



## wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 10:31 AM JST

PDB ID : 8IWH  
EMDB ID : EMD-35766  
Title : Structure and characteristics of a photosystem II supercomplex containing monomeric LHCX and dimeric FCP II antennae from the diatom *Thalassiosira pseudonana*  
Authors : Feng, Y.; Li, Z.H.; Wang, W.D.; Shen, J.R.  
Deposited on : 2023-03-30  
Resolution : 2.68 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](mailto: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>.

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

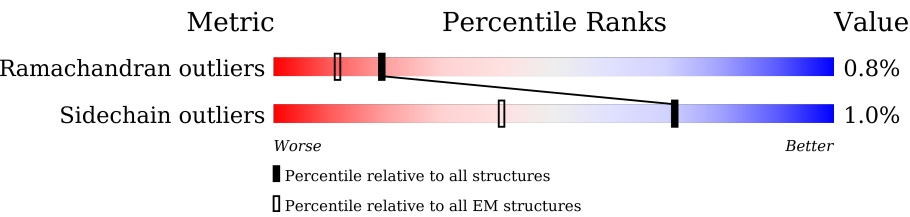
EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 2.68 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.







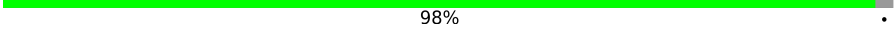
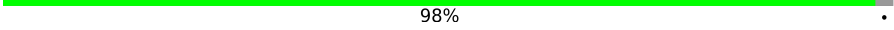
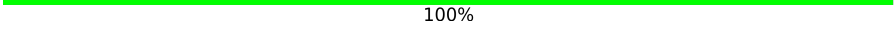
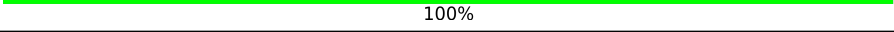



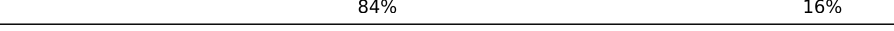
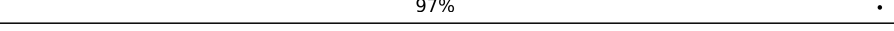
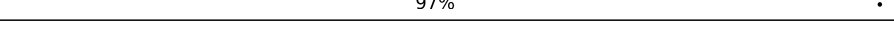


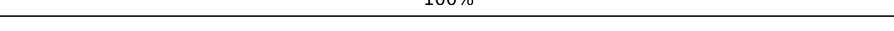
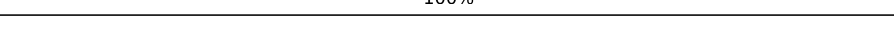

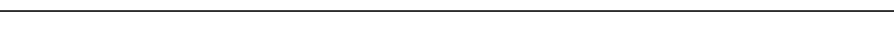

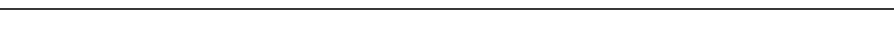
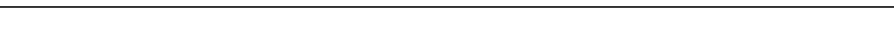


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	333	<div><div></div><div>99%</div><div>.</div></div>
1	a	333	<div><div></div><div>100%</div><div></div></div>
2	B	509	<div><div></div><div>94%</div><div>6%</div></div>
2	b	509	<div><div></div><div>94%</div><div>6%</div></div>
3	C	470	<div><div></div><div>96%</div><div>.</div></div>
3	c	470	<div><div></div><div>96%</div><div>.</div></div>
4	D	351	<div><div></div><div>97%</div><div>.</div></div>
4	d	351	<div><div></div><div>97%</div><div>..</div></div>
5	E	84	<div><div></div><div>90%</div><div>10%</div></div>
5	e	84	<div><div></div><div>90%</div><div>10%</div></div>


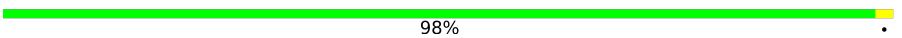



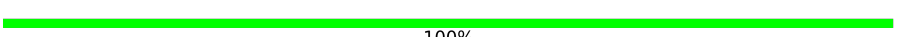
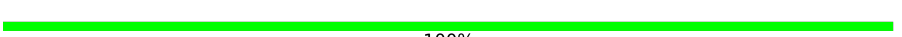



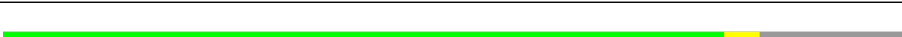

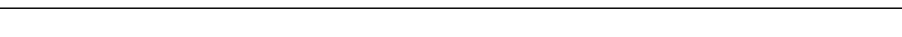
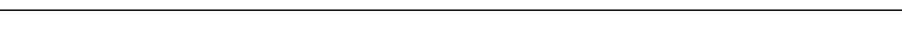
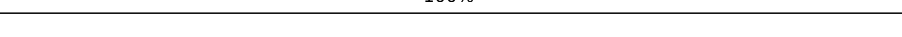
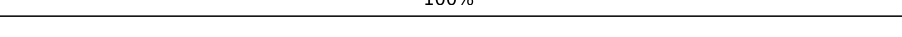

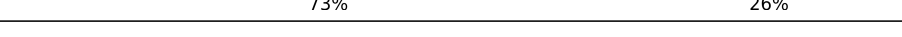

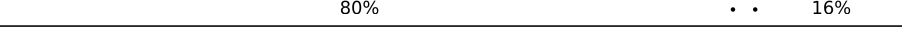
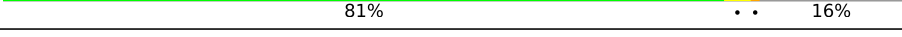
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Mol	Chain	Length	Quality of chain
6	F	43	 63%9%28%
6	f	43	 72%28%
7	G	176	 68%32%
7	g	176	 68%32%
8	H	66	 98%. .
8	h	66	 98%. .
9	I	34	 100%
9	i	34	 100%
10	J	39	 85%15%
10	j	39	 85%15%
11	K	44	 84%16%
11	k	44	 84%16%
12	L	38	 97%. .
12	l	38	 97%. .
13	M	113	 36%64%
13	m	113	 36%64%
14	N	30	 100%
14	n	30	 100%
15	O	305	 79%..19%
15	o	305	 79%.19%
16	T	28	 100%
16	t	28	 100%
17	U	148	 62%38%
17	u	148	 60%.38%
18	V	162	 81%..17%

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Mol	Chain	Length	Quality of chain
18	v	162	
19	W	54	
19	w	54	
20	X	38	
20	x	38	
21	Z	61	
21	z	61	
22	3	220	
23	4	196	
24	5	192	
25	6	199	
26	0	199	
26	7	199	
27	Y	34	
27	y	34	
28	Q	211	
28	q	211	
29	1	193	
29	2	193	
29	8	193	
29	9	193	

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
33	CLA	0	304	X	-	-	-
33	CLA	0	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	0	307	X	-	-	-
33	CLA	0	308	X	-	-	-
33	CLA	0	309	X	-	-	-
33	CLA	0	310	X	-	-	-
33	CLA	0	311	X	-	-	-
33	CLA	0	312	X	-	-	-
33	CLA	0	313	X	-	-	-
33	CLA	1	305	X	-	-	-
33	CLA	1	306	X	-	-	-
33	CLA	1	307	X	-	-	-
33	CLA	1	308	X	-	-	-
33	CLA	1	309	X	-	-	-
33	CLA	1	310	X	-	-	-
33	CLA	1	311	X	-	-	-
33	CLA	1	312	X	-	-	-
33	CLA	1	313	X	-	-	-
33	CLA	1	314	X	-	-	-
33	CLA	1	315	X	-	-	-
33	CLA	1	316	X	-	-	-
33	CLA	2	305	X	-	-	-
33	CLA	2	306	X	-	-	-
33	CLA	2	307	X	-	-	-
33	CLA	2	308	X	-	-	-
33	CLA	2	309	X	-	-	-
33	CLA	2	310	X	-	-	-
33	CLA	2	311	X	-	-	-
33	CLA	2	312	X	-	-	-
33	CLA	2	314	X	-	-	-
33	CLA	2	315	X	-	-	-
33	CLA	2	316	X	-	-	-
33	CLA	2	317	X	-	-	-
33	CLA	3	302	X	-	-	-
33	CLA	3	303	X	-	-	-
33	CLA	3	304	X	-	-	-
33	CLA	3	305	X	-	-	-
33	CLA	3	306	X	-	-	-
33	CLA	3	307	X	-	-	-
33	CLA	3	308	X	-	-	-
33	CLA	3	309	X	-	-	-
33	CLA	3	311	X	-	-	-
33	CLA	3	312	X	-	-	-
33	CLA	3	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	3	319	X	-	-	-
33	CLA	4	305	X	-	-	-
33	CLA	4	306	X	-	-	-
33	CLA	4	308	X	-	-	-
33	CLA	4	309	X	-	-	-
33	CLA	4	310	X	-	-	-
33	CLA	4	311	X	-	-	-
33	CLA	4	312	X	-	-	-
33	CLA	4	313	X	-	-	-
33	CLA	4	314	X	-	-	-
33	CLA	4	315	X	-	-	-
33	CLA	4	316	X	-	-	-
33	CLA	5	308	X	-	-	-
33	CLA	5	309	X	-	-	-
33	CLA	5	311	X	-	-	-
33	CLA	5	312	X	-	-	-
33	CLA	5	313	X	-	-	-
33	CLA	5	314	X	-	-	-
33	CLA	5	316	X	-	-	-
33	CLA	5	317	X	-	-	-
33	CLA	6	307	X	-	-	-
33	CLA	6	308	X	-	-	-
33	CLA	6	310	X	-	-	-
33	CLA	6	311	X	-	-	-
33	CLA	6	312	X	-	-	-
33	CLA	6	313	X	-	-	-
33	CLA	6	315	X	-	-	-
33	CLA	6	316	X	-	-	-
33	CLA	7	304	X	-	-	-
33	CLA	7	305	X	-	-	-
33	CLA	7	307	X	-	-	-
33	CLA	7	308	X	-	-	-
33	CLA	7	309	X	-	-	-
33	CLA	7	310	X	-	-	-
33	CLA	7	311	X	-	-	-
33	CLA	7	312	X	-	-	-
33	CLA	7	313	X	-	-	-
33	CLA	7	314	X	-	-	-
33	CLA	8	305	X	-	-	-
33	CLA	8	306	X	-	-	-
33	CLA	8	307	X	-	-	-
33	CLA	8	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	8	309	X	-	-	-
33	CLA	8	310	X	-	-	-
33	CLA	8	311	X	-	-	-
33	CLA	8	312	X	-	-	-
33	CLA	8	313	X	-	-	-
33	CLA	8	314	X	-	-	-
33	CLA	8	315	X	-	-	-
33	CLA	8	316	X	-	-	-
33	CLA	9	305	X	-	-	-
33	CLA	9	306	X	-	-	-
33	CLA	9	307	X	-	-	-
33	CLA	9	308	X	-	-	-
33	CLA	9	309	X	-	-	-
33	CLA	9	310	X	-	-	-
33	CLA	9	311	X	-	-	-
33	CLA	9	312	X	-	-	-
33	CLA	9	313	X	-	-	-
33	CLA	9	314	X	-	-	-
33	CLA	9	315	X	-	-	-
33	CLA	9	316	X	-	-	-
33	CLA	9	317	X	-	-	-
33	CLA	A	404	X	-	-	-
33	CLA	A	405	X	-	-	-
33	CLA	A	408	X	-	-	-
33	CLA	B	601	X	-	-	-
33	CLA	B	602	X	-	-	-
33	CLA	B	603	X	-	-	-
33	CLA	B	604	X	-	-	-
33	CLA	B	605	X	-	-	-
33	CLA	B	606	X	-	-	-
33	CLA	B	607	X	-	-	-
33	CLA	B	608	X	-	-	-
33	CLA	B	609	X	-	-	-
33	CLA	B	610	X	-	-	-
33	CLA	B	611	X	-	-	-
33	CLA	B	612	X	-	-	-
33	CLA	B	613	X	-	-	-
33	CLA	B	614	X	-	-	-
33	CLA	B	615	X	-	-	-
33	CLA	B	616	X	-	-	-
33	CLA	C	501	X	-	-	-
33	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	C	503	X	-	-	-
33	CLA	C	504	X	-	-	-
33	CLA	C	505	X	-	-	-
33	CLA	C	506	X	-	-	-
33	CLA	C	507	X	-	-	-
33	CLA	C	508	X	-	-	-
33	CLA	C	509	X	-	-	-
33	CLA	C	510	X	-	-	-
33	CLA	C	511	X	-	-	-
33	CLA	C	512	X	-	-	-
33	CLA	C	513	X	-	-	-
33	CLA	D	402	X	-	-	-
33	CLA	D	405	X	-	-	-
33	CLA	D	406	X	-	-	-
33	CLA	H	103	X	-	-	-
33	CLA	W	303	X	-	-	-
33	CLA	Z	101	X	-	-	-
33	CLA	a	407	X	-	-	-
33	CLA	a	408	X	-	-	-
33	CLA	a	411	X	-	-	-
33	CLA	b	602	X	-	-	-
33	CLA	b	603	X	-	-	-
33	CLA	b	604	X	-	-	-
33	CLA	b	605	X	-	-	-
33	CLA	b	606	X	-	-	-
33	CLA	b	607	X	-	-	-
33	CLA	b	608	X	-	-	-
33	CLA	b	609	X	-	-	-
33	CLA	b	610	X	-	-	-
33	CLA	b	611	X	-	-	-
33	CLA	b	612	X	-	-	-
33	CLA	b	613	X	-	-	-
33	CLA	b	614	X	-	-	-
33	CLA	b	615	X	-	-	-
33	CLA	b	616	X	-	-	-
33	CLA	b	617	X	-	-	-
33	CLA	c	501	X	-	-	-
33	CLA	c	502	X	-	-	-
33	CLA	c	503	X	-	-	-
33	CLA	c	504	X	-	-	-
33	CLA	c	505	X	-	-	-
33	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	c	507	X	-	-	-
33	CLA	c	508	X	-	-	-
33	CLA	c	509	X	-	-	-
33	CLA	c	510	X	-	-	-
33	CLA	c	511	X	-	-	-
33	CLA	c	512	X	-	-	-
33	CLA	c	513	X	-	-	-
33	CLA	d	401	X	-	-	-
33	CLA	d	402	X	-	-	-
33	CLA	d	409	X	-	-	-
33	CLA	w	303	X	-	-	-
33	CLA	z	101	X	-	-	-

## 2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 75511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2614	1709	427	462	16		
1	a	333	Total	C	N	O	S	0	0
			2614	1709	427	462	16		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3772	2466	639	654	13		
2	b	478	Total	C	N	O	S	0	0
			3772	2466	639	654	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3489	2277	588	608	16		
3	c	450	Total	C	N	O	S	0	0
			3489	2277	588	608	16		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2699	1784	442	463	10		
4	d	341	Total	C	N	O	S	0	0
			2699	1784	442	463	10		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	76	Total	C	N	O	0	0
			626	407	103	116		
5	e	76	Total	C	N	O	0	0
			626	407	103	116		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	31	Total	C	N	O	S	0	0
			253	173	42	37	1		
6	f	31	Total	C	N	O	S	0	0
			253	173	42	37	1		

- Molecule 7 is a protein called Photosystem II Psb31 protein domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	120	Total	C	N	O	0	0
			890	556	160	174		
7	g	120	Total	C	N	O	0	0
			890	556	160	174		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			512	339	82	89	2		
8	h	65	Total	C	N	O	S	0	0
			512	339	82	89	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			279	188	43	47	1		
9	i	34	Total	C	N	O	S	0	0
			279	188	43	47	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	33	Total	C	N	O	0	0
			243	165	37	41		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	33	Total	C	N	O	0	0
			243	165	37	41		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			303	213	45	45		
11	k	37	Total	C	N	O	0	0
			303	213	45	45		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			302	203	47	52		
12	l	37	Total	C	N	O	0	0
			302	203	47	52		

- Molecule 13 is a protein called Photosystem II reaction center M protein, plastid.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	41	Total	C	N	O	0	0
			317	208	51	58		
13	m	41	Total	C	N	O	0	0
			317	208	51	58		

- Molecule 14 is a protein called Photosystem II subunit, PsbN..

Mol	Chain	Residues	Atoms				AltConf	Trace
14	n	30	Total	C	N	O	0	0
			150	90	30	30		
14	N	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	248	Total	C	N	O	S	0	0
			1867	1176	309	374	8		
15	o	248	Total	C	N	O	S	0	0
			1867	1176	309	374	8		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	28	Total	C	N	O	S	0	0
			233	161	34	36	2		
16	t	28	Total	C	N	O	S	0	0
			233	161	34	36	2		

- Molecule 17 is a protein called PS II complex 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	92	Total	C	N	O	S	0	0
			708	451	121	134	2		
17	u	92	Total	C	N	O	S	0	0
			708	451	121	134	2		

- Molecule 18 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	135	Total	C	N	O	S	0	0
			1029	640	179	206	4		
18	v	135	Total	C	N	O	S	0	0
			1029	640	179	206	4		

- Molecule 19 is a protein called Photosystem II subunit, PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	W	54	Total	C	N	O	0	0
			434	281	64	89		
19	w	54	Total	C	N	O	0	0
			434	281	64	89		

- Molecule 20 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	35	Total	C	N	O	S	0	0
			248	160	41	46	1		
20	x	35	Total	C	N	O	S	0	0
			248	160	41	46	1		

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			453	301	68	83	1		
21	z	61	Total	C	N	O	S	0	0
			453	301	68	83	1		

- Molecule 22 is a protein called Fucoxanthin chl a/c protein, lhca clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	220	Total	C	N	O	S	0	0
			1710	1110	281	315	4		

- Molecule 23 is a protein called Fucoxanthin-chlorophyll a-c binding protein, plastid.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	163	Total	C	N	O	S	0	0
			1249	809	204	232	4		

- Molecule 24 is a protein called Fucoxanthin chlorophyll a/c protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	160	Total	C	N	O	S	0	0
			1229	780	217	227	5		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	168	Total	C	N	O	S	0	0
			1296	833	219	238	6		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c protein-LI818 clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	165	Total	C	N	O	S	0	0
			1269	819	213	233	4		
26	0	165	Total	C	N	O	S	0	0
			1269	819	213	233	4		

- Molecule 27 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	34	Total	C	N	O	S	0	0
			251	167	41	41	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	34	Total	C	N	O	S	0	0
			251	167	41	41	2		

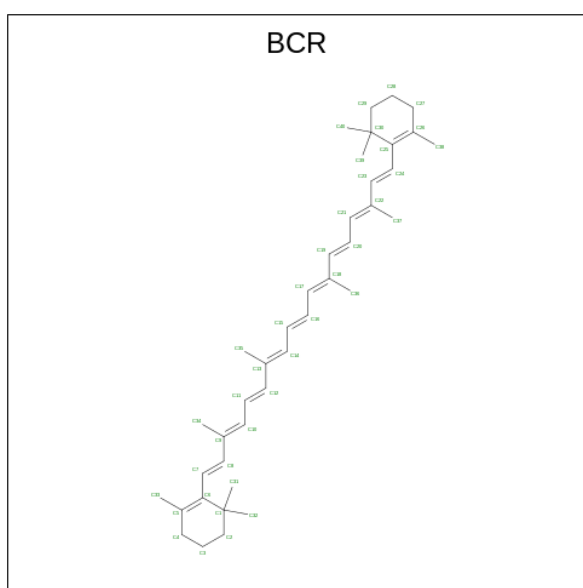
- Molecule 28 is a protein called Photosystem II subunit, PsbQ..

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	156	Total	C	N	O	S	0	0
			1198	757	202	237	2		
28	q	156	Total	C	N	O	S	0	0
			1198	757	202	237	2		

- Molecule 29 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein, major type.

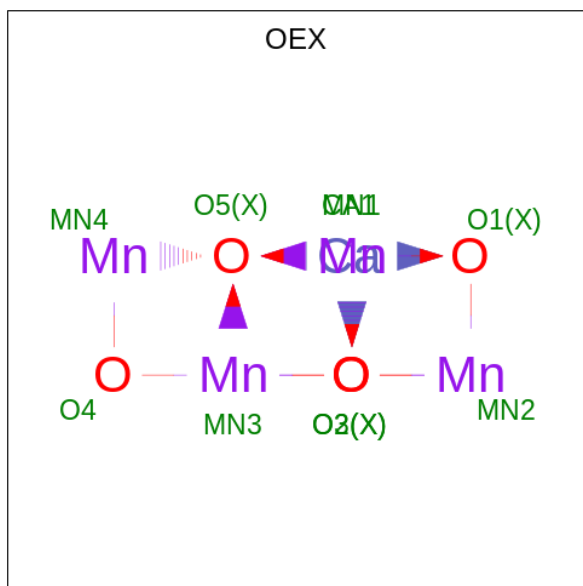
Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	163	Total	C	N	O	S	0	0
			1214	788	206	218	2		
29	2	163	Total	C	N	O	S	0	0
			1214	788	206	218	2		
29	8	163	Total	C	N	O	S	0	0
			1206	783	206	216	1		
29	1	163	Total	C	N	O	S	0	0
			1206	783	206	216	1		

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	d	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	h	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	k	1	Total C 40 40	0
30	k	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).

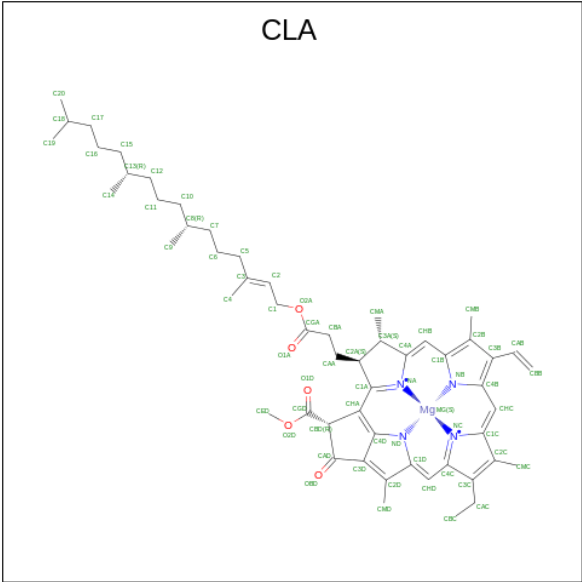


Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
31	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula:  $\text{Cl}$ ).

Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Cl	0
			1	1	
32	a	1	Total	Cl	0
			1	1	

- Molecule 33 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
33	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	D	1	Total 59	C 49	Mg 1	N 4	O 5	0
33	D	1	Total 57	C 47	Mg 1	N 4	O 5	0
33	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	d	1	Total 57	C 47	Mg 1	N 4	O 5	0
33	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	d	1	Total 59	C 49	Mg 1	N 4	O 5	0
33	H	1	Total 43	C 35	Mg 1	N 4	O 3	0
33	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	Z	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	z	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
33	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
33	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	4	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	5	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
33	6	1	Total 54	C 44	Mg 1	N 4	O 5	0
33	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	6	1	Total 39	C 30	Mg 1	N 4	O 4	0
33	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 34	C 28	Mg 1	N 4	O 1	0
33	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
33	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	b	1	Total 61	C 52	Mg 1	N 4	O 4	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	0	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 34	C 28	Mg 1	N 4	O 1	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	2	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	8	1	Total 45	C 35	Mg 1	N 4	O 5	0

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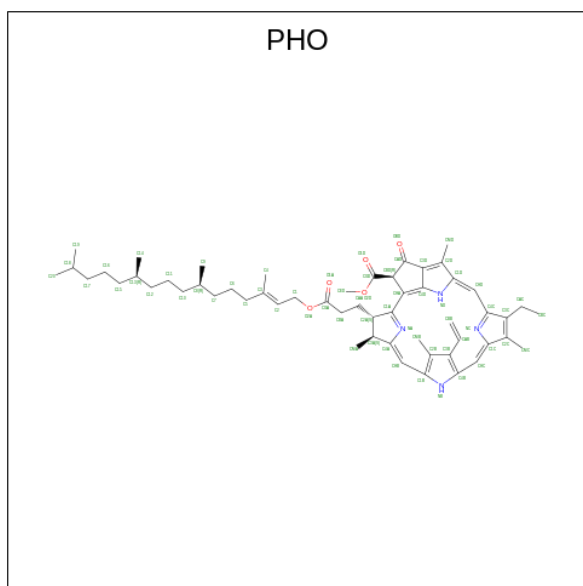
Mol	Chain	Residues	Atoms					AltConf
33	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	8	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	1	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	1	1	Total 38	C 32	Mg 1	N 4	O 1	0

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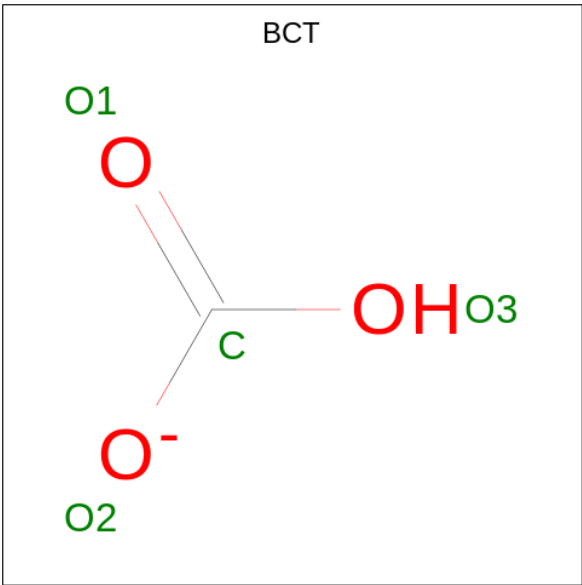
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	1	1	38	32	1	4	1	0

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



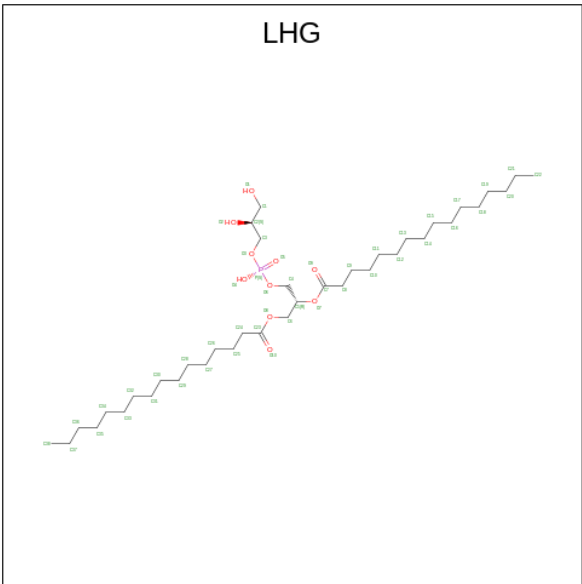
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
34	A	1	64	55	4	5	0
34	A	1	64	55	4	5	0
34	a	1	64	55	4	5	0
34	a	1	64	55	4	5	0

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			4	1	3	
35	a	1	Total	C	O	0
			4	1	3	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



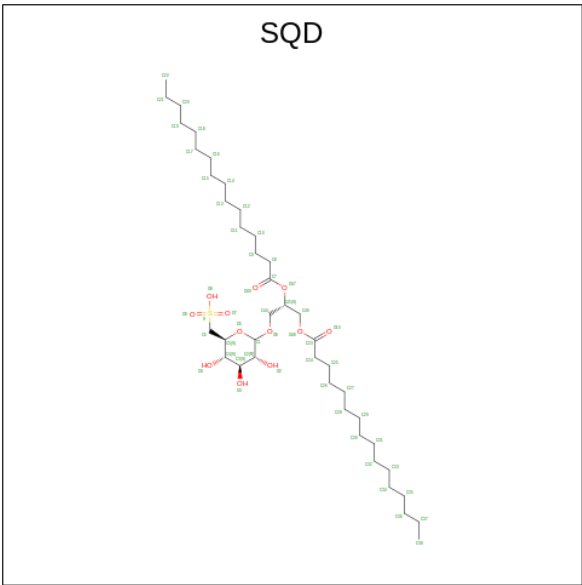
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			43	32	10	1	

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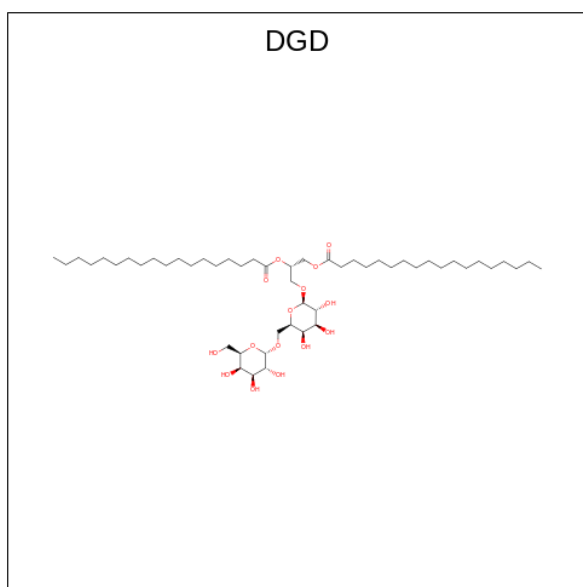
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			49	38	10	1	
36	A	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			48	38	9	1	
36	D	1	Total	C	O	P	0
			42	31	10	1	
36	d	1	Total	C	O	P	0
			48	38	9	1	
36	d	1	Total	C	O	P	0
			42	31	10	1	
36	H	1	Total	C	O	P	0
			42	31	10	1	
36	h	1	Total	C	O	P	0
			42	31	10	1	
36	W	1	Total	C	O	P	0
			35	24	10	1	
36	w	1	Total	C	O	P	0
			35	24	10	1	
36	3	1	Total	C	O	P	0
			27	16	10	1	
36	3	1	Total	C	O	P	0
			49	38	10	1	
36	4	1	Total	C	O	P	0
			49	38	10	1	
36	5	1	Total	C	O	P	0
			33	24	8	1	
36	7	1	Total	C	O	P	0
			28	19	8	1	
36	a	1	Total	C	O	P	0
			43	32	10	1	
36	a	1	Total	C	O	P	0
			49	38	10	1	
36	b	1	Total	C	O	P	0
			49	38	10	1	
36	0	1	Total	C	O	P	0
			28	19	8	1	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



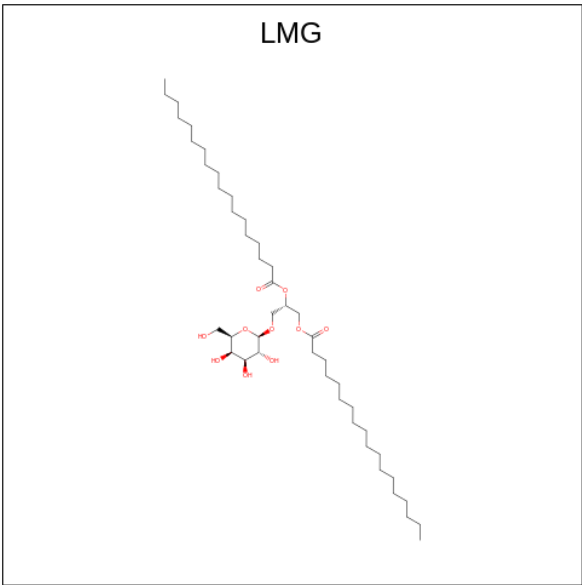
Mol	Chain	Residues	Atoms				AltConf
37	A	1	Total	C	O	S	0
			40	27	12	1	
37	B	1	Total	C	O	S	0
			54	41	12	1	
37	D	1	Total	C	O	S	0
			54	41	12	1	
37	i	1	Total	C	O	S	0
			40	27	12	1	
37	L	1	Total	C	O	S	0
			54	41	12	1	
37	l	1	Total	C	O	S	0
			54	41	12	1	
37	T	1	Total	C	O	S	0
			40	27	12	1	
37	T	1	Total	C	O	S	0
			54	41	12	1	
37	t	1	Total	C	O	S	0
			40	27	12	1	
37	7	1	Total	C	O	S	0
			48	35	12	1	
37	a	1	Total	C	O	S	0
			54	41	12	1	
37	0	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			53	39	14	
38	C	1	Total	C	O	0
			55	40	15	
38	C	1	Total	C	O	0
			56	41	15	
38	C	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			56	41	15	
38	c	1	Total	C	O	0
			55	40	15	
38	H	1	Total	C	O	0
			62	47	15	
38	h	1	Total	C	O	0
			62	47	15	
38	3	1	Total	C	O	0
			39	34	5	
38	a	1	Total	C	O	0
			53	39	14	

- Molecule 39 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			51	41	10	
39	B	1	Total	C	O	0
			28	18	10	
39	C	1	Total	C	O	0
			46	36	10	
39	C	1	Total	C	O	0
			48	38	10	
39	C	1	Total	C	O	0
			27	17	10	
39	C	1	Total	C	O	0
			23	13	10	
39	c	1	Total	C	O	0
			48	38	10	
39	c	1	Total	C	O	0
			27	17	10	
39	D	1	Total	C	O	0
			40	30	10	
39	D	1	Total	C	O	0
			46	36	10	
39	d	1	Total	C	O	0
			46	36	10	
39	d	1	Total	C	O	0
			37	27	10	
39	M	1	Total	C	O	0
			40	30	10	
39	m	1	Total	C	O	0
			40	30	10	

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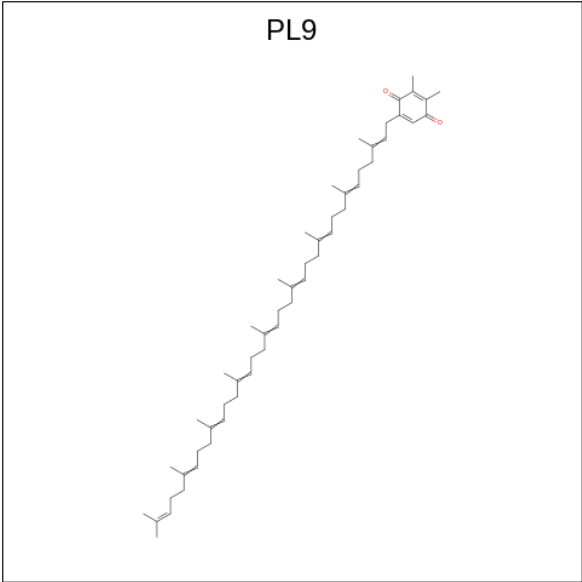
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Mol	Chain	Residues	Atoms			AltConf
39	W	1	Total	C	O	0
			48	38	10	
39	w	1	Total	C	O	0
			48	38	10	
39	3	1	Total	C	O	0
			31	21	10	
39	5	1	Total	C	O	0
			31	21	10	
39	7	1	Total	C	O	0
			55	45	10	
39	b	1	Total	C	O	0
			51	41	10	
39	b	1	Total	C	O	0
			28	18	10	
39	b	1	Total	C	O	0
			40	30	10	
39	Q	1	Total	C	O	0
			37	27	10	
39	q	1	Total	C	O	0
			46	36	10	
39	q	1	Total	C	O	0
			37	27	10	
39	0	1	Total	C	O	0
			42	32	10	

- Molecule 40 is FE (II) ION (three-letter code: FE2) (formula: Fe).

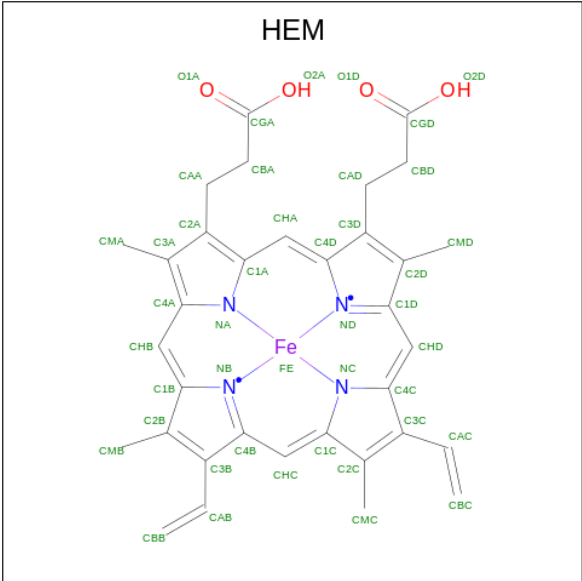
Mol	Chain	Residues	Atoms		AltConf
40	D	1	Total	Fe	0
			1	1	
40	d	1	Total	Fe	0
			1	1	

- Molecule 41 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			55	53	2	
41	d	1	Total	C	O	0
			55	53	2	

- Molecule 42 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



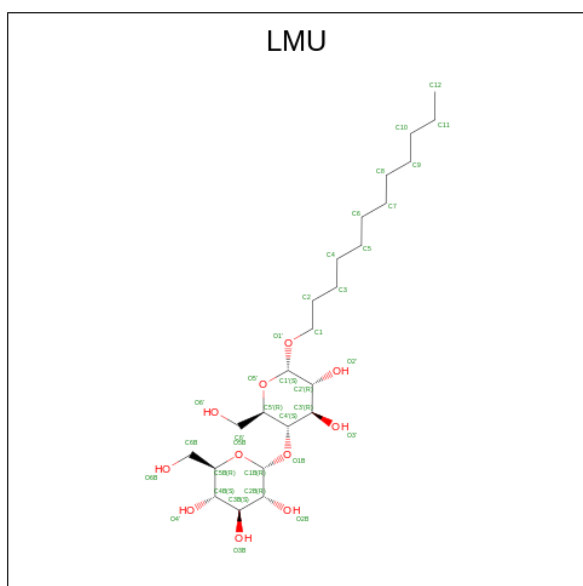
Mol	Chain	Residues	Atoms					AltConf
42	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
42	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
42	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
42	v	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 43 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
43	T	1	Total	C	O	0
			31	20	11	
43	t	1	Total	C	O	0
			31	20	11	
43	w	1	Total	C	O	0
			35	24	11	
43	3	1	Total	C	O	0
			35	24	11	
43	4	1	Total	C	O	0
			35	24	11	
43	5	1	Total	C	O	0
			31	20	11	

- Molecule 44 is Chlorophyll c1 (three-letter code: KC1) (formula:  $C_{35}H_{30}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
44	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
44	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
44	6	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 45 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 (three-letter code: A86) (formula:  $C_{42}H_{58}O_6$ ).



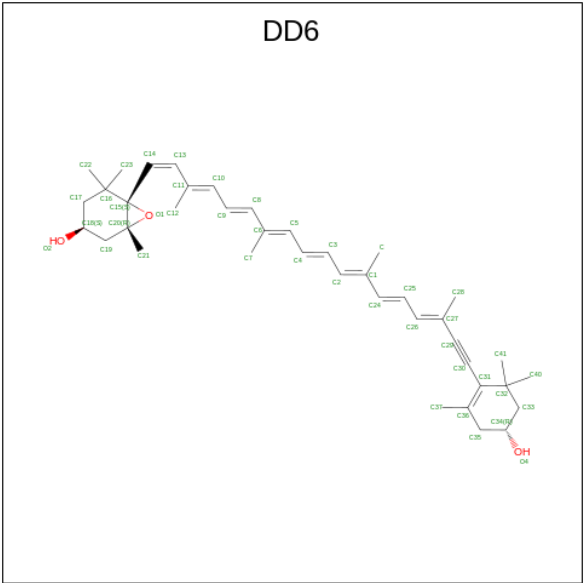
Mol	Chain	Residues	Atoms			AltConf
45	3	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			47	41	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	7	1	Total	C	O	0
			48	42	6	
45	7	1	Total	C	O	0
			48	42	6	
45	0	1	Total	C	O	0
			48	42	6	
45	0	1	Total	C	O	0
			48	42	6	
45	9	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	C	O	0
			48	42	6	
45	2	1	Total	C	O	0
			48	42	6	
45	2	1	Total	C	O	0
			48	42	6	
45	8	1	Total	C	O	0
			48	42	6	
45	8	1	Total	C	O	0
			48	42	6	
45	1	1	Total	C	O	0
			48	42	6	
45	1	1	Total	C	O	0
			48	42	6	

- Molecule 46 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
46	3	1	Total	C	O	0
			43	40	3	
46	4	1	Total	C	O	0
			43	40	3	
46	9	1	Total	C	O	0
			43	40	3	
46	9	1	Total	C	O	0
			43	40	3	

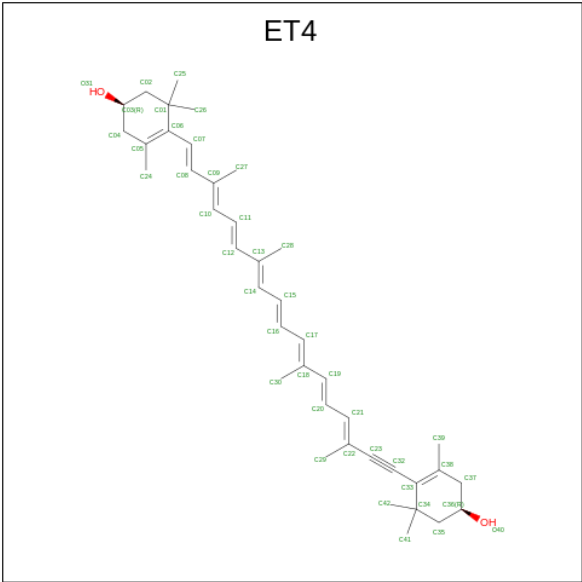
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Mol	Chain	Residues	Atoms			AltConf
46	2	1	Total 43	C 40	O 3	0
46	2	1	Total 43	C 40	O 3	0
46	8	1	Total 43	C 40	O 3	0
46	8	1	Total 43	C 40	O 3	0
46	1	1	Total 43	C 40	O 3	0
46	1	1	Total 43	C 40	O 3	0

- ## KC2

Mol	Chain	Residues	Atoms					AltConf
47	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	0	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 48 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (three-letter code: ET4) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
48	7	1	Total	C	O	0
			42	40	2	
48	0	1	Total	C	O	0
			42	40	2	

### 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem II protein D1

Chain A:  99%



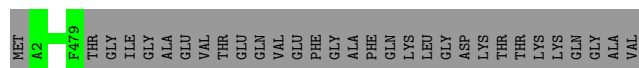
- Molecule 1: Photosystem II protein D1

Chain a:  100%

There are no outlier residues recorded for this chain.

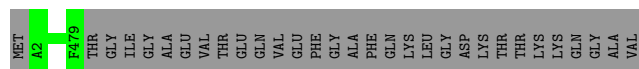
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  94% 6%



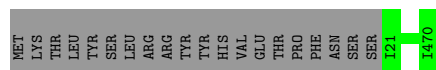
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  94% 6%



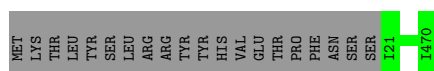
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  96%



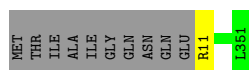
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  96%



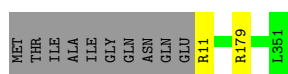
- Molecule 4: Photosystem II D2 protein

Chain D: 97%



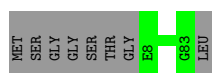
- Molecule 4: Photosystem II D2 protein

Chain d: 97%



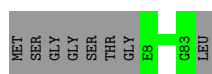
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 90%



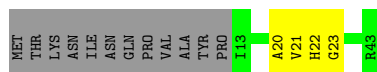
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 90%



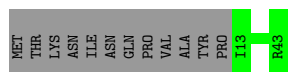
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 63%



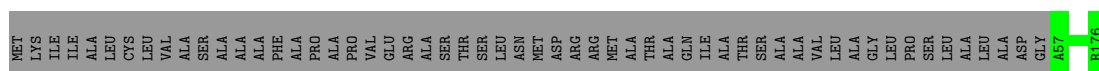
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 72%

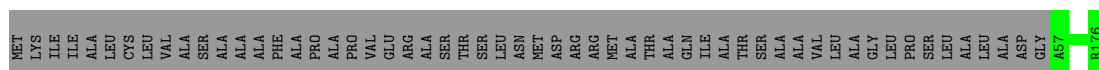


- Molecule 7: Photosystem II Psb31 protein domain-containing protein

Chain G: 68%



- Molecule 7: Photosystem II Psb31 protein domain-containing protein



- Molecule 8: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein H



- Molecule 9: Photosystem II reaction center protein I



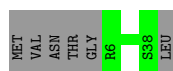
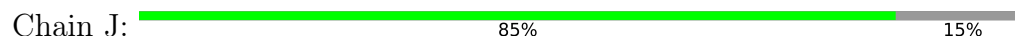
There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein I

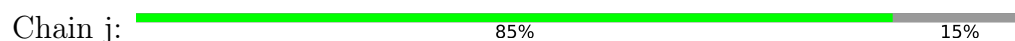


There are no outlier residues recorded for this chain.

- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J



- Chain n:  100%


There are no outlier residues recorded for this chain.

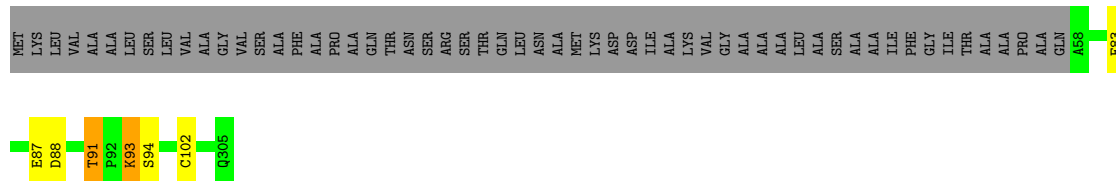
- Molecule 14: Photosystem II subunit, PsbN.

Chain N:  100%


There are no outlier residues recorded for this chain.

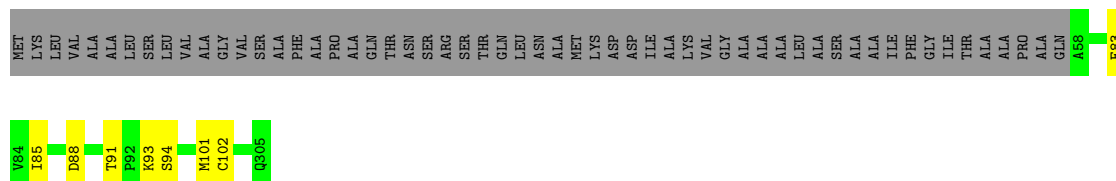
- Molecule 15: Oxygen-evolving enhancer protein 1

Chain O:  79% .. 19%



- Molecule 15: Oxygen-evolving enhancer protein 1

Chain o:  79% . 19%



- Molecule 16: Photosystem II reaction center protein T

Chain T:  100%

There are no outlier residues recorded for this chain.

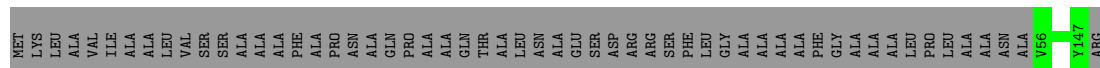
- Molecule 16: Photosystem II reaction center protein T

Chain t:  100%

There are no outlier residues recorded for this chain.

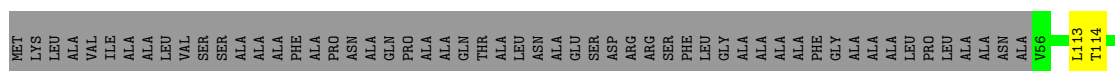
- Molecule 17: PS II complex 12 kDa extrinsic protein

Chain U:  62% 38%



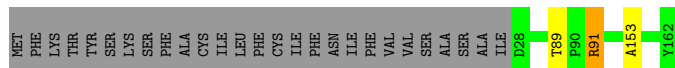
- Molecule 17: PS II complex 12 kDa extrinsic protein

Chain u:  60% . 38%



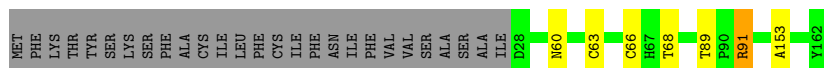
- Molecule 18: Cytochrome c-550

Chain V: 81% 17%



- Molecule 18: Cytochrome c-550

Chain v: 79% 17%



- Molecule 19: Photosystem II subunit, PsbW

Chain W: 98%



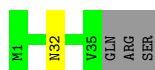
- Molecule 19: Photosystem II subunit, PsbW

Chain w: 100%

There are no outlier residues recorded for this chain.

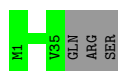
- Molecule 20: Photosystem II reaction center X protein

Chain X: 89% 8%



- Molecule 20: Photosystem II reaction center X protein

Chain x: 92% 8%



- Molecule 21: Photosystem II reaction center protein Z

Chain Z: 100%

There are no outlier residues recorded for this chain.

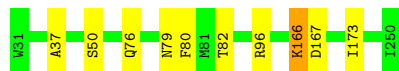
- Molecule 21: Photosystem II reaction center protein Z

Chain z:  100%

There are no outlier residues recorded for this chain.

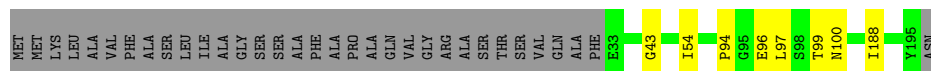
- Molecule 22: Fucoxanthin chl a/c protein, lhca clade

Chain 3:  95%




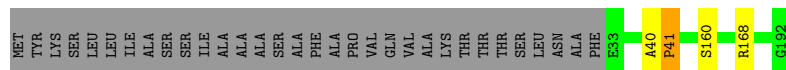
- Molecule 23: Fucoxanthin-chlorophyll a-c binding protein, plastid

Chain 4:  79%




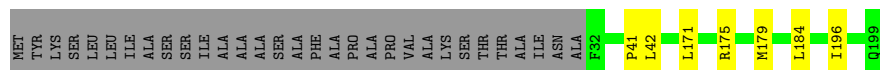
- Molecule 24: Fucoxanthin chlorophyll a/c protein 6

Chain 5:  81%




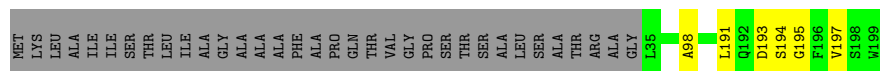
- Molecule 25: Fucoxanthin chlorophyll a/c protein 5

Chain 6:  81%




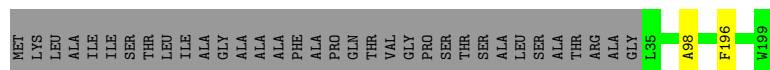
- Molecule 26: Fucoxanthin chlorophyll a/c protein-LI818 clade

Chain 7:  80%



- Molecule 26: Fucoxanthin chlorophyll a/c protein-LI818 clade

Chain 0:  82%



- Molecule 27: Photosystem II reaction center protein Ycf12

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Photosystem II reaction center protein Ycf12

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: Photosystem II subunit, PsbQ.

Chain Q:  74% 26%


MET LYS ILE VAL LEU LEU VAL ALA ALA ALA SER SER VAL SER ALA PHE PHE ALA PRO PRO GLN SER SER ASN ASN ARG ARG GLN GLU ASN SER ARG ARG GLU ALA LEU SER THR THR ILE ALA ALA THR ALA ALA ILE LEU PRO ALA ALA ALA ALA ASN ALA A56 L211

- Molecule 28: Photosystem II subunit, PsbQ.

Chain q:  73% 26%


MET LYS ILE VAL LEU LEU VAL ALA ALA ALA SER SER VAL SER ALA PHE PHE ALA PRO PRO GLN SER SER ASN ASN ARG ARG GLU ALA LEU SER THR THR ILE ALA ALA THR ALA ALA ILE LEU PRO ALA ALA ALA ALA ASN ALA A56 Y93 L211

- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type

Chain 9:  80% 16%


MET LYS SER VAL ILE ILE ALA SER LEU LEU ALA CYS SER SER ALA ALA ALA PHE PHE ALA PRO PRO GLN VAL VAL ARG ARG SER SER THR VAL VAL GLN GLY F31 A39 A39 Y79 A92 G143 L158 D183 N184 L186 Y193

- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type

Chain 2:  80% 16%


MET LYS SER VAL ILE ILE ALA SER LEU LEU ALA CYS SER SER ALA ALA ALA PHE PHE ALA PRO PRO GLN VAL VAL ARG ARG SER SER THR VAL VAL GLN GLY F31 A39 A39 A92 P139 D140 I163 L164 L185 I186 I187 Y193

- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type

Chain 8:  81% 16%

MET LYS SER VAL ILE ILE ALA SER LEU LEU ALA CYS SER SER ALA ALA ALA PHE PHE ALA PRO PRO GLN VAL VAL ARG ARG SER SER THR VAL VAL GLN GLY F31 A39 A39 A92 D140 L166 L185 I186 Y193

- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type

Chain 1:  80% 5% 16%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97098	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PHO, BCT, CLA, LMG, KC2, HEM, DD6, SQD, KC1, OEX, ET4, DGD, A86, FE2, PL9, LMU, BCR, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.32	0/2697	0.49	0/3674
1	a	0.31	0/2697	0.47	0/3674
2	B	0.32	0/3901	0.50	0/5308
2	b	0.32	0/3901	0.49	0/5308
3	C	0.33	0/3604	0.49	0/4909
3	c	0.31	0/3604	0.48	0/4909
4	D	0.32	0/2791	0.48	0/3804
4	d	0.33	0/2791	0.50	0/3804
5	E	0.28	0/644	0.47	0/878
5	e	0.29	0/644	0.50	0/878
6	F	0.35	0/261	0.53	0/352
6	f	0.28	0/261	0.48	0/352
7	G	0.26	0/900	0.47	0/1207
7	g	0.25	0/900	0.48	0/1207
8	H	0.30	0/522	0.49	0/712
8	h	0.29	0/522	0.51	0/712
9	I	0.35	0/286	0.50	0/386
9	i	0.31	0/286	0.48	0/386
10	J	0.36	0/249	0.51	0/339
10	j	0.26	0/249	0.43	0/339
11	K	0.33	0/315	0.47	0/432
11	k	0.32	0/315	0.47	0/432
12	L	0.36	0/311	0.42	0/423
12	l	0.33	0/311	0.42	0/423
13	M	0.32	0/322	0.47	0/435
13	m	0.31	0/322	0.48	0/435
15	O	0.33	0/1896	0.50	0/2549
15	o	0.32	0/1896	0.49	0/2549
16	T	0.33	0/239	0.47	0/323
16	t	0.31	0/239	0.46	0/323
17	U	0.33	0/722	0.51	0/982

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	u	0.33	0/722	0.49	0/982
18	V	0.33	0/1047	0.51	0/1422
18	v	0.31	0/1047	0.51	0/1422
19	W	0.33	0/446	0.46	0/606
19	w	0.29	0/446	0.44	0/606
20	X	0.25	0/248	0.45	0/336
20	x	0.25	0/248	0.44	0/336
21	Z	0.27	0/461	0.41	0/633
21	z	0.25	0/461	0.40	0/633
22	3	0.31	0/1765	0.46	0/2405
23	4	0.32	0/1282	0.53	0/1746
24	5	0.30	0/1255	0.52	1/1696 (0.1%)
25	6	0.33	0/1324	0.55	0/1780
26	0	0.27	0/1298	0.48	0/1764
26	7	0.32	0/1298	0.51	0/1764
27	Y	0.24	0/253	0.42	0/341
27	y	0.23	0/253	0.39	0/341
28	Q	0.29	0/1220	0.46	0/1638
28	q	0.28	0/1220	0.49	0/1638
29	1	0.31	0/1237	0.48	0/1687
29	2	0.32	0/1246	0.50	0/1700
29	8	0.31	0/1237	0.48	0/1687
29	9	0.33	0/1246	0.49	0/1700
All	All	0.31	0/59858	0.49	1/81307 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	41	PRO	N-CA-CB	5.23	109.58	103.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	331/333 (99%)	311 (94%)	19 (6%)	1 (0%)	37	59
1	a	331/333 (99%)	314 (95%)	17 (5%)	0	100	100
2	B	476/509 (94%)	463 (97%)	13 (3%)	0	100	100
2	b	476/509 (94%)	464 (98%)	12 (2%)	0	100	100
3	C	448/470 (95%)	430 (96%)	18 (4%)	0	100	100
3	c	448/470 (95%)	433 (97%)	15 (3%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
5	e	74/84 (88%)	71 (96%)	3 (4%)	0	100	100
6	F	29/43 (67%)	26 (90%)	0	3 (10%)	0	0
6	f	29/43 (67%)	29 (100%)	0	0	100	100
7	G	118/176 (67%)	108 (92%)	10 (8%)	0	100	100
7	g	118/176 (67%)	108 (92%)	10 (8%)	0	100	100
8	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
8	h	63/66 (96%)	56 (89%)	7 (11%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	J	31/39 (80%)	29 (94%)	2 (6%)	0	100	100
10	j	31/39 (80%)	29 (94%)	2 (6%)	0	100	100
11	K	35/44 (80%)	34 (97%)	1 (3%)	0	100	100
11	k	35/44 (80%)	34 (97%)	1 (3%)	0	100	100
12	L	35/38 (92%)	35 (100%)	0	0	100	100
12	l	35/38 (92%)	35 (100%)	0	0	100	100
13	M	39/113 (34%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	39/113 (34%)	38 (97%)	1 (3%)	0	100	100
15	O	246/305 (81%)	230 (94%)	14 (6%)	2 (1%)	16	35
15	o	246/305 (81%)	228 (93%)	16 (6%)	2 (1%)	16	35
16	T	26/28 (93%)	26 (100%)	0	0	100	100
16	t	26/28 (93%)	26 (100%)	0	0	100	100
17	U	90/148 (61%)	88 (98%)	2 (2%)	0	100	100
17	u	90/148 (61%)	82 (91%)	8 (9%)	0	100	100
18	V	133/162 (82%)	125 (94%)	6 (4%)	2 (2%)	8	20
18	v	133/162 (82%)	123 (92%)	7 (5%)	3 (2%)	5	12
19	W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
19	w	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
20	X	33/38 (87%)	31 (94%)	1 (3%)	1 (3%)	3	8
20	x	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
21	Z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
21	z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
22	3	218/220 (99%)	186 (85%)	27 (12%)	5 (2%)	5	12
23	4	161/196 (82%)	139 (86%)	16 (10%)	6 (4%)	2	5
24	5	158/192 (82%)	137 (87%)	18 (11%)	3 (2%)	6	15
25	6	166/199 (83%)	136 (82%)	27 (16%)	3 (2%)	7	16
26	0	163/199 (82%)	148 (91%)	13 (8%)	2 (1%)	11	25
26	7	163/199 (82%)	148 (91%)	13 (8%)	2 (1%)	11	25
27	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
27	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
28	Q	154/211 (73%)	145 (94%)	9 (6%)	0	100	100
28	q	154/211 (73%)	144 (94%)	10 (6%)	0	100	100
29	1	161/193 (83%)	128 (80%)	26 (16%)	7 (4%)	2	4
29	2	161/193 (83%)	141 (88%)	14 (9%)	6 (4%)	2	5
29	8	161/193 (83%)	144 (89%)	13 (8%)	4 (2%)	4	10
29	9	161/193 (83%)	138 (86%)	17 (11%)	6 (4%)	2	5
All	All	7423/8659 (86%)	6918 (93%)	447 (6%)	58 (1%)	19	35

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	4	99	THR
24	5	41	PRO
25	6	42	LEU
25	6	196	ILE
29	9	39	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/271 (100%)	270 (100%)	1 (0%)	89	96
1	a	271/271 (100%)	271 (100%)	0	100	100
2	B	385/408 (94%)	385 (100%)	0	100	100
2	b	385/408 (94%)	385 (100%)	0	100	100
3	C	355/375 (95%)	355 (100%)	0	100	100
3	c	355/375 (95%)	355 (100%)	0	100	100
4	D	272/280 (97%)	271 (100%)	1 (0%)	89	96
4	d	272/280 (97%)	270 (99%)	2 (1%)	81	92
5	E	70/75 (93%)	70 (100%)	0	100	100
5	e	70/75 (93%)	70 (100%)	0	100	100
6	F	25/36 (69%)	24 (96%)	1 (4%)	27	51
6	f	25/36 (69%)	25 (100%)	0	100	100
7	G	84/122 (69%)	84 (100%)	0	100	100
7	g	84/122 (69%)	84 (100%)	0	100	100
8	H	56/57 (98%)	56 (100%)	0	100	100
8	h	56/57 (98%)	56 (100%)	0	100	100
9	I	33/33 (100%)	33 (100%)	0	100	100
9	i	33/33 (100%)	33 (100%)	0	100	100
10	J	26/31 (84%)	26 (100%)	0	100	100
10	j	26/31 (84%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	32/38 (84%)	32 (100%)	0	100	100
11	k	32/38 (84%)	32 (100%)	0	100	100
12	L	33/34 (97%)	33 (100%)	0	100	100
12	l	33/34 (97%)	33 (100%)	0	100	100
13	M	33/86 (38%)	33 (100%)	0	100	100
13	m	33/86 (38%)	33 (100%)	0	100	100
15	O	199/236 (84%)	192 (96%)	7 (4%)	31	57
15	o	199/236 (84%)	193 (97%)	6 (3%)	36	63
16	T	25/25 (100%)	25 (100%)	0	100	100
16	t	25/25 (100%)	25 (100%)	0	100	100
17	U	73/105 (70%)	73 (100%)	0	100	100
17	u	73/105 (70%)	70 (96%)	3 (4%)	26	50
18	V	114/138 (83%)	112 (98%)	2 (2%)	54	78
18	v	114/138 (83%)	109 (96%)	5 (4%)	24	48
19	W	44/44 (100%)	43 (98%)	1 (2%)	45	72
19	w	44/44 (100%)	44 (100%)	0	100	100
20	X	27/30 (90%)	27 (100%)	0	100	100
20	x	27/30 (90%)	27 (100%)	0	100	100
21	Z	49/49 (100%)	49 (100%)	0	100	100
21	z	49/49 (100%)	49 (100%)	0	100	100
22	3	171/171 (100%)	165 (96%)	6 (4%)	31	57
23	4	128/152 (84%)	126 (98%)	2 (2%)	58	80
24	5	120/147 (82%)	119 (99%)	1 (1%)	79	91
25	6	131/152 (86%)	127 (97%)	4 (3%)	35	61
26	0	128/151 (85%)	128 (100%)	0	100	100
26	7	128/151 (85%)	124 (97%)	4 (3%)	35	61
27	Y	27/27 (100%)	27 (100%)	0	100	100
27	y	27/27 (100%)	27 (100%)	0	100	100
28	Q	120/157 (76%)	120 (100%)	0	100	100
28	q	120/157 (76%)	119 (99%)	1 (1%)	79	91
29	1	109/148 (74%)	107 (98%)	2 (2%)	54	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	2	113/148 (76%)	108 (96%)	5 (4%)	24	48
29	8	109/148 (74%)	106 (97%)	3 (3%)	38	65
29	9	113/148 (76%)	109 (96%)	4 (4%)	31	57
All	All	5956/6830 (87%)	5895 (99%)	61 (1%)	71	88

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	W	191	ARG
29	2	187	THR
23	4	96	GLU
29	2	186	ILE
29	1	89	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
26	7	192	GLN
26	7	190	ASN
25	6	39	GLN
26	7	183	ASN
24	5	104	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 347 ligands modelled in this entry, 4 are monoatomic - leaving 343 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	DD6	4	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.77	15 (28%)
33	CLA	c	501	-	65,73,73	1.46	7 (10%)	76,113,113	1.32	6 (7%)
33	CLA	W	303	-	65,73,73	1.50	7 (10%)	76,113,113	1.41	10 (13%)
33	CLA	b	607	-	65,73,73	1.44	7 (10%)	76,113,113	1.36	7 (9%)
33	CLA	2	308	-	55,63,73	1.60	5 (9%)	64,101,113	1.49	8 (12%)
33	CLA	2	310	29	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
33	CLA	8	312	-	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
33	CLA	B	602	-	61,69,73	1.47	7 (11%)	67,106,113	1.40	6 (8%)
36	LHG	4	318	-	48,48,48	0.57	0	51,54,54	1.26	6 (11%)
38	DGD	C	517	-	57,57,67	0.99	2 (3%)	71,71,81	1.46	10 (14%)
33	CLA	2	305	-	41,49,73	1.88	6 (14%)	47,84,113	1.61	8 (17%)
30	BCR	K	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	7 (12%)
33	CLA	B	611	-	64,72,73	1.46	7 (10%)	74,111,113	1.38	10 (13%)
33	CLA	2	315	-	37,46,73	1.93	6 (16%)	44,80,113	1.69	8 (18%)
33	CLA	3	302	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
33	CLA	9	315	-	37,46,73	1.91	6 (16%)	44,80,113	1.67	7 (15%)
30	BCR	h	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	4 (7%)
33	CLA	6	308	25	54,62,73	1.63	5 (9%)	62,99,113	1.51	8 (12%)
33	CLA	b	617	-	65,73,73	1.48	8 (12%)	76,113,113	1.38	7 (9%)
33	CLA	C	510	-	65,73,73	1.46	6 (9%)	76,113,113	1.43	8 (10%)
38	DGD	3	320	-	38,38,67	0.63	0	40,40,81	1.49	6 (15%)
33	CLA	8	308	-	55,63,73	1.58	6 (10%)	64,101,113	1.56	8 (12%)
37	SQD	t	102	-	39,40,54	1.14	5 (12%)	48,51,65	2.03	12 (25%)
38	DGD	C	518	-	56,56,67	0.99	2 (3%)	70,70,81	1.40	10 (14%)
47	KC2	4	307	-	48,53,53	1.78	9 (18%)	54,89,89	2.47	15 (27%)
33	CLA	c	510	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	1	306	29	45,53,73	1.78	5 (11%)	52,89,113	1.62	7 (13%)
33	CLA	b	603	-	61,69,73	1.49	6 (9%)	67,106,113	1.22	5 (7%)
33	CLA	1	308	-	55,63,73	1.59	5 (9%)	64,101,113	1.51	8 (12%)
38	DGD	A	415	-	54,54,67	1.00	3 (5%)	67,67,81	1.47	12 (17%)
36	LHG	W	302	-	34,34,48	0.75	1 (2%)	37,40,54	1.21	3 (8%)
33	CLA	z	101	-	51,59,73	1.69	5 (9%)	59,96,113	1.48	7 (11%)
33	CLA	5	309	24	55,63,73	1.59	5 (9%)	64,101,113	1.49	7 (10%)
39	LMG	w	304	-	48,48,55	0.77	1 (2%)	56,56,63	1.33	6 (10%)
33	CLA	C	502	-	64,72,73	1.48	8 (12%)	74,111,113	1.36	8 (10%)
33	CLA	0	309	26	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
45	A86	5	303	-	44,50,50	1.23	3 (6%)	51,76,76	11.73	23 (45%)
33	CLA	6	311	-	46,54,73	1.77	5 (10%)	53,90,113	1.57	8 (15%)
30	BCR	k	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
33	CLA	8	316	29	37,46,73	1.91	6 (16%)	44,80,113	1.67	7 (15%)
33	CLA	4	309	23	65,73,73	1.48	5 (7%)	76,113,113	1.37	6 (7%)
34	PHO	a	409	-	51,69,69	1.00	4 (7%)	47,99,99	1.20	6 (12%)
36	LHG	a	403	-	42,42,48	0.68	1 (2%)	45,48,54	1.21	4 (8%)
33	CLA	C	506	-	45,53,73	1.76	7 (15%)	52,89,113	1.59	7 (13%)
33	CLA	6	307	-	53,61,73	1.63	6 (11%)	61,98,113	1.57	9 (14%)
46	DD6	9	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.18	13 (25%)
34	PHO	a	410	-	51,69,69	1.01	4 (7%)	47,99,99	1.22	6 (12%)
33	CLA	b	616	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	7 (9%)
30	BCR	C	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	8 (14%)
44	KC1	3	310	-	48,53,53	1.50	7 (14%)	55,89,89	1.88	9 (16%)
33	CLA	4	305	-	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
39	LMG	B	621	-	28,28,55	0.97	0	36,36,63	1.30	4 (11%)
33	CLA	2	309	-	44,51,73	1.88	6 (13%)	50,86,113	1.70	9 (18%)
33	CLA	d	401	-	57,65,73	1.63	8 (14%)	70,103,113	1.47	10 (14%)
33	CLA	2	317	-	55,63,73	1.61	6 (10%)	64,101,113	1.45	8 (12%)
31	OEX	a	405	1,3	0,15,15	-	-	-	-	-
45	A86	1	301	-	44,50,50	1.22	3 (6%)	51,76,76	1.99	13 (25%)
33	CLA	8	307	-	44,52,73	1.83	7 (15%)	55,88,113	1.61	8 (14%)
30	BCR	A	401	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	7 (12%)
30	BCR	b	619	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	6 (10%)
39	LMG	c	520	-	27,27,55	1.03	0	35,35,63	1.18	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
43	LMU	w	302	-	36,36,36	0.34	0	47,47,47	1.02	3 (6%)
36	LHG	3	317	33	26,26,48	0.85	1 (3%)	29,32,54	1.35	3 (10%)
41	PL9	d	404	-	55,55,55	1.28	5 (9%)	68,69,69	1.48	10 (14%)
44	KC1	5	315	-	48,53,53	1.51	7 (14%)	55,89,89	1.77	11 (20%)
30	BCR	B	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.16	4 (7%)
39	LMG	C	519	-	46,46,55	0.77	1 (2%)	54,54,63	1.37	7 (12%)
33	CLA	B	607	-	41,49,73	1.77	7 (17%)	47,84,113	1.73	7 (14%)
33	CLA	4	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	8 (10%)
33	CLA	4	310	-	46,54,73	1.73	7 (15%)	53,90,113	1.59	6 (11%)
33	CLA	2	316	29	37,46,73	1.93	6 (16%)	44,80,113	1.65	7 (15%)
45	A86	5	305	-	43,49,50	1.42	5 (11%)	48,74,76	7.05	25 (52%)
39	LMG	m	201	-	40,40,55	0.86	1 (2%)	48,48,63	1.29	4 (8%)
45	A86	7	301	-	44,50,50	1.33	5 (11%)	51,76,76	2.05	16 (31%)
33	CLA	8	310	29	65,73,73	1.50	7 (10%)	76,113,113	1.39	6 (7%)
33	CLA	c	511	3	65,73,73	1.44	7 (10%)	76,113,113	1.43	7 (9%)
43	LMU	5	320	-	32,32,36	0.37	0	43,43,47	0.74	1 (2%)
33	CLA	A	405	-	49,57,73	1.65	7 (14%)	55,93,113	1.62	8 (14%)
33	CLA	Z	101	-	51,59,73	1.66	6 (11%)	59,96,113	1.49	7 (11%)
33	CLA	3	313	-	61,69,73	1.52	6 (9%)	71,108,113	1.40	7 (9%)
39	LMG	0	314	-	42,42,55	0.92	2 (4%)	50,50,63	1.26	3 (6%)
30	BCR	d	403	-	41,41,41	1.14	2 (4%)	56,56,56	1.18	4 (7%)
33	CLA	d	409	-	59,67,73	1.50	7 (11%)	68,105,113	1.53	8 (11%)
33	CLA	7	308	26	41,49,73	1.83	6 (14%)	47,84,113	1.63	8 (17%)
39	LMG	q	301	-	46,46,55	0.76	1 (2%)	54,54,63	1.33	6 (11%)
46	DD6	8	303	-	39,45,45	1.96	3 (7%)	52,67,67	2.10	12 (23%)
33	CLA	c	502	-	64,72,73	1.49	8 (12%)	74,111,113	1.37	7 (9%)
48	ET4	7	302	-	41,43,43	2.05	14 (34%)	54,60,60	2.39	19 (35%)
35	BCT	a	402	40	2,3,3	1.17	0	2,3,3	4.27	2 (100%)
33	CLA	B	610	-	65,73,73	1.47	8 (12%)	76,113,113	1.37	7 (9%)
33	CLA	4	306	23	65,73,73	1.46	7 (10%)	76,113,113	1.37	7 (9%)
33	CLA	8	309	-	44,51,73	1.89	7 (15%)	50,86,113	1.70	7 (14%)
36	LHG	d	407	-	41,41,48	0.66	1 (2%)	44,47,54	1.28	5 (11%)
33	CLA	B	604	-	61,69,73	1.49	6 (9%)	71,108,113	1.47	9 (12%)
33	CLA	2	307	-	44,52,73	1.88	7 (15%)	55,88,113	1.62	8 (14%)
43	LMU	3	301	-	36,36,36	0.38	0	47,47,47	0.81	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	9	307	-	44,52,73	1.86	7 (15%)	55,88,113	1.60	8 (14%)
38	DGD	c	516	-	56,56,67	0.96	2 (3%)	70,70,81	1.46	11 (15%)
46	DD6	1	304	-	39,45,45	2.10	4 (10%)	52,67,67	2.35	16 (30%)
33	CLA	2	313	29	36,44,73	2.36	9 (25%)	42,77,113	1.66	8 (19%)
33	CLA	7	311	-	51,59,73	1.62	6 (11%)	59,96,113	1.60	6 (10%)
33	CLA	9	313	-	36,44,73	2.09	6 (16%)	42,77,113	1.79	9 (21%)
39	LMG	b	621	-	51,51,55	0.75	1 (1%)	59,59,63	1.33	6 (10%)
33	CLA	C	508	-	65,73,73	1.46	7 (10%)	76,113,113	1.38	8 (10%)
33	CLA	5	312	-	46,54,73	1.77	5 (10%)	53,90,113	1.52	7 (13%)
45	A86	4	301	-	44,50,50	1.29	4 (9%)	51,76,76	2.20	13 (25%)
33	CLA	4	312	-	51,59,73	1.68	7 (13%)	59,96,113	1.52	7 (11%)
33	CLA	c	506	-	45,53,73	1.75	6 (13%)	52,89,113	1.59	7 (13%)
33	CLA	b	609	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	7 (9%)
33	CLA	9	316	29	37,46,73	1.92	6 (16%)	44,80,113	1.66	8 (18%)
33	CLA	3	309	36	51,59,73	1.66	6 (11%)	59,96,113	1.49	7 (11%)
39	LMG	3	316	-	31,31,55	0.93	0	39,39,63	1.25	5 (12%)
39	LMG	b	623	-	40,40,55	0.86	1 (2%)	48,48,63	1.30	5 (10%)
39	LMG	C	520	-	48,48,55	0.80	1 (2%)	56,56,63	1.33	6 (10%)
39	LMG	c	519	-	48,48,55	0.86	2 (4%)	56,56,63	1.28	5 (8%)
33	CLA	B	614	-	64,72,73	1.45	7 (10%)	74,111,113	1.40	7 (9%)
33	CLA	1	307	-	44,52,73	1.87	6 (13%)	55,88,113	1.61	8 (14%)
33	CLA	C	503	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
45	A86	6	303	-	44,50,50	1.24	4 (9%)	51,76,76	8.48	24 (47%)
33	CLA	B	603	-	64,72,73	1.47	7 (10%)	74,111,113	1.36	8 (10%)
34	PHO	A	407	-	51,69,69	1.01	4 (7%)	47,99,99	1.17	6 (12%)
33	CLA	7	310	26	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
45	A86	0	301	-	44,50,50	1.32	5 (11%)	51,76,76	2.05	16 (31%)
33	CLA	C	509	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	7 (9%)
39	LMG	D	410	-	46,46,55	0.81	1 (2%)	54,54,63	1.34	5 (9%)
45	A86	6	305	-	44,50,50	1.25	4 (9%)	51,76,76	9.10	23 (45%)
33	CLA	3	308	22	65,73,73	1.46	5 (7%)	76,113,113	1.36	7 (9%)
39	LMG	C	522	-	23,23,55	1.37	2 (8%)	31,31,63	1.50	7 (22%)
48	ET4	0	302	-	41,43,43	2.13	13 (31%)	54,60,60	2.45	19 (35%)
33	CLA	C	513	-	49,57,73	1.65	7 (14%)	55,93,113	1.63	8 (14%)
33	CLA	c	508	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	LHG	w	301	-	34,34,48	0.73	1 (2%)	37,40,54	1.23	4 (10%)
33	CLA	C	512	-	64,72,73	1.44	7 (10%)	74,111,113	1.42	6 (8%)
37	SQD	T	101	-	39,40,54	1.14	5 (12%)	48,51,65	2.02	11 (22%)
33	CLA	D	406	-	60,68,73	1.48	7 (11%)	70,107,113	1.53	7 (10%)
30	BCR	a	414	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	7 (12%)
33	CLA	d	402	-	60,68,73	1.51	7 (11%)	70,107,113	1.53	8 (11%)
33	CLA	9	305	-	41,49,73	1.86	5 (12%)	47,84,113	1.62	8 (17%)
45	A86	0	303	-	44,50,50	1.26	4 (9%)	51,76,76	2.07	14 (27%)
33	CLA	1	309	-	44,51,73	1.93	7 (15%)	50,86,113	1.68	8 (16%)
42	HEM	v	201	18	41,50,50	1.48	3 (7%)	45,82,82	1.28	4 (8%)
36	LHG	7	316	-	27,27,48	0.88	2 (7%)	31,32,54	1.70	4 (12%)
33	CLA	1	312	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	6 (11%)
38	DGD	H	102	-	63,63,67	0.89	2 (3%)	77,77,81	1.39	10 (12%)
33	CLA	3	311	-	41,49,73	1.81	6 (14%)	47,84,113	1.69	7 (14%)
33	CLA	9	310	29	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
33	CLA	8	305	-	41,49,73	1.84	5 (12%)	47,84,113	1.64	7 (14%)
36	LHG	d	405	-	46,47,48	0.63	2 (4%)	45,51,54	1.18	5 (11%)
39	LMG	M	201	-	40,40,55	0.85	2 (5%)	48,48,63	1.31	5 (10%)
46	DD6	1	303	-	39,45,45	1.96	3 (7%)	52,67,67	2.10	12 (23%)
39	LMG	B	620	-	51,51,55	0.74	0	59,59,63	1.36	7 (11%)
33	CLA	9	317	-	55,63,73	1.62	7 (12%)	64,101,113	1.48	7 (10%)
33	CLA	c	509	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	7 (9%)
33	CLA	a	411	-	60,68,73	1.54	7 (11%)	70,107,113	1.50	9 (12%)
30	BCR	B	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.20	4 (7%)
33	CLA	C	504	-	64,72,73	1.44	7 (10%)	74,111,113	1.44	6 (8%)
33	CLA	5	313	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
33	CLA	9	309	29	44,51,73	1.91	7 (15%)	50,86,113	1.68	8 (16%)
33	CLA	0	310	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	7 (13%)
38	DGD	c	517	-	57,57,67	0.95	2 (3%)	71,71,81	1.46	12 (16%)
46	DD6	2	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.17	13 (25%)
33	CLA	a	408	-	49,57,73	1.66	8 (16%)	55,93,113	1.59	8 (14%)
33	CLA	1	311	29	55,63,73	1.61	5 (9%)	64,101,113	1.47	8 (12%)
33	CLA	3	312	-	56,64,73	1.62	6 (10%)	65,102,113	1.45	7 (10%)
33	CLA	0	305	26	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
43	LMU	4	317	-	36,36,36	0.38	0	47,47,47	0.85	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	B	606	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	6 (7%)
33	CLA	b	613	-	65,73,73	1.46	7 (10%)	76,113,113	1.45	7 (9%)
30	BCR	k	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
33	CLA	3	319	-	55,63,73	1.60	6 (10%)	64,101,113	1.46	6 (9%)
33	CLA	0	307	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	8 (10%)
45	A86	9	302	-	44,50,50	1.29	5 (11%)	51,76,76	2.47	18 (35%)
37	SQD	D	403	-	53,54,54	0.95	5 (9%)	62,65,65	1.48	9 (14%)
33	CLA	1	305	-	41,49,73	1.86	5 (12%)	47,84,113	1.64	7 (14%)
33	CLA	7	304	-	47,55,73	1.71	6 (12%)	54,91,113	1.58	6 (11%)
33	CLA	7	309	26	65,73,73	1.46	7 (10%)	76,113,113	1.38	8 (10%)
37	SQD	l	101	-	53,54,54	0.96	5 (9%)	62,65,65	1.46	9 (14%)
33	CLA	7	313	26	35,42,73	2.42	8 (22%)	41,73,113	1.68	7 (17%)
33	CLA	8	313	29	36,44,73	2.03	7 (19%)	42,77,113	1.79	9 (21%)
45	A86	7	303	-	44,50,50	1.24	3 (6%)	51,76,76	2.23	16 (31%)
36	LHG	b	601	-	48,48,48	0.65	1 (2%)	51,54,54	1.28	6 (11%)
45	A86	5	304	-	44,50,50	1.23	3 (6%)	51,76,76	11.21	22 (43%)
39	LMG	b	622	-	28,28,55	0.98	0	36,36,63	1.31	5 (13%)
39	LMG	D	404	-	40,40,55	0.83	1 (2%)	48,48,63	1.31	5 (10%)
41	PL9	D	408	-	55,55,55	1.32	5 (9%)	68,69,69	1.50	12 (17%)
39	LMG	W	301	-	48,48,55	0.79	1 (2%)	56,56,63	1.35	6 (10%)
45	A86	6	304	-	44,50,50	1.24	3 (6%)	51,76,76	11.87	21 (41%)
33	CLA	5	317	-	37,46,73	1.92	5 (13%)	44,80,113	1.67	8 (18%)
37	SQD	i	101	-	39,40,54	1.12	5 (12%)	48,51,65	1.73	11 (22%)
45	A86	3	314	-	44,50,50	1.24	3 (6%)	51,76,76	2.23	17 (33%)
33	CLA	9	314	-	37,46,73	1.91	6 (16%)	44,80,113	1.62	7 (15%)
37	SQD	0	316	-	47,48,54	1.03	5 (10%)	56,59,65	1.52	9 (16%)
33	CLA	6	310	-	52,60,73	1.66	6 (11%)	60,97,113	1.50	7 (11%)
30	BCR	c	514	-	41,41,41	1.14	2 (4%)	56,56,56	1.24	7 (12%)
33	CLA	B	616	-	65,73,73	1.51	8 (12%)	76,113,113	1.36	8 (10%)
37	SQD	a	413	-	53,54,54	0.94	5 (9%)	62,65,65	1.60	11 (17%)
37	SQD	L	101	-	53,54,54	0.96	5 (9%)	62,65,65	1.51	9 (14%)
33	CLA	9	312	-	45,53,73	1.78	5 (11%)	52,89,113	1.56	6 (11%)
33	CLA	9	306	-	45,53,73	1.77	6 (13%)	52,89,113	1.60	6 (11%)
45	A86	5	306	-	44,50,50	1.24	4 (9%)	51,76,76	7.71	25 (49%)
33	CLA	4	311	23	60,68,73	1.52	7 (11%)	70,107,113	1.39	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
42	HEM	V	201	18	41,50,50	1.38	7 (17%)	45,82,82	1.84	8 (17%)
45	A86	8	302	-	44,50,50	1.25	3 (6%)	51,76,76	2.25	17 (33%)
45	A86	6	306	-	44,50,50	1.20	3 (6%)	51,76,76	8.91	22 (43%)
33	CLA	b	605	-	61,69,73	1.49	7 (11%)	71,108,113	1.49	10 (14%)
33	CLA	1	310	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	7 (9%)
33	CLA	0	311	-	51,59,73	1.65	6 (11%)	59,96,113	1.60	7 (11%)
33	CLA	7	305	26	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
33	CLA	5	314	24	55,63,73	1.60	5 (9%)	64,101,113	1.45	7 (10%)
37	SQD	T	103	-	53,54,54	0.94	5 (9%)	62,65,65	1.59	11 (17%)
33	CLA	b	606	-	65,73,73	1.47	7 (10%)	76,113,113	1.29	8 (10%)
36	LHG	5	318	-	32,32,48	0.83	2 (6%)	36,37,54	1.71	6 (16%)
38	DGD	c	518	-	56,56,67	0.94	2 (3%)	70,70,81	1.38	10 (14%)
33	CLA	b	615	-	64,72,73	1.45	7 (10%)	74,111,113	1.40	7 (9%)
33	CLA	0	304	-	47,55,73	1.70	6 (12%)	54,91,113	1.57	7 (12%)
33	CLA	C	507	-	65,73,73	1.44	7 (10%)	76,113,113	1.41	7 (9%)
33	CLA	3	304	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	6 (7%)
39	LMG	d	410	-	37,37,55	0.86	0	45,45,63	1.28	6 (13%)
33	CLA	8	306	29	45,53,73	1.76	6 (13%)	52,89,113	1.62	7 (13%)
35	BCT	A	410	40	2,3,3	1.32	0	2,3,3	4.05	2 (100%)
47	KC2	0	306	-	48,53,53	1.82	9 (18%)	54,89,89	2.27	15 (27%)
33	CLA	b	612	-	64,72,73	1.47	7 (10%)	74,111,113	1.44	9 (12%)
45	A86	5	302	-	44,50,50	1.26	4 (9%)	51,76,76	12.11	24 (47%)
45	A86	5	301	-	44,50,50	1.24	4 (9%)	51,76,76	11.32	26 (50%)
37	SQD	7	317	-	47,48,54	1.03	5 (10%)	56,59,65	1.55	10 (17%)
36	LHG	D	411	-	41,41,48	0.65	1 (2%)	44,47,54	1.28	4 (9%)
33	CLA	8	315	29	37,46,73	1.86	6 (16%)	44,80,113	1.74	8 (18%)
38	DGD	C	516	-	56,56,67	0.98	2 (3%)	70,70,81	1.44	11 (15%)
33	CLA	9	311	29	55,63,73	1.61	6 (10%)	64,101,113	1.48	7 (10%)
45	A86	6	302	-	44,50,50	1.20	3 (6%)	51,76,76	11.14	24 (47%)
39	LMG	5	319	-	31,31,55	0.95	0	39,39,63	1.33	5 (12%)
45	A86	5	307	-	44,50,50	1.24	4 (9%)	51,76,76	11.49	23 (45%)
30	BCR	C	515	-	41,41,41	0.75	0	56,56,56	1.92	15 (26%)
45	A86	6	301	-	44,50,50	1.25	5 (11%)	51,76,76	11.60	24 (47%)
33	CLA	B	613	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	7 (9%)
33	CLA	6	312	-	65,73,73	1.49	6 (9%)	76,113,113	1.33	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	KC2	6	309	-	48,53,53	1.88	9 (18%)	54,89,89	2.20	14 (25%)
33	CLA	2	306	-	45,53,73	1.77	5 (11%)	52,89,113	1.64	6 (11%)
33	CLA	8	314	-	37,46,73	1.93	6 (16%)	44,80,113	1.63	7 (15%)
39	LMG	Q	301	-	37,37,55	0.87	1 (2%)	45,45,63	1.27	4 (8%)
43	LMU	t	101	-	32,32,36	0.35	0	43,43,47	0.80	1 (2%)
33	CLA	a	407	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	6 (7%)
33	CLA	1	314	-	37,46,73	1.95	5 (13%)	44,80,113	1.61	7 (15%)
33	CLA	B	601	-	47,55,73	1.70	7 (14%)	54,91,113	1.53	6 (11%)
37	SQD	B	622	-	53,54,54	0.96	5 (9%)	62,65,65	1.78	10 (16%)
33	CLA	2	312	-	45,53,73	1.79	6 (13%)	52,89,113	1.58	6 (11%)
46	DD6	9	304	-	39,45,45	2.05	3 (7%)	52,67,67	2.23	15 (28%)
37	SQD	A	413	-	39,40,54	1.11	5 (12%)	48,51,65	1.76	12 (25%)
33	CLA	b	602	-	47,55,73	1.67	6 (12%)	54,91,113	1.60	7 (12%)
36	LHG	a	404	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
36	LHG	0	315	-	27,27,48	0.91	2 (7%)	31,32,54	1.68	4 (12%)
33	CLA	b	611	-	65,73,73	1.47	8 (12%)	76,113,113	1.38	7 (9%)
43	LMU	T	102	-	32,32,36	0.35	0	43,43,47	0.83	0
33	CLA	2	311	29	55,63,73	1.61	5 (9%)	64,101,113	1.44	6 (9%)
30	BCR	K	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	6 (10%)
33	CLA	9	308	-	55,63,73	1.60	6 (10%)	64,101,113	1.50	8 (12%)
33	CLA	3	303	-	65,73,73	1.48	7 (10%)	76,113,113	1.35	8 (10%)
33	CLA	7	307	-	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
30	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.15	4 (7%)
33	CLA	0	313	-	35,42,73	2.41	8 (22%)	41,73,113	1.67	8 (19%)
33	CLA	7	314	-	42,51,73	1.75	6 (14%)	50,86,113	1.61	6 (12%)
33	CLA	6	316	-	38,46,73	2.39	8 (21%)	47,79,113	1.61	9 (19%)
33	CLA	7	312	-	65,73,73	1.47	6 (9%)	76,113,113	1.35	7 (9%)
36	LHG	H	104	-	41,41,48	0.67	1 (2%)	44,47,54	1.30	5 (11%)
45	A86	1	302	-	44,50,50	1.25	3 (6%)	51,76,76	2.25	17 (33%)
33	CLA	6	315	-	41,49,73	1.83	6 (14%)	47,84,113	1.68	7 (14%)
33	CLA	B	608	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	8 (10%)
45	A86	2	302	-	44,50,50	1.29	5 (11%)	51,76,76	2.47	18 (35%)
38	DGD	a	401	-	54,54,67	1.01	4 (7%)	67,67,81	1.48	13 (19%)
33	CLA	0	308	-	41,49,73	1.82	6 (14%)	47,84,113	1.67	9 (19%)
33	CLA	B	612	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	1	316	29	37,46,73	1.93	5 (13%)	44,80,113	1.67	7 (15%)
33	CLA	2	314	-	37,46,73	1.91	5 (13%)	44,80,113	1.66	7 (15%)
31	OEX	A	402	1,3	0,15,15	-	-	-	-	-
33	CLA	A	404	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	7 (9%)
45	A86	2	301	-	44,50,50	1.20	3 (6%)	51,76,76	2.17	16 (31%)
45	A86	9	301	-	44,50,50	1.19	3 (6%)	51,76,76	2.18	16 (31%)
36	LHG	D	409	-	46,47,48	0.64	2 (4%)	45,51,54	1.18	5 (11%)
47	KC2	7	306	-	48,53,53	1.84	9 (18%)	54,89,89	2.29	14 (25%)
46	DD6	8	304	-	39,45,45	2.05	3 (7%)	52,67,67	2.52	18 (34%)
33	CLA	1	315	-	37,46,73	1.89	5 (13%)	44,80,113	1.69	7 (15%)
33	CLA	D	405	-	57,65,73	1.63	8 (14%)	70,103,113	1.49	10 (14%)
30	BCR	D	407	-	41,41,41	1.17	3 (7%)	56,56,56	1.20	6 (10%)
33	CLA	6	313	25	46,54,73	1.75	5 (10%)	53,90,113	1.54	7 (13%)
30	BCR	H	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.18	3 (5%)
39	LMG	7	315	-	55,55,55	0.73	1 (1%)	63,63,63	1.35	6 (9%)
47	KC2	5	310	-	48,53,53	1.81	9 (18%)	54,89,89	2.31	13 (24%)
33	CLA	C	505	-	65,73,73	1.47	6 (9%)	76,113,113	1.29	7 (9%)
45	A86	8	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.15	16 (31%)
30	BCR	a	412	-	41,41,41	1.17	2 (4%)	56,56,56	1.16	3 (5%)
33	CLA	5	308	-	46,54,73	1.74	5 (10%)	53,90,113	1.55	6 (11%)
36	LHG	A	414	-	48,48,48	0.65	1 (2%)	51,54,54	1.27	6 (11%)
33	CLA	c	507	-	65,73,73	1.45	7 (10%)	76,113,113	1.40	6 (7%)
45	A86	4	304	-	44,50,50	1.22	3 (6%)	51,76,76	2.21	17 (33%)
33	CLA	w	303	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	8 (10%)
46	DD6	2	304	-	39,45,45	2.05	3 (7%)	52,67,67	2.23	15 (28%)
44	KC1	6	314	25	48,53,53	1.59	7 (14%)	55,89,89	1.88	12 (21%)
33	CLA	4	316	-	52,60,73	1.64	7 (13%)	60,97,113	1.54	8 (13%)
36	LHG	A	411	-	42,42,48	0.68	1 (2%)	45,48,54	1.21	4 (8%)
39	LMG	d	406	-	46,46,55	0.80	1 (2%)	54,54,63	1.35	6 (11%)
33	CLA	H	103	26	42,51,73	1.79	6 (14%)	50,86,113	1.57	6 (12%)
33	CLA	c	505	-	65,73,73	1.46	7 (10%)	76,113,113	1.33	7 (9%)
30	BCR	B	617	-	41,41,41	1.21	3 (7%)	56,56,56	1.21	7 (12%)
34	PHO	A	406	-	51,69,69	1.02	4 (7%)	47,99,99	1.17	6 (12%)
33	CLA	c	504	-	64,72,73	1.46	7 (10%)	74,111,113	1.43	6 (8%)
46	DD6	3	315	-	39,45,45	1.99	3 (7%)	52,67,67	1.99	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	BCR	c	515	-	41,41,41	0.80	1 (2%)	56,56,56	2.00	15 (26%)
33	CLA	0	312	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
38	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.38	9 (11%)
33	CLA	C	501	-	65,73,73	1.43	7 (10%)	76,113,113	1.39	7 (9%)
33	CLA	B	615	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	7 (9%)
33	CLA	5	311	-	55,63,73	1.61	5 (9%)	64,101,113	1.48	8 (12%)
33	CLA	B	609	-	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)
33	CLA	3	306	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
33	CLA	4	315	-	47,55,73	1.72	6 (12%)	54,91,113	1.58	8 (14%)
33	CLA	D	402	-	59,67,73	1.51	7 (11%)	68,105,113	1.49	8 (11%)
30	BCR	b	618	-	41,41,41	1.20	3 (7%)	56,56,56	1.23	7 (12%)
39	LMG	q	302	-	37,37,55	0.84	0	45,45,63	1.27	5 (11%)
33	CLA	b	610	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	8 (10%)
33	CLA	c	503	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	7 (9%)
36	LHG	A	412	-	48,48,48	0.60	1 (2%)	51,54,54	1.25	6 (11%)
33	CLA	1	313	29	36,44,73	2.06	7 (19%)	42,77,113	1.77	8 (19%)
33	CLA	c	513	-	49,57,73	1.68	7 (14%)	55,93,113	1.62	7 (12%)
33	CLA	b	604	-	64,72,73	1.46	7 (10%)	74,111,113	1.37	8 (10%)
33	CLA	3	305	-	48,56,73	1.70	7 (14%)	55,92,113	1.59	8 (14%)
33	CLA	C	511	3	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
33	CLA	c	512	-	64,72,73	1.46	7 (10%)	74,111,113	1.39	7 (9%)
33	CLA	4	314	23	56,64,73	1.58	6 (10%)	65,102,113	1.45	7 (10%)
45	A86	4	302	-	44,50,50	1.25	4 (9%)	51,76,76	12.51	29 (56%)
33	CLA	4	313	23	41,49,73	1.82	6 (14%)	47,84,113	1.66	8 (17%)
33	CLA	3	307	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
33	CLA	b	608	-	41,49,73	1.77	7 (17%)	47,84,113	1.74	7 (14%)
36	LHG	h	103	-	41,41,48	0.68	1 (2%)	44,47,54	1.30	5 (11%)
39	LMG	C	521	-	27,27,55	1.06	1 (3%)	35,35,63	1.15	5 (14%)
33	CLA	5	316	-	41,49,73	1.84	5 (12%)	47,84,113	1.65	8 (17%)
30	BCR	b	620	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	6 (10%)
42	HEM	F	101	6	41,50,50	1.46	3 (7%)	45,82,82	1.33	5 (11%)
42	HEM	e	101	6	41,50,50	1.35	6 (14%)	45,82,82	1.86	9 (20%)
33	CLA	A	408	-	60,68,73	1.52	7 (11%)	70,107,113	1.42	8 (11%)
33	CLA	8	311	29	55,63,73	1.59	6 (10%)	64,101,113	1.46	8 (12%)
36	LHG	3	318	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	B	605	-	65,73,73	1.45	7 (10%)	76,113,113	1.31	8 (10%)
33	CLA	b	614	-	65,73,73	1.47	8 (12%)	76,113,113	1.37	7 (9%)

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
46	DD6	4	303	-	-	3/26/80/80	0/3/3/3
33	CLA	c	501	-	1/1/15/20	21/37/115/115	-
33	CLA	W	303	-	1/1/15/20	15/37/115/115	-
33	CLA	b	607	-	1/1/15/20	8/37/115/115	-
33	CLA	2	308	-	1/1/13/20	13/25/103/115	-
33	CLA	2	310	29	1/1/15/20	13/37/115/115	-
33	CLA	8	312	-	1/1/11/20	4/13/91/115	-
33	CLA	B	602	-	1/1/12/20	12/27/107/115	-
36	LHG	4	318	-	-	31/53/53/53	-
38	DGD	C	517	-	-	18/45/85/95	0/2/2/2
33	CLA	2	305	-	1/1/10/20	2/8/86/115	-
30	BCR	K	102	-	-	4/29/63/63	0/2/2/2
33	CLA	B	611	-	1/1/14/20	10/35/113/115	-
33	CLA	2	315	-	1/1/9/20	0/2/80/115	-
33	CLA	3	302	-	1/1/15/20	18/37/115/115	-
33	CLA	9	315	-	1/1/9/20	0/2/80/115	-
30	BCR	h	101	-	-	4/29/63/63	0/2/2/2
33	CLA	6	308	25	1/1/12/20	4/24/102/115	-
33	CLA	b	617	-	1/1/15/20	16/37/115/115	-
33	CLA	C	510	-	1/1/15/20	8/37/115/115	-
38	DGD	3	320	-	-	20/40/40/95	-
33	CLA	8	308	-	1/1/13/20	11/25/103/115	-
37	SQD	t	102	-	-	18/34/54/69	0/1/1/1
38	DGD	C	518	-	-	13/44/84/95	0/2/2/2
47	KC2	4	307	-	-	8/15/71/71	-
33	CLA	c	510	-	1/1/15/20	12/37/115/115	-
33	CLA	1	306	29	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	b	603	-	1/1/12/20	9/27/107/115	-
33	CLA	1	308	-	1/1/13/20	8/25/103/115	-
38	DGD	A	415	-	-	24/43/79/95	0/2/2/2
36	LHG	W	302	-	-	23/39/39/53	-
33	CLA	z	101	-	1/1/12/20	4/21/99/115	-
33	CLA	5	309	24	1/1/13/20	3/25/103/115	-
39	LMG	w	304	-	-	20/43/63/70	0/1/1/1
33	CLA	C	502	-	1/1/14/20	17/35/113/115	-
33	CLA	0	309	26	1/1/15/20	13/37/115/115	-
45	A86	5	303	-	-	9/34/90/90	0/3/3/3
33	CLA	6	311	-	1/1/11/20	8/15/93/115	-
33	CLA	8	316	29	1/1/9/20	0/2/80/115	-
30	BCR	k	102	-	-	4/29/63/63	0/2/2/2
33	CLA	4	309	23	1/1/15/20	3/37/115/115	-
34	PHO	a	409	-	-	13/37/103/103	0/5/6/6
36	LHG	a	403	-	-	12/47/47/53	-
33	CLA	C	506	-	1/1/11/20	5/13/91/115	-
33	CLA	6	307	-	1/1/12/20	6/23/101/115	-
46	DD6	9	303	-	-	4/26/80/80	0/3/3/3
34	PHO	a	410	-	-	3/37/103/103	0/5/6/6
33	CLA	b	616	-	1/1/15/20	6/37/115/115	-
30	BCR	C	514	-	-	4/29/63/63	0/2/2/2
44	KC1	3	310	-	-	9/15/71/71	-
33	CLA	4	305	-	1/1/13/20	7/25/103/115	-
39	LMG	B	621	-	-	6/23/43/70	0/1/1/1
33	CLA	2	309	-	1/1/11/20	6/11/89/115	-
33	CLA	d	401	-	1/1/13/20	6/28/104/115	-
33	CLA	2	317	-	1/1/13/20	8/25/103/115	-
45	A86	1	301	-	-	5/34/90/90	0/3/3/3
33	CLA	8	307	-	1/1/11/20	5/13/89/115	-
30	BCR	A	401	-	-	5/29/63/63	0/2/2/2
30	BCR	b	619	-	-	5/29/63/63	0/2/2/2
39	LMG	c	520	-	-	7/21/41/70	0/1/1/1
43	LMU	w	302	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	3	317	33	-	12/31/31/53	-
41	PL9	d	404	-	-	7/53/73/73	0/1/1/1
44	KC1	5	315	-	-	8/15/71/71	-
30	BCR	B	618	-	-	5/29/63/63	0/2/2/2
39	LMG	C	519	-	-	18/41/61/70	0/1/1/1
33	CLA	B	607	-	1/1/10/20	3/8/86/115	-
33	CLA	4	308	-	1/1/15/20	10/37/115/115	-
33	CLA	4	310	-	1/1/11/20	5/15/93/115	-
33	CLA	2	316	29	1/1/9/20	0/2/80/115	-
45	A86	5	305	-	-	8/33/89/90	0/3/3/3
39	LMG	m	201	-	-	16/35/55/70	0/1/1/1
45	A86	7	301	-	-	8/34/90/90	0/3/3/3
33	CLA	8	310	29	1/1/15/20	16/37/115/115	-
33	CLA	c	511	3	1/1/15/20	8/37/115/115	-
43	LMU	5	320	-	-	9/17/57/61	0/2/2/2
33	CLA	A	405	-	1/1/11/20	3/18/96/115	-
33	CLA	Z	101	-	1/1/12/20	2/21/99/115	-
33	CLA	3	313	-	1/1/14/20	16/33/111/115	-
39	LMG	0	314	-	-	20/37/57/70	0/1/1/1
33	CLA	d	409	-	1/1/13/20	6/30/108/115	-
30	BCR	d	403	-	-	8/29/63/63	0/2/2/2
33	CLA	7	308	26	1/1/10/20	2/8/86/115	-
39	LMG	q	301	-	-	22/41/61/70	0/1/1/1
46	DD6	8	303	-	-	3/26/80/80	0/3/3/3
33	CLA	c	502	-	1/1/14/20	14/35/113/115	-
48	ET4	7	302	-	-	11/25/67/67	0/2/2/2
33	CLA	B	610	-	1/1/15/20	5/37/115/115	-
33	CLA	4	306	23	1/1/15/20	5/37/115/115	-
33	CLA	8	309	-	1/1/11/20	6/11/89/115	-
36	LHG	d	407	-	-	18/46/46/53	-
33	CLA	B	604	-	1/1/14/20	10/33/111/115	-
33	CLA	2	307	-	1/1/11/20	7/13/89/115	-
43	LMU	3	301	-	-	17/21/61/61	0/2/2/2
33	CLA	9	307	-	1/1/11/20	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	DGD	c	516	-	-	14/44/84/95	0/2/2/2
46	DD6	1	304	-	-	7/26/80/80	0/3/3/3
33	CLA	2	313	29	-	0/0/78/115	-
33	CLA	7	311	-	1/1/12/20	11/21/99/115	-
33	CLA	9	313	-	1/1/9/20	0/0/78/115	-
39	LMG	b	621	-	-	20/46/66/70	0/1/1/1
33	CLA	C	508	-	1/1/15/20	7/37/115/115	-
33	CLA	5	312	-	1/1/11/20	7/15/93/115	-
45	A86	4	301	-	-	9/34/90/90	0/3/3/3
33	CLA	4	312	-	1/1/12/20	7/21/99/115	-
33	CLA	c	506	-	1/1/11/20	5/13/91/115	-
33	CLA	b	609	-	1/1/15/20	5/37/115/115	-
33	CLA	9	316	29	1/1/9/20	0/2/80/115	-
33	CLA	3	309	36	1/1/12/20	5/21/99/115	-
39	LMG	3	316	-	-	7/26/46/70	0/1/1/1
39	LMG	b	623	-	-	22/35/55/70	0/1/1/1
39	LMG	C	520	-	-	19/43/63/70	0/1/1/1
39	LMG	c	519	-	-	21/43/63/70	0/1/1/1
33	CLA	B	614	-	1/1/14/20	13/35/113/115	-
33	CLA	1	307	-	1/1/11/20	3/13/89/115	-
33	CLA	C	503	-	1/1/15/20	15/37/115/115	-
45	A86	6	303	-	-	8/34/90/90	0/3/3/3
33	CLA	B	603	-	1/1/14/20	11/35/113/115	-
34	PHO	A	407	-	-	8/37/103/103	0/5/6/6
33	CLA	7	310	26	1/1/11/20	6/13/91/115	-
45	A86	0	301	-	-	8/34/90/90	0/3/3/3
33	CLA	C	509	-	1/1/15/20	10/37/115/115	-
39	LMG	D	410	-	-	15/41/61/70	0/1/1/1
45	A86	6	305	-	-	8/34/90/90	0/3/3/3
33	CLA	3	308	22	1/1/15/20	16/37/115/115	-
39	LMG	C	522	-	-	7/16/36/70	0/1/1/1
48	ET4	0	302	-	-	13/25/67/67	0/2/2/2
33	CLA	C	513	-	1/1/11/20	5/18/96/115	-
33	CLA	c	508	-	1/1/15/20	10/37/115/115	-
36	LHG	w	301	-	-	22/39/39/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	C	512	-	1/1/14/20	12/35/113/115	-
37	SQD	T	101	-	-	16/34/54/69	0/1/1/1
33	CLA	D	406	-	1/1/14/20	10/31/109/115	-
33	CLA	d	402	-	1/1/14/20	10/31/109/115	-
30	BCR	a	414	-	-	4/29/63/63	0/2/2/2
33	CLA	9	305	-	1/1/10/20	2/8/86/115	-
45	A86	0	303	-	-	4/34/90/90	0/3/3/3
33	CLA	1	309	-	1/1/11/20	7/11/89/115	-
42	HEM	v	201	18	-	5/12/54/54	-
36	LHG	7	316	-	-	15/29/29/53	-
33	CLA	1	312	-	1/1/11/20	6/13/91/115	-
38	DGD	H	102	-	-	16/51/91/95	0/2/2/2
33	CLA	3	311	-	1/1/10/20	3/8/86/115	-
33	CLA	9	310	29	1/1/15/20	15/37/115/115	-
33	CLA	8	305	-	1/1/10/20	2/8/86/115	-
36	LHG	d	405	-	-	22/47/51/53	-
39	LMG	M	201	-	-	14/35/55/70	0/1/1/1
46	DD6	1	303	-	-	3/26/80/80	0/3/3/3
39	LMG	B	620	-	-	19/46/66/70	0/1/1/1
33	CLA	9	317	-	1/1/13/20	9/25/103/115	-
33	CLA	c	509	-	1/1/15/20	6/37/115/115	-
33	CLA	a	411	-	1/1/14/20	5/31/109/115	-
30	BCR	B	619	-	-	8/29/63/63	0/2/2/2
33	CLA	C	504	-	1/1/14/20	13/35/113/115	-
33	CLA	5	313	-	1/1/15/20	11/37/115/115	-
33	CLA	9	309	29	1/1/11/20	5/11/89/115	-
33	CLA	0	310	-	1/1/11/20	8/13/91/115	-
38	DGD	c	517	-	-	21/45/85/95	0/2/2/2
46	DD6	2	303	-	-	4/26/80/80	0/3/3/3
33	CLA	a	408	-	1/1/11/20	4/18/96/115	-
33	CLA	1	311	29	1/1/13/20	7/25/103/115	-
33	CLA	3	312	-	1/1/13/20	12/27/105/115	-
33	CLA	0	305	26	1/1/15/20	18/37/115/115	-
43	LMU	4	317	-	-	14/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	B	606	-	1/1/15/20	8/37/115/115	-
33	CLA	b	613	-	1/1/15/20	15/37/115/115	-
33	CLA	3	319	-	1/1/13/20	9/25/103/115	-
30	BCR	k	101	-	-	24/29/63/63	0/2/2/2
33	CLA	0	307	-	1/1/15/20	13/37/115/115	-
45	A86	9	302	-	-	8/34/90/90	0/3/3/3
37	SQD	D	403	-	-	21/49/69/69	0/1/1/1
33	CLA	1	305	-	1/1/10/20	4/8/86/115	-
33	CLA	7	304	-	1/1/11/20	7/16/94/115	-
33	CLA	7	309	26	1/1/15/20	18/37/115/115	-
37	SQD	l	101	-	-	21/49/69/69	0/1/1/1
33	CLA	7	313	26	1/1/8/20	0/2/74/115	-
33	CLA	8	313	29	1/1/9/20	0/0/78/115	-
45	A86	7	303	-	-	6/34/90/90	0/3/3/3
36	LHG	b	601	-	-	21/53/53/53	-
45	A86	5	304	-	-	8/34/90/90	0/3/3/3
39	LMG	b	622	-	-	4/23/43/70	0/1/1/1
39	LMG	D	404	-	-	20/35/55/70	0/1/1/1
41	PL9	D	408	-	-	5/53/73/73	0/1/1/1
39	LMG	W	301	-	-	18/43/63/70	0/1/1/1
45	A86	6	304	-	-	9/34/90/90	0/3/3/3
33	CLA	5	317	-	1/1/9/20	0/2/80/115	-
37	SQD	i	101	-	-	9/35/55/69	0/1/1/1
45	A86	3	314	-	-	7/34/90/90	0/3/3/3
33	CLA	9	314	-	1/1/9/20	0/2/80/115	-
37	SQD	0	316	-	-	14/43/63/69	0/1/1/1
33	CLA	6	310	-	1/1/12/20	7/22/100/115	-
30	BCR	c	514	-	-	5/29/63/63	0/2/2/2
33	CLA	B	616	-	1/1/15/20	12/37/115/115	-
37	SQD	a	413	-	-	17/49/69/69	0/1/1/1
37	SQD	L	101	-	-	23/49/69/69	0/1/1/1
33	CLA	9	312	-	1/1/11/20	5/13/91/115	-
33	CLA	9	306	-	1/1/11/20	7/13/91/115	-
45	A86	5	306	-	-	8/34/90/90	0/3/3/3
33	CLA	4	311	23	1/1/14/20	13/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	HEM	V	201	18	-	4/12/54/54	-
45	A86	8	302	-	-	8/34/90/90	0/3/3/3
45	A86	6	306	-	-	8/34/90/90	0/3/3/3
33	CLA	b	605	-	1/1/14/20	9/33/111/115	-
33	CLA	1	310	-	1/1/15/20	17/37/115/115	-
33	CLA	0	311	-	1/1/12/20	7/21/99/115	-
33	CLA	7	305	26	1/1/15/20	21/37/115/115	-
33	CLA	5	314	24	1/1/13/20	4/25/103/115	-
37	SQD	T	103	-	-	21/49/69/69	0/1/1/1
33	CLA	b	606	-	1/1/15/20	10/37/115/115	-
36	LHG	5	318	-	-	13/34/34/53	-
38	DGD	c	518	-	-	15/44/84/95	0/2/2/2
33	CLA	b	615	-	1/1/14/20	14/35/113/115	-
33	CLA	0	304	-	1/1/11/20	10/16/94/115	-
33	CLA	C	507	-	1/1/15/20	15/37/115/115	-
33	CLA	3	304	-	1/1/15/20	12/37/115/115	-
39	LMG	d	410	-	-	17/32/52/70	0/1/1/1
33	CLA	8	306	29	1/1/11/20	6/13/91/115	-
47	KC2	0	306	-	-	11/15/71/71	-
33	CLA	b	612	-	1/1/14/20	6/35/113/115	-
45	A86	5	302	-	-	9/34/90/90	0/3/3/3
45	A86	5	301	-	-	11/34/90/90	0/3/3/3
37	SQD	7	317	-	-	13/43/63/69	0/1/1/1
36	LHG	D	411	-	-	19/46/46/53	-
33	CLA	8	315	29	1/1/9/20	0/2/80/115	-
38	DGD	C	516	-	-	19/44/84/95	0/2/2/2
33	CLA	9	311	29	1/1/13/20	8/25/103/115	-
45	A86	6	302	-	-	8/34/90/90	0/3/3/3
39	LMG	5	319	-	-	13/26/46/70	0/1/1/1
45	A86	5	307	-	-	8/34/90/90	0/3/3/3
30	BCR	C	515	-	-	9/29/63/63	0/2/2/2
45	A86	6	301	-	-	7/34/90/90	0/3/3/3
33	CLA	B	613	-	1/1/15/20	14/37/115/115	-
33	CLA	6	312	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	KC2	6	309	-	-	7/15/71/71	-
33	CLA	2	306	-	1/1/11/20	5/13/91/115	-
33	CLA	8	314	-	1/1/9/20	0/2/80/115	-
39	LMG	Q	301	-	-	16/32/52/70	0/1/1/1
43	LMU	t	101	-	-	12/17/57/61	0/2/2/2
33	CLA	a	407	-	1/1/15/20	8/37/115/115	-
33	CLA	1	314	-	1/1/9/20	0/2/80/115	-
33	CLA	B	601	-	1/1/11/20	7/16/94/115	-
37	SQD	B	622	-	-	21/49/69/69	0/1/1/1
33	CLA	2	312	-	1/1/11/20	3/13/91/115	-
46	DD6	9	304	-	-	10/26/80/80	0/3/3/3
37	SQD	A	413	-	-	13/35/55/69	0/1/1/1
33	CLA	b	602	-	1/1/11/20	8/16/94/115	-
36	LHG	a	404	-	-	26/53/53/53	-
36	LHG	0	315	-	-	17/29/29/53	-
33	CLA	b	611	-	1/1/15/20	7/37/115/115	-
43	LMU	T	102	-	-	9/17/57/61	0/2/2/2
33	CLA	2	311	29	1/1/13/20	9/25/103/115	-
30	BCR	K	101	-	-	19/29/63/63	0/2/2/2
33	CLA	9	308	-	1/1/13/20	11/25/103/115	-
33	CLA	3	303	-	1/1/15/20	15/37/115/115	-
33	CLA	7	307	-	1/1/15/20	13/37/115/115	-
30	BCR	A	409	-	-	4/29/63/63	0/2/2/2
33	CLA	0	313	-	1/1/8/20	0/2/74/115	-
33	CLA	7	314	-	1/1/10/20	4/9/87/115	-
33	CLA	6	316	-	1/1/9/20	2/8/80/115	-
33	CLA	7	312	-	1/1/15/20	15/37/115/115	-
36	LHG	H	104	-	-	20/46/46/53	-
45	A86	1	302	-	-	8/34/90/90	0/3/3/3
33	CLA	6	315	-	1/1/10/20	3/8/86/115	-
33	CLA	B	608	-	1/1/15/20	5/37/115/115	-
45	A86	2	302	-	-	8/34/90/90	0/3/3/3
38	DGD	a	401	-	-	27/43/79/95	0/2/2/2
33	CLA	0	308	-	1/1/10/20	2/8/86/115	-
33	CLA	B	612	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	1	316	29	1/1/9/20	0/2/80/115	-
33	CLA	2	314	-	1/1/9/20	0/2/80/115	-
33	CLA	A	404	-	1/1/15/20	9/37/115/115	-
45	A86	2	301	-	-	7/34/90/90	0/3/3/3
45	A86	9	301	-	-	7/34/90/90	0/3/3/3
36	LHG	D	409	-	-	18/47/51/53	-
47	KC2	7	306	-	-	8/15/71/71	-
46	DD6	8	304	-	-	10/26/80/80	0/3/3/3
33	CLA	1	315	-	1/1/9/20	0/2/80/115	-
33	CLA	D	405	-	1/1/13/20	5/28/104/115	-
30	BCR	D	407	-	-	4/29/63/63	0/2/2/2
33	CLA	6	313	25	1/1/11/20	5/15/93/115	-
30	BCR	H	101	-	-	5/29/63/63	0/2/2/2
39	LMG	7	315	-	-	26/50/70/70	0/1/1/1
47	KC2	5	310	-	-	6/15/71/71	-
33	CLA	C	505	-	1/1/15/20	16/37/115/115	-
45	A86	8	301	-	-	8/34/90/90	0/3/3/3
30	BCR	a	412	-	-	4/29/63/63	0/2/2/2
33	CLA	5	308	-	1/1/11/20	9/15/93/115	-
36	LHG	A	414	-	-	17/53/53/53	-
33	CLA	c	507	-	1/1/15/20	13/37/115/115	-
45	A86	4	304	-	-	3/34/90/90	0/3/3/3
33	CLA	w	303	-	1/1/15/20	17/37/115/115	-
46	DD6	2	304	-	-	10/26/80/80	0/3/3/3
44	KC1	6	314	25	-	7/15/71/71	-
33	CLA	4	316	-	1/1/12/20	4/22/100/115	-
36	LHG	A	411	-	-	14/47/47/53	-
39	LMG	d	406	-	-	16/41/61/70	0/1/1/1
33	CLA	H	103	26	1/1/10/20	4/9/87/115	-
33	CLA	c	505	-	1/1/15/20	16/37/115/115	-
30	BCR	B	617	-	-	2/29/63/63	0/2/2/2
34	PHO	A	406	-	-	14/37/103/103	0/5/6/6
33	CLA	c	504	-	1/1/14/20	12/35/113/115	-
46	DD6	3	315	-	-	5/26/80/80	0/3/3/3
30	BCR	c	515	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	0	312	-	1/1/15/20	18/37/115/115	-
38	DGD	h	102	-	-	16/51/91/95	0/2/2/2
33	CLA	C	501	-	1/1/15/20	21/37/115/115	-
33	CLA	B	615	-	1/1/15/20	6/37/115/115	-
33	CLA	5	311	-	1/1/13/20	7/25/103/115	-
33	CLA	B	609	-	1/1/15/20	11/37/115/115	-
33	CLA	3	306	-	1/1/15/20	12/37/115/115	-
33	CLA	4	315	-	1/1/11/20	4/16/94/115	-
33	CLA	D	402	-	1/1/13/20	4/30/108/115	-
30	BCR	b	618	-	-	3/29/63/63	0/2/2/2
39	LMG	q	302	-	-	18/32/52/70	0/1/1/1
33	CLA	b	610	-	1/1/15/20	10/37/115/115	-
33	CLA	c	503	-	1/1/15/20	13/37/115/115	-
36	LHG	A	412	-	-	27/53/53/53	-
33	CLA	1	313	29	1/1/9/20	0/0/78/115	-
33	CLA	c	513	-	1/1/11/20	5/18/96/115	-
33	CLA	b	604	-	1/1/14/20	14/35/113/115	-
33	CLA	3	305	-	1/1/11/20	10/17/95/115	-
33	CLA	C	511	3	1/1/15/20	9/37/115/115	-
33	CLA	c	512	-	1/1/14/20	11/35/113/115	-
33	CLA	4	314	23	1/1/13/20	5/27/105/115	-
45	A86	4	302	-	-	9/34/90/90	0/3/3/3
33	CLA	4	313	23	1/1/10/20	0/8/86/115	-
33	CLA	3	307	-	1/1/15/20	11/37/115/115	-
33	CLA	b	608	-	1/1/10/20	5/8/86/115	-
36	LHG	h	103	-	-	18/46/46/53	-
39	LMG	C	521	-	-	4/21/41/70	0/1/1/1
33	CLA	5	316	-	1/1/10/20	2/8/86/115	-
30	BCR	b	620	-	-	8/29/63/63	0/2/2/2
42	HEM	F	101	6	-	3/12/54/54	-
42	HEM	e	101	6	-	7/12/54/54	-
33	CLA	A	408	-	1/1/14/20	7/31/109/115	-
33	CLA	8	311	29	1/1/13/20	6/25/103/115	-
36	LHG	3	318	-	-	23/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	B	605	-	1/1/15/20	15/37/115/115	-
33	CLA	b	614	-	1/1/15/20	12/37/115/115	-

The worst 5 of 1627 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2	313	CLA	C4B-NB	9.58	1.43	1.35
46	9	304	DD6	C29-C27	-8.81	1.25	1.42
46	1	304	DD6	C29-C27	-8.79	1.25	1.42
46	2	304	DD6	C29-C27	-8.78	1.25	1.42
46	8	304	DD6	C29-C27	-8.72	1.25	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	5	302	A86	C23-C16-C22	-71.43	2.00	107.37
45	6	304	A86	C23-C16-C22	-71.27	2.25	107.37
45	5	303	A86	C23-C16-C22	-70.78	2.97	107.37
45	4	302	A86	C23-C16-C22	-70.28	3.70	107.37
45	5	307	A86	C23-C16-C22	-68.88	5.76	107.37

5 of 182 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	A	404	CLA	ND
33	A	405	CLA	ND
33	A	408	CLA	ND
33	B	601	CLA	ND
33	B	602	CLA	ND

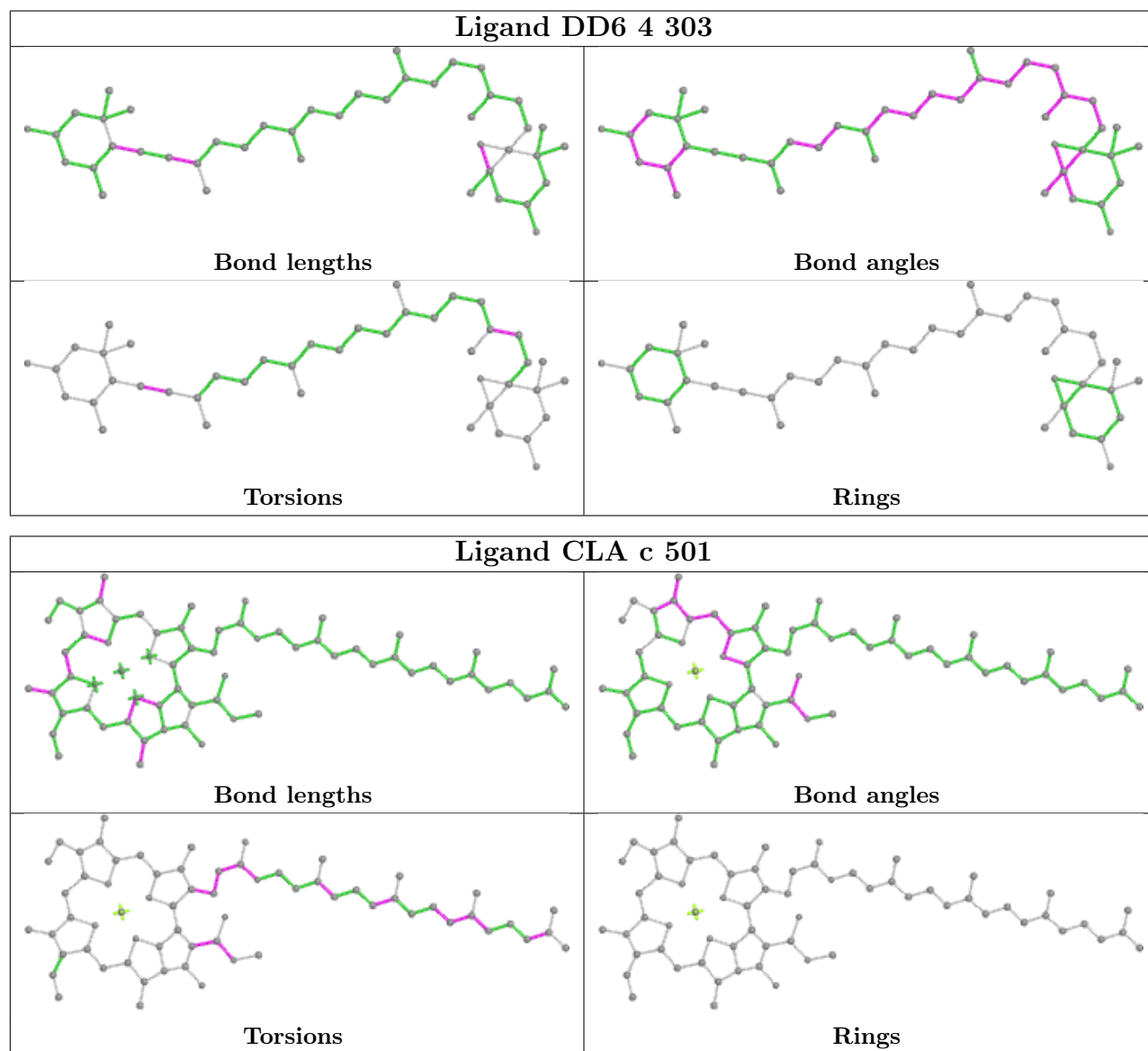
5 of 3309 torsion outliers are listed below:

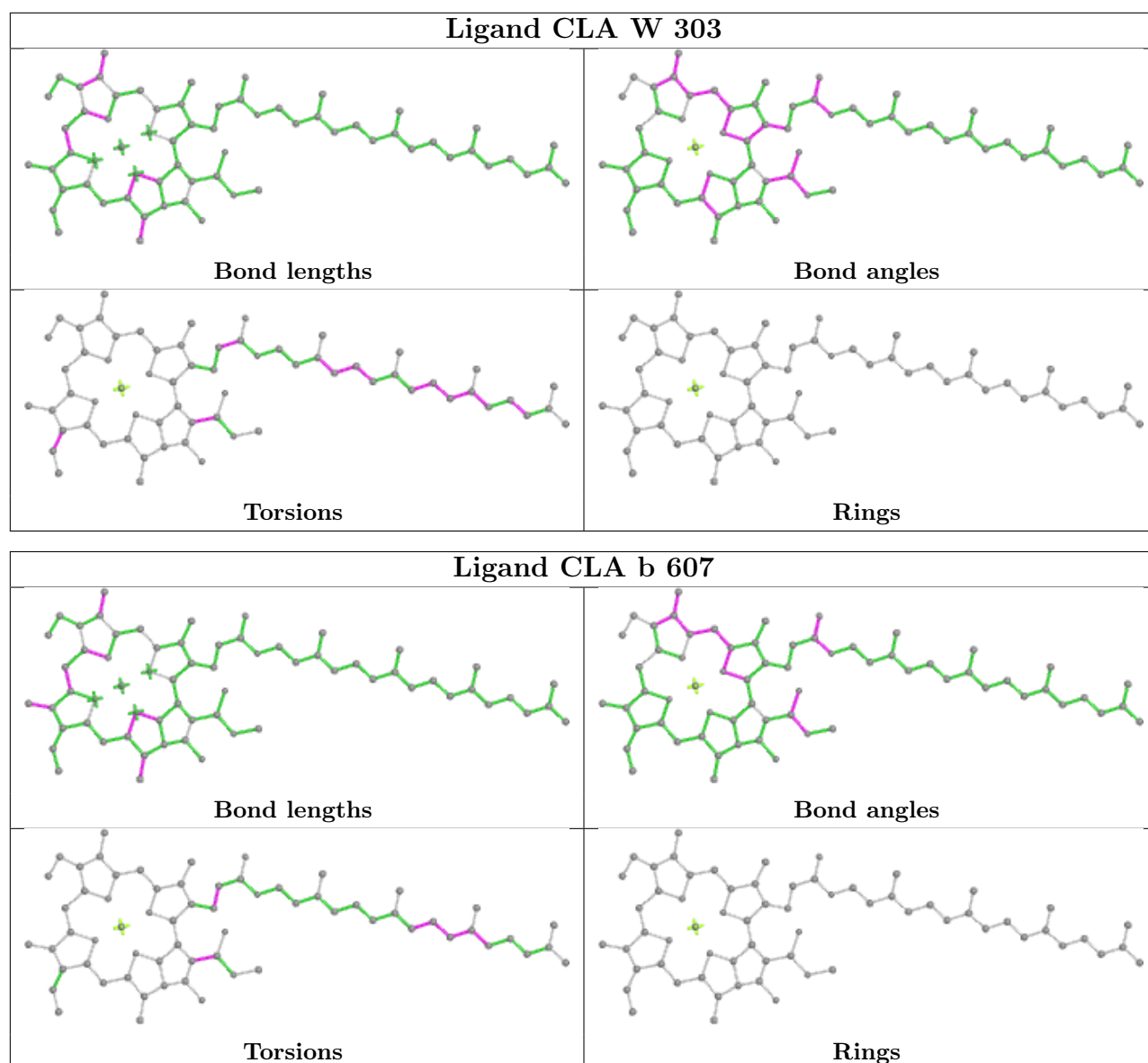
Mol	Chain	Res	Type	Atoms
30	A	401	BCR	C1-C6-C7-C8
30	B	618	BCR	C7-C8-C9-C34
30	B	619	BCR	C7-C8-C9-C10
30	B	619	BCR	C21-C22-C23-C24
30	B	619	BCR	C37-C22-C23-C24

There are no ring outliers.

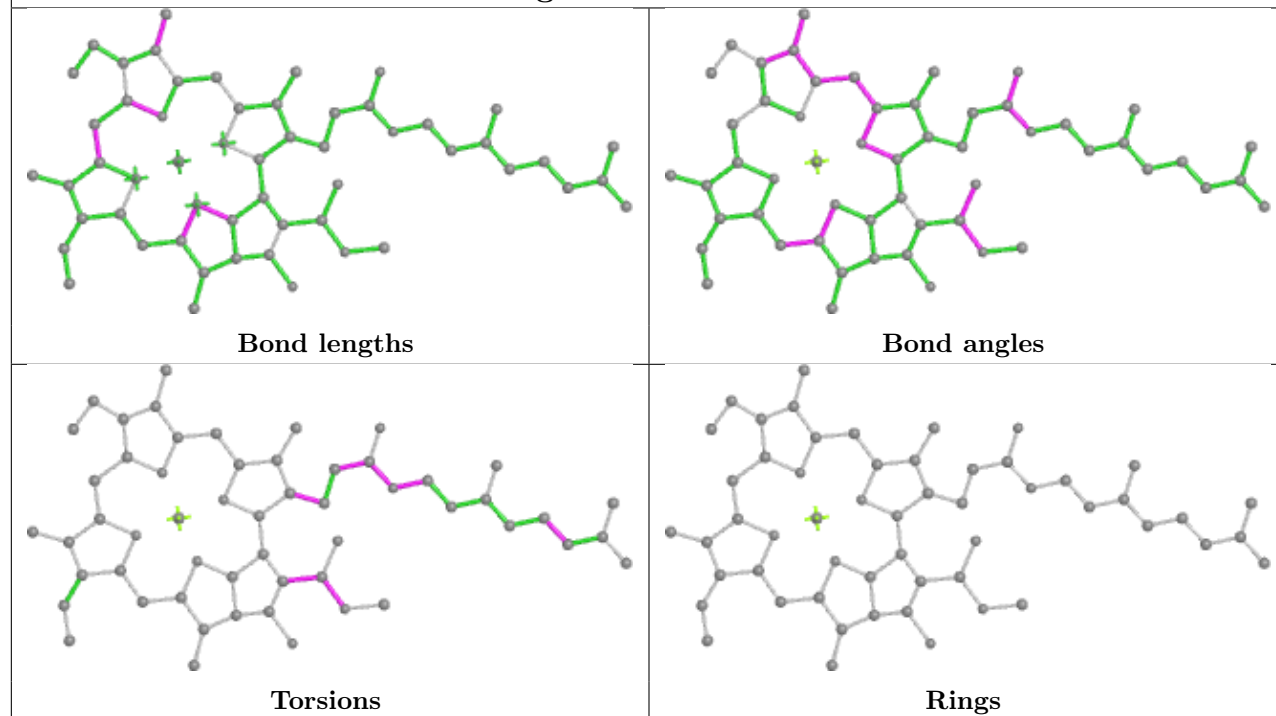
No monomer is involved in short contacts.

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.

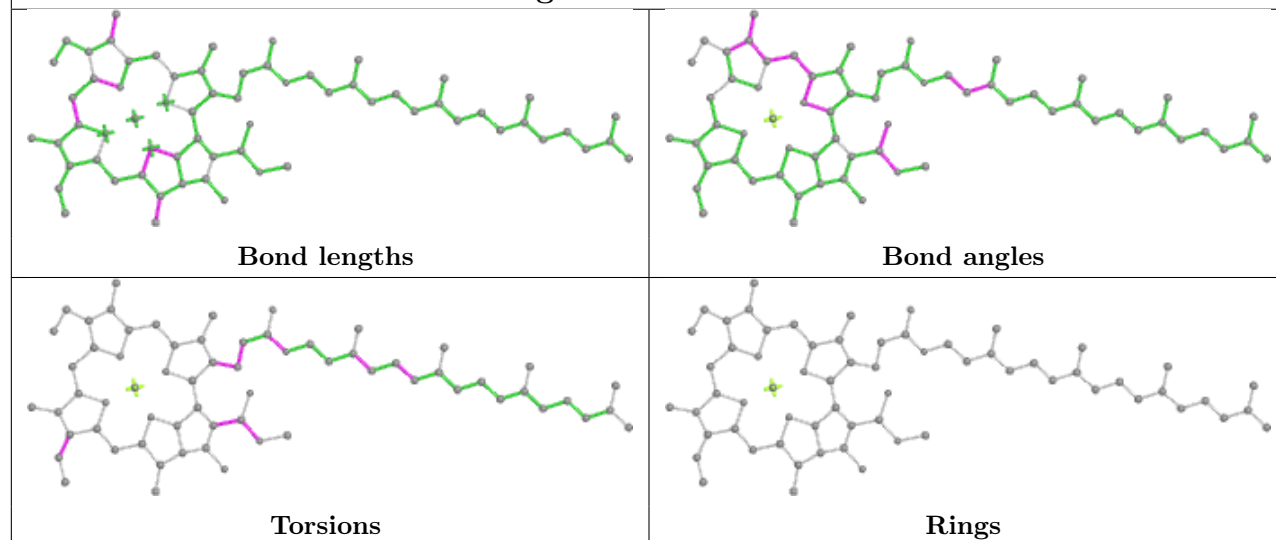




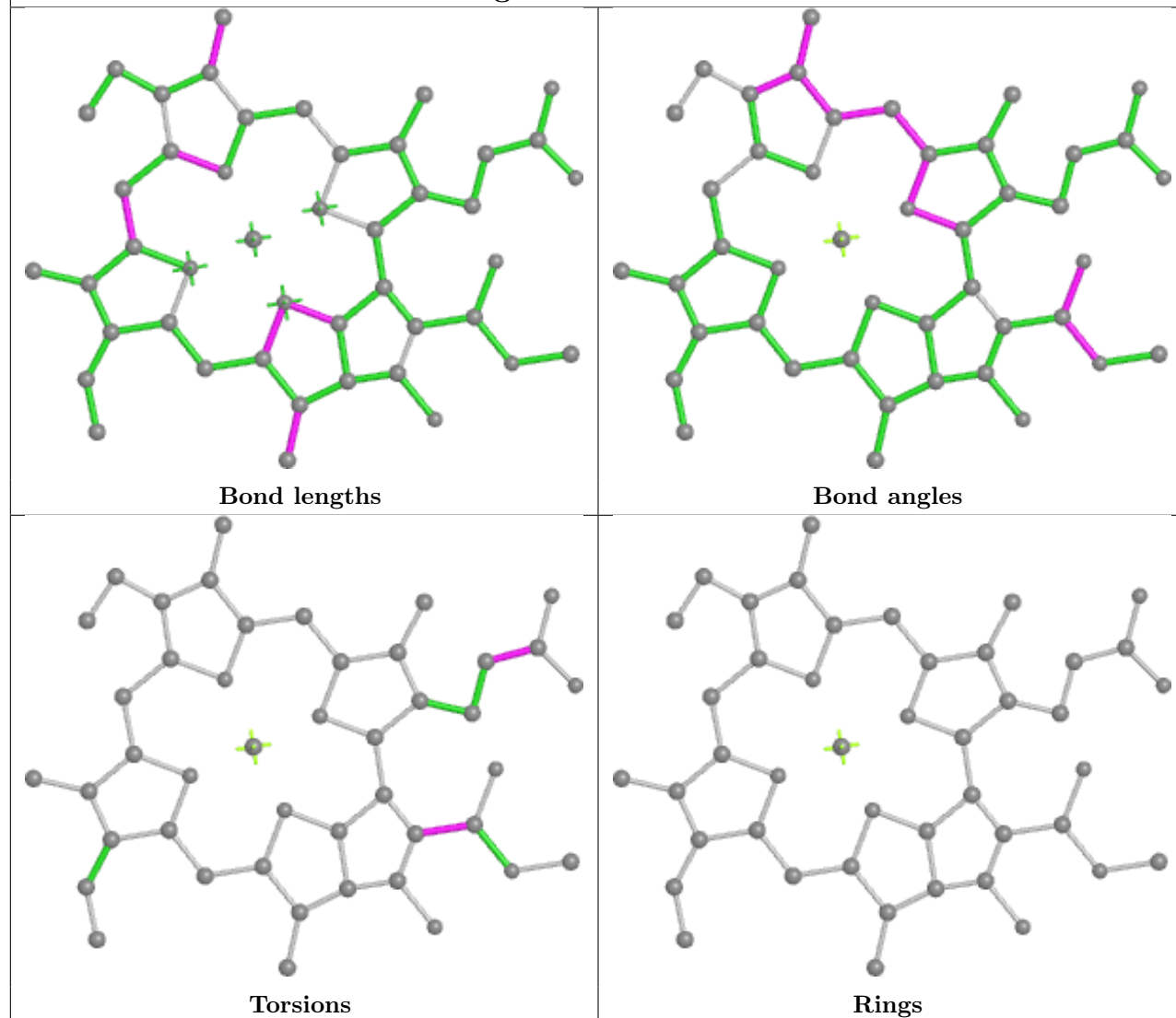
## Ligand CLA 2 308



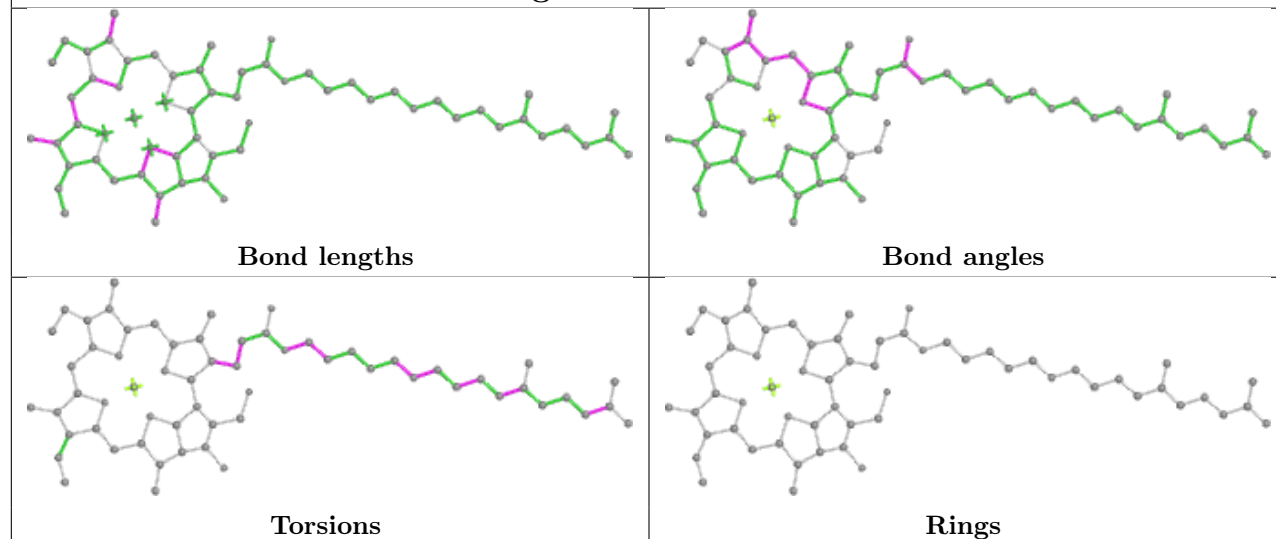
## Ligand CLA 2 310

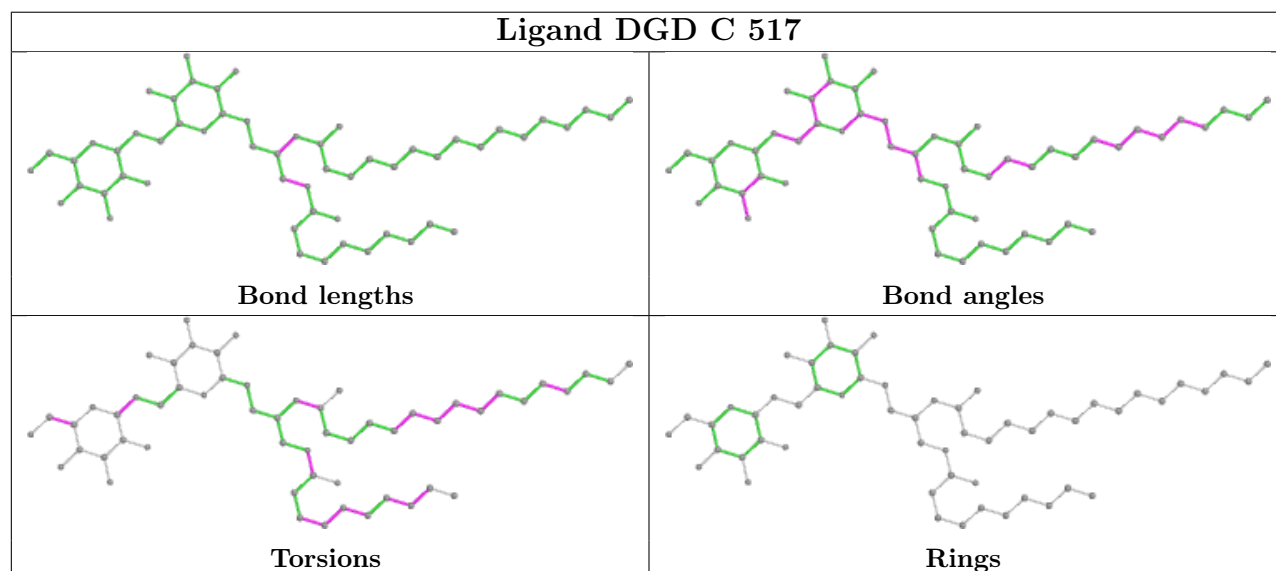
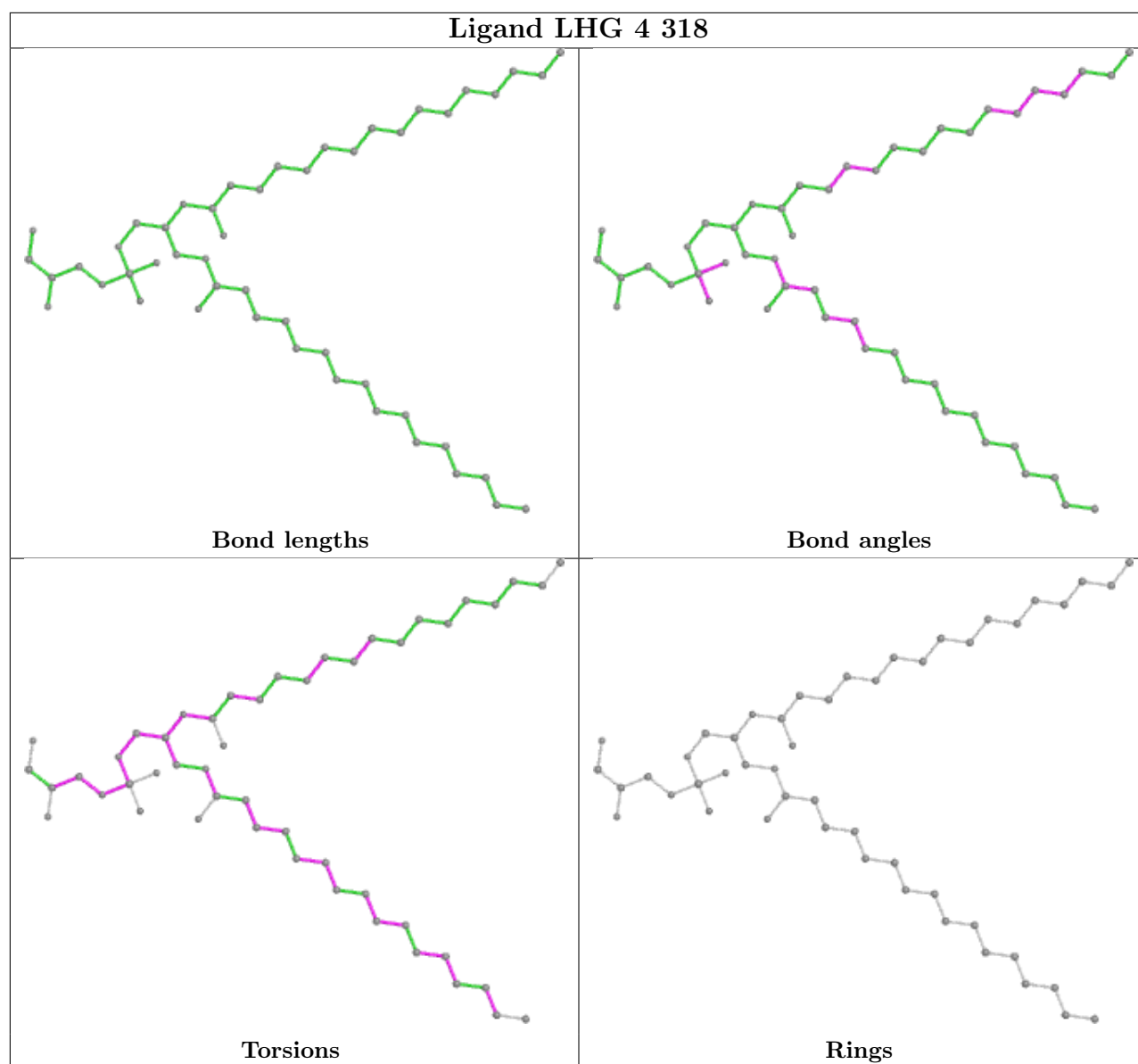


## Ligand CLA 8 312

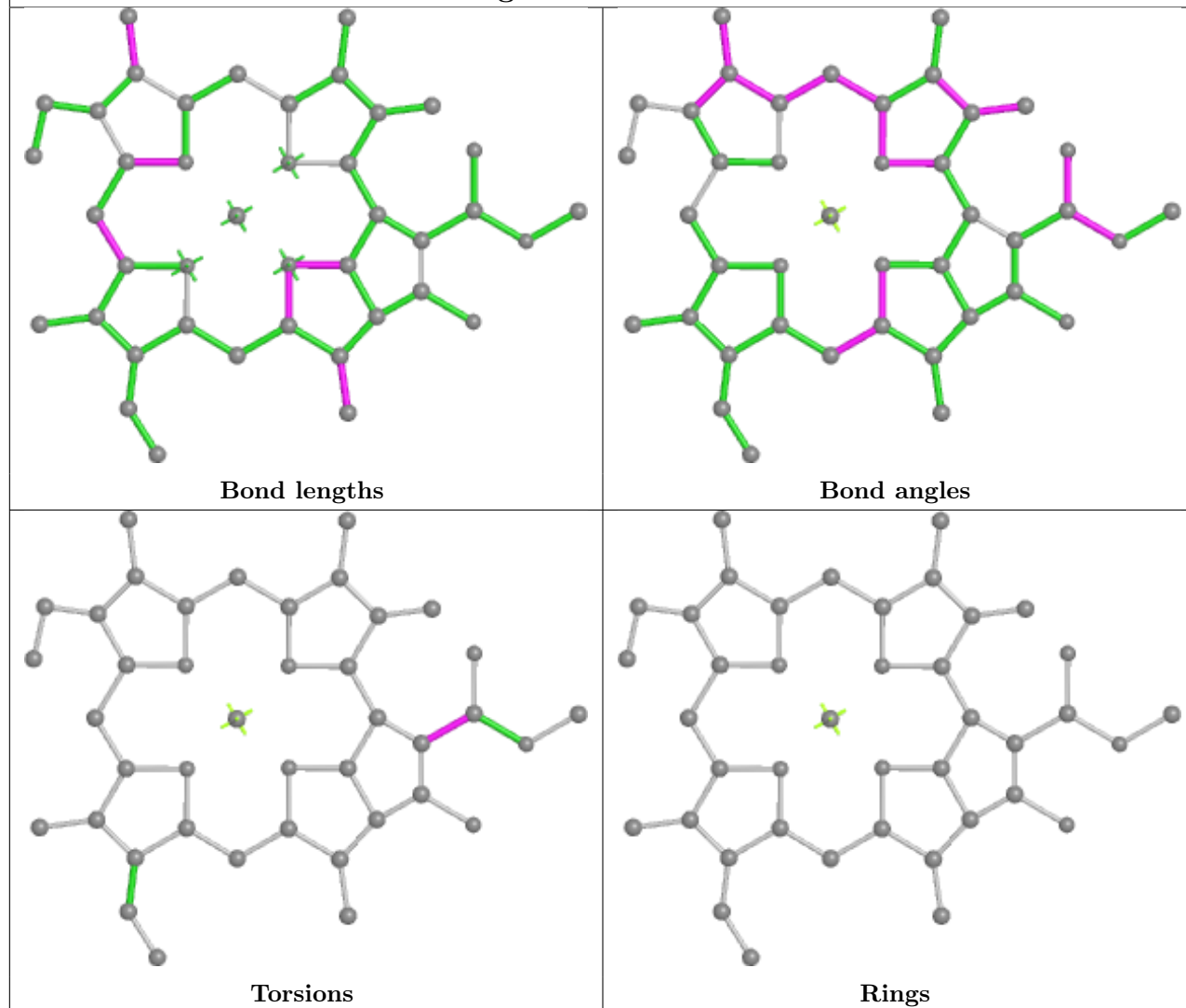


## Ligand CLA B 602

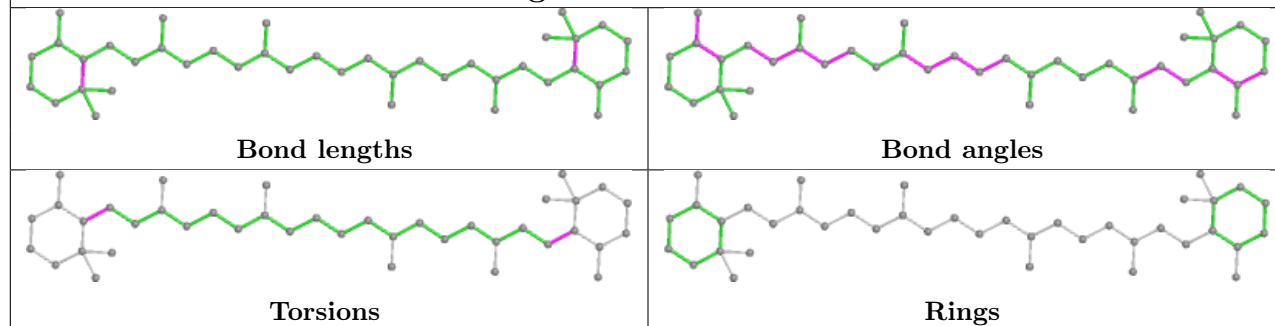


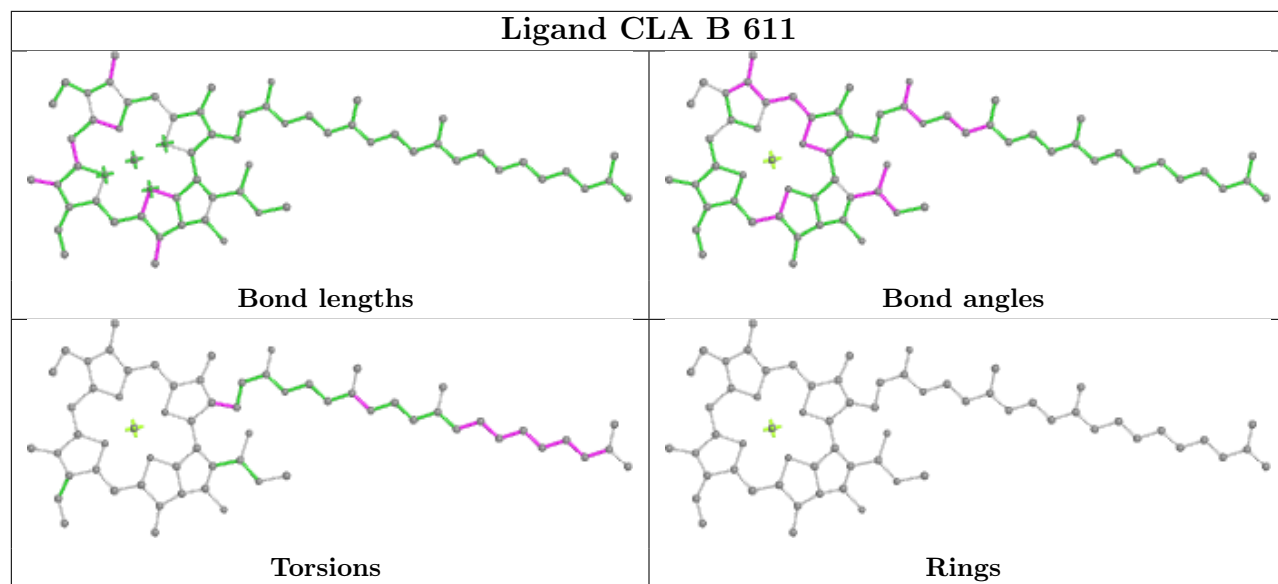


## Ligand CLA 2 305

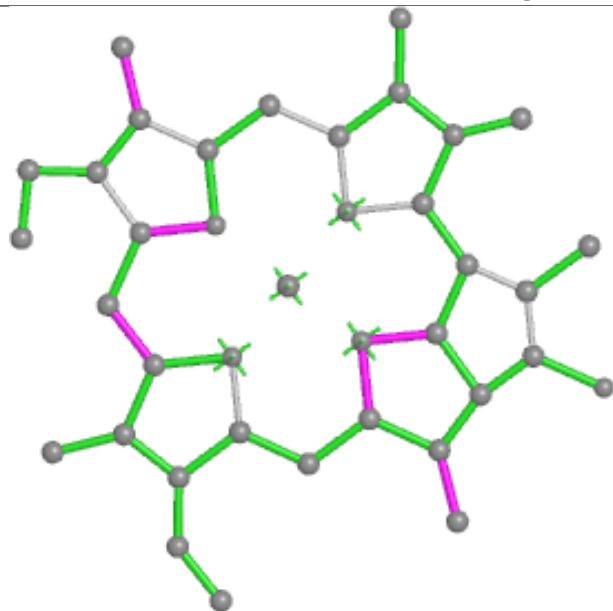


## Ligand BCR K 102

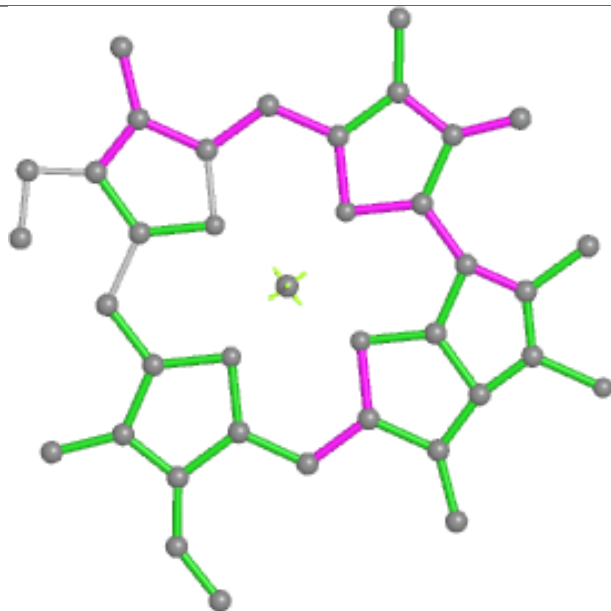




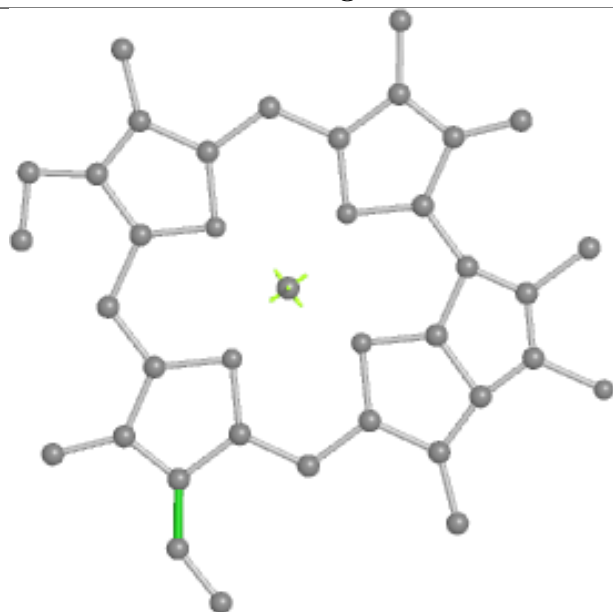
## Ligand CLA 2 315



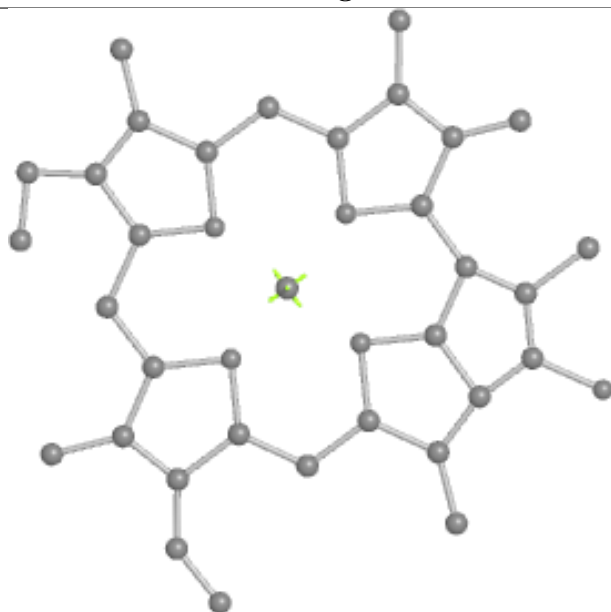
Bond lengths



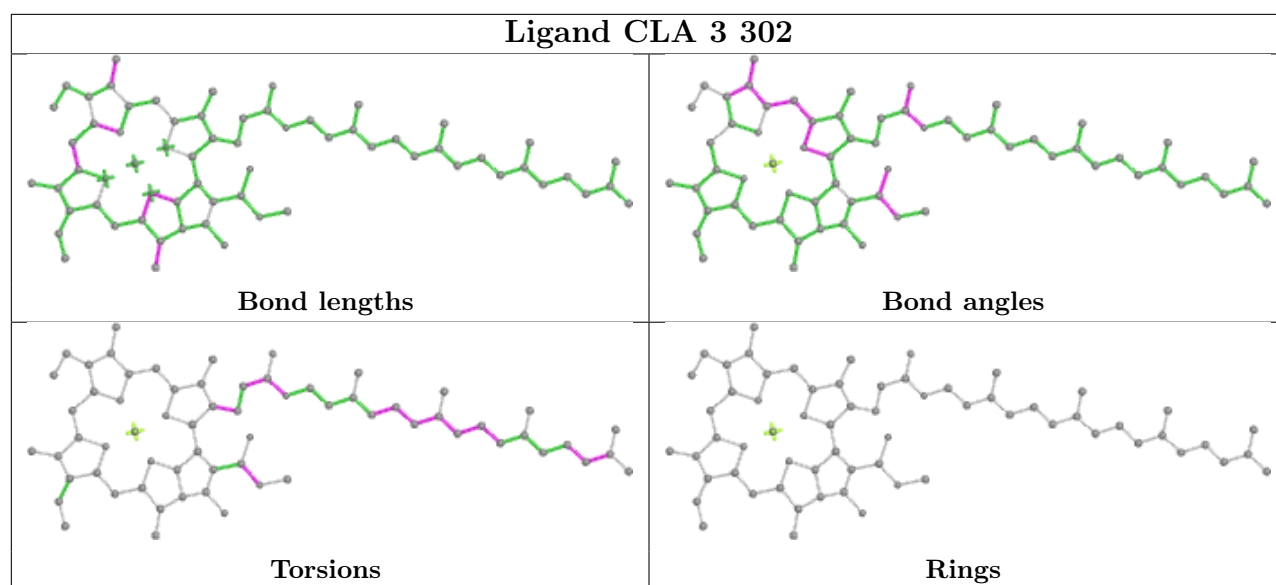
Bond angles



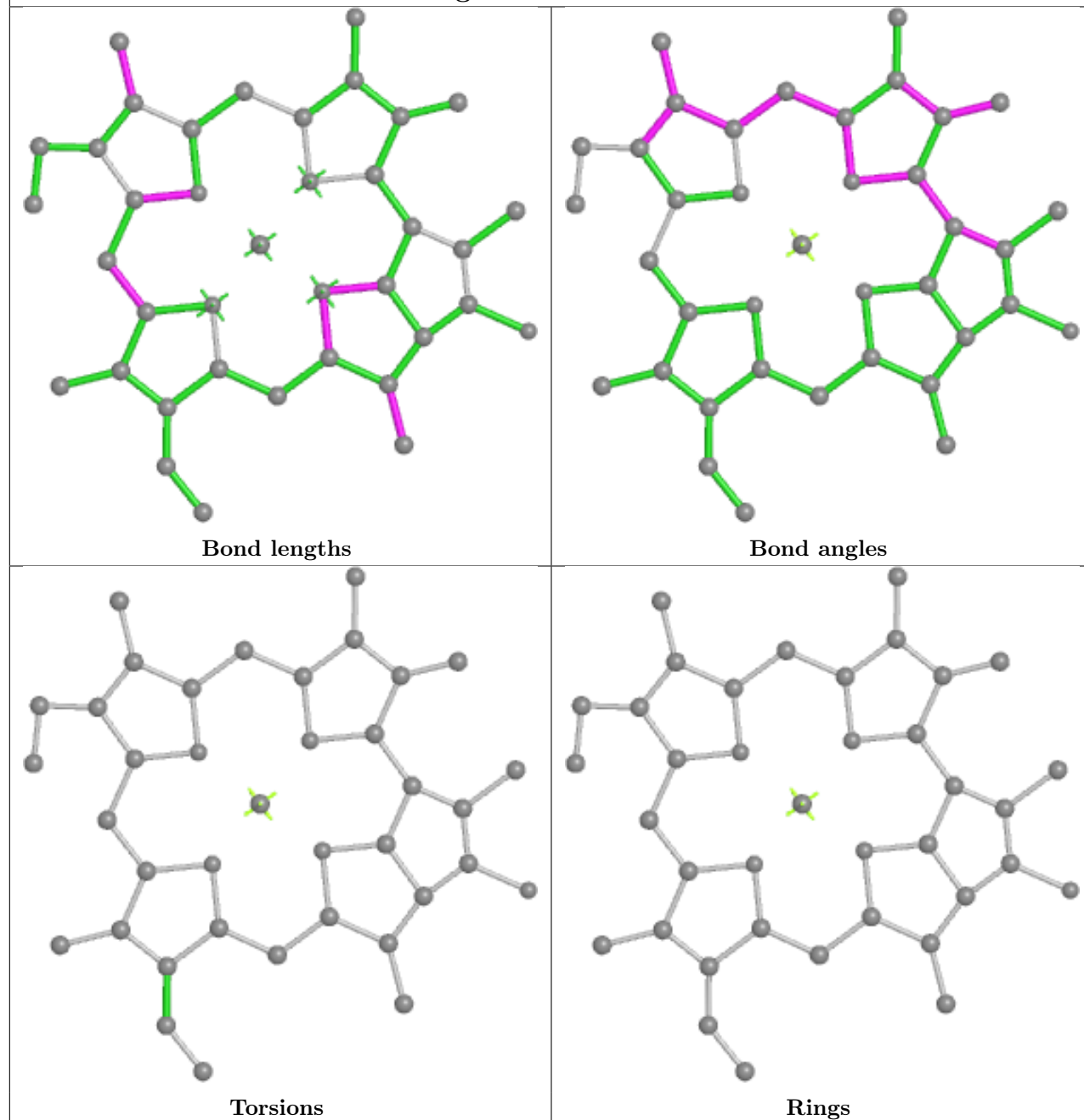
Torsions



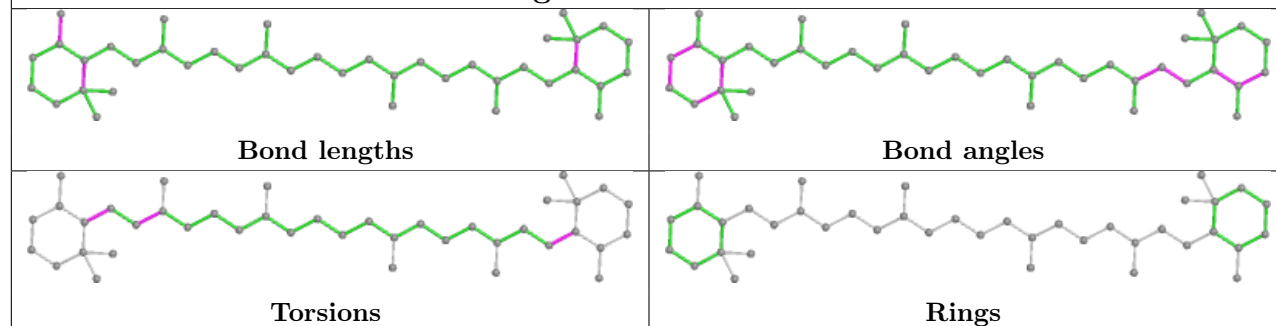
Rings

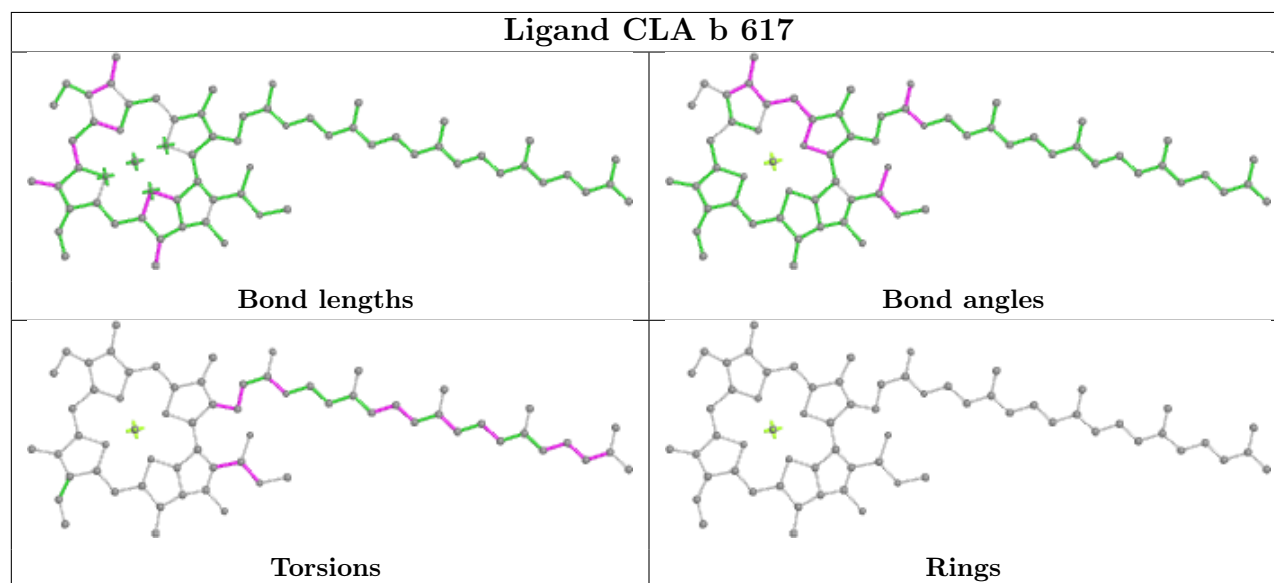
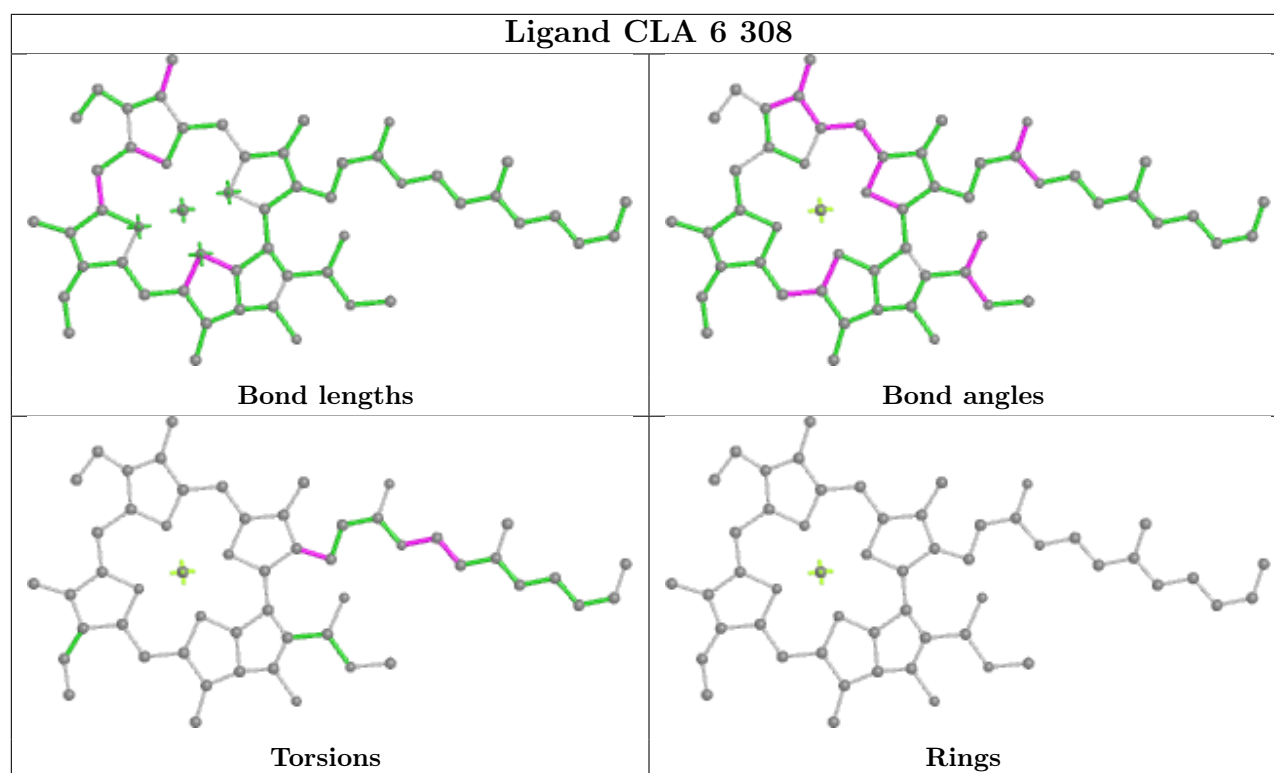


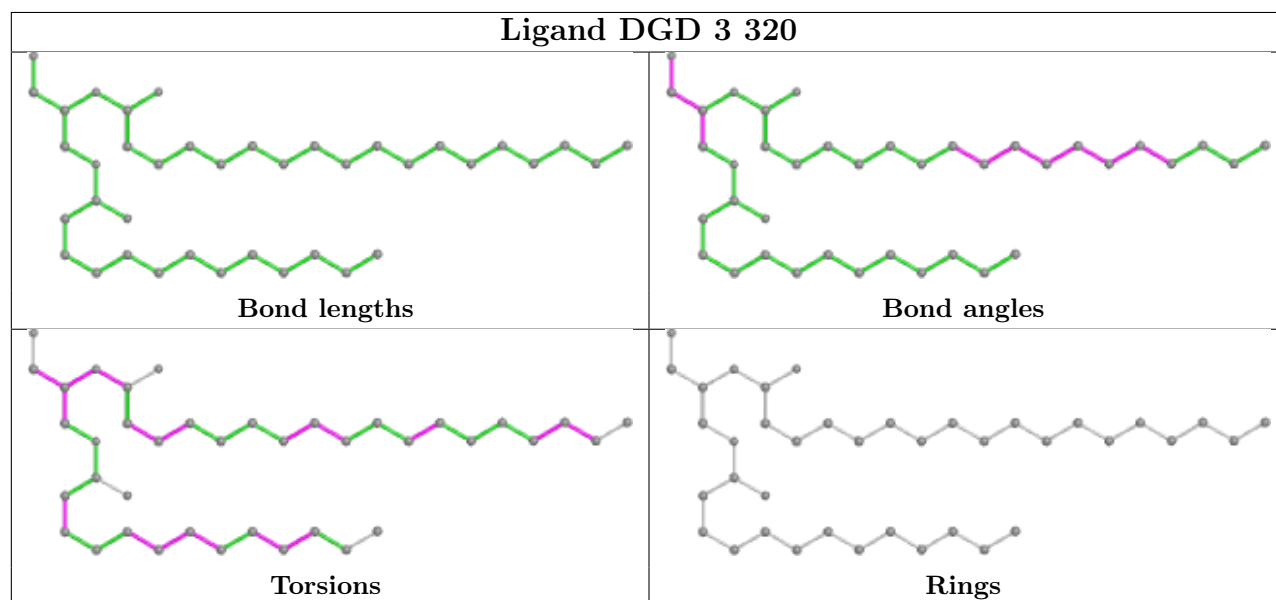
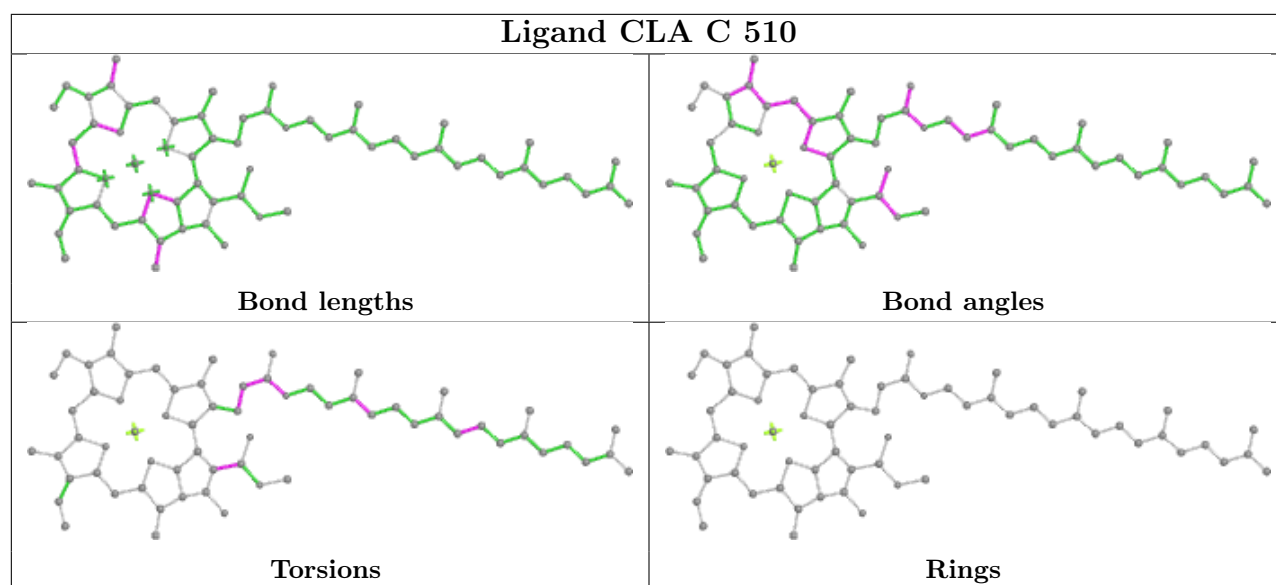
## Ligand CLA 9 315



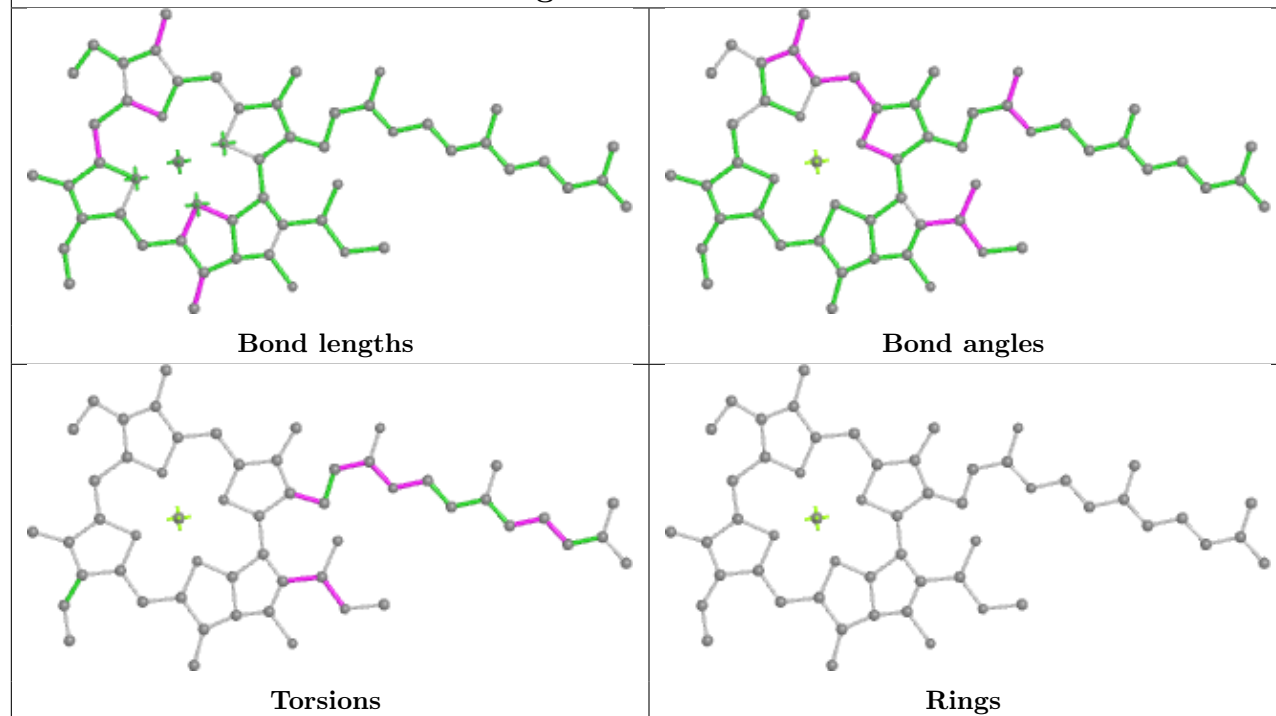
## Ligand BCR h 101



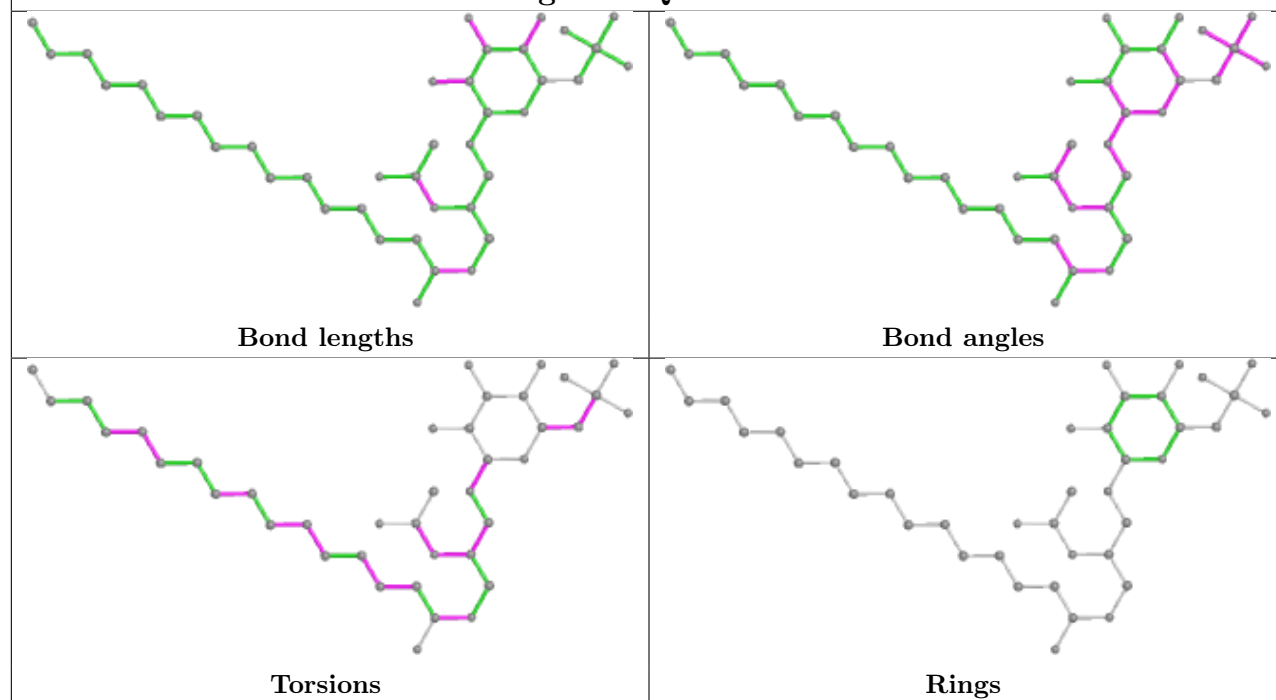


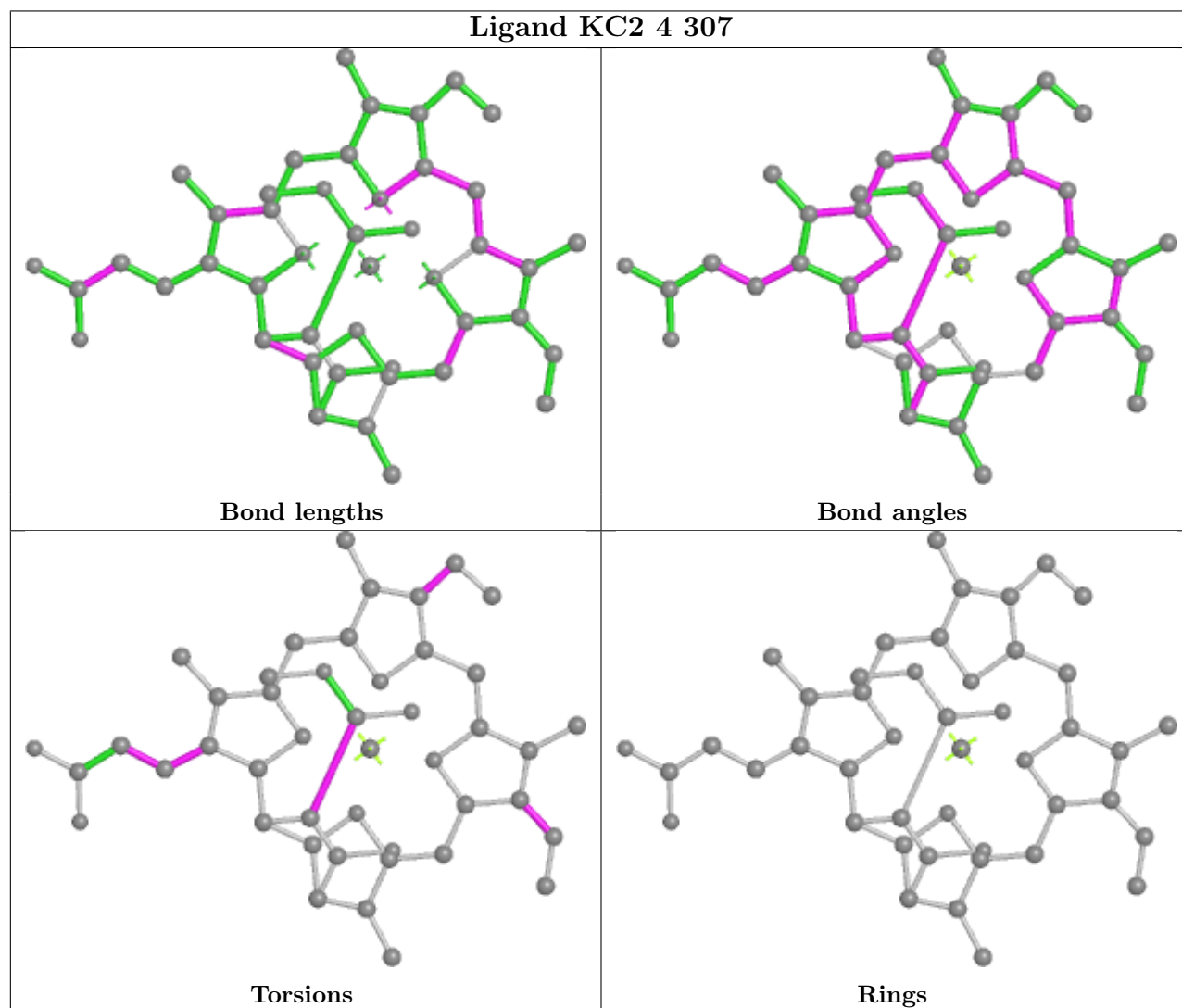
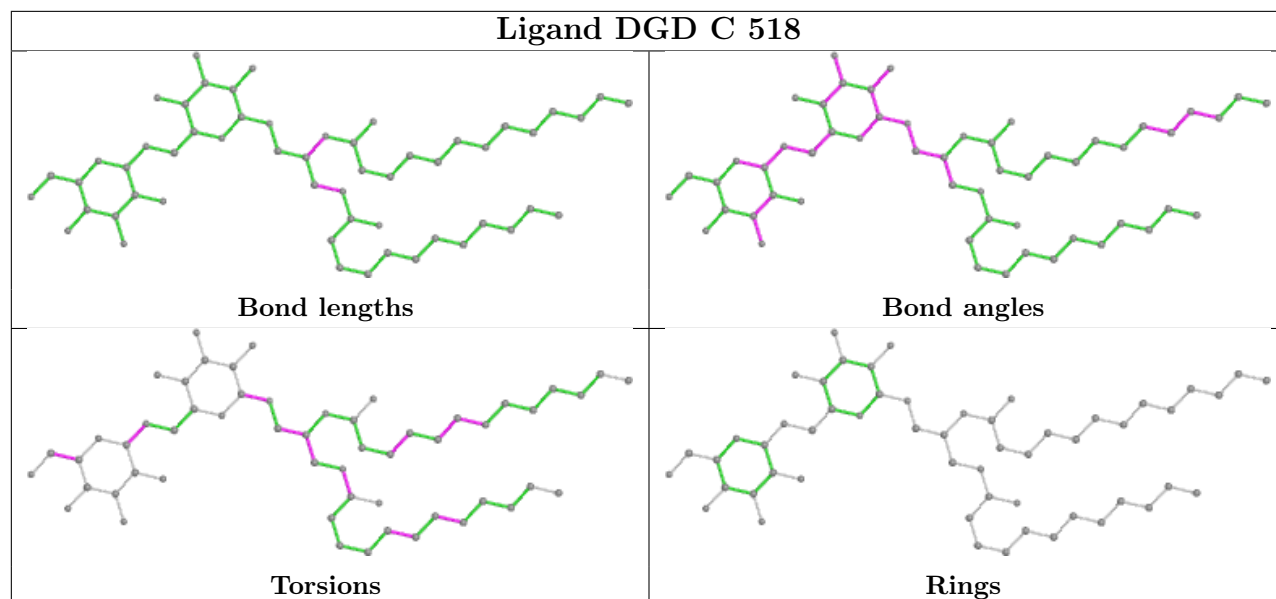


## Ligand CLA 8 308

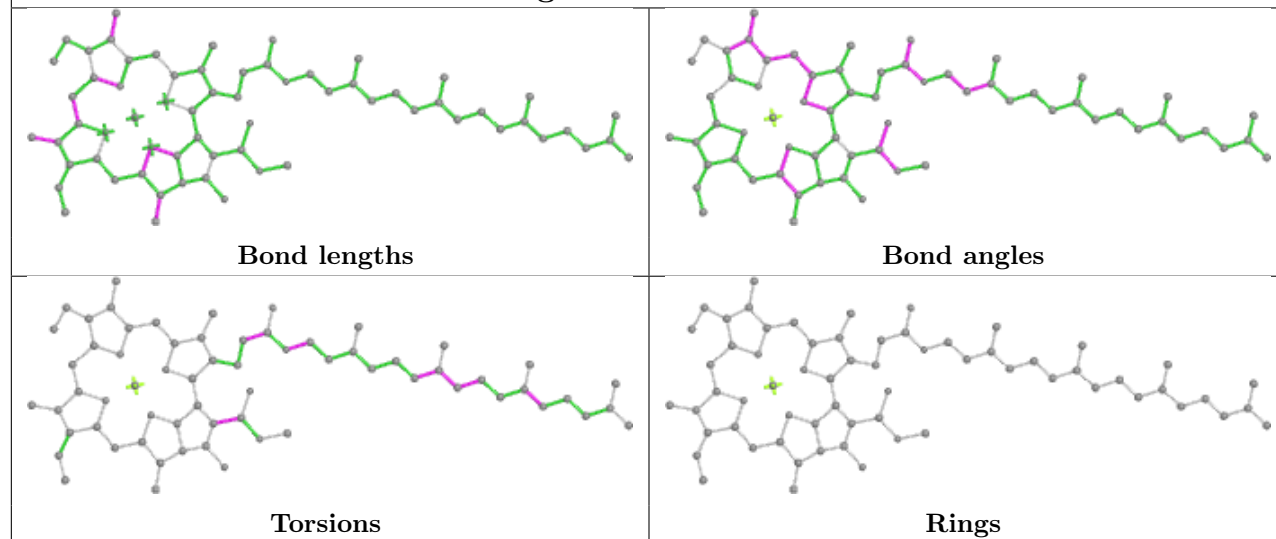


## Ligand SQD t 102

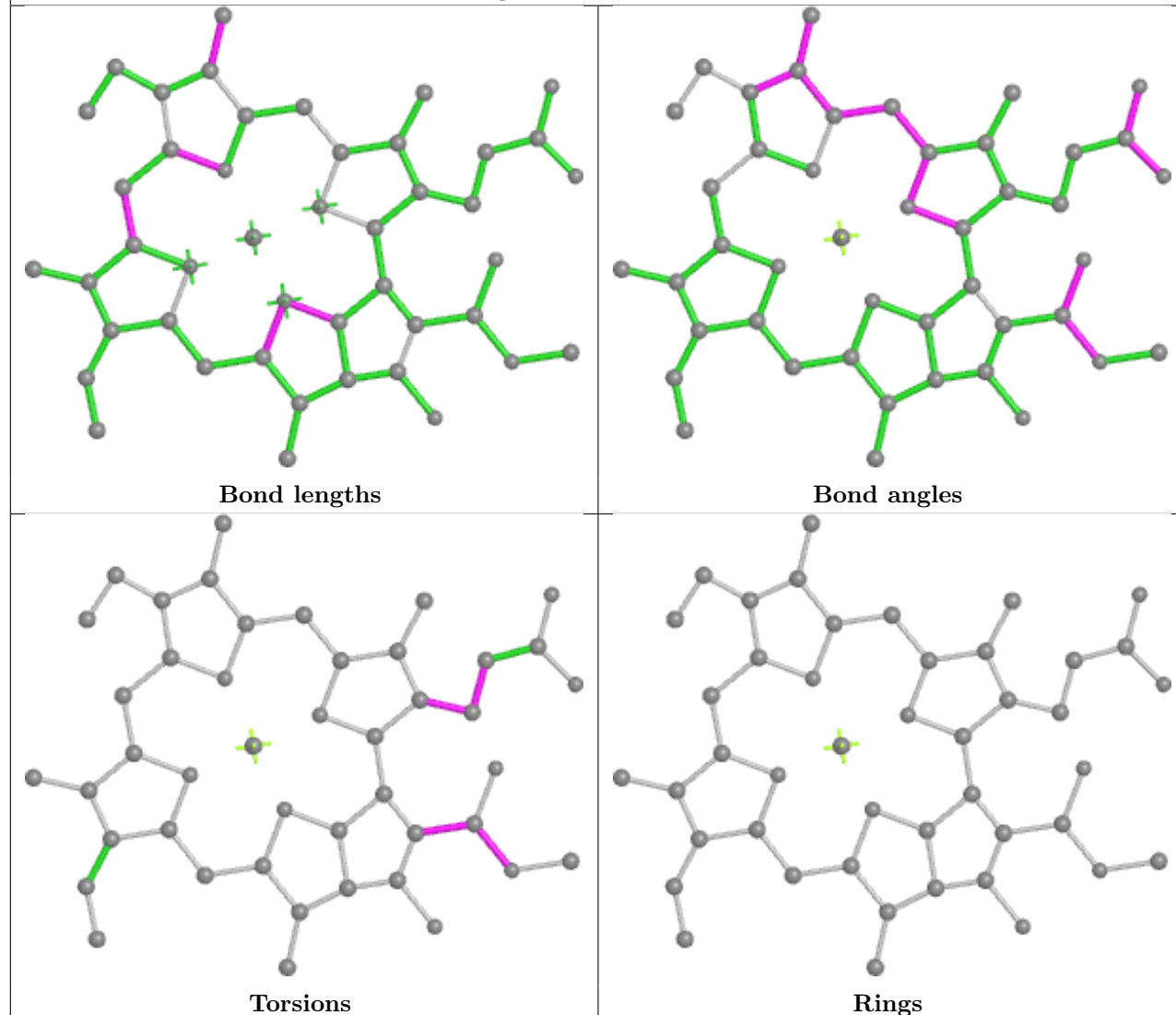


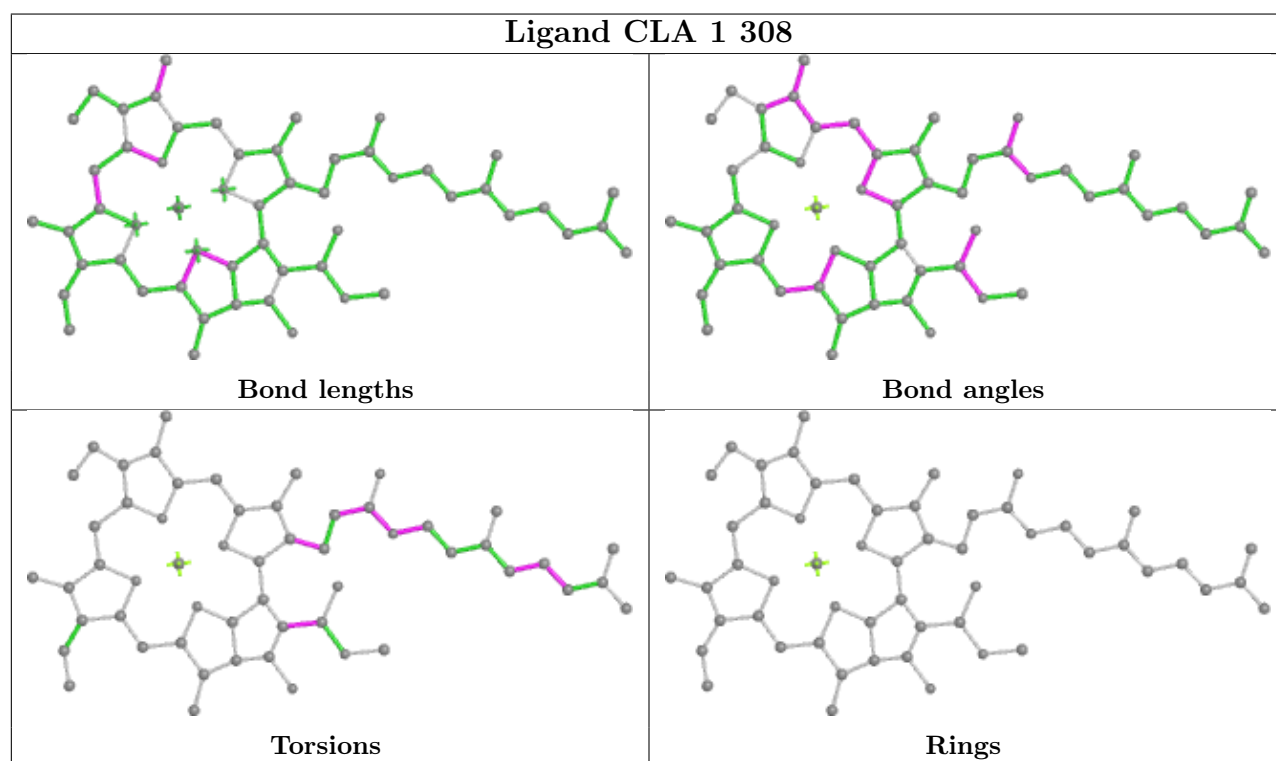
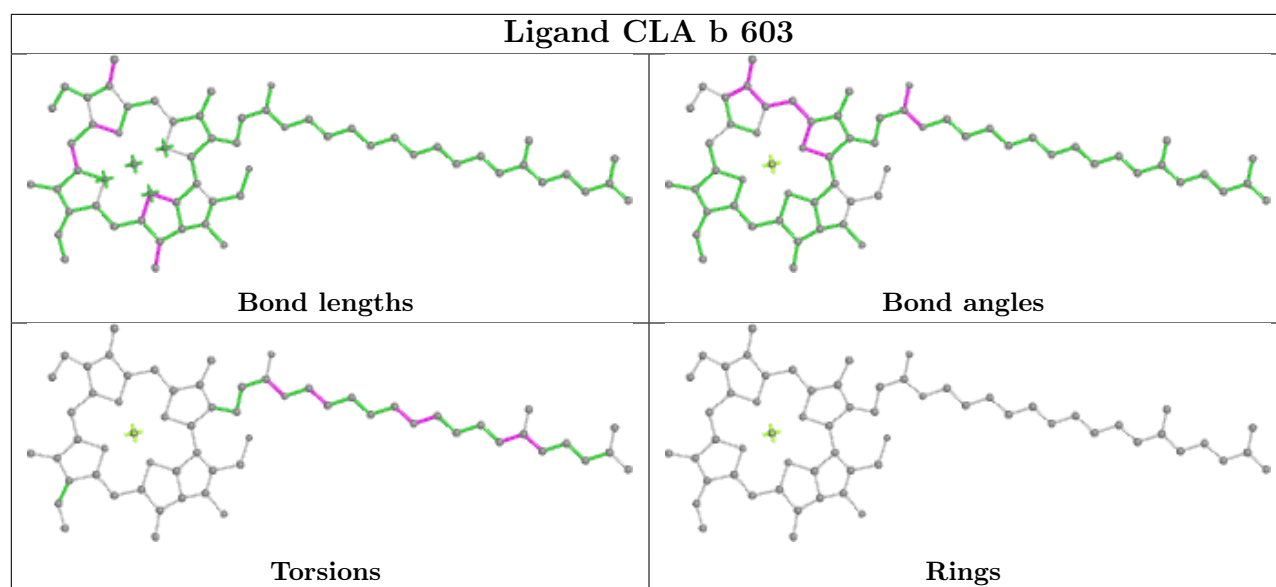


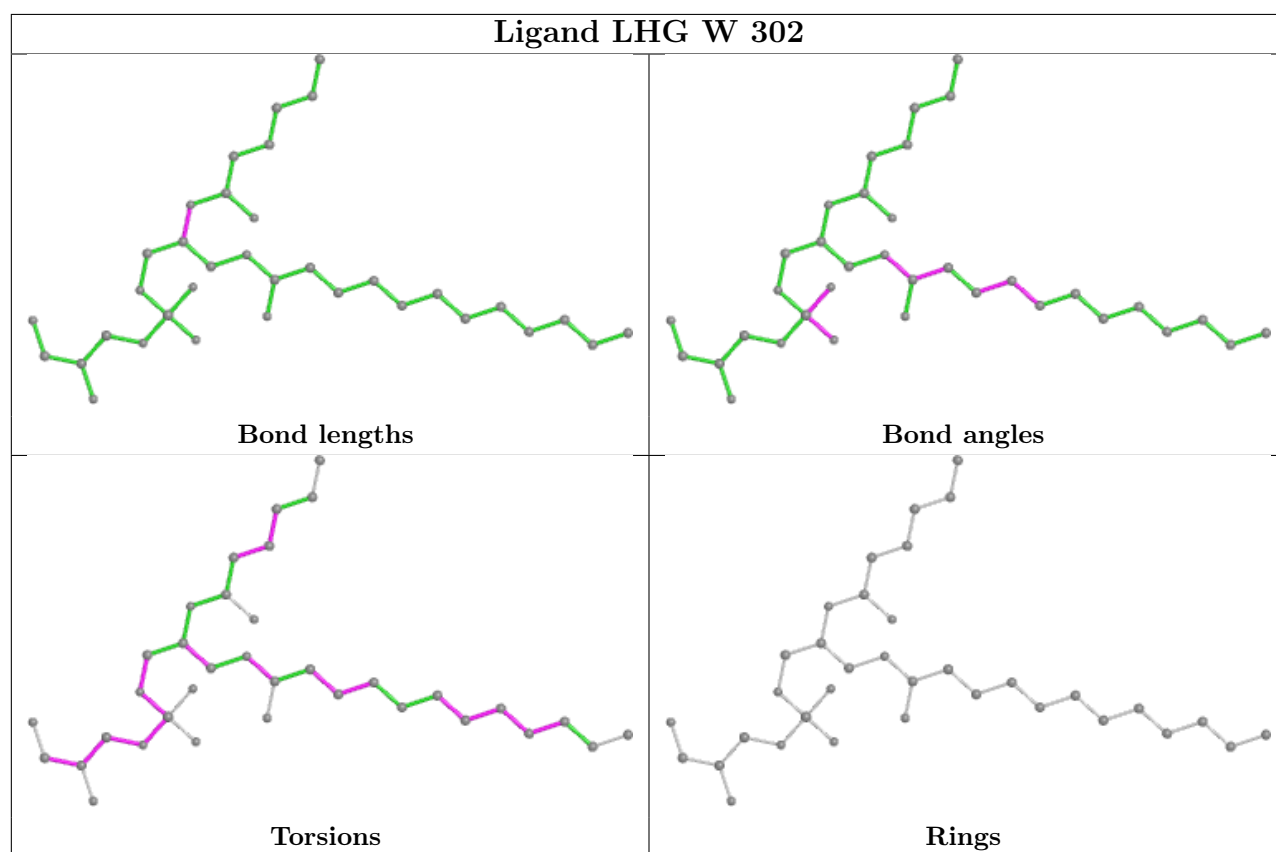
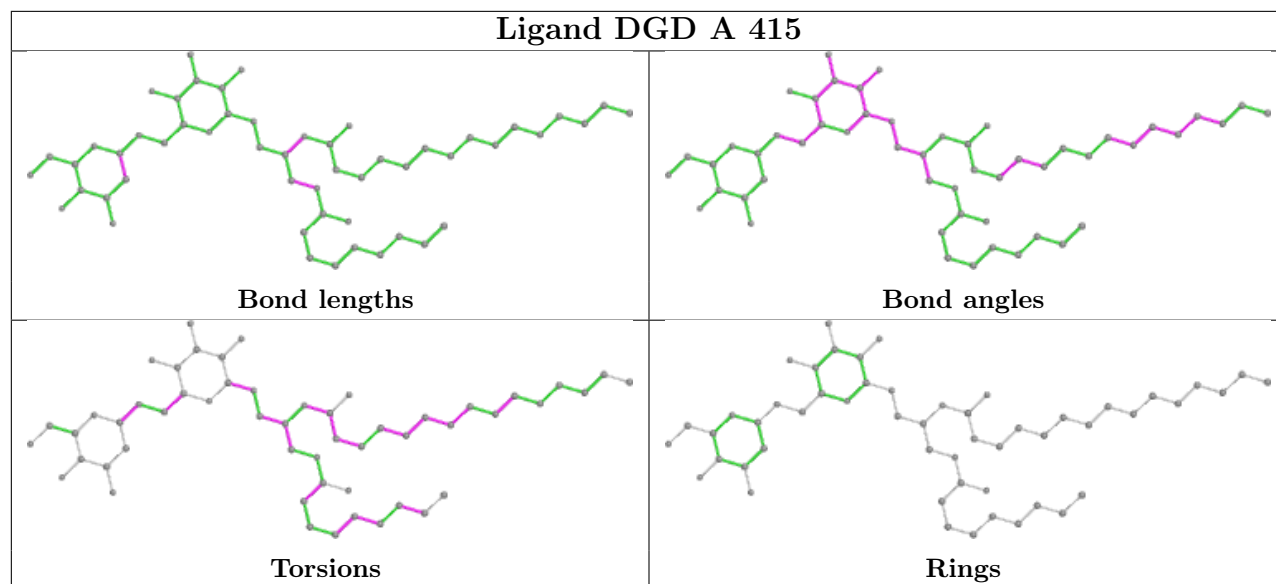
## Ligand CLA c 510



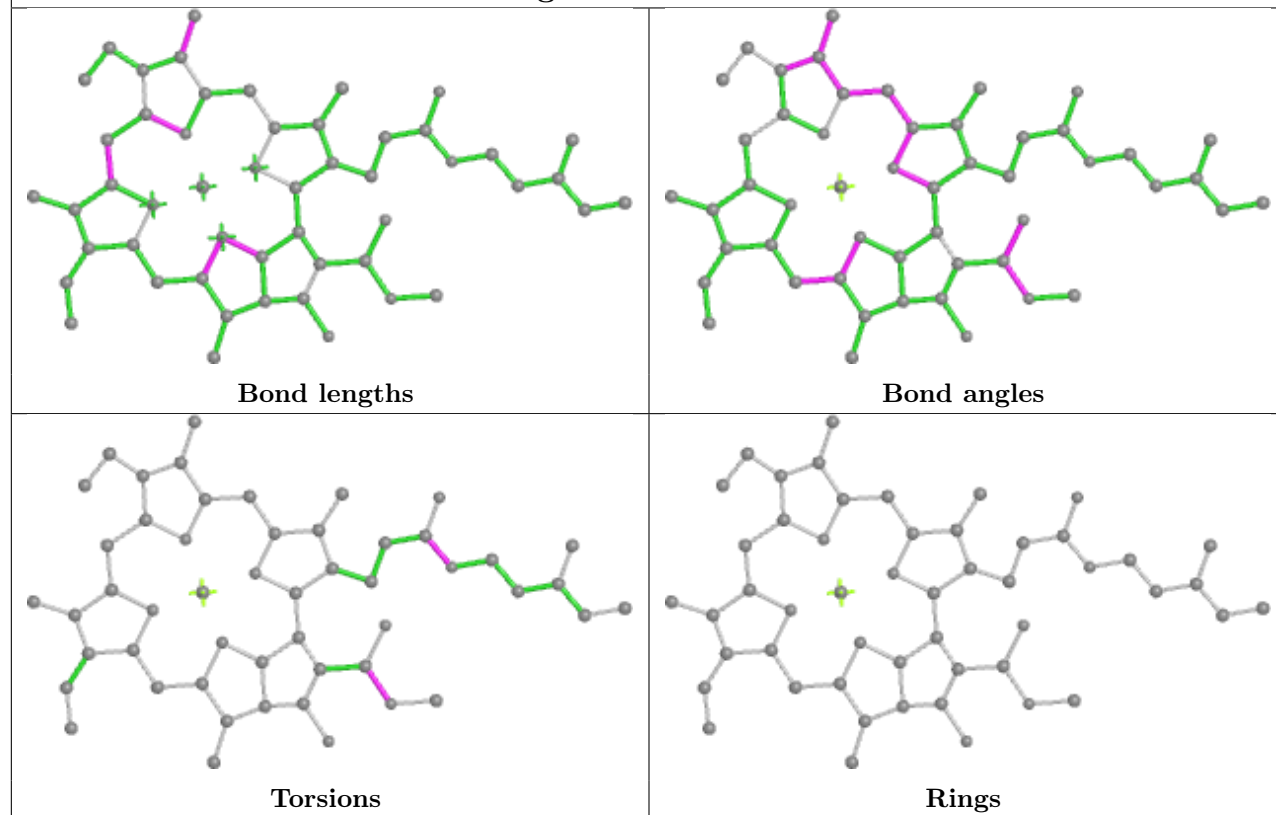
## Ligand CLA 1 306



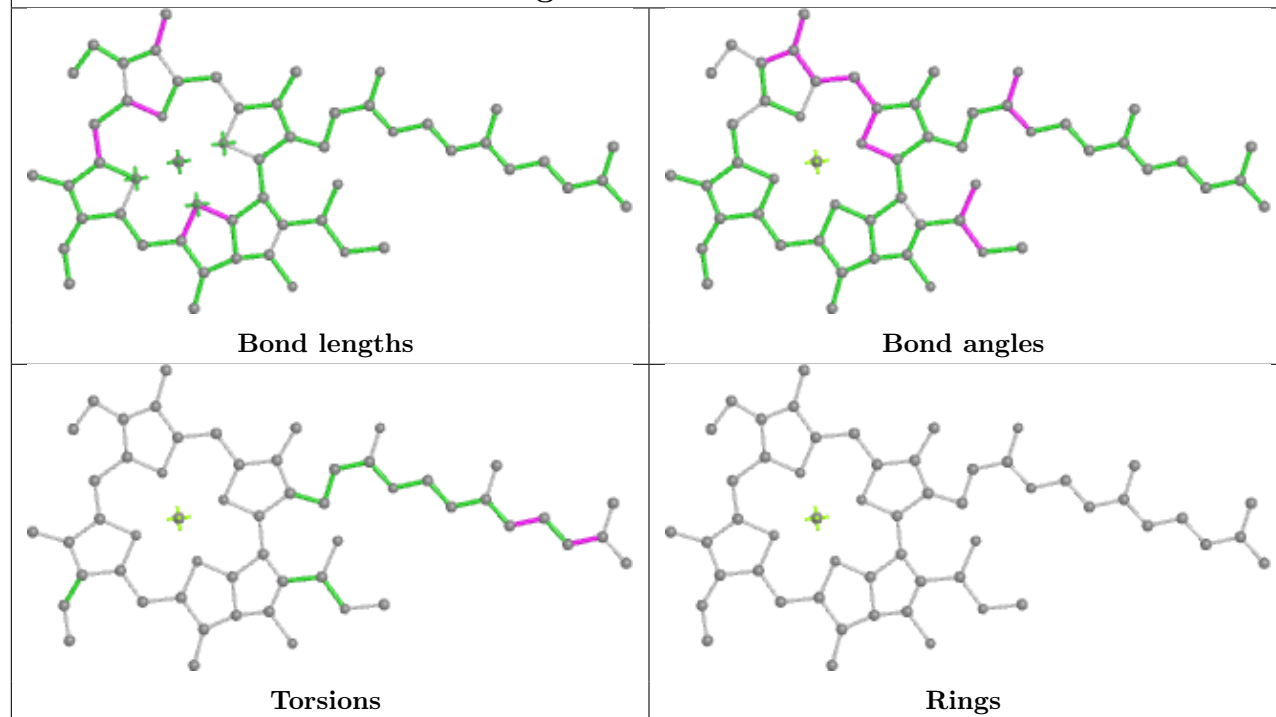


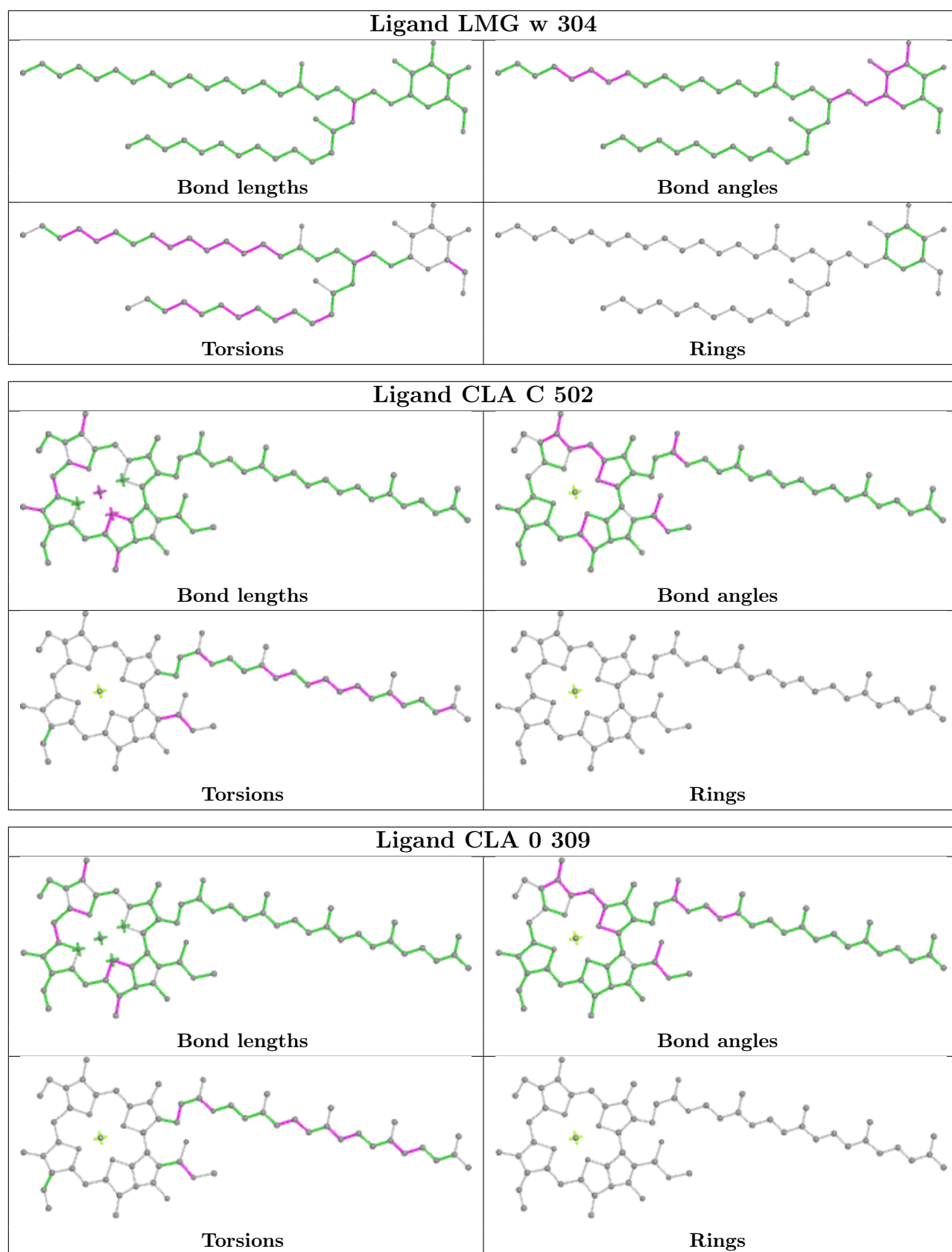


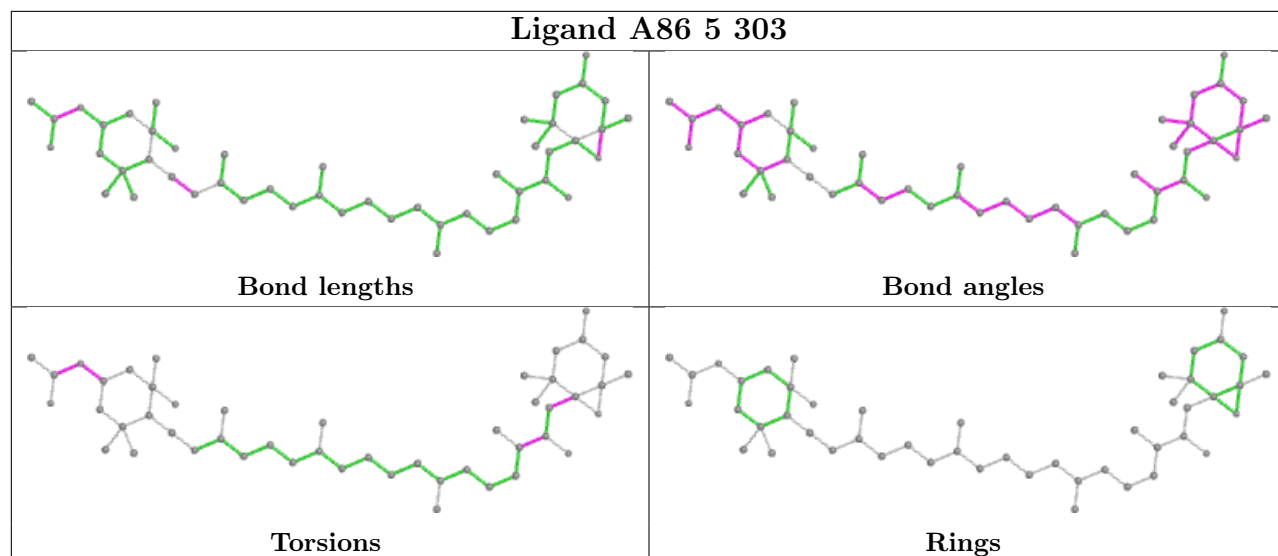
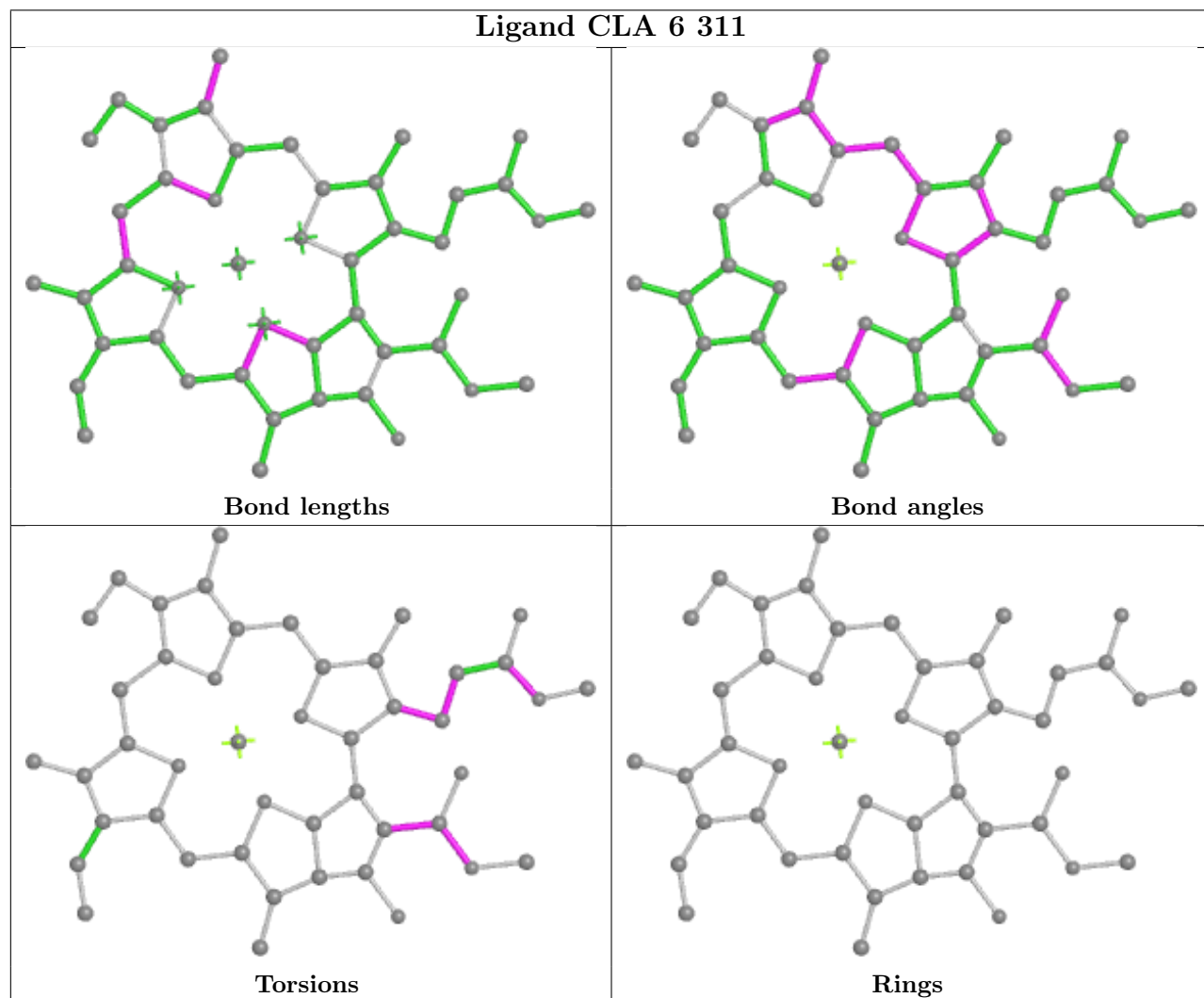
## Ligand CLA z 101

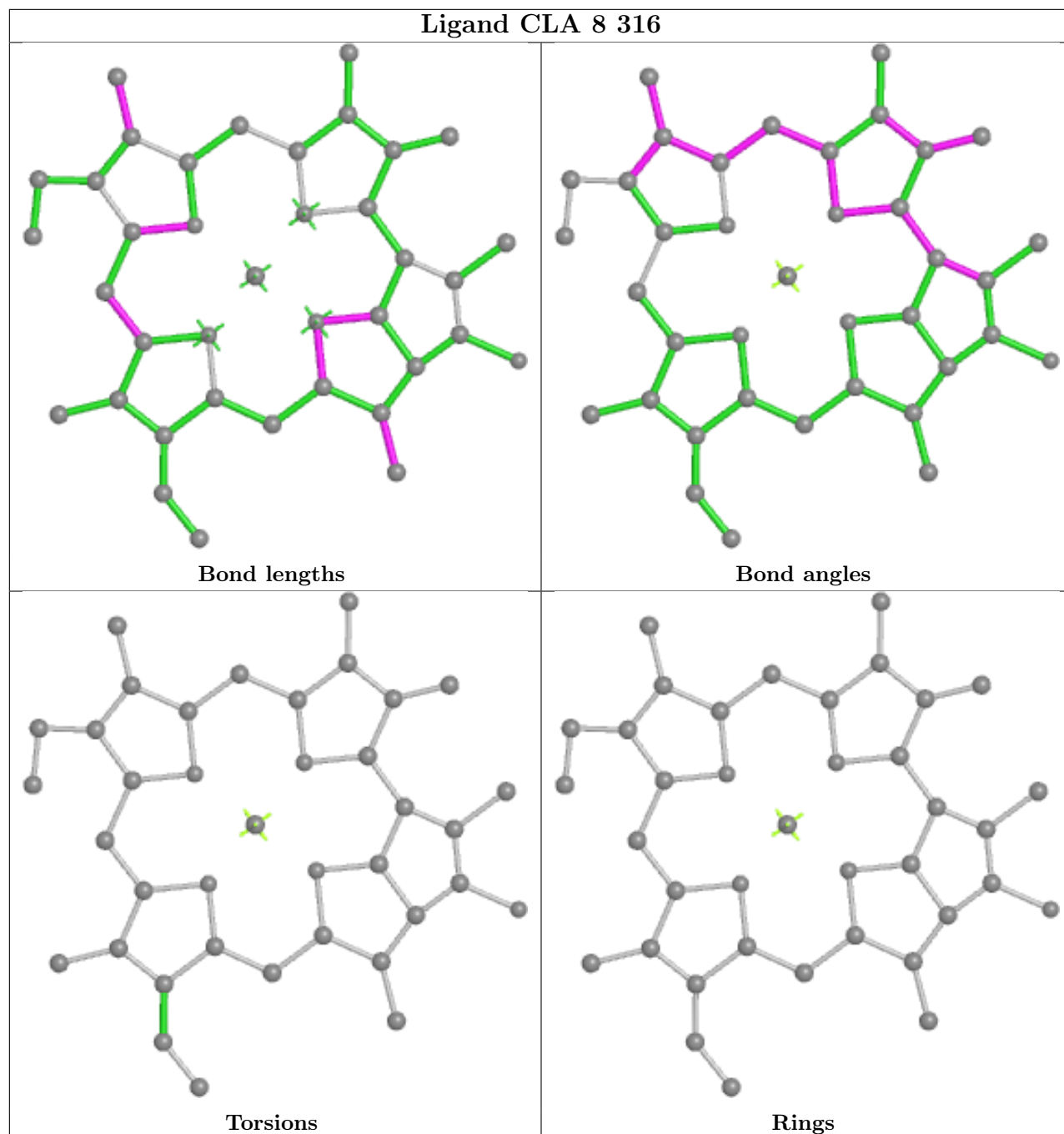
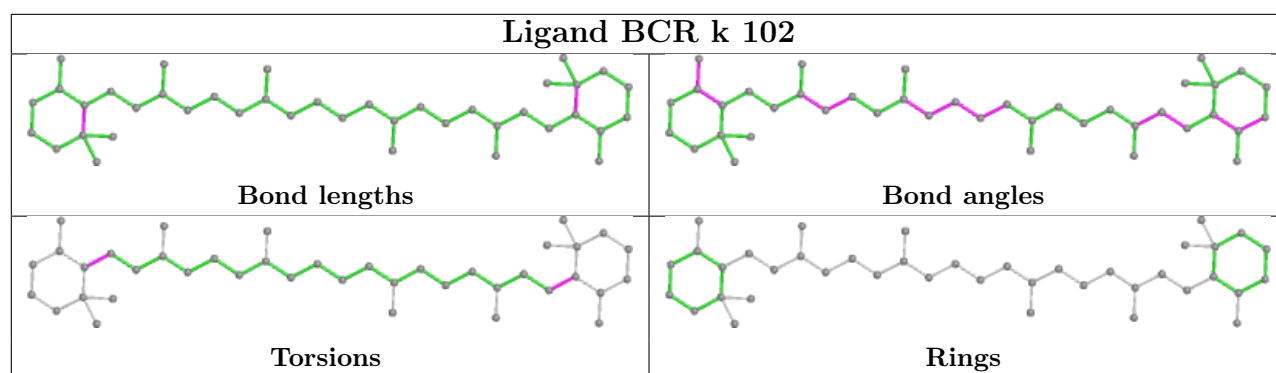


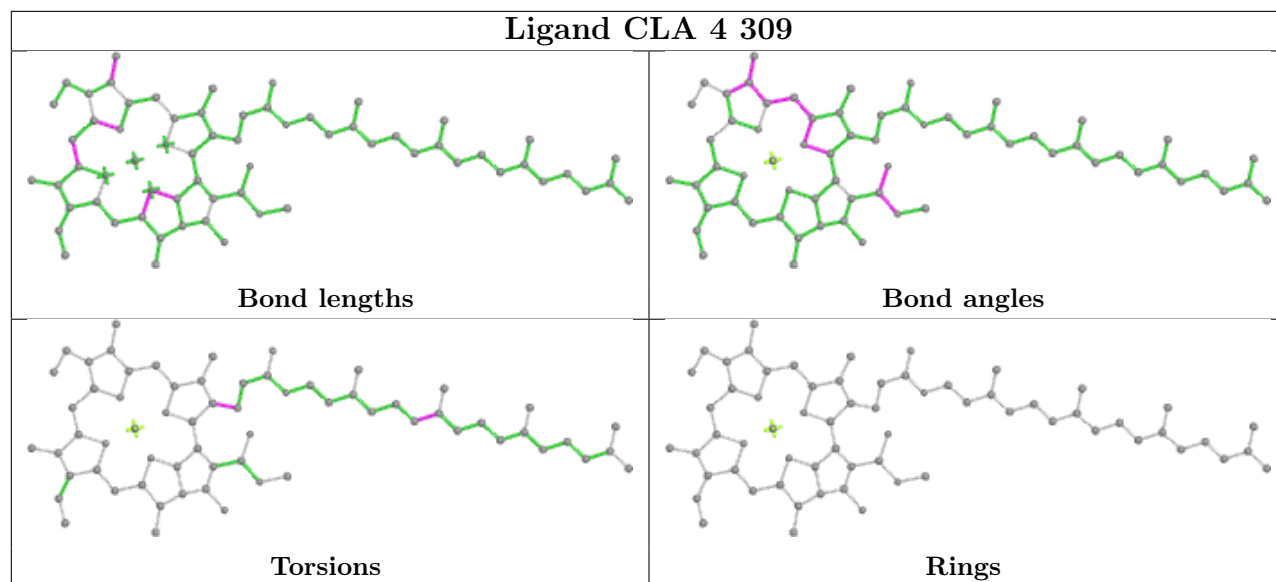
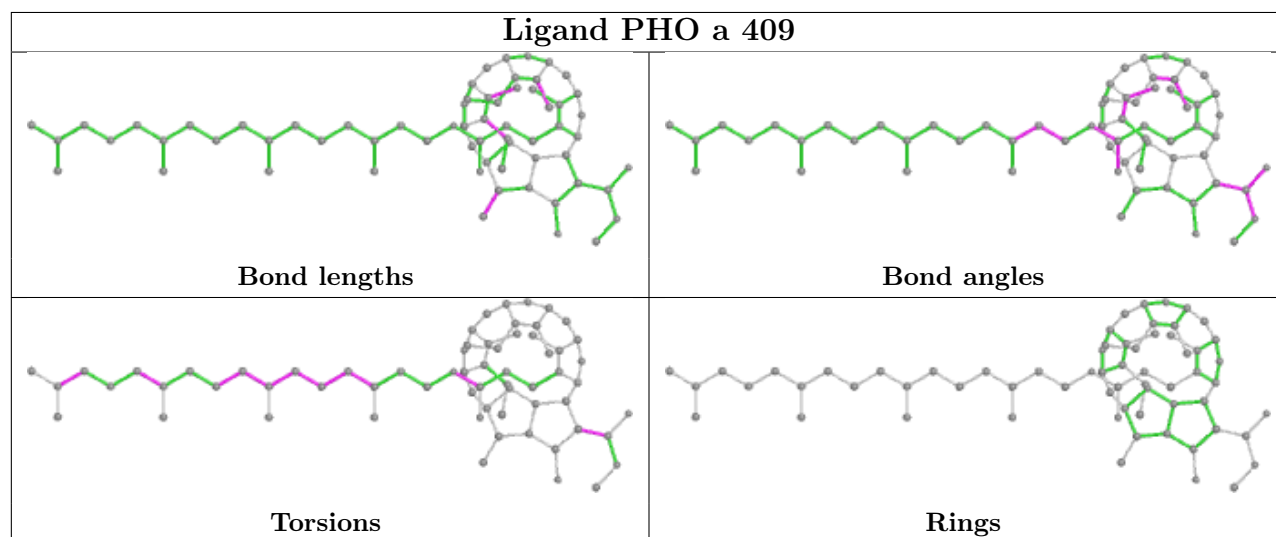
## Ligand CLA 5 309



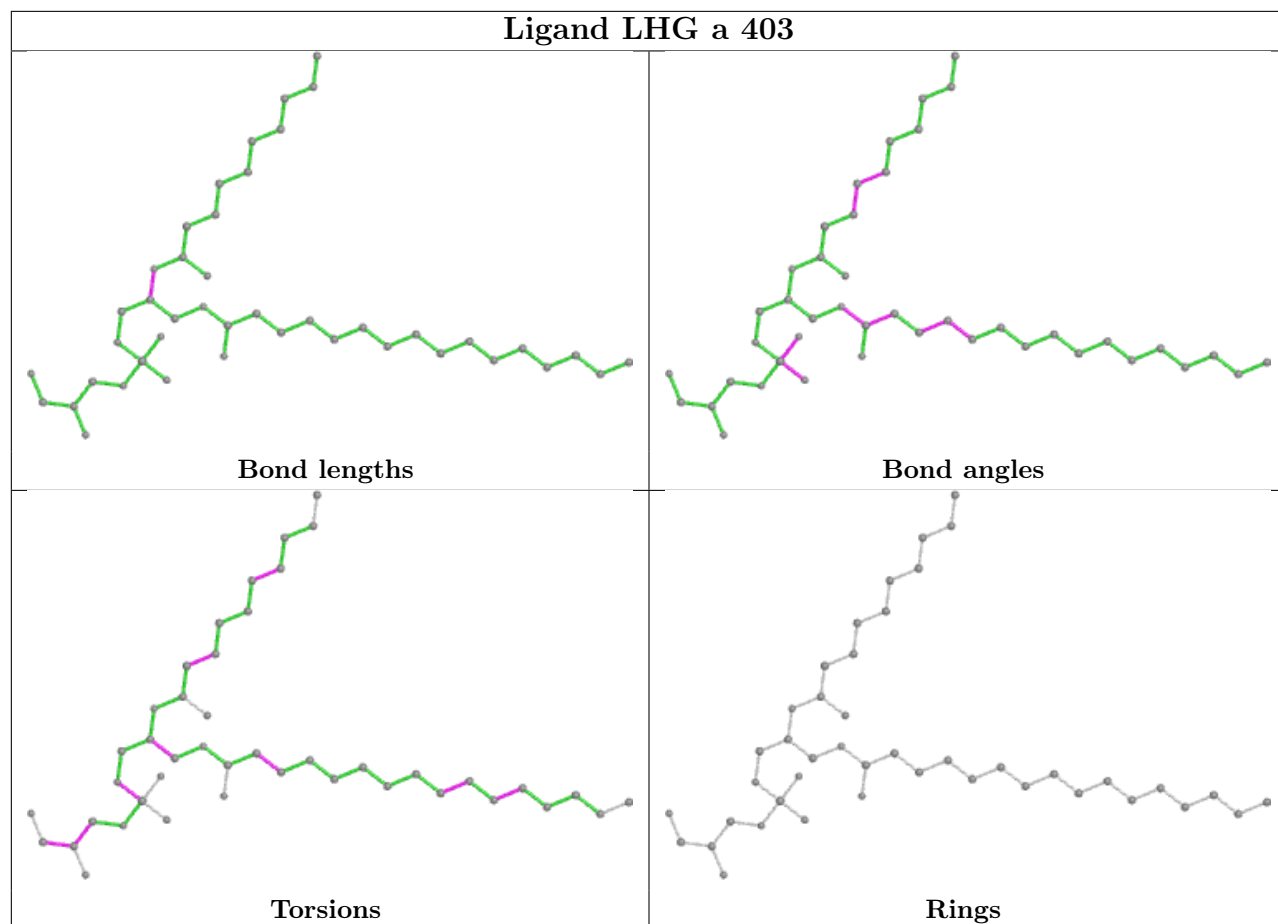


**Ligand A86 5 303****Ligand CLA 6 311**

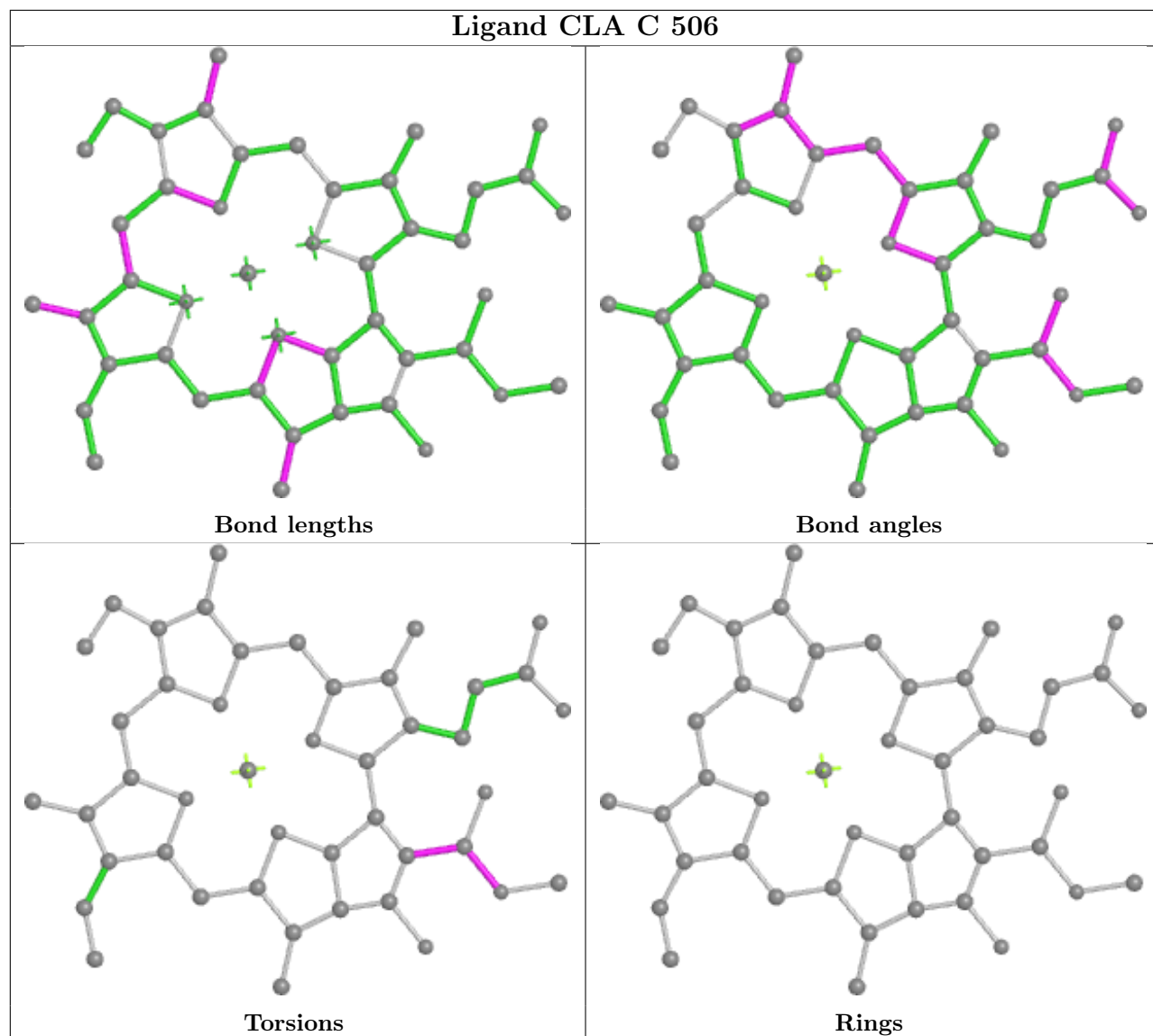


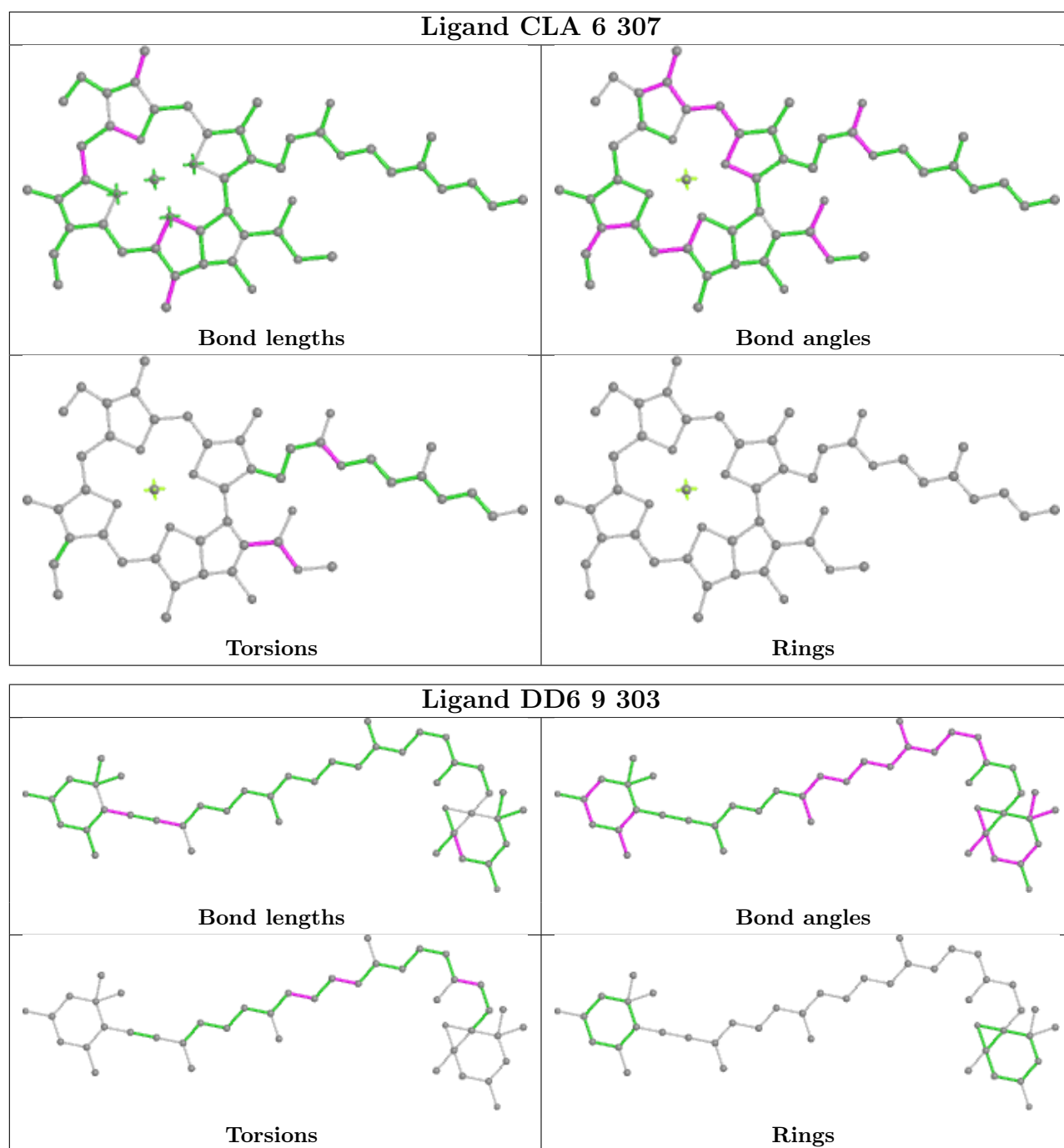
**Ligand CLA 4 309****Ligand PHO a 409**

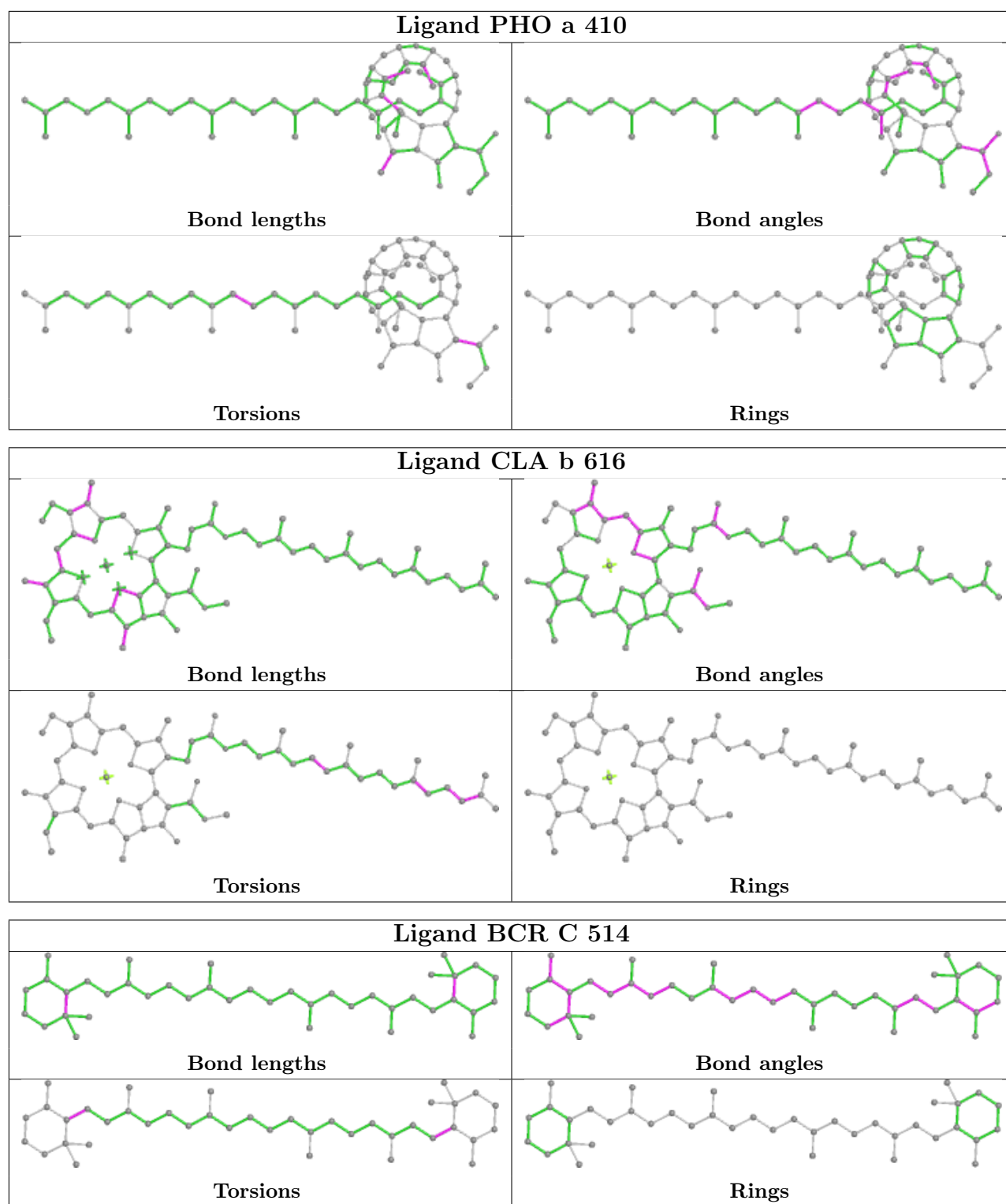
## Ligand LHG a 403



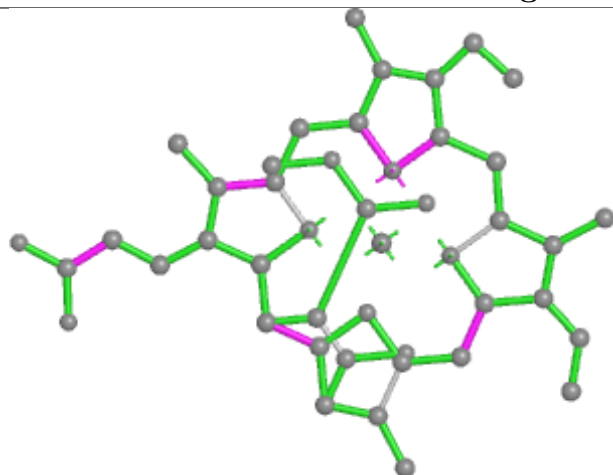
## Ligand CLA C 506



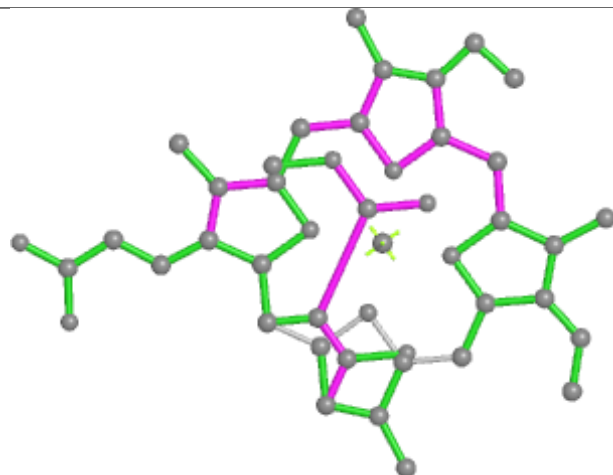




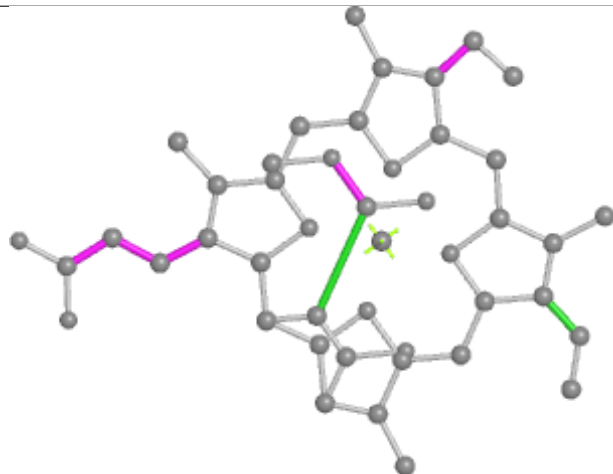
## Ligand KC1 3 310



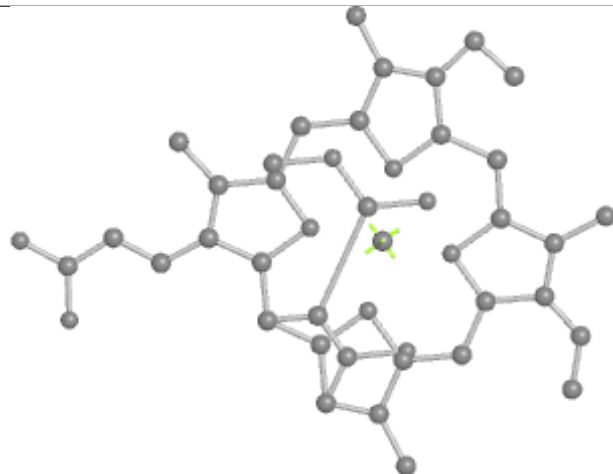
Bond lengths



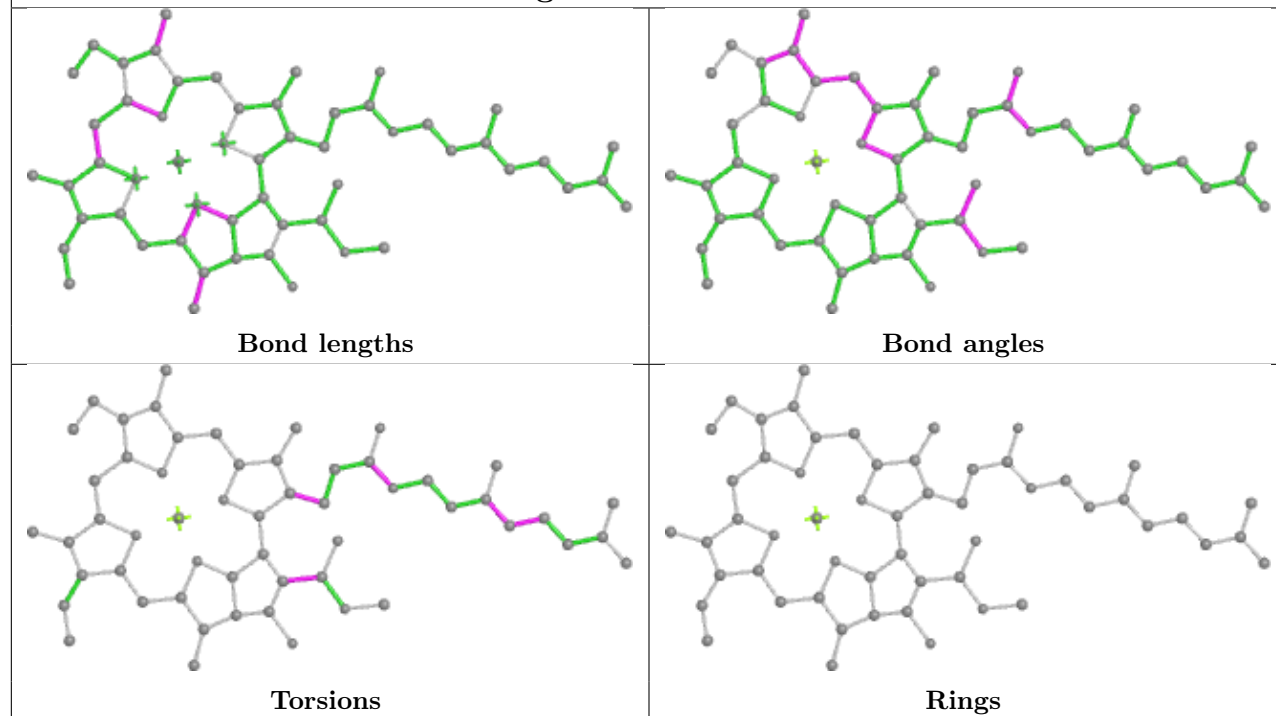
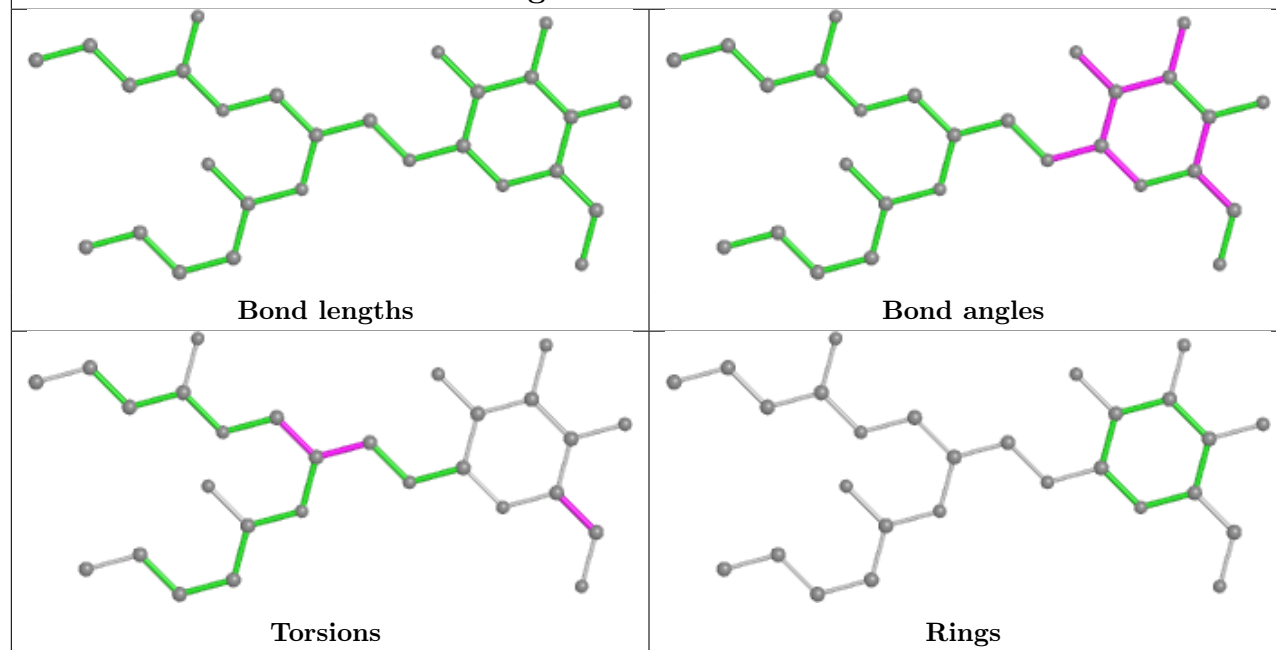
Bond angles



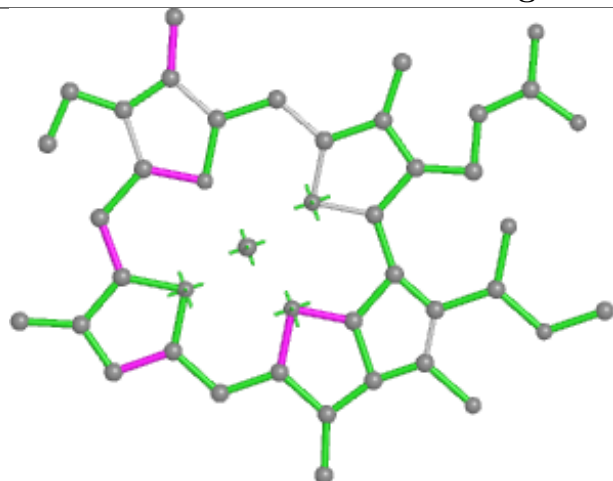
Torsions



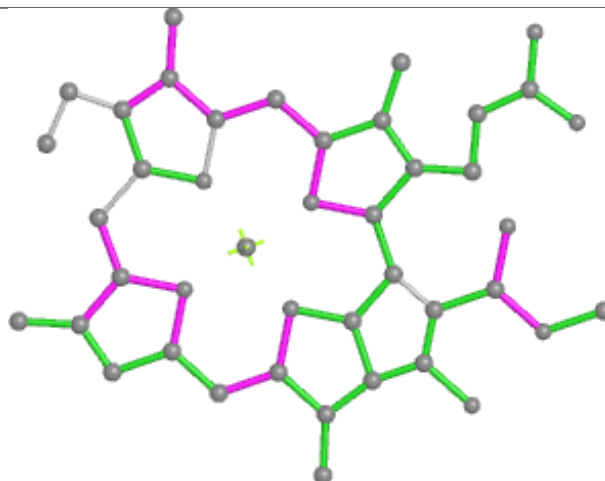
Rings

**Ligand CLA 4 305****Ligand LMG B 621**

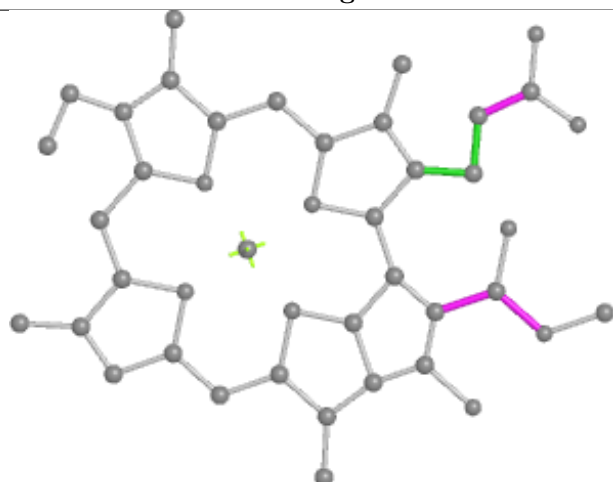
## Ligand CLA 2 309



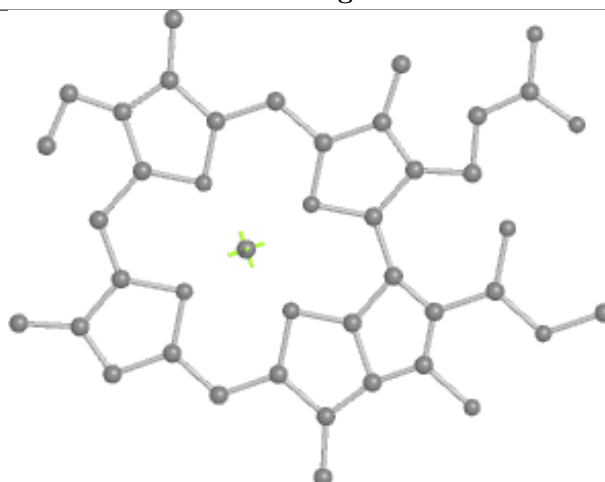
Bond lengths



Bond angles

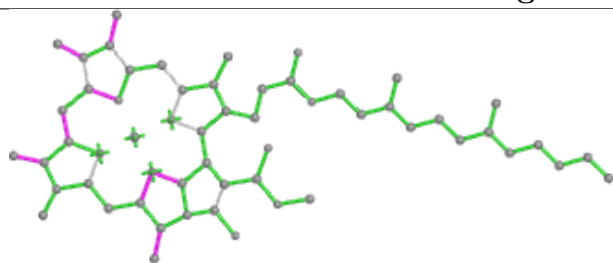


Torsions

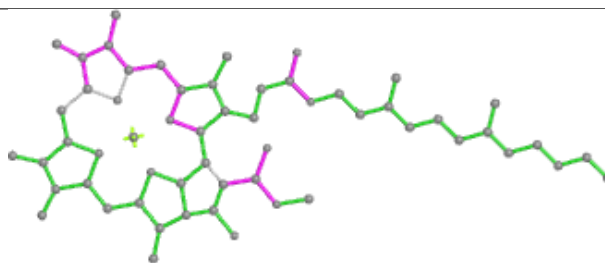


Rings

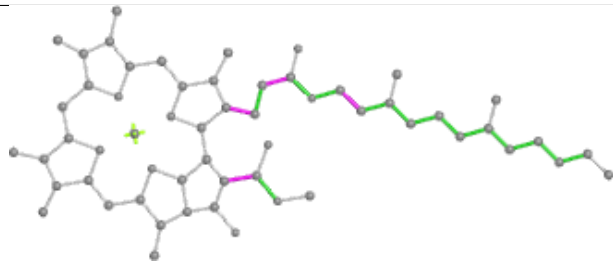
## Ligand CLA d 401



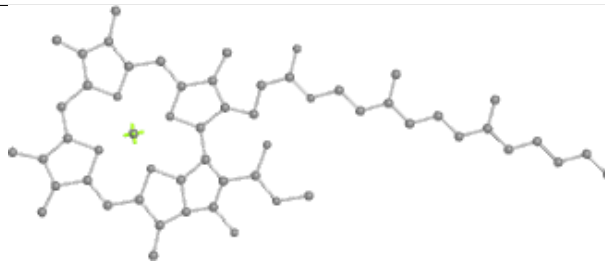
Bond lengths



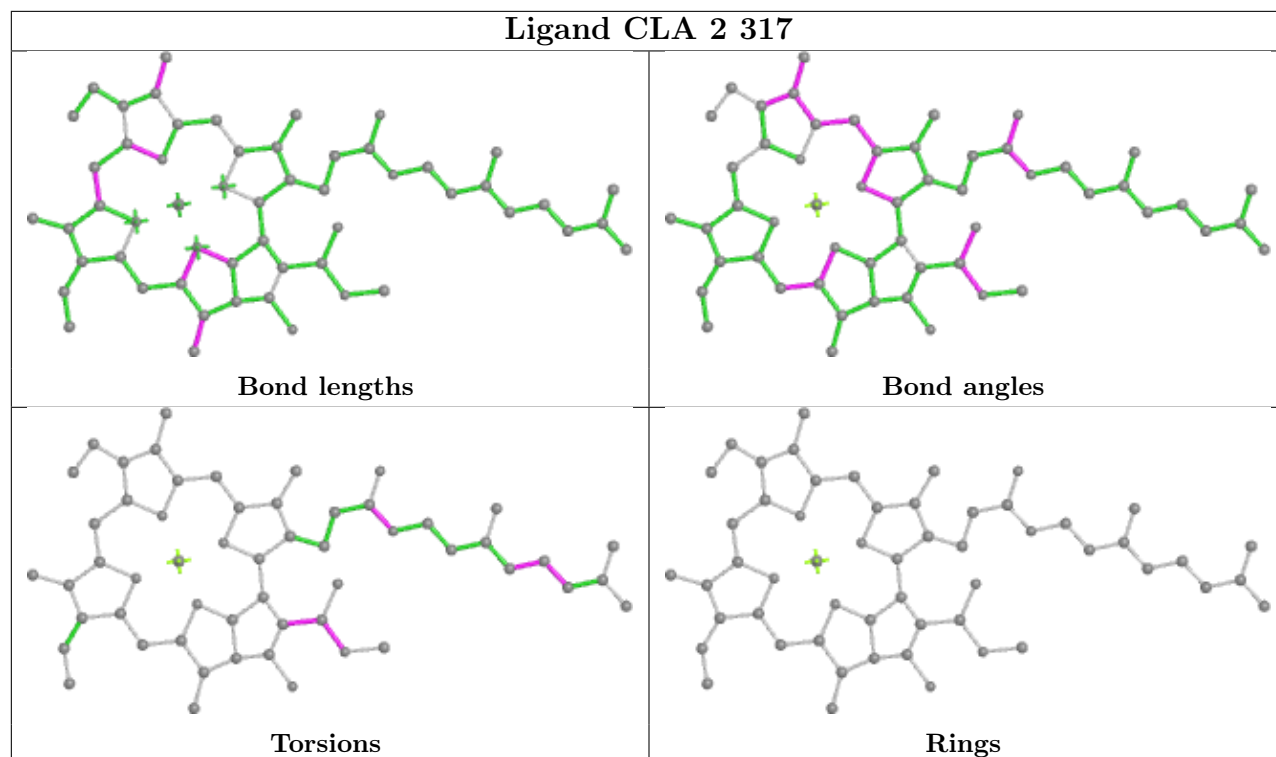
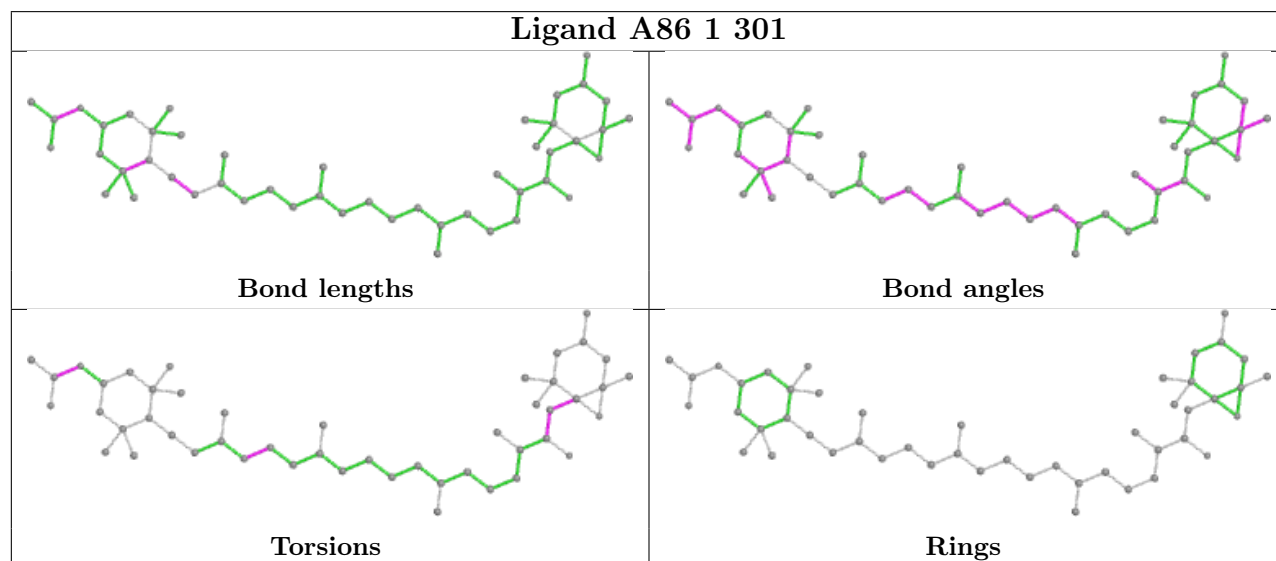
Bond angles



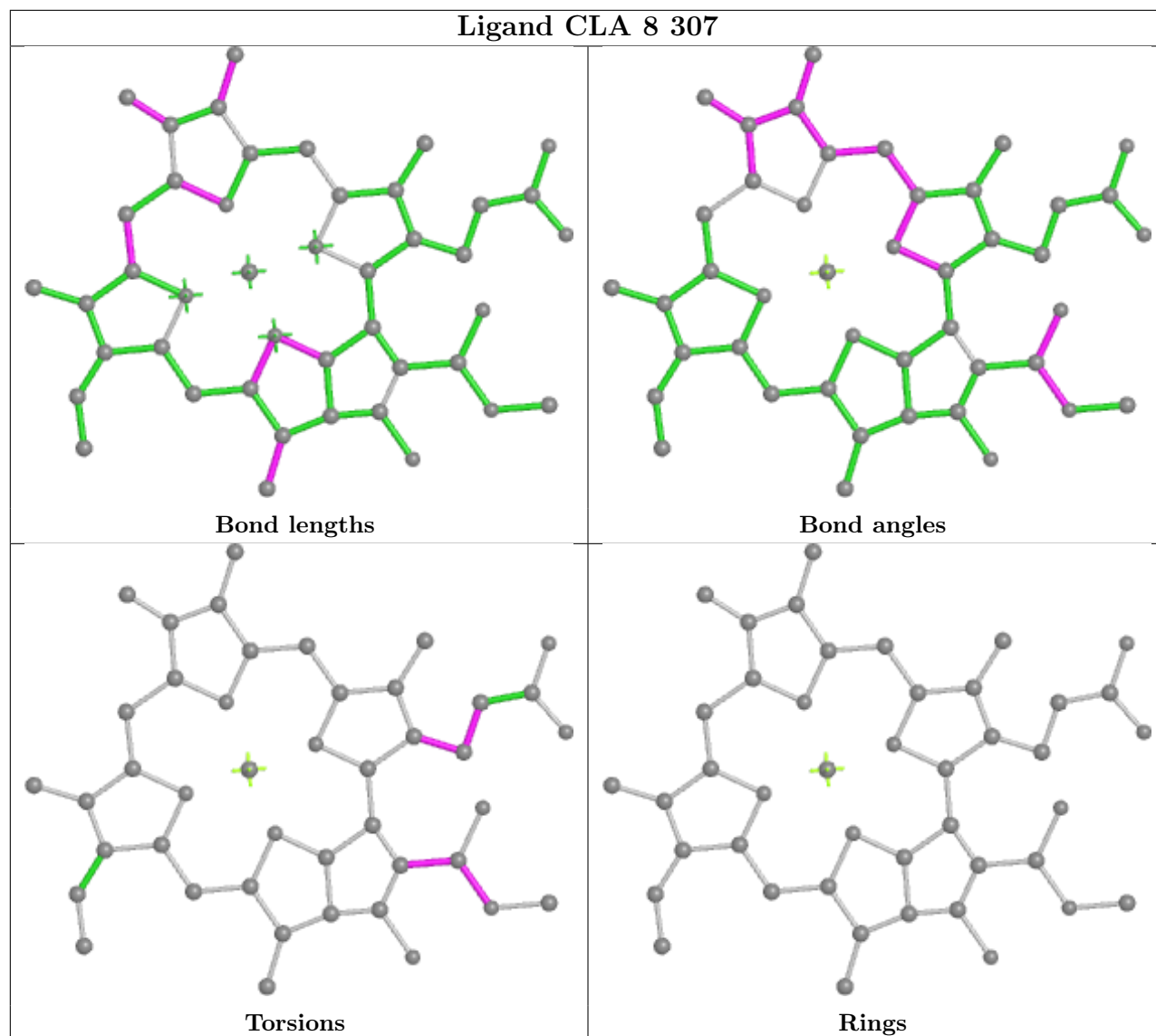
Torsions



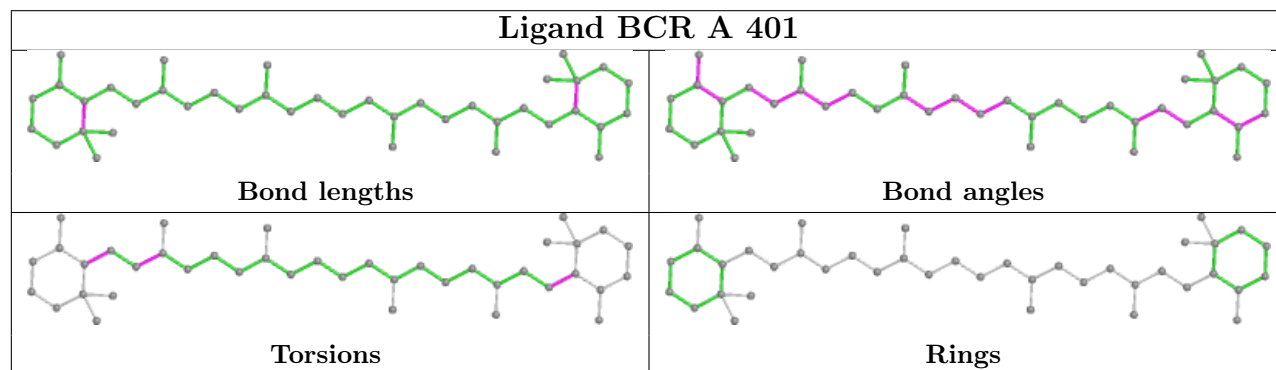
Rings

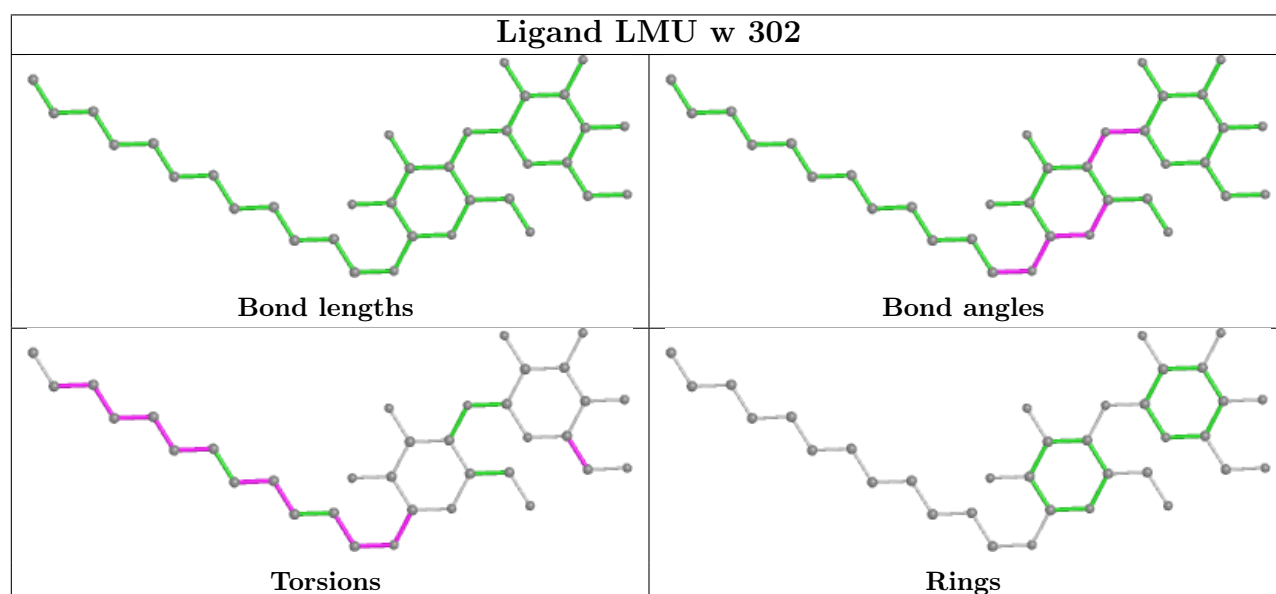
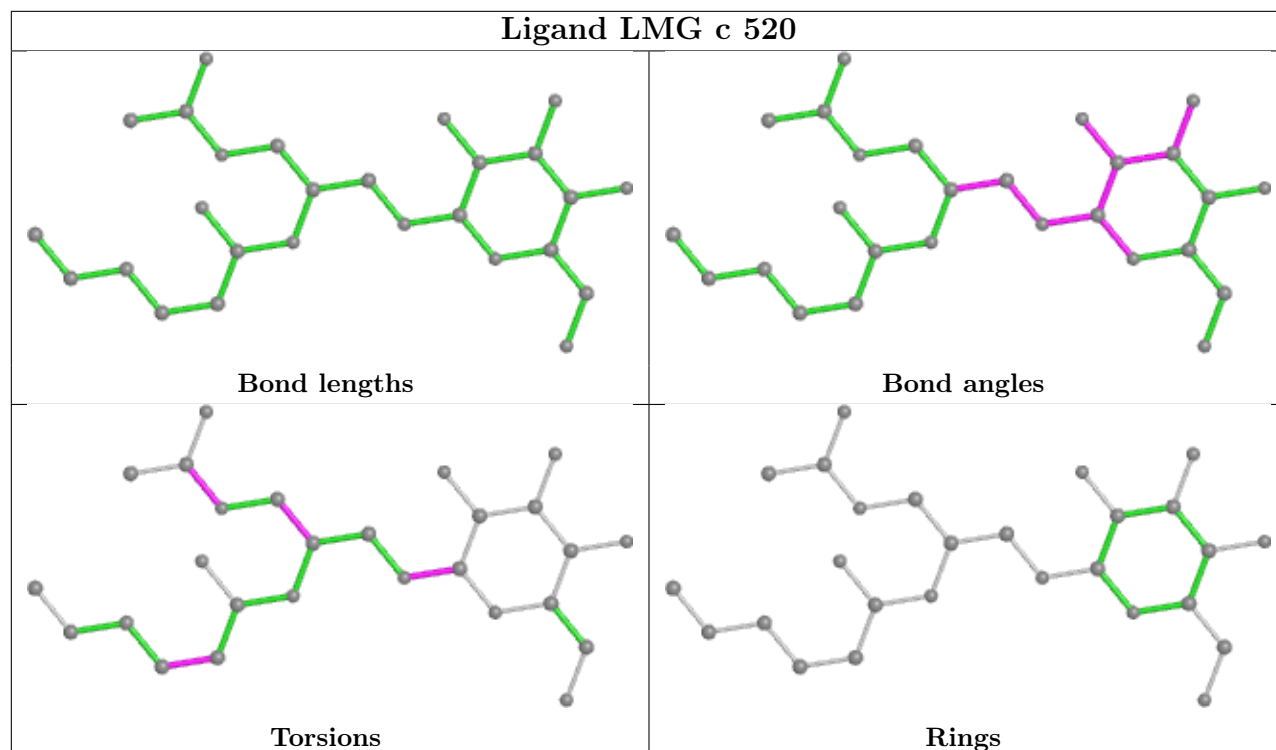
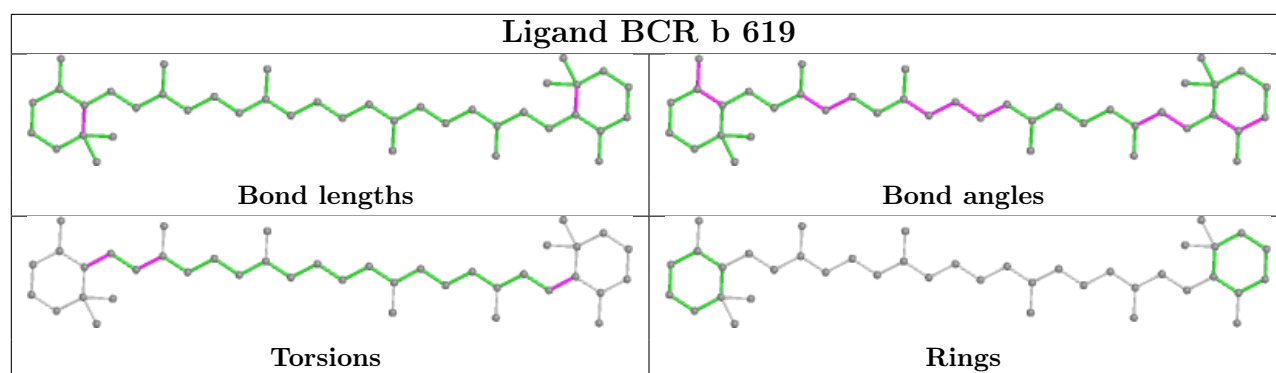
**Ligand CLA 2 317****Ligand A86 1 301**

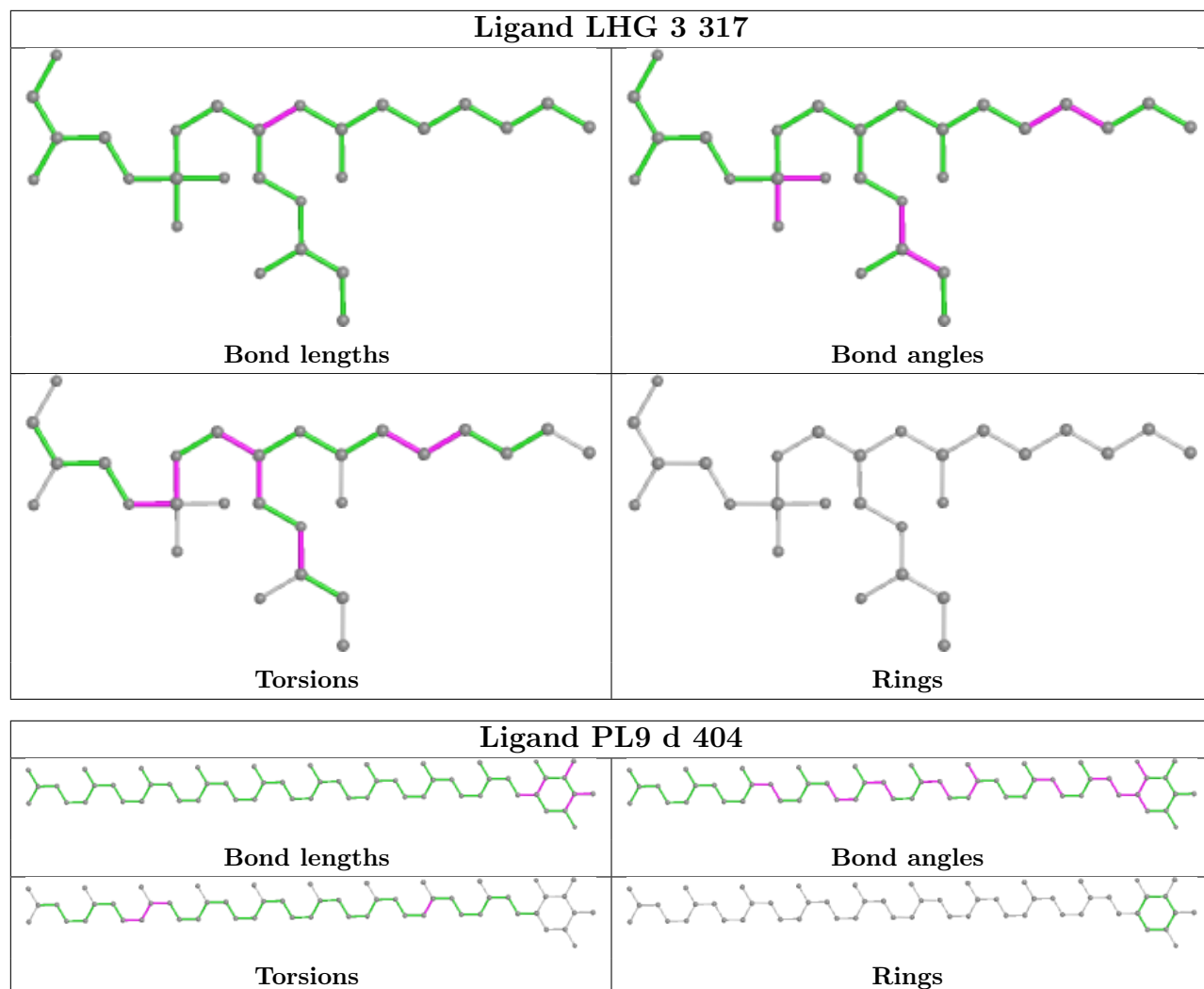
## Ligand CLA 8 307



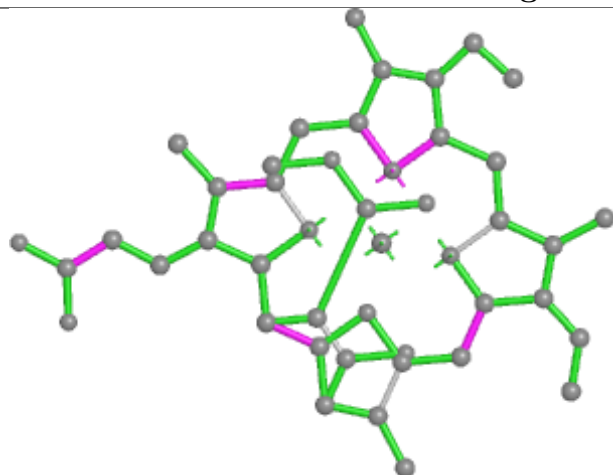
## Ligand BCR A 401



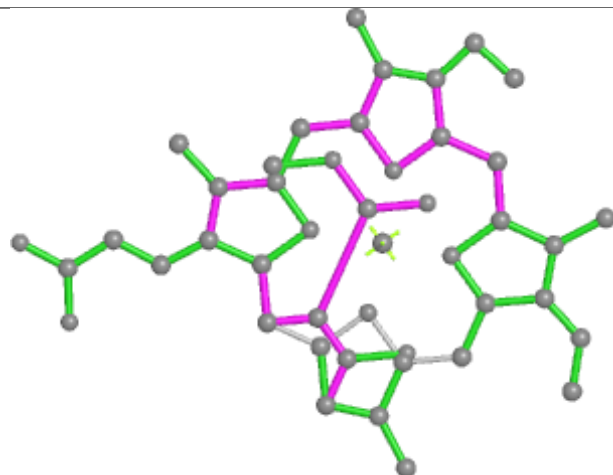




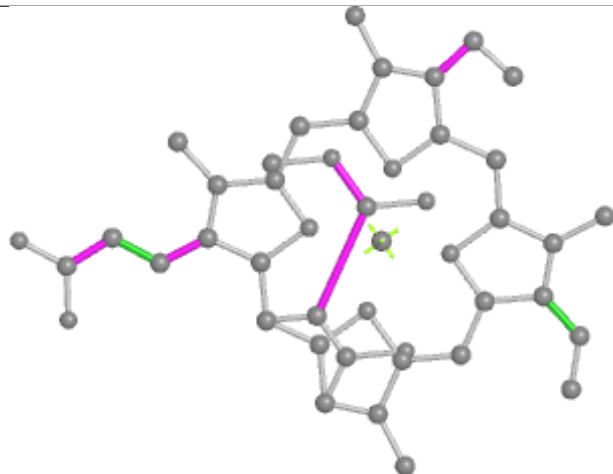
## Ligand KC1 5 315



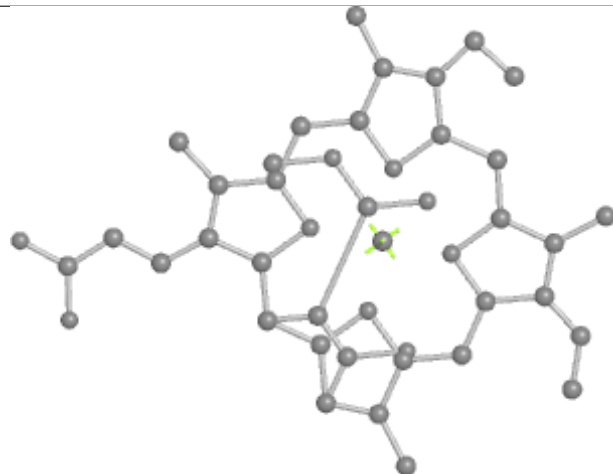
Bond lengths



Bond angles

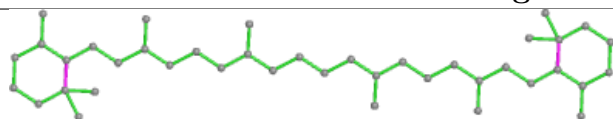


Torsions

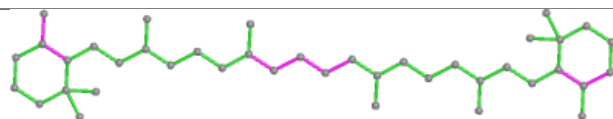


Rings

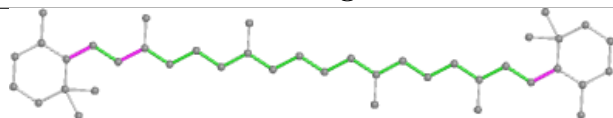
## Ligand BCR B 618



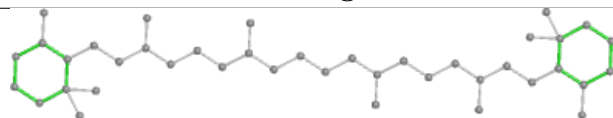
Bond lengths



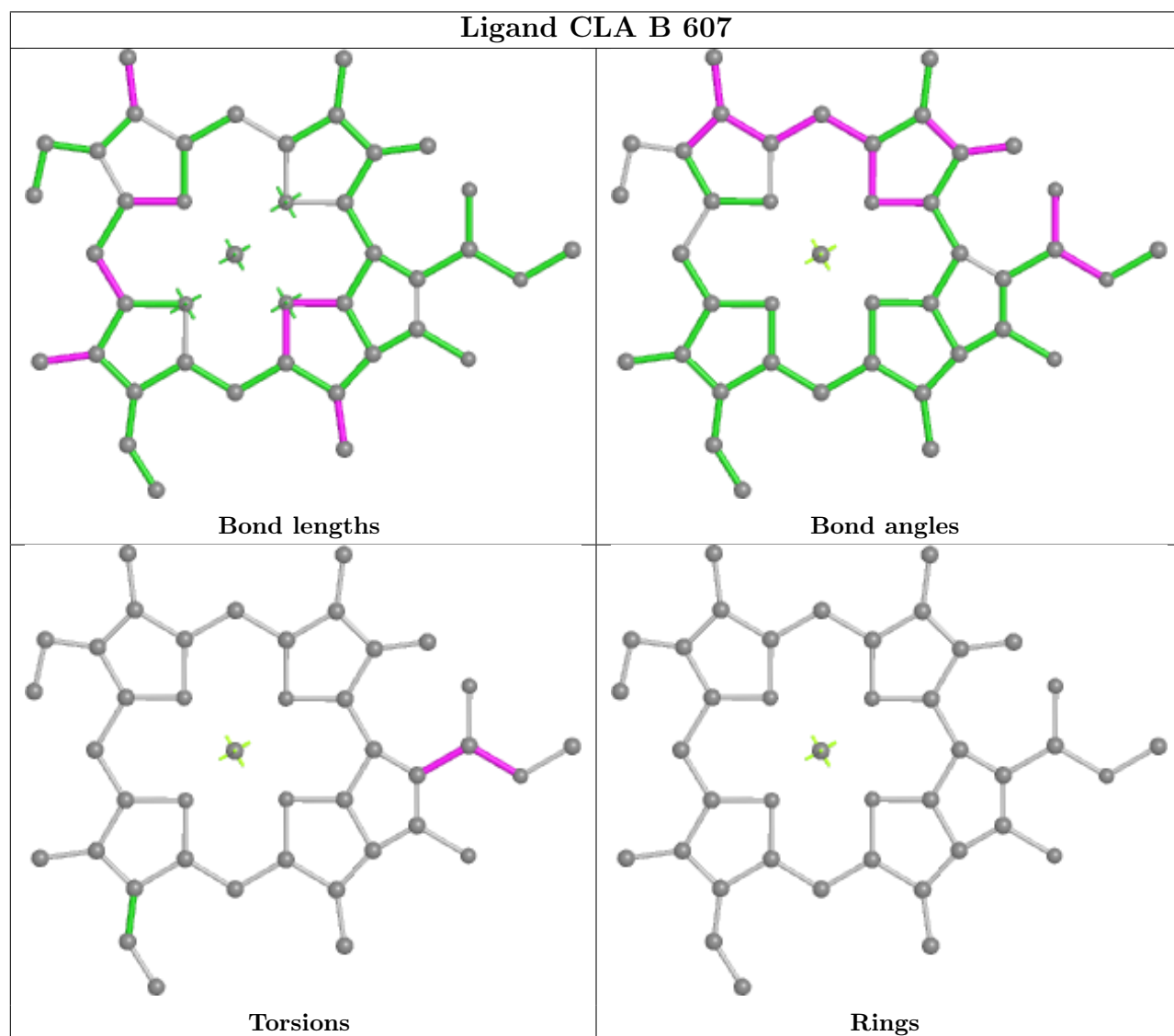
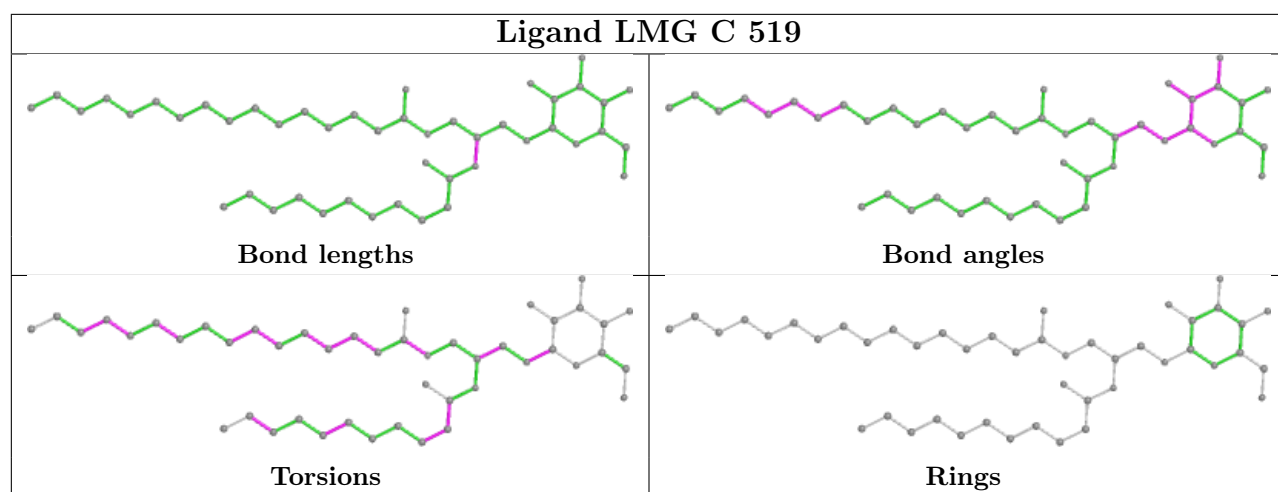
Bond angles



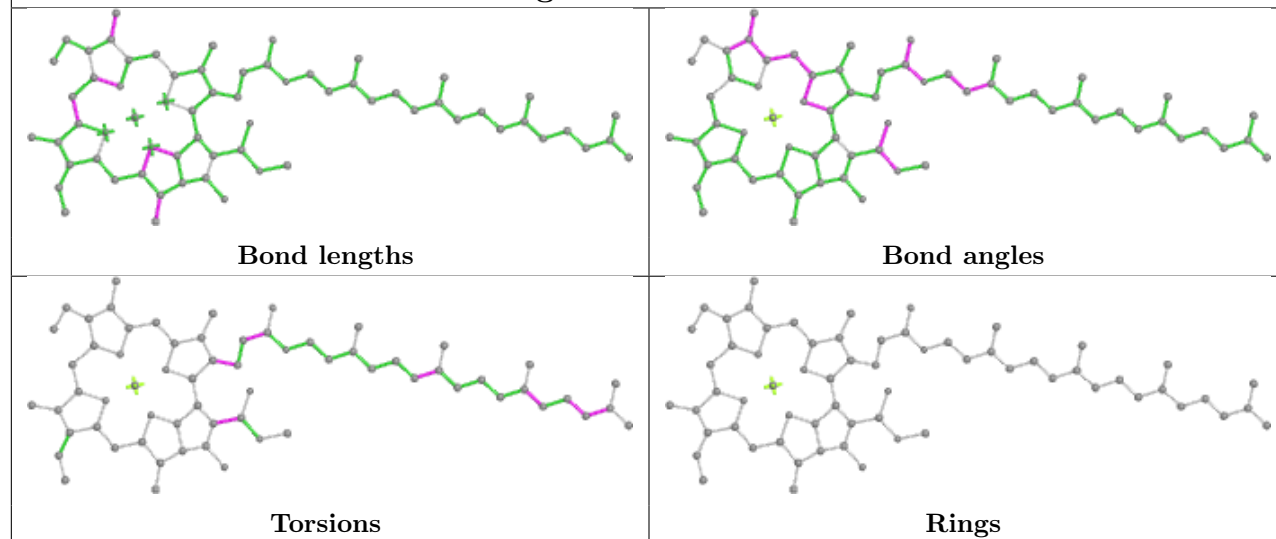
Torsions



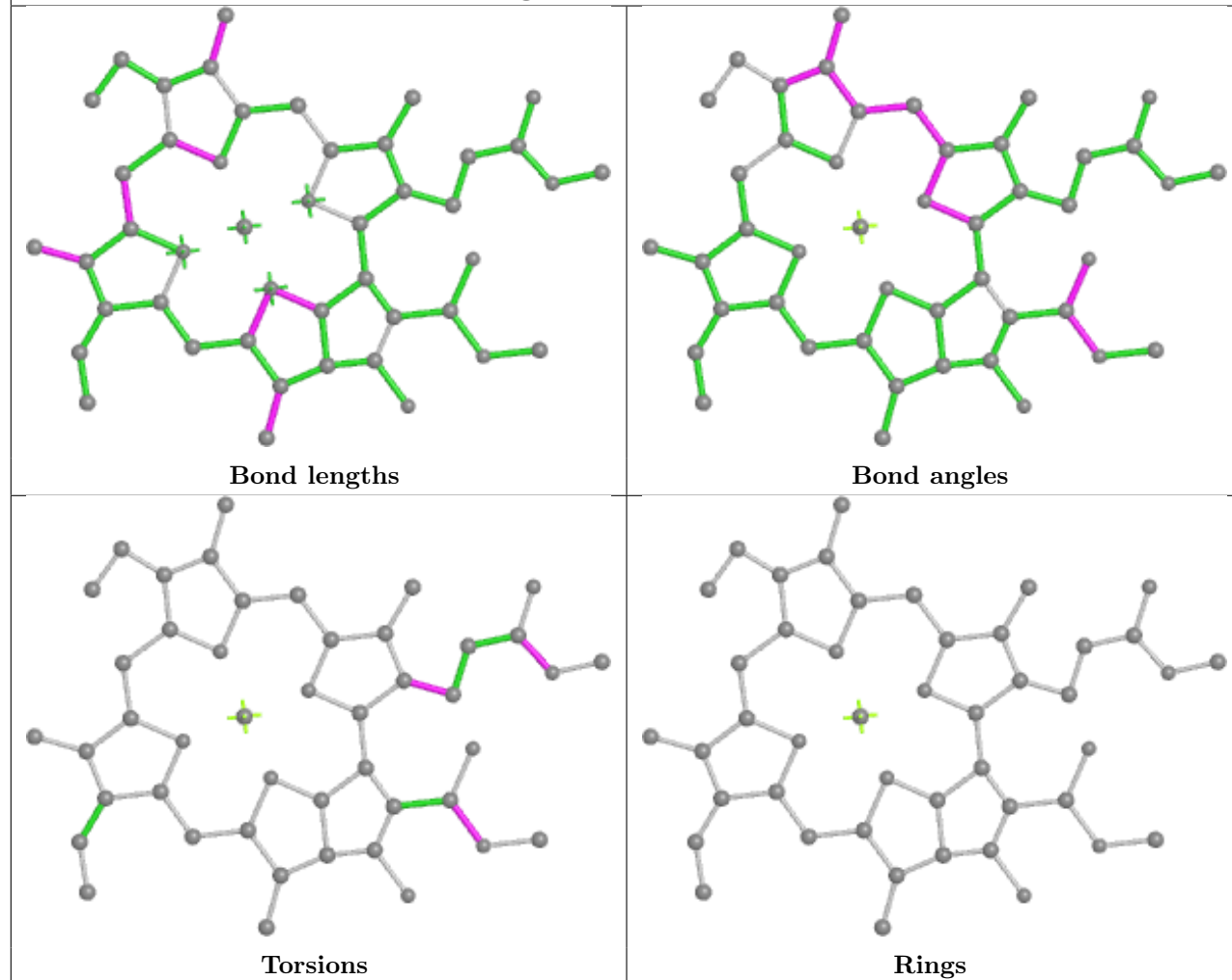
Rings



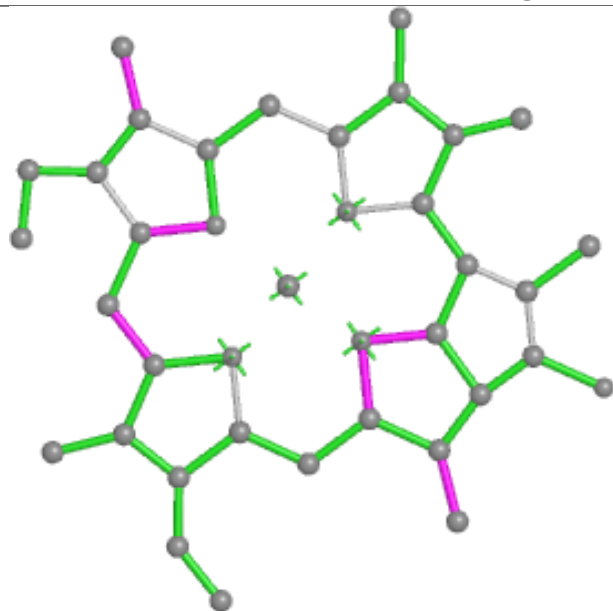
## Ligand CLA 4 308



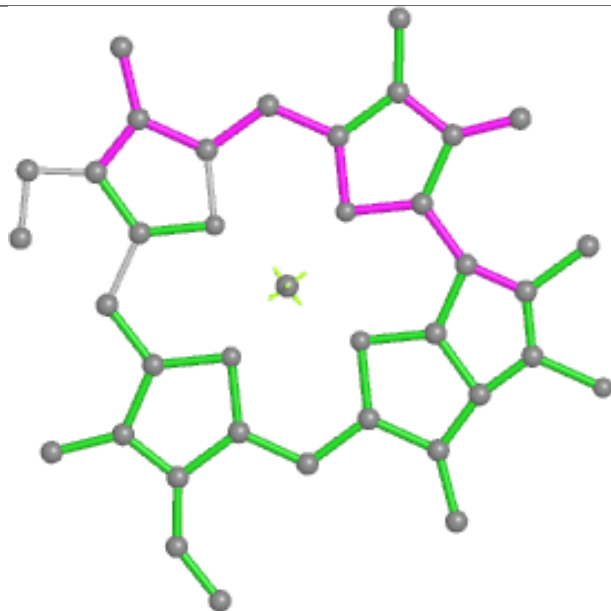
## Ligand CLA 4 310



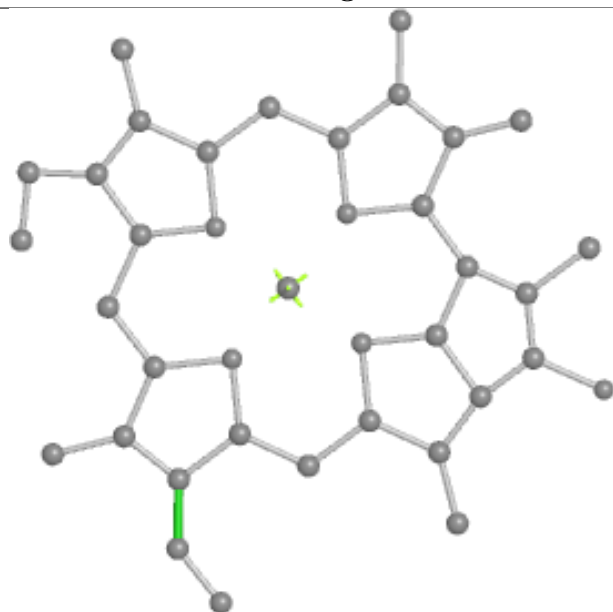
## Ligand CLA 2 316



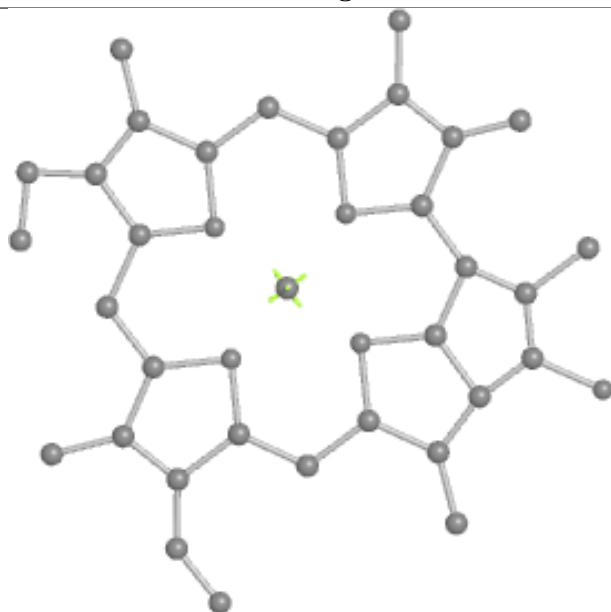
Bond lengths



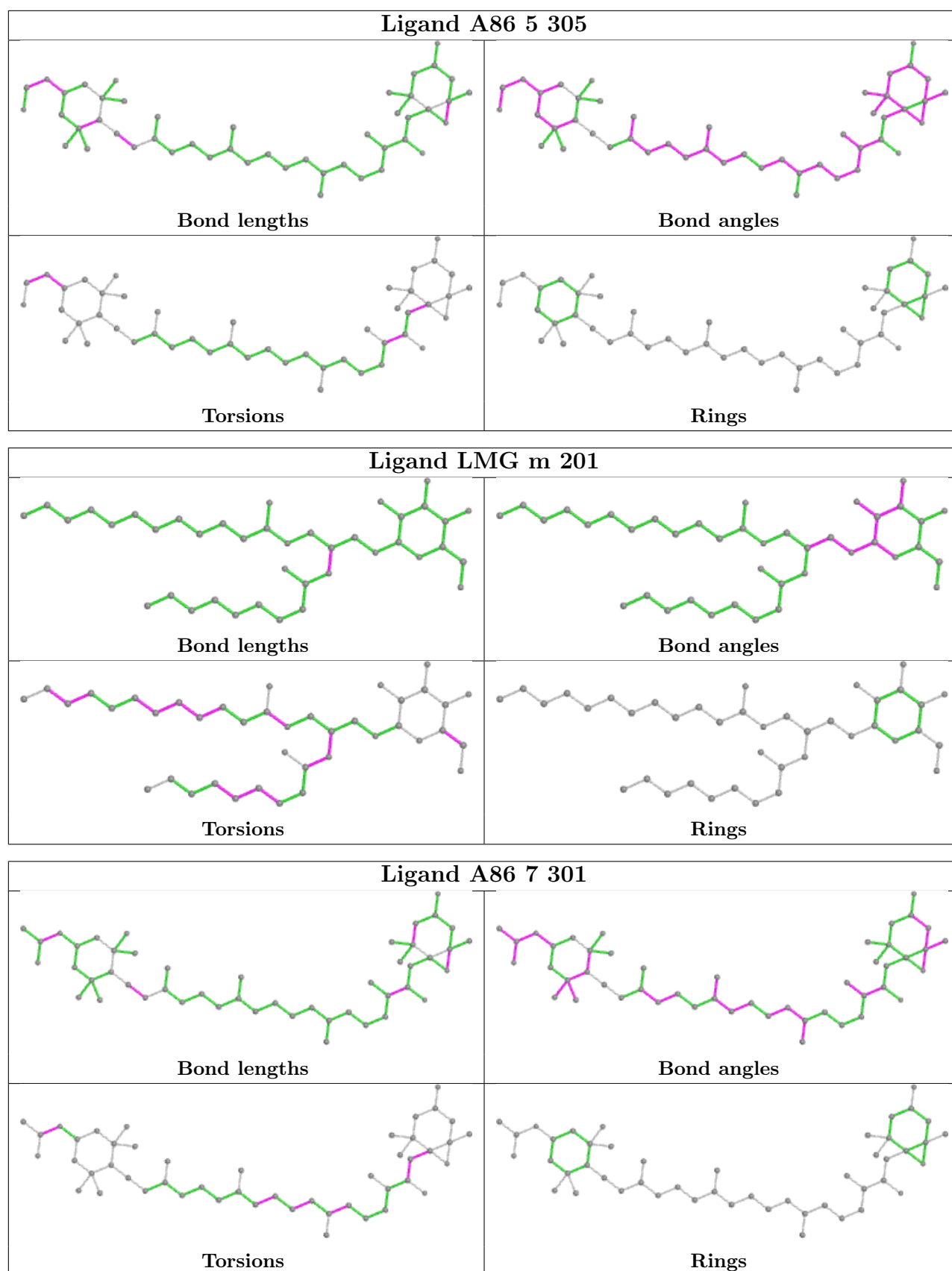
Bond angles

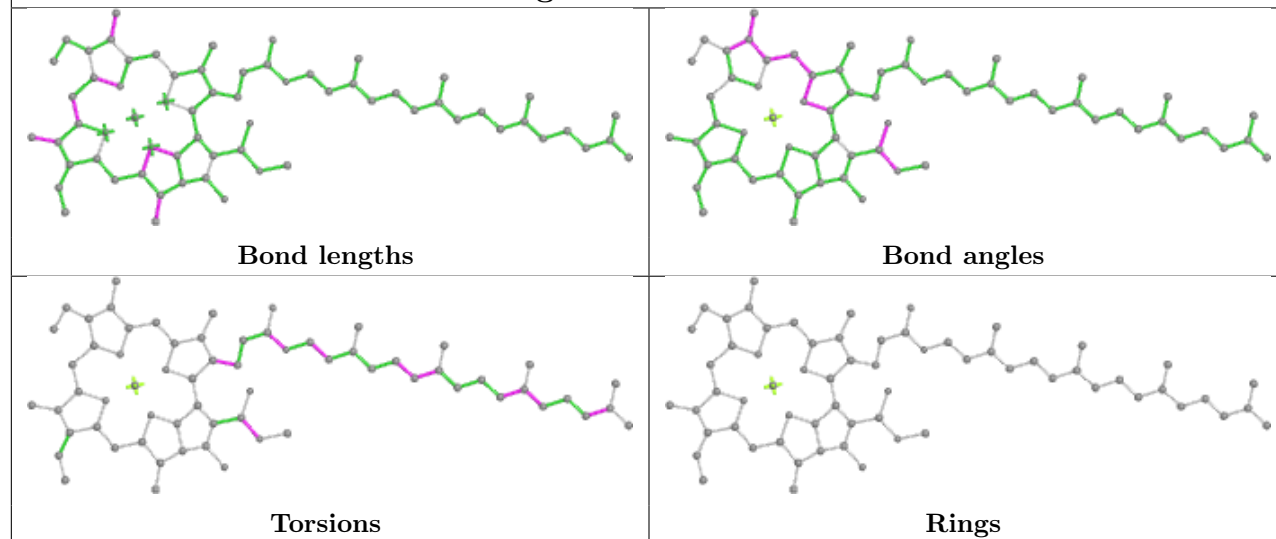
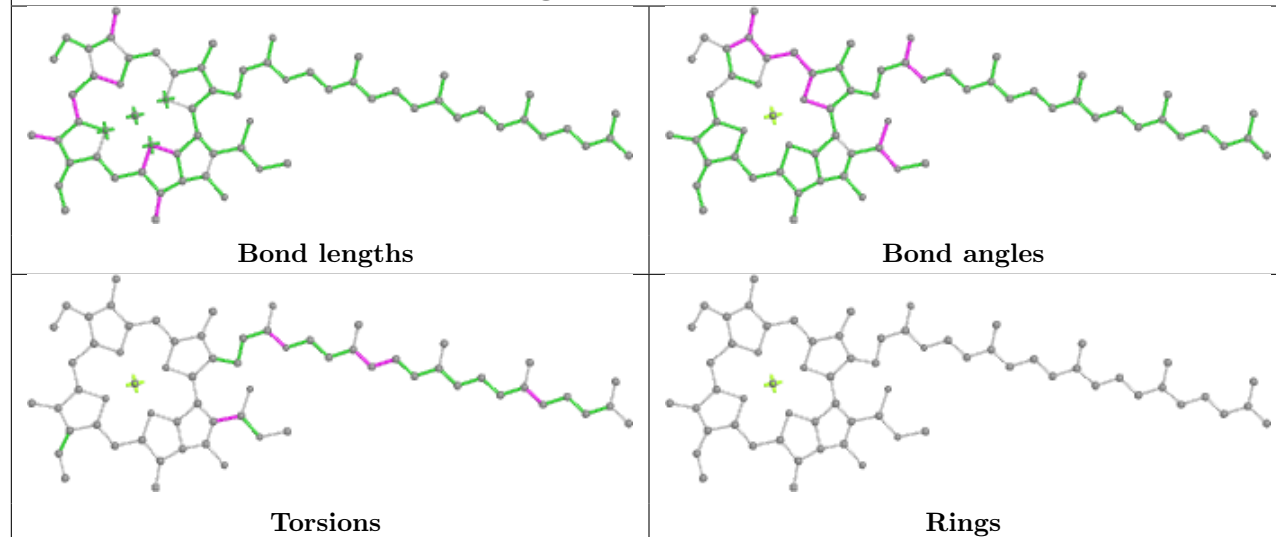


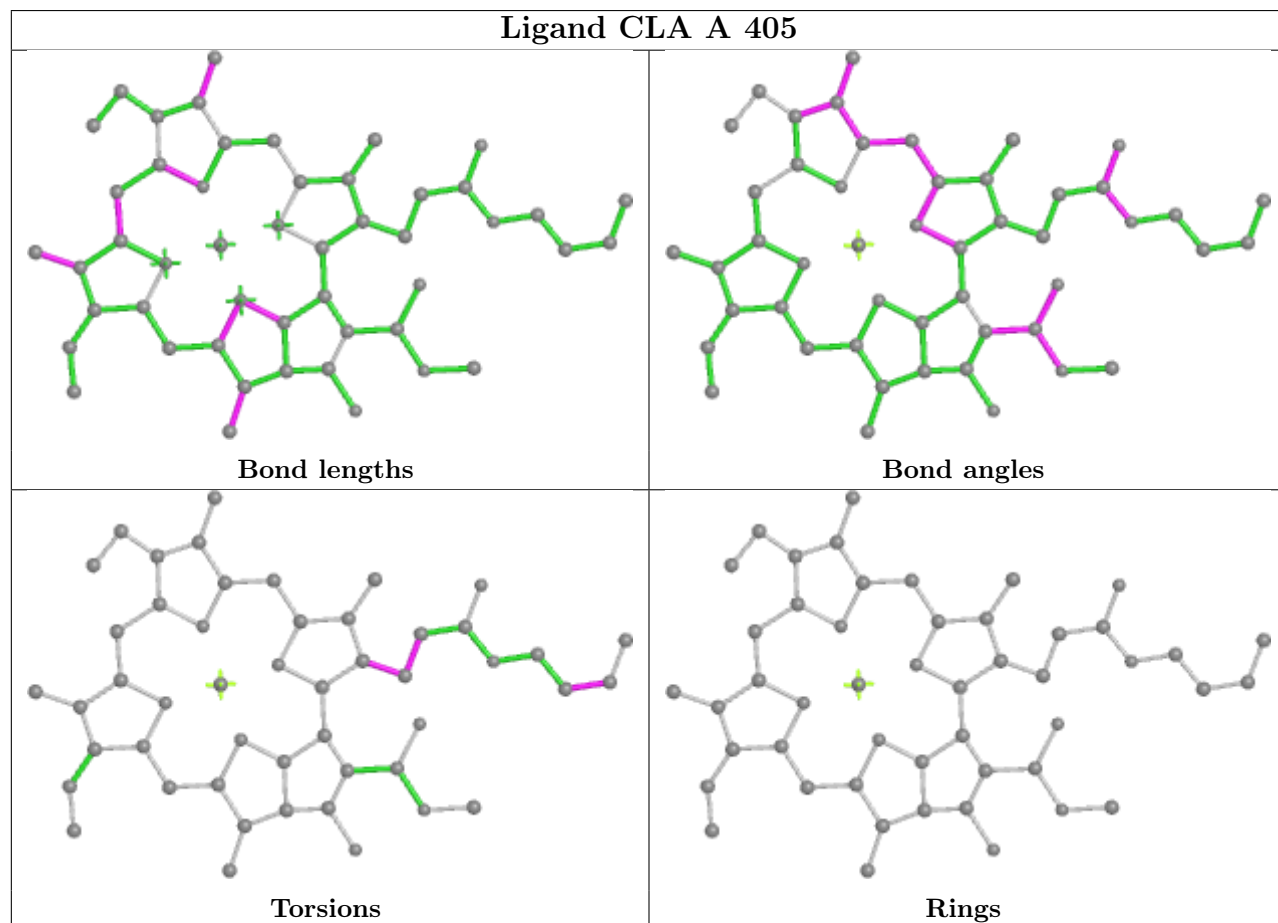
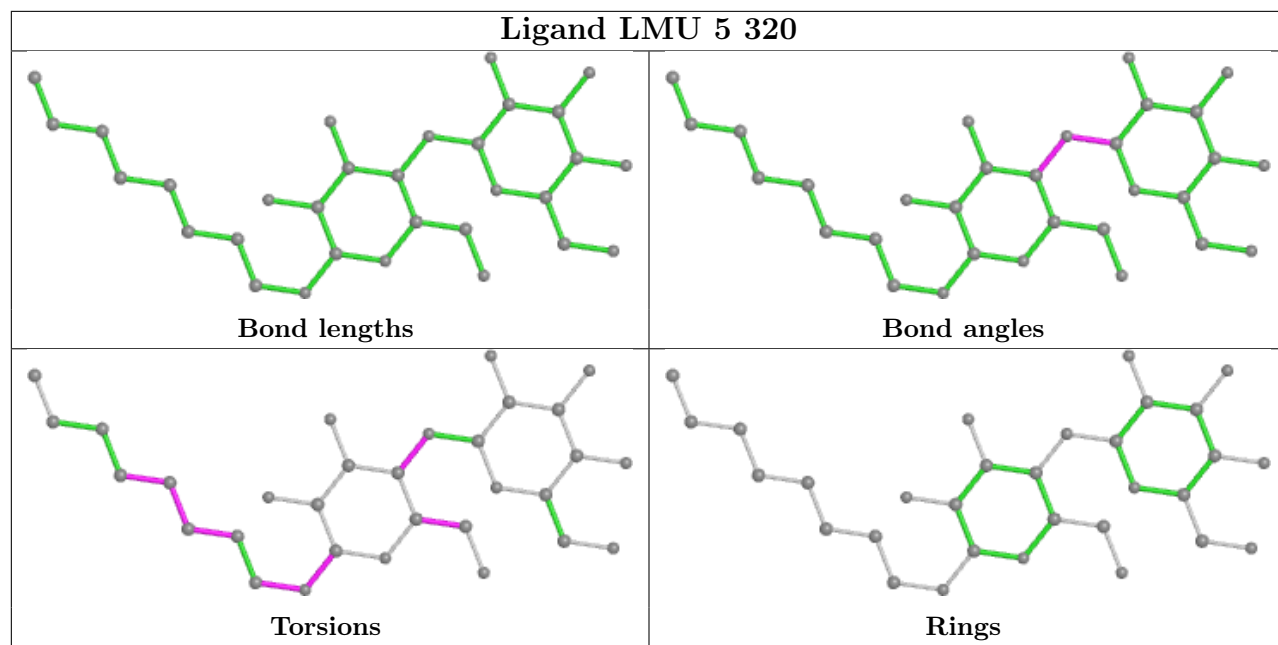
Torsions



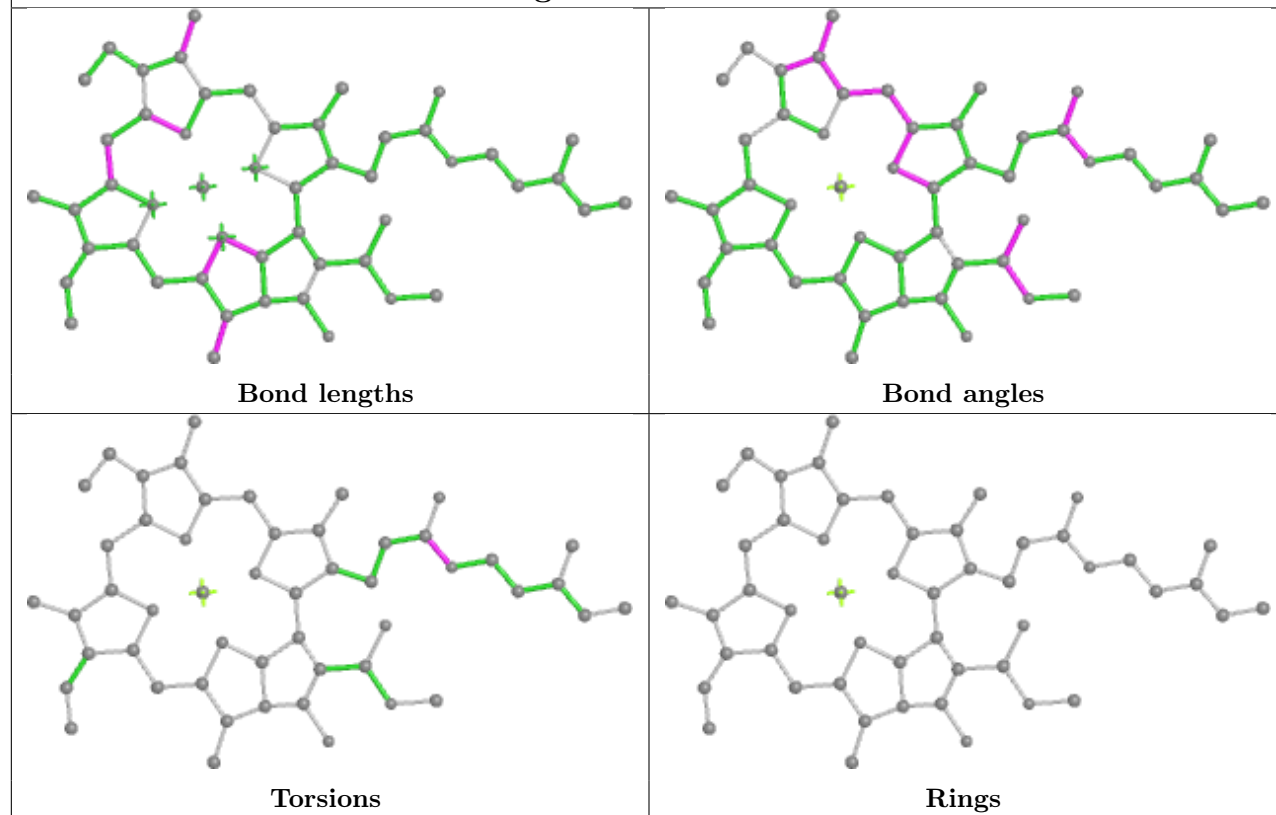
Rings



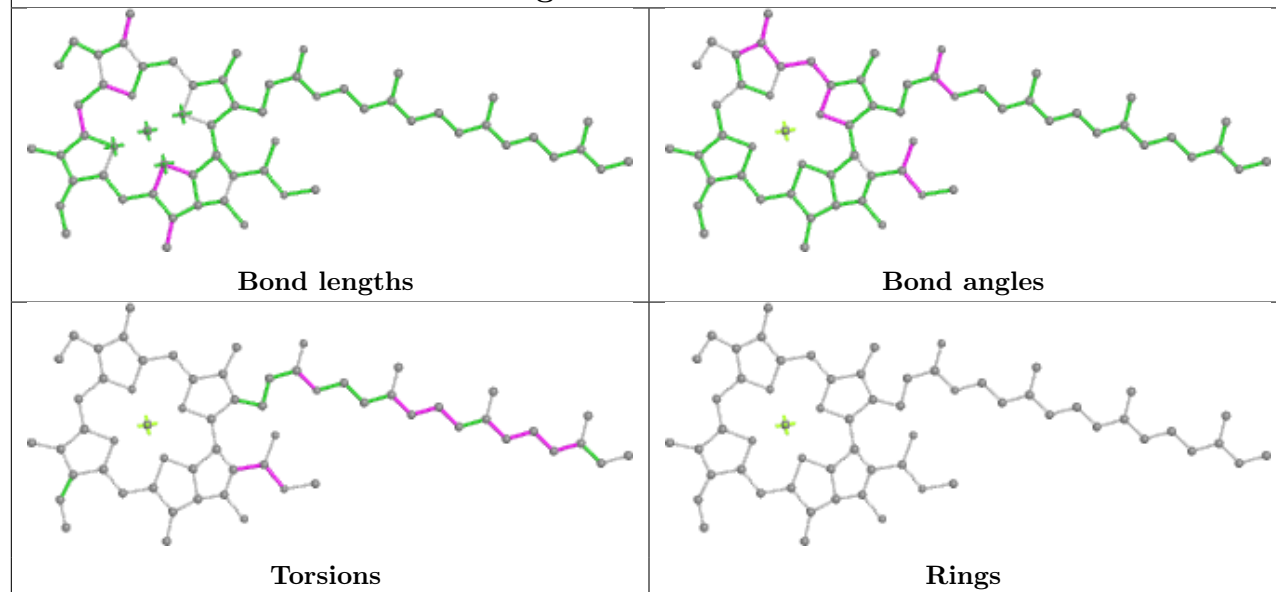
**Ligand CLA 8 310****Ligand CLA c 511**

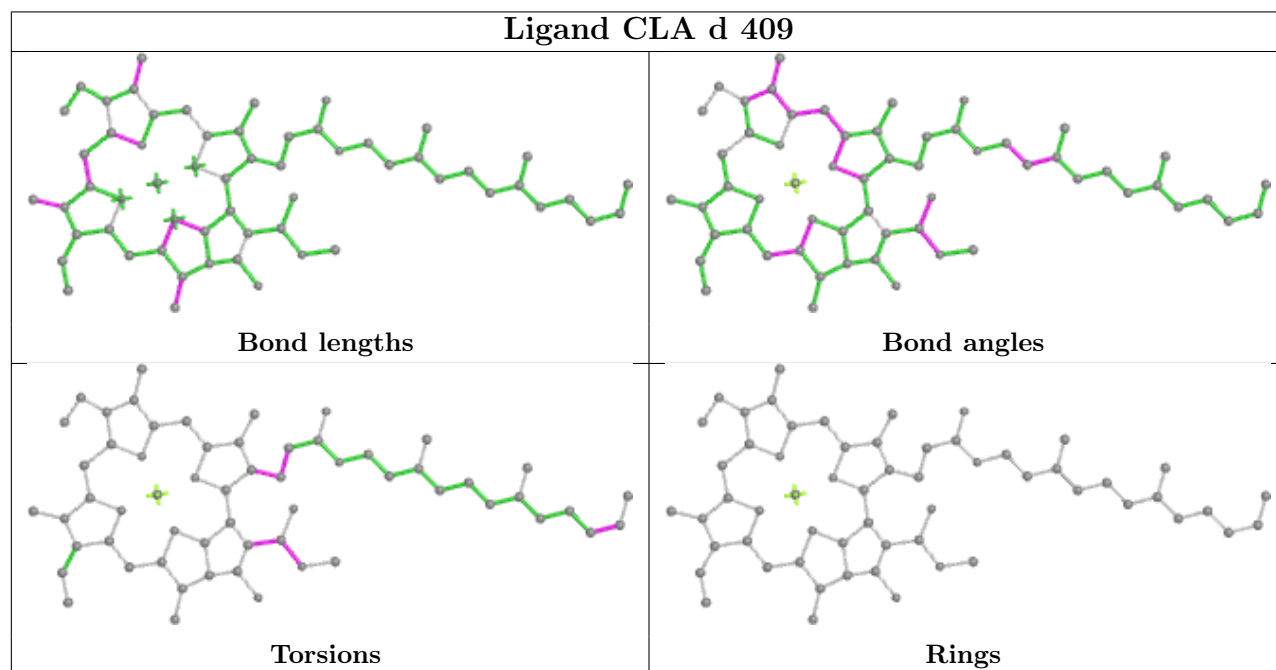
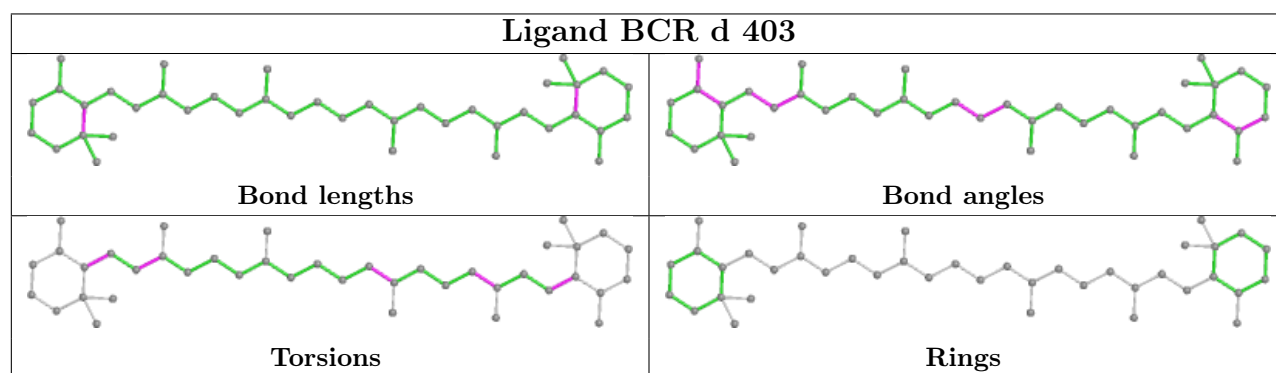
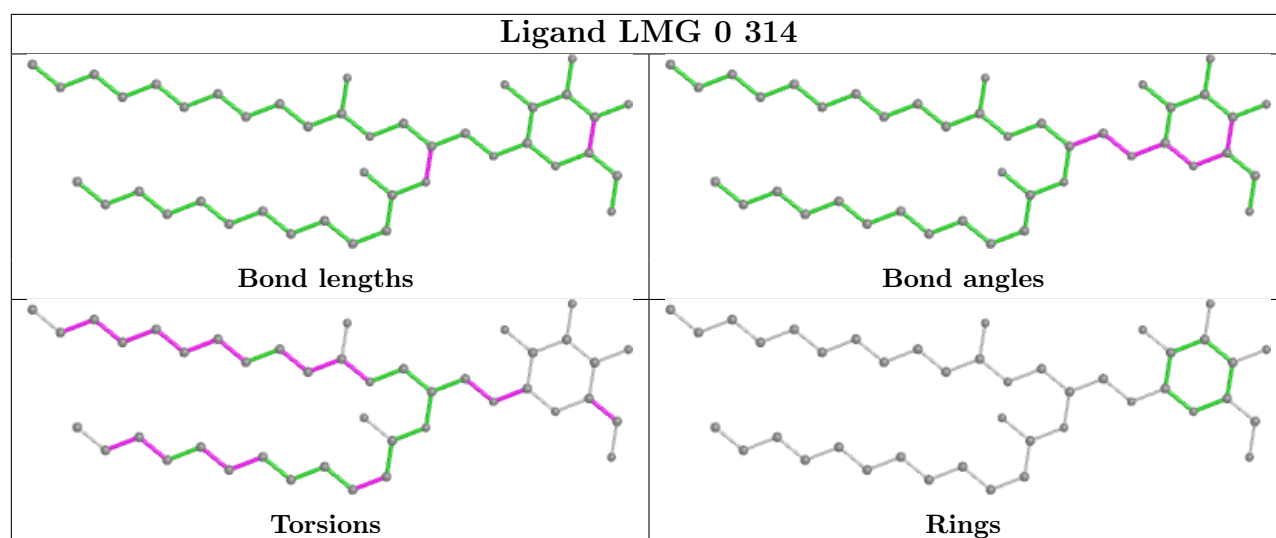


## Ligand CLA Z 101

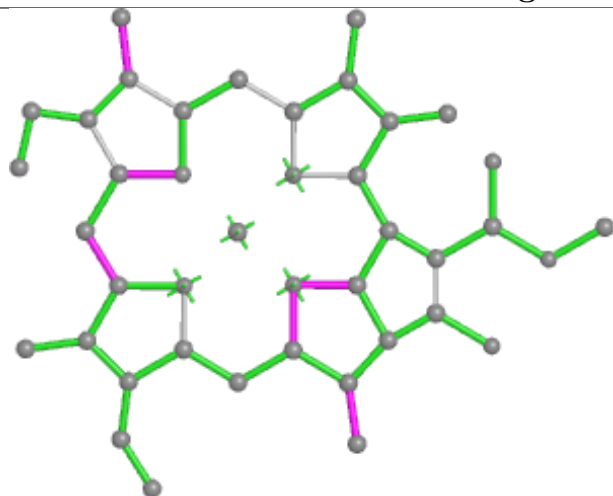


## Ligand CLA 3 313

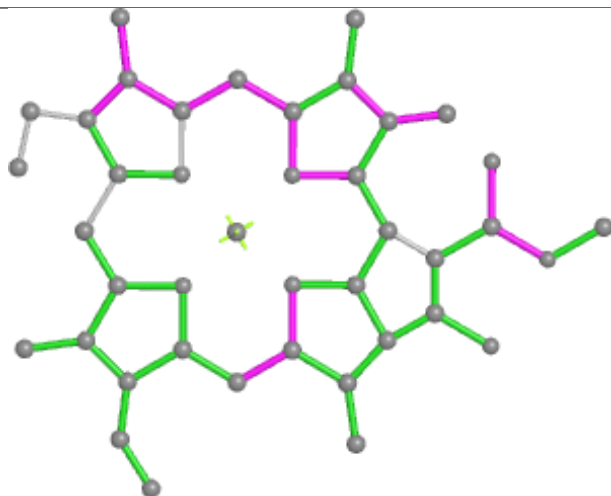




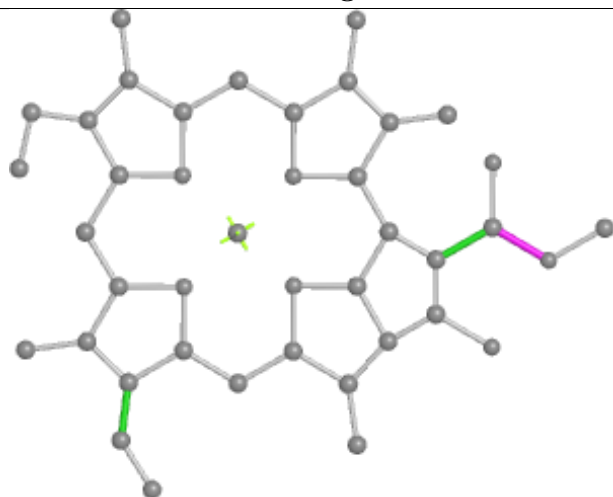
## Ligand CLA 7 308



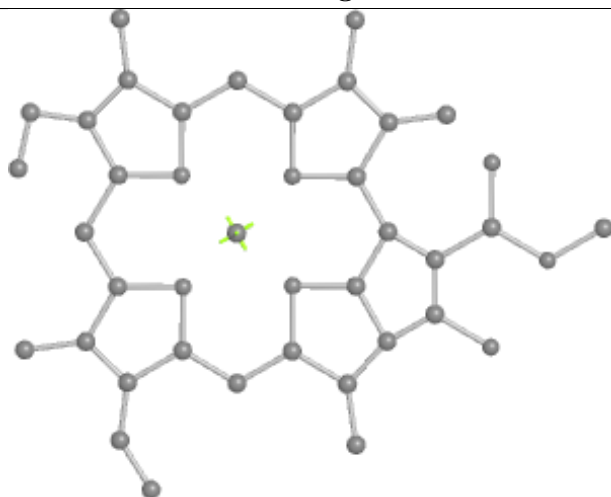
Bond lengths



Bond angles

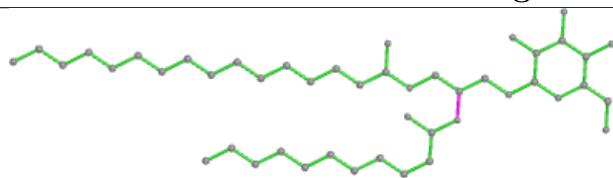


Torsions

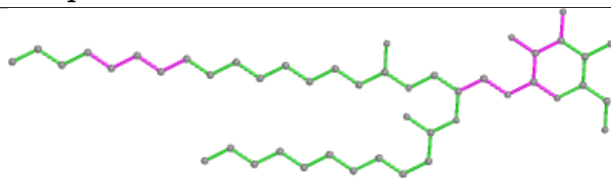


Rings

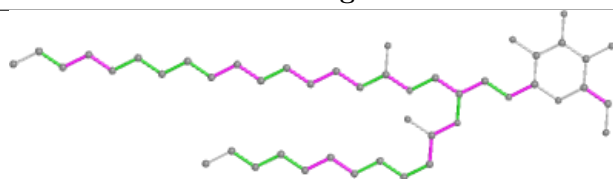
## Ligand LMG q 301



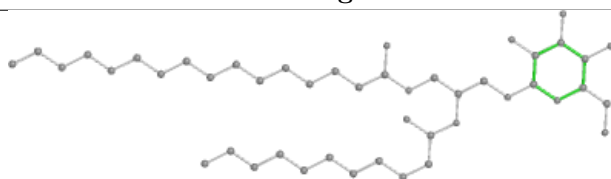
Bond lengths



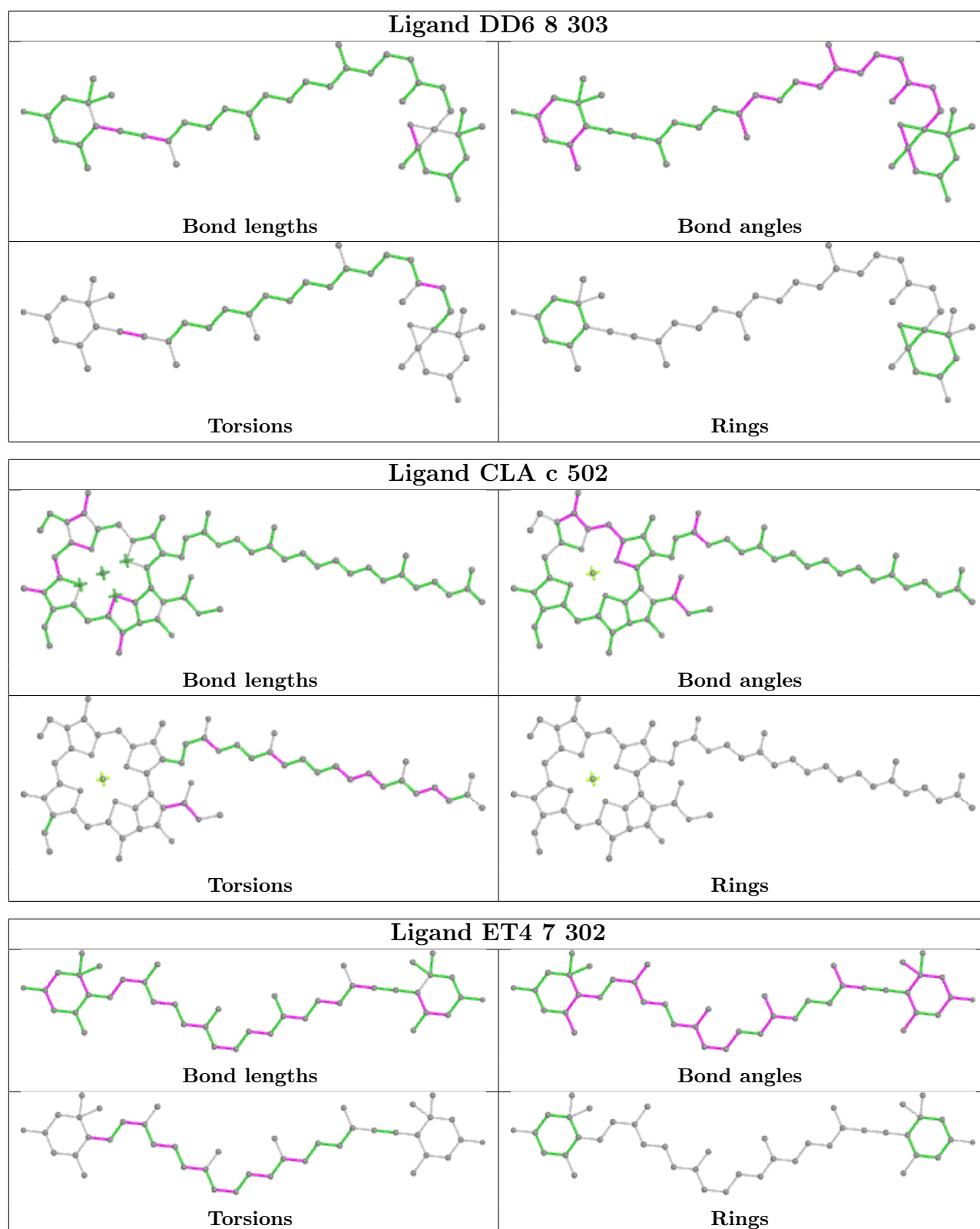
Bond angles

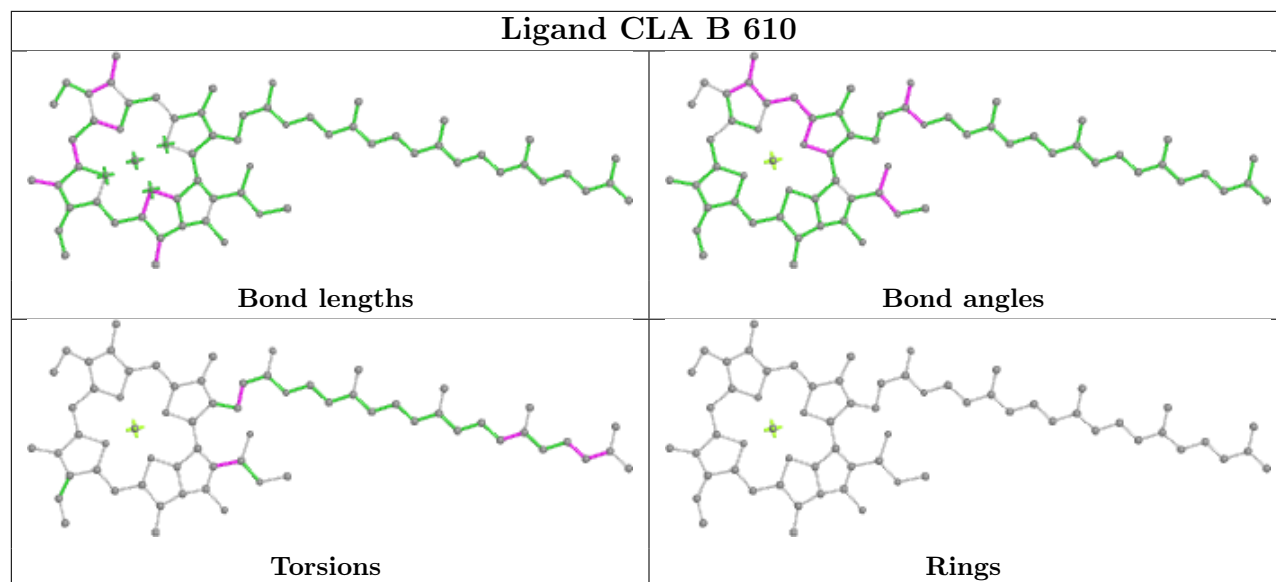
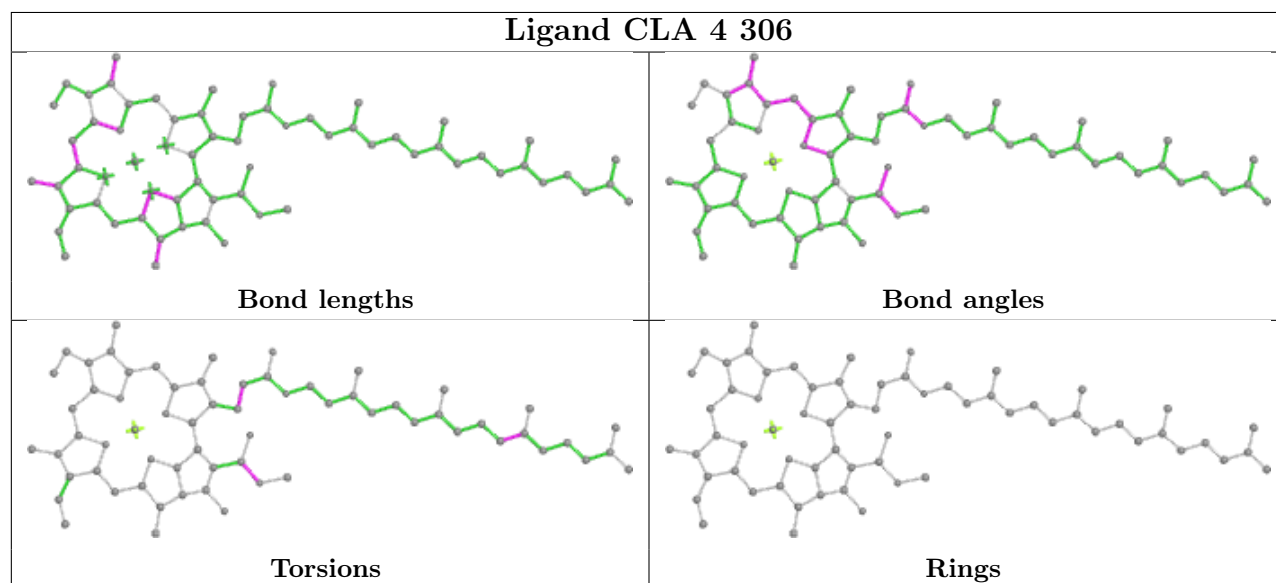


Torsions

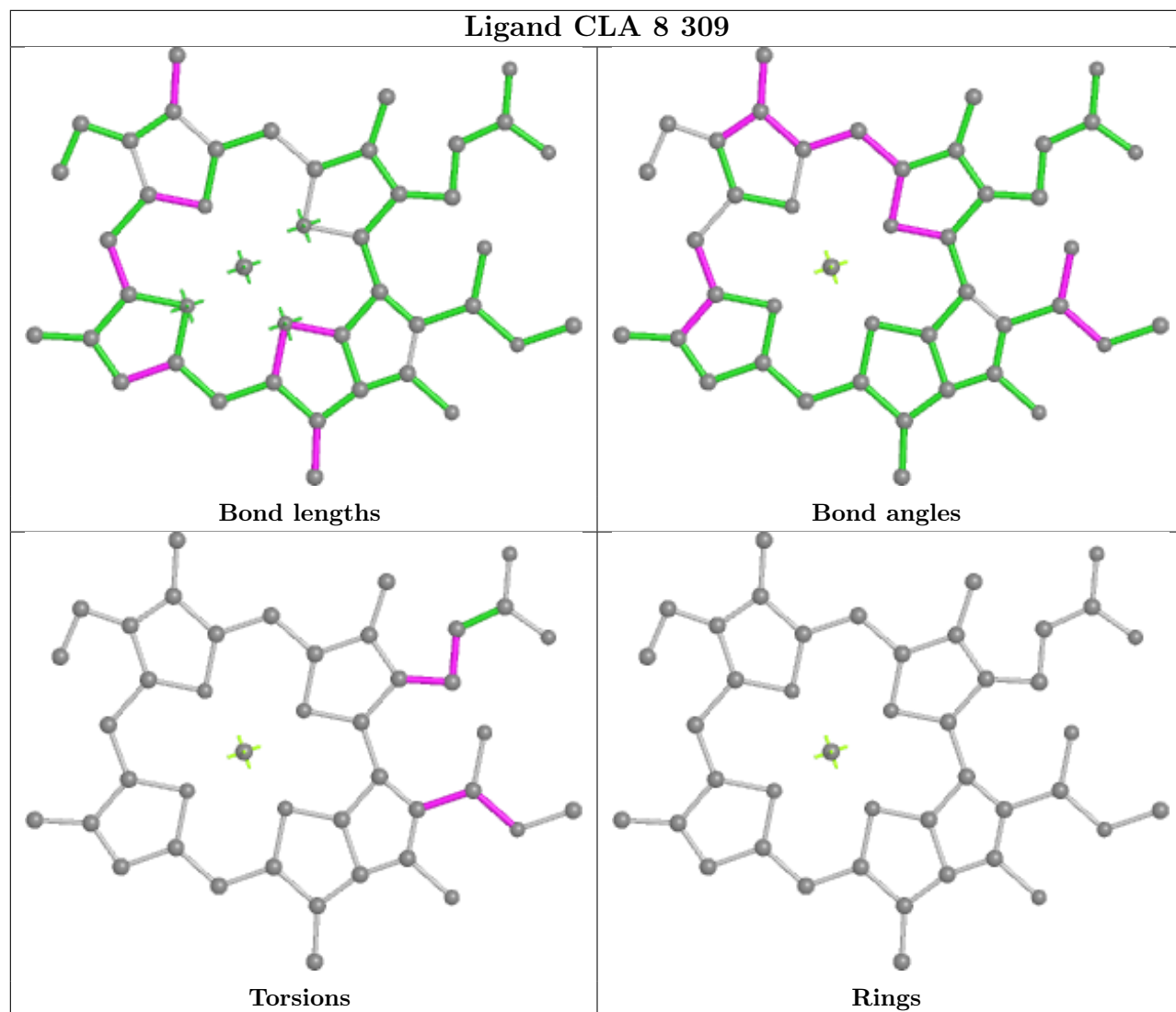


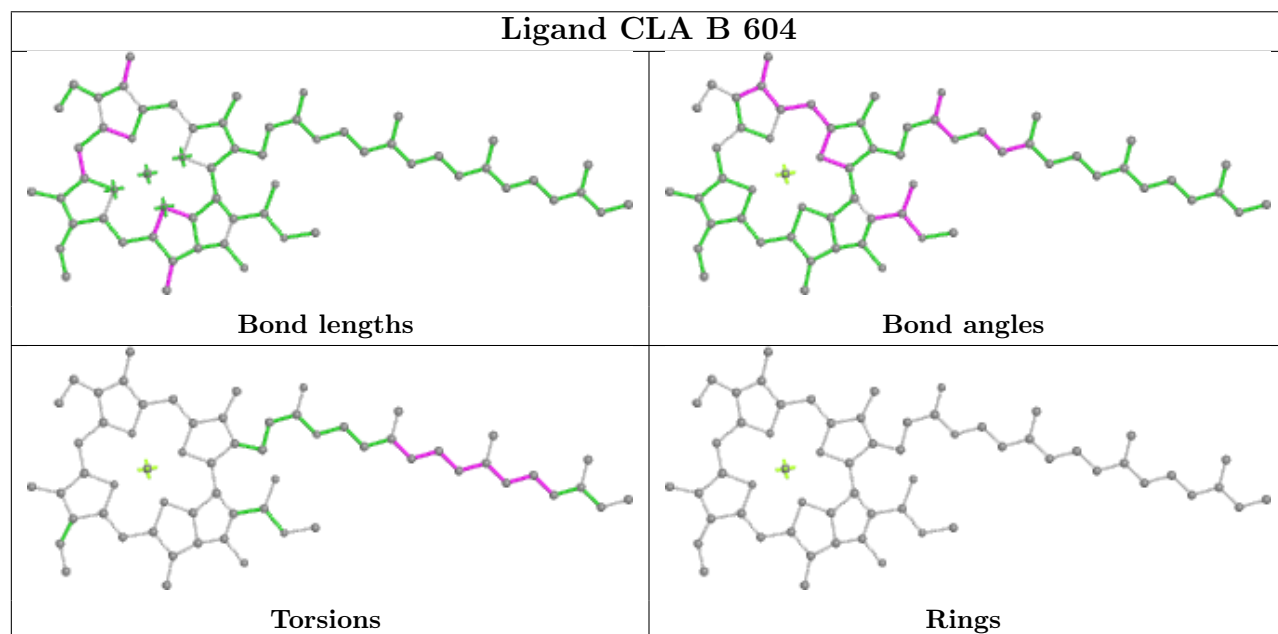
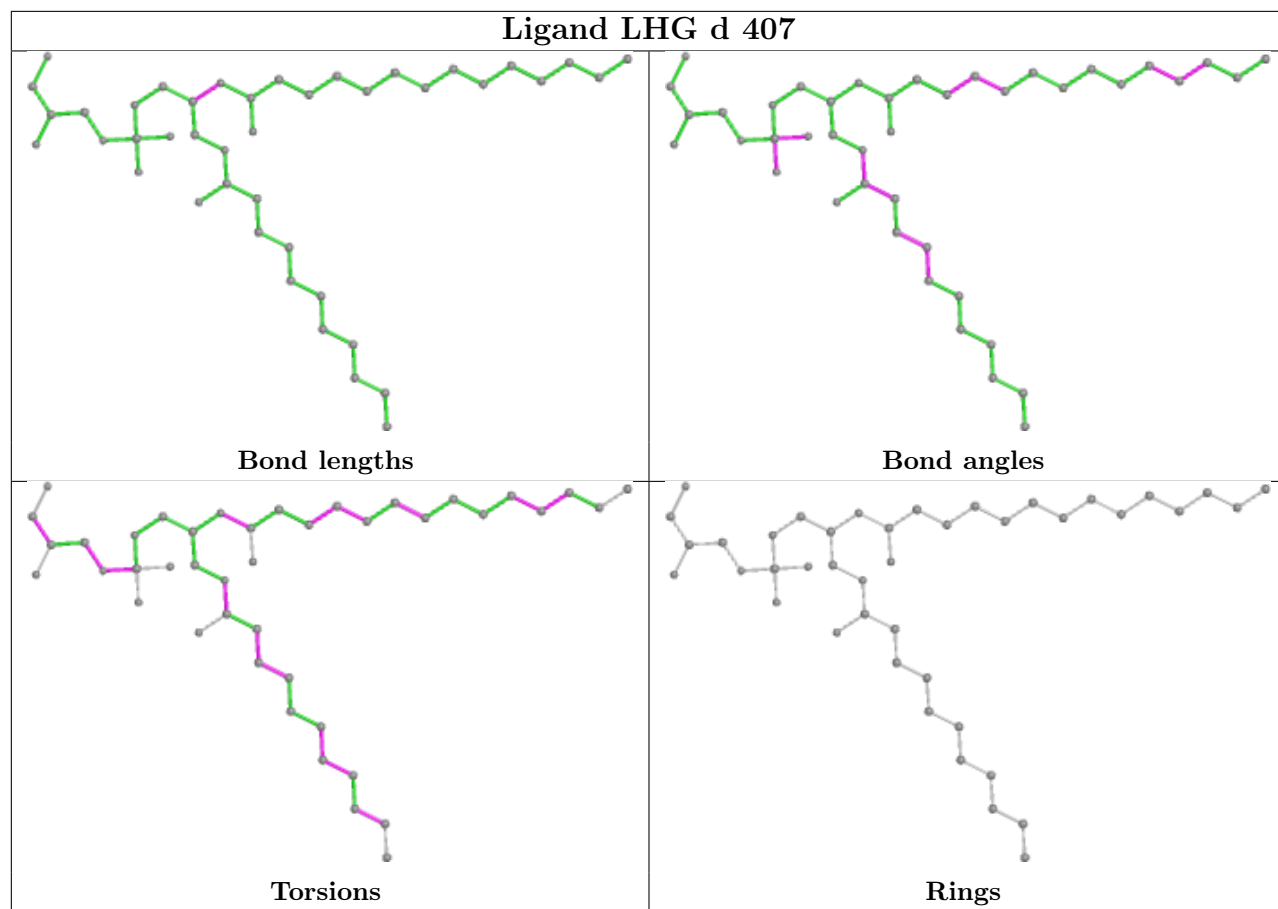
Rings



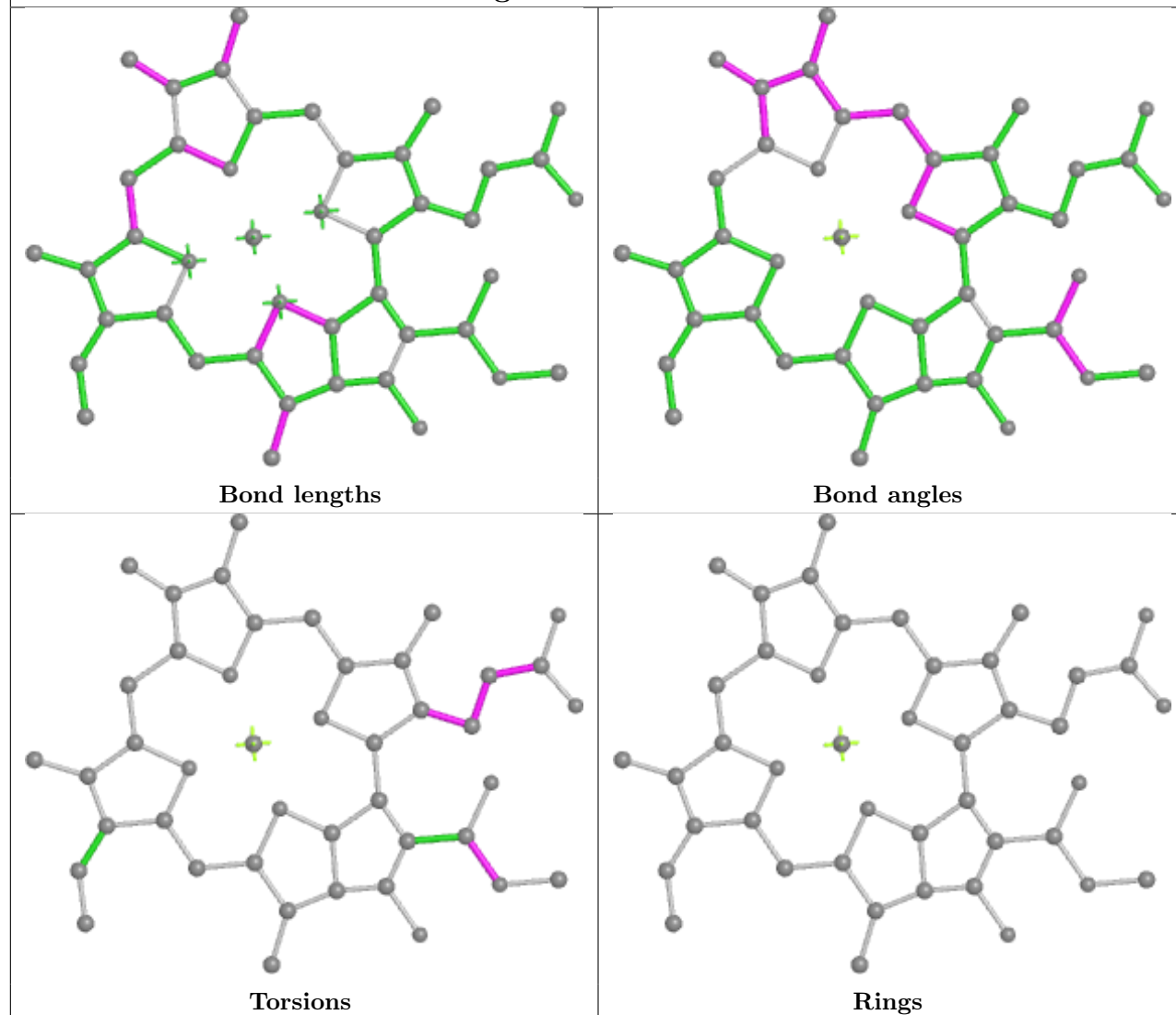
**Ligand CLA B 610****Ligand CLA 4 306**

## Ligand CLA 8 309

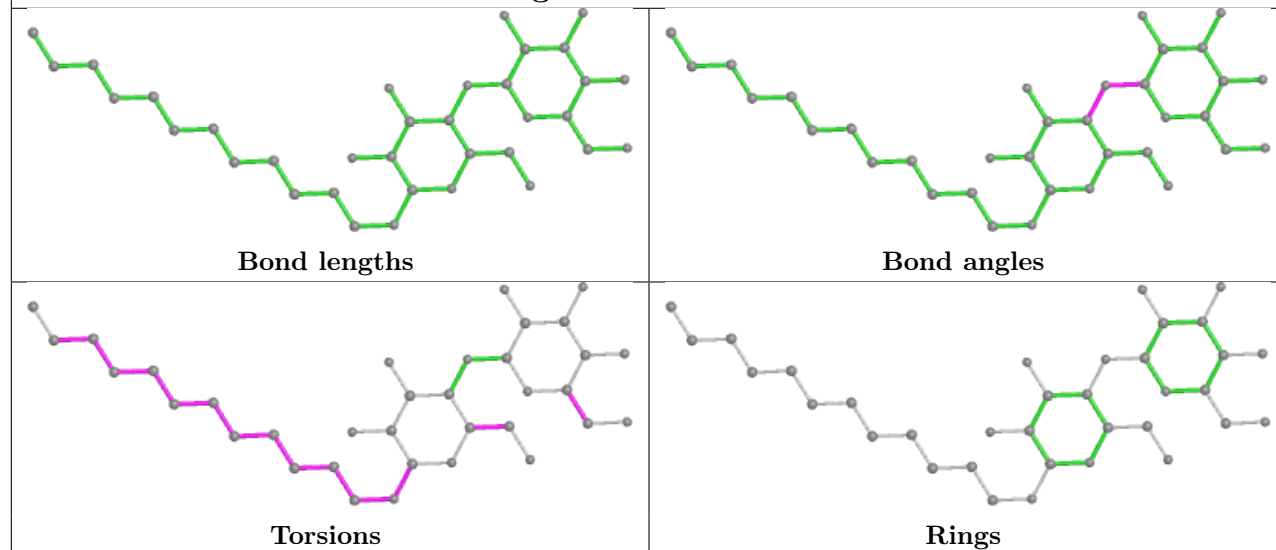




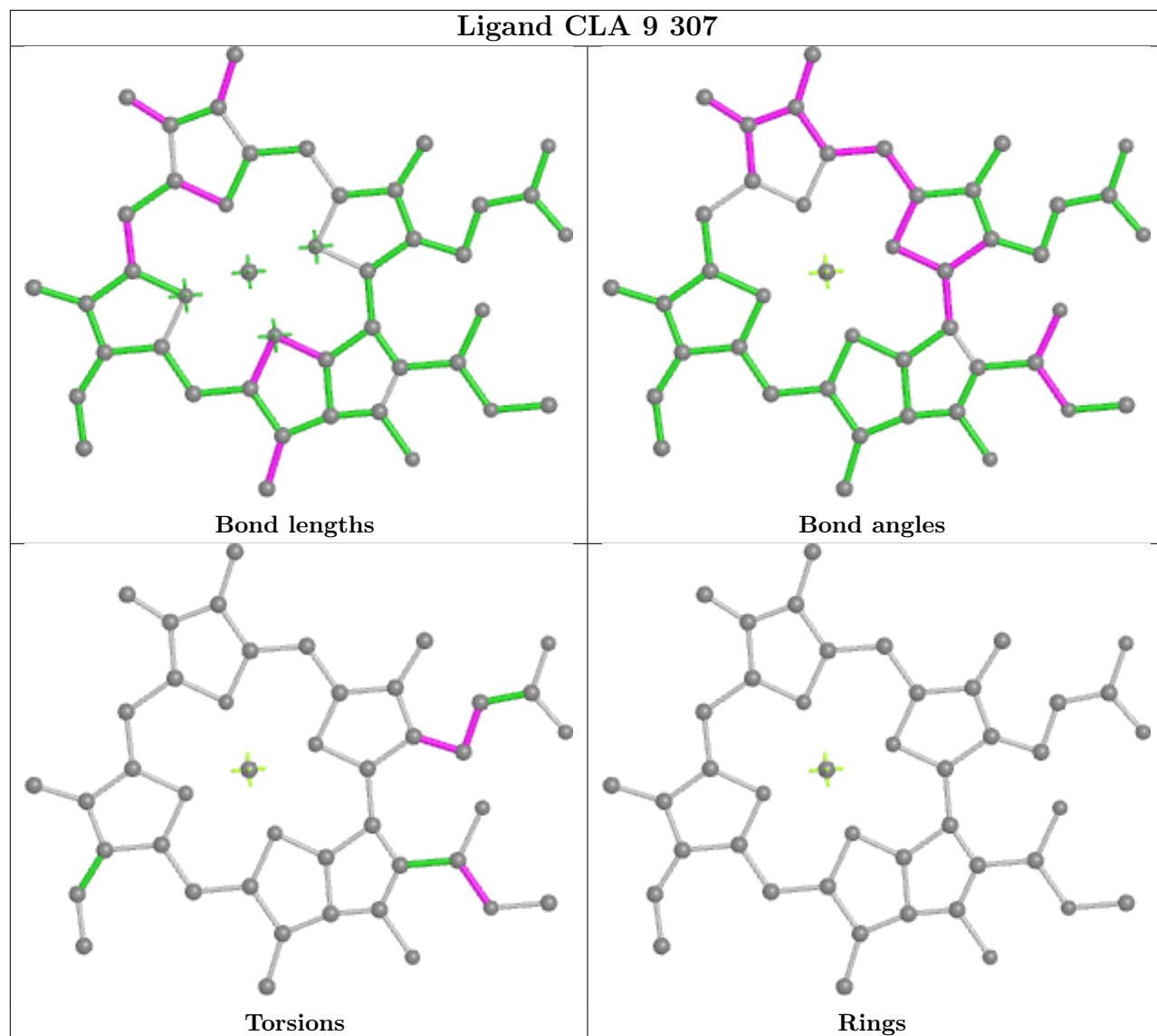
## Ligand CLA 2 307



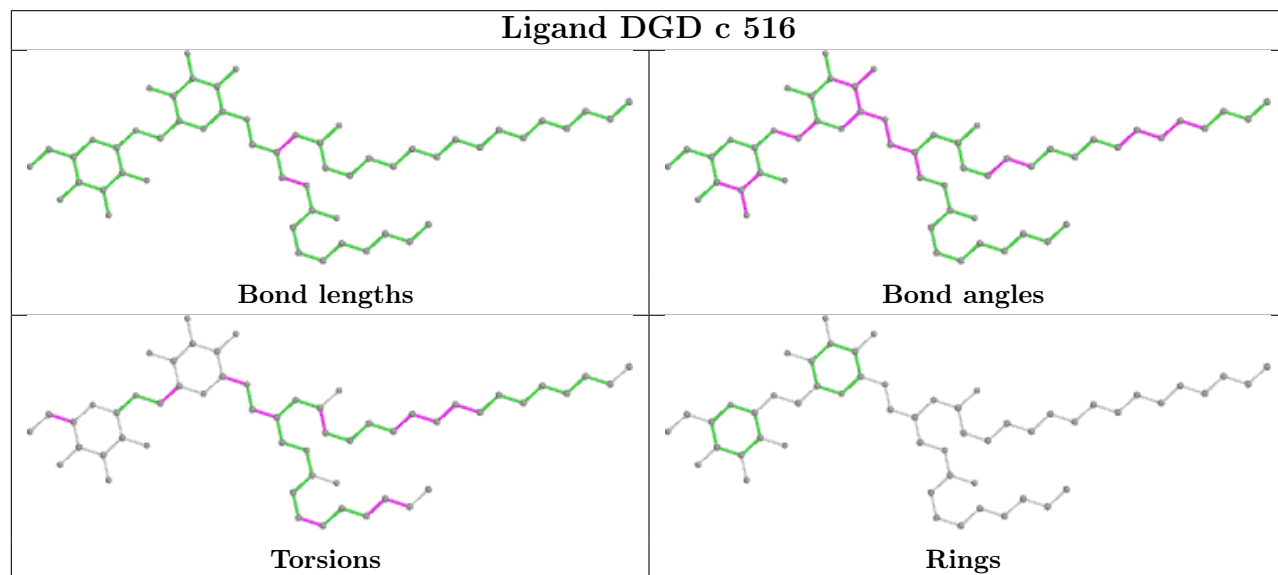
## Ligand LMU 3 301

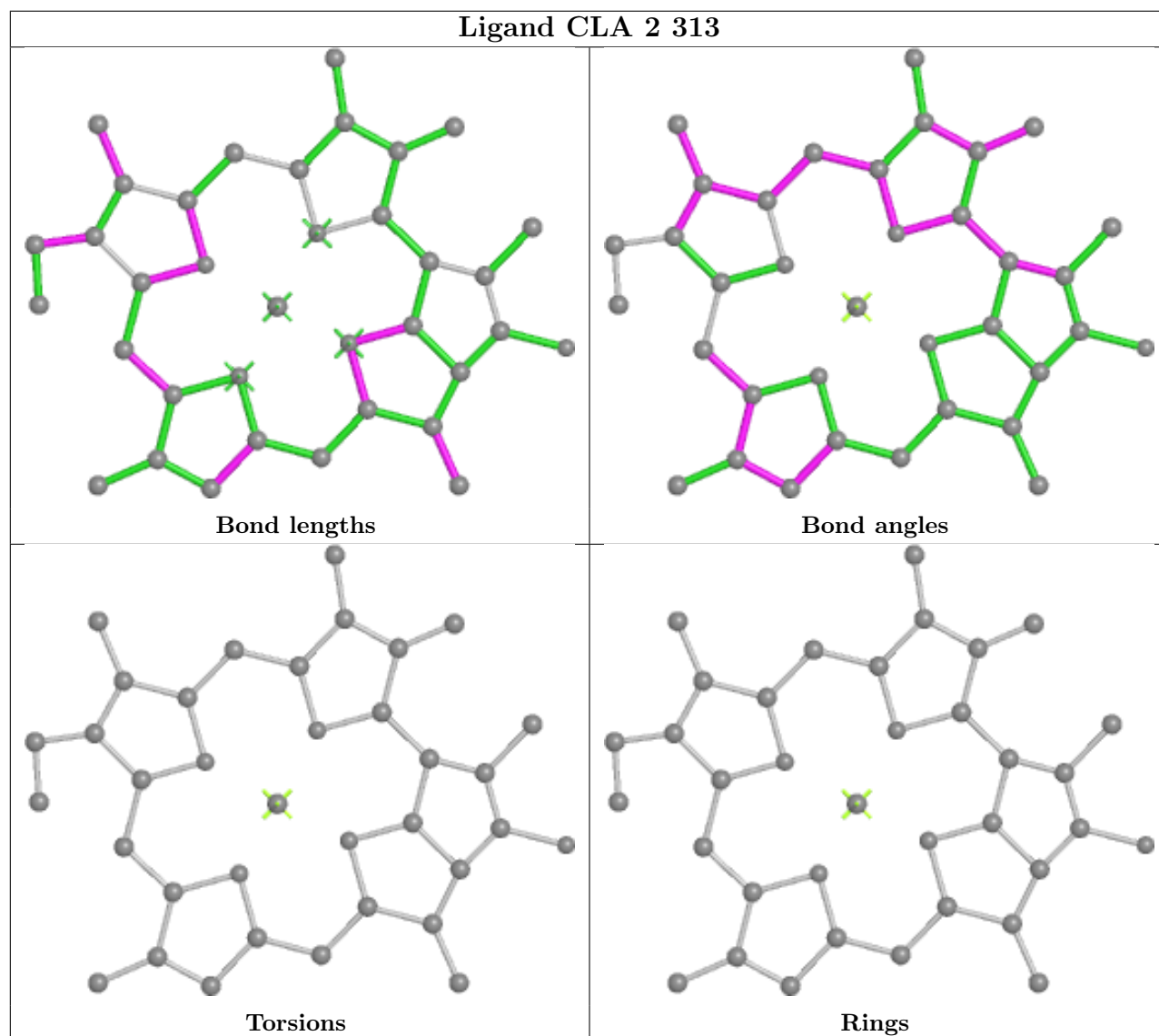
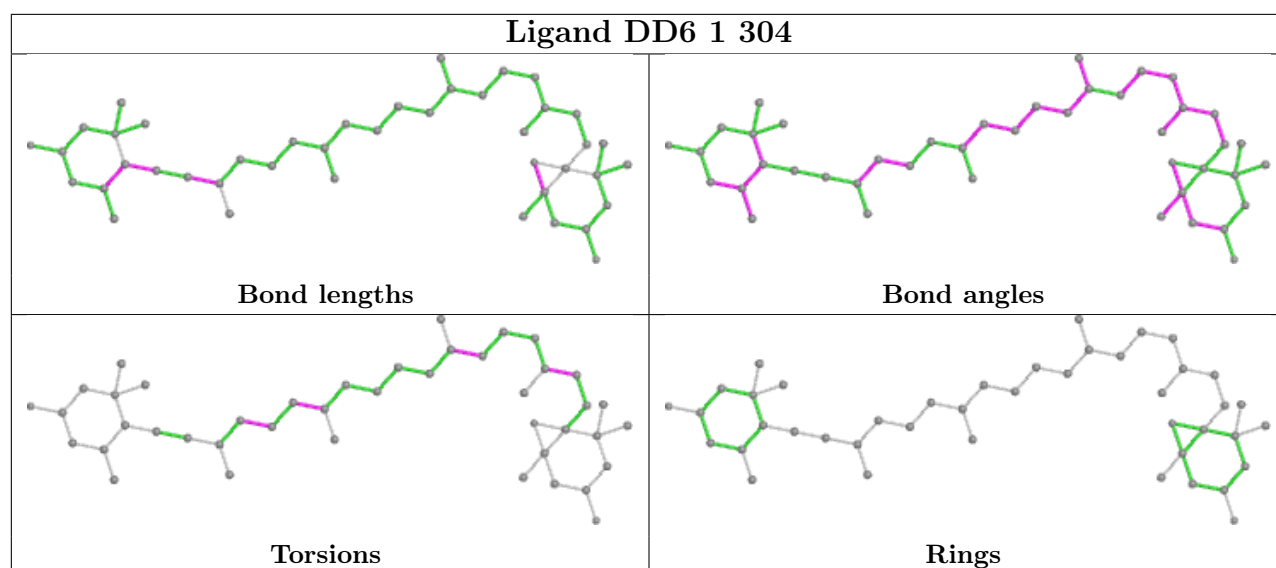


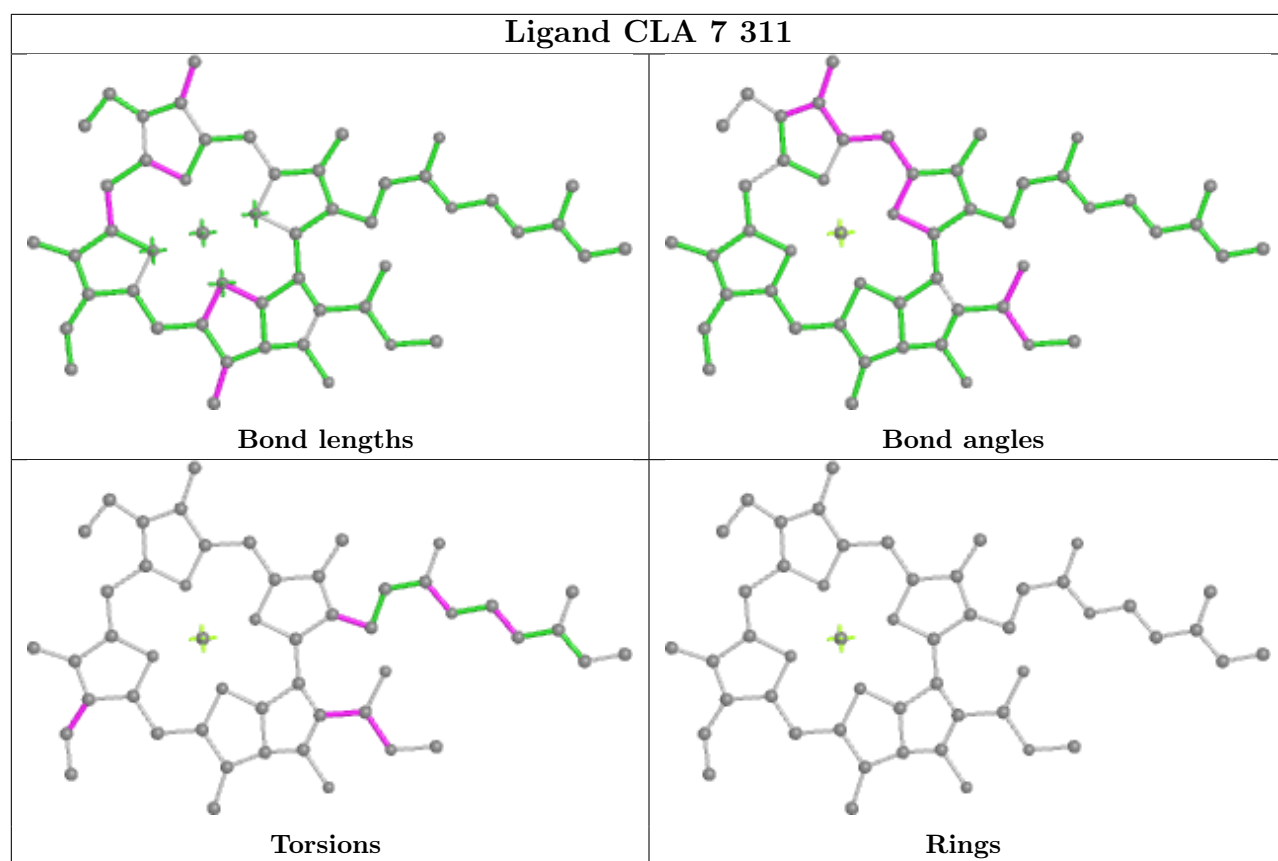
## Ligand CLA 9 307



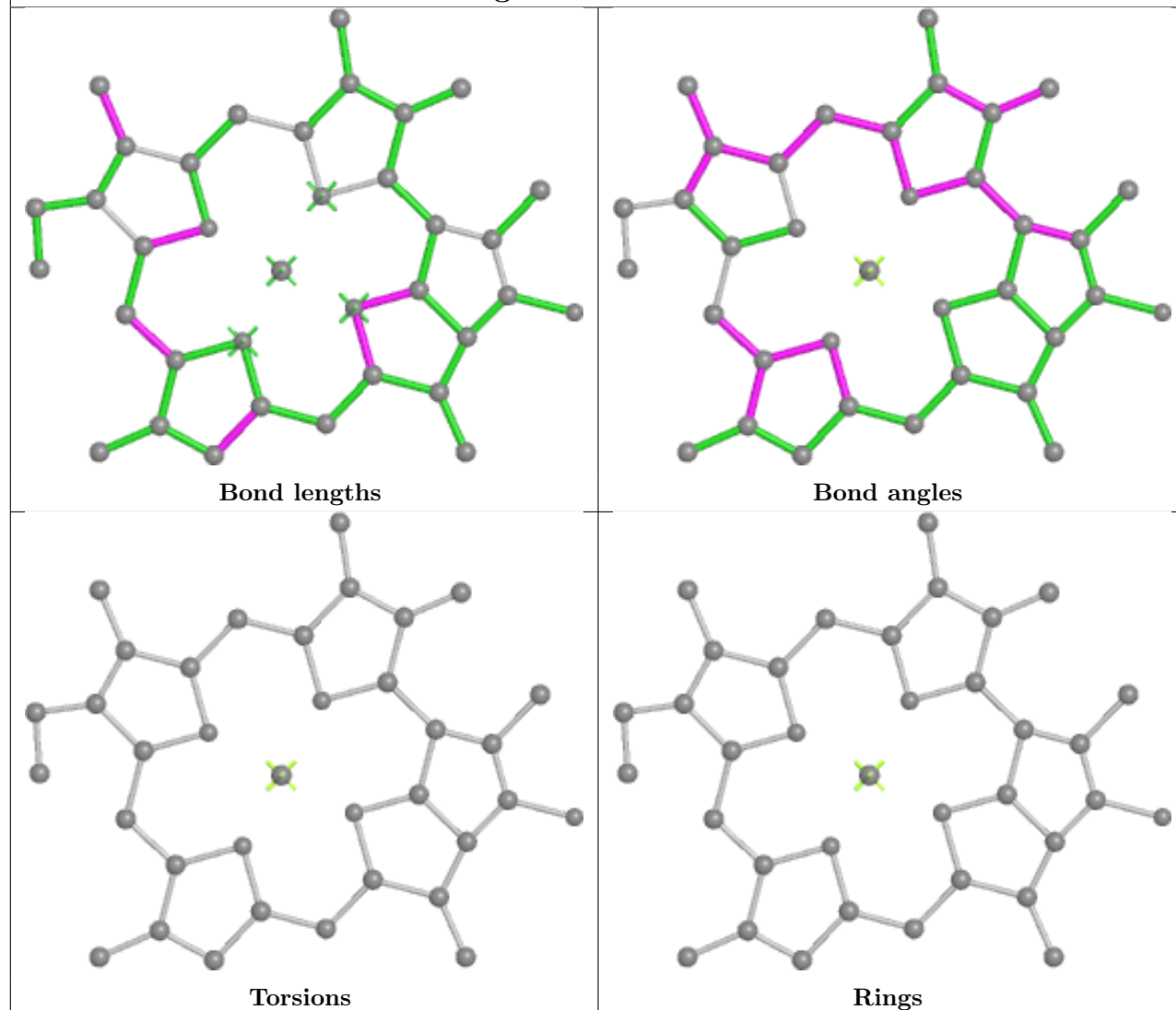
## Ligand DGD c 516



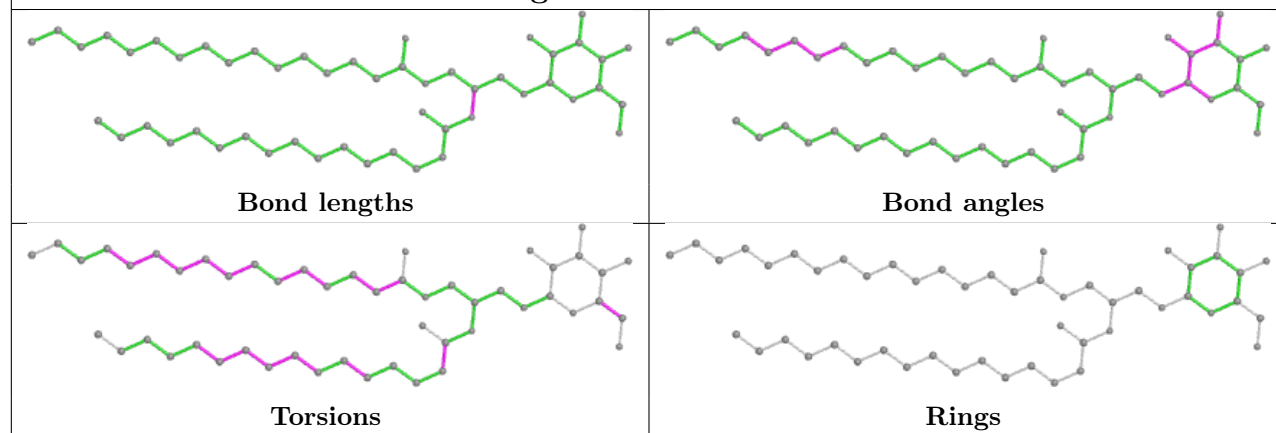




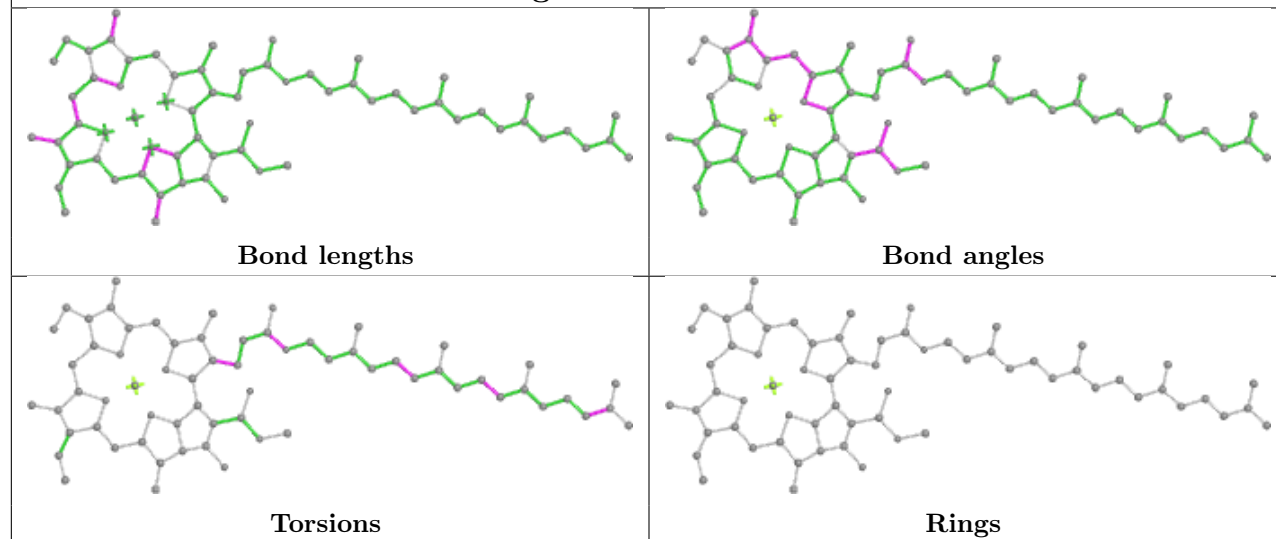
## Ligand CLA 9 313



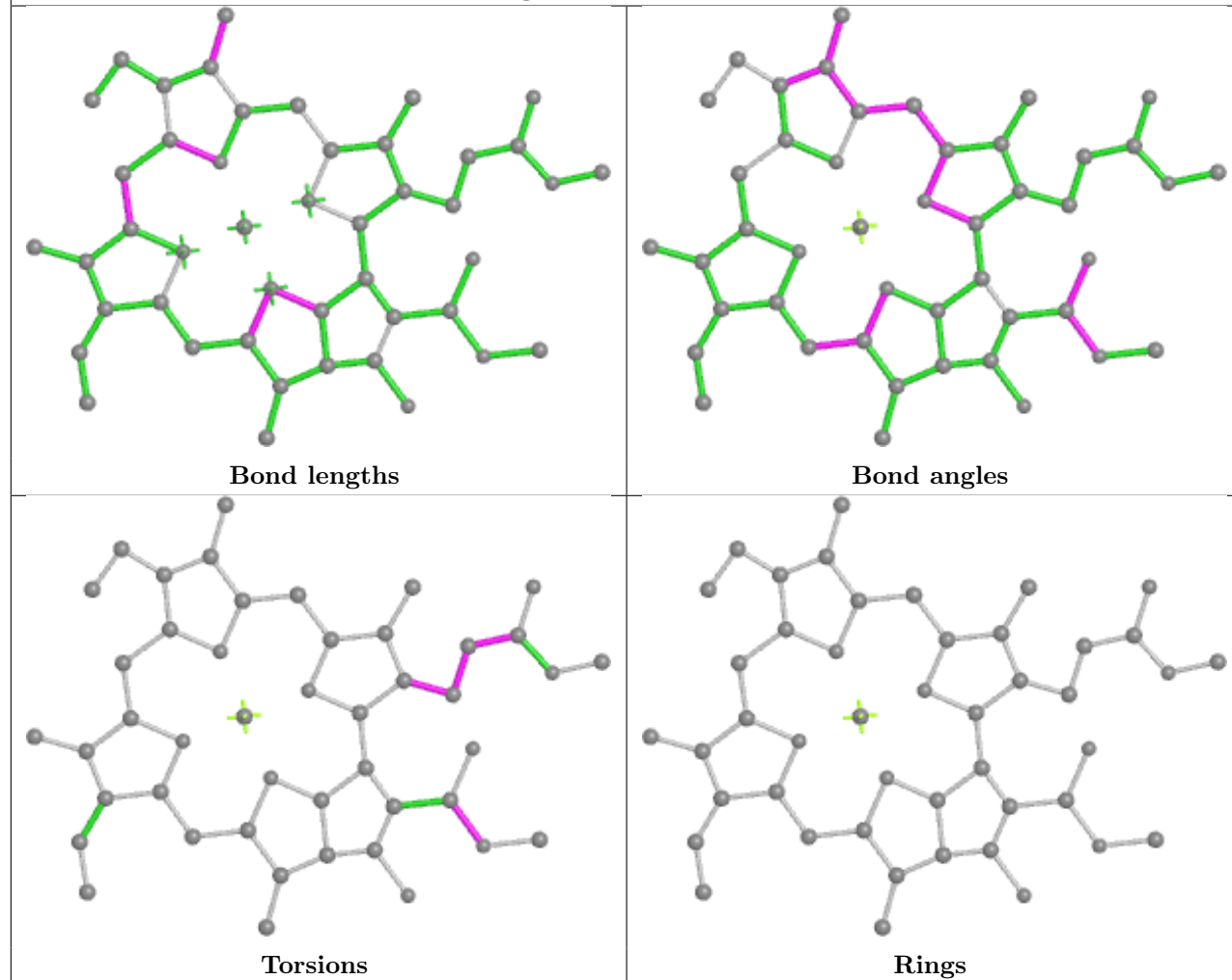
## Ligand LMG b 621

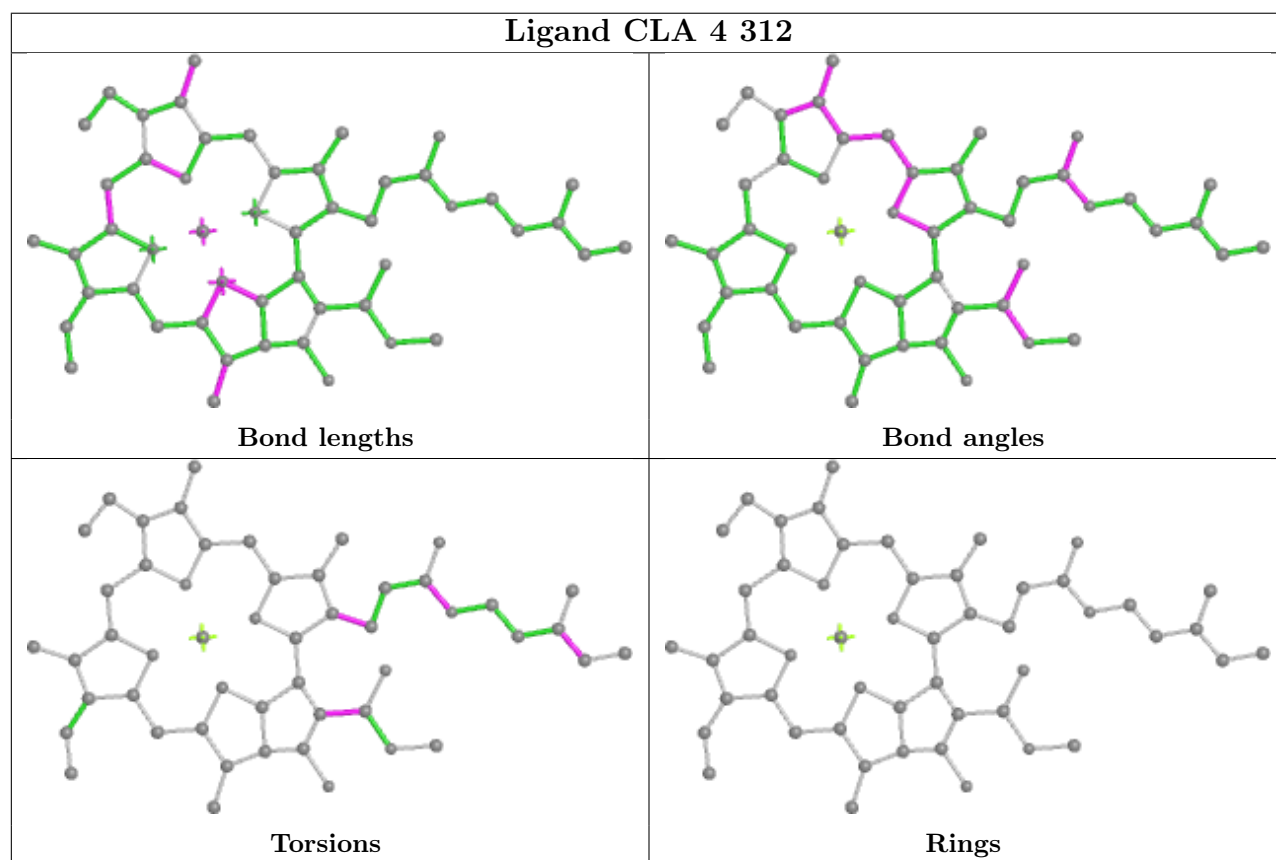
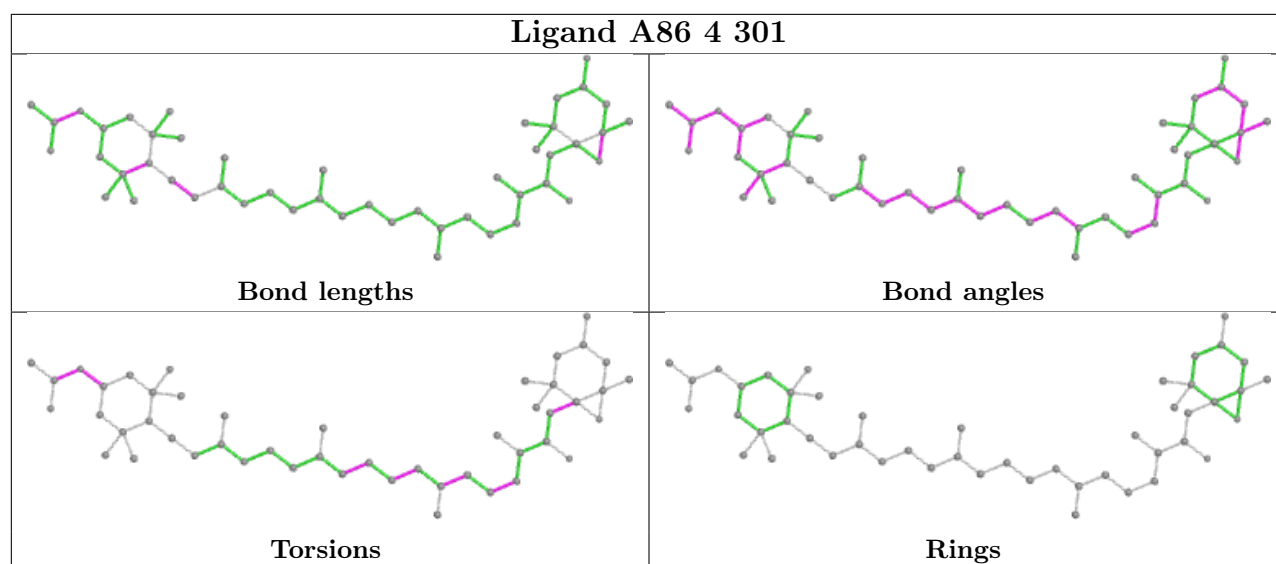


## Ligand CLA C 508

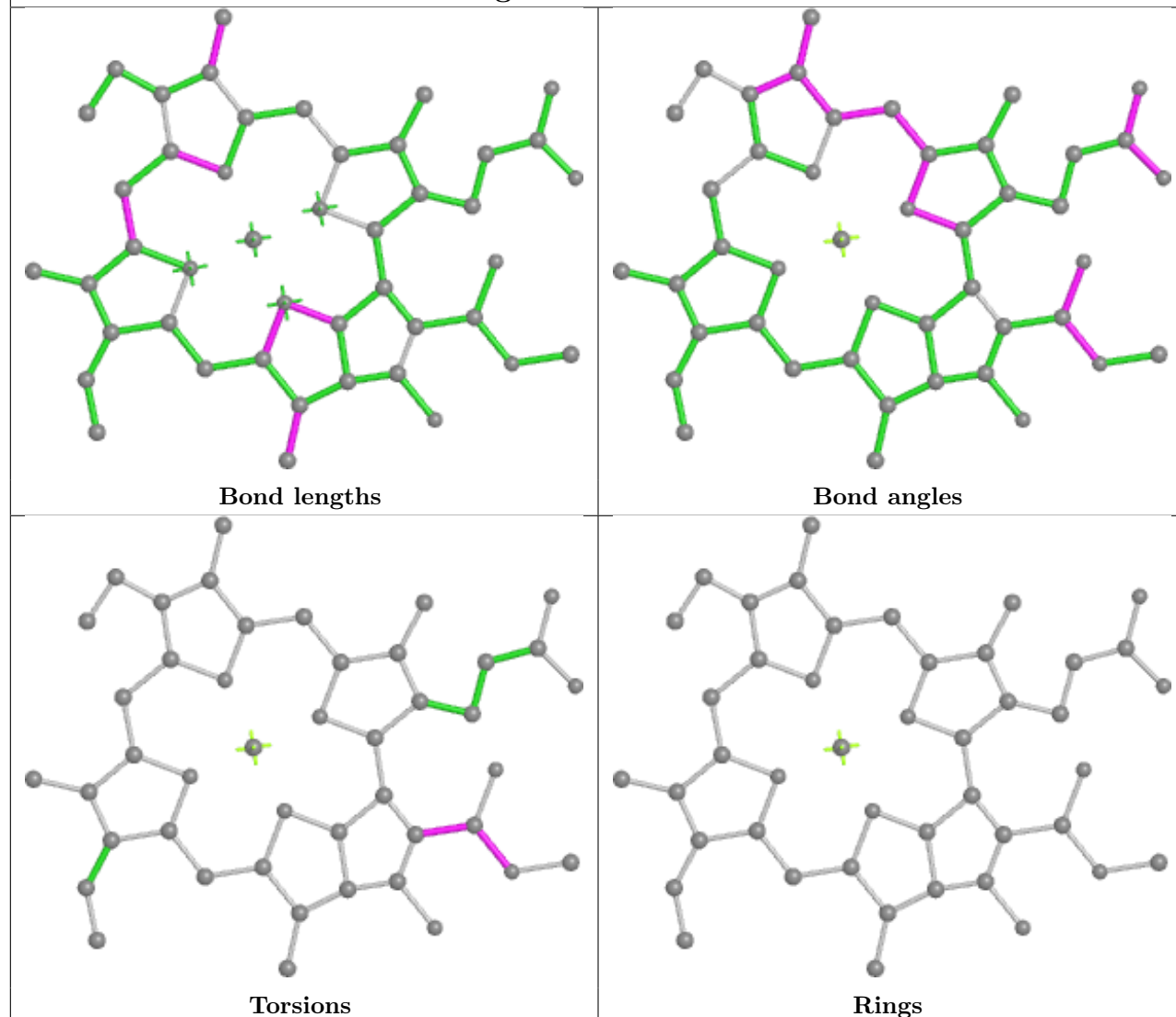


## Ligand CLA 5 312

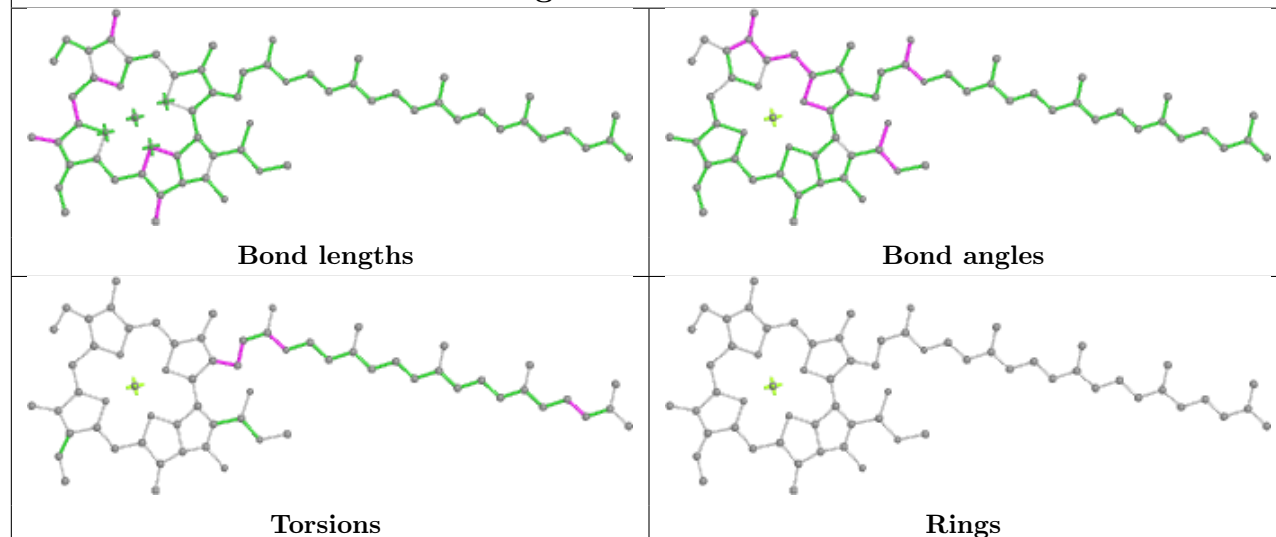




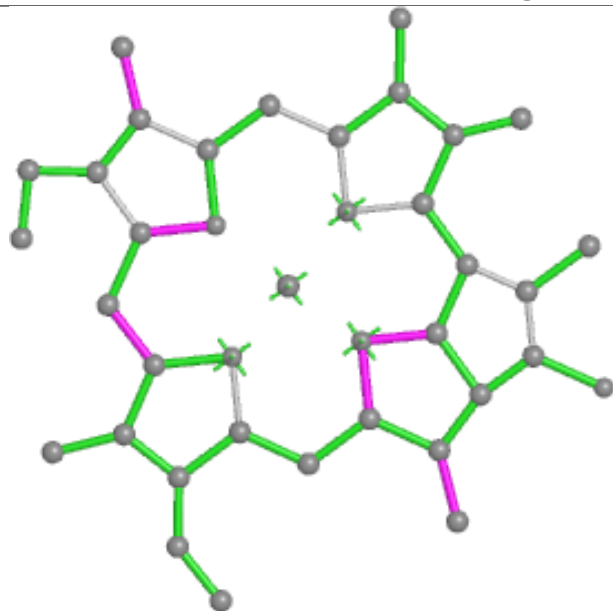
## Ligand CLA c 506



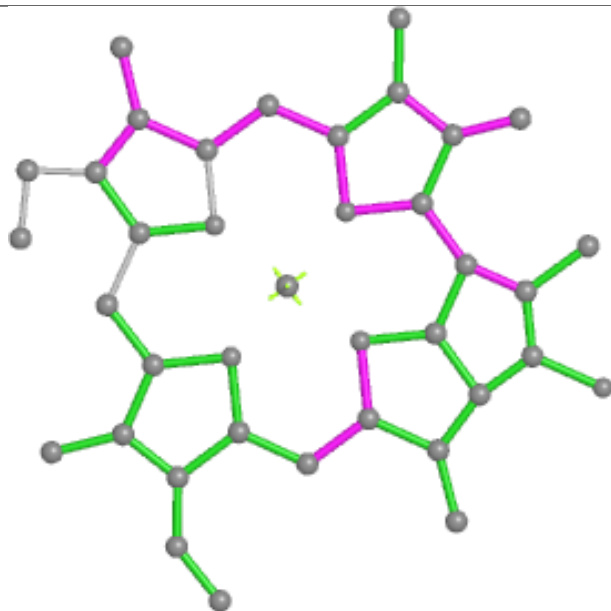
## Ligand CLA b 609



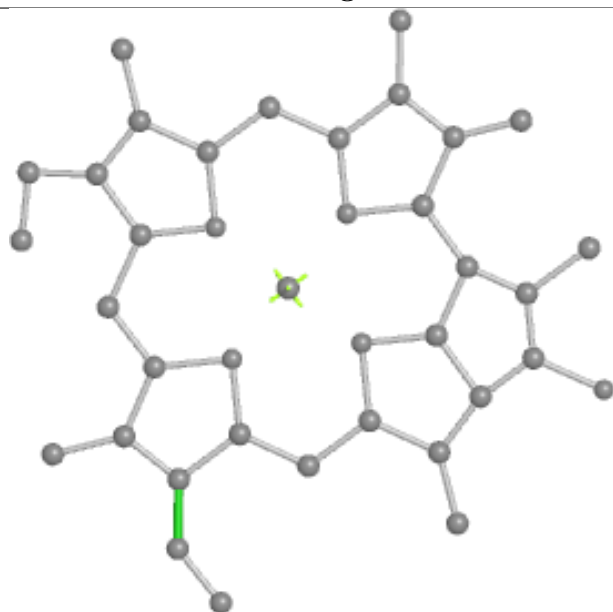
## Ligand CLA 9 316



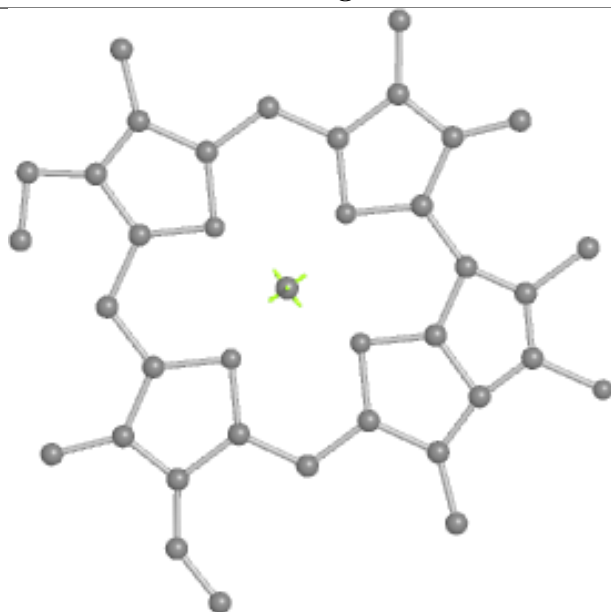
Bond lengths



Bond angles

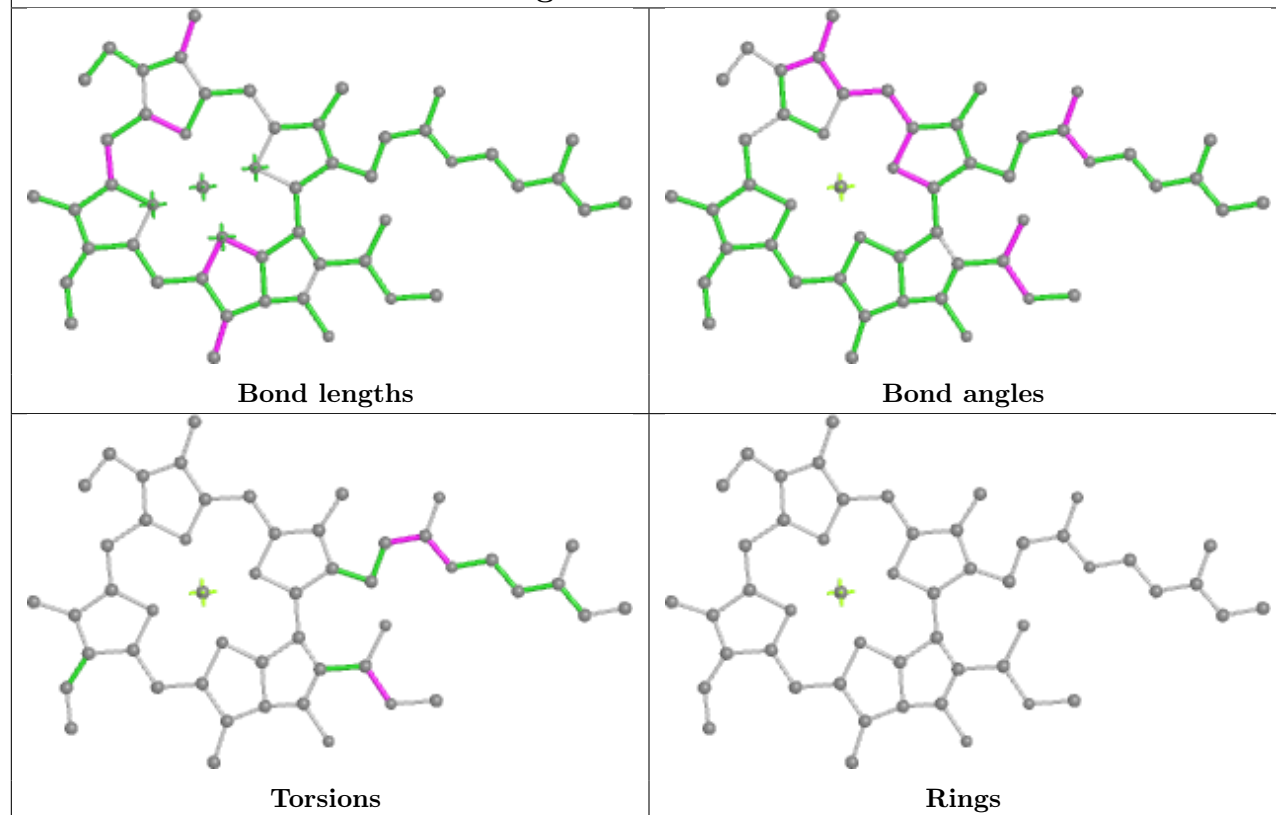


Torsions

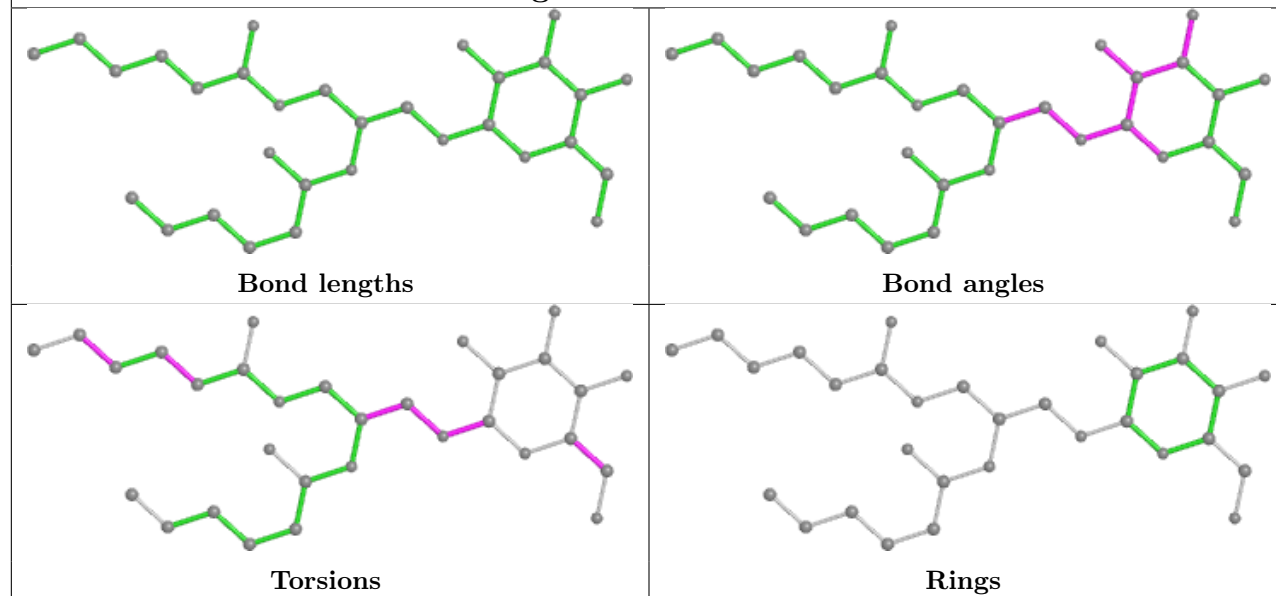


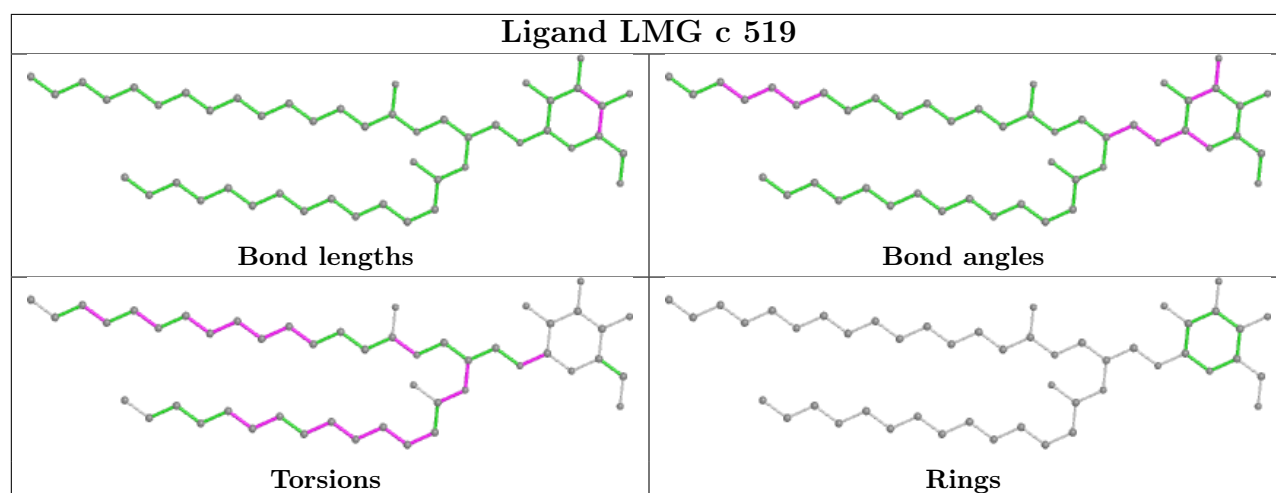
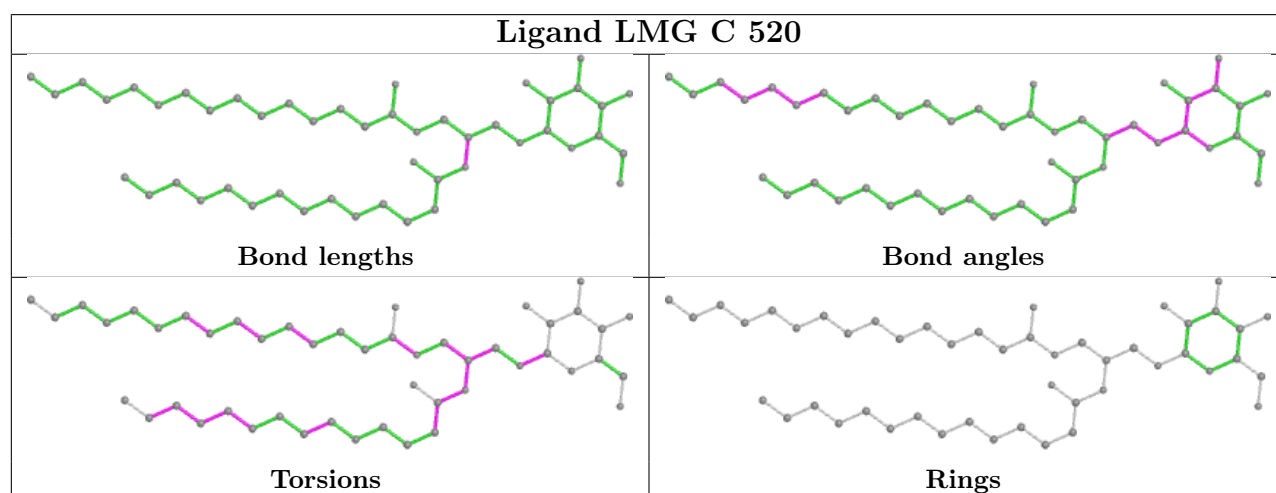
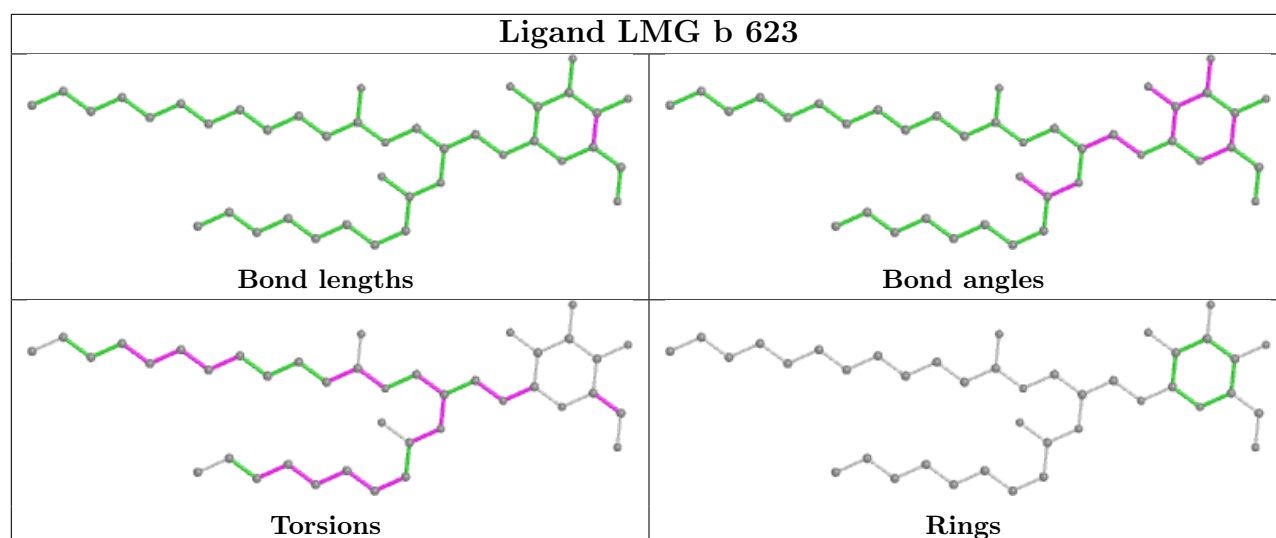
Rings

## Ligand CLA 3 309

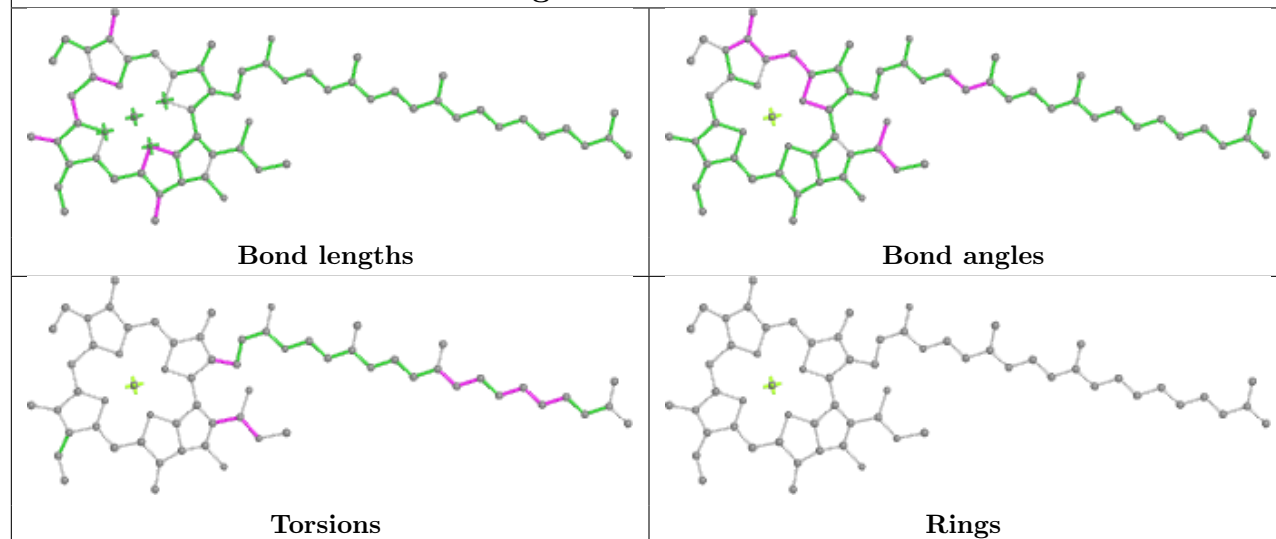


## Ligand LMG 3 316

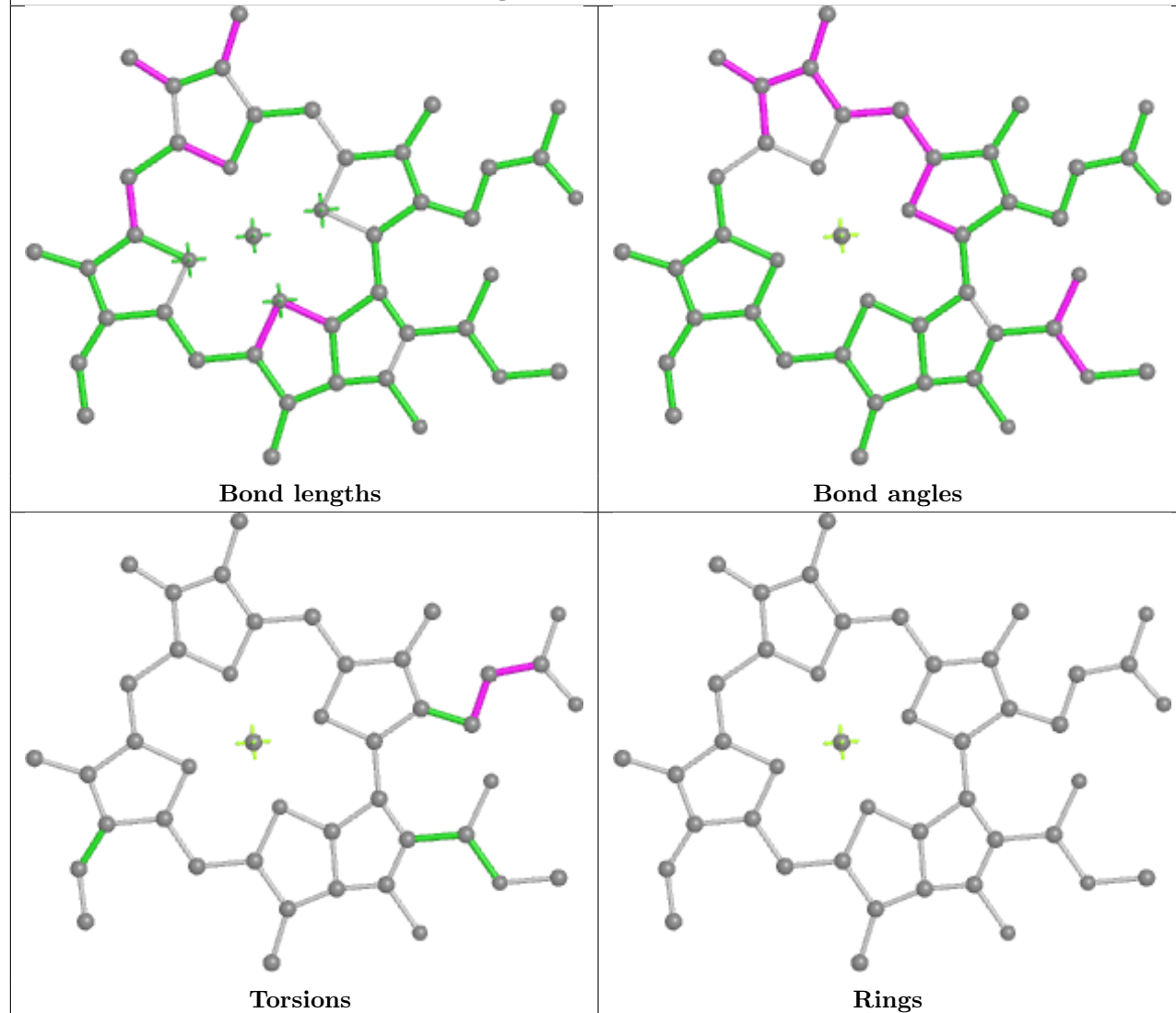




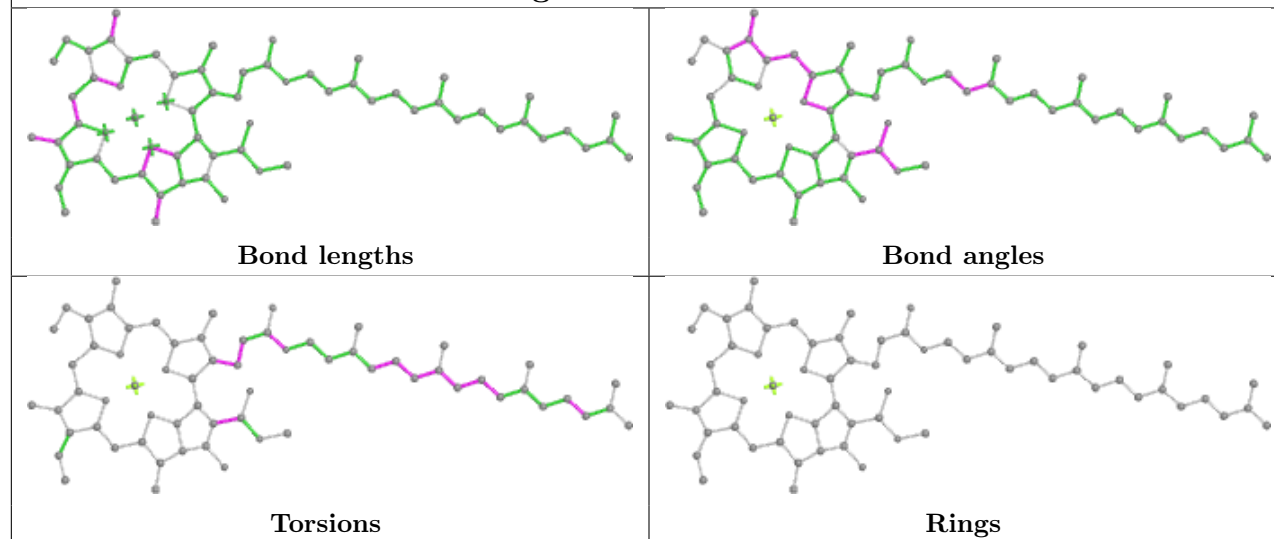
## Ligand CLA B 614



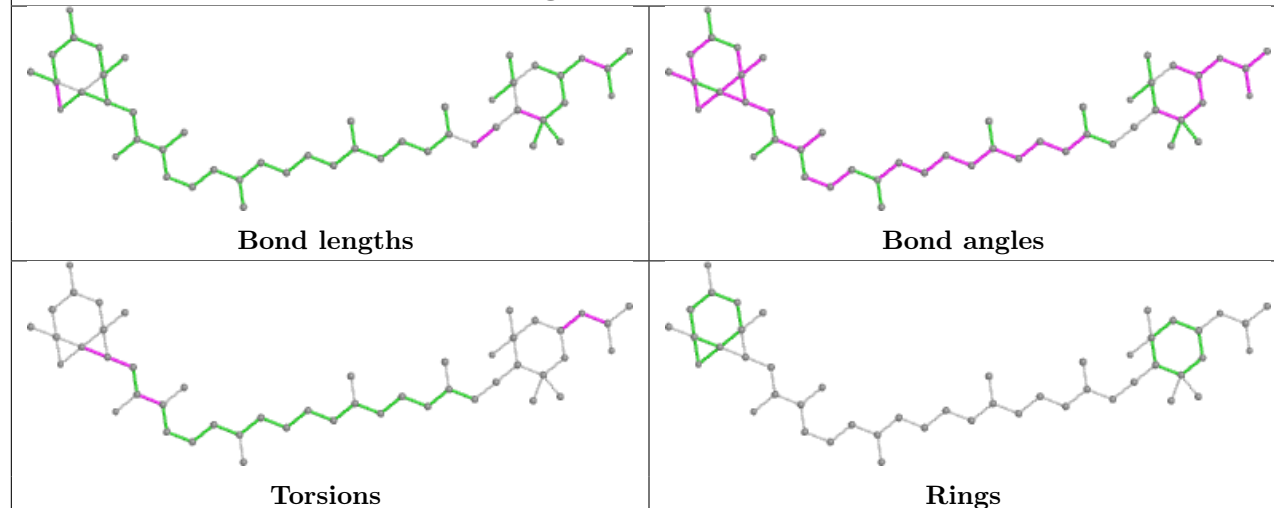
## Ligand CLA 1 307



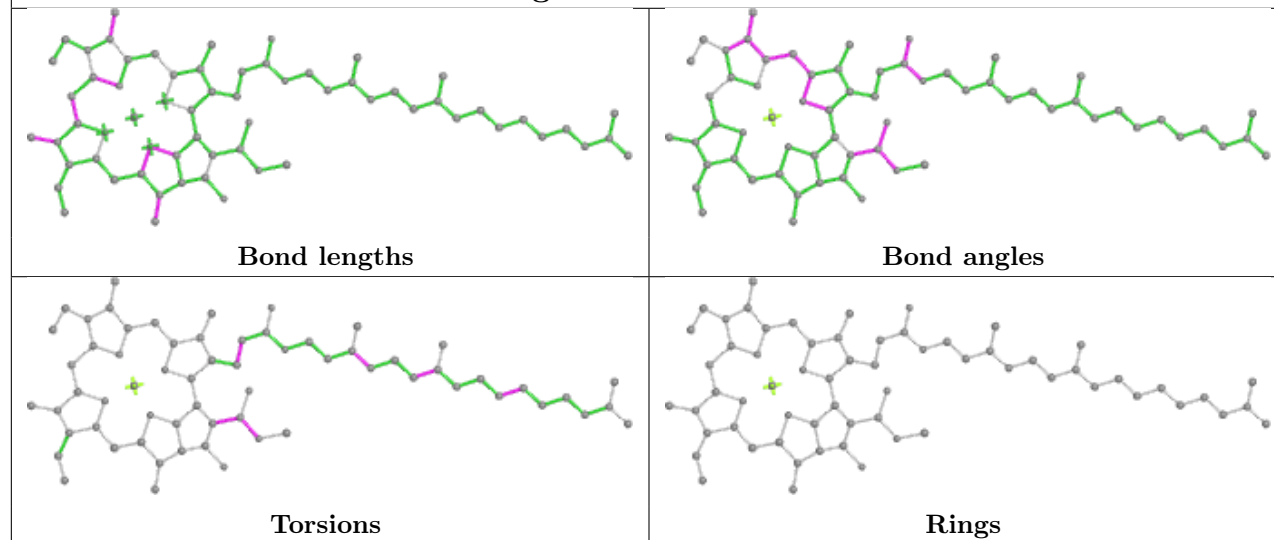
## Ligand CLA C 503

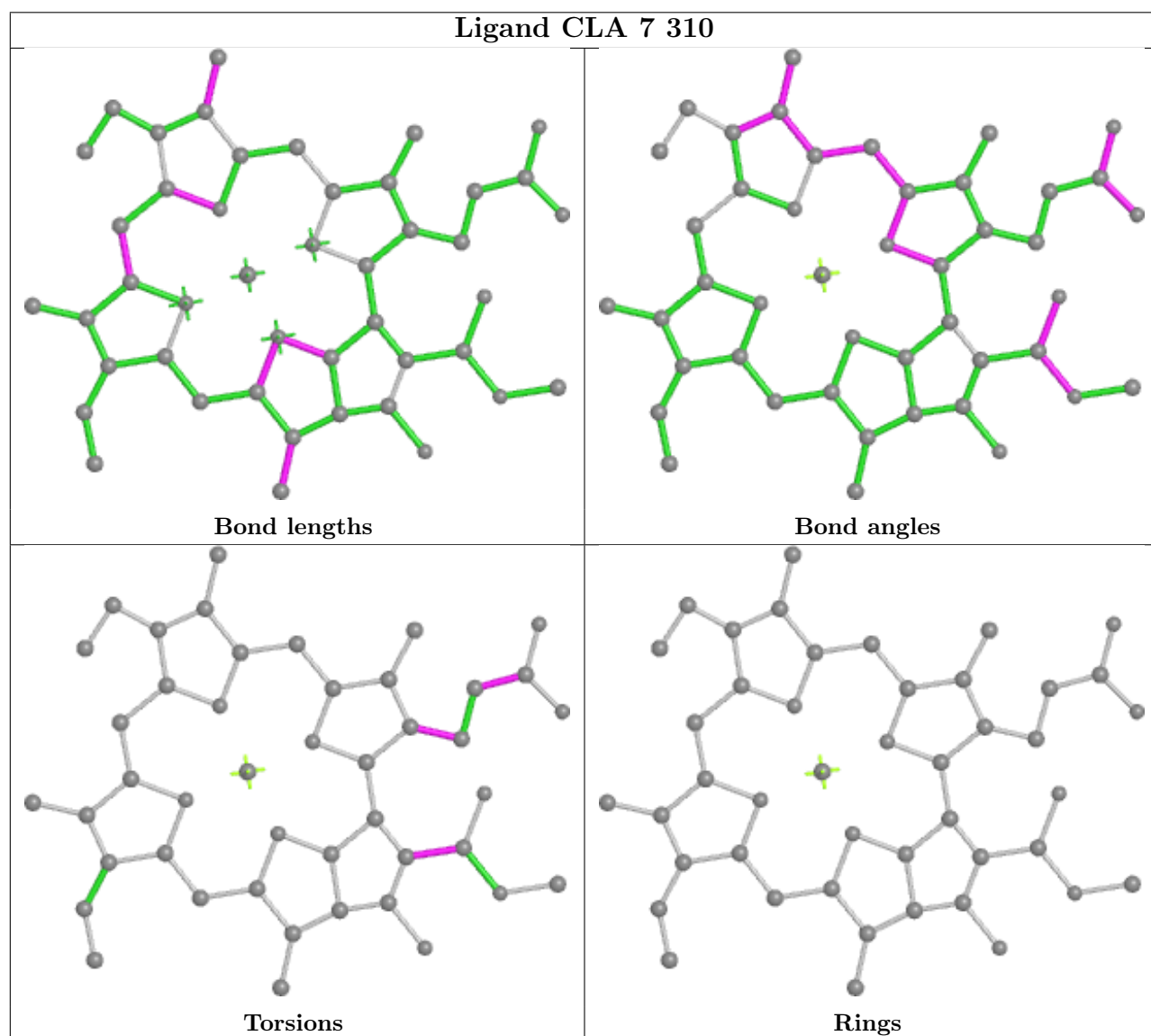
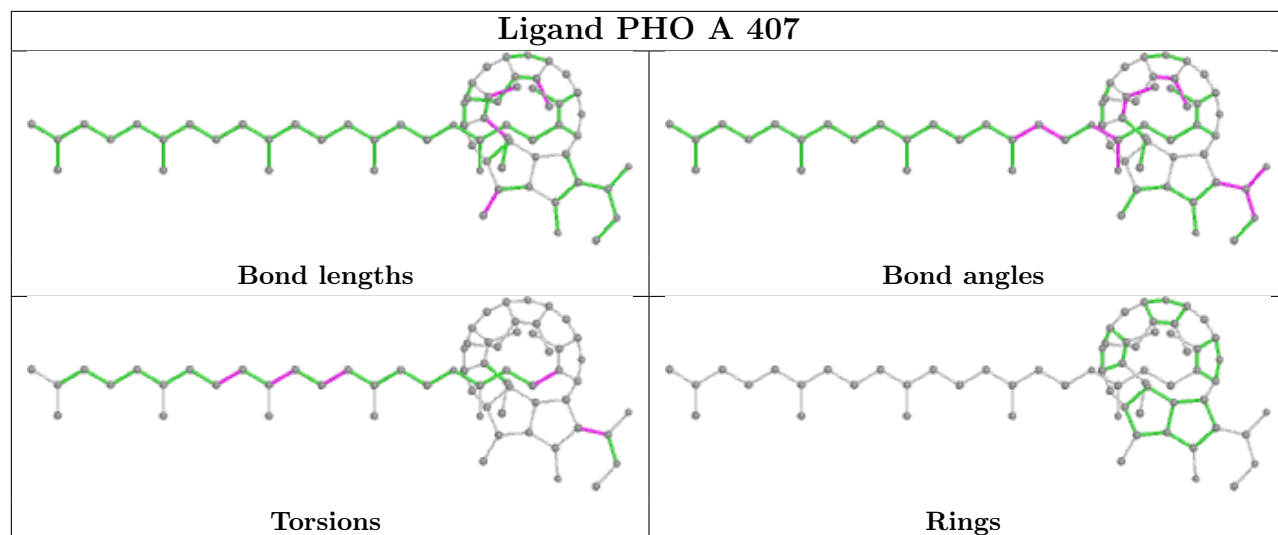


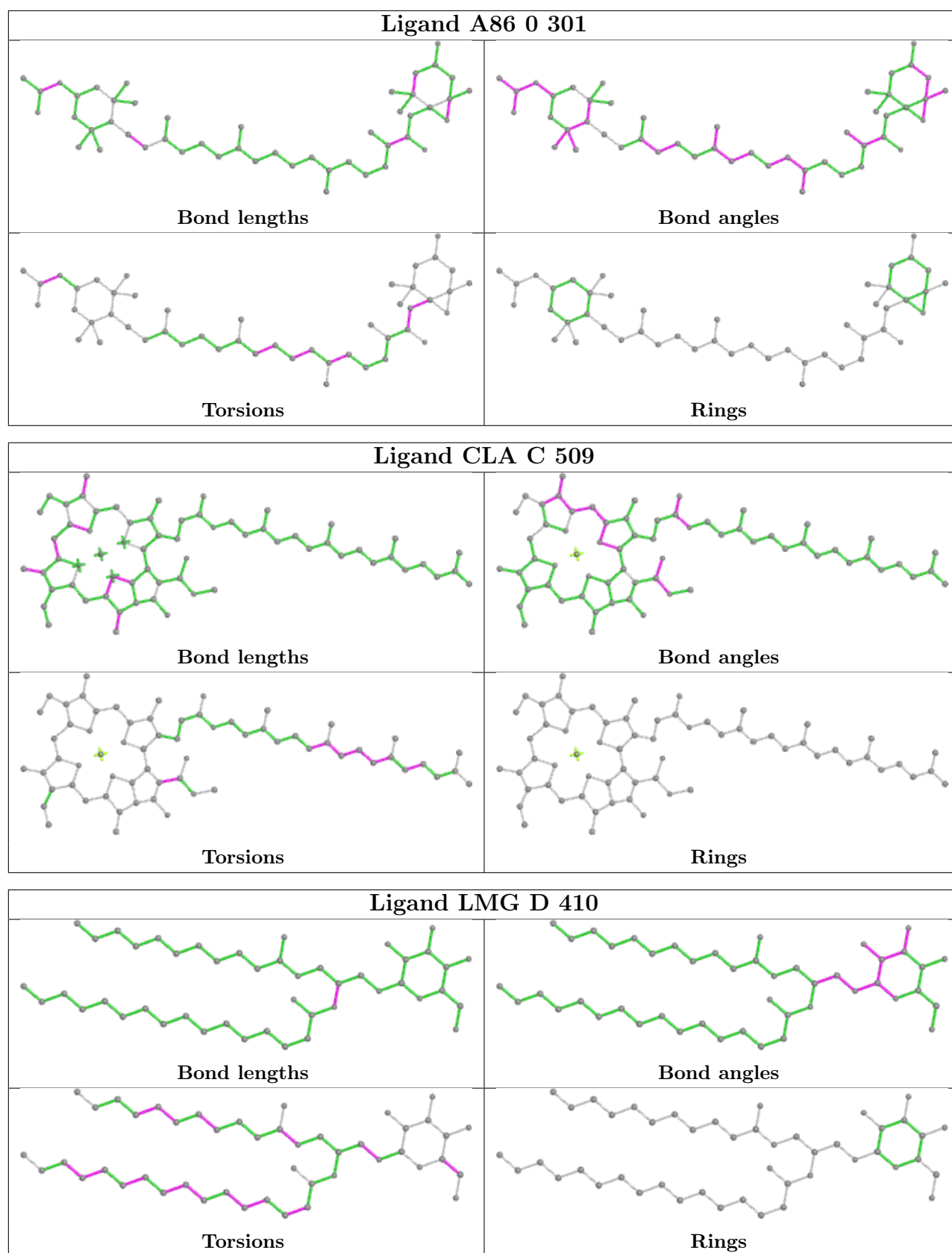
## Ligand A86 6 303

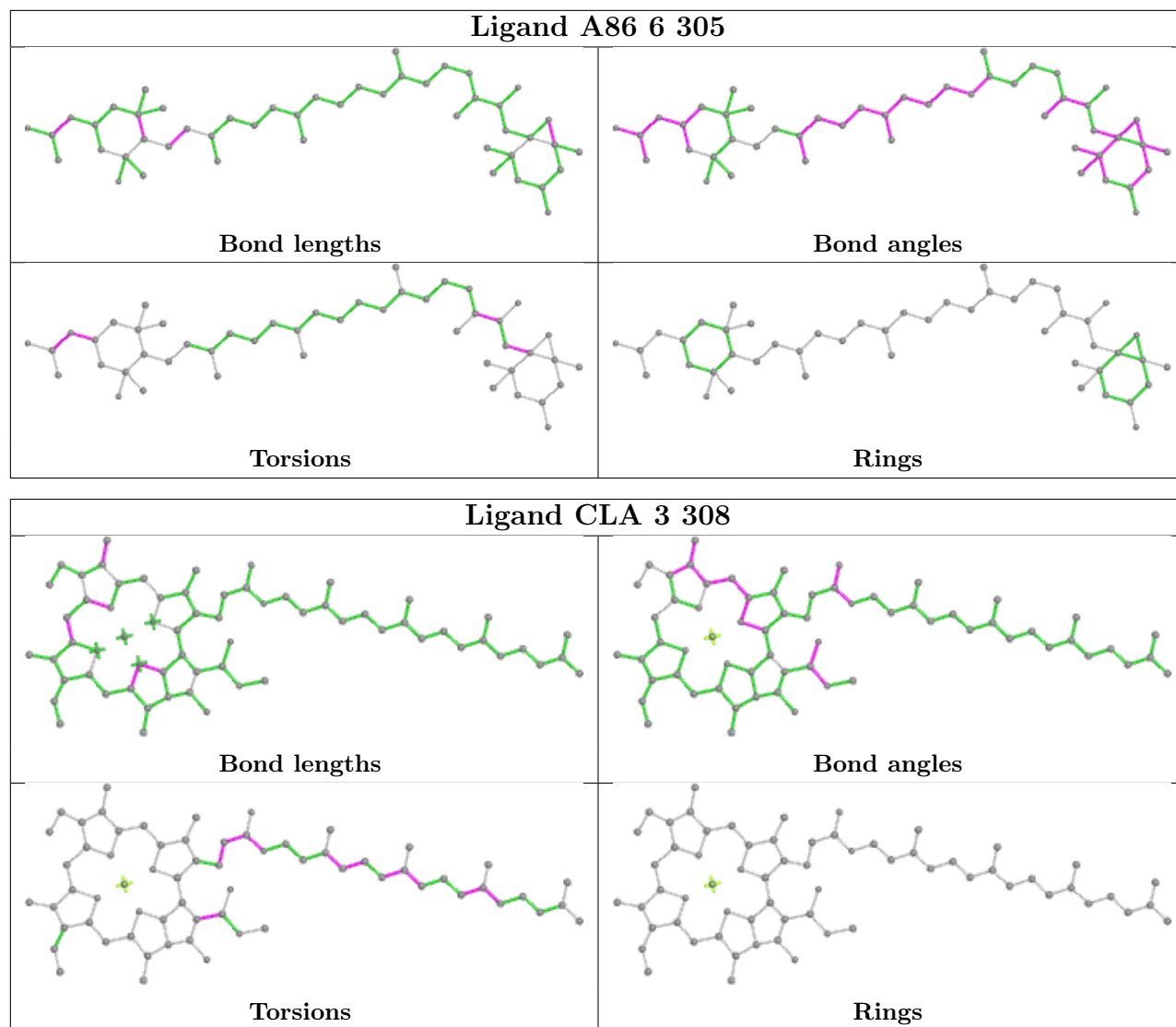


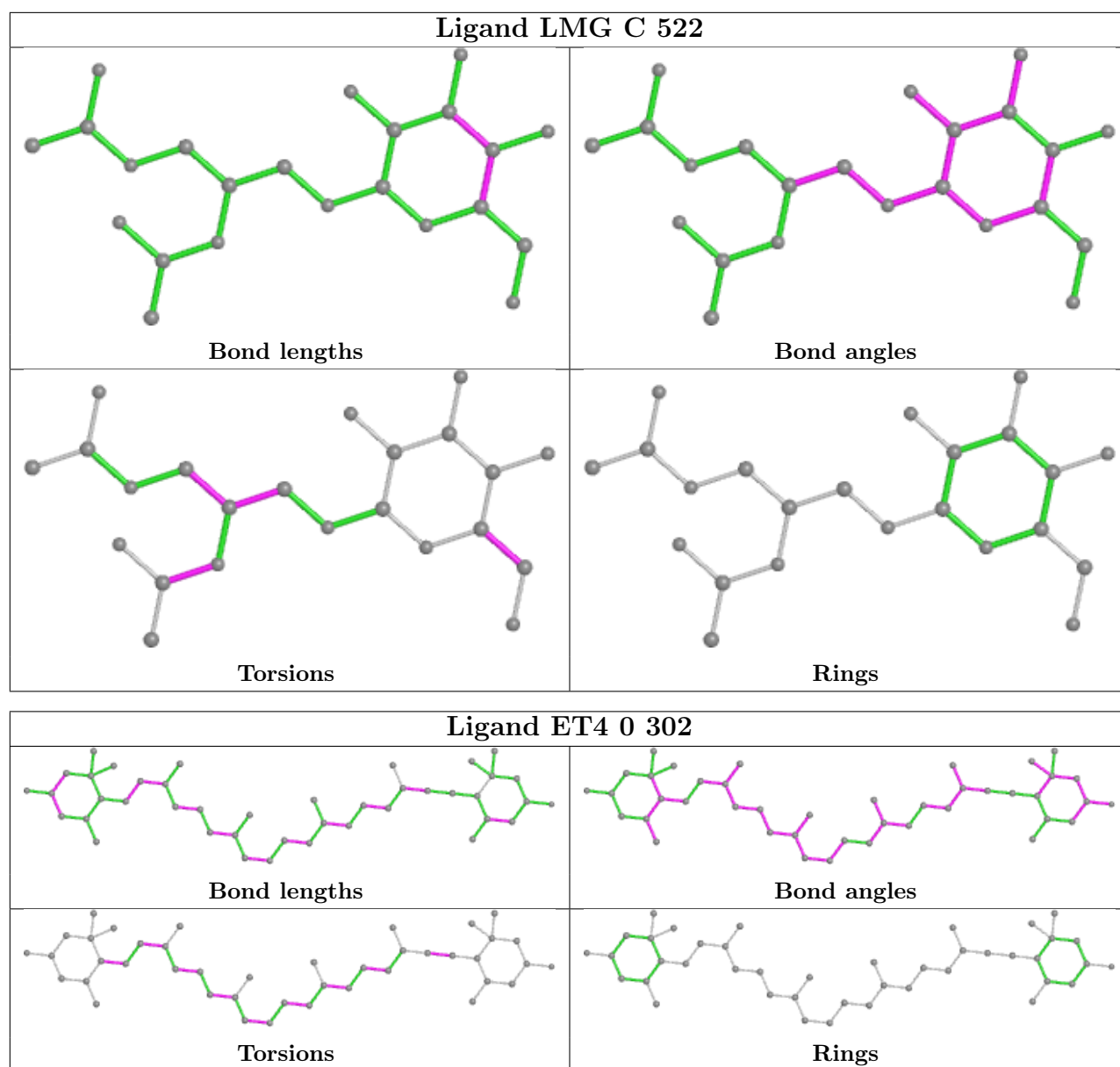
## Ligand CLA B 603



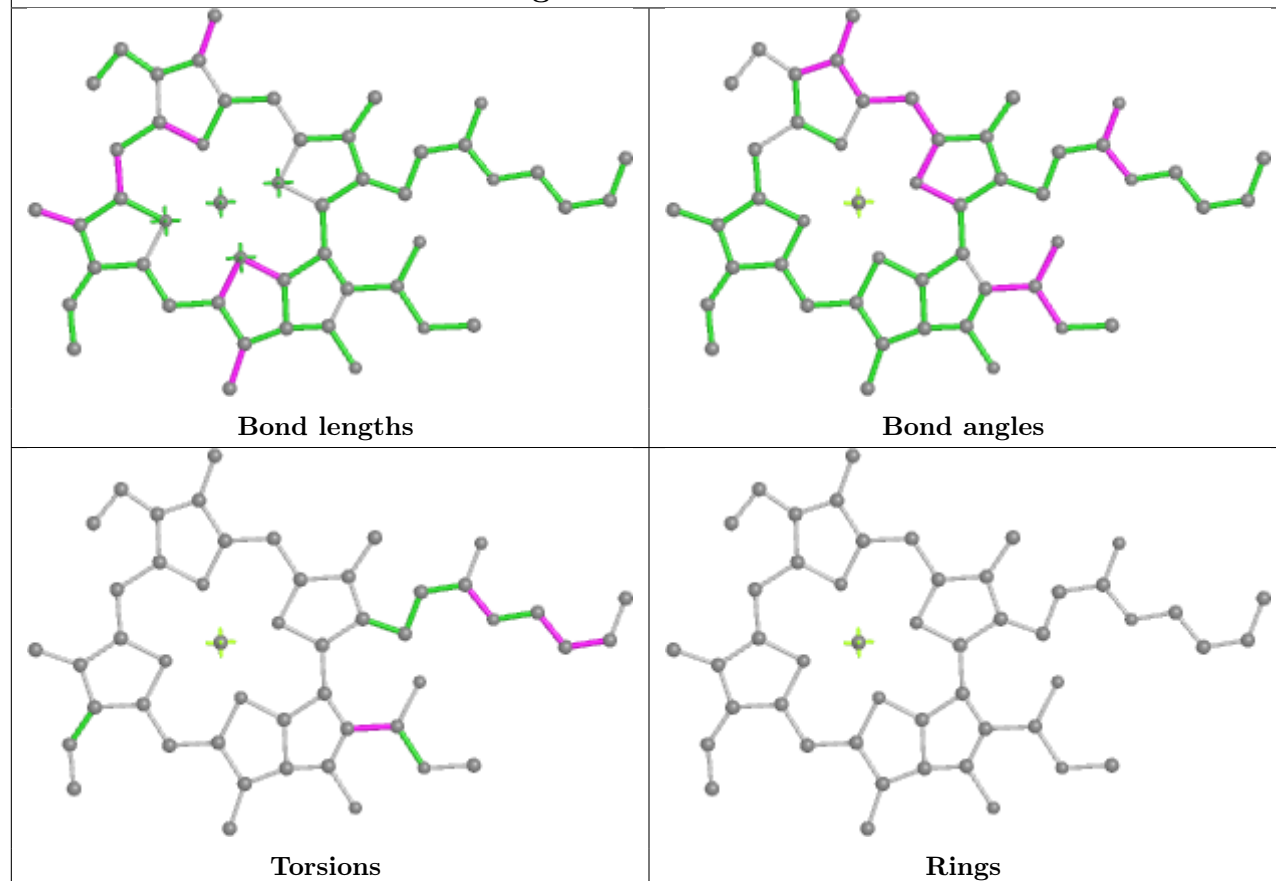




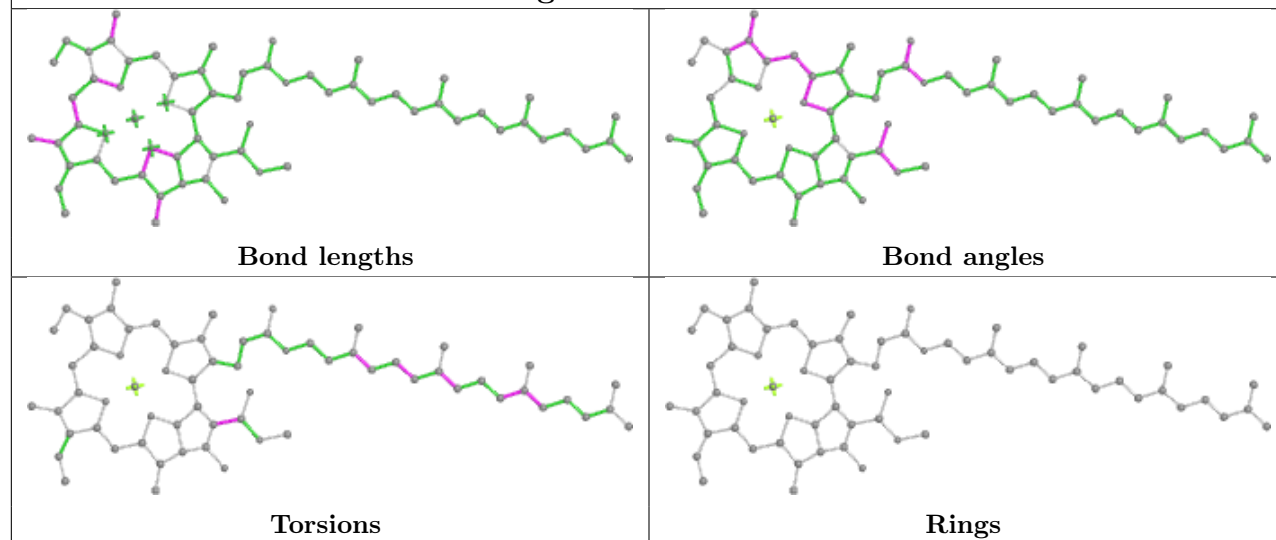


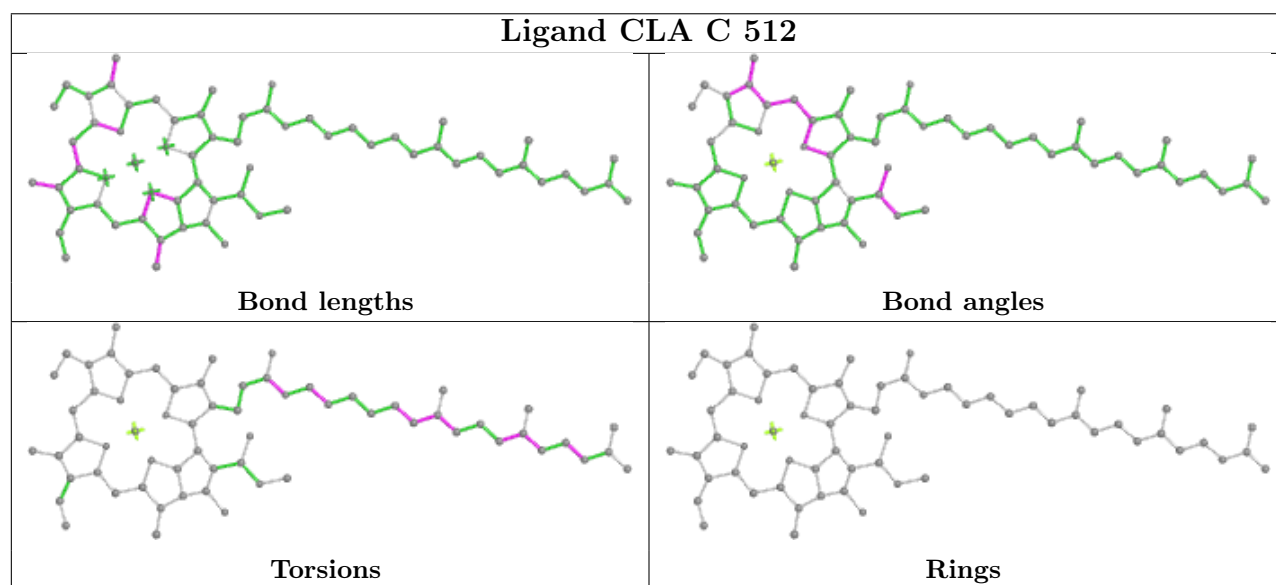
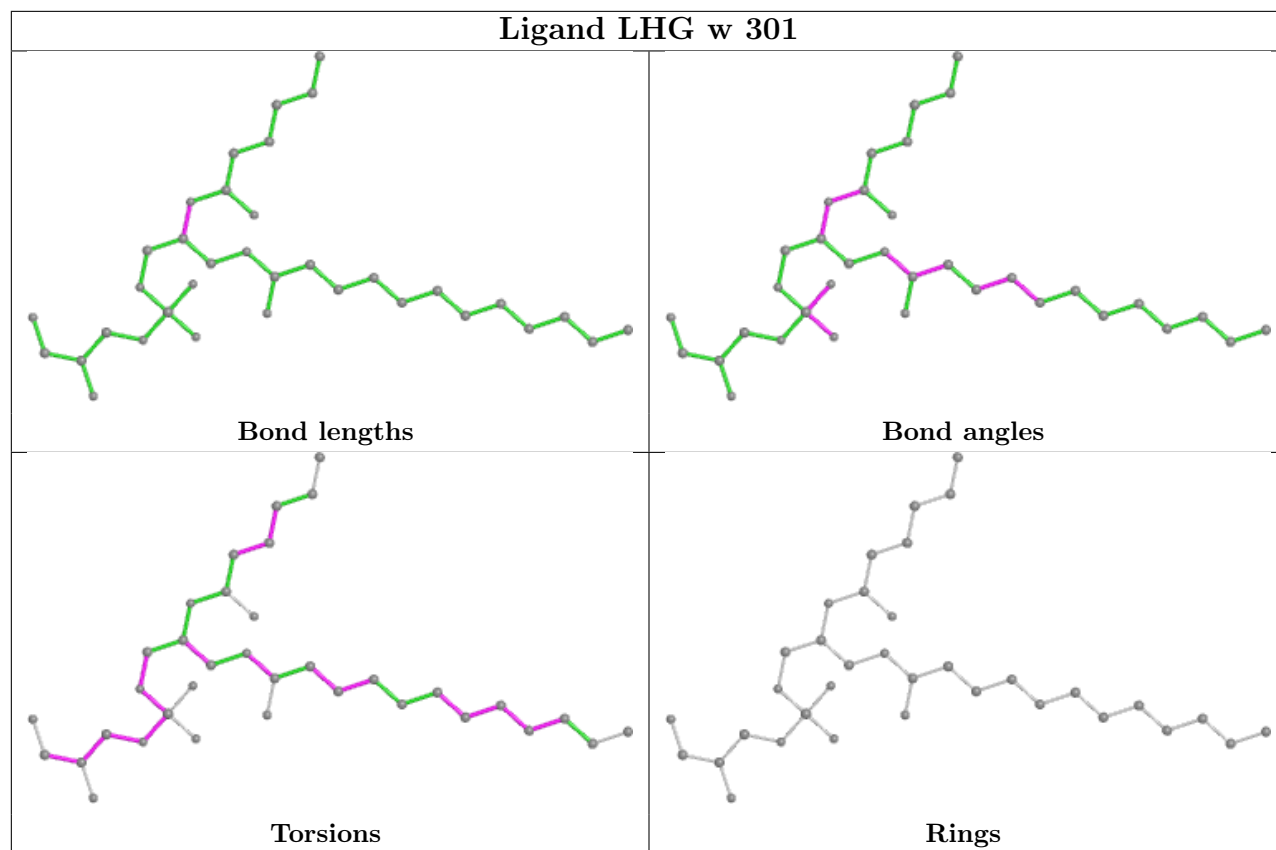


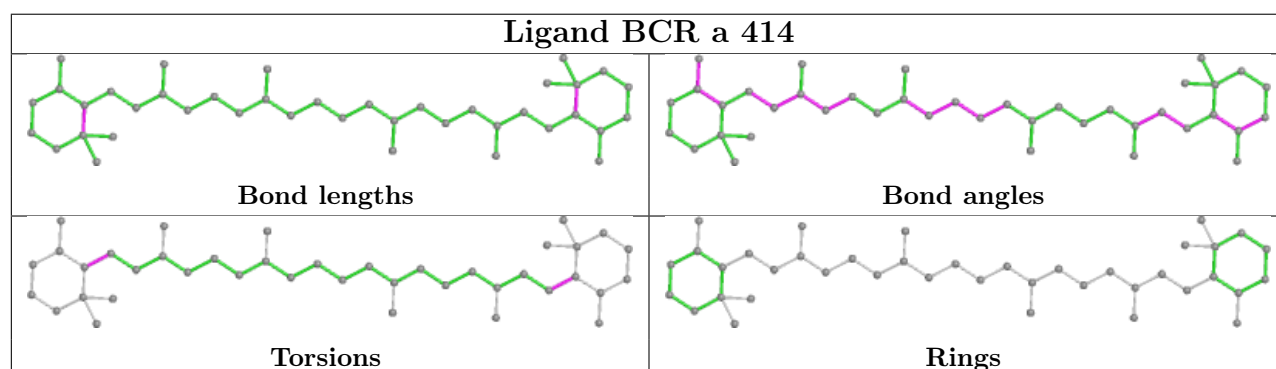
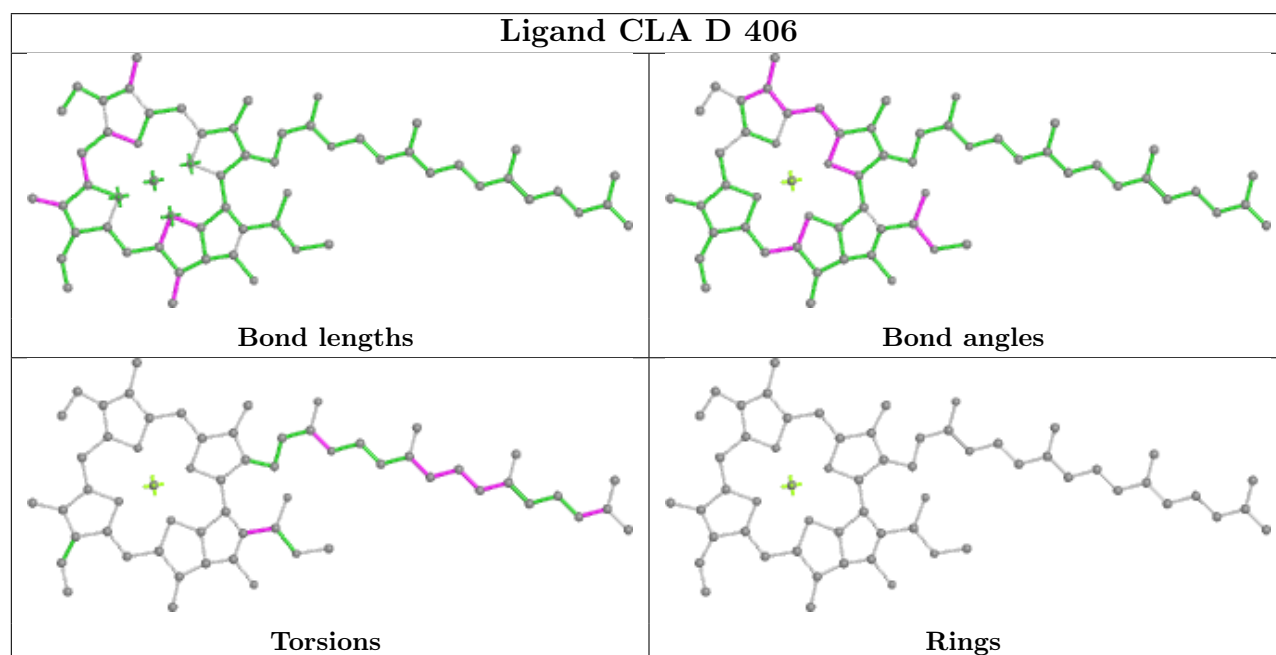
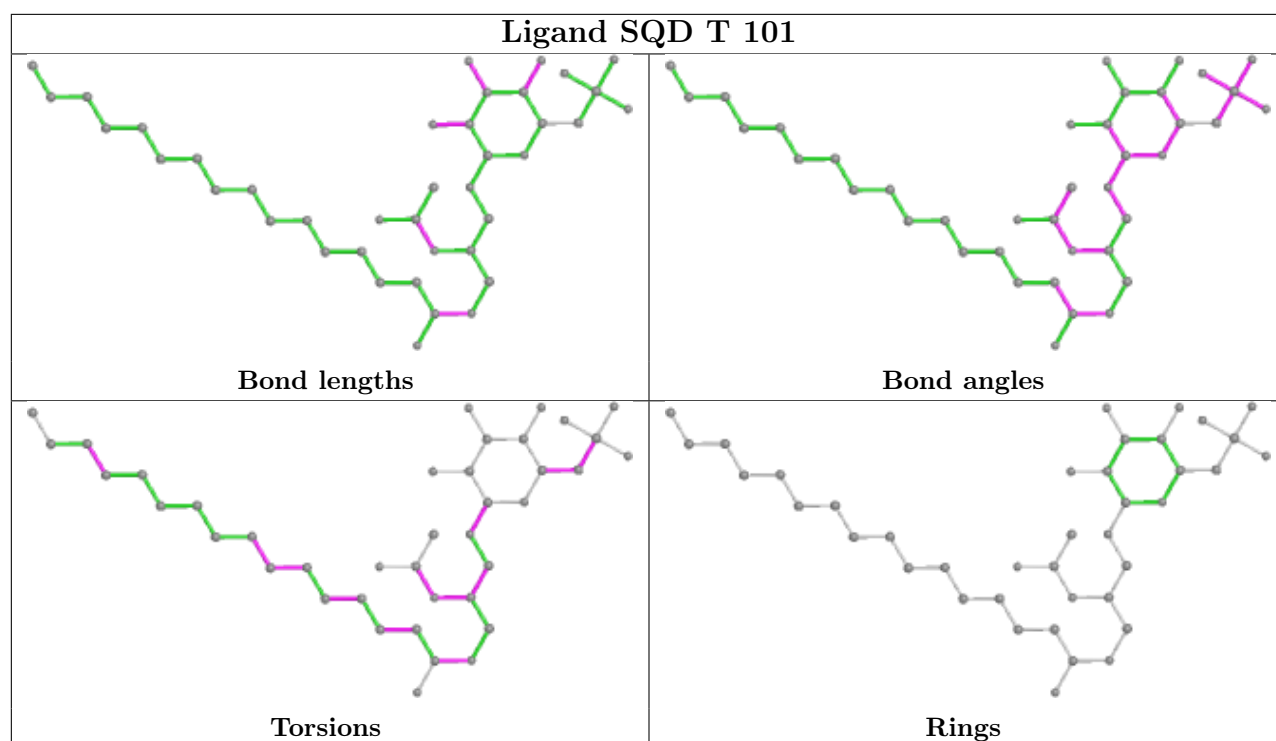
## Ligand CLA C 513



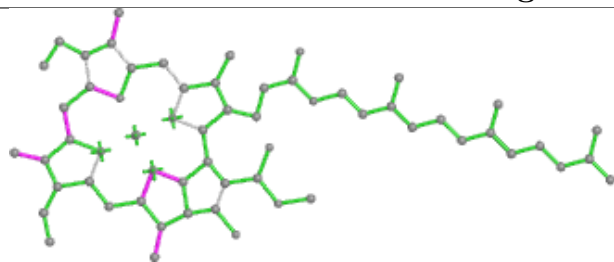
## Ligand CLA c 508



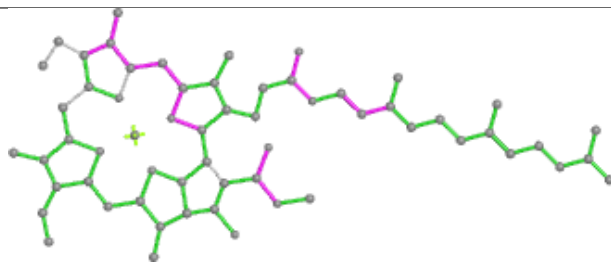




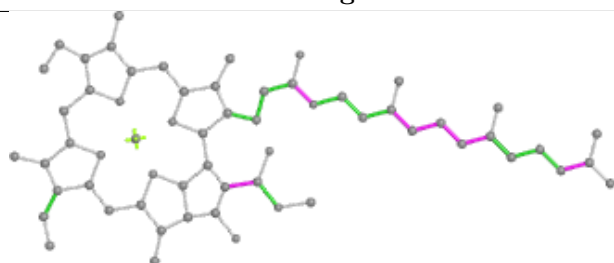
## Ligand CLA d 402



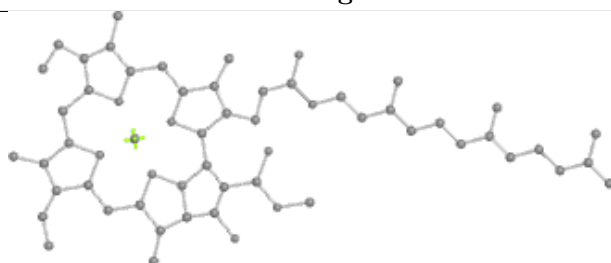
Bond lengths



Bond angles

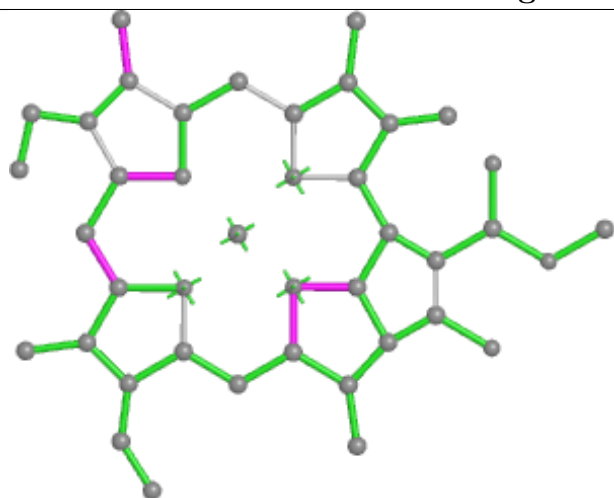


Torsions

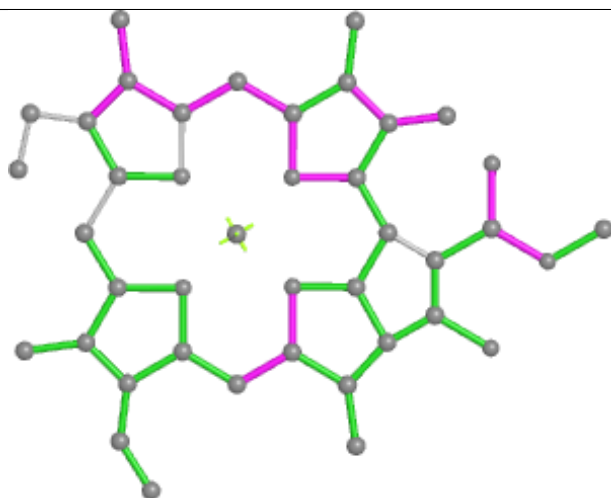


Rings

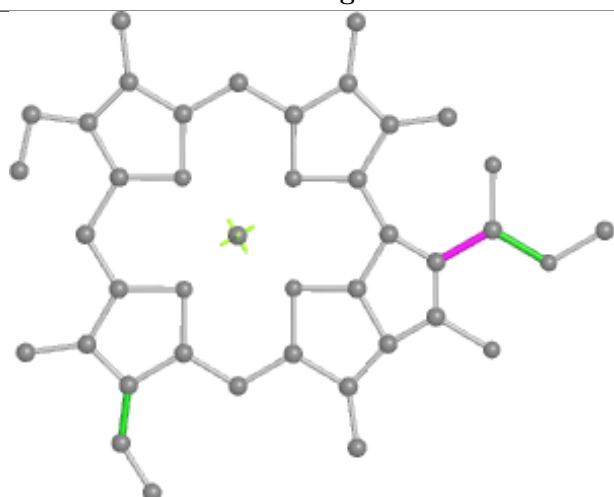
## Ligand CLA 9 305



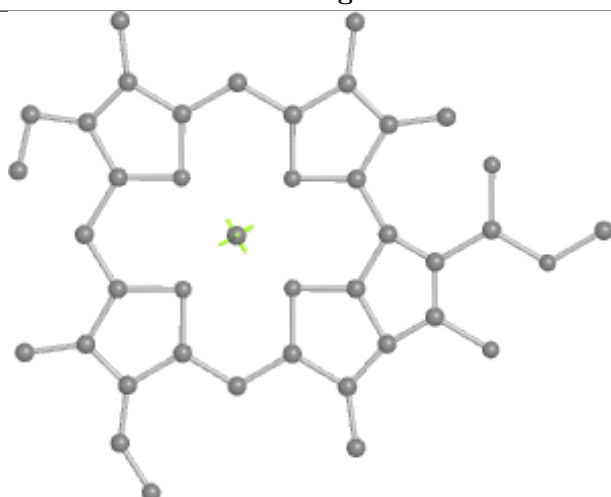
Bond lengths



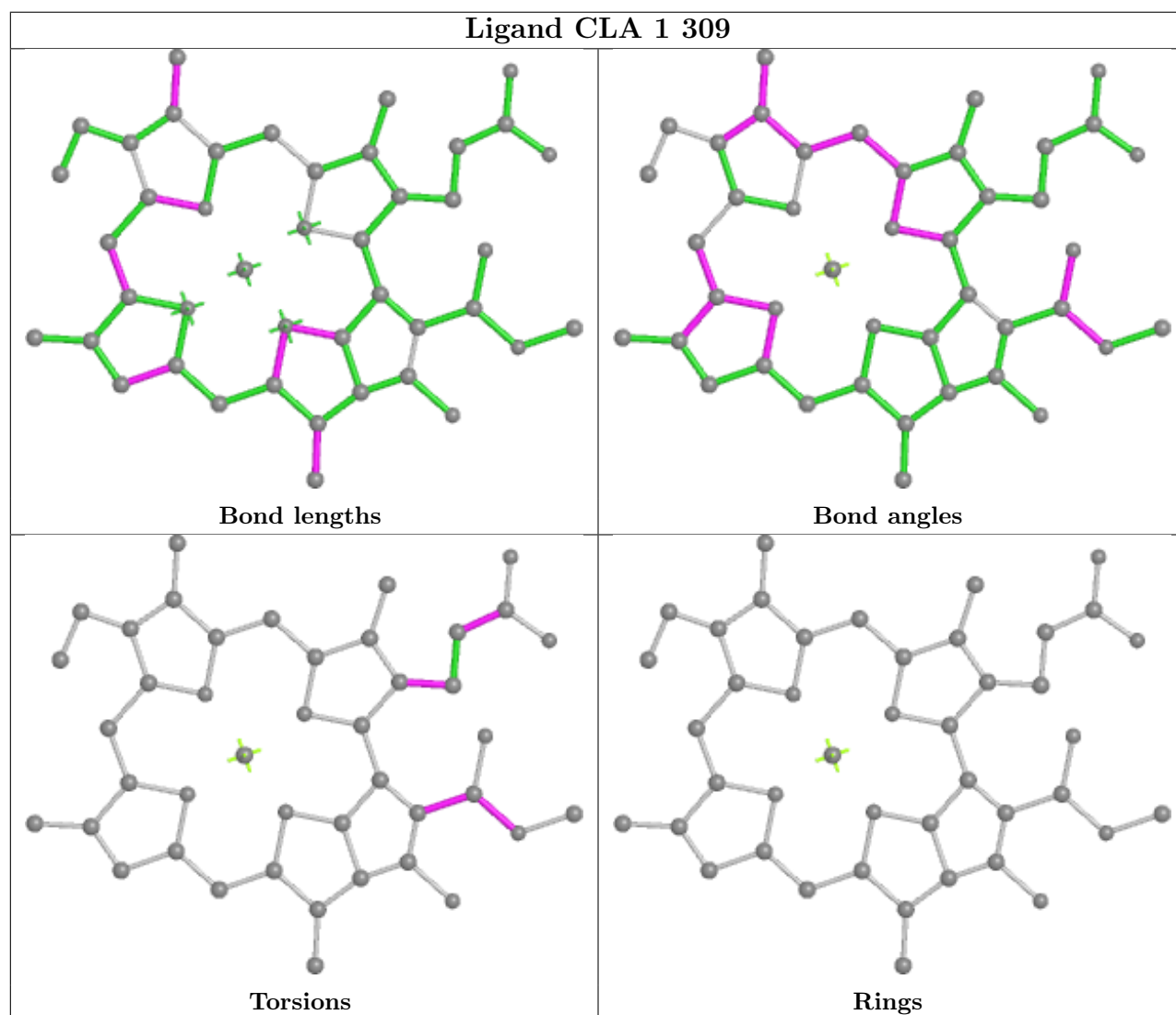
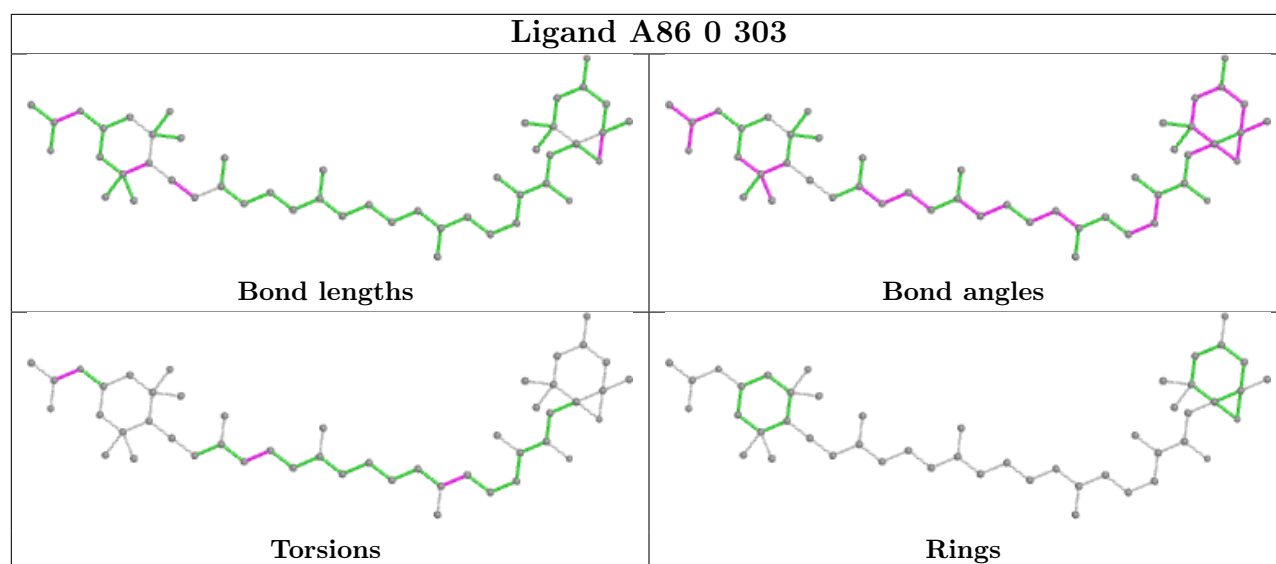
Bond angles

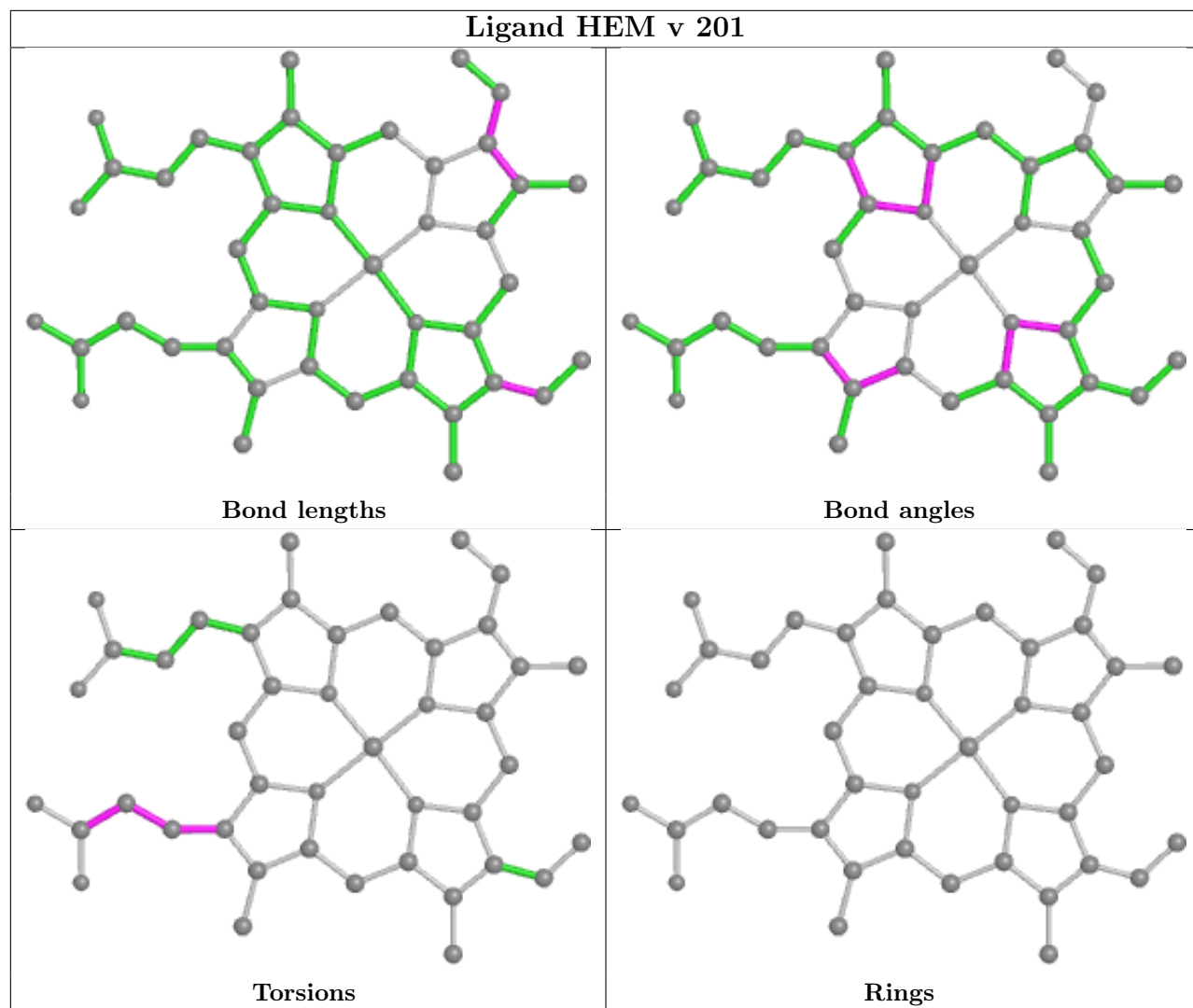


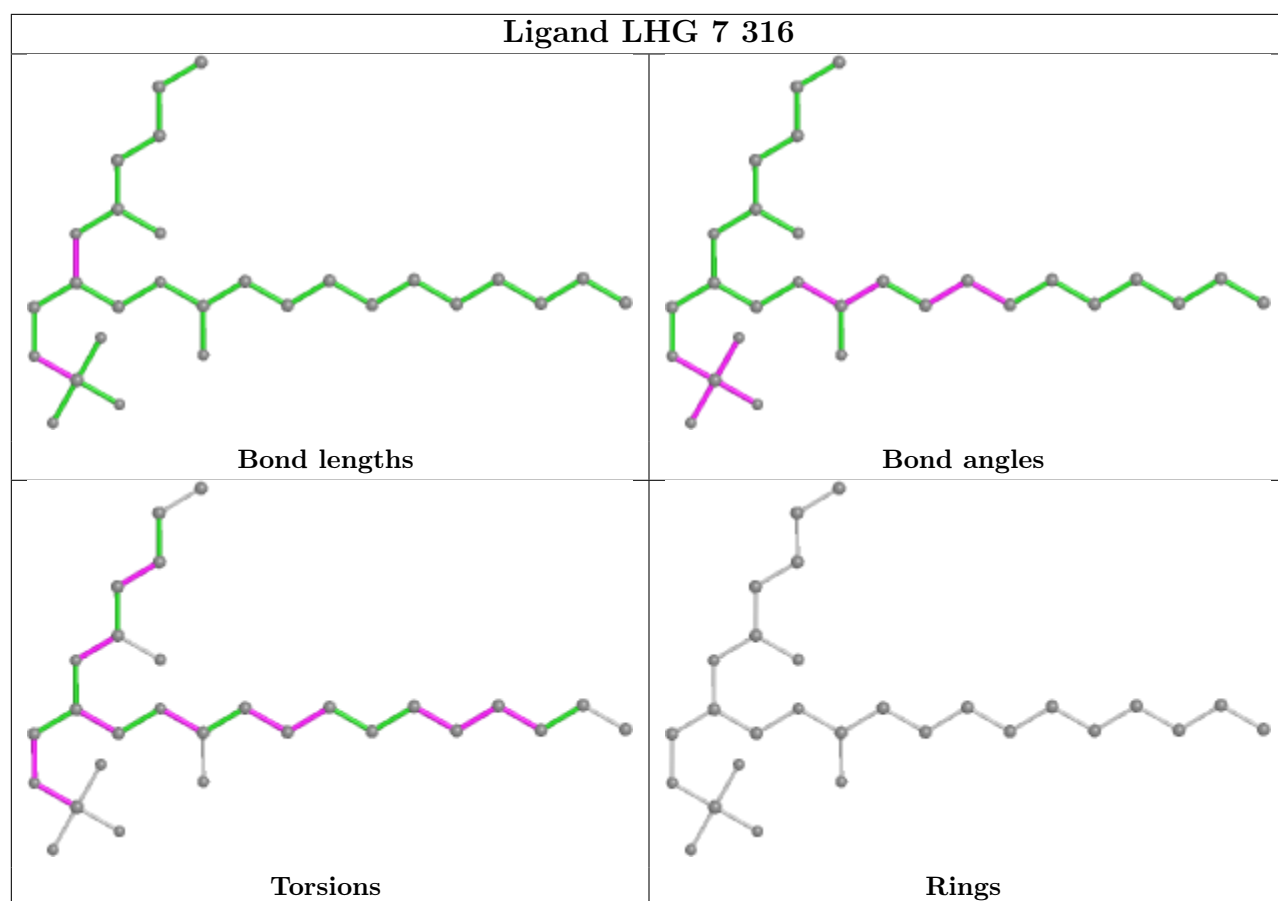
Torsions



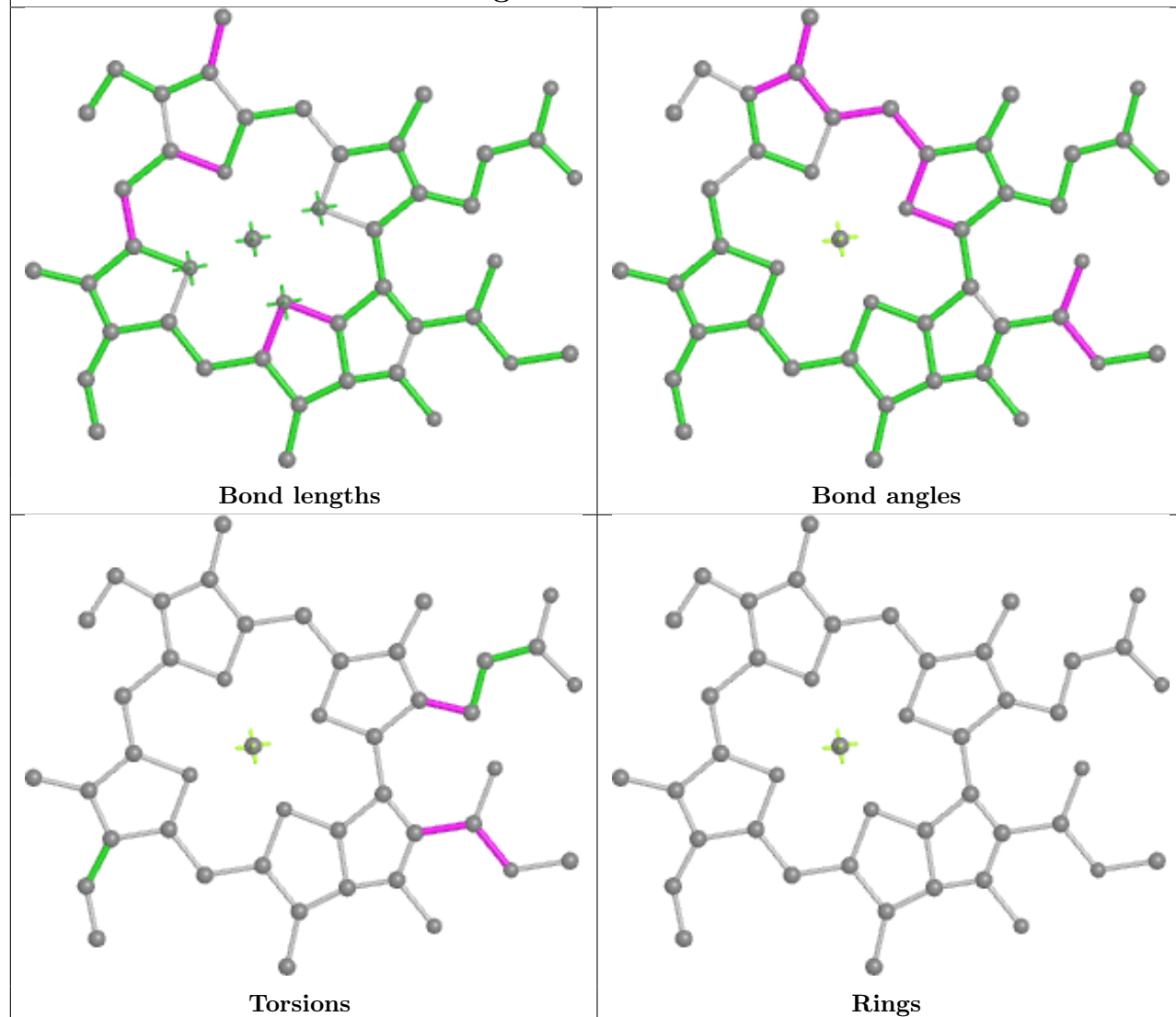
Rings



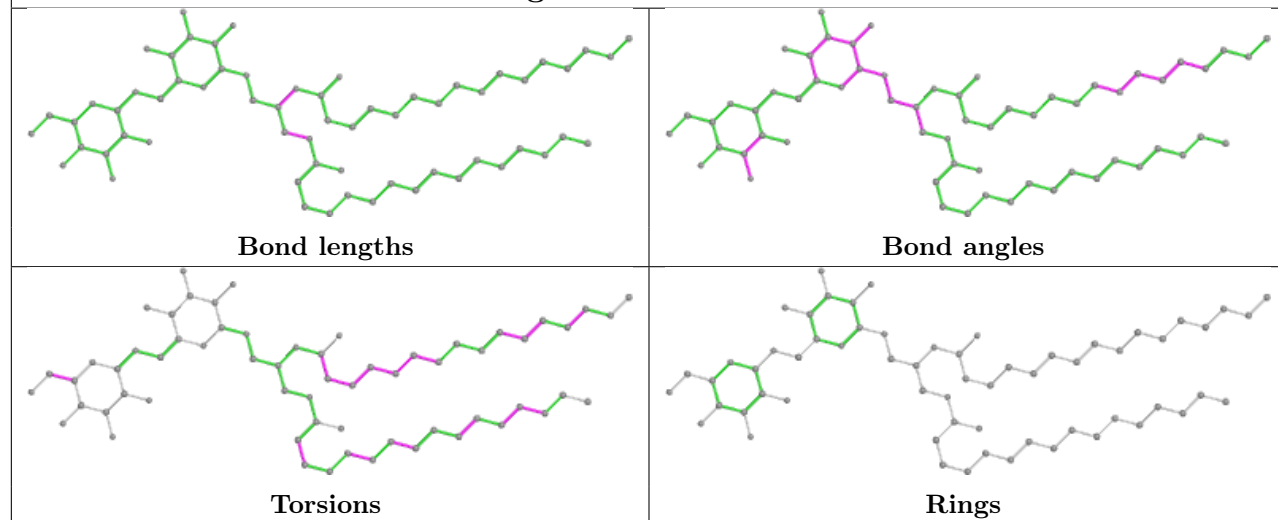




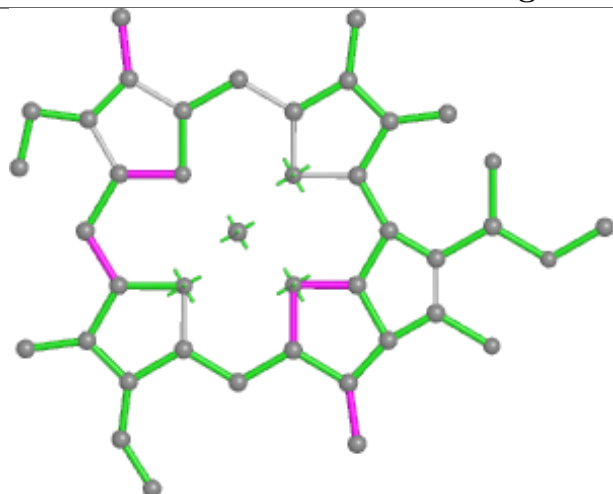
## Ligand CLA 1 312



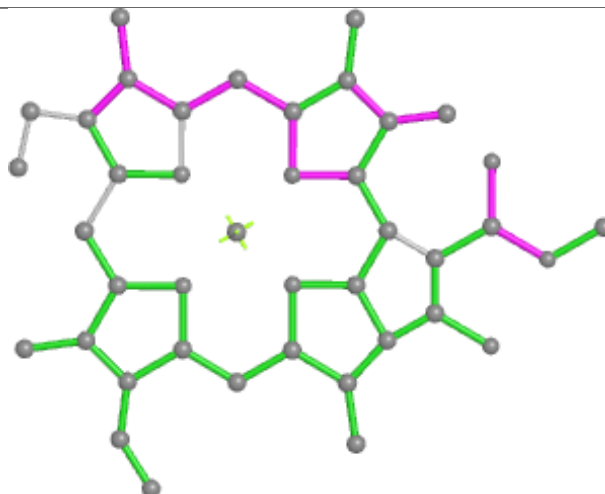
## Ligand DGD H 102



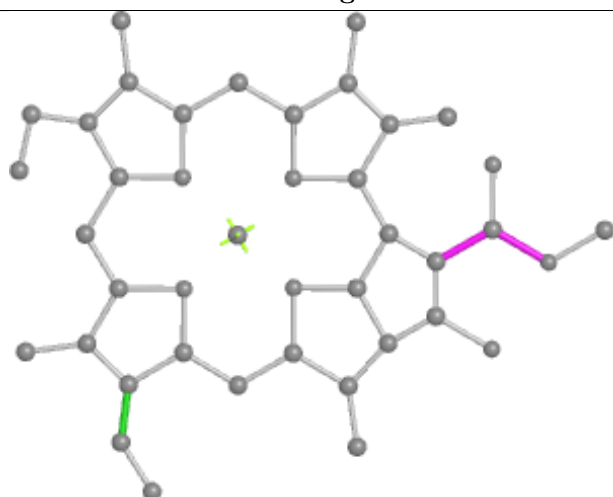
## Ligand CLA 3 311



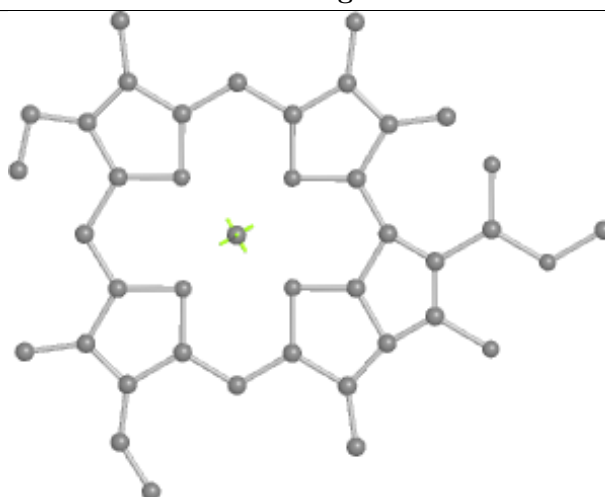
Bond lengths



Bond angles

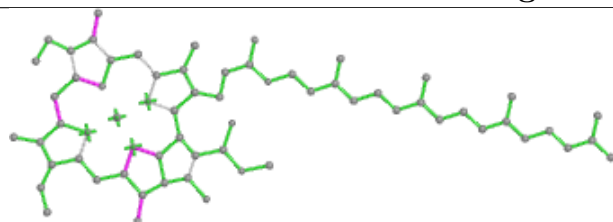


Torsions

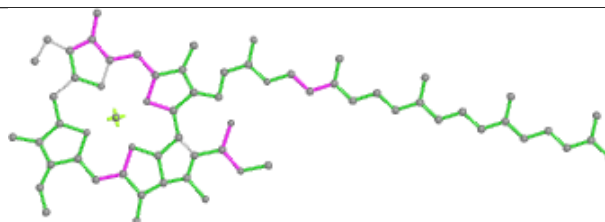


Rings

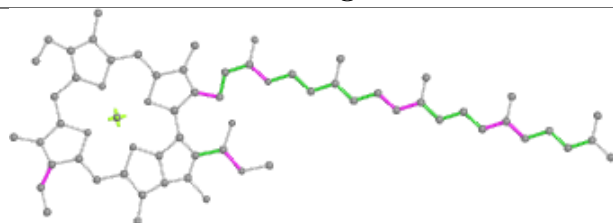
## Ligand CLA 9 310



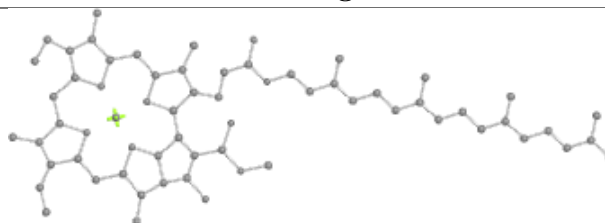
Bond lengths



Bond angles

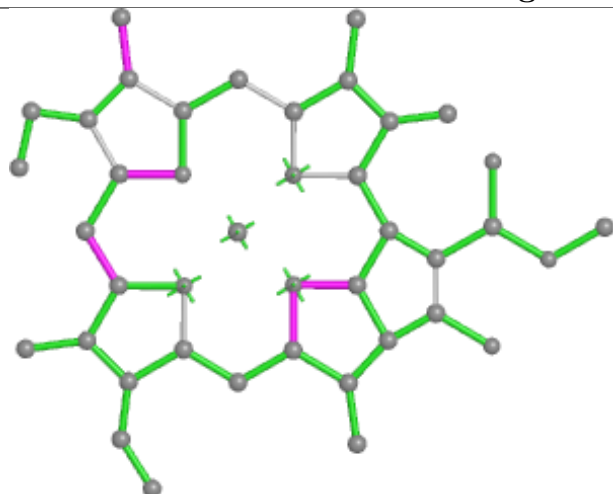


Torsions

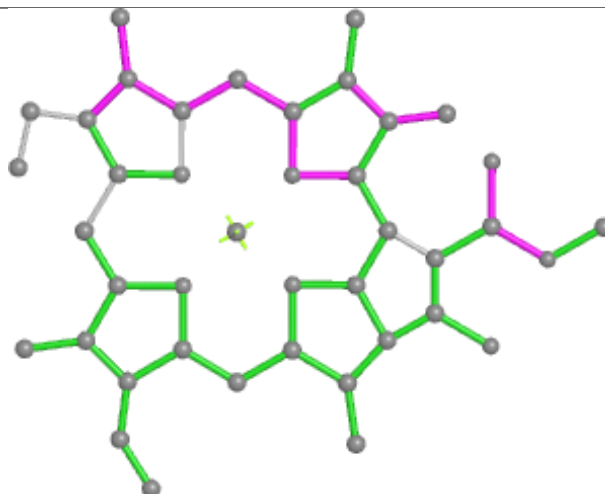


Rings

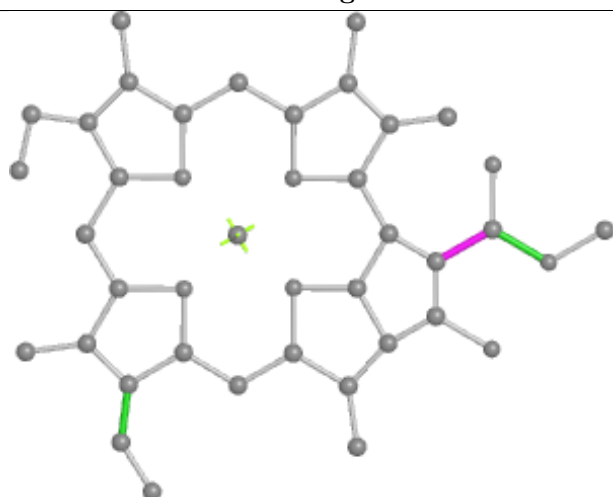
## Ligand CLA 8 305



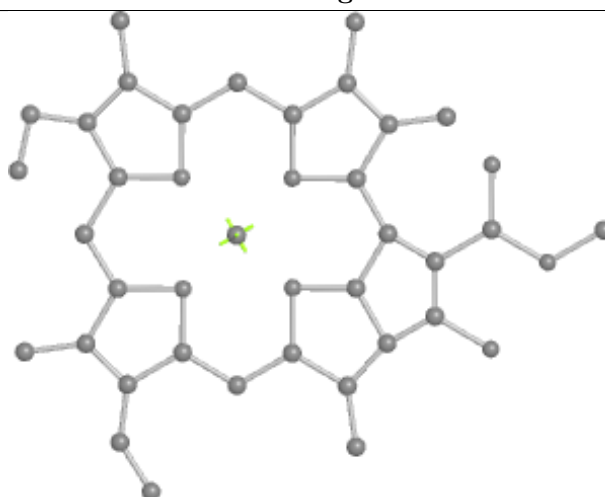
Bond lengths



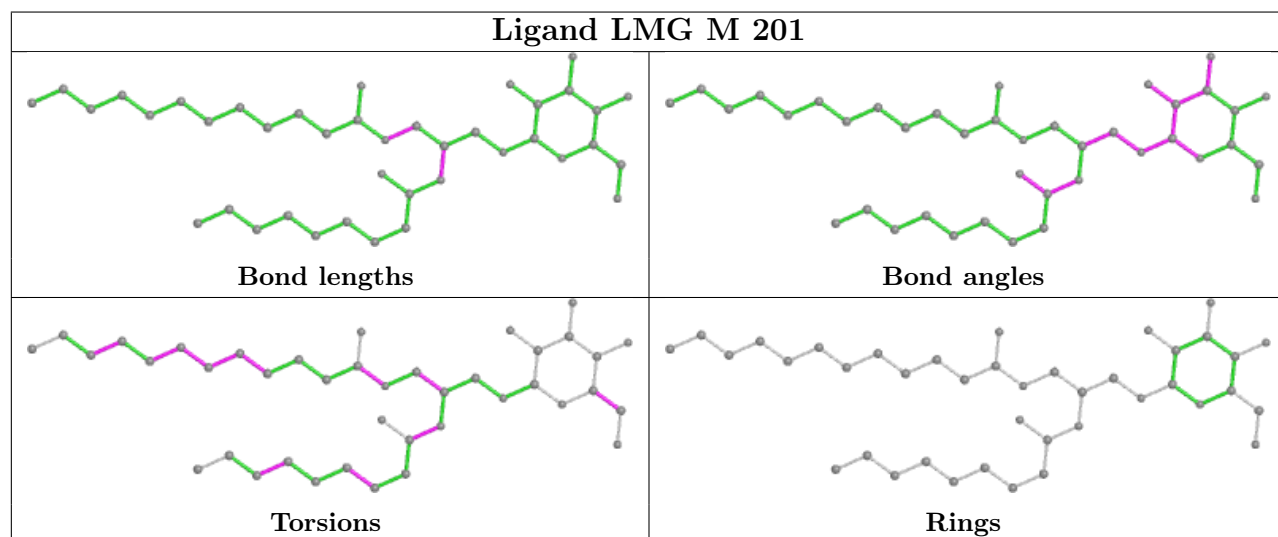
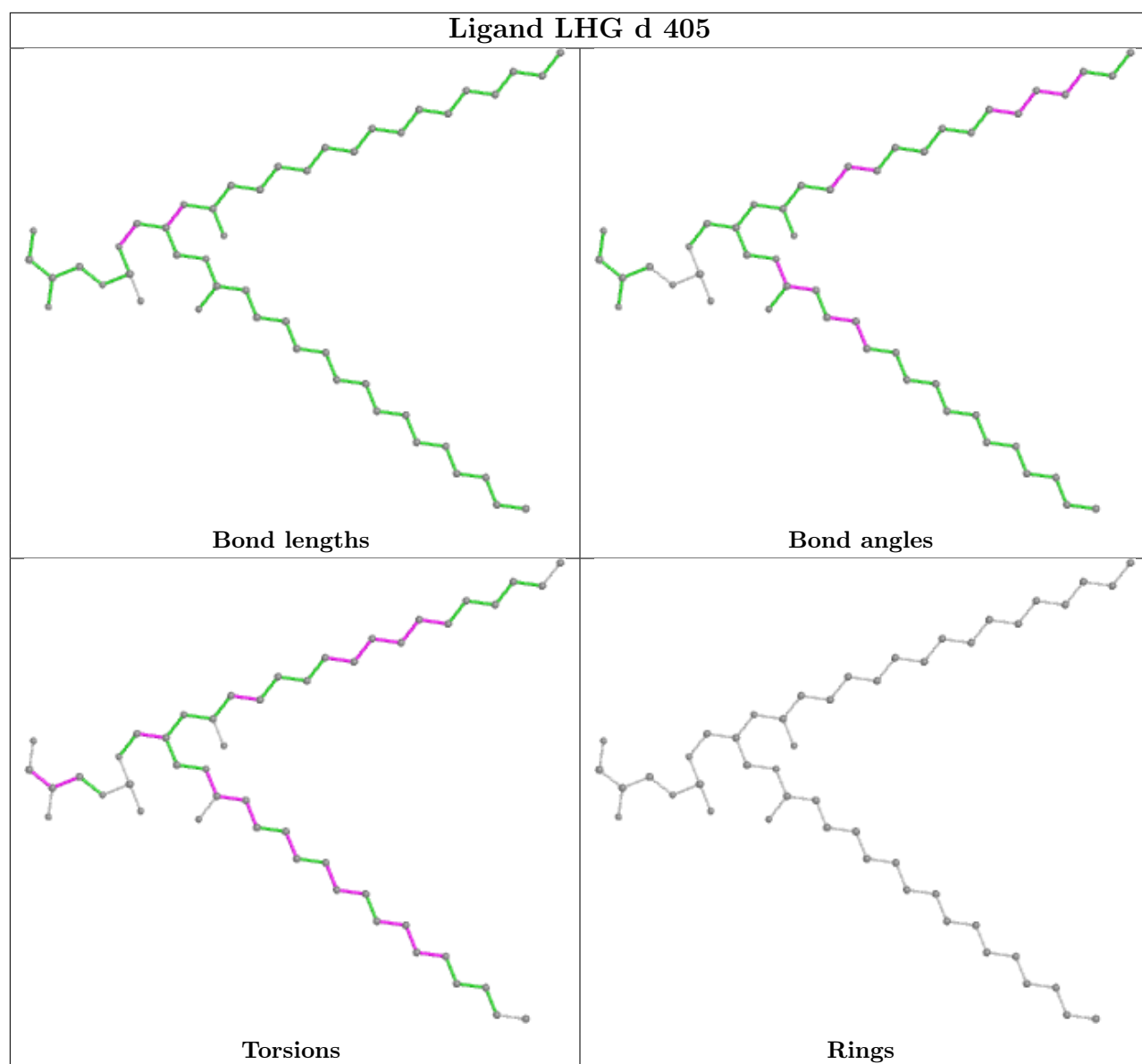
Bond angles

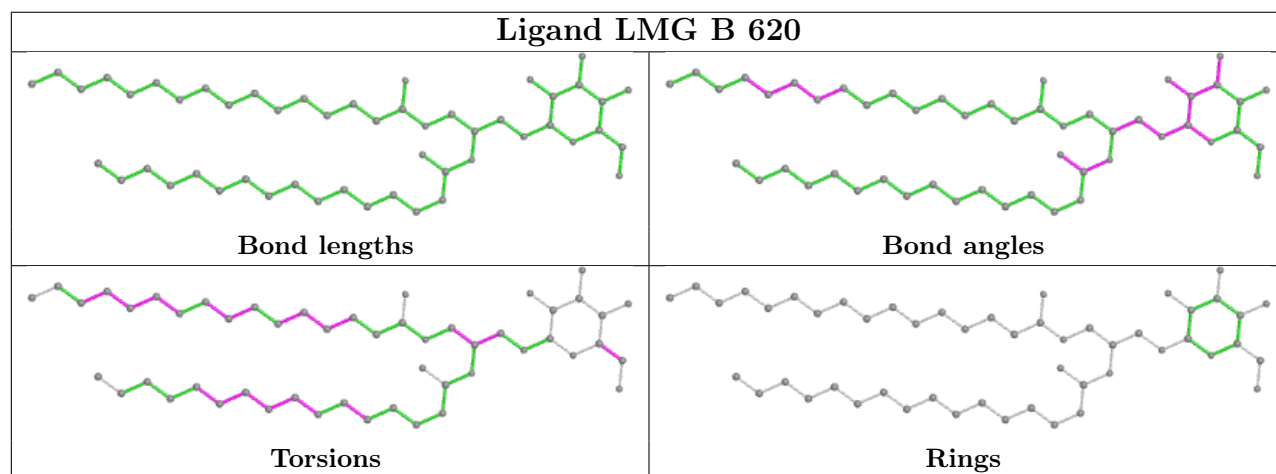
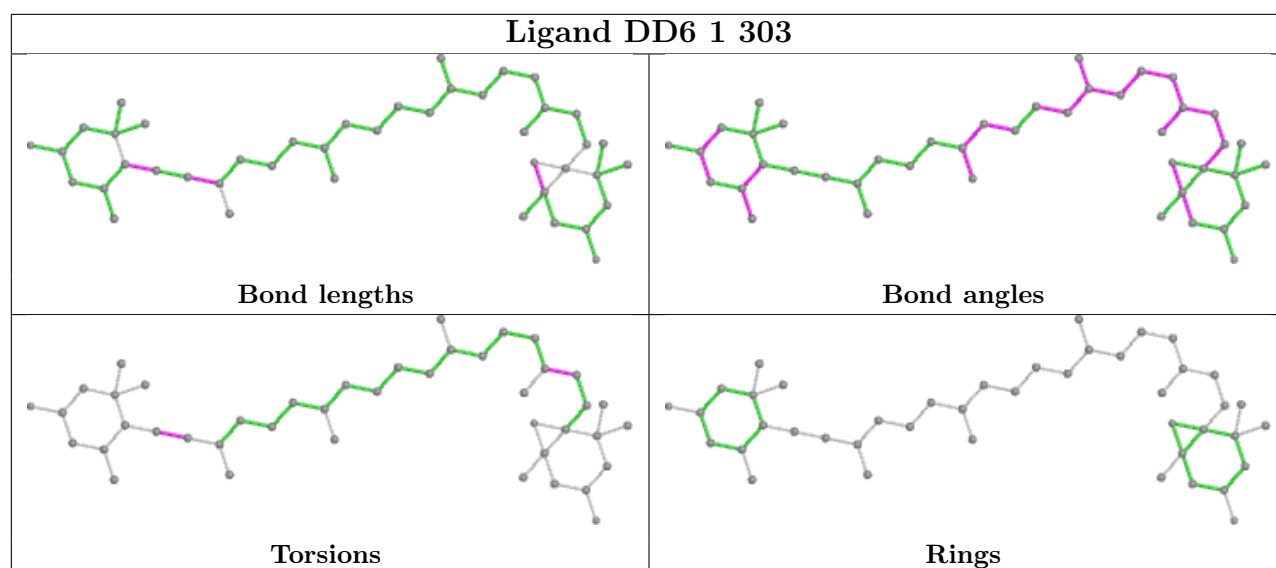


Torsions

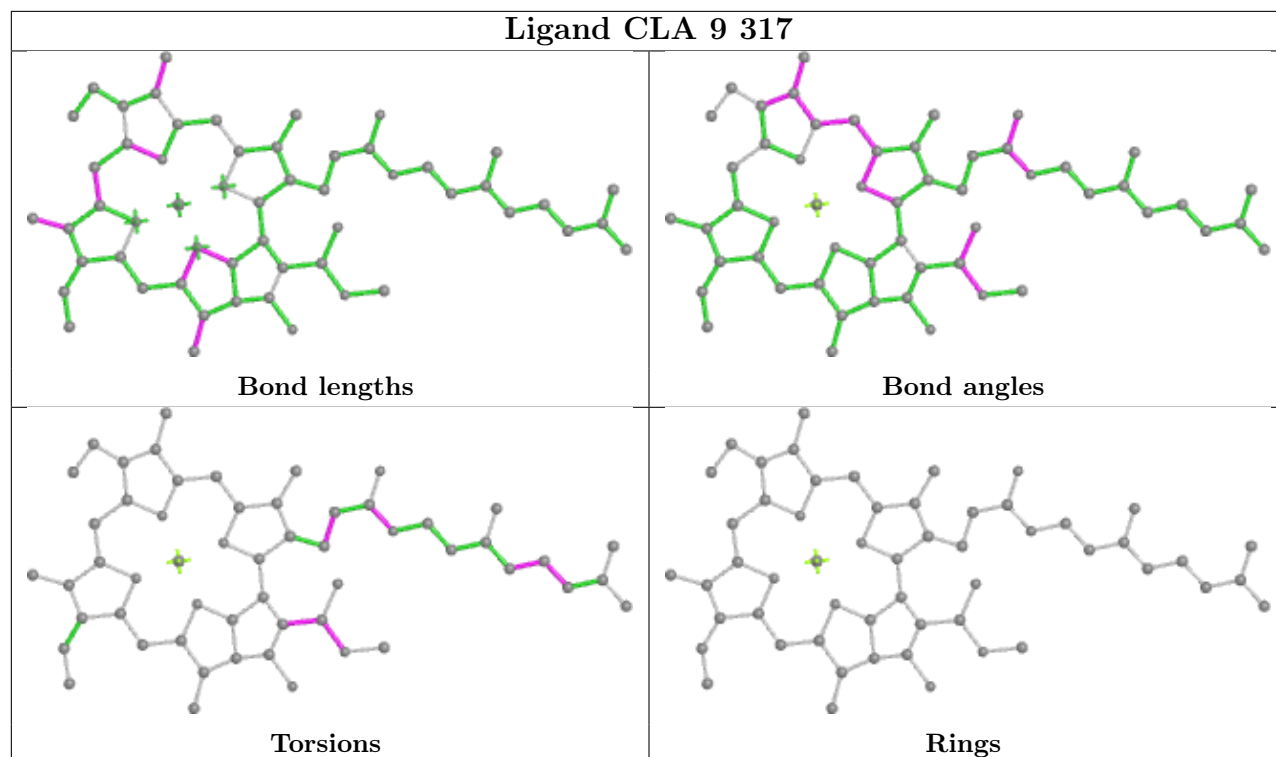


Rings

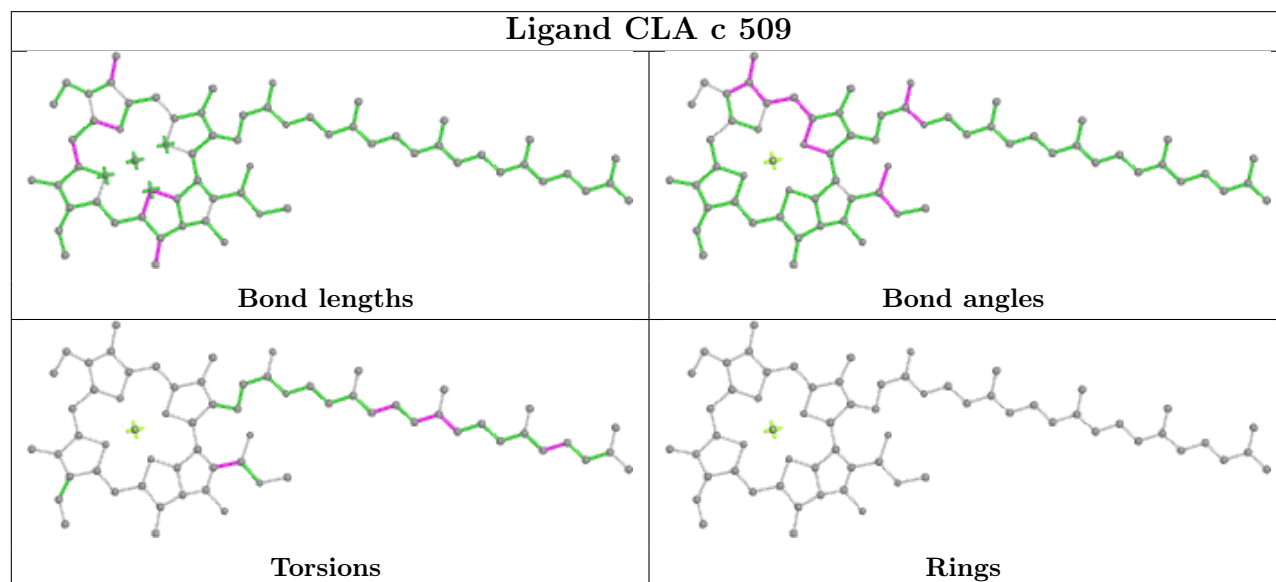


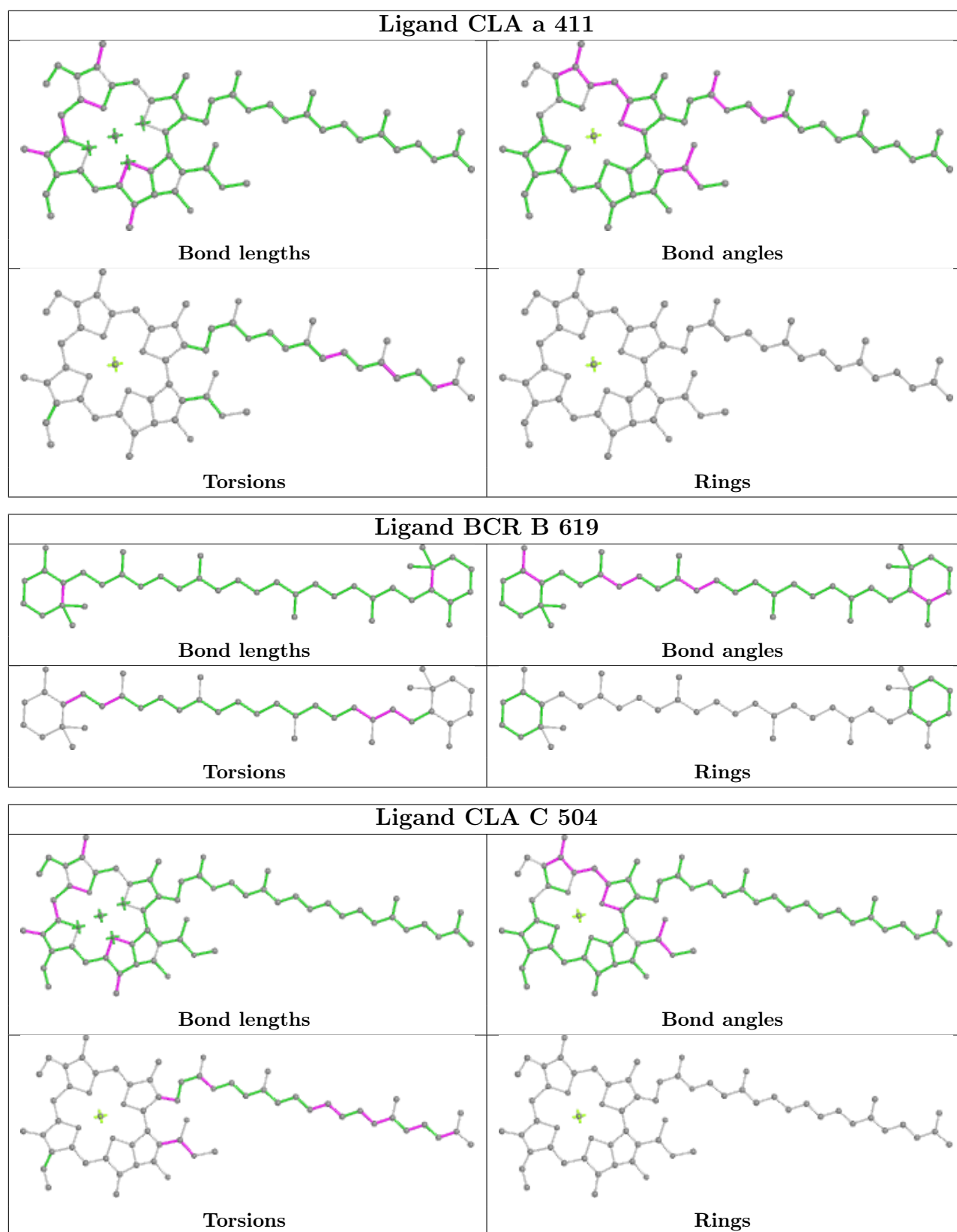


## Ligand CLA 9 317

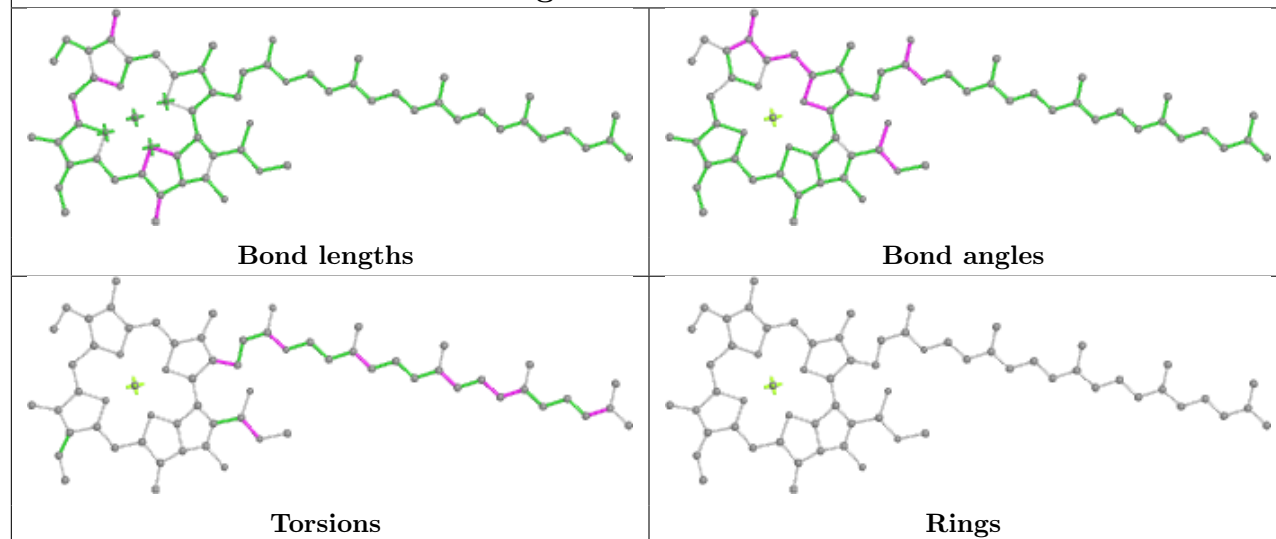


## Ligand CLA c 509

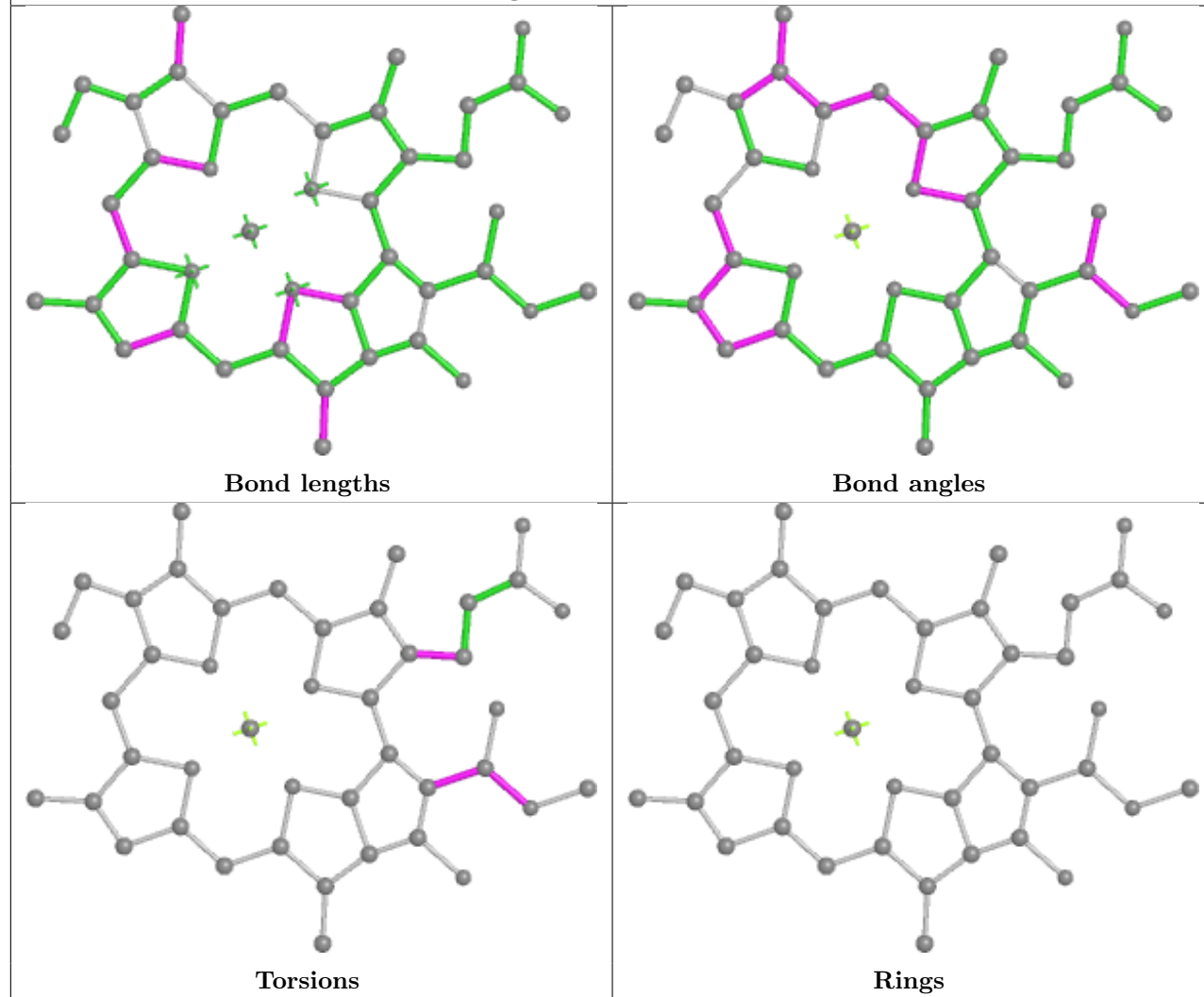




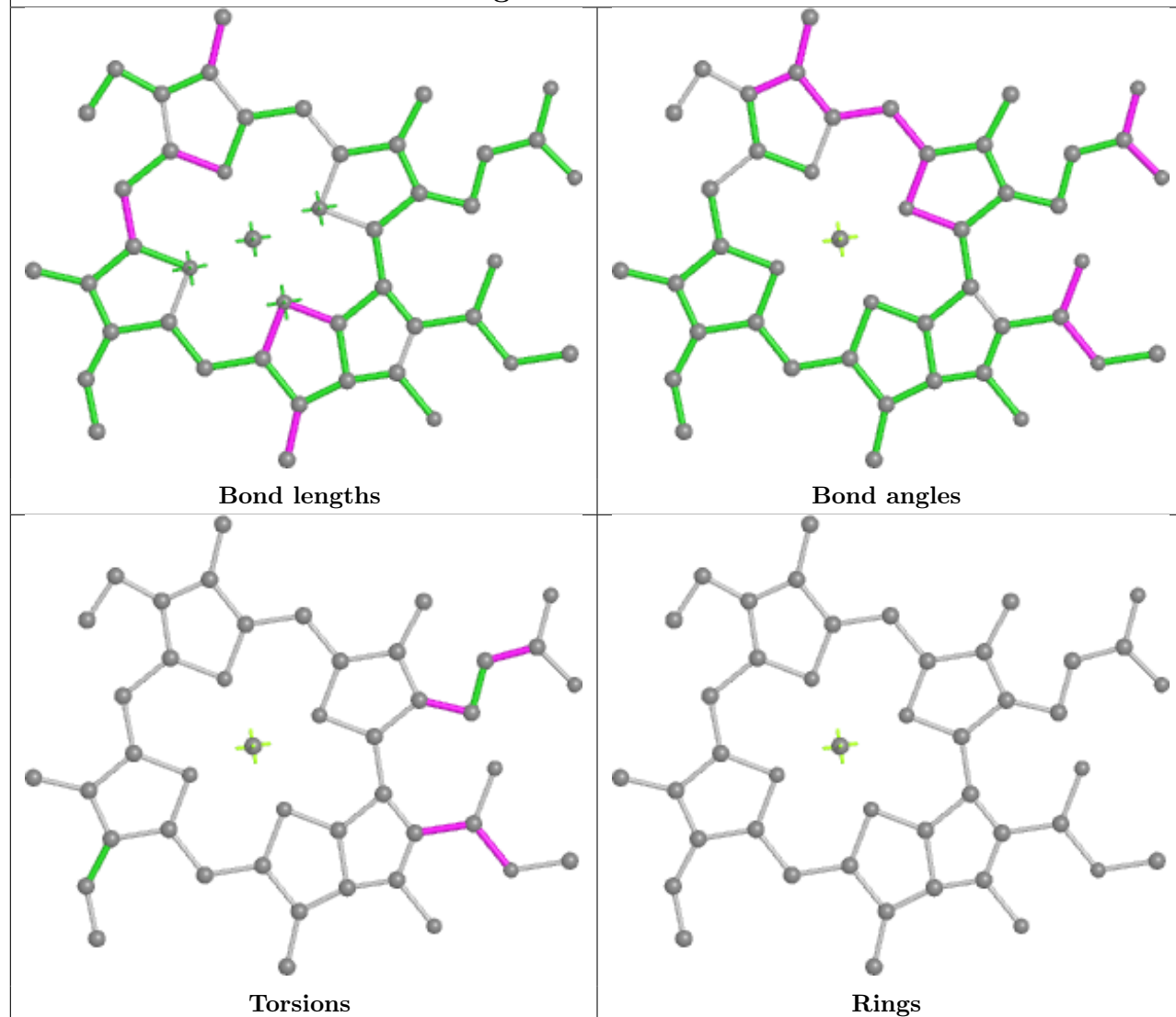
## Ligand CLA 5 313



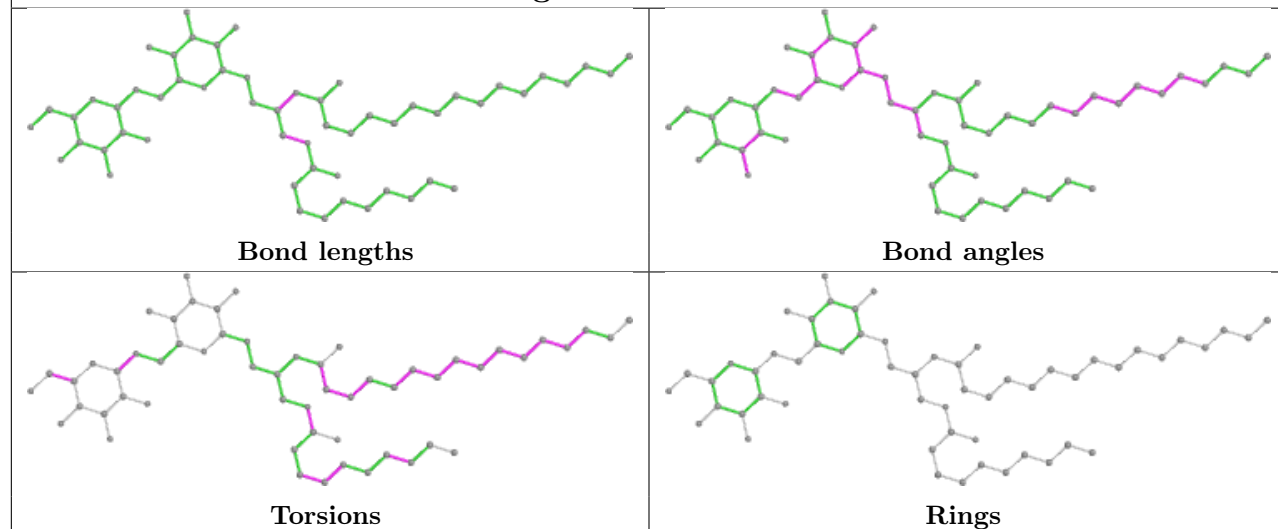
## Ligand CLA 9 309

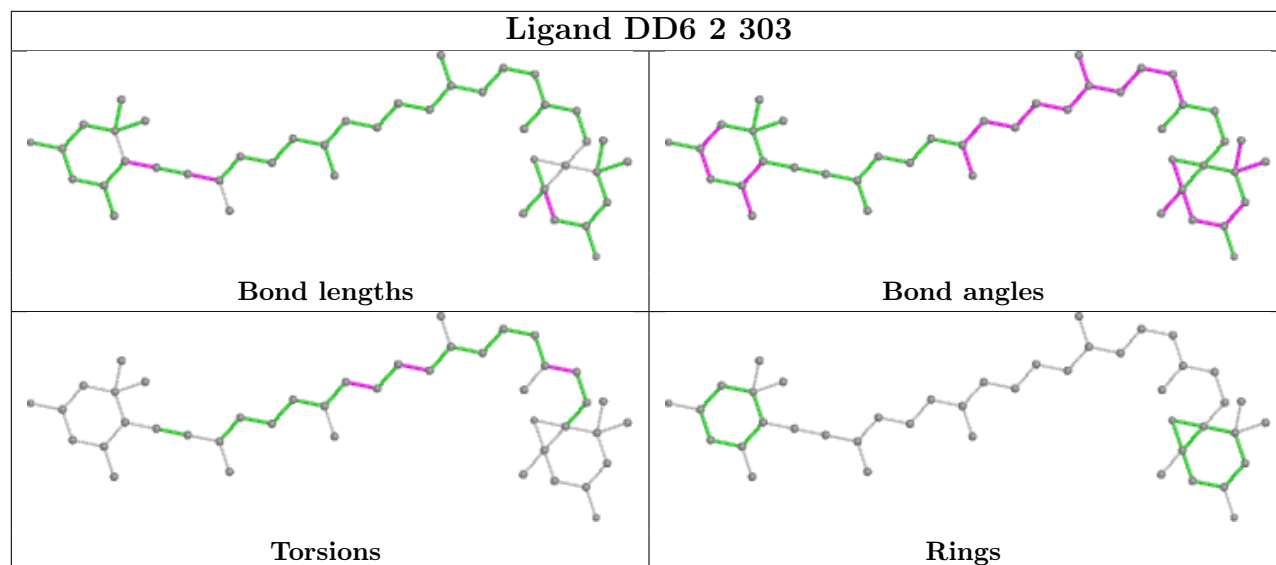
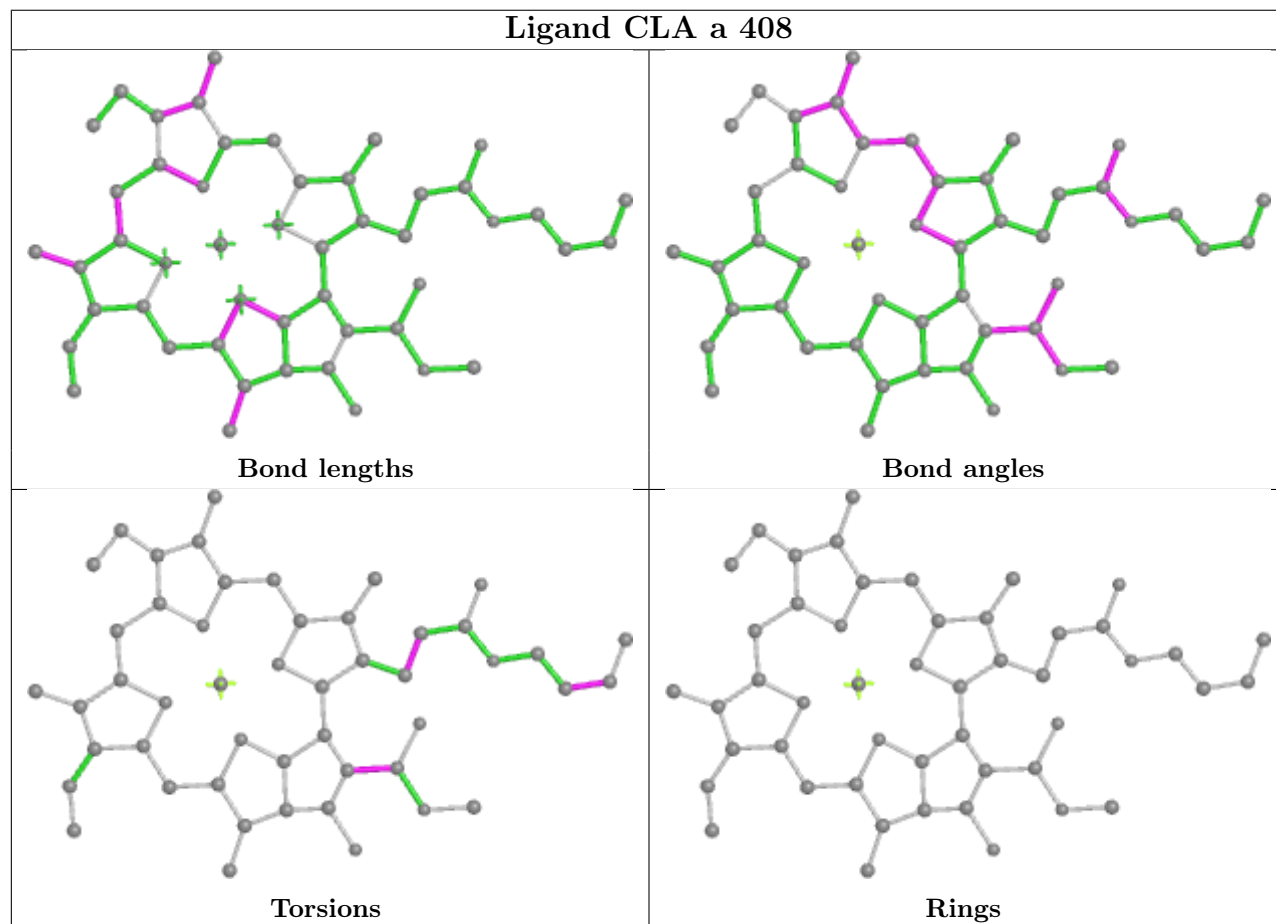


## Ligand CLA 0 310

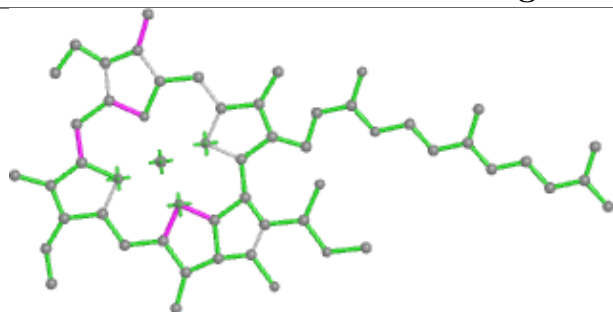


## Ligand DGD c 517

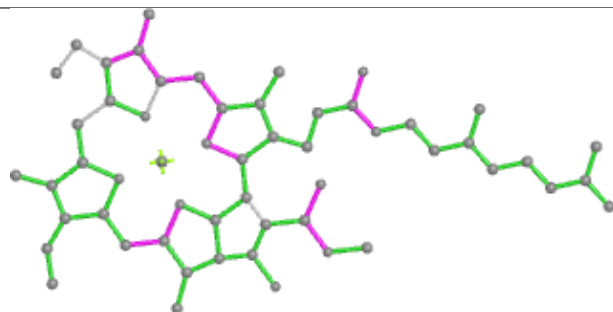


**Ligand DD6 2 303****Ligand CLA a 408**

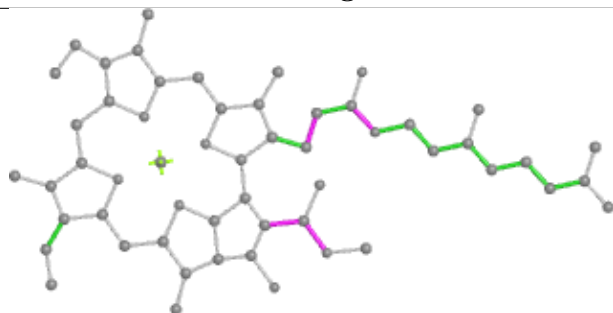
## Ligand CLA 1 311



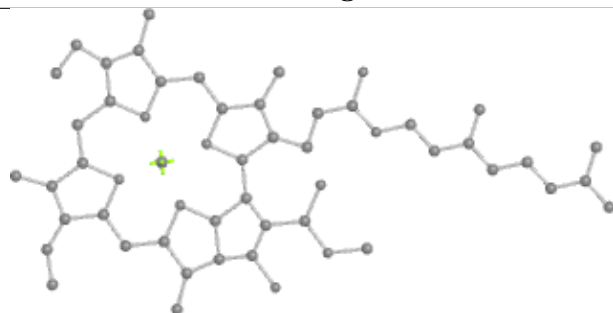
Bond lengths



Bond angles

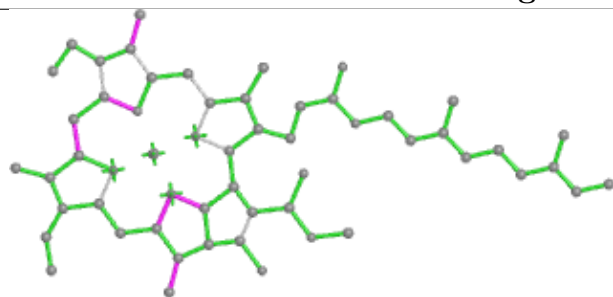


Torsions

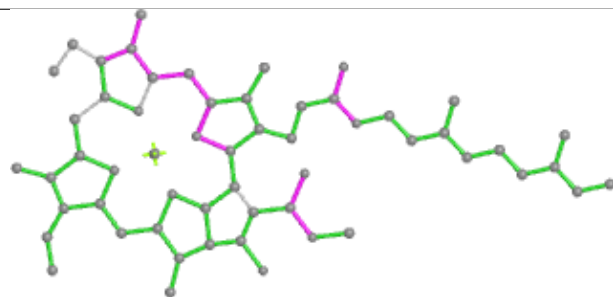


Rings

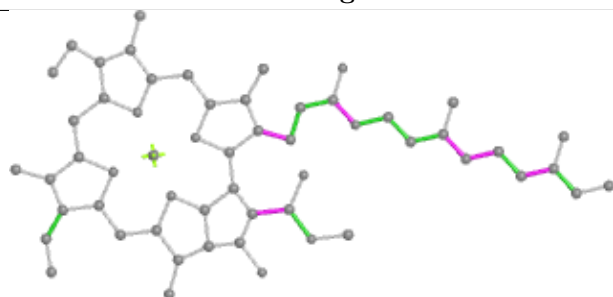
## Ligand CLA 3 312



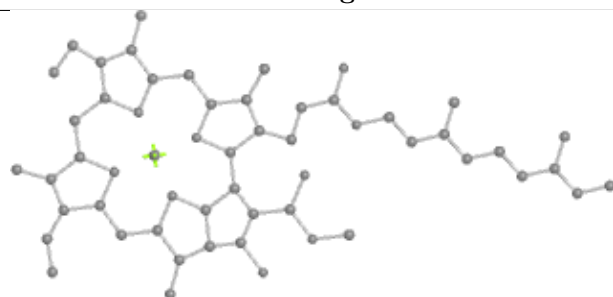
Bond lengths



Bond angles

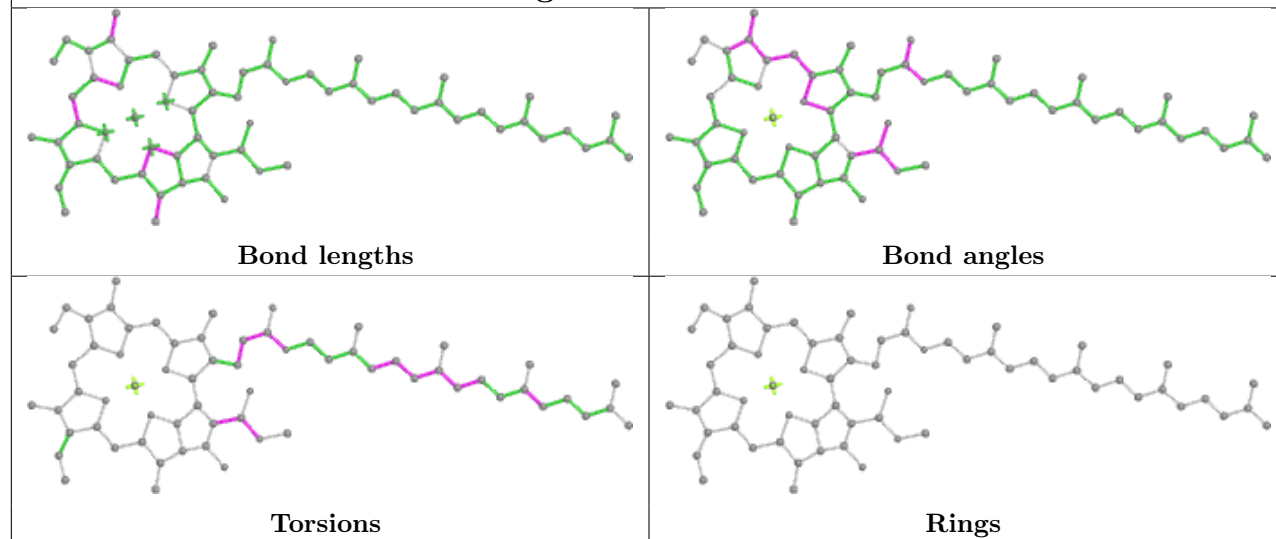


Torsions

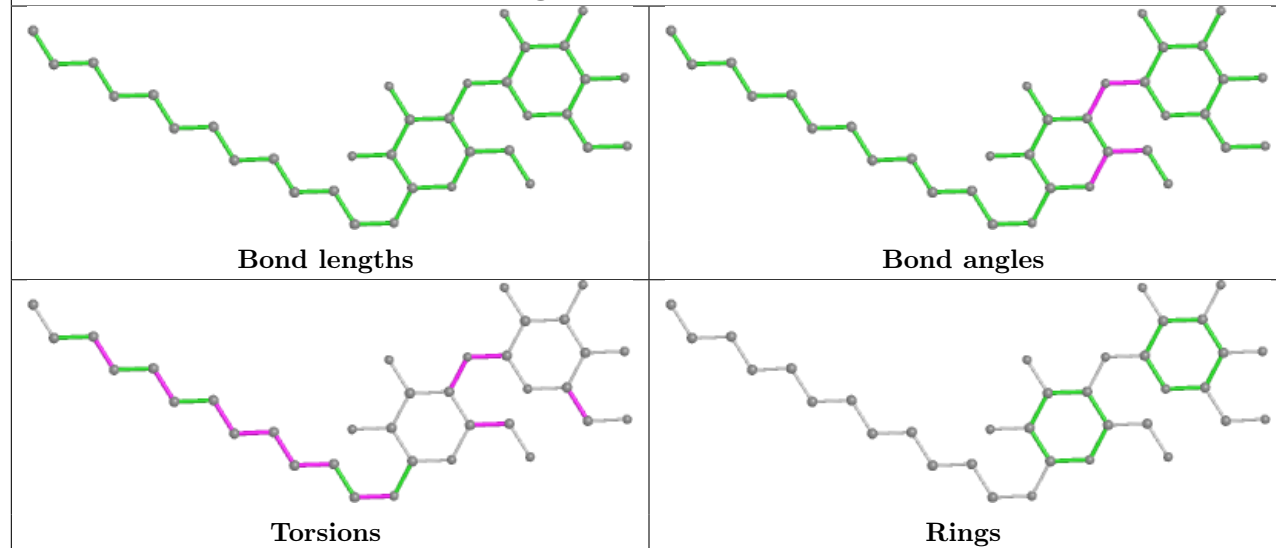


Rings

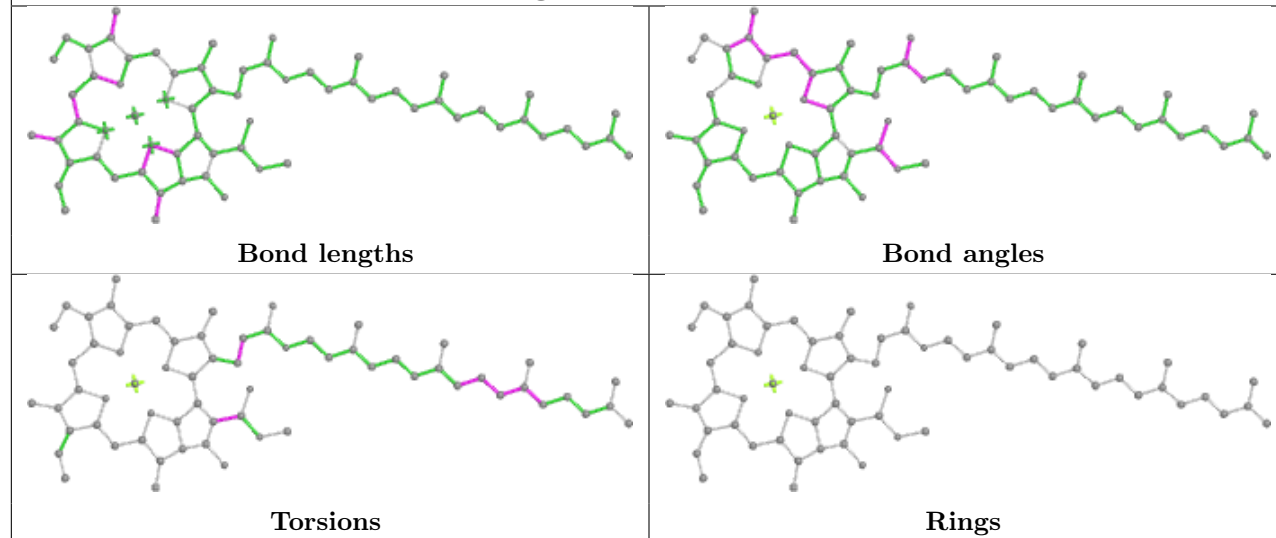
## Ligand CLA 0 305



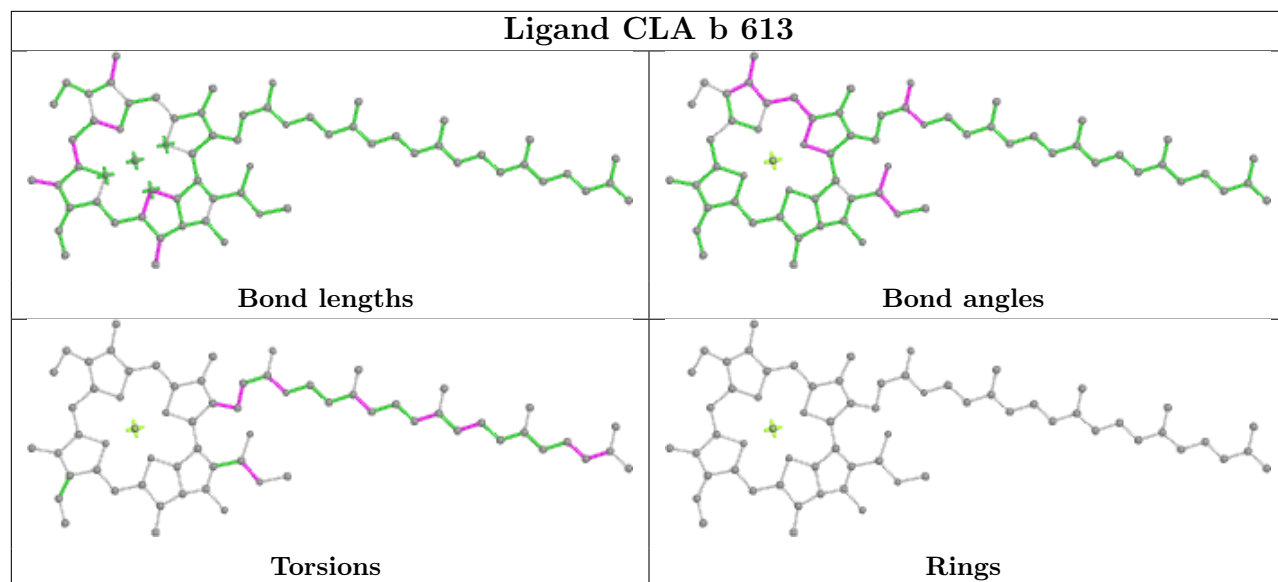
## Ligand LMU 4 317



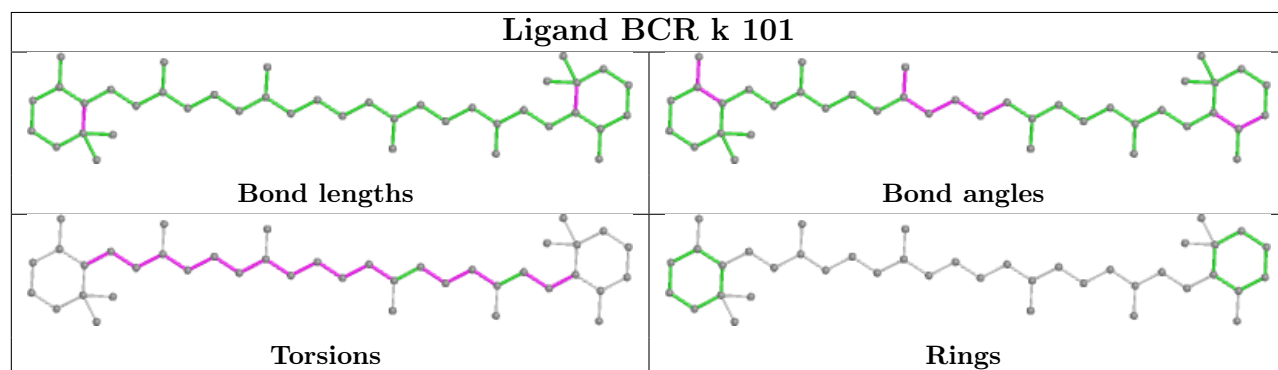
## Ligand CLA B 606



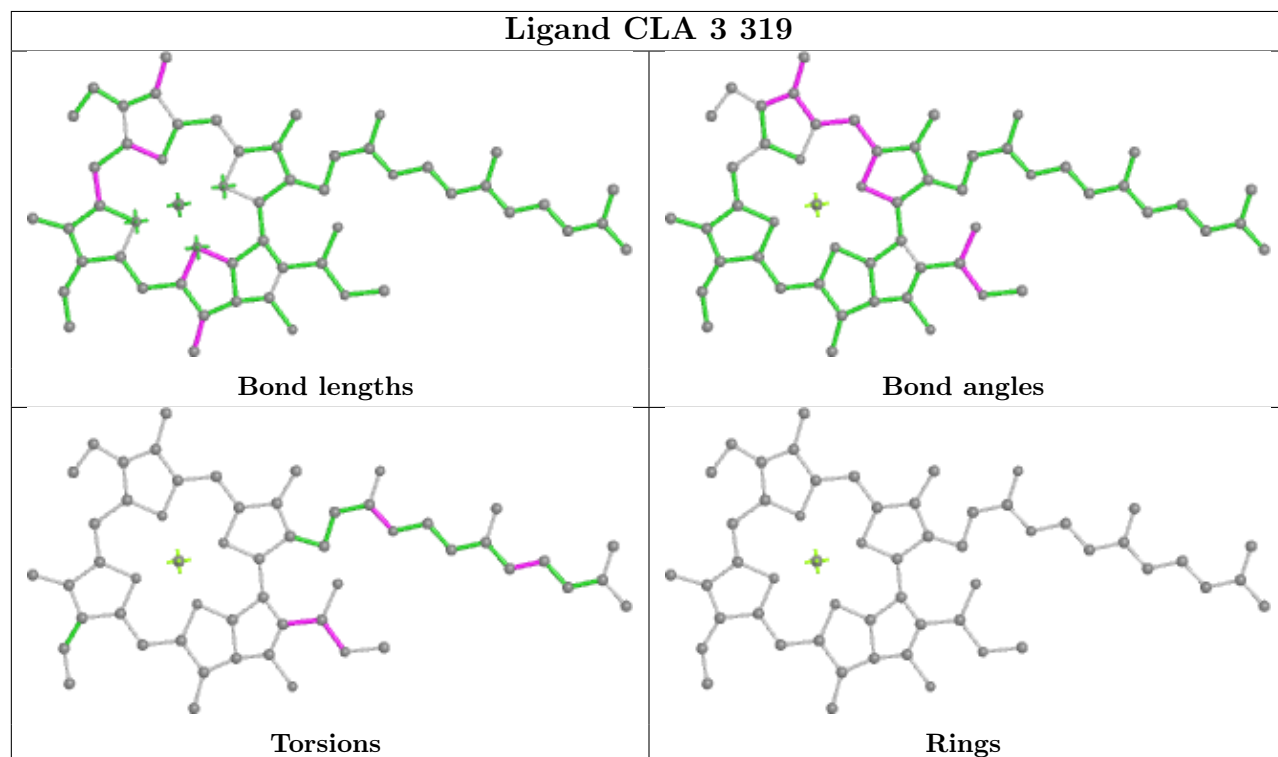
## Ligand CLA b 613

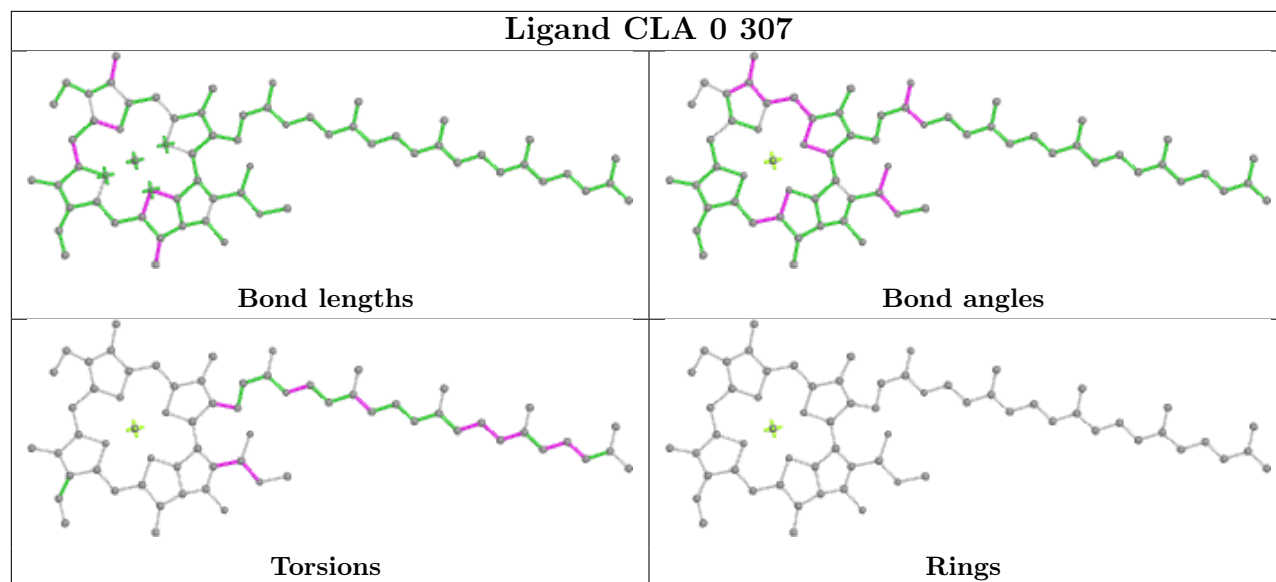
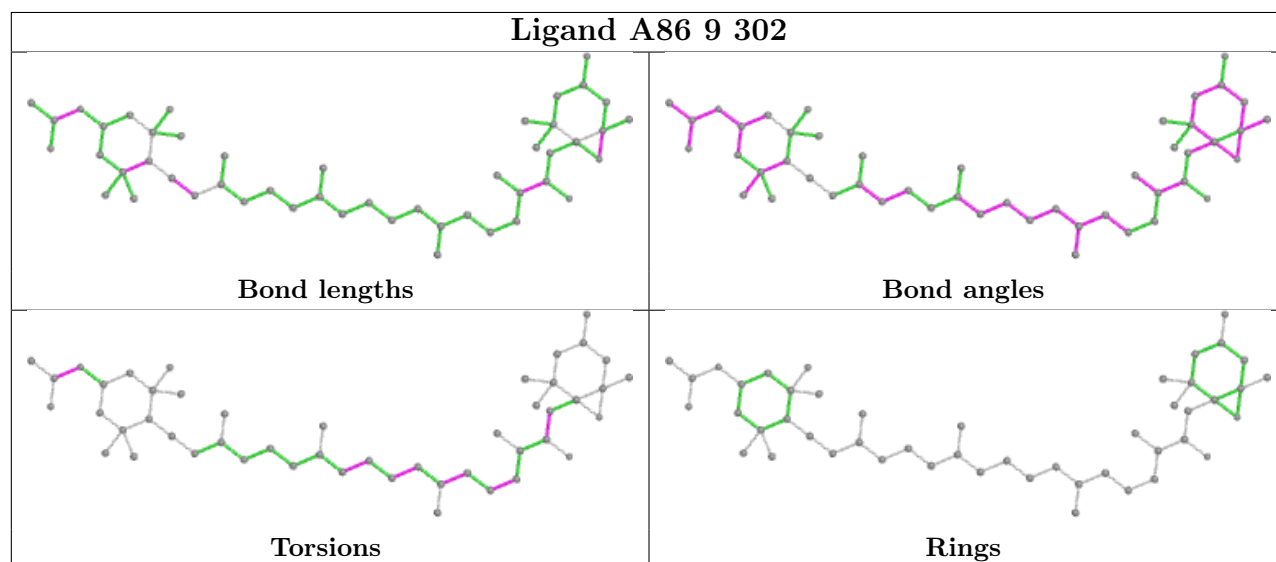


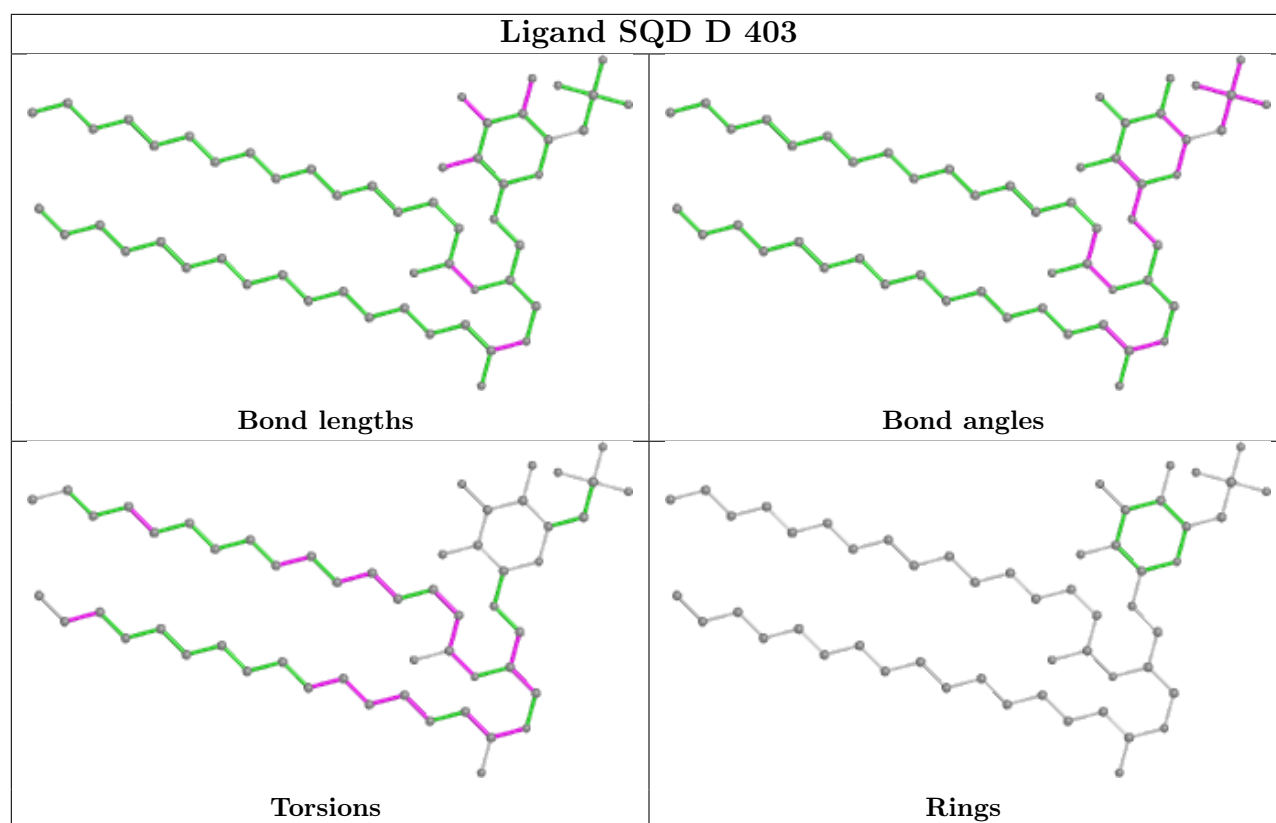
## Ligand BCR k 101



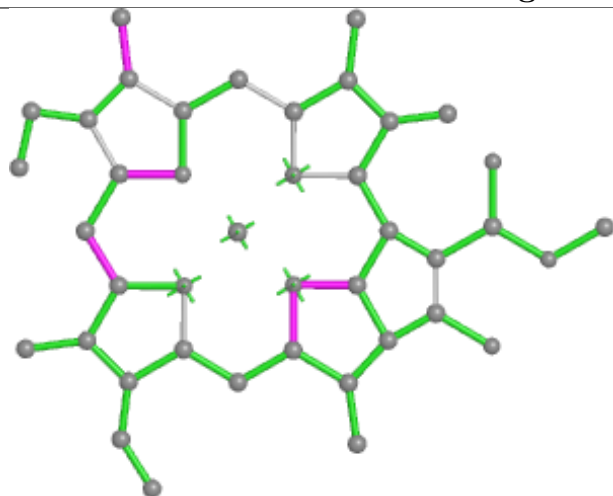
## Ligand CLA 3 319



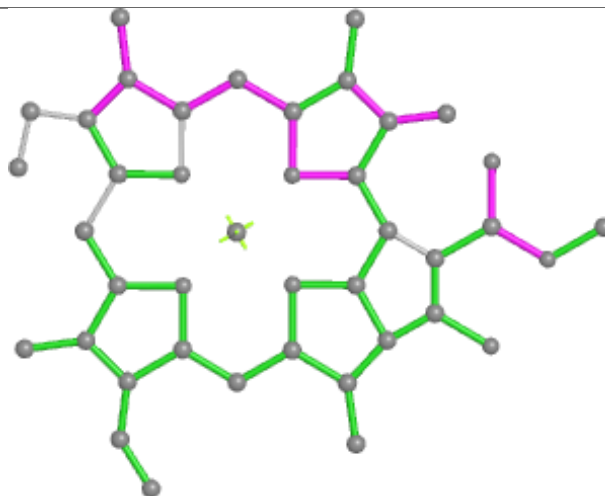
**Ligand CLA 0 307****Ligand A86 9 302**



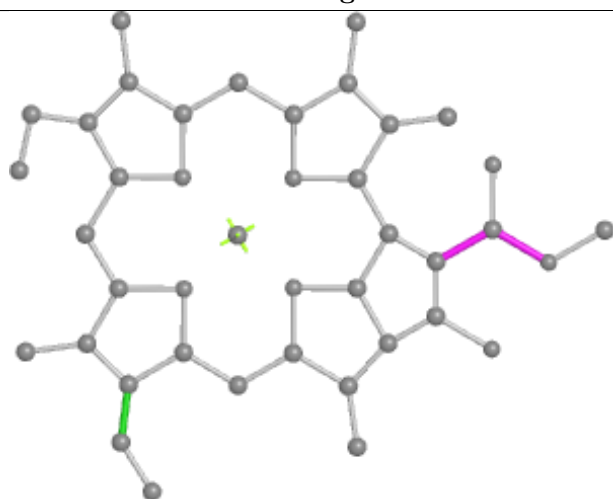
## Ligand CLA 1 305



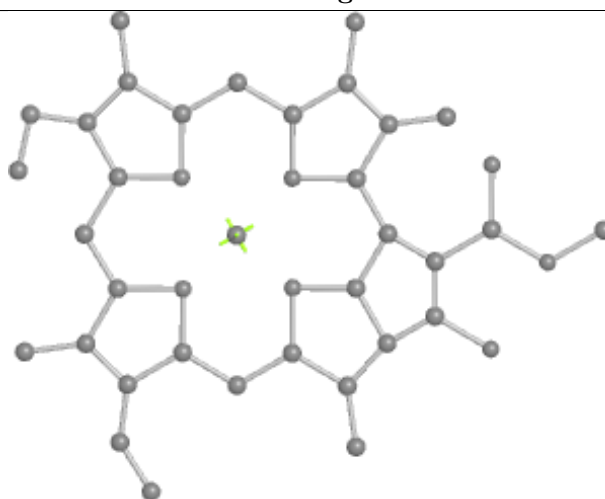
Bond lengths



Bond angles

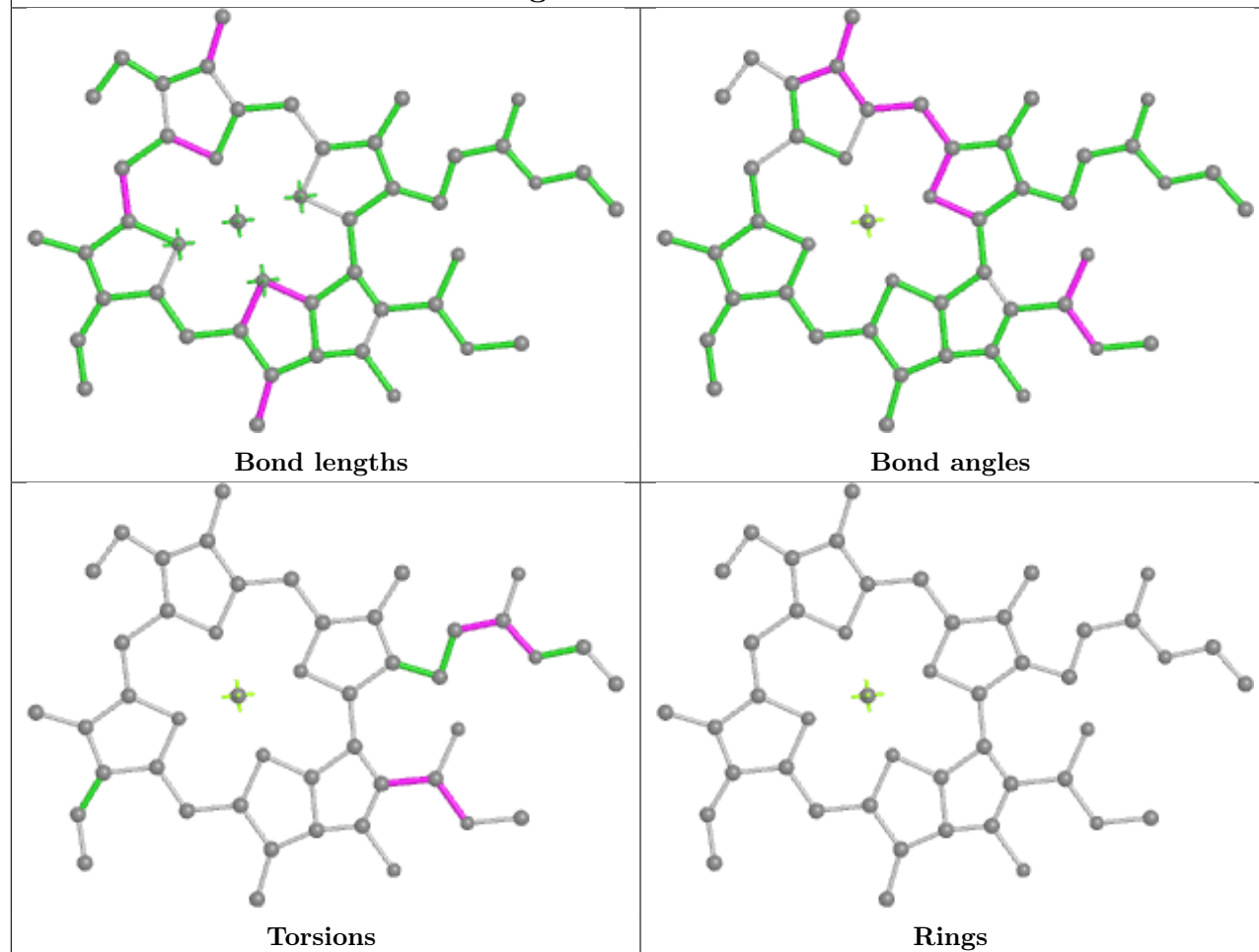


Torsions

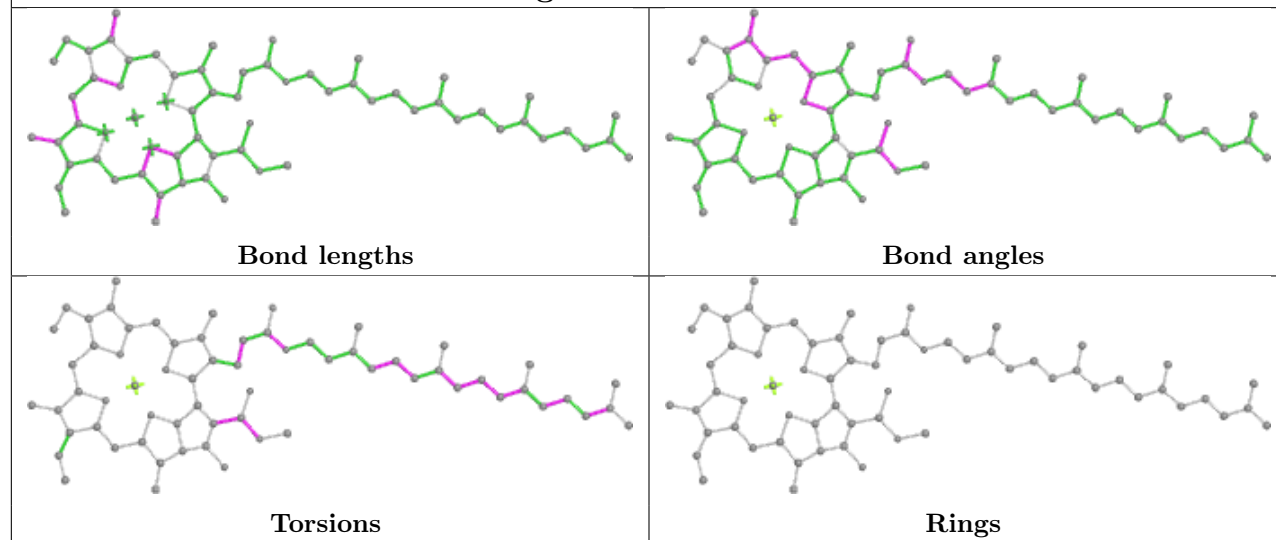


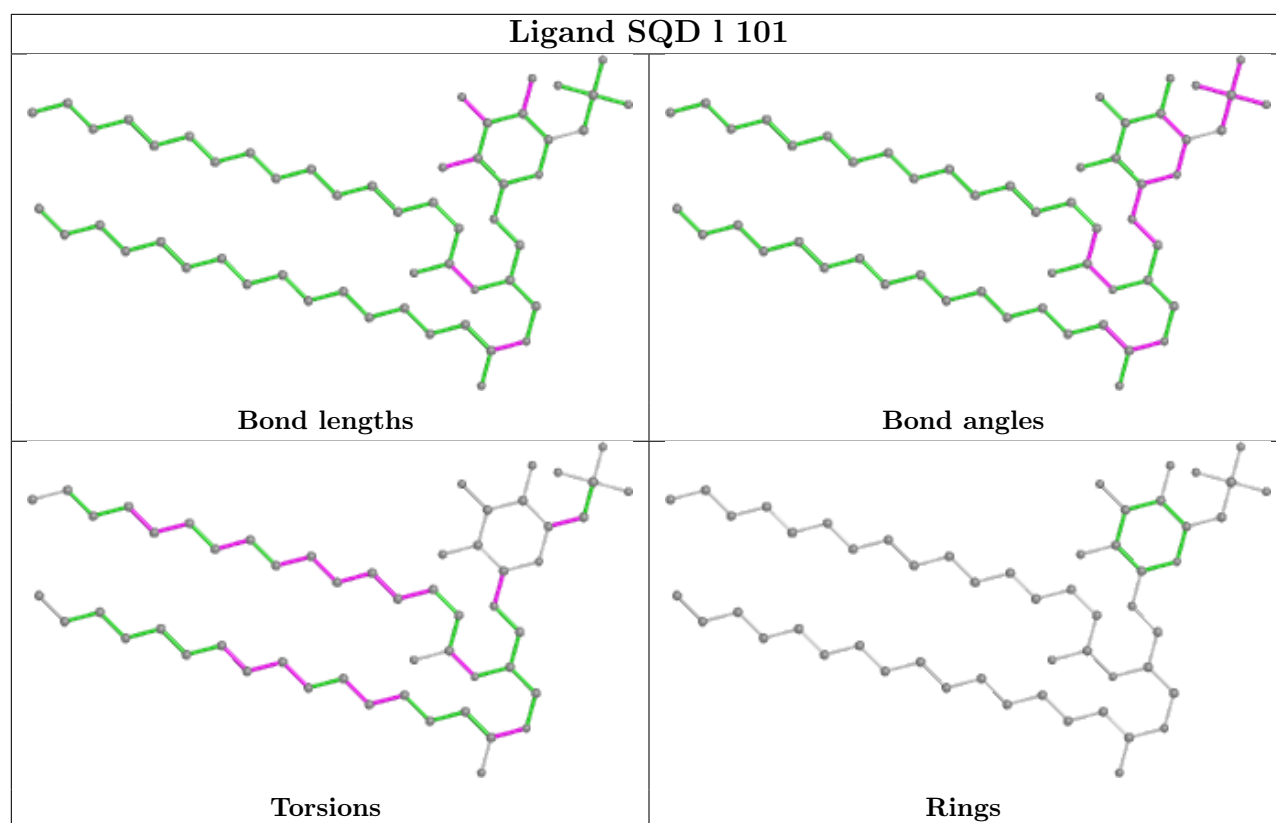
Rings

## Ligand CLA 7 304

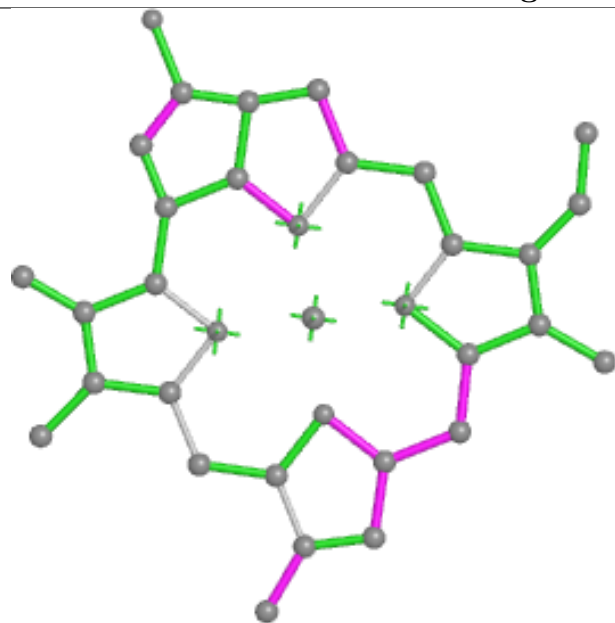


## Ligand CLA 7 309

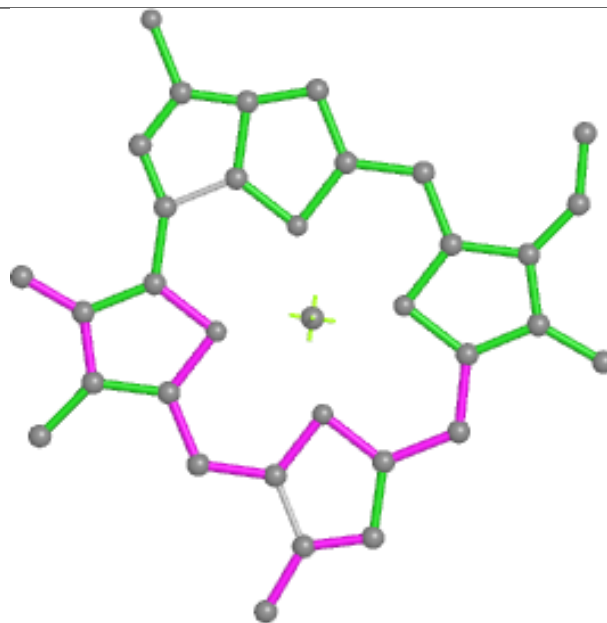




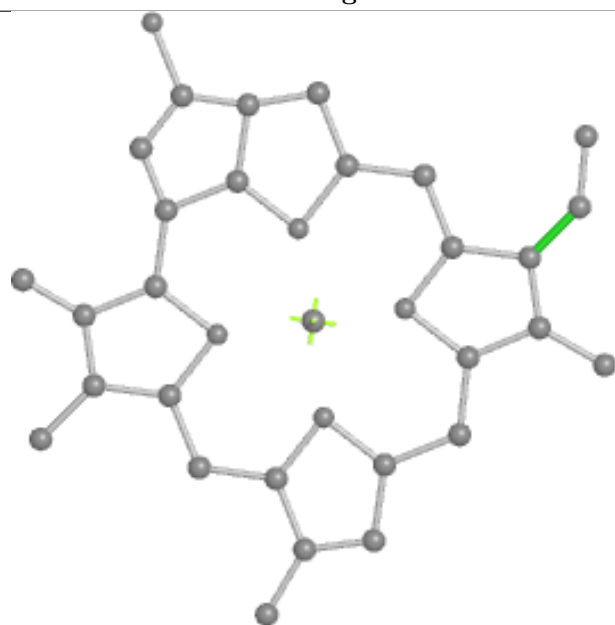
## Ligand CLA 7 313



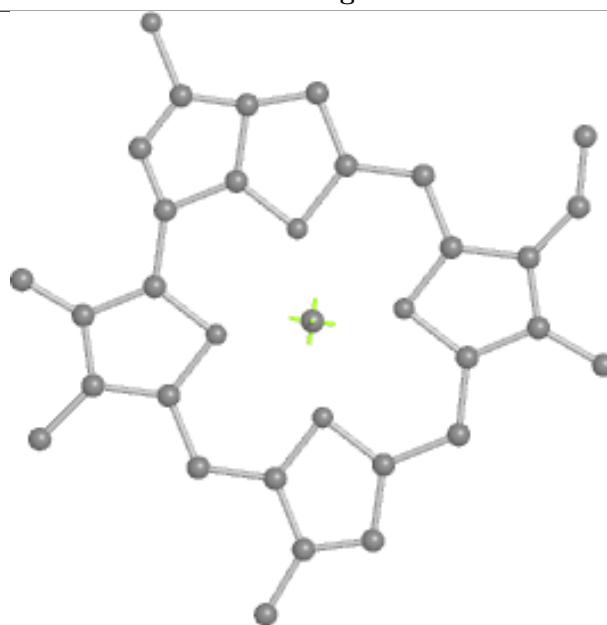
Bond lengths



Bond angles

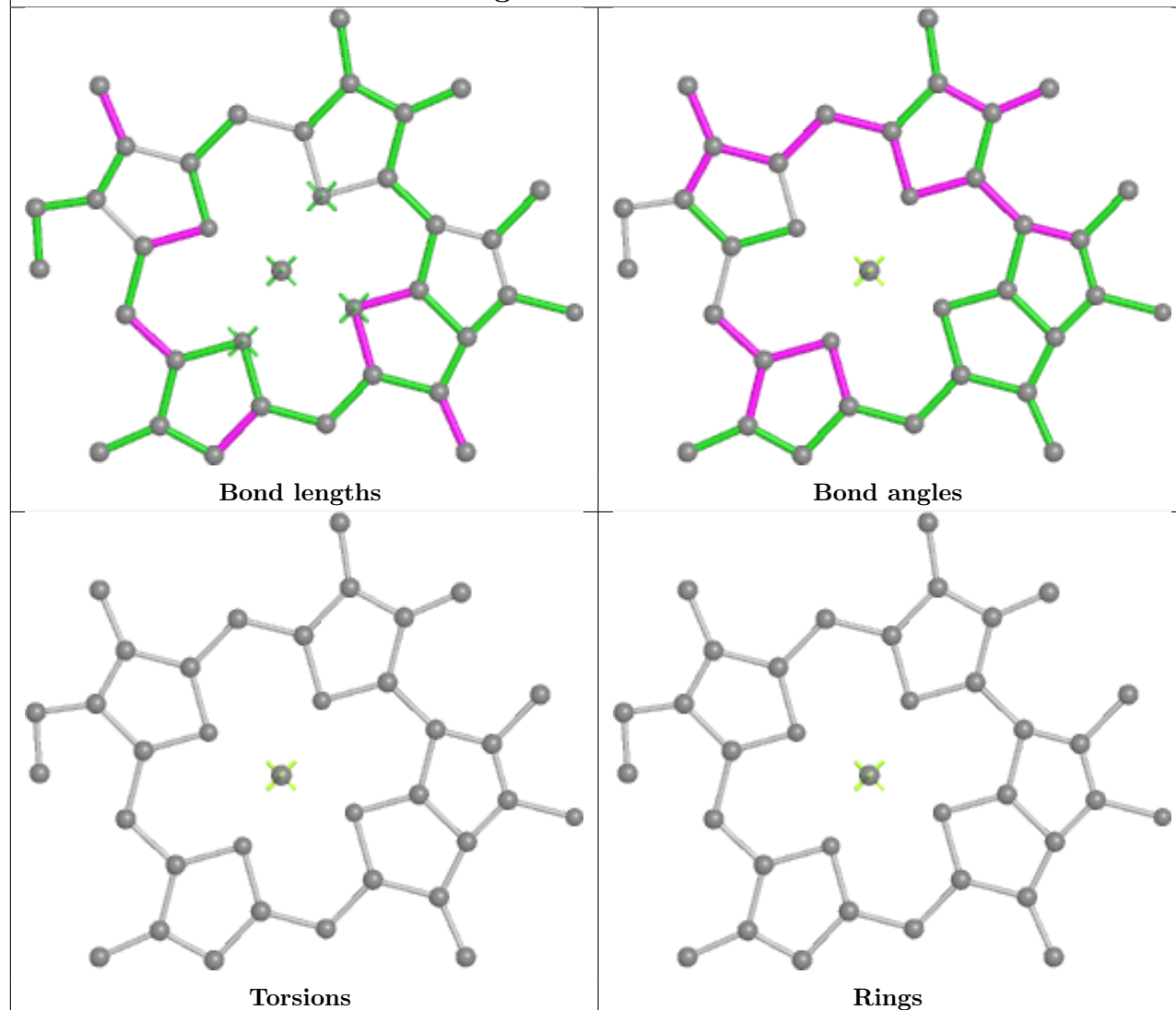


Torsions

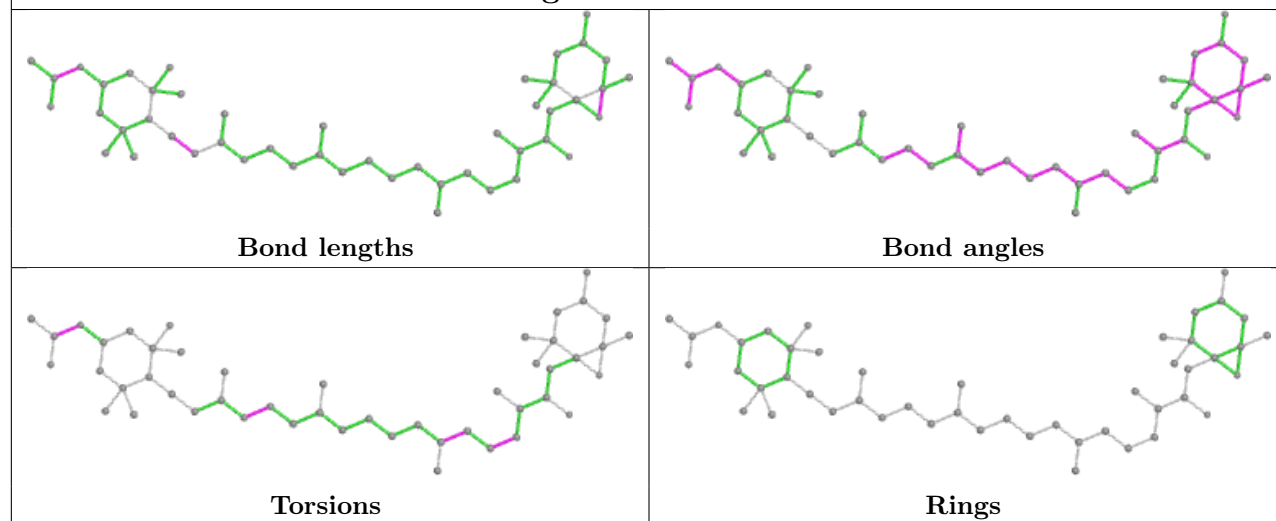


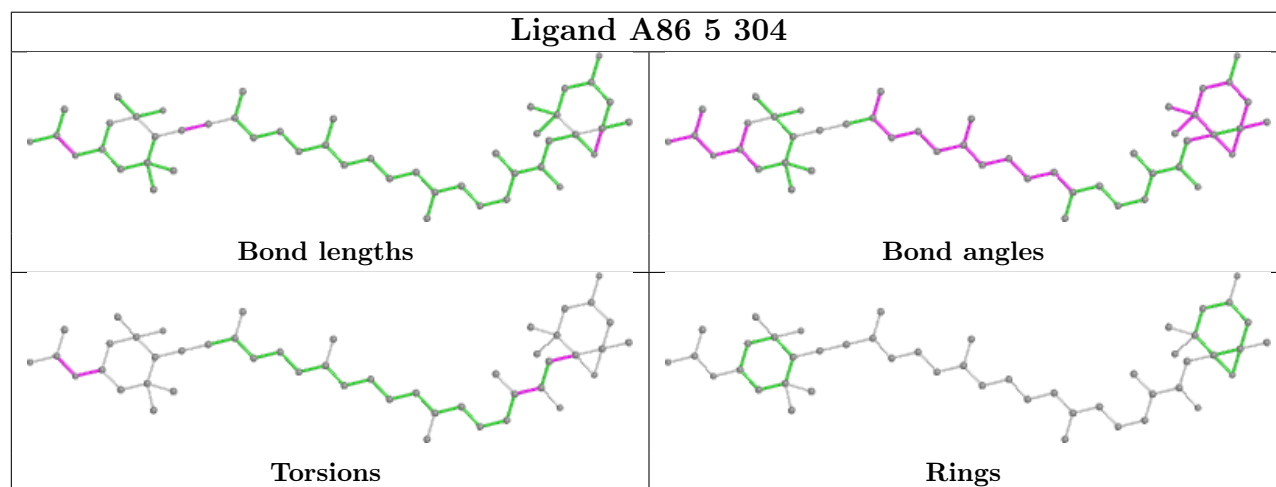
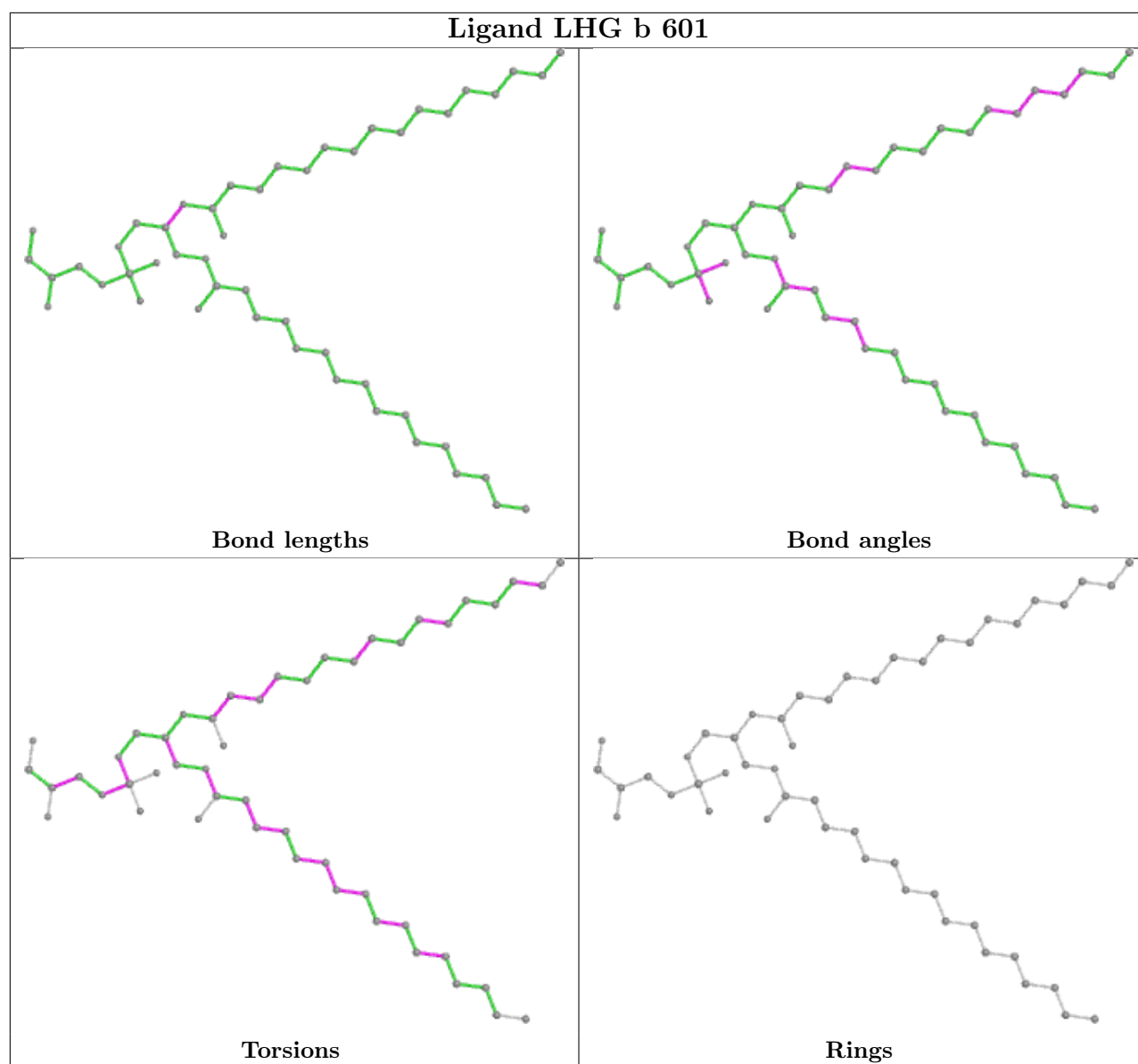
Rings

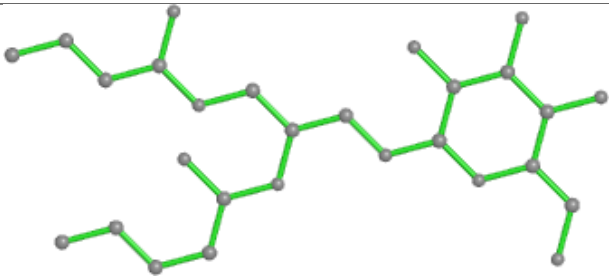
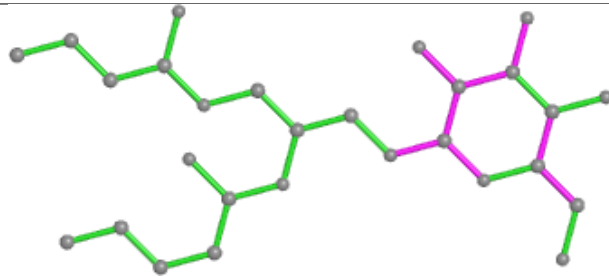
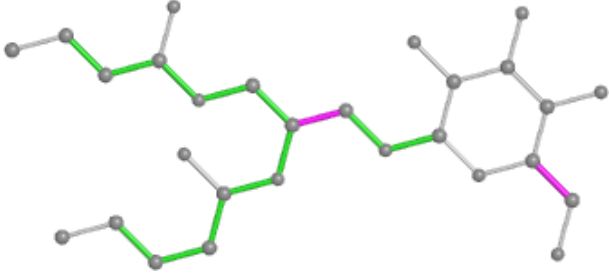
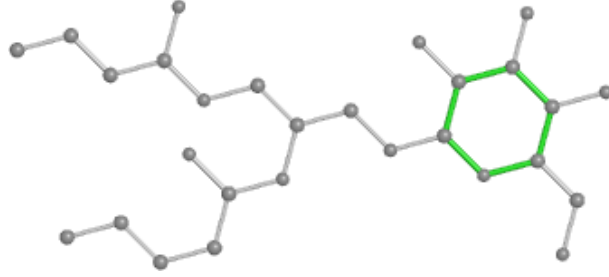
## Ligand CLA 8 313

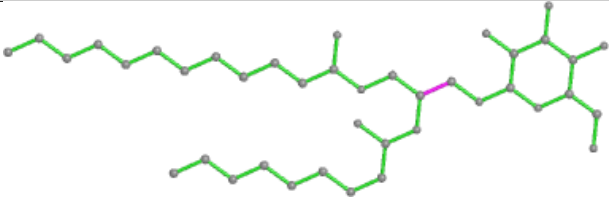
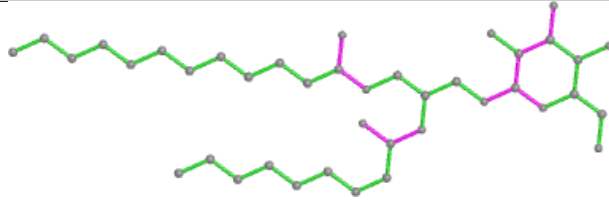
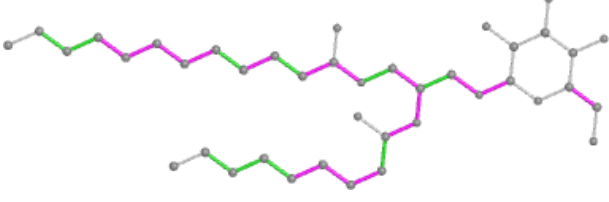
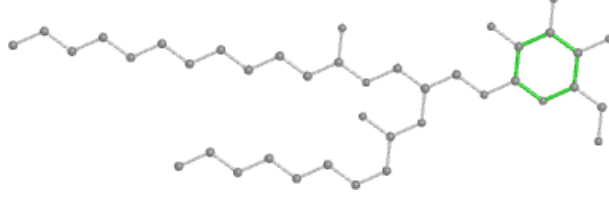


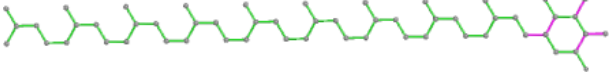
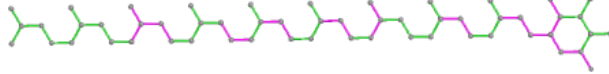
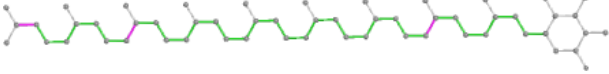
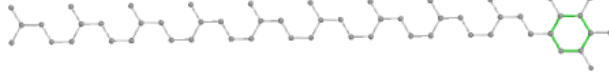
## Ligand A86 7 303

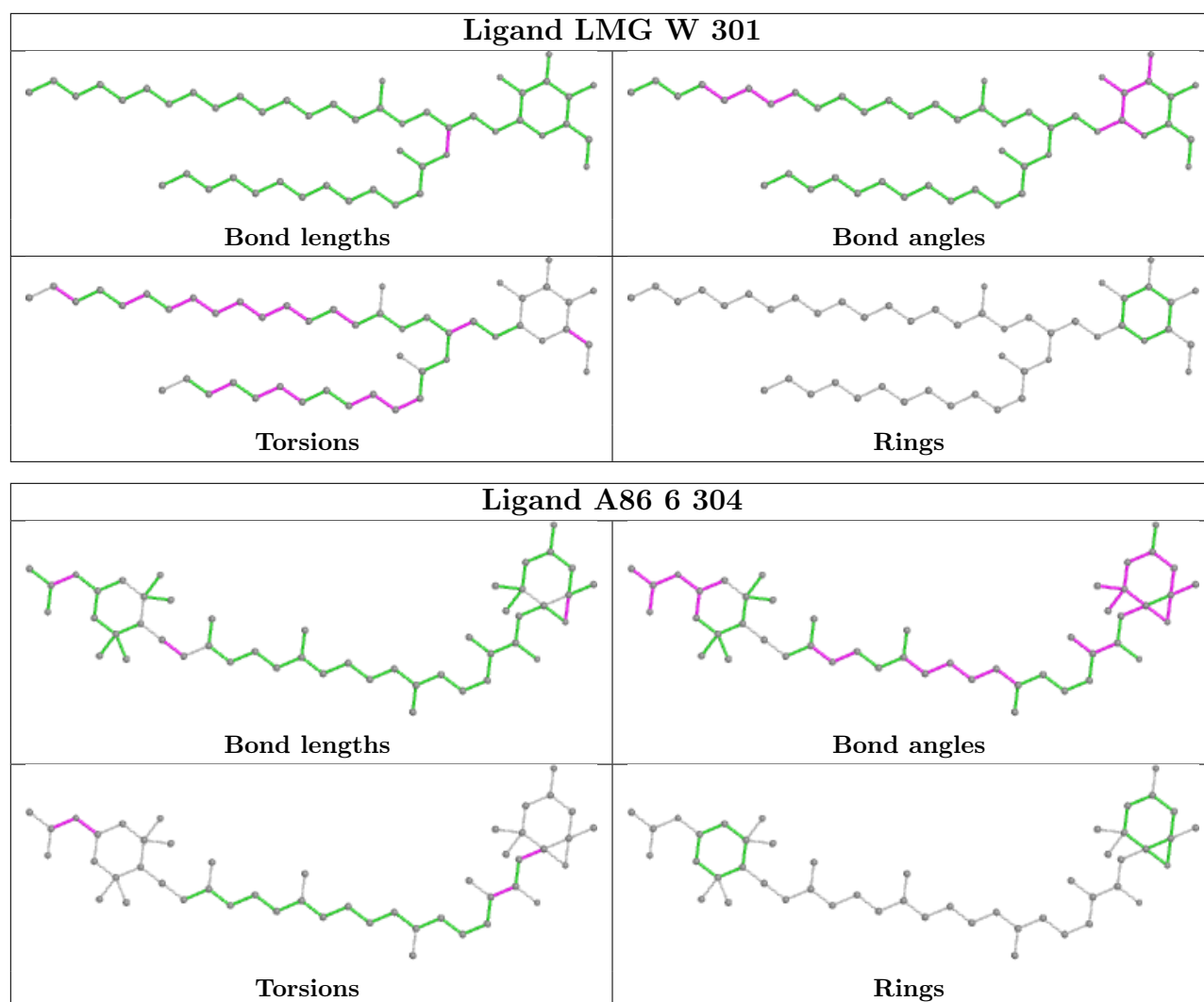




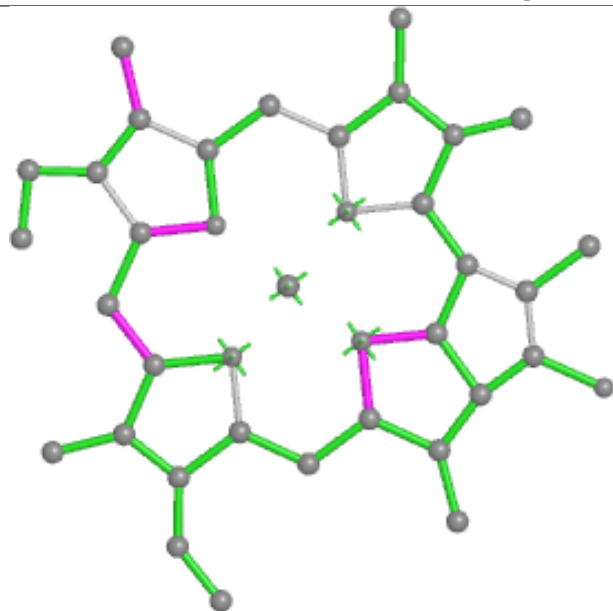
Ligand LMG b 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

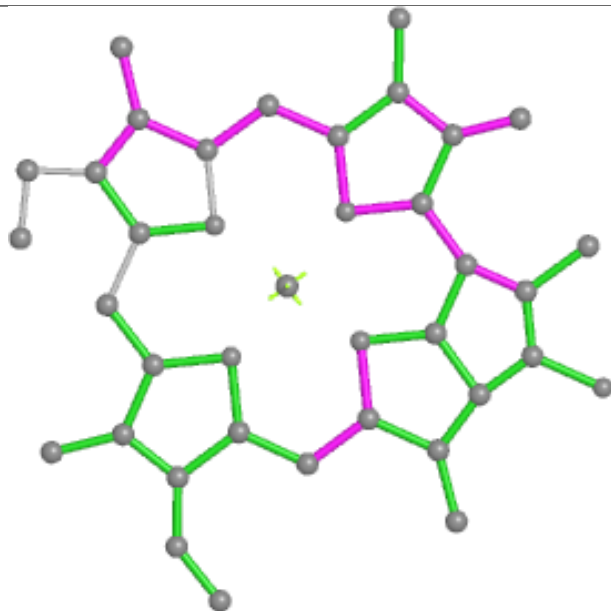
Ligand PL9 D 408	
	
Bond lengths	Bond angles
	
Torsions	Rings



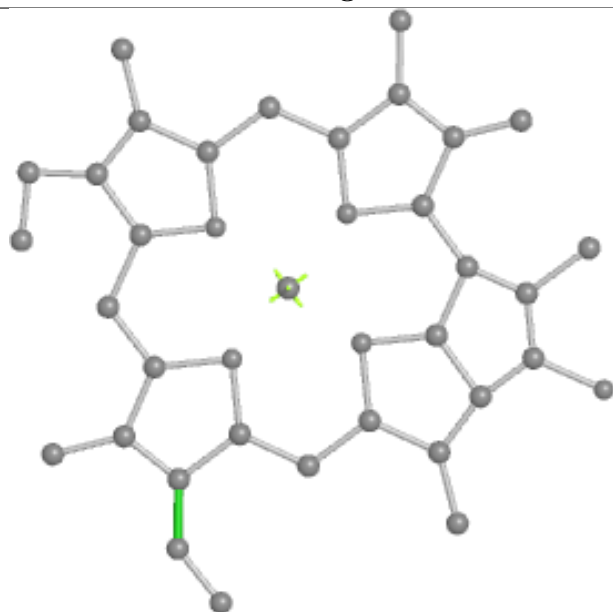
## Ligand CLA 5 317



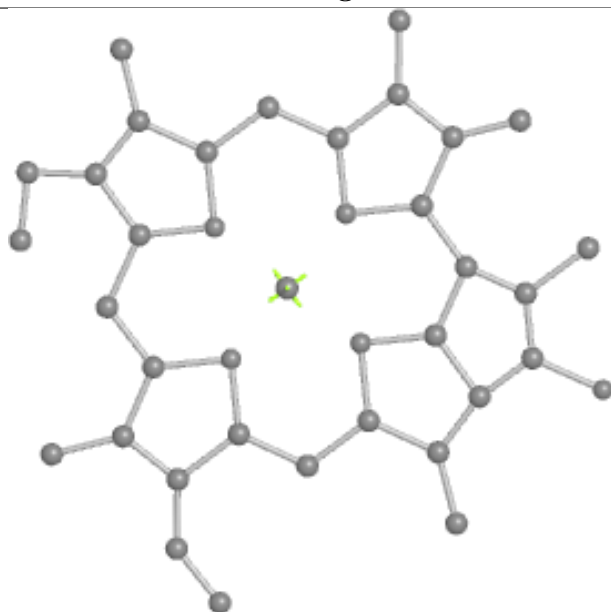
Bond lengths



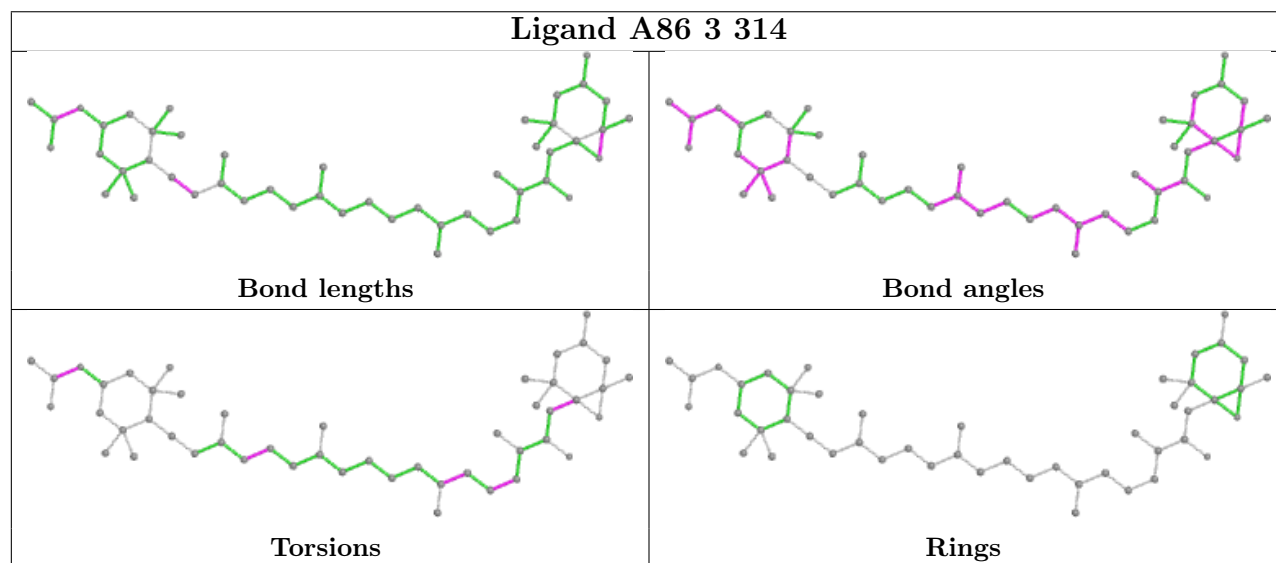
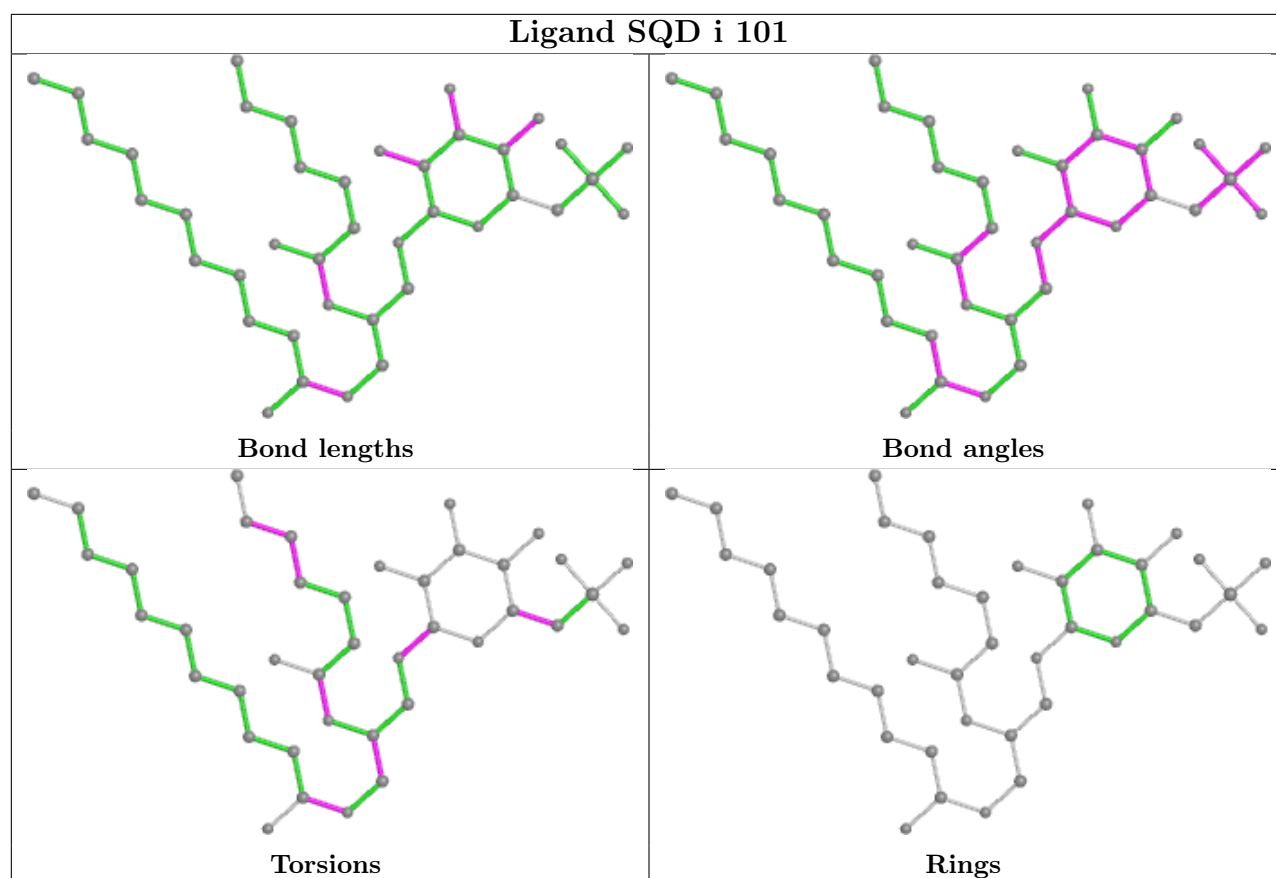
Bond angles



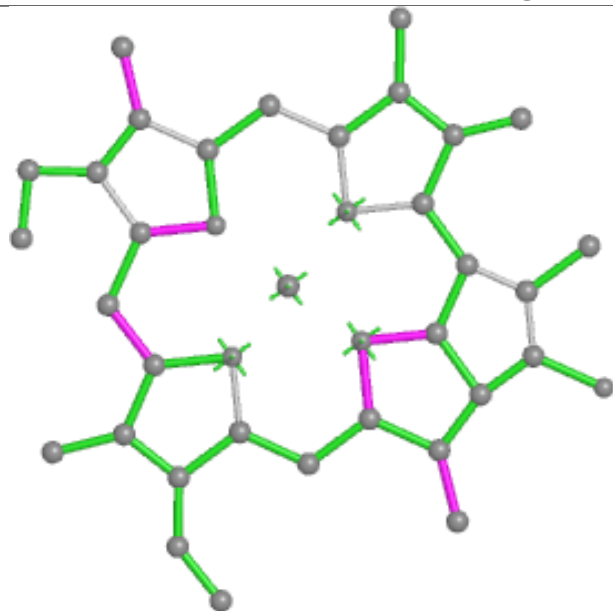
Torsions



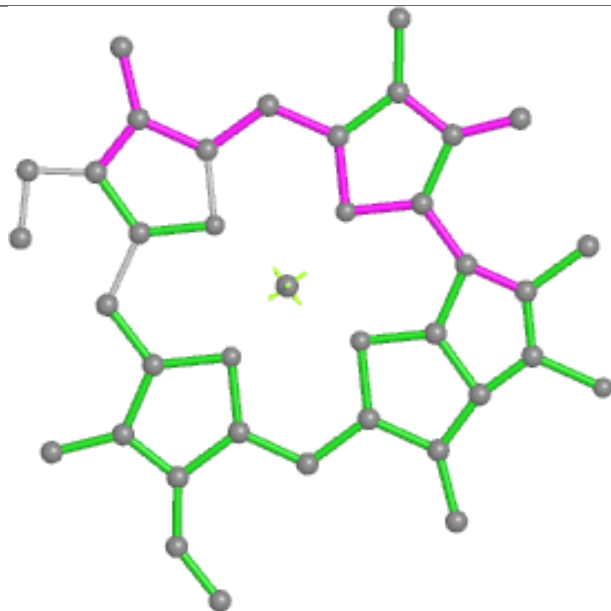
Rings



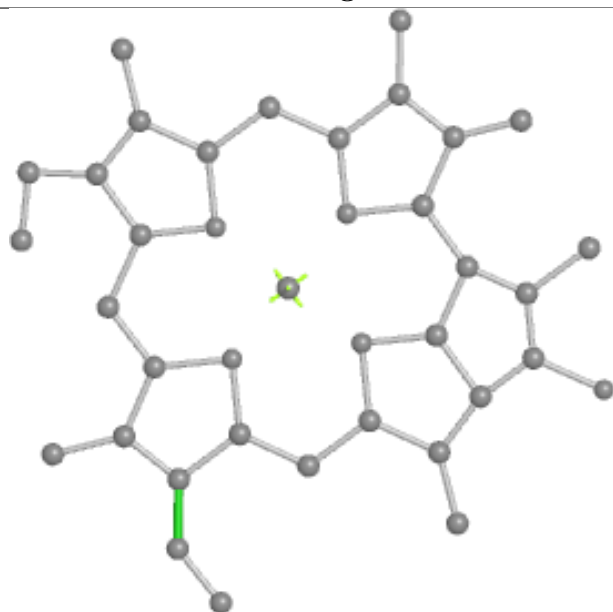
## Ligand CLA 9 314



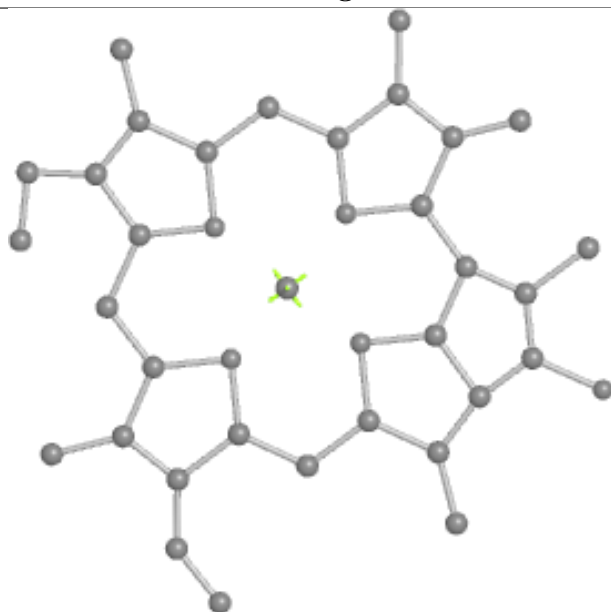
Bond lengths



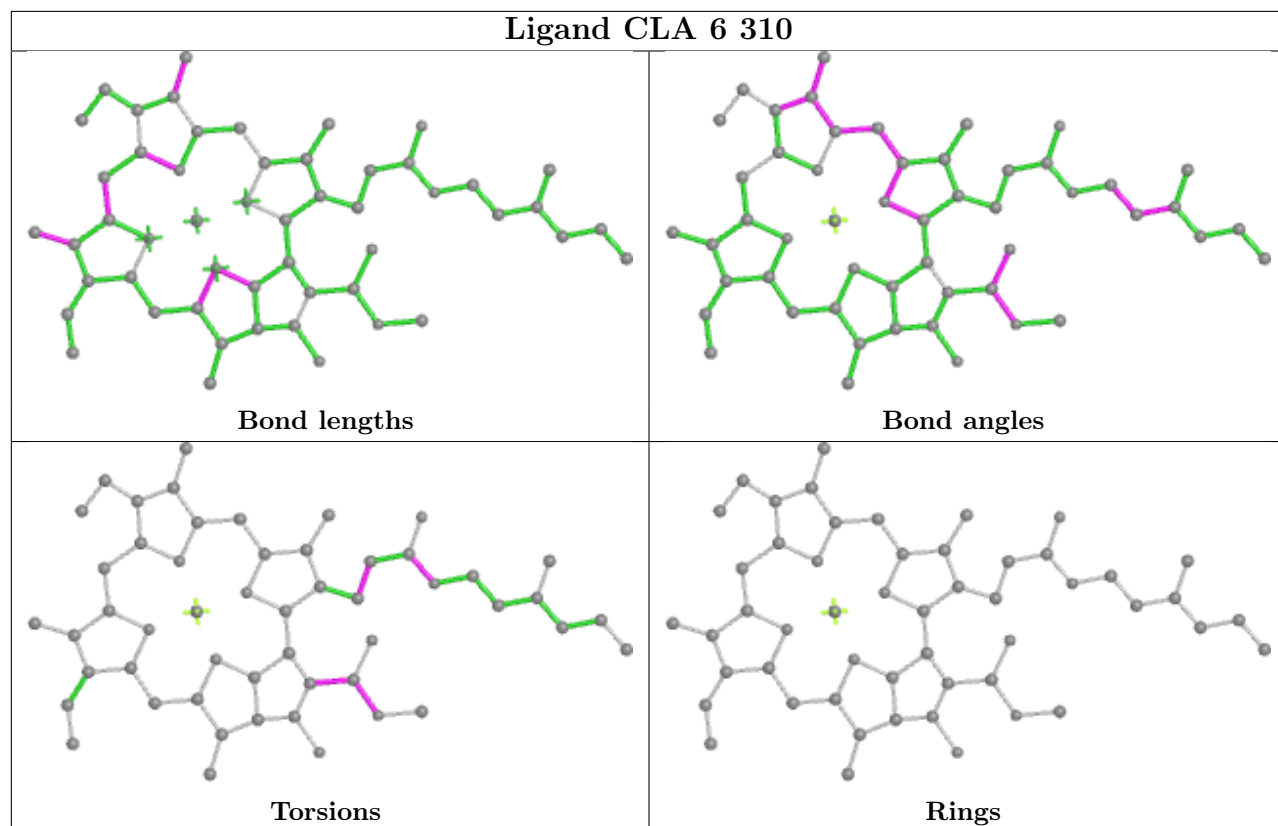
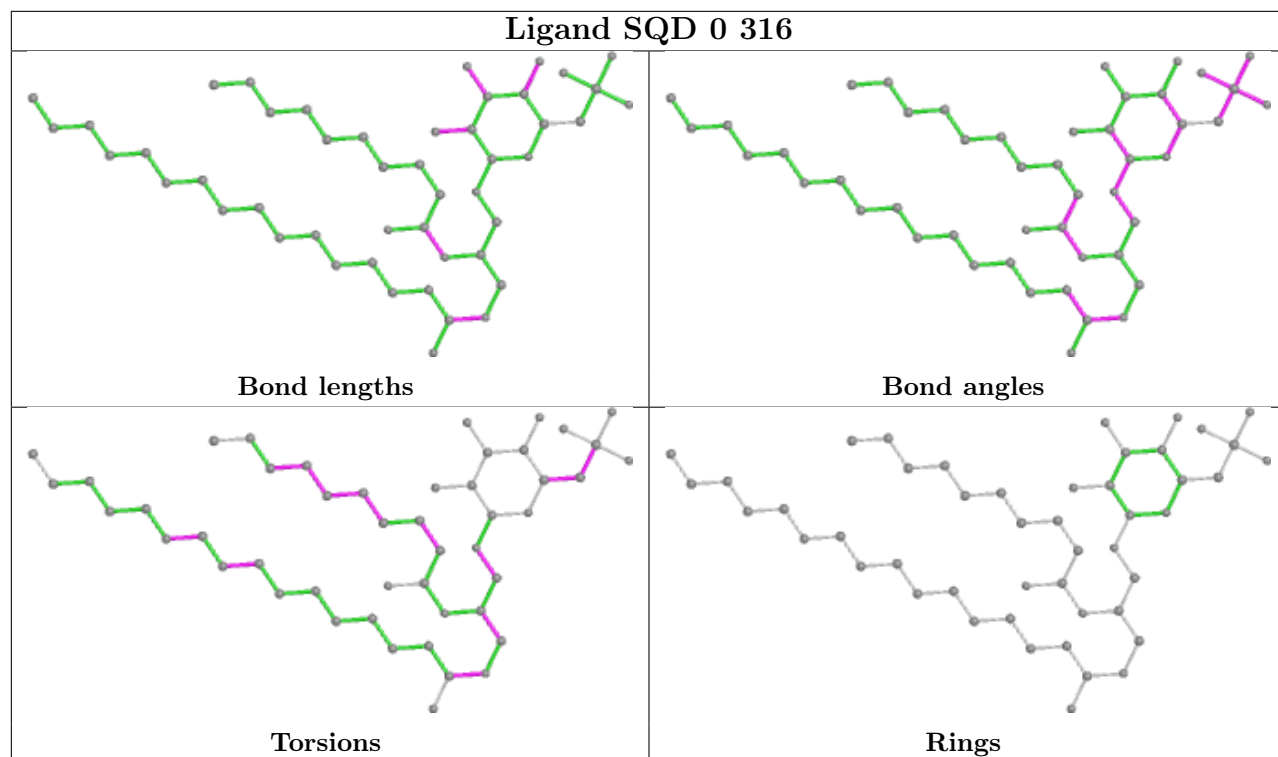
Bond angles

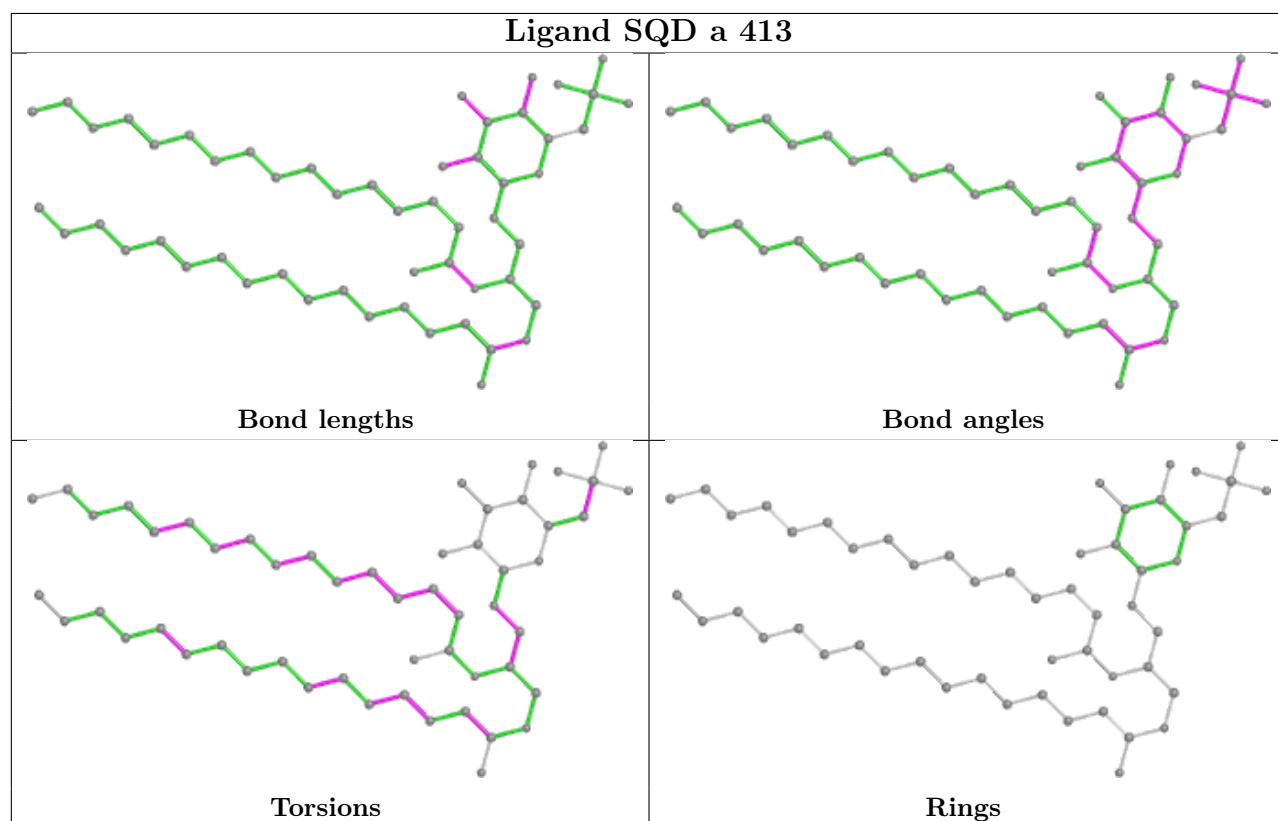
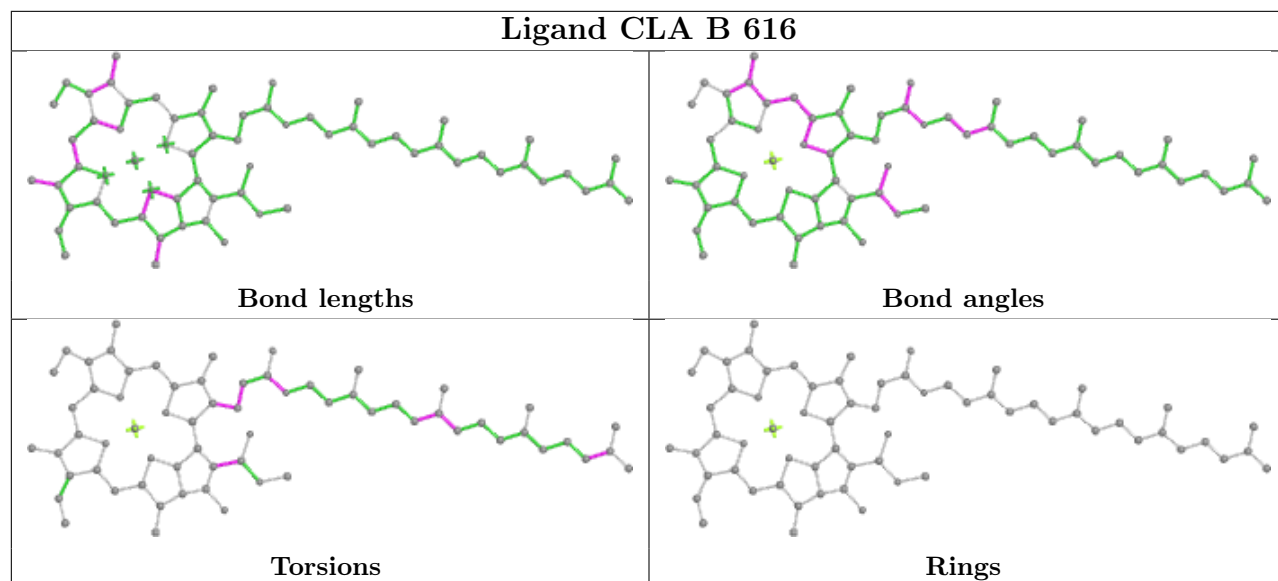
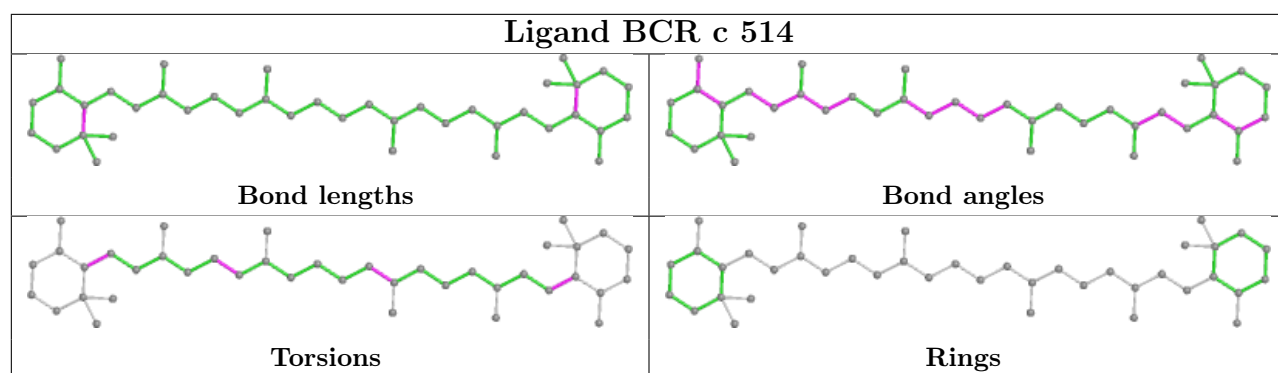


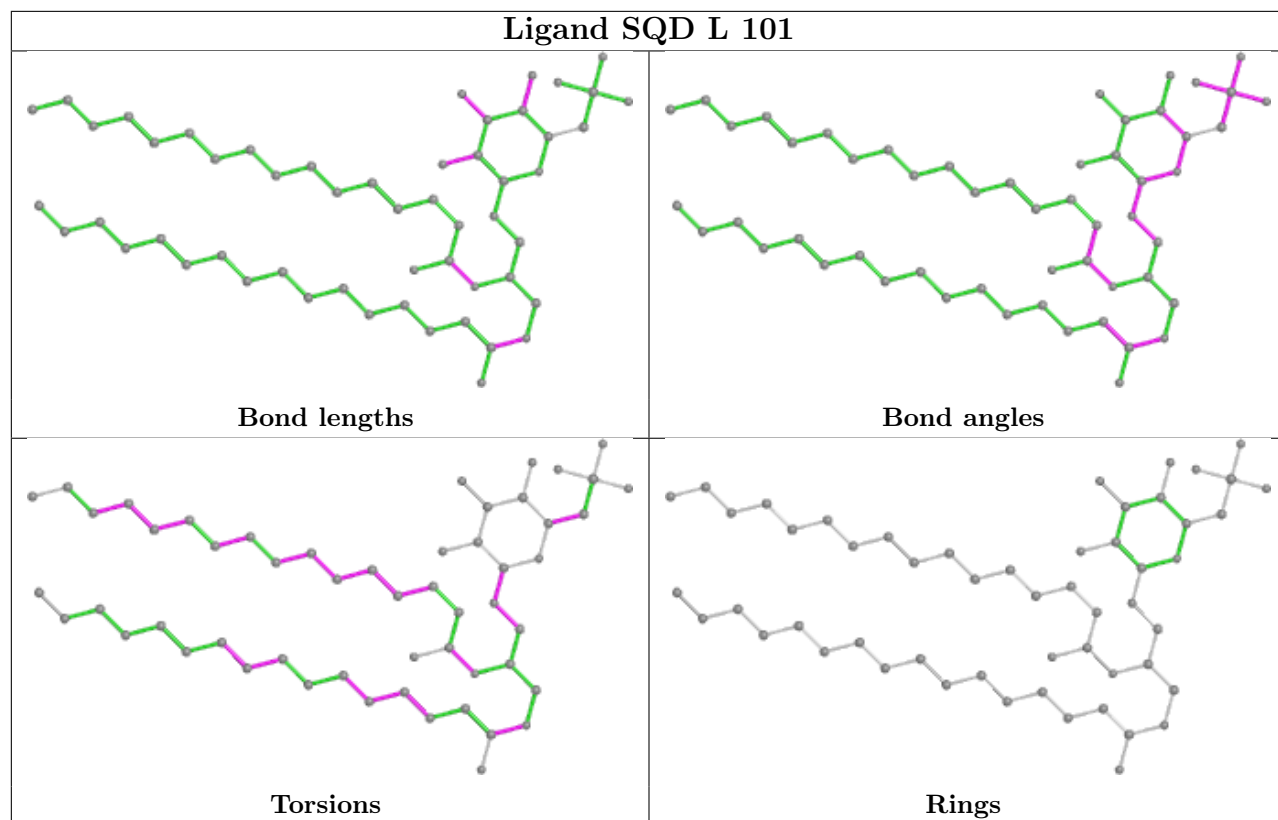
Torsions



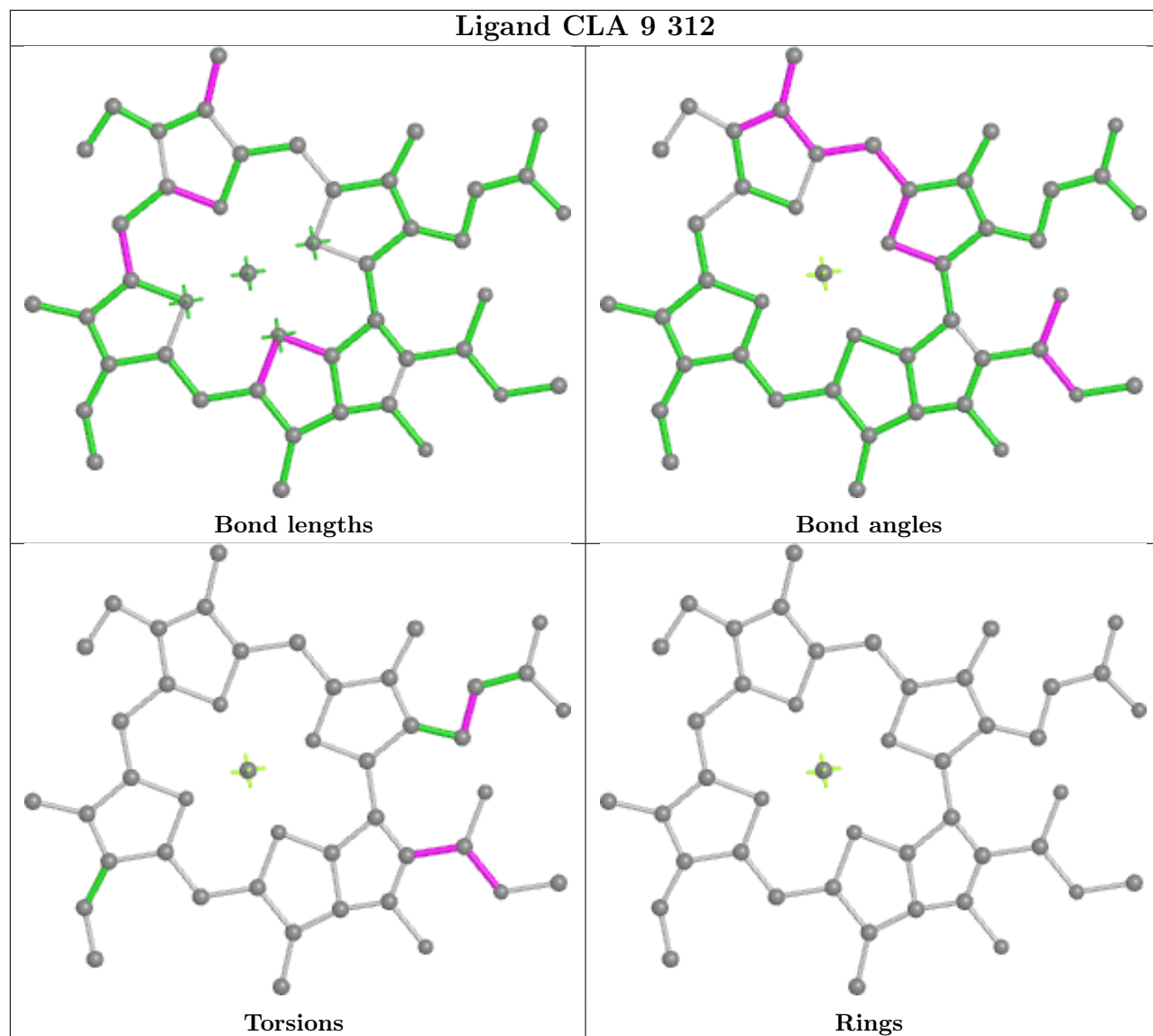
Rings



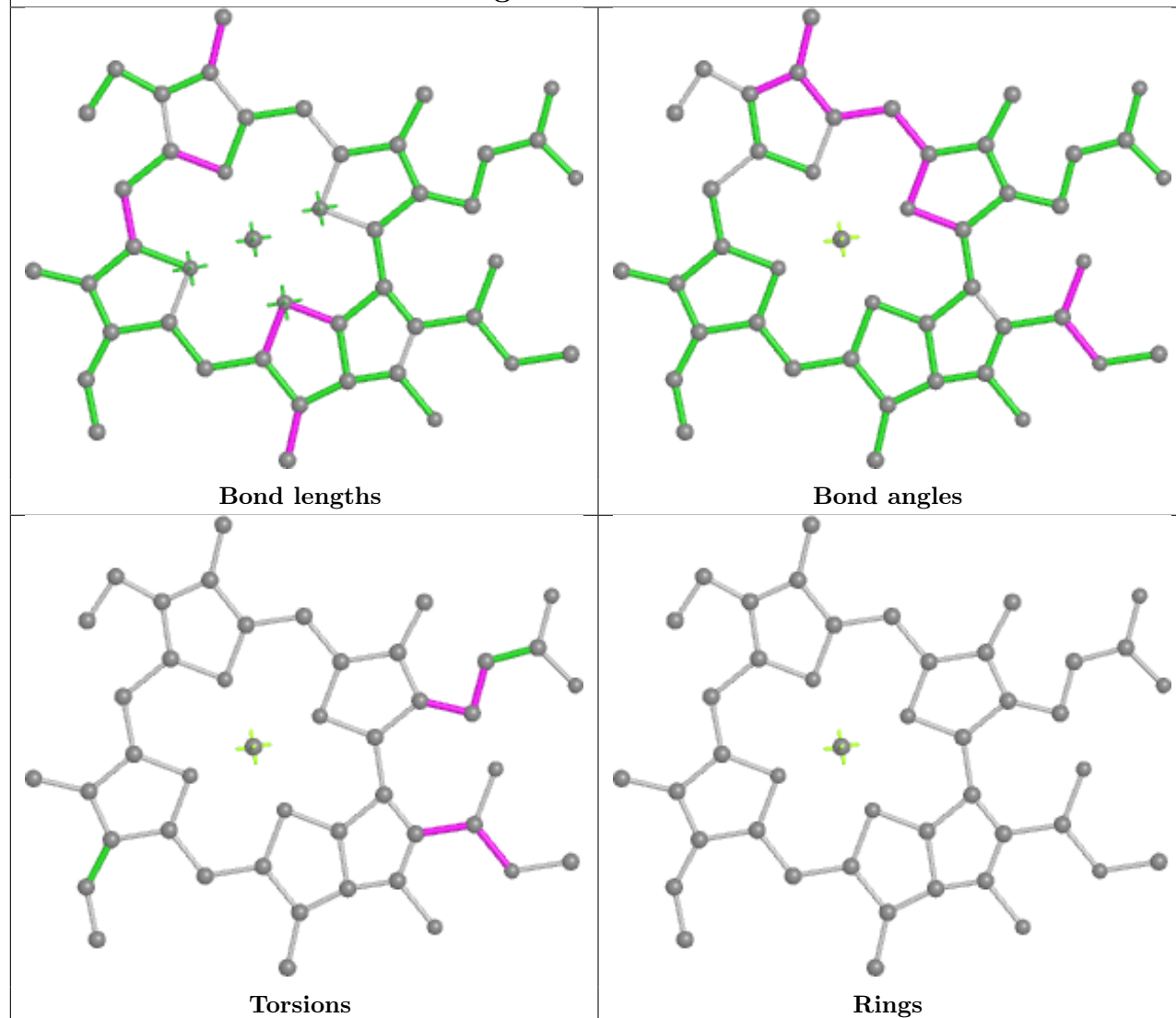




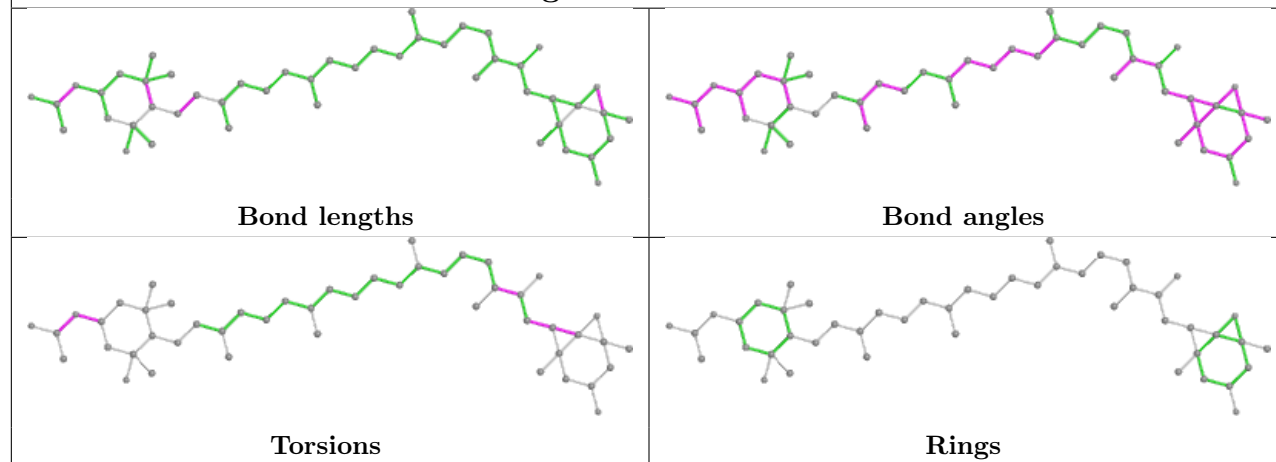
## Ligand CLA 9 312



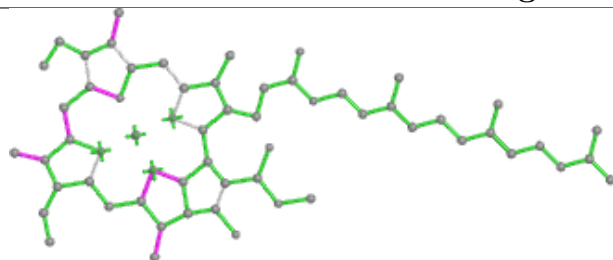
## Ligand CLA 9 306



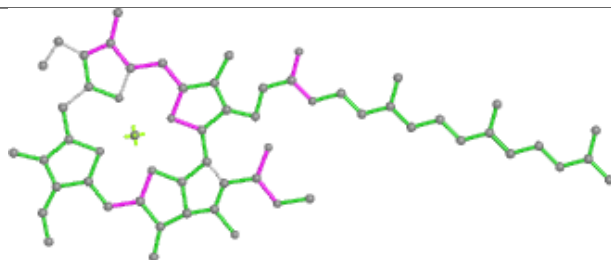
## Ligand A86 5 306



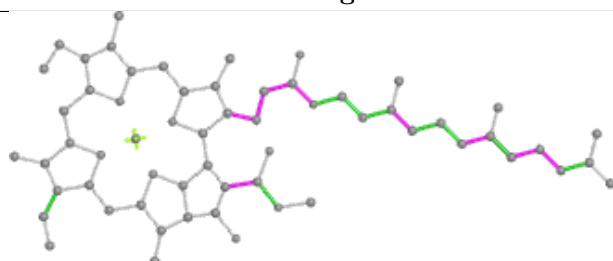
## Ligand CLA 4 311



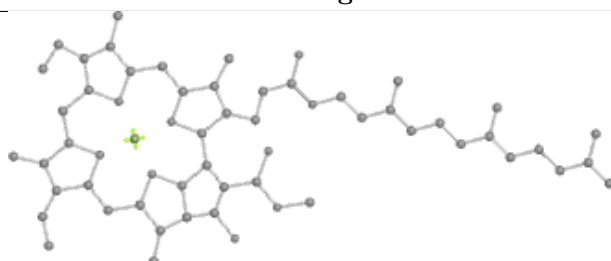
Bond lengths



Bond angles

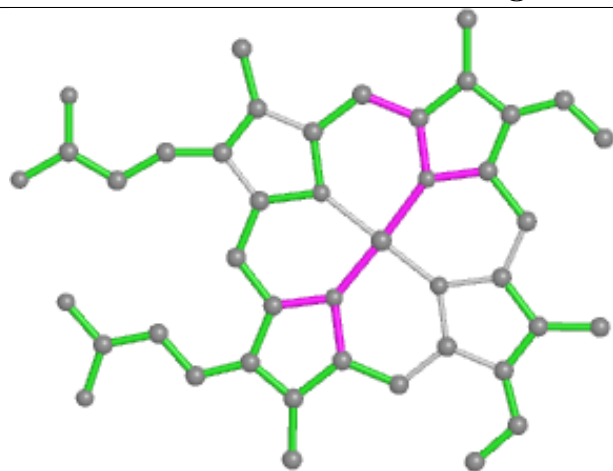


Torsions

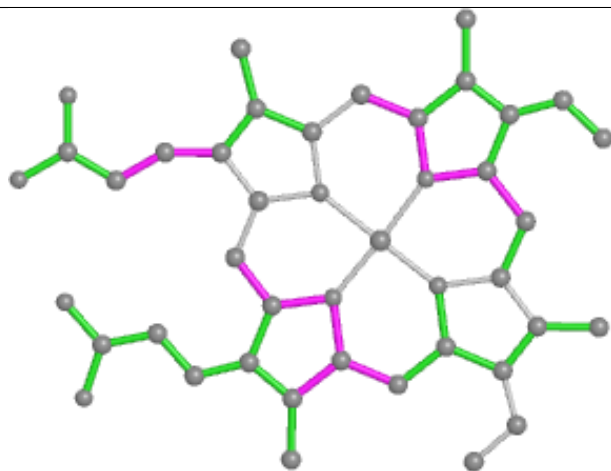


Rings

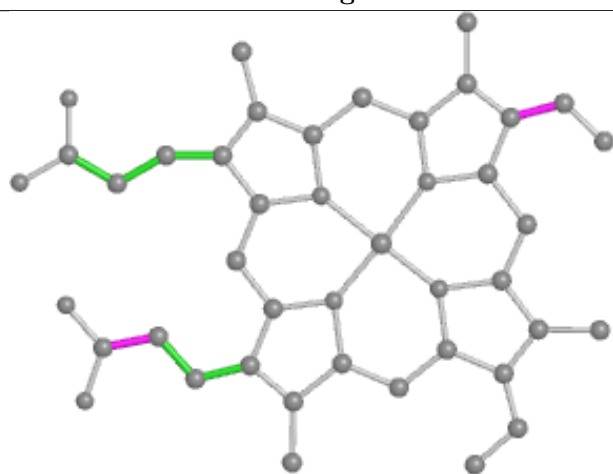
## Ligand HEM V 201



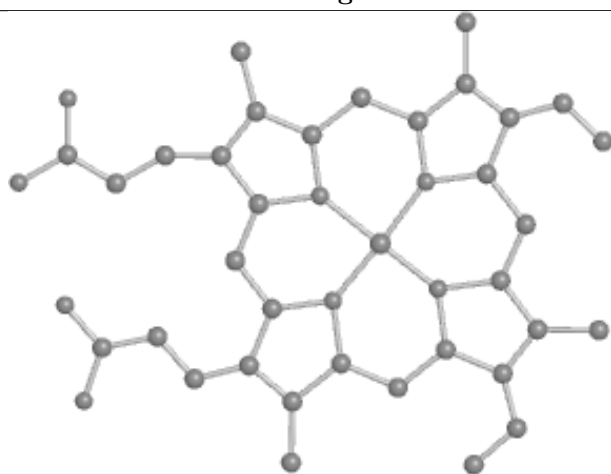
Bond lengths



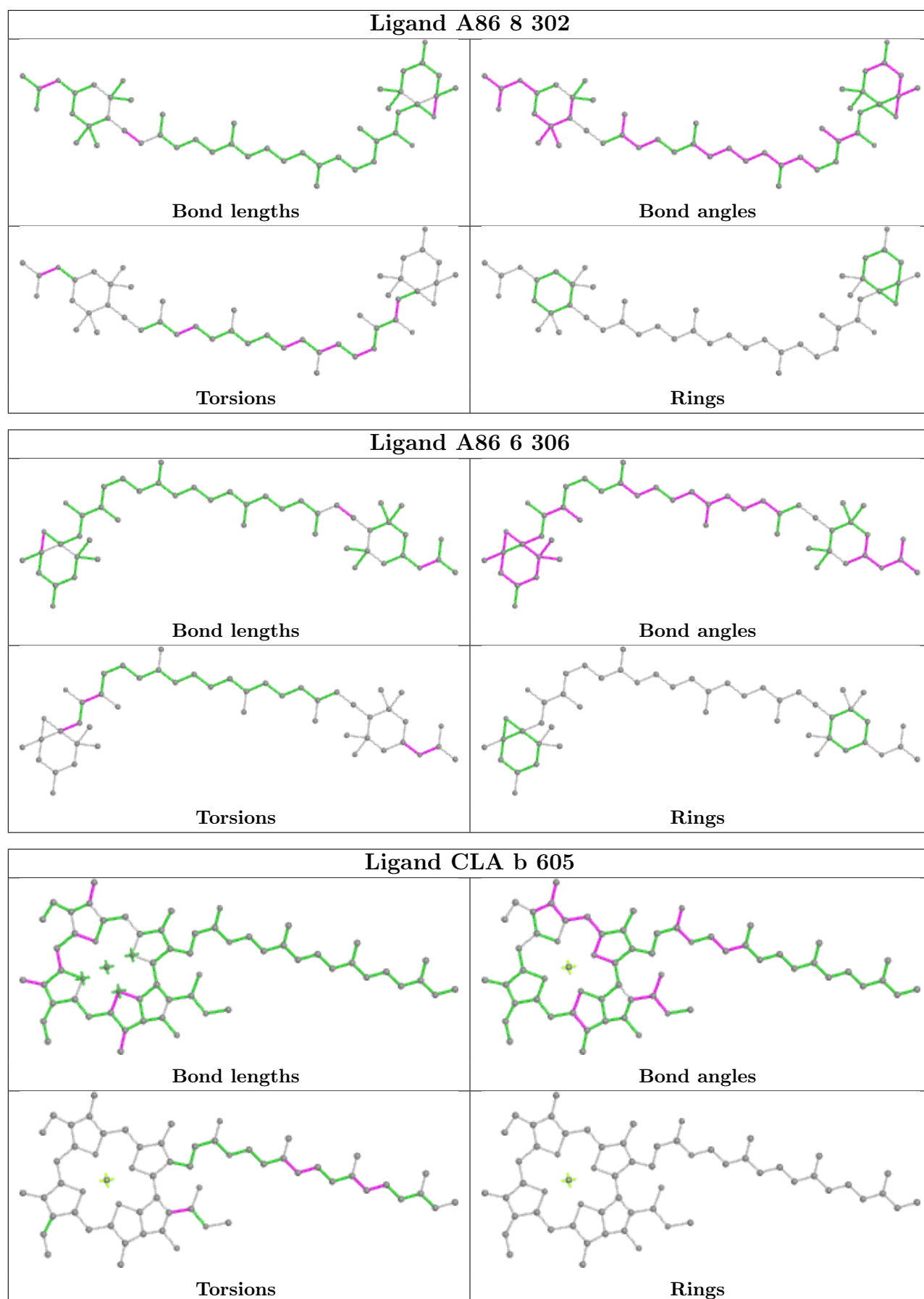
Bond angles



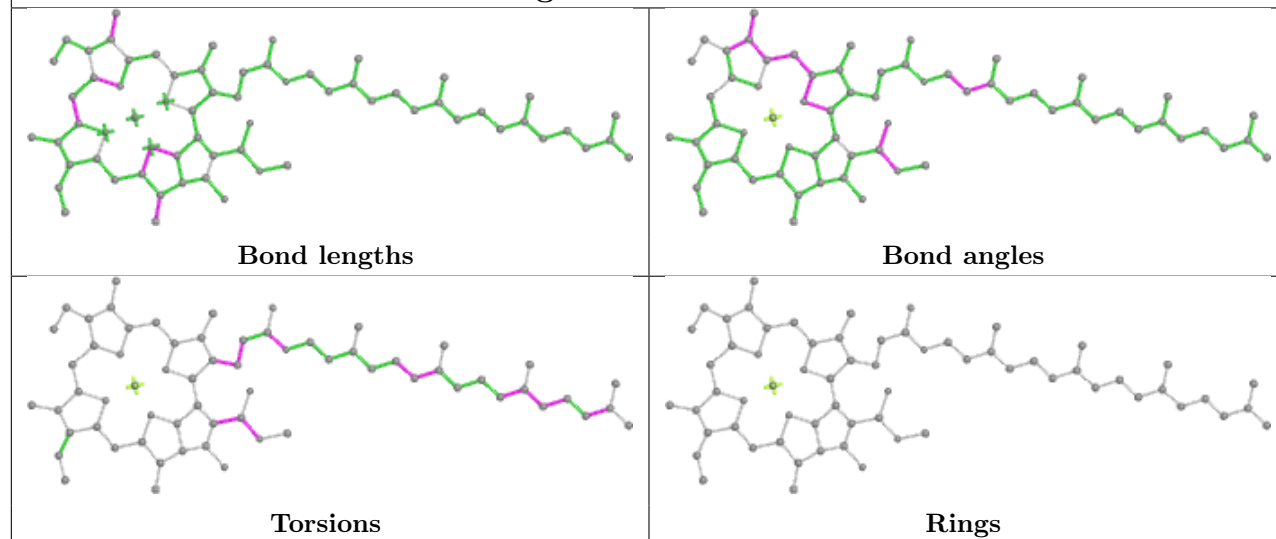
Torsions



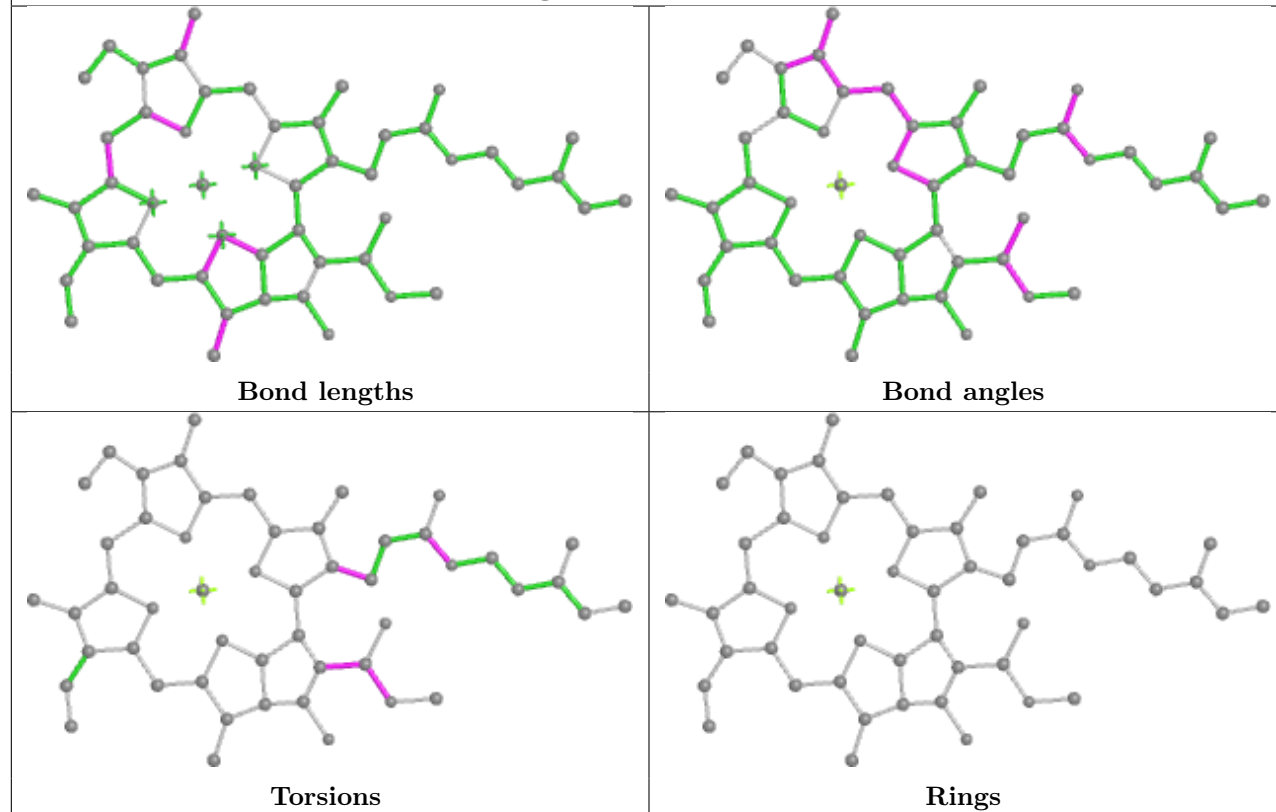
Rings



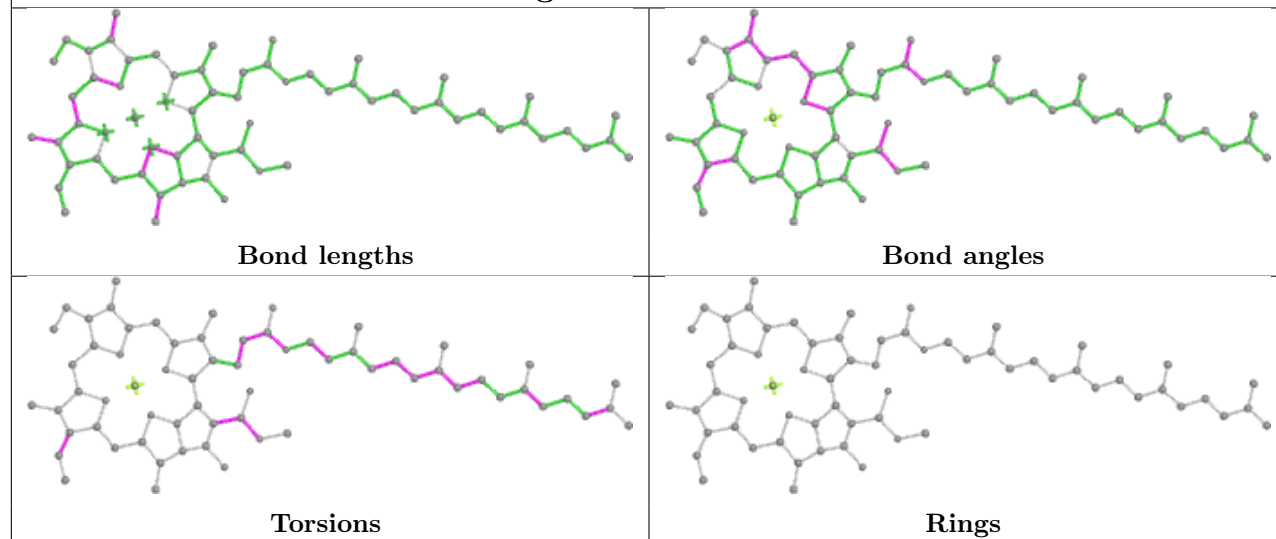
## Ligand CLA 1 310



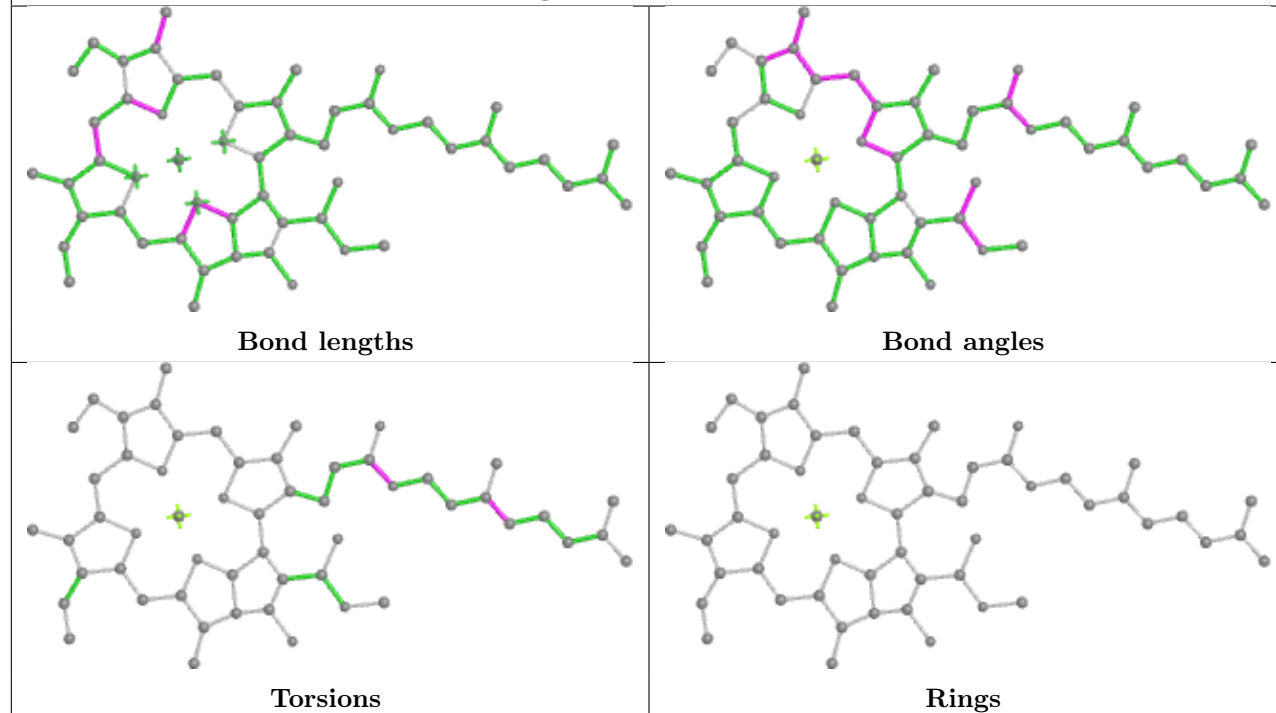
## Ligand CLA 0 311

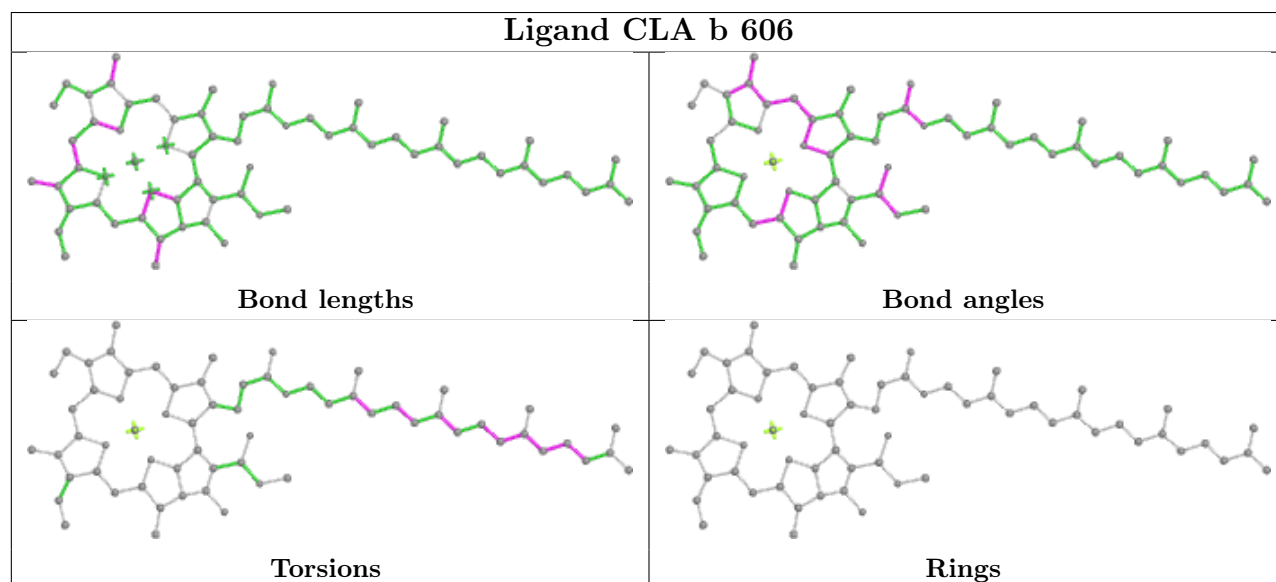
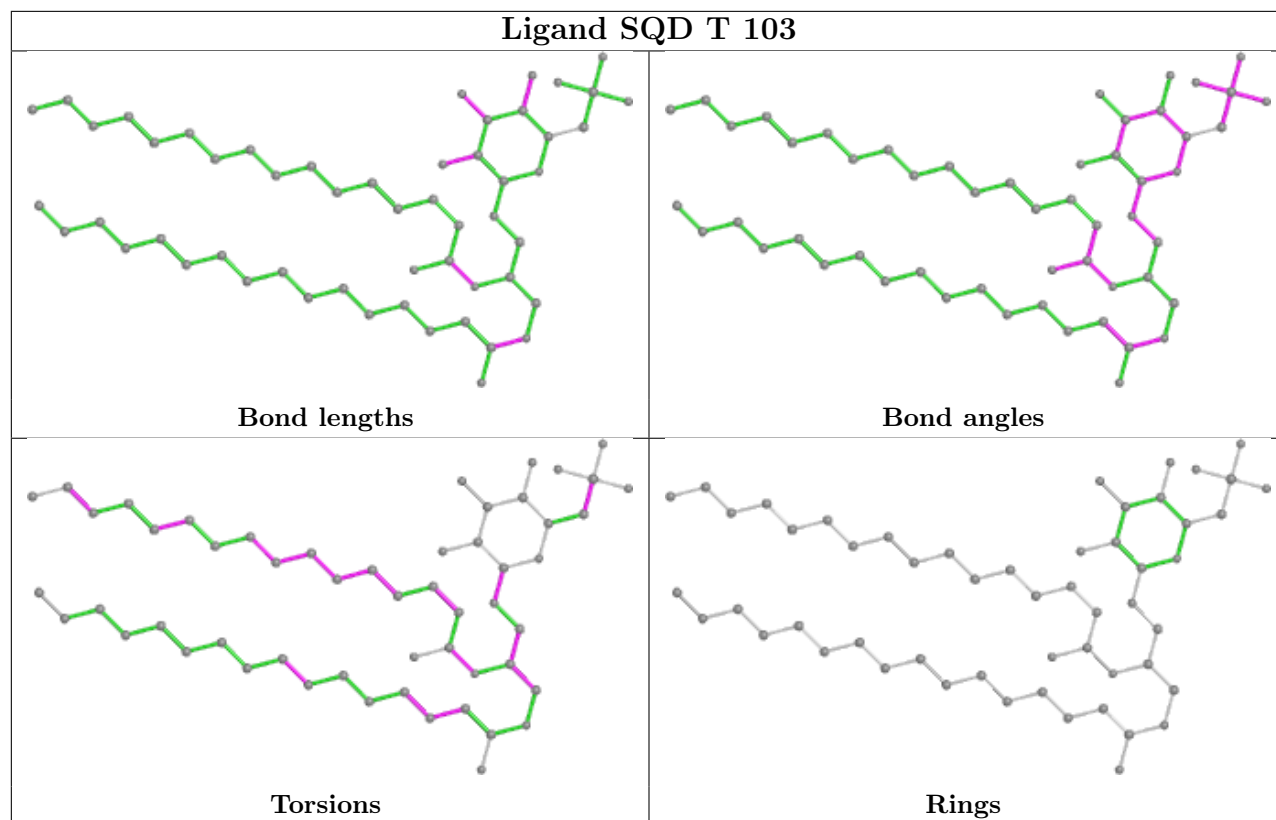


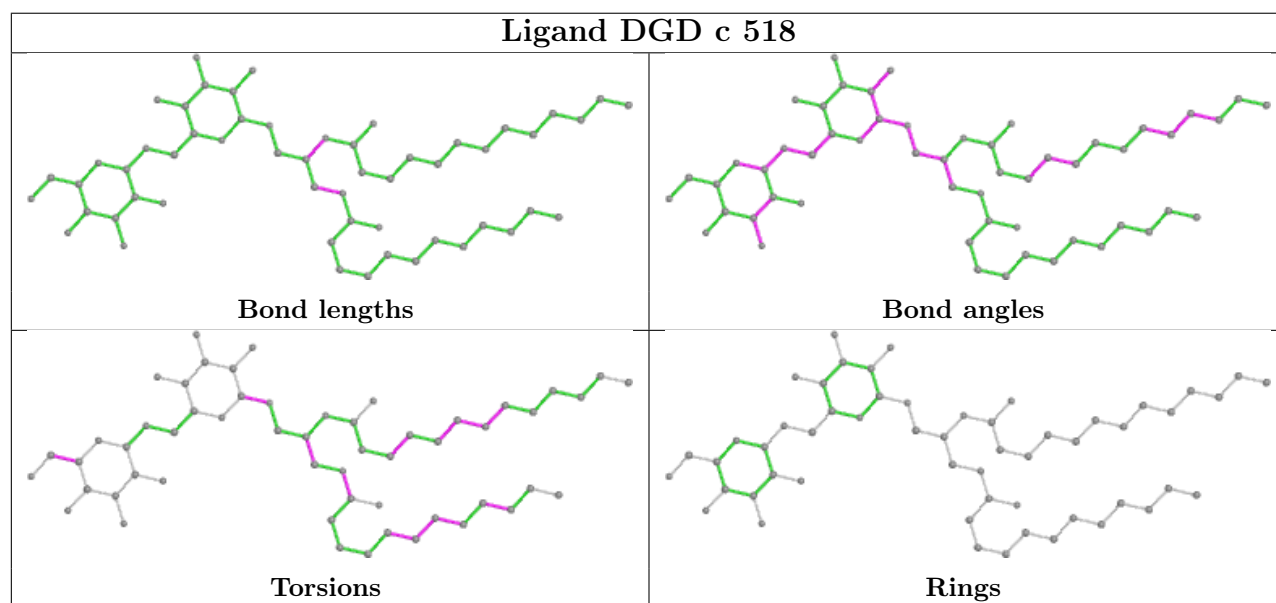
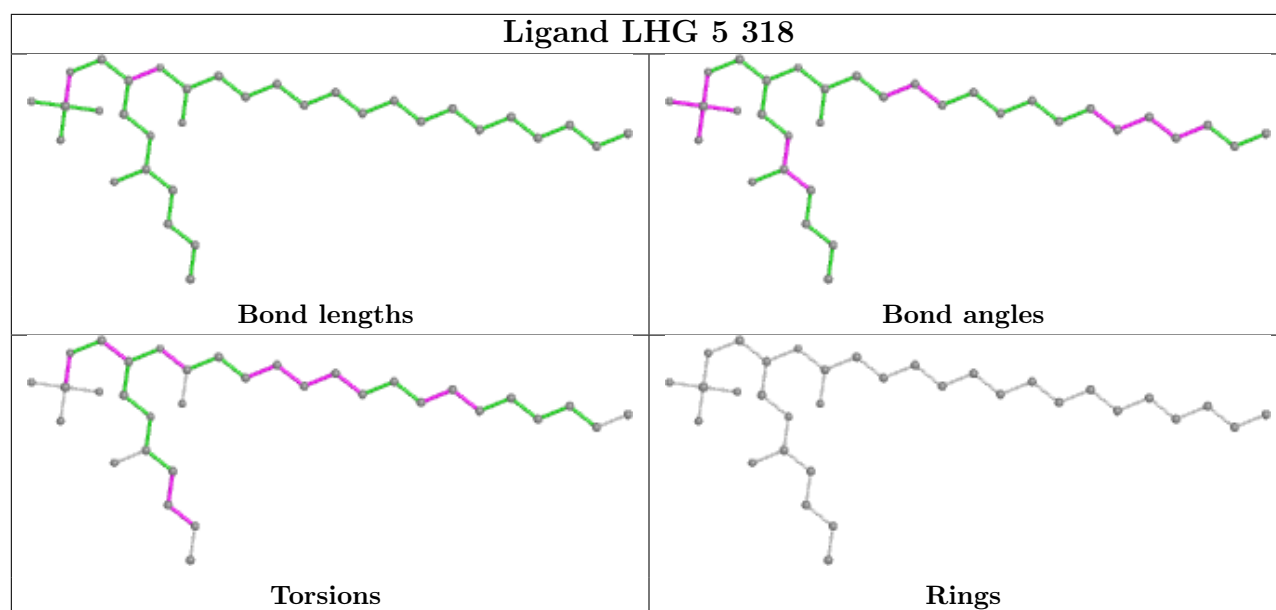
## Ligand CLA 7 305



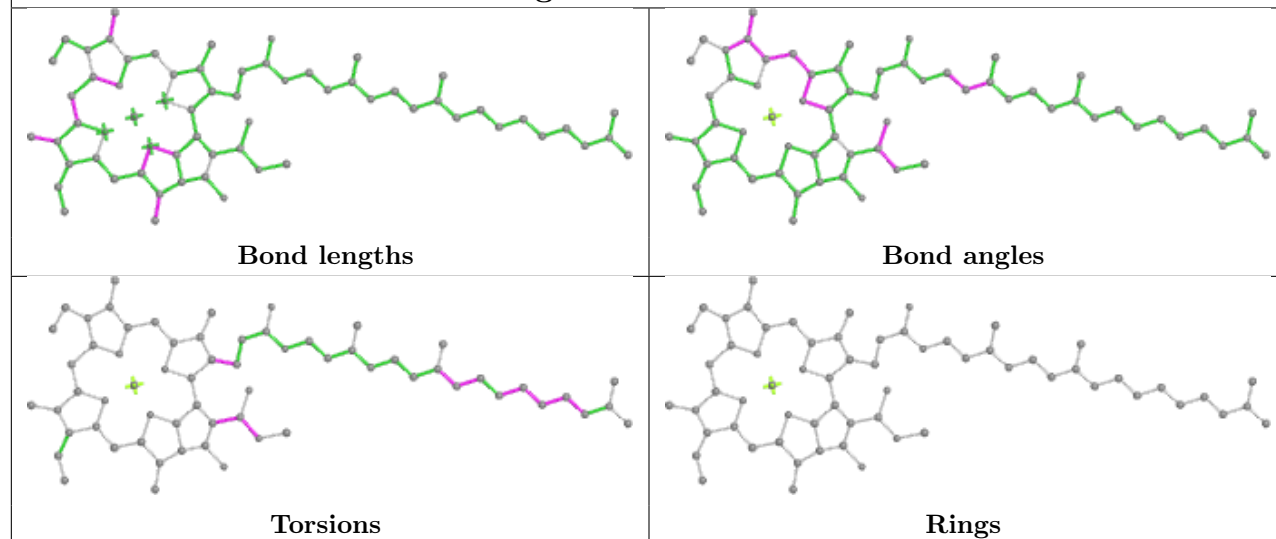
## Ligand CLA 5 314



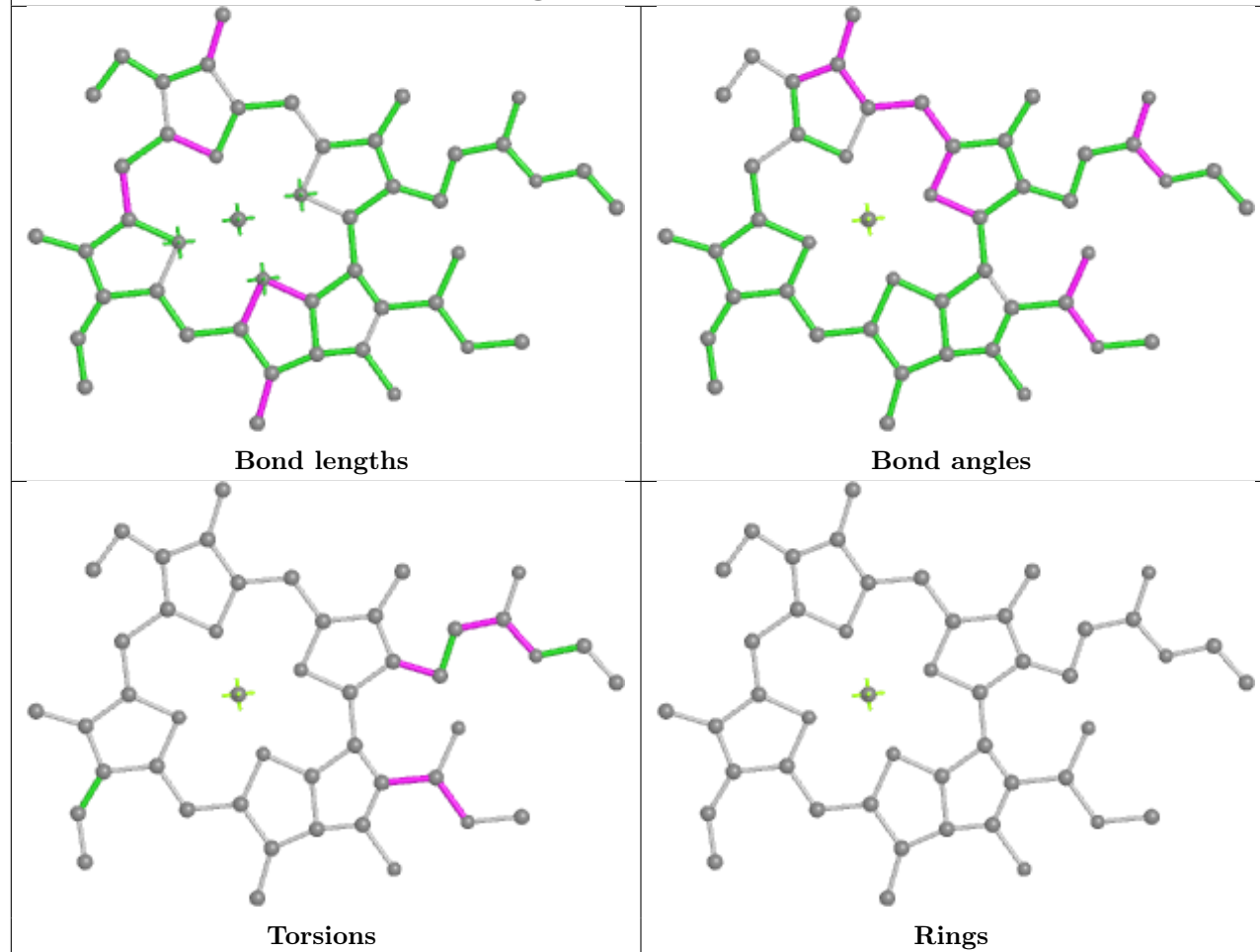


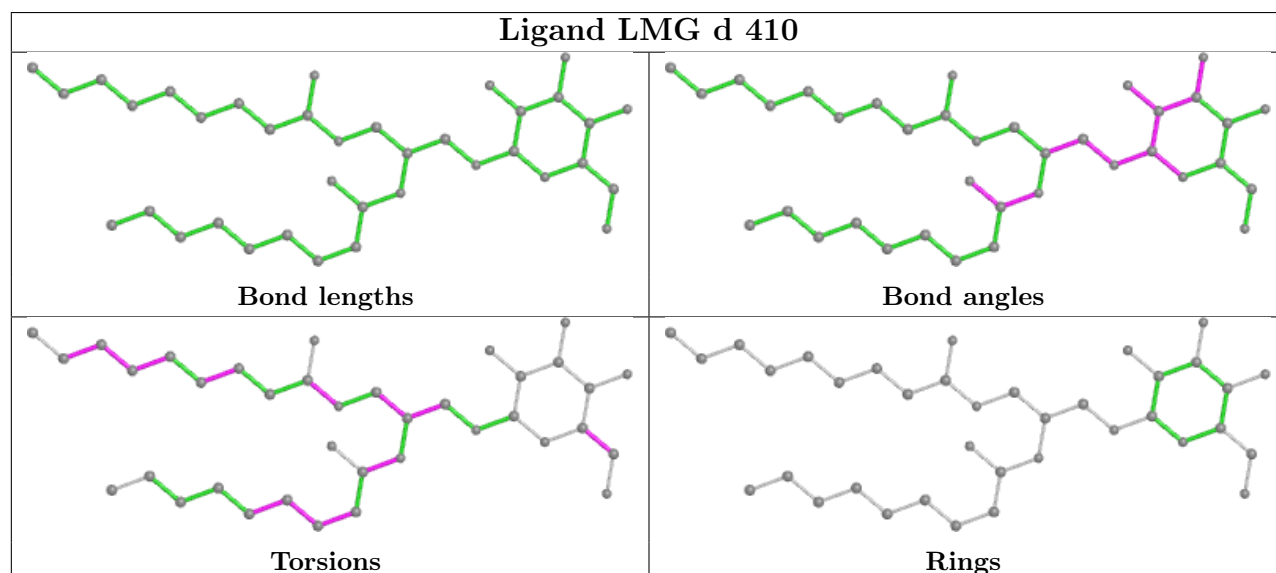
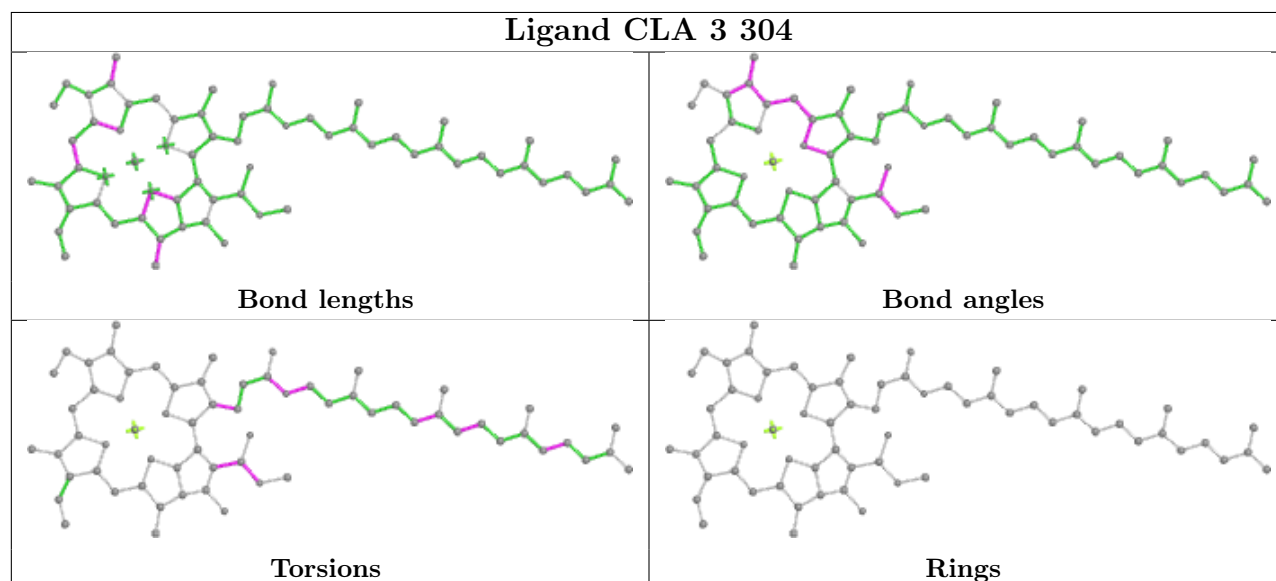
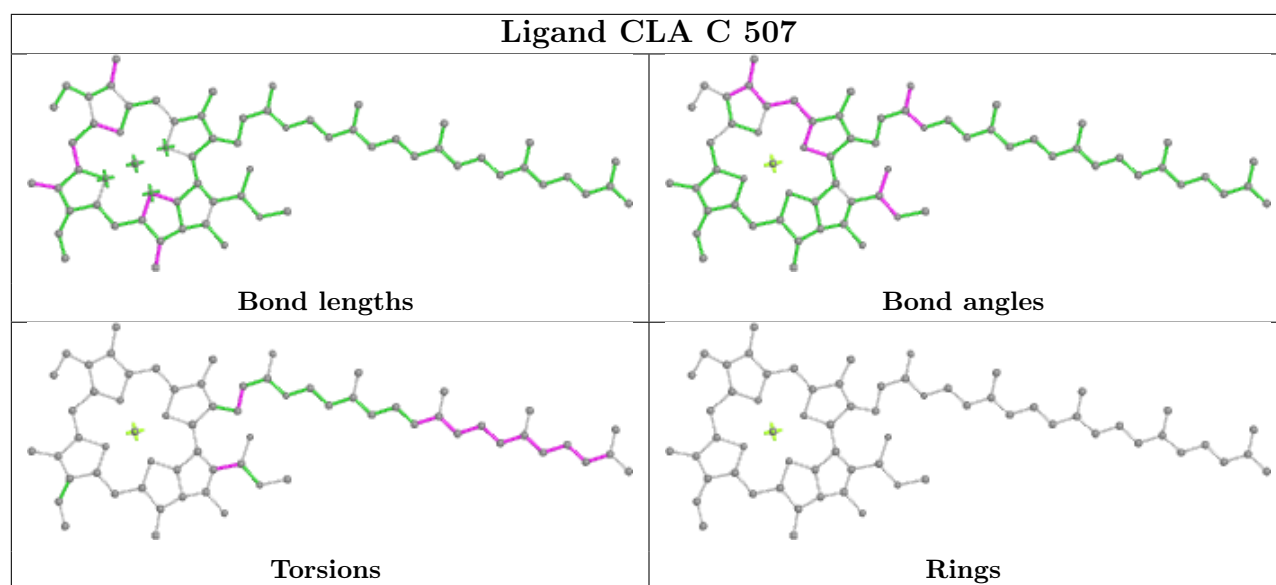


## Ligand CLA b 615

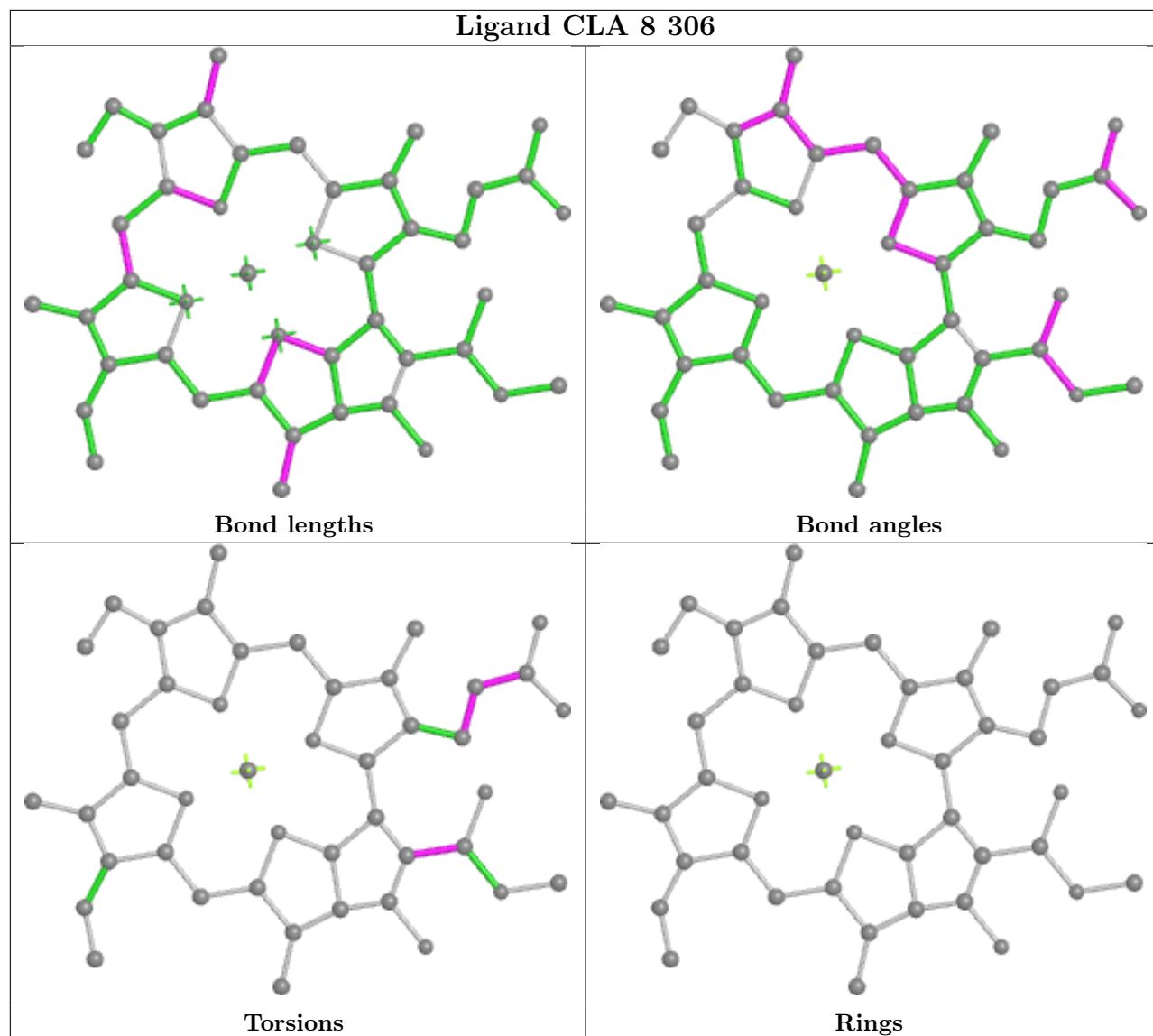


## Ligand CLA 0 304

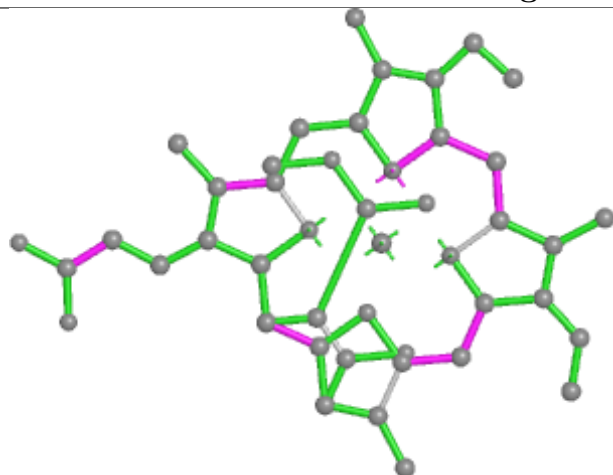




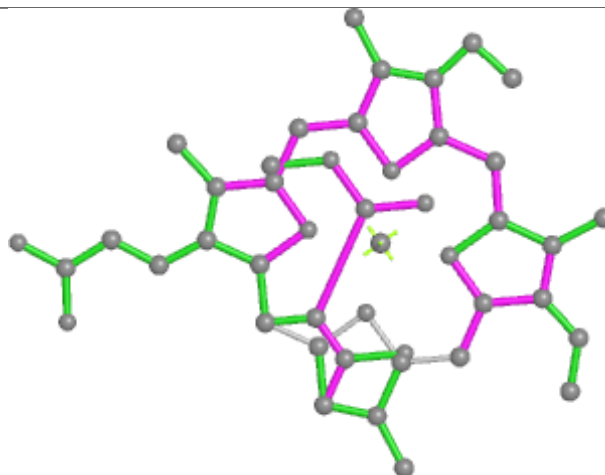
## Ligand CLA 8 306



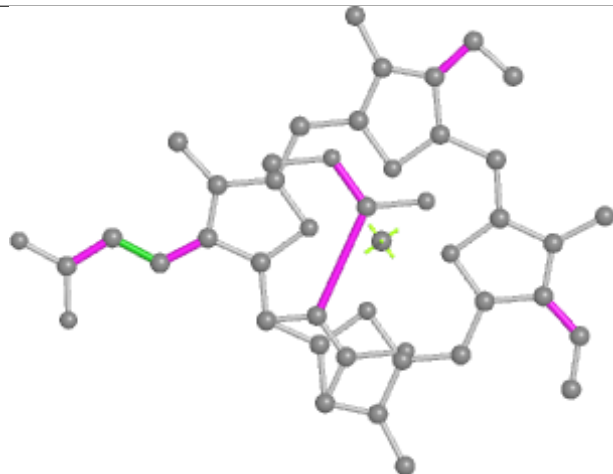
## Ligand KC2 0 306



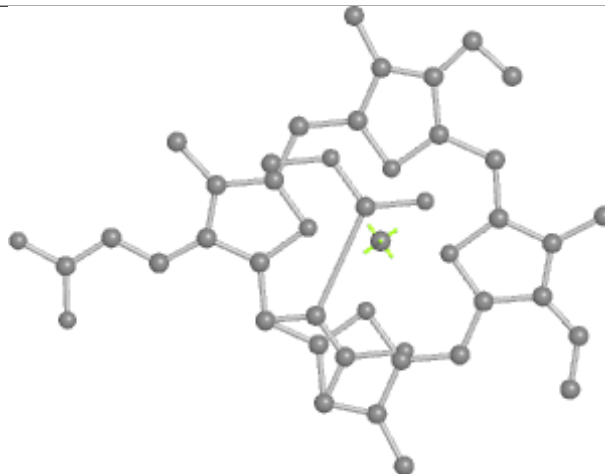
Bond lengths



Bond angles

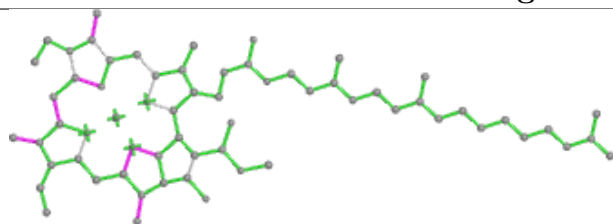


Torsions

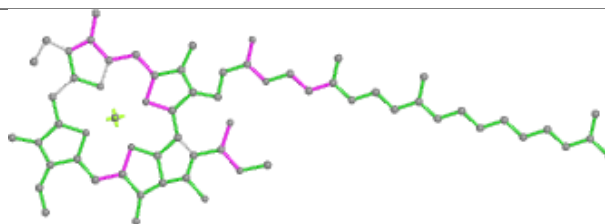


Rings

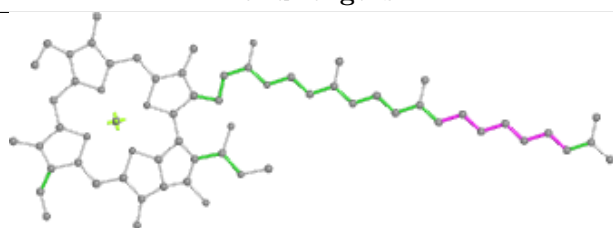
## Ligand CLA b 612



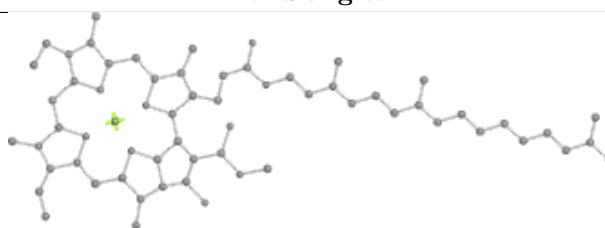
Bond lengths



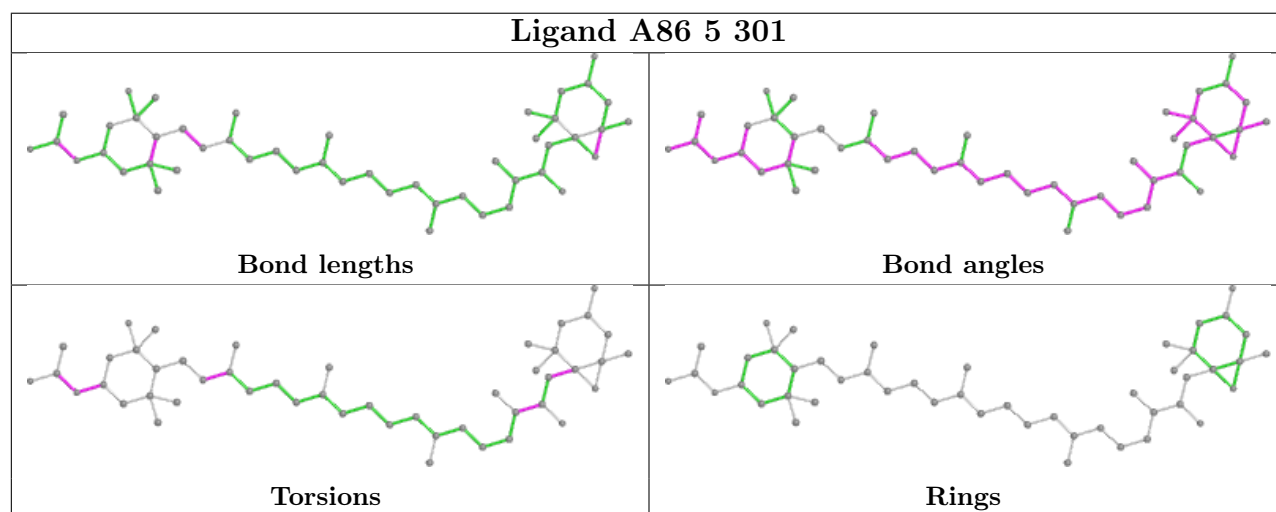
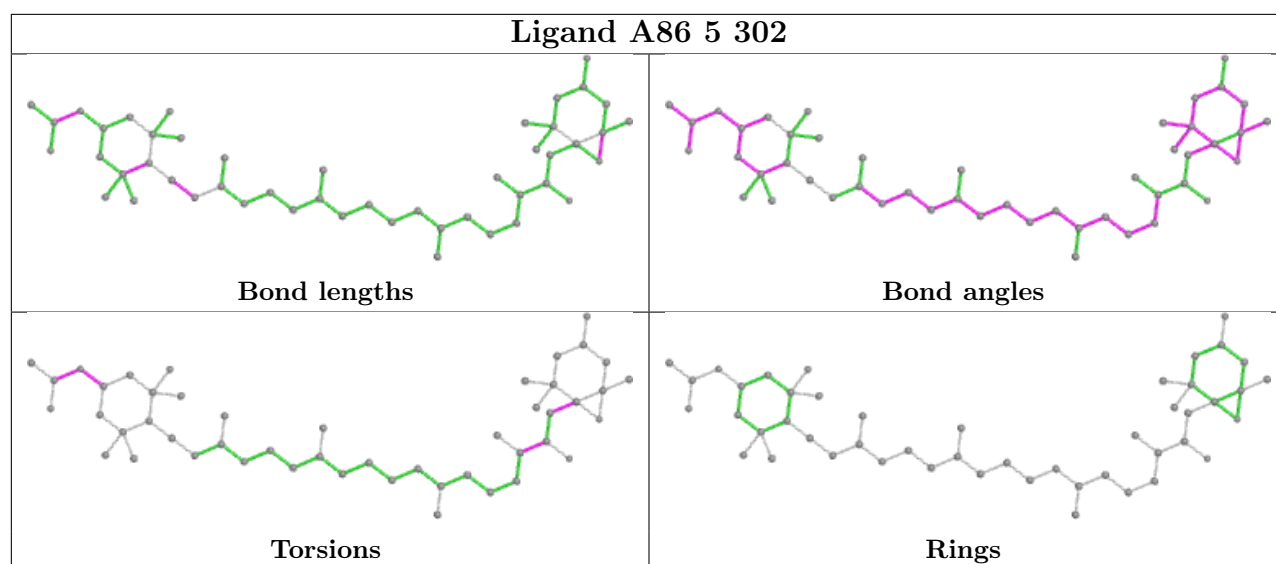
Bond angles

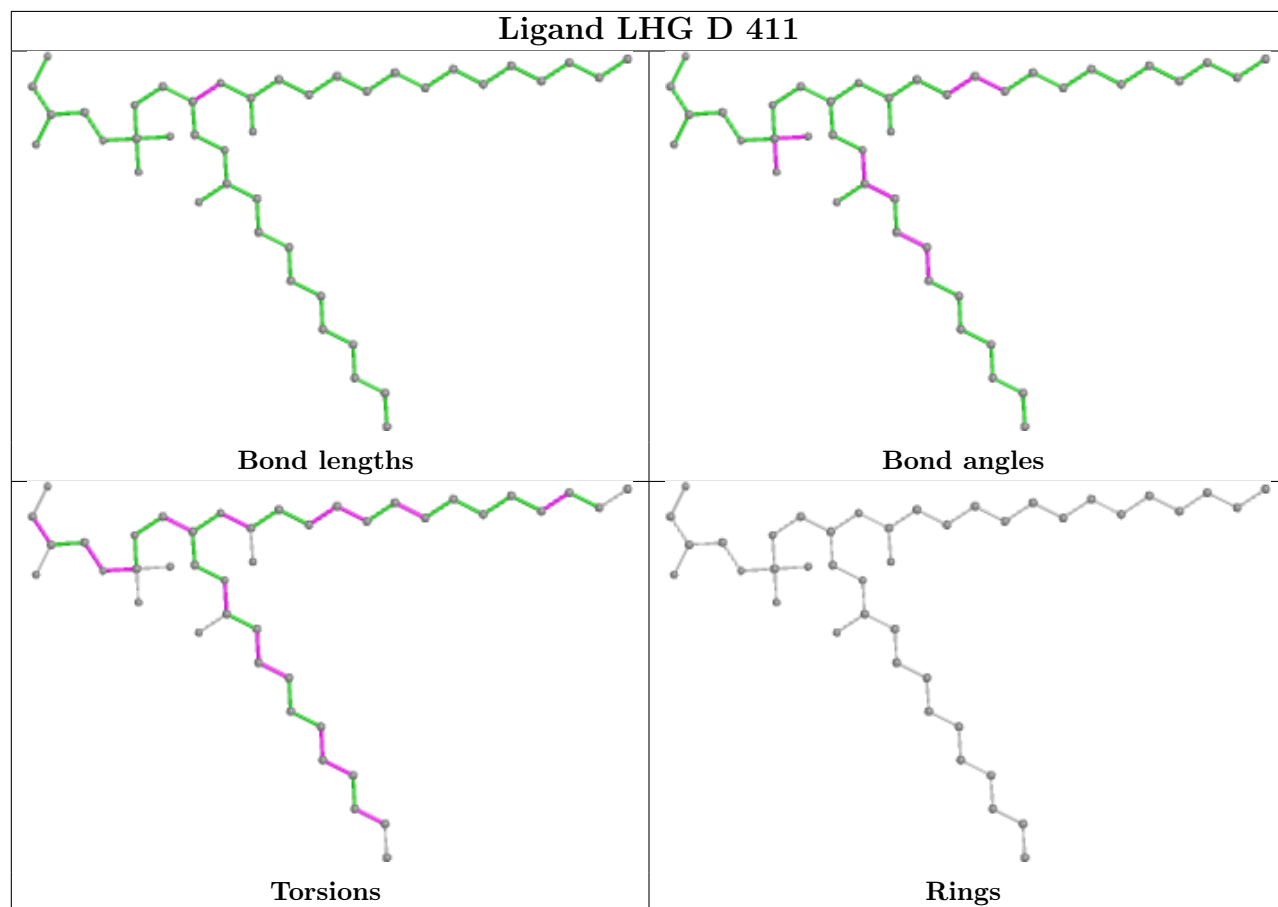
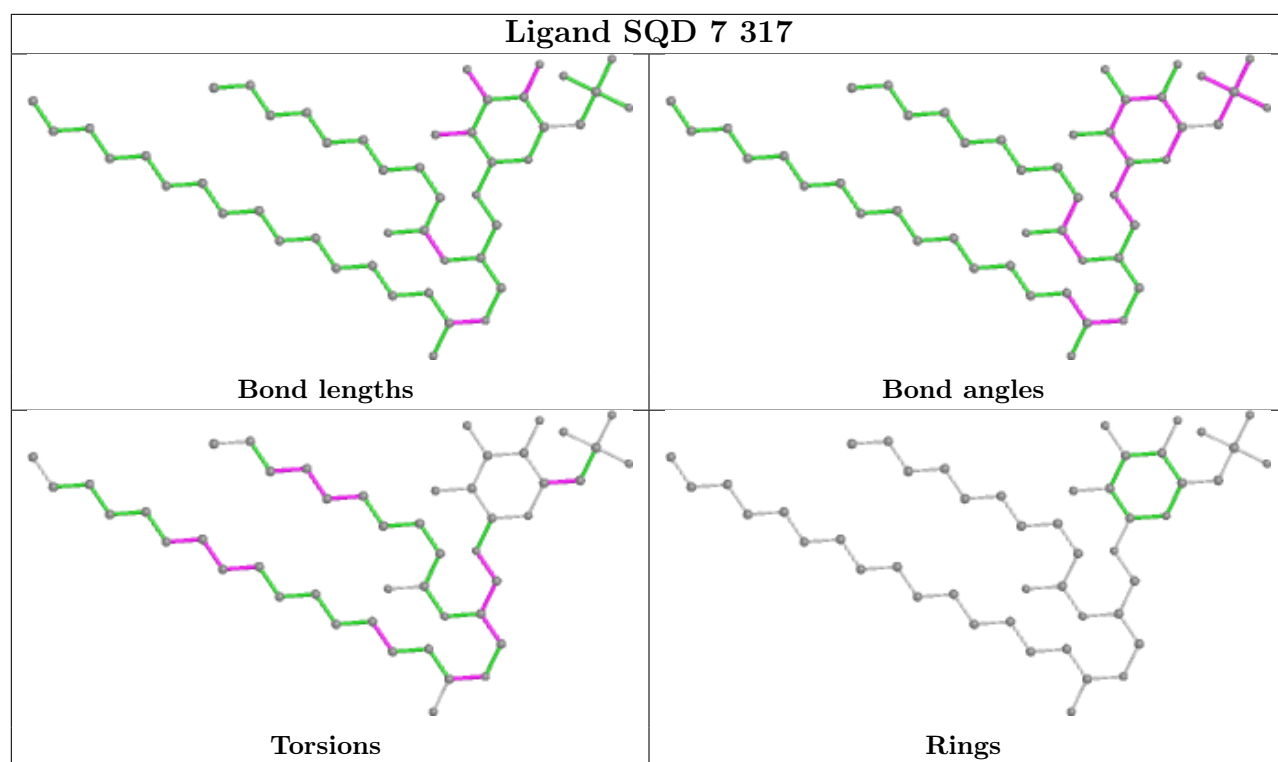


Torsions

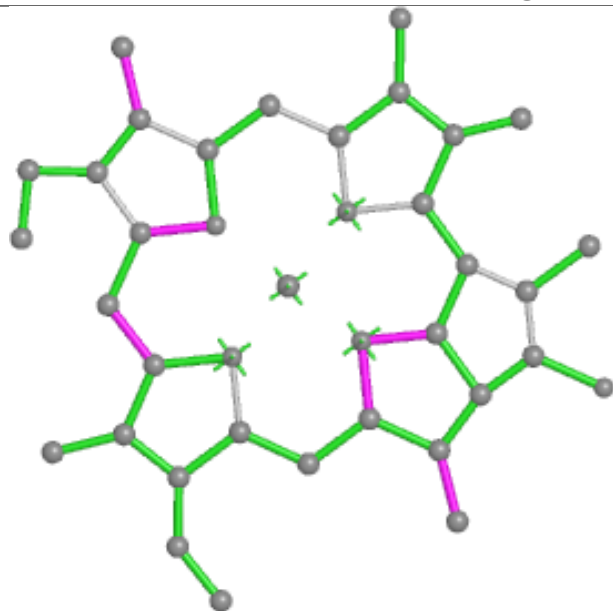


Rings

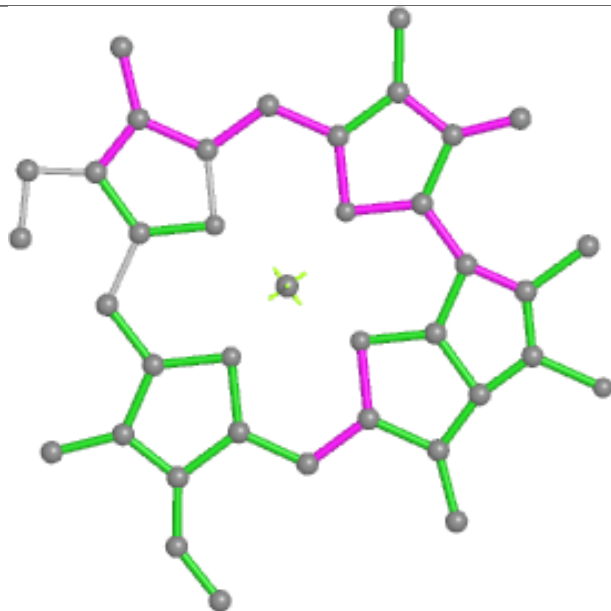




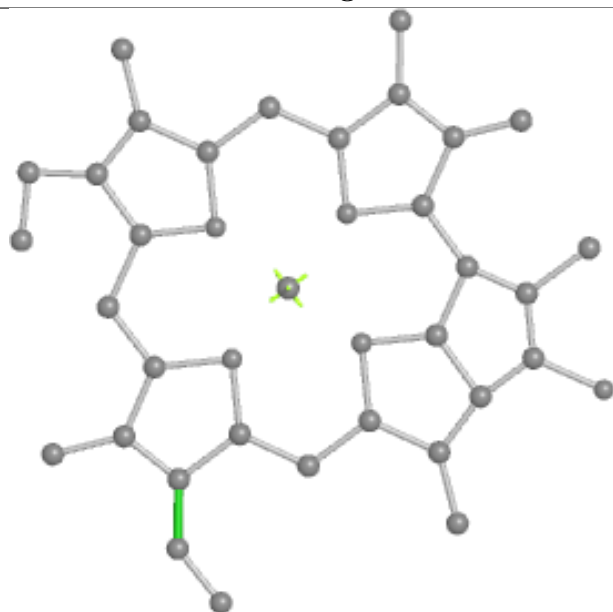
## Ligand CLA 8 315



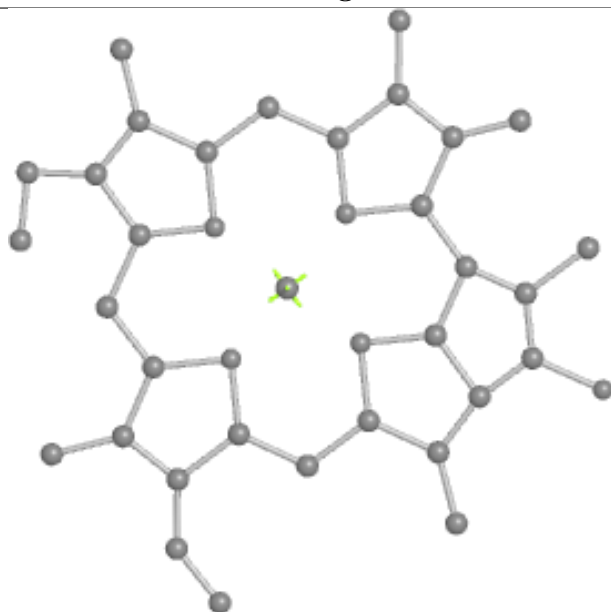
Bond lengths



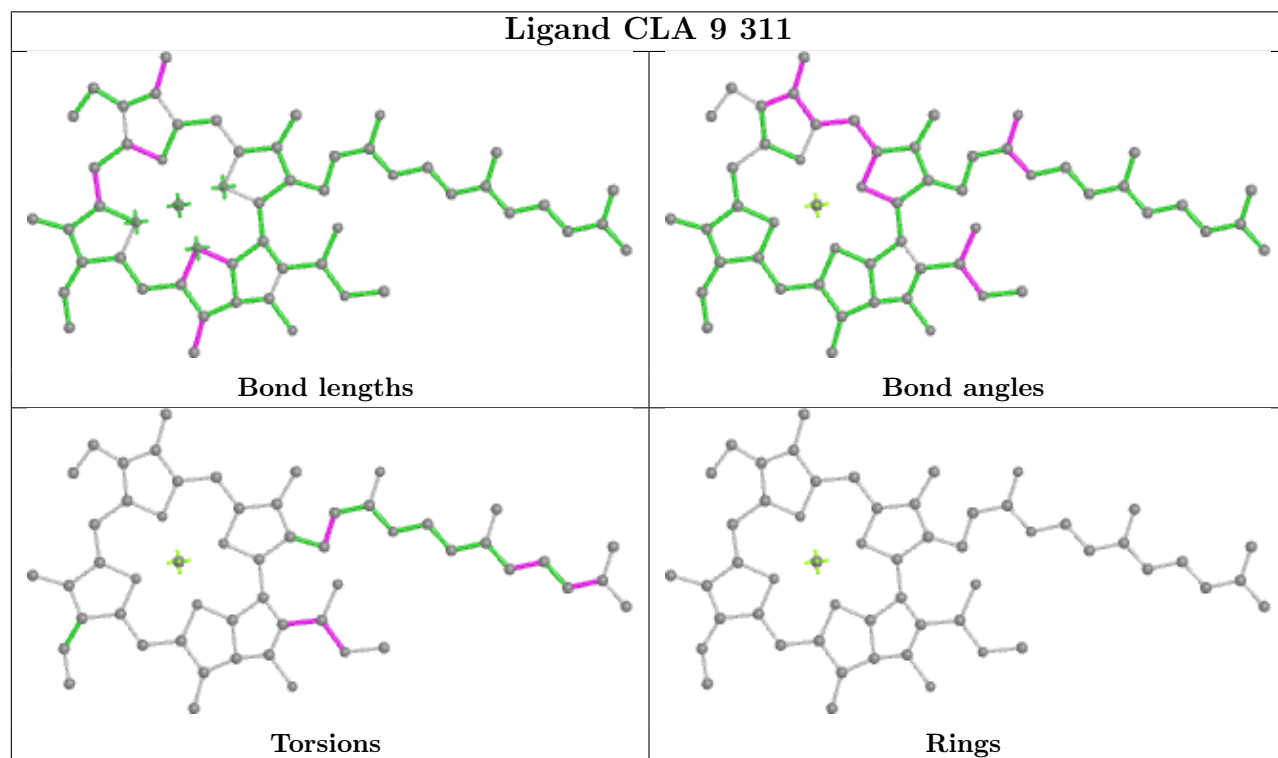
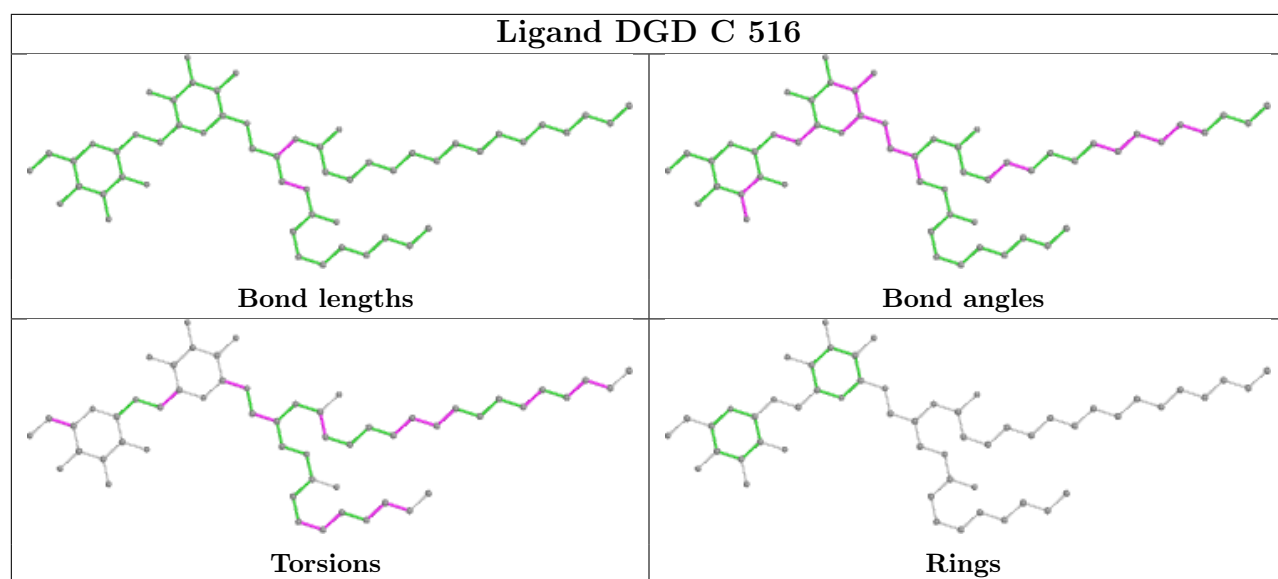
Bond angles

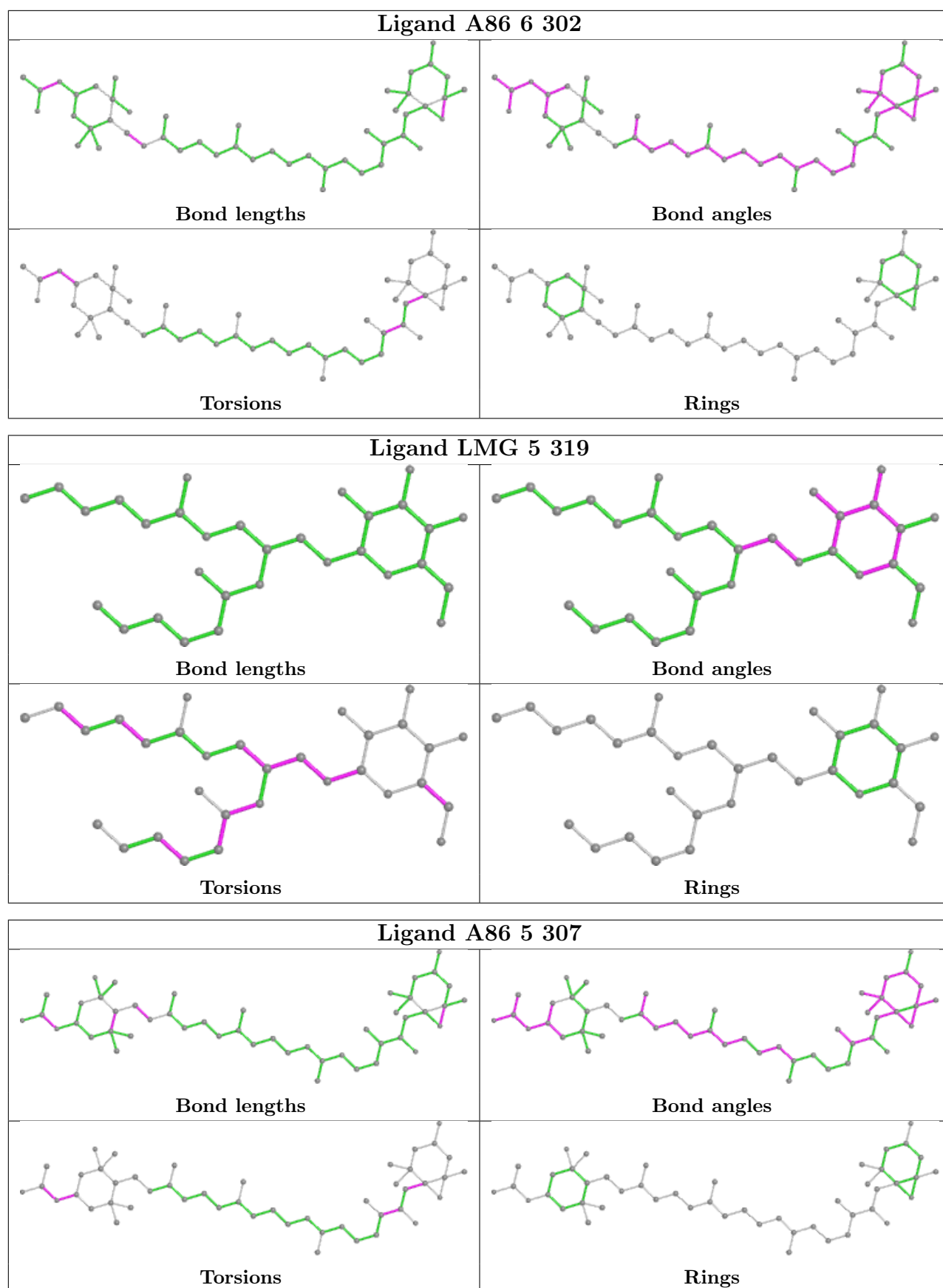


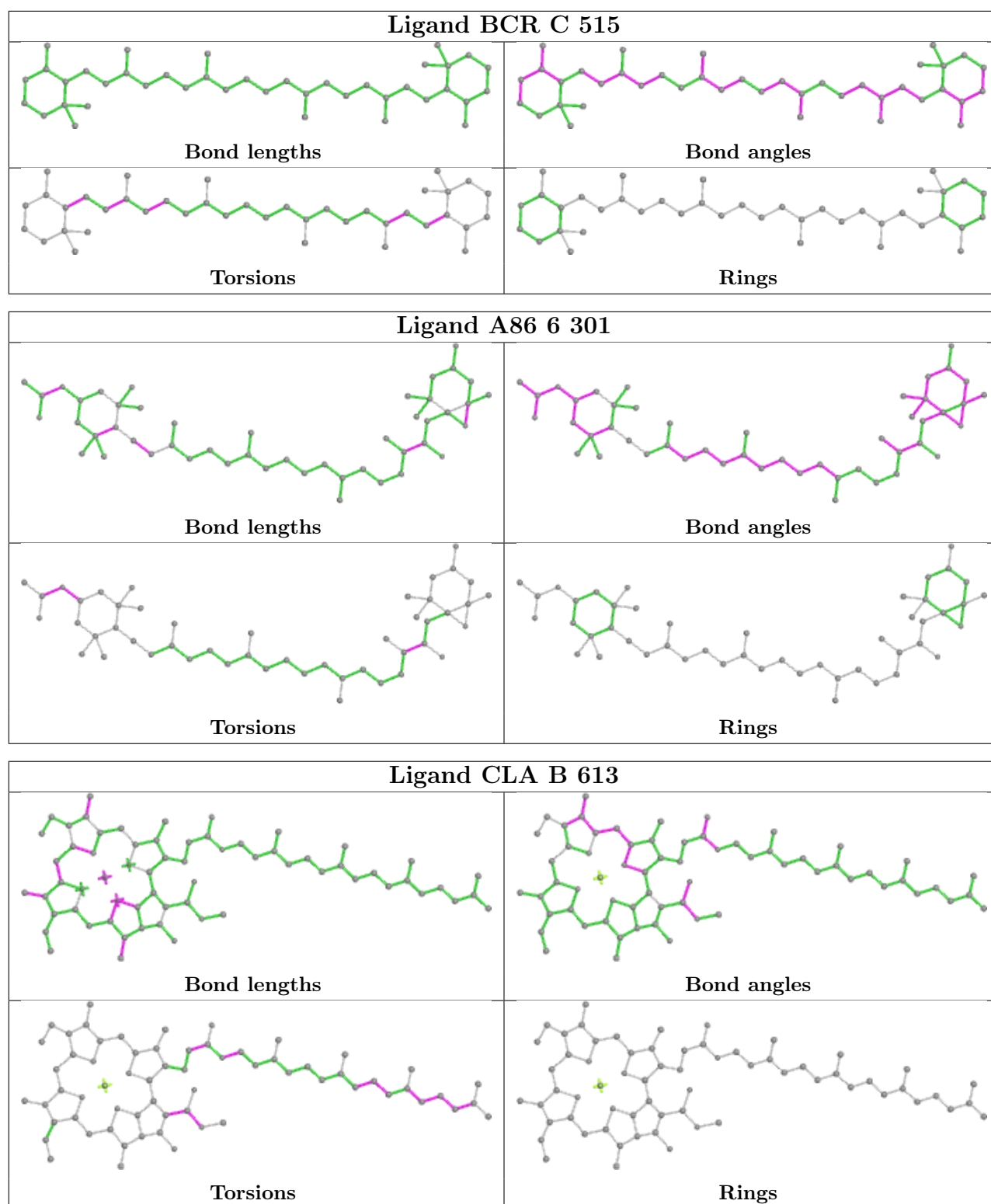
Torsions



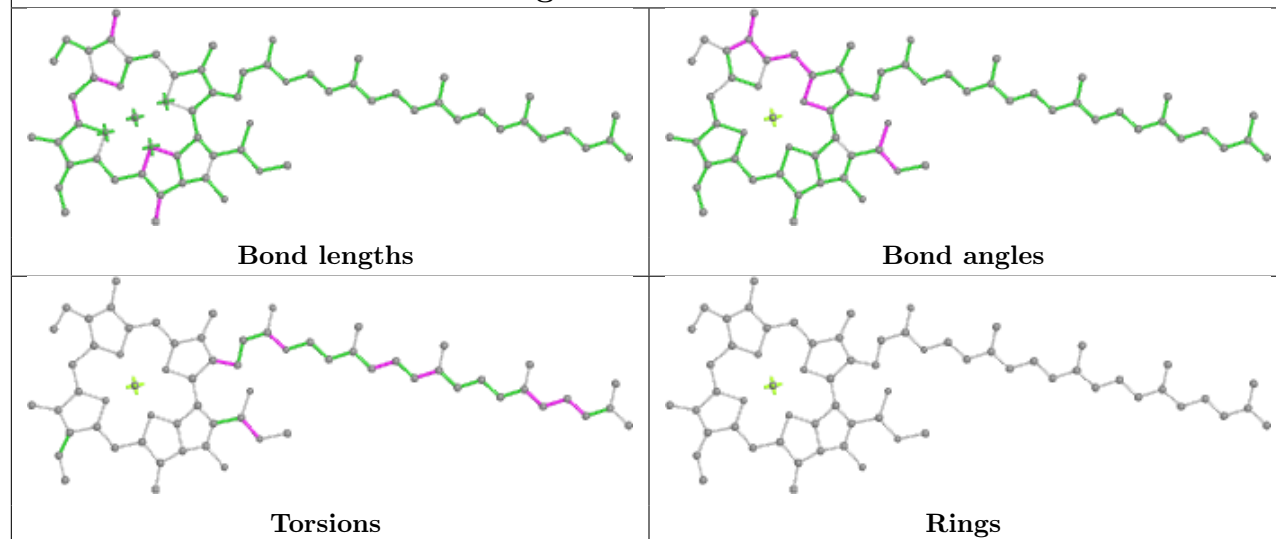
Rings



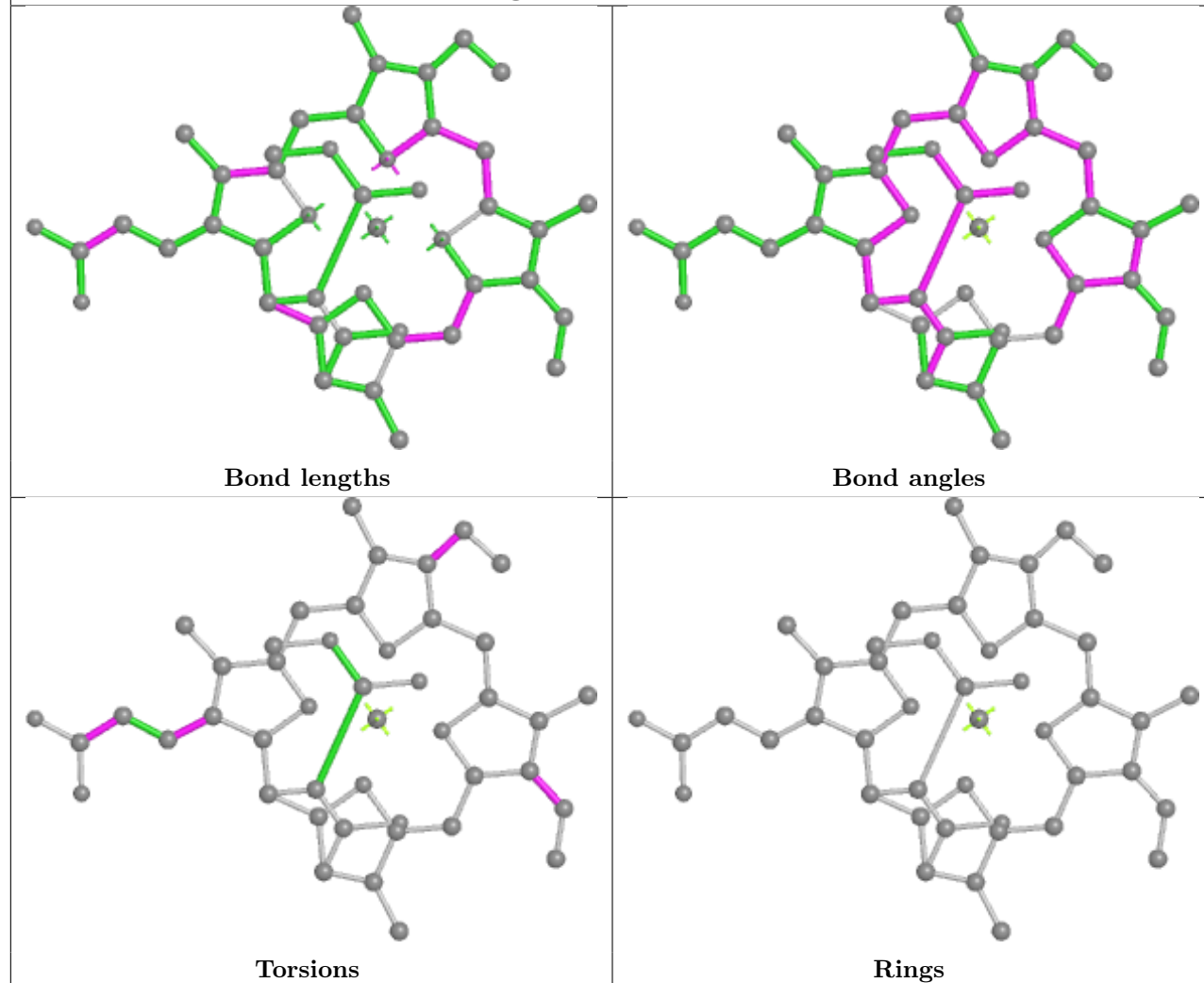




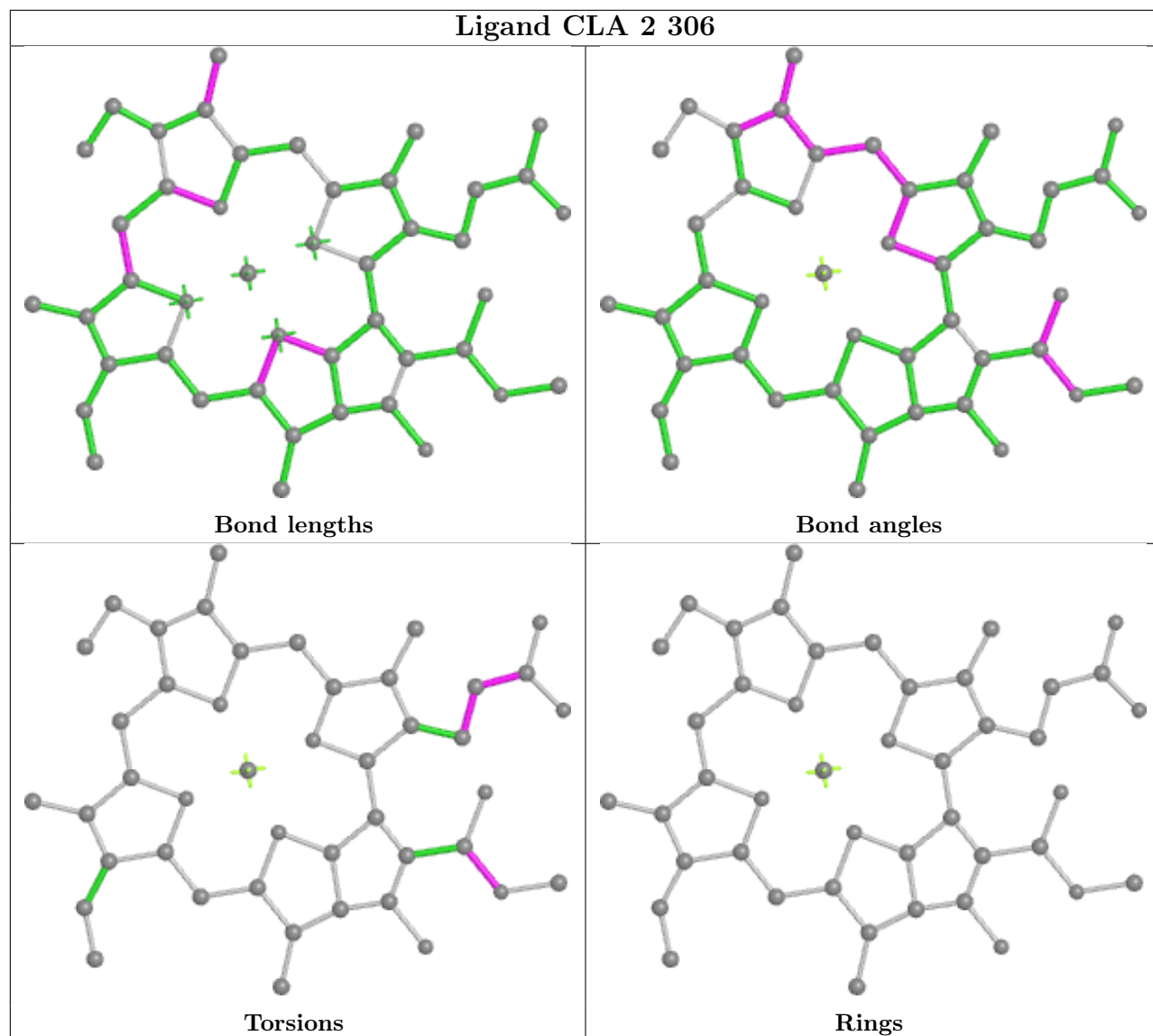
## Ligand CLA 6 312



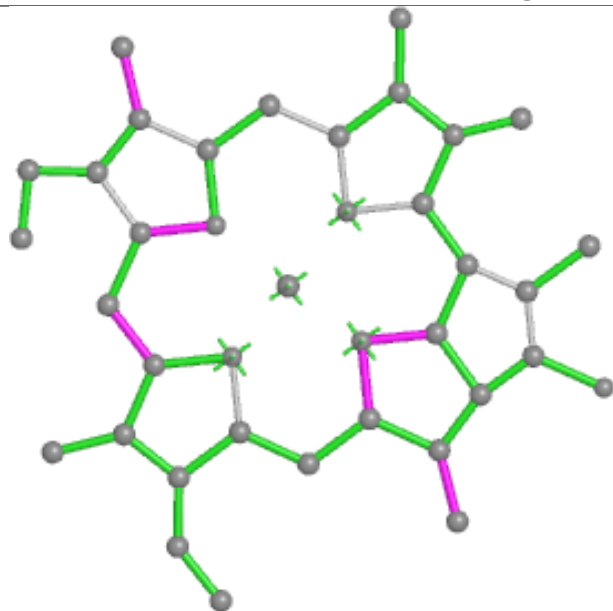
## Ligand KC2 6 309



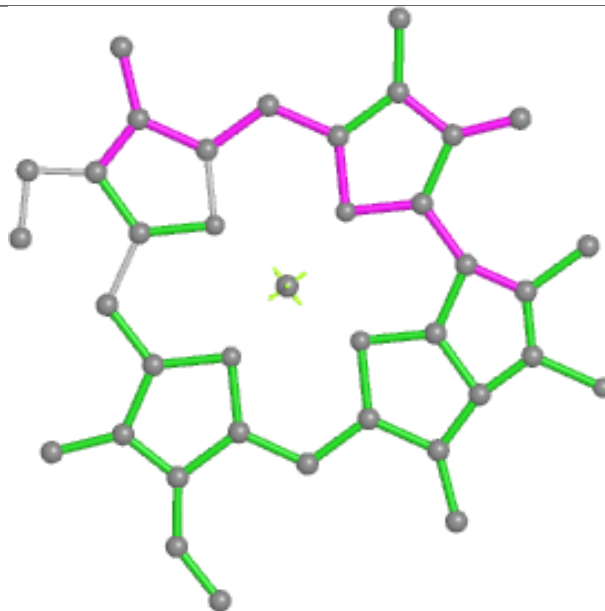
## Ligand CLA 2 306



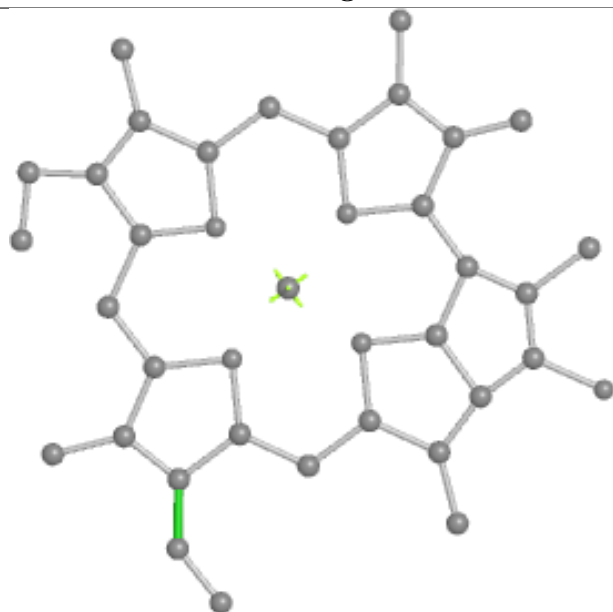
## Ligand CLA 8 314



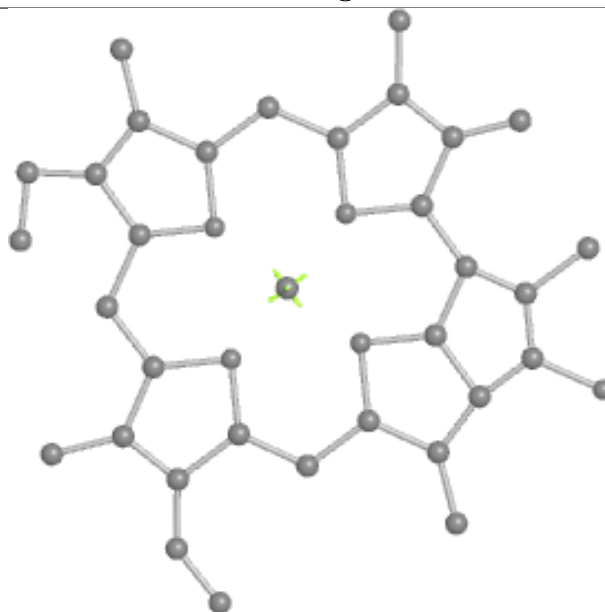
Bond lengths



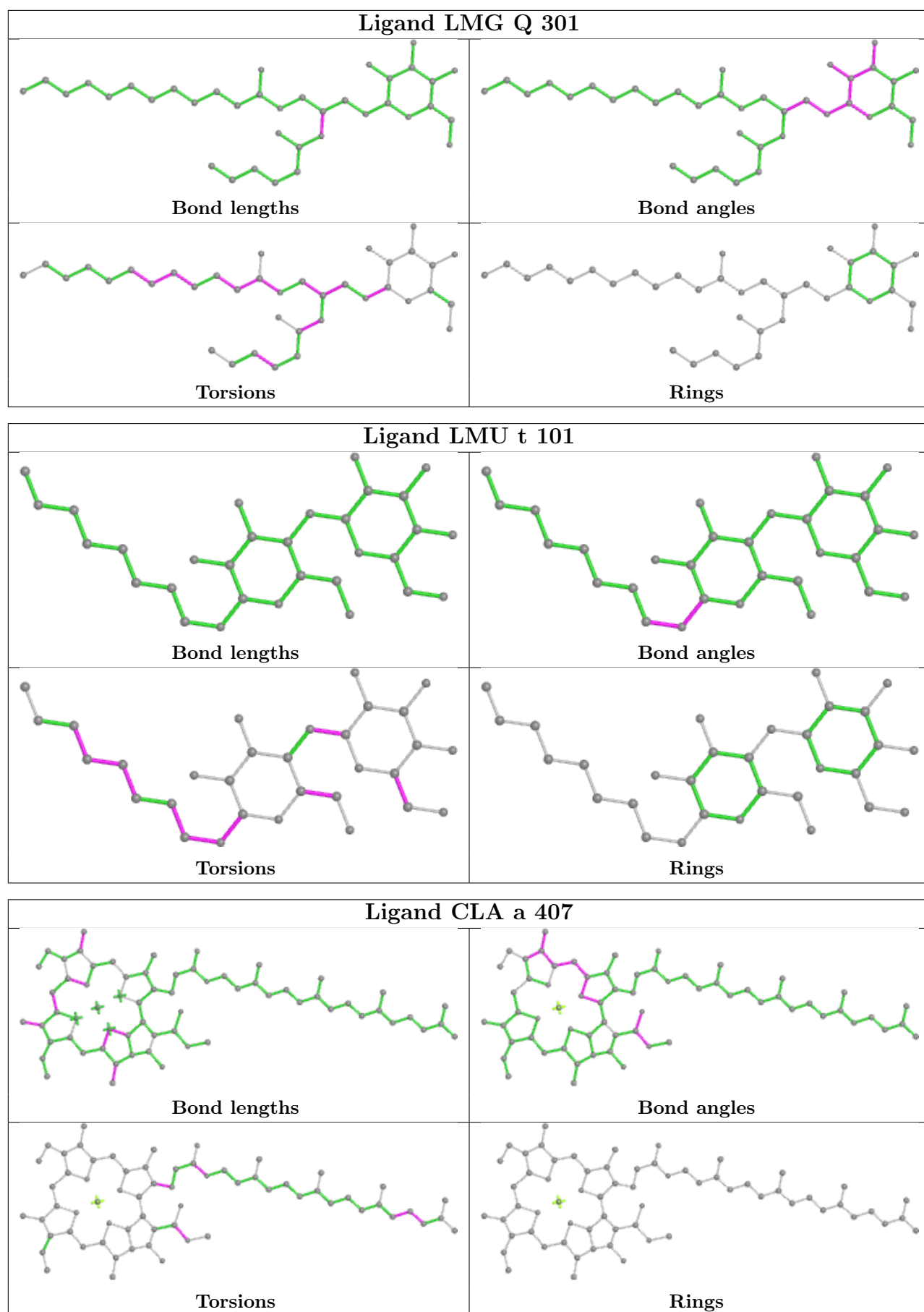
Bond angles



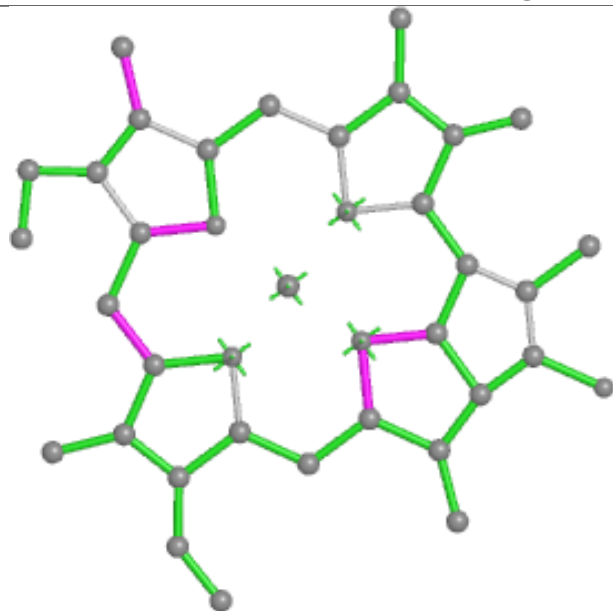
Torsions



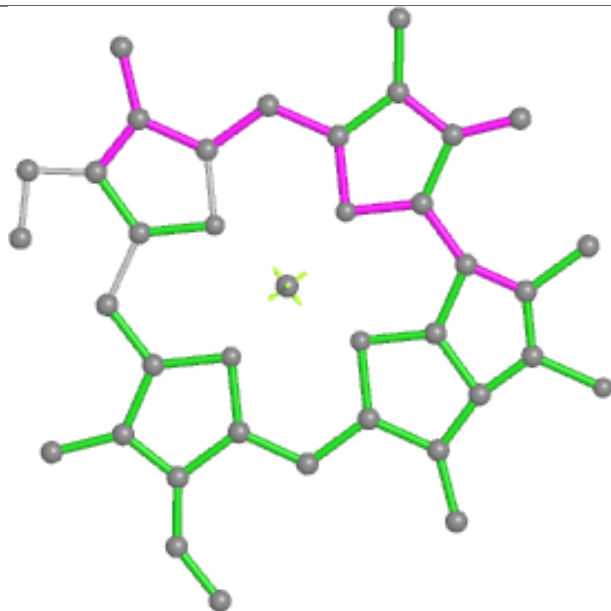
Rings



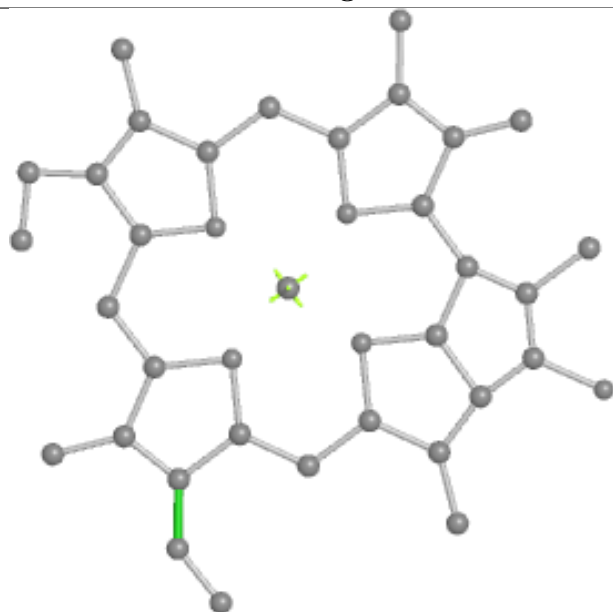
## Ligand CLA 1 314



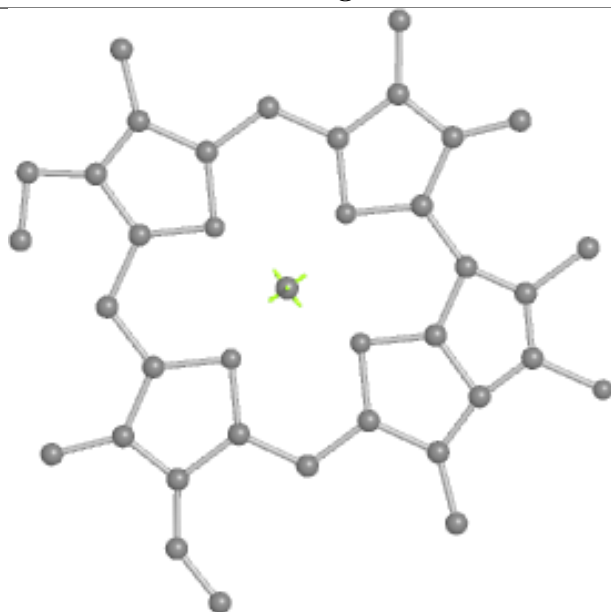
Bond lengths



Bond angles

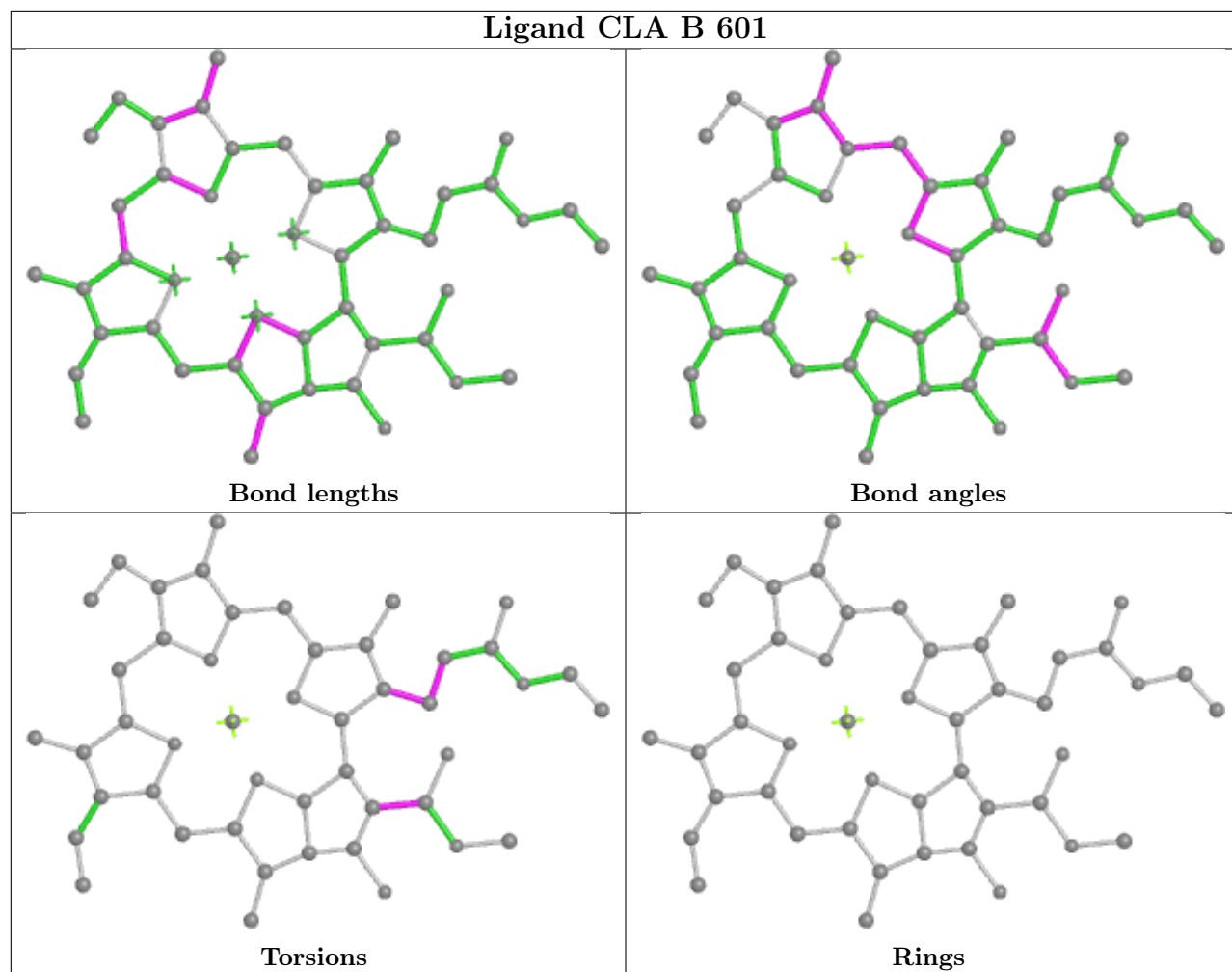


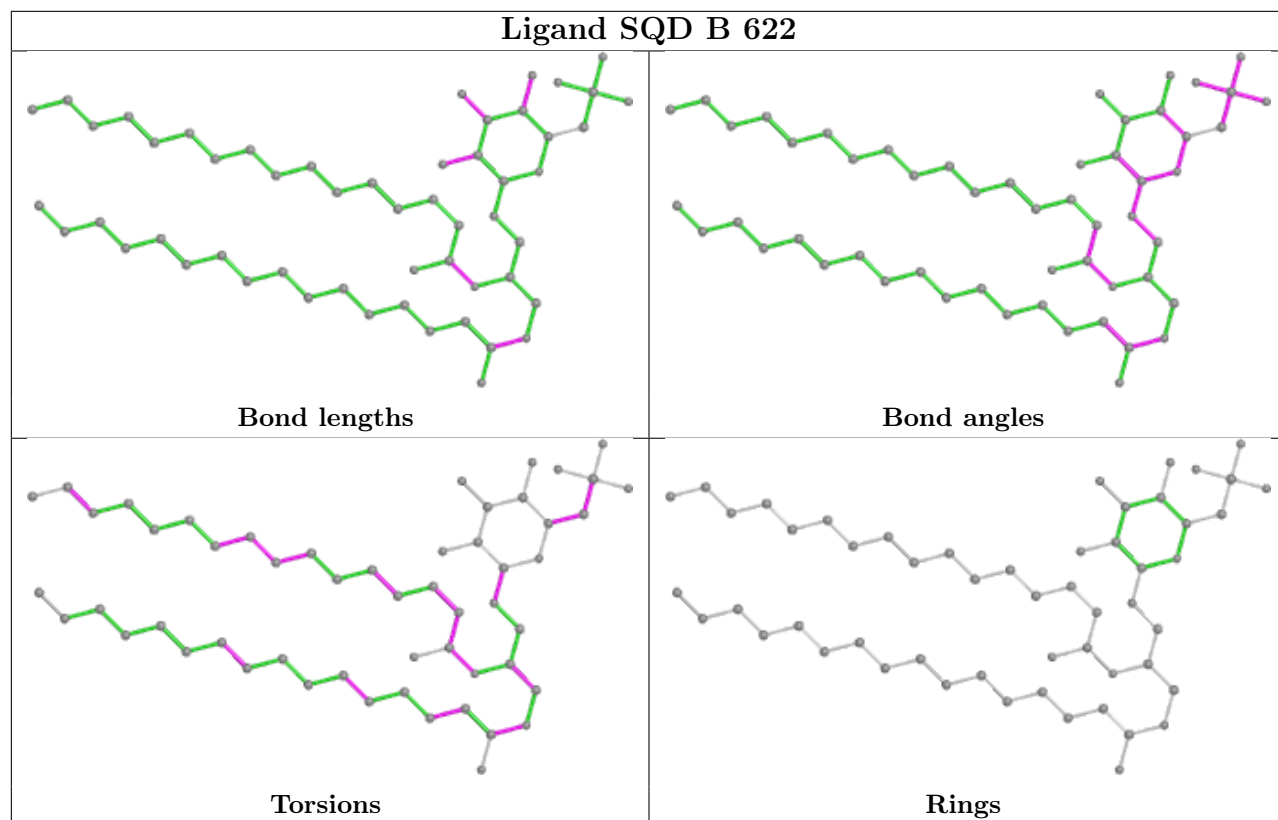
Torsions



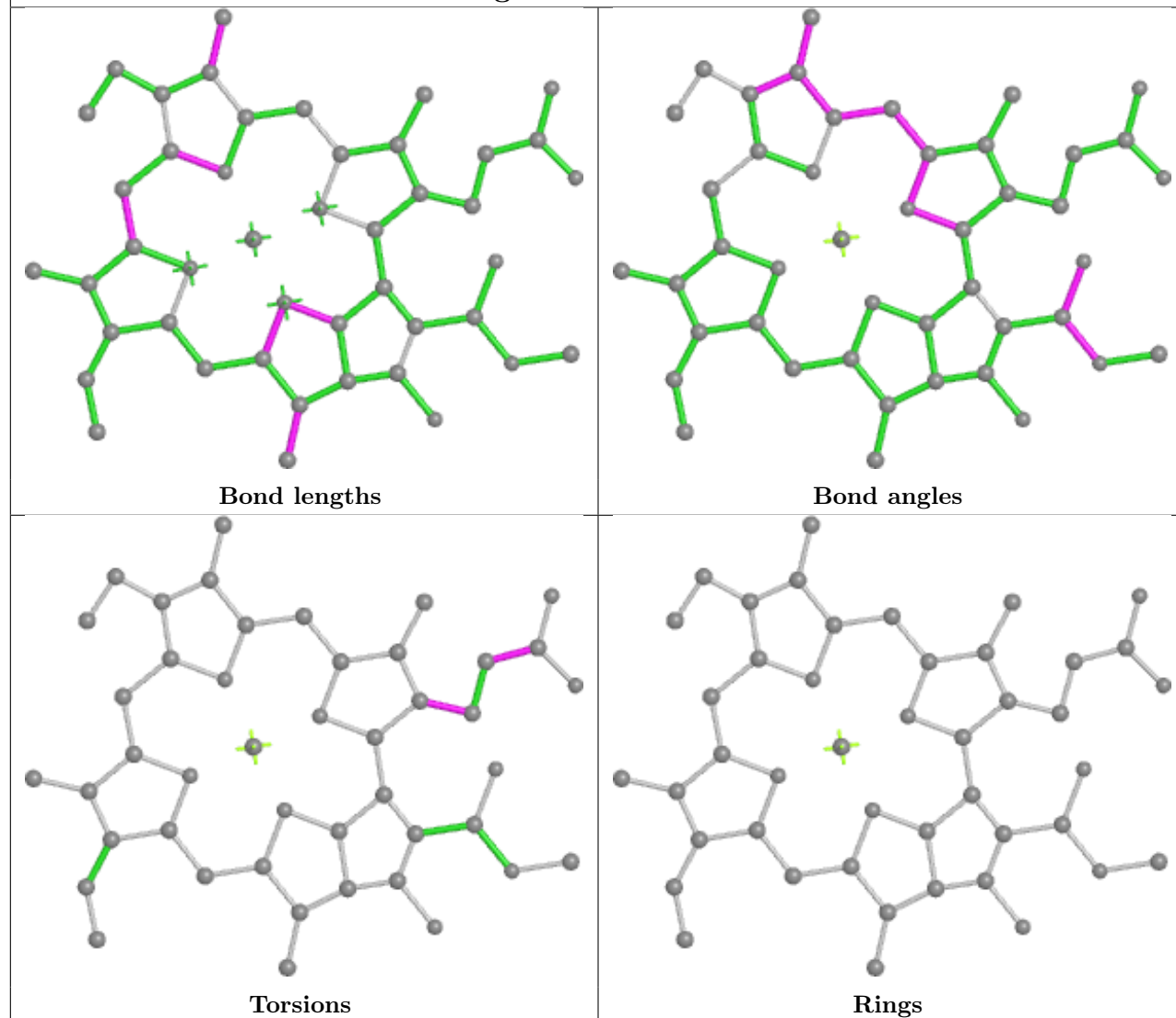
Rings

## Ligand CLA B 601

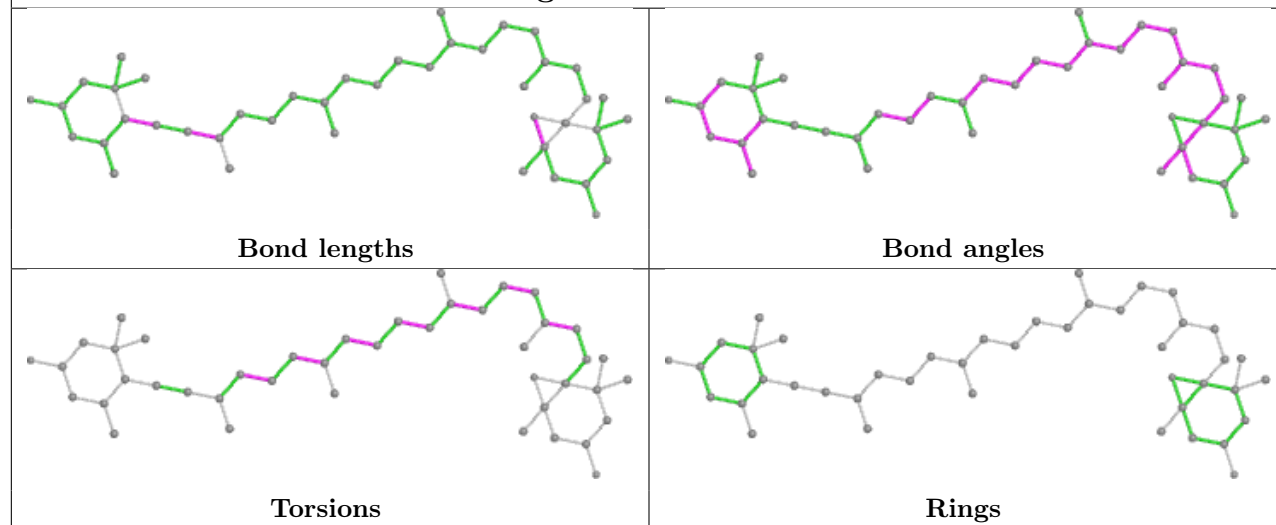


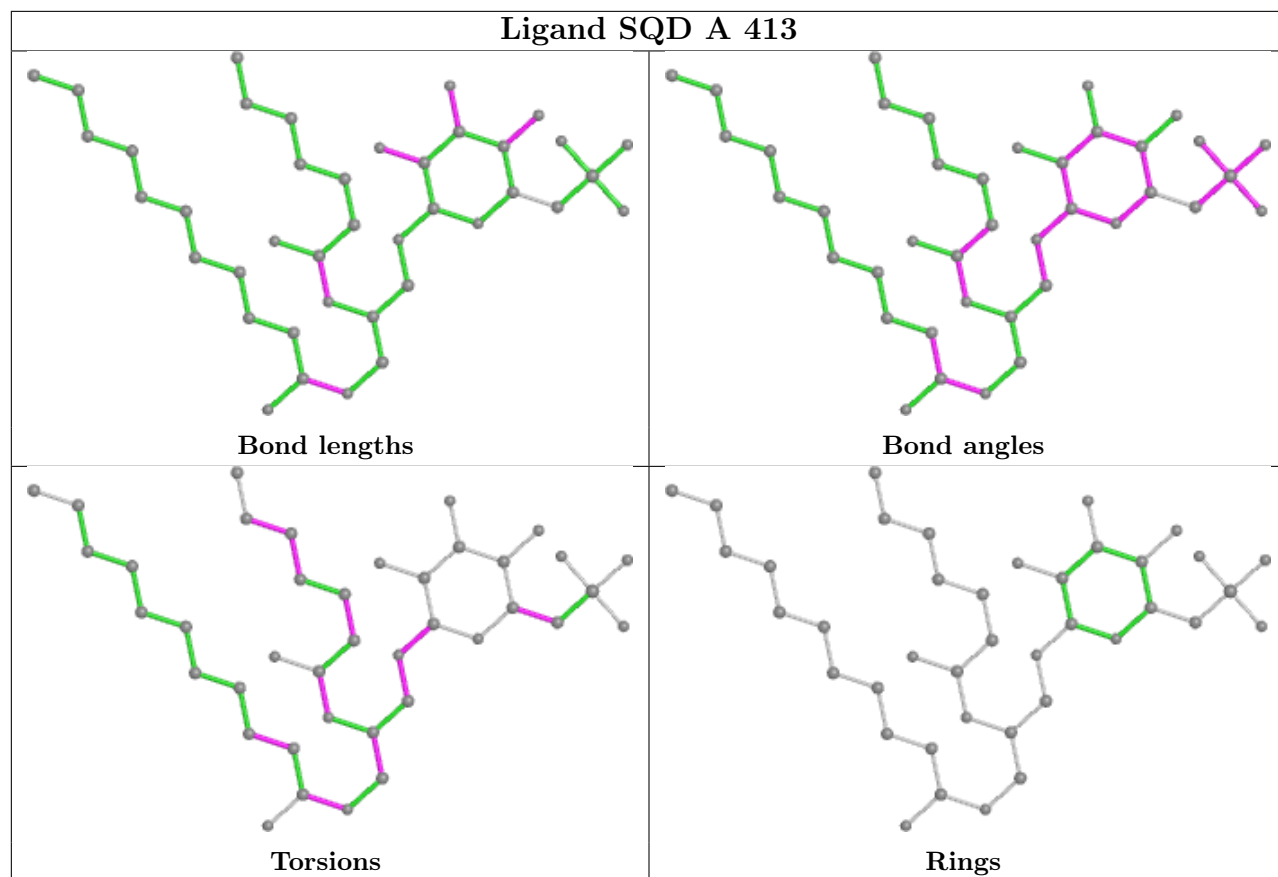


## Ligand CLA 2 312

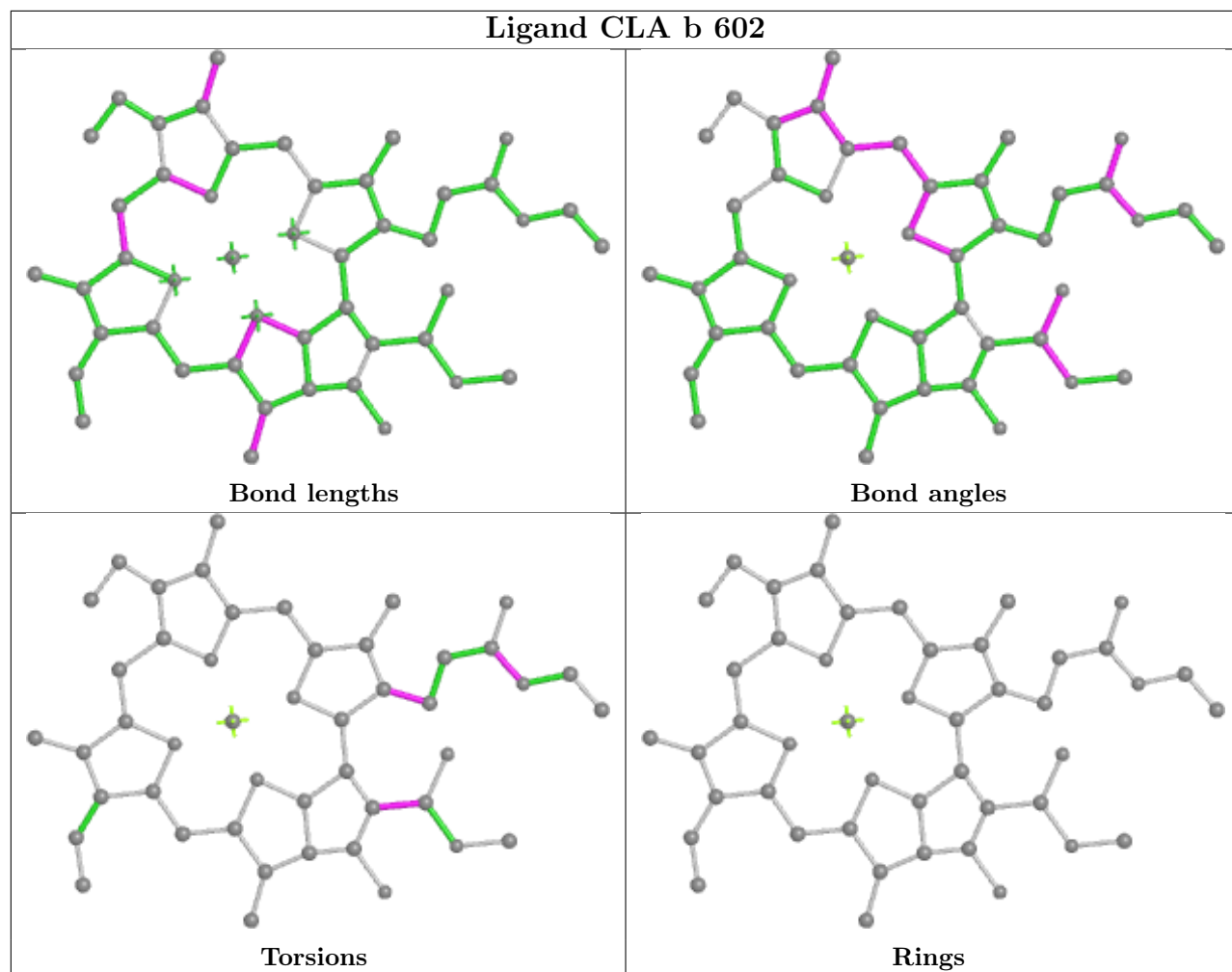


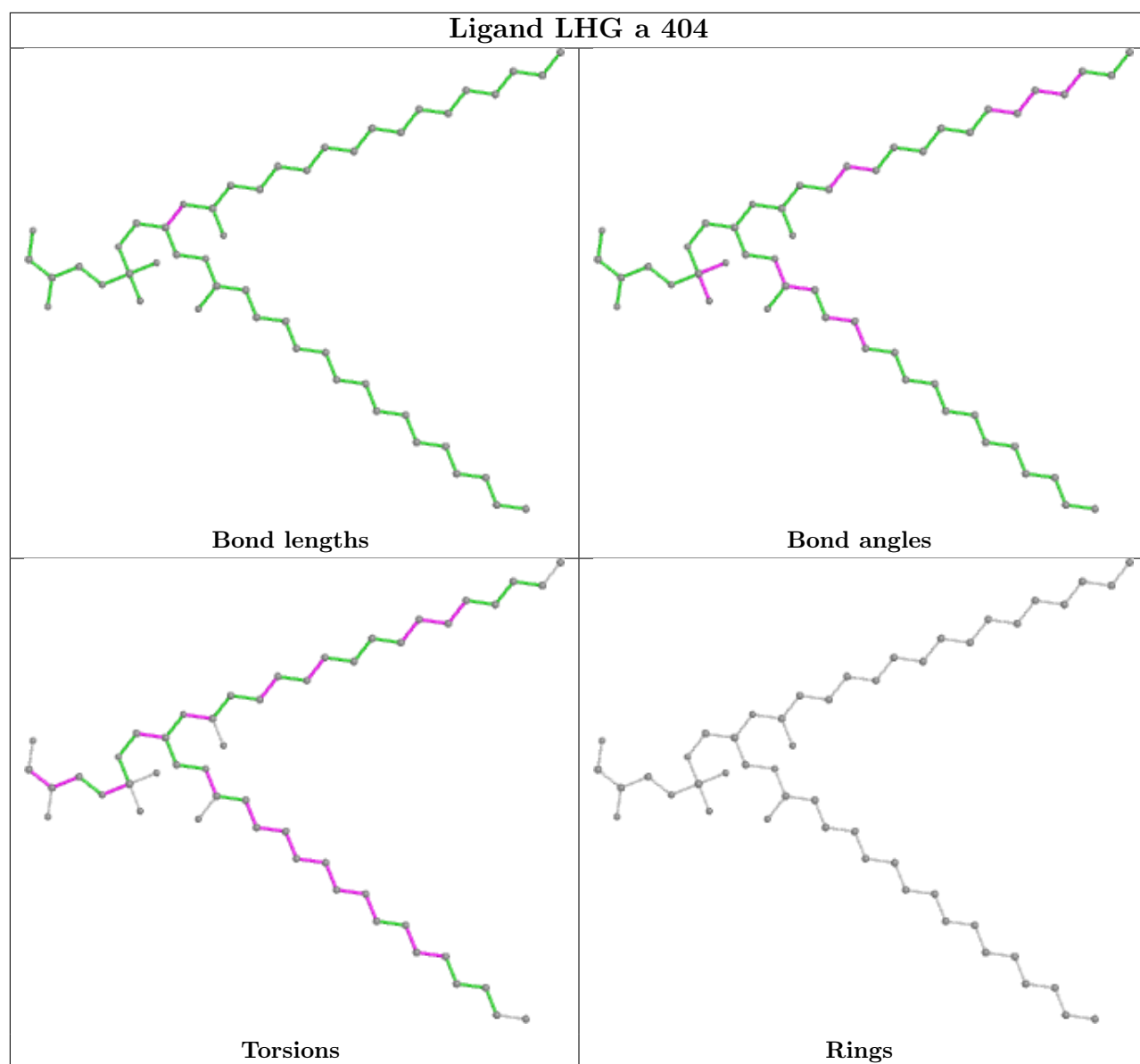
## Ligand DD6 9 304



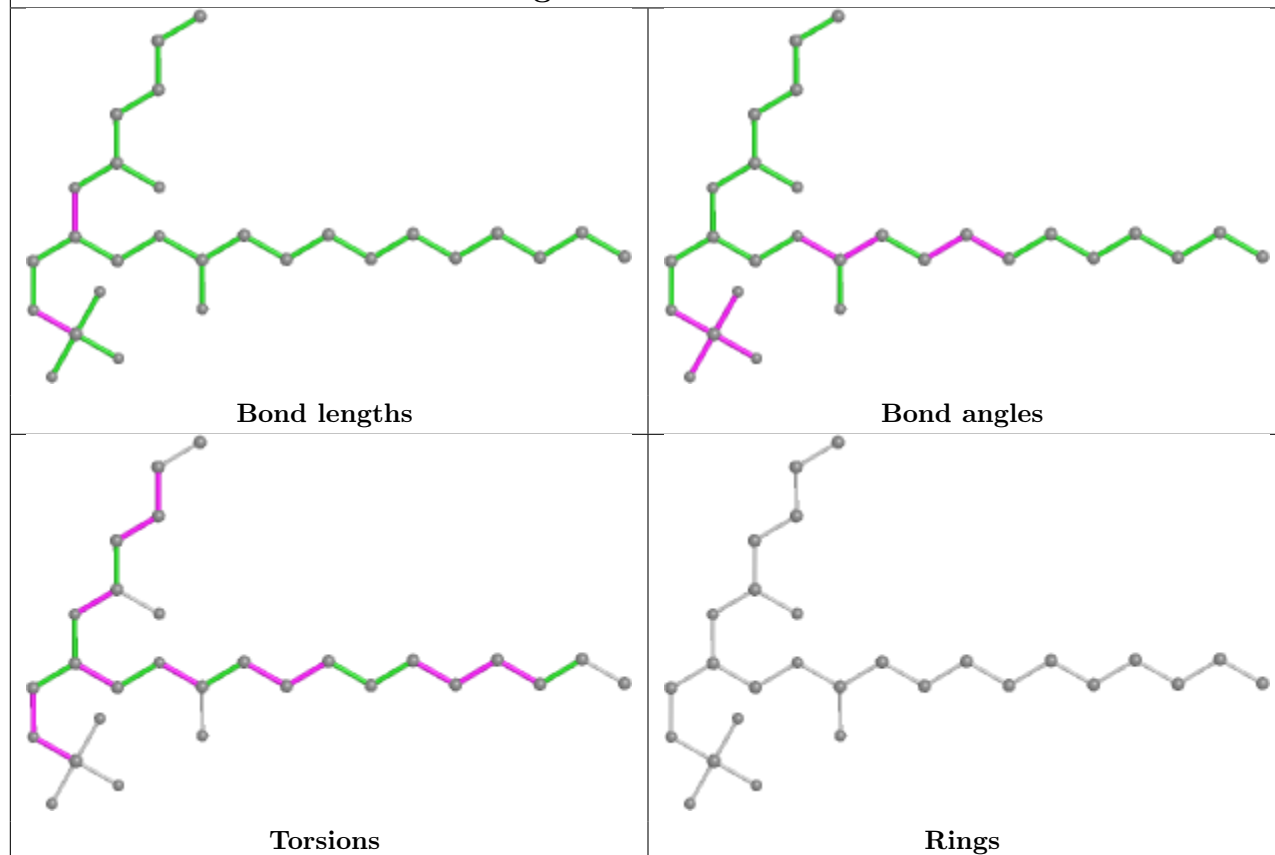


## Ligand CLA b 602

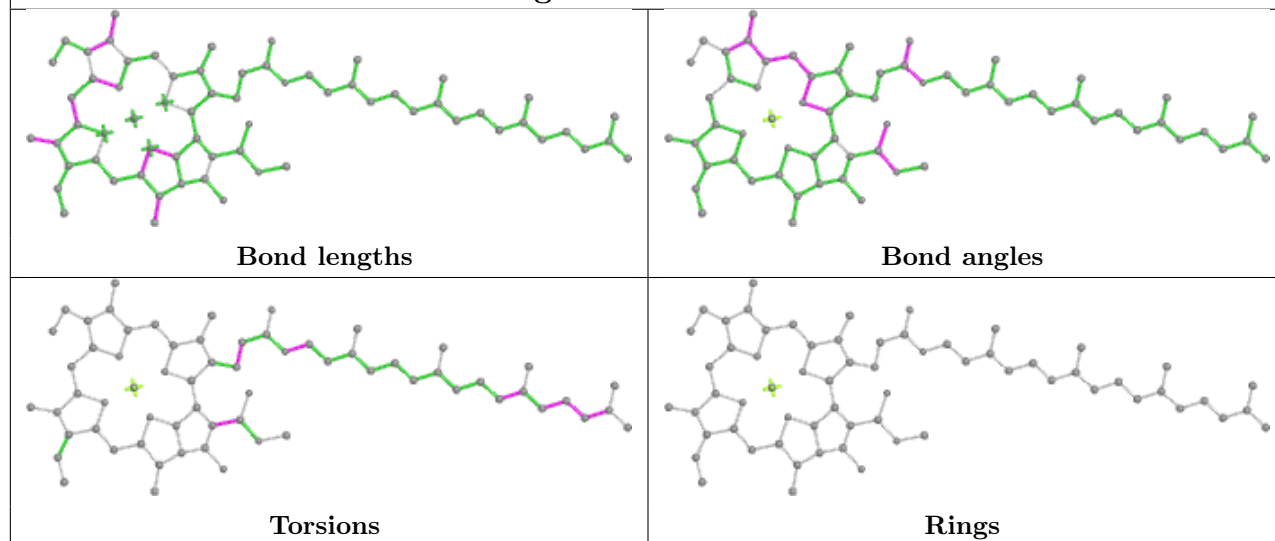


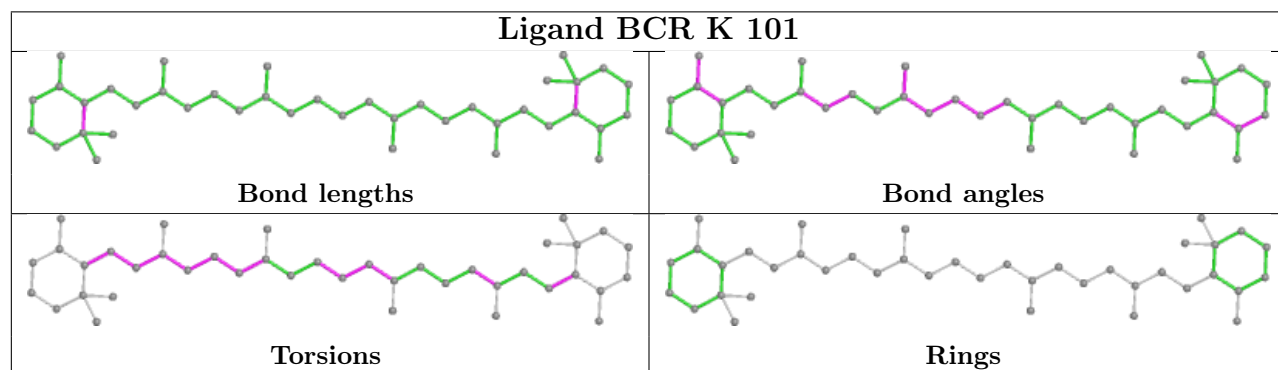
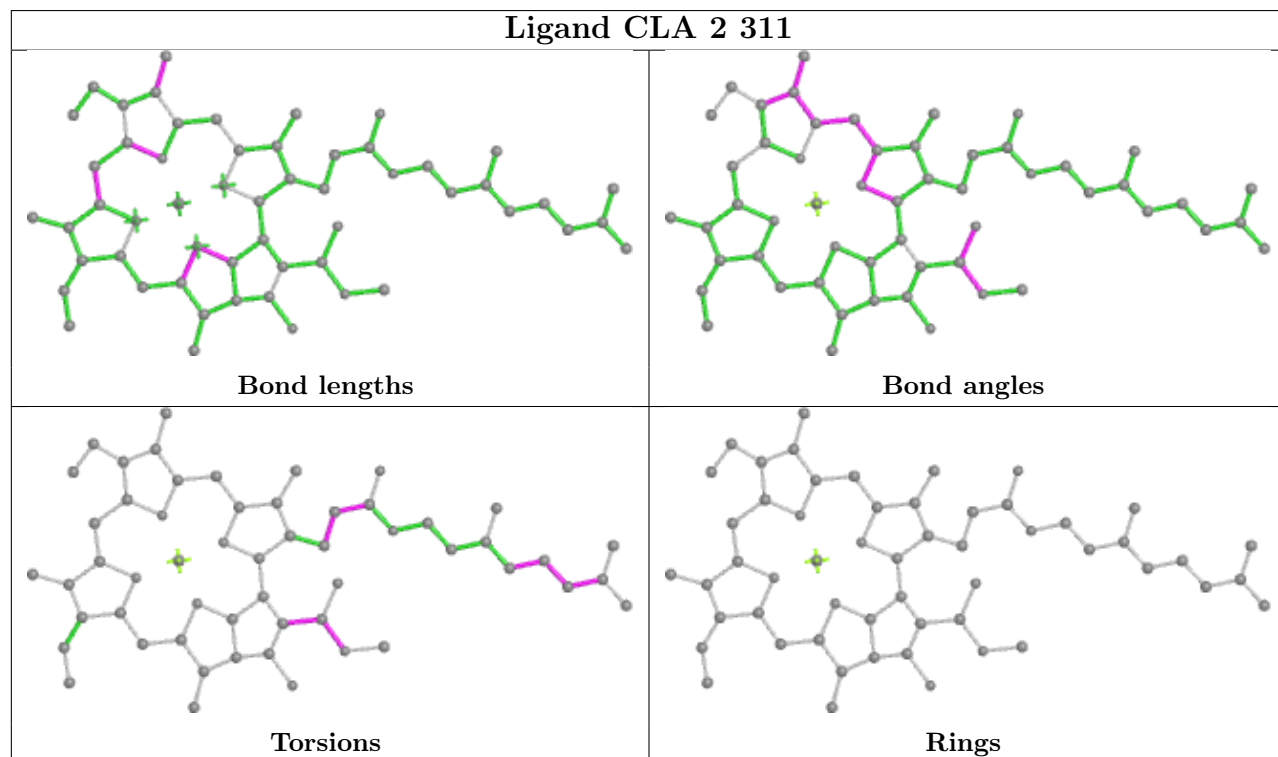
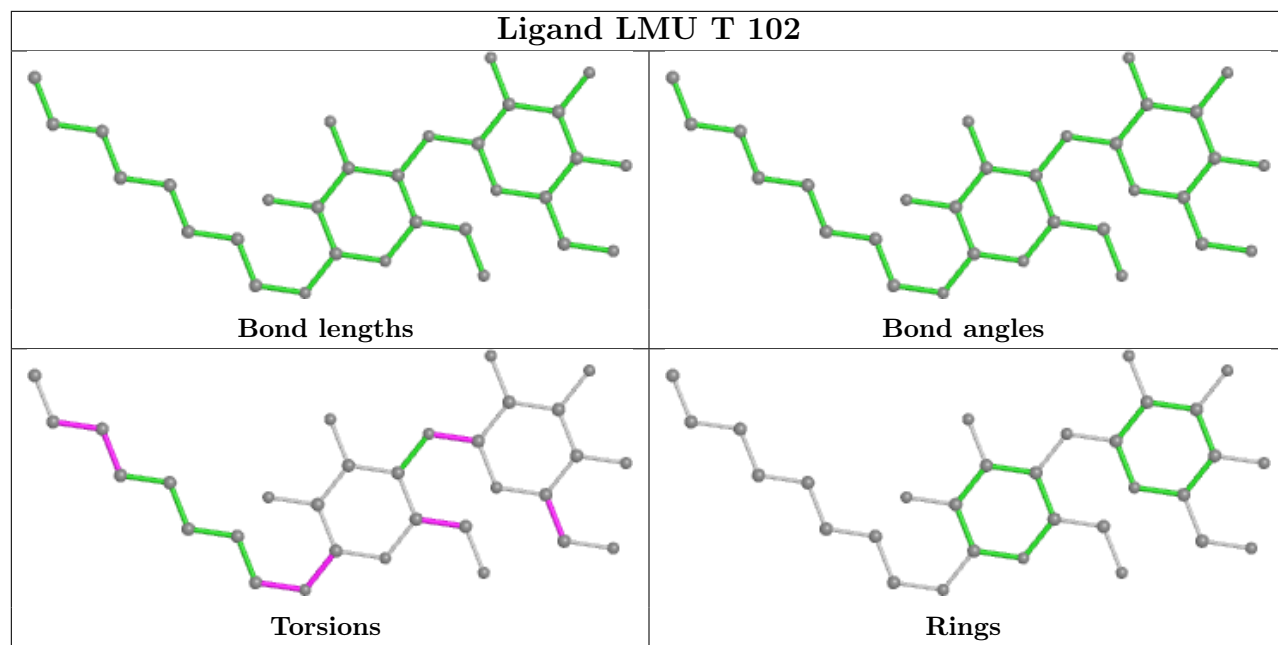


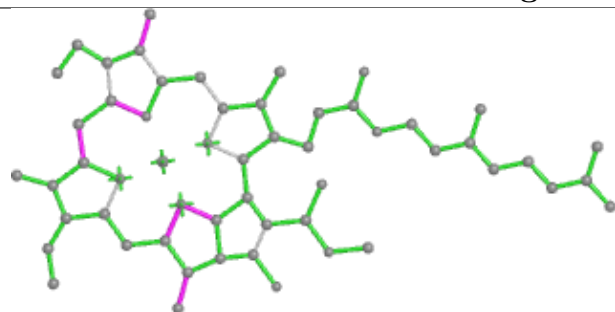
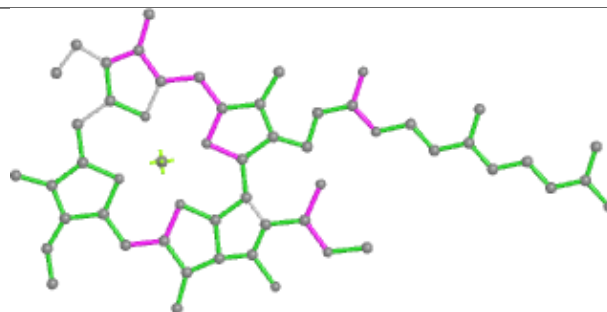
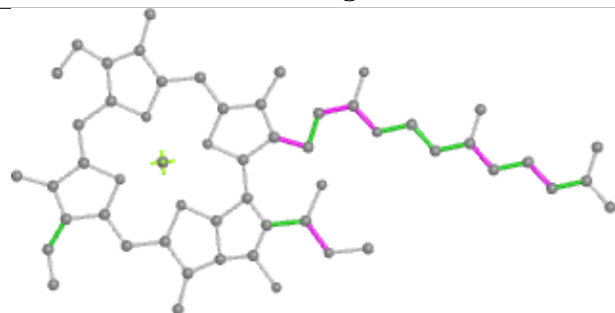
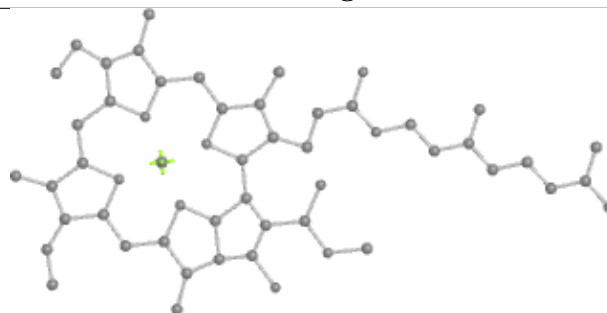
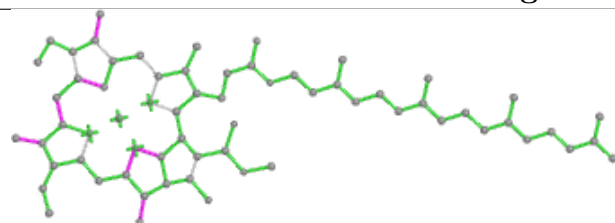
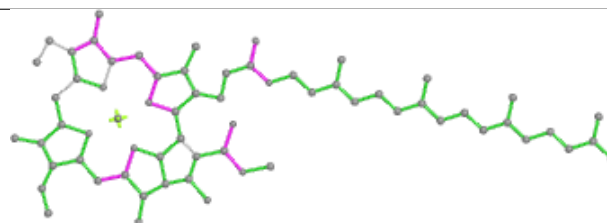
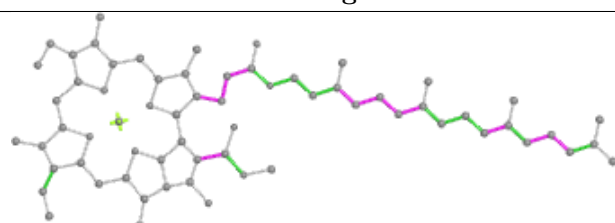
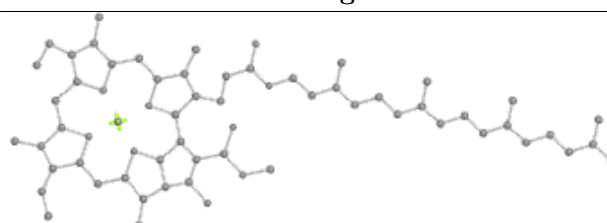
## Ligand LHG 0 315

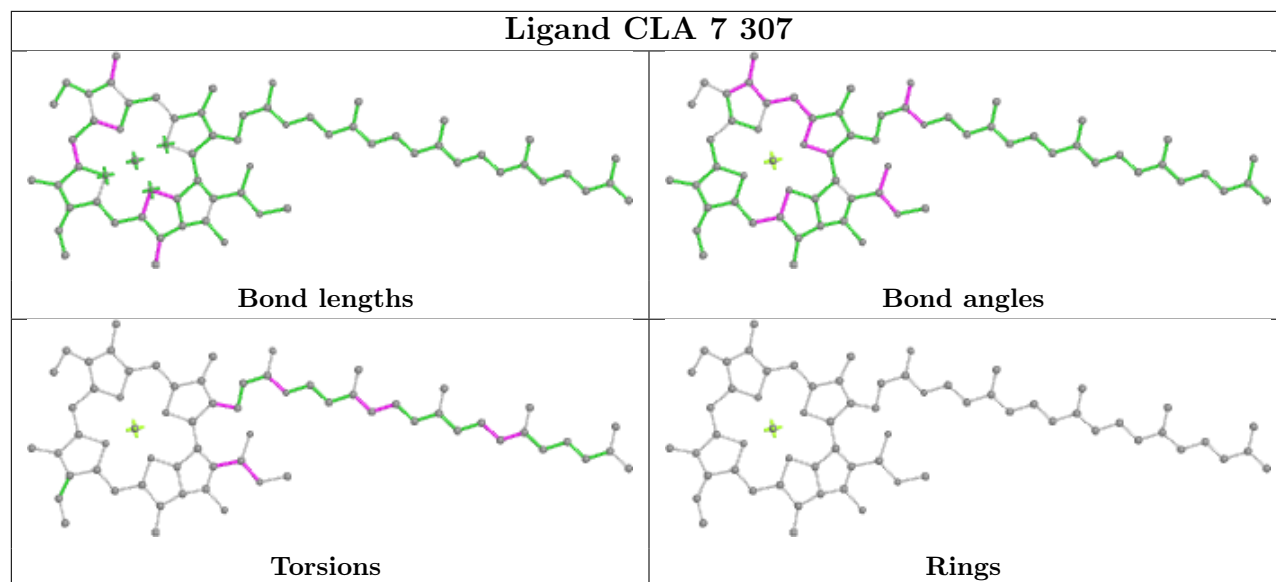
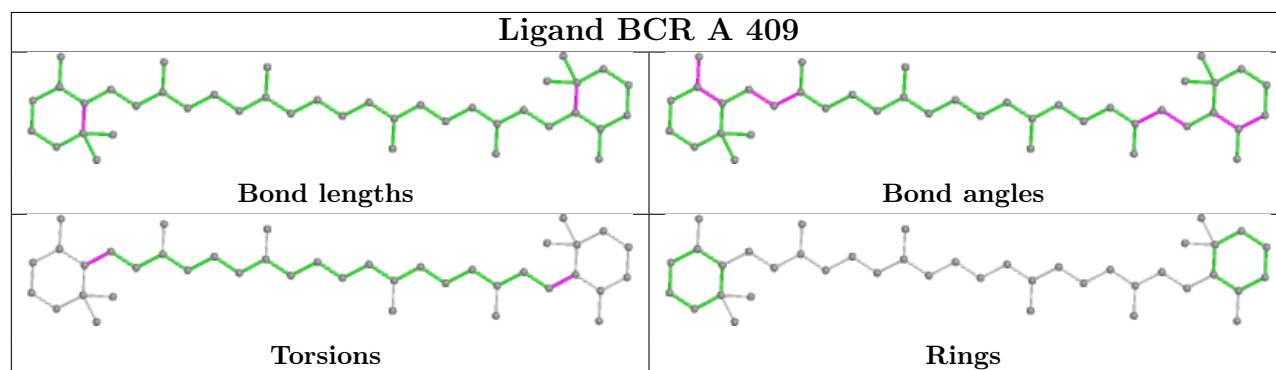


## Ligand CLA b 611

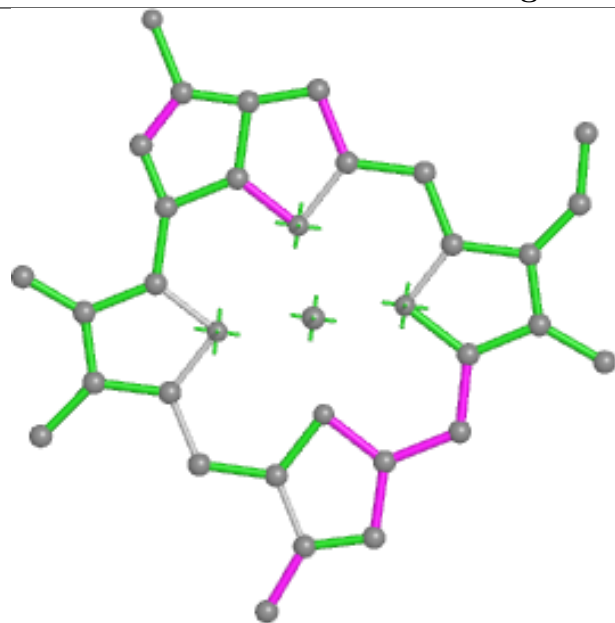




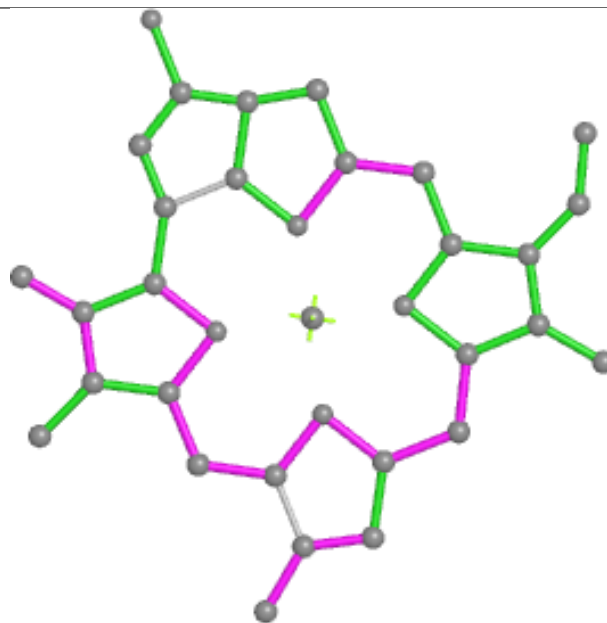
**Ligand CLA 9 308****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 3 303****Bond lengths****Bond angles****Torsions****Rings**

**Ligand CLA 7 307****Ligand BCR A 409**

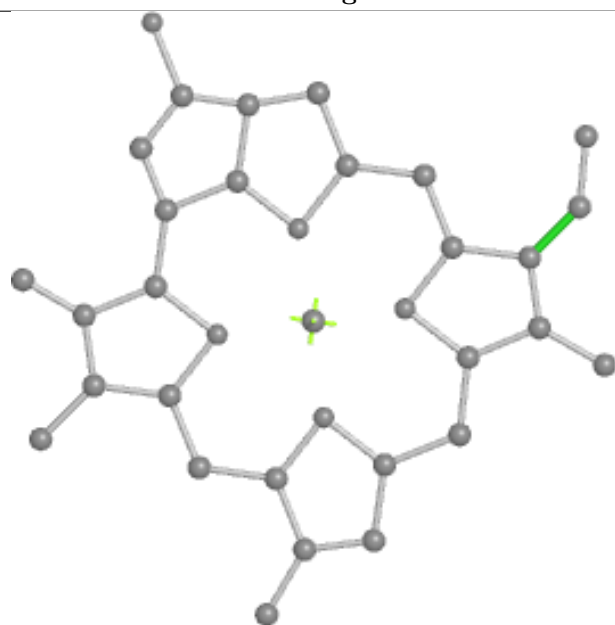
## Ligand CLA 0 313



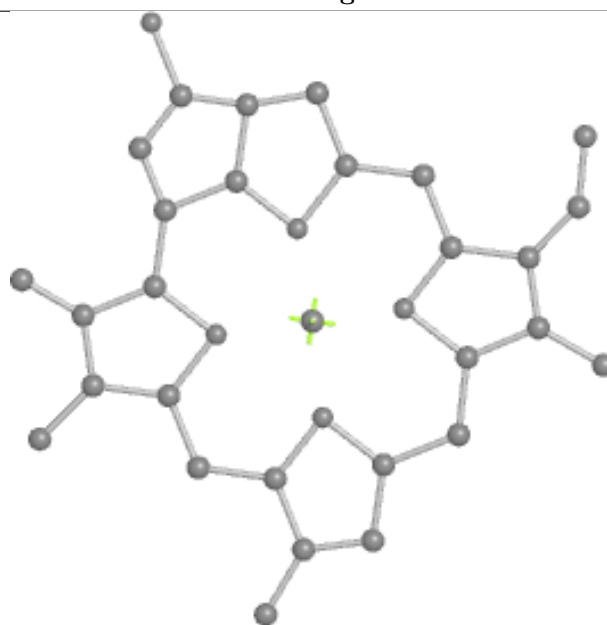
Bond lengths



Bond angles

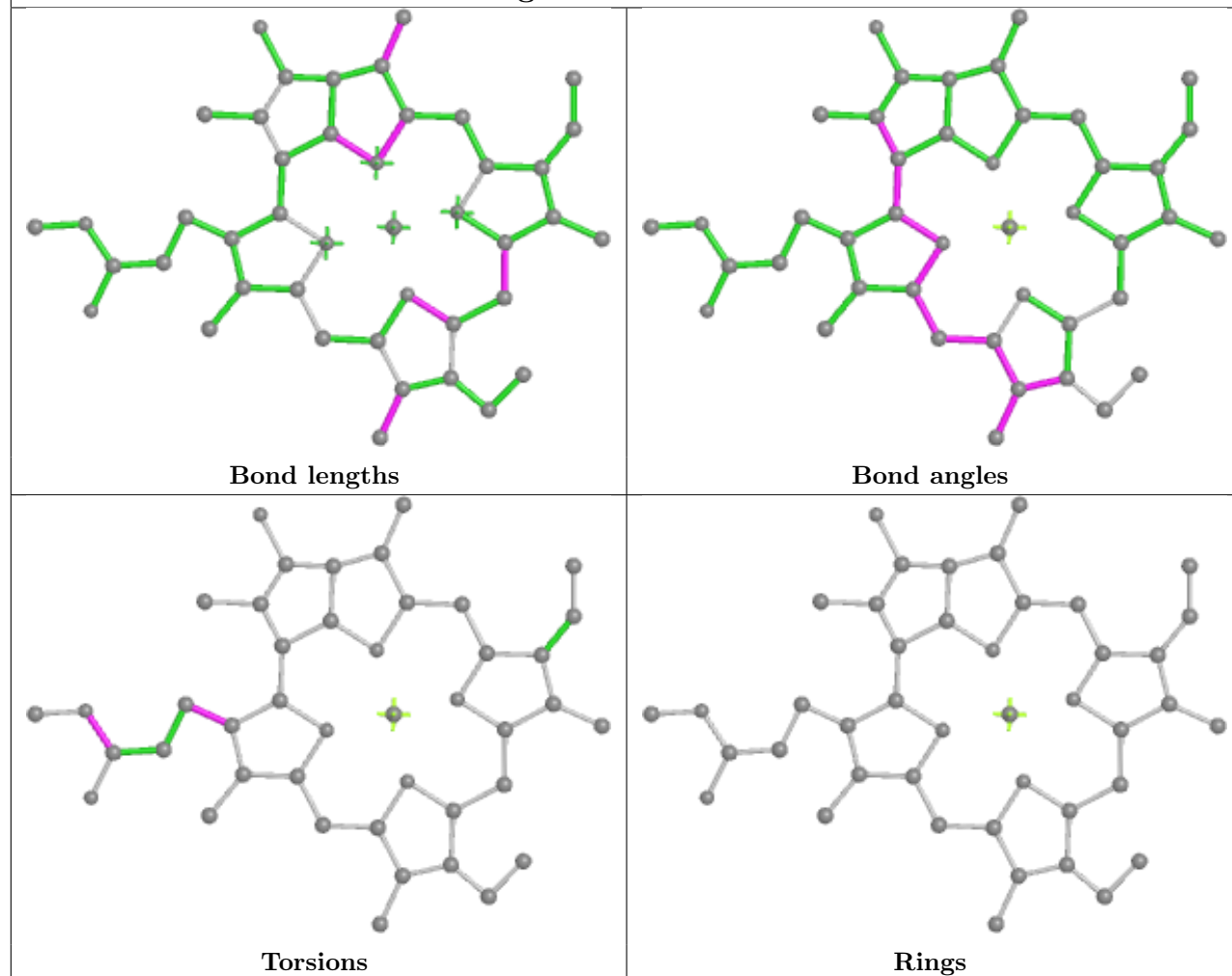


Torsions

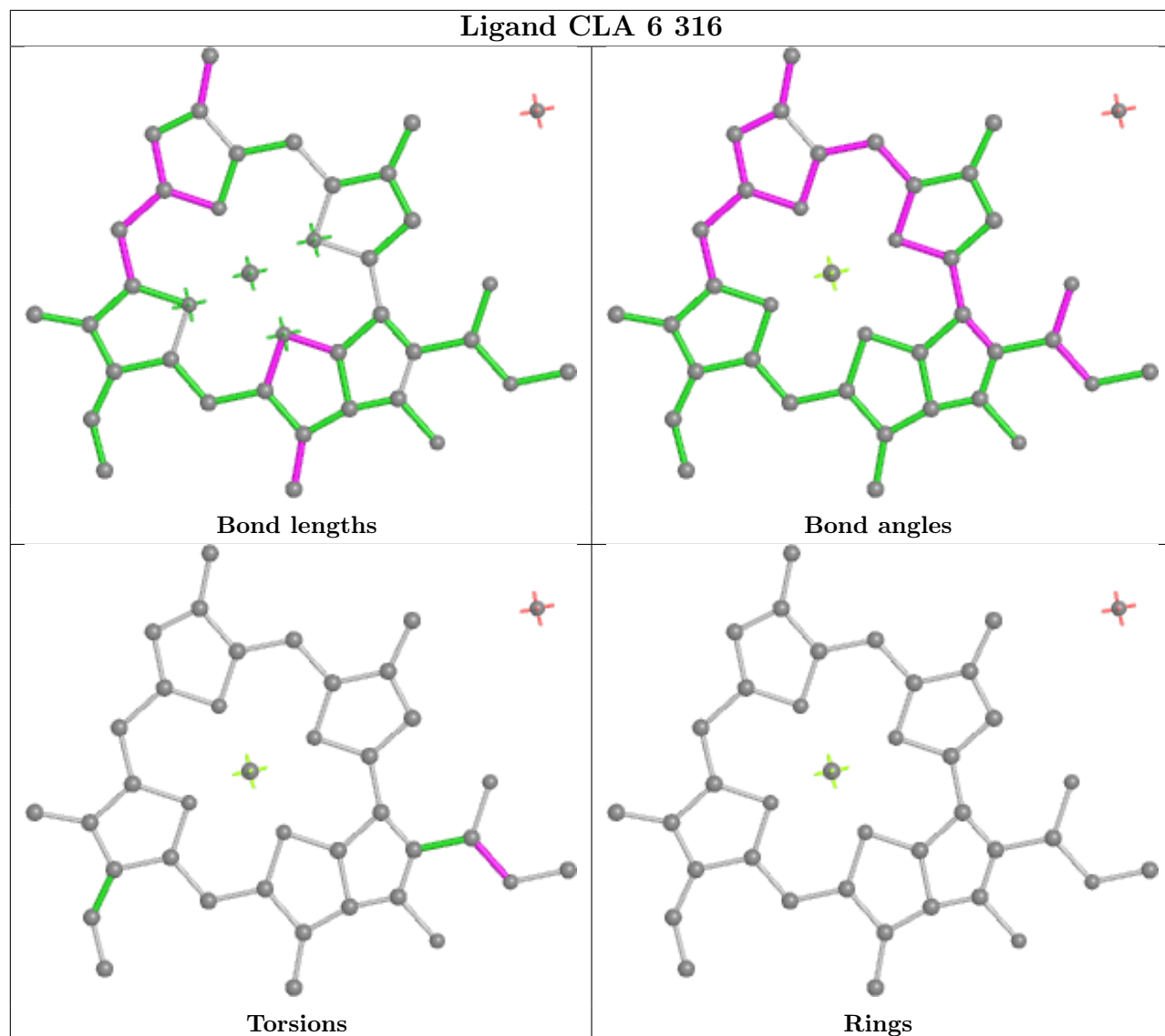


Rings

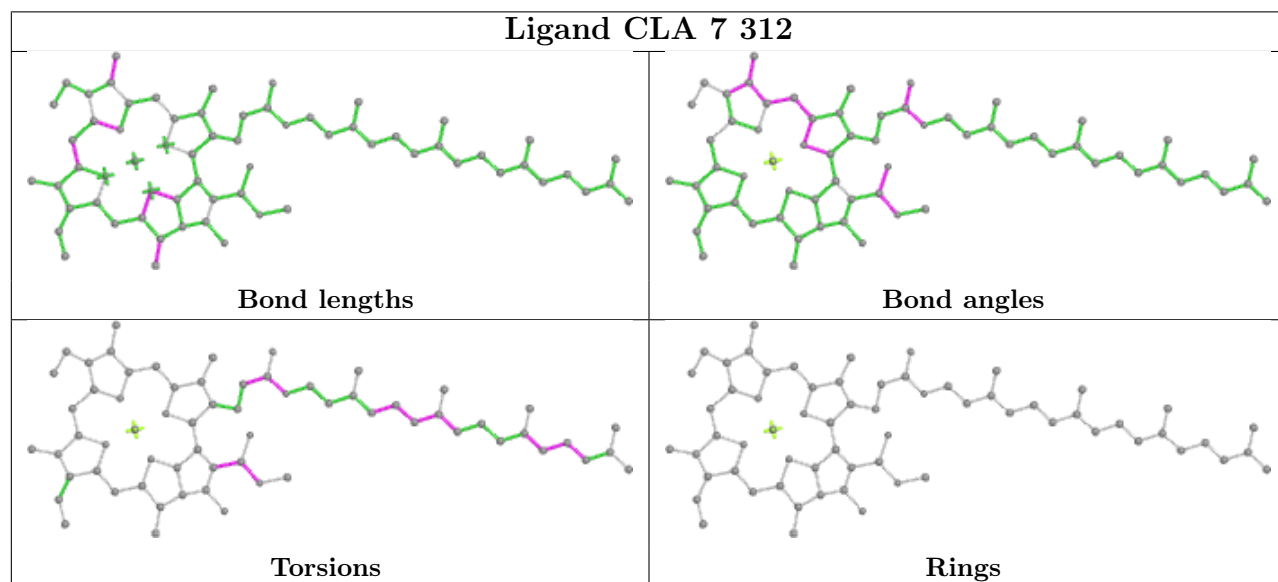
## Ligand CLA 7 314

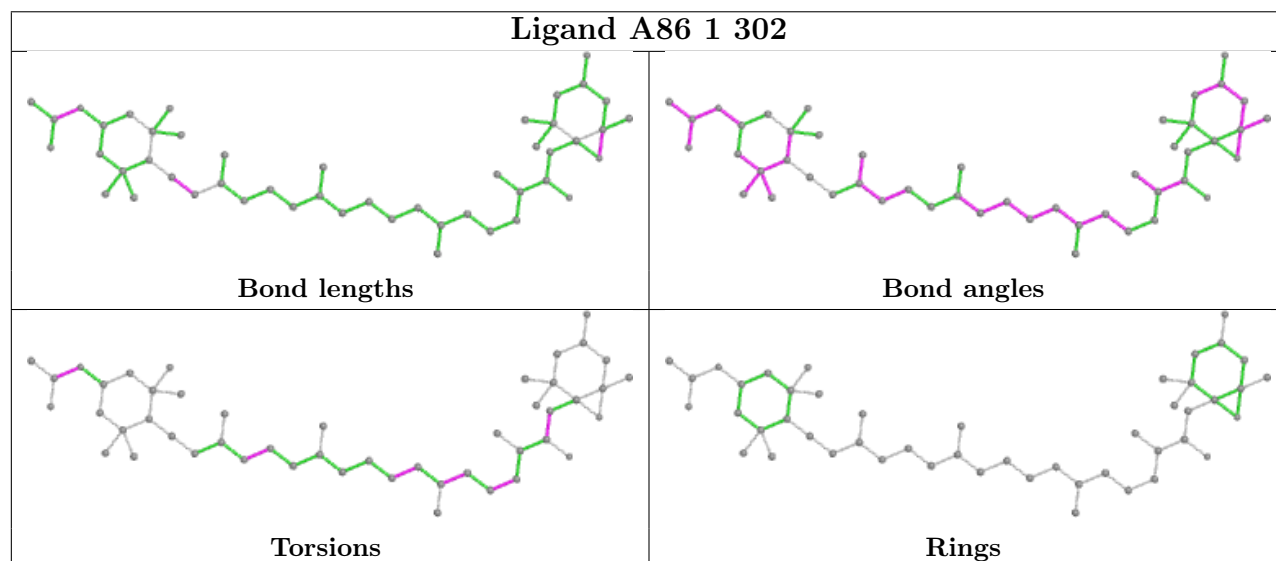
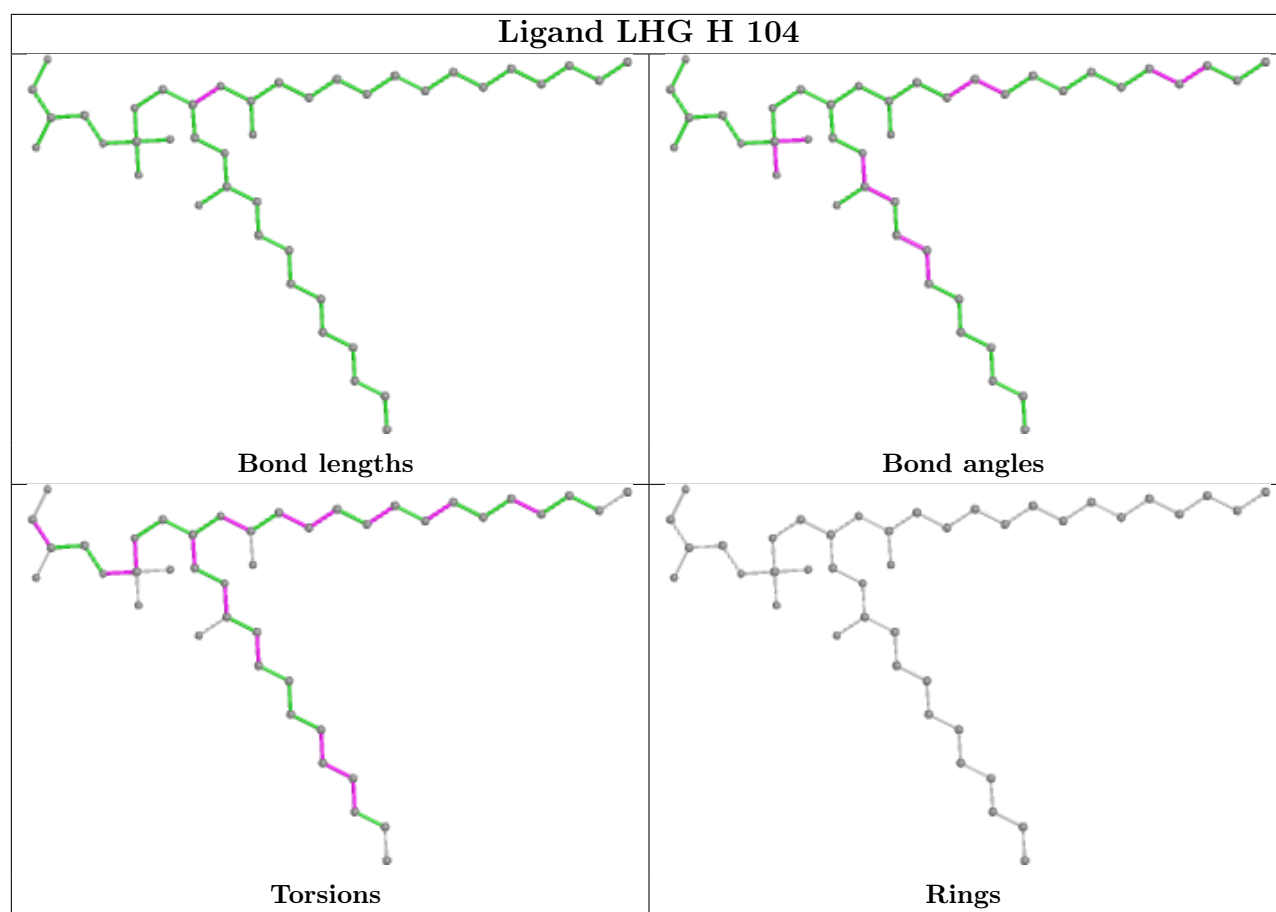


## Ligand CLA 6 316

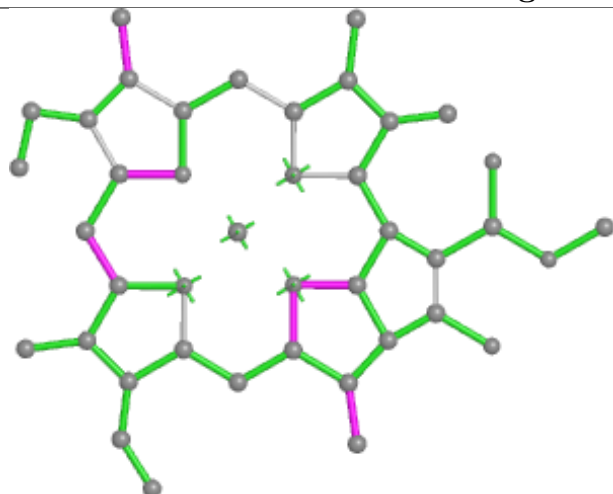


## Ligand CLA 7 312

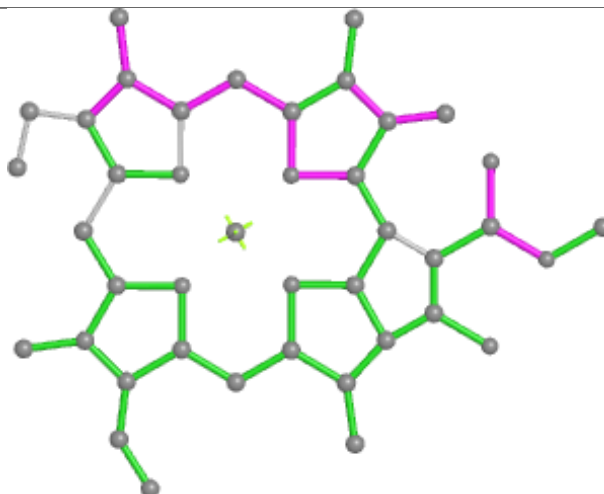




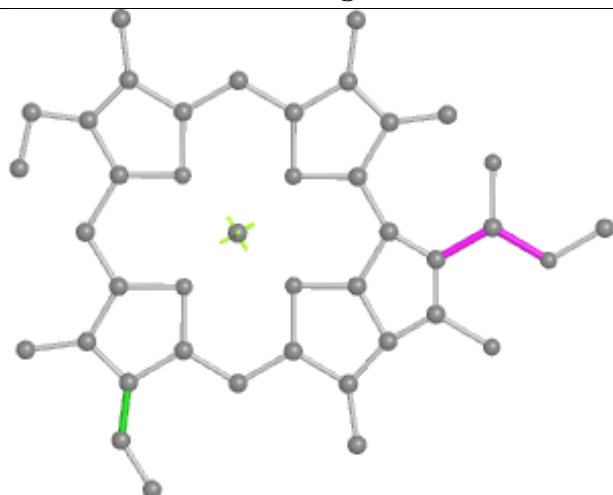
## Ligand CLA 6 315



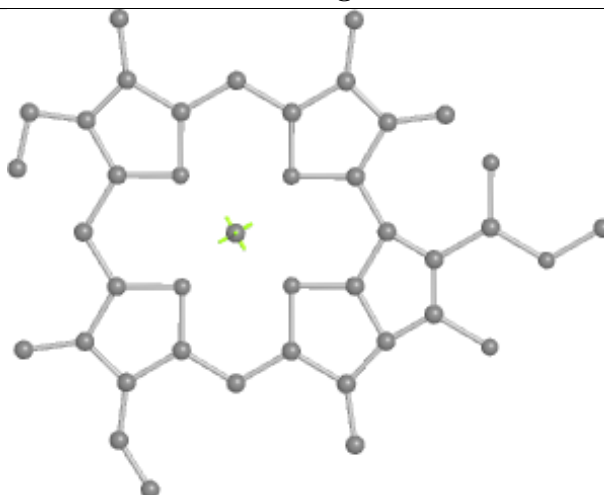
Bond lengths



Bond angles

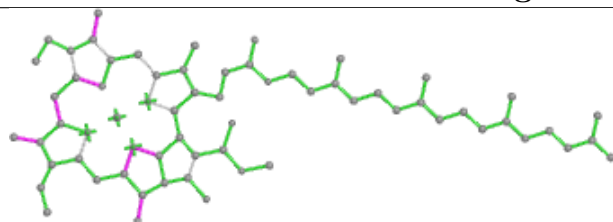


Torsions

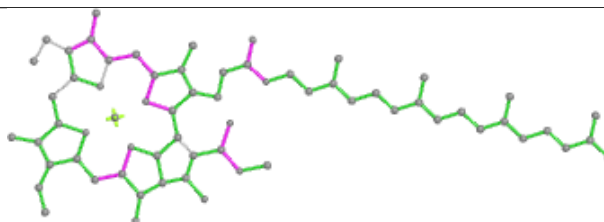


Rings

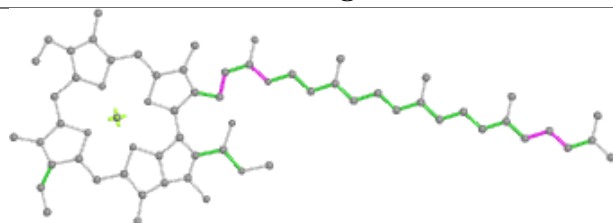
## Ligand CLA B 608



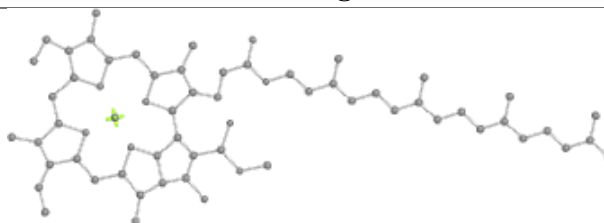
Bond lengths



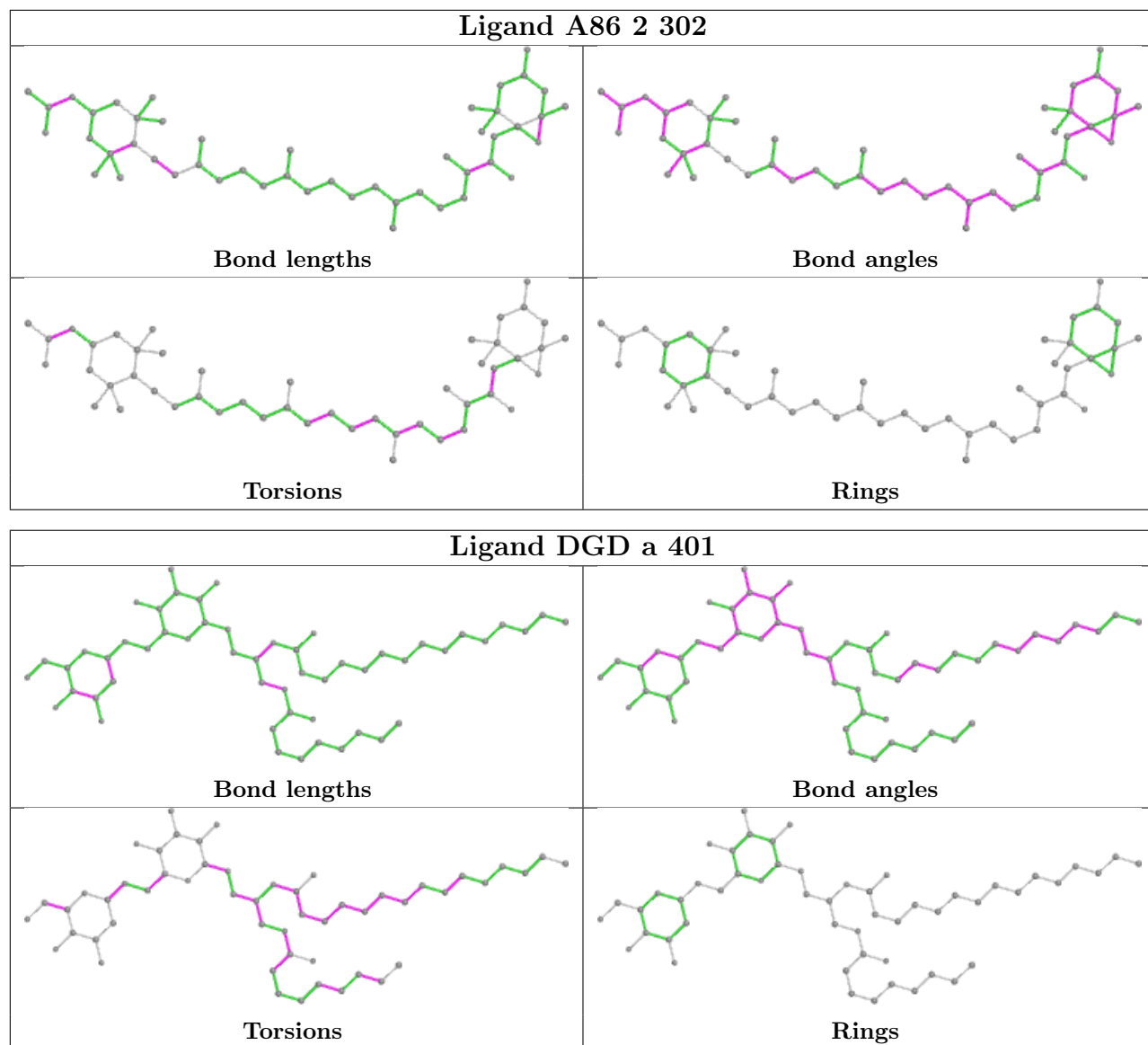
Bond angles



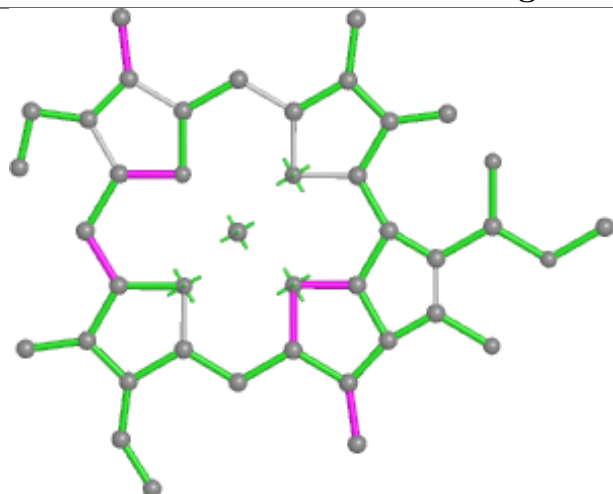
Torsions



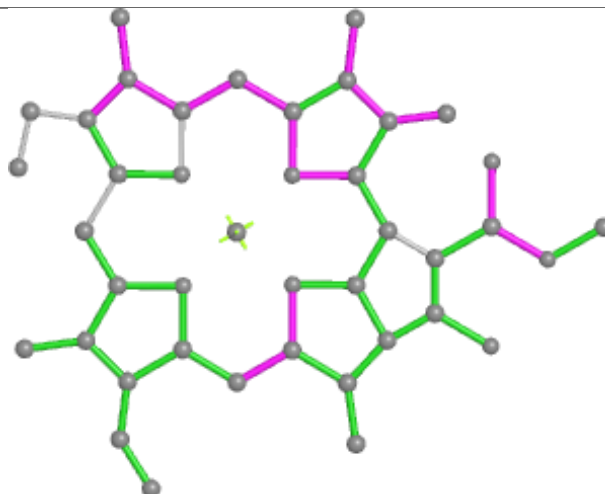
Rings



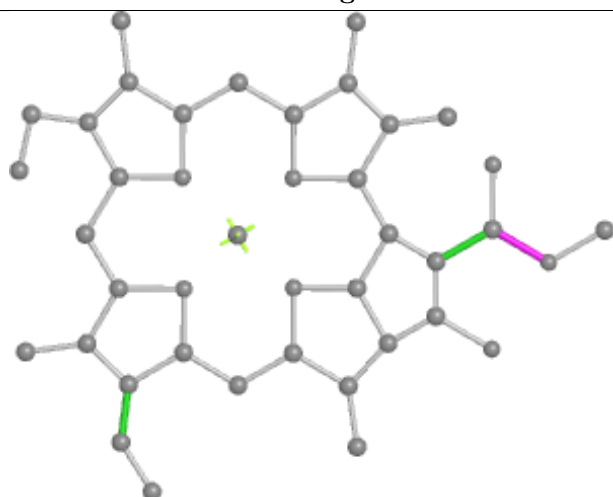
## Ligand CLA 0 308



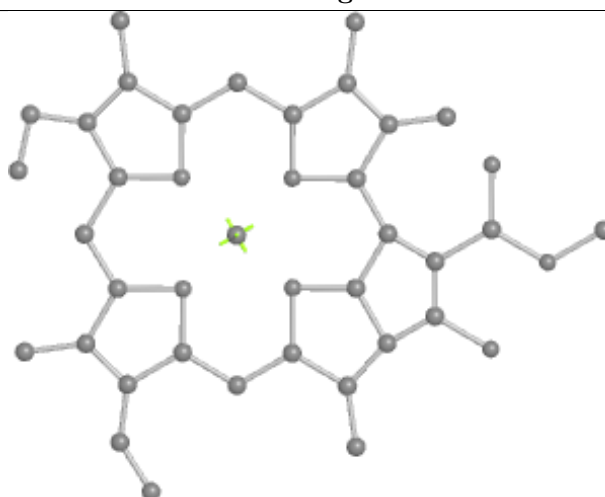
Bond lengths



Bond angles

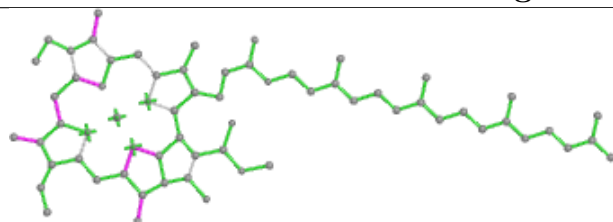


Torsions

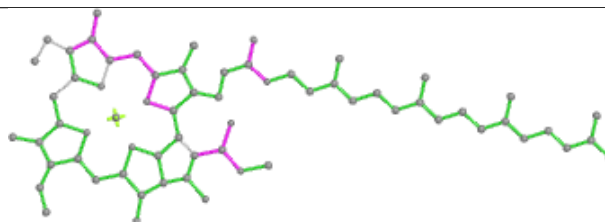


Rings

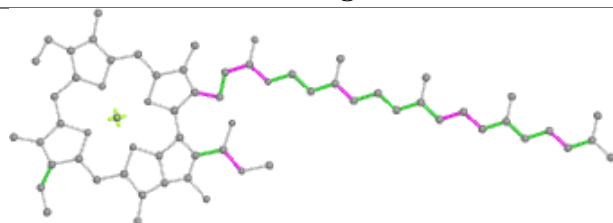
## Ligand CLA B 612



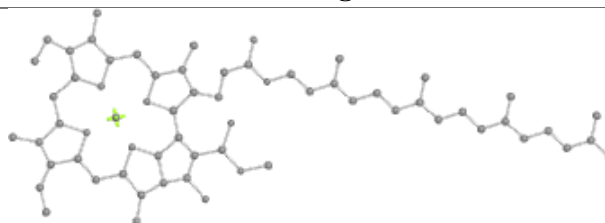
Bond lengths



Bond angles

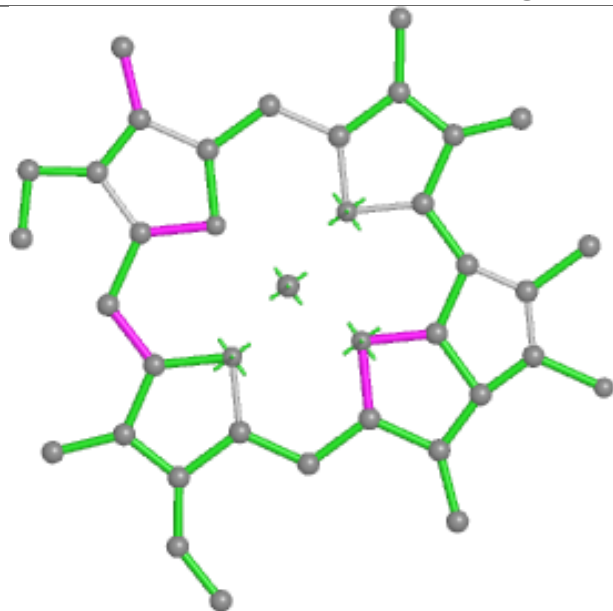


Torsions

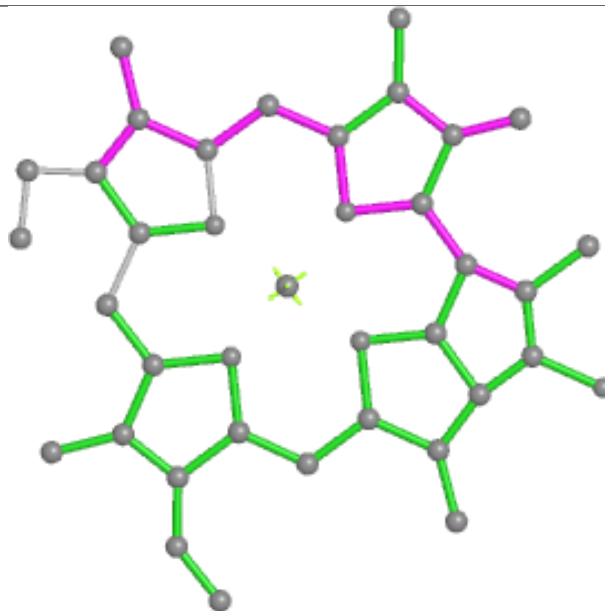


Rings

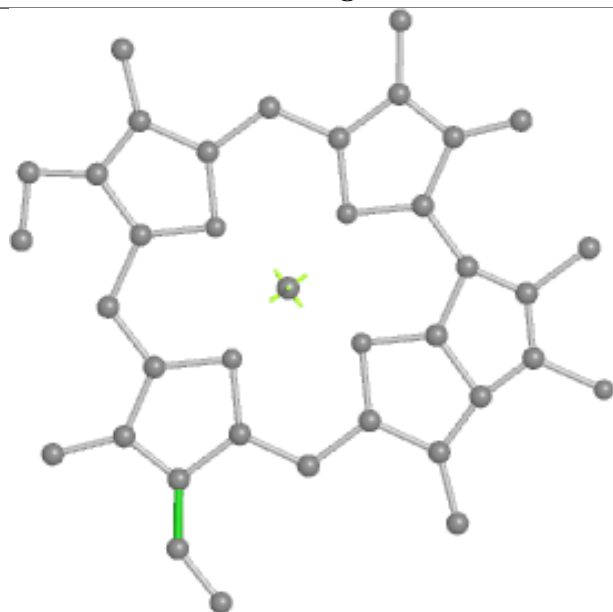
## Ligand CLA 1 316



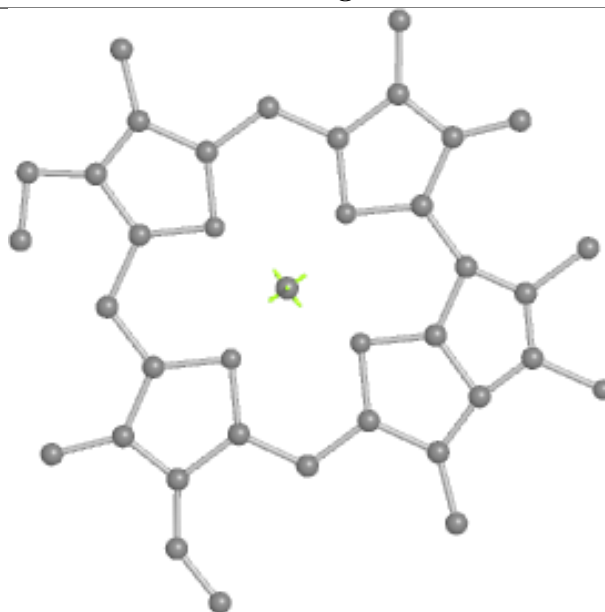
Bond lengths



Bond angles

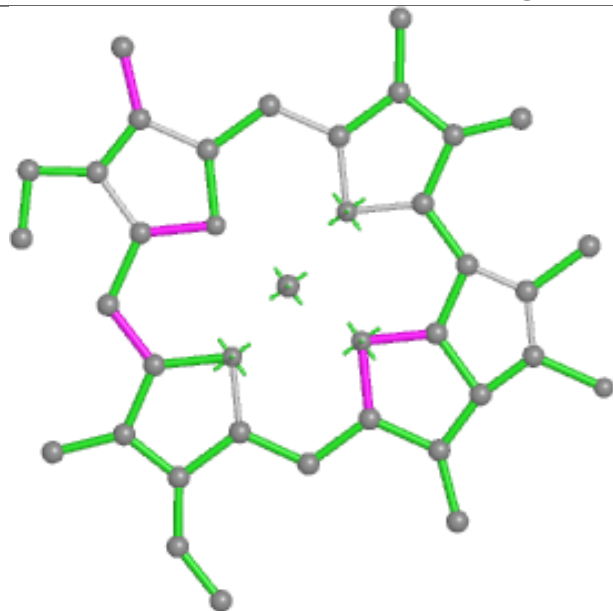


Torsions

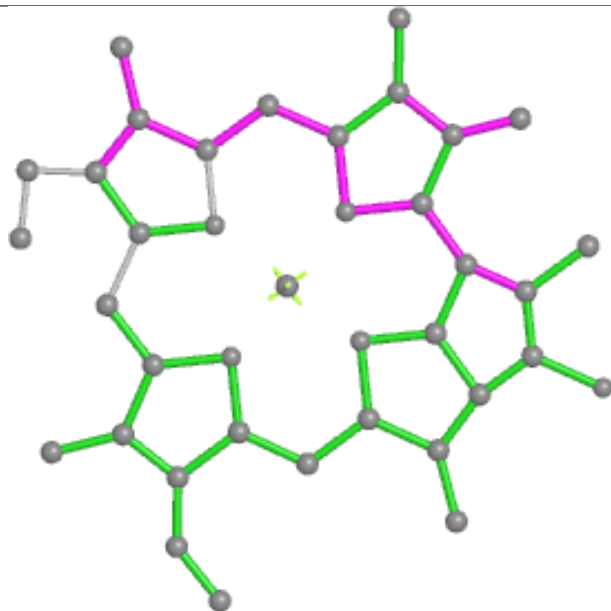


Rings

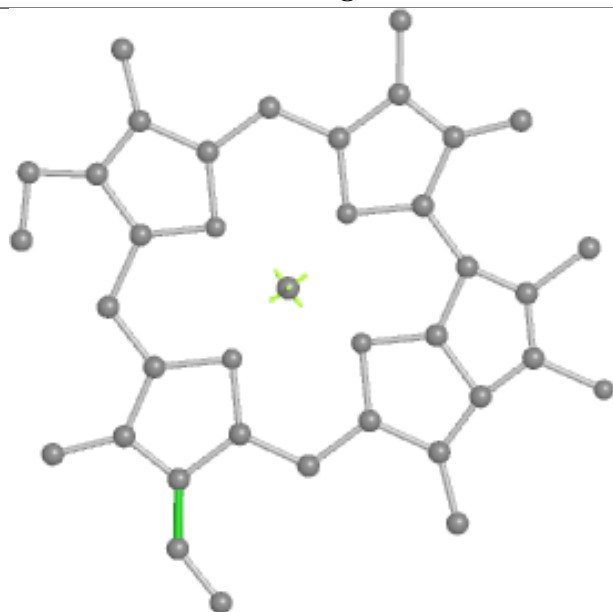
## Ligand CLA 2 314



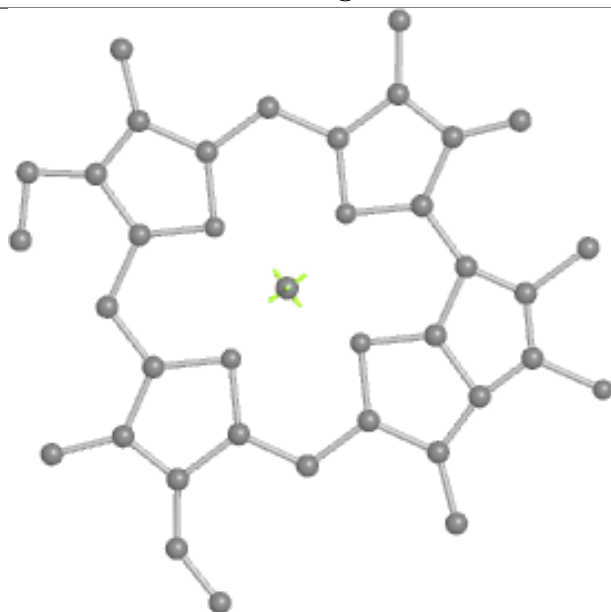
Bond lengths



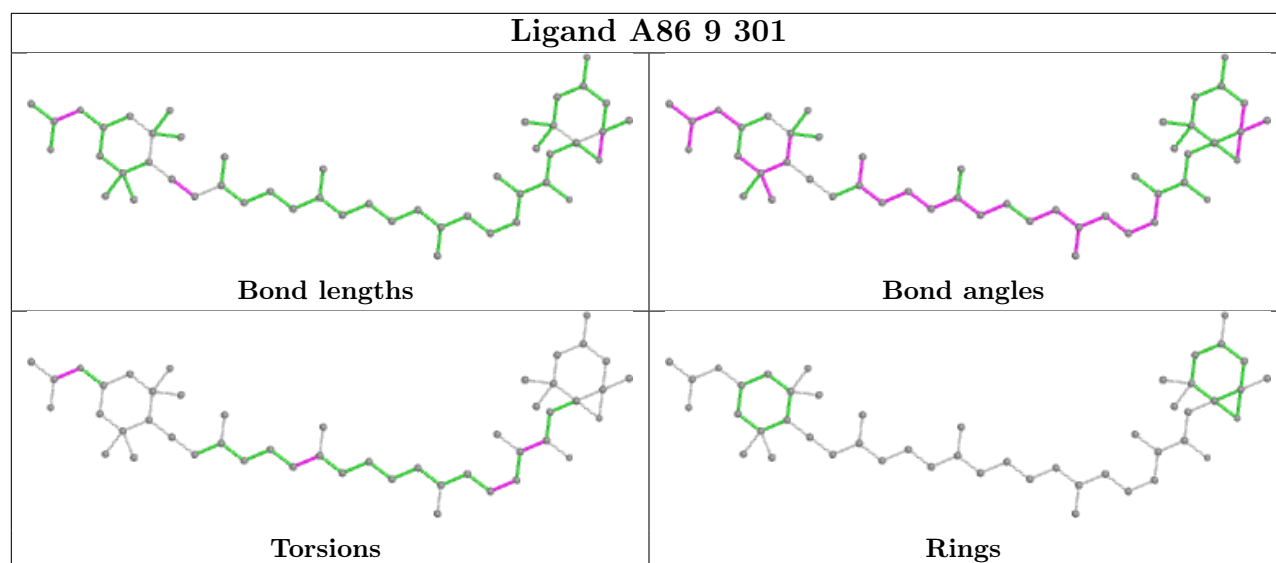
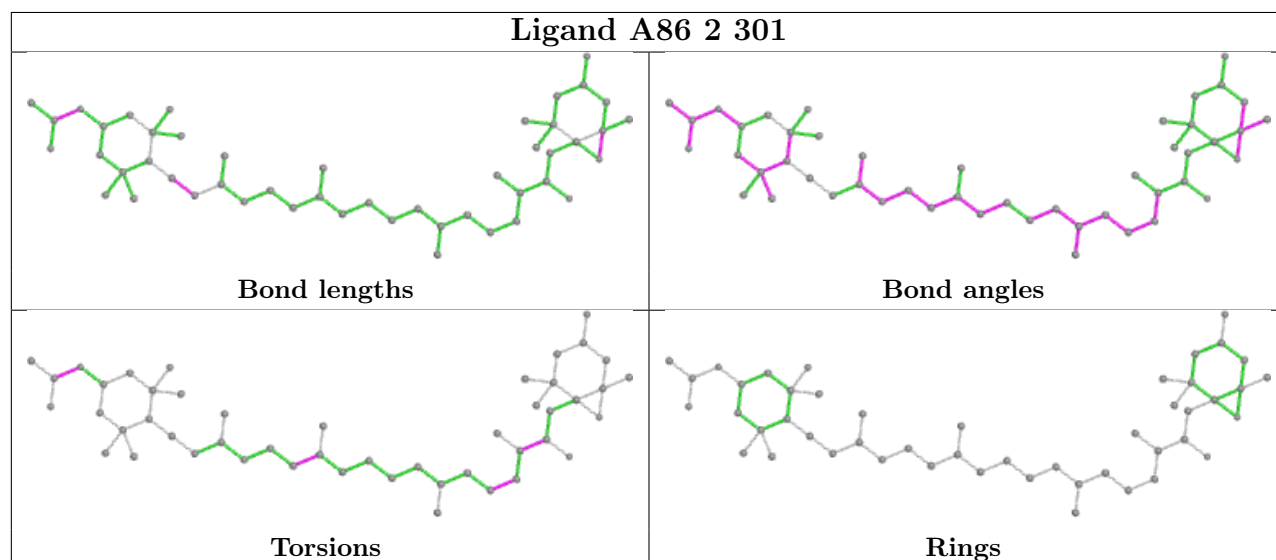
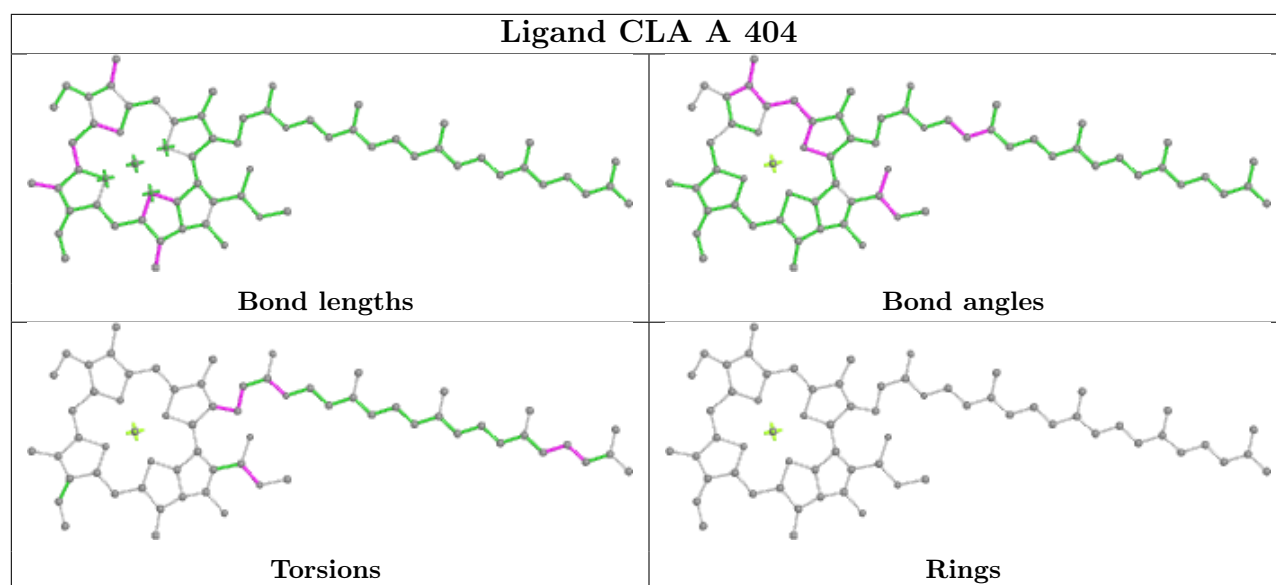
Bond angles

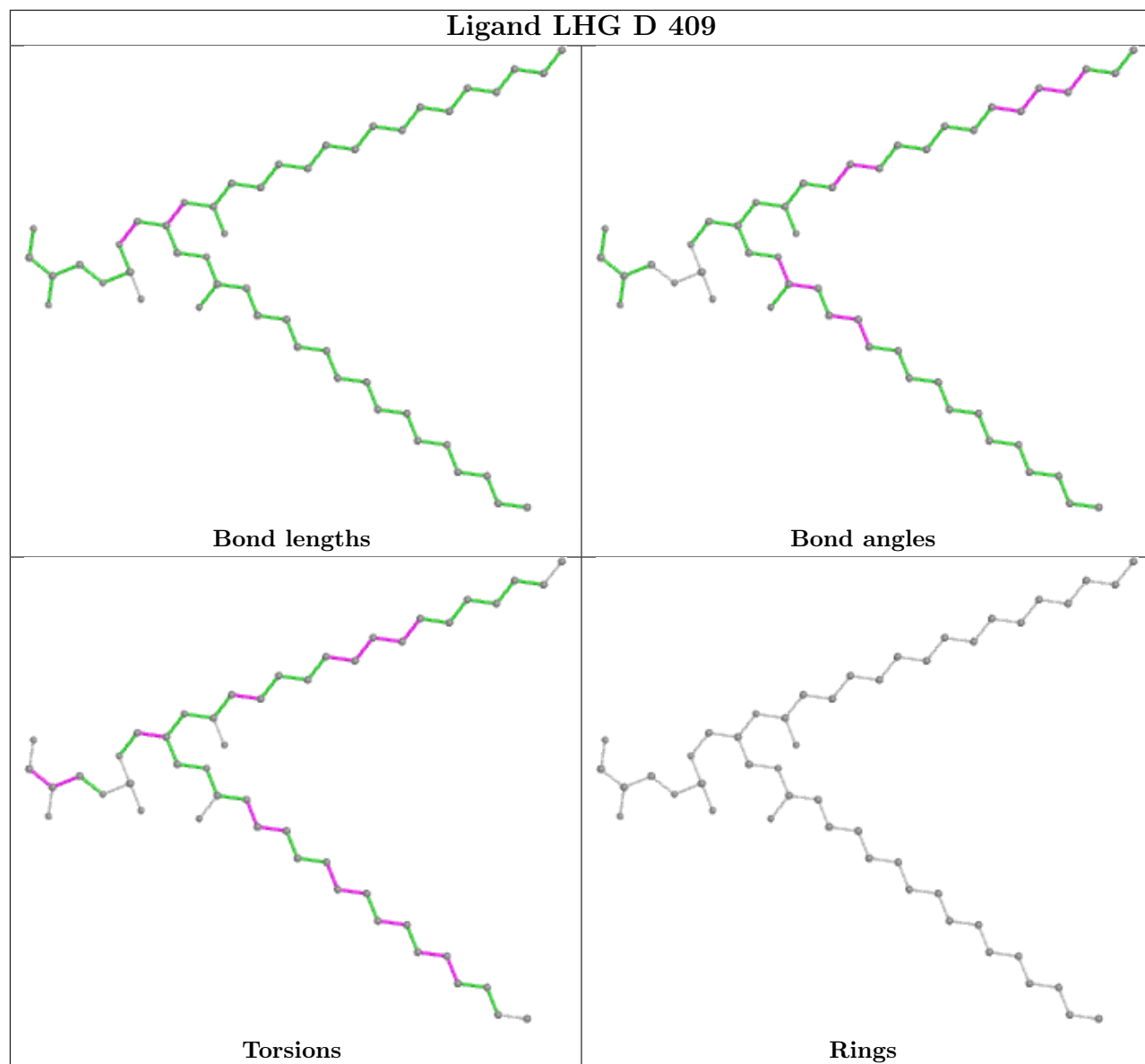


Torsions

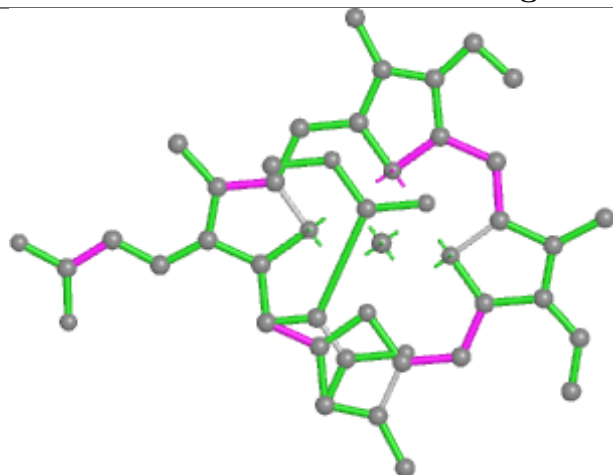


Rings

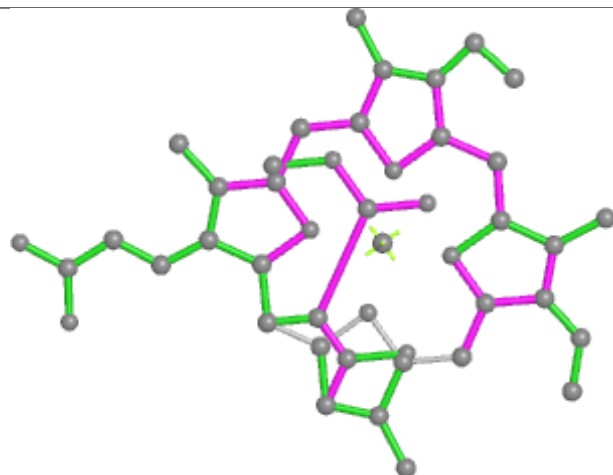




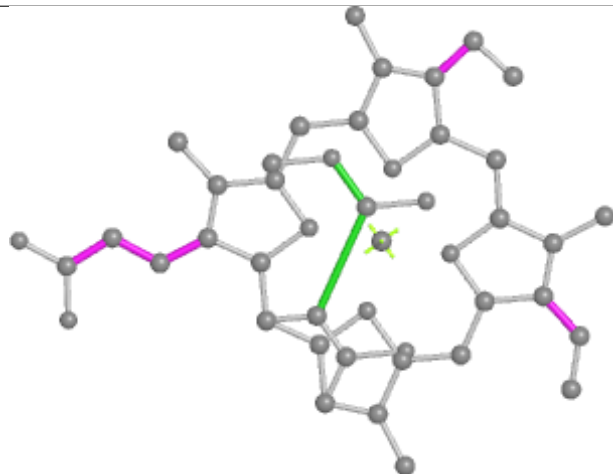
## Ligand KC2 7 306



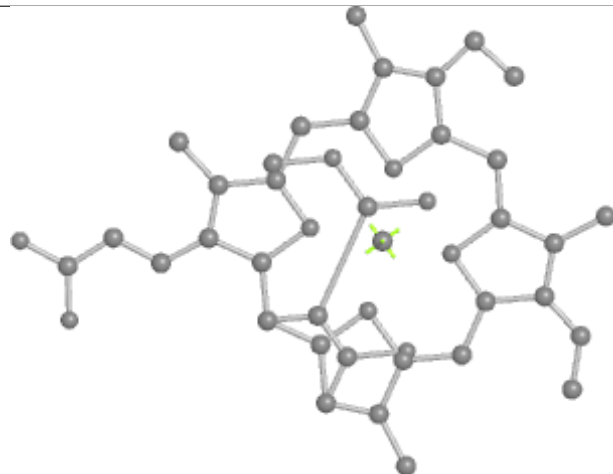
Bond lengths



Bond angles

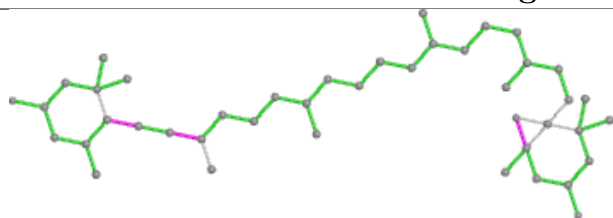


Torsions

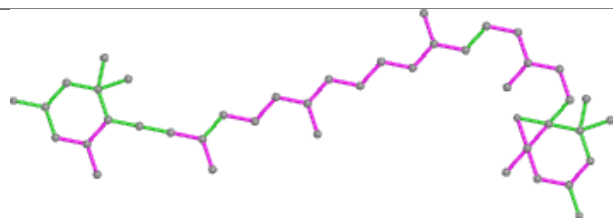


Rings

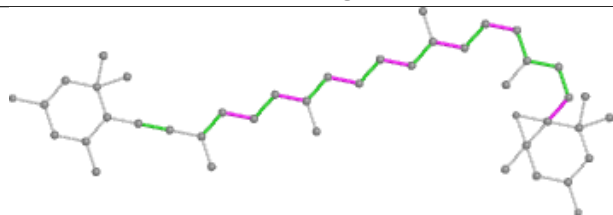
## Ligand DD6 8 304



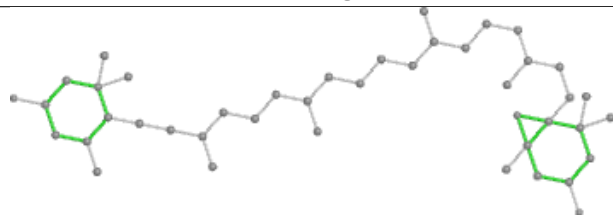
Bond lengths



Bond angles

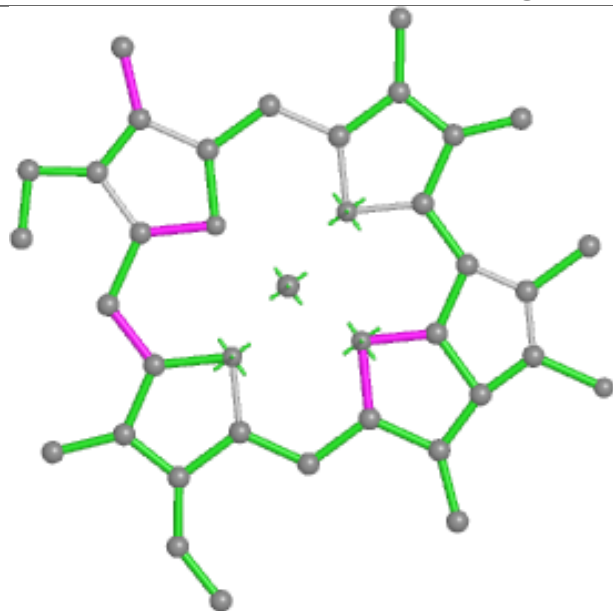


Torsions

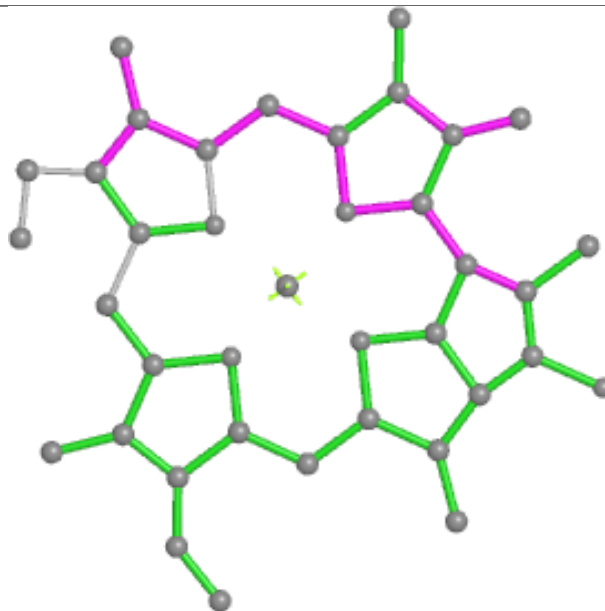


Rings

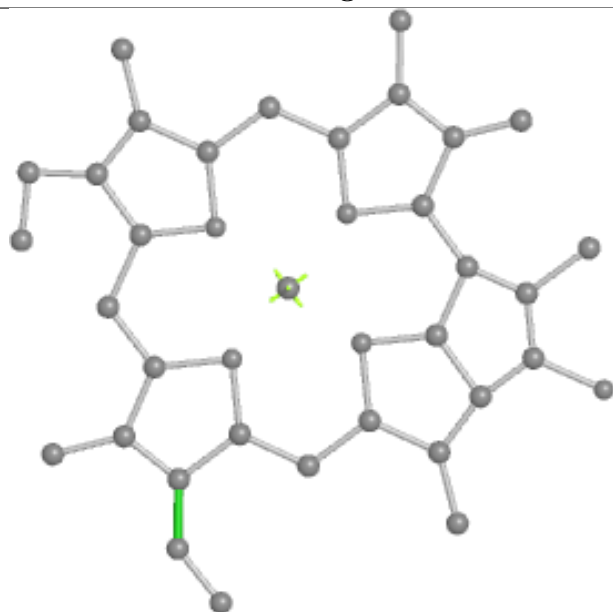
## Ligand CLA 1 315



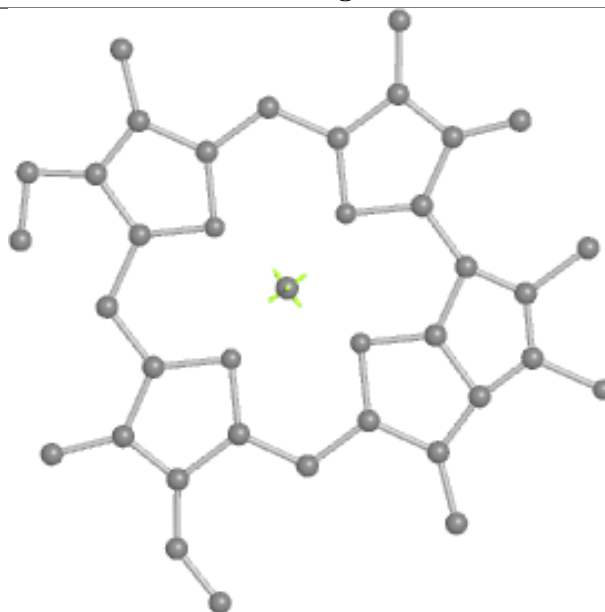
Bond lengths



Bond angles

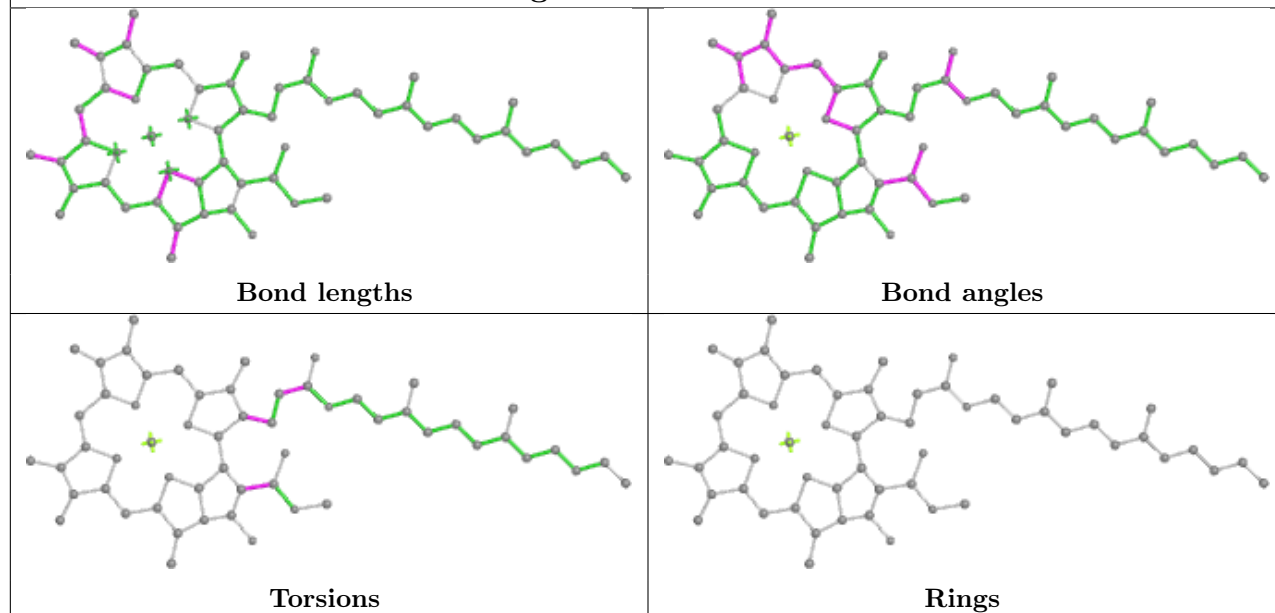


Torsions

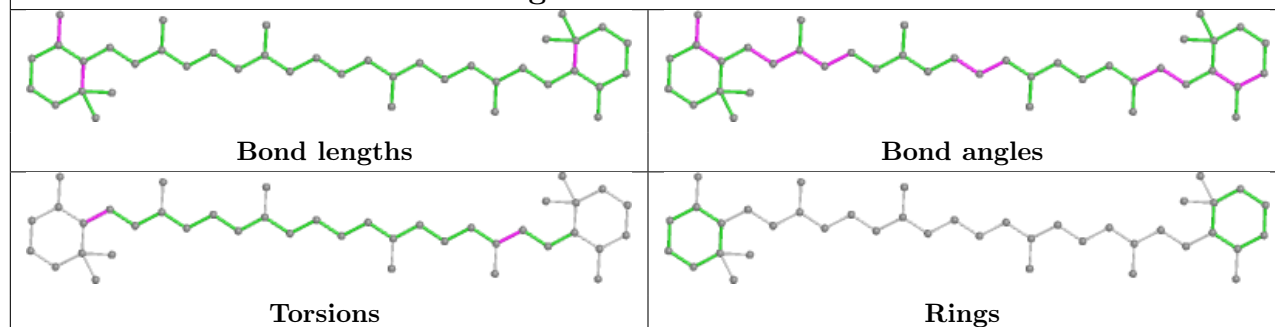


Rings

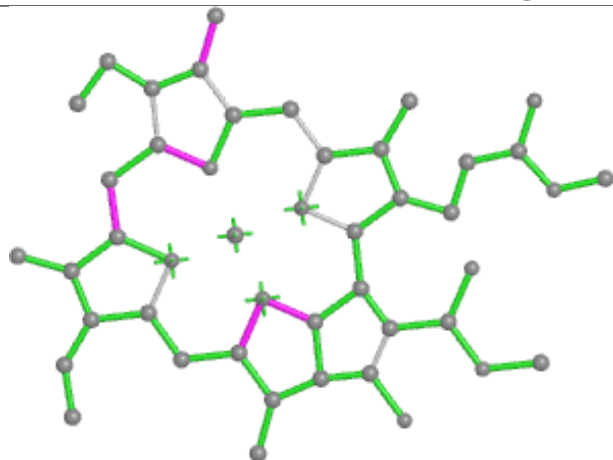
## Ligand CLA D 405



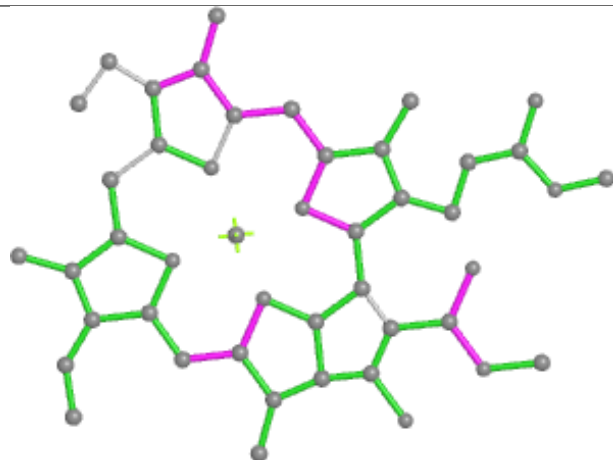
## Ligand BCR D 407



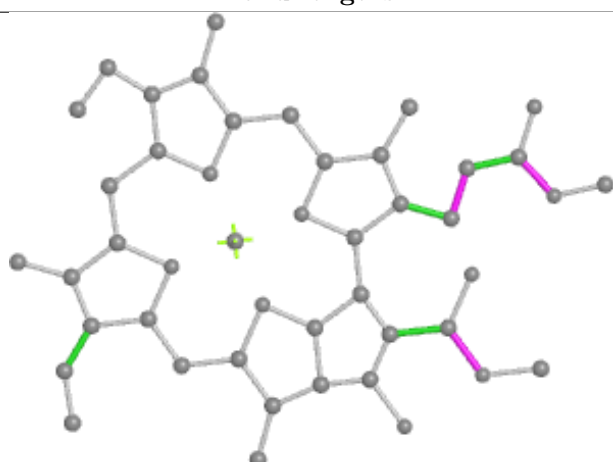
## Ligand CLA 6 313



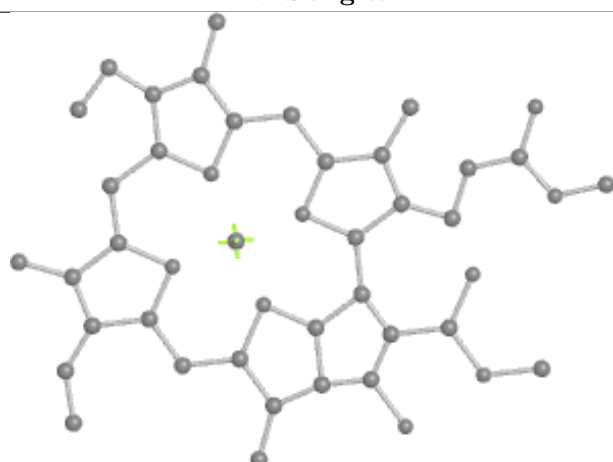
Bond lengths



Bond angles

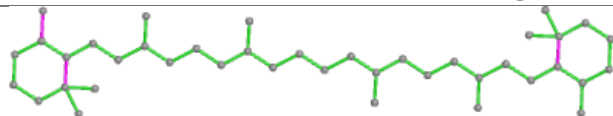


Torsions

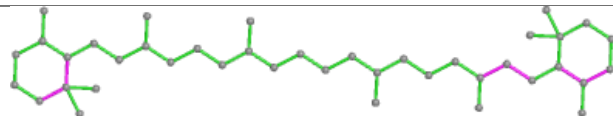


Rings

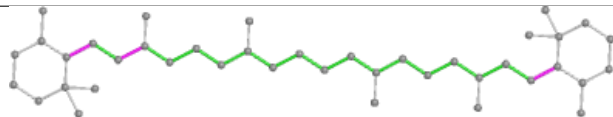
## Ligand BCR H 101



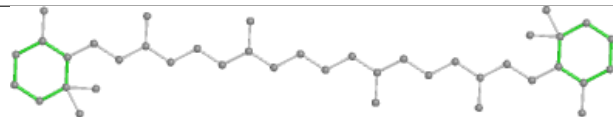
Bond lengths



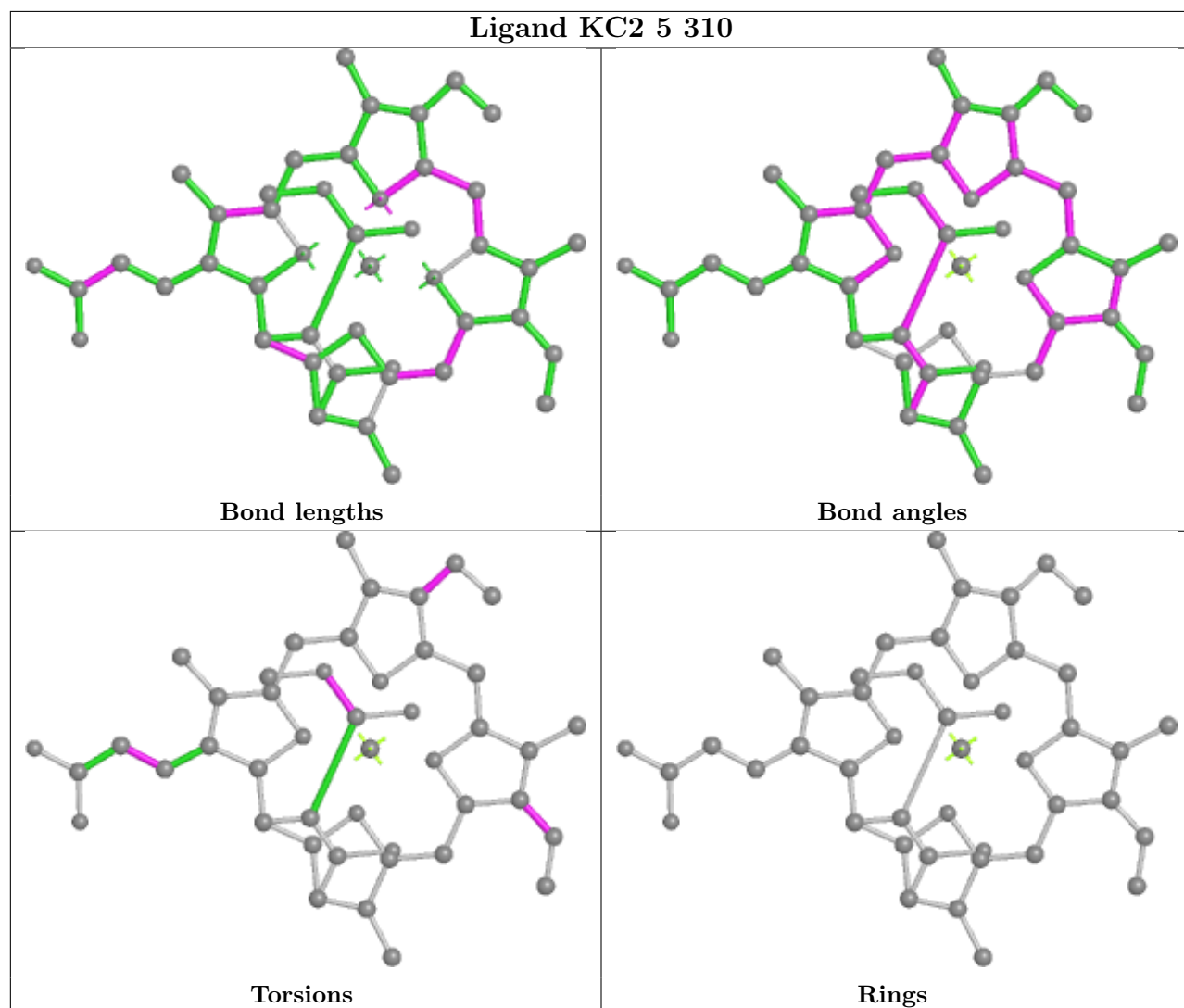
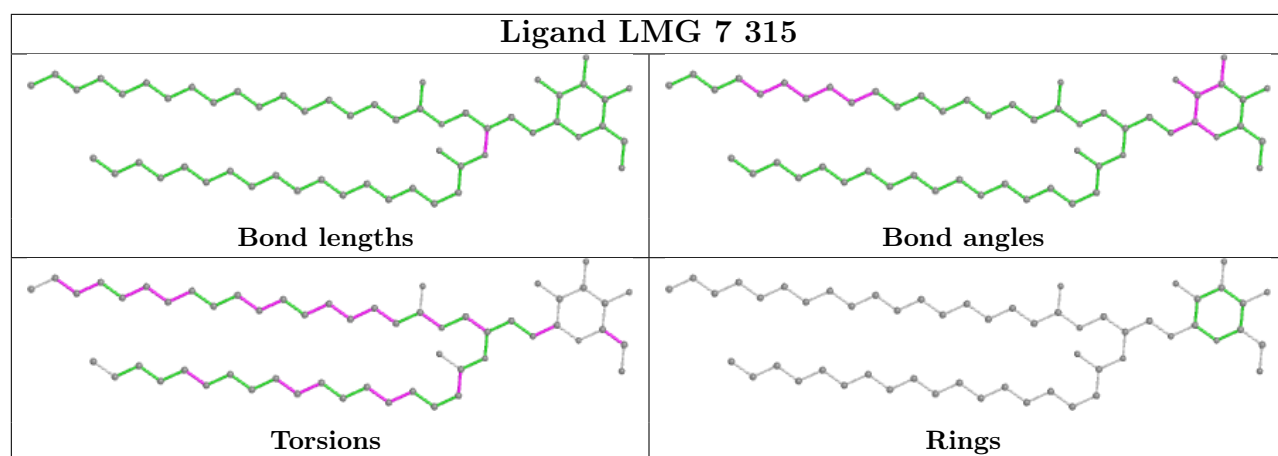
Bond angles

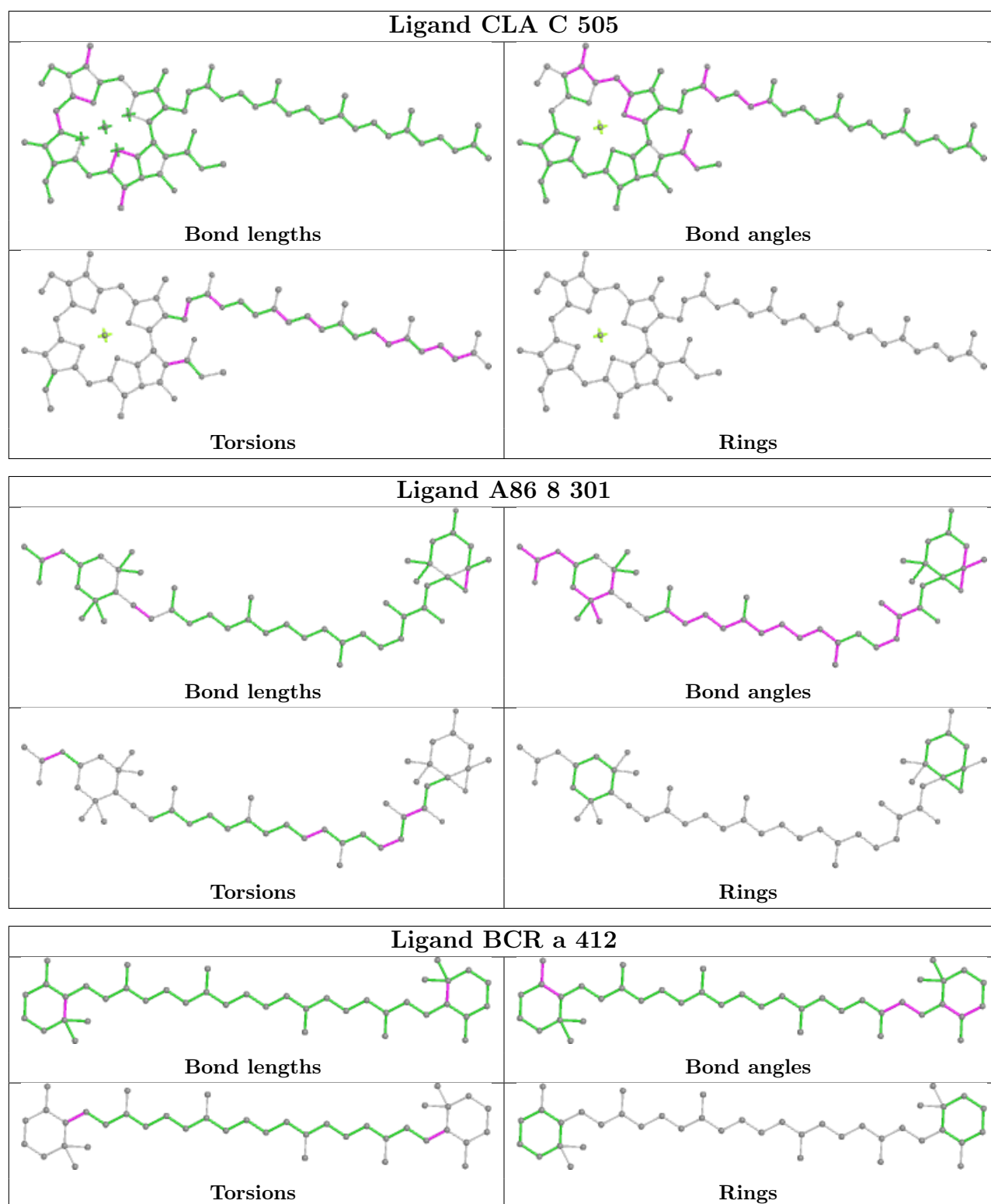


Torsions

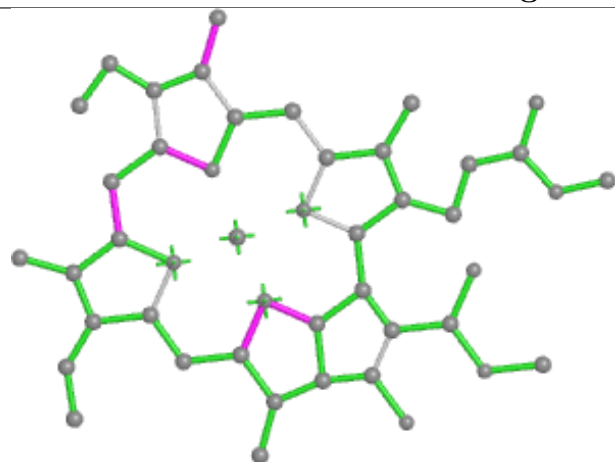


Rings

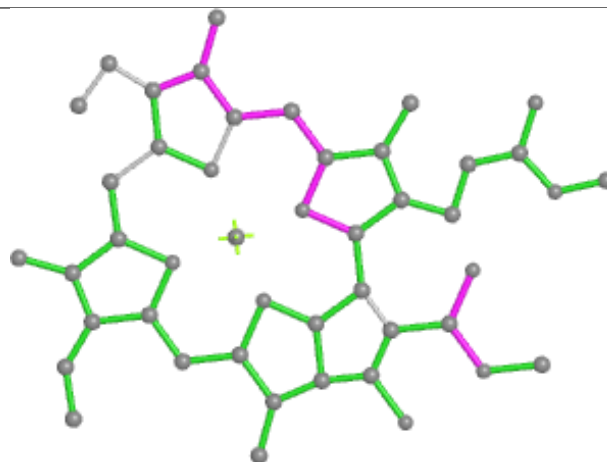




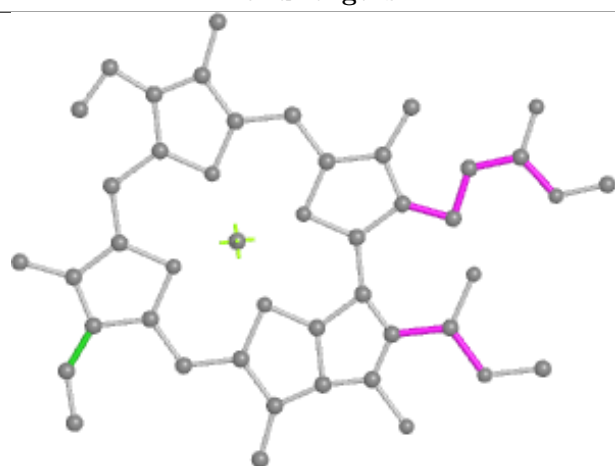
## Ligand CLA 5 308



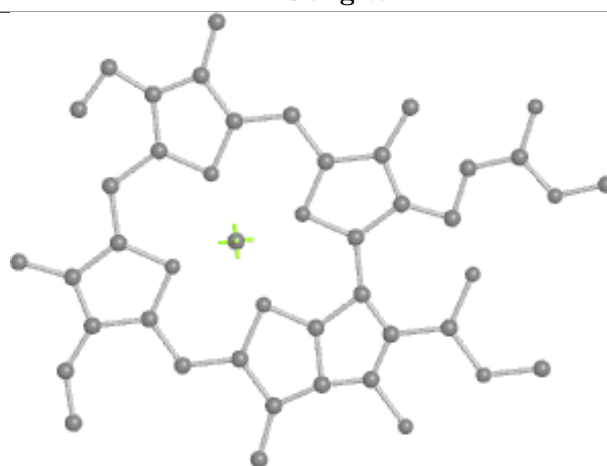
Bond lengths



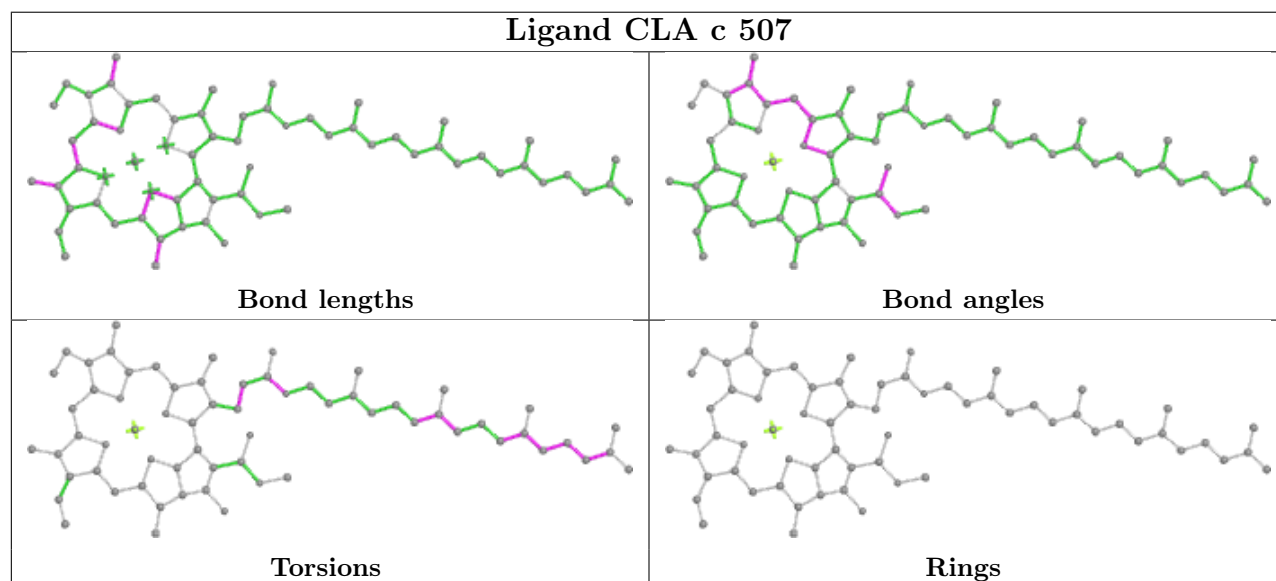
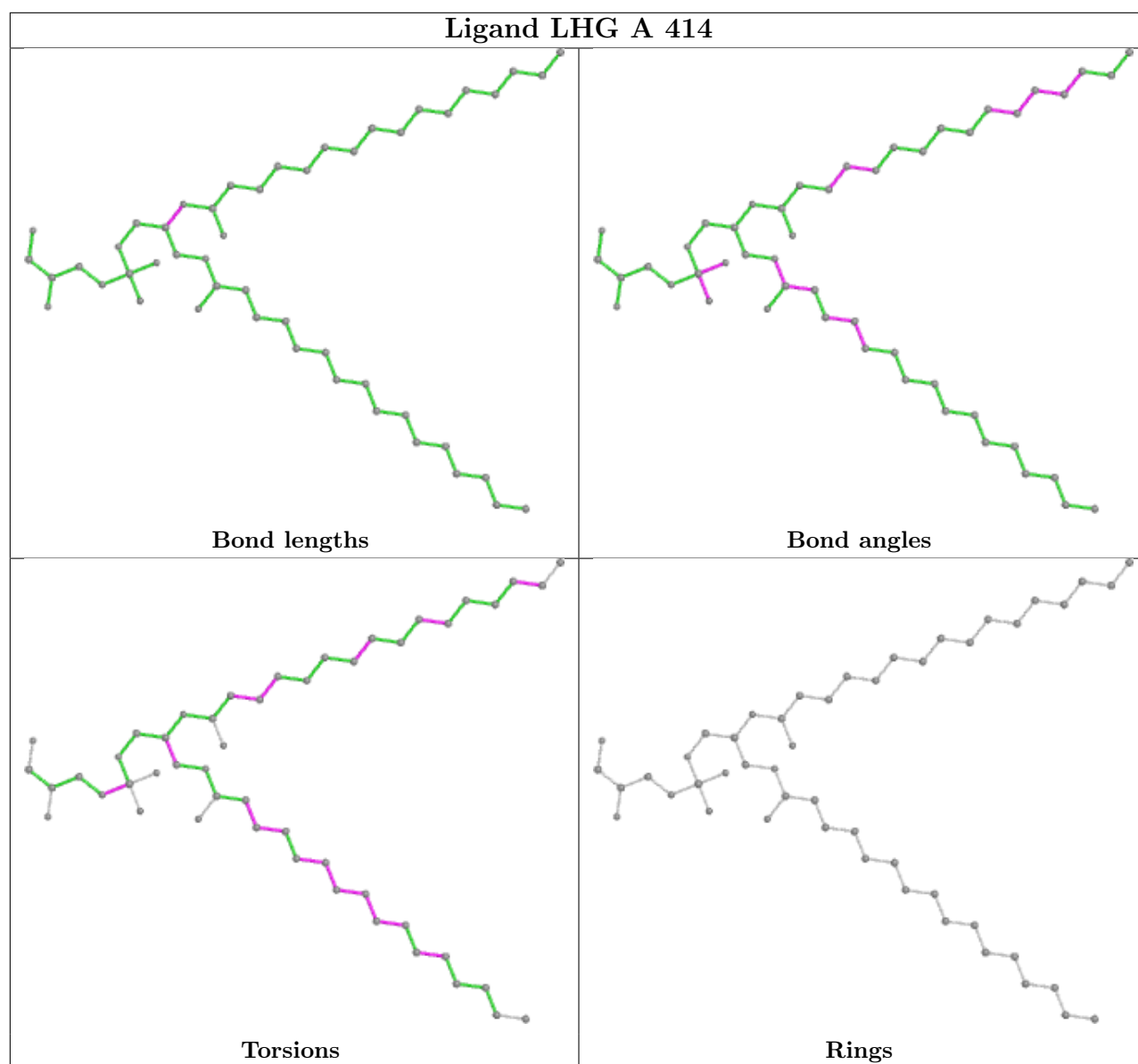
Bond angles

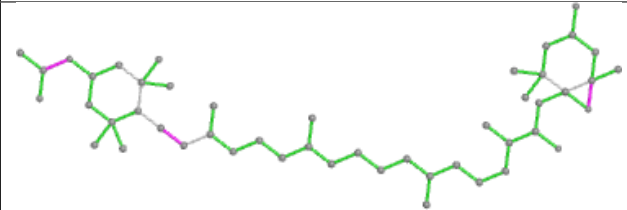
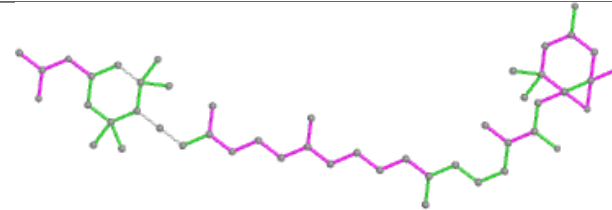
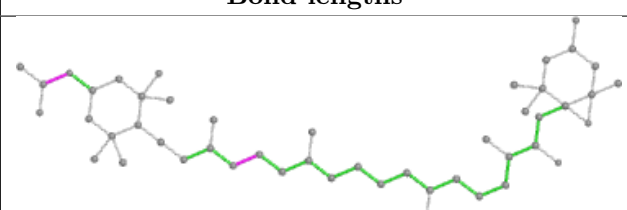
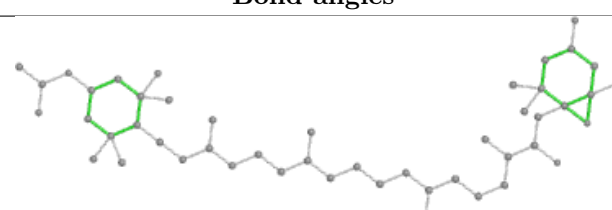


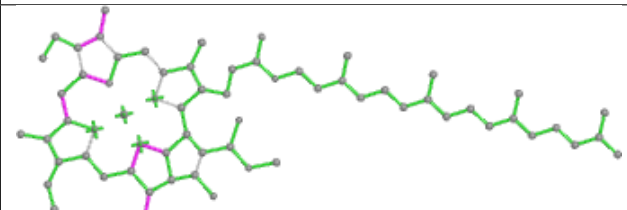
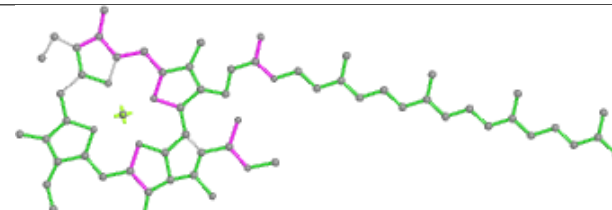
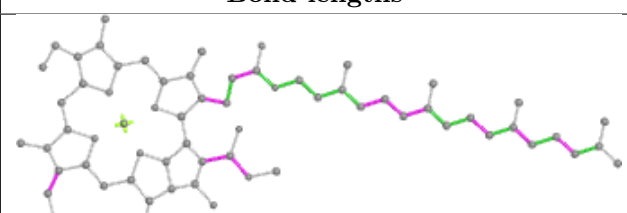
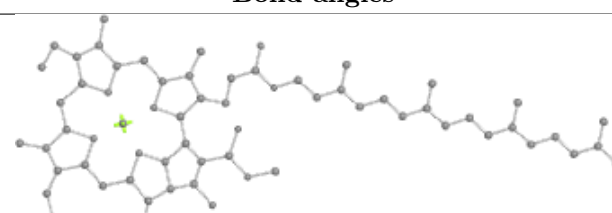
Torsions

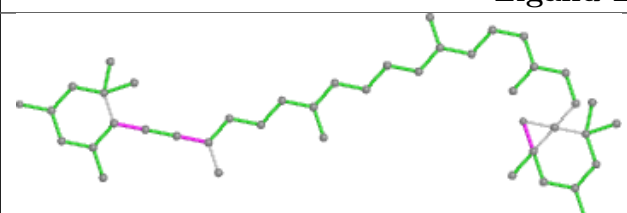
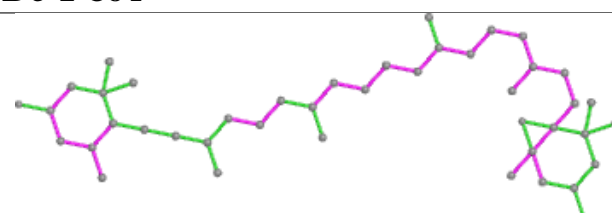
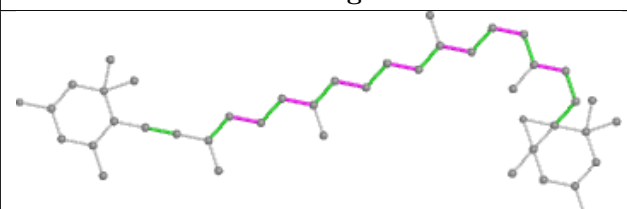
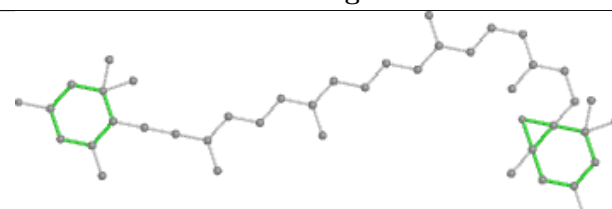


Rings

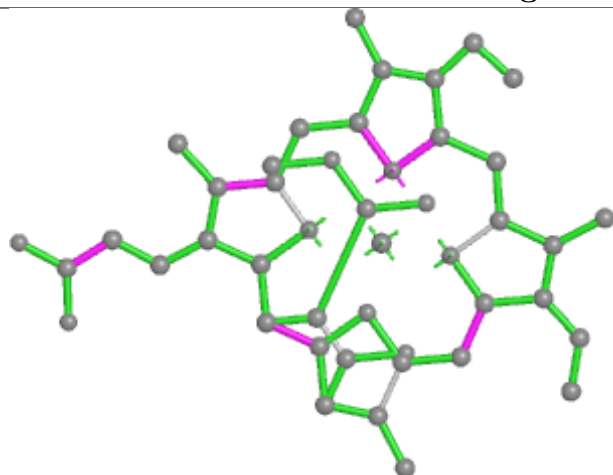


Ligand A86 4 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

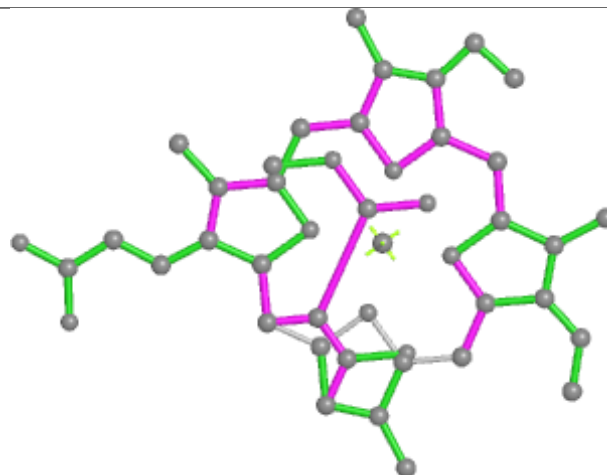
Ligand CLA w 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 2 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

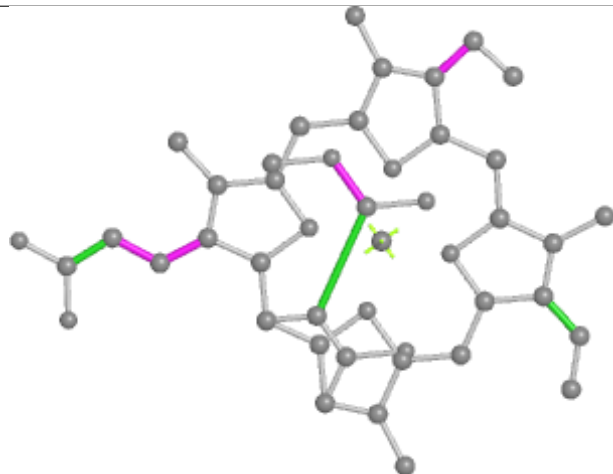
## Ligand KC1 6 314



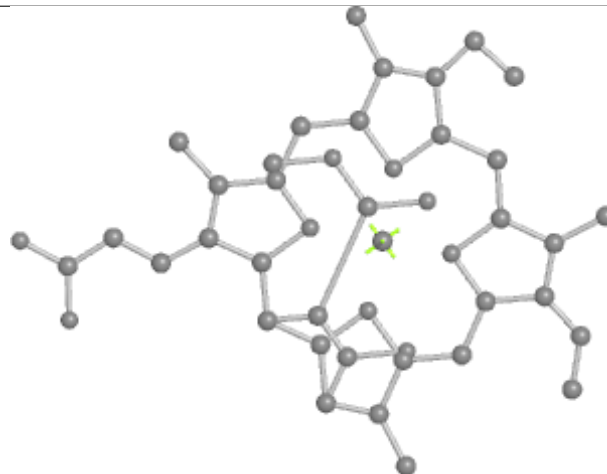
Bond lengths



Bond angles

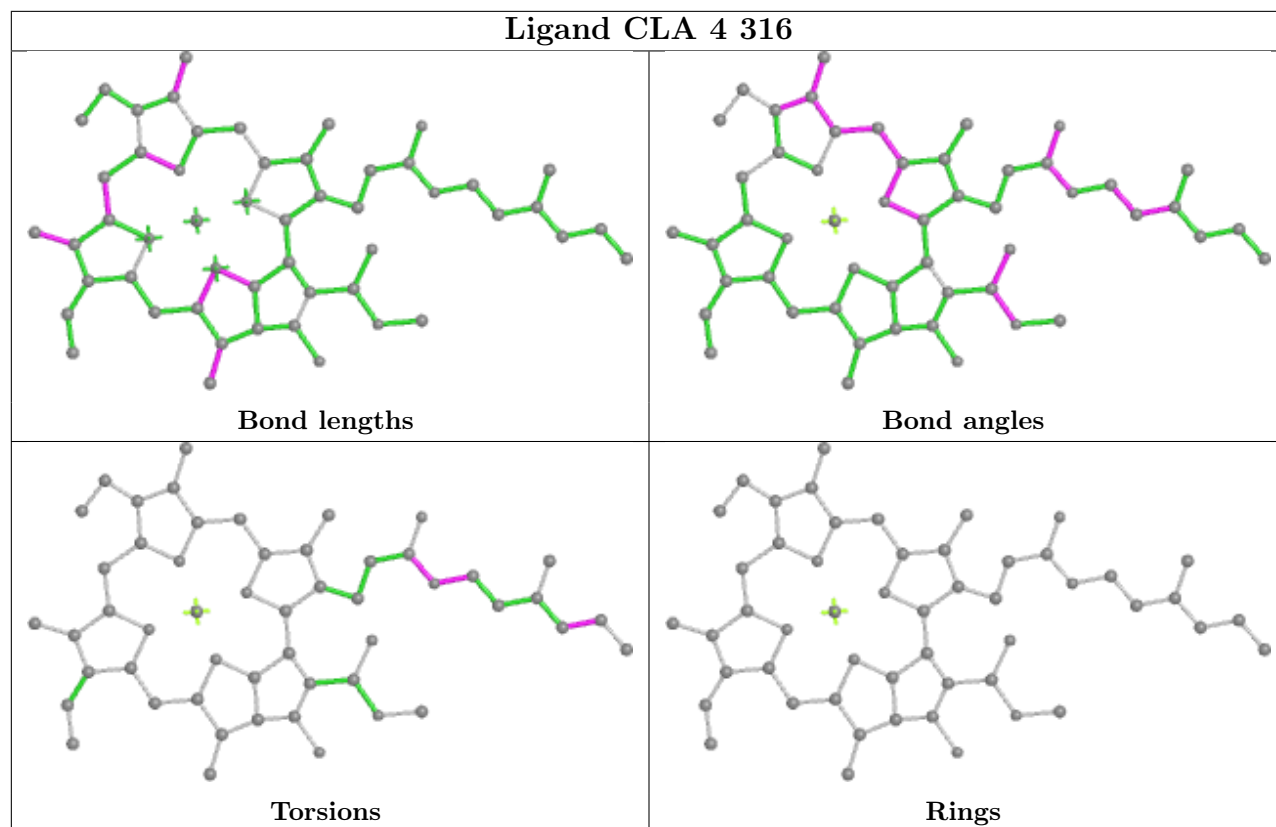


Torsions

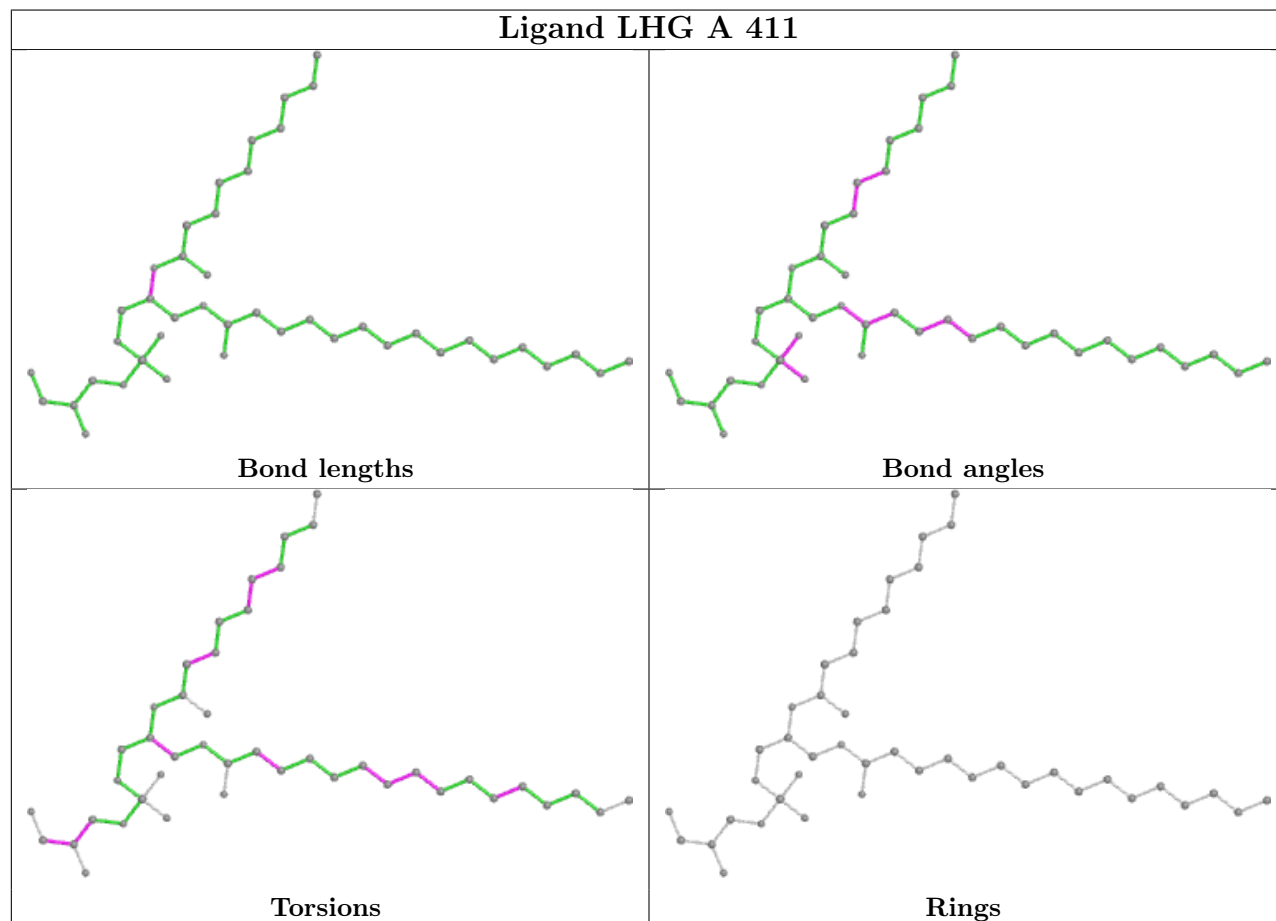


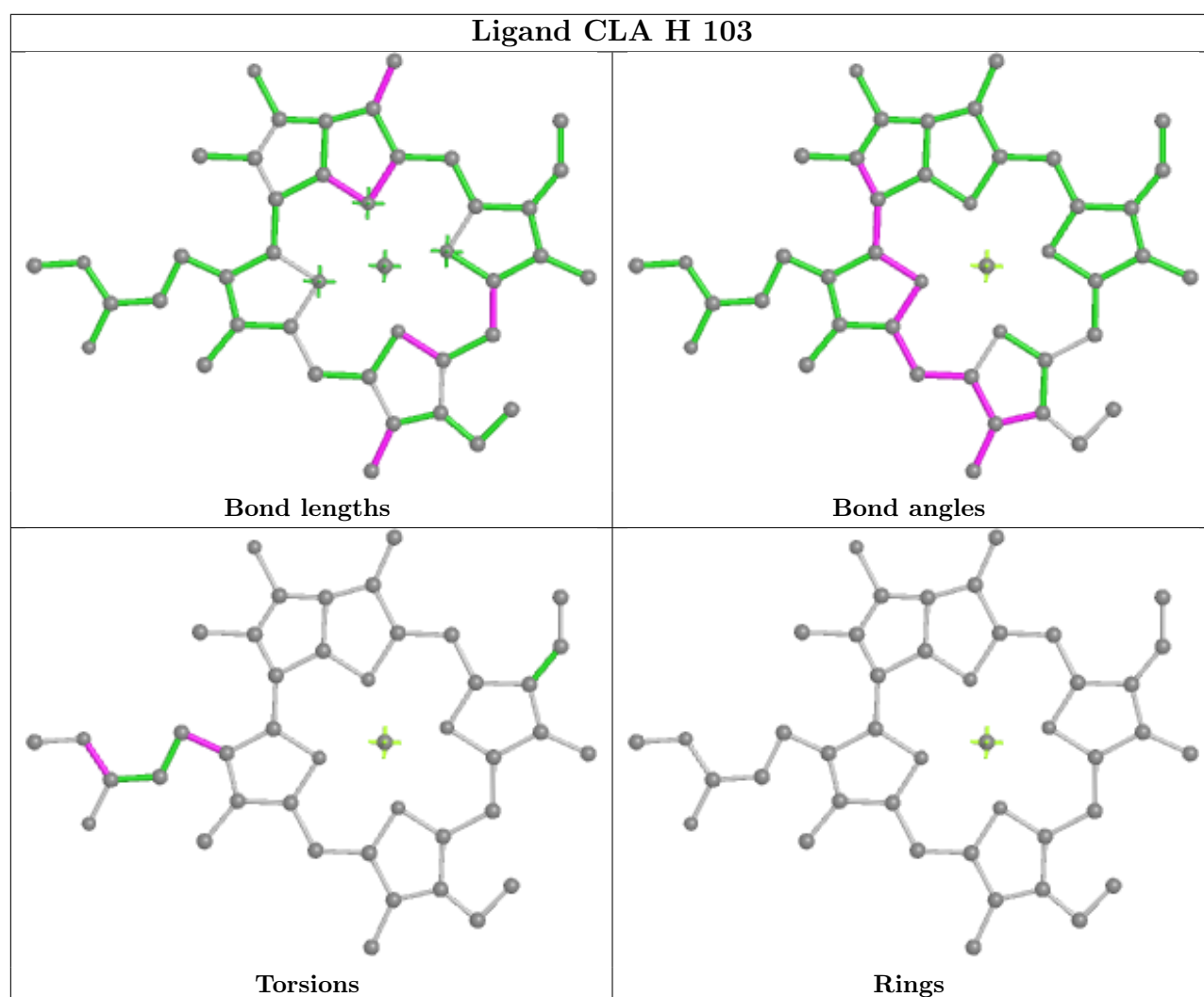
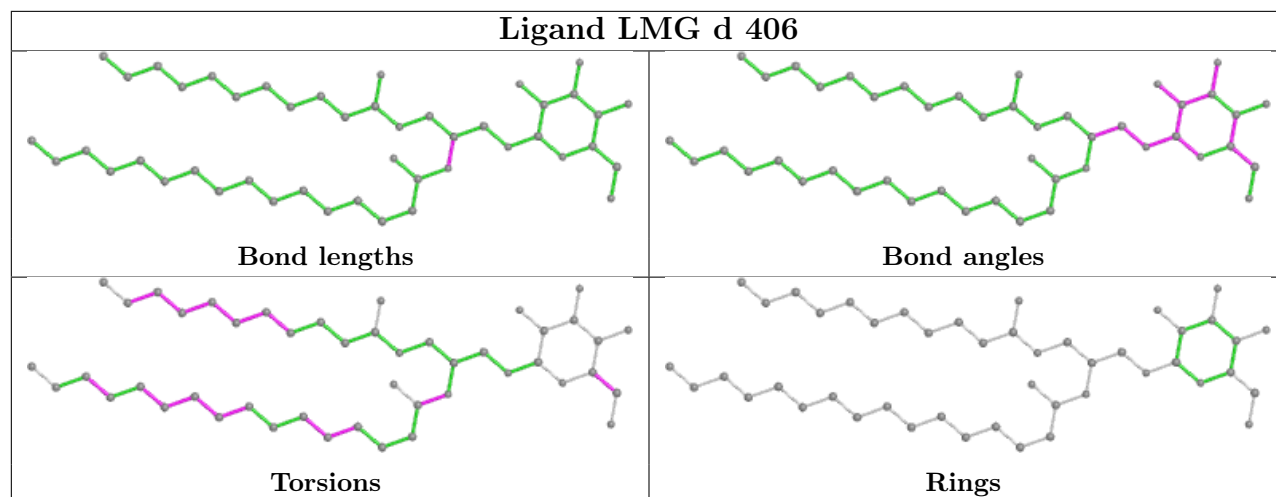
Rings

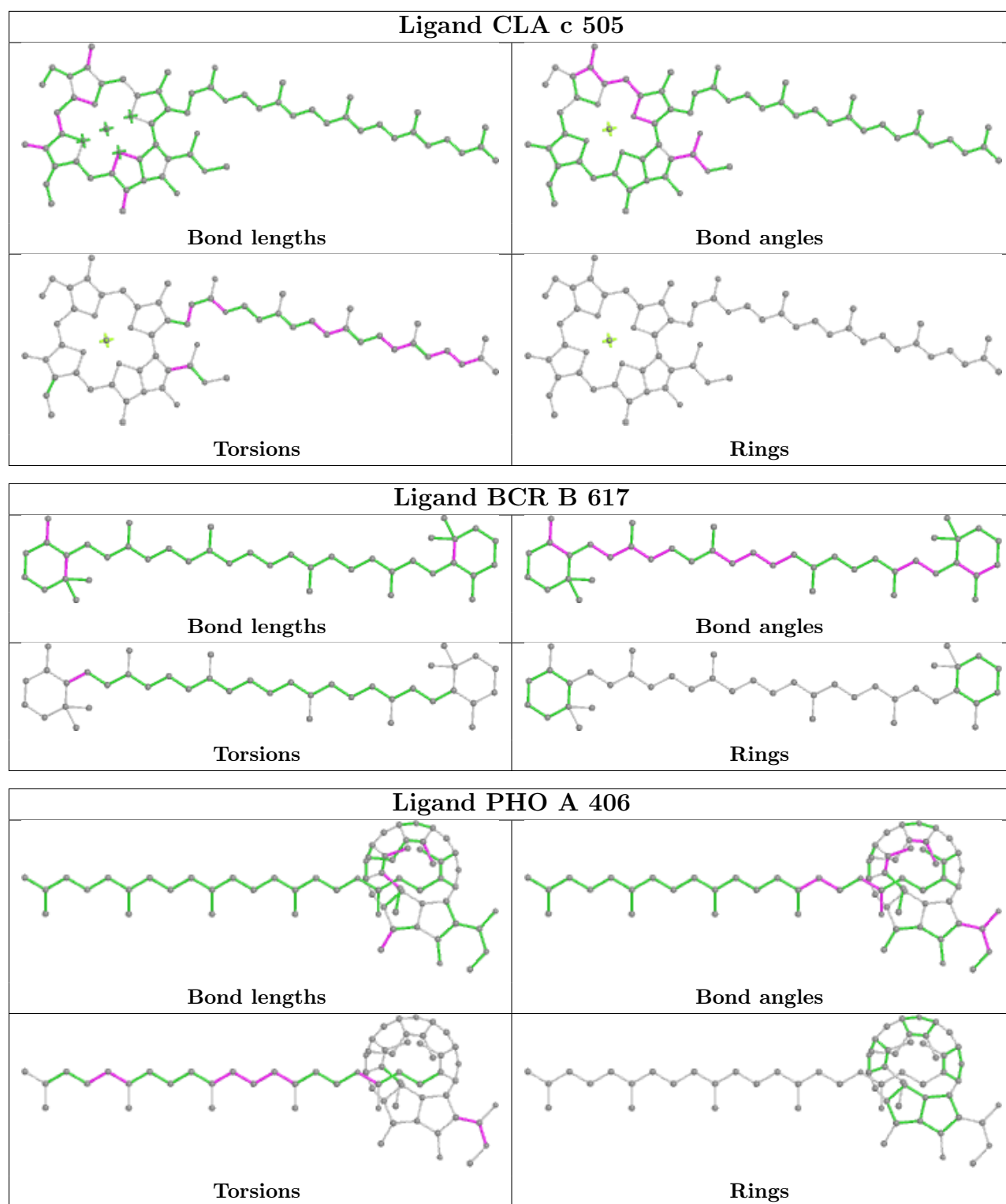
## Ligand CLA 4 316

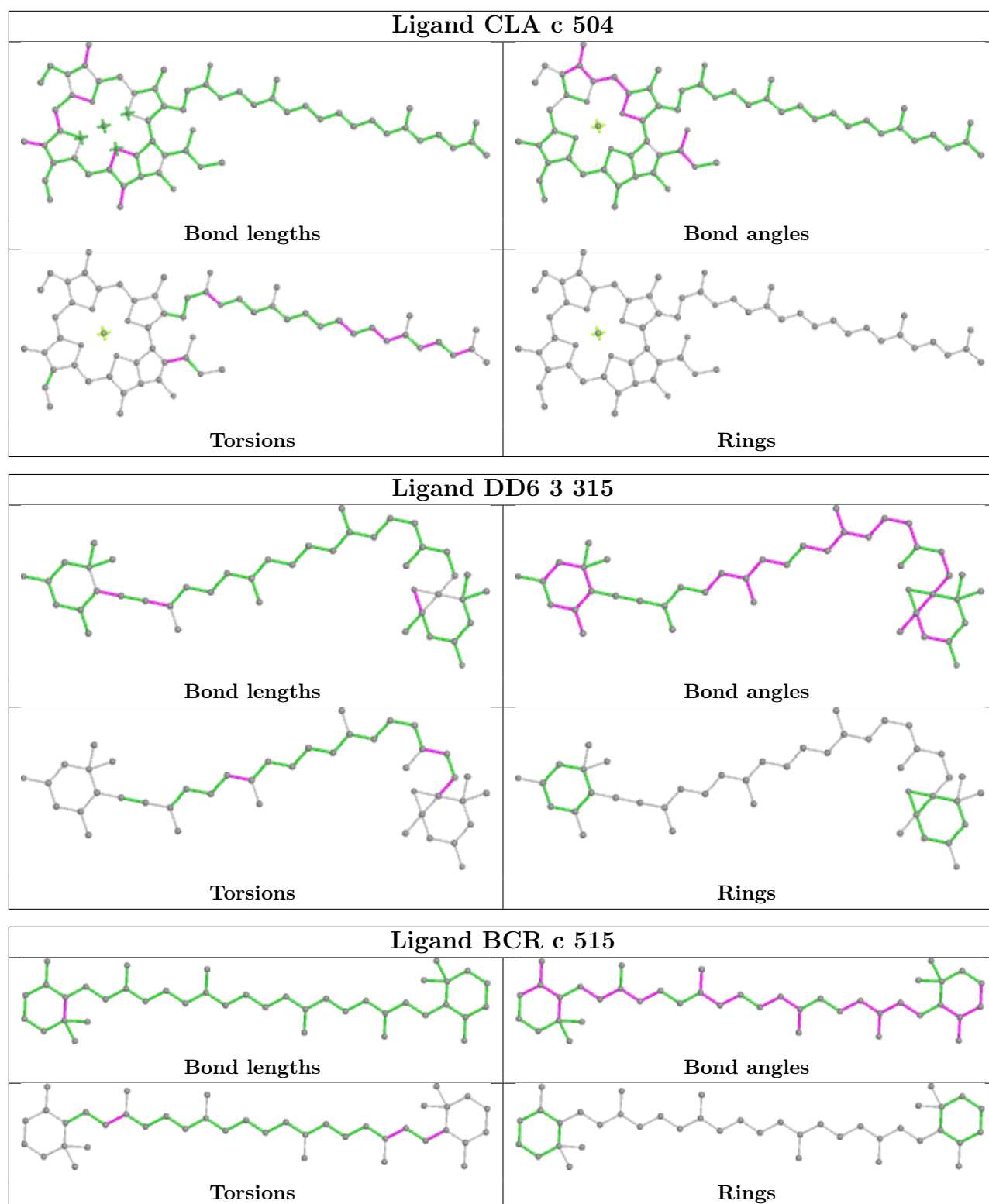


## Ligand LHG A 411

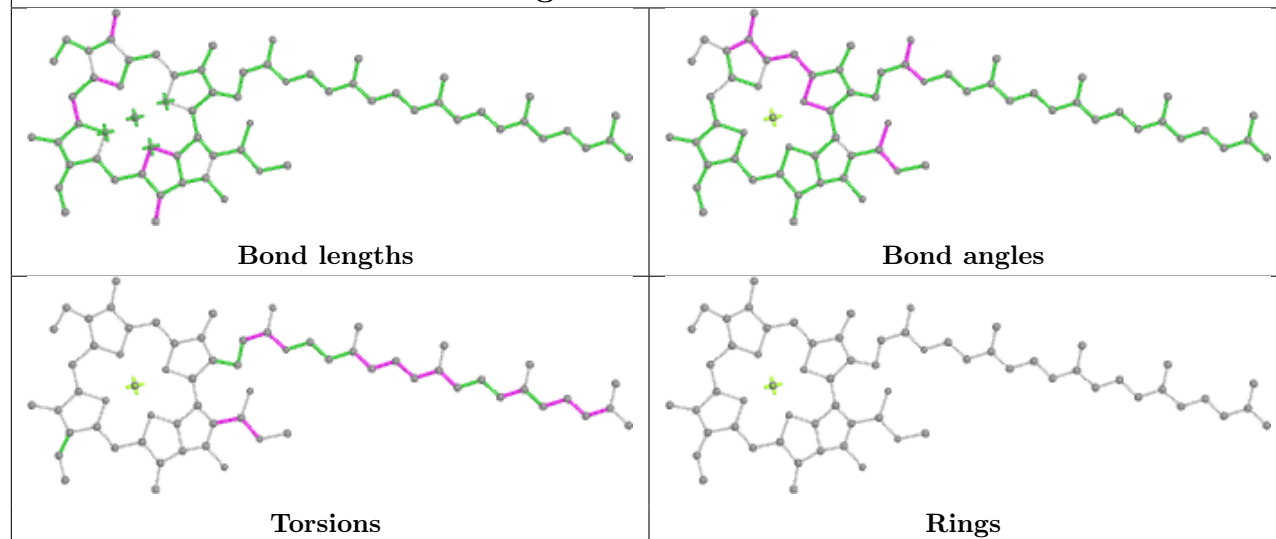




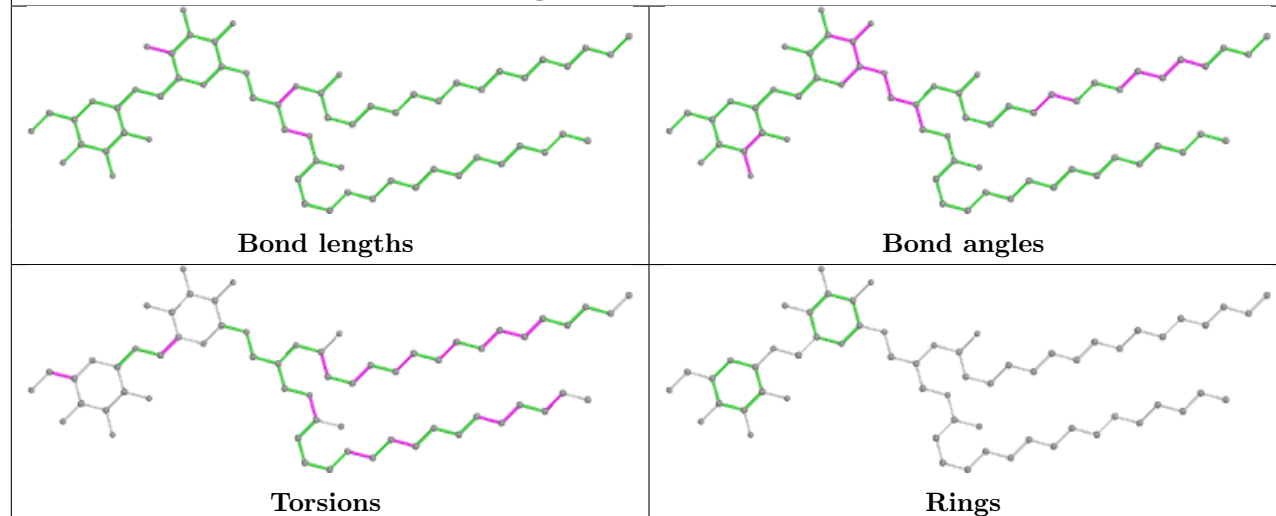




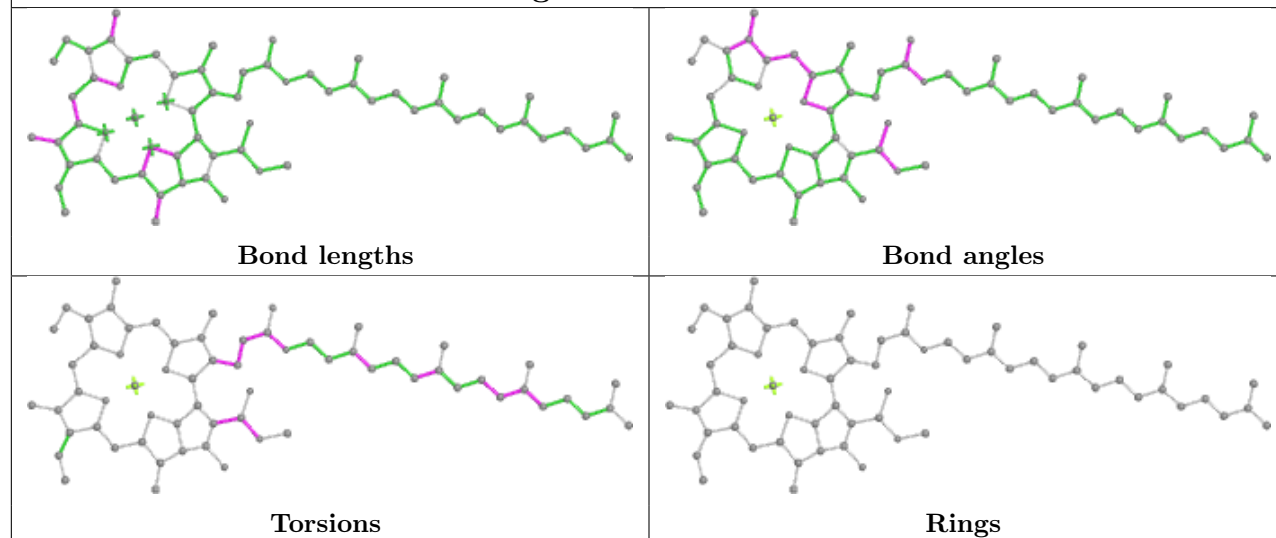
## Ligand CLA 0 312



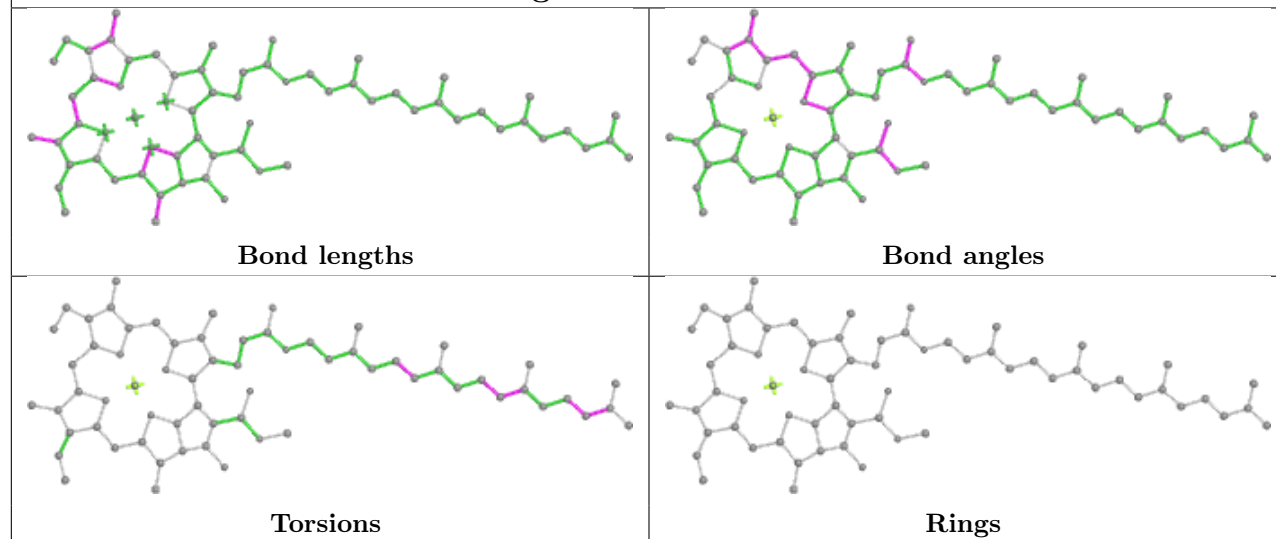
## Ligand DGD h 102



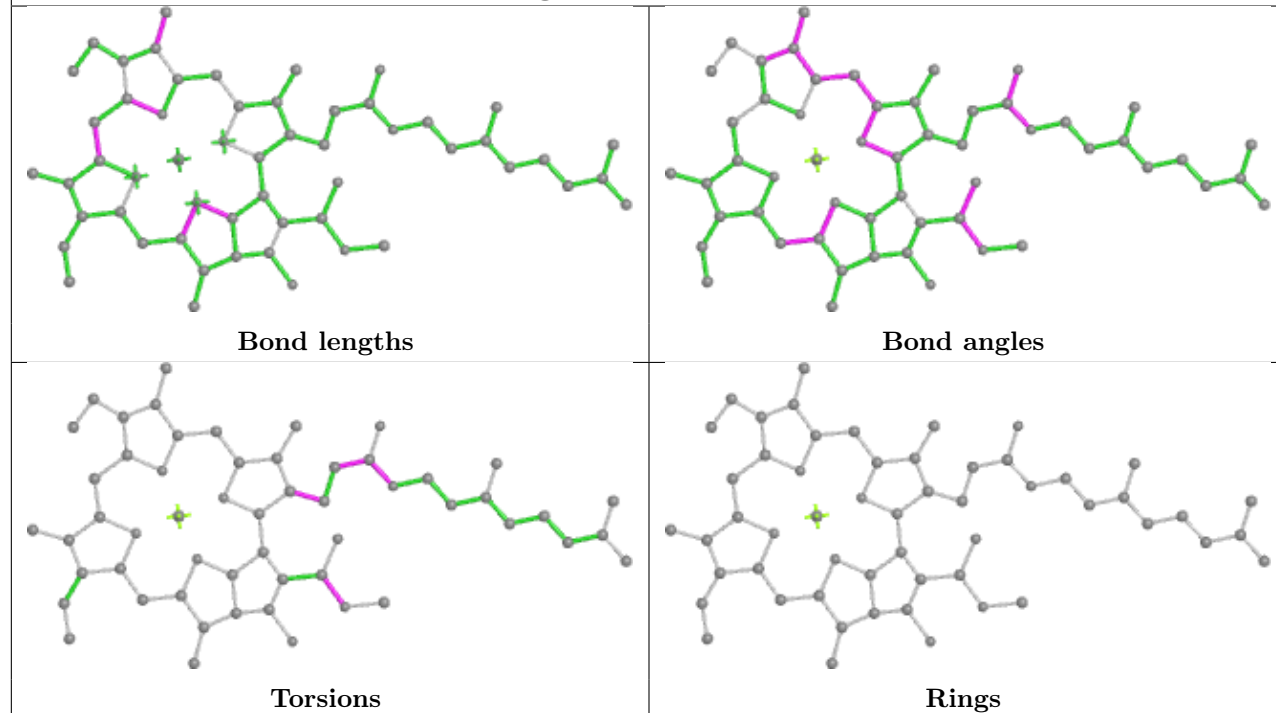
## Ligand CLA C 501

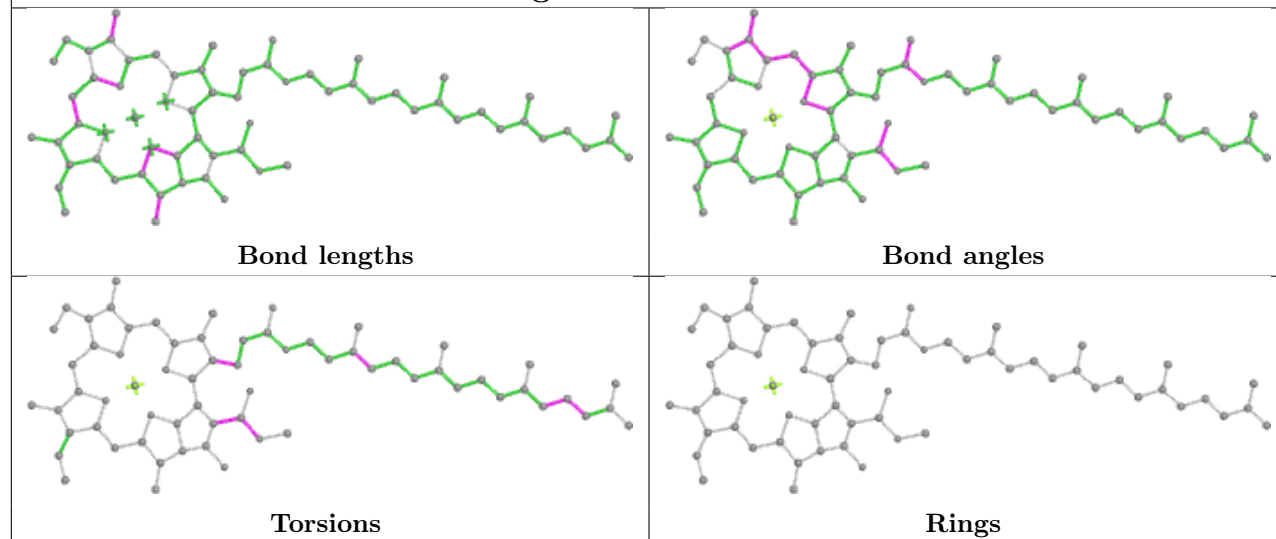
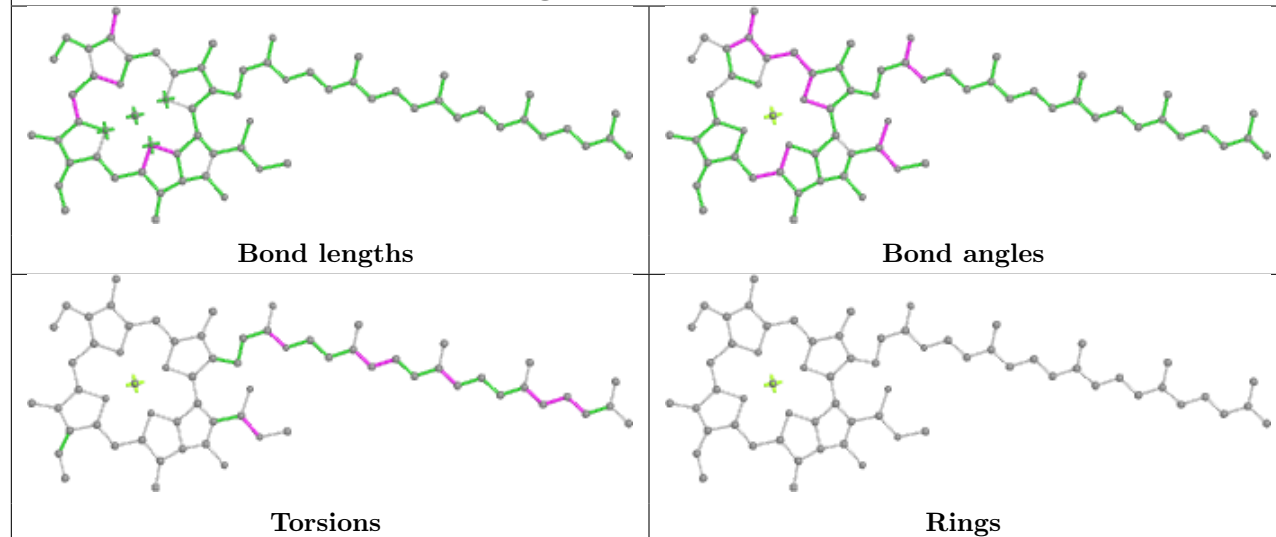


## Ligand CLA B 615

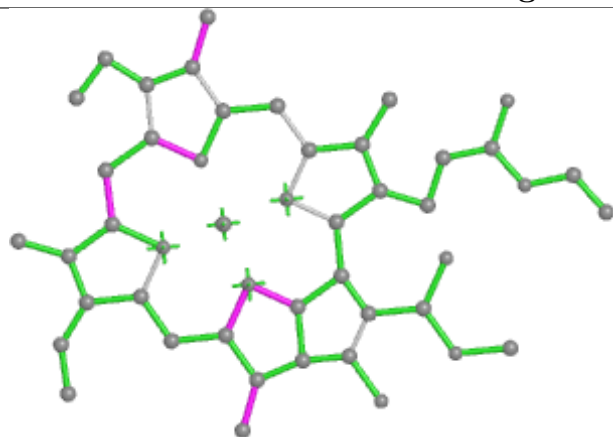


## Ligand CLA 5 311

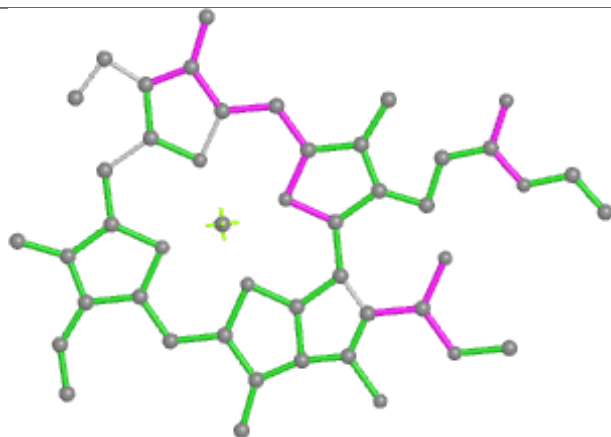


**Ligand CLA B 609****Ligand CLA 3 306**

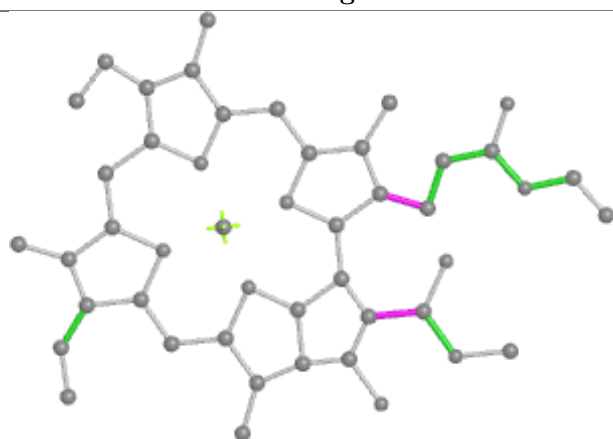
## Ligand CLA 4 315



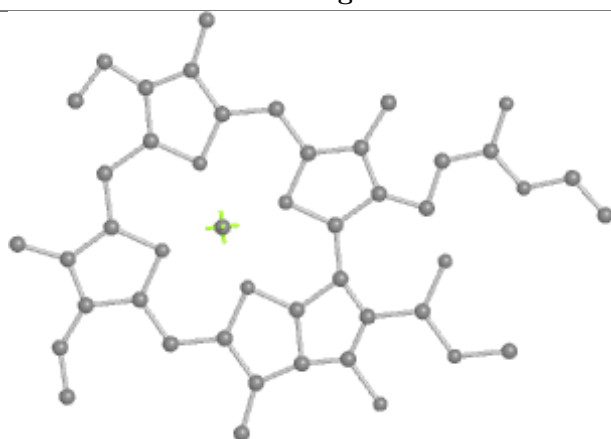
Bond lengths



Bond angles

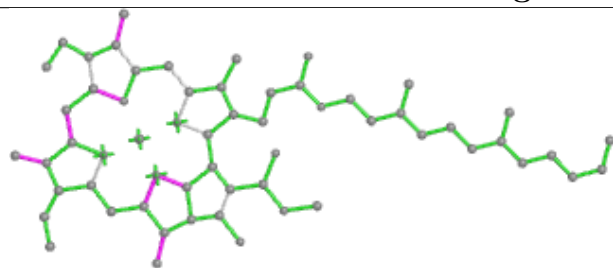


Torsions

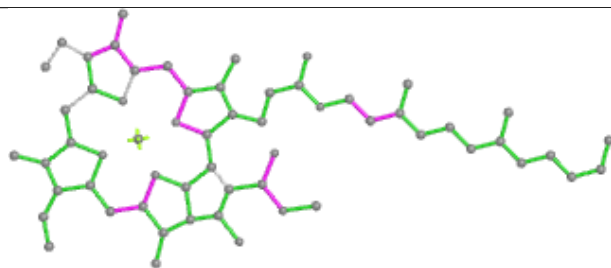


Rings

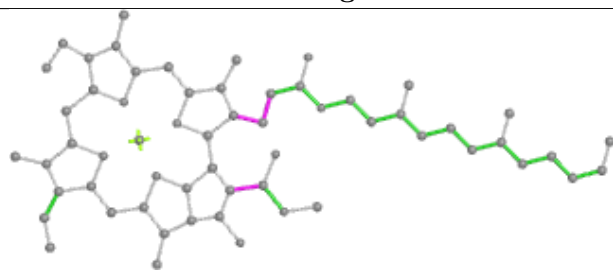
## Ligand CLA D 402



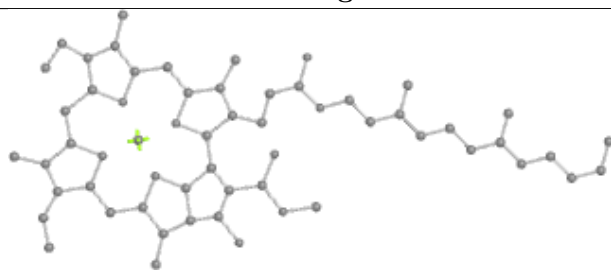
Bond lengths



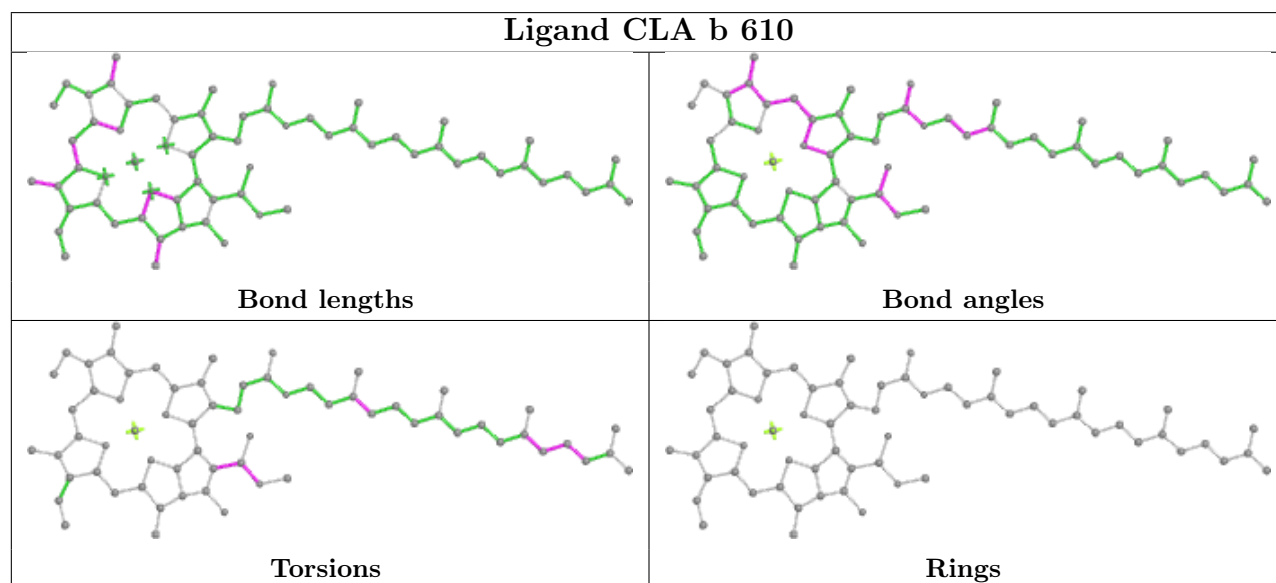
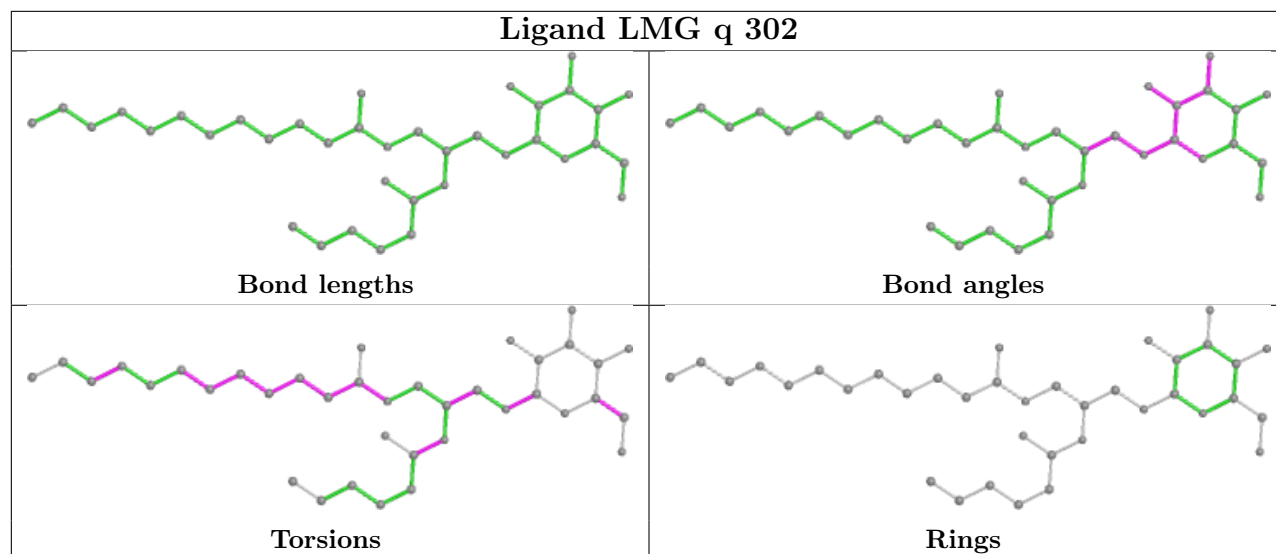
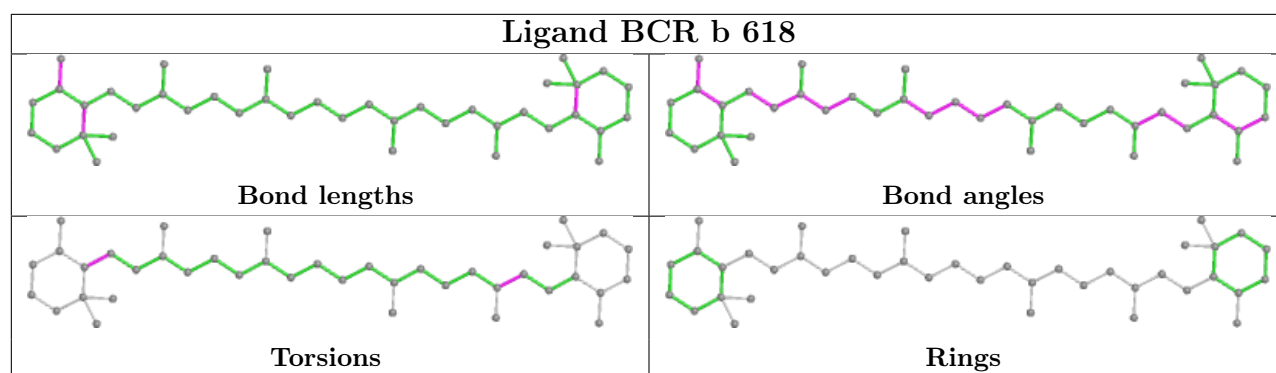
Bond angles

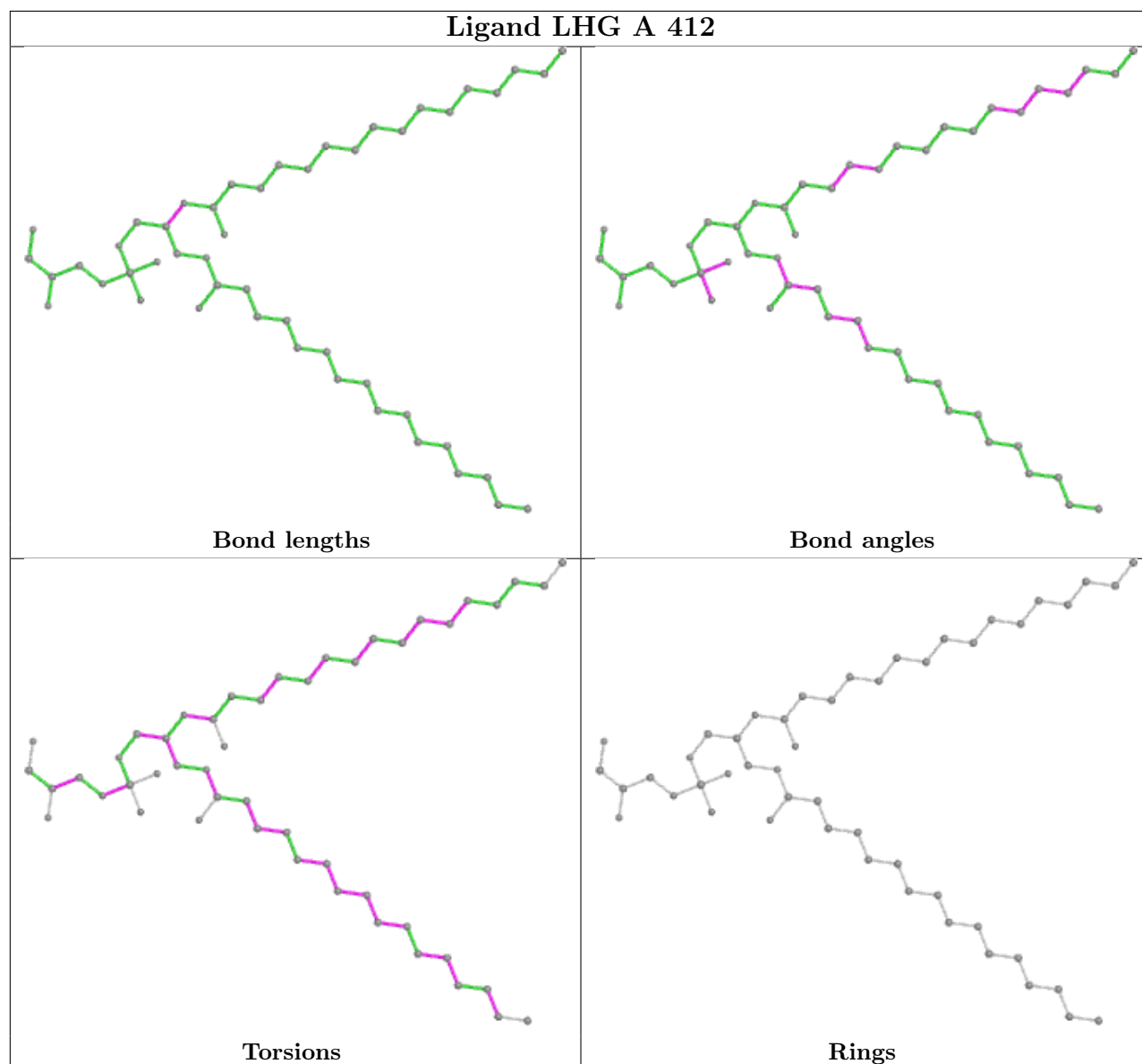
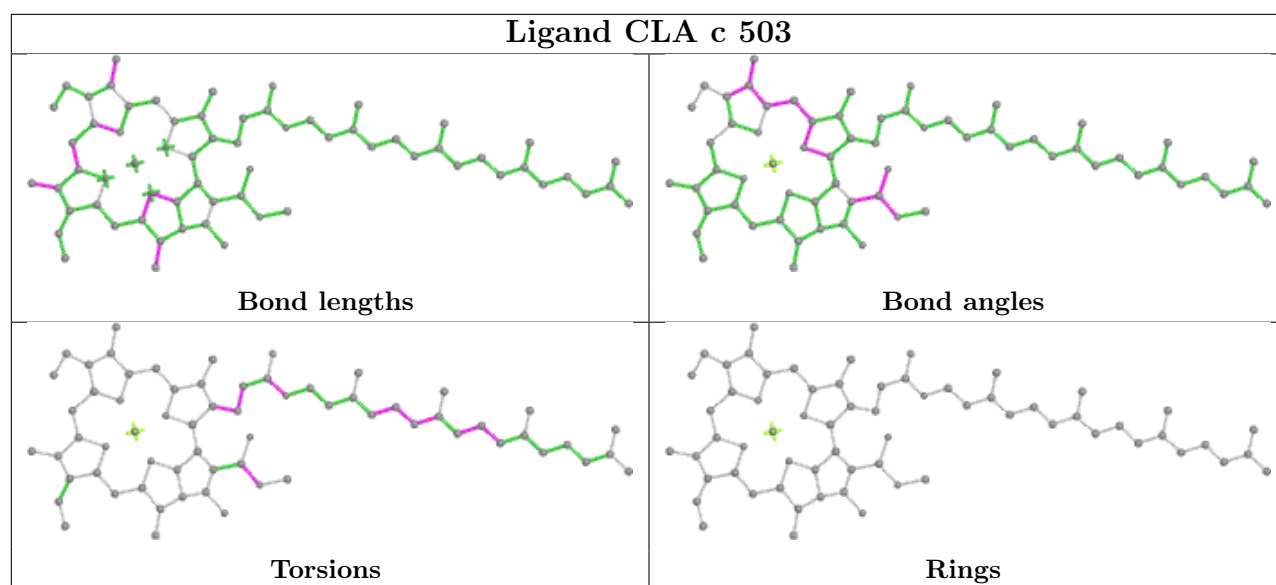


Torsions

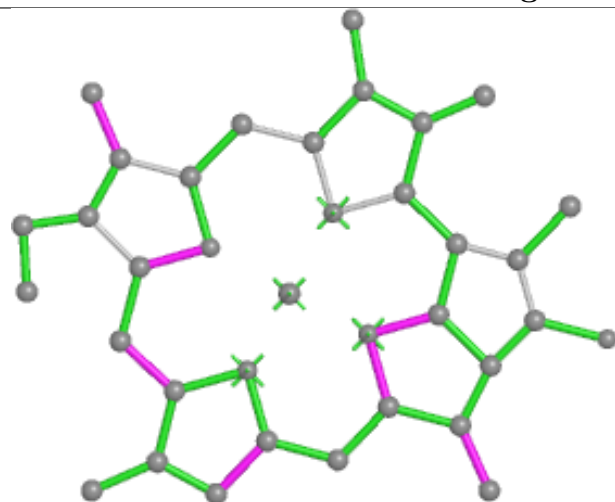


Rings

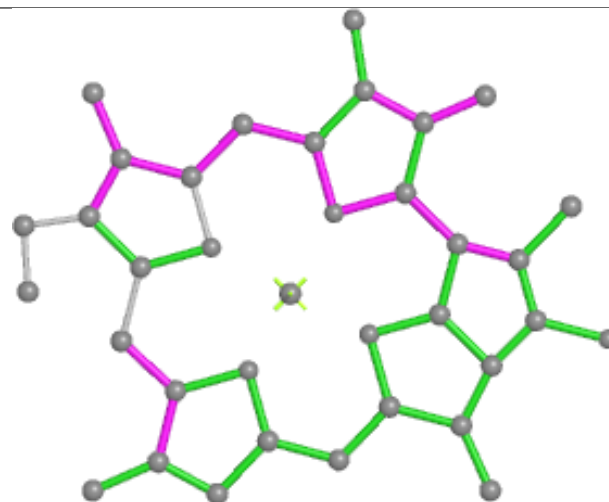




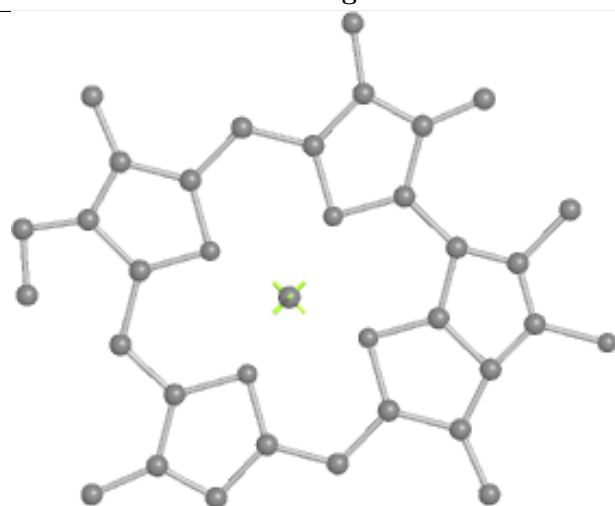
## Ligand CLA 1 313



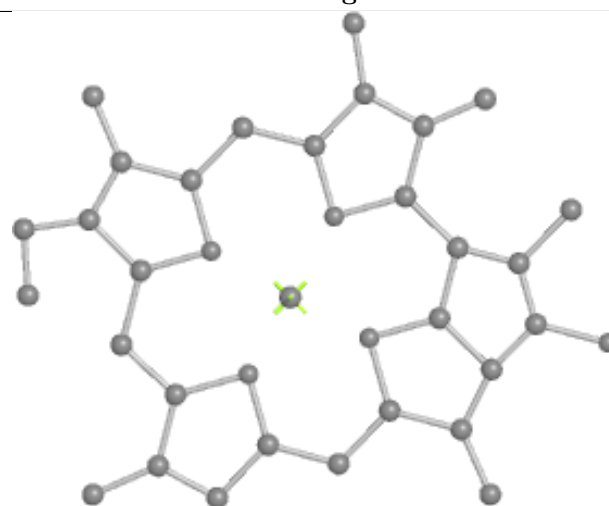
Bond lengths



Bond angles

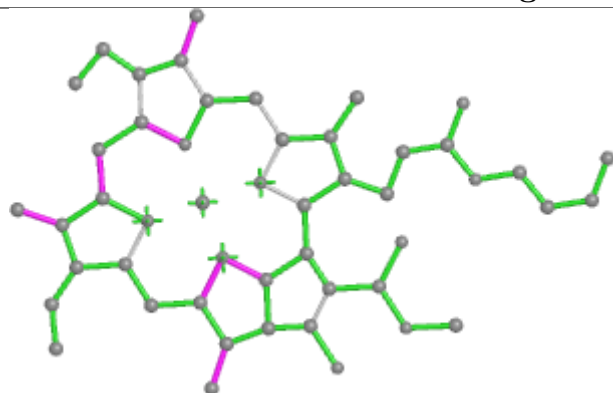


Torsions

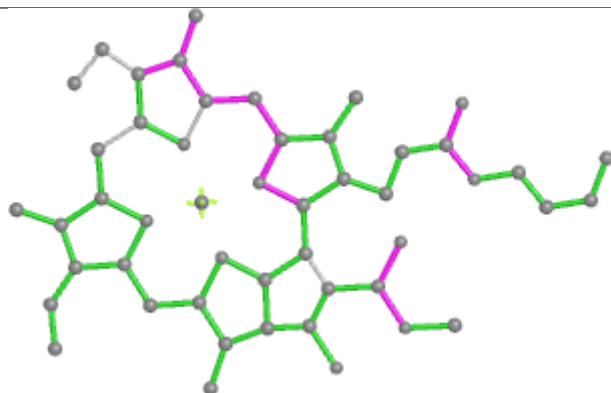


Rings

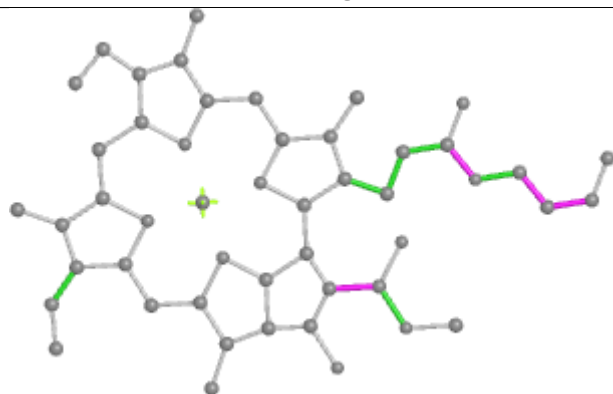
## Ligand CLA c 513



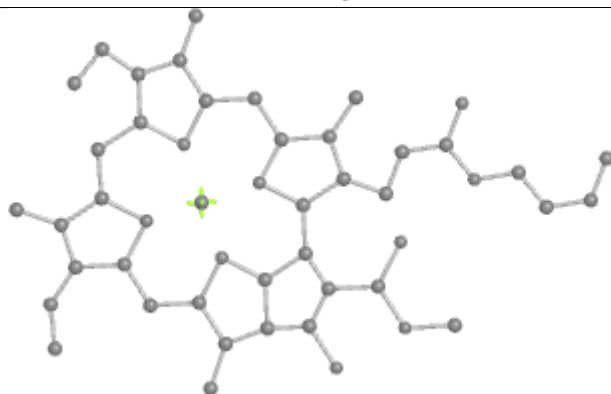
Bond lengths



Bond angles

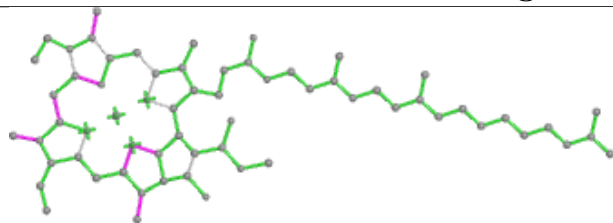


Torsions

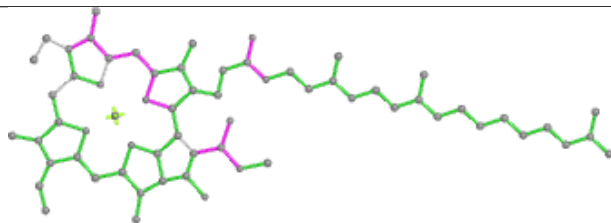


Rings

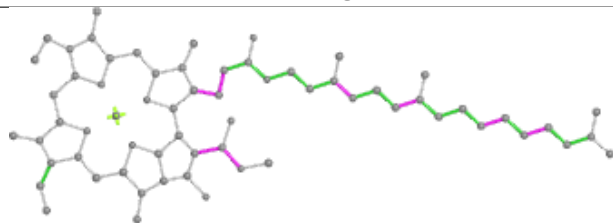
## Ligand CLA b 604



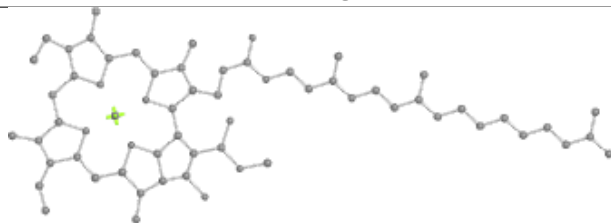
Bond lengths



Bond angles

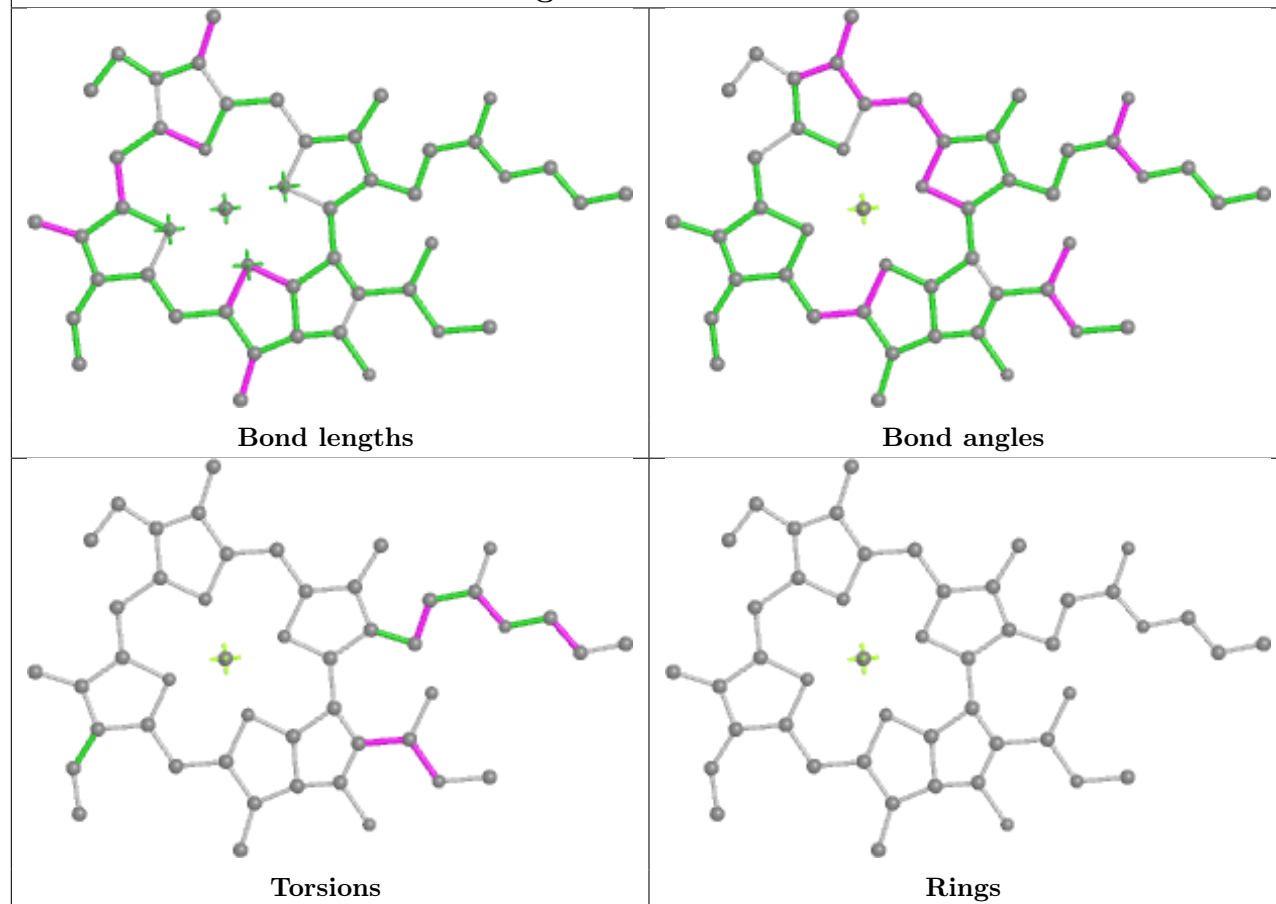


Torsions

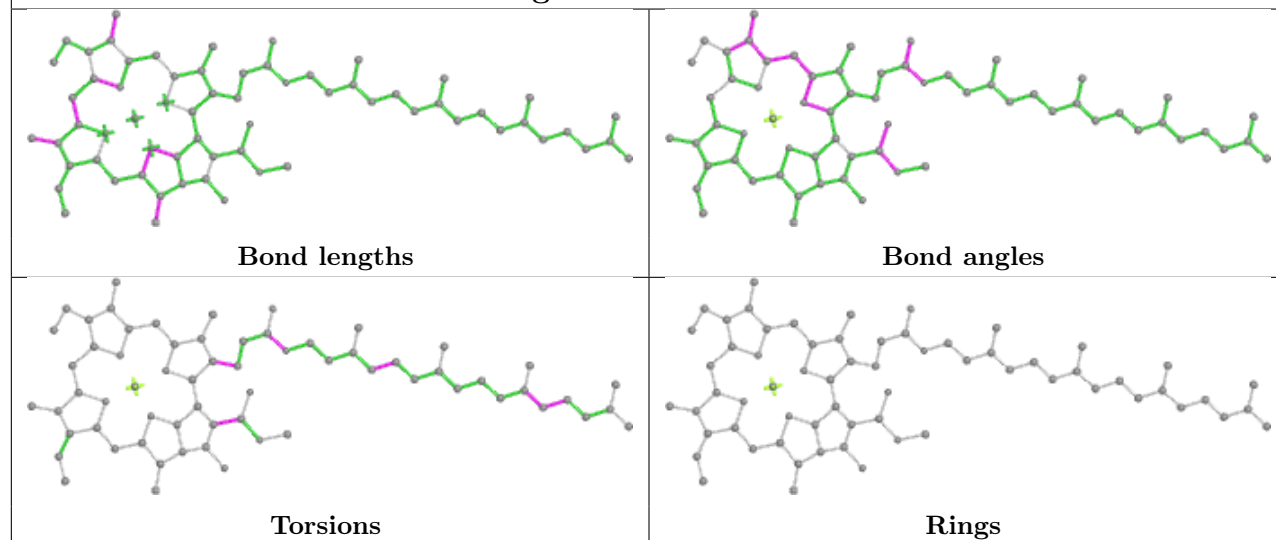


Rings

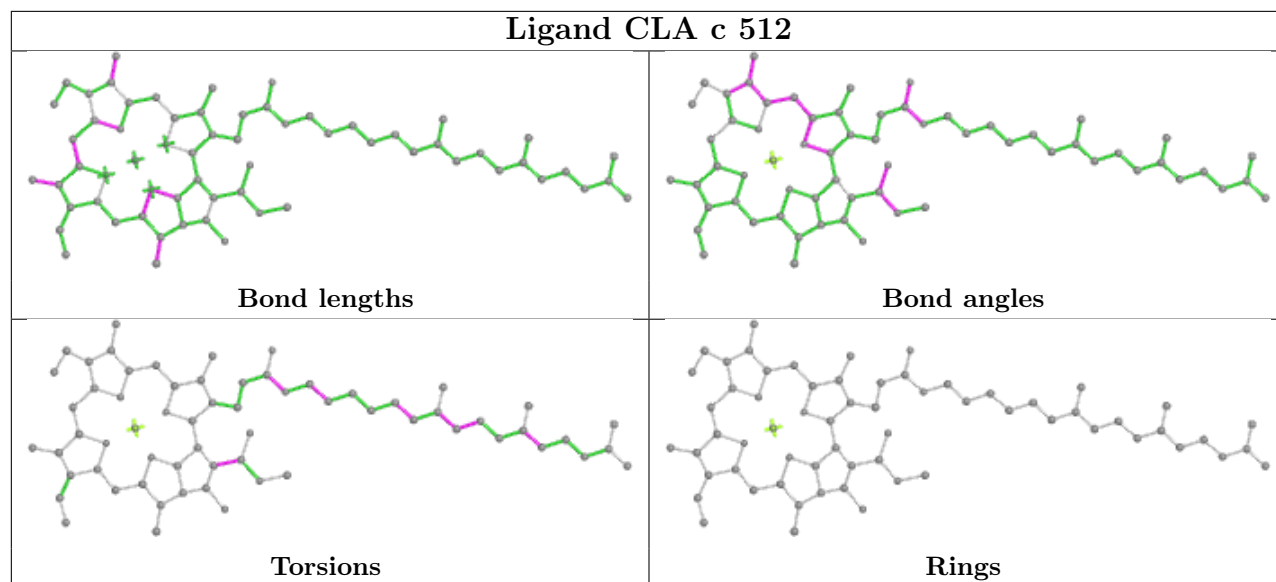
## Ligand CLA 3 305



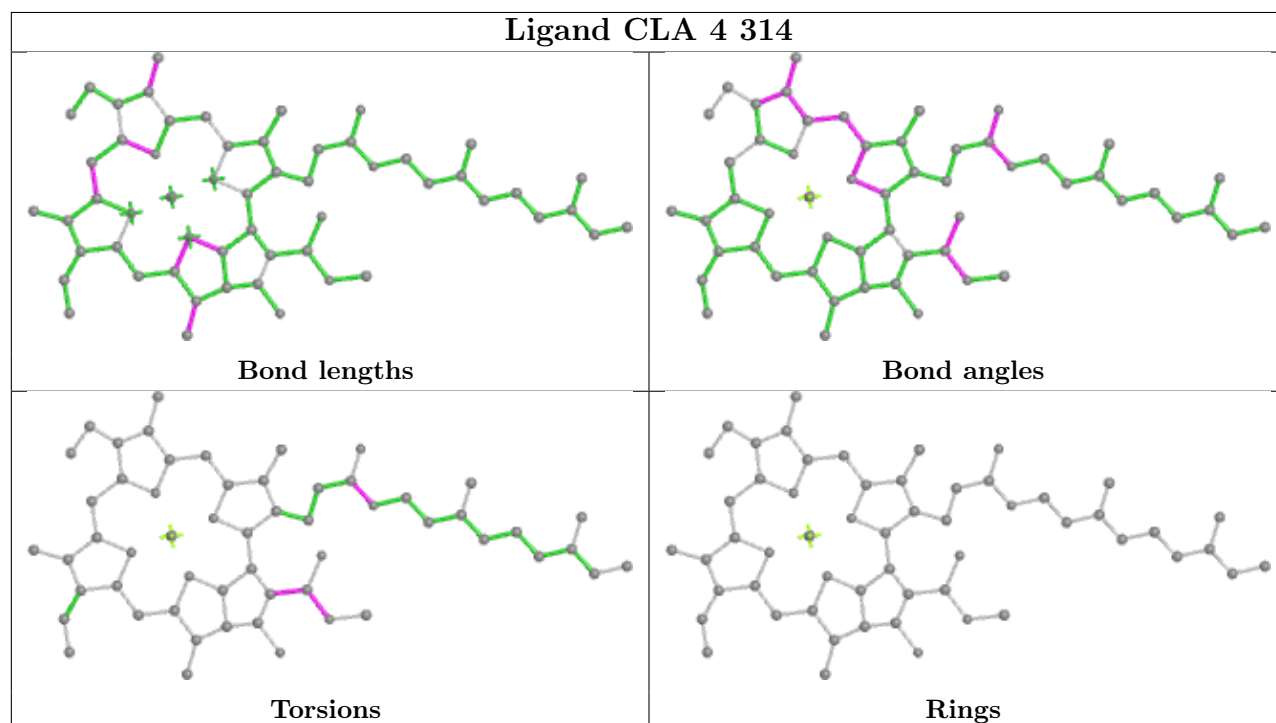
## Ligand CLA C 511

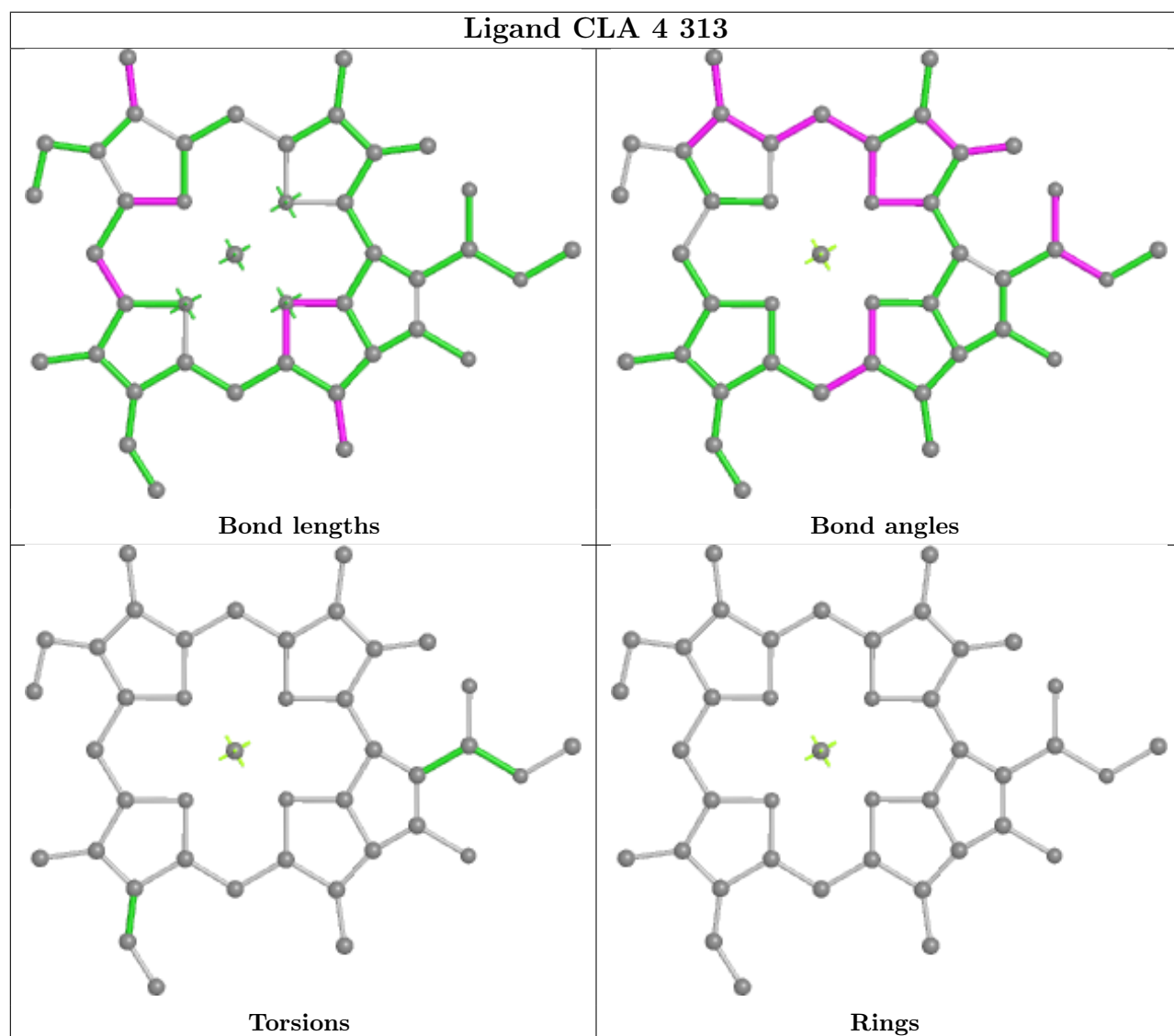
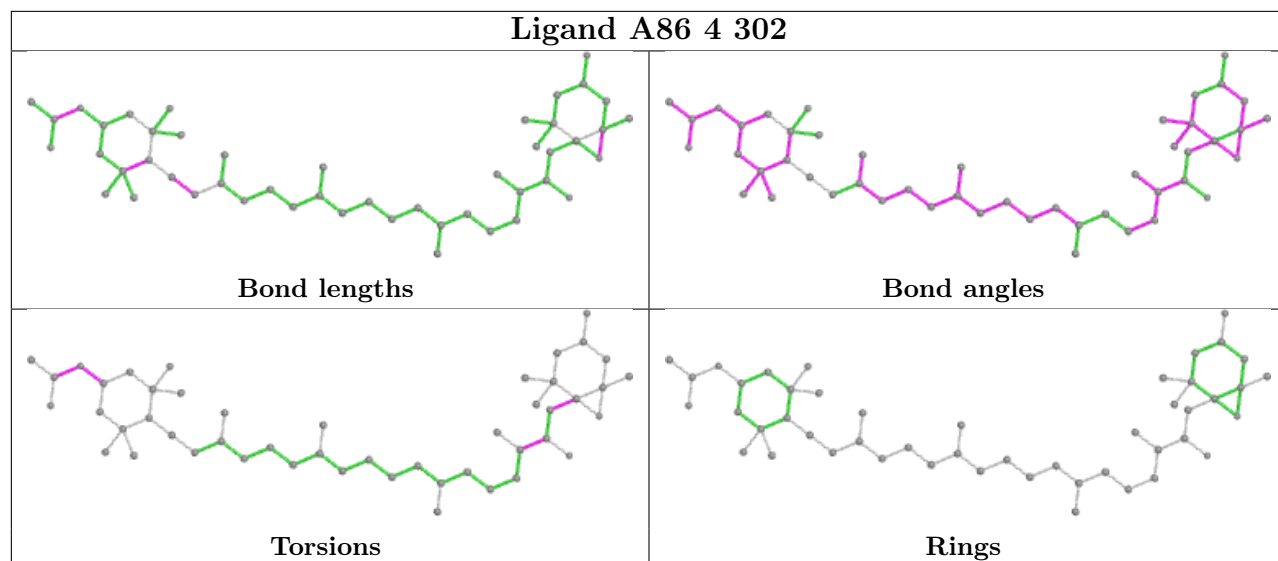


## Ligand CLA c 512

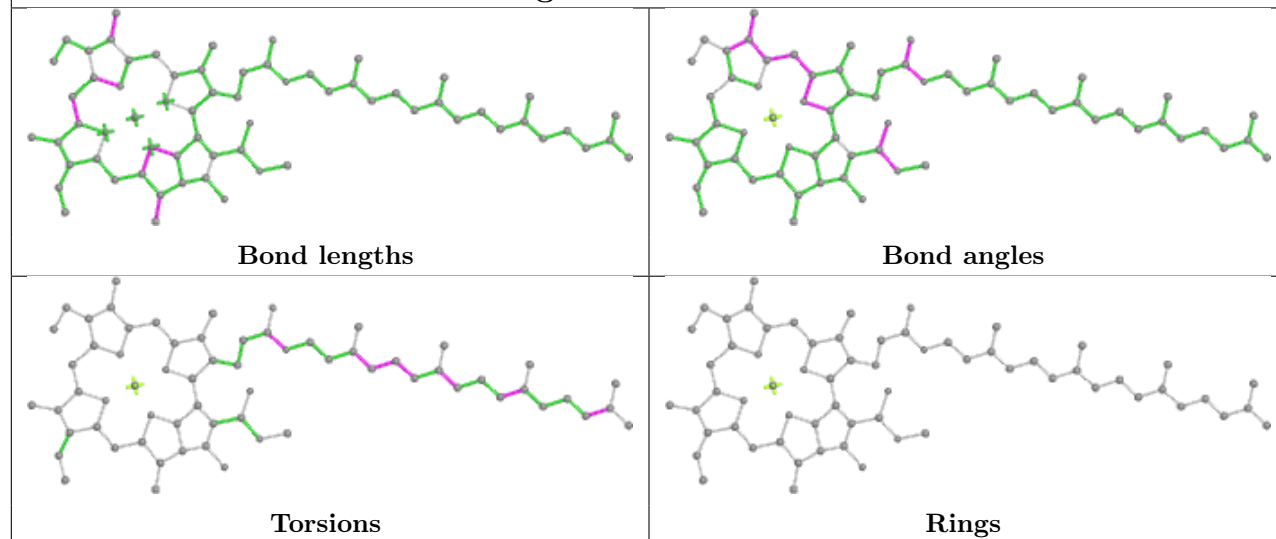


## Ligand CLA 4 314

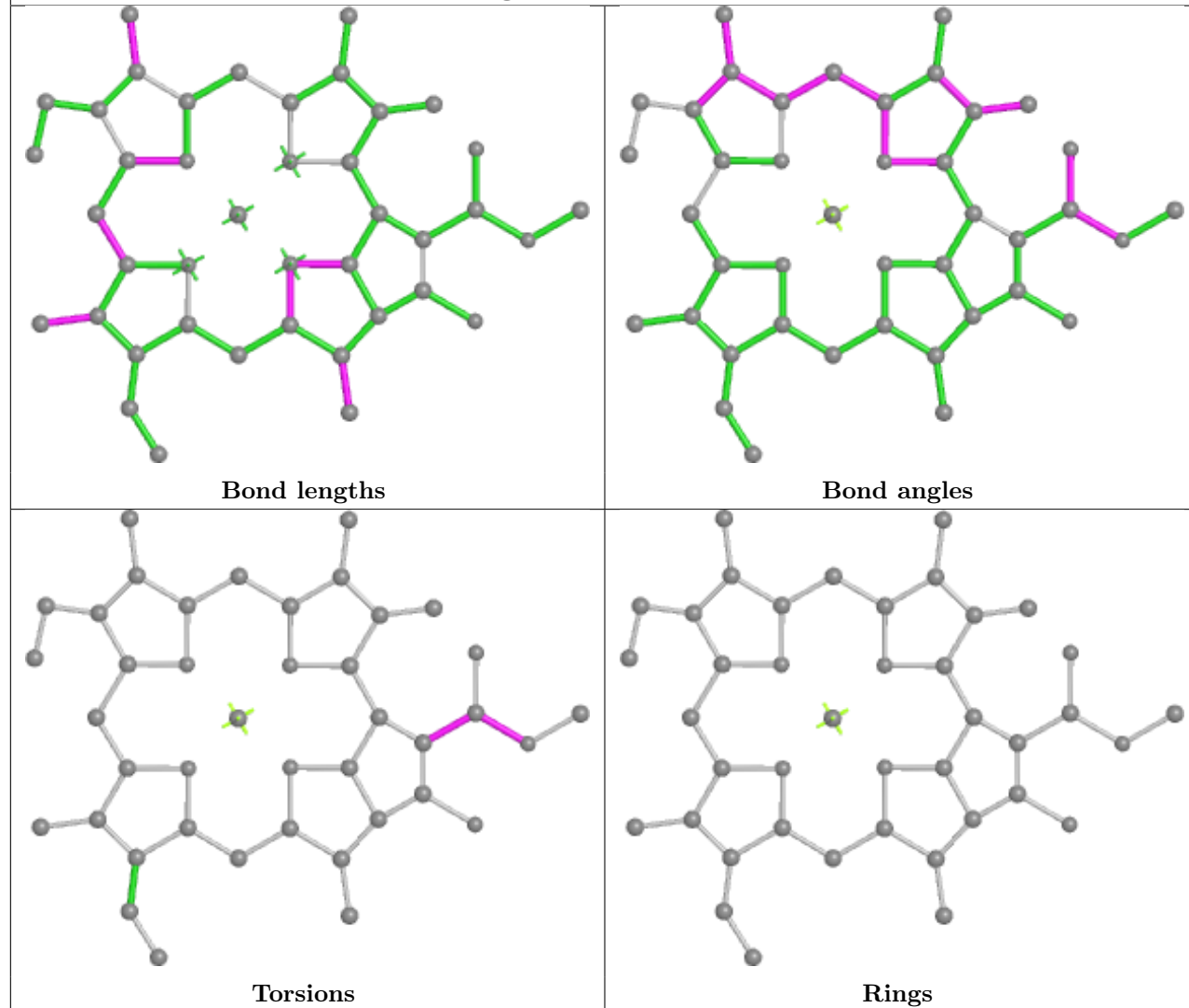


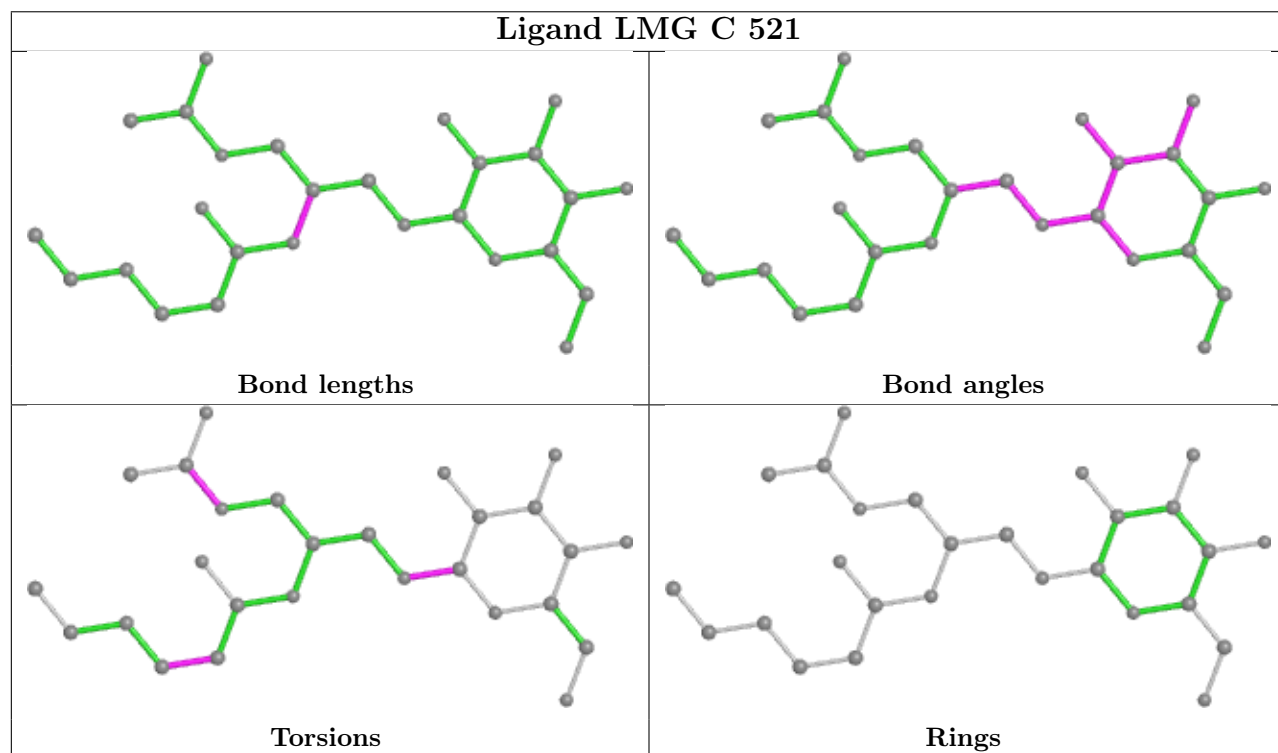
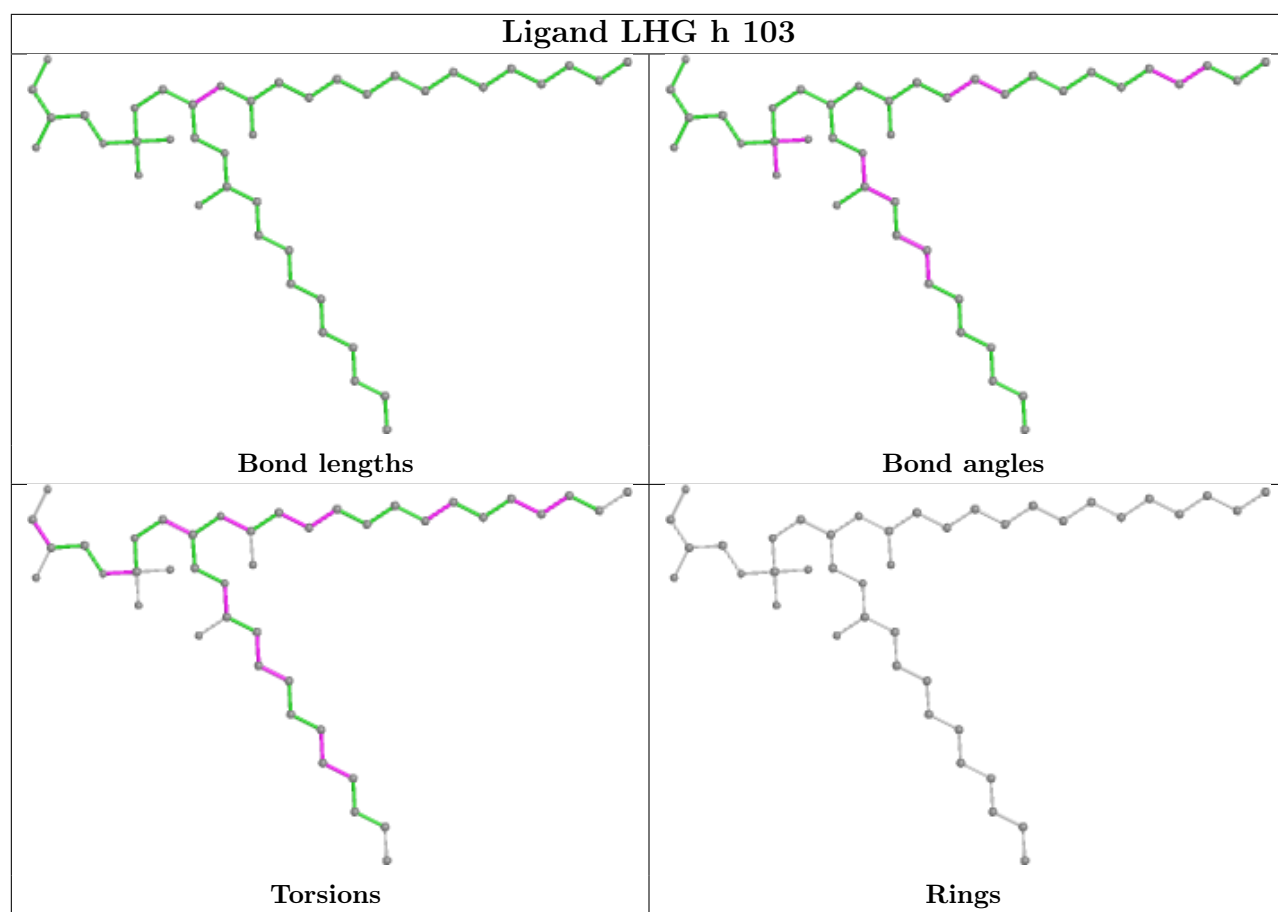


## Ligand CLA 3 307

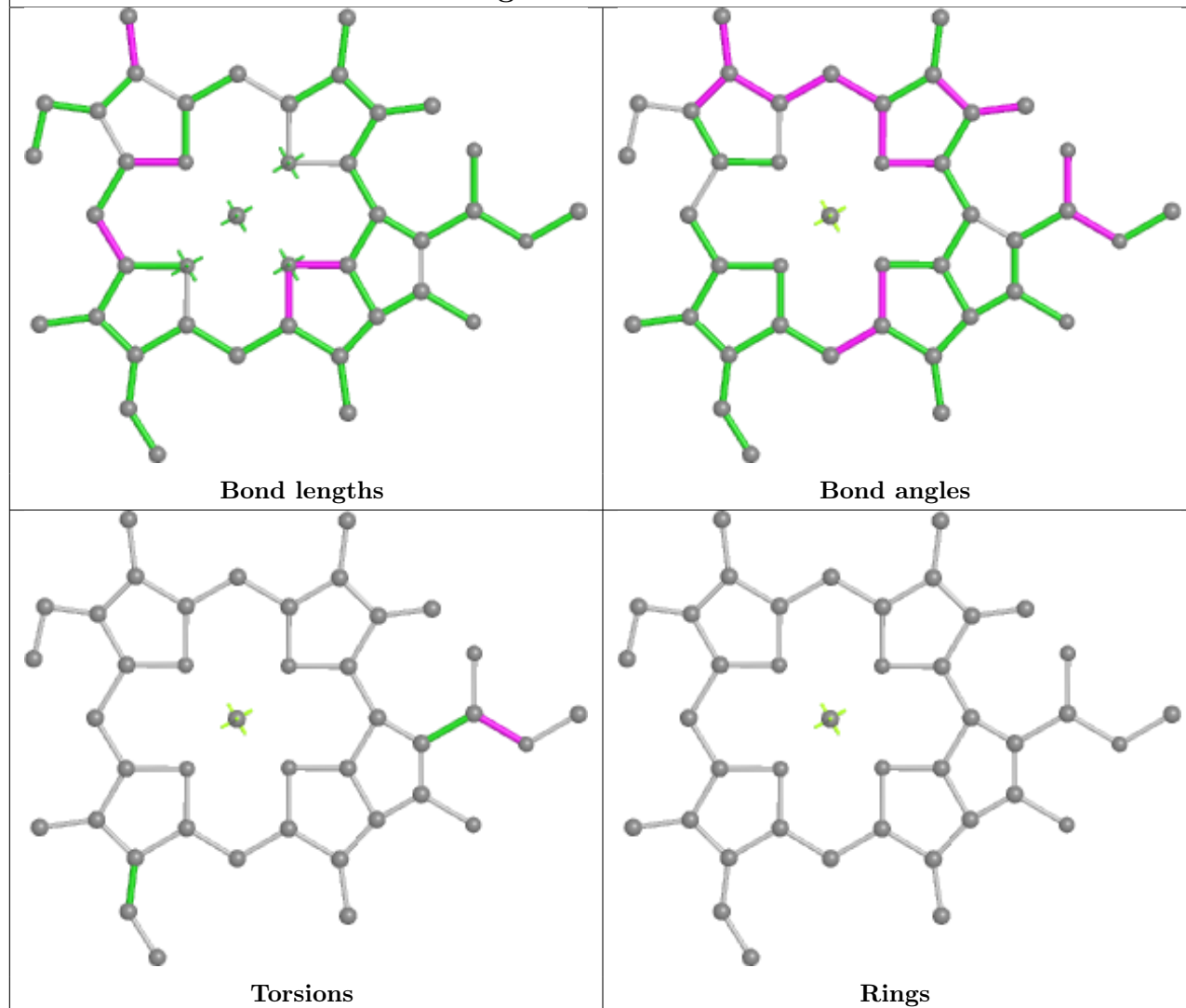


## Ligand CLA b 608

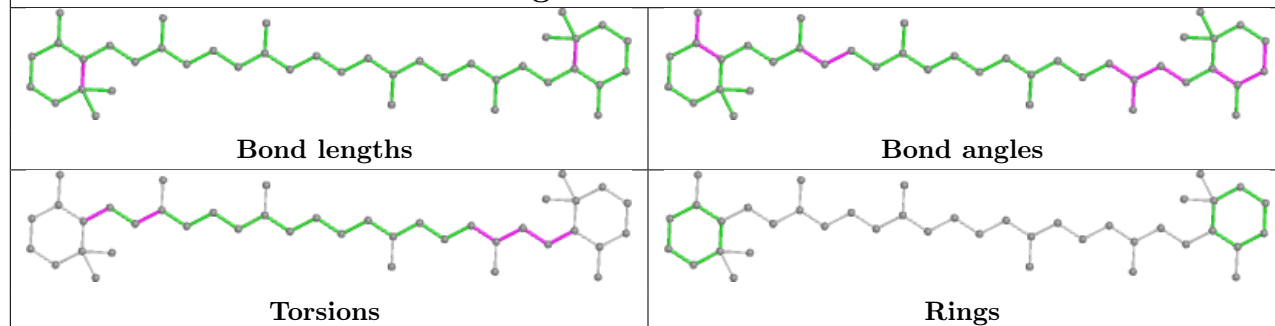


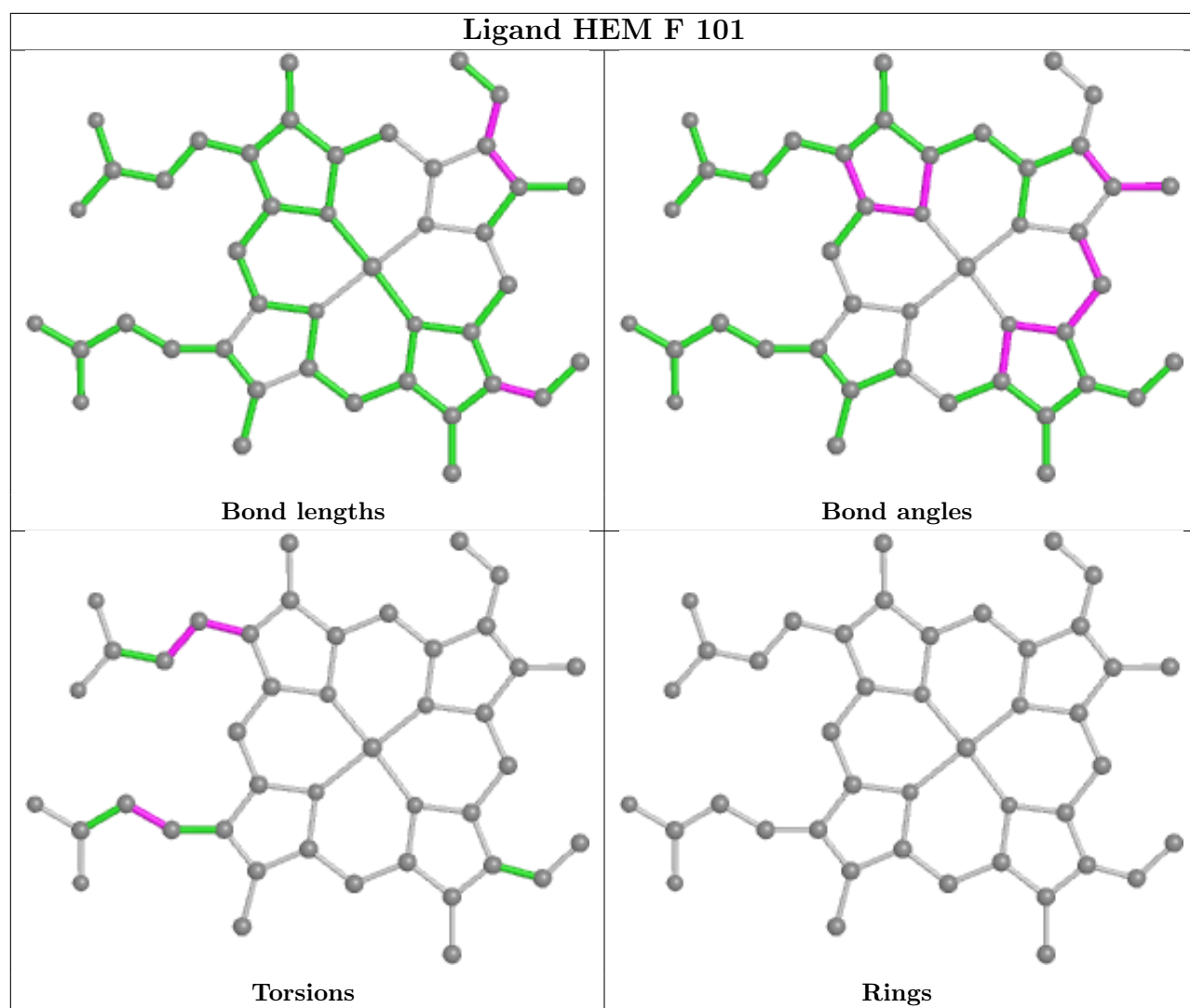


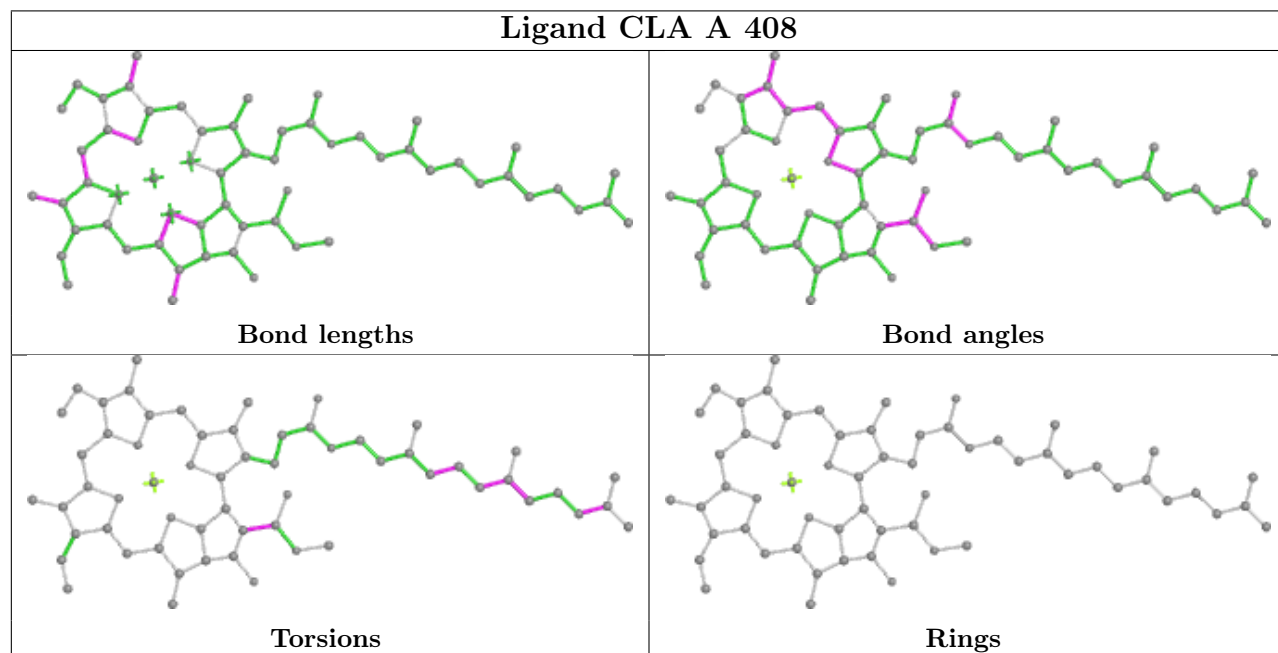
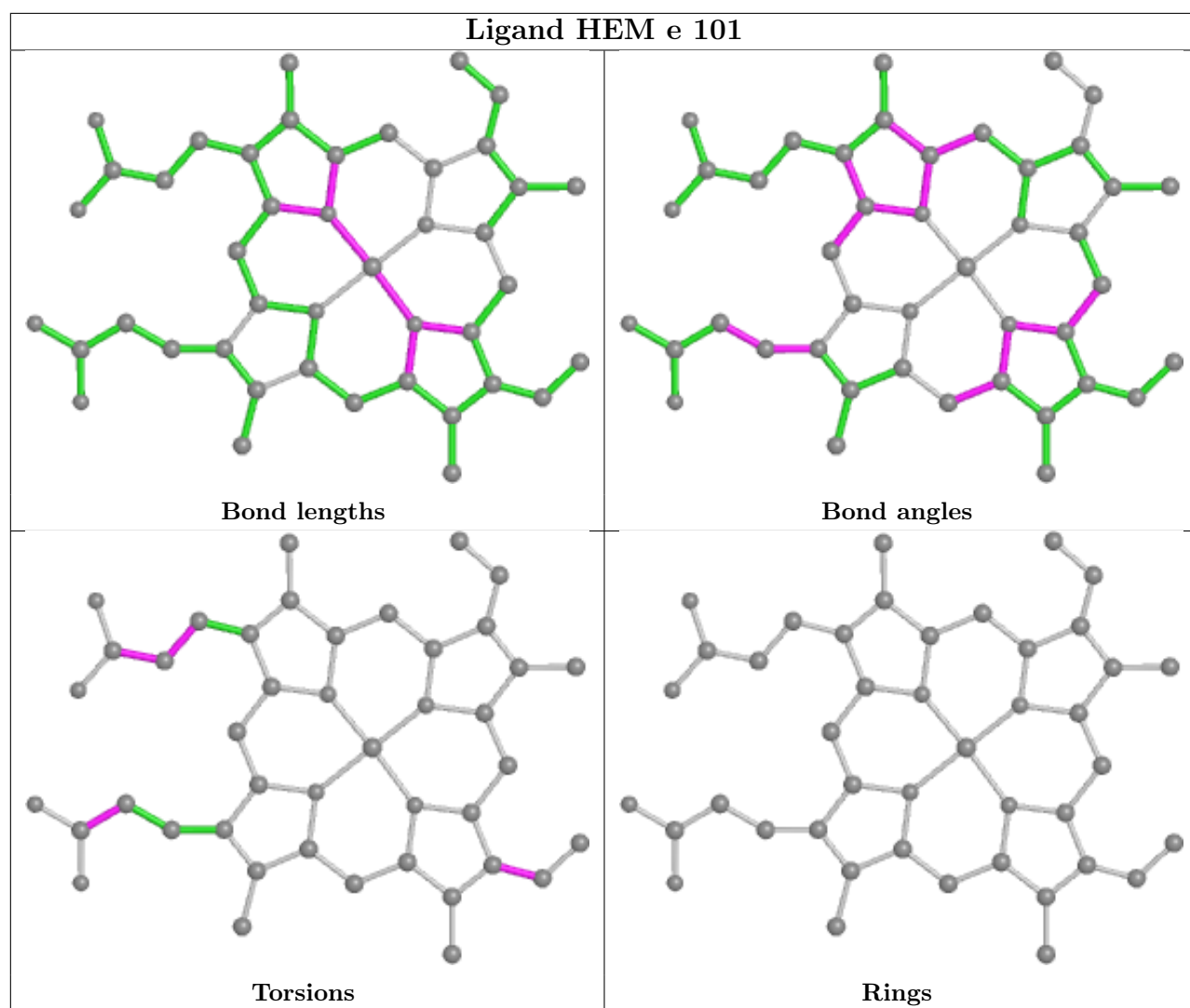
## Ligand CLA 5 316

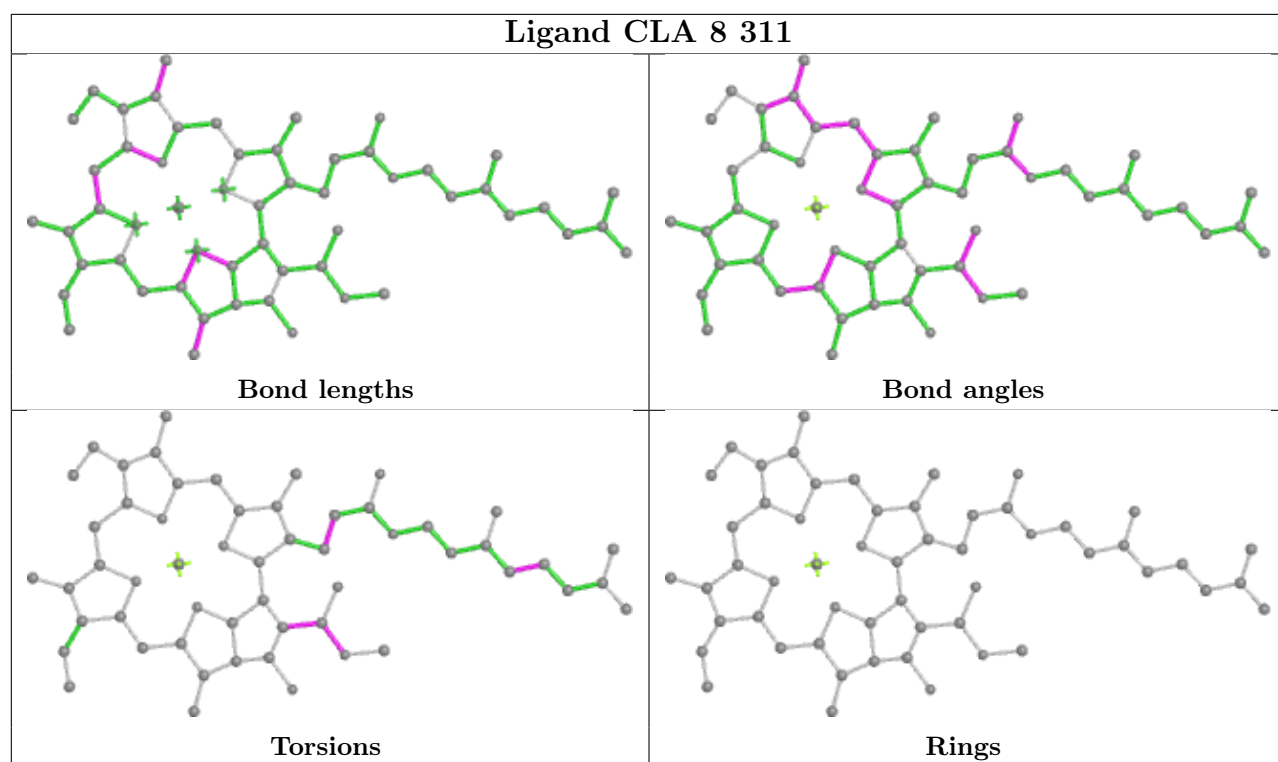


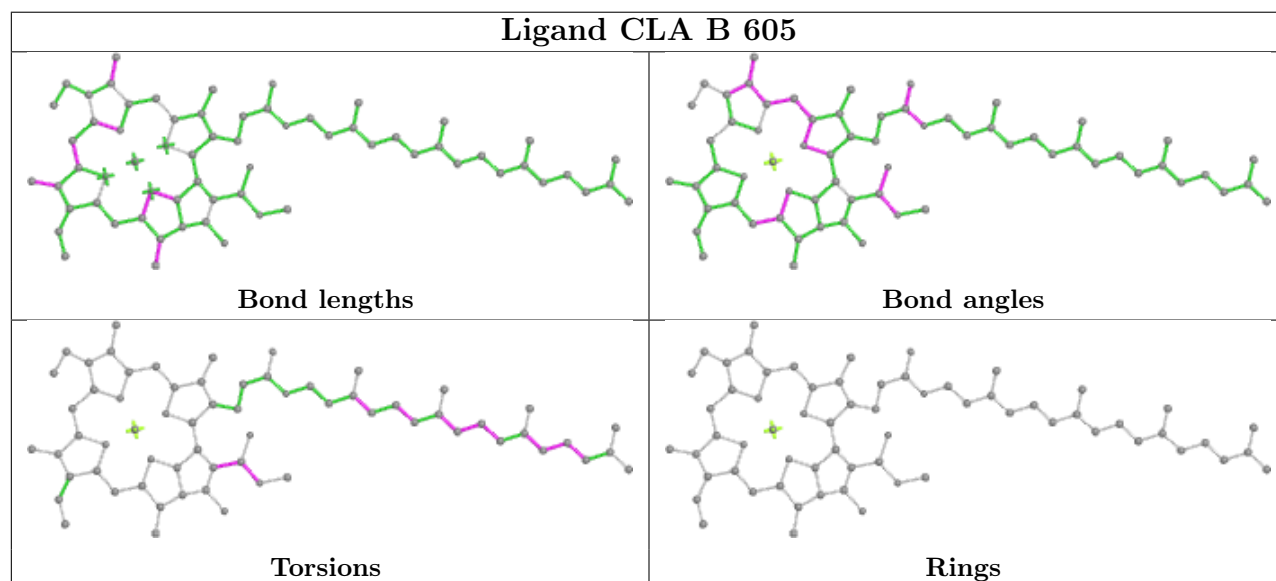
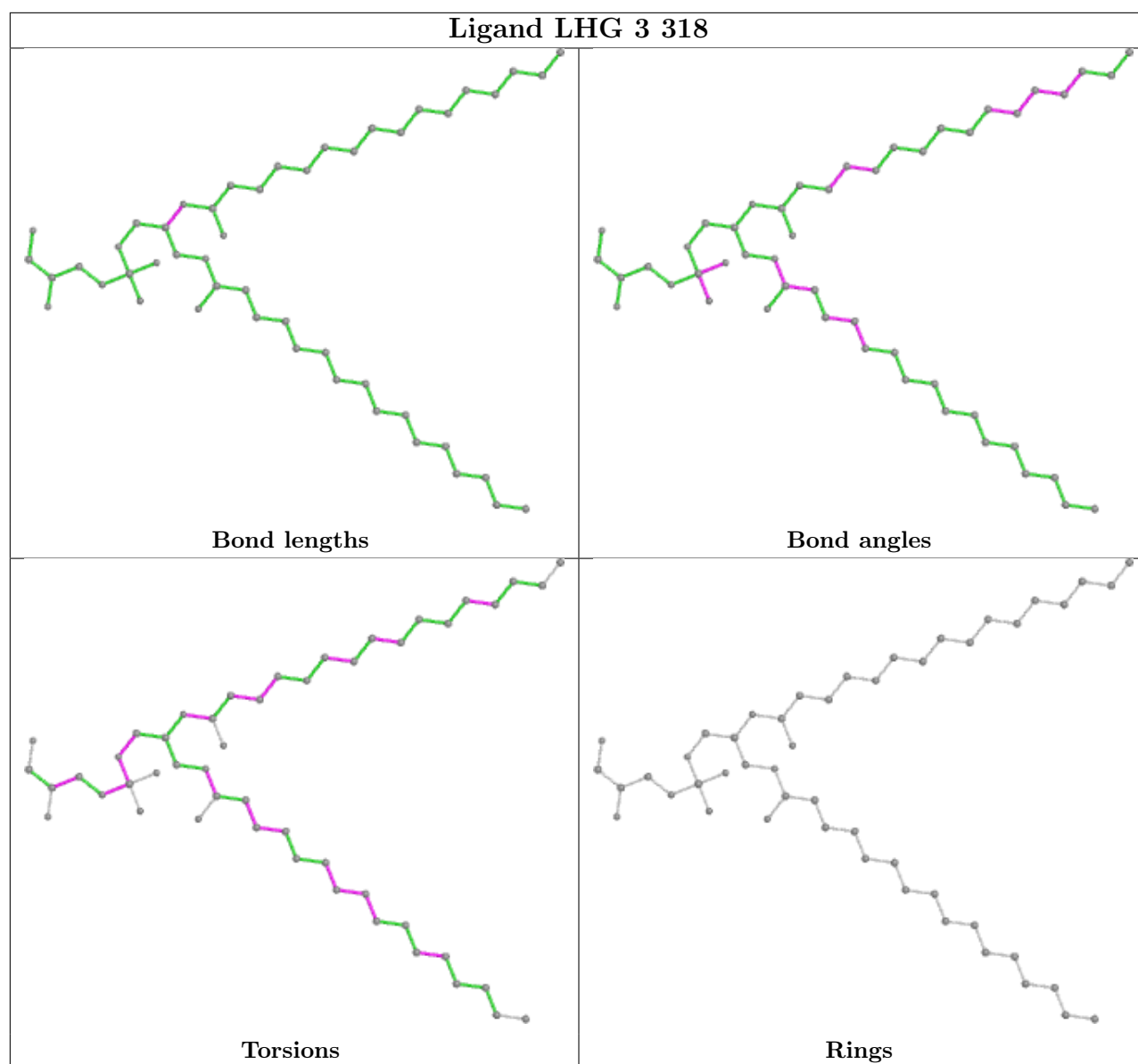
## Ligand BCR b 620

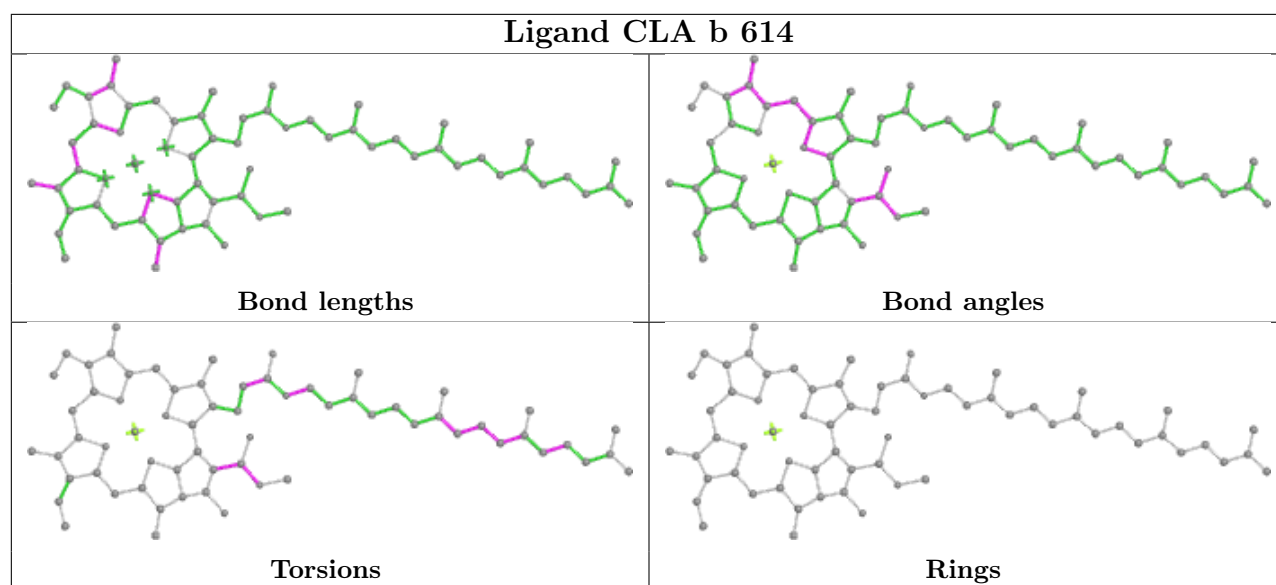












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.