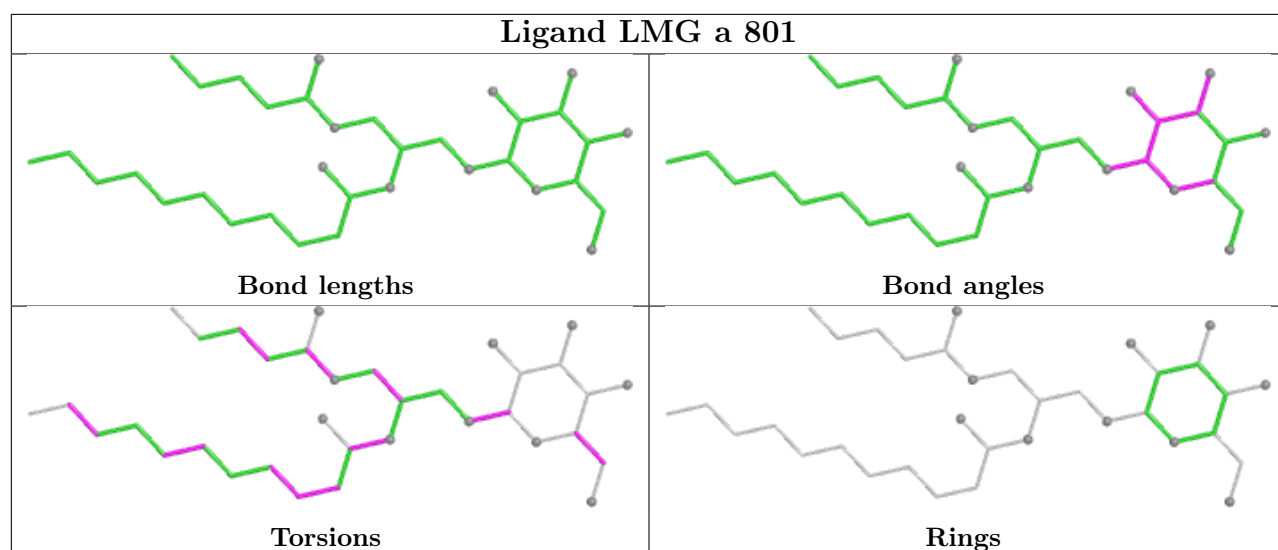




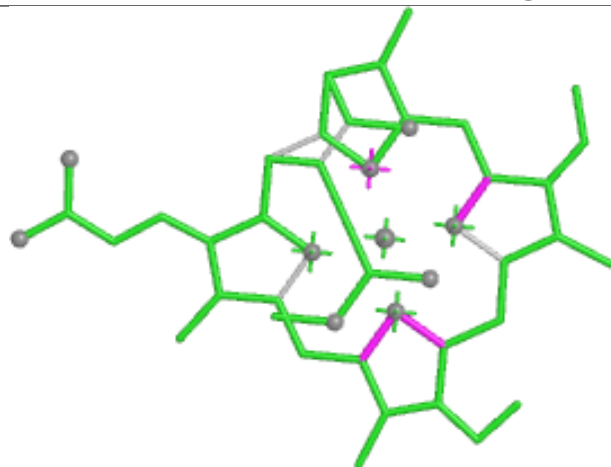




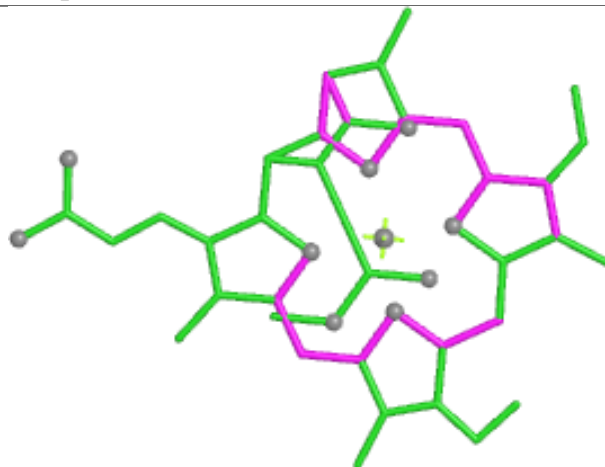




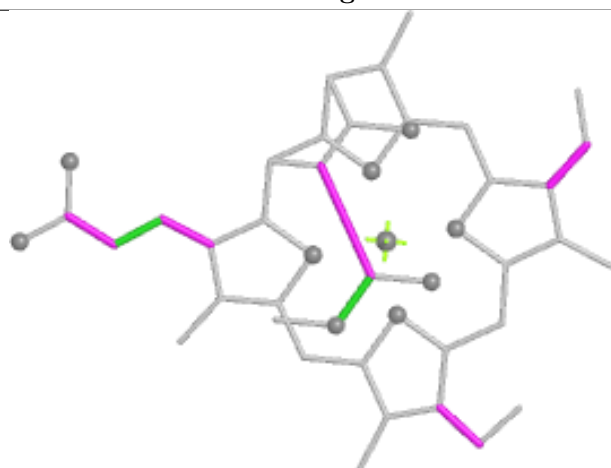
Ligand KC2 q 308



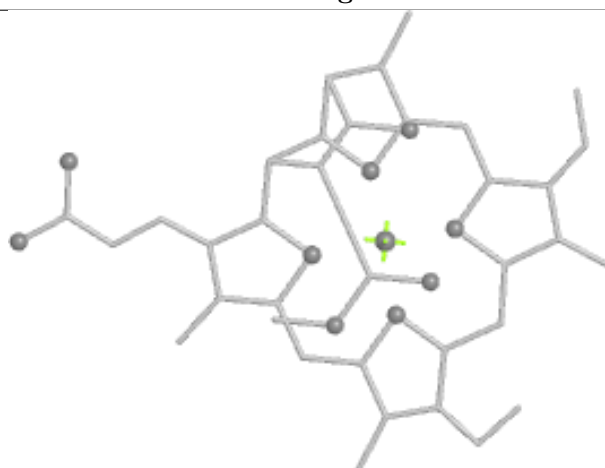
Bond lengths



Bond angles



Torsions



Rings

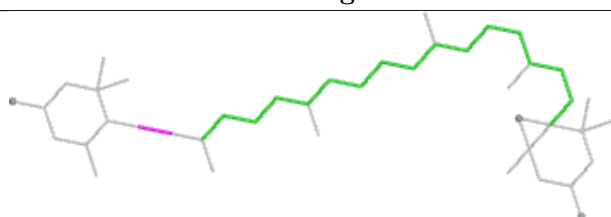
Ligand DD6 T 314



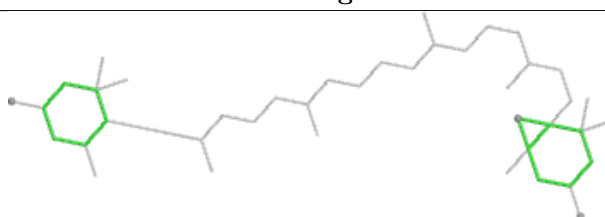
Bond lengths



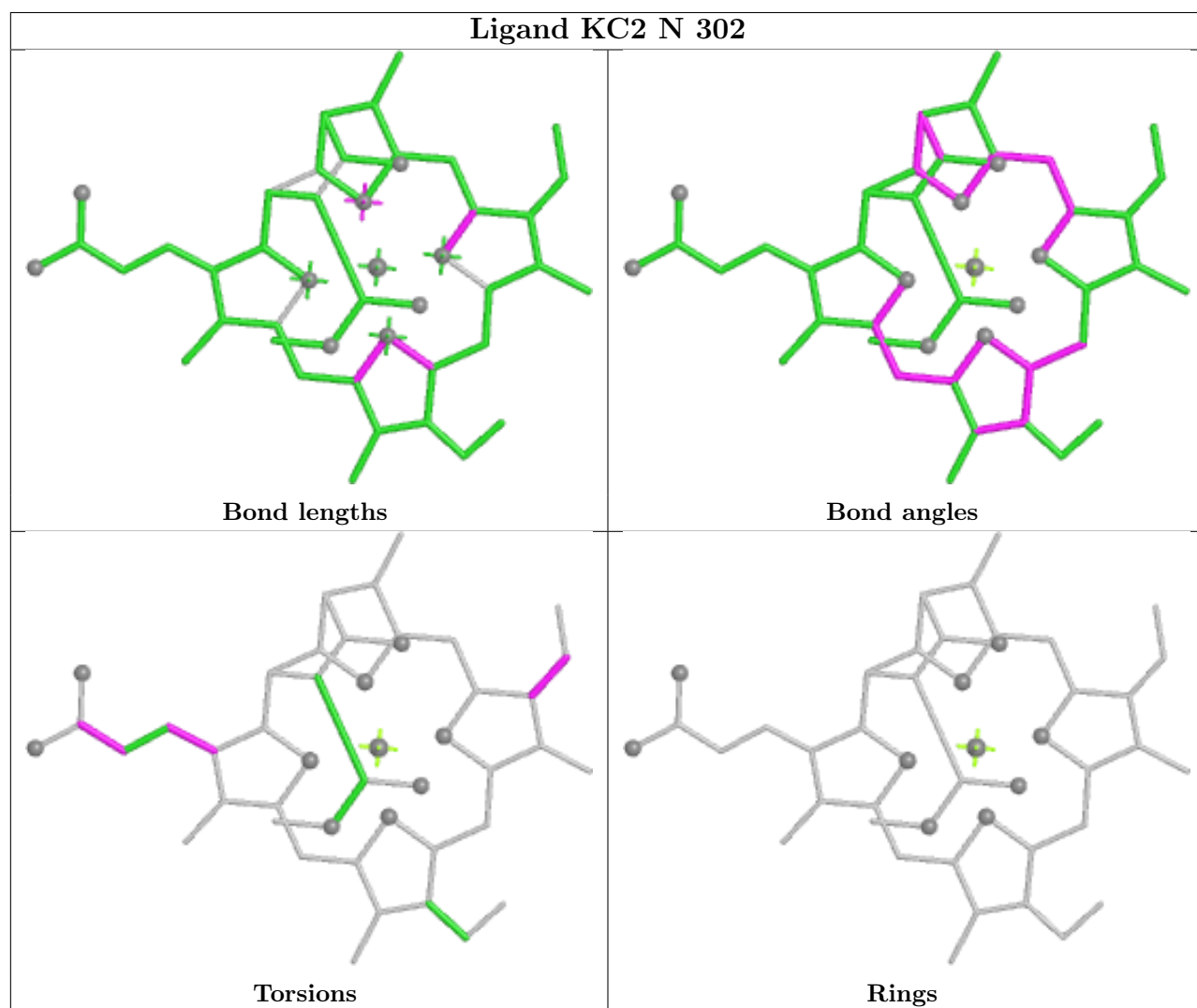
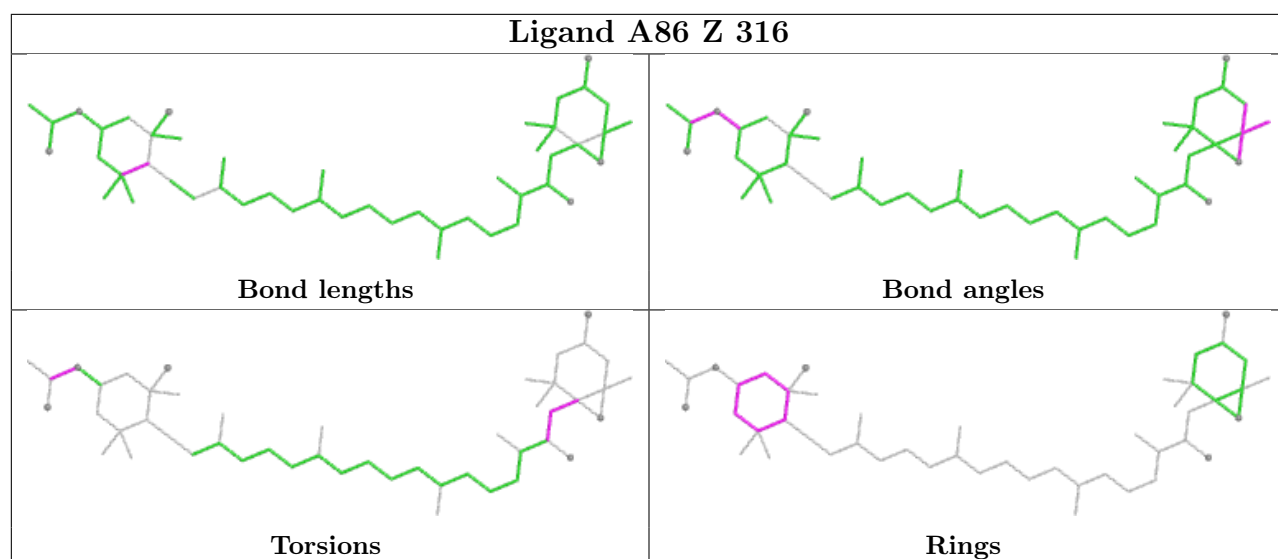
Bond angles



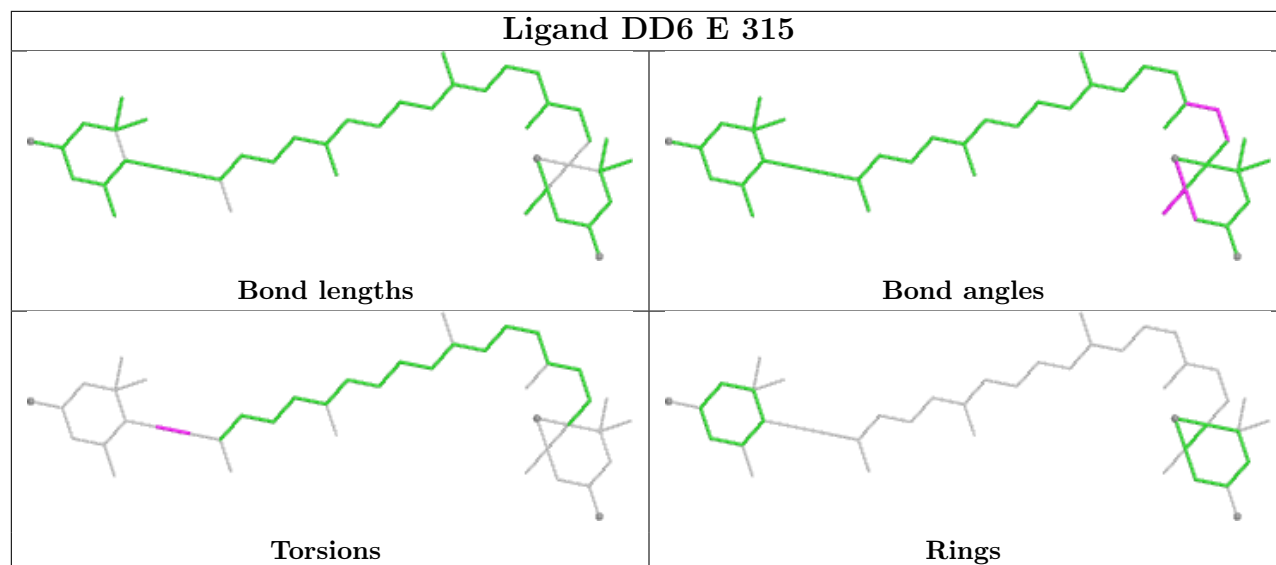
Torsions



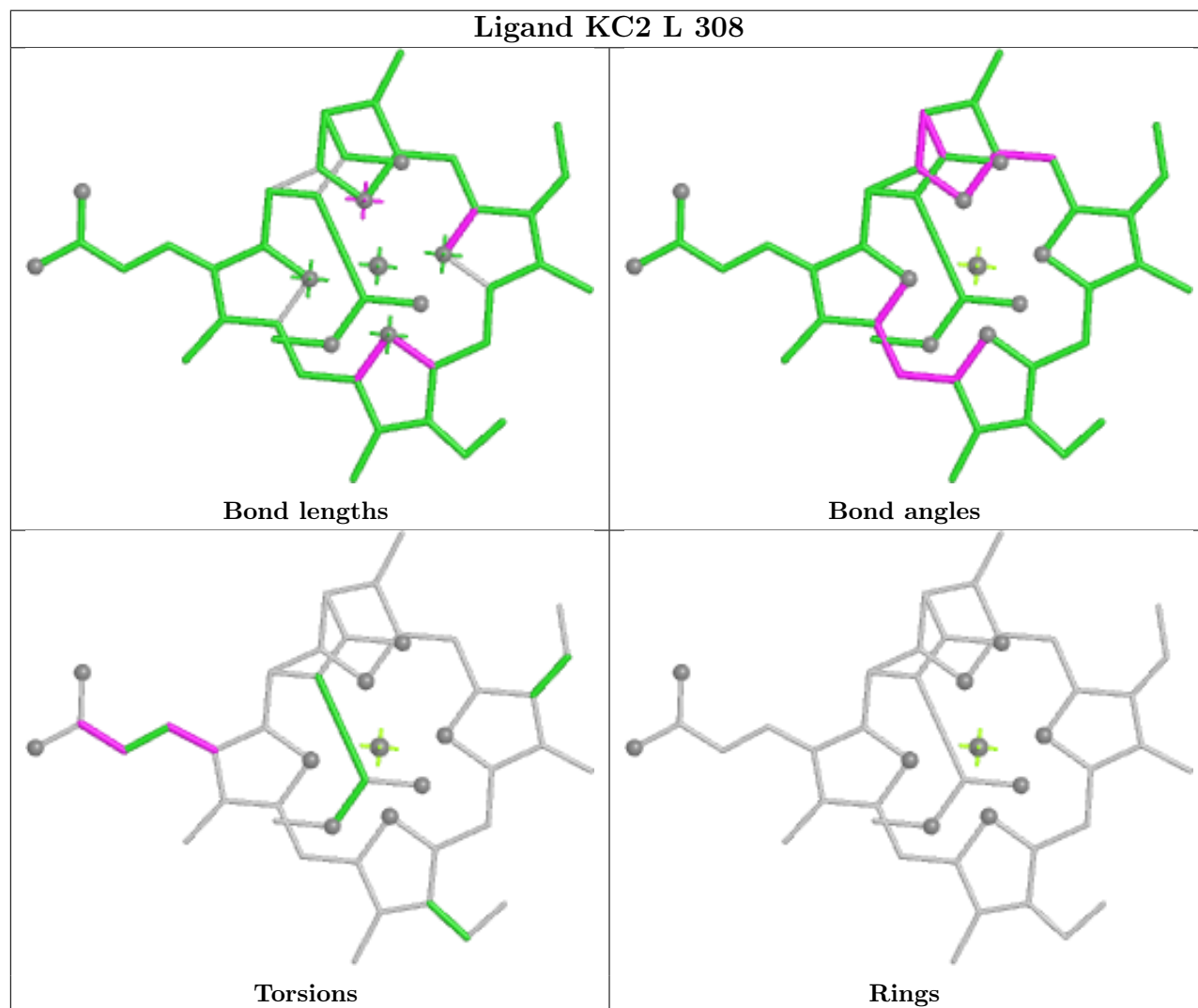
Rings

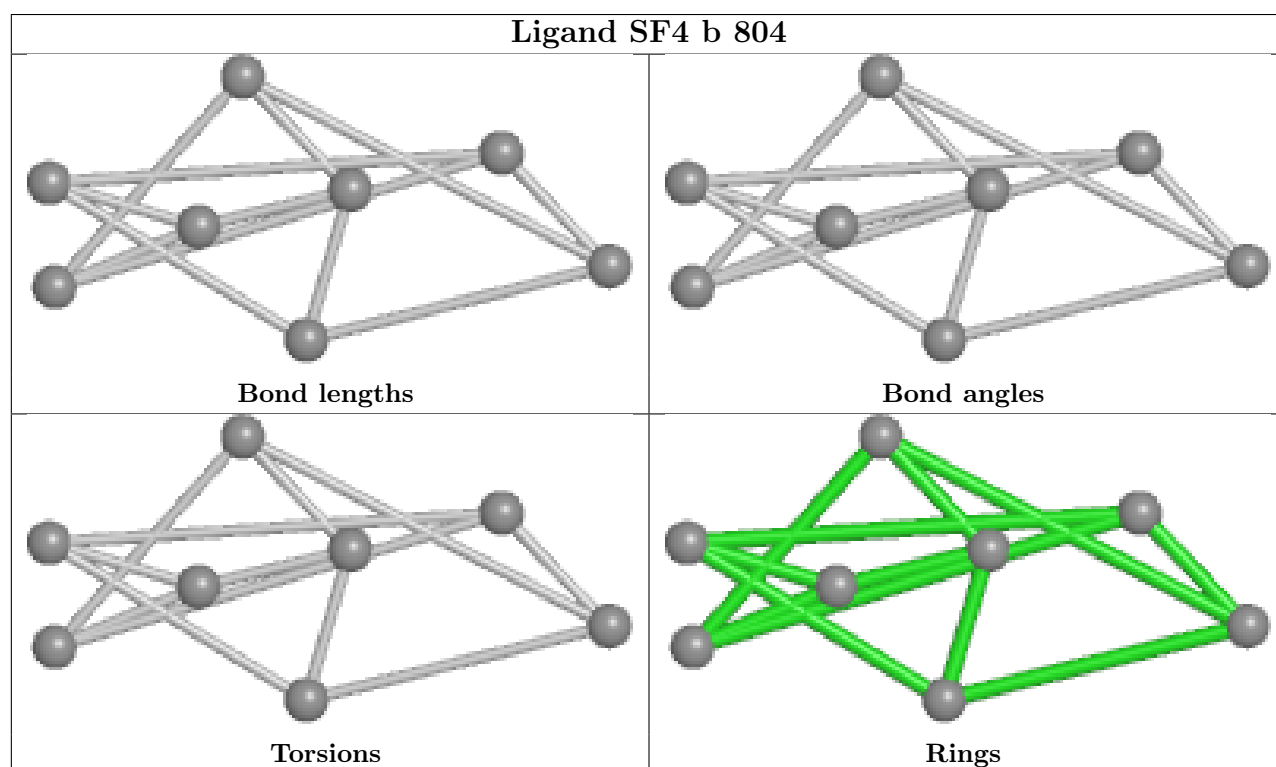
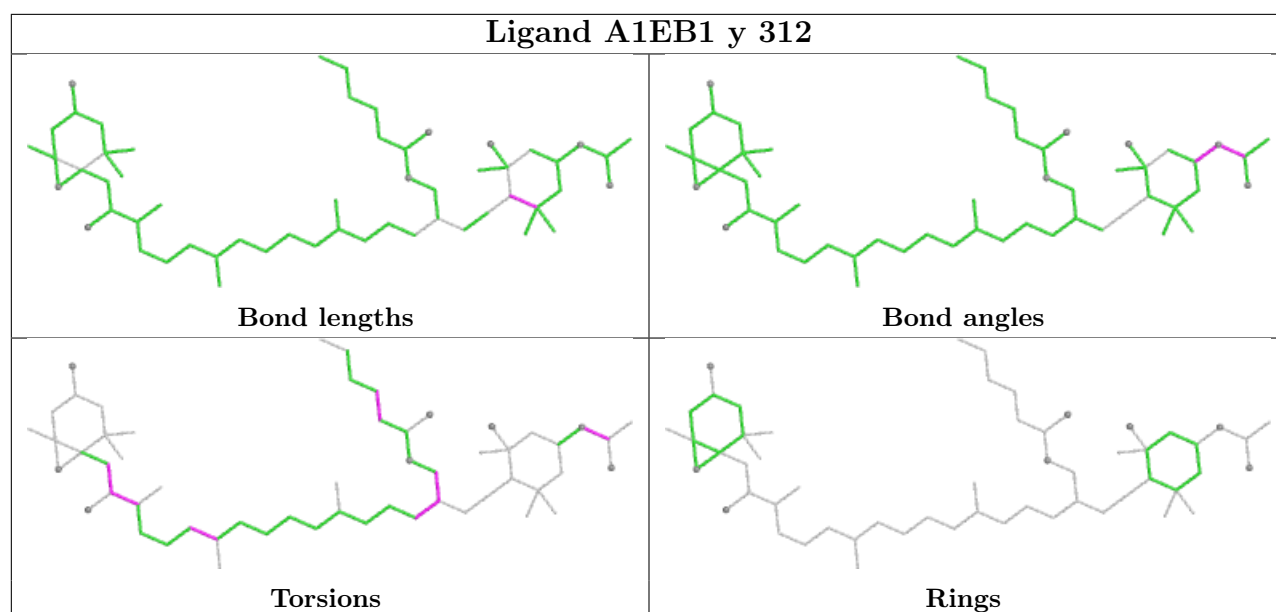


Ligand DD6 E 315

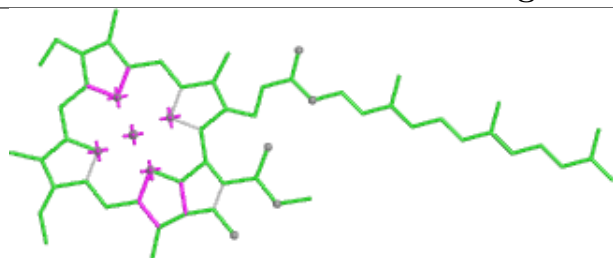


Ligand KC2 L 308

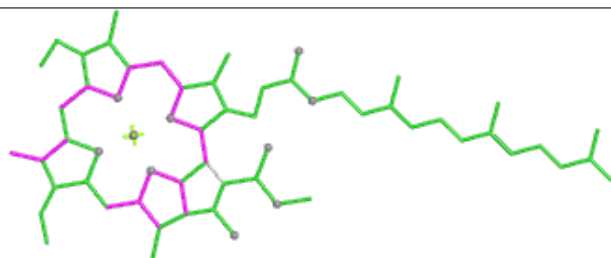




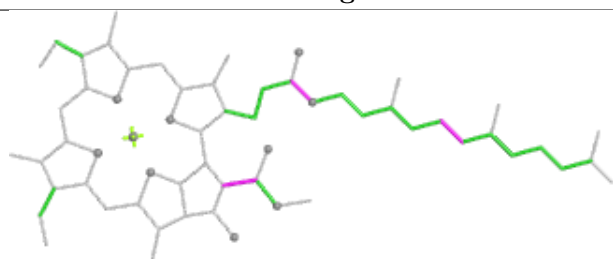
Ligand CLA v 305



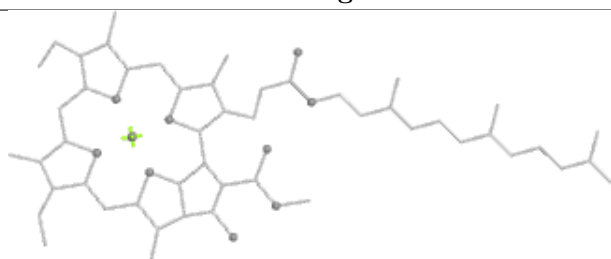
Bond lengths



Bond angles

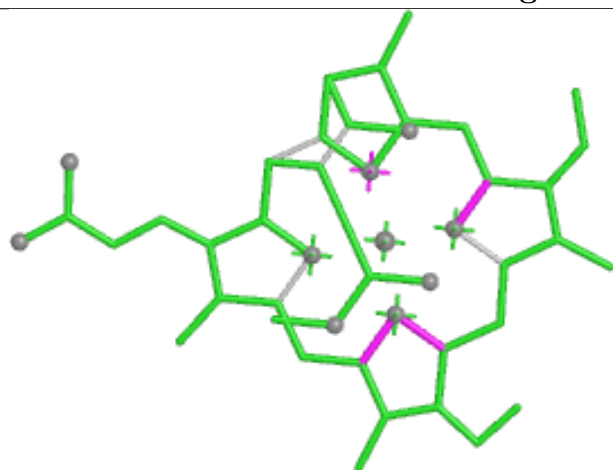


Torsions

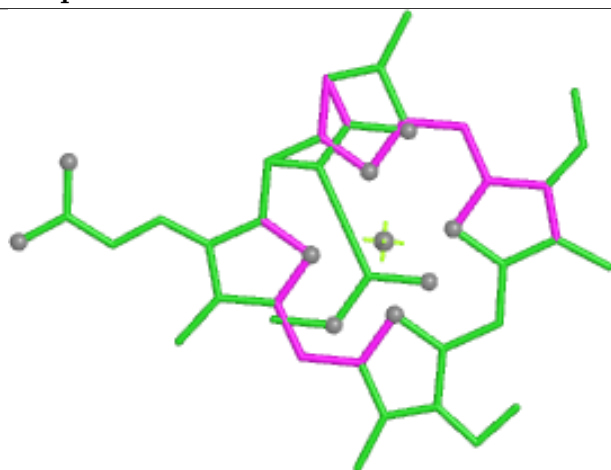


Rings

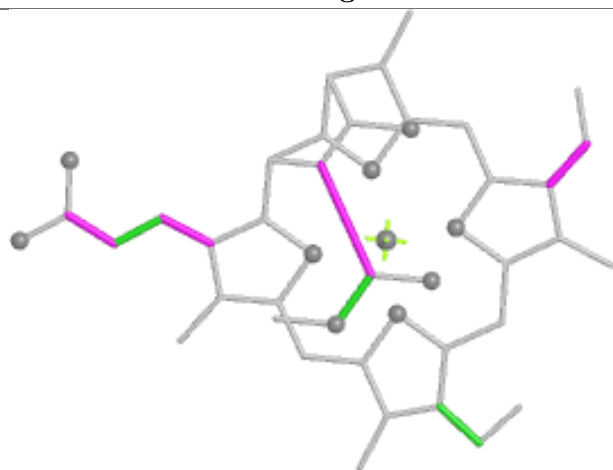
Ligand KC2 q 302



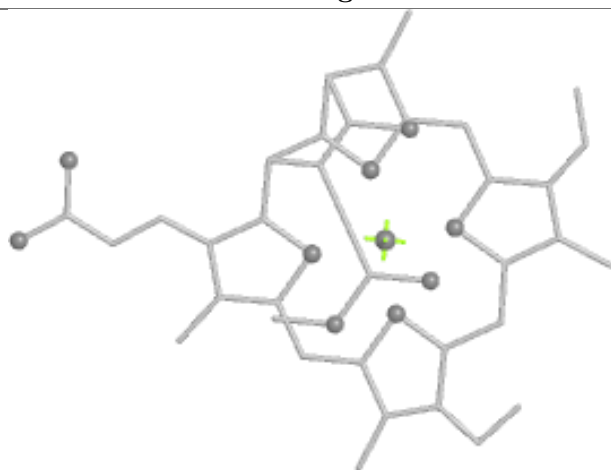
Bond lengths



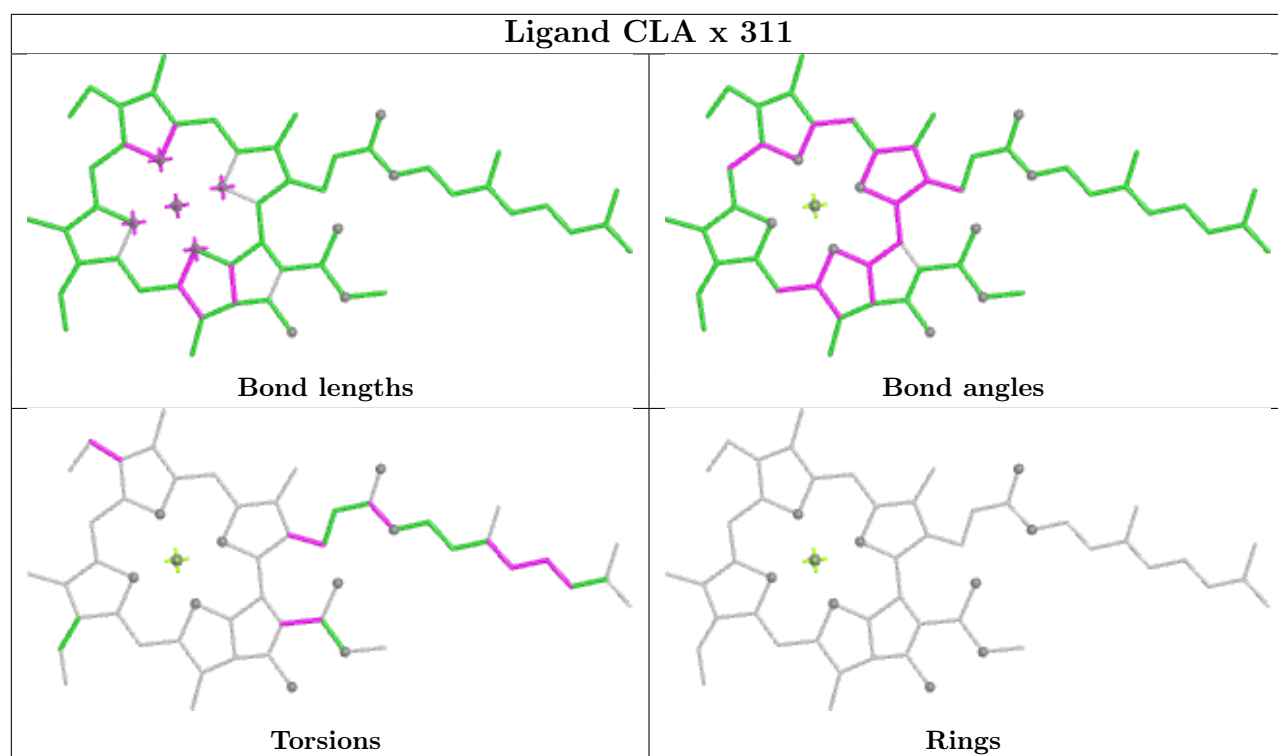
Bond angles



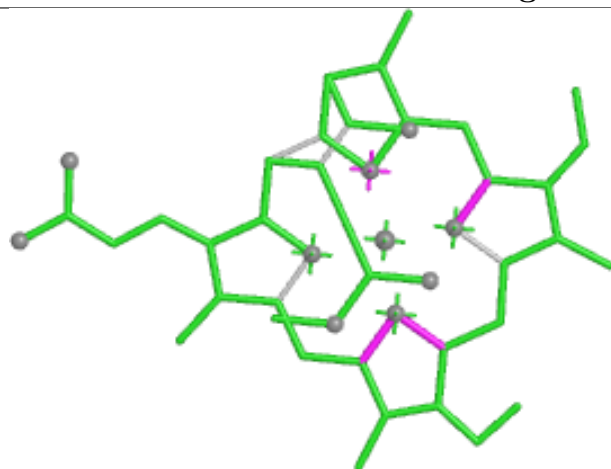
Torsions



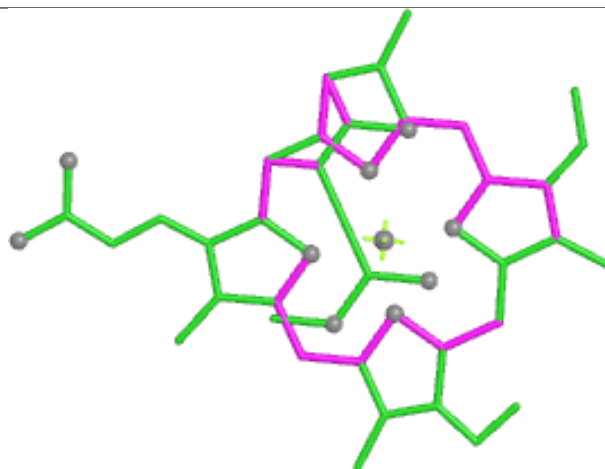
Rings



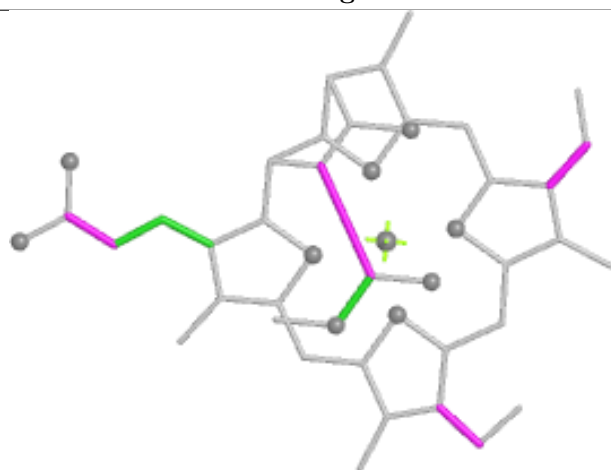
Ligand KC2 u 315



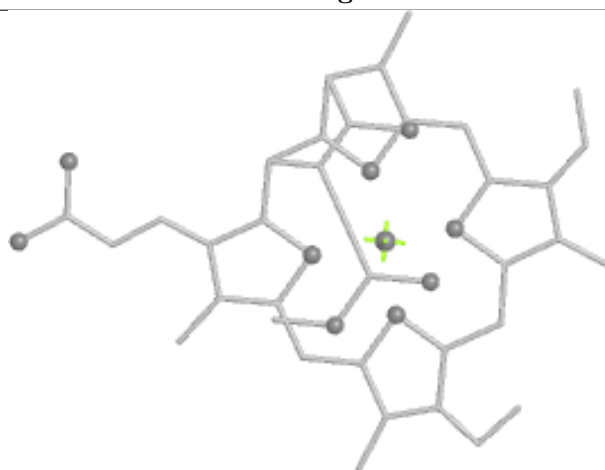
Bond lengths



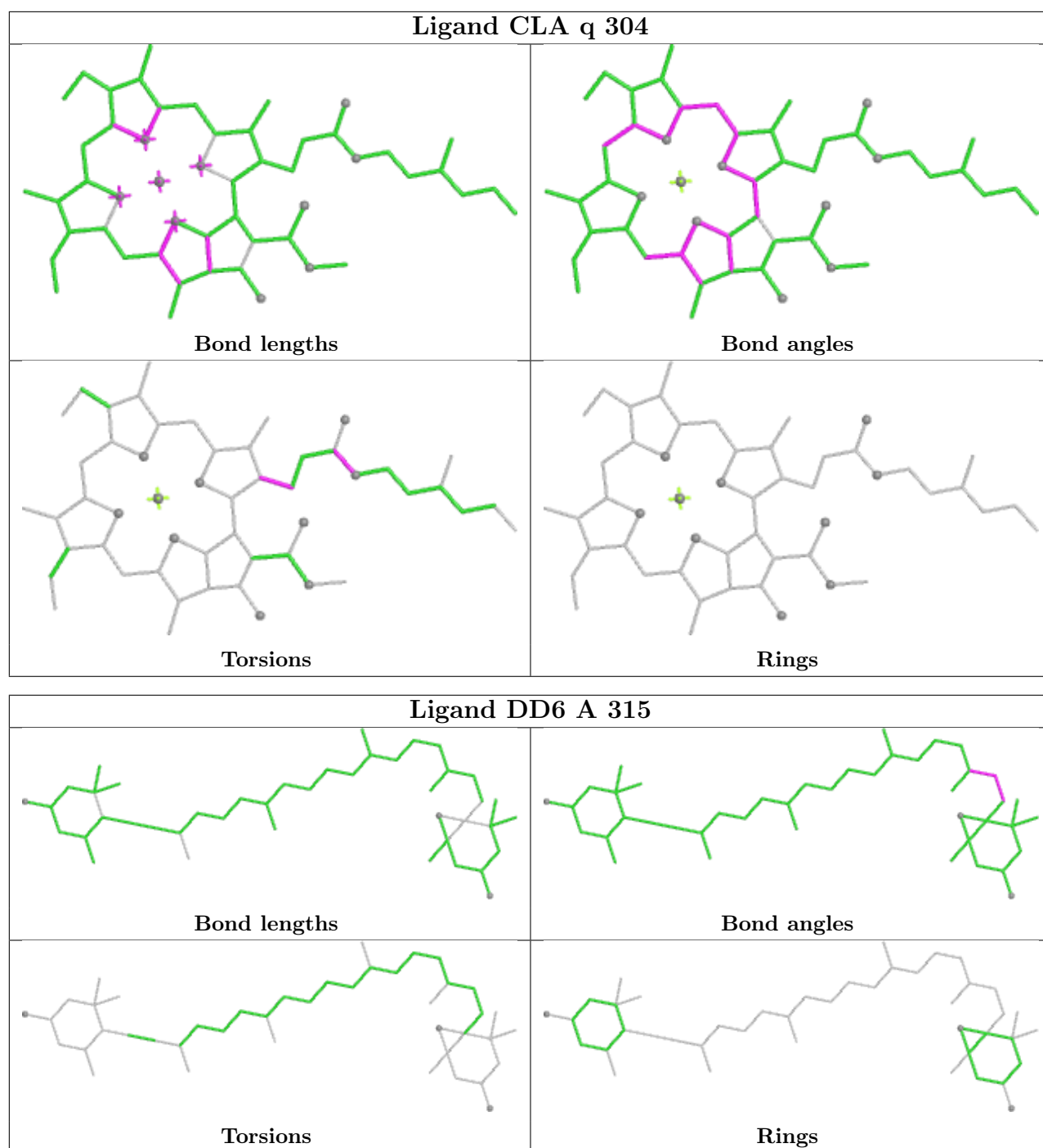
Bond angles



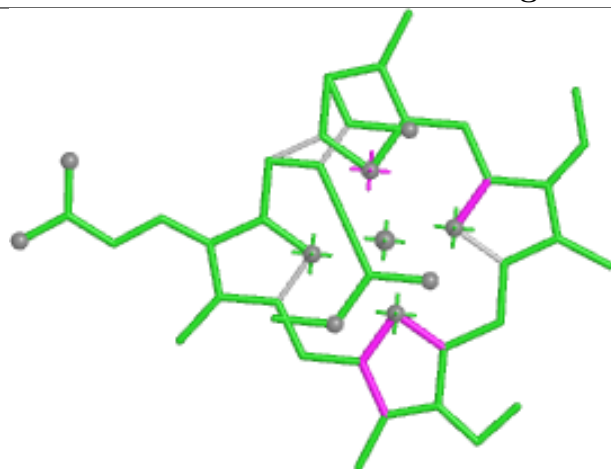
Torsions



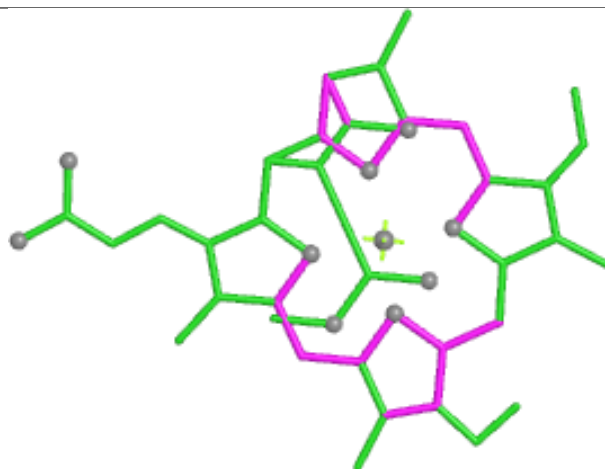
Rings



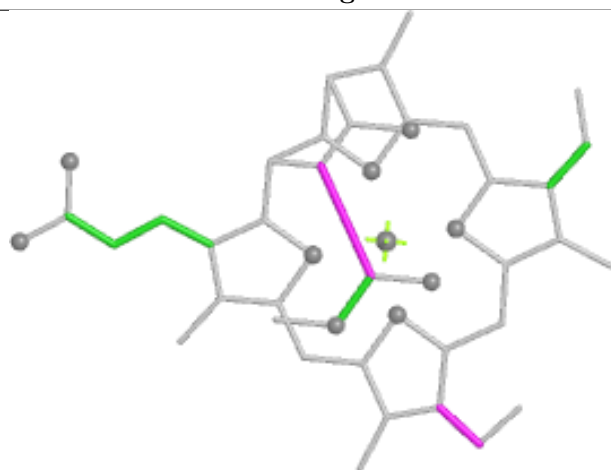
Ligand KC2 o 303



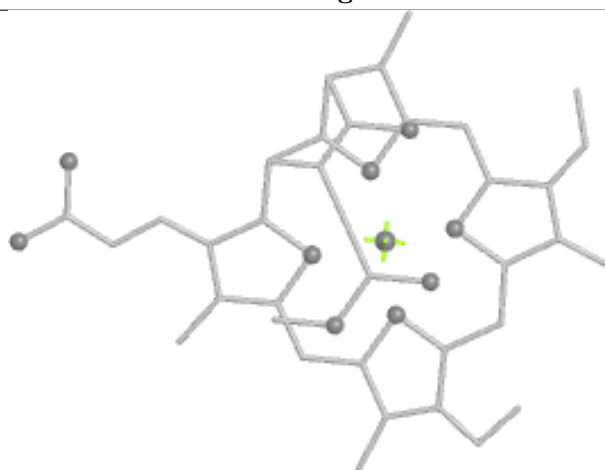
Bond lengths



Bond angles

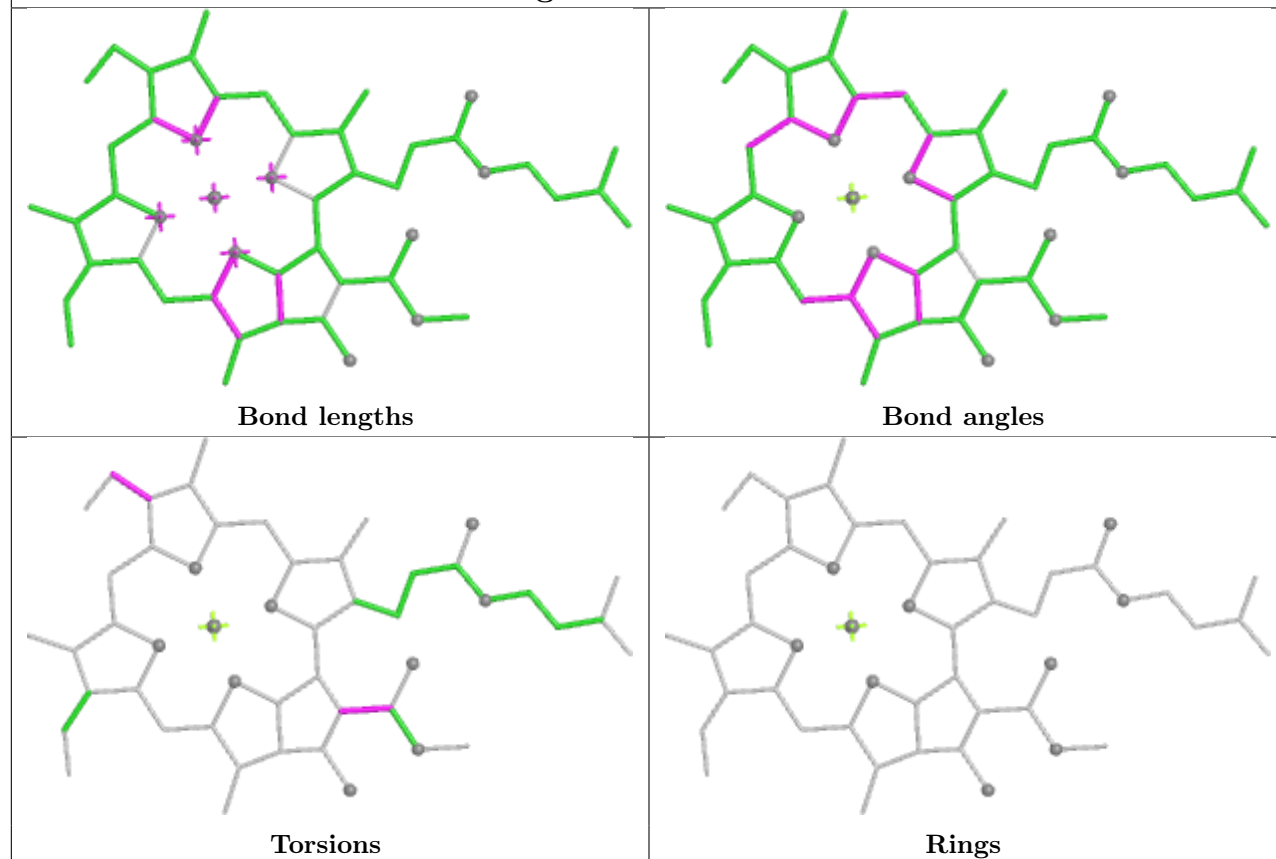


Torsions

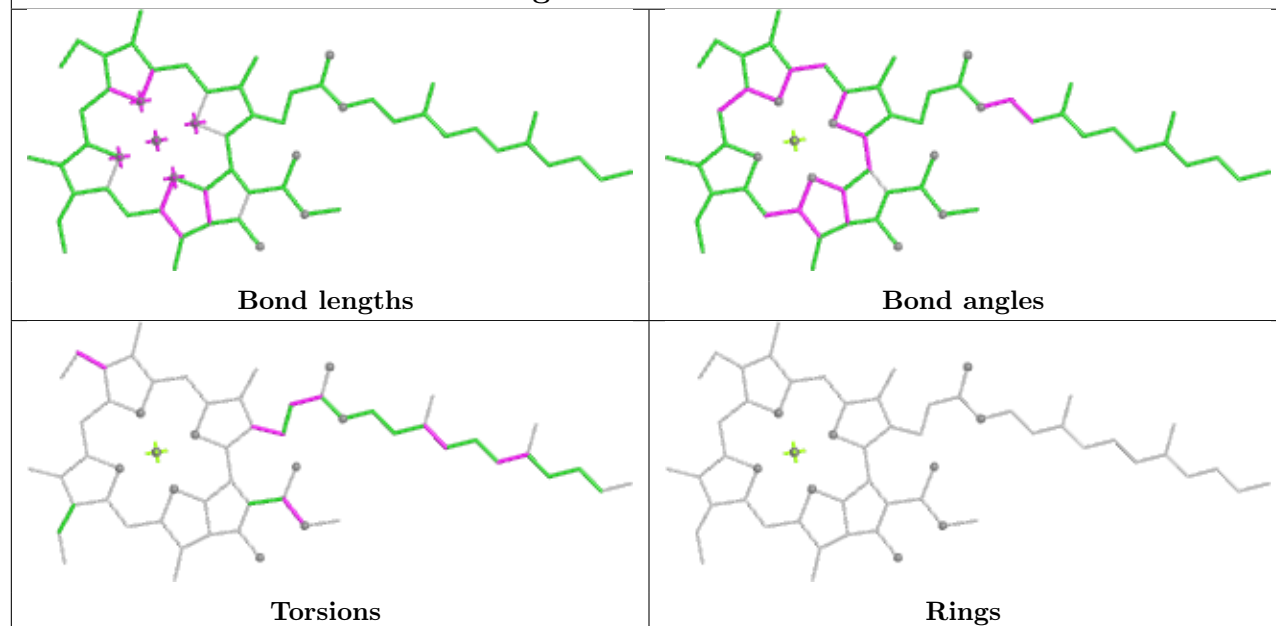


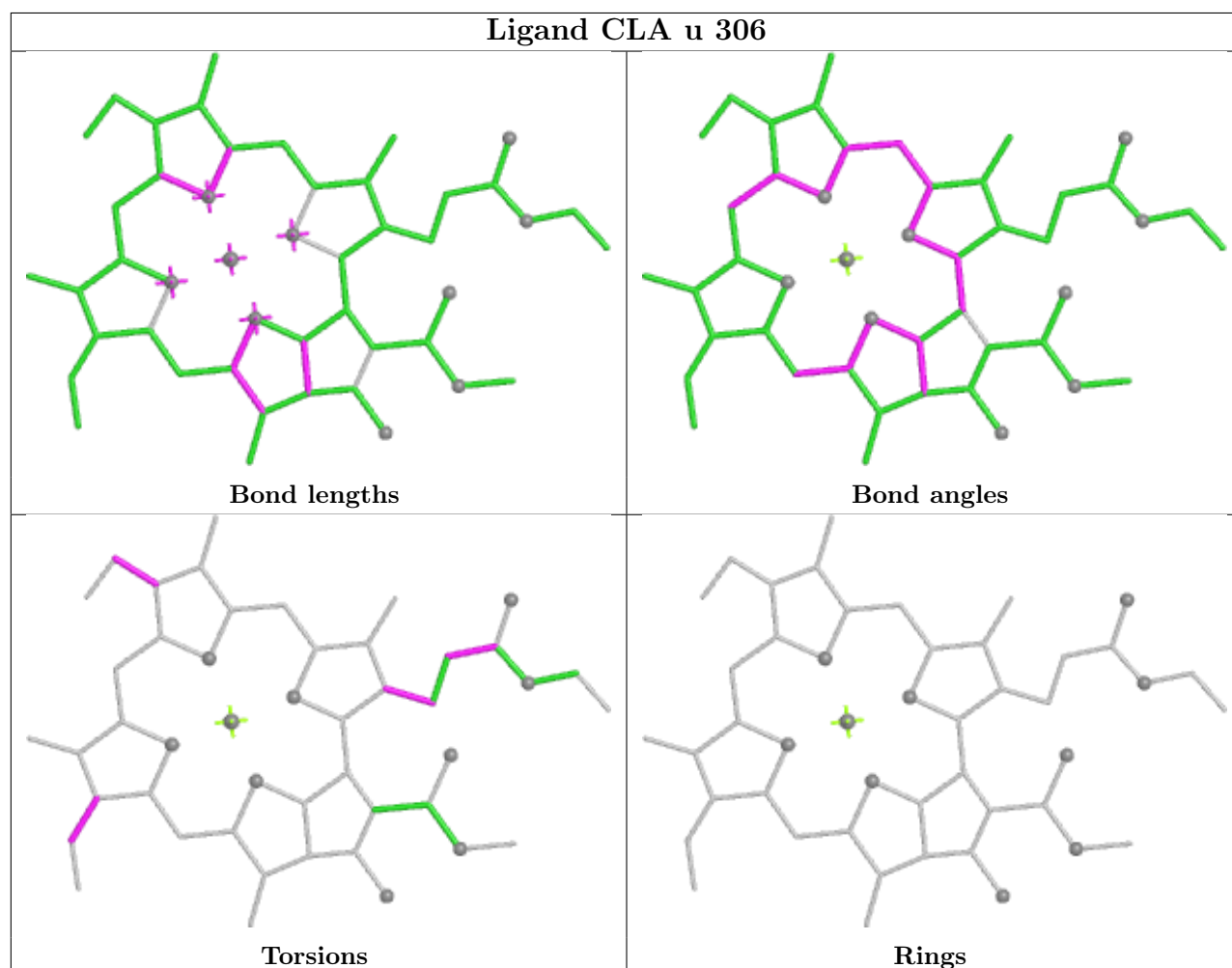
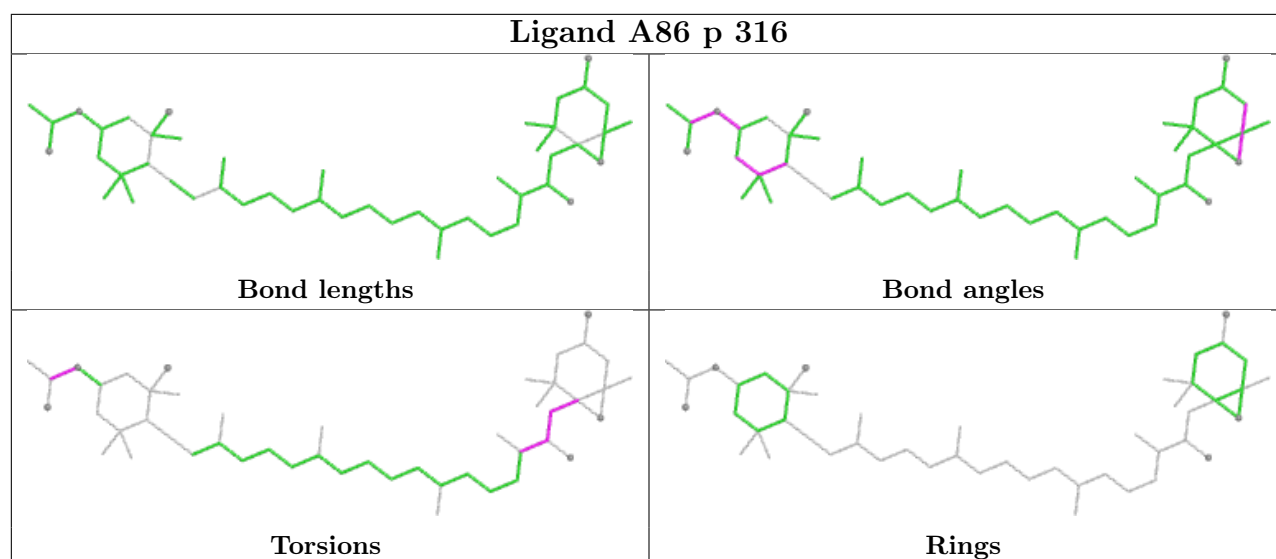
Rings

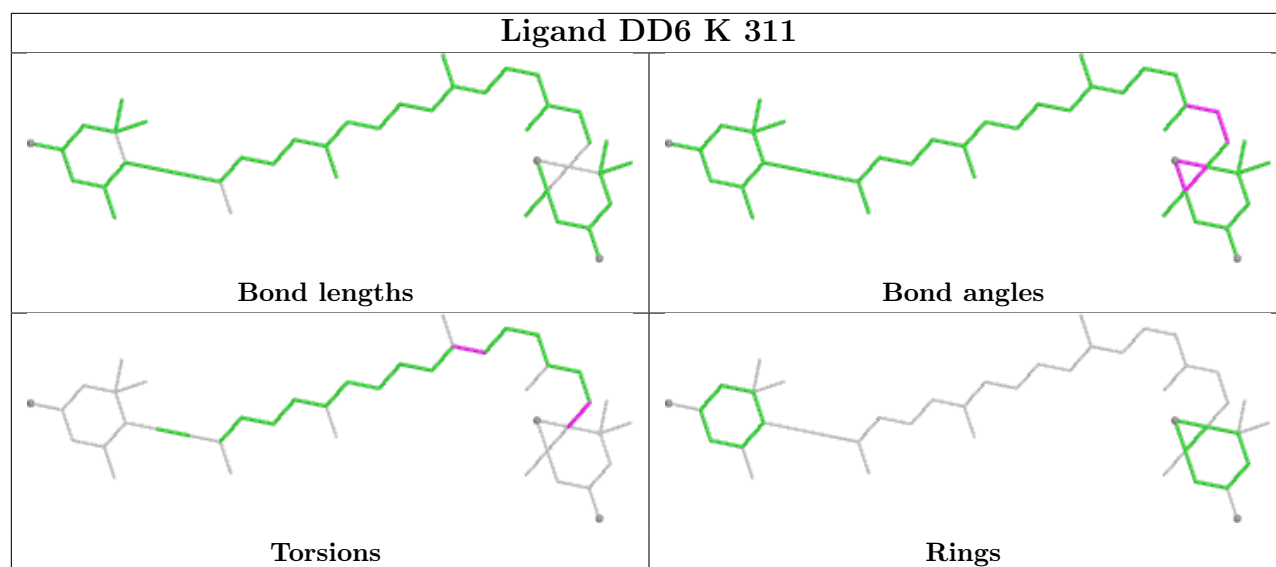
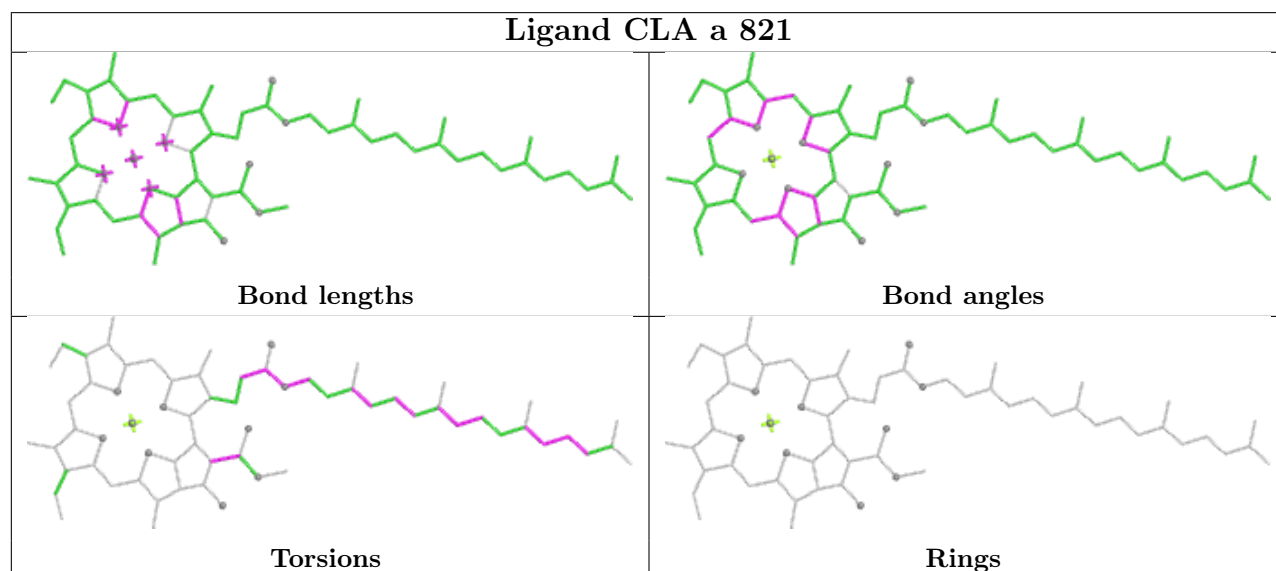
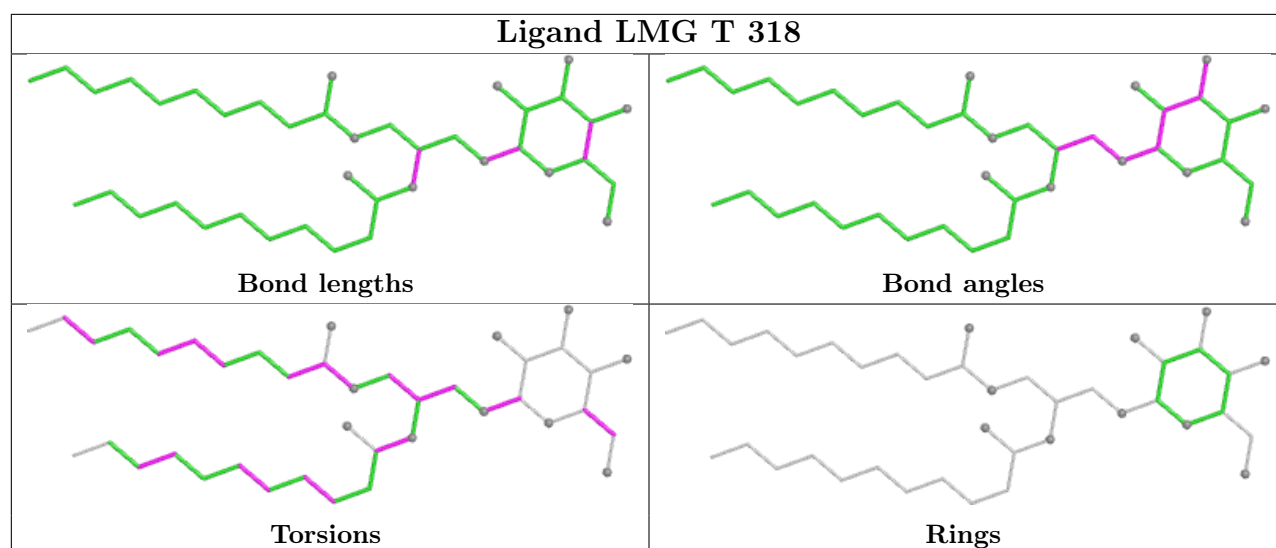
Ligand CLA a 814

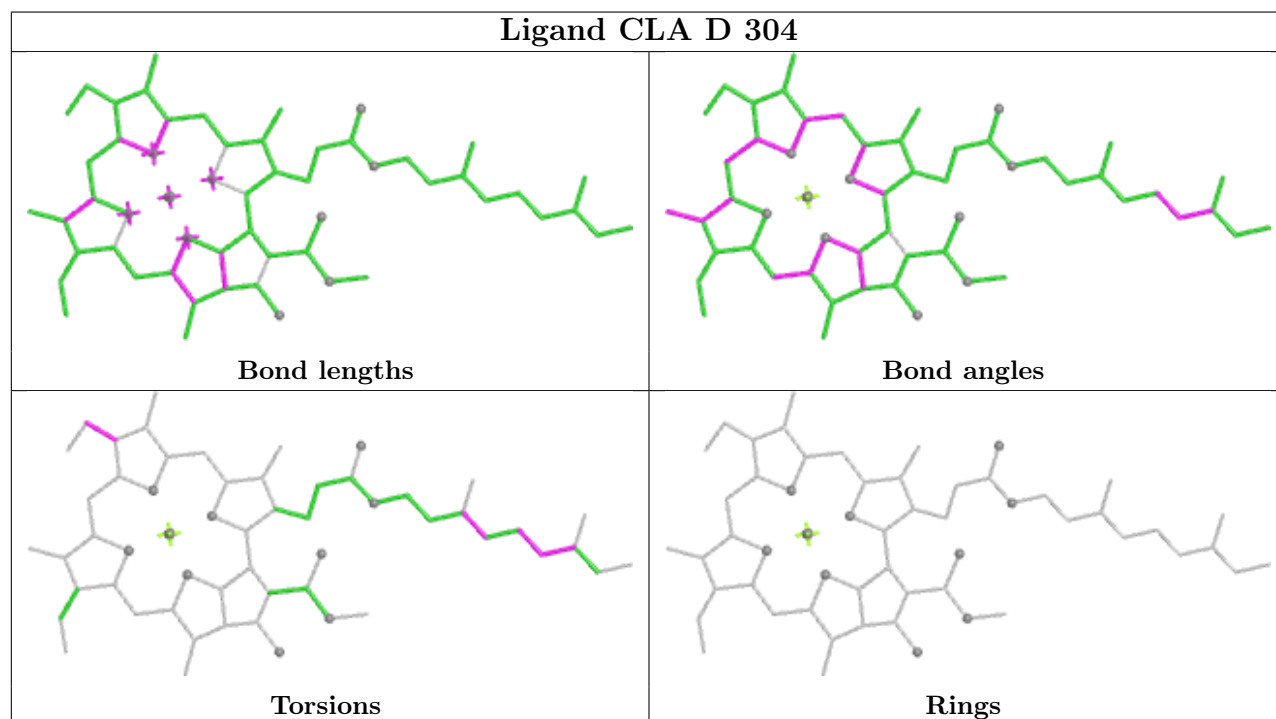
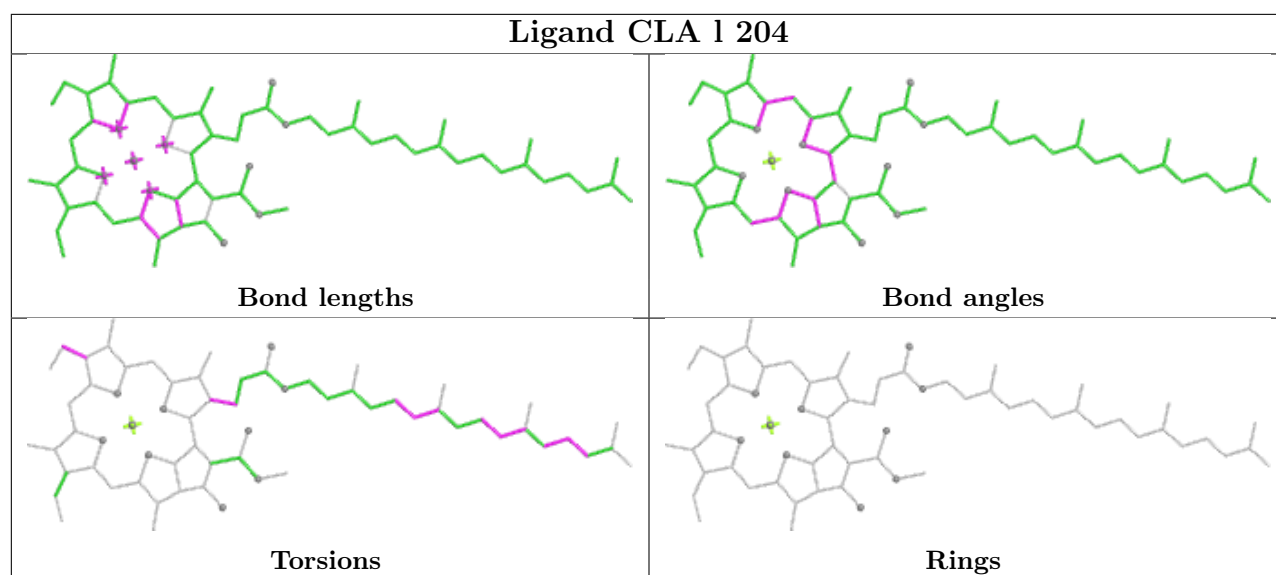


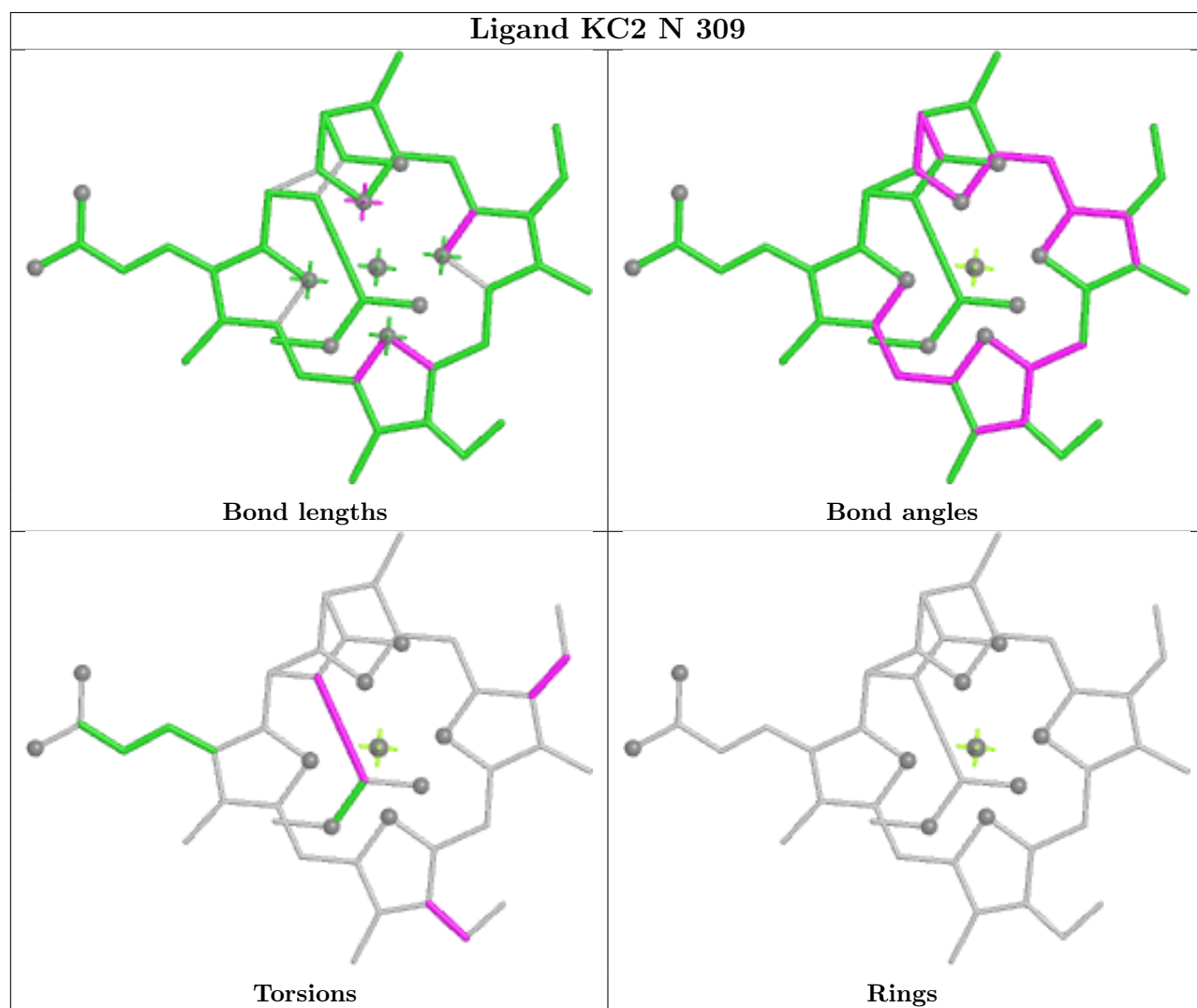
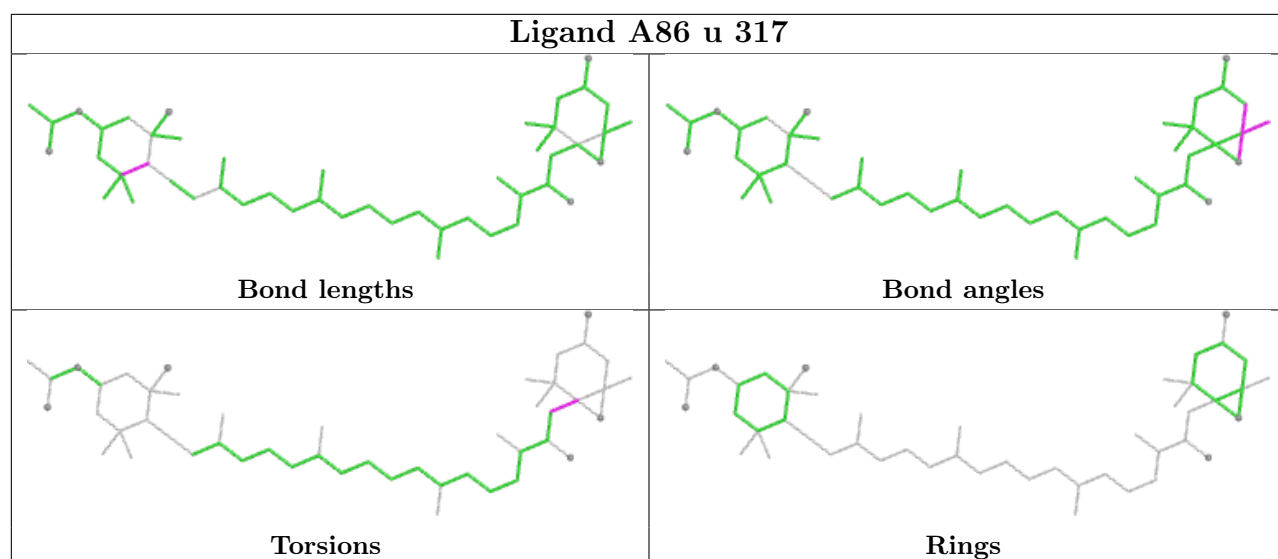
Ligand CLA T 310



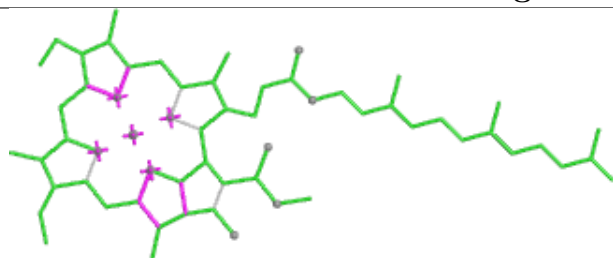




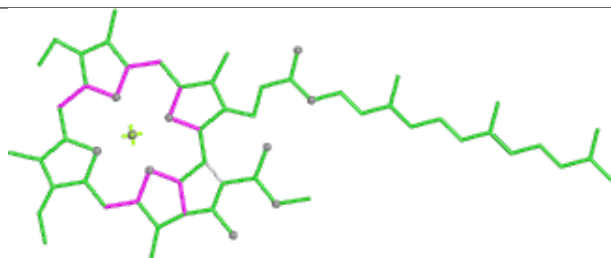




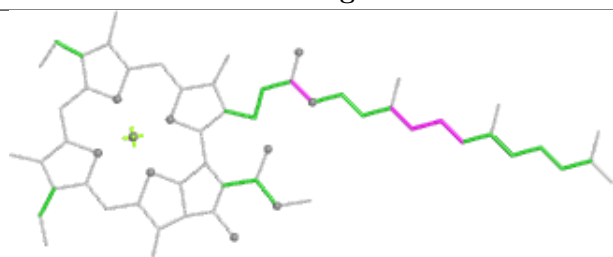
Ligand CLA R 305



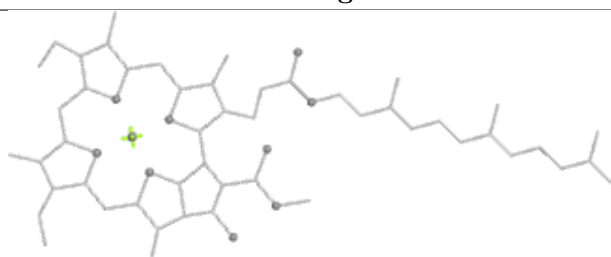
Bond lengths



Bond angles

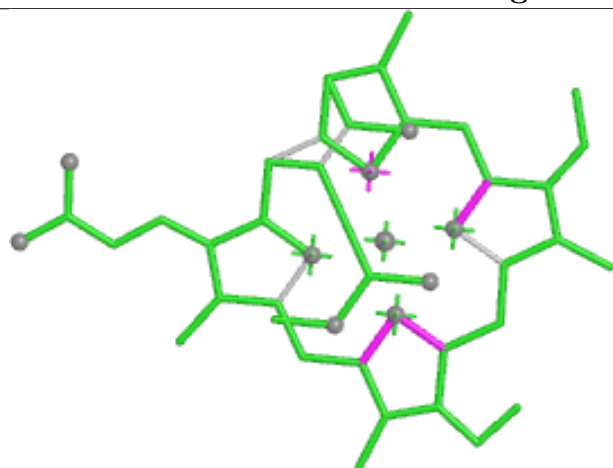


Torsions

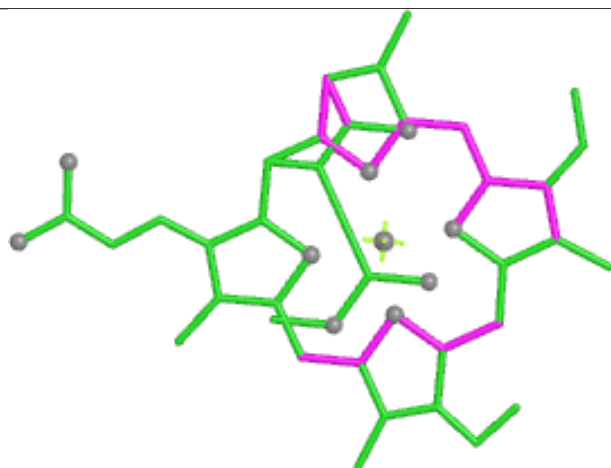


Rings

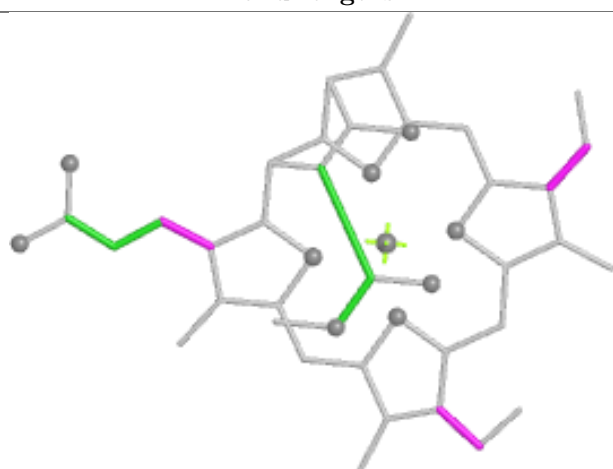
Ligand KC2 W 302



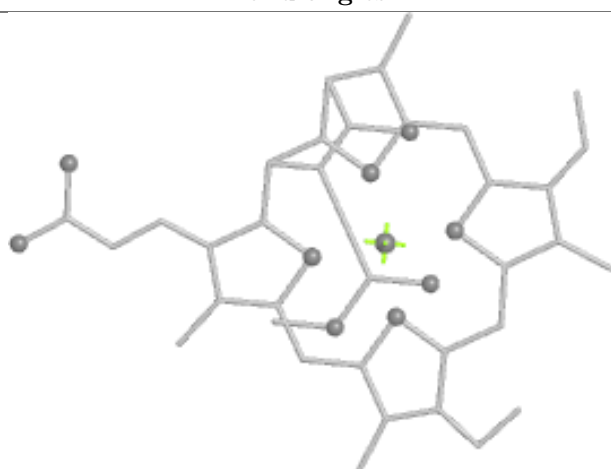
Bond lengths



Bond angles

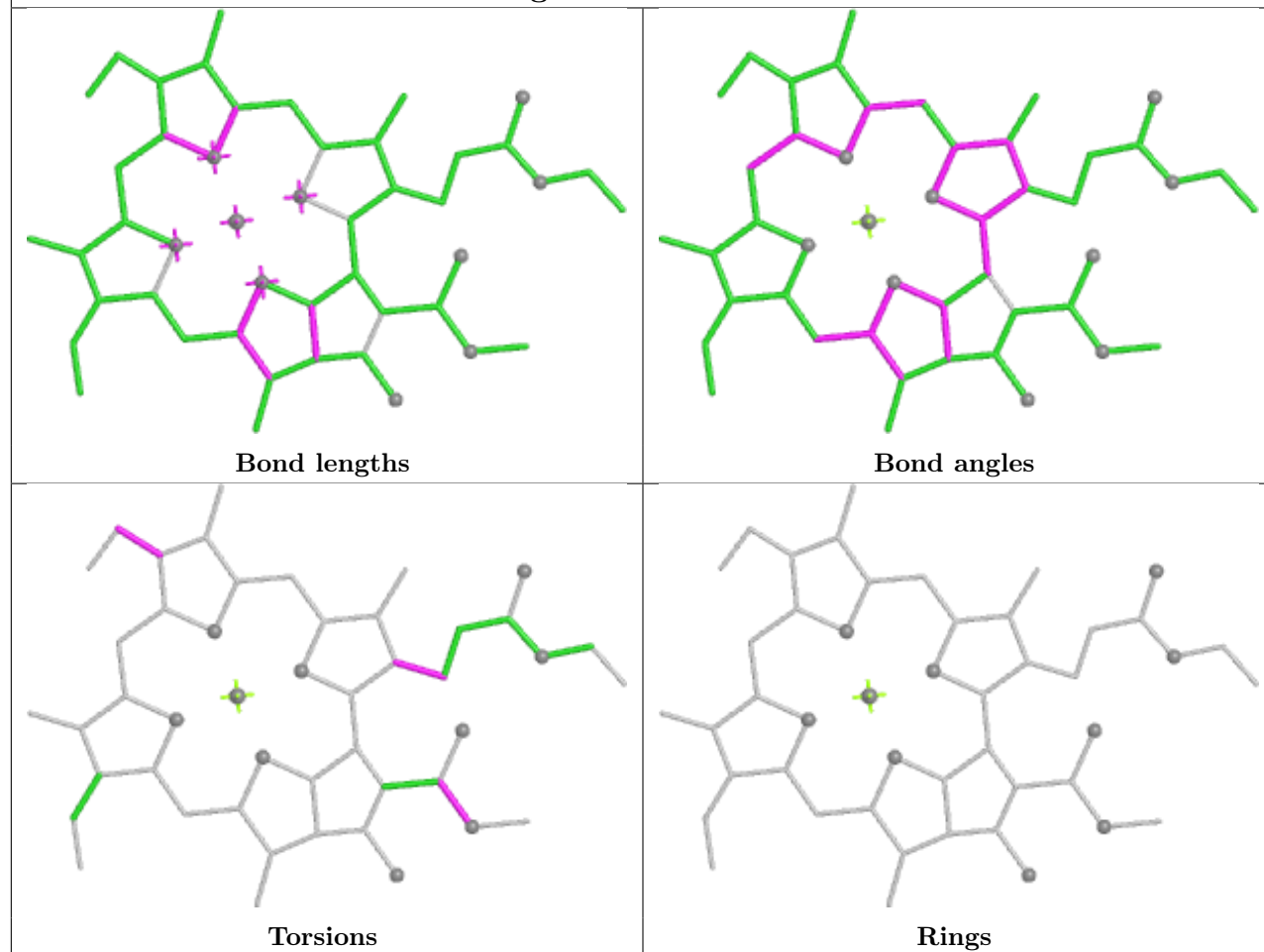


Torsions

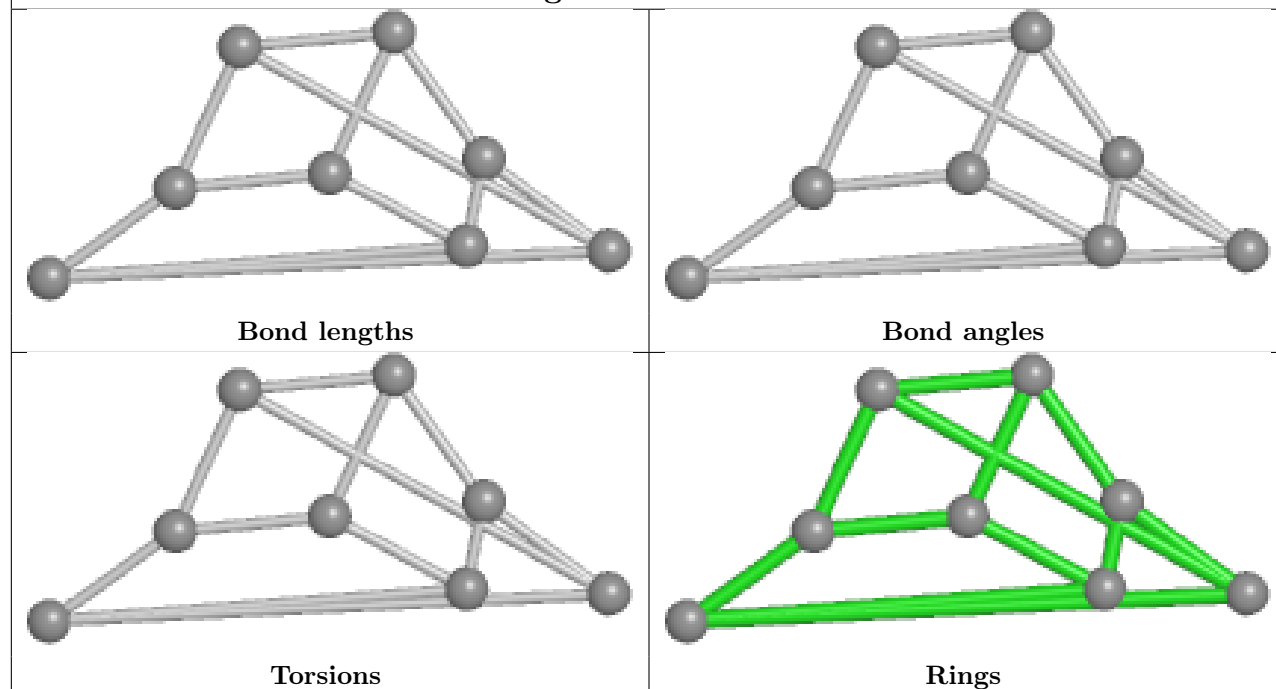


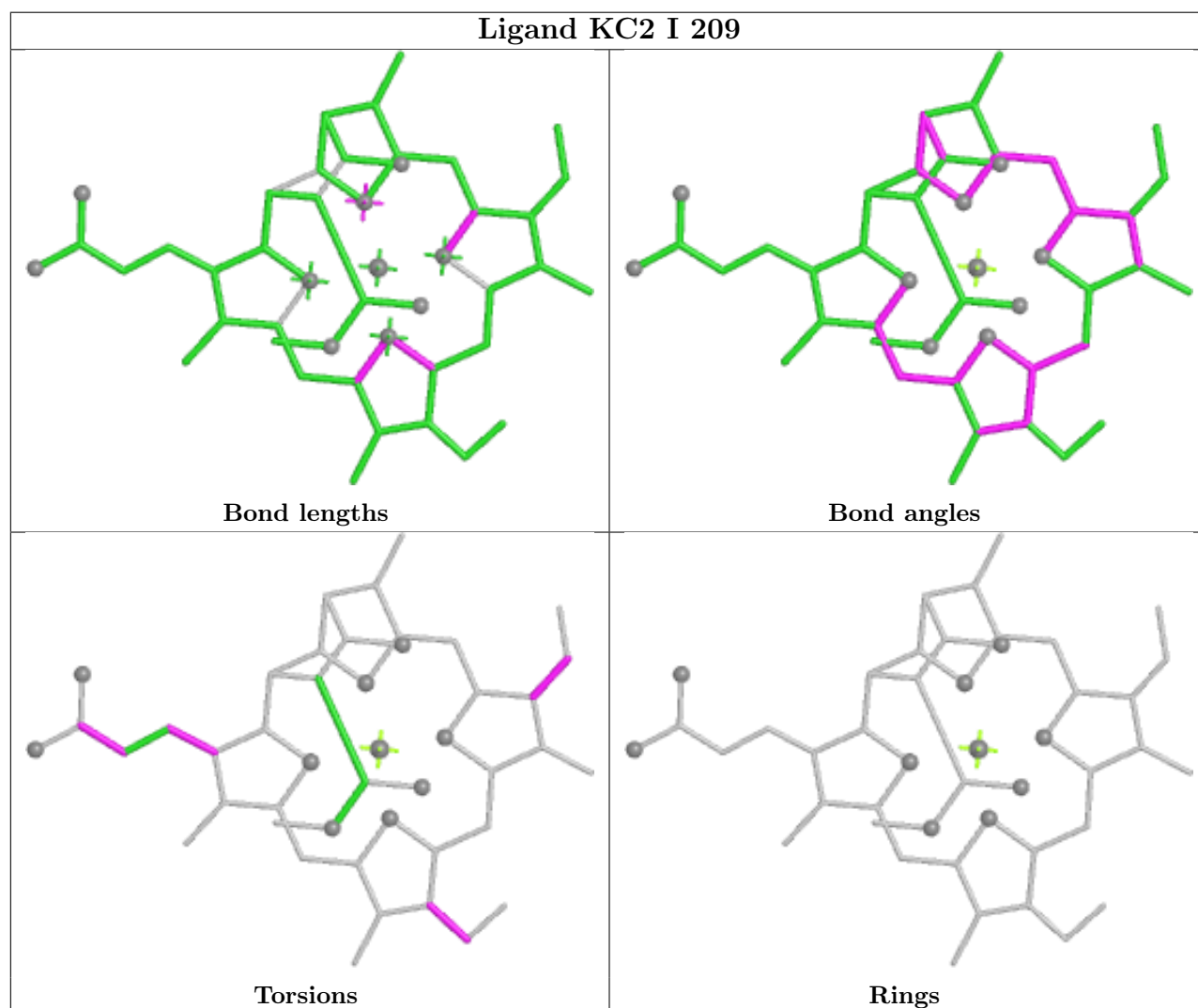
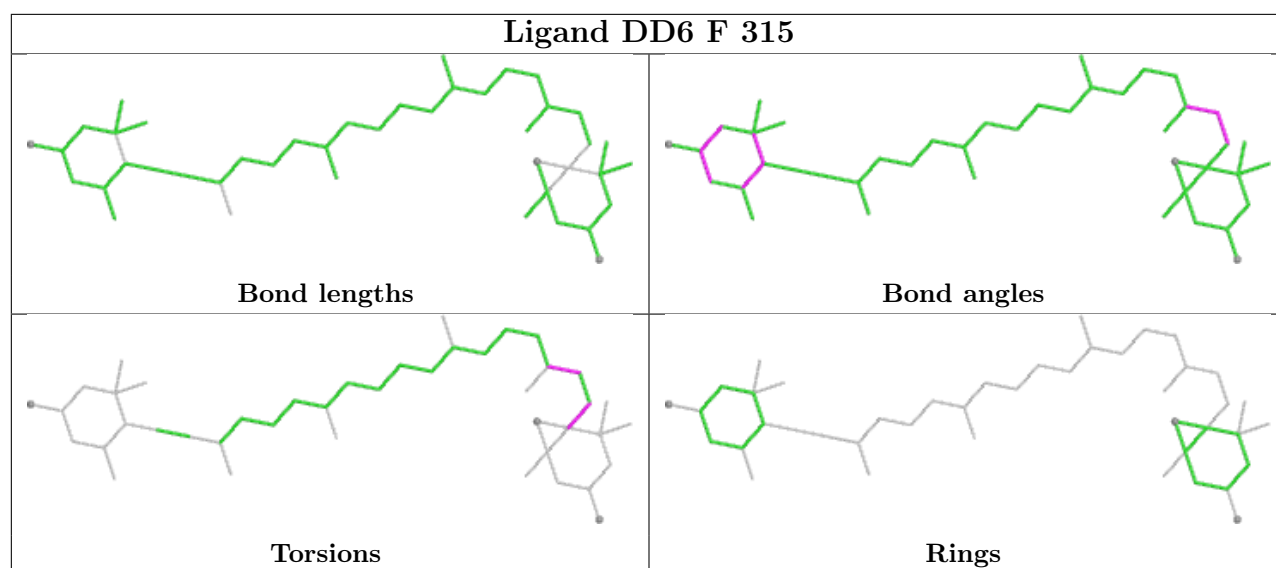
Rings

Ligand CLA S 311

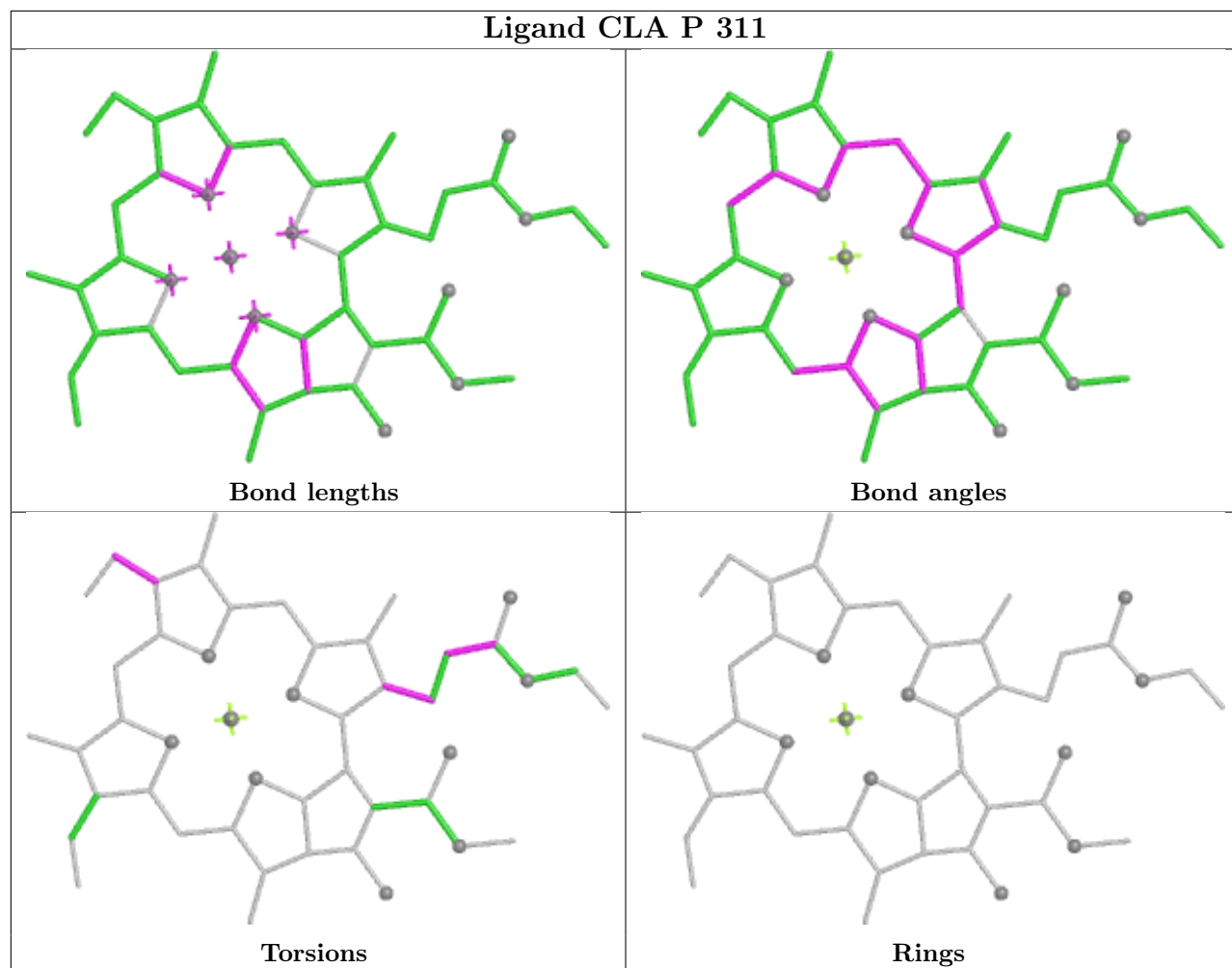


Ligand SF4 c 102

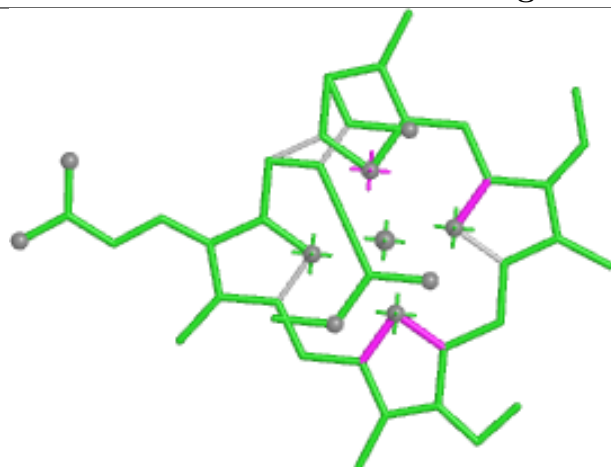




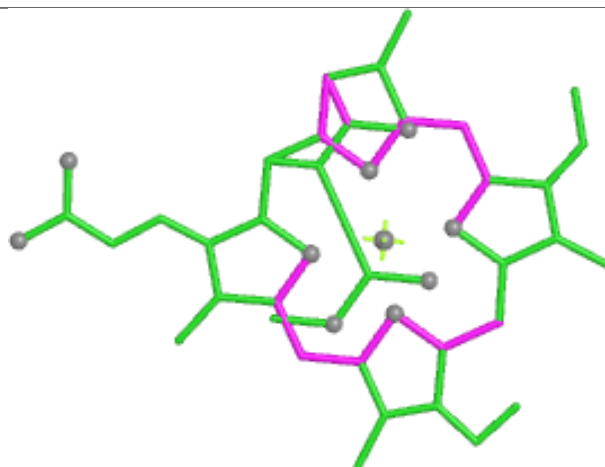
Ligand CLA P 311



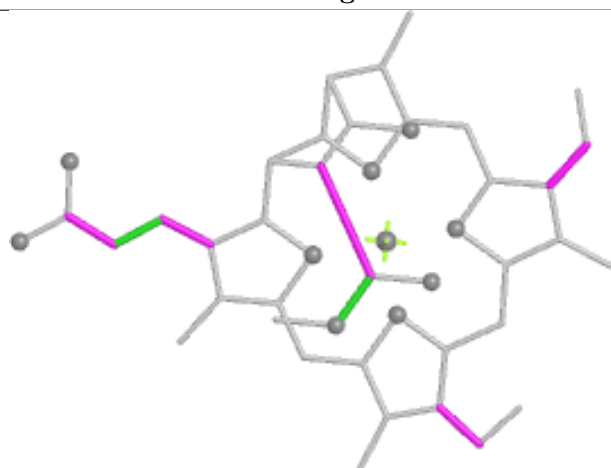
Ligand KC2 E 319



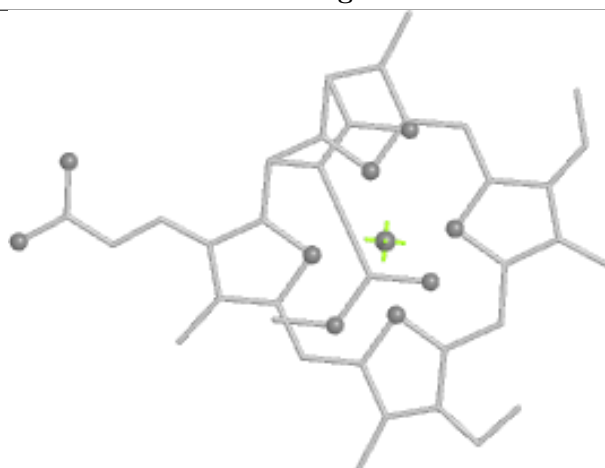
Bond lengths



Bond angles



Torsions



Rings

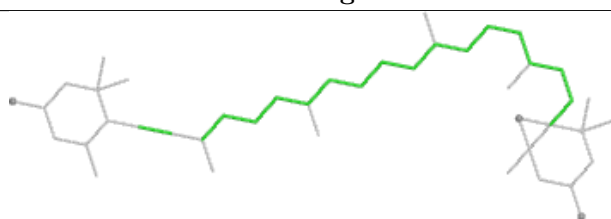
Ligand DD6 y 311



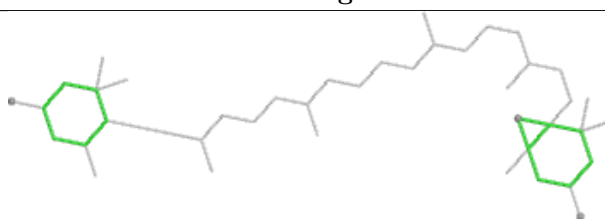
Bond lengths



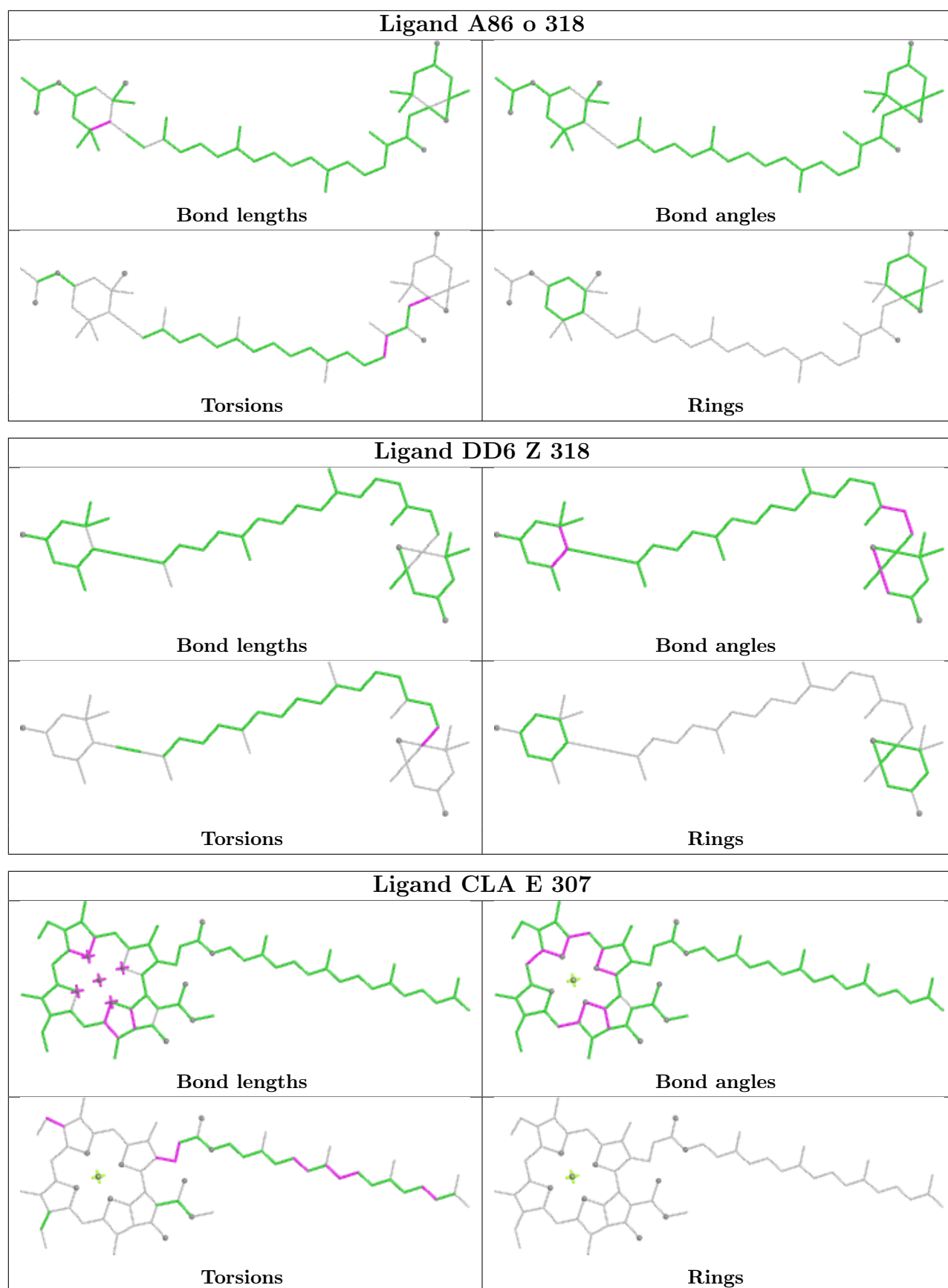
Bond angles

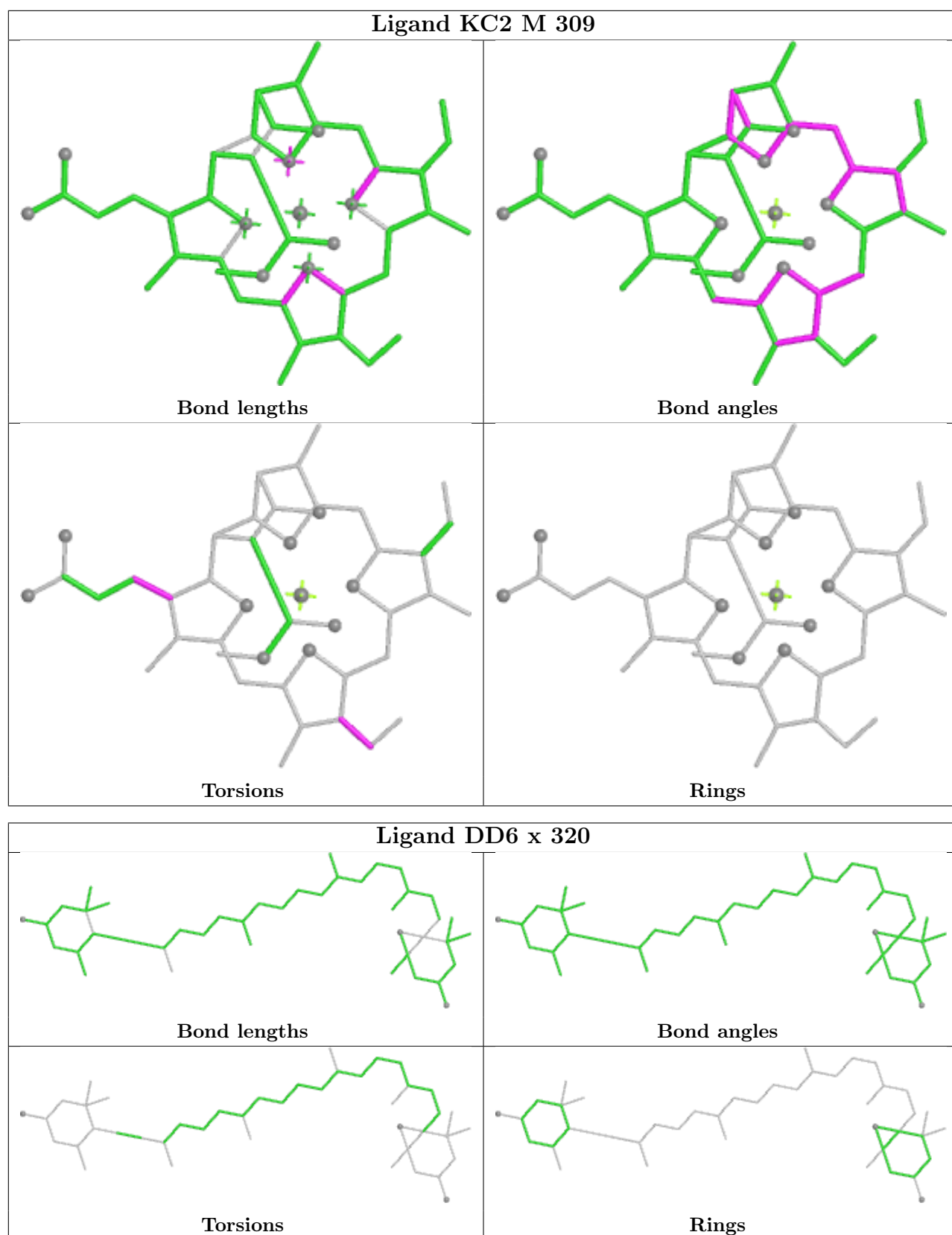


Torsions

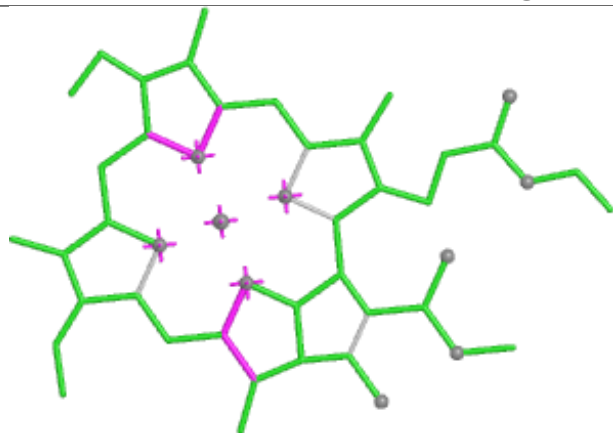


Rings

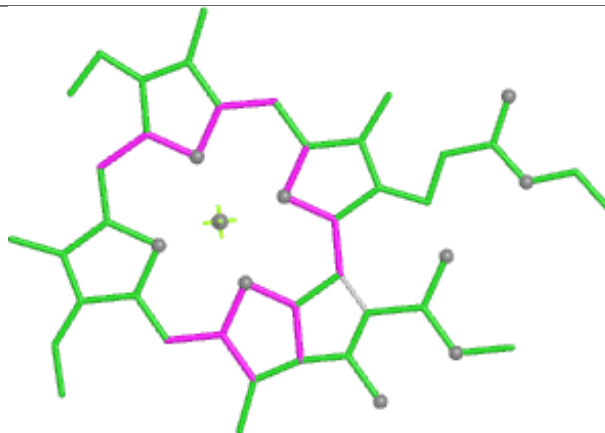




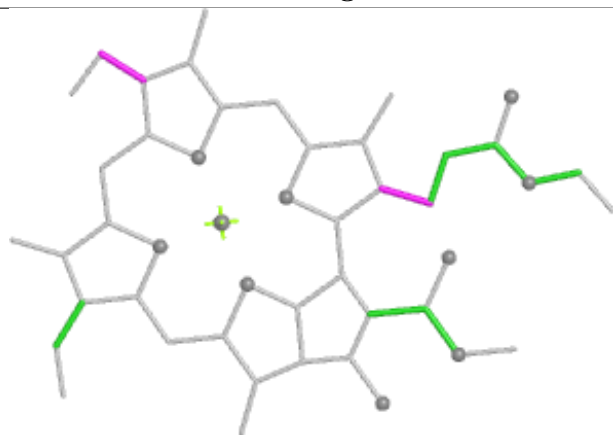
Ligand CLA J 303



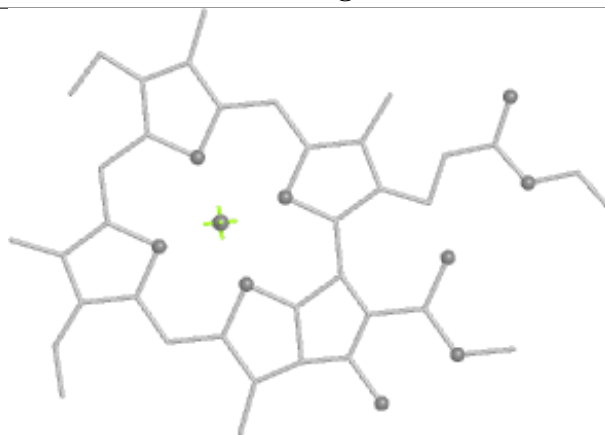
Bond lengths



Bond angles

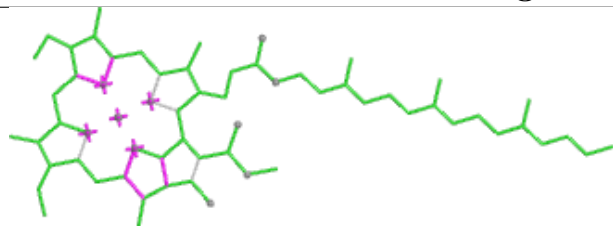


Torsions

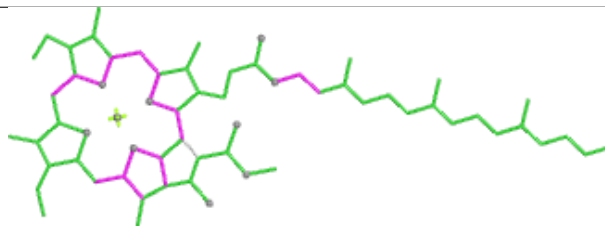


Rings

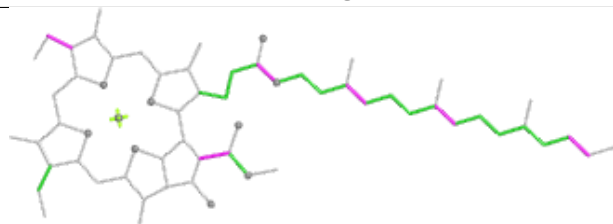
Ligand CLA Z 311



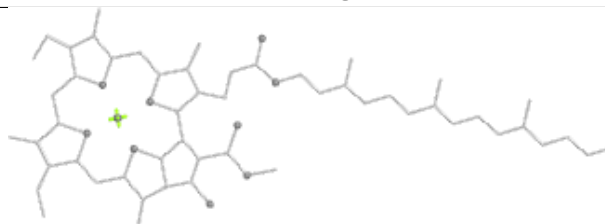
Bond lengths



Bond angles

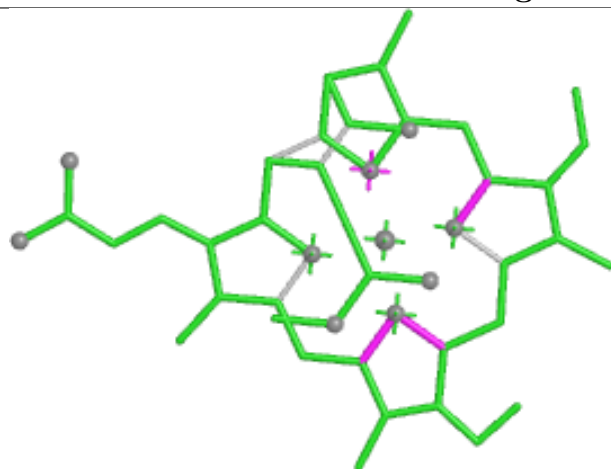


Torsions

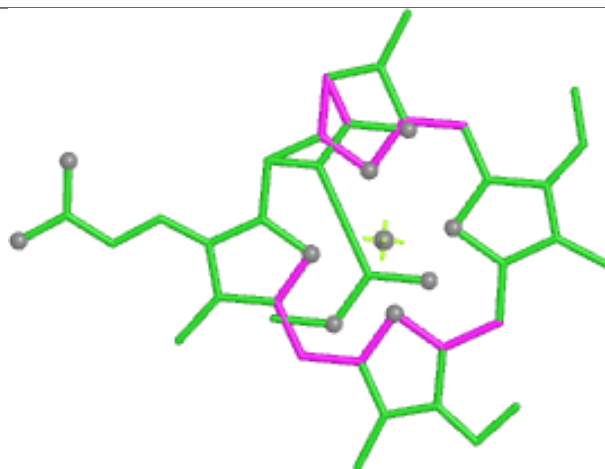


Rings

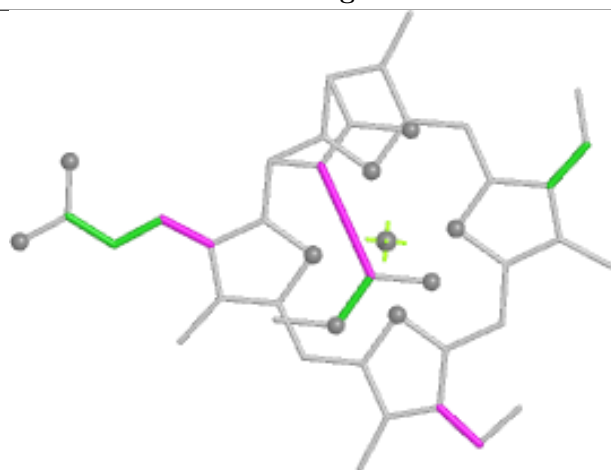
Ligand KC2 G 208



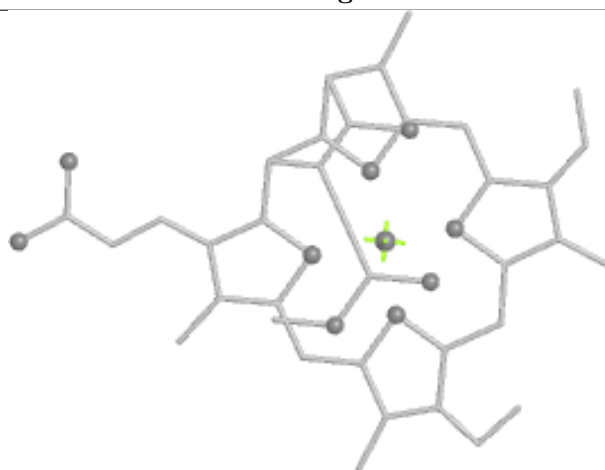
Bond lengths



Bond angles



Torsions



Rings

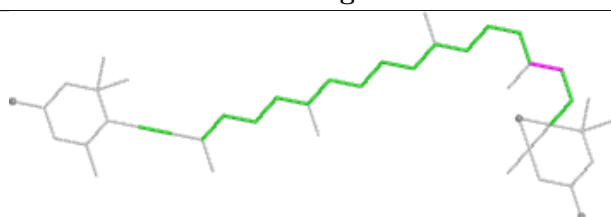
Ligand DD6 N 316



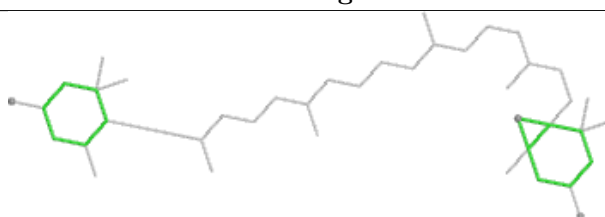
Bond lengths



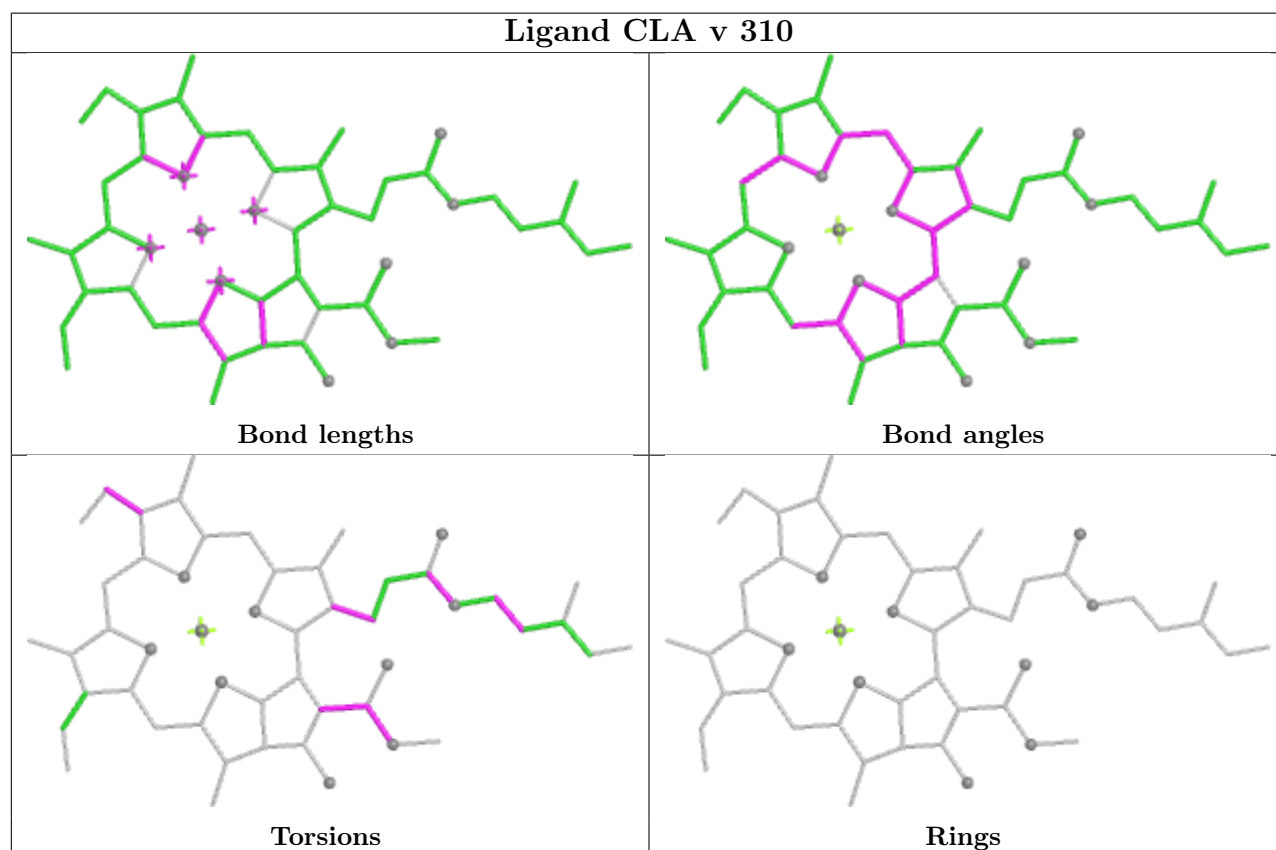
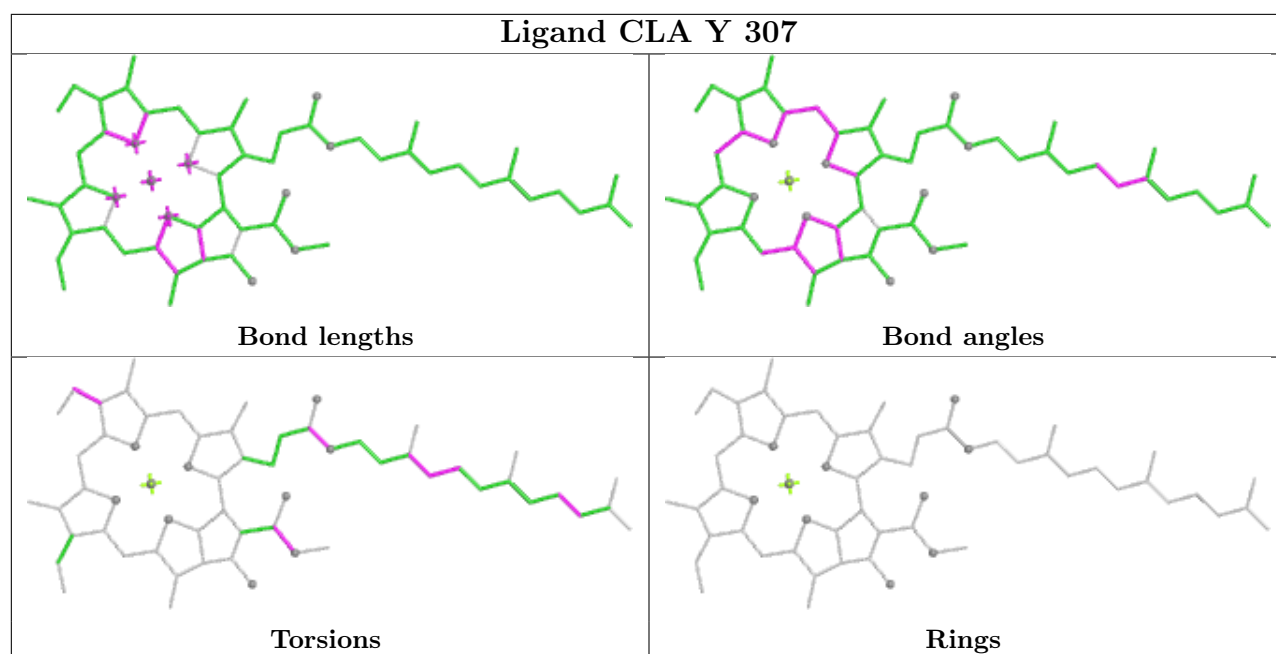
Bond angles



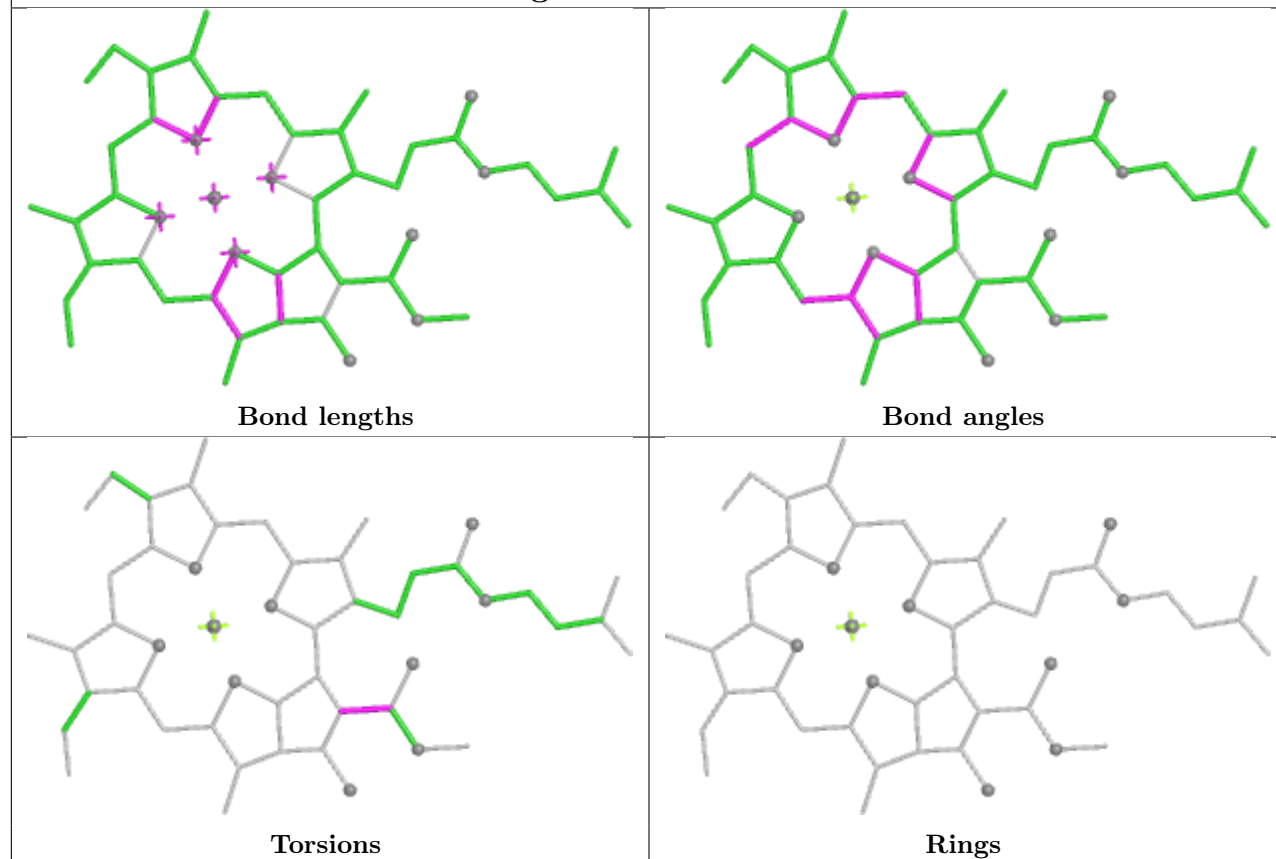
Torsions



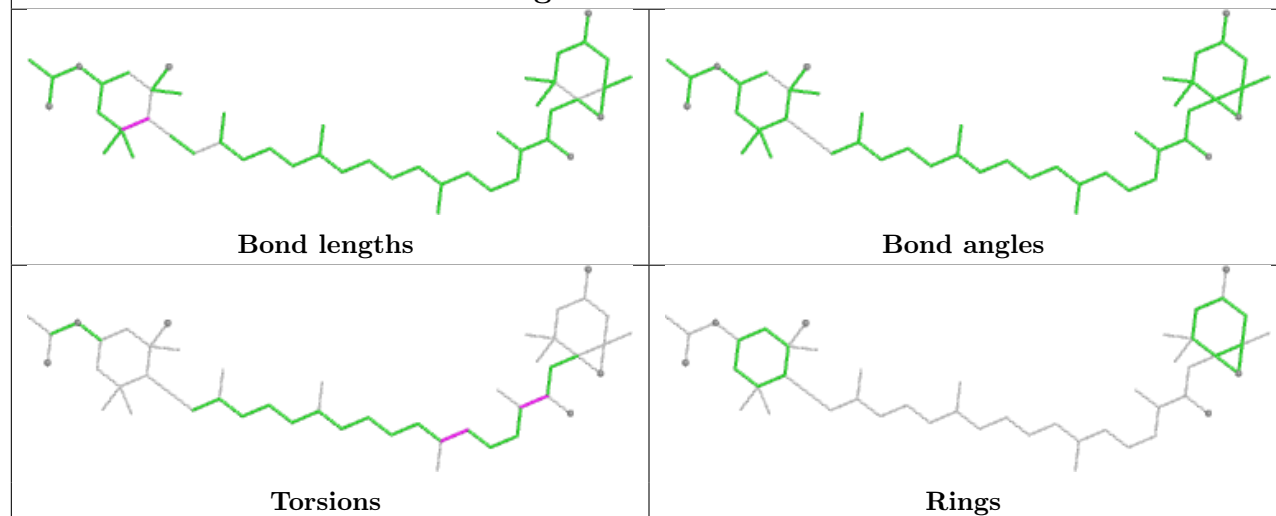
Rings

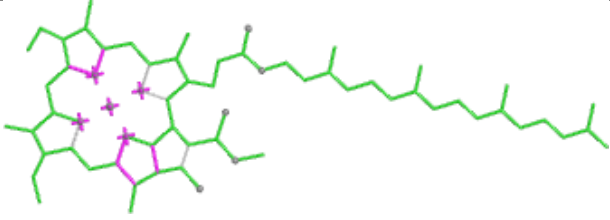
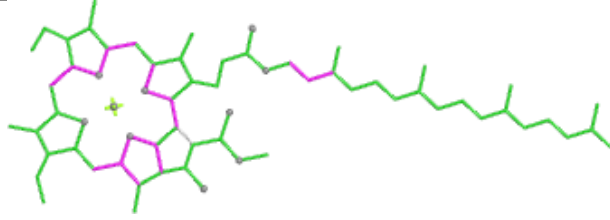
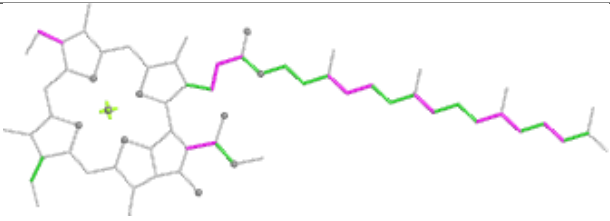
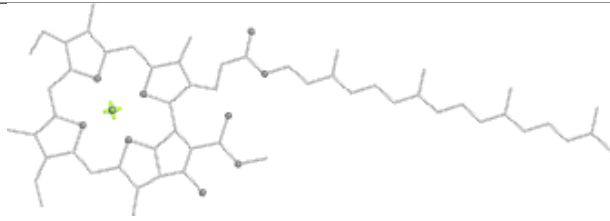
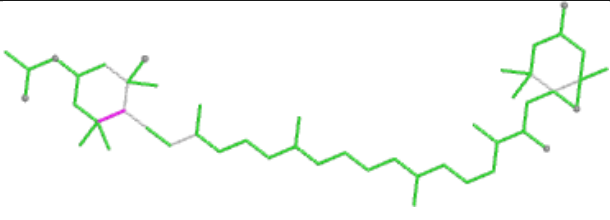
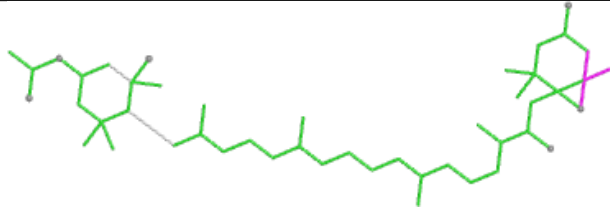
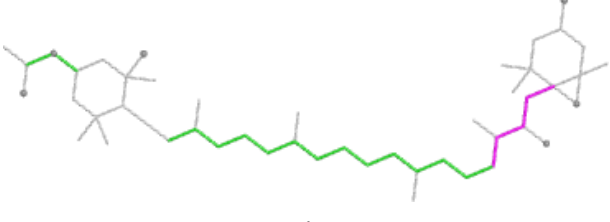
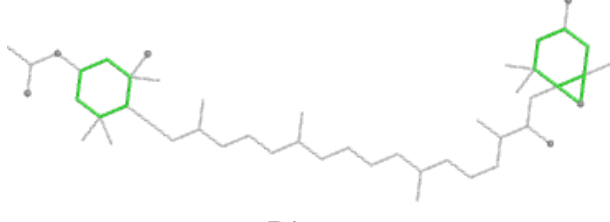
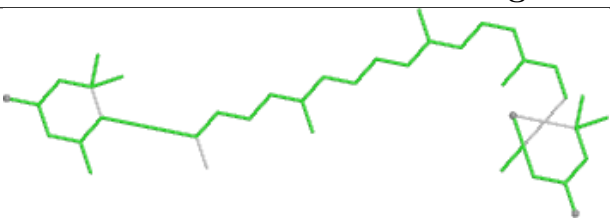
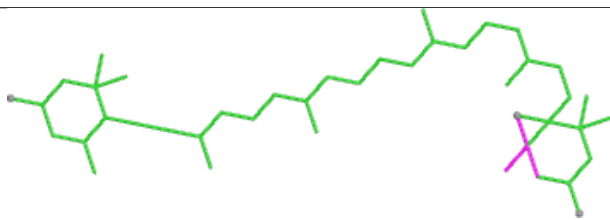
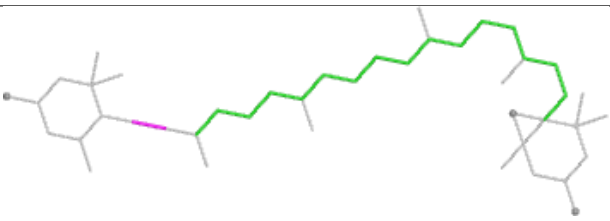
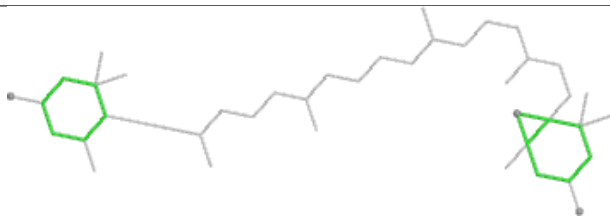


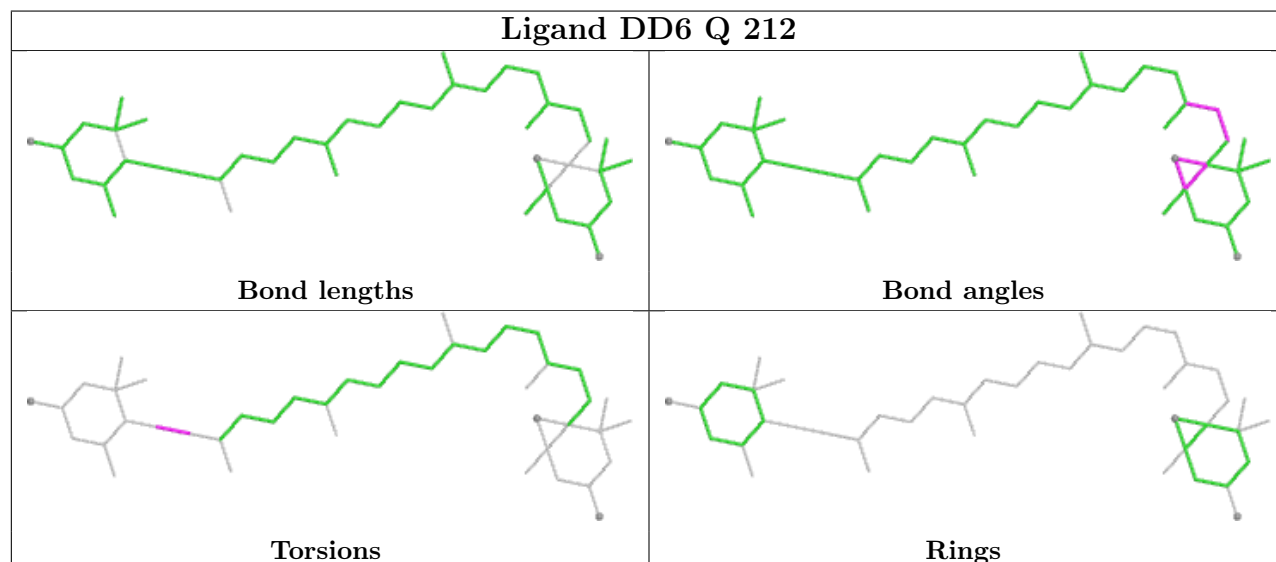
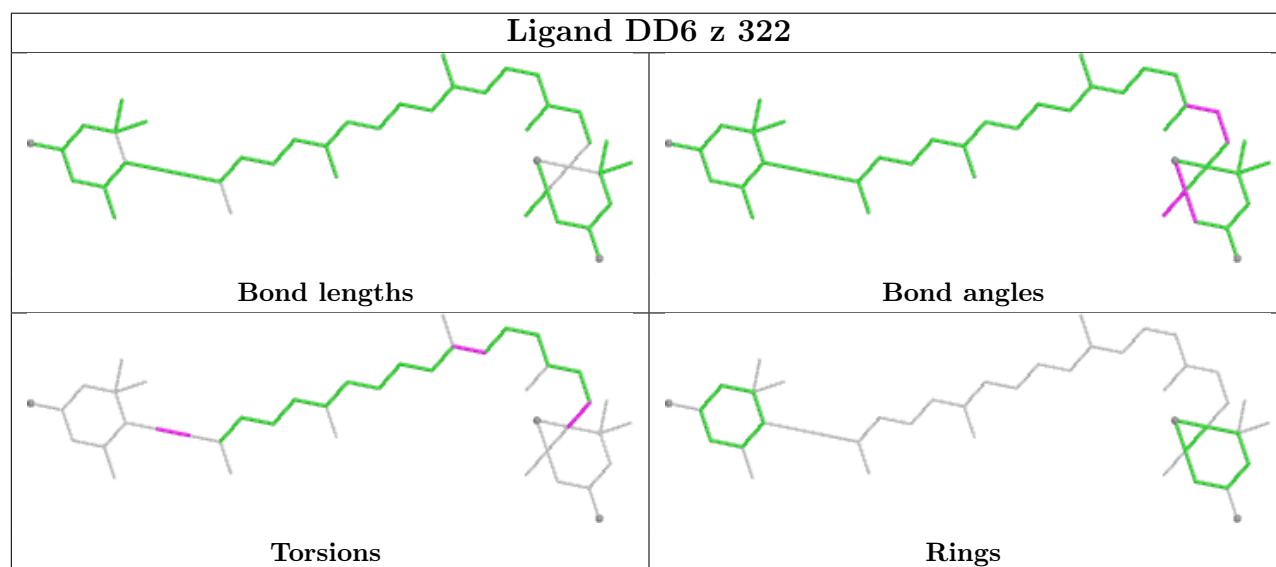
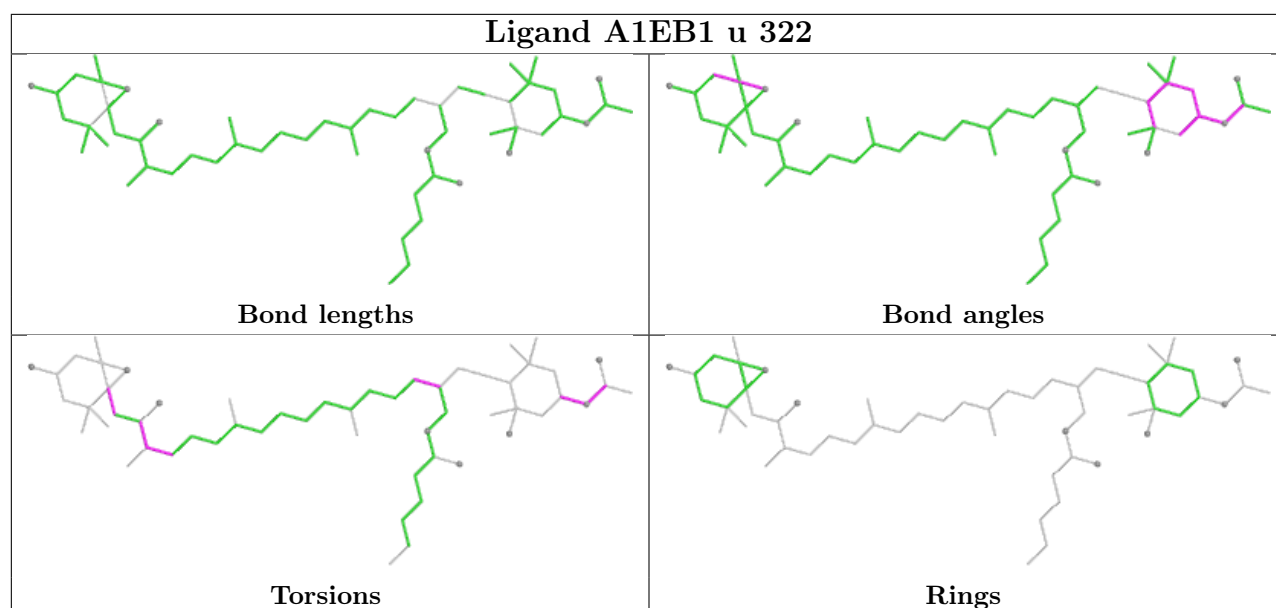
Ligand CLA G 205

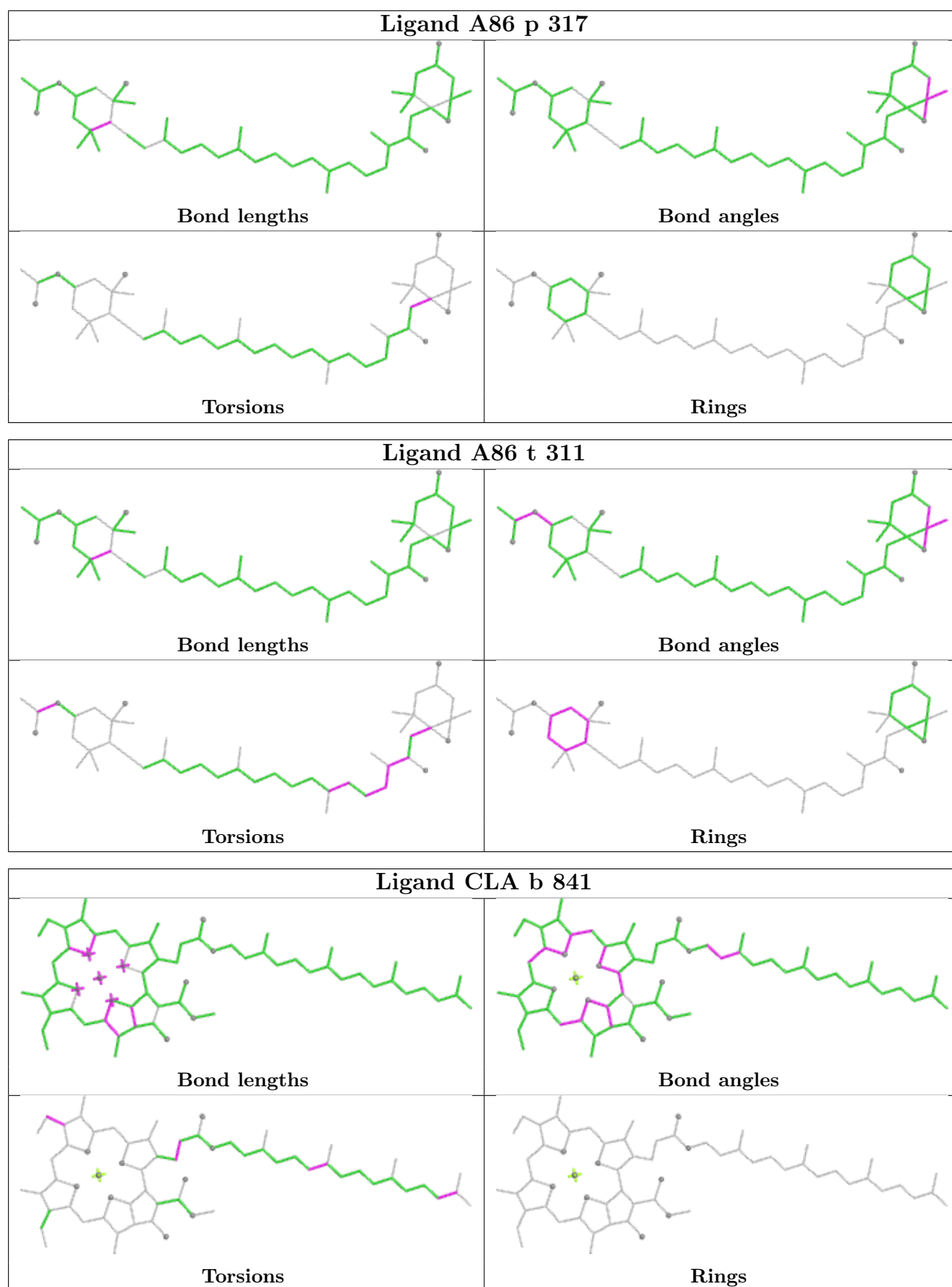


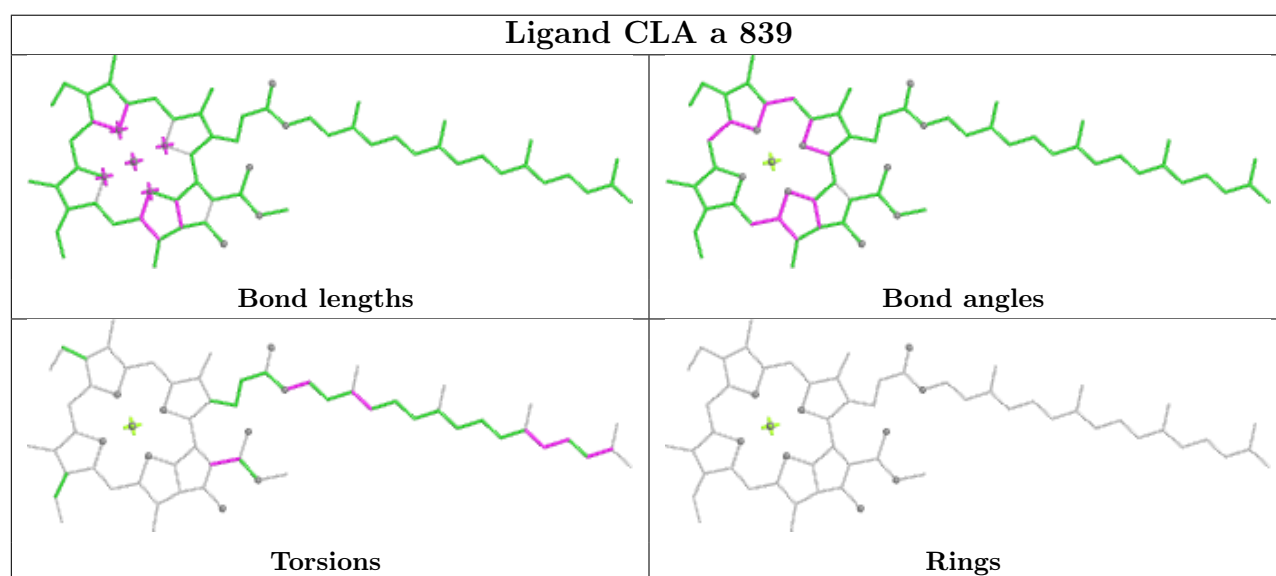
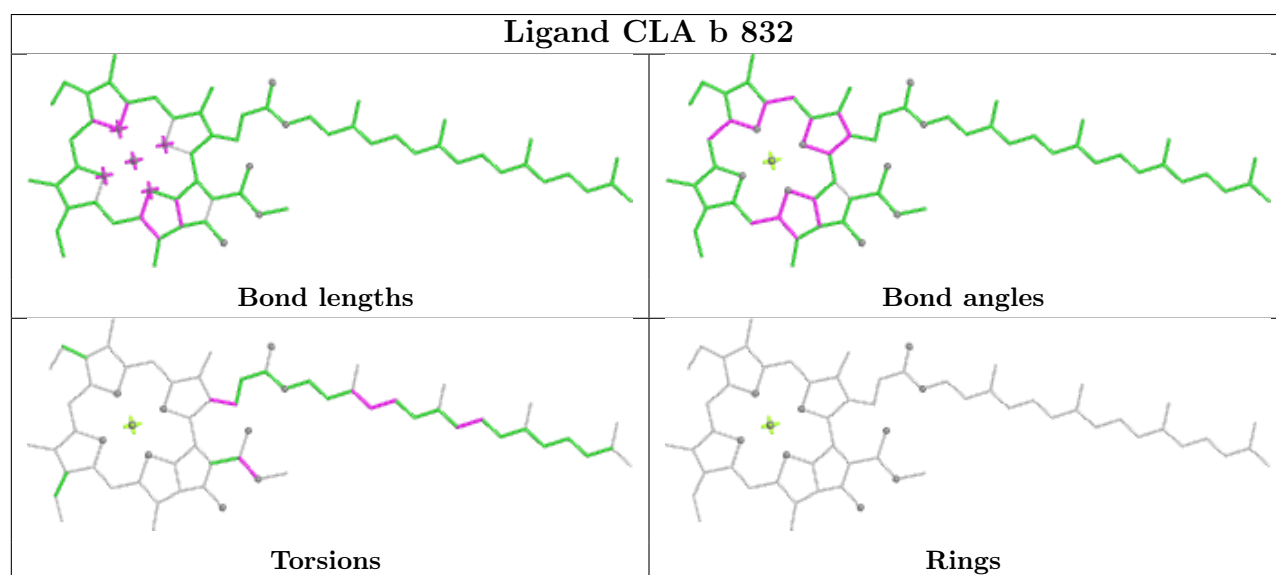
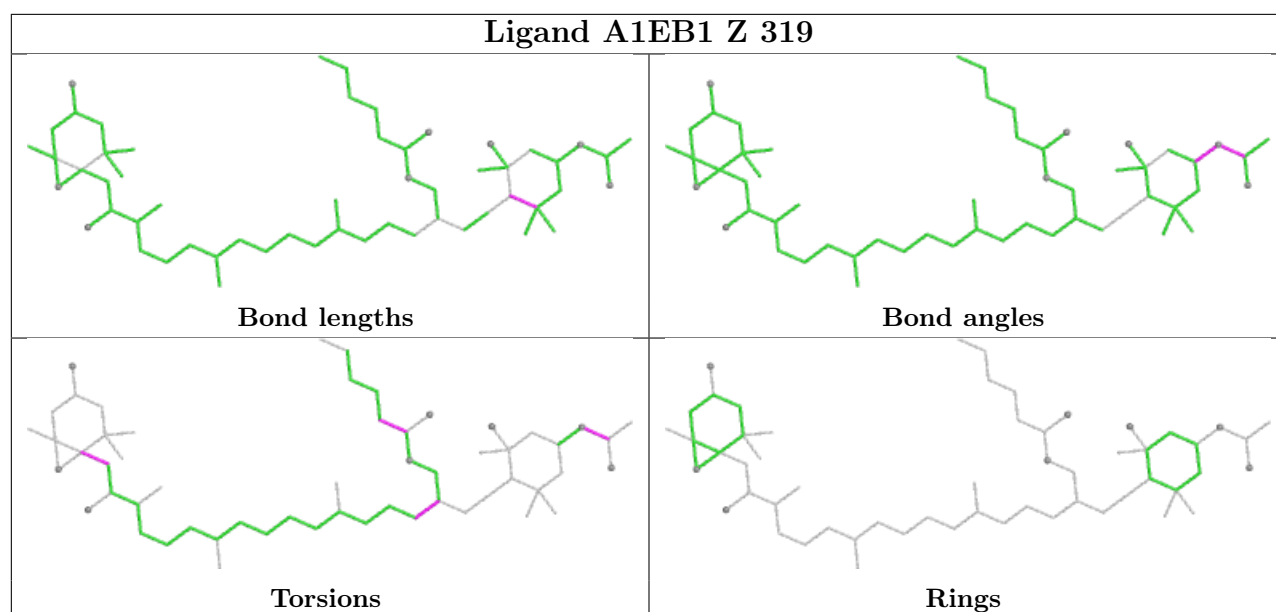
Ligand A86 M 320

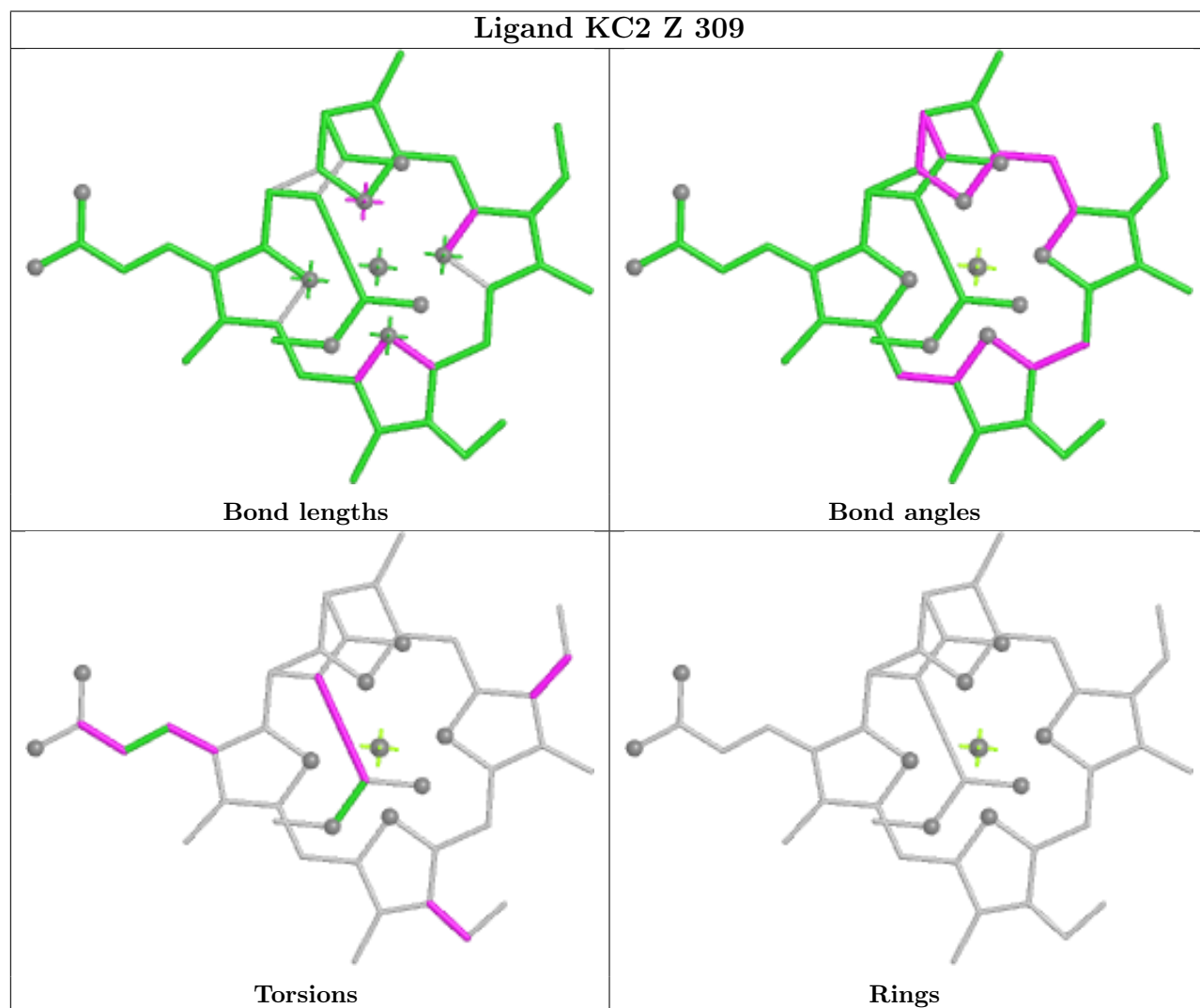
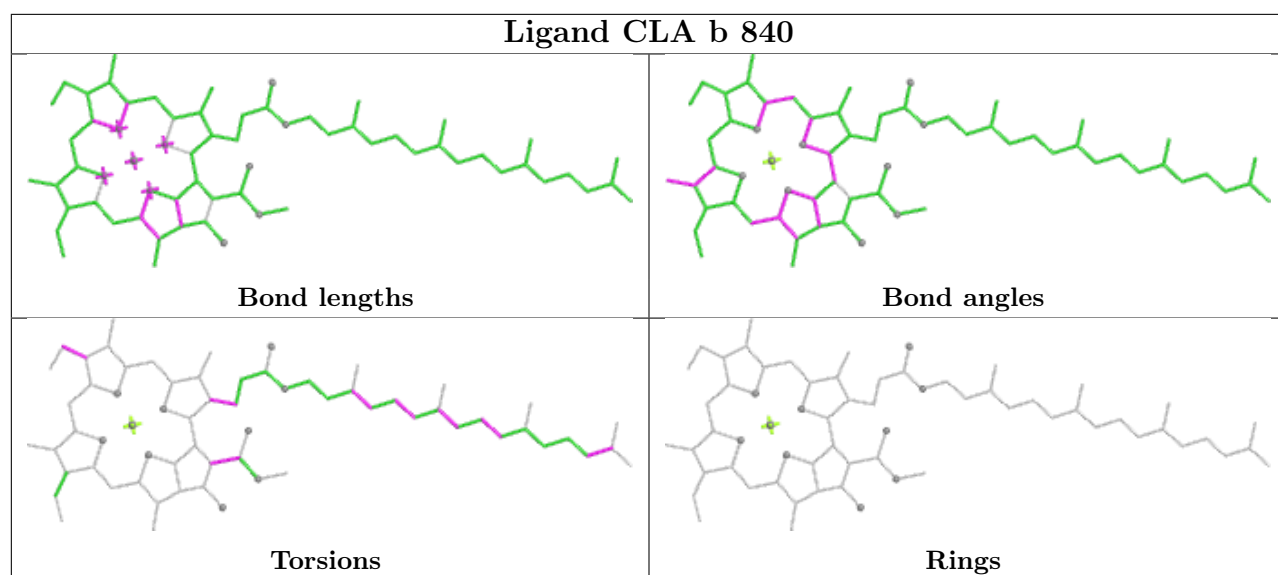


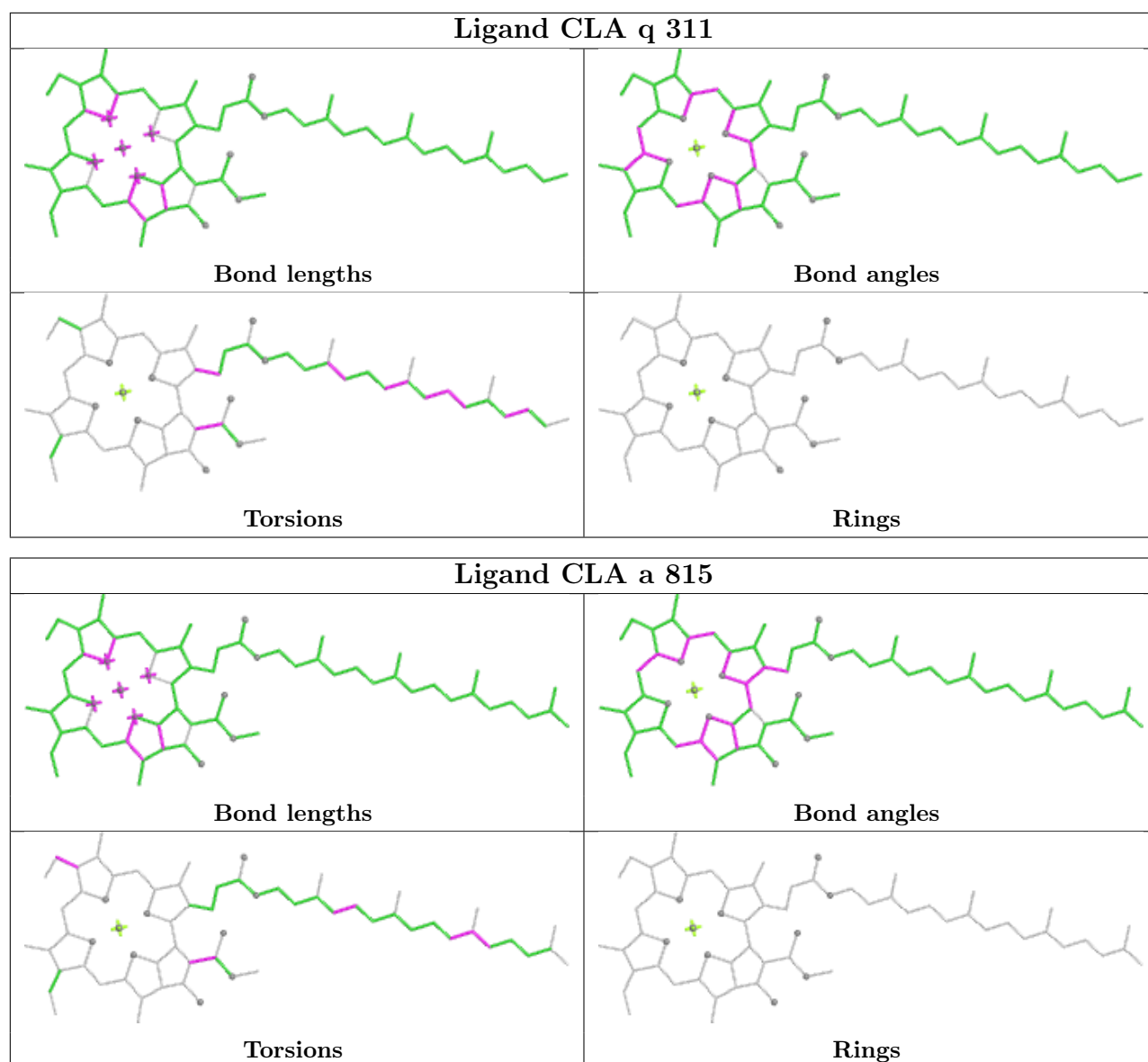
Ligand CLA b 803	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A86 O 312	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DD6 U 209	
 Bond lengths	 Bond angles
 Torsions	 Rings

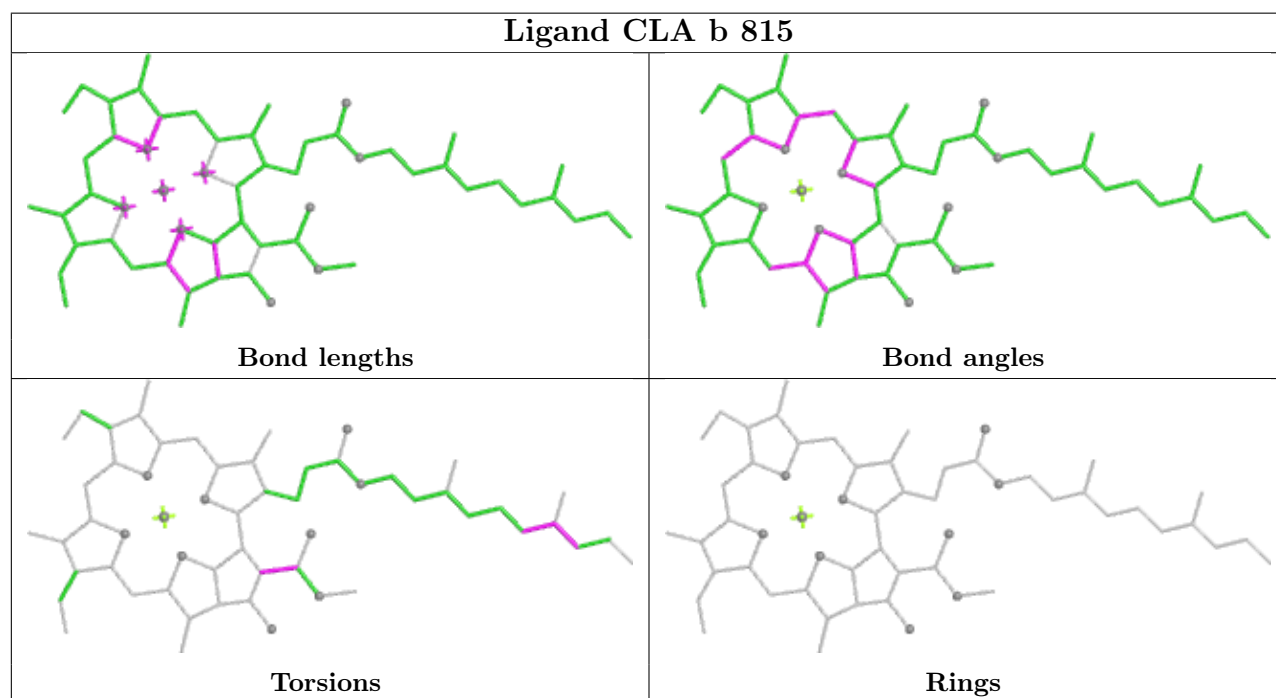
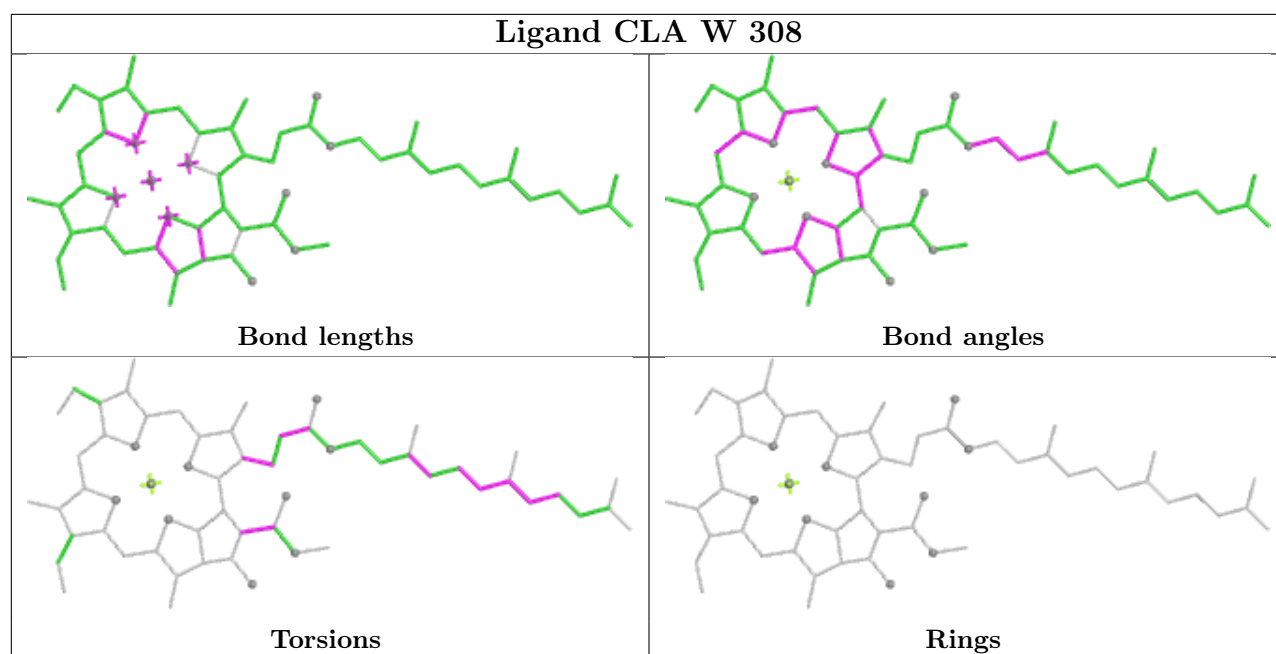


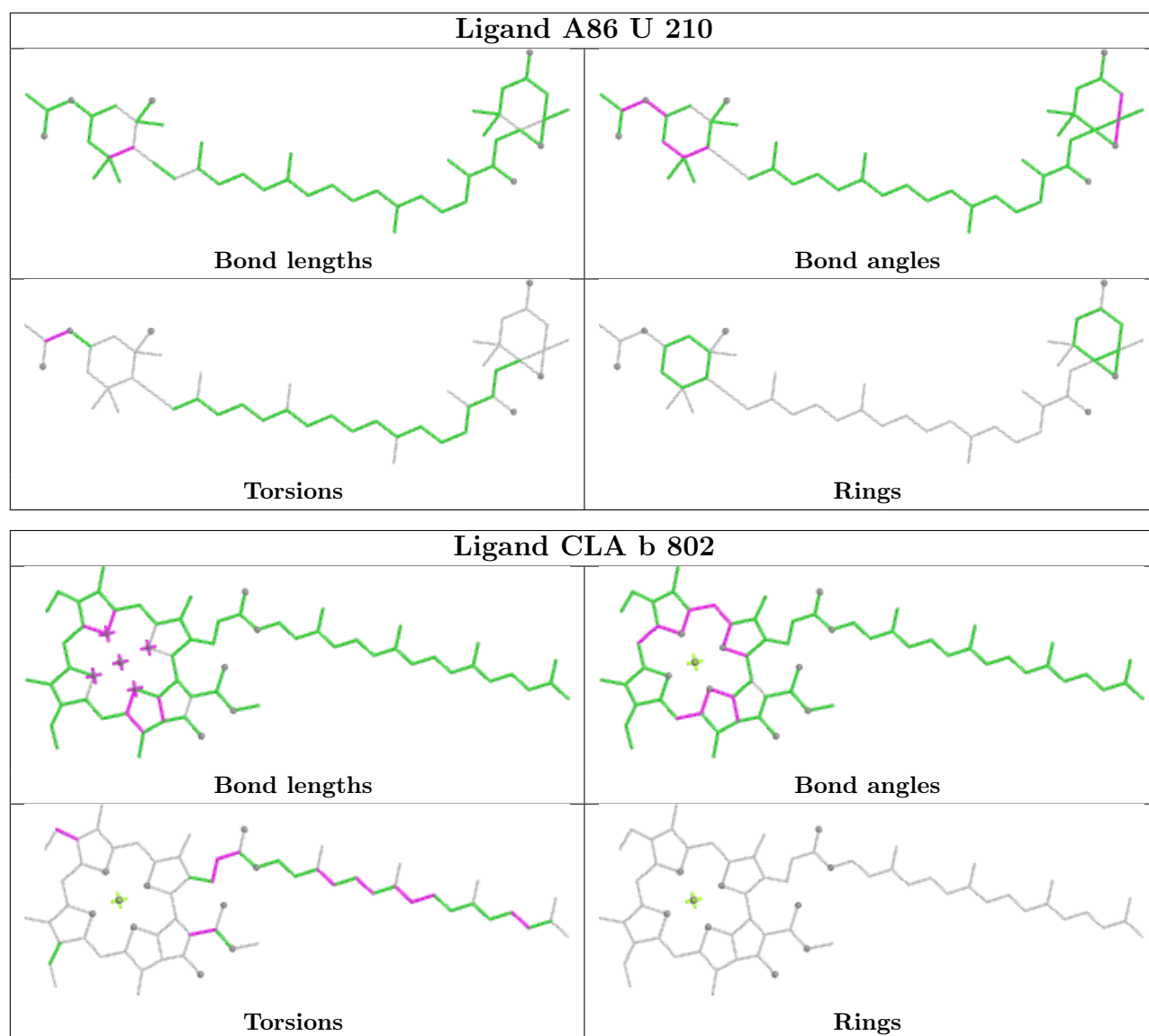




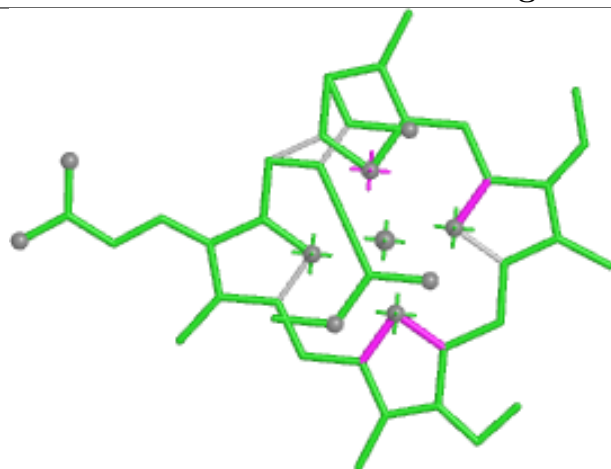




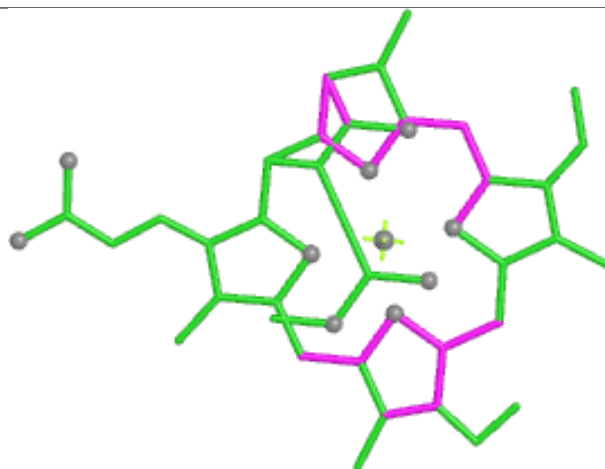




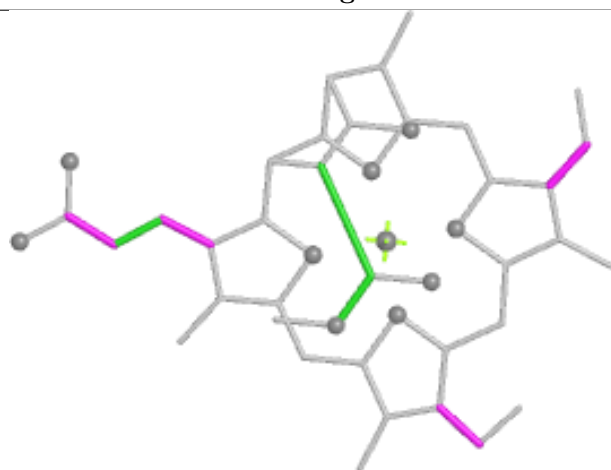
Ligand KC2 L 309



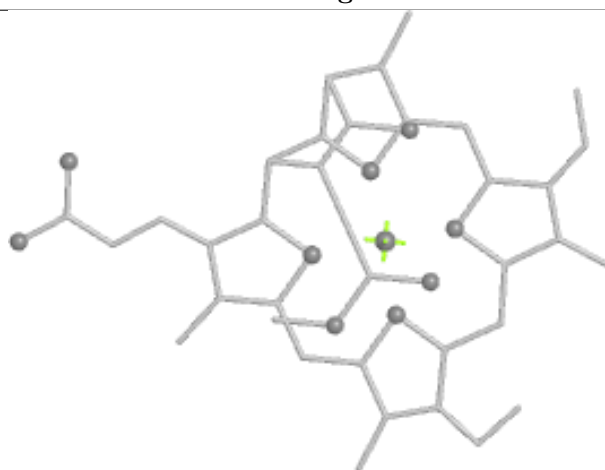
Bond lengths



Bond angles

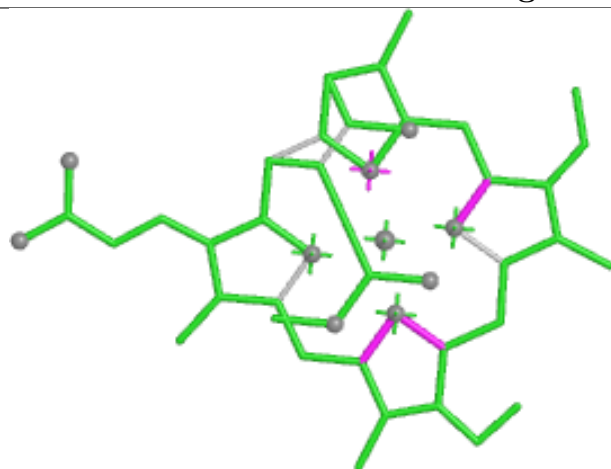


Torsions

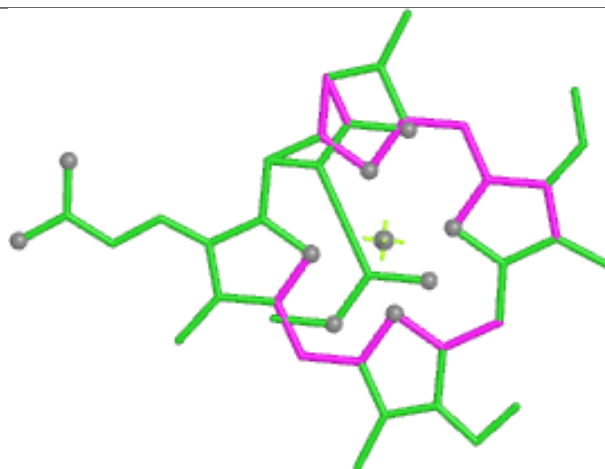


Rings

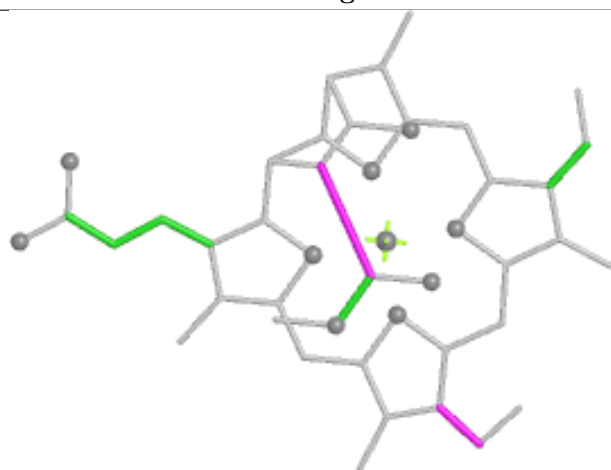
Ligand KC2 Z 303



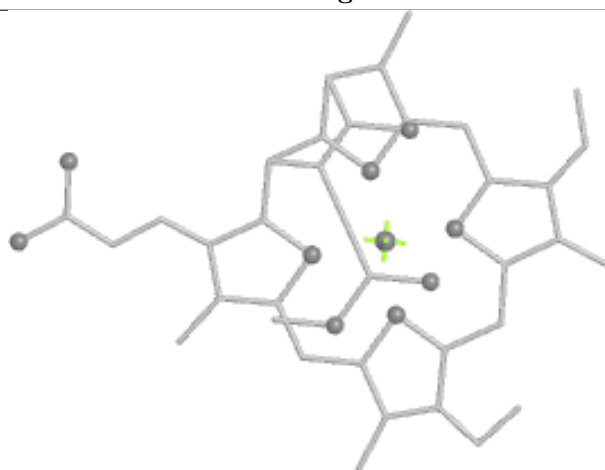
Bond lengths



Bond angles

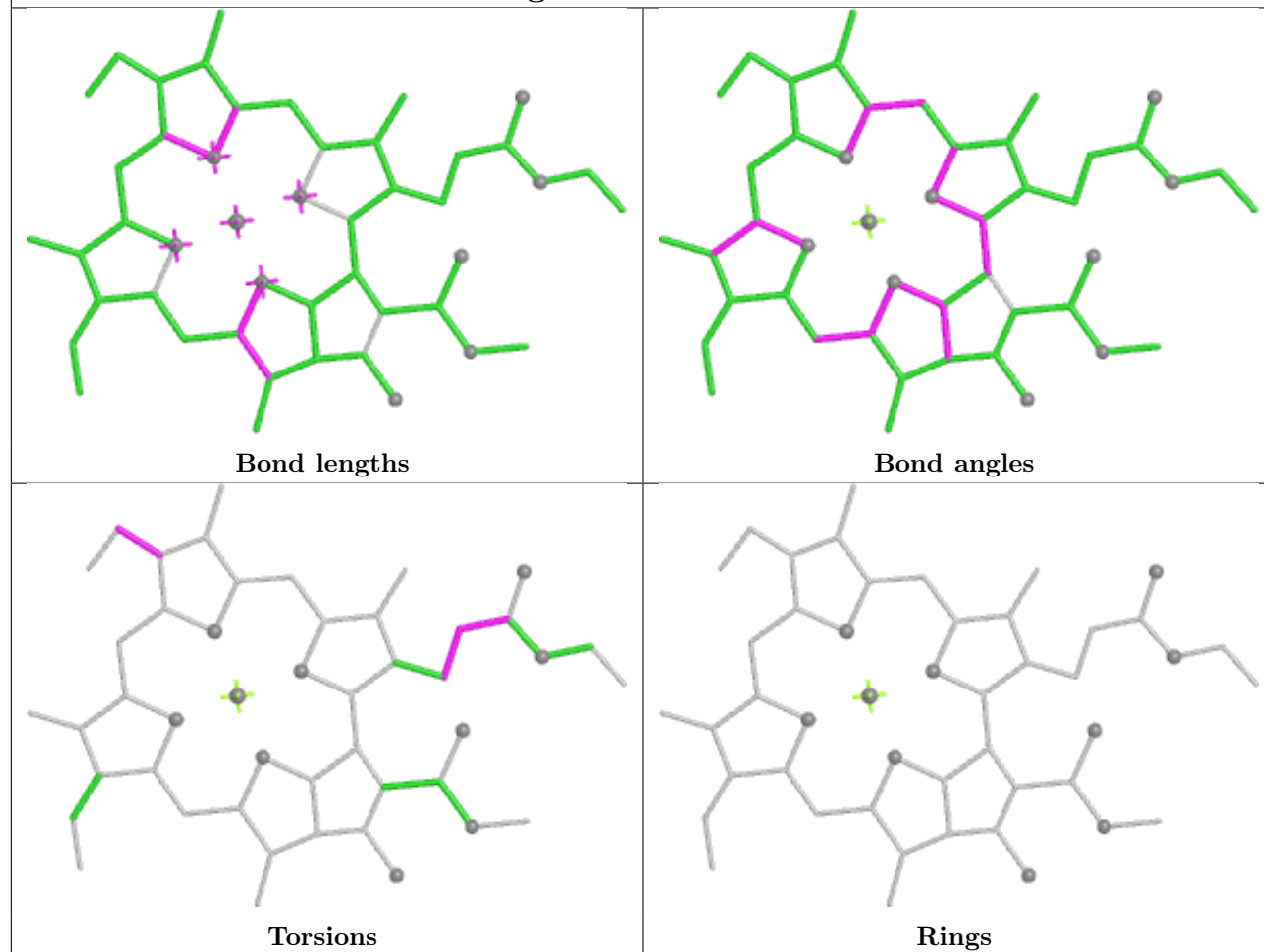


Torsions

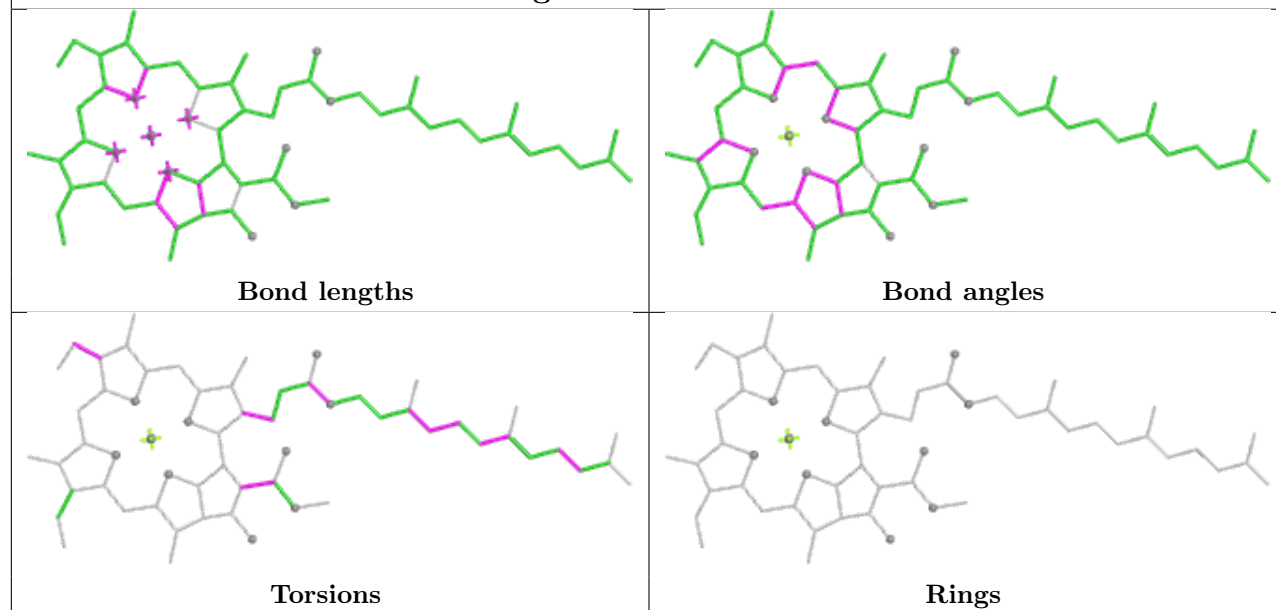


Rings

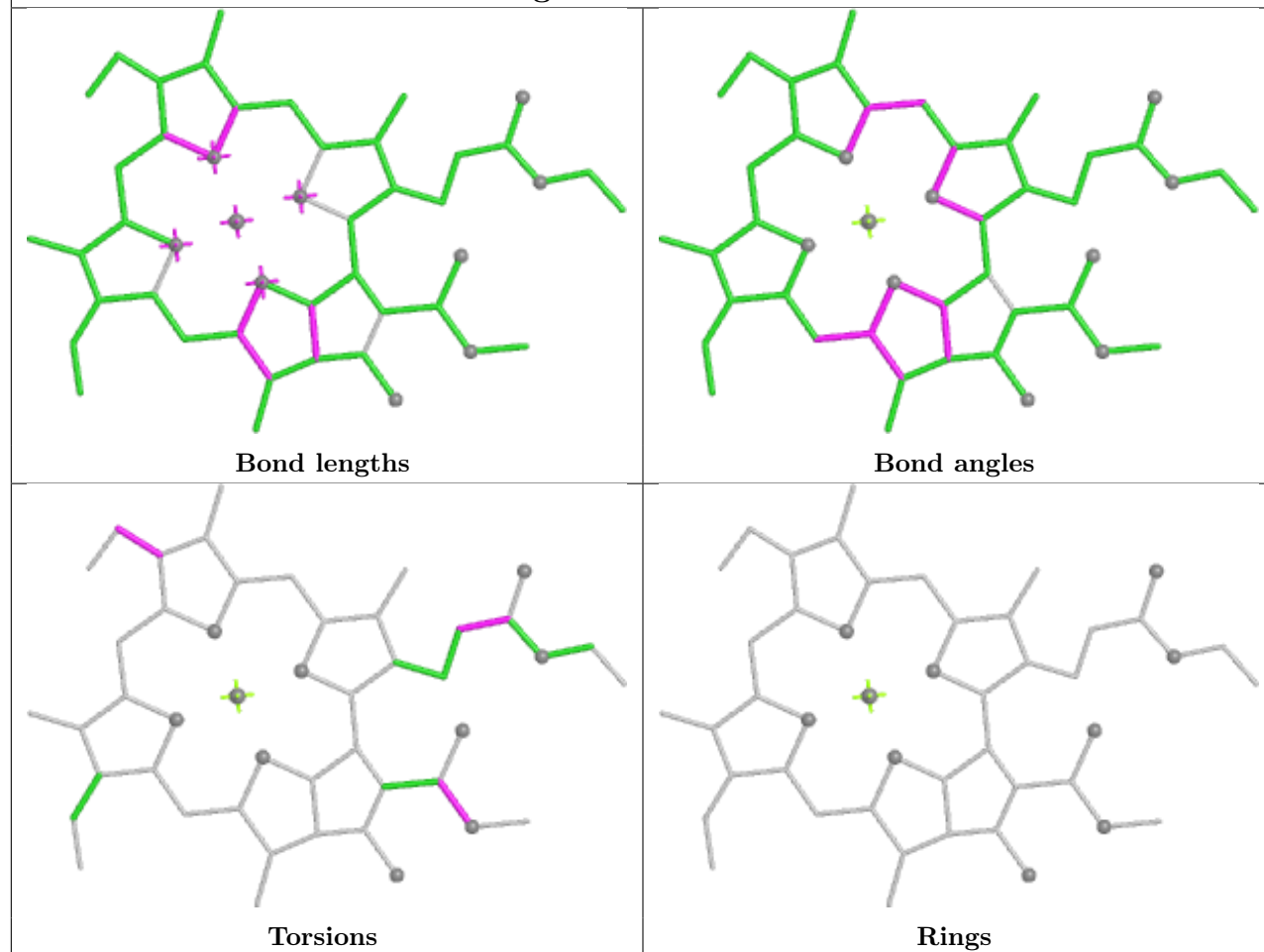
Ligand CLA T 317



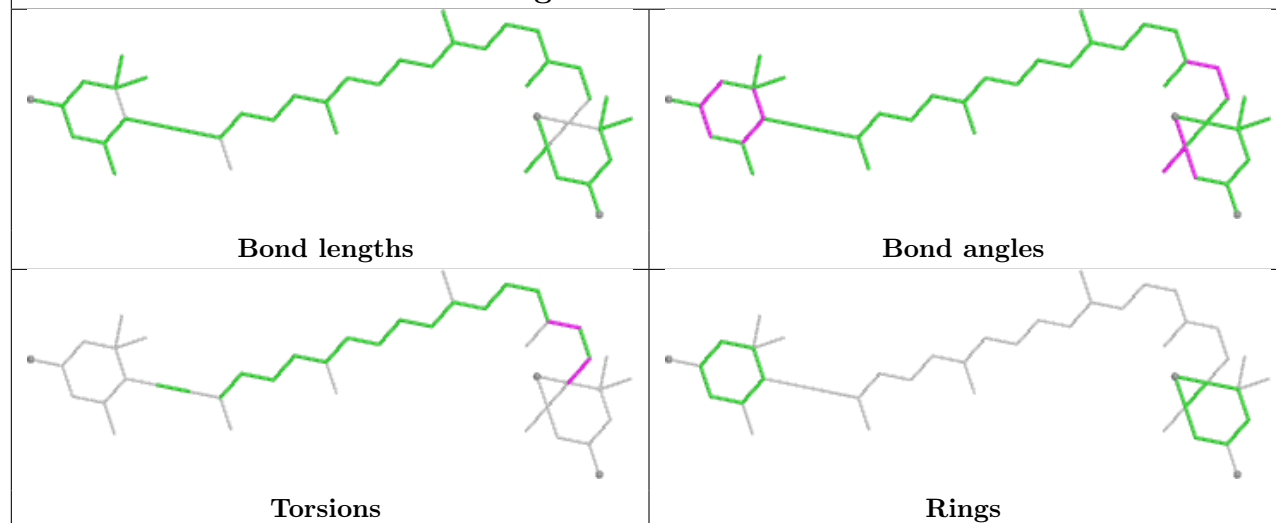
Ligand CLA P 313

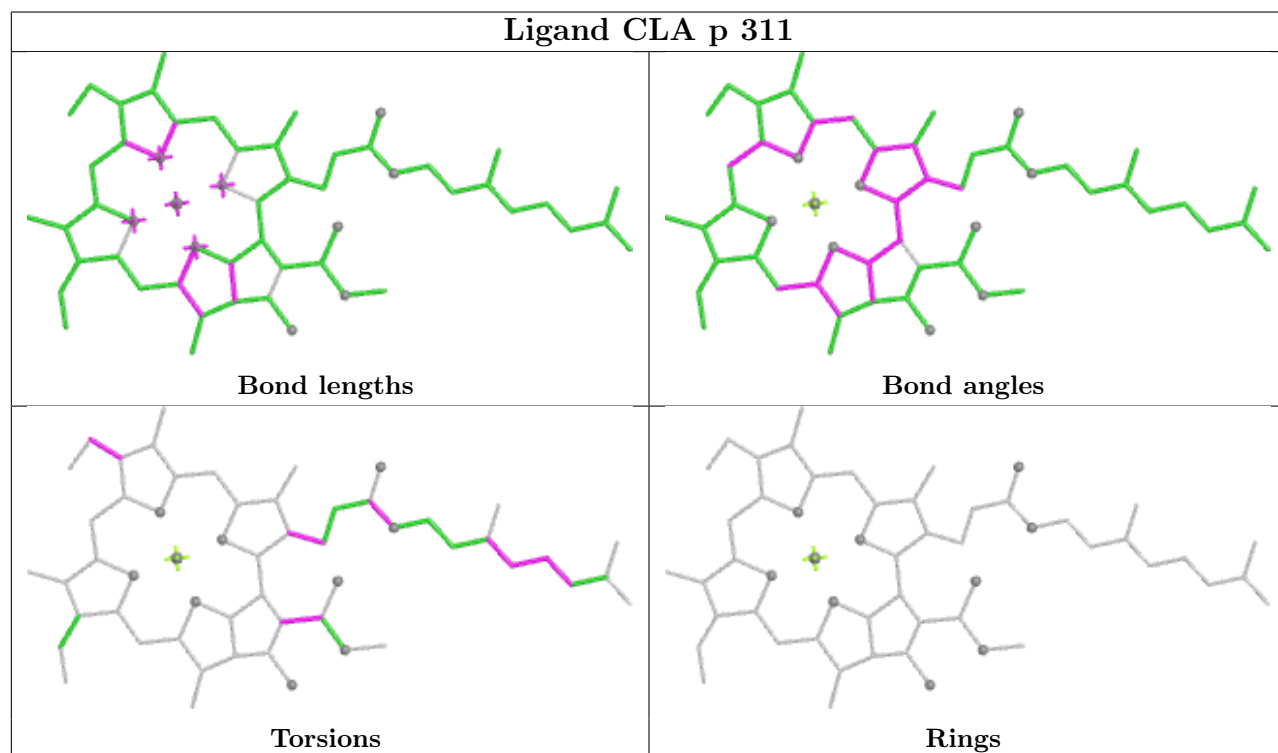
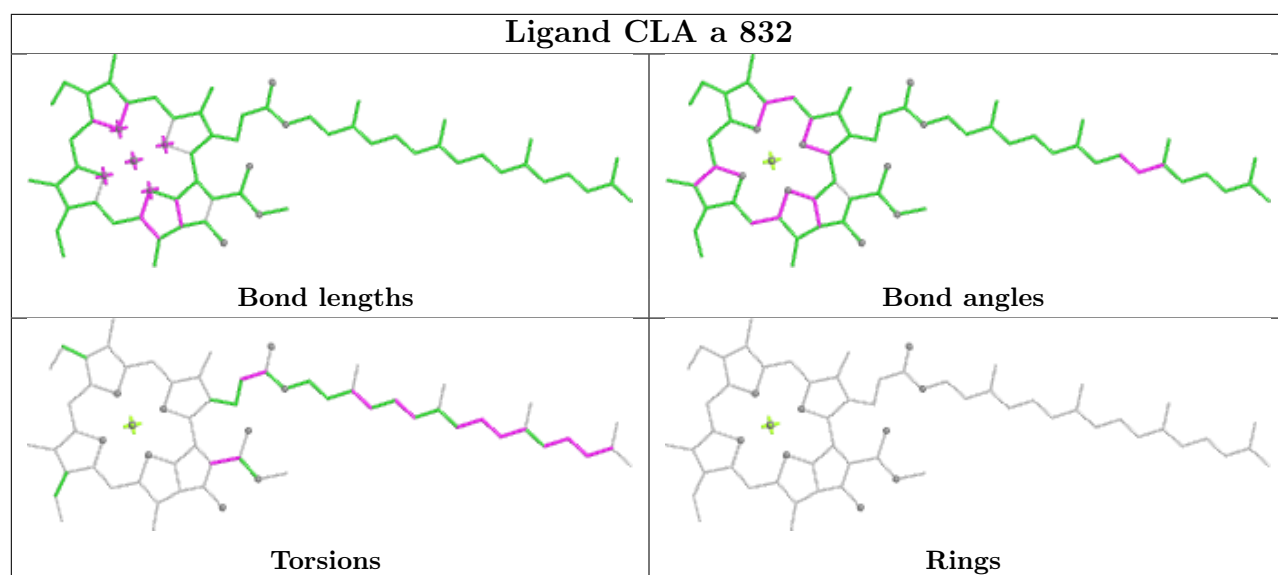


Ligand CLA t 309

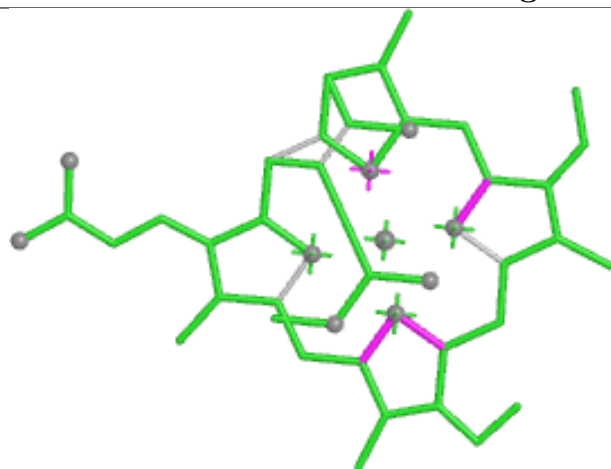


Ligand DD6 E 318

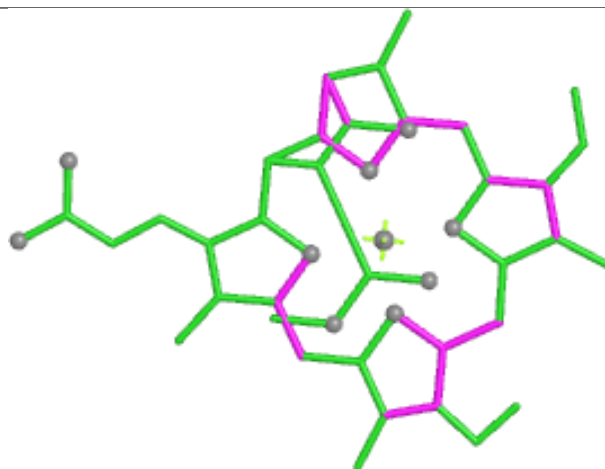




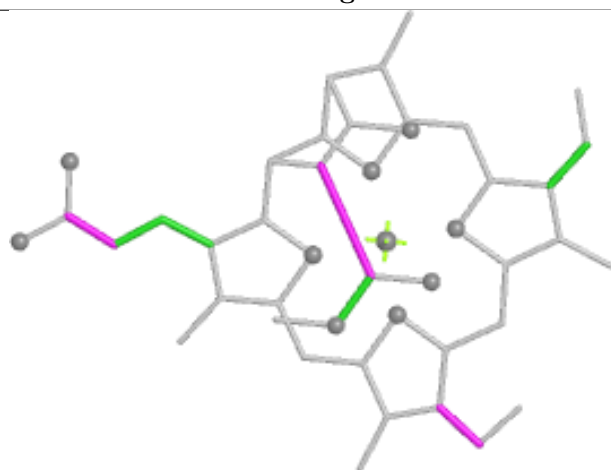
Ligand KC2 v 303



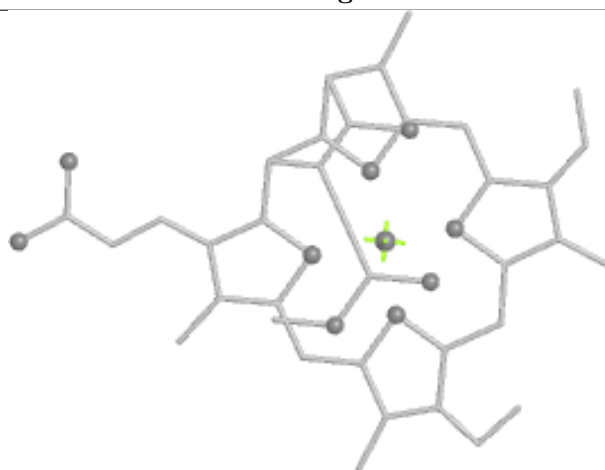
Bond lengths



Bond angles

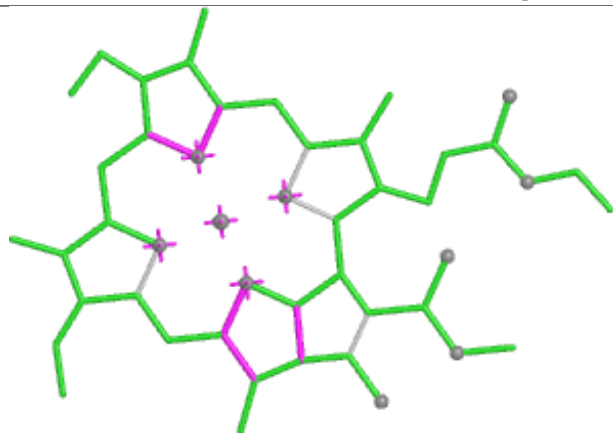


Torsions

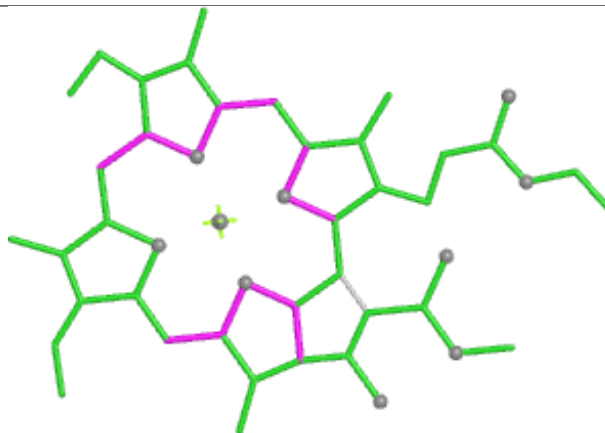


Rings

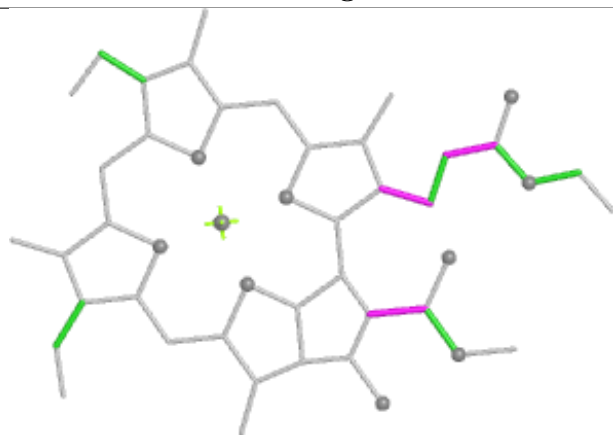
Ligand CLA L 305



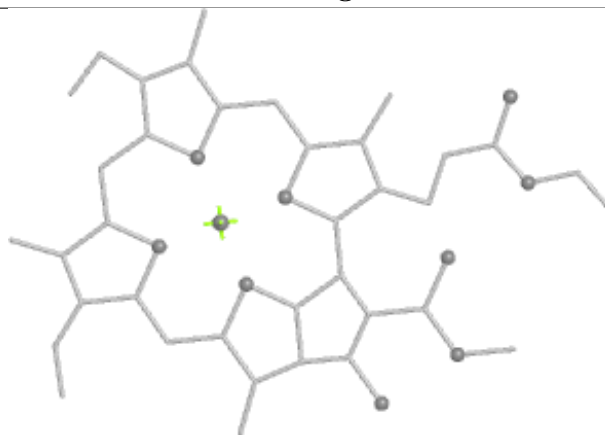
Bond lengths



Bond angles

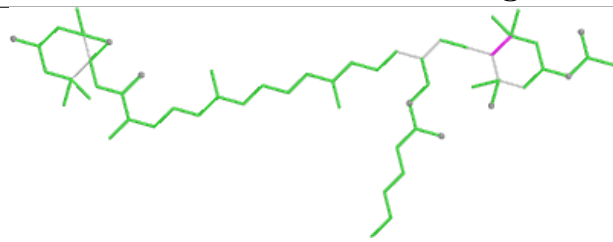


Torsions

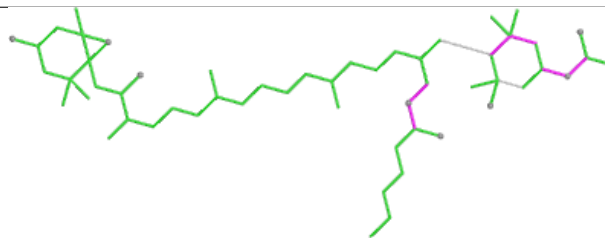


Rings

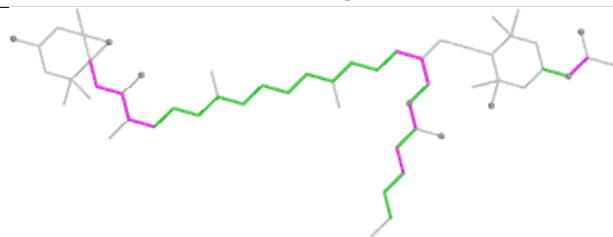
Ligand A1EB1 t 314



Bond lengths



Bond angles

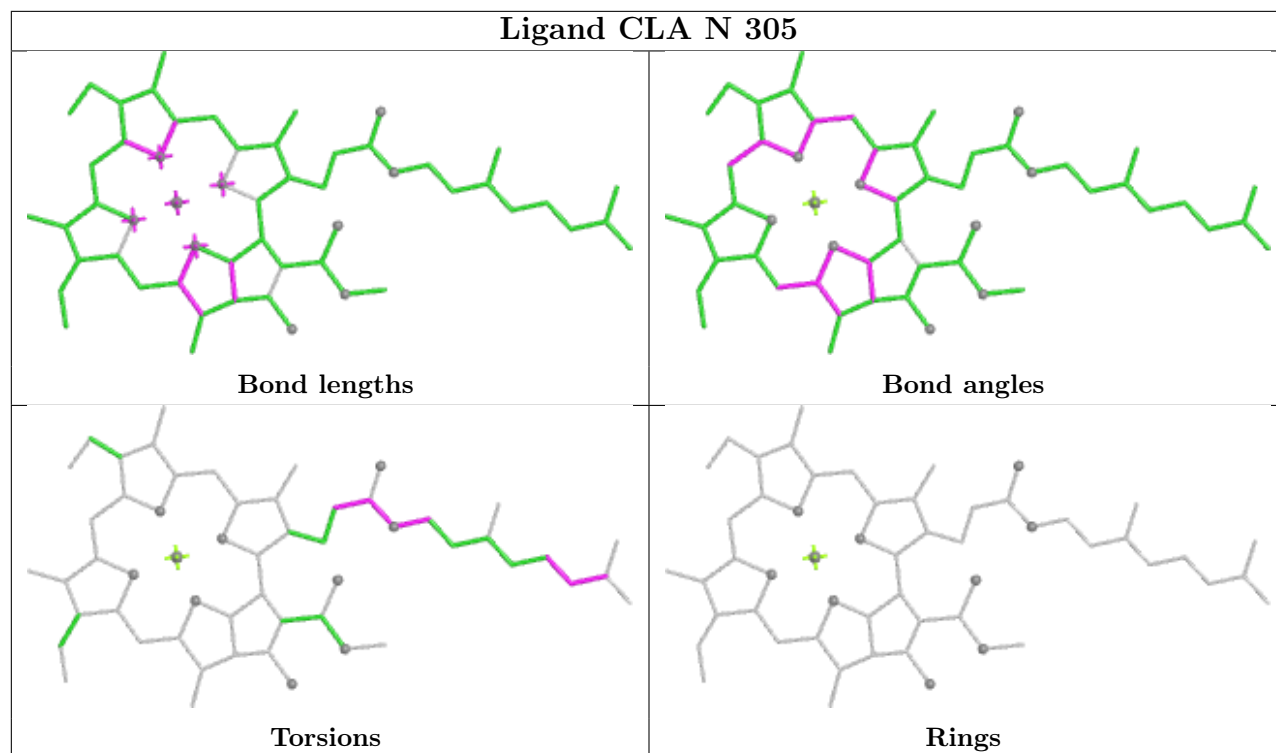


Torsions

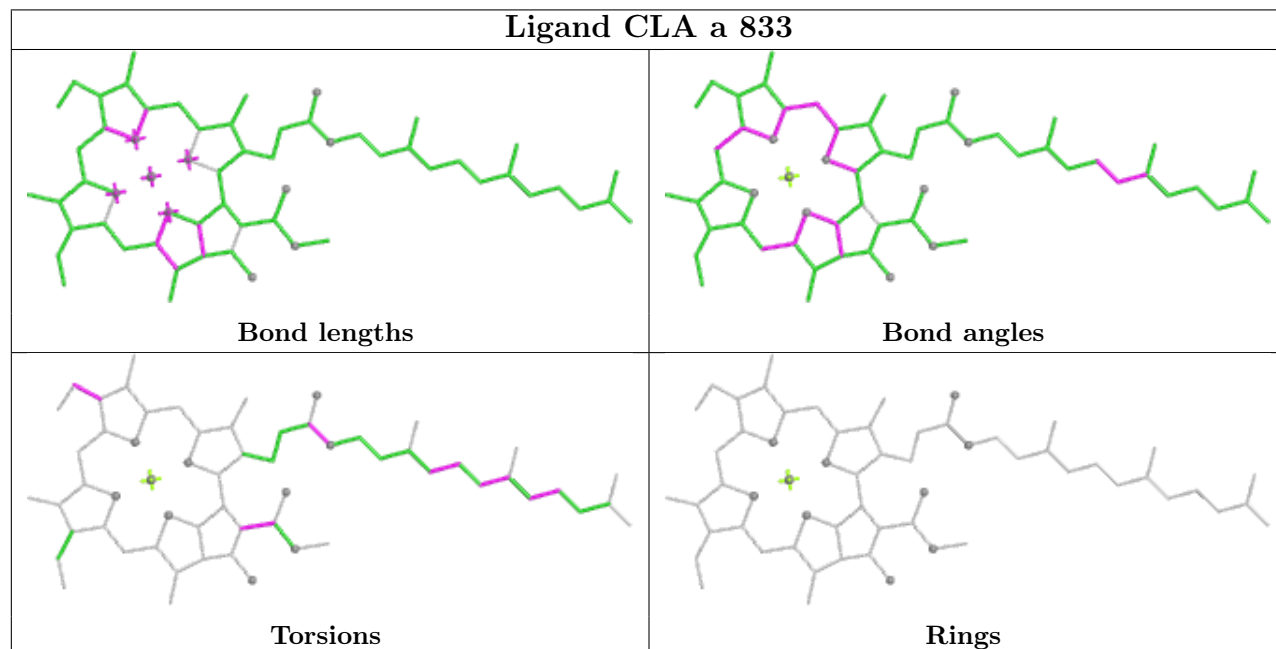


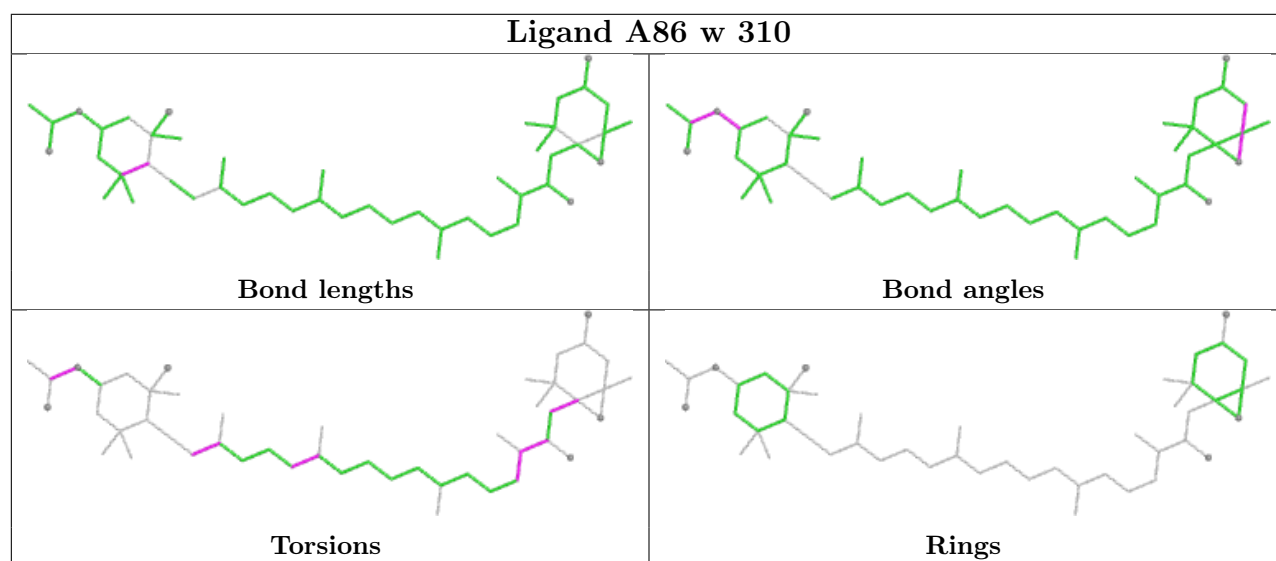
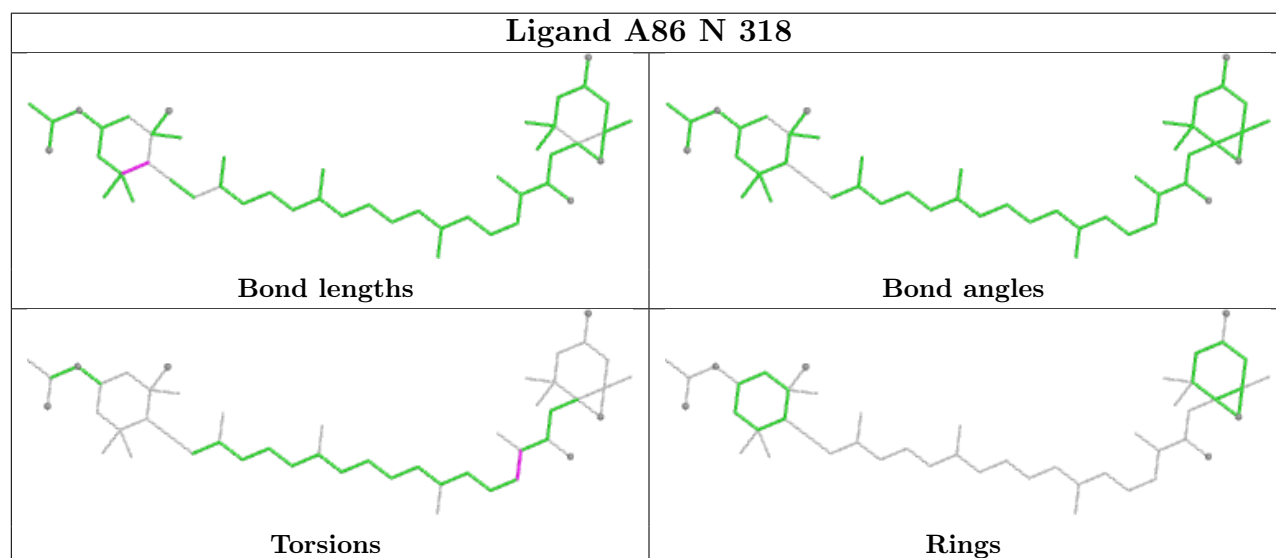
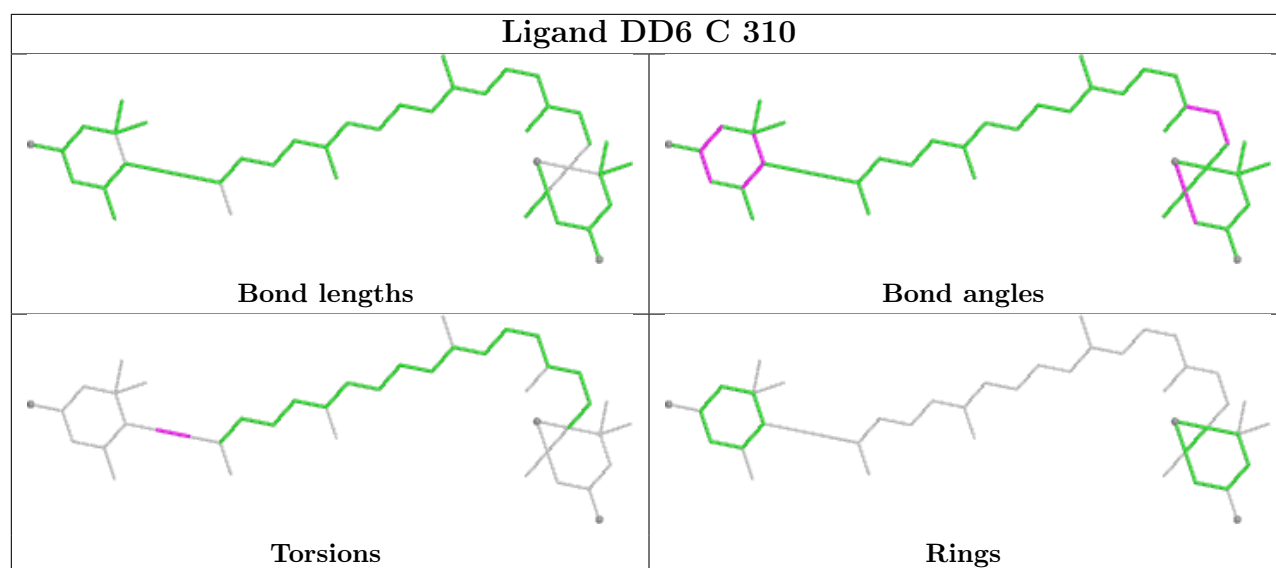
Rings

Ligand CLA N 305

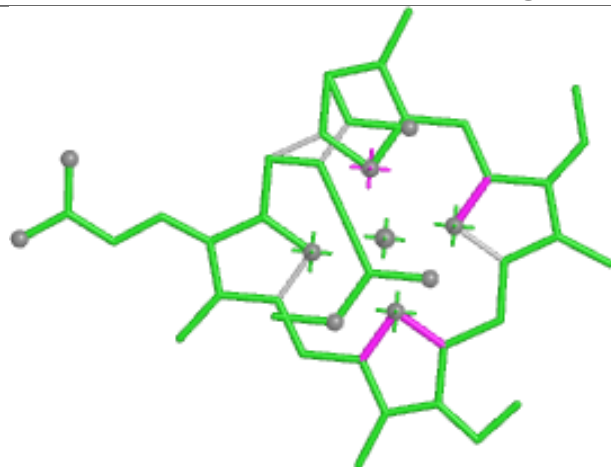


Ligand CLA a 833

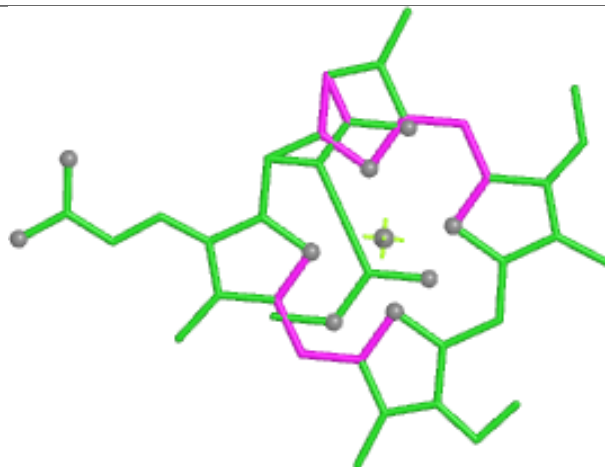




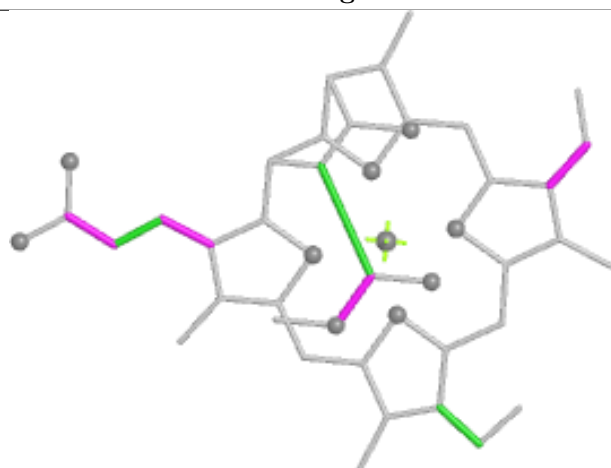
Ligand KC2 x 303



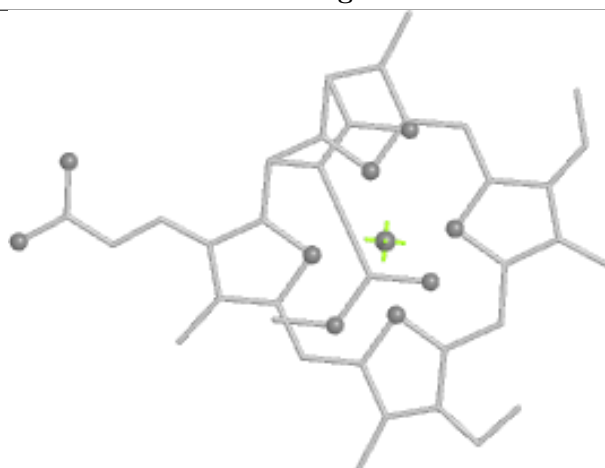
Bond lengths



Bond angles

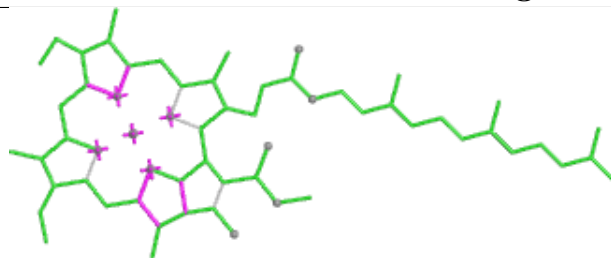


Torsions

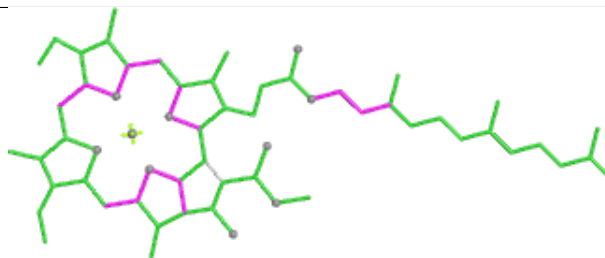


Rings

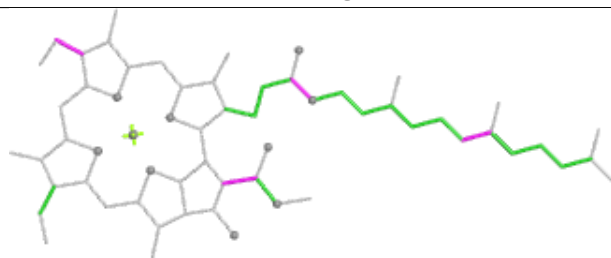
Ligand CLA E 310



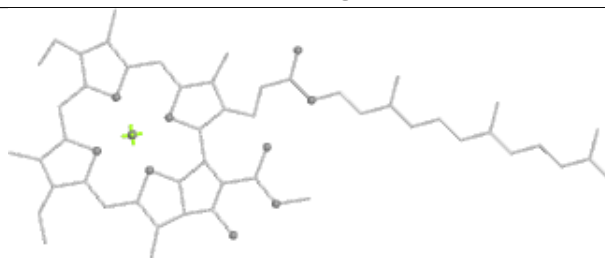
Bond lengths



Bond angles

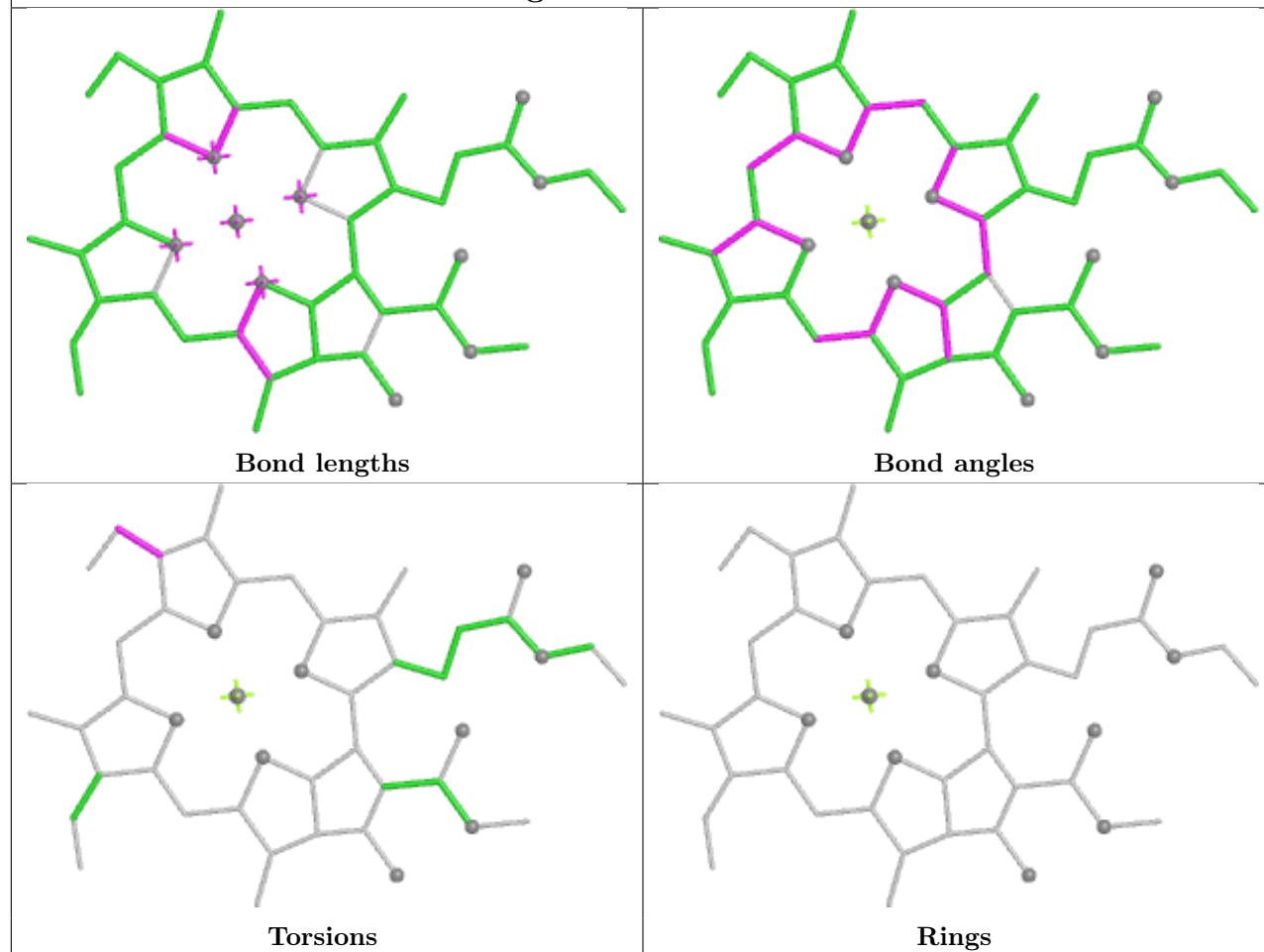


Torsions

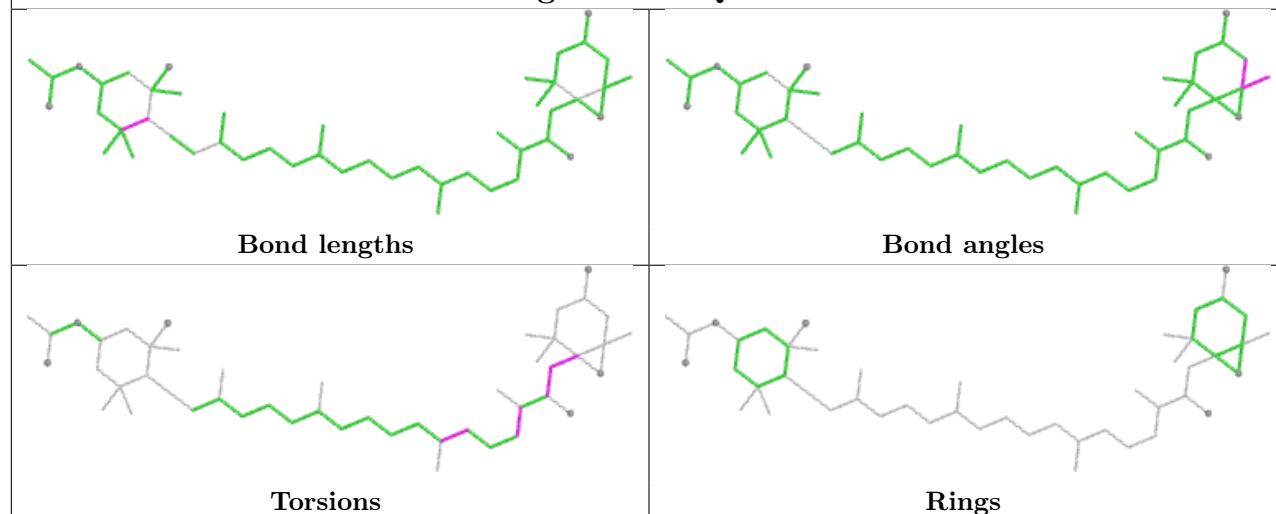


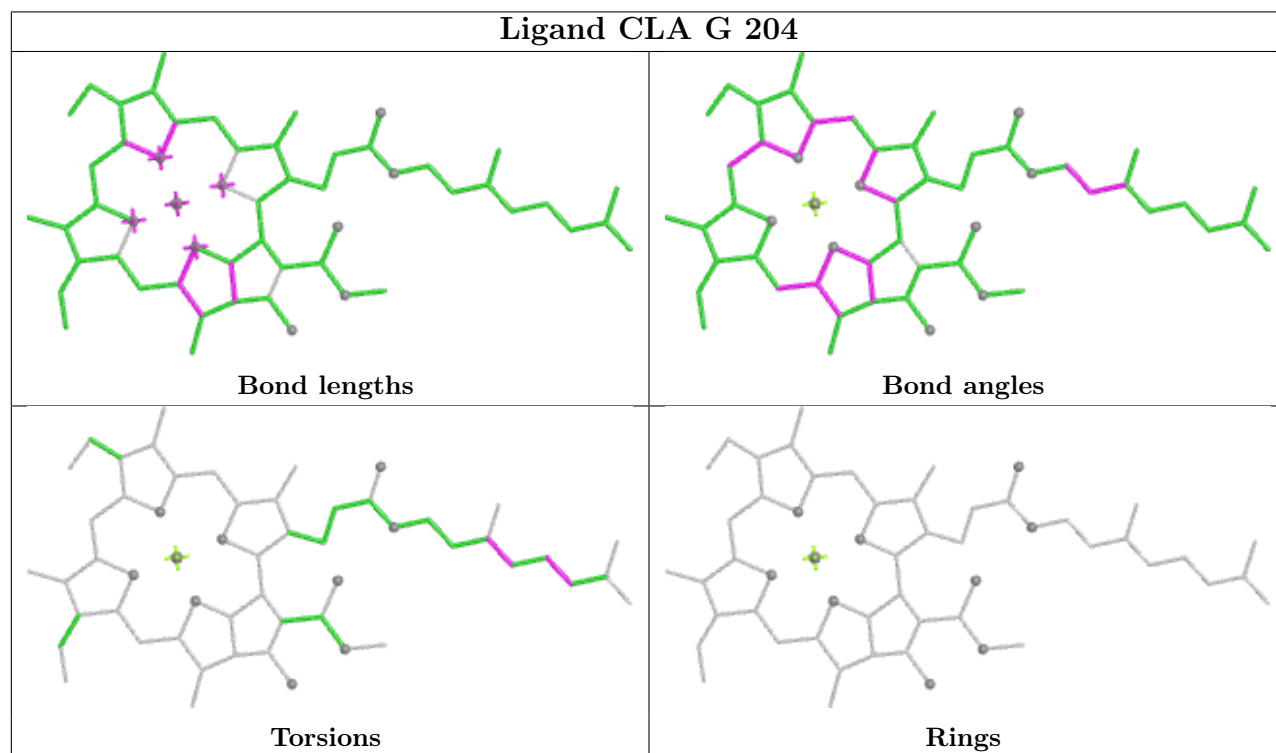
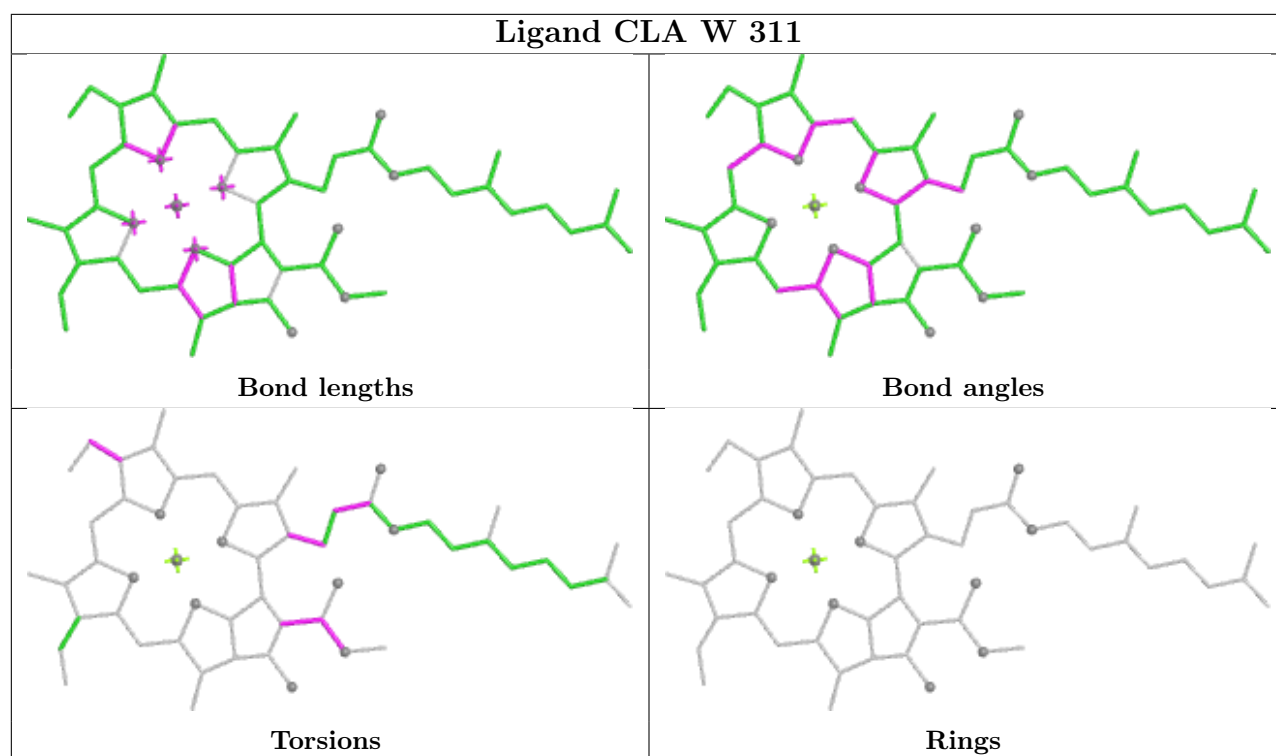
Rings

Ligand CLA R 316

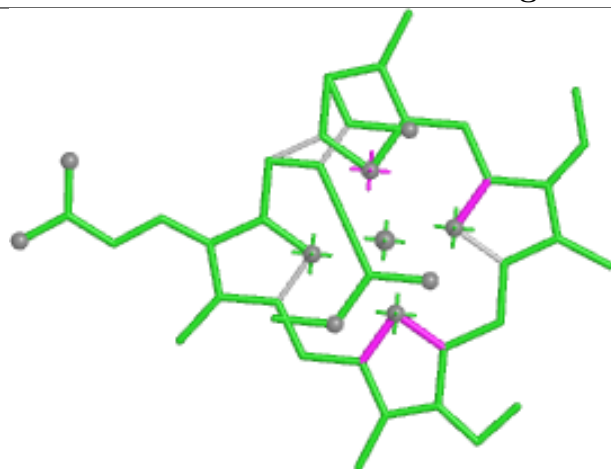


Ligand A86 Q 210

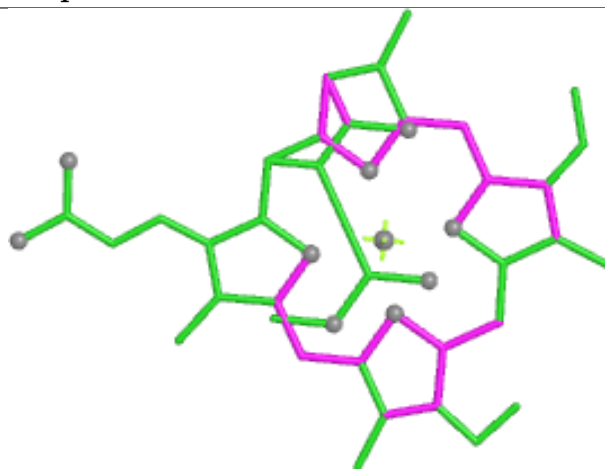




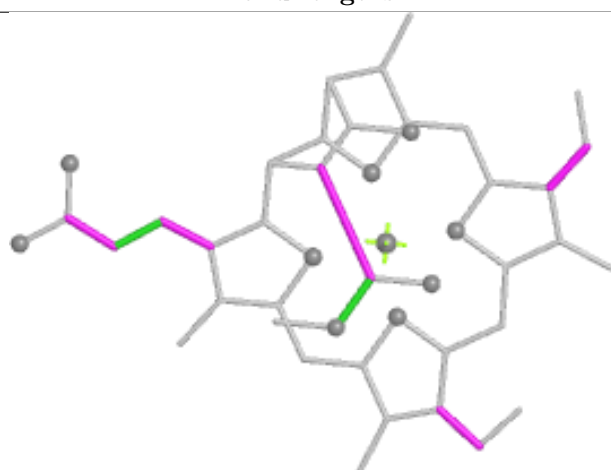
Ligand KC2 q 309



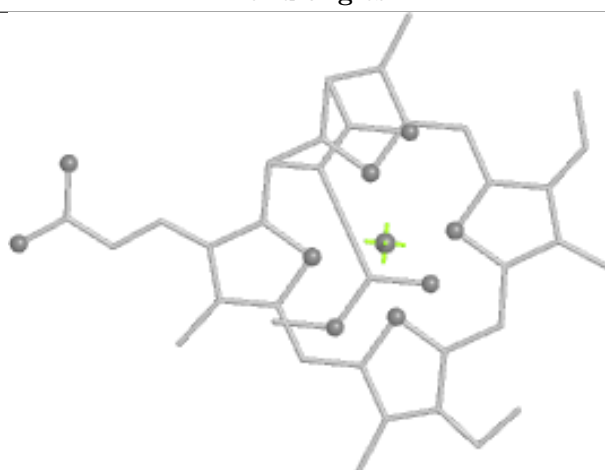
Bond lengths



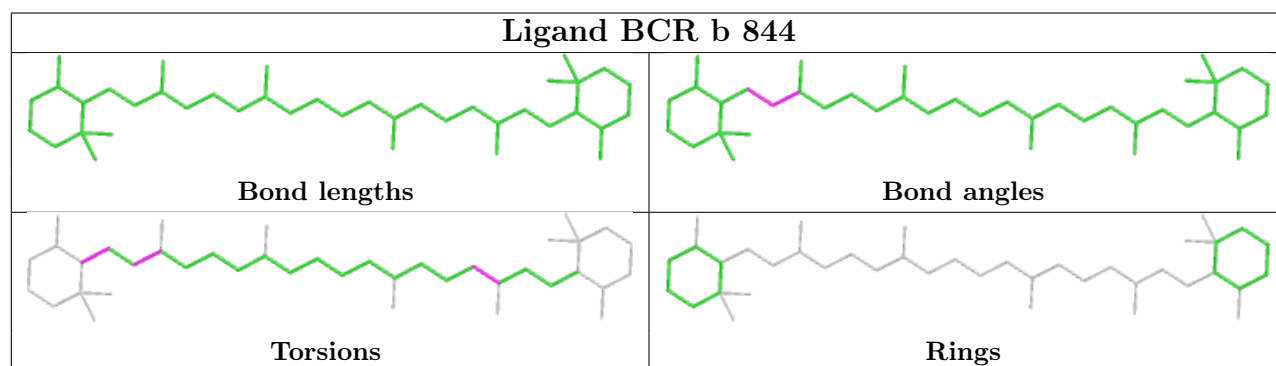
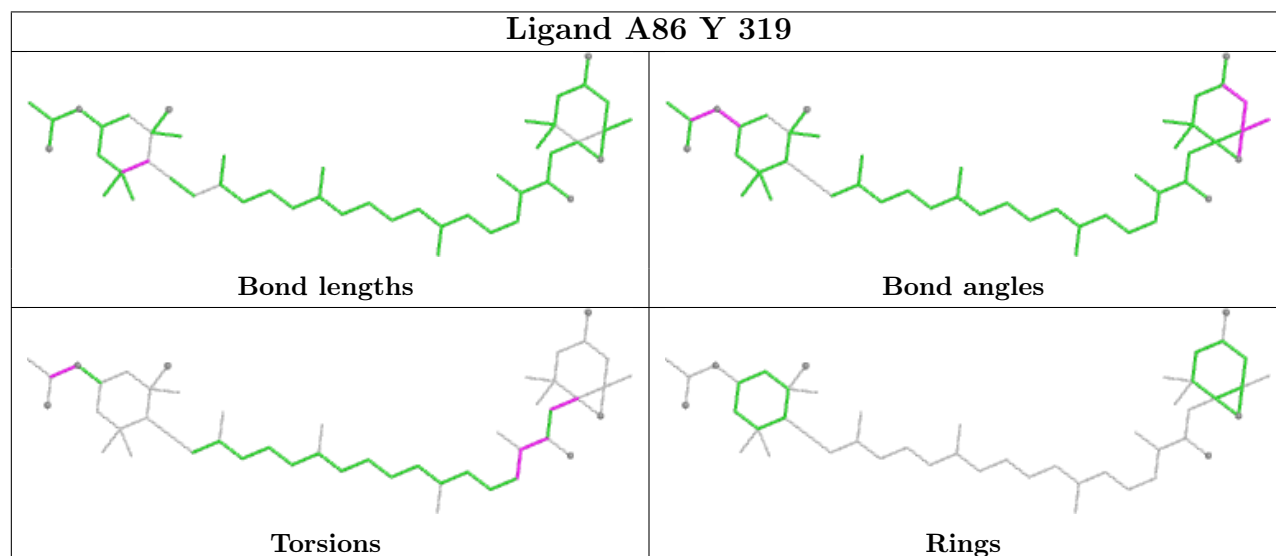
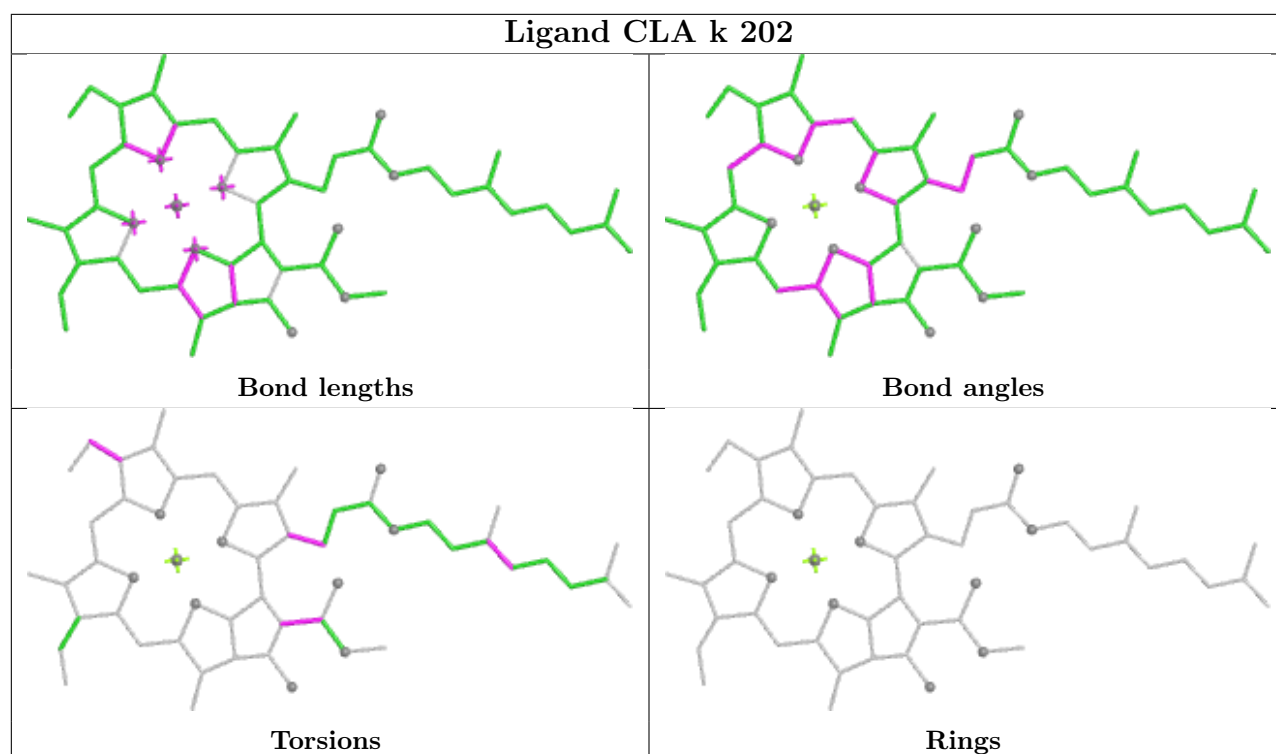
Bond angles

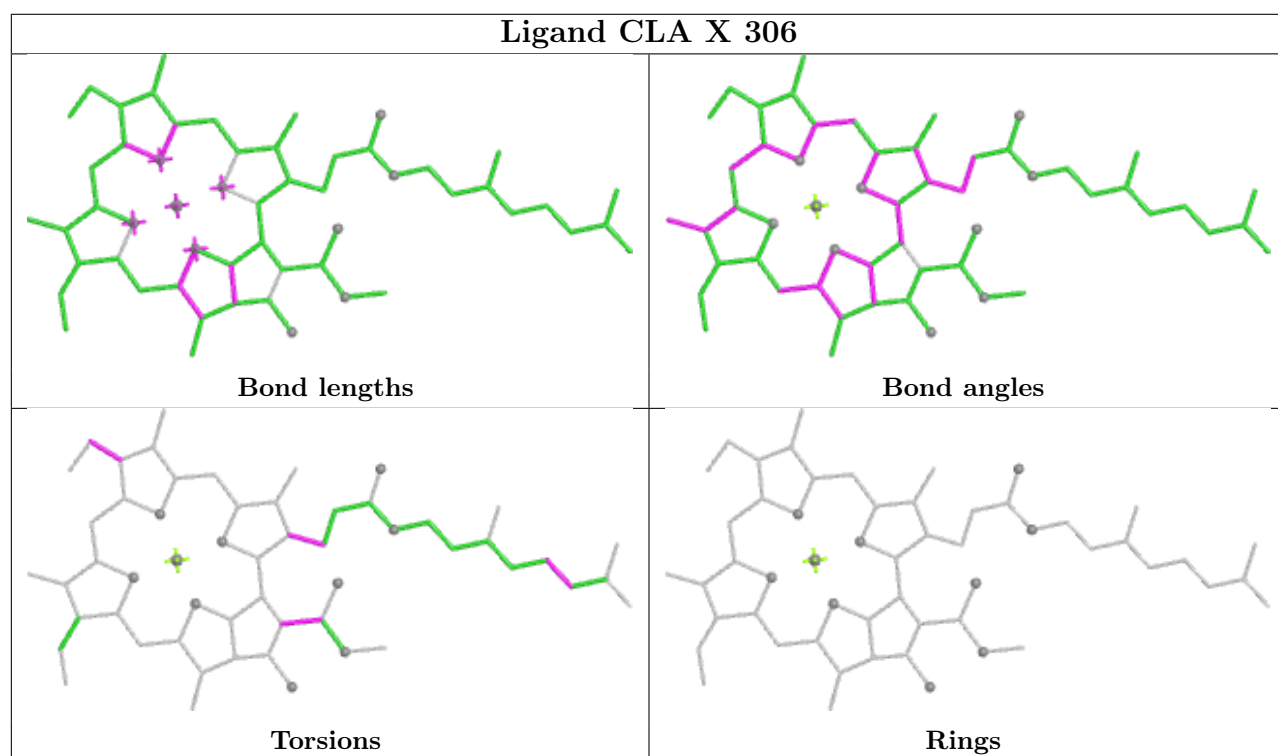
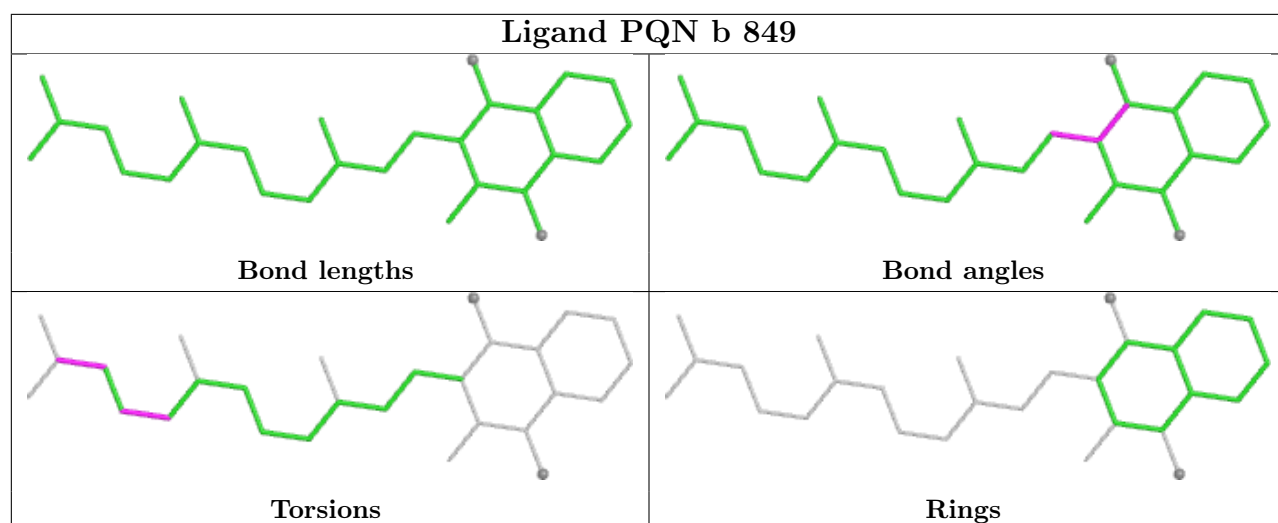


Torsions

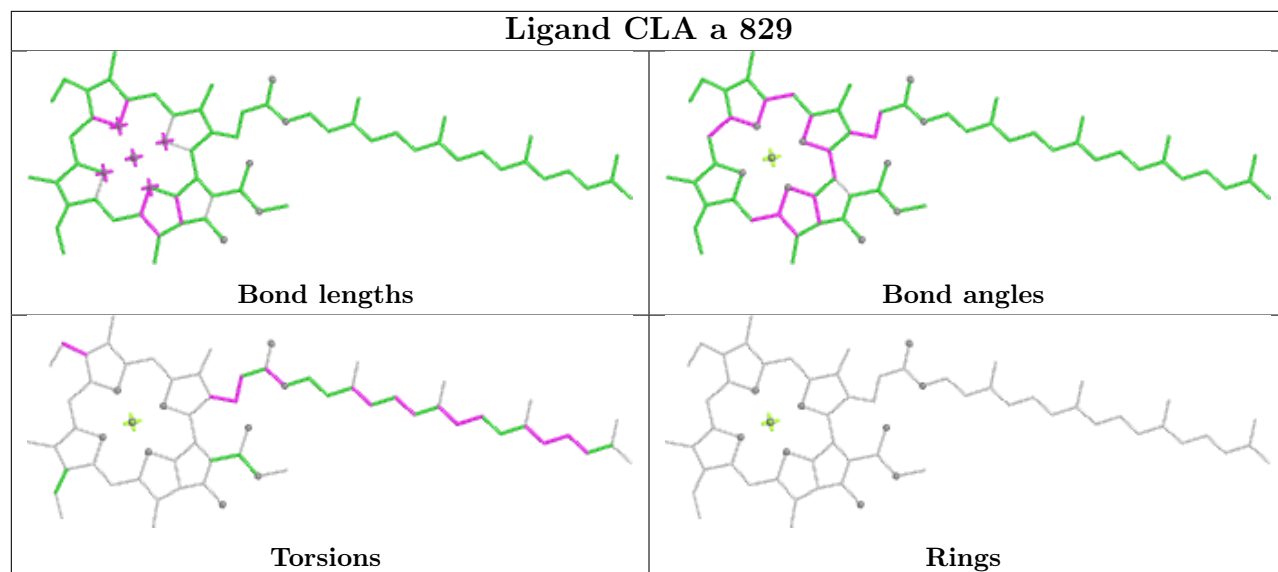


Rings

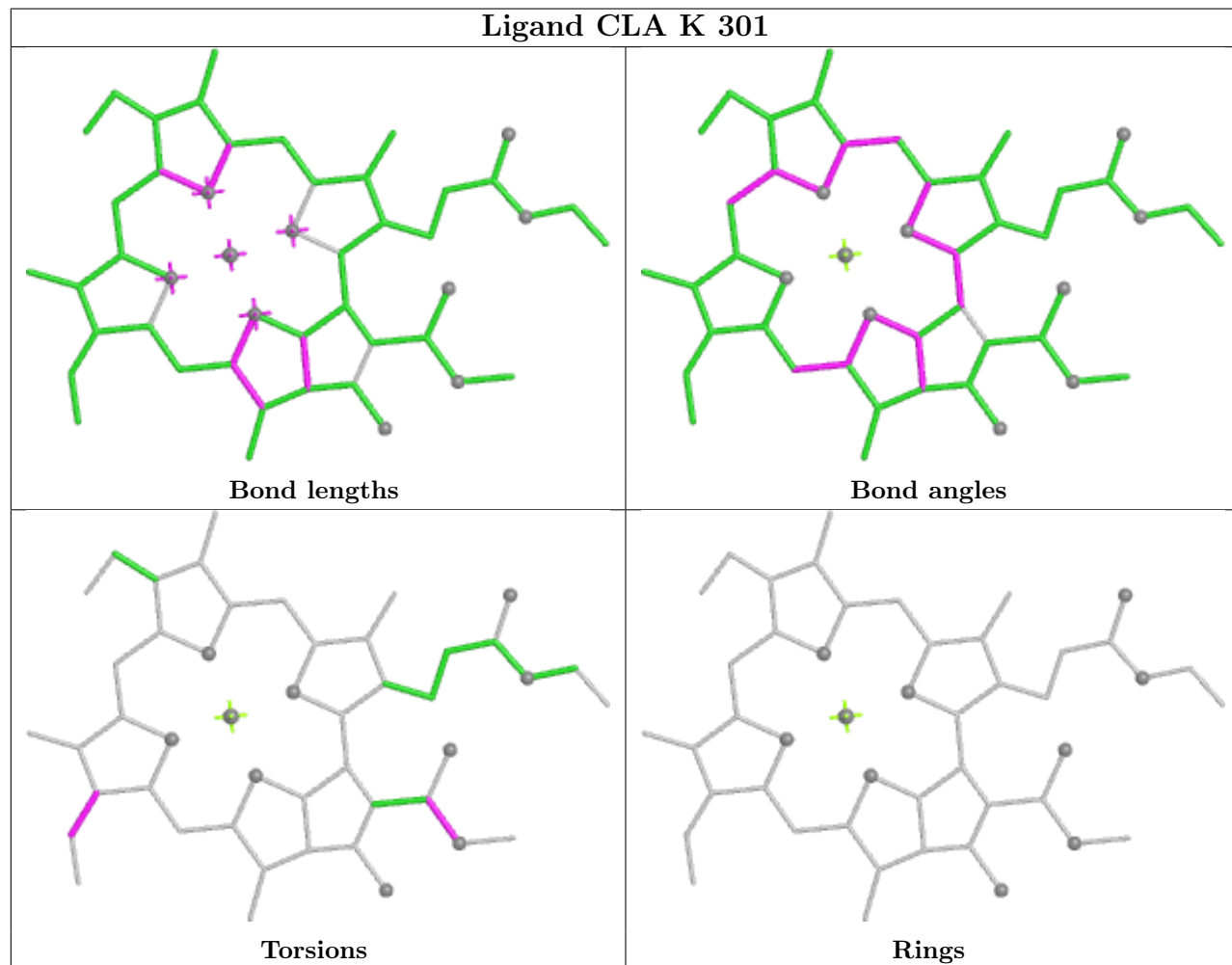


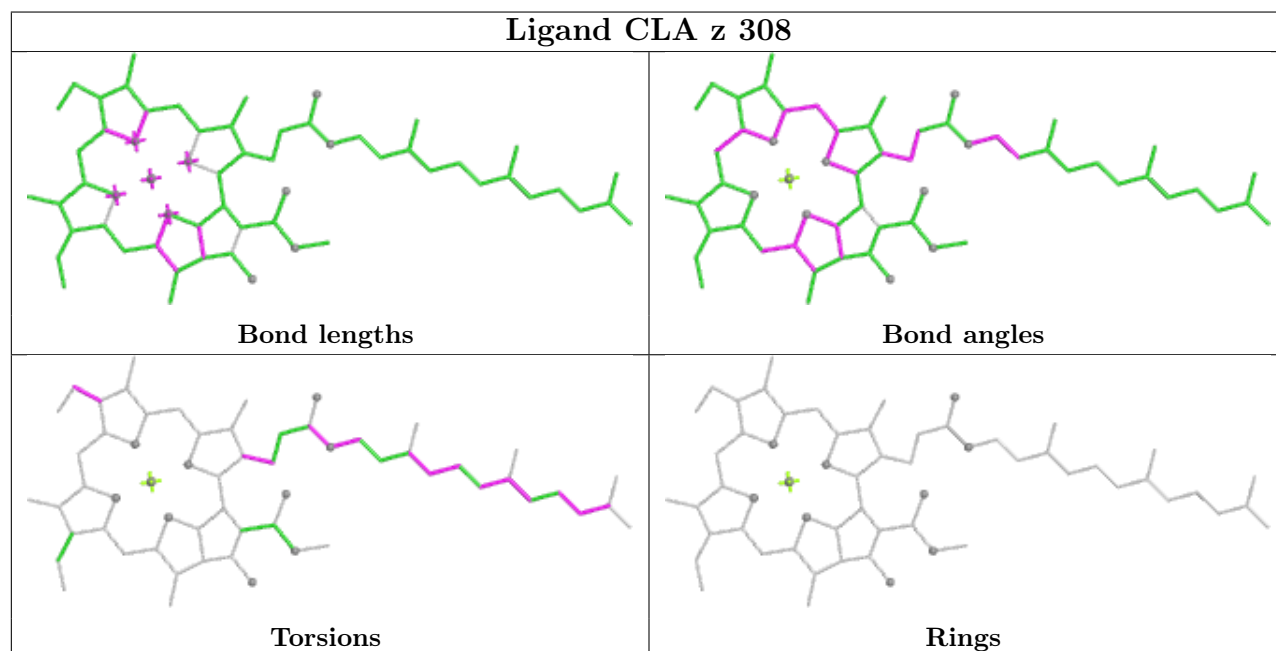
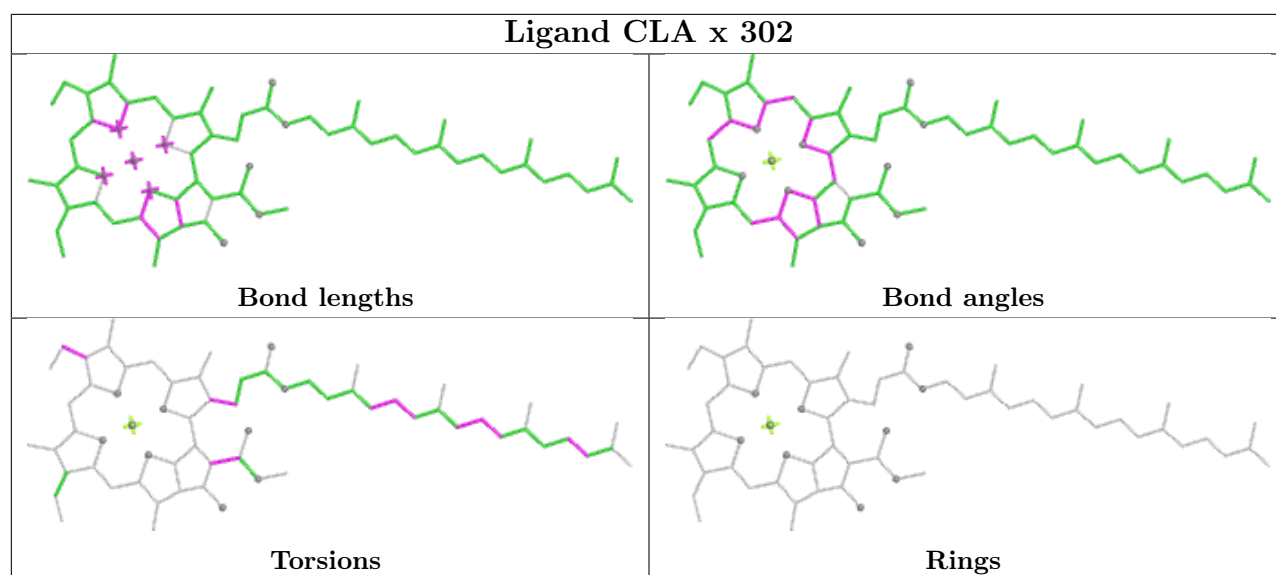


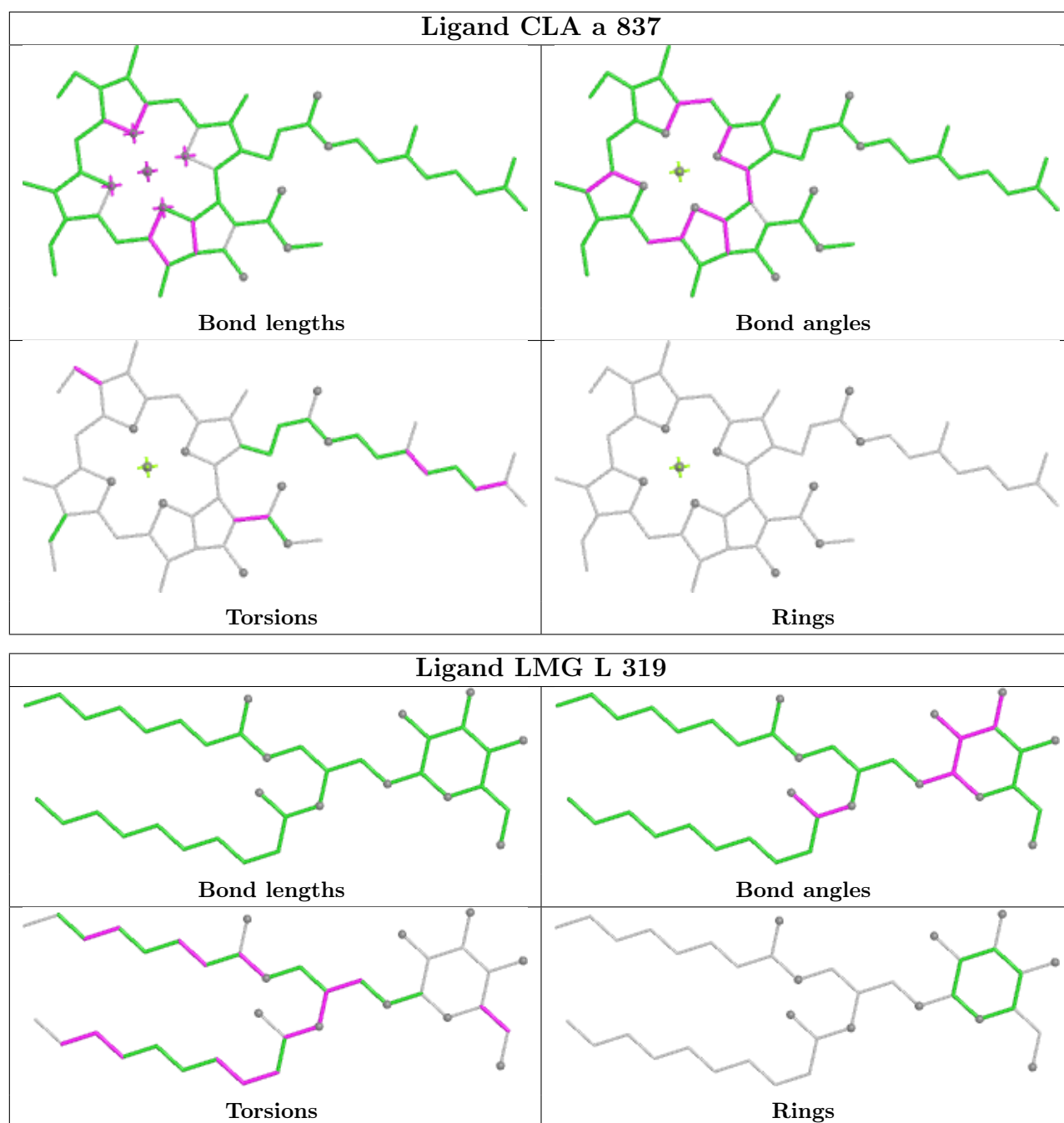
Ligand CLA a 829

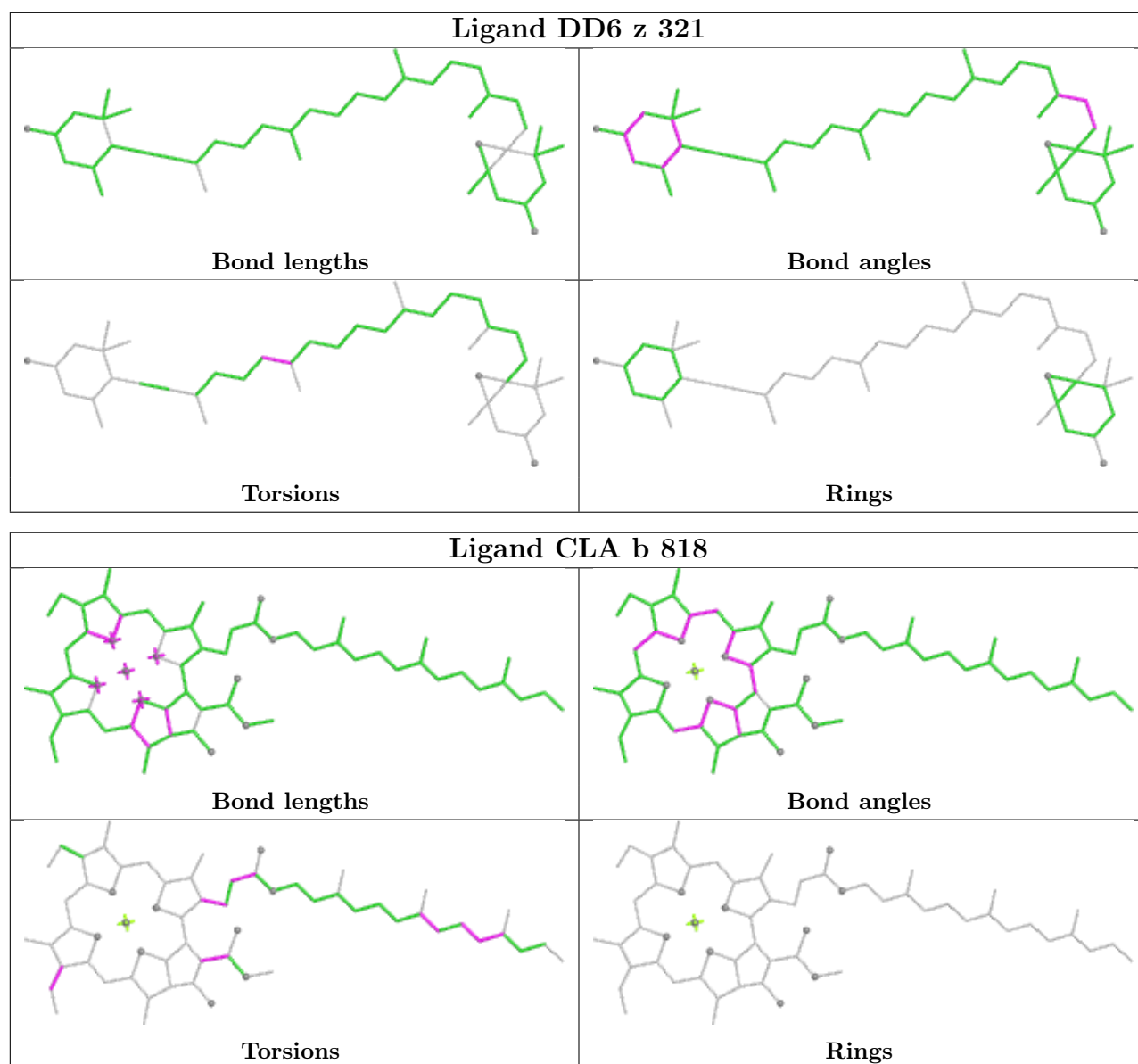


Ligand CLA K 301

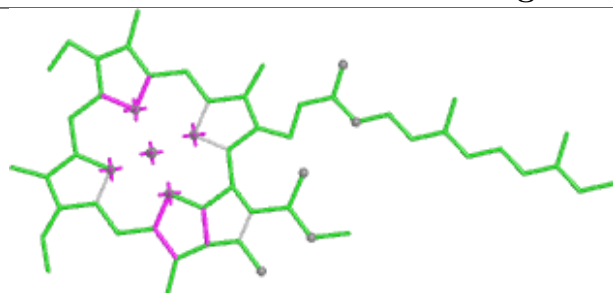




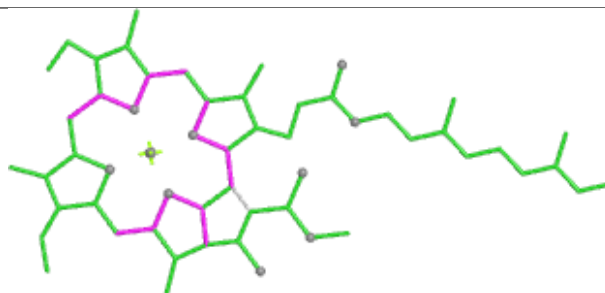




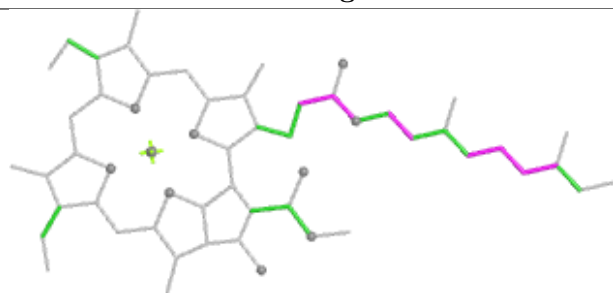
Ligand CLA S 306



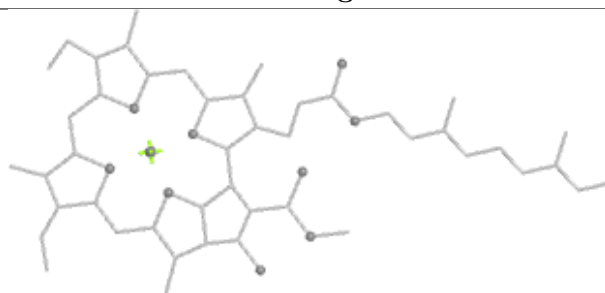
Bond lengths



Bond angles

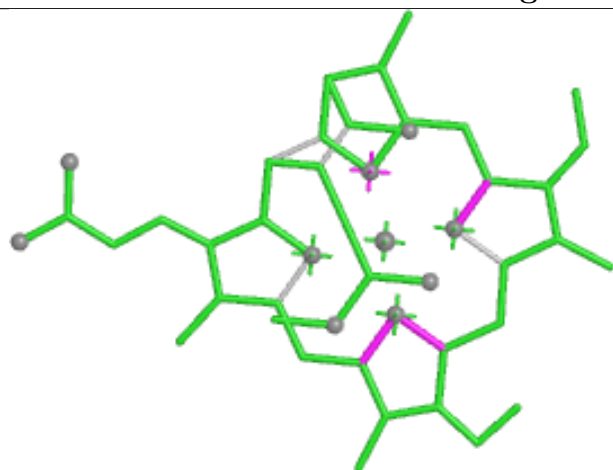


Torsions

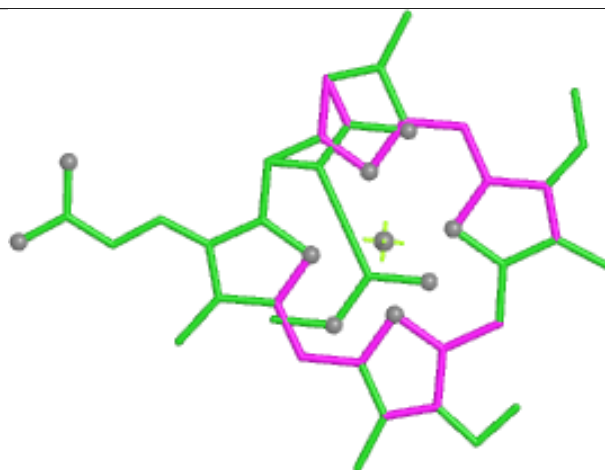


Rings

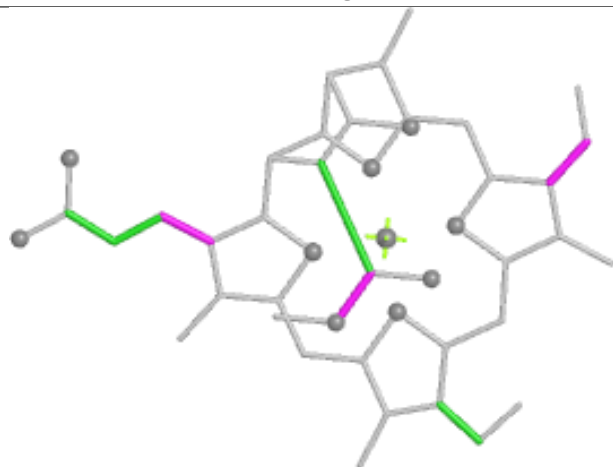
Ligand KC2 o 302



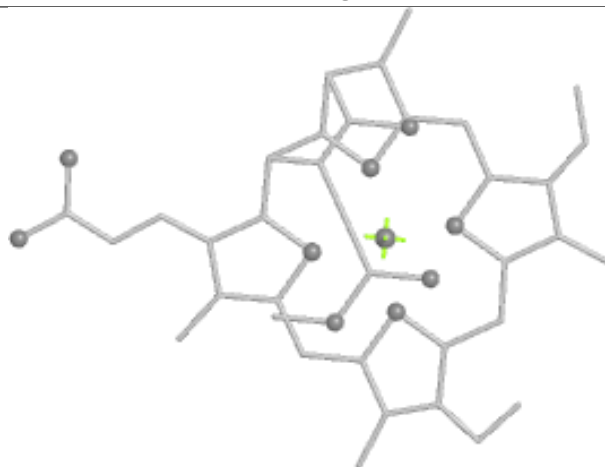
Bond lengths



Bond angles

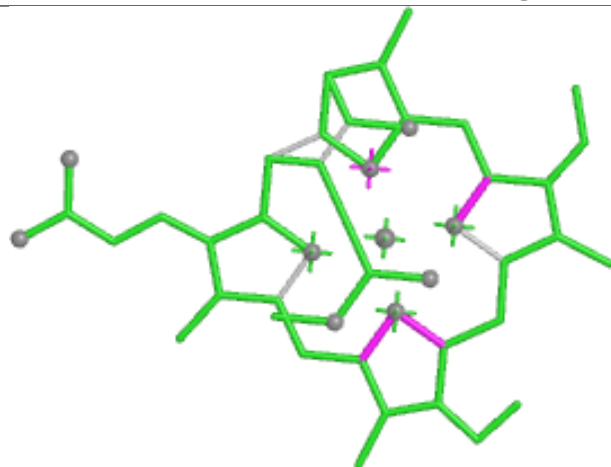


Torsions

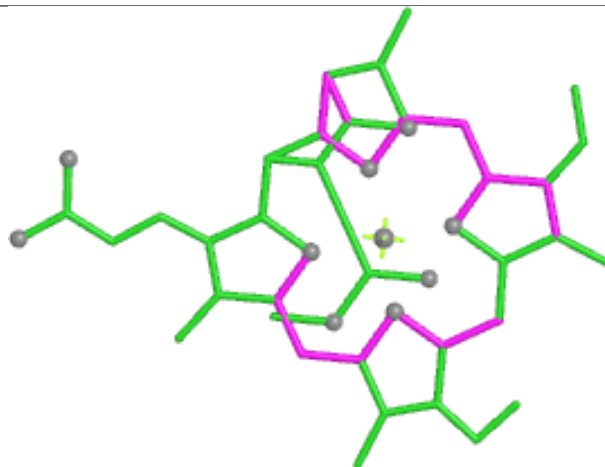


Rings

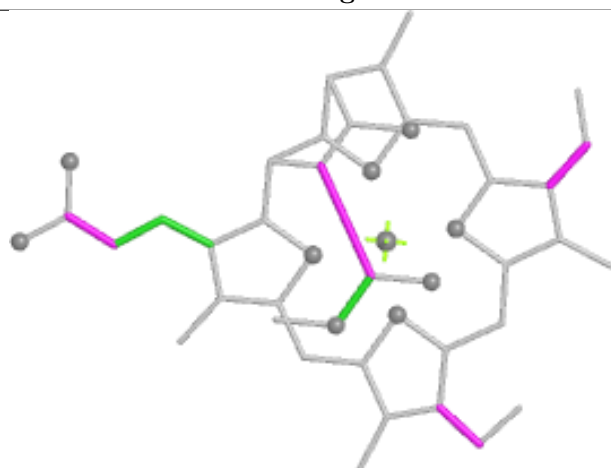
Ligand KC2 Y 308



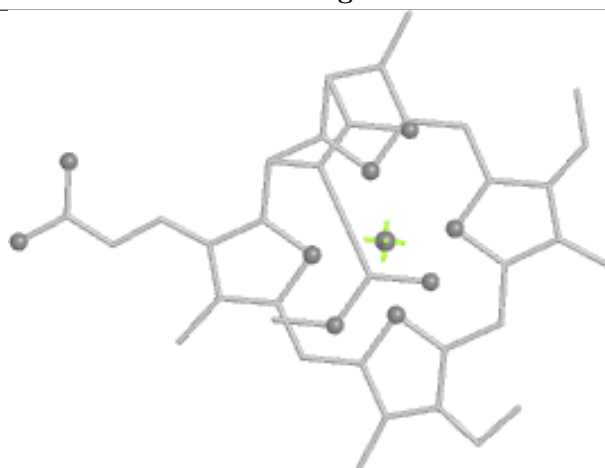
Bond lengths



Bond angles

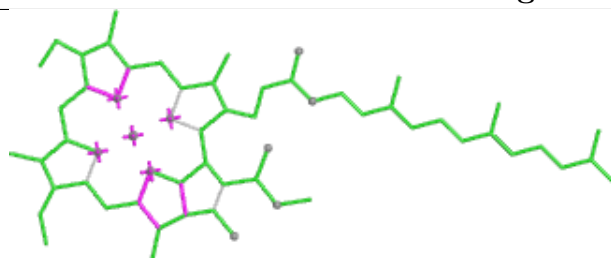


Torsions

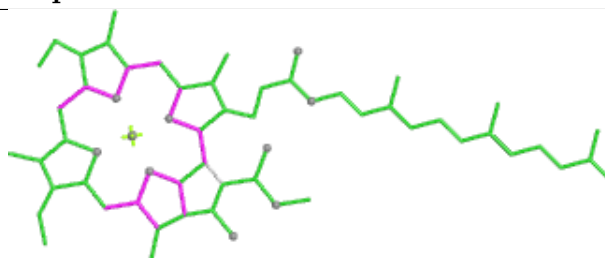


Rings

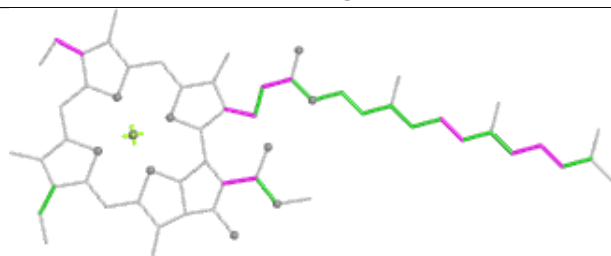
Ligand CLA p 308



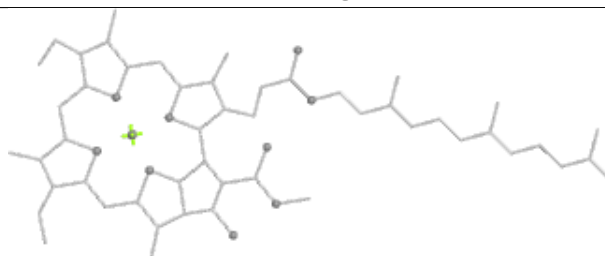
Bond lengths



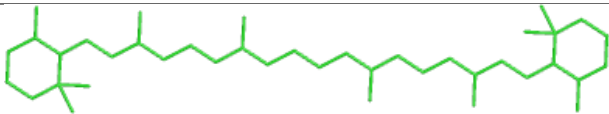
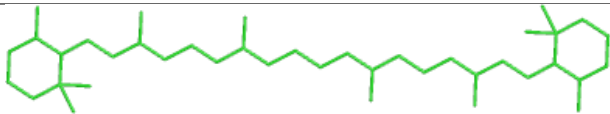
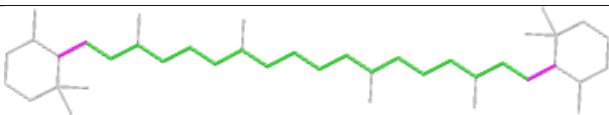
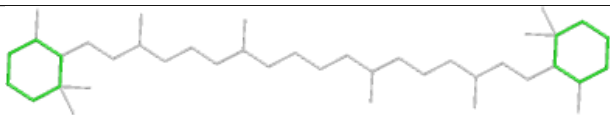
Bond angles

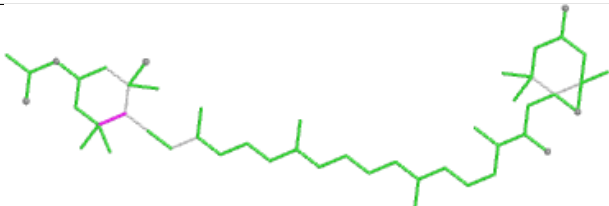
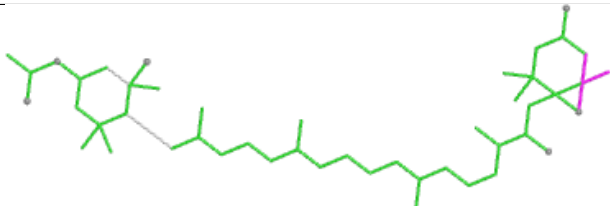
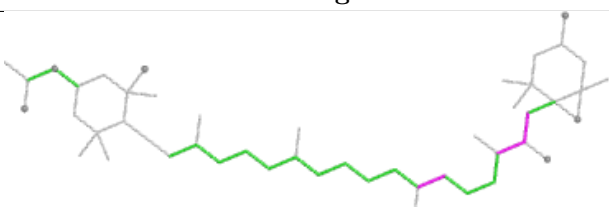
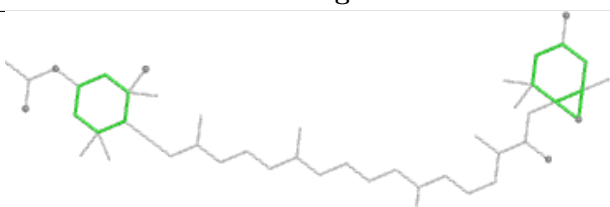


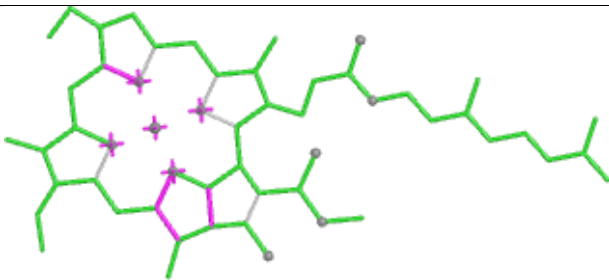
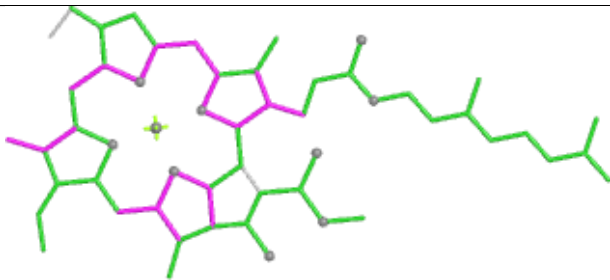
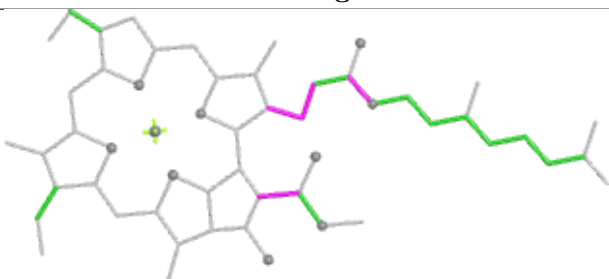
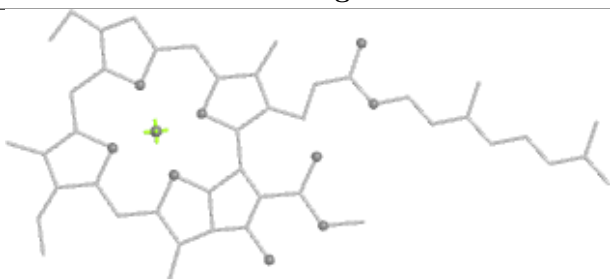
Torsions



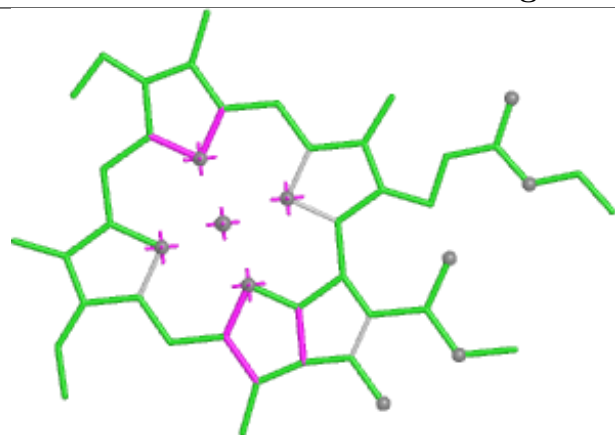
Rings

Ligand BCR a 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

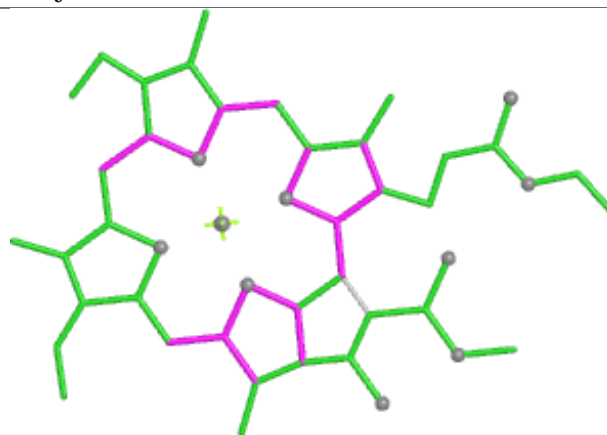
Ligand A86 z 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

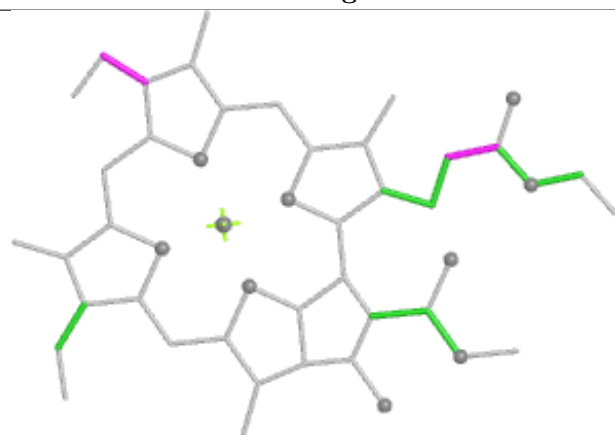
Ligand CLA y 302



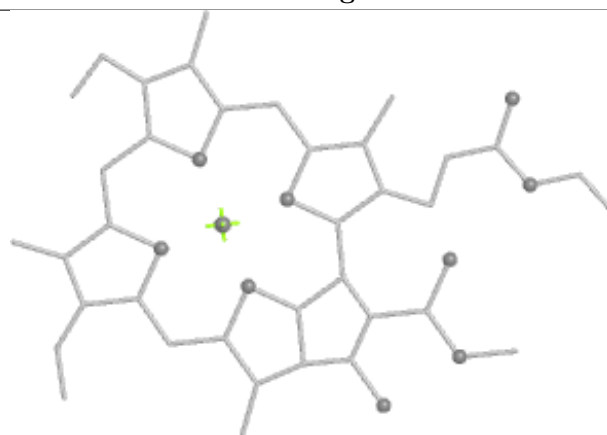
Bond lengths



Bond angles

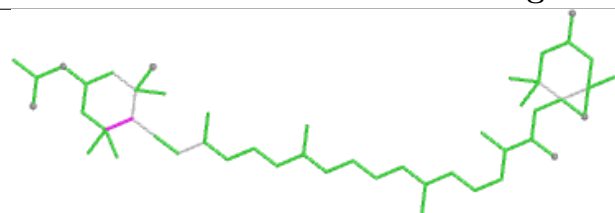


Torsions

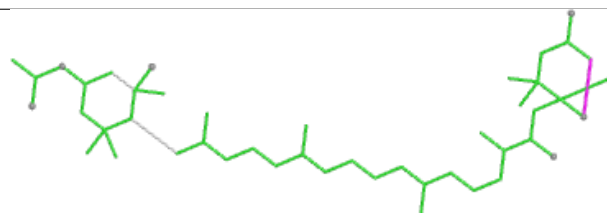


Rings

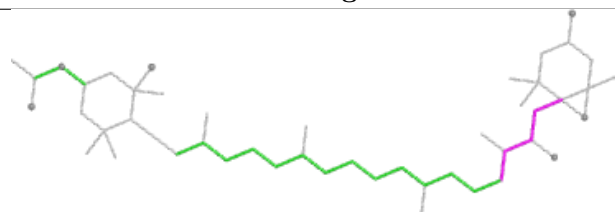
Ligand A86 z 319



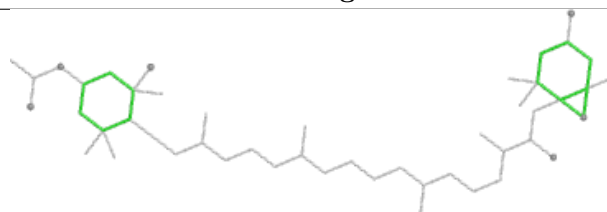
Bond lengths



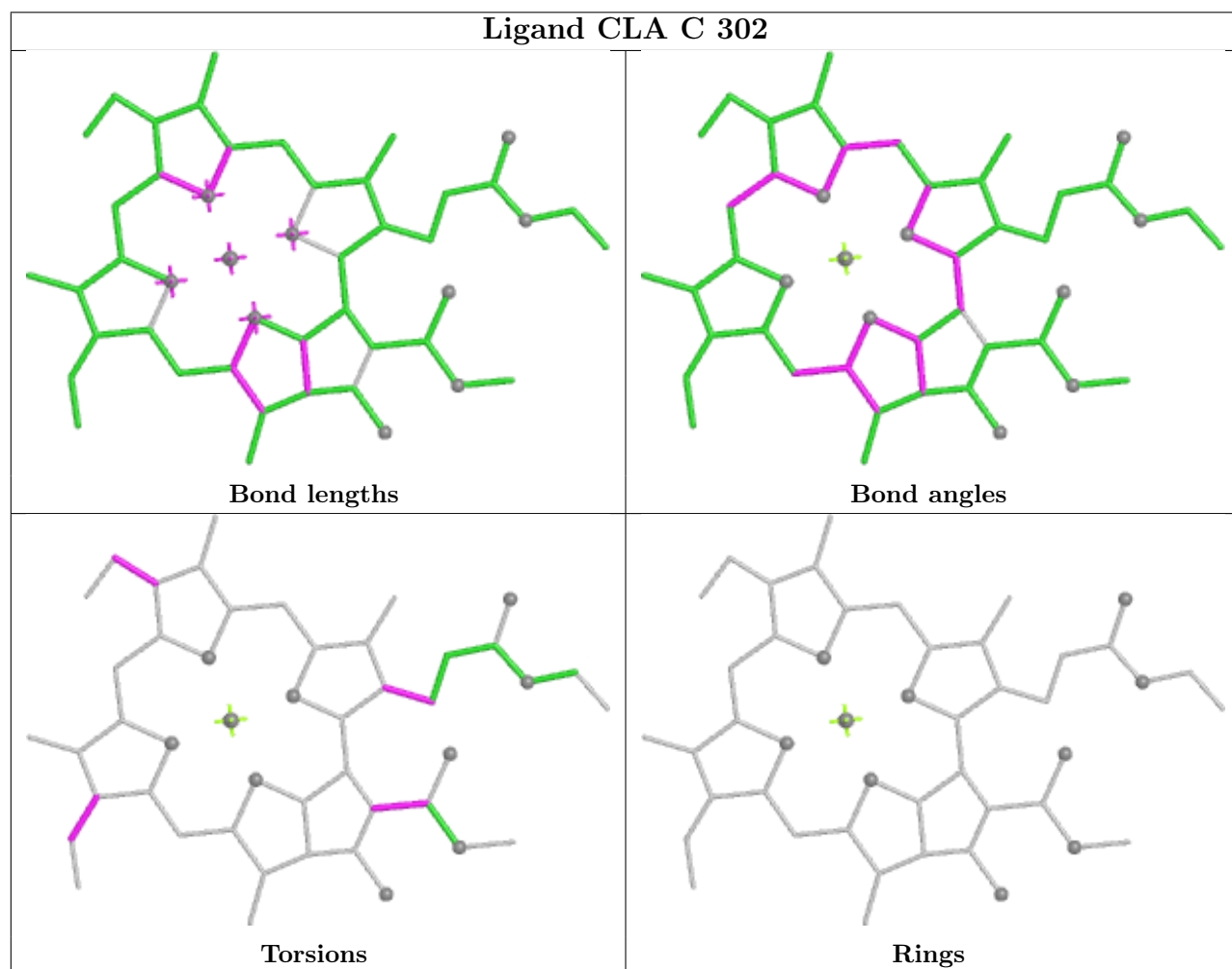
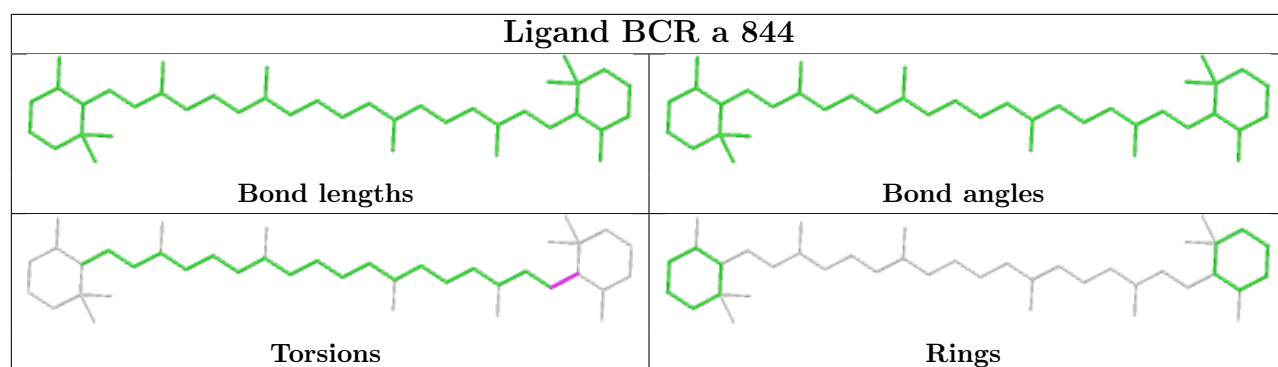
Bond angles



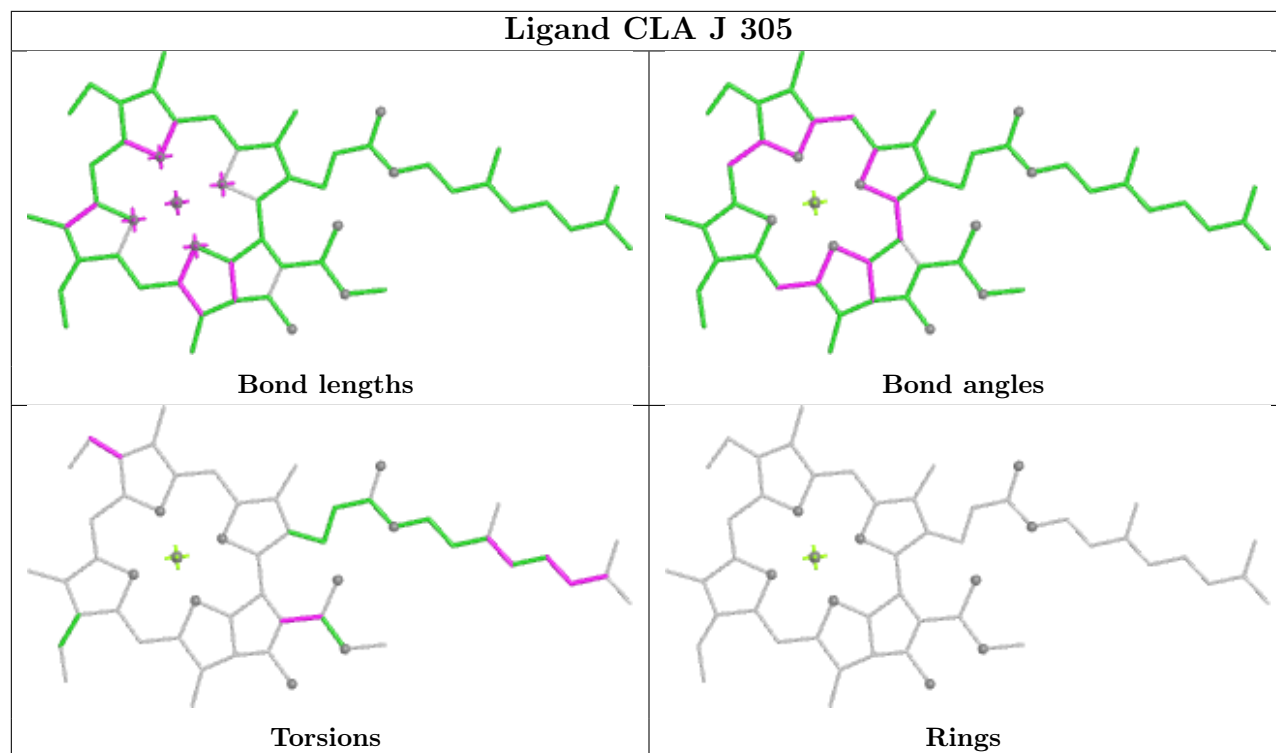
Torsions



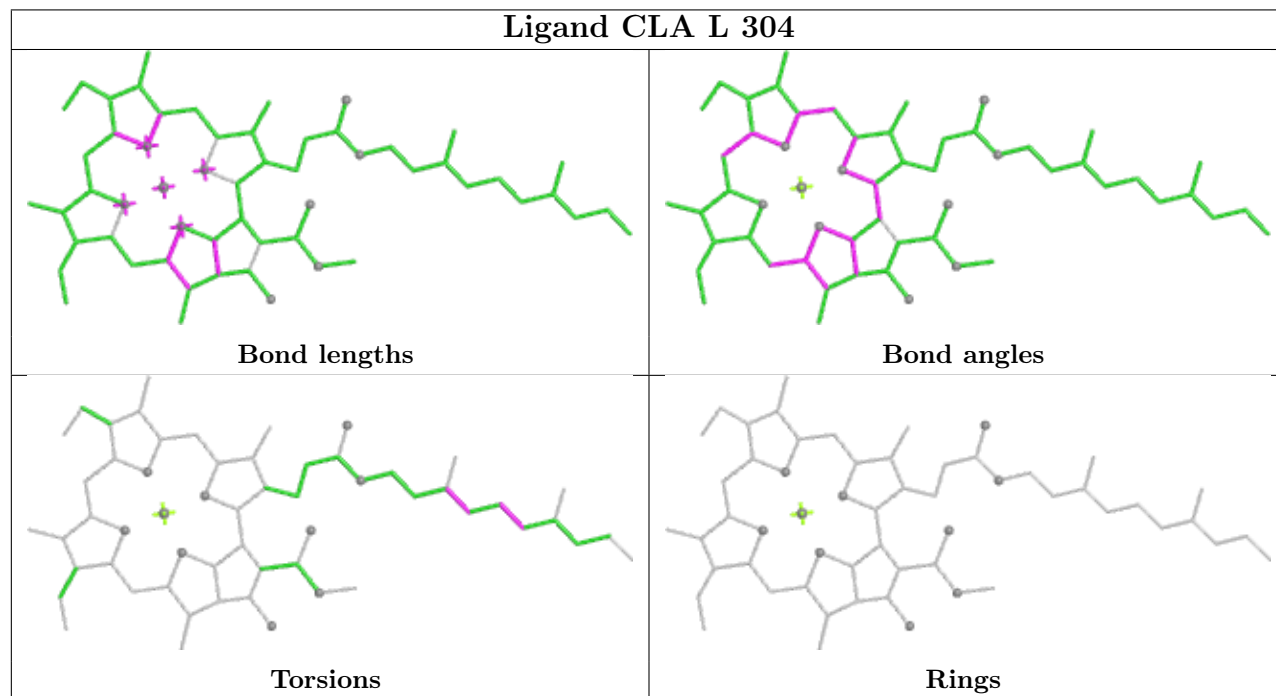
Rings



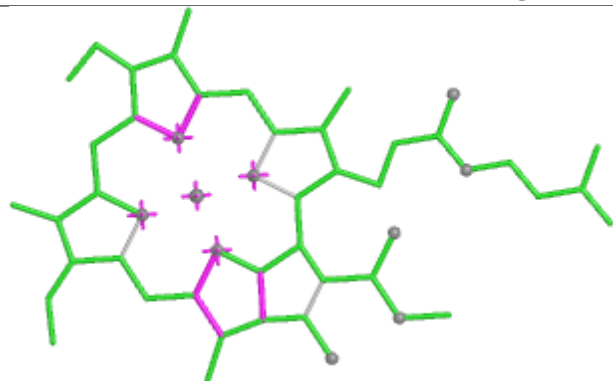
Ligand CLA J 305



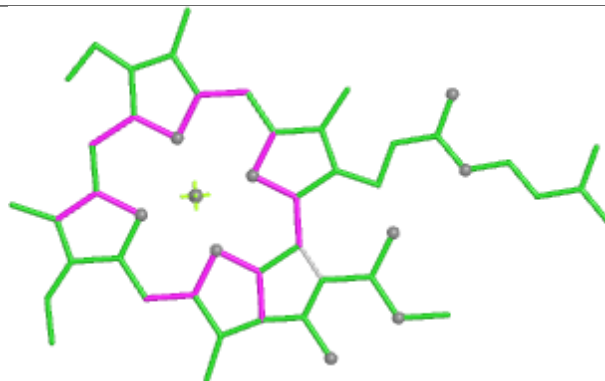
Ligand CLA L 304



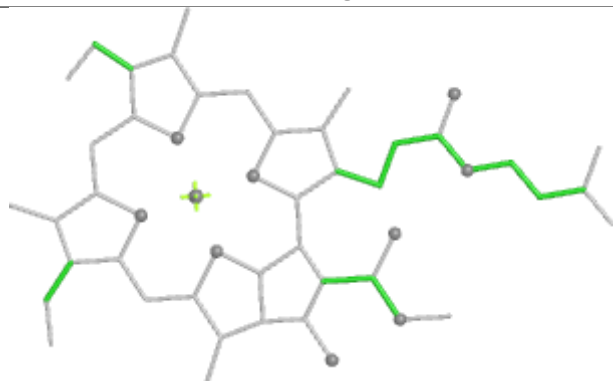
Ligand CLA H 306



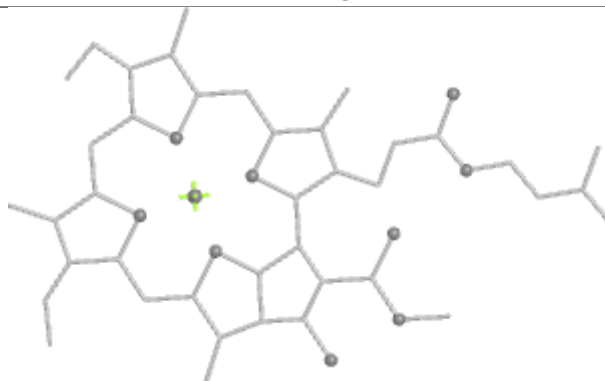
Bond lengths



Bond angles

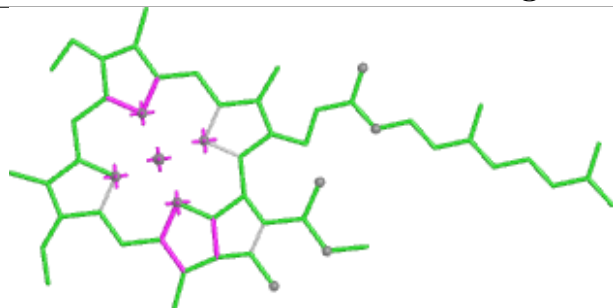


Torsions

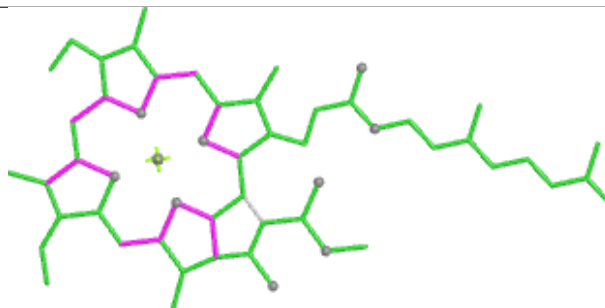


Rings

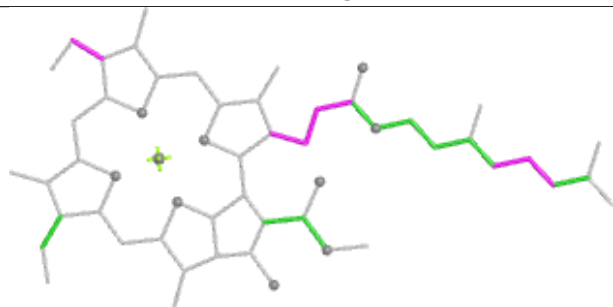
Ligand CLA I 202



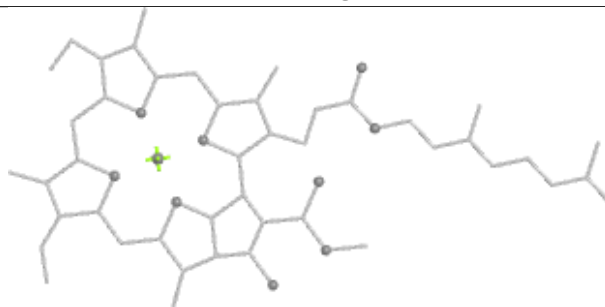
Bond lengths



Bond angles

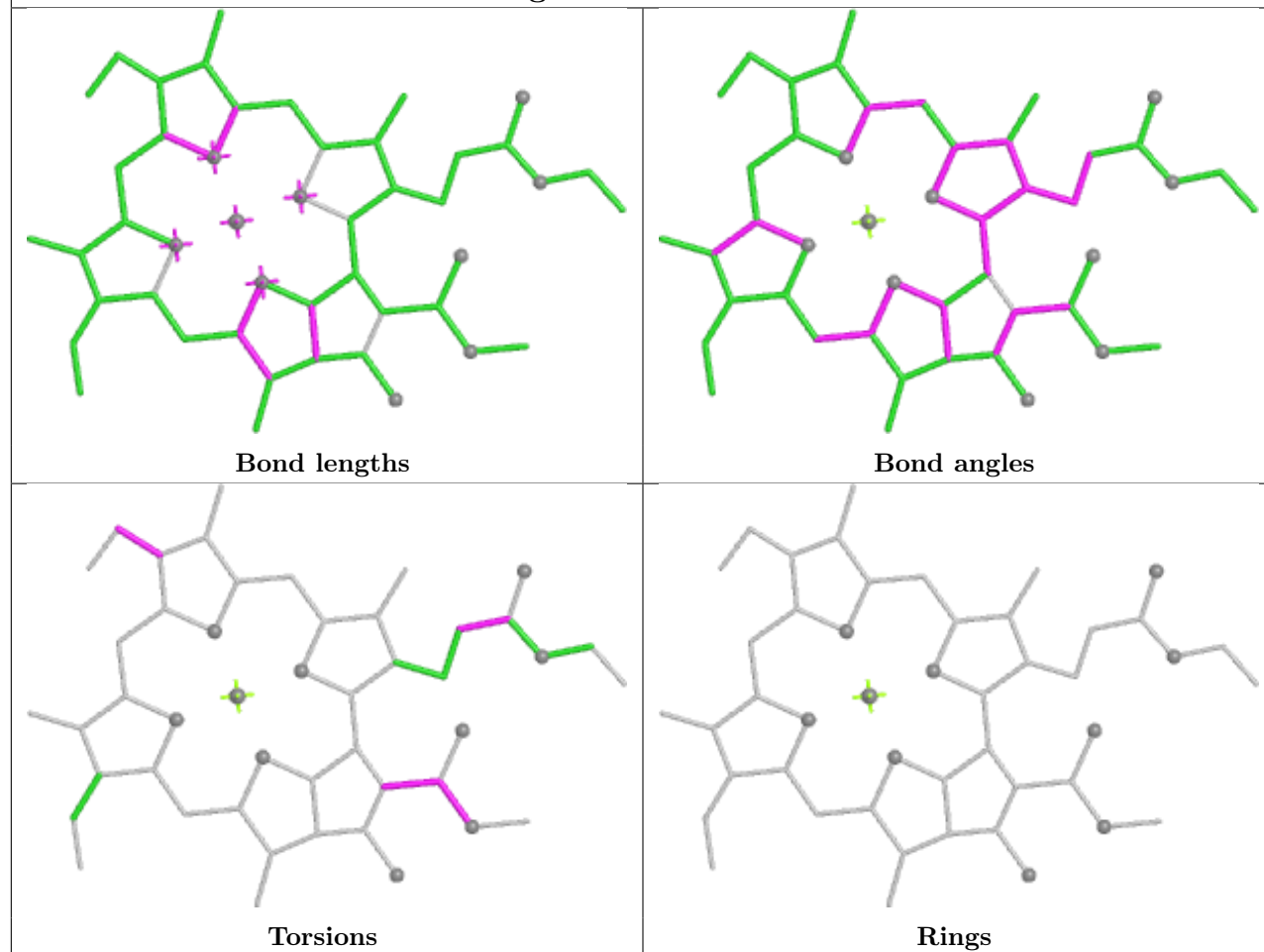


Torsions

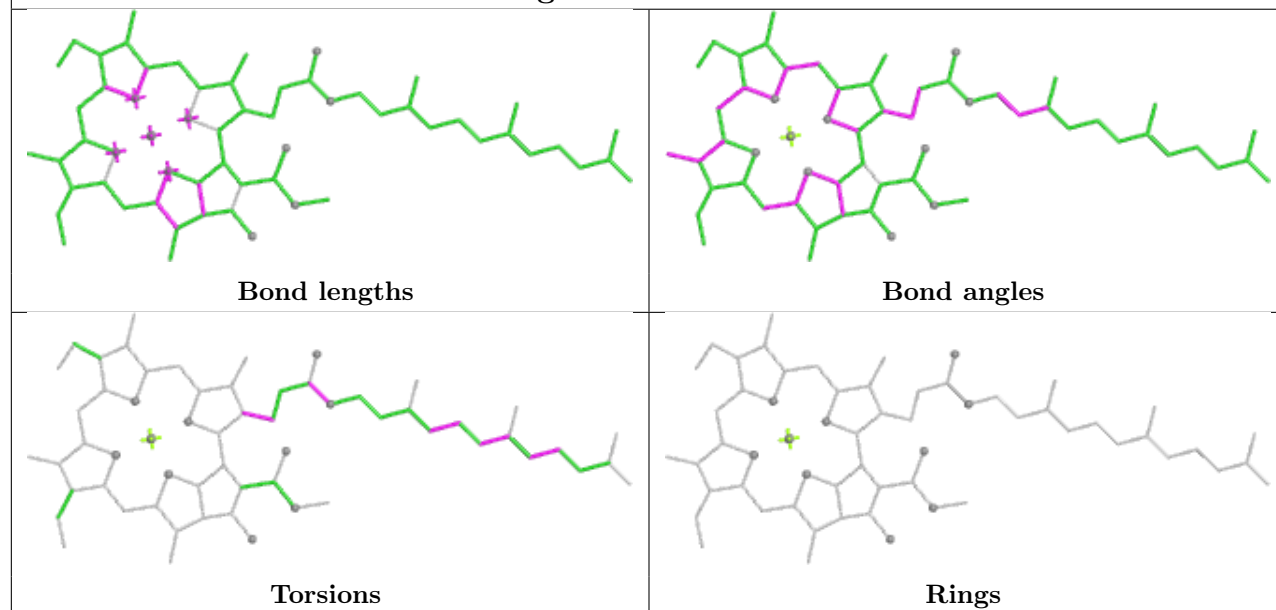


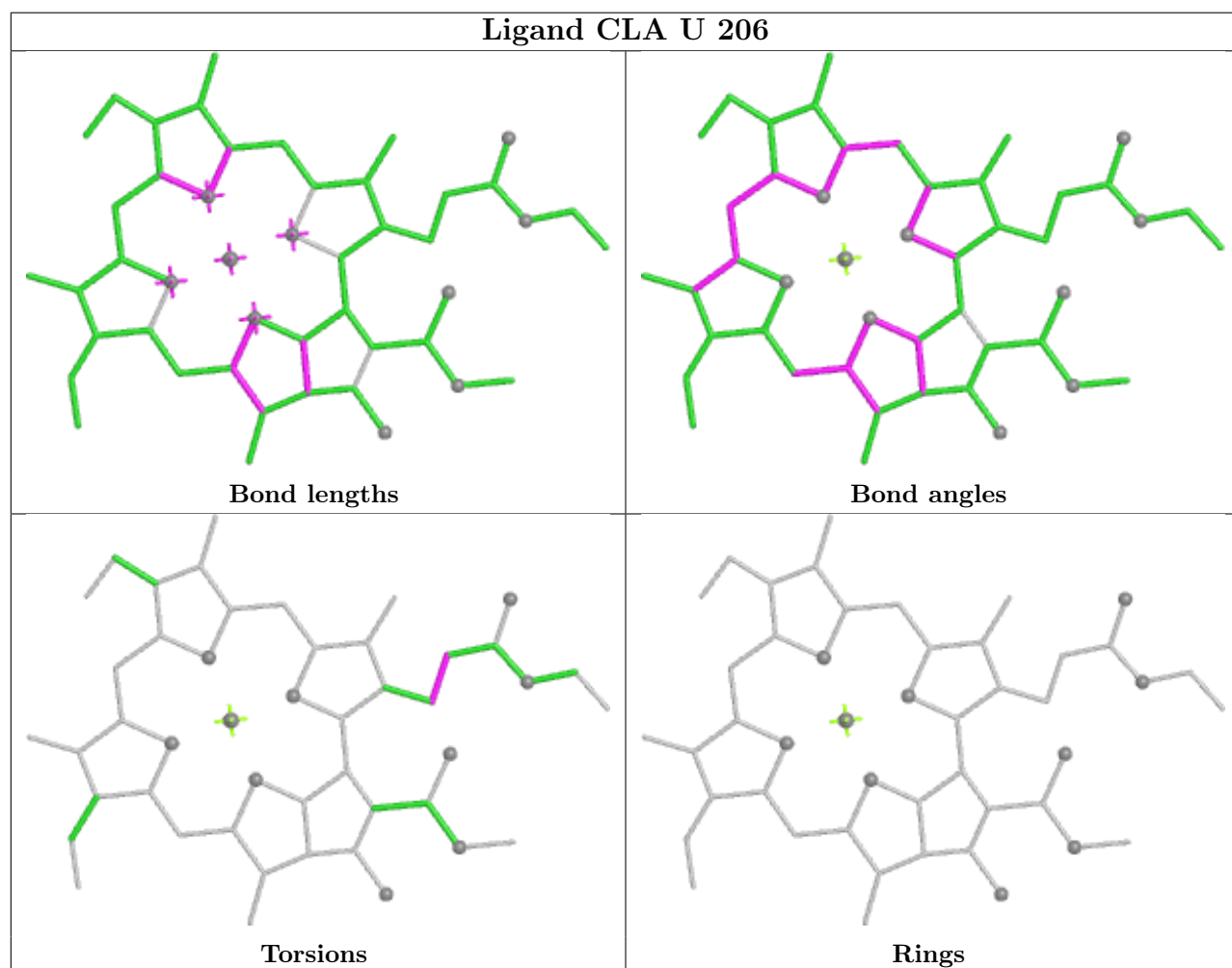
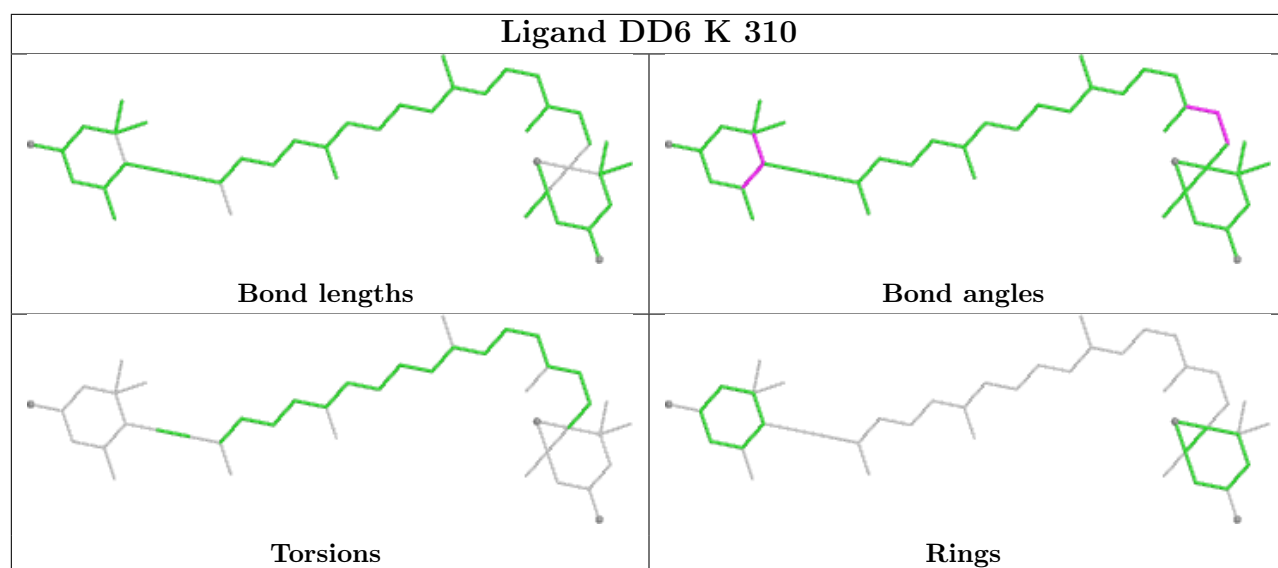
Rings

Ligand CLA F 310

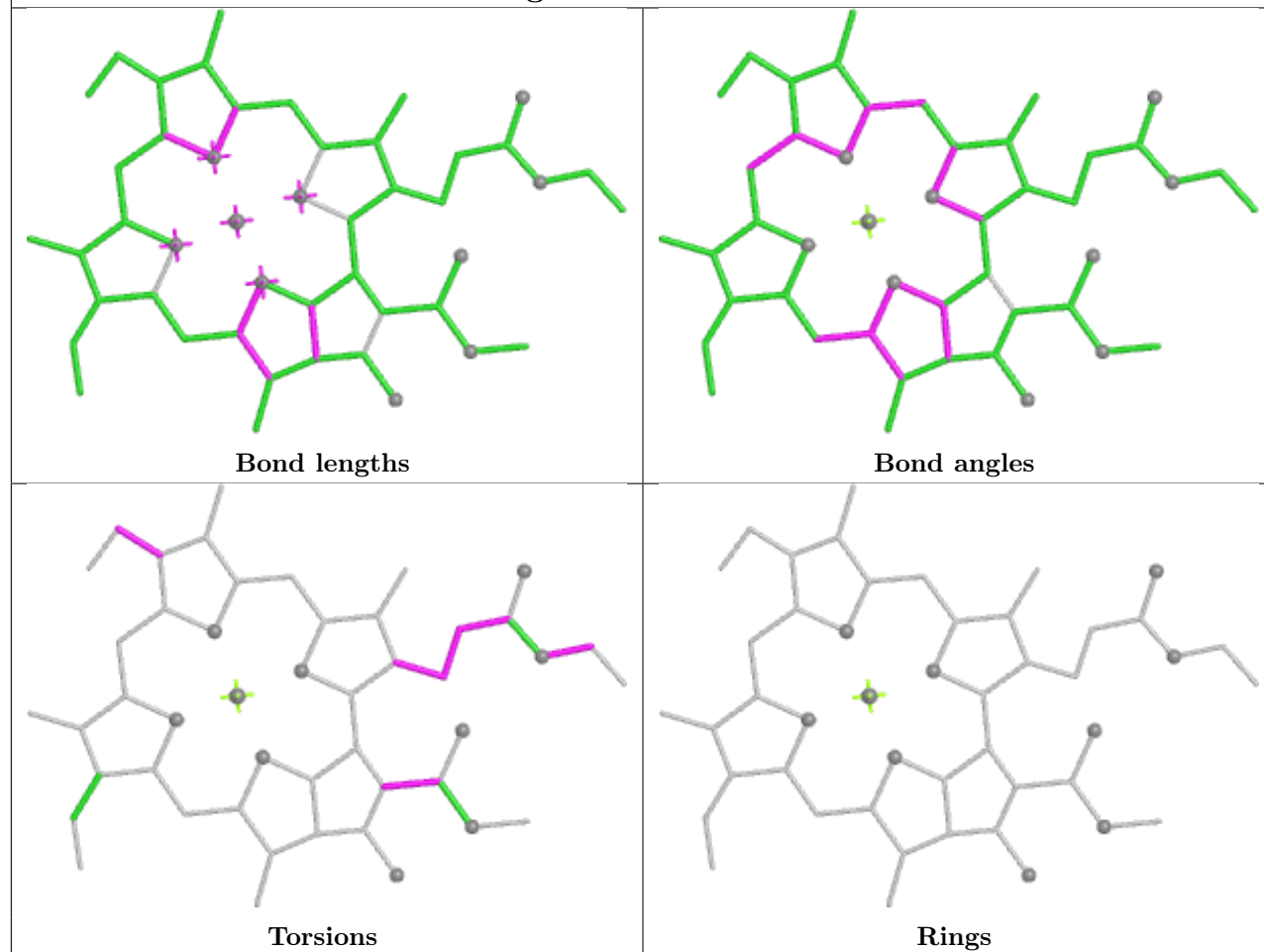


Ligand CLA z 307

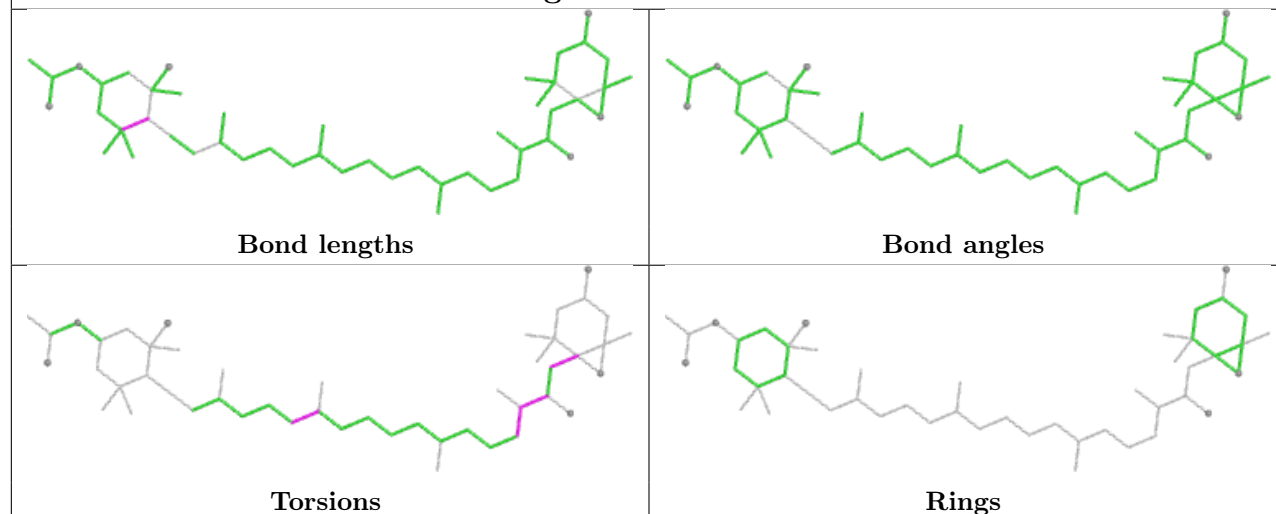


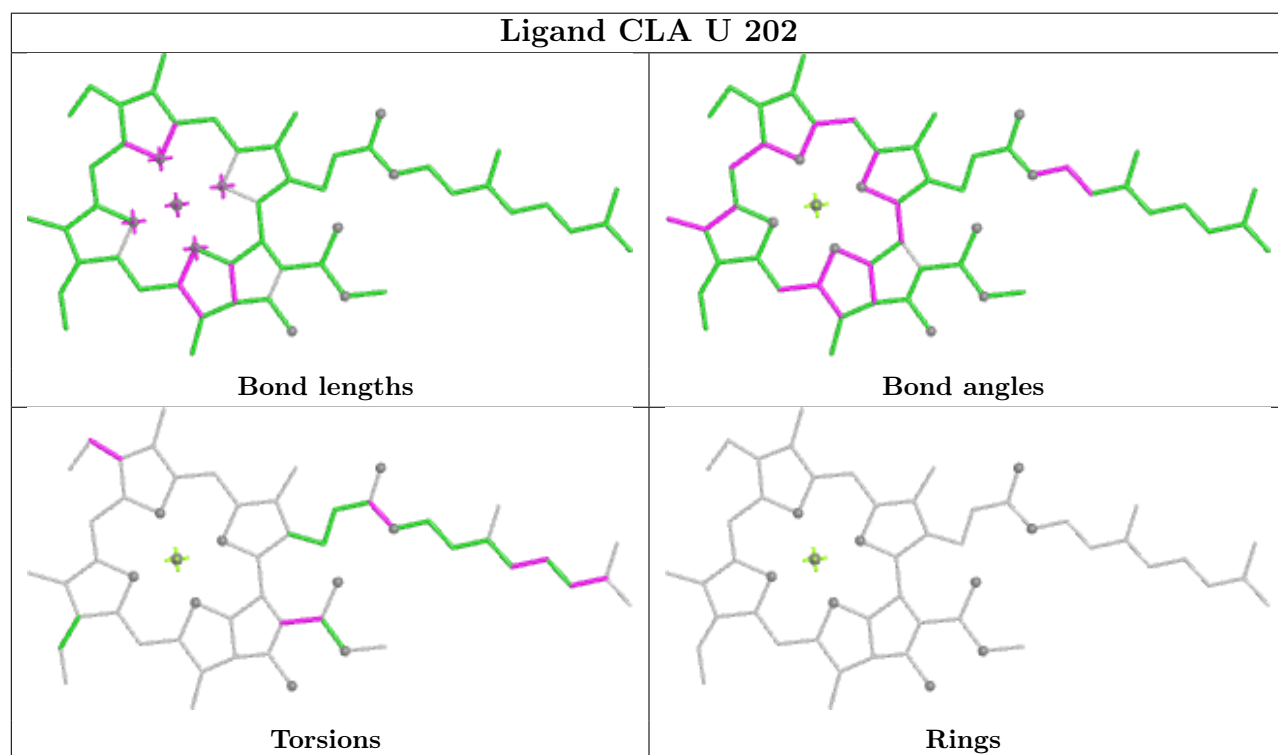
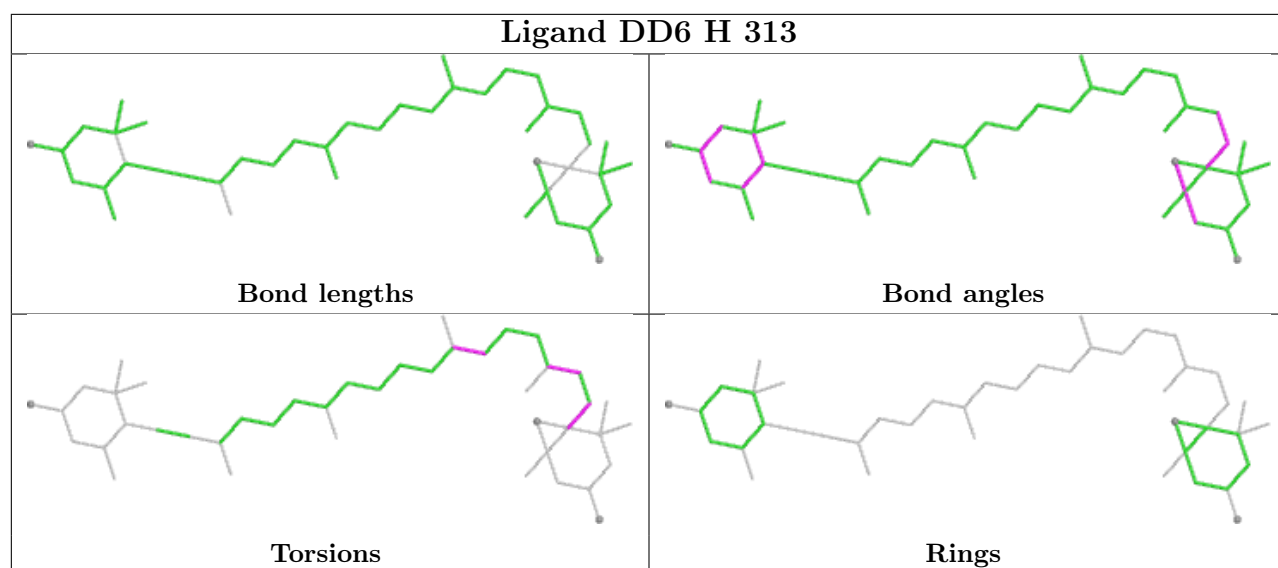


Ligand CLA U 204

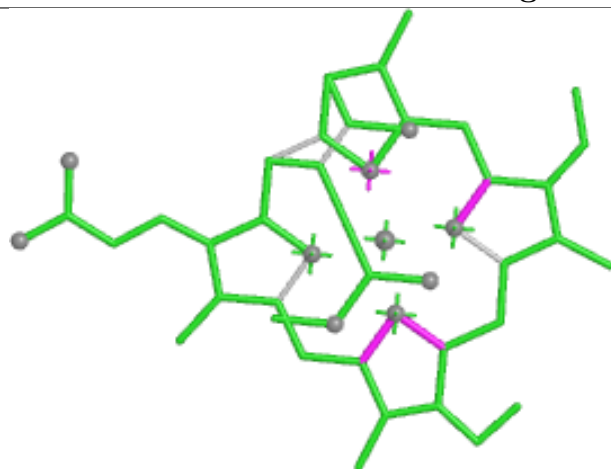


Ligand A86 t 316

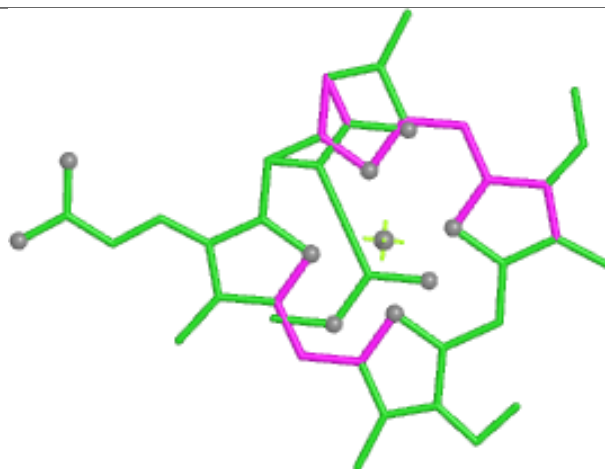




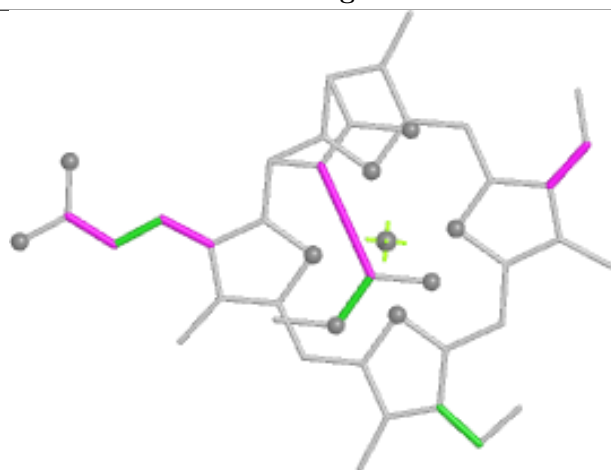
Ligand KC2 v 302



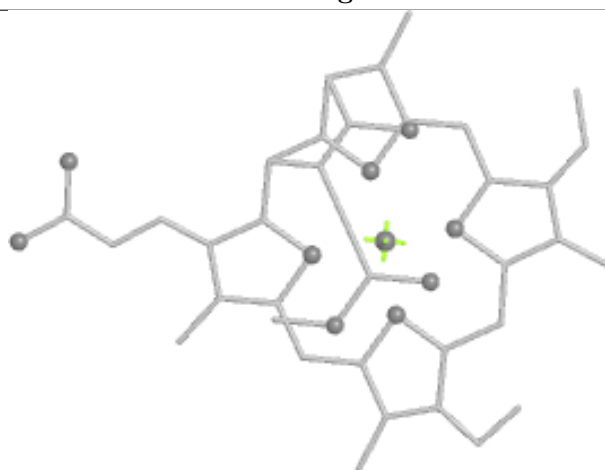
Bond lengths



Bond angles

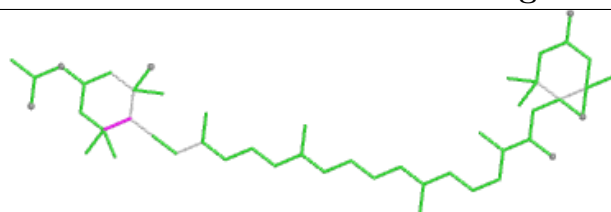


Torsions

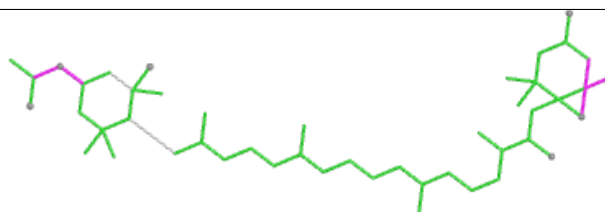


Rings

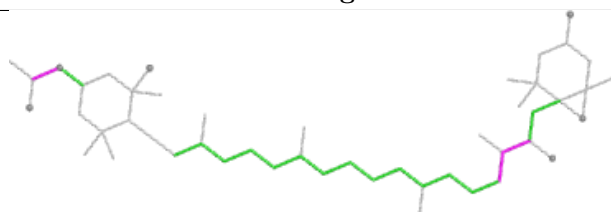
Ligand A86 X 321



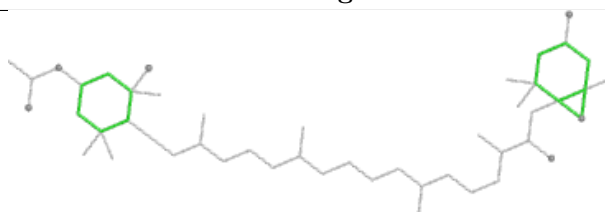
Bond lengths



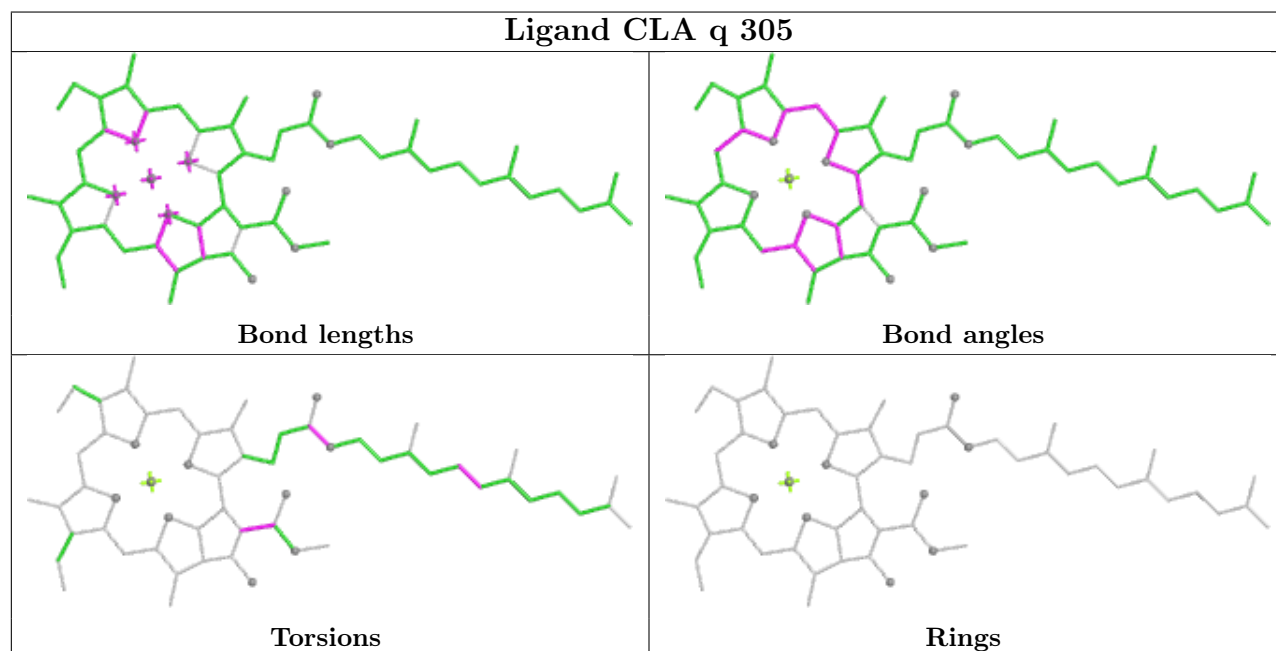
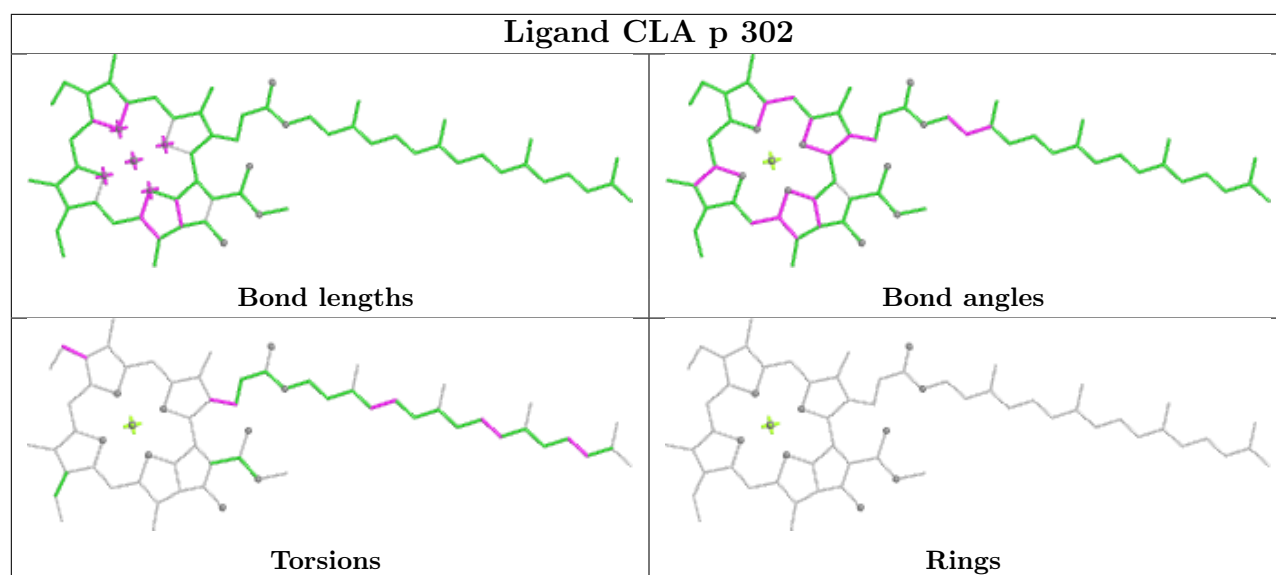
Bond angles

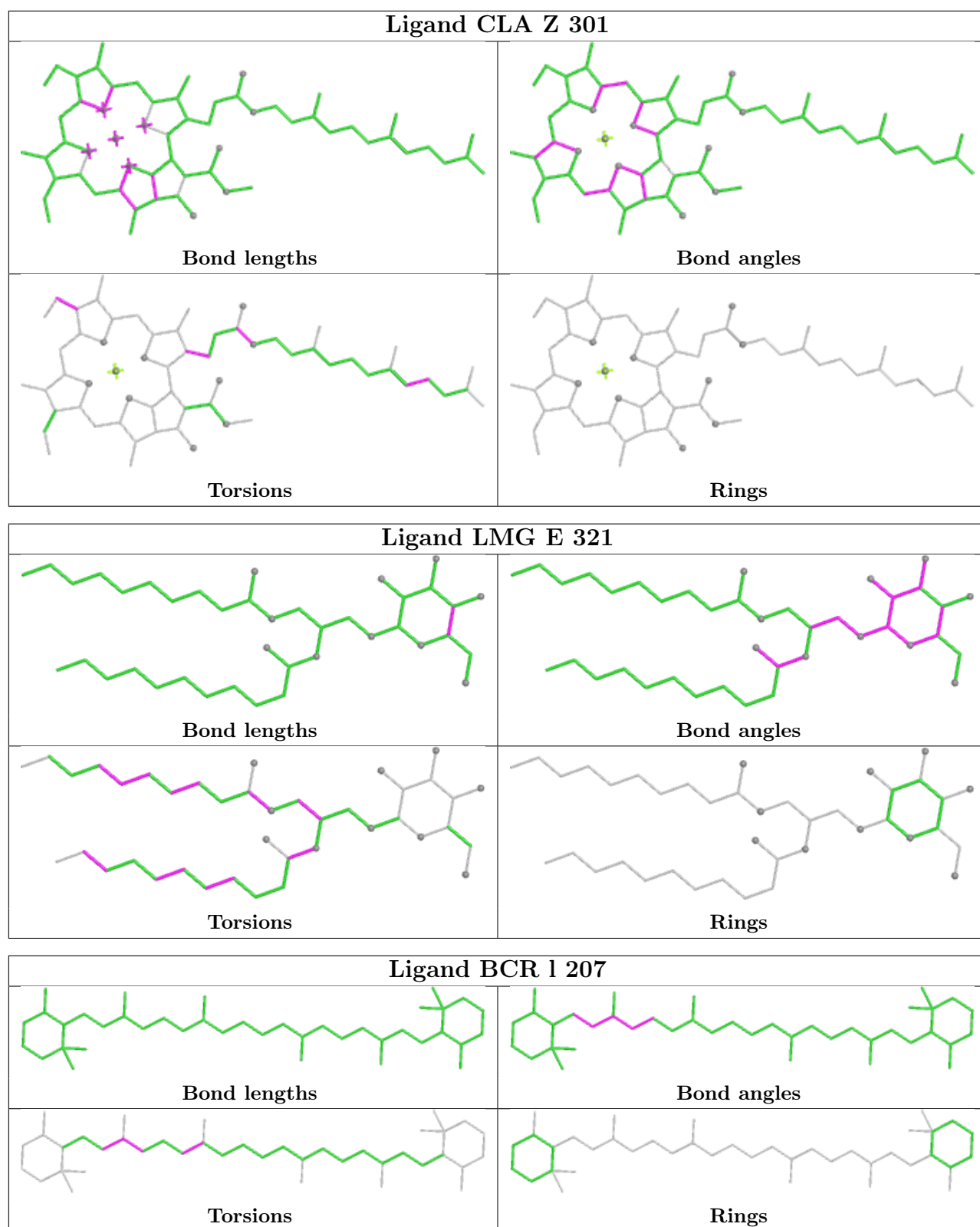


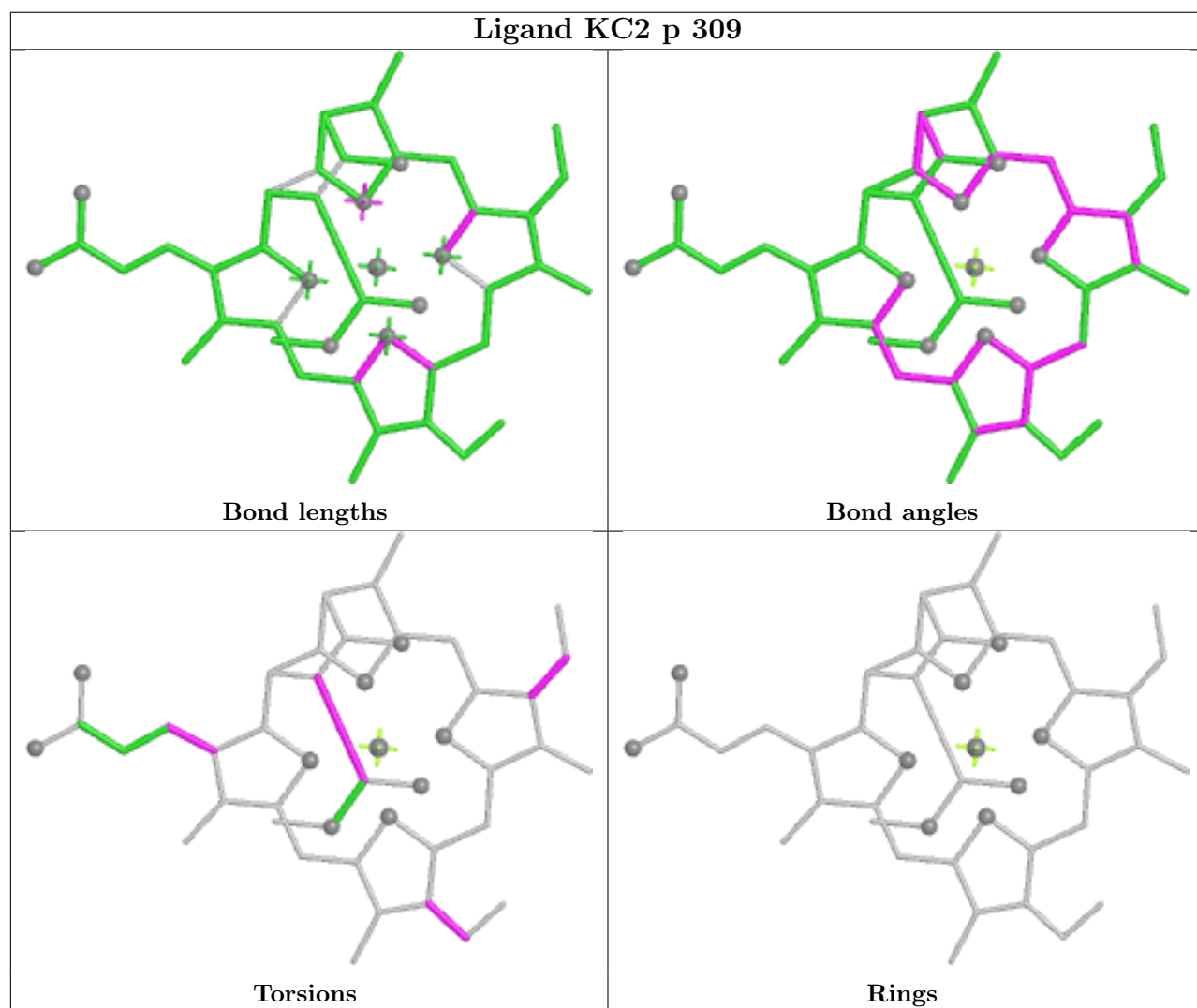
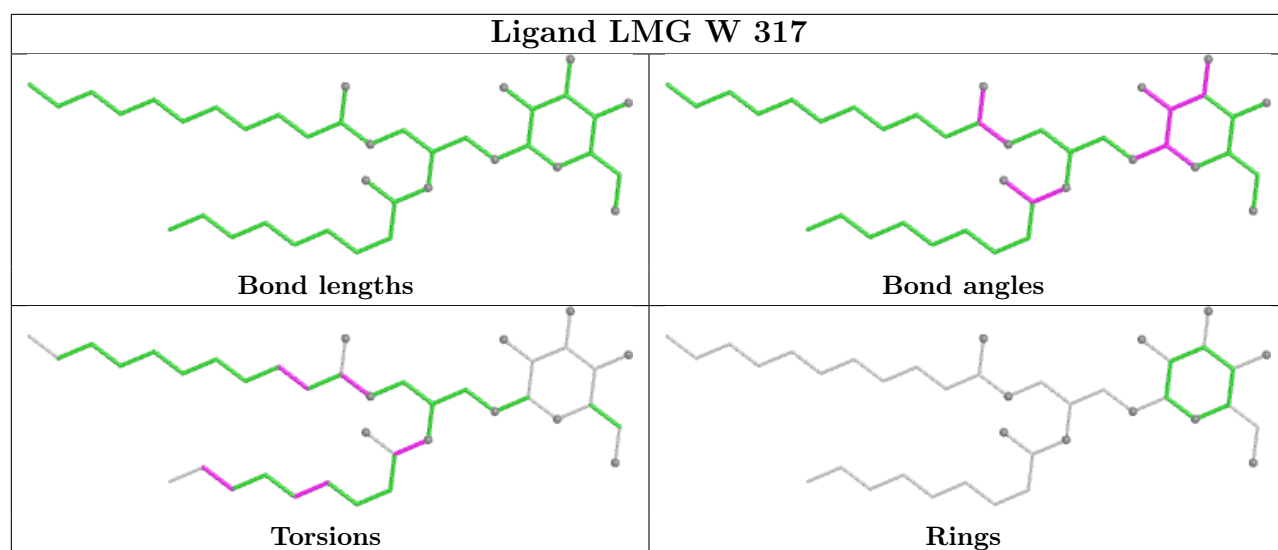
Torsions

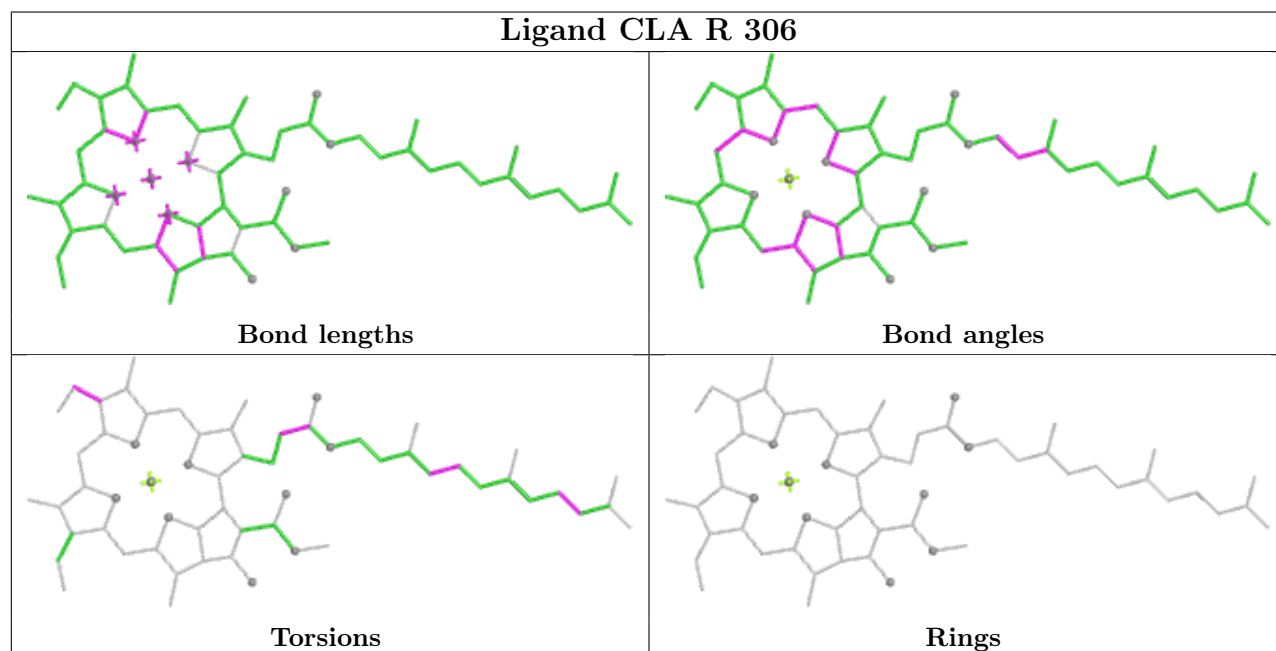
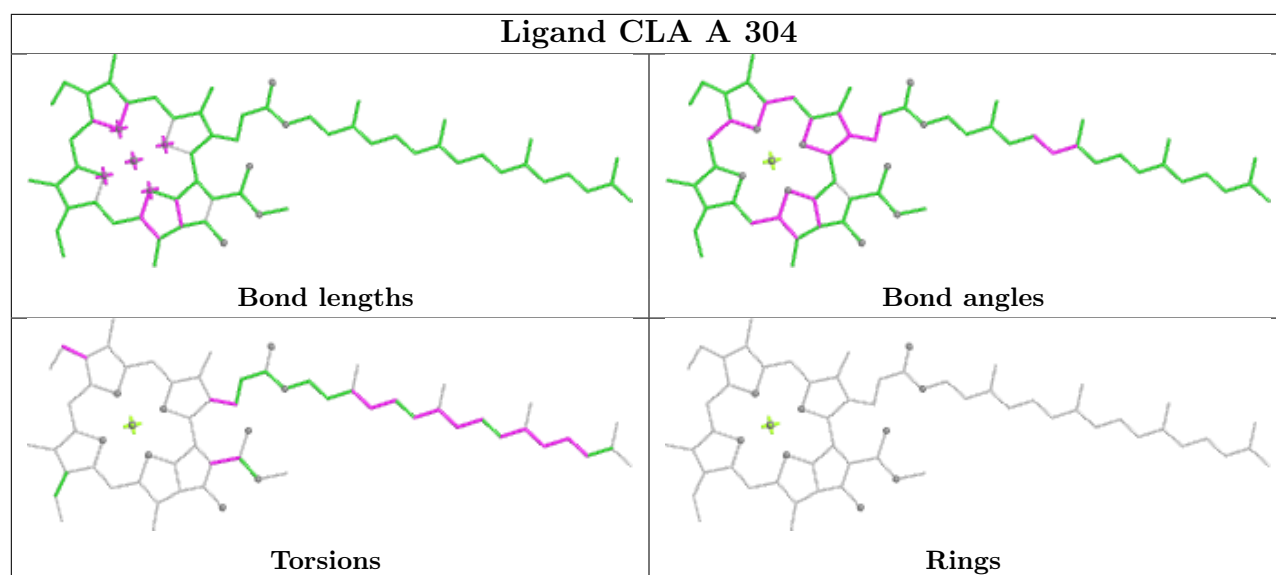


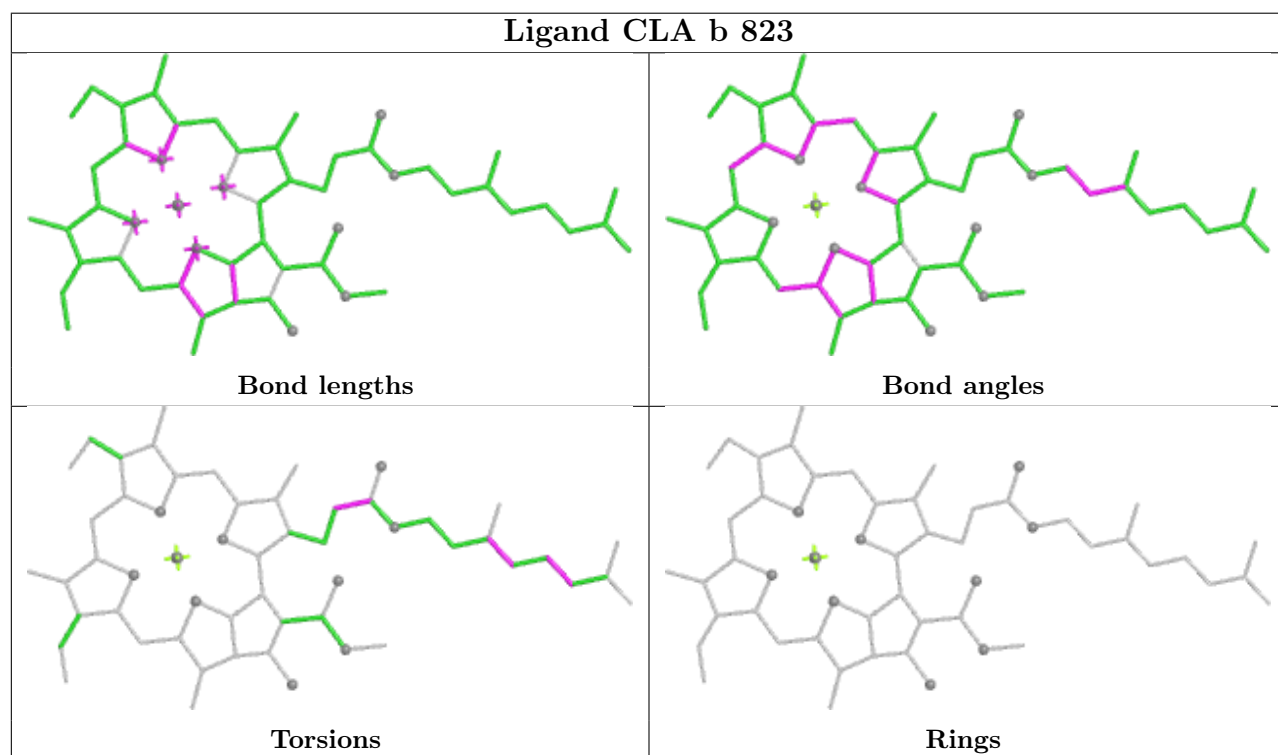
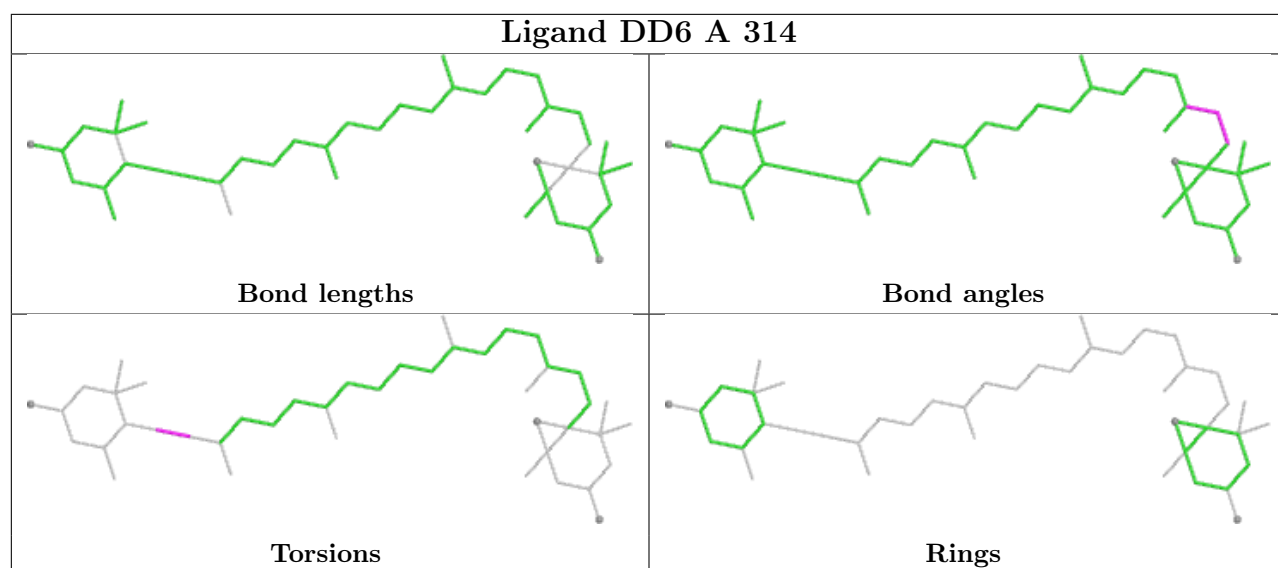
Rings



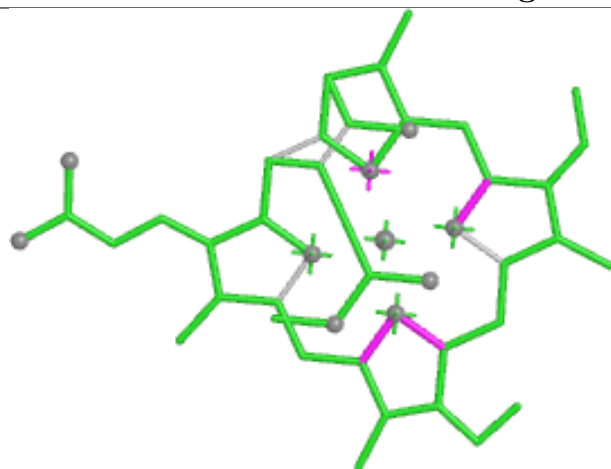




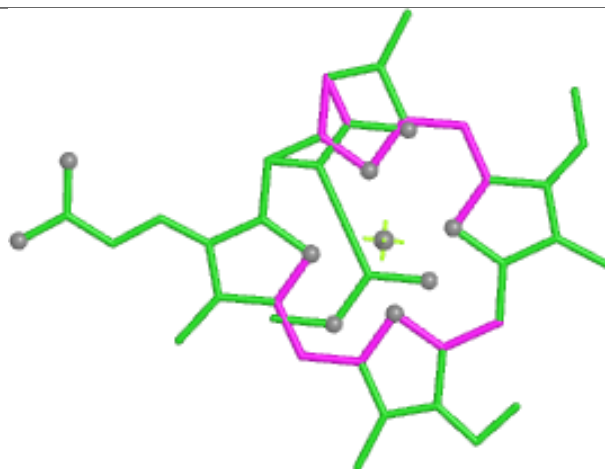




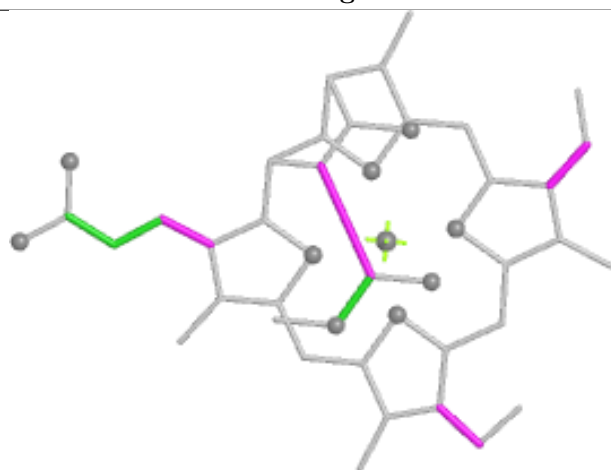
Ligand KC2 L 313



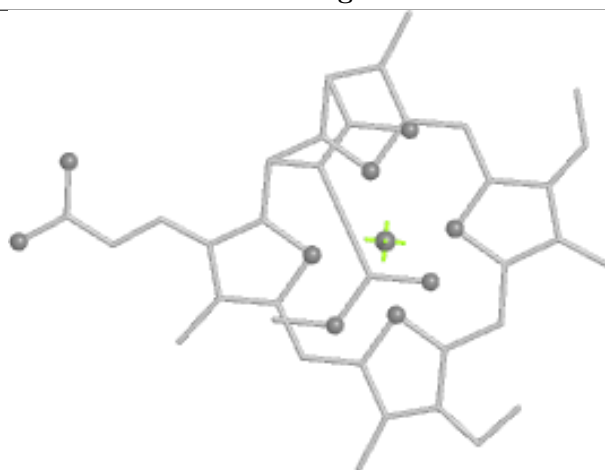
Bond lengths



Bond angles

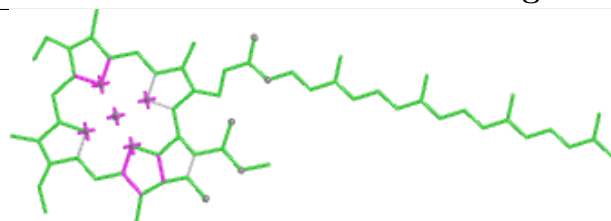


Torsions

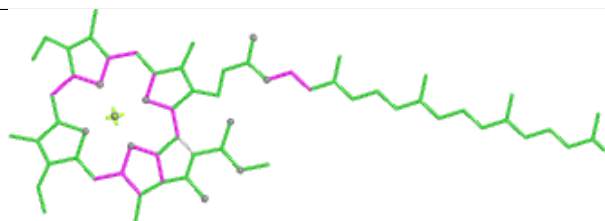


Rings

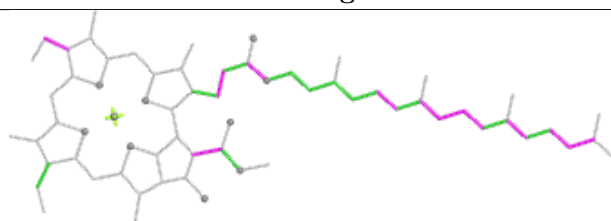
Ligand CLA 1 202



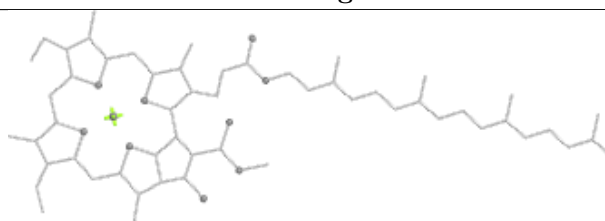
Bond lengths



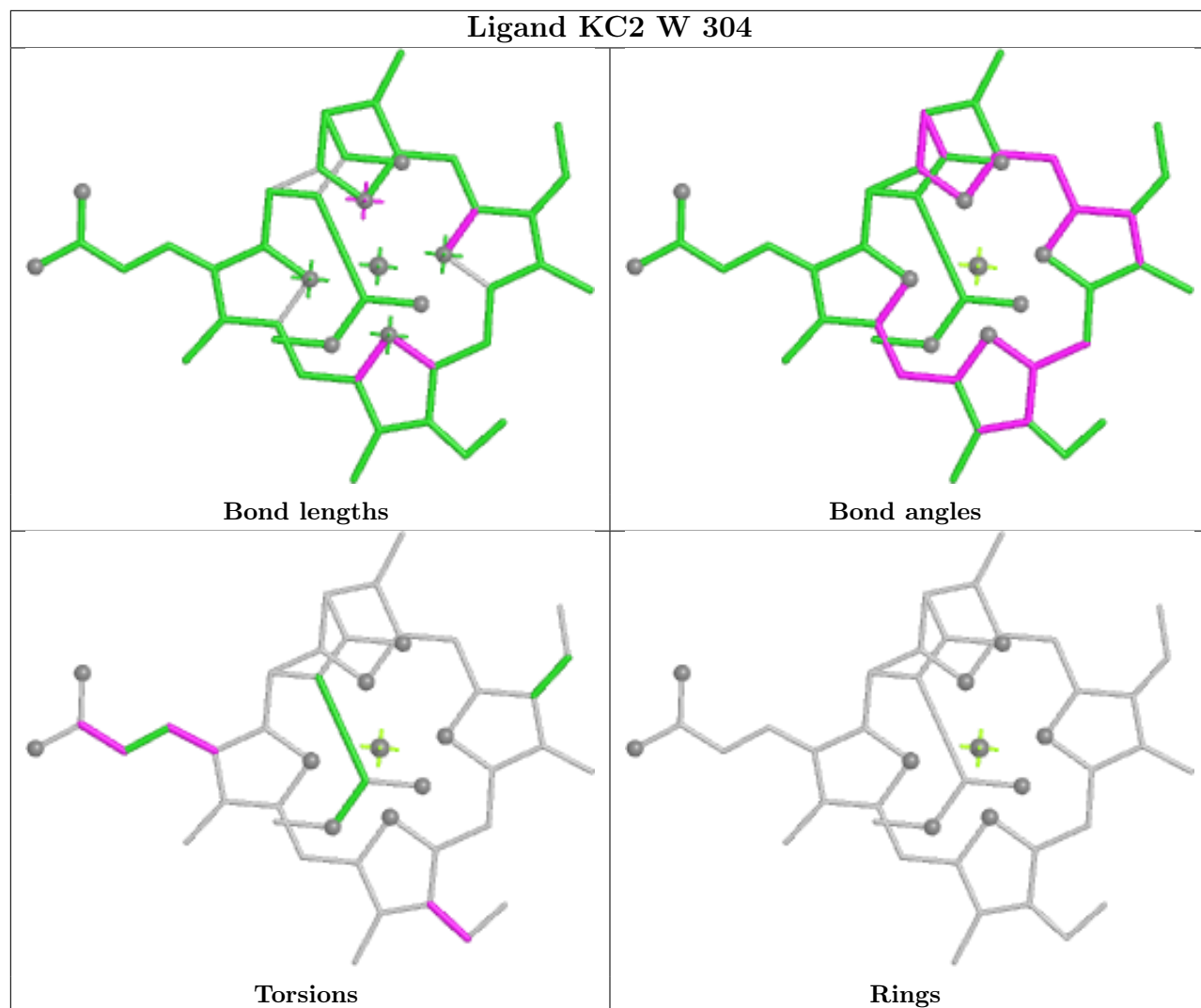
Bond angles



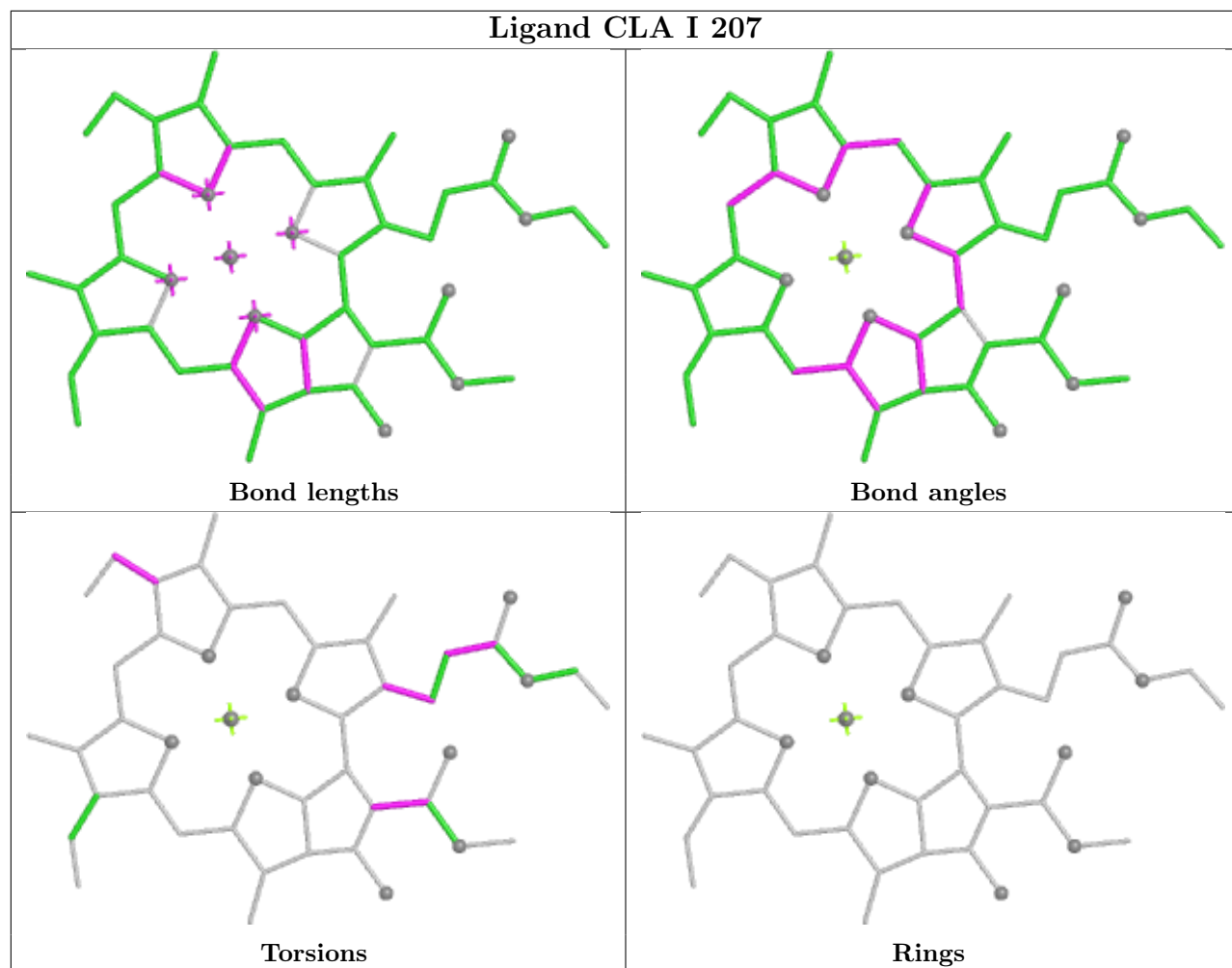
Torsions



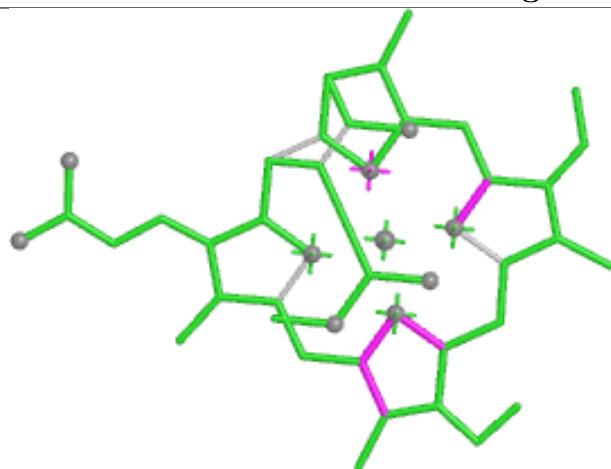
Rings



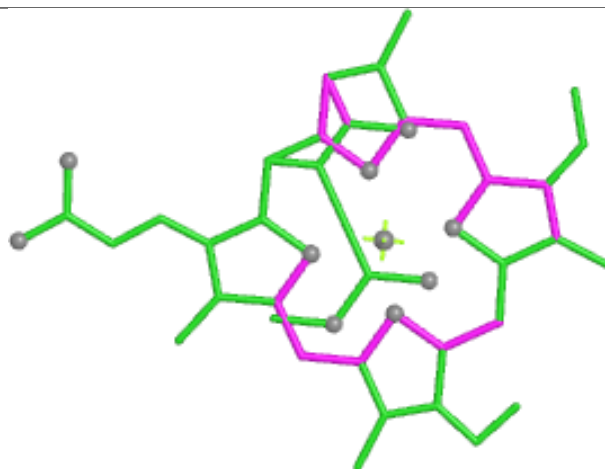
Ligand CLA I 207



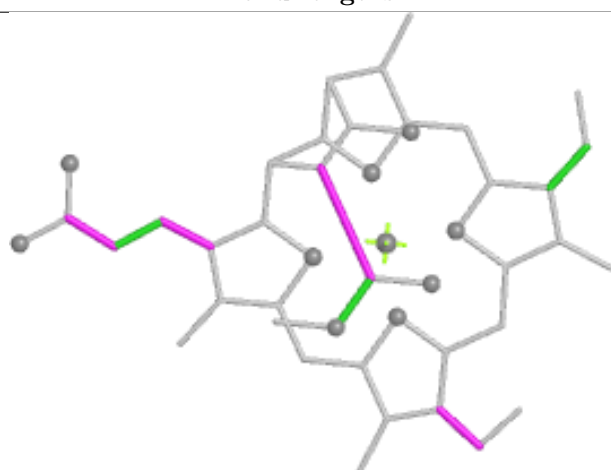
Ligand KC2 t 301



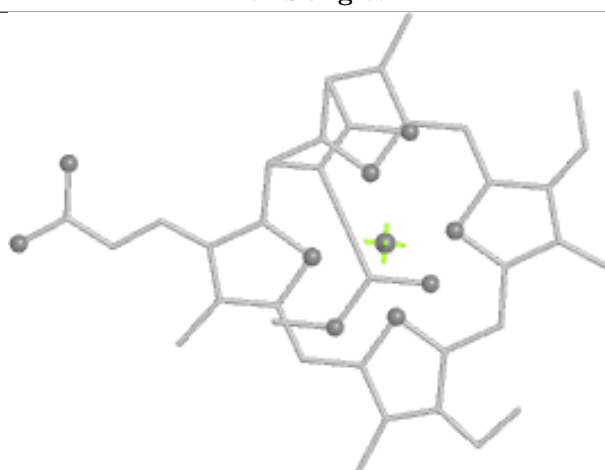
Bond lengths



Bond angles

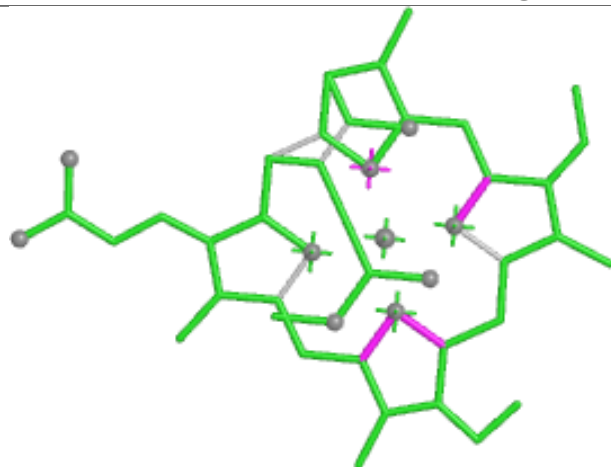


Torsions

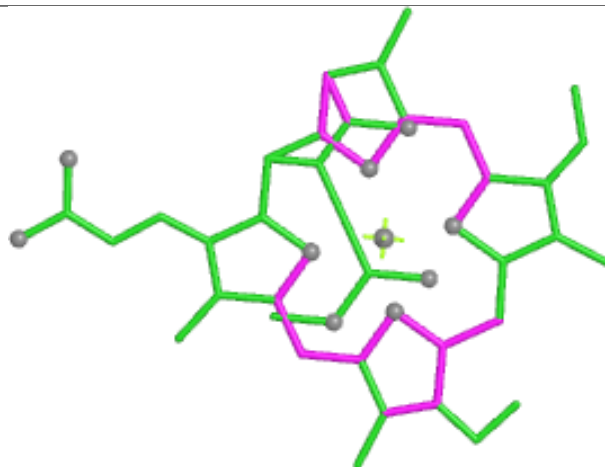


Rings

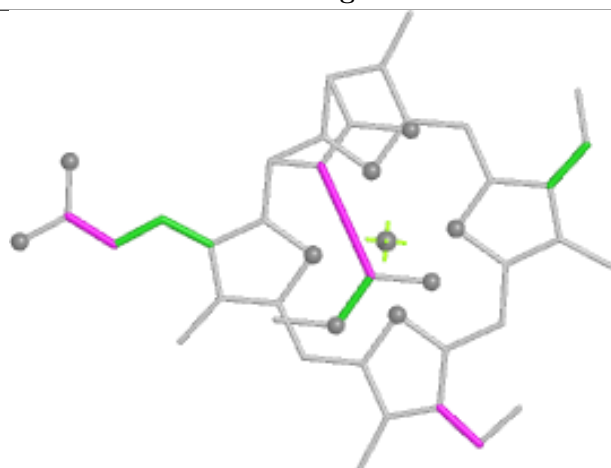
Ligand KC2 X 308



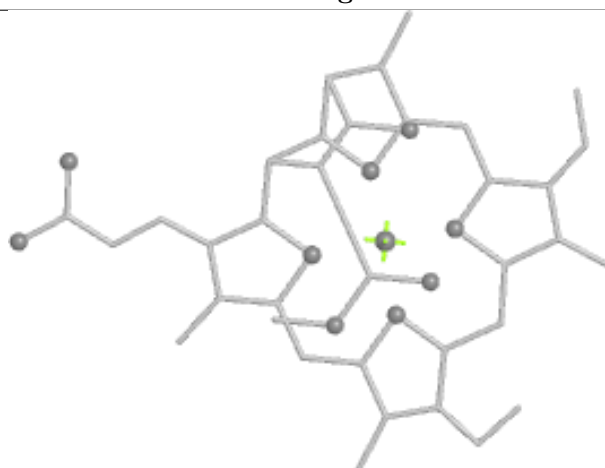
Bond lengths



Bond angles

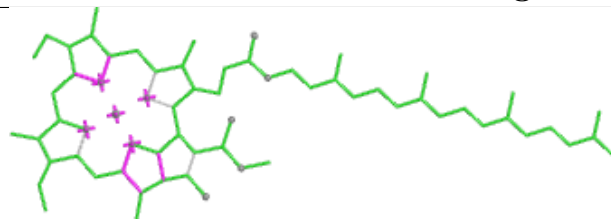


Torsions

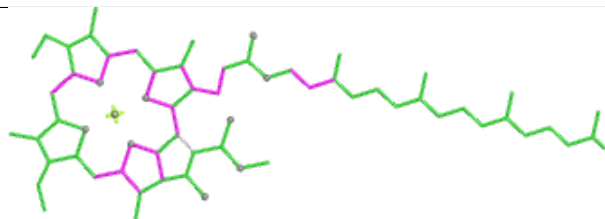


Rings

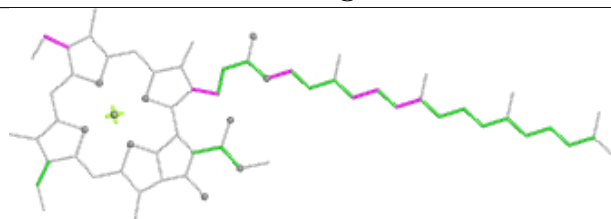
Ligand CLA D 307



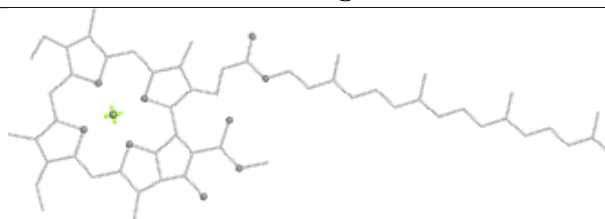
Bond lengths



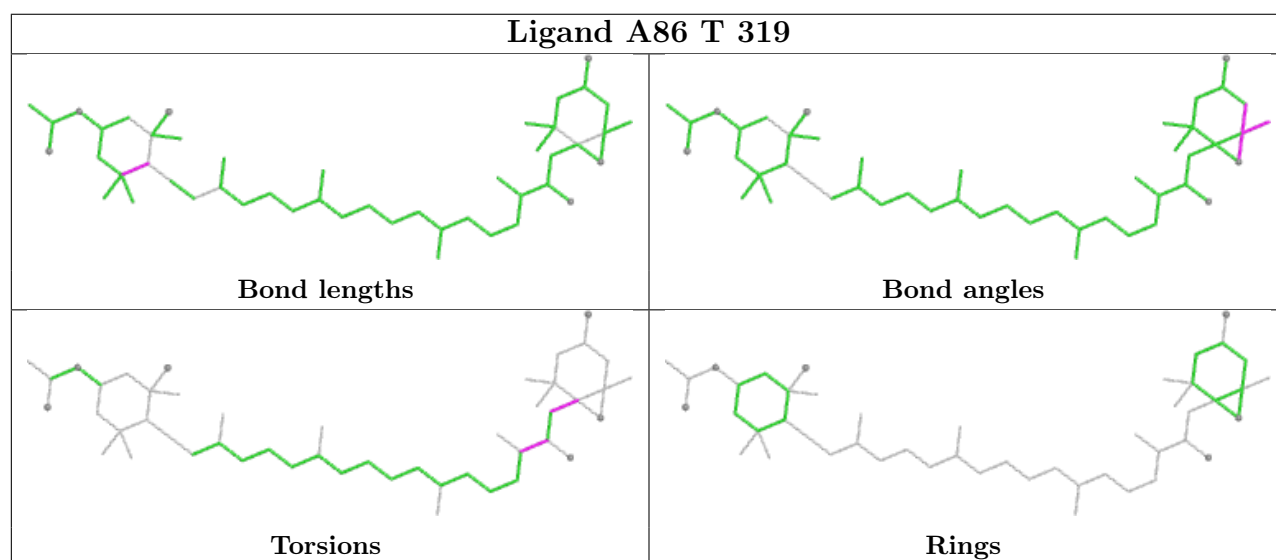
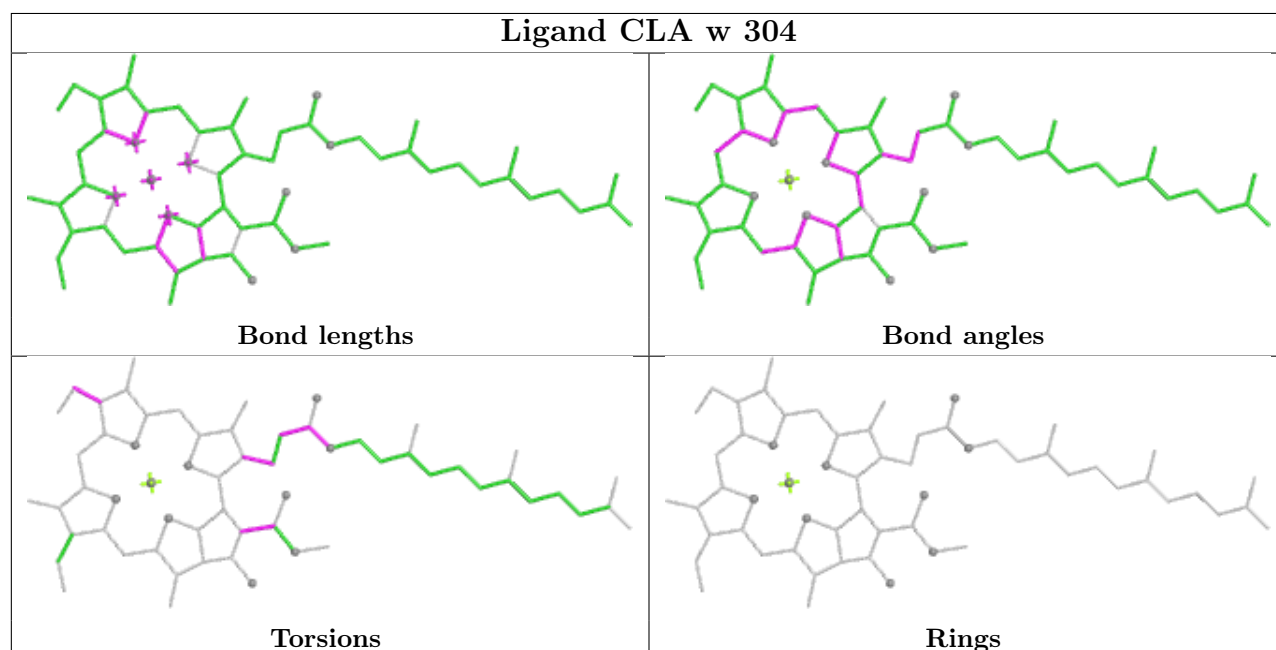
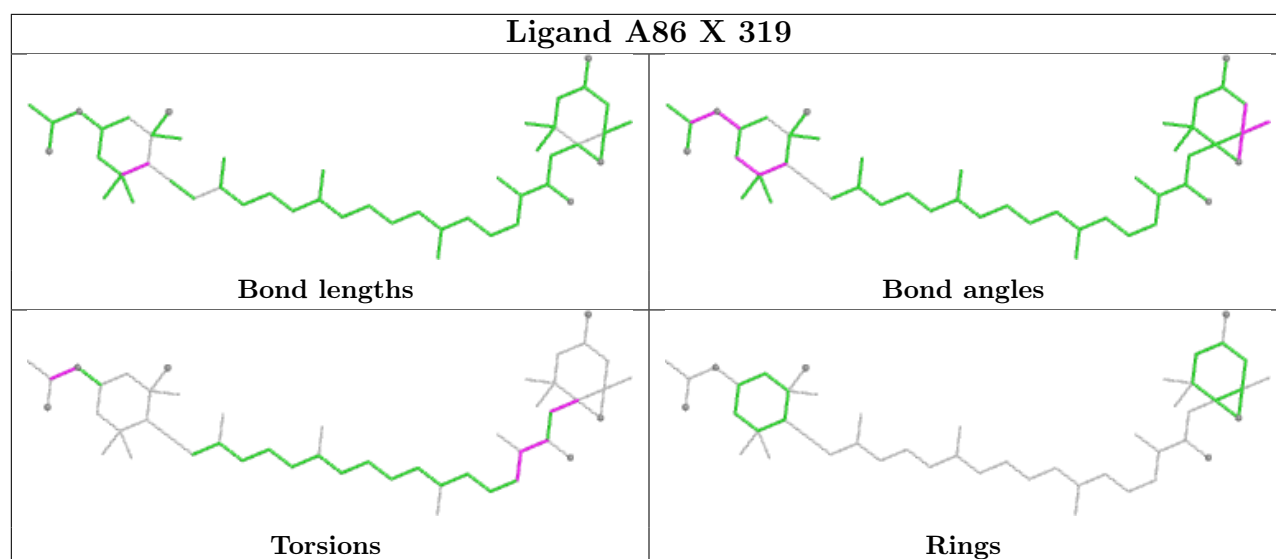
Bond angles

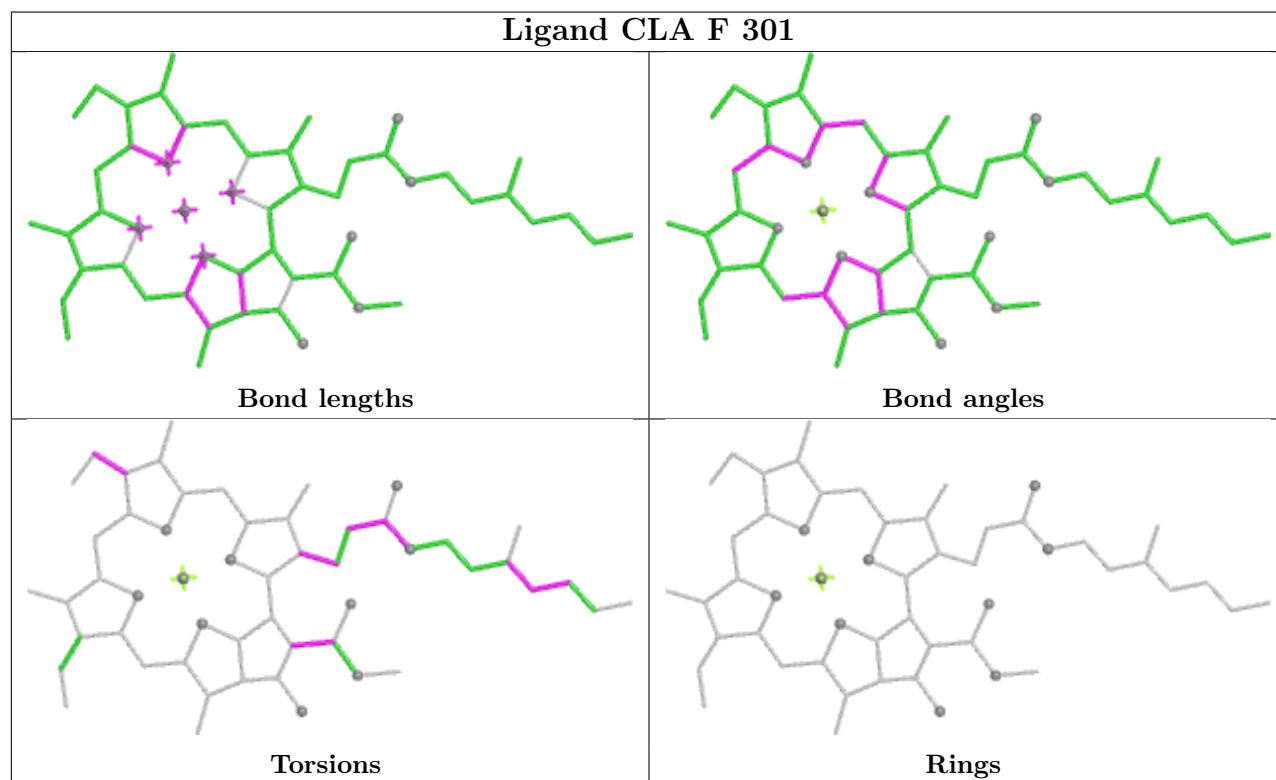
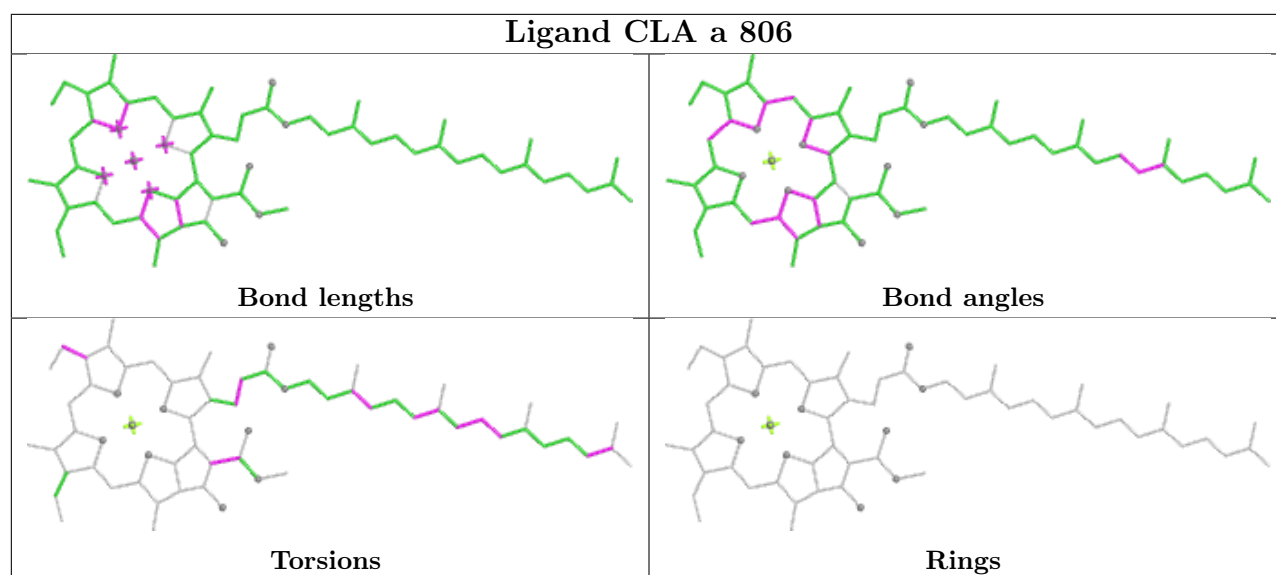


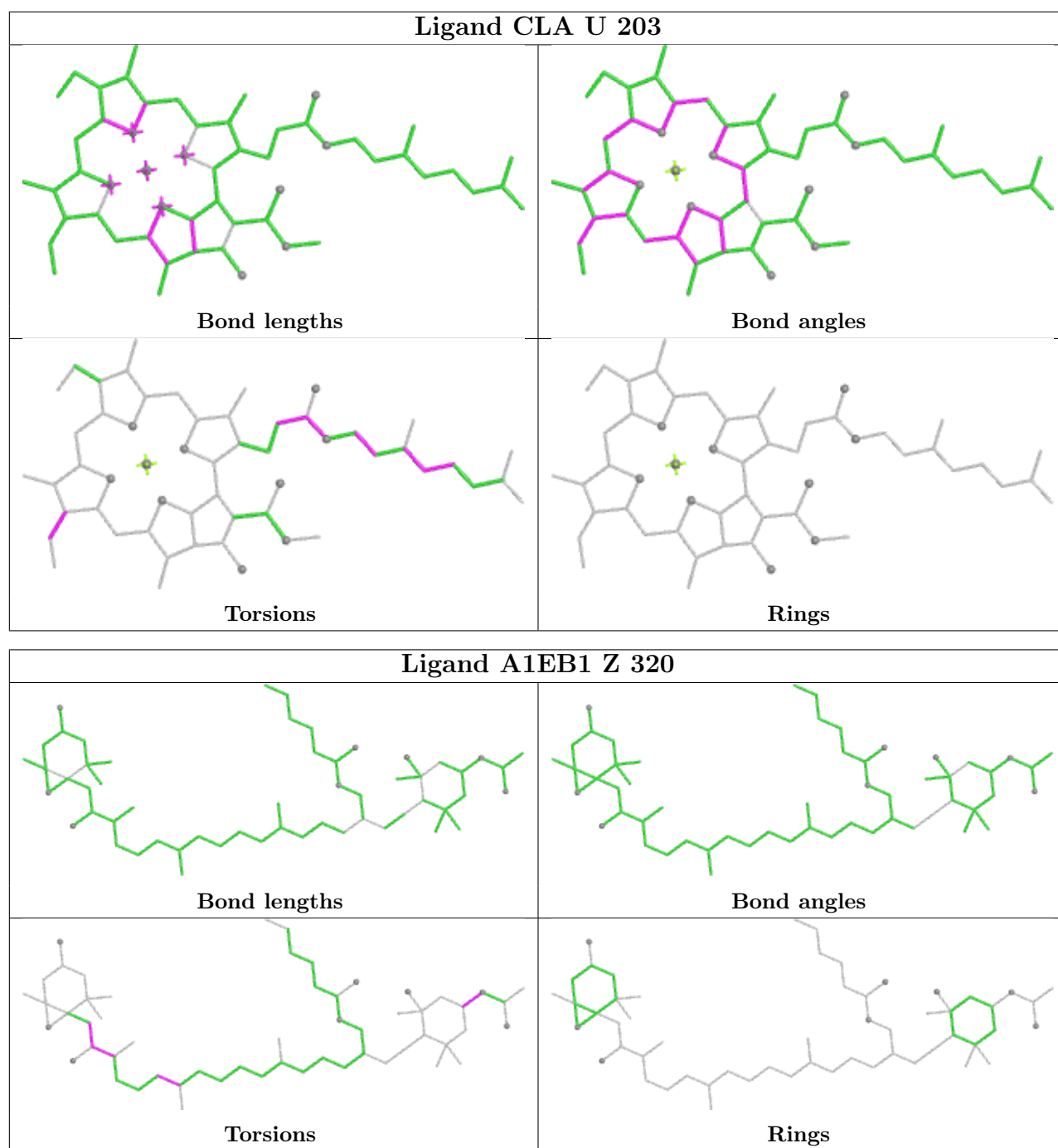
Torsions

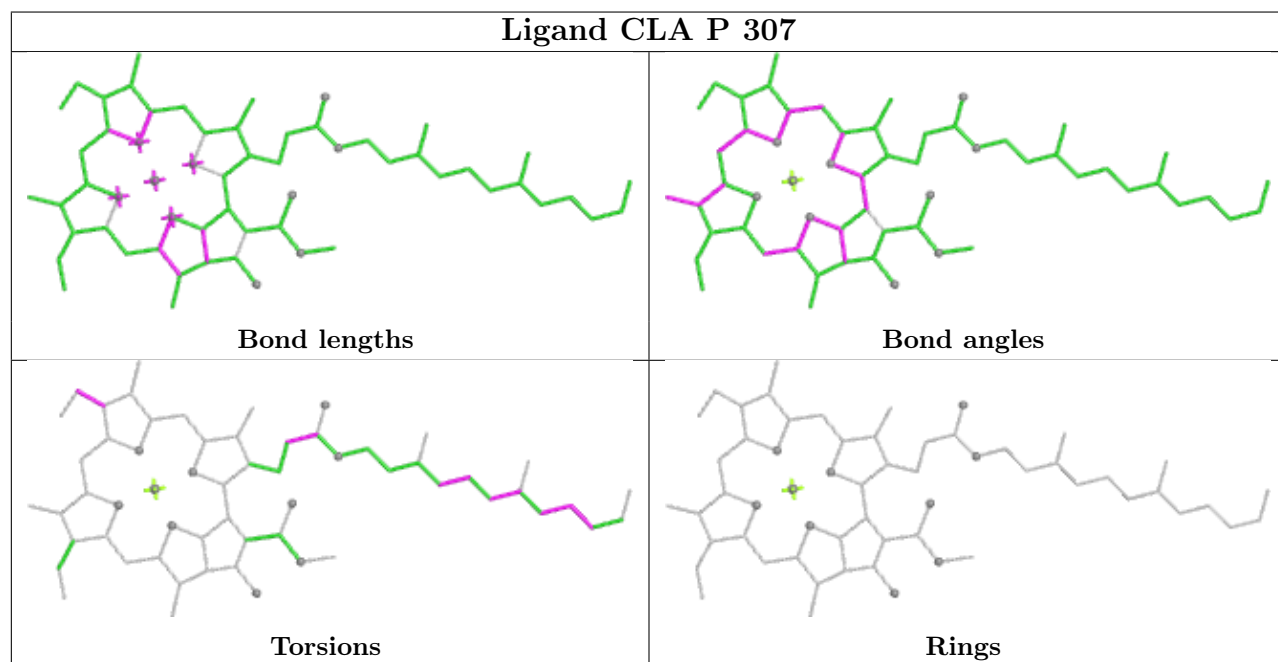
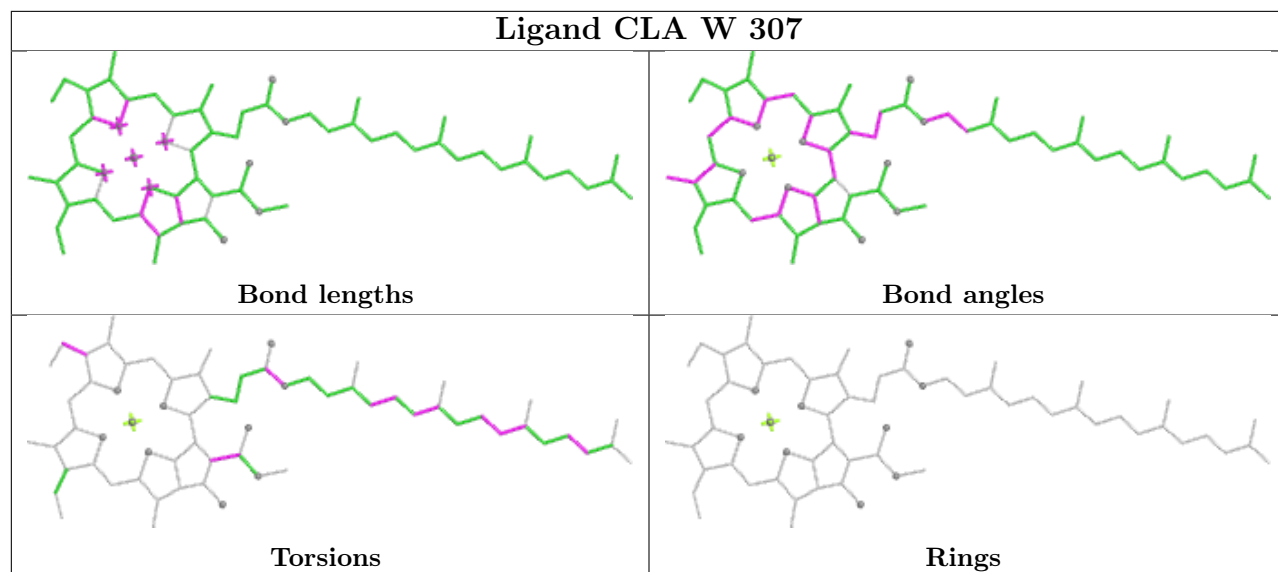


Rings

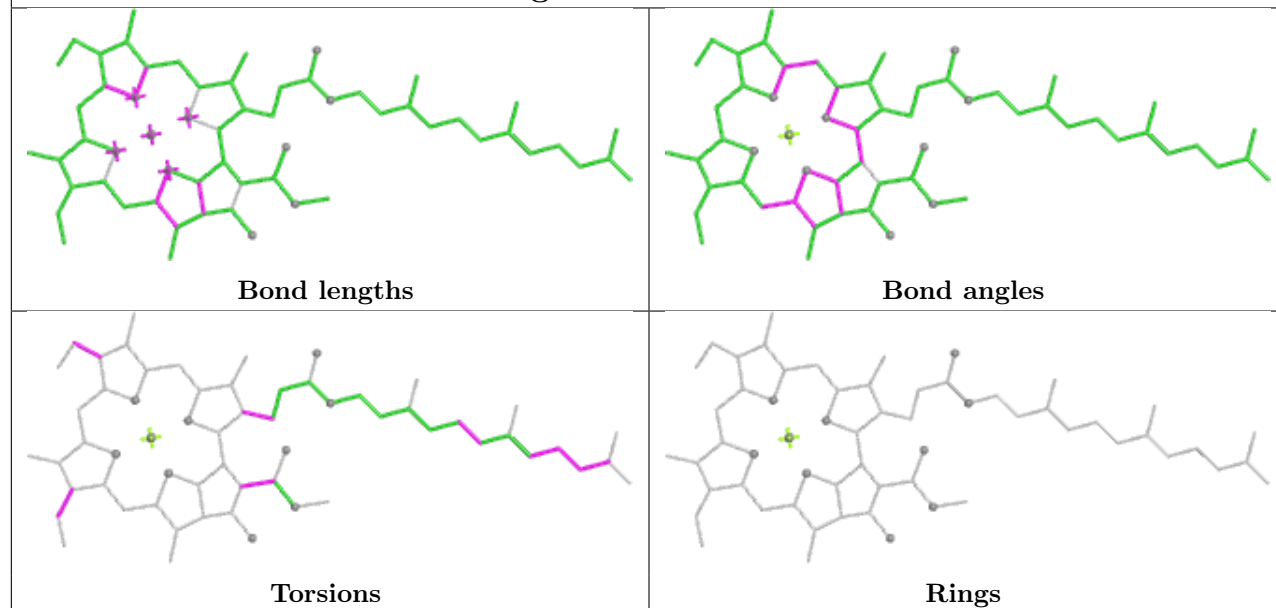




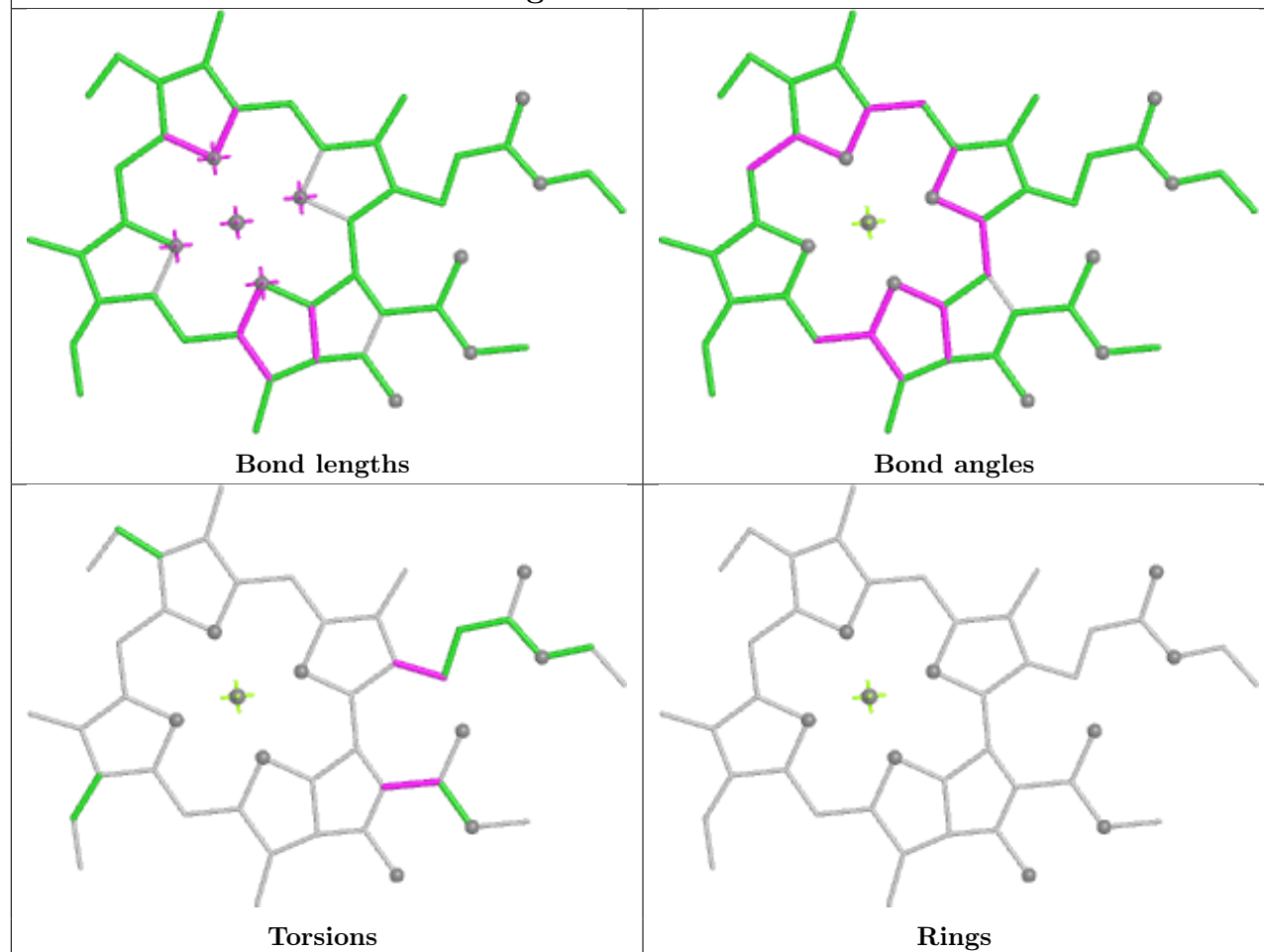


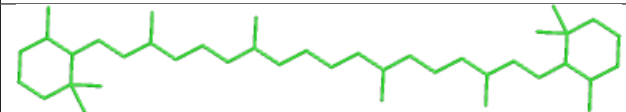
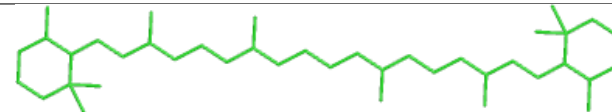
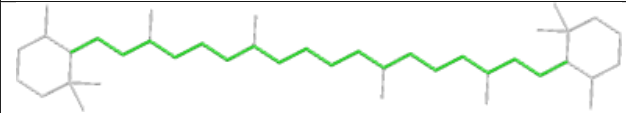
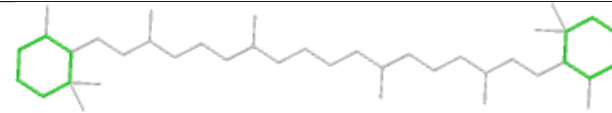


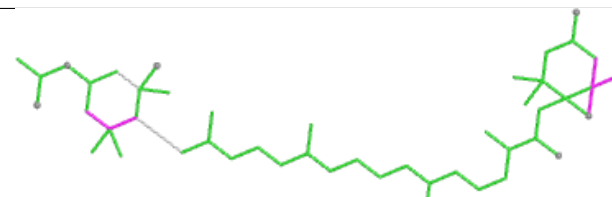
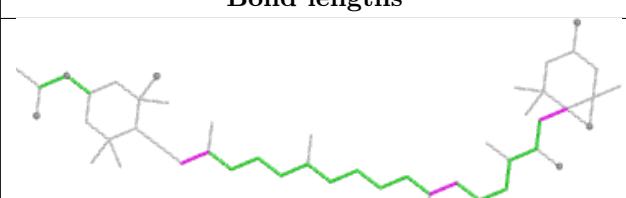
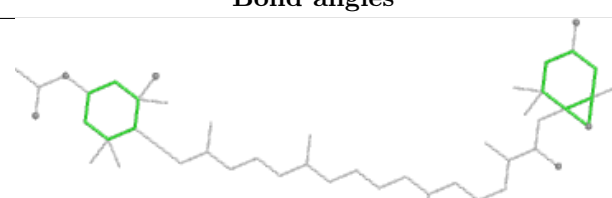
Ligand CLA D 303

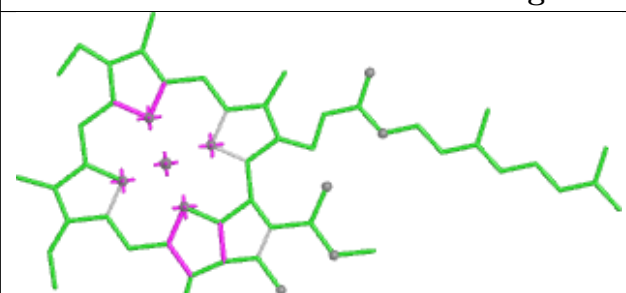
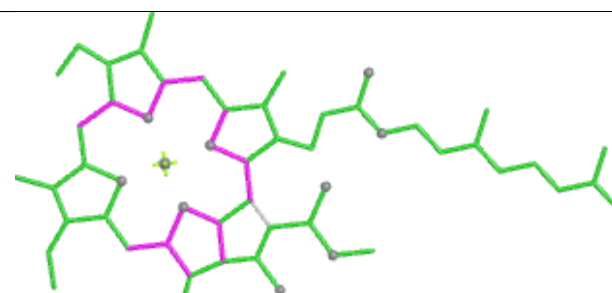
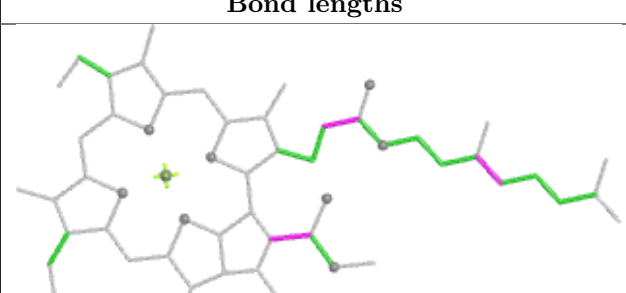
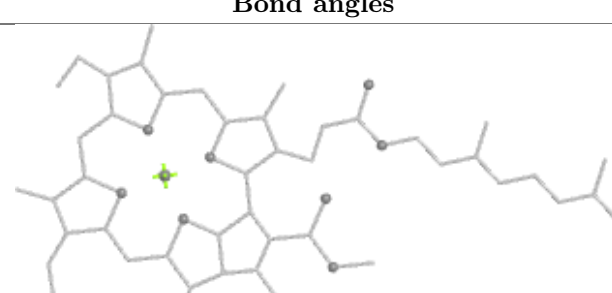


Ligand CLA Y 304

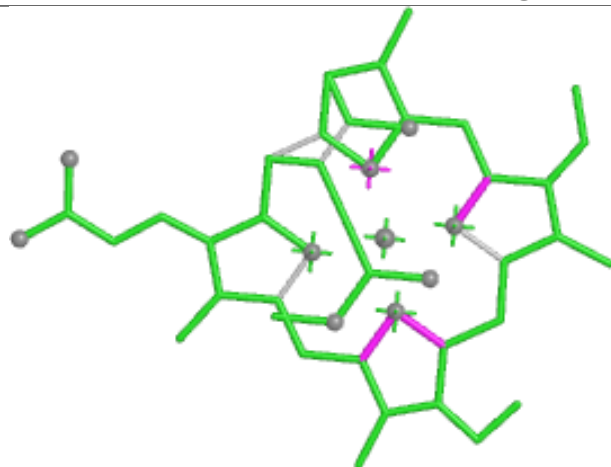


Ligand BCR m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

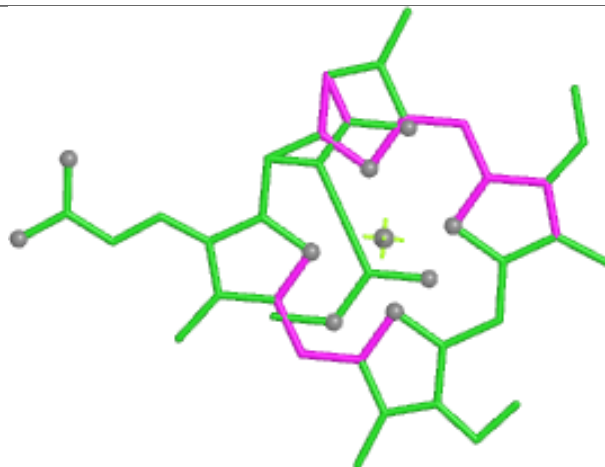
Ligand A86 K 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA I 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

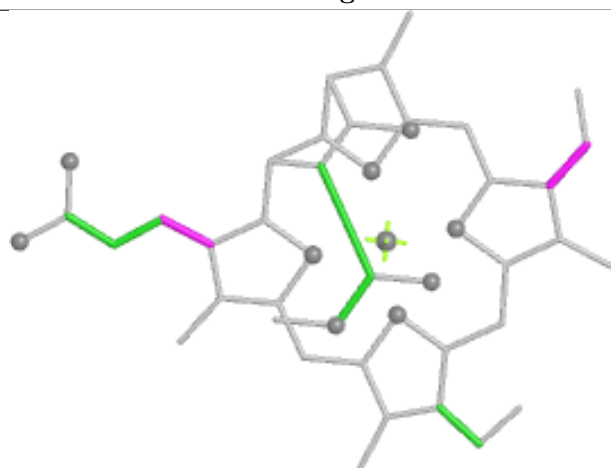
Ligand KC2 X 302



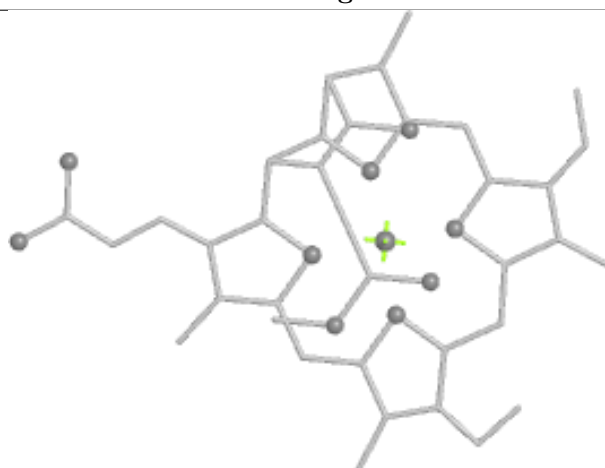
Bond lengths



Bond angles



Torsions



Rings

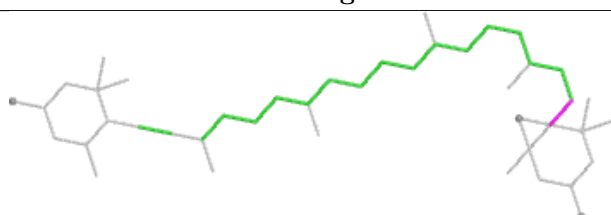
Ligand DD6 Q 214



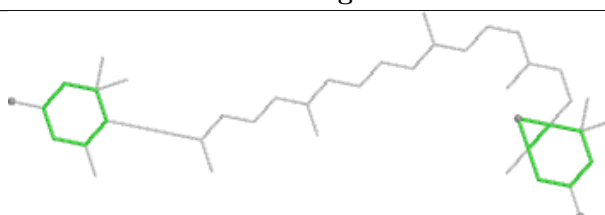
Bond lengths



Bond angles

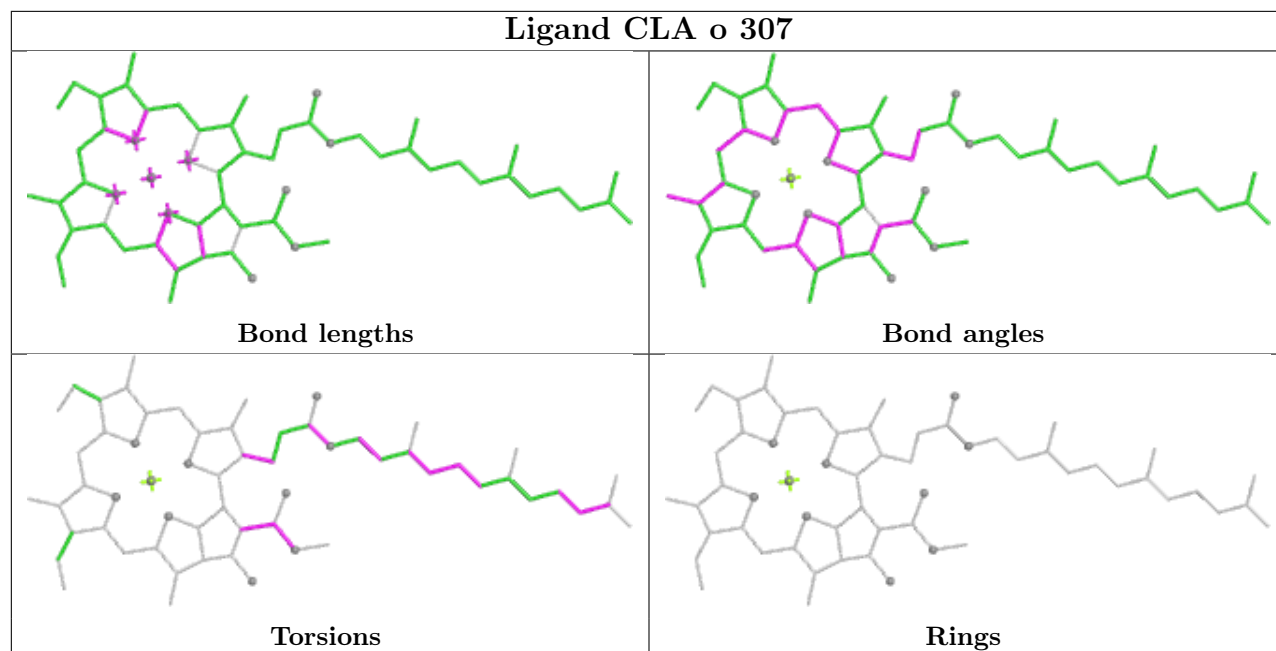


Torsions

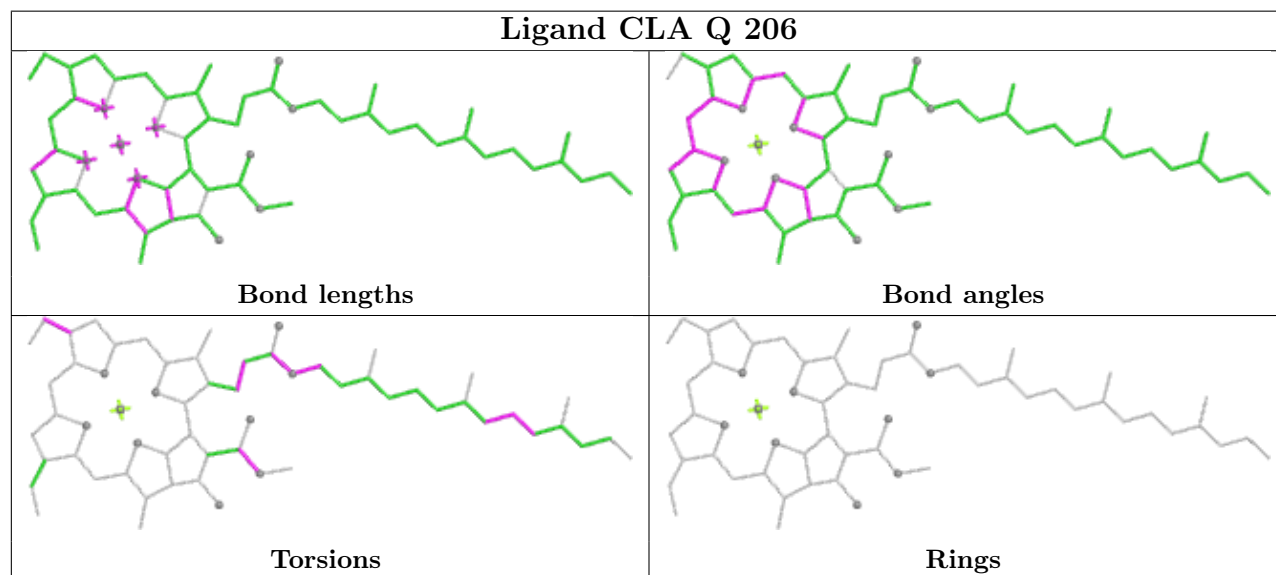


Rings

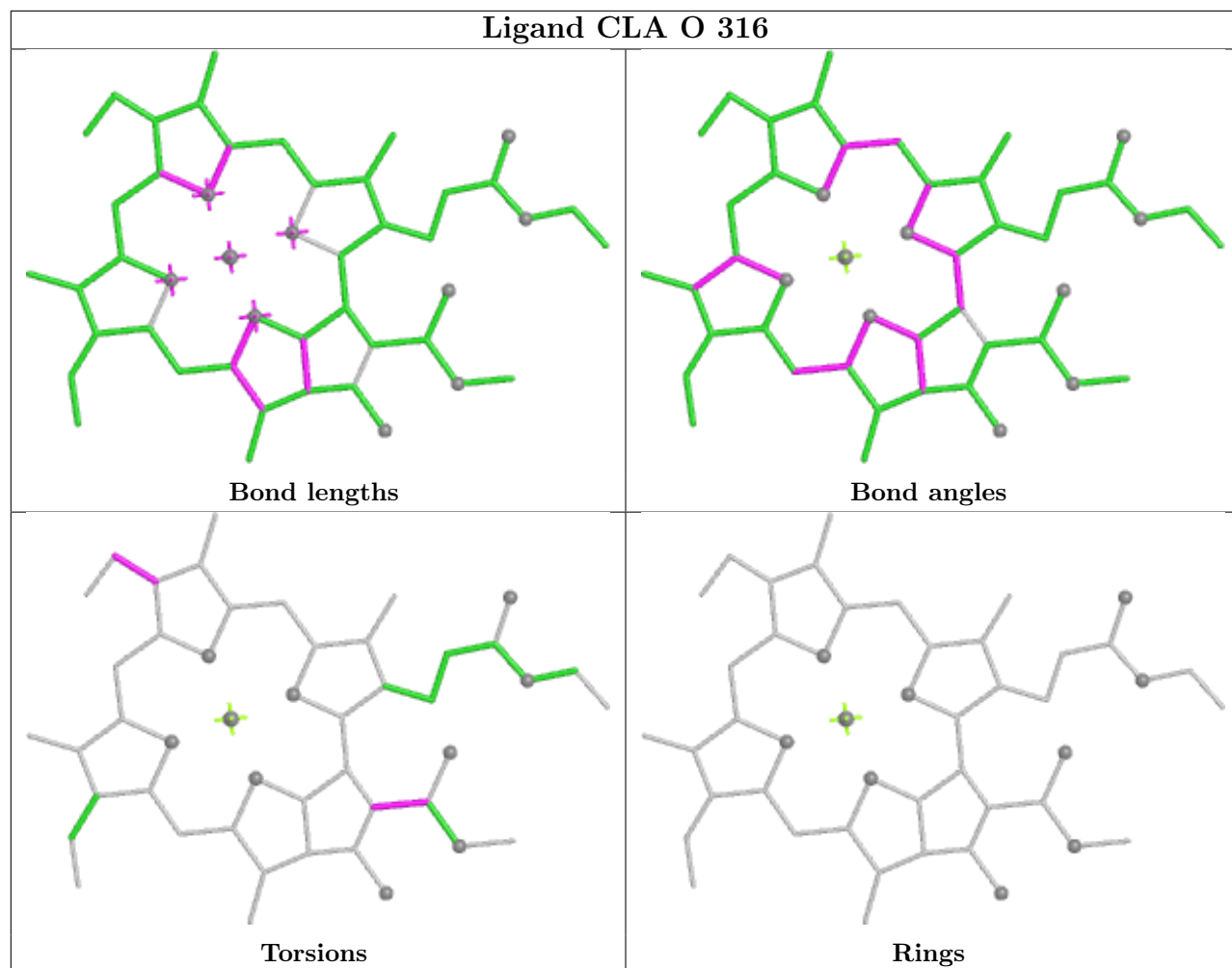
Ligand CLA o 307

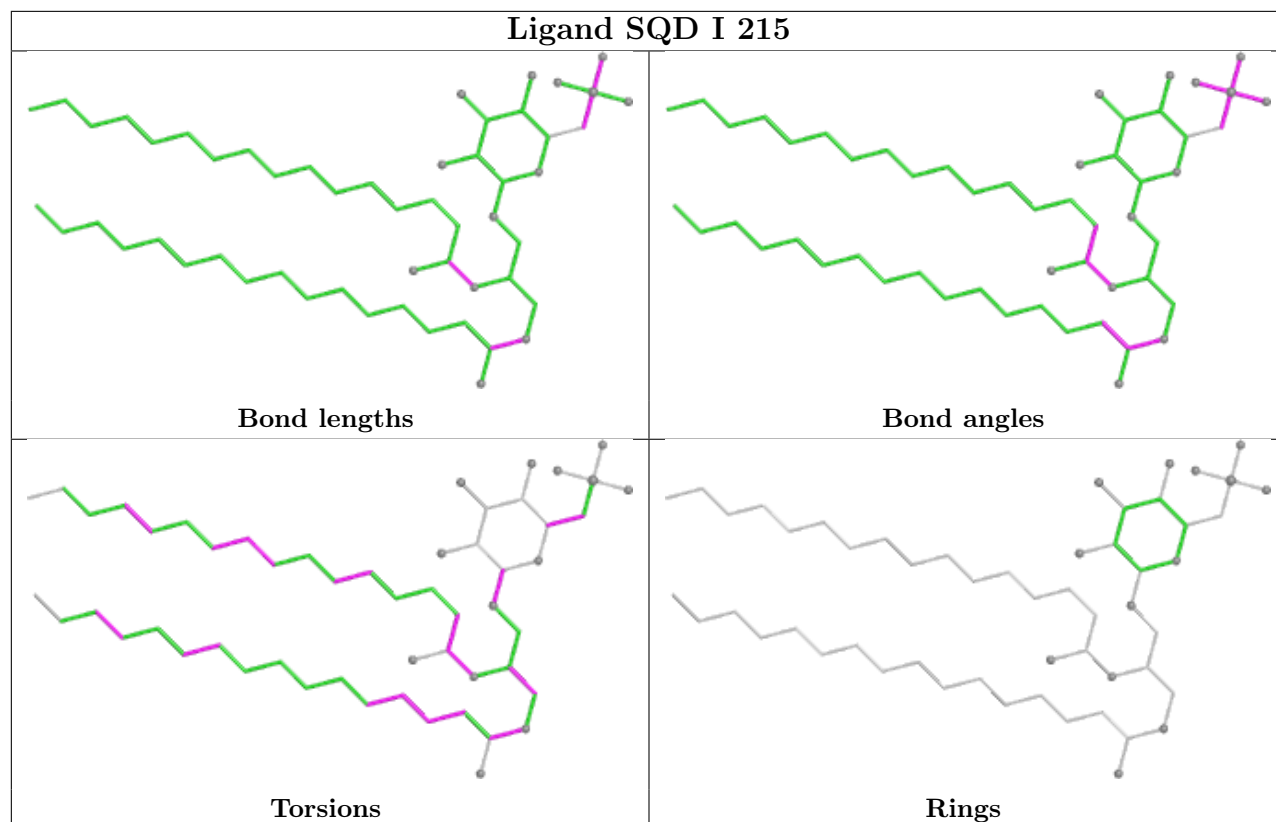


Ligand CLA Q 206

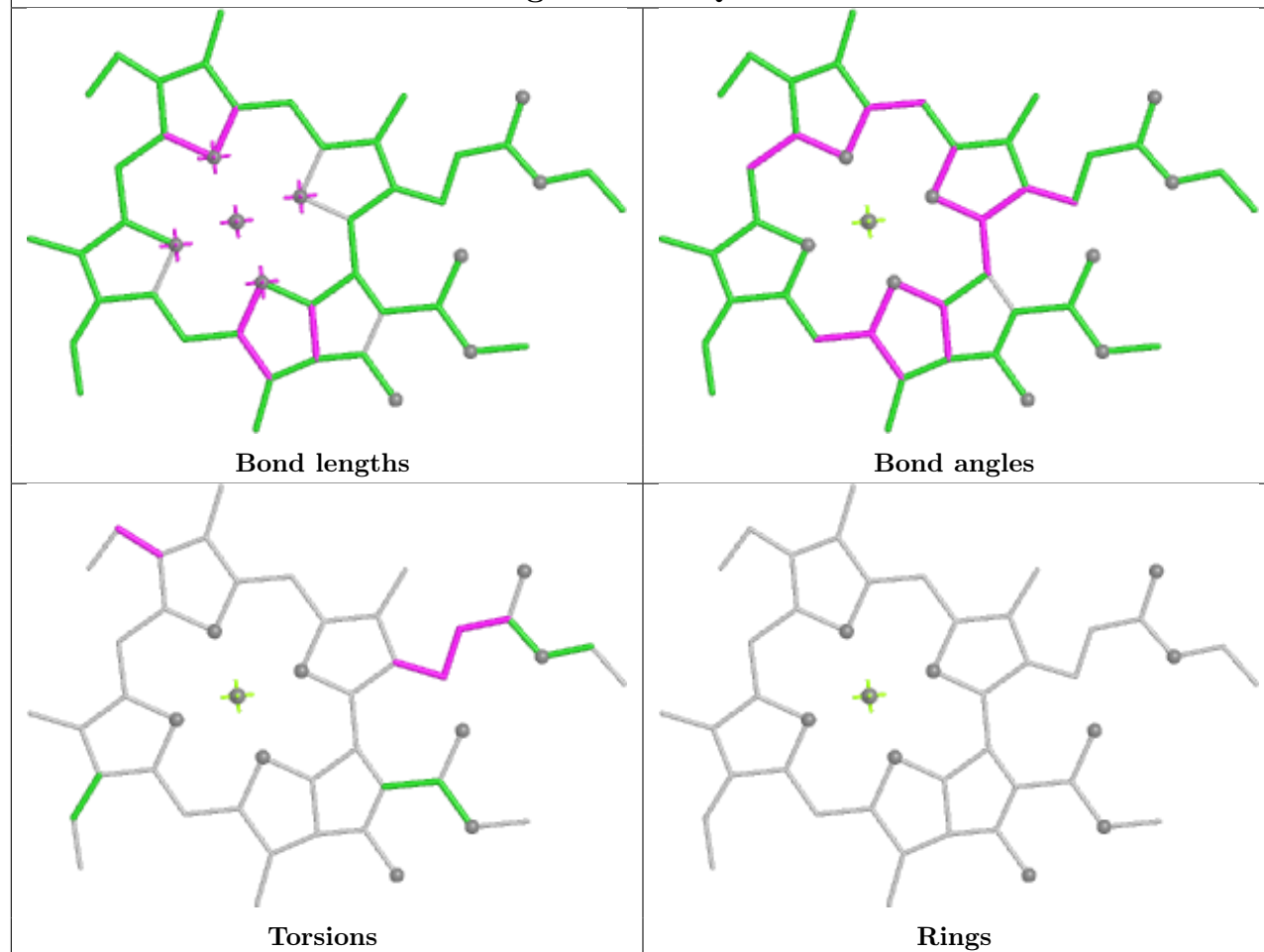


Ligand CLA O 316

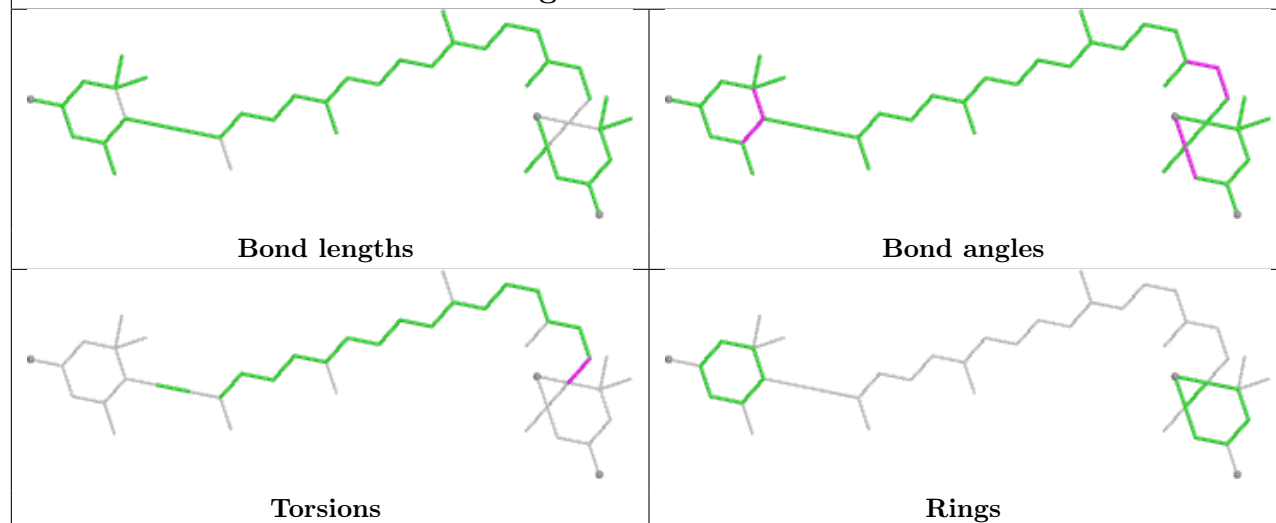


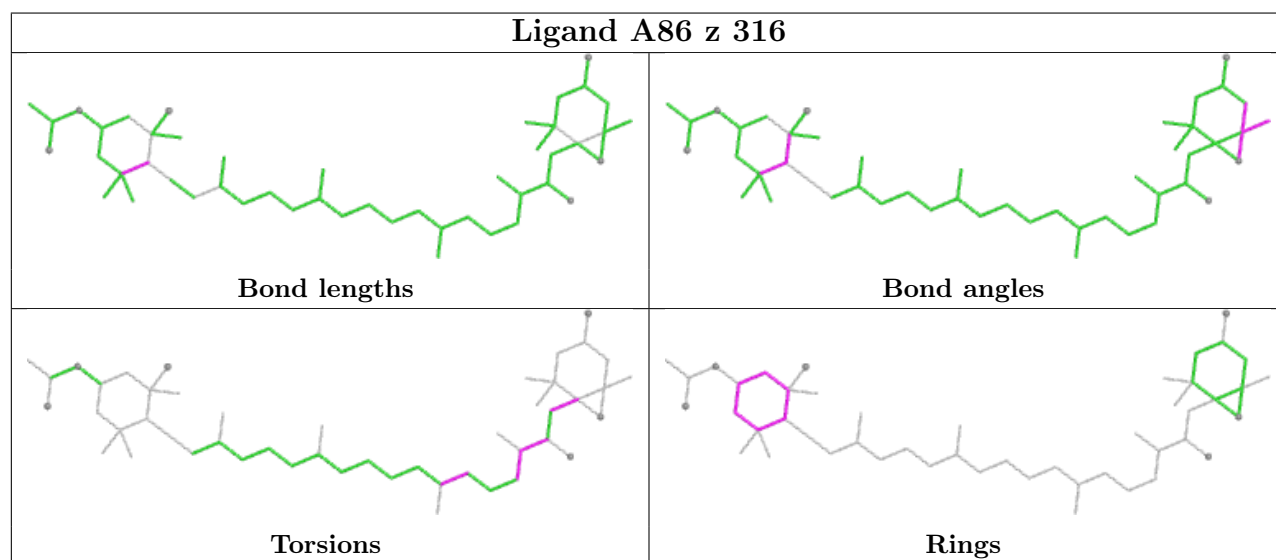
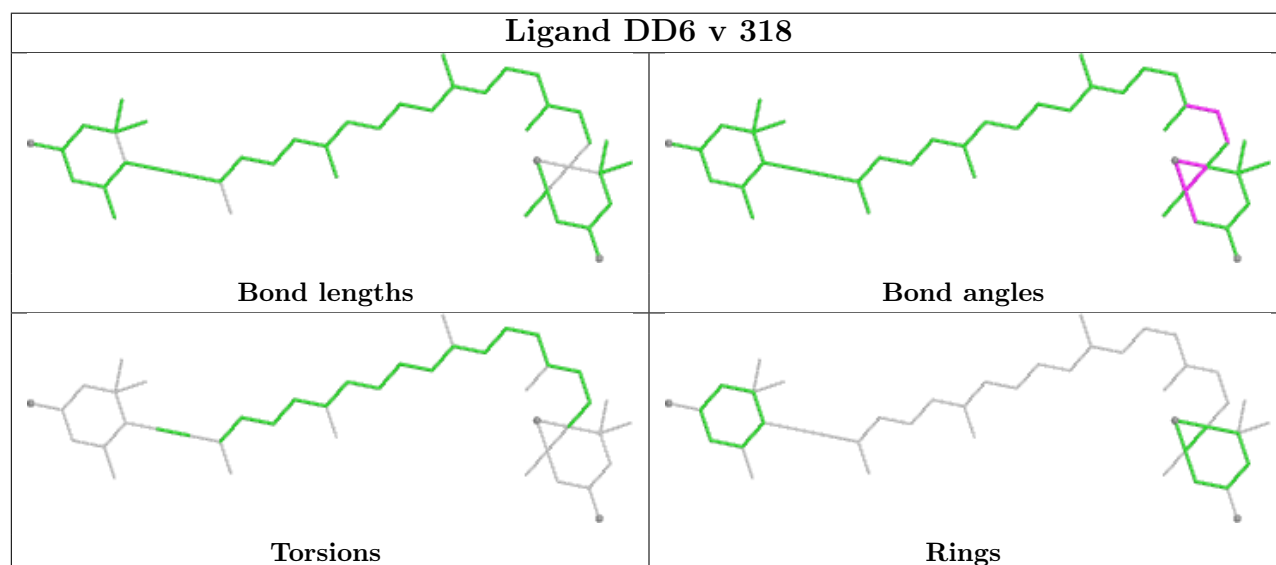
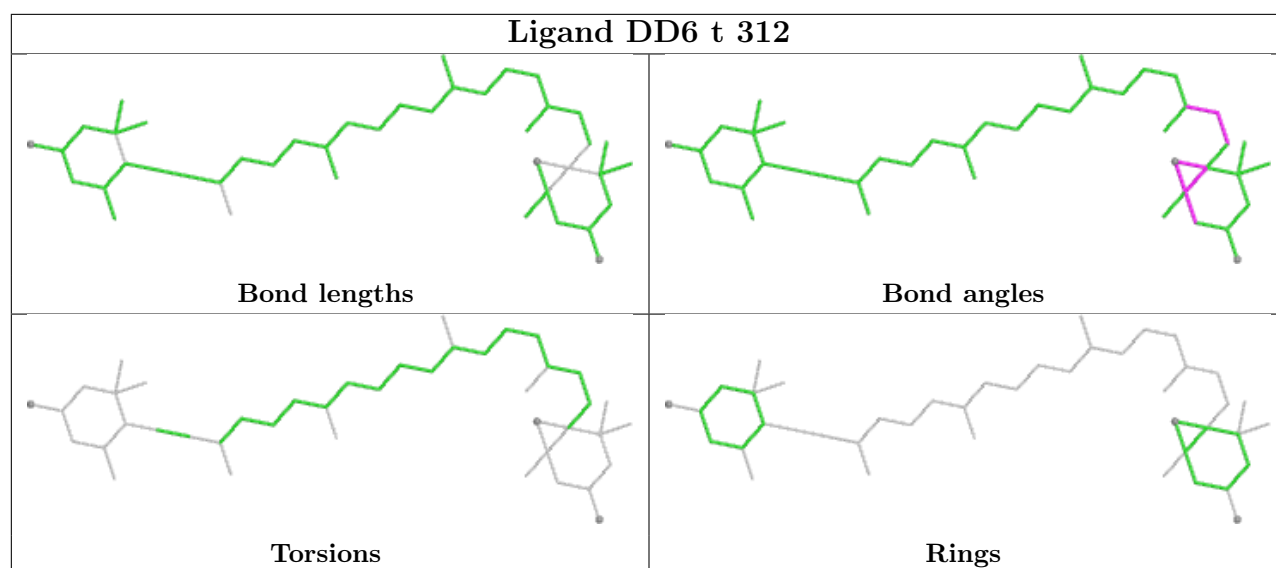


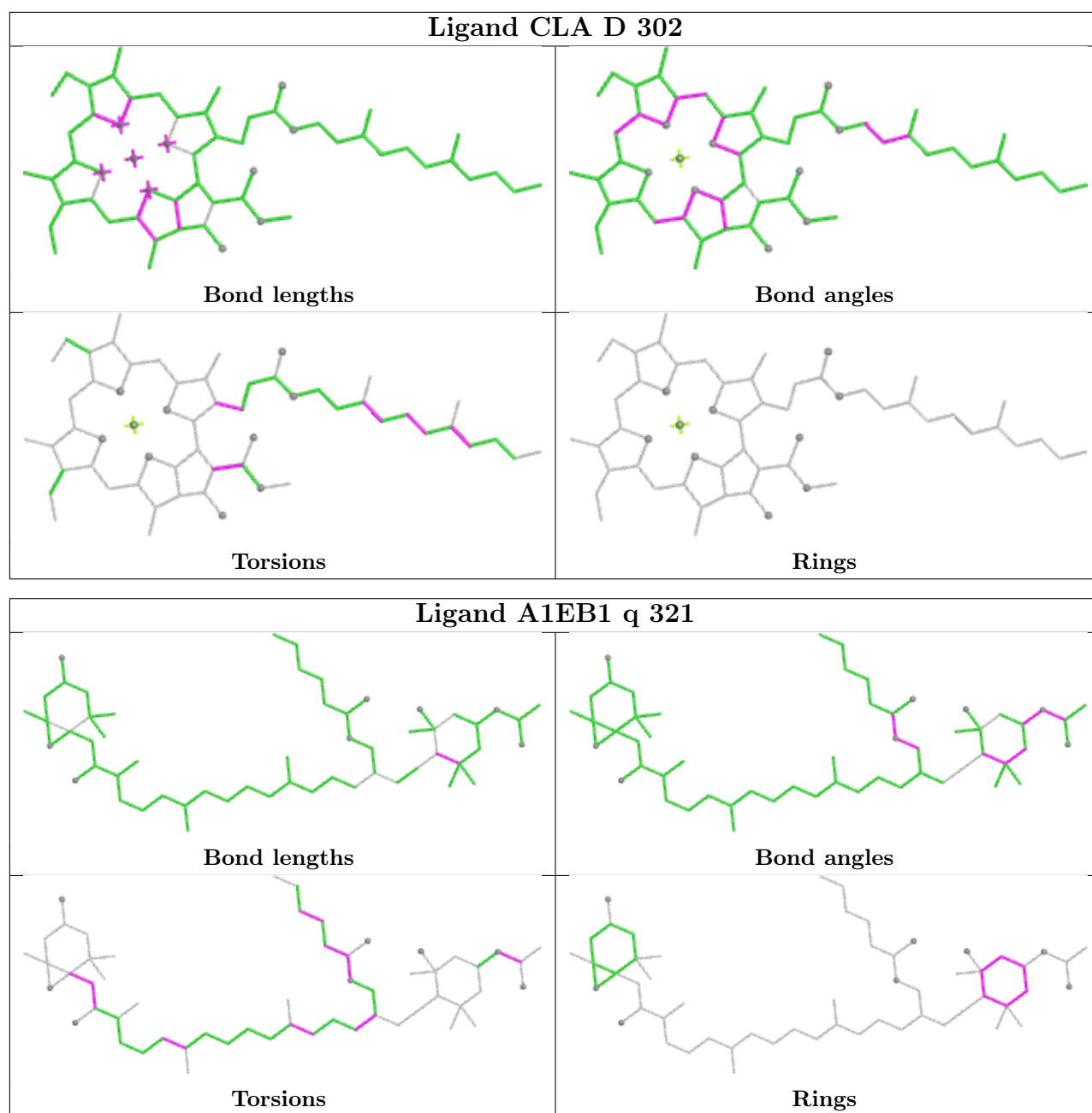
Ligand CLA Q 209

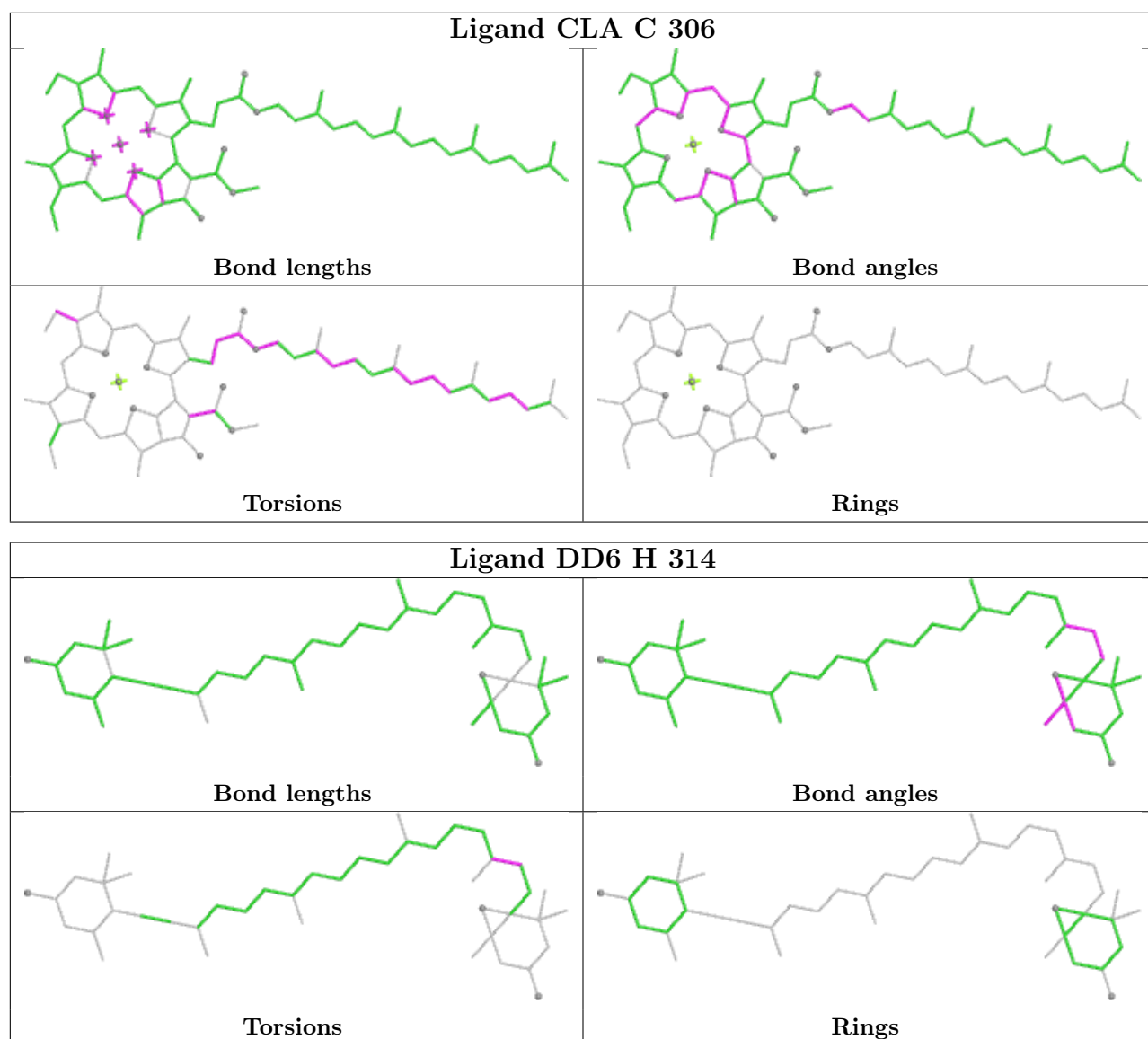


Ligand DD6 I 213

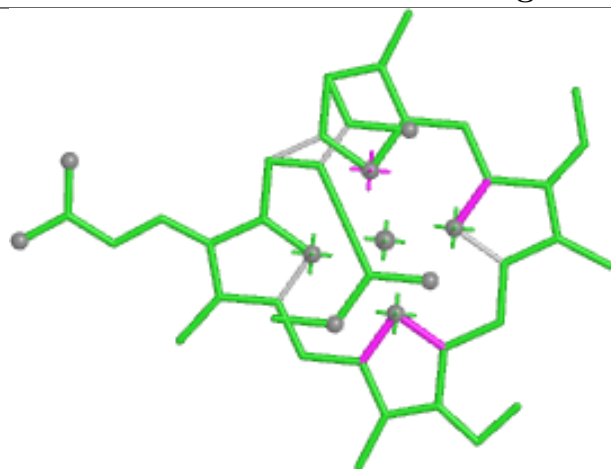




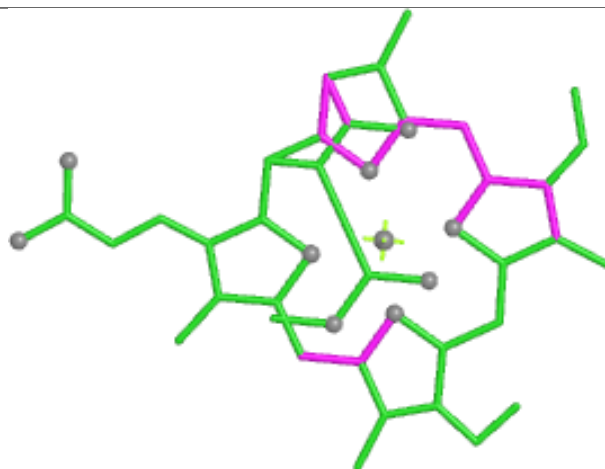




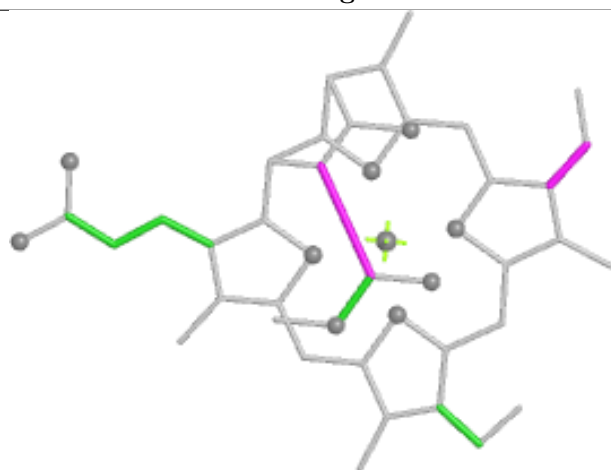
Ligand KC2 P 303



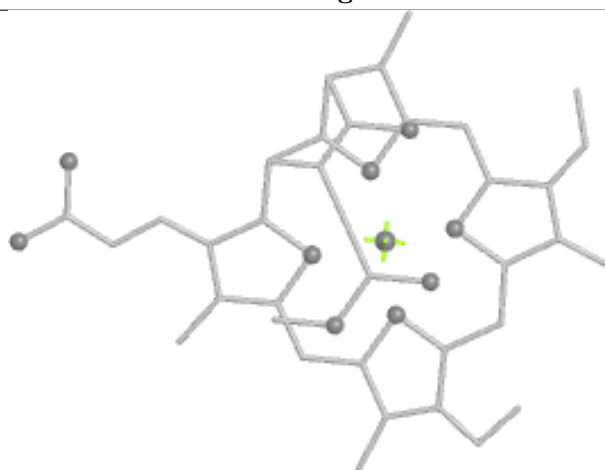
Bond lengths



Bond angles

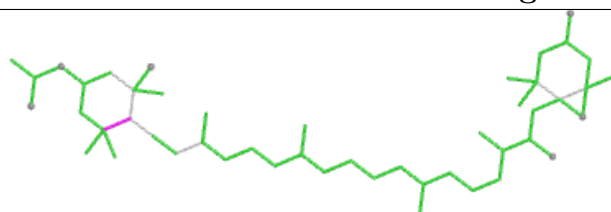


Torsions

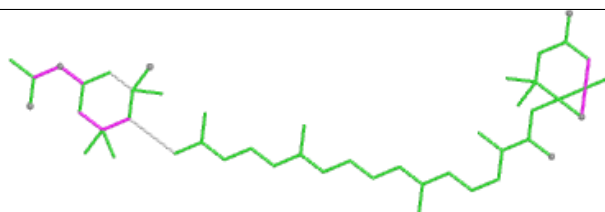


Rings

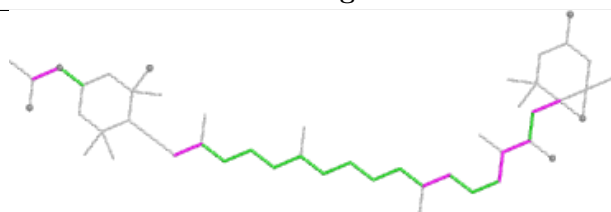
Ligand A86 Y 320



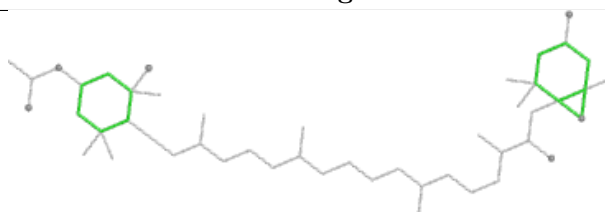
Bond lengths



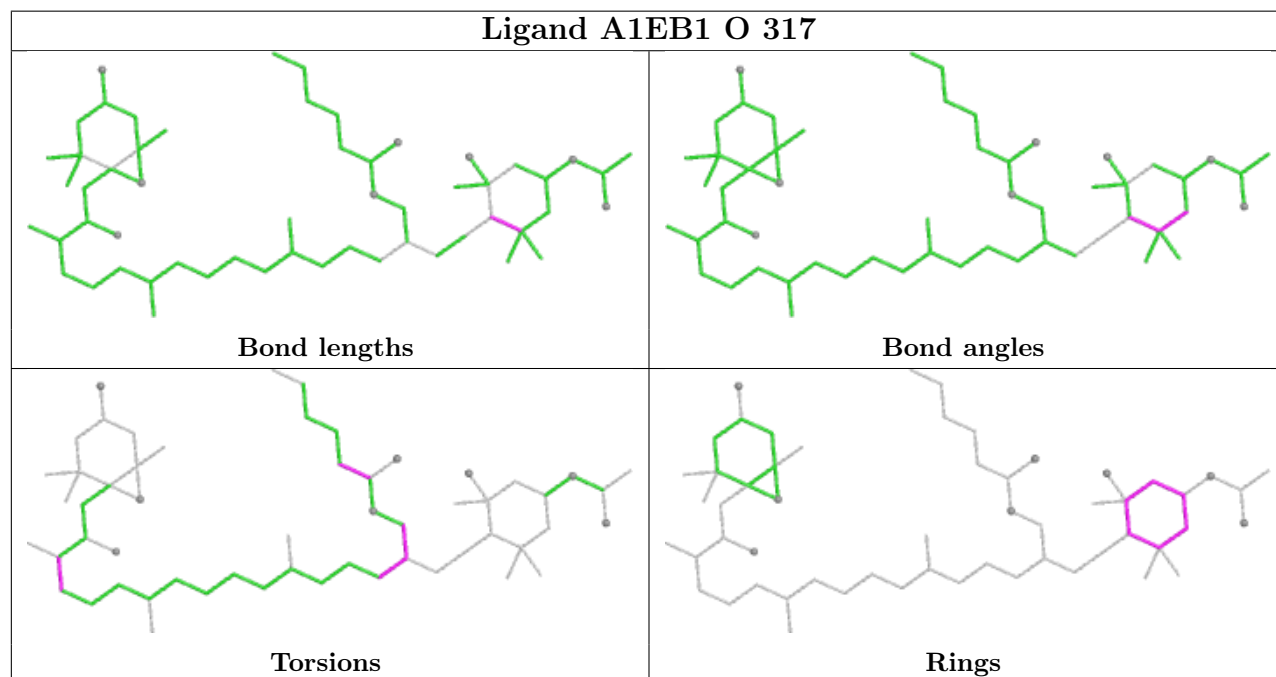
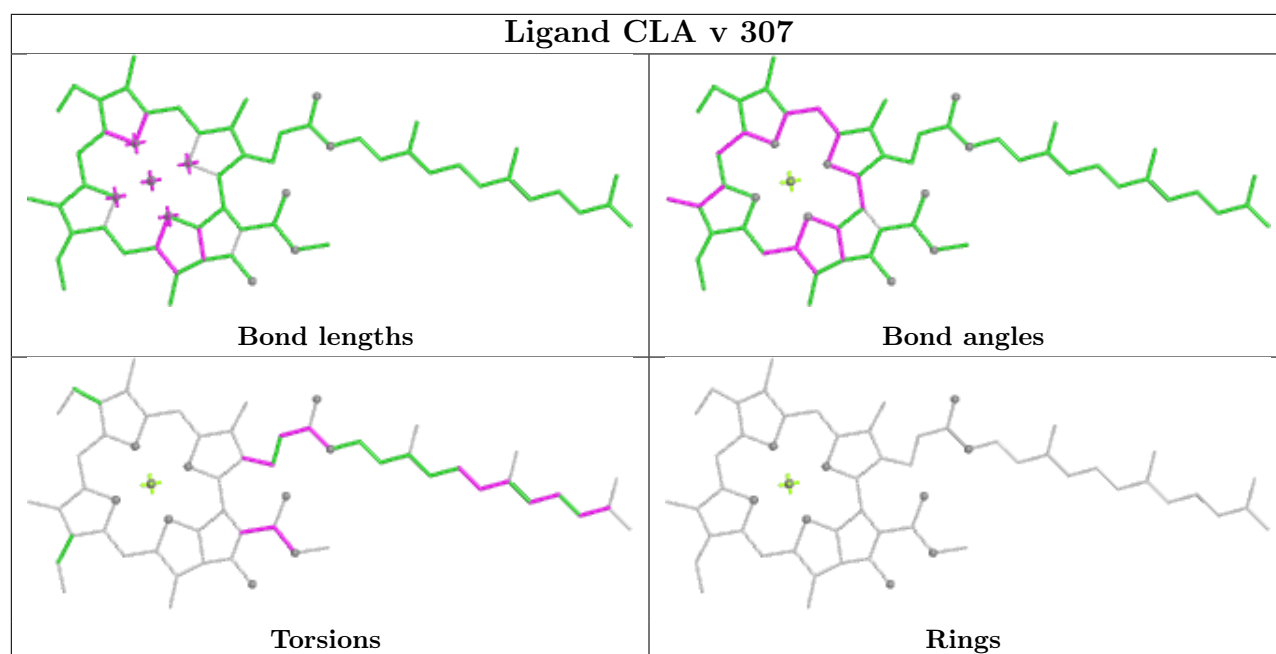
Bond angles

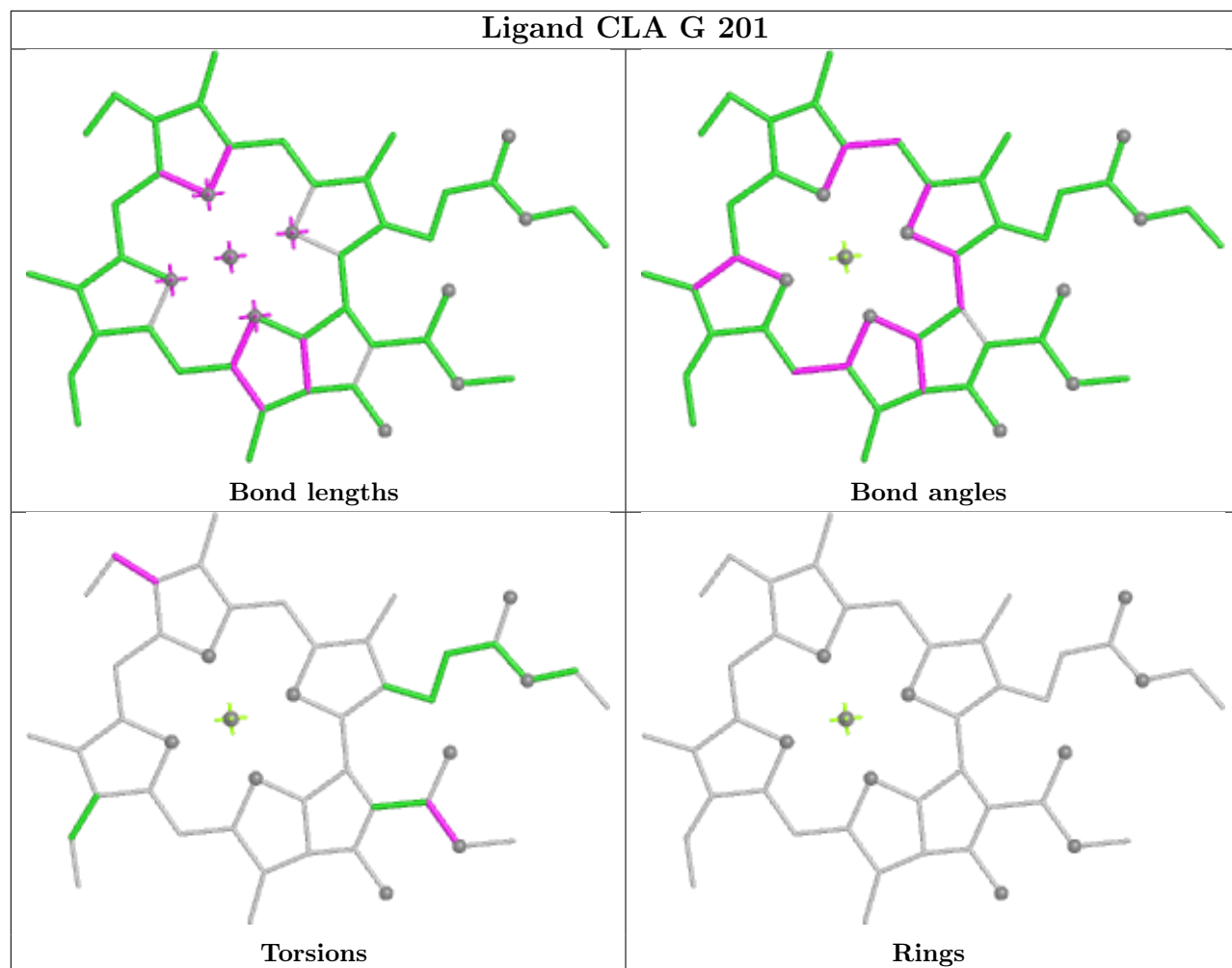


Torsions

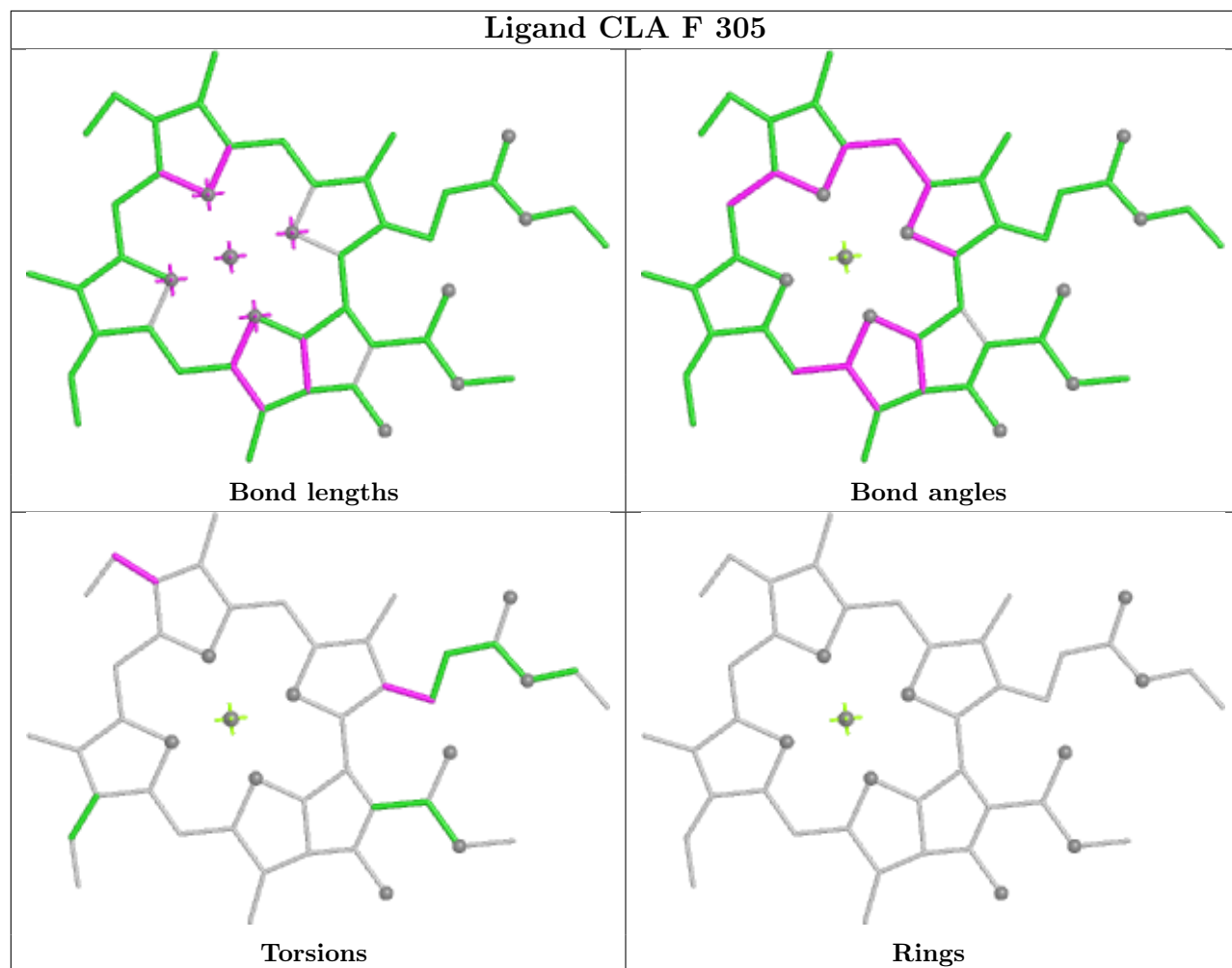


Rings

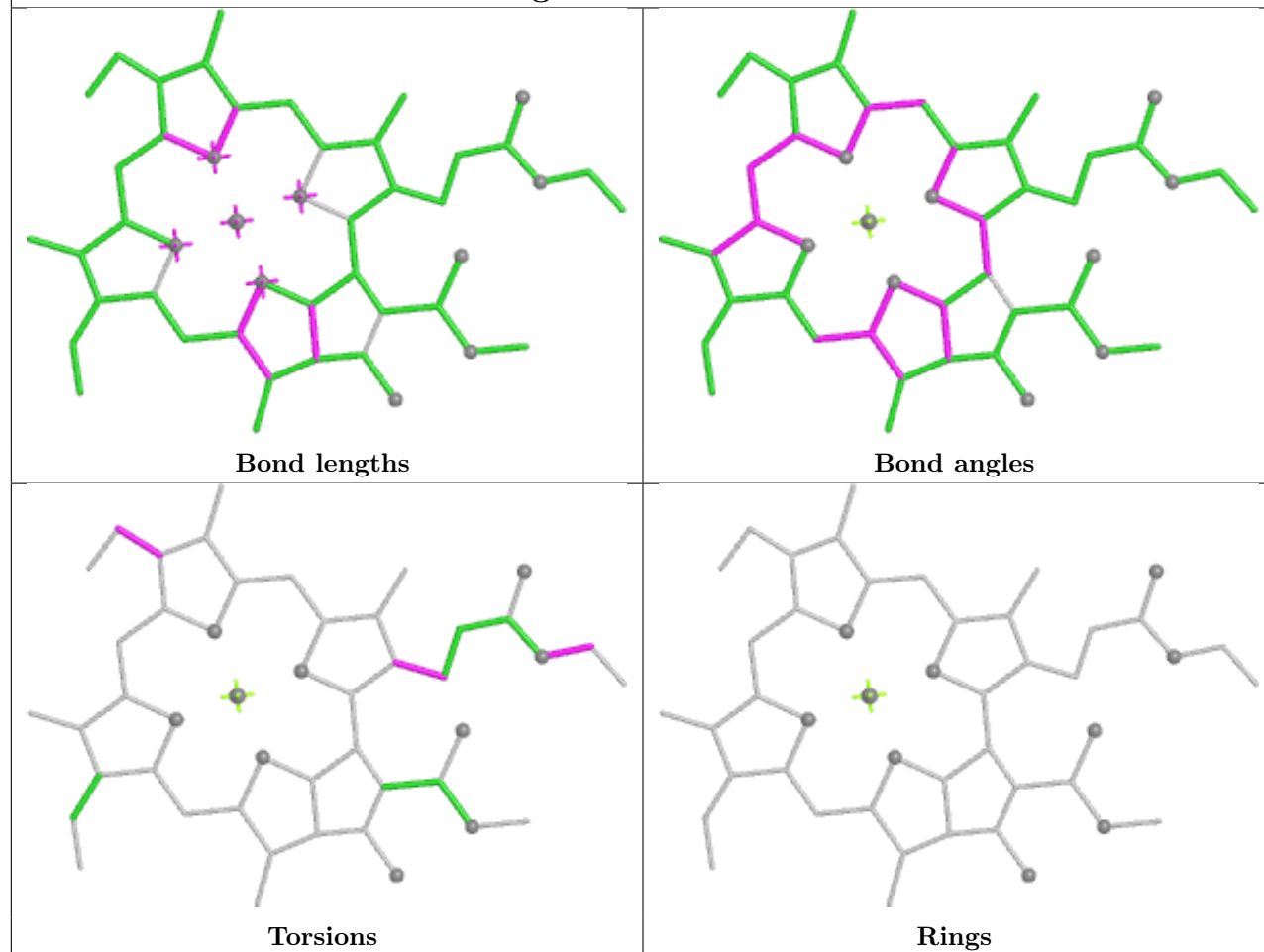




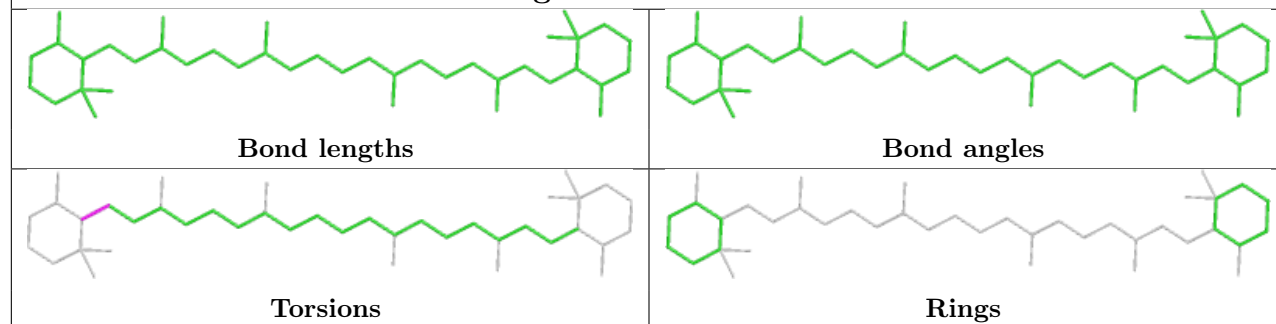
Ligand CLA F 305

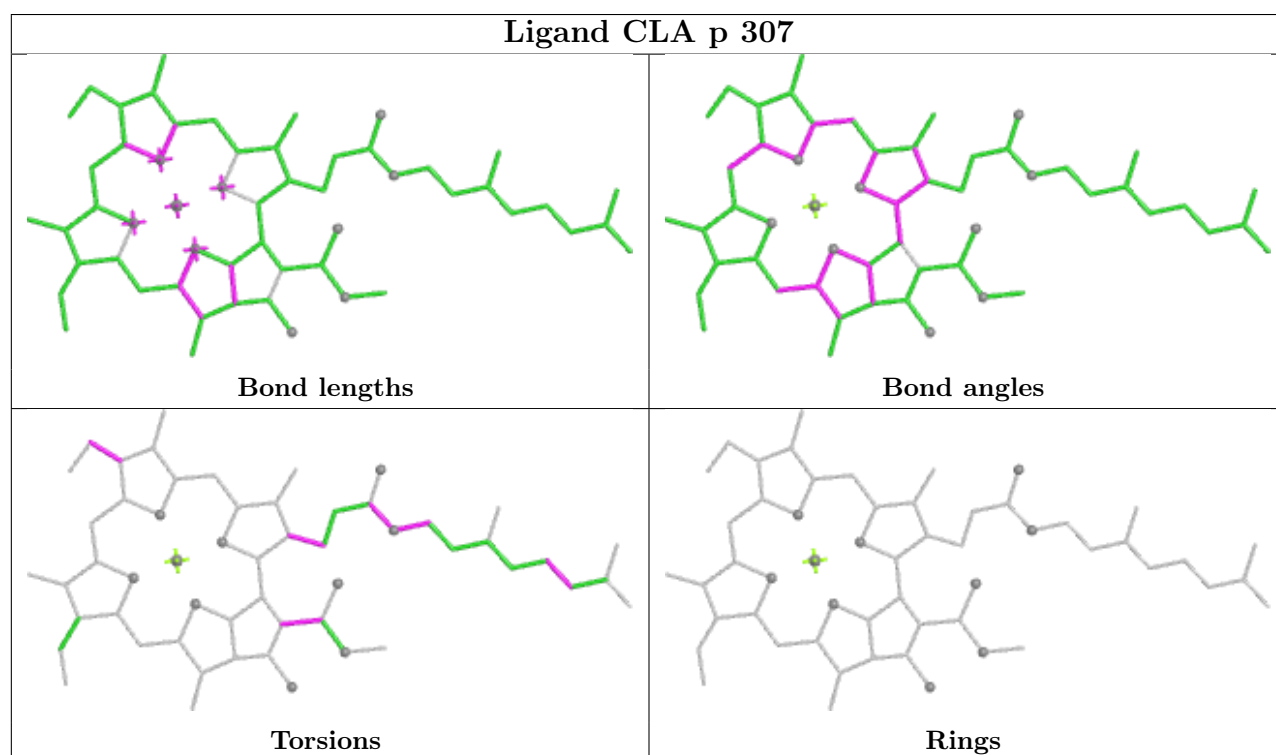
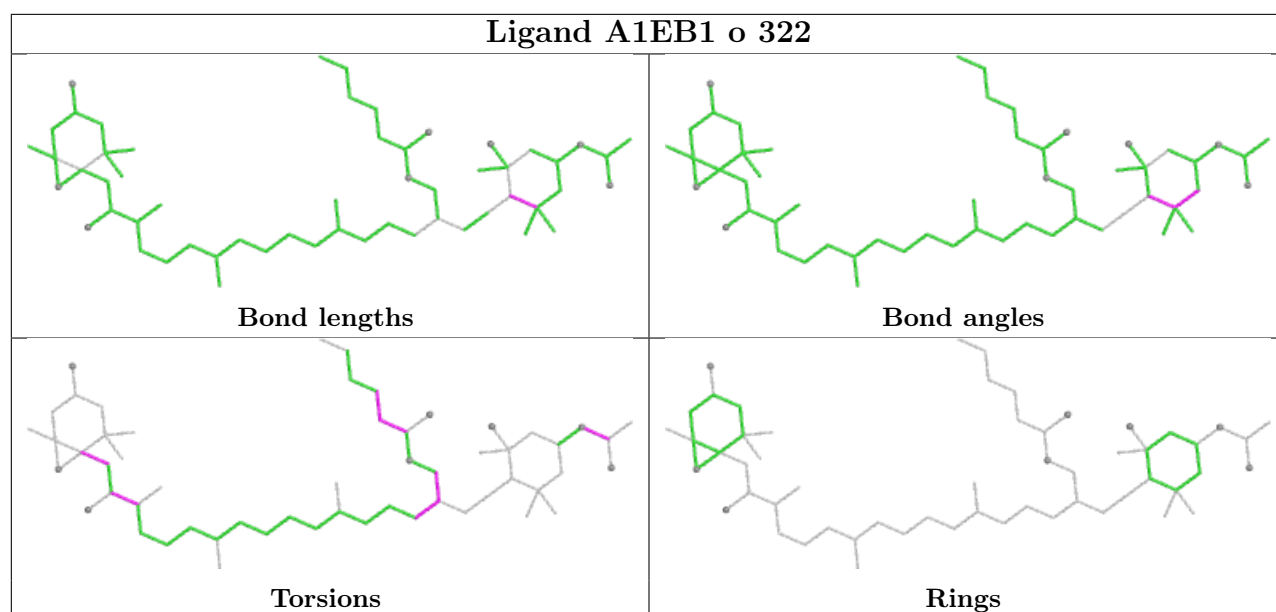


Ligand CLA z 324

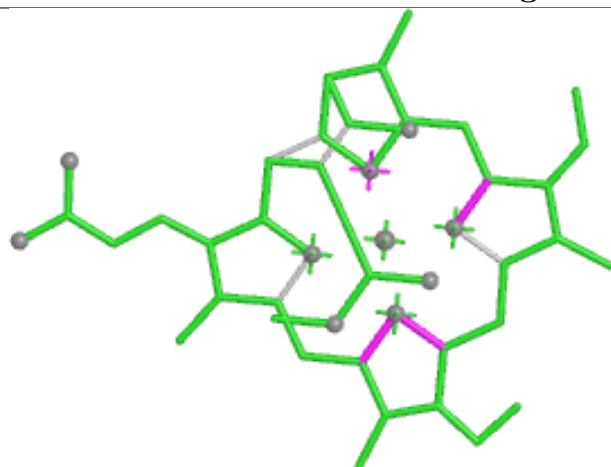


Ligand BCR b 843

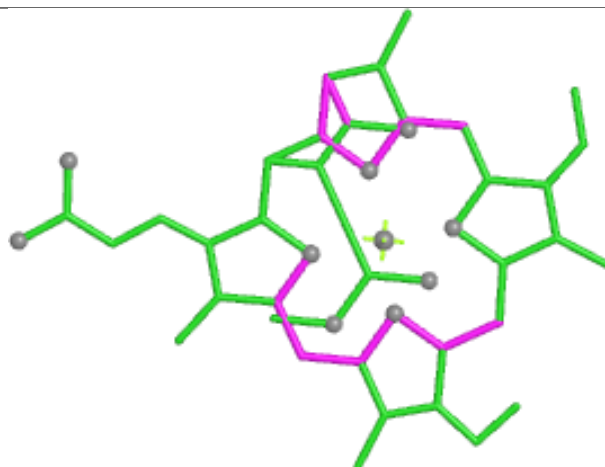




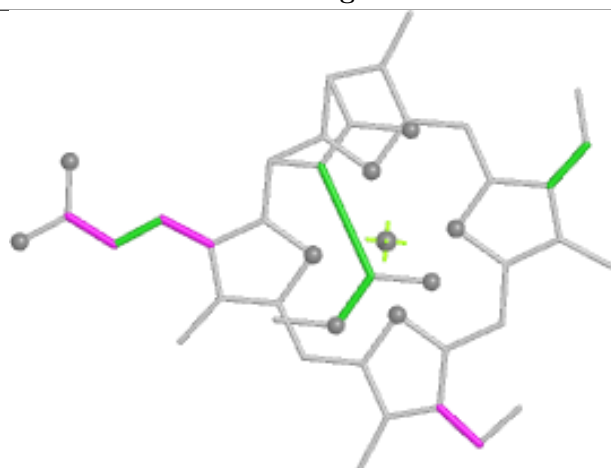
Ligand KC2 x 304



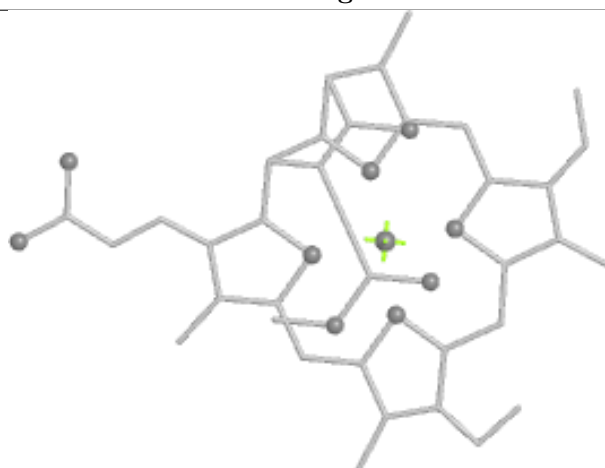
Bond lengths



Bond angles

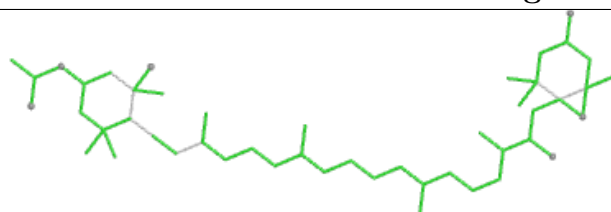


Torsions

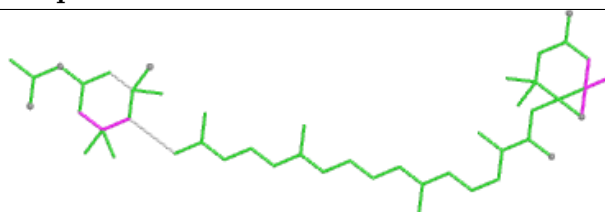


Rings

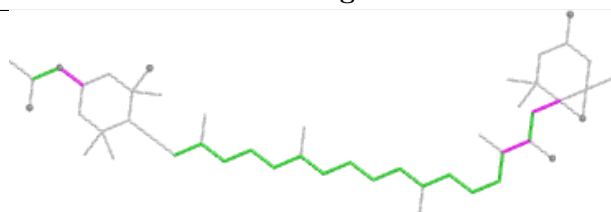
Ligand A86 q 324



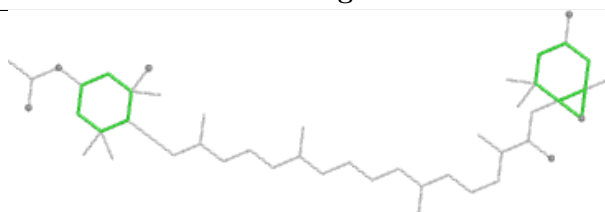
Bond lengths



Bond angles

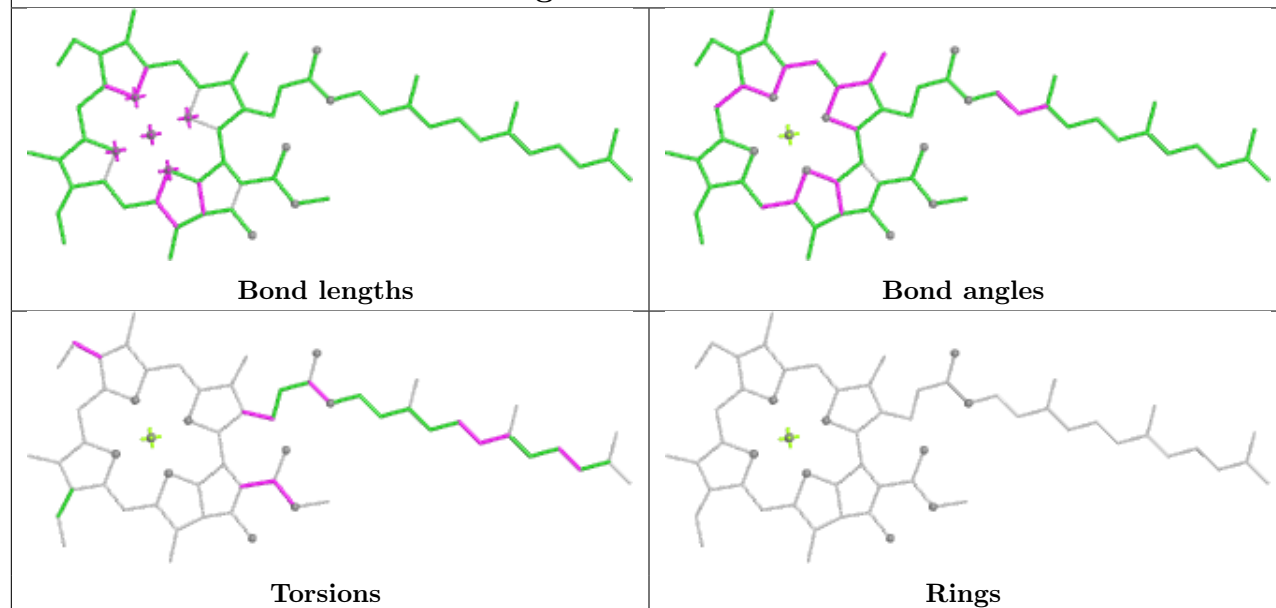


Torsions

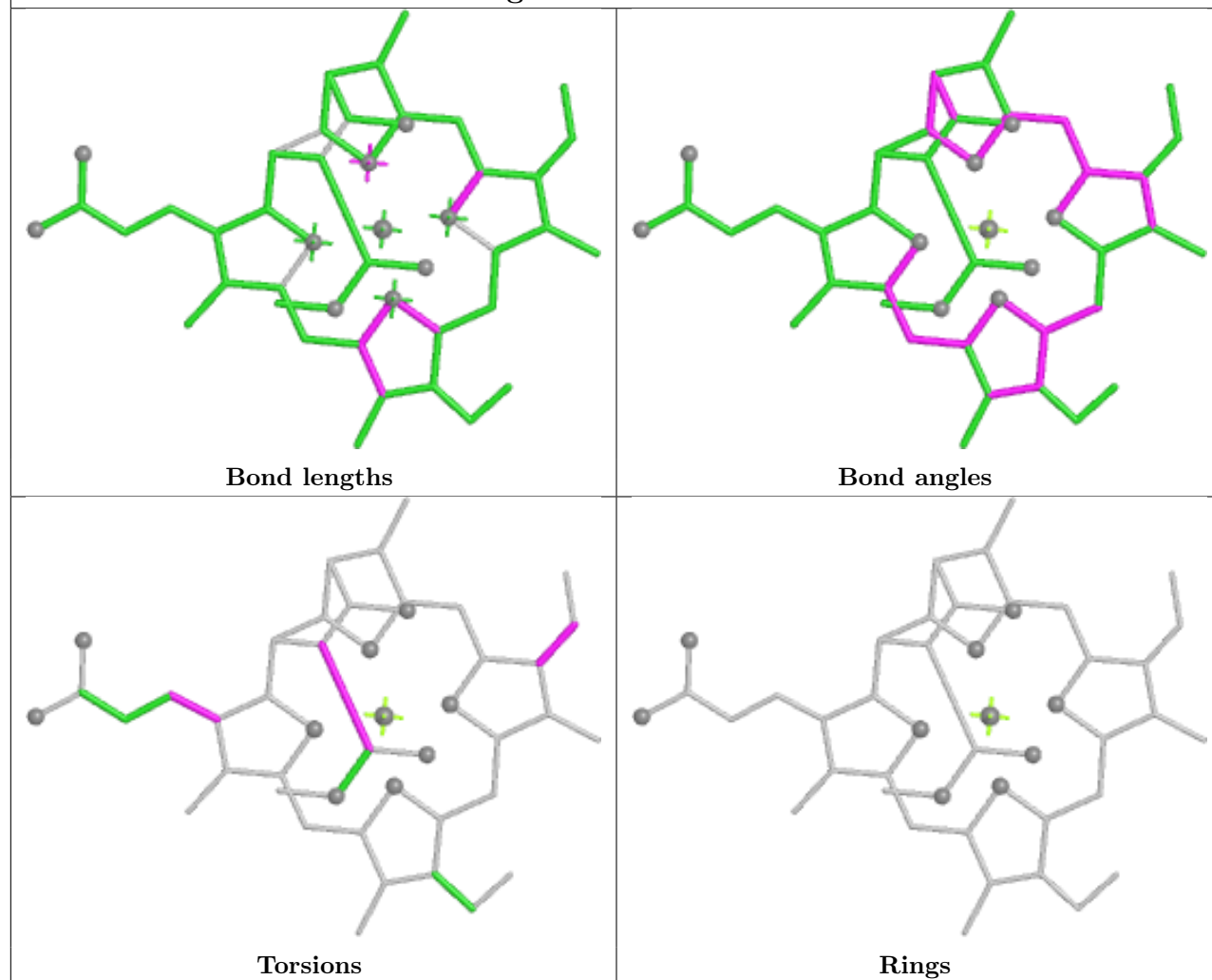


Rings

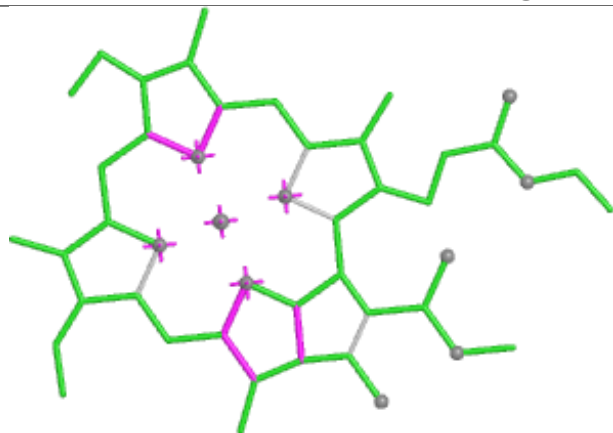
Ligand CLA x 312



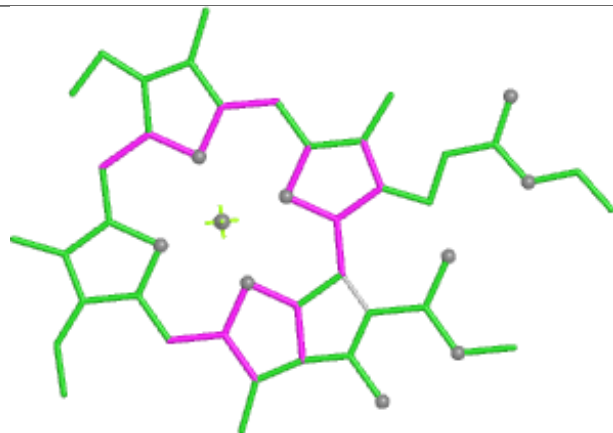
Ligand KC2 R 302



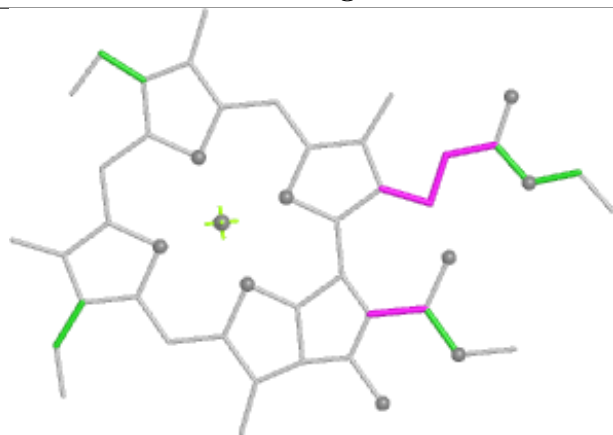
Ligand CLA u 314



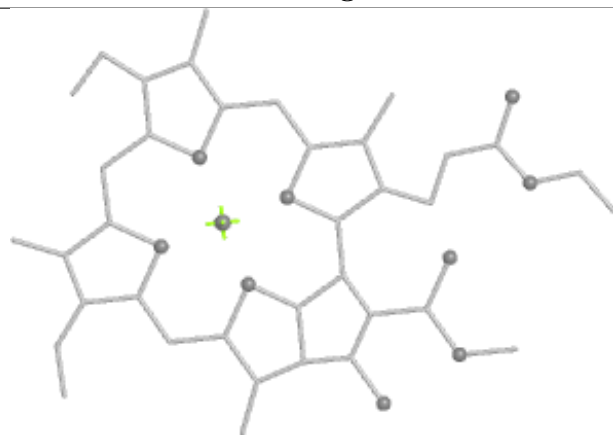
Bond lengths



Bond angles

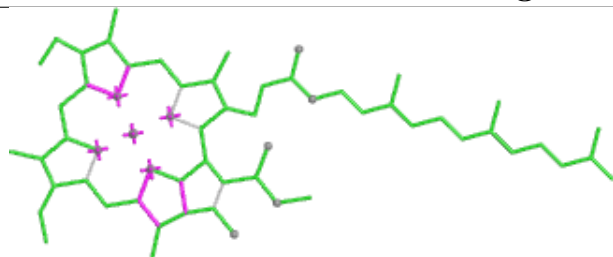


Torsions

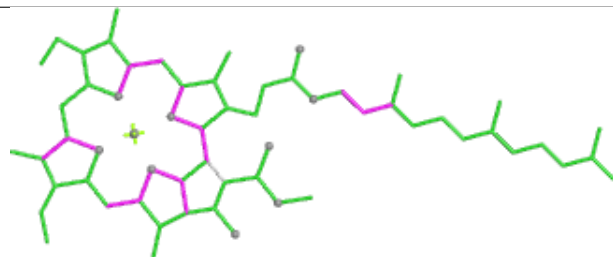


Rings

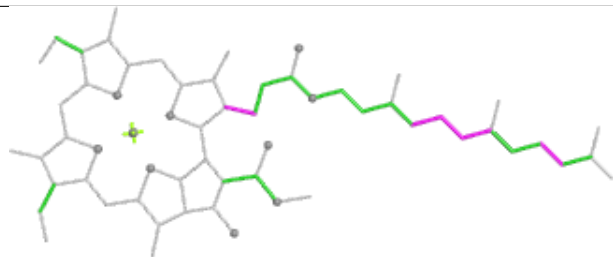
Ligand CLA F 306



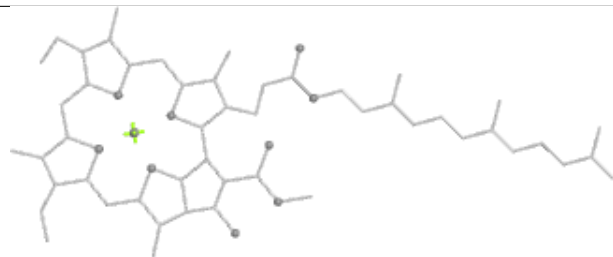
Bond lengths



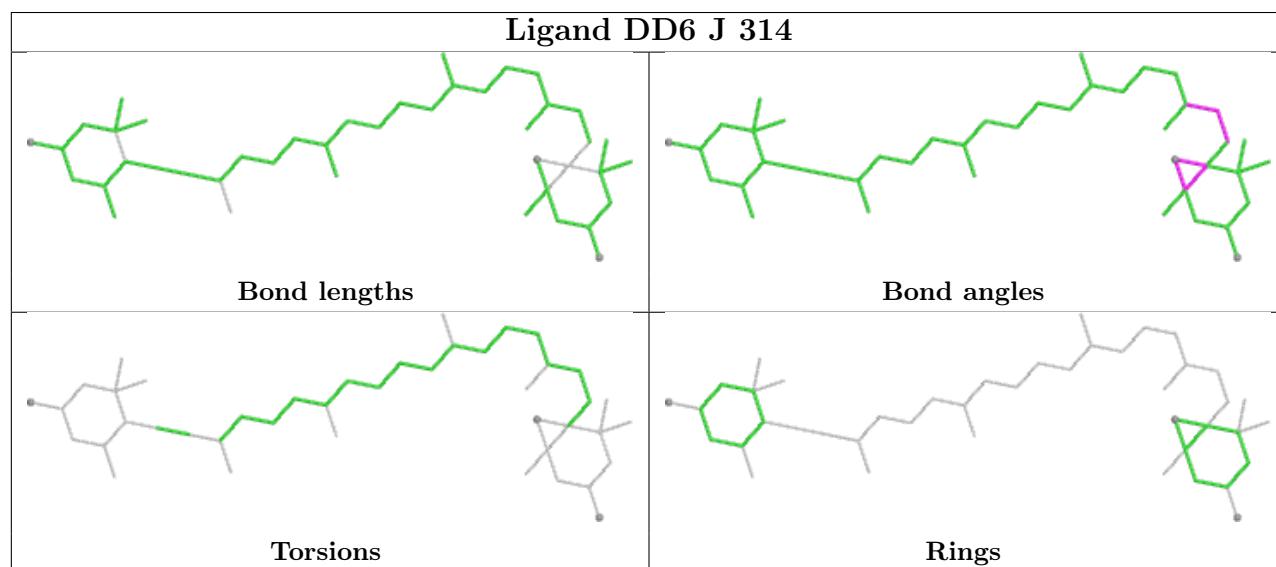
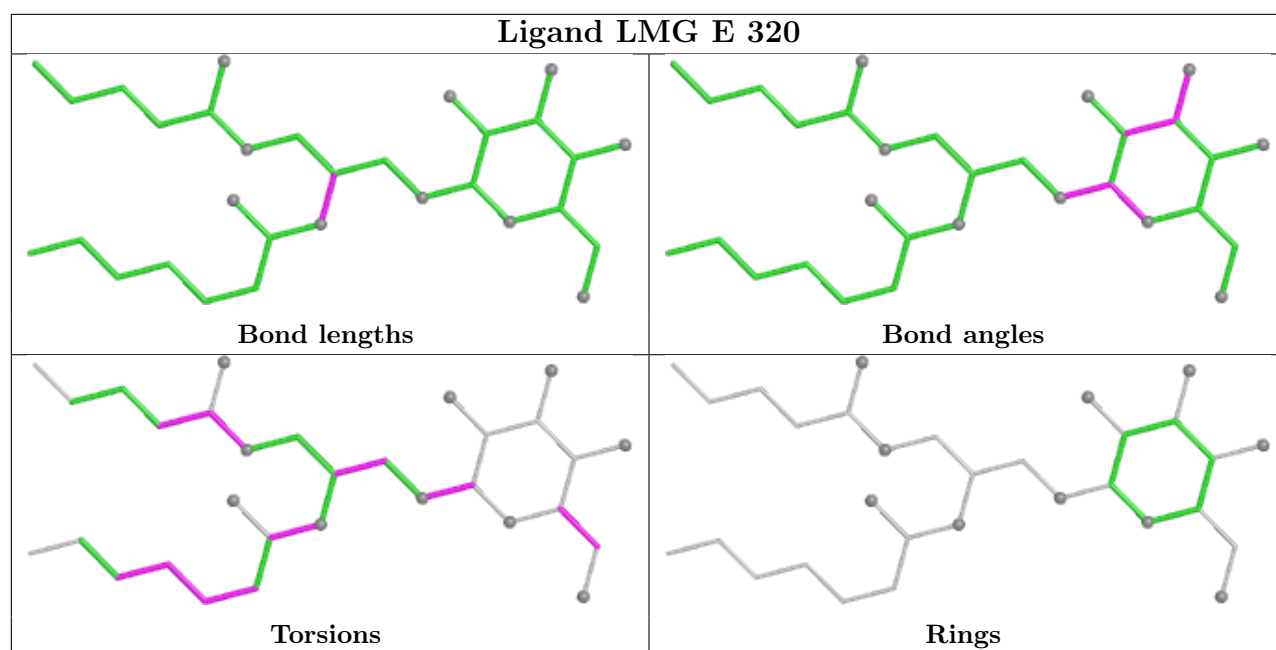
Bond angles

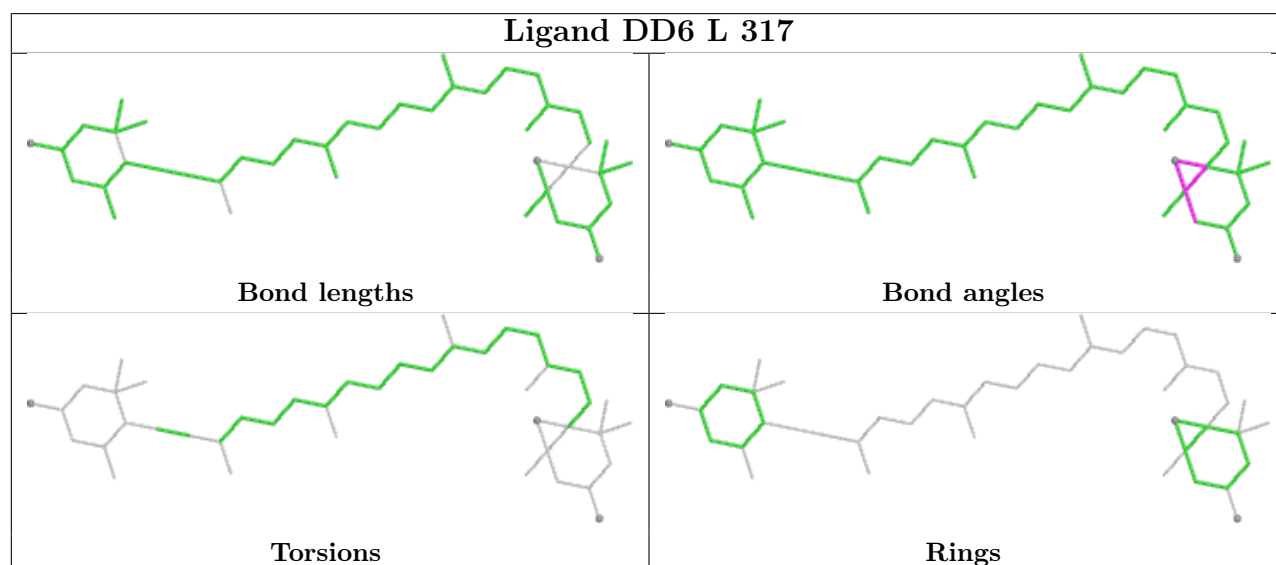
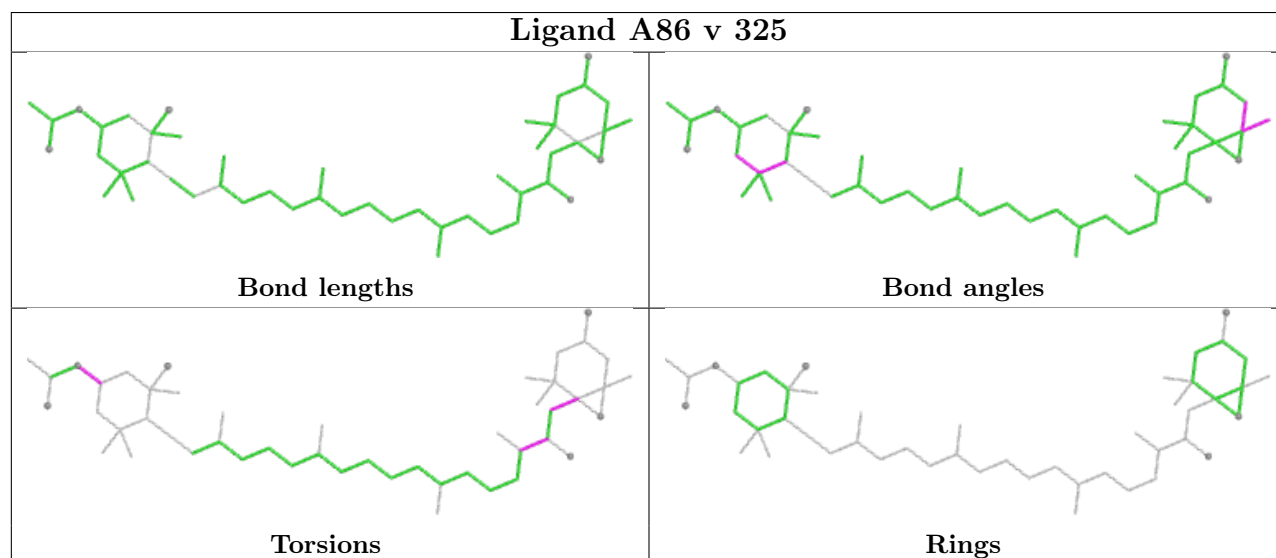
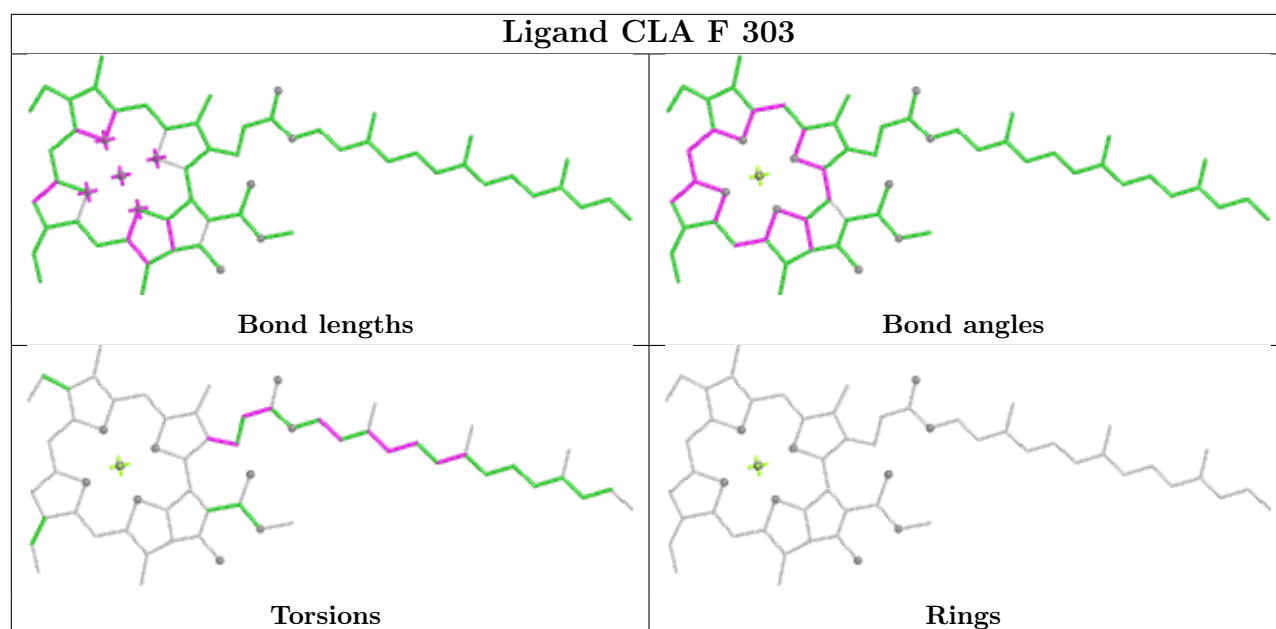


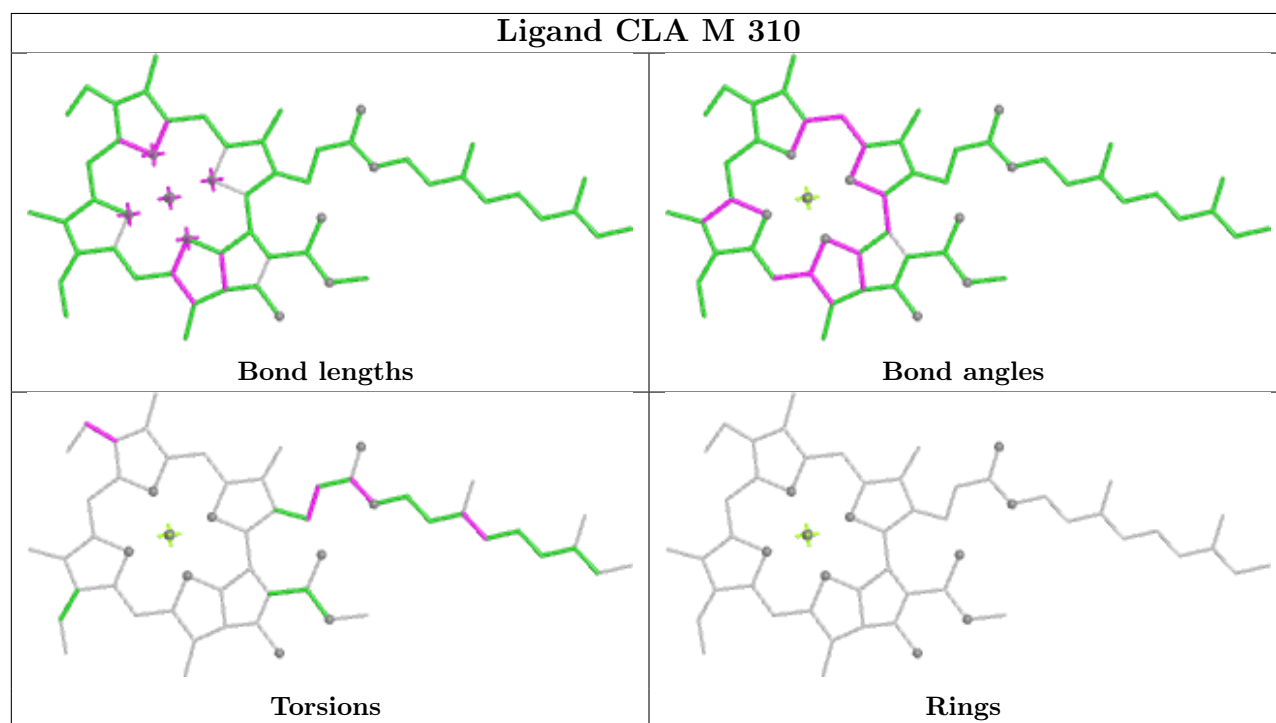
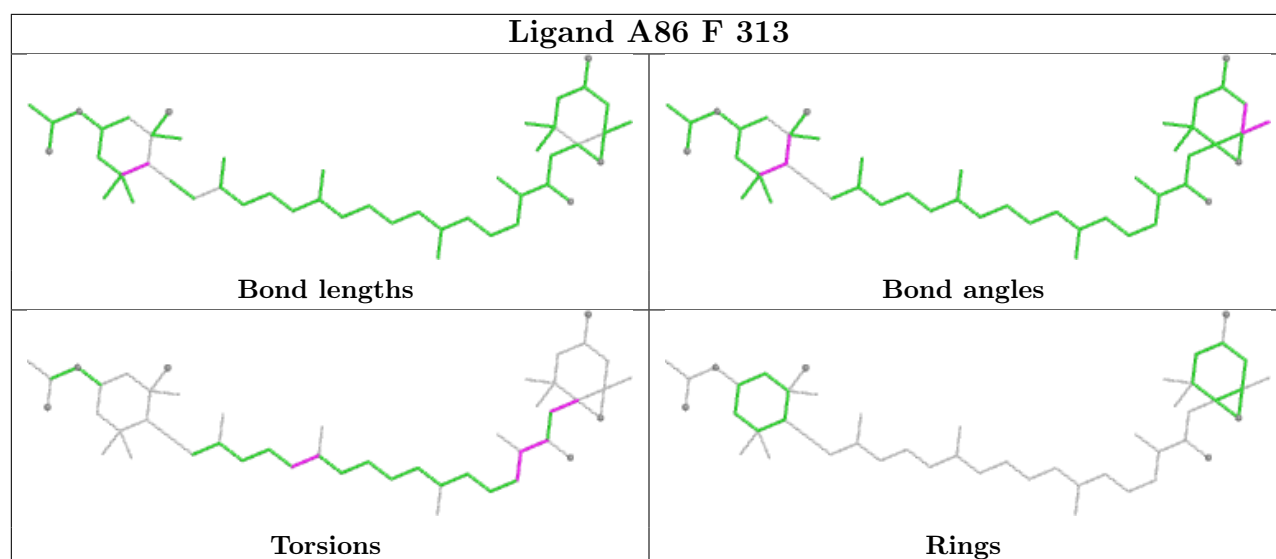
Torsions

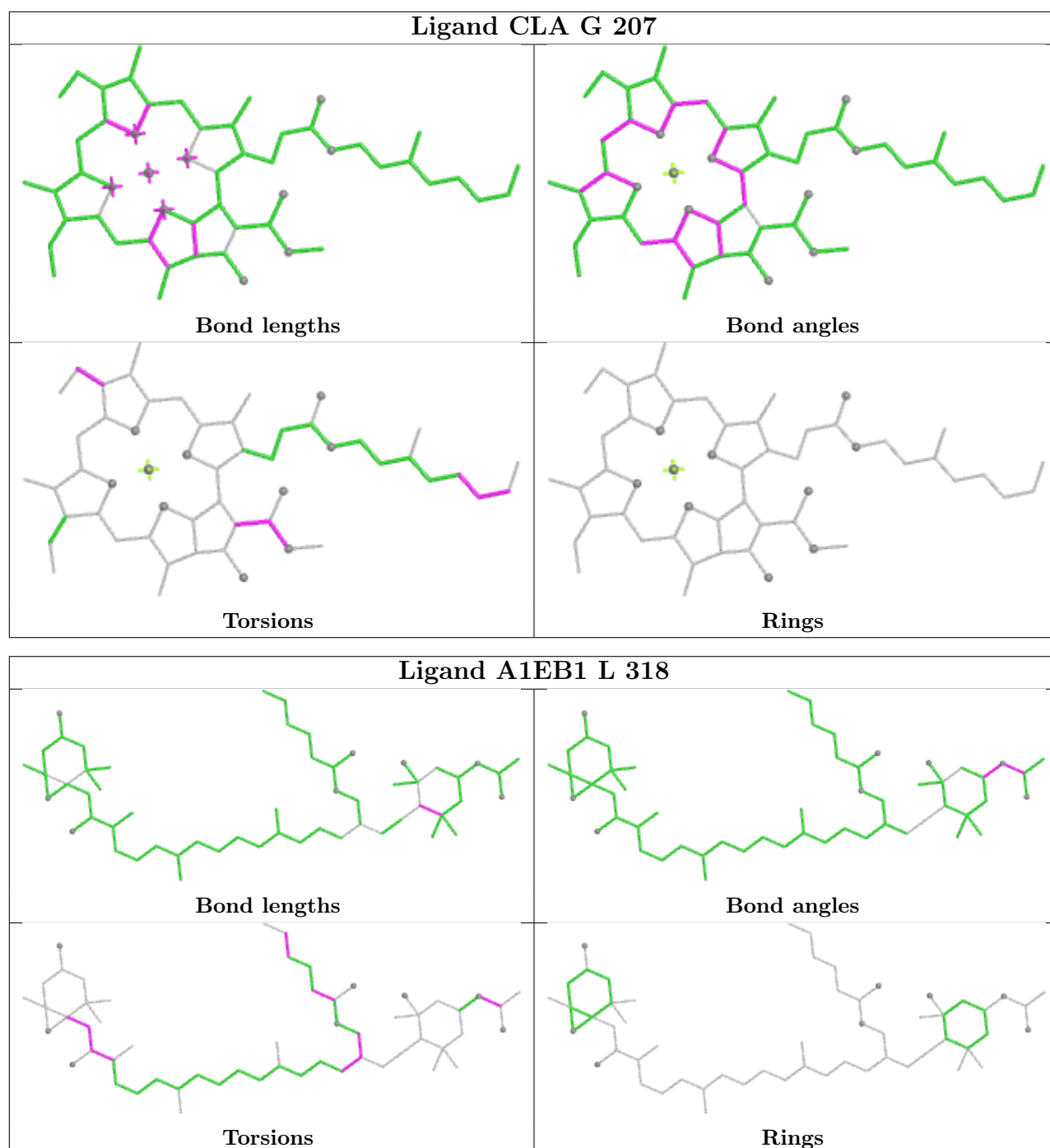


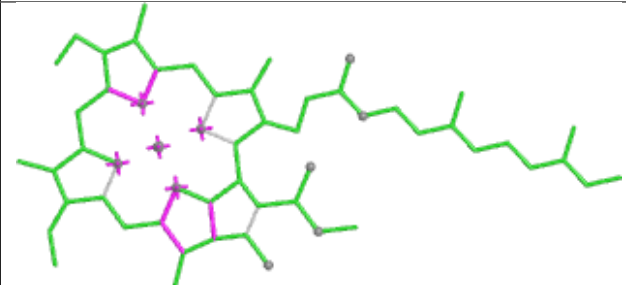
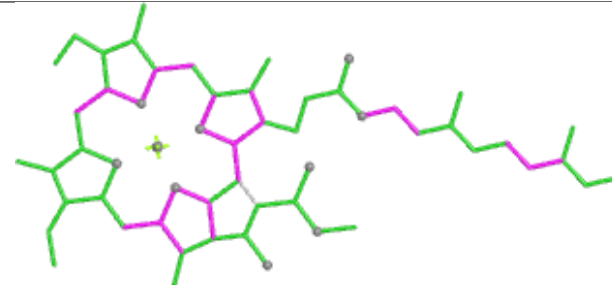
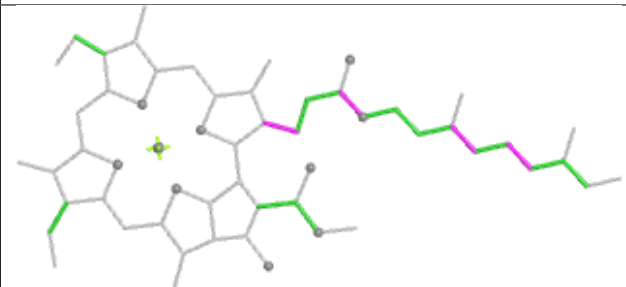
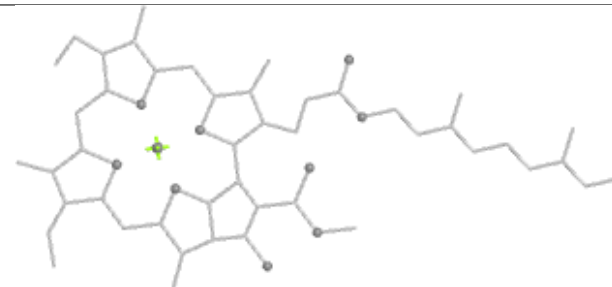
Rings

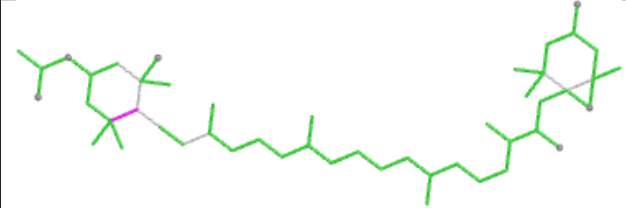
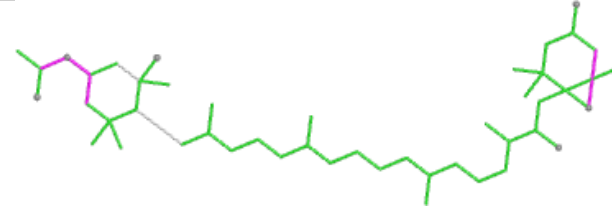
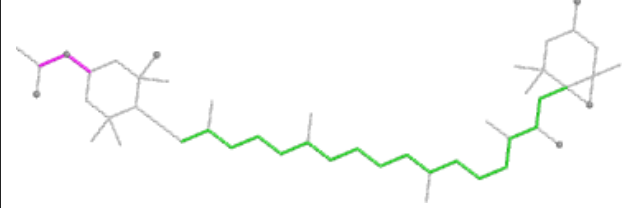
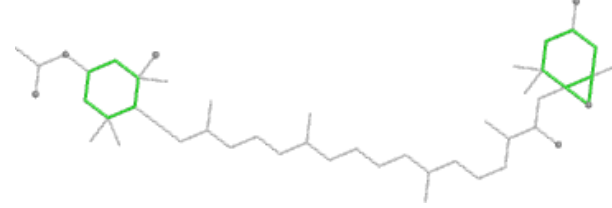


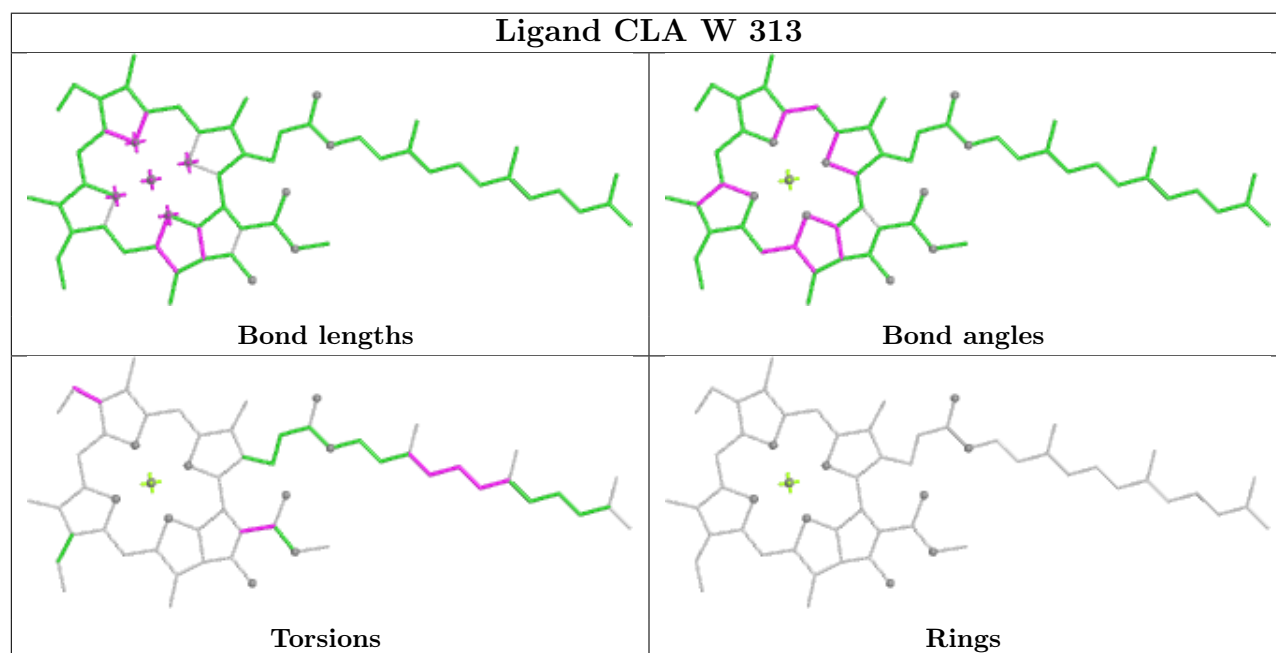
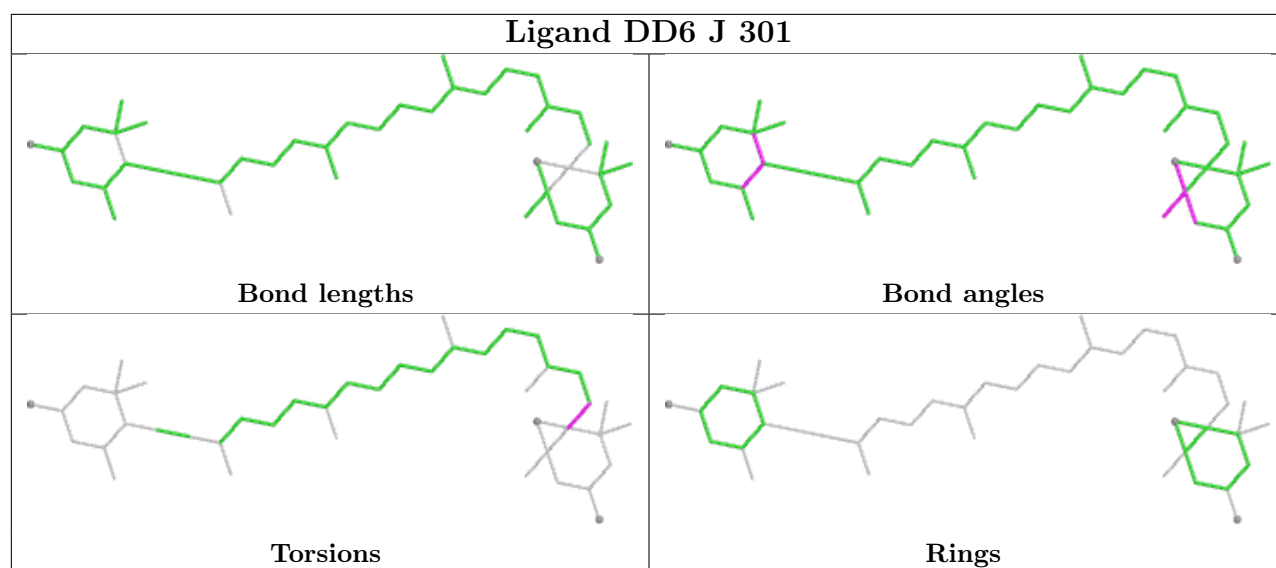




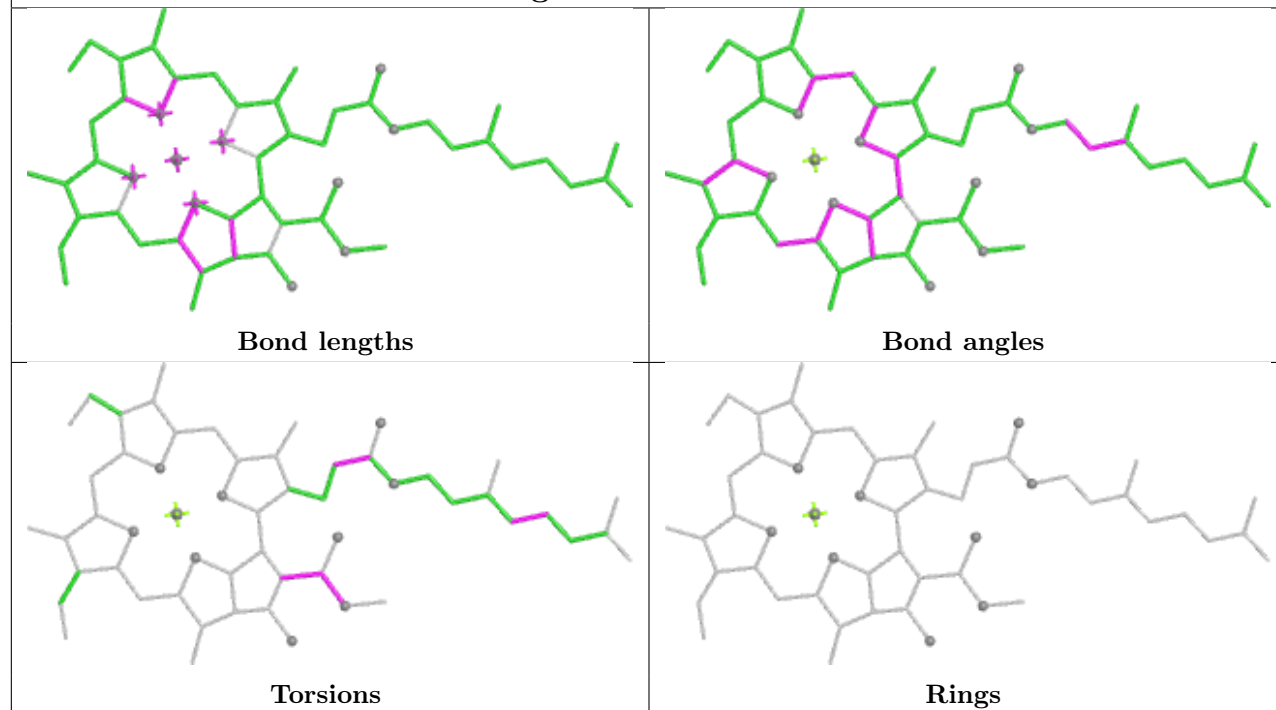


Ligand CLA H 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

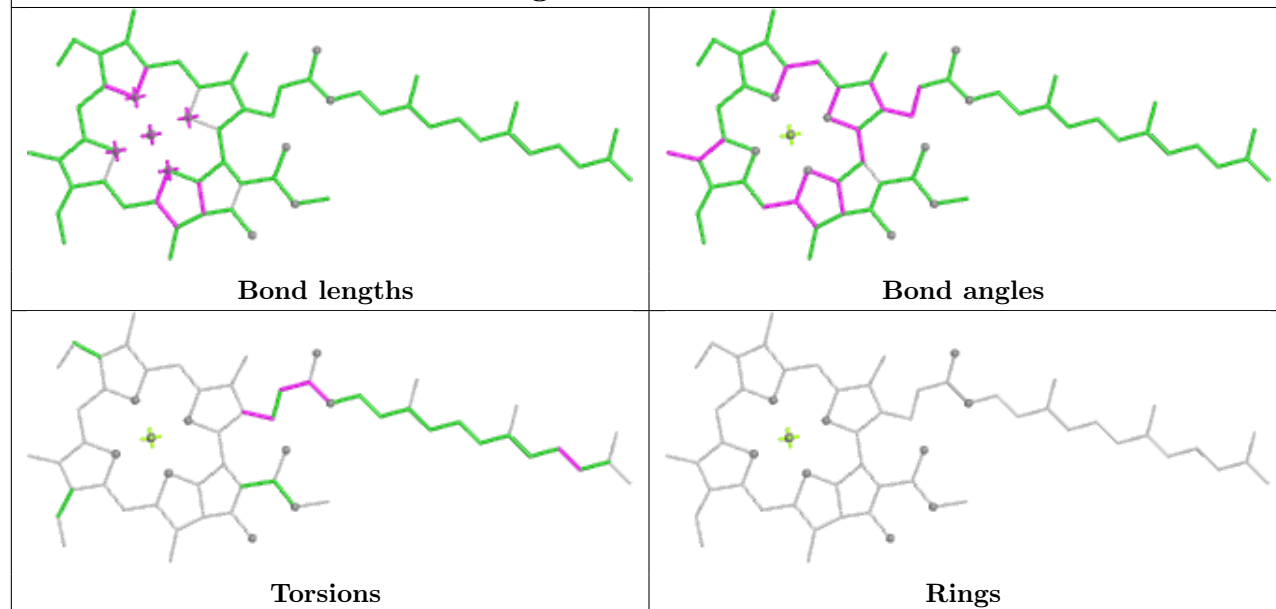
Ligand A86 Z 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

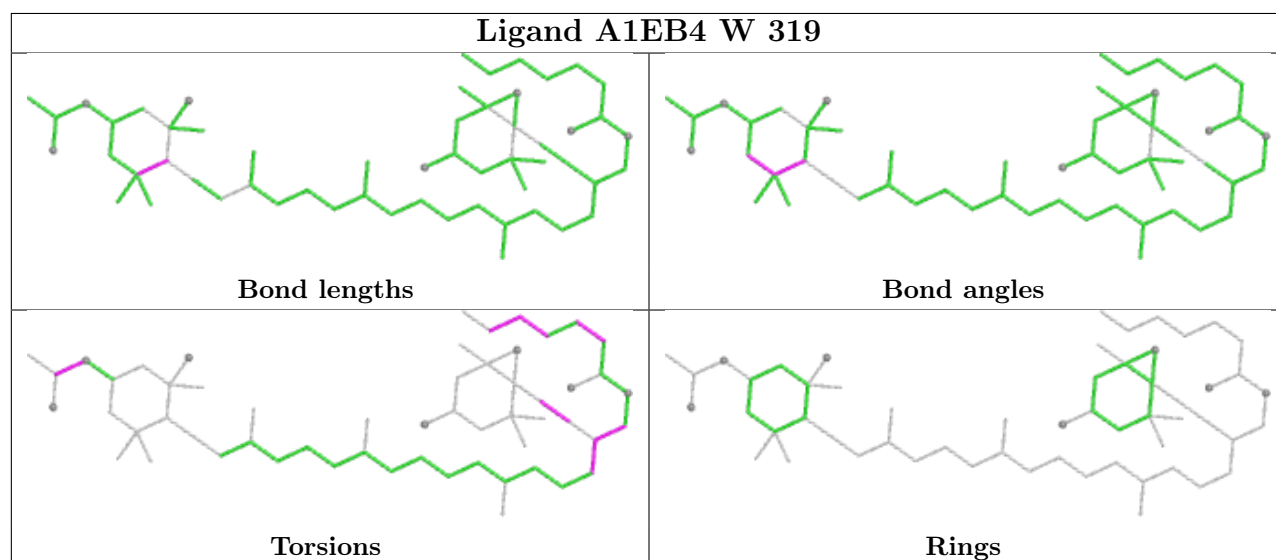
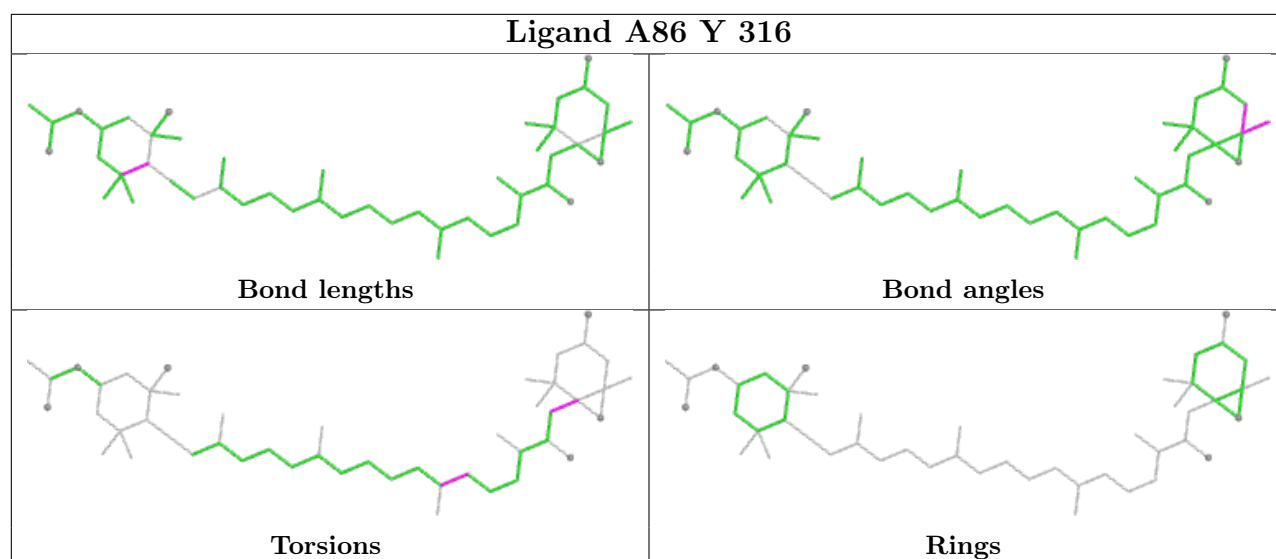


Ligand CLA D 306

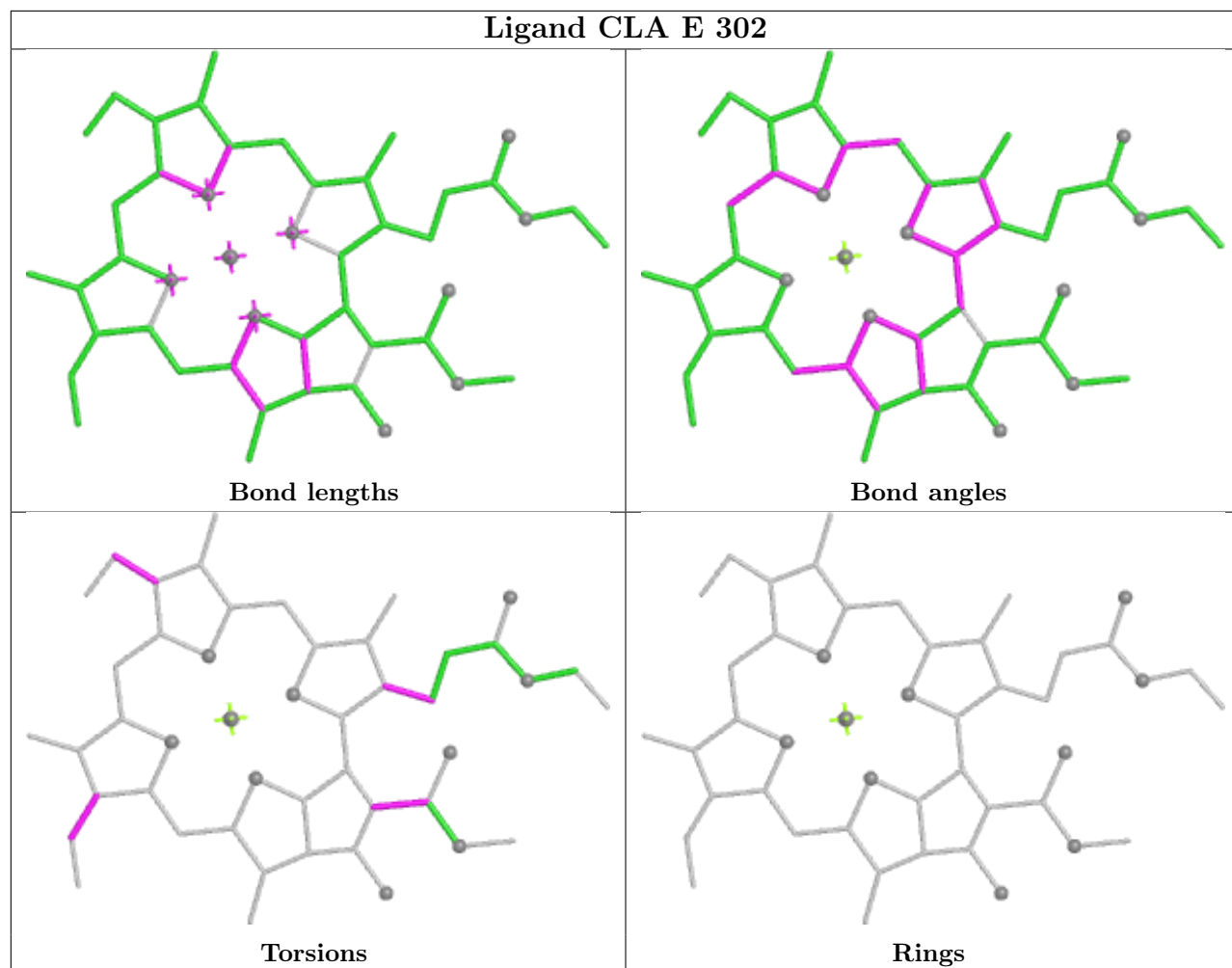


Ligand CLA K 306

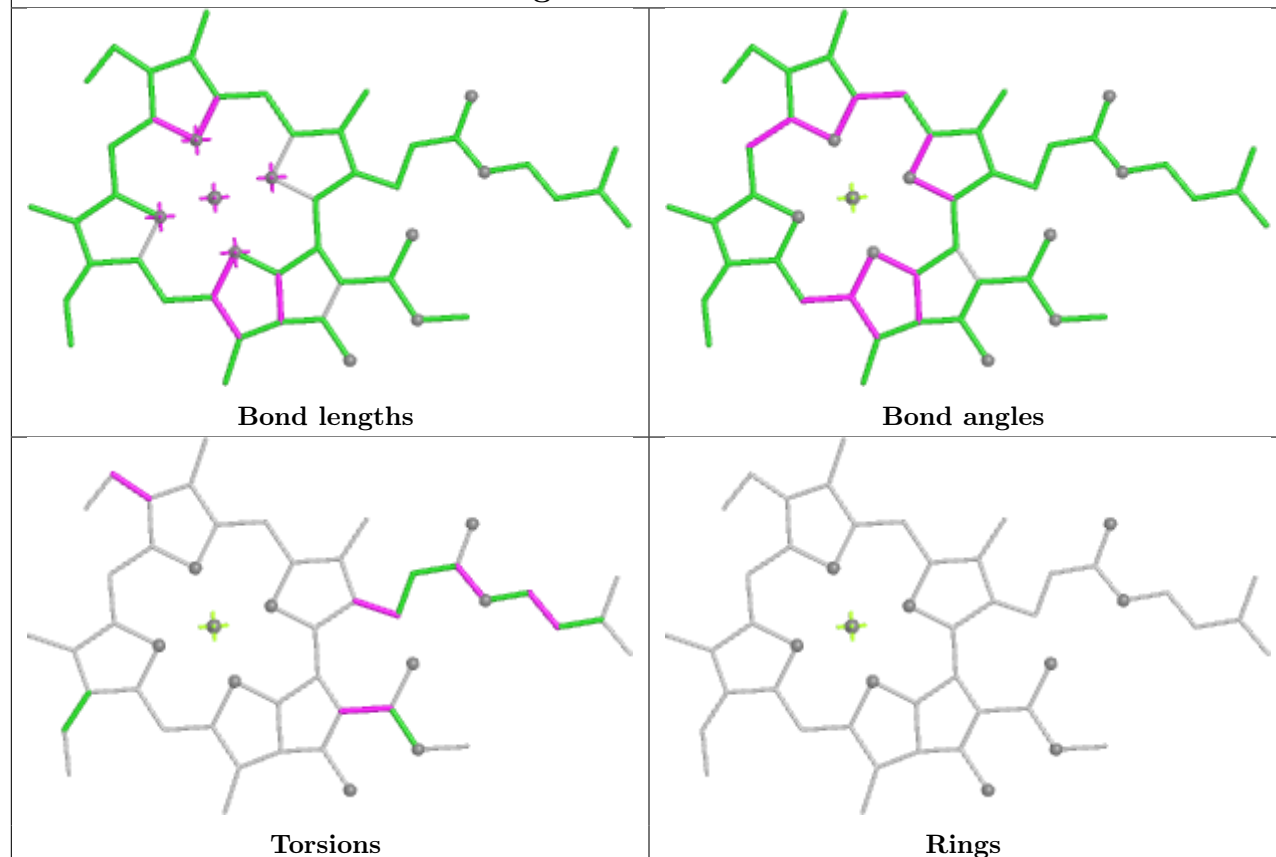




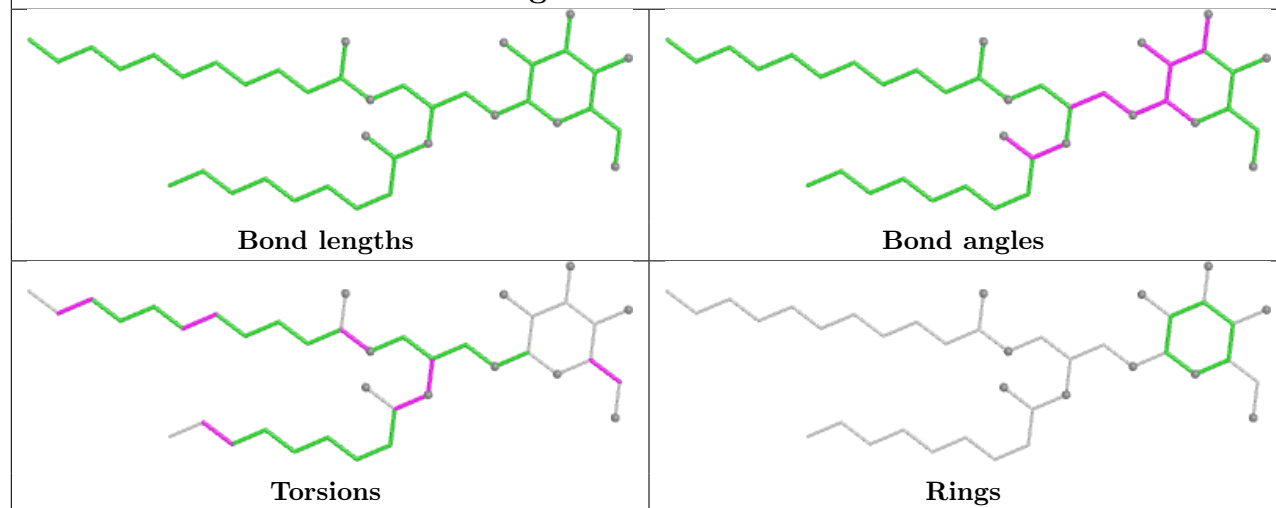
Ligand CLA E 302



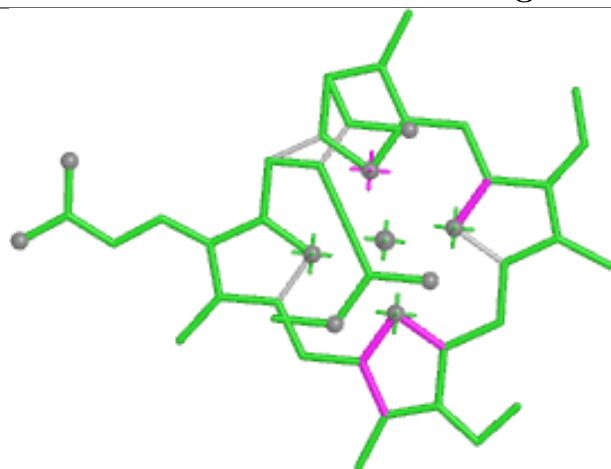
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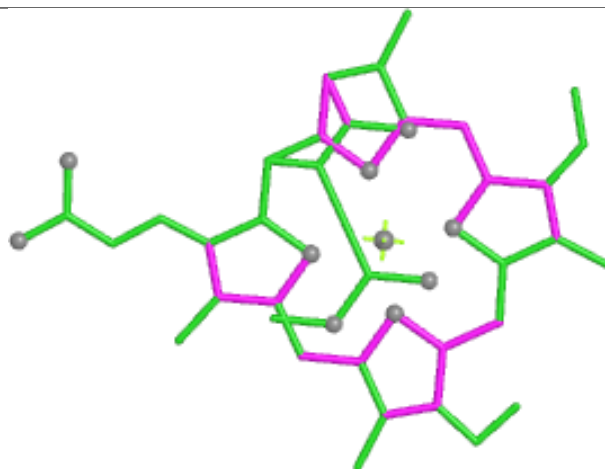
Ligand LMG F 318



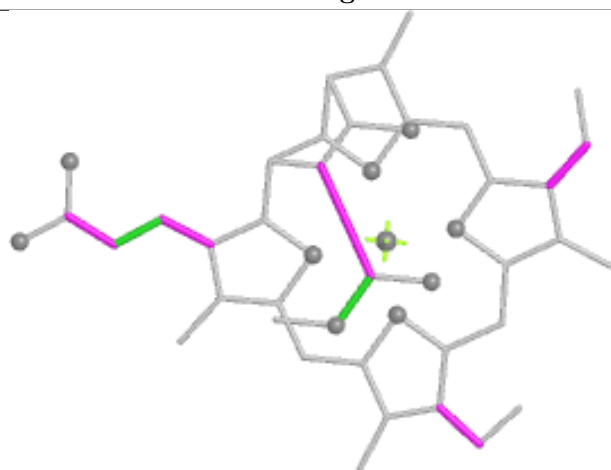
Ligand KC2 O 302



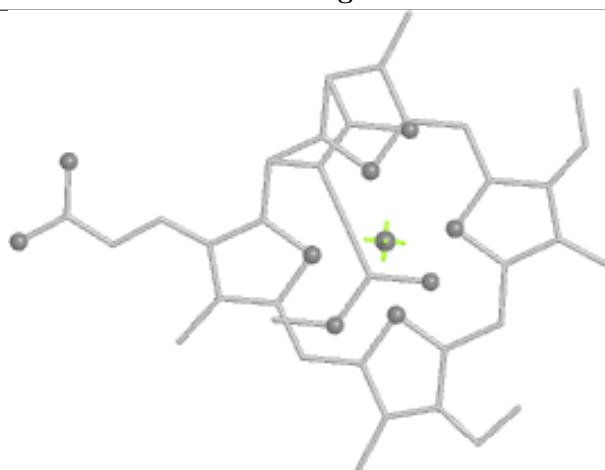
Bond lengths



Bond angles

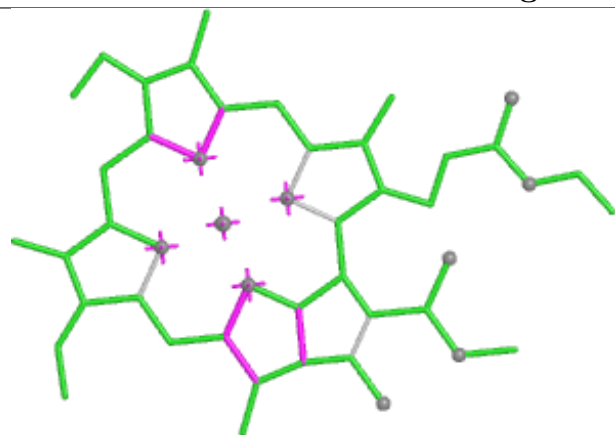


Torsions

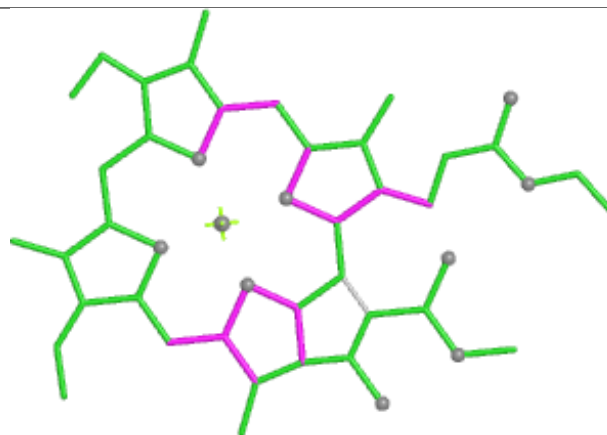


Rings

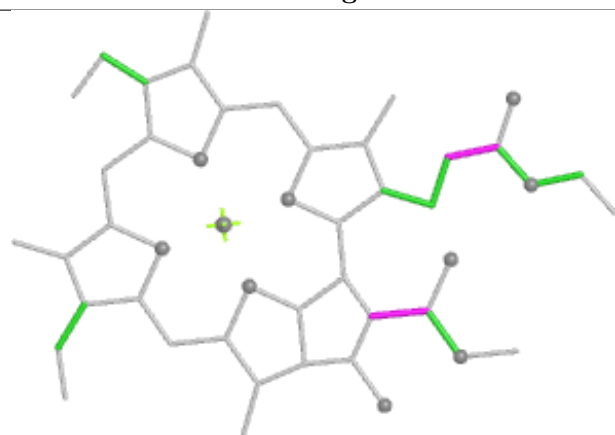
Ligand CLA J 311



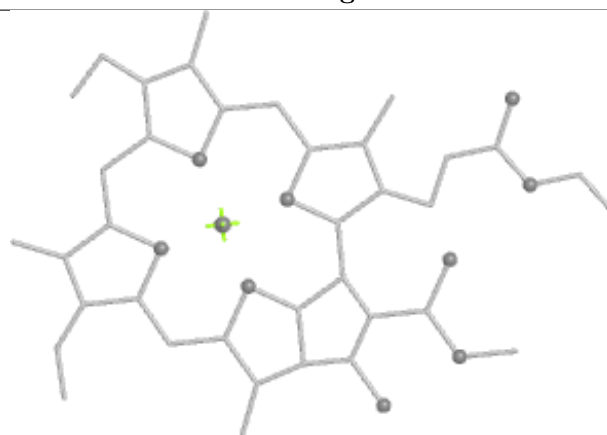
Bond lengths



Bond angles

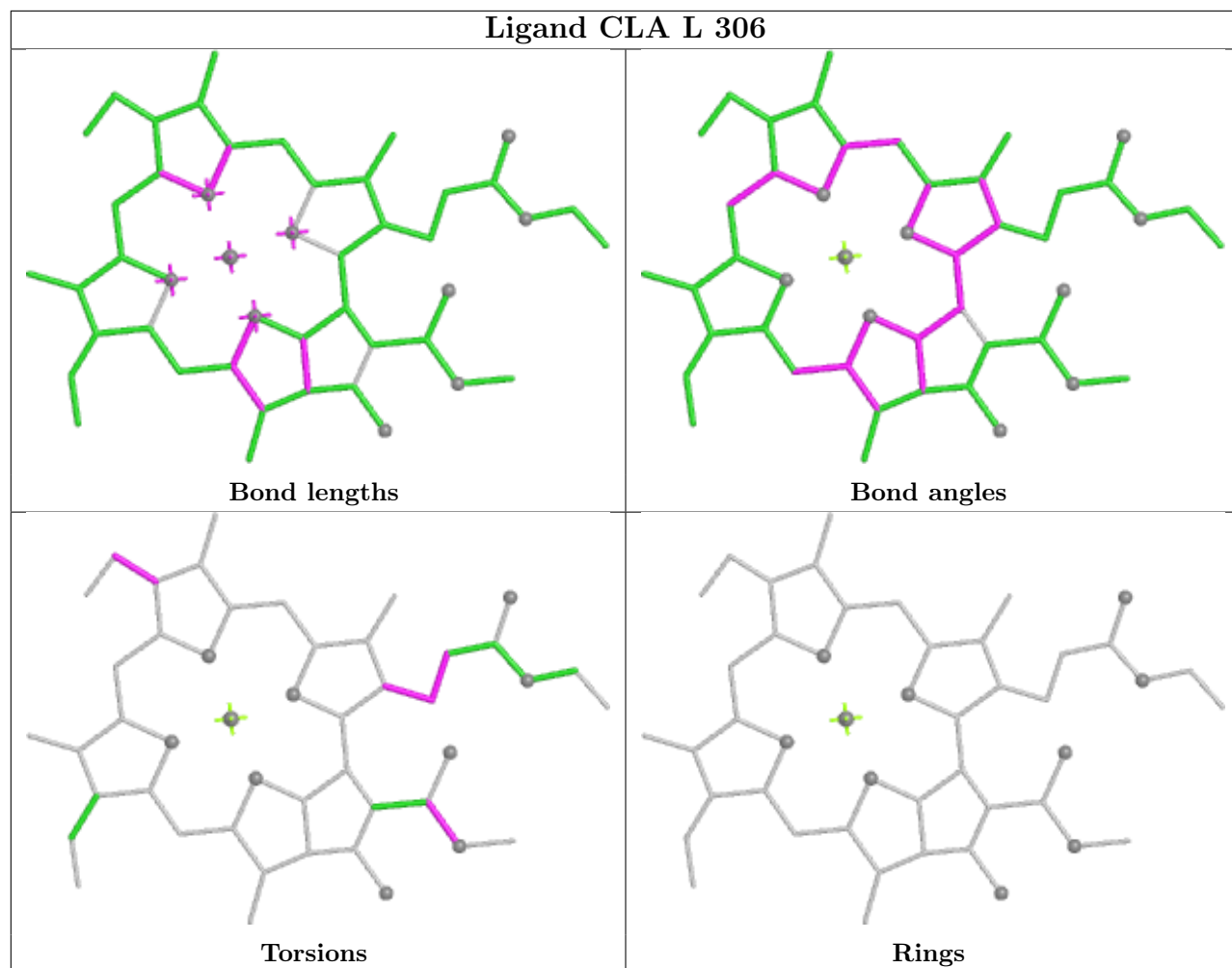


Torsions

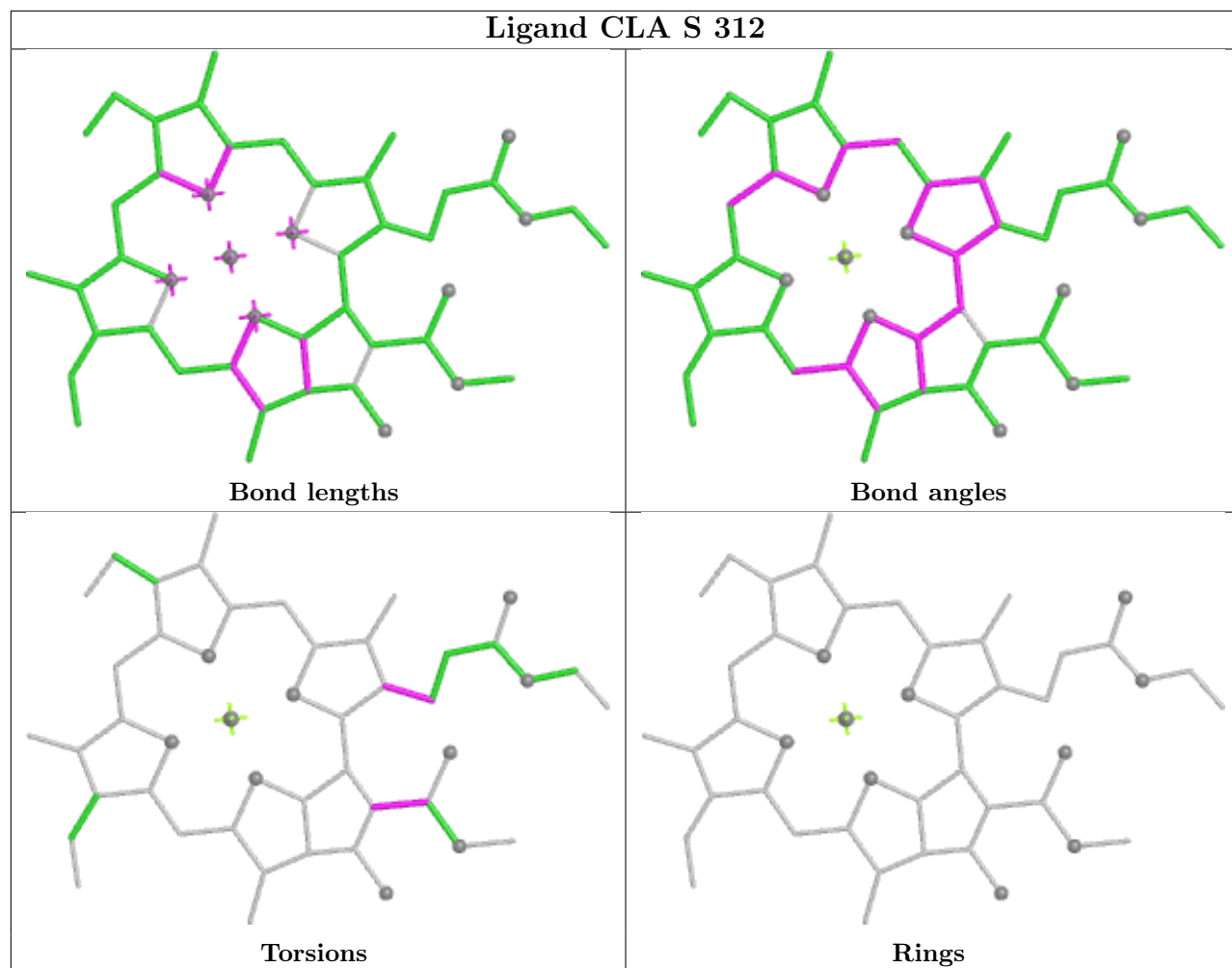


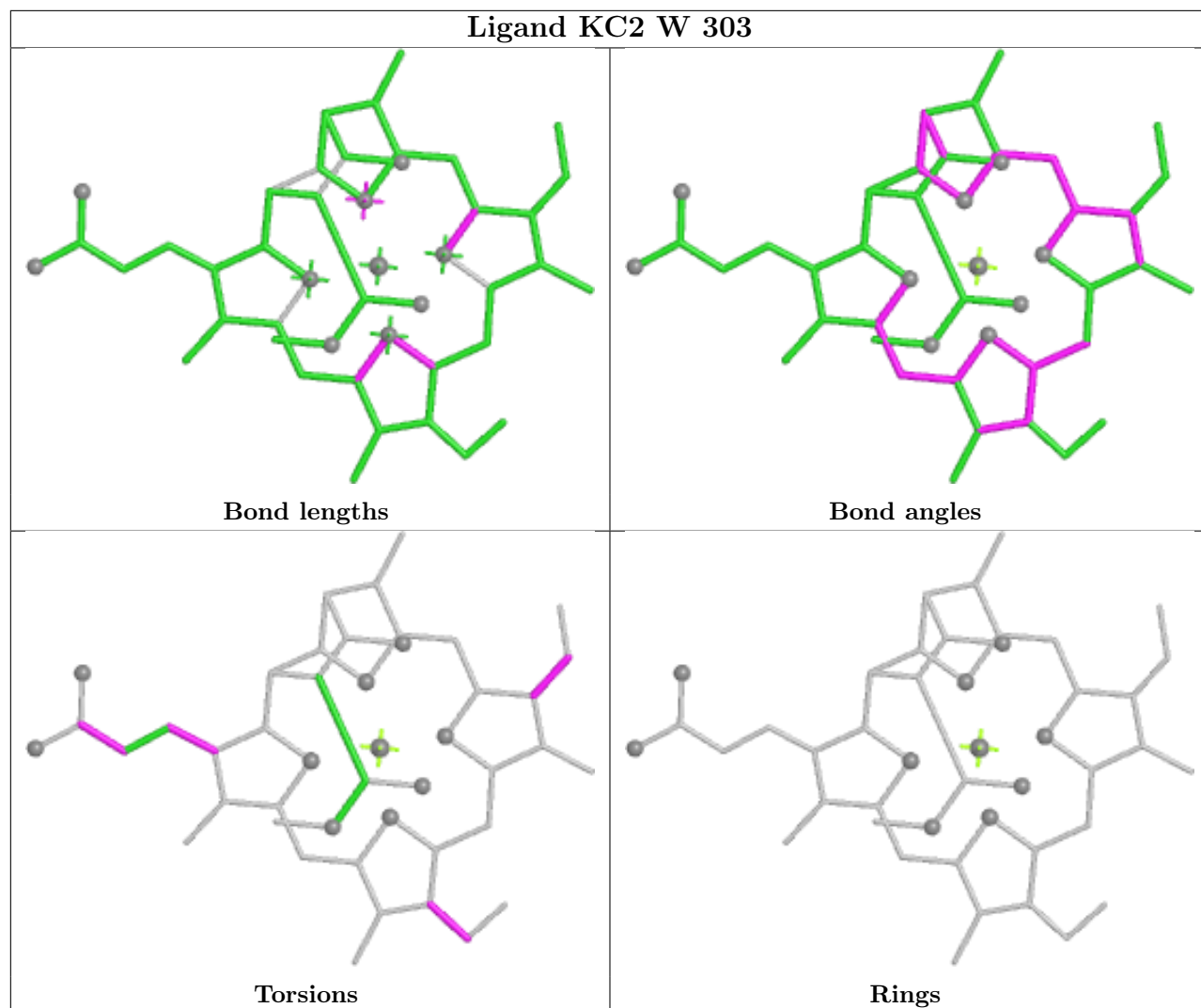
Rings

Ligand CLA L 306

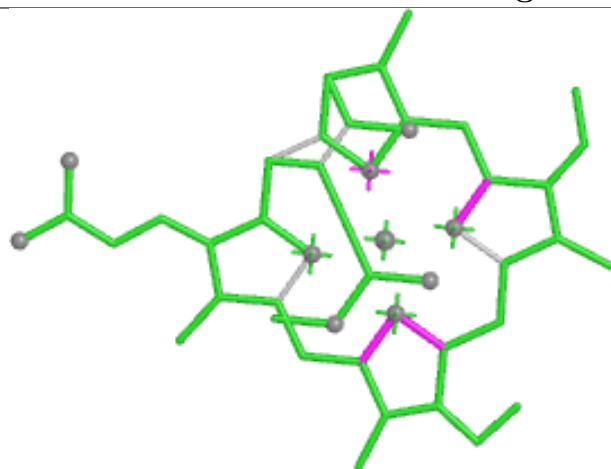


Ligand CLA S 312

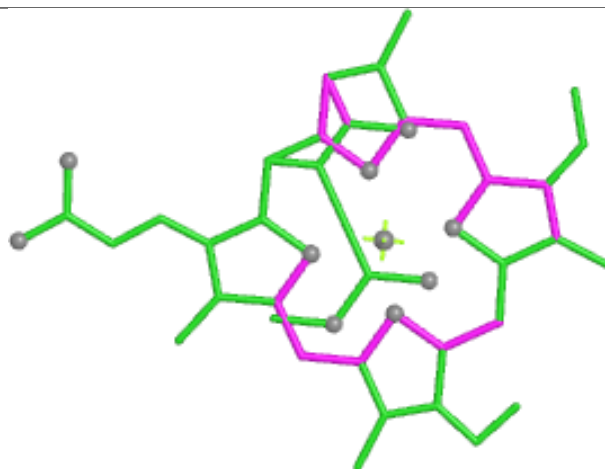




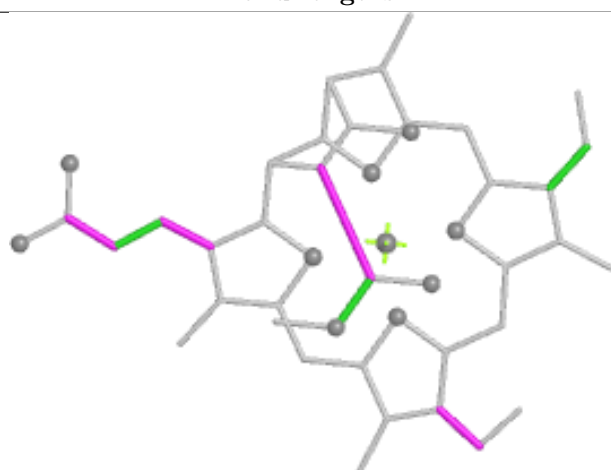
Ligand KC2 w 301



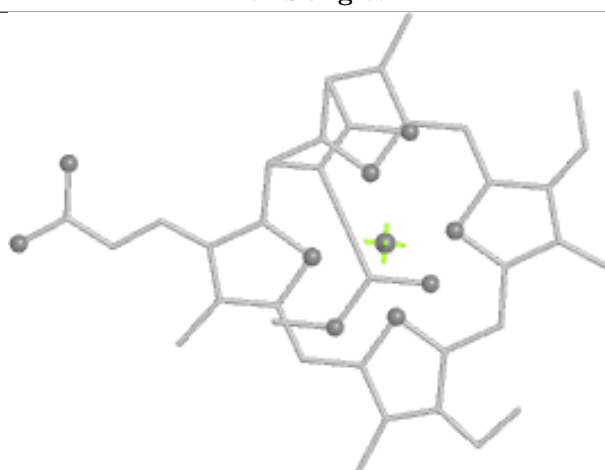
Bond lengths



Bond angles

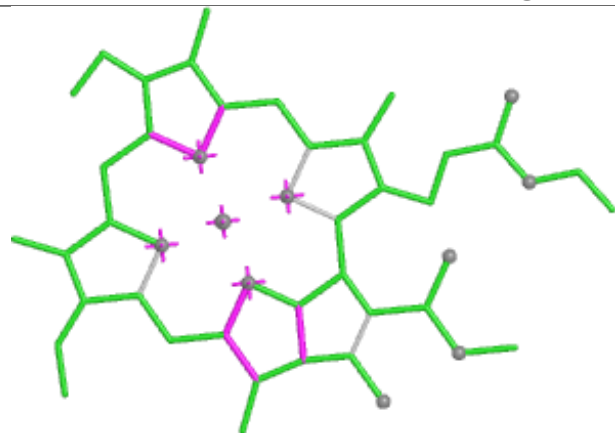


Torsions

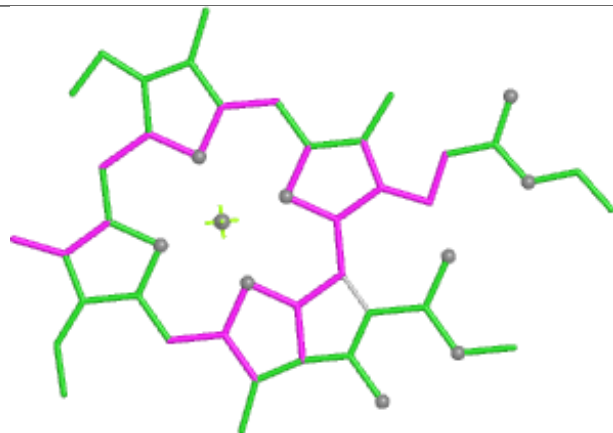


Rings

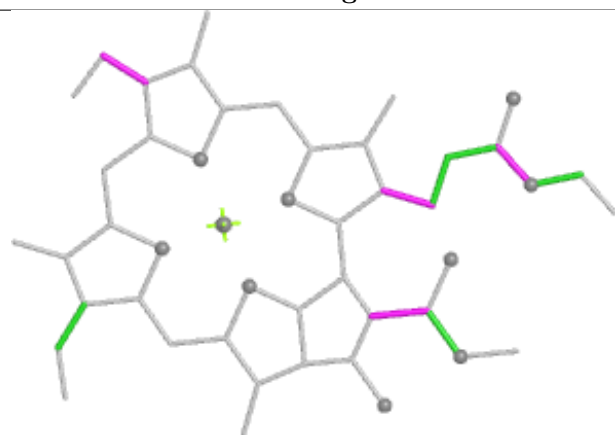
Ligand CLA Z 312



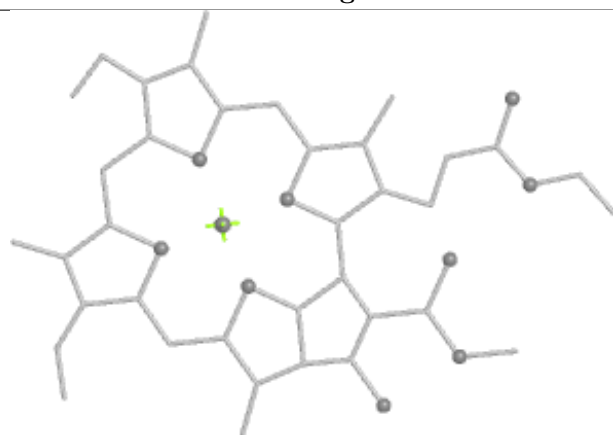
Bond lengths



Bond angles

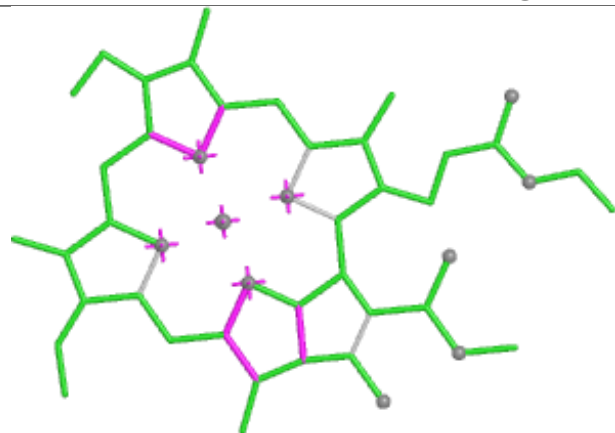


Torsions

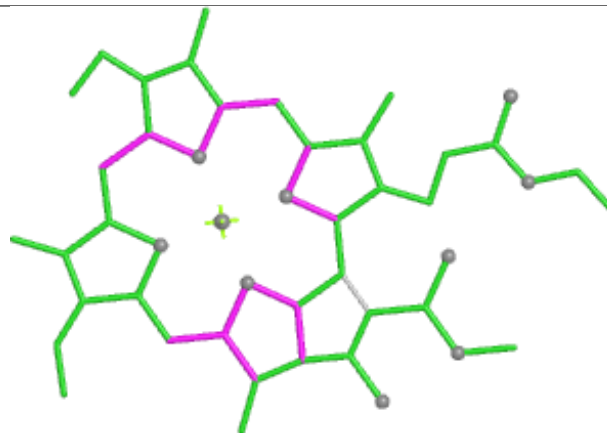


Rings

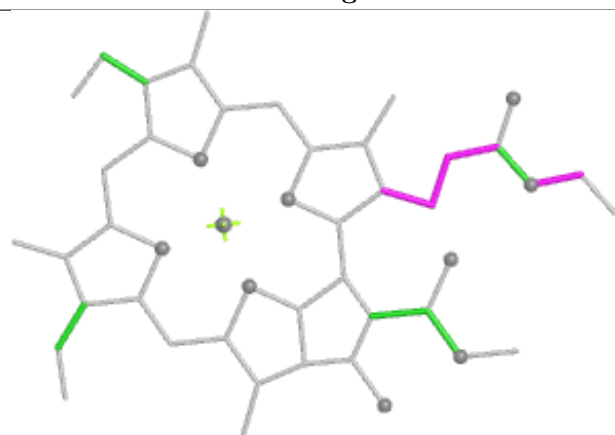
Ligand CLA w 303



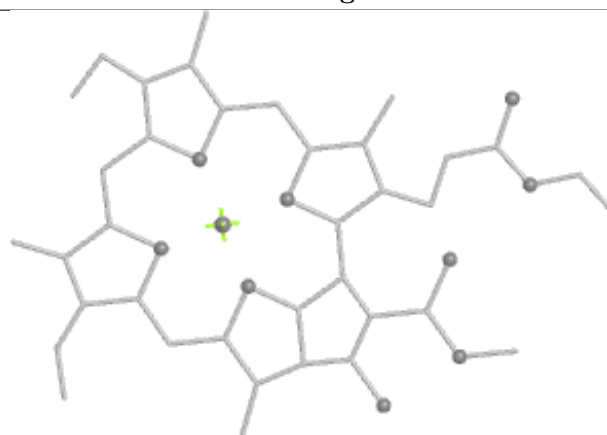
Bond lengths



Bond angles

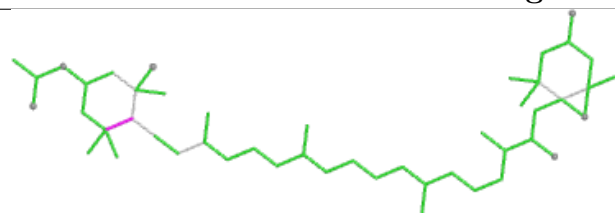


Torsions

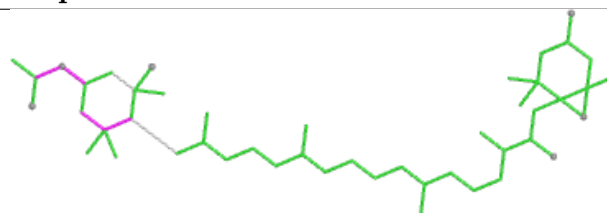


Rings

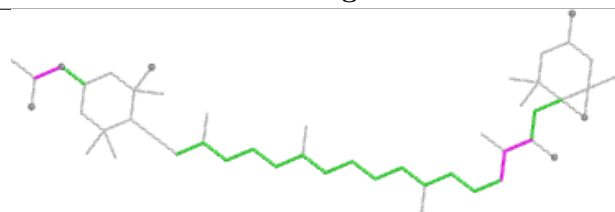
Ligand A86 q 315



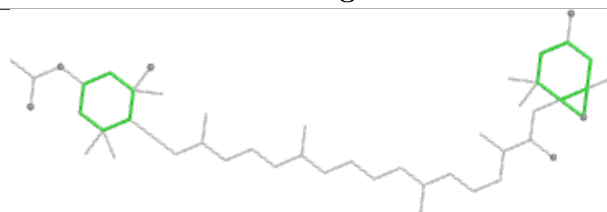
Bond lengths



Bond angles

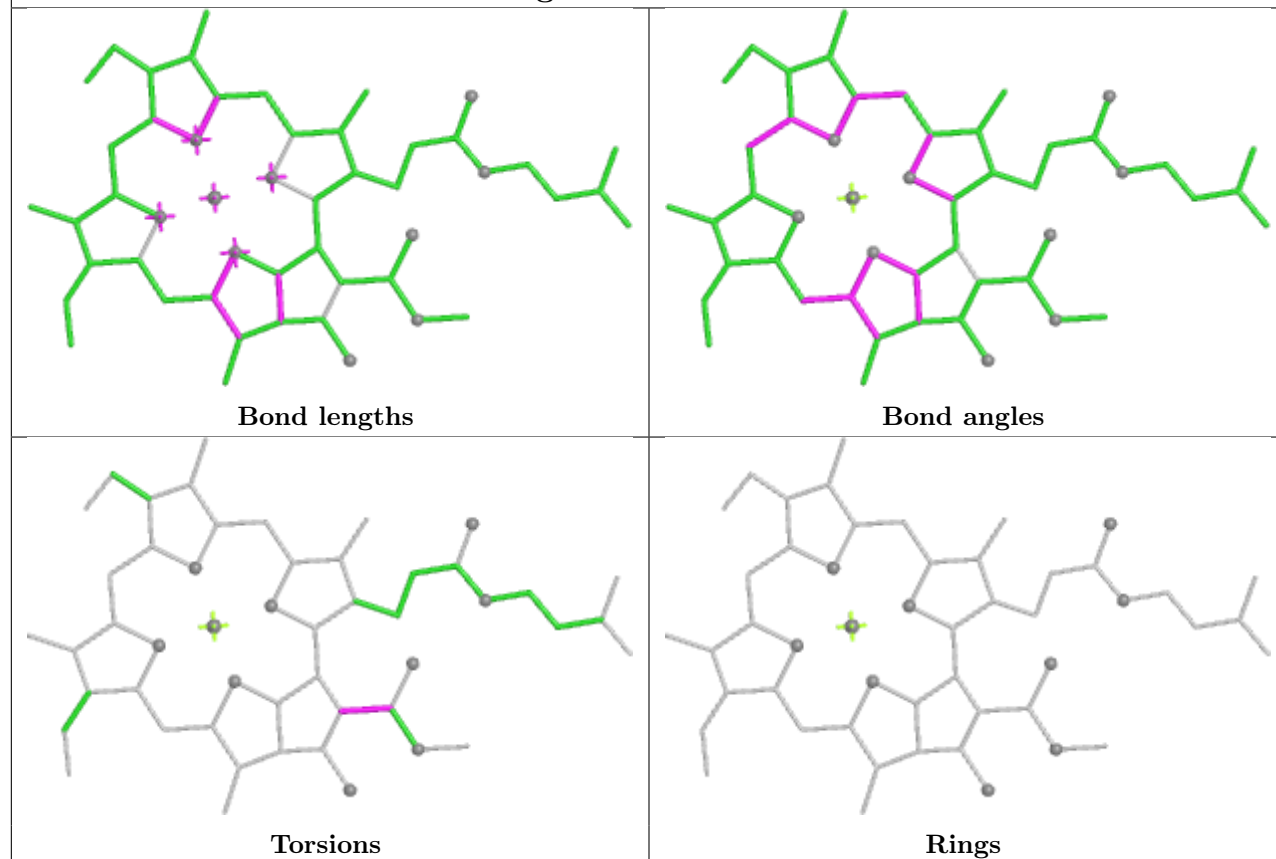


Torsions

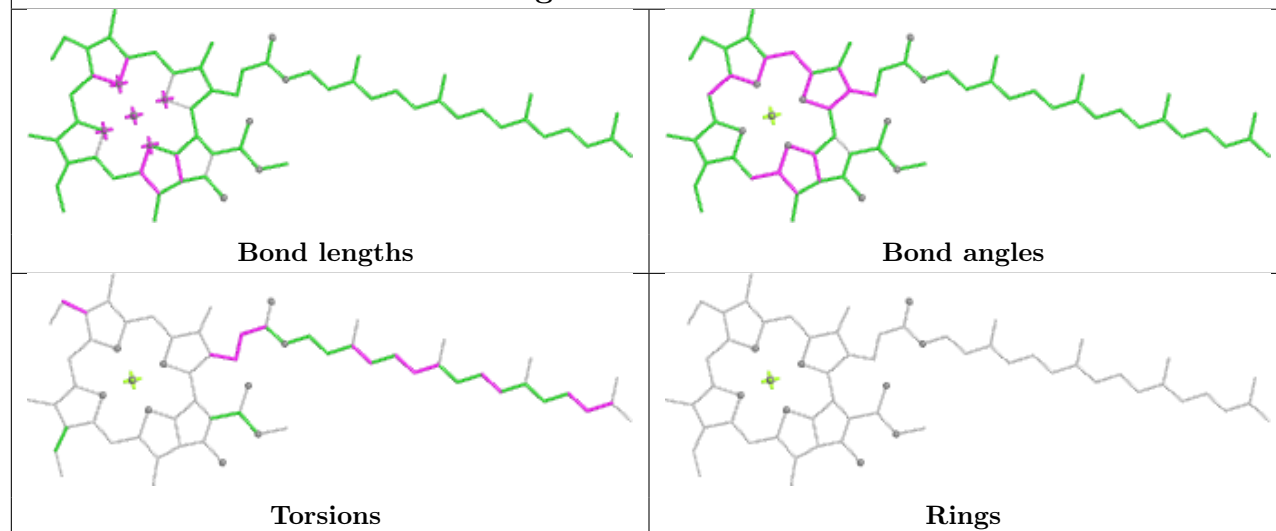


Rings

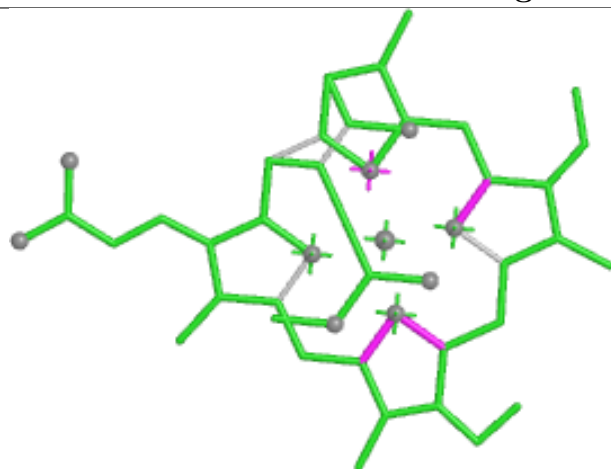
Ligand CLA a 817



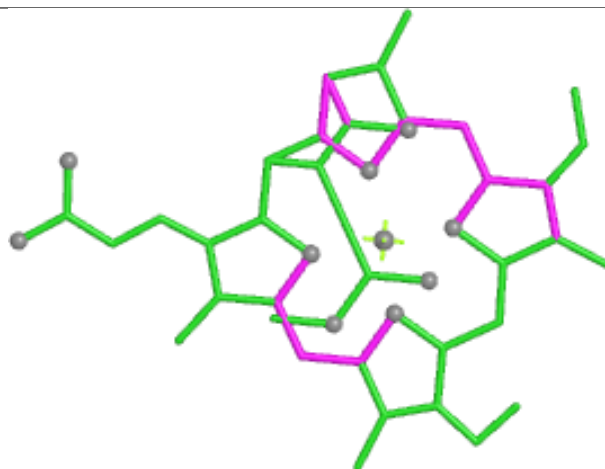
Ligand CLA b 824



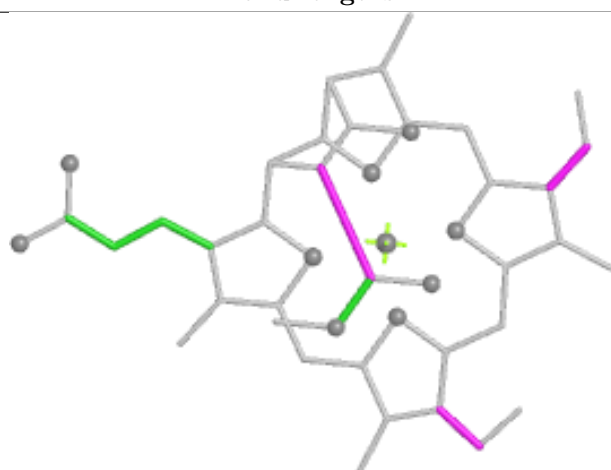
Ligand KC2 H 303



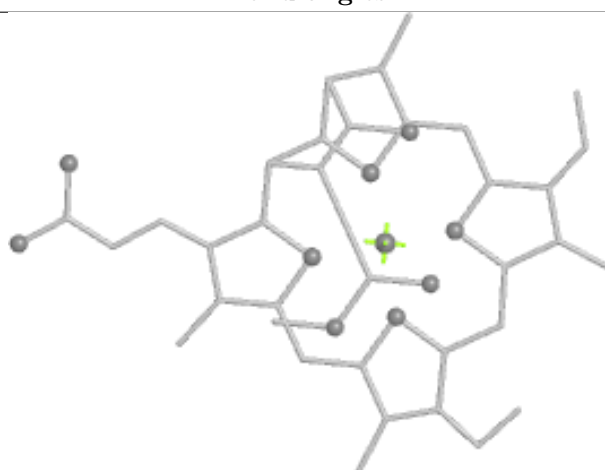
Bond lengths



Bond angles

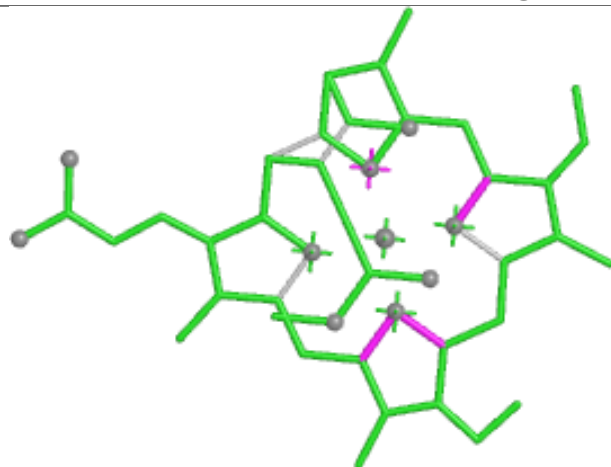


Torsions

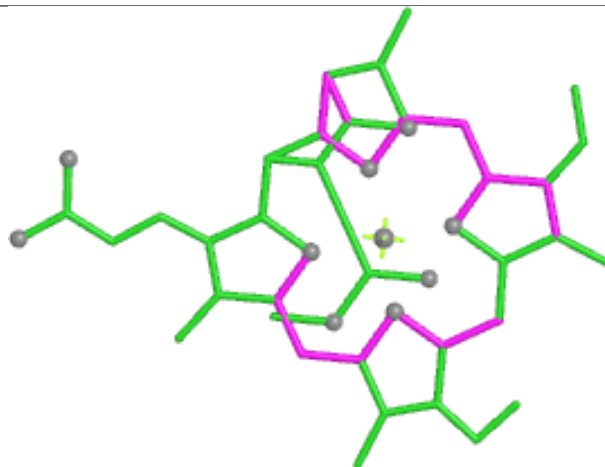


Rings

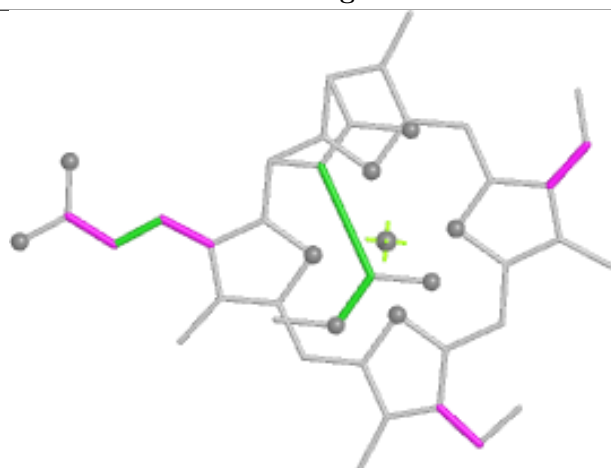
Ligand KC2 K 309



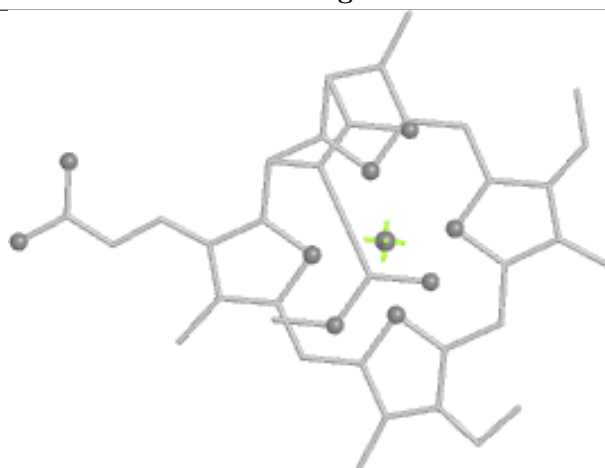
Bond lengths



Bond angles

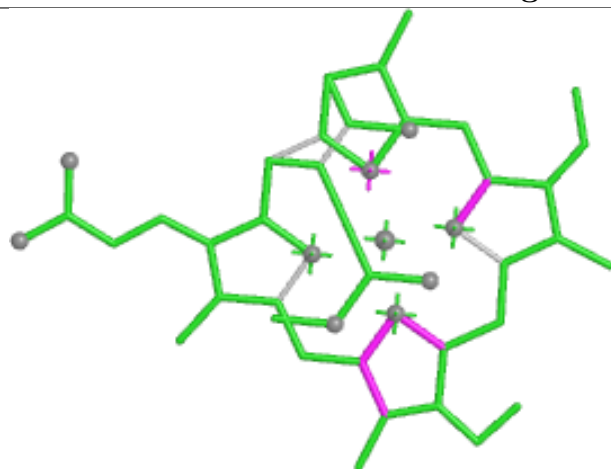


Torsions

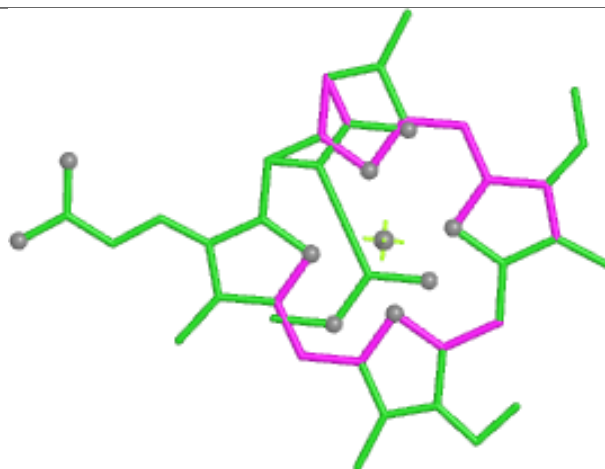


Rings

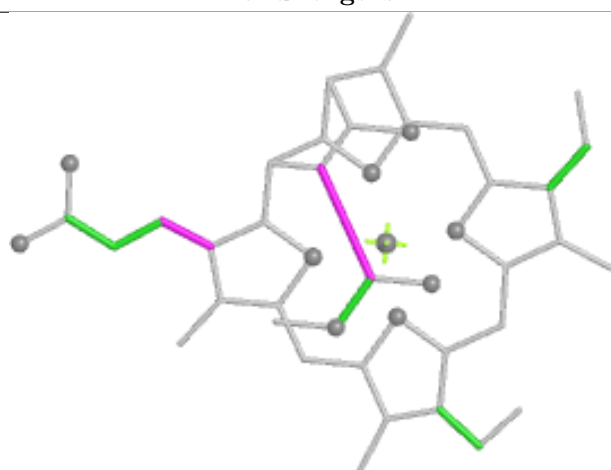
Ligand KC2 z 304



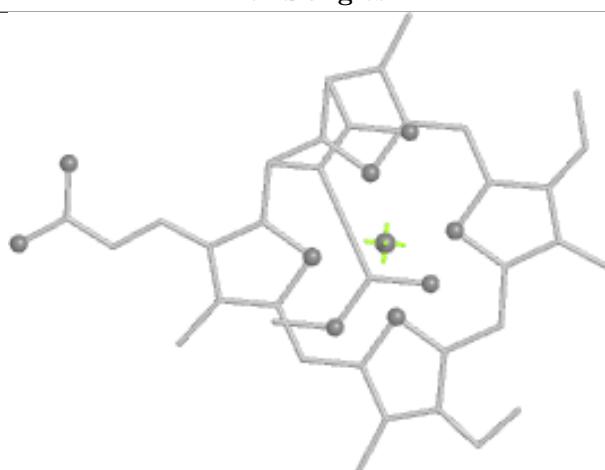
Bond lengths



Bond angles

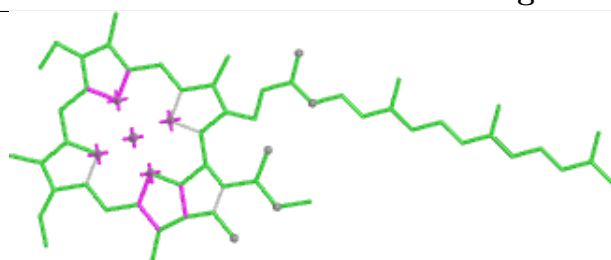


Torsions

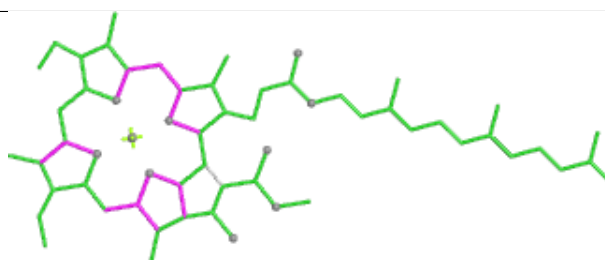


Rings

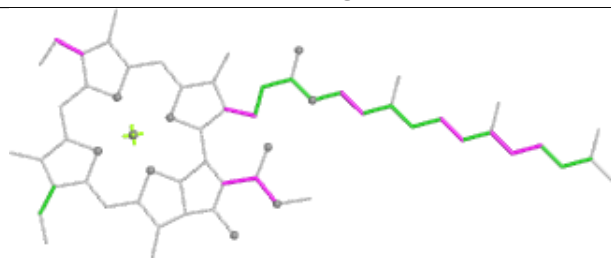
Ligand CLA b 833



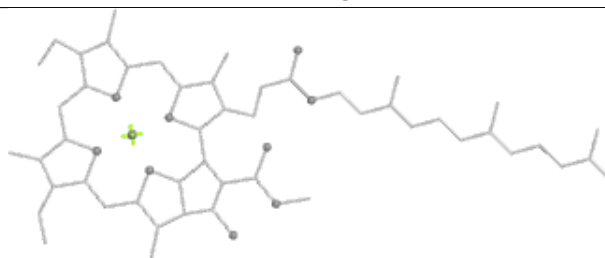
Bond lengths



Bond angles

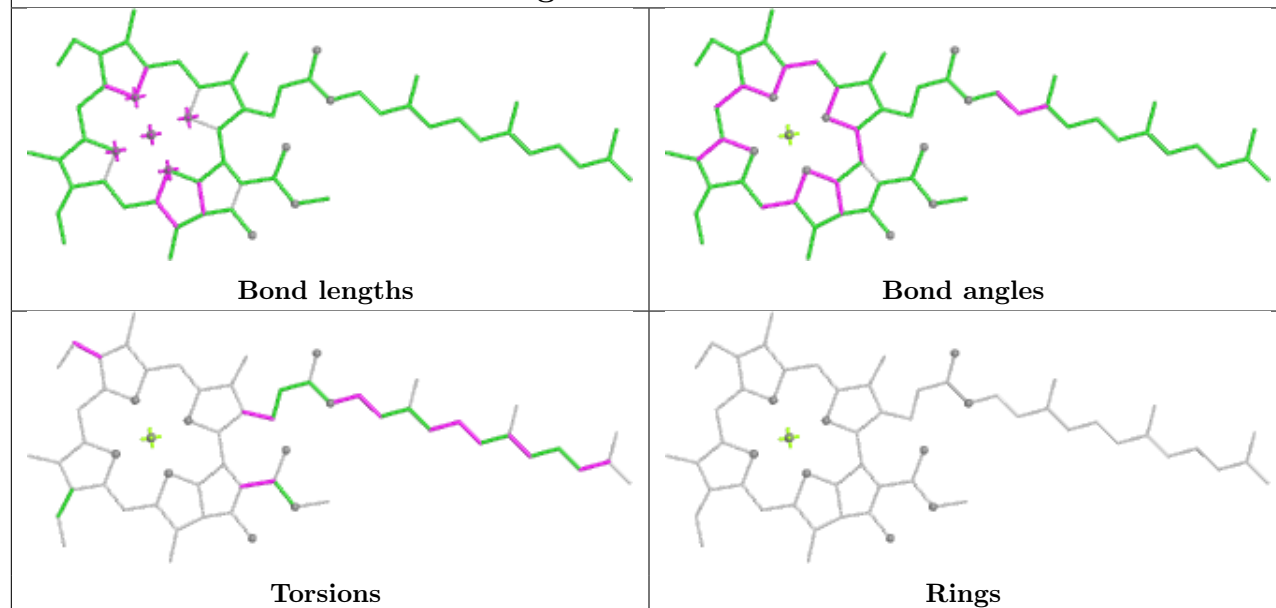


Torsions

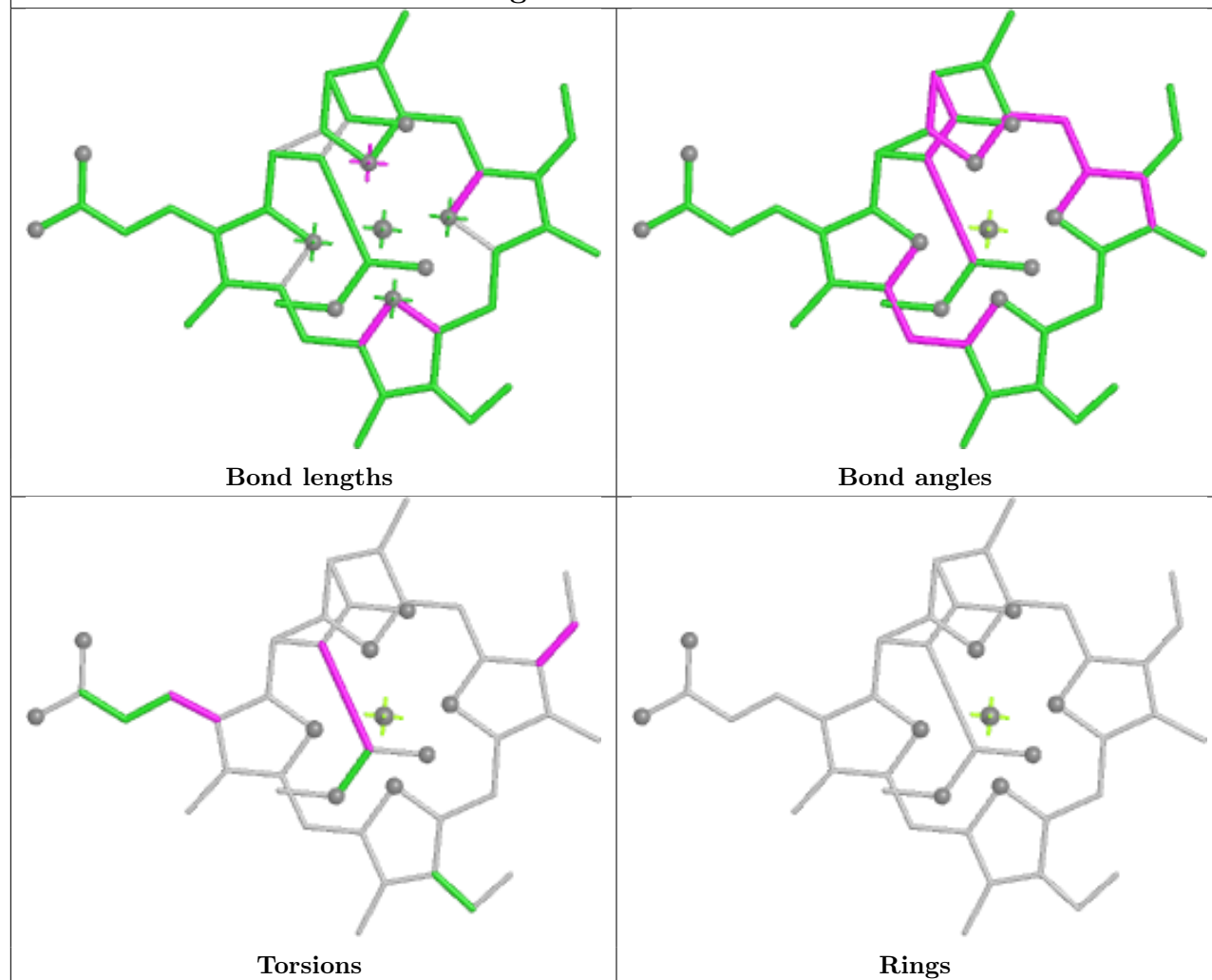


Rings

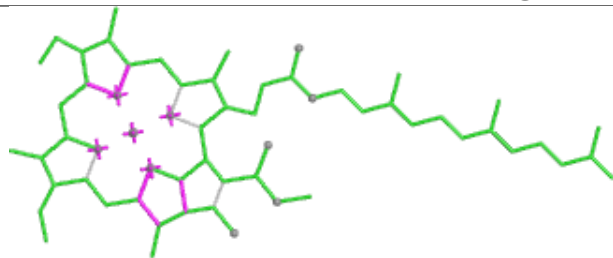
Ligand CLA z 312



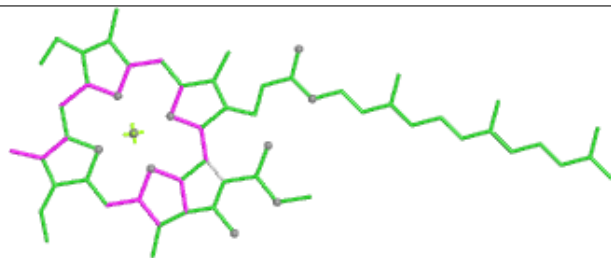
Ligand KC2 S 303



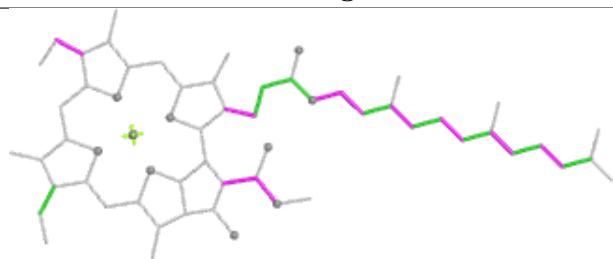
Ligand CLA Z 306



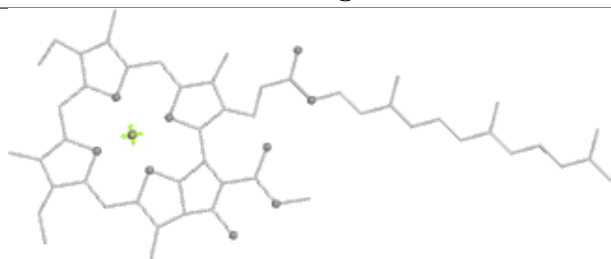
Bond lengths



Bond angles

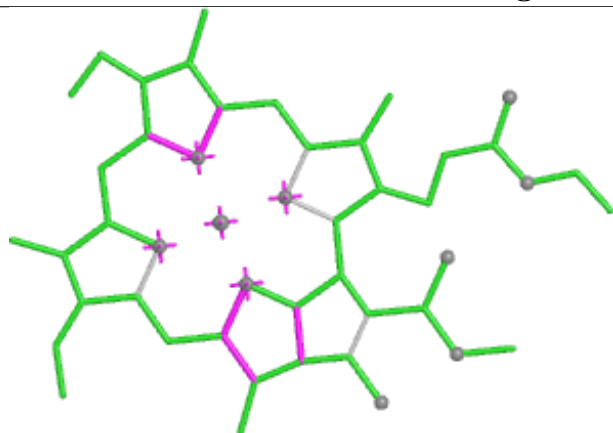


Torsions

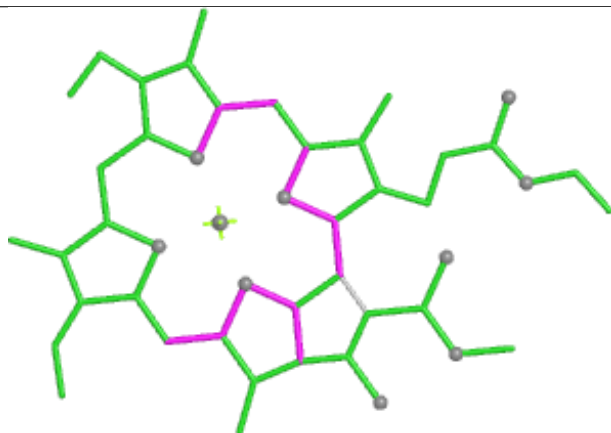


Rings

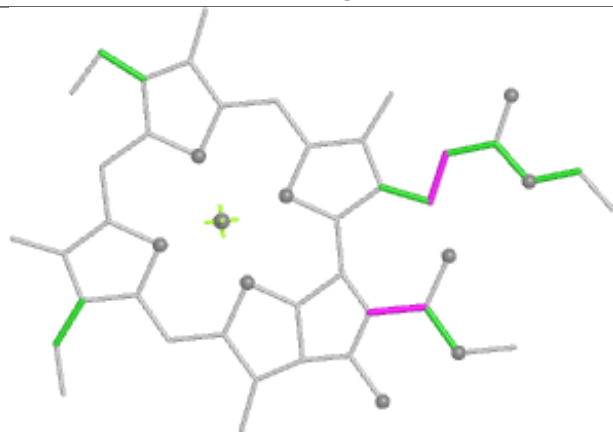
Ligand CLA E 313



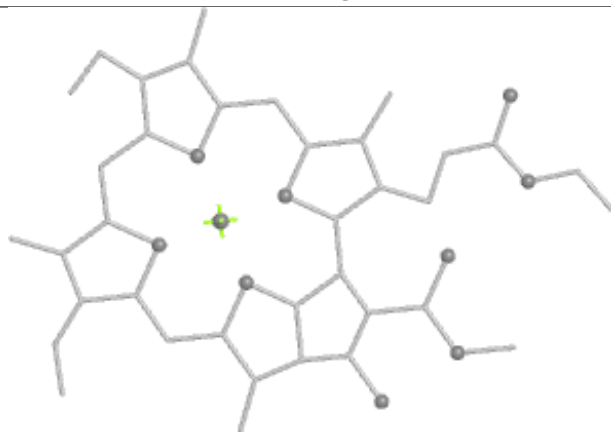
Bond lengths



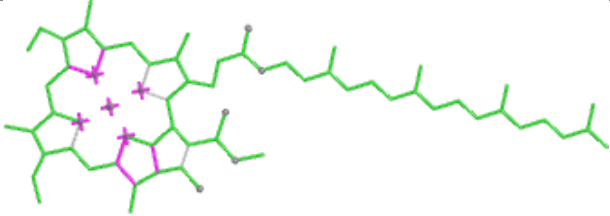
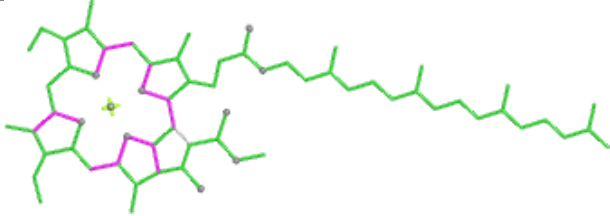
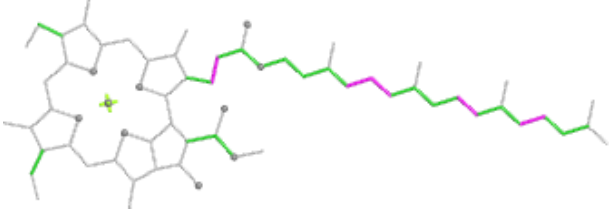
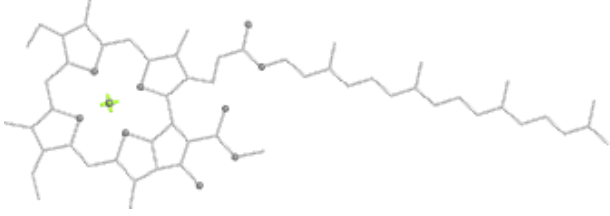
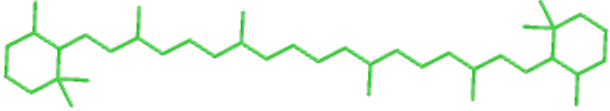
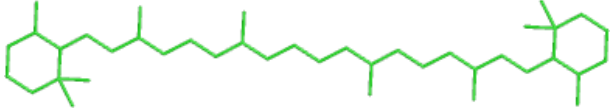
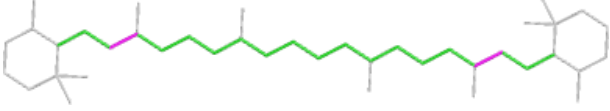
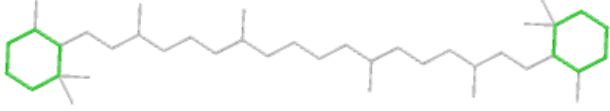
Bond angles



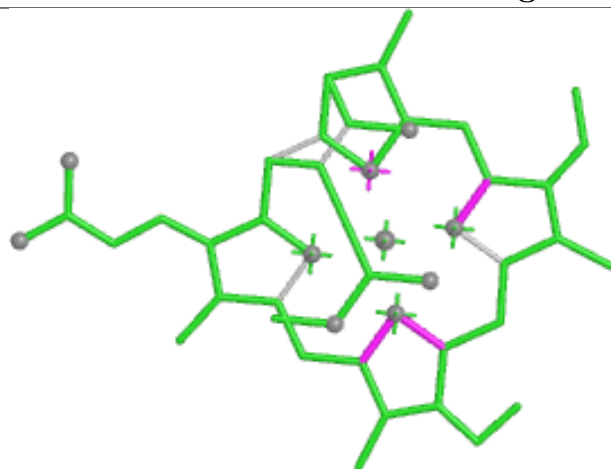
Torsions



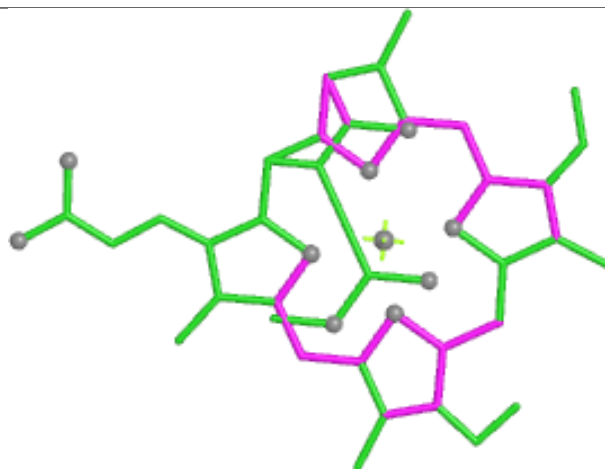
Rings

Ligand CLA a 825	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

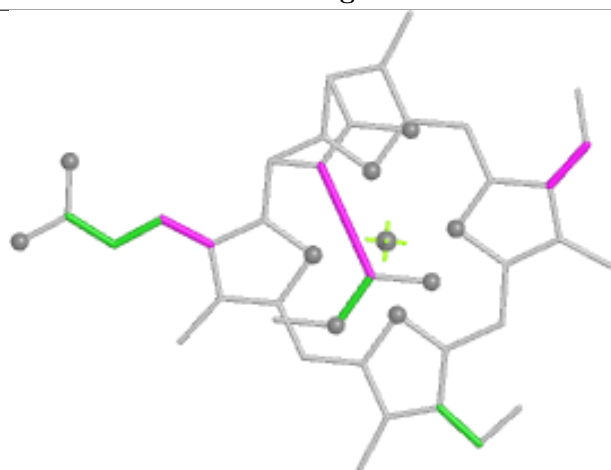
Ligand KC2 L 302



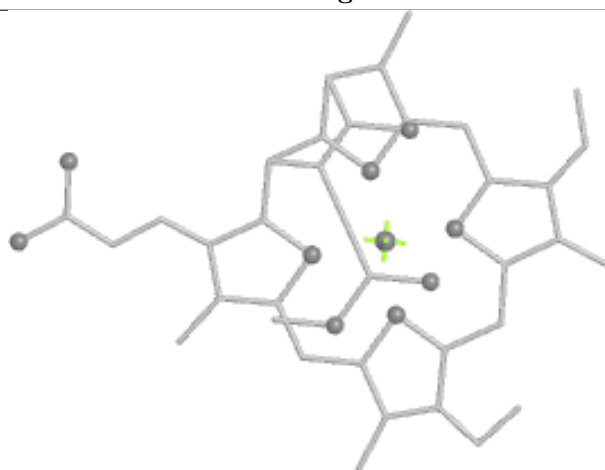
Bond lengths



Bond angles

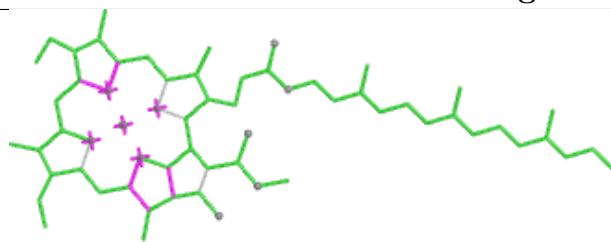


Torsions

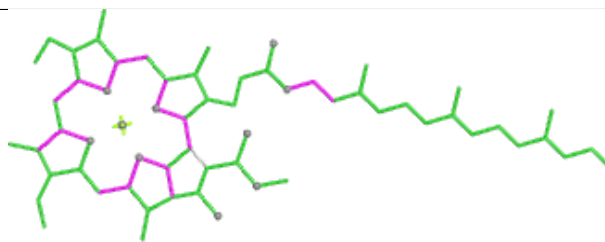


Rings

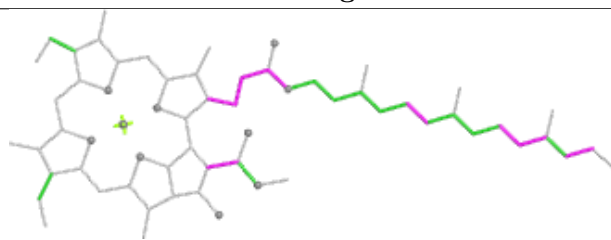
Ligand CLA a 824



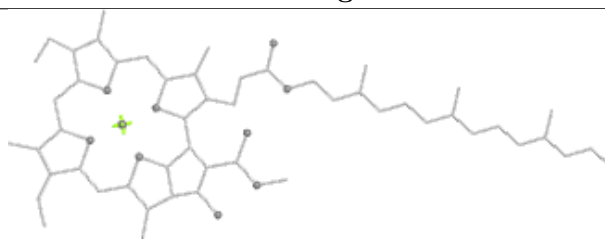
Bond lengths



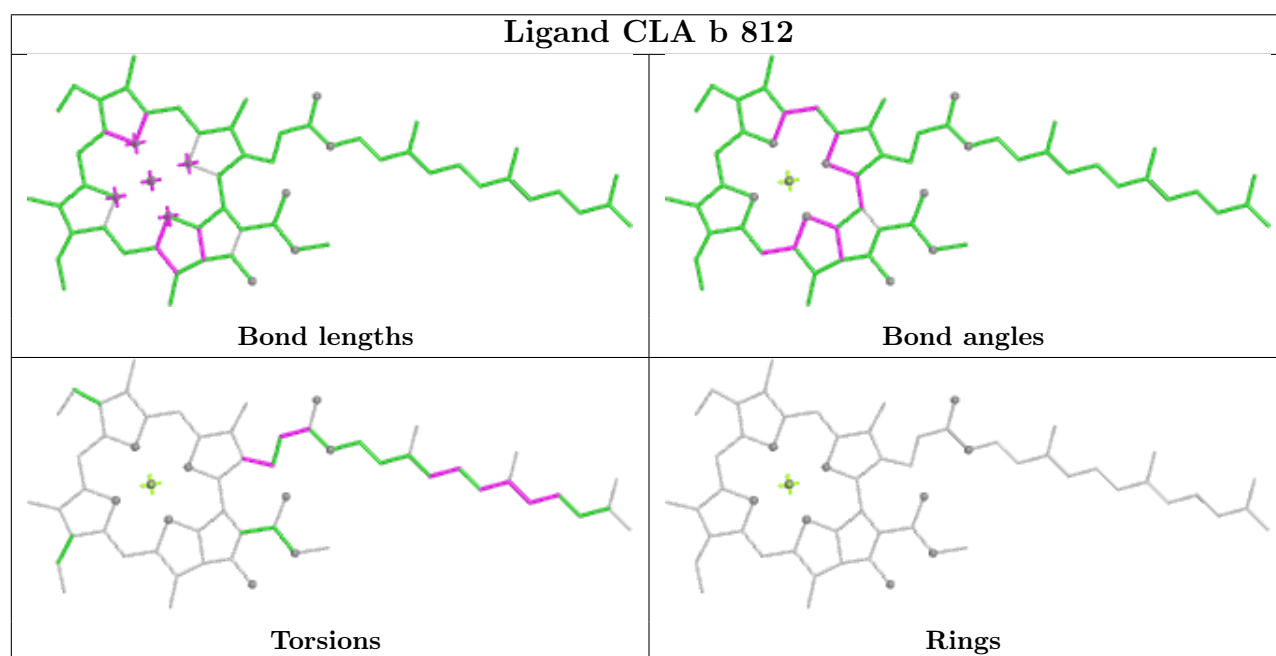
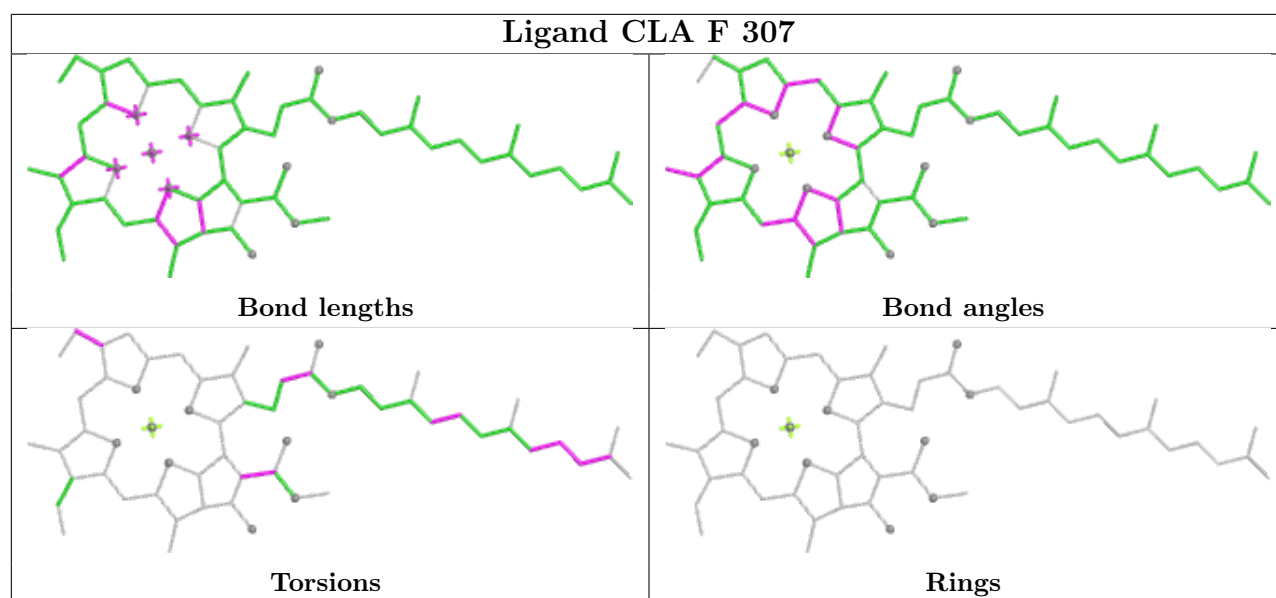
Bond angles



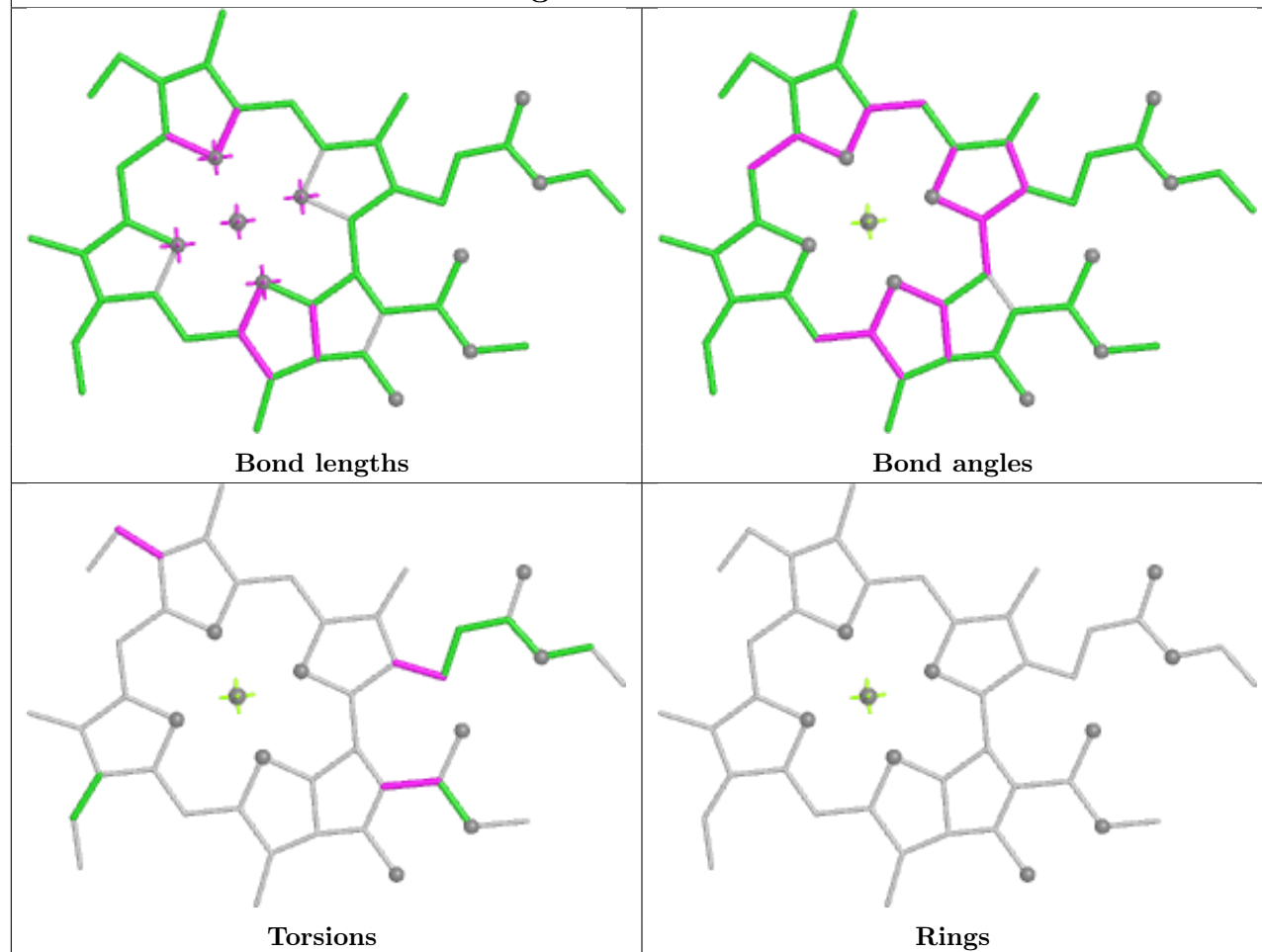
Torsions



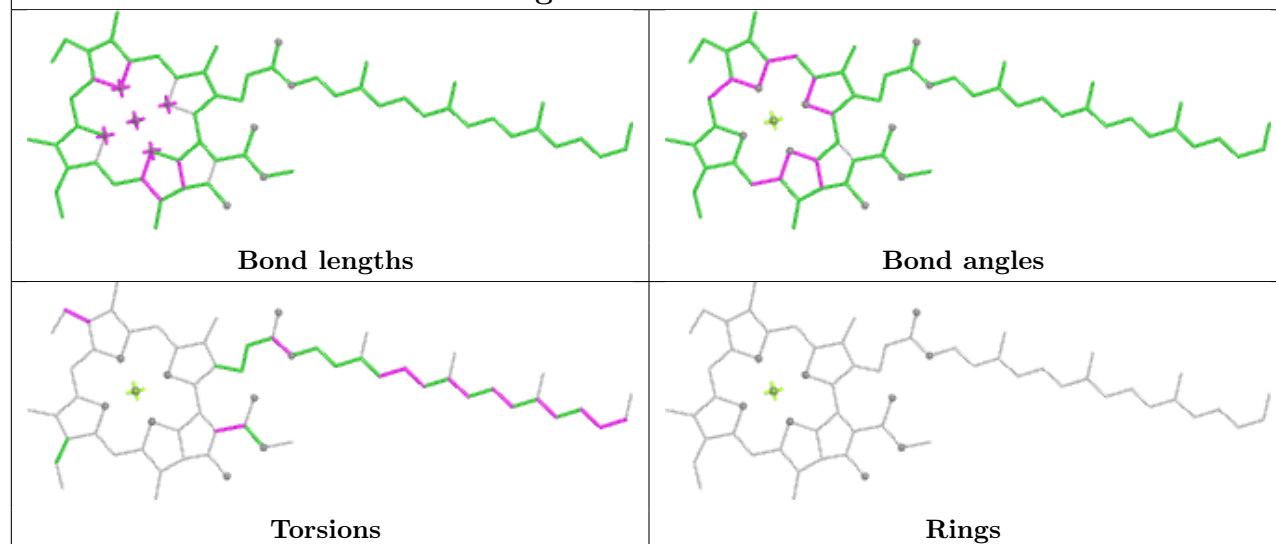
Rings

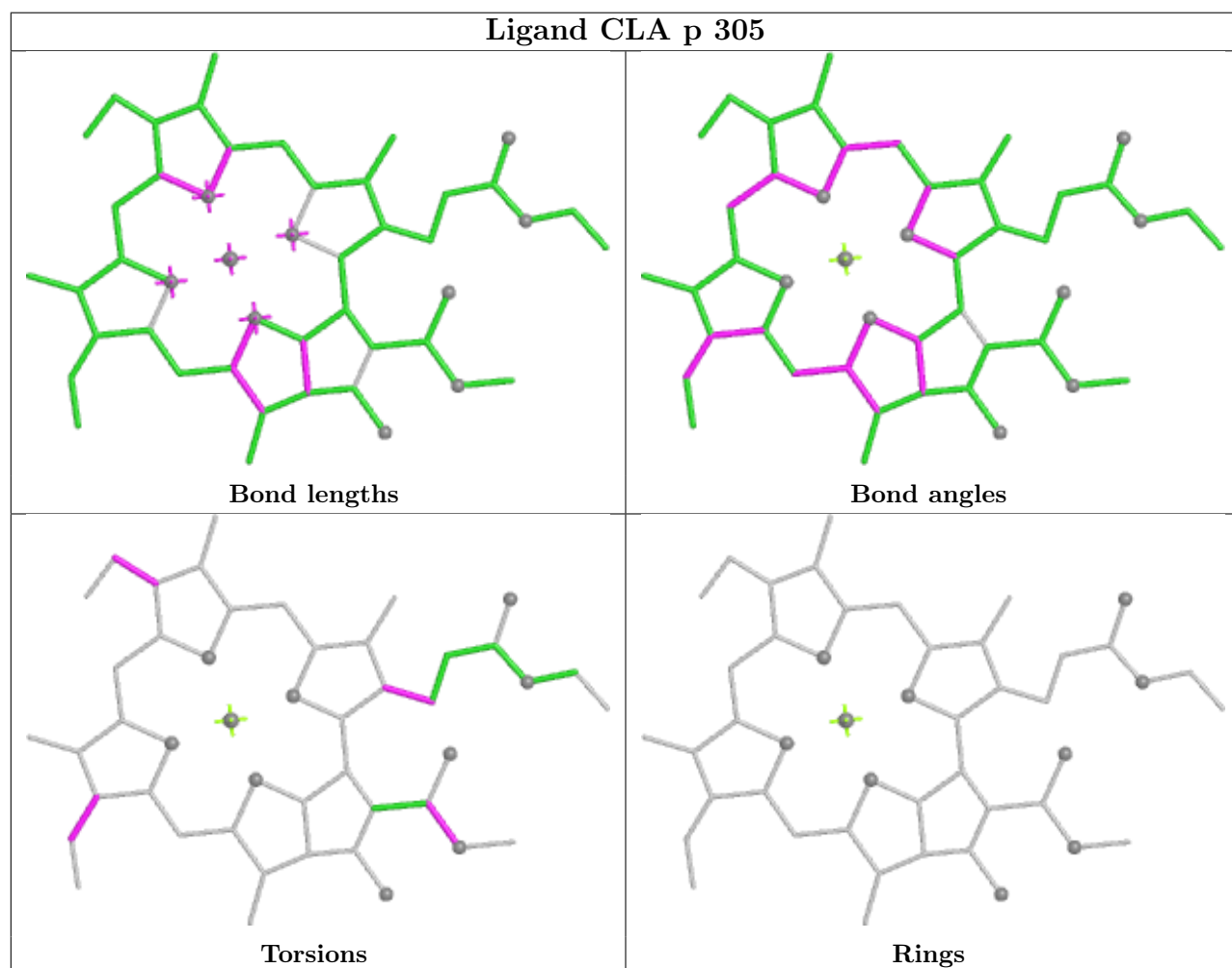
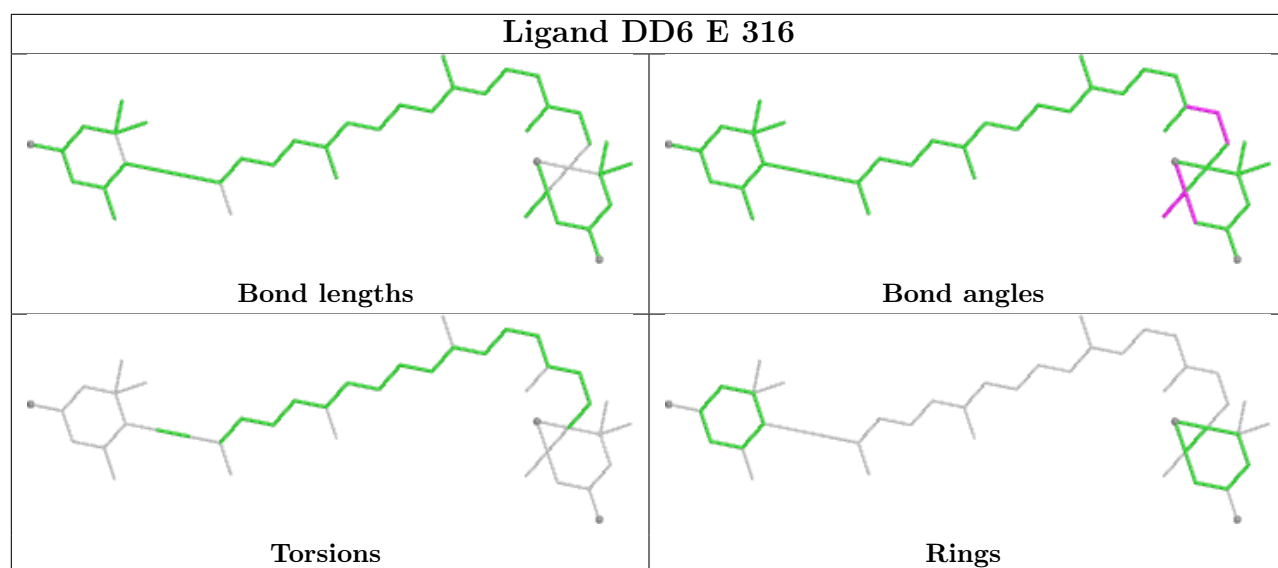


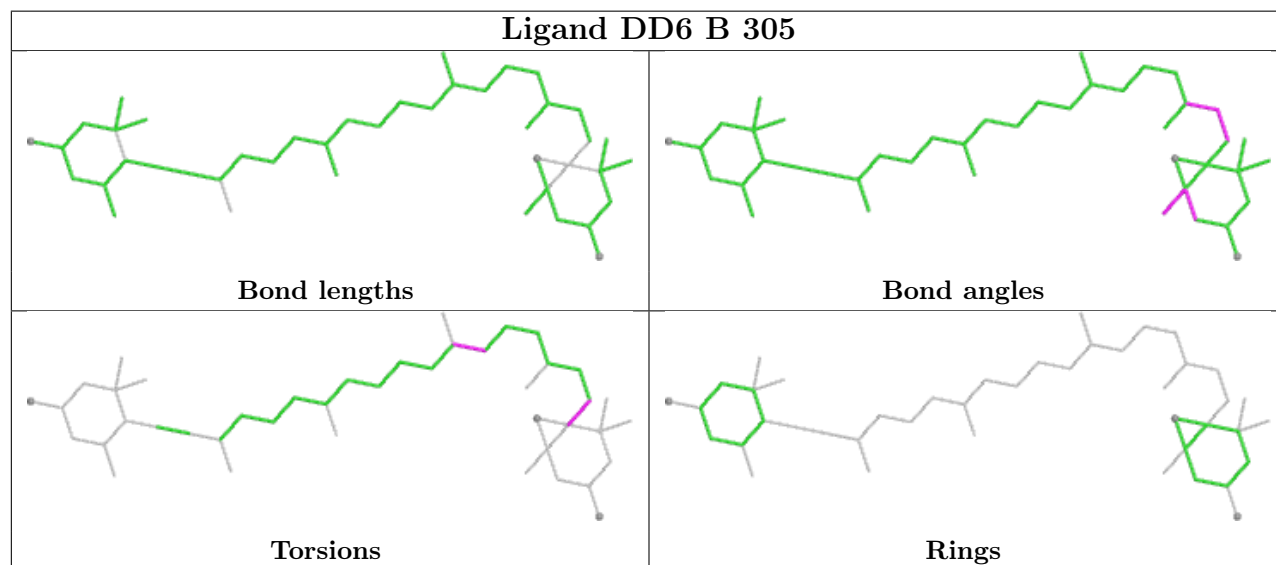
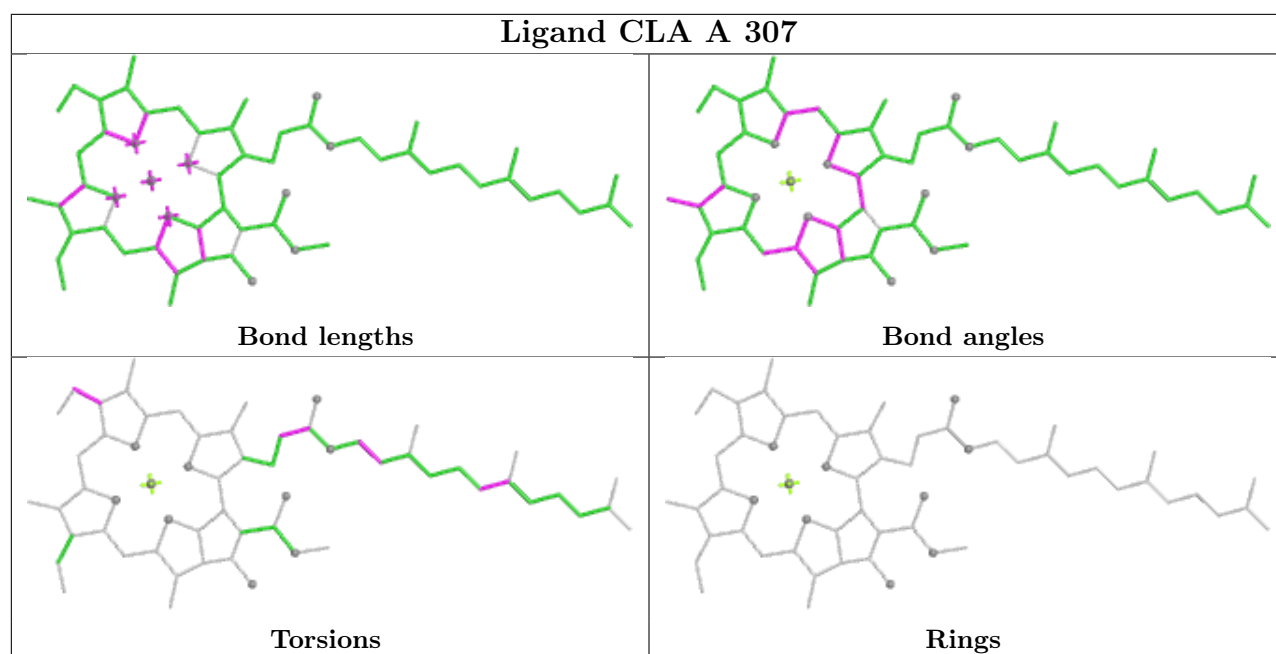
Ligand CLA z 313



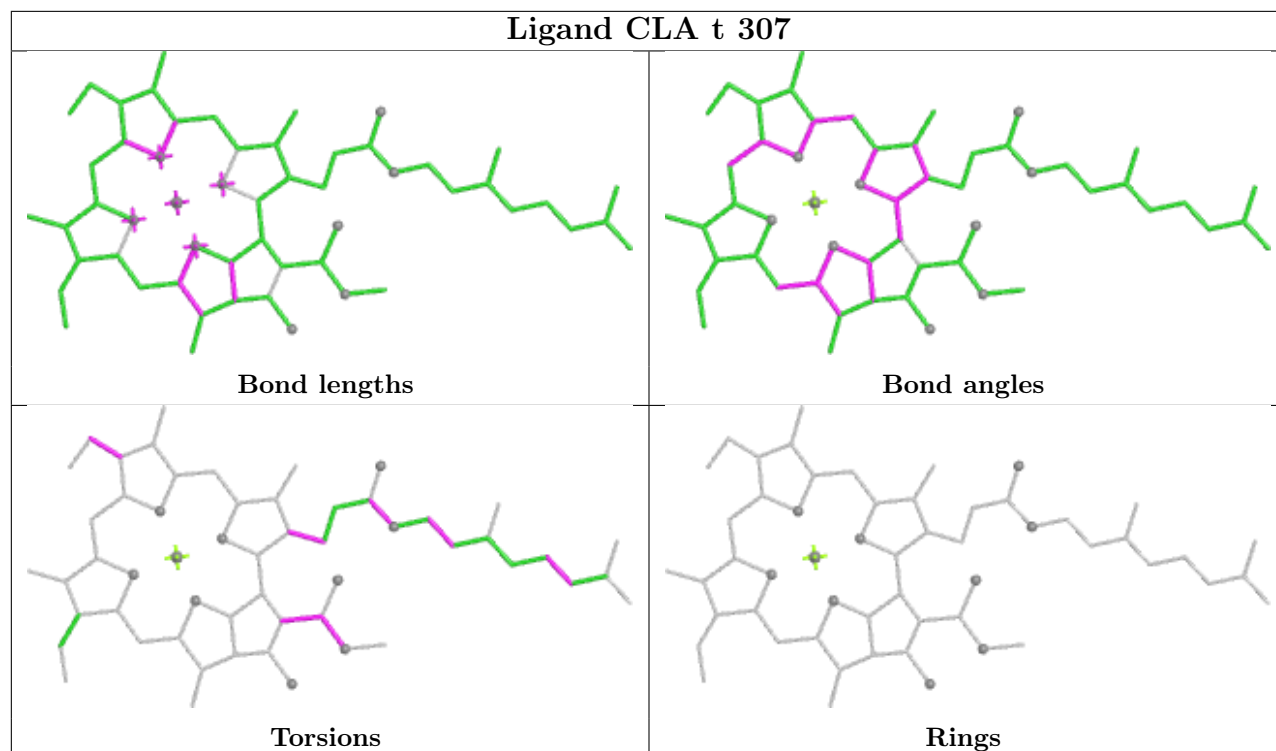
Ligand CLA b 819



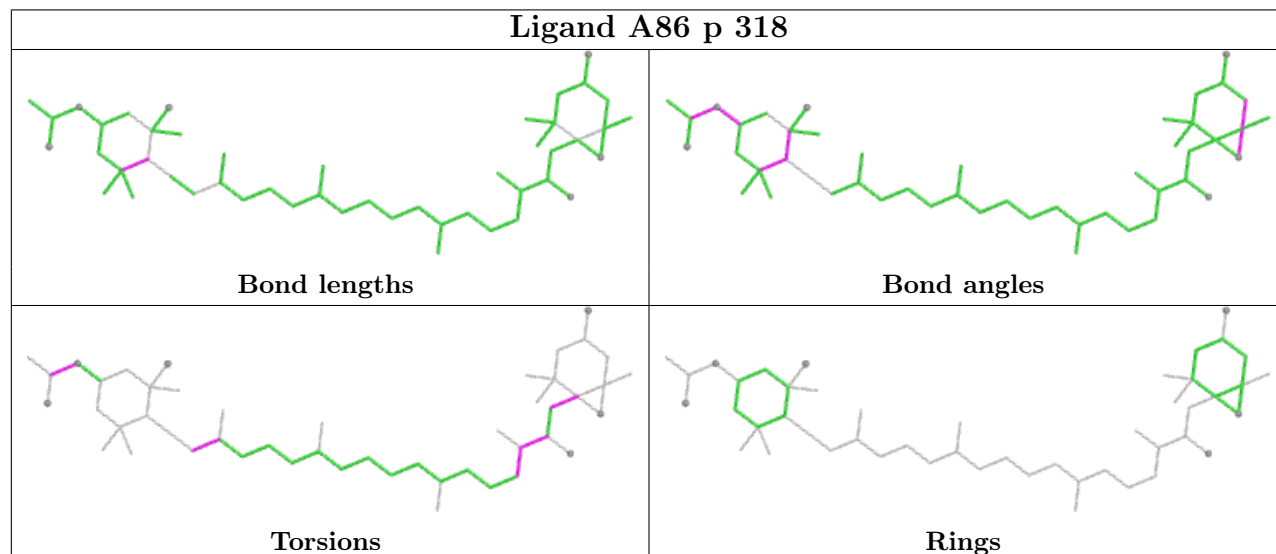




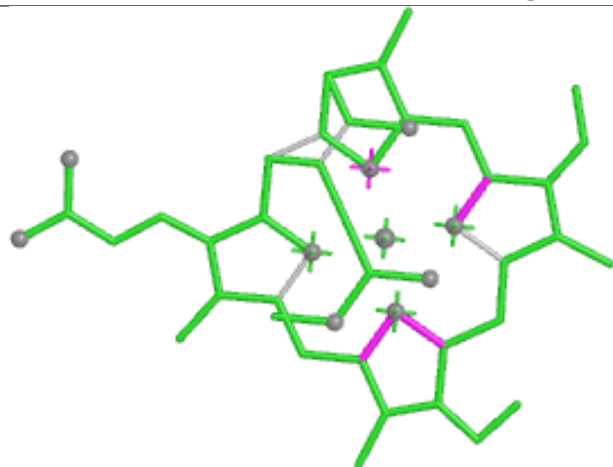
Ligand CLA t 307



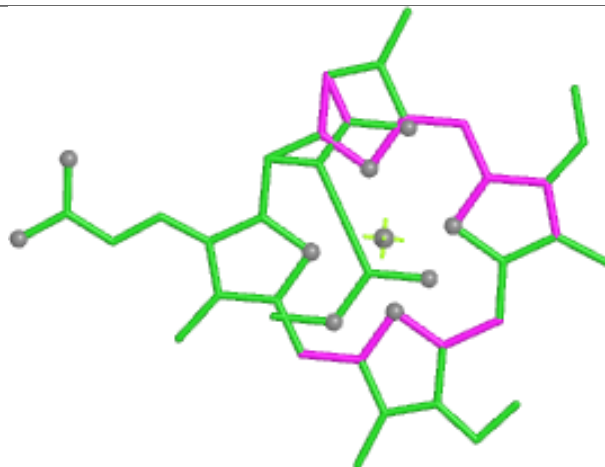
Ligand A86 p 318



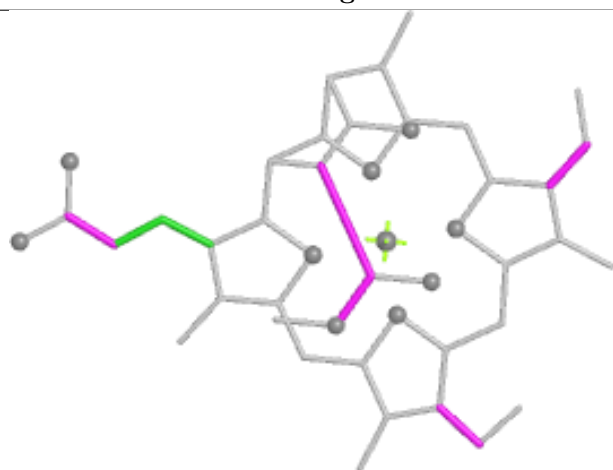
Ligand KC2 t 306



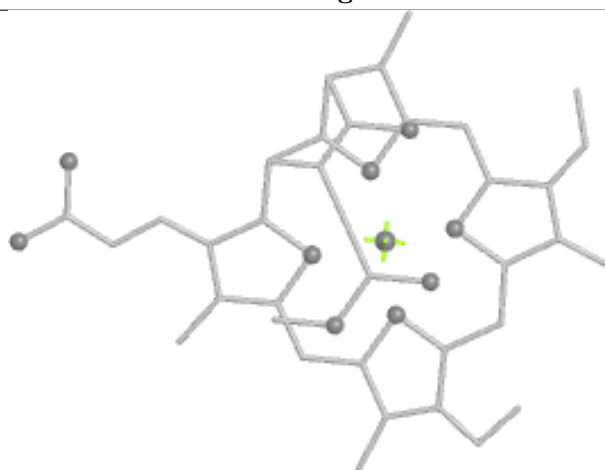
Bond lengths



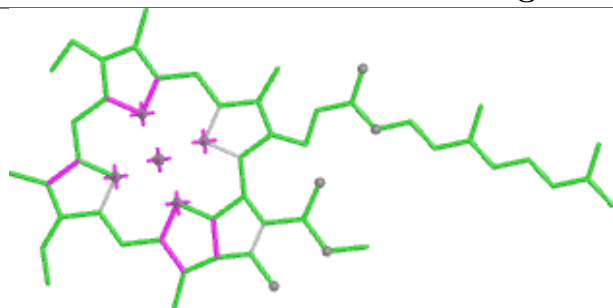
Bond angles



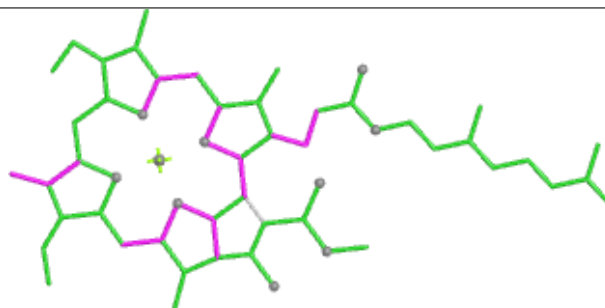
Torsions



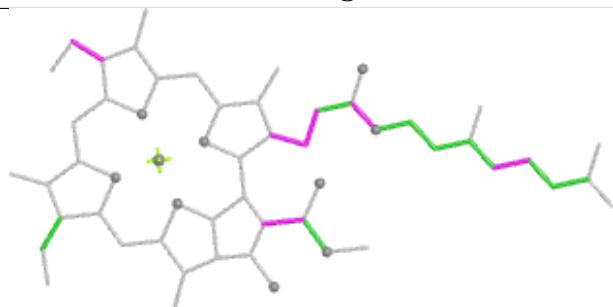
Rings

Ligand CLA J 308

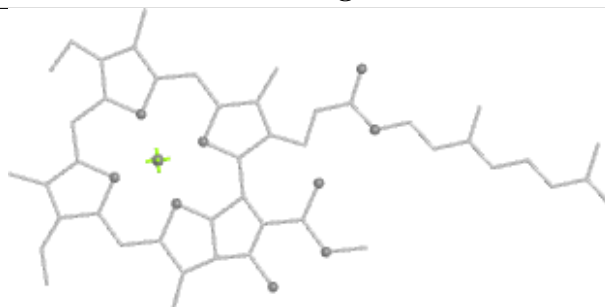
Bond lengths



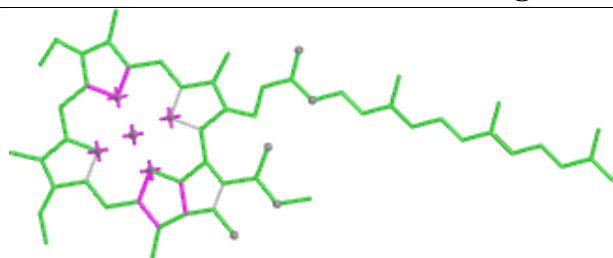
Bond angles



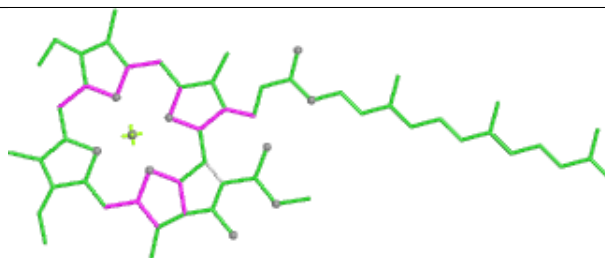
Torsions



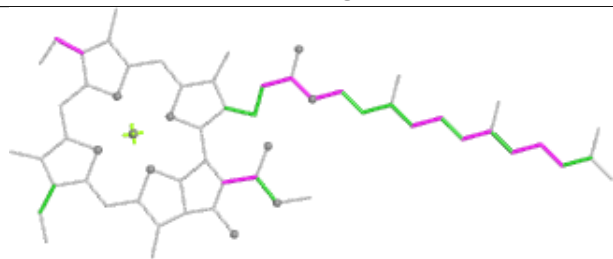
Rings

Ligand CLA N 311

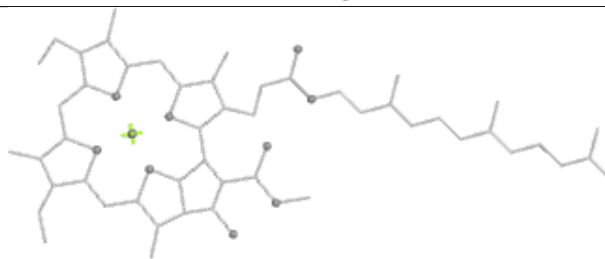
Bond lengths



Bond angles

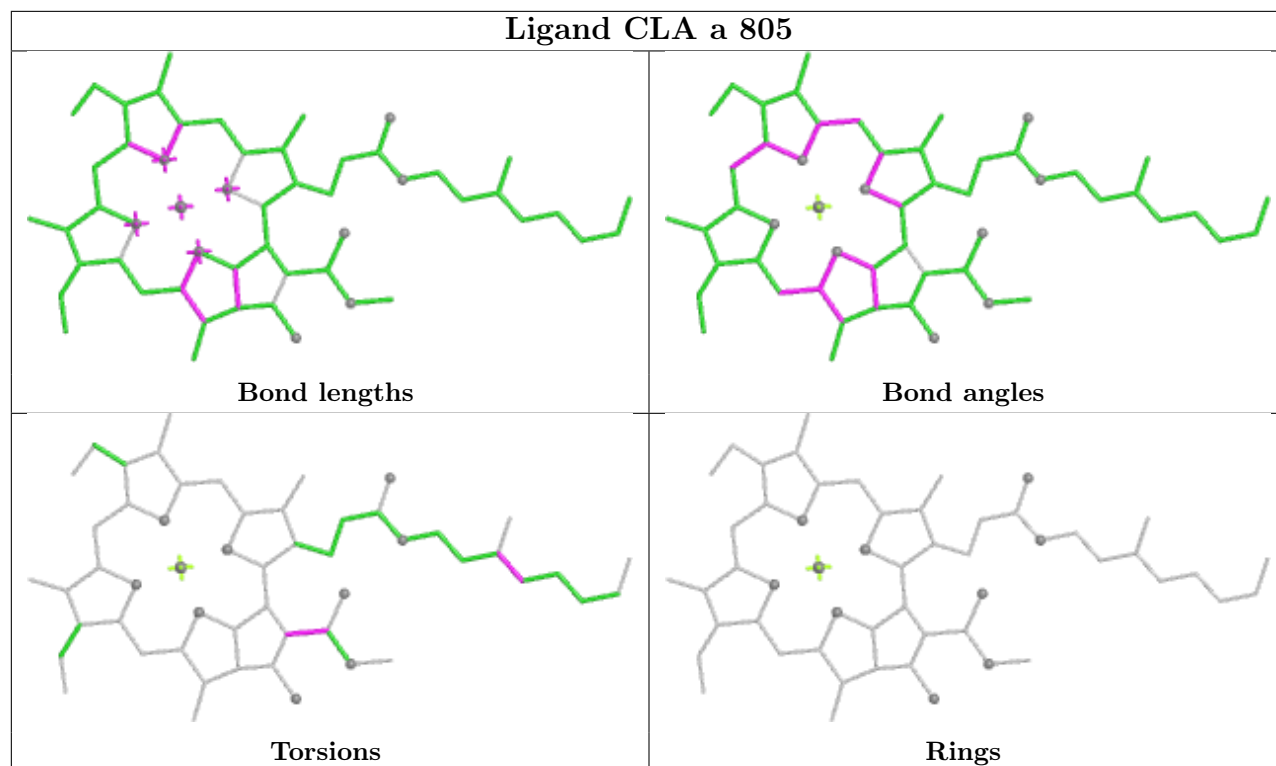


Torsions

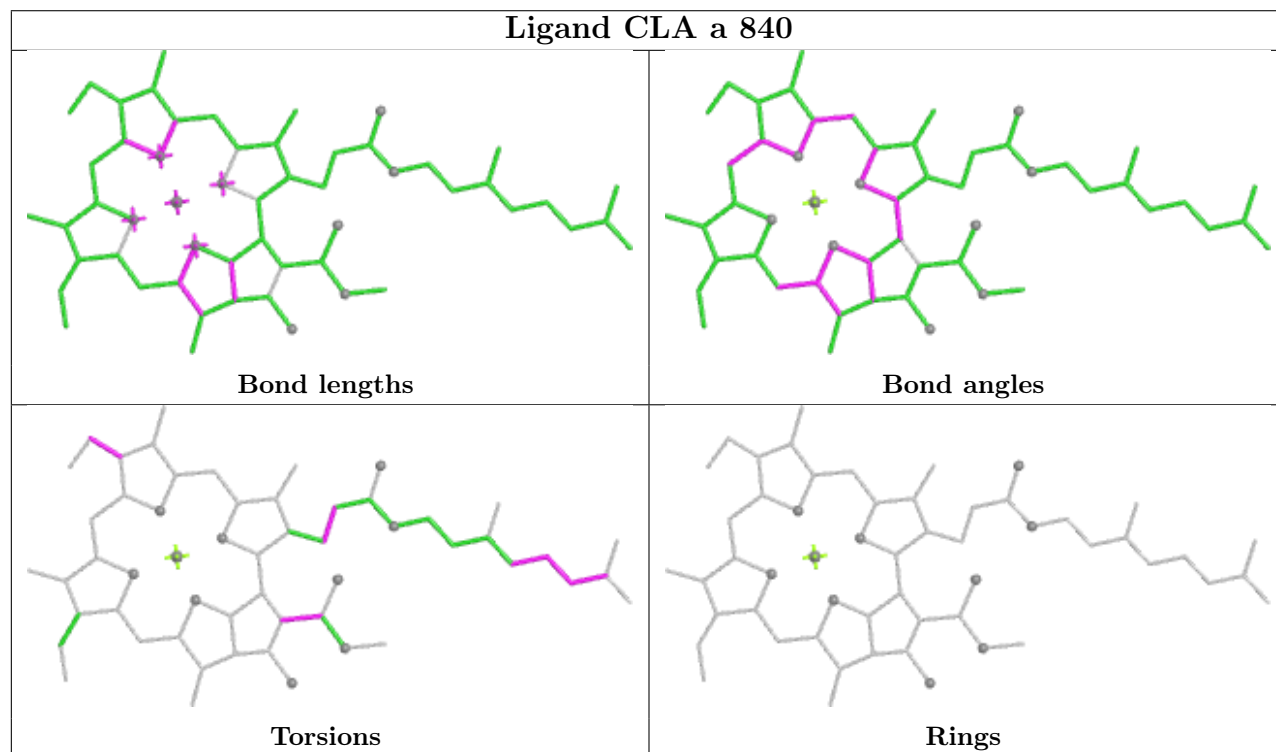


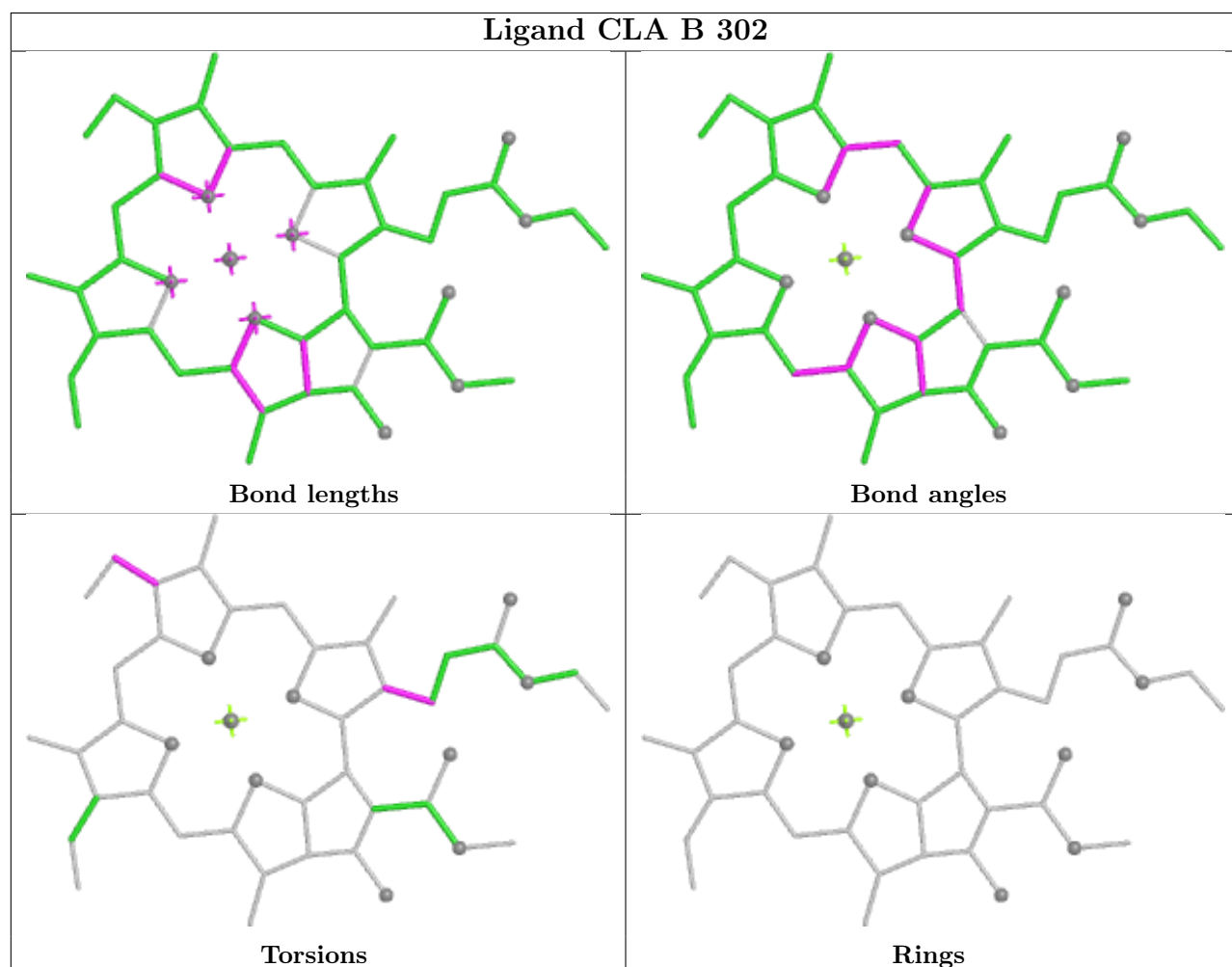
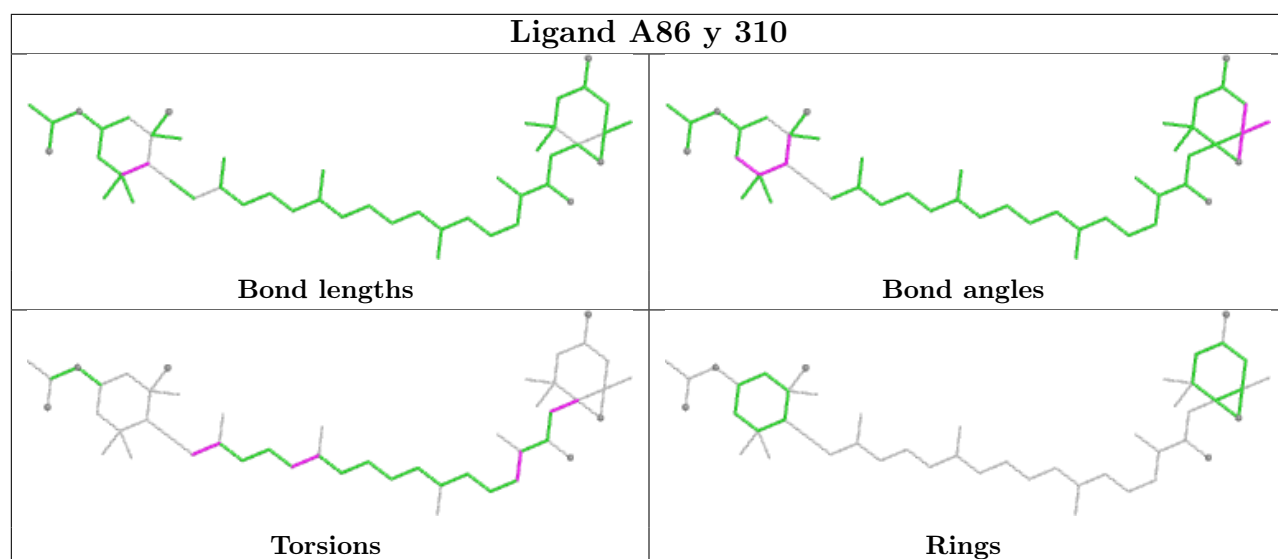
Rings

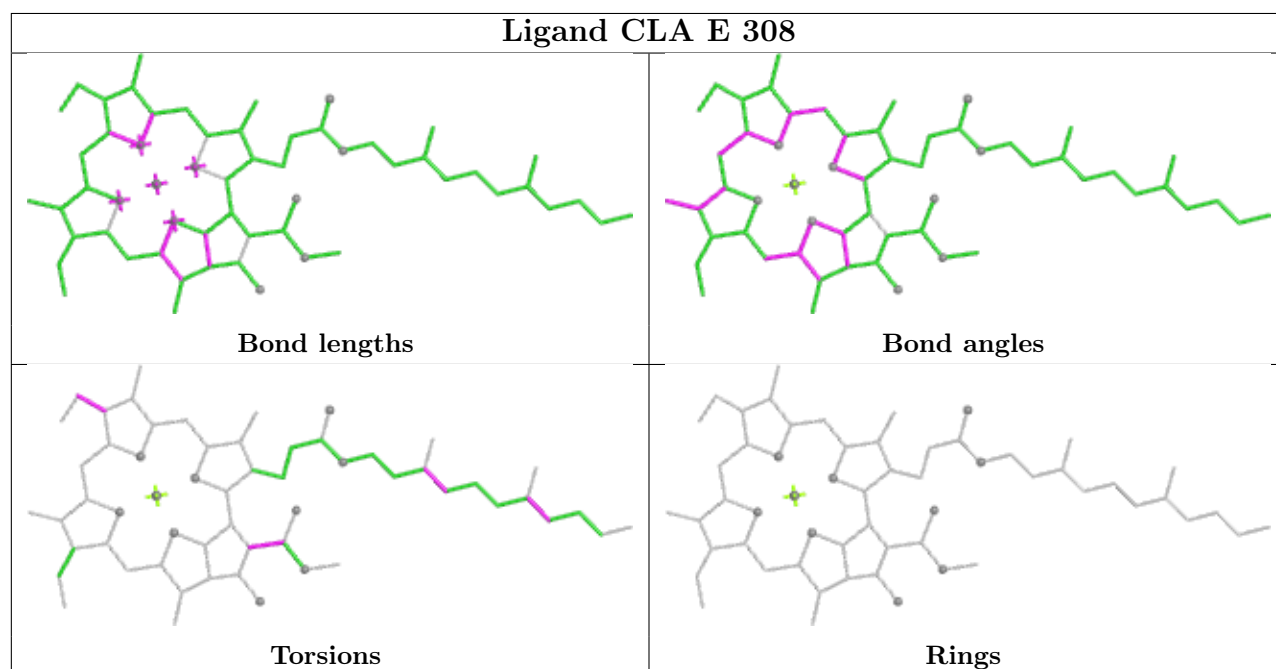
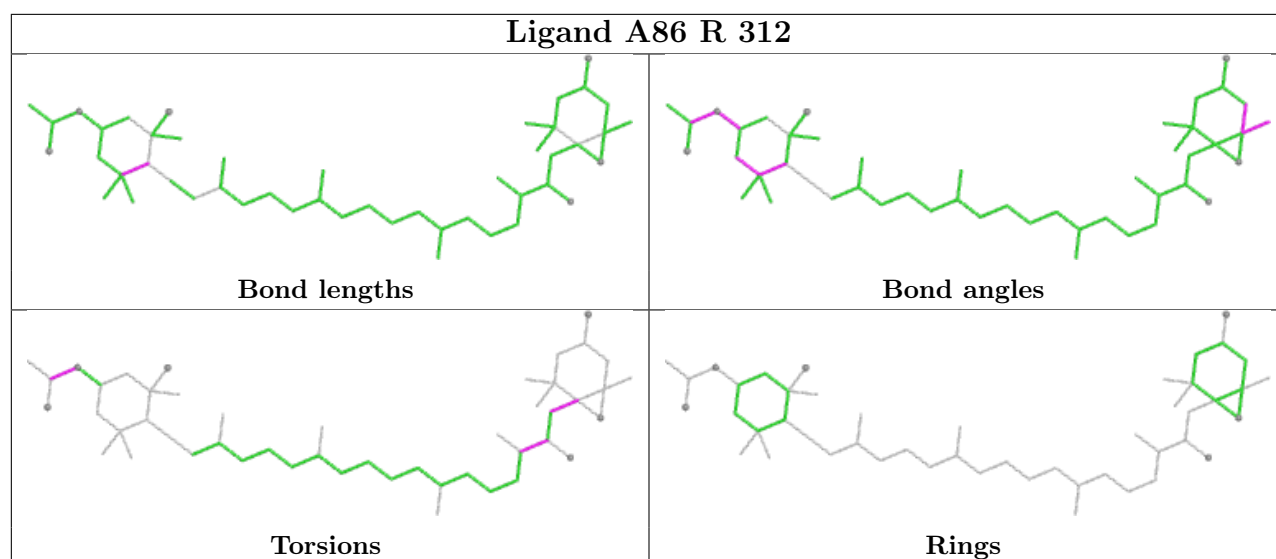
Ligand CLA a 805

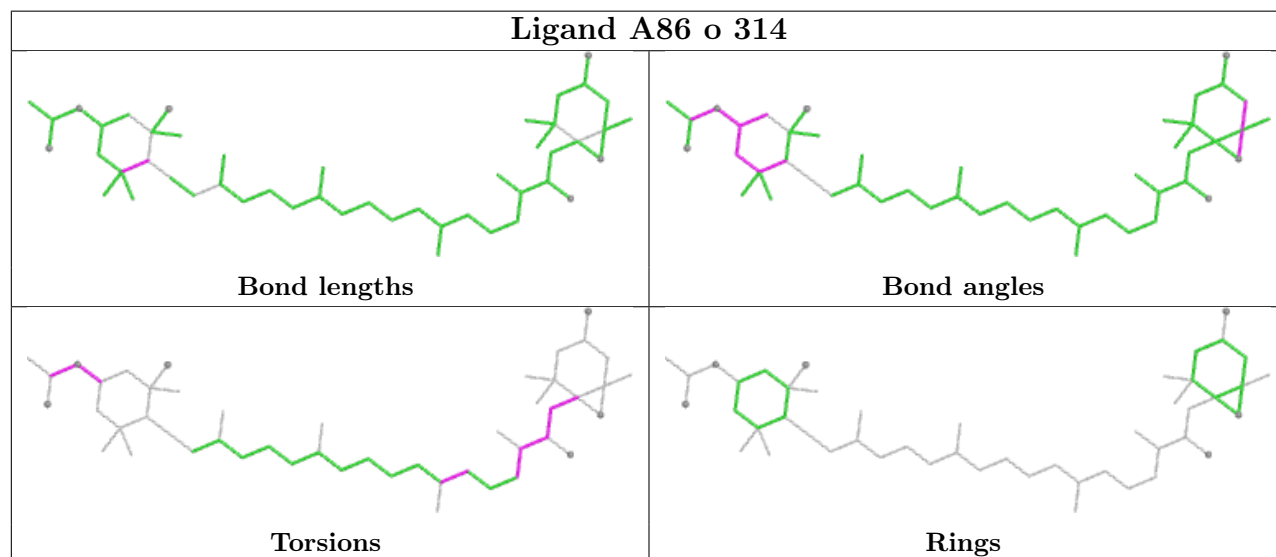
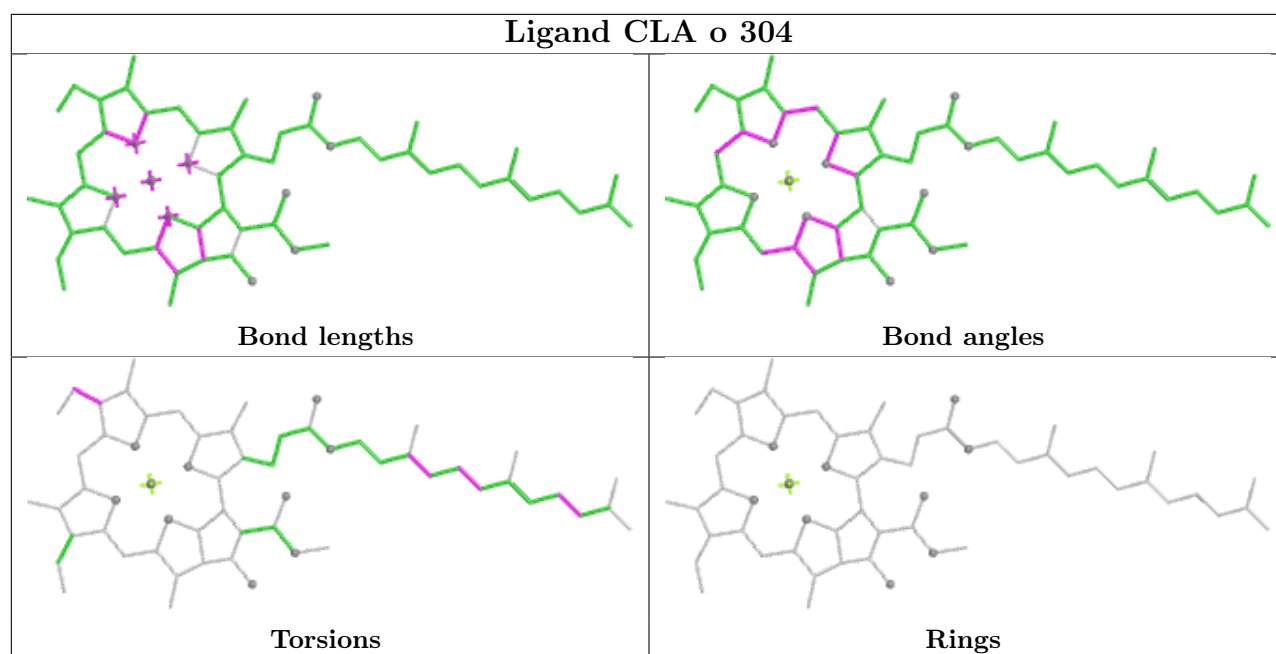


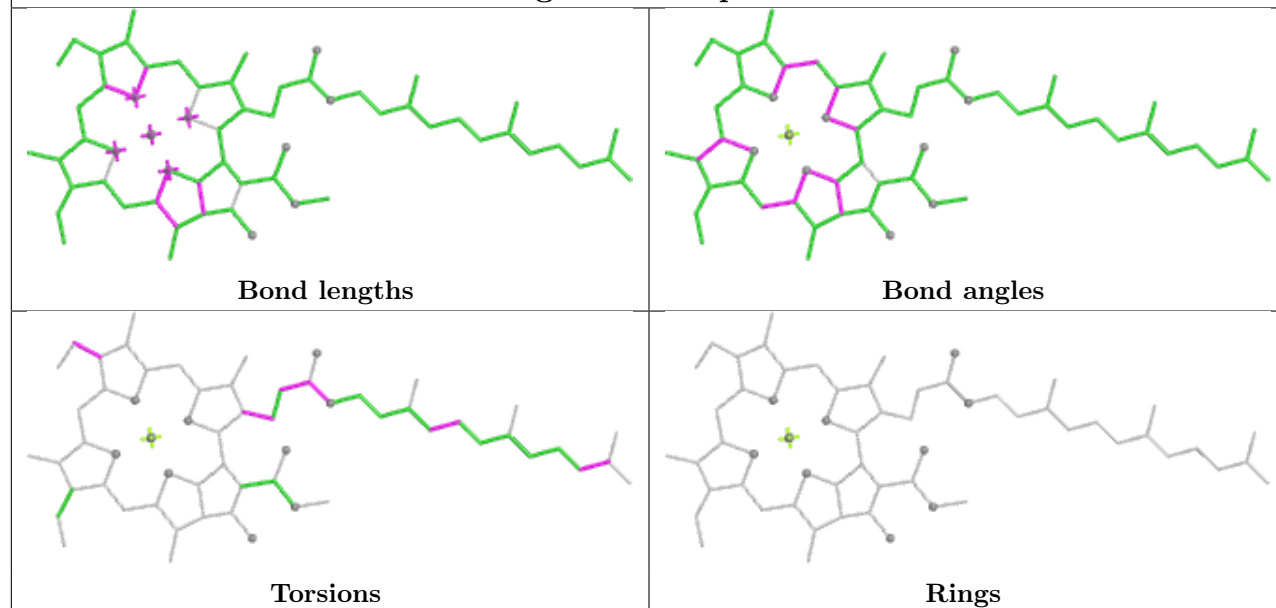
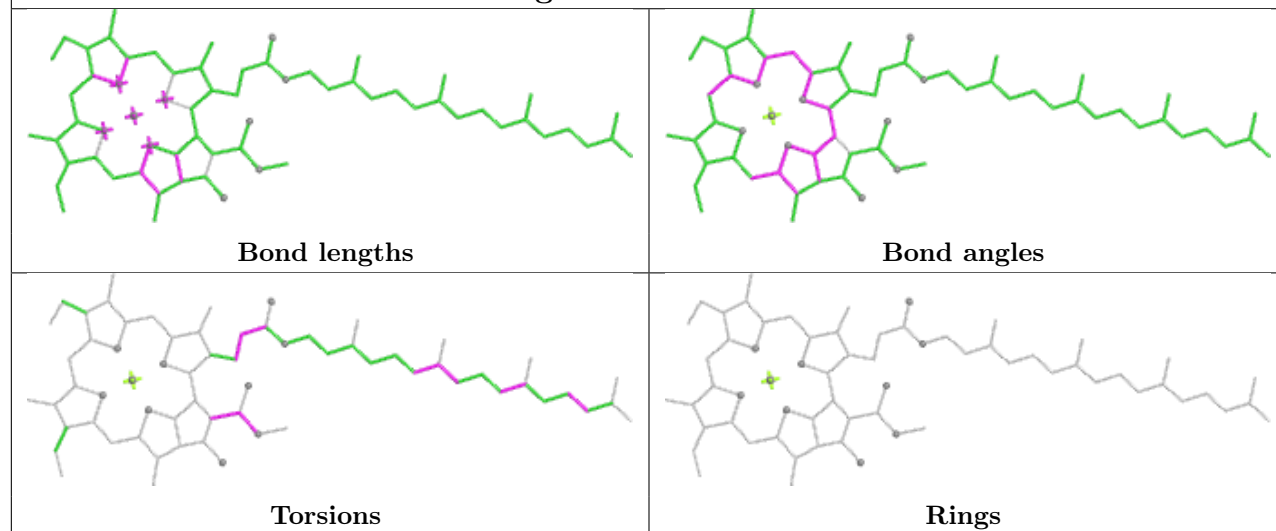
Ligand CLA a 840



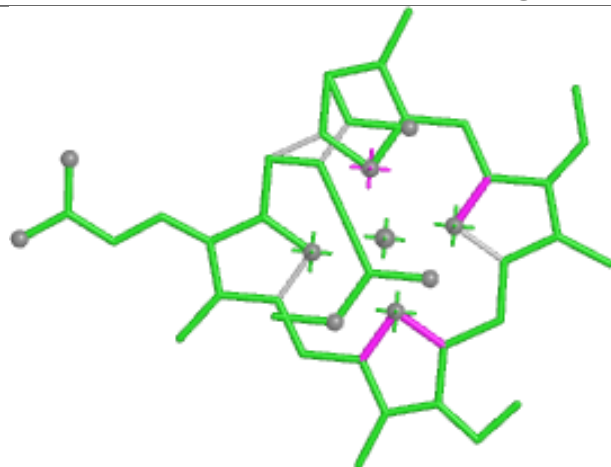




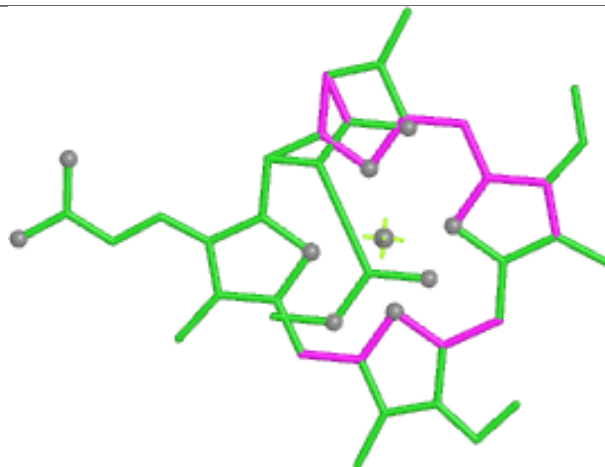


Ligand CLA q 312**Ligand CLA b 808**

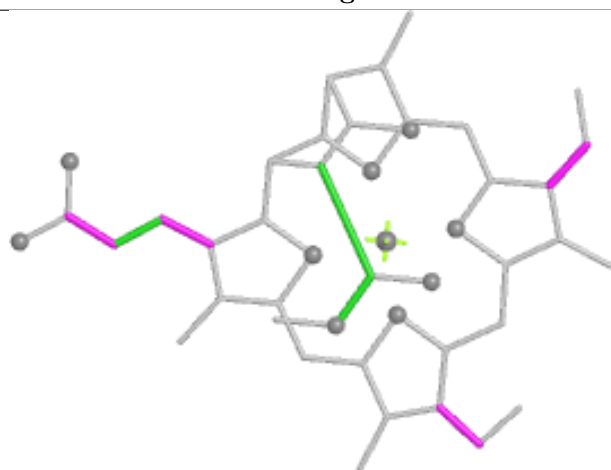
Ligand KC2 N 308



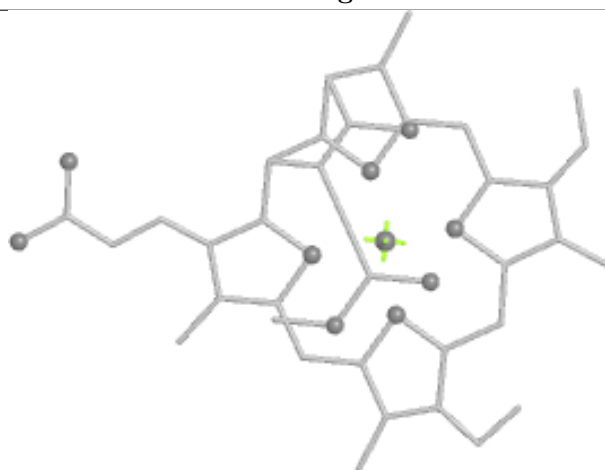
Bond lengths



Bond angles

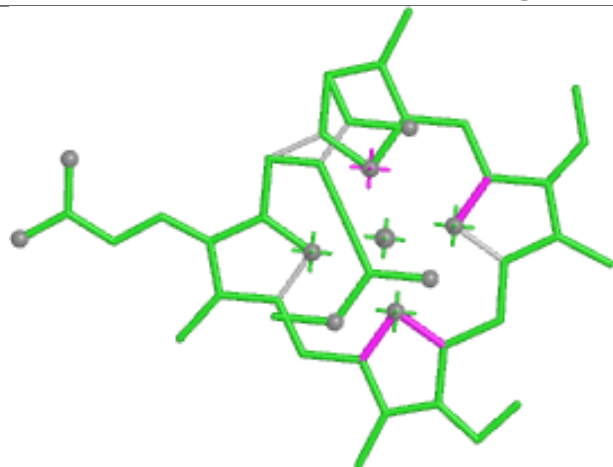


Torsions

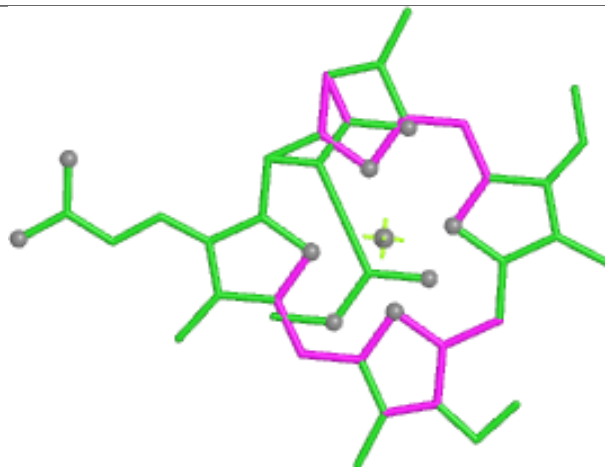


Rings

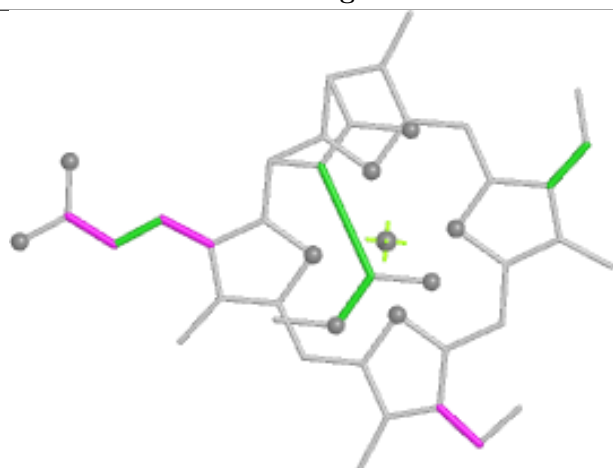
Ligand KC2 O 303



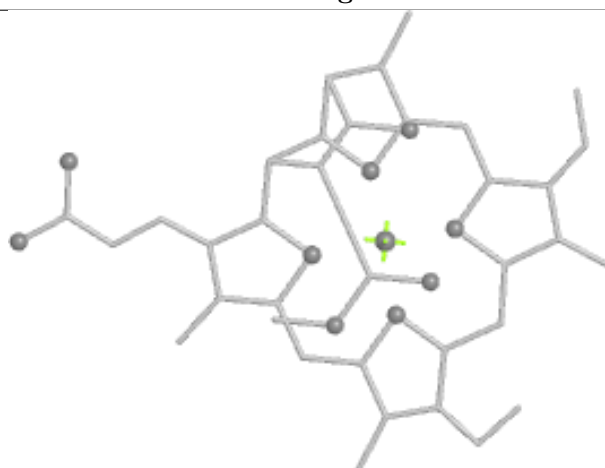
Bond lengths



Bond angles



Torsions



Rings

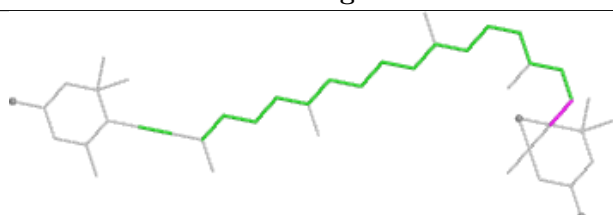
Ligand DD6 N 319



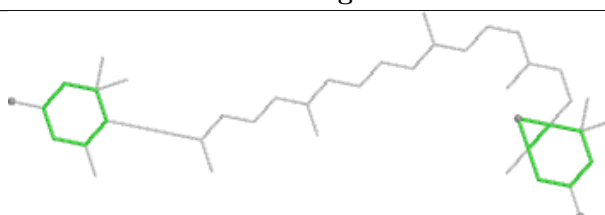
Bond lengths



Bond angles

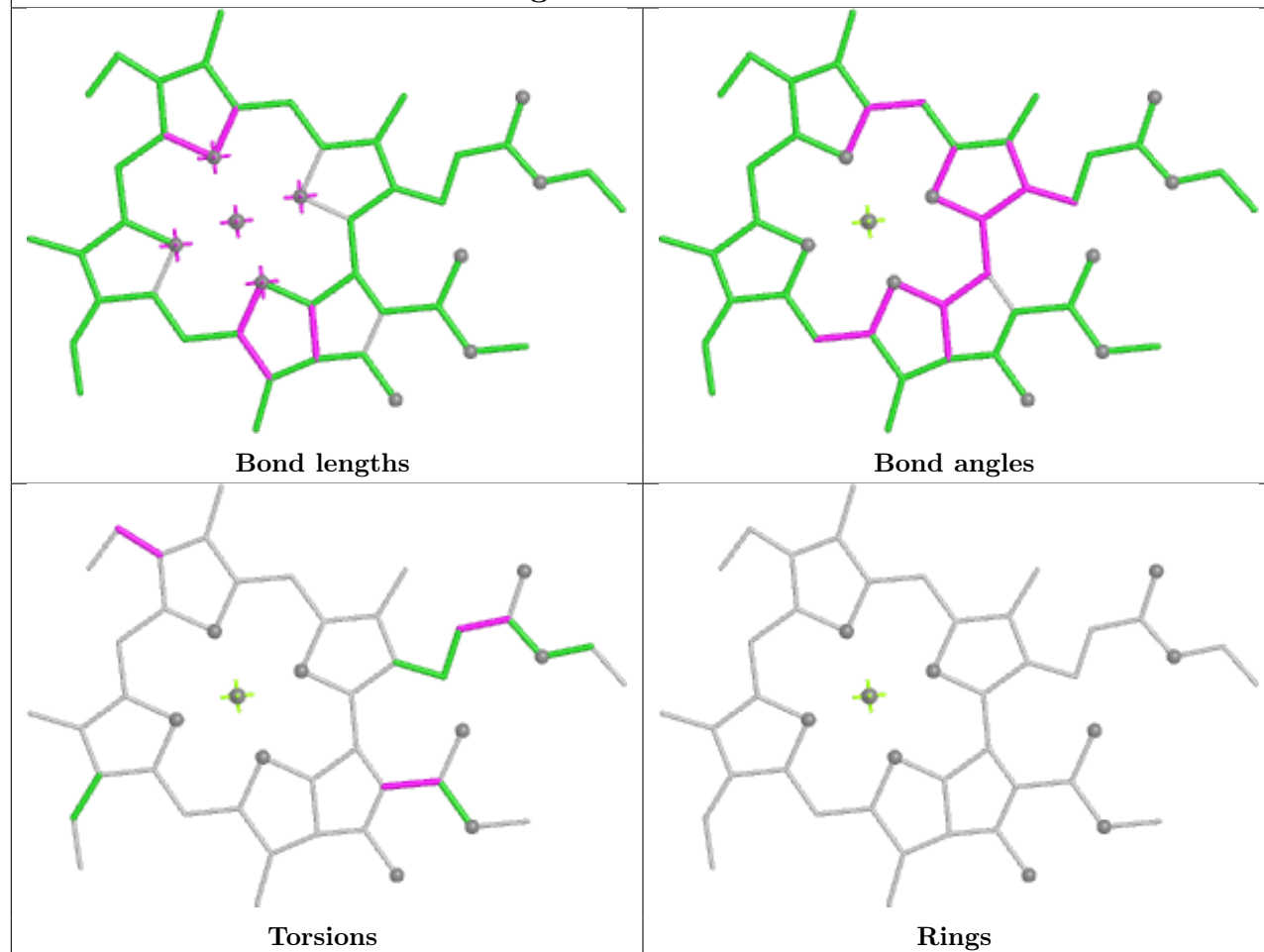


Torsions

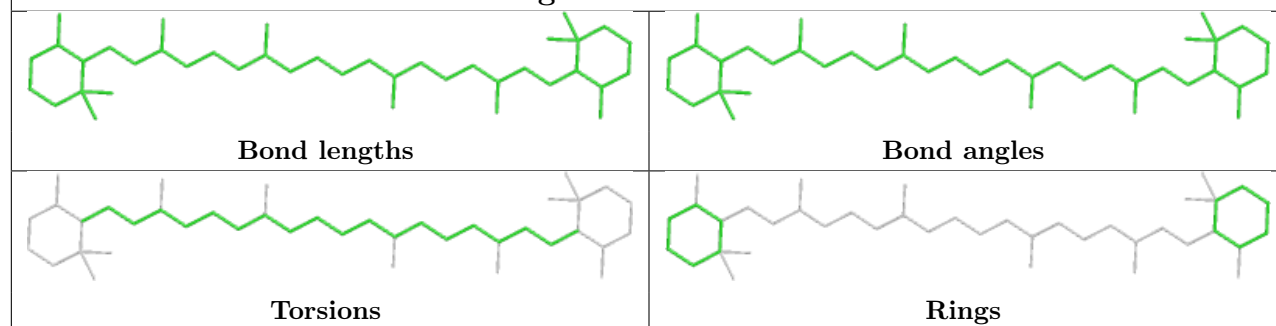


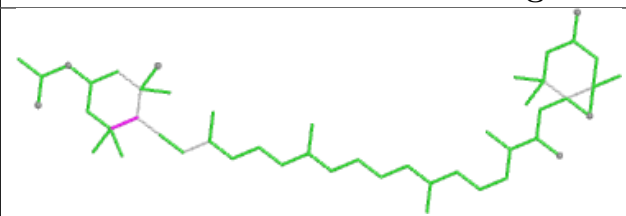
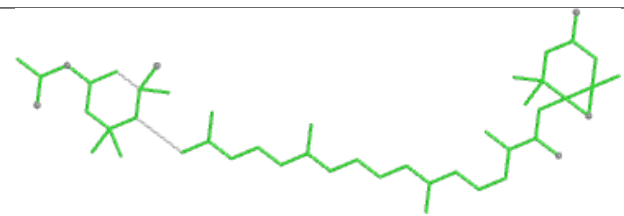
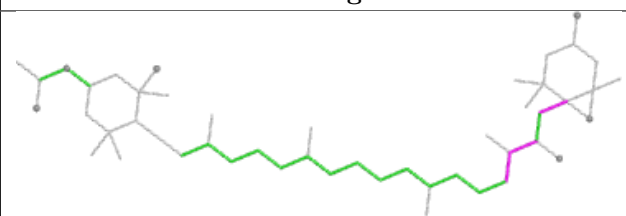
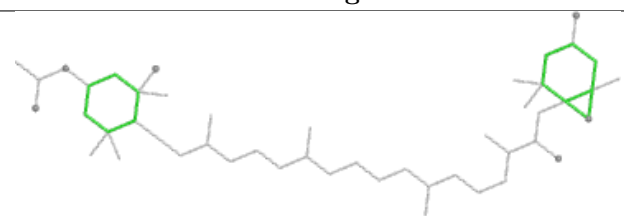
Rings

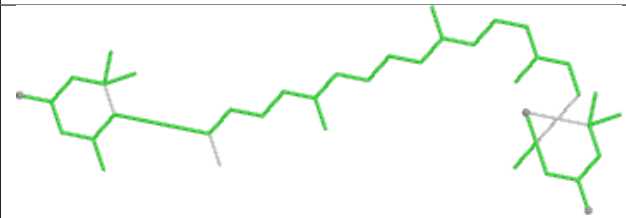
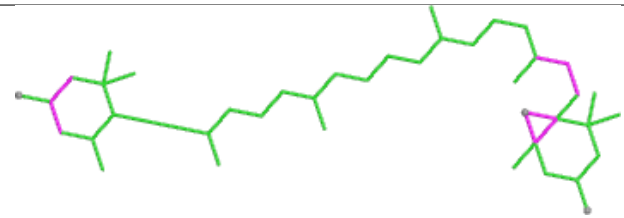
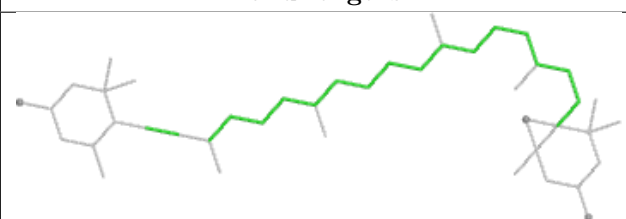
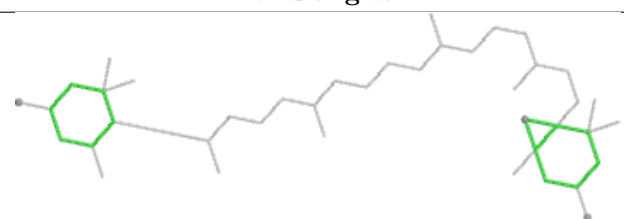
Ligand CLA b 816

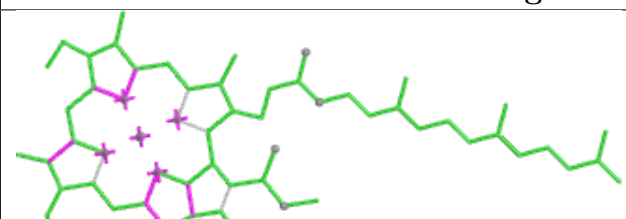
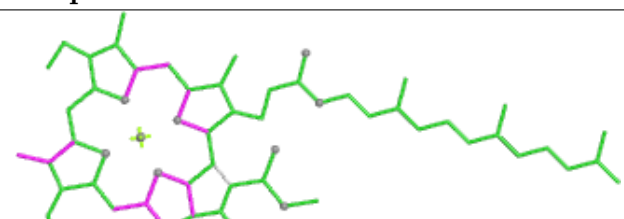
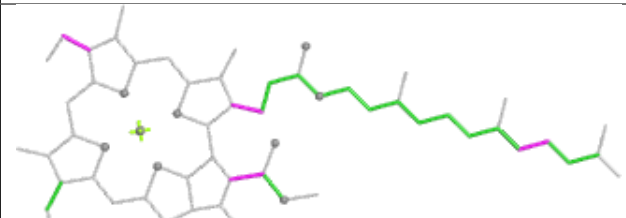
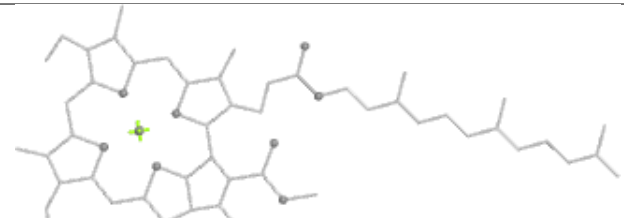


Ligand BCR f 203

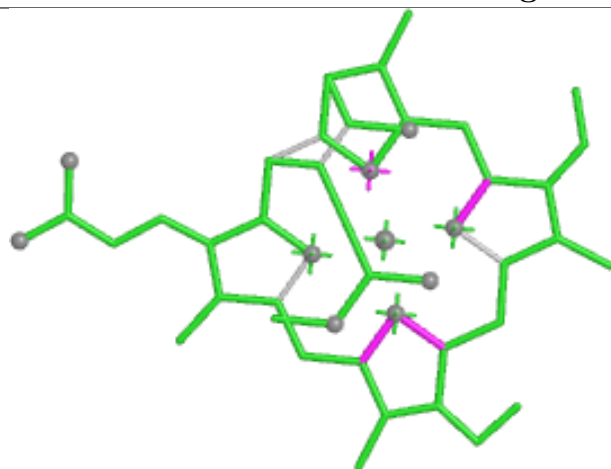


Ligand A86 R 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

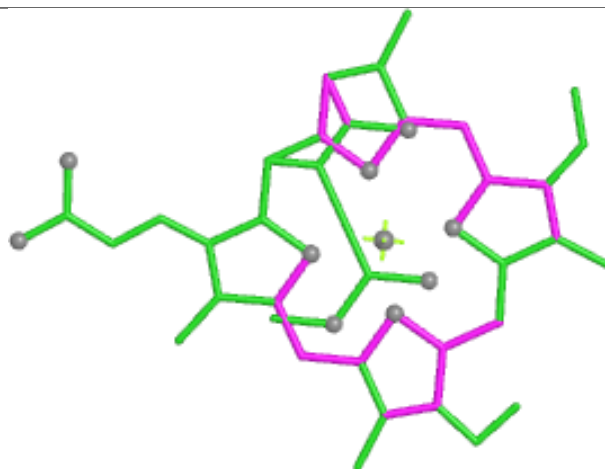
Ligand DD6 D 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA q 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

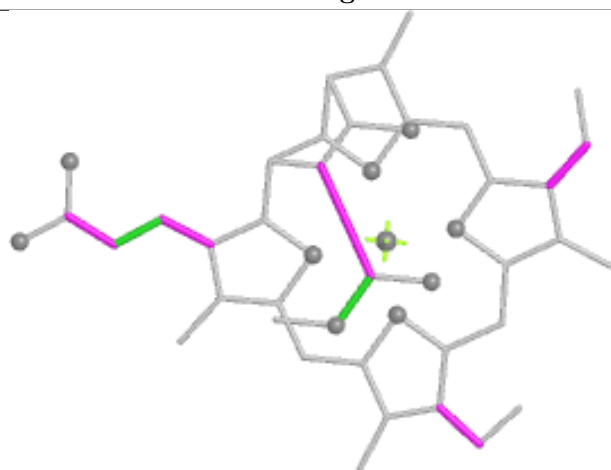
Ligand KC2 J 304



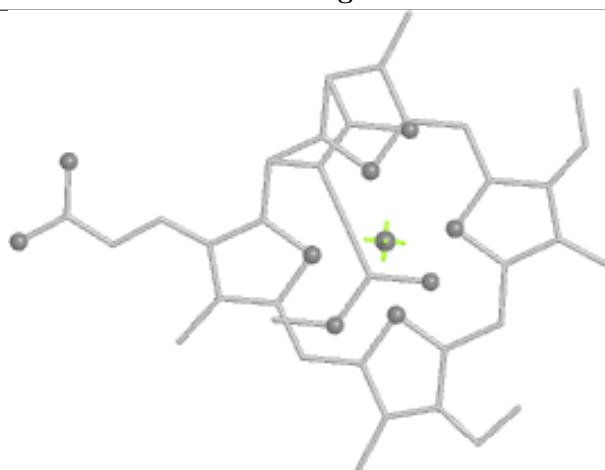
Bond lengths



Bond angles

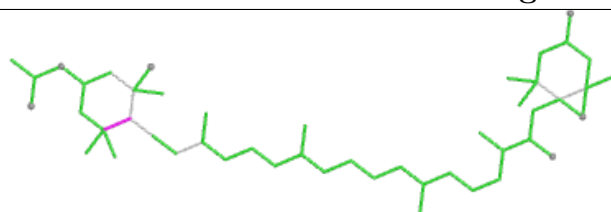


Torsions

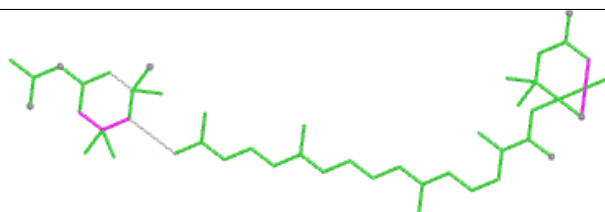


Rings

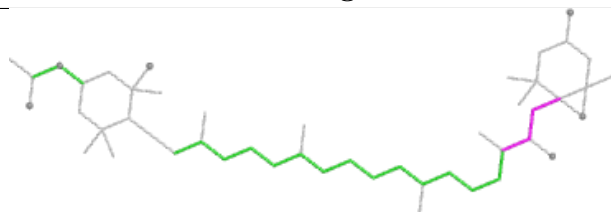
Ligand A86 X 320



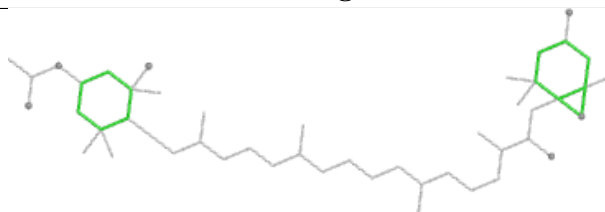
Bond lengths



Bond angles

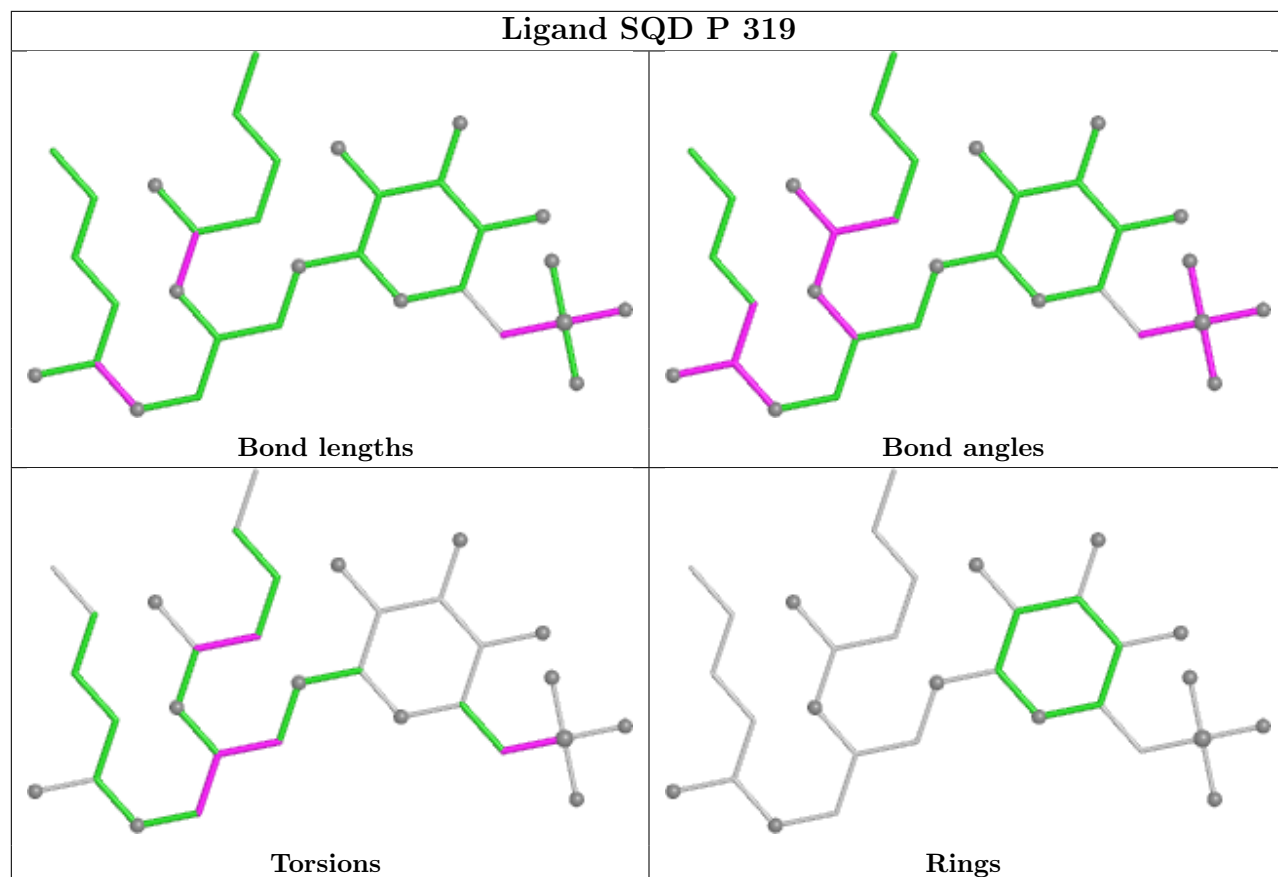


Torsions

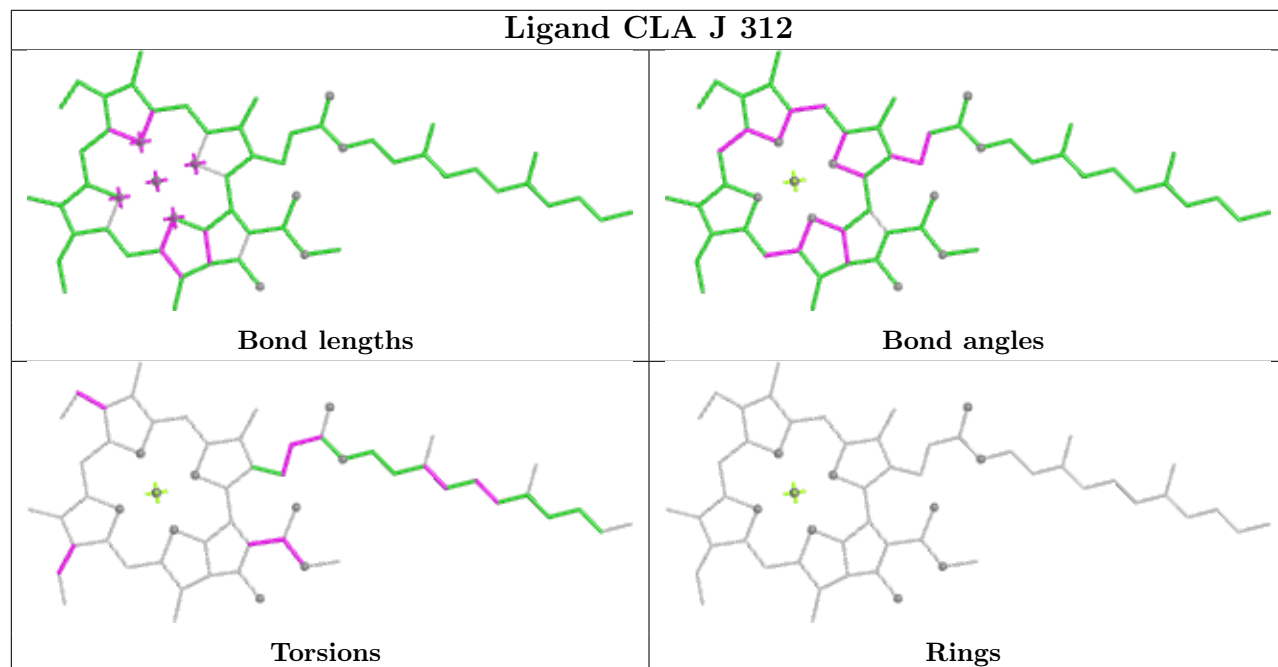


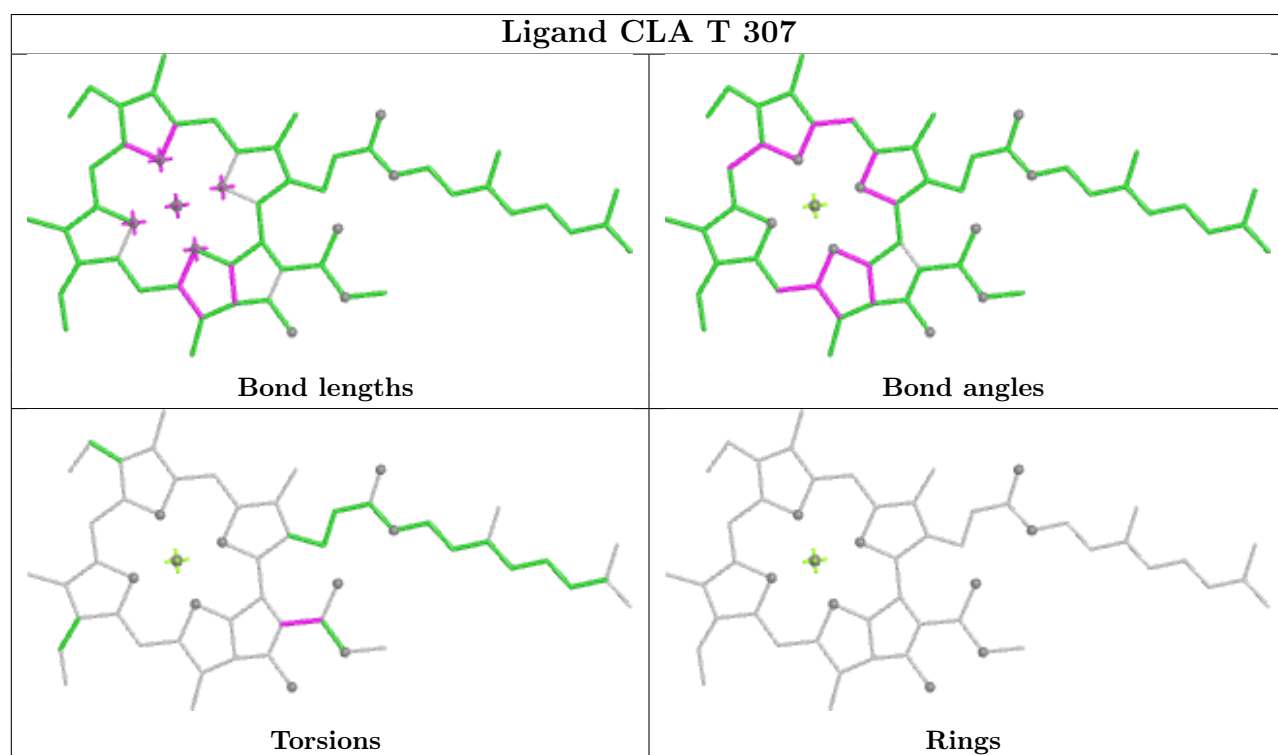
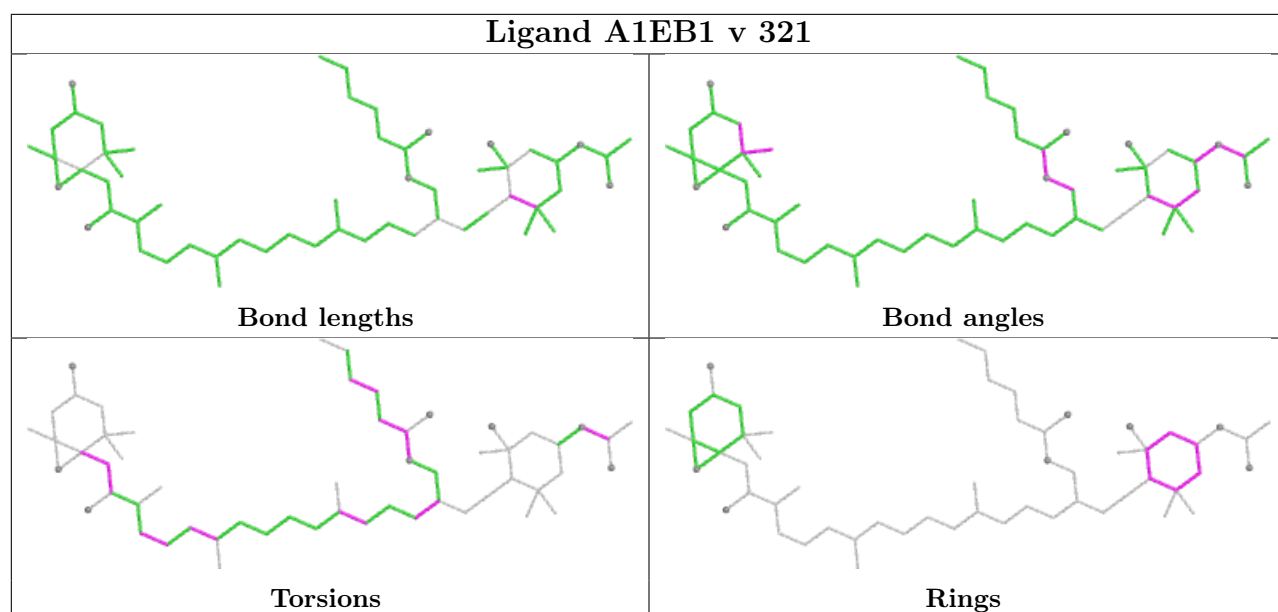
Rings

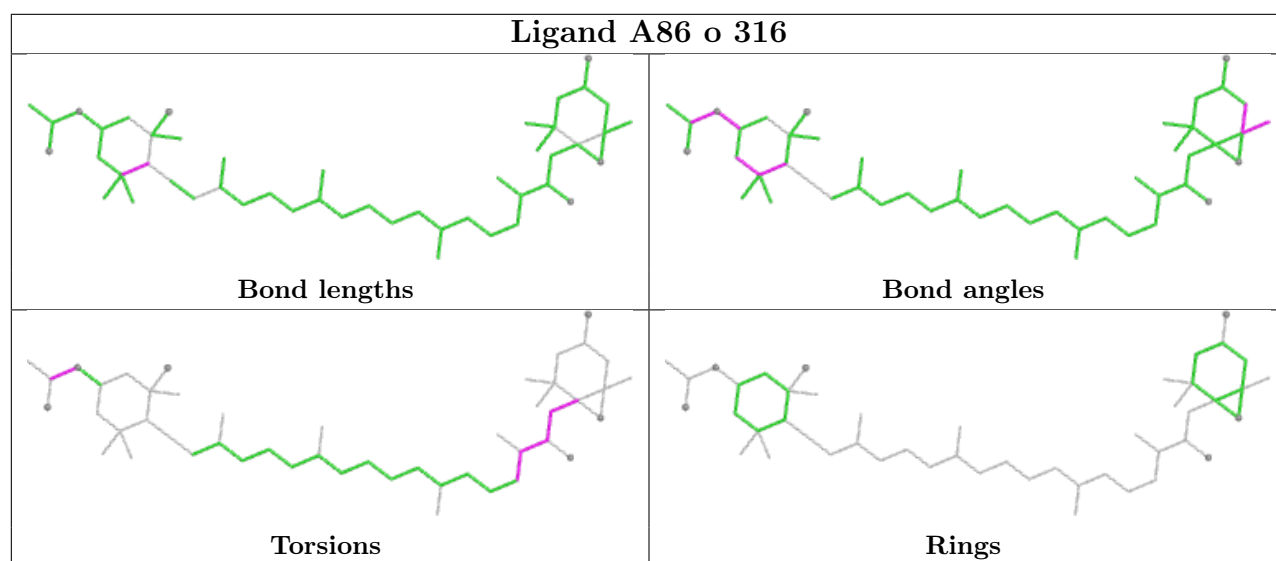
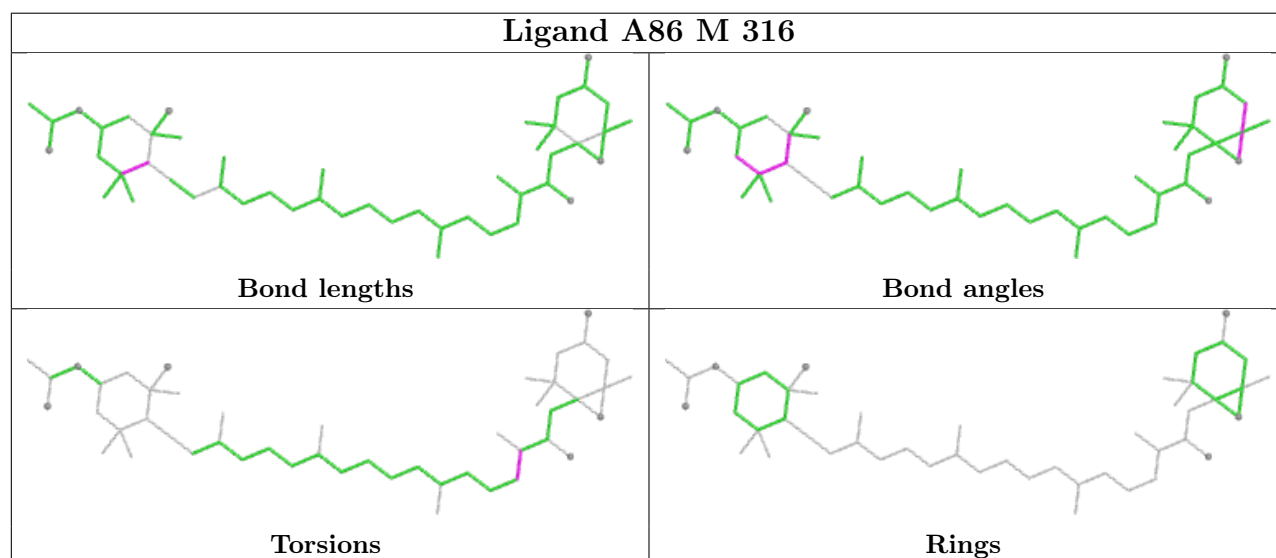
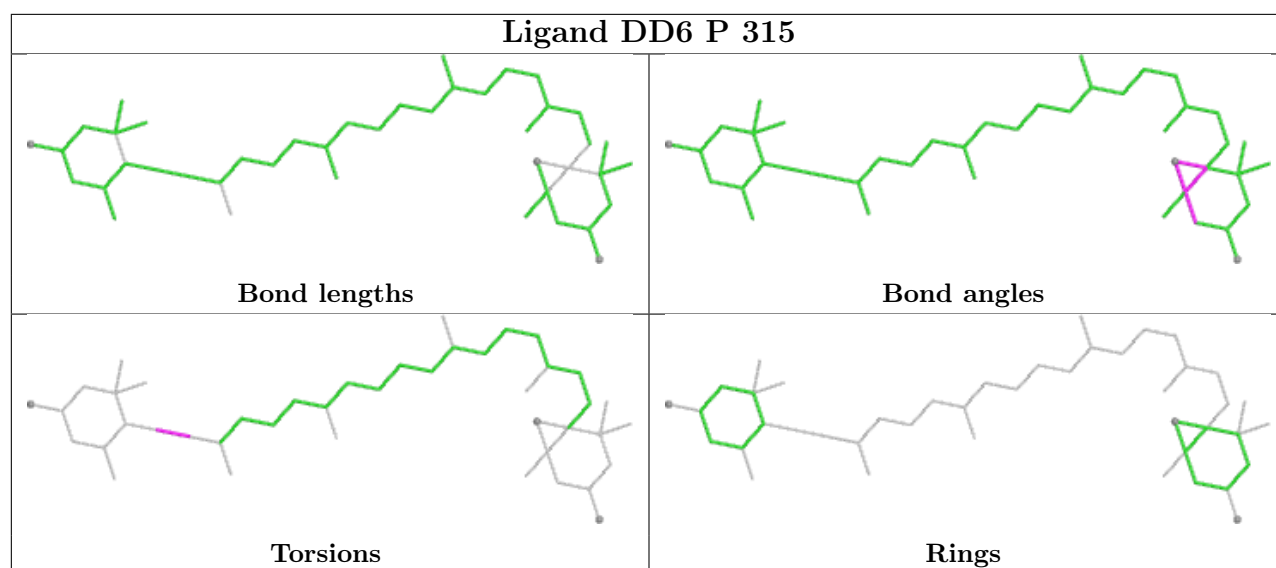
Ligand SQD P 319



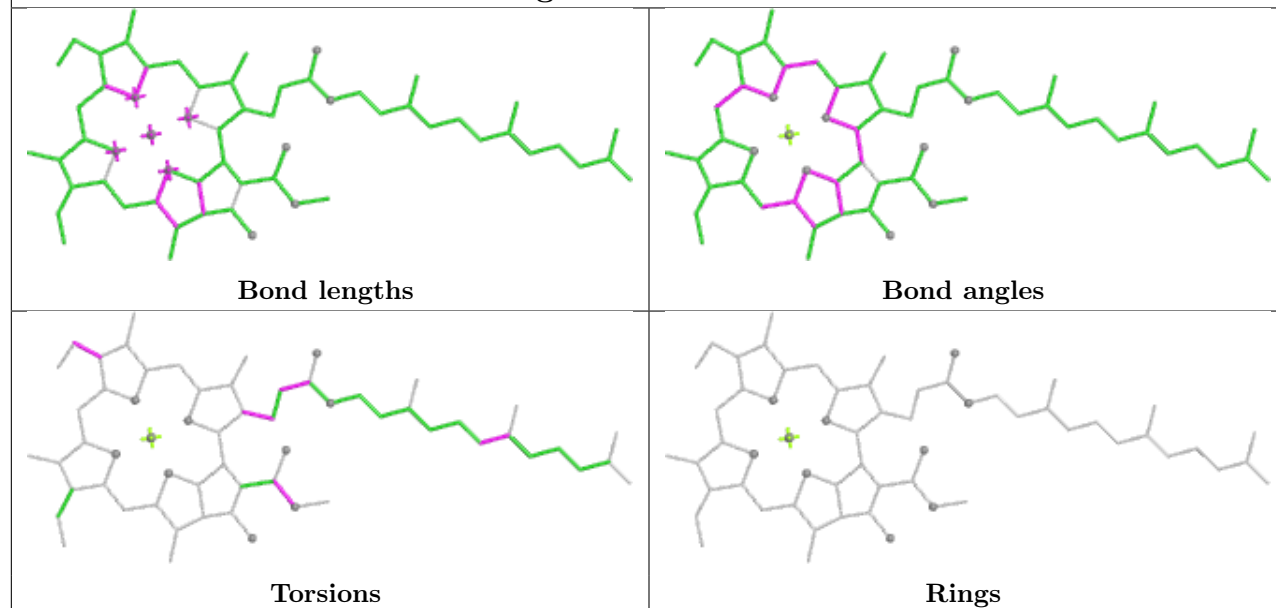
Ligand CLA J 312



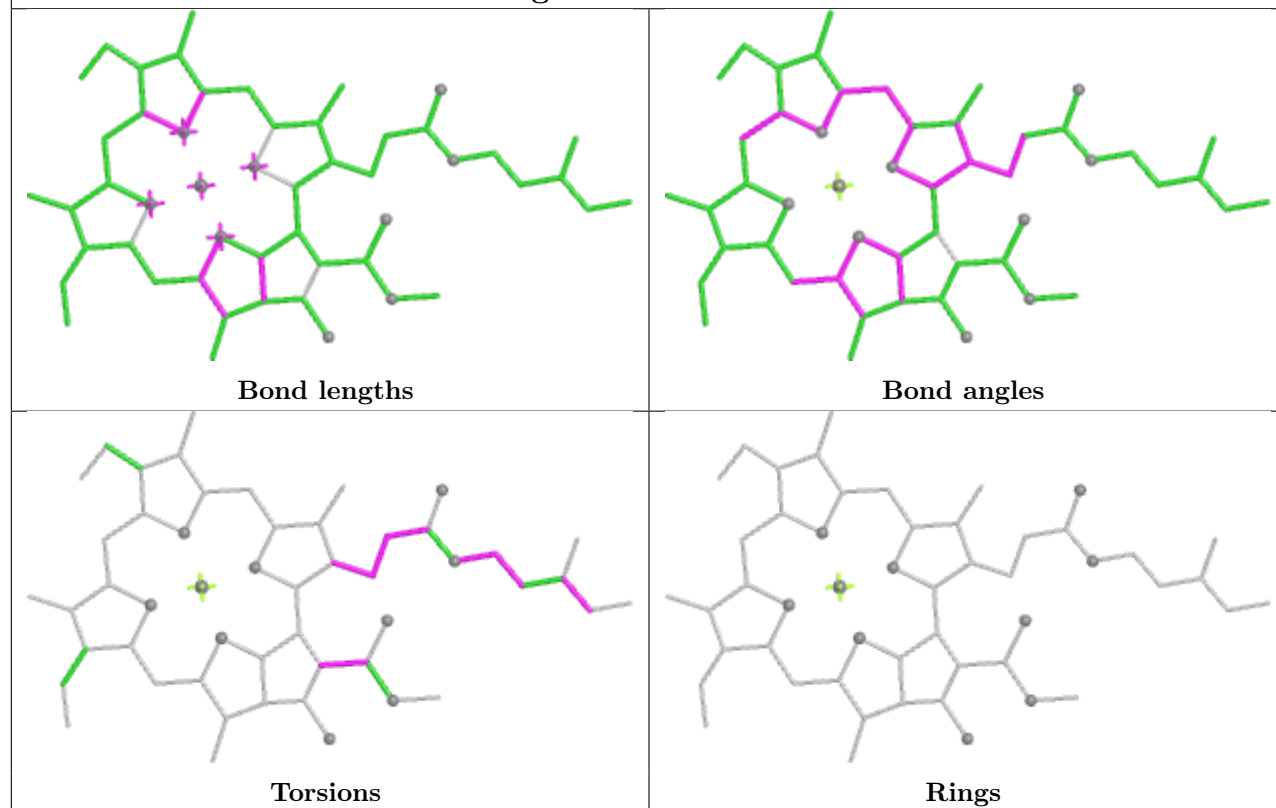




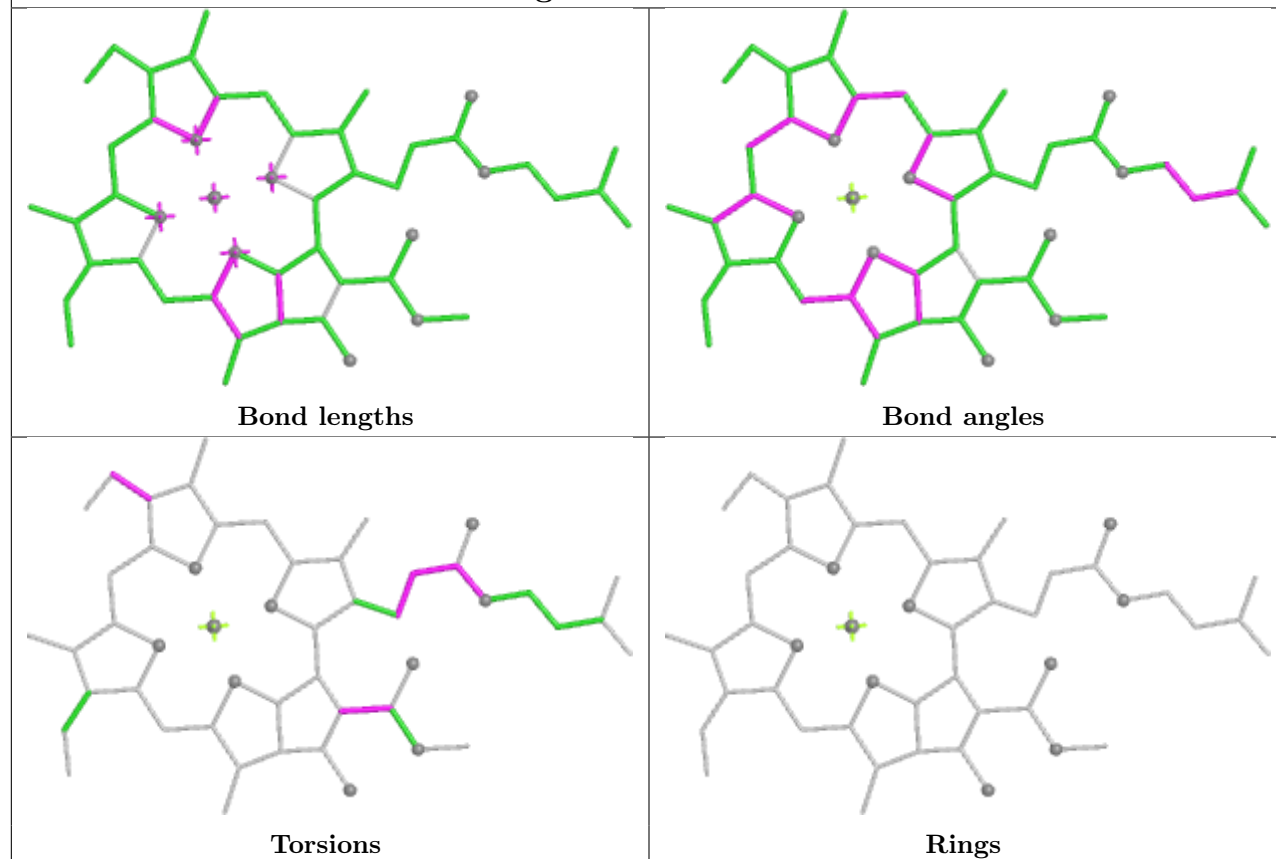
Ligand CLA a 813



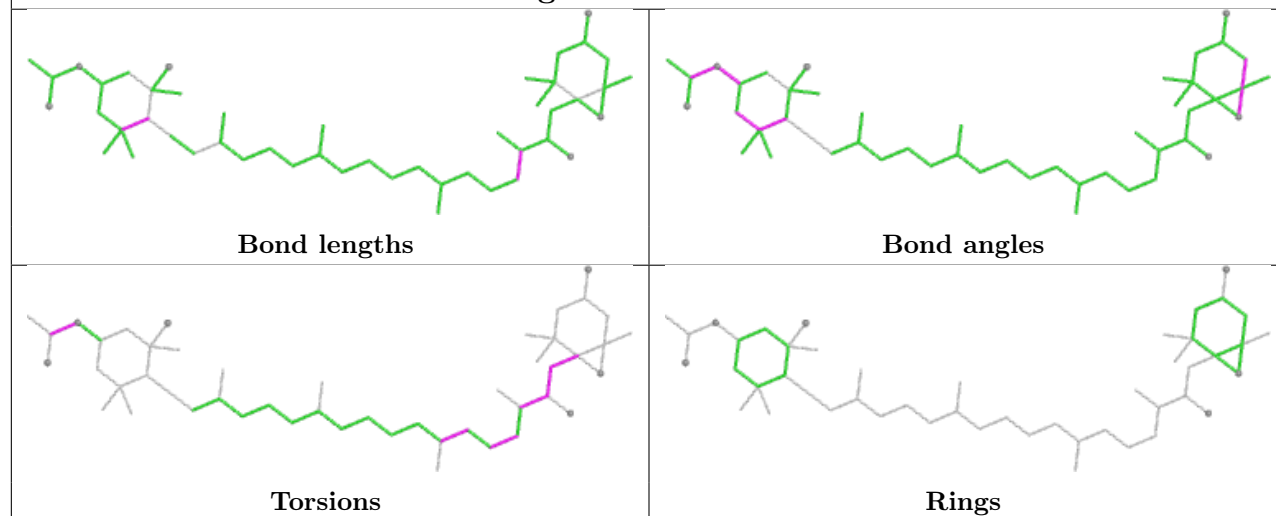
Ligand CLA R 304

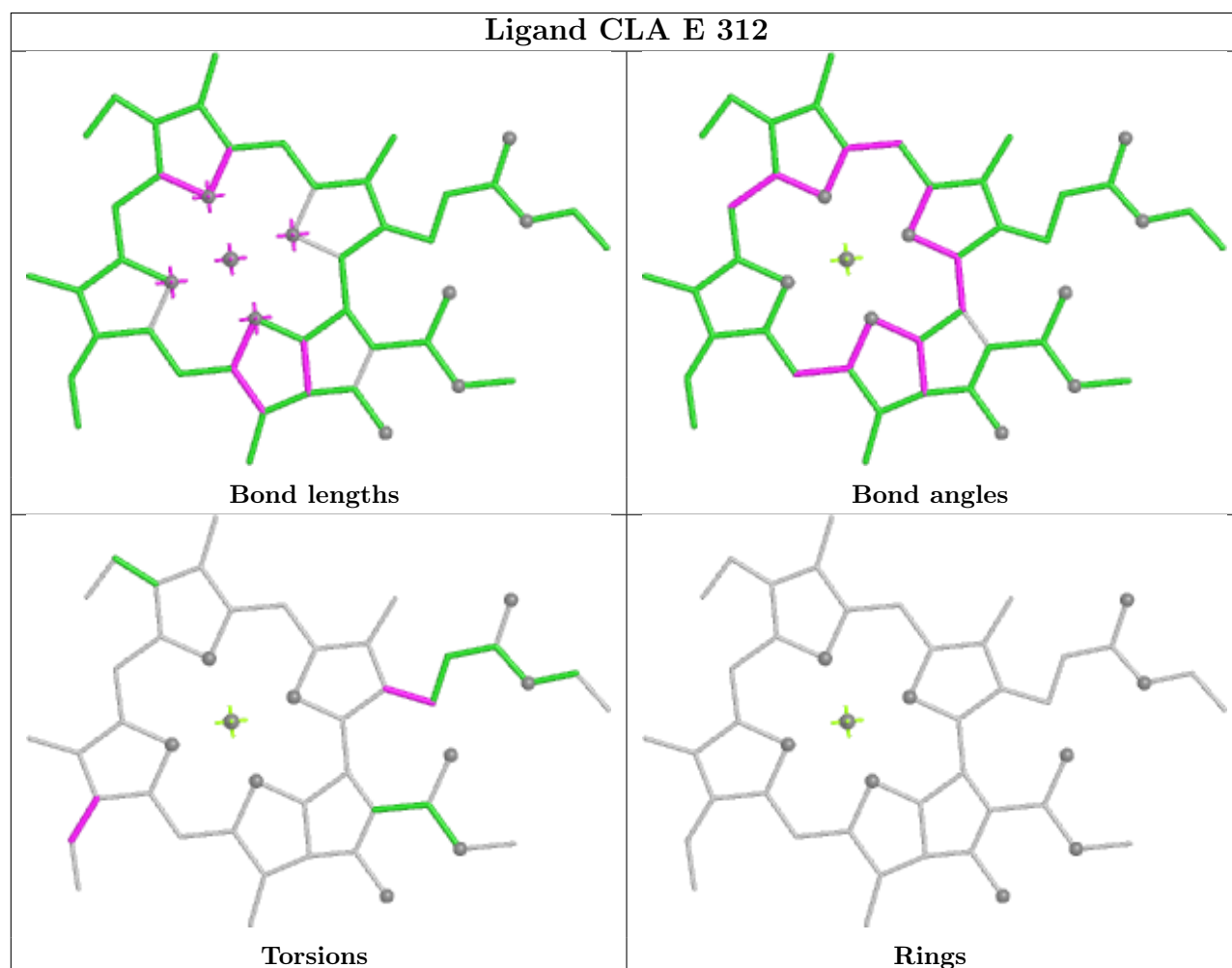
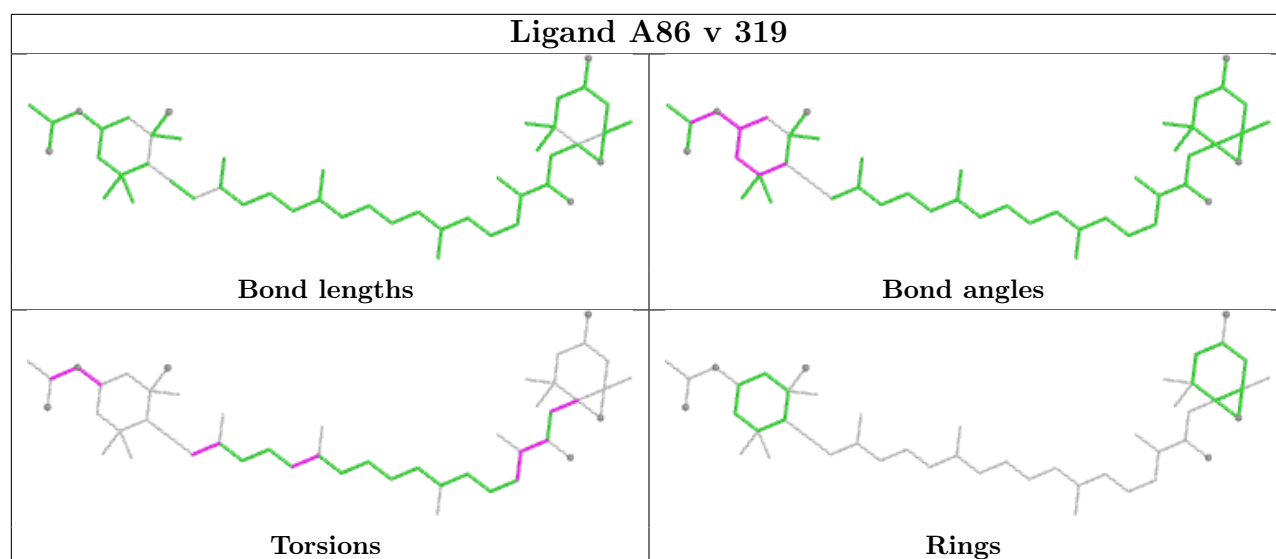


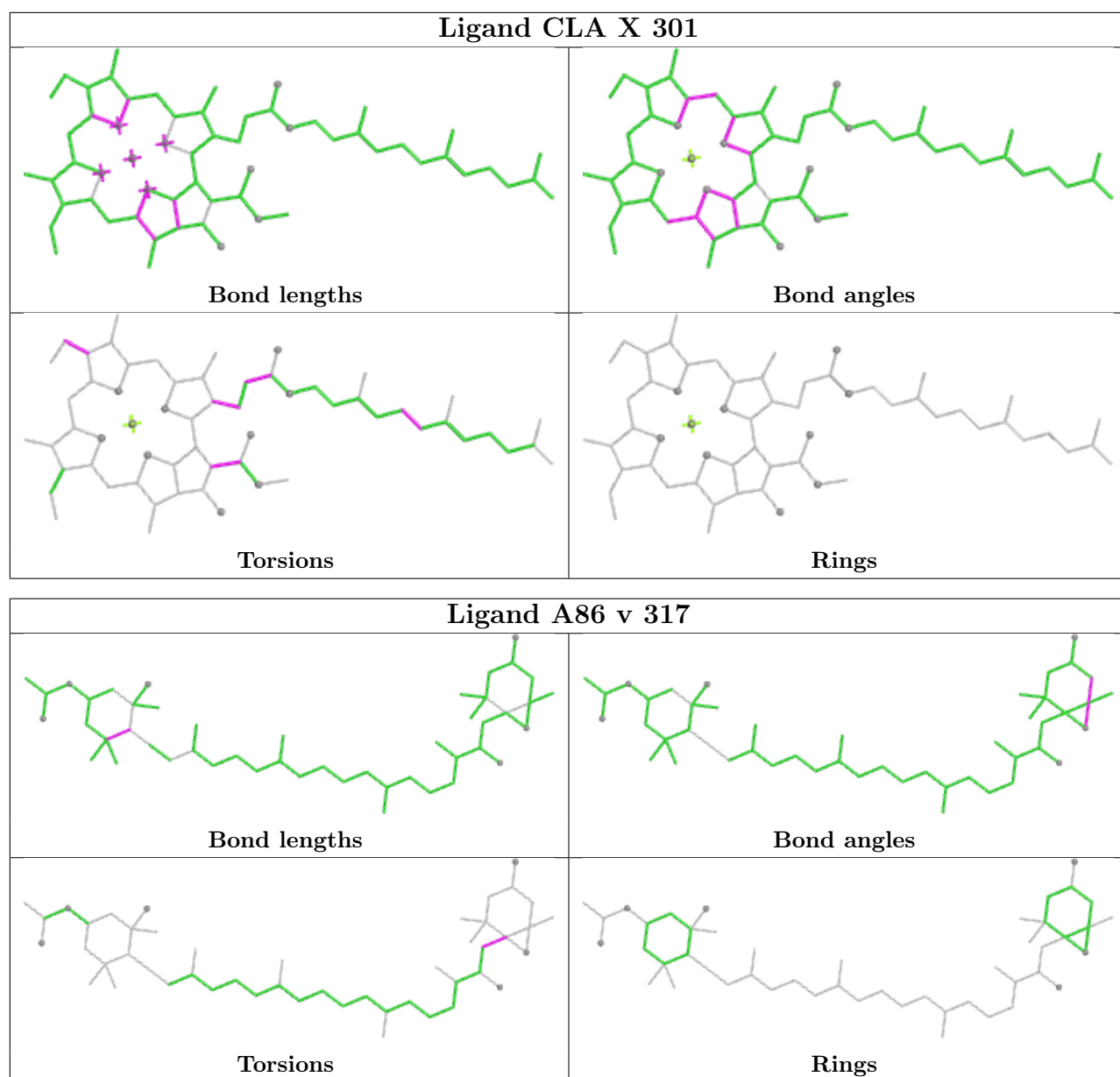
Ligand CLA b 813



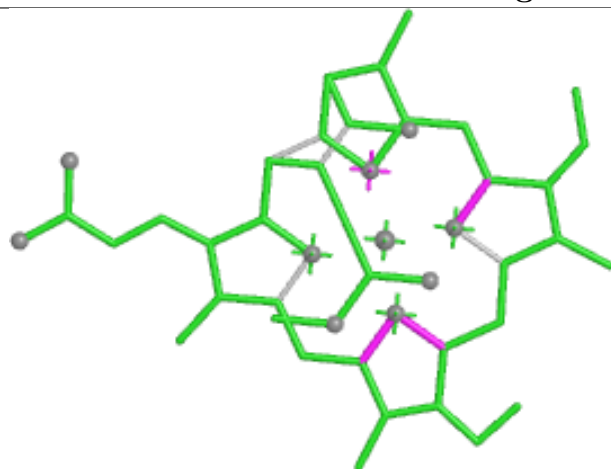
Ligand A86 w 311



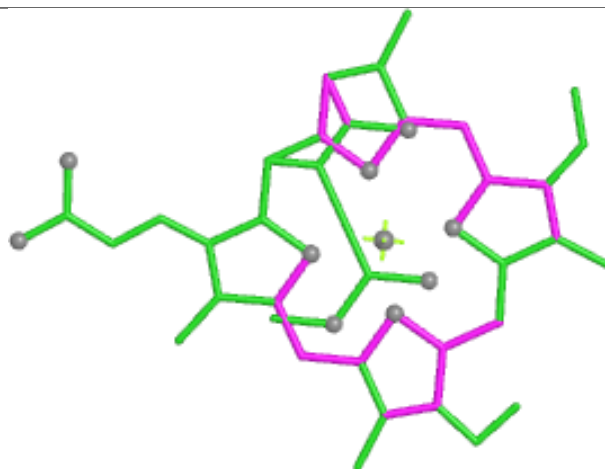




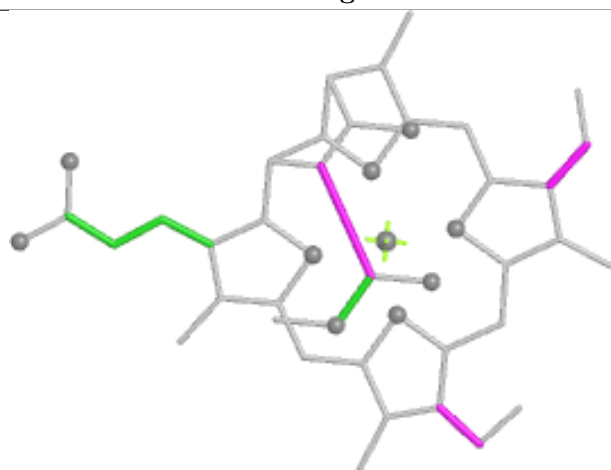
Ligand KC2 R 301



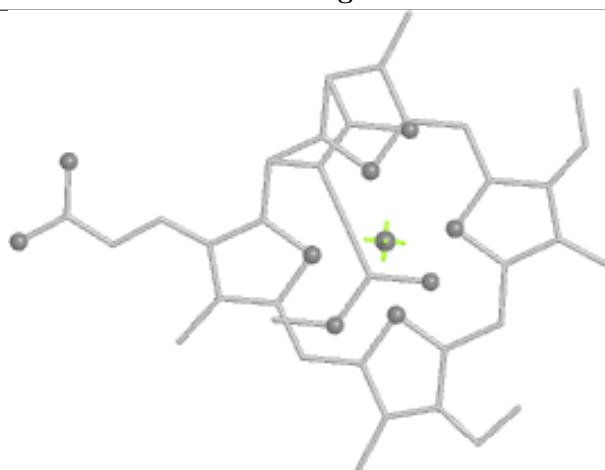
Bond lengths



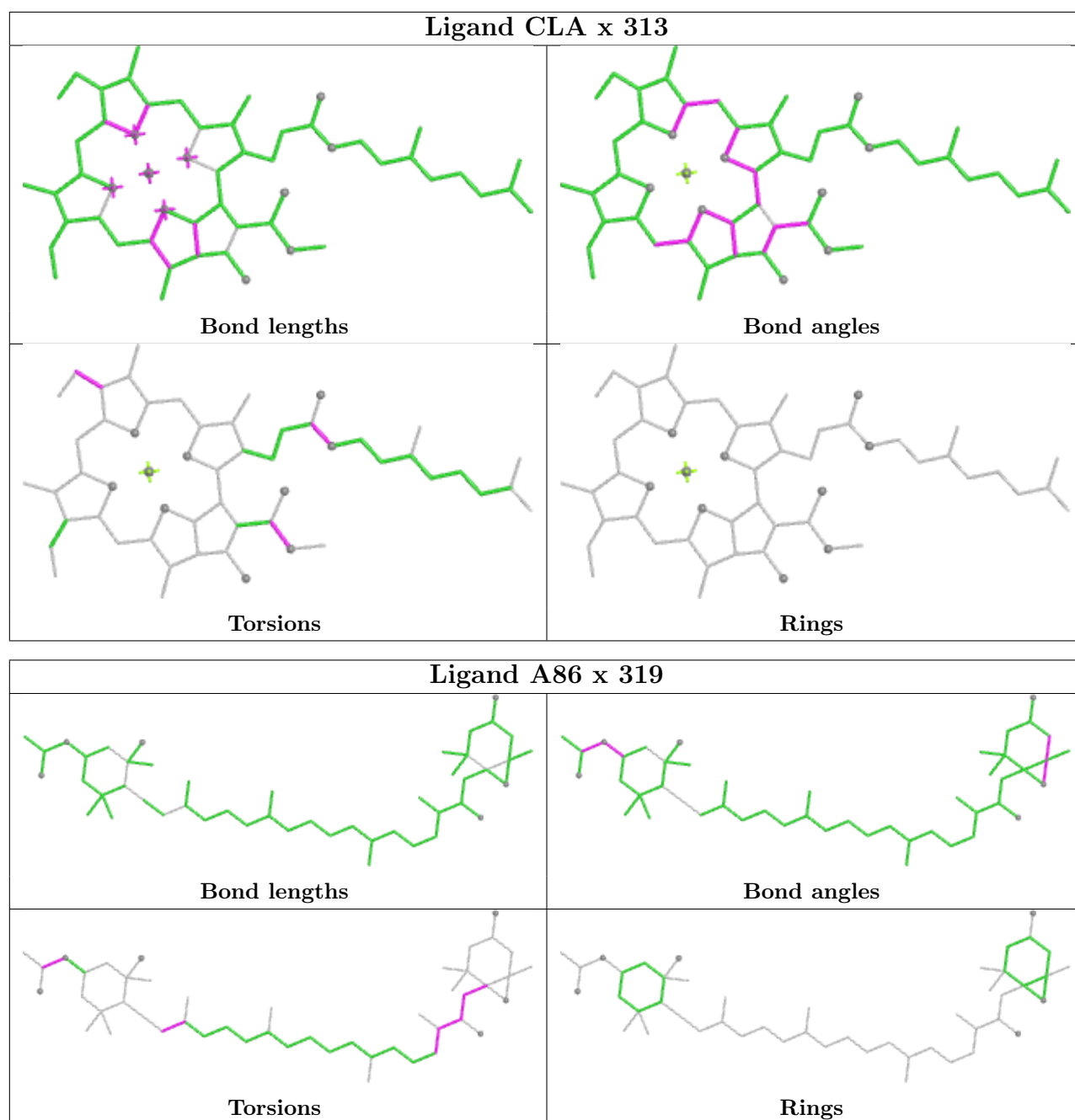
Bond angles

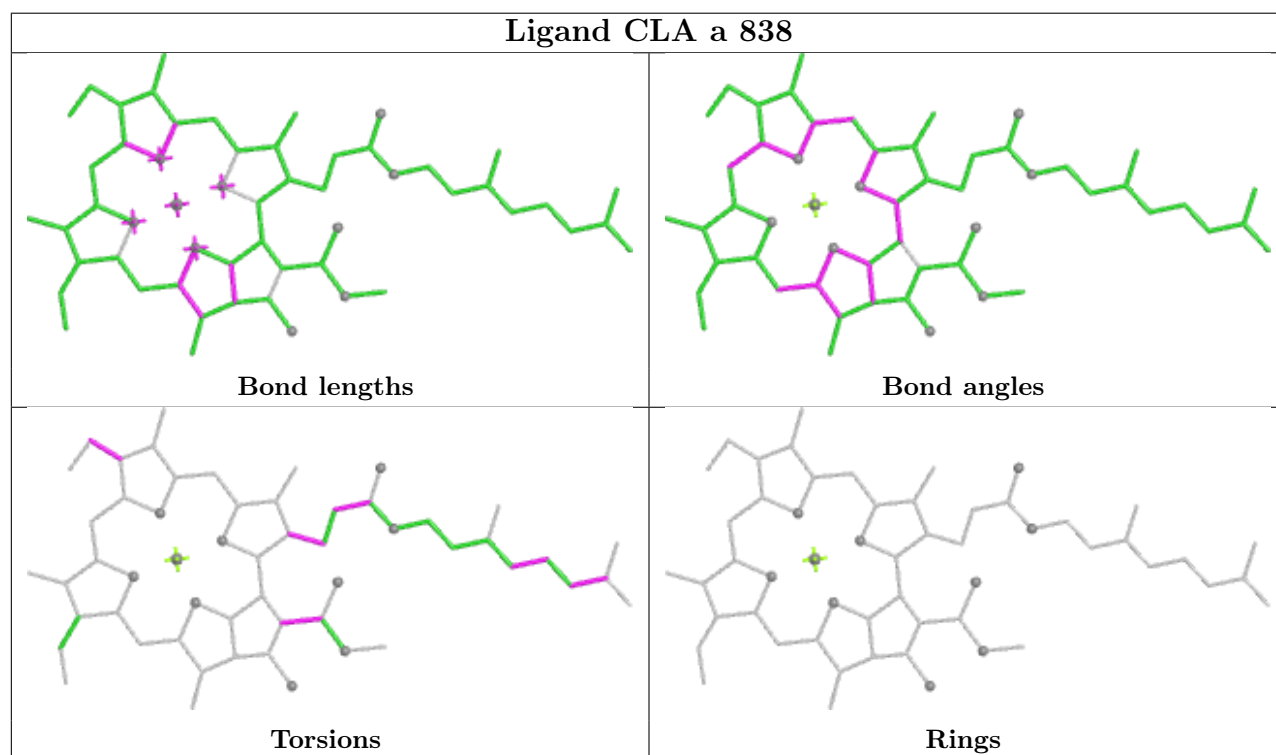
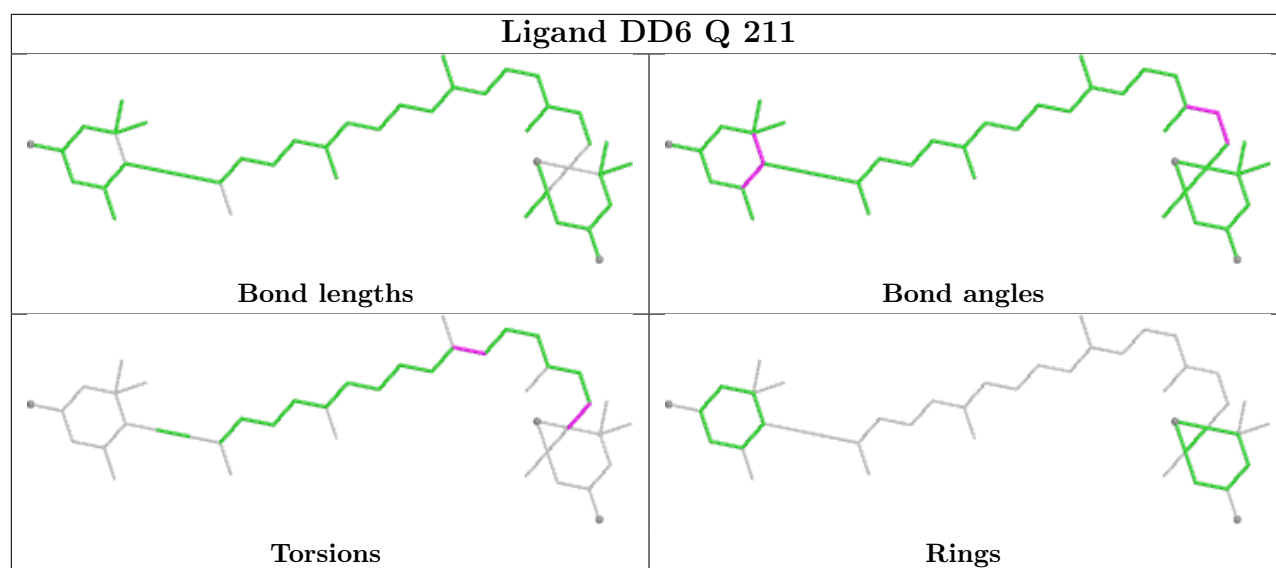


Torsions

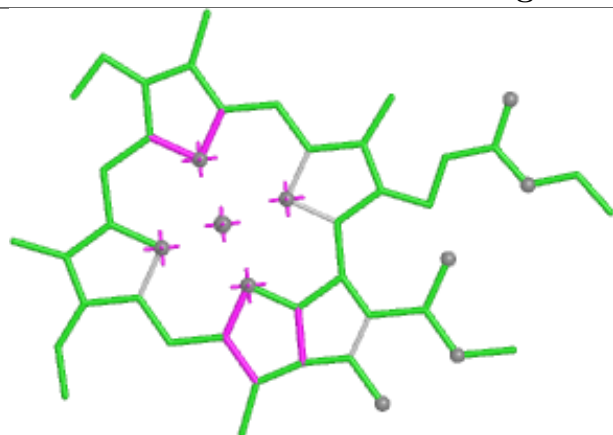


Rings

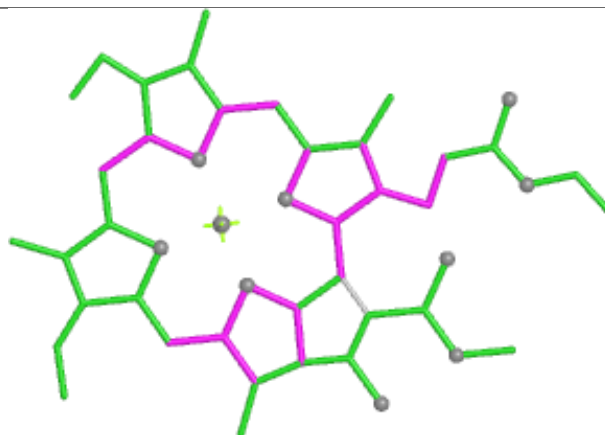




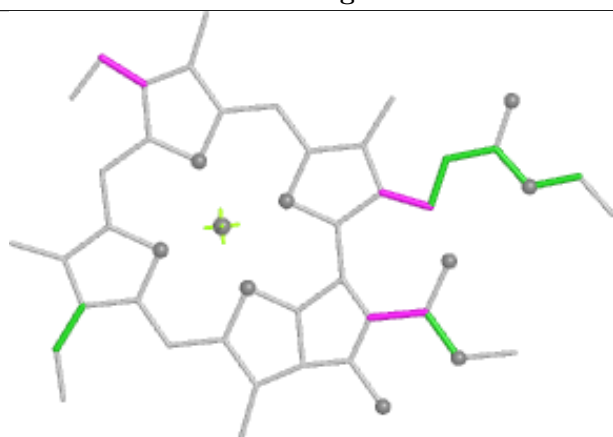
Ligand CLA Z 313



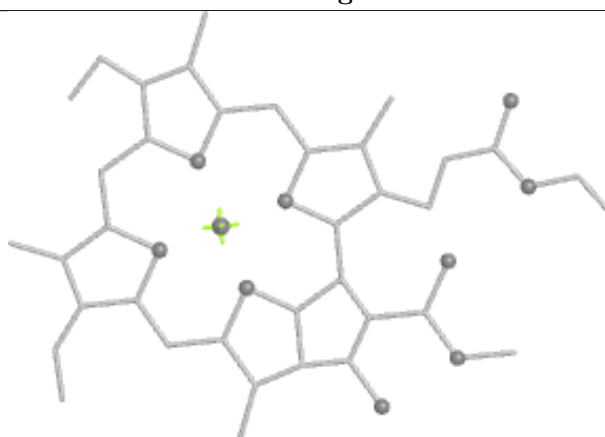
Bond lengths



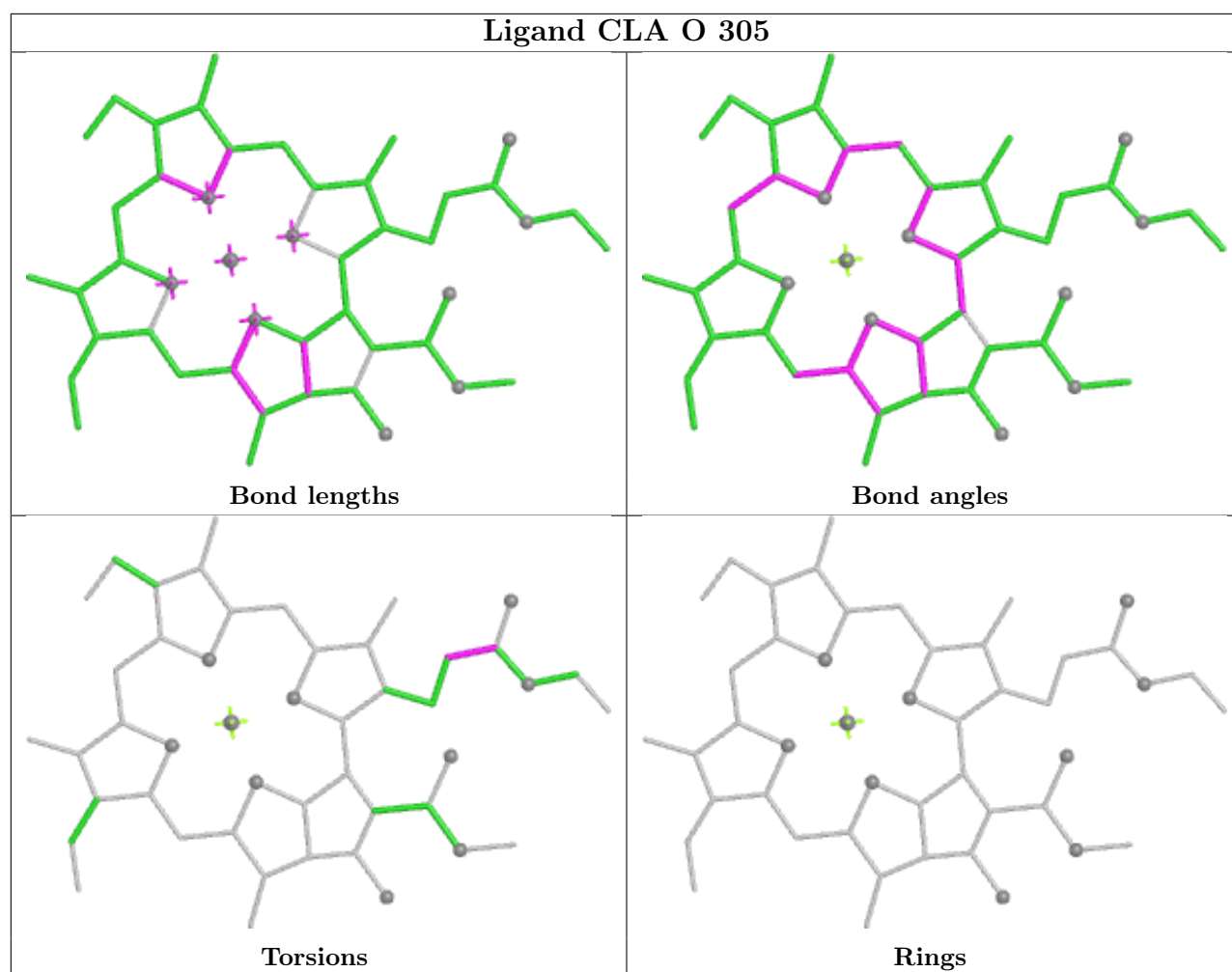
Bond angles



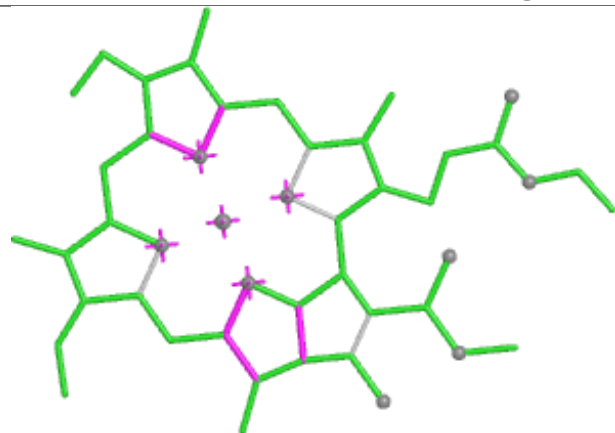
Torsions



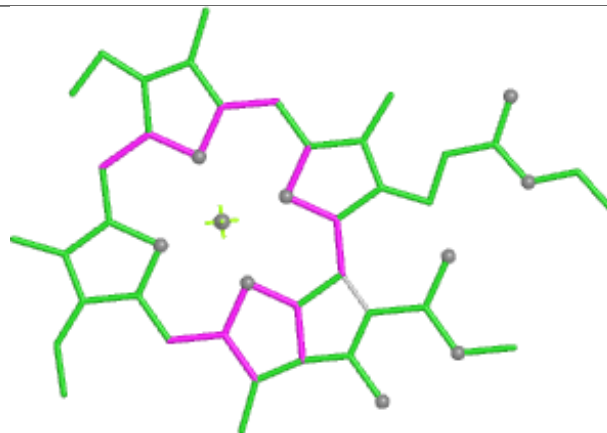
Rings



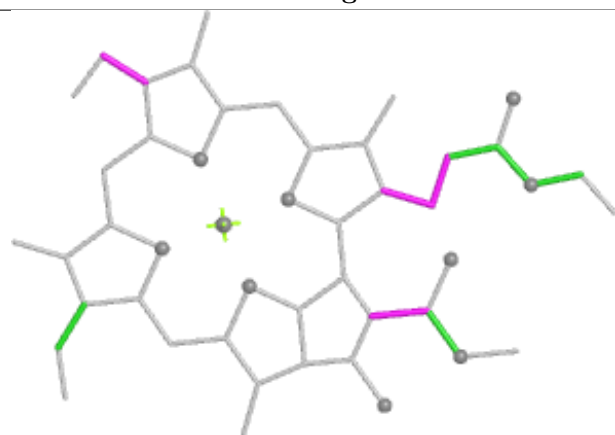
Ligand CLA L 311



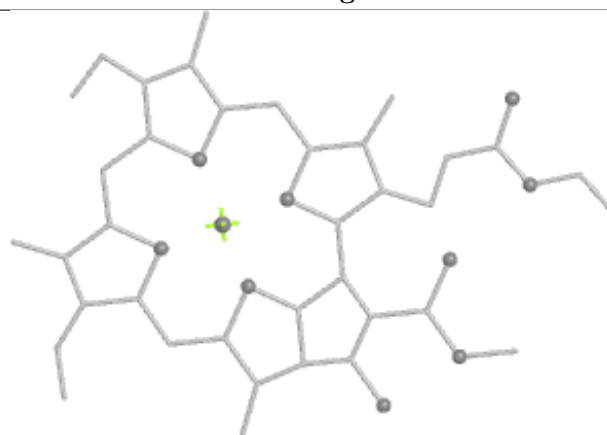
Bond lengths



Bond angles

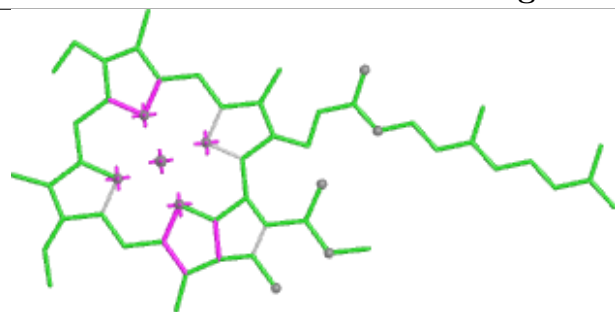


Torsions

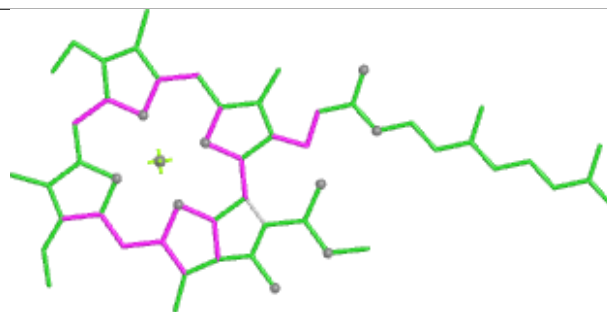


Rings

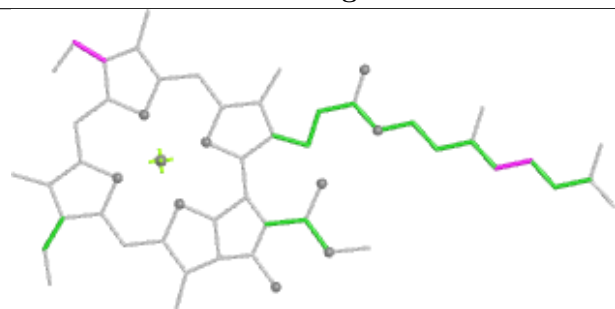
Ligand CLA F 304



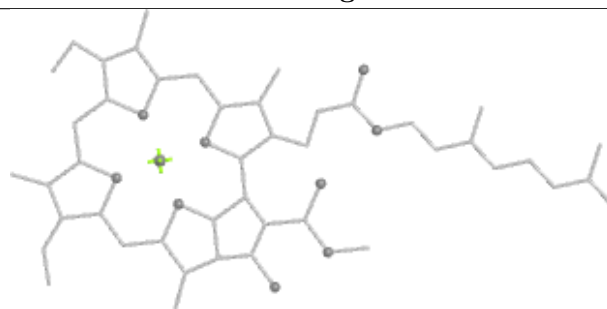
Bond lengths



Bond angles

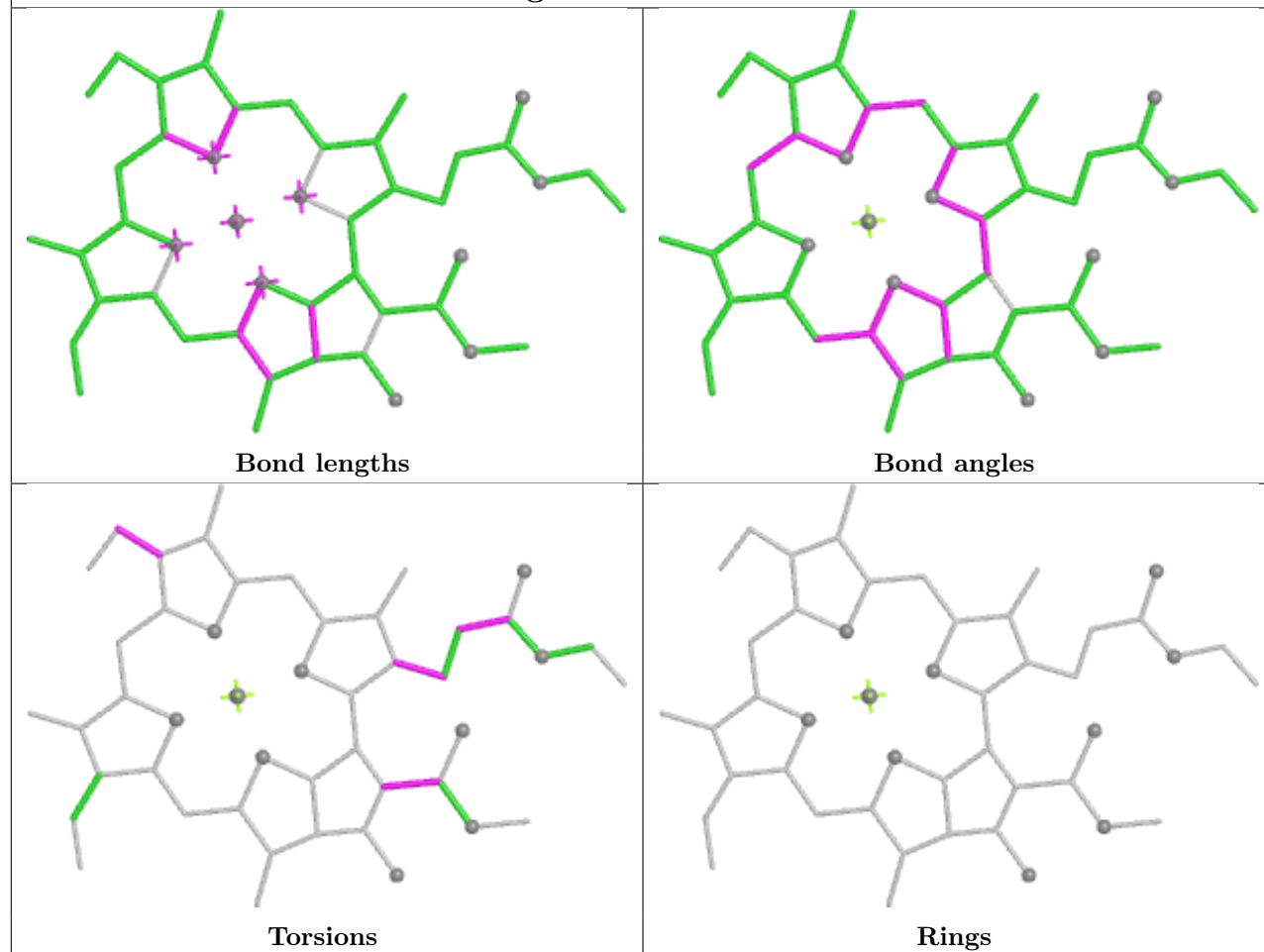


Torsions

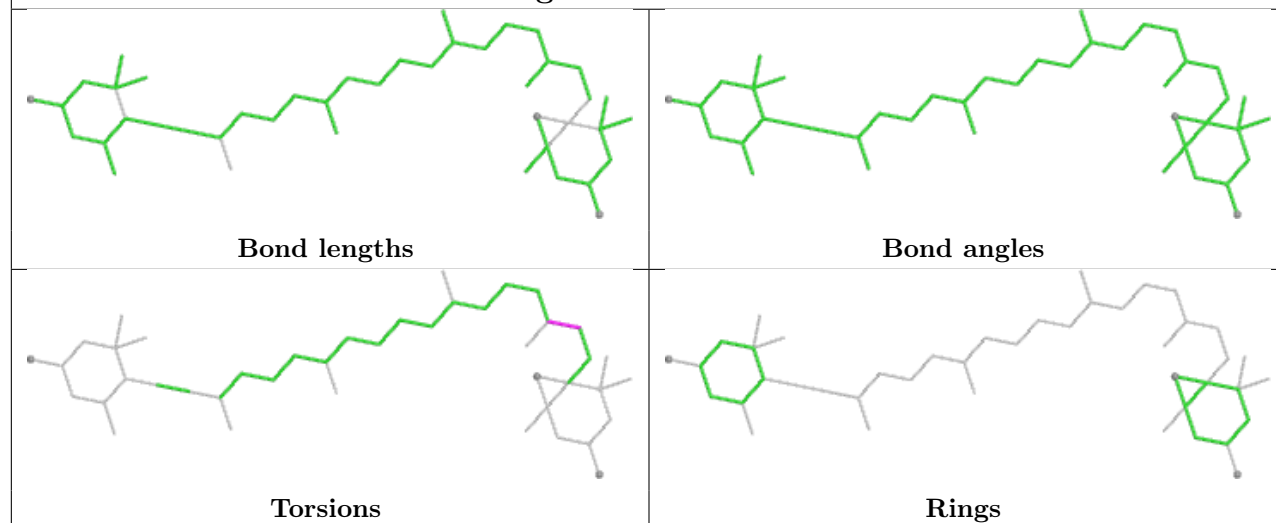


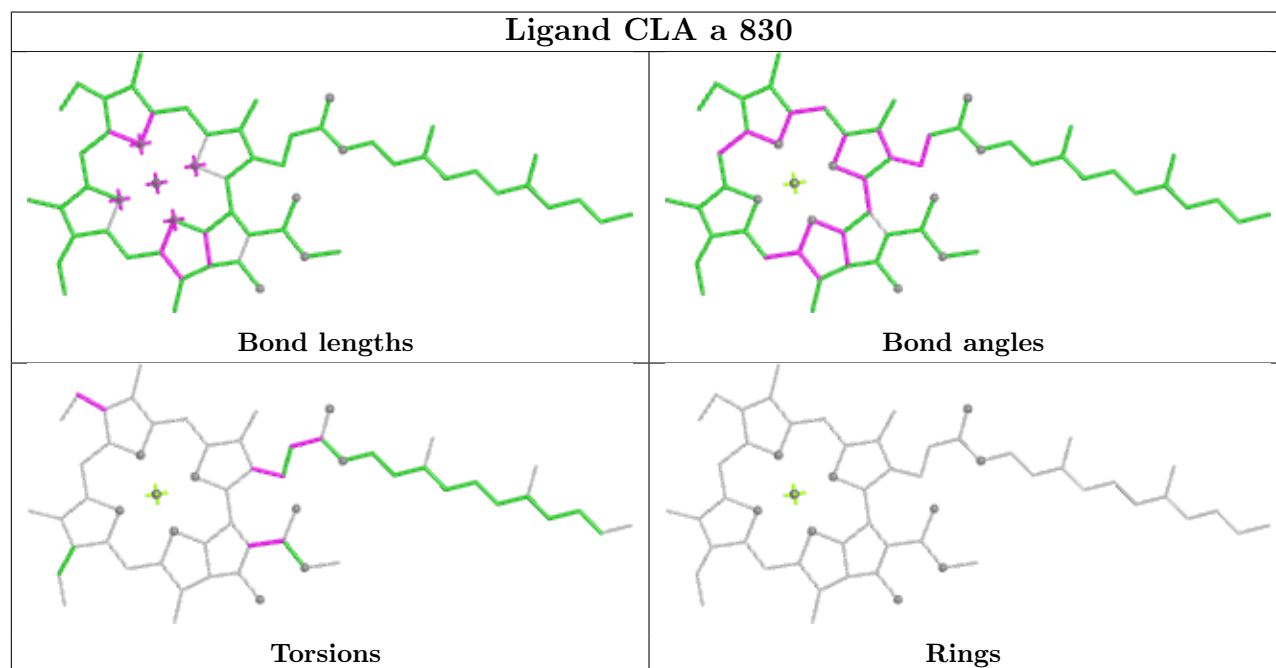
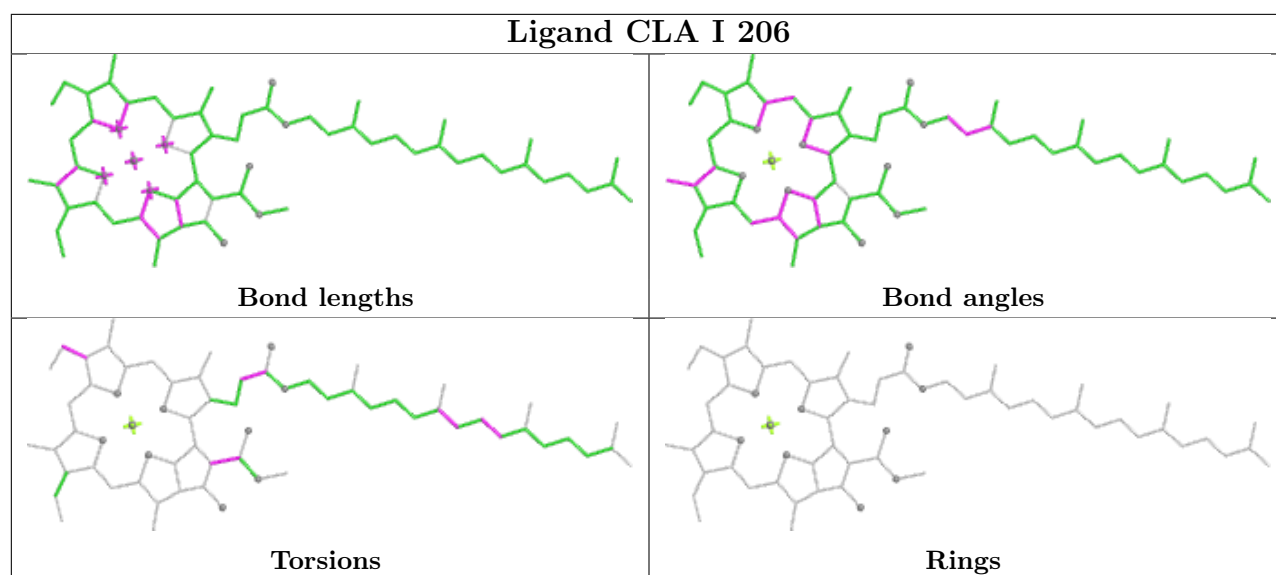
Rings

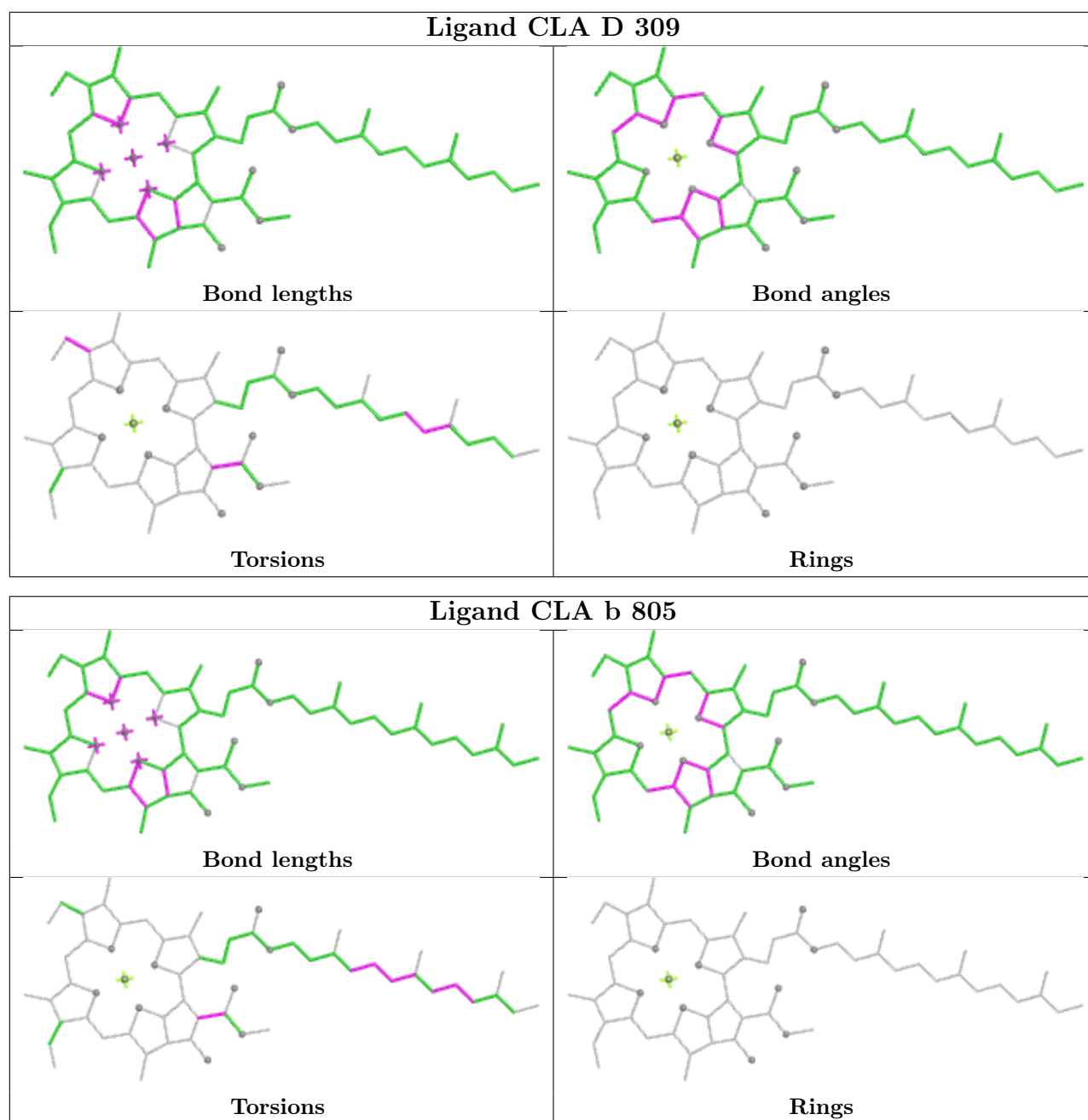
Ligand CLA R 310

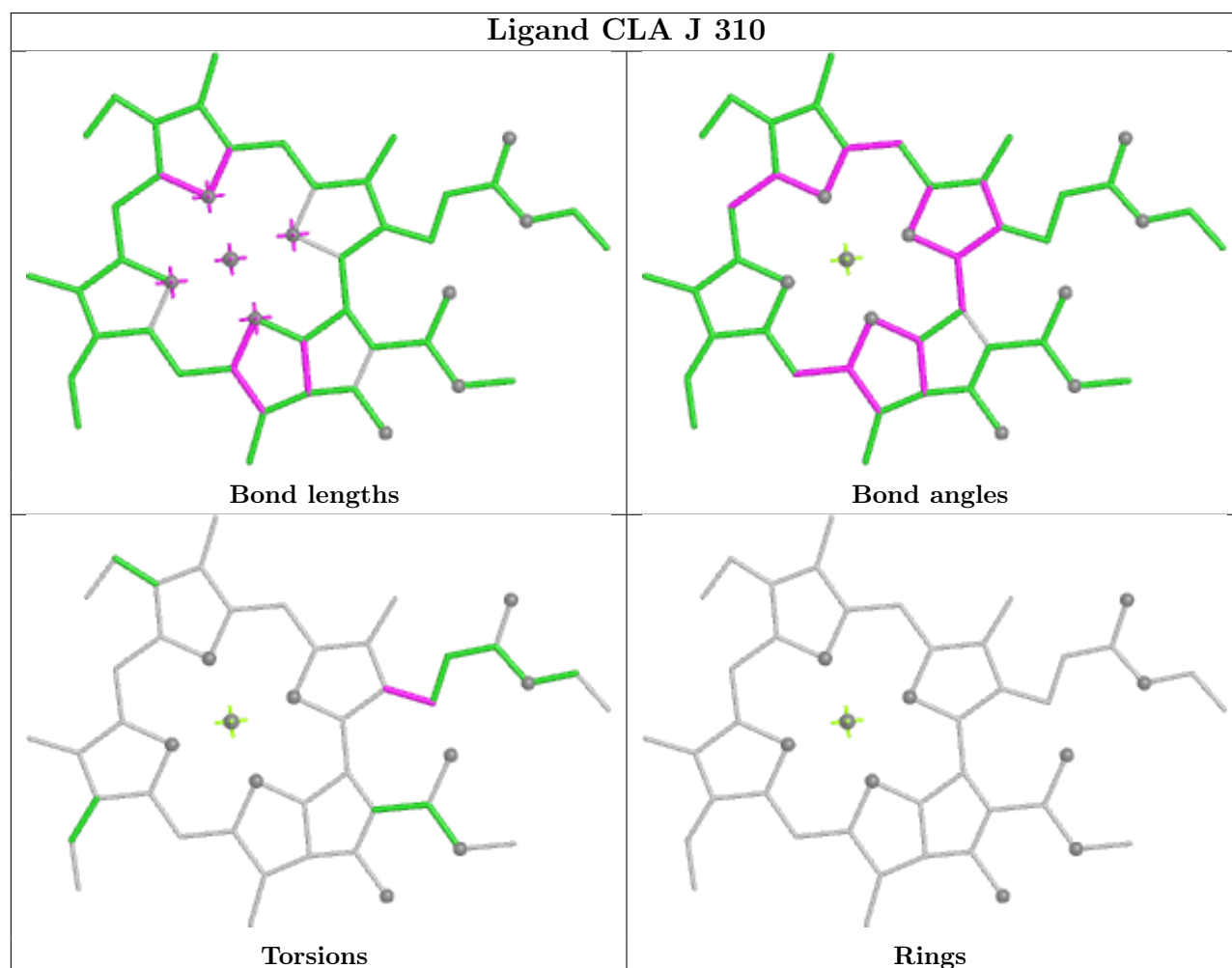
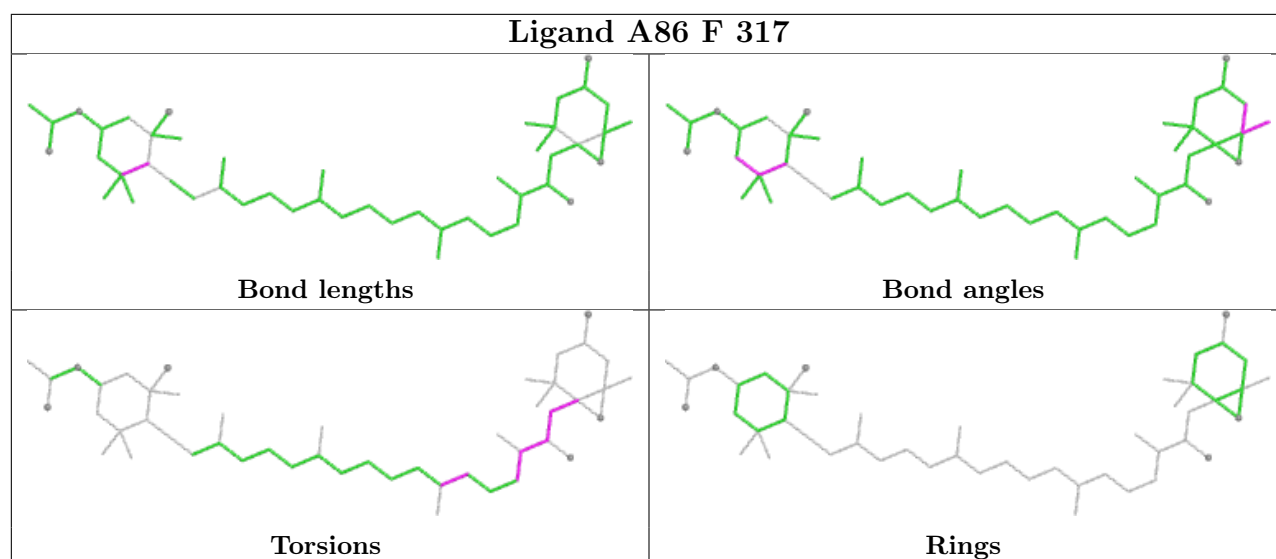


Ligand DD6 u 321

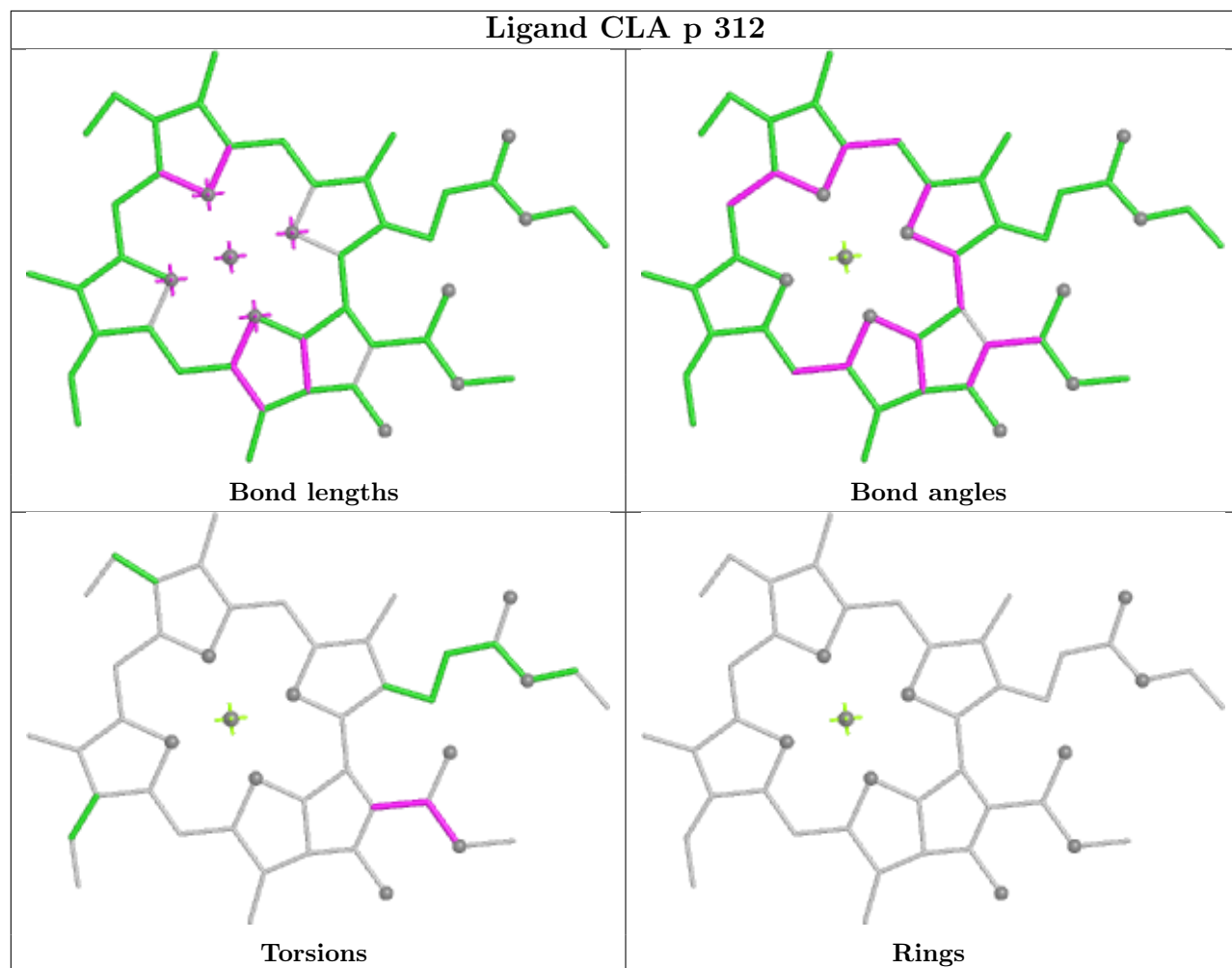




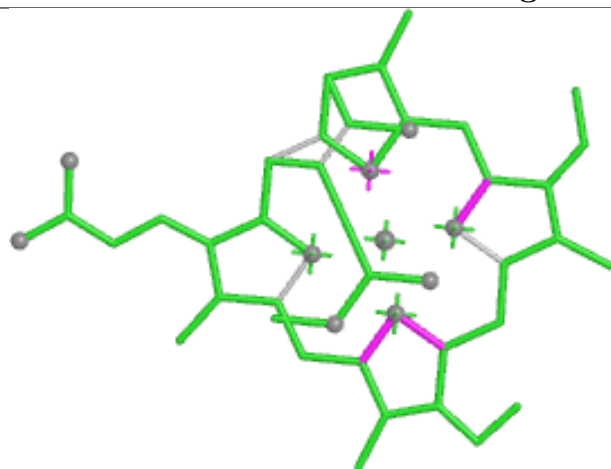




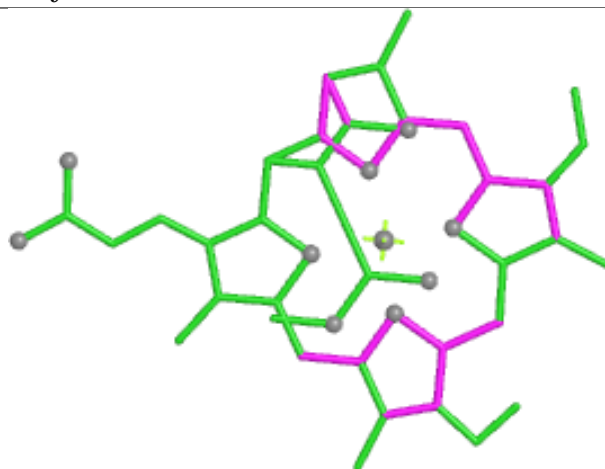
Ligand CLA p 312



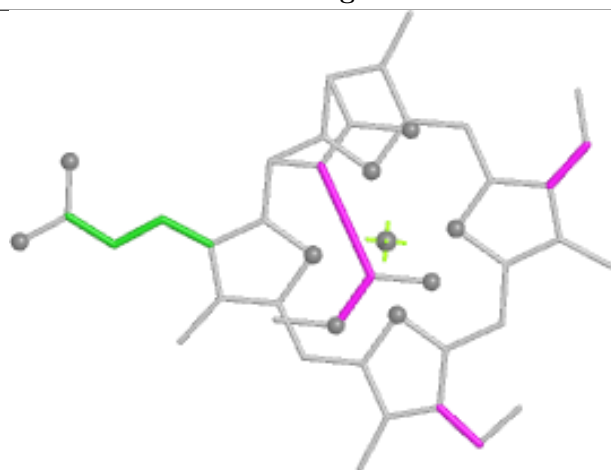
Ligand KC2 y 306



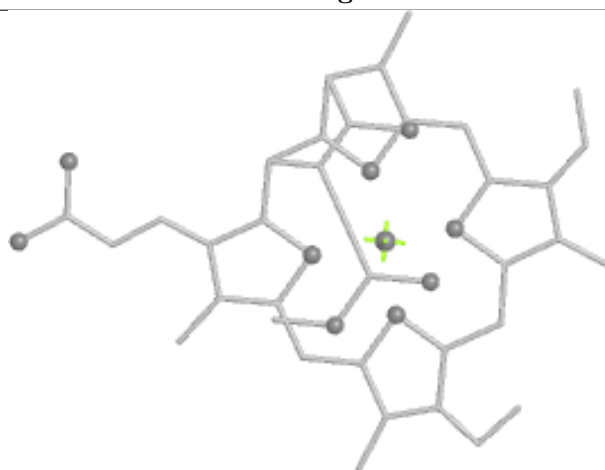
Bond lengths



Bond angles



Torsions

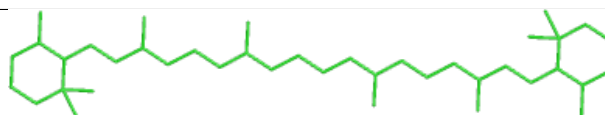


Rings

Ligand BCR a 843



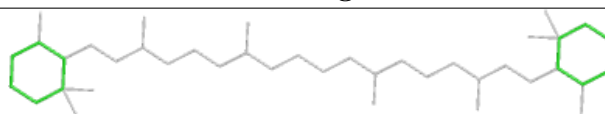
Bond lengths



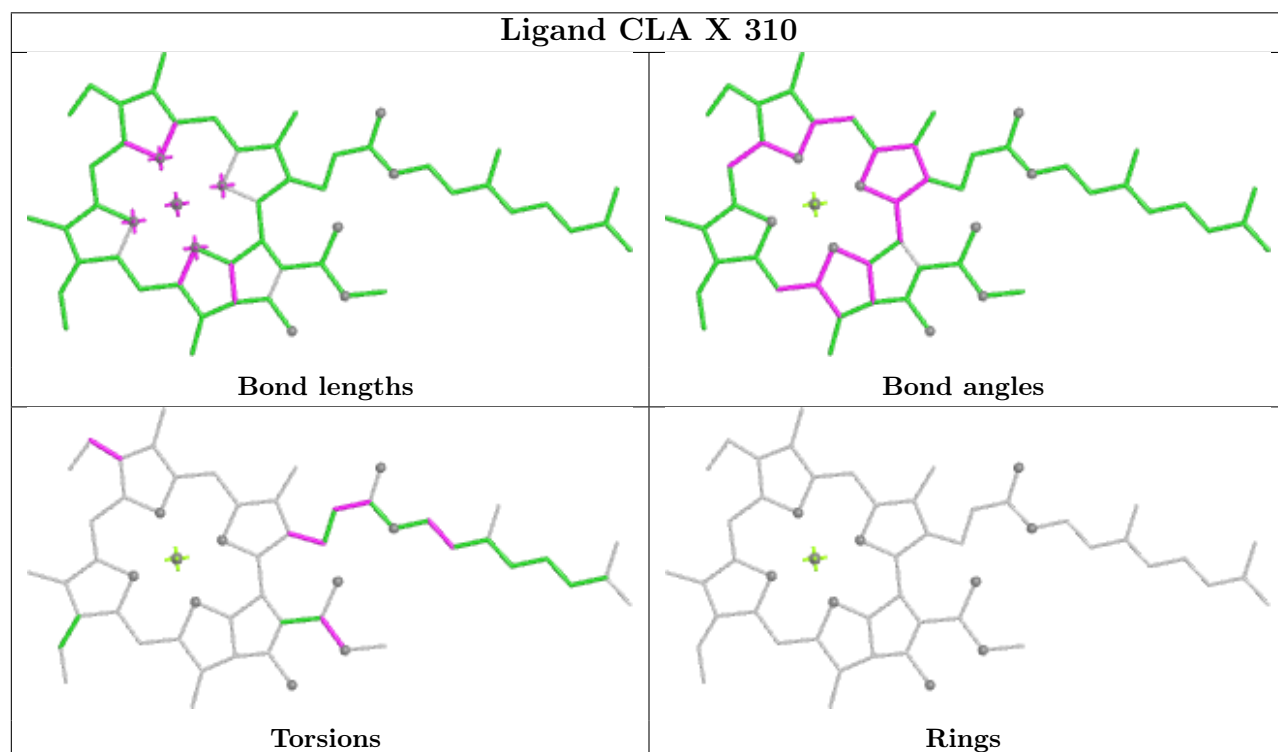
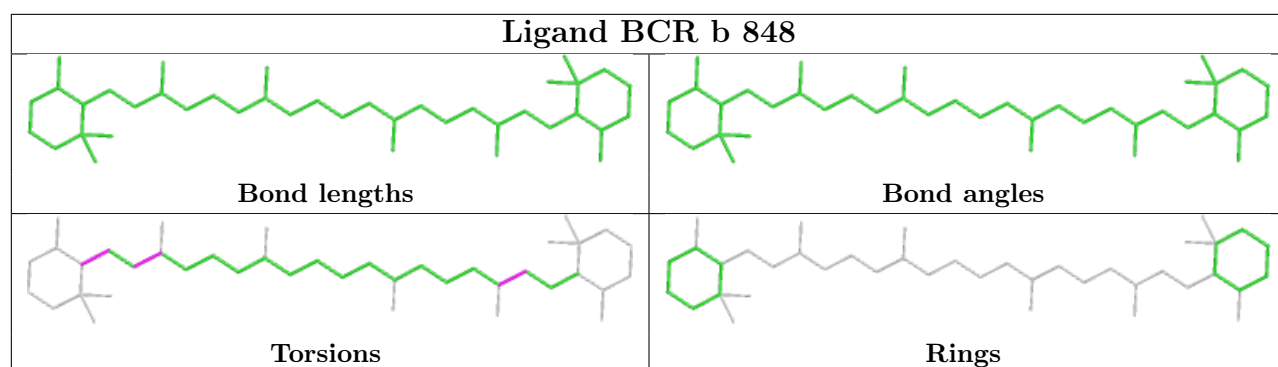
Bond angles



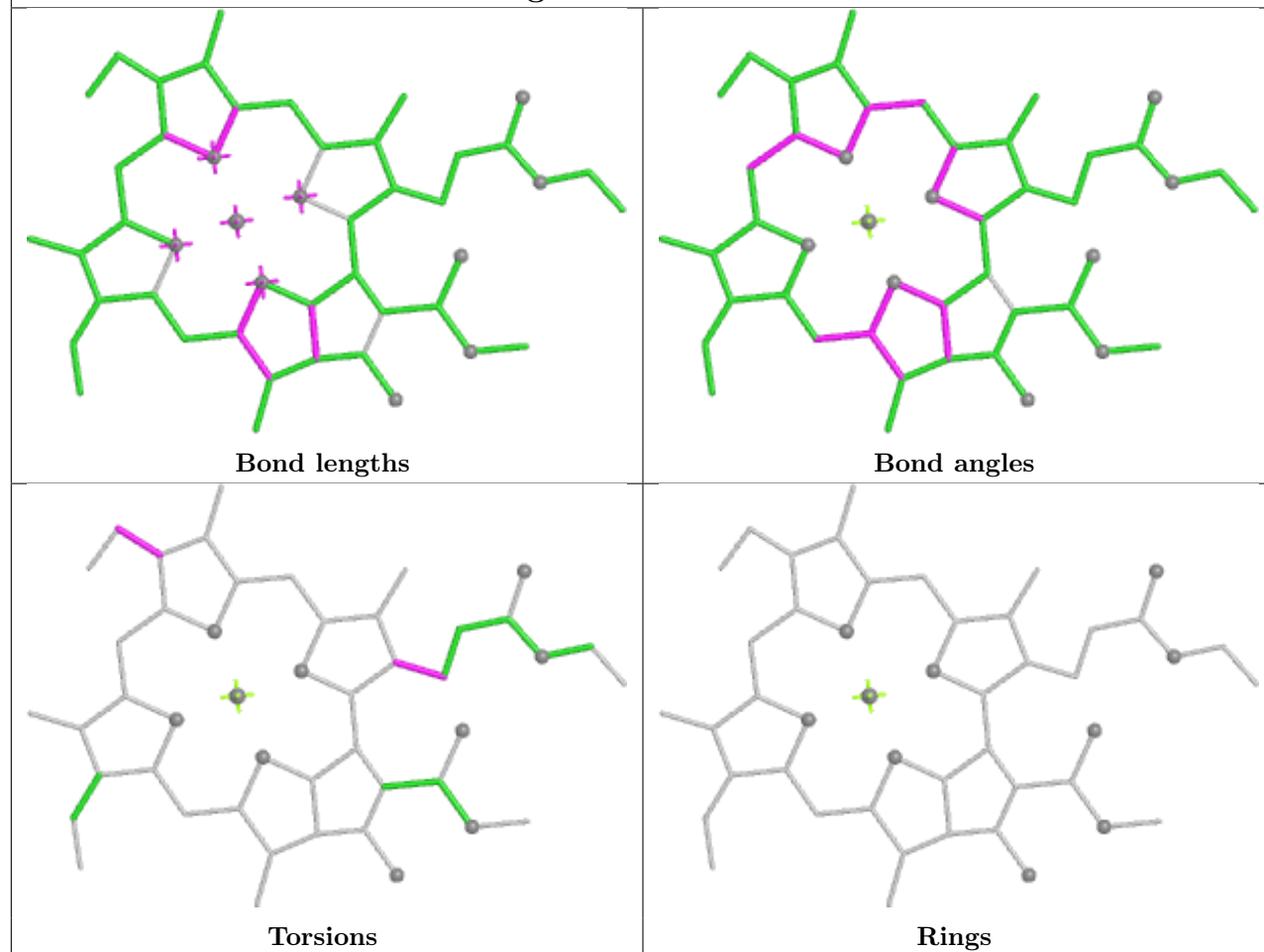
Torsions



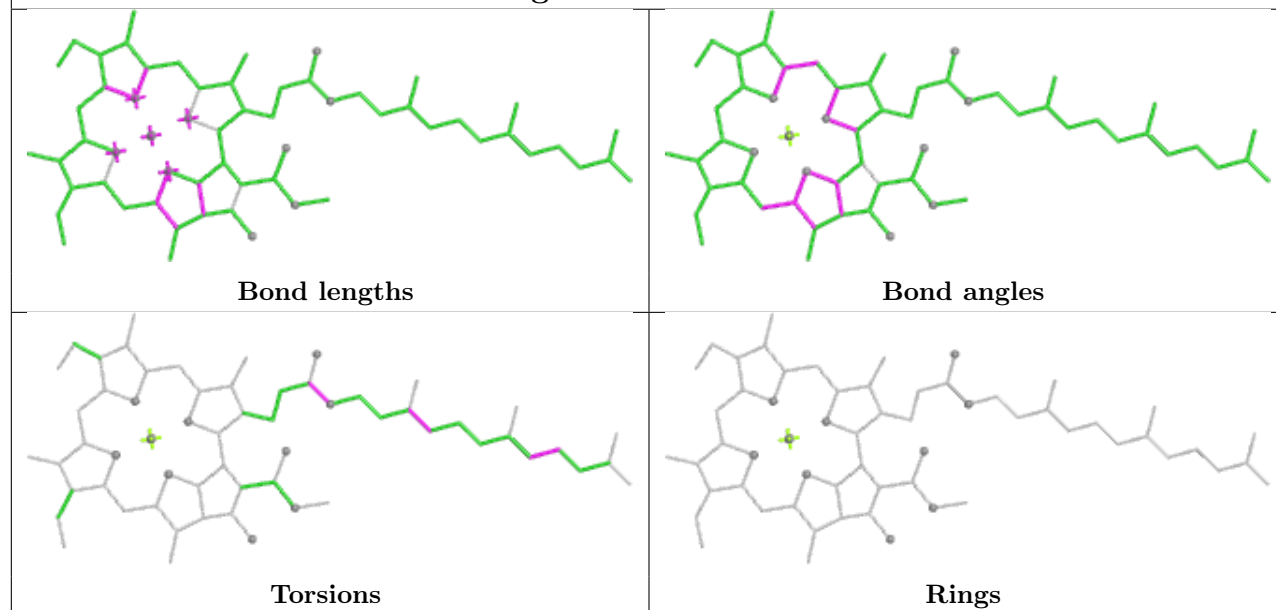
Rings

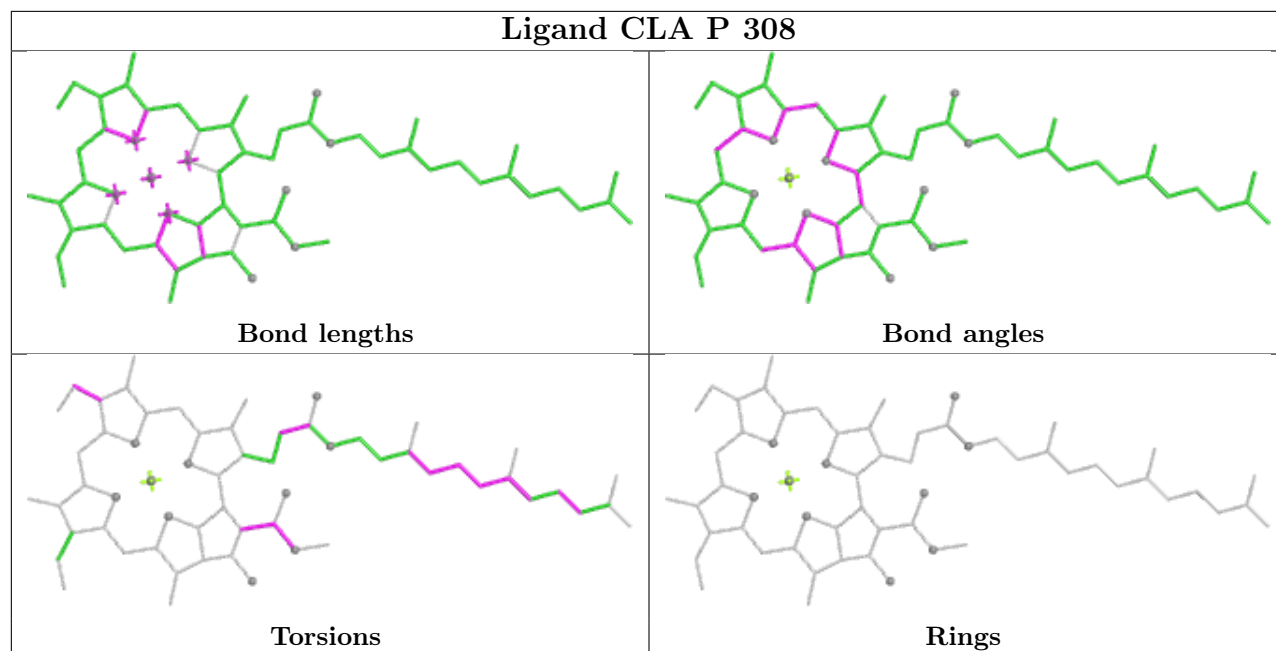
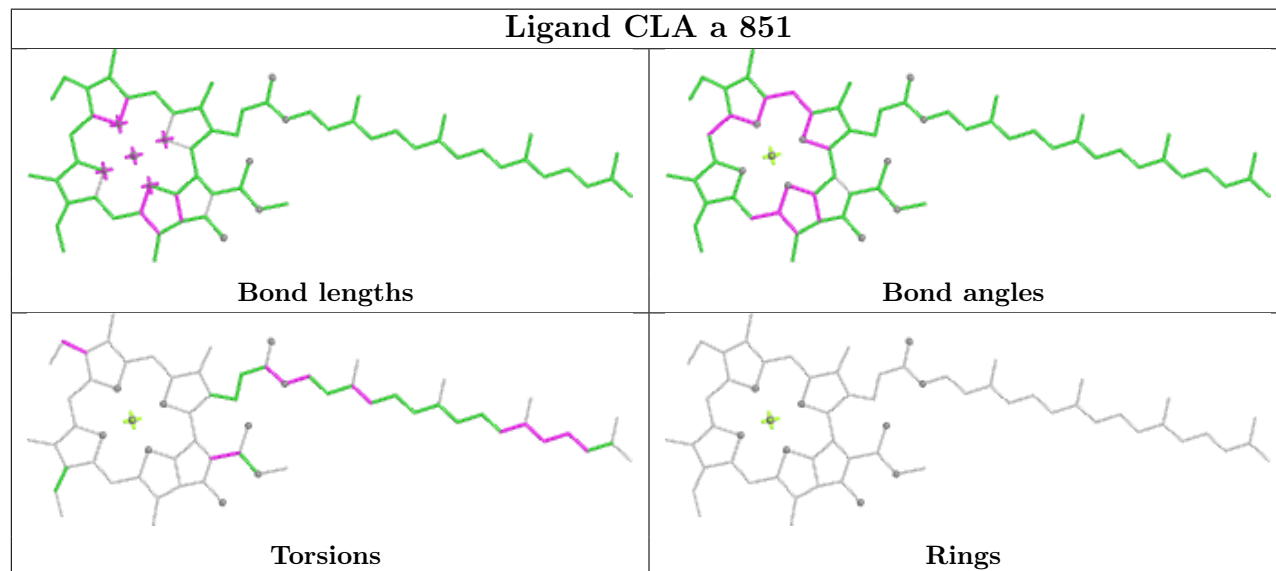


Ligand CLA B 303

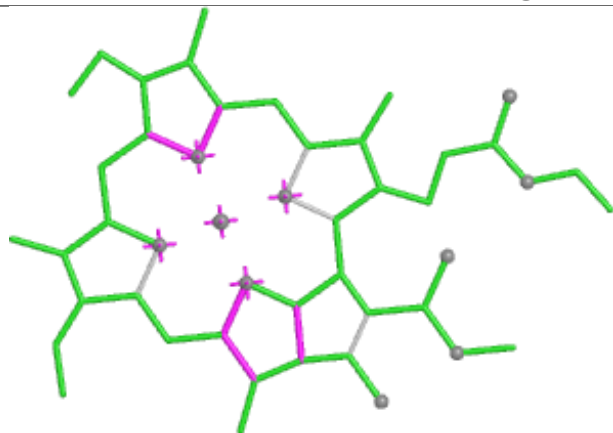


Ligand CLA H 310

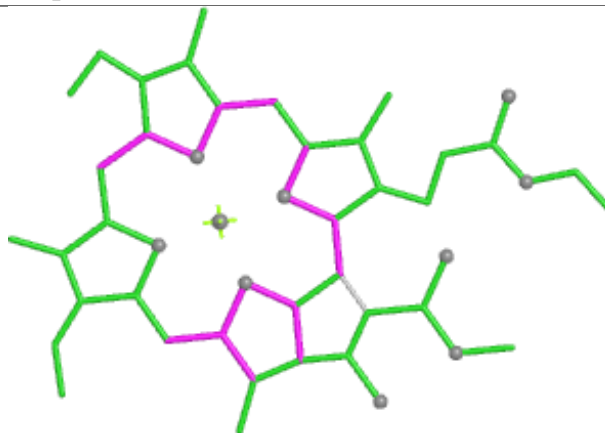


Ligand CLA P 308**Ligand CLA a 851**

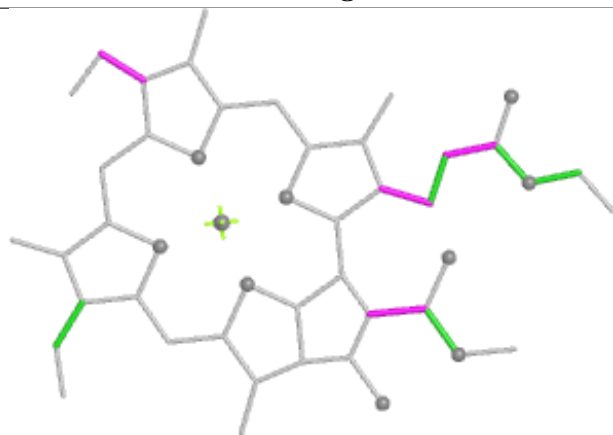
Ligand CLA p 306



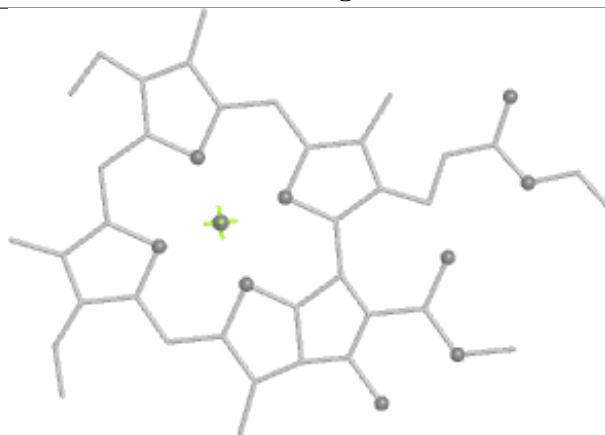
Bond lengths



Bond angles

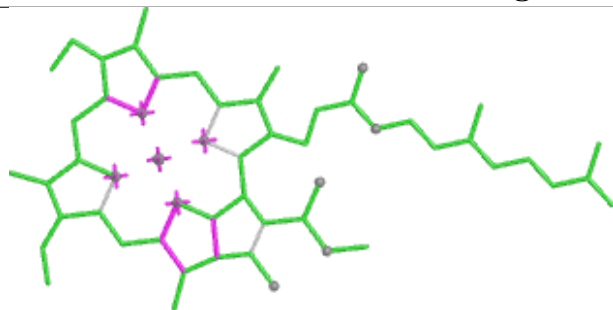


Torsions

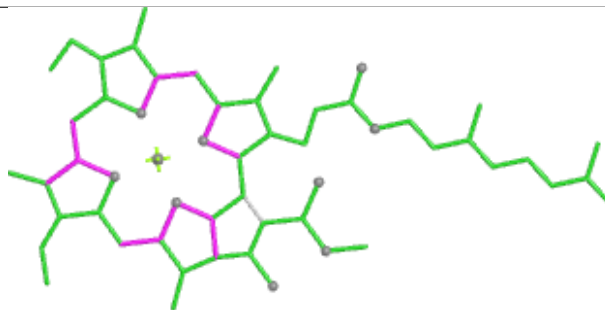


Rings

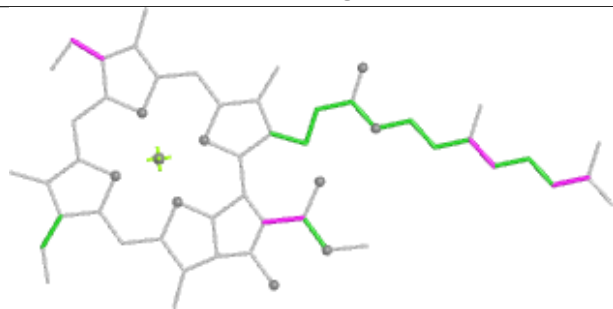
Ligand CLA D 301



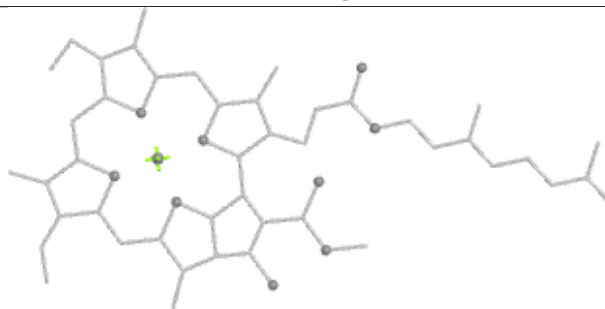
Bond lengths



Bond angles

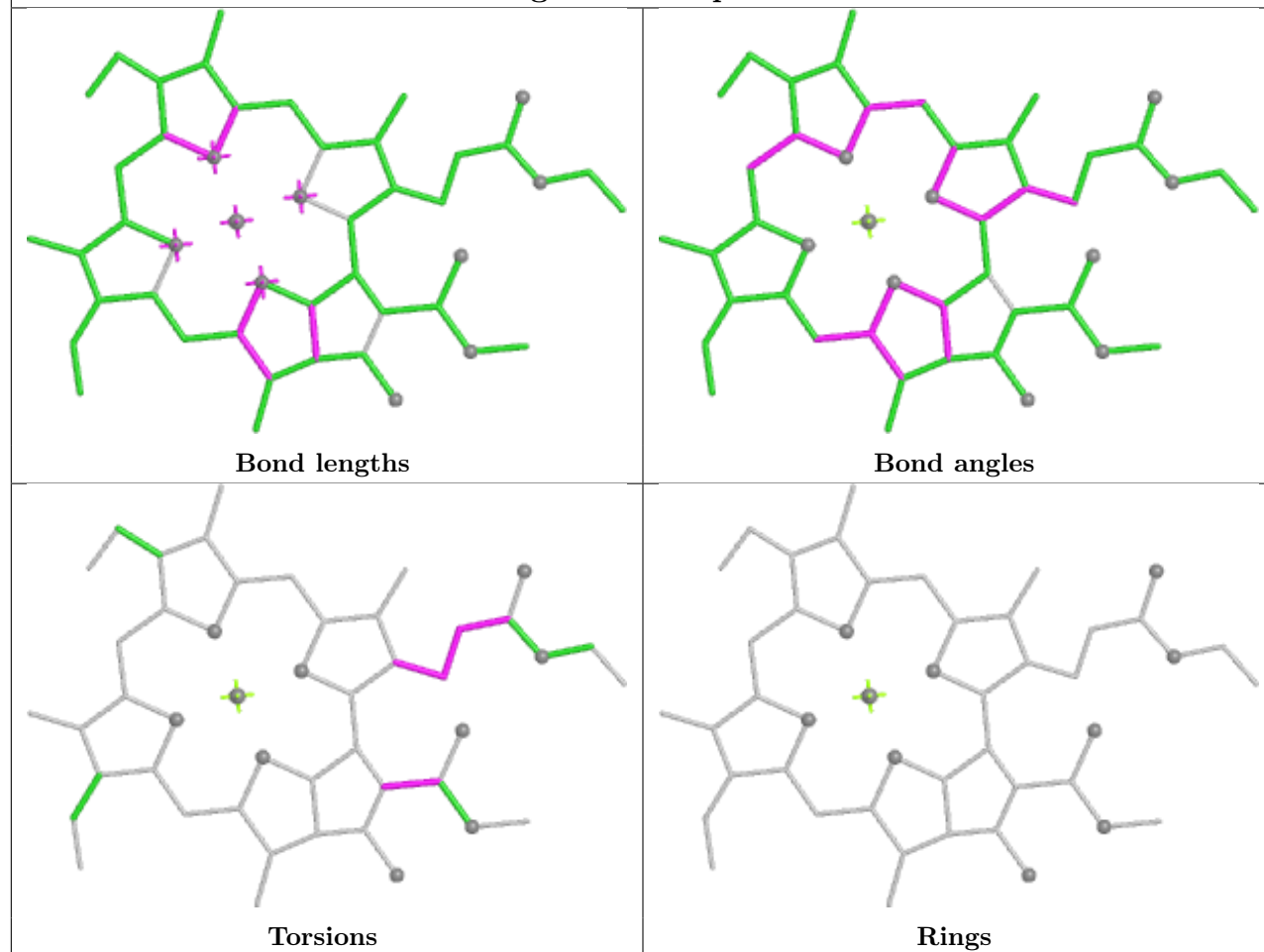


Torsions

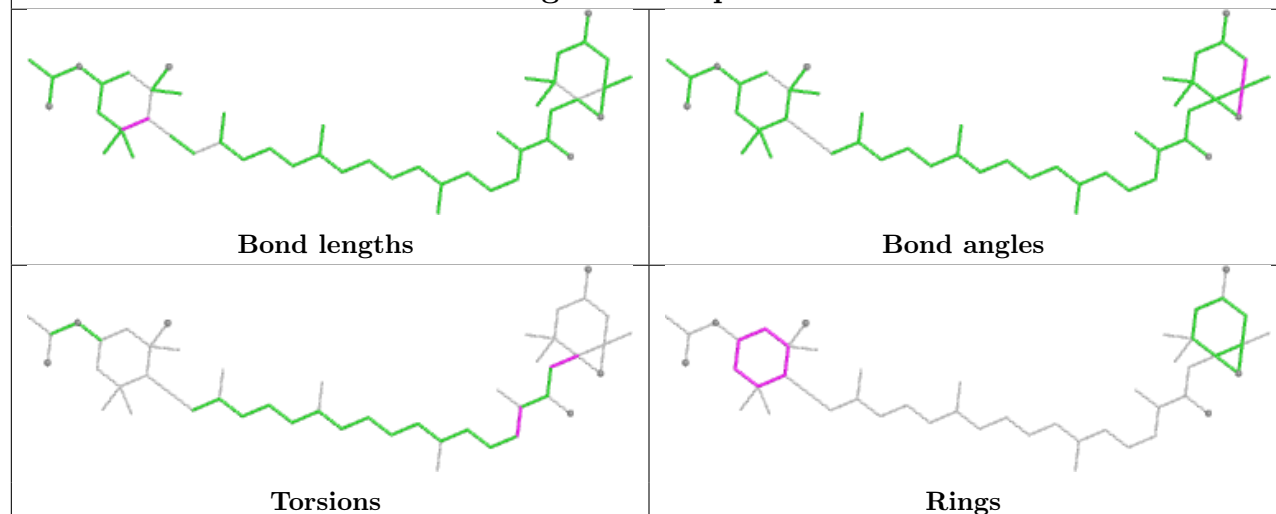


Rings

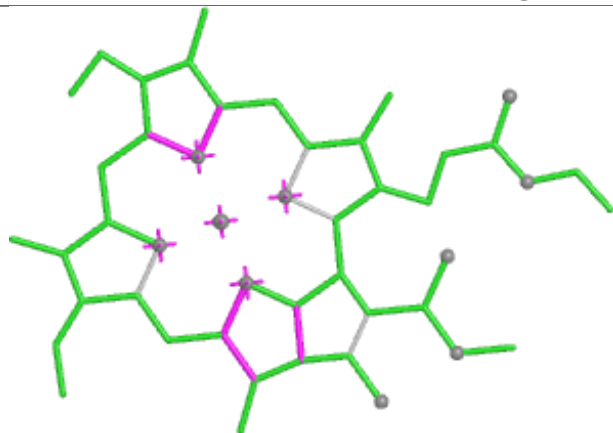
Ligand CLA q 313



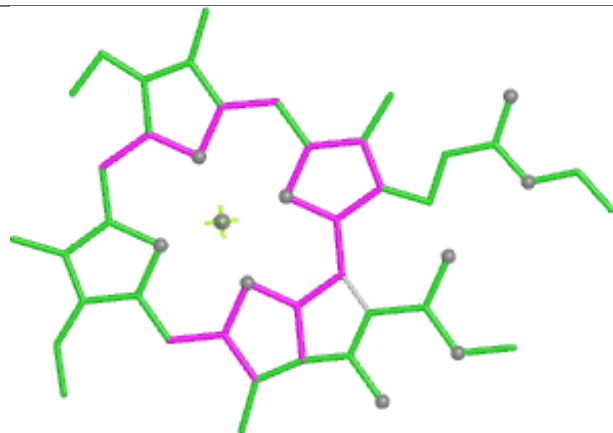
Ligand A86 q 316



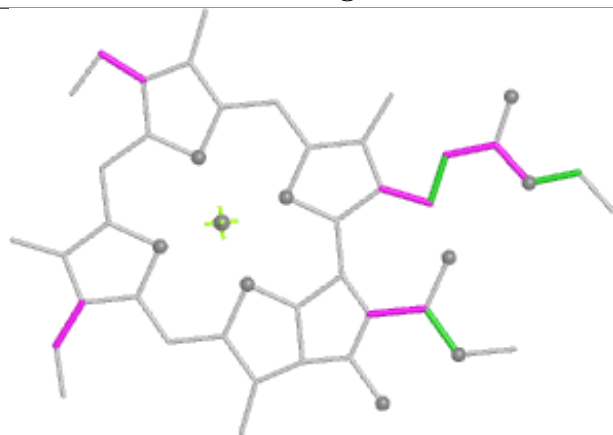
Ligand CLA E 314



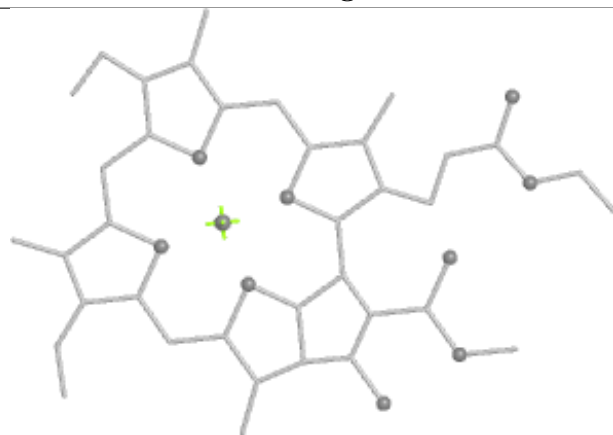
Bond lengths



Bond angles

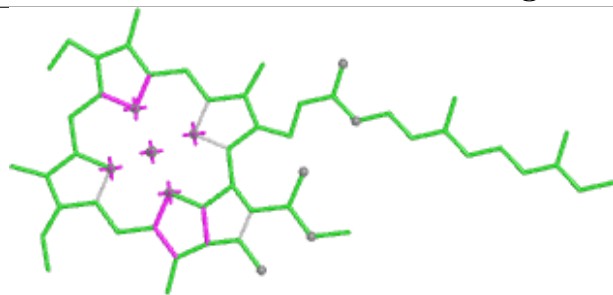


Torsions

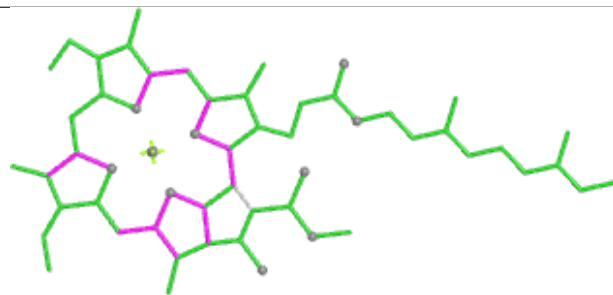


Rings

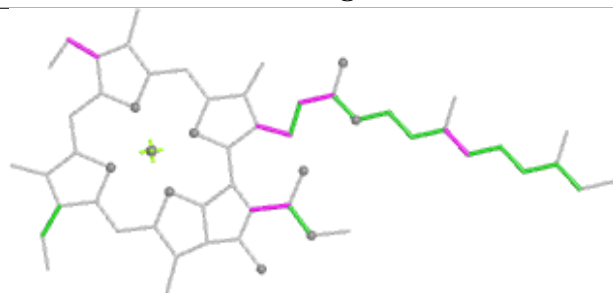
Ligand CLA I 205



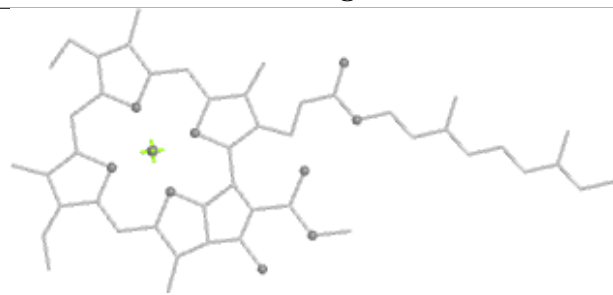
Bond lengths



Bond angles

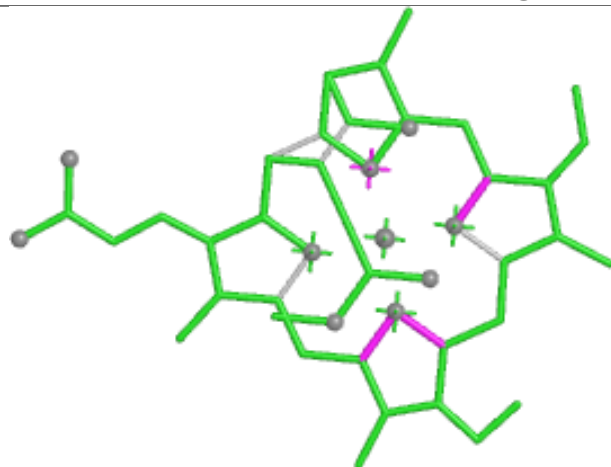


Torsions

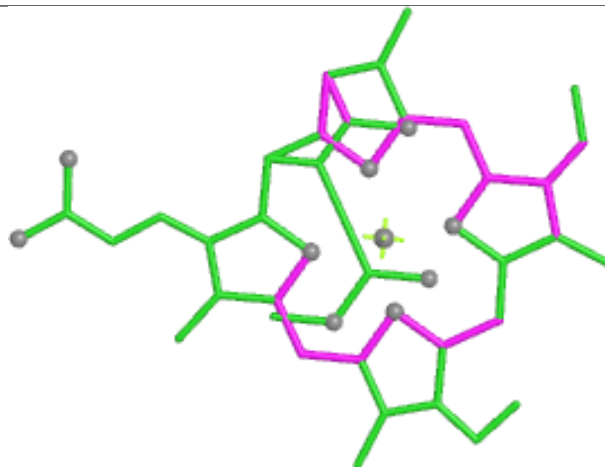


Rings

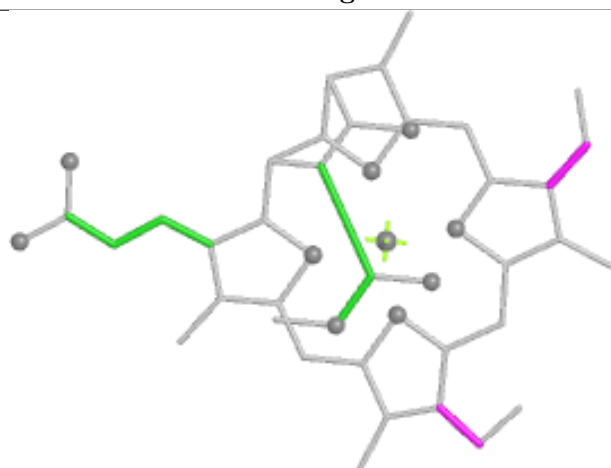
Ligand KC2 N 303



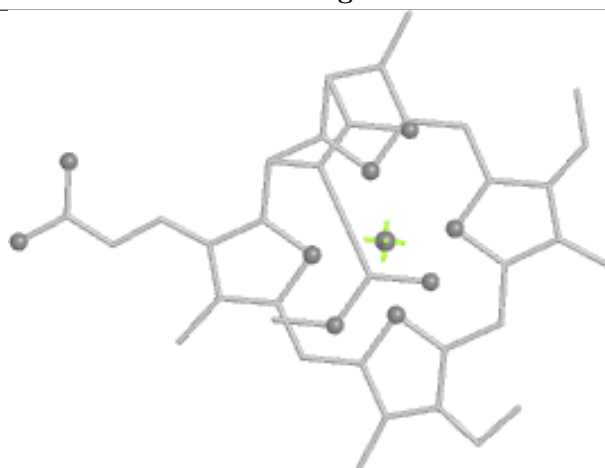
Bond lengths



Bond angles



Torsions



Rings

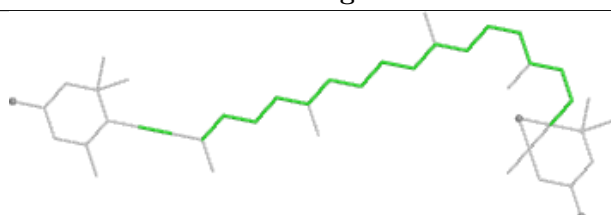
Ligand DD6 X 322



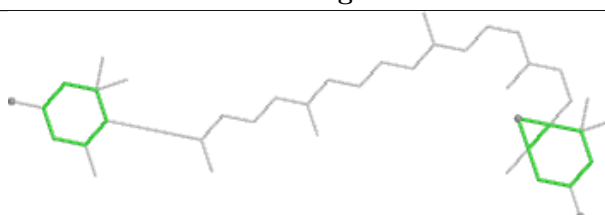
Bond lengths



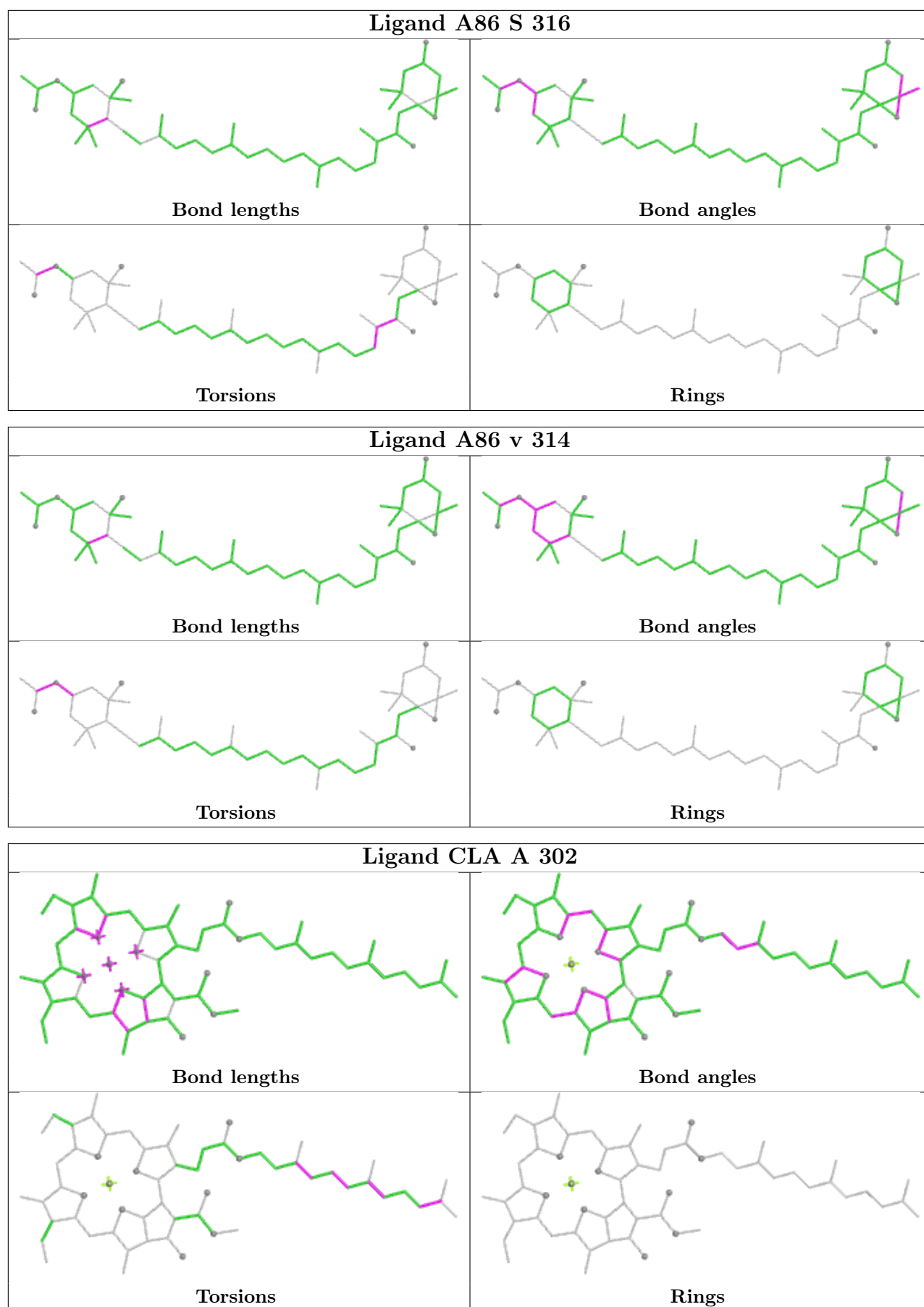
Bond angles

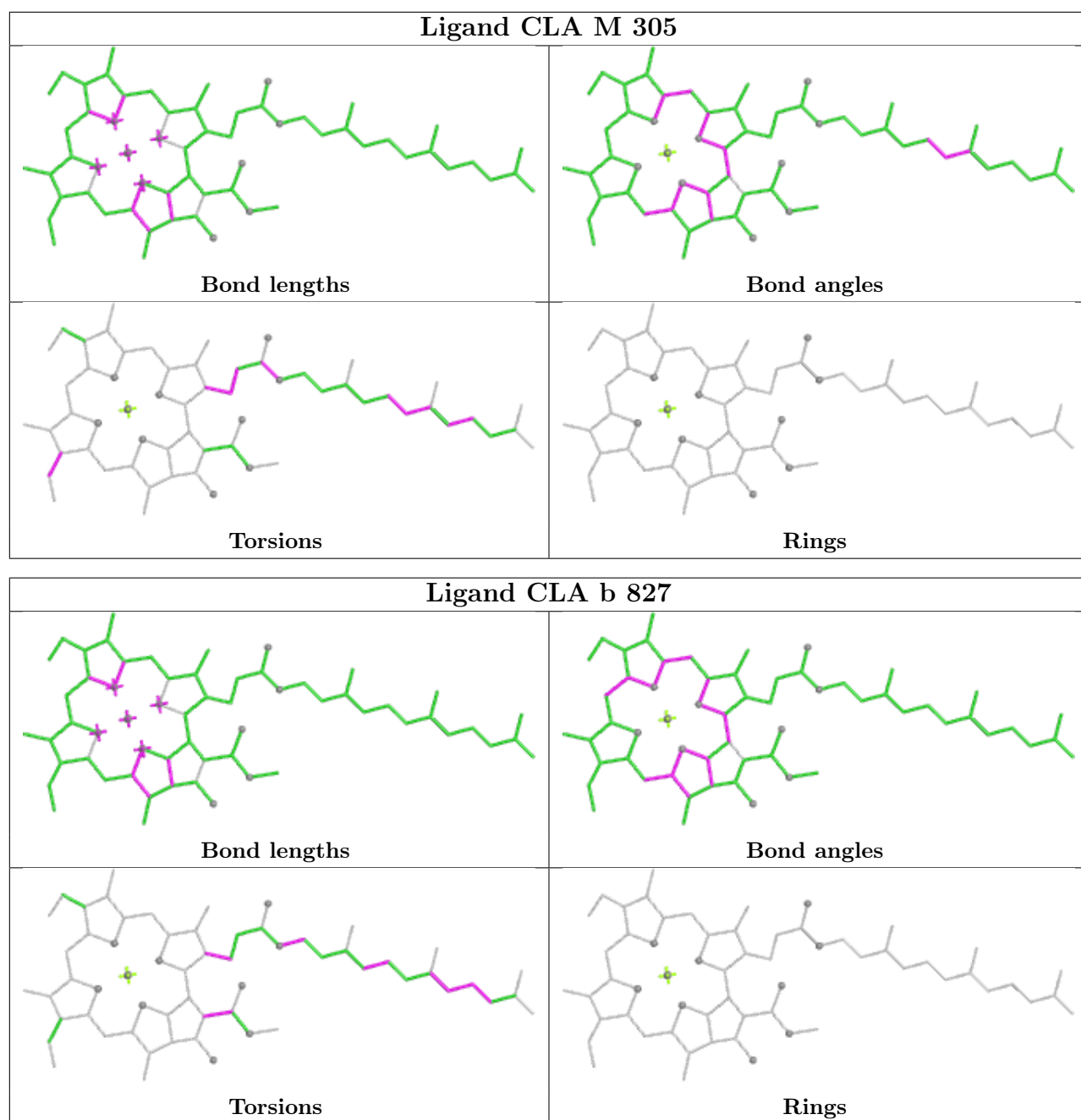


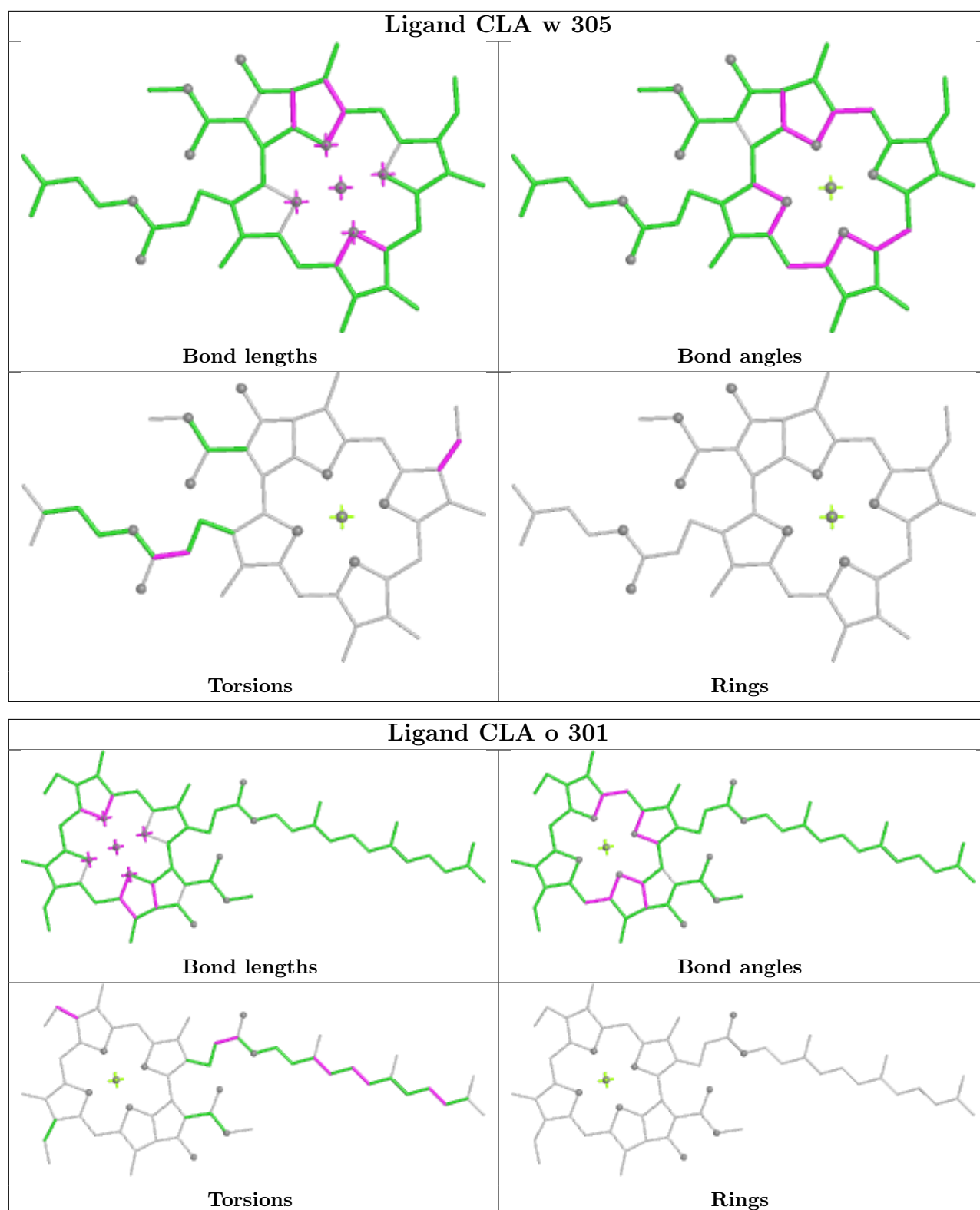
Torsions

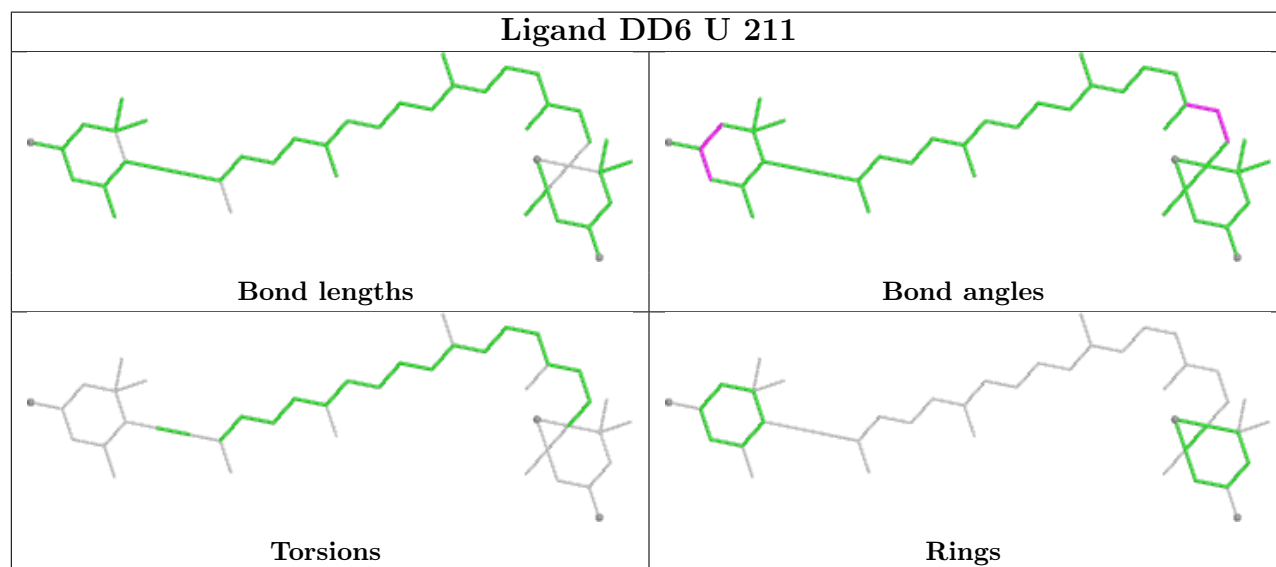
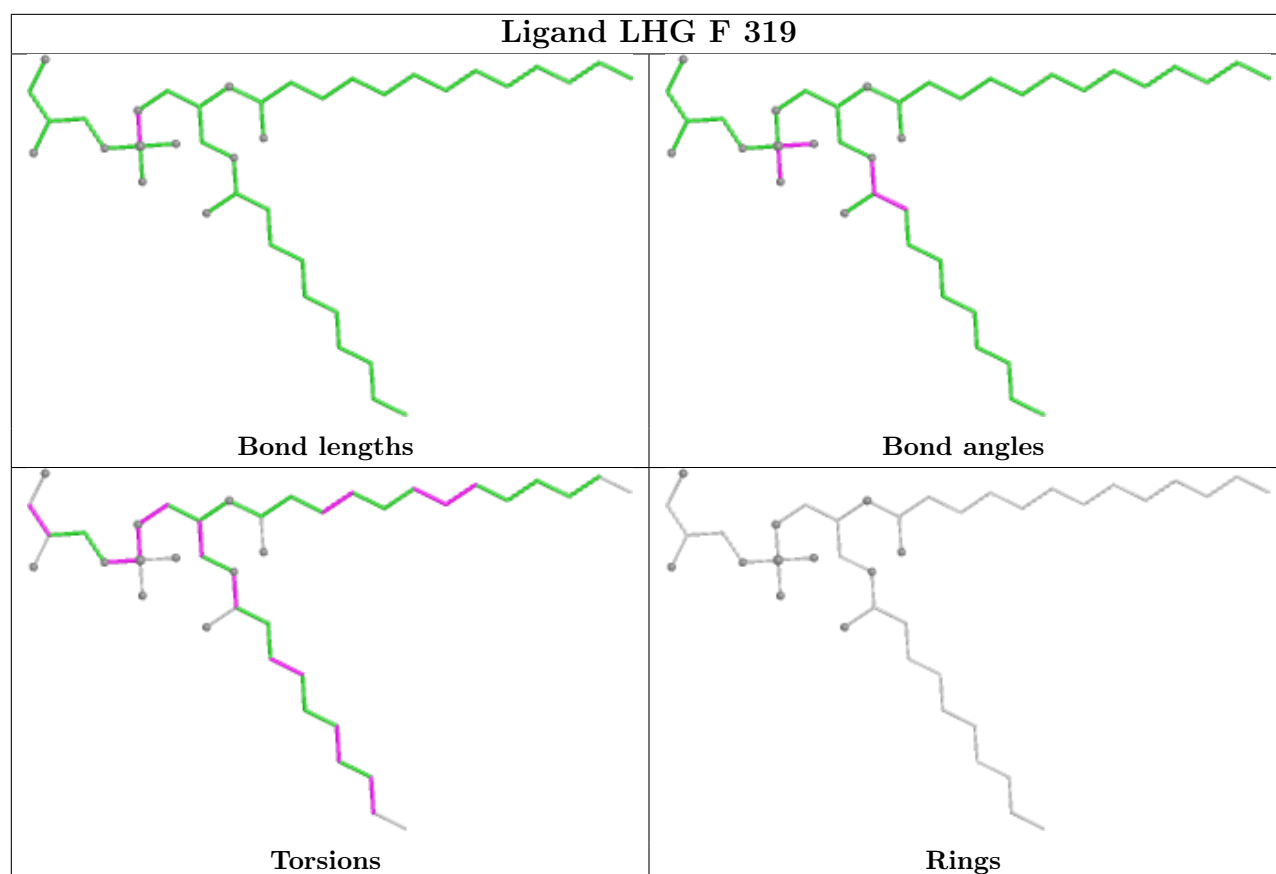


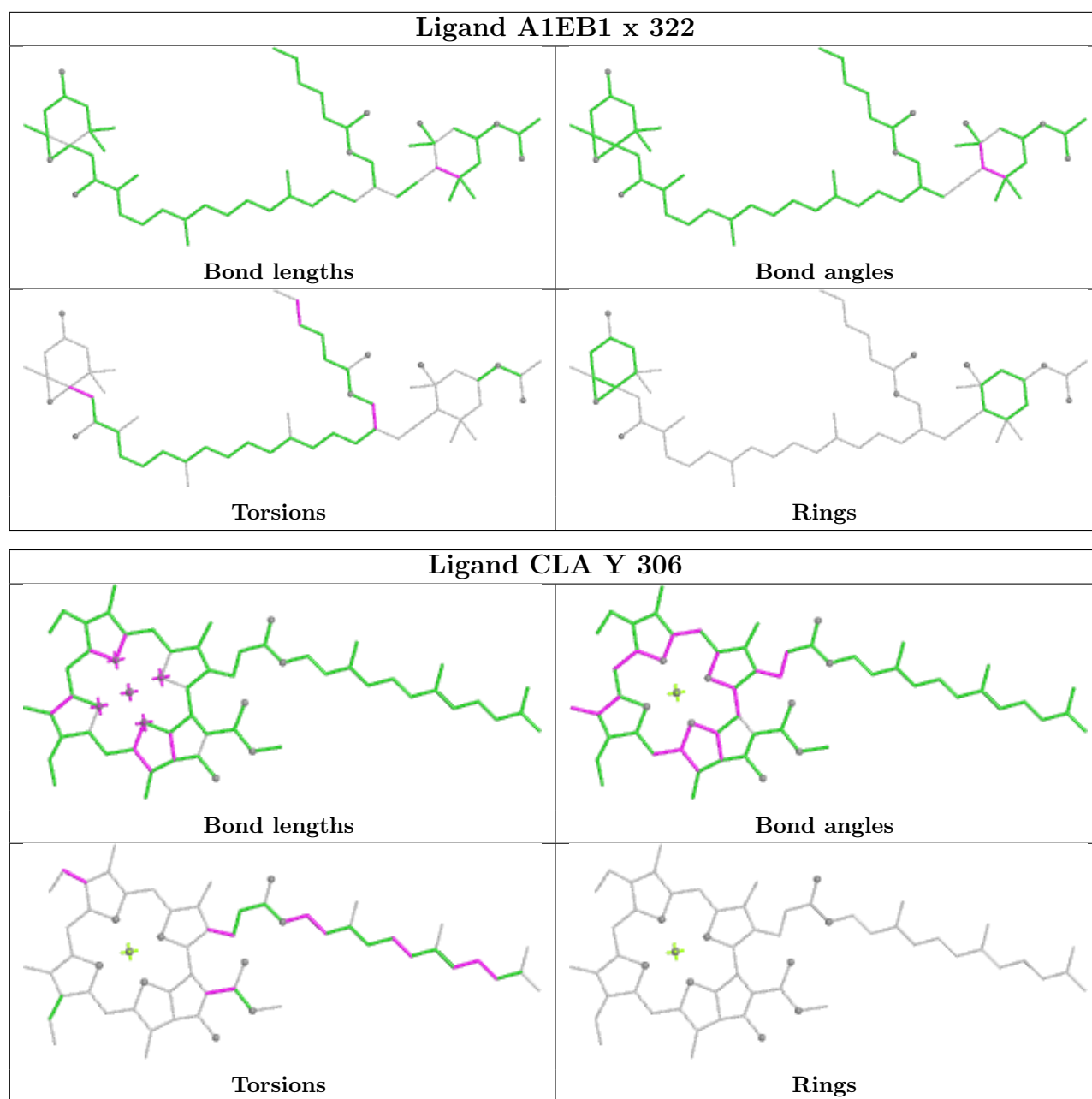
Rings

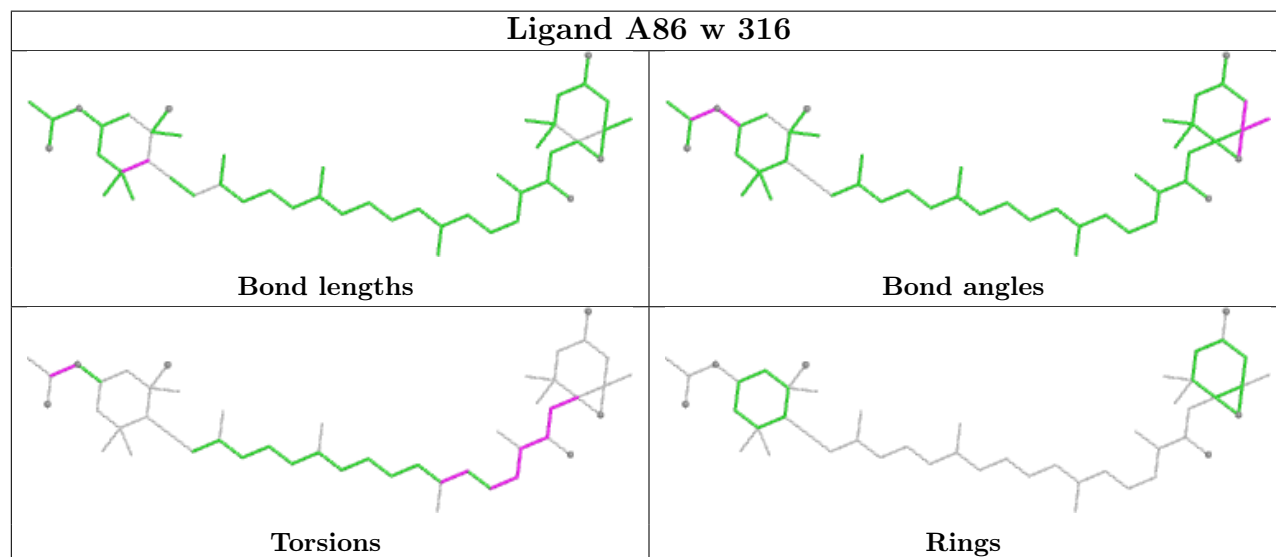
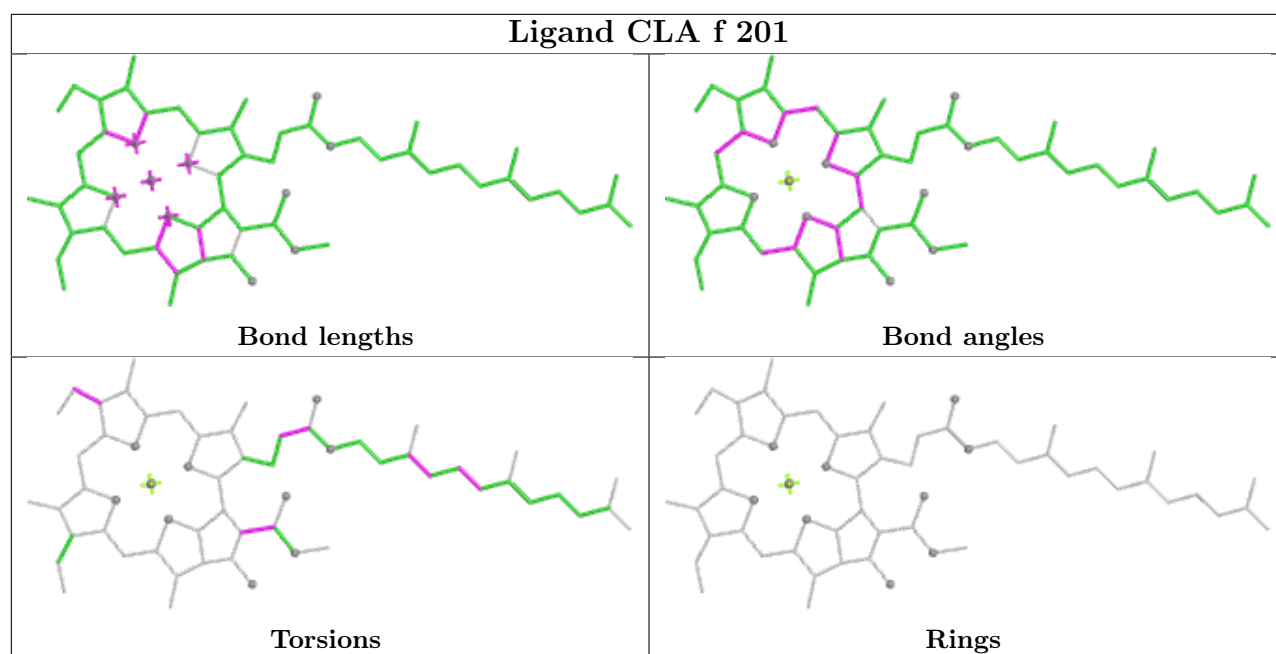


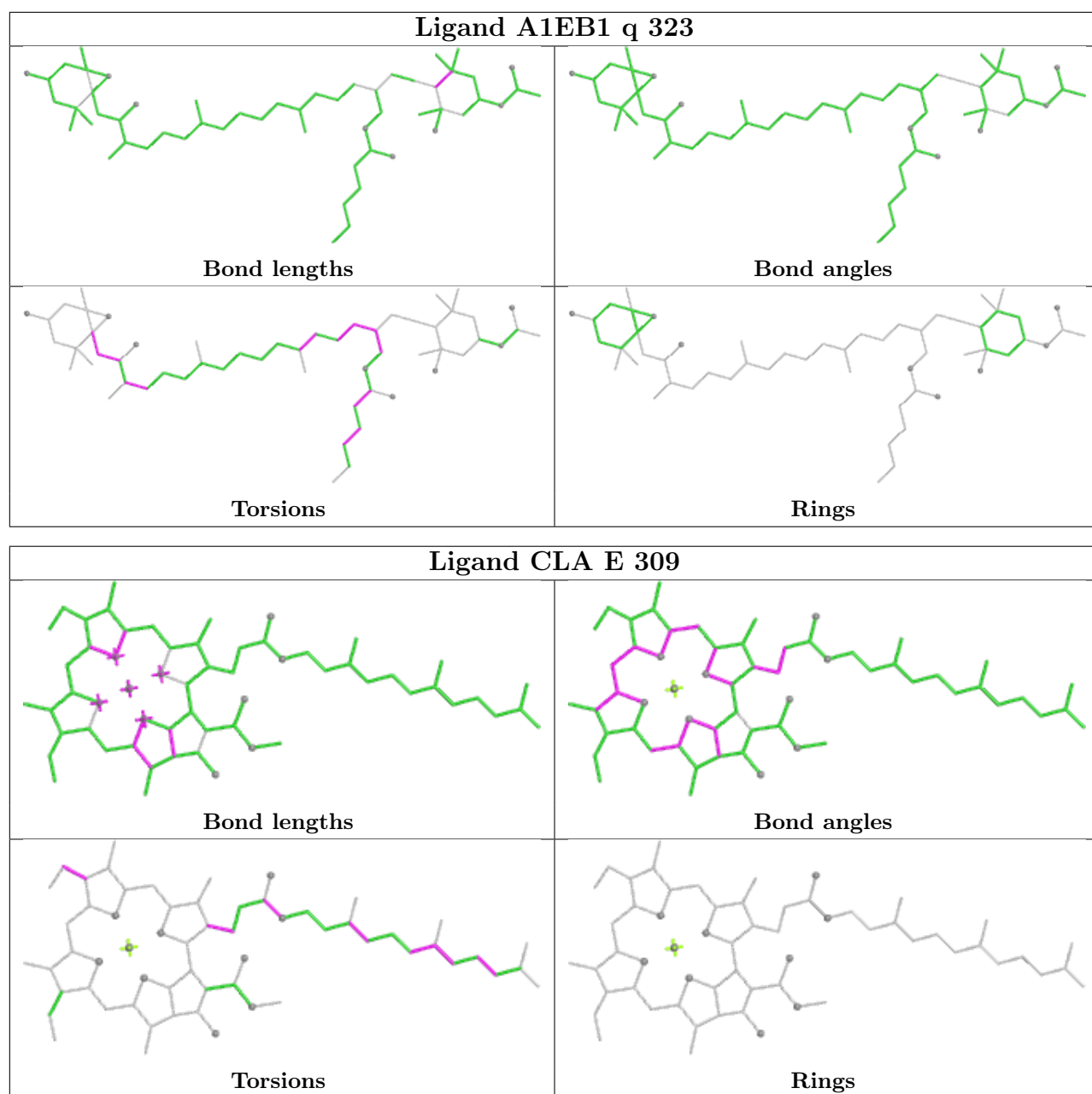


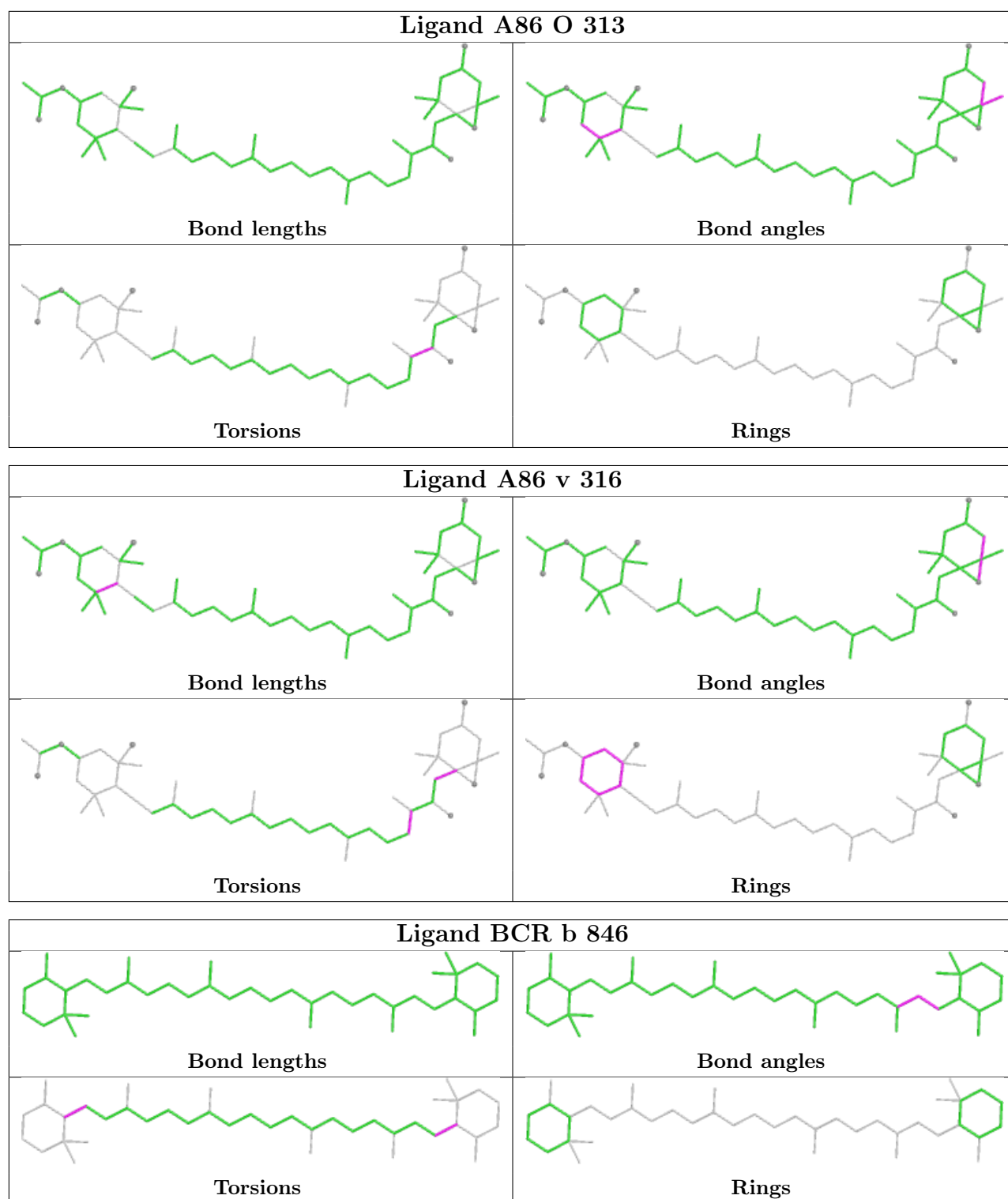


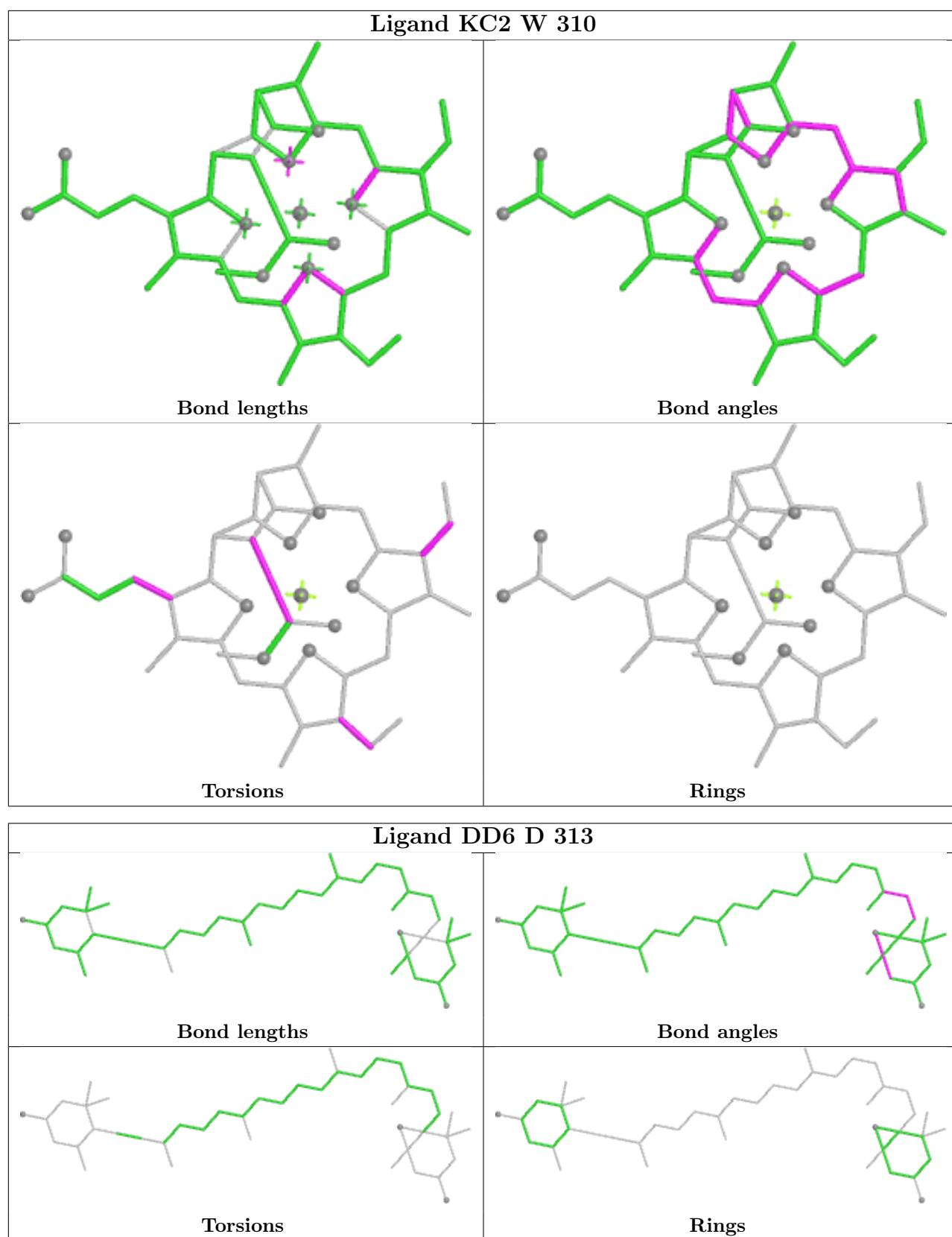


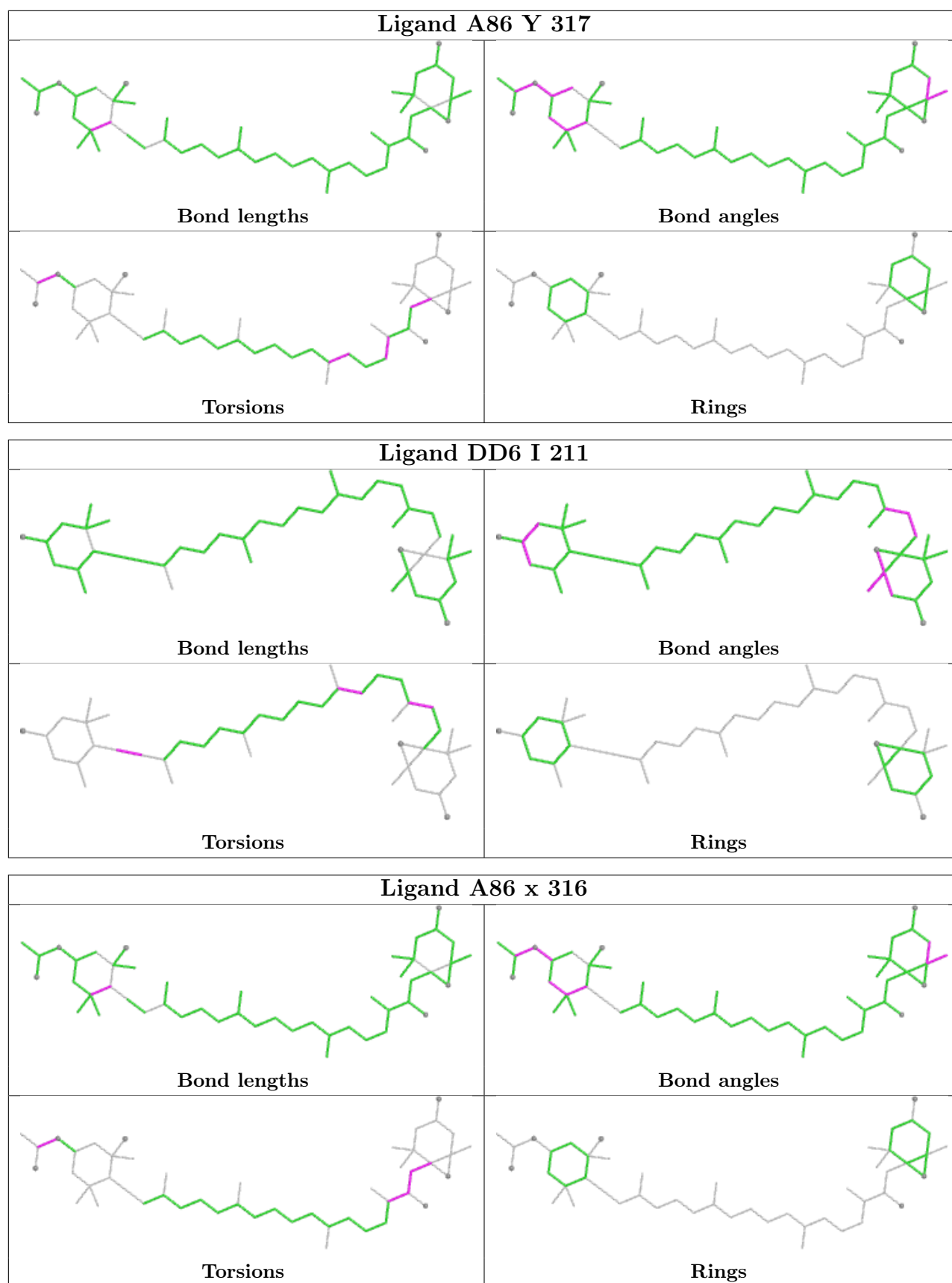




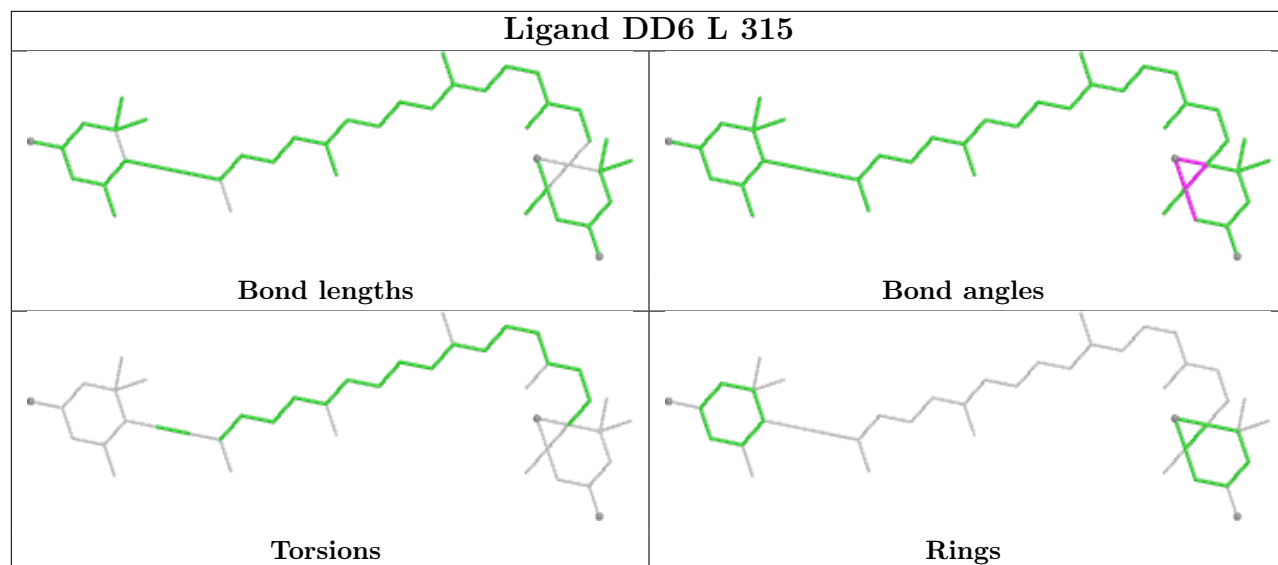




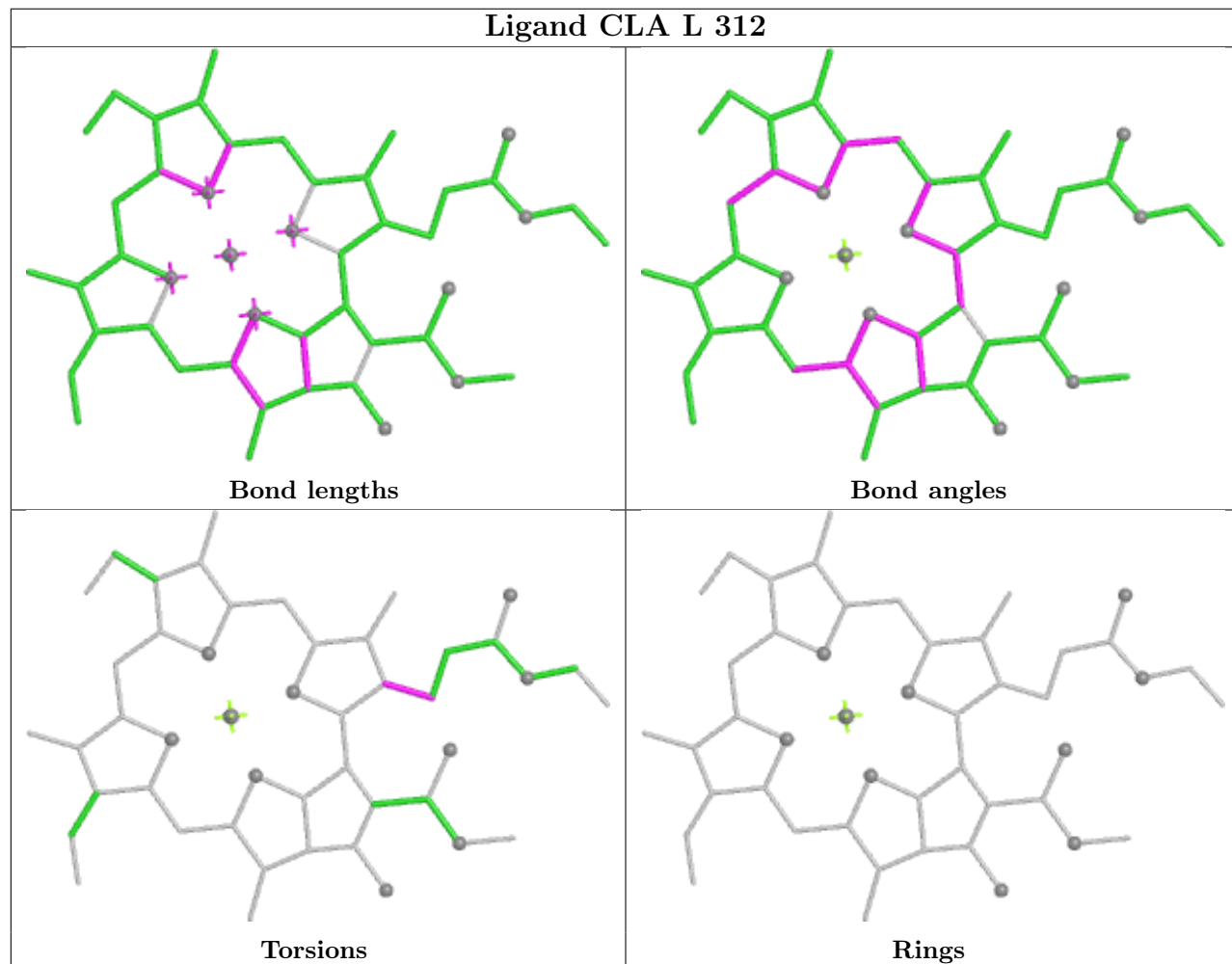


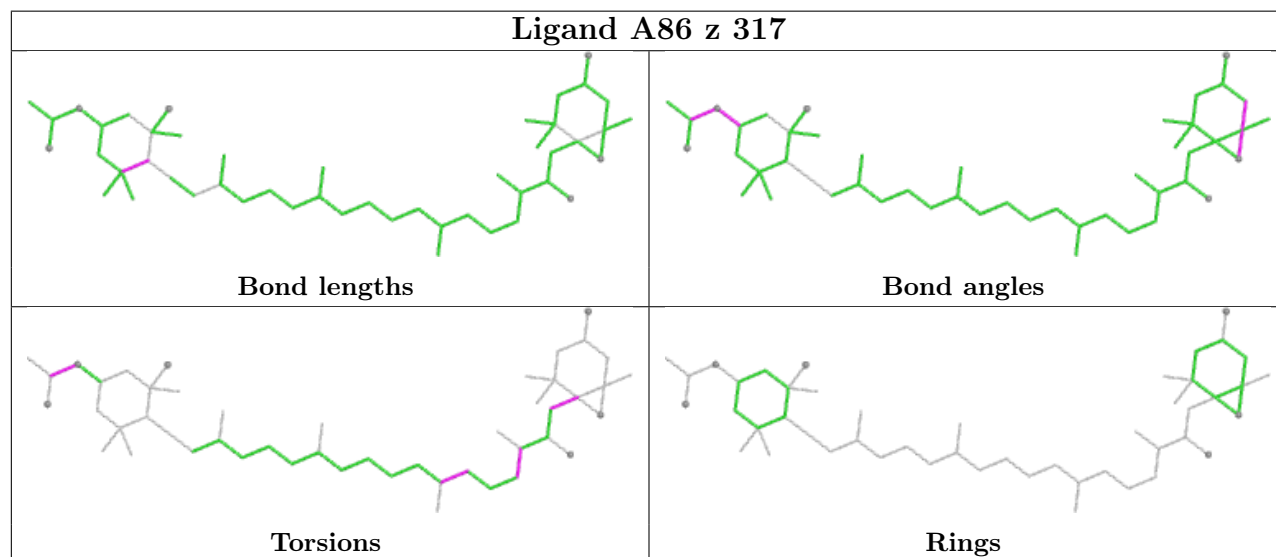
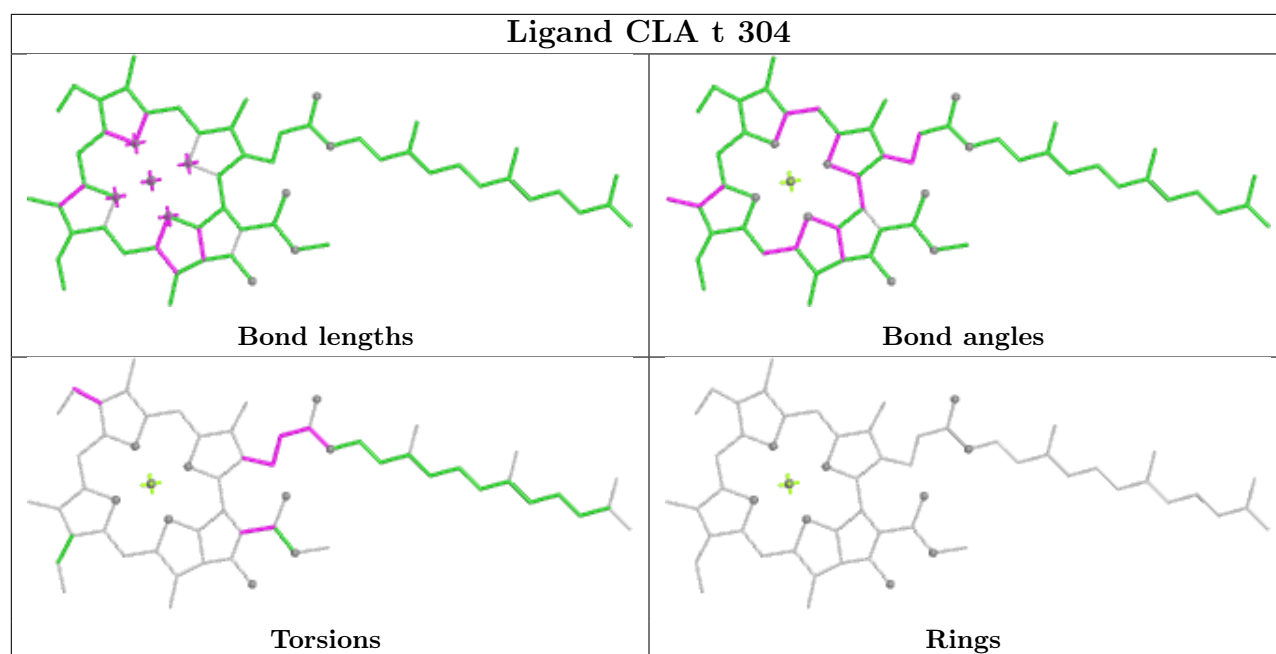


Ligand DD6 L 315

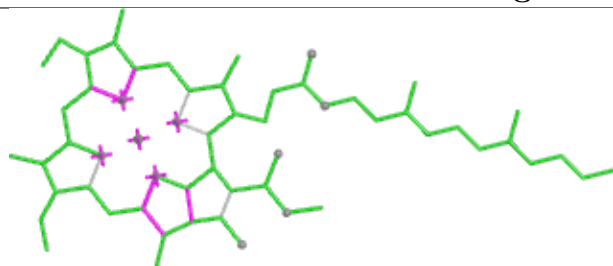


Ligand CLA L 312

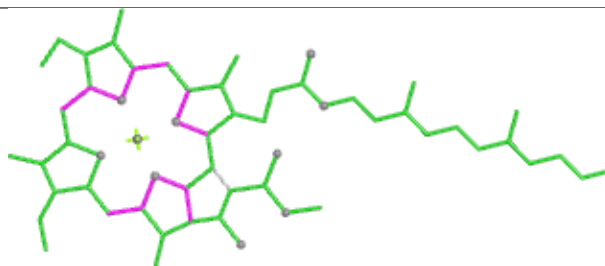




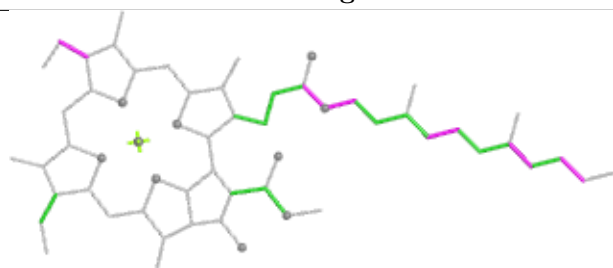
Ligand CLA V 201



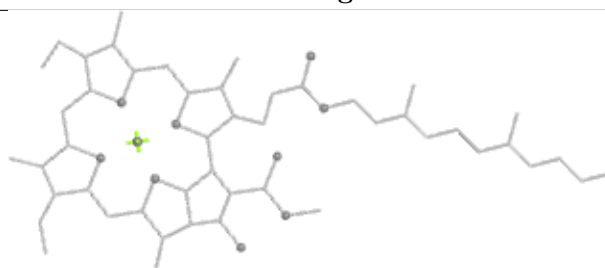
Bond lengths



Bond angles

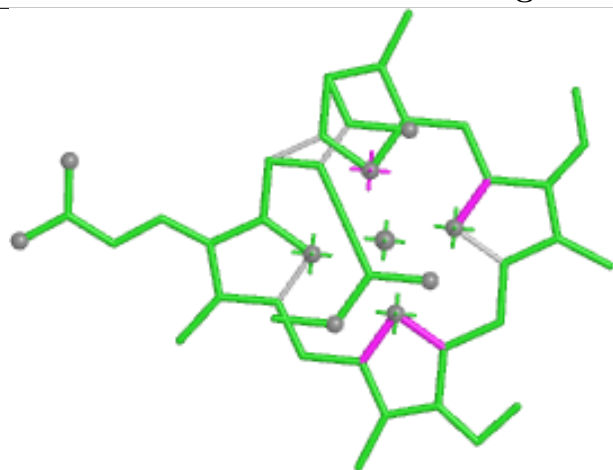


Torsions

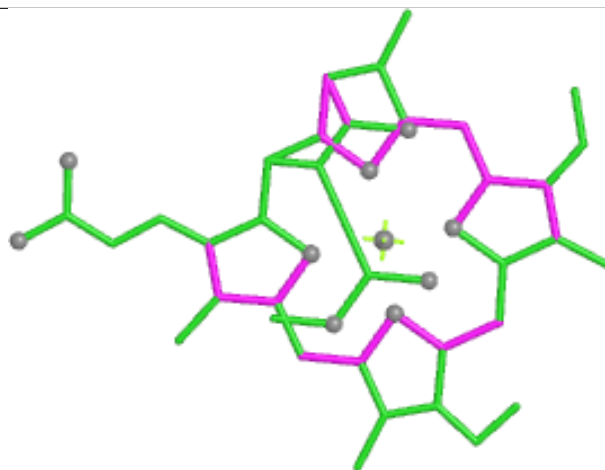


Rings

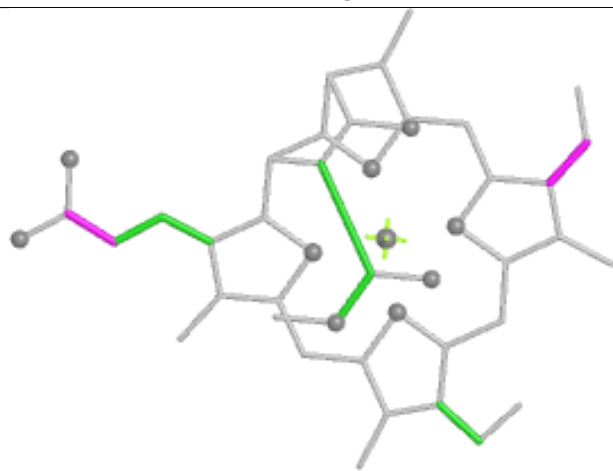
Ligand KC2 w 307



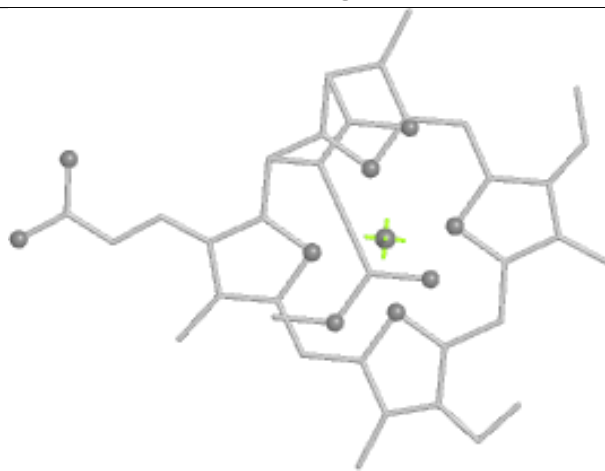
Bond lengths



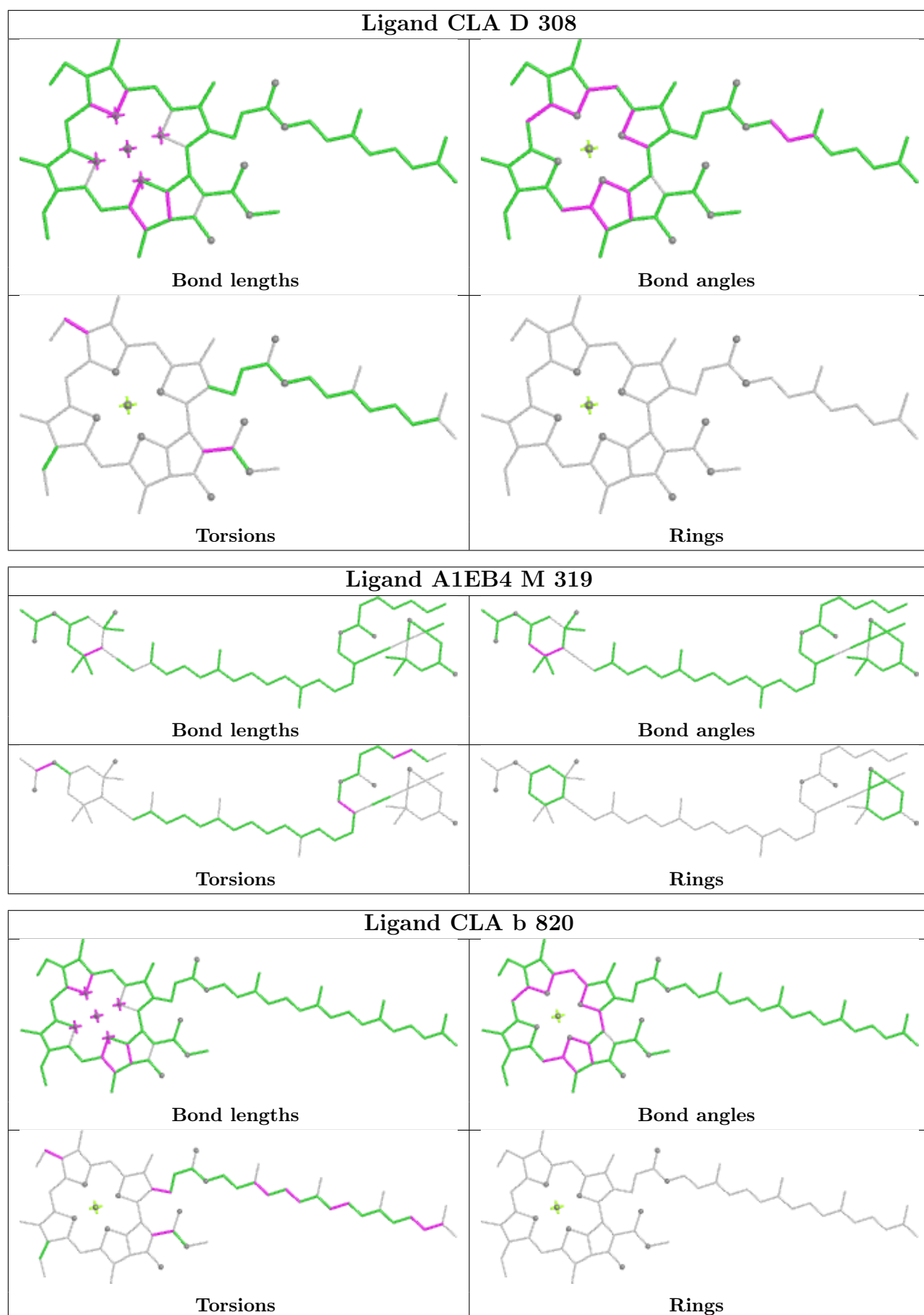
Bond angles

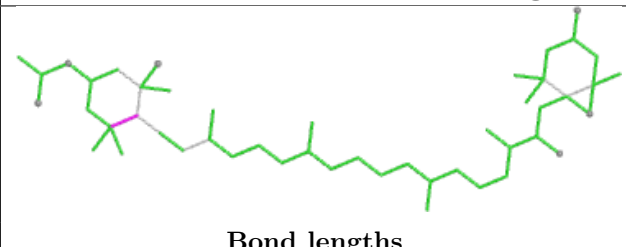
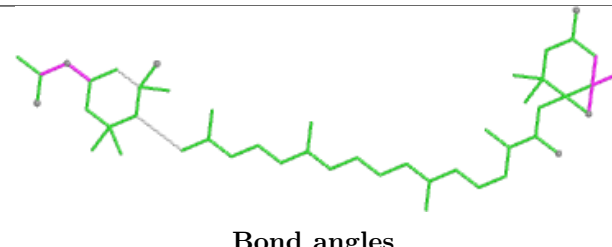
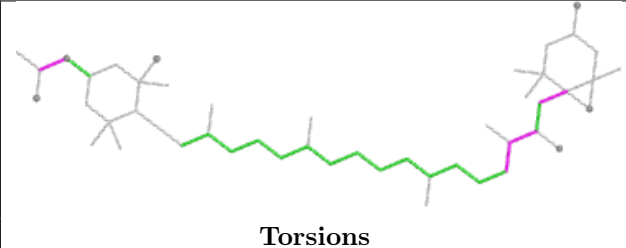
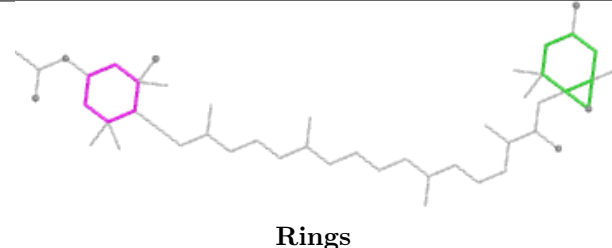


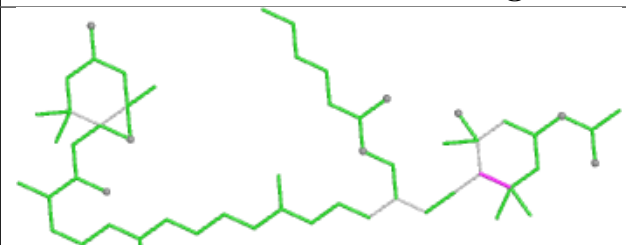
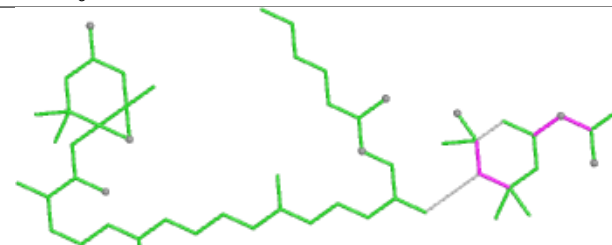
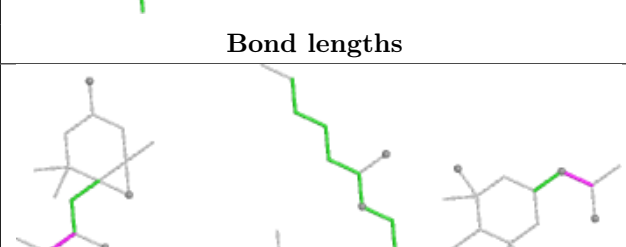
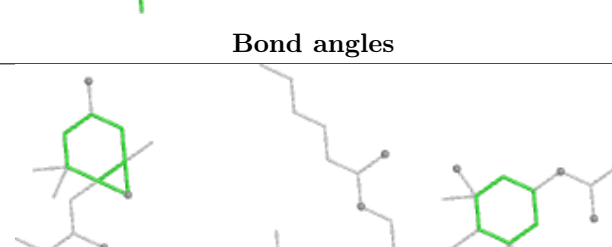
Torsions

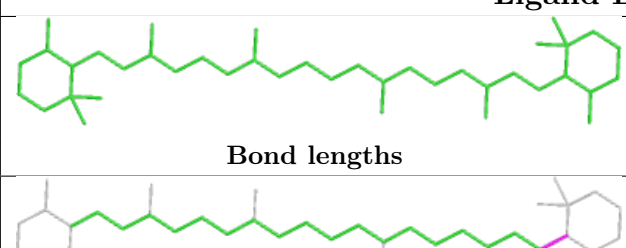
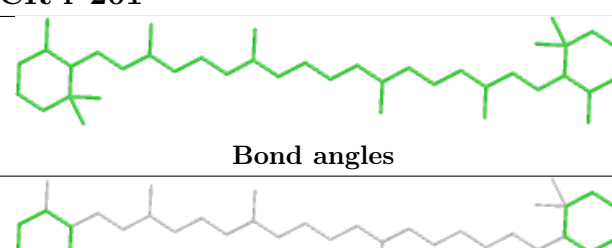


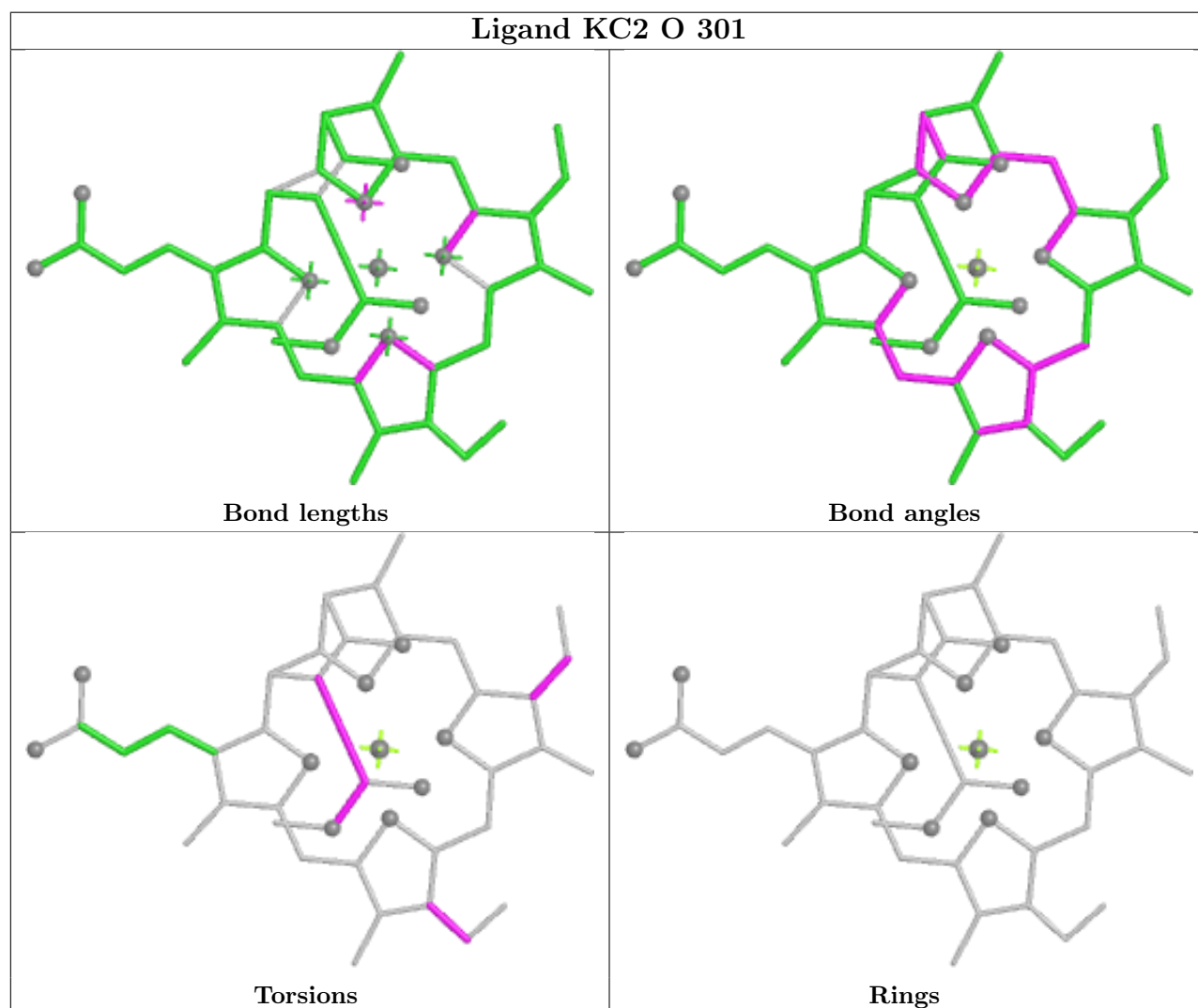
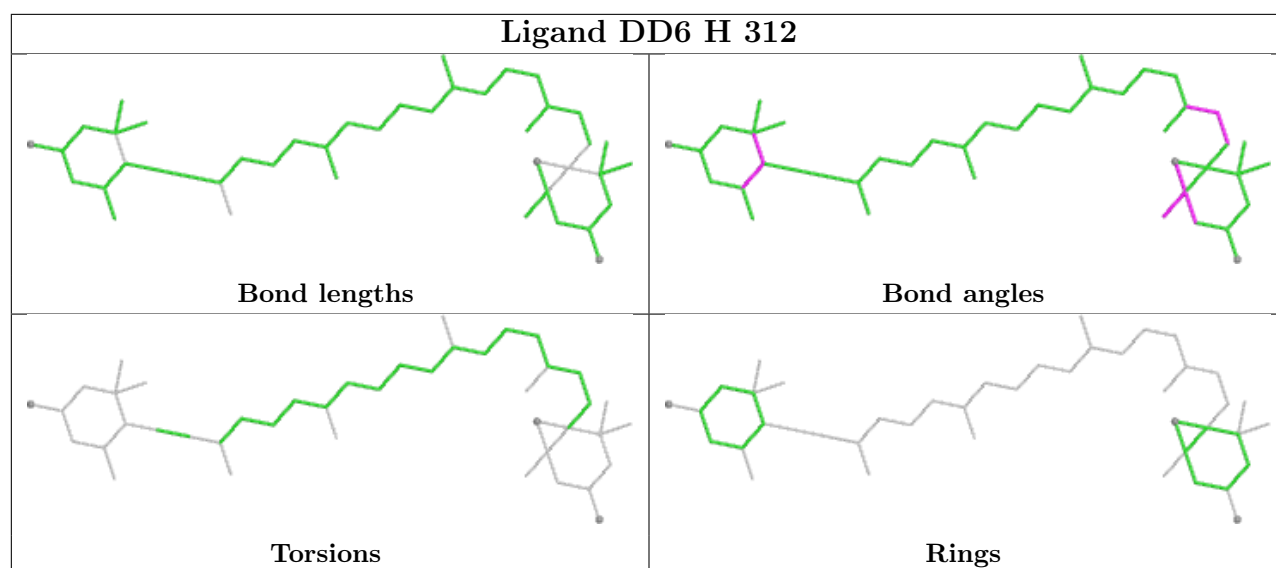
Rings



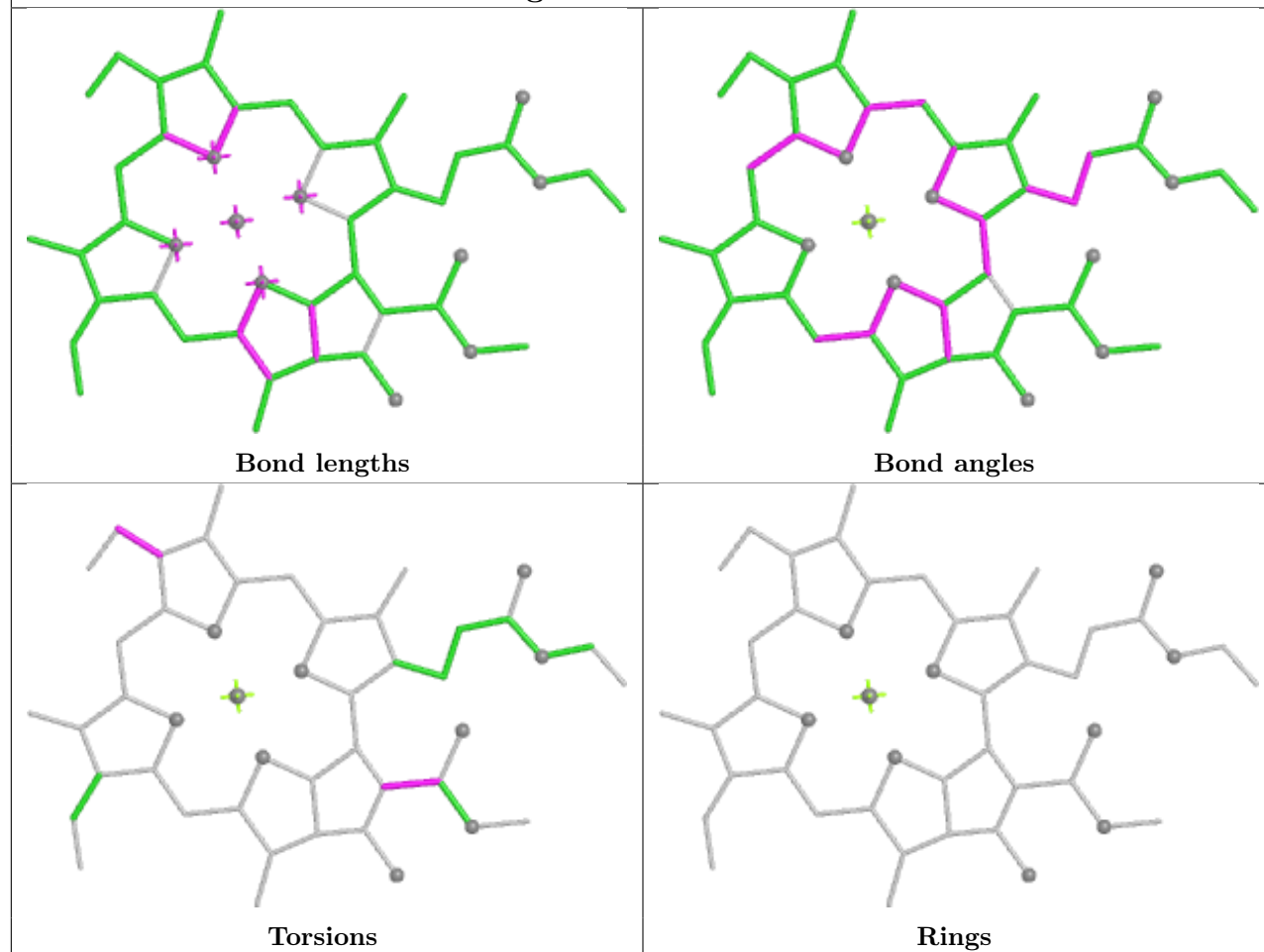
Ligand A86 C 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EB1 y 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

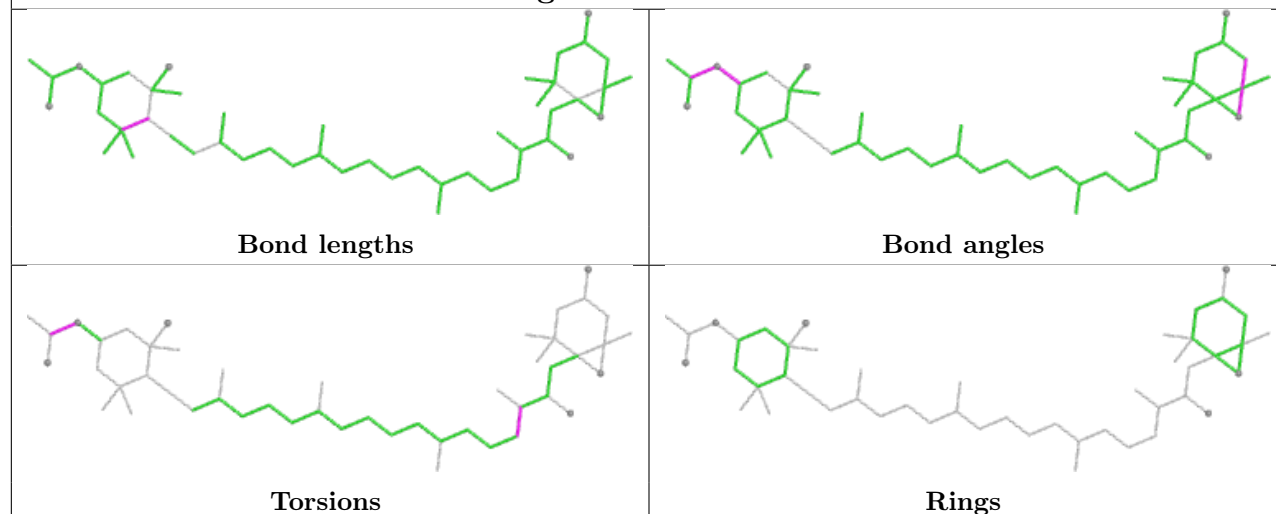
Ligand BCR r 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

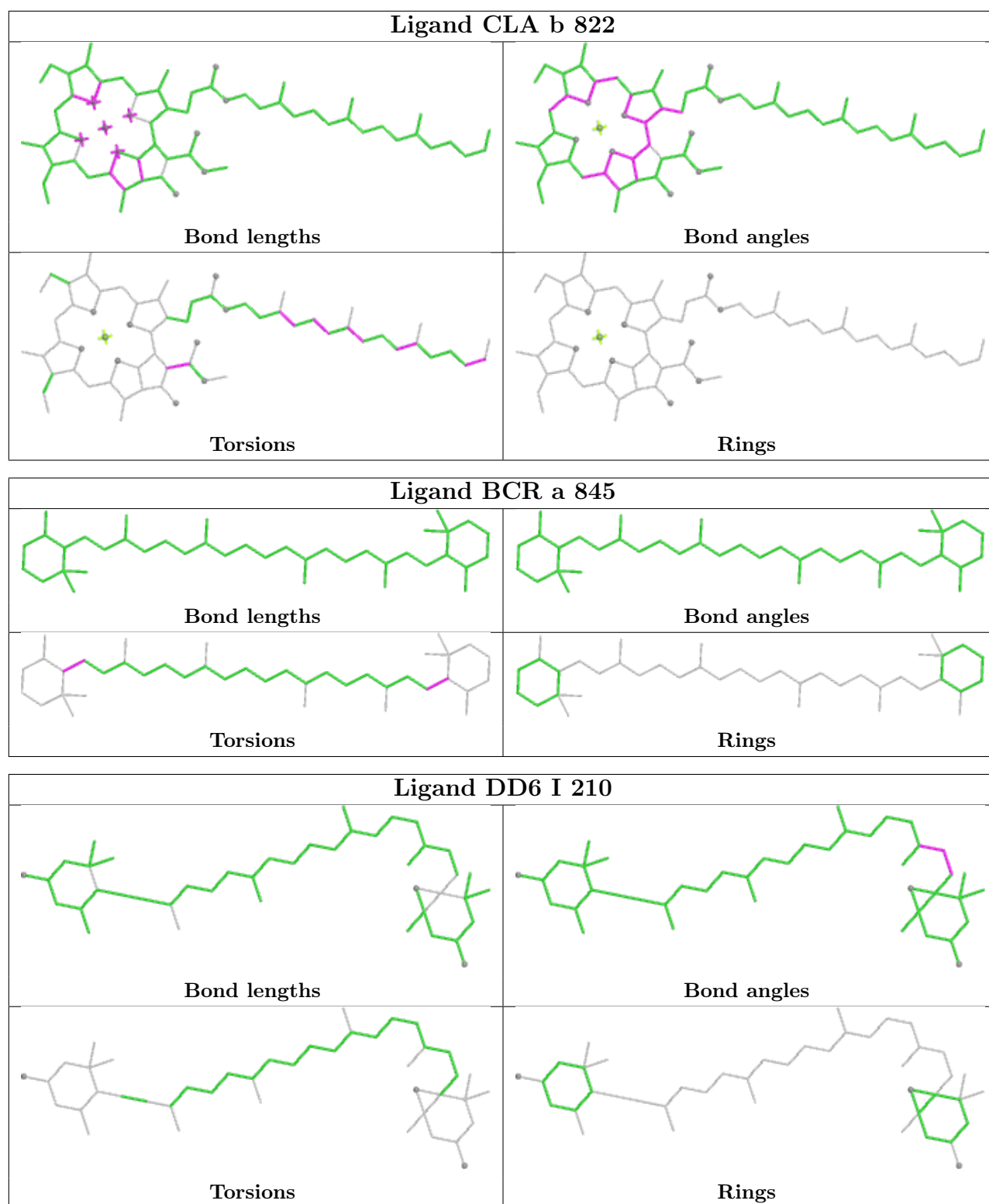


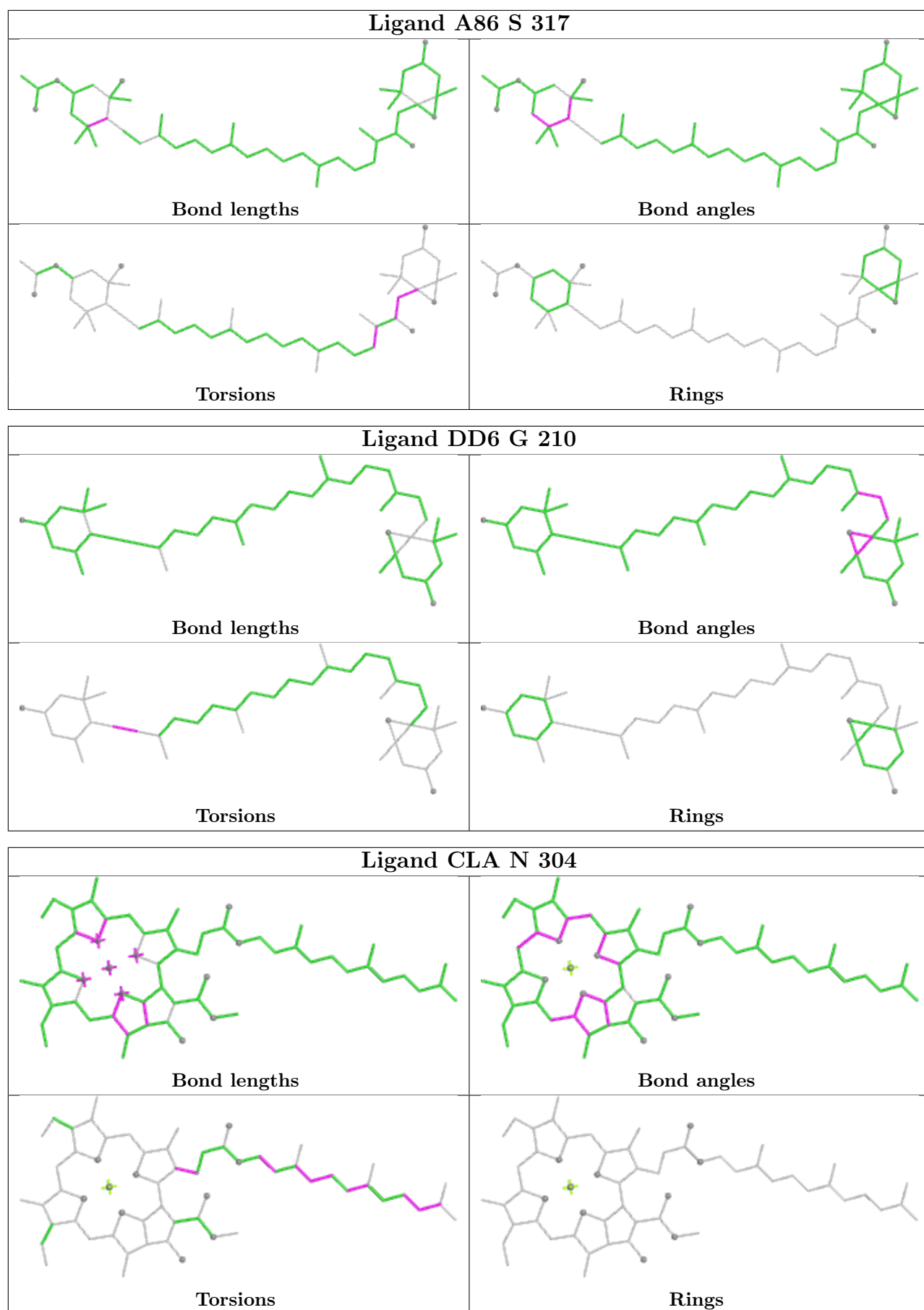
Ligand CLA U 205



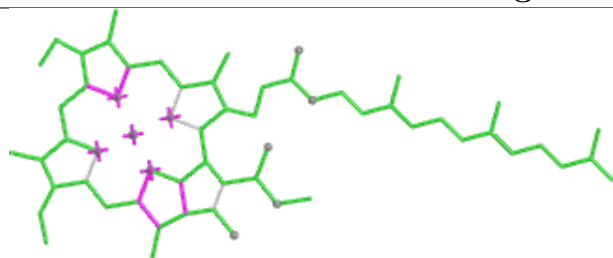
Ligand A86 D 319



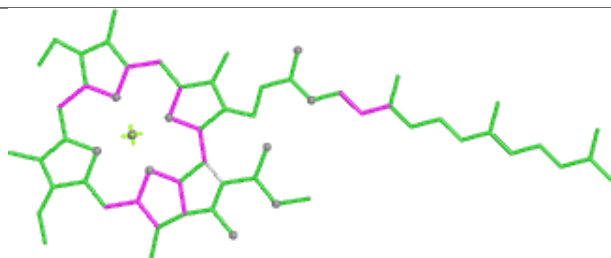




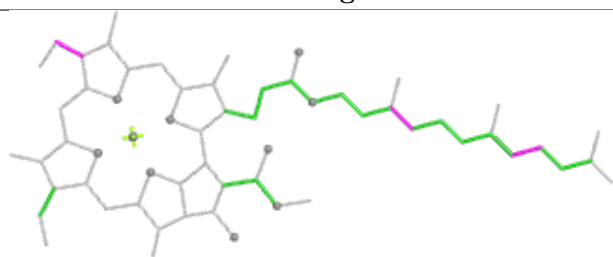
Ligand CLA C 305



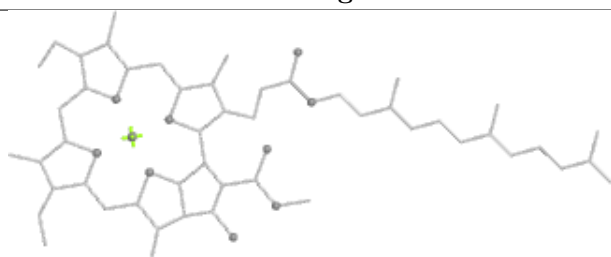
Bond lengths



Bond angles

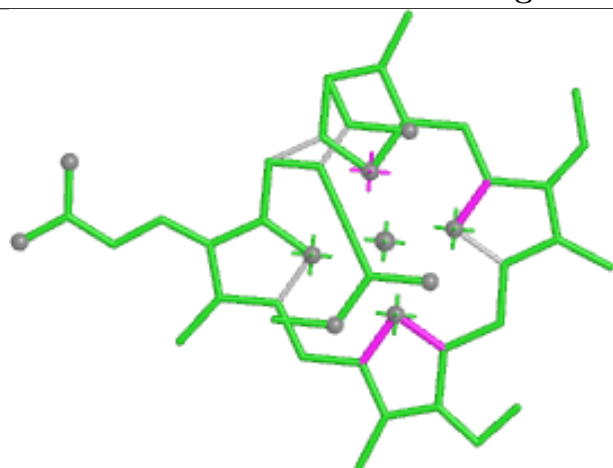


Torsions

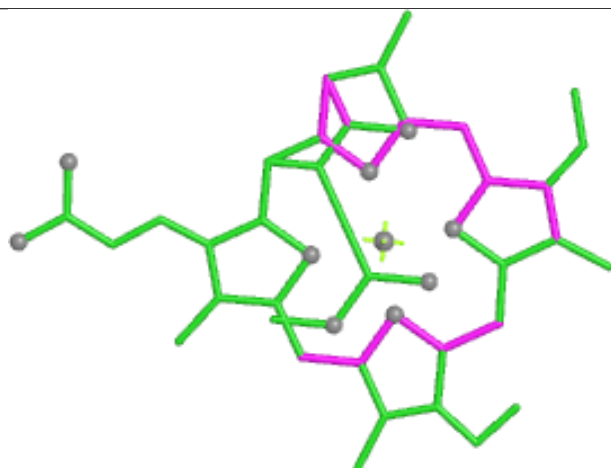


Rings

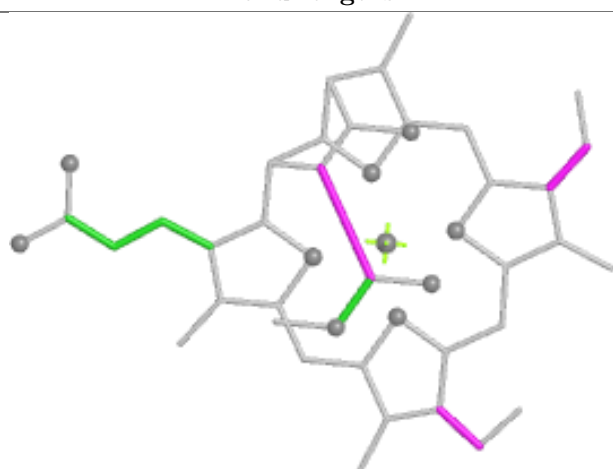
Ligand KC2 N 301



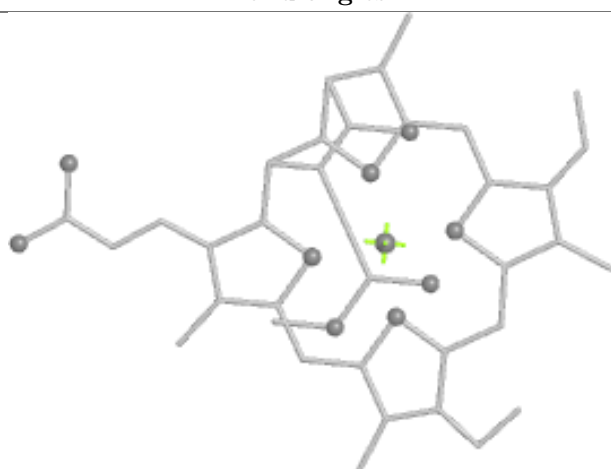
Bond lengths



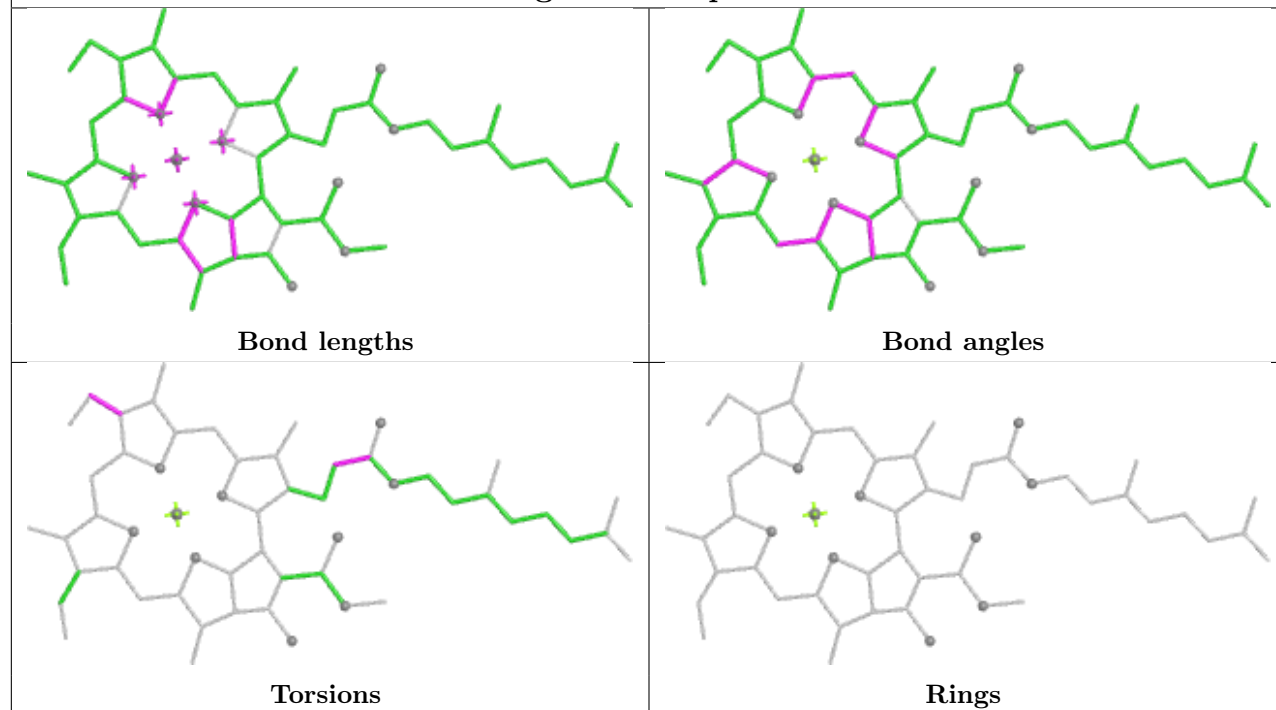
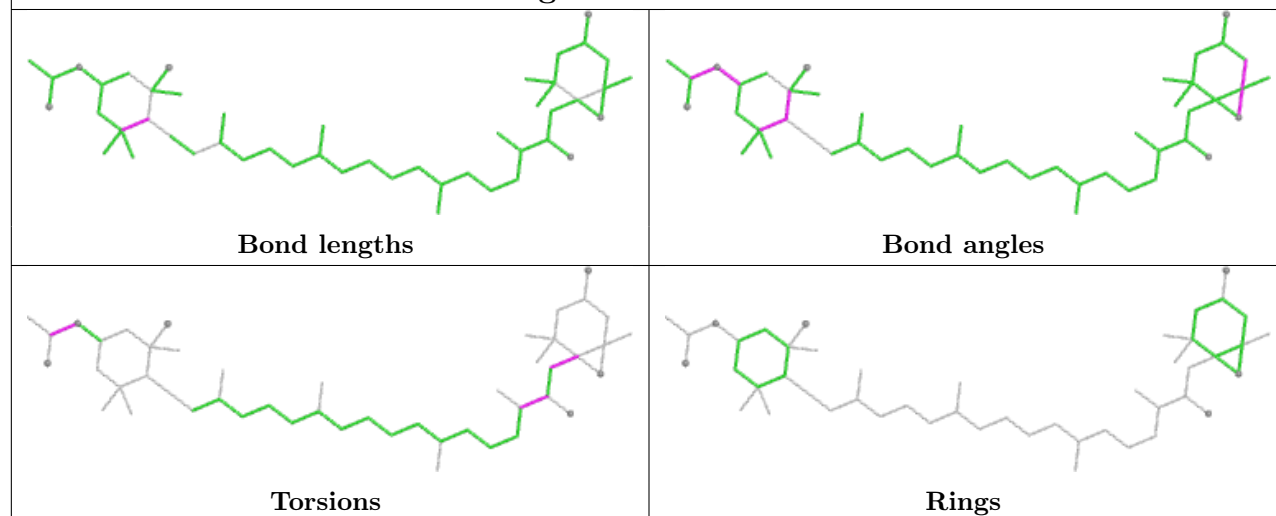
Bond angles

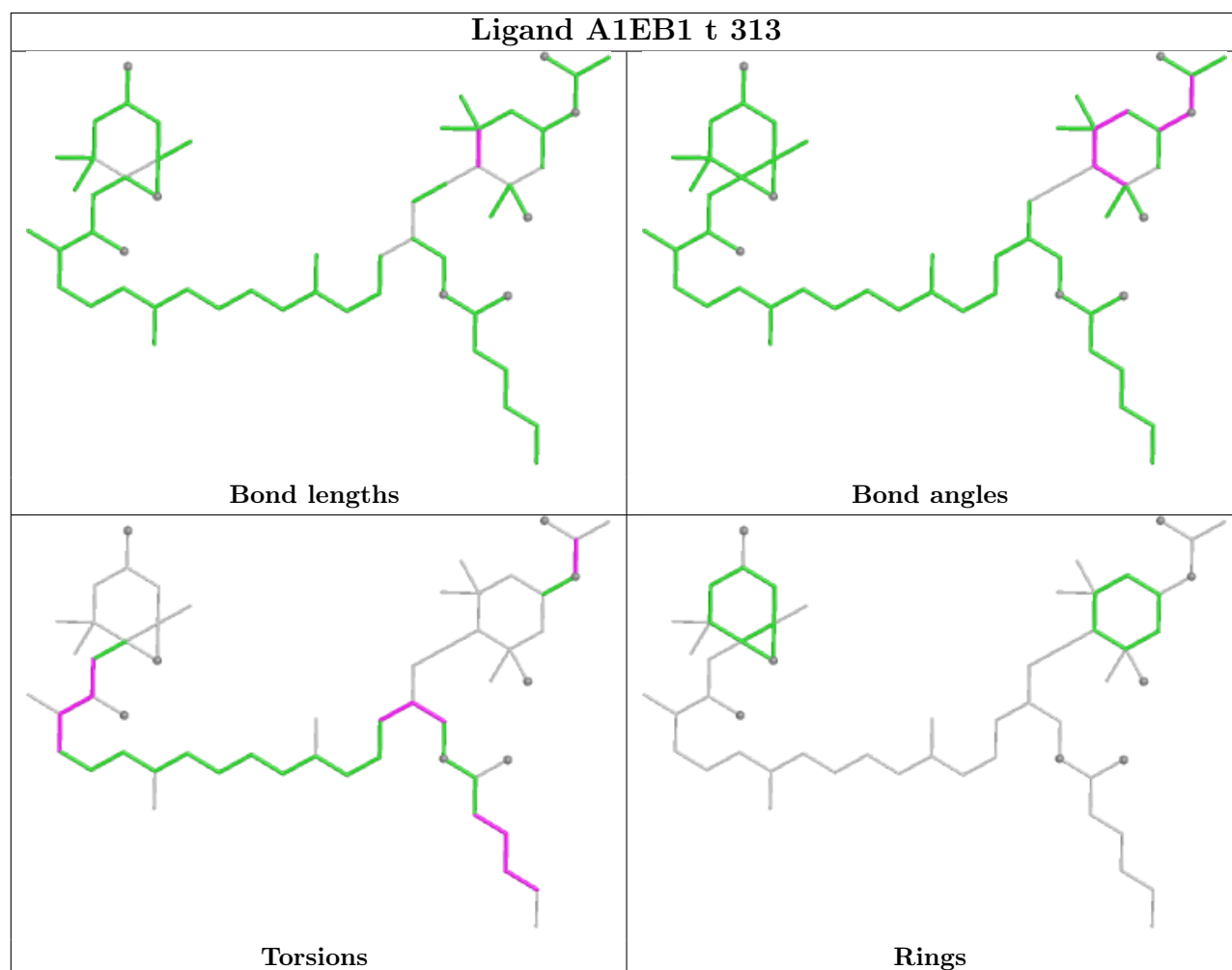
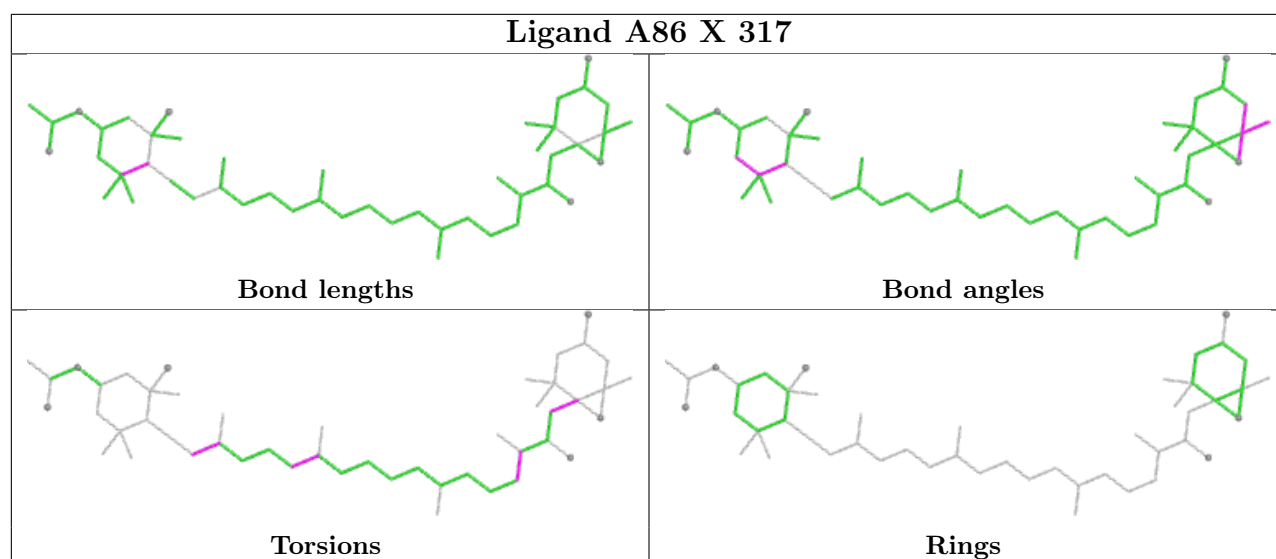


Torsions

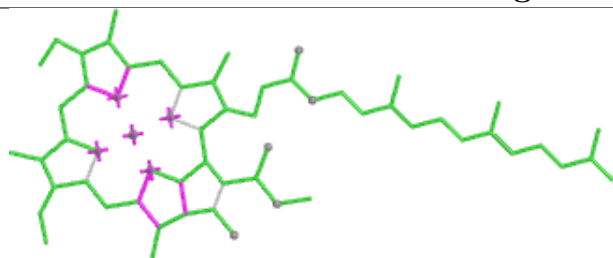


Rings

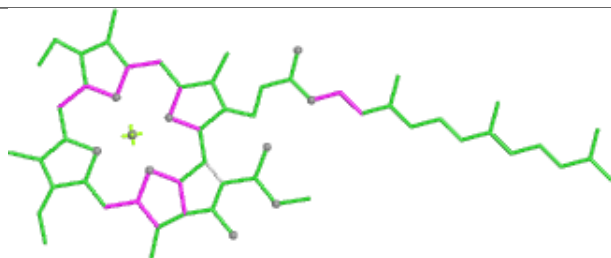
Ligand CLA p 313**Ligand A86 P 316**



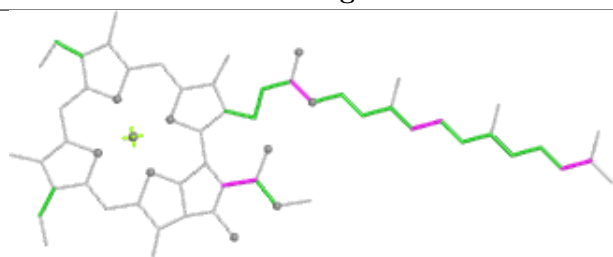
Ligand CLA X 307



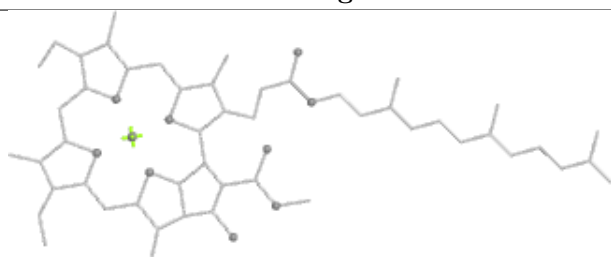
Bond lengths



Bond angles

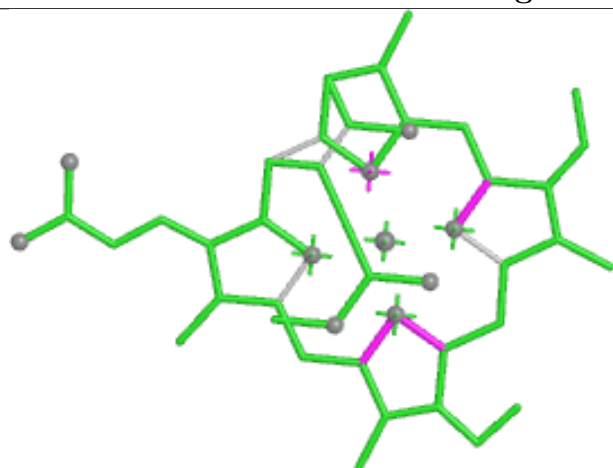


Torsions

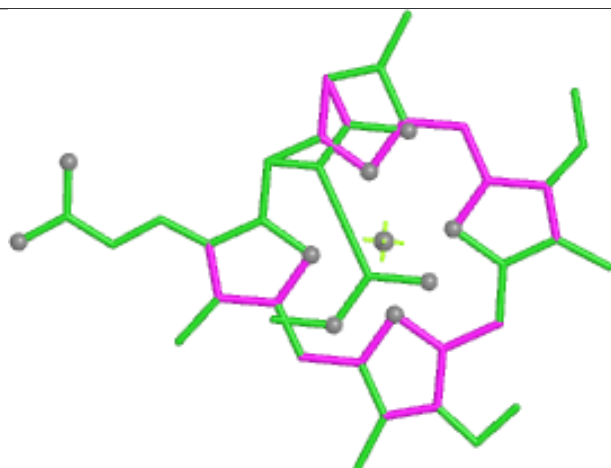


Rings

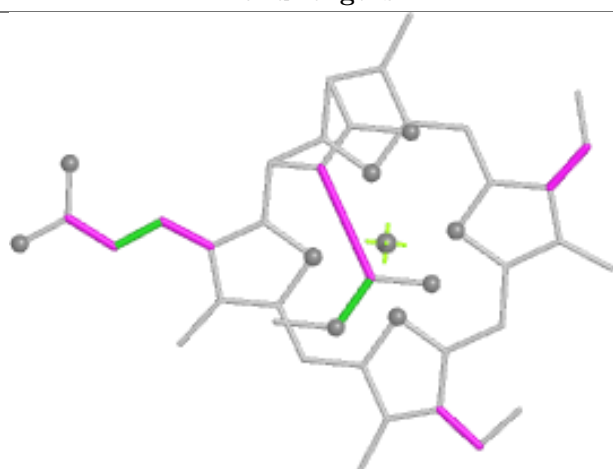
Ligand KC2 G 202



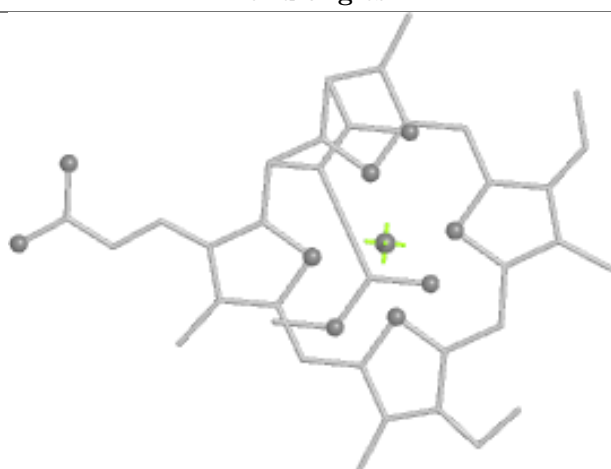
Bond lengths



Bond angles

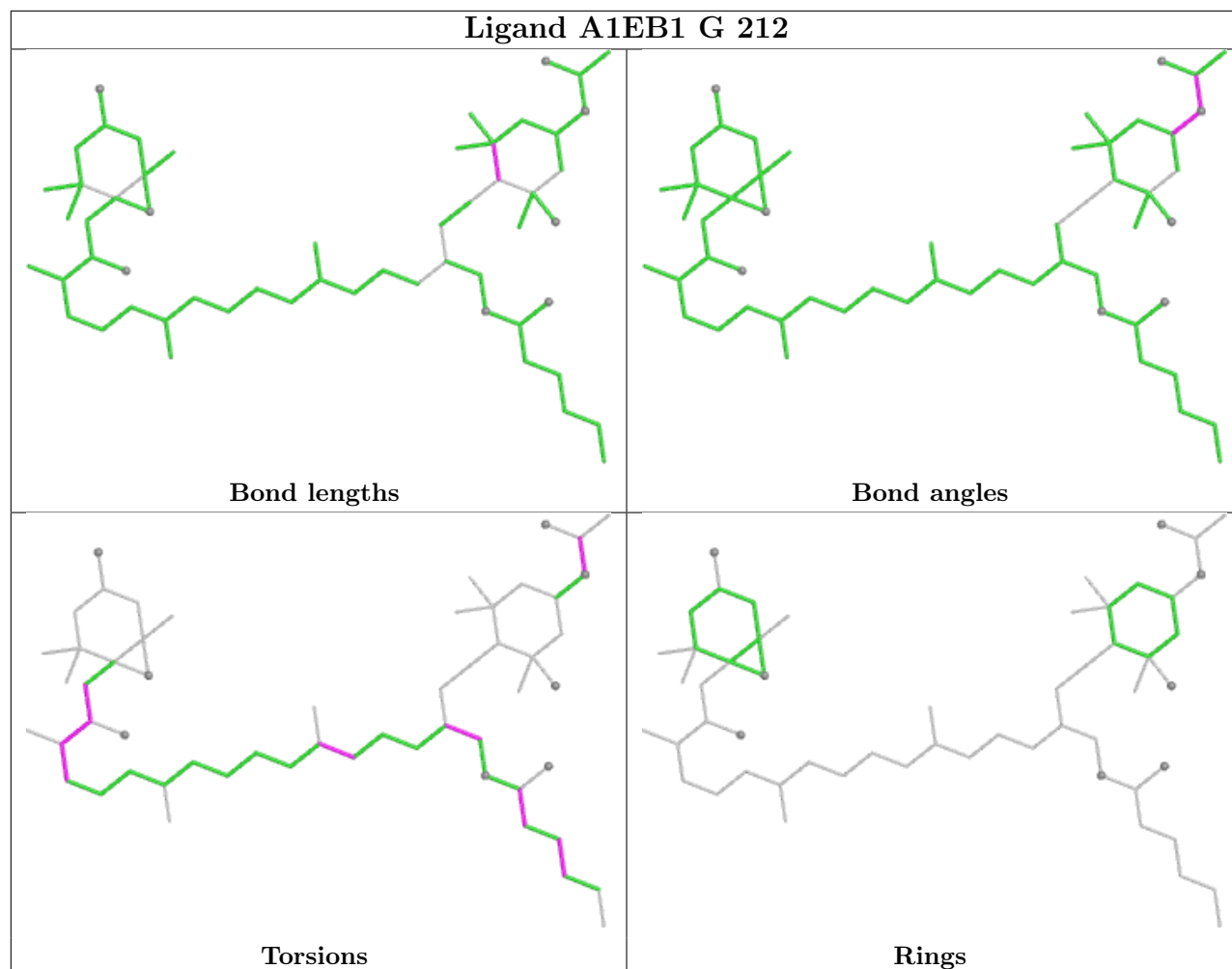


Torsions

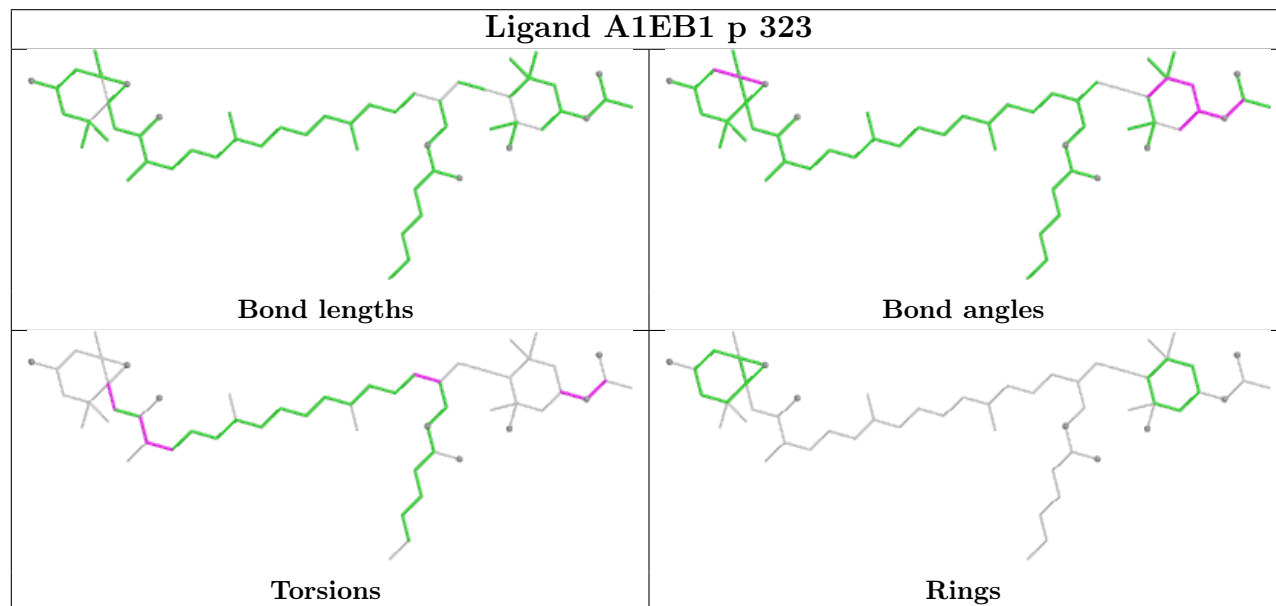


Rings

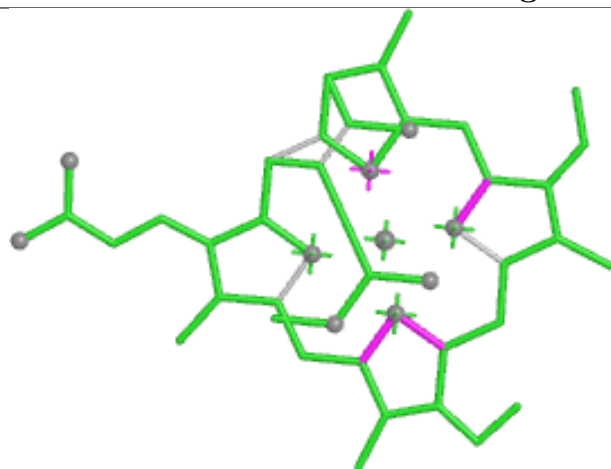
Ligand A1EB1 G 212



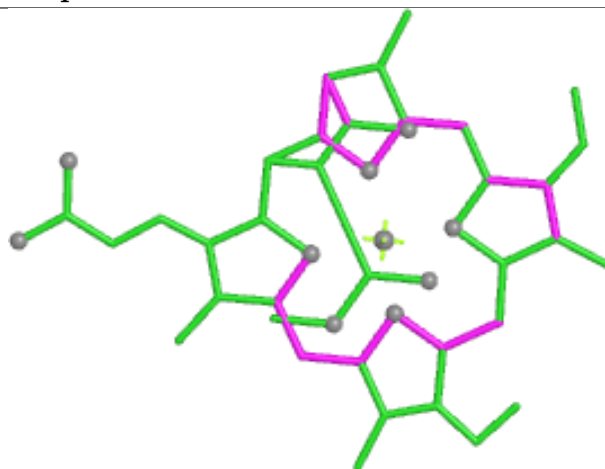
Ligand A1EB1 p 323



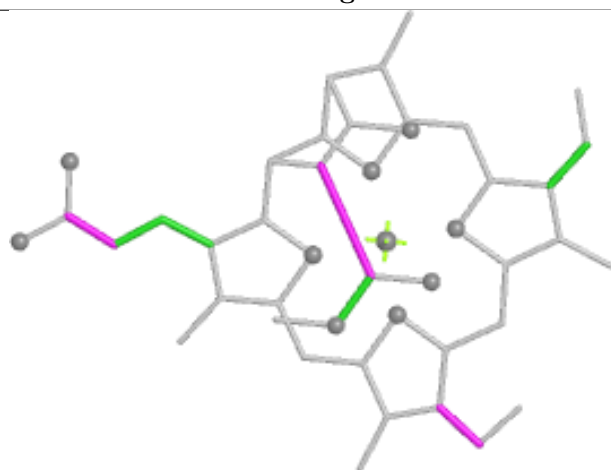
Ligand KC2 q 303



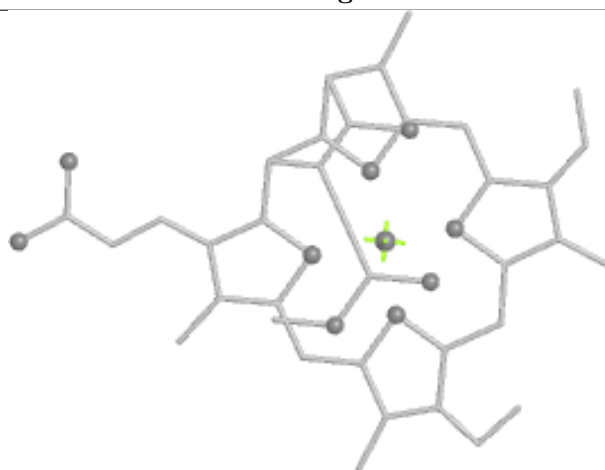
Bond lengths



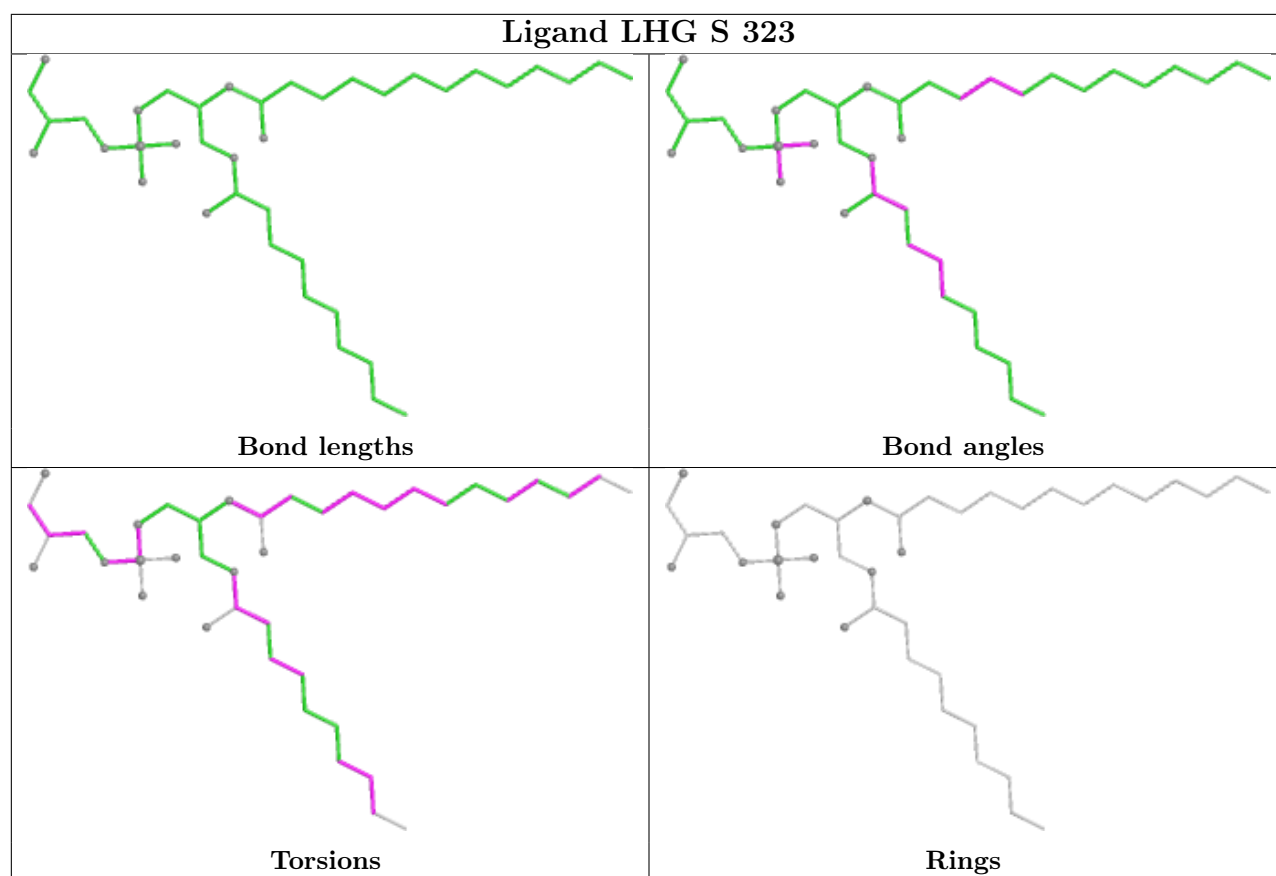
Bond angles



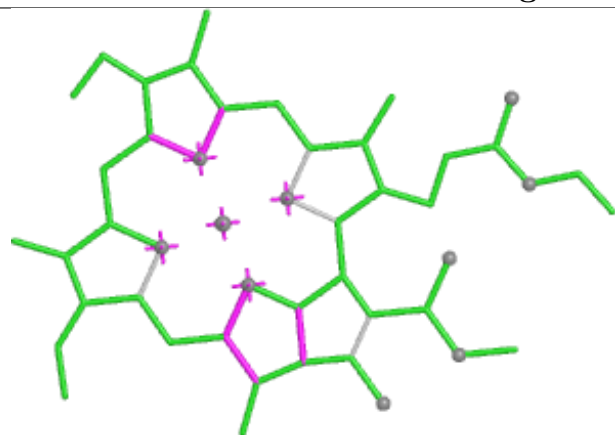
Torsions



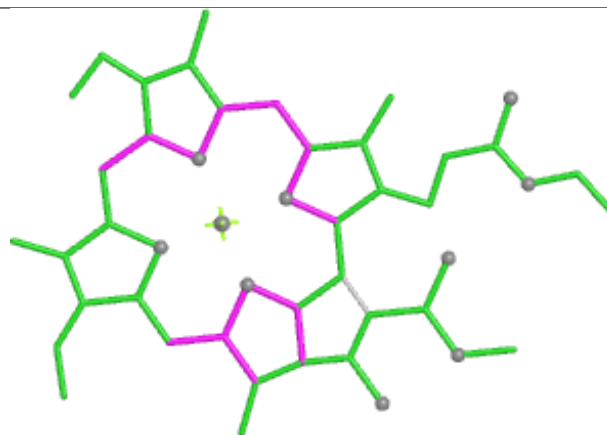
Rings



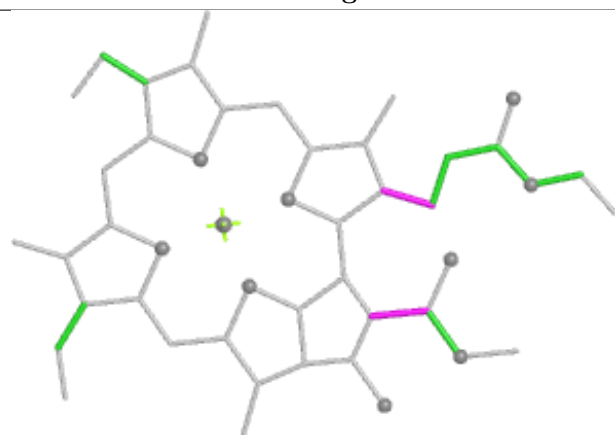
Ligand CLA S 313



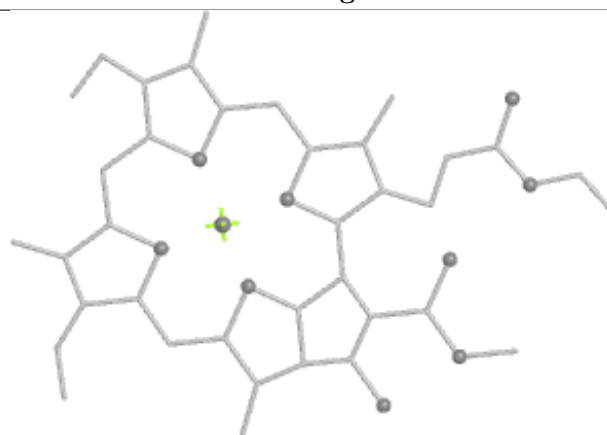
Bond lengths



Bond angles

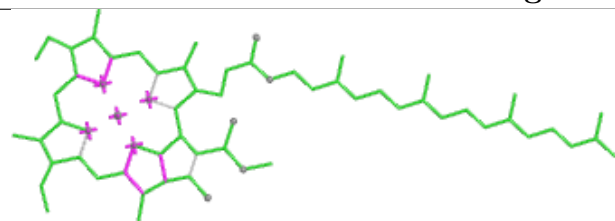


Torsions

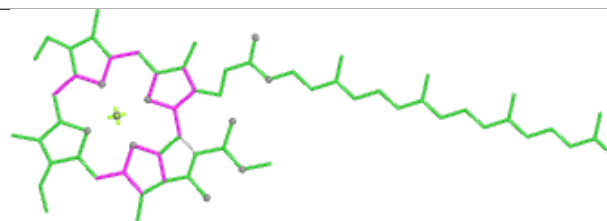


Rings

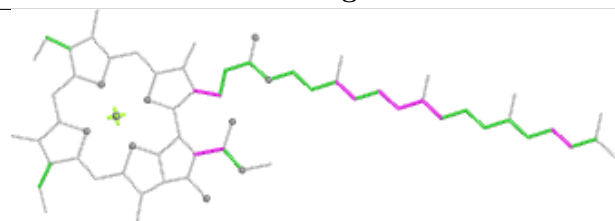
Ligand CLA 1 205



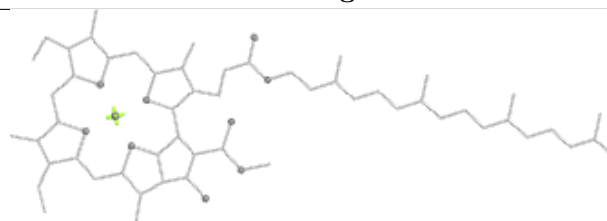
Bond lengths



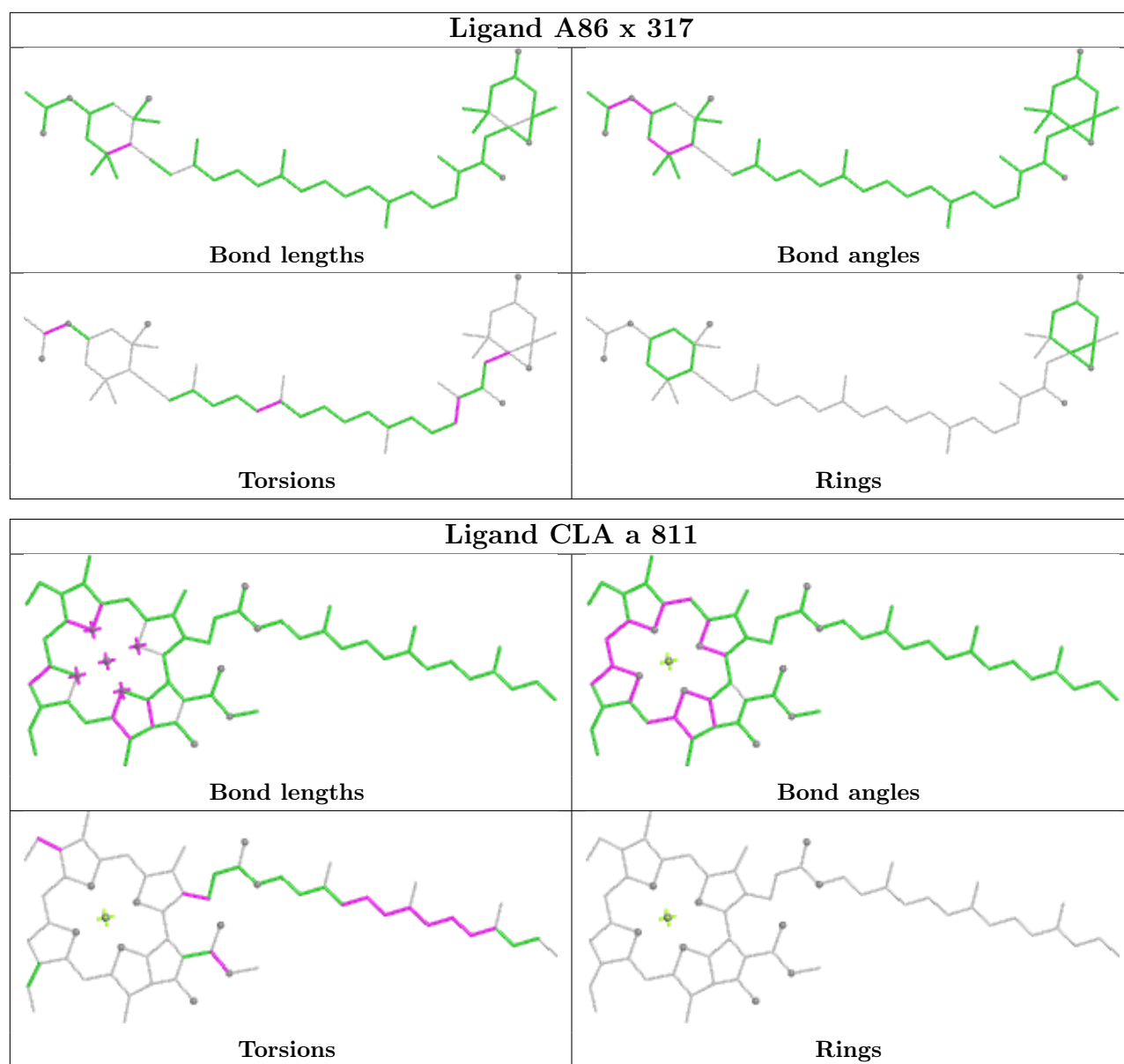
Bond angles

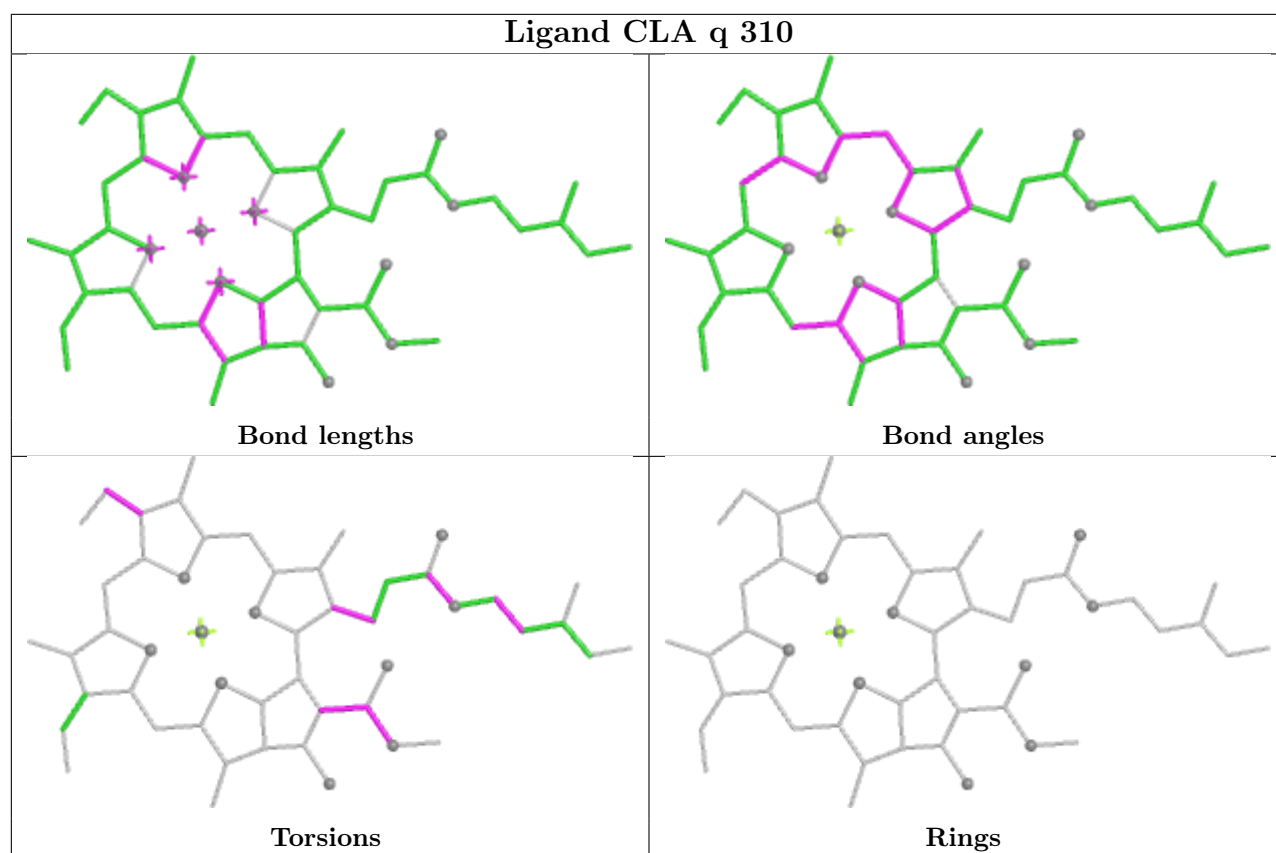


Torsions

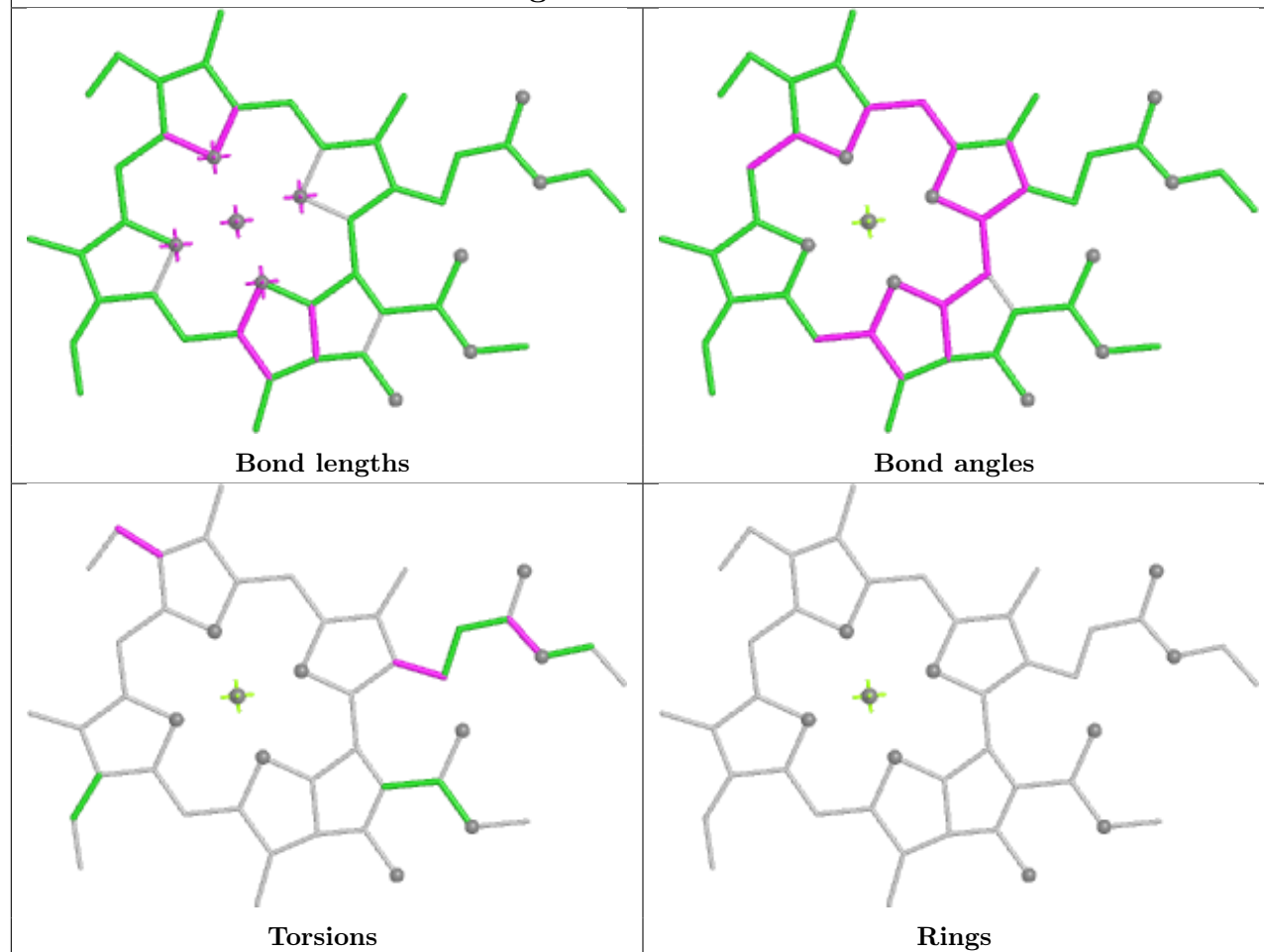


Rings

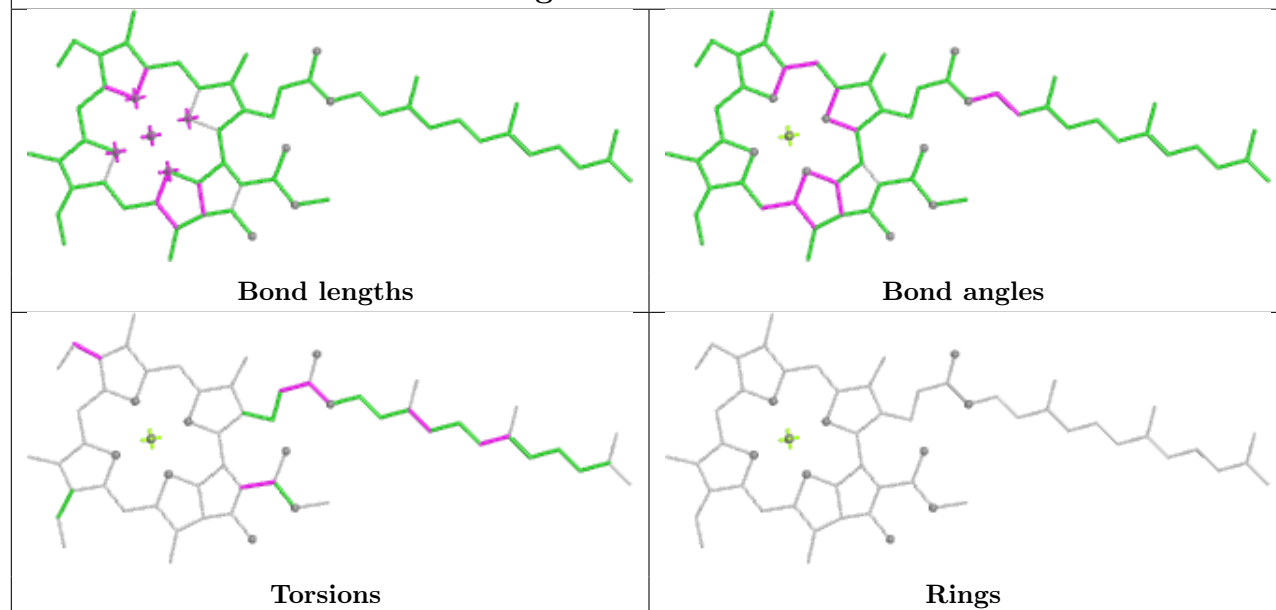


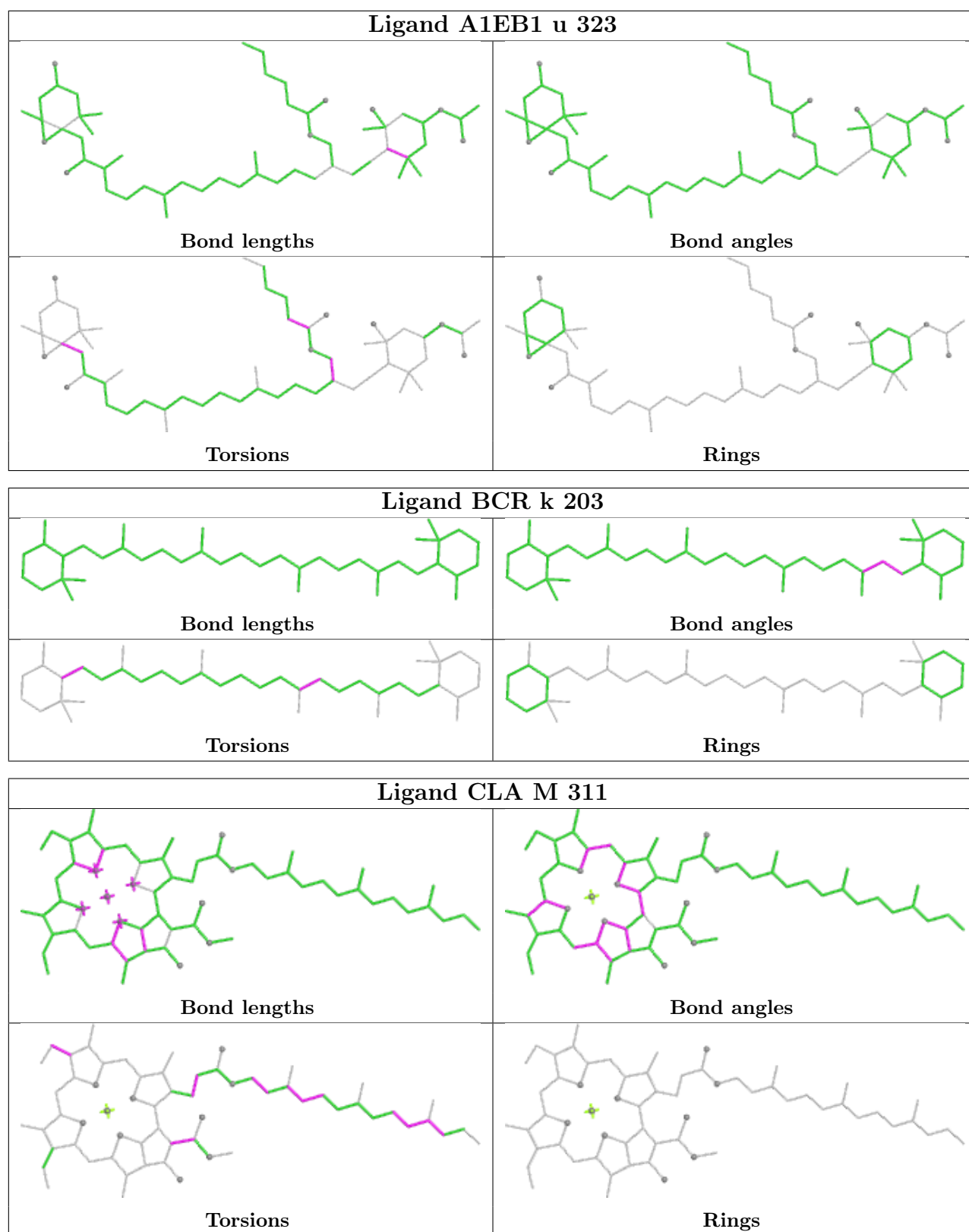


Ligand CLA L 310

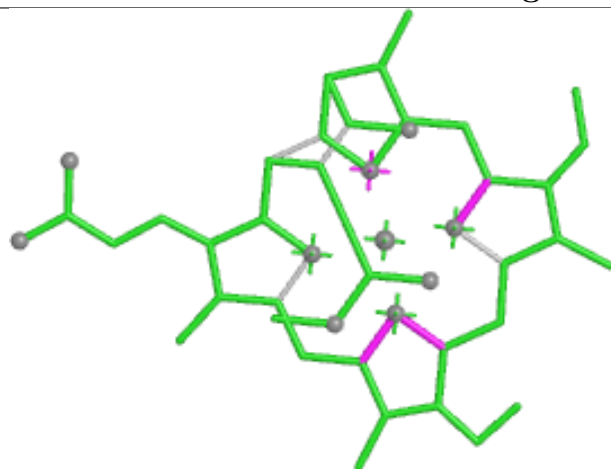


Ligand CLA S 307

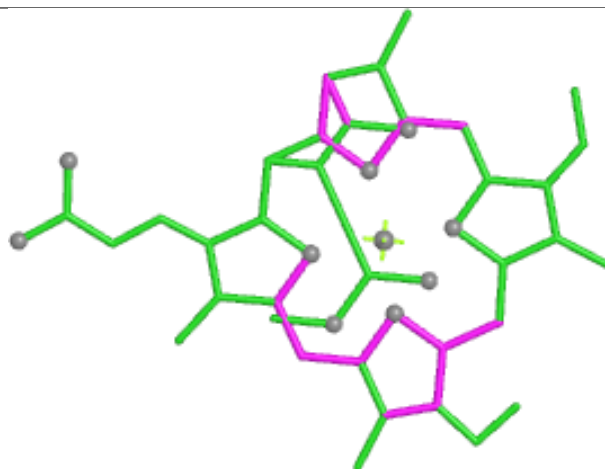




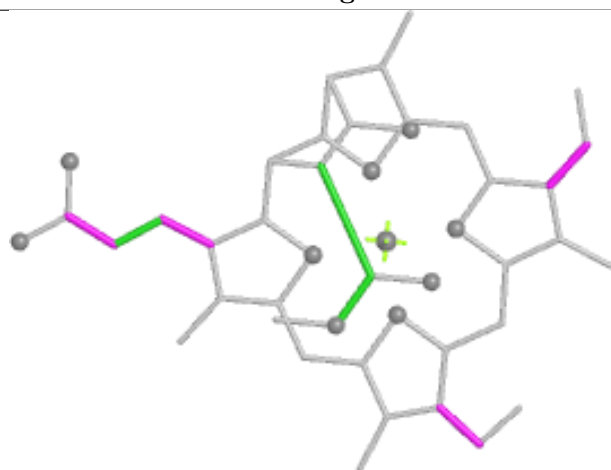
Ligand KC2 I 214



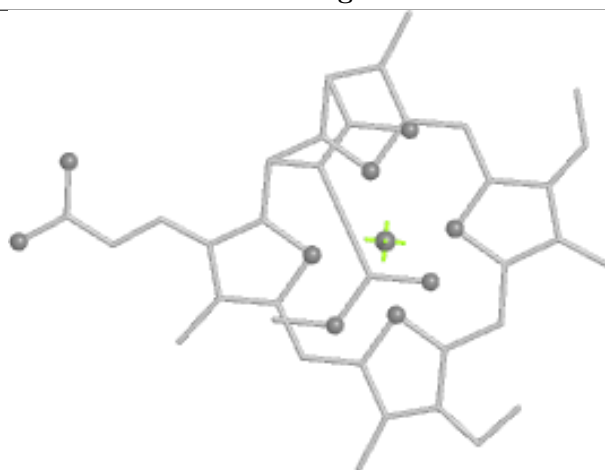
Bond lengths



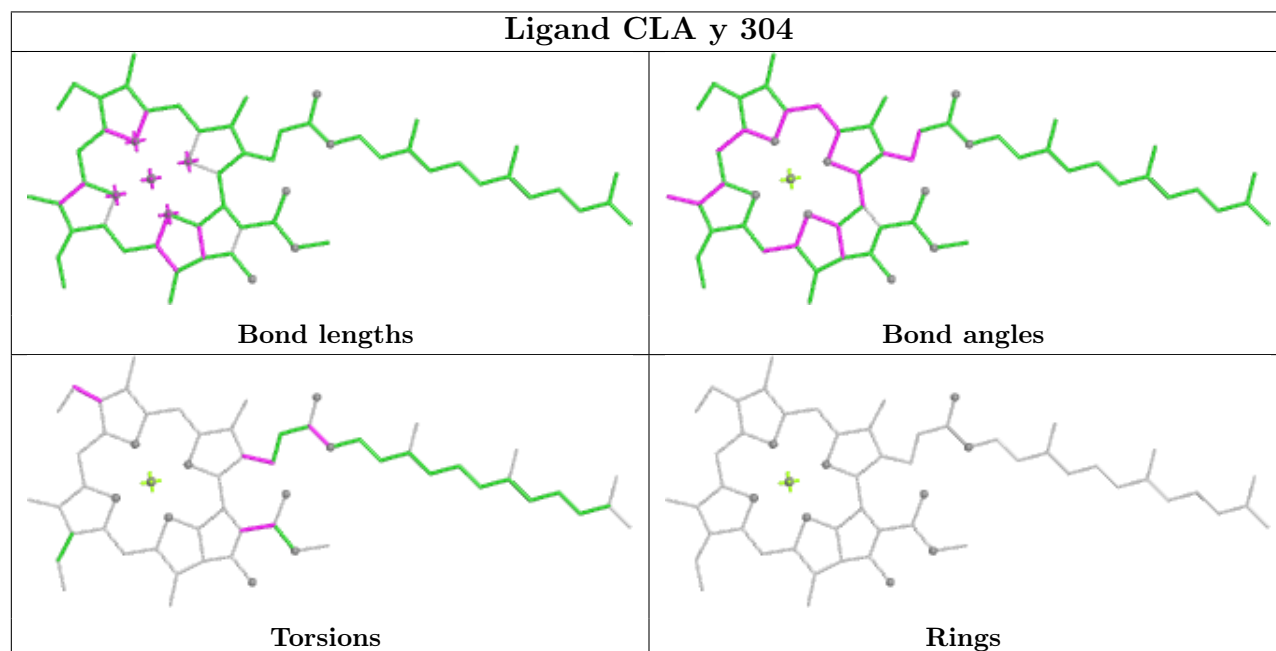
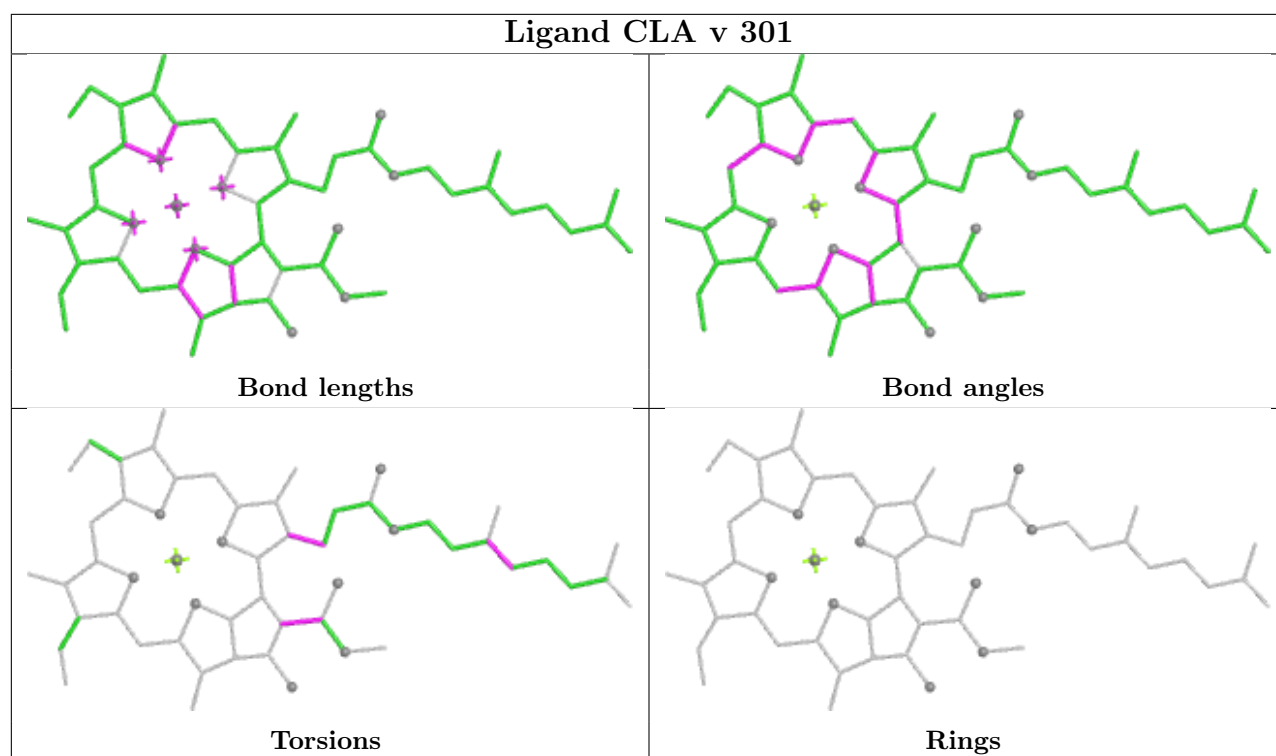
Bond angles



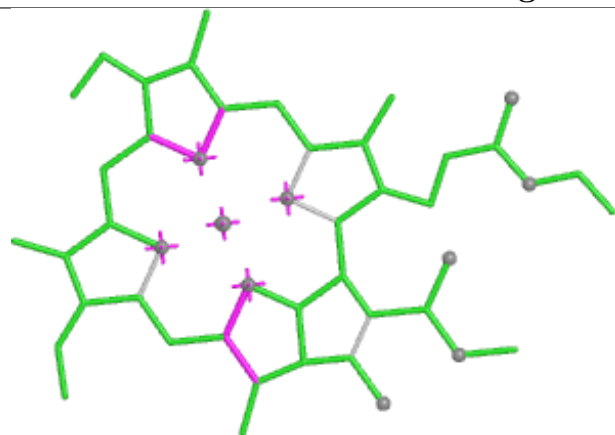
Torsions



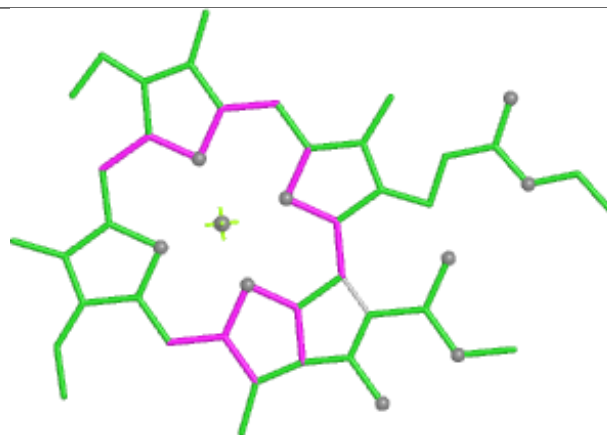
Rings



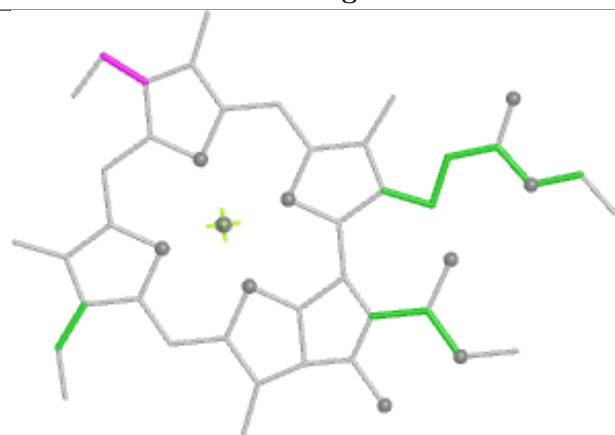
Ligand CLA L 301



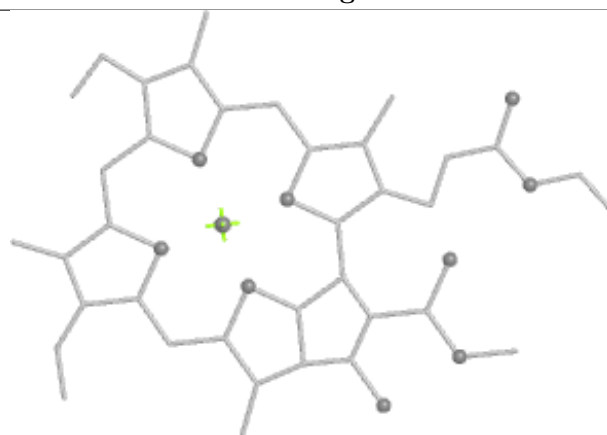
Bond lengths



Bond angles

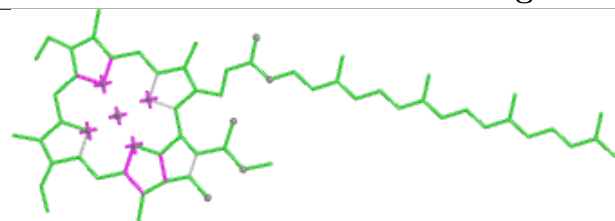


Torsions

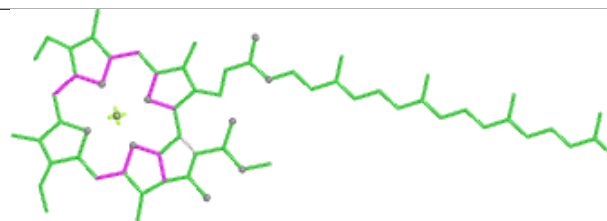


Rings

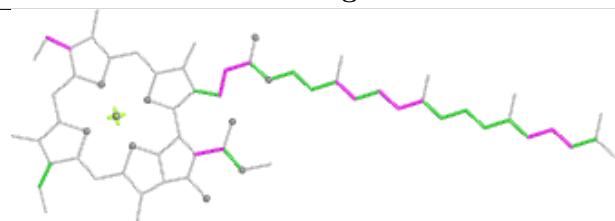
Ligand CLA A 309



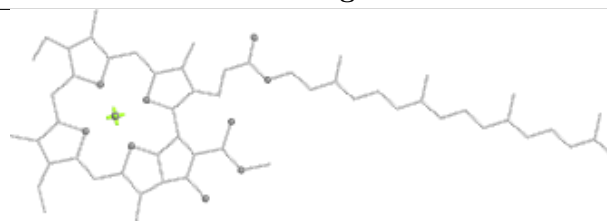
Bond lengths



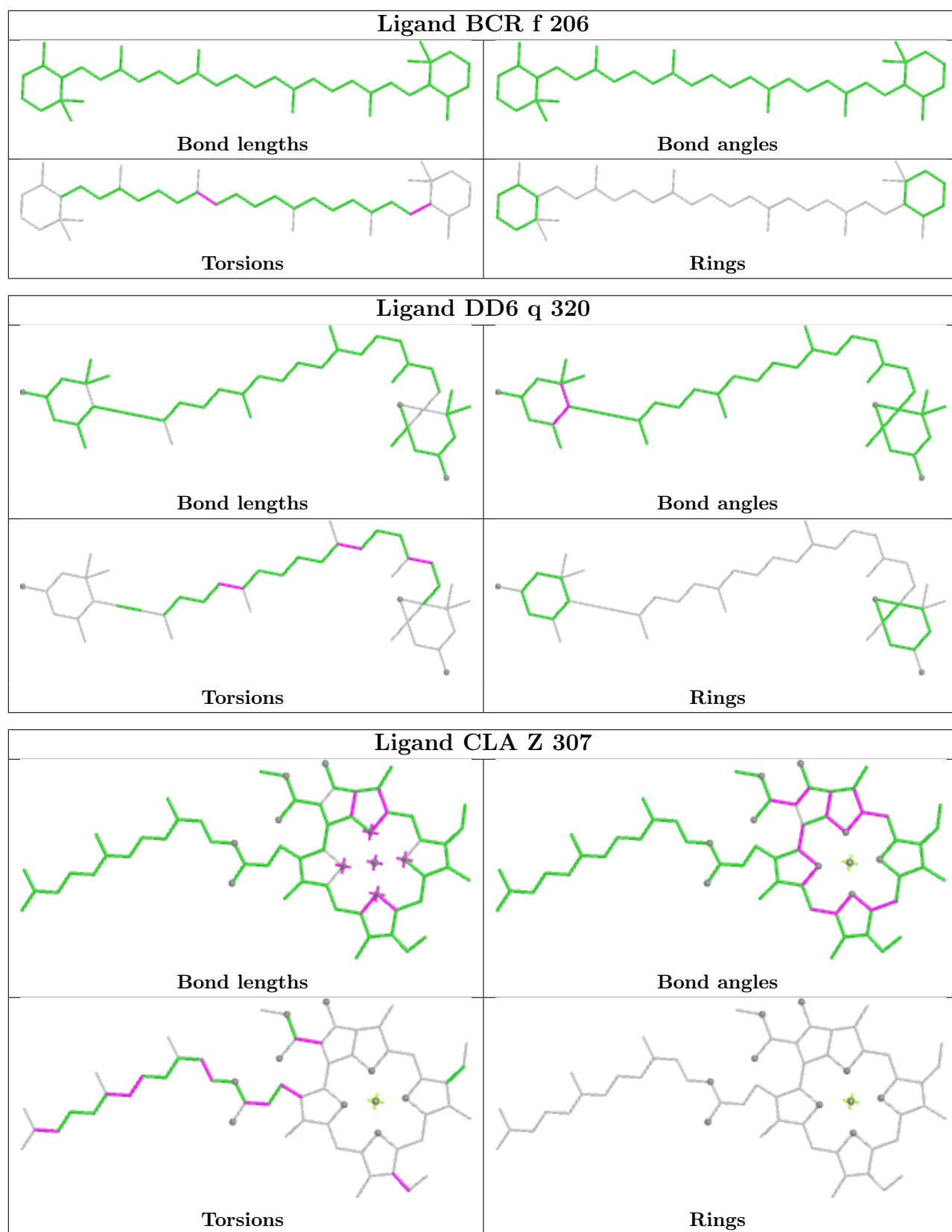
Bond angles



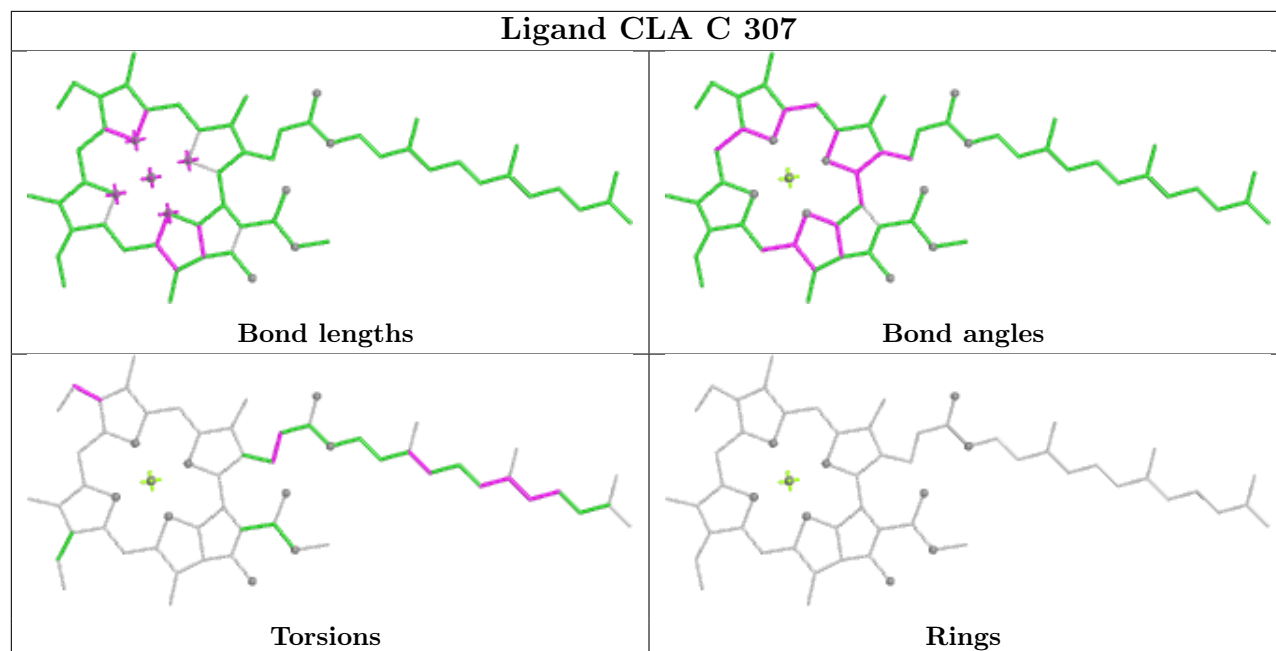
Torsions



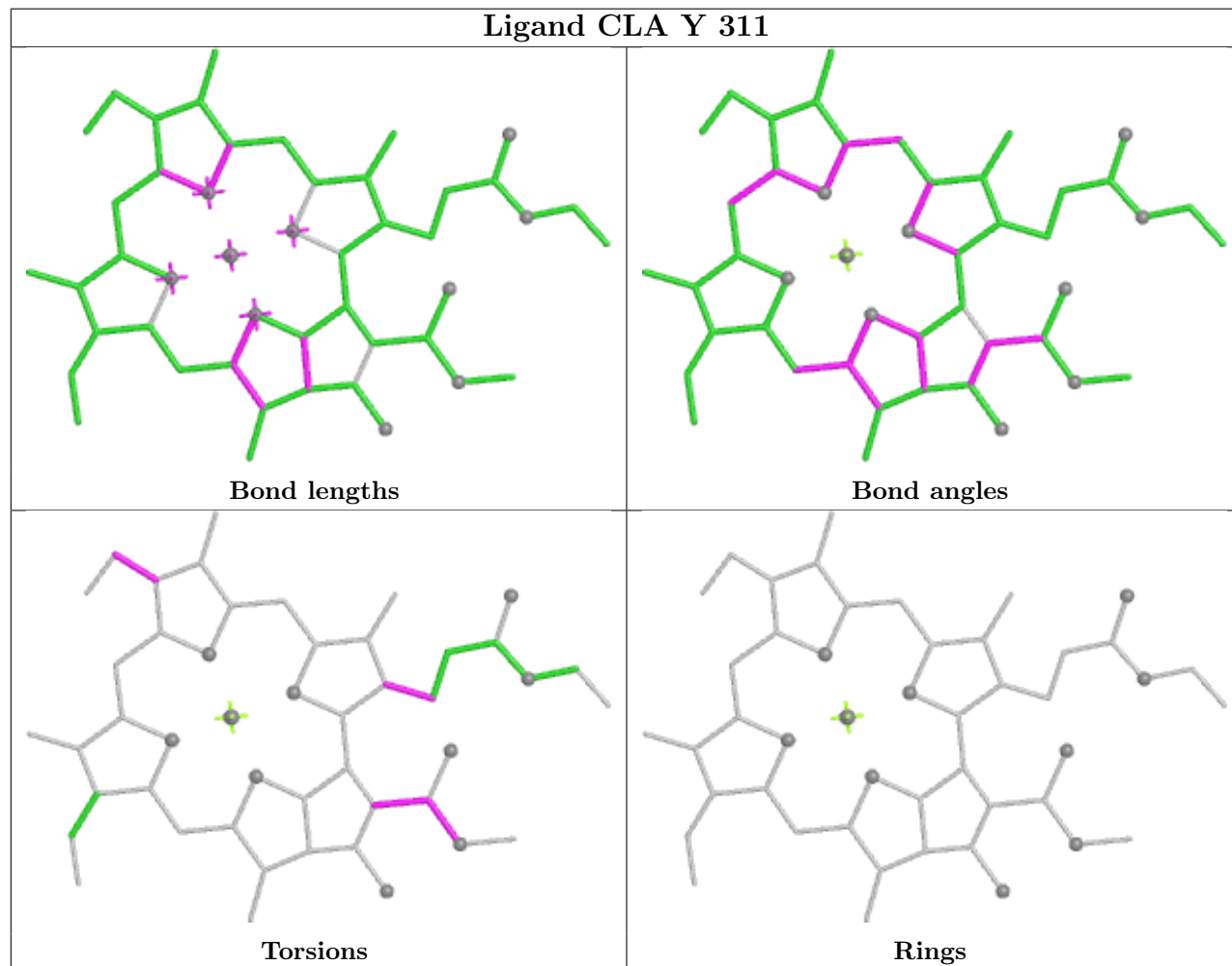
Rings

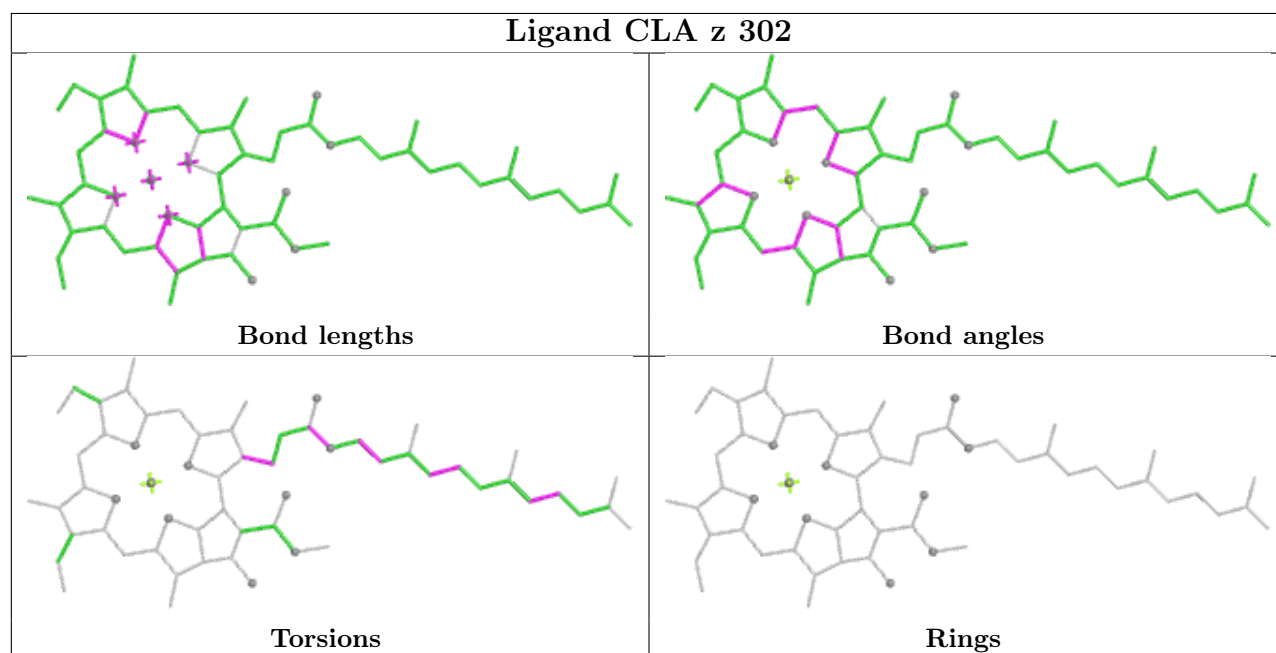
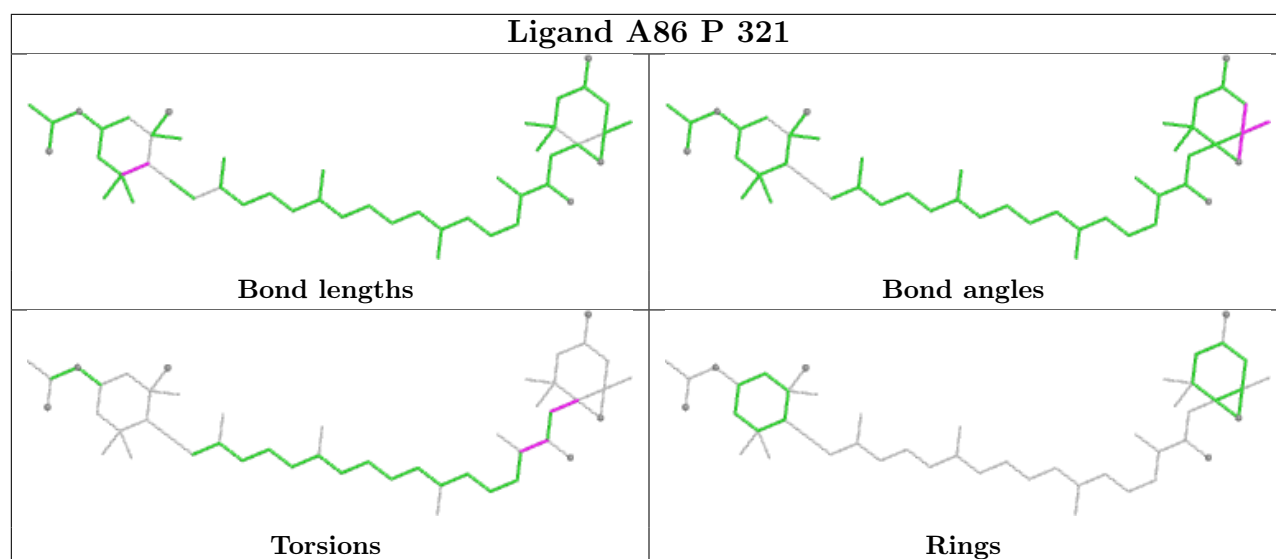


Ligand CLA C 307

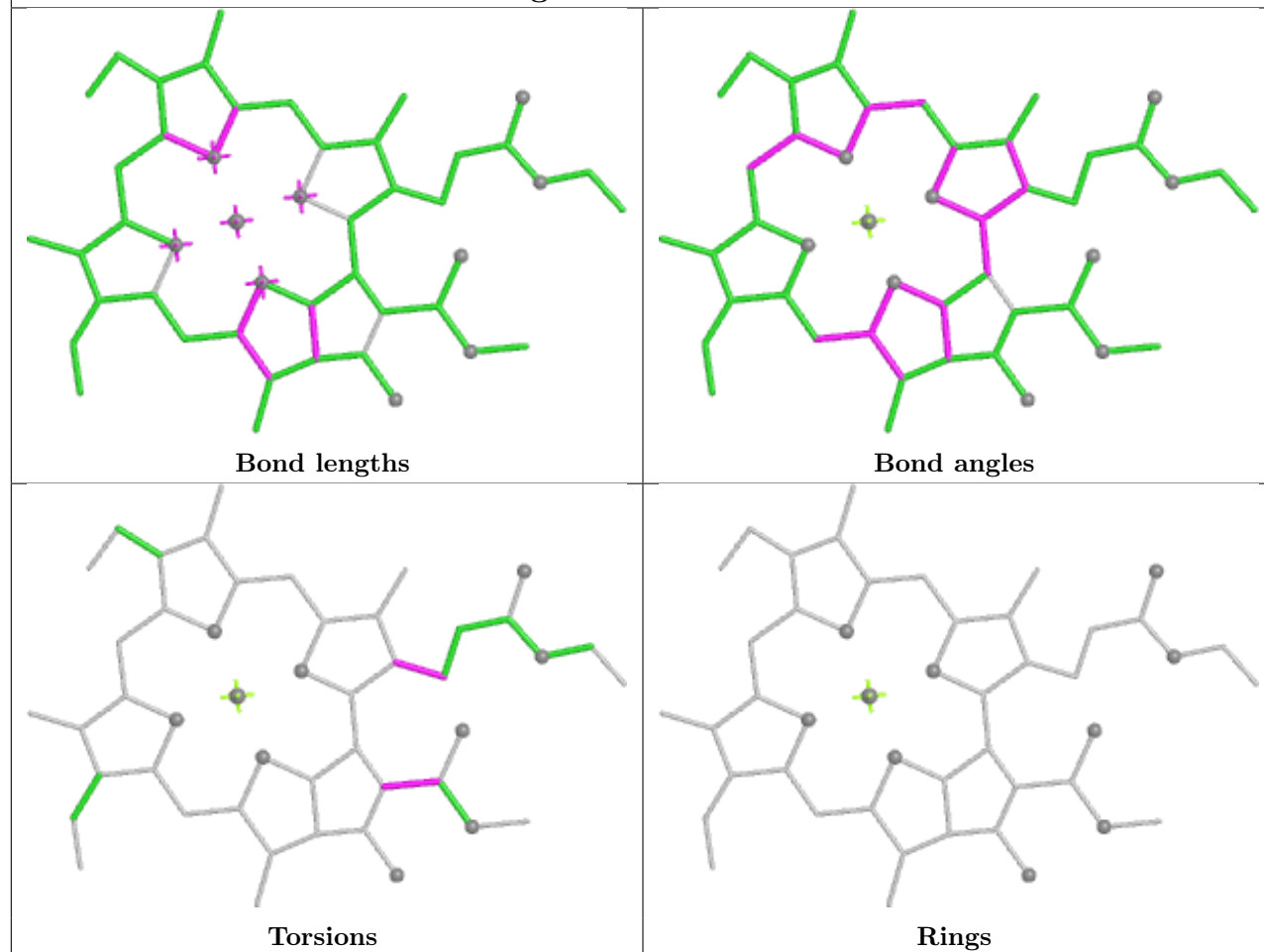


Ligand CLA Y 311

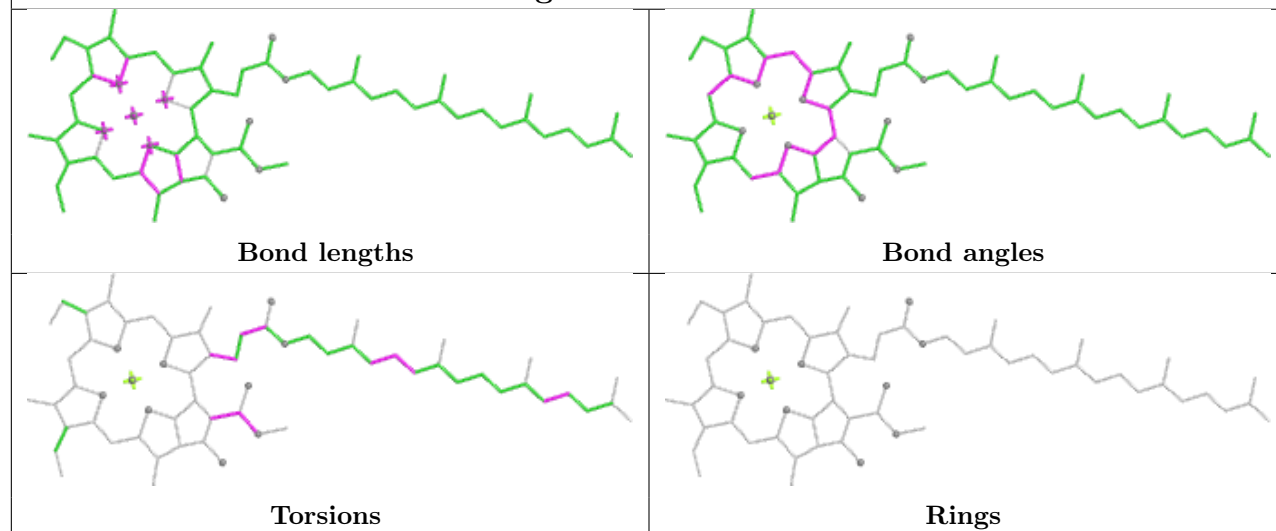


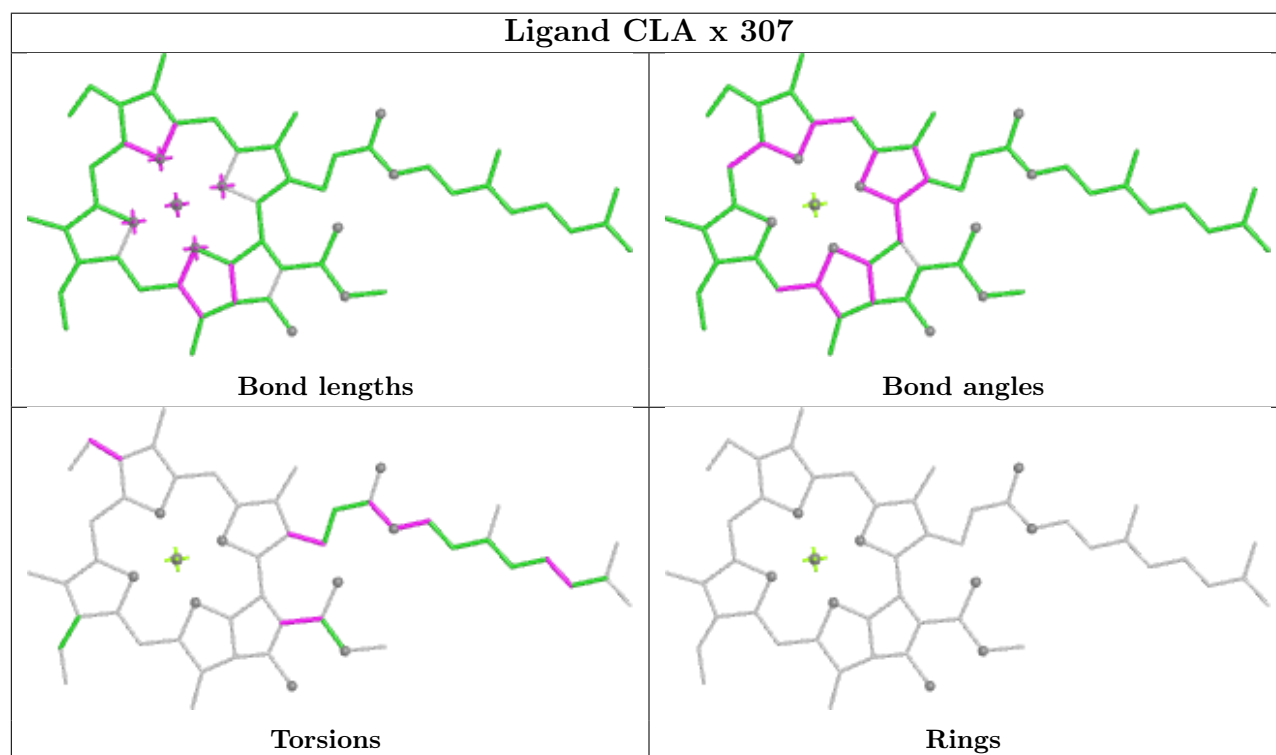
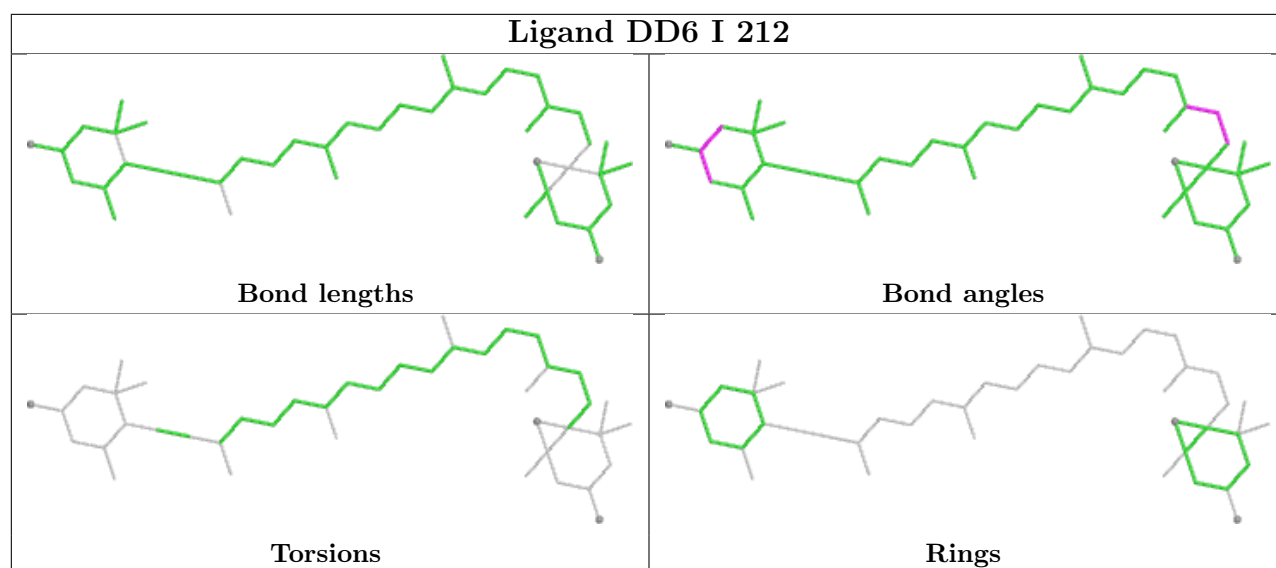


Ligand CLA v 313

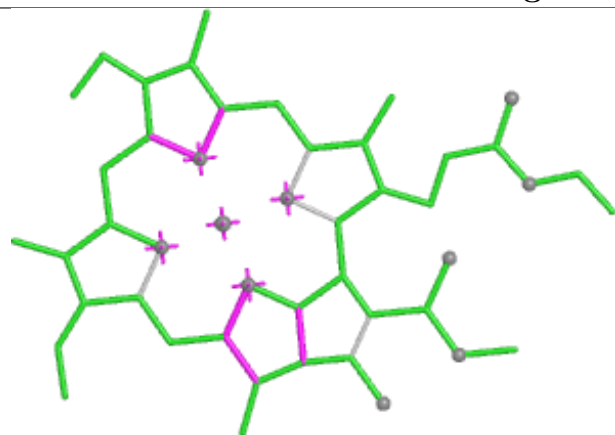


Ligand CLA b 807

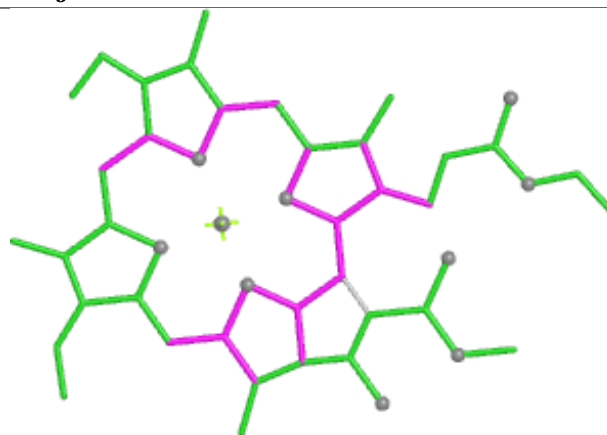




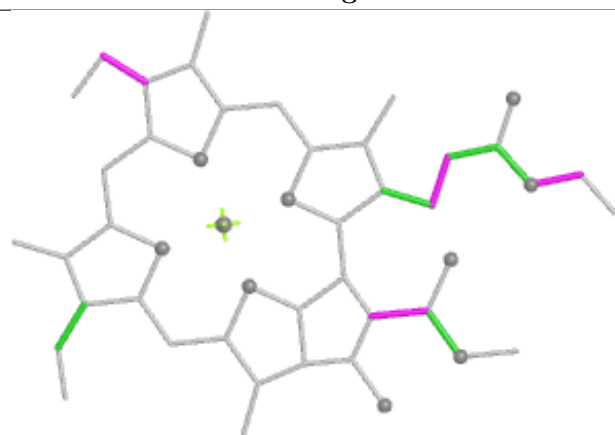
Ligand CLA j 102



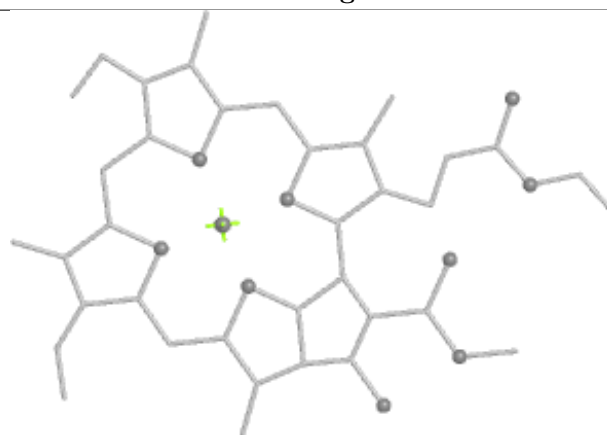
Bond lengths



Bond angles

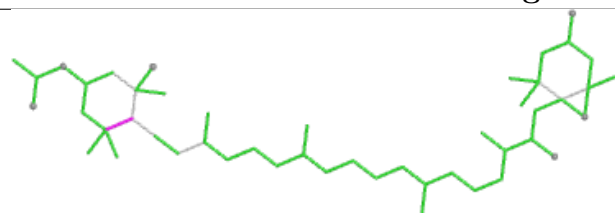


Torsions

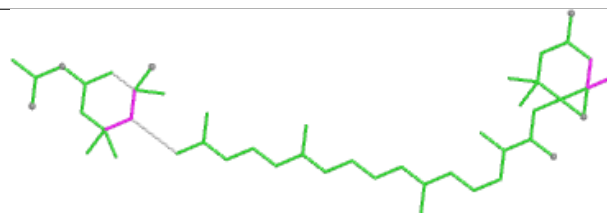


Rings

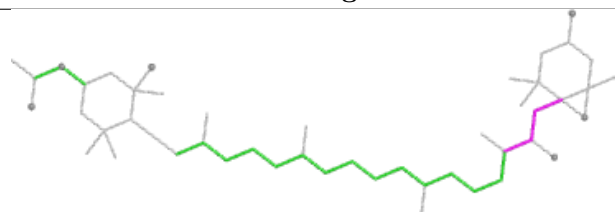
Ligand A86 P 317



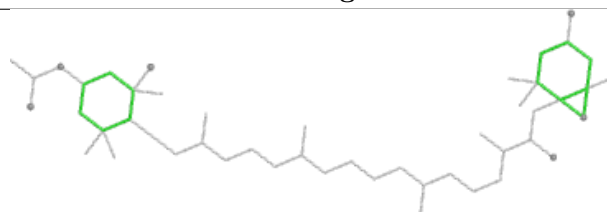
Bond lengths



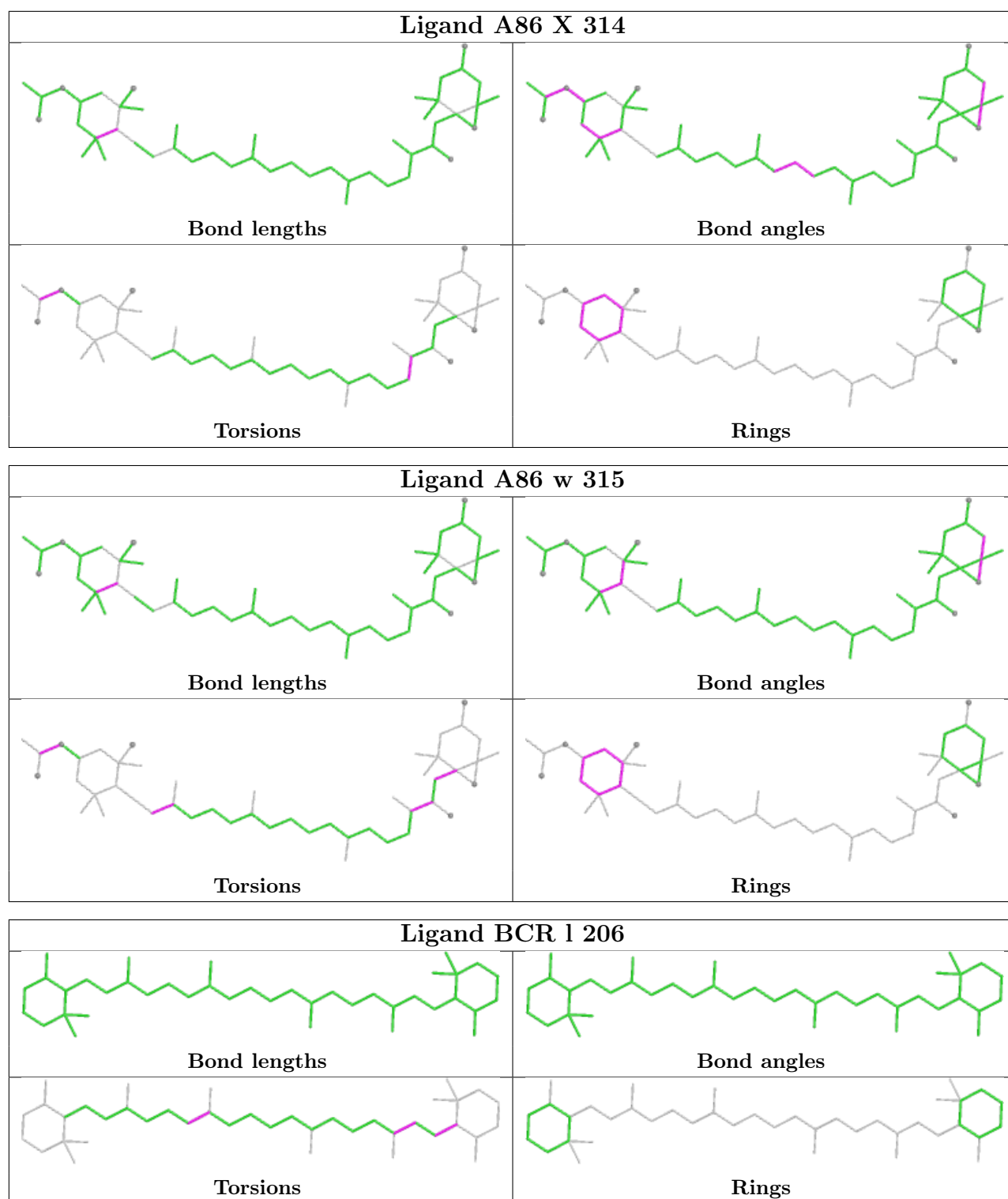
Bond angles

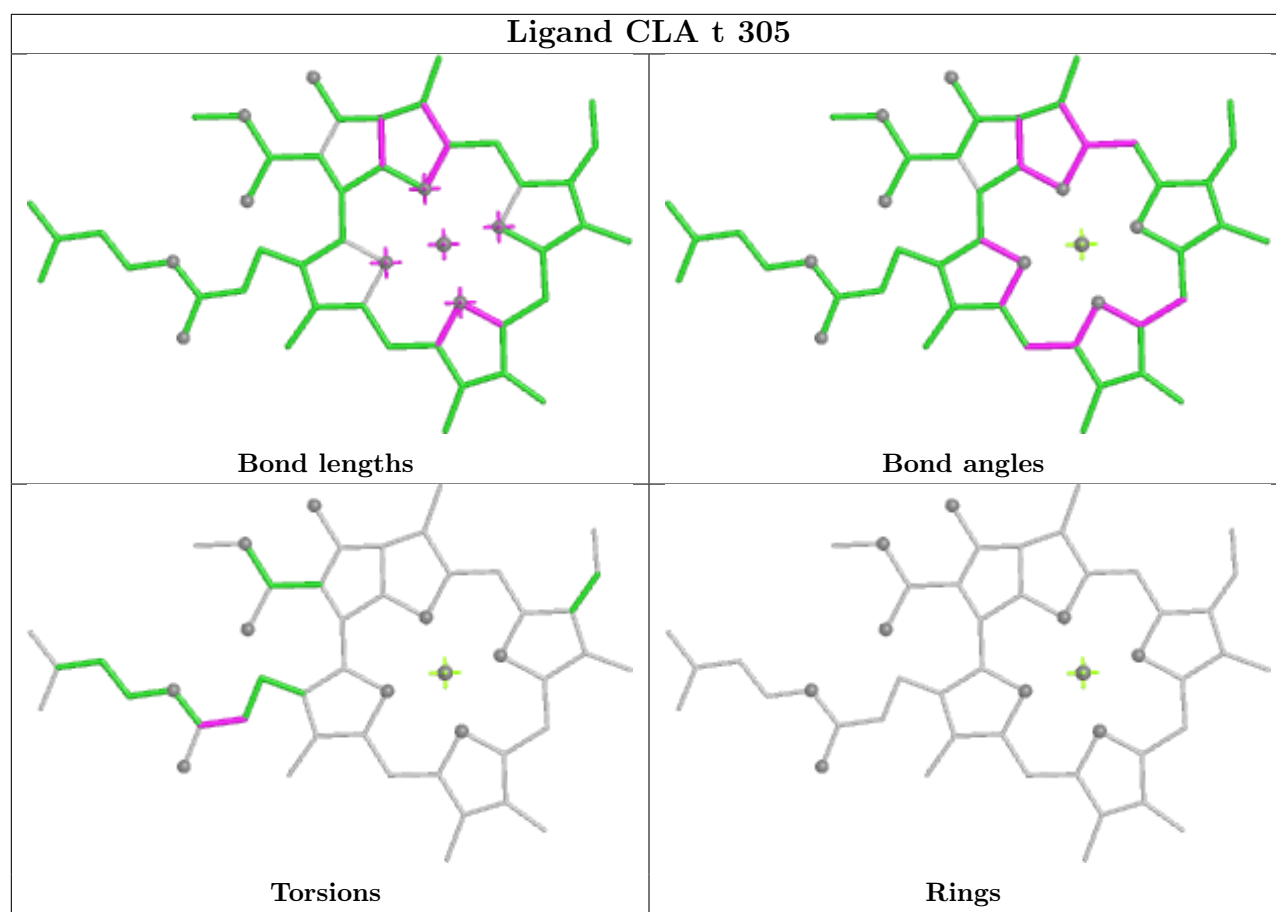


Torsions

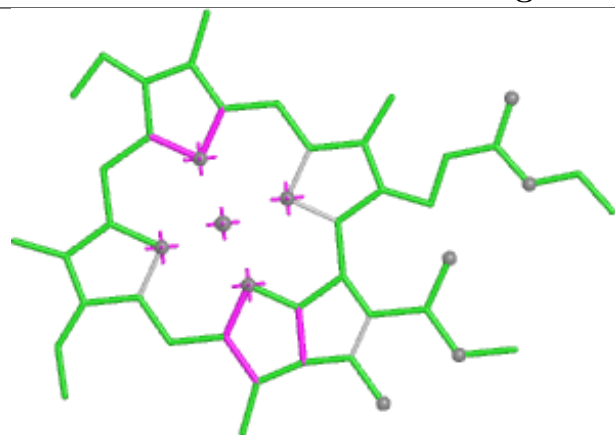


Rings





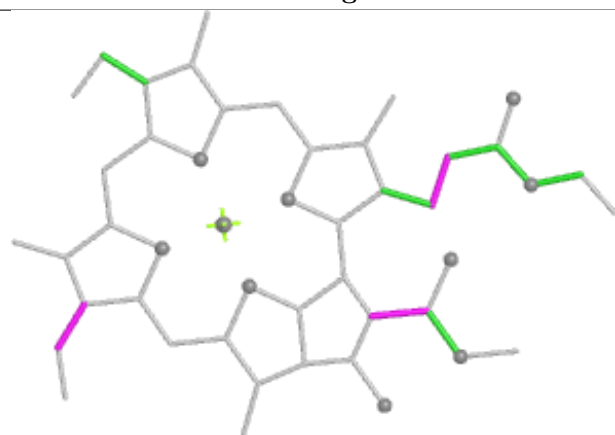
Ligand CLA A 301



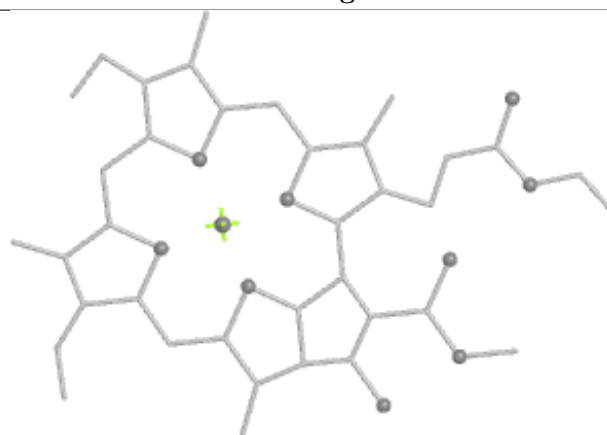
Bond lengths



Bond angles

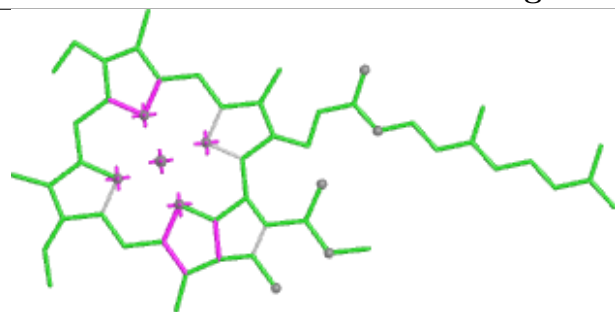


Torsions

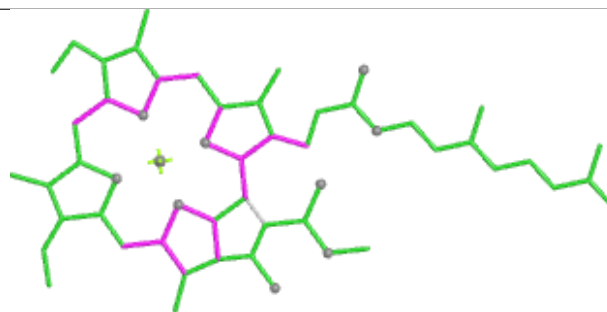


Rings

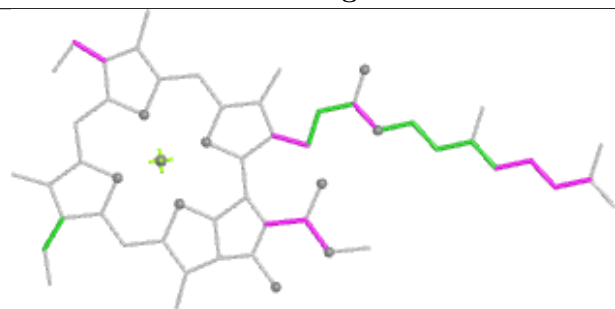
Ligand CLA i 101



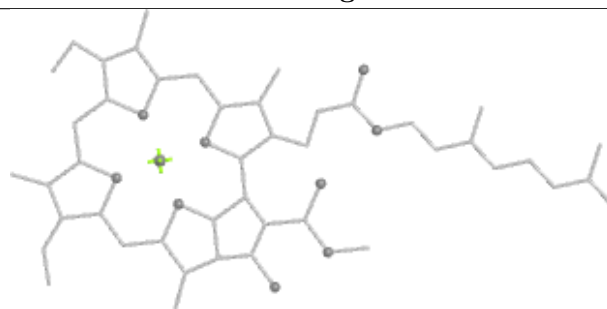
Bond lengths



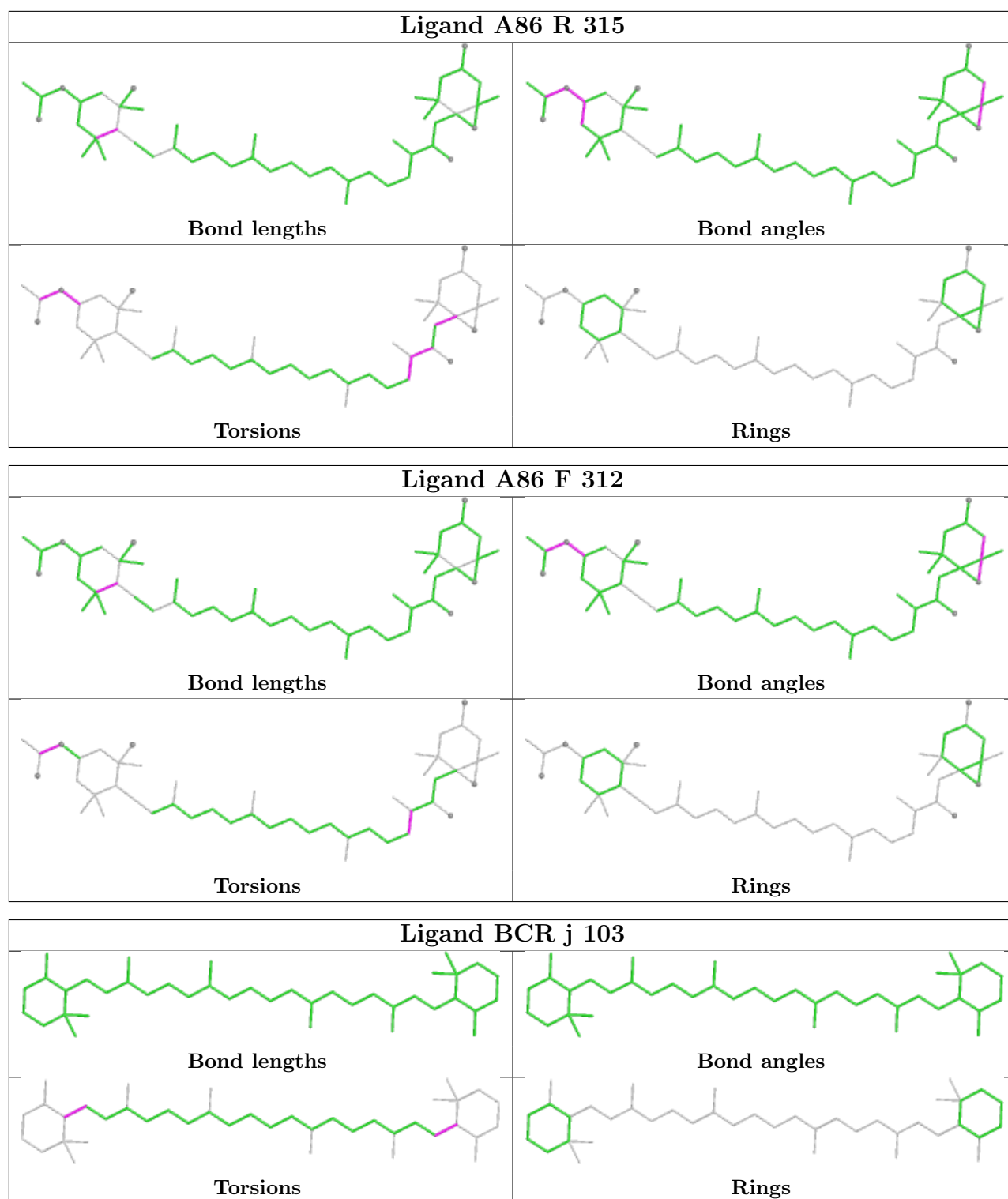
Bond angles

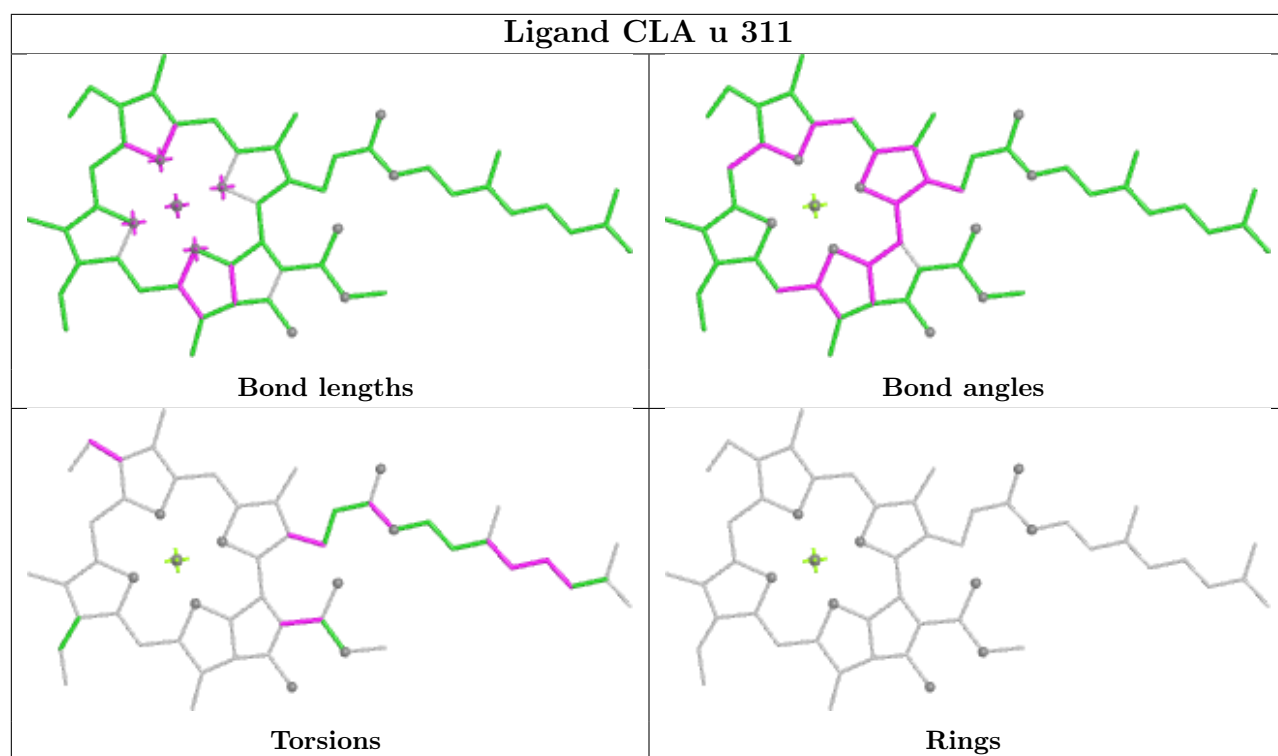


Torsions

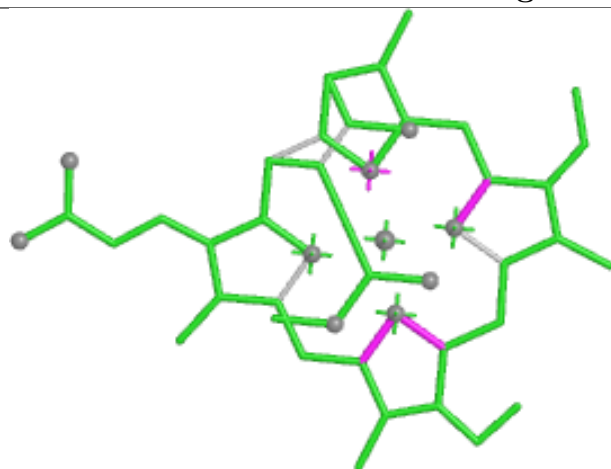


Rings

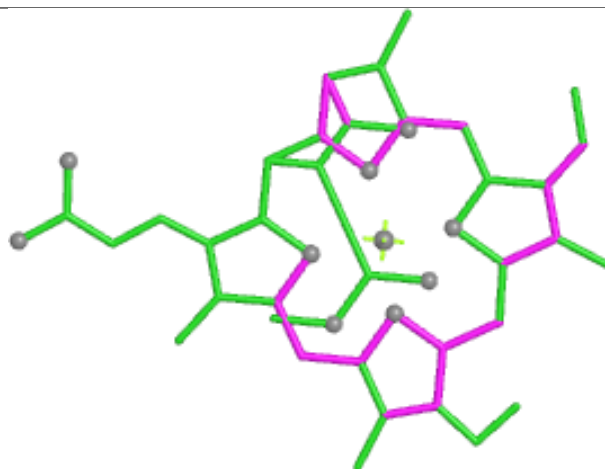




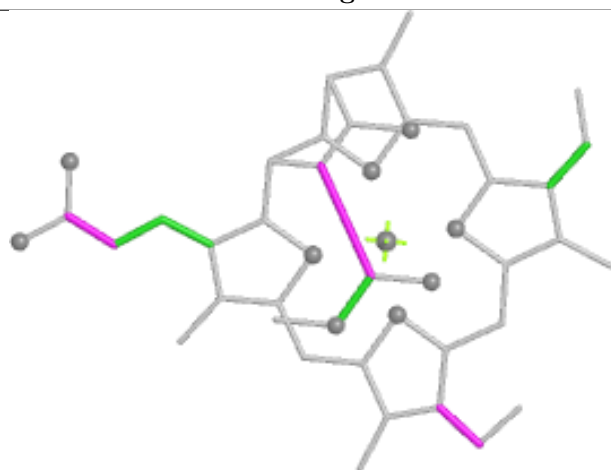
Ligand KC2 T 303



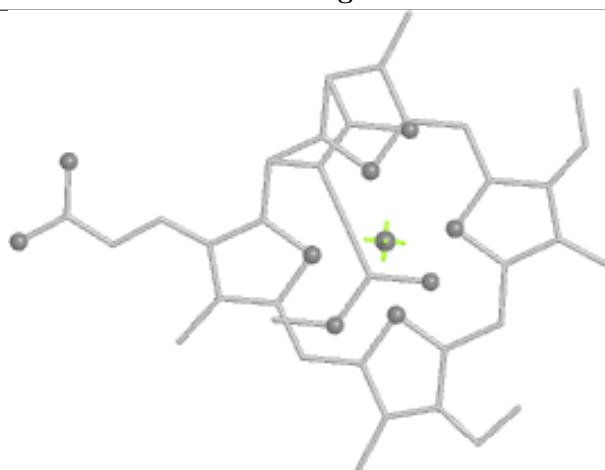
Bond lengths



Bond angles

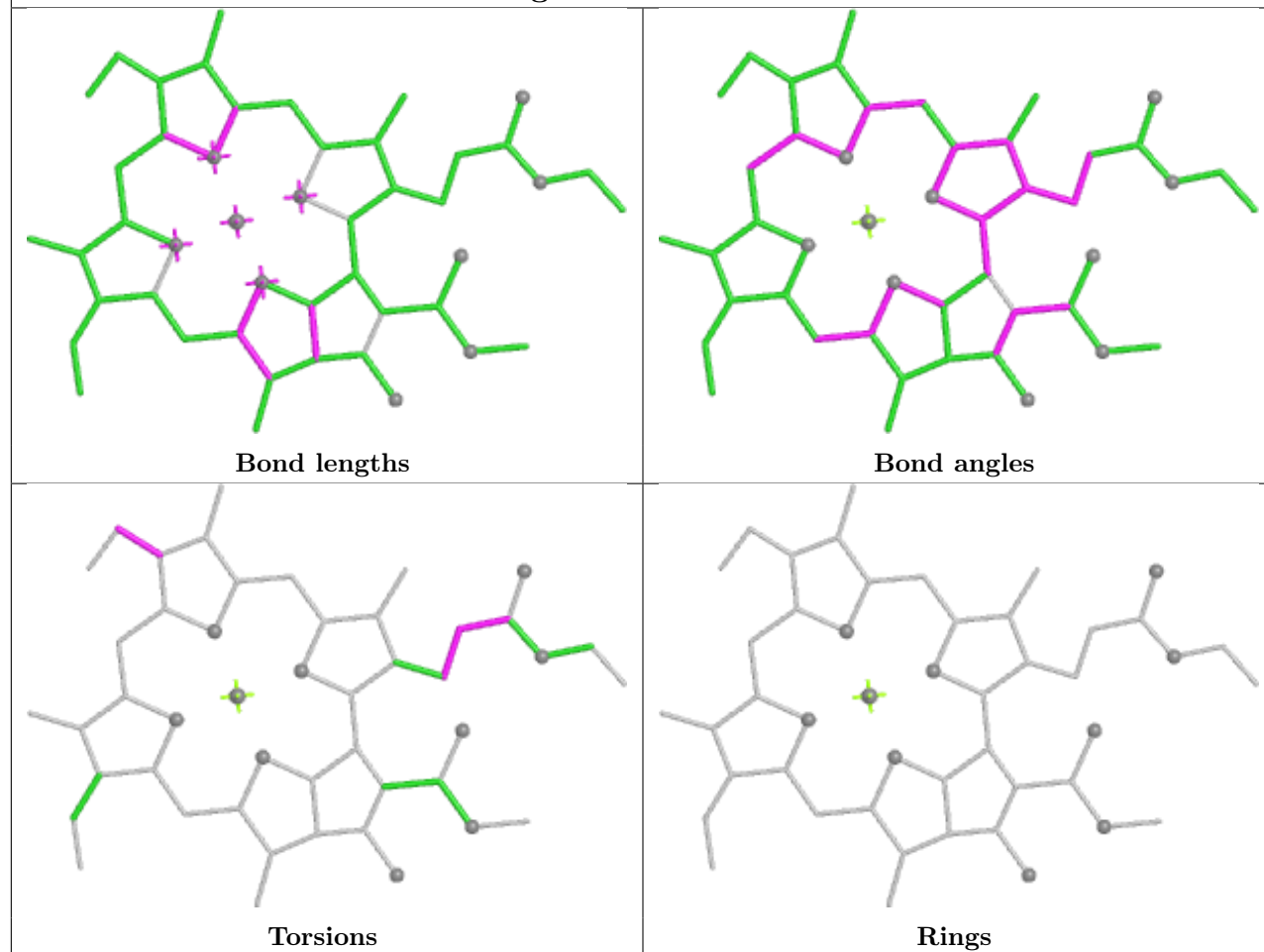


Torsions

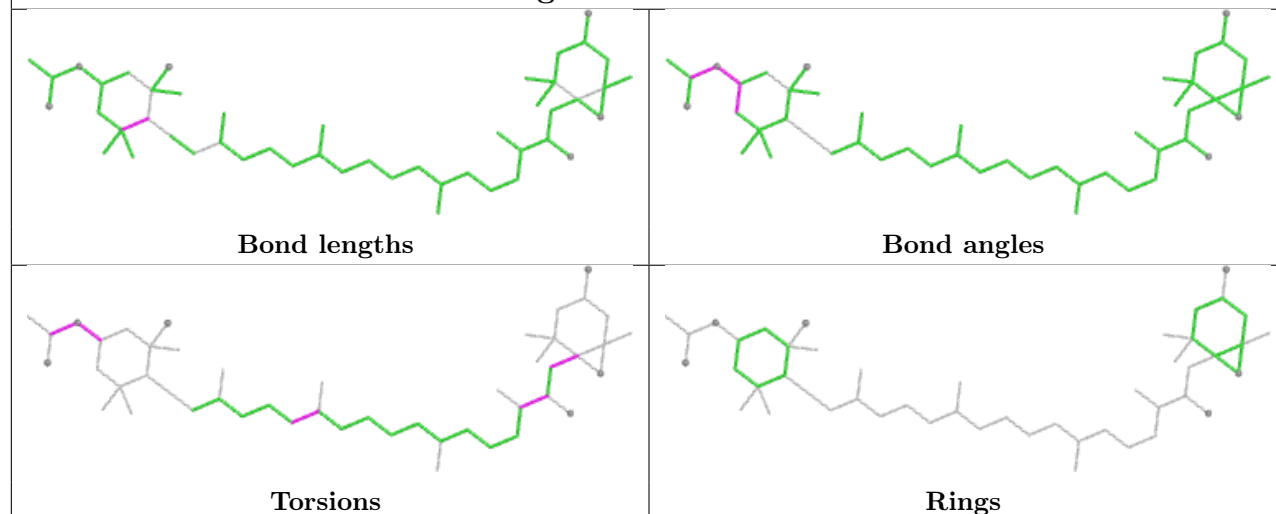


Rings

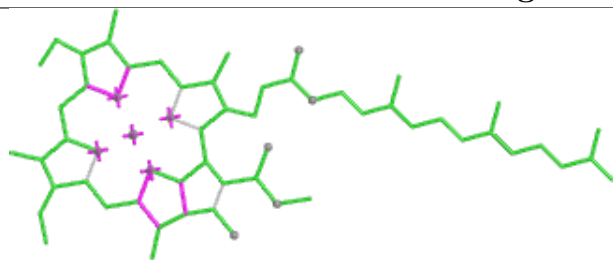
Ligand CLA J 307



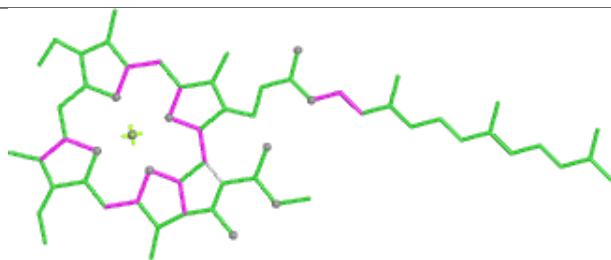
Ligand A86 Y 315



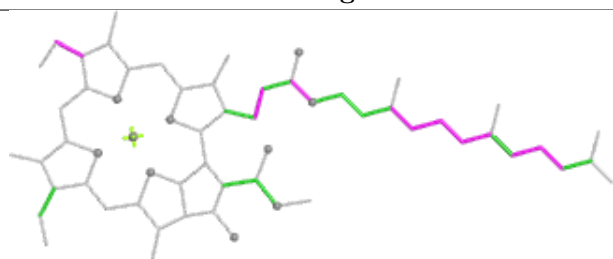
Ligand CLA S 302



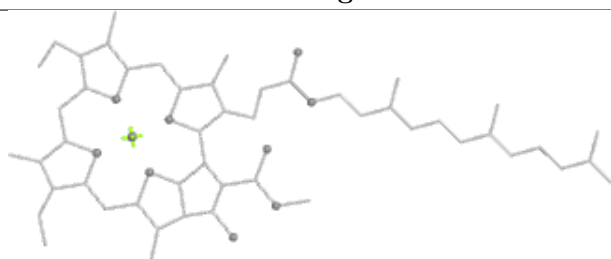
Bond lengths



Bond angles

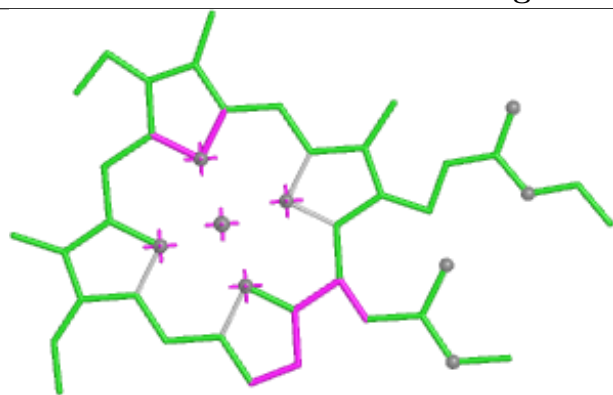


Torsions

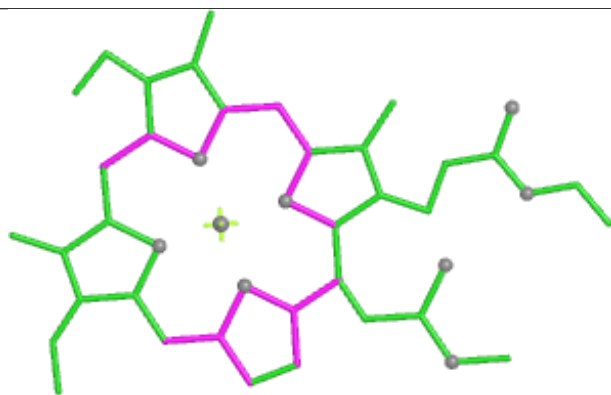


Rings

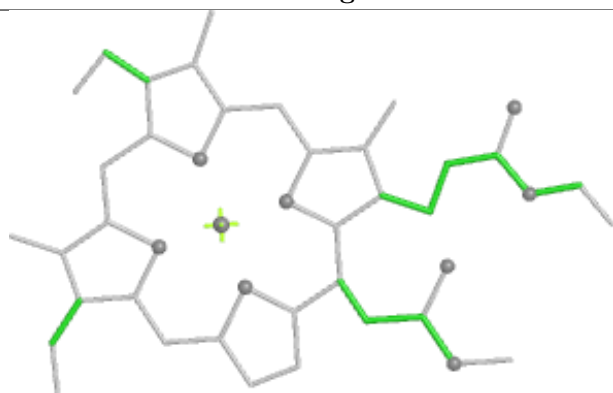
Ligand CLA D 305



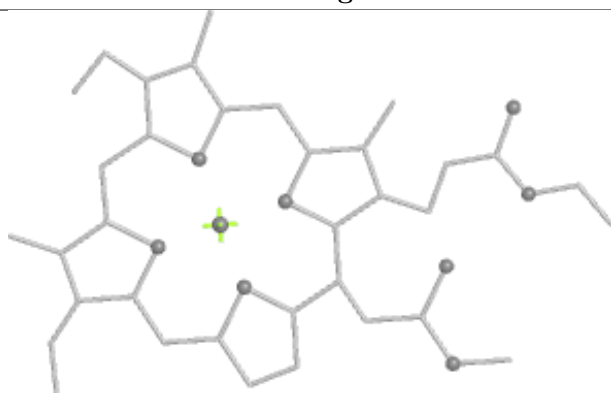
Bond lengths



Bond angles

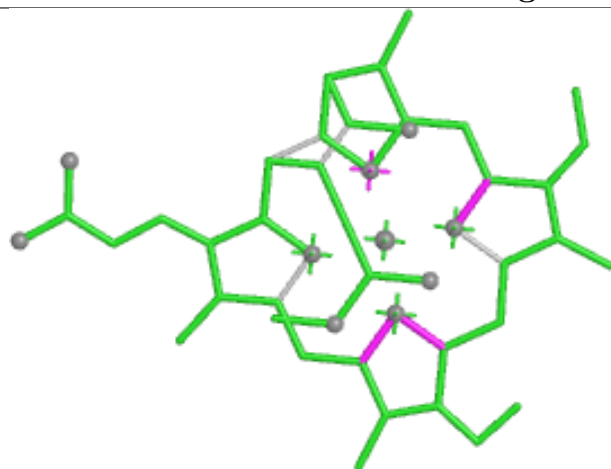


Torsions

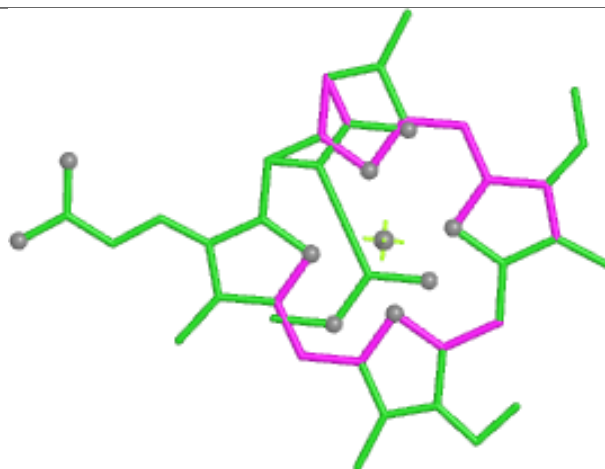


Rings

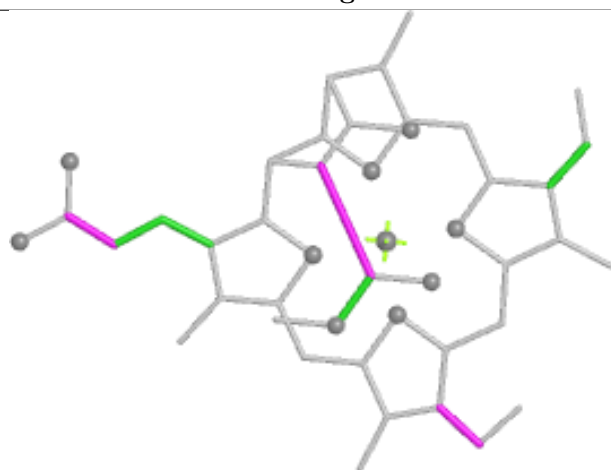
Ligand KC2 L 303



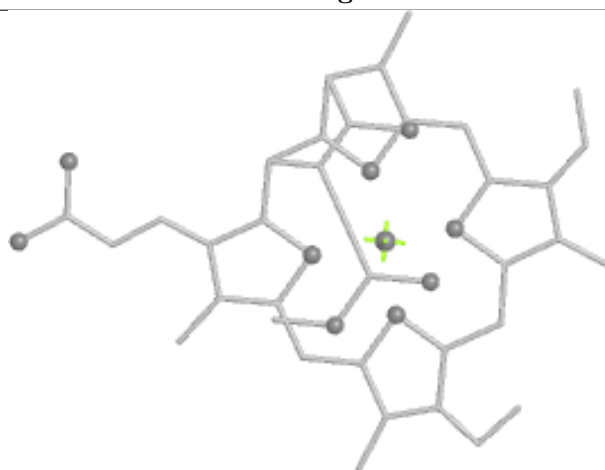
Bond lengths



Bond angles

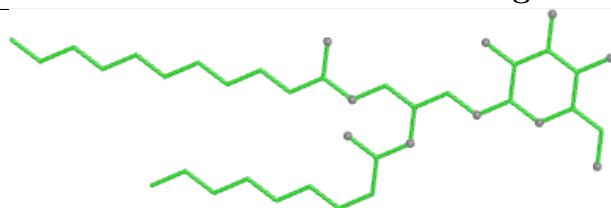


Torsions

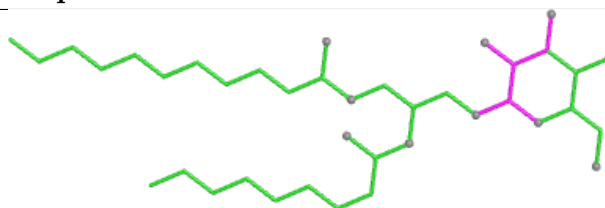


Rings

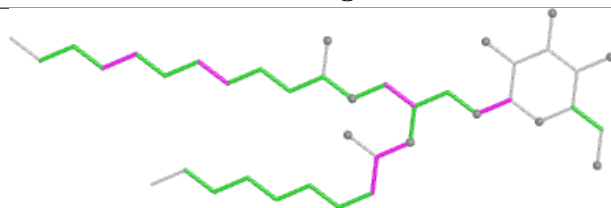
Ligand LMG p 301



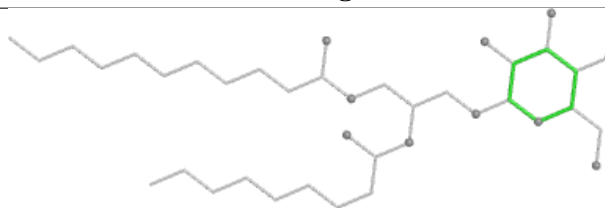
Bond lengths



Bond angles

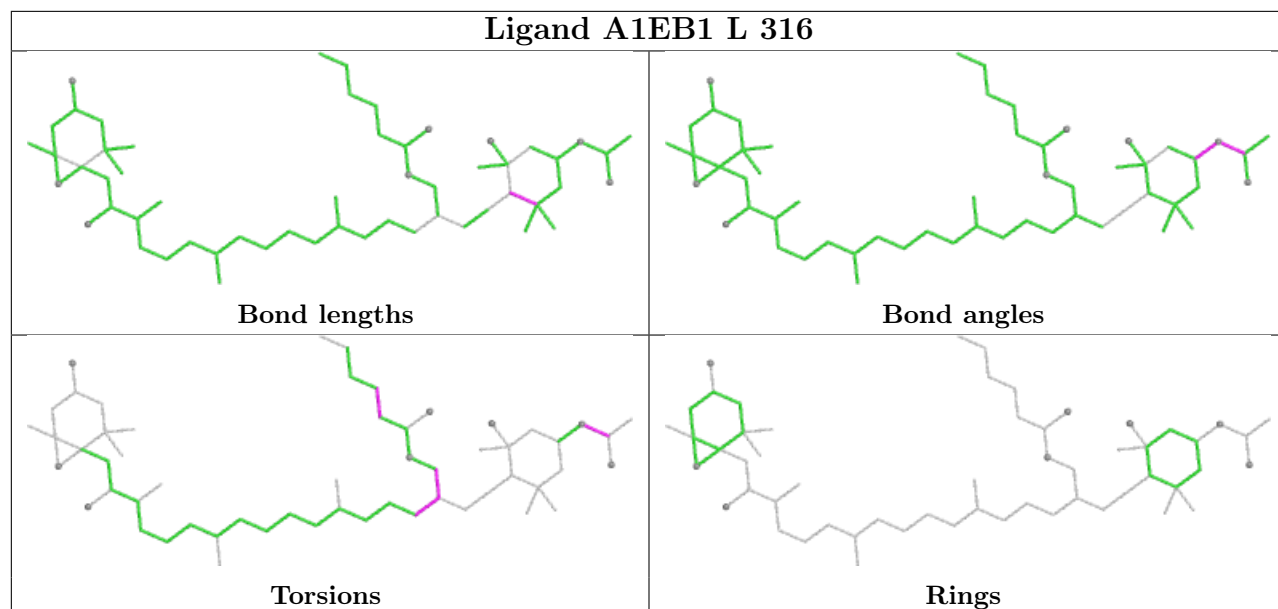


Torsions

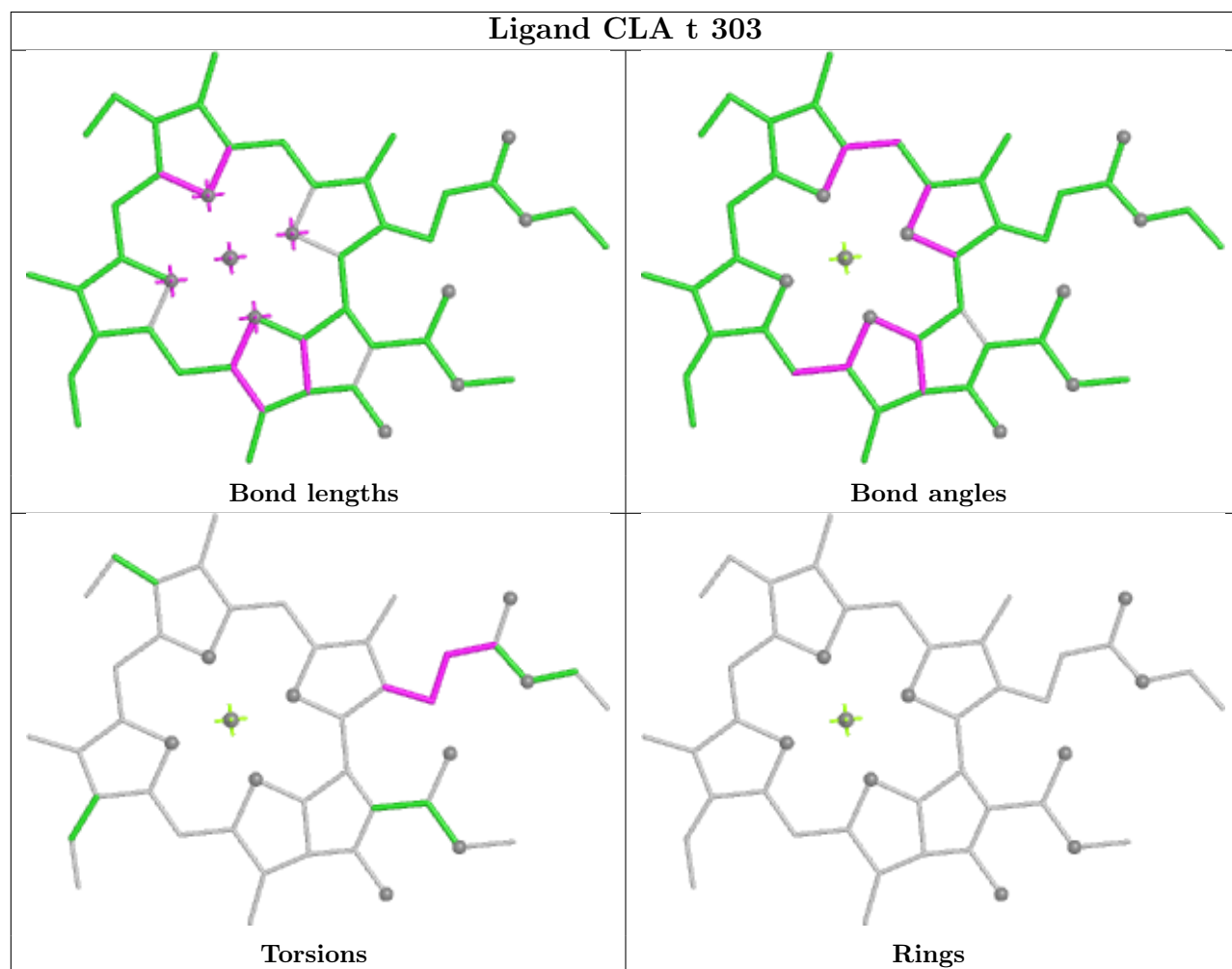


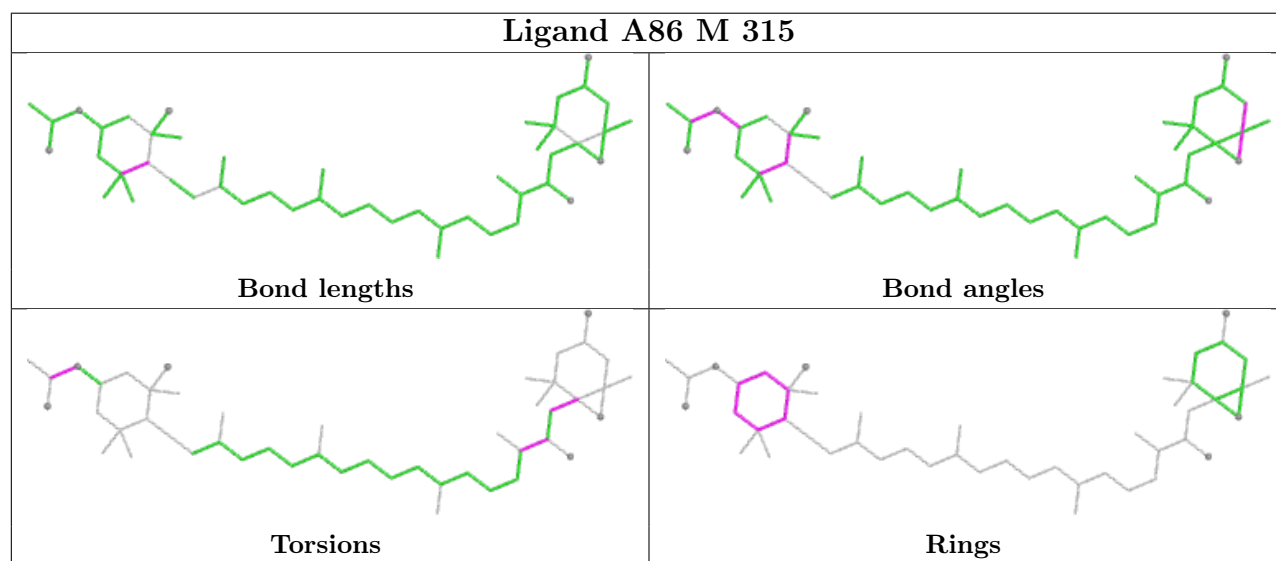
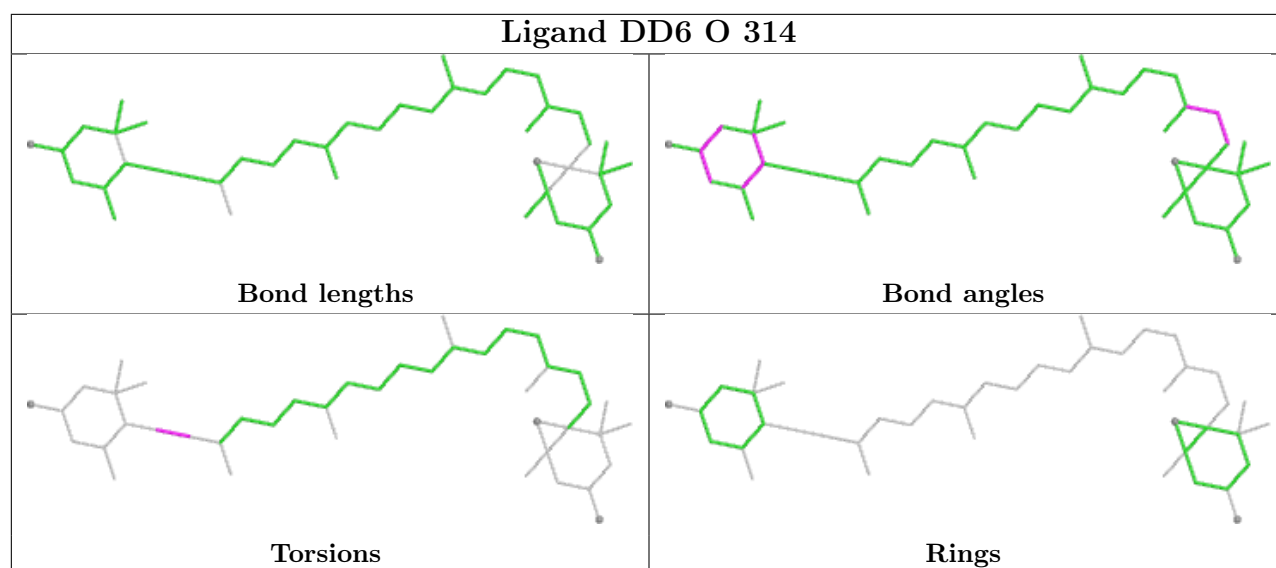
Rings

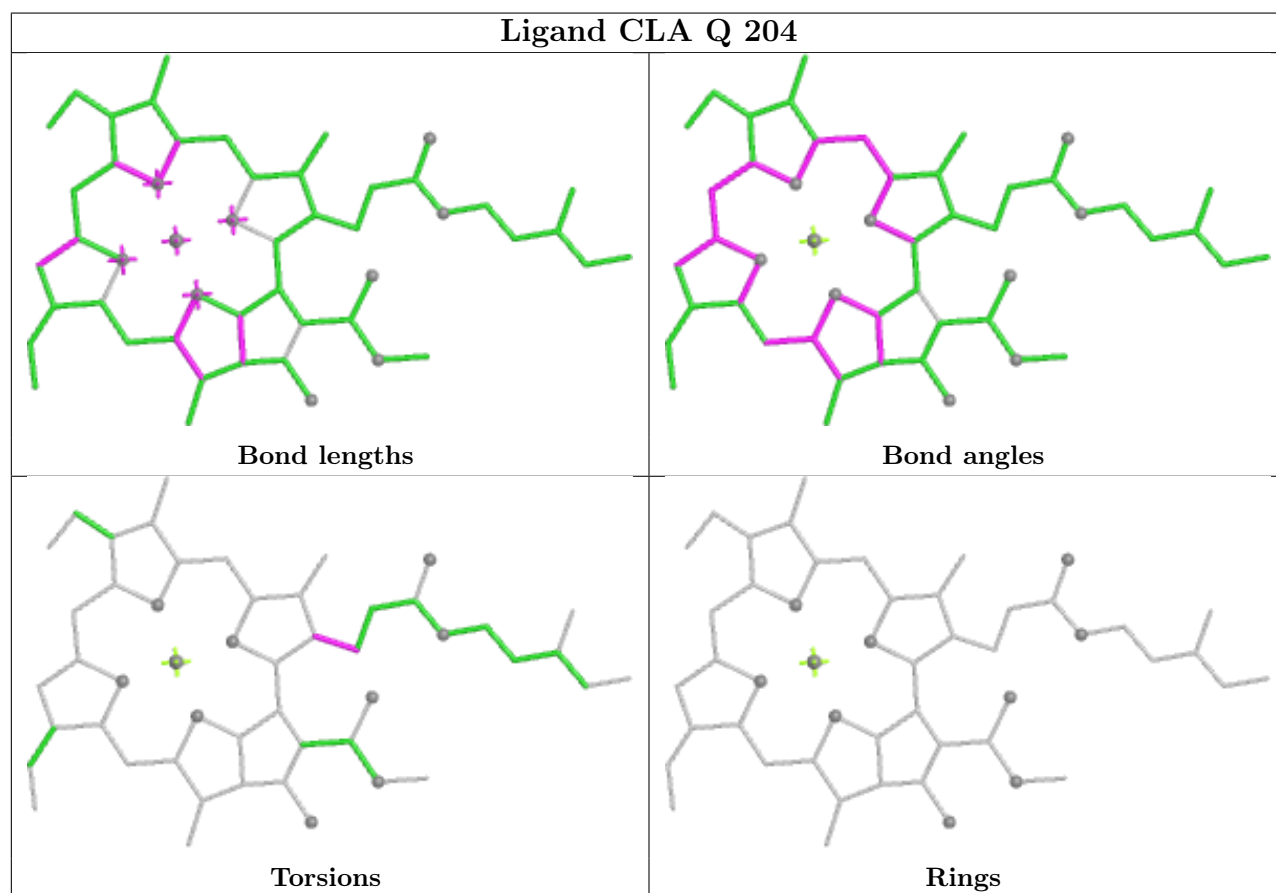
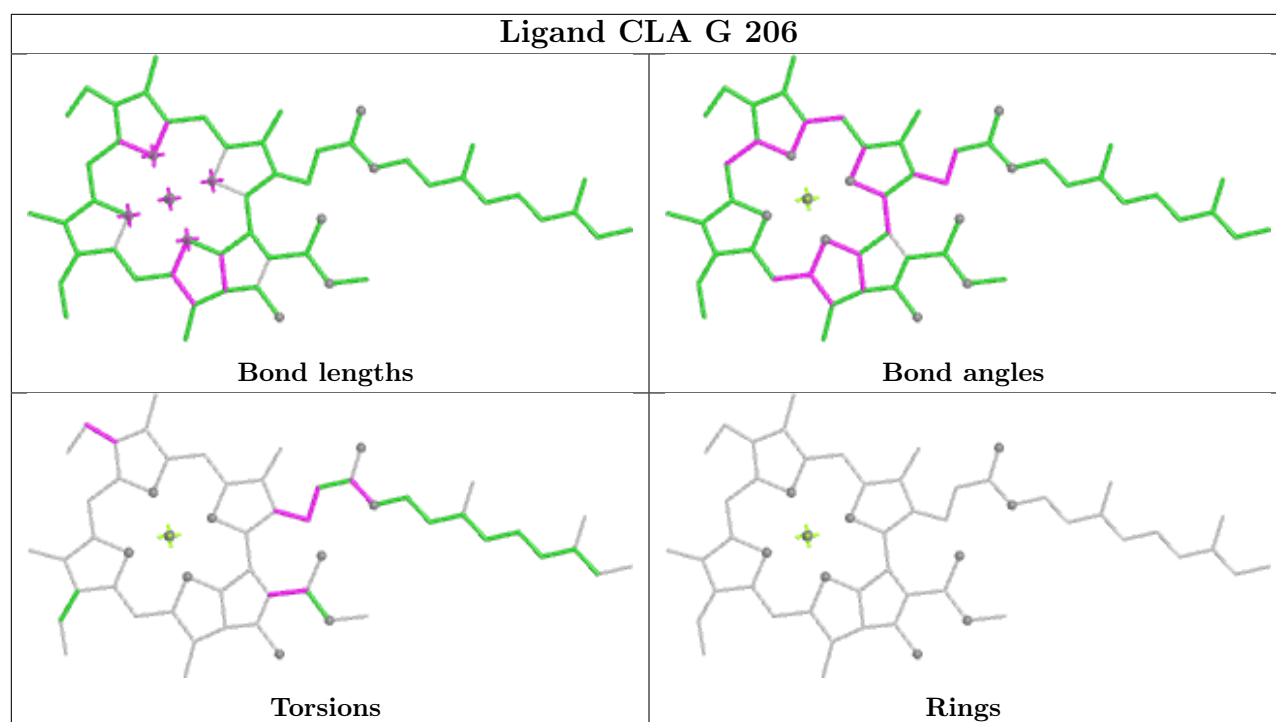
Ligand A1EB1 L 316

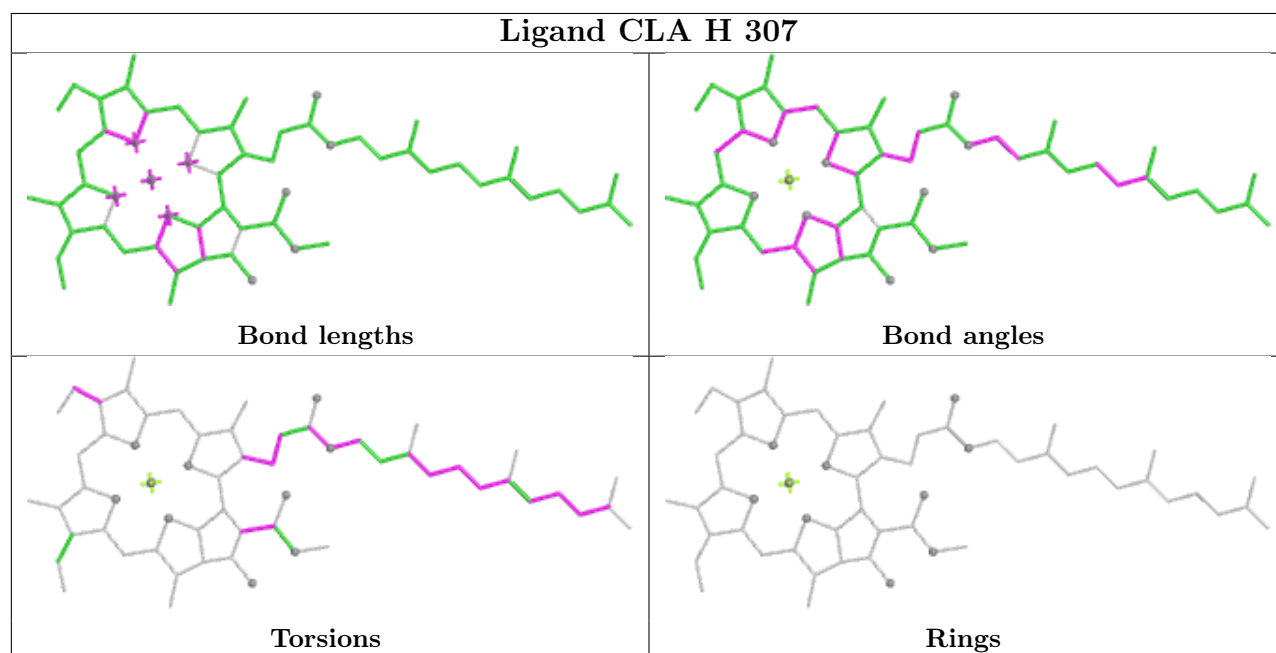
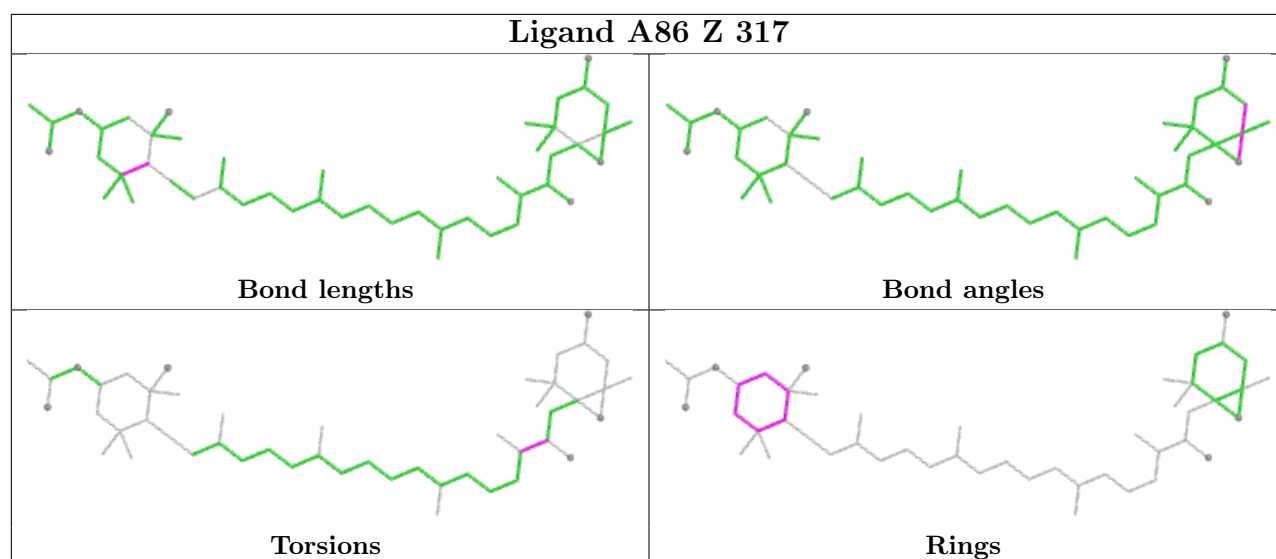


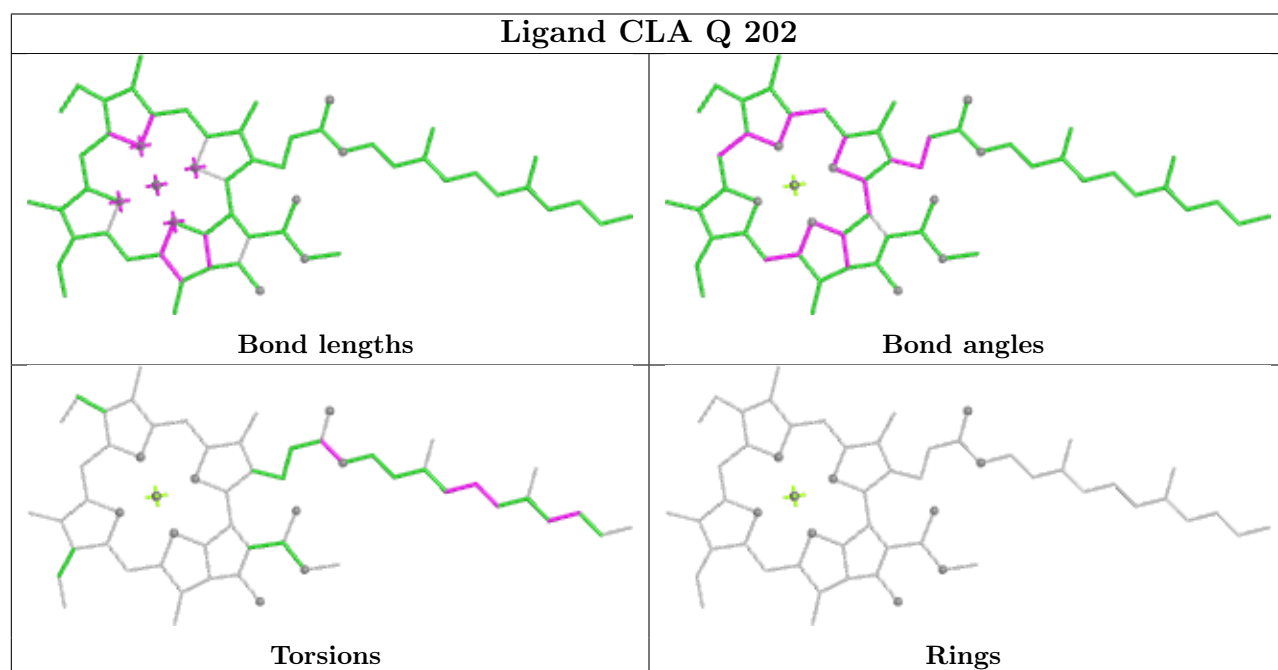
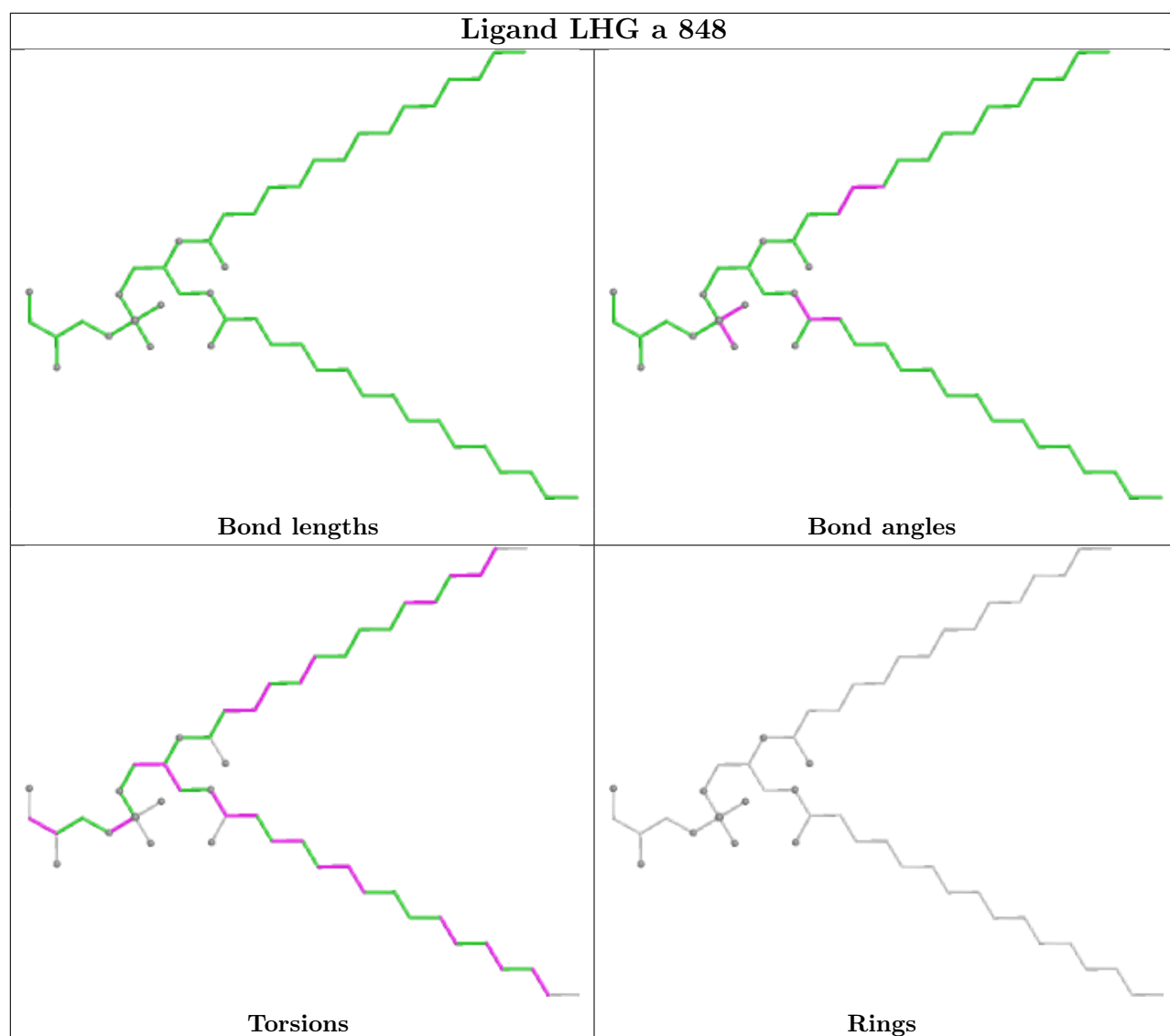
Ligand CLA t 303



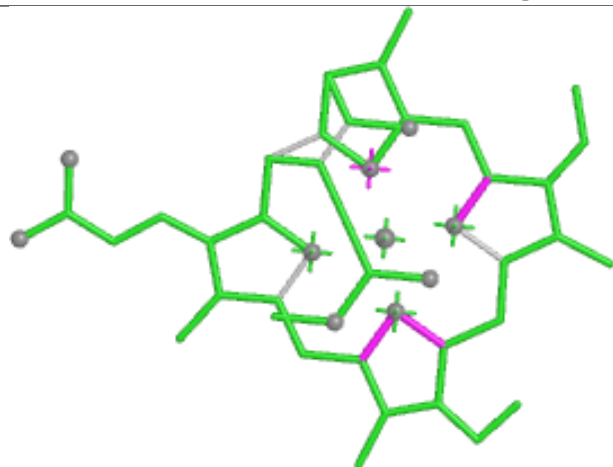




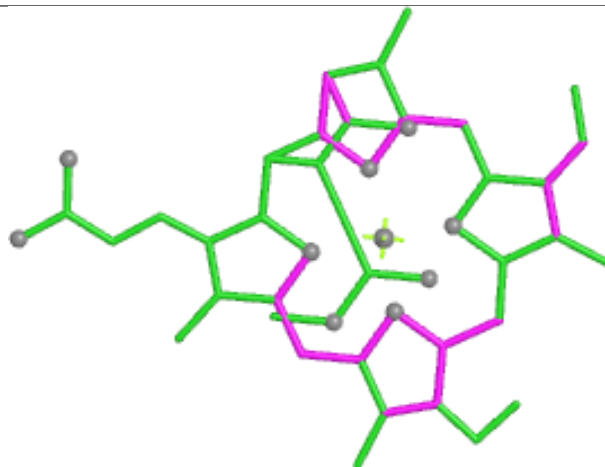




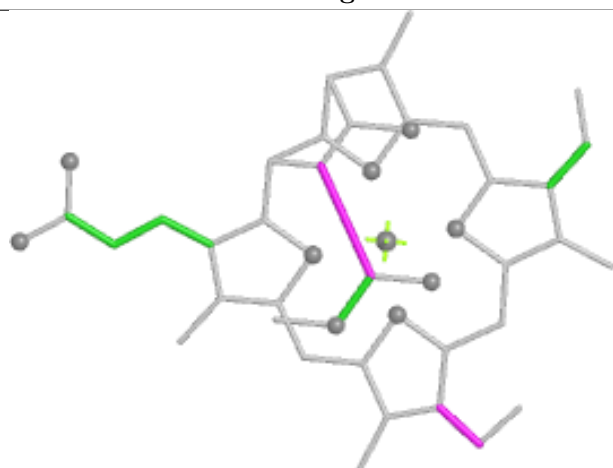
Ligand KC2 P 304



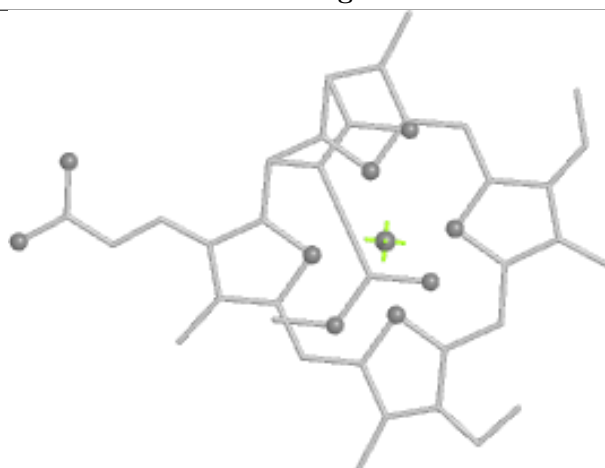
Bond lengths



Bond angles



Torsions



Rings

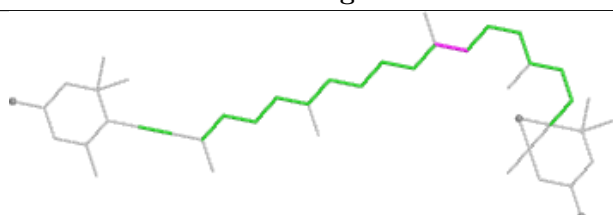
Ligand DD6 D 317



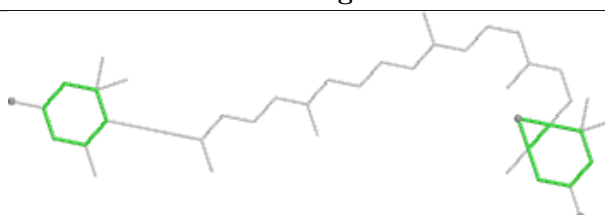
Bond lengths



Bond angles

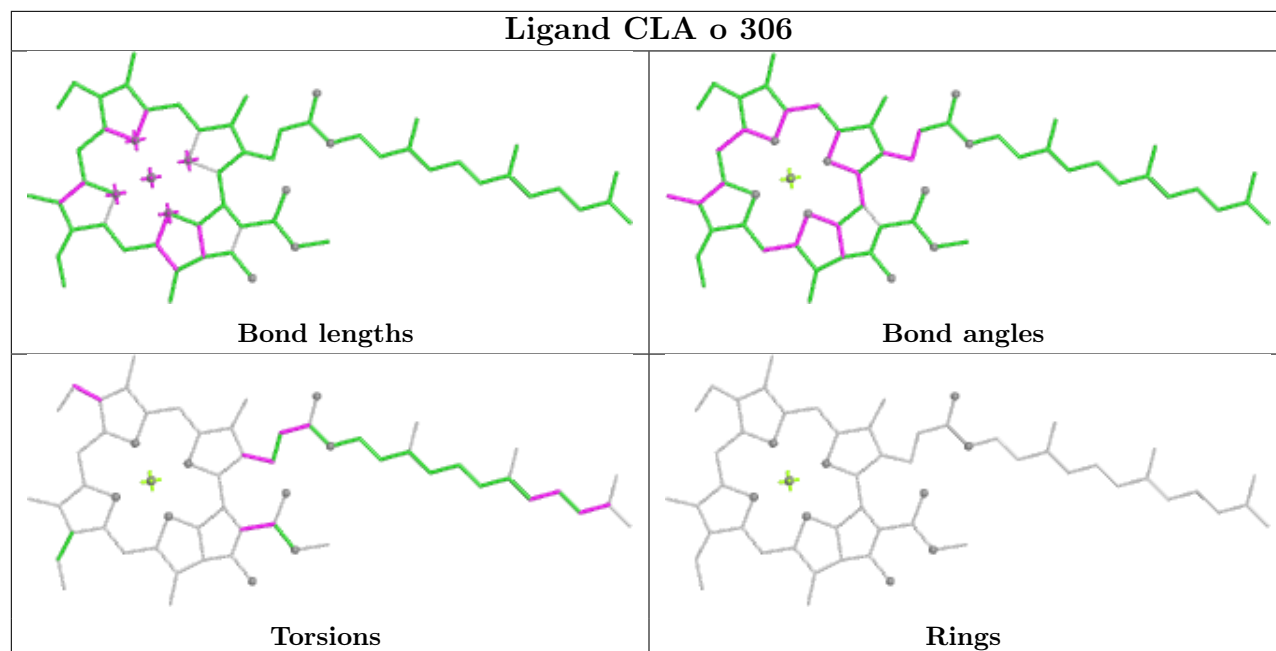


Torsions

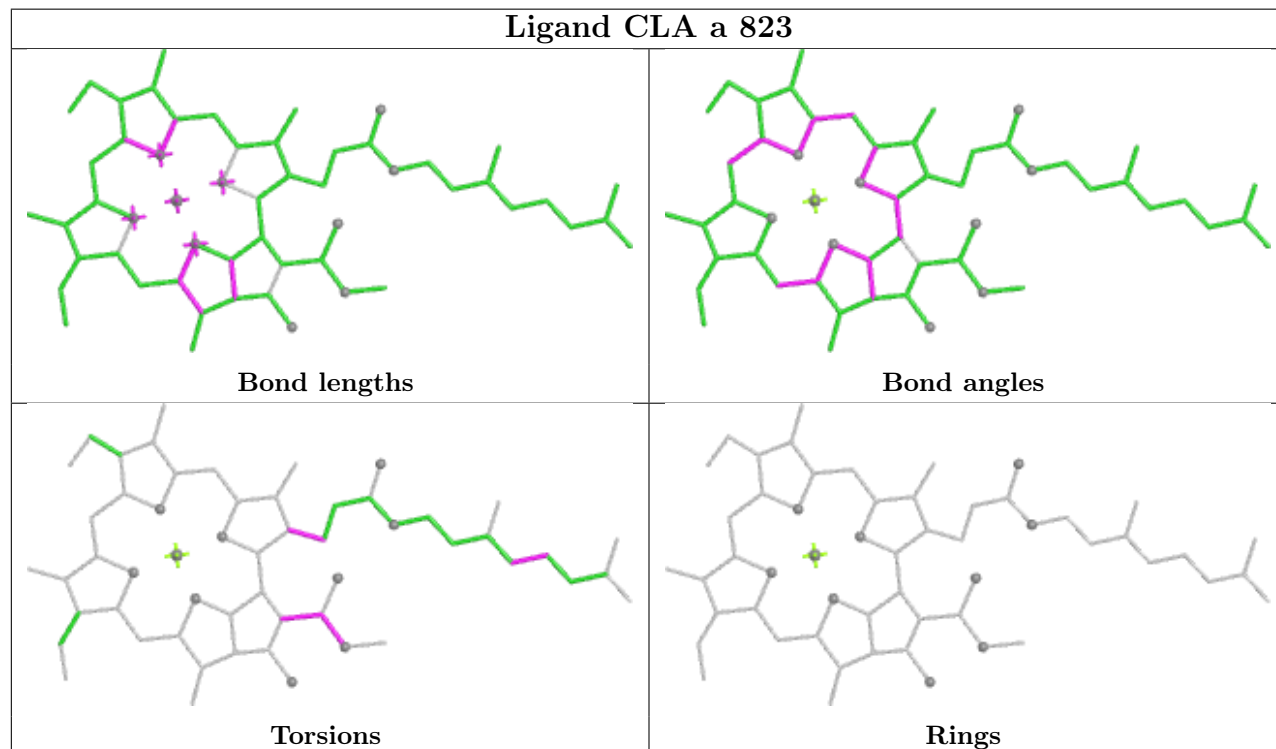


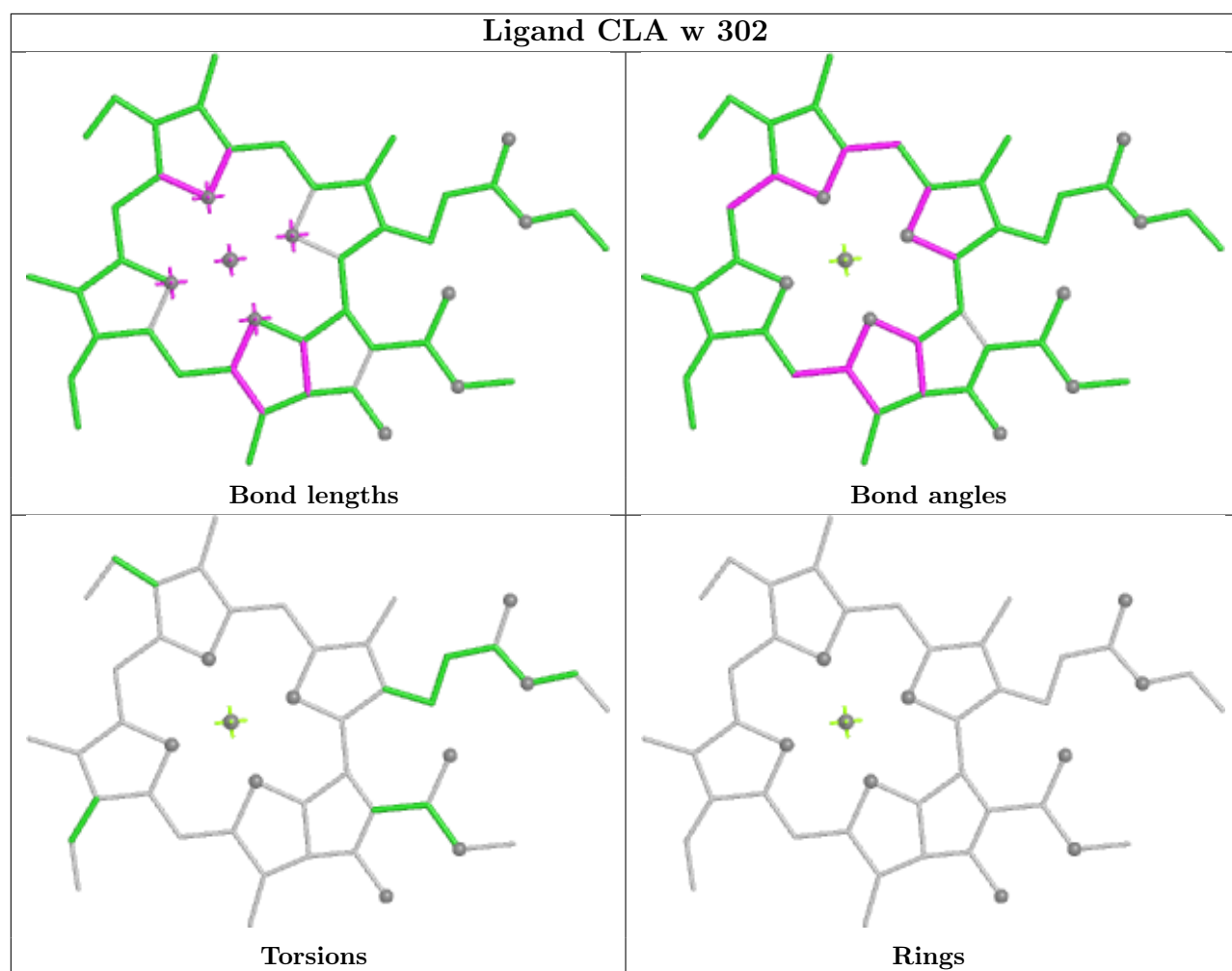
Rings

Ligand CLA o 306

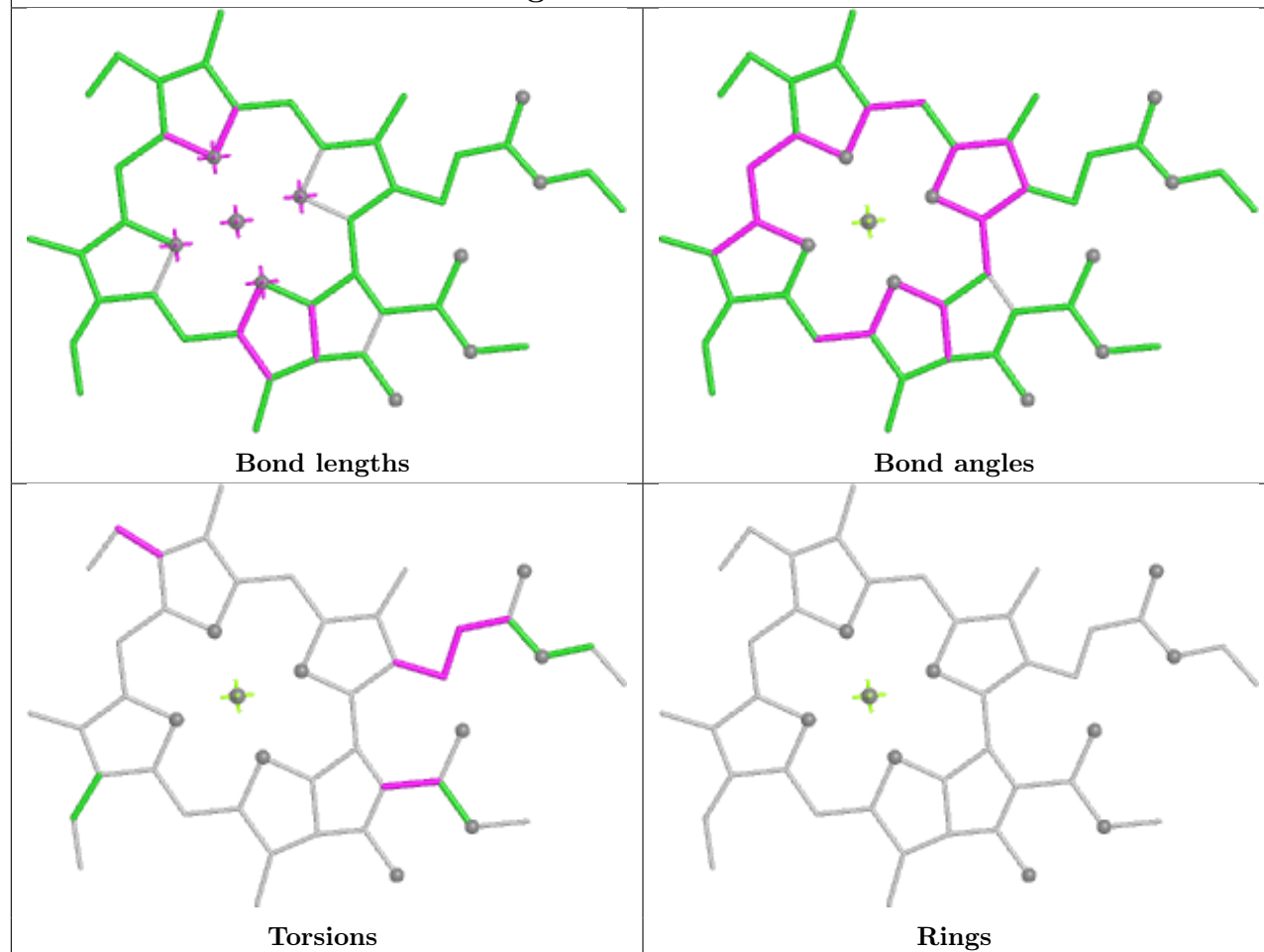


Ligand CLA a 823

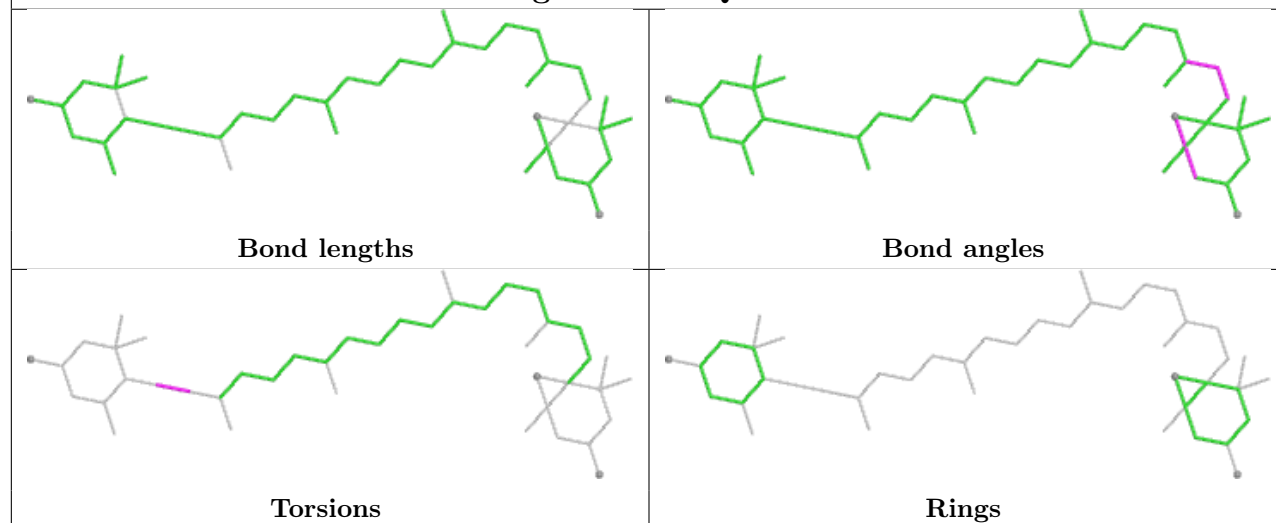


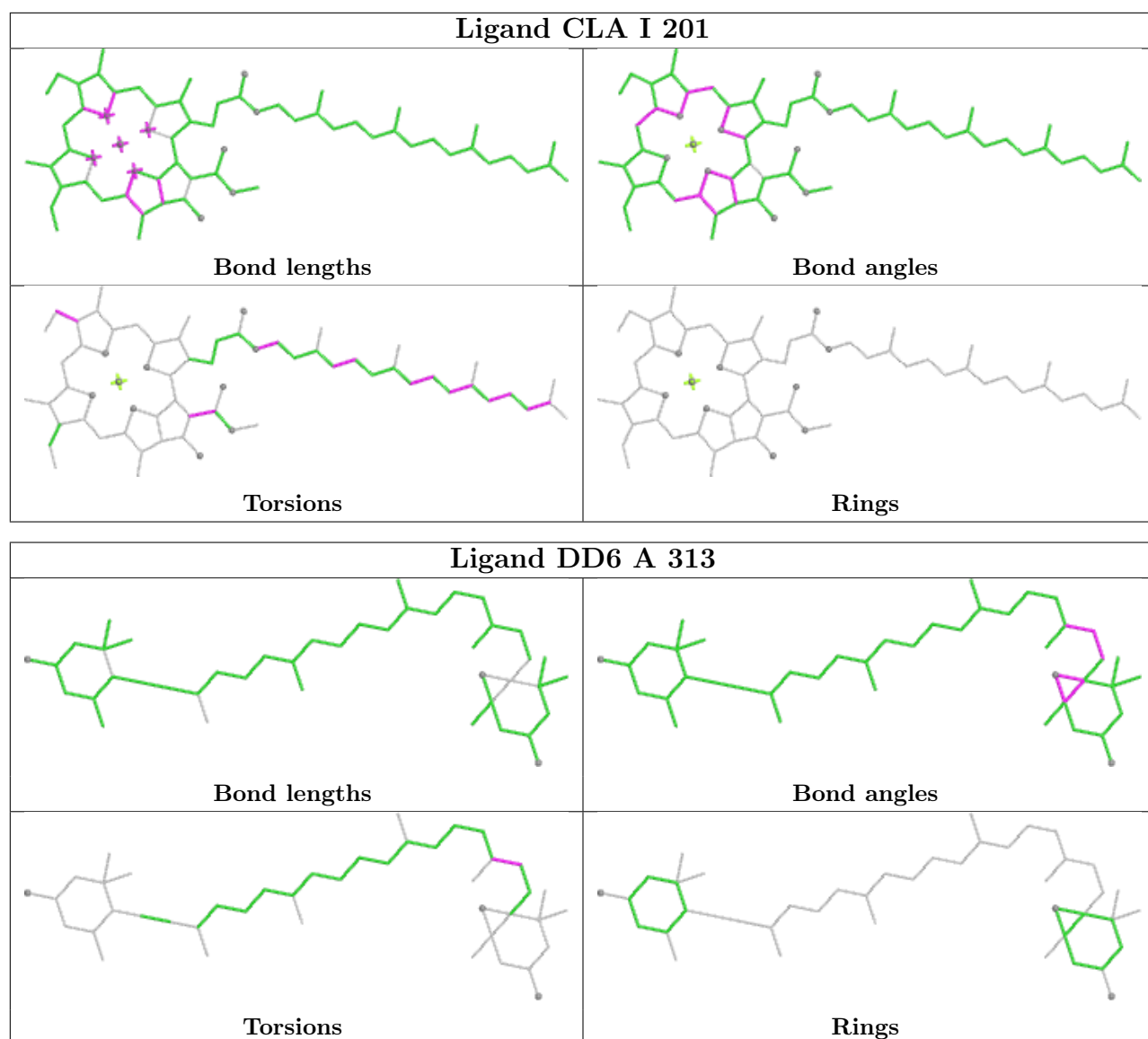


Ligand CLA B 307

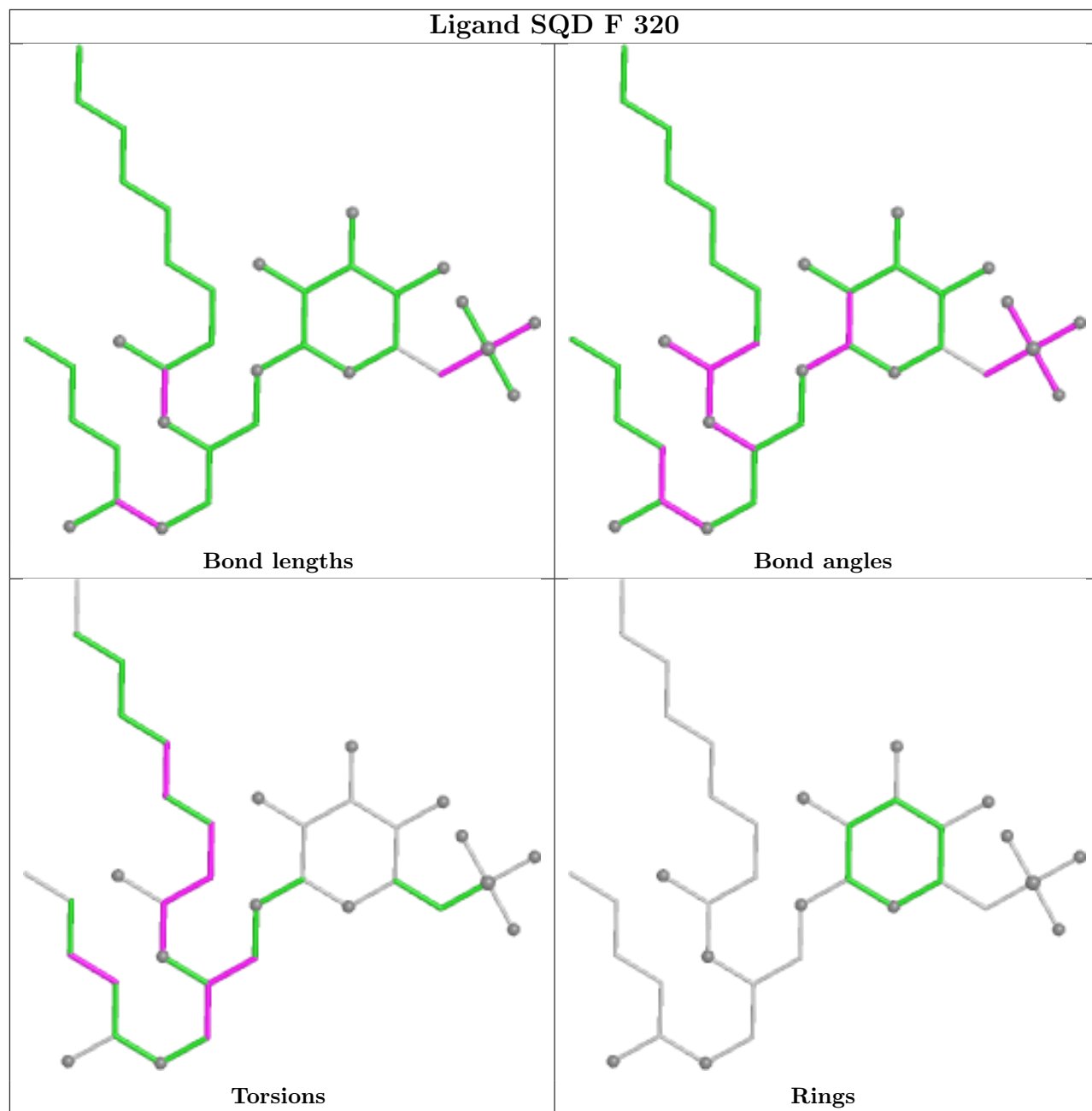


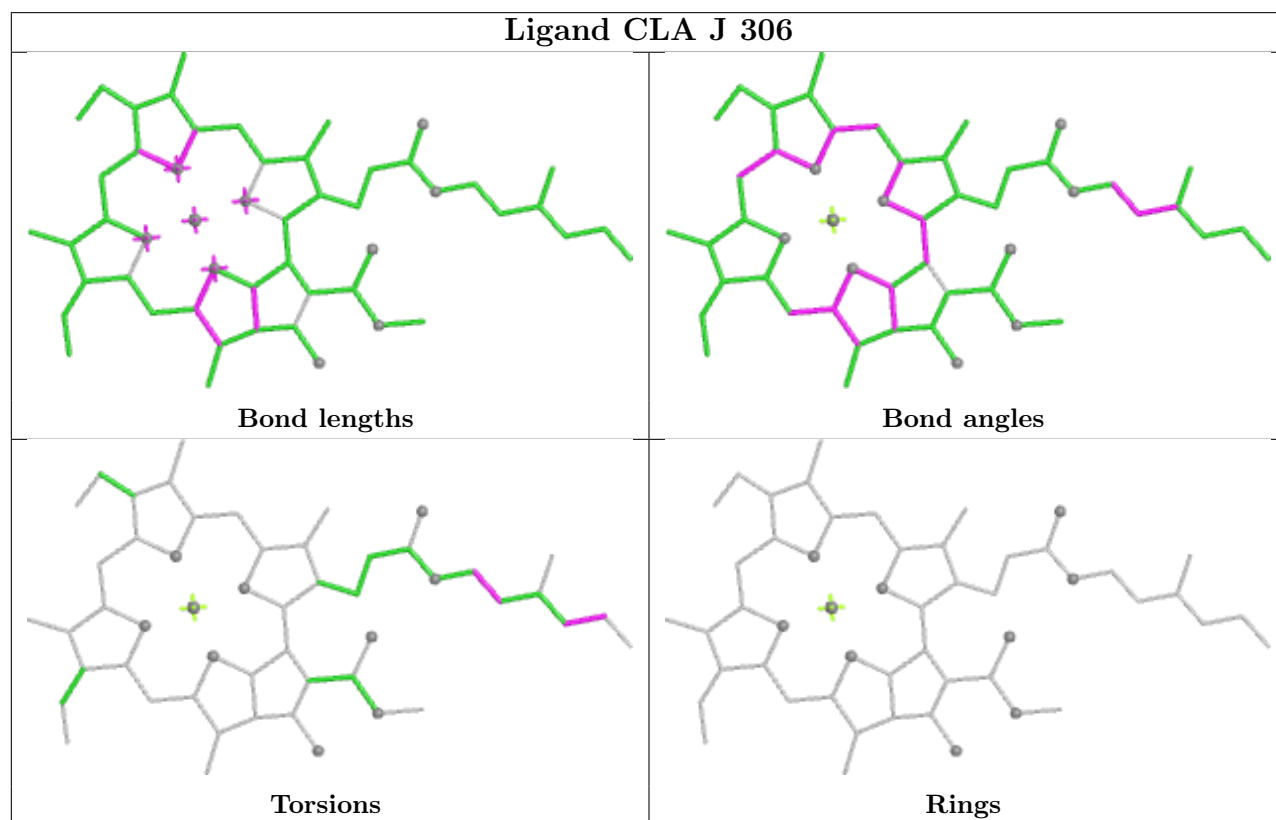
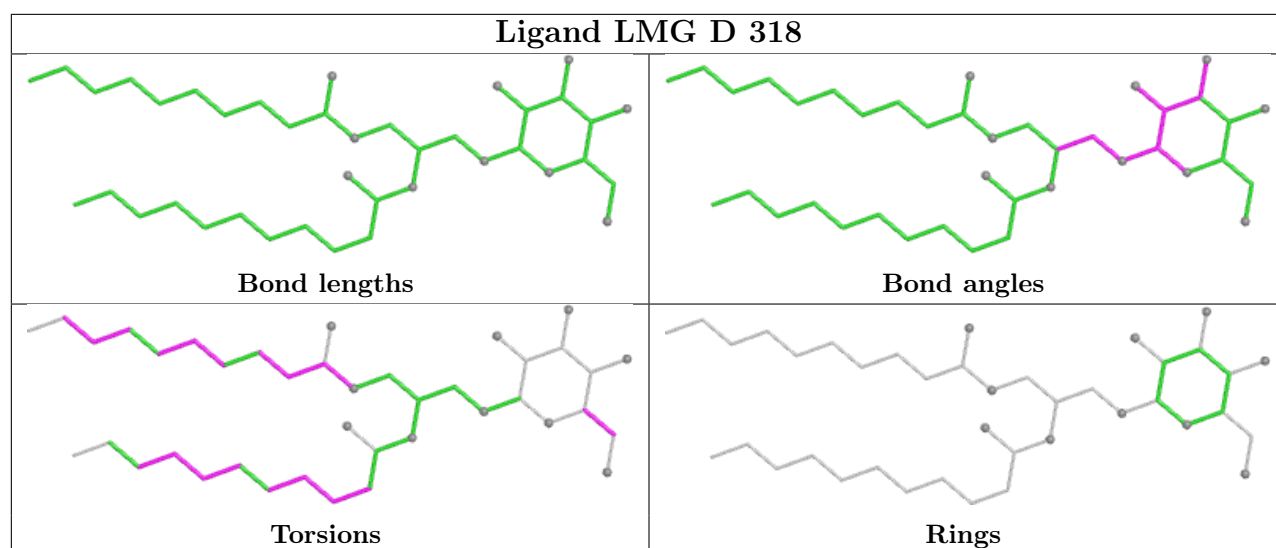
Ligand DD6 Q 213

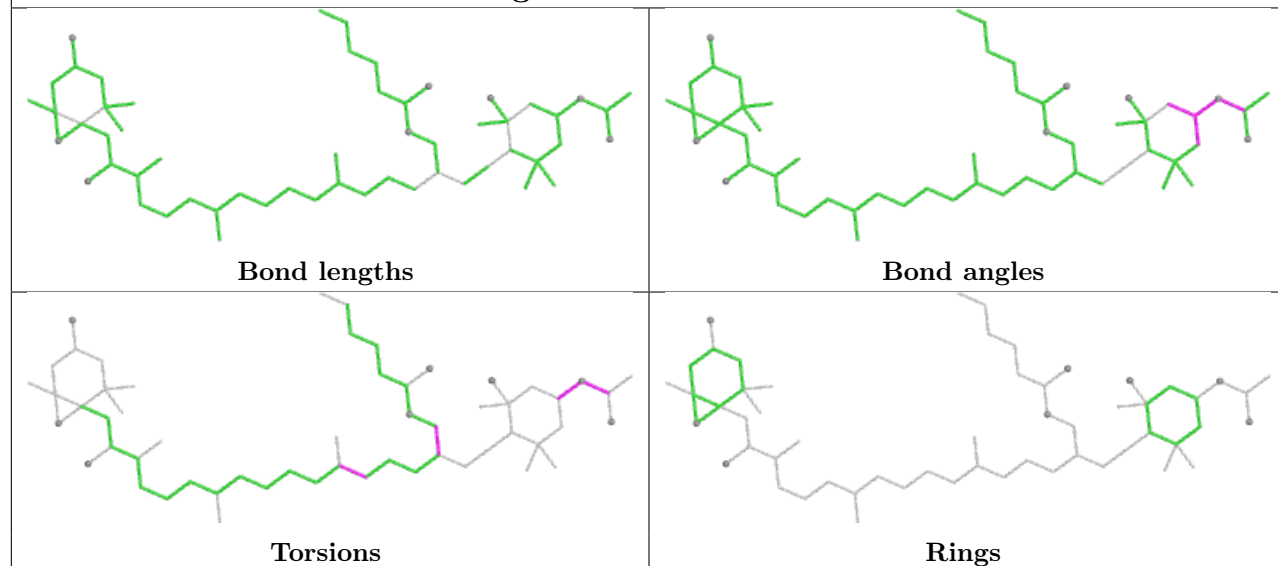
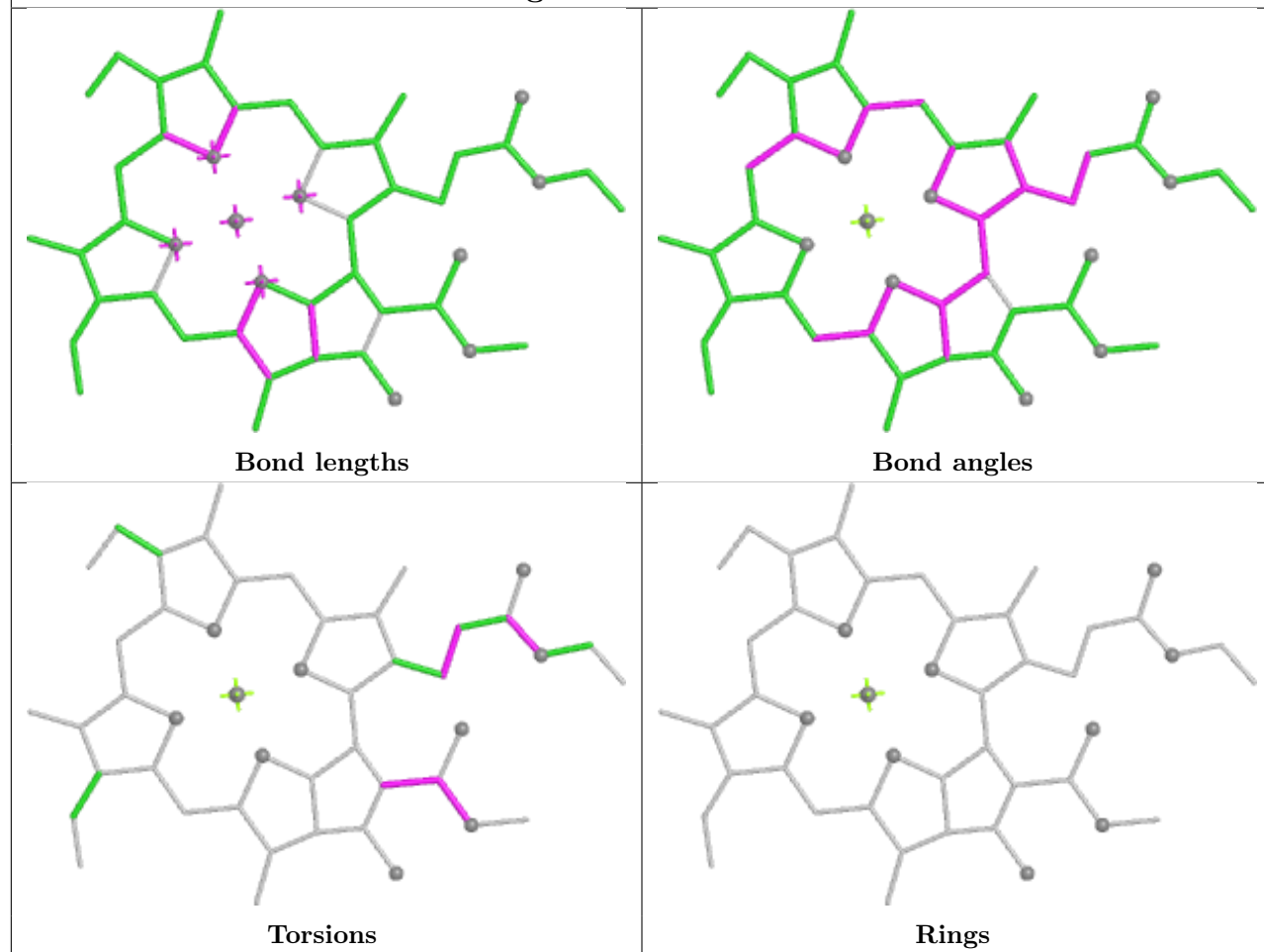


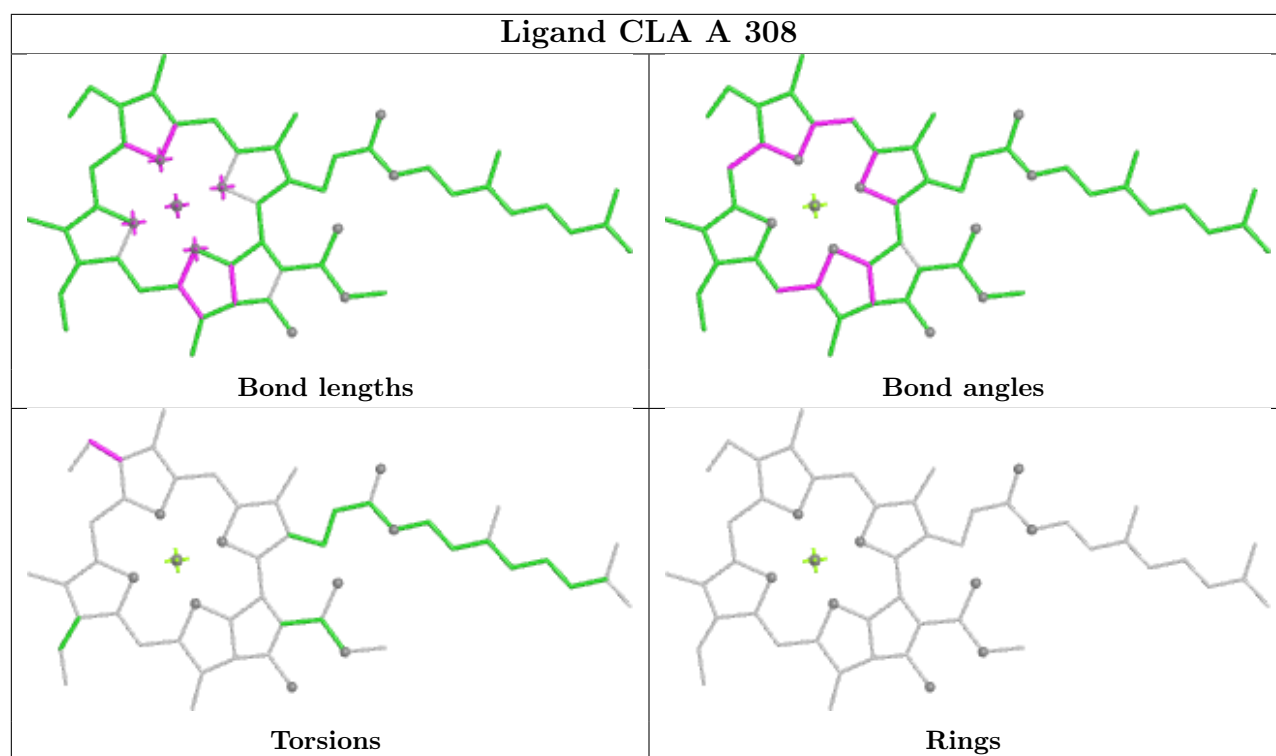


Ligand SQD F 320

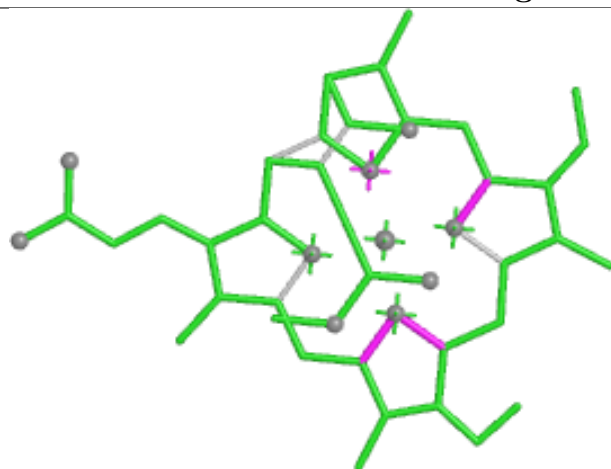




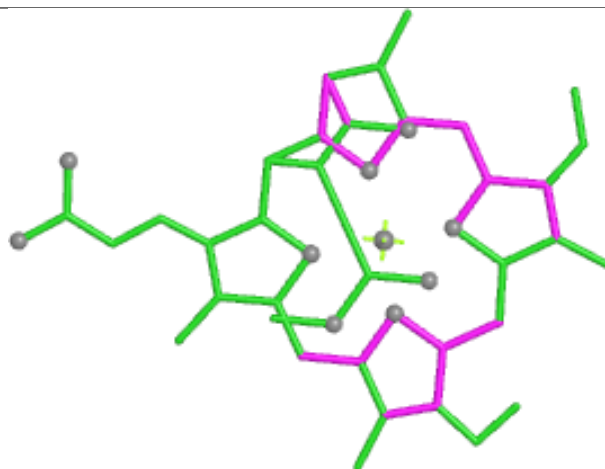
Ligand A1EB1 N 320**Ligand CLA C 308**



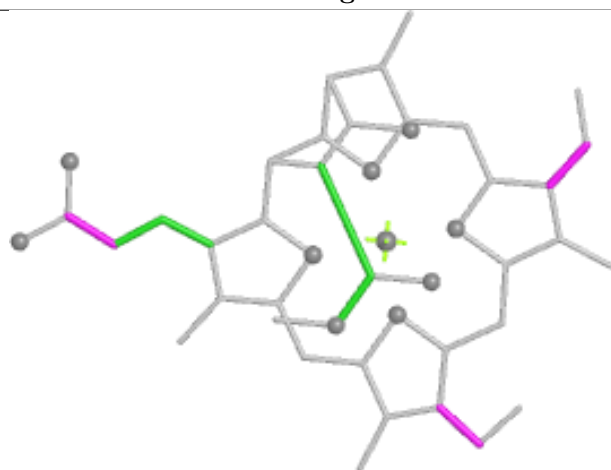
Ligand KC2 K 302



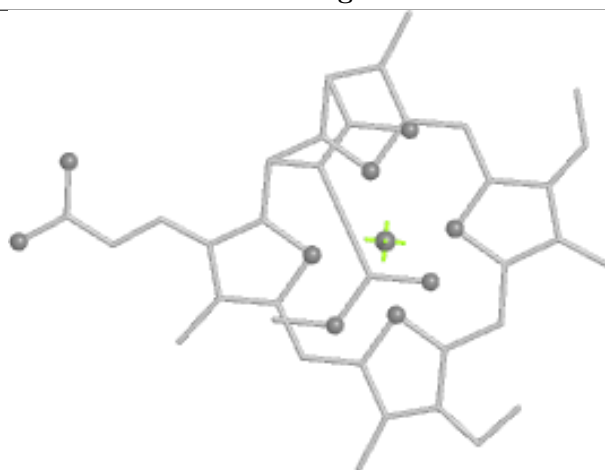
Bond lengths



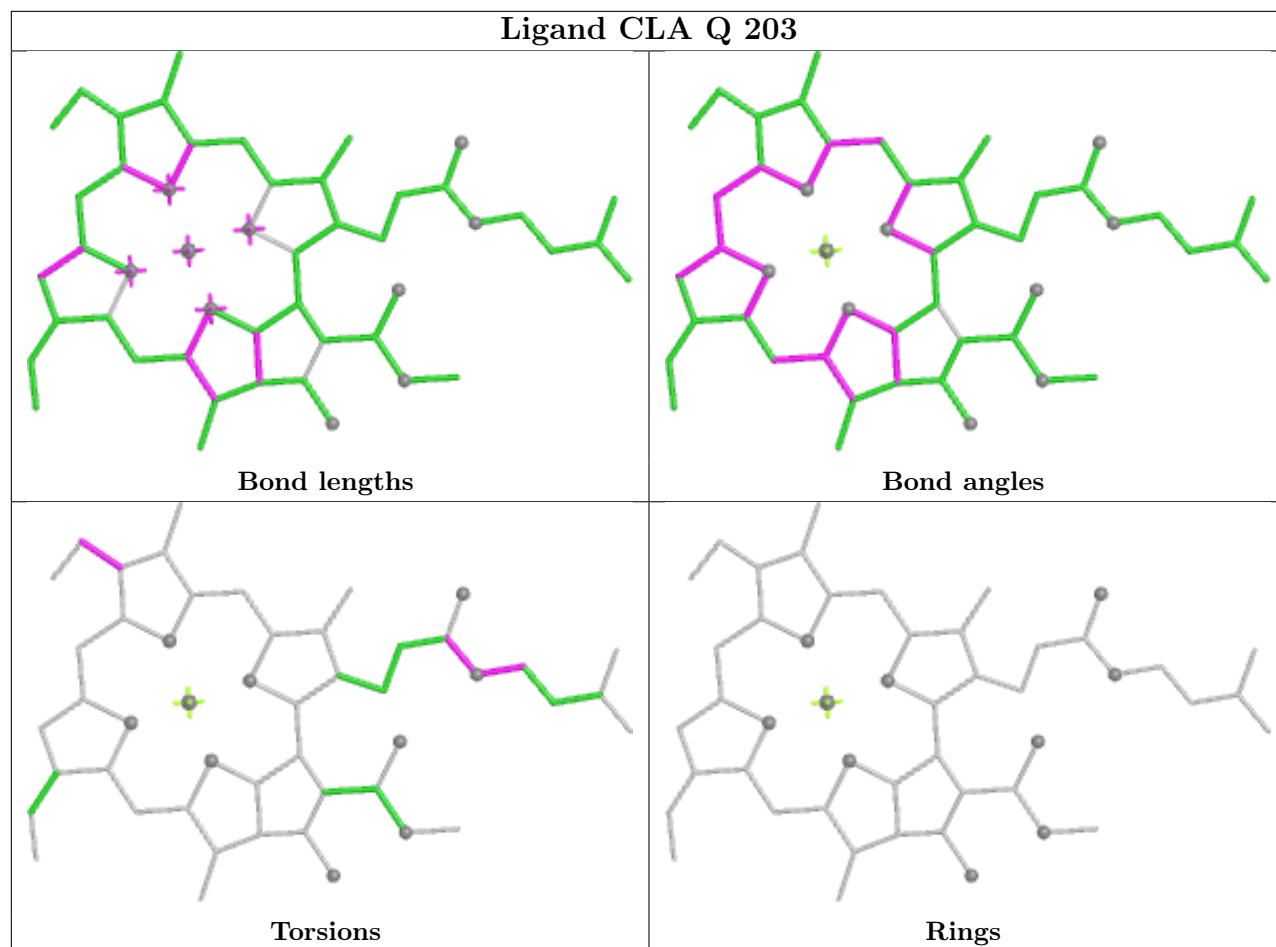
Bond angles

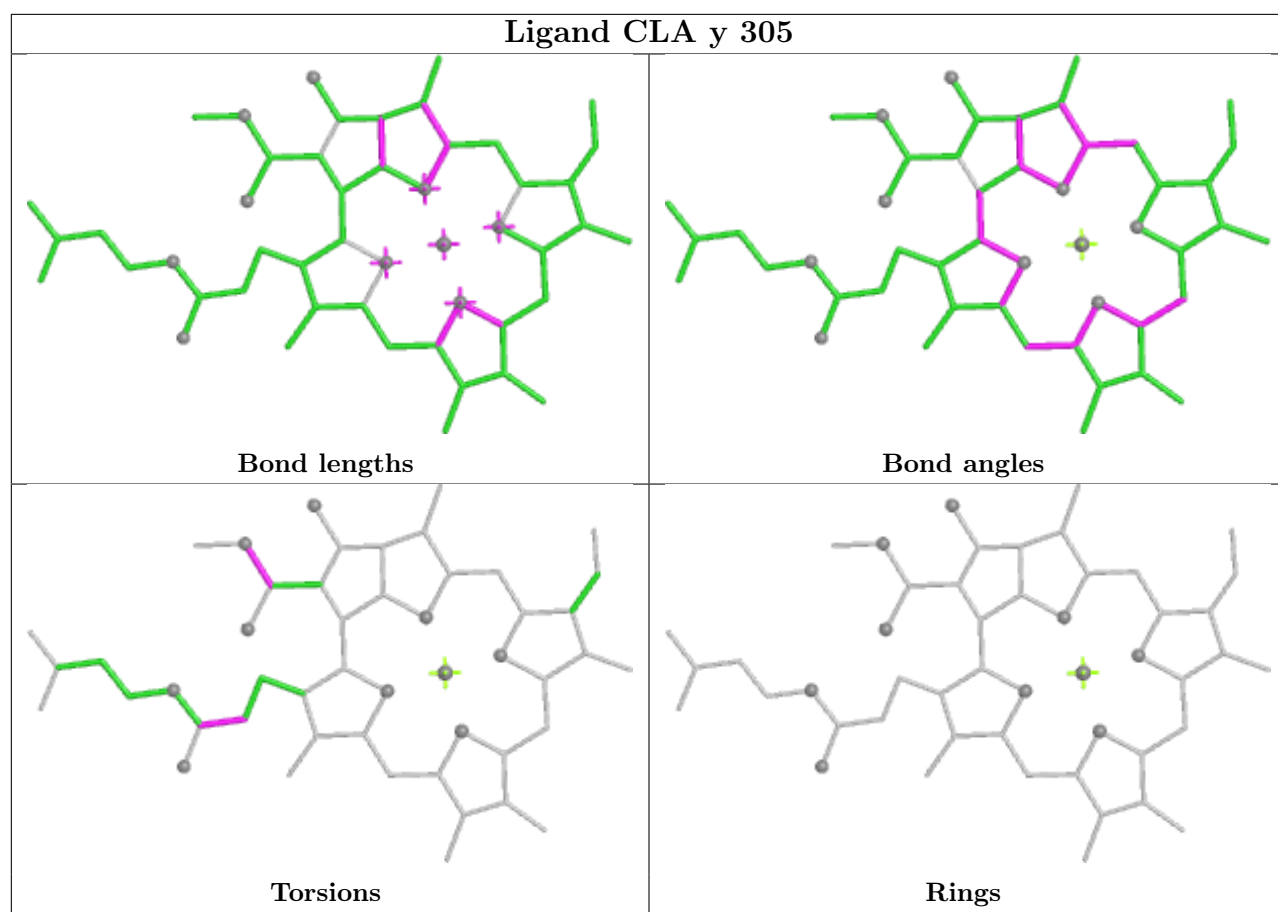


Torsions

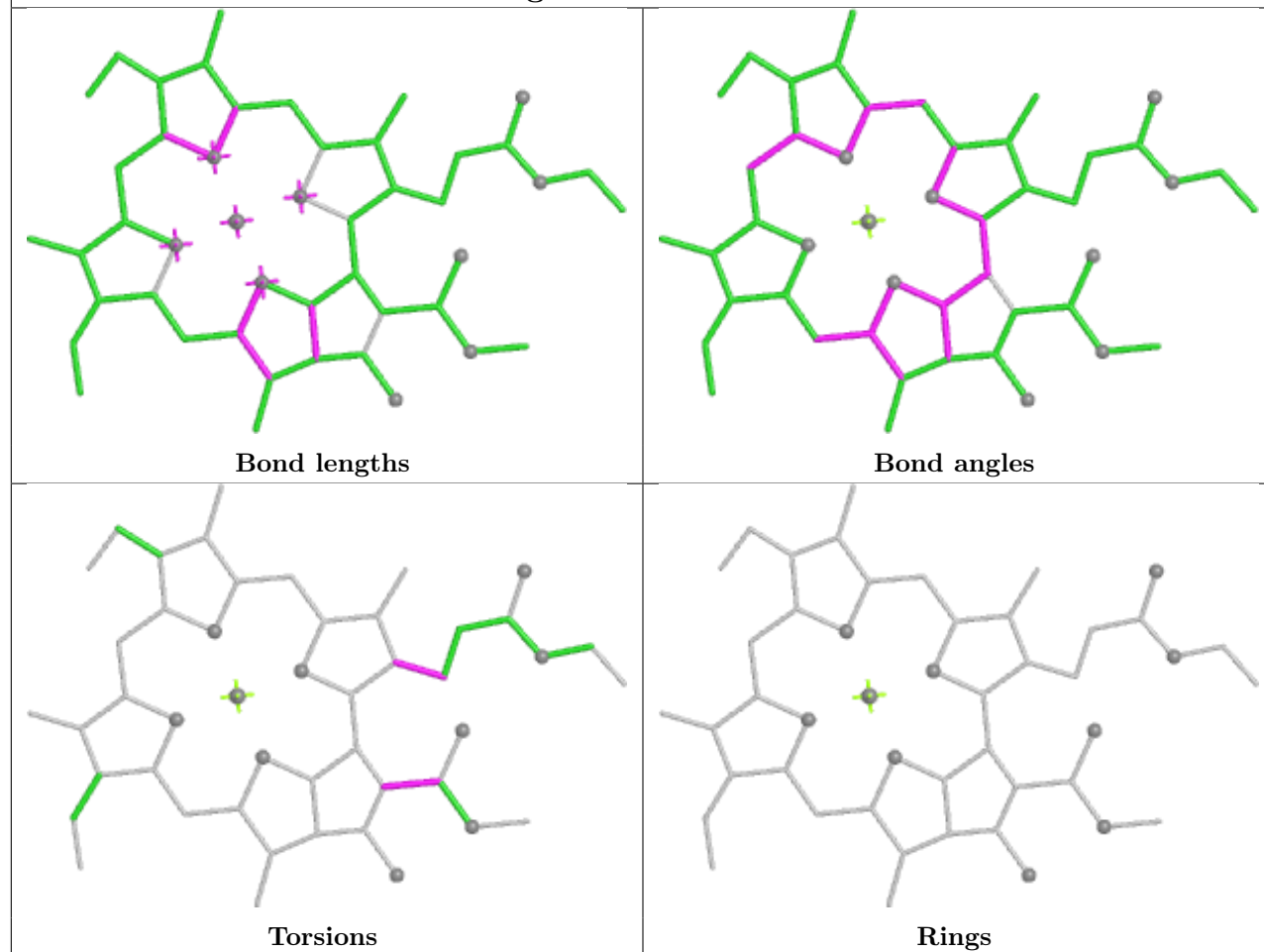


Rings

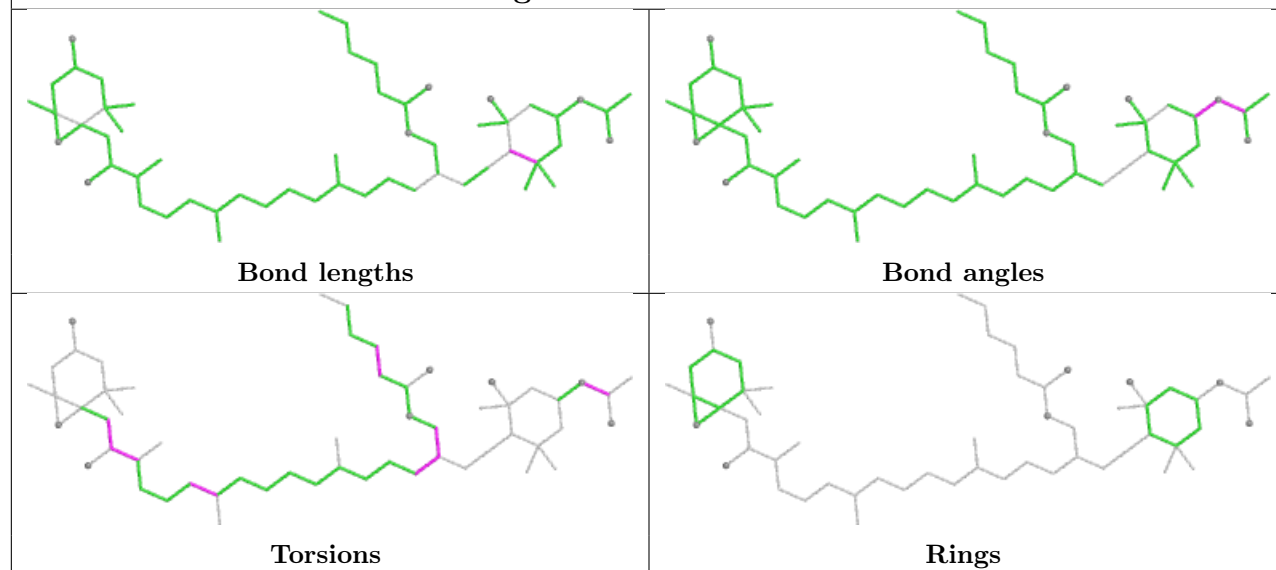




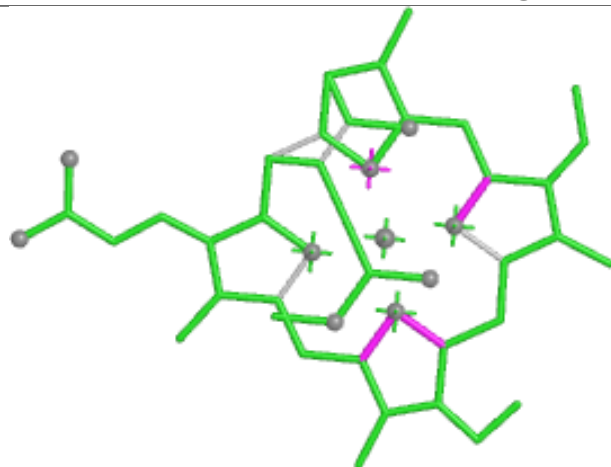
Ligand CLA X 313



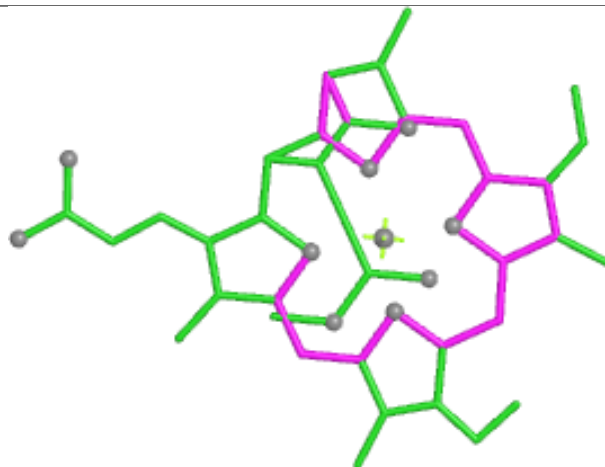
Ligand A1EB1 w 313



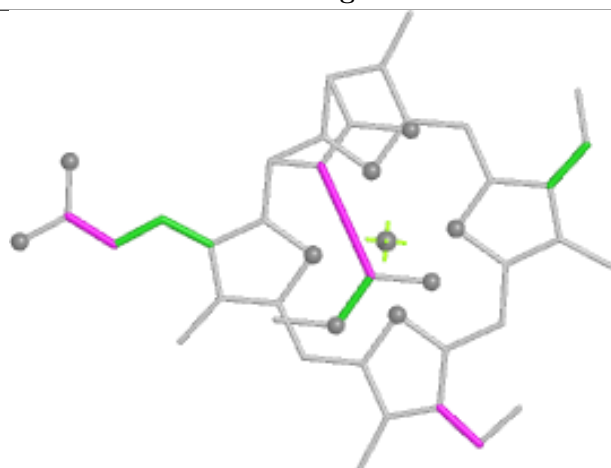
Ligand KC2 H 316



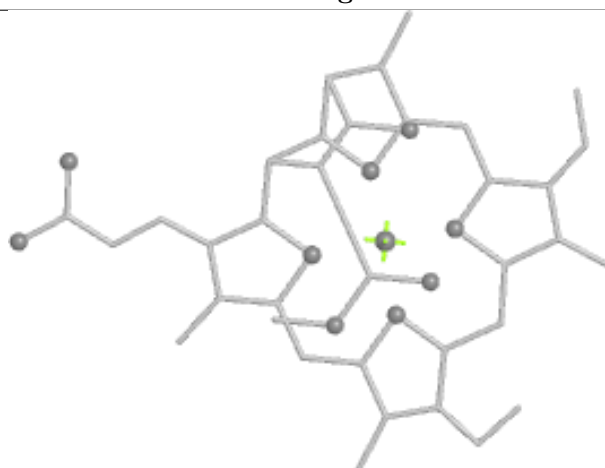
Bond lengths



Bond angles

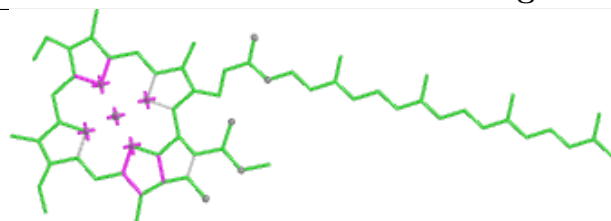


Torsions

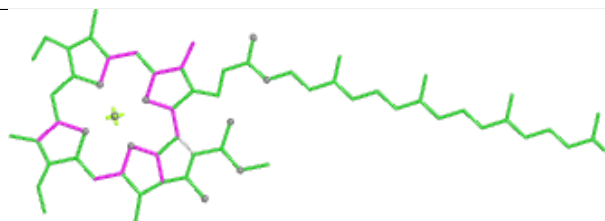


Rings

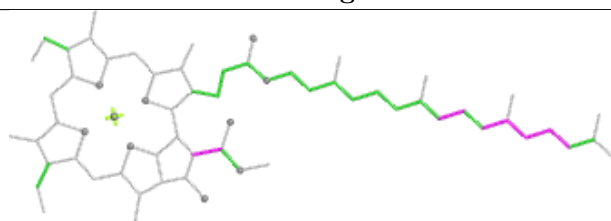
Ligand CLA b 821



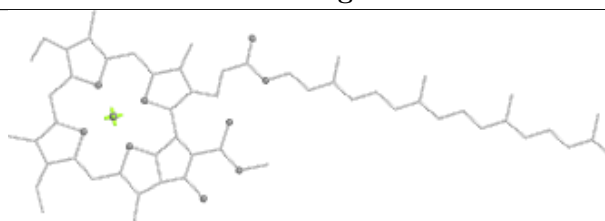
Bond lengths



Bond angles

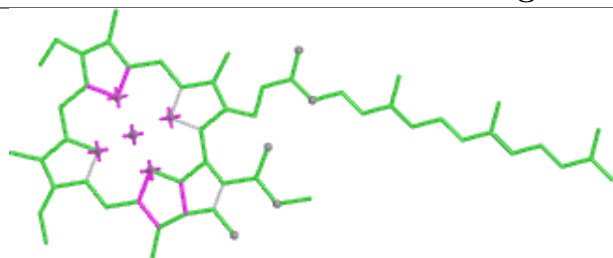


Torsions

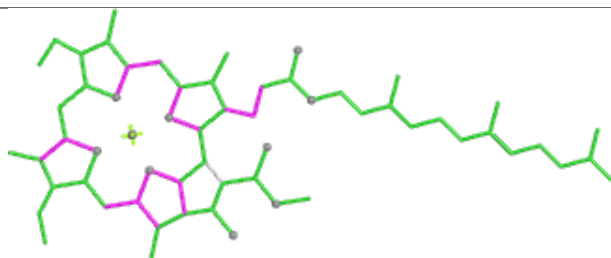


Rings

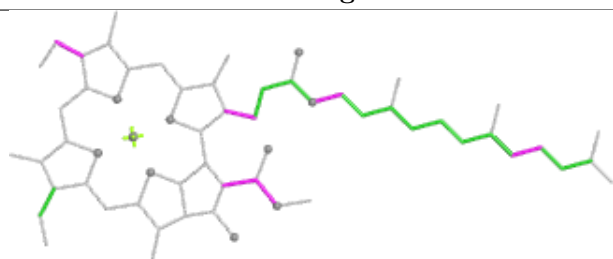
Ligand CLA v 306



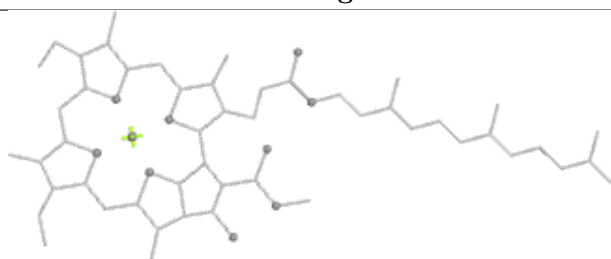
Bond lengths



Bond angles

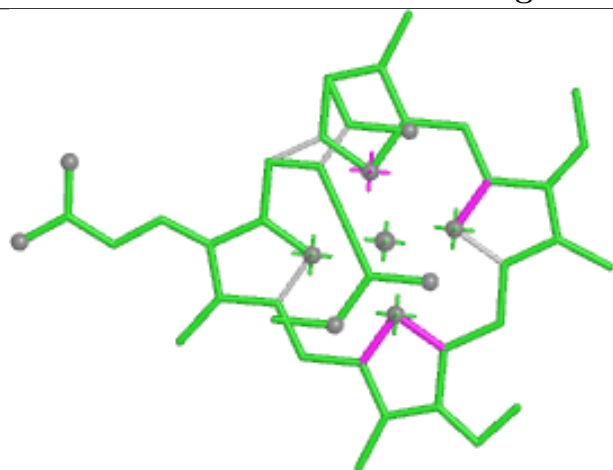


Torsions

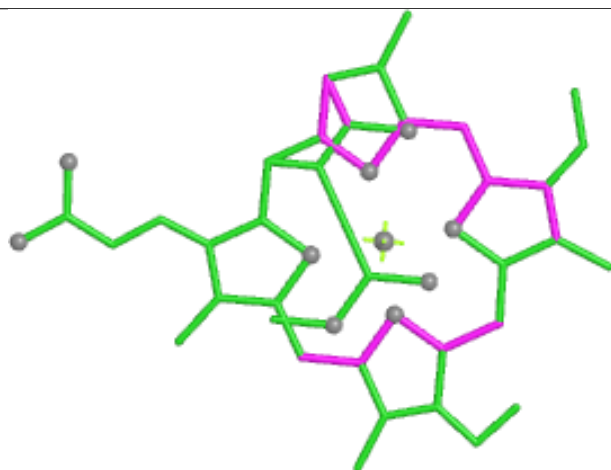


Rings

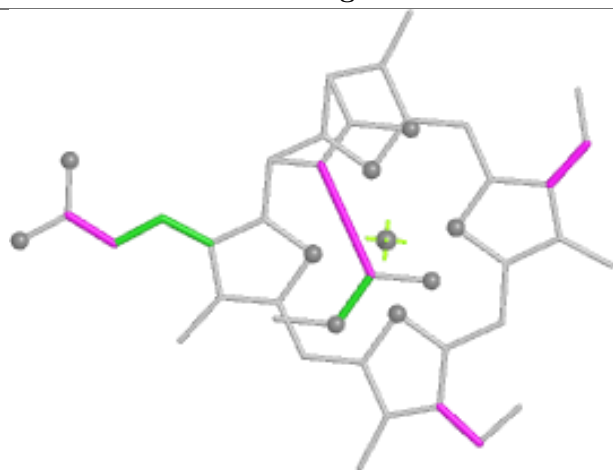
Ligand KC2 Y 309



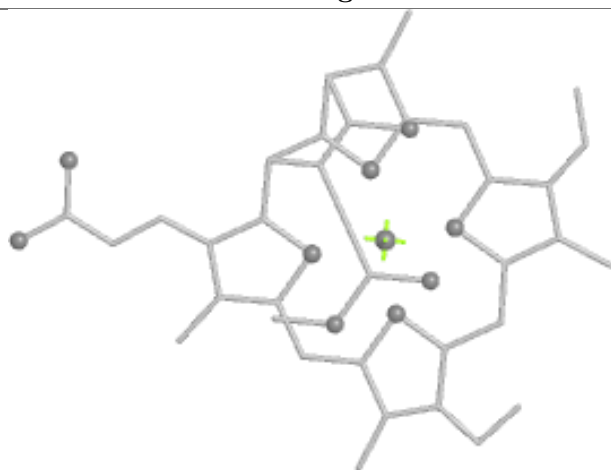
Bond lengths



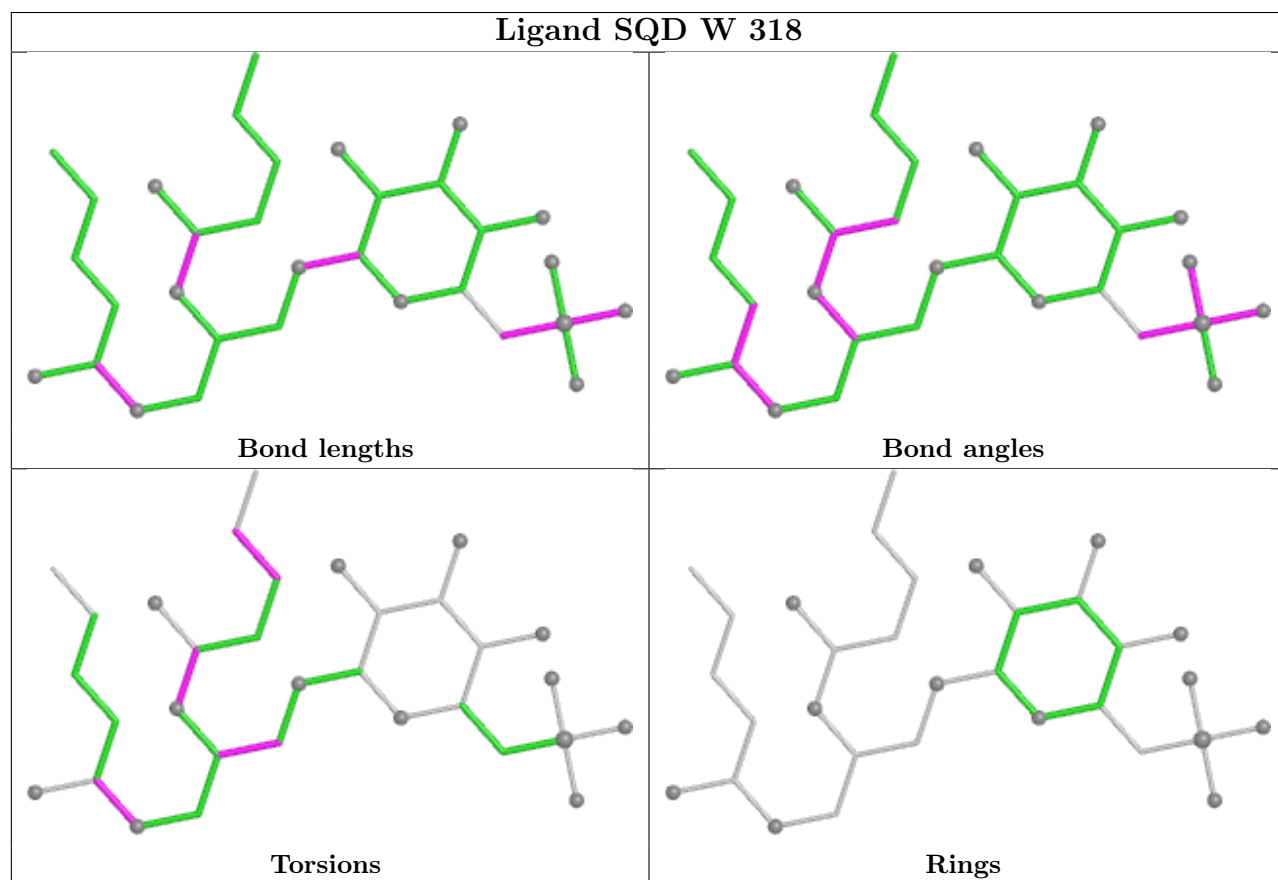
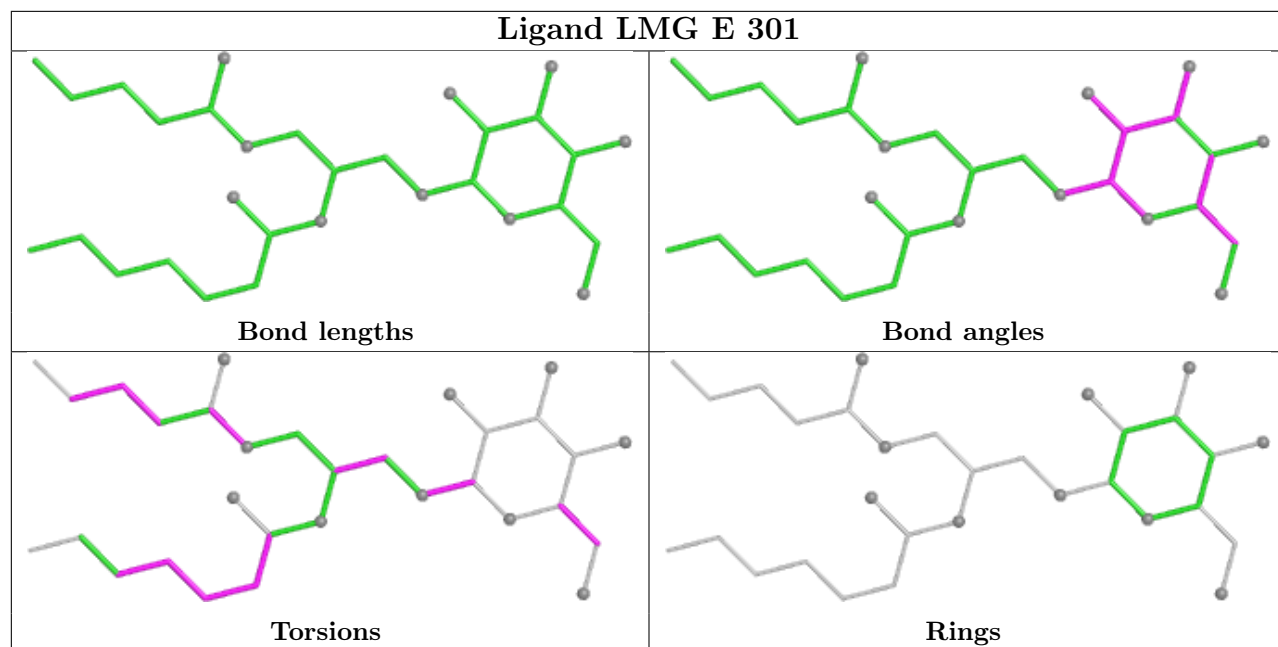
Bond angles

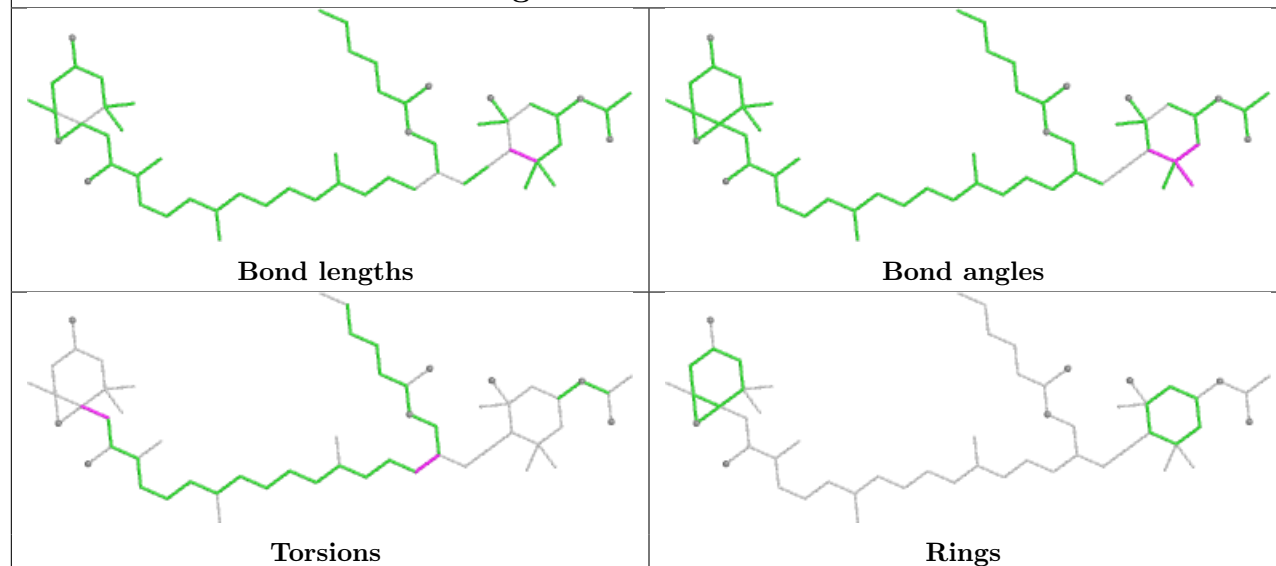
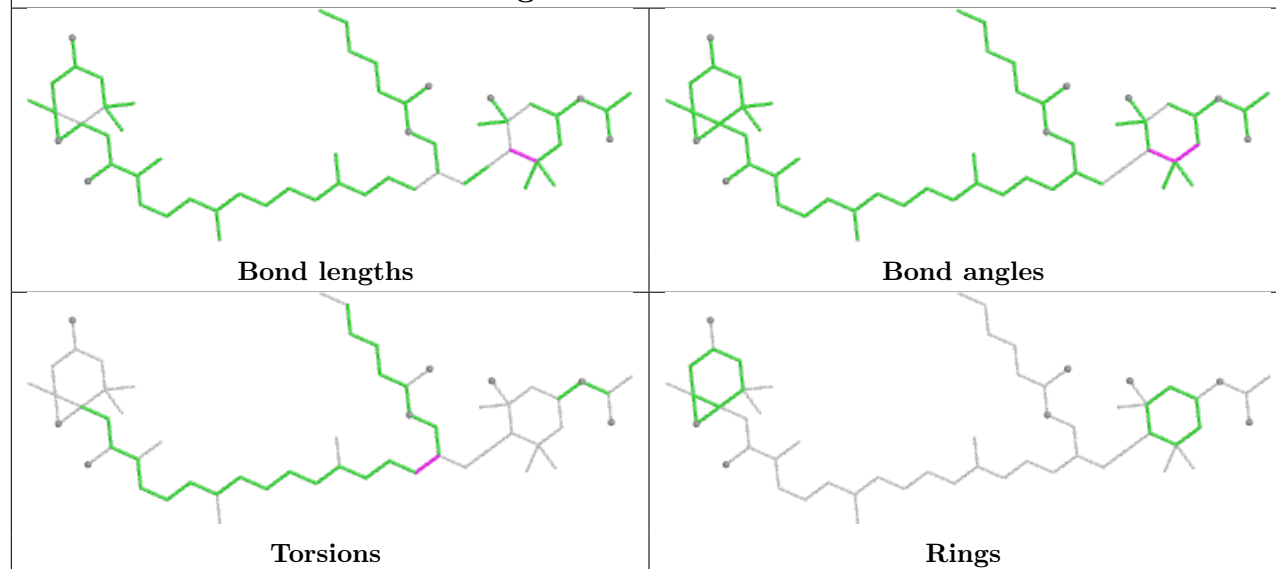


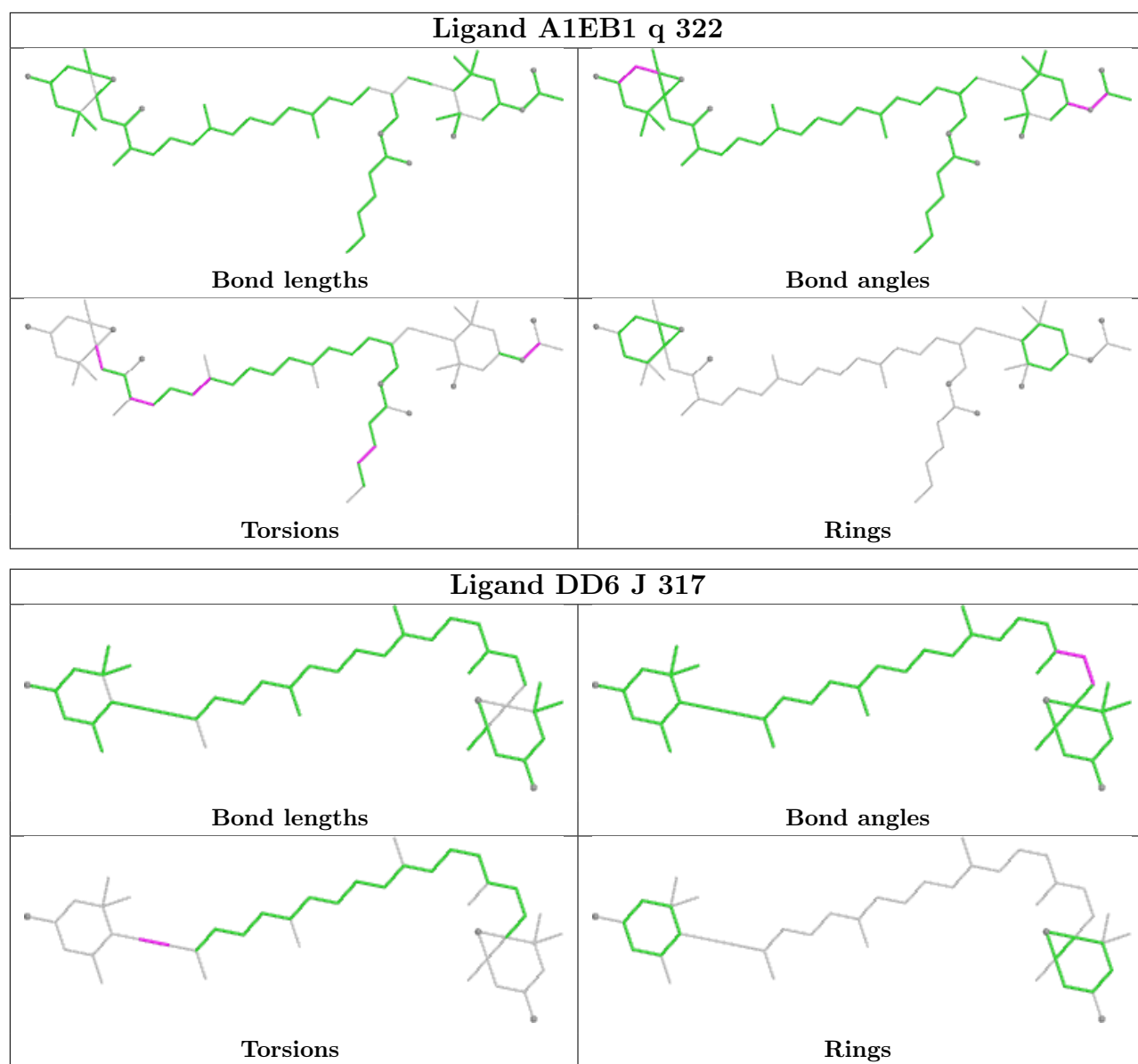
Torsions



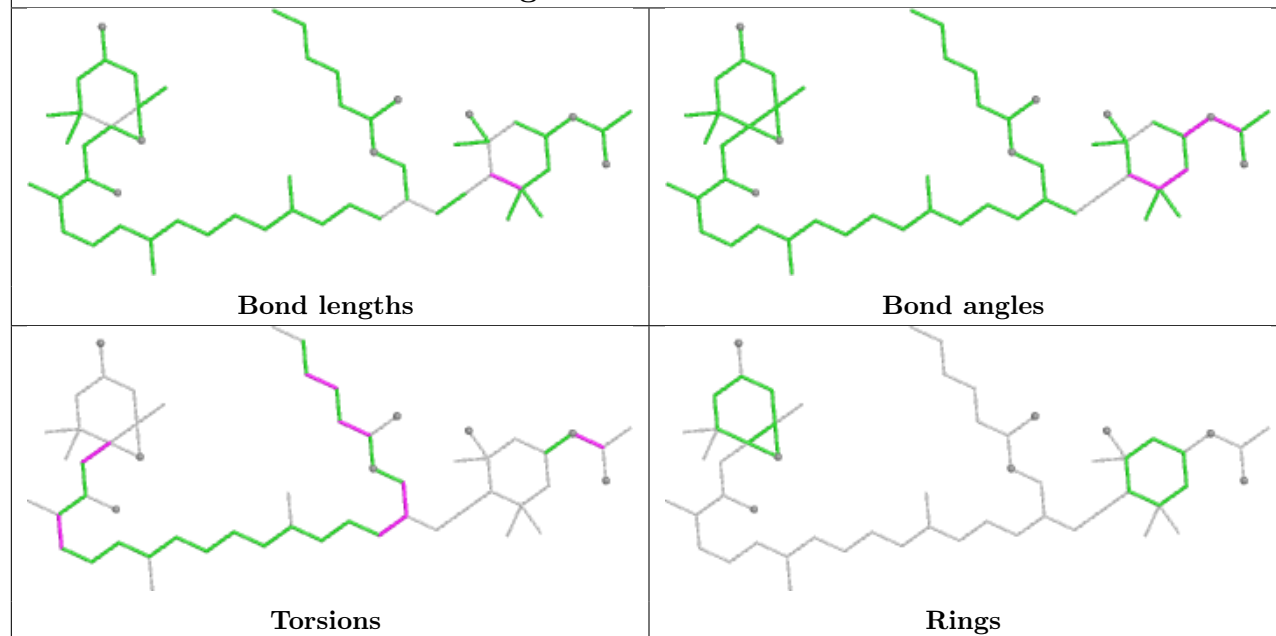
Rings



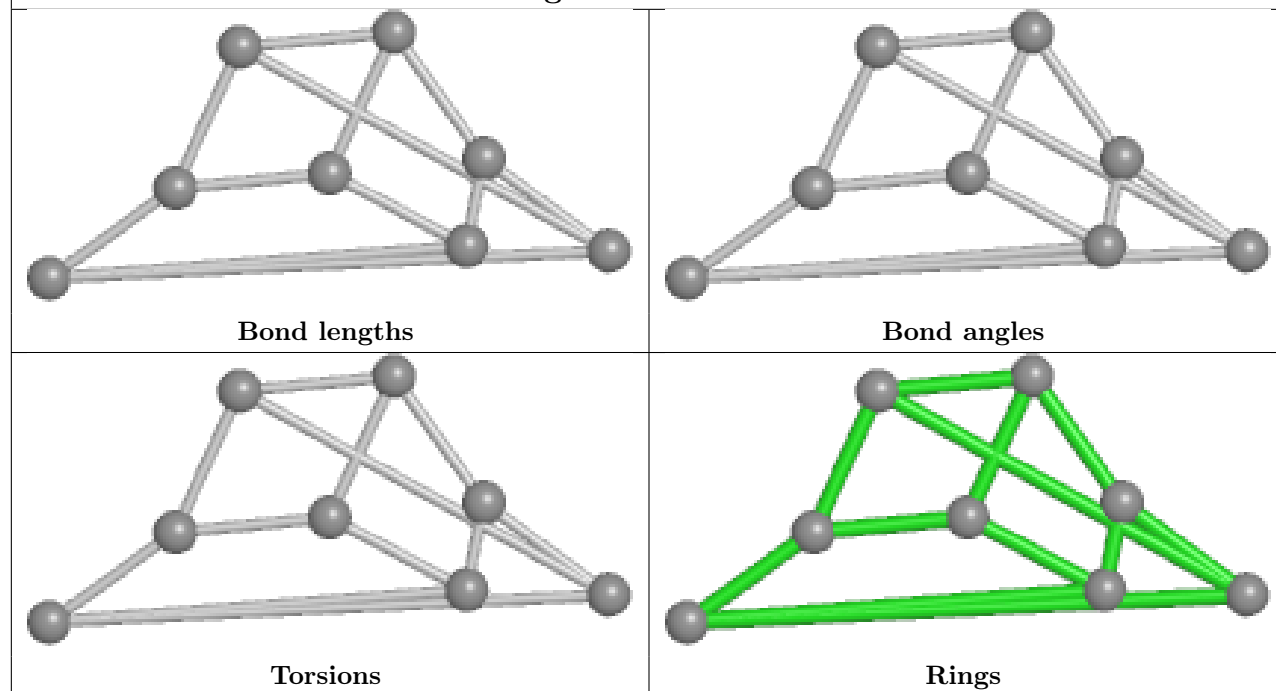
Ligand A1EB1 K 313**Ligand A1EB1 x 321**

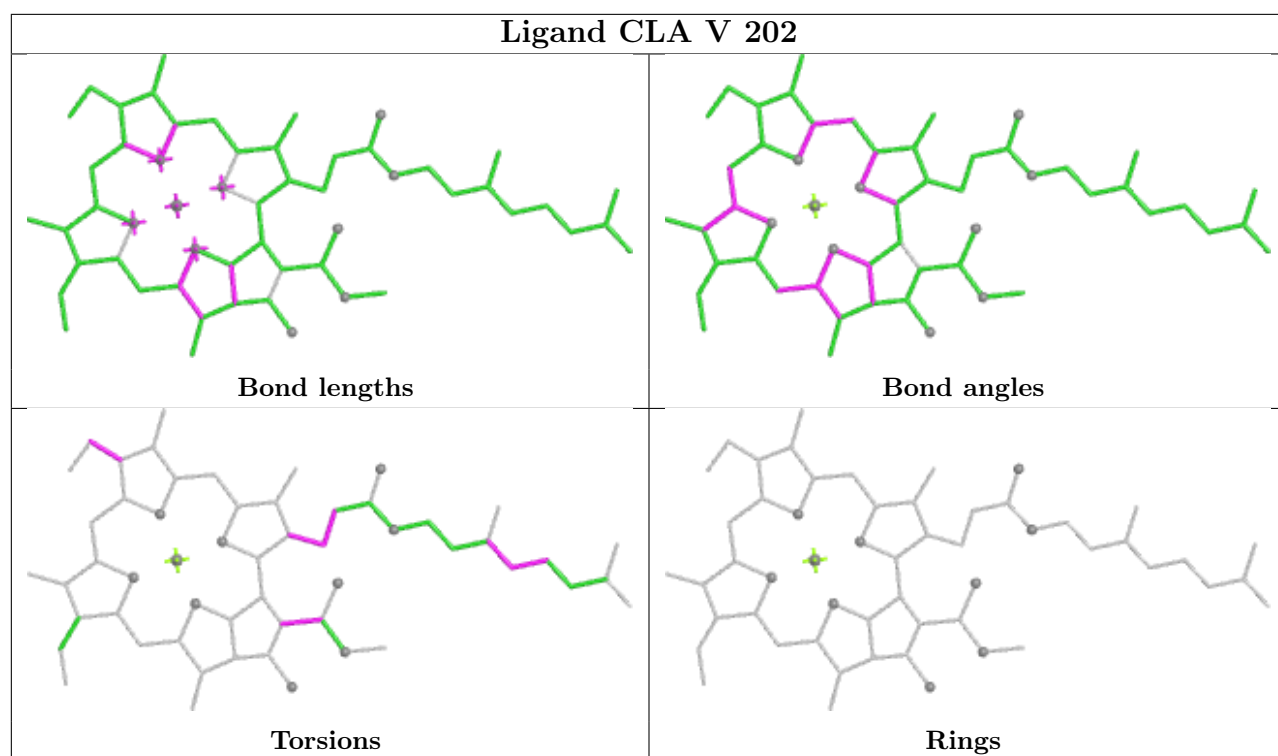


Ligand A1EB1 t 315

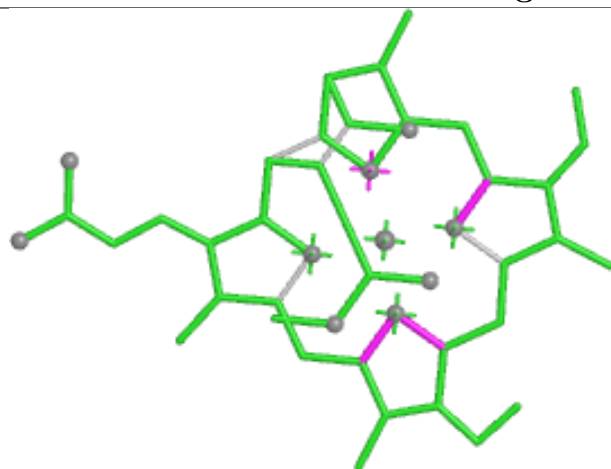


Ligand SF4 c 101

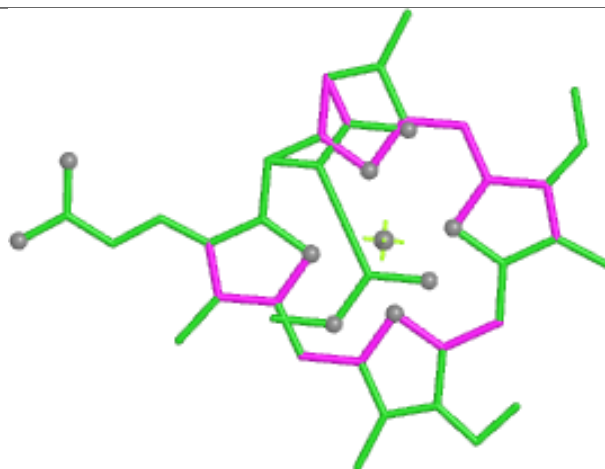




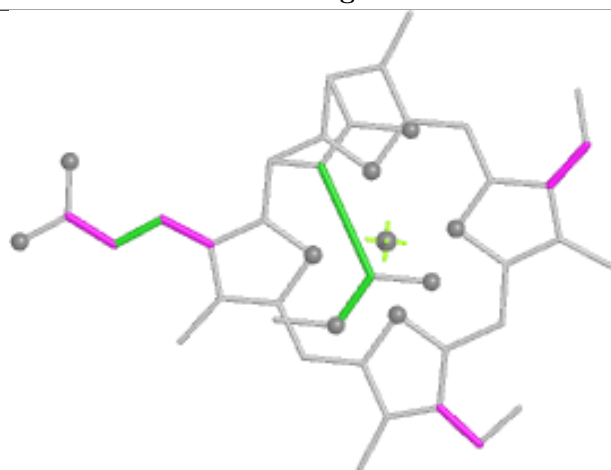
Ligand KC2 O 308



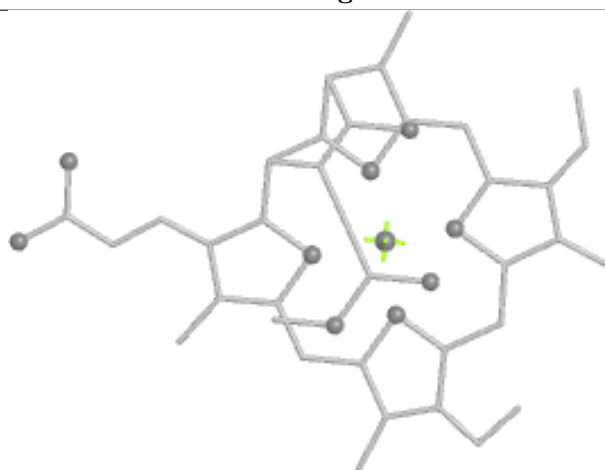
Bond lengths



Bond angles

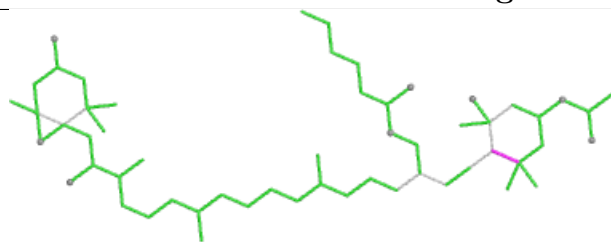


Torsions

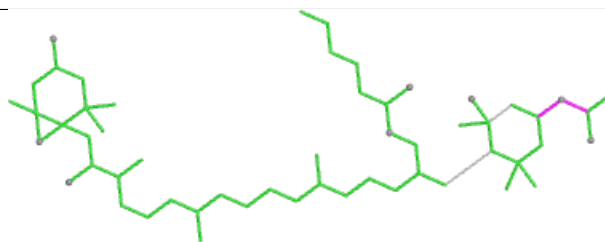


Rings

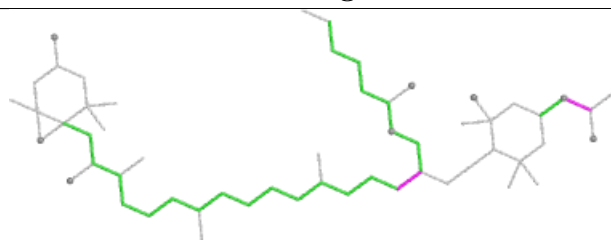
Ligand A1EB1 T 316



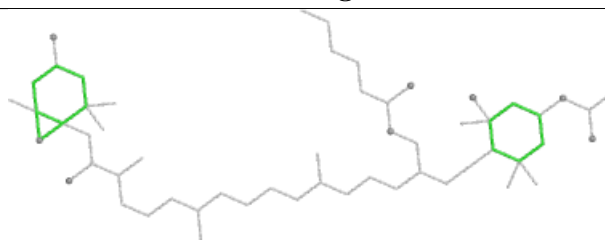
Bond lengths



Bond angles

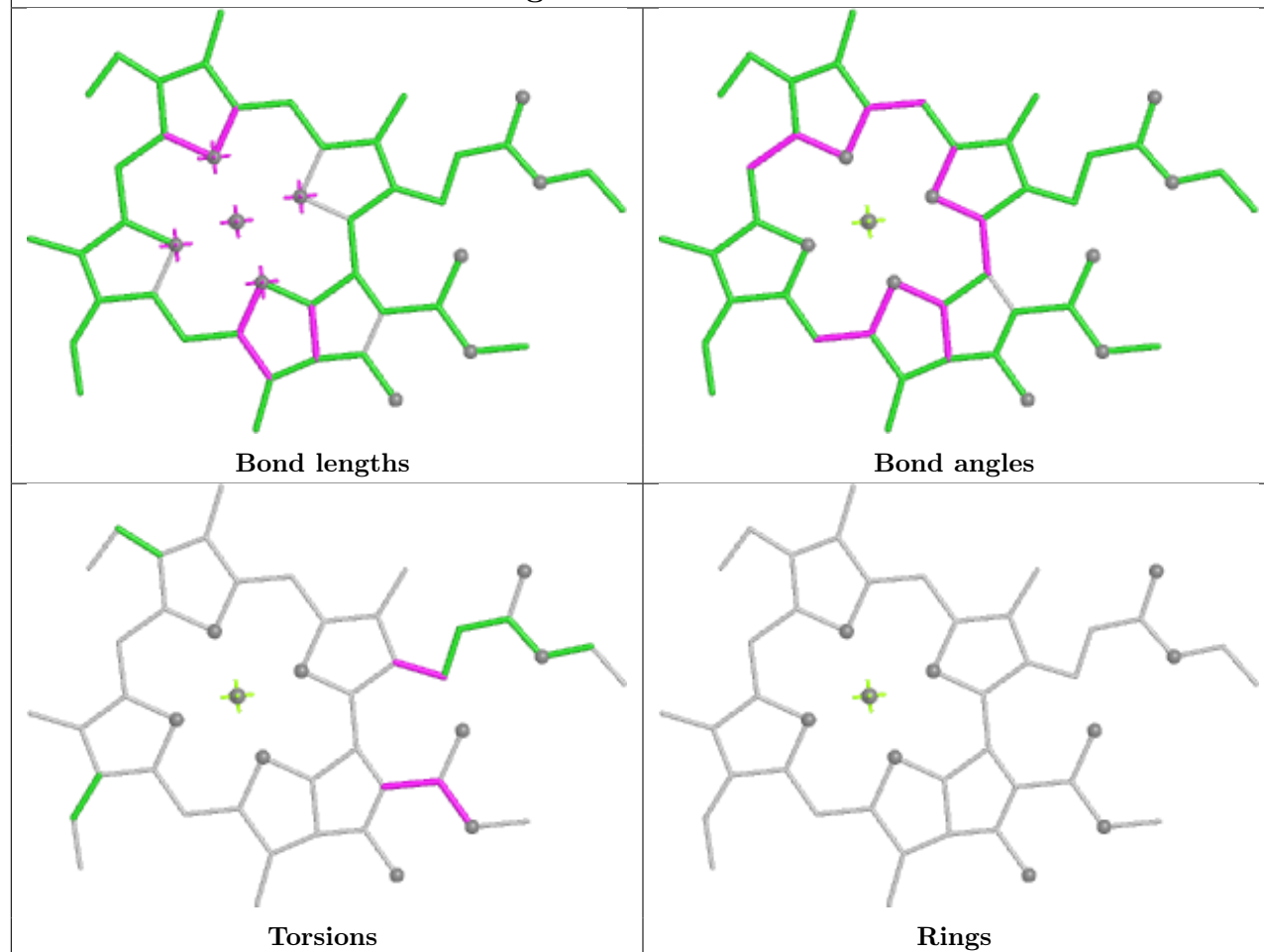


Torsions

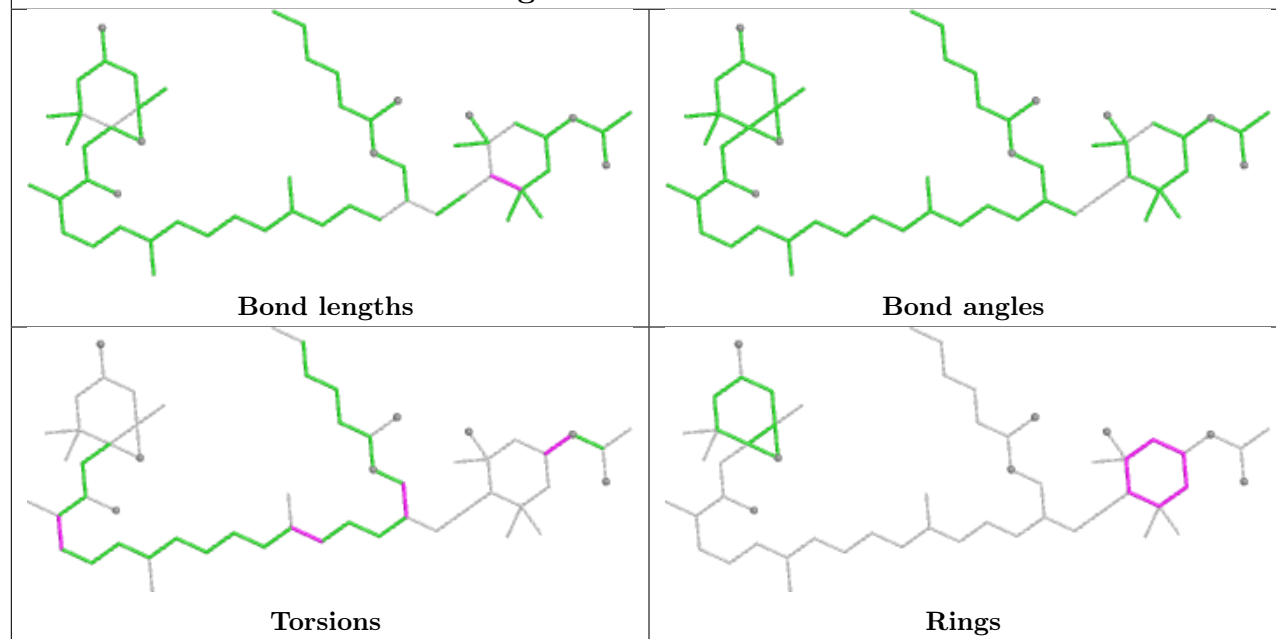


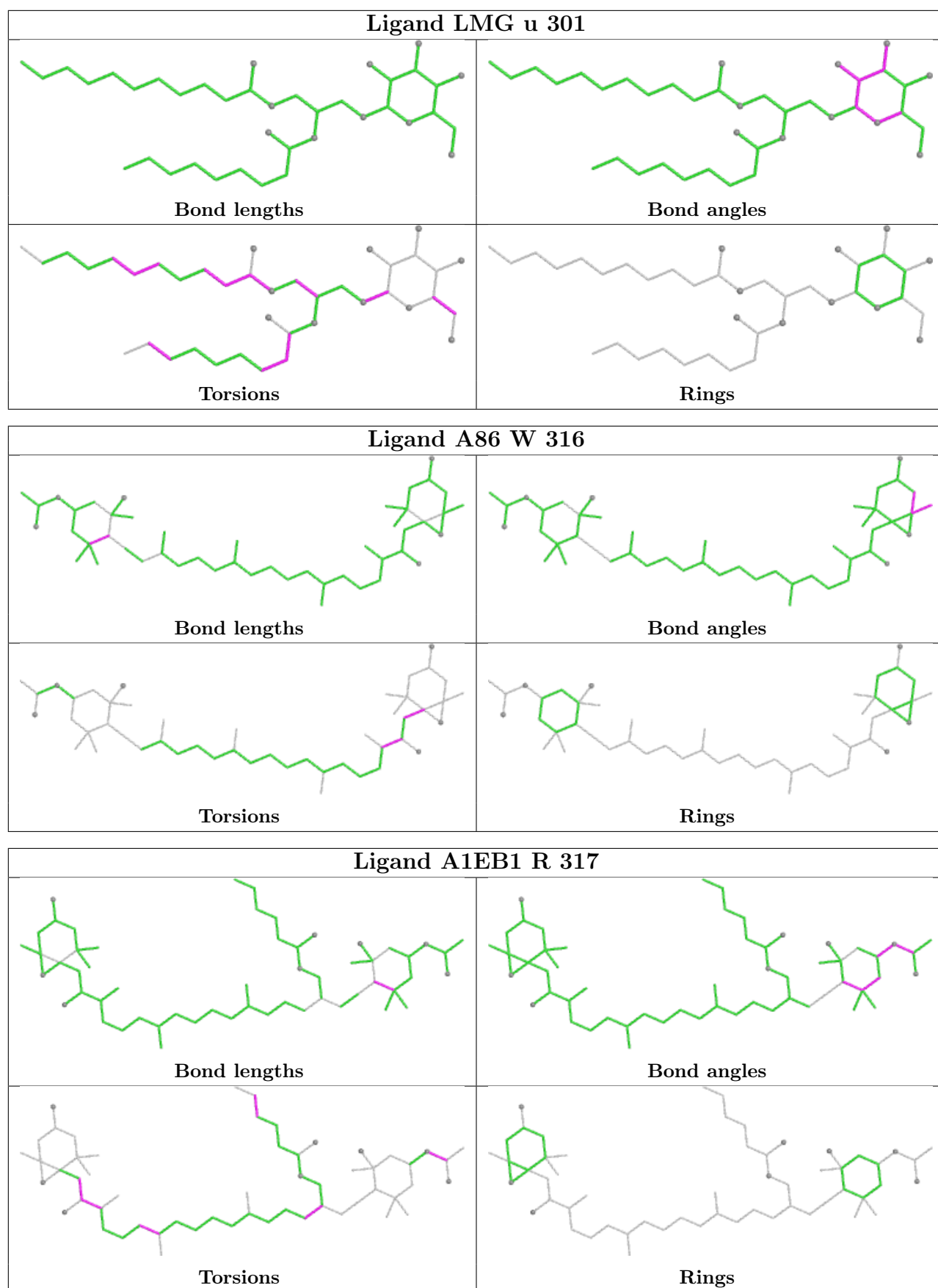
Rings

Ligand CLA U 207

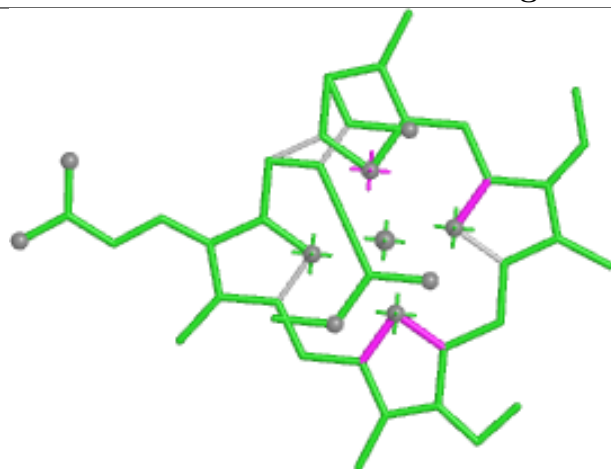


Ligand A1EB1 o 321

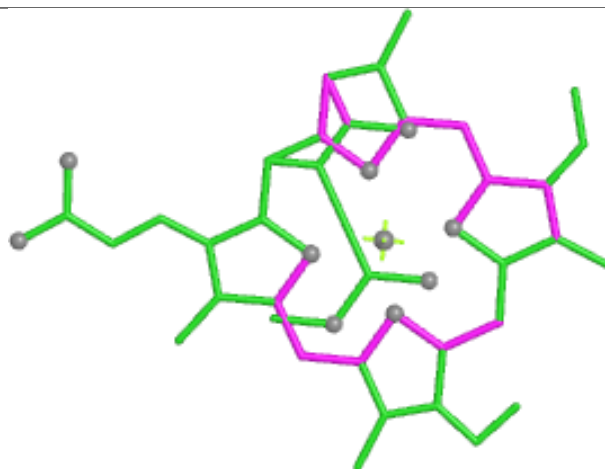




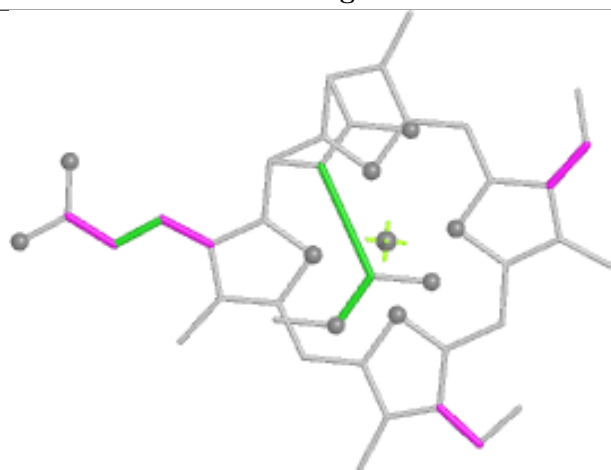
Ligand KC2 o 308



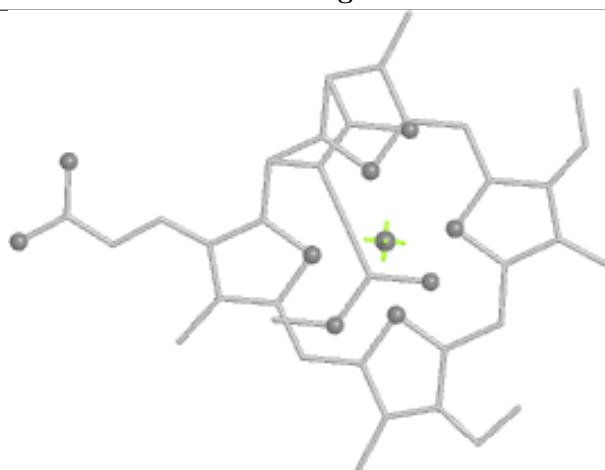
Bond lengths



Bond angles

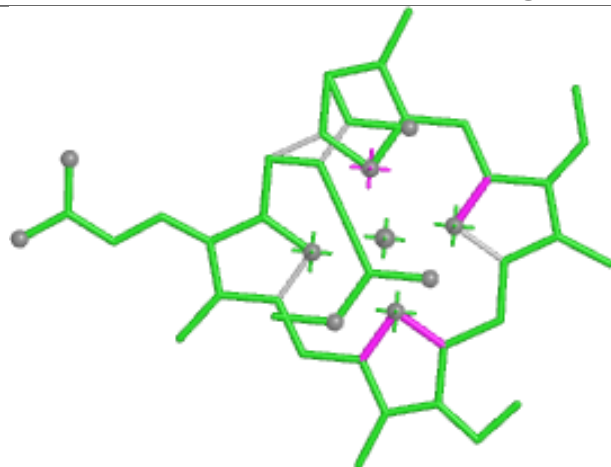


Torsions

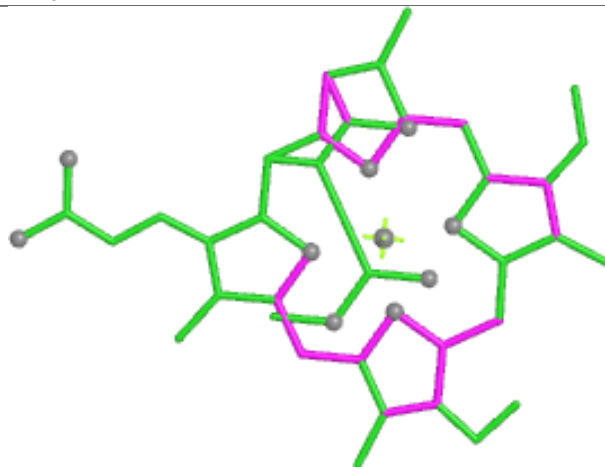


Rings

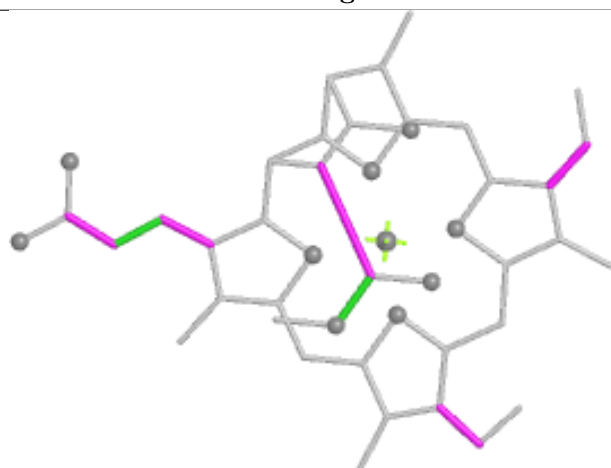
Ligand KC2 y 301



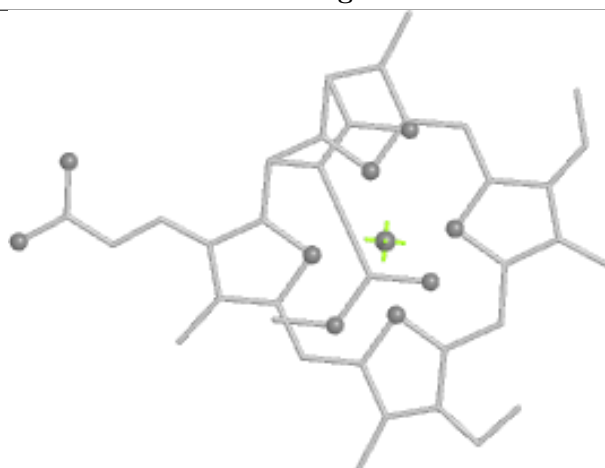
Bond lengths



Bond angles

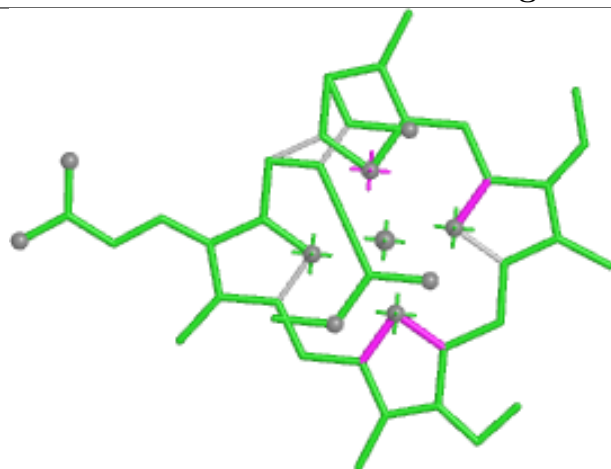


Torsions

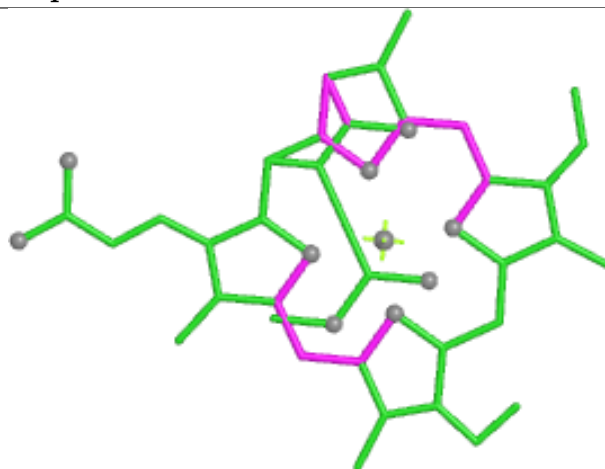


Rings

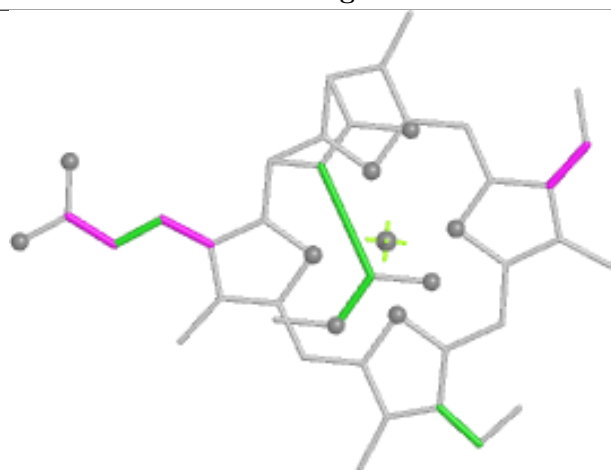
Ligand KC2 p 303



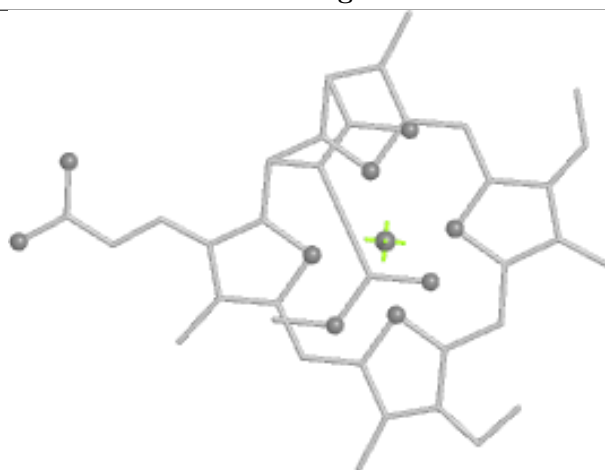
Bond lengths



Bond angles

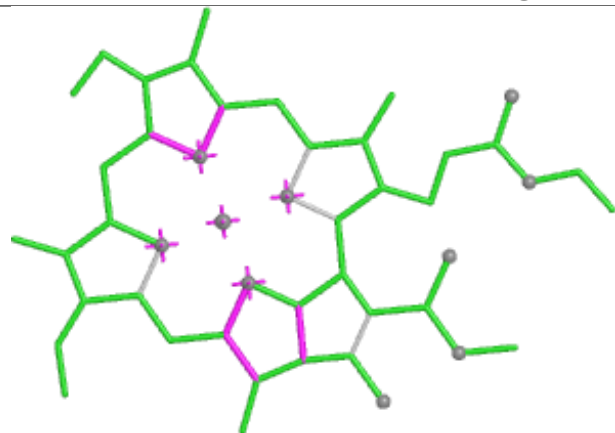


Torsions

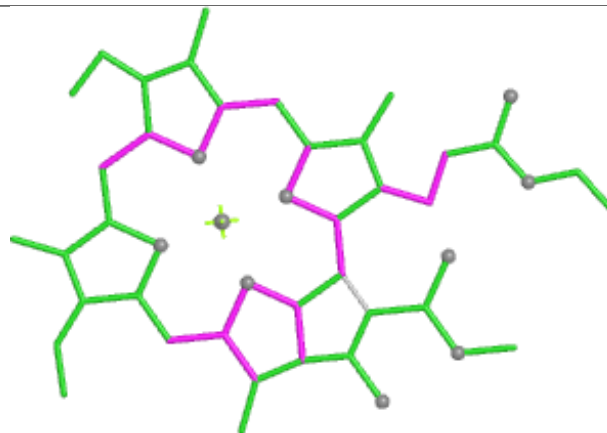


Rings

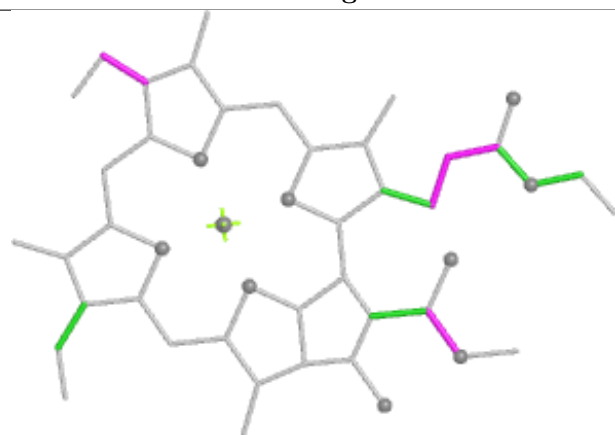
Ligand CLA H 302



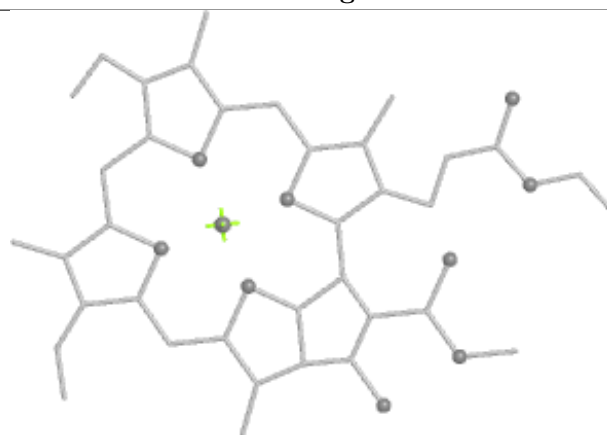
Bond lengths



Bond angles

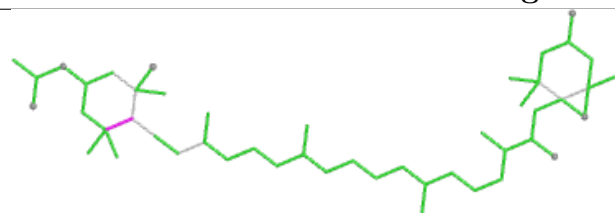


Torsions

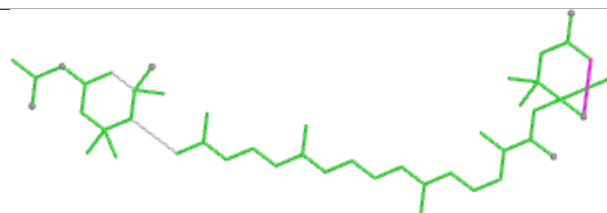


Rings

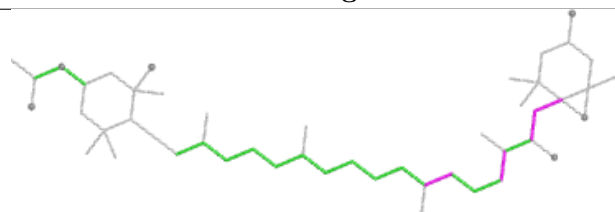
Ligand A86 Y 321



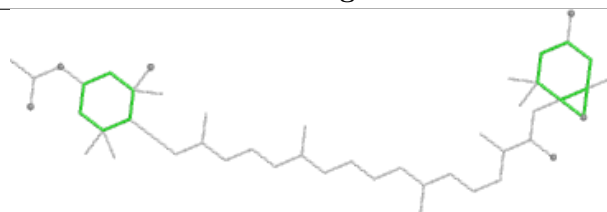
Bond lengths



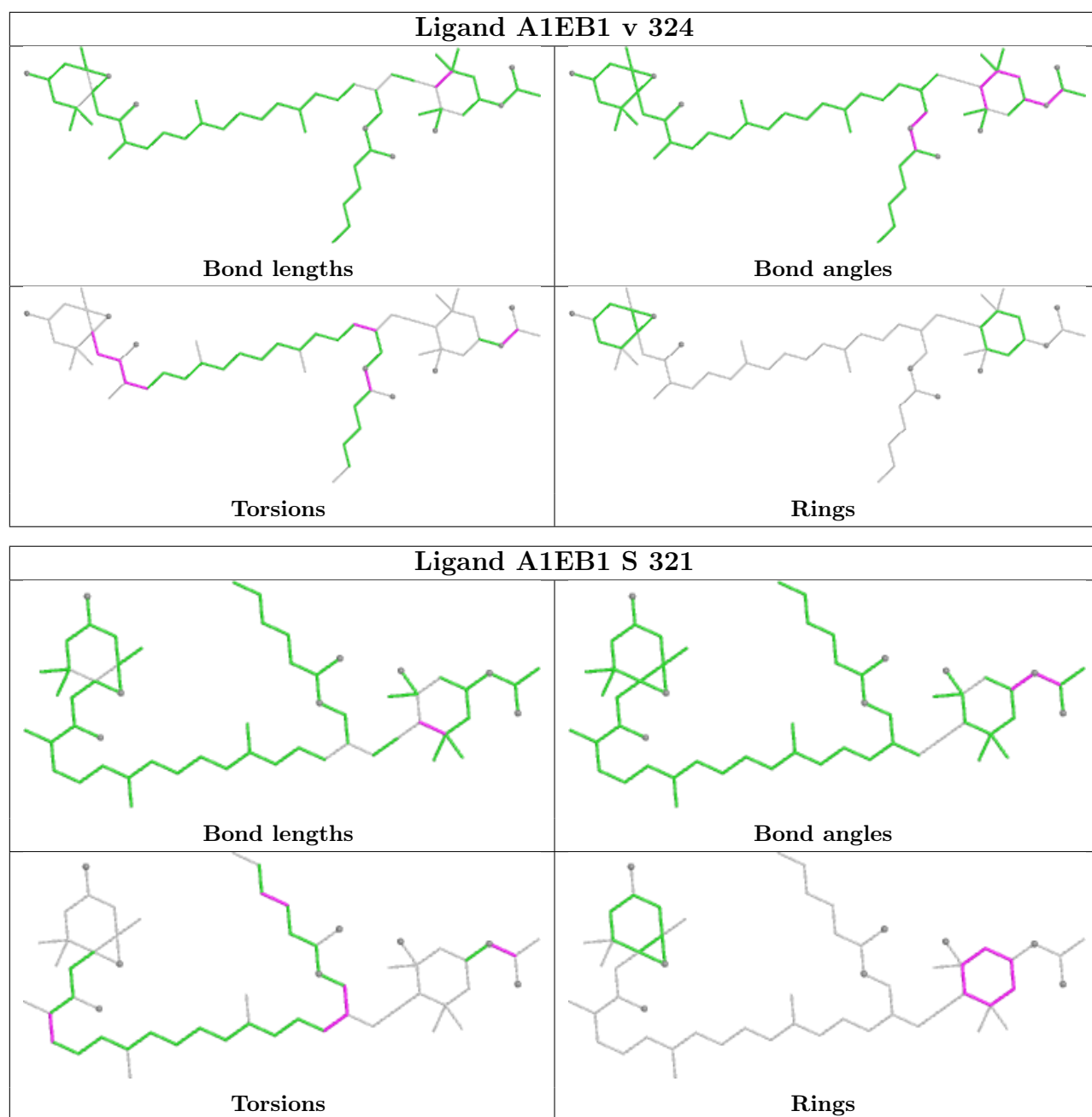
Bond angles

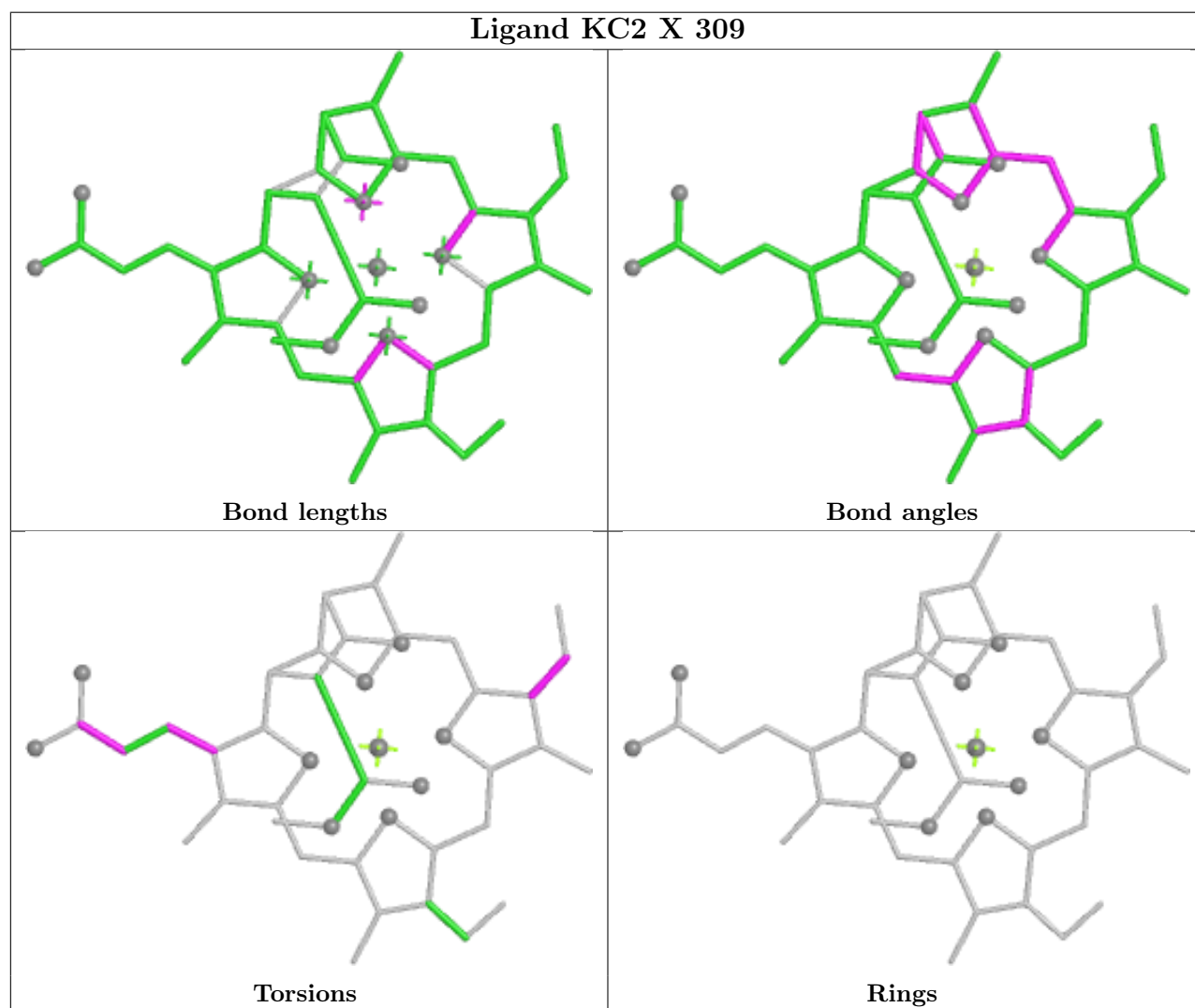
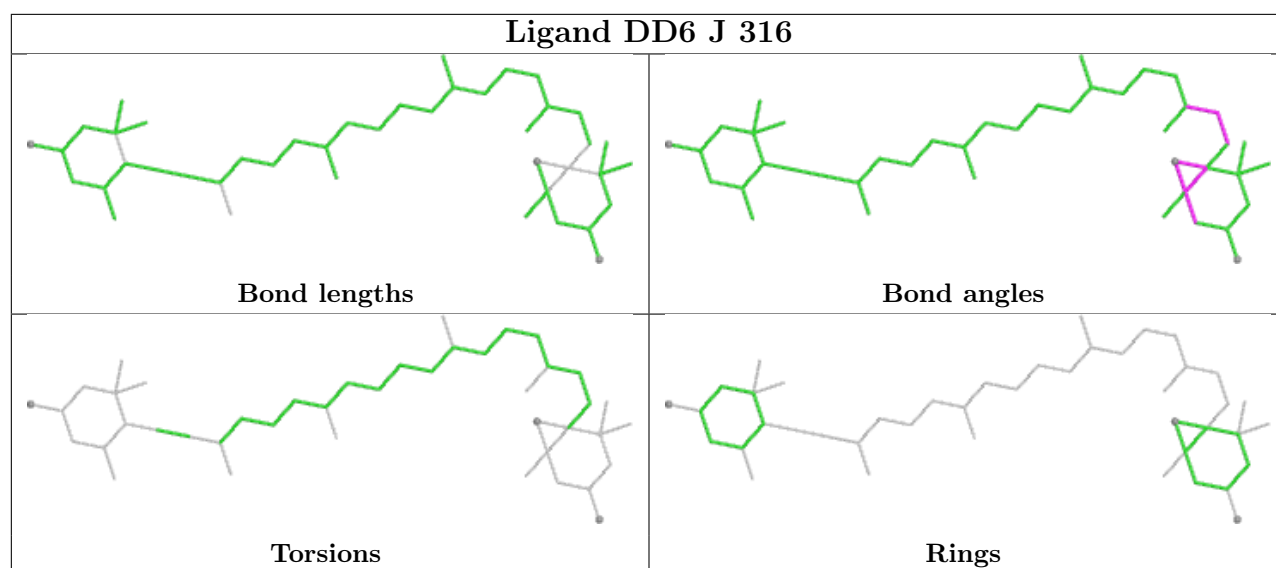


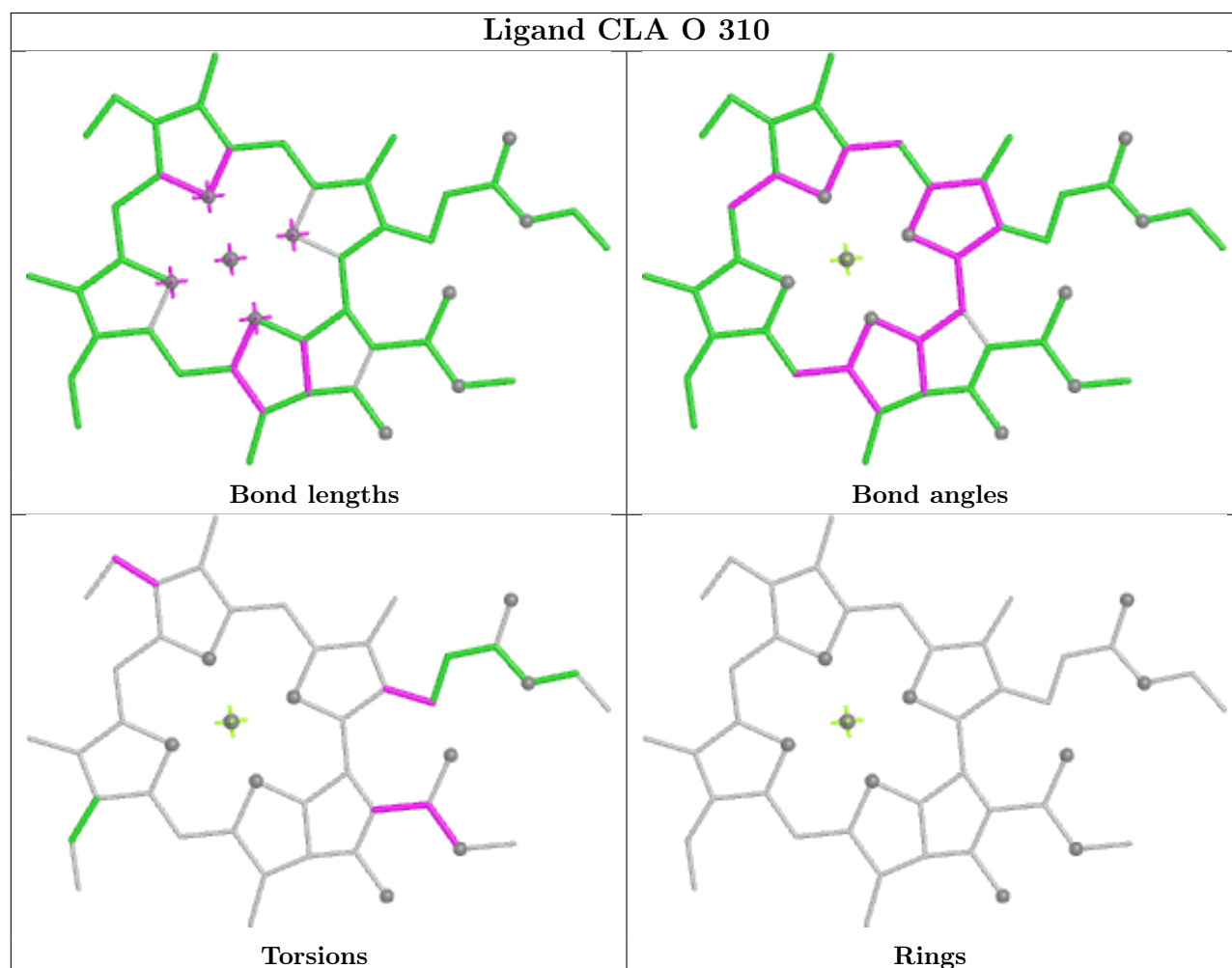
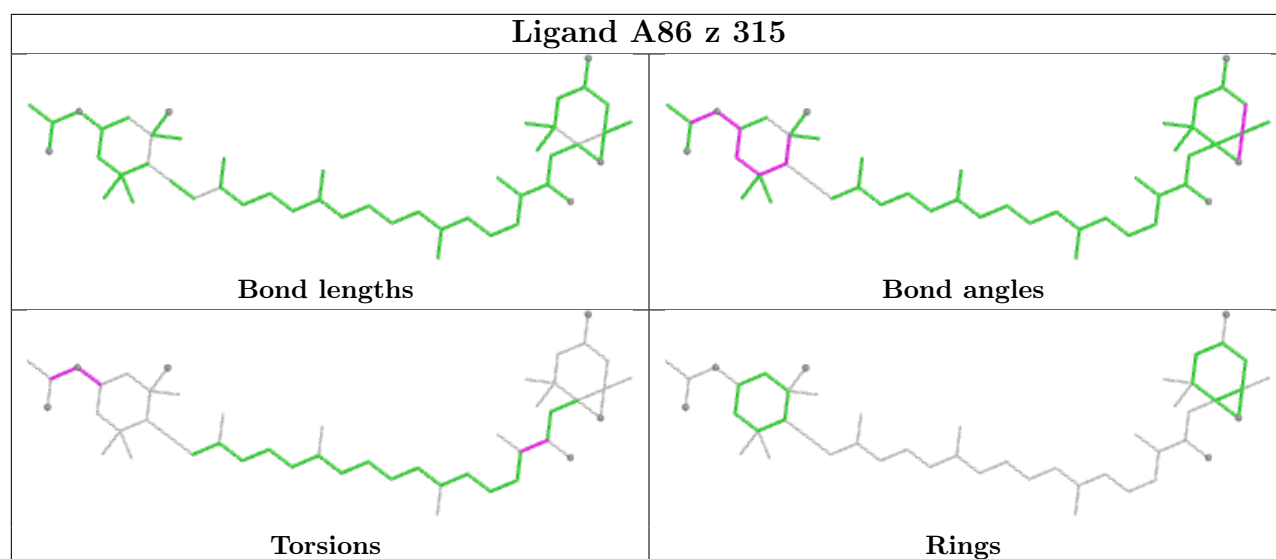
Torsions

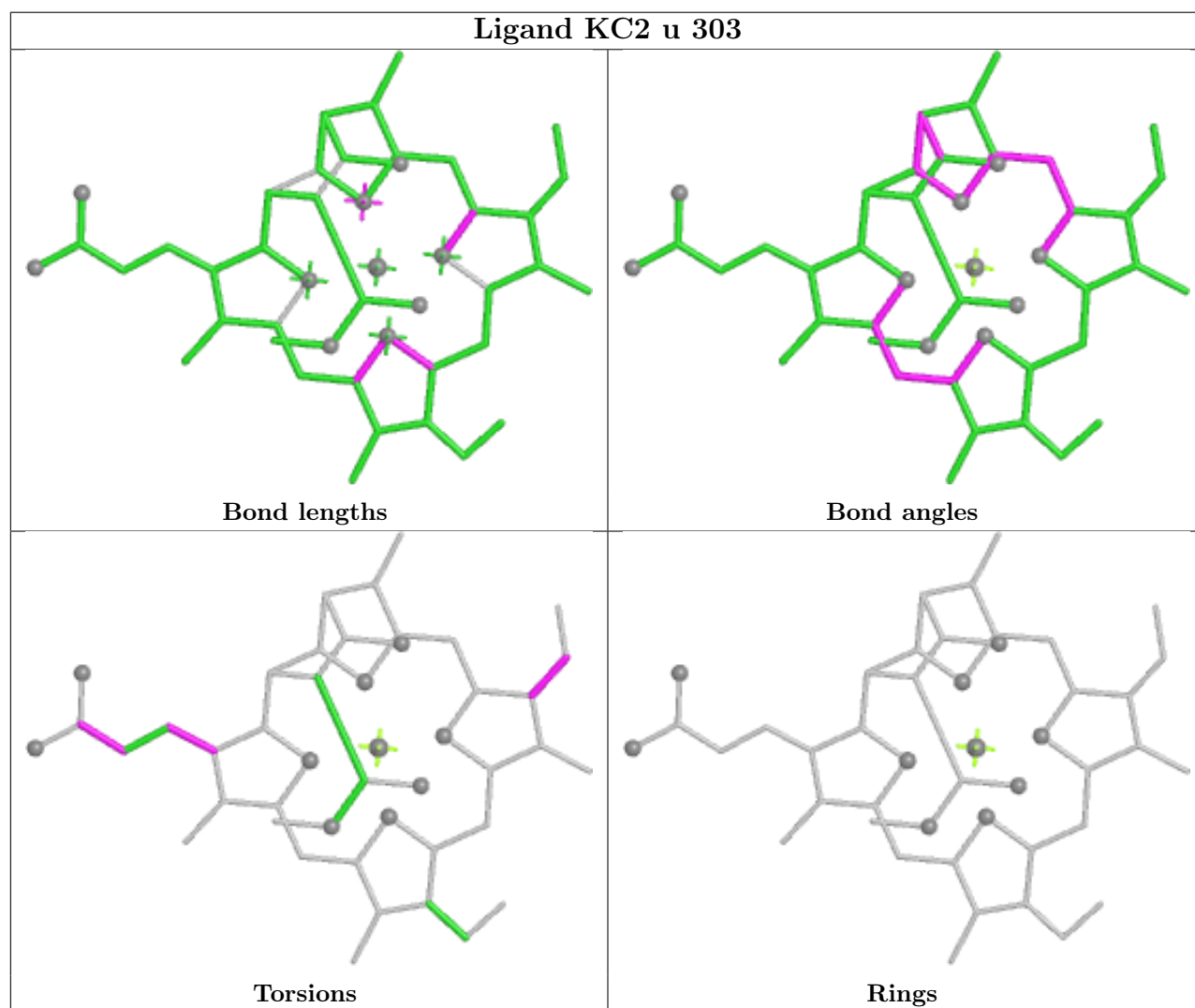
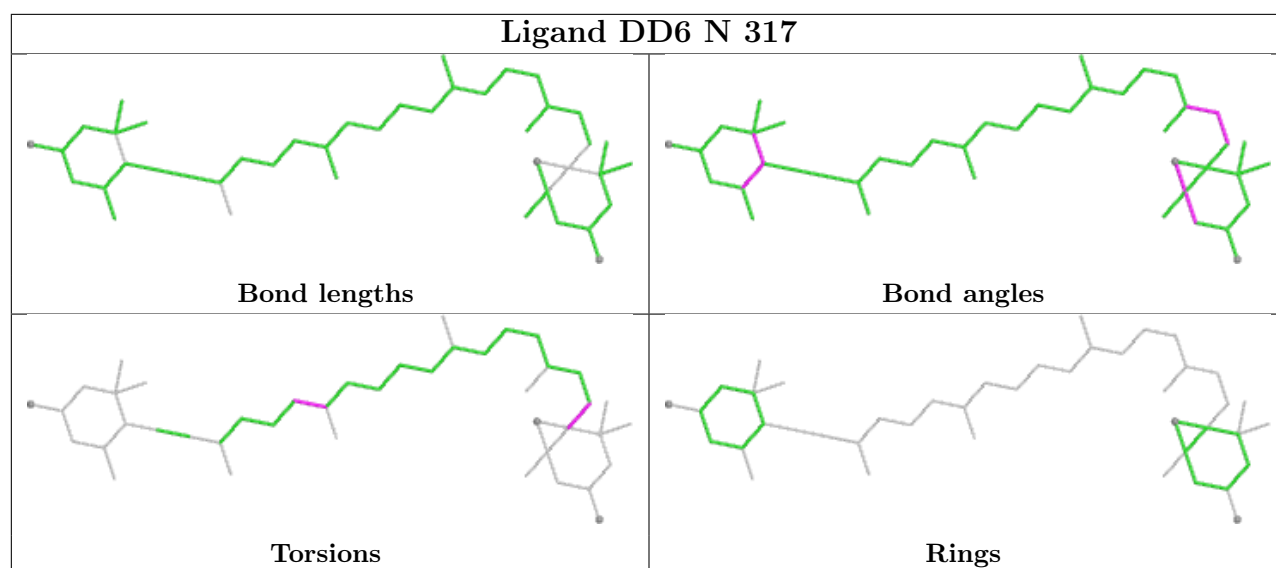


Rings

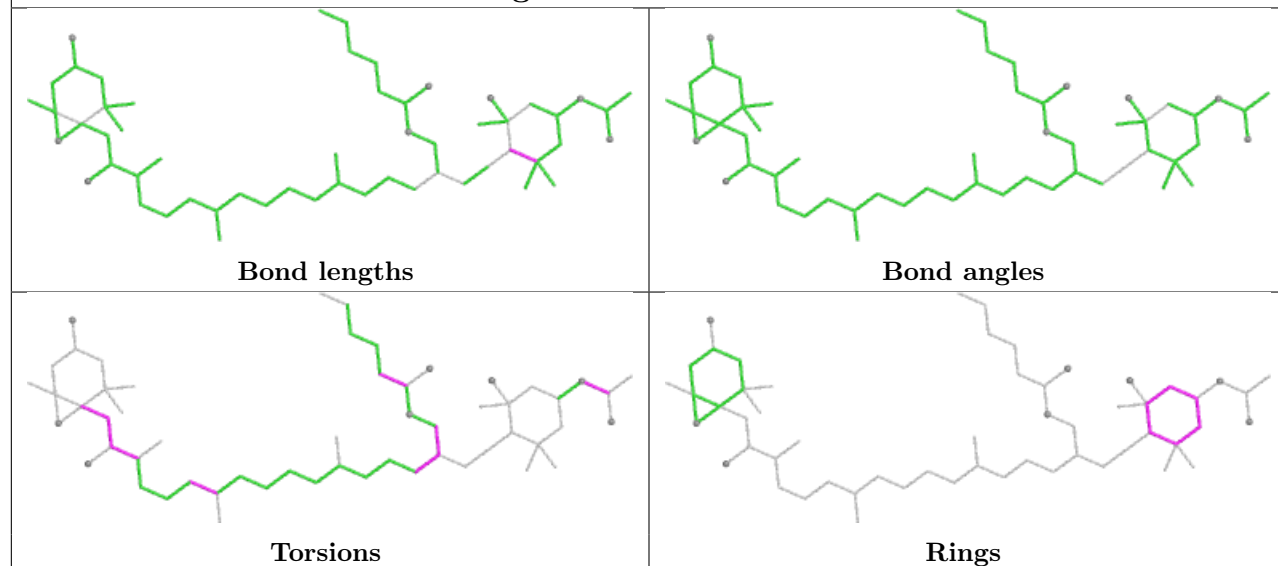




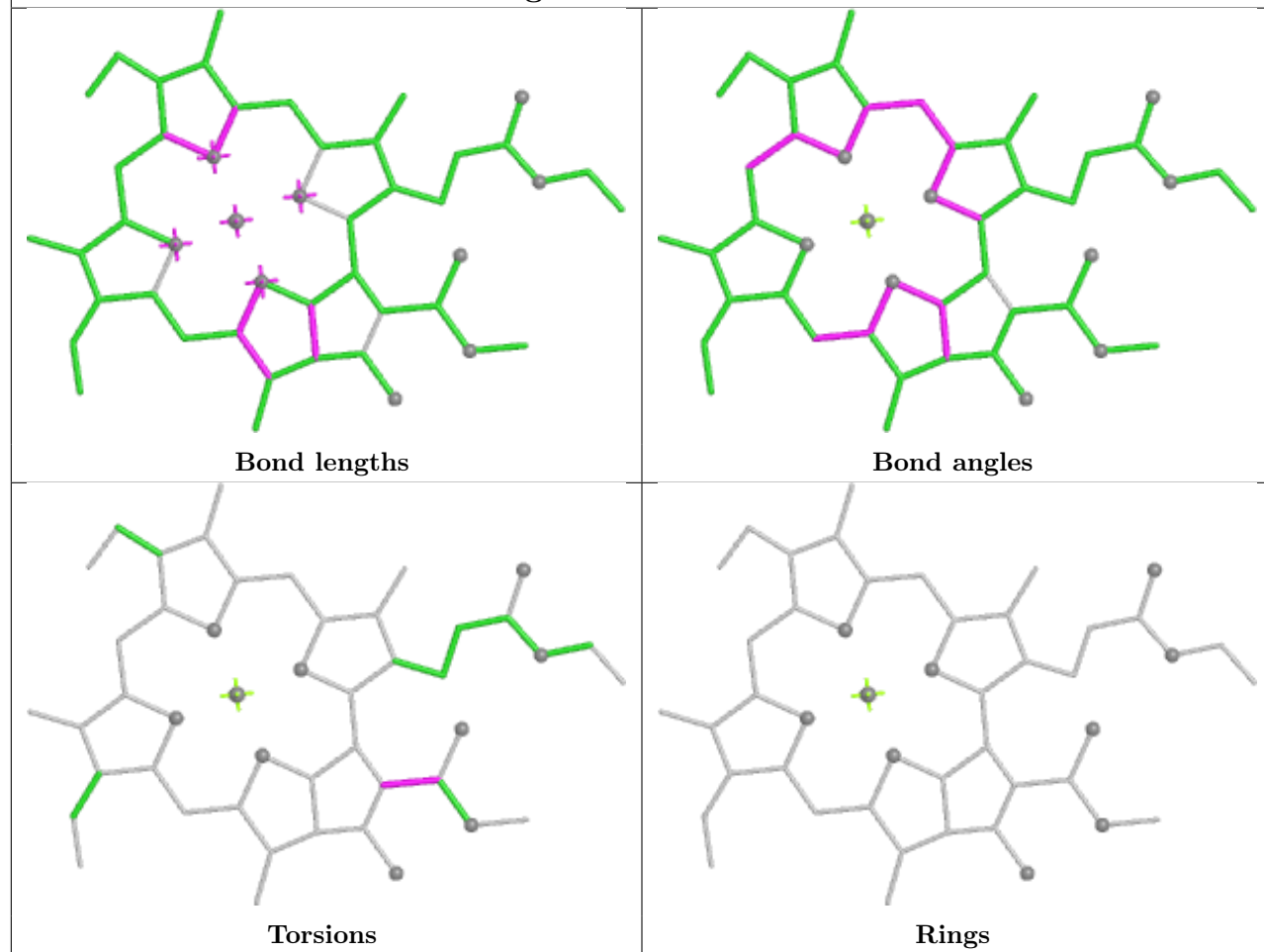


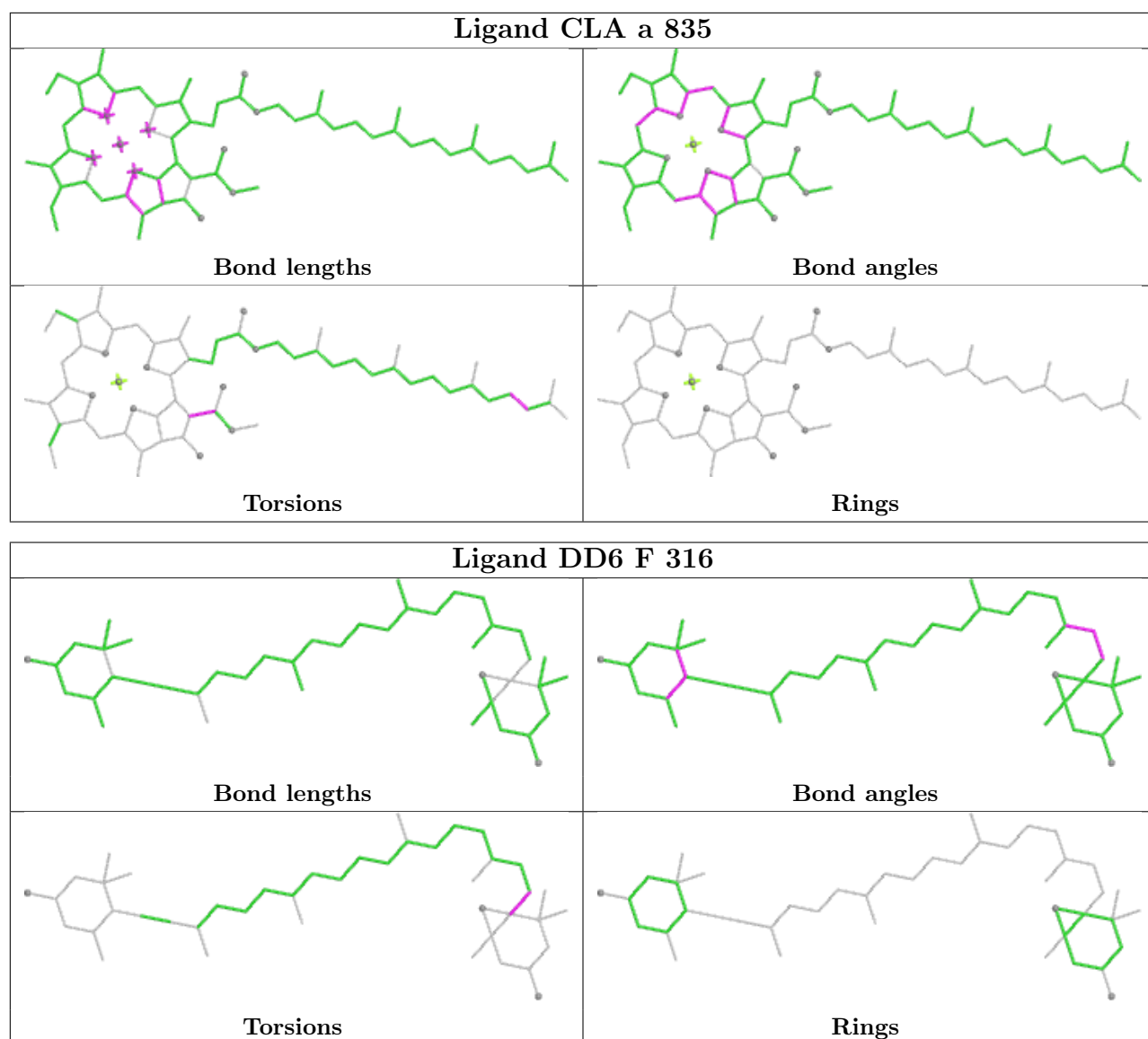


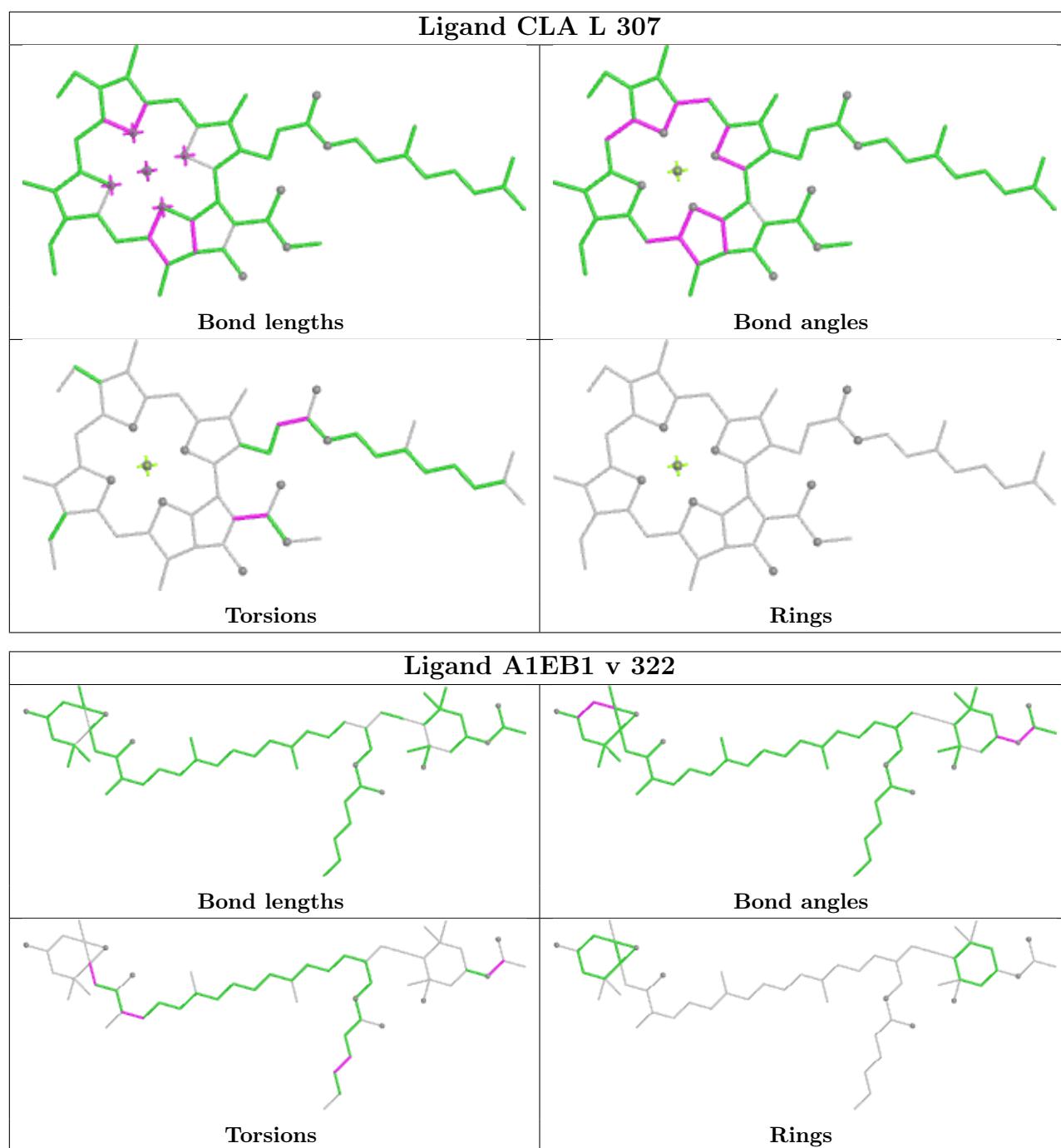
Ligand A1EB1 K 315



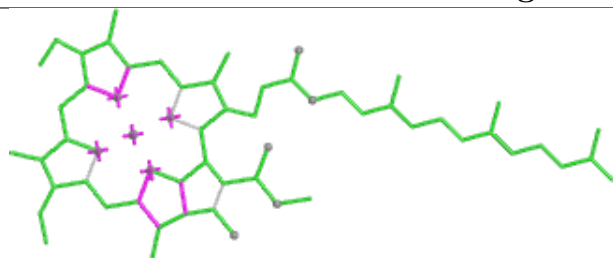
Ligand CLA K 312



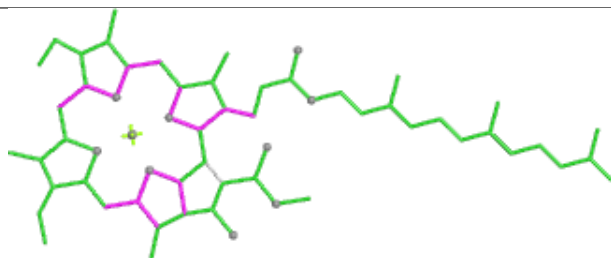




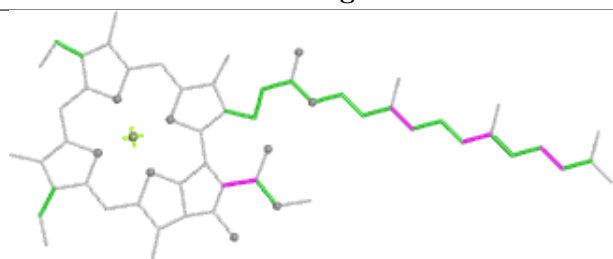
Ligand CLA b 836



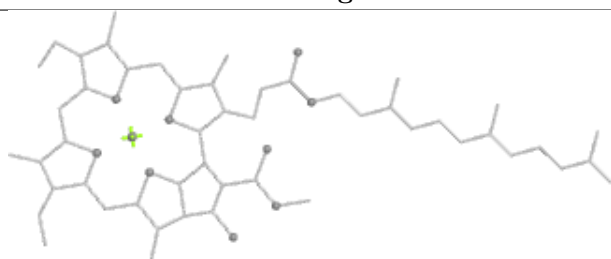
Bond lengths



Bond angles

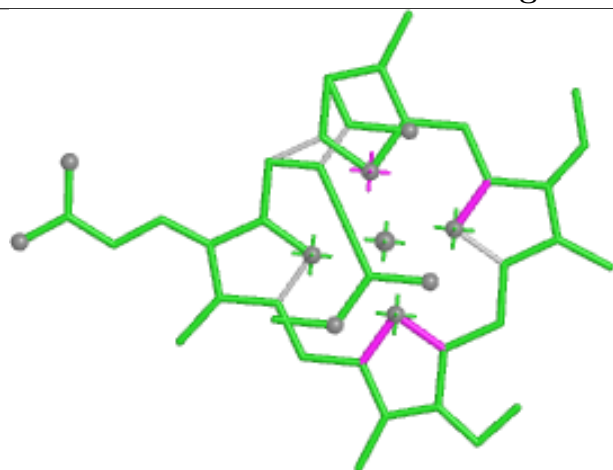


Torsions

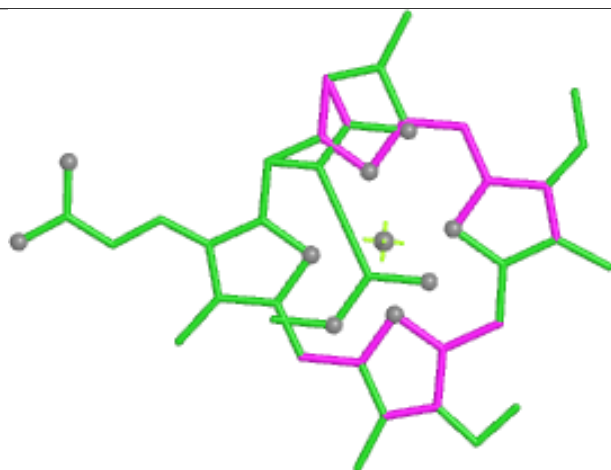


Rings

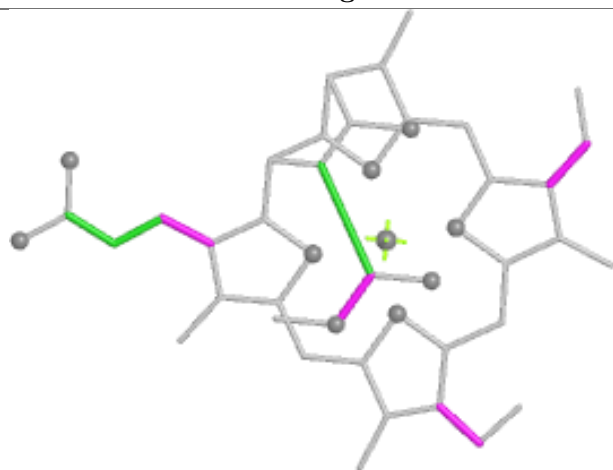
Ligand KC2 x 310



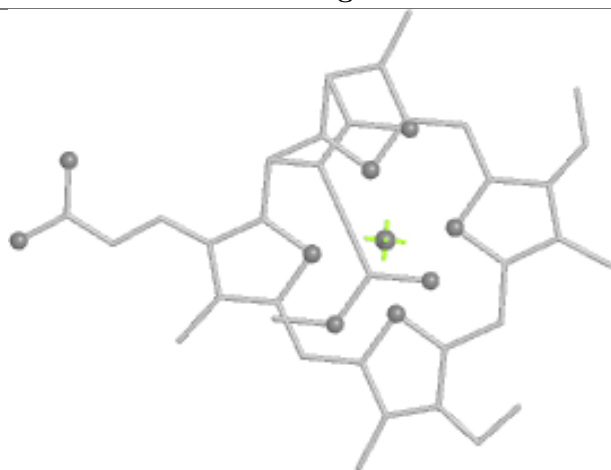
Bond lengths



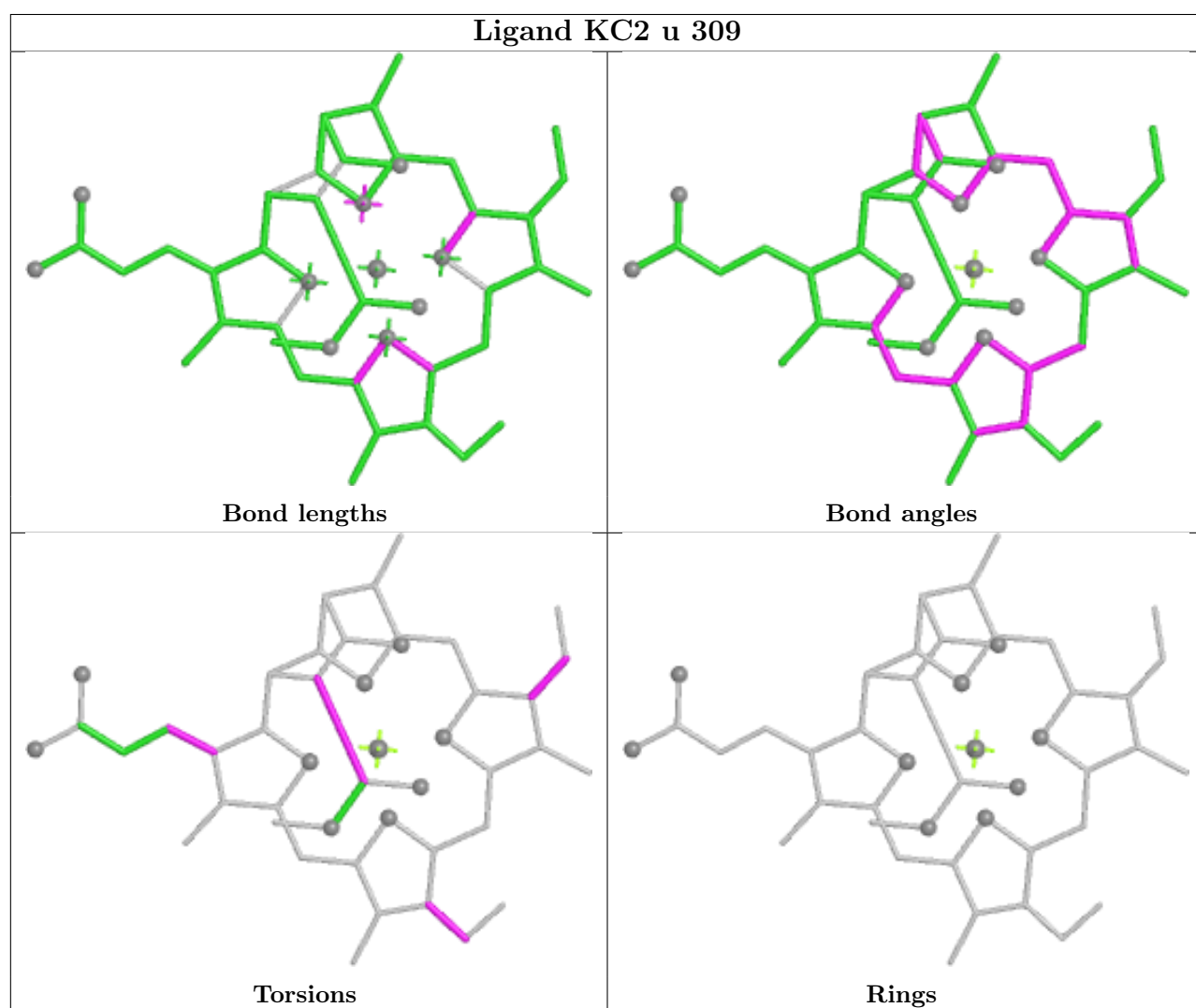
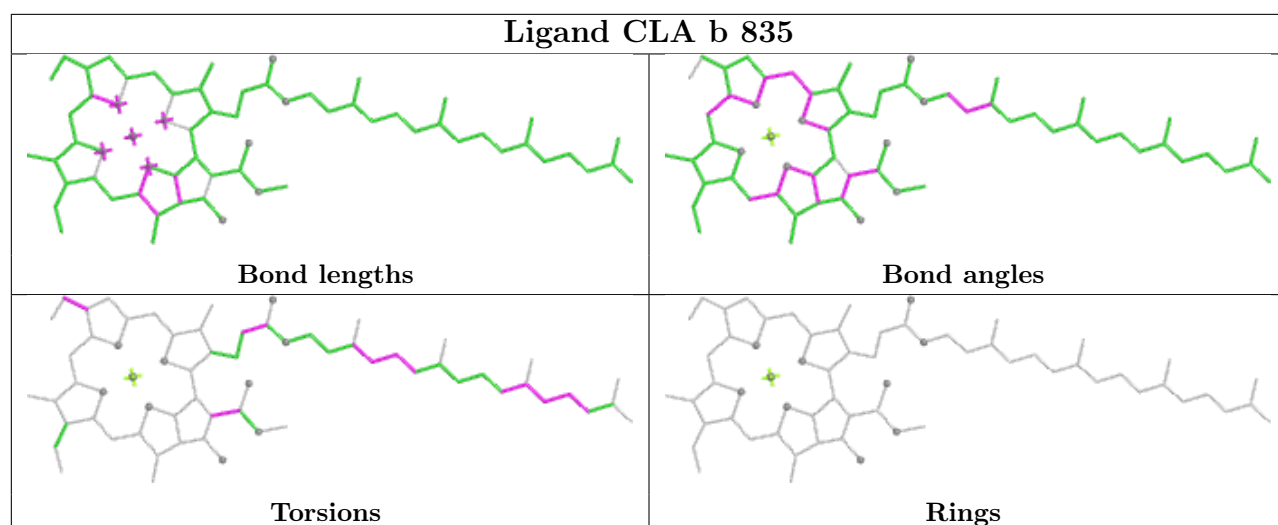
Bond angles

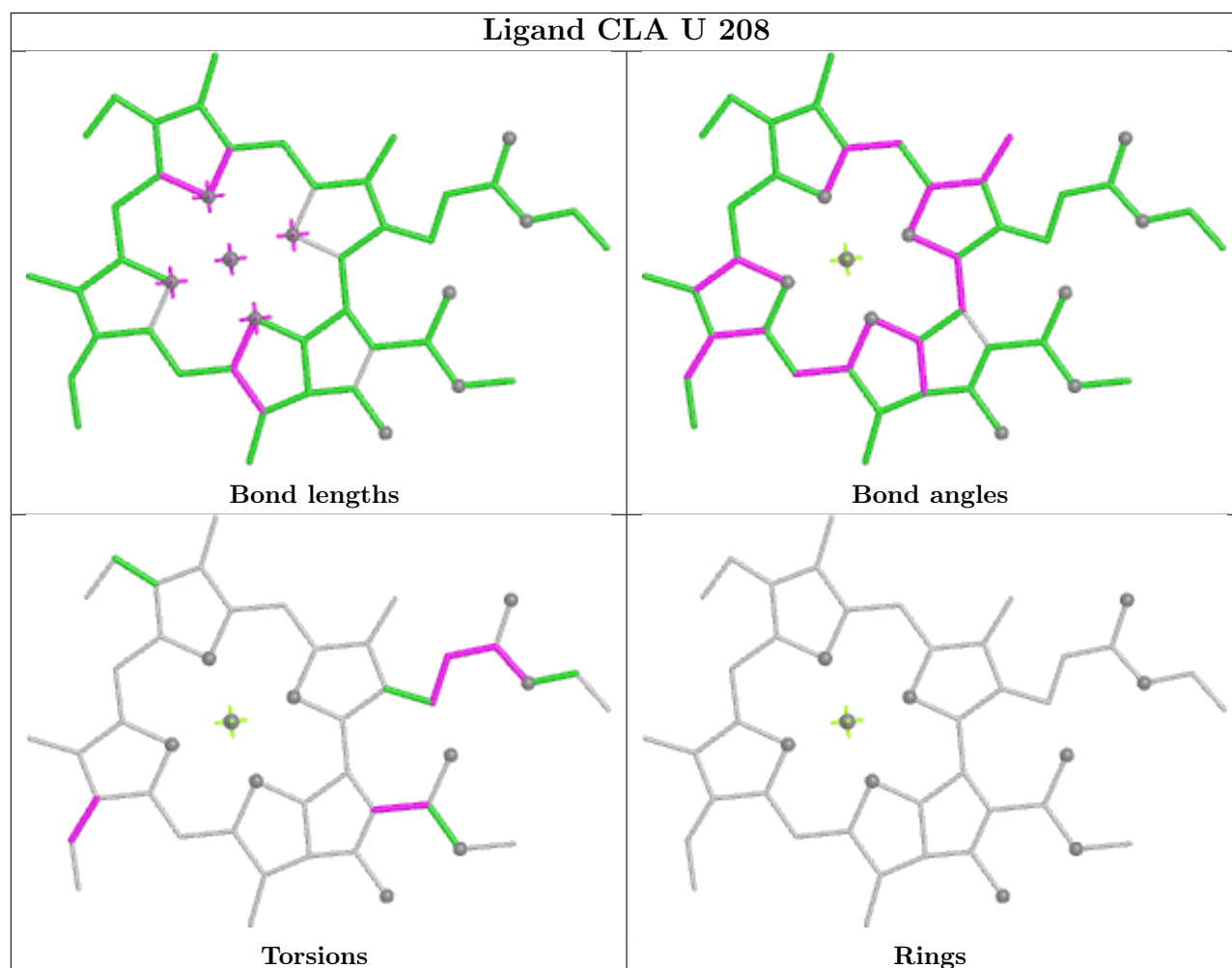
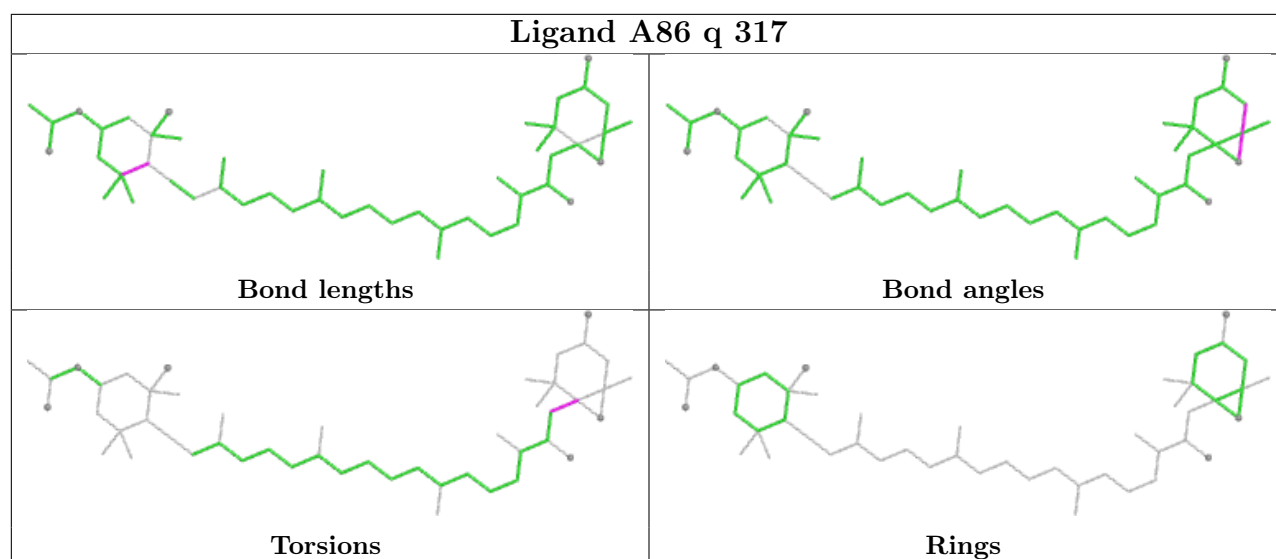


Torsions

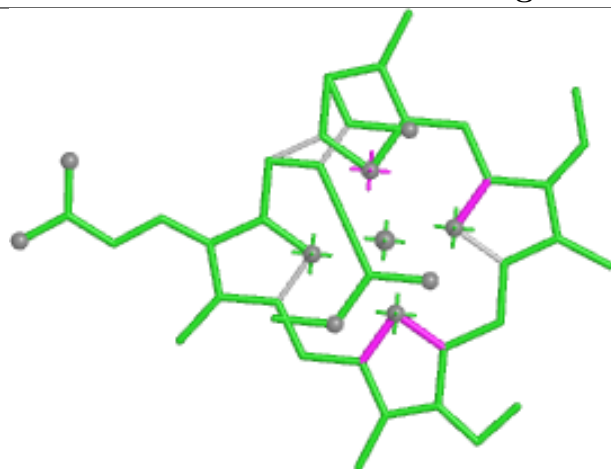


Rings

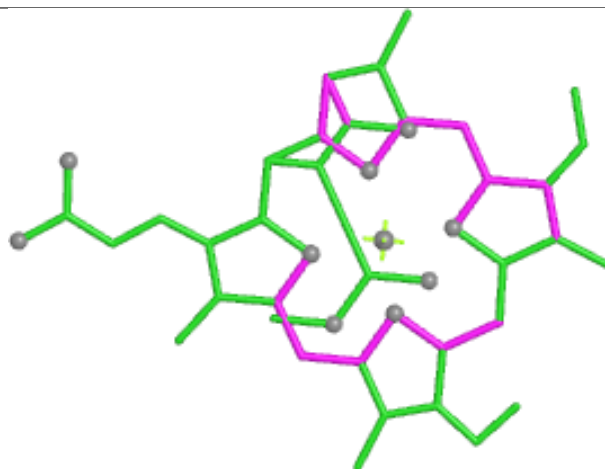




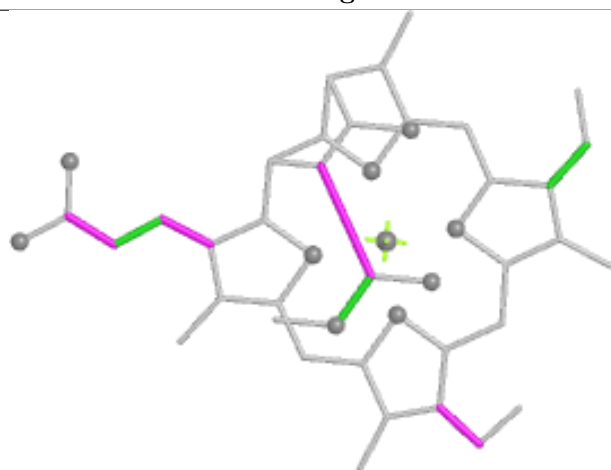
Ligand KC2 R 308



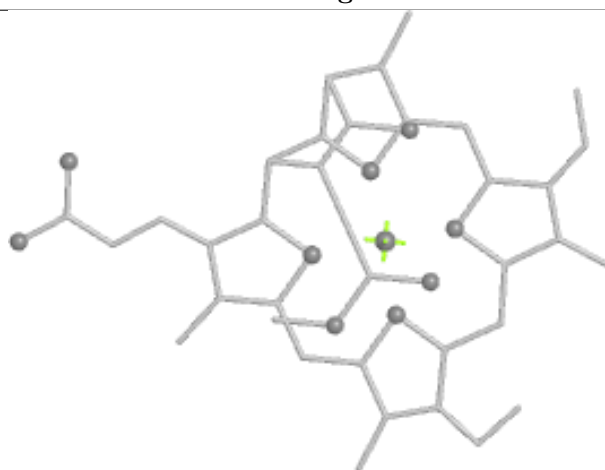
Bond lengths



Bond angles



Torsions



Rings

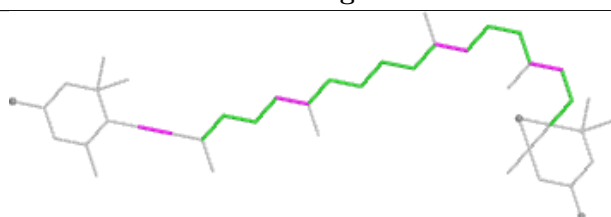
Ligand DD6 v 320



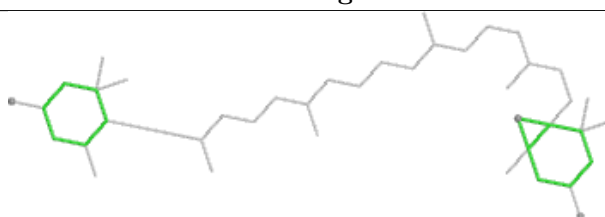
Bond lengths



Bond angles

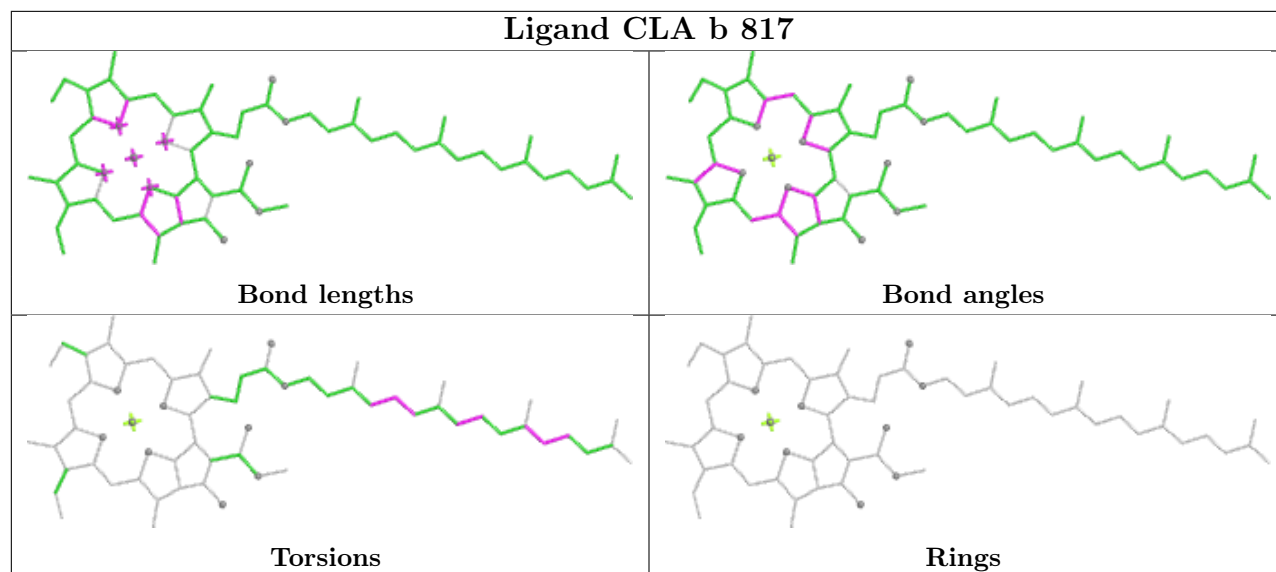


Torsions

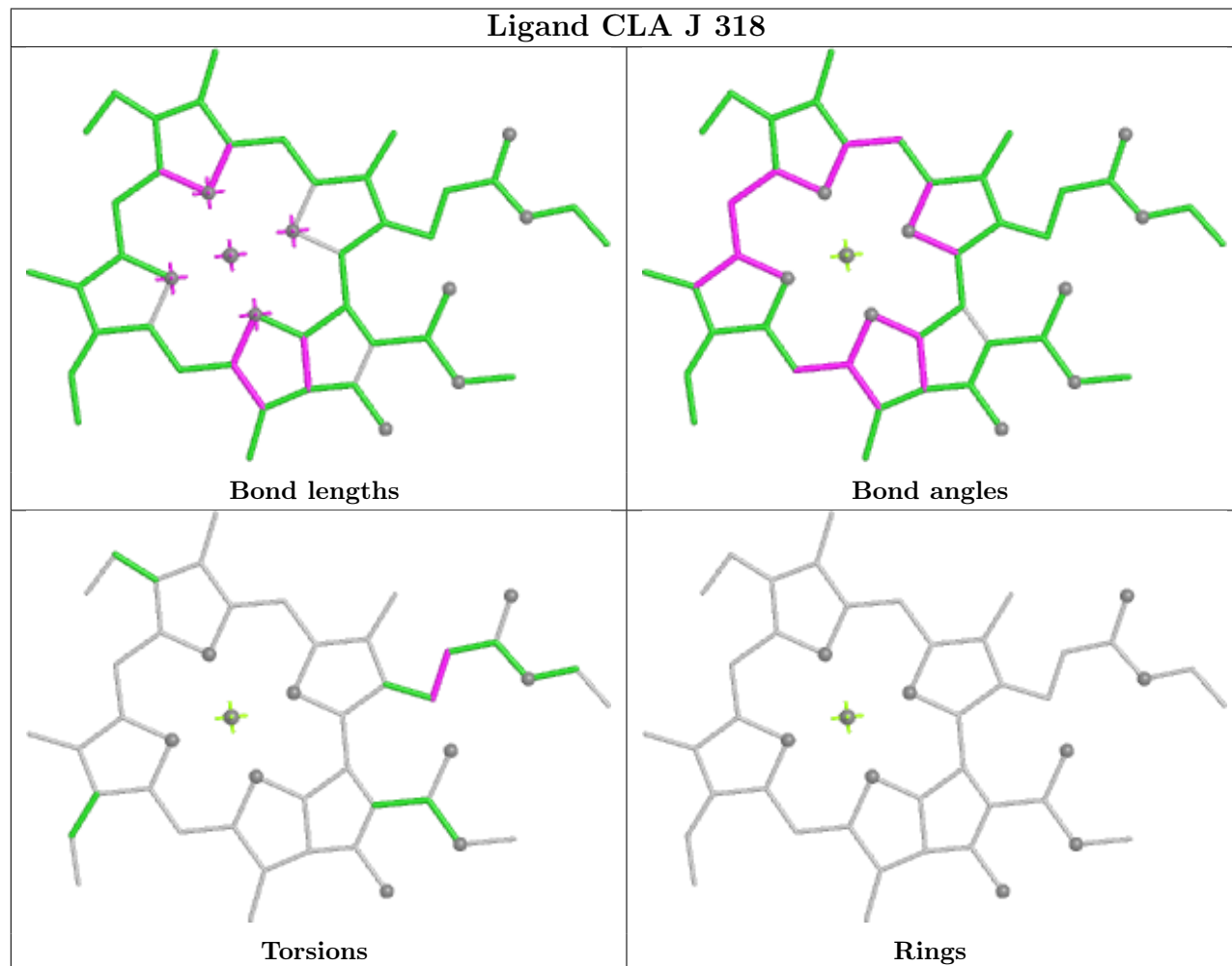


Rings

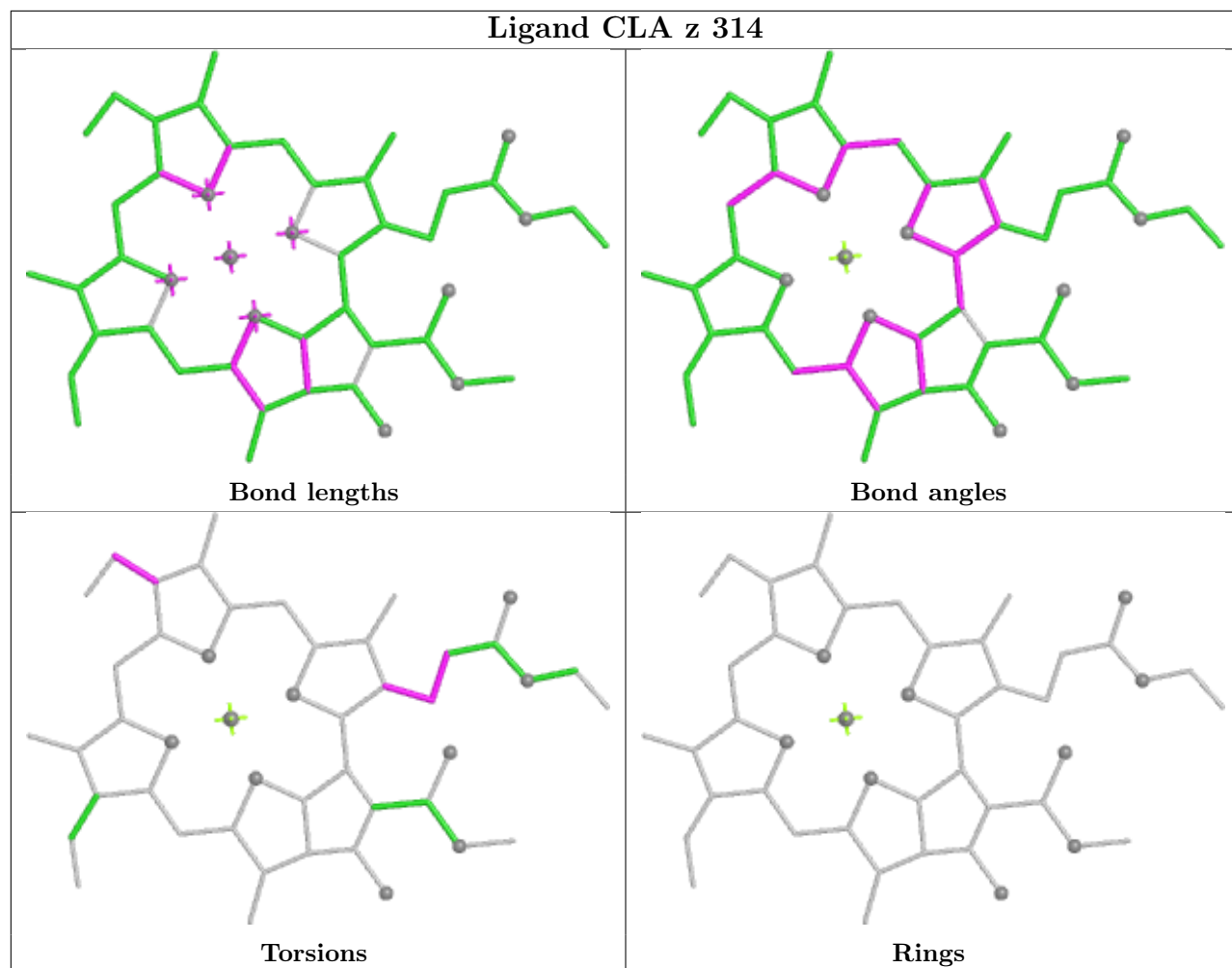
Ligand CLA b 817



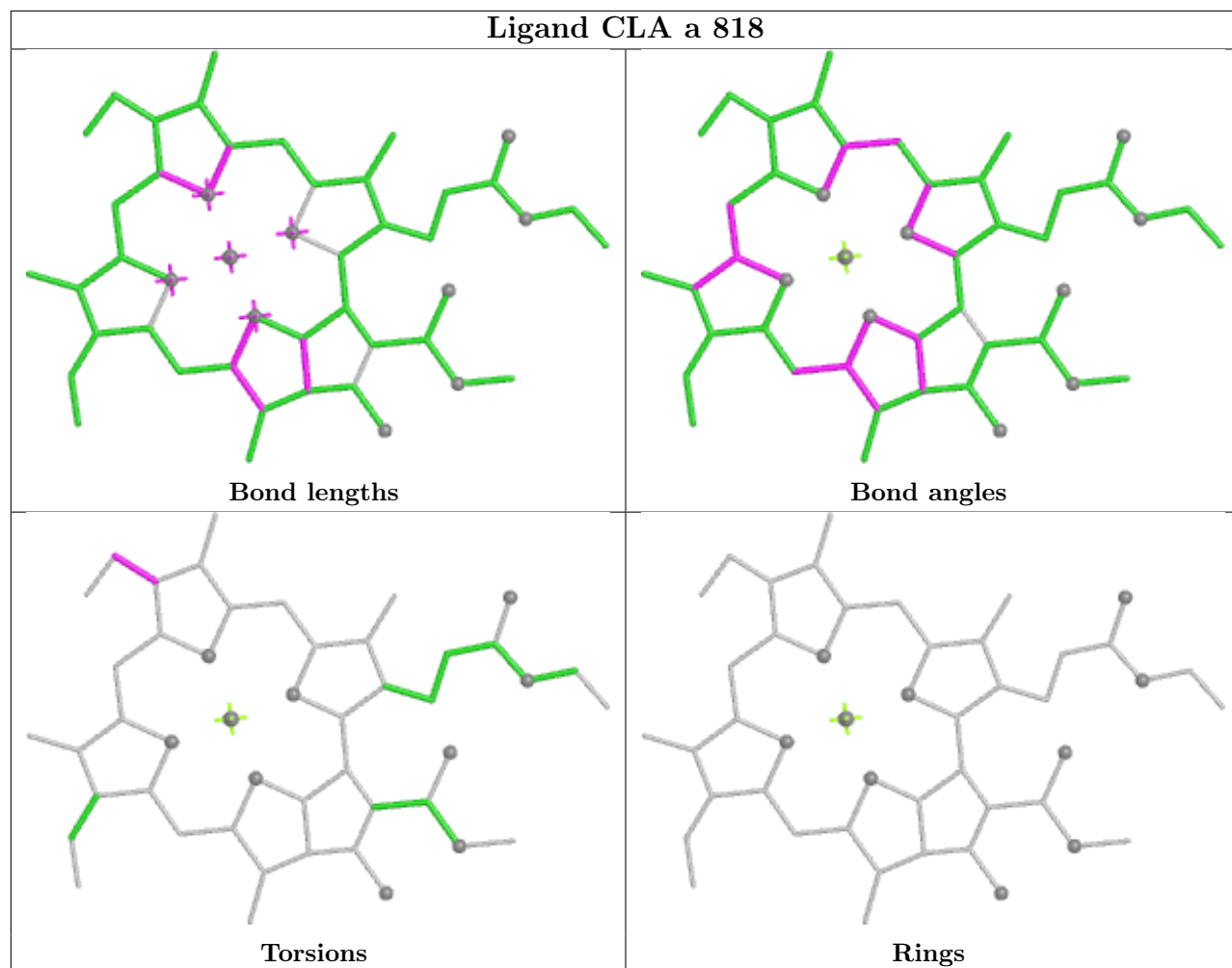
Ligand CLA J 318



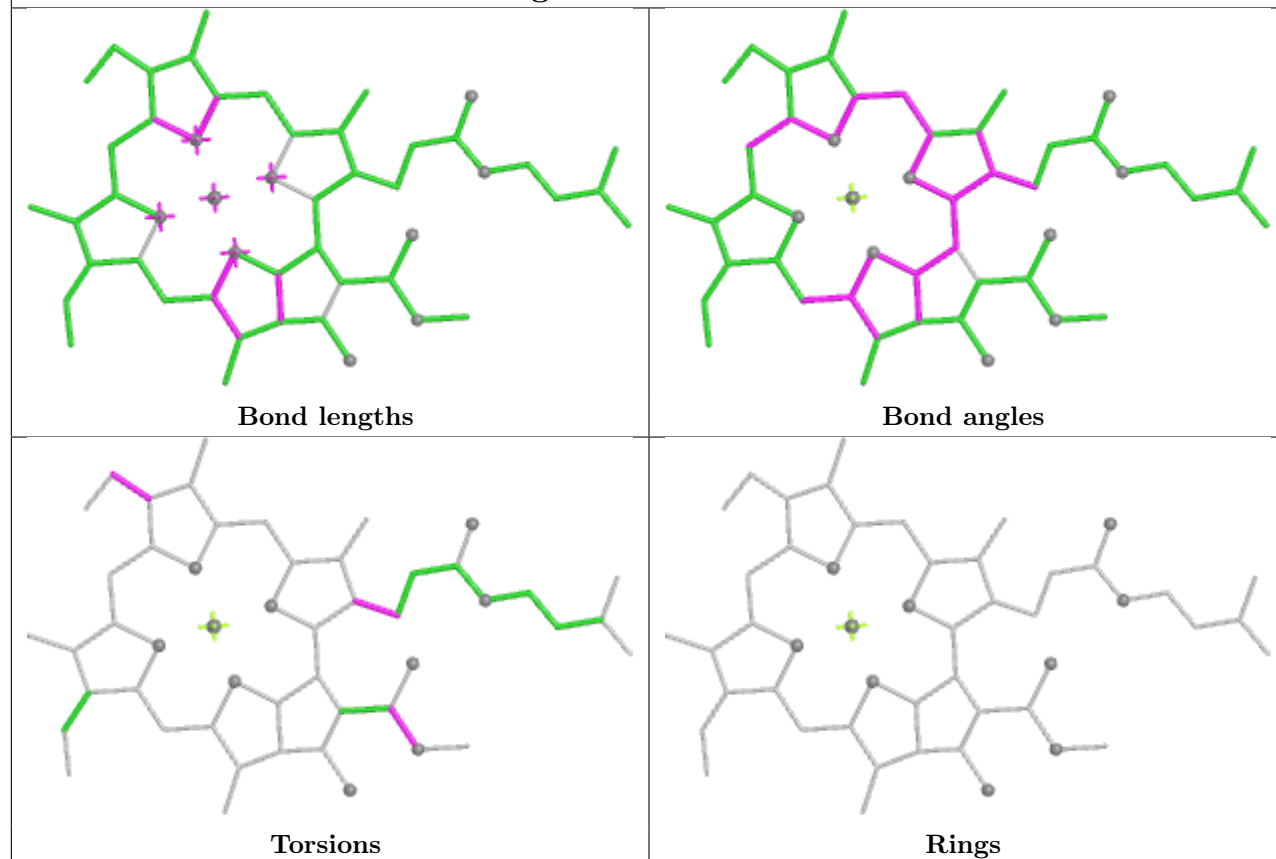
Ligand CLA z 314



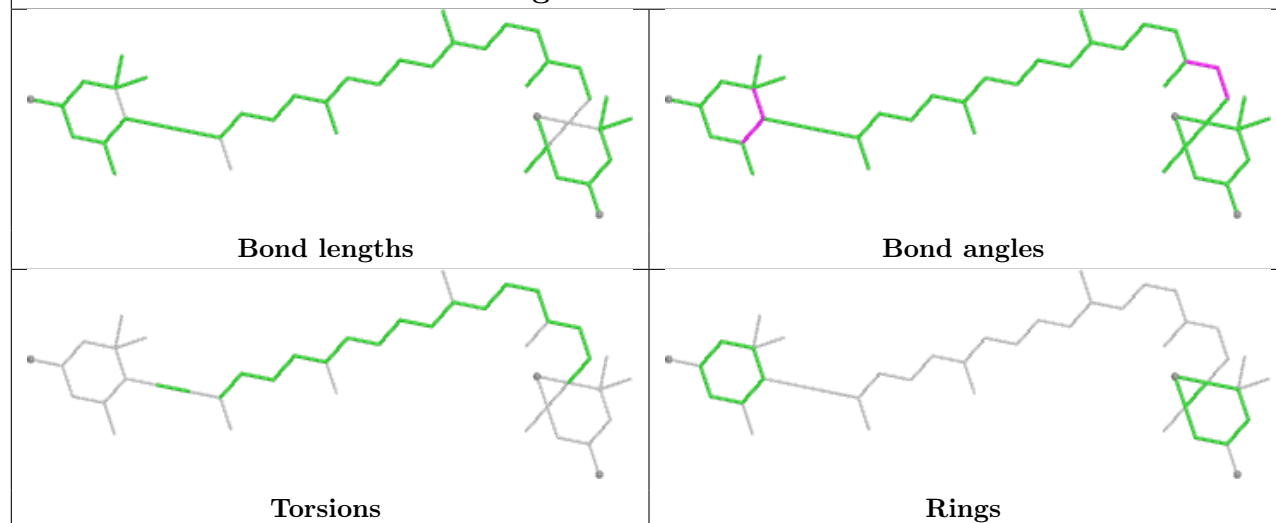
Ligand CLA a 818

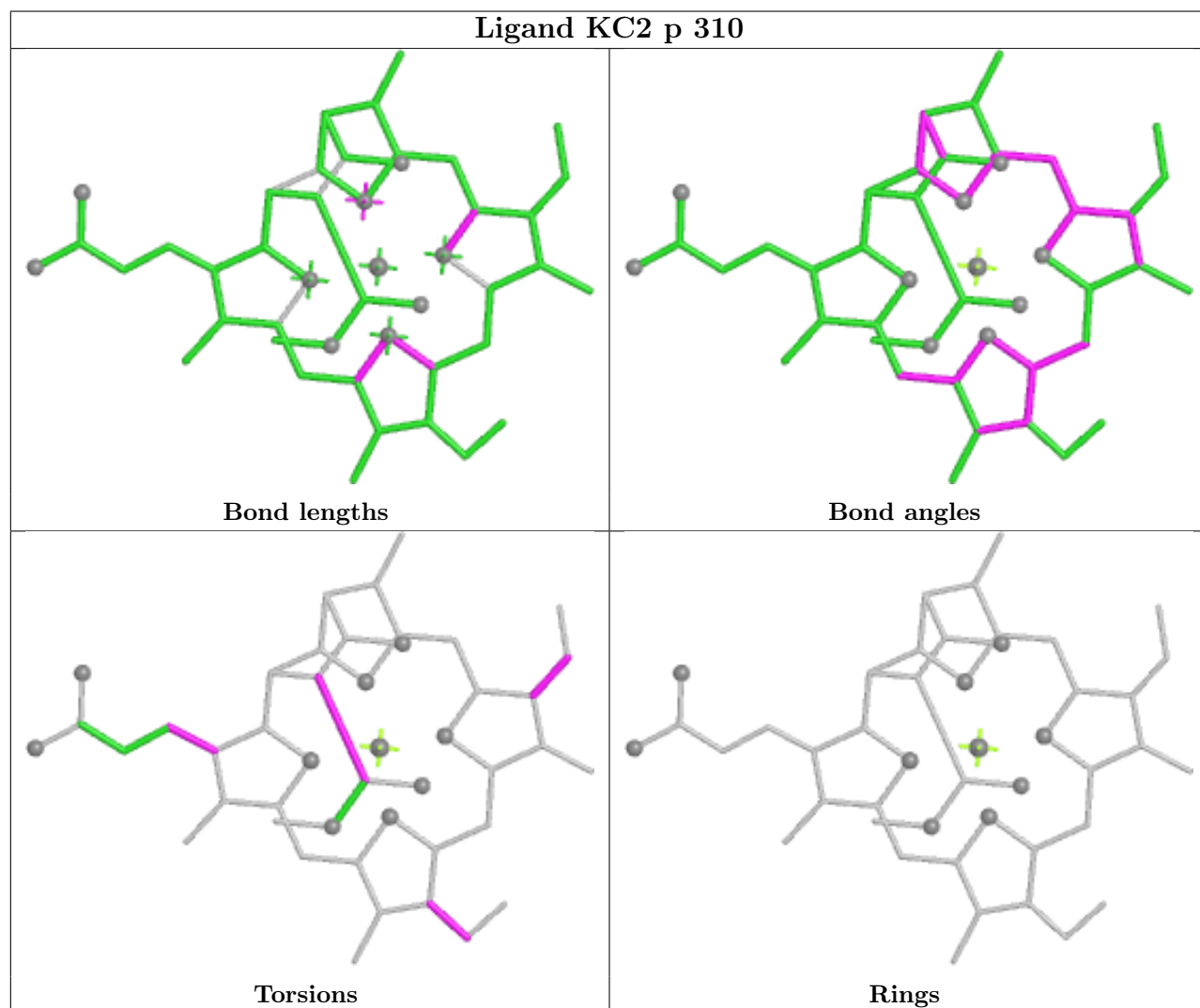
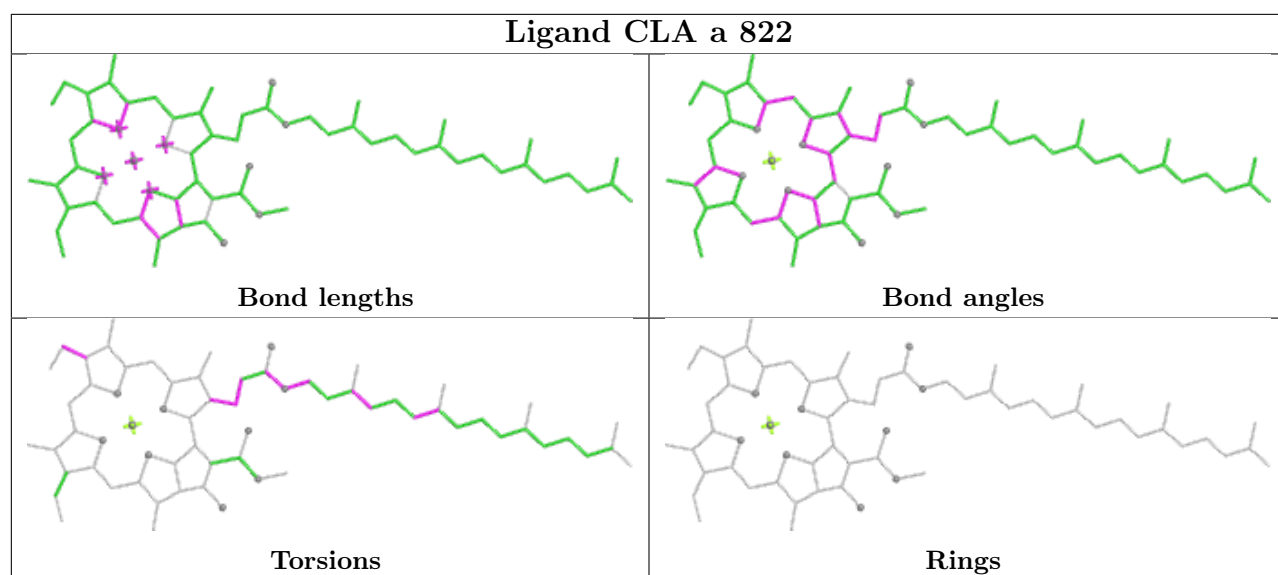


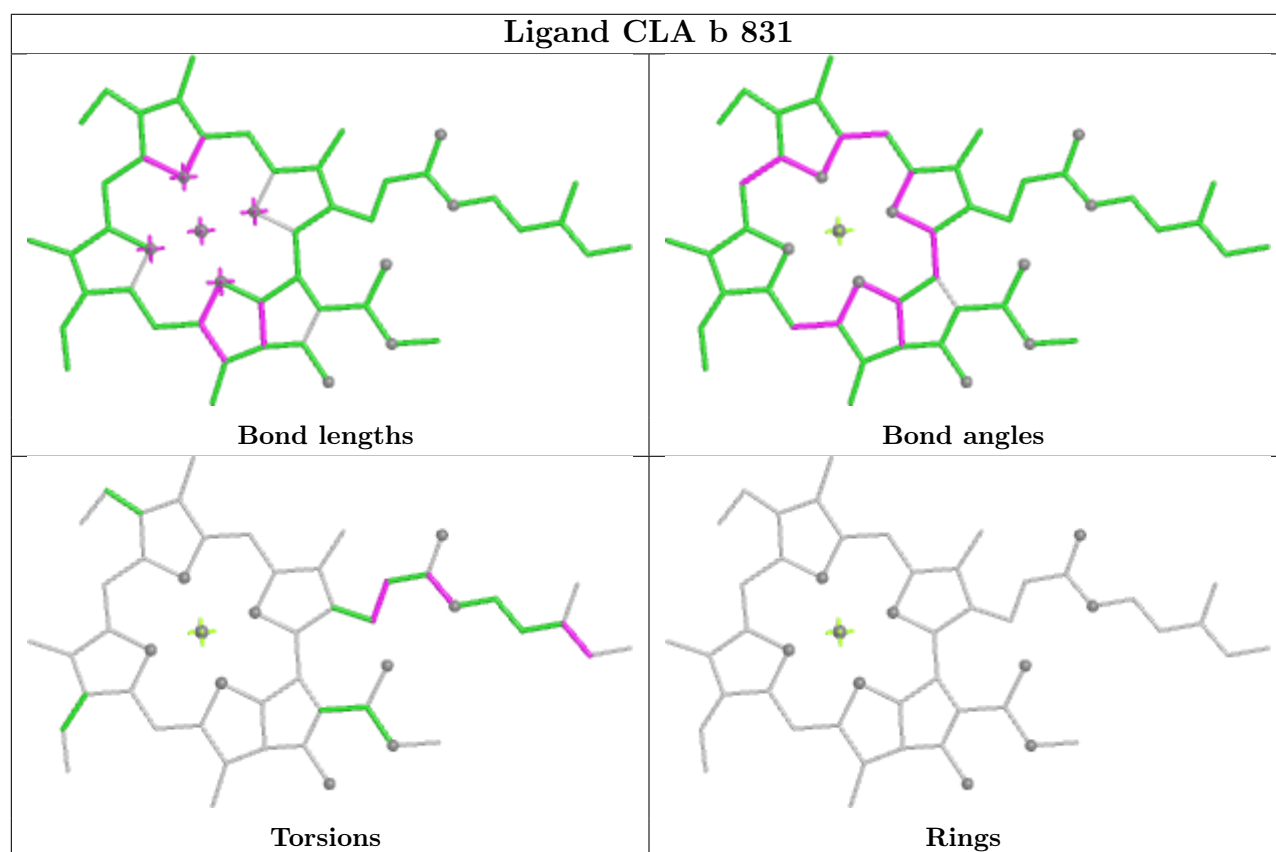
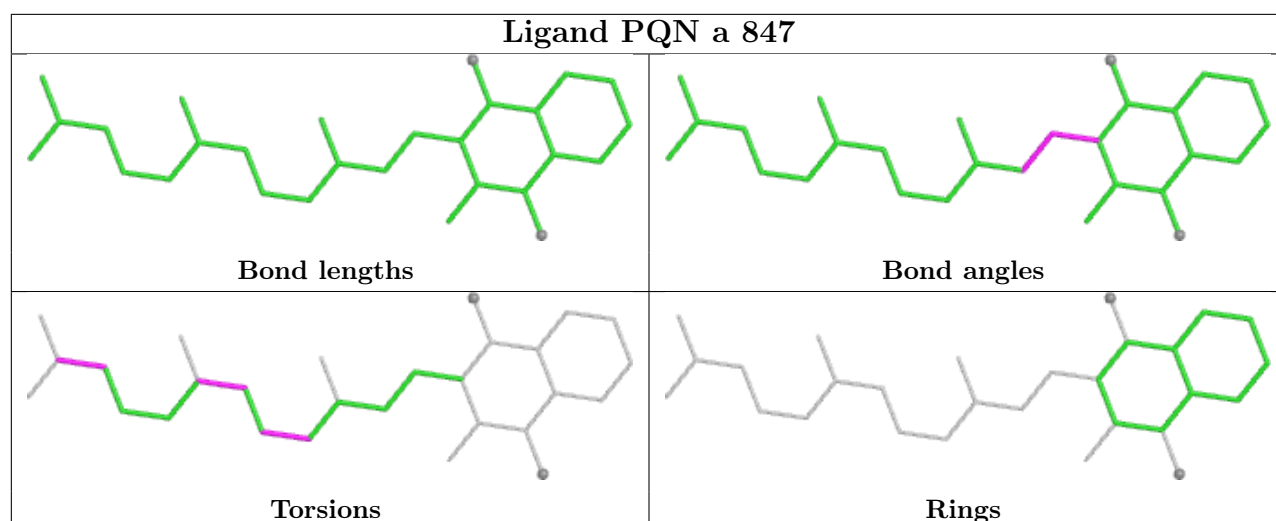
Ligand CLA N 310

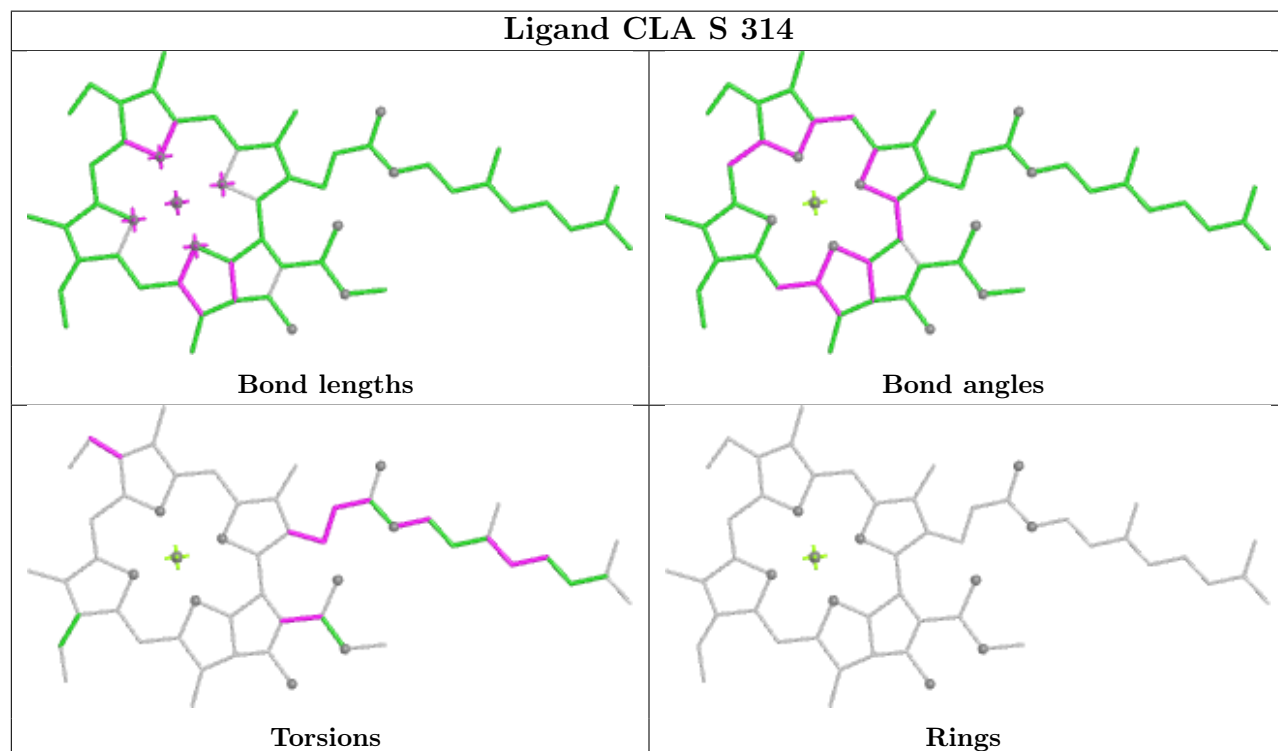
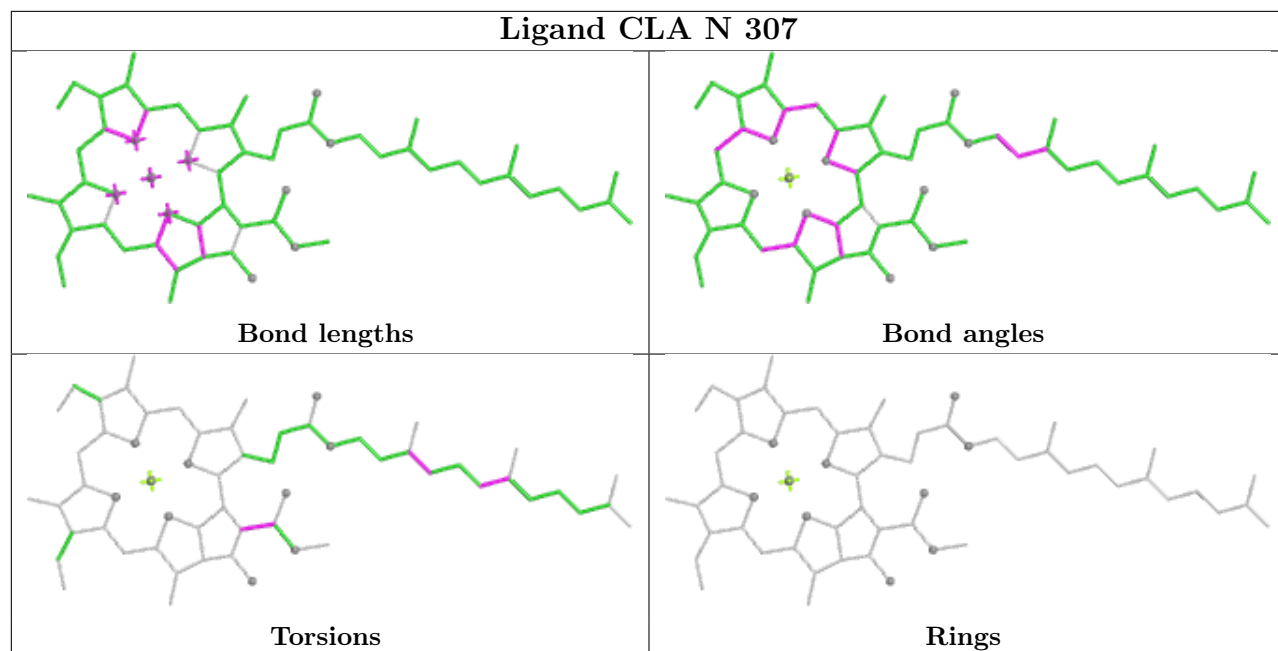


Ligand DD6 A 312

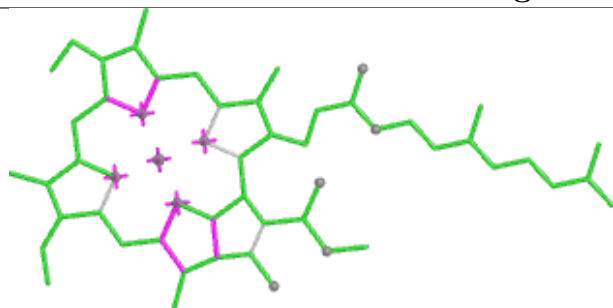




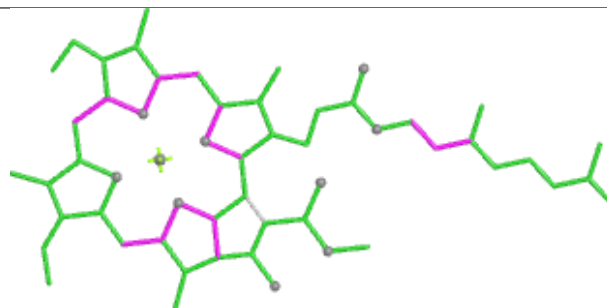




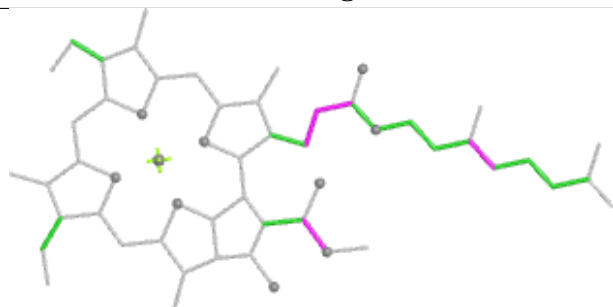
Ligand CLA Y 305



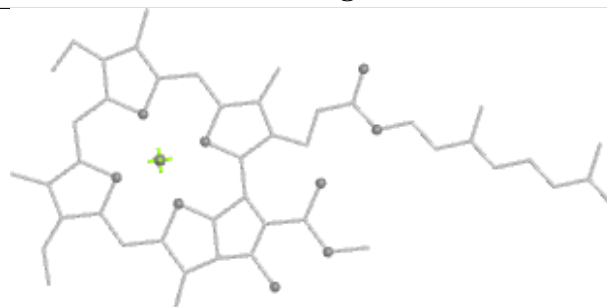
Bond lengths



Bond angles

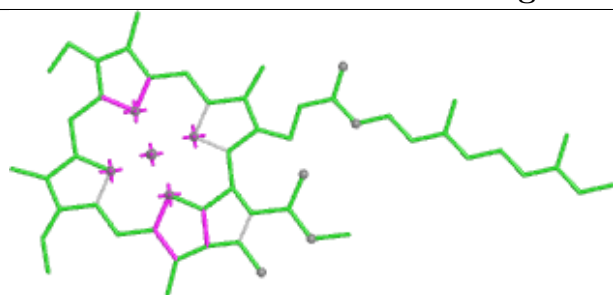


Torsions

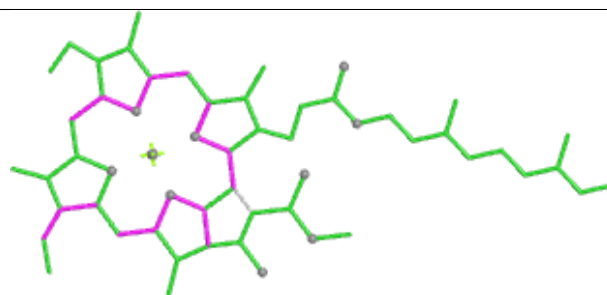


Rings

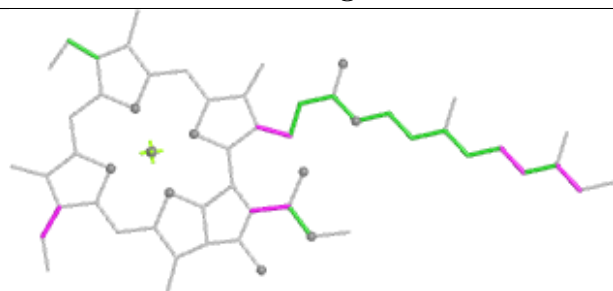
Ligand CLA a 807



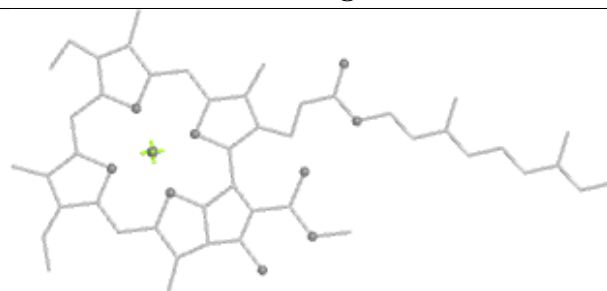
Bond lengths



Bond angles

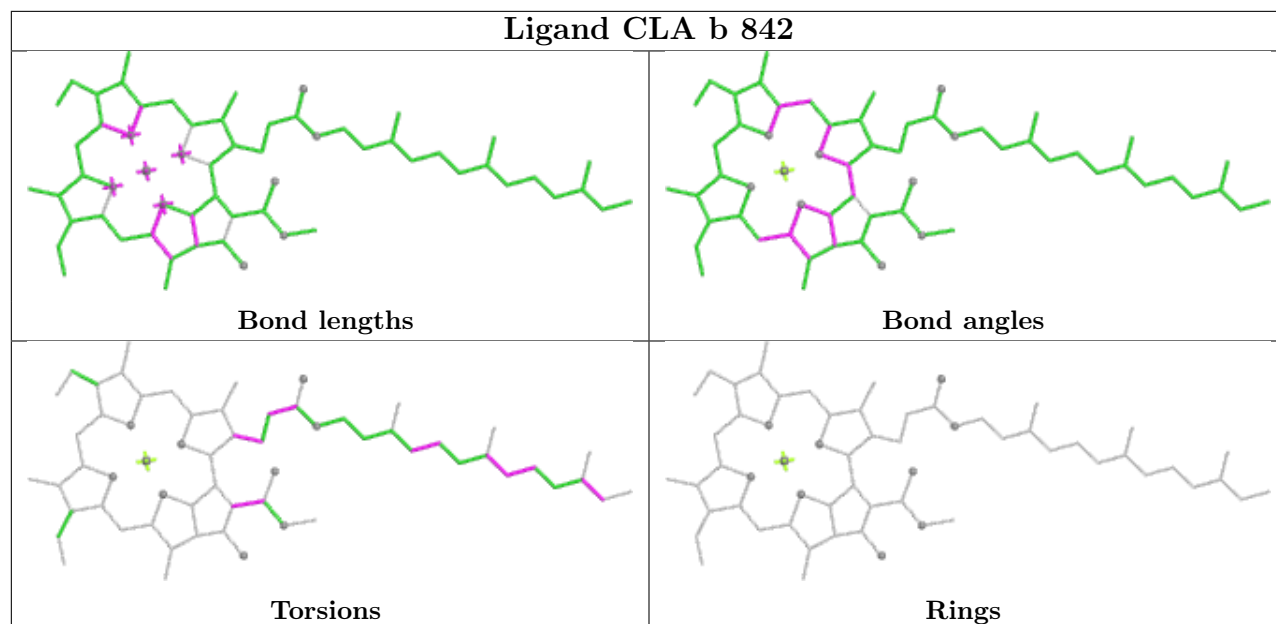


Torsions

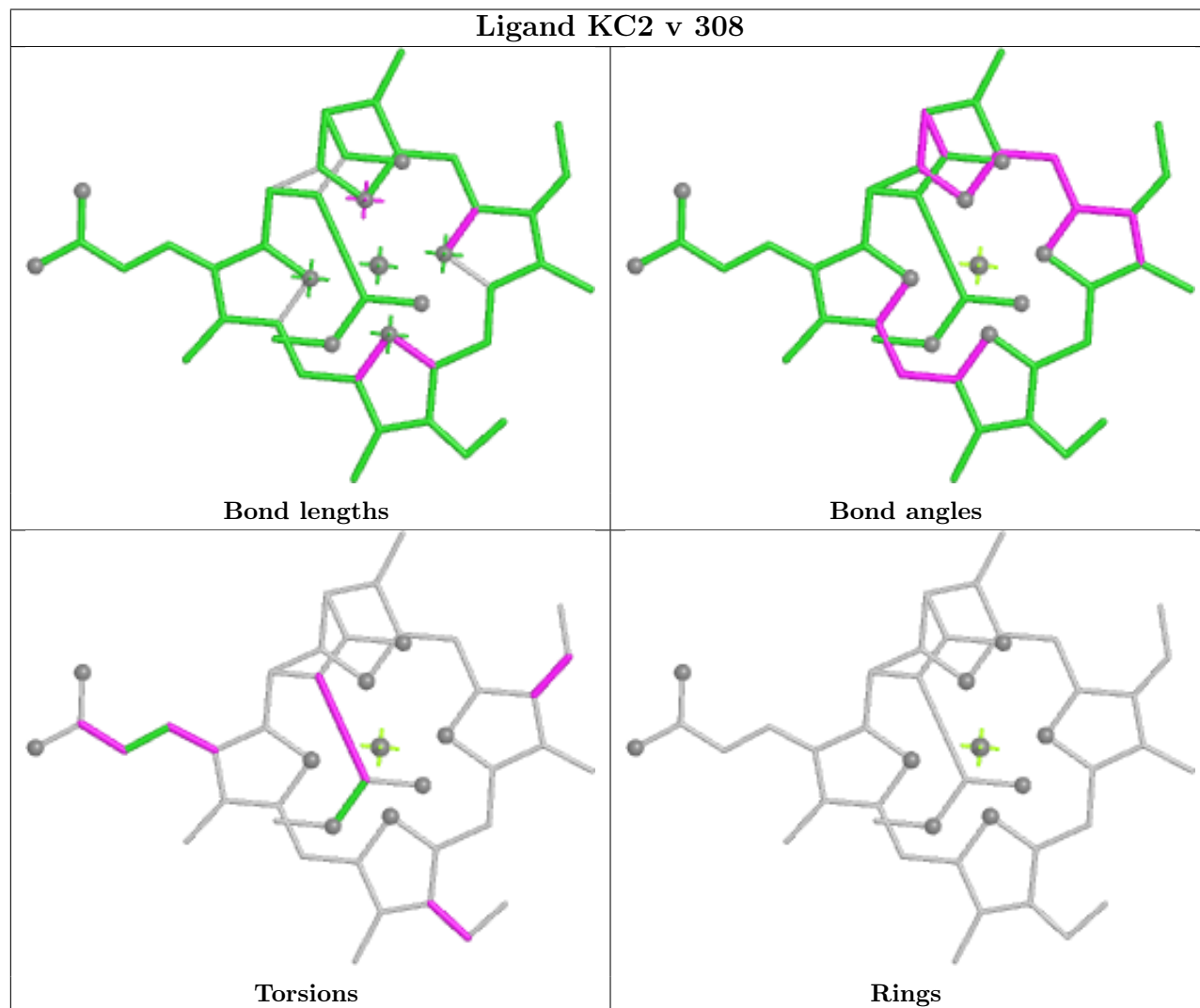


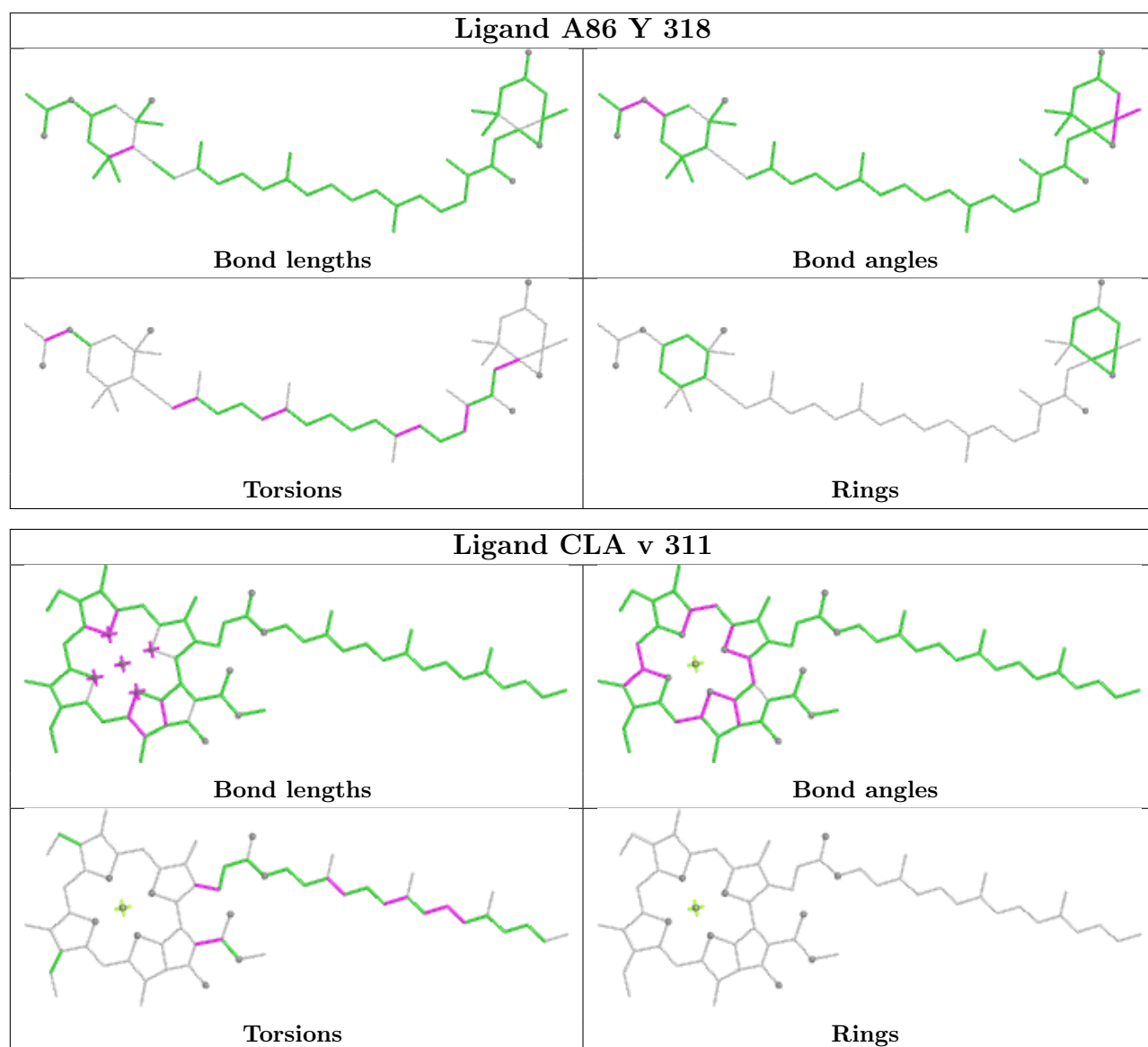
Rings

Ligand CLA b 842

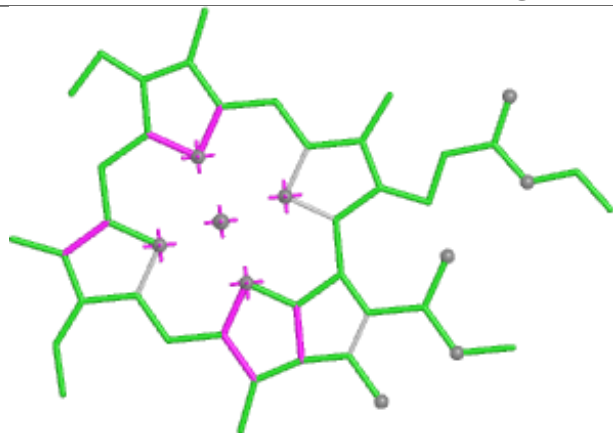


Ligand KC2 v 308

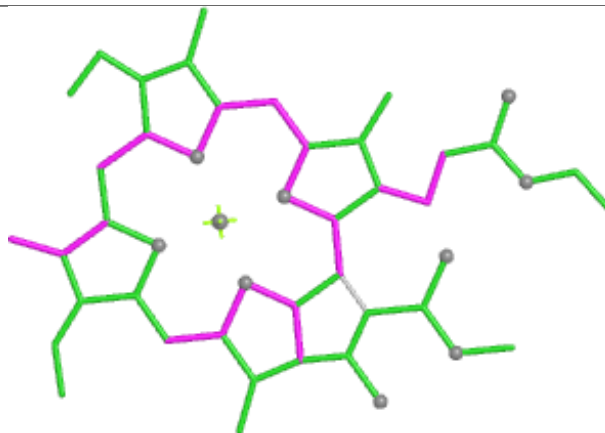




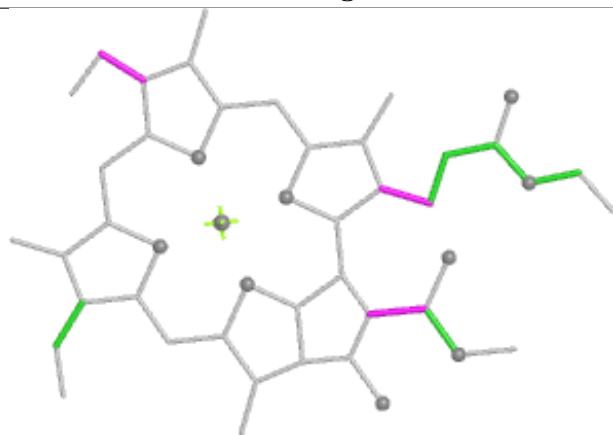
Ligand CLA H 304



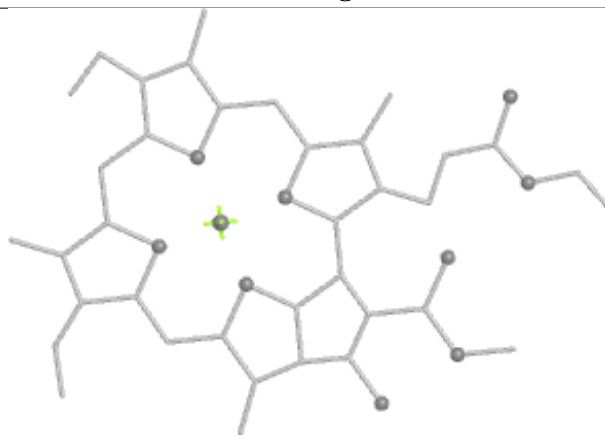
Bond lengths



Bond angles

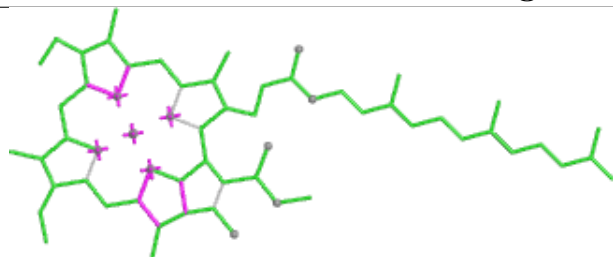


Torsions

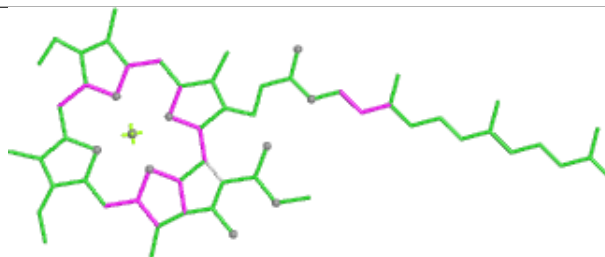


Rings

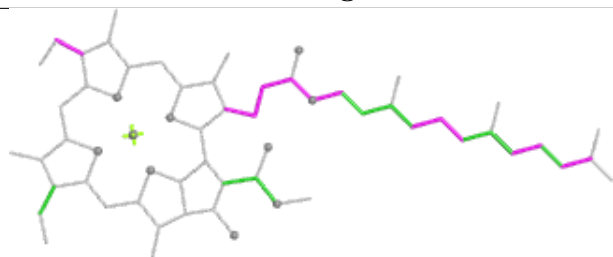
Ligand CLA a 820



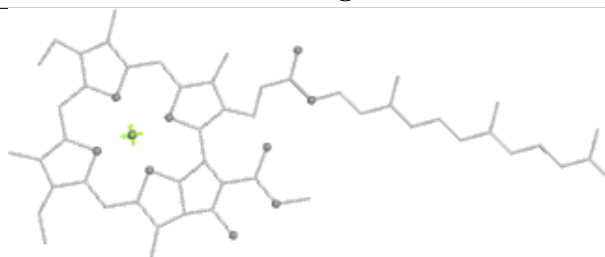
Bond lengths



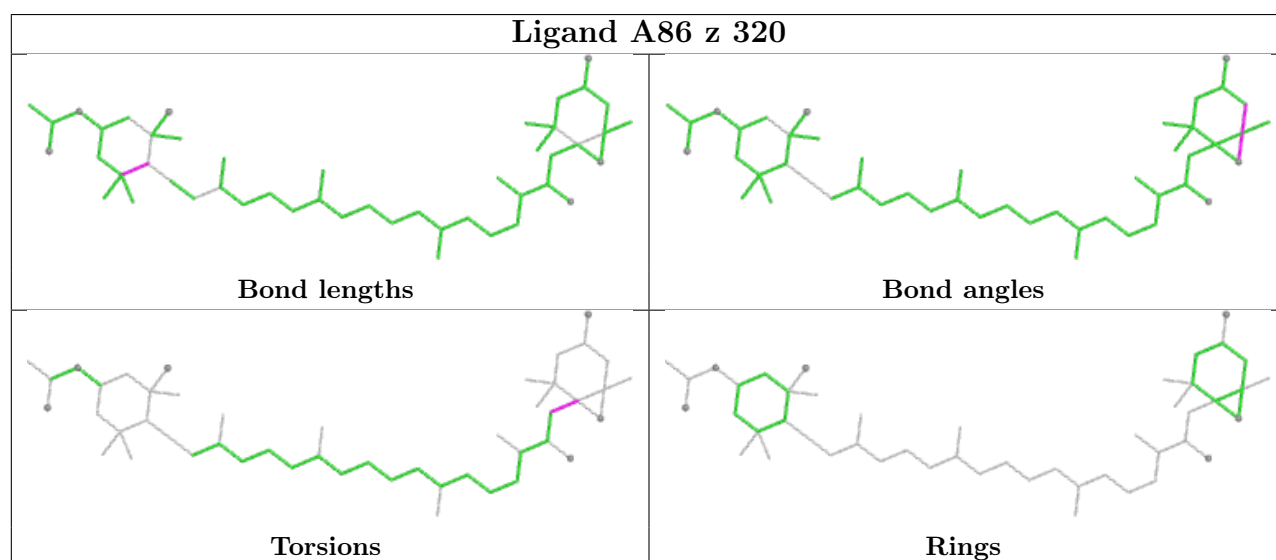
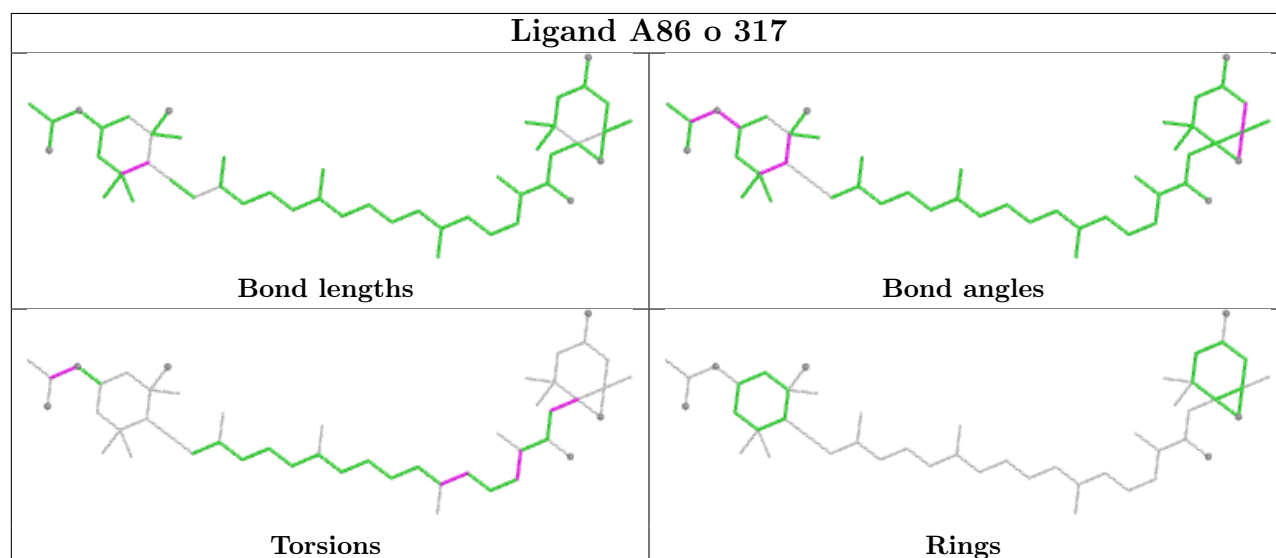
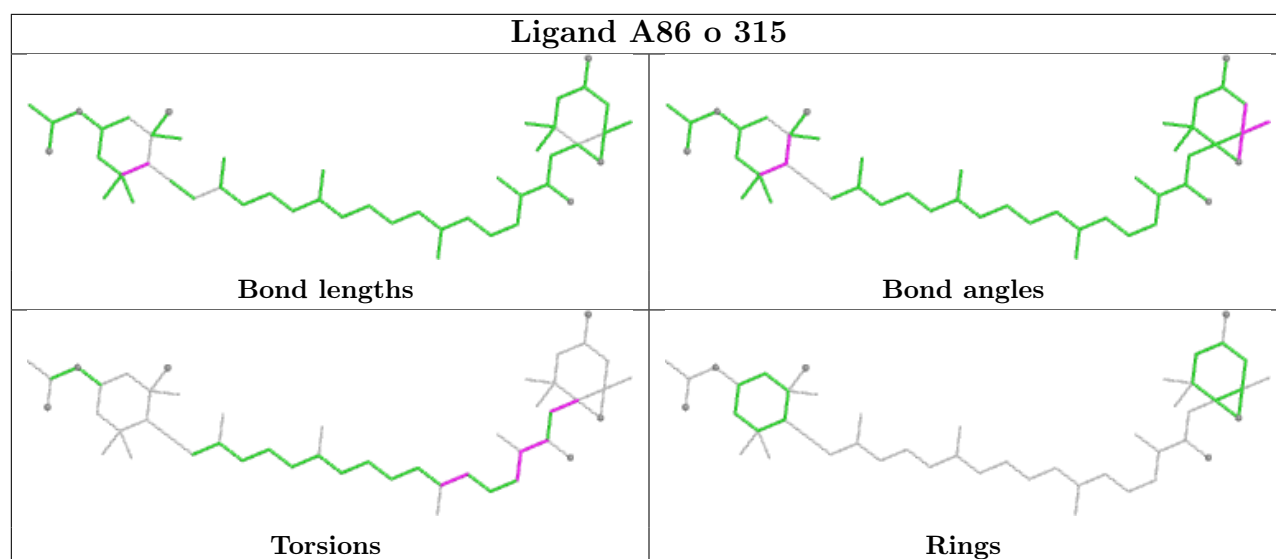
Bond angles



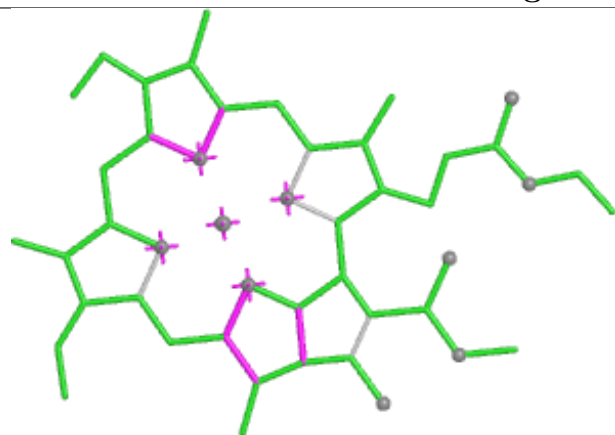
Torsions



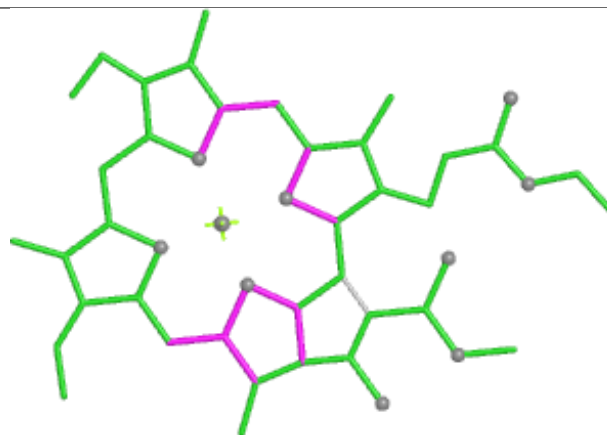
Rings



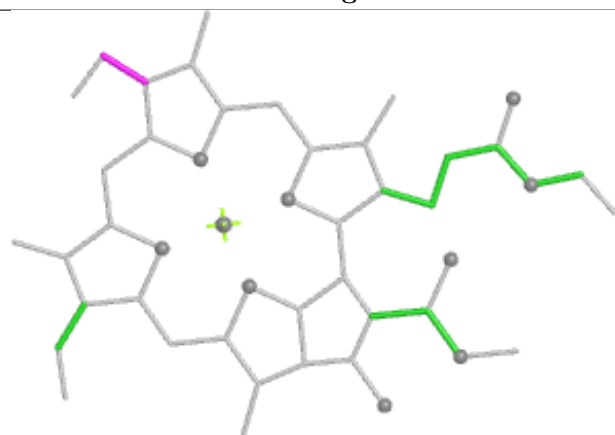
Ligand CLA f 204



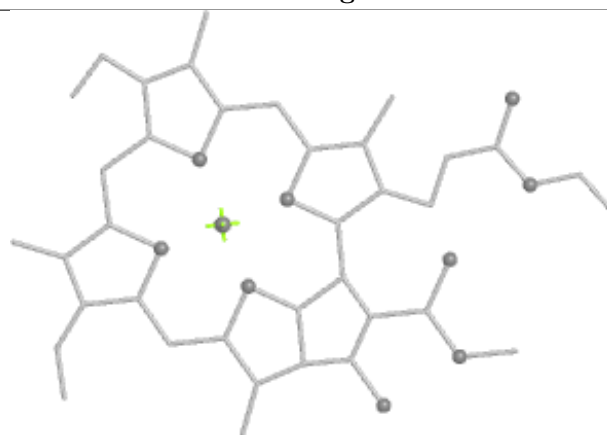
Bond lengths



Bond angles

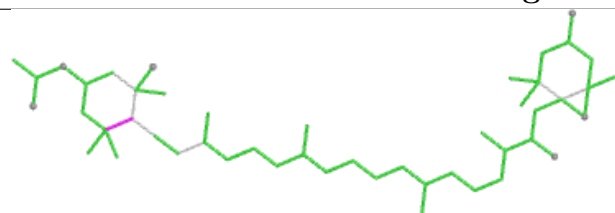


Torsions

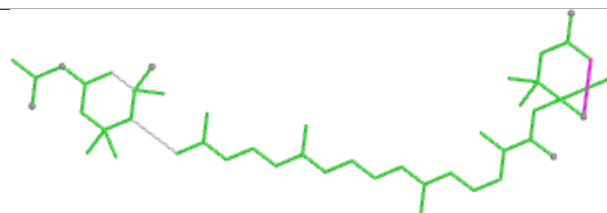


Rings

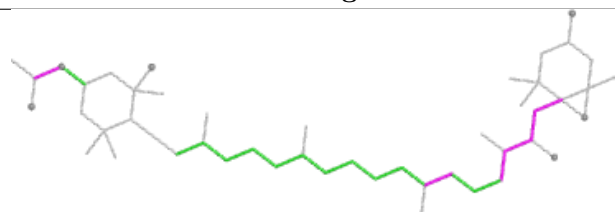
Ligand A86 T 315



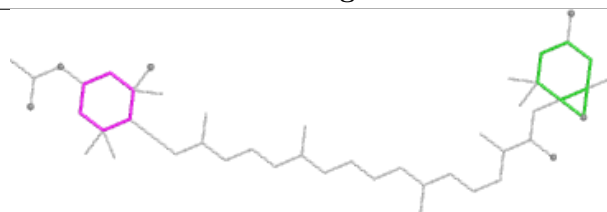
Bond lengths



Bond angles

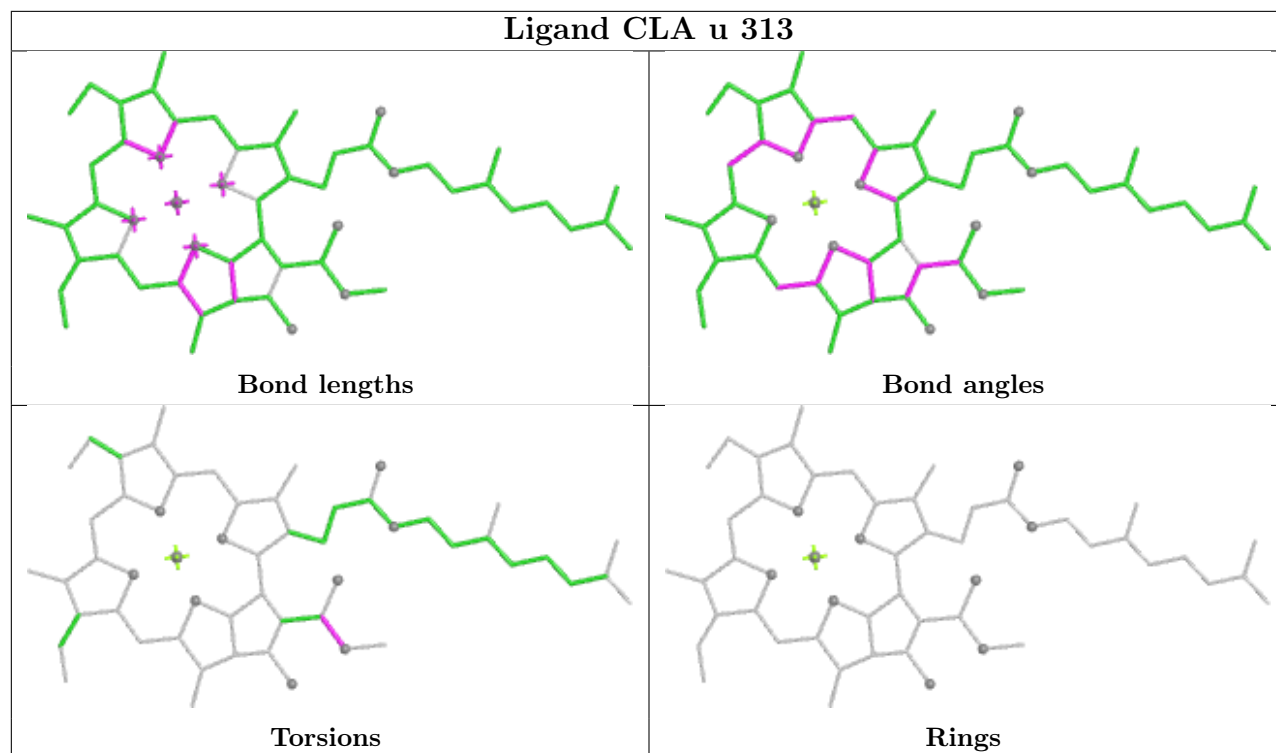


Torsions

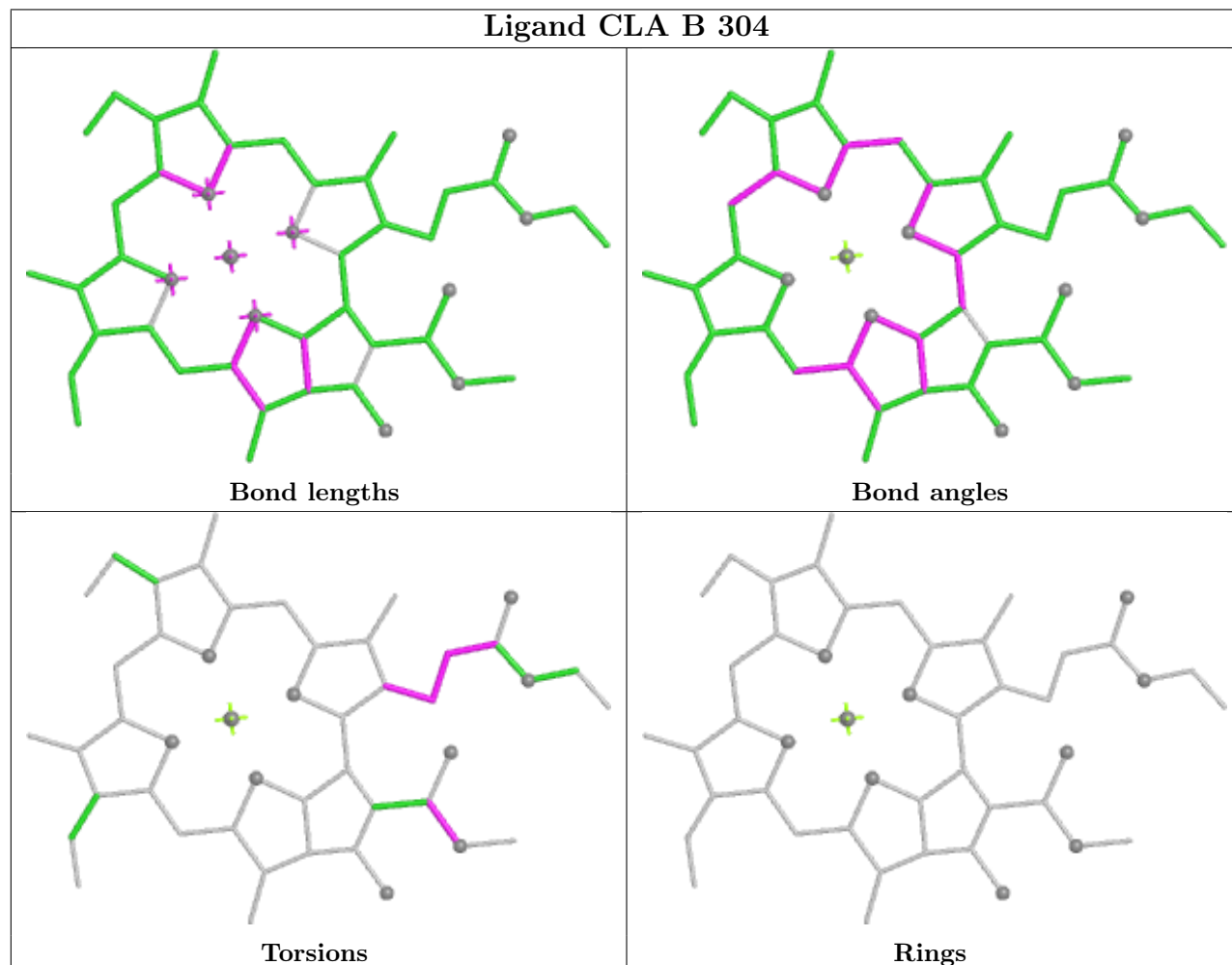


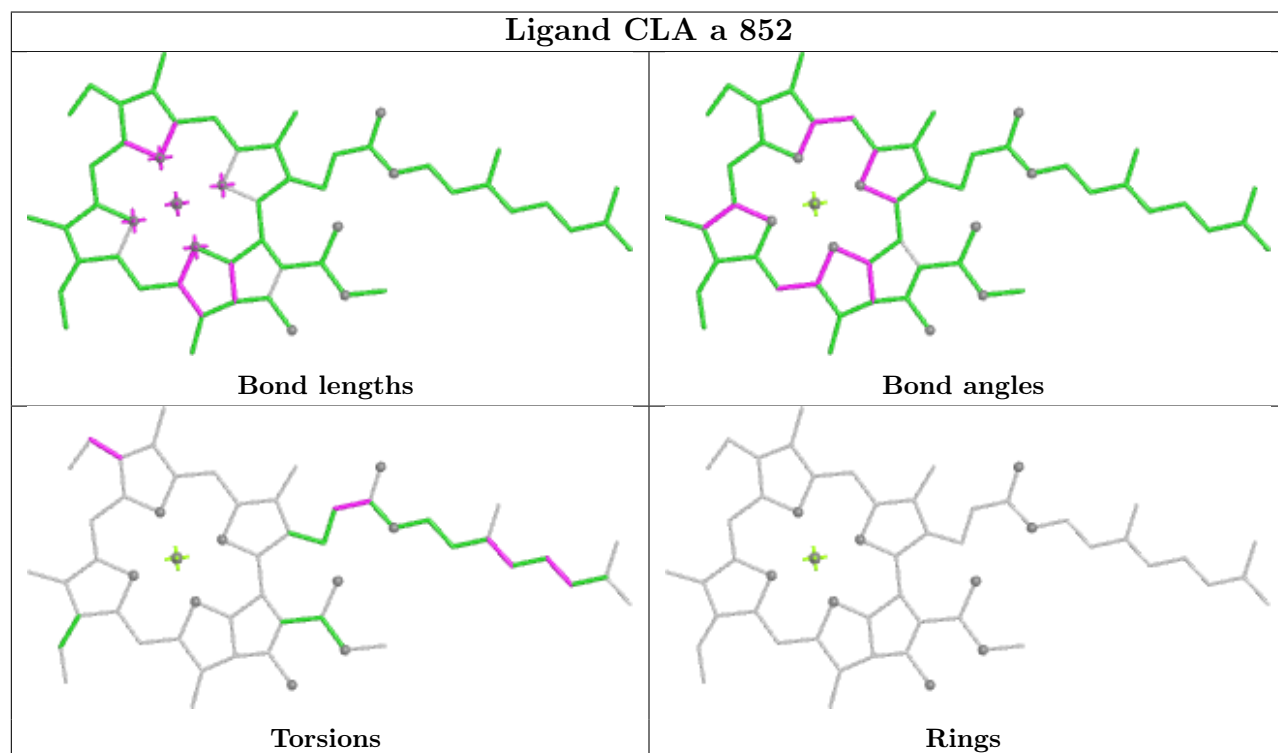
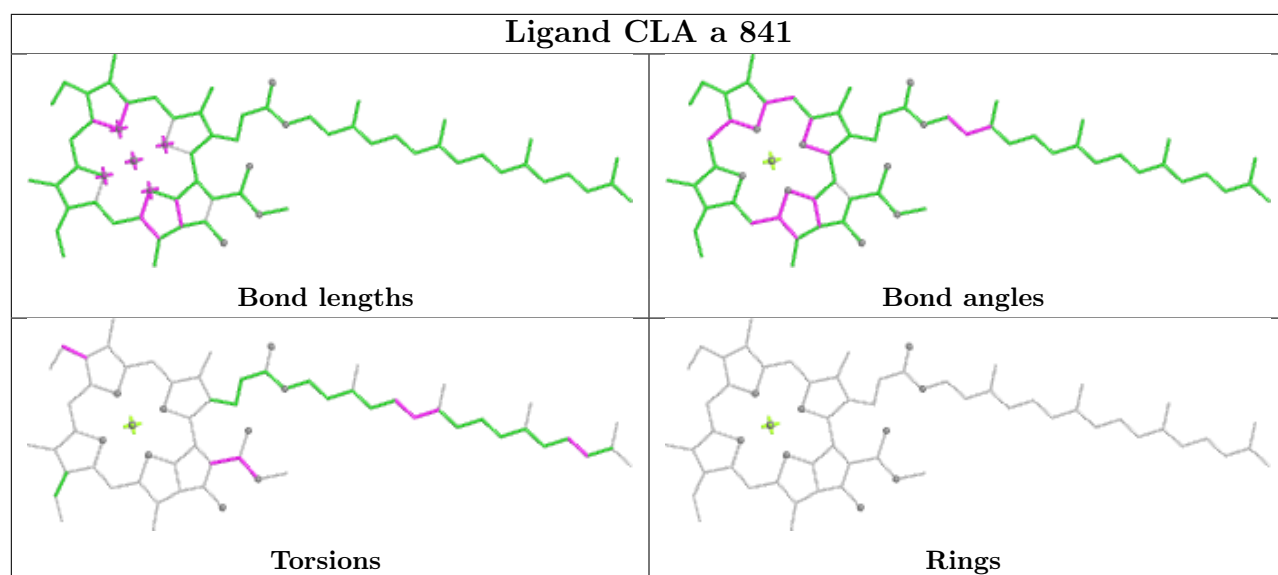
Rings

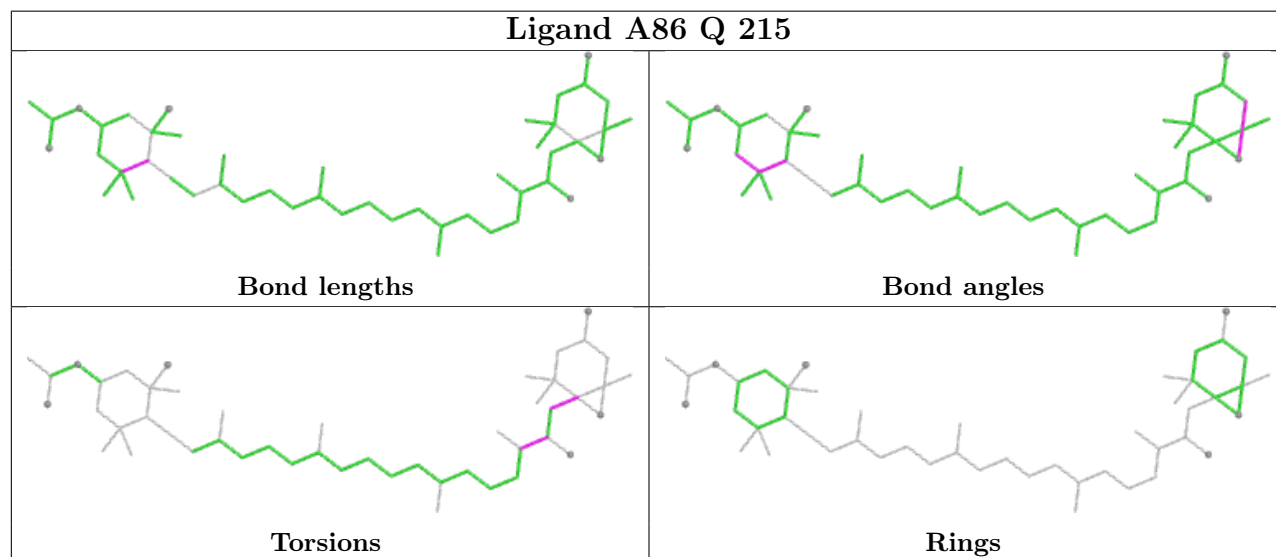
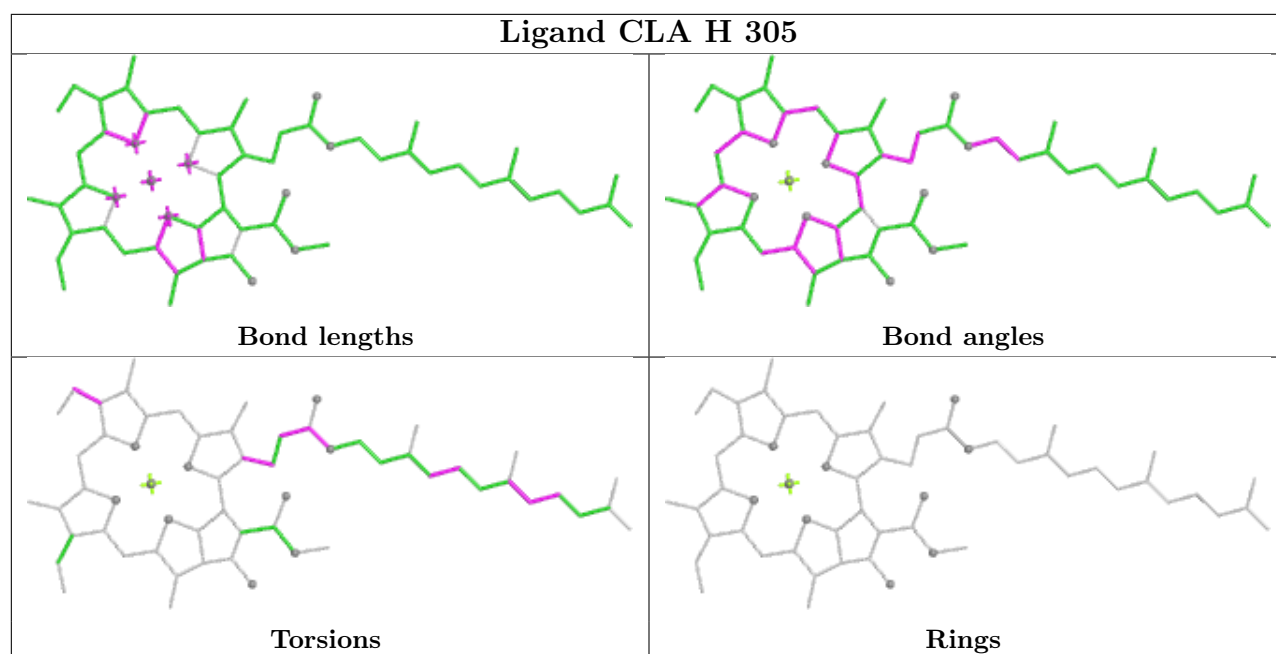
Ligand CLA u 313

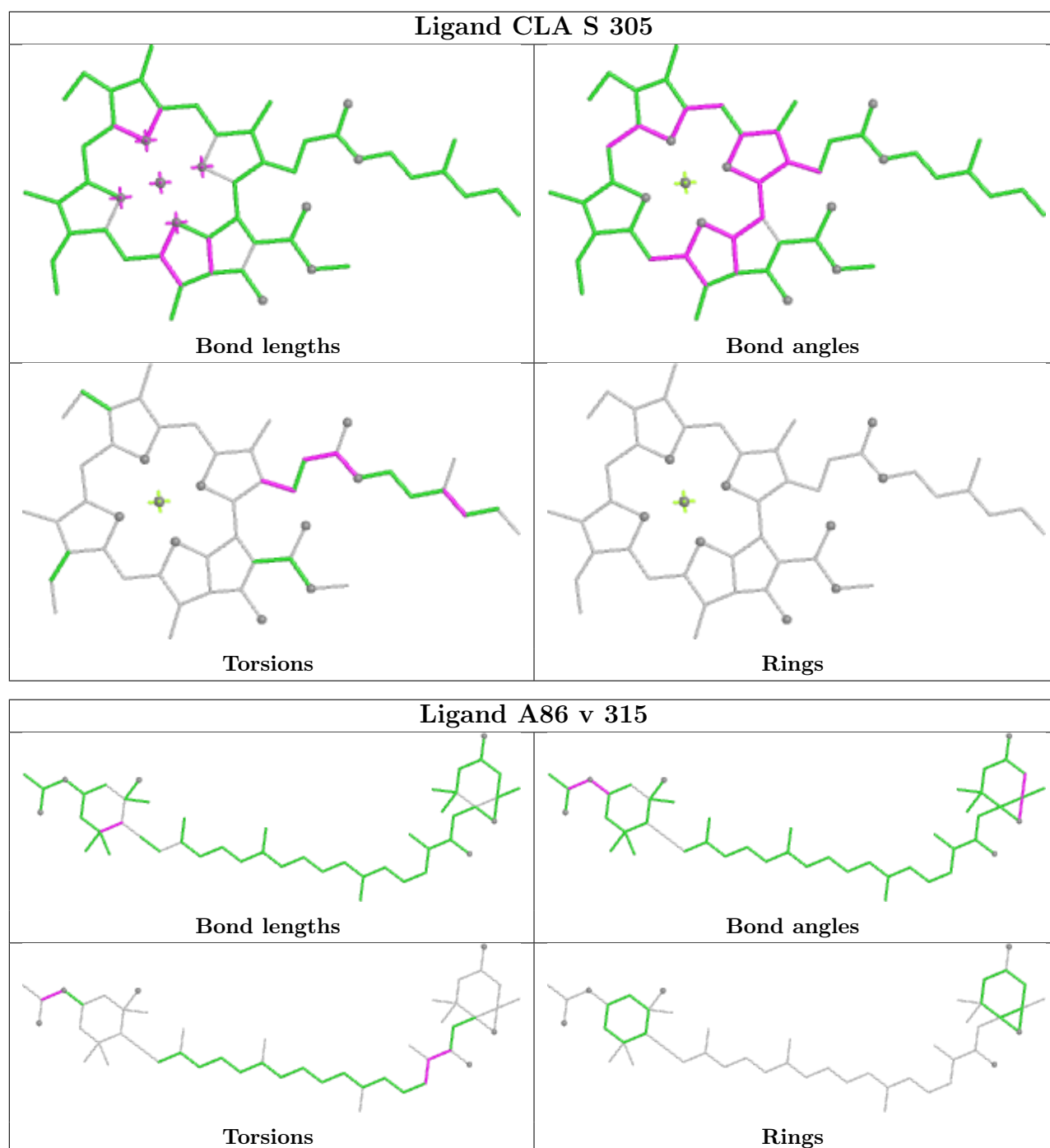


Ligand CLA B 304

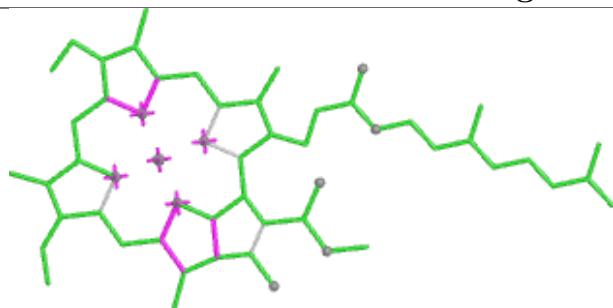




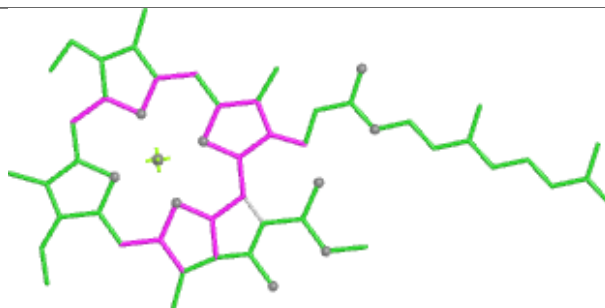




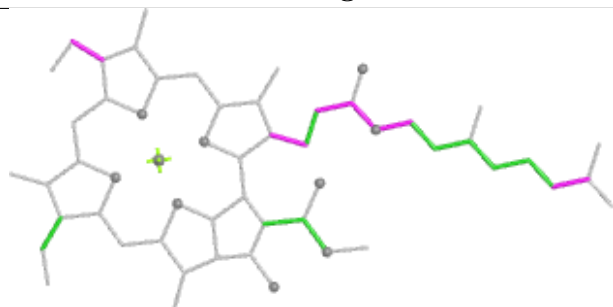
Ligand CLA Z 310



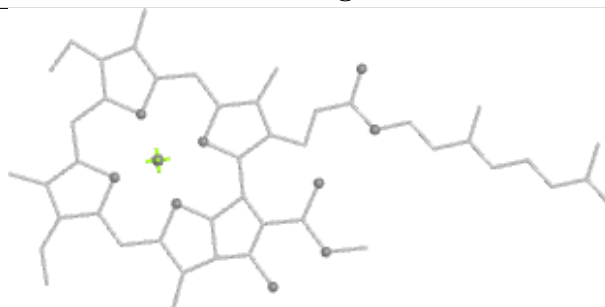
Bond lengths



Bond angles

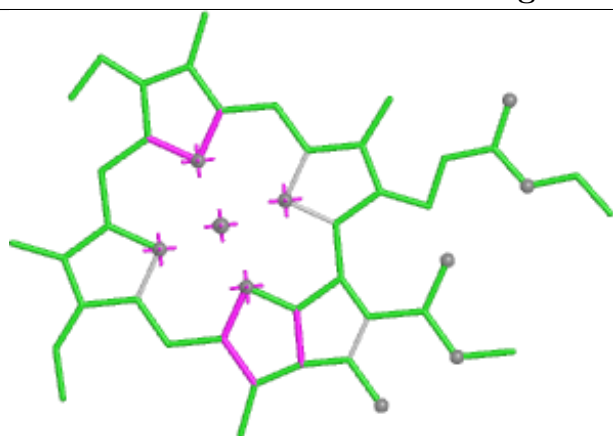


Torsions

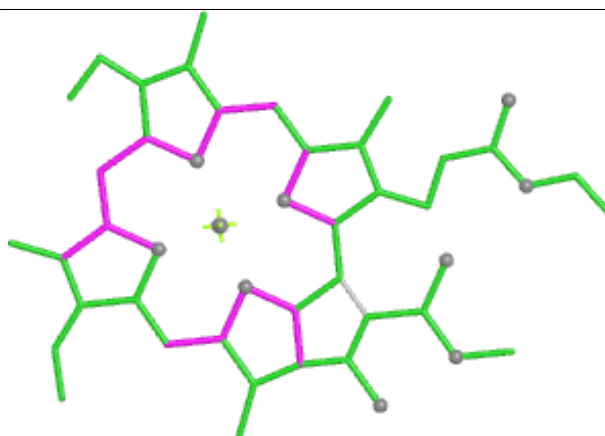


Rings

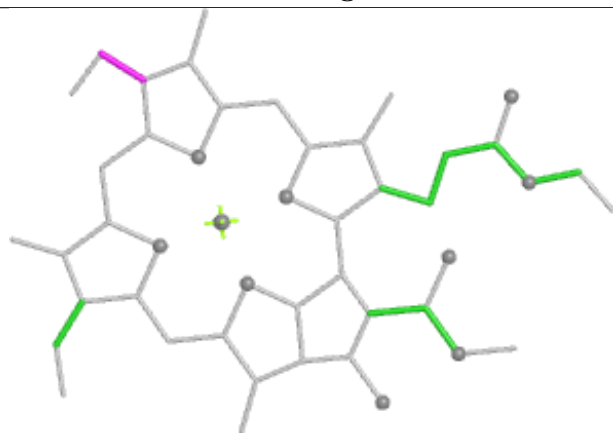
Ligand CLA J 309



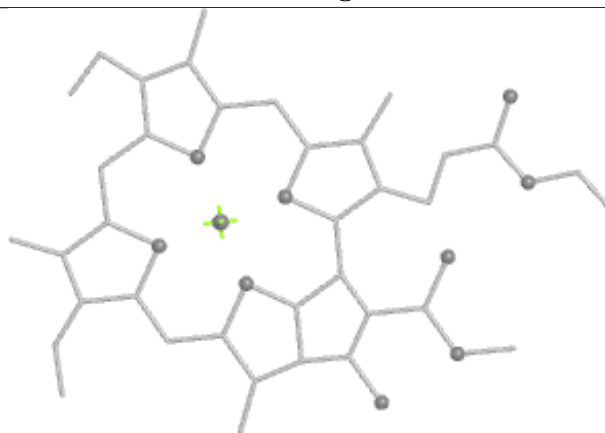
Bond lengths



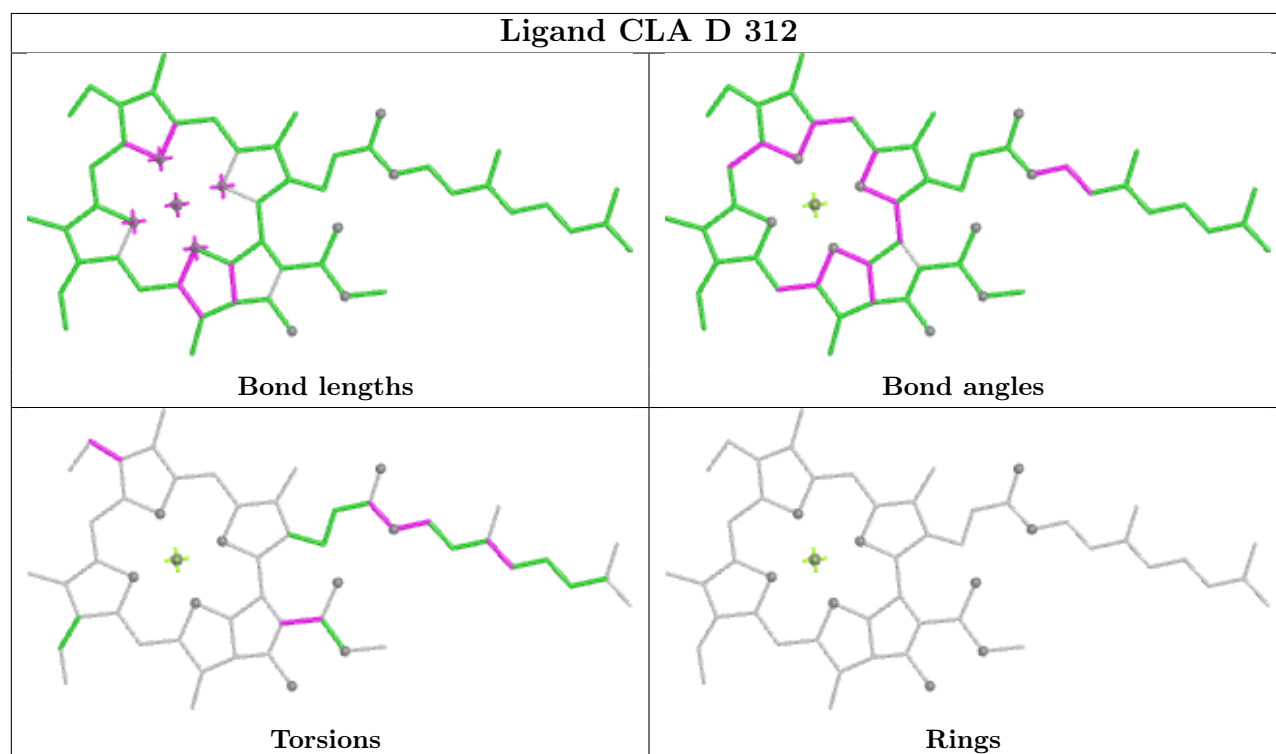
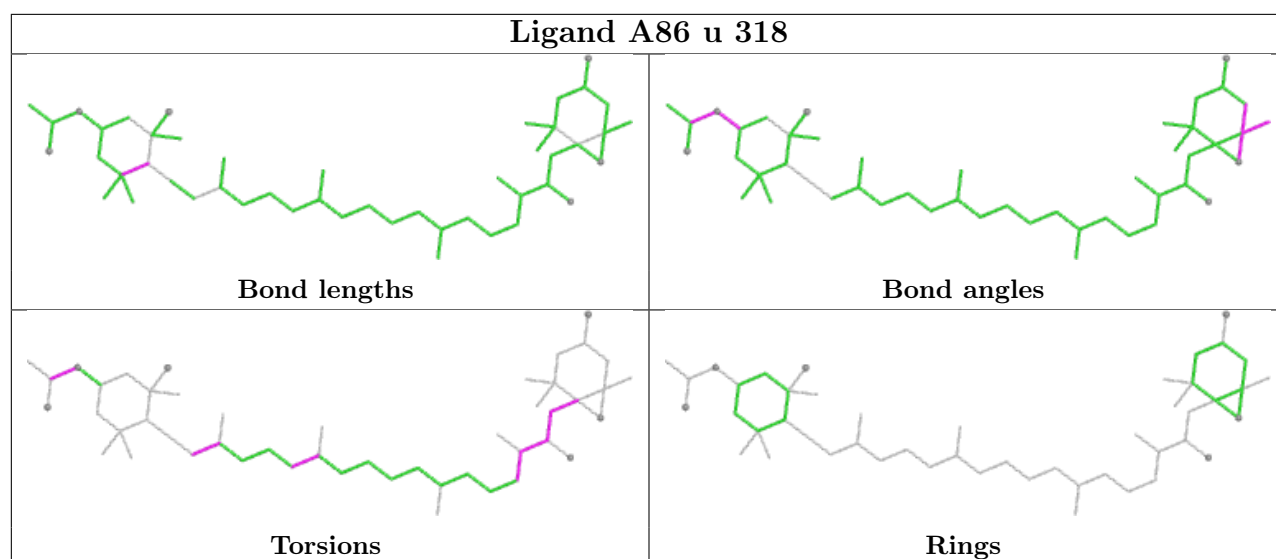
Bond angles

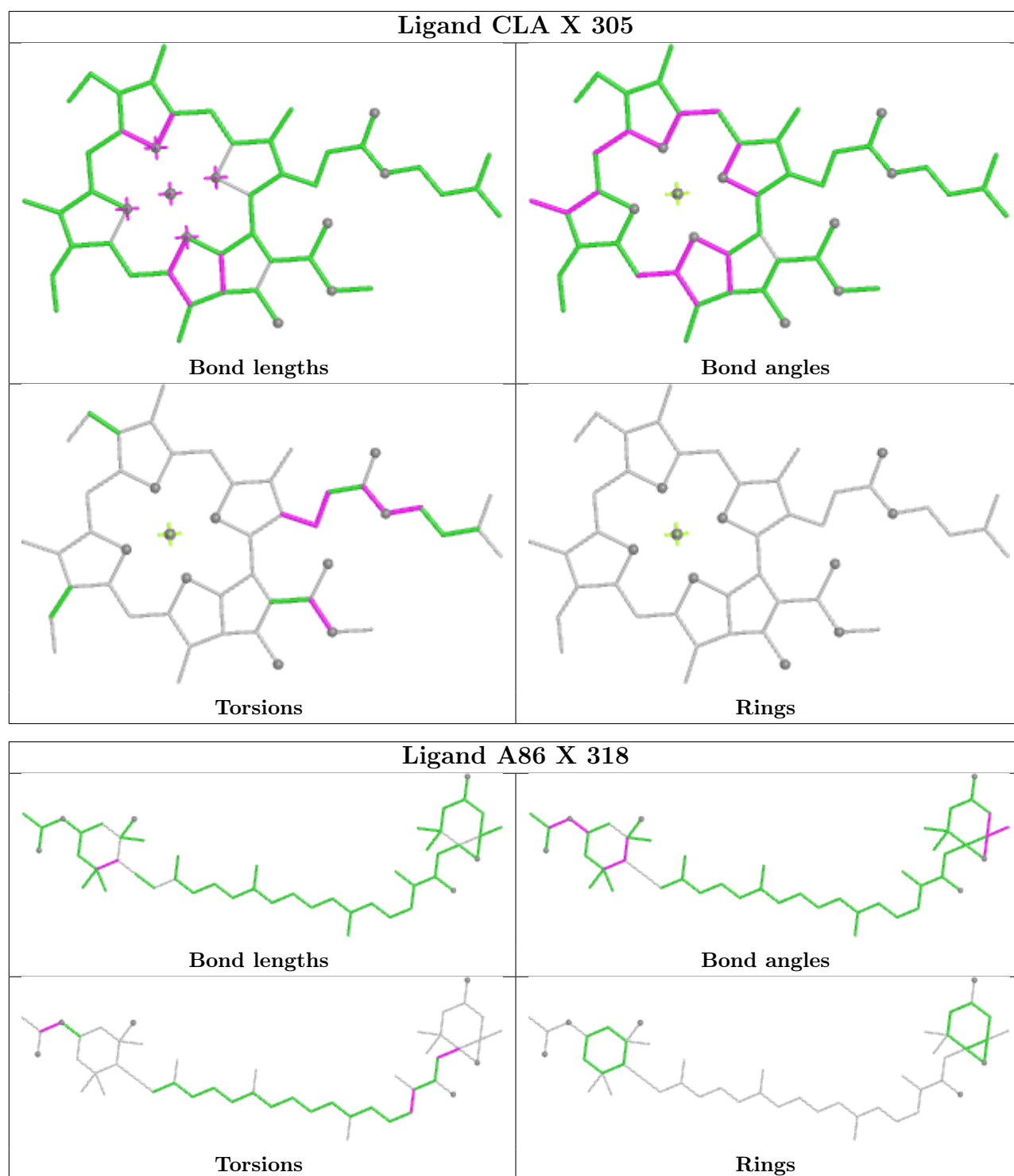


Torsions

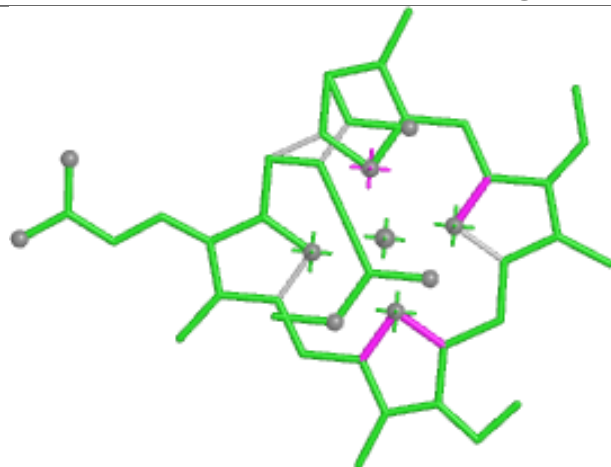


Rings

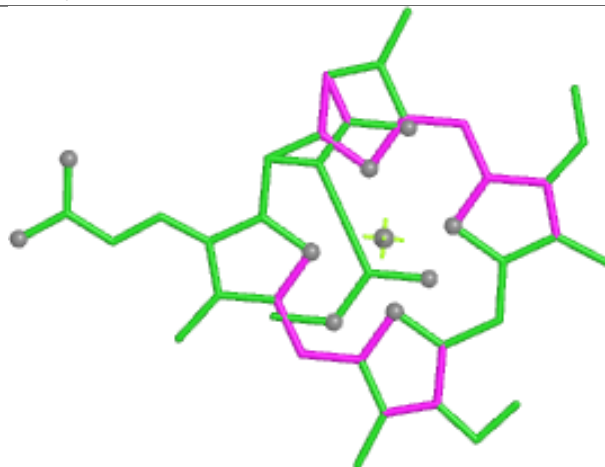




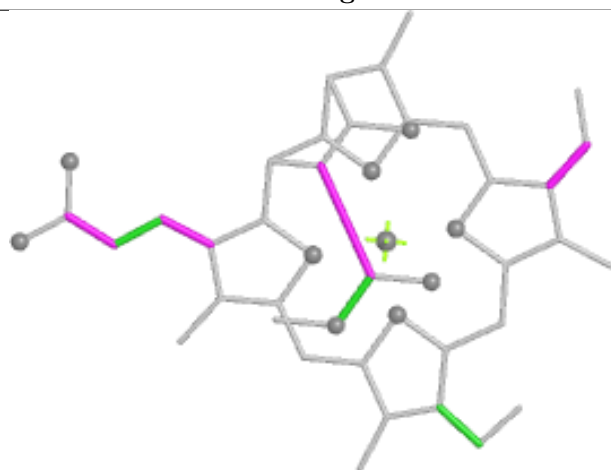
Ligand KC2 Q 216



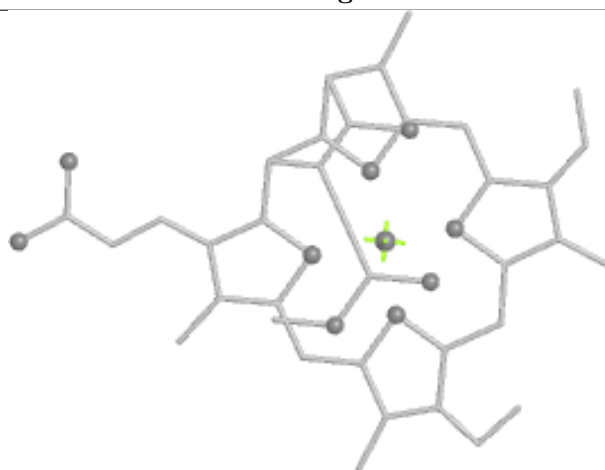
Bond lengths



Bond angles

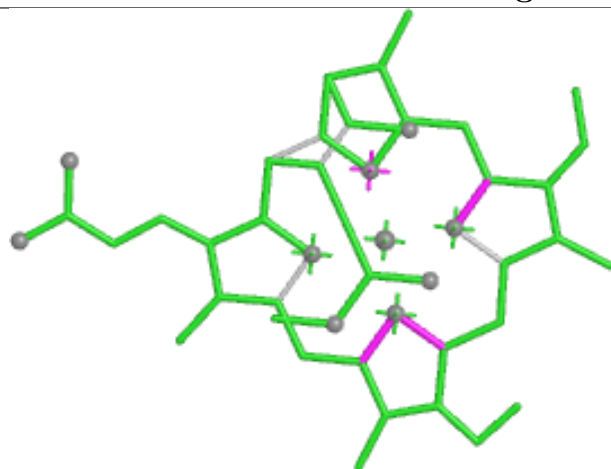


Torsions

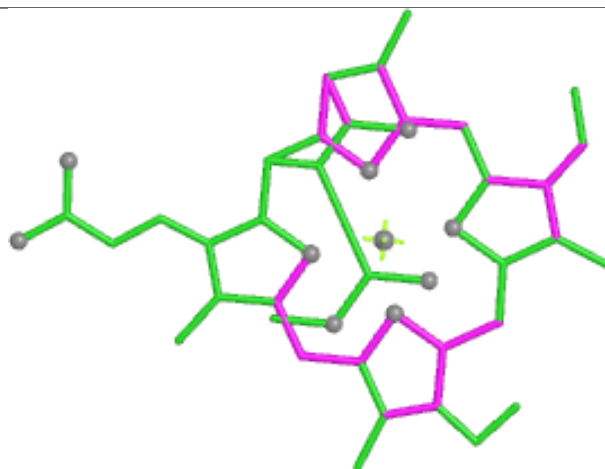


Rings

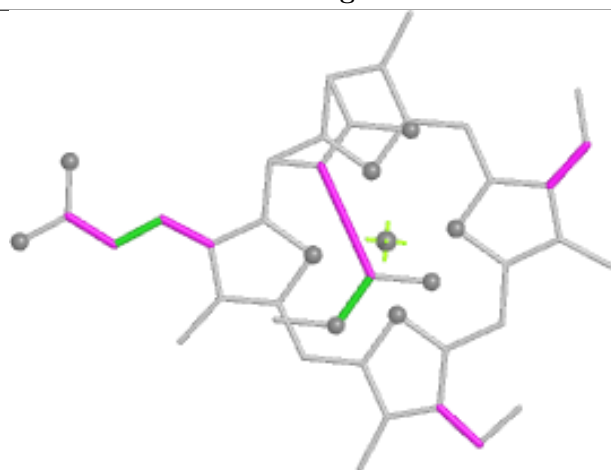
Ligand KC2 R 303



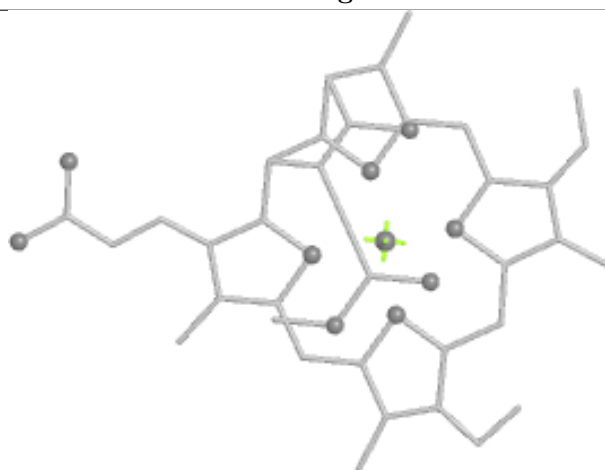
Bond lengths



Bond angles

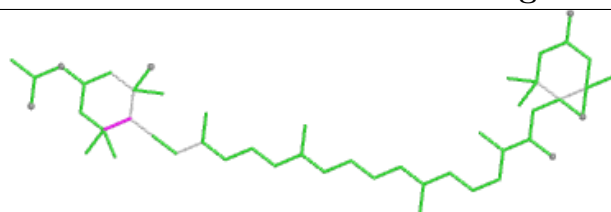


Torsions

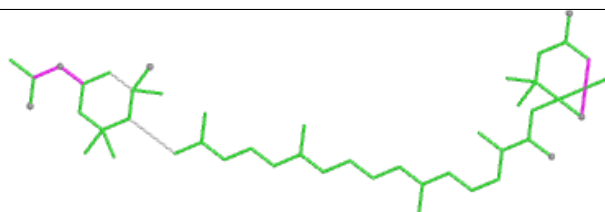


Rings

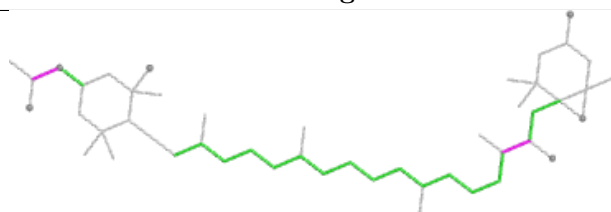
Ligand A86 X 316



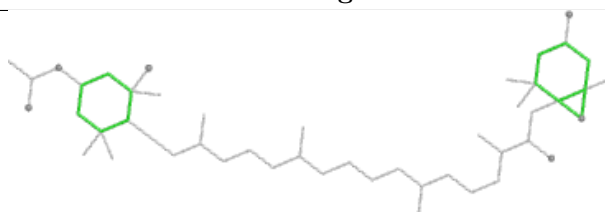
Bond lengths



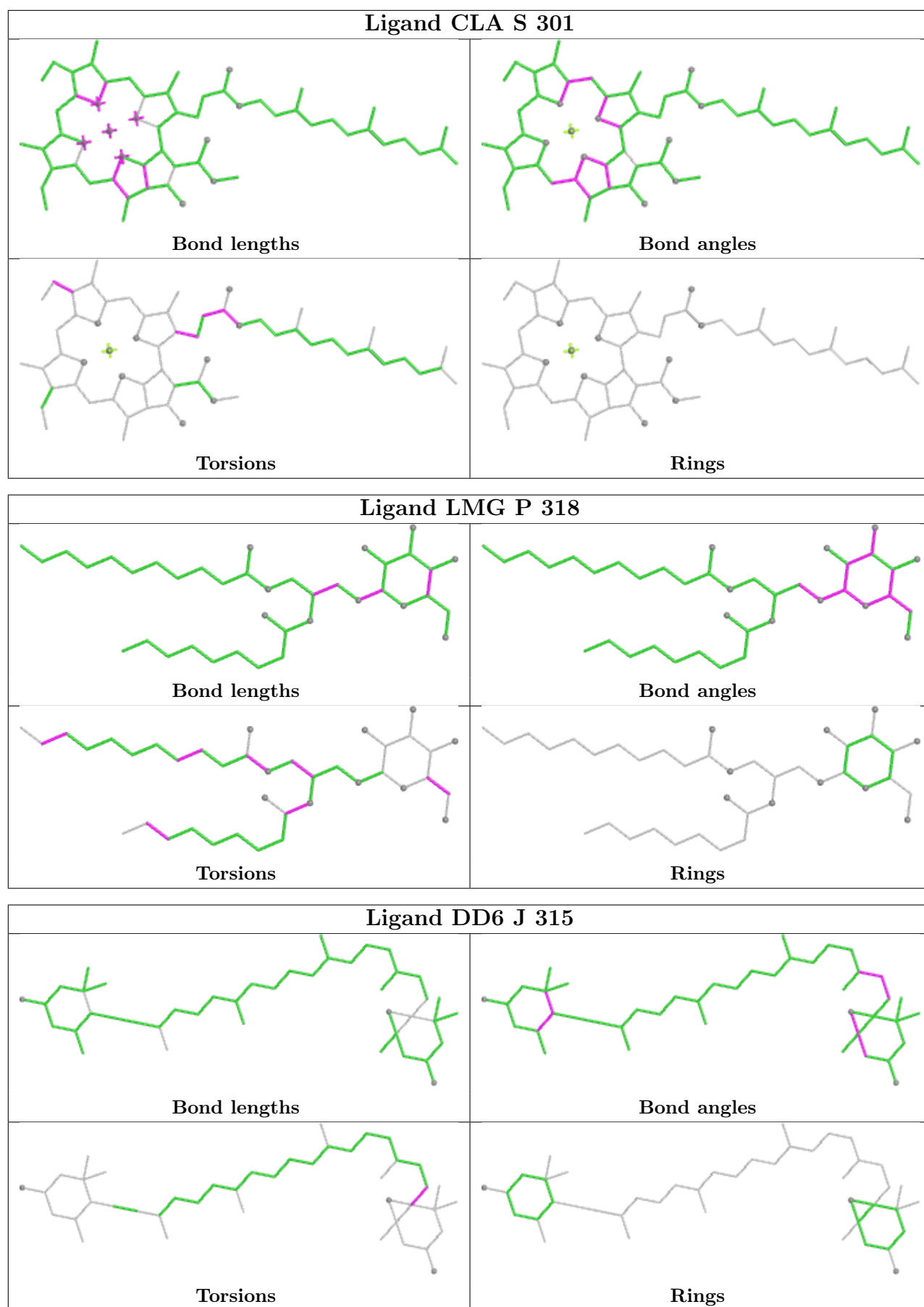
Bond angles



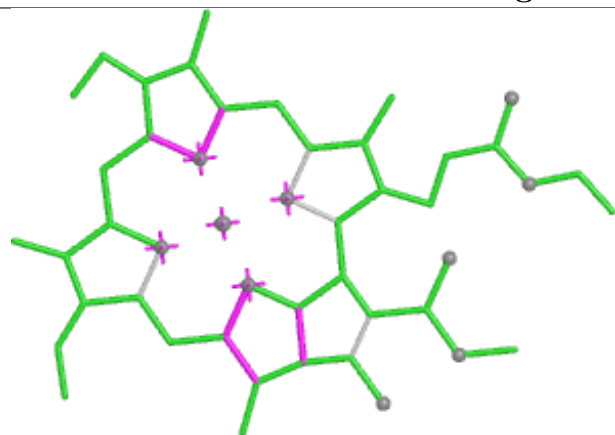
Torsions



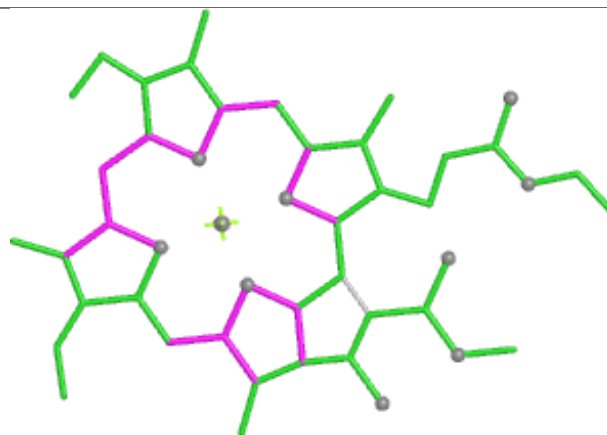
Rings



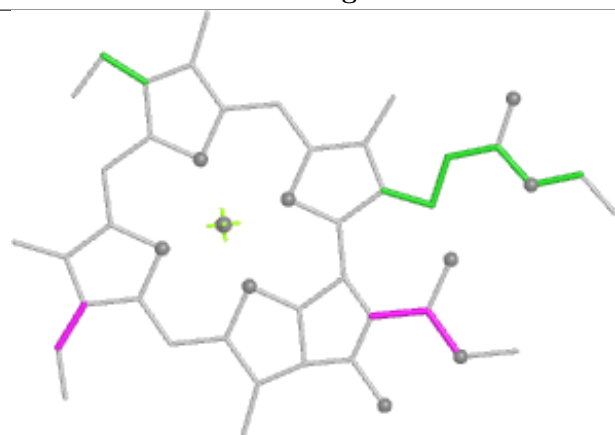
Ligand CLA H 301



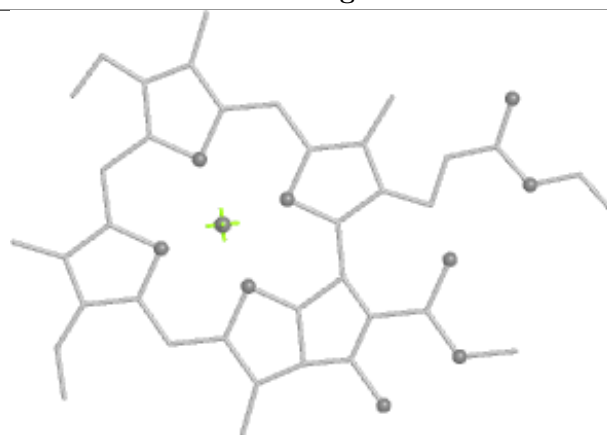
Bond lengths



Bond angles

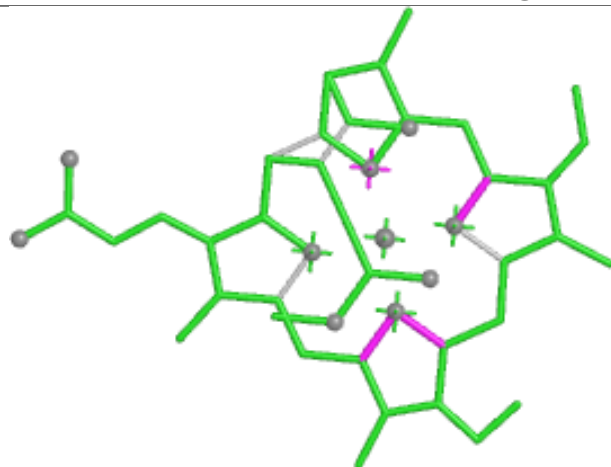


Torsions

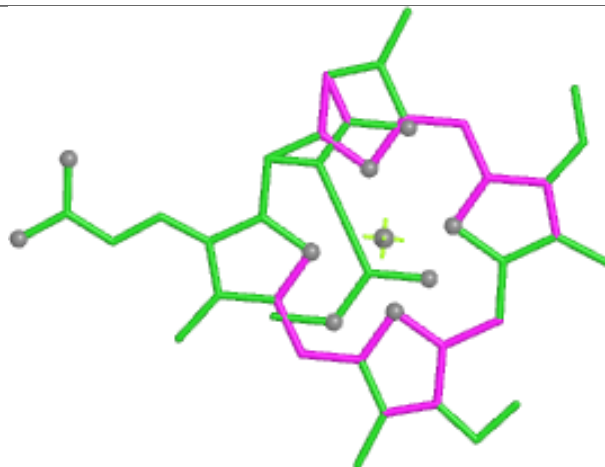


Rings

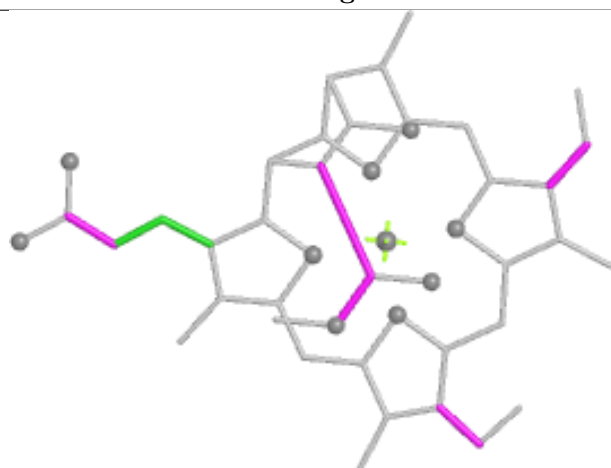
Ligand KC2 w 306



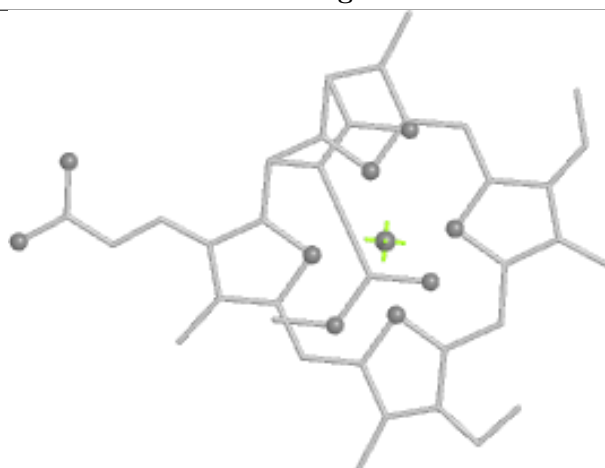
Bond lengths



Bond angles

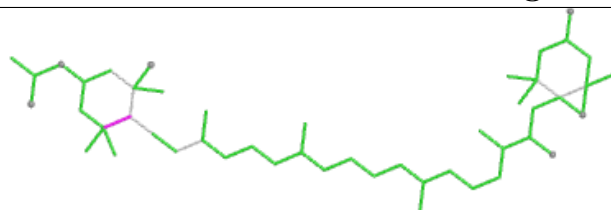


Torsions

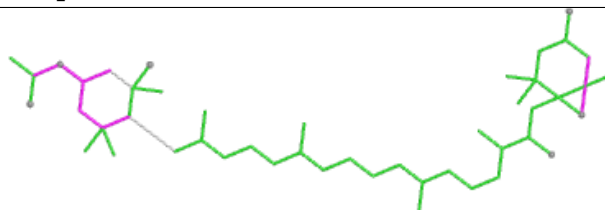


Rings

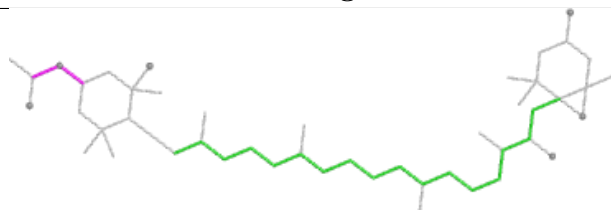
Ligand A86 q 314



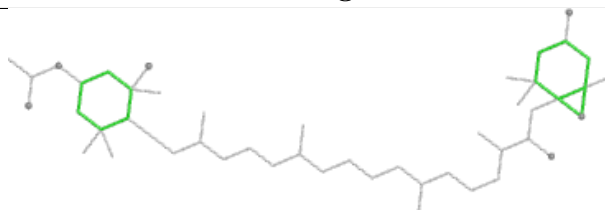
Bond lengths



Bond angles

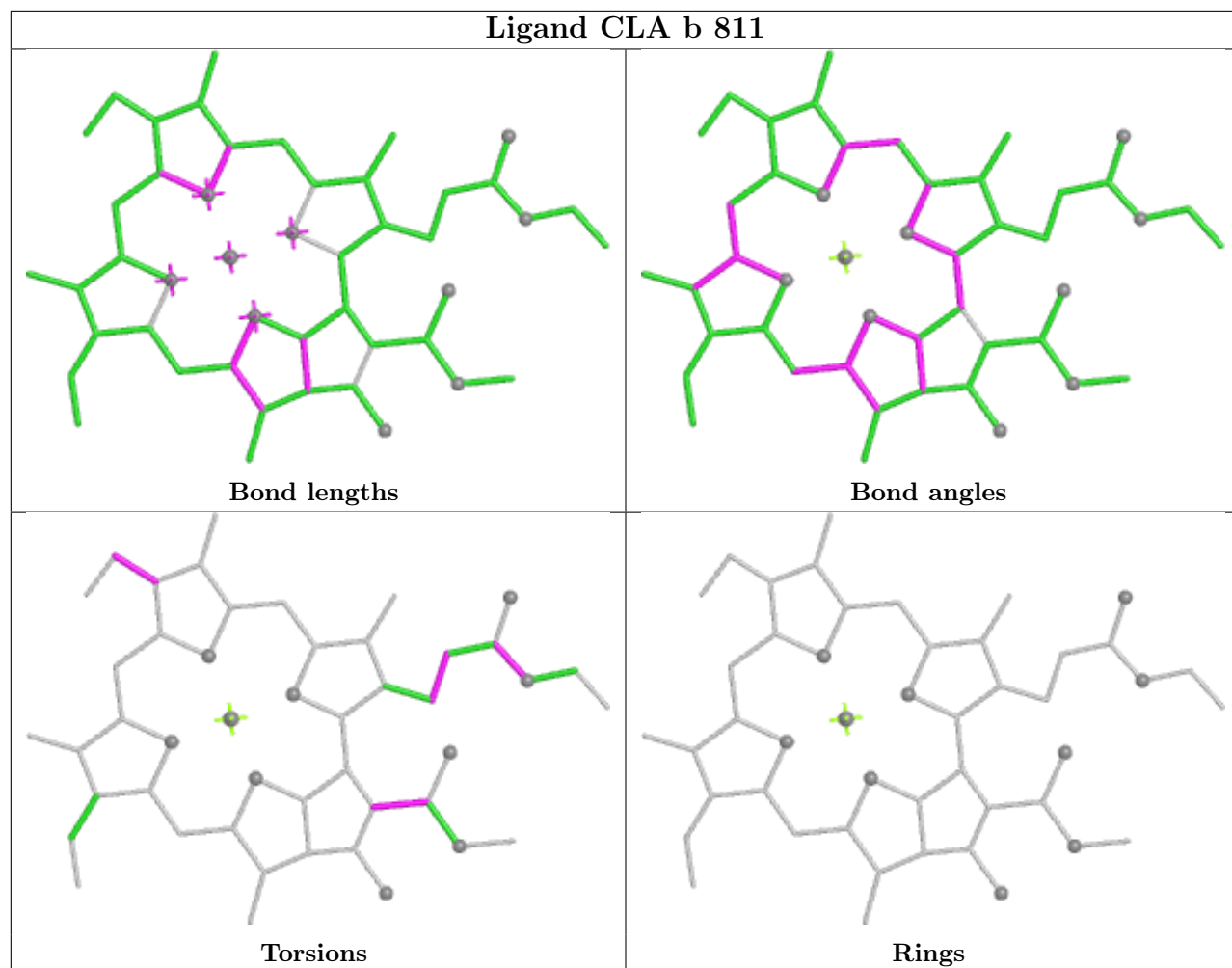


Torsions

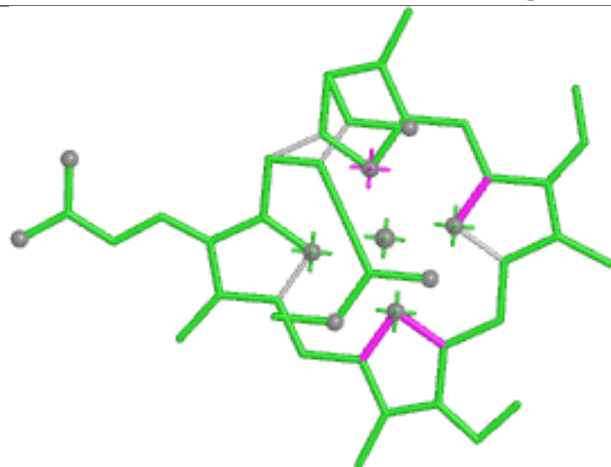


Rings

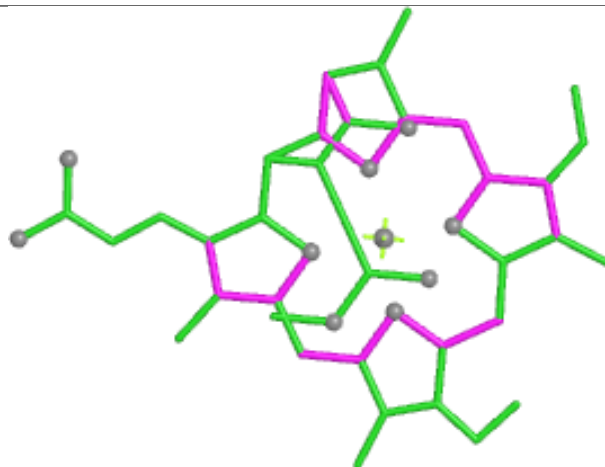
Ligand CLA b 811



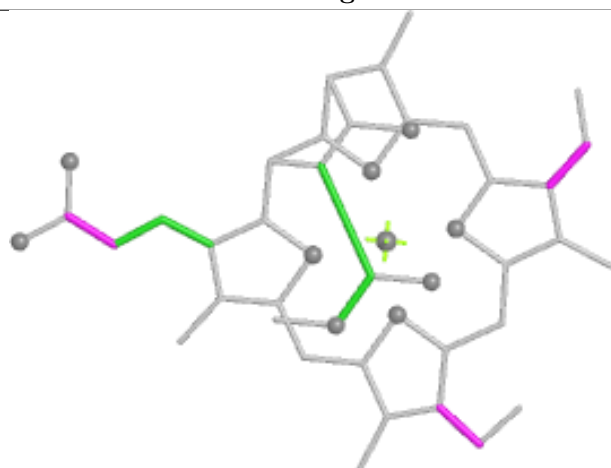
Ligand KC2 t 308



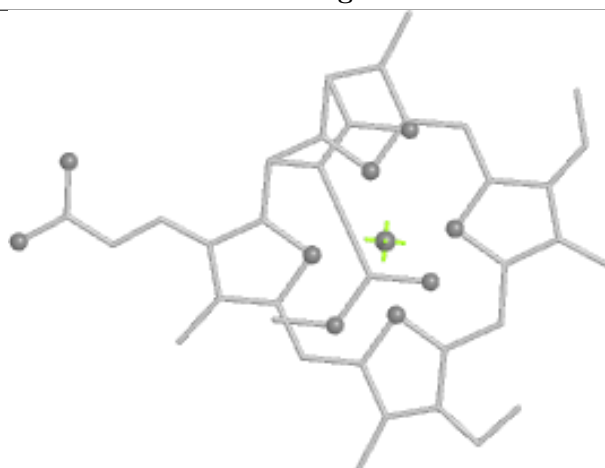
Bond lengths



Bond angles

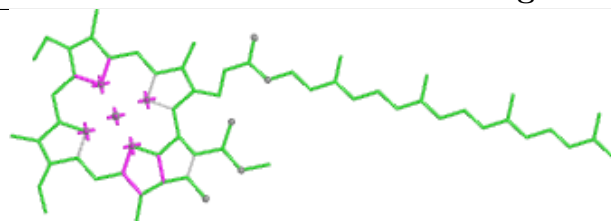


Torsions

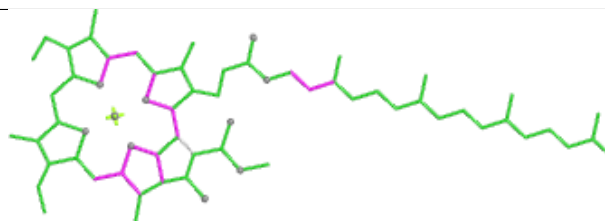


Rings

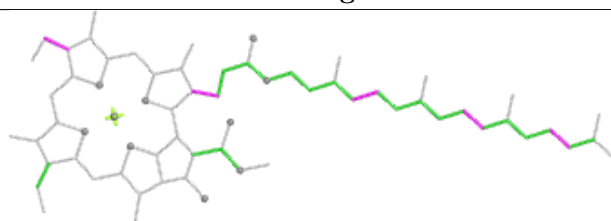
Ligand CLA u 302



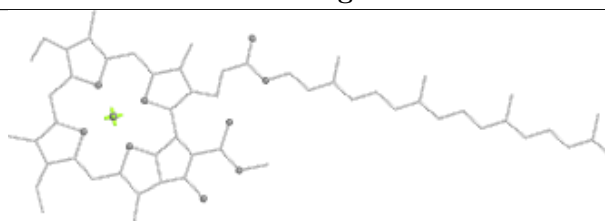
Bond lengths



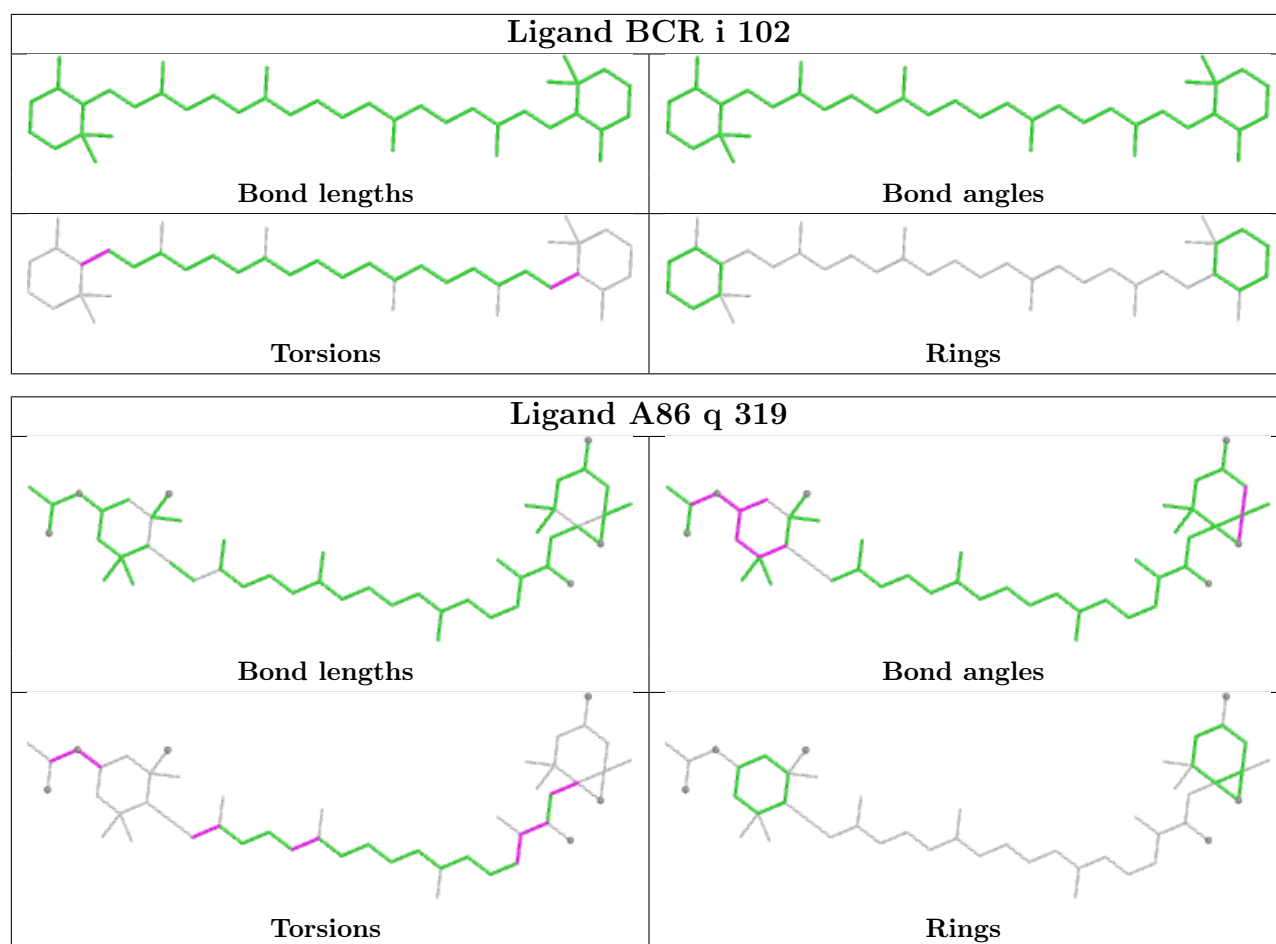
Bond angles



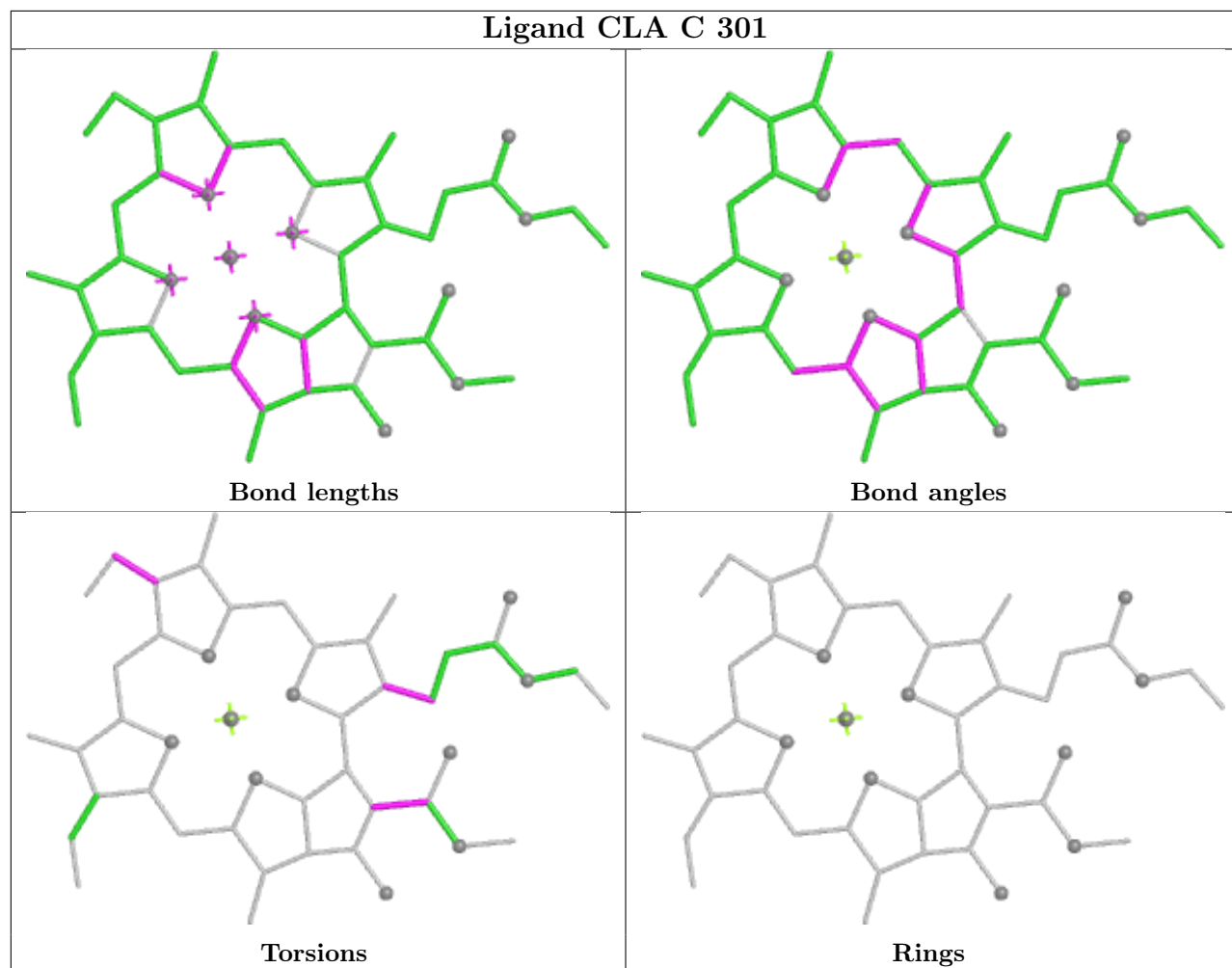
Torsions



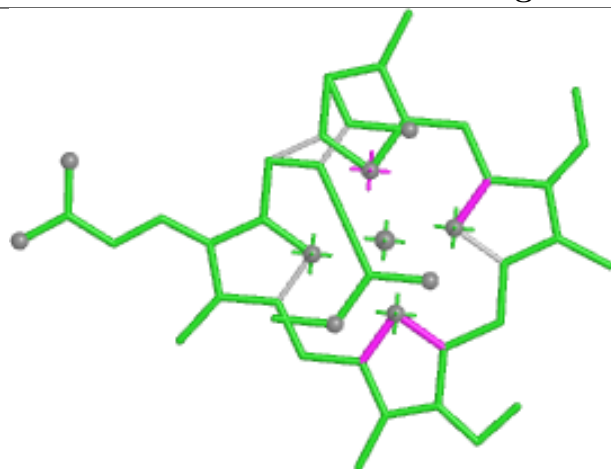
Rings



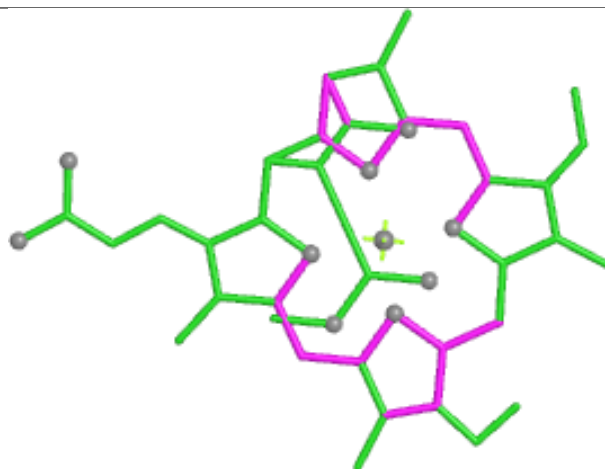
Ligand CLA C 301



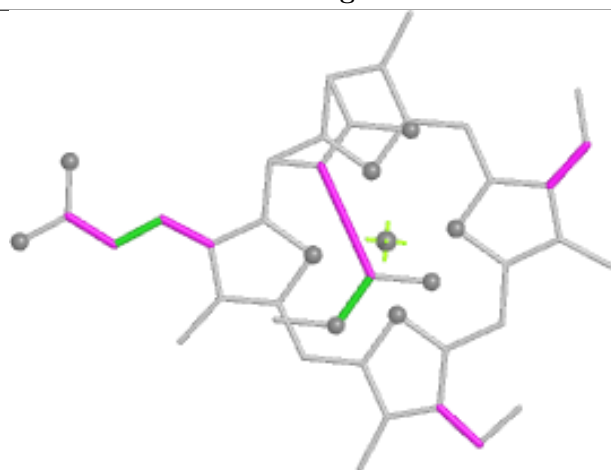
Ligand KC2 K 303



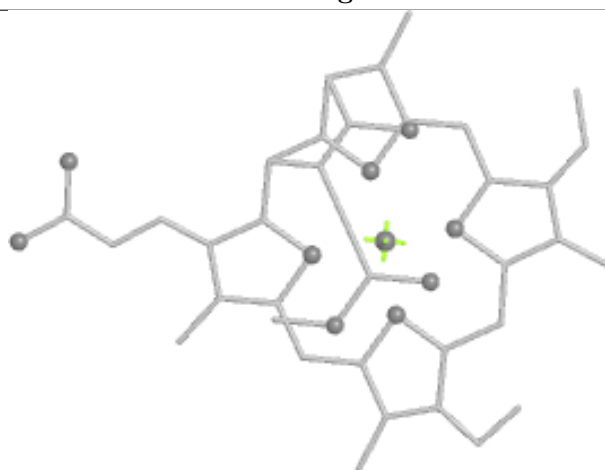
Bond lengths



Bond angles

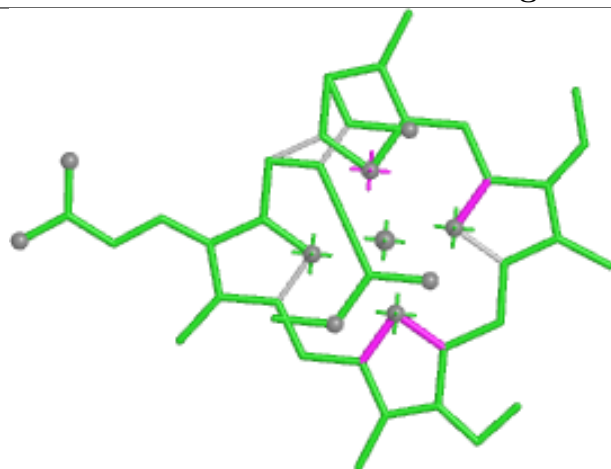


Torsions

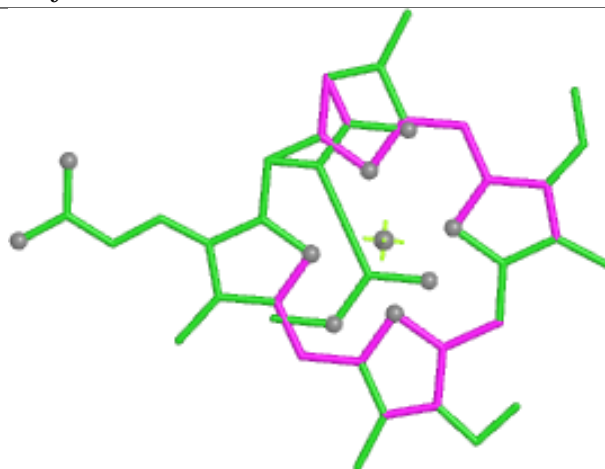


Rings

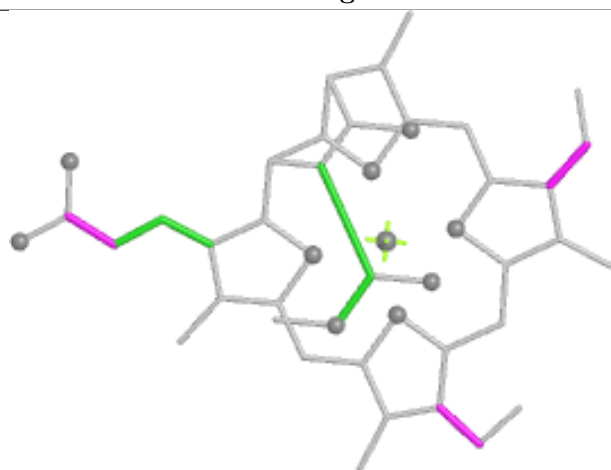
Ligand KC2 y 307



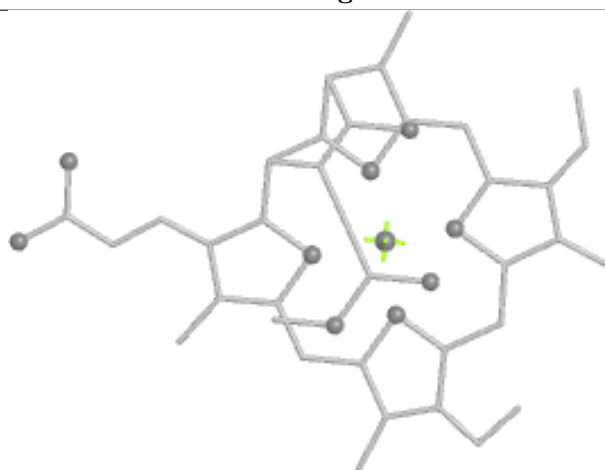
Bond lengths



Bond angles

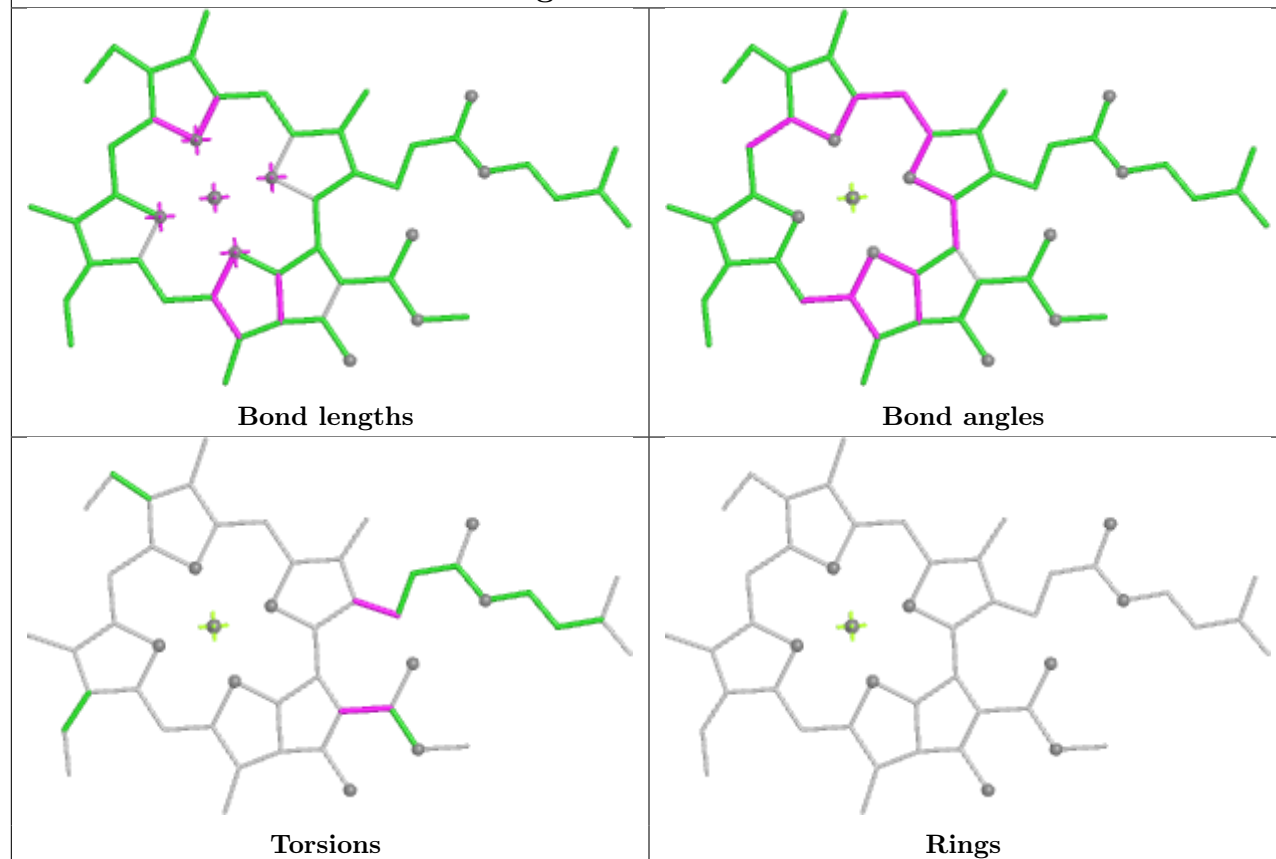


Torsions

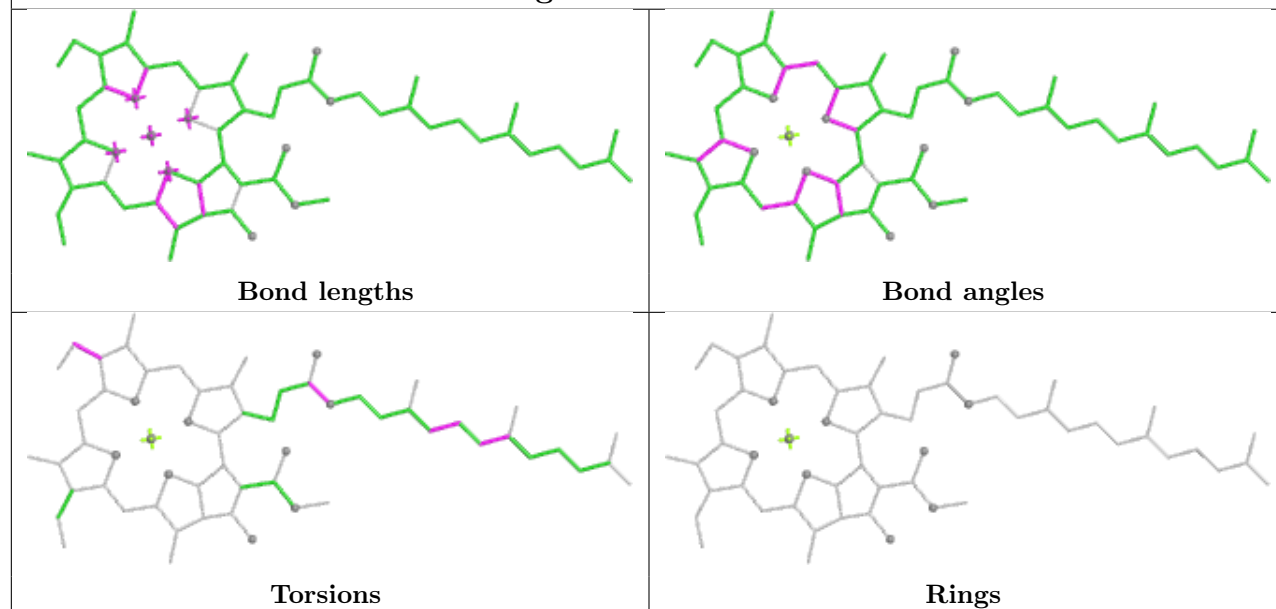


Rings

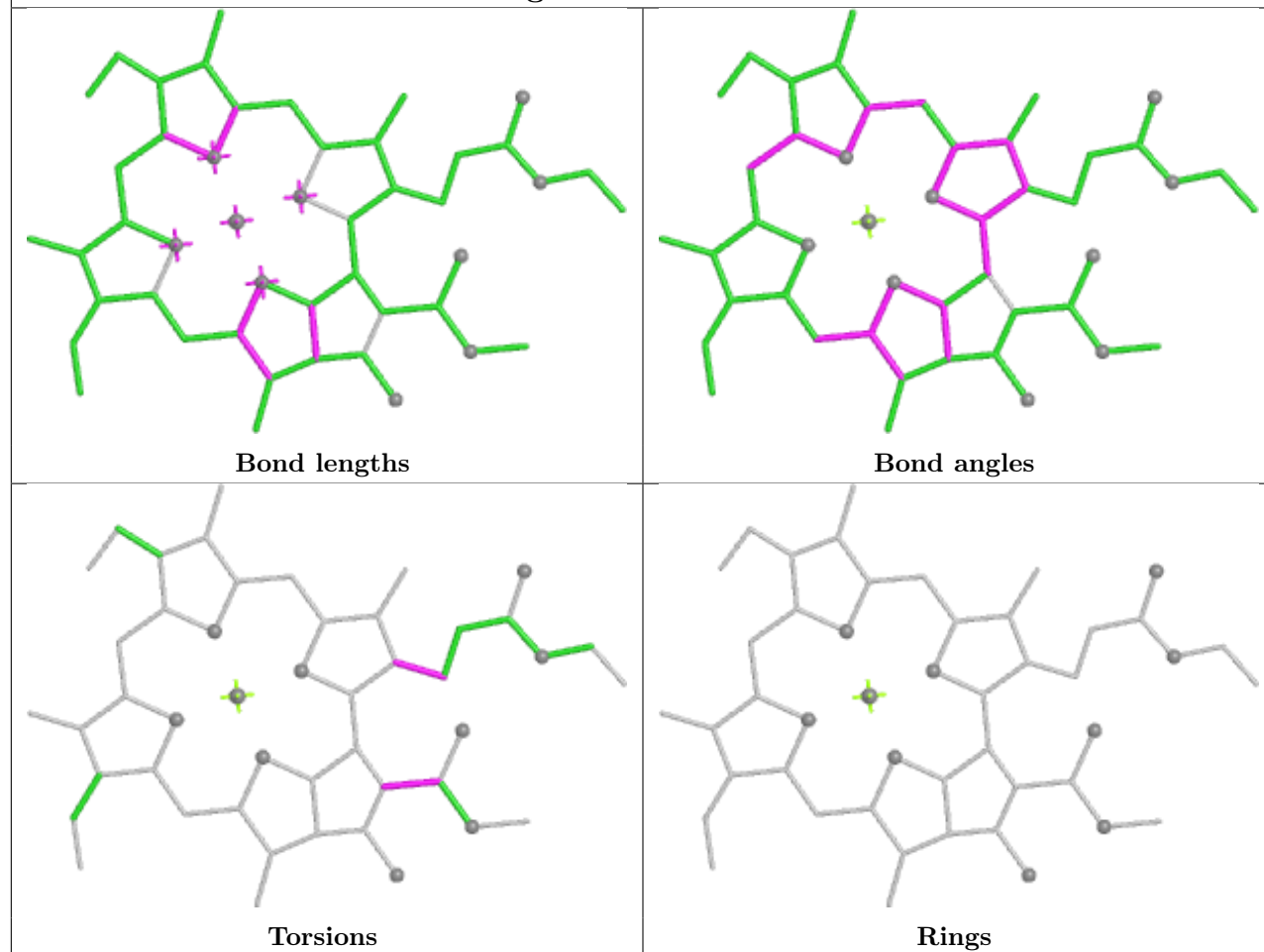
Ligand CLA a 809



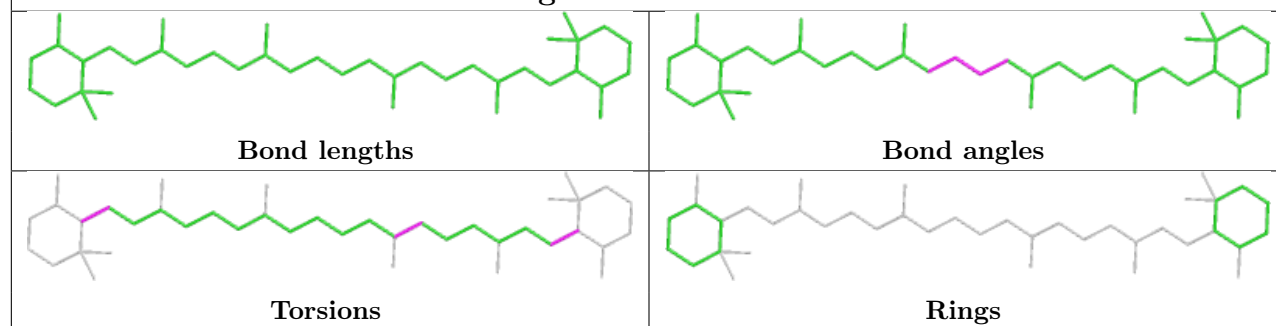
Ligand CLA v 312



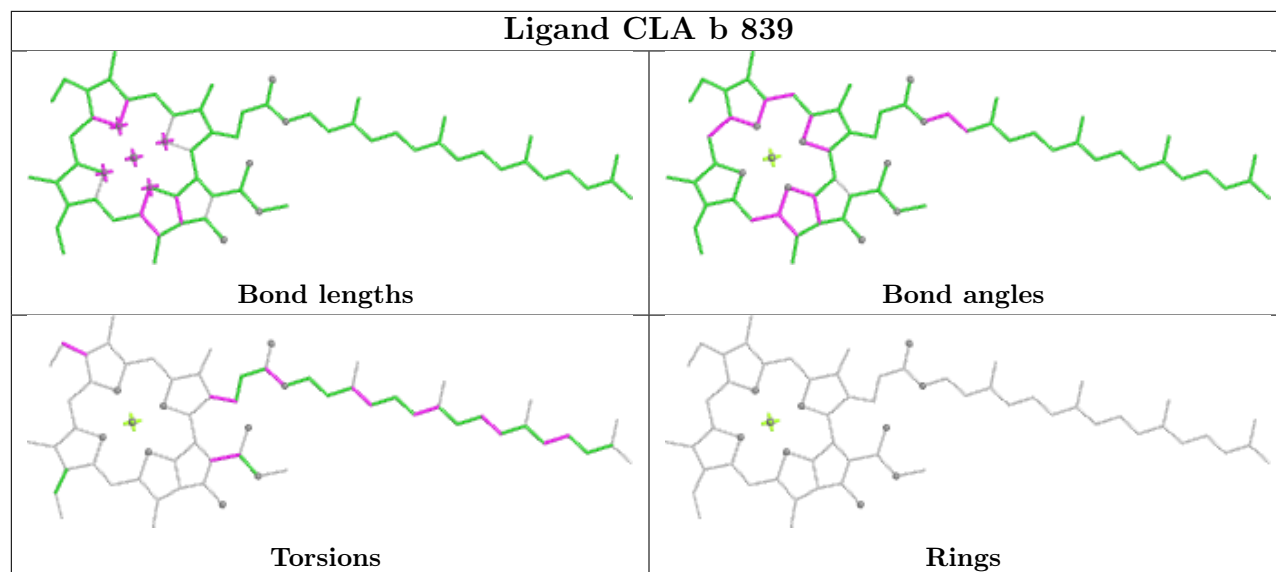
Ligand CLA Y 312



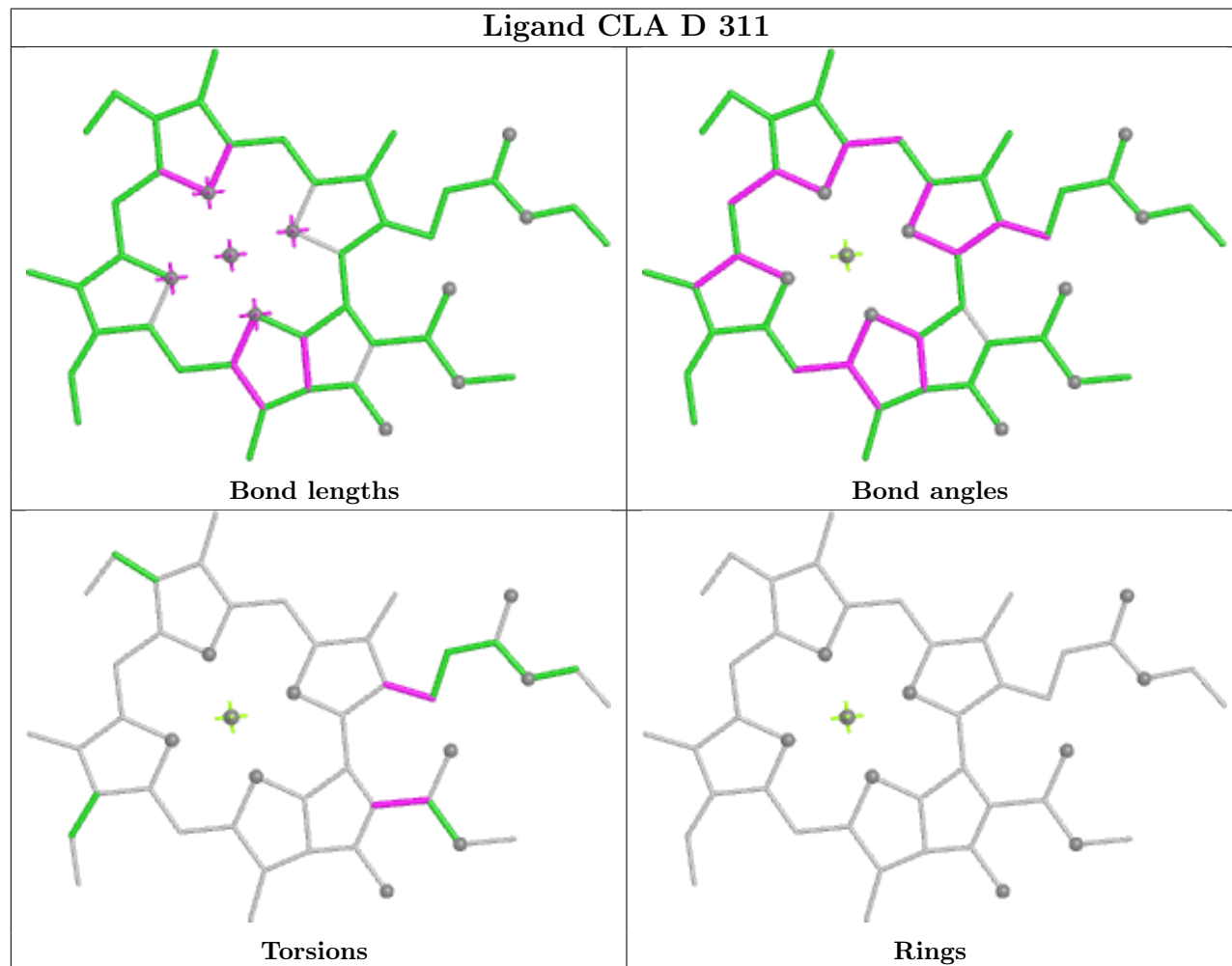
Ligand BCR 1 208



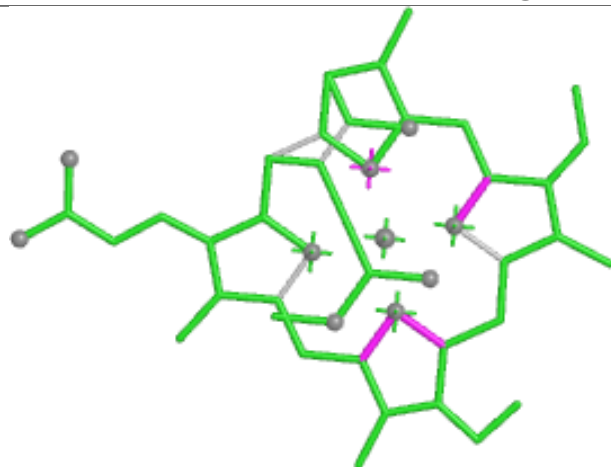
Ligand CLA b 839



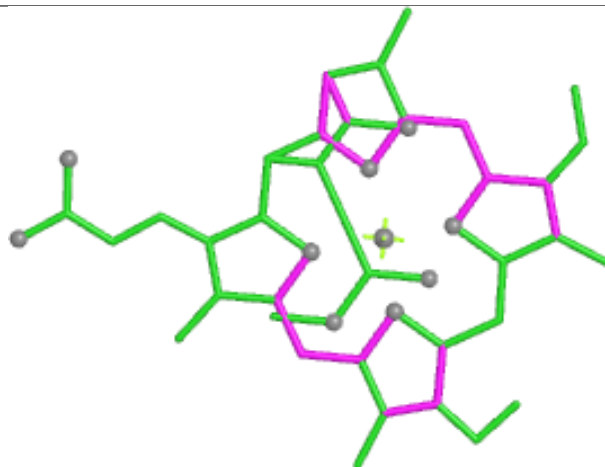
Ligand CLA D 311



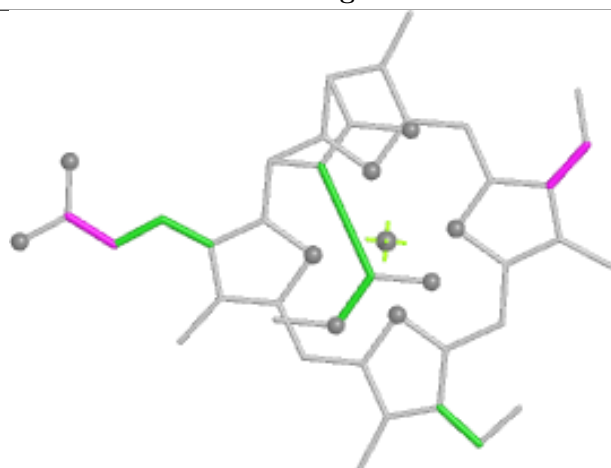
Ligand KC2 P 309



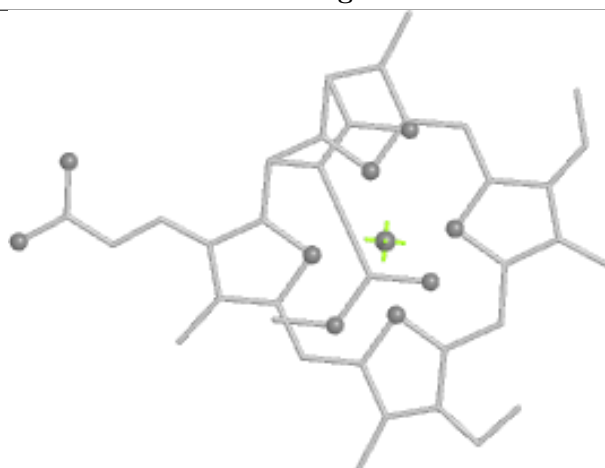
Bond lengths



Bond angles

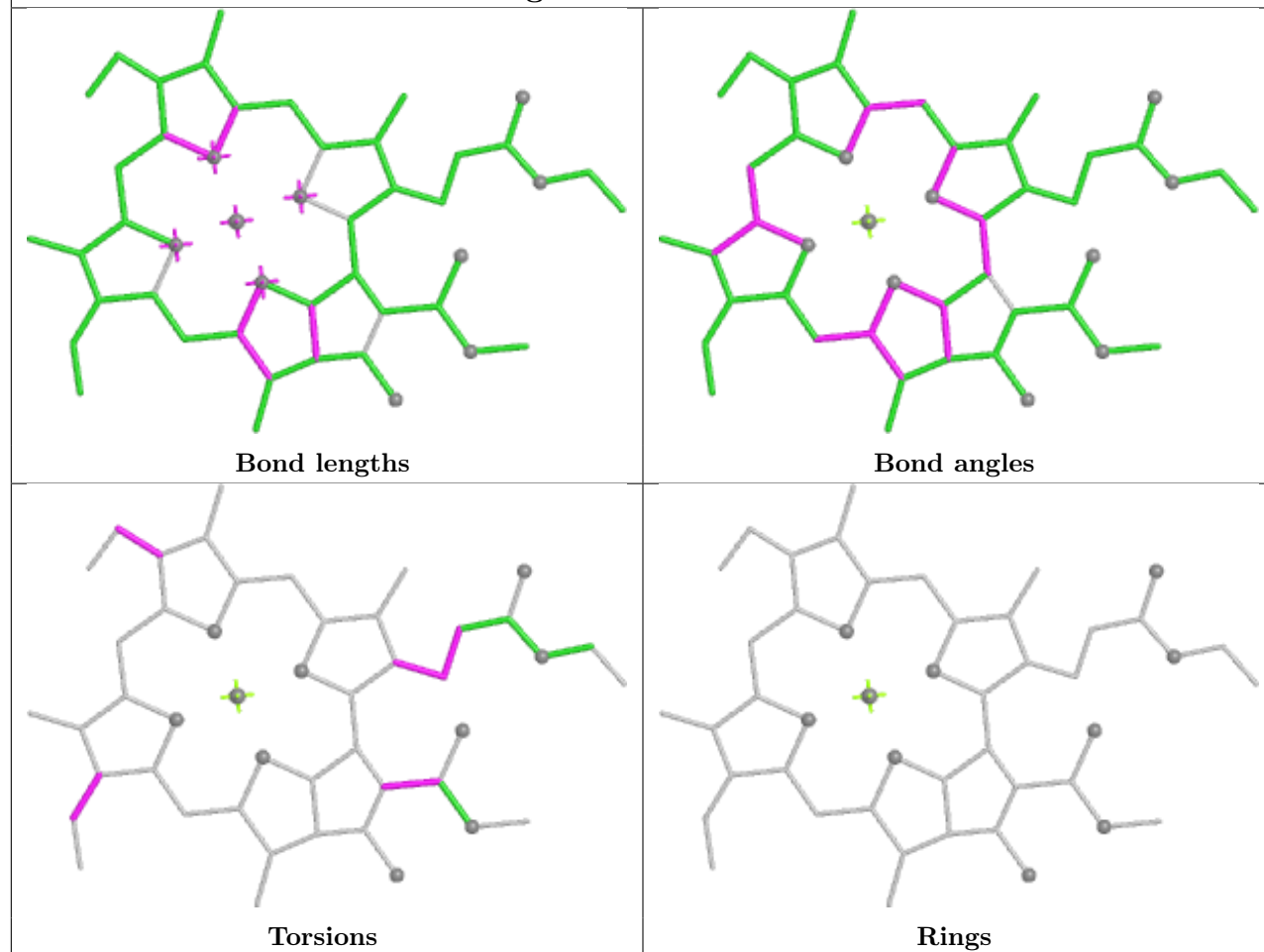


Torsions

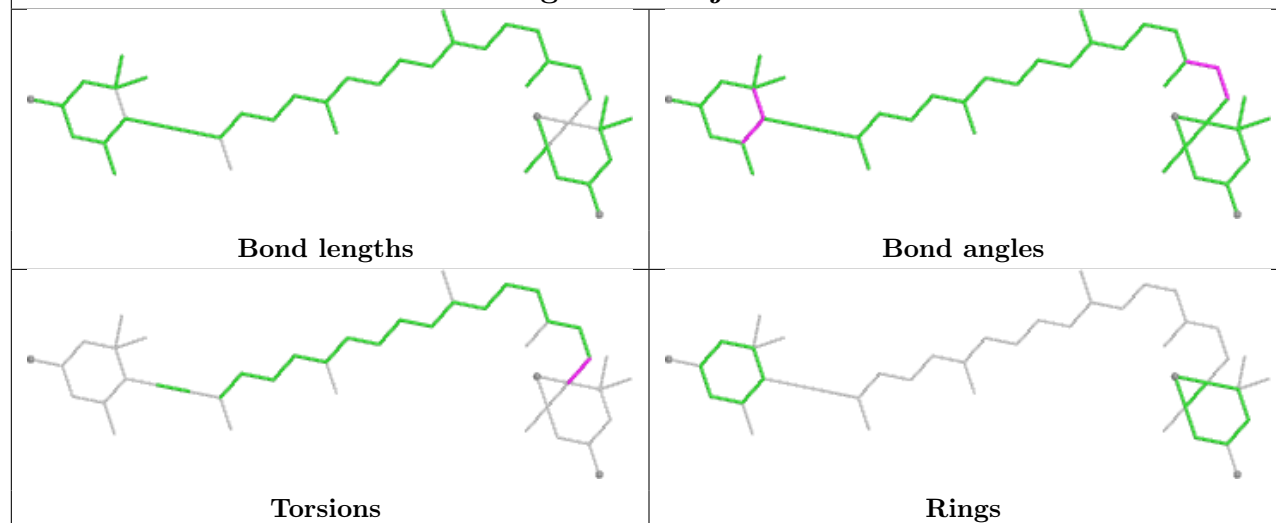


Rings

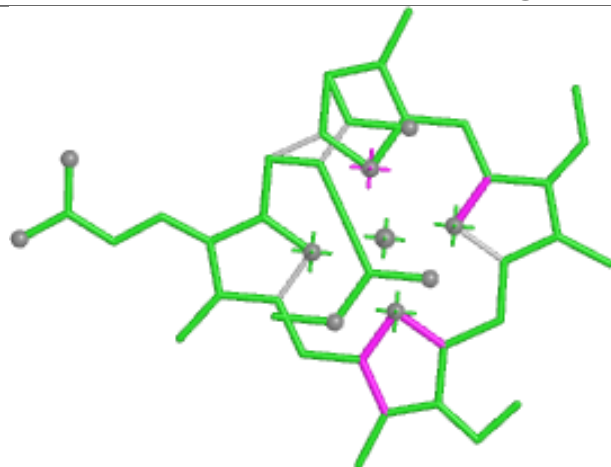
Ligand CLA G 213



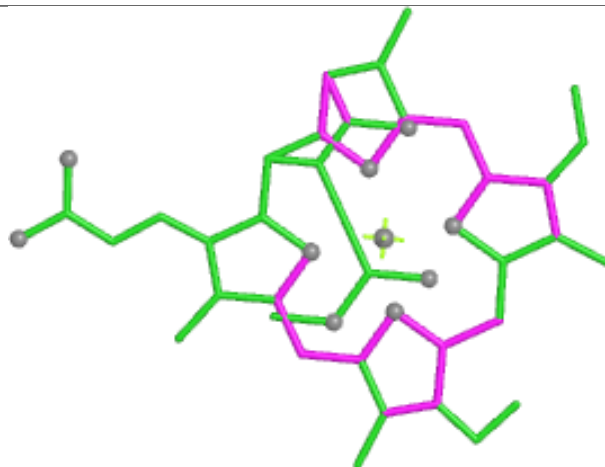
Ligand DD6 j 104



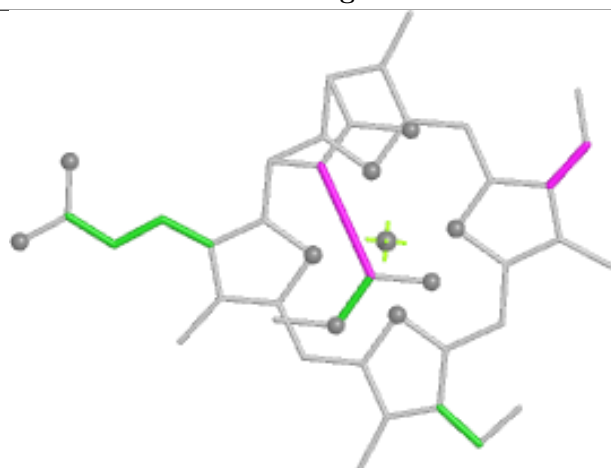
Ligand KC2 T 302



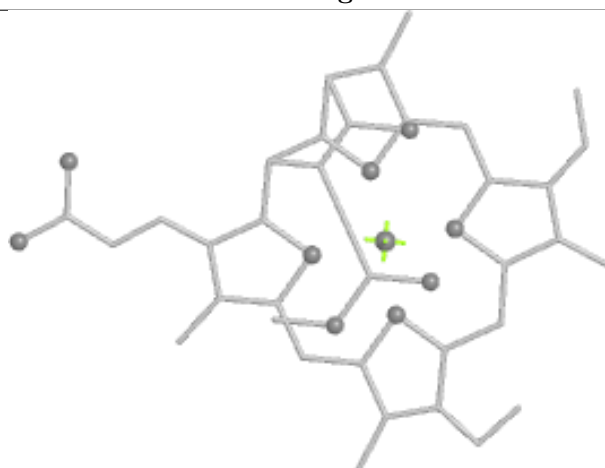
Bond lengths



Bond angles

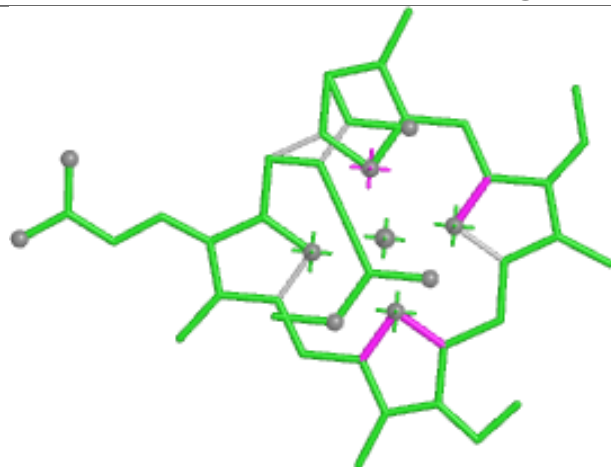


Torsions

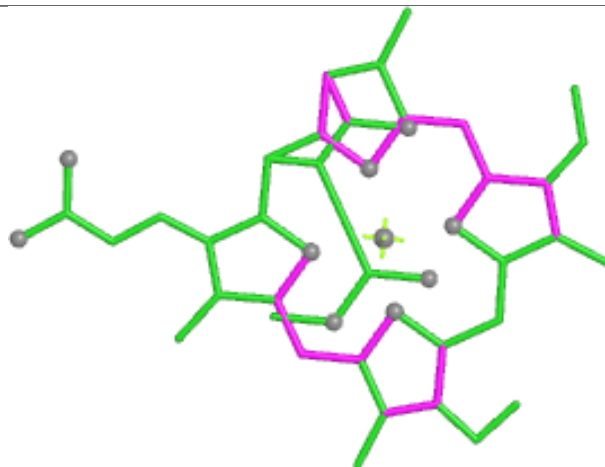


Rings

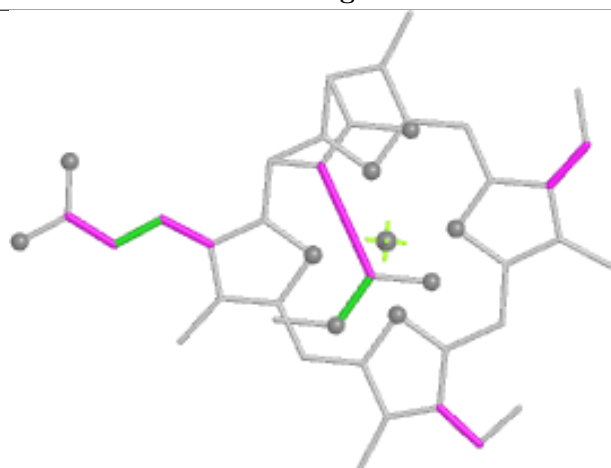
Ligand KC2 T 311



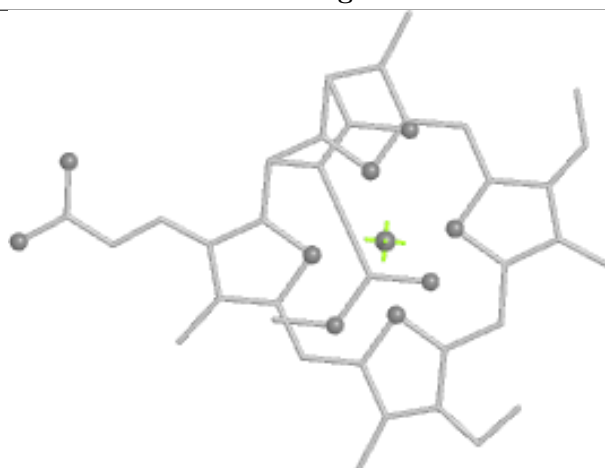
Bond lengths



Bond angles



Torsions



Rings

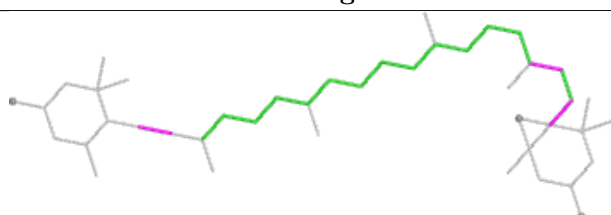
Ligand DD6 p 322



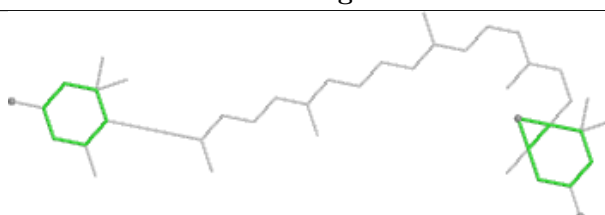
Bond lengths



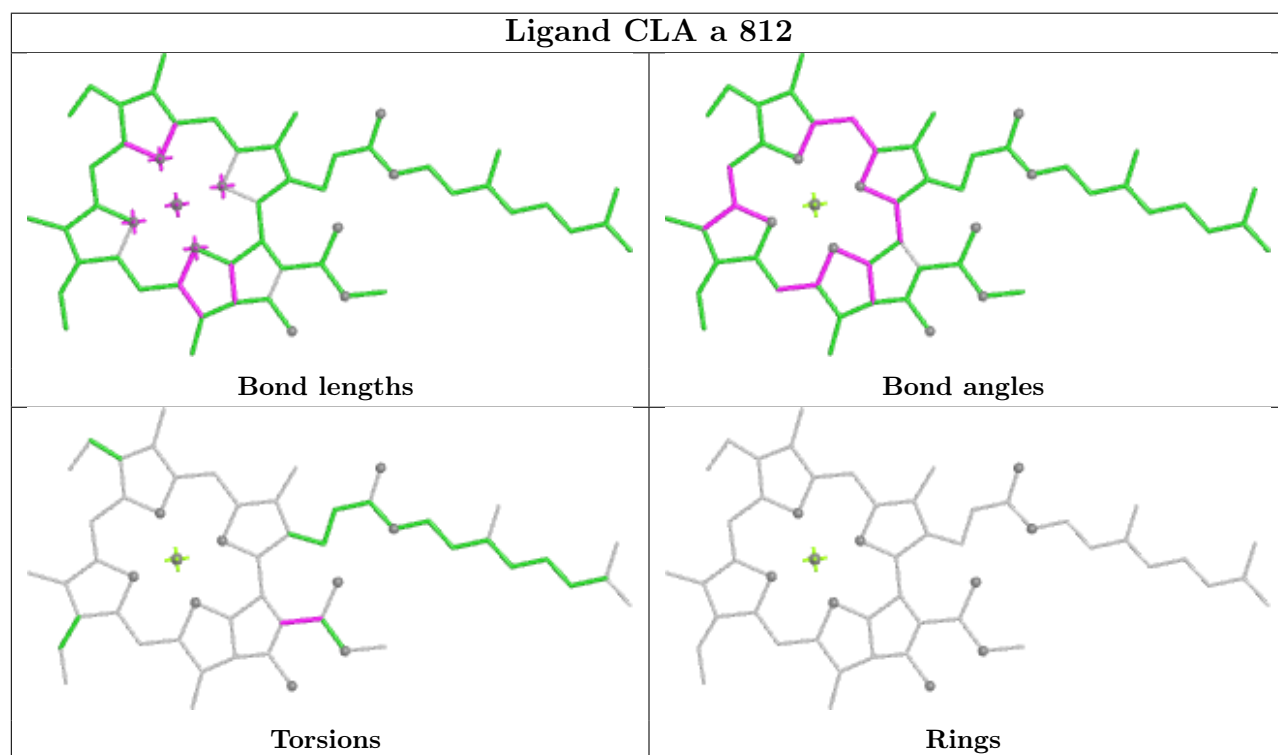
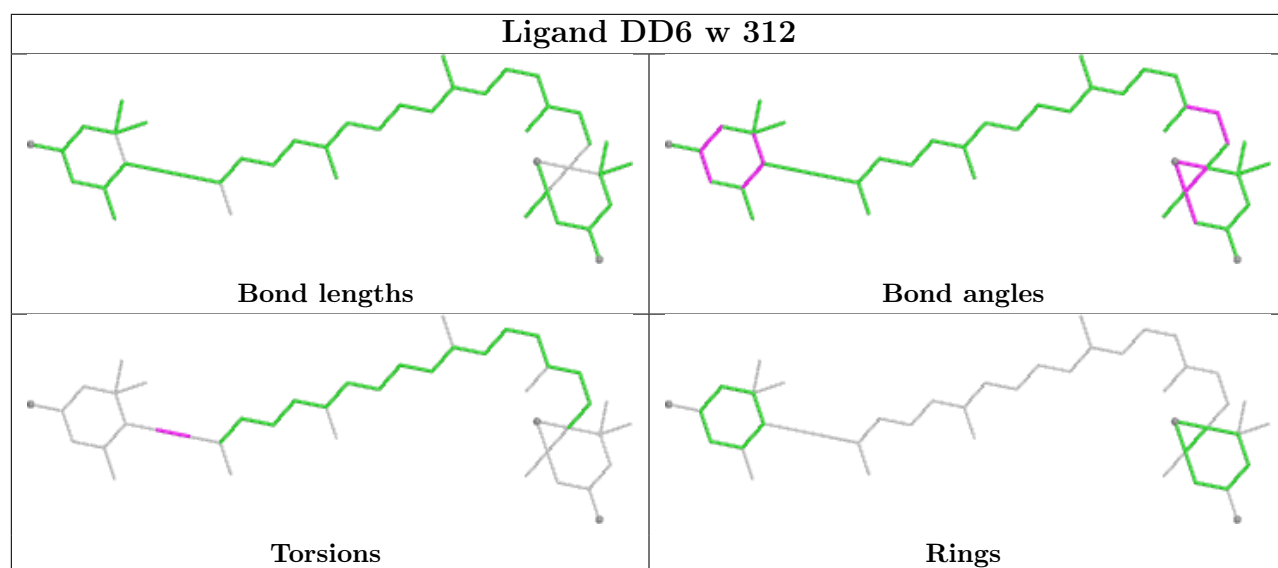
Bond angles



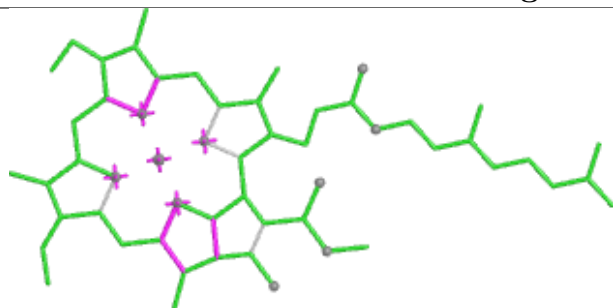
Torsions



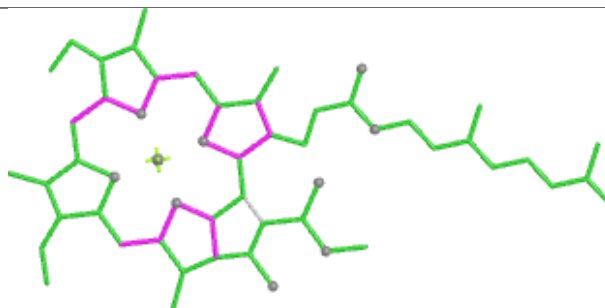
Rings



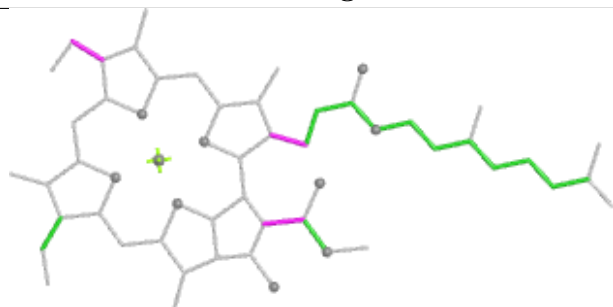
Ligand CLA I 208



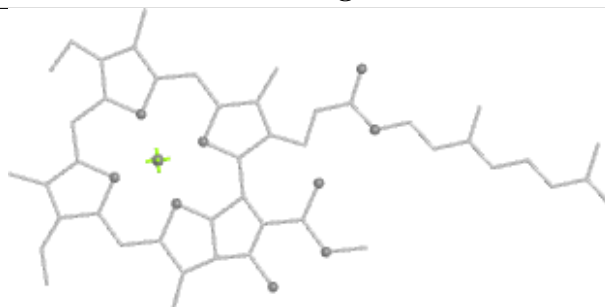
Bond lengths



Bond angles

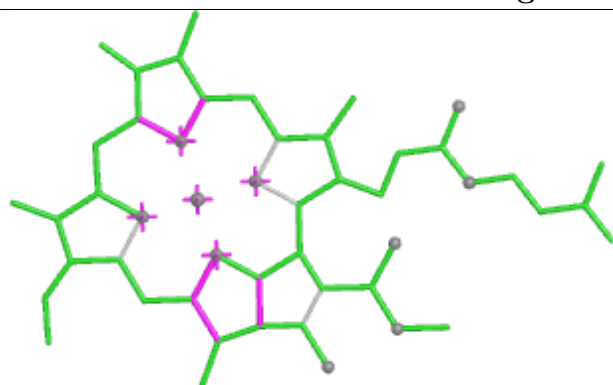


Torsions

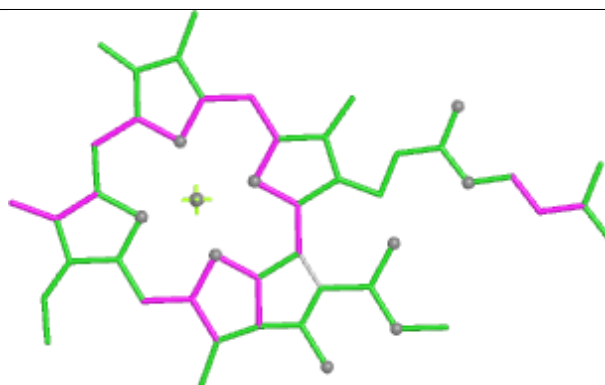


Rings

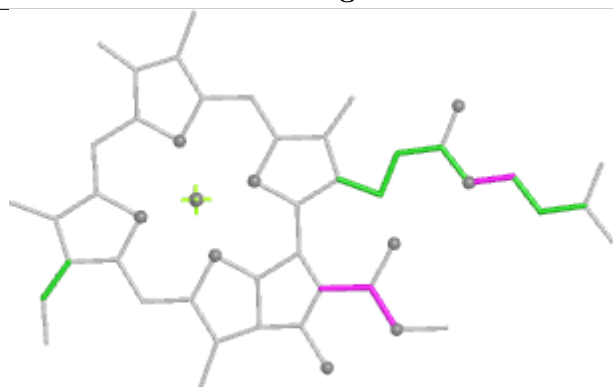
Ligand CLA S 308



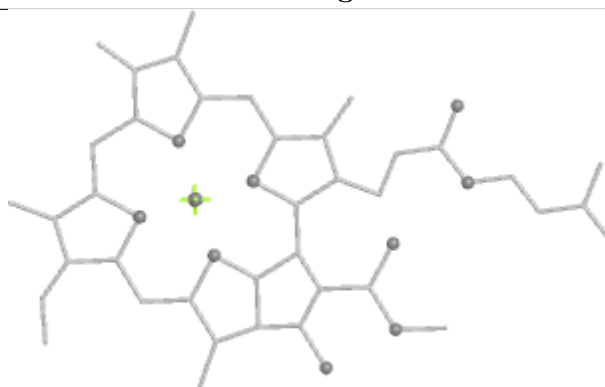
Bond lengths



Bond angles

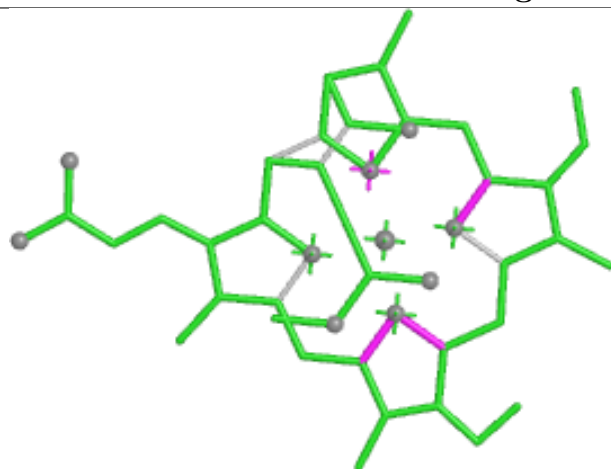


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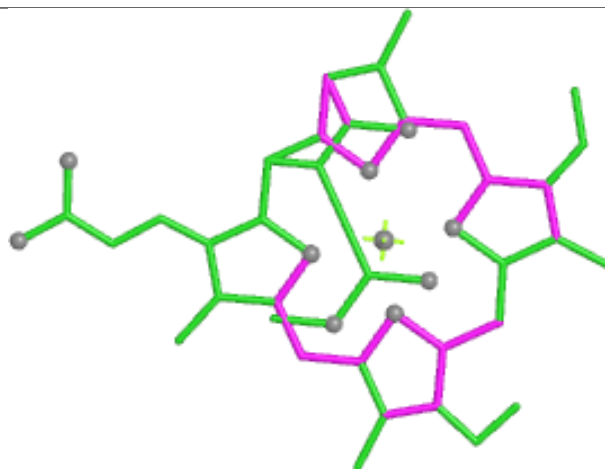


Rings

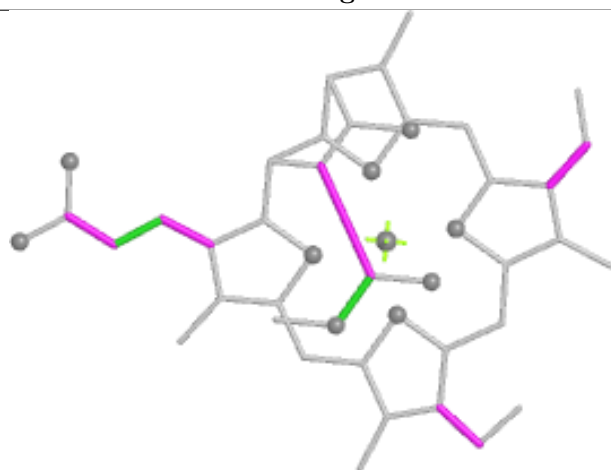
Ligand KC2 N 312



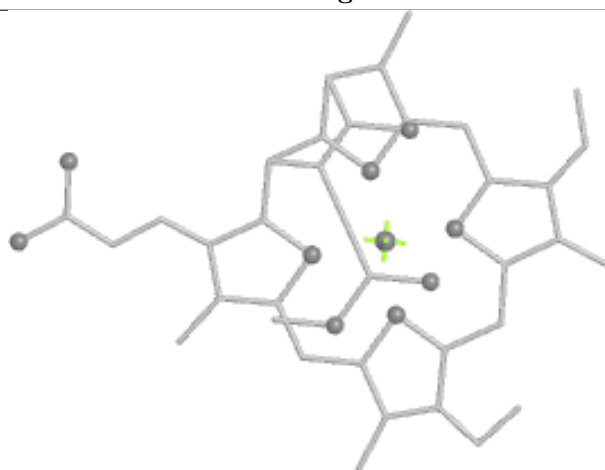
Bond lengths



Bond angles

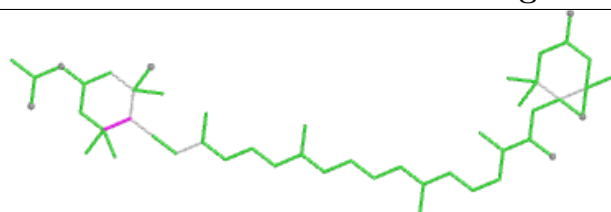


Torsions

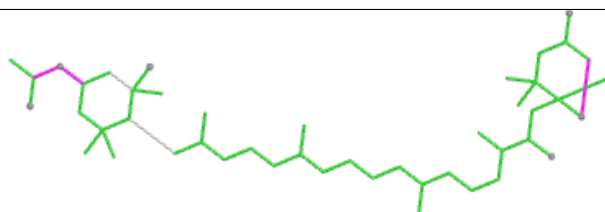


Rings

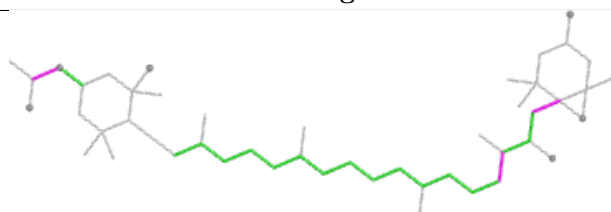
Ligand A86 D 320



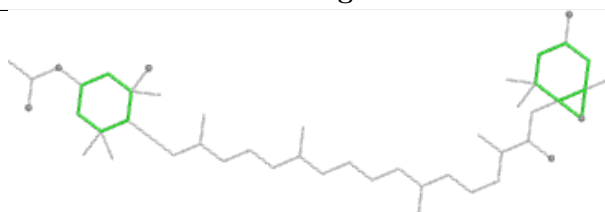
Bond lengths



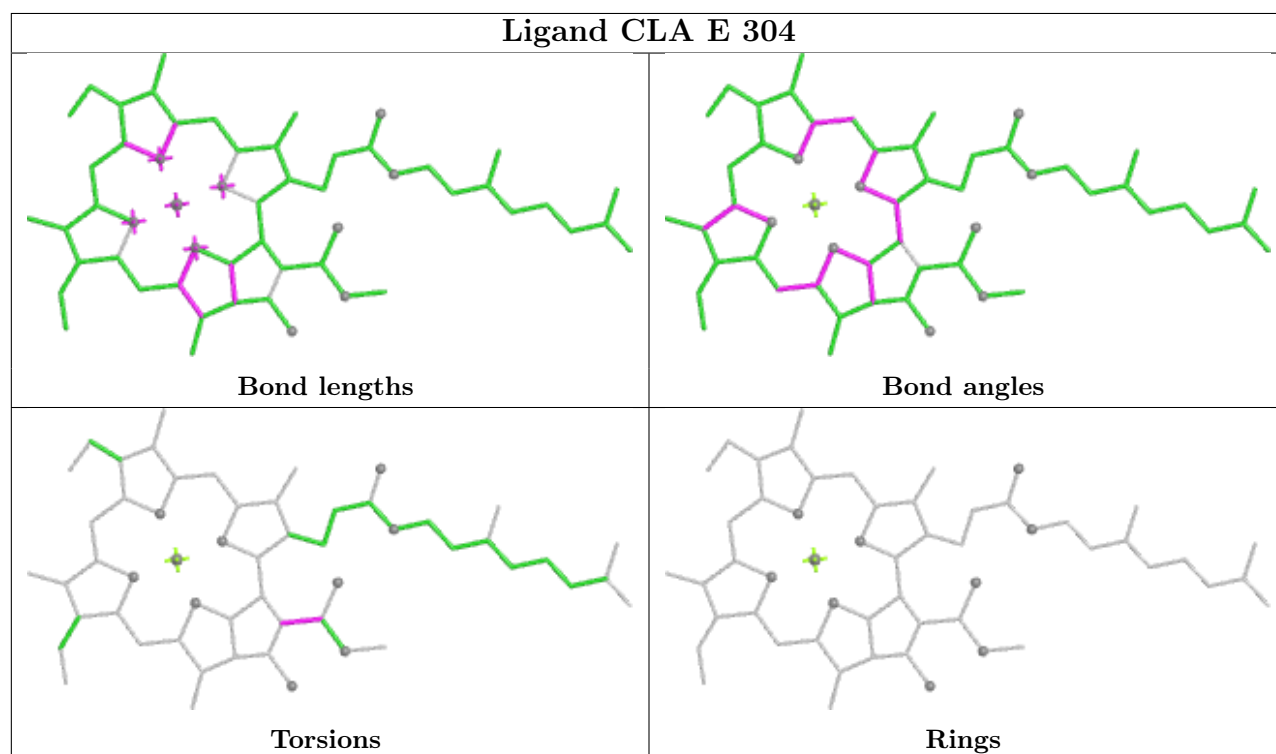
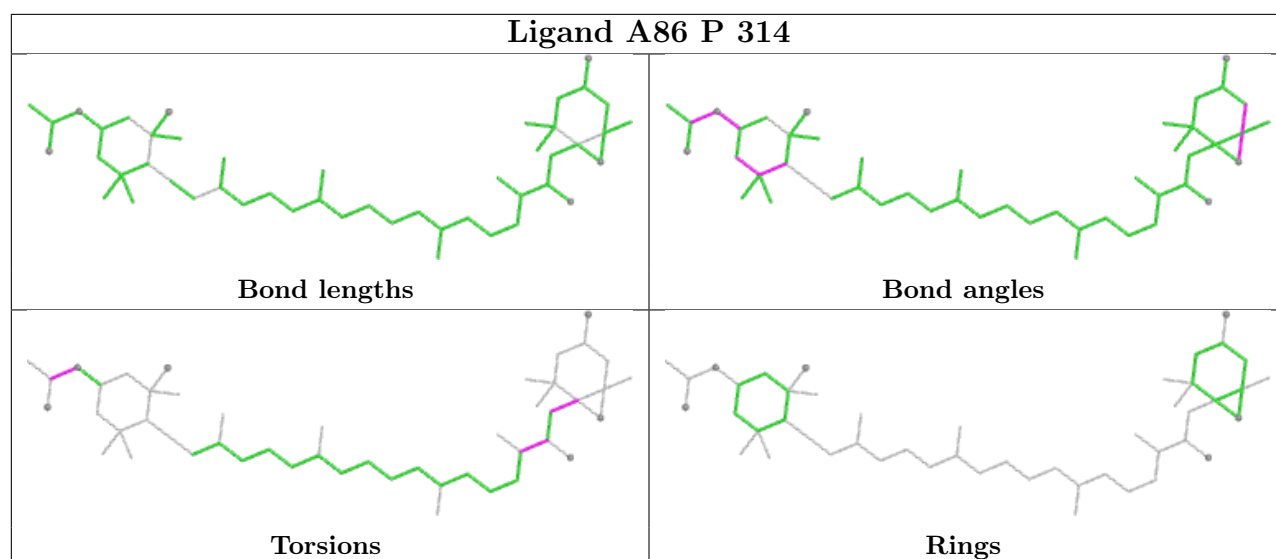
Bond angles



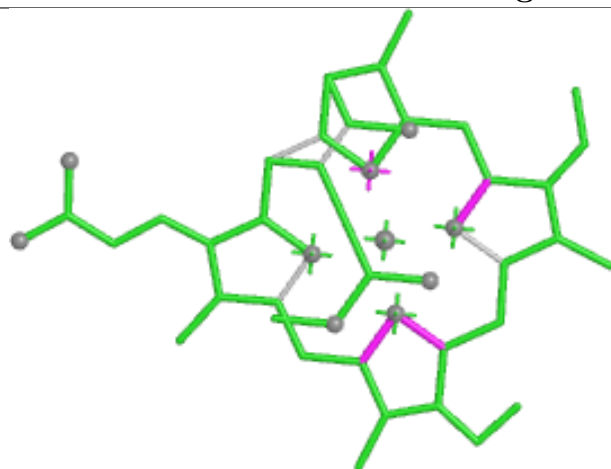
Torsions



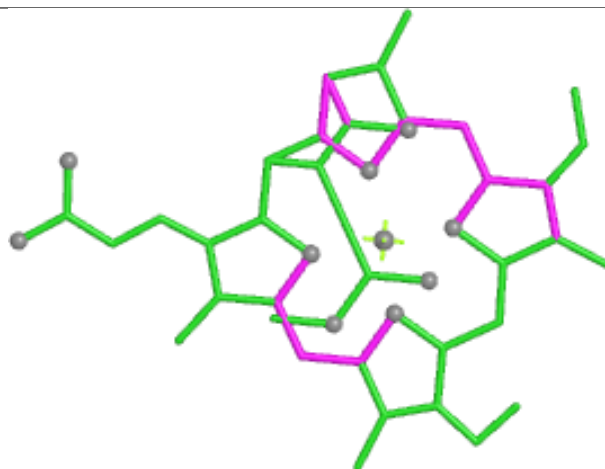
Rings



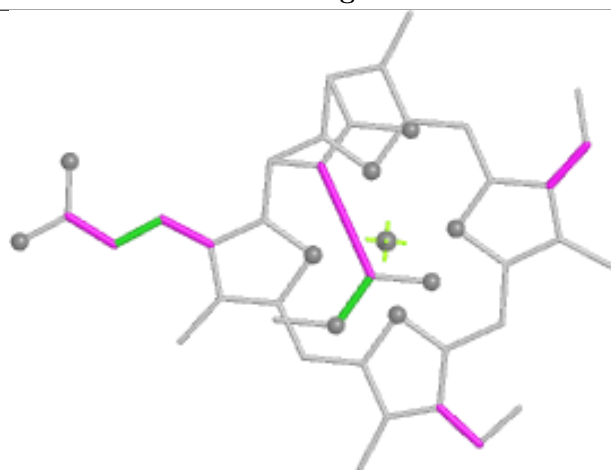
Ligand KC2 C 303



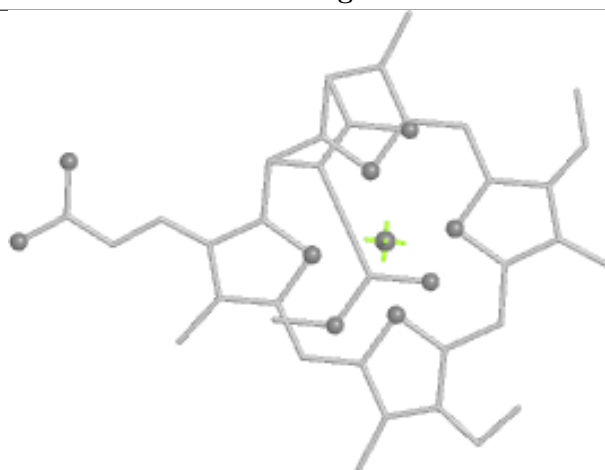
Bond lengths



Bond angles

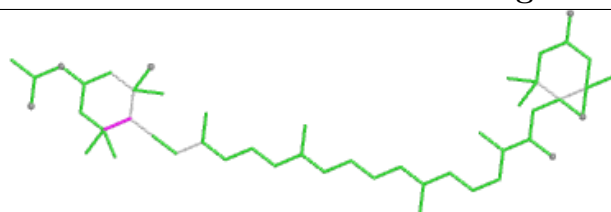


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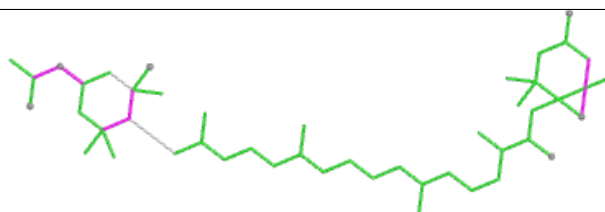


Rings

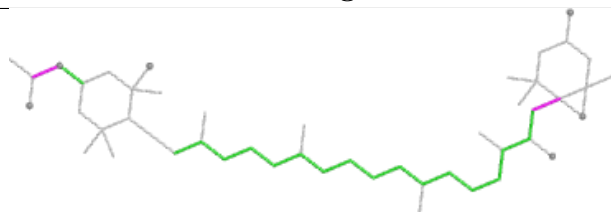
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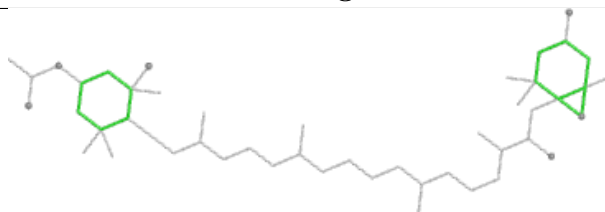
Bond lengths



Bond angles

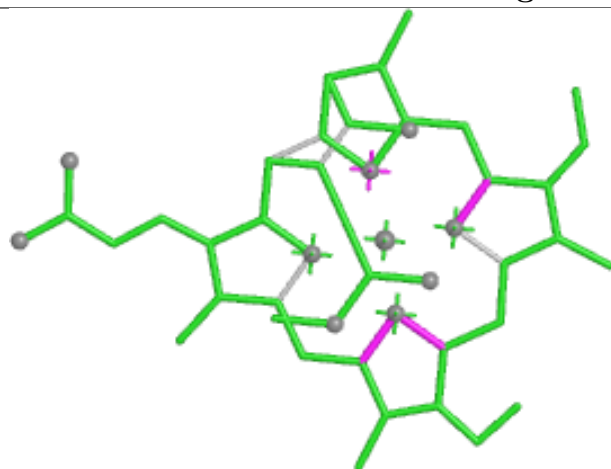


Torsions

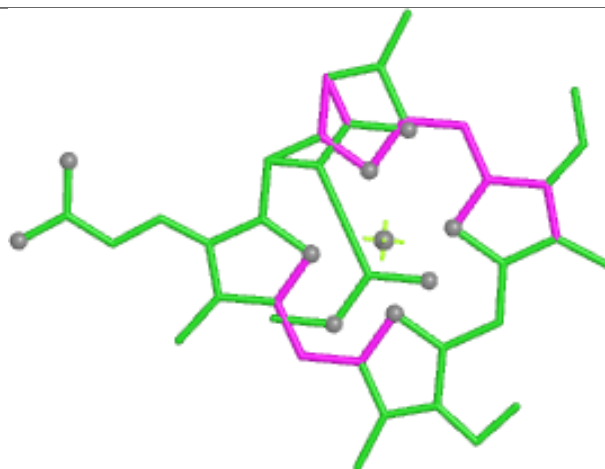


Rings

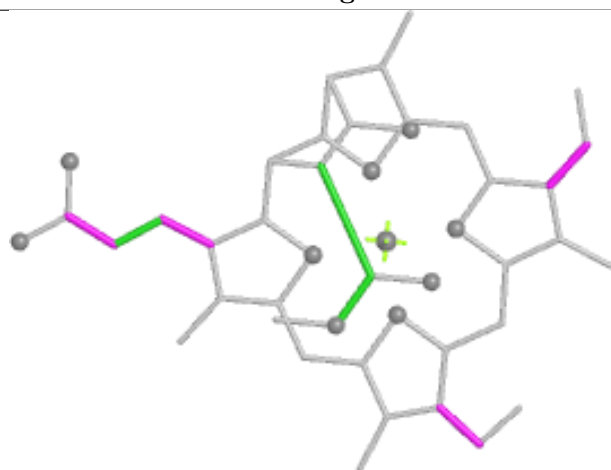
Ligand KC2 P 310



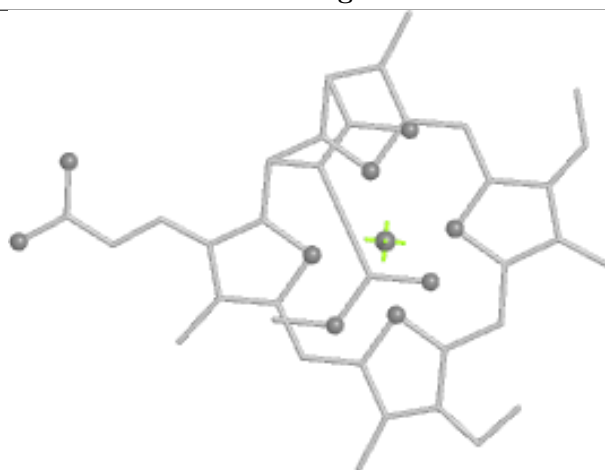
Bond lengths



Bond angles



Torsions



Rings

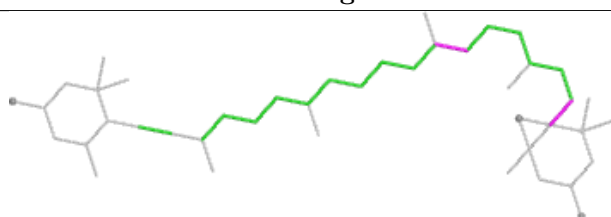
Ligand DD6 C 313



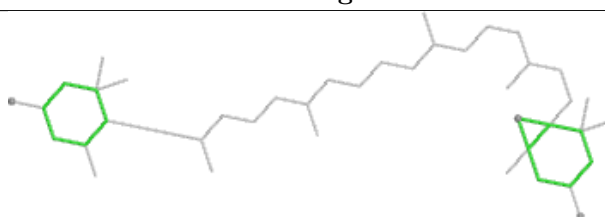
Bond lengths



Bond angles

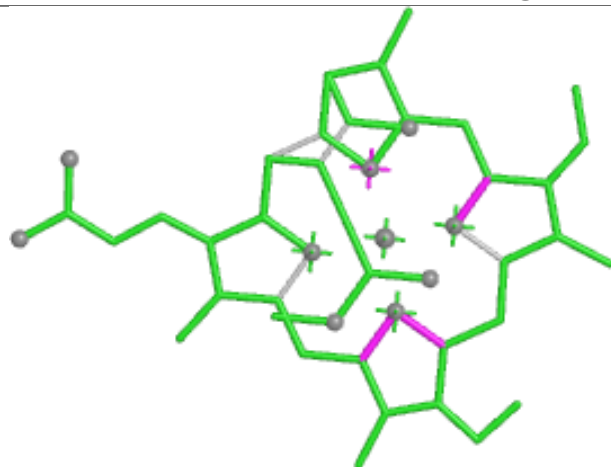


Torsions

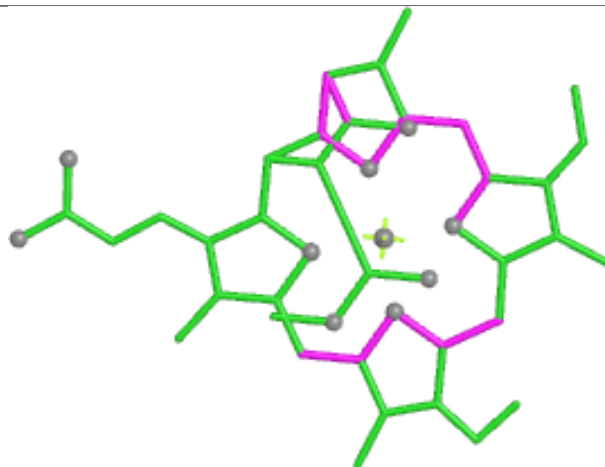


Rings

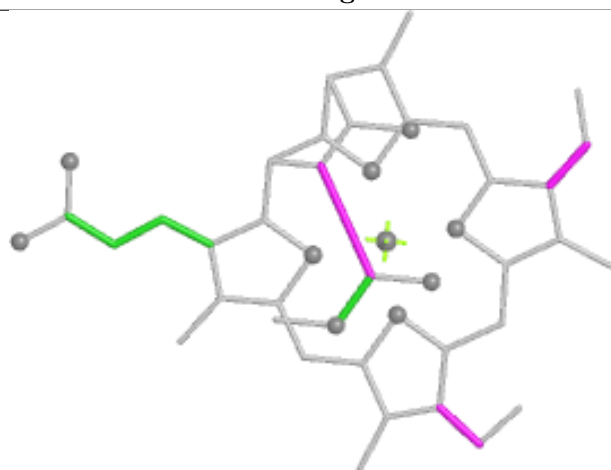
Ligand KC2 T 309



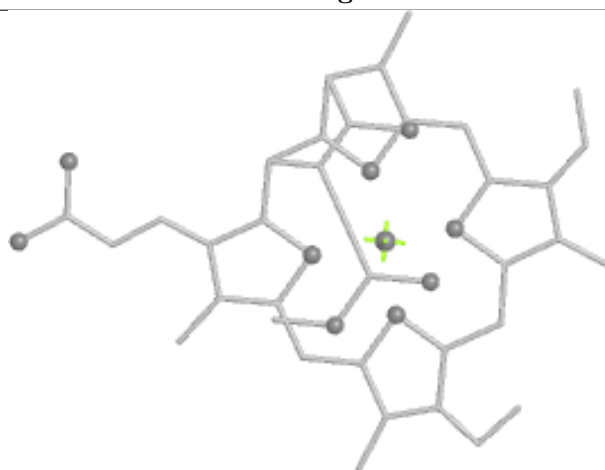
Bond lengths



Bond angles

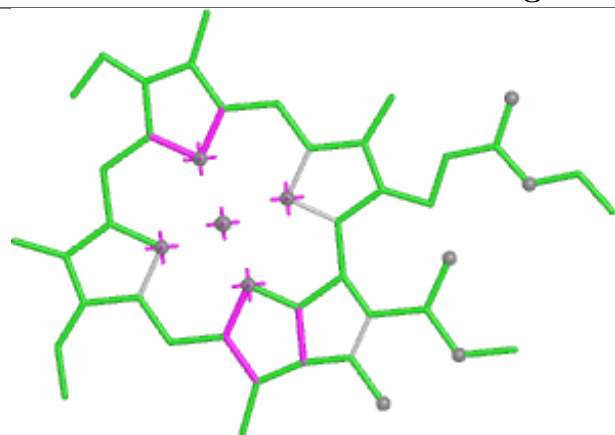


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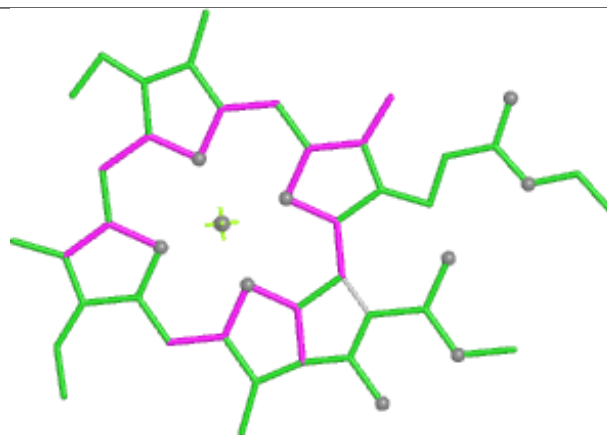


Rings

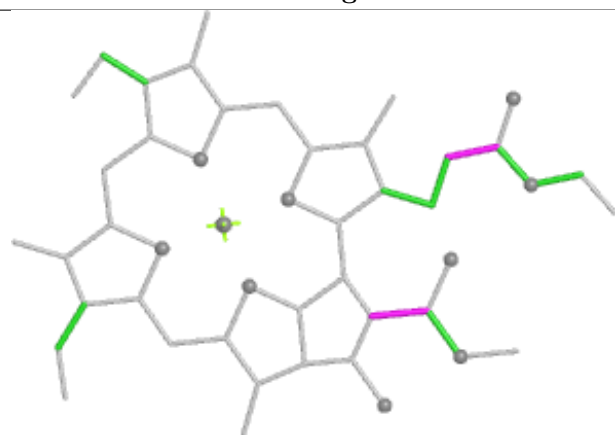
Ligand CLA f 205



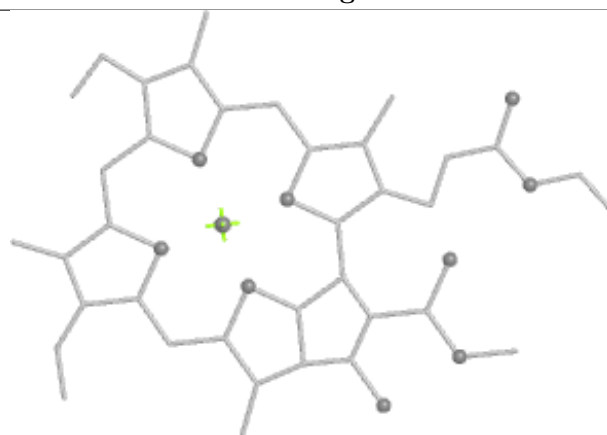
Bond lengths



Bond angles

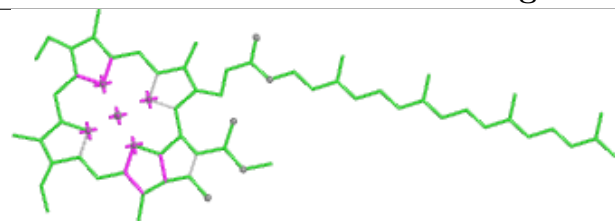


Torsions

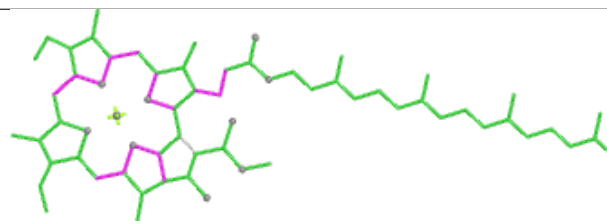


Rings

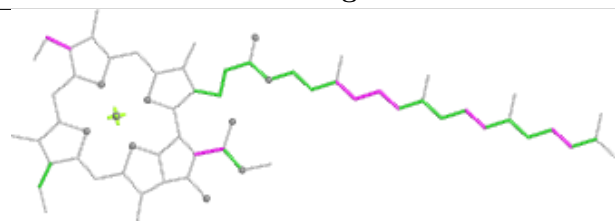
Ligand CLA b 825



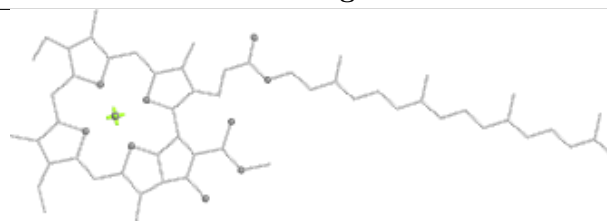
Bond lengths



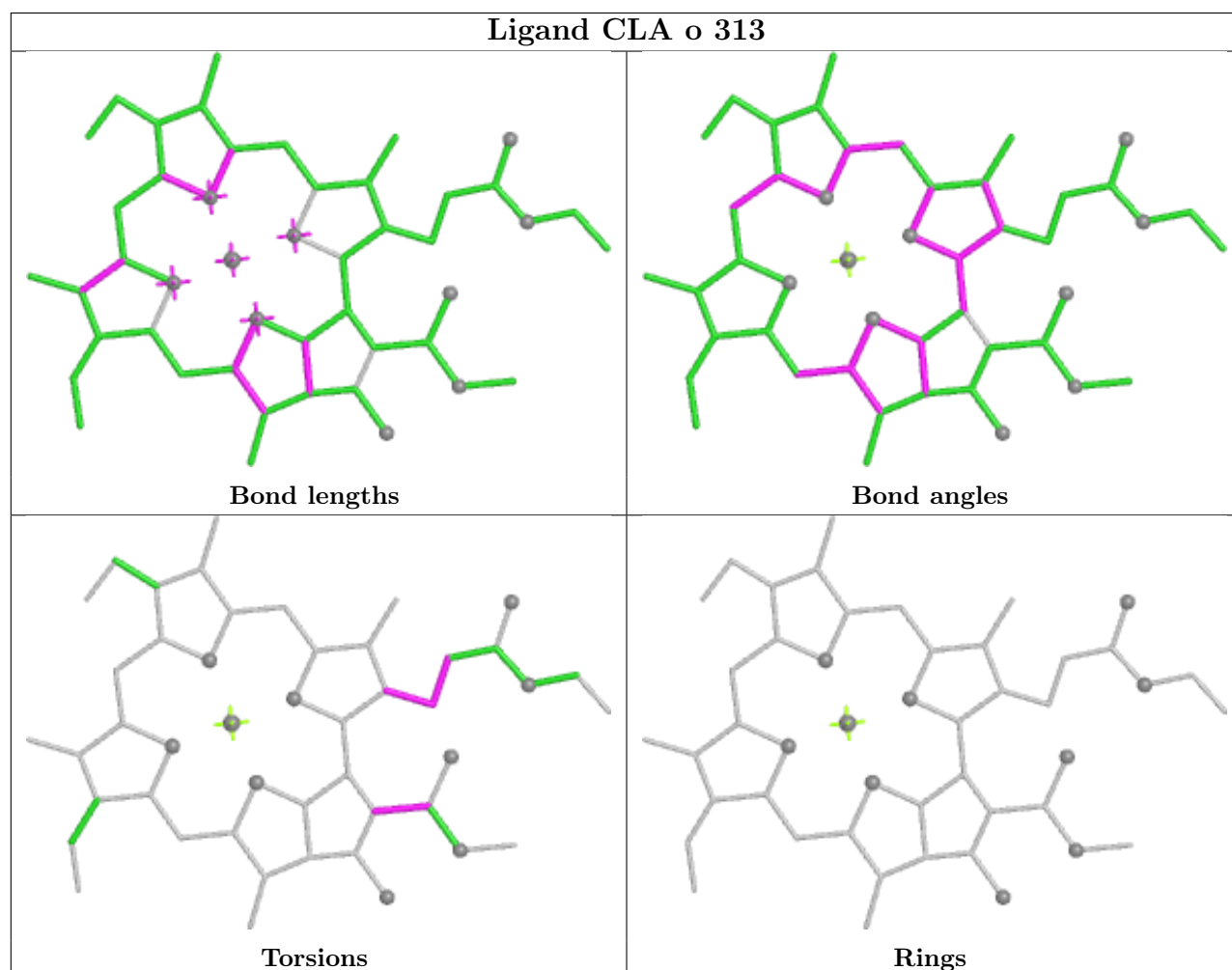
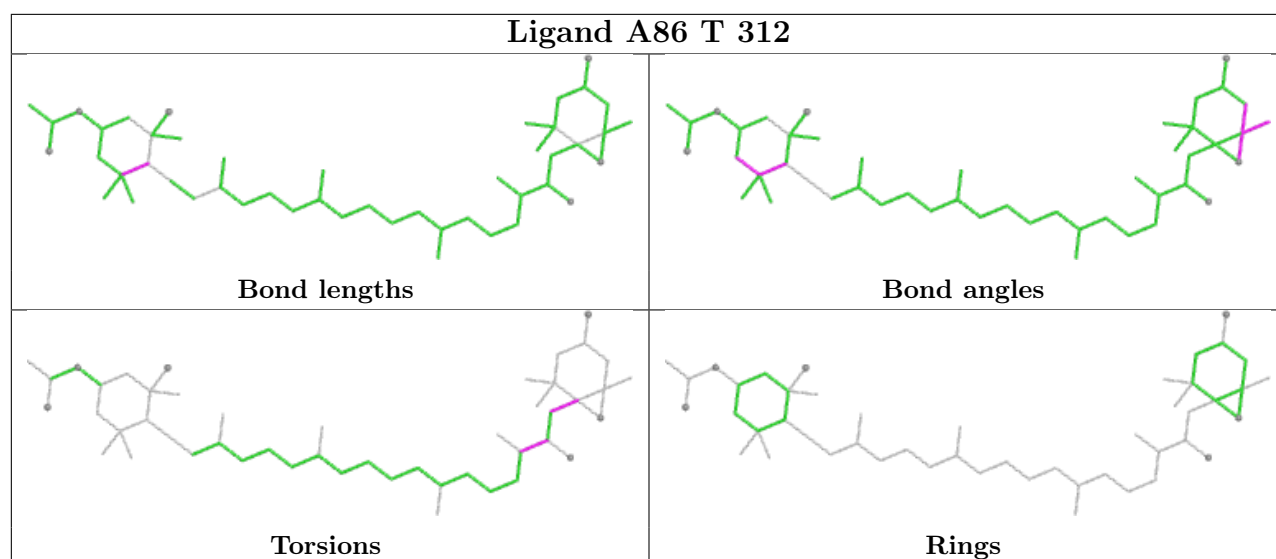
Bond angles



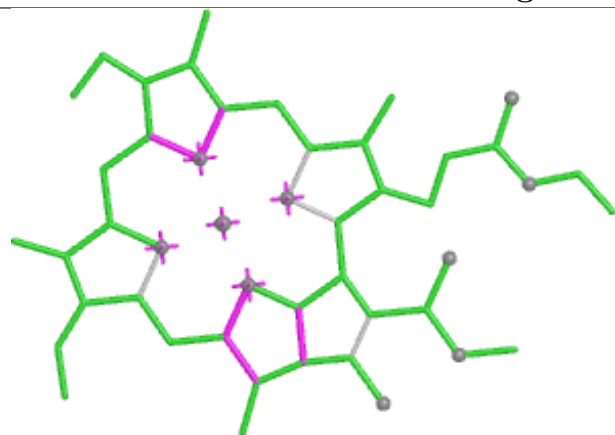
Torsions



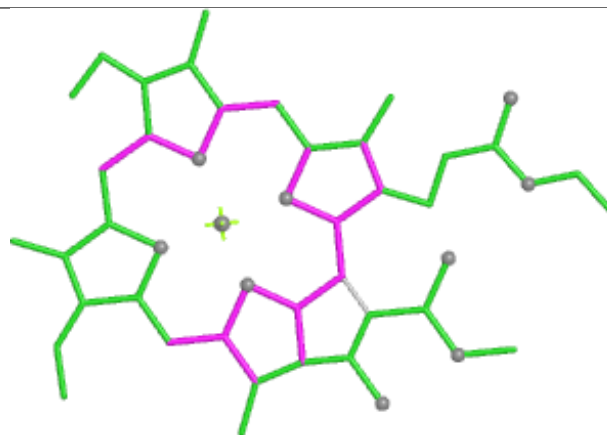
Rings



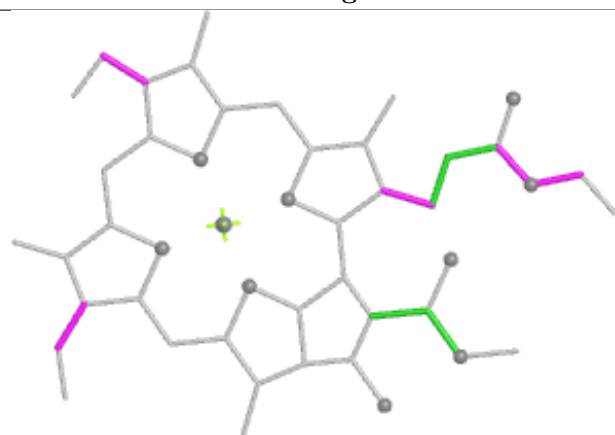
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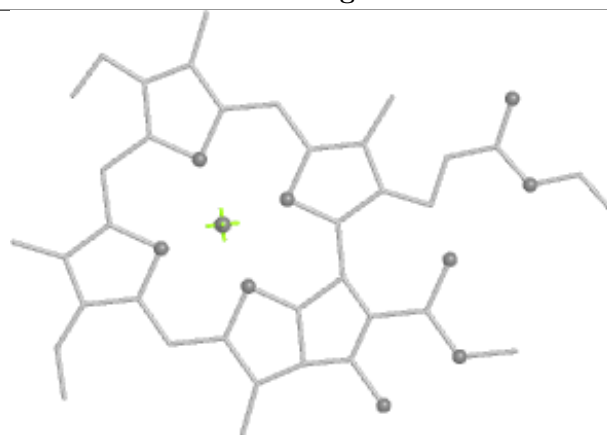
Bond lengths



Bond angles

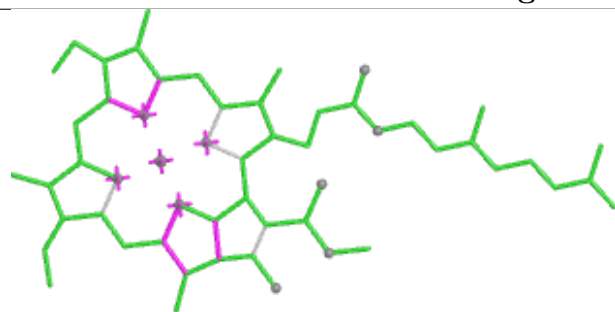


Torsions

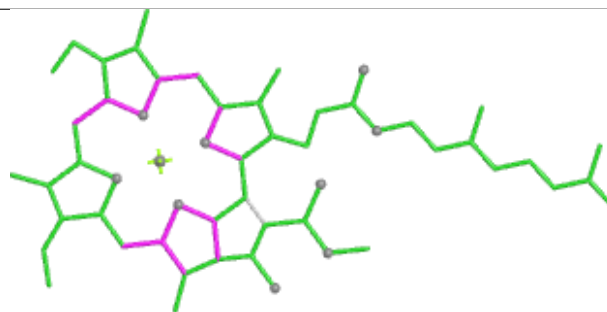


Rings

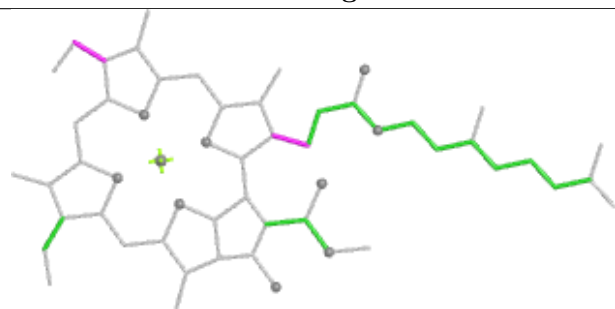
Ligand CLA F 308



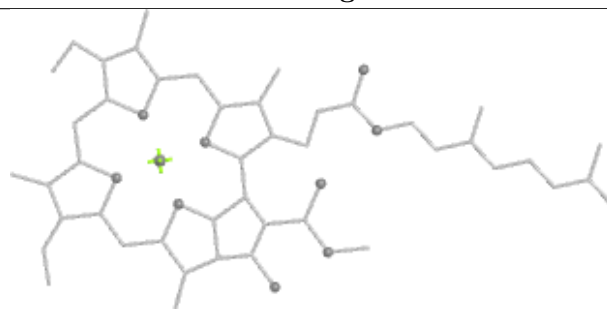
Bond lengths



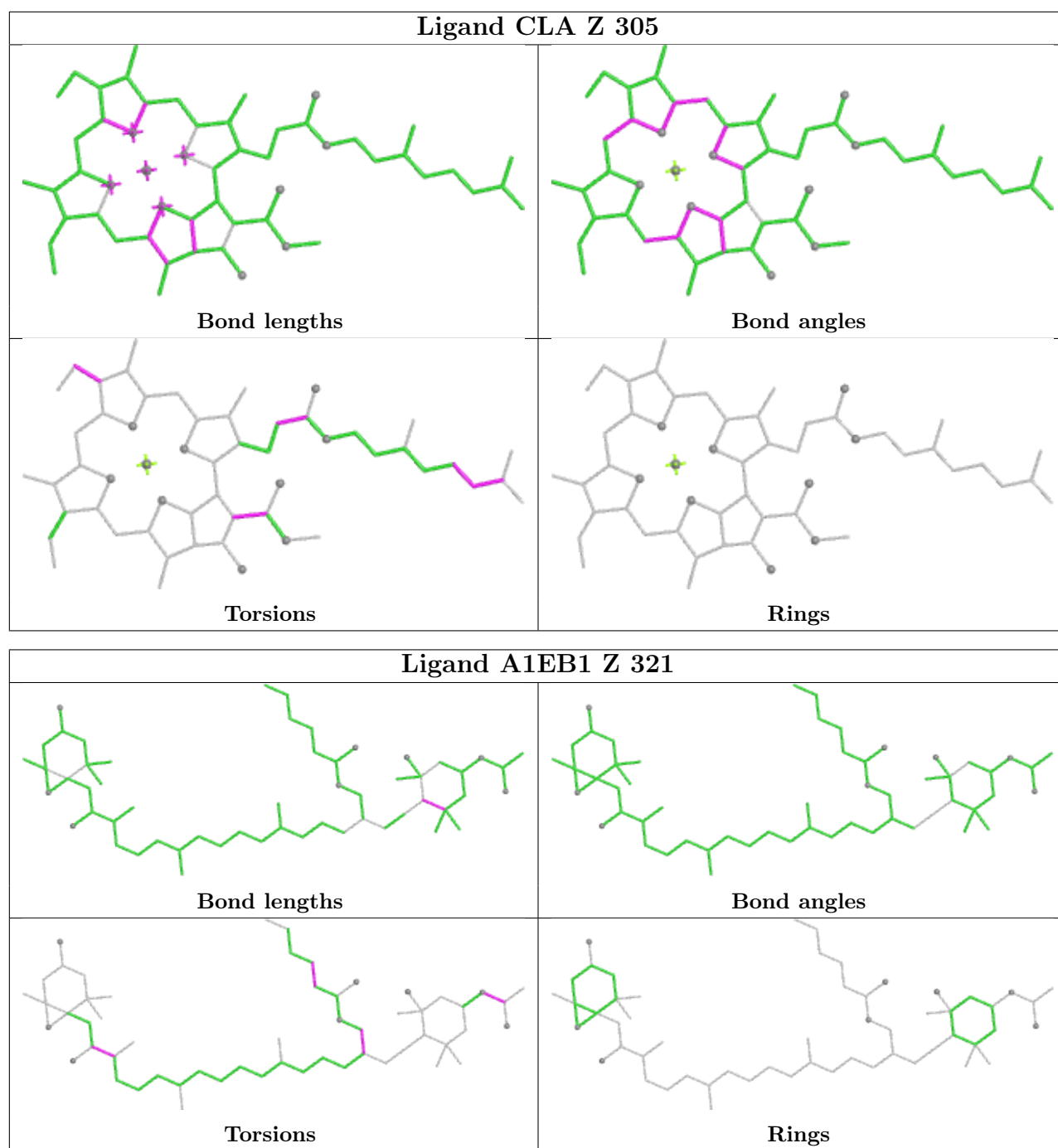
Bond angles

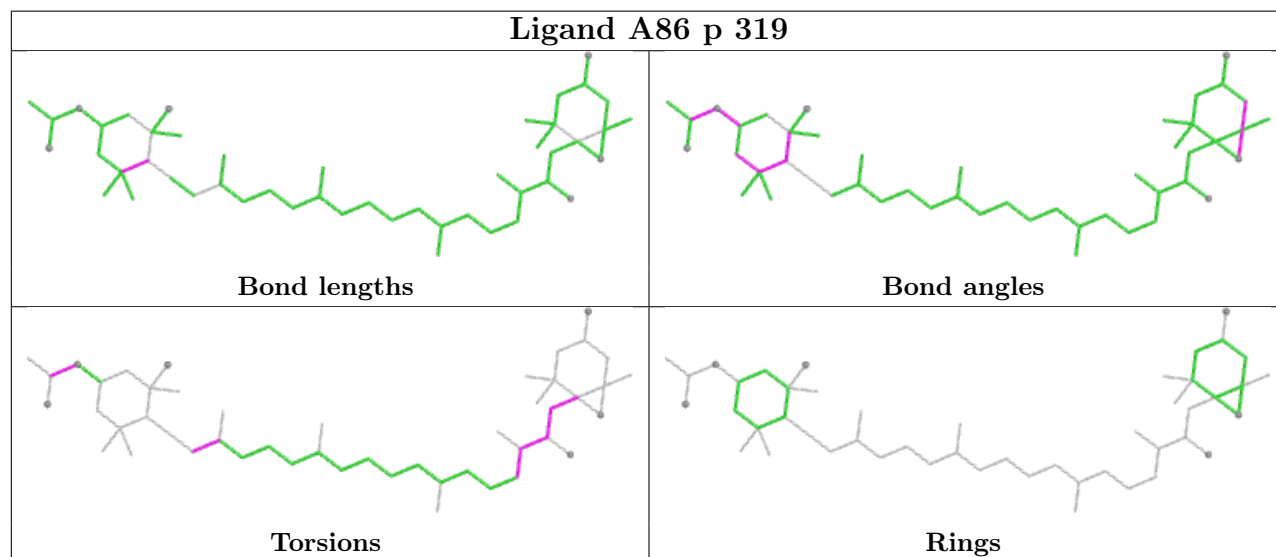
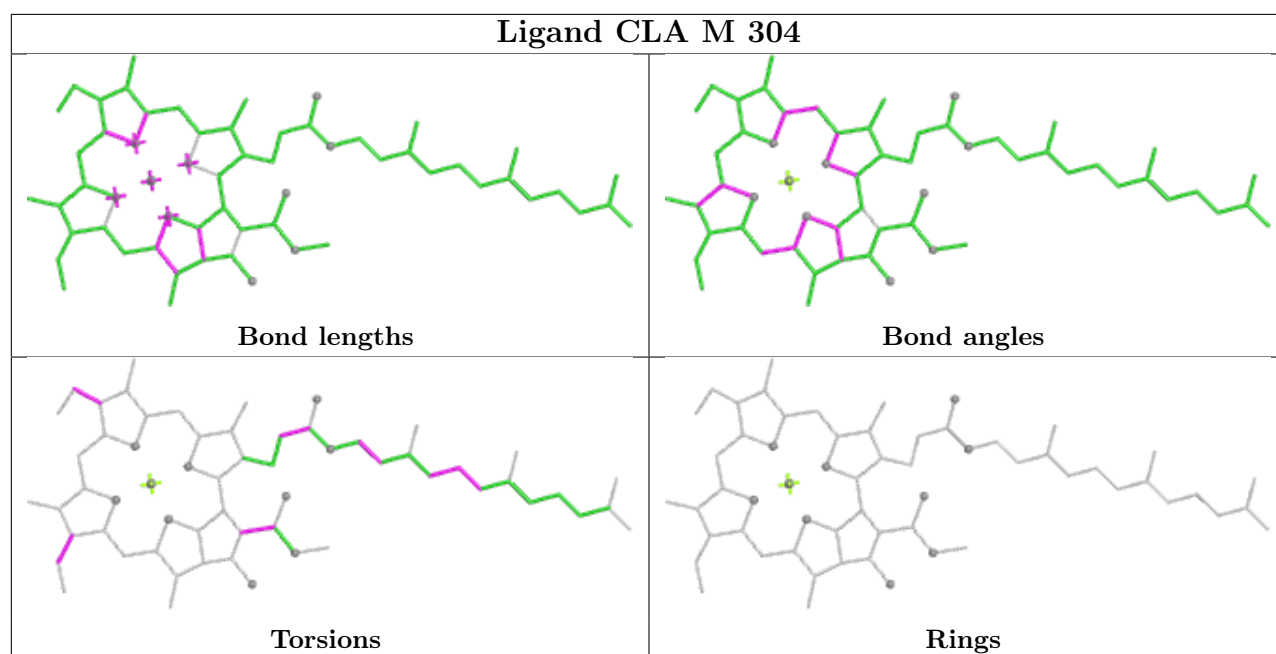


Torsions

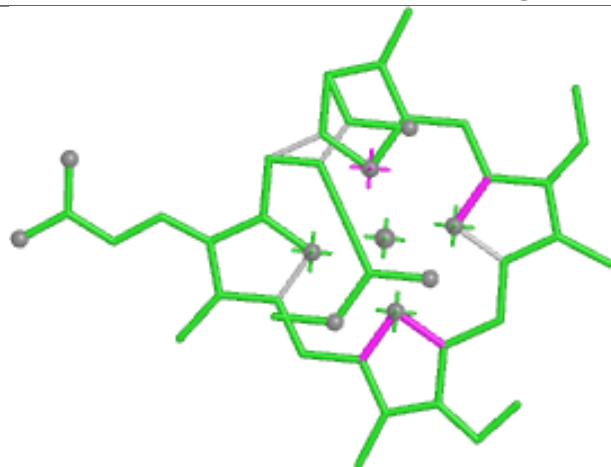


Rings

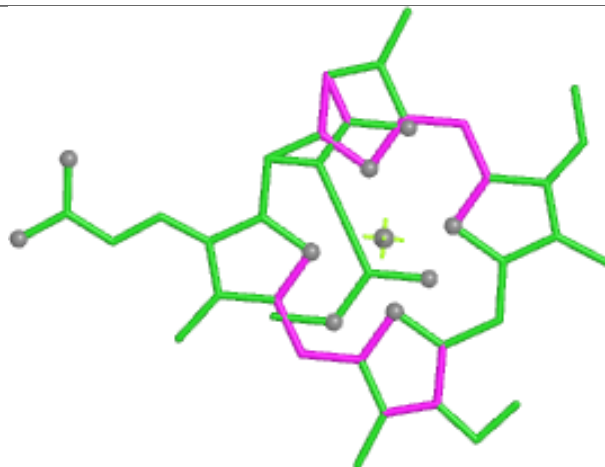




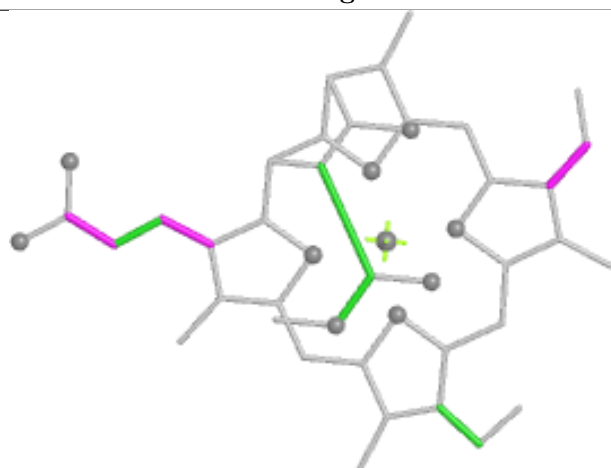
Ligand KC2 Y 302



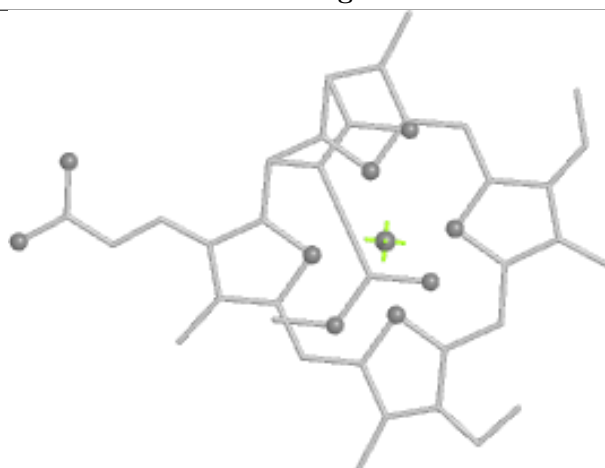
Bond lengths



Bond angles

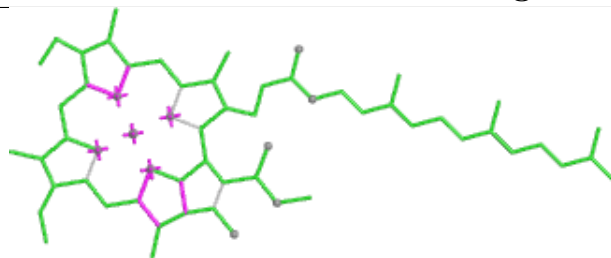


Torsions

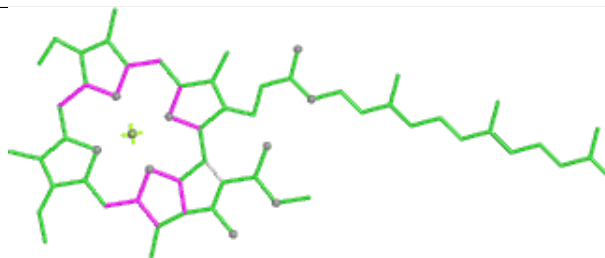


Rings

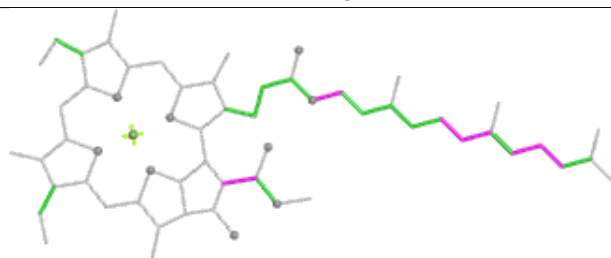
Ligand CLA K 304



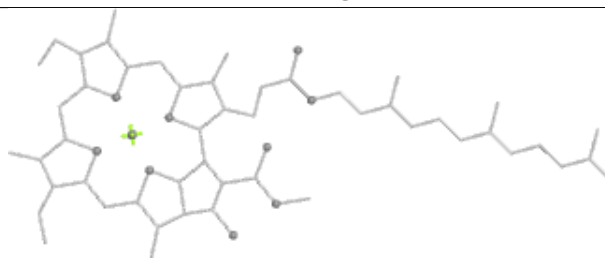
Bond lengths



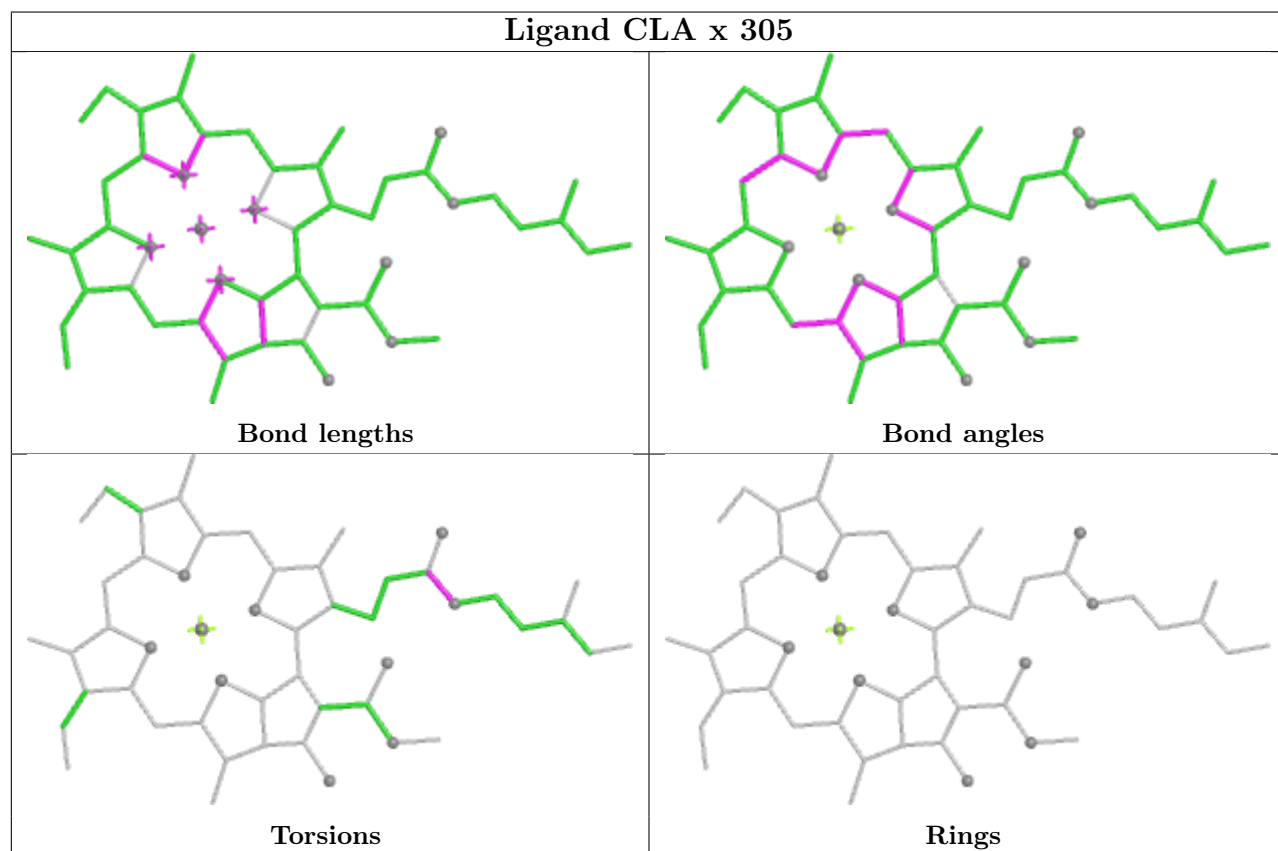
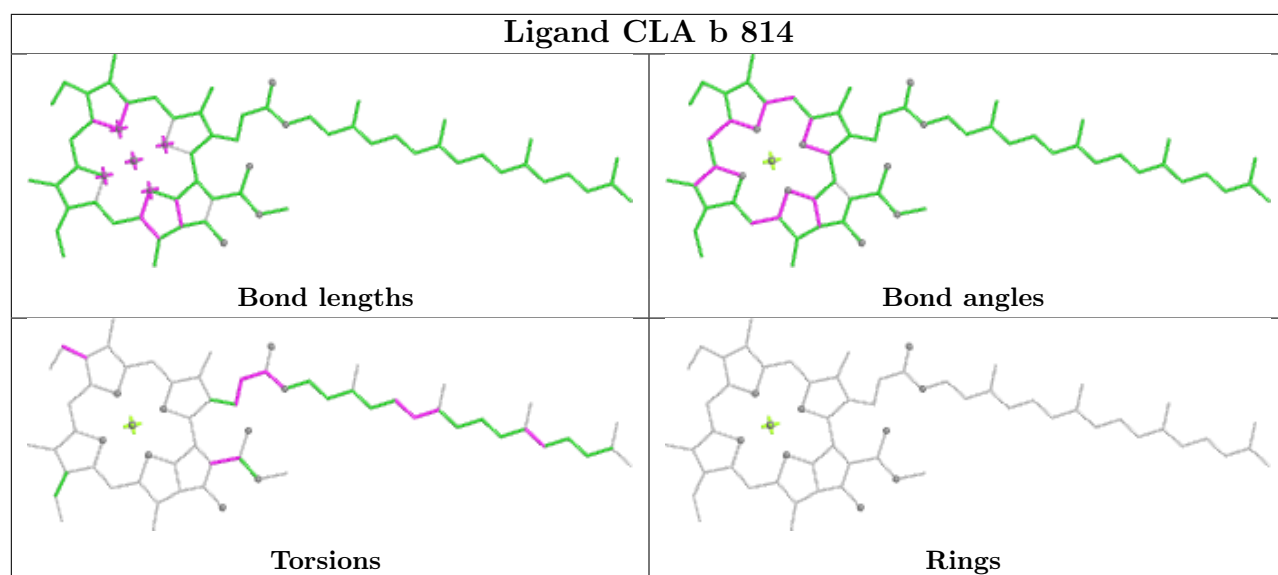
Bond angles

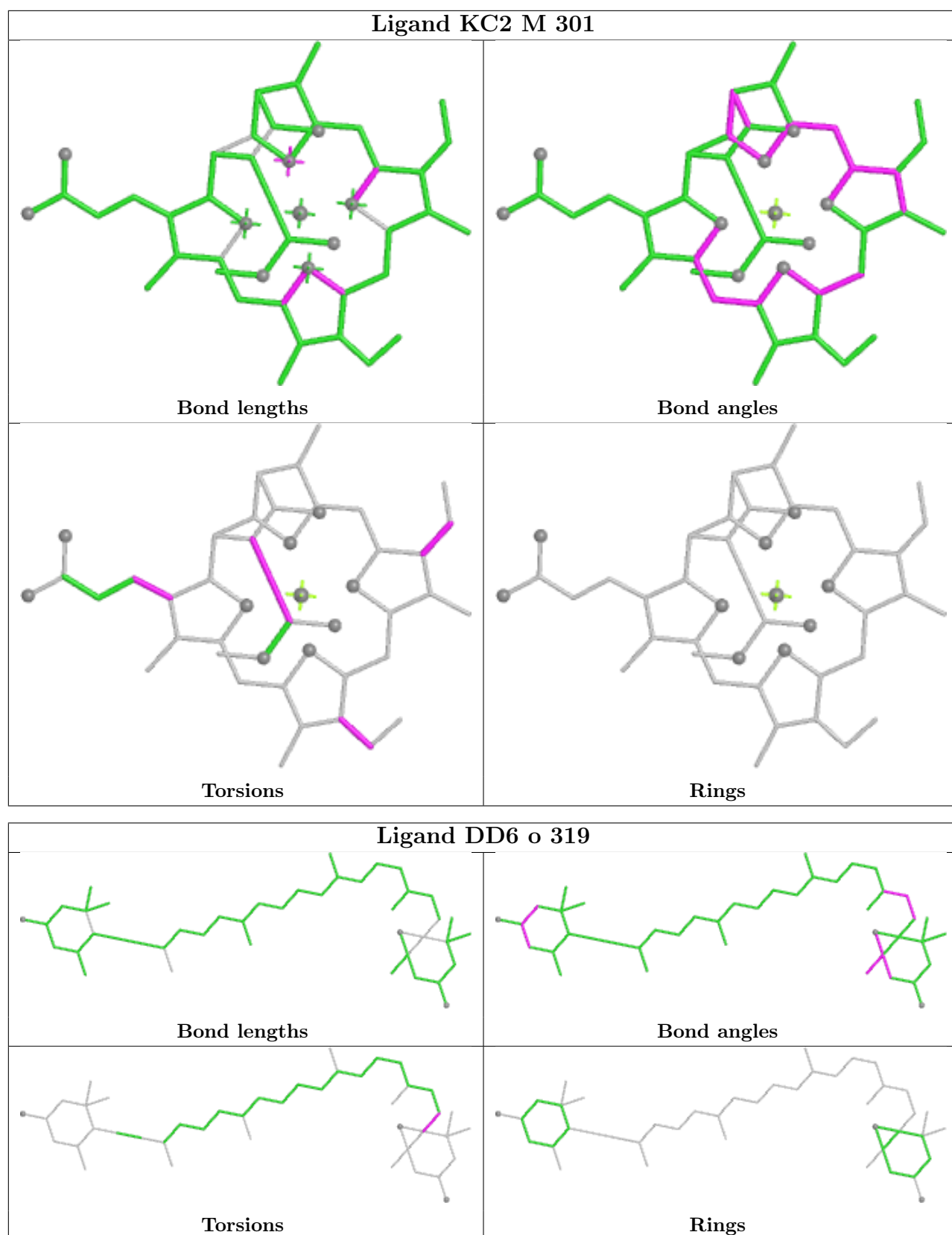


Torsions

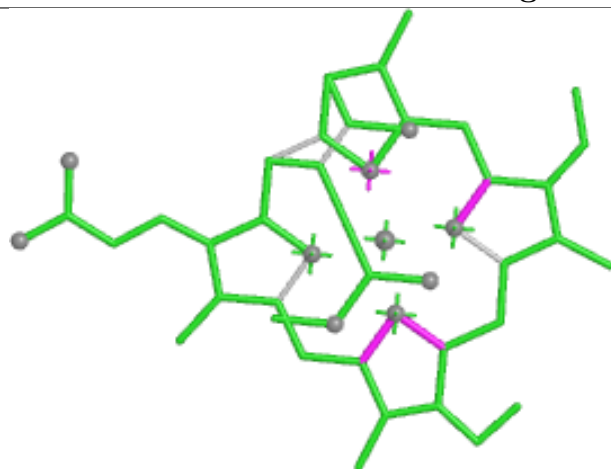


Rings

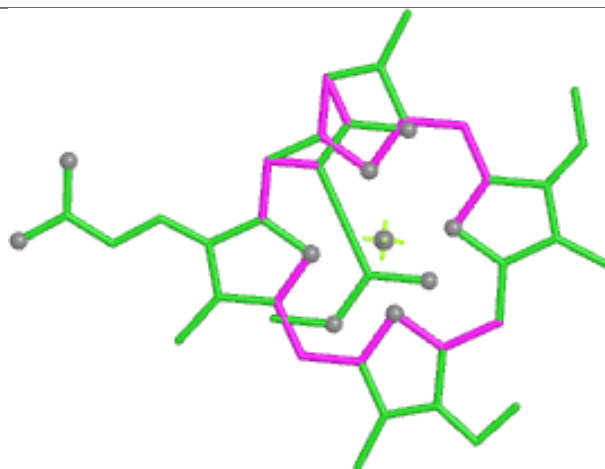




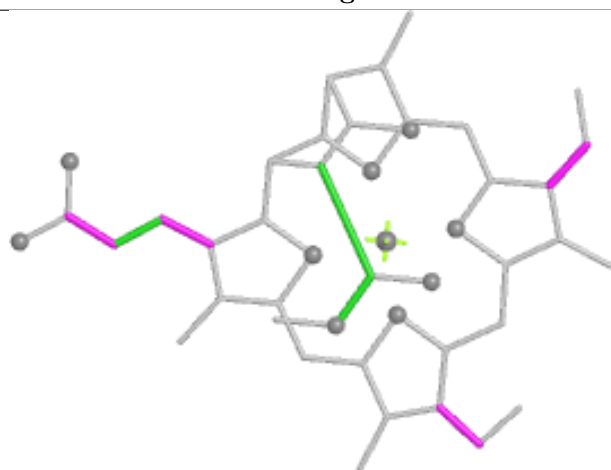
Ligand KC2 x 315



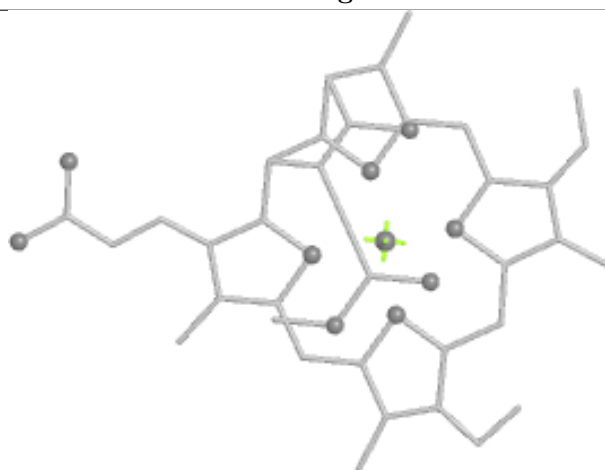
Bond lengths



Bond angles

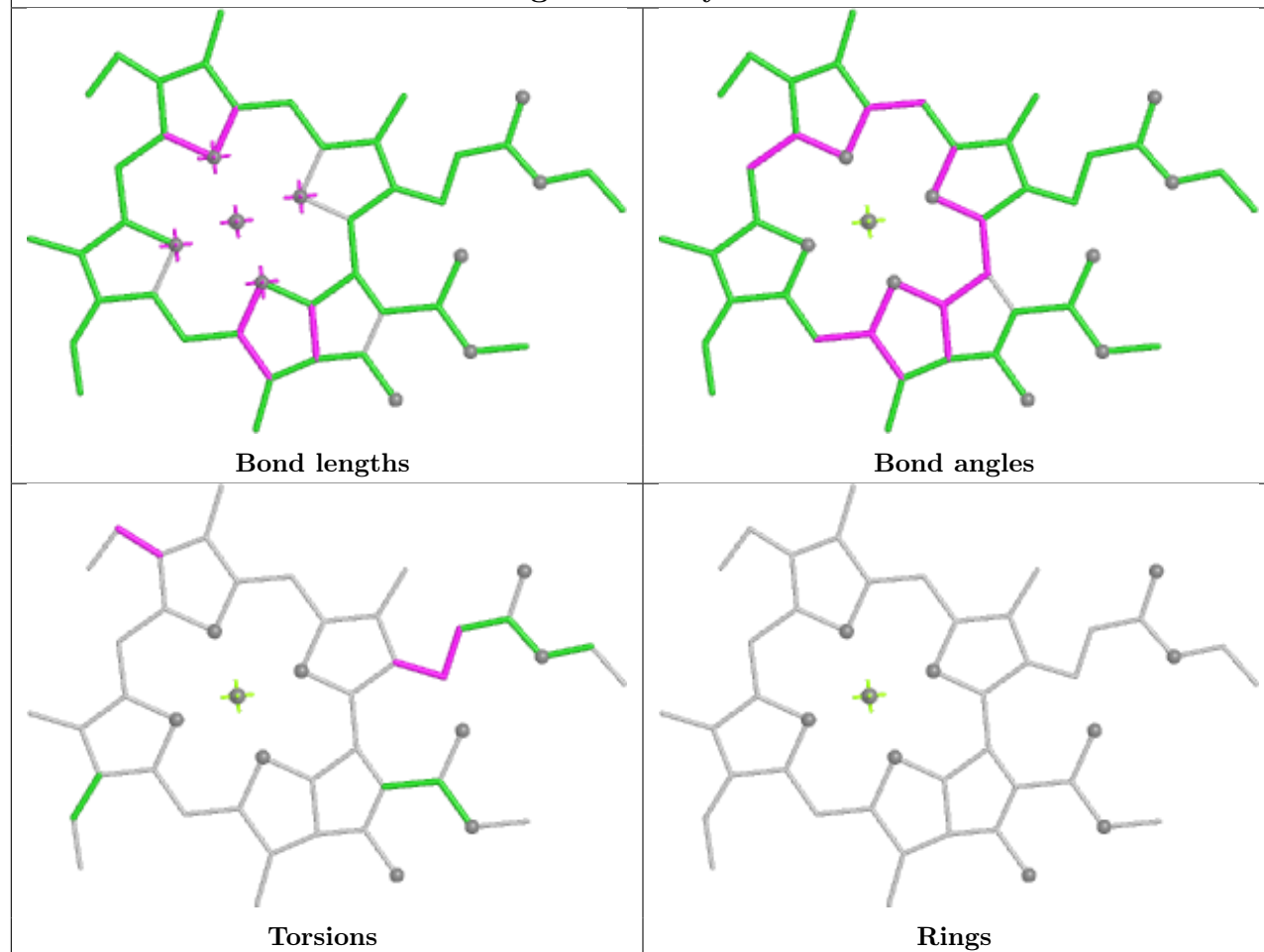


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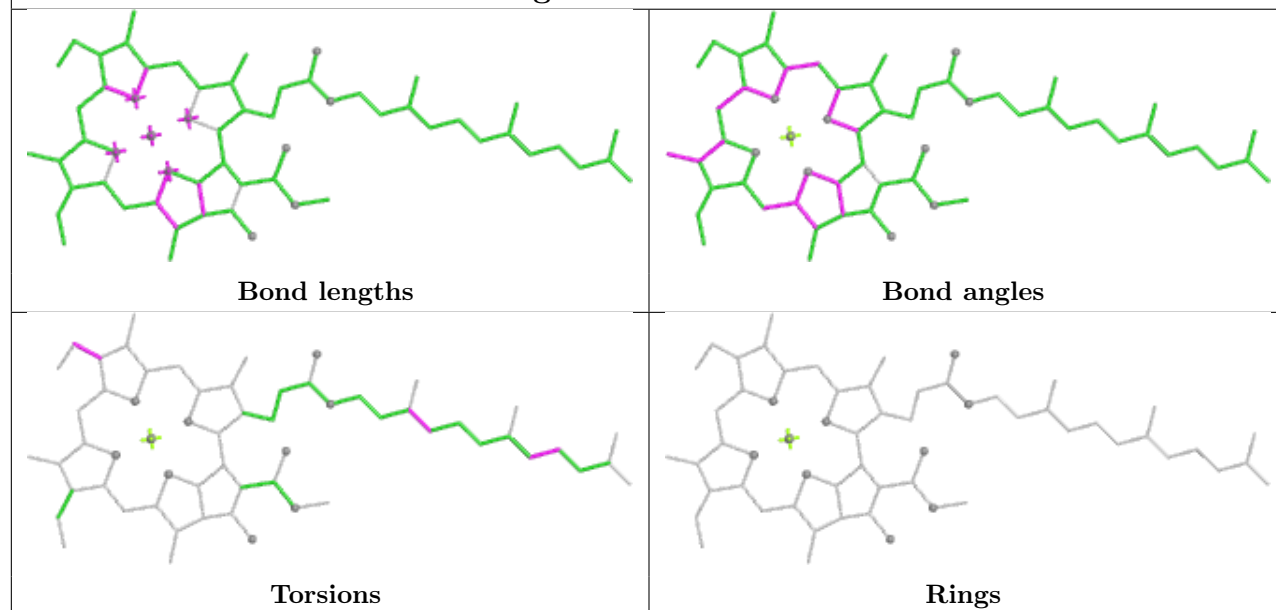


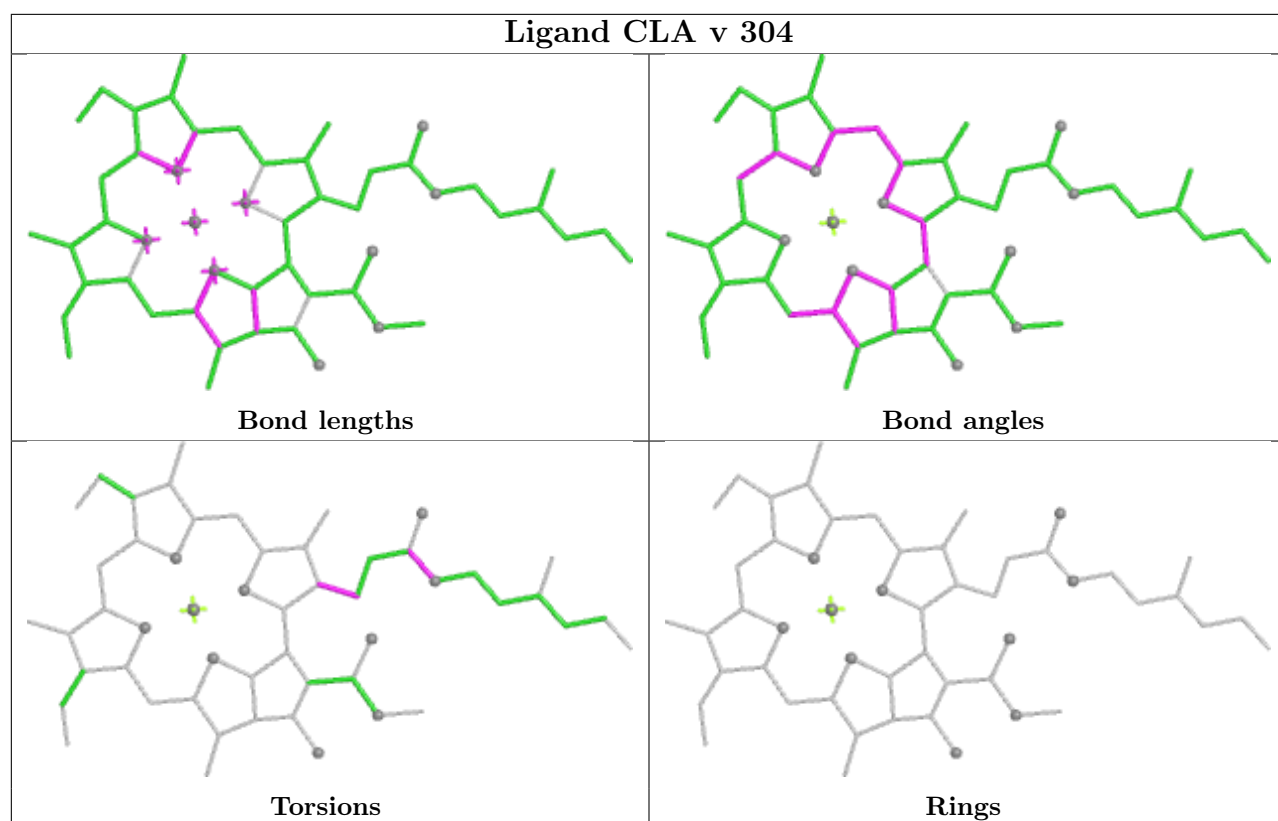
Rings

Ligand CLA y 303

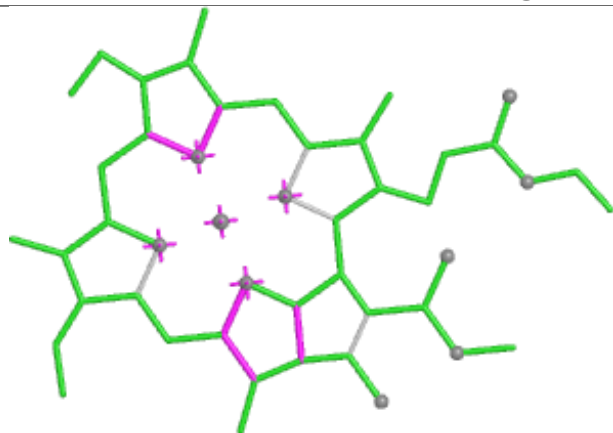


Ligand CLA E 305

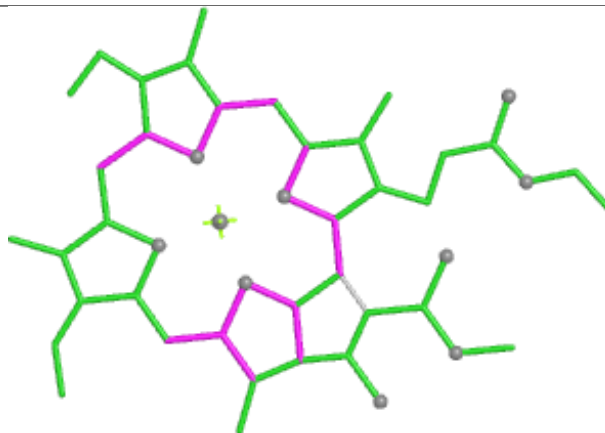




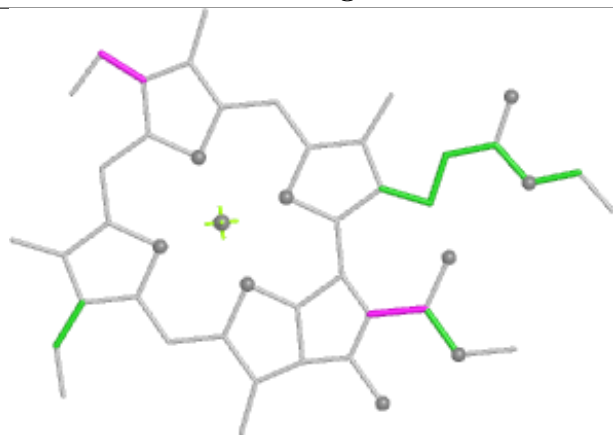
Ligand CLA x 314



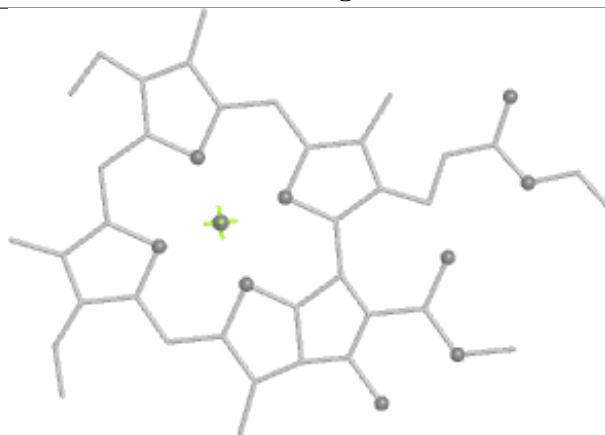
Bond lengths



Bond angles

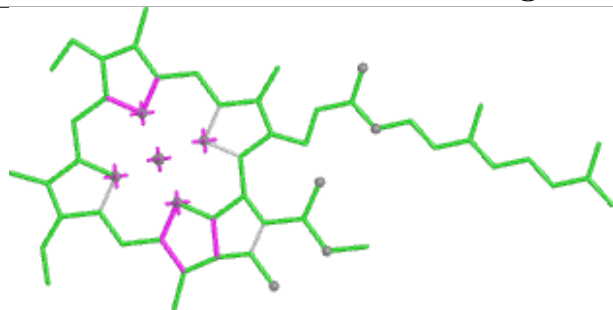


Torsions

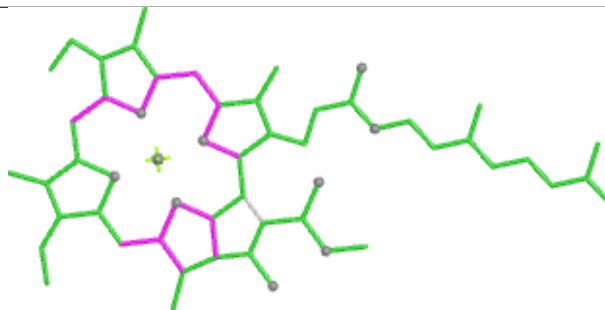


Rings

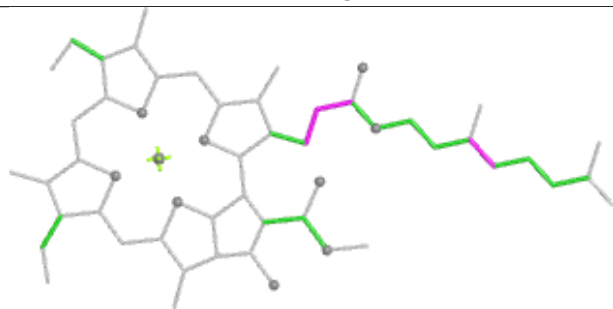
Ligand CLA z 306



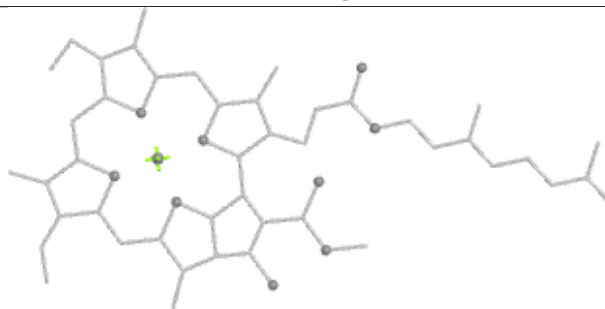
Bond lengths



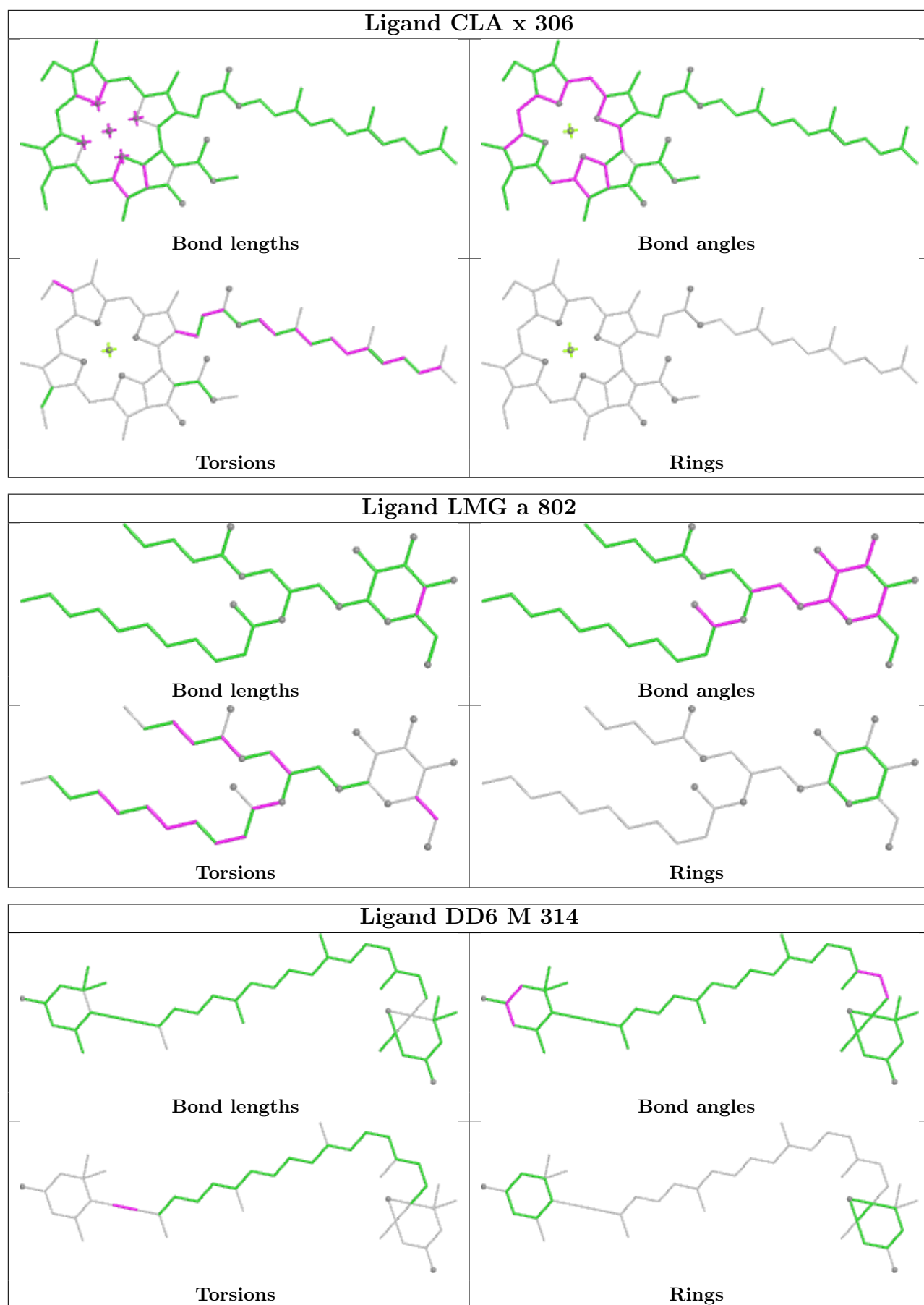
Bond angles

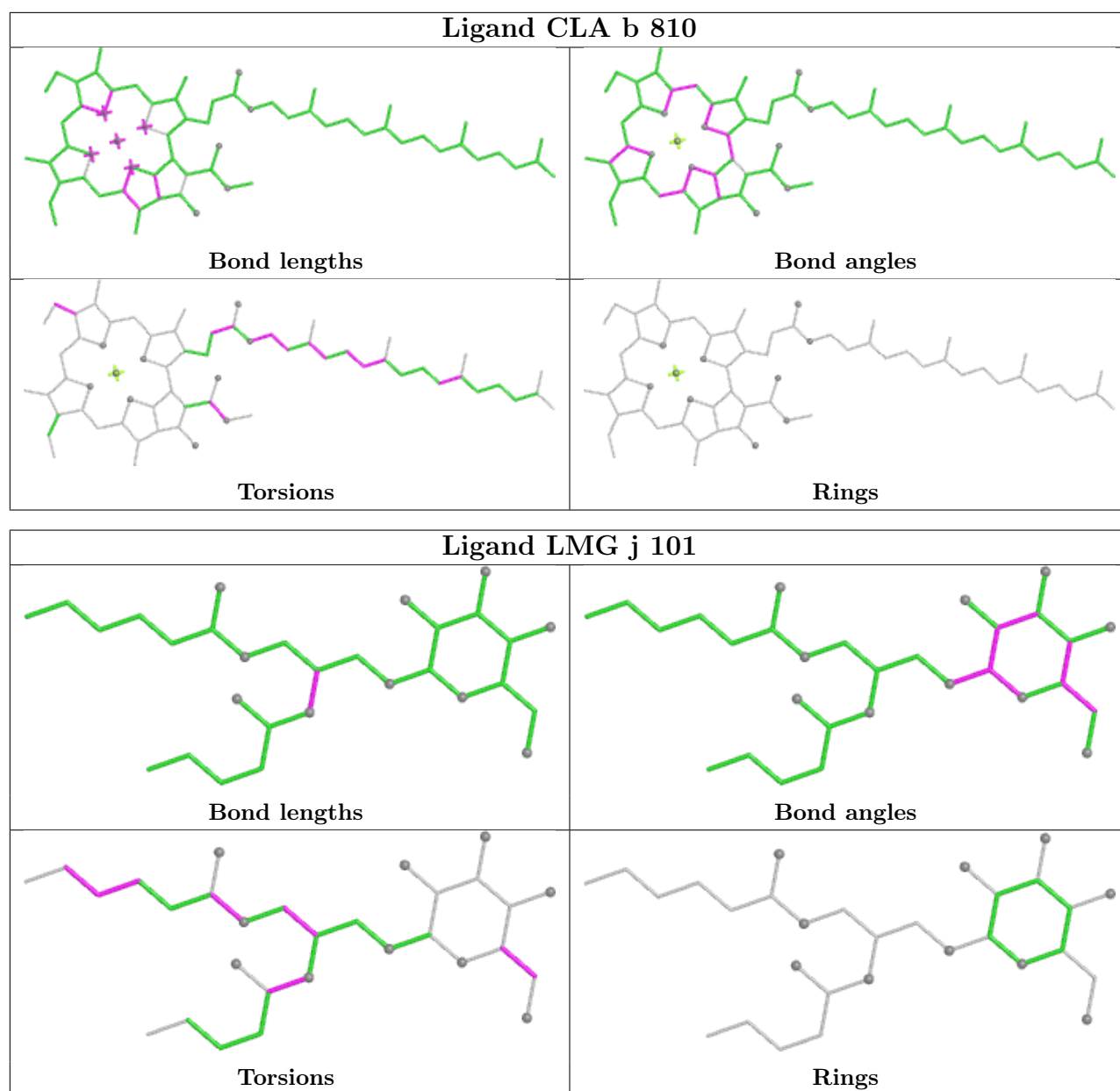


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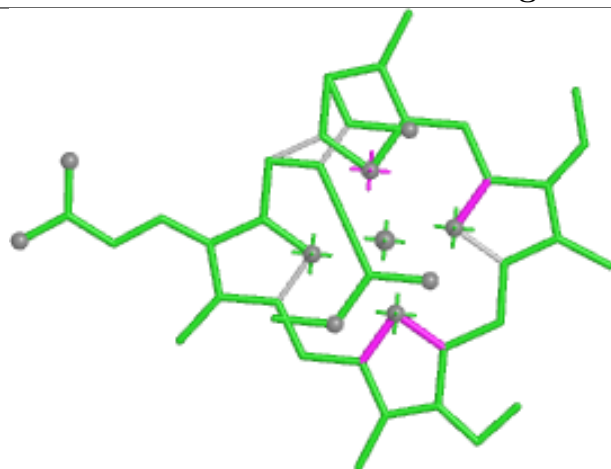


Rings

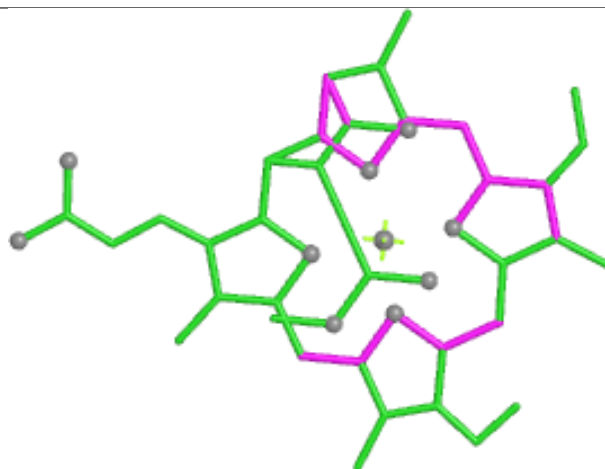




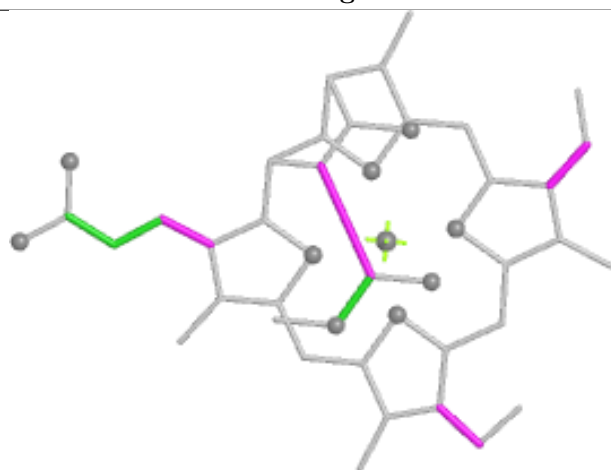
Ligand KC2 u 310



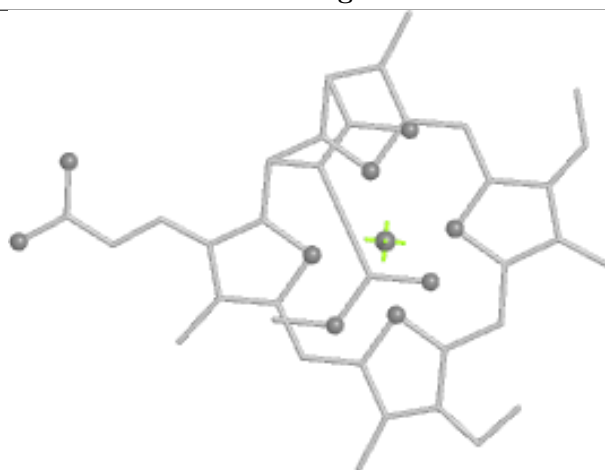
Bond lengths



Bond angles

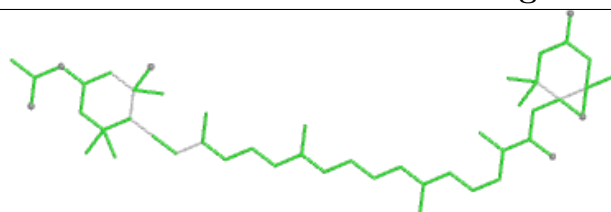


Torsions

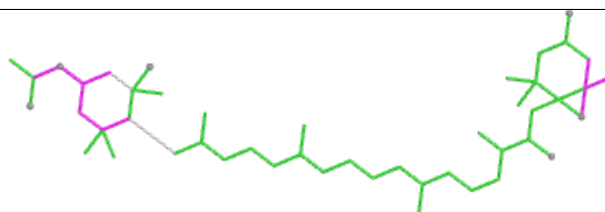


Rings

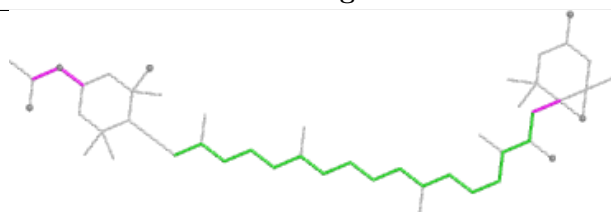
Ligand A86 X 315



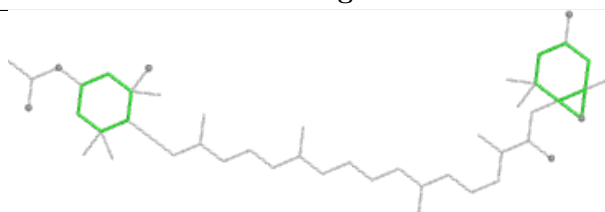
Bond lengths



Bond angles

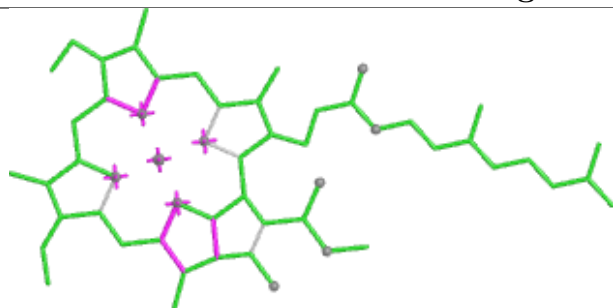


Torsions

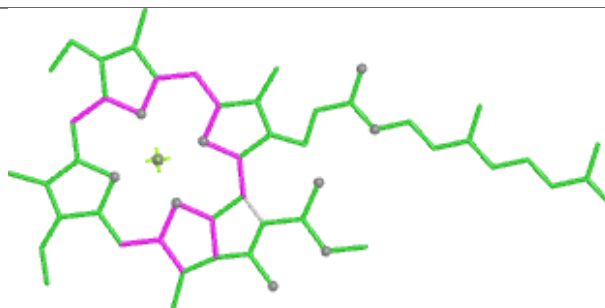


Rings

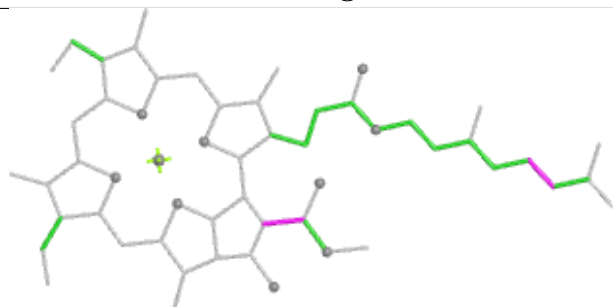
Ligand CLA b 828



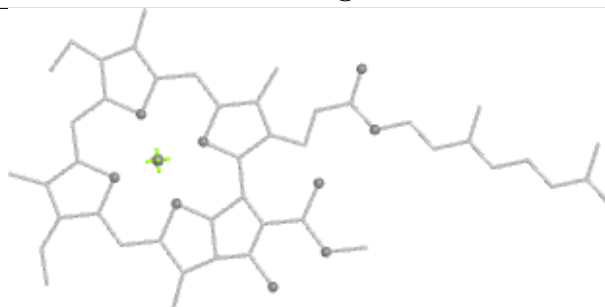
Bond lengths



Bond angles

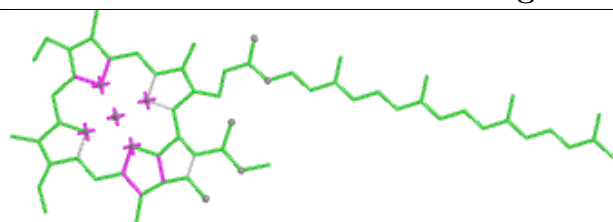


Torsions

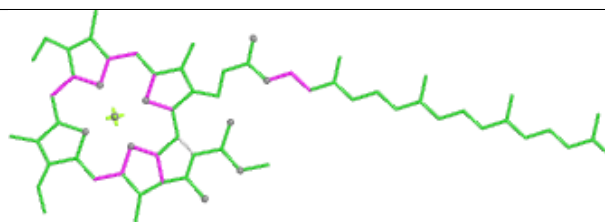


Rings

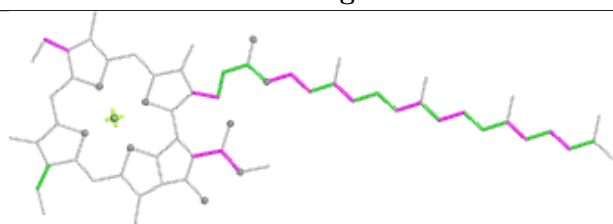
Ligand CLA b 806



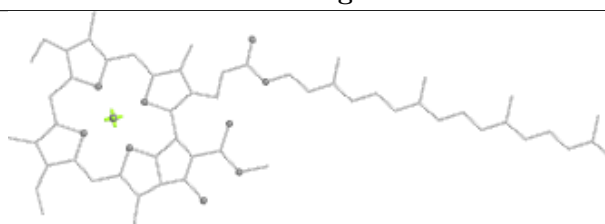
Bond lengths



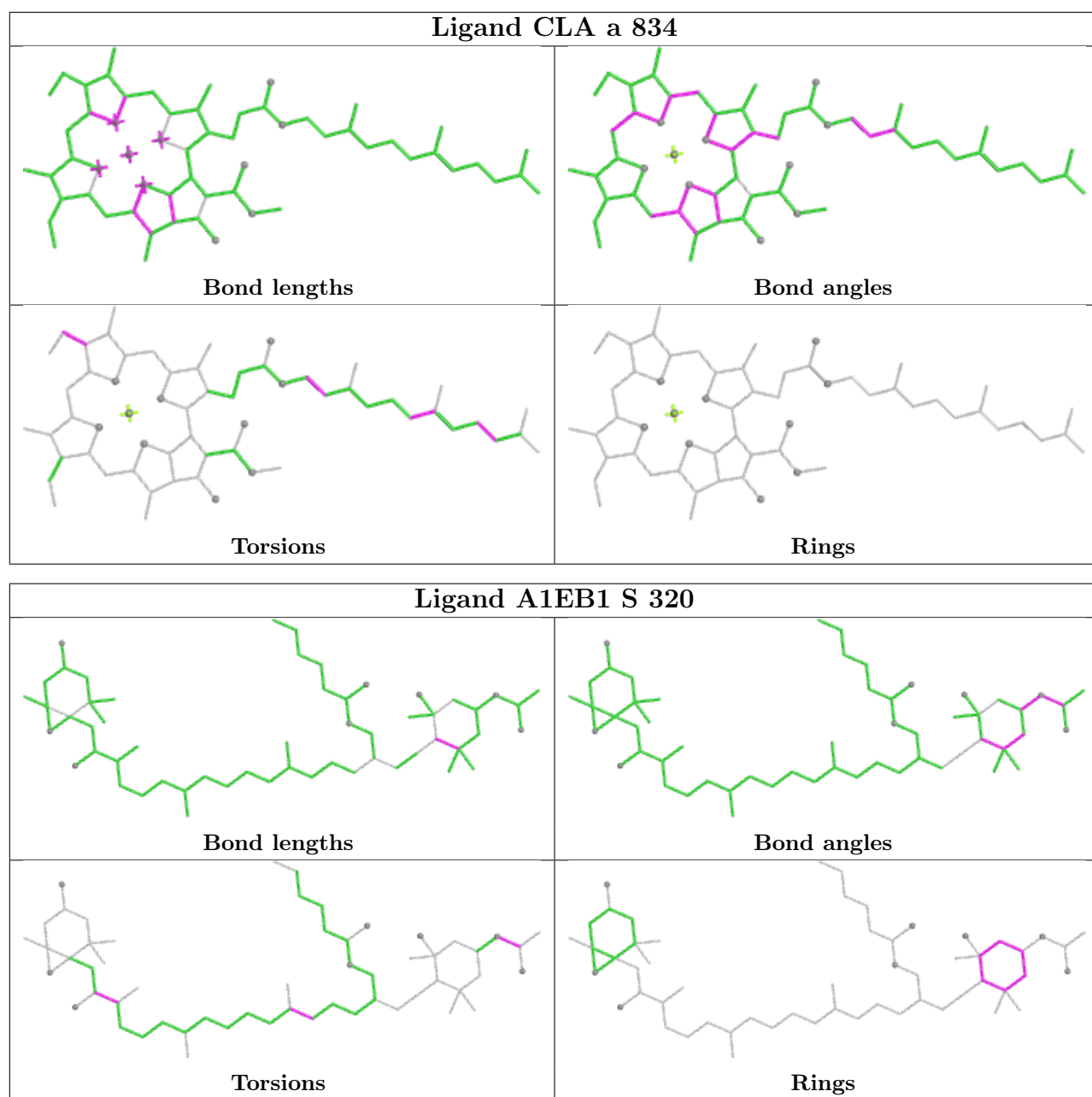
Bond angles



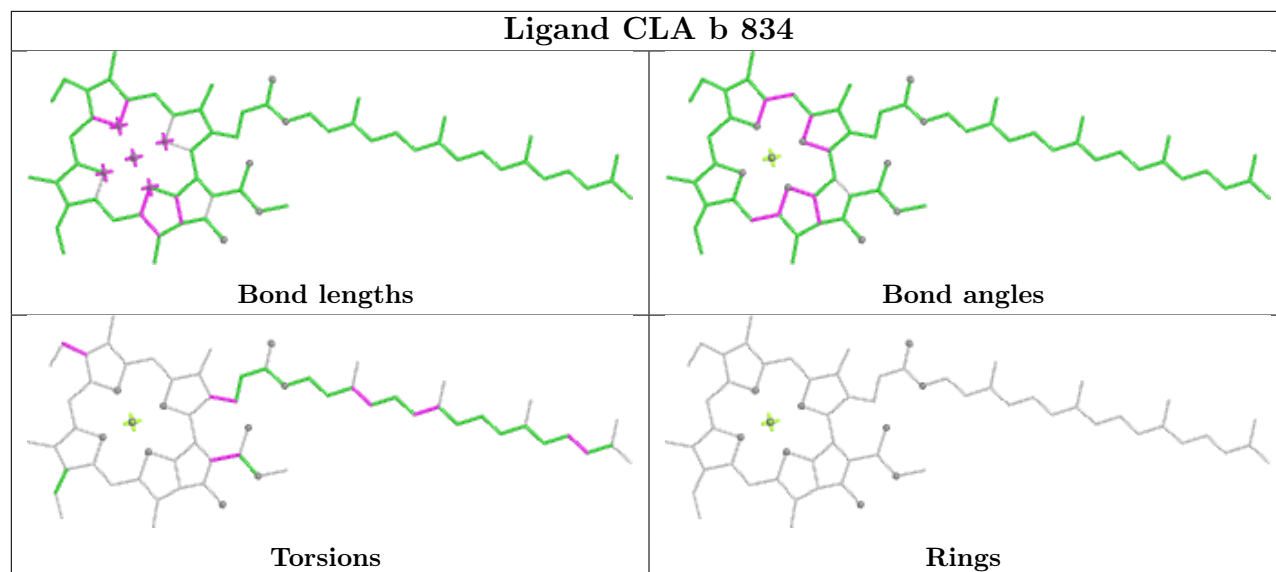
Torsions



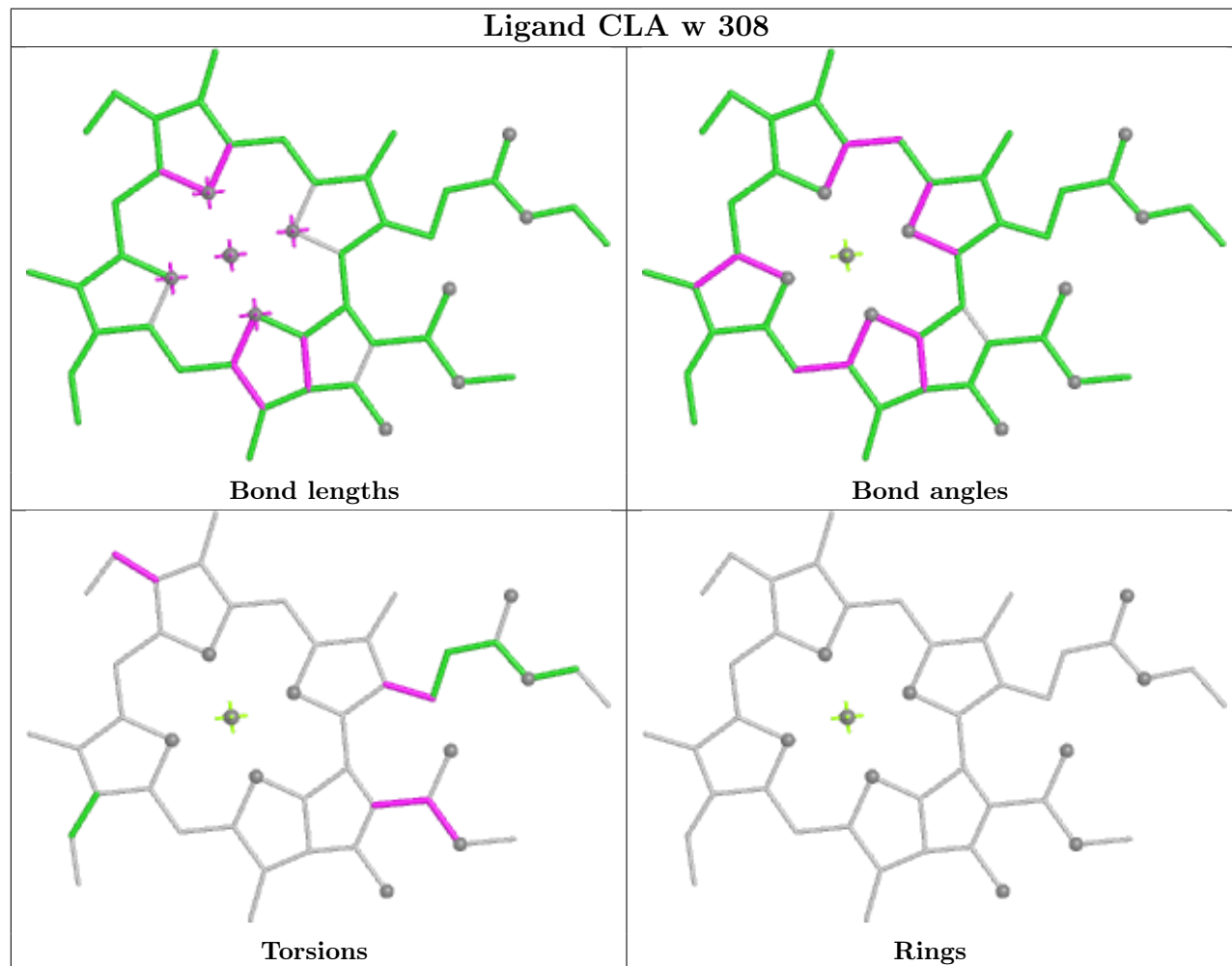
Rings

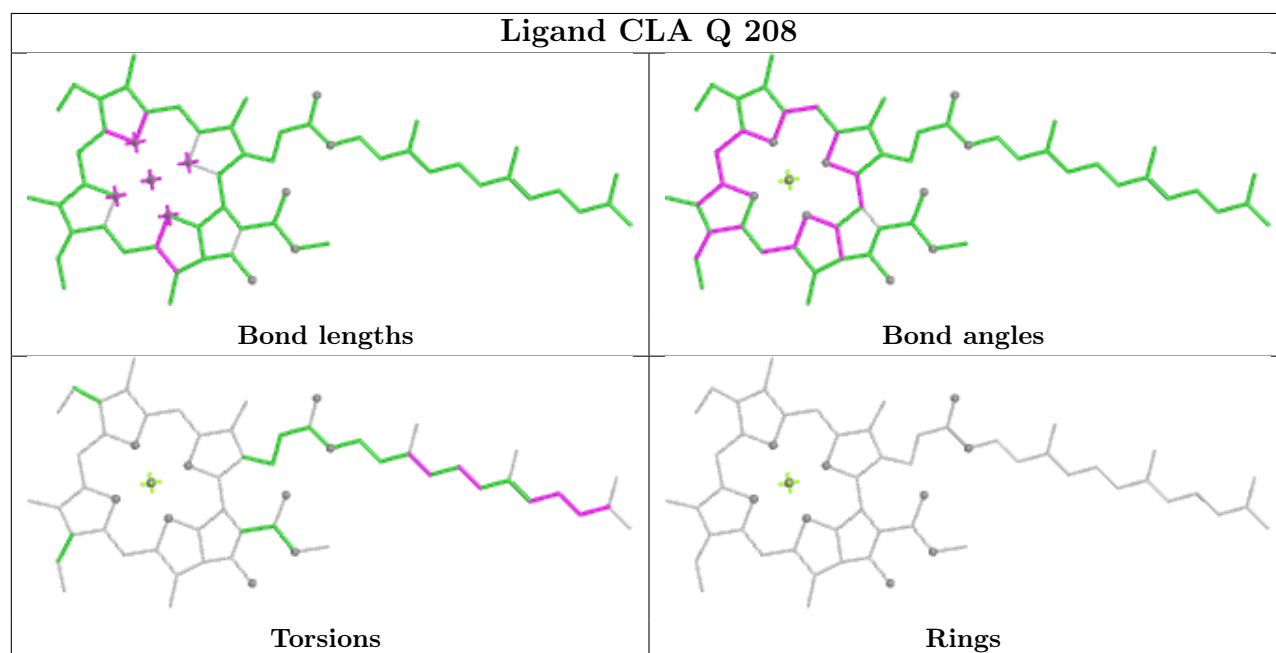
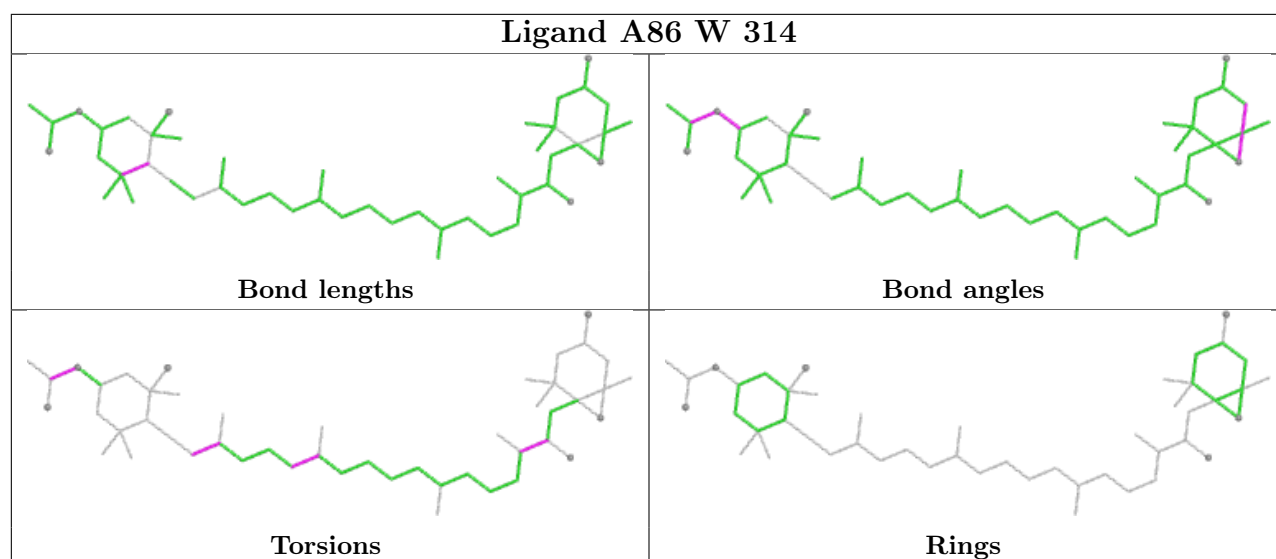


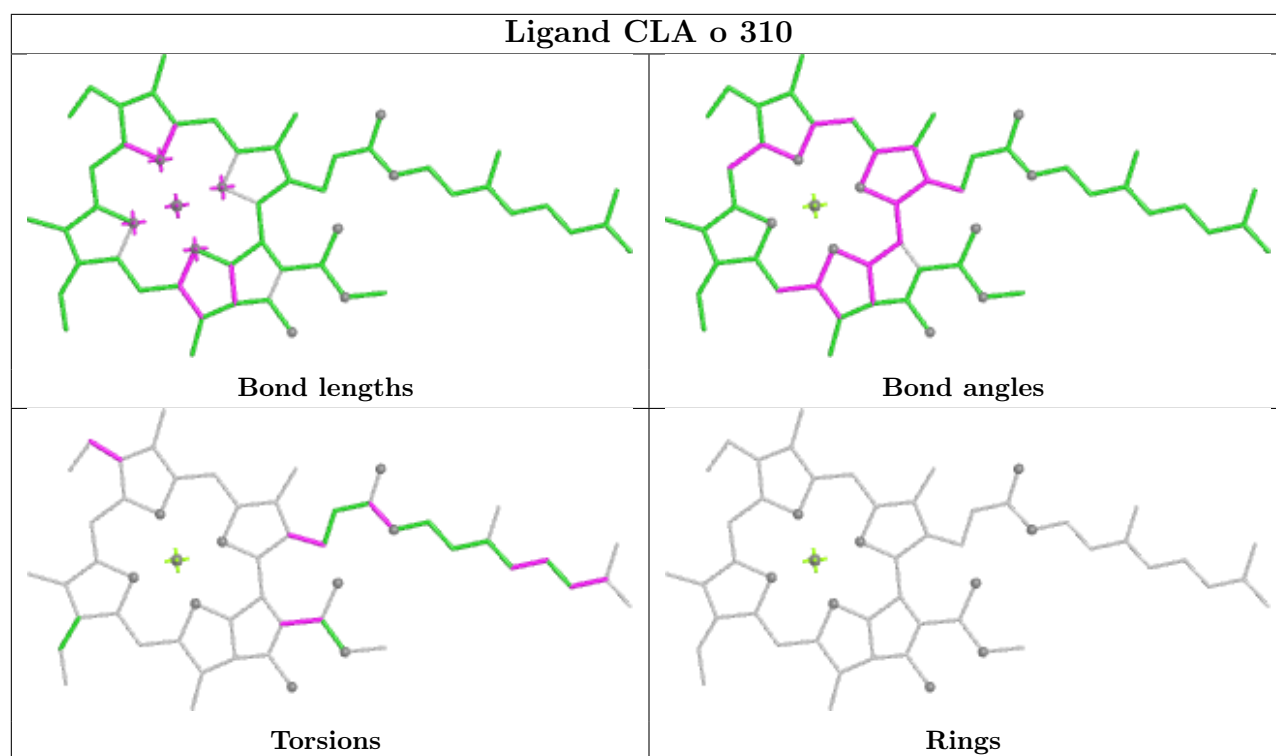
Ligand CLA b 834



Ligand CLA w 308







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.

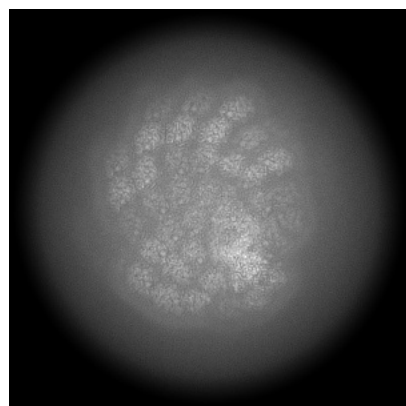
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64087. These allow visual inspection of the internal detail of the map and identification of artifacts.

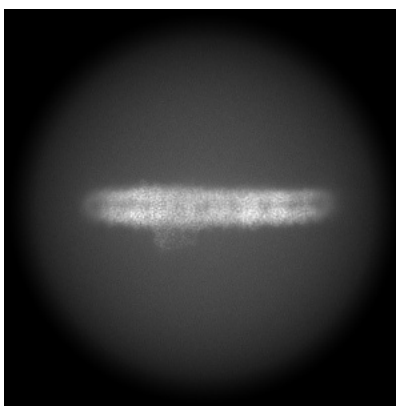
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

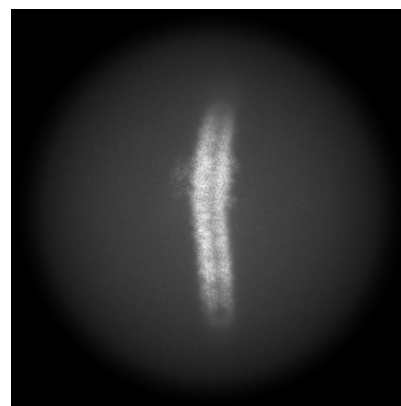
6.1.1 Primary map



X

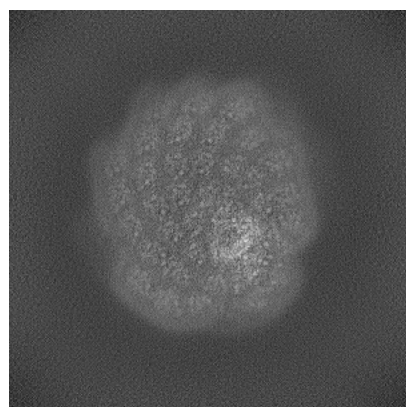


Y

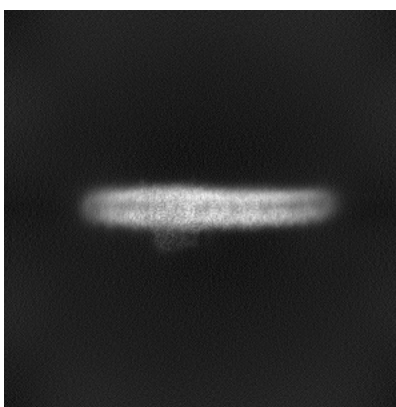


Z

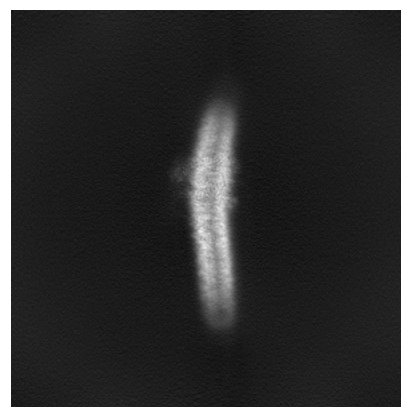
6.1.2 Raw map



X



Y

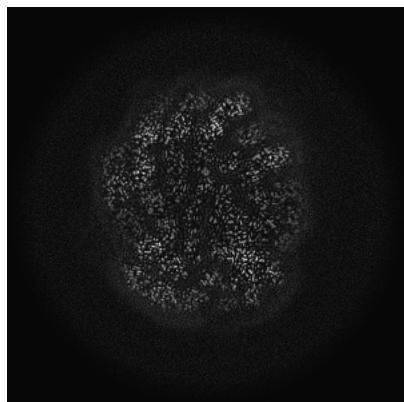


Z

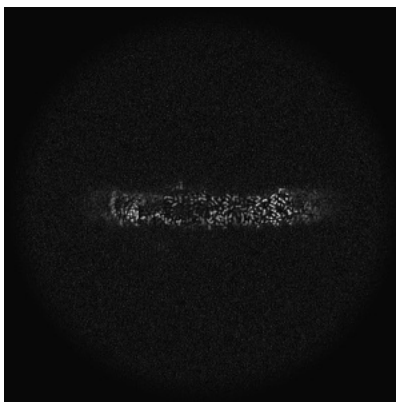
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

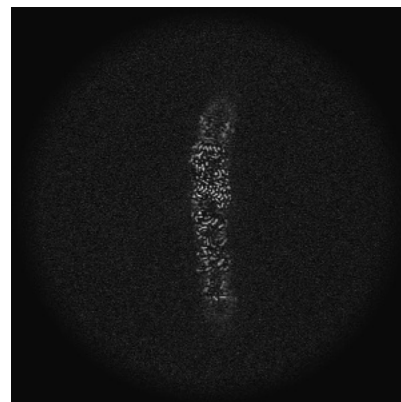
6.2.1 Primary map



X Index: 250

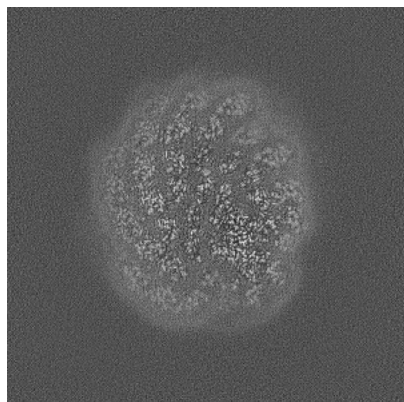


Y Index: 250

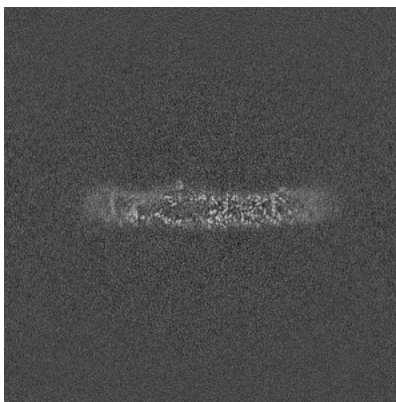


Z Index: 250

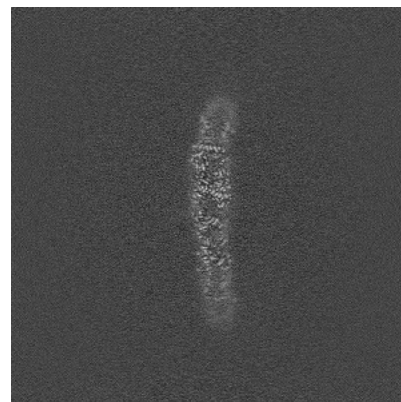
6.2.2 Raw map



X Index: 250



Y Index: 250

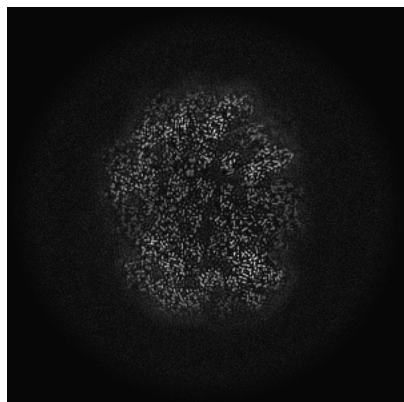


Z Index: 250

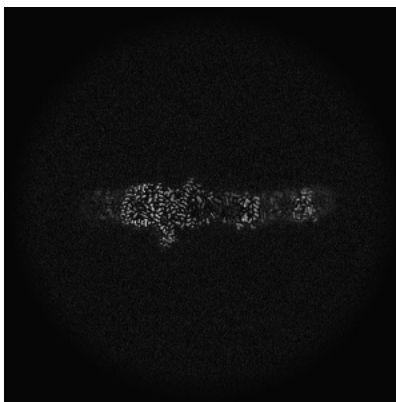
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

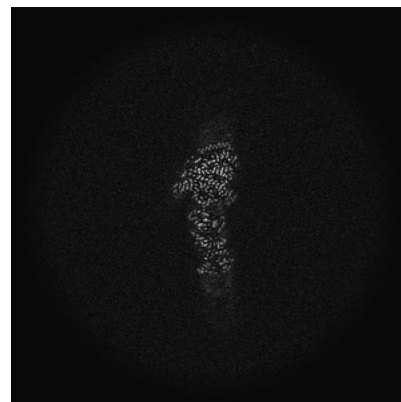
6.3.1 Primary map



X Index: 244

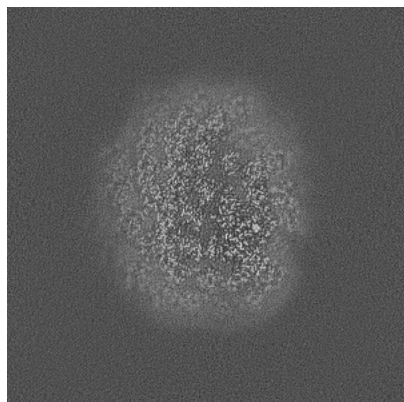


Y Index: 285



Z Index: 191

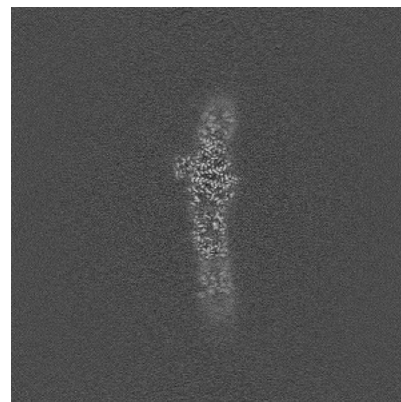
6.3.2 Raw map



X Index: 242



Y Index: 295

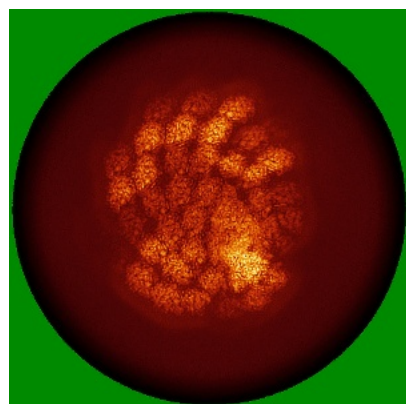


Z Index: 230

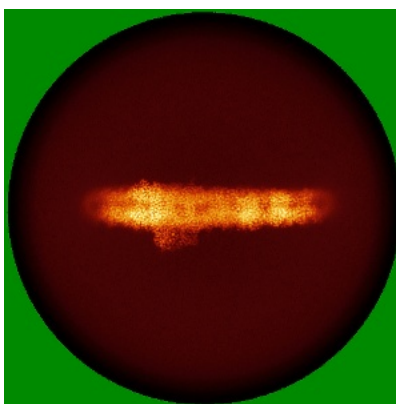
The images above show the largest variance slices of the map in three orthogonal directions.

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

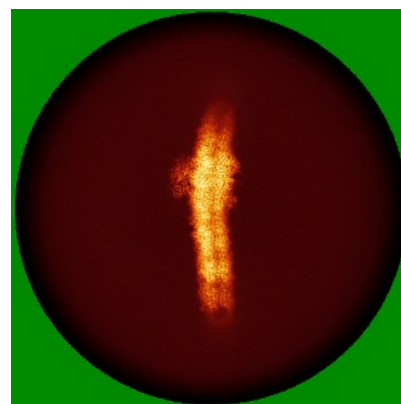
6.4.1 Primary map



X

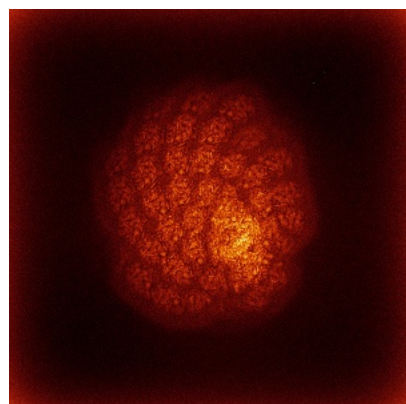


Y

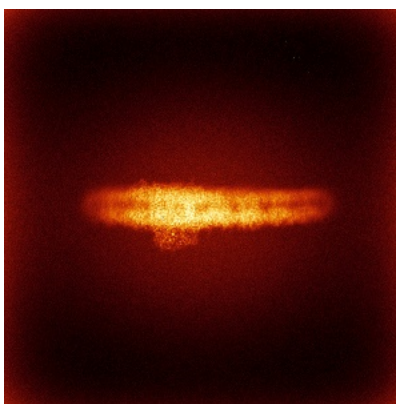


Z

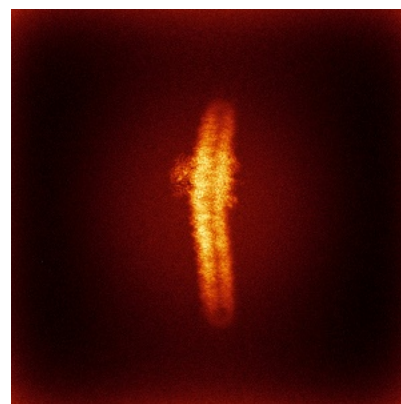
6.4.2 Raw map



X



Y

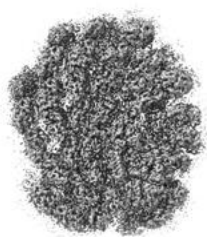


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



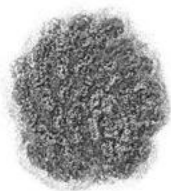
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

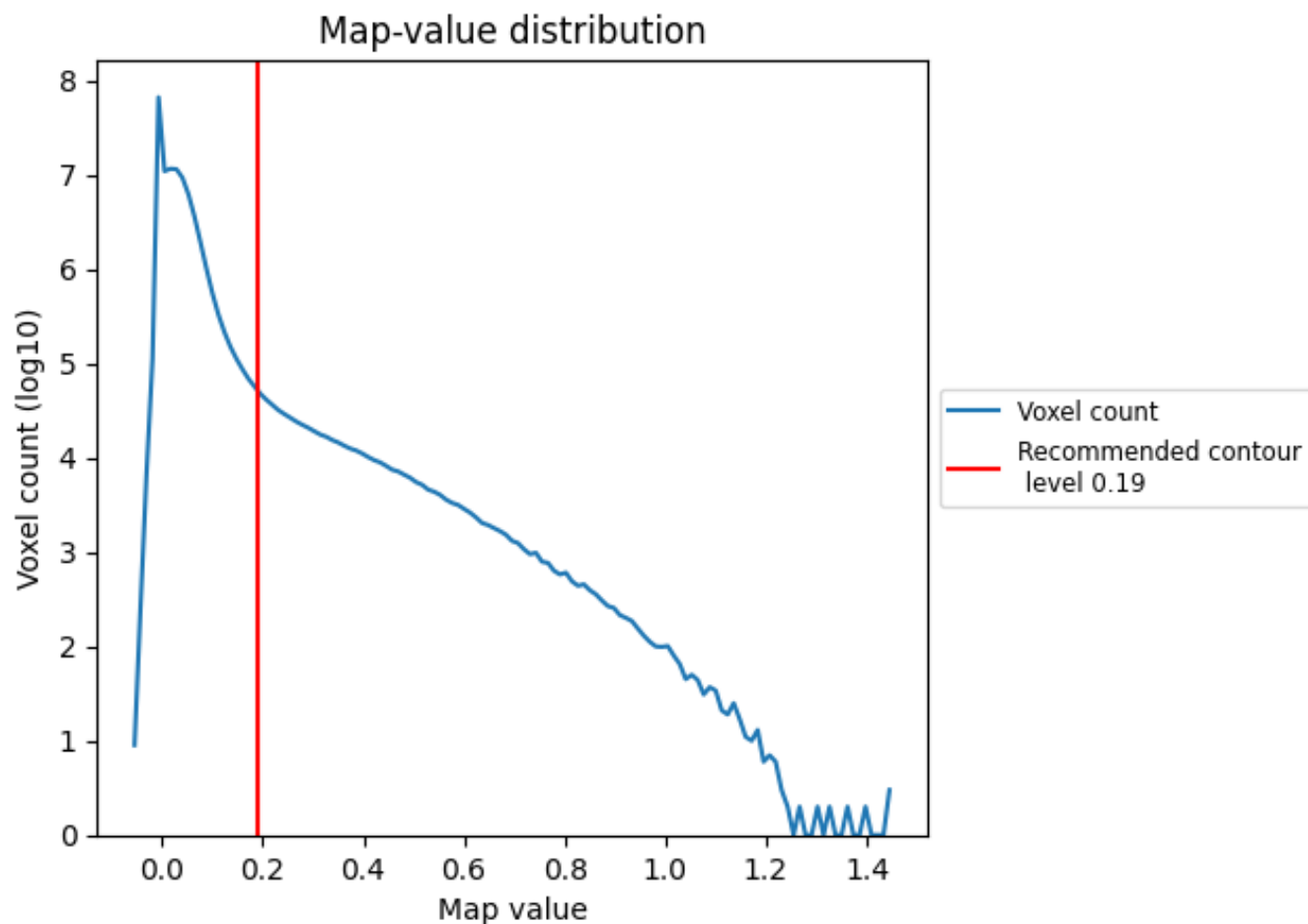
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

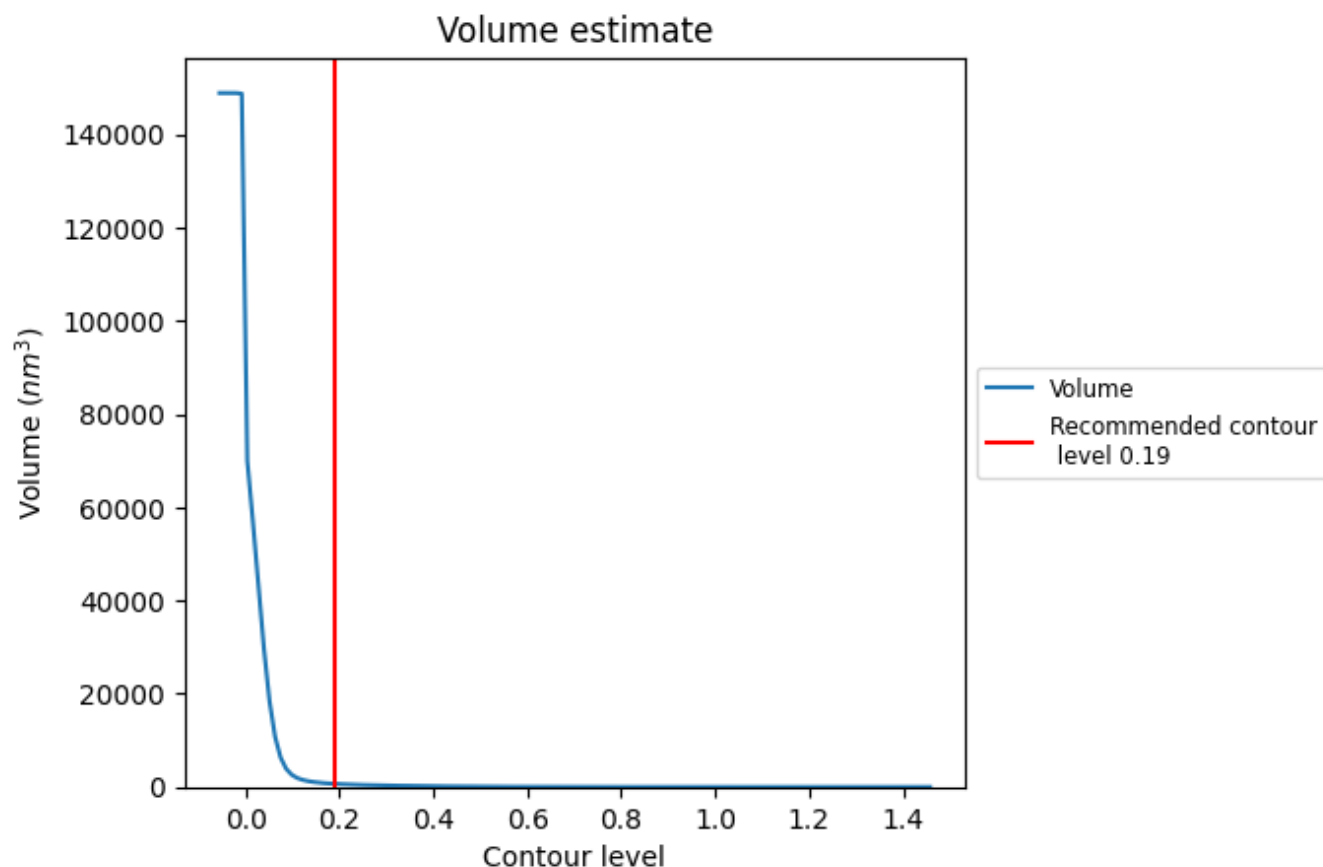
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

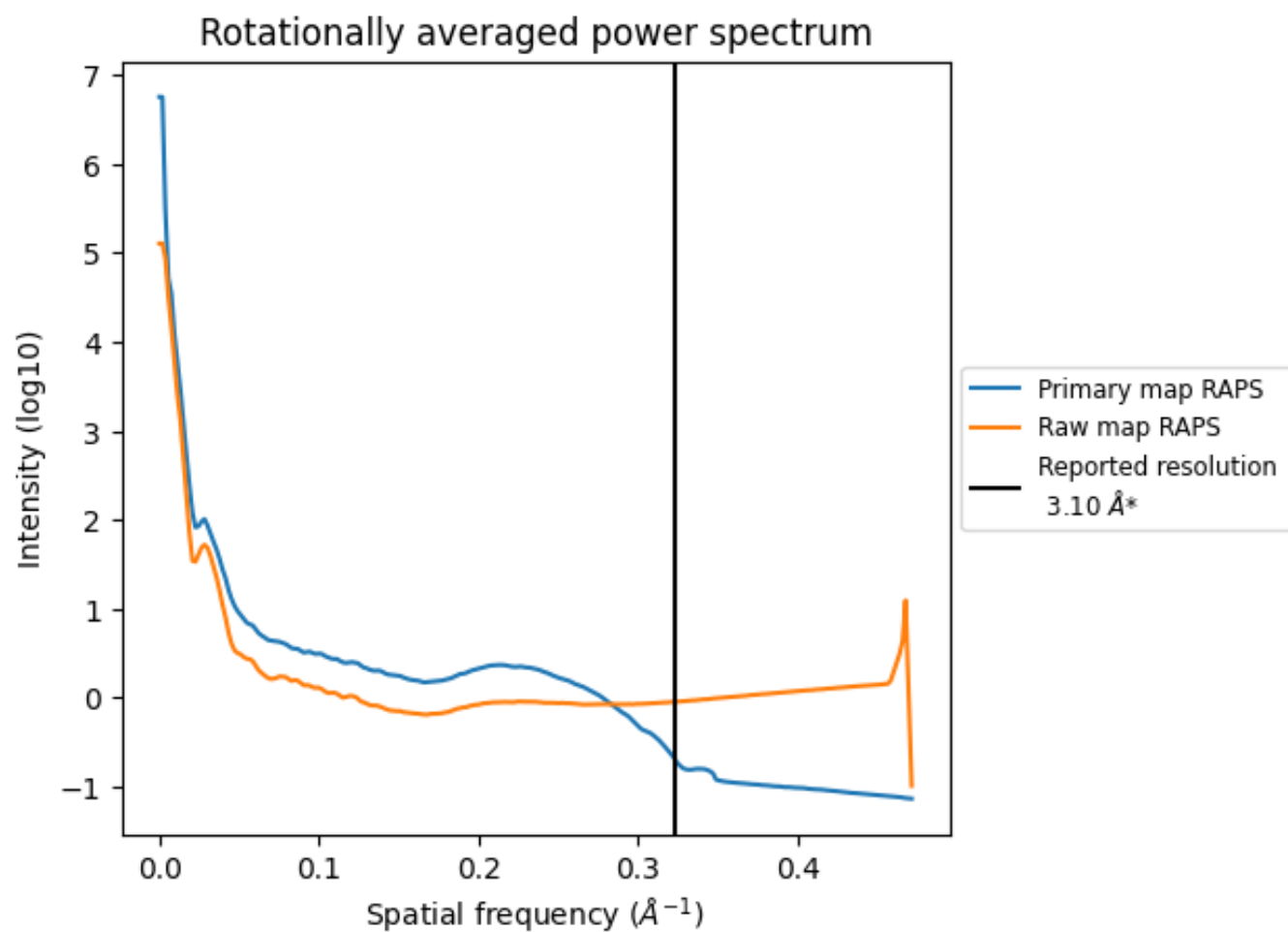
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 675 nm^3 ; this corresponds to an approximate mass of 610 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 ⓘ

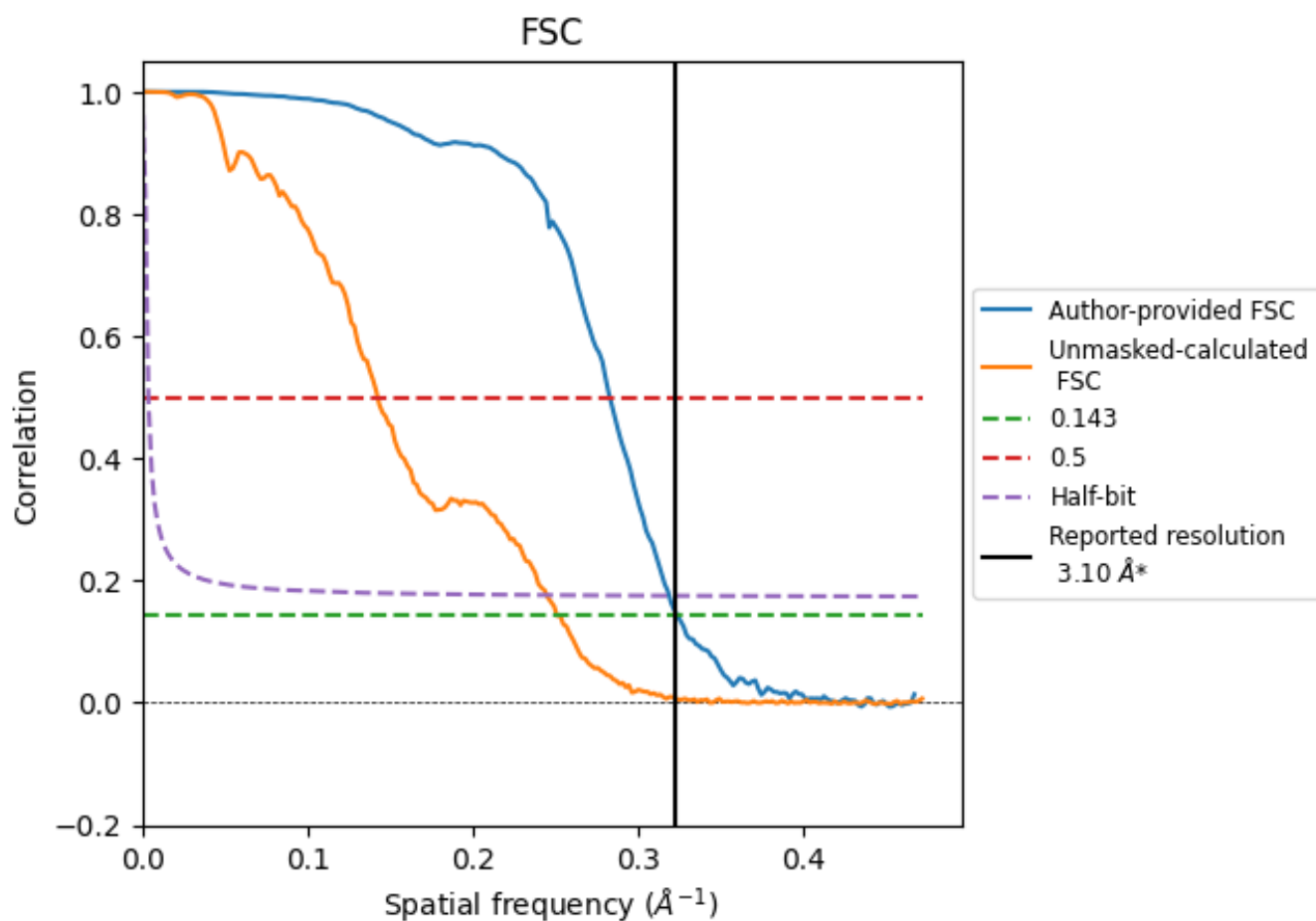


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

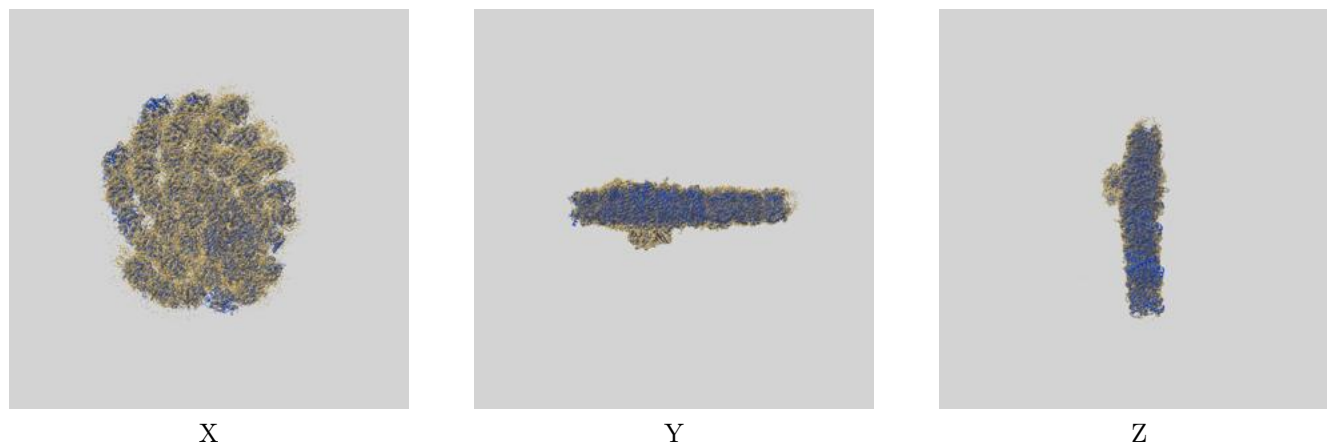
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.54	3.14
Unmasked-calculated*	3.99	7.02	4.09

*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 3.99 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

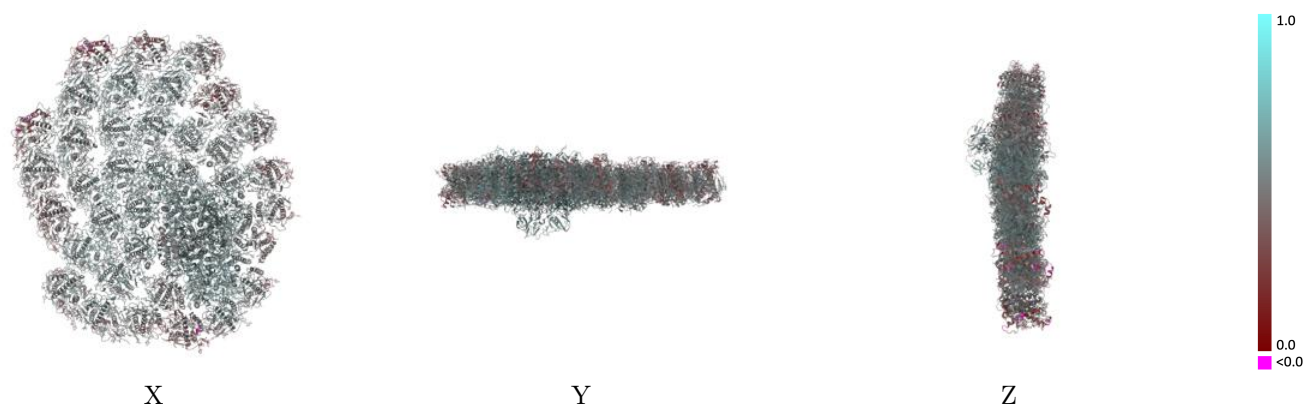
This section contains information regarding the fit between EMDB map EMD-64087 and PDB model 9UEN. Per-residue inclusion information can be found in section 3 on page 56.

9.1 Map-model overlay [i](#)



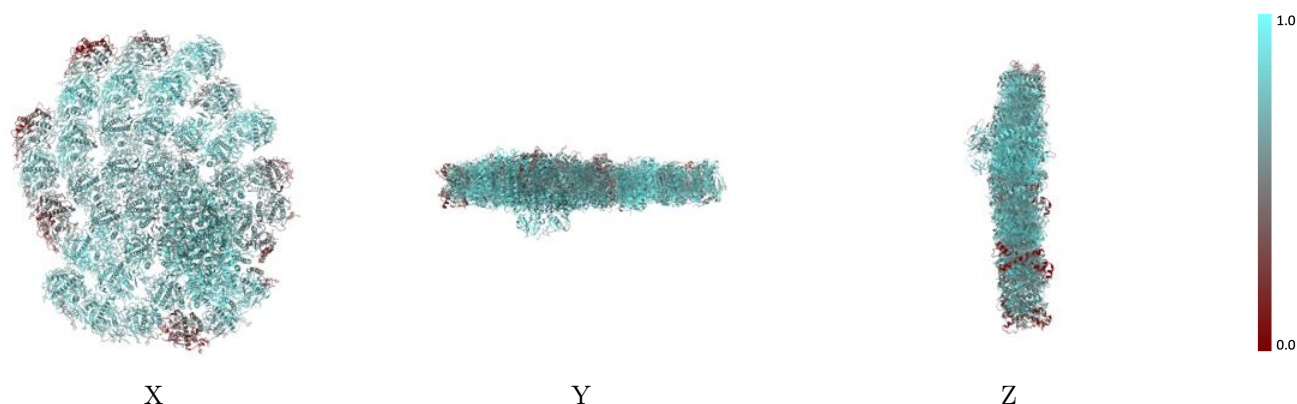
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



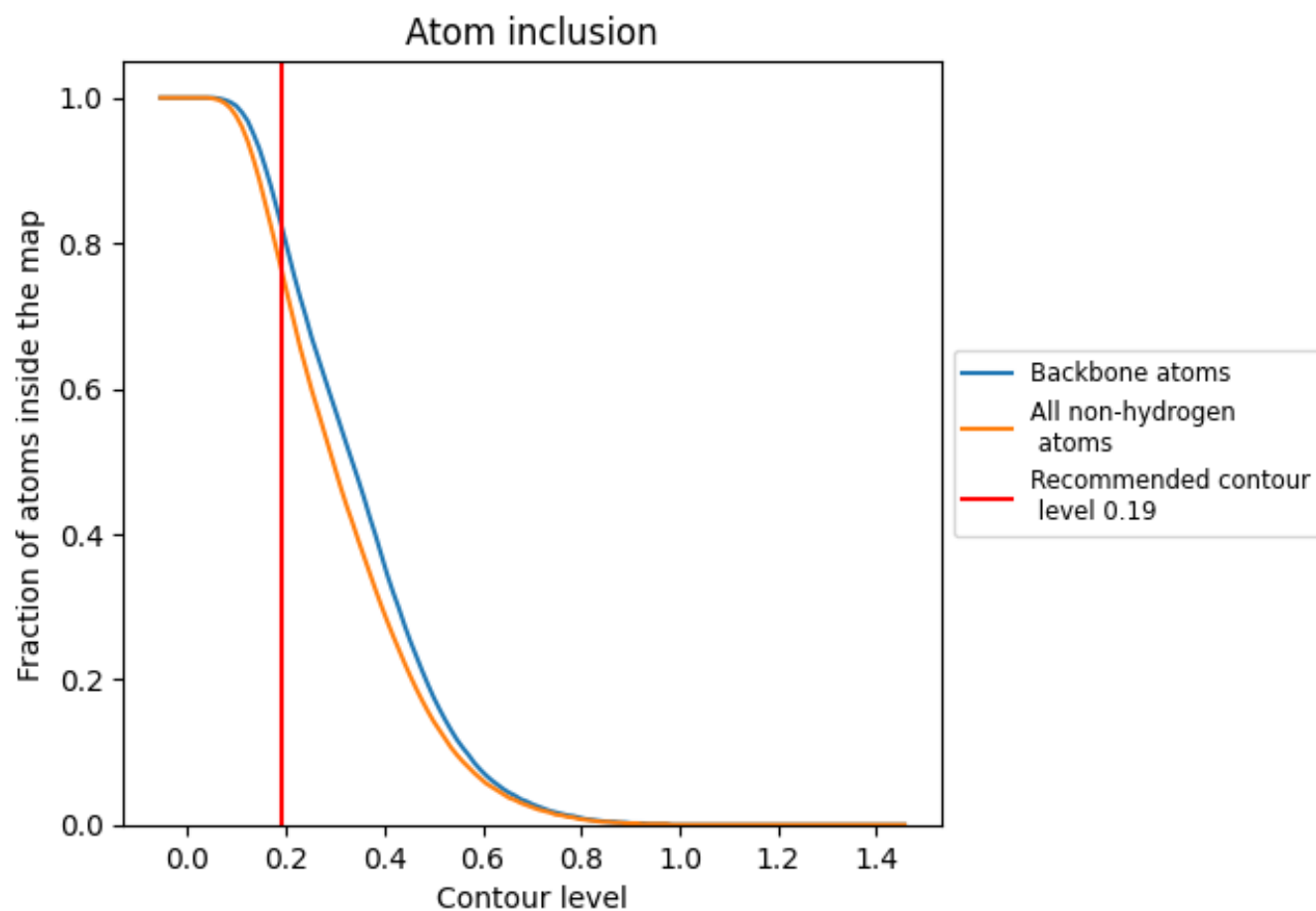
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7660	 0.5070
A	 0.8540	 0.5430
B	 0.5090	 0.4400
C	 0.7470	 0.4950
D	 0.8110	 0.5570
E	 0.8030	 0.5560
F	 0.8020	 0.4930
G	 0.8550	 0.5160
H	 0.7410	 0.4910
I	 0.7790	 0.5340
J	 0.3120	 0.3700
K	 0.8660	 0.5290
L	 0.5510	 0.4440
M	 0.7940	 0.5510
N	 0.8930	 0.5440
O	 0.7300	 0.5150
P	 0.8450	 0.5380
Q	 0.7710	 0.4710
R	 0.7610	 0.5210
S	 0.7700	 0.4820
T	 0.8420	 0.5370
U	 0.5700	 0.4500
V	 0.6860	 0.5350
W	 0.8160	 0.5330
X	 0.8200	 0.4800
Y	 0.6790	 0.3930
Z	 0.8280	 0.4820
a	 0.8520	 0.5670
b	 0.9260	 0.5770
c	 0.8680	 0.5250
d	 0.7420	 0.5330
e	 0.8640	 0.5520
f	 0.8090	 0.5240
i	 0.8080	 0.5410
j	 0.7870	 0.5320



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Chain	Atom inclusion	Q-score
k	 0.7620	 0.5340
l	 0.7870	 0.5340
m	 0.7740	 0.5160
o	 0.7600	 0.4860
p	 0.4340	 0.4220
q	 0.7230	 0.4690
r	 0.8990	 0.5550
t	 0.4880	 0.3920
u	 0.8180	 0.5080
v	 0.8360	 0.5130
w	 0.3790	 0.3720
x	 0.8920	 0.5460
y	 0.5790	 0.4230
z	 0.9090	 0.5450