



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:25 PM UTC

PDB ID : 8Z9D / pdb_00008z9d
EMDB ID : EMD-39860
Title : cryo-EM structure of PSII-LHCII megacomplex from spinach
Authors : Shan, J.Y.; Liu, Z.F.
Deposited on : 2024-04-23
Resolution : 3.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

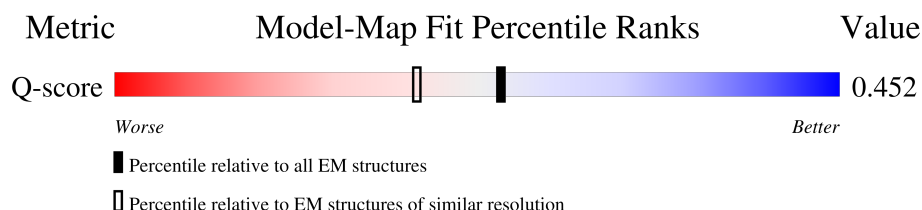
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.22 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	14612 (2.72 - 3.72)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
35	PL9	A	410	-	X	-	-
35	PL9	AA	410	-	X	-	-
35	PL9	D	407	-	X	-	-
35	PL9	DD	406	-	X	-	-
35	PL9	Dd	404	-	X	-	-
35	PL9	d	404	-	X	-	-

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 339330 atoms, of which 168031 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	335	Total	C	H	N	O	S	0	0
			5145	1710	2526	431	465	13		
1	a	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		
1	AA	335	Total	C	H	N	O	S	0	0
			5146	1710	2527	431	465	13		
1	Aa	334	Total	C	H	N	O	S	0	0
			5134	1707	2521	430	463	13		

- Molecule 2 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Oo	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	O	236	Total	C	H	N	O	S	0	0
			3559	1136	1765	292	363	3		
2	o	234	Total	C	H	N	O	S	0	0
			3524	1125	1748	289	359	3		
2	OO	236	Total	C	H	N	O	S	0	0
			3561	1136	1767	292	363	3		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Rr	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	R	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		
3	r	228	Total	C	H	N	O	S	0	0
			3541	1155	1763	289	330	4		
3	RR	227	Total	C	H	N	O	S	0	0
			3526	1150	1753	290	329	4		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Ss	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	S	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		
4	s	213	Total	C	H	N	O	S	0	0
			3266	1078	1617	268	298	5		
4	SS	222	Total	C	H	N	O	S	0	0
			3395	1117	1683	280	310	5		

- Molecule 5 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Tt	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	T	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	t	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		
5	TT	30	Total	C	H	N	O	S	0	0
			505	171	260	34	39	1		

- Molecule 6 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	Uu	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	U	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		
6	u	26	Total	C	H	N	O	S	0	0
			420	129	218	37	33	3		
6	UU	27	Total	C	H	N	O	S	0	0
			435	134	226	38	34	3		

- Molecule 7 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	Ww	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	W	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		
7	w	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	WW	54	Total	C	H	N	O	S	0	0
			820	276	401	61	81	1		

- Molecule 8 is a protein called Photosystem II reaction center X protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Xx	34	Total	C	H	N	O		0	0
			487	158	250	37	42			
8	X	46	Total	C	H	N	O		0	0
			667	213	341	53	60			
8	x	34	Total	C	H	N	O		0	0
			487	158	250	37	42			
8	XX	48	Total	C	H	N	O	S	0	0
			701	223	359	55	62	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Xx	45	GLY	SER	conflict	UNP A0A9R0JQ89
X	45	GLY	SER	conflict	UNP A0A9R0JQ89
x	45	GLY	SER	conflict	UNP A0A9R0JQ89
XX	45	GLY	SER	conflict	UNP A0A9R0JQ89

- Molecule 9 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Yy	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	G	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	N	217	Total	C	H	N	O	S	0	0
			3245	1077	1589	269	303	7		
9	Y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	g	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	n	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	y	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	GG	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	NN	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	YY	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		
9	Gg	215	Total	C	H	N	O	S	0	0
			3207	1065	1571	264	300	7		
9	Nn	218	Total	C	H	N	O	S	0	0
			3252	1079	1592	270	304	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Zz	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	Z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	z	61	Total	C	H	N	O	0	0
			933	306	479	68	80		
10	ZZ	61	Total	C	H	N	O	0	0
			933	306	479	68	80		

- Molecule 11 is a protein called Chlorophyll a-b binding protein CP24, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	44	186	Total	C	H	N	O	S	0	0
			2847	952	1395	234	262	4		
11	4	186	Total	C	H	N	O	S	0	0
			2847	952	1395	234	262	4		

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	Pp	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	p	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	P	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0
12	PP	187	Total 2827	C 912	H 1394	N 234	O 285	S 2	0	0

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Qq	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	Q	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		
13	QQ	147	Total	C	H	N	O	0	0
			2334	731	1181	201	221		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	11	206	Total	C	H	N	O	S	0	0
			3075	1021	1505	254	288	7		
14	22	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		
14	1	207	Total	C	H	N	O	S	0	0
			3086	1024	1510	255	290	7		
14	2	218	Total	C	H	N	O	S	0	0
			3253	1079	1592	270	305	7		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	33	207	Total	C	H	N	O	S	0	0
			3189	1061	1575	258	290	5		
15	3	209	Total	C	H	N	O	S	0	0
			3195	1063	1573	260	294	5		

- Molecule 16 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	0	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		
16	00	99	Total	C	H	N	O	S	0	0
			1448	462	726	120	139	1		

- Molecule 17 is a protein called Photosystem II reaction center proteins PsbY, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	5	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
17	55	40	Total	C	H	N	O	S	0	0
			633	199	325	55	53	1		

- Molecule 18 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	C	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	c	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		
18	CC	449	Total	C	H	N	O	S	0	0
			6892	2284	3417	581	599	11		
18	Cc	449	Total	C	H	N	O	S	0	0
			6891	2284	3416	581	599	11		

- Molecule 19 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	D	339	Total	C	H	N	O	S	0	0
			5274	1780	2580	441	461	12		
19	d	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		
19	DD	339	Total	C	H	N	O	S	0	0
			5275	1780	2581	441	461	12		
19	Dd	340	Total	C	H	N	O	S	0	0
			5295	1786	2592	443	462	12		

- Molecule 20 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	e	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		
20	EE	80	Total	C	H	N	O	0	0
			1255	414	615	105	121		
20	Ee	75	Total	C	H	N	O	0	0
			1201	398	591	100	112		

- Molecule 21 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	34	Total	C	H	N	O	S	
			558	187	282	45	43	1	0
21	f	31	Total	C	H	N	O	S	
			509	169	259	42	38	1	0
21	FF	34	Total	C	H	N	O	S	
			558	187	282	45	43	1	0
21	Ff	31	Total	C	H	N	O	S	
			509	169	259	42	38	1	0

- Molecule 22 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	h	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	HH	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0
22	Hh	59	Total	C	H	N	O	S	
			893	288	459	65	78	3	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	35	Total	C	H	N	O	S	
			581	195	295	44	46	1	0
23	i	33	Total	C	H	N	O	S	
			542	184	276	39	42	1	0
23	II	35	Total	C	H	N	O	S	
			581	195	295	44	46	1	0
23	Ii	33	Total	C	H	N	O	S	
			542	184	276	39	42	1	0

- Molecule 24 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	J	37	Total	C	H	N	O	
			552	182	283	41	46	0
24	j	34	Total	C	H	N	O	
			505	168	258	38	41	0
24	JJ	37	Total	C	H	N	O	
			552	182	283	41	46	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	Jj	34	Total	C	H	N	O	0	0
			505	168	258	38	41		

- Molecule 25 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	K	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	k	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	KK	37	Total 617	C 217	H 310	N 43	O 46	S 1	0	0
25	Kk	37	Total 616	C 217	H 310	N 43	O 45	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	35	Total 579	C 196	H 284	N 46	O 53	0	0
26	l	36	Total 596	C 201	H 292	N 48	O 55	0	0
26	LL	35	Total 579	C 196	H 284	N 46	O 53	0	0
26	Ll	36	Total 596	C 201	H 292	N 48	O 55	0	0

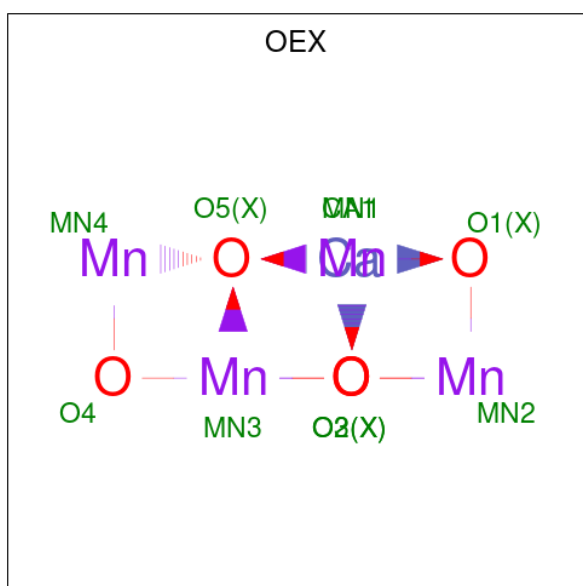
- Molecule 27 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	M	33	Total 543	C 177	H 285	N 37	O 43	S 1	0	0
27	m	32	Total 523	C 172	H 273	N 36	O 42		0	0
27	MM	33	Total 543	C 177	H 285	N 37	O 43	S 1	0	0
27	Mm	32	Total 523	C 172	H 273	N 36	O 42		0	0

- Molecule 28 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		
28	BB	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	B	499	Total	C	H	N	O	S	0	0
			7692	2562	3778	655	685	12		
28	Bb	487	Total	C	H	N	O	S	0	0
			7510	2501	3690	640	667	12		

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Fe	0
			1	1	
30	a	1	Total	Fe	0
			1	1	

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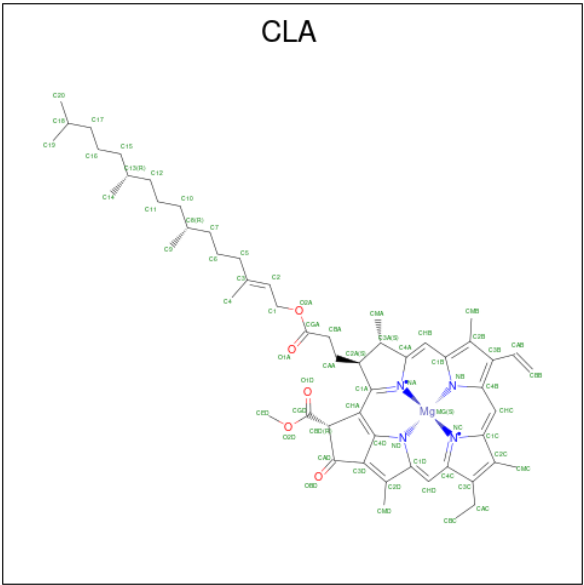
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Mol	Chain	Residues	Atoms		AltConf
30	AA	1	Total	Fe	0
			1	1	
30	Aa	1	Total	Fe	0
			1	1	

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Cl	0
			2	2	
31	a	2	Total	Cl	0
			2	2	
31	AA	2	Total	Cl	0
			2	2	
31	Aa	2	Total	Cl	0
			2	2	

- Molecule 32 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						AltConf
32	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	A	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Rr	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Ss	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Yy	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	Yy	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	44	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	11	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	22	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	33	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms						AltConf
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	1	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	2	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	3	1	Total 68	C 32	H 28	Mg 1	N 4	O 3	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	C	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	D	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	G	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
32	G	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	N	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	N	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	R	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	R	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	S	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	S	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	S	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
32	X	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Y	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			114	49	55	1	4	5	
32	Y	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	a	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	b	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	c	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	d	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	g	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	g	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	n	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	n	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	n	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	r	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	s	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	y	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	y	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	y	1	Total 114	C 49	H 55	Mg 1	N 4	O 5	0
32	y	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	AA	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	AA	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	AA	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0



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Mol	Chain	Residues	Atoms						AltConf
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
32	BB	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	BB	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	CC	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	DD	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	GG	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	GG	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	NN	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	NN	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
32	RR	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	RR	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
32	RR	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	RR	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	RR	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	RR	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	RR	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	RR	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	RR	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	RR	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	SS	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	SS	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
32	SS	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	SS	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	SS	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	SS	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	SS	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	SS	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	SS	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	XX	1	Total 70	C 33	H 29	Mg 1	N 4	O 3	0
32	YY	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	YY	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	YY	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
32	YY	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	YY	1	Total 73	C 34	H 31	Mg 1	N 4	O 3	0
32	YY	1	Total 113	C 48	H 55	Mg 1	N 4	O 5	0
32	YY	1	Total 114	C 49	H 55	Mg 1	N 4	O 5	0
32	YY	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	Aa	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Aa	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Aa	1	Total 88	C 39	H 39	Mg 1	N 4	O 5	0
32	Aa	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
32	Bb	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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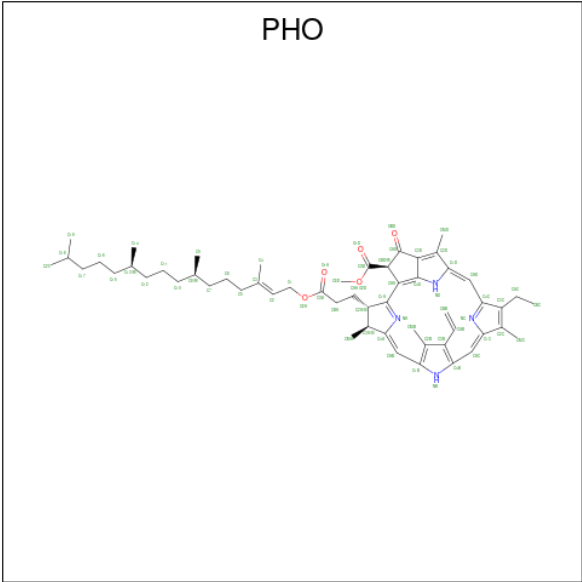
Mol	Chain	Residues	Atoms						AltConf
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Bb	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Cc	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Dd	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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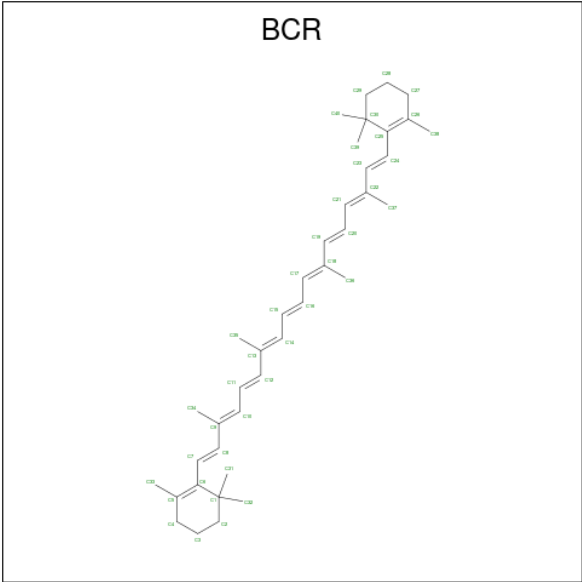
Mol	Chain	Residues	Atoms						AltConf
32	Gg	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Gg	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
32	Gg	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
32	Nn	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	

- Molecule 33 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	D	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	a	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	AA	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	DD	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	
33	Aa	1	Total	C	H	N	O	0
			138	55	74	4	5	

- Molecule 34 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	C	1	Total	C	H	0
			96	40	56	
34	D	1	Total	C	H	0
			96	40	56	
34	H	1	Total	C	H	0
			96	40	56	
34	K	1	Total	C	H	0
			96	40	56	
34	T	1	Total	C	H	0
			96	40	56	
34	a	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	b	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	
34	c	1	Total	C	H	0
			96	40	56	

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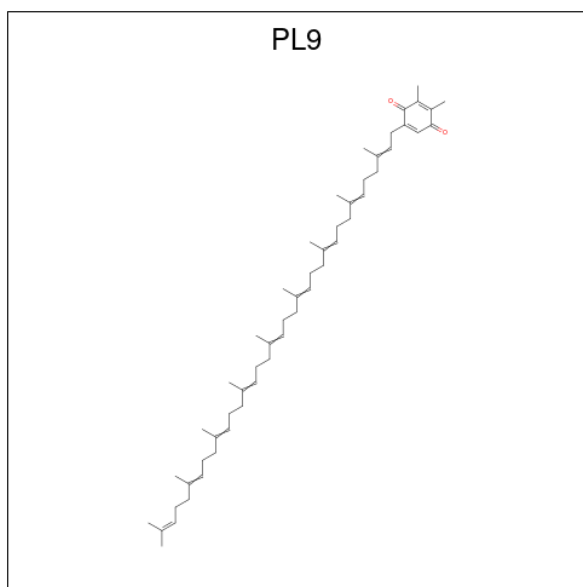
Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total 96	C 40	H 56	0
34	d	1	Total 96	C 40	H 56	0
34	h	1	Total 96	C 40	H 56	0
34	k	1	Total 96	C 40	H 56	0
34	AA	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	BB	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	CC	1	Total 96	C 40	H 56	0
34	DD	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	B	1	Total 96	C 40	H 56	0
34	KK	1	Total 96	C 40	H 56	0
34	TT	1	Total 96	C 40	H 56	0
34	XX	1	Total 96	C 40	H 56	0
34	Aa	1	Total 96	C 40	H 56	0

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Mol	Chain	Residues	Atoms			AltConf
34	Bb	1	Total	C	H	0
			96	40	56	
34	Bb	1	Total	C	H	0
			96	40	56	
34	Bb	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Cc	1	Total	C	H	0
			96	40	56	
34	Dd	1	Total	C	H	0
			96	40	56	
34	Hh	1	Total	C	H	0
			96	40	56	
34	Kk	1	Total	C	H	0
			96	40	56	

- Molecule 35 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



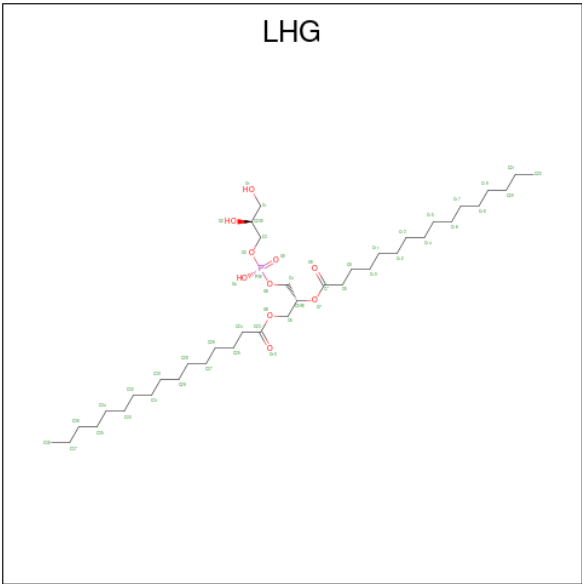
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			55	53	2	

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Mol	Chain	Residues	Atoms			AltConf
35	D	1	Total	C	O	0
			55	53	2	
35	d	1	Total	C	O	0
			55	53	2	
35	AA	1	Total	C	O	0
			55	53	2	
35	DD	1	Total	C	O	0
			55	53	2	
35	Dd	1	Total	C	O	0
			55	53	2	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	A	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	A	1	Total	C	H	O	P	0
			108	34	63	10	1	
36	Rr	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Ss	1	Total	C	H	O	P	0
			117	37	69	10	1	
36	Yy	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
36	44	1	Total	C	H	O	P	0
			33	10	12	10	1	
36	44	1	Total	C	H	O	P	0
			31	8	12	10	1	
36	11	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	22	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	33	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	1	1	Total	C	H	O	P	0
			60	19	30	10	1	
36	3	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	0	1	Total	C	H	O	P	0
			114	36	67	10	1	
36	C	1	Total	C	H	O	P	0
			63	20	32	10	1	
36	D	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	D	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	D	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	G	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	J	1	Total	C	H	O	P	0
			51	16	24	10	1	
36	K	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	N	1	Total	C	H	O	P	0
			84	27	46	10	1	
36	Y	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	a	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	d	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	d	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	g	1	Total	C	H	O	P	0
			72	23	38	10	1	

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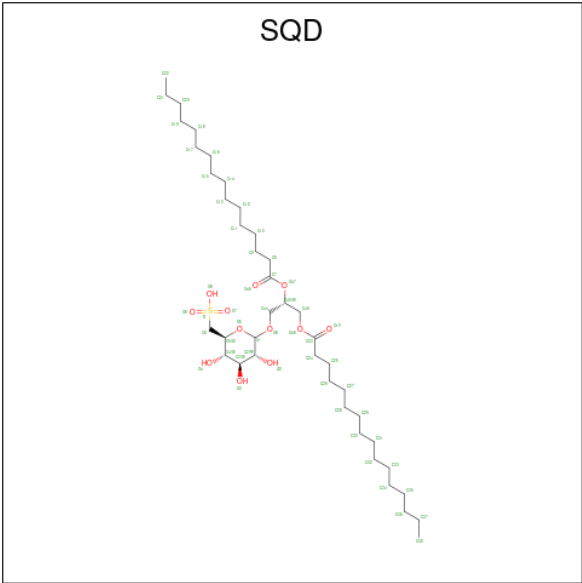
Mol	Chain	Residues	Atoms					AltConf
36	l	1	Total 123	C 38	H 74	O 10	P 1	0
36	n	1	Total 123	C 38	H 74	O 10	P 1	0
36	r	1	Total 123	C 38	H 74	O 10	P 1	0
36	s	1	Total 117	C 37	H 69	O 10	P 1	0
36	y	1	Total 123	C 38	H 74	O 10	P 1	0
36	4	1	Total 31	C 8	H 12	O 10	P 1	0
36	4	1	Total 33	C 10	H 12	O 10	P 1	0
36	AA	1	Total 72	C 23	H 38	O 10	P 1	0
36	AA	1	Total 108	C 34	H 63	O 10	P 1	0
36	BB	1	Total 72	C 23	H 38	O 10	P 1	0
36	CC	1	Total 72	C 23	H 38	O 10	P 1	0
36	CC	1	Total 81	C 26	H 44	O 10	P 1	0
36	DD	1	Total 102	C 32	H 59	O 10	P 1	0
36	DD	1	Total 123	C 38	H 74	O 10	P 1	0
36	EE	1	Total 93	C 29	H 53	O 10	P 1	0
36	GG	1	Total 72	C 23	H 38	O 10	P 1	0
36	II	1	Total 72	C 23	H 38	O 10	P 1	0
36	JJ	1	Total 69	C 22	H 36	O 10	P 1	0
36	KK	1	Total 72	C 23	H 38	O 10	P 1	0
36	NN	1	Total 84	C 27	H 46	O 10	P 1	0
36	SS	1	Total 48	C 15	H 22	O 10	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
36	YY	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			102	32	59	10	1	
36	Dd	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Dd	1	Total	C	H	O	P	0
			81	26	44	10	1	
36	Gg	1	Total	C	H	O	P	0
			72	23	38	10	1	
36	Ll	1	Total	C	H	O	P	0
			123	38	74	10	1	
36	Nn	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



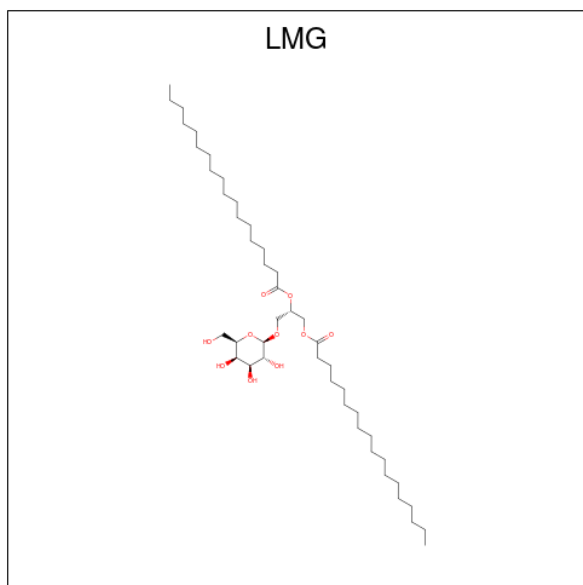
Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	C	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	L	1	Total	C	H	O	S	0
			72	23	36	12	1	

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Mol	Chain	Residues	Atoms					AltConf
37	l	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	AA	1	Total	C	H	O	S	0
			69	22	34	12	1	
37	BB	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	CC	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	B	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	B	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			72	23	36	12	1	
37	LL	1	Total	C	H	O	S	0
			132	41	78	12	1	
37	Aa	1	Total	C	H	O	S	0
			108	34	61	12	1	
37	Ll	1	Total	C	H	O	S	0
			132	41	78	12	1	

- Molecule 38 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



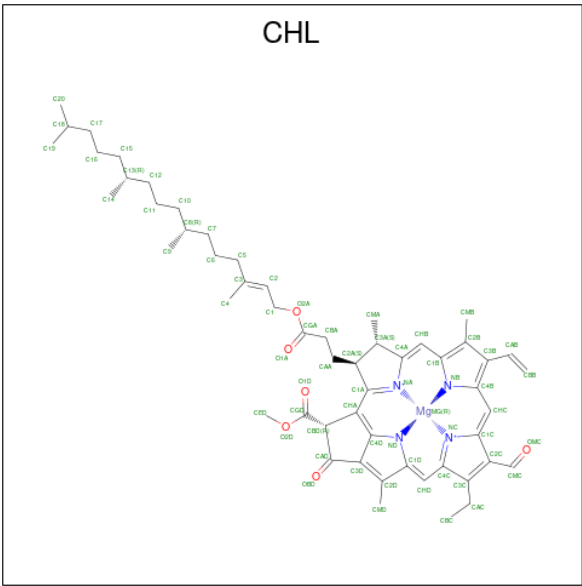
Mol	Chain	Residues	Atoms				AltConf
38	A	1	Total	C	H	O	0
			78	26	42	10	

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Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total 123	C 41	H 72	O 10	0
38	F	1	Total 108	C 36	H 62	O 10	0
38	W	1	Total 114	C 38	H 66	O 10	0
38	a	1	Total 97	C 33	H 54	O 10	0
38	b	1	Total 78	C 26	H 42	O 10	0
38	b	1	Total 78	C 26	H 42	O 10	0
38	c	1	Total 72	C 24	H 38	O 10	0
38	j	1	Total 108	C 36	H 62	O 10	0
38	m	1	Total 123	C 41	H 72	O 10	0
38	AA	1	Total 78	C 26	H 42	O 10	0
38	BB	1	Total 105	C 35	H 60	O 10	0
38	CC	1	Total 87	C 29	H 48	O 10	0
38	DD	1	Total 108	C 36	H 62	O 10	0
38	B	1	Total 105	C 35	H 60	O 10	0
38	WW	1	Total 114	C 38	H 66	O 10	0
38	Aa	1	Total 97	C 33	H 54	O 10	0
38	Bb	1	Total 78	C 26	H 42	O 10	0
38	Bb	1	Total 78	C 26	H 42	O 10	0
38	Cc	1	Total 72	C 24	H 38	O 10	0
38	Dd	1	Total 108	C 36	H 62	O 10	0
38	Mm	1	Total 123	C 41	H 72	O 10	0

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



Mol	Chain	Residues	Atoms						AltConf
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Rr	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Ss	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Yy	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Yy	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
39	44	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	44	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	11	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	22	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	33	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	
39	1	1	Total	C	H	Mg	N	O	0
			67	32	26	1	4	4	

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Mol	Chain	Residues	Atoms						AltConf
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	1	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	2	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	3	1	Total 67	C 32	H 26	Mg 1	N 4	O 4	0
39	G	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	G	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	G	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	G	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
39	G	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	G	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	N	1	Total 75	C 35	H 31	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms						AltConf
39	N	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	N	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	N	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	N	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	N	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	R	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	R	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	R	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	S	1	Total 91	C 41	H 39	Mg 1	N 4	O 6	0
39	S	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	S	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	S	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	Y	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	Y	1	Total 81	C 37	H 33	Mg 1	N 4	O 6	0
39	Y	1	Total 75	C 35	H 31	Mg 1	N 4	O 4	0
39	Y	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	Y	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	Y	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	g	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	g	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	g	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms						AltConf
39	g	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	g	1	Total 69	C 33	H 27	Mg 1	N 4	O 4	0
39	g	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	n	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	n	1	Total 81	C 37	H 33	Mg 1	N 4	O 6	0
39	n	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	n	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	n	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	n	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	r	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	r	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	r	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	s	1	Total 91	C 41	H 39	Mg 1	N 4	O 6	0
39	s	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	s	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0
39	s	1	Total 83	C 38	H 34	Mg 1	N 4	O 6	0
39	y	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
39	y	1	Total 81	C 37	H 33	Mg 1	N 4	O 6	0
39	y	1	Total 75	C 35	H 31	Mg 1	N 4	O 4	0
39	y	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
39	y	1	Total 87	C 39	H 37	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms						AltConf
39	y	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			73	34	28	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
39	GG	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	GG	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	NN	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	NN	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			86	39	36	1	4	6	
39	RR	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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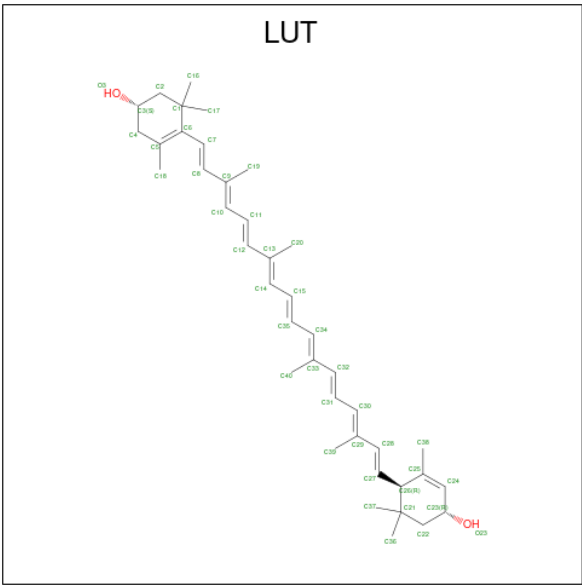
Mol	Chain	Residues	Atoms						AltConf
39	SS	1	Total	C	H	Mg	N	O	0
			91	41	39	1	4	6	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	SS	1	Total	C	H	Mg	N	O	0
			83	38	34	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			75	35	31	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	YY	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	YY	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Gg	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
39	Gg	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			81	37	33	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
39	Nn	1	Total	C	H	Mg	N	O	0
			87	39	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
39	Nn	1	87	39	37	1	4	6	0

- Molecule 40 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
40	Rr	1	98	40	56	2	0
40	Ss	1	98	40	56	2	0
40	Ss	1	98	40	56	2	0
40	Yy	1	98	40	56	2	0
40	Yy	1	98	40	56	2	0
40	44	1	98	40	56	2	0
40	22	1	98	40	56	2	0
40	2	1	98	40	56	2	0
40	G	1	98	40	56	2	0
40	G	1	98	40	56	2	0

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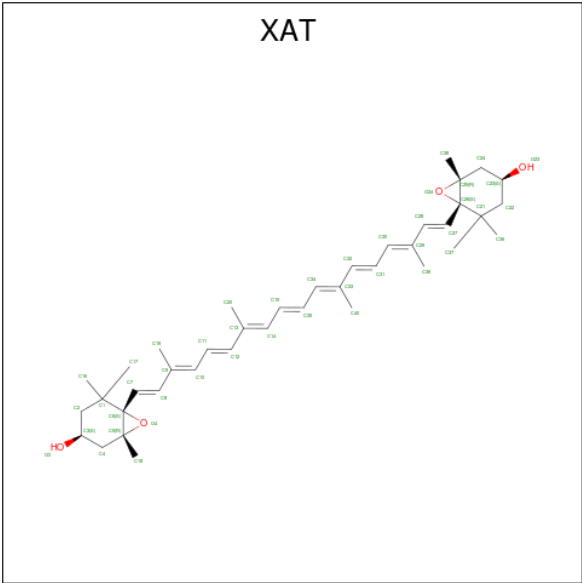
Mol	Chain	Residues	Atoms				AltConf
40	N	1	Total 98	C 40	H 56	O 2	0
40	N	1	Total 98	C 40	H 56	O 2	0
40	R	1	Total 98	C 40	H 56	O 2	0
40	S	1	Total 98	C 40	H 56	O 2	0
40	Y	1	Total 98	C 40	H 56	O 2	0
40	Y	1	Total 98	C 40	H 56	O 2	0
40	g	1	Total 98	C 40	H 56	O 2	0
40	g	1	Total 98	C 40	H 56	O 2	0
40	n	1	Total 98	C 40	H 56	O 2	0
40	n	1	Total 98	C 40	H 56	O 2	0
40	r	1	Total 98	C 40	H 56	O 2	0
40	s	1	Total 98	C 40	H 56	O 2	0
40	s	1	Total 98	C 40	H 56	O 2	0
40	y	1	Total 98	C 40	H 56	O 2	0
40	y	1	Total 98	C 40	H 56	O 2	0
40	4	1	Total 98	C 40	H 56	O 2	0
40	GG	1	Total 98	C 40	H 56	O 2	0
40	GG	1	Total 98	C 40	H 56	O 2	0
40	NN	1	Total 98	C 40	H 56	O 2	0
40	NN	1	Total 98	C 40	H 56	O 2	0
40	RR	1	Total 98	C 40	H 56	O 2	0

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Mol	Chain	Residues	Atoms				AltConf
40	SS	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	YY	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Gg	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	
40	Nn	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 41 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



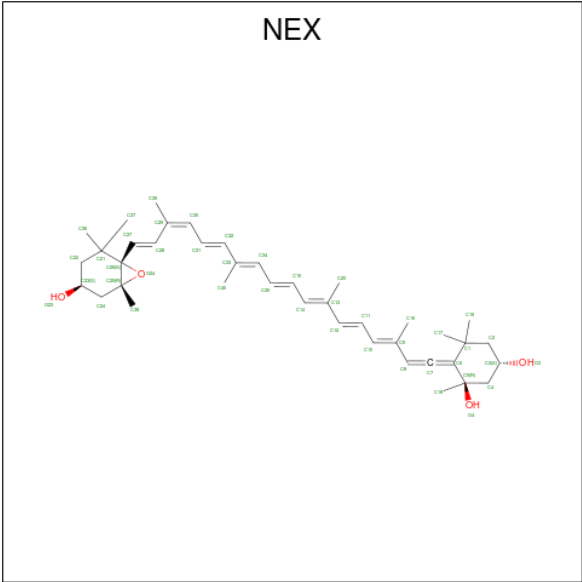
Mol	Chain	Residues	Atoms				AltConf
41	Rr	1	Total	C	H	O	0
			100	40	56	4	
41	Yy	1	Total	C	H	O	0
			100	40	56	4	
41	44	1	Total	C	H	O	0
			100	40	56	4	
41	G	1	Total	C	H	O	0
			100	40	56	4	

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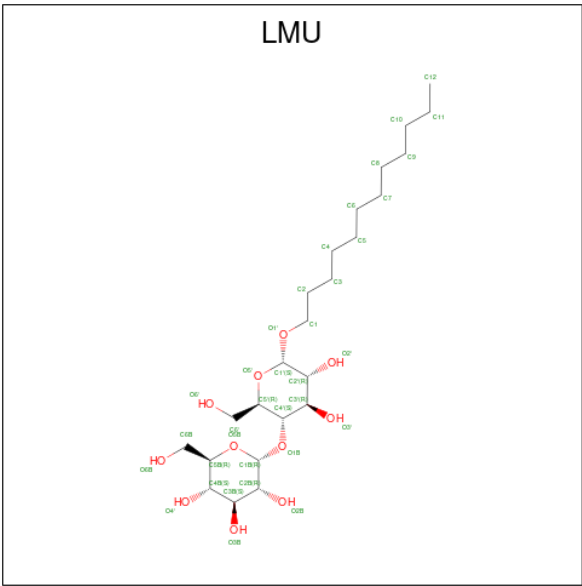
Mol	Chain	Residues	Atoms				AltConf
41	G	1	Total 100	C 40	H 56	O 4	0
41	N	1	Total 100	C 40	H 56	O 4	0
41	R	1	Total 100	C 40	H 56	O 4	0
41	g	1	Total 100	C 40	H 56	O 4	0
41	r	1	Total 100	C 40	H 56	O 4	0
41	y	1	Total 100	C 40	H 56	O 4	0
41	y	1	Total 100	C 40	H 56	O 4	0
41	4	1	Total 100	C 40	H 56	O 4	0
41	GG	1	Total 100	C 40	H 56	O 4	0
41	GG	1	Total 100	C 40	H 56	O 4	0
41	NN	1	Total 100	C 40	H 56	O 4	0
41	RR	1	Total 100	C 40	H 56	O 4	0
41	Gg	1	Total 100	C 40	H 56	O 4	0
41	Nn	1	Total 100	C 40	H 56	O 4	0

- Molecule 42 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



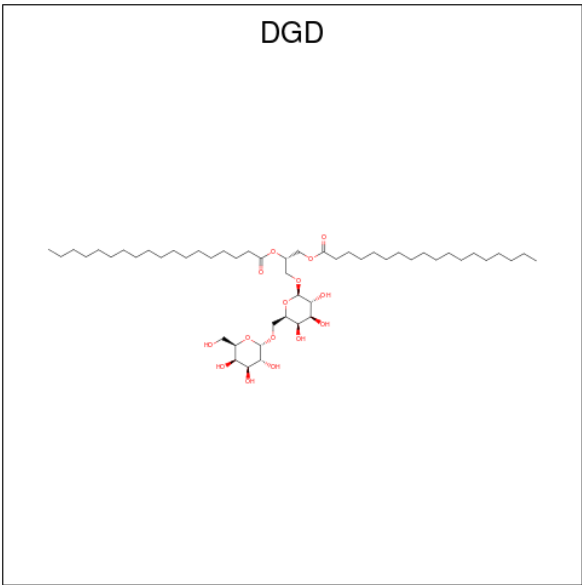
Mol	Chain	Residues	Atoms				AltConf
42	Rr	1	Total	C	H	O	0
			100	40	56	4	
42	Yy	1	Total	C	H	O	0
			100	40	56	4	
42	N	1	Total	C	H	O	0
			100	40	56	4	
42	R	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	Y	1	Total	C	H	O	0
			100	40	56	4	
42	g	1	Total	C	H	O	0
			100	40	56	4	
42	n	1	Total	C	H	O	0
			100	40	56	4	
42	y	1	Total	C	H	O	0
			100	40	56	4	
42	NN	1	Total	C	H	O	0
			100	40	56	4	
42	RR	1	Total	C	H	O	0
			100	40	56	4	
42	YY	1	Total	C	H	O	0
			100	40	56	4	
42	Gg	1	Total	C	H	O	0
			100	40	56	4	
42	Nn	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 43 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				AltConf
43	C	1	Total	C	H	O	0
			54	16	27	11	
43	R	1	Total	C	H	O	0
			54	16	27	11	
43	KK	1	Total	C	H	O	0
			54	16	27	11	
43	RR	1	Total	C	H	O	0
			53	16	26	11	

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



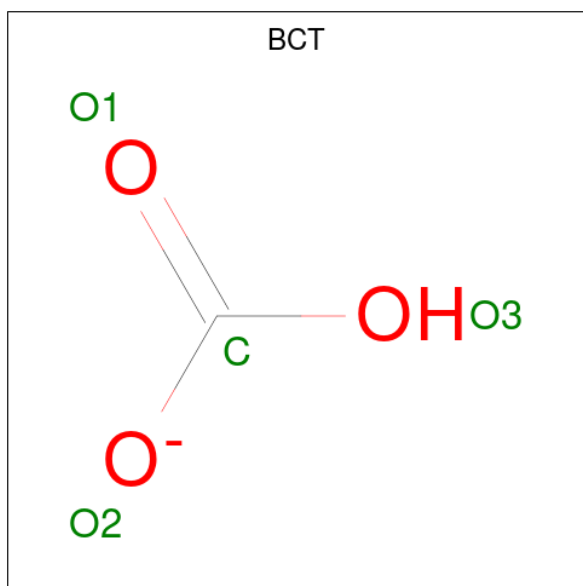
Mol	Chain	Residues	Atoms				AltConf
44	C	1	Total	C	H	O	0
			117	40	62	15	
44	C	1	Total	C	H	O	0
			132	47	70	15	
44	C	1	Total	C	H	O	0
			110	37	58	15	
44	D	1	Total	C	H	O	0
			132	47	70	15	
44	a	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			117	40	62	15	
44	c	1	Total	C	H	O	0
			108	37	56	15	
44	h	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			132	47	70	15	
44	BB	1	Total	C	H	O	0
			117	40	62	15	
44	BB	1	Total	C	H	O	0
			121	42	64	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	
44	CC	1	Total	C	H	O	0
			132	47	70	15	
44	CC	1	Total	C	H	O	0
			117	40	62	15	

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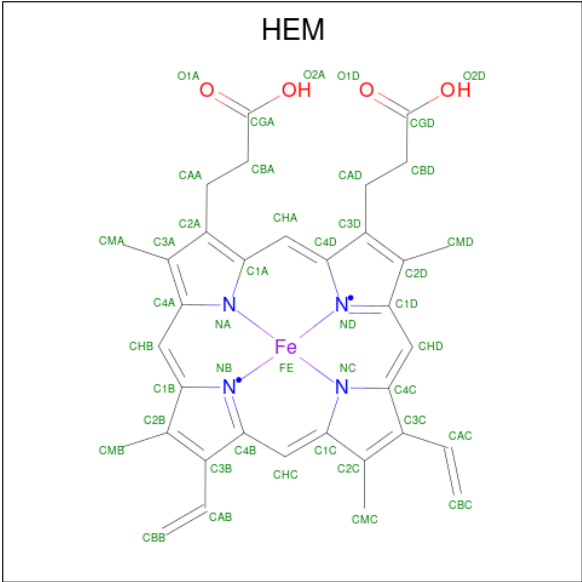
Mol	Chain	Residues	Atoms				AltConf
44	B	1	Total	C	H	O	0
			117	40	62	15	
44	B	1	Total	C	H	O	0
			121	42	64	15	
44	Aa	1	Total	C	H	O	0
			117	40	62	15	
44	Cc	1	Total	C	H	O	0
			117	40	62	15	
44	Cc	1	Total	C	H	O	0
			108	37	56	15	
44	Hh	1	Total	C	H	O	0
			132	47	70	15	

- Molecule 45 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				AltConf
45	D	1	Total	C	O		0
			4	1	3		
45	a	1	Total	C	H	O	0
			5	1	1	3	
45	AA	1	Total	C	O		0
			4	1	3		
45	Aa	1	Total	C	H	O	0
			5	1	1	3	

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						AltConf
46	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
46	e	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
46	EE	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
46	Ee	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93684	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	34.286	Depositor
Minimum map value	-20.735	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 781 ligands modelled in this entry, 12 are monoatomic - leaving 769 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
37	SQD	l	102	-	52,54,54	1.11	3 (5%)	62,65,65	1.00	3 (4%)
39	CHL	11	607	-	35,49,74	3.24	8 (22%)	30,83,114	2.05	12 (40%)
39	CHL	r	607	-	44,58,74	2.90	8 (18%)	37,94,114	1.84	13 (35%)
32	CLA	Ss	602	4	53,57,73	1.31	6 (11%)	61,93,113	1.20	4 (6%)
36	LHG	y	320	32	48,48,48	0.92	2 (4%)	51,54,54	0.96	3 (5%)
39	CHL	Gg	309	-	36,50,74	3.17	10 (27%)	29,85,114	1.91	9 (31%)
32	CLA	s	602	4	53,57,73	1.30	6 (11%)	61,93,113	1.18	4 (6%)
36	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.95	2 (3%)
32	CLA	C	513	18	69,73,73	1.16	7 (10%)	82,113,113	1.14	4 (4%)
32	CLA	a	406	1	69,73,73	1.17	9 (13%)	82,113,113	1.12	8 (9%)
32	CLA	SS	309	4	45,49,73	1.41	6 (13%)	54,84,113	1.22	4 (7%)
39	CHL	NN	608	-	36,50,74	3.20	10 (27%)	29,85,114	1.94	9 (31%)
32	CLA	1	602	14	44,48,73	1.44	6 (13%)	51,82,113	1.30	4 (7%)
32	CLA	1	610	36	44,48,73	1.45	5 (11%)	51,82,113	1.27	3 (5%)
32	CLA	d	402	-	69,73,73	1.16	6 (8%)	82,113,113	1.01	4 (4%)
33	PHO	A	407	-	58,69,69	2.15	10 (17%)	55,99,99	1.63	9 (16%)
32	CLA	44	602	11	49,53,73	1.36	8 (16%)	58,89,113	1.21	5 (8%)
32	CLA	11	612	-	44,48,73	1.51	8 (18%)	51,82,113	1.52	9 (17%)
44	DGD	CC	518	-	56,56,67	0.93	2 (3%)	70,70,81	0.95	3 (4%)
36	LHG	D	408	-	42,42,48	1.00	2 (4%)	45,48,54	1.03	2 (4%)
32	CLA	b	606	-	69,73,73	1.15	6 (8%)	82,113,113	1.11	7 (8%)
39	CHL	1	606	-	35,49,74	3.29	8 (22%)	30,83,114	1.89	8 (26%)
42	NEX	Yy	617	-	40,46,46	1.23	3 (7%)	50,70,70	1.94	15 (30%)
32	CLA	Aa	406	1	69,73,73	1.16	8 (11%)	82,113,113	1.11	7 (8%)
32	CLA	3	613	-	44,48,73	1.44	6 (13%)	51,82,113	1.31	4 (7%)
42	NEX	R	617	-	40,46,46	1.25	4 (10%)	50,70,70	1.91	12 (24%)
44	DGD	CC	522	-	56,56,67	0.93	3 (5%)	70,70,81	1.12	5 (7%)
36	LHG	BB	622	-	33,33,48	1.12	2 (6%)	36,39,54	1.02	2 (5%)
32	CLA	C	507	-	69,73,73	1.13	6 (8%)	82,113,113	1.08	6 (7%)
43	LMU	RR	301	-	28,28,36	0.75	0	39,39,47	0.76	0
39	CHL	YY	607	-	37,51,74	3.16	9 (24%)	30,86,114	2.08	12 (40%)
33	PHO	a	409	-	58,69,69	2.18	11 (18%)	55,99,99	1.49	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	XAT	Nn	308	-	41,47,47	1.20	3 (7%)	54,74,74	2.47	13 (24%)
32	CLA	2	611	14	44,48,73	1.45	6 (13%)	51,82,113	1.29	4 (7%)
36	LHG	NN	619	32	37,37,48	1.08	2 (5%)	40,43,54	1.05	2 (5%)
39	CHL	Ss	601	4	46,60,74	2.84	10 (21%)	40,97,114	1.74	13 (32%)
41	XAT	N	617	-	41,47,47	1.17	4 (9%)	54,74,74	2.27	14 (25%)
41	XAT	R	616	-	41,47,47	1.06	2 (4%)	54,74,74	2.19	16 (29%)
44	DGD	D	411	-	63,63,67	0.88	2 (3%)	77,77,81	0.89	3 (3%)
32	CLA	B	620	-	69,73,73	1.15	7 (10%)	82,113,113	1.13	5 (6%)
32	CLA	c	511	18	69,73,73	1.18	5 (7%)	82,113,113	1.04	3 (3%)
32	CLA	y	313	36	46,50,73	1.38	7 (15%)	53,85,113	1.27	4 (7%)
45	BCT	a	413	30	3,3,3	1.14	0	2,3,3	3.88	2 (100%)
32	CLA	D	401	-	69,73,73	1.13	6 (8%)	82,113,113	1.13	7 (8%)
32	CLA	AA	405	-	69,73,73	1.15	7 (10%)	82,113,113	1.09	5 (6%)
39	CHL	N	601	9	38,52,74	3.14	8 (21%)	31,87,114	1.89	9 (29%)
40	LUT	Rr	614	-	42,43,43	0.93	1 (2%)	51,60,60	1.41	9 (17%)
44	DGD	Aa	401	-	56,56,67	0.96	2 (3%)	70,70,81	0.89	3 (4%)
36	LHG	11	614	32	33,33,48	1.14	2 (6%)	36,39,54	1.13	3 (8%)
44	DGD	C	520	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	3 (3%)
42	NEX	Rr	616	-	40,46,46	1.23	3 (7%)	50,70,70	2.09	17 (34%)
32	CLA	RR	302	3	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
32	CLA	S	613	-	49,53,73	1.37	7 (14%)	58,89,113	1.17	4 (6%)
39	CHL	S	601	4	46,60,74	2.84	9 (19%)	40,97,114	1.73	11 (27%)
41	XAT	4	314	-	41,47,47	1.04	2 (4%)	54,74,74	2.38	15 (27%)
39	CHL	NN	601	9	38,52,74	3.11	9 (23%)	31,87,114	1.91	9 (29%)
39	CHL	g	609	9	37,51,74	3.10	10 (27%)	30,86,114	1.96	9 (30%)
41	XAT	r	615	-	41,47,47	1.11	3 (7%)	54,74,74	2.30	15 (27%)
32	CLA	3	602	15	44,48,73	1.44	5 (11%)	51,82,113	1.26	4 (7%)
39	CHL	Rr	607	-	44,58,74	2.89	8 (18%)	37,94,114	1.85	13 (35%)
32	CLA	GG	602	9	53,57,73	1.34	5 (9%)	61,93,113	1.36	6 (9%)
32	CLA	Bb	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.20	6 (7%)
37	SQD	BB	621	-	34,36,54	1.43	4 (11%)	44,47,65	3.79	10 (22%)
32	CLA	S	603	-	49,53,73	1.39	6 (12%)	58,89,113	1.23	4 (6%)
32	CLA	R	609	3	69,73,73	1.16	8 (11%)	82,113,113	1.06	5 (6%)
41	XAT	44	613	-	41,47,47	1.03	2 (4%)	54,74,74	2.28	12 (22%)
32	CLA	g	602	9	53,57,73	1.35	6 (11%)	61,93,113	1.83	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	B	622	-	69,73,73	1.15	6 (8%)	82,113,113	1.16	7 (8%)
40	LUT	GG	615	-	42,43,43	0.94	0	51,60,60	1.49	10 (19%)
42	NEX	Y	617	-	40,46,46	1.25	3 (7%)	50,70,70	1.97	12 (24%)
32	CLA	g	603	-	69,73,73	1.16	6 (8%)	82,113,113	1.01	4 (4%)
32	CLA	Cc	512	-	69,73,73	1.15	8 (11%)	82,113,113	1.09	4 (4%)
39	CHL	Nn	319	9	44,58,74	2.82	12 (27%)	37,94,114	1.83	10 (27%)
32	CLA	N	611	36	53,57,73	1.31	7 (13%)	61,93,113	1.26	6 (9%)
32	CLA	Gg	311	9	53,57,73	1.29	6 (11%)	61,93,113	1.21	5 (8%)
32	CLA	Bb	611	-	69,73,73	1.14	7 (10%)	82,113,113	1.07	4 (4%)
34	BCR	k	101	-	41,41,41	0.91	1 (2%)	56,56,56	1.94	17 (30%)
32	CLA	b	614	-	69,73,73	1.14	6 (8%)	82,113,113	1.09	3 (3%)
39	CHL	3	608	15	35,49,74	3.23	8 (22%)	30,83,114	1.81	8 (26%)
42	NEX	N	618	-	40,46,46	1.25	3 (7%)	50,70,70	2.08	14 (28%)
39	CHL	Y	606	-	38,52,74	3.11	11 (28%)	31,87,114	1.93	8 (25%)
32	CLA	RR	312	3	46,50,73	1.40	5 (10%)	53,85,113	1.17	3 (5%)
32	CLA	Cc	508	-	69,73,73	1.14	7 (10%)	82,113,113	1.17	7 (8%)
32	CLA	YY	604	-	53,57,73	1.30	5 (9%)	61,93,113	1.27	5 (8%)
32	CLA	Y	604	-	53,57,73	1.30	6 (11%)	61,93,113	1.20	5 (8%)
39	CHL	Yy	609	9	60,74,74	2.45	11 (18%)	58,114,114	1.61	9 (15%)
34	BCR	b	619	-	41,41,41	0.90	1 (2%)	56,56,56	1.94	12 (21%)
32	CLA	R	608	3	53,57,73	1.31	7 (13%)	61,93,113	1.28	4 (6%)
32	CLA	N	610	9	69,73,73	1.16	6 (8%)	82,113,113	1.04	6 (7%)
34	BCR	B	614	-	41,41,41	0.98	2 (4%)	56,56,56	1.85	14 (25%)
32	CLA	B	623	-	69,73,73	1.15	6 (8%)	82,113,113	1.03	3 (3%)
33	PHO	Aa	409	-	58,69,69	2.16	11 (18%)	55,99,99	1.50	8 (14%)
35	PL9	A	410	-	55,55,55	4.42	23 (41%)	68,69,69	3.73	38 (55%)
39	CHL	YY	609	9	60,74,74	2.46	10 (16%)	58,114,114	1.51	12 (20%)
32	CLA	Cc	510	-	64,68,73	1.18	6 (9%)	76,107,113	1.05	3 (3%)
39	CHL	G	601	9	60,74,74	2.47	11 (18%)	58,114,114	1.56	13 (22%)
32	CLA	YY	611	36	46,50,73	1.41	9 (19%)	53,85,113	1.26	4 (7%)
42	NEX	n	617	-	40,46,46	1.22	3 (7%)	50,70,70	2.01	12 (24%)
32	CLA	D	405	-	69,73,73	1.15	6 (8%)	82,113,113	1.05	4 (4%)
40	LUT	g	616	-	42,43,43	0.88	1 (2%)	51,60,60	1.58	10 (19%)
32	CLA	Rr	610	36	53,57,73	1.35	6 (11%)	61,93,113	1.24	4 (6%)
34	BCR	DD	405	-	41,41,41	0.85	0	56,56,56	1.94	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	c	502	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	8 (9%)
32	CLA	r	604	-	53,57,73	1.30	5 (9%)	61,93,113	1.21	6 (9%)
42	NEX	y	319	-	40,46,46	1.24	3 (7%)	50,70,70	1.94	12 (24%)
32	CLA	3	610	36	44,48,73	1.45	5 (11%)	51,82,113	1.35	6 (11%)
32	CLA	y	315	9	63,67,73	1.20	6 (9%)	74,105,113	1.14	3 (4%)
39	CHL	S	606	-	36,50,74	3.19	8 (22%)	29,85,114	1.98	10 (34%)
32	CLA	BB	613	-	64,68,73	1.19	6 (9%)	76,107,113	1.14	5 (6%)
34	BCR	CC	516	-	41,41,41	0.97	1 (2%)	56,56,56	1.92	14 (25%)
32	CLA	44	611	-	49,53,73	1.37	5 (10%)	58,89,113	1.22	3 (5%)
32	CLA	Rr	608	3	53,57,73	1.30	6 (11%)	61,93,113	1.19	5 (8%)
34	BCR	C	516	-	41,41,41	0.97	1 (2%)	56,56,56	2.09	18 (32%)
34	BCR	b	618	-	41,41,41	0.91	1 (2%)	56,56,56	1.94	12 (21%)
32	CLA	C	504	-	69,73,73	1.15	7 (10%)	82,113,113	1.20	4 (4%)
32	CLA	r	610	36	53,57,73	1.34	5 (9%)	61,93,113	1.24	4 (6%)
37	SQD	LL	101	-	34,36,54	1.37	3 (8%)	44,47,65	1.12	2 (4%)
44	DGD	C	519	-	56,56,67	0.94	2 (3%)	70,70,81	0.94	3 (4%)
32	CLA	g	611	36	69,73,73	1.17	7 (10%)	82,113,113	1.23	8 (9%)
39	CHL	Nn	316	-	44,58,74	2.86	10 (22%)	37,94,114	1.92	11 (29%)
39	CHL	g	607	-	44,58,74	2.89	11 (25%)	37,94,114	1.75	10 (27%)
46	HEM	Ee	101	21,20	50,50,50	1.42	10 (20%)	67,82,82	1.10	3 (4%)
32	CLA	r	612	3	53,57,73	1.33	5 (9%)	61,93,113	1.24	6 (9%)
38	LMG	CC	520	-	39,39,55	1.07	2 (5%)	47,47,63	0.95	2 (4%)
34	BCR	C	518	-	41,41,41	0.89	0	56,56,56	2.09	14 (25%)
32	CLA	r	602	3	69,73,73	1.16	6 (8%)	82,113,113	1.08	6 (7%)
39	CHL	Nn	311	9	44,58,74	2.90	9 (20%)	37,94,114	1.78	11 (29%)
32	CLA	b	605	-	69,73,73	1.14	6 (8%)	82,113,113	1.09	4 (4%)
41	XAT	Gg	301	-	41,47,47	1.22	4 (9%)	54,74,74	2.46	12 (22%)
42	NEX	Nn	309	-	40,46,46	1.23	3 (7%)	50,70,70	1.99	12 (24%)
32	CLA	22	604	-	44,48,73	1.45	5 (11%)	51,82,113	1.27	4 (7%)
32	CLA	Nn	314	-	53,57,73	1.30	8 (15%)	61,93,113	1.17	6 (9%)
32	CLA	Gg	314	9	44,48,73	1.43	5 (11%)	51,82,113	1.37	5 (9%)
32	CLA	n	610	9	69,73,73	1.16	6 (8%)	82,113,113	1.04	8 (9%)
32	CLA	Cc	515	-	47,51,73	1.36	7 (14%)	55,86,113	1.23	5 (9%)
39	CHL	r	605	3	44,58,74	2.87	9 (20%)	37,94,114	1.94	9 (24%)
35	PL9	Dd	404	-	55,55,55	4.36	21 (38%)	68,69,69	3.81	38 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	33	610	36	44,48,73	1.44	6 (13%)	51,82,113	1.31	5 (9%)
36	LHG	CC	523	-	36,36,48	1.06	2 (5%)	39,42,54	1.05	3 (7%)
32	CLA	2	609	14	44,48,73	1.44	6 (13%)	51,82,113	1.21	3 (5%)
32	CLA	CC	508	-	69,73,73	1.15	6 (8%)	82,113,113	1.25	7 (8%)
32	CLA	d	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.17	7 (8%)
38	LMG	W	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.06	2 (3%)
32	CLA	11	602	14	44,48,73	1.45	5 (11%)	51,82,113	1.29	5 (9%)
32	CLA	11	611	14	44,48,73	1.45	6 (13%)	51,82,113	1.28	4 (7%)
46	HEM	E	101	21,20	50,50,50	1.40	8 (16%)	67,82,82	1.06	1 (1%)
36	LHG	Nn	310	32	48,48,48	0.95	2 (4%)	51,54,54	1.06	2 (3%)
32	CLA	N	614	-	45,49,73	1.39	7 (15%)	54,84,113	1.18	3 (5%)
36	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.97	3 (5%)
32	CLA	RR	310	36	53,57,73	1.31	4 (7%)	61,93,113	1.17	5 (8%)
40	LUT	r	614	-	42,43,43	0.94	1 (2%)	51,60,60	1.40	8 (15%)
32	CLA	Aa	410	-	64,68,73	1.19	7 (10%)	76,107,113	1.13	7 (9%)
40	LUT	NN	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.34	8 (15%)
32	CLA	B	606	-	69,73,73	1.14	7 (10%)	82,113,113	1.14	6 (7%)
32	CLA	y	305	-	53,57,73	1.31	7 (13%)	61,93,113	1.19	3 (4%)
33	PHO	a	408	-	58,69,69	2.18	11 (18%)	55,99,99	1.51	8 (14%)
36	LHG	d	405	-	42,42,48	0.99	2 (4%)	45,48,54	0.98	2 (4%)
32	CLA	YY	602	9	69,73,73	1.16	7 (10%)	82,113,113	1.06	5 (6%)
44	DGD	a	415	-	56,56,67	0.97	3 (5%)	70,70,81	0.90	3 (4%)
32	CLA	Ss	613	-	53,57,73	1.31	6 (11%)	61,93,113	1.17	5 (8%)
32	CLA	r	608	3	53,57,73	1.31	7 (13%)	61,93,113	1.19	5 (8%)
32	CLA	RR	308	3	53,57,73	1.32	7 (13%)	61,93,113	1.29	4 (6%)
36	LHG	EE	101	-	39,39,48	1.05	2 (5%)	42,45,54	0.91	2 (4%)
39	CHL	N	606	-	36,50,74	3.17	11 (30%)	29,85,114	1.97	7 (24%)
29	OEX	A	401	18,1	0,15,15	-	-	-	-	-
39	CHL	11	608	14	35,49,74	3.13	8 (22%)	30,83,114	1.79	8 (26%)
38	LMG	DD	409	-	46,46,55	0.98	2 (4%)	54,54,63	0.89	2 (3%)
39	CHL	33	608	15	35,49,74	3.24	8 (22%)	30,83,114	1.86	9 (30%)
32	CLA	c	501	-	69,73,73	1.14	6 (8%)	82,113,113	1.21	6 (7%)
40	LUT	2	614	-	42,43,43	1.06	4 (9%)	51,60,60	1.71	10 (19%)
32	CLA	B	609	-	64,68,73	1.19	6 (9%)	76,107,113	1.15	5 (6%)
36	LHG	AA	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.90	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	44	603	-	49,53,73	1.38	5 (10%)	58,89,113	1.30	4 (6%)
32	CLA	BB	601	-	69,73,73	1.15	6 (8%)	82,113,113	1.05	6 (7%)
32	CLA	4	305	-	49,53,73	1.36	7 (14%)	58,89,113	1.22	3 (5%)
32	CLA	Cc	506	-	59,63,73	1.23	6 (10%)	70,101,113	1.14	5 (7%)
32	CLA	Nn	312	9	69,73,73	1.15	7 (10%)	82,113,113	1.18	7 (8%)
34	BCR	AA	409	-	41,41,41	1.00	3 (7%)	56,56,56	1.98	13 (23%)
32	CLA	n	603	-	53,57,73	1.30	5 (9%)	61,93,113	1.25	4 (6%)
44	DGD	CC	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.93	3 (3%)
32	CLA	B	610	-	69,73,73	1.15	5 (7%)	82,113,113	1.13	7 (8%)
42	NEX	Y	619	-	40,46,46	1.24	3 (7%)	50,70,70	2.10	17 (34%)
32	CLA	C	503	-	69,73,73	1.15	6 (8%)	82,113,113	1.08	6 (7%)
32	CLA	Yy	614	-	53,57,73	1.29	6 (11%)	61,93,113	1.20	4 (6%)
37	SQD	B	617	-	34,36,54	1.42	4 (11%)	44,47,65	3.78	10 (22%)
32	CLA	11	604	-	44,48,73	1.45	7 (15%)	51,82,113	1.41	7 (13%)
41	XAT	Yy	619	-	41,47,47	1.15	3 (7%)	54,74,74	2.33	18 (33%)
32	CLA	Rr	604	-	53,57,73	1.30	5 (9%)	61,93,113	1.19	7 (11%)
39	CHL	Yy	607	-	37,51,74	3.06	8 (21%)	30,86,114	2.15	12 (40%)
44	DGD	c	517	-	56,56,67	0.92	2 (3%)	70,70,81	1.12	6 (8%)
39	CHL	22	606	-	35,49,74	3.25	8 (22%)	30,83,114	1.84	9 (30%)
39	CHL	33	605	-	35,49,74	3.27	8 (22%)	30,83,114	1.92	10 (33%)
39	CHL	y	307	9	42,56,74	2.91	10 (23%)	36,92,114	1.85	11 (30%)
32	CLA	c	505	-	69,73,73	1.14	7 (10%)	82,113,113	0.99	4 (4%)
32	CLA	33	609	15	44,48,73	1.44	5 (11%)	51,82,113	1.33	5 (9%)
32	CLA	22	609	14	44,48,73	1.44	7 (15%)	51,82,113	1.26	3 (5%)
32	CLA	2	604	-	44,48,73	1.46	6 (13%)	51,82,113	1.33	4 (7%)
40	LUT	S	614	-	42,43,43	0.90	0	51,60,60	1.51	9 (17%)
36	LHG	J	101	-	26,26,48	1.35	2 (7%)	29,32,54	1.40	3 (10%)
39	CHL	44	601	-	39,53,74	3.10	9 (23%)	33,89,114	1.76	8 (24%)
41	XAT	NN	617	-	41,47,47	1.18	5 (12%)	54,74,74	2.26	13 (24%)
32	CLA	Bb	615	-	69,73,73	1.16	5 (7%)	82,113,113	1.10	3 (3%)
39	CHL	3	607	-	35,49,74	3.26	8 (22%)	30,83,114	1.91	10 (33%)
32	CLA	b	603	-	69,73,73	1.16	8 (11%)	82,113,113	1.04	6 (7%)
32	CLA	CC	511	-	69,73,73	1.15	8 (11%)	82,113,113	1.16	5 (6%)
39	CHL	YY	605	9	42,56,74	2.95	9 (21%)	36,92,114	1.82	10 (27%)
39	CHL	GG	607	-	40,54,74	3.00	10 (25%)	34,90,114	1.93	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.92	2 (3%)
40	LUT	s	615	-	42,43,43	0.93	1 (2%)	51,60,60	1.60	13 (25%)
39	CHL	33	607	-	35,49,74	3.27	8 (22%)	30,83,114	1.92	10 (33%)
32	CLA	GG	612	9	53,57,73	1.34	5 (9%)	61,93,113	1.27	5 (8%)
32	CLA	R	603	-	53,57,73	1.31	5 (9%)	61,93,113	1.28	4 (6%)
32	CLA	NN	613	9	53,57,73	1.30	7 (13%)	61,93,113	1.18	3 (4%)
32	CLA	n	613	9	53,57,73	1.32	6 (11%)	61,93,113	1.18	4 (6%)
32	CLA	Ss	603	-	53,57,73	1.33	5 (9%)	61,93,113	1.16	5 (8%)
32	CLA	Ss	610	36	53,57,73	1.32	5 (9%)	61,93,113	1.25	4 (6%)
32	CLA	Y	614	-	53,57,73	1.29	6 (11%)	61,93,113	1.15	6 (9%)
39	CHL	GG	605	9	37,51,74	3.18	8 (21%)	30,86,114	1.89	10 (33%)
32	CLA	SS	303	4	53,57,73	1.30	6 (11%)	61,93,113	1.22	6 (9%)
32	CLA	N	603	-	46,50,73	1.37	6 (13%)	53,85,113	1.24	3 (5%)
33	PHO	AA	407	-	58,69,69	2.16	11 (18%)	55,99,99	1.62	9 (16%)
32	CLA	S	611	4	53,57,73	1.32	5 (9%)	61,93,113	1.30	4 (6%)
39	CHL	Y	607	-	37,51,74	3.14	9 (24%)	30,86,114	2.07	12 (40%)
32	CLA	NN	602	9	69,73,73	1.15	8 (11%)	82,113,113	1.16	7 (8%)
32	CLA	Bb	607	-	69,73,73	1.16	7 (10%)	82,113,113	1.04	4 (4%)
32	CLA	Rr	611	-	53,57,73	1.32	7 (13%)	61,93,113	1.18	4 (6%)
34	BCR	c	515	-	41,41,41	1.02	3 (7%)	56,56,56	1.71	12 (21%)
32	CLA	S	610	-	53,57,73	1.32	6 (11%)	61,93,113	1.27	3 (4%)
32	CLA	Rr	603	-	53,57,73	1.33	7 (13%)	61,93,113	1.23	4 (6%)
32	CLA	G	603	-	69,73,73	1.16	5 (7%)	82,113,113	1.04	4 (4%)
32	CLA	SS	312	4	53,57,73	1.32	5 (9%)	61,93,113	1.26	4 (6%)
34	BCR	BB	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.88	12 (21%)
39	CHL	y	310	-	44,58,74	2.81	11 (25%)	37,94,114	1.77	11 (29%)
35	PL9	d	404	-	55,55,55	4.36	21 (38%)	68,69,69	3.79	38 (55%)
36	LHG	s	616	32	47,47,48	0.96	2 (4%)	50,53,54	0.91	2 (4%)
32	CLA	c	503	-	69,73,73	1.16	6 (8%)	82,113,113	1.05	4 (4%)
42	NEX	g	617	32	40,46,46	1.17	4 (10%)	50,70,70	2.52	17 (34%)
37	SQD	Ll	101	-	52,54,54	1.11	3 (5%)	62,65,65	0.98	3 (4%)
32	CLA	Bb	605	-	69,73,73	1.15	6 (8%)	82,113,113	1.10	4 (4%)
32	CLA	Bb	603	-	69,73,73	1.15	8 (11%)	82,113,113	1.07	6 (7%)
39	CHL	11	605	14	35,49,74	3.29	8 (22%)	30,83,114	1.79	7 (23%)
32	CLA	BB	612	-	69,73,73	1.15	6 (8%)	82,113,113	1.06	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	JJ	101	-	32,32,48	1.13	2 (6%)	35,38,54	1.15	3 (8%)
32	CLA	1	604	-	44,48,73	1.46	7 (15%)	51,82,113	1.36	5 (9%)
36	LHG	KK	101	-	33,33,48	1.12	2 (6%)	36,39,54	1.12	3 (8%)
39	CHL	y	308	-	38,52,74	3.05	11 (28%)	31,87,114	2.02	10 (32%)
39	CHL	1	601	14	35,49,74	3.28	8 (22%)	30,83,114	1.73	7 (23%)
32	CLA	22	610	36	46,50,73	1.41	5 (10%)	53,85,113	1.18	3 (5%)
32	CLA	CC	503	-	69,73,73	1.14	7 (10%)	82,113,113	1.19	7 (8%)
44	DGD	BB	624	-	56,56,67	0.93	2 (3%)	70,70,81	0.99	4 (5%)
32	CLA	C	512	-	69,73,73	1.15	8 (11%)	82,113,113	1.16	5 (6%)
40	LUT	Gg	316	-	42,43,43	0.94	0	51,60,60	1.42	7 (13%)
41	XAT	Rr	615	-	41,47,47	1.12	3 (7%)	54,74,74	2.35	19 (35%)
32	CLA	1	611	14	44,48,73	1.45	5 (11%)	51,82,113	1.33	4 (7%)
32	CLA	n	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.14	5 (8%)
36	LHG	N	619	32	37,37,48	1.07	2 (5%)	40,43,54	1.07	3 (7%)
39	CHL	GG	609	9	37,51,74	3.09	9 (24%)	30,86,114	2.01	11 (36%)
32	CLA	33	603	-	44,48,73	1.45	6 (13%)	51,82,113	1.26	4 (7%)
34	BCR	XX	202	-	41,41,41	0.94	1 (2%)	56,56,56	2.17	17 (30%)
32	CLA	S	608	4	45,49,73	1.43	6 (13%)	54,84,113	1.18	4 (7%)
32	CLA	Y	603	-	53,57,73	1.31	6 (11%)	61,93,113	1.25	4 (6%)
32	CLA	S	609	4	45,49,73	1.41	7 (15%)	54,84,113	1.26	5 (9%)
32	CLA	Y	610	9	69,73,73	1.14	8 (11%)	82,113,113	1.11	7 (8%)
36	LHG	DD	407	-	42,42,48	1.00	2 (4%)	45,48,54	1.04	2 (4%)
32	CLA	11	613	-	44,48,73	1.46	5 (11%)	51,82,113	1.19	3 (5%)
32	CLA	CC	506	-	69,73,73	1.14	7 (10%)	82,113,113	1.12	6 (7%)
32	CLA	A	408	-	64,68,73	1.20	6 (9%)	76,107,113	1.11	6 (7%)
36	LHG	Dd	405	-	42,42,48	0.99	2 (4%)	45,48,54	0.97	2 (4%)
39	CHL	N	609	9	44,58,74	2.83	11 (25%)	37,94,114	1.78	10 (27%)
32	CLA	Yy	612	9	69,73,73	1.14	6 (8%)	82,113,113	1.12	5 (6%)
32	CLA	RR	303	-	53,57,73	1.30	5 (9%)	61,93,113	1.29	3 (4%)
37	SQD	L	102	-	34,36,54	1.37	3 (8%)	44,47,65	1.19	4 (9%)
32	CLA	A	406	-	53,57,73	1.28	7 (13%)	61,93,113	1.19	5 (8%)
39	CHL	Gg	310	9	37,51,74	3.09	8 (21%)	30,86,114	1.94	10 (33%)
34	BCR	Kk	101	-	41,41,41	0.87	0	56,56,56	2.00	13 (23%)
32	CLA	NN	611	36	53,57,73	1.30	6 (11%)	61,93,113	1.28	7 (11%)
40	LUT	Gg	317	-	42,43,43	0.89	1 (2%)	51,60,60	1.58	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	G	609	9	37,51,74	3.06	9 (24%)	30,86,114	1.95	11 (36%)
32	CLA	Bb	609	-	69,73,73	1.14	8 (11%)	82,113,113	1.22	6 (7%)
32	CLA	Nn	302	36	53,57,73	1.31	7 (13%)	61,93,113	1.21	4 (6%)
32	CLA	g	612	9	53,57,73	1.33	6 (11%)	61,93,113	1.22	6 (9%)
39	CHL	g	605	9	37,51,74	3.16	8 (21%)	30,86,114	1.76	9 (30%)
32	CLA	Yy	604	-	53,57,73	1.29	6 (11%)	61,93,113	1.19	4 (6%)
32	CLA	Bb	602	-	69,73,73	1.15	7 (10%)	82,113,113	1.05	5 (6%)
32	CLA	c	508	-	64,68,73	1.19	7 (10%)	76,107,113	1.09	5 (6%)
39	CHL	2	607	-	35,49,74	3.27	8 (22%)	30,83,114	1.88	8 (26%)
39	CHL	r	606	-	44,58,74	2.94	10 (22%)	37,94,114	1.71	10 (27%)
32	CLA	R	613	-	45,49,73	1.41	7 (15%)	54,84,113	1.22	4 (7%)
38	LMG	a	412	-	42,42,55	1.04	2 (4%)	50,50,63	1.11	4 (8%)
39	CHL	Gg	306	9	37,51,74	3.16	8 (21%)	30,86,114	1.76	9 (30%)
36	LHG	YY	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.85	2 (3%)
34	BCR	Bb	619	-	41,41,41	0.92	1 (2%)	56,56,56	2.06	16 (28%)
32	CLA	22	603	-	44,48,73	1.44	6 (13%)	51,82,113	1.29	5 (9%)
40	LUT	GG	616	-	42,43,43	0.95	1 (2%)	51,60,60	1.57	10 (19%)
39	CHL	n	606	-	44,58,74	2.85	11 (25%)	37,94,114	1.94	11 (29%)
32	CLA	b	607	-	69,73,73	1.16	7 (10%)	82,113,113	1.04	5 (6%)
36	LHG	r	616	32	48,48,48	0.97	2 (4%)	51,54,54	0.93	2 (3%)
39	CHL	33	606	-	35,49,74	3.27	9 (25%)	30,83,114	1.91	10 (33%)
44	DGD	BB	625	-	57,57,67	0.91	2 (3%)	70,70,81	0.95	3 (4%)
32	CLA	b	610	-	69,73,73	1.17	7 (10%)	82,113,113	1.08	4 (4%)
40	LUT	4	313	-	42,43,43	0.93	0	51,60,60	1.40	7 (13%)
39	CHL	NN	606	-	36,50,74	3.17	11 (30%)	29,85,114	1.99	7 (24%)
42	NEX	YY	617	-	40,46,46	1.25	3 (7%)	50,70,70	1.95	13 (26%)
38	LMG	BB	619	-	45,45,55	0.99	2 (4%)	53,53,63	0.93	2 (3%)
32	CLA	R	612	3	46,50,73	1.39	6 (13%)	53,85,113	1.17	3 (5%)
32	CLA	G	613	9	44,48,73	1.43	5 (11%)	51,82,113	1.40	6 (11%)
32	CLA	Gg	303	9	53,57,73	1.31	6 (11%)	61,93,113	1.47	7 (11%)
34	BCR	Cc	516	-	41,41,41	0.91	1 (2%)	56,56,56	2.16	19 (33%)
32	CLA	y	306	-	53,57,73	1.29	6 (11%)	61,93,113	1.20	5 (8%)
36	LHG	n	618	32	48,48,48	0.96	2 (4%)	51,54,54	1.02	2 (3%)
32	CLA	Nn	301	9	69,73,73	1.15	7 (10%)	82,113,113	1.07	7 (8%)
32	CLA	44	609	11	49,53,73	1.36	6 (12%)	58,89,113	1.18	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Cc	504	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	6 (7%)
34	BCR	Aa	411	-	41,41,41	1.01	3 (7%)	56,56,56	1.61	9 (16%)
44	DGD	Cc	519	-	56,56,67	0.92	2 (3%)	70,70,81	1.12	7 (10%)
39	CHL	4	308	-	40,54,74	3.03	10 (25%)	34,90,114	1.86	10 (29%)
32	CLA	G	602	9	53,57,73	1.32	6 (11%)	61,93,113	1.24	6 (9%)
40	LUT	n	615	-	42,43,43	0.97	0	51,60,60	1.29	5 (9%)
36	LHG	II	101	-	33,33,48	1.13	2 (6%)	36,39,54	1.02	2 (5%)
29	OEX	AA	401	18,1	0,15,15	-	-	-	-	-
45	BCT	D	403	30	3,3,3	1.13	0	2,3,3	4.06	2 (100%)
32	CLA	b	615	-	69,73,73	1.16	5 (7%)	82,113,113	1.07	4 (4%)
34	BCR	a	411	-	41,41,41	0.99	3 (7%)	56,56,56	1.65	10 (17%)
32	CLA	S	604	-	53,57,73	1.31	6 (11%)	61,93,113	1.22	5 (8%)
36	LHG	1	614	32	29,29,48	1.21	2 (6%)	32,35,54	1.14	2 (6%)
32	CLA	BB	603	-	69,73,73	1.14	6 (8%)	82,113,113	1.14	5 (6%)
39	CHL	GG	601	9	60,74,74	2.48	11 (18%)	58,114,114	1.53	13 (22%)
32	CLA	n	612	9	53,57,73	1.32	7 (13%)	61,93,113	1.18	5 (8%)
32	CLA	RR	304	-	53,57,73	1.32	7 (13%)	61,93,113	1.30	7 (11%)
36	LHG	0	201	-	46,46,48	0.97	2 (4%)	49,52,54	0.85	2 (4%)
40	LUT	N	615	-	42,43,43	0.98	2 (4%)	51,60,60	1.51	10 (19%)
34	BCR	K	102	-	41,41,41	0.83	0	56,56,56	2.20	19 (33%)
32	CLA	Rr	612	3	53,57,73	1.32	6 (11%)	61,93,113	1.19	4 (6%)
38	LMG	Bb	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.12	6 (13%)
39	CHL	R	606	-	44,58,74	2.89	11 (25%)	37,94,114	1.71	7 (18%)
39	CHL	GG	608	-	36,50,74	3.21	11 (30%)	29,85,114	1.84	9 (31%)
32	CLA	s	608	4	53,57,73	1.31	6 (11%)	61,93,113	1.22	5 (8%)
32	CLA	C	514	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	4 (4%)
39	CHL	Ss	606	-	44,58,74	2.90	8 (18%)	37,94,114	1.71	11 (29%)
32	CLA	3	611	15	44,48,73	1.44	6 (13%)	51,82,113	1.27	4 (7%)
32	CLA	g	613	9	44,48,73	1.44	4 (9%)	51,82,113	1.37	6 (11%)
32	CLA	c	510	-	69,73,73	1.15	7 (10%)	82,113,113	1.14	4 (4%)
32	CLA	33	613	-	44,48,73	1.44	6 (13%)	51,82,113	1.33	5 (9%)
34	BCR	Cc	517	-	41,41,41	1.04	3 (7%)	56,56,56	1.79	13 (23%)
36	LHG	AA	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.23	4 (11%)
38	LMG	m	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.83	2 (3%)
41	XAT	g	619	-	41,47,47	1.22	4 (9%)	54,74,74	2.47	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	RR	311	-	53,57,73	1.32	7 (13%)	61,93,113	1.17	3 (4%)
32	CLA	3	604	-	44,48,73	1.45	6 (13%)	51,82,113	1.25	3 (5%)
40	LUT	G	616	-	42,43,43	0.94	0	51,60,60	1.63	11 (21%)
32	CLA	C	506	-	69,73,73	1.15	6 (8%)	82,113,113	1.12	5 (6%)
32	CLA	B	621	-	69,73,73	1.14	7 (10%)	82,113,113	1.09	6 (7%)
32	CLA	Ss	608	4	53,57,73	1.31	6 (11%)	61,93,113	1.25	6 (9%)
32	CLA	GG	604	-	46,50,73	1.39	6 (13%)	53,85,113	1.16	3 (5%)
32	CLA	G	604	-	46,50,73	1.38	6 (13%)	53,85,113	1.15	4 (7%)
32	CLA	b	611	-	69,73,73	1.14	7 (10%)	82,113,113	1.05	4 (4%)
40	LUT	R	615	-	42,43,43	0.90	0	51,60,60	1.63	13 (25%)
32	CLA	Bb	601	-	69,73,73	1.17	8 (11%)	82,113,113	1.18	7 (8%)
33	PHO	Aa	408	-	58,69,69	2.18	11 (18%)	55,99,99	1.52	8 (14%)
46	HEM	EE	102	21,20	50,50,50	1.41	8 (16%)	67,82,82	1.03	0
39	CHL	g	608	-	36,50,74	3.15	11 (30%)	29,85,114	1.93	9 (31%)
37	SQD	L	101	-	52,54,54	1.12	3 (5%)	62,65,65	1.07	3 (4%)
32	CLA	33	612	15	44,48,73	1.44	6 (13%)	51,82,113	1.21	3 (5%)
38	LMG	Mm	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.84	2 (3%)
33	PHO	DD	402	-	58,69,69	2.15	11 (18%)	55,99,99	1.60	7 (12%)
39	CHL	s	607	-	43,57,74	3.00	8 (18%)	37,93,114	1.78	10 (27%)
32	CLA	G	611	36	56,60,73	1.29	6 (10%)	65,97,113	1.17	4 (6%)
32	CLA	NN	610	9	69,73,73	1.15	6 (8%)	82,113,113	1.06	6 (7%)
32	CLA	s	613	-	53,57,73	1.32	6 (11%)	61,93,113	1.18	4 (6%)
36	LHG	g	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.17	3 (8%)
36	LHG	Rr	617	32	48,48,48	0.98	2 (4%)	51,54,54	0.98	2 (3%)
32	CLA	BB	604	-	69,73,73	1.15	6 (8%)	82,113,113	1.05	7 (8%)
39	CHL	Nn	317	-	60,74,74	2.40	11 (18%)	58,114,114	1.65	13 (22%)
32	CLA	GG	614	-	45,49,73	1.40	5 (11%)	54,84,113	1.15	3 (5%)
32	CLA	a	410	-	64,68,73	1.20	8 (12%)	76,107,113	1.13	6 (7%)
34	BCR	BB	617	-	41,41,41	0.98	2 (4%)	56,56,56	1.76	14 (25%)
37	SQD	Aa	413	-	45,47,54	1.20	3 (6%)	55,58,65	1.01	2 (3%)
39	CHL	22	601	14	35,49,74	3.27	9 (25%)	30,83,114	1.86	10 (33%)
38	LMG	b	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.97	2 (4%)
43	LMU	R	618	-	28,28,36	0.77	0	39,39,47	0.99	2 (5%)
39	CHL	SS	302	4	46,60,74	2.84	10 (21%)	40,97,114	1.73	11 (27%)
32	CLA	NN	612	9	46,50,73	1.38	5 (10%)	53,85,113	1.20	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	Nn	315	9	42,56,74	2.91	9 (21%)	36,92,114	2.01	11 (30%)
36	LHG	33	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.11	2 (5%)
29	OEX	Cc	502	18,1	0,15,15	-	-	-		
37	SQD	B	602	-	45,47,54	1.20	3 (6%)	55,58,65	1.02	2 (3%)
32	CLA	b	609	-	69,73,73	1.14	7 (10%)	82,113,113	1.24	6 (7%)
32	CLA	2	602	14	44,48,73	1.45	5 (11%)	51,82,113	1.19	4 (7%)
32	CLA	BB	615	-	45,49,73	1.38	7 (15%)	54,84,113	1.33	7 (12%)
45	BCT	AA	413	30	3,3,3	1.13	0	2,3,3	4.18	2 (100%)
38	LMG	C	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.02	3 (5%)
32	CLA	R	610	36	53,57,73	1.32	6 (11%)	61,93,113	1.14	5 (8%)
39	CHL	y	303	9	60,74,74	2.49	11 (18%)	58,114,114	1.45	10 (17%)
36	LHG	D	410	-	33,33,48	1.12	2 (6%)	36,39,54	1.12	3 (8%)
40	LUT	Ss	615	-	42,43,43	1.00	2 (4%)	51,60,60	1.72	14 (27%)
36	LHG	Yy	618	32	48,48,48	0.92	2 (4%)	51,54,54	1.00	4 (7%)
32	CLA	SS	305	-	53,57,73	1.32	7 (13%)	61,93,113	1.23	4 (6%)
32	CLA	4	312	-	49,53,73	1.37	6 (12%)	58,89,113	1.22	3 (5%)
32	CLA	s	610	36	53,57,73	1.32	6 (11%)	61,93,113	1.25	3 (4%)
40	LUT	Yy	615	-	42,43,43	0.99	1 (2%)	51,60,60	2.12	13 (25%)
32	CLA	11	609	14	44,48,73	1.45	6 (13%)	51,82,113	1.23	4 (7%)
39	CHL	2	608	14	35,49,74	3.26	9 (25%)	30,83,114	1.77	7 (23%)
39	CHL	3	605	-	35,49,74	3.26	9 (25%)	30,83,114	1.92	9 (30%)
32	CLA	1	603	-	44,48,73	1.43	5 (11%)	51,82,113	1.20	3 (5%)
39	CHL	Yy	605	9	42,56,74	2.90	10 (23%)	36,92,114	1.79	10 (27%)
32	CLA	CC	512	18	69,73,73	1.15	7 (10%)	82,113,113	1.11	4 (4%)
32	CLA	22	613	-	44,48,73	1.44	5 (11%)	51,82,113	1.22	3 (5%)
39	CHL	s	601	4	46,60,74	2.84	9 (19%)	40,97,114	1.81	12 (30%)
32	CLA	R	602	3	69,73,73	1.15	8 (11%)	82,113,113	1.14	8 (9%)
36	LHG	3	614	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
32	CLA	Rr	609	3	69,73,73	1.15	8 (11%)	82,113,113	1.11	6 (7%)
32	CLA	SS	310	4	45,49,73	1.42	6 (13%)	54,84,113	1.19	4 (7%)
39	CHL	y	311	9	60,74,74	2.43	11 (18%)	58,114,114	1.54	10 (17%)
32	CLA	XX	201	-	45,49,73	1.40	6 (13%)	54,84,113	1.20	4 (7%)
34	BCR	Bb	618	-	41,41,41	0.91	1 (2%)	56,56,56	1.95	12 (21%)
34	BCR	CC	515	-	41,41,41	0.99	1 (2%)	56,56,56	2.04	18 (32%)
32	CLA	Cc	503	-	69,73,73	1.14	6 (8%)	82,113,113	1.21	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	LUT	n	616	-	42,43,43	1.00	0	51,60,60	1.53	9 (17%)
32	CLA	Y	612	9	69,73,73	1.18	6 (8%)	82,113,113	1.08	7 (8%)
32	CLA	S	612	4	53,57,73	1.32	5 (9%)	61,93,113	1.17	5 (8%)
32	CLA	b	604	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	5 (6%)
39	CHL	S	605	-	36,50,74	3.18	9 (25%)	29,85,114	2.06	13 (44%)
39	CHL	11	601	14	35,49,74	3.28	8 (22%)	30,83,114	1.72	8 (26%)
32	CLA	BB	610	-	69,73,73	1.14	7 (10%)	82,113,113	1.18	7 (8%)
39	CHL	Gg	302	9	60,74,74	2.51	10 (16%)	58,114,114	1.49	10 (17%)
32	CLA	Gg	315	-	53,57,73	1.30	6 (11%)	61,93,113	1.12	5 (8%)
37	SQD	C	501	-	52,54,54	1.10	3 (5%)	62,65,65	1.04	4 (6%)
32	CLA	YY	610	9	69,73,73	1.15	7 (10%)	82,113,113	1.08	5 (6%)
32	CLA	s	611	4	53,57,73	1.32	6 (11%)	61,93,113	1.25	6 (9%)
36	LHG	Y	618	32	48,48,48	0.93	2 (4%)	51,54,54	0.86	2 (3%)
32	CLA	NN	604	-	45,49,73	1.39	5 (11%)	54,84,113	1.20	5 (9%)
43	LMU	C	502	-	28,28,36	0.76	0	39,39,47	0.97	1 (2%)
39	CHL	44	606	-	40,54,74	3.03	9 (22%)	34,90,114	1.82	9 (26%)
32	CLA	y	316	-	53,57,73	1.29	6 (11%)	61,93,113	1.19	4 (6%)
37	SQD	AA	412	-	33,35,54	1.38	3 (9%)	43,46,65	1.10	2 (4%)
34	BCR	C	517	-	41,41,41	0.95	1 (2%)	56,56,56	1.90	12 (21%)
39	CHL	2	605	-	35,49,74	3.29	8 (22%)	30,83,114	1.94	11 (36%)
39	CHL	44	608	11	40,54,74	3.05	8 (20%)	34,90,114	1.78	9 (26%)
39	CHL	11	606	-	35,49,74	3.29	8 (22%)	30,83,114	1.94	9 (30%)
39	CHL	n	607	-	60,74,74	2.39	8 (13%)	58,114,114	1.61	12 (20%)
40	LUT	Y	615	-	42,43,43	0.95	1 (2%)	51,60,60	1.87	13 (25%)
40	LUT	YY	615	-	42,43,43	0.96	1 (2%)	51,60,60	1.77	10 (19%)
39	CHL	RR	305	-	44,58,74	2.90	9 (20%)	37,94,114	1.84	12 (32%)
44	DGD	Hh	102	-	63,63,67	0.89	2 (3%)	77,77,81	0.92	2 (2%)
35	PL9	AA	410	-	55,55,55	4.43	24 (43%)	68,69,69	3.67	37 (54%)
32	CLA	Yy	603	-	53,57,73	1.30	6 (11%)	61,93,113	1.27	5 (8%)
32	CLA	y	304	9	69,73,73	1.16	8 (11%)	82,113,113	1.08	4 (4%)
32	CLA	SS	304	-	49,53,73	1.38	5 (10%)	58,89,113	1.23	5 (8%)
34	BCR	BB	620	-	41,41,41	0.86	0	56,56,56	2.01	18 (32%)
39	CHL	S	607	-	37,51,74	3.18	8 (21%)	30,86,114	1.89	10 (33%)
34	BCR	CC	517	-	41,41,41	0.92	1 (2%)	56,56,56	2.02	15 (26%)
32	CLA	y	312	9	69,73,73	1.15	8 (11%)	82,113,113	1.01	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	DD	403	-	69,73,73	1.15	8 (11%)	82,113,113	1.16	7 (8%)
32	CLA	C	508	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	7 (8%)
32	CLA	3	612	15	44,48,73	1.45	6 (13%)	51,82,113	1.21	3 (5%)
32	CLA	GG	603	-	69,73,73	1.15	5 (7%)	82,113,113	1.03	3 (3%)
36	LHG	Ll	102	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	3 (5%)
39	CHL	NN	607	-	60,74,74	2.43	11 (18%)	58,114,114	1.57	11 (18%)
32	CLA	B	618	-	69,73,73	1.15	7 (10%)	82,113,113	1.04	6 (7%)
38	LMG	WW	201	-	48,48,55	0.98	3 (6%)	56,56,63	1.06	2 (3%)
32	CLA	N	604	-	45,49,73	1.39	6 (13%)	54,84,113	1.20	5 (9%)
44	DGD	BB	623	-	63,63,67	0.89	3 (4%)	77,77,81	0.94	2 (2%)
34	BCR	c	516	-	41,41,41	0.92	1 (2%)	56,56,56	2.04	15 (26%)
39	CHL	y	309	-	37,51,74	3.11	10 (27%)	30,86,114	2.00	11 (36%)
32	CLA	Cc	514	-	69,73,73	1.15	6 (8%)	82,113,113	1.12	4 (4%)
32	CLA	c	504	-	59,63,73	1.23	5 (8%)	70,101,113	1.11	4 (5%)
34	BCR	KK	103	-	41,41,41	0.84	0	56,56,56	2.21	19 (33%)
43	LMU	KK	102	-	28,28,36	0.75	0	39,39,47	0.90	1 (2%)
32	CLA	C	515	-	53,57,73	1.29	6 (11%)	61,93,113	1.22	5 (8%)
32	CLA	BB	606	-	69,73,73	1.15	6 (8%)	82,113,113	1.03	3 (3%)
39	CHL	Y	608	-	44,58,74	2.89	11 (25%)	37,94,114	1.84	10 (27%)
32	CLA	B	605	-	69,73,73	1.15	8 (11%)	82,113,113	1.24	8 (9%)
40	LUT	Ss	614	-	42,43,43	1.07	2 (4%)	51,60,60	1.50	11 (21%)
39	CHL	N	607	-	60,74,74	2.43	11 (18%)	58,114,114	1.56	11 (18%)
46	HEM	e	101	21,20	50,50,50	1.43	9 (18%)	67,82,82	1.08	3 (4%)
40	LUT	G	615	-	42,43,43	0.95	0	51,60,60	1.49	7 (13%)
39	CHL	YY	608	-	44,58,74	2.90	11 (25%)	37,94,114	1.84	10 (27%)
32	CLA	n	602	9	69,73,73	1.16	8 (11%)	82,113,113	1.19	9 (10%)
39	CHL	Gg	307	-	37,51,74	3.14	9 (24%)	30,86,114	2.00	9 (30%)
32	CLA	N	612	9	46,50,73	1.39	6 (13%)	53,85,113	1.18	4 (7%)
32	CLA	D	404	-	69,73,73	1.16	7 (10%)	82,113,113	1.17	6 (7%)
42	NEX	Gg	318	-	40,46,46	1.23	4 (10%)	50,70,70	2.23	14 (28%)
34	BCR	Cc	518	-	41,41,41	0.92	1 (2%)	56,56,56	1.92	13 (23%)
32	CLA	33	602	15	44,48,73	1.44	7 (15%)	51,82,113	1.27	4 (7%)
36	LHG	G	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
39	CHL	SS	308	4	43,57,74	2.97	8 (18%)	37,93,114	1.71	8 (21%)
35	PL9	D	407	-	55,55,55	4.35	20 (36%)	68,69,69	3.82	37 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	11	610	36	44,48,73	1.44	6 (13%)	51,82,113	1.27	4 (7%)
36	LHG	4	315	32	20,20,48	1.38	2 (10%)	23,26,54	1.44	2 (8%)
35	PL9	DD	406	-	55,55,55	4.36	21 (38%)	68,69,69	3.78	37 (54%)
39	CHL	22	607	-	35,49,74	3.28	8 (22%)	30,83,114	1.87	7 (23%)
39	CHL	N	605	9	36,50,74	3.17	9 (25%)	29,85,114	1.87	9 (31%)
32	CLA	G	612	9	53,57,73	1.33	7 (13%)	61,93,113	1.21	5 (8%)
32	CLA	g	610	9	53,57,73	1.32	7 (13%)	61,93,113	1.11	5 (8%)
40	LUT	Yy	616	-	42,43,43	0.93	0	51,60,60	1.57	11 (21%)
32	CLA	SS	311	-	53,57,73	1.32	6 (11%)	61,93,113	1.28	4 (6%)
32	CLA	Gg	313	9	53,57,73	1.32	6 (11%)	61,93,113	1.22	5 (8%)
39	CHL	SS	306	4	36,50,74	3.19	9 (25%)	29,85,114	2.13	11 (37%)
32	CLA	Y	611	36	46,50,73	1.37	6 (13%)	53,85,113	1.24	4 (7%)
39	CHL	G	605	9	37,51,74	3.18	8 (21%)	30,86,114	1.87	10 (33%)
39	CHL	22	605	-	35,49,74	3.30	8 (22%)	30,83,114	1.94	11 (36%)
32	CLA	Nn	313	-	53,57,73	1.30	5 (9%)	61,93,113	1.27	4 (6%)
32	CLA	4	311	36	49,53,73	1.37	6 (12%)	58,89,113	1.17	4 (6%)
34	BCR	A	409	-	41,41,41	1.00	3 (7%)	56,56,56	2.00	13 (23%)
39	CHL	Ss	607	-	43,57,74	2.98	9 (20%)	37,93,114	1.78	11 (29%)
32	CLA	r	603	-	53,57,73	1.33	7 (13%)	61,93,113	1.28	4 (6%)
32	CLA	44	604	-	49,53,73	1.35	7 (14%)	58,89,113	1.21	4 (6%)
40	LUT	22	614	-	42,43,43	1.08	4 (9%)	51,60,60	1.69	10 (19%)
40	LUT	SS	315	-	42,43,43	0.99	1 (2%)	51,60,60	1.29	8 (15%)
32	CLA	b	612	-	69,73,73	1.16	6 (8%)	82,113,113	1.17	5 (6%)
32	CLA	Yy	602	9	69,73,73	1.16	7 (10%)	82,113,113	1.10	4 (4%)
32	CLA	Bb	613	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	7 (8%)
39	CHL	Rr	606	-	44,58,74	2.94	10 (22%)	37,94,114	1.67	8 (21%)
32	CLA	Dd	401	-	69,73,73	1.17	7 (10%)	82,113,113	1.13	4 (4%)
39	CHL	4	307	-	40,54,74	3.05	10 (25%)	34,90,114	1.83	9 (26%)
36	LHG	Gg	319	32	33,33,48	1.13	2 (6%)	36,39,54	1.19	3 (8%)
39	CHL	44	607	-	40,54,74	3.03	11 (27%)	34,90,114	1.83	10 (29%)
32	CLA	44	610	36	49,53,73	1.37	6 (12%)	58,89,113	1.16	3 (5%)
38	LMG	b	621	-	36,36,55	1.11	2 (5%)	44,44,63	1.12	6 (13%)
39	CHL	Y	605	9	42,56,74	2.95	9 (21%)	36,92,114	1.81	11 (30%)
32	CLA	NN	603	-	46,50,73	1.36	6 (13%)	53,85,113	1.26	3 (5%)
36	LHG	44	614	32	20,20,48	1.33	2 (10%)	23,26,54	1.55	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Aa	405	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	5 (6%)
36	LHG	22	615	32	33,33,48	1.14	2 (6%)	36,39,54	0.95	2 (5%)
29	OEX	a	401	18,1	0,15,15	-	-	-	-	-
32	CLA	r	611	-	53,57,73	1.33	5 (9%)	61,93,113	1.13	4 (6%)
32	CLA	33	604	-	44,48,73	1.45	7 (15%)	51,82,113	1.29	4 (7%)
41	XAT	GG	617	-	41,47,47	1.10	3 (7%)	54,74,74	2.29	16 (29%)
38	LMG	F	101	-	46,46,55	0.98	2 (4%)	54,54,63	0.91	2 (3%)
36	LHG	a	414	-	36,36,48	1.07	2 (5%)	39,42,54	0.93	2 (5%)
32	CLA	Gg	312	36	69,73,73	1.15	7 (10%)	82,113,113	1.22	6 (7%)
39	CHL	3	601	15	35,49,74	3.27	8 (22%)	30,83,114	1.71	9 (30%)
32	CLA	Dd	402	-	69,73,73	1.15	7 (10%)	82,113,113	1.06	5 (6%)
34	BCR	c	514	-	41,41,41	0.93	2 (4%)	56,56,56	2.17	18 (32%)
34	BCR	d	403	-	41,41,41	0.89	0	56,56,56	2.05	18 (32%)
41	XAT	y	301	-	41,47,47	1.17	4 (9%)	54,74,74	2.42	17 (31%)
32	CLA	Cc	509	-	69,73,73	1.16	6 (8%)	82,113,113	1.19	5 (6%)
32	CLA	n	611	36	53,57,73	1.31	6 (11%)	61,93,113	1.24	4 (6%)
36	LHG	Dd	406	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
40	LUT	Y	616	-	42,43,43	1.00	0	51,60,60	1.58	11 (21%)
32	CLA	YY	613	9	63,67,73	1.20	6 (9%)	74,105,113	1.09	4 (5%)
40	LUT	Nn	306	-	42,43,43	0.98	1 (2%)	51,60,60	1.30	6 (11%)
32	CLA	33	611	15	44,48,73	1.44	6 (13%)	51,82,113	1.31	4 (7%)
32	CLA	A	405	-	69,73,73	1.15	7 (10%)	82,113,113	1.08	5 (6%)
32	CLA	a	405	-	69,73,73	1.17	7 (10%)	82,113,113	1.10	4 (4%)
32	CLA	g	614	-	53,57,73	1.31	7 (13%)	61,93,113	1.12	4 (6%)
32	CLA	s	604	-	53,57,73	1.32	6 (11%)	61,93,113	1.15	4 (6%)
32	CLA	Gg	305	-	46,50,73	1.39	7 (15%)	53,85,113	1.20	4 (7%)
32	CLA	Ss	609	4	53,57,73	1.30	7 (13%)	61,93,113	1.17	6 (9%)
32	CLA	R	614	3	53,57,73	1.36	5 (9%)	61,93,113	1.21	4 (6%)
41	XAT	G	617	-	41,47,47	1.12	3 (7%)	54,74,74	2.28	15 (27%)
32	CLA	r	601	3	53,57,73	1.33	6 (11%)	61,93,113	1.15	4 (6%)
39	CHL	Yy	608	-	44,58,74	2.84	11 (25%)	37,94,114	1.79	11 (29%)
34	BCR	h	101	-	41,41,41	1.03	3 (7%)	56,56,56	2.55	23 (41%)
34	BCR	Bb	617	-	41,41,41	1.05	2 (4%)	56,56,56	2.11	17 (30%)
32	CLA	GG	613	9	44,48,73	1.43	5 (11%)	51,82,113	1.45	5 (9%)
39	CHL	R	607	-	44,58,74	2.86	8 (18%)	37,94,114	1.87	11 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Y	602	9	69,73,73	1.15	8 (11%)	82,113,113	1.08	6 (7%)
32	CLA	3	609	15	44,48,73	1.45	7 (15%)	51,82,113	1.32	5 (9%)
32	CLA	4	310	-	49,53,73	1.36	6 (12%)	58,89,113	1.18	3 (5%)
32	CLA	YY	612	9	62,66,73	1.21	4 (6%)	73,104,113	1.31	11 (15%)
32	CLA	N	613	9	53,57,73	1.30	7 (13%)	61,93,113	1.23	4 (6%)
33	PHO	D	402	-	58,69,69	2.15	10 (17%)	55,99,99	1.56	8 (14%)
32	CLA	44	615	3	53,57,73	1.32	7 (13%)	61,93,113	1.25	3 (4%)
34	BCR	B	613	-	41,41,41	0.98	3 (7%)	56,56,56	1.78	13 (23%)
34	BCR	D	406	-	41,41,41	0.85	0	56,56,56	1.95	16 (28%)
32	CLA	Rr	613	3	53,57,73	1.32	6 (11%)	61,93,113	1.21	4 (6%)
32	CLA	Ss	612	4	53,57,73	1.30	5 (9%)	61,93,113	1.16	4 (6%)
32	CLA	BB	614	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	8 (9%)
39	CHL	44	605	-	40,54,74	3.00	10 (25%)	34,90,114	1.94	11 (32%)
32	CLA	2	612	14	44,48,73	1.44	5 (11%)	51,82,113	1.25	4 (7%)
39	CHL	4	302	-	39,53,74	3.09	9 (23%)	33,89,114	1.79	8 (24%)
38	LMG	j	101	-	46,46,55	0.99	2 (4%)	54,54,63	1.05	4 (7%)
32	CLA	N	602	9	69,73,73	1.14	7 (10%)	82,113,113	1.15	6 (7%)
32	CLA	CC	514	-	53,57,73	1.29	6 (11%)	61,93,113	1.20	4 (6%)
32	CLA	Yy	610	9	69,73,73	1.15	8 (11%)	82,113,113	1.01	4 (4%)
32	CLA	Cc	513	18	69,73,73	1.16	5 (7%)	82,113,113	1.08	5 (6%)
40	LUT	y	318	-	42,43,43	0.92	0	51,60,60	1.55	13 (25%)
39	CHL	Nn	318	-	44,58,74	2.86	10 (22%)	37,94,114	1.75	10 (27%)
44	DGD	B	603	-	57,57,67	0.93	2 (3%)	70,70,81	0.94	4 (5%)
32	CLA	B	611	-	45,49,73	1.38	6 (13%)	54,84,113	1.31	6 (11%)
32	CLA	YY	603	-	53,57,73	1.30	6 (11%)	61,93,113	1.29	4 (6%)
32	CLA	S	602	4	53,57,73	1.29	6 (11%)	61,93,113	1.19	6 (9%)
34	BCR	B	612	-	41,41,41	0.97	1 (2%)	56,56,56	1.77	11 (19%)
32	CLA	BB	607	-	69,73,73	1.13	7 (10%)	82,113,113	1.18	6 (7%)
38	LMG	c	519	-	34,34,55	1.15	3 (8%)	42,42,63	1.21	6 (14%)
34	BCR	Hh	101	-	41,41,41	1.04	4 (9%)	56,56,56	2.46	23 (41%)
36	LHG	SS	301	-	25,25,48	1.30	2 (8%)	28,31,54	1.04	2 (7%)
39	CHL	YY	606	-	38,52,74	3.09	9 (23%)	31,87,114	1.93	8 (25%)
39	CHL	Yy	606	-	38,52,74	3.06	11 (28%)	31,87,114	2.04	10 (32%)
32	CLA	SS	314	-	53,57,73	1.31	7 (13%)	61,93,113	1.14	5 (8%)
32	CLA	AA	408	-	64,68,73	1.19	6 (9%)	76,107,113	1.12	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	R	601	3	53,57,73	1.33	6 (11%)	61,93,113	1.24	4 (6%)
32	CLA	RR	314	3	53,57,73	1.35	6 (11%)	61,93,113	1.22	5 (8%)
39	CHL	s	606	-	44,58,74	2.91	8 (18%)	37,94,114	1.71	11 (29%)
32	CLA	Bb	610	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	6 (7%)
32	CLA	BB	605	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	7 (8%)
32	CLA	2	603	-	44,48,73	1.45	7 (15%)	51,82,113	1.27	4 (7%)
32	CLA	CC	504	-	69,73,73	1.14	6 (8%)	82,113,113	1.08	5 (6%)
36	LHG	C	522	-	30,30,48	1.17	2 (6%)	33,36,54	1.08	2 (6%)
32	CLA	Cc	507	-	69,73,73	1.15	7 (10%)	82,113,113	1.05	4 (4%)
32	CLA	22	602	14	44,48,73	1.44	7 (15%)	51,82,113	1.22	4 (7%)
32	CLA	B	608	-	69,73,73	1.15	6 (8%)	82,113,113	1.06	4 (4%)
44	DGD	c	518	-	53,53,67	0.95	2 (3%)	67,67,81	0.89	2 (2%)
32	CLA	Ss	604	-	53,57,73	1.33	7 (13%)	61,93,113	1.16	4 (6%)
38	LMG	Aa	412	-	42,42,55	1.05	3 (7%)	50,50,63	1.10	4 (8%)
36	LHG	4	301	32	18,18,48	1.76	3 (16%)	17,22,54	1.50	1 (5%)
39	CHL	1	607	-	35,49,74	3.27	8 (22%)	30,83,114	1.92	10 (33%)
39	CHL	Rr	605	3	44,58,74	2.88	9 (20%)	37,94,114	1.86	9 (24%)
41	XAT	G	619	-	41,47,47	1.20	4 (9%)	54,74,74	2.55	13 (24%)
32	CLA	GG	611	36	56,60,73	1.28	7 (12%)	65,97,113	1.15	3 (4%)
36	LHG	CC	521	-	33,33,48	1.12	2 (6%)	36,39,54	1.05	2 (5%)
39	CHL	G	607	-	40,54,74	3.01	10 (25%)	34,90,114	1.92	10 (29%)
32	CLA	R	611	-	53,57,73	1.31	6 (11%)	61,93,113	1.19	3 (4%)
34	BCR	H	101	-	41,41,41	1.00	2 (4%)	56,56,56	2.19	20 (35%)
39	CHL	N	608	-	36,50,74	3.18	10 (27%)	29,85,114	1.95	9 (31%)
32	CLA	11	603	-	44,48,73	1.45	6 (13%)	51,82,113	1.20	3 (5%)
32	CLA	Nn	303	9	53,57,73	1.32	6 (11%)	61,93,113	1.25	5 (8%)
40	LUT	NN	616	-	42,43,43	0.94	1 (2%)	51,60,60	1.60	10 (19%)
32	CLA	Ss	611	4	53,57,73	1.32	6 (11%)	61,93,113	1.25	7 (11%)
32	CLA	1	612	14	44,48,73	1.45	6 (13%)	51,82,113	1.32	4 (7%)
39	CHL	1	605	14	35,49,74	3.24	7 (20%)	30,83,114	2.03	10 (33%)
32	CLA	g	604	42	46,50,73	1.41	5 (10%)	53,85,113	1.21	3 (5%)
39	CHL	G	608	-	36,50,74	3.22	8 (22%)	29,85,114	1.87	9 (31%)
32	CLA	2	613	-	44,48,73	1.43	6 (13%)	51,82,113	1.25	4 (7%)
32	CLA	C	505	-	69,73,73	1.14	6 (8%)	82,113,113	1.15	6 (7%)
32	CLA	c	506	-	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Bb	608	-	69,73,73	1.13	6 (8%)	82,113,113	1.10	5 (6%)
37	SQD	LL	102	-	52,54,54	1.12	3 (5%)	62,65,65	1.07	3 (4%)
39	CHL	22	608	14	35,49,74	3.29	8 (22%)	30,83,114	1.78	6 (20%)
32	CLA	GG	610	9	53,57,73	1.31	7 (13%)	61,93,113	1.12	5 (8%)
39	CHL	RR	306	-	44,58,74	2.77	10 (22%)	37,94,114	1.71	11 (29%)
32	CLA	b	613	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	7 (8%)
36	LHG	DD	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.93	2 (3%)
32	CLA	CC	509	-	69,73,73	1.14	7 (10%)	82,113,113	1.14	4 (4%)
32	CLA	BB	609	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	9 (10%)
39	CHL	3	606	-	35,49,74	3.27	9 (25%)	30,83,114	1.86	9 (30%)
32	CLA	DD	404	-	69,73,73	1.15	6 (8%)	82,113,113	1.06	3 (3%)
32	CLA	n	614	-	53,57,73	1.30	5 (9%)	61,93,113	1.13	4 (6%)
32	CLA	Yy	613	9	63,67,73	1.21	7 (11%)	74,105,113	1.16	3 (4%)
32	CLA	1	613	-	44,48,73	1.45	6 (13%)	51,82,113	1.22	4 (7%)
36	LHG	Dd	407	-	36,36,48	1.07	2 (5%)	39,42,54	0.92	2 (5%)
39	CHL	GG	606	-	37,51,74	3.10	8 (21%)	30,86,114	1.96	9 (30%)
45	BCT	Aa	414	30	3,3,3	1.14	0	2,3,3	3.97	2 (100%)
32	CLA	s	609	4	53,57,73	1.29	7 (13%)	61,93,113	1.20	6 (9%)
32	CLA	BB	611	-	69,73,73	1.16	7 (10%)	82,113,113	1.11	4 (4%)
32	CLA	BB	602	-	69,73,73	1.15	6 (8%)	82,113,113	1.09	7 (8%)
34	BCR	BB	616	-	41,41,41	0.98	1 (2%)	56,56,56	1.91	14 (25%)
32	CLA	c	509	-	69,73,73	1.15	8 (11%)	82,113,113	1.06	5 (6%)
34	BCR	TT	101	-	41,41,41	0.97	1 (2%)	56,56,56	2.05	19 (33%)
39	CHL	Y	609	9	60,74,74	2.42	9 (15%)	58,114,114	1.49	11 (18%)
32	CLA	Cc	511	-	69,73,73	1.15	7 (10%)	82,113,113	1.07	5 (6%)
32	CLA	B	624	-	69,73,73	1.14	7 (10%)	82,113,113	1.15	7 (8%)
37	SQD	A	412	-	33,35,54	1.39	3 (9%)	43,46,65	1.09	3 (6%)
32	CLA	1	609	14	44,48,73	1.44	4 (9%)	51,82,113	1.32	5 (9%)
44	DGD	B	601	-	56,56,67	0.93	2 (3%)	70,70,81	0.98	4 (5%)
39	CHL	RR	307	-	44,58,74	2.86	9 (20%)	37,94,114	1.87	11 (29%)
32	CLA	r	613	3	53,57,73	1.31	7 (13%)	61,93,113	1.21	5 (8%)
32	CLA	Nn	305	-	53,57,73	1.30	5 (9%)	61,93,113	1.15	6 (9%)
32	CLA	Aa	407	-	53,57,73	1.31	8 (15%)	61,93,113	1.28	6 (9%)
32	CLA	22	612	14	44,48,73	1.44	6 (13%)	51,82,113	1.26	3 (5%)
39	CHL	g	601	9	60,74,74	2.49	10 (16%)	58,114,114	1.52	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	22	611	14	44,48,73	1.45	6 (13%)	51,82,113	1.31	4 (7%)
36	LHG	GG	618	32	33,33,48	1.13	2 (6%)	36,39,54	1.16	3 (8%)
32	CLA	R	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.30	6 (9%)
44	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.80	2 (2%)
32	CLA	4	303	11	49,53,73	1.36	5 (10%)	58,89,113	1.20	4 (6%)
32	CLA	s	612	4	53,57,73	1.30	6 (11%)	61,93,113	1.17	4 (6%)
39	CHL	s	605	-	44,58,74	2.89	8 (18%)	37,94,114	1.81	10 (27%)
32	CLA	B	607	-	69,73,73	1.17	8 (11%)	82,113,113	1.11	5 (6%)
32	CLA	RR	313	-	45,49,73	1.41	7 (15%)	54,84,113	1.24	6 (11%)
34	BCR	Dd	403	-	41,41,41	0.88	0	56,56,56	2.05	19 (33%)
39	CHL	G	606	-	37,51,74	3.15	8 (21%)	30,86,114	1.97	8 (26%)
32	CLA	Bb	606	-	69,73,73	1.14	6 (8%)	82,113,113	1.11	7 (8%)
37	SQD	CC	501	-	52,54,54	1.09	4 (7%)	62,65,65	1.19	4 (6%)
40	LUT	N	616	-	42,43,43	0.97	0	51,60,60	1.63	10 (19%)
32	CLA	CC	502	-	69,73,73	1.14	9 (13%)	82,113,113	1.26	6 (7%)
39	CHL	g	606	-	37,51,74	3.14	10 (27%)	30,86,114	2.04	10 (33%)
44	DGD	Cc	520	-	53,53,67	0.96	2 (3%)	67,67,81	0.88	2 (2%)
32	CLA	a	407	-	53,57,73	1.31	7 (13%)	61,93,113	1.25	5 (8%)
34	BCR	b	617	-	41,41,41	1.01	2 (4%)	56,56,56	2.10	16 (28%)
40	LUT	y	317	-	42,43,43	0.97	1 (2%)	51,60,60	2.07	12 (23%)
32	CLA	b	601	-	69,73,73	1.17	8 (11%)	82,113,113	1.17	7 (8%)
32	CLA	Bb	616	-	69,73,73	1.15	7 (10%)	82,113,113	1.10	5 (6%)
38	LMG	Bb	620	-	36,36,55	1.11	2 (5%)	44,44,63	0.96	2 (4%)
39	CHL	2	601	14	35,49,74	3.23	9 (25%)	30,83,114	1.89	10 (33%)
39	CHL	2	606	-	35,49,74	3.26	8 (22%)	30,83,114	1.88	10 (33%)
32	CLA	b	602	-	69,73,73	1.15	6 (8%)	82,113,113	1.08	6 (7%)
40	LUT	s	614	-	42,43,43	1.04	2 (4%)	51,60,60	1.52	10 (19%)
39	CHL	n	605	9	42,56,74	2.92	10 (23%)	36,92,114	1.78	10 (27%)
36	LHG	K	101	-	33,33,48	1.13	2 (6%)	36,39,54	1.09	2 (5%)
32	CLA	CC	513	-	69,73,73	1.15	6 (8%)	82,113,113	1.15	3 (3%)
39	CHL	n	609	9	44,58,74	2.84	11 (25%)	37,94,114	1.87	9 (24%)
39	CHL	4	306	-	40,54,74	2.96	9 (22%)	34,90,114	2.03	9 (26%)
39	CHL	SS	307	-	36,50,74	3.18	8 (22%)	29,85,114	1.97	10 (34%)
32	CLA	Y	613	9	63,67,73	1.20	5 (7%)	74,105,113	1.11	4 (5%)
32	CLA	C	511	-	69,73,73	1.17	8 (11%)	82,113,113	1.13	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	NN	605	9	36,50,74	3.15	9 (25%)	29,85,114	2.03	9 (31%)
38	LMG	B	615	-	45,45,55	0.99	2 (4%)	53,53,63	0.93	2 (3%)
39	CHL	NN	609	9	44,58,74	2.83	11 (25%)	37,94,114	1.77	9 (24%)
39	CHL	Yy	601	9	60,74,74	2.50	11 (18%)	58,114,114	1.44	9 (15%)
32	CLA	y	314	9	69,73,73	1.15	7 (10%)	82,113,113	1.08	5 (6%)
38	LMG	Cc	501	-	34,34,55	1.15	3 (8%)	42,42,63	1.28	7 (16%)
32	CLA	Rr	602	3	69,73,73	1.17	8 (11%)	82,113,113	1.10	5 (6%)
32	CLA	AA	406	-	53,57,73	1.29	7 (13%)	61,93,113	1.21	6 (9%)
39	CHL	Gg	308	-	44,58,74	2.86	11 (25%)	37,94,114	1.78	10 (27%)
32	CLA	Bb	612	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	5 (6%)
32	CLA	Cc	505	-	69,73,73	1.16	7 (10%)	82,113,113	1.12	6 (7%)
32	CLA	NN	614	-	45,49,73	1.39	6 (13%)	54,84,113	1.19	4 (7%)
32	CLA	Yy	611	36	46,50,73	1.38	7 (15%)	53,85,113	1.28	4 (7%)
32	CLA	CC	507	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	7 (8%)
41	XAT	y	302	-	41,47,47	1.21	3 (7%)	54,74,74	2.45	17 (31%)
32	CLA	Nn	304	9	53,57,73	1.33	6 (11%)	61,93,113	1.19	4 (6%)
32	CLA	Rr	601	3	53,57,73	1.34	6 (11%)	61,93,113	1.15	4 (6%)
40	LUT	YY	616	-	42,43,43	0.95	0	51,60,60	1.46	9 (17%)
32	CLA	2	610	-	44,48,73	1.44	6 (13%)	51,82,113	1.34	5 (9%)
32	CLA	b	616	-	69,73,73	1.15	7 (10%)	82,113,113	1.09	5 (6%)
32	CLA	c	507	-	69,73,73	1.16	6 (8%)	82,113,113	1.20	5 (6%)
32	CLA	Bb	614	-	69,73,73	1.13	5 (7%)	82,113,113	1.09	3 (3%)
34	BCR	T	101	-	41,41,41	0.96	1 (2%)	56,56,56	2.07	19 (33%)
32	CLA	SS	313	4	53,57,73	1.31	5 (9%)	61,93,113	1.15	5 (8%)
32	CLA	X	201	-	45,49,73	1.41	7 (15%)	54,84,113	1.25	4 (7%)
38	LMG	AA	415	-	36,36,55	1.11	2 (5%)	44,44,63	1.15	3 (6%)
36	LHG	A	414	-	44,44,48	0.97	2 (4%)	47,50,54	0.90	2 (4%)
39	CHL	33	601	15	35,49,74	3.26	8 (22%)	30,83,114	1.77	8 (26%)
32	CLA	CC	510	-	69,73,73	1.16	8 (11%)	82,113,113	1.14	5 (6%)
39	CHL	R	605	-	44,58,74	2.89	10 (22%)	37,94,114	1.79	11 (29%)
32	CLA	s	603	-	53,57,73	1.32	5 (9%)	61,93,113	1.16	4 (6%)
40	LUT	RR	315	-	42,43,43	0.89	1 (2%)	51,60,60	1.60	15 (29%)
32	CLA	c	512	-	69,73,73	1.15	6 (8%)	82,113,113	1.10	4 (4%)
40	LUT	Nn	307	-	42,43,43	1.00	1 (2%)	51,60,60	1.55	8 (15%)
32	CLA	BB	608	-	69,73,73	1.16	7 (10%)	82,113,113	1.08	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCR	B	616	-	41,41,41	0.87	0	56,56,56	1.99	19 (33%)
36	LHG	44	616	32	18,18,48	1.76	3 (16%)	17,22,54	1.44	1 (5%)
39	CHL	Ss	605	-	44,58,74	2.88	8 (18%)	37,94,114	1.84	11 (29%)
42	NEX	RR	317	-	40,46,46	1.24	4 (10%)	50,70,70	1.93	13 (26%)
32	CLA	C	509	-	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
32	CLA	G	610	9	53,57,73	1.33	6 (11%)	61,93,113	1.37	6 (9%)
40	LUT	44	612	-	42,43,43	0.92	0	51,60,60	1.40	7 (13%)
32	CLA	r	609	3	69,73,73	1.15	6 (8%)	82,113,113	1.06	3 (3%)
32	CLA	c	513	-	47,51,73	1.36	7 (14%)	55,86,113	1.24	4 (7%)
36	LHG	A	413	-	36,36,48	1.07	2 (5%)	39,42,54	1.03	3 (7%)
39	CHL	Y	601	9	60,74,74	2.49	11 (18%)	58,114,114	1.50	9 (15%)
32	CLA	B	619	-	69,73,73	1.14	6 (8%)	82,113,113	1.09	6 (7%)
32	CLA	YY	614	-	53,57,73	1.30	7 (13%)	61,93,113	1.18	6 (9%)
39	CHL	YY	601	9	60,74,74	2.49	10 (16%)	58,114,114	1.54	9 (15%)
32	CLA	4	304	-	49,53,73	1.38	6 (12%)	58,89,113	1.37	5 (8%)
39	CHL	4	309	11	40,54,74	3.05	8 (20%)	34,90,114	1.72	8 (23%)
40	LUT	g	615	-	42,43,43	0.95	1 (2%)	51,60,60	1.49	7 (13%)
32	CLA	RR	309	3	69,73,73	1.16	7 (10%)	82,113,113	1.05	5 (6%)
44	DGD	C	523	-	53,53,67	0.94	2 (3%)	67,67,81	0.94	2 (2%)
41	XAT	GG	619	-	41,47,47	1.20	4 (9%)	54,74,74	2.55	12 (22%)
41	XAT	RR	316	-	41,47,47	1.08	2 (4%)	54,74,74	2.21	16 (29%)
32	CLA	DD	401	-	69,73,73	1.14	7 (10%)	82,113,113	1.14	6 (7%)
32	CLA	b	608	-	69,73,73	1.14	7 (10%)	82,113,113	1.10	5 (6%)
39	CHL	1	608	14	35,49,74	3.05	7 (20%)	30,83,114	1.79	9 (30%)
32	CLA	CC	505	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	6 (7%)
38	LMG	A	415	-	36,36,55	1.10	2 (5%)	44,44,63	1.13	3 (6%)
36	LHG	Ss	616	32	47,47,48	0.94	2 (4%)	50,53,54	0.90	2 (4%)
39	CHL	n	601	9	44,58,74	2.91	10 (22%)	37,94,114	1.78	11 (29%)
32	CLA	C	510	-	69,73,73	1.14	7 (10%)	82,113,113	1.15	4 (4%)
32	CLA	B	604	-	69,73,73	1.17	7 (10%)	82,113,113	1.08	4 (4%)
38	LMG	Dd	408	-	46,46,55	0.98	2 (4%)	54,54,63	1.03	3 (5%)
42	NEX	NN	618	-	40,46,46	1.21	3 (7%)	50,70,70	2.08	14 (28%)
32	CLA	G	614	-	45,49,73	1.39	5 (11%)	54,84,113	1.14	3 (5%)
32	CLA	3	603	-	44,48,73	1.45	6 (13%)	51,82,113	1.24	4 (7%)
36	LHG	A	411	-	33,33,48	1.12	2 (6%)	36,39,54	1.23	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CLA	Gg	304	-	69,73,73	1.16	5 (7%)	82,113,113	1.03	4 (4%)
39	CHL	n	608	-	44,58,74	2.90	9 (20%)	37,94,114	1.80	10 (27%)

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
39	CHL	r	607	-	3/3/22/26	7/20/118/137	-
39	CHL	11	607	-	3/3/19/26	4/10/104/137	-
37	SQD	l	102	-	-	10/49/69/69	0/1/1/1
32	CLA	Ss	602	4	1/1/16/20	13/20/96/115	-
36	LHG	y	320	32	-	22/53/53/53	-
39	CHL	Gg	309	-	3/3/20/26	2/10/108/137	-
32	CLA	s	602	4	1/1/16/20	12/20/96/115	-
36	LHG	d	406	-	-	11/53/53/53	-
32	CLA	C	513	18	1/1/20/20	14/39/115/115	-
32	CLA	a	406	1	1/1/20/20	8/39/115/115	-
32	CLA	SS	309	4	1/1/14/20	6/10/86/115	-
39	CHL	NN	608	-	3/3/20/26	2/10/108/137	-
32	CLA	1	602	14	1/1/13/20	2/10/82/115	-
32	CLA	1	610	36	1/1/13/20	5/10/82/115	-
32	CLA	d	402	-	1/1/20/20	10/39/115/115	-
33	PHO	A	407	-	-	8/37/103/103	0/5/6/6
32	CLA	44	602	11	1/1/15/20	8/15/91/115	-
32	CLA	11	612	-	1/1/13/20	6/10/82/115	-
44	DGD	CC	518	-	-	10/44/84/95	0/2/2/2
36	LHG	D	408	-	-	12/47/47/53	-
32	CLA	b	606	-	1/1/20/20	9/39/115/115	-
39	CHL	1	606	-	3/3/19/26	2/10/104/137	-
42	NEX	Yy	617	-	-	3/27/83/83	0/3/3/3
32	CLA	Aa	406	1	1/1/20/20	9/39/115/115	-
32	CLA	3	613	-	1/1/13/20	6/10/82/115	-
42	NEX	R	617	-	-	2/27/83/83	0/3/3/3
44	DGD	CC	522	-	-	12/44/84/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	BB	622	-	-	8/38/38/53	-
32	CLA	C	507	-	1/1/20/20	11/39/115/115	-
43	LMU	RR	301	-	-	3/13/53/61	0/2/2/2
39	CHL	YY	607	-	3/3/20/26	2/12/110/137	-
33	PHO	a	409	-	-	15/37/103/103	0/5/6/6
41	XAT	Nn	308	-	-	1/31/93/93	0/4/4/4
32	CLA	2	611	14	1/1/13/20	5/10/82/115	-
36	LHG	NN	619	32	-	9/42/42/53	-
39	CHL	Ss	601	4	3/3/23/26	4/23/121/137	-
41	XAT	N	617	-	-	0/31/93/93	0/4/4/4
41	XAT	R	616	-	-	0/31/93/93	0/4/4/4
44	DGD	D	411	-	-	7/51/91/95	0/2/2/2
32	CLA	B	620	-	1/1/20/20	10/39/115/115	-
32	CLA	c	511	18	1/1/20/20	10/39/115/115	-
32	CLA	y	313	36	1/1/14/20	5/12/88/115	-
32	CLA	D	401	-	1/1/20/20	8/39/115/115	-
32	CLA	AA	405	-	1/1/20/20	14/39/115/115	-
39	CHL	N	601	9	3/3/20/26	5/13/111/137	-
40	LUT	Rr	614	-	-	2/29/67/67	0/2/2/2
44	DGD	Aa	401	-	-	9/44/84/95	0/2/2/2
36	LHG	11	614	32	-	16/38/38/53	-
44	DGD	C	520	-	-	4/51/91/95	0/2/2/2
42	NEX	Rr	616	-	-	3/27/83/83	0/3/3/3
32	CLA	RR	302	3	1/1/20/20	17/39/115/115	-
32	CLA	S	613	-	1/1/15/20	2/15/91/115	-
39	CHL	S	601	4	3/3/23/26	7/23/121/137	-
41	XAT	4	314	-	-	0/31/93/93	0/4/4/4
39	CHL	NN	601	9	3/3/20/26	3/13/111/137	-
39	CHL	g	609	9	3/3/20/26	5/12/110/137	-
41	XAT	r	615	-	-	1/31/93/93	0/4/4/4
32	CLA	3	602	15	1/1/13/20	4/10/82/115	-
39	CHL	Rr	607	-	3/3/22/26	7/20/118/137	-
32	CLA	GG	602	9	1/1/16/20	10/20/96/115	-
32	CLA	Bb	604	-	1/1/20/20	7/39/115/115	-
37	SQD	BB	621	-	-	5/31/51/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	S	603	-	1/1/15/20	8/15/91/115	-
32	CLA	R	609	3	1/1/20/20	11/39/115/115	-
41	XAT	44	613	-	-	0/31/93/93	0/4/4/4
32	CLA	g	602	9	-	9/20/96/115	-
32	CLA	B	622	-	1/1/20/20	17/39/115/115	-
40	LUT	GG	615	-	-	2/29/67/67	0/2/2/2
42	NEX	Y	617	-	-	2/27/83/83	0/3/3/3
32	CLA	g	603	-	1/1/20/20	14/39/115/115	-
32	CLA	Cc	512	-	1/1/20/20	12/39/115/115	-
39	CHL	Nn	319	9	3/3/22/26	4/20/118/137	-
32	CLA	N	611	36	1/1/16/20	10/20/96/115	-
32	CLA	Gg	311	9	1/1/16/20	8/20/96/115	-
32	CLA	Bb	611	-	1/1/20/20	7/39/115/115	-
34	BCR	k	101	-	-	6/29/63/63	0/2/2/2
32	CLA	b	614	-	1/1/20/20	6/39/115/115	-
39	CHL	3	608	15	3/3/19/26	2/10/104/137	-
42	NEX	N	618	-	-	2/27/83/83	0/3/3/3
39	CHL	Y	606	-	3/3/20/26	4/13/111/137	-
32	CLA	RR	312	3	1/1/14/20	1/12/88/115	-
32	CLA	Cc	508	-	1/1/20/20	18/39/115/115	-
32	CLA	YY	604	-	-	10/20/96/115	-
32	CLA	Y	604	-	-	11/20/96/115	-
39	CHL	Yy	609	9	3/3/26/26	13/39/137/137	-
34	BCR	b	619	-	-	4/29/63/63	0/2/2/2
32	CLA	R	608	3	1/1/16/20	9/20/96/115	-
32	CLA	N	610	9	1/1/20/20	15/39/115/115	-
39	CHL	YY	609	9	3/3/26/26	9/39/137/137	-
32	CLA	B	623	-	1/1/20/20	10/39/115/115	-
33	PHO	Aa	409	-	-	15/37/103/103	0/5/6/6
34	BCR	B	614	-	-	4/29/63/63	0/2/2/2
35	PL9	A	410	-	-	26/53/73/73	0/1/1/1
32	CLA	Cc	510	-	1/1/19/20	6/33/109/115	-
39	CHL	G	601	9	3/3/26/26	12/39/137/137	-
32	CLA	YY	611	36	1/1/14/20	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	n	617	-	-	3/27/83/83	0/3/3/3
32	CLA	D	405	-	1/1/20/20	8/39/115/115	-
40	LUT	g	616	-	-	2/29/67/67	0/2/2/2
32	CLA	Rr	610	36	1/1/16/20	11/20/96/115	-
34	BCR	DD	405	-	-	2/29/63/63	0/2/2/2
32	CLA	c	502	-	1/1/20/20	9/39/115/115	-
32	CLA	r	604	-	1/1/16/20	15/20/96/115	-
42	NEX	y	319	-	-	3/27/83/83	0/3/3/3
32	CLA	3	610	36	1/1/13/20	5/10/82/115	-
32	CLA	y	315	9	1/1/18/20	9/32/108/115	-
39	CHL	S	606	-	3/3/20/26	0/10/108/137	-
32	CLA	BB	613	-	1/1/19/20	6/33/109/115	-
34	BCR	CC	516	-	-	5/29/63/63	0/2/2/2
32	CLA	44	611	-	1/1/15/20	9/15/91/115	-
32	CLA	Rr	608	3	1/1/16/20	13/20/96/115	-
34	BCR	C	516	-	-	6/29/63/63	0/2/2/2
34	BCR	b	618	-	-	4/29/63/63	0/2/2/2
32	CLA	r	610	36	1/1/16/20	9/20/96/115	-
32	CLA	C	504	-	-	11/39/115/115	-
37	SQD	LL	101	-	-	9/31/51/69	0/1/1/1
44	DGD	C	519	-	-	9/44/84/95	0/2/2/2
32	CLA	g	611	36	1/1/20/20	18/39/115/115	-
39	CHL	Nn	316	-	3/3/22/26	3/20/118/137	-
39	CHL	g	607	-	3/3/22/26	7/20/118/137	-
46	HEM	Ee	101	21,20	-	6/14/54/54	-
32	CLA	r	612	3	1/1/16/20	4/20/96/115	-
38	LMG	CC	520	-	-	3/34/54/70	0/1/1/1
34	BCR	C	518	-	-	2/29/63/63	0/2/2/2
32	CLA	r	602	3	1/1/20/20	13/39/115/115	-
39	CHL	Nn	311	9	3/3/22/26	5/20/118/137	-
32	CLA	b	605	-	1/1/20/20	11/39/115/115	-
41	XAT	Gg	301	-	-	1/31/93/93	0/4/4/4
42	NEX	Nn	309	-	-	2/27/83/83	0/3/3/3
32	CLA	22	604	-	1/1/13/20	4/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Nn	314	-	1/1/16/20	4/20/96/115	-
32	CLA	Gg	314	9	1/1/13/20	3/10/82/115	-
32	CLA	n	610	9	1/1/20/20	12/39/115/115	-
32	CLA	Cc	515	-	1/1/14/20	7/13/89/115	-
39	CHL	r	605	3	3/3/22/26	8/20/118/137	-
35	PL9	Dd	404	-	-	28/53/73/73	0/1/1/1
32	CLA	33	610	36	1/1/13/20	4/10/82/115	-
36	LHG	CC	523	-	-	10/41/41/53	-
32	CLA	2	609	14	1/1/13/20	6/10/82/115	-
32	CLA	CC	508	-	1/1/20/20	12/39/115/115	-
32	CLA	d	401	-	-	10/39/115/115	-
38	LMG	W	201	-	-	6/43/63/70	0/1/1/1
32	CLA	11	602	14	1/1/13/20	4/10/82/115	-
32	CLA	11	611	14	1/1/13/20	2/10/82/115	-
46	HEM	E	101	21,20	-	1/14/54/54	-
36	LHG	Nn	310	32	-	14/53/53/53	-
32	CLA	N	614	-	1/1/14/20	4/10/86/115	-
36	LHG	l	101	-	-	12/53/53/53	-
32	CLA	RR	310	36	1/1/16/20	11/20/96/115	-
40	LUT	r	614	-	-	2/29/67/67	0/2/2/2
32	CLA	Aa	410	-	1/1/19/20	10/33/109/115	-
40	LUT	NN	615	-	-	1/29/67/67	0/2/2/2
32	CLA	B	606	-	1/1/20/20	14/39/115/115	-
32	CLA	y	305	-	1/1/16/20	6/20/96/115	-
33	PHO	a	408	-	-	7/37/103/103	0/5/6/6
36	LHG	d	405	-	-	8/47/47/53	-
32	CLA	YY	602	9	1/1/20/20	14/39/115/115	-
44	DGD	a	415	-	-	9/44/84/95	0/2/2/2
32	CLA	Ss	613	-	1/1/16/20	7/20/96/115	-
32	CLA	r	608	3	1/1/16/20	10/20/96/115	-
32	CLA	RR	308	3	1/1/16/20	9/20/96/115	-
36	LHG	EE	101	-	-	7/44/44/53	-
39	CHL	N	606	-	3/3/20/26	0/10/108/137	-
39	CHL	11	608	14	3/3/19/26	2/10/104/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	33	608	15	3/3/19/26	2/10/104/137	-
38	LMG	DD	409	-	-	4/41/61/70	0/1/1/1
32	CLA	c	501	-	1/1/20/20	18/39/115/115	-
40	LUT	2	614	-	-	4/29/67/67	0/2/2/2
32	CLA	B	609	-	1/1/19/20	5/33/109/115	-
36	LHG	AA	414	-	-	9/49/49/53	-
32	CLA	44	603	-	1/1/15/20	11/15/91/115	-
32	CLA	BB	601	-	1/1/20/20	7/39/115/115	-
32	CLA	4	305	-	1/1/15/20	5/15/91/115	-
32	CLA	Cc	506	-	1/1/18/20	8/27/103/115	-
32	CLA	Nn	312	9	1/1/20/20	13/39/115/115	-
34	BCR	AA	409	-	-	5/29/63/63	0/2/2/2
32	CLA	n	603	-	1/1/16/20	9/20/96/115	-
44	DGD	CC	519	-	-	5/51/91/95	0/2/2/2
32	CLA	B	610	-	1/1/20/20	7/39/115/115	-
42	NEX	Y	619	-	-	3/27/83/83	0/3/3/3
32	CLA	C	503	-	1/1/20/20	11/39/115/115	-
32	CLA	Yy	614	-	1/1/16/20	10/20/96/115	-
37	SQD	B	617	-	-	5/31/51/69	0/1/1/1
32	CLA	11	604	-	1/1/13/20	2/10/82/115	-
41	XAT	Yy	619	-	-	3/31/93/93	0/4/4/4
32	CLA	Rr	604	-	1/1/16/20	12/20/96/115	-
39	CHL	Yy	607	-	3/3/20/26	4/12/110/137	-
44	DGD	c	517	-	-	5/44/84/95	0/2/2/2
39	CHL	22	606	-	3/3/19/26	4/10/104/137	-
39	CHL	33	605	-	3/3/19/26	2/10/104/137	-
39	CHL	y	307	9	3/3/21/26	6/18/116/137	-
32	CLA	c	505	-	1/1/20/20	10/39/115/115	-
32	CLA	33	609	15	1/1/13/20	2/10/82/115	-
32	CLA	22	609	14	1/1/13/20	6/10/82/115	-
32	CLA	2	604	-	1/1/13/20	4/10/82/115	-
40	LUT	S	614	-	-	1/29/67/67	0/2/2/2
39	CHL	44	601	-	3/3/21/26	2/13/111/137	-
36	LHG	J	101	-	-	10/30/30/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	XAT	NN	617	-	-	0/31/93/93	0/4/4/4
32	CLA	Bb	615	-	1/1/20/20	13/39/115/115	-
39	CHL	3	607	-	3/3/19/26	2/10/104/137	-
32	CLA	b	603	-	1/1/20/20	16/39/115/115	-
32	CLA	CC	511	-	1/1/20/20	8/39/115/115	-
39	CHL	YY	605	9	3/3/21/26	5/18/116/137	-
39	CHL	GG	607	-	3/3/21/26	4/15/113/137	-
36	LHG	D	409	-	-	5/53/53/53	-
40	LUT	s	615	-	-	2/29/67/67	0/2/2/2
39	CHL	33	607	-	3/3/19/26	2/10/104/137	-
32	CLA	GG	612	9	1/1/16/20	10/20/96/115	-
32	CLA	R	603	-	1/1/16/20	2/20/96/115	-
32	CLA	NN	613	9	1/1/16/20	10/20/96/115	-
32	CLA	n	613	9	1/1/16/20	8/20/96/115	-
32	CLA	Ss	603	-	1/1/16/20	12/20/96/115	-
32	CLA	Ss	610	36	1/1/16/20	9/20/96/115	-
32	CLA	Y	614	-	1/1/16/20	12/20/96/115	-
39	CHL	GG	605	9	3/3/20/26	2/12/110/137	-
32	CLA	SS	303	4	1/1/16/20	12/20/96/115	-
32	CLA	N	603	-	1/1/14/20	4/12/88/115	-
33	PHO	AA	407	-	-	6/37/103/103	0/5/6/6
32	CLA	S	611	4	1/1/16/20	9/20/96/115	-
39	CHL	Y	607	-	3/3/20/26	2/12/110/137	-
32	CLA	NN	602	9	1/1/20/20	13/39/115/115	-
32	CLA	Bb	607	-	1/1/20/20	13/39/115/115	-
32	CLA	Rr	611	-	1/1/16/20	11/20/96/115	-
34	BCR	c	515	-	-	5/29/63/63	0/2/2/2
32	CLA	S	610	-	1/1/16/20	9/20/96/115	-
32	CLA	Rr	603	-	1/1/16/20	7/20/96/115	-
32	CLA	G	603	-	1/1/20/20	13/39/115/115	-
32	CLA	SS	312	4	1/1/16/20	9/20/96/115	-
34	BCR	BB	618	-	-	4/29/63/63	0/2/2/2
39	CHL	y	310	-	3/3/22/26	4/20/118/137	-
35	PL9	d	404	-	-	29/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	s	616	32	-	7/52/52/53	-
32	CLA	c	503	-	1/1/20/20	9/39/115/115	-
42	NEX	g	617	32	-	3/27/83/83	0/3/3/3
37	SQD	Ll	101	-	-	9/49/69/69	0/1/1/1
32	CLA	Bb	605	-	1/1/20/20	12/39/115/115	-
32	CLA	Bb	603	-	1/1/20/20	17/39/115/115	-
39	CHL	11	605	14	3/3/19/26	4/10/104/137	-
32	CLA	BB	612	-	1/1/20/20	10/39/115/115	-
36	LHG	JJ	101	-	-	8/37/37/53	-
32	CLA	1	604	-	1/1/13/20	4/10/82/115	-
36	LHG	KK	101	-	-	8/38/38/53	-
39	CHL	y	308	-	3/3/20/26	2/13/111/137	-
39	CHL	1	601	14	3/3/19/26	2/10/104/137	-
32	CLA	22	610	36	1/1/14/20	7/12/88/115	-
32	CLA	CC	503	-	-	12/39/115/115	-
44	DGD	BB	624	-	-	9/44/84/95	0/2/2/2
32	CLA	C	512	-	1/1/20/20	10/39/115/115	-
40	LUT	Gg	316	-	-	1/29/67/67	0/2/2/2
41	XAT	Rr	615	-	-	3/31/93/93	0/4/4/4
32	CLA	1	611	14	1/1/13/20	2/10/82/115	-
32	CLA	n	604	-	1/1/16/20	6/20/96/115	-
36	LHG	N	619	32	-	9/42/42/53	-
39	CHL	GG	609	9	3/3/20/26	2/12/110/137	-
32	CLA	33	603	-	1/1/13/20	6/10/82/115	-
34	BCR	XX	202	-	-	6/29/63/63	0/2/2/2
32	CLA	S	608	4	1/1/14/20	6/10/86/115	-
32	CLA	Y	603	-	1/1/16/20	10/20/96/115	-
32	CLA	S	609	4	1/1/14/20	2/10/86/115	-
32	CLA	Y	610	9	1/1/20/20	17/39/115/115	-
36	LHG	DD	407	-	-	14/47/47/53	-
32	CLA	11	613	-	1/1/13/20	4/10/82/115	-
32	CLA	CC	506	-	1/1/20/20	14/39/115/115	-
32	CLA	A	408	-	1/1/19/20	7/33/109/115	-
36	LHG	Dd	405	-	-	8/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	N	609	9	3/3/22/26	4/20/118/137	-
32	CLA	Yy	612	9	1/1/20/20	10/39/115/115	-
32	CLA	RR	303	-	1/1/16/20	2/20/96/115	-
37	SQD	L	102	-	-	10/31/51/69	0/1/1/1
32	CLA	A	406	-	1/1/16/20	9/20/96/115	-
39	CHL	Gg	310	9	3/3/20/26	5/12/110/137	-
34	BCR	Kk	101	-	-	4/29/63/63	0/2/2/2
32	CLA	NN	611	36	1/1/16/20	12/20/96/115	-
40	LUT	Gg	317	-	-	1/29/67/67	0/2/2/2
39	CHL	G	609	9	3/3/20/26	2/12/110/137	-
32	CLA	Bb	609	-	1/1/20/20	14/39/115/115	-
32	CLA	Nn	302	36	1/1/16/20	5/20/96/115	-
32	CLA	g	612	9	1/1/16/20	12/20/96/115	-
39	CHL	g	605	9	3/3/20/26	6/12/110/137	-
32	CLA	Yy	604	-	1/1/16/20	10/20/96/115	-
32	CLA	Bb	602	-	1/1/20/20	9/39/115/115	-
32	CLA	c	508	-	1/1/19/20	7/33/109/115	-
39	CHL	2	607	-	3/3/19/26	2/10/104/137	-
39	CHL	r	606	-	3/3/22/26	4/20/118/137	-
32	CLA	R	613	-	1/1/14/20	6/10/86/115	-
39	CHL	Gg	306	9	3/3/20/26	6/12/110/137	-
38	LMG	a	412	-	-	10/37/57/70	0/1/1/1
36	LHG	YY	618	32	-	19/53/53/53	-
34	BCR	Bb	619	-	-	2/29/63/63	0/2/2/2
32	CLA	22	603	-	1/1/13/20	2/10/82/115	-
40	LUT	GG	616	-	-	2/29/67/67	0/2/2/2
39	CHL	n	606	-	3/3/22/26	2/20/118/137	-
32	CLA	b	607	-	1/1/20/20	13/39/115/115	-
36	LHG	r	616	32	-	13/53/53/53	-
39	CHL	33	606	-	3/3/19/26	2/10/104/137	-
44	DGD	BB	625	-	-	3/43/83/95	0/2/2/2
32	CLA	b	610	-	1/1/20/20	11/39/115/115	-
40	LUT	4	313	-	-	2/29/67/67	0/2/2/2
39	CHL	NN	606	-	3/3/20/26	2/10/108/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	NEX	YY	617	-	-	2/27/83/83	0/3/3/3
38	LMG	BB	619	-	-	10/40/60/70	0/1/1/1
32	CLA	R	612	3	1/1/14/20	3/12/88/115	-
32	CLA	G	613	9	1/1/13/20	5/10/82/115	-
32	CLA	Gg	303	9	-	11/20/96/115	-
34	BCR	Cc	516	-	-	4/29/63/63	0/2/2/2
32	CLA	y	306	-	1/1/16/20	8/20/96/115	-
36	LHG	n	618	32	-	11/53/53/53	-
32	CLA	Nn	301	9	1/1/20/20	11/39/115/115	-
32	CLA	44	609	11	1/1/15/20	6/15/91/115	-
32	CLA	Cc	504	-	-	12/39/115/115	-
34	BCR	Aa	411	-	-	4/29/63/63	0/2/2/2
44	DGD	Cc	519	-	-	9/44/84/95	0/2/2/2
39	CHL	4	308	-	3/3/21/26	6/15/113/137	-
32	CLA	G	602	9	1/1/16/20	9/20/96/115	-
40	LUT	n	615	-	-	1/29/67/67	0/2/2/2
36	LHG	II	101	-	-	10/38/38/53	-
32	CLA	b	615	-	1/1/20/20	13/39/115/115	-
34	BCR	a	411	-	-	4/29/63/63	0/2/2/2
32	CLA	S	604	-	1/1/16/20	8/20/96/115	-
36	LHG	1	614	32	-	7/34/34/53	-
32	CLA	BB	603	-	1/1/20/20	11/39/115/115	-
39	CHL	GG	601	9	3/3/26/26	10/39/137/137	-
32	CLA	n	612	9	1/1/16/20	8/20/96/115	-
32	CLA	RR	304	-	1/1/16/20	8/20/96/115	-
36	LHG	0	201	-	-	9/51/51/53	-
40	LUT	N	615	-	-	1/29/67/67	0/2/2/2
34	BCR	K	102	-	-	5/29/63/63	0/2/2/2
32	CLA	Rr	612	3	1/1/16/20	6/20/96/115	-
39	CHL	GG	608	-	3/3/20/26	4/10/108/137	-
39	CHL	R	606	-	3/3/22/26	10/20/118/137	-
38	LMG	Bb	621	-	-	8/31/51/70	0/1/1/1
32	CLA	s	608	4	1/1/16/20	8/20/96/115	-
32	CLA	C	514	-	1/1/20/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Ss	606	-	3/3/22/26	9/20/118/137	-
32	CLA	3	611	15	1/1/13/20	6/10/82/115	-
32	CLA	g	613	9	1/1/13/20	5/10/82/115	-
32	CLA	c	510	-	1/1/20/20	16/39/115/115	-
32	CLA	33	613	-	1/1/13/20	6/10/82/115	-
34	BCR	Cc	517	-	-	5/29/63/63	0/2/2/2
36	LHG	AA	411	-	-	13/38/38/53	-
38	LMG	m	101	-	-	14/46/66/70	0/1/1/1
41	XAT	g	619	-	-	1/31/93/93	0/4/4/4
32	CLA	RR	311	-	1/1/16/20	8/20/96/115	-
32	CLA	3	604	-	1/1/13/20	3/10/82/115	-
40	LUT	G	616	-	-	2/29/67/67	0/2/2/2
32	CLA	C	506	-	1/1/20/20	10/39/115/115	-
32	CLA	B	621	-	1/1/20/20	13/39/115/115	-
32	CLA	Ss	608	4	1/1/16/20	10/20/96/115	-
32	CLA	GG	604	-	1/1/14/20	4/12/88/115	-
32	CLA	G	604	-	1/1/14/20	7/12/88/115	-
32	CLA	b	611	-	1/1/20/20	7/39/115/115	-
40	LUT	R	615	-	-	0/29/67/67	0/2/2/2
32	CLA	Bb	601	-	1/1/20/20	15/39/115/115	-
33	PHO	Aa	408	-	-	7/37/103/103	0/5/6/6
46	HEM	EE	102	21,20	-	1/14/54/54	-
39	CHL	g	608	-	3/3/20/26	2/10/108/137	-
37	SQD	L	101	-	-	16/49/69/69	0/1/1/1
32	CLA	33	612	15	1/1/13/20	4/10/82/115	-
38	LMG	Mm	101	-	-	11/46/66/70	0/1/1/1
33	PHO	DD	402	-	-	10/37/103/103	0/5/6/6
39	CHL	s	607	-	3/3/22/26	5/19/117/137	-
32	CLA	G	611	36	1/1/17/20	11/24/100/115	-
32	CLA	NN	610	9	1/1/20/20	14/39/115/115	-
32	CLA	s	613	-	1/1/16/20	6/20/96/115	-
36	LHG	g	618	32	-	7/38/38/53	-
36	LHG	Rr	617	32	-	11/53/53/53	-
32	CLA	BB	604	-	1/1/20/20	13/39/115/115	-
39	CHL	Nn	317	-	3/3/26/26	12/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	GG	614	-	1/1/14/20	4/10/86/115	-
32	CLA	a	410	-	1/1/19/20	10/33/109/115	-
34	BCR	BB	617	-	-	4/29/63/63	0/2/2/2
37	SQD	Aa	413	-	-	10/42/62/69	0/1/1/1
39	CHL	22	601	14	3/3/19/26	2/10/104/137	-
38	LMG	b	620	-	-	4/31/51/70	0/1/1/1
43	LMU	R	618	-	-	5/13/53/61	0/2/2/2
39	CHL	SS	302	4	3/3/23/26	7/23/121/137	-
32	CLA	NN	612	9	1/1/14/20	3/12/88/115	-
39	CHL	Nn	315	9	3/3/21/26	6/18/116/137	-
36	LHG	33	614	32	-	10/38/38/53	-
37	SQD	B	602	-	-	10/42/62/69	0/1/1/1
32	CLA	b	609	-	1/1/20/20	17/39/115/115	-
32	CLA	2	602	14	1/1/13/20	6/10/82/115	-
32	CLA	BB	615	-	1/1/14/20	2/10/86/115	-
38	LMG	C	521	-	-	10/46/66/70	0/1/1/1
32	CLA	R	610	36	1/1/16/20	10/20/96/115	-
39	CHL	y	303	9	3/3/26/26	12/39/137/137	-
36	LHG	D	410	-	-	10/38/38/53	-
40	LUT	Ss	615	-	-	0/29/67/67	0/2/2/2
36	LHG	Yy	618	32	-	19/53/53/53	-
32	CLA	SS	305	-	1/1/16/20	8/20/96/115	-
32	CLA	4	312	-	1/1/15/20	9/15/91/115	-
32	CLA	s	610	36	1/1/16/20	9/20/96/115	-
40	LUT	Yy	615	-	-	2/29/67/67	0/2/2/2
32	CLA	11	609	14	1/1/13/20	4/10/82/115	-
39	CHL	2	608	14	3/3/19/26	2/10/104/137	-
39	CHL	3	605	-	3/3/19/26	4/10/104/137	-
32	CLA	1	603	-	1/1/13/20	6/10/82/115	-
39	CHL	Yy	605	9	3/3/21/26	7/18/116/137	-
32	CLA	CC	512	18	1/1/20/20	13/39/115/115	-
32	CLA	22	613	-	1/1/13/20	4/10/82/115	-
39	CHL	s	601	4	3/3/23/26	7/23/121/137	-
32	CLA	R	602	3	1/1/20/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LHG	3	614	32	-	10/38/38/53	-
32	CLA	Rr	609	3	1/1/20/20	11/39/115/115	-
32	CLA	SS	310	4	1/1/14/20	2/10/86/115	-
39	CHL	y	311	9	3/3/26/26	14/39/137/137	-
32	CLA	XX	201	-	1/1/14/20	4/10/86/115	-
34	BCR	Bb	618	-	-	4/29/63/63	0/2/2/2
34	BCR	CC	515	-	-	6/29/63/63	0/2/2/2
32	CLA	Cc	503	-	1/1/20/20	17/39/115/115	-
40	LUT	n	616	-	-	3/29/67/67	0/2/2/2
32	CLA	Y	612	9	1/1/20/20	11/39/115/115	-
32	CLA	S	612	4	1/1/16/20	8/20/96/115	-
32	CLA	b	604	-	1/1/20/20	9/39/115/115	-
39	CHL	S	605	-	3/3/20/26	2/10/108/137	-
39	CHL	11	601	14	3/3/19/26	2/10/104/137	-
32	CLA	BB	610	-	1/1/20/20	13/39/115/115	-
39	CHL	Gg	302	9	3/3/26/26	10/39/137/137	-
32	CLA	Gg	315	-	1/1/16/20	10/20/96/115	-
37	SQD	C	501	-	-	16/49/69/69	0/1/1/1
32	CLA	YY	610	9	1/1/20/20	13/39/115/115	-
32	CLA	s	611	4	1/1/16/20	9/20/96/115	-
36	LHG	Y	618	32	-	18/53/53/53	-
32	CLA	NN	604	-	1/1/14/20	4/10/86/115	-
43	LMU	C	502	-	-	4/13/53/61	0/2/2/2
39	CHL	44	606	-	3/3/21/26	4/15/113/137	-
32	CLA	y	316	-	1/1/16/20	11/20/96/115	-
39	CHL	2	605	-	3/3/19/26	2/10/104/137	-
34	BCR	C	517	-	-	5/29/63/63	0/2/2/2
37	SQD	AA	412	-	-	8/30/50/69	0/1/1/1
39	CHL	44	608	11	3/3/21/26	4/15/113/137	-
39	CHL	11	606	-	3/3/19/26	2/10/104/137	-
39	CHL	n	607	-	3/3/26/26	15/39/137/137	-
40	LUT	Y	615	-	-	4/29/67/67	0/2/2/2
40	LUT	YY	615	-	-	4/29/67/67	0/2/2/2
39	CHL	RR	305	-	3/3/22/26	7/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DGD	Hh	102	-	-	12/51/91/95	0/2/2/2
35	PL9	AA	410	-	-	28/53/73/73	0/1/1/1
32	CLA	Yy	603	-	1/1/16/20	6/20/96/115	-
32	CLA	y	304	9	1/1/20/20	12/39/115/115	-
32	CLA	SS	304	-	1/1/15/20	6/15/91/115	-
34	BCR	BB	620	-	-	5/29/63/63	0/2/2/2
39	CHL	S	607	-	3/3/20/26	0/12/110/137	-
34	BCR	CC	517	-	-	2/29/63/63	0/2/2/2
32	CLA	y	312	9	1/1/20/20	13/39/115/115	-
32	CLA	DD	403	-	1/1/20/20	10/39/115/115	-
32	CLA	C	508	-	1/1/20/20	10/39/115/115	-
32	CLA	3	612	15	1/1/13/20	4/10/82/115	-
32	CLA	GG	603	-	1/1/20/20	12/39/115/115	-
36	LHG	Ll	102	-	-	14/53/53/53	-
39	CHL	NN	607	-	3/3/26/26	9/39/137/137	-
32	CLA	B	618	-	1/1/20/20	9/39/115/115	-
38	LMG	WW	201	-	-	7/43/63/70	0/1/1/1
32	CLA	N	604	-	1/1/14/20	4/10/86/115	-
44	DGD	BB	623	-	-	9/51/91/95	0/2/2/2
34	BCR	c	516	-	-	4/29/63/63	0/2/2/2
39	CHL	y	309	-	3/3/20/26	2/12/110/137	-
32	CLA	Cc	514	-	1/1/20/20	9/39/115/115	-
32	CLA	c	504	-	1/1/18/20	7/27/103/115	-
34	BCR	KK	103	-	-	4/29/63/63	0/2/2/2
43	LMU	KK	102	-	-	5/13/53/61	0/2/2/2
32	CLA	C	515	-	1/1/16/20	6/20/96/115	-
32	CLA	BB	606	-	1/1/20/20	10/39/115/115	-
39	CHL	Y	608	-	3/3/22/26	6/20/118/137	-
32	CLA	B	605	-	-	15/39/115/115	-
40	LUT	Ss	614	-	-	2/29/67/67	0/2/2/2
39	CHL	N	607	-	3/3/26/26	10/39/137/137	-
46	HEM	e	101	21,20	-	3/14/54/54	-
40	LUT	G	615	-	-	2/29/67/67	0/2/2/2
39	CHL	YY	608	-	3/3/22/26	7/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	n	602	9	1/1/20/20	14/39/115/115	-
39	CHL	Gg	307	-	3/3/20/26	4/12/110/137	-
32	CLA	N	612	9	1/1/14/20	3/12/88/115	-
32	CLA	D	404	-	1/1/20/20	15/39/115/115	-
42	NEX	Gg	318	-	-	3/27/83/83	0/3/3/3
34	BCR	Cc	518	-	-	3/29/63/63	0/2/2/2
32	CLA	33	602	15	1/1/13/20	4/10/82/115	-
36	LHG	G	618	32	-	6/38/38/53	-
39	CHL	SS	308	4	3/3/22/26	3/19/117/137	-
35	PL9	D	407	-	-	29/53/73/73	0/1/1/1
32	CLA	11	610	36	1/1/13/20	4/10/82/115	-
39	CHL	22	607	-	3/3/19/26	2/10/104/137	-
35	PL9	DD	406	-	-	26/53/73/73	0/1/1/1
36	LHG	4	315	32	-	8/23/23/53	-
39	CHL	N	605	9	3/3/20/26	4/10/108/137	-
32	CLA	G	612	9	1/1/16/20	10/20/96/115	-
32	CLA	g	610	9	1/1/16/20	6/20/96/115	-
40	LUT	Yy	616	-	-	3/29/67/67	0/2/2/2
32	CLA	SS	311	-	1/1/16/20	7/20/96/115	-
32	CLA	Gg	313	9	1/1/16/20	14/20/96/115	-
39	CHL	SS	306	4	3/3/20/26	2/10/108/137	-
32	CLA	Y	611	36	1/1/14/20	5/12/88/115	-
39	CHL	G	605	9	3/3/20/26	2/12/110/137	-
39	CHL	22	605	-	3/3/19/26	2/10/104/137	-
32	CLA	Nn	313	-	1/1/16/20	10/20/96/115	-
32	CLA	4	311	36	1/1/15/20	5/15/91/115	-
39	CHL	Ss	607	-	3/3/22/26	5/19/117/137	-
34	BCR	A	409	-	-	5/29/63/63	0/2/2/2
32	CLA	r	603	-	1/1/16/20	8/20/96/115	-
32	CLA	44	604	-	1/1/15/20	7/15/91/115	-
40	LUT	22	614	-	-	4/29/67/67	0/2/2/2
40	LUT	SS	315	-	-	2/29/67/67	0/2/2/2
32	CLA	b	612	-	1/1/20/20	14/39/115/115	-
32	CLA	Yy	602	9	1/1/20/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Bb	613	-	1/1/20/20	14/39/115/115	-
39	CHL	Rr	606	-	3/3/22/26	5/20/118/137	-
39	CHL	4	307	-	3/3/21/26	4/15/113/137	-
32	CLA	Dd	401	-	-	13/39/115/115	-
36	LHG	Gg	319	32	-	6/38/38/53	-
39	CHL	44	607	-	3/3/21/26	6/15/113/137	-
32	CLA	44	610	36	1/1/15/20	8/15/91/115	-
38	LMG	b	621	-	-	9/31/51/70	0/1/1/1
39	CHL	Y	605	9	3/3/21/26	5/18/116/137	-
32	CLA	NN	603	-	1/1/14/20	4/12/88/115	-
36	LHG	44	614	32	-	8/23/23/53	-
32	CLA	Aa	405	-	1/1/20/20	10/39/115/115	-
36	LHG	22	615	32	-	8/38/38/53	-
32	CLA	r	611	-	1/1/16/20	13/20/96/115	-
32	CLA	33	604	-	1/1/13/20	4/10/82/115	-
41	XAT	GG	617	-	-	2/31/93/93	0/4/4/4
38	LMG	F	101	-	-	3/41/61/70	0/1/1/1
36	LHG	a	414	-	-	3/41/41/53	-
32	CLA	Gg	312	36	1/1/20/20	17/39/115/115	-
39	CHL	3	601	15	3/3/19/26	4/10/104/137	-
32	CLA	Dd	402	-	1/1/20/20	13/39/115/115	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
34	BCR	d	403	-	-	4/29/63/63	0/2/2/2
41	XAT	y	301	-	-	3/31/93/93	0/4/4/4
32	CLA	Cc	509	-	1/1/20/20	12/39/115/115	-
32	CLA	n	611	36	1/1/16/20	7/20/96/115	-
36	LHG	Dd	406	-	-	10/53/53/53	-
40	LUT	Y	616	-	-	2/29/67/67	0/2/2/2
32	CLA	YY	613	9	1/1/18/20	7/32/108/115	-
40	LUT	Nn	306	-	-	1/29/67/67	0/2/2/2
32	CLA	33	611	15	1/1/13/20	6/10/82/115	-
32	CLA	A	405	-	1/1/20/20	13/39/115/115	-
32	CLA	a	405	-	1/1/20/20	13/39/115/115	-
32	CLA	g	614	-	1/1/16/20	10/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	s	604	-	1/1/16/20	10/20/96/115	-
32	CLA	Gg	305	-	1/1/14/20	5/12/88/115	-
32	CLA	Ss	609	4	1/1/16/20	10/20/96/115	-
32	CLA	R	614	3	-	6/20/96/115	-
41	XAT	G	617	-	-	2/31/93/93	0/4/4/4
32	CLA	r	601	3	1/1/16/20	13/20/96/115	-
39	CHL	Yy	608	-	3/3/22/26	4/20/118/137	-
34	BCR	h	101	-	-	7/29/63/63	0/2/2/2
34	BCR	Bb	617	-	-	5/29/63/63	0/2/2/2
32	CLA	GG	613	9	1/1/13/20	5/10/82/115	-
39	CHL	R	607	-	3/3/22/26	6/20/118/137	-
32	CLA	Y	602	9	1/1/20/20	15/39/115/115	-
32	CLA	3	609	15	1/1/13/20	3/10/82/115	-
32	CLA	4	310	-	1/1/15/20	6/15/91/115	-
32	CLA	YY	612	9	1/1/18/20	10/31/107/115	-
32	CLA	N	613	9	1/1/16/20	9/20/96/115	-
33	PHO	D	402	-	-	9/37/103/103	0/5/6/6
32	CLA	44	615	3	1/1/16/20	10/20/96/115	-
34	BCR	B	613	-	-	4/29/63/63	0/2/2/2
34	BCR	D	406	-	-	2/29/63/63	0/2/2/2
32	CLA	Rr	613	3	1/1/16/20	8/20/96/115	-
32	CLA	Ss	612	4	1/1/16/20	7/20/96/115	-
32	CLA	BB	614	-	1/1/20/20	7/39/115/115	-
39	CHL	44	605	-	3/3/21/26	4/15/113/137	-
32	CLA	2	612	14	1/1/13/20	4/10/82/115	-
39	CHL	4	302	-	3/3/21/26	2/13/111/137	-
38	LMG	j	101	-	-	3/41/61/70	0/1/1/1
32	CLA	N	602	9	1/1/20/20	13/39/115/115	-
32	CLA	CC	514	-	1/1/16/20	6/20/96/115	-
32	CLA	Yy	610	9	1/1/20/20	12/39/115/115	-
32	CLA	Cc	513	18	1/1/20/20	8/39/115/115	-
40	LUT	y	318	-	-	2/29/67/67	0/2/2/2
39	CHL	Nn	318	-	3/3/22/26	6/20/118/137	-
44	DGD	B	603	-	-	6/43/83/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	B	611	-	1/1/14/20	2/10/86/115	-
32	CLA	YY	603	-	1/1/16/20	8/20/96/115	-
32	CLA	S	602	4	1/1/16/20	10/20/96/115	-
34	BCR	B	612	-	-	4/29/63/63	0/2/2/2
32	CLA	BB	607	-	1/1/20/20	11/39/115/115	-
38	LMG	c	519	-	-	7/29/49/70	0/1/1/1
34	BCR	Hh	101	-	-	9/29/63/63	0/2/2/2
39	CHL	YY	606	-	3/3/20/26	4/13/111/137	-
36	LHG	SS	301	-	-	4/30/30/53	-
39	CHL	Yy	606	-	3/3/20/26	2/13/111/137	-
32	CLA	SS	314	-	1/1/16/20	5/20/96/115	-
32	CLA	AA	408	-	1/1/19/20	6/33/109/115	-
32	CLA	R	601	3	1/1/16/20	7/20/96/115	-
32	CLA	RR	314	3	-	9/20/96/115	-
39	CHL	s	606	-	3/3/22/26	9/20/118/137	-
32	CLA	Bb	610	-	1/1/20/20	16/39/115/115	-
32	CLA	BB	605	-	1/1/20/20	14/39/115/115	-
32	CLA	2	603	-	1/1/13/20	4/10/82/115	-
32	CLA	CC	504	-	1/1/20/20	15/39/115/115	-
36	LHG	C	522	-	-	9/35/35/53	-
32	CLA	Cc	507	-	1/1/20/20	10/39/115/115	-
32	CLA	22	602	14	1/1/13/20	4/10/82/115	-
32	CLA	B	608	-	1/1/20/20	11/39/115/115	-
44	DGD	c	518	-	-	8/41/81/95	0/2/2/2
32	CLA	Ss	604	-	1/1/16/20	10/20/96/115	-
38	LMG	Aa	412	-	-	7/37/57/70	0/1/1/1
36	LHG	4	301	32	-	6/21/21/53	-
39	CHL	1	607	-	3/3/19/26	4/10/104/137	-
39	CHL	Rr	605	3	3/3/22/26	7/20/118/137	-
41	XAT	G	619	-	-	1/31/93/93	0/4/4/4
32	CLA	GG	611	36	1/1/17/20	9/24/100/115	-
36	LHG	CC	521	-	-	7/38/38/53	-
39	CHL	G	607	-	3/3/21/26	4/15/113/137	-
32	CLA	R	611	-	1/1/16/20	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	N	608	-	3/3/20/26	2/10/108/137	-
34	BCR	H	101	-	-	3/29/63/63	0/2/2/2
32	CLA	11	603	-	1/1/13/20	4/10/82/115	-
32	CLA	Nn	303	9	1/1/16/20	5/20/96/115	-
40	LUT	NN	616	-	-	2/29/67/67	0/2/2/2
32	CLA	Ss	611	4	1/1/16/20	9/20/96/115	-
32	CLA	1	612	14	1/1/13/20	0/10/82/115	-
39	CHL	1	605	14	3/3/19/26	2/10/104/137	-
32	CLA	g	604	42	1/1/14/20	5/12/88/115	-
39	CHL	G	608	-	3/3/20/26	5/10/108/137	-
32	CLA	2	613	-	1/1/13/20	4/10/82/115	-
32	CLA	C	505	-	1/1/20/20	17/39/115/115	-
32	CLA	c	506	-	1/1/20/20	18/39/115/115	-
32	CLA	Bb	608	-	1/1/20/20	12/39/115/115	-
39	CHL	22	608	14	3/3/19/26	2/10/104/137	-
37	SQD	LL	102	-	-	16/49/69/69	0/1/1/1
32	CLA	GG	610	9	1/1/16/20	6/20/96/115	-
39	CHL	RR	306	-	3/3/21/26	9/20/118/137	-
32	CLA	b	613	-	1/1/20/20	14/39/115/115	-
36	LHG	DD	408	-	-	8/53/53/53	-
32	CLA	CC	509	-	1/1/20/20	11/39/115/115	-
32	CLA	BB	609	-	-	12/39/115/115	-
39	CHL	3	606	-	3/3/19/26	2/10/104/137	-
32	CLA	DD	404	-	1/1/20/20	10/39/115/115	-
32	CLA	n	614	-	1/1/16/20	8/20/96/115	-
32	CLA	Yy	613	9	1/1/18/20	7/32/108/115	-
32	CLA	1	613	-	1/1/13/20	6/10/82/115	-
36	LHG	Dd	407	-	-	3/41/41/53	-
39	CHL	GG	606	-	3/3/20/26	4/12/110/137	-
32	CLA	s	609	4	1/1/16/20	10/20/96/115	-
32	CLA	BB	611	-	1/1/20/20	5/39/115/115	-
32	CLA	BB	602	-	1/1/20/20	17/39/115/115	-
34	BCR	BB	616	-	-	4/29/63/63	0/2/2/2
32	CLA	c	509	-	1/1/20/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	Y	609	9	3/3/26/26	10/39/137/137	-
34	BCR	TT	101	-	-	5/29/63/63	0/2/2/2
32	CLA	Cc	511	-	1/1/20/20	15/39/115/115	-
32	CLA	B	624	-	1/1/20/20	11/39/115/115	-
37	SQD	A	412	-	-	6/30/50/69	0/1/1/1
32	CLA	1	609	14	1/1/13/20	4/10/82/115	-
44	DGD	B	601	-	-	7/44/84/95	0/2/2/2
39	CHL	RR	307	-	3/3/22/26	6/20/118/137	-
32	CLA	r	613	3	1/1/16/20	9/20/96/115	-
32	CLA	Nn	305	-	-	9/20/96/115	-
32	CLA	Aa	407	-	1/1/16/20	8/20/96/115	-
32	CLA	22	612	14	1/1/13/20	2/10/82/115	-
39	CHL	g	601	9	3/3/26/26	11/39/137/137	-
32	CLA	22	611	14	1/1/13/20	6/10/82/115	-
36	LHG	GG	618	32	-	6/38/38/53	-
32	CLA	R	604	-	1/1/16/20	8/20/96/115	-
44	DGD	h	102	-	-	8/51/91/95	0/2/2/2
32	CLA	4	303	11	1/1/15/20	8/15/91/115	-
32	CLA	s	612	4	1/1/16/20	7/20/96/115	-
39	CHL	s	605	-	3/3/22/26	9/20/118/137	-
32	CLA	B	607	-	1/1/20/20	7/39/115/115	-
32	CLA	RR	313	-	1/1/14/20	4/10/86/115	-
34	BCR	Dd	403	-	-	4/29/63/63	0/2/2/2
39	CHL	G	606	-	3/3/20/26	4/12/110/137	-
32	CLA	Bb	606	-	1/1/20/20	8/39/115/115	-
37	SQD	CC	501	-	-	13/49/69/69	0/1/1/1
40	LUT	N	616	-	-	2/29/67/67	0/2/2/2
32	CLA	CC	502	-	1/1/20/20	12/39/115/115	-
39	CHL	g	606	-	3/3/20/26	4/12/110/137	-
44	DGD	Cc	520	-	-	9/41/81/95	0/2/2/2
32	CLA	a	407	-	1/1/16/20	6/20/96/115	-
34	BCR	b	617	-	-	4/29/63/63	0/2/2/2
40	LUT	y	317	-	-	3/29/67/67	0/2/2/2
32	CLA	b	601	-	1/1/20/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	Bb	616	-	1/1/20/20	12/39/115/115	-
39	CHL	2	601	14	3/3/19/26	2/10/104/137	-
38	LMG	Bb	620	-	-	4/31/51/70	0/1/1/1
39	CHL	2	606	-	3/3/19/26	4/10/104/137	-
32	CLA	b	602	-	1/1/20/20	11/39/115/115	-
40	LUT	s	614	-	-	2/29/67/67	0/2/2/2
39	CHL	n	605	9	3/3/21/26	6/18/116/137	-
36	LHG	K	101	-	-	11/38/38/53	-
32	CLA	CC	513	-	1/1/20/20	9/39/115/115	-
39	CHL	n	609	9	3/3/22/26	4/20/118/137	-
39	CHL	4	306	-	3/3/21/26	4/15/113/137	-
39	CHL	SS	307	-	3/3/20/26	0/10/108/137	-
32	CLA	Y	613	9	1/1/18/20	11/32/108/115	-
32	CLA	C	511	-	1/1/20/20	14/39/115/115	-
39	CHL	NN	605	9	3/3/20/26	4/10/108/137	-
38	LMG	B	615	-	-	8/40/60/70	0/1/1/1
39	CHL	NN	609	9	3/3/22/26	4/20/118/137	-
39	CHL	Yy	601	9	3/3/26/26	12/39/137/137	-
32	CLA	y	314	9	1/1/20/20	12/39/115/115	-
38	LMG	Cc	501	-	-	7/29/49/70	0/1/1/1
32	CLA	Rr	602	3	1/1/20/20	12/39/115/115	-
32	CLA	AA	406	-	1/1/16/20	9/20/96/115	-
39	CHL	Gg	308	-	3/3/22/26	8/20/118/137	-
32	CLA	Bb	612	-	1/1/20/20	15/39/115/115	-
32	CLA	Cc	505	-	1/1/20/20	11/39/115/115	-
32	CLA	Yy	611	36	1/1/14/20	5/12/88/115	-
32	CLA	NN	614	-	1/1/14/20	4/10/86/115	-
32	CLA	CC	507	-	1/1/20/20	10/39/115/115	-
41	XAT	y	302	-	-	1/31/93/93	0/4/4/4
32	CLA	Nn	304	9	1/1/16/20	7/20/96/115	-
32	CLA	Rr	601	3	1/1/16/20	13/20/96/115	-
40	LUT	YY	616	-	-	2/29/67/67	0/2/2/2
32	CLA	2	610	-	1/1/13/20	4/10/82/115	-
32	CLA	b	616	-	1/1/20/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CLA	c	507	-	1/1/20/20	10/39/115/115	-
32	CLA	Bb	614	-	1/1/20/20	7/39/115/115	-
34	BCR	T	101	-	-	3/29/63/63	0/2/2/2
32	CLA	SS	313	4	1/1/16/20	8/20/96/115	-
32	CLA	X	201	-	1/1/14/20	4/10/86/115	-
39	CHL	33	601	15	3/3/19/26	4/10/104/137	-
36	LHG	A	414	-	-	9/49/49/53	-
38	LMG	AA	415	-	-	4/31/51/70	0/1/1/1
32	CLA	CC	510	-	1/1/20/20	14/39/115/115	-
39	CHL	R	605	-	3/3/22/26	7/20/118/137	-
32	CLA	s	603	-	1/1/16/20	12/20/96/115	-
40	LUT	RR	315	-	-	2/29/67/67	0/2/2/2
32	CLA	c	512	-	1/1/20/20	8/39/115/115	-
40	LUT	Nh	307	-	-	2/29/67/67	0/2/2/2
32	CLA	BB	608	-	1/1/20/20	11/39/115/115	-
34	BCR	B	616	-	-	4/29/63/63	0/2/2/2
36	LHG	44	616	32	-	7/21/21/53	-
39	CHL	Ss	605	-	3/3/22/26	11/20/118/137	-
42	NEX	RR	317	-	-	3/27/83/83	0/3/3/3
32	CLA	C	509	-	1/1/20/20	12/39/115/115	-
32	CLA	G	610	9	1/1/16/20	9/20/96/115	-
40	LUT	44	612	-	-	2/29/67/67	0/2/2/2
32	CLA	r	609	3	1/1/20/20	11/39/115/115	-
32	CLA	c	513	-	1/1/14/20	9/13/89/115	-
36	LHG	A	413	-	-	11/41/41/53	-
39	CHL	Y	601	9	3/3/26/26	12/39/137/137	-
32	CLA	B	619	-	1/1/20/20	18/39/115/115	-
32	CLA	YY	614	-	1/1/16/20	12/20/96/115	-
39	CHL	YY	601	9	3/3/26/26	13/39/137/137	-
32	CLA	4	304	-	1/1/15/20	8/15/91/115	-
39	CHL	4	309	11	3/3/21/26	6/15/113/137	-
40	LUT	g	615	-	-	1/29/67/67	0/2/2/2
32	CLA	RR	309	3	1/1/20/20	11/39/115/115	-
44	DGD	C	523	-	-	9/41/81/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	XAT	GG	619	-	-	1/31/93/93	0/4/4/4
41	XAT	RR	316	-	-	0/31/93/93	0/4/4/4
32	CLA	DD	401	-	1/1/20/20	8/39/115/115	-
32	CLA	b	608	-	1/1/20/20	10/39/115/115	-
39	CHL	1	608	14	3/3/19/26	2/10/104/137	-
32	CLA	CC	505	-	1/1/20/20	9/39/115/115	-
38	LMG	A	415	-	-	4/31/51/70	0/1/1/1
36	LHG	Ss	616	32	-	7/52/52/53	-
39	CHL	n	601	9	3/3/22/26	5/20/118/137	-
32	CLA	C	510	-	1/1/20/20	10/39/115/115	-
32	CLA	B	604	-	1/1/20/20	10/39/115/115	-
38	LMG	Dd	408	-	-	5/41/61/70	0/1/1/1
42	NEX	NN	618	-	-	2/27/83/83	0/3/3/3
32	CLA	G	614	-	1/1/14/20	4/10/86/115	-
32	CLA	3	603	-	1/1/13/20	6/10/82/115	-
36	LHG	A	411	-	-	11/38/38/53	-
32	CLA	Gg	304	-	1/1/20/20	13/39/115/115	-
39	CHL	n	608	-	3/3/22/26	7/20/118/137	-

The worst 5 of 4369 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	r	606	CHL	C3B-C4B	11.64	1.52	1.41
39	22	605	CHL	C3B-C4B	11.60	1.52	1.41
39	33	607	CHL	C3B-C4B	11.54	1.52	1.41
39	22	606	CHL	C3B-C4B	11.51	1.52	1.41
39	Rr	605	CHL	C3B-C4B	11.50	1.52	1.41

The worst 5 of 5348 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BB	621	SQD	O9-S-C6	-15.25	83.99	106.76
37	B	617	SQD	O9-S-C6	-15.19	84.07	106.76
41	G	619	XAT	O24-C25-C24	11.36	124.14	113.49
41	GG	619	XAT	O24-C25-C24	11.33	124.11	113.49
37	BB	621	SQD	O8-S-O9	-11.31	83.10	111.40

5 of 780 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
32	A	405	CLA	ND
32	A	406	CLA	ND
32	A	408	CLA	ND
32	Rr	601	CLA	ND
32	Rr	602	CLA	ND

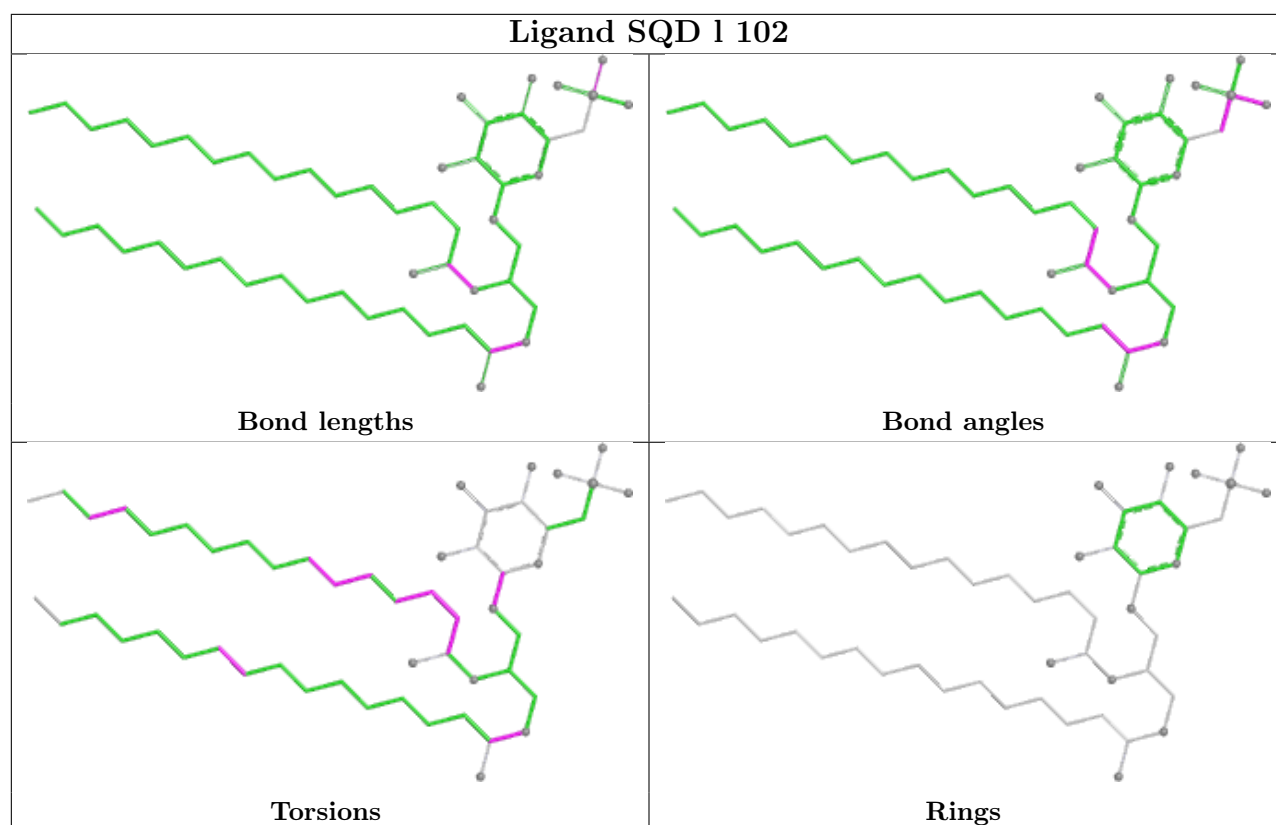
5 of 5624 torsion outliers are listed below:

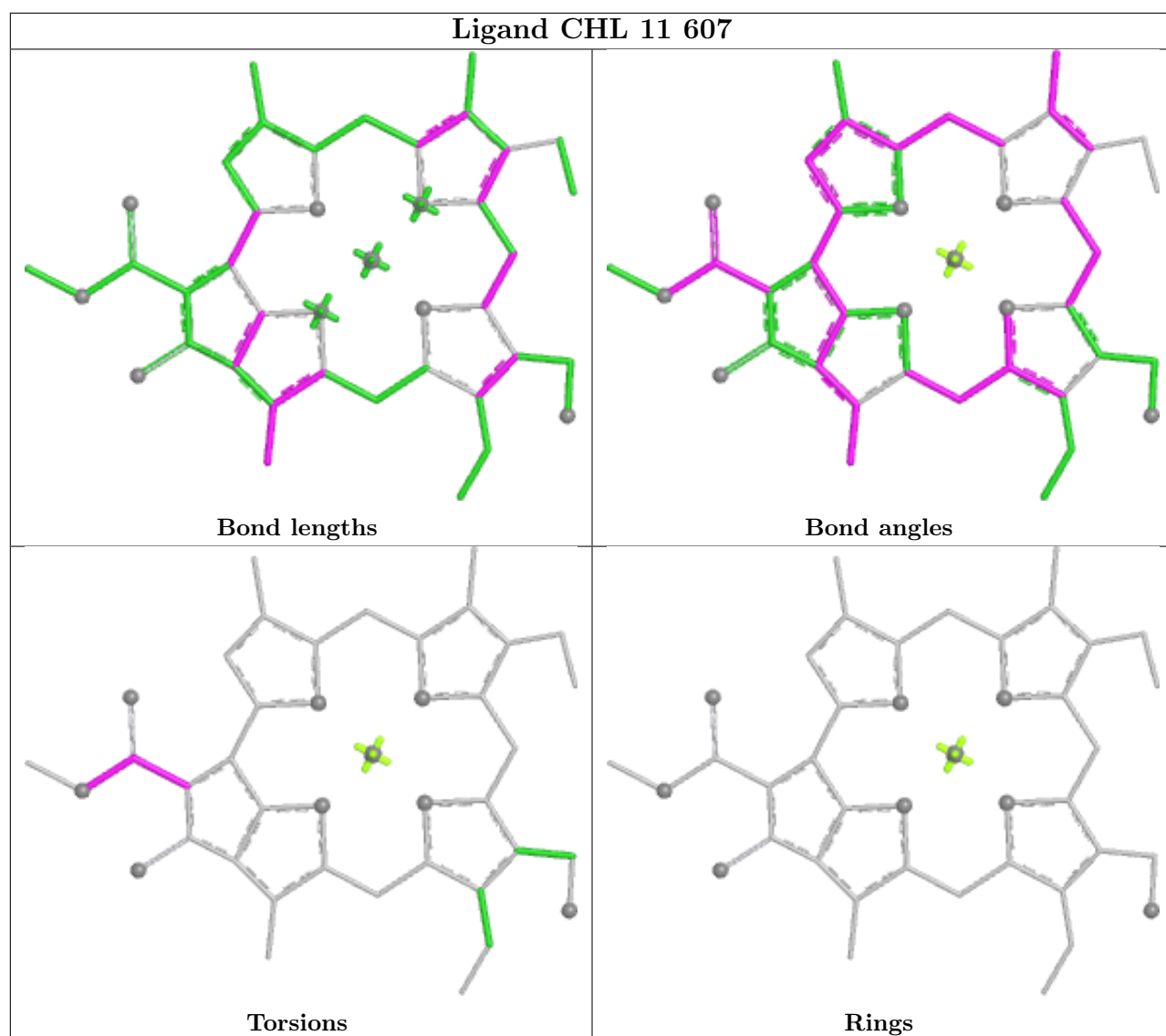
Mol	Chain	Res	Type	Atoms
32	A	408	CLA	CAD-CBD-CGD-O1D
32	A	408	CLA	CAD-CBD-CGD-O2D
32	Rr	601	CLA	C2B-C3B-CAB-CBB
32	Rr	601	CLA	C4B-C3B-CAB-CBB
32	Rr	601	CLA	CHA-CBD-CGD-O1D

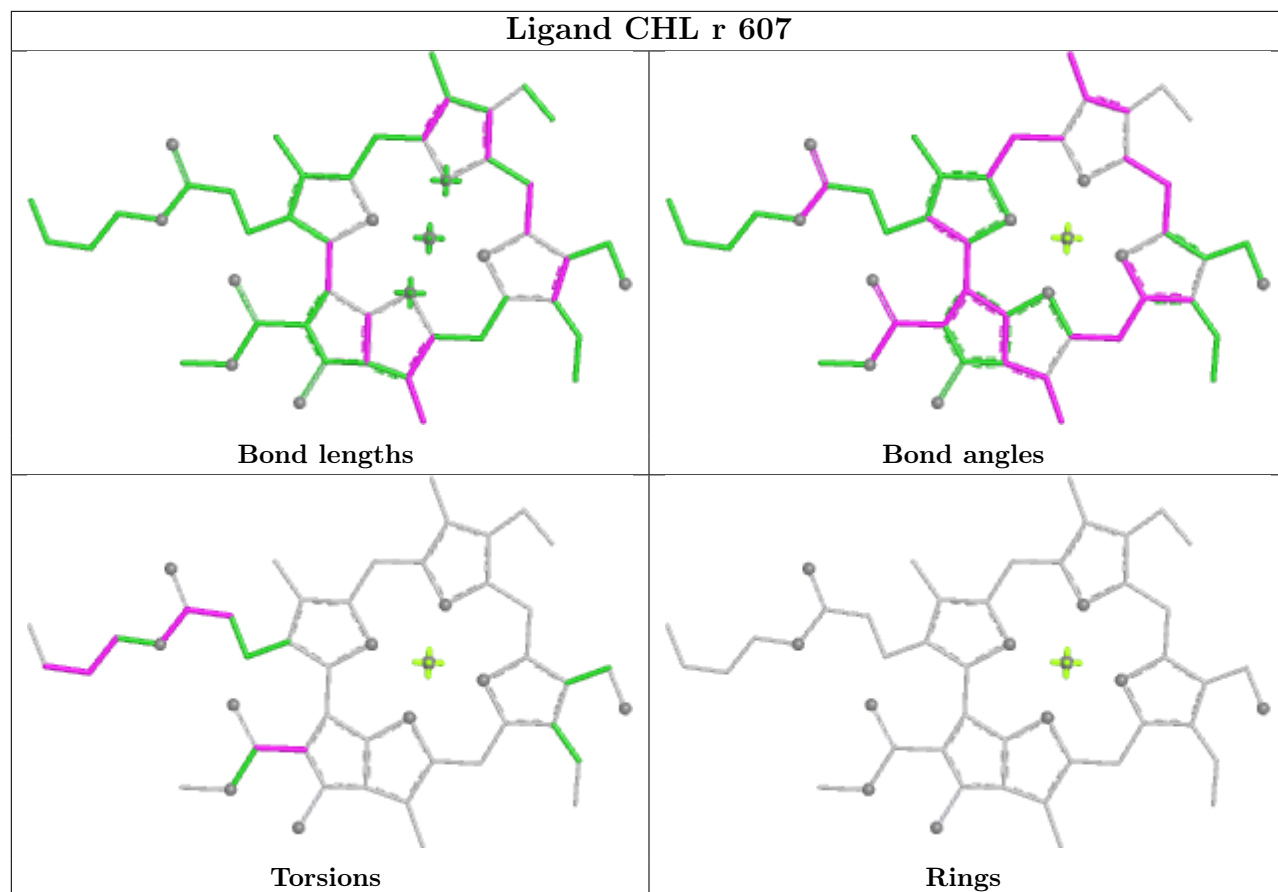
There are no ring outliers.

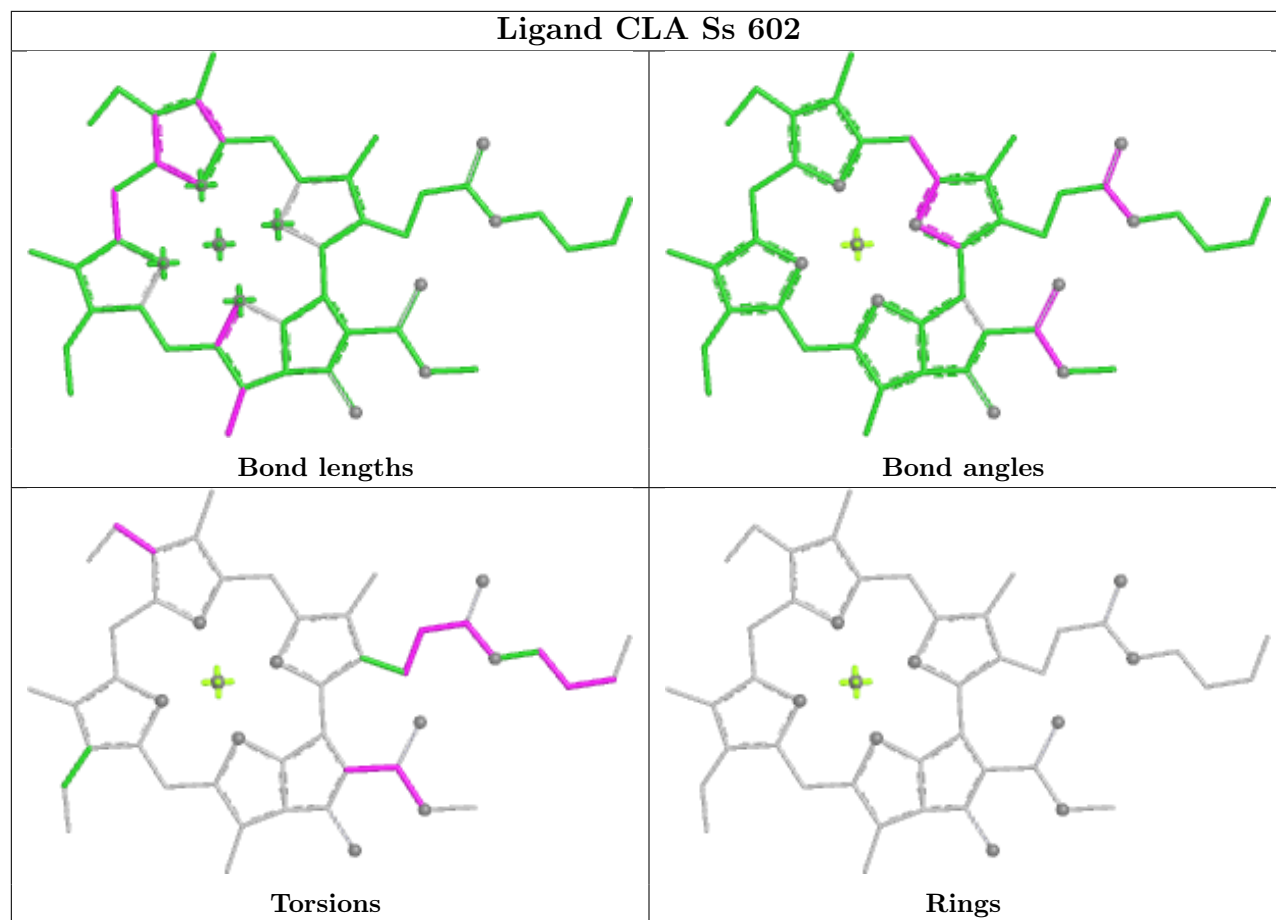
No monomer is involved in short contacts.

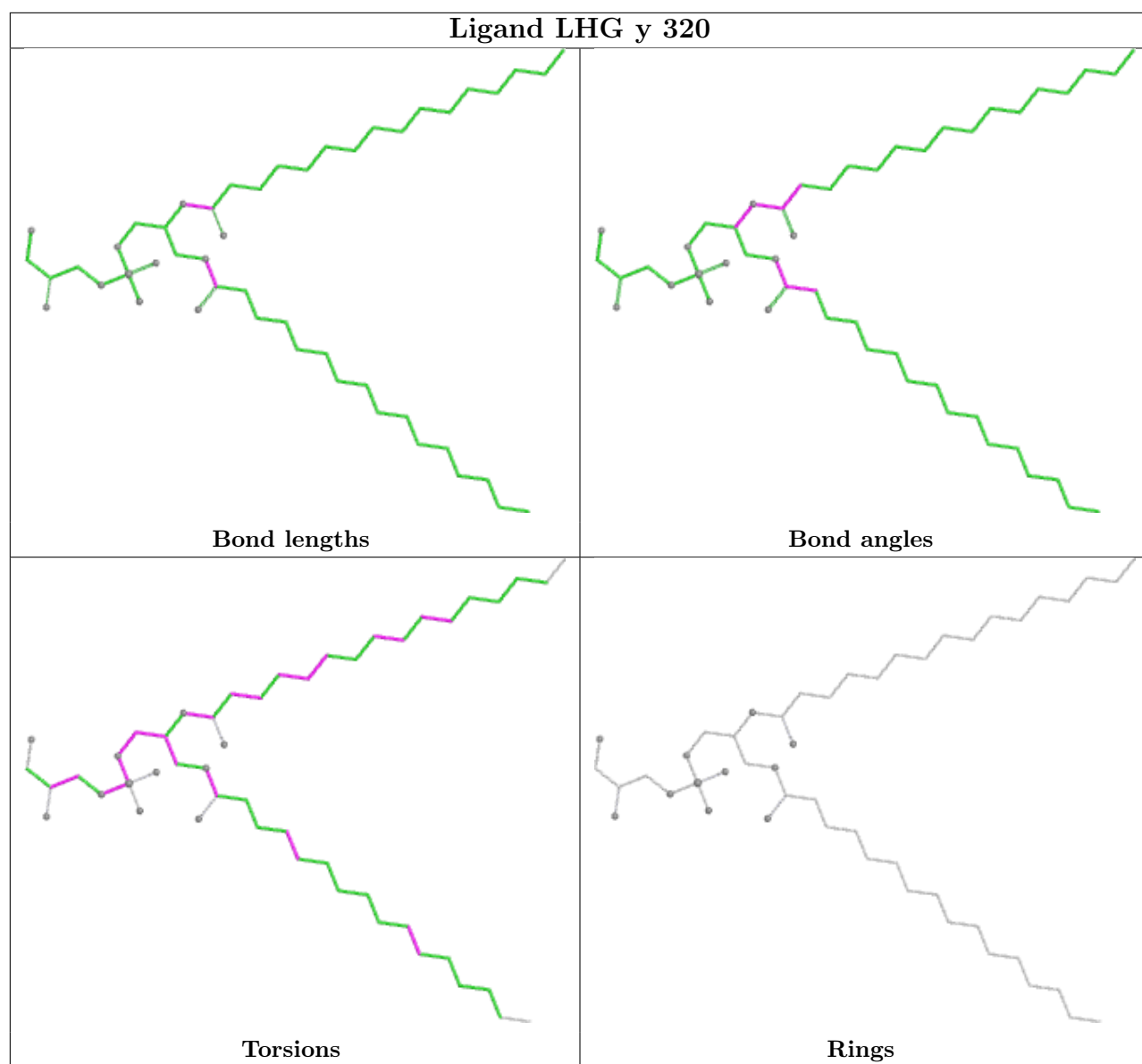
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



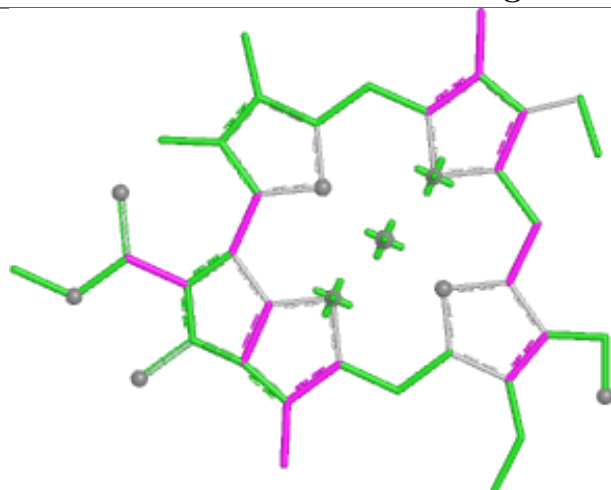




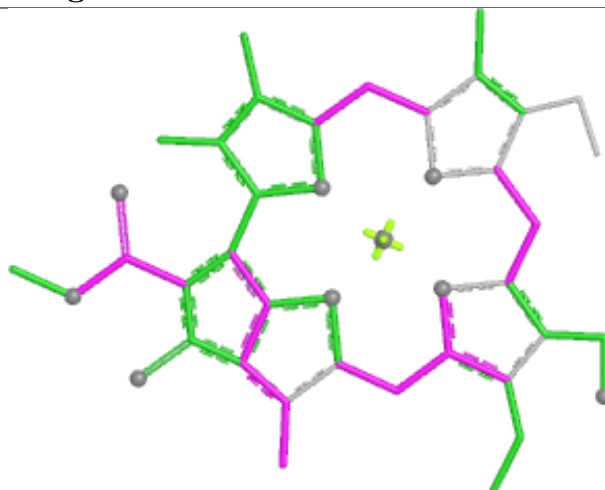




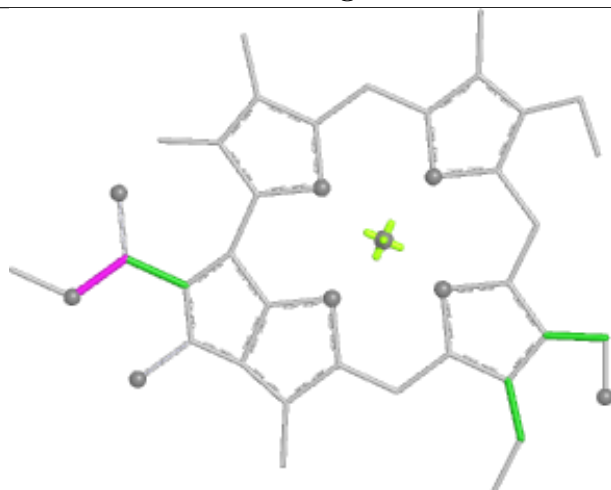
Ligand CHL Gg 309



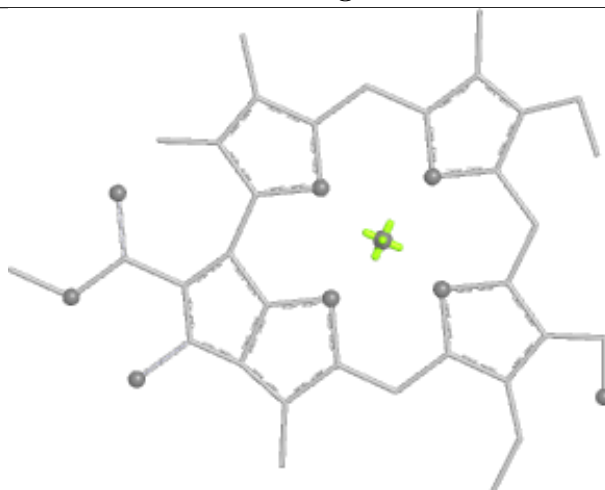
Bond lengths



Bond angles

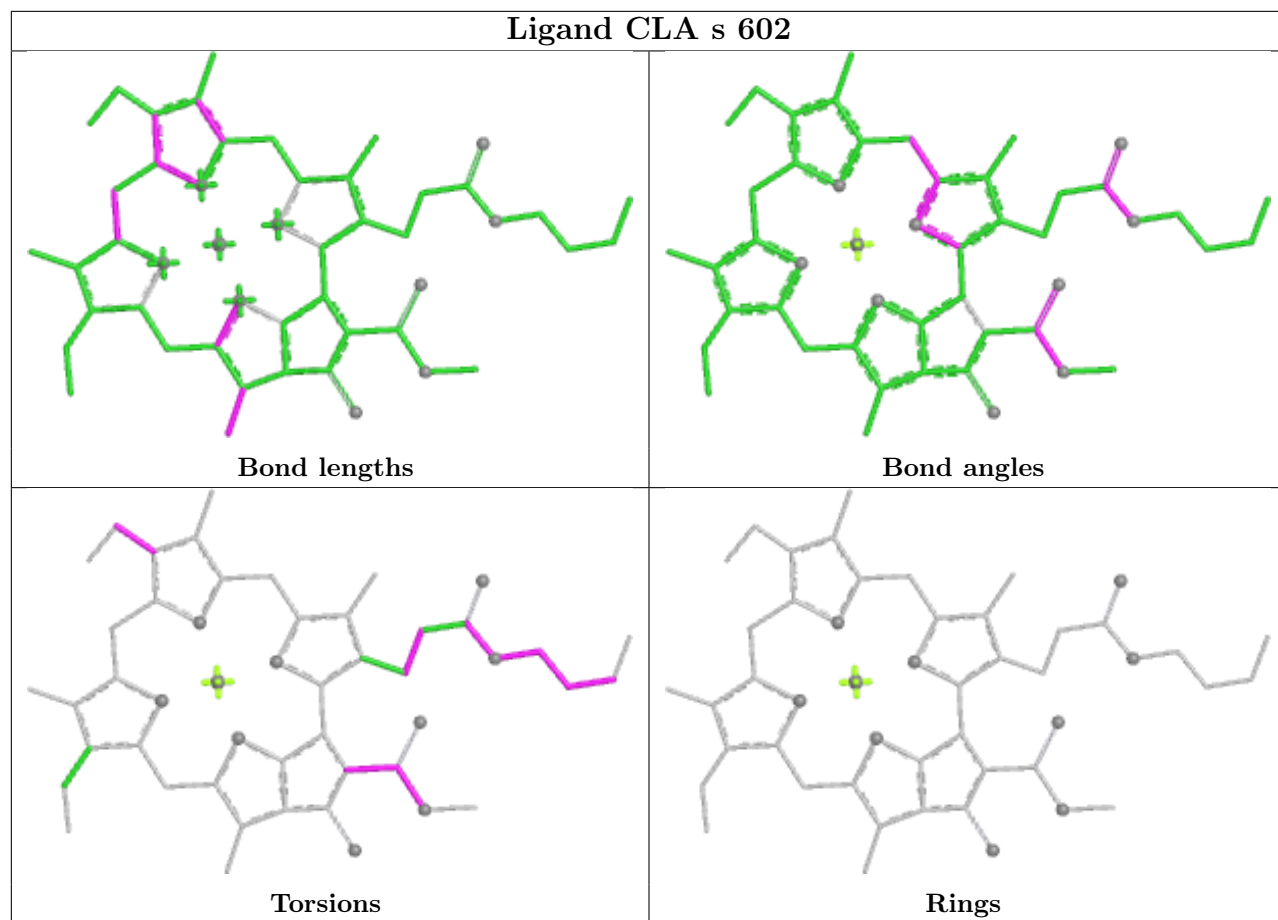


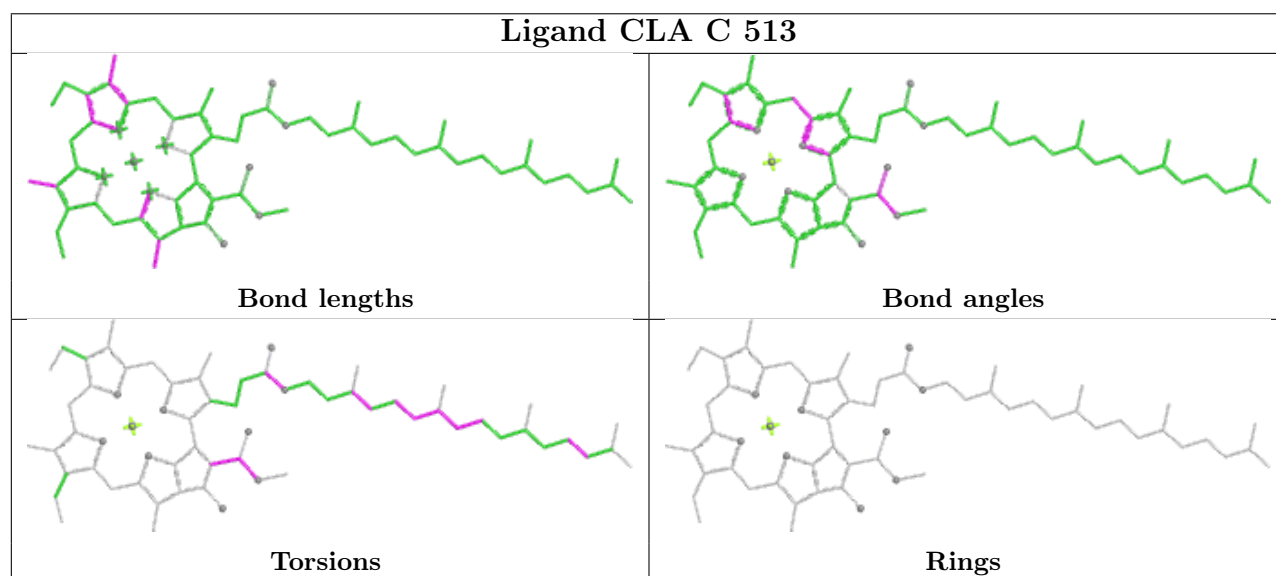
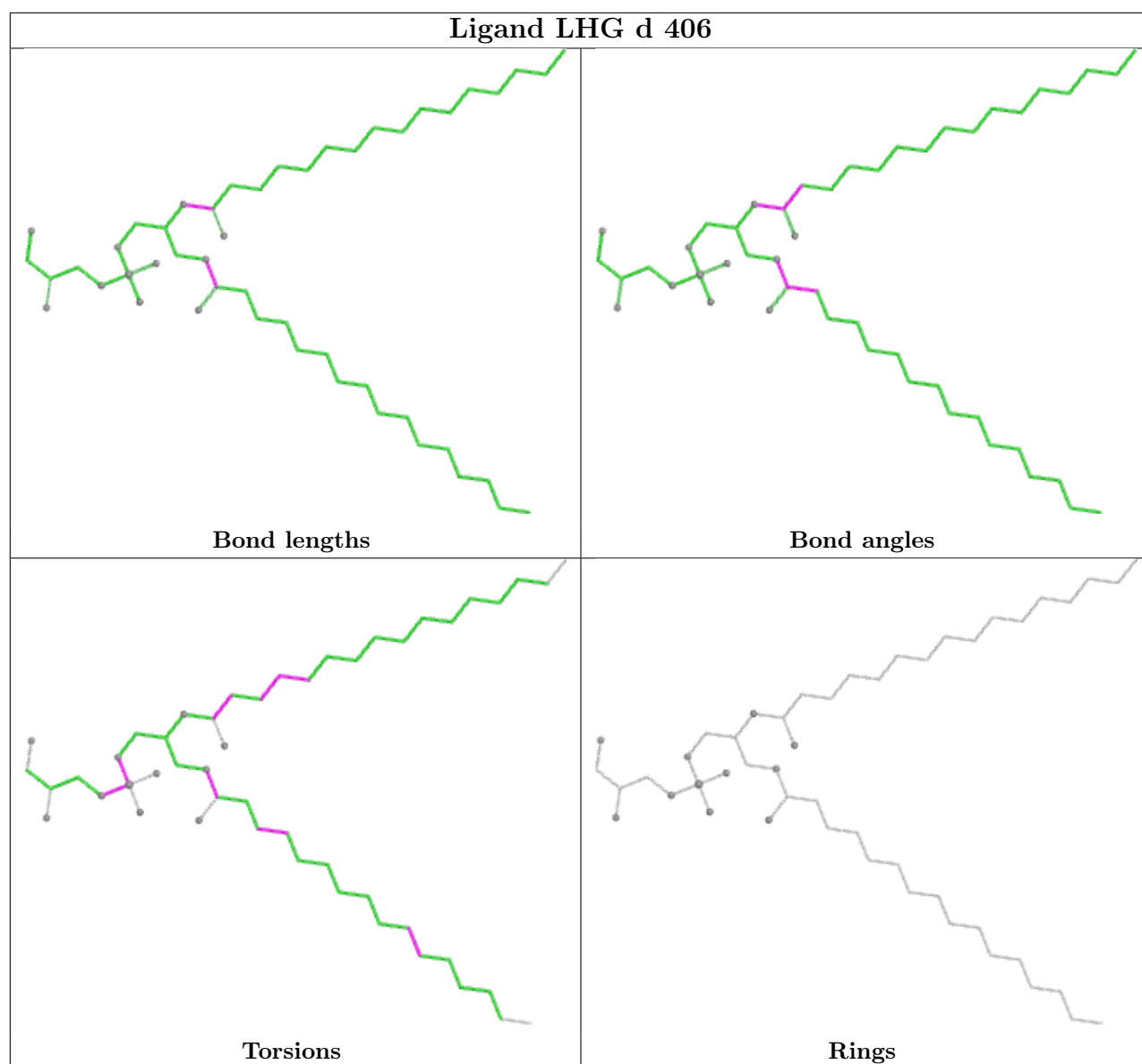
Torsions



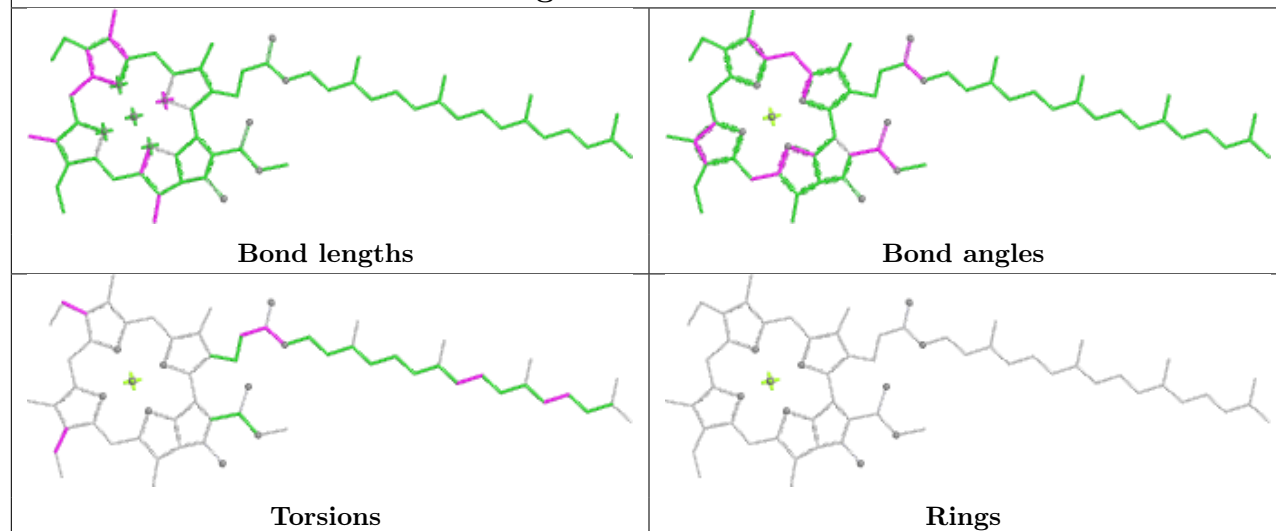
Rings

Ligand CLA s 602

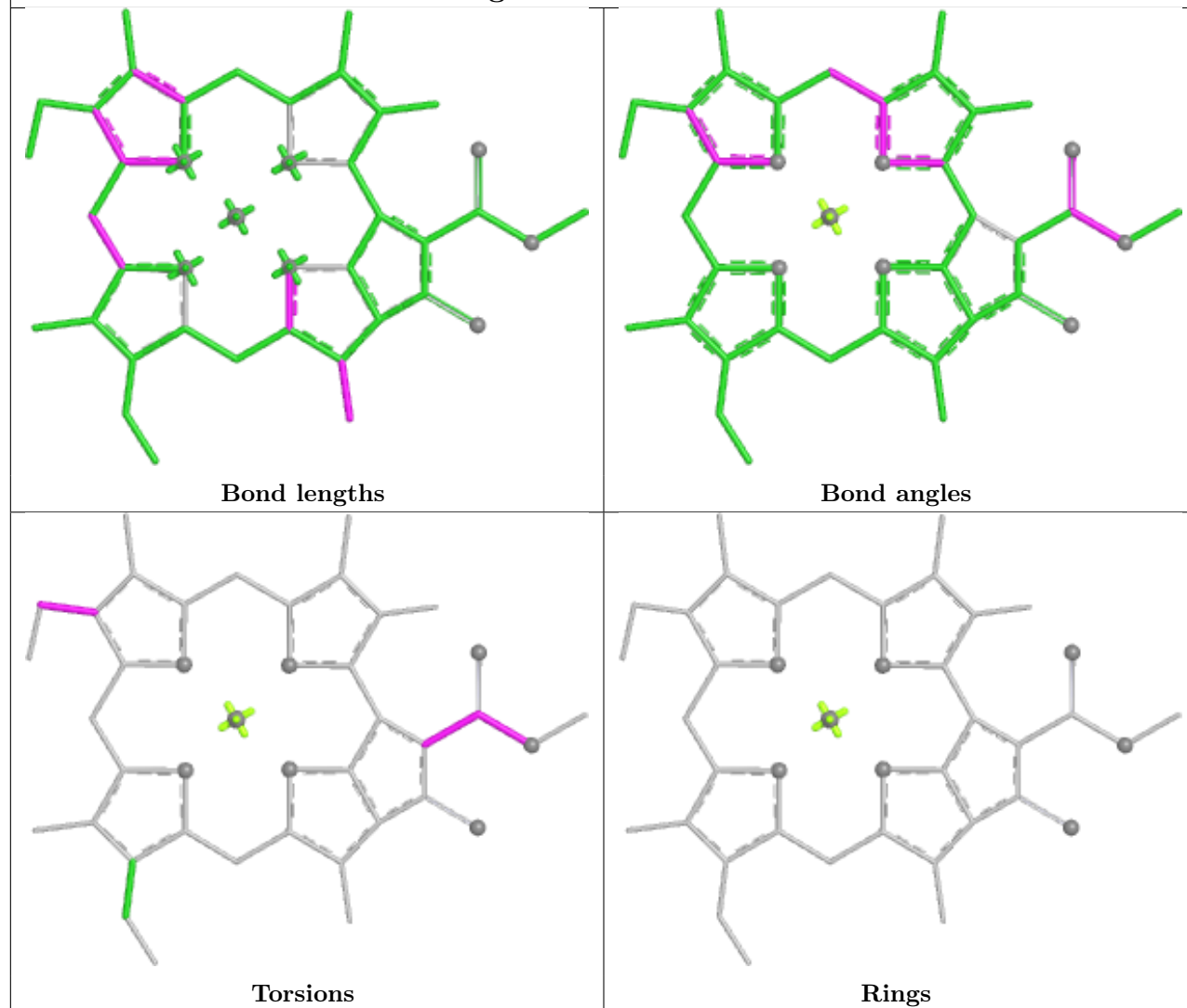




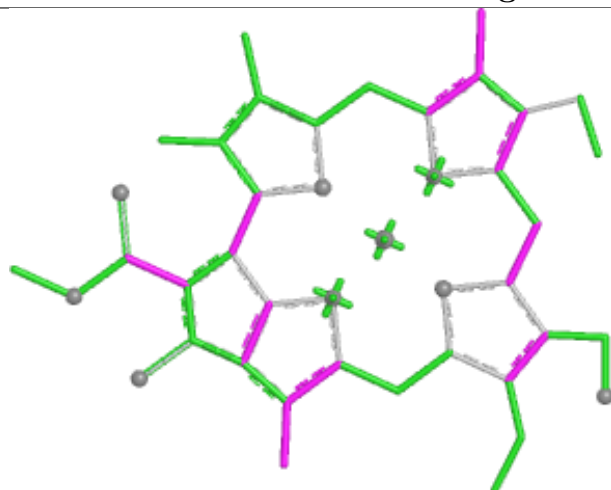
Ligand CLA a 406



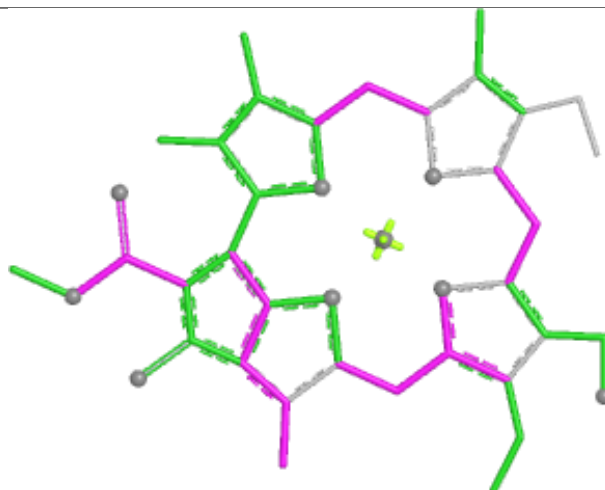
Ligand CLA SS 309



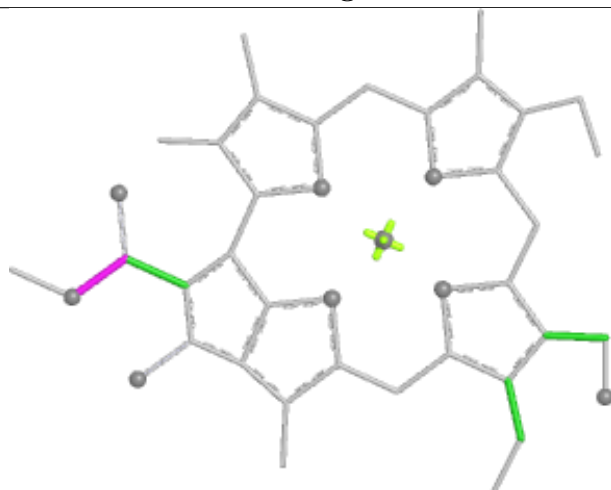
Ligand CHL NN 608



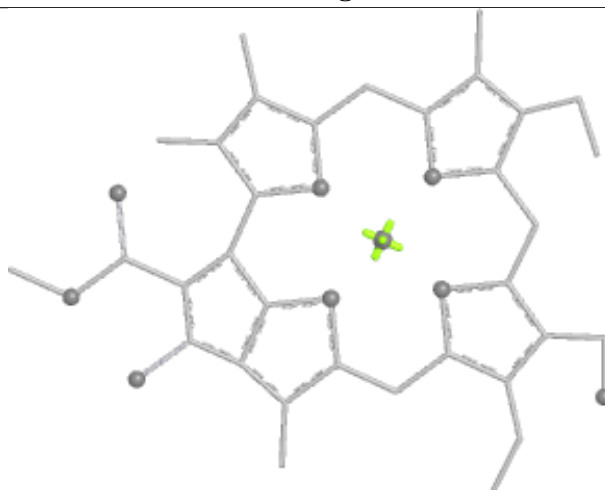
Bond lengths



Bond angles

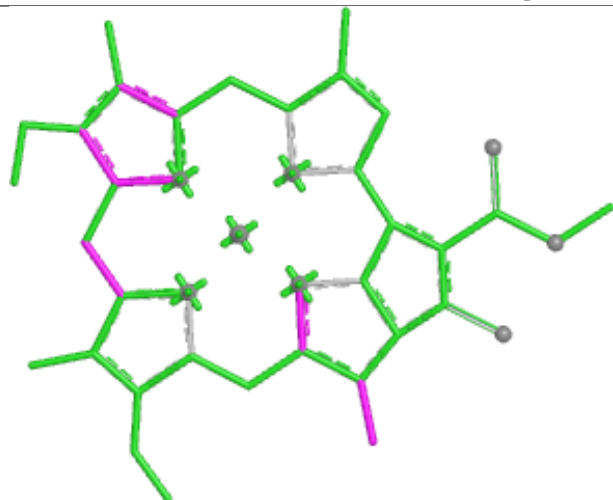


Torsions

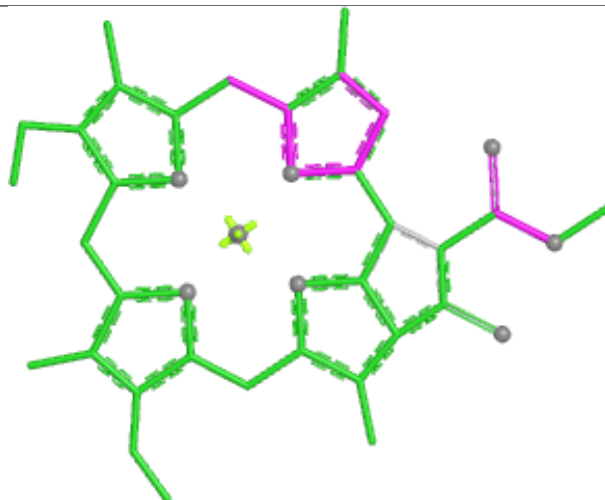


Rings

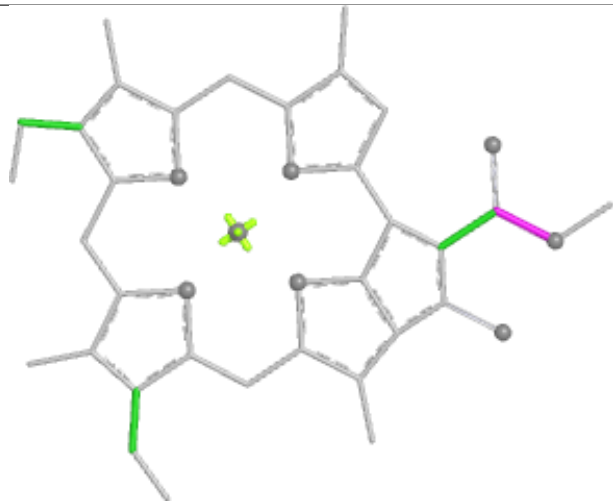
Ligand CLA 1 602



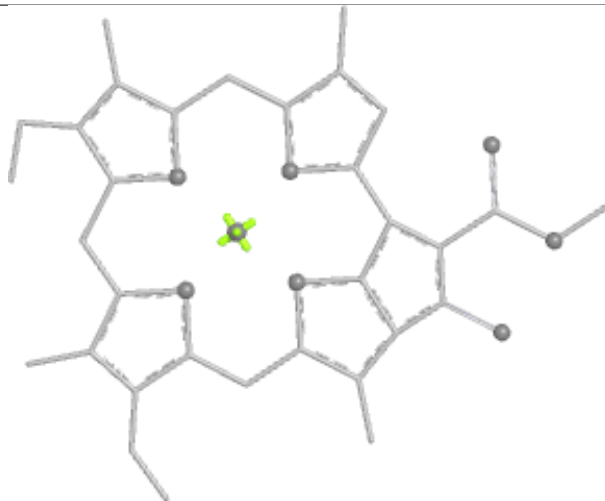
Bond lengths



Bond angles

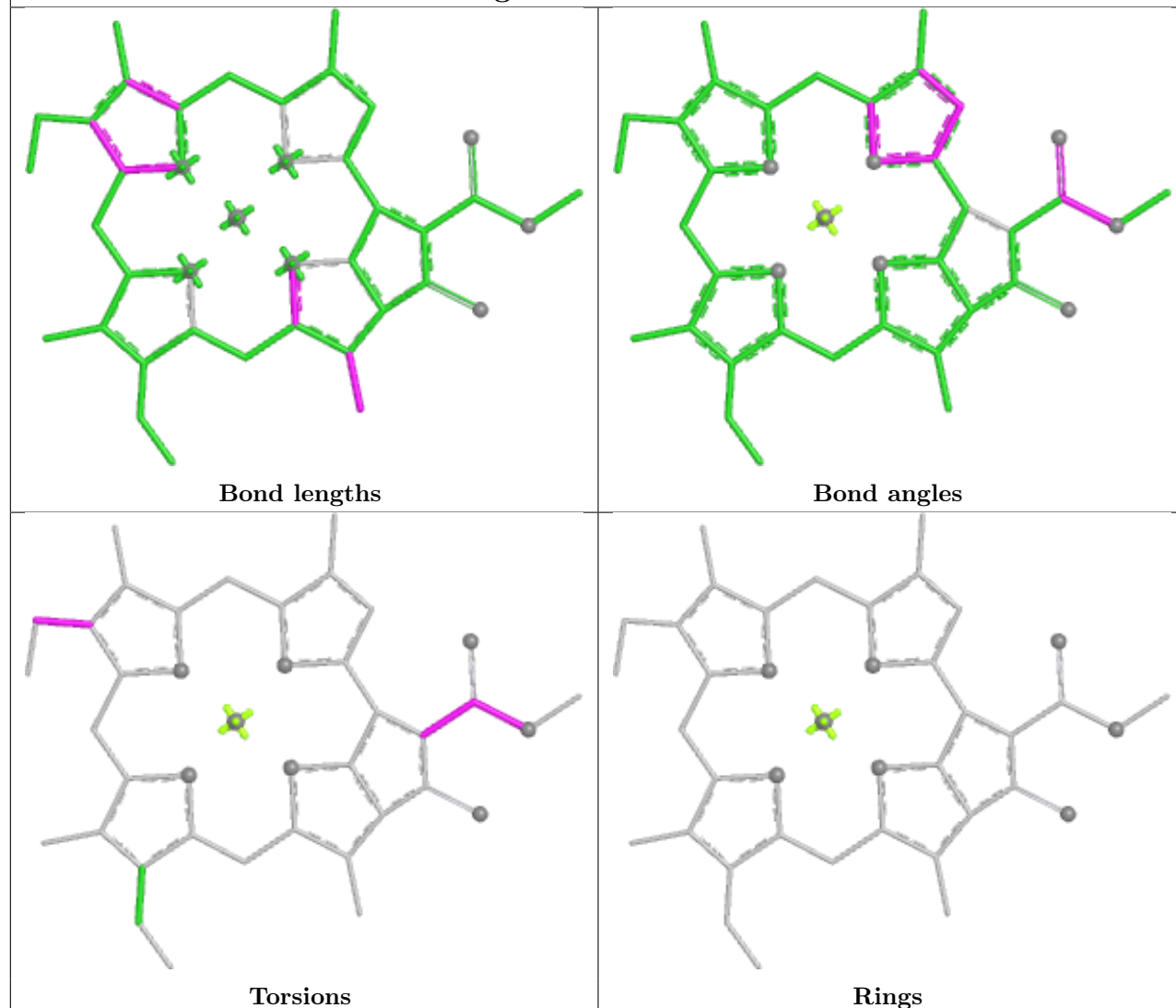


Torsions

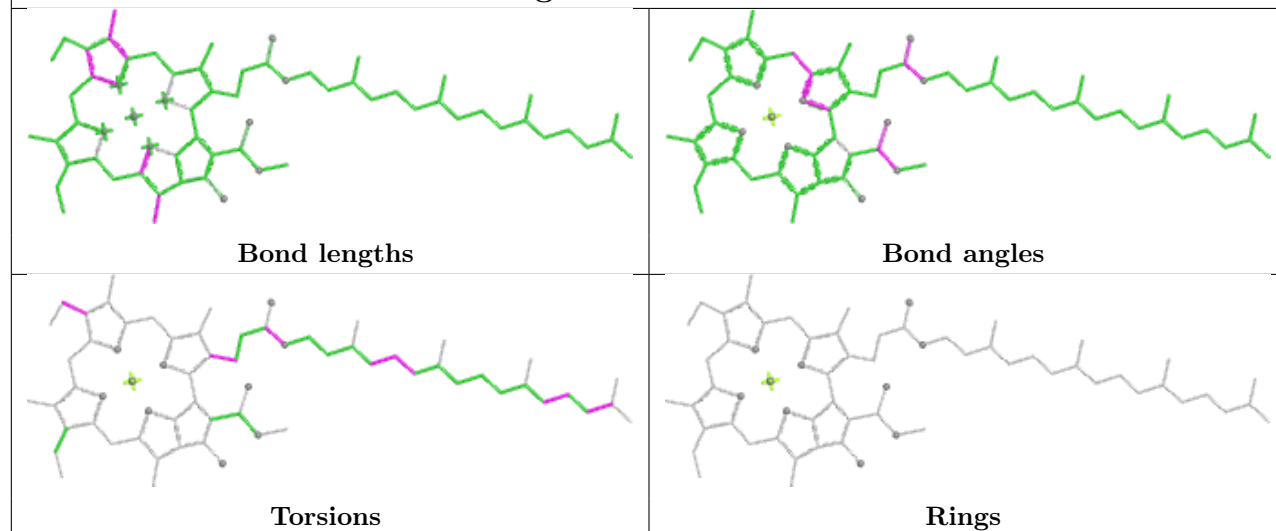


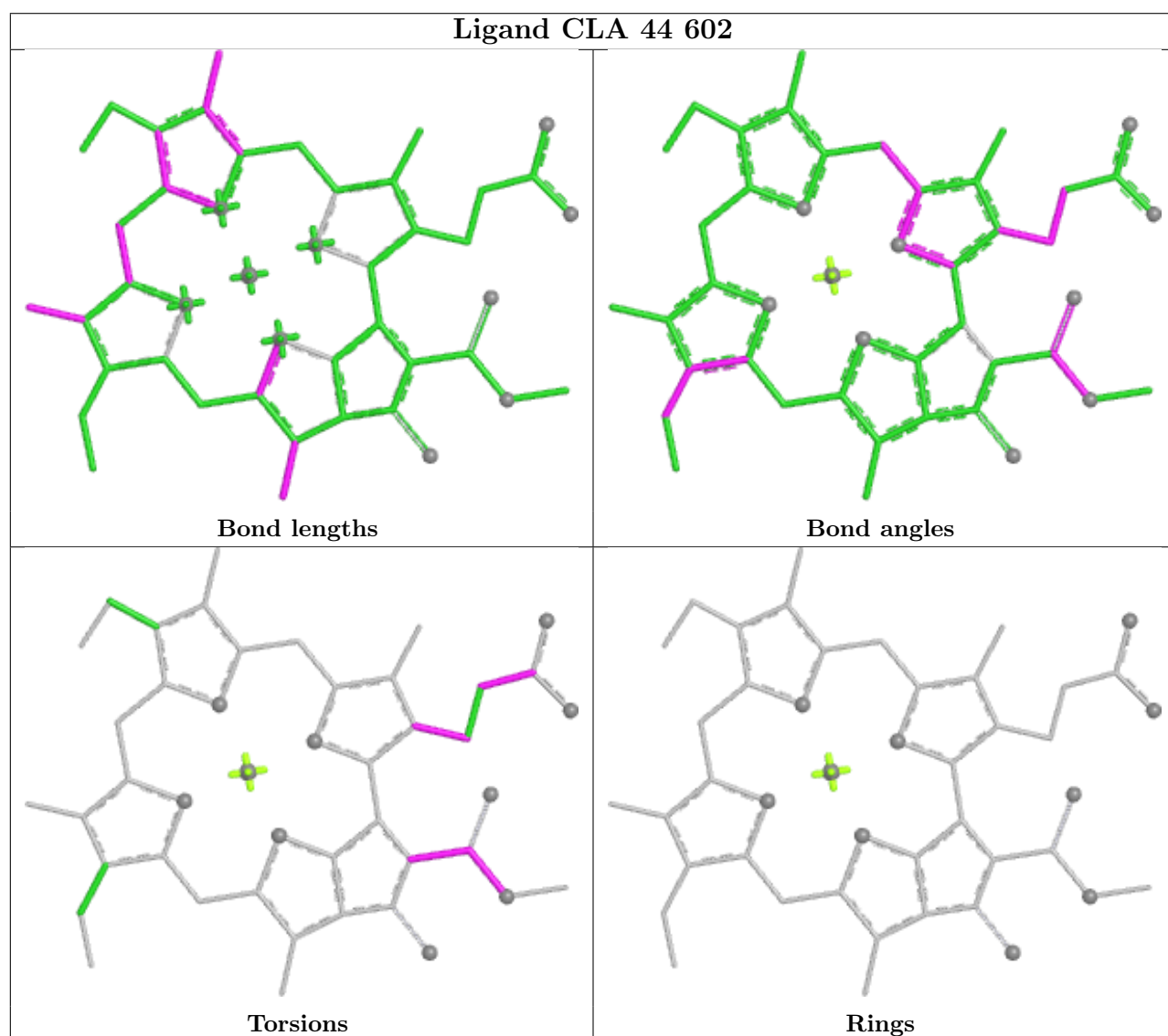
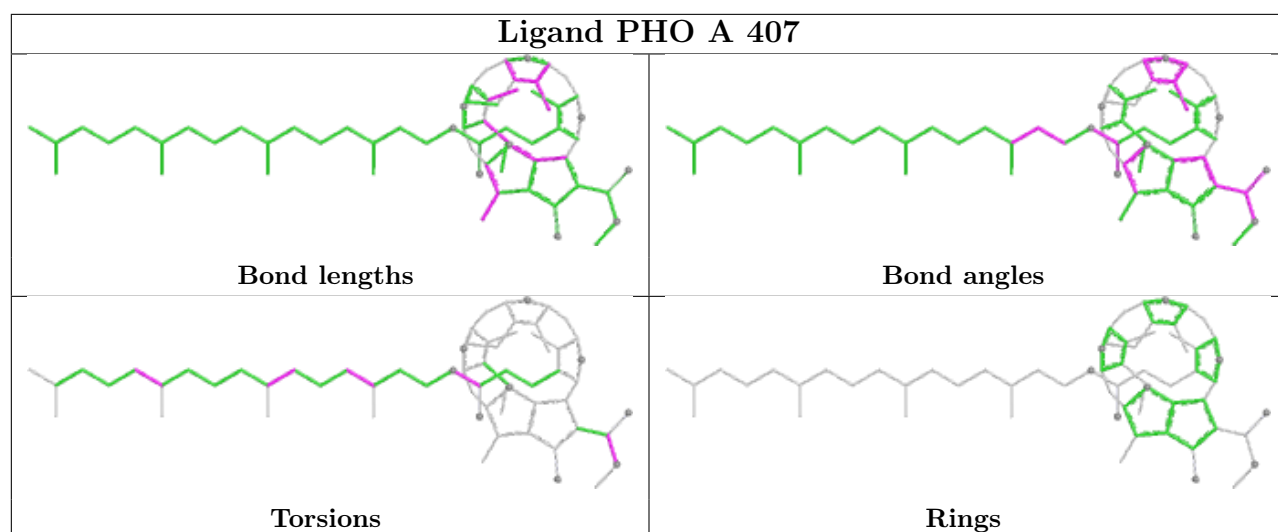
Rings

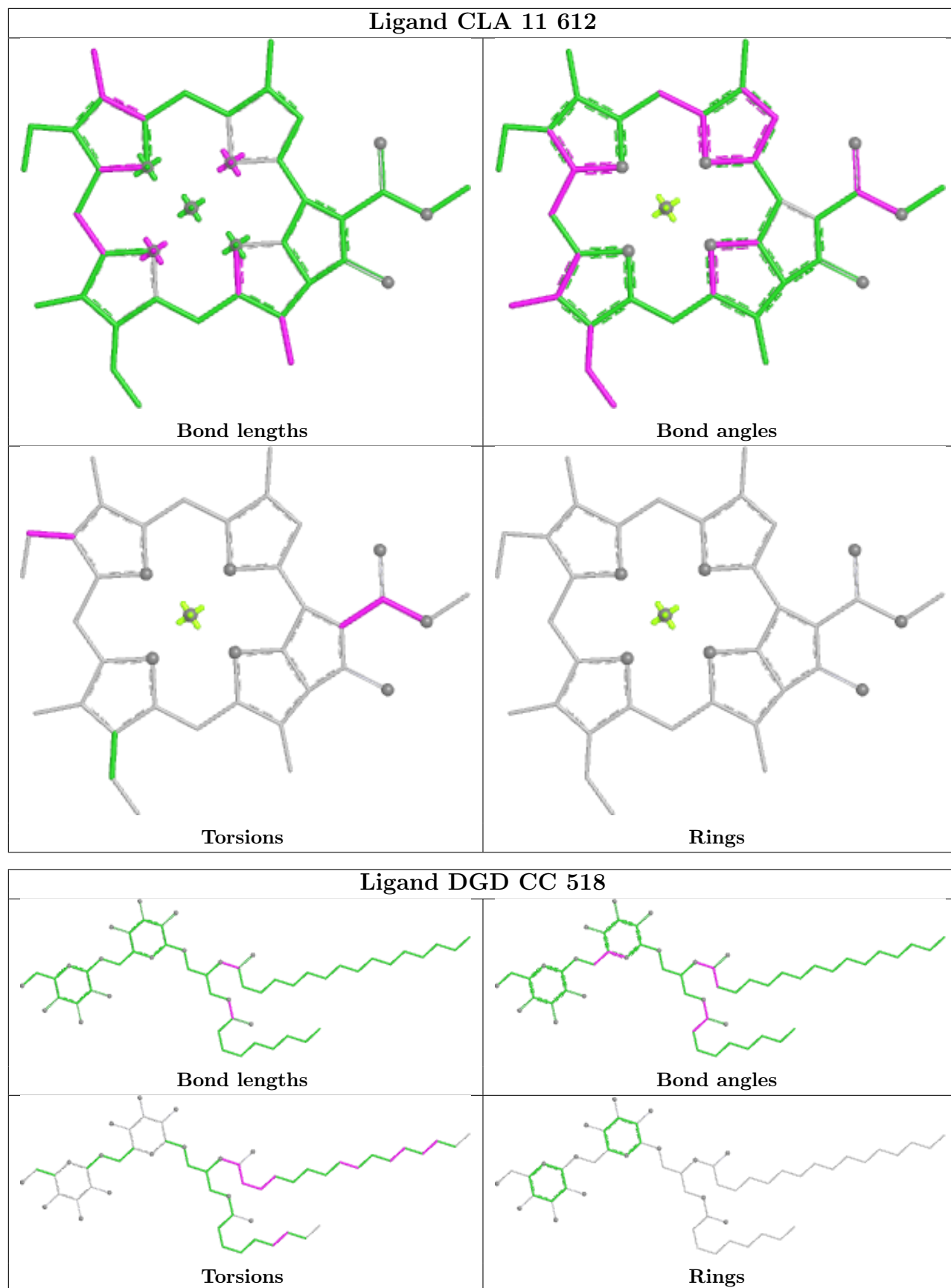
Ligand CLA 1 610

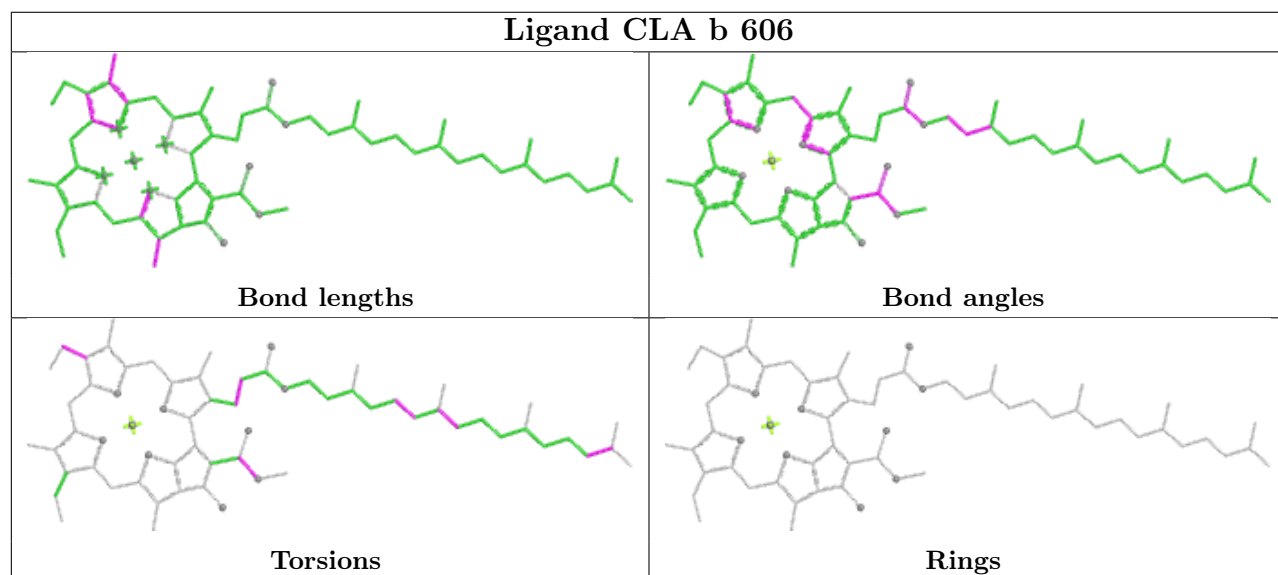
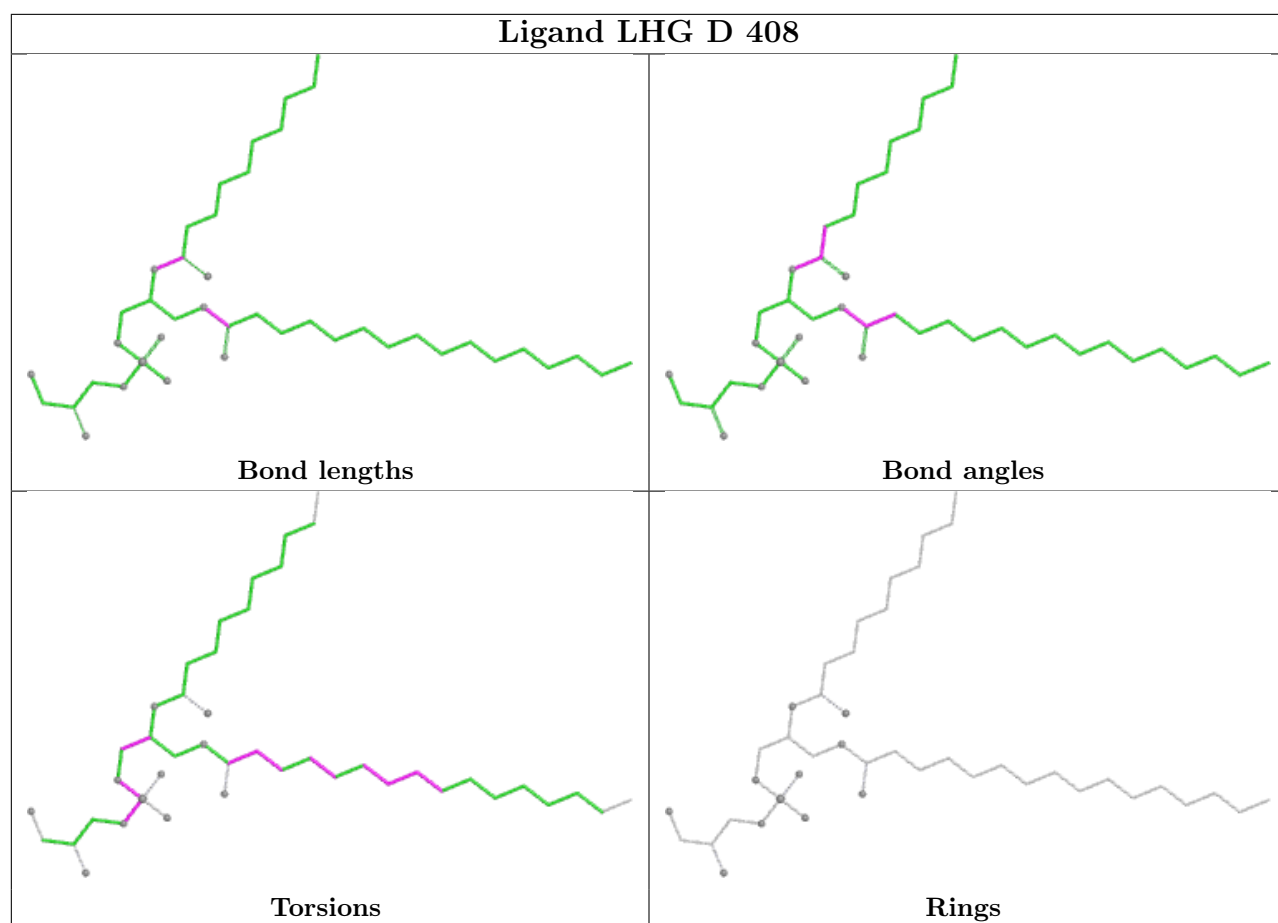


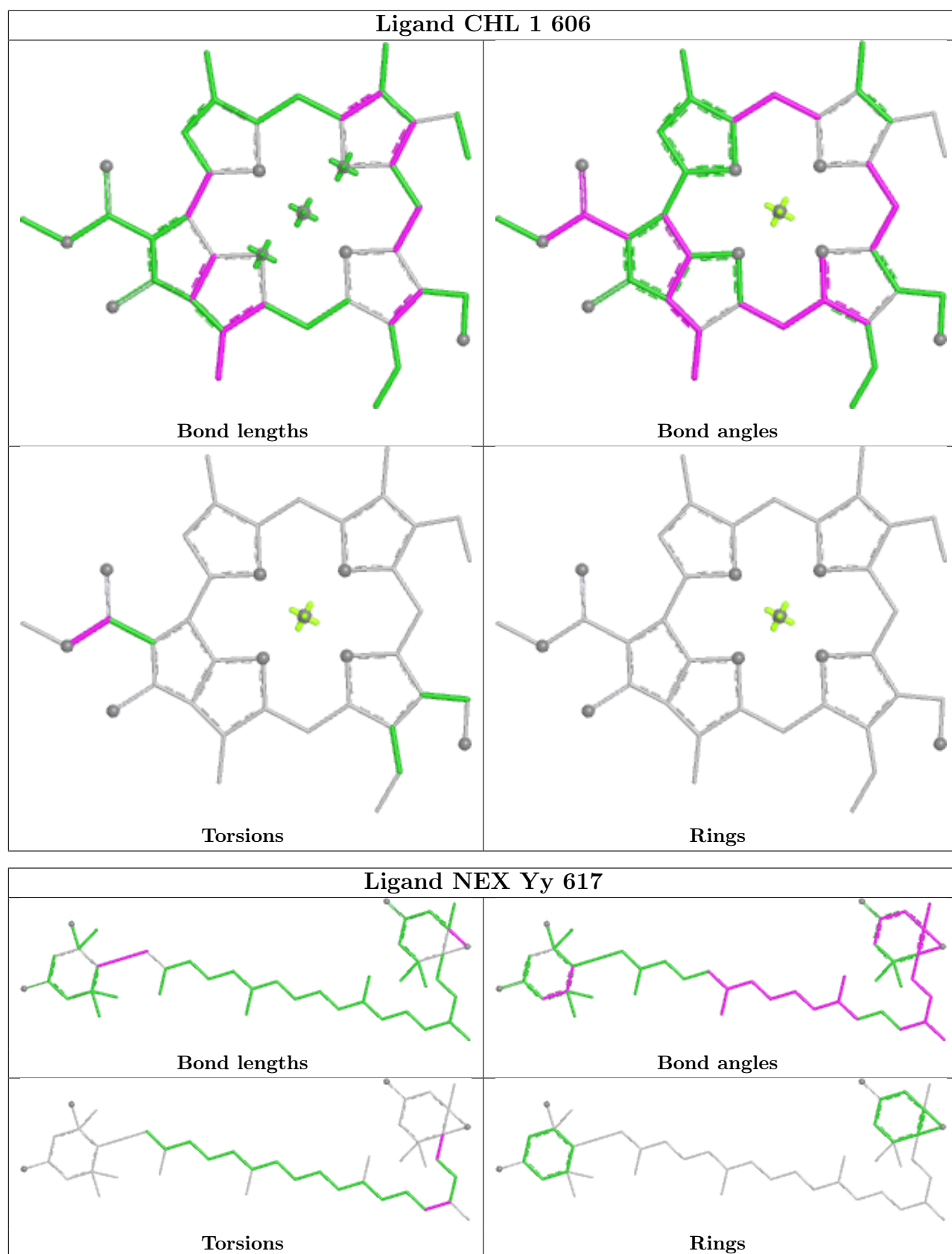
Ligand CLA d 402

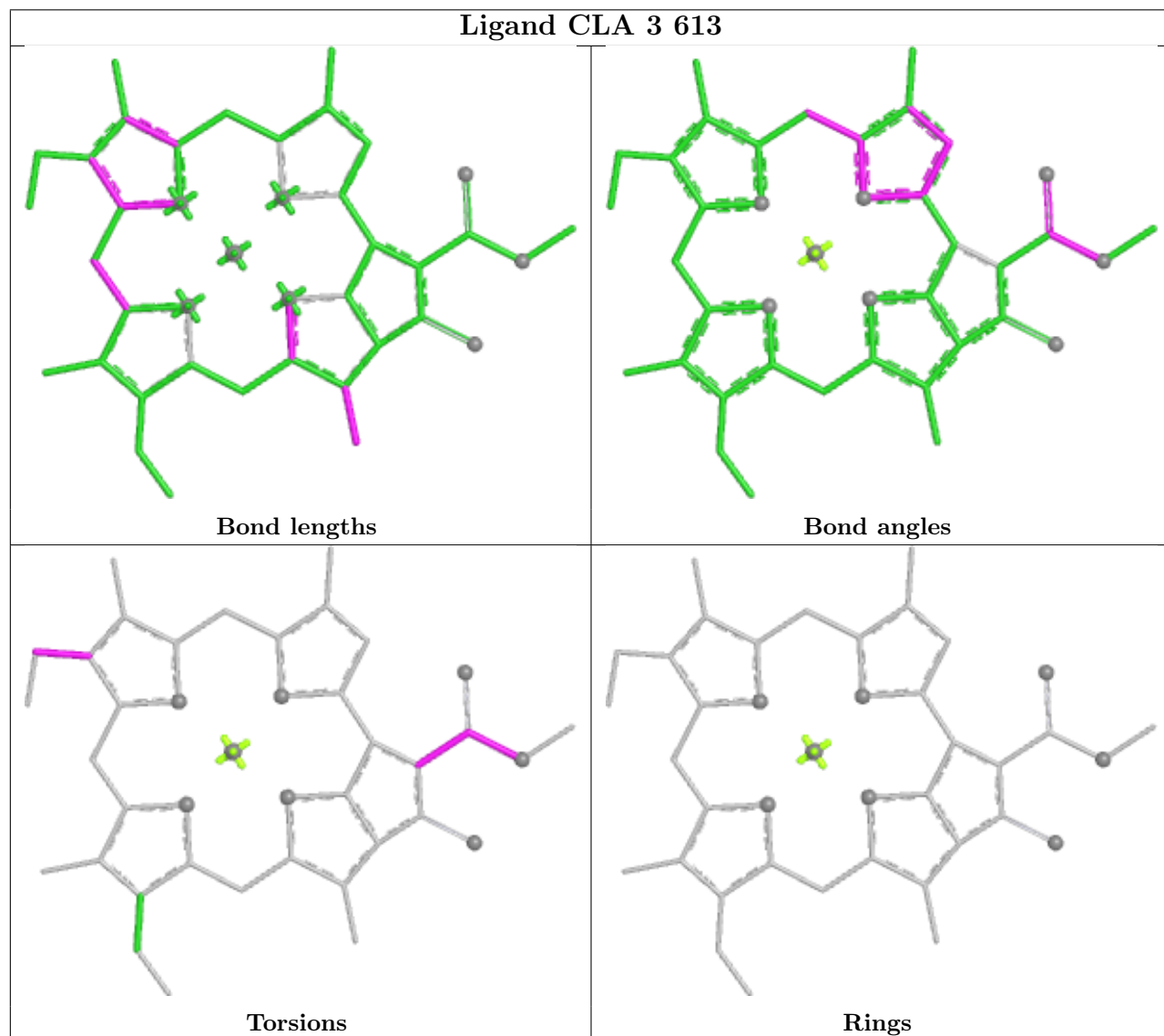
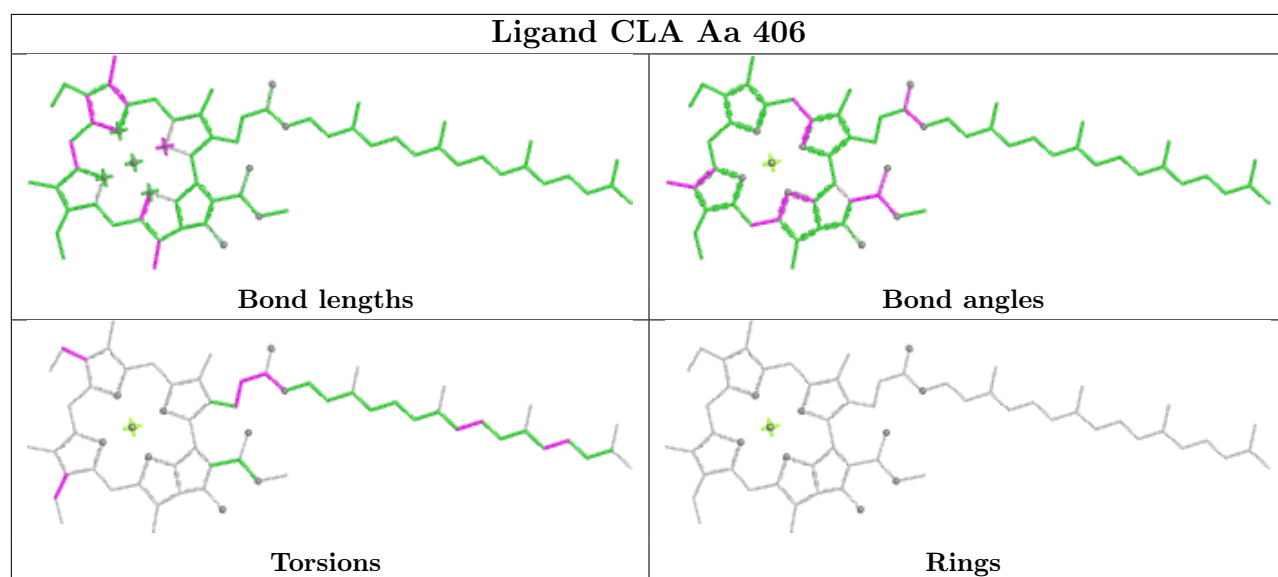


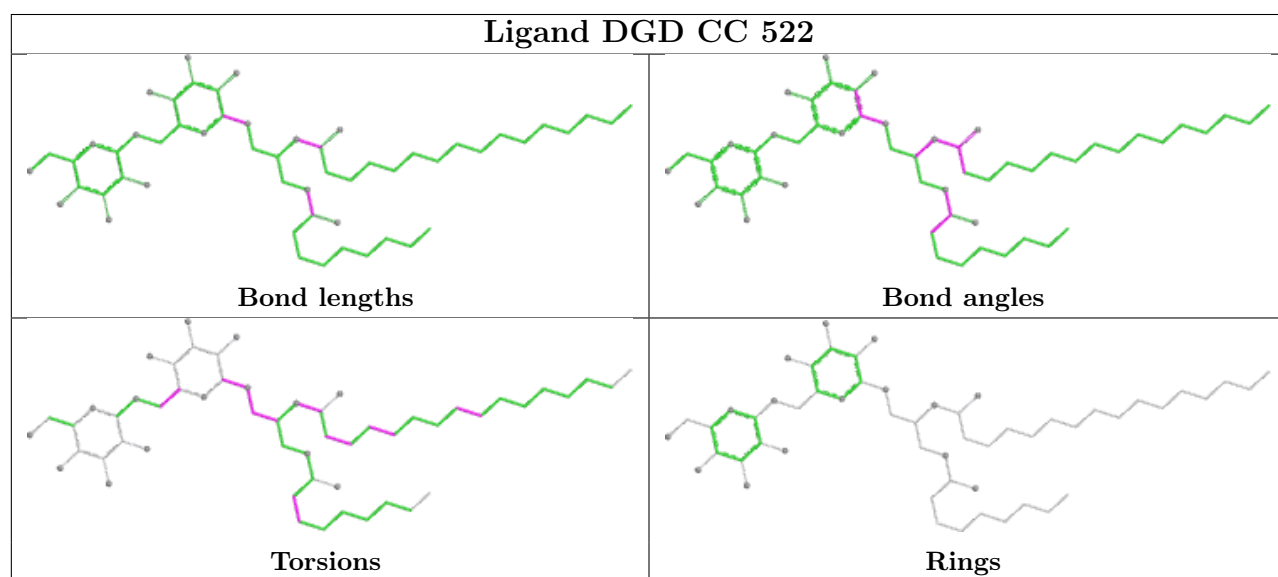
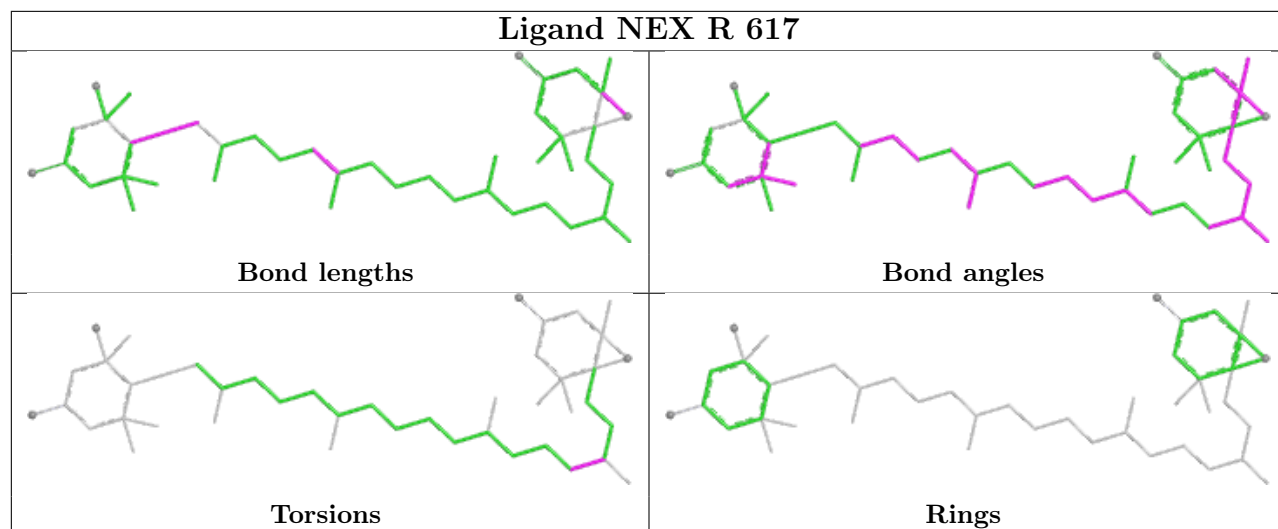


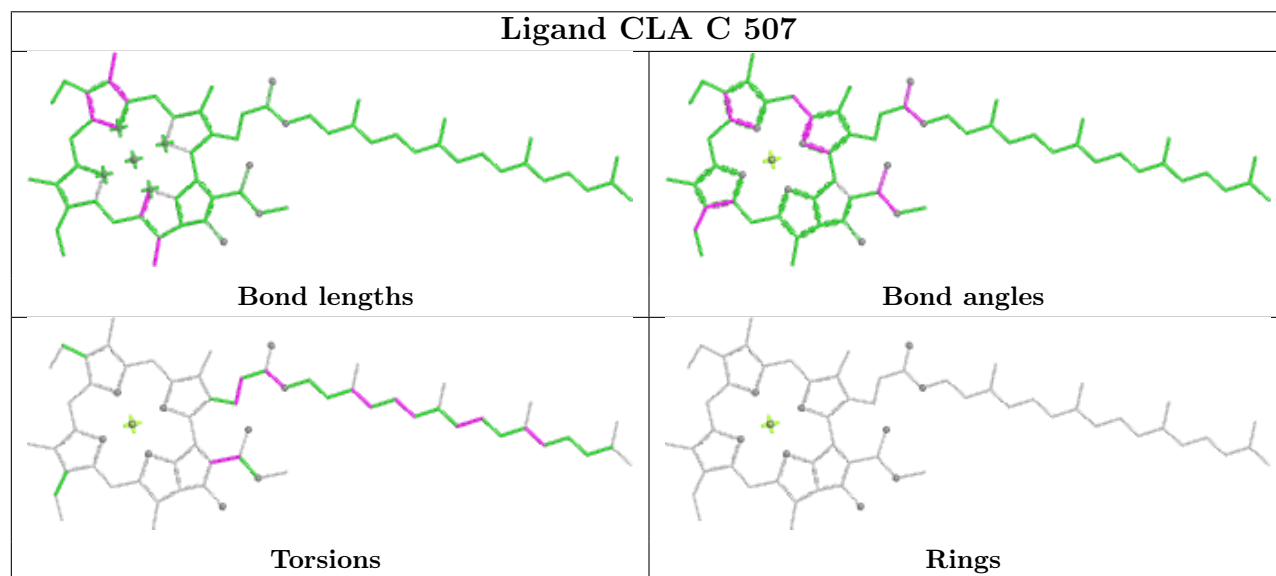
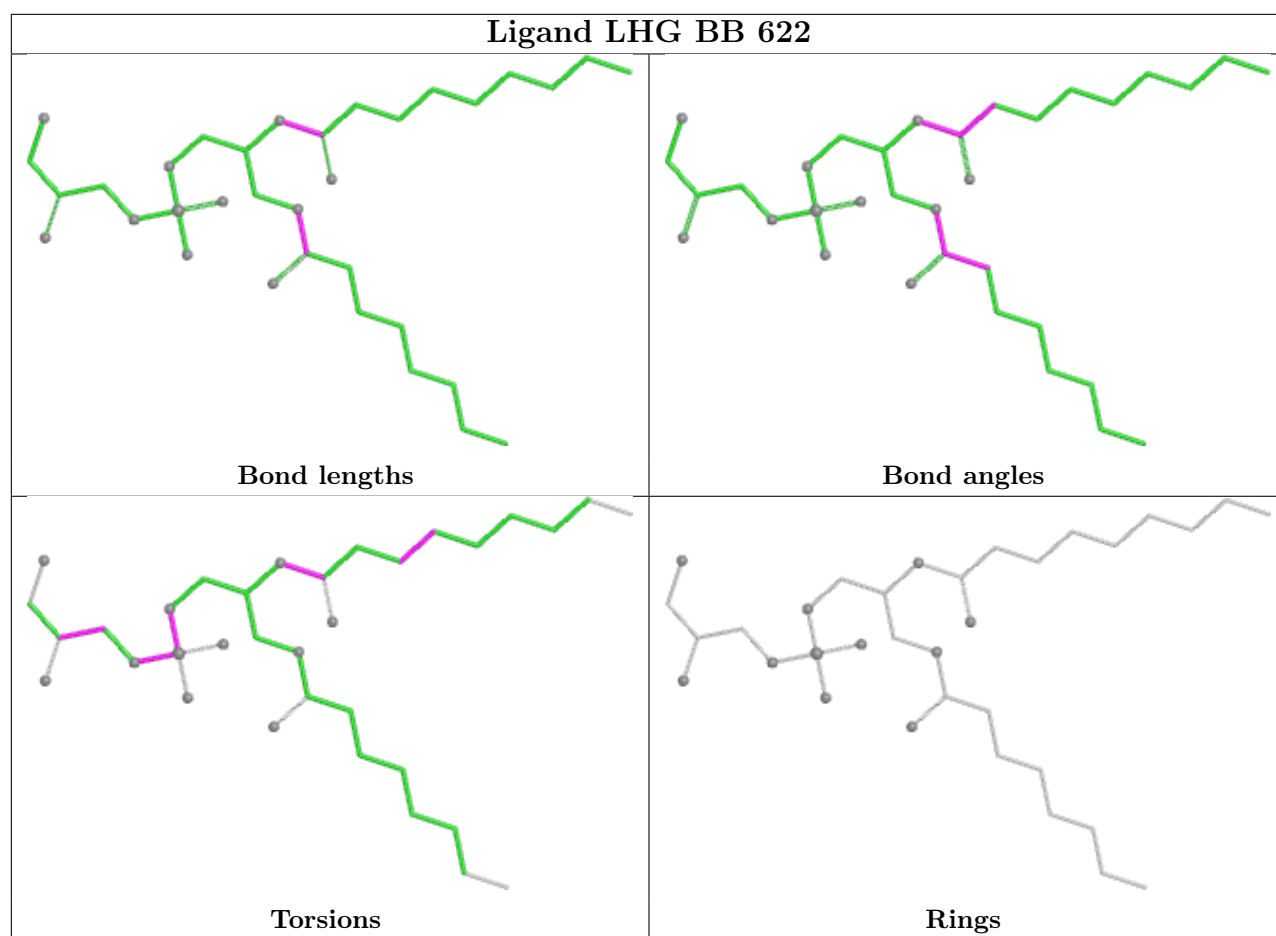


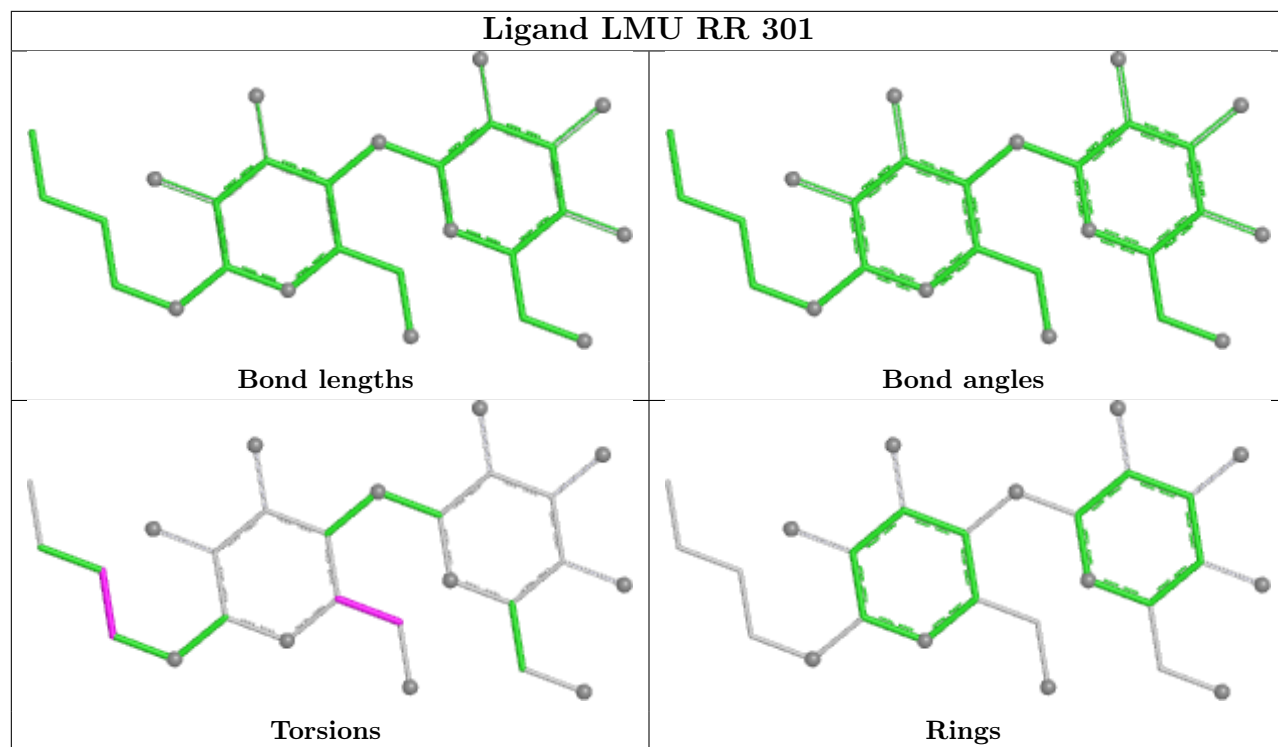




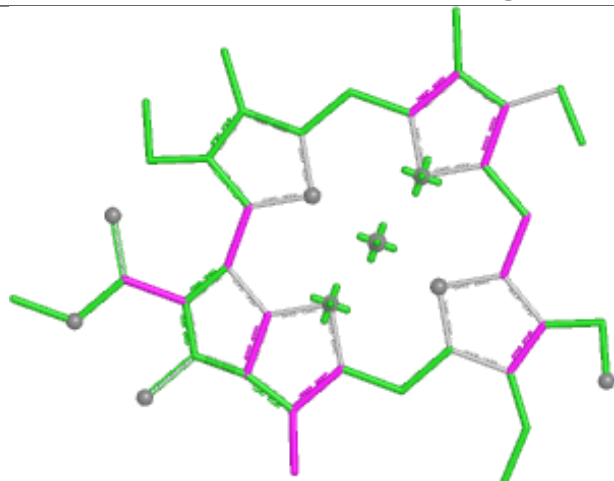




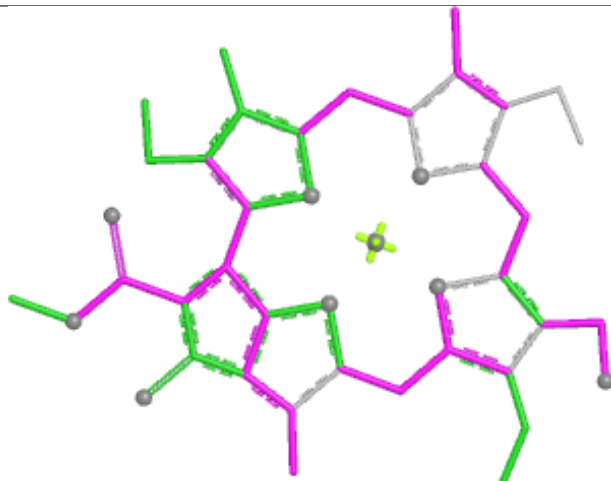




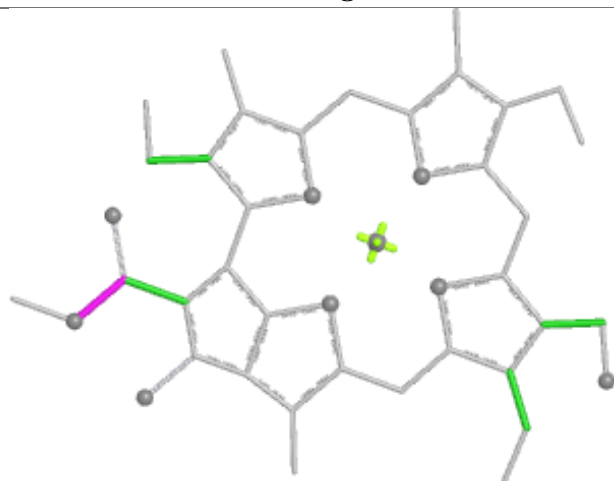
Ligand CHL YY 607



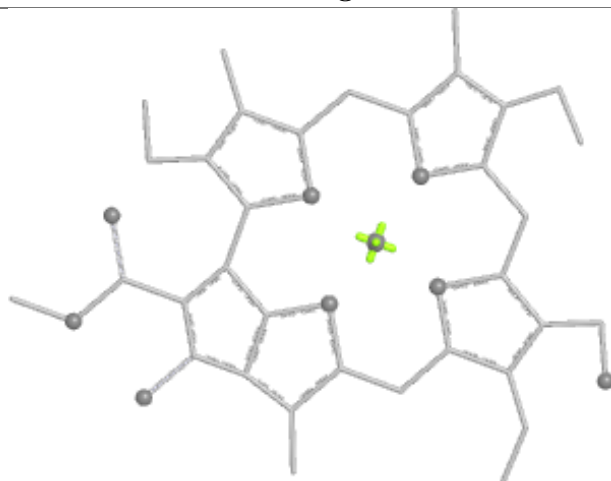
Bond lengths



Bond angles

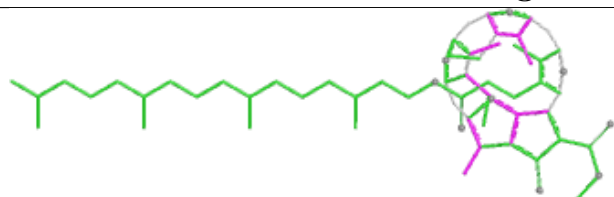


Torsions

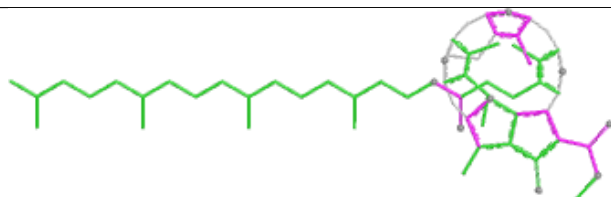


Rings

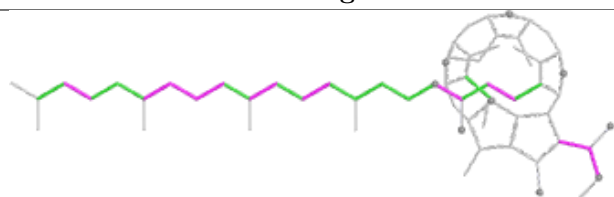
Ligand PHO a 409



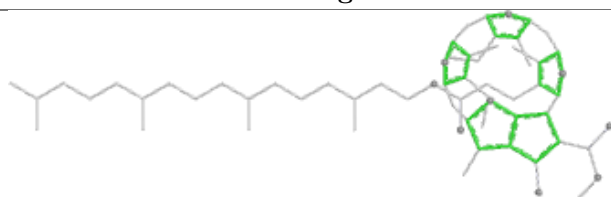
Bond lengths



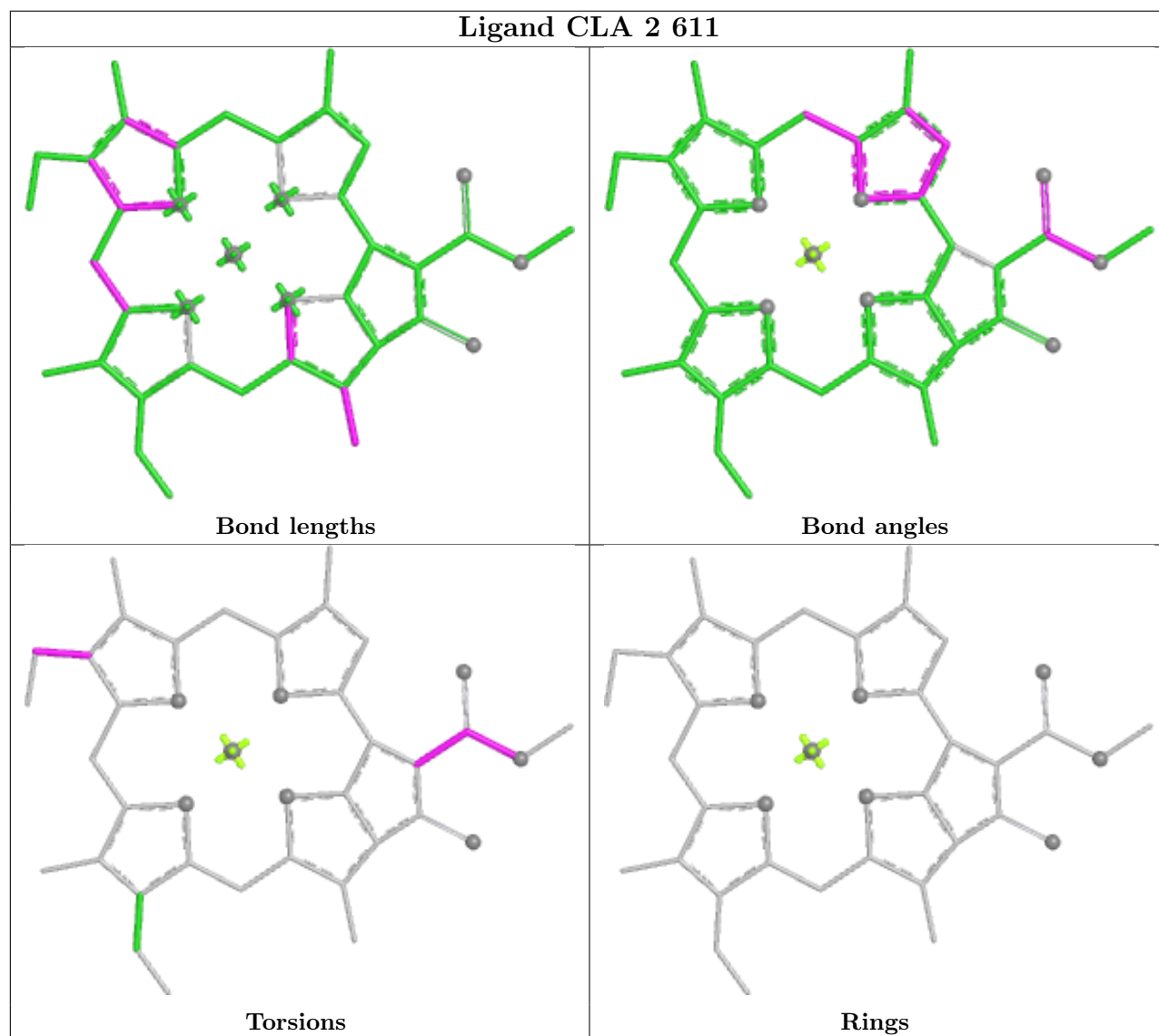
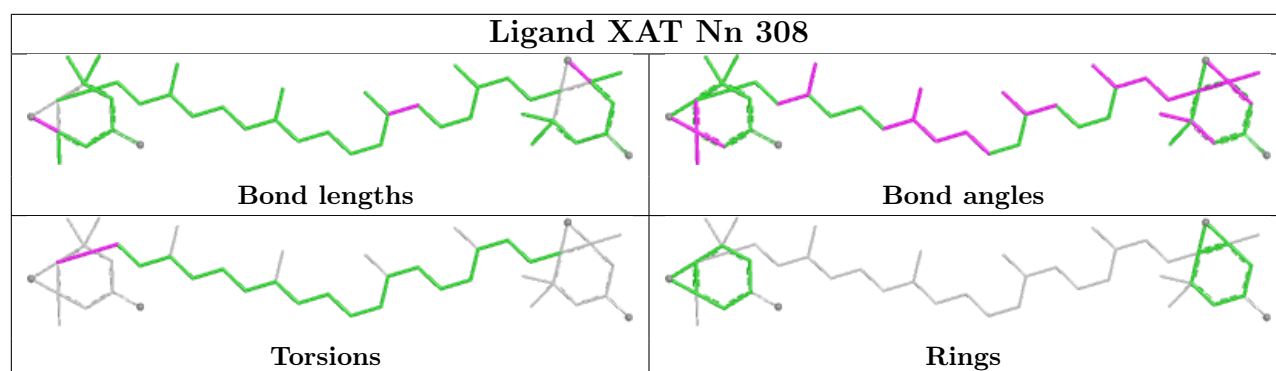
Bond angles

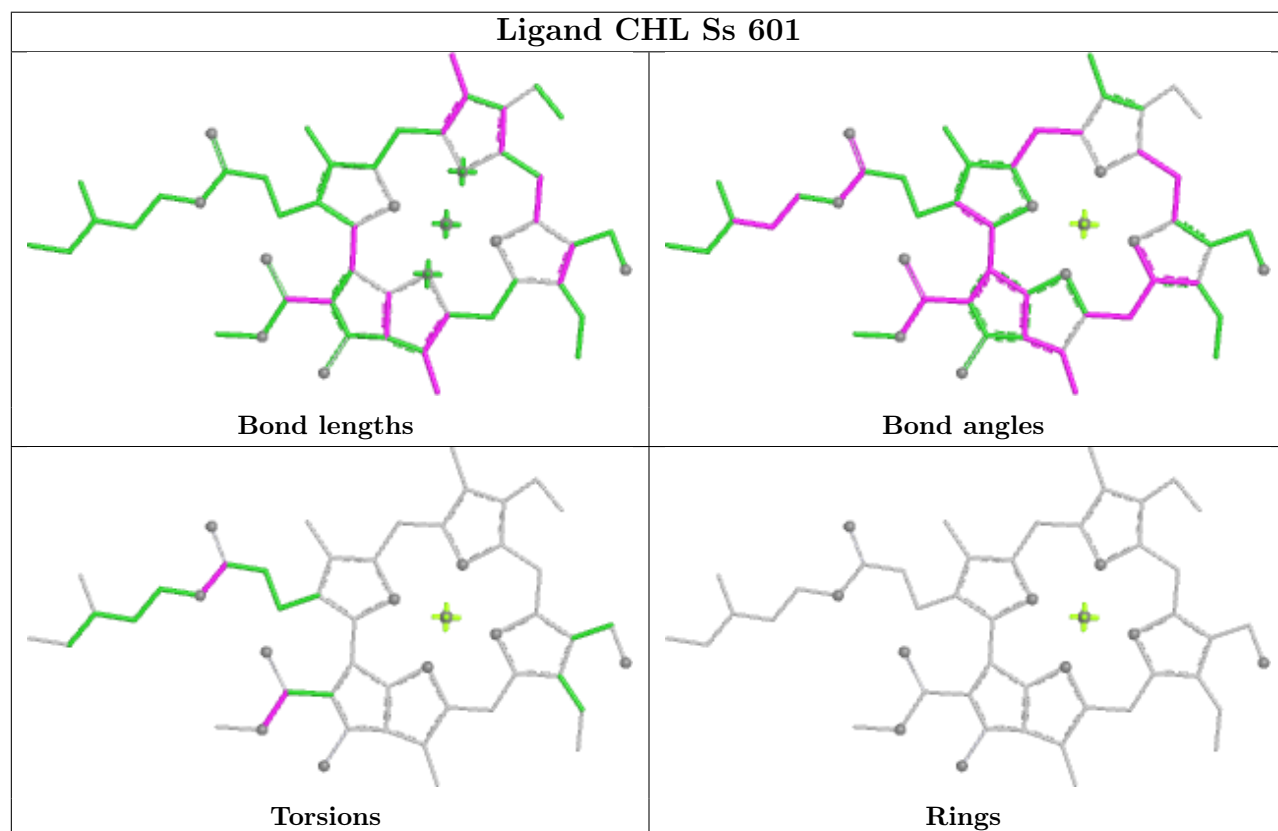
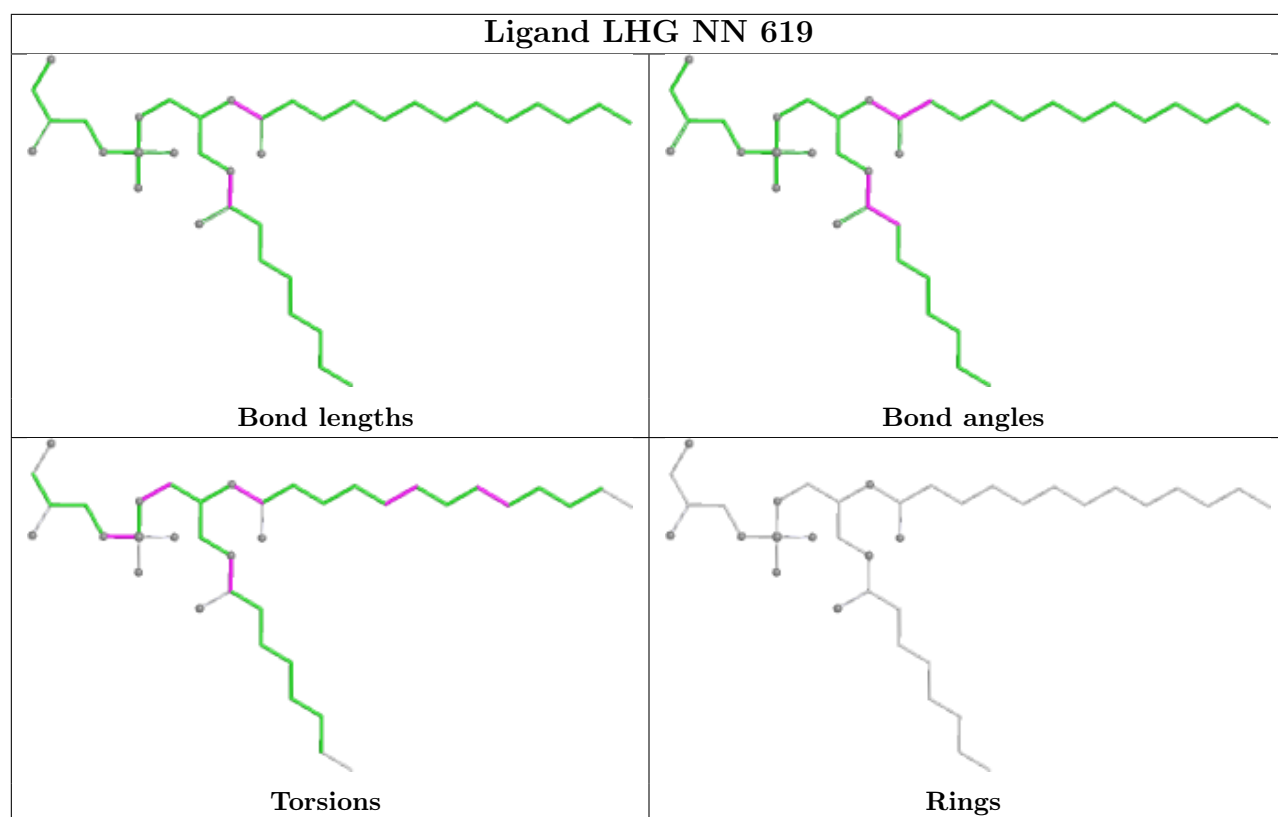


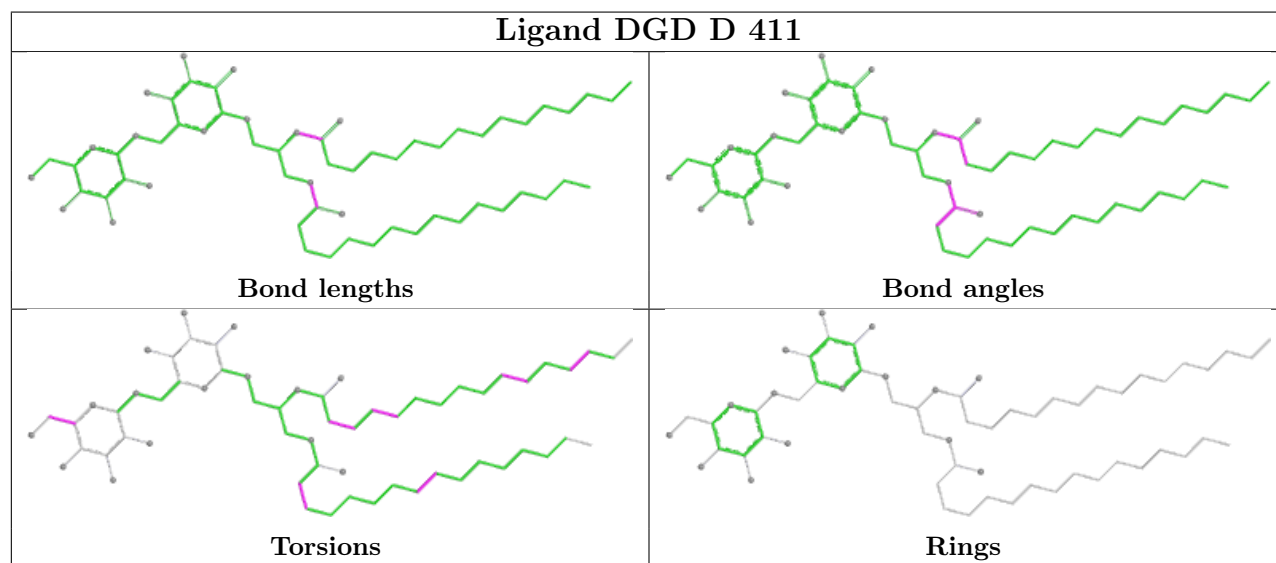
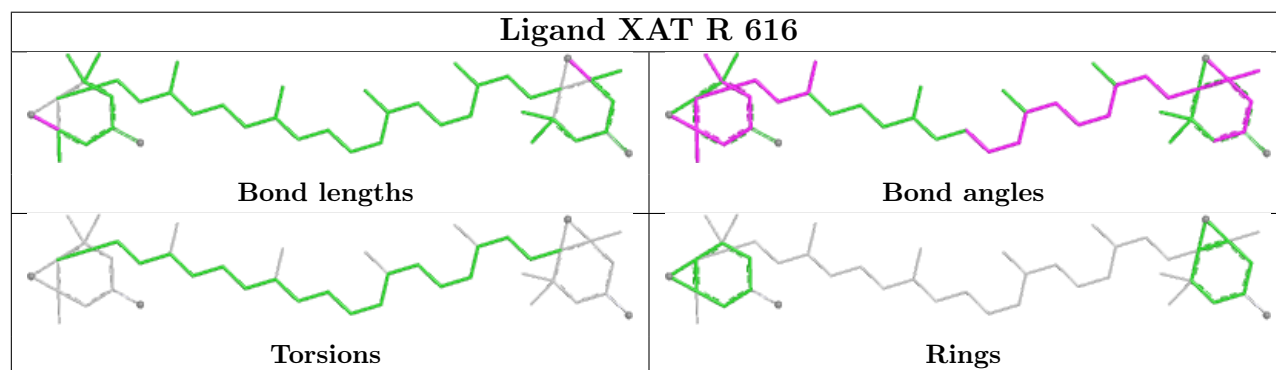
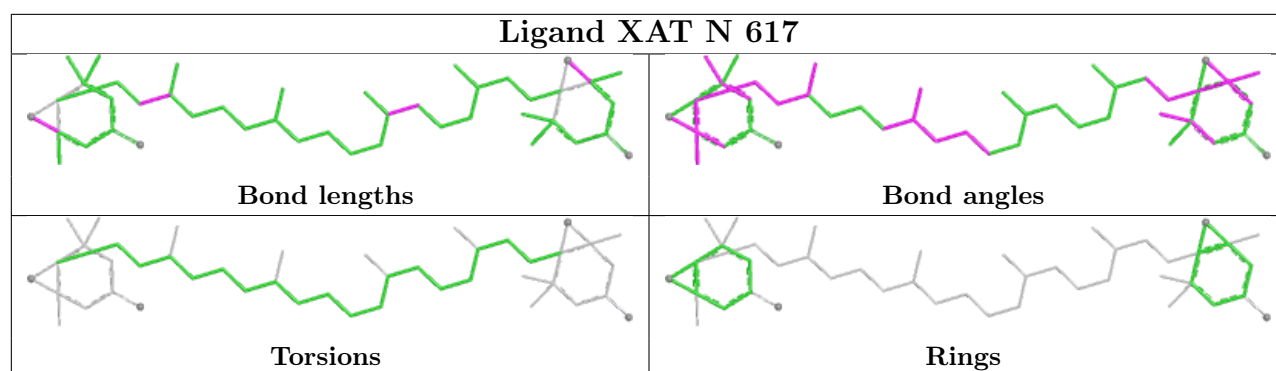
Torsions

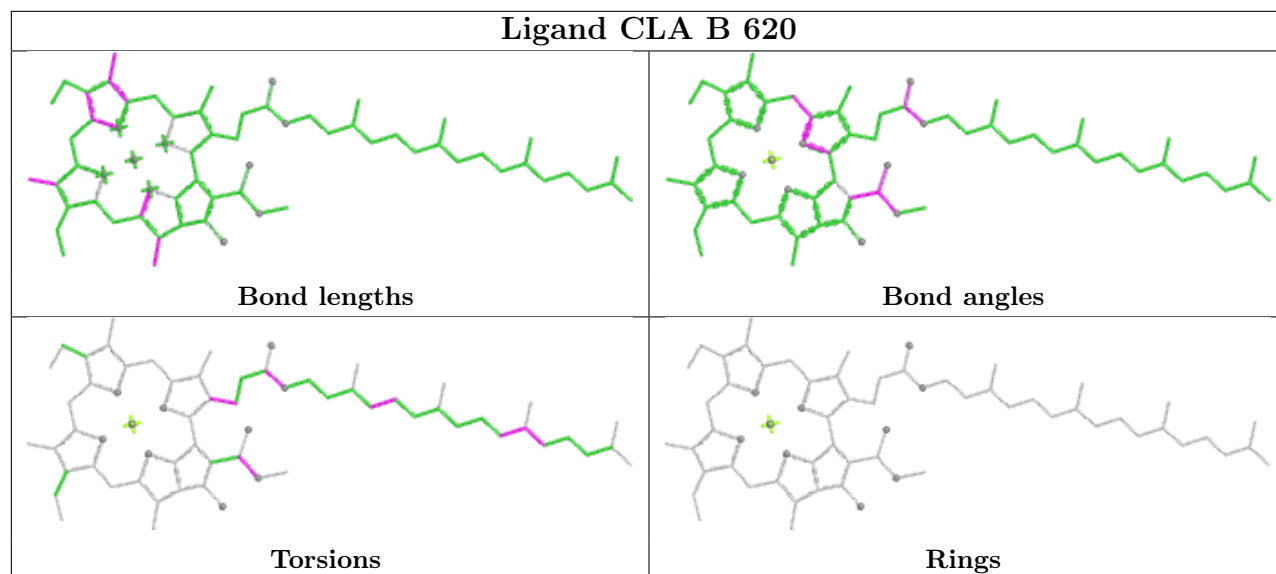
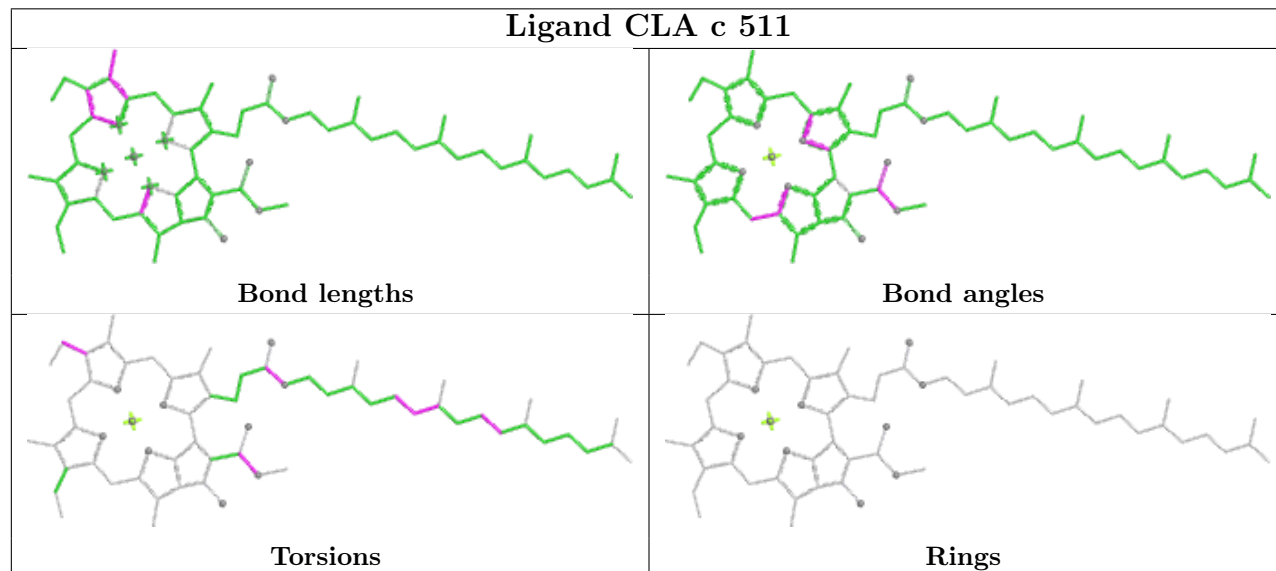


Rings

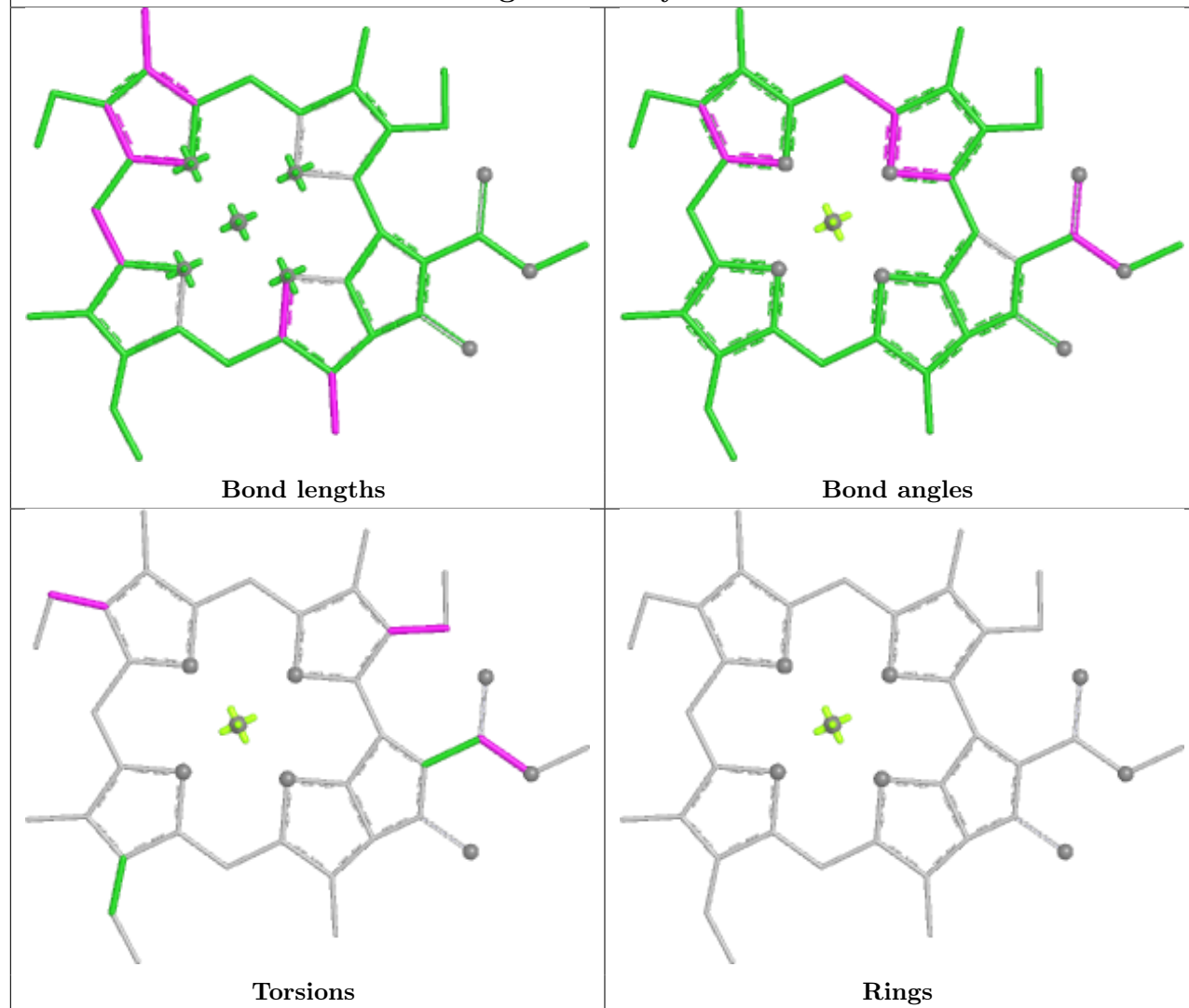




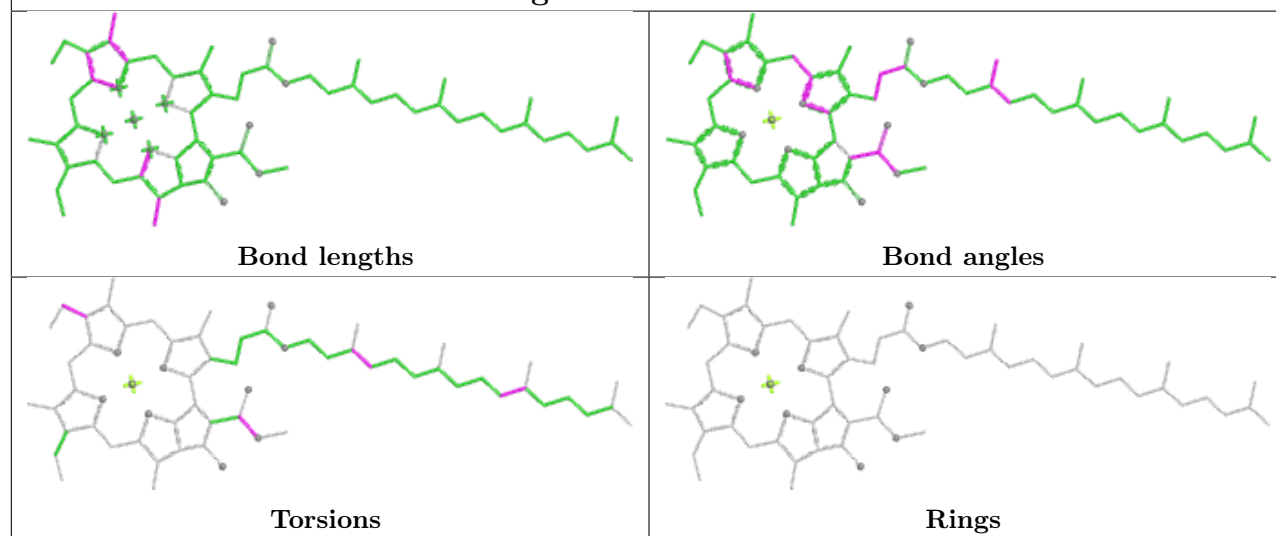


Ligand CLA B 620**Ligand CLA c 511**

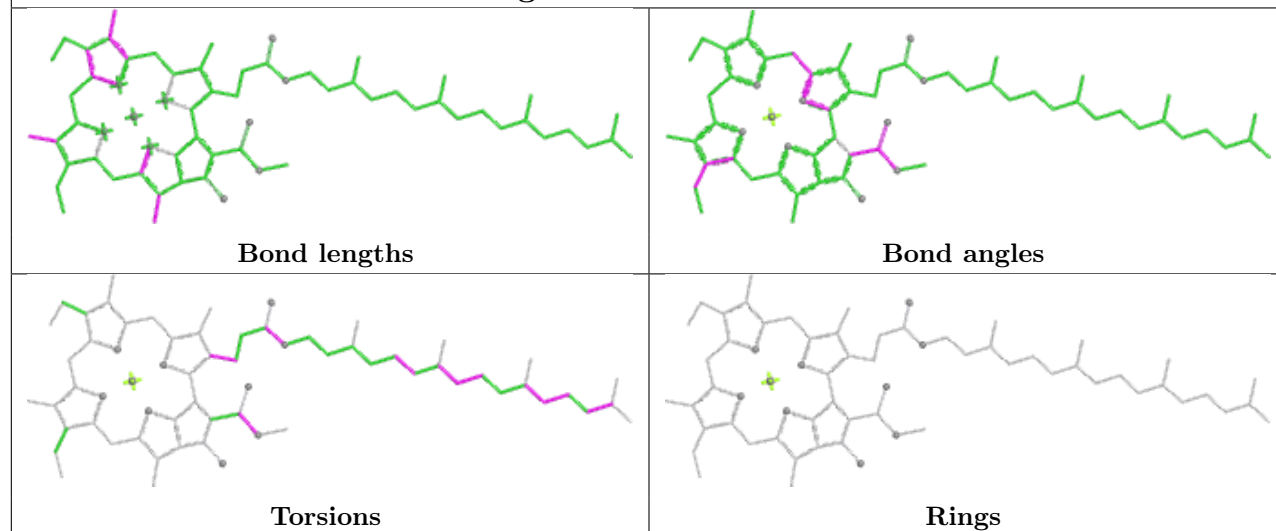
Ligand CLA y 313



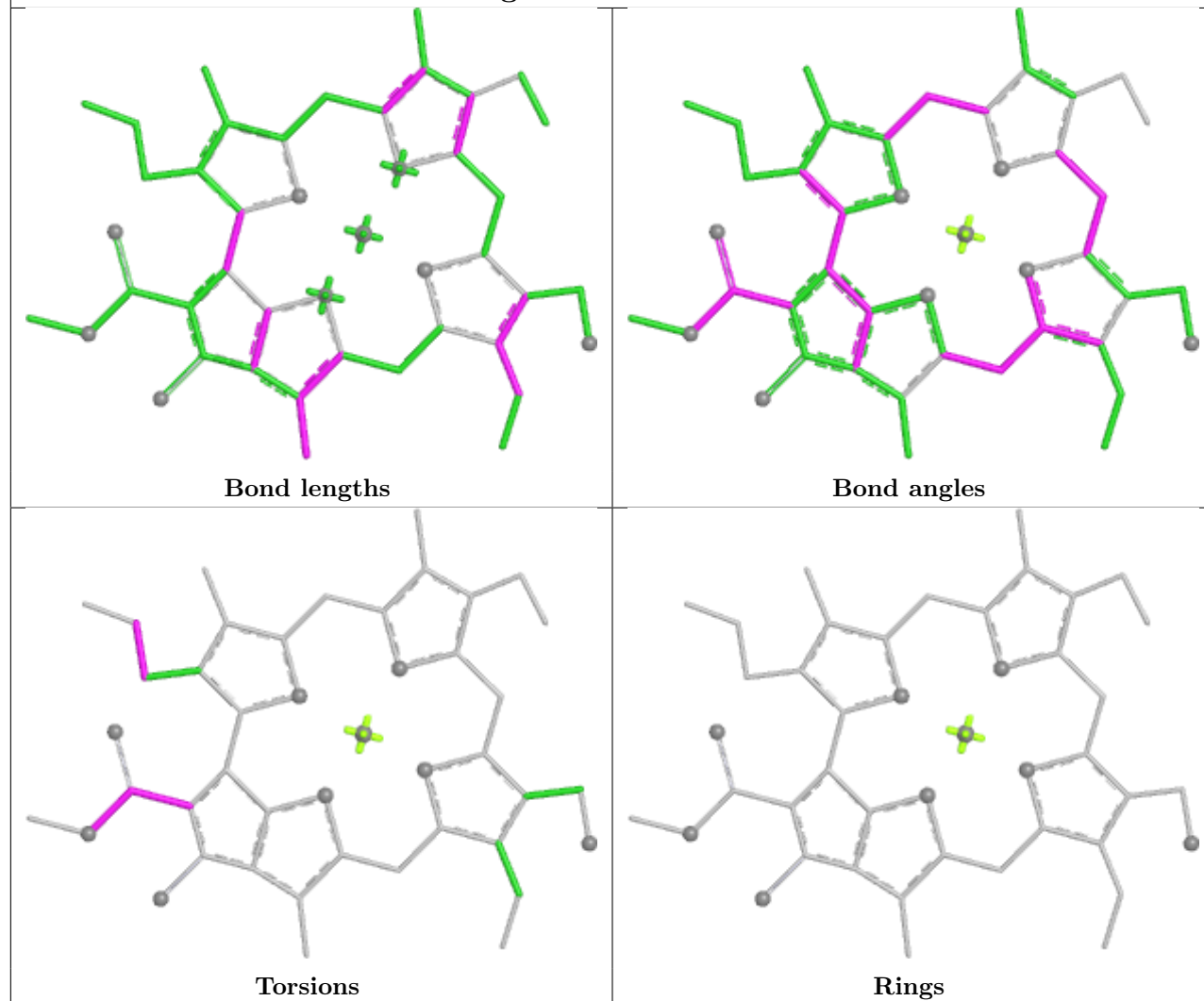
Ligand CLA D 401

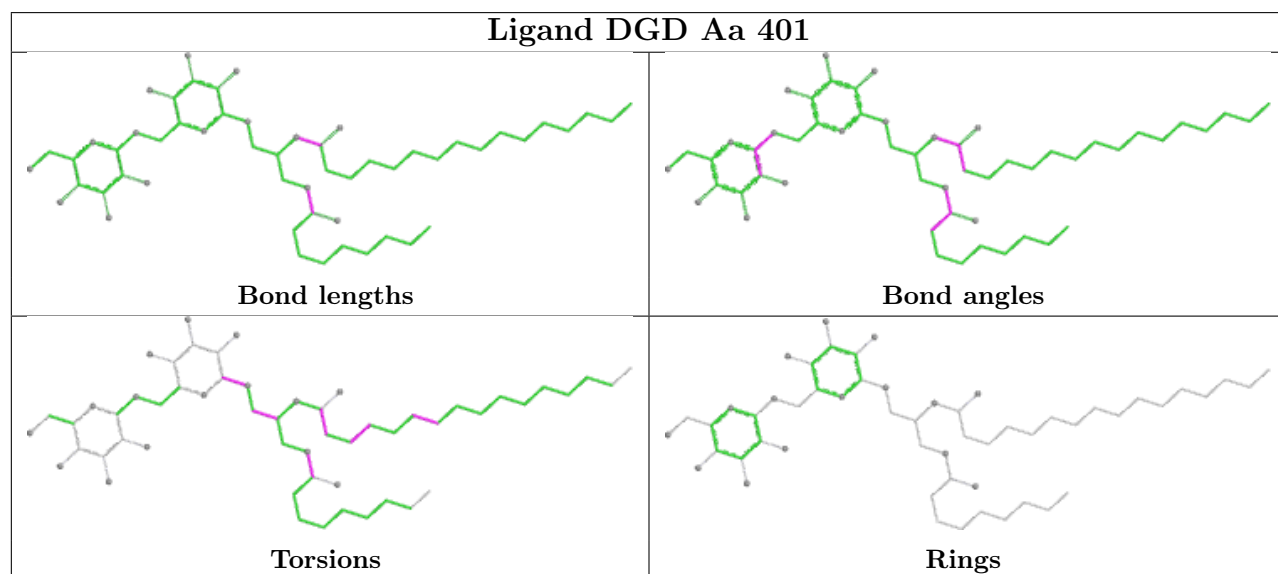
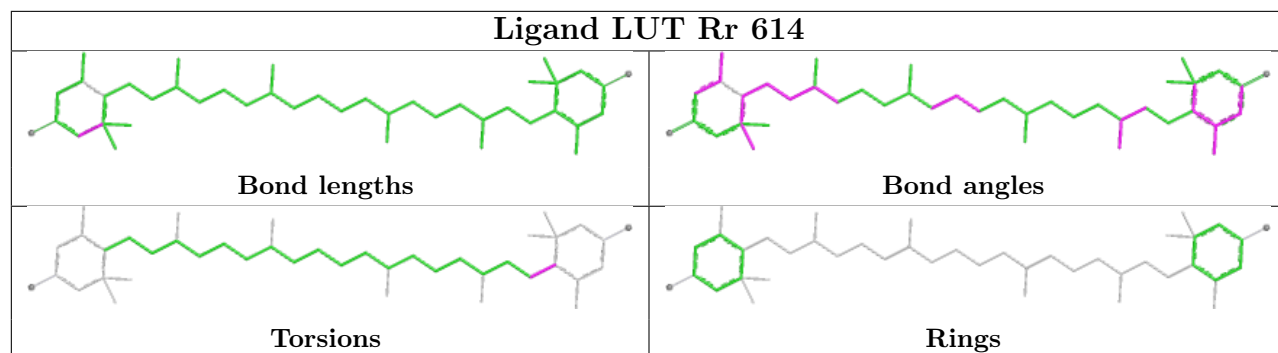


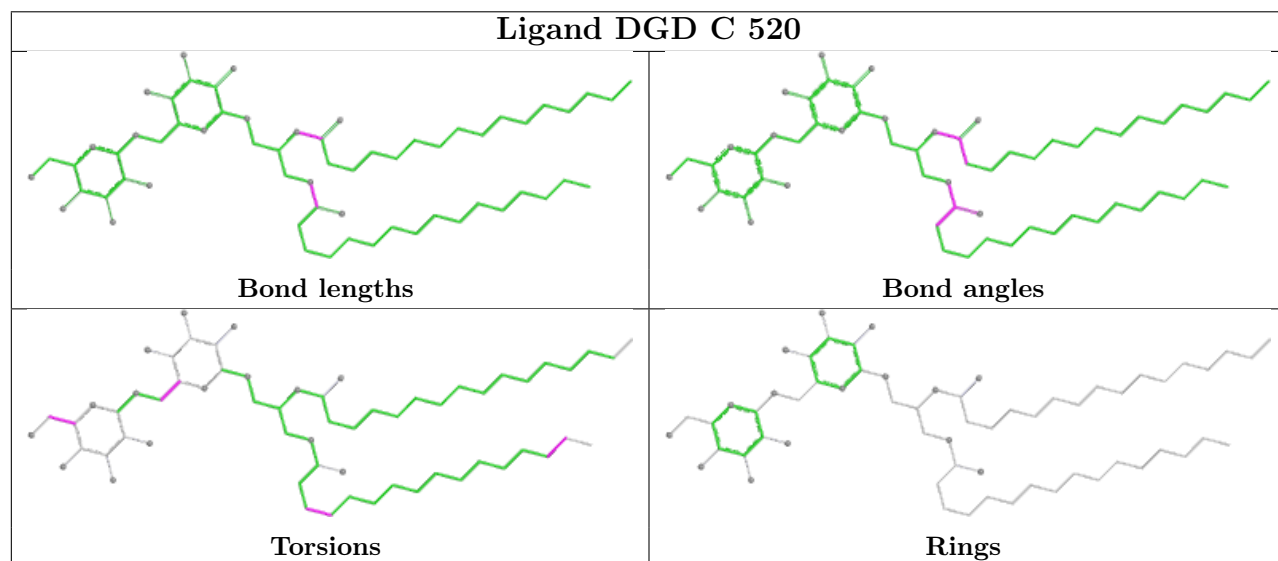
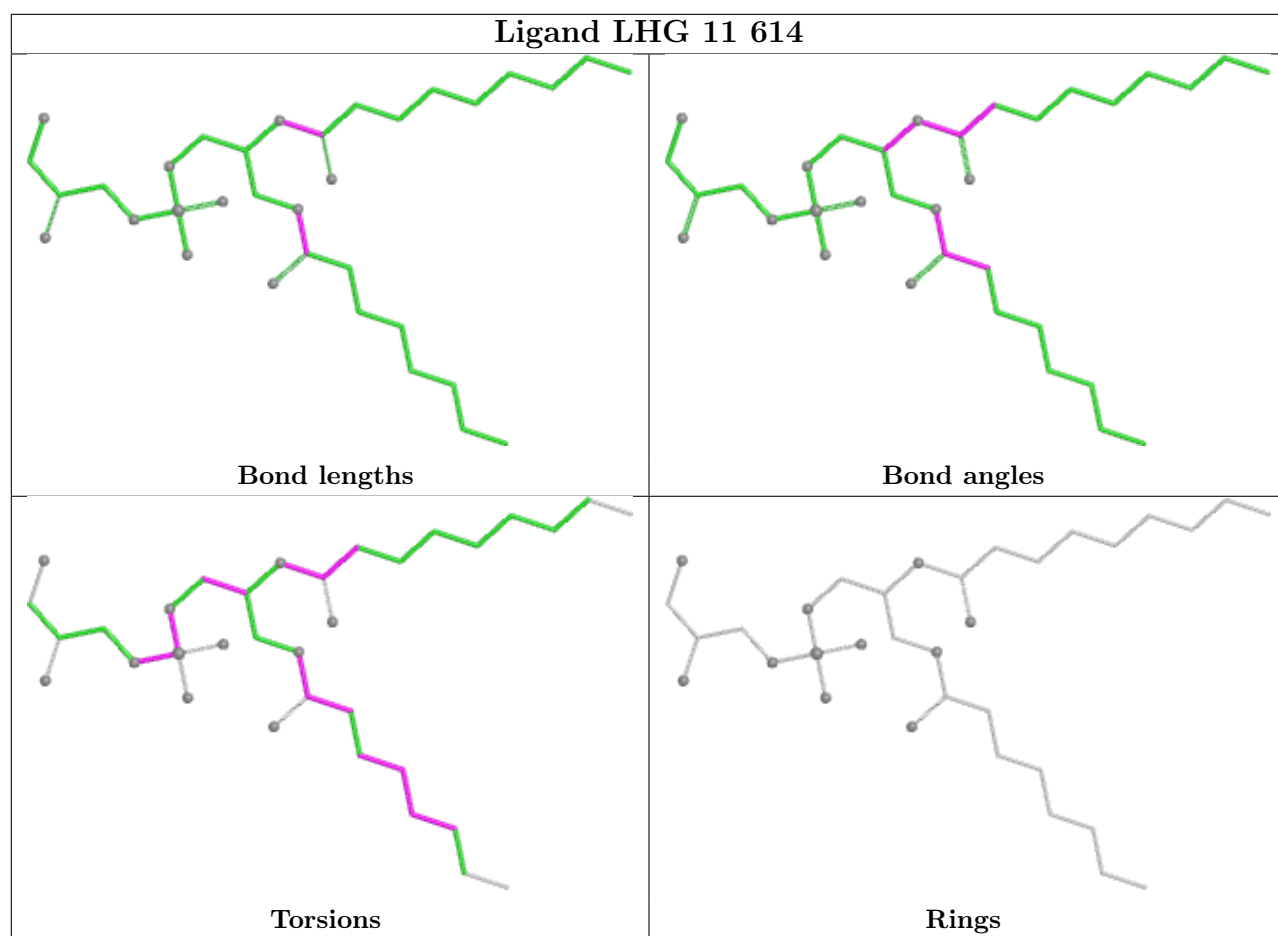
Ligand CLA AA 405

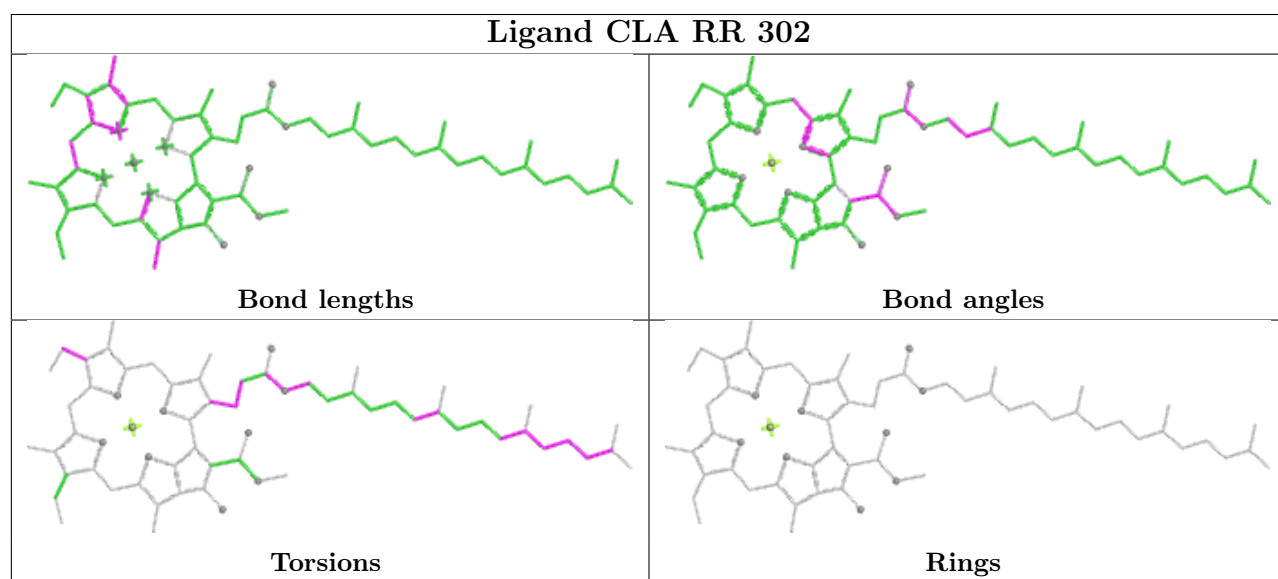
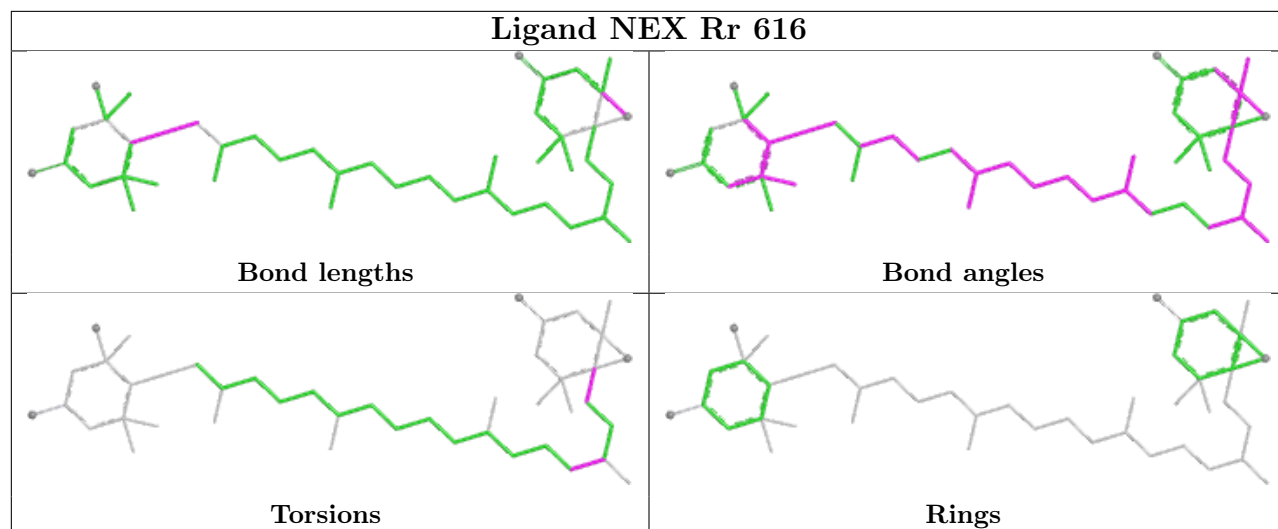


Ligand CHL N 601

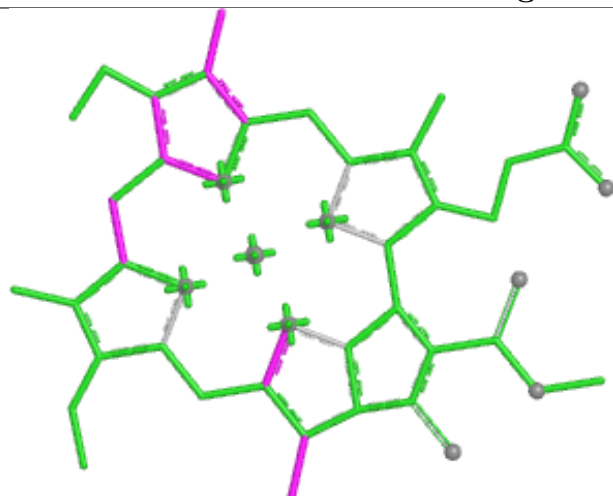




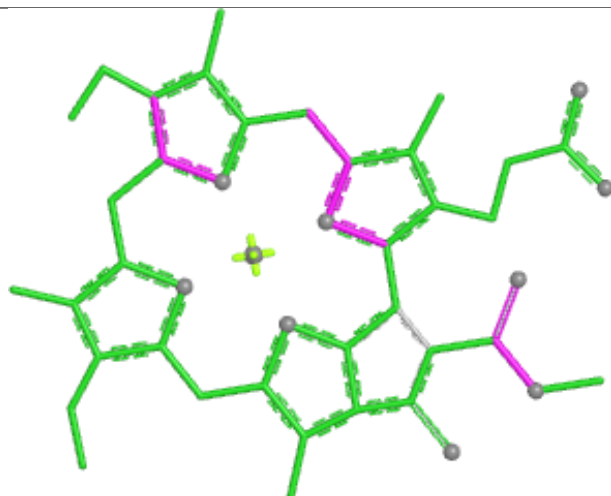




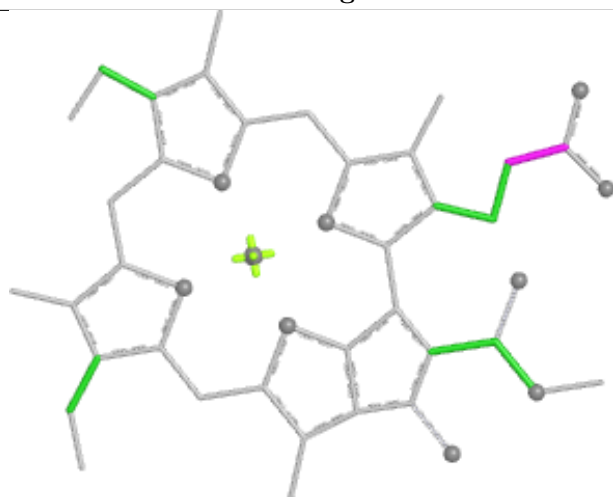
Ligand CLA S 613



Bond lengths



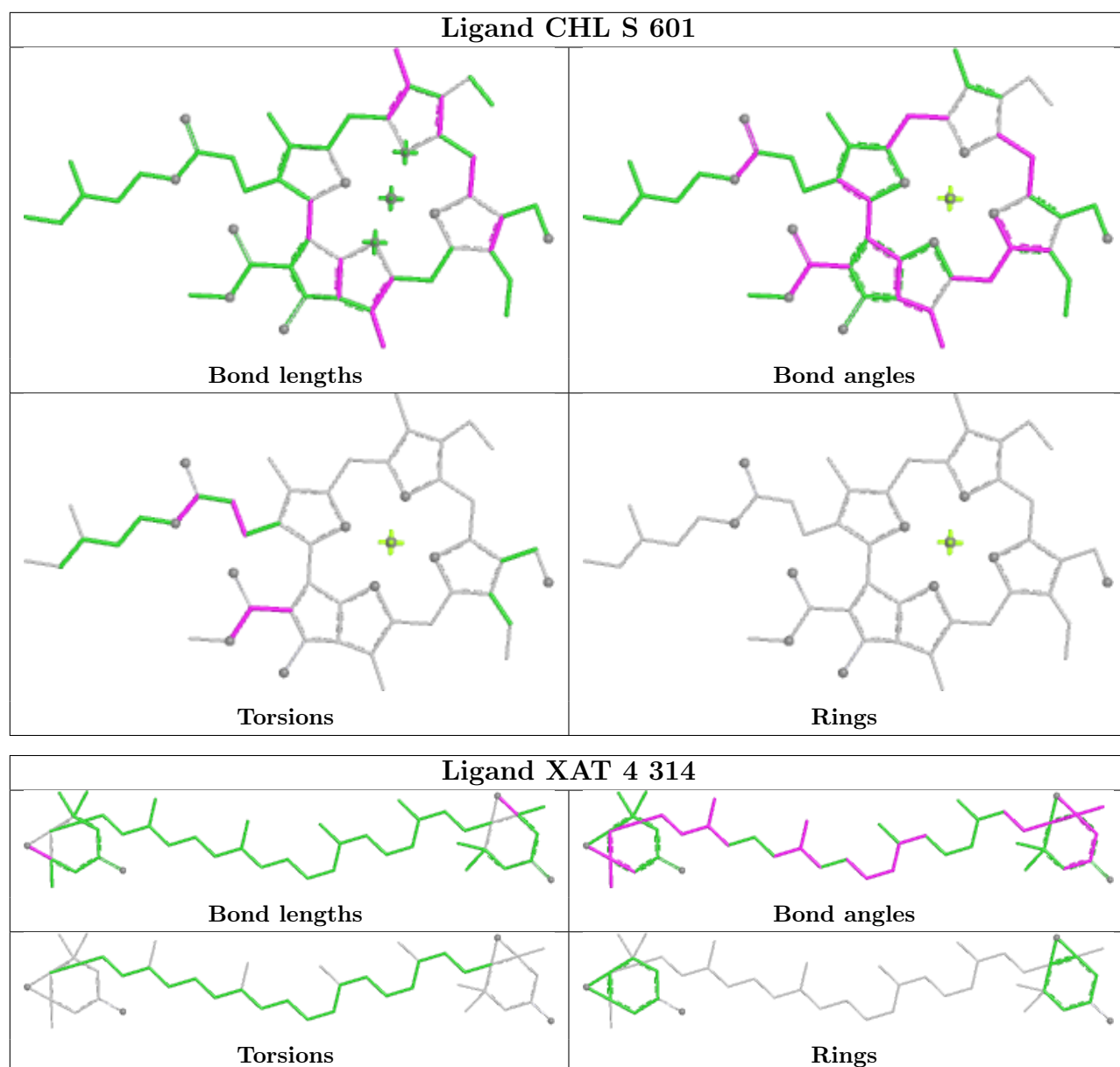
Bond angles



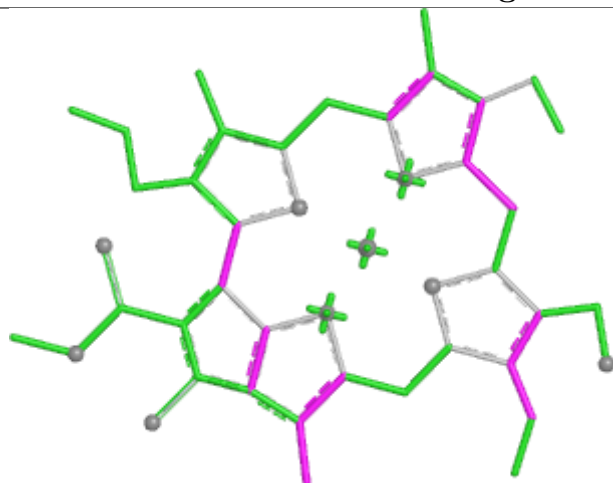
Torsions



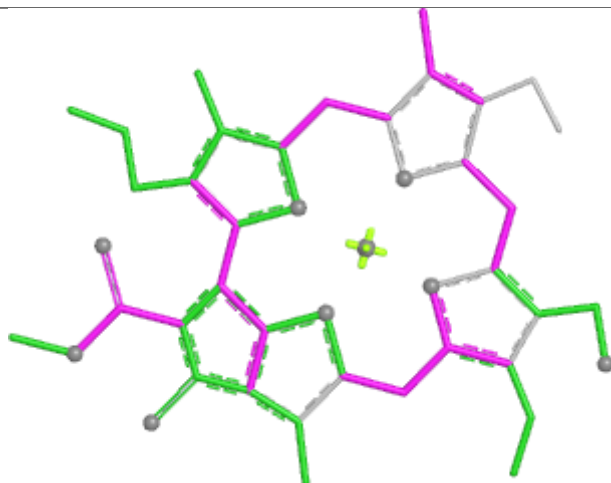
Rings



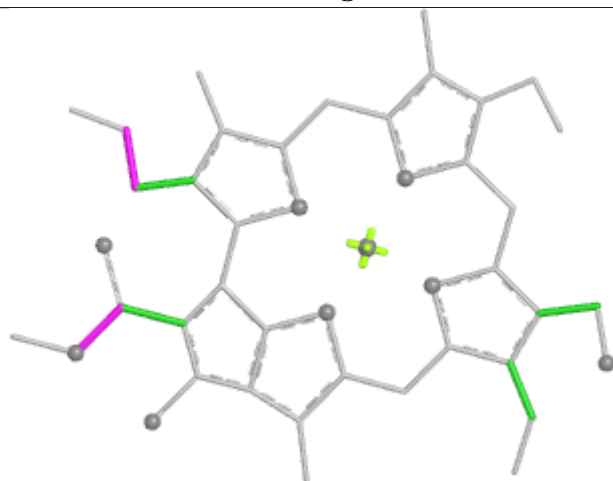
Ligand CHL NN 601



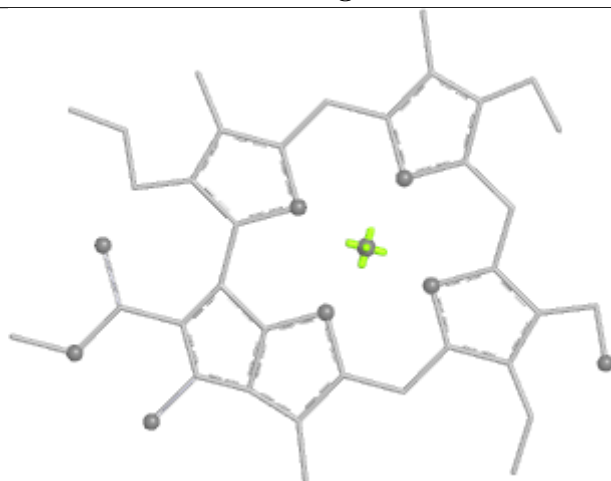
Bond lengths



Bond angles

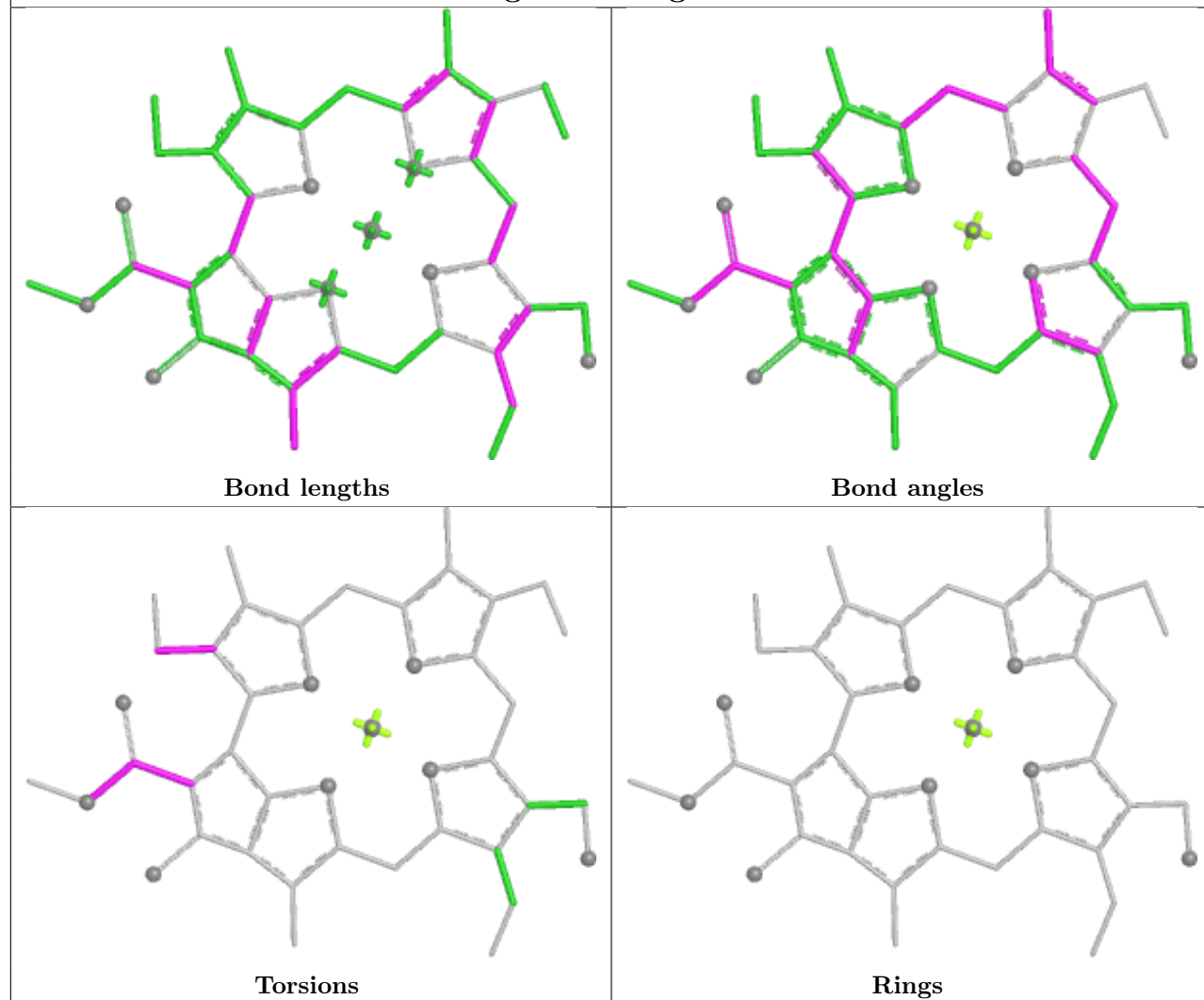


Torsions

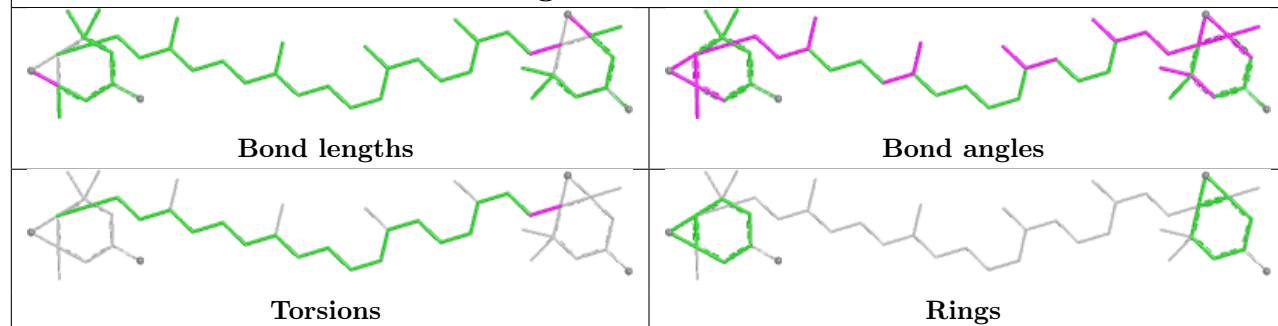


Rings

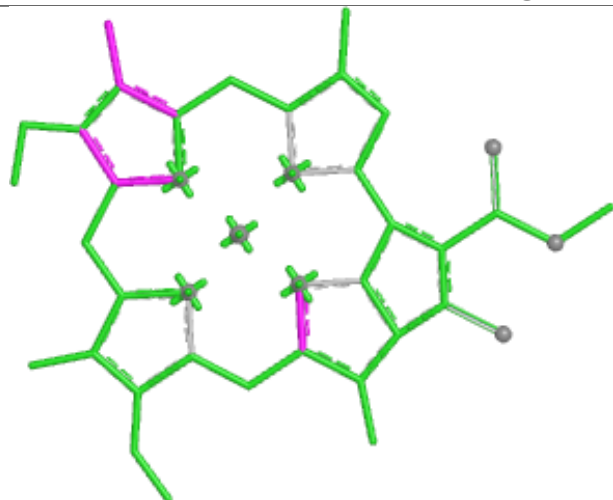
Ligand CHL g 609



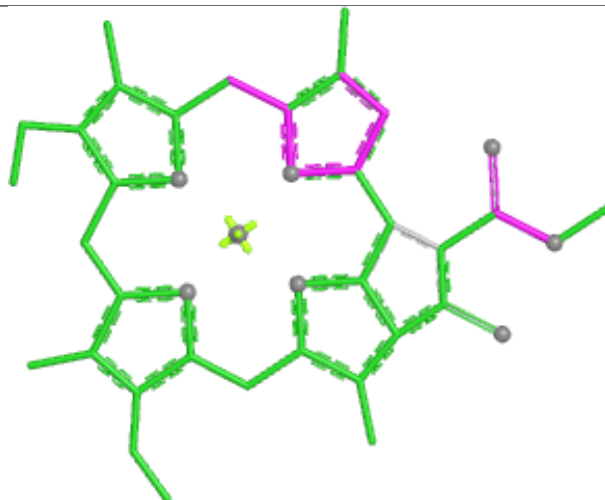
Ligand XAT r 615



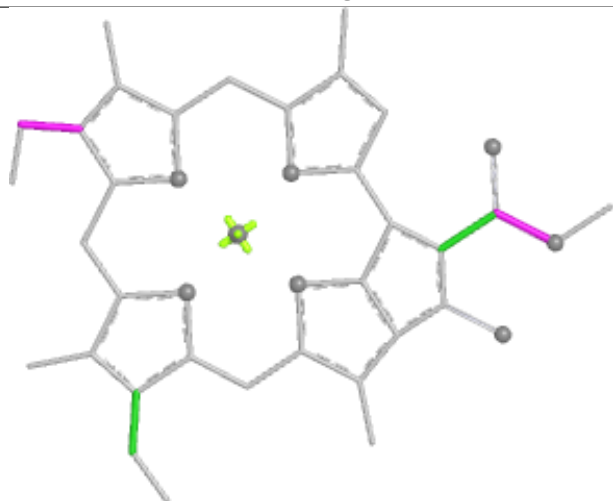
Ligand CLA 3 602



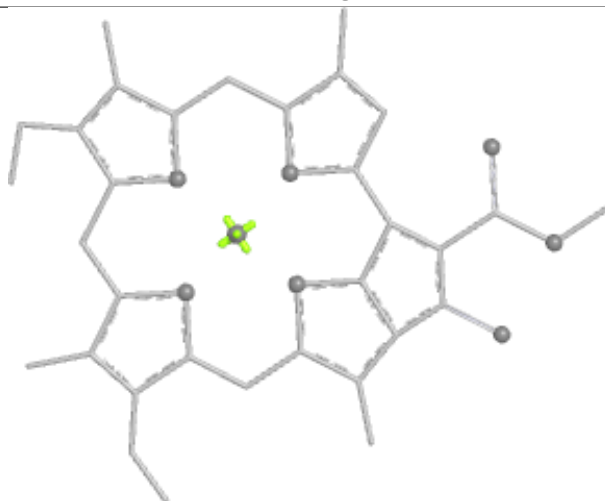
Bond lengths



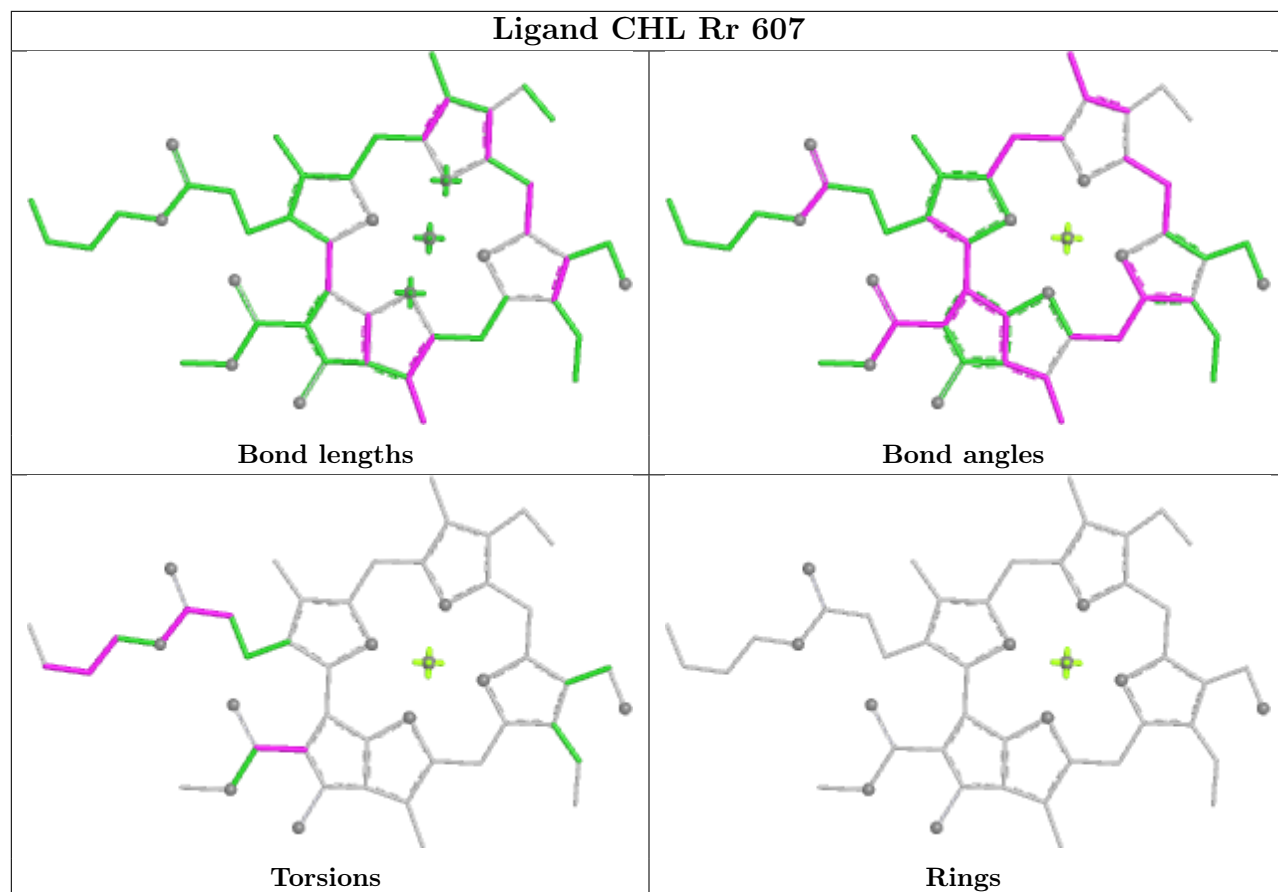
Bond angles



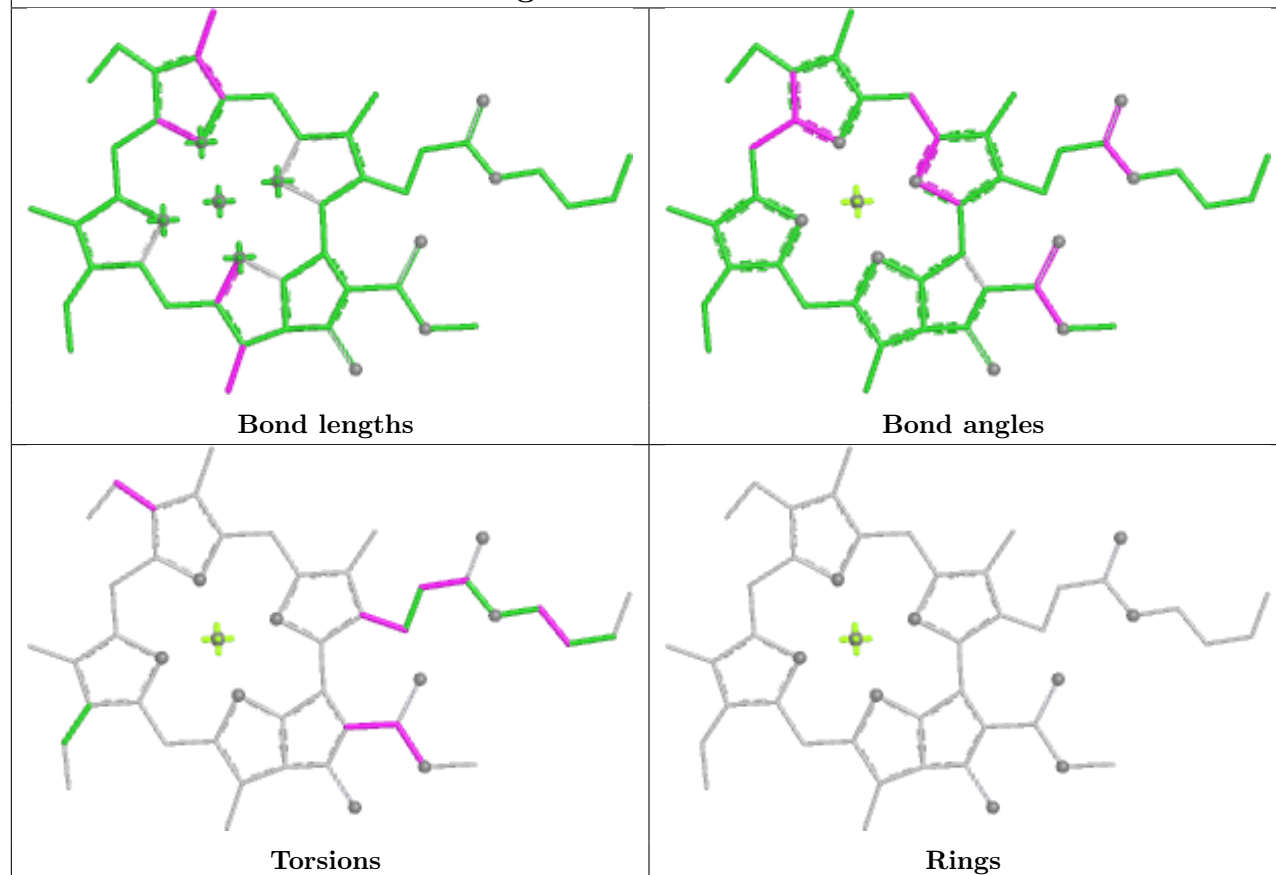
Torsions



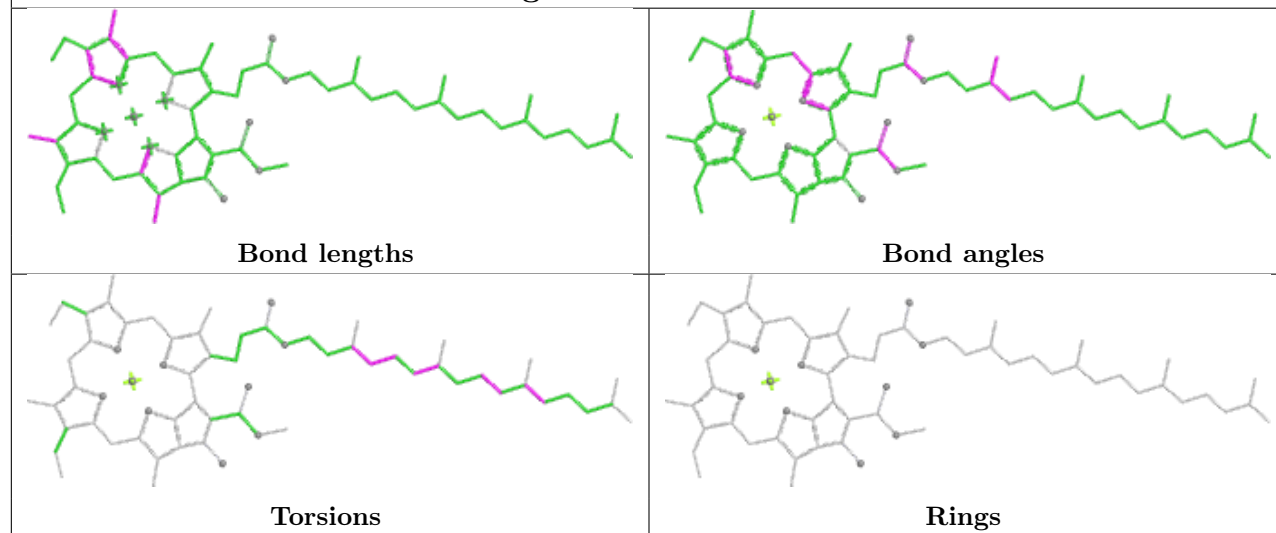
Rings

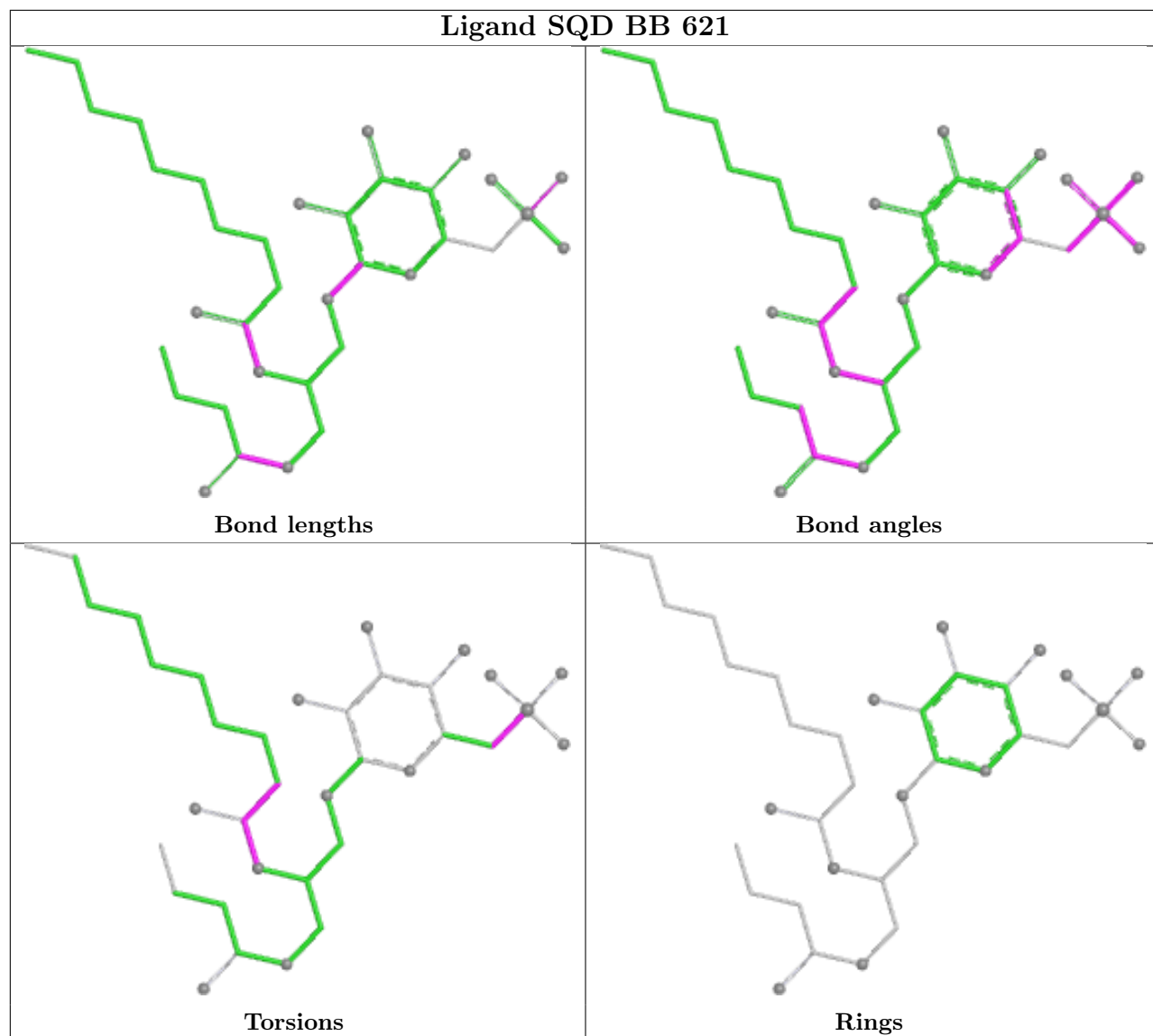


Ligand CLA GG 602

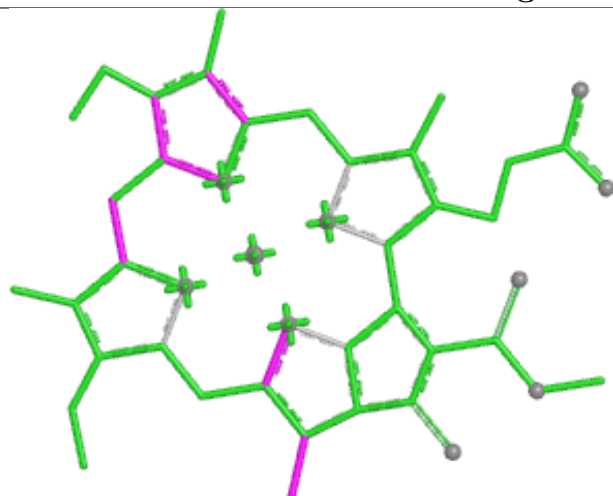


Ligand CLA Bb 604

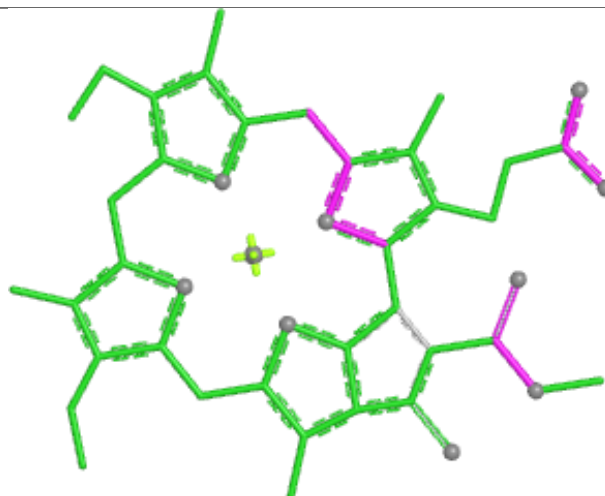




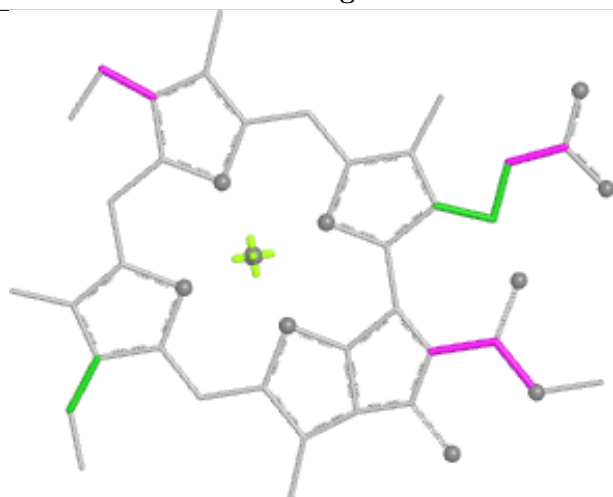
Ligand CLA S 603



Bond lengths



Bond angles

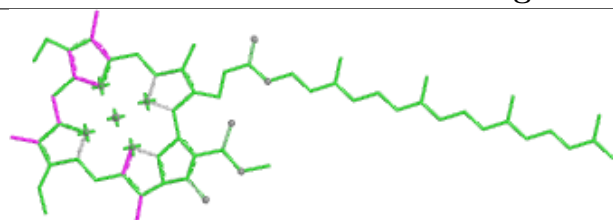


Torsions

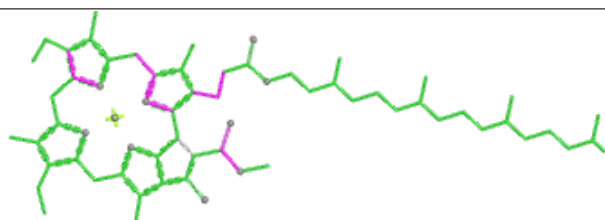


Rings

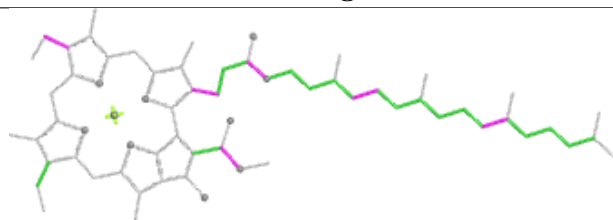
Ligand CLA R 609



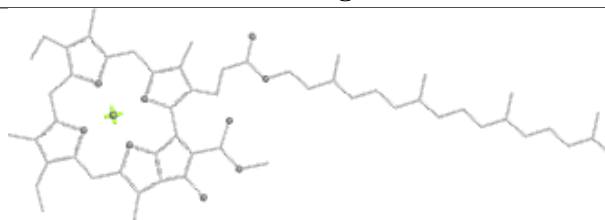
Bond lengths



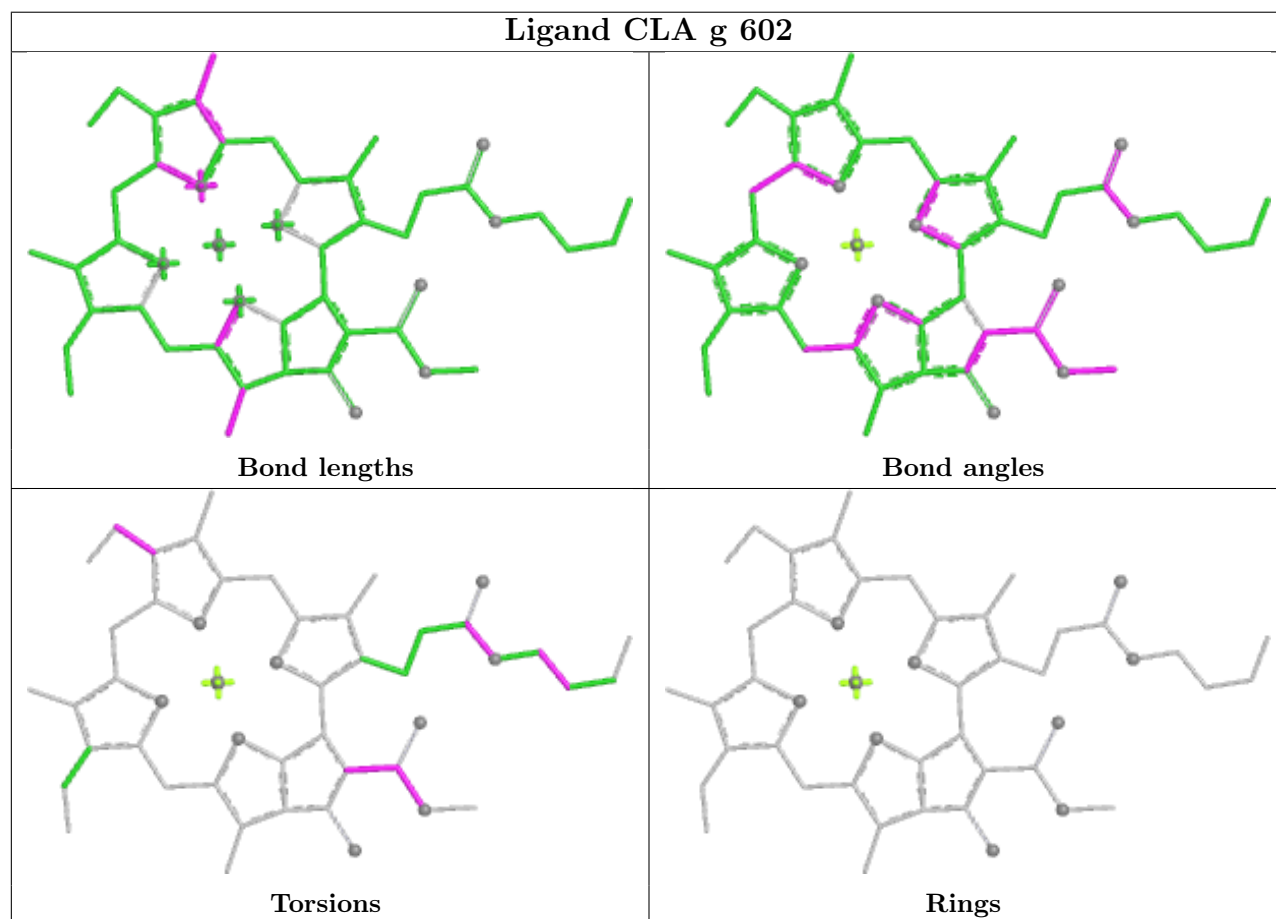
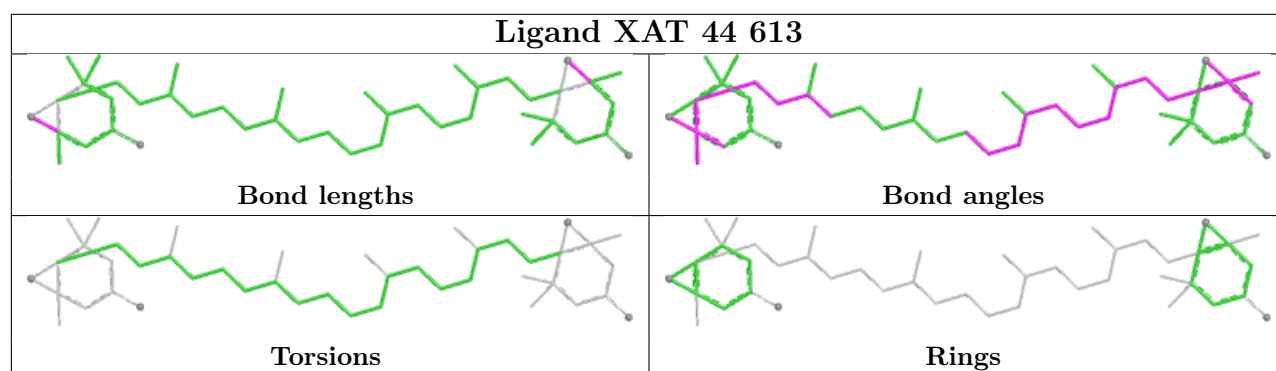
Bond angles

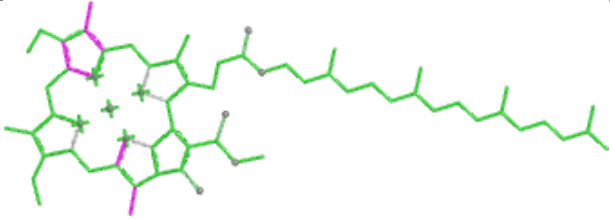
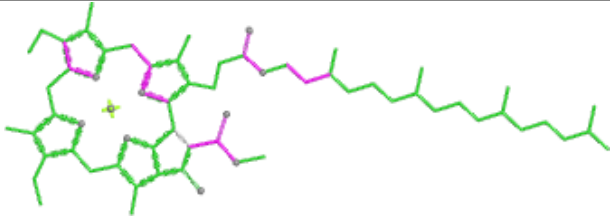
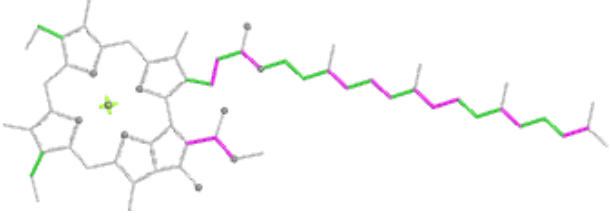
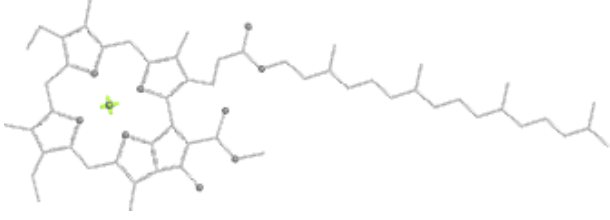
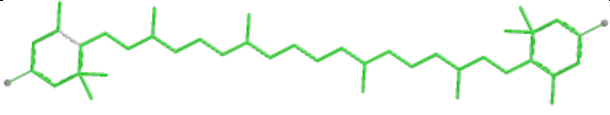
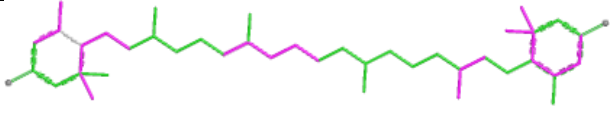
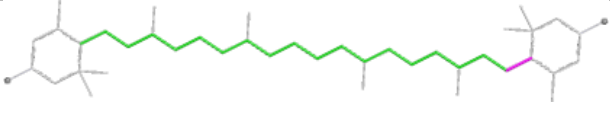
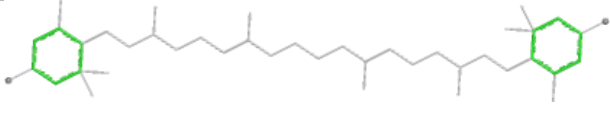
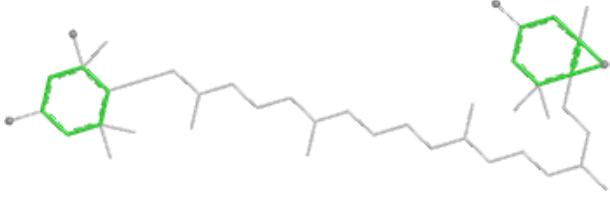


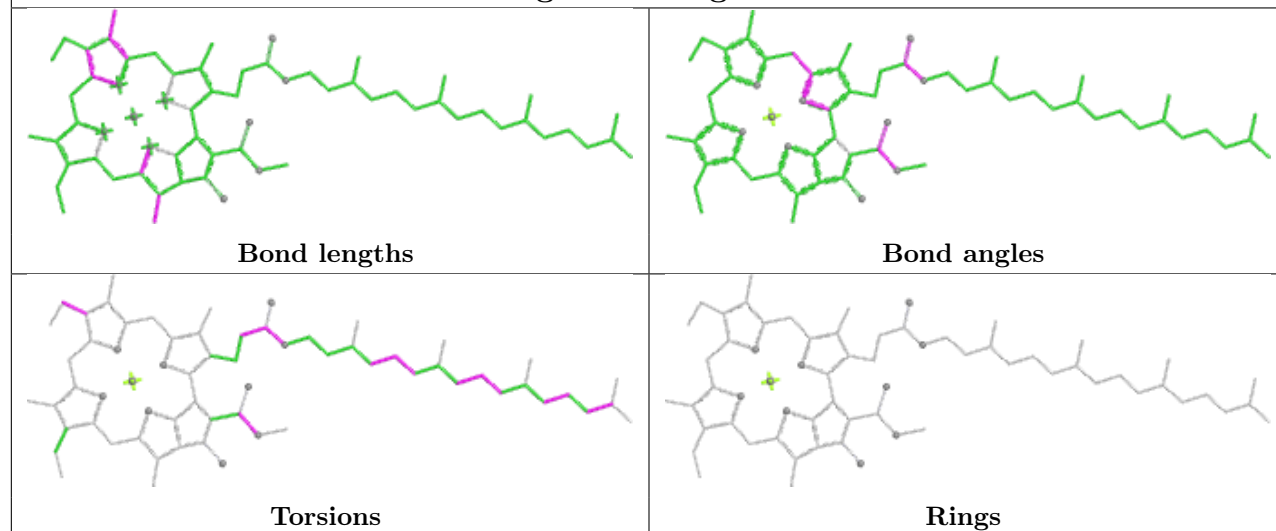
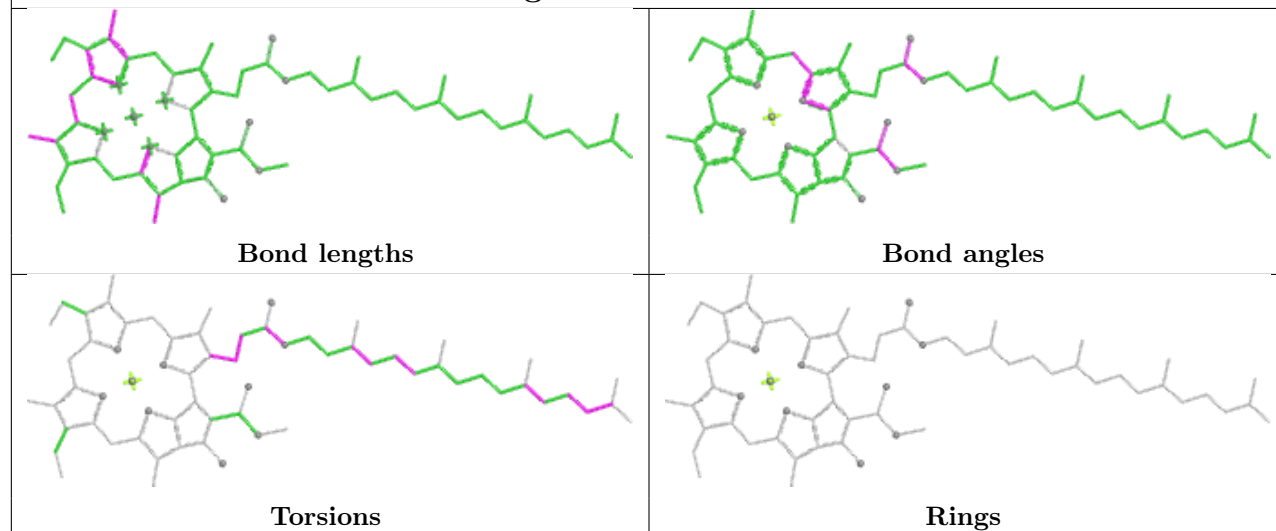
Torsions

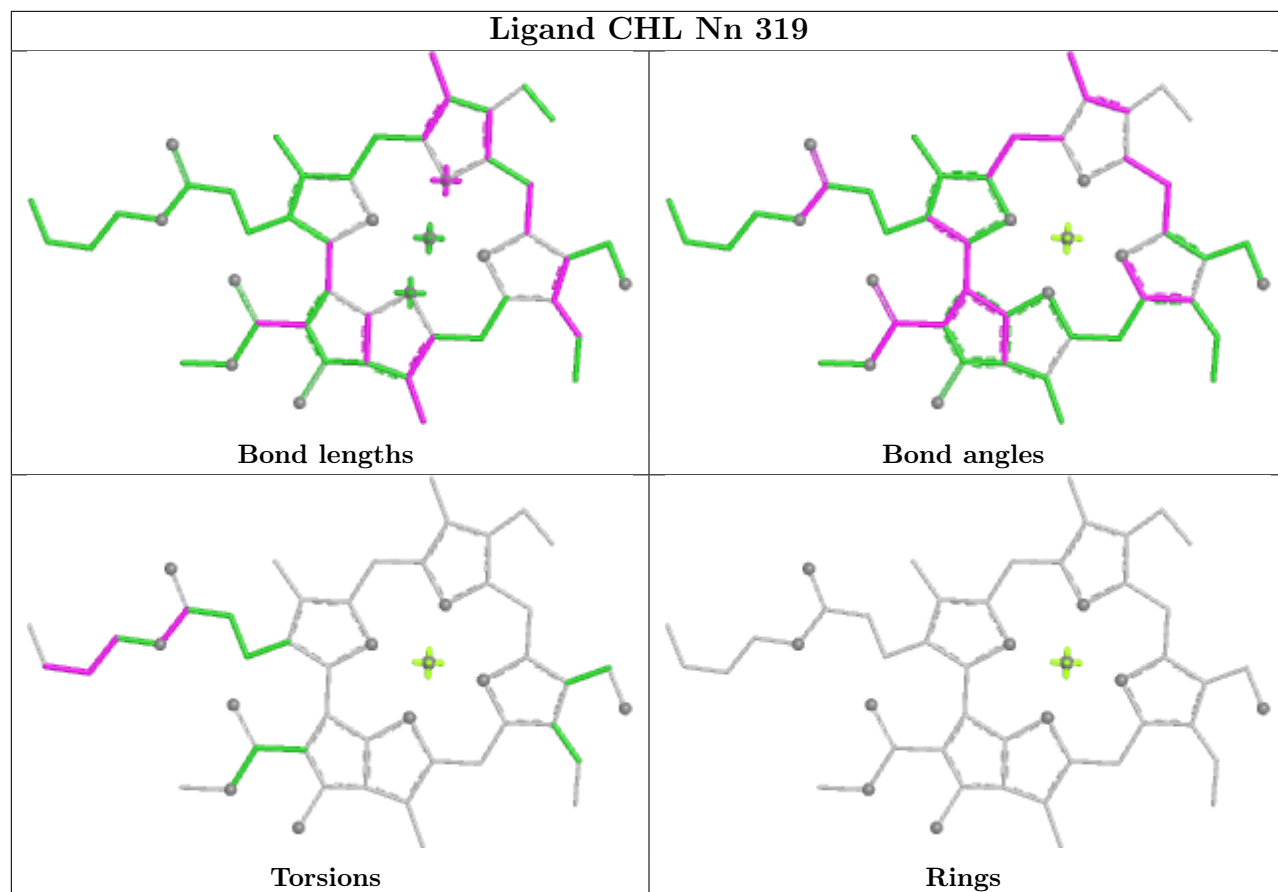


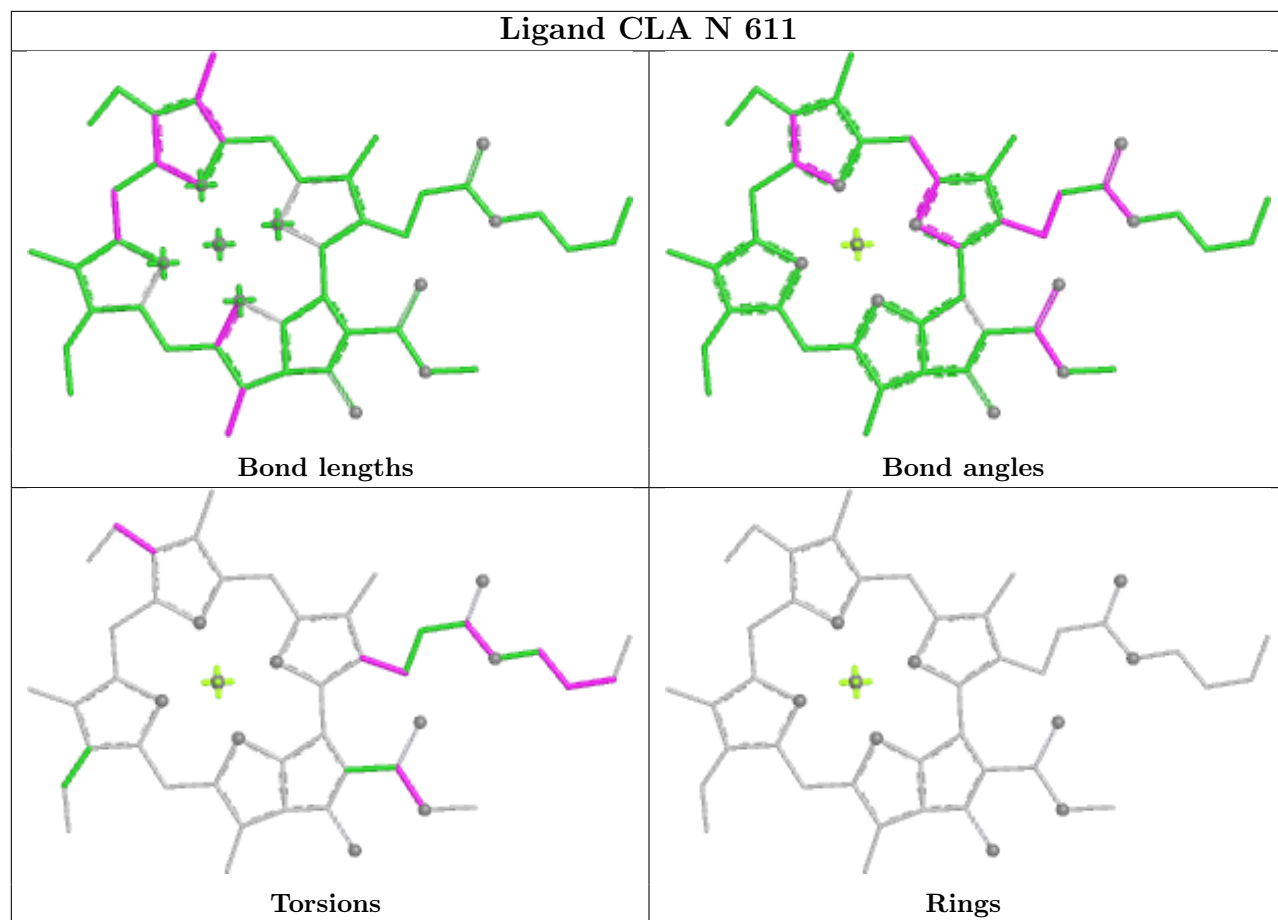
Rings



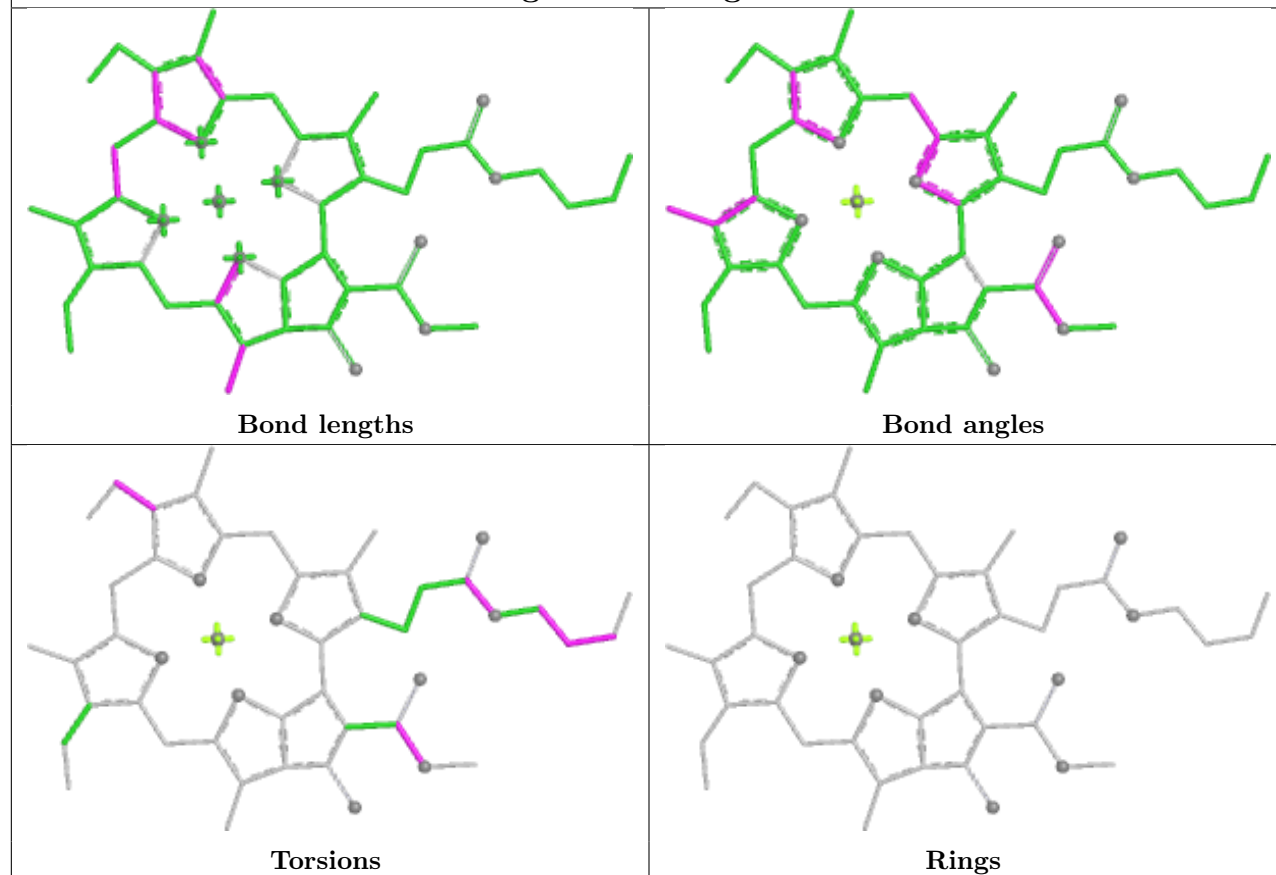
Ligand CLA B 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT GG 615	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand NEX Y 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 603**Ligand CLA Cc 512**

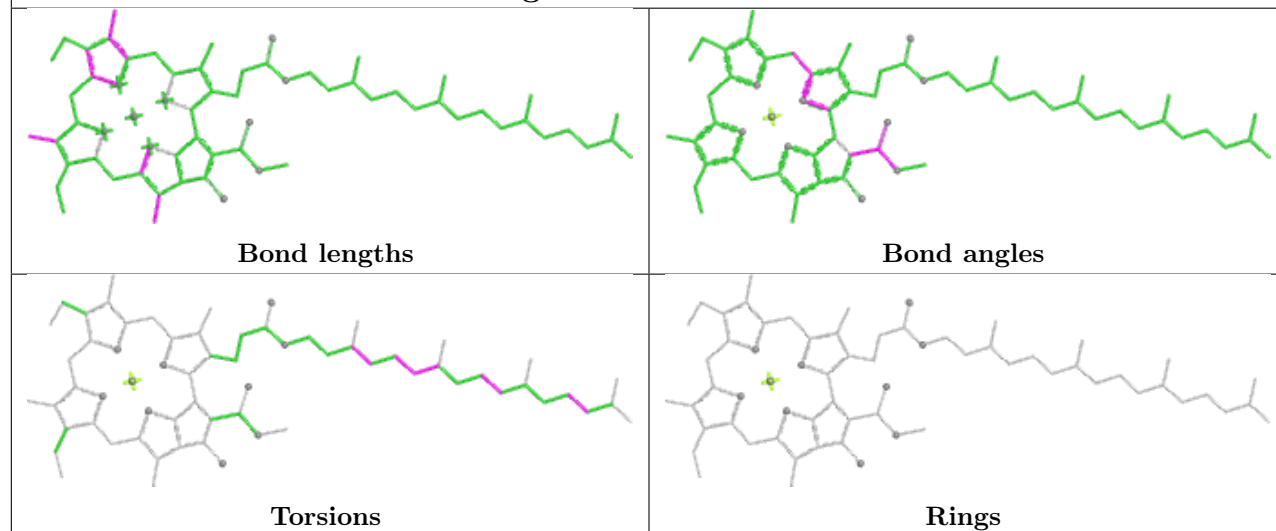


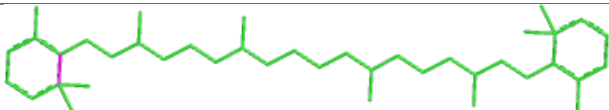
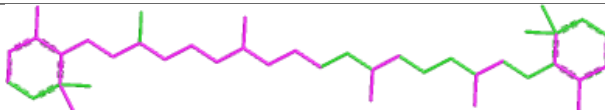
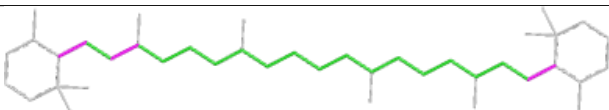
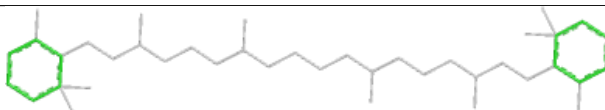


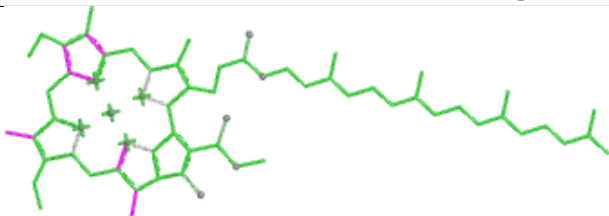
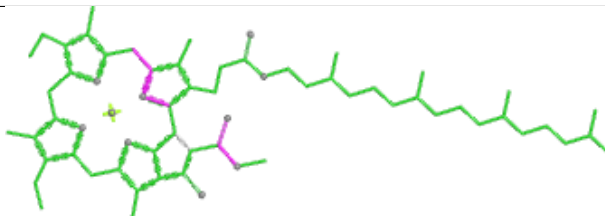
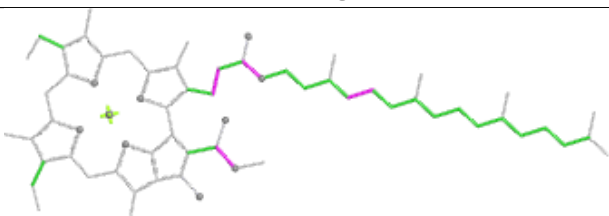
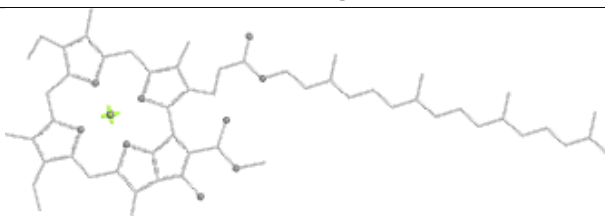
Ligand CLA Gg 311

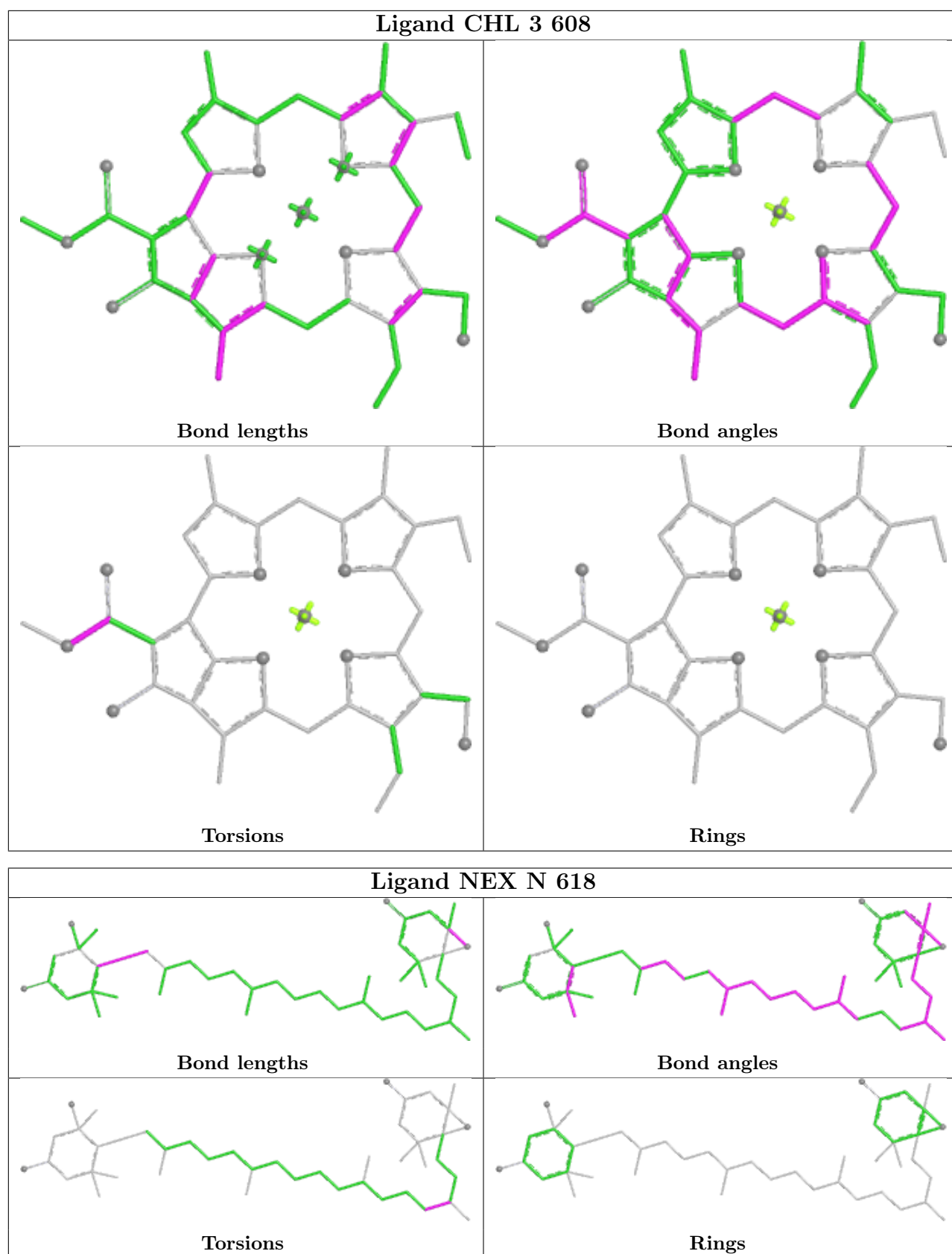


Ligand CLA Bb 611

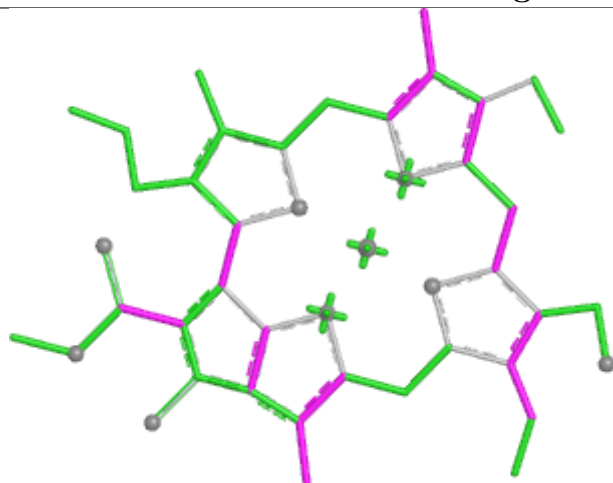


Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

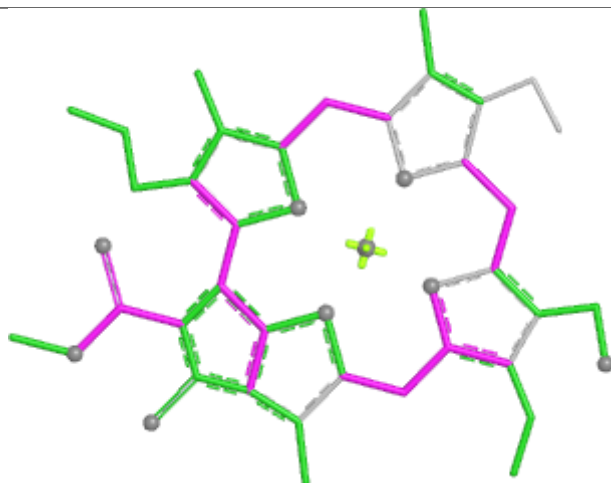
Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings



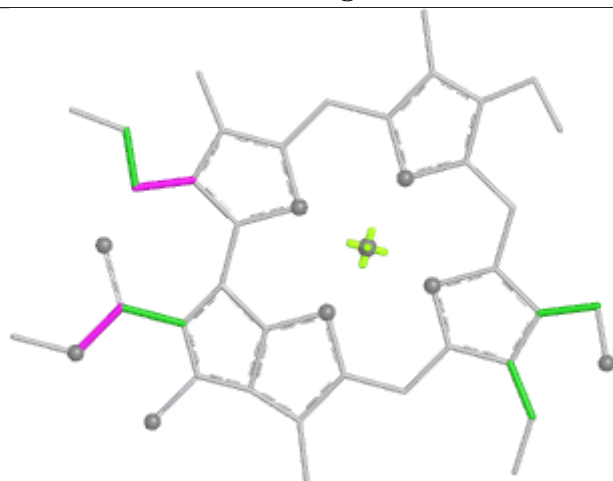
Ligand CHL Y 606



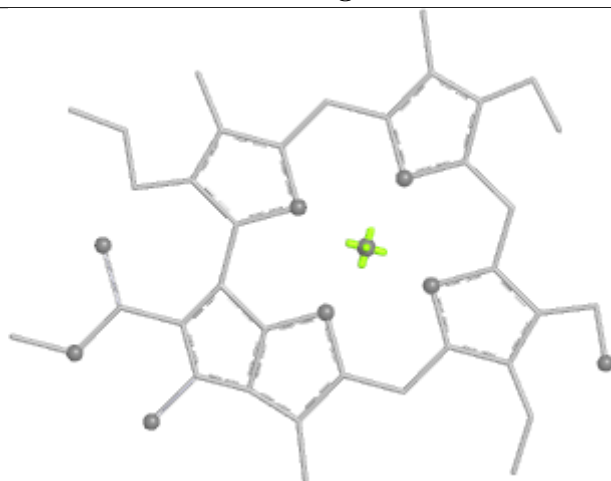
Bond lengths



Bond angles

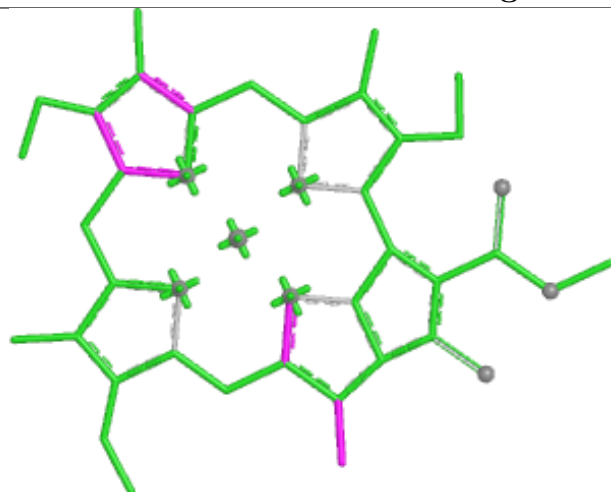


Torsions

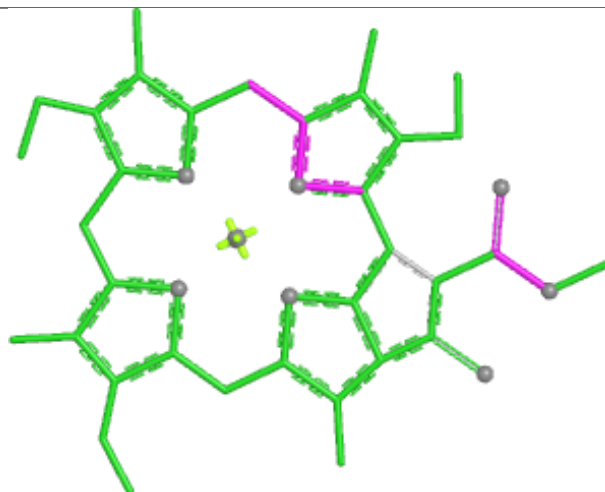


Rings

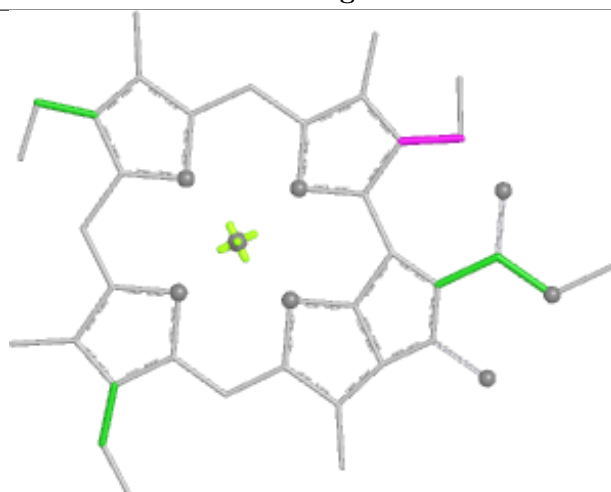
Ligand CLA RR 312



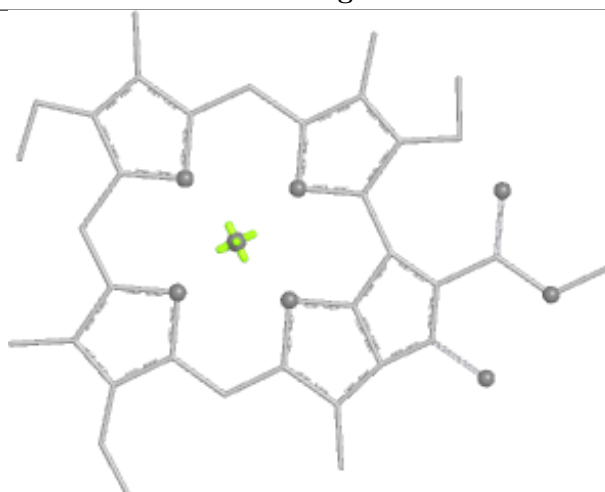
Bond lengths



Bond angles

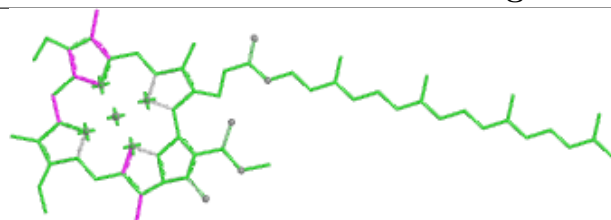


Torsions

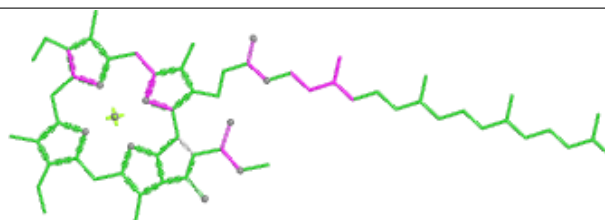


Rings

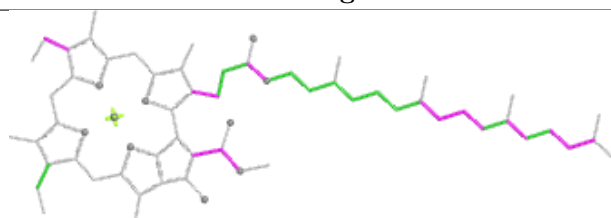
Ligand CLA Cc 508



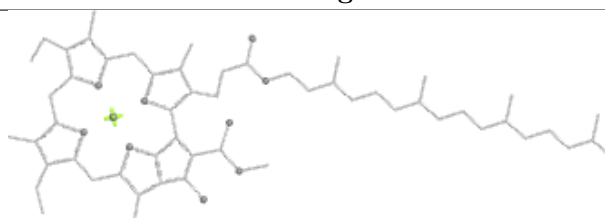
Bond lengths



Bond angles

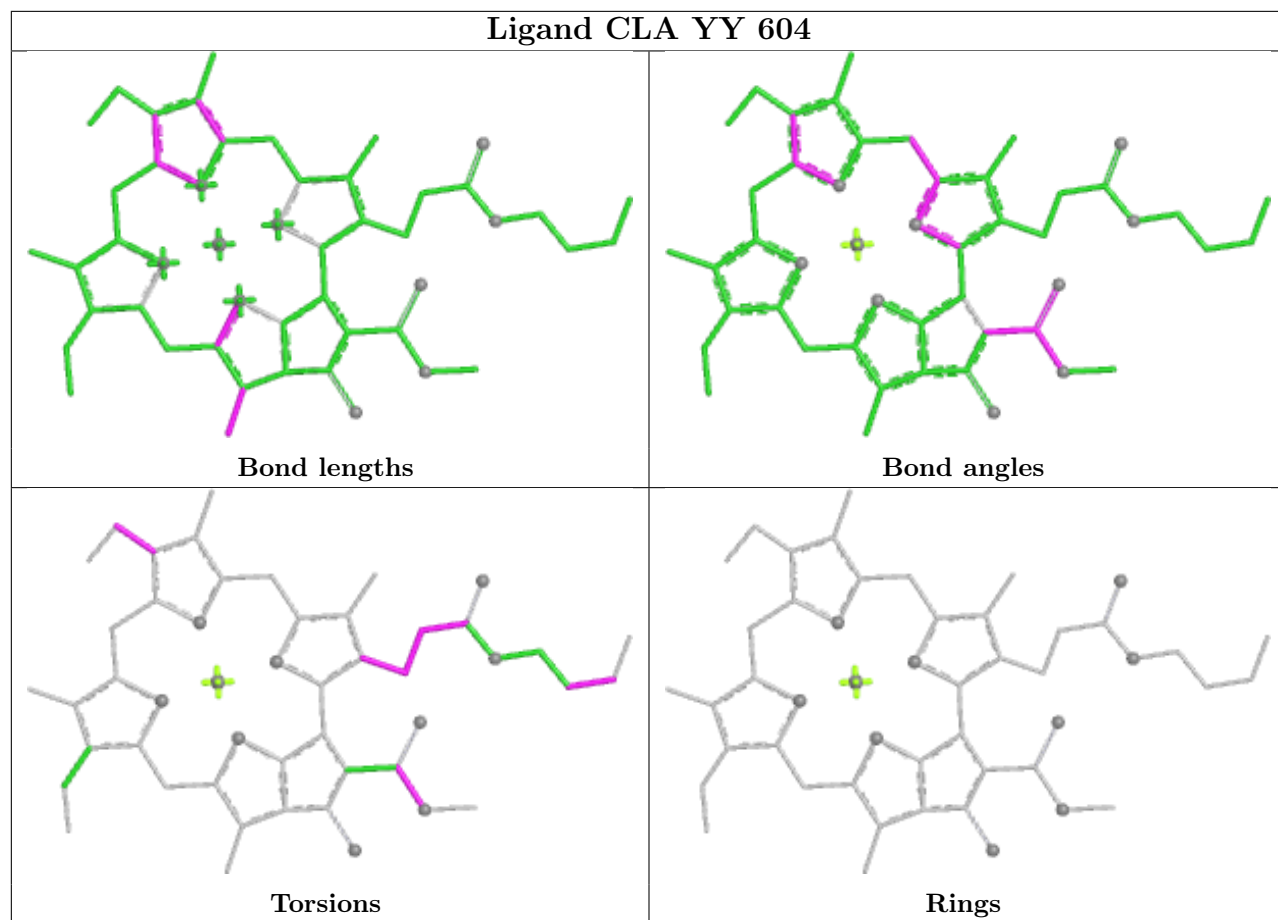


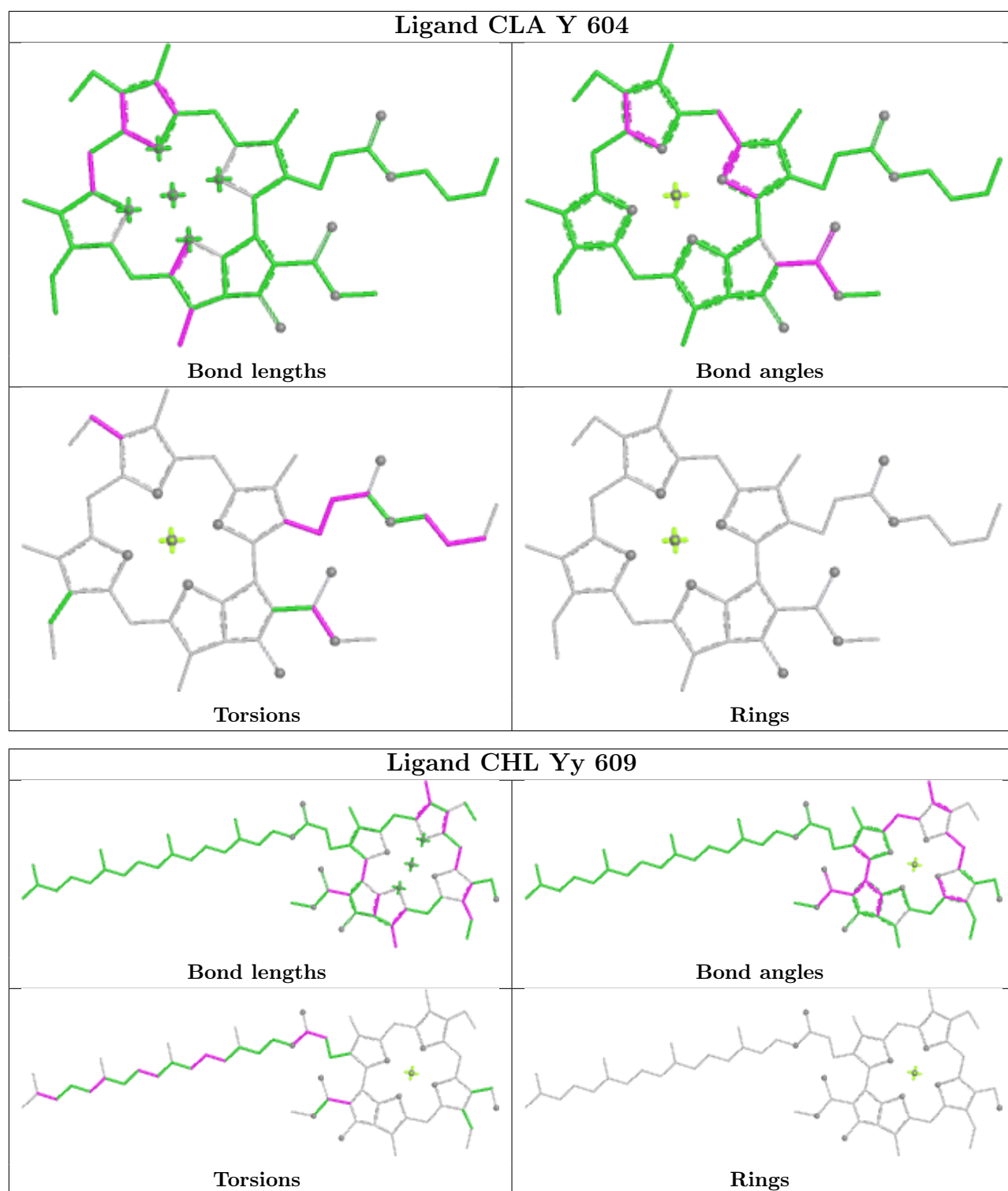
Torsions

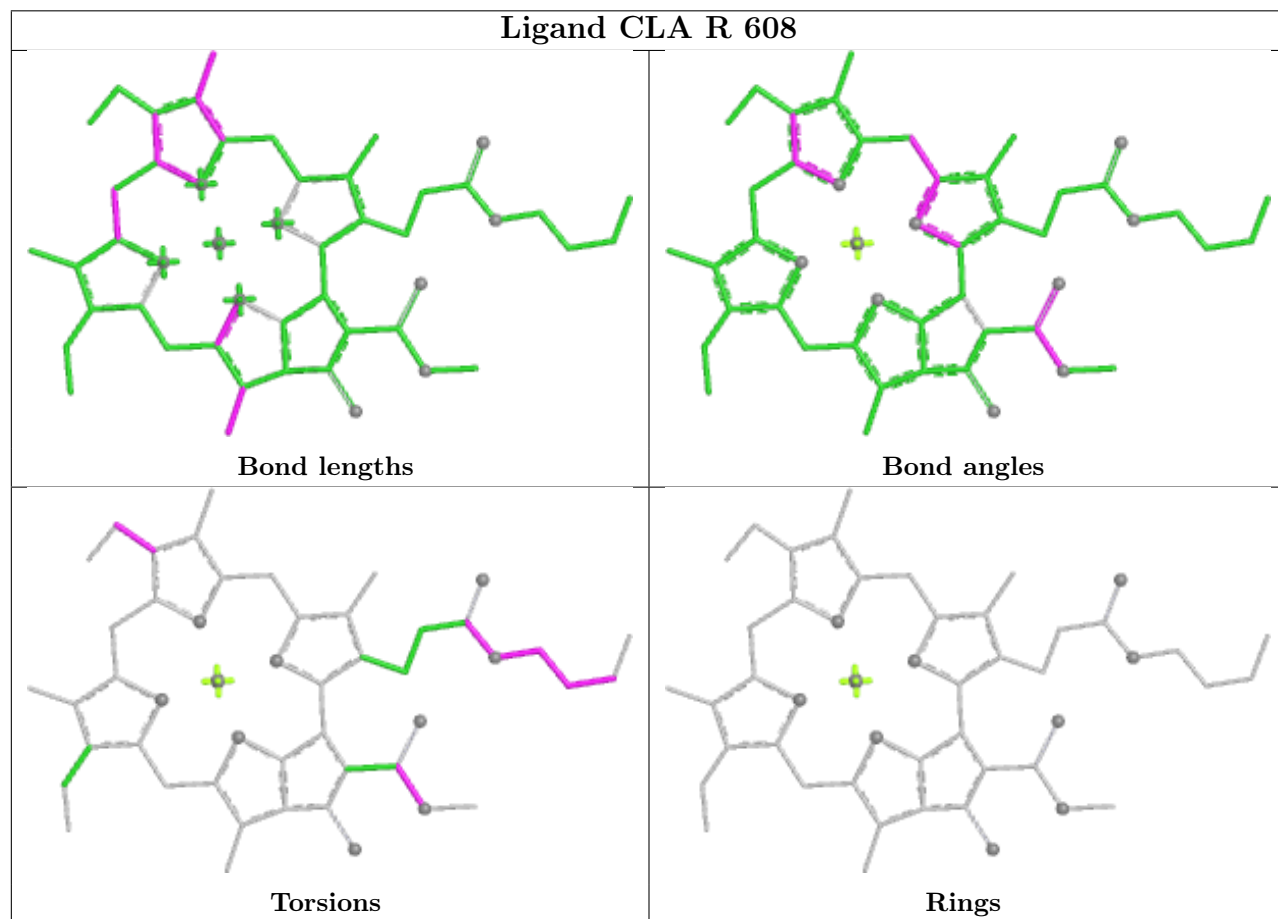
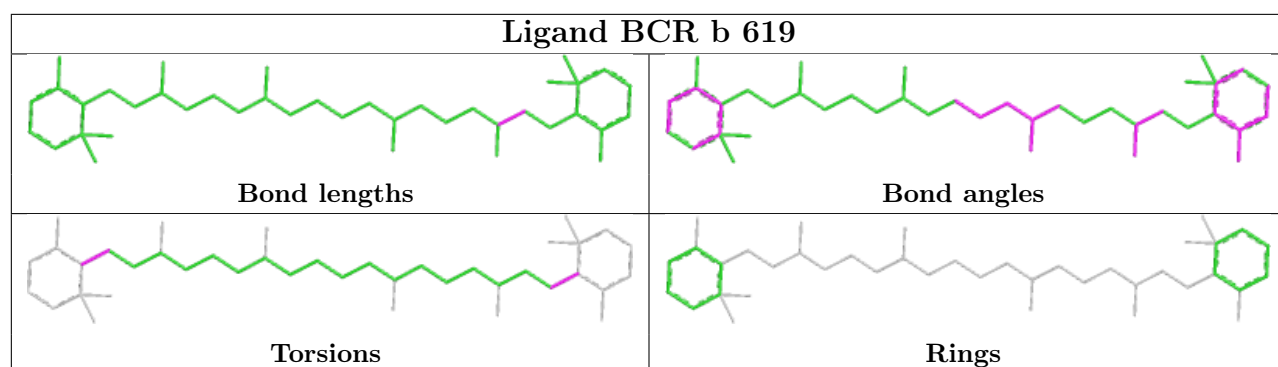


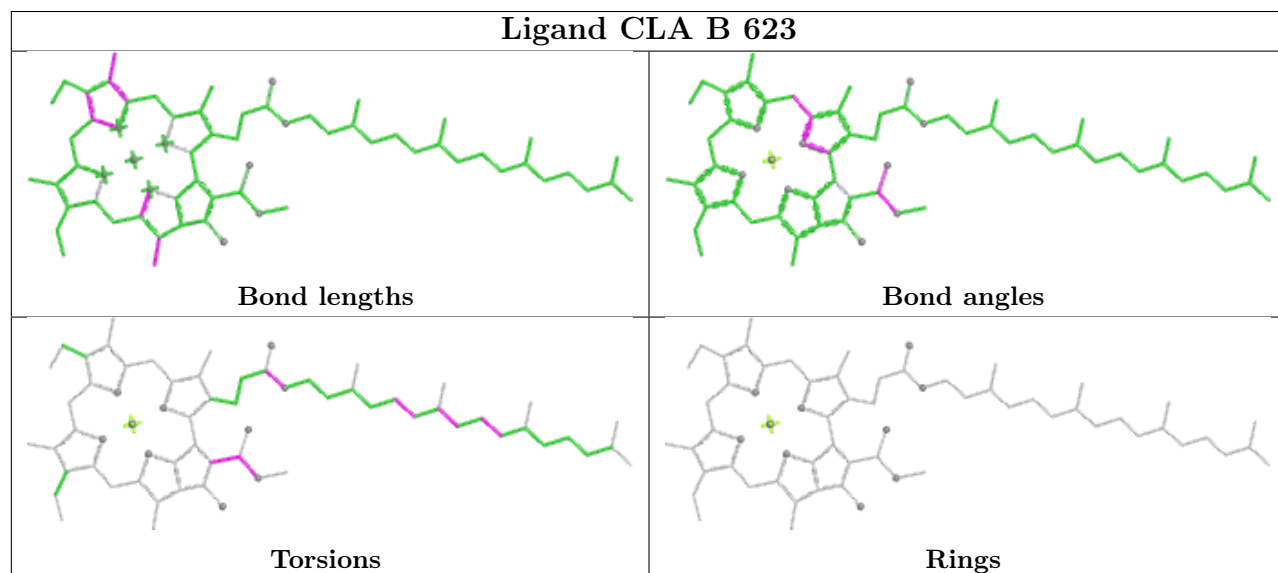
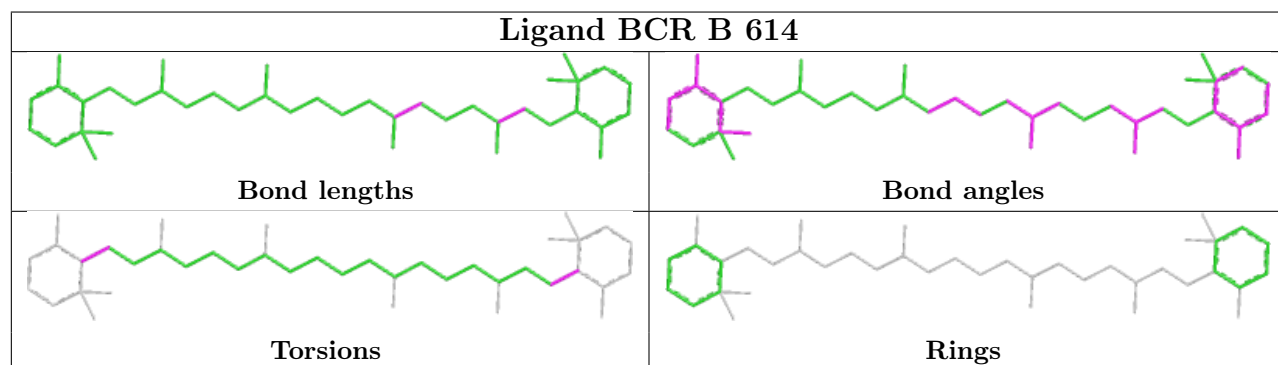
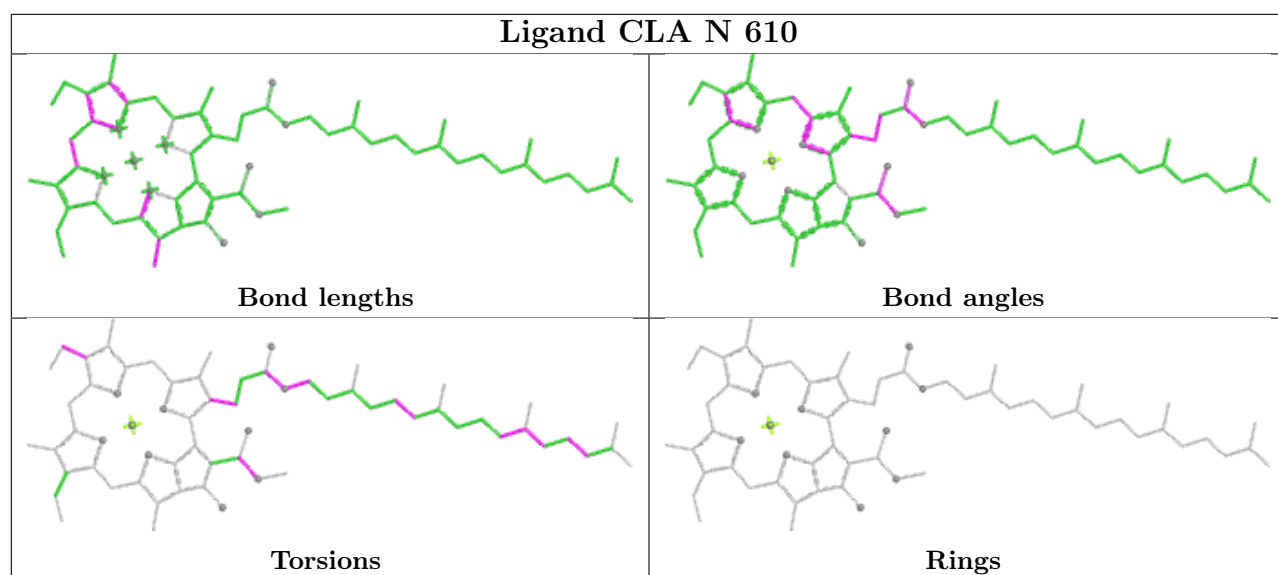
Rings

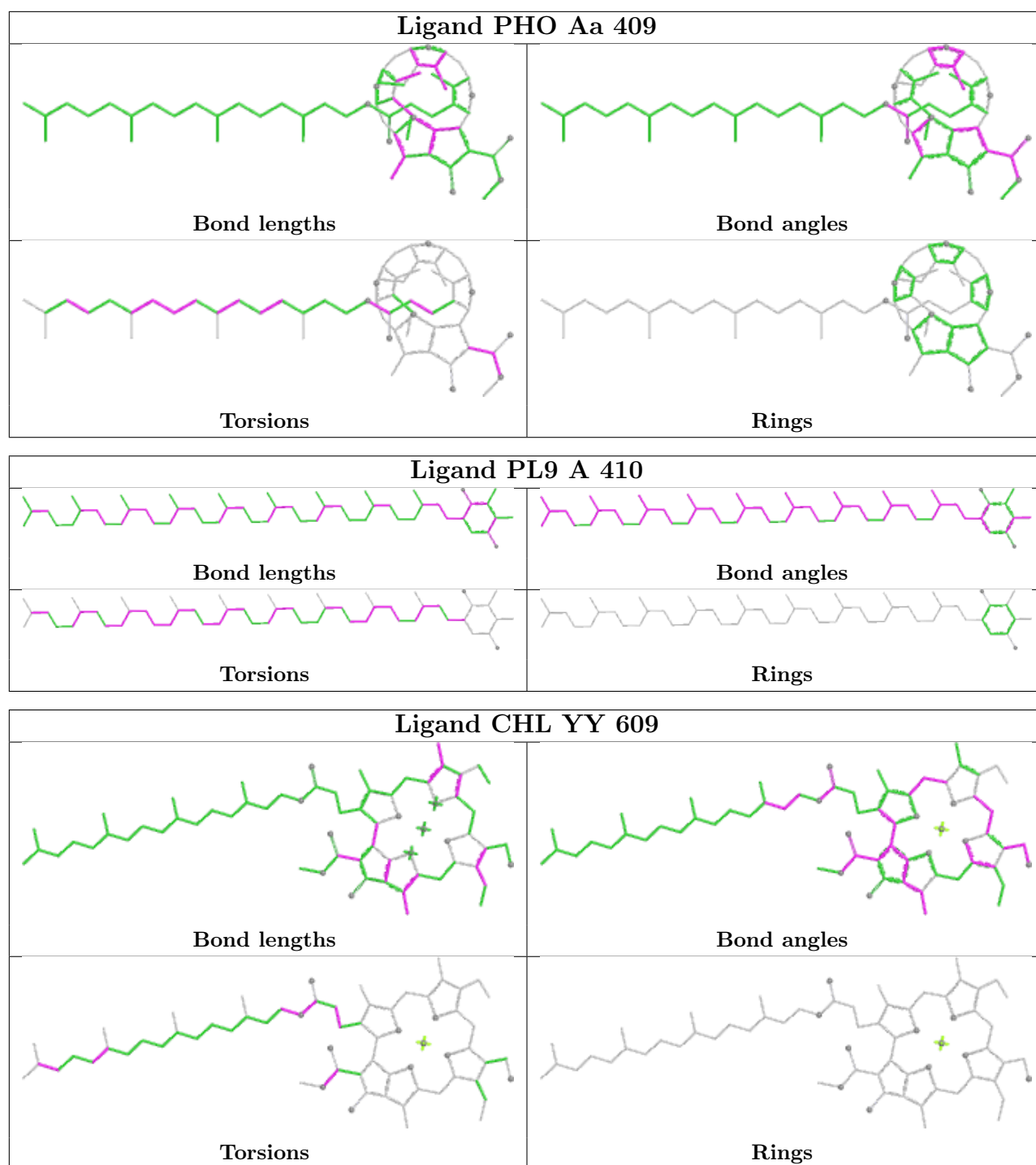
Ligand CLA YY 604

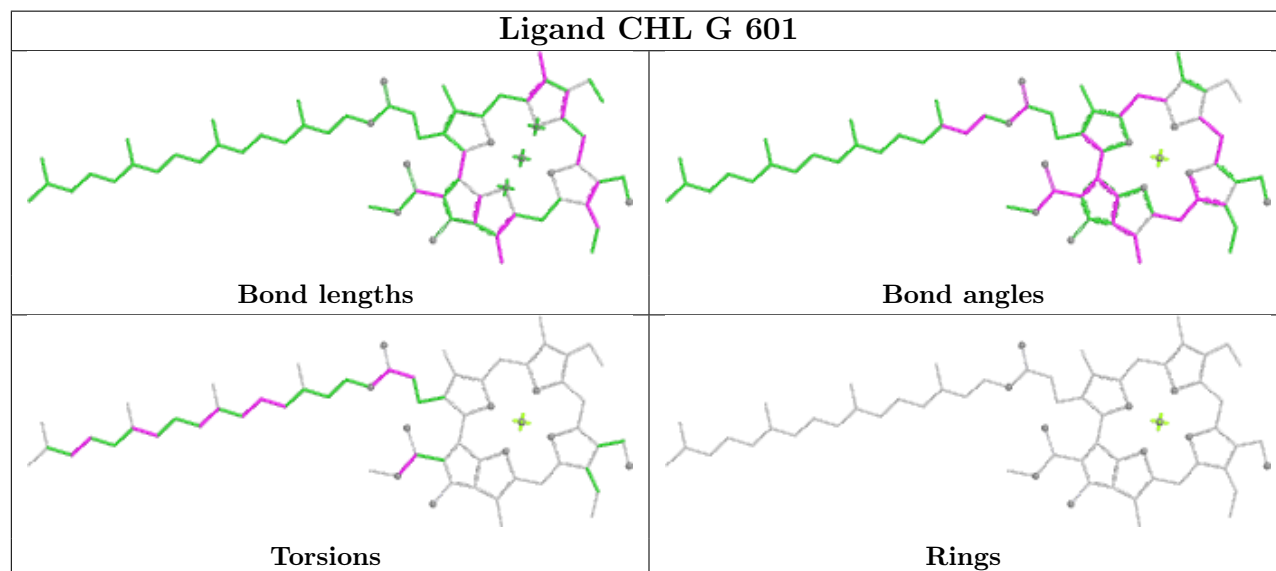
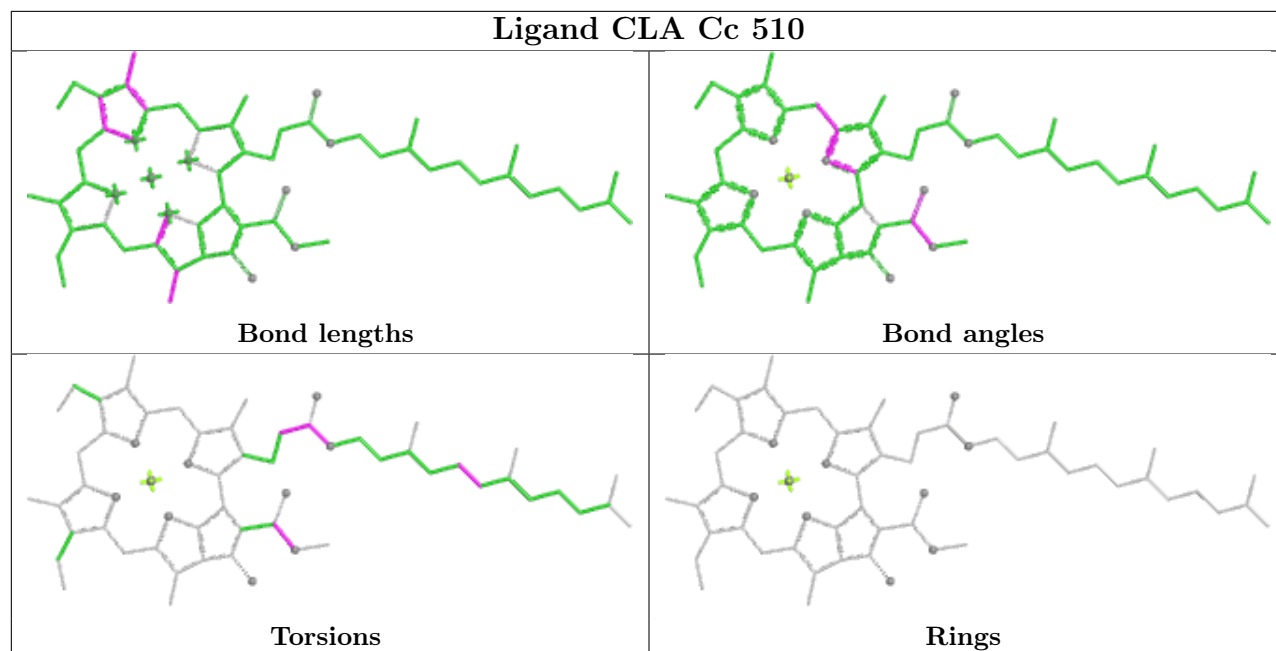




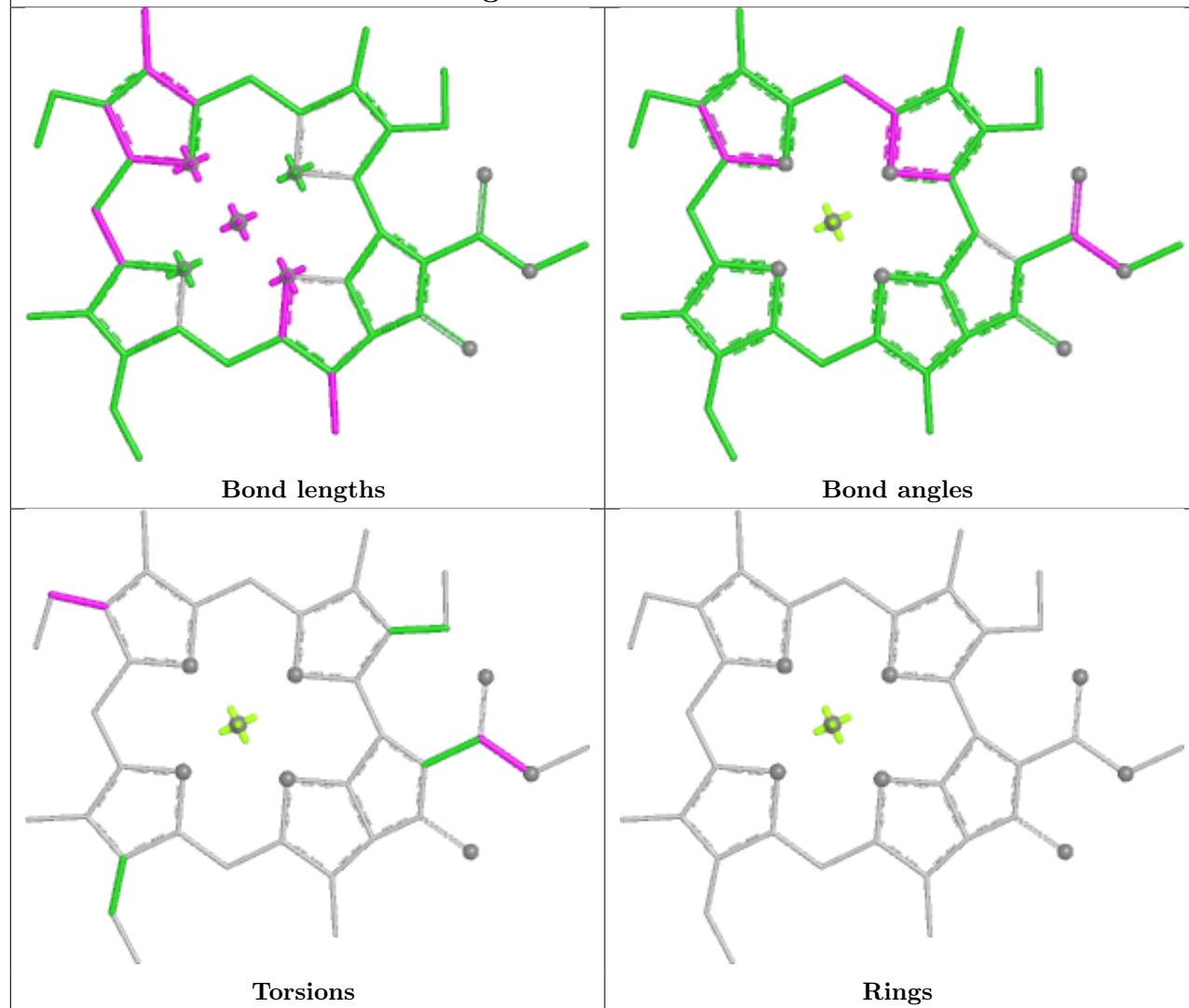




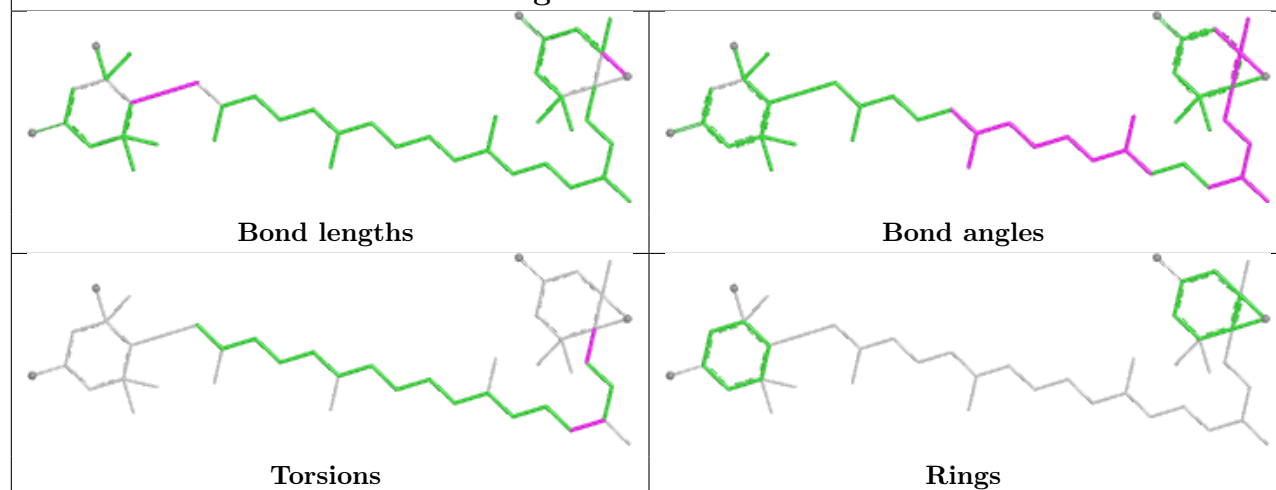


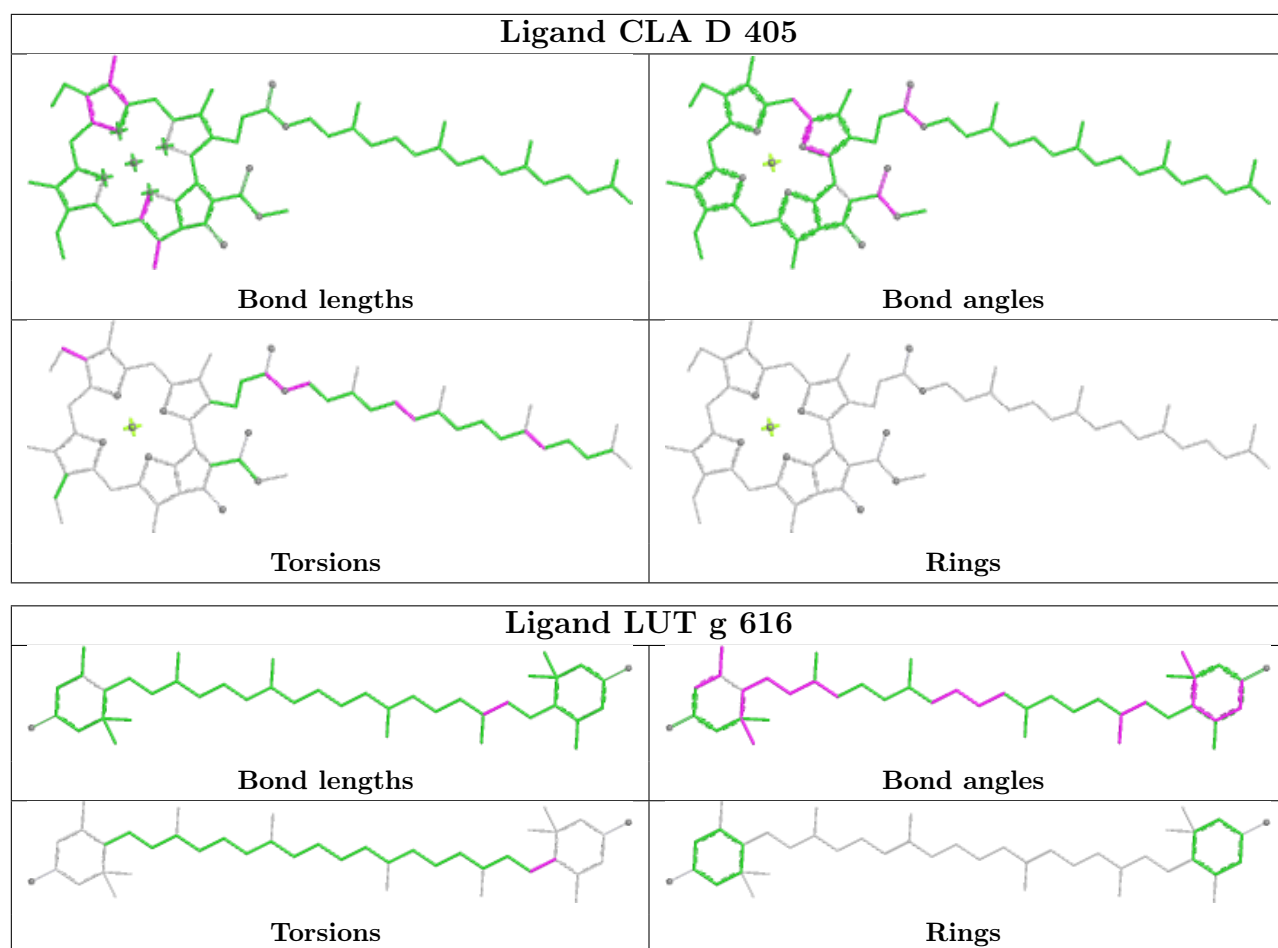


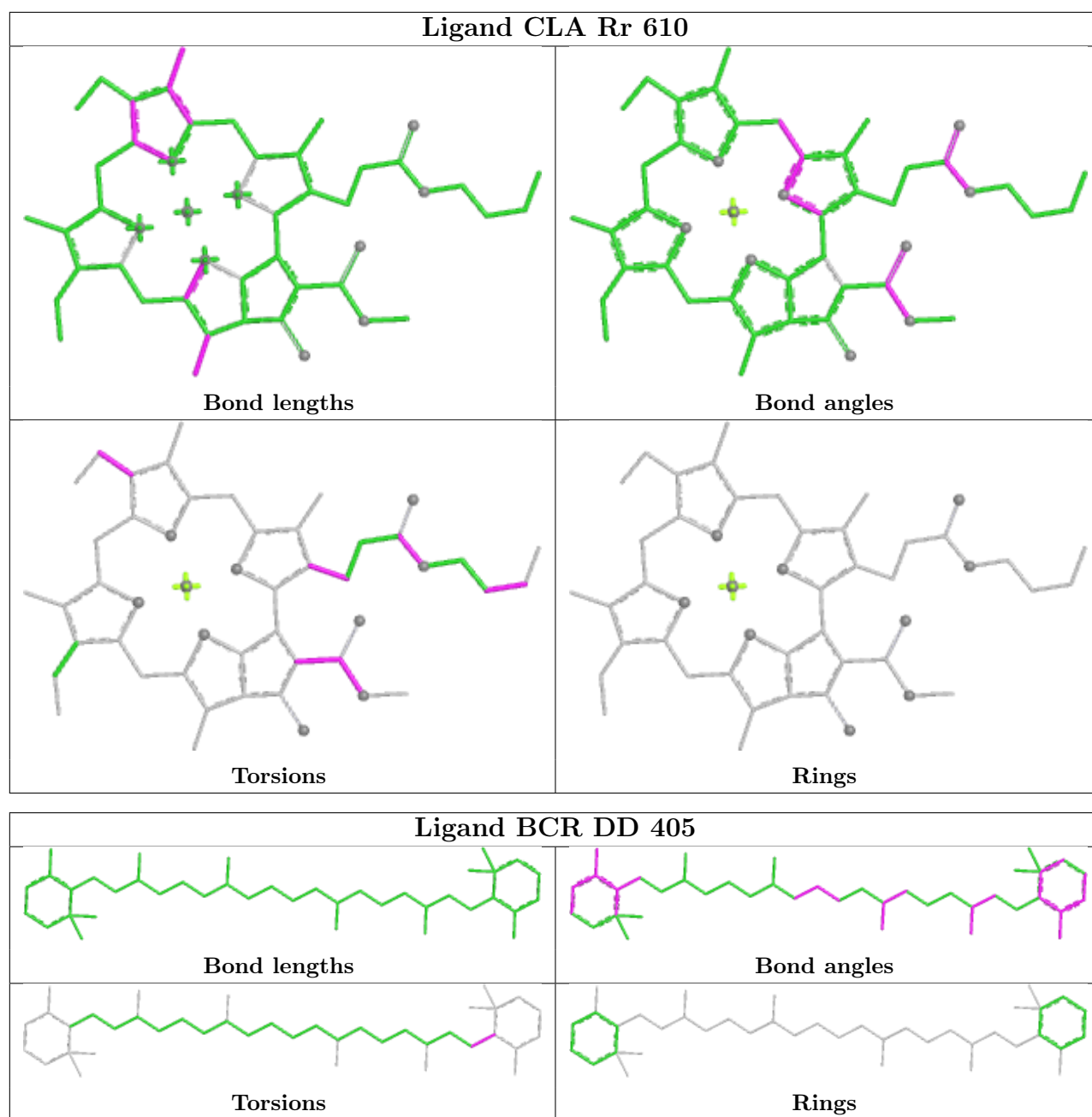
Ligand CLA YY 611



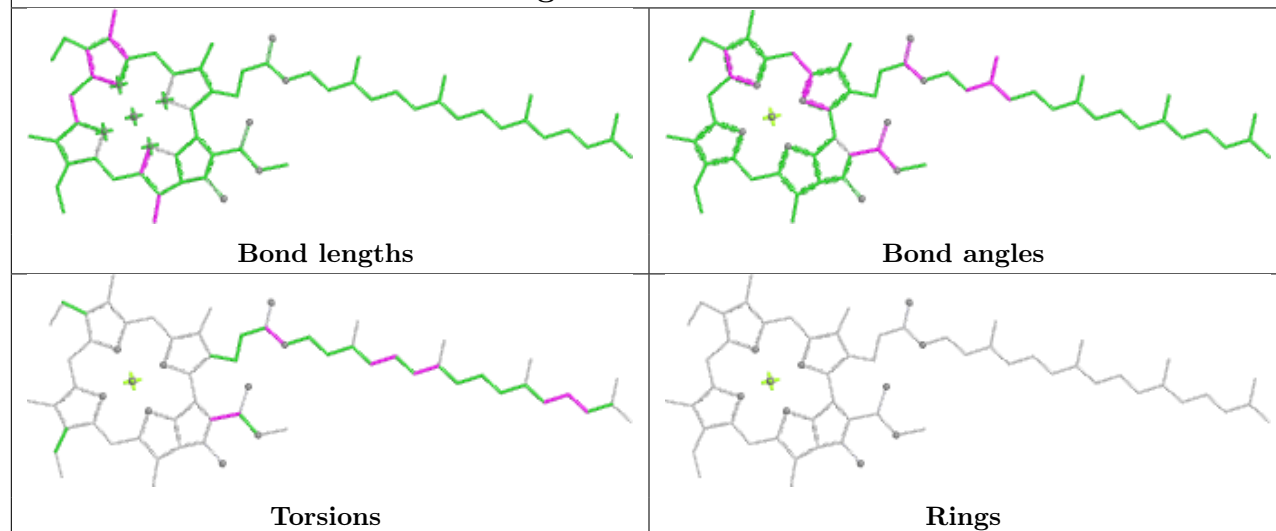
Ligand NEX n 617



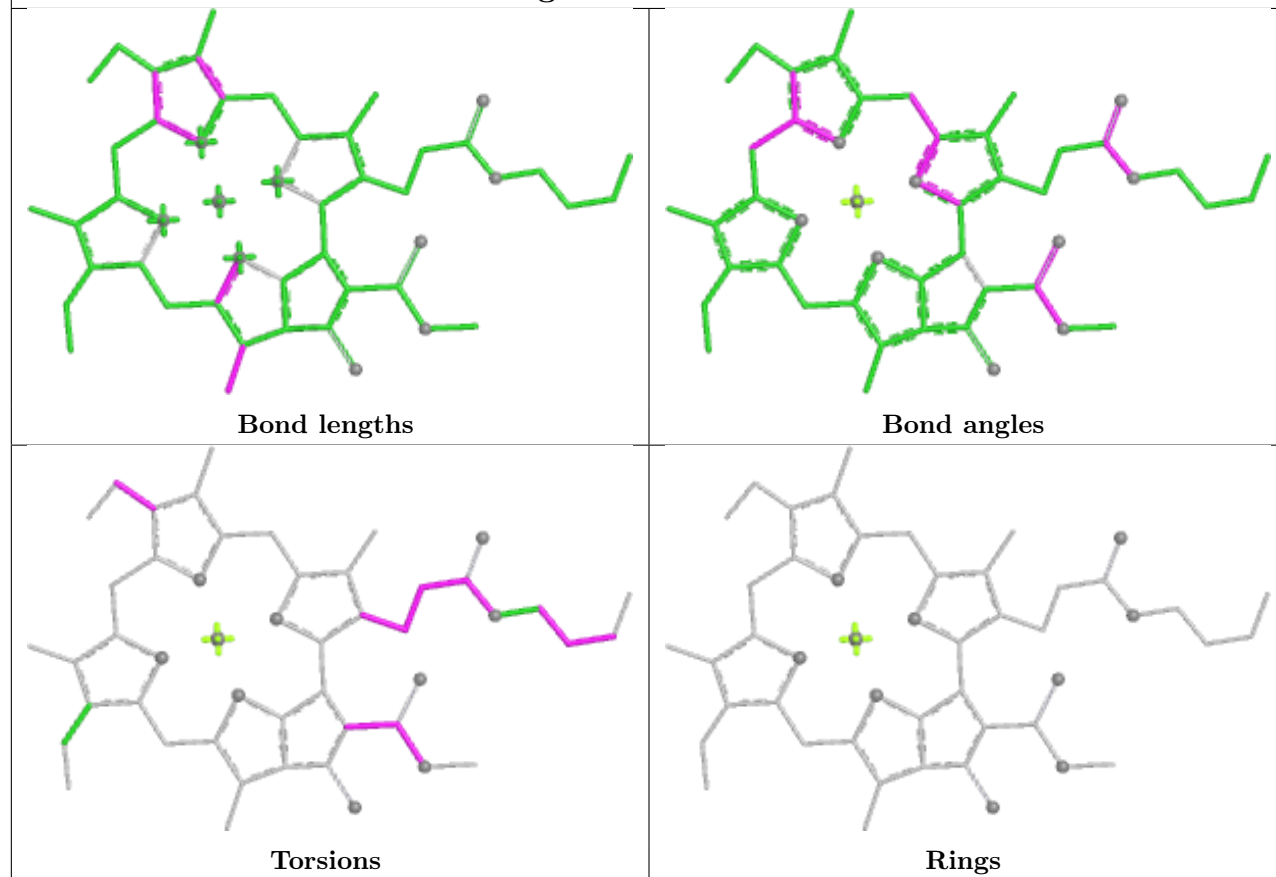


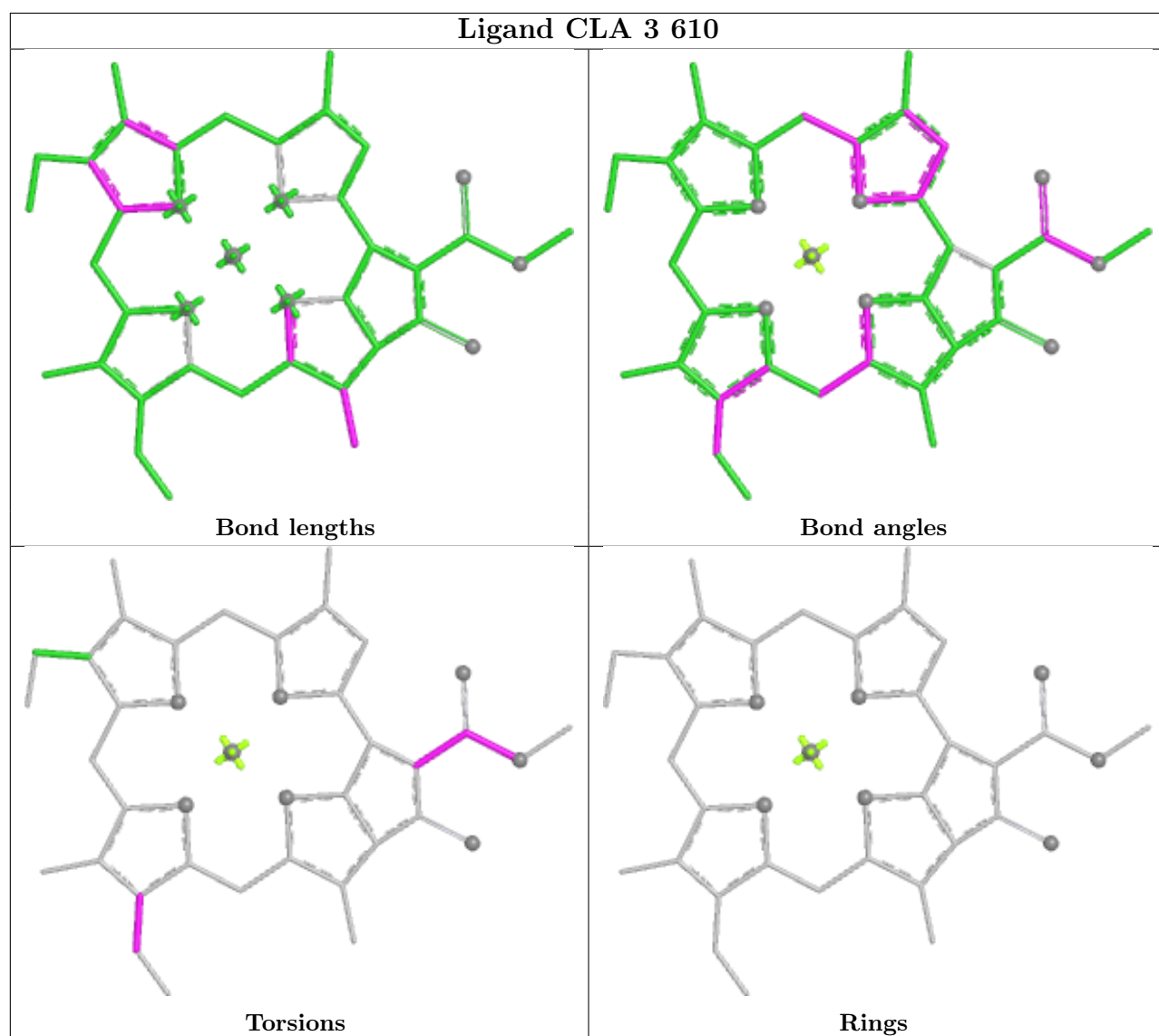
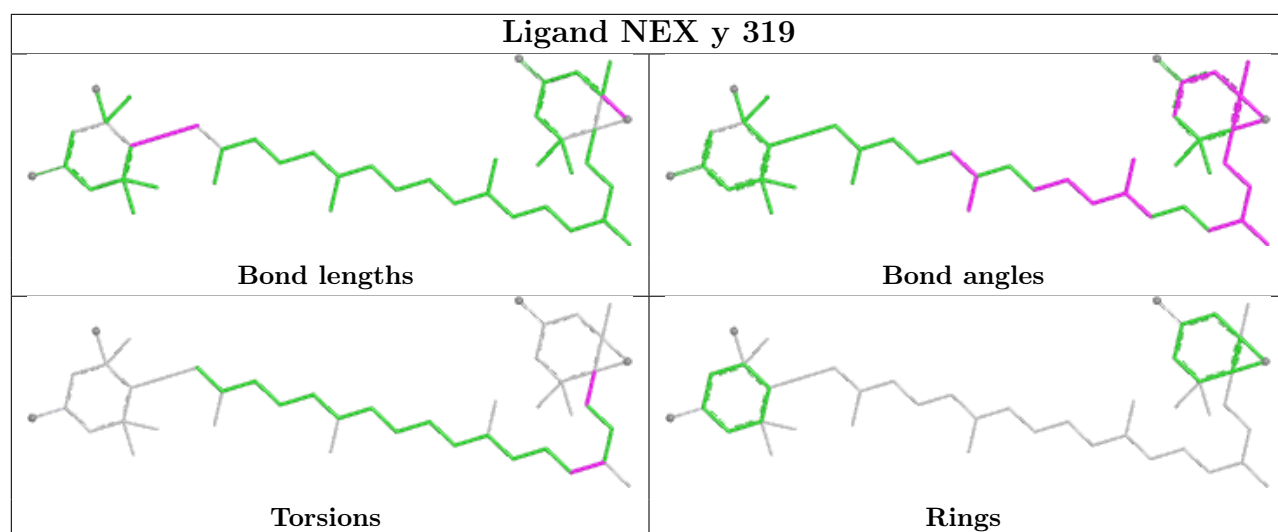


Ligand CLA c 502

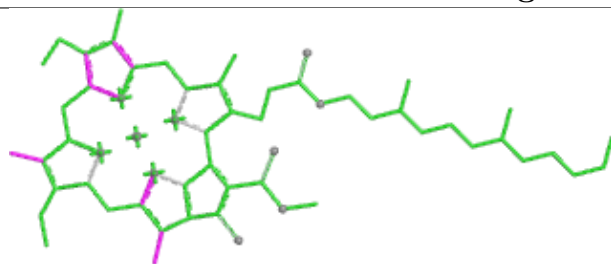


Ligand CLA r 604

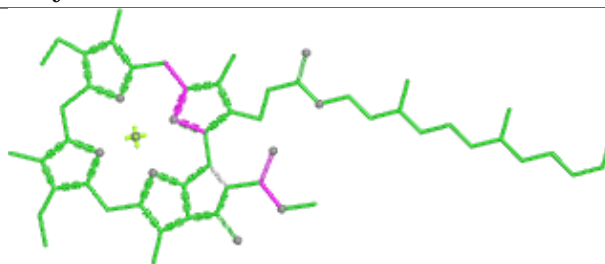




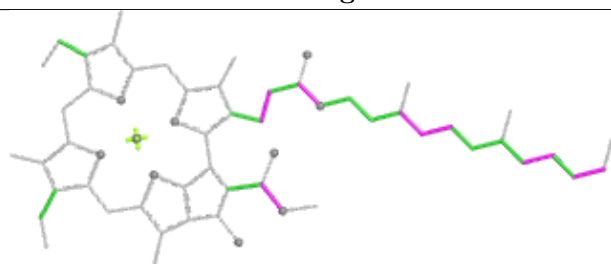
Ligand CLA y 315



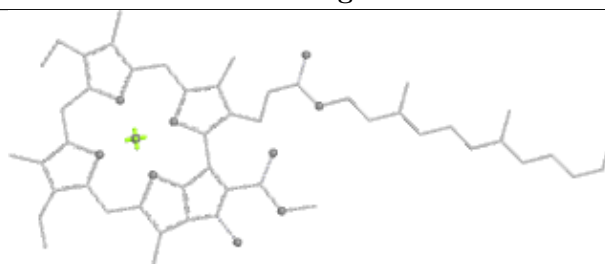
Bond lengths



Bond angles

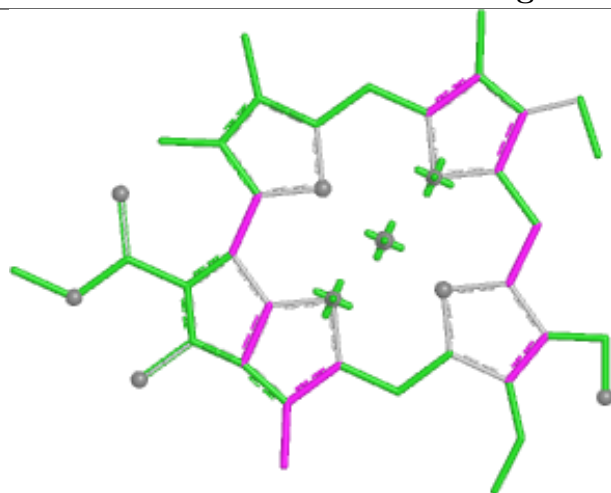


Torsions



Rings

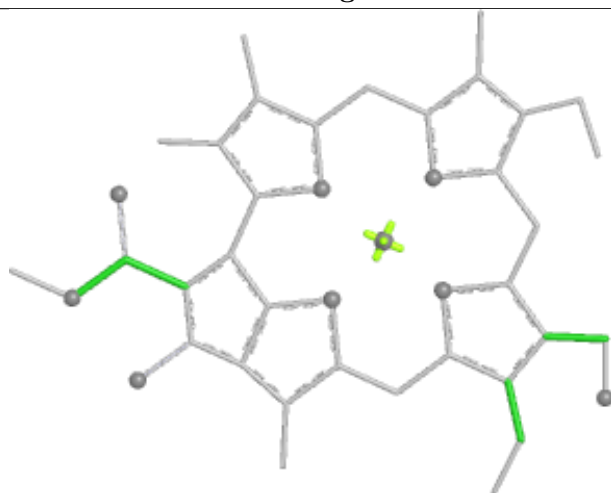
Ligand CHL S 606



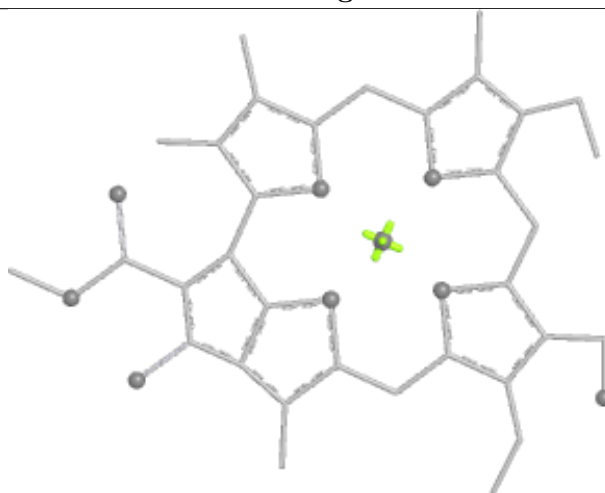
Bond lengths



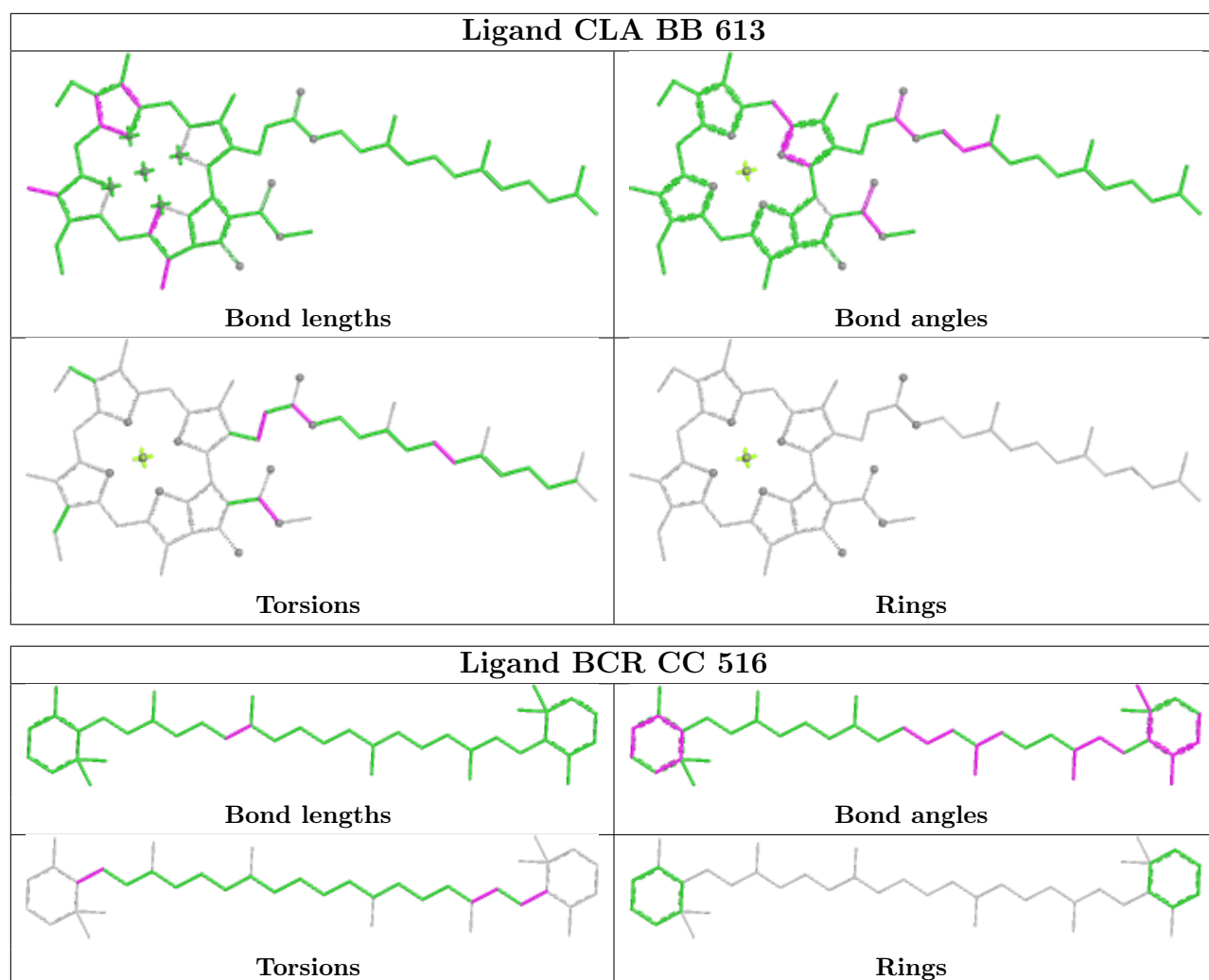
Bond angles

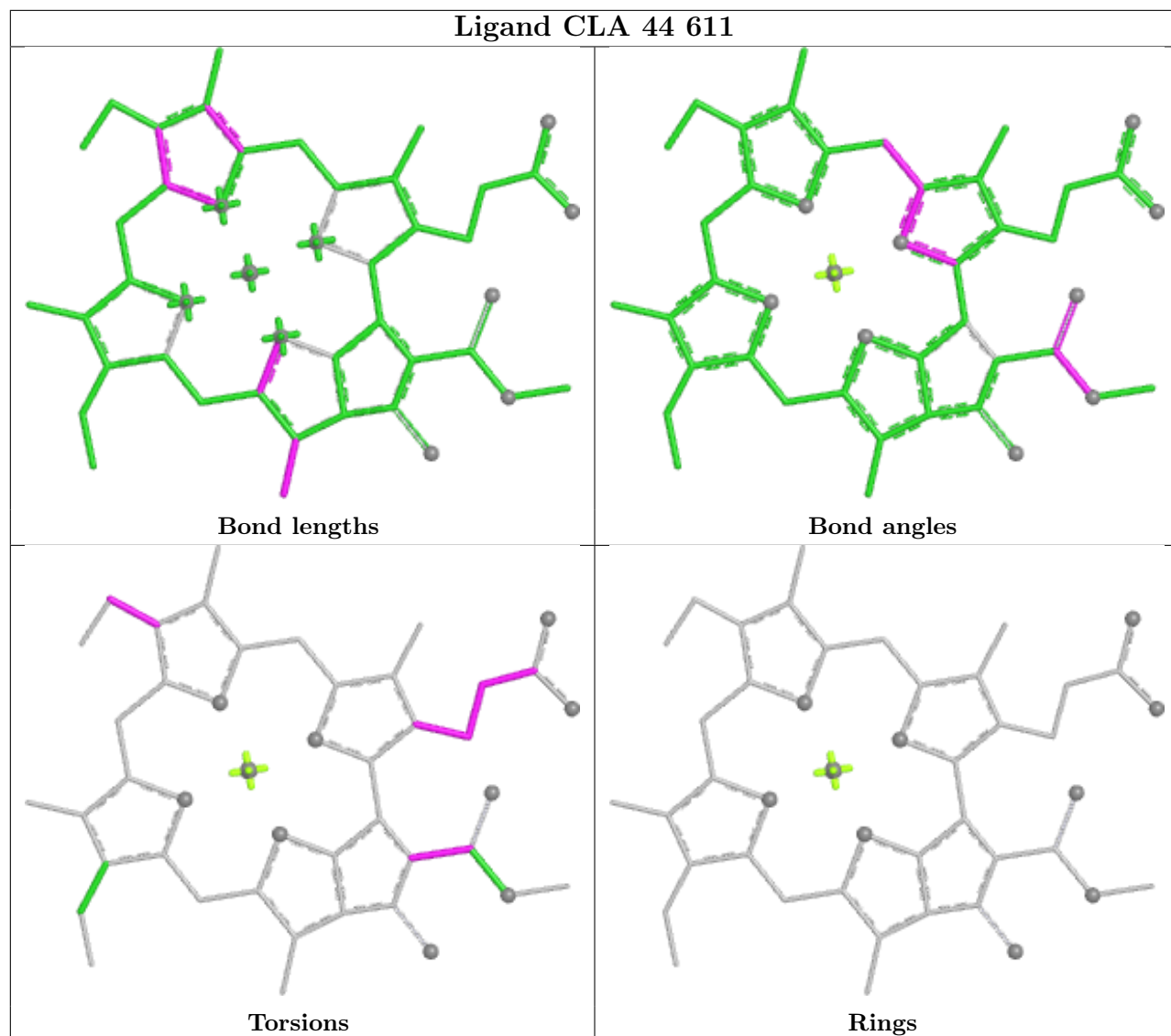


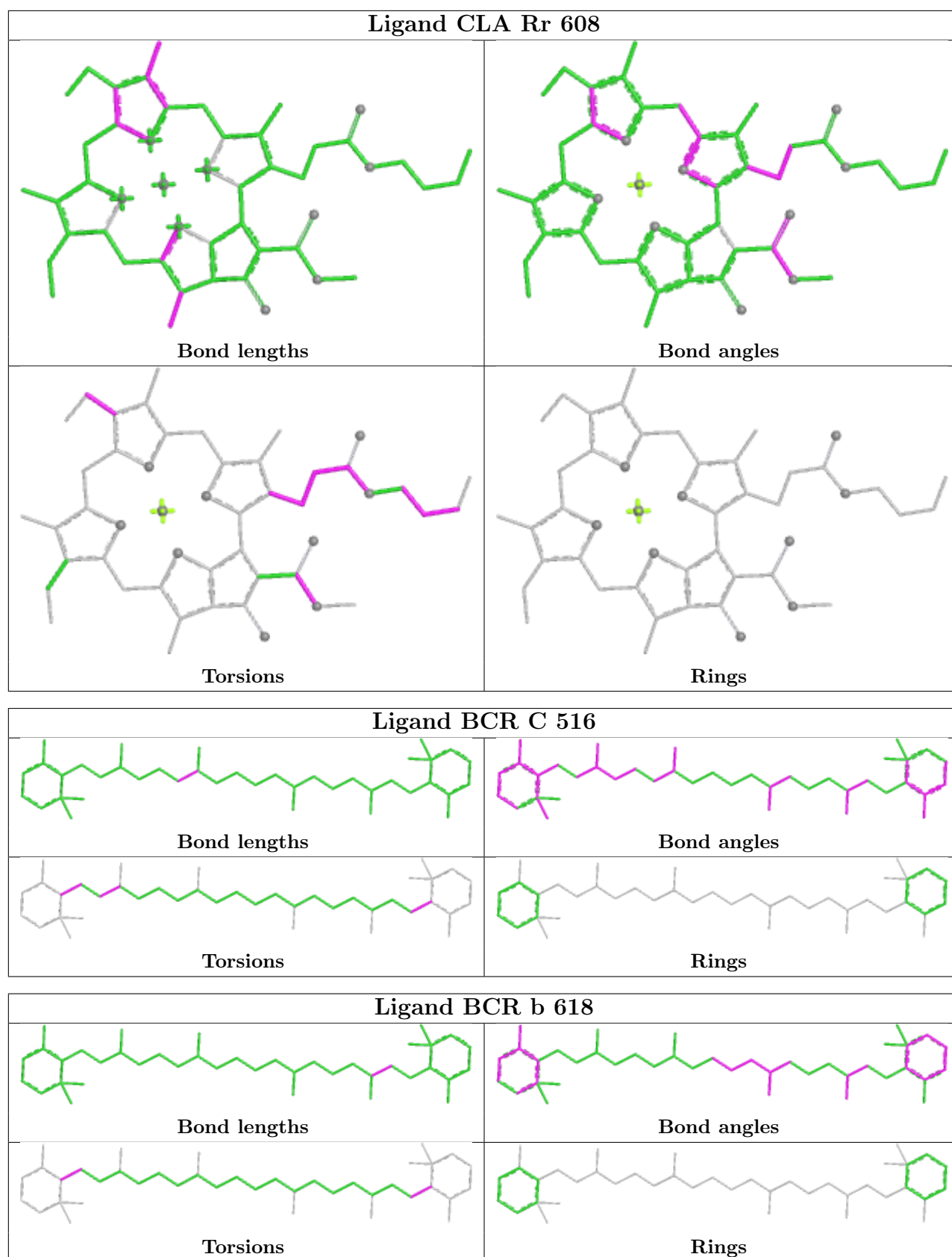
Torsions



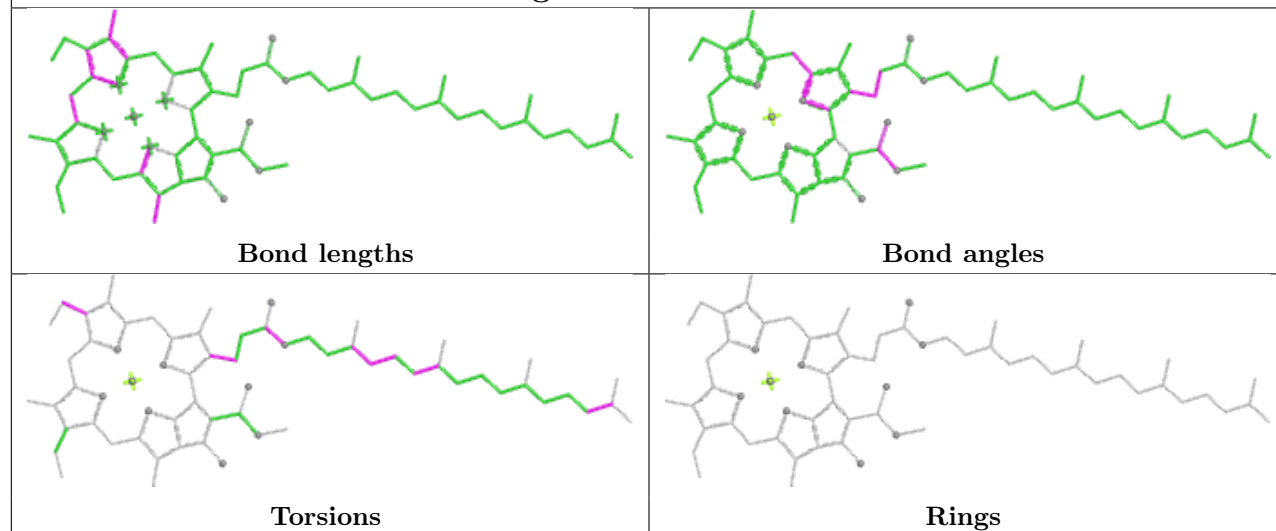
Rings



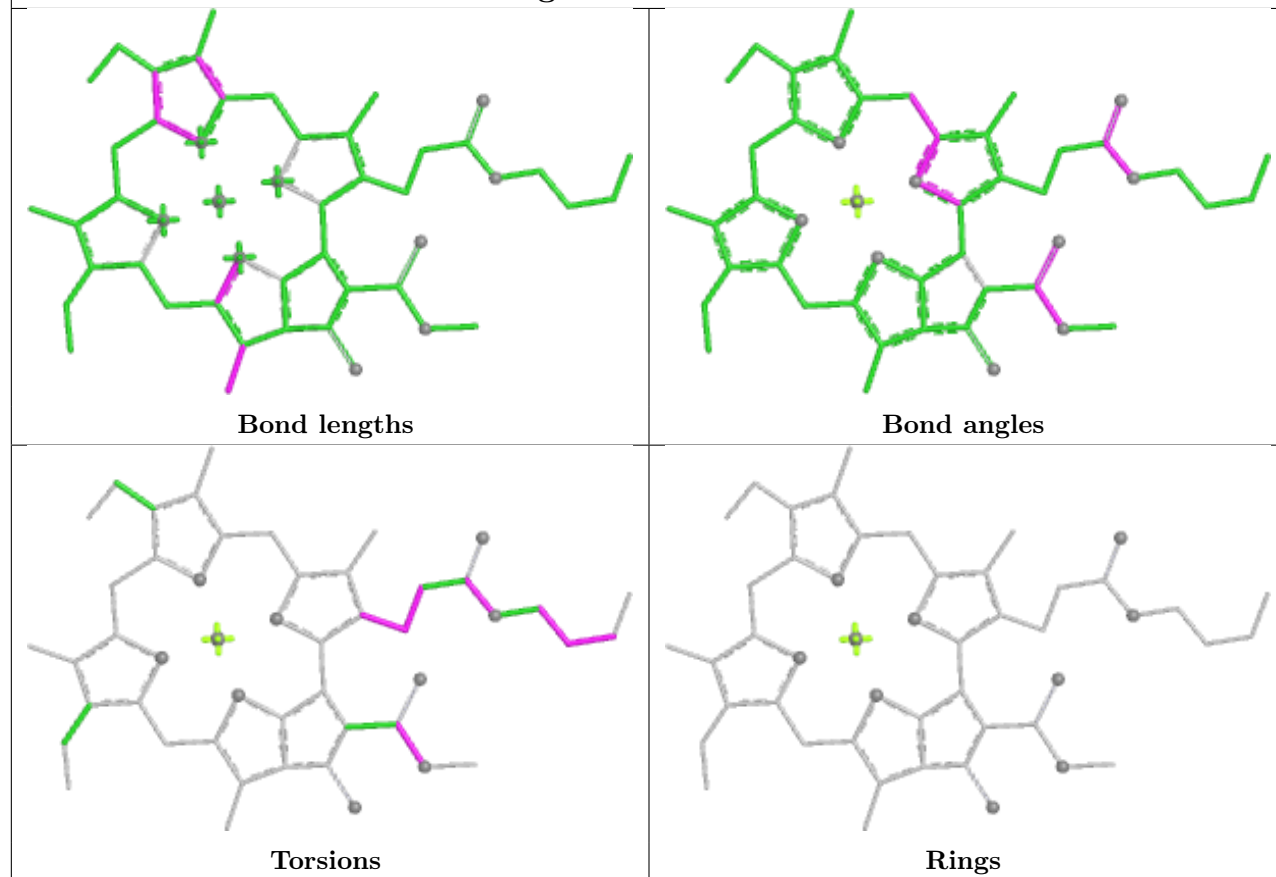


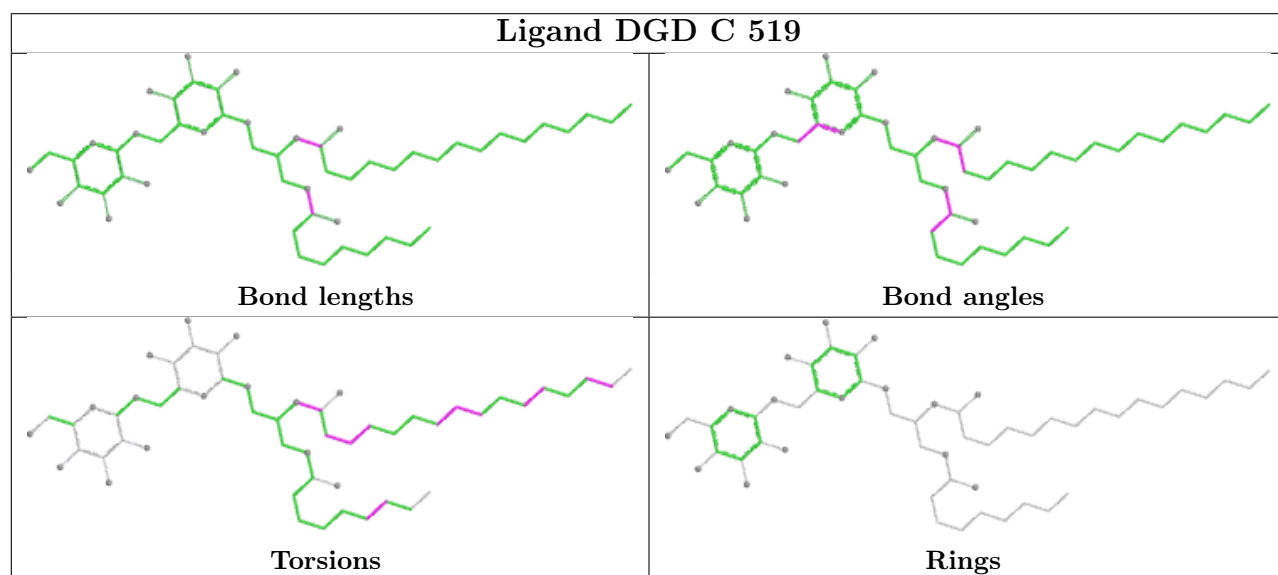
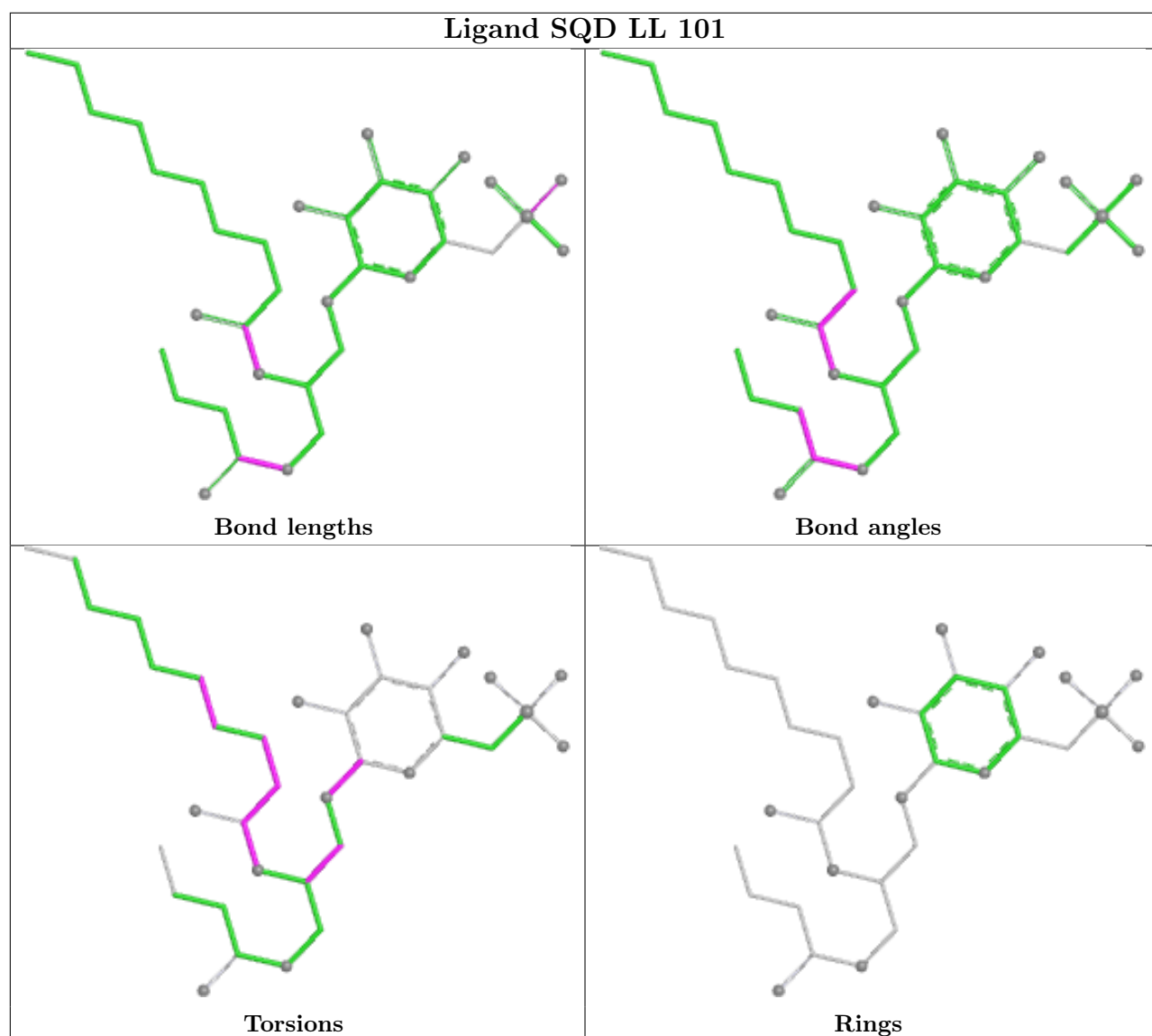


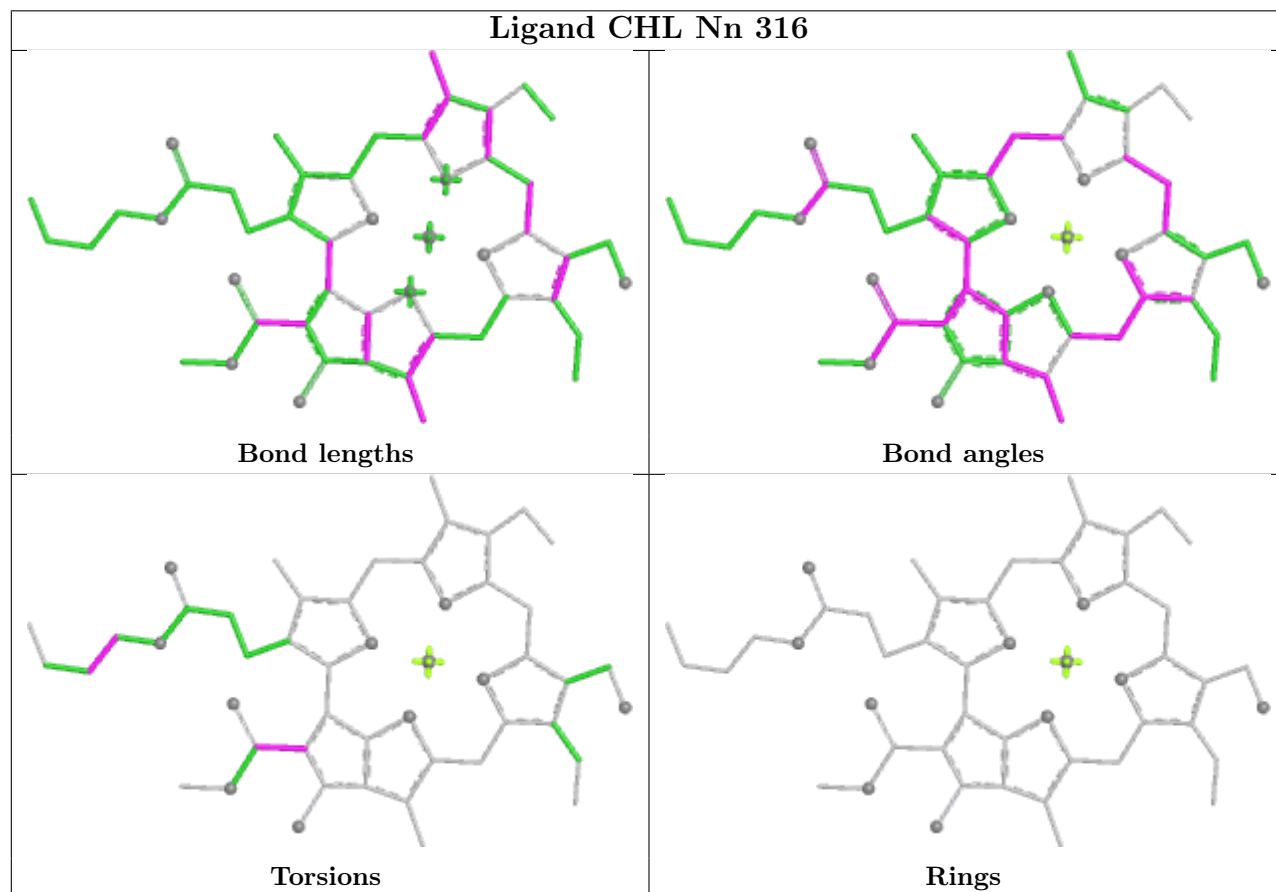
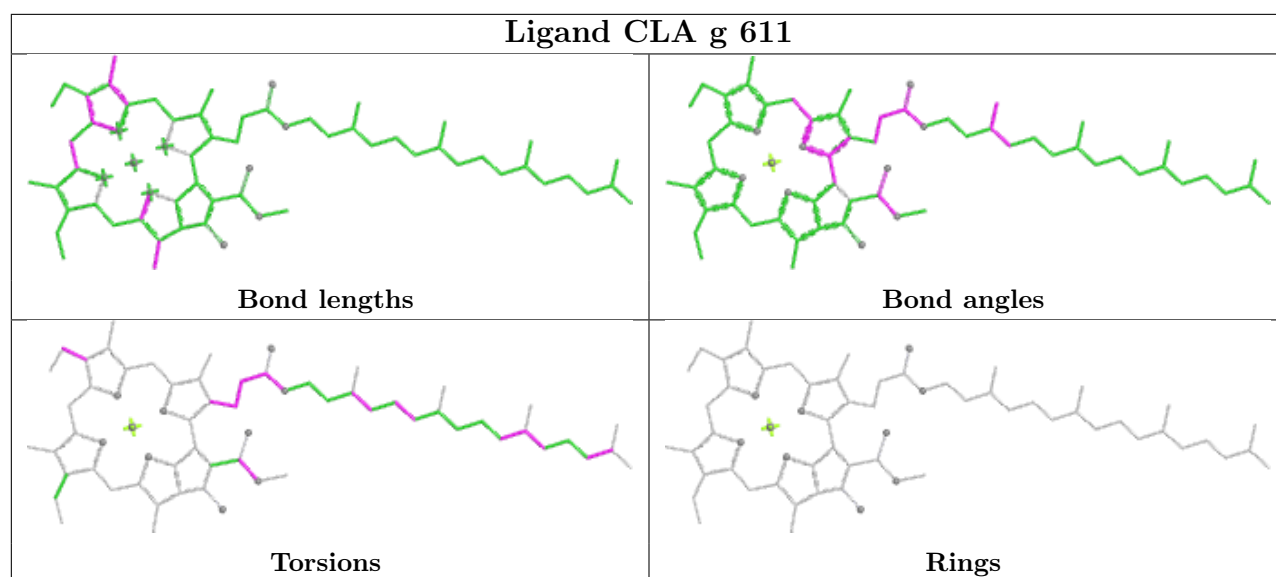
Ligand CLA C 504

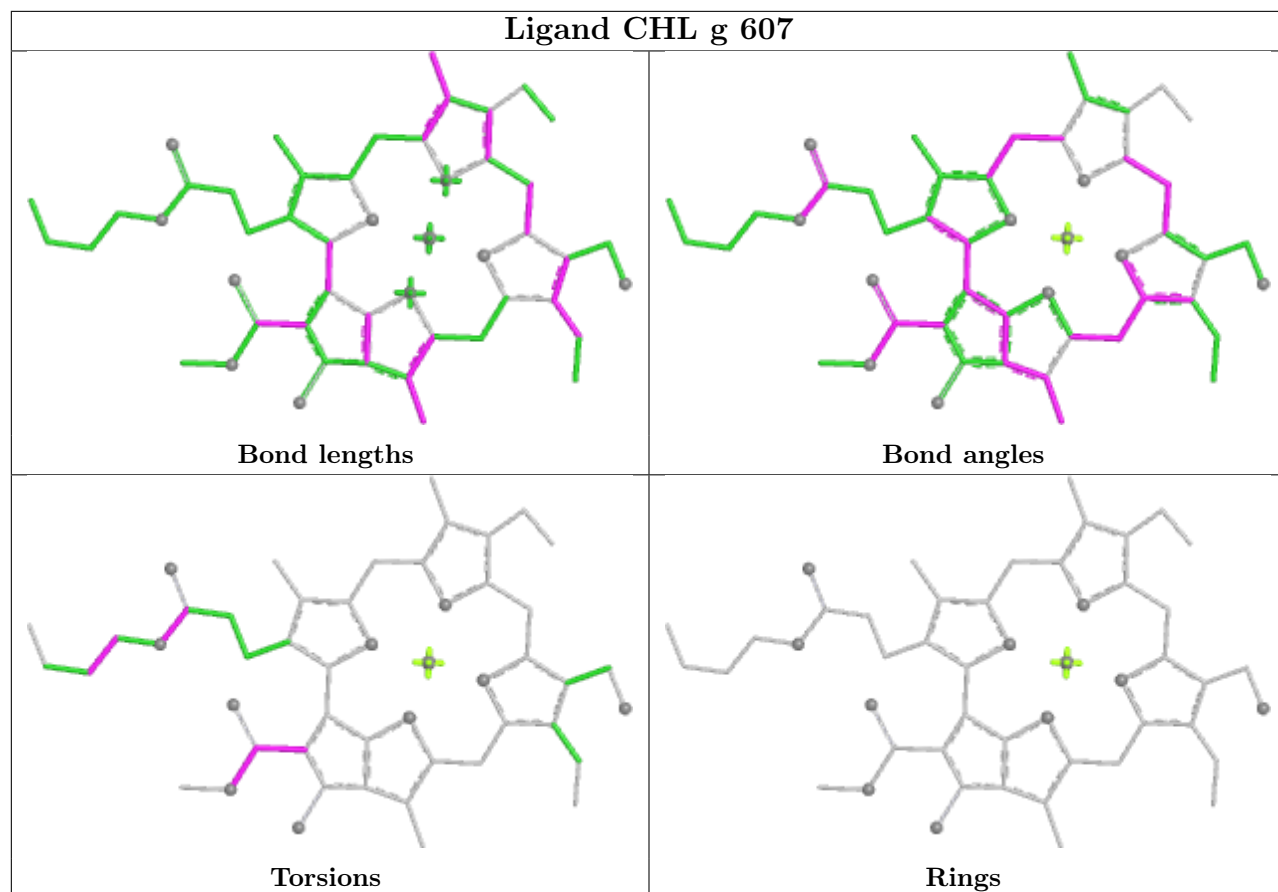


Ligand CLA r 610

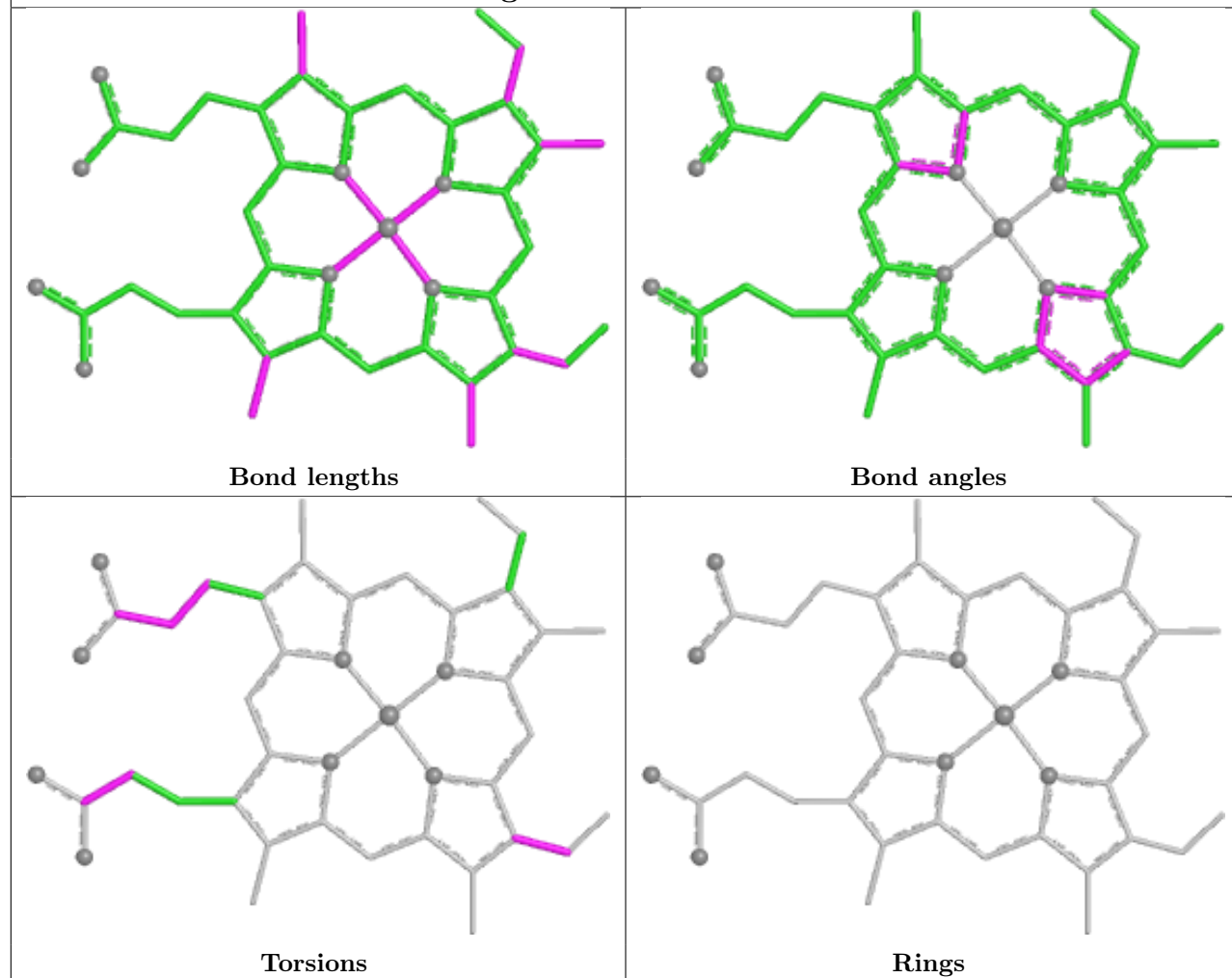




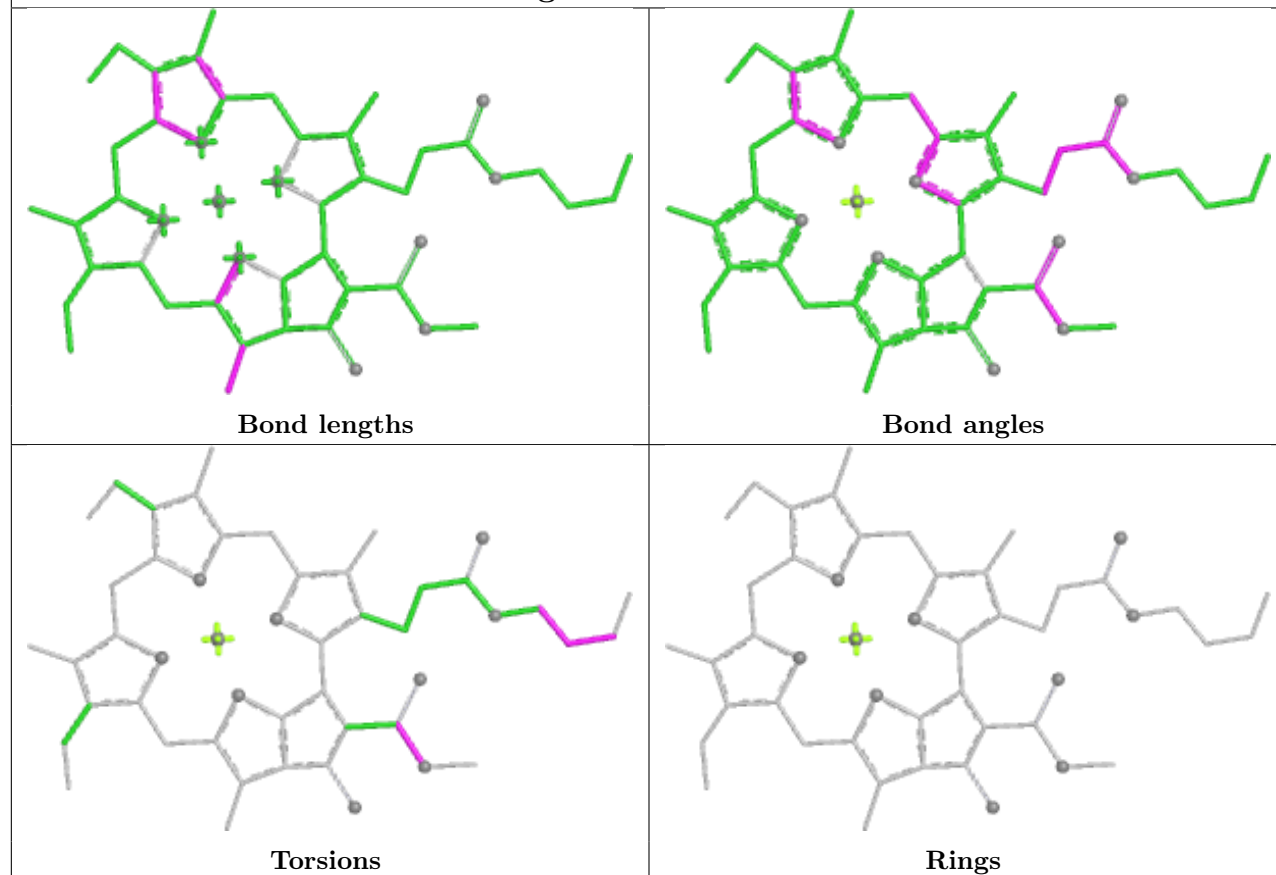




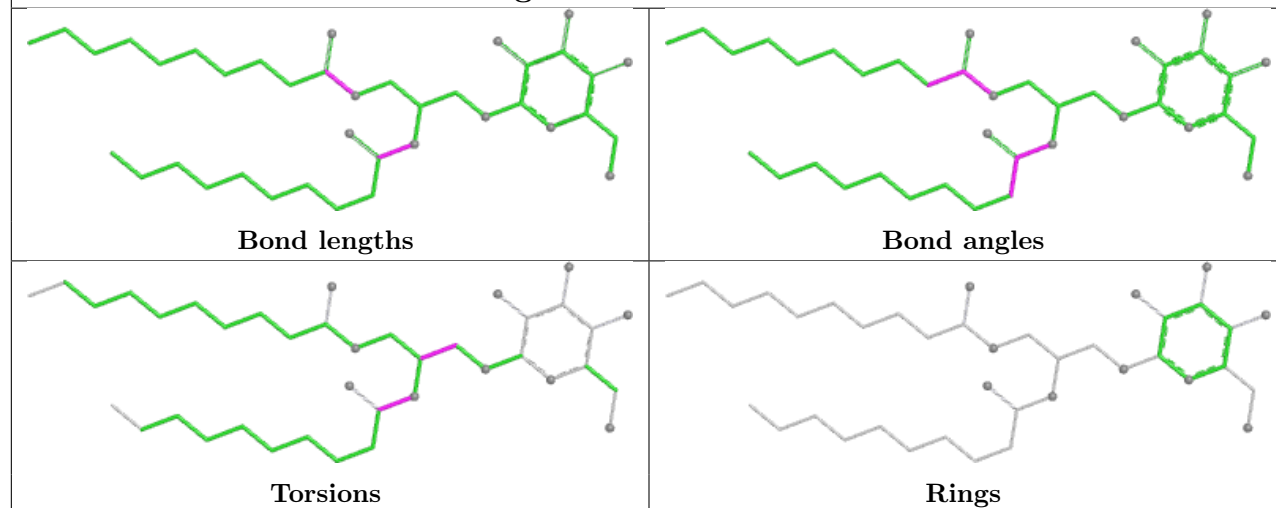
Ligand HEM Ee 101

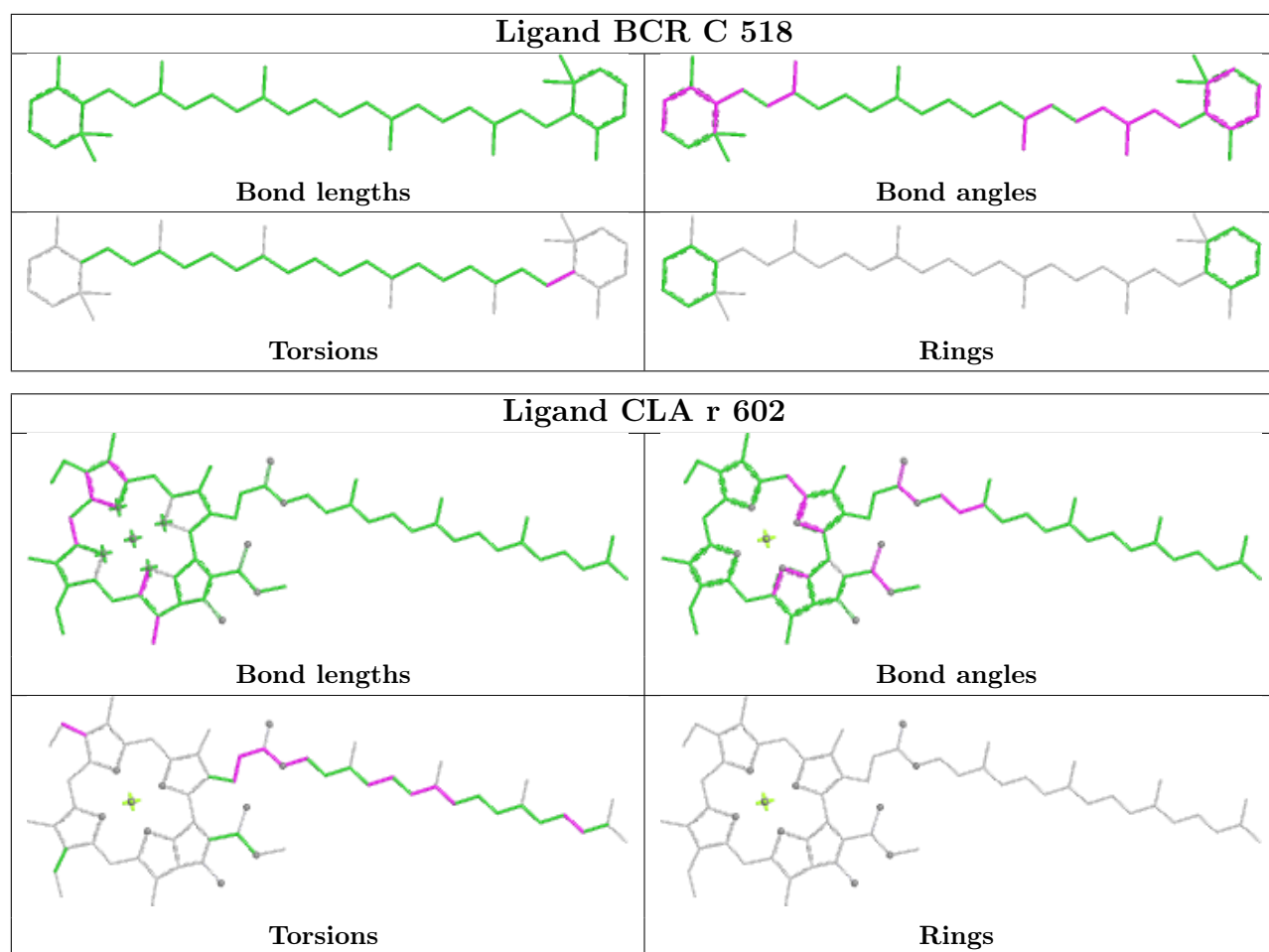


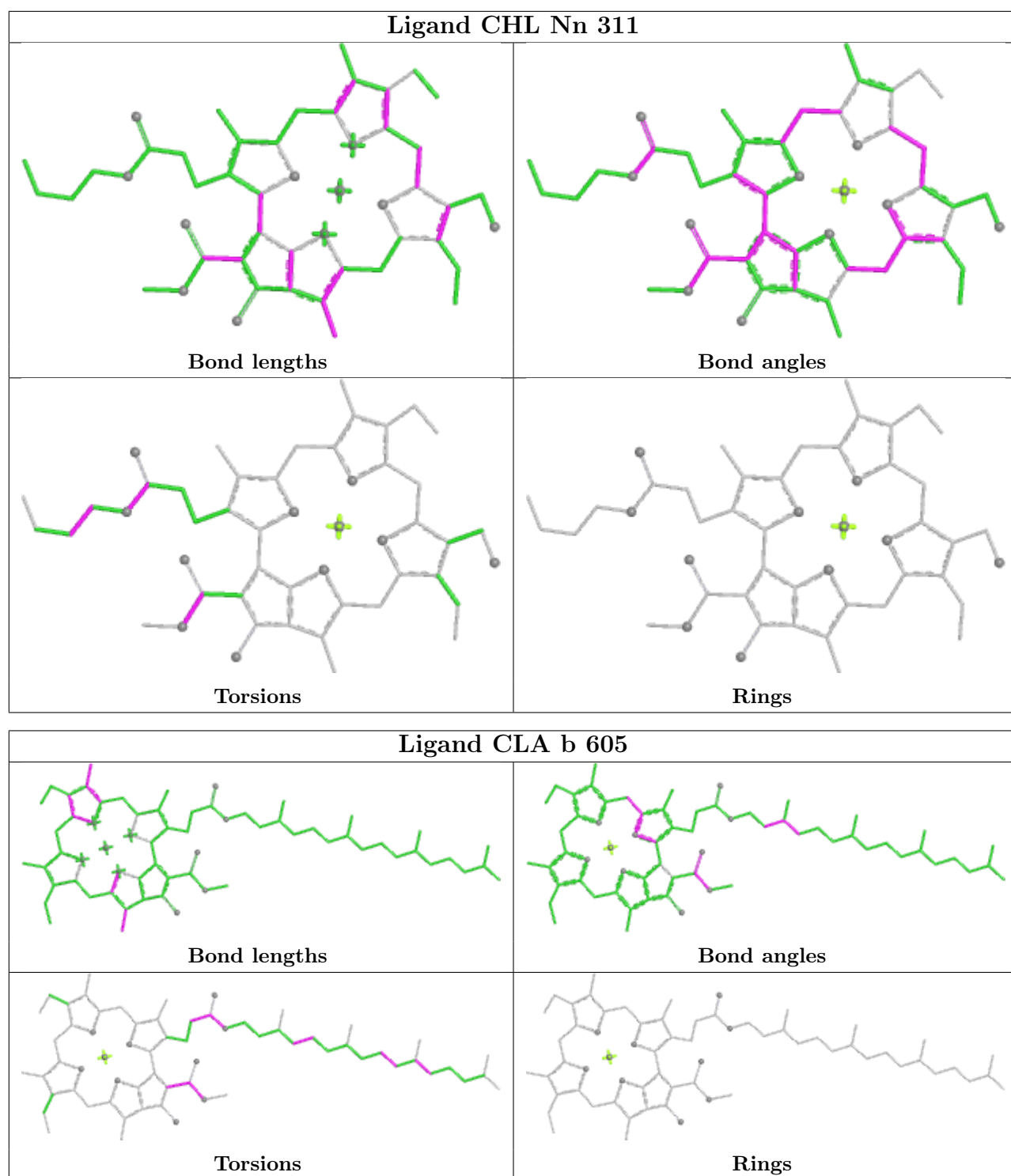
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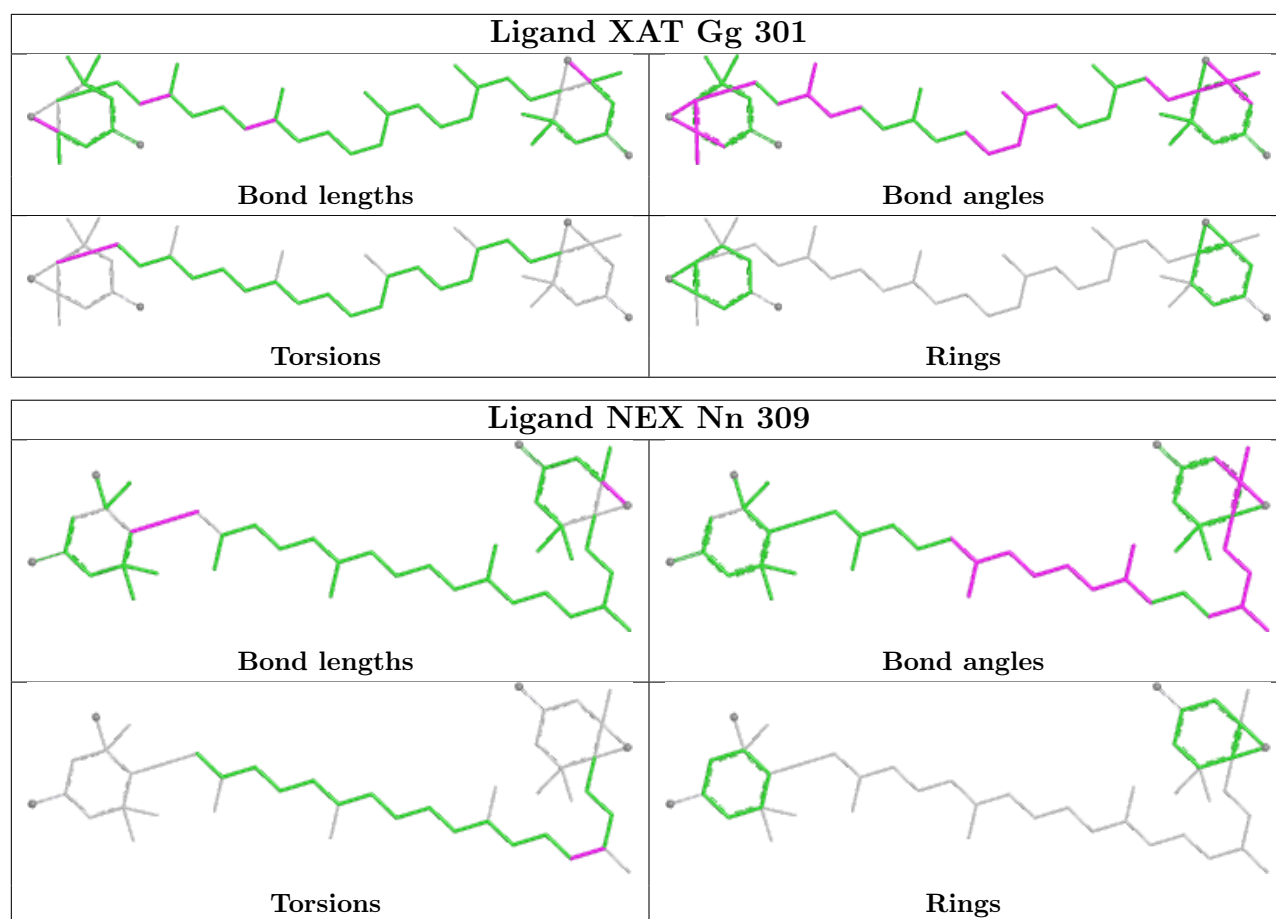


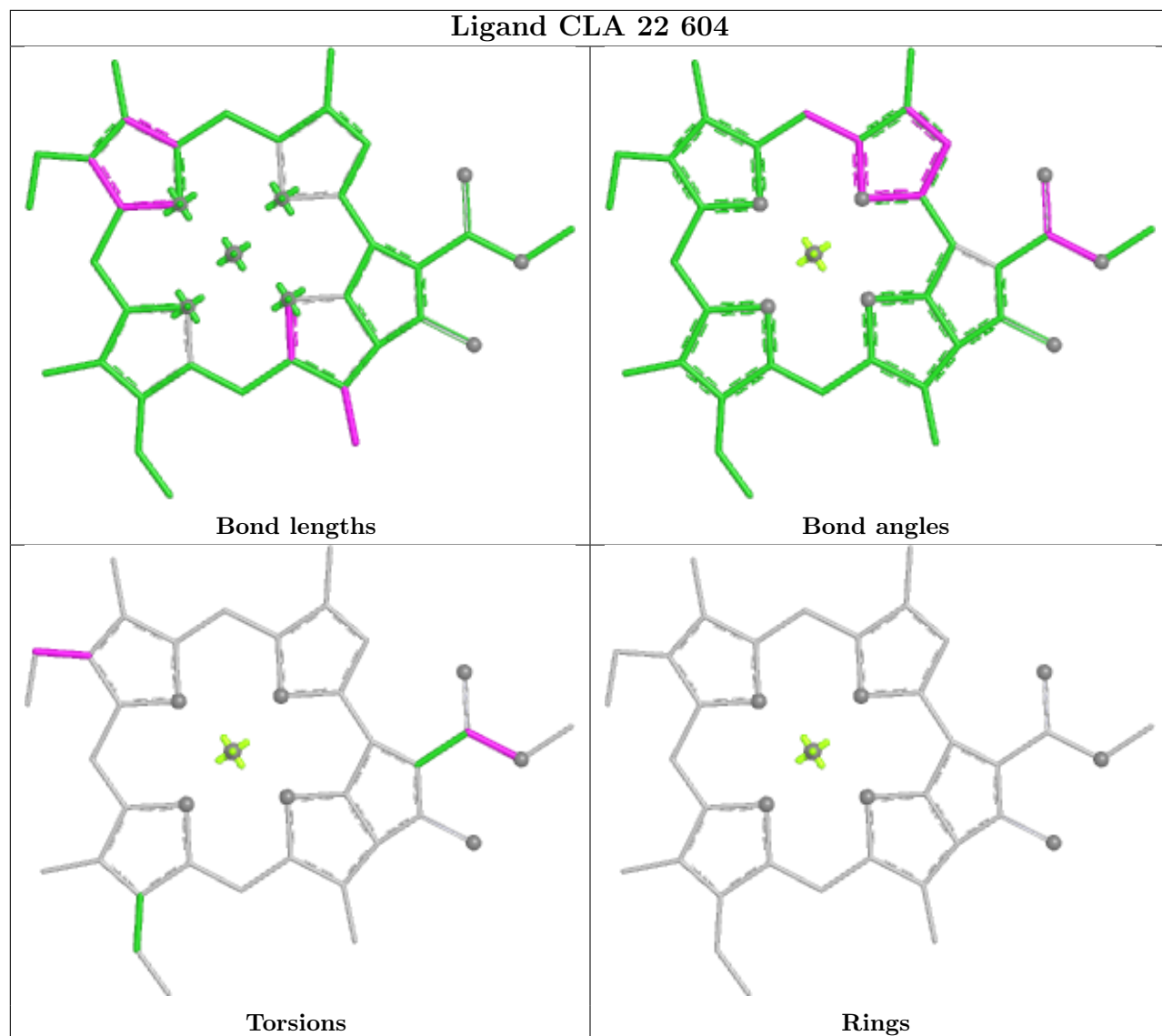
Ligand LMG CC 520

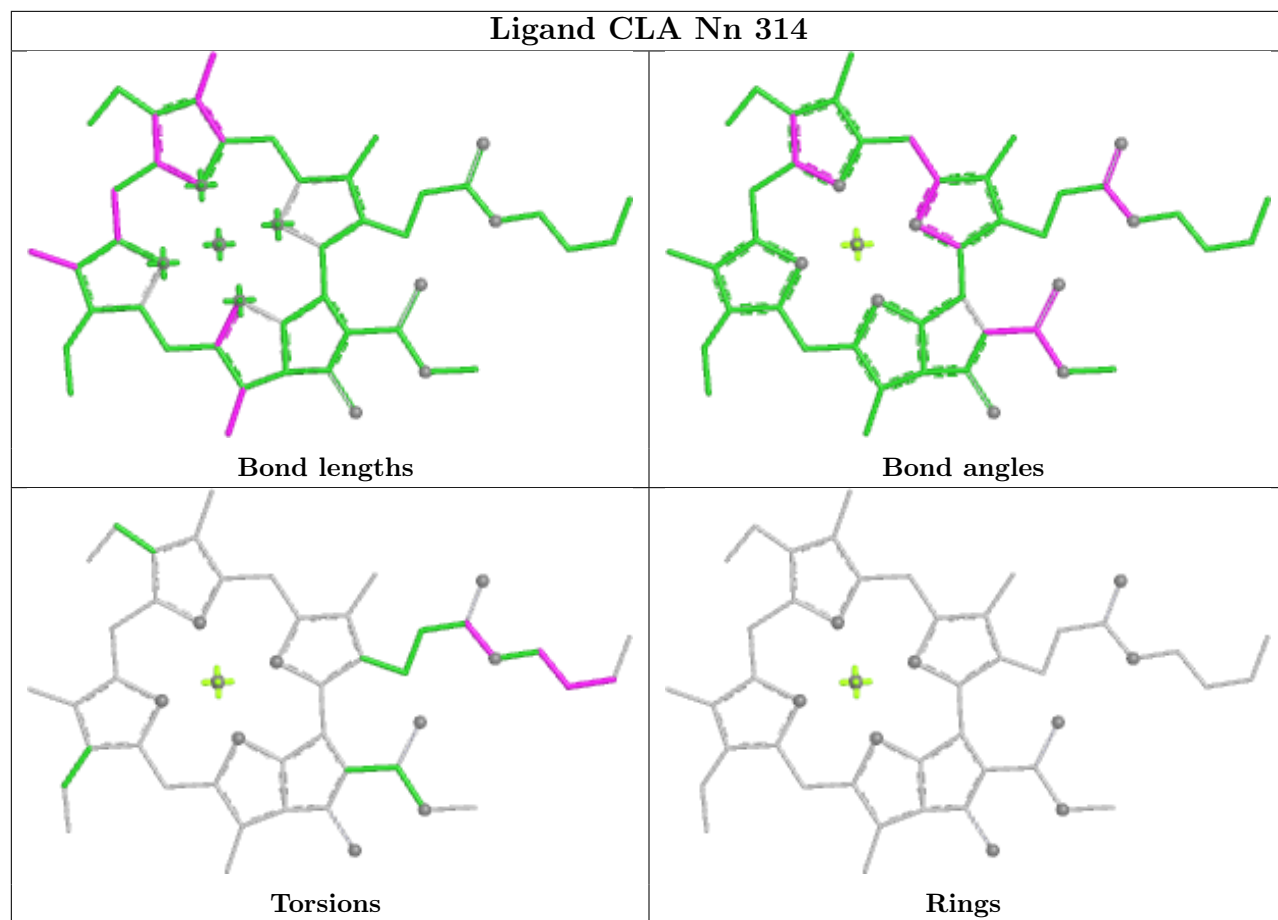




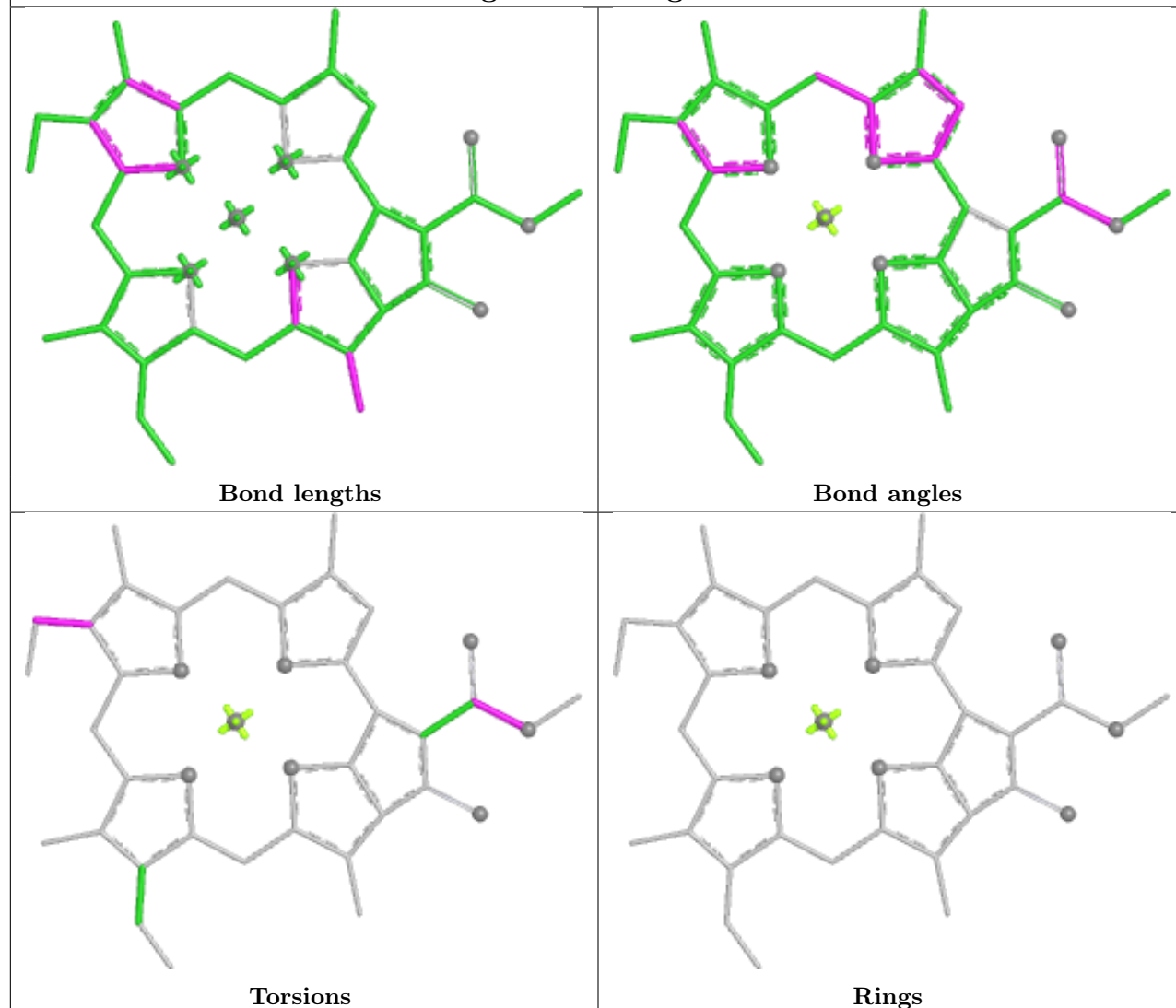




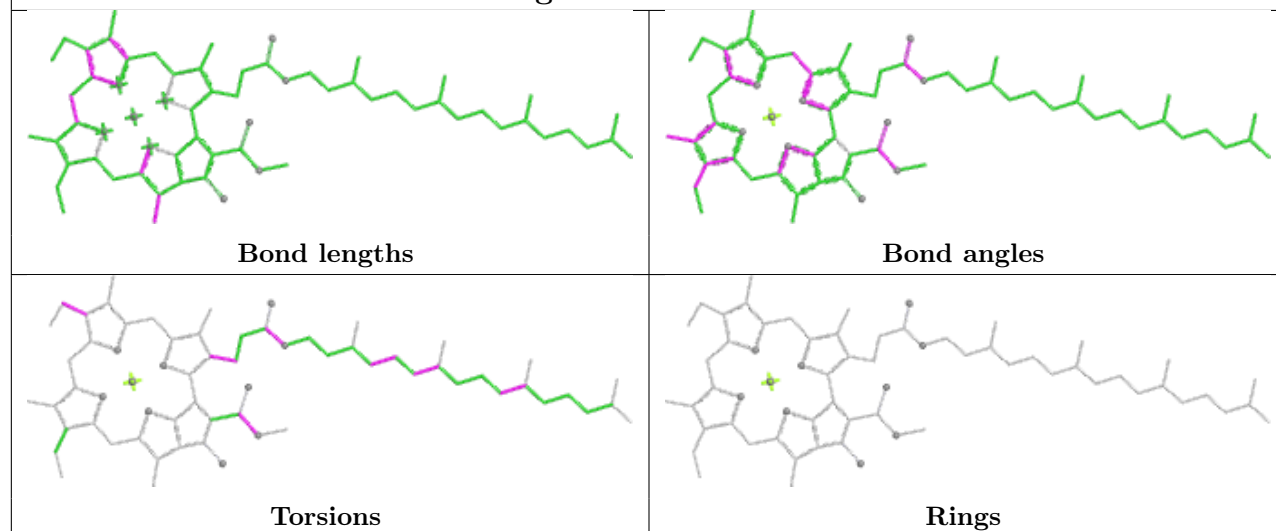




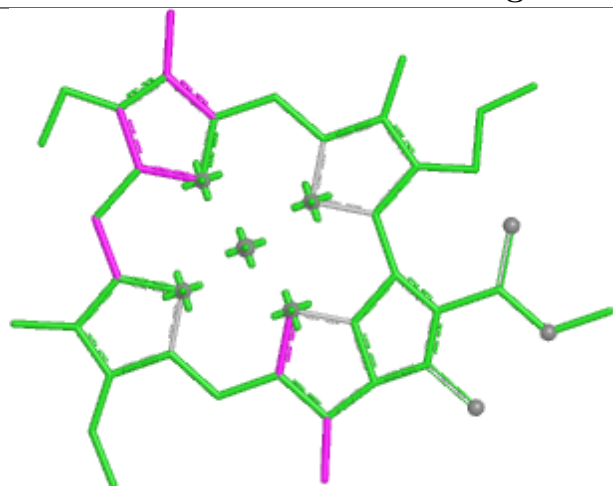
Ligand CLA Gg 314



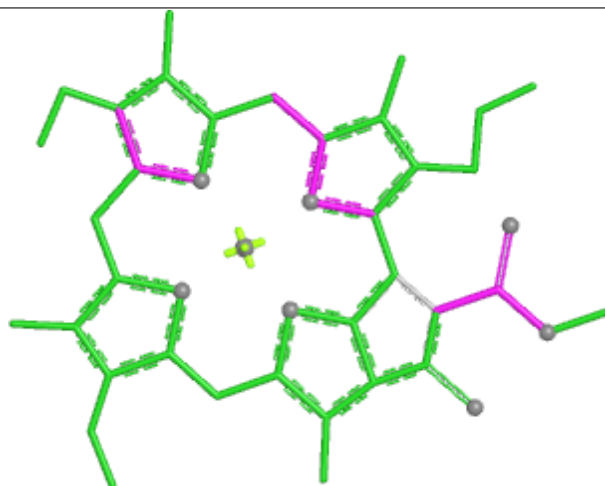
Ligand CLA n 610



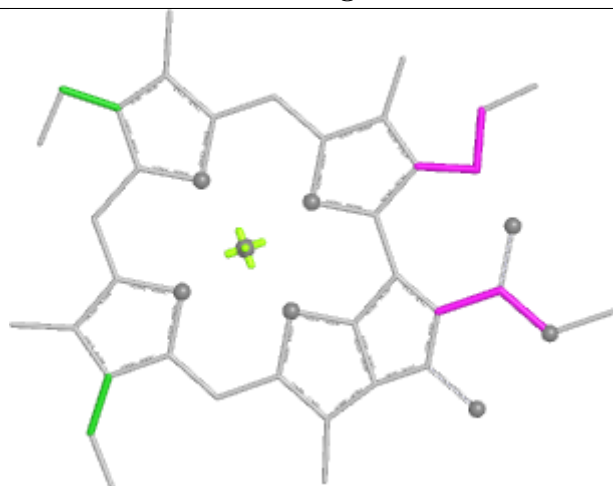
Ligand CLA Cc 515



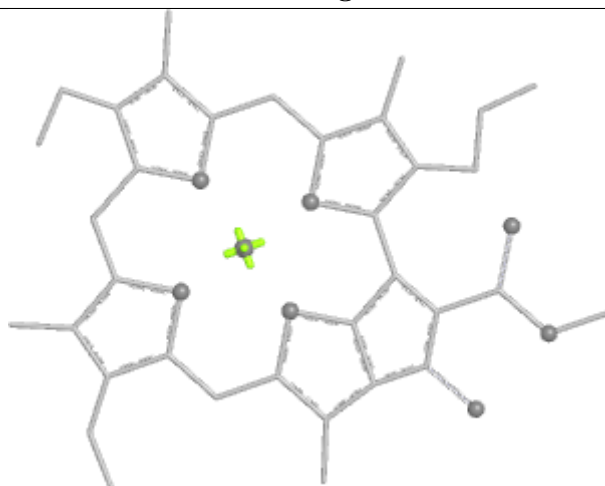
Bond lengths



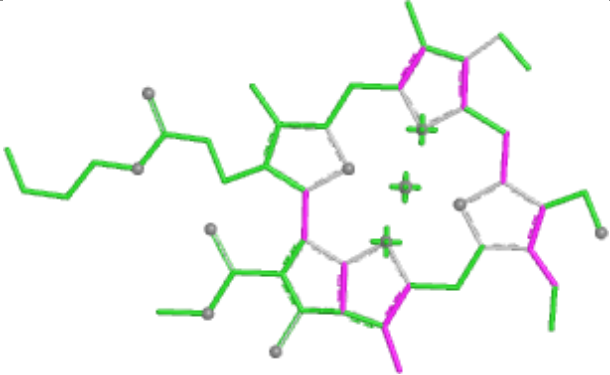
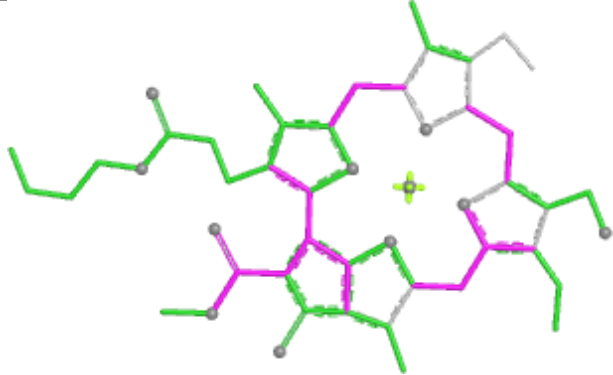
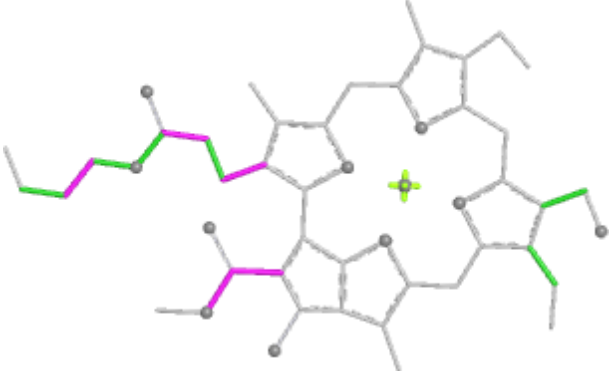
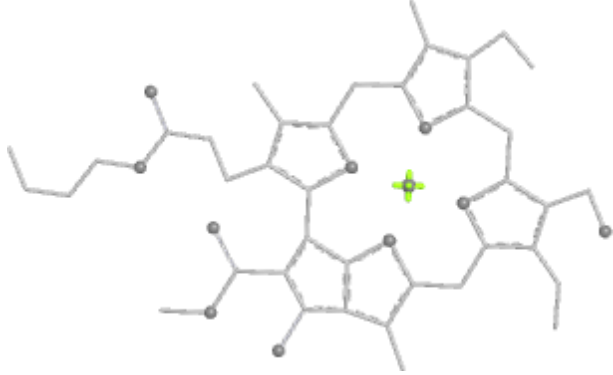
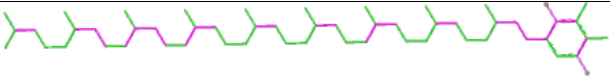
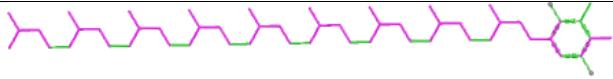
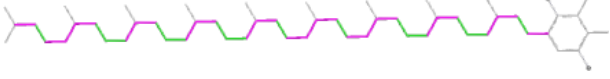
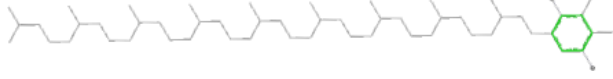
Bond angles

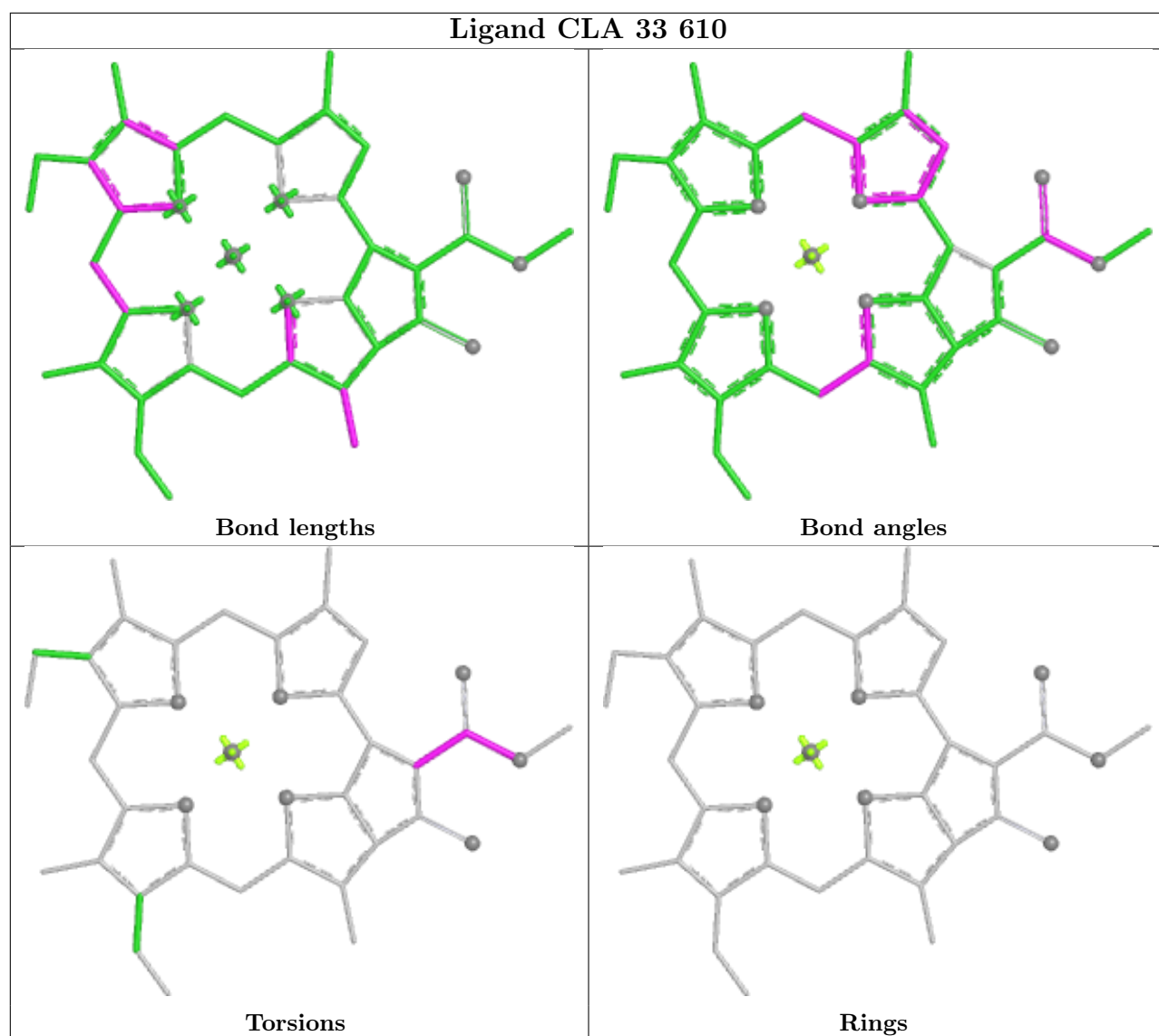


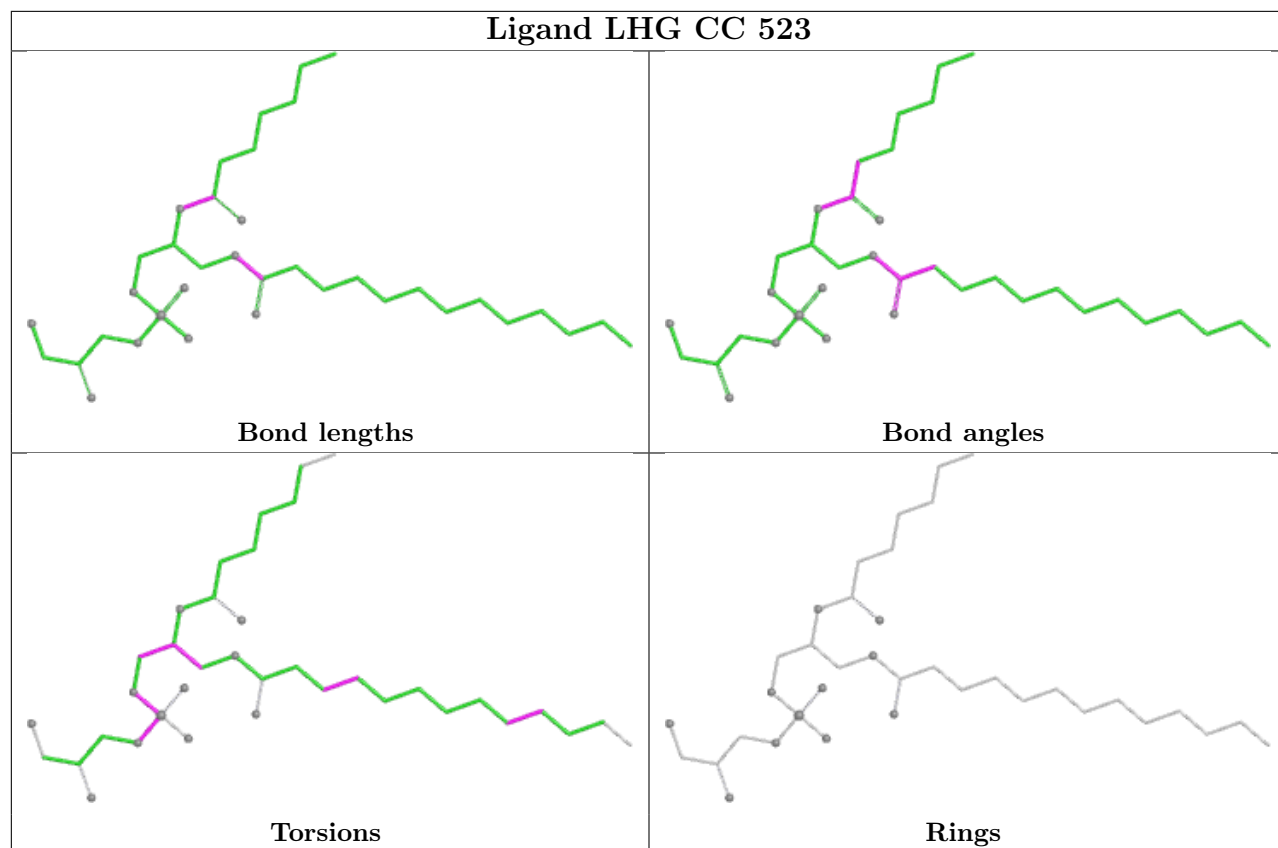
Torsions



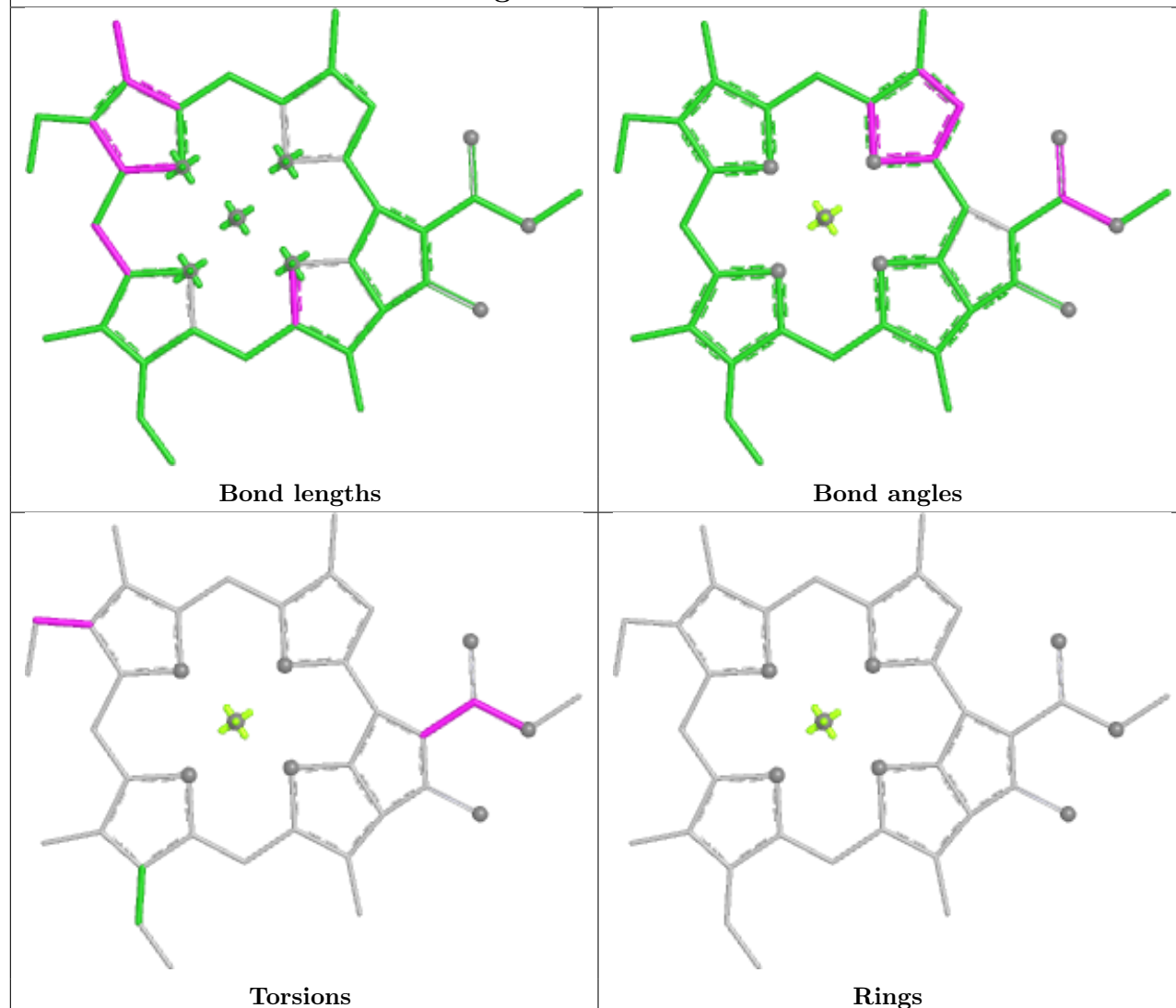
Rings

Ligand CHL r 605	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 Dd 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

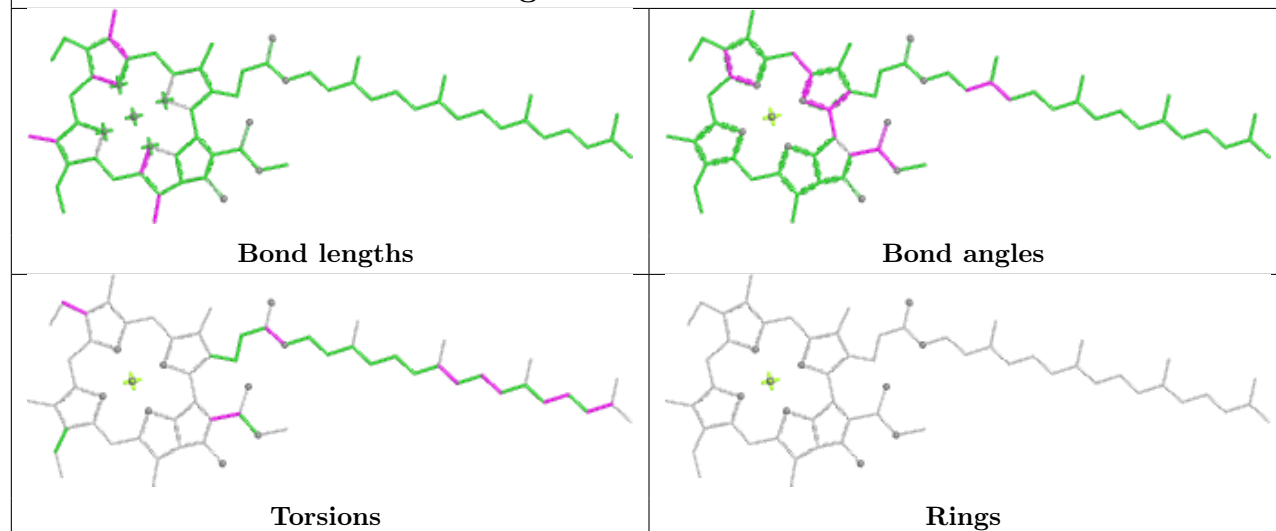


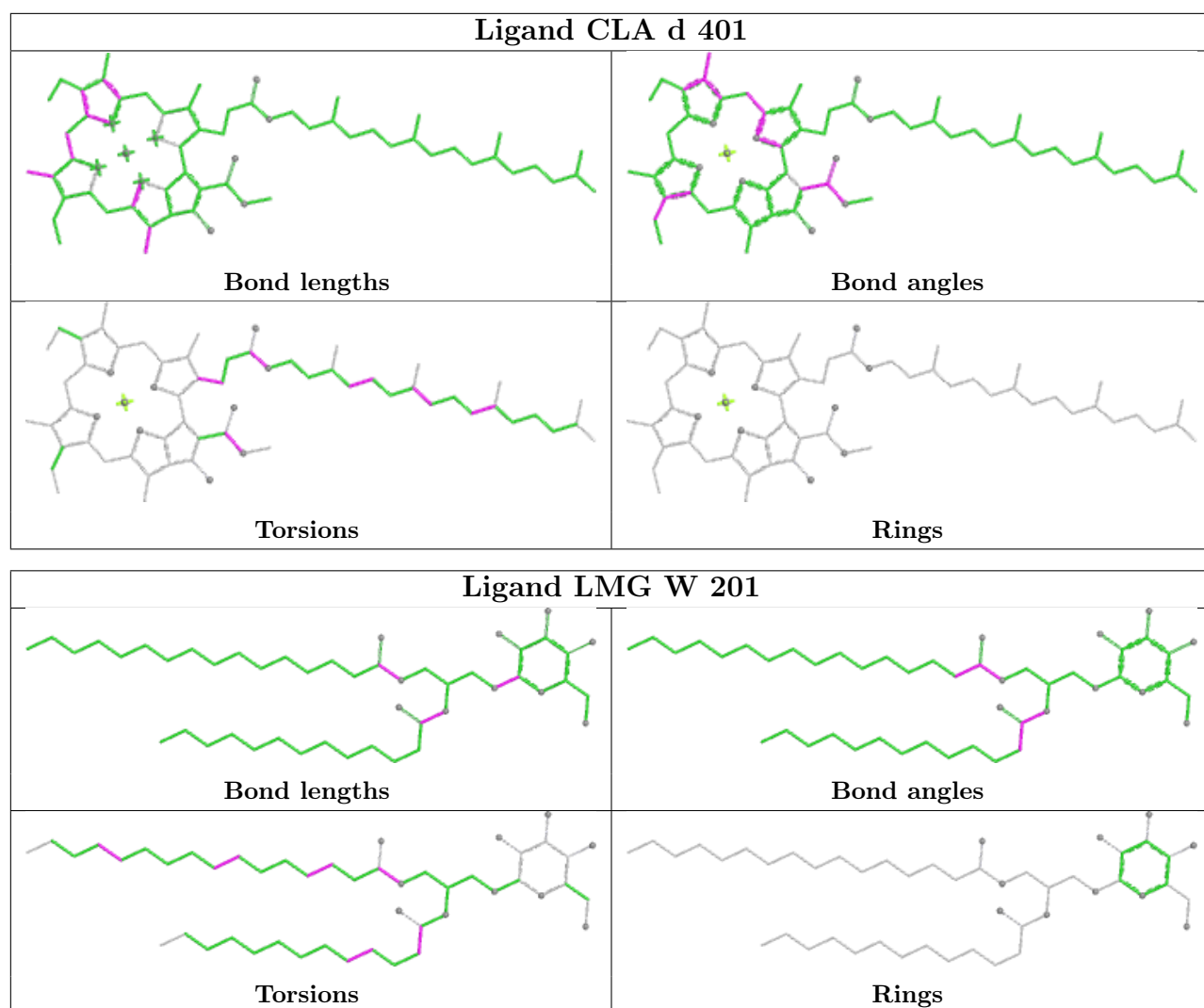


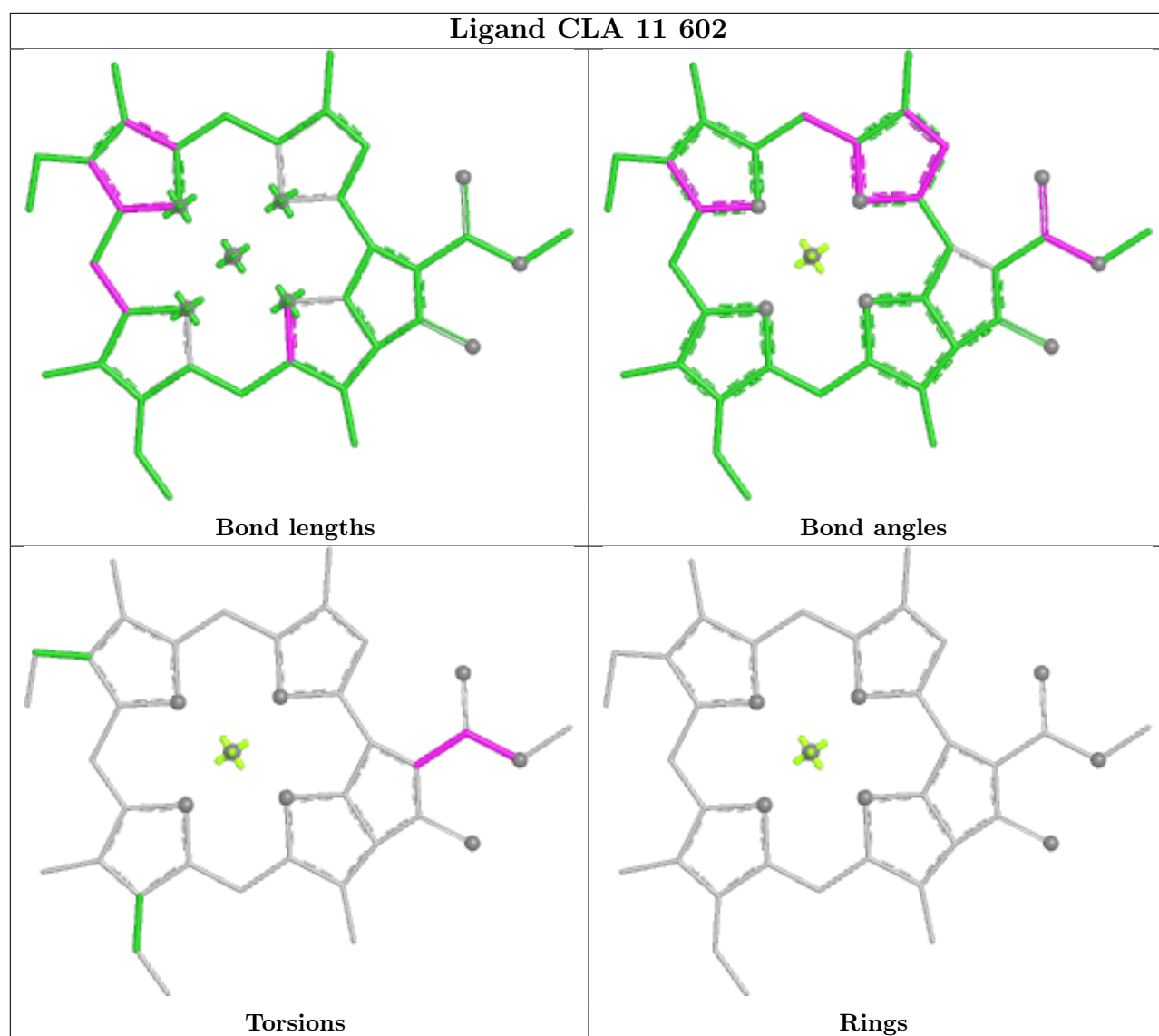
Ligand CLA 2 609

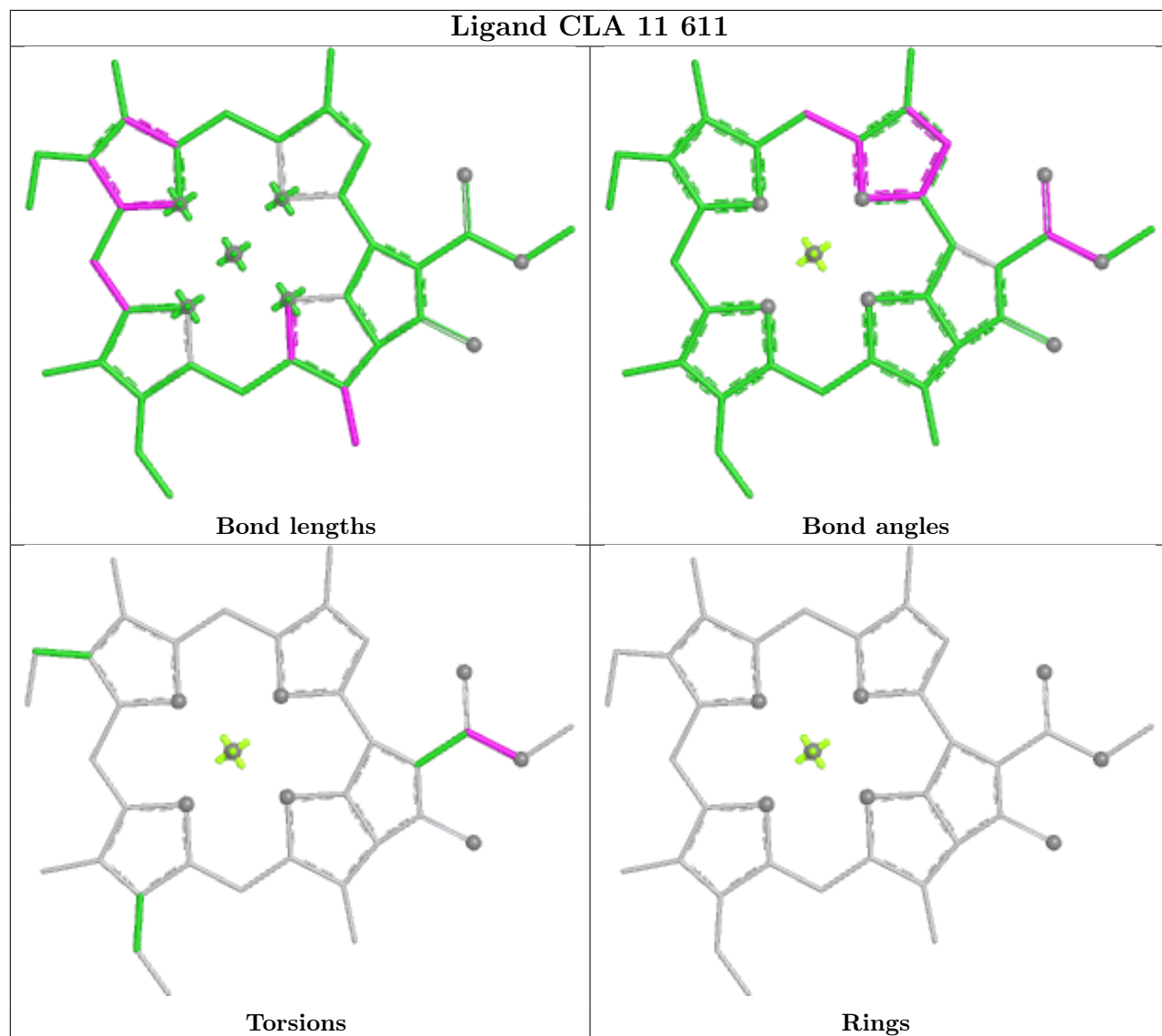


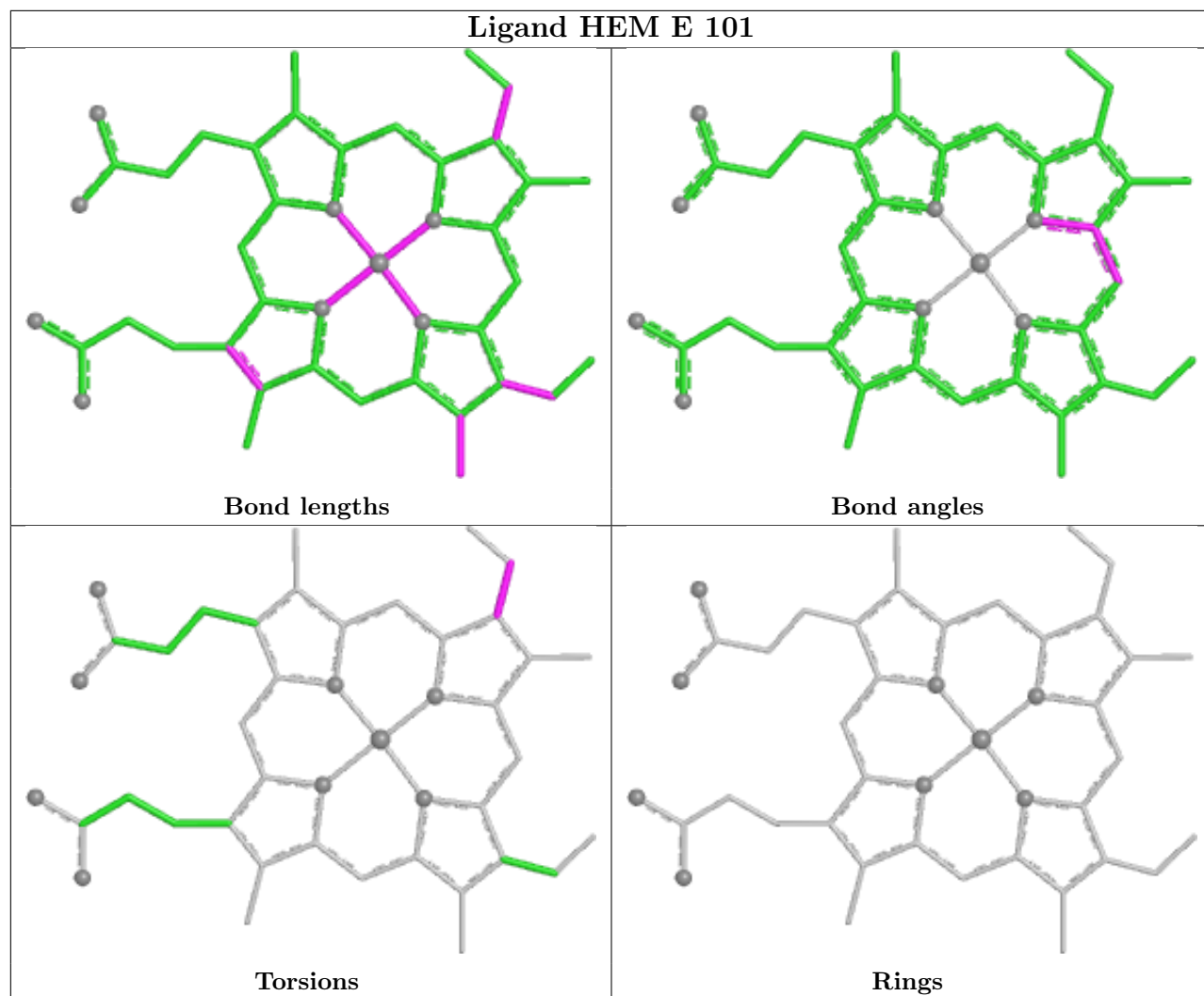
Ligand CLA CC 508

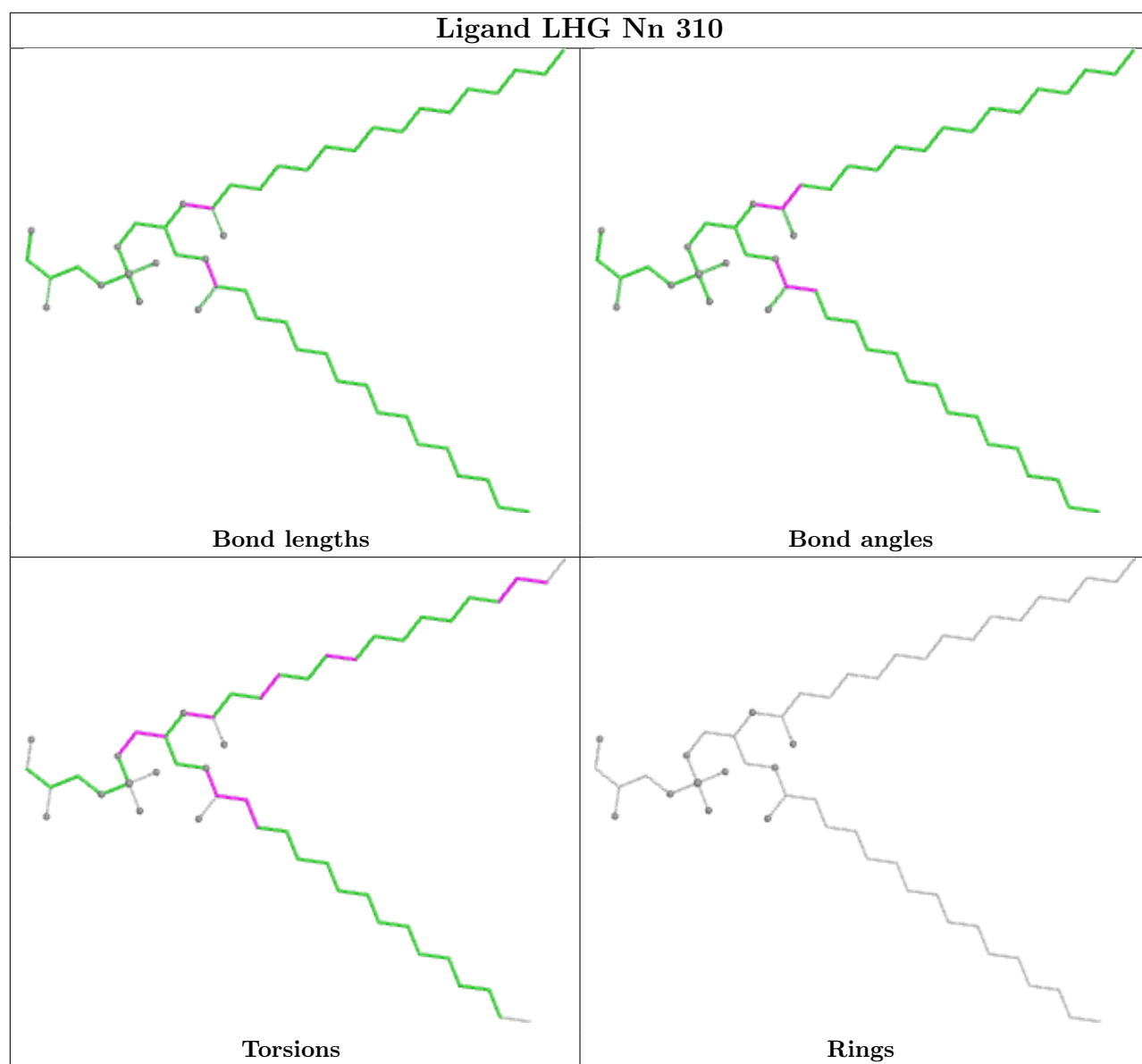




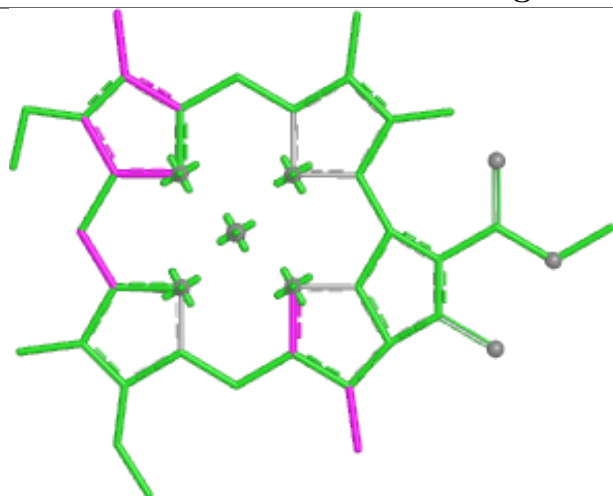




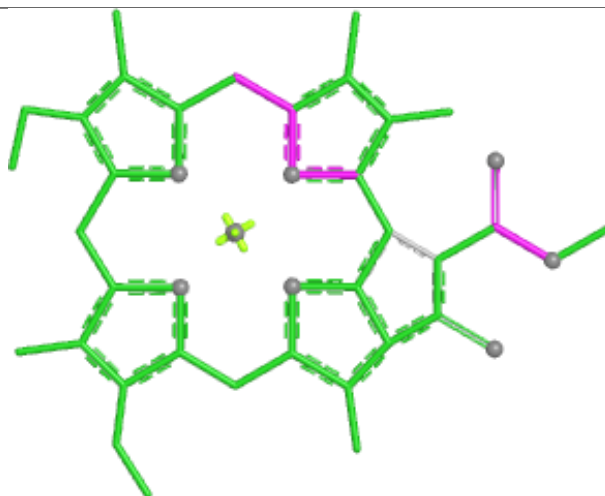




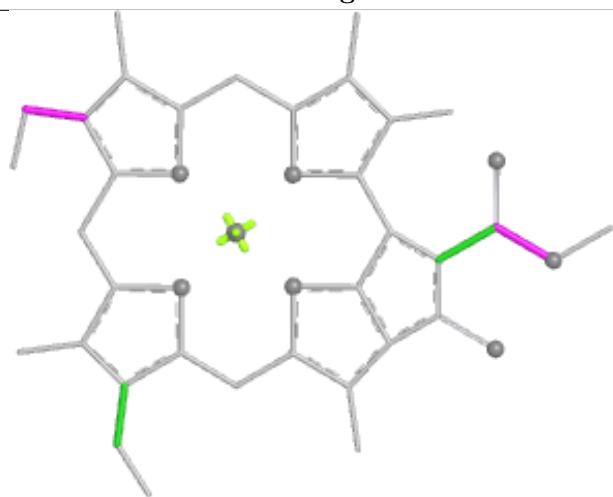
Ligand CLA N 614



Bond lengths



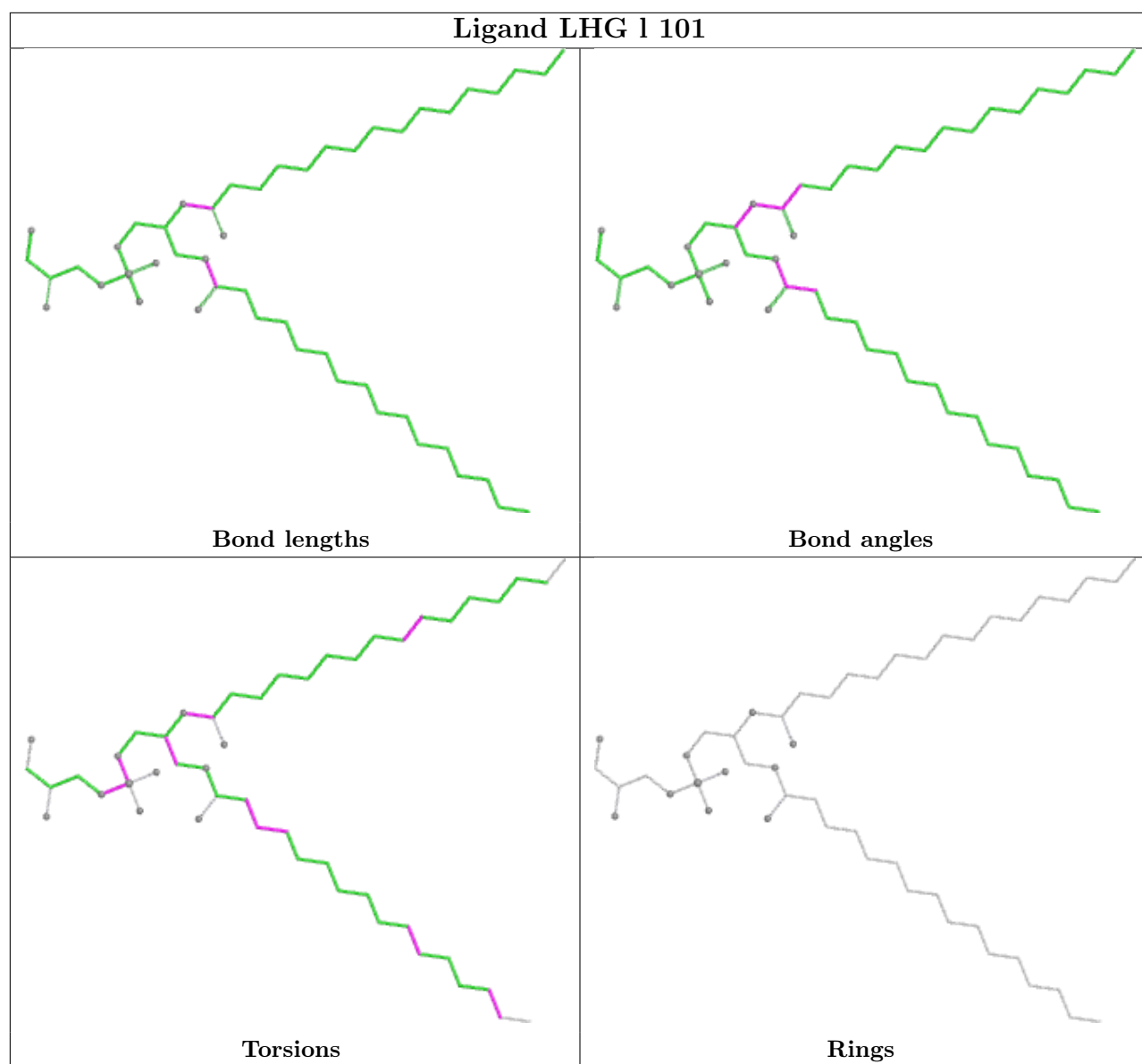
Bond angles

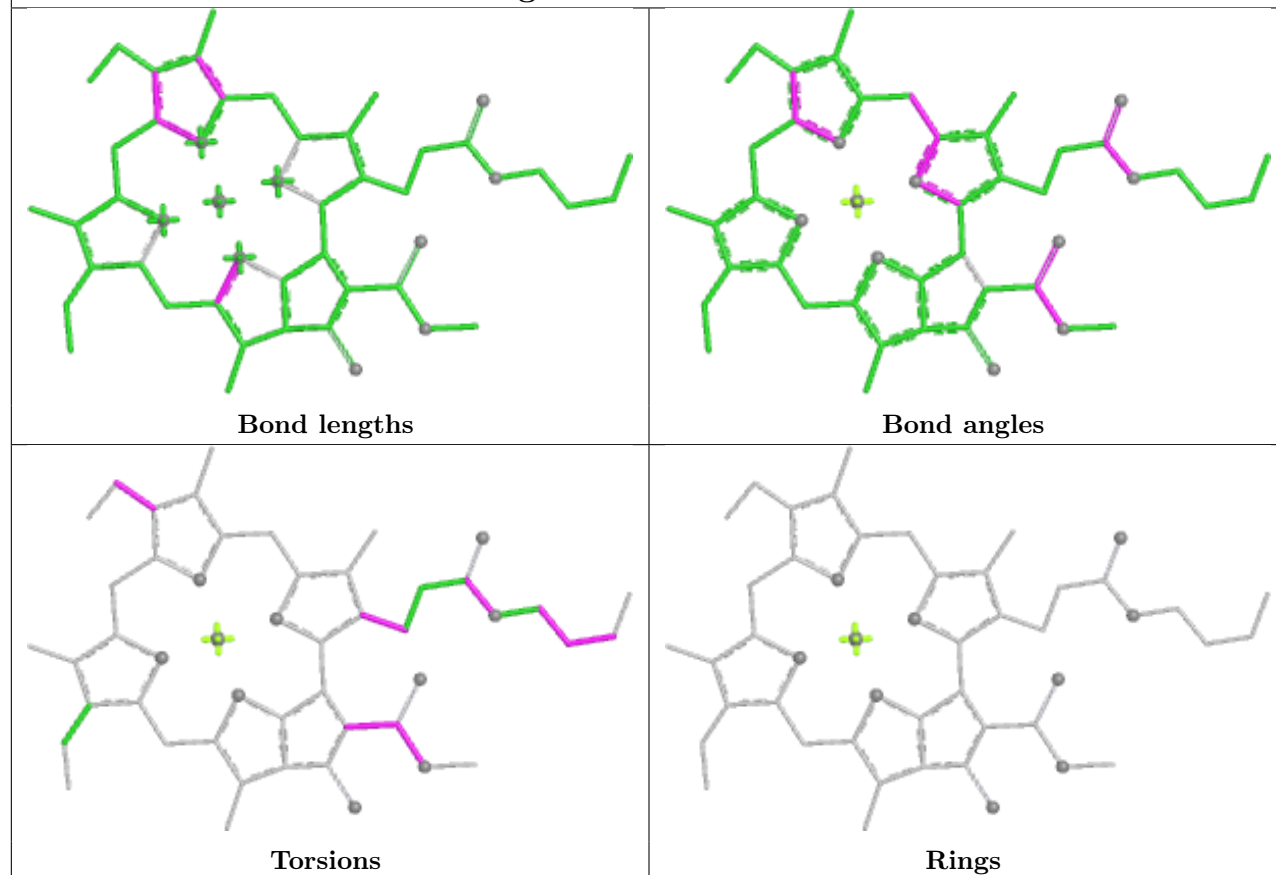
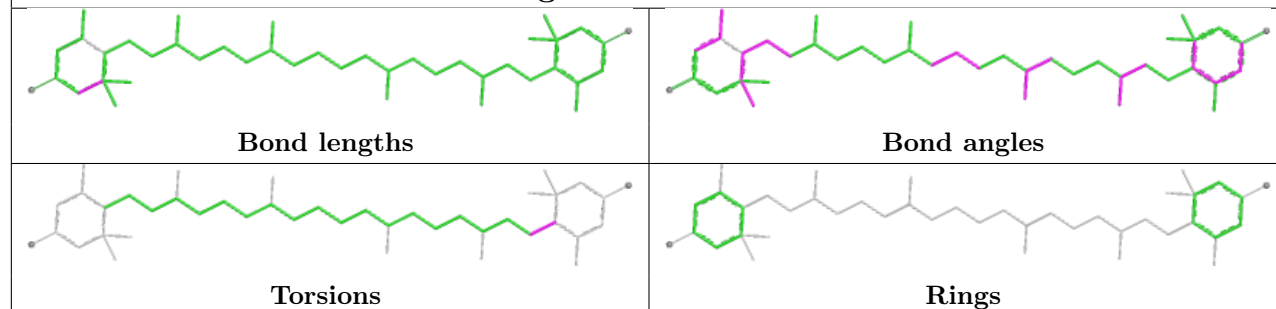


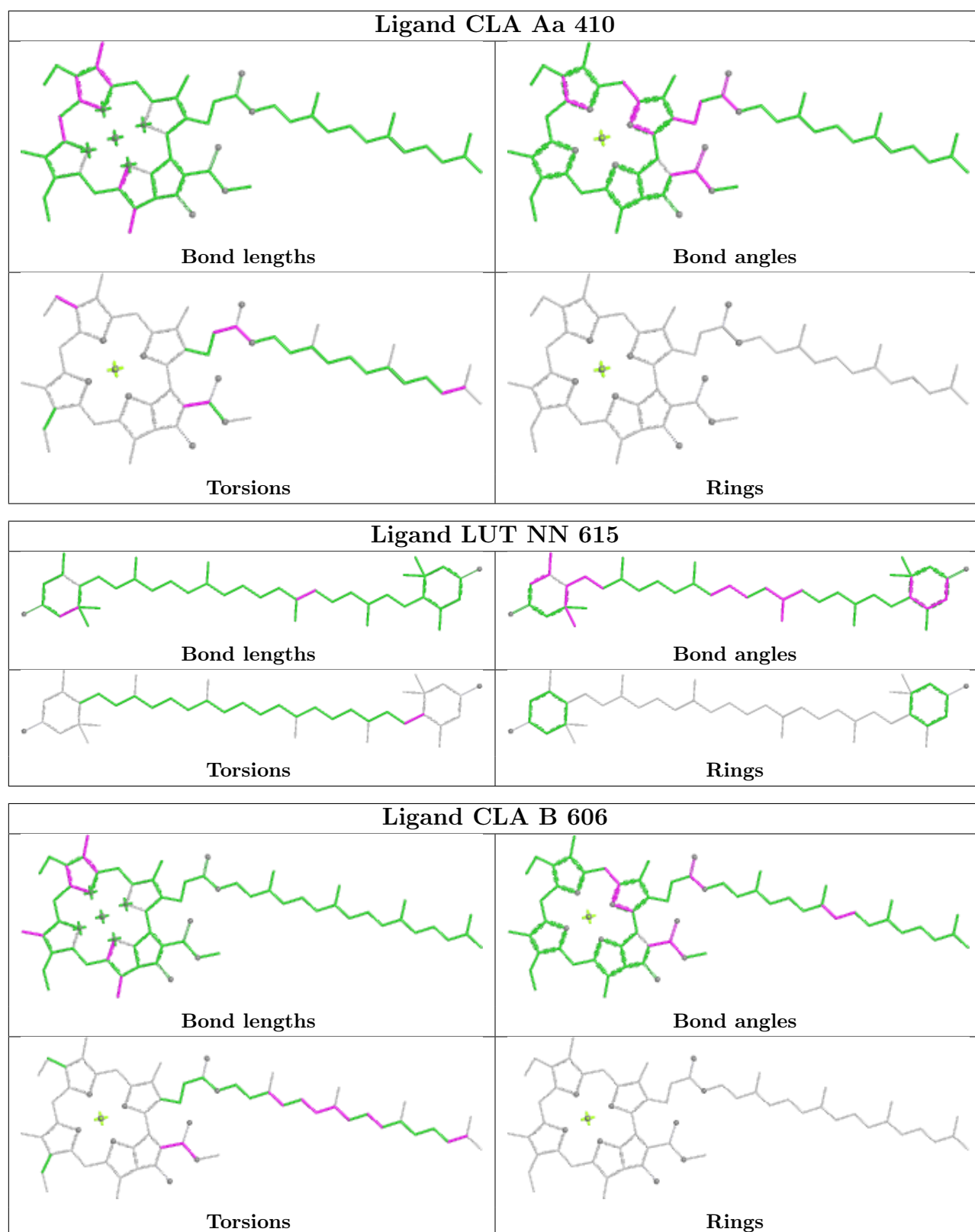
Torsions



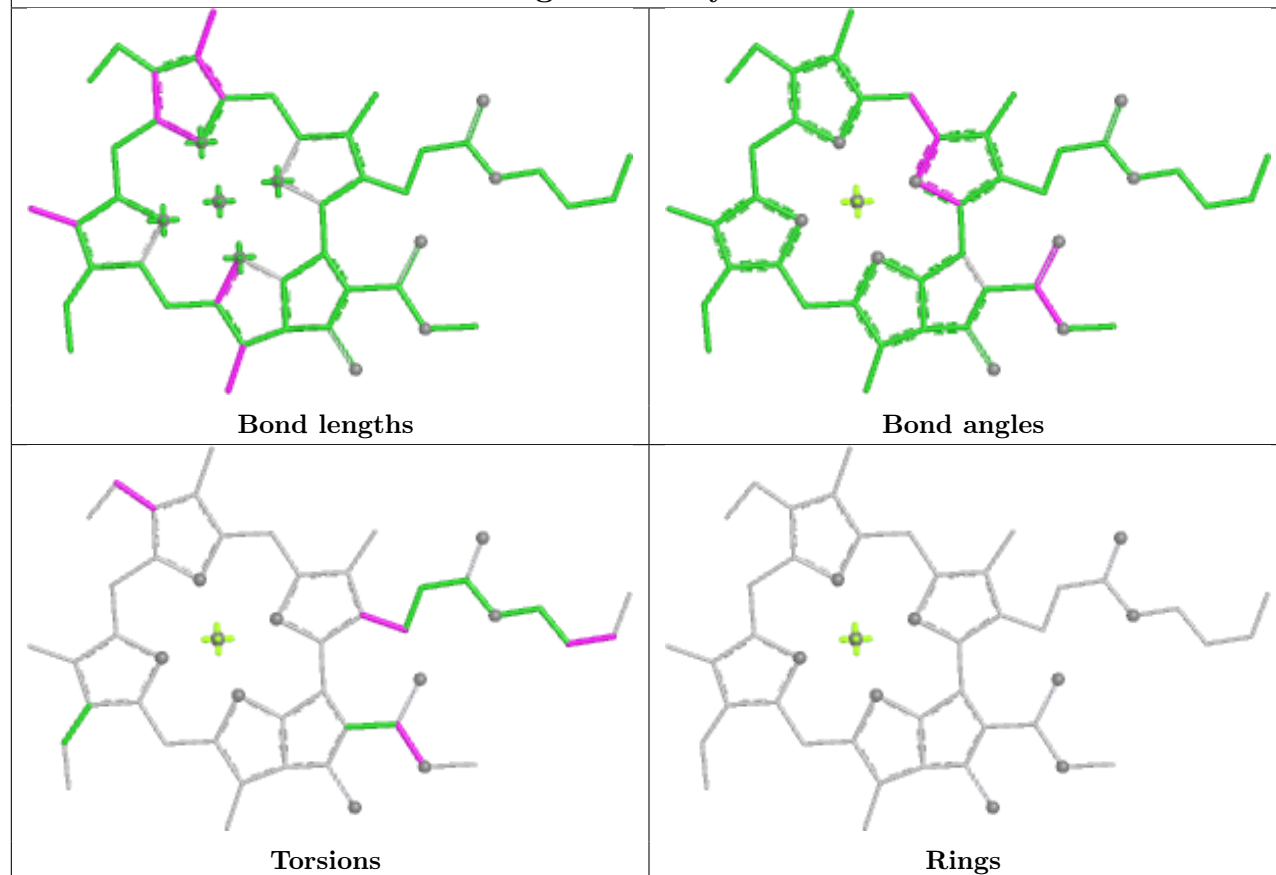
Rings



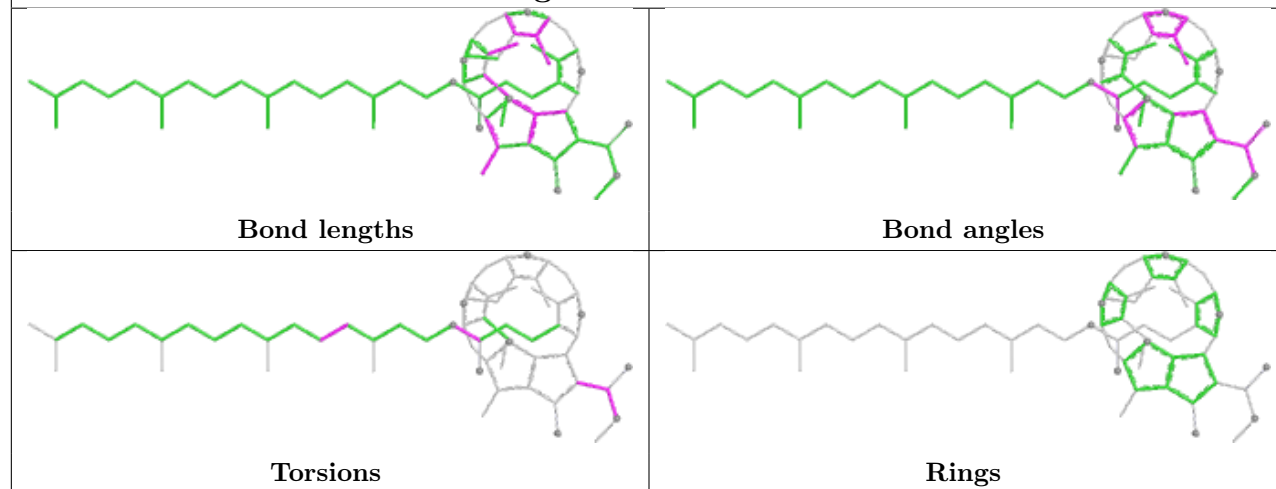
Ligand CLA RR 310**Ligand LUT r 614**

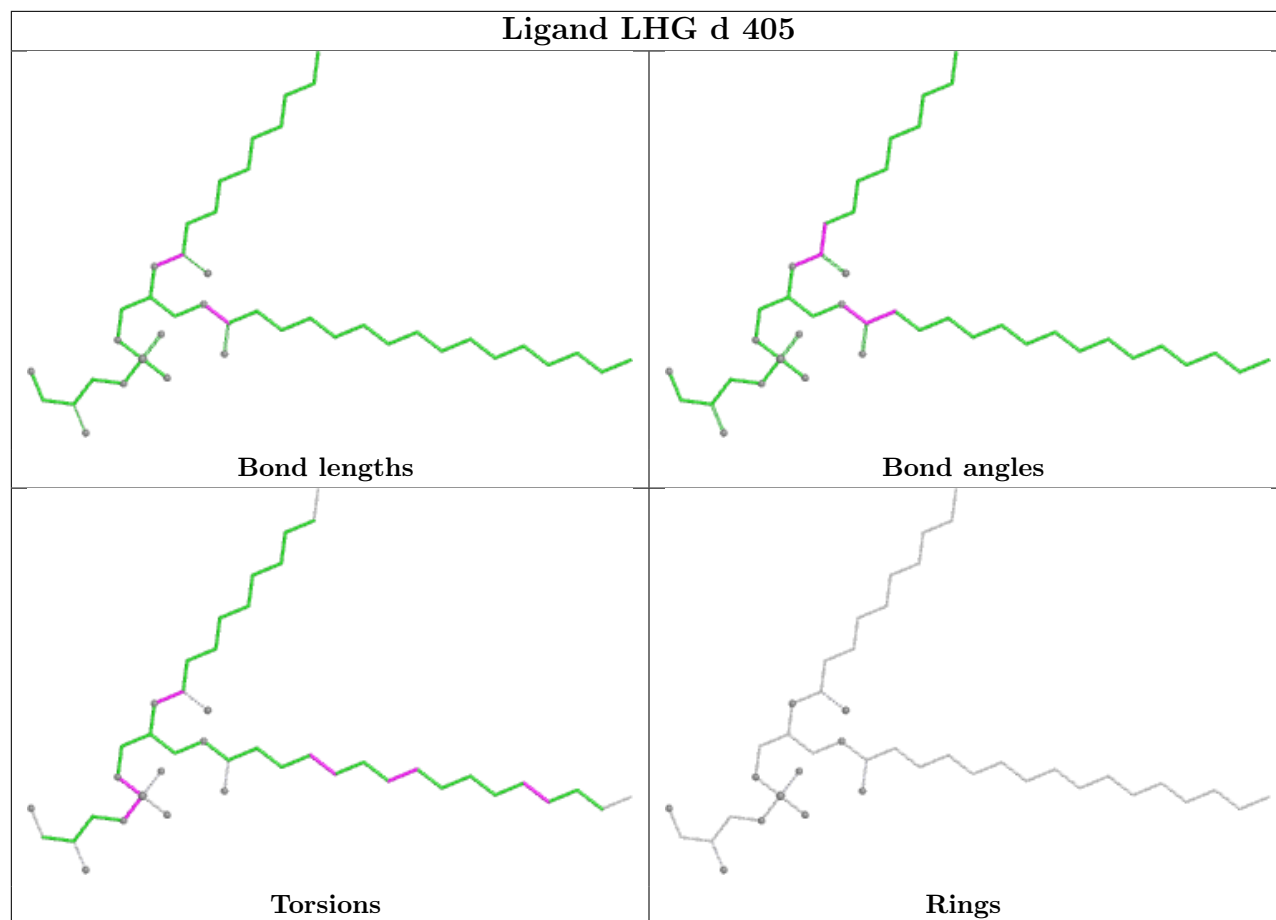
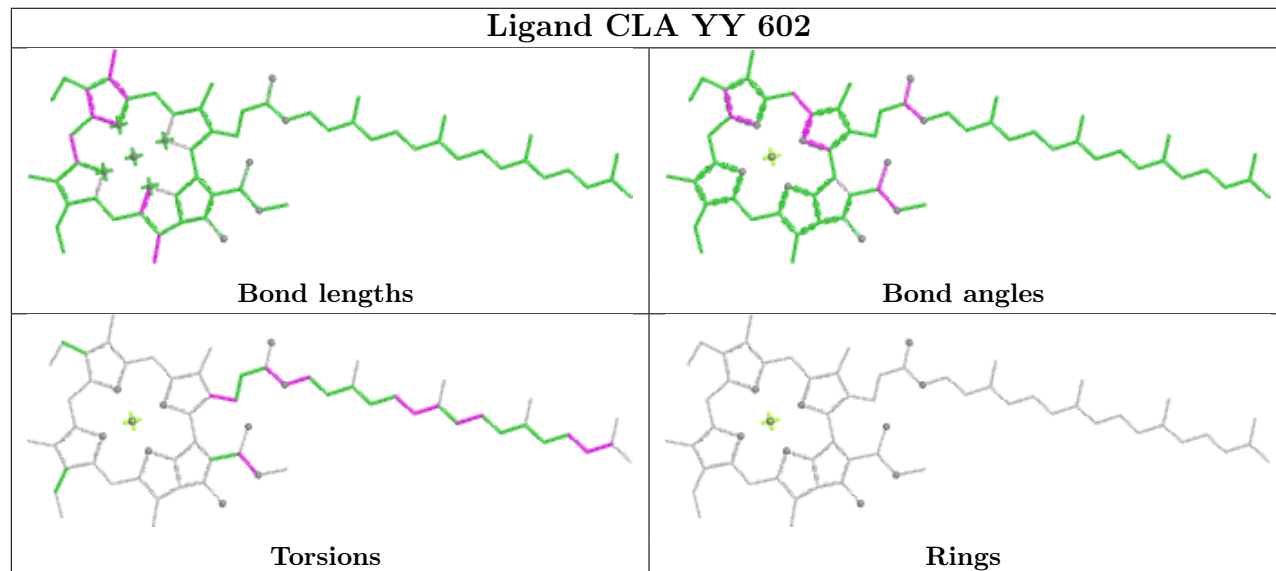


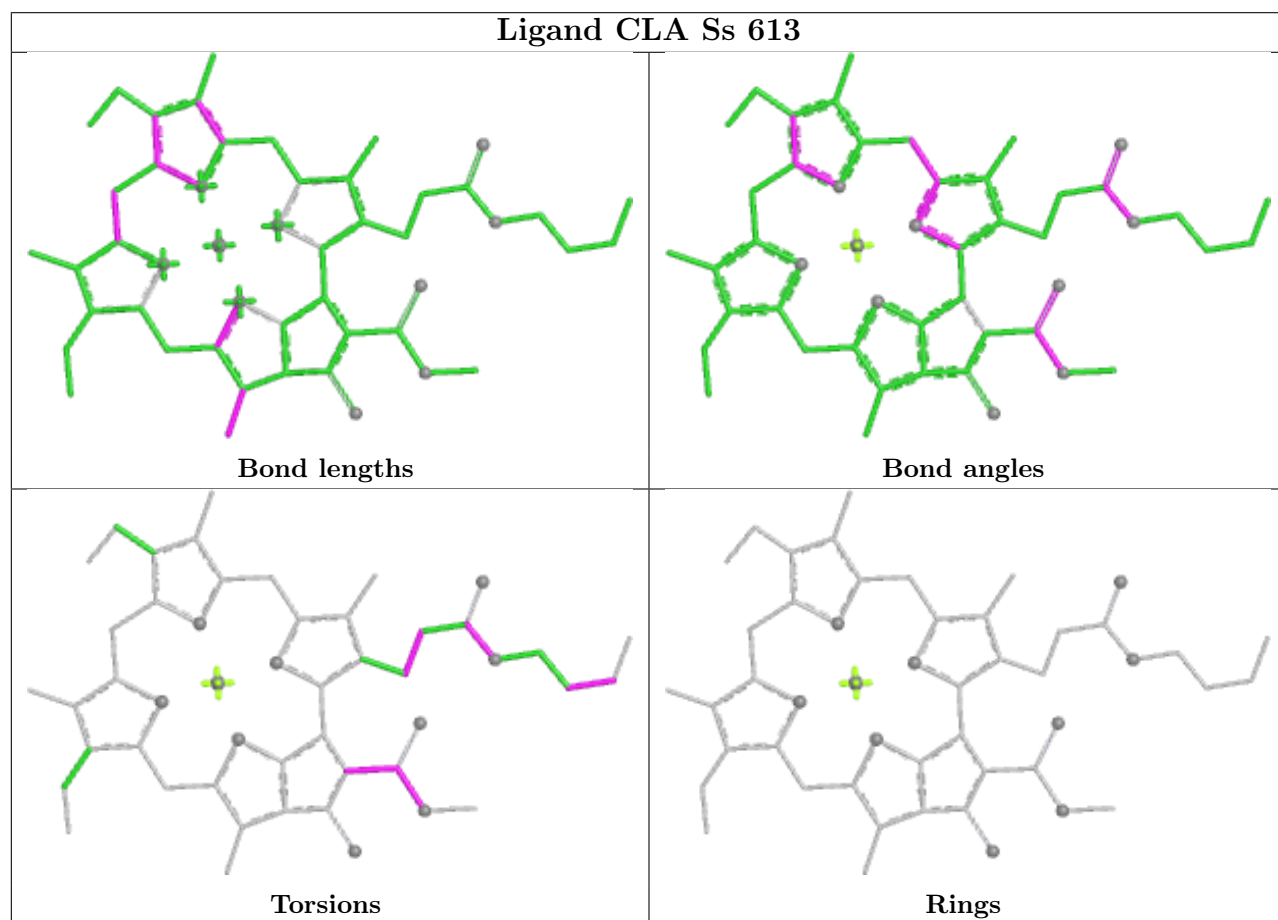
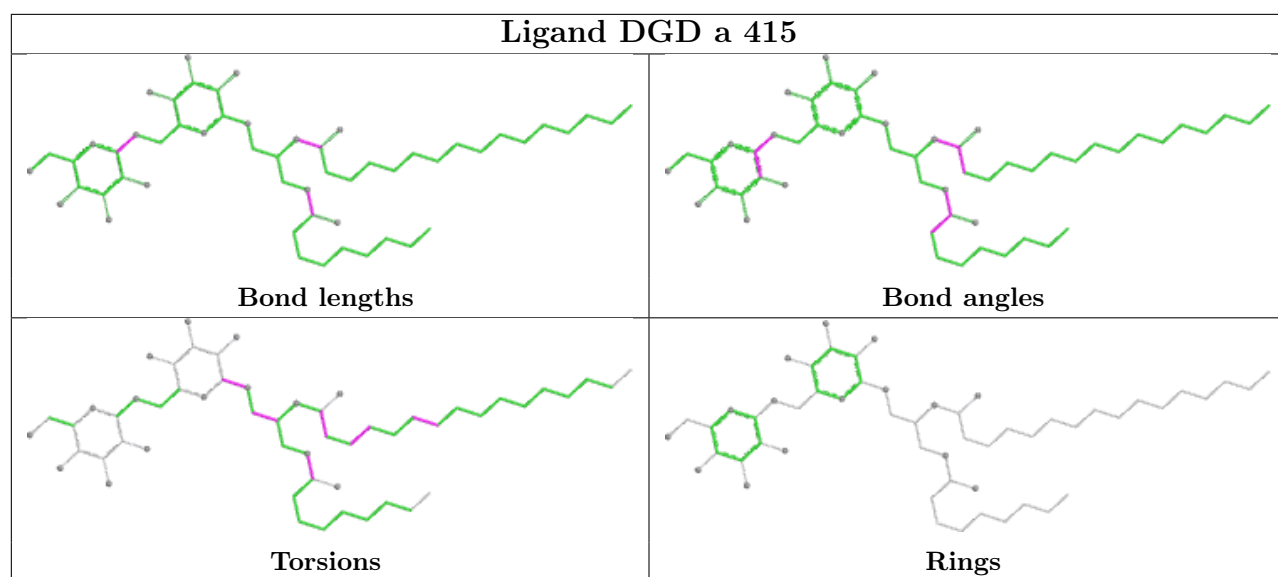
Ligand CLA y 305



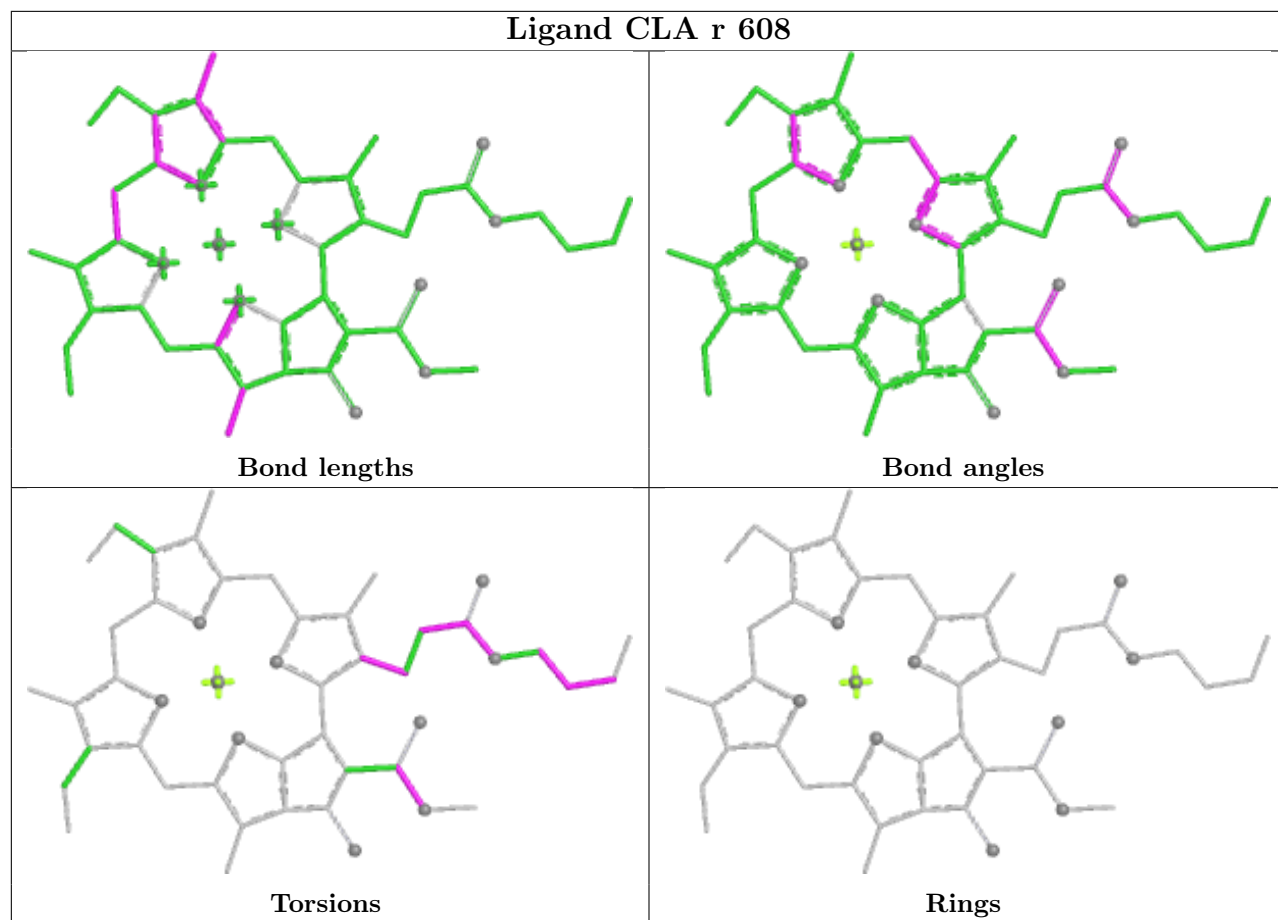
Ligand PHO a 408



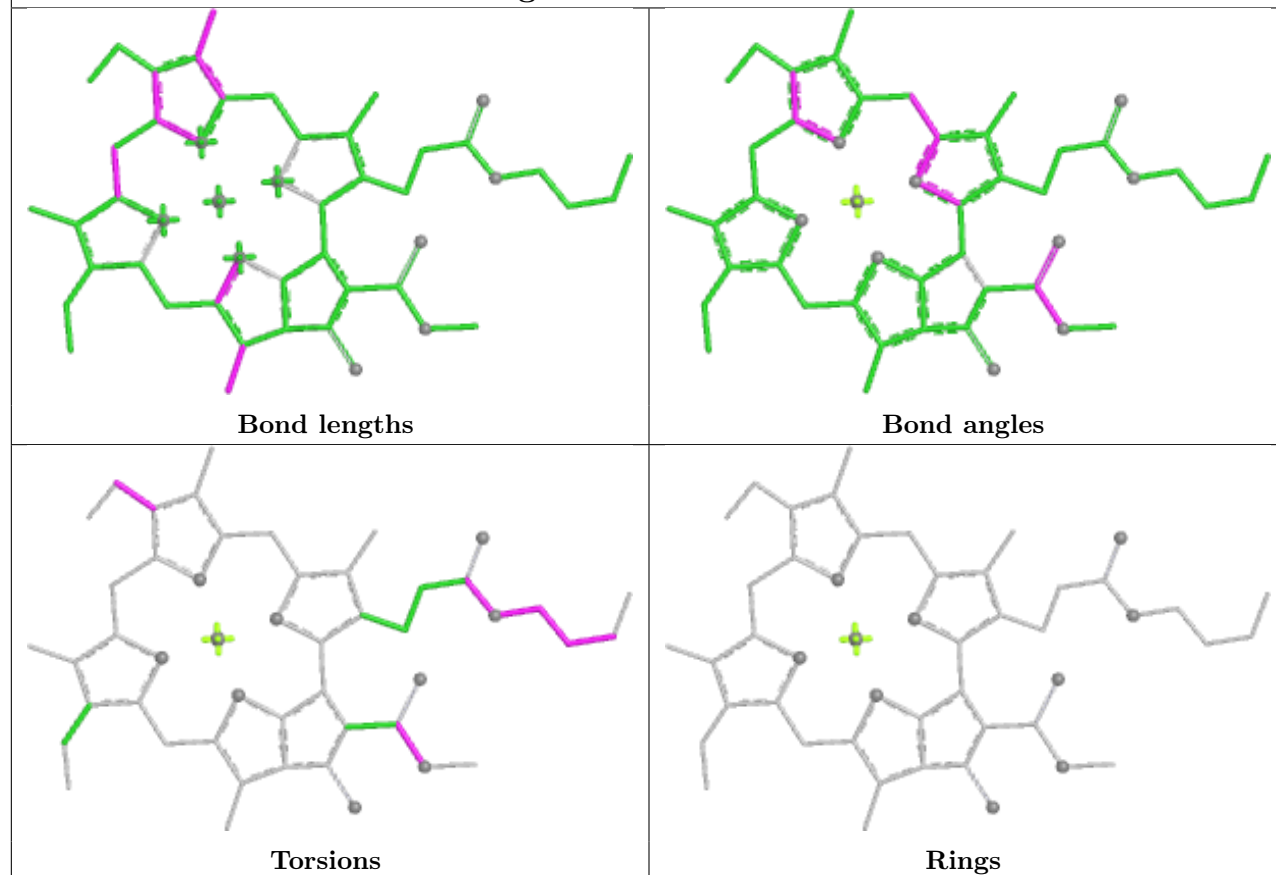
Ligand LHG d 405**Ligand CLA YY 602**



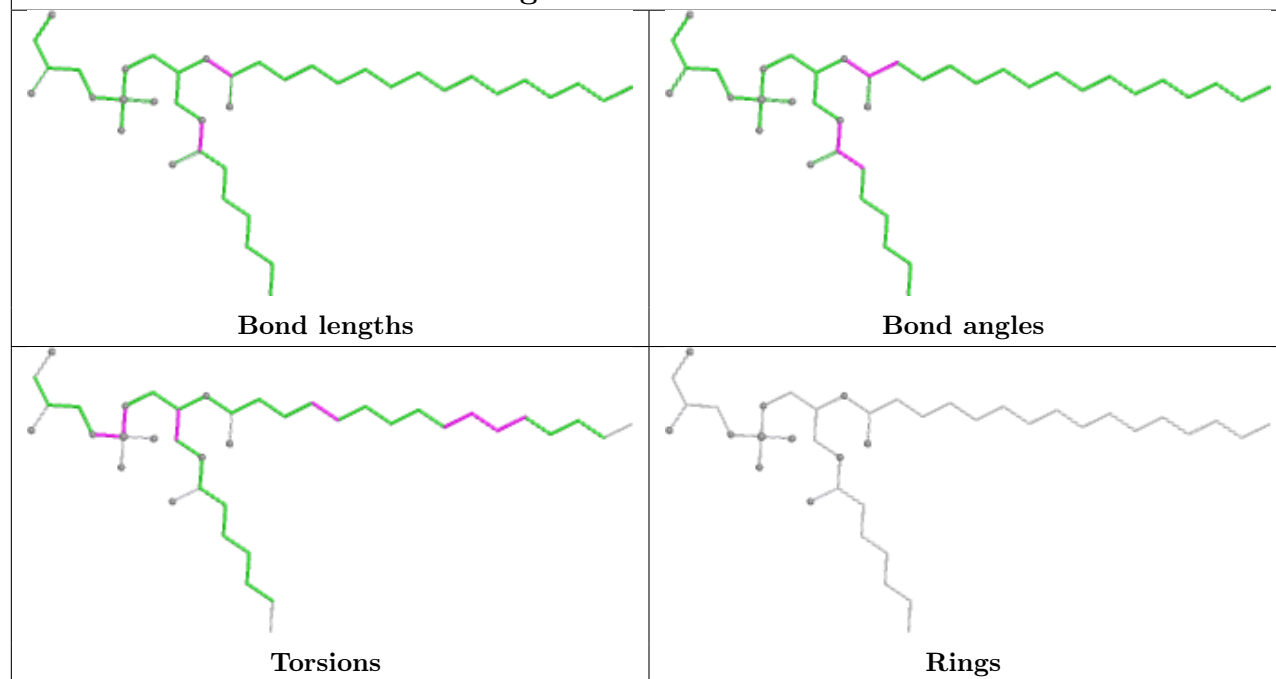
Ligand CLA r 608

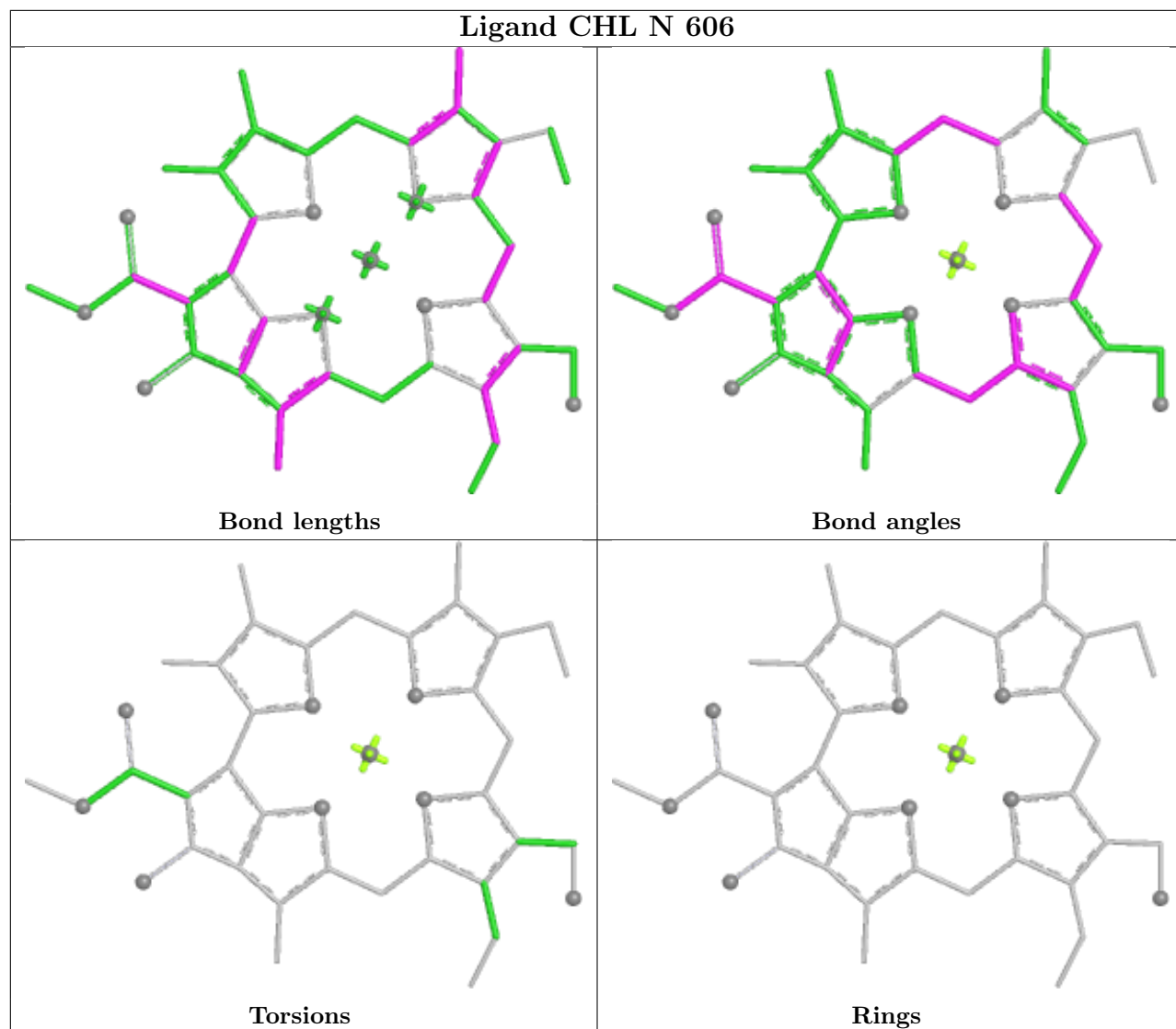


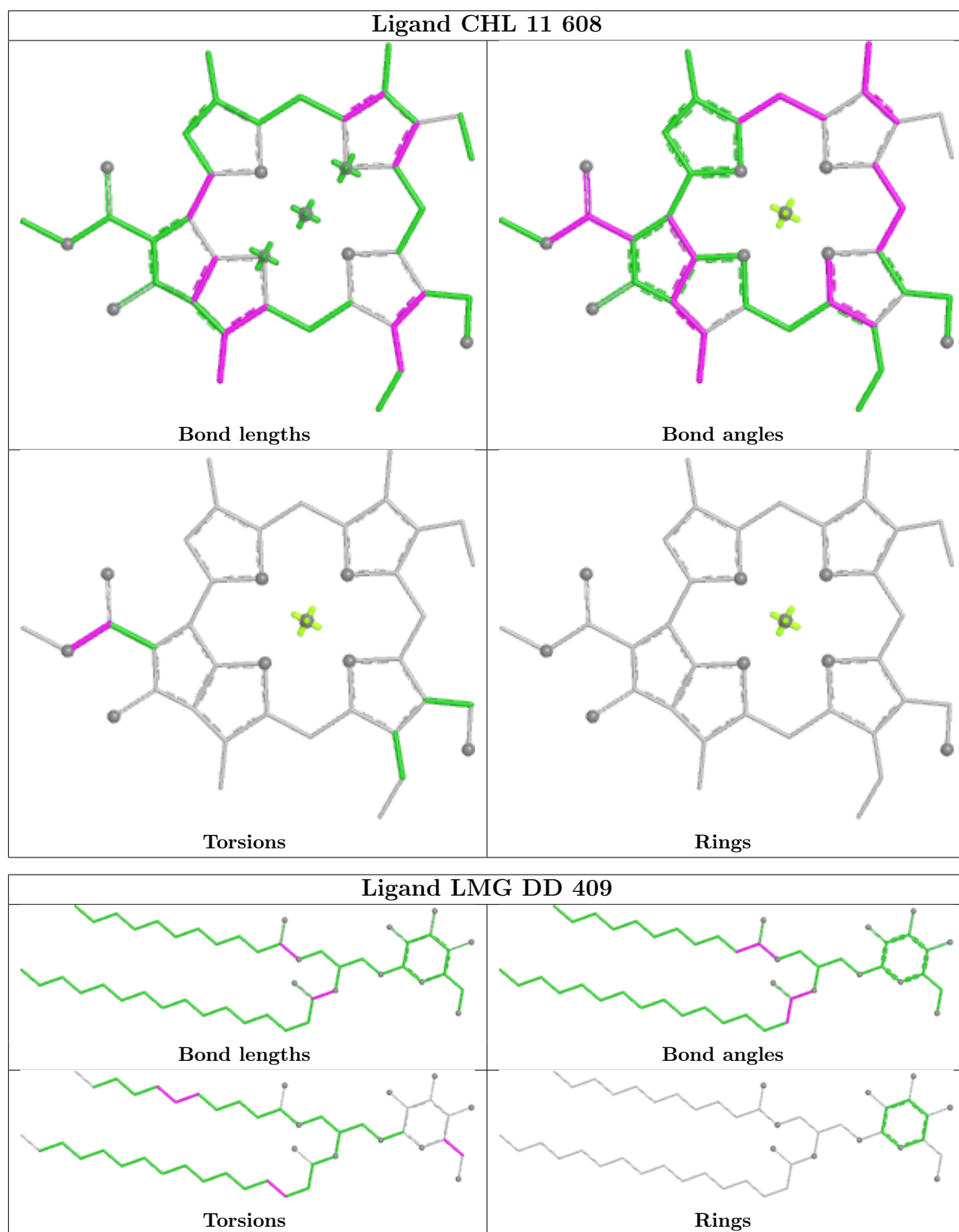
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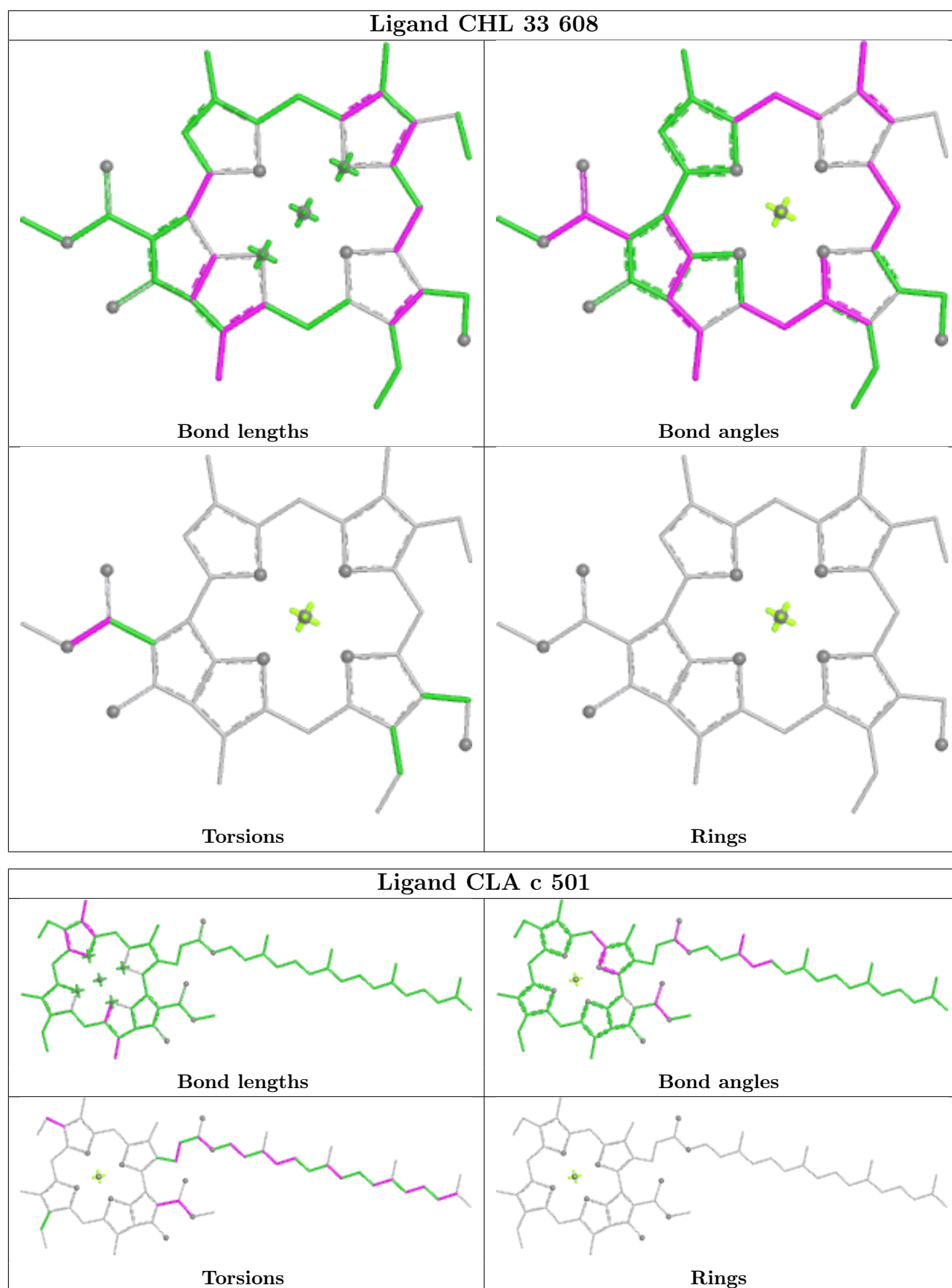


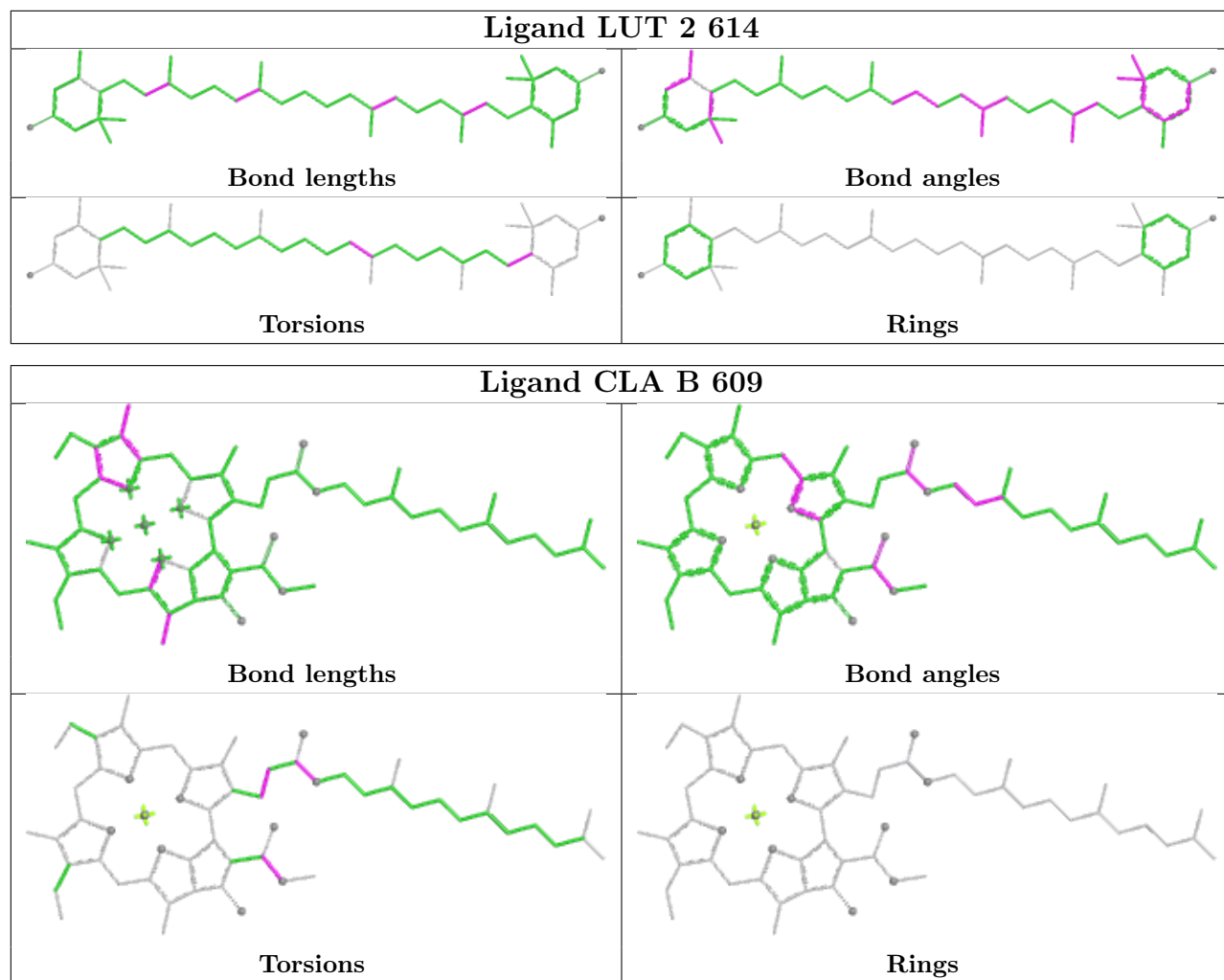
Ligand LHG EE 101

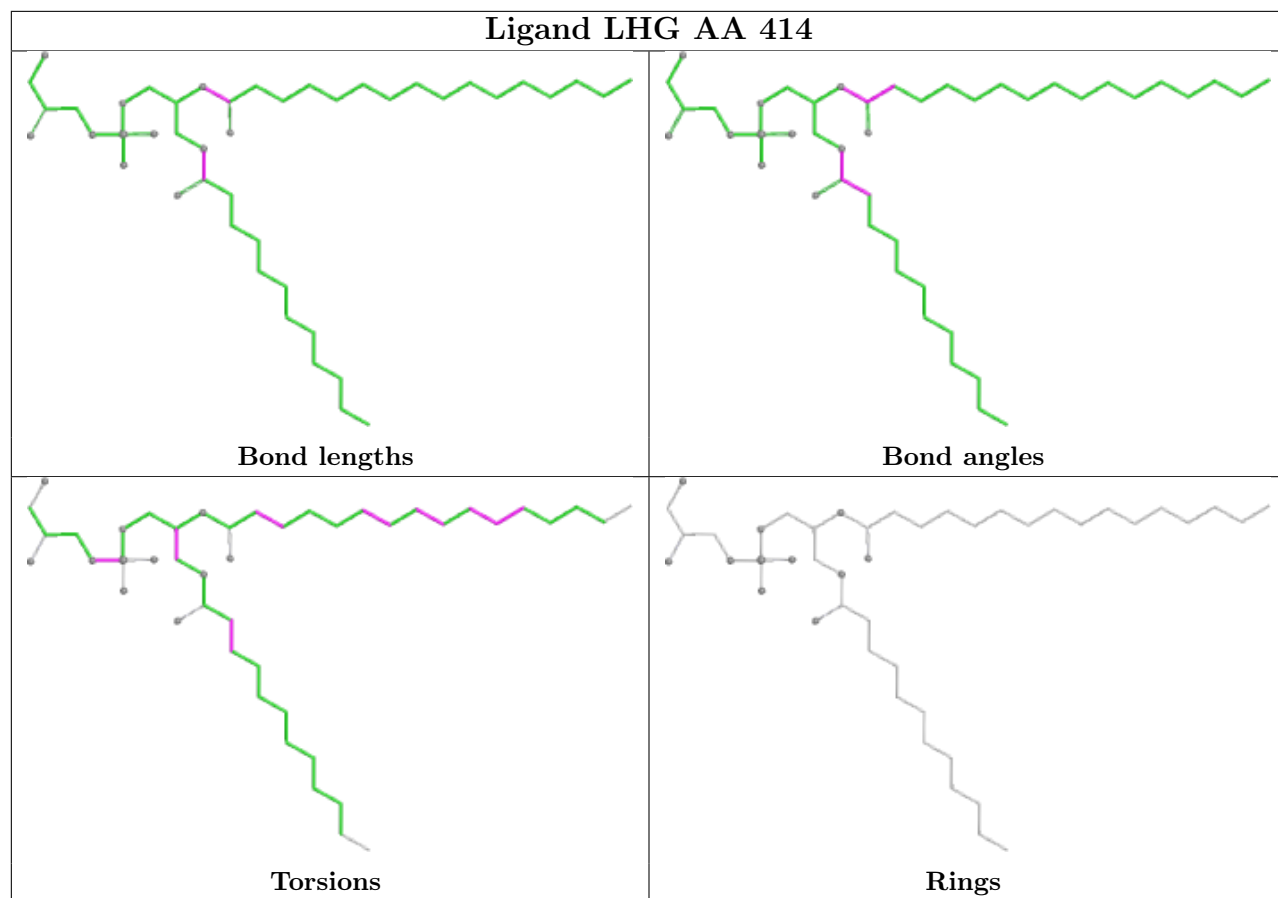


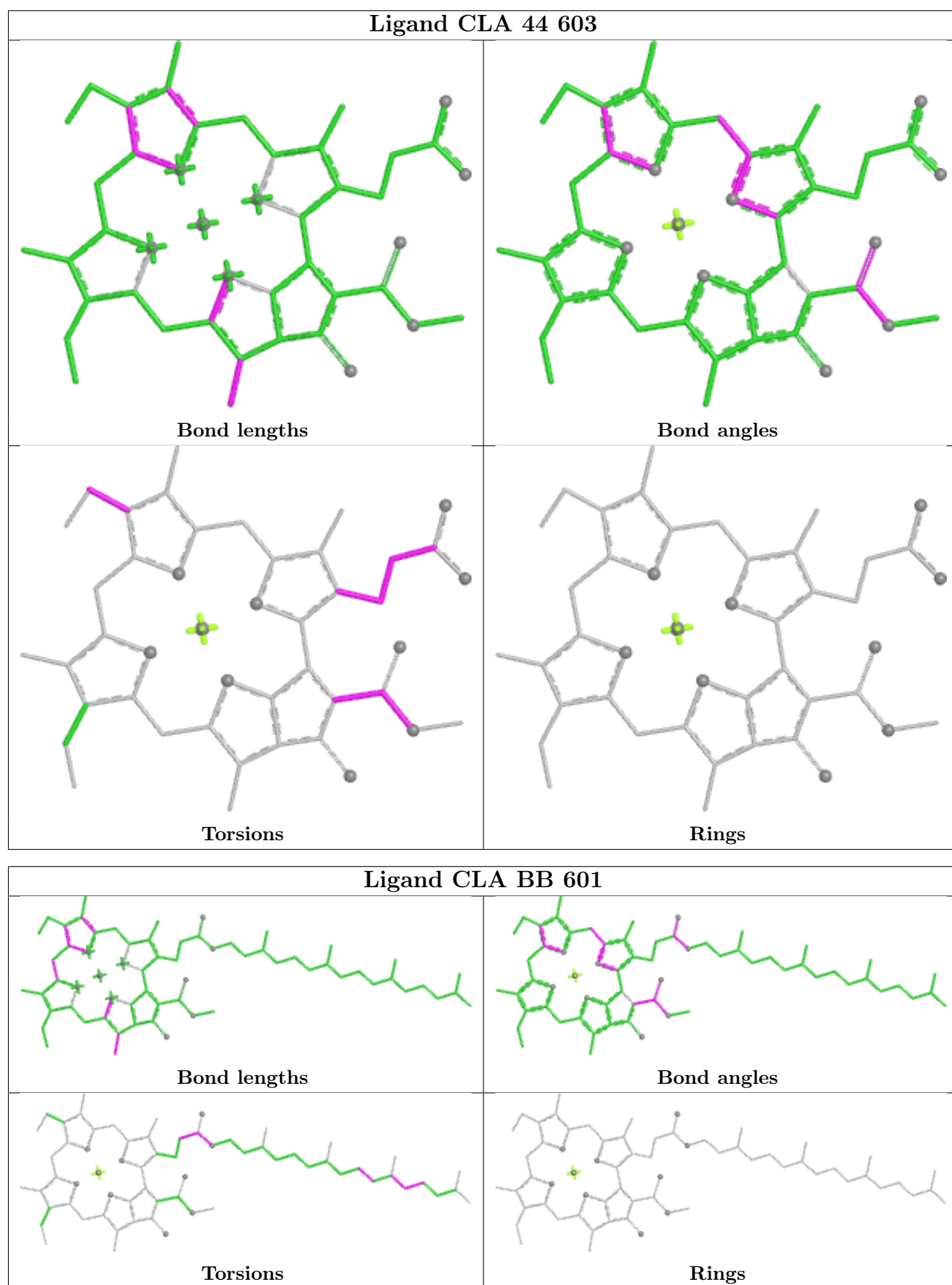




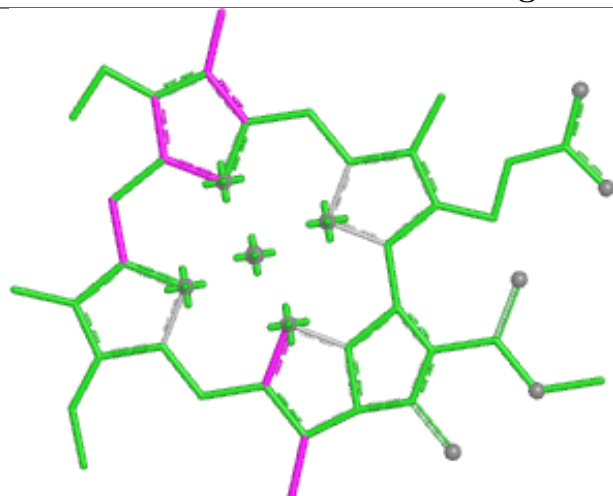




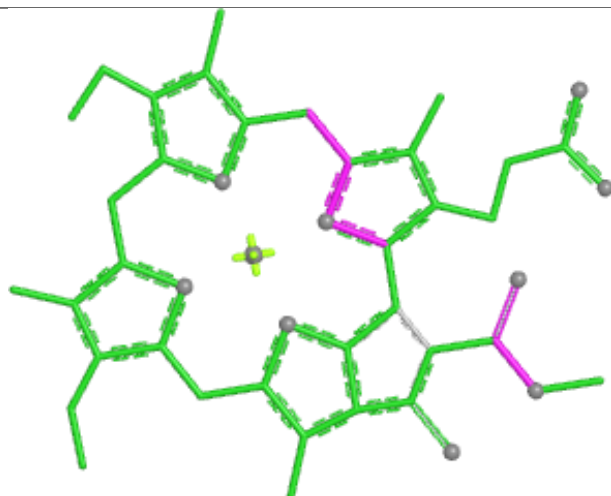




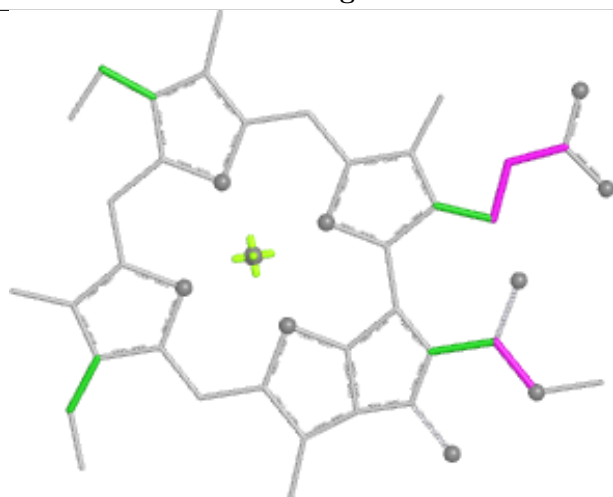
Ligand CLA 4 305



Bond lengths



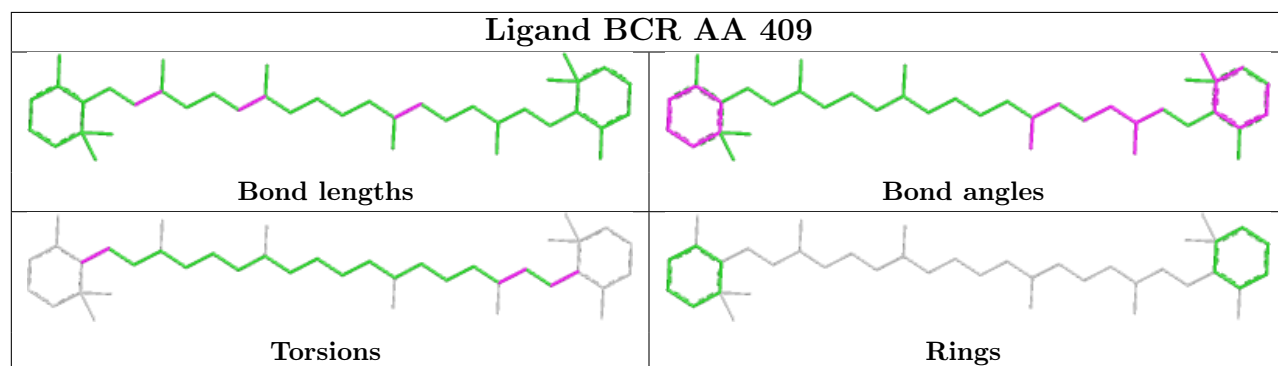
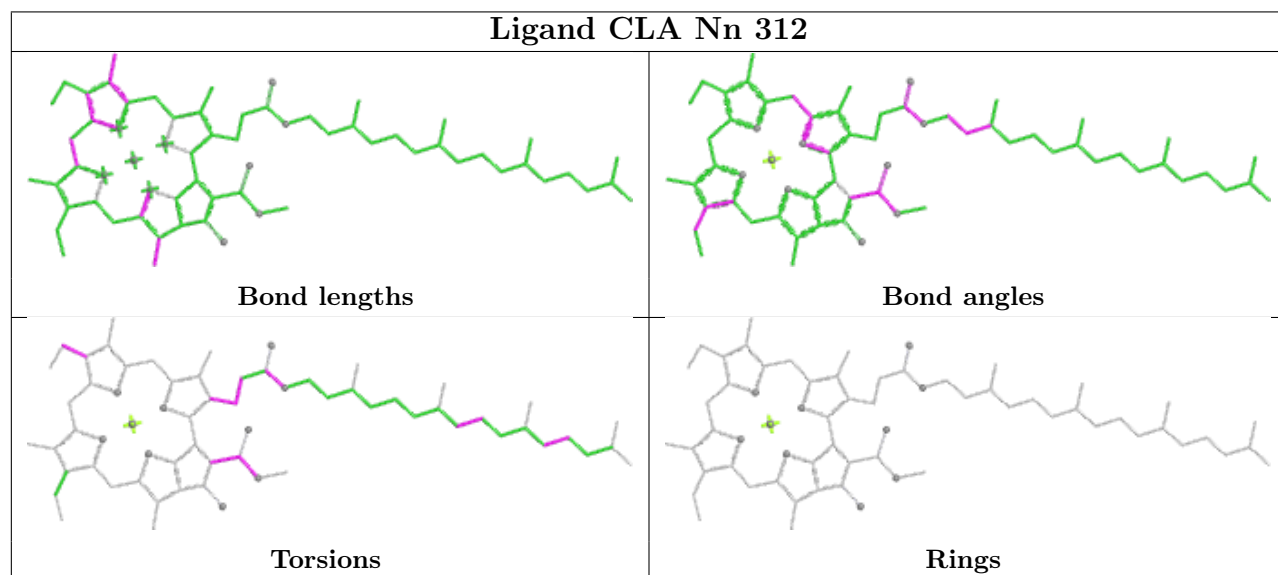
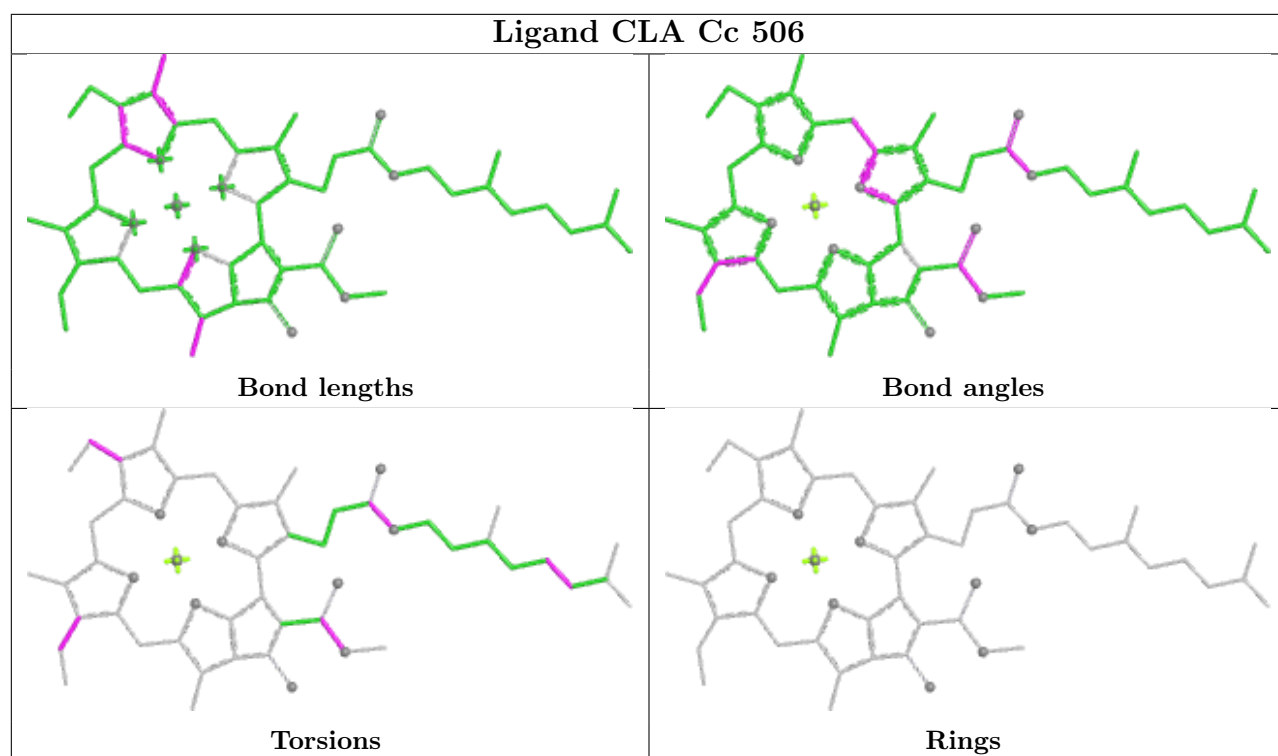
Bond angles



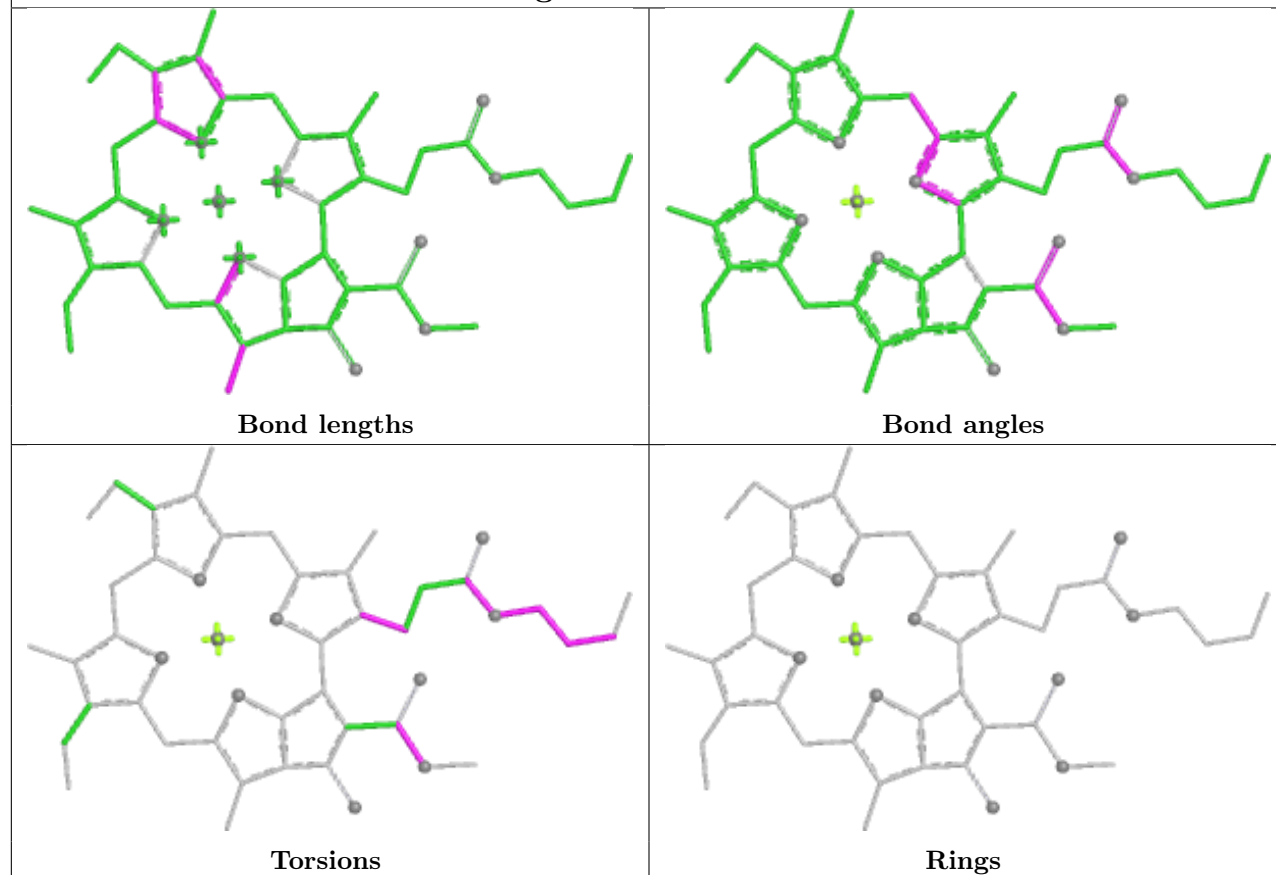
Torsions



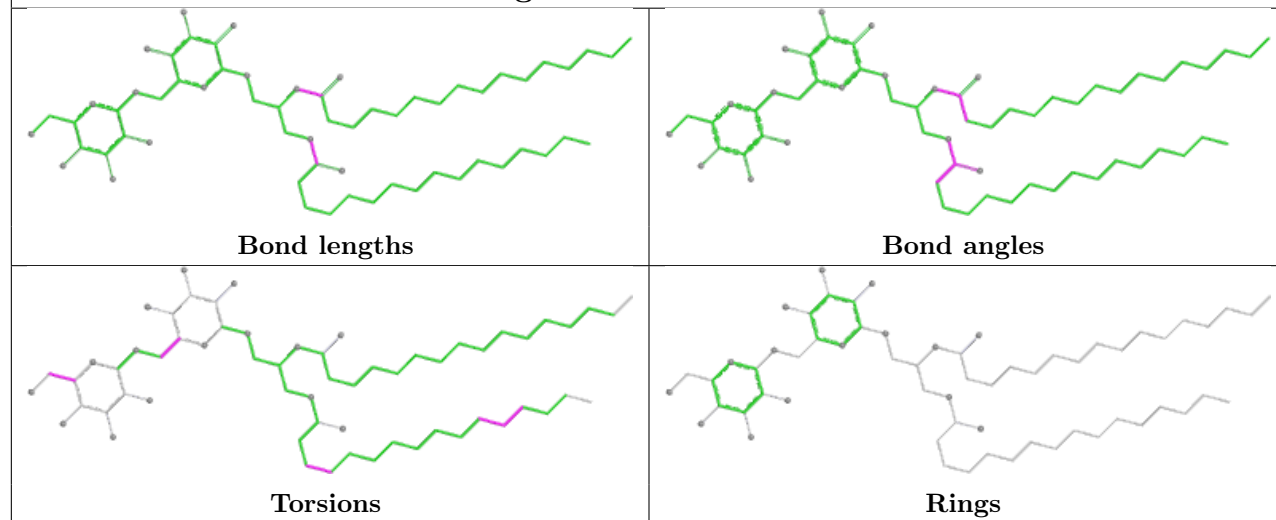
Rings

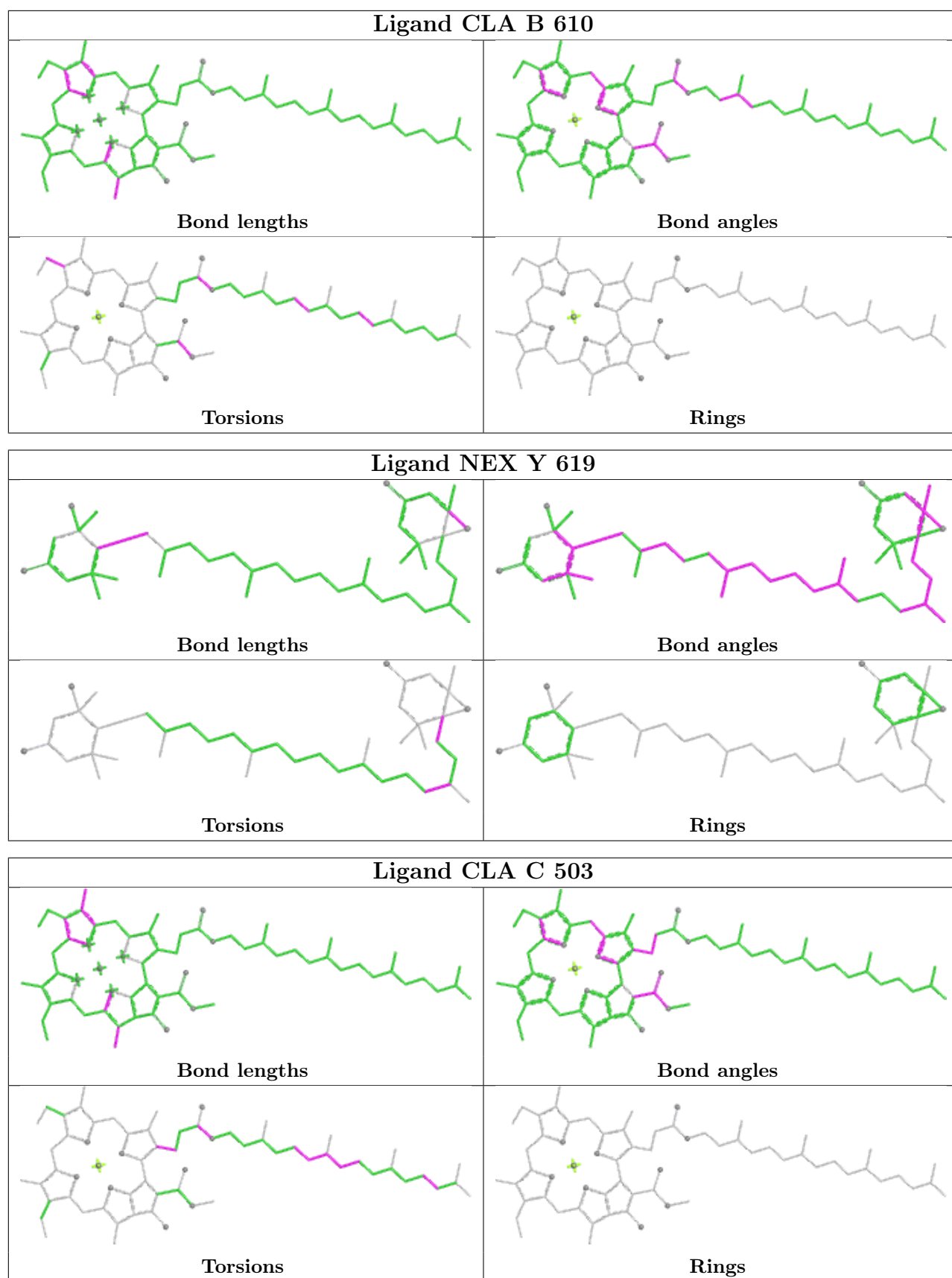


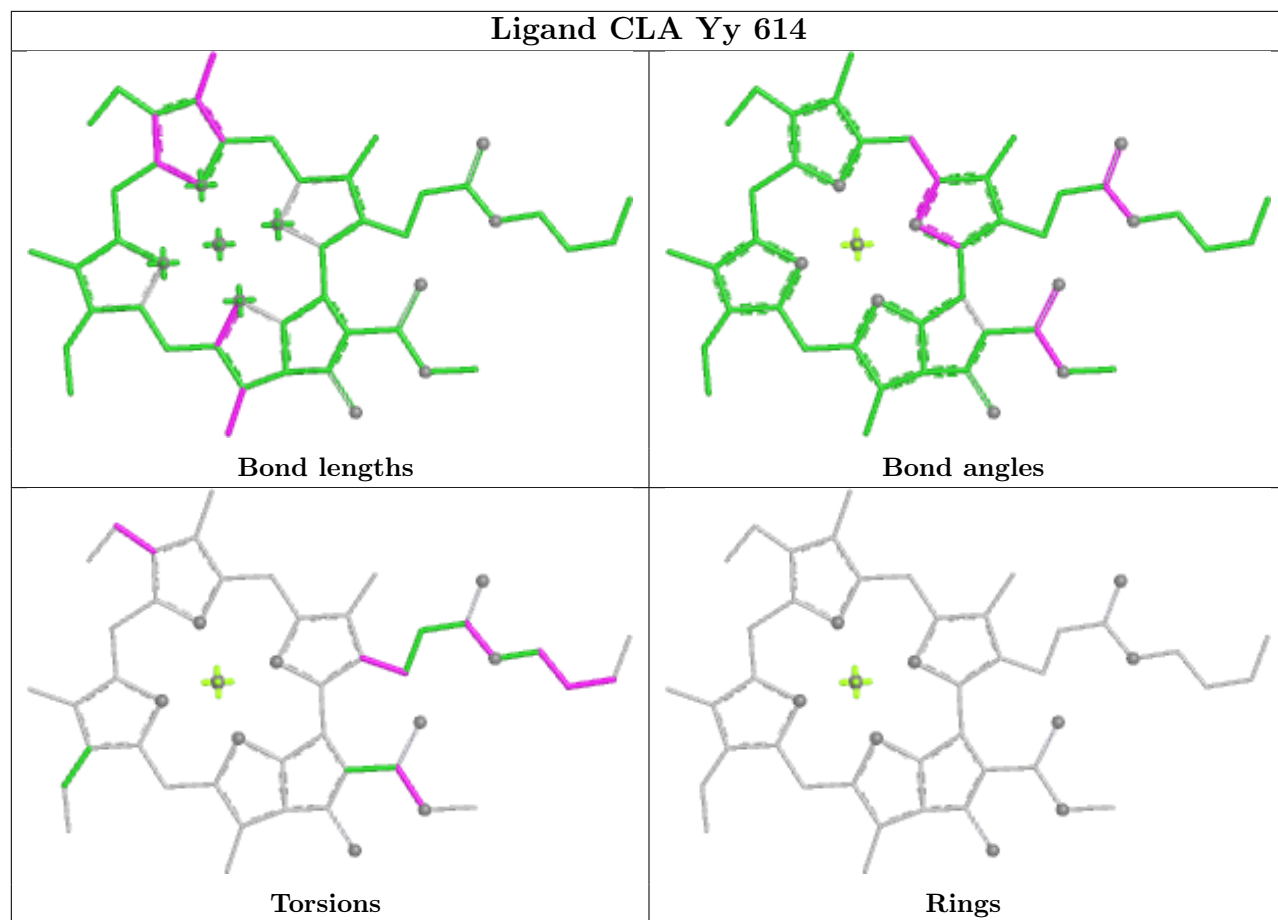
Ligand CLA n 603

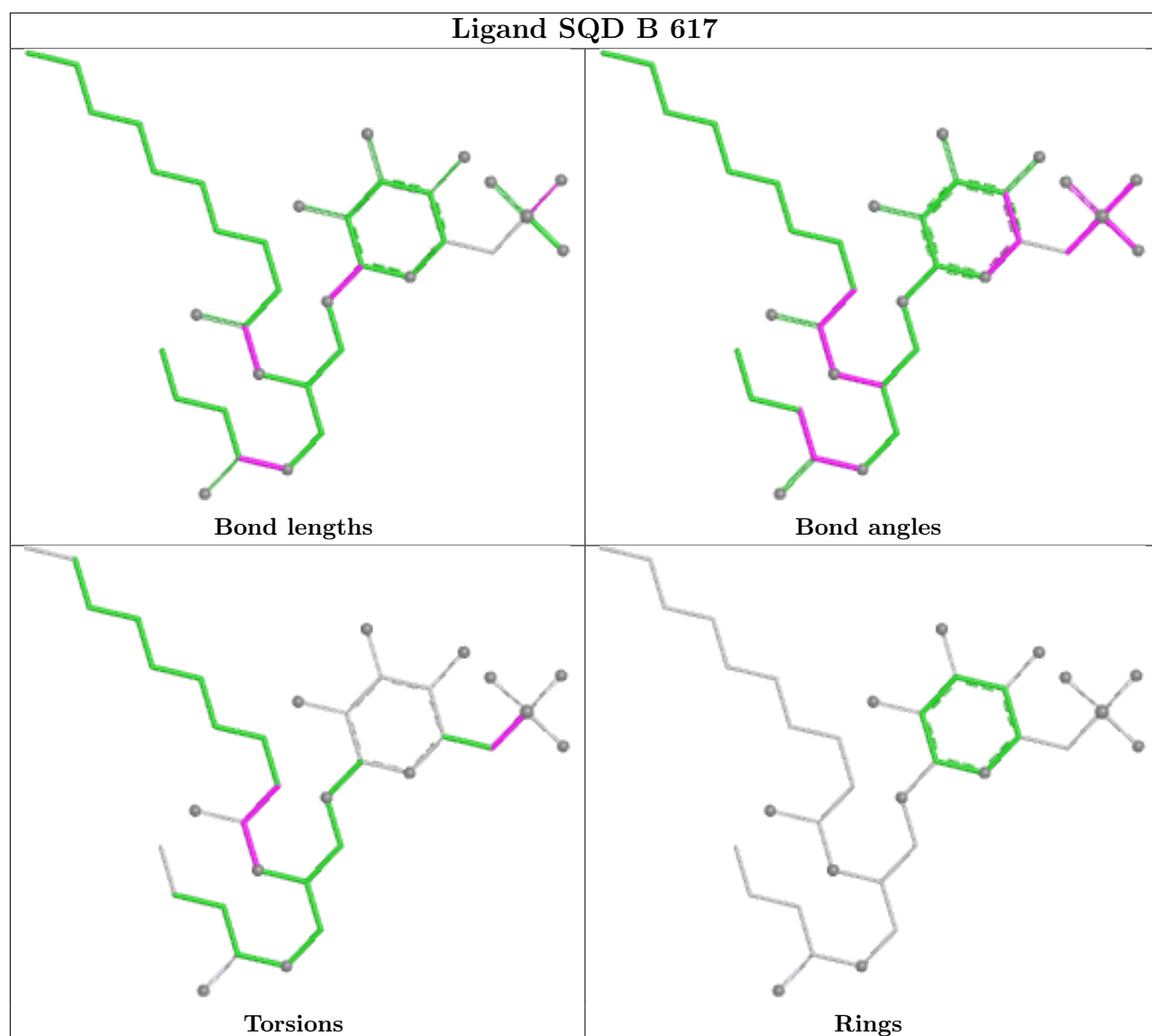


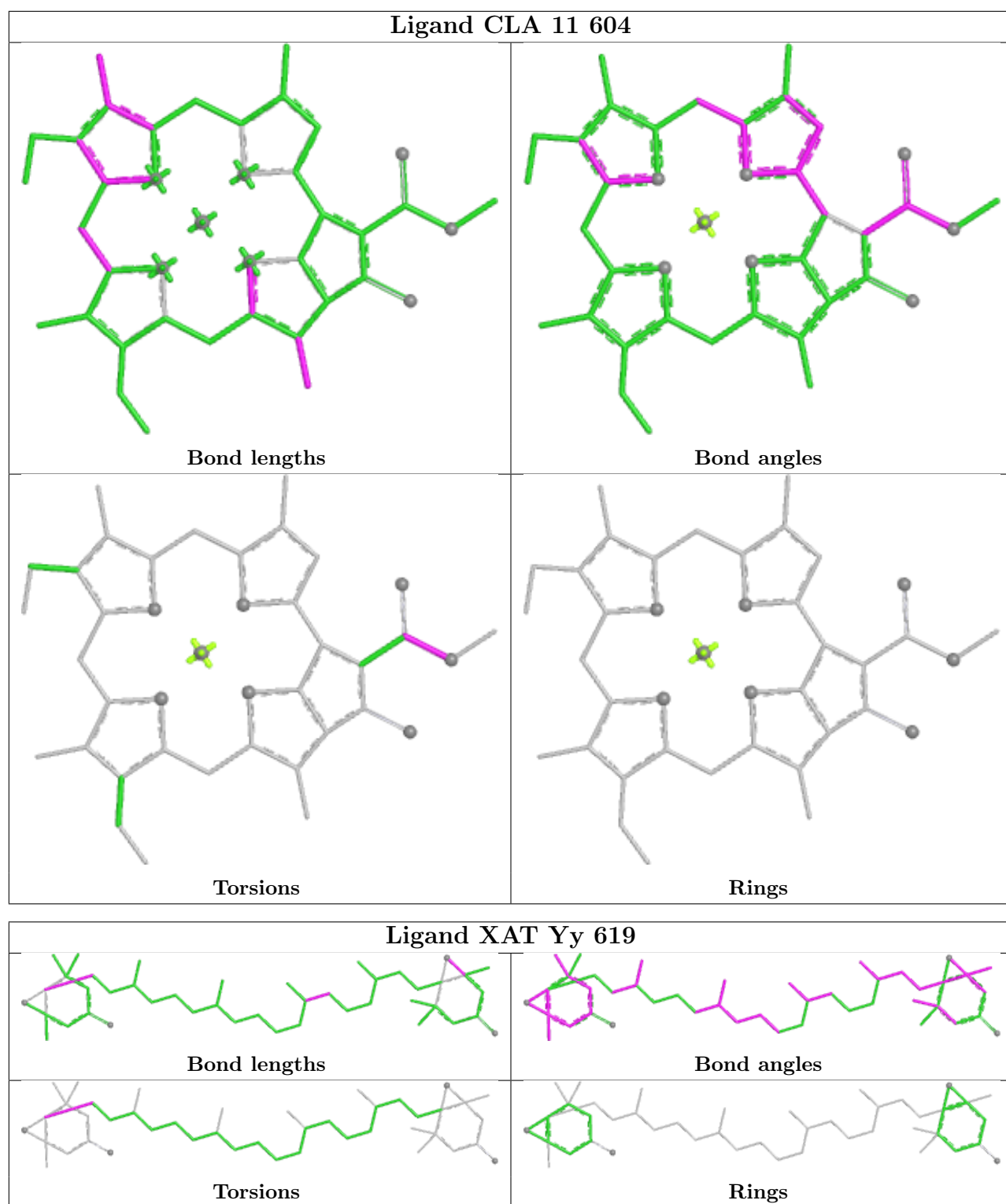
Ligand DGD CC 519

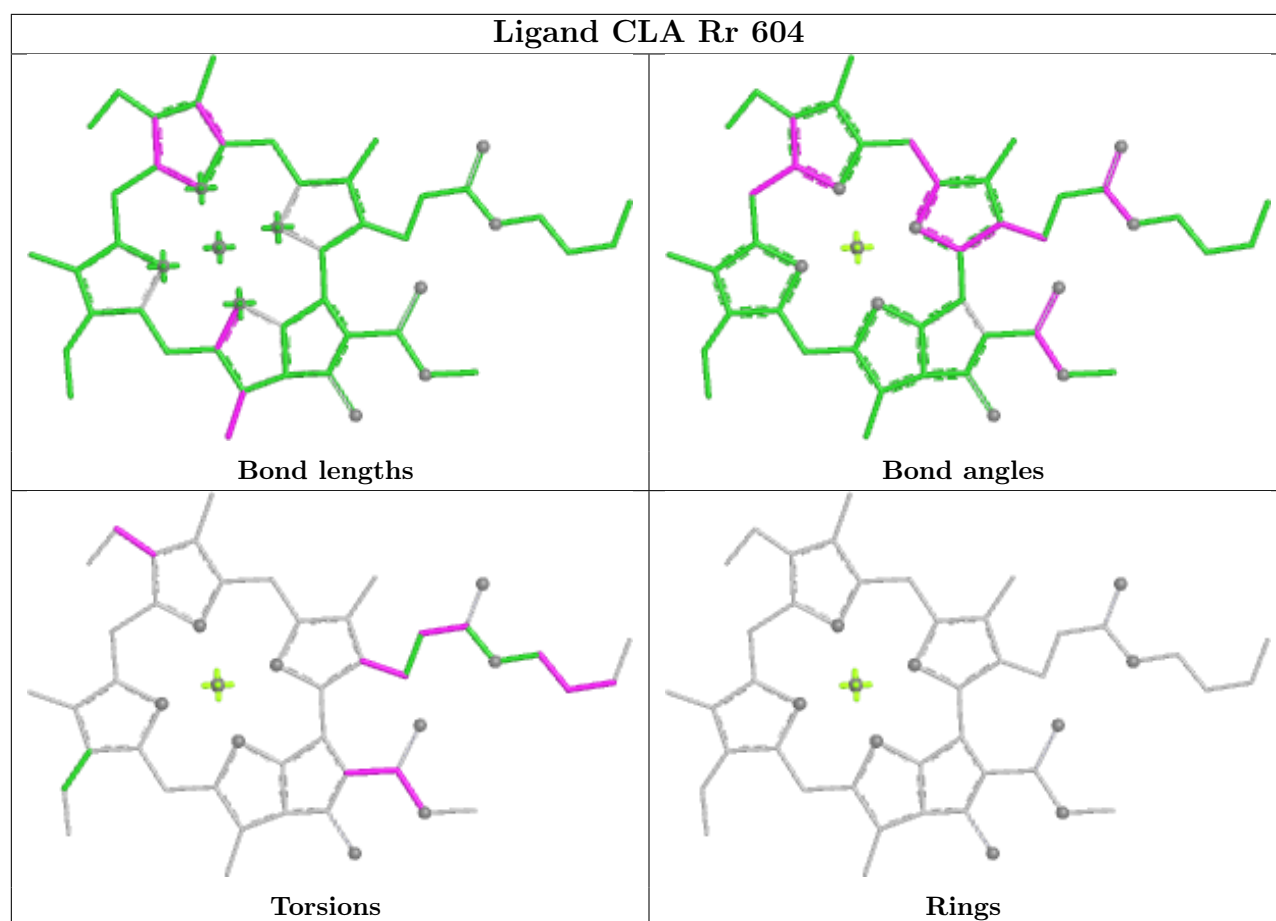




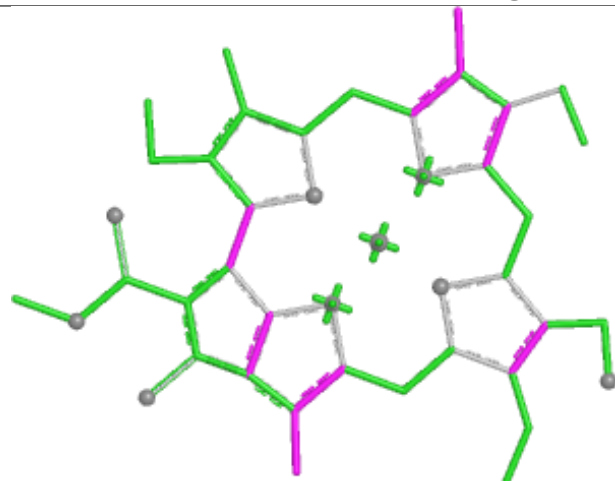




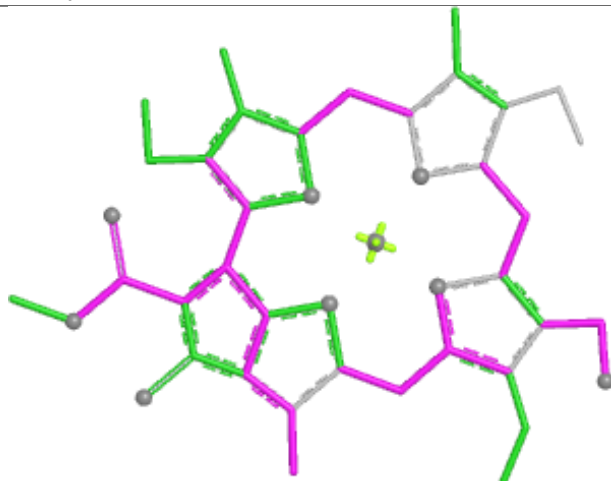




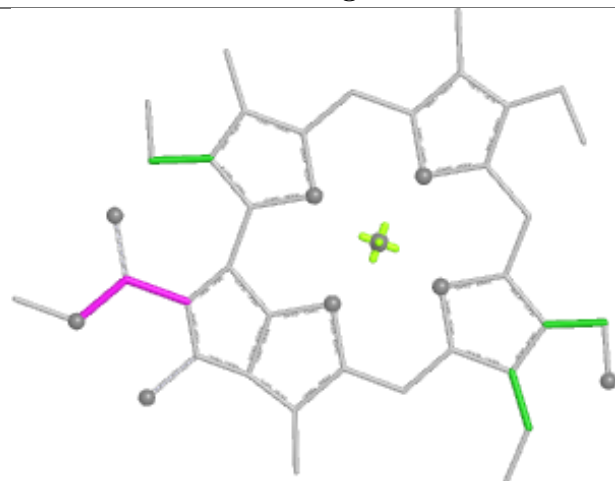
Ligand CHL Yy 607



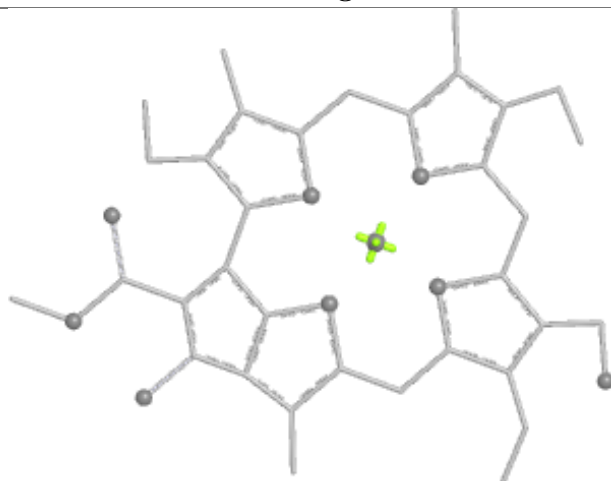
Bond lengths



Bond angles

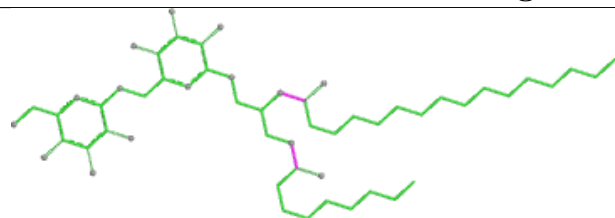


Torsions

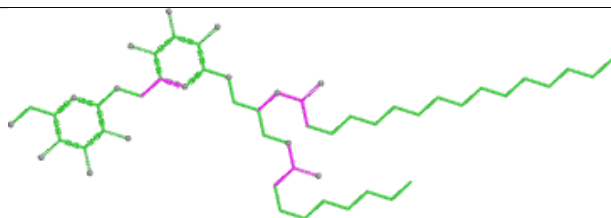


Rings

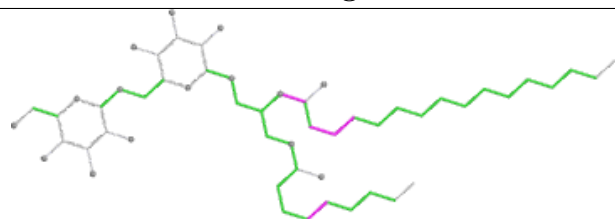
Ligand DGD c 517



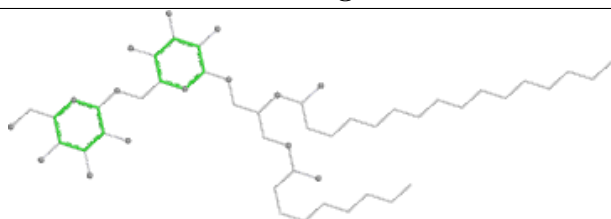
Bond lengths



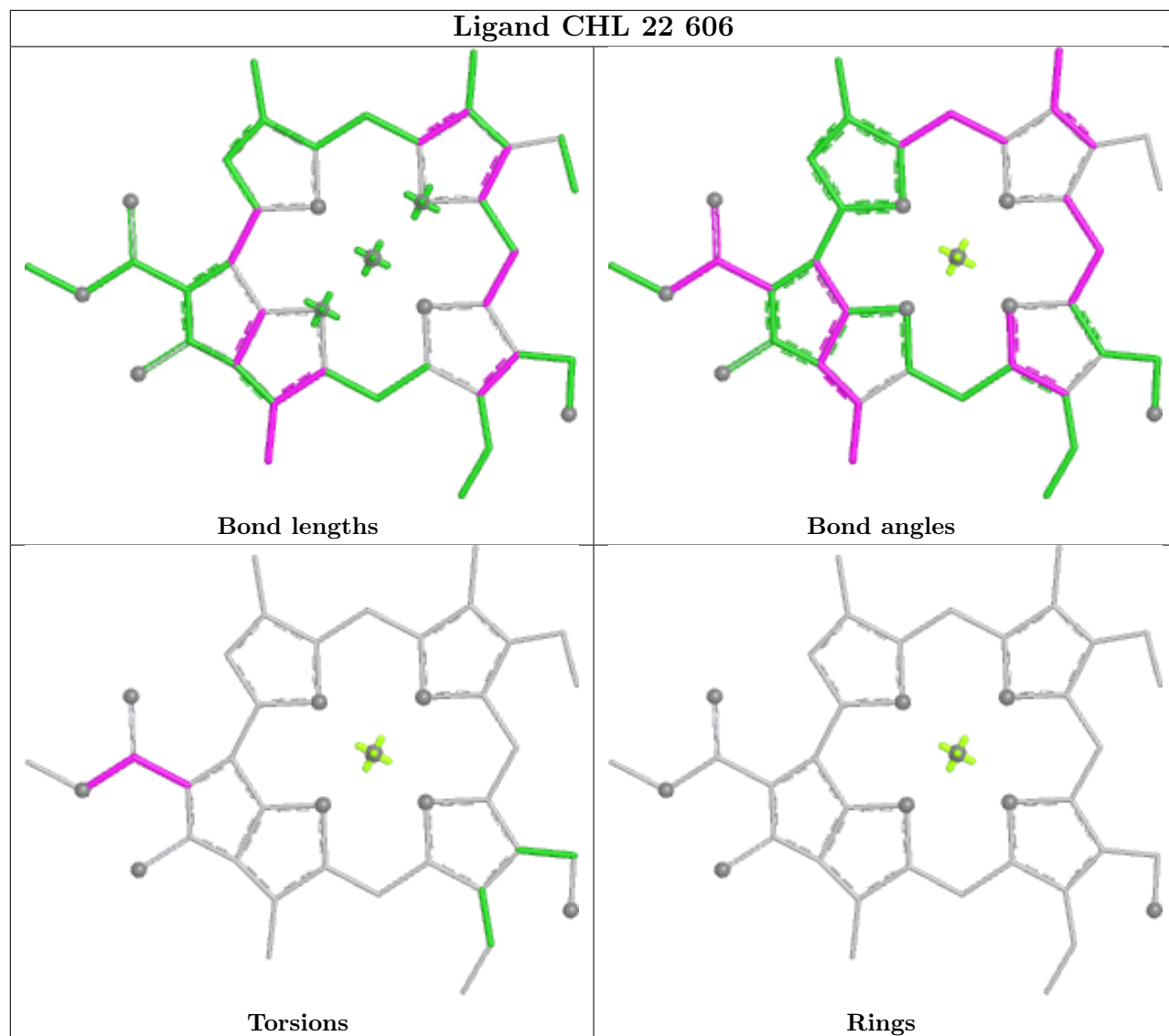
Bond angles

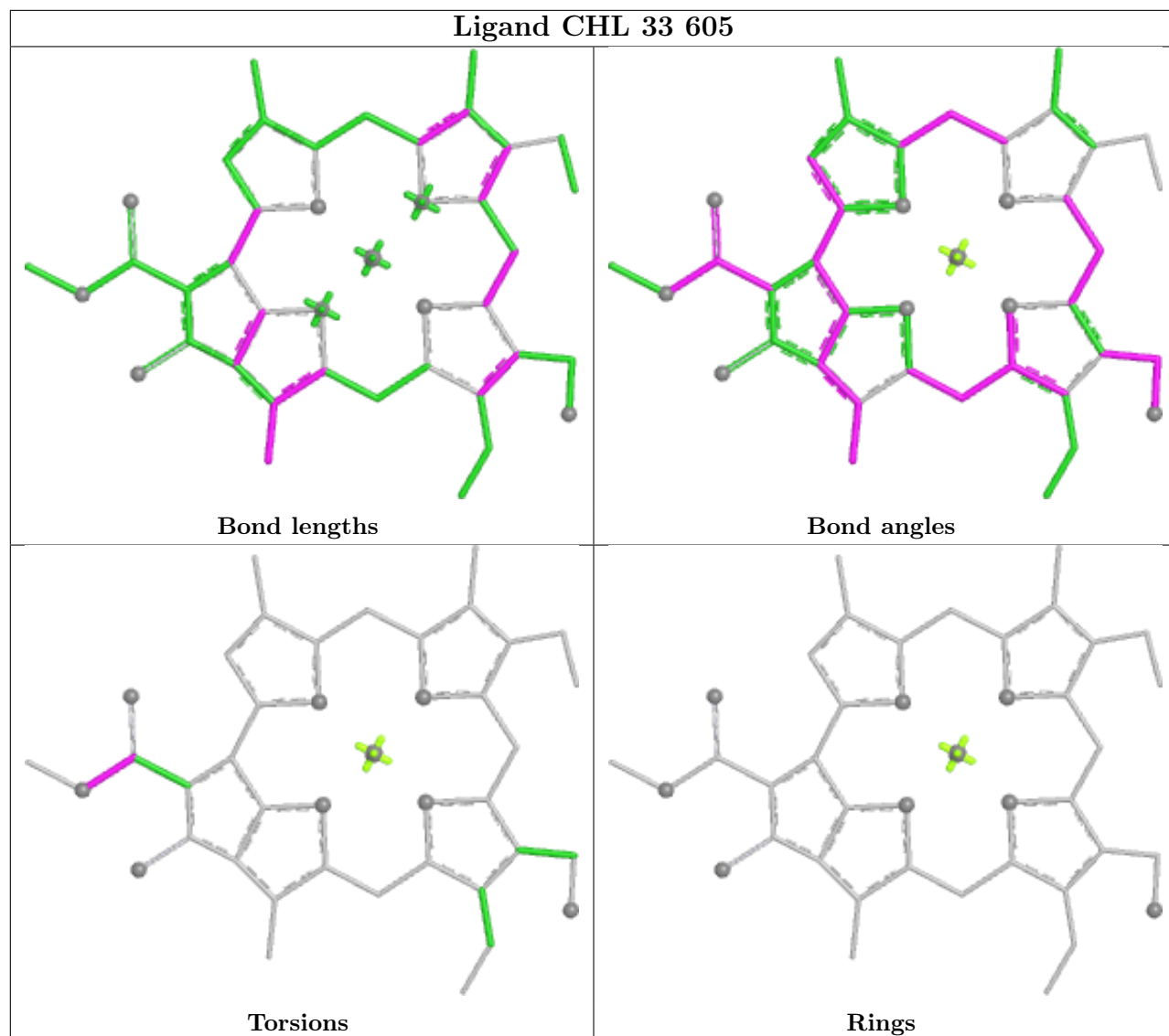


Torsions

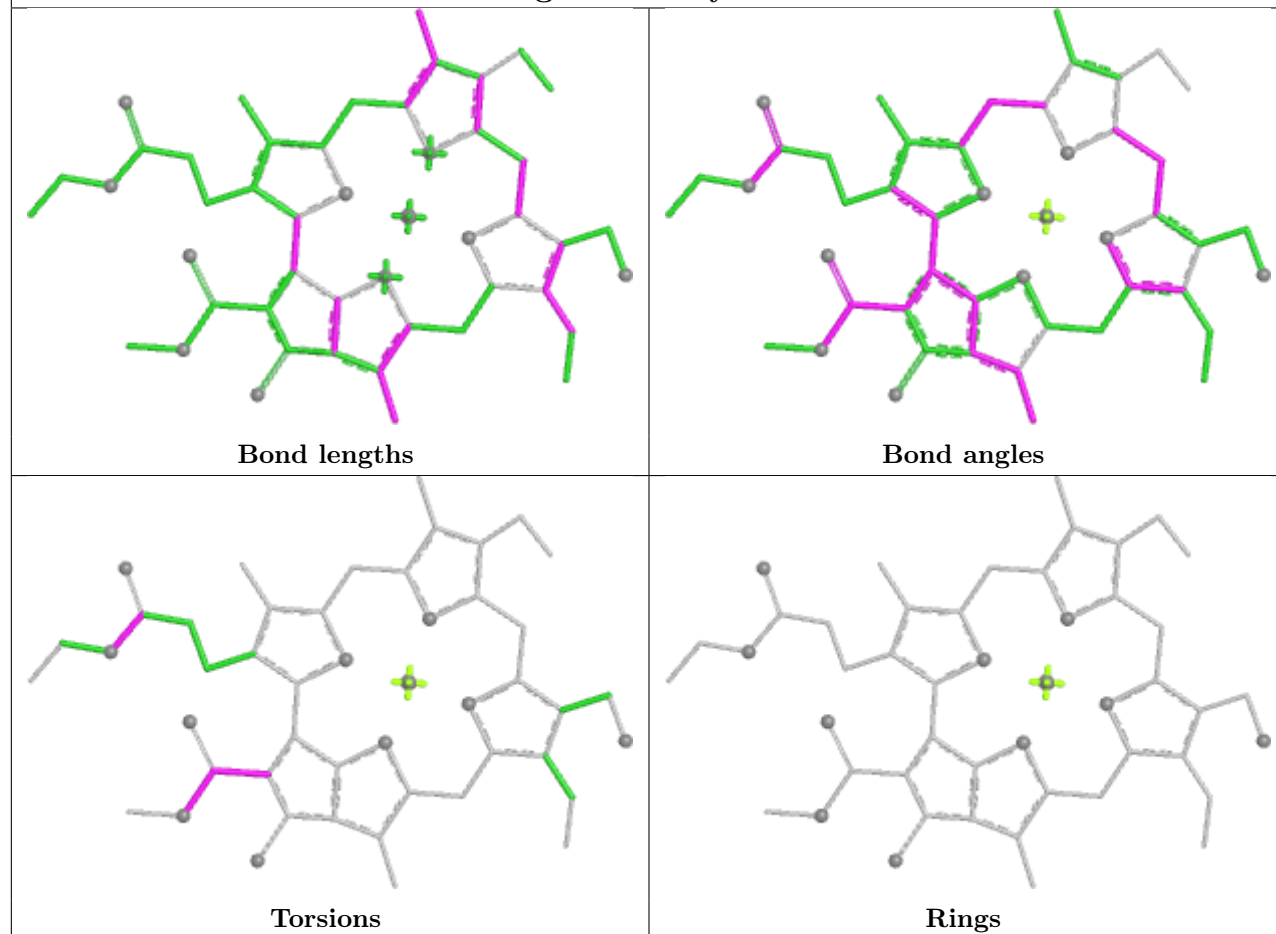


Rings

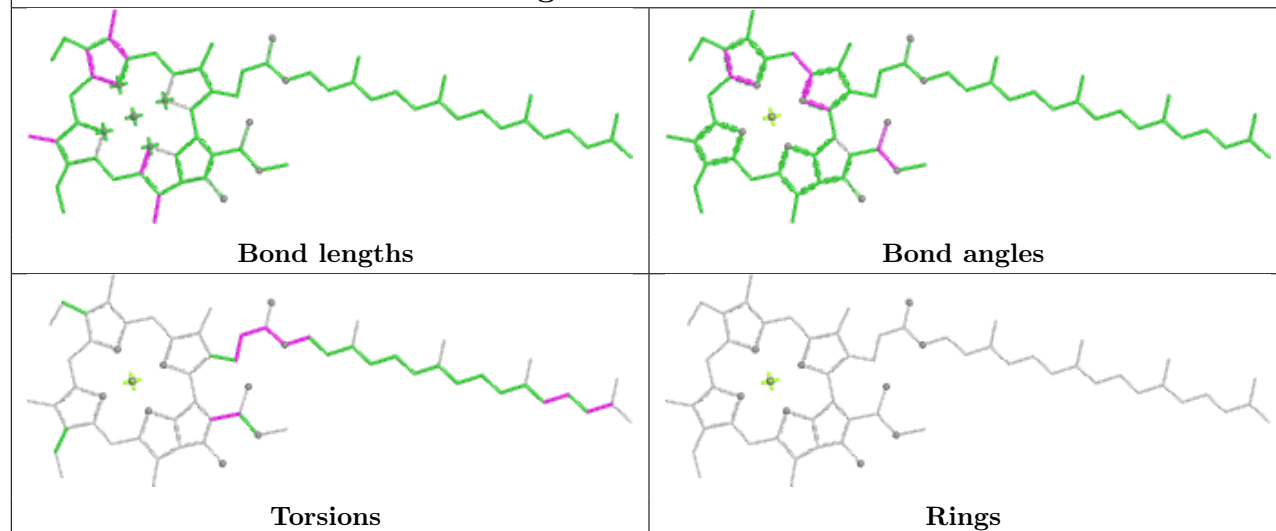


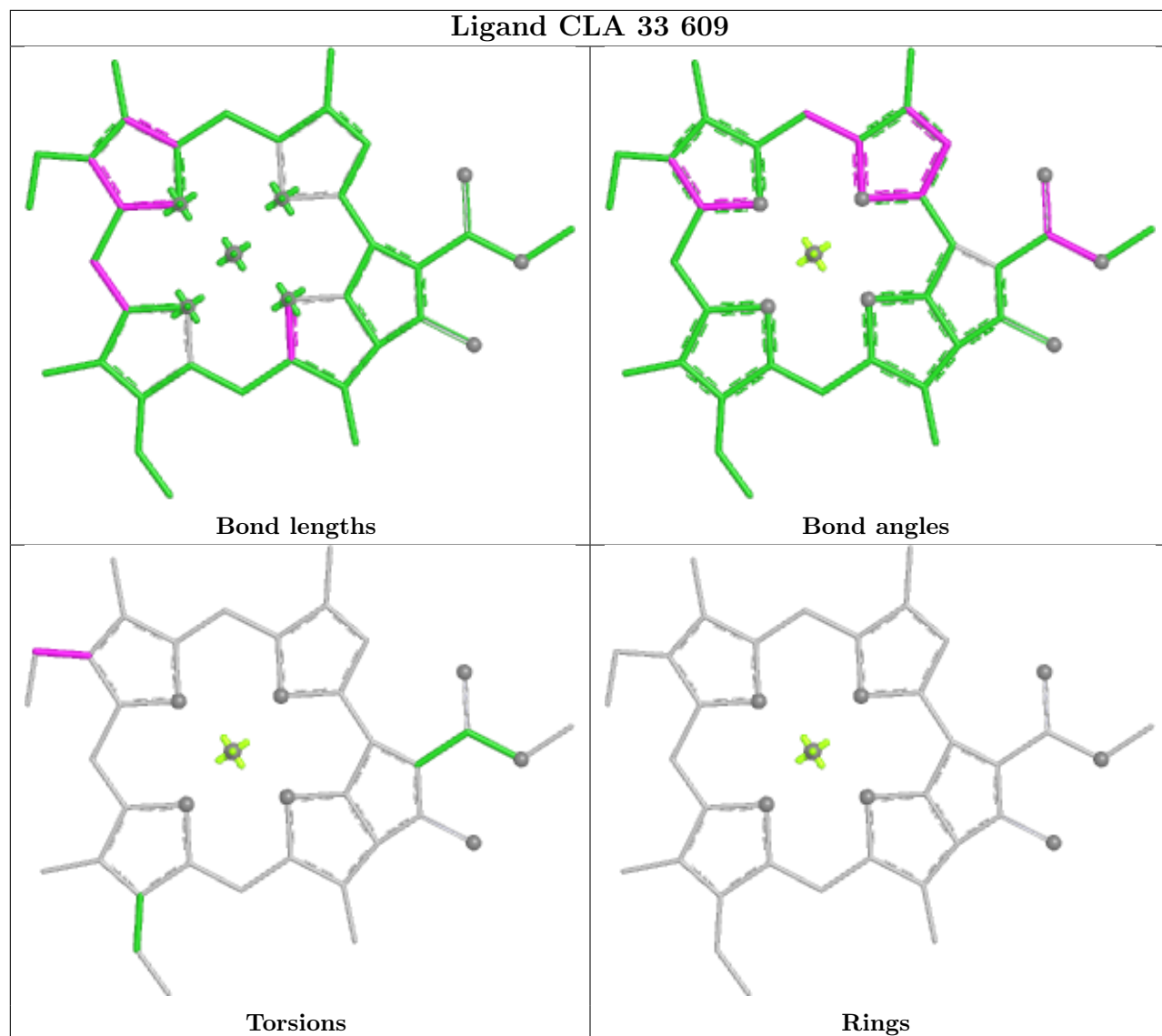


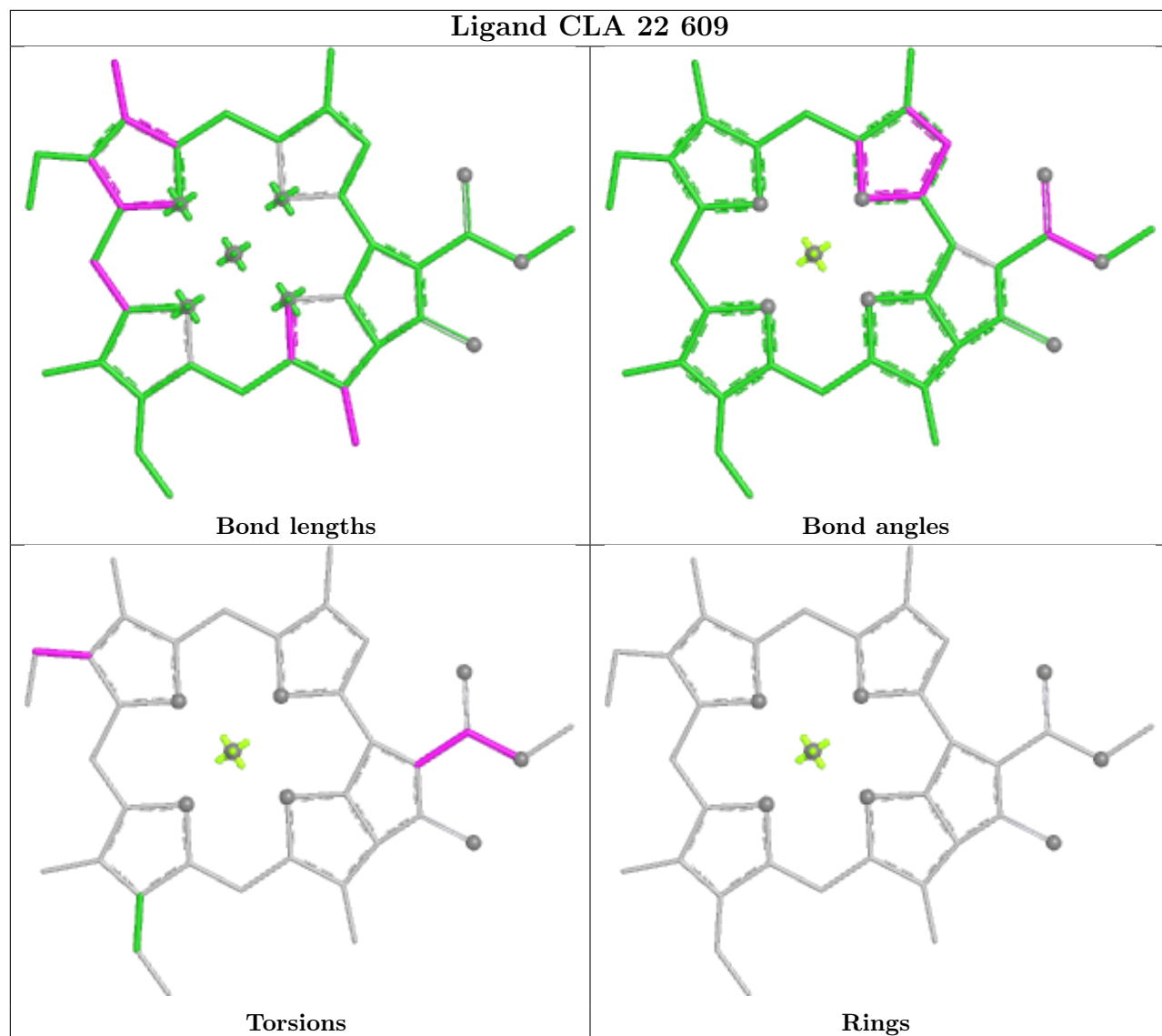
Ligand CHL y 307



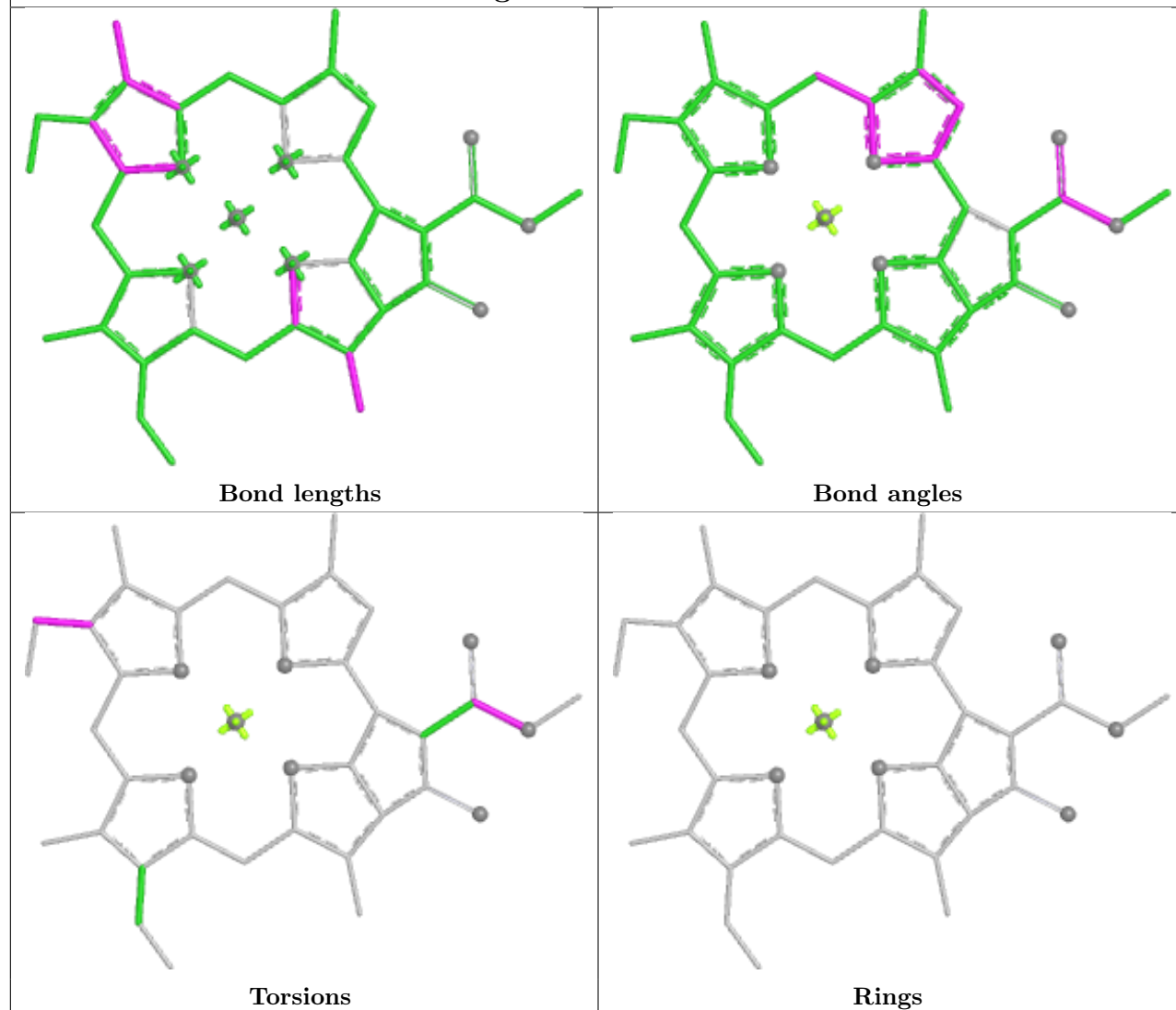
Ligand CLA c 505



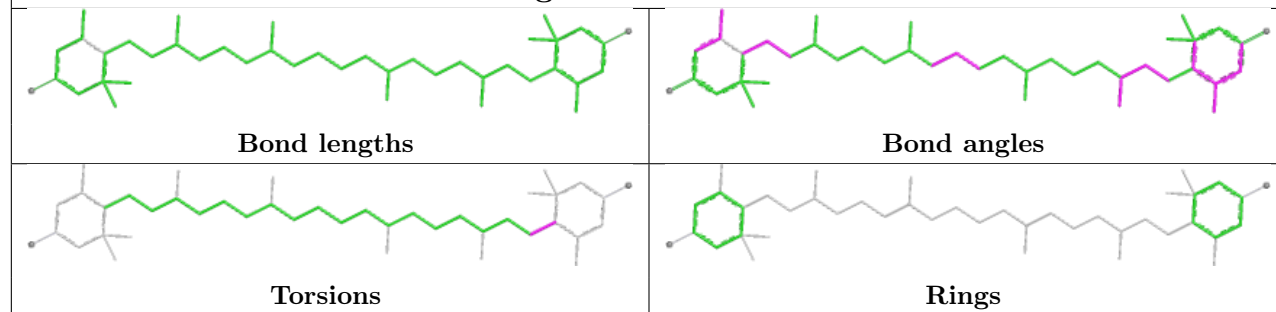




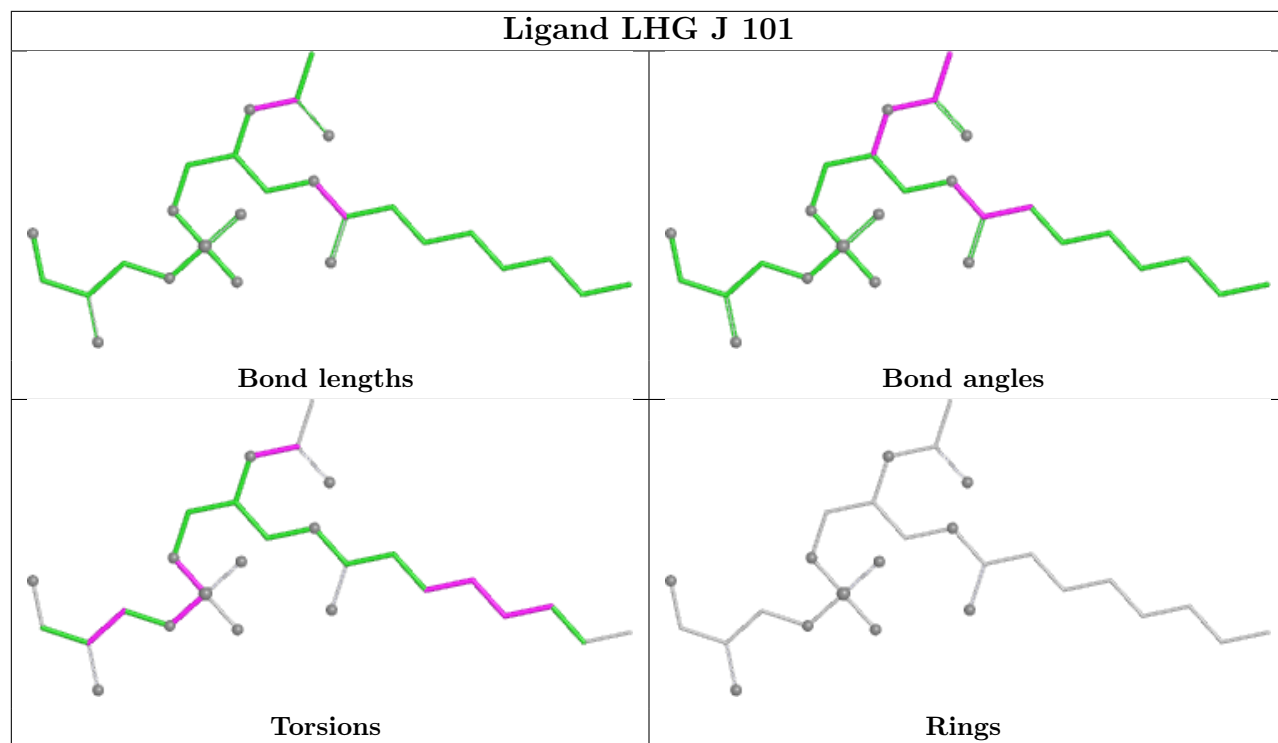
Ligand CLA 2 604

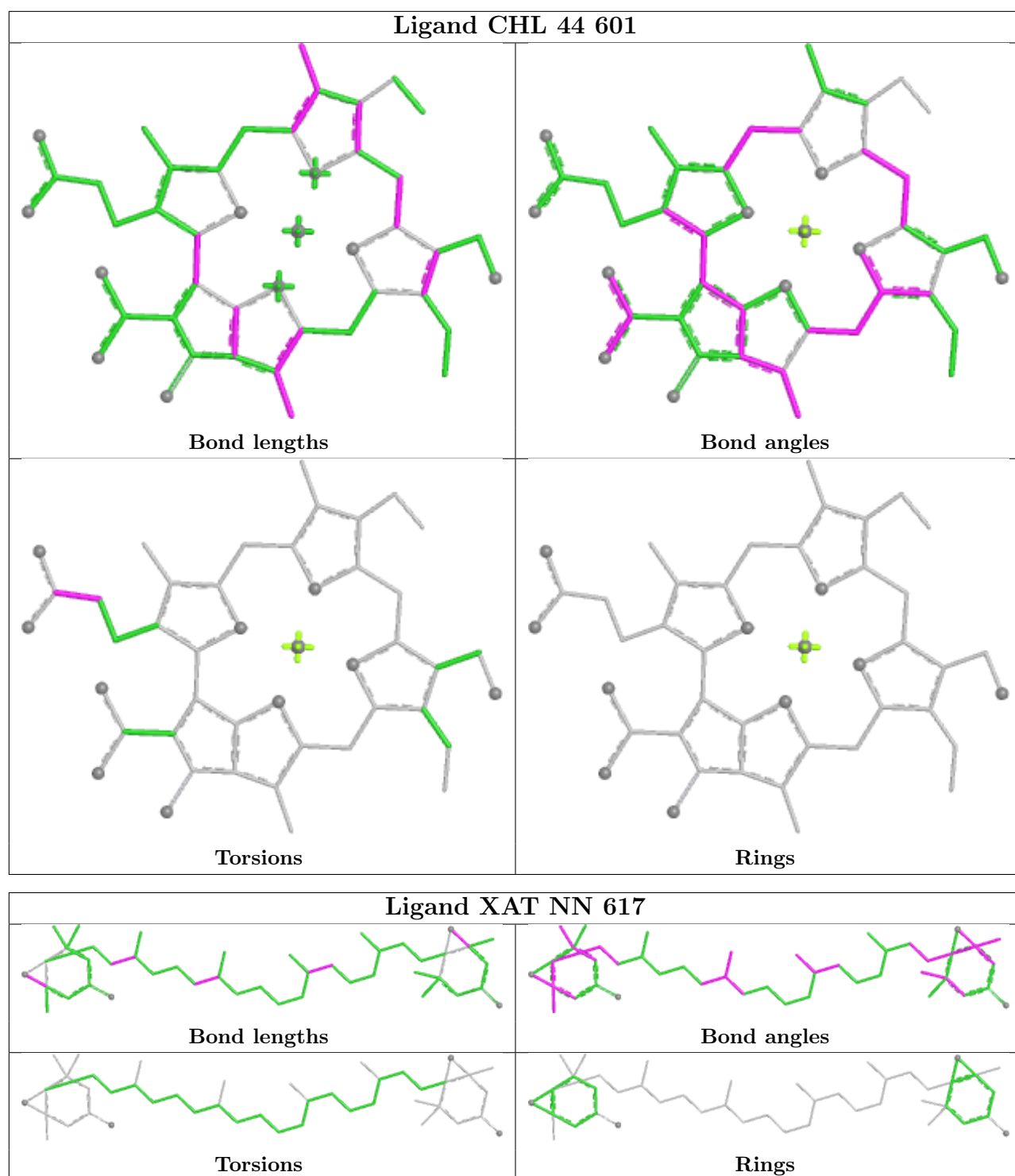


Ligand LUT S 614

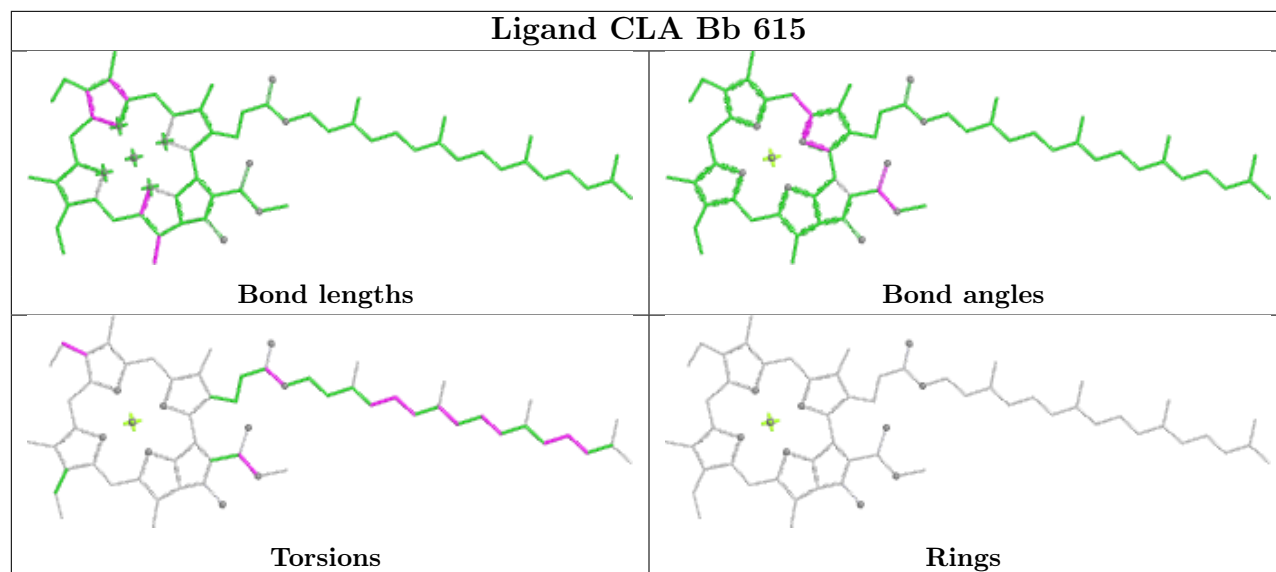


Ligand LHG J 101

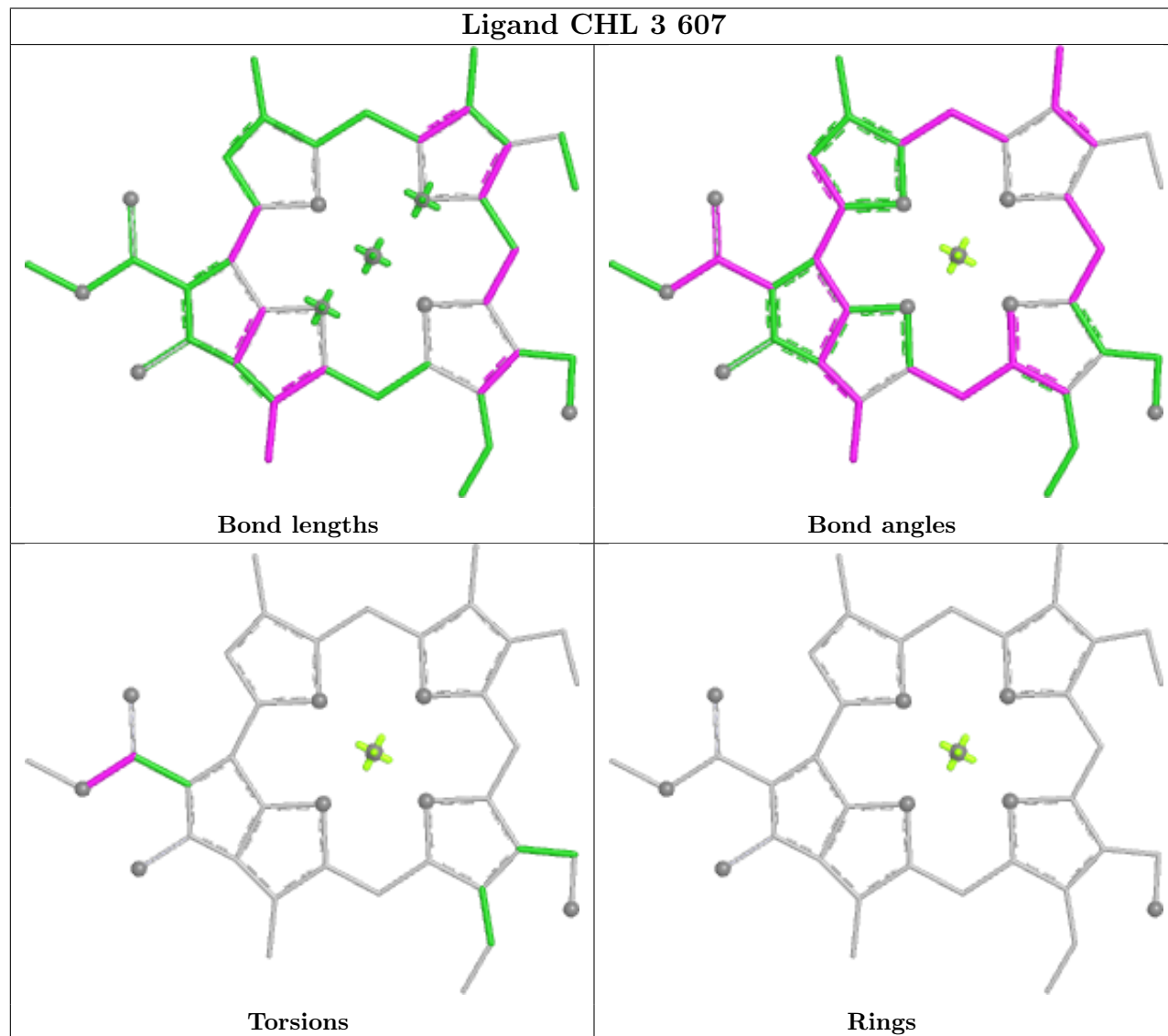


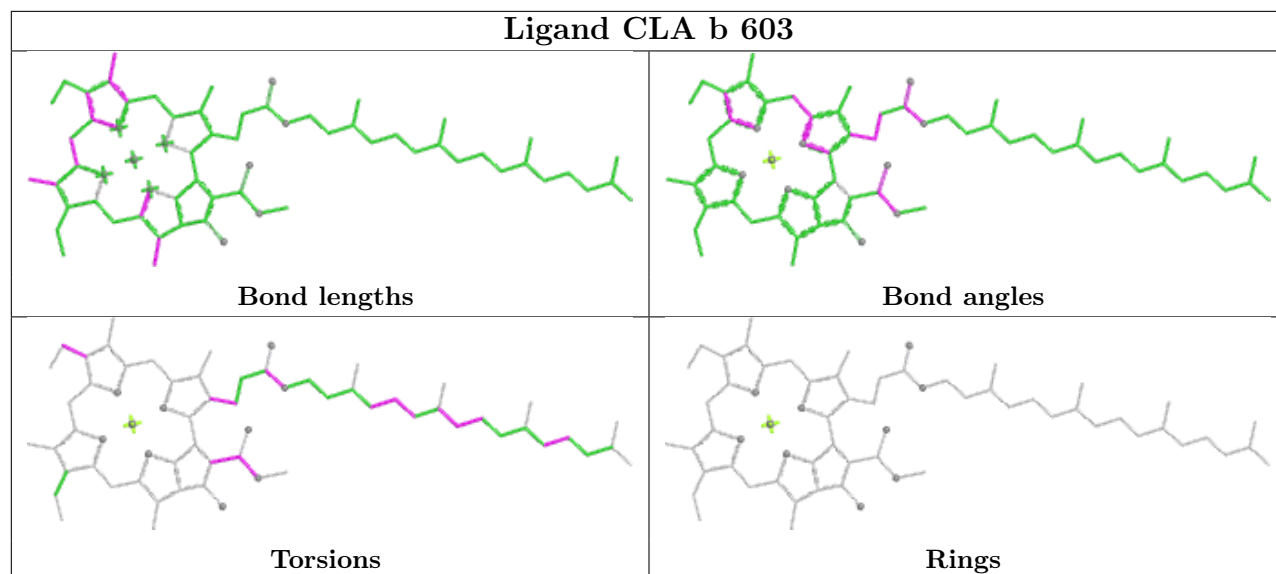
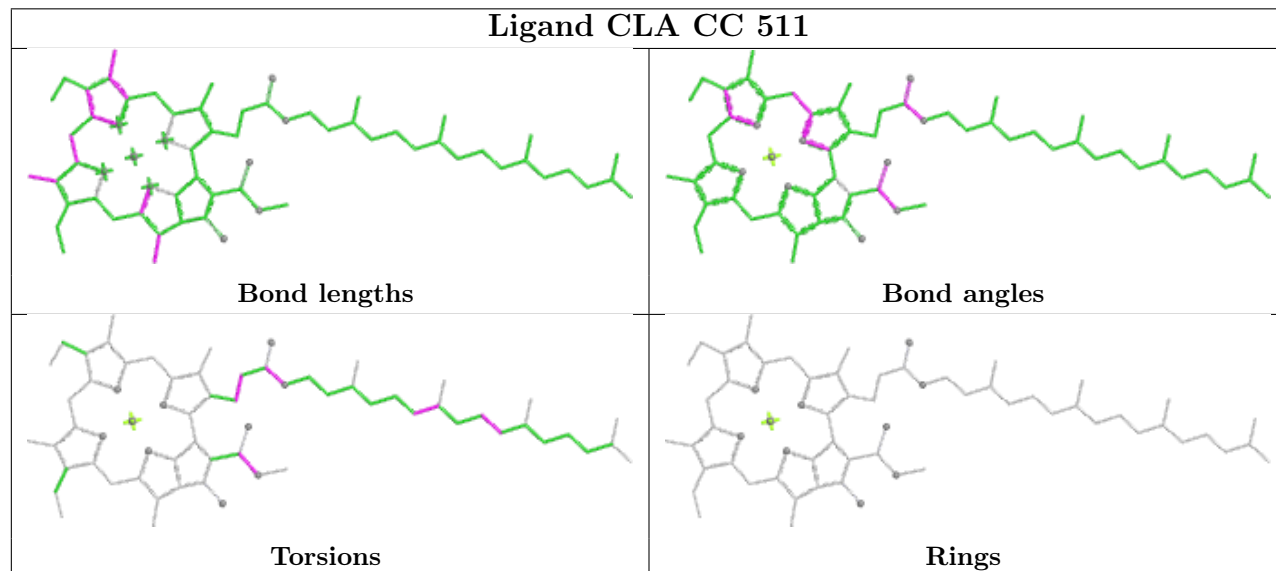


Ligand CLA Bb 615

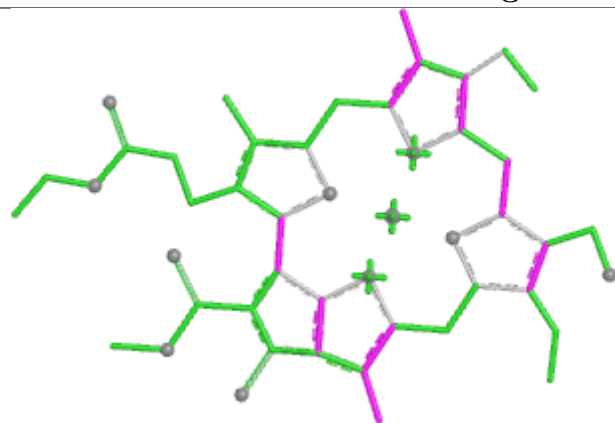


Ligand CHL 3 607

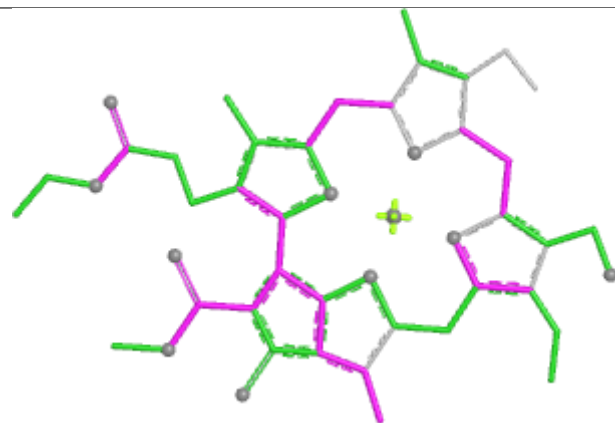


Ligand CLA b 603**Ligand CLA CC 511**

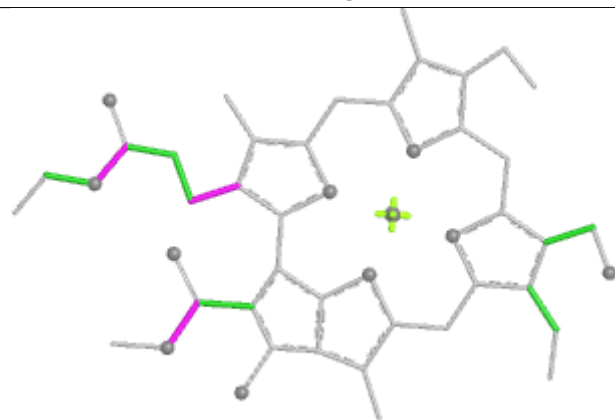
Ligand CHL YY 605



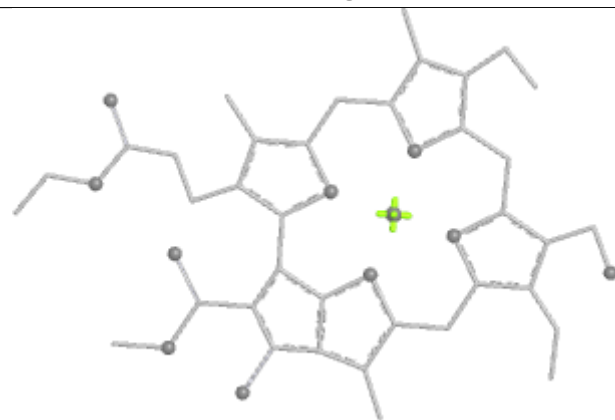
Bond lengths



Bond angles

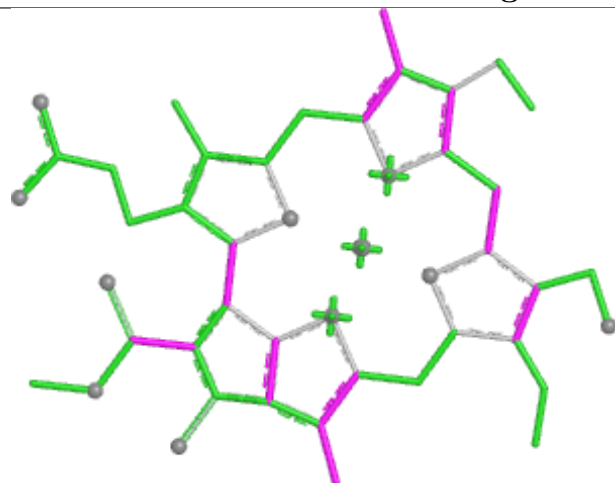


Torsions

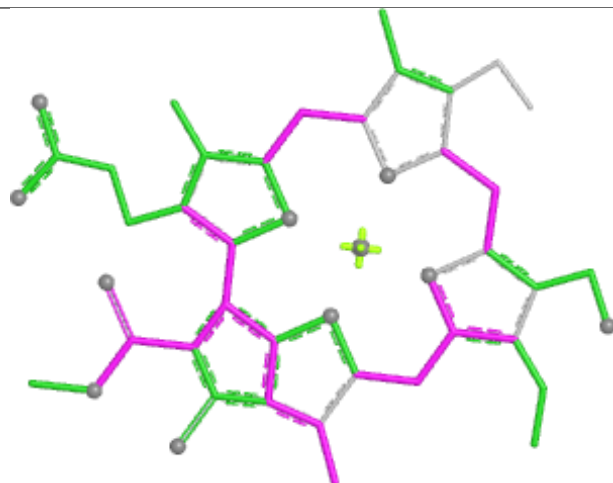


Rings

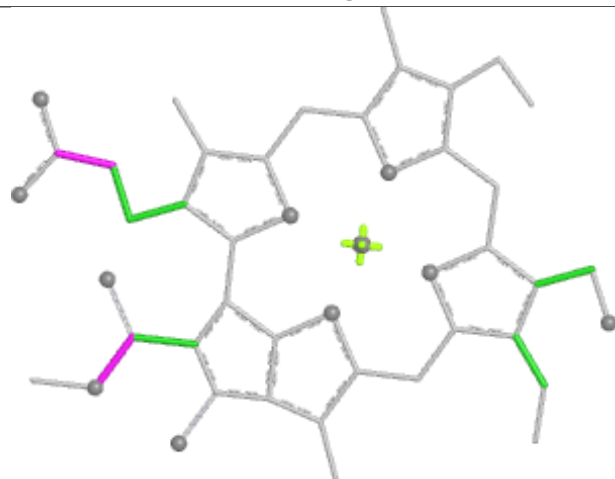
Ligand CHL GG 607



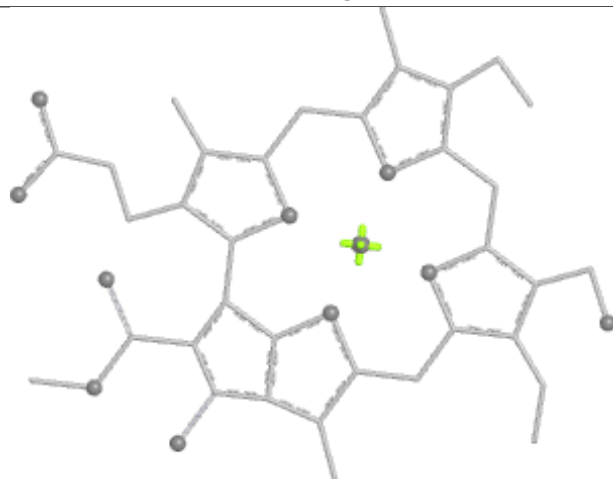
Bond lengths



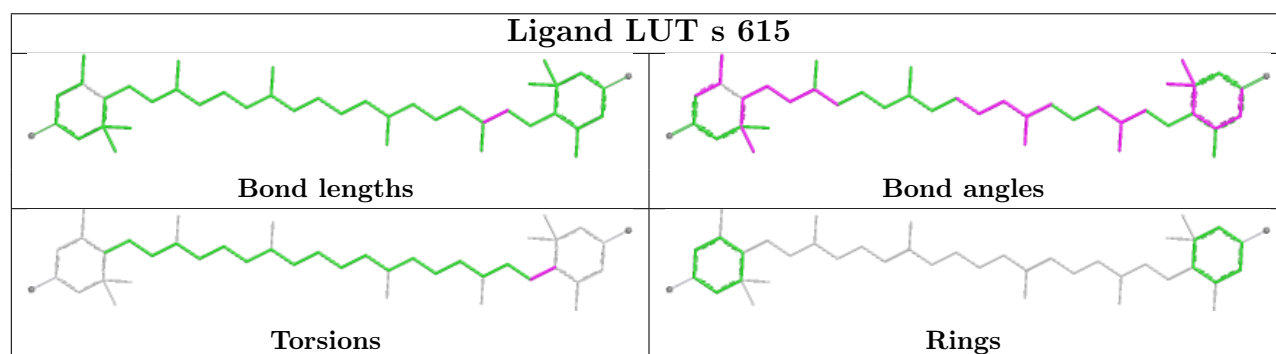
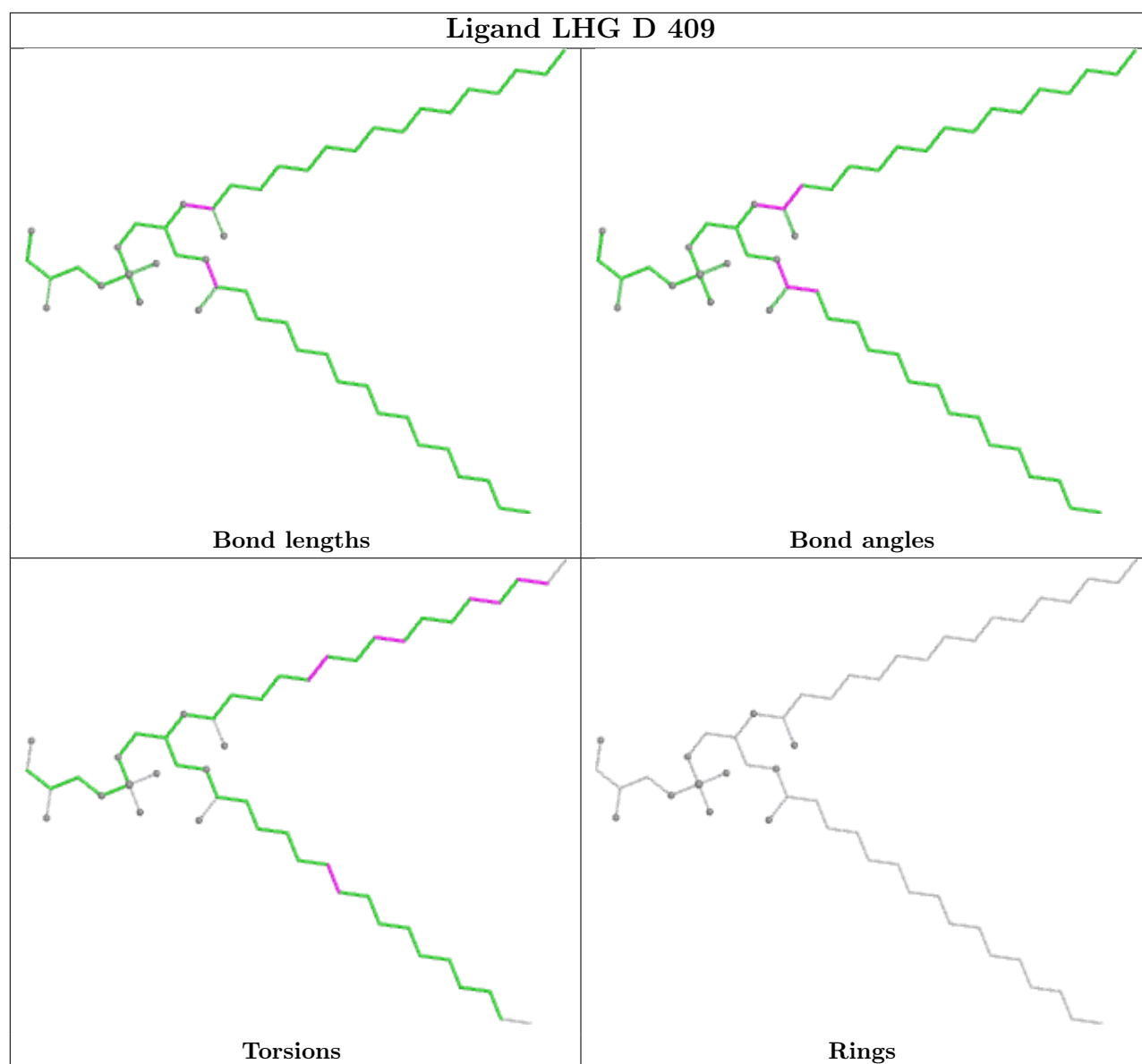
Bond angles

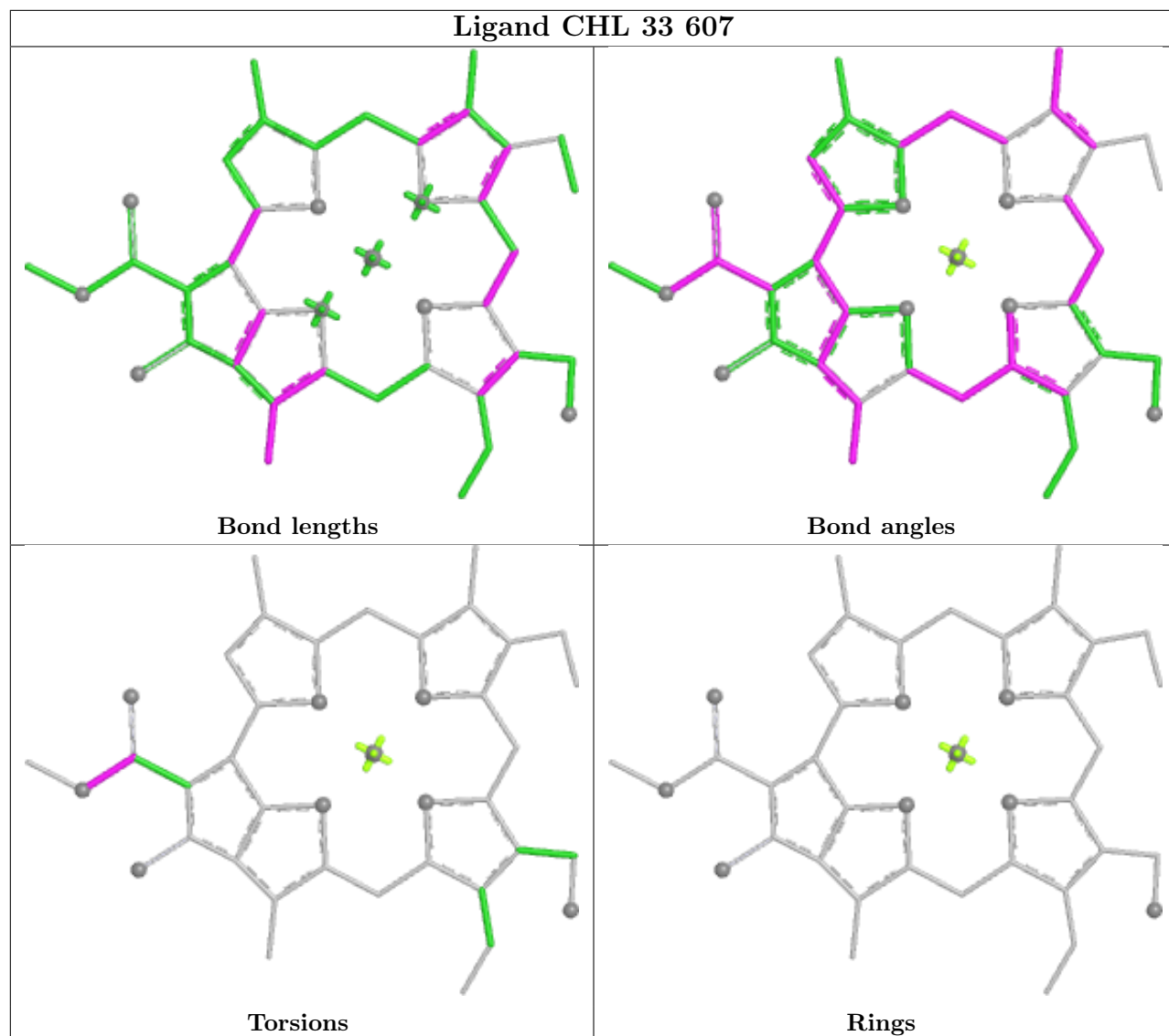


Torsions

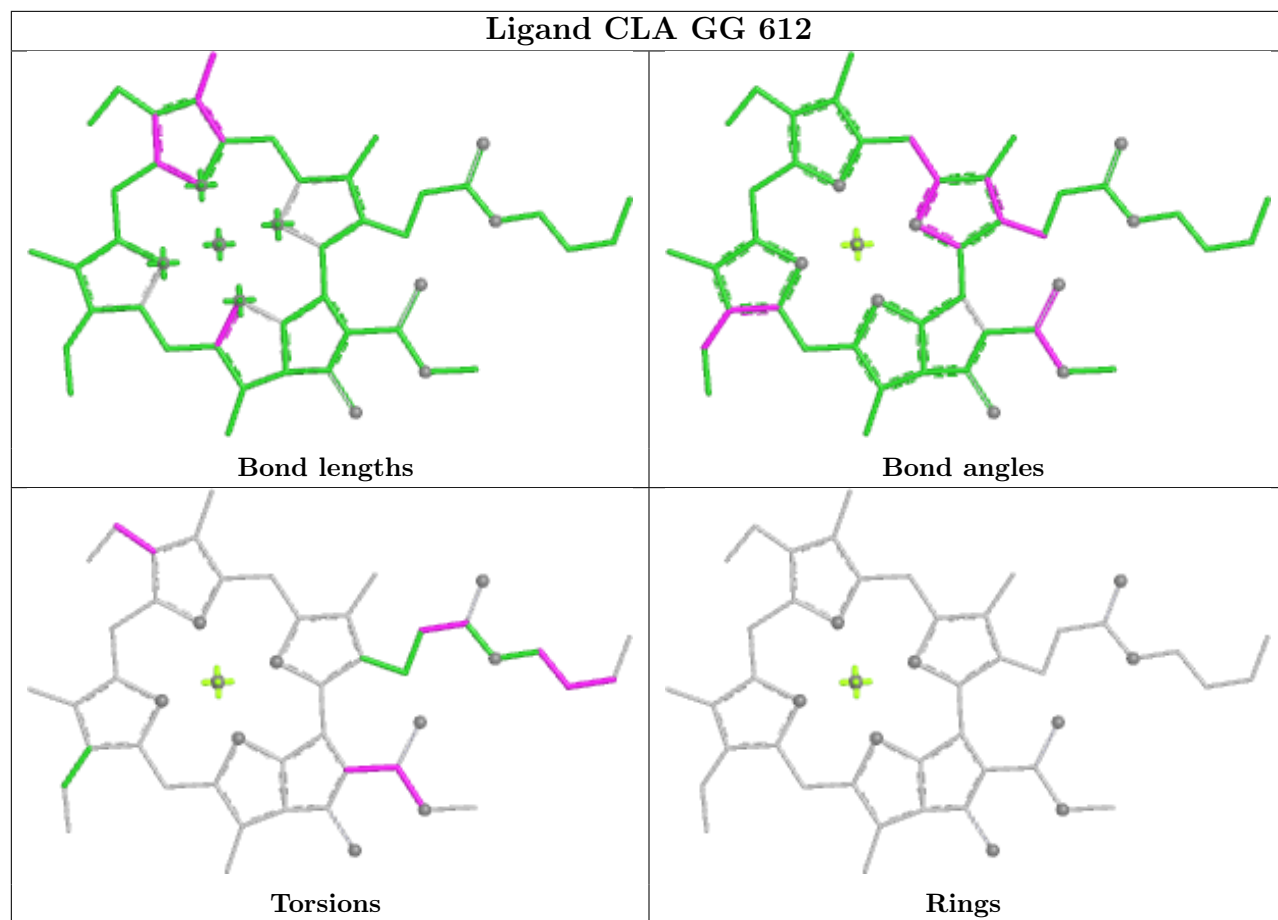


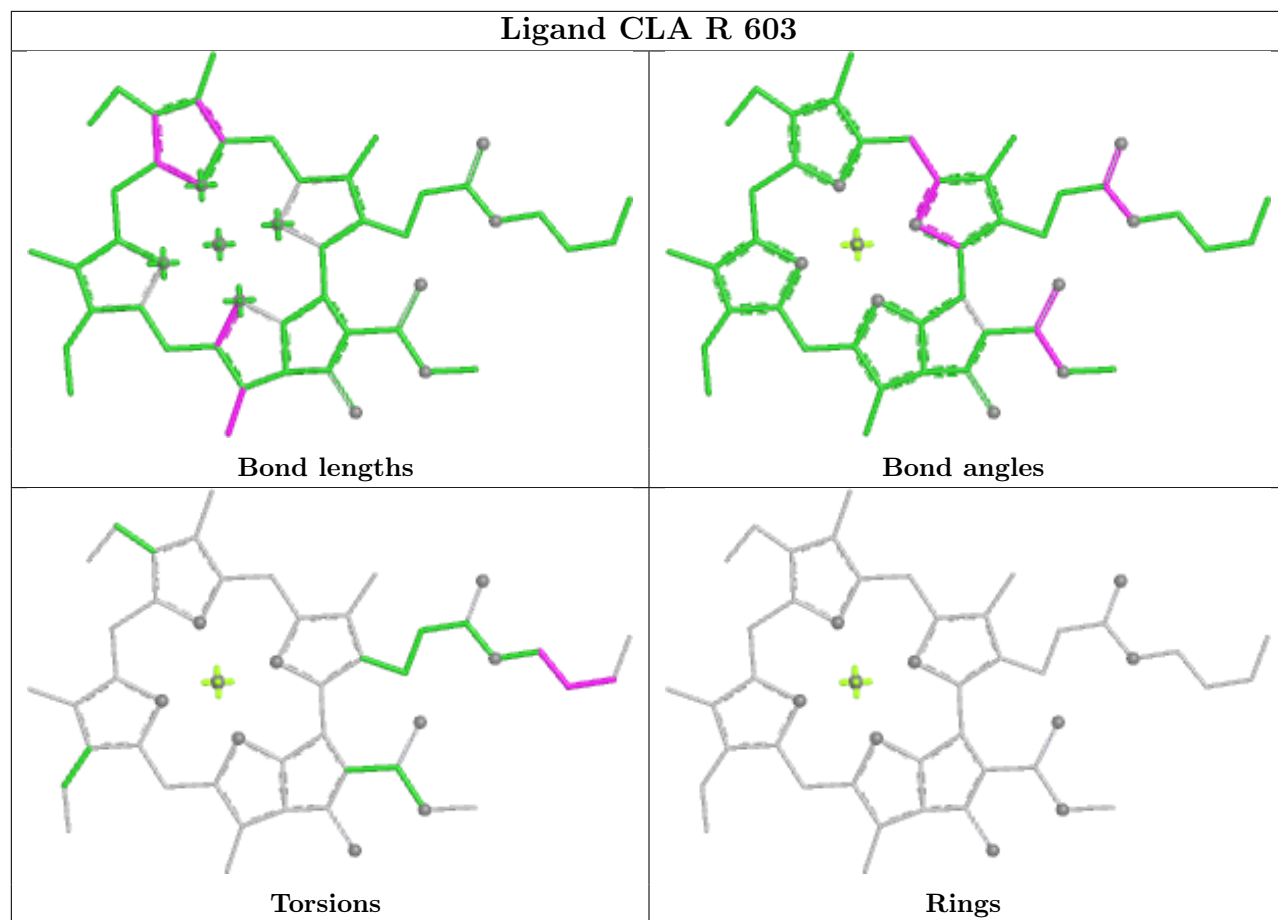
Rings



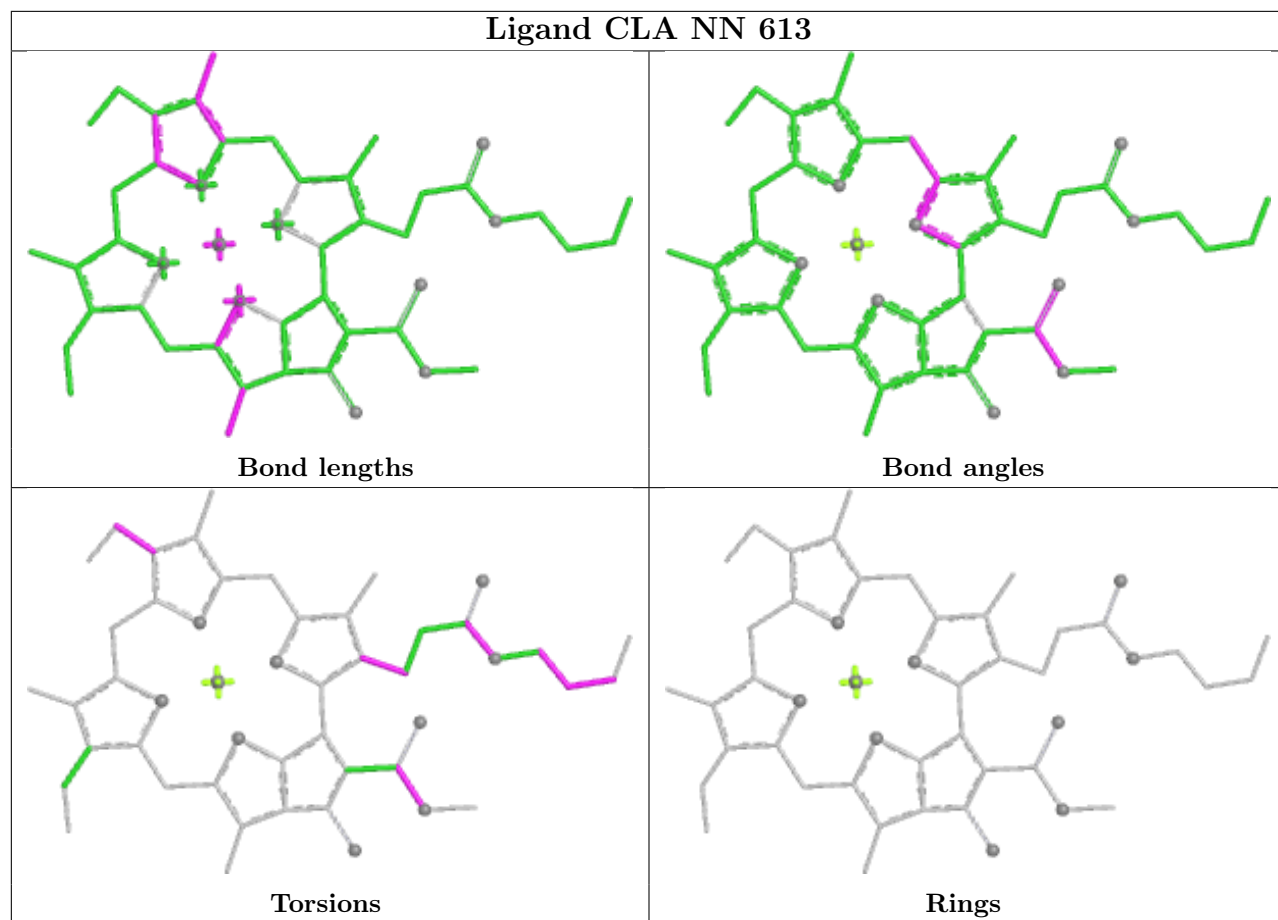


Ligand CLA GG 612

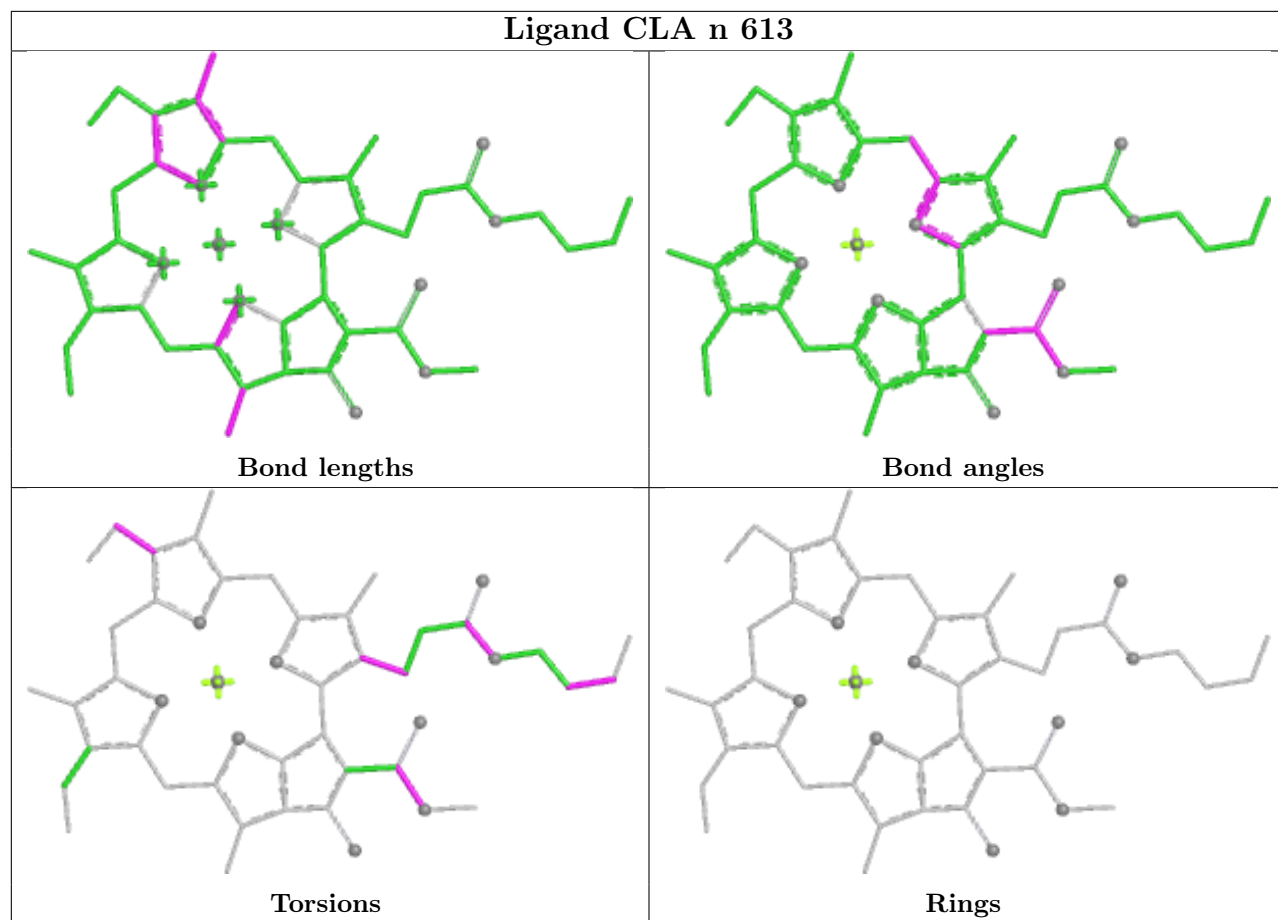


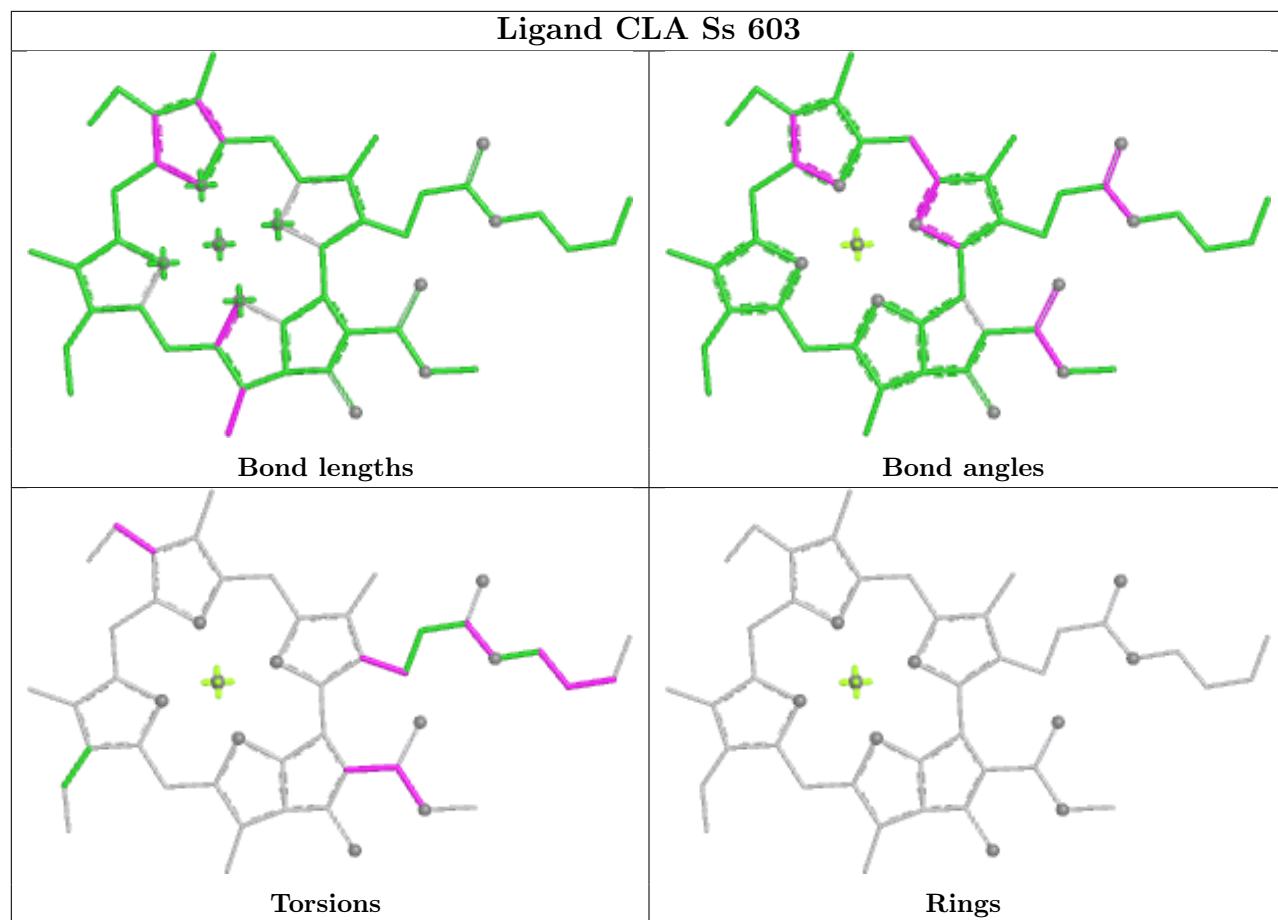


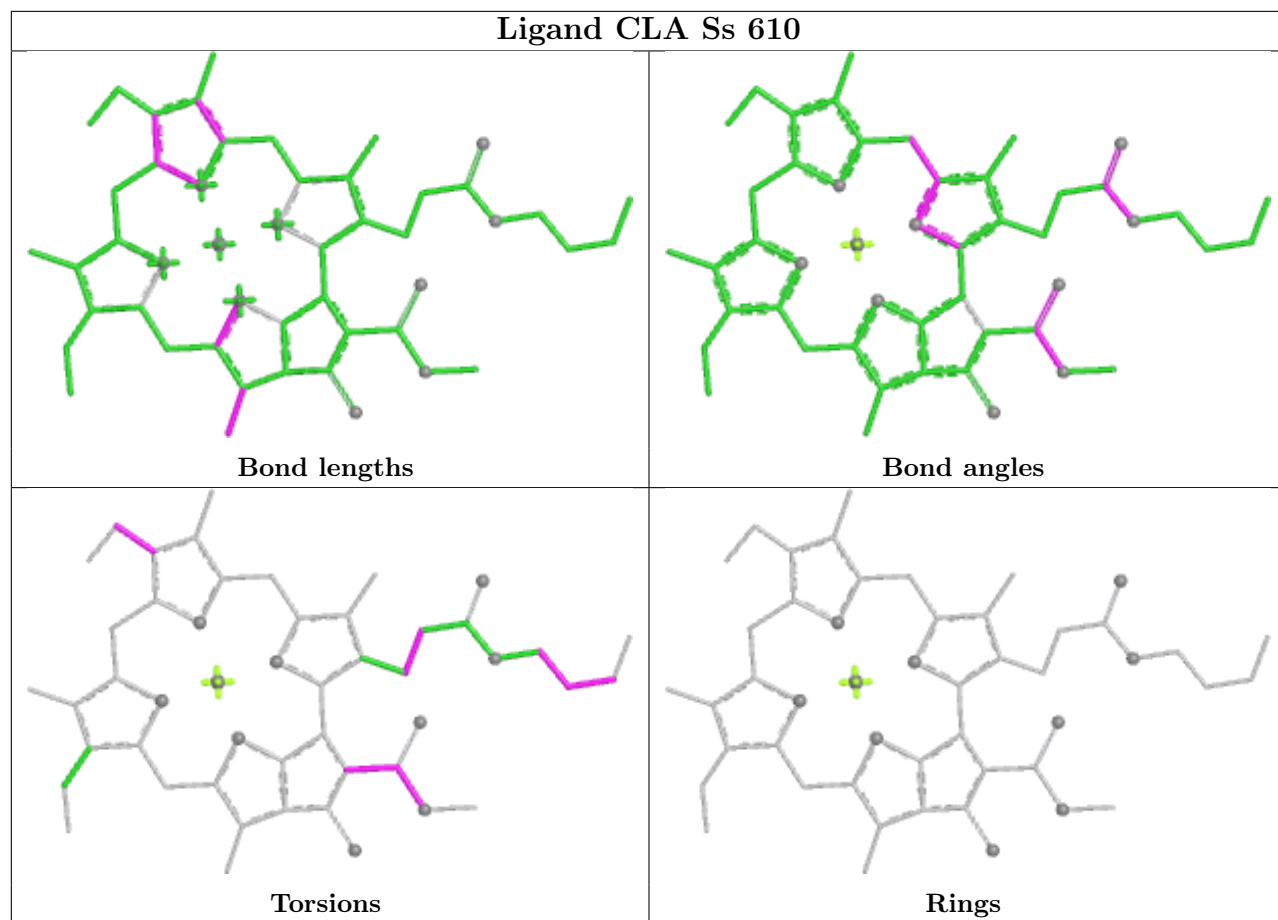
Ligand CLA NN 613



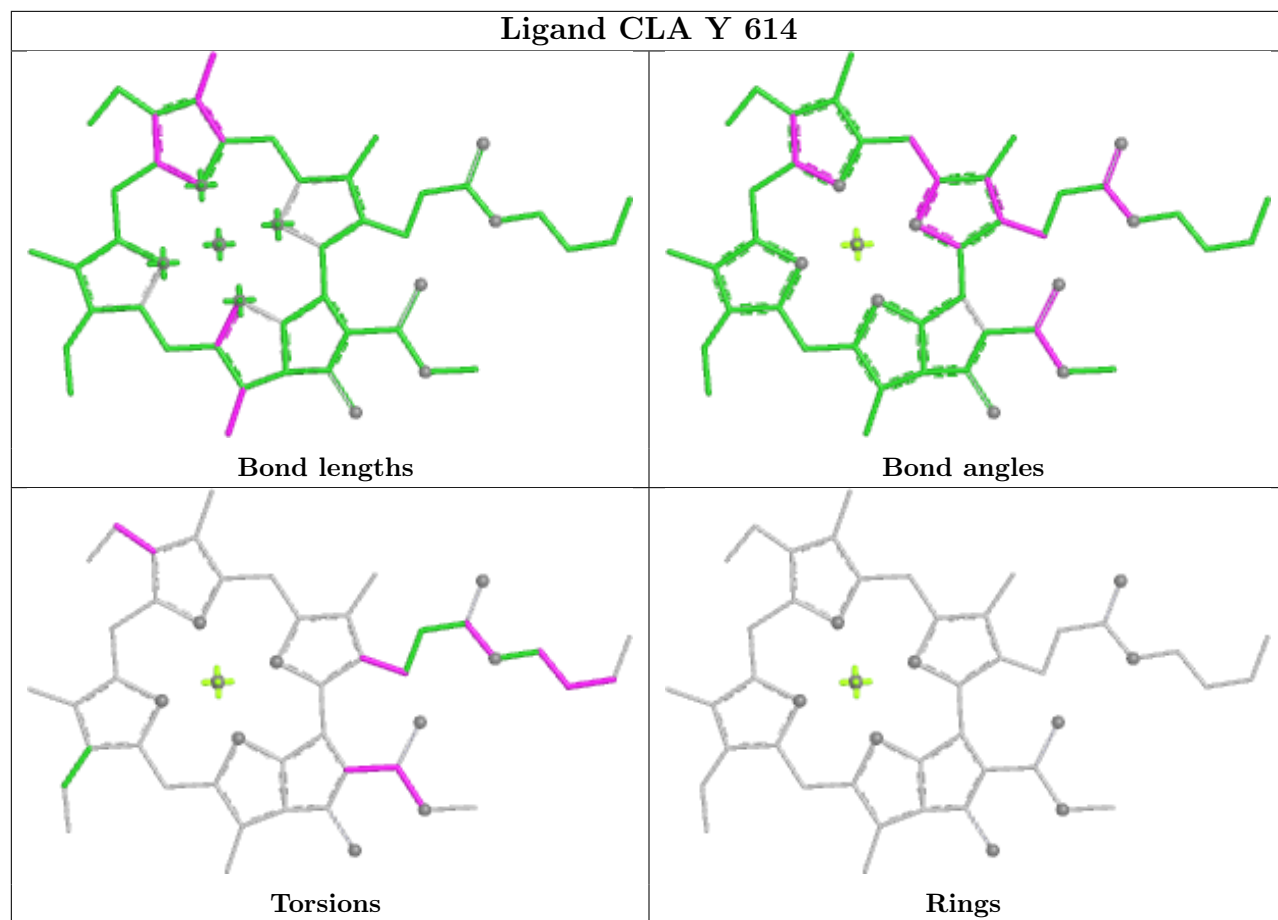
Ligand CLA n 613



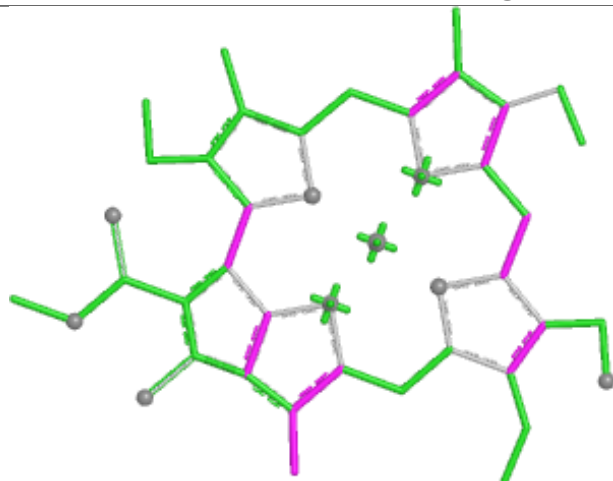




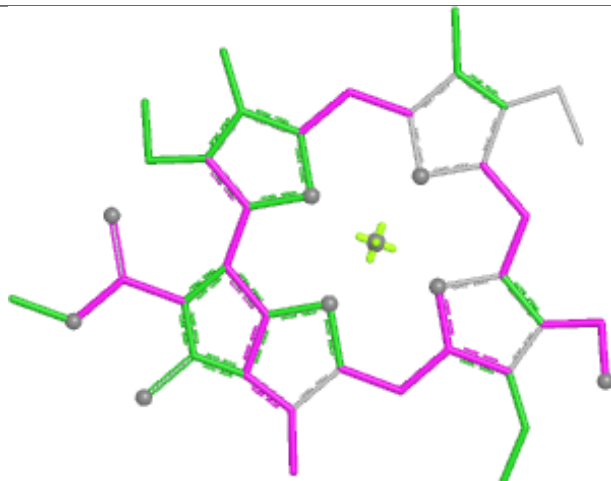
Ligand CLA Y 614



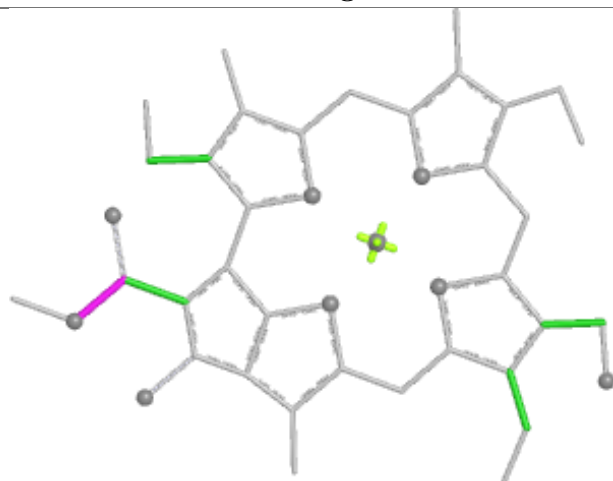
Ligand CHL GG 605



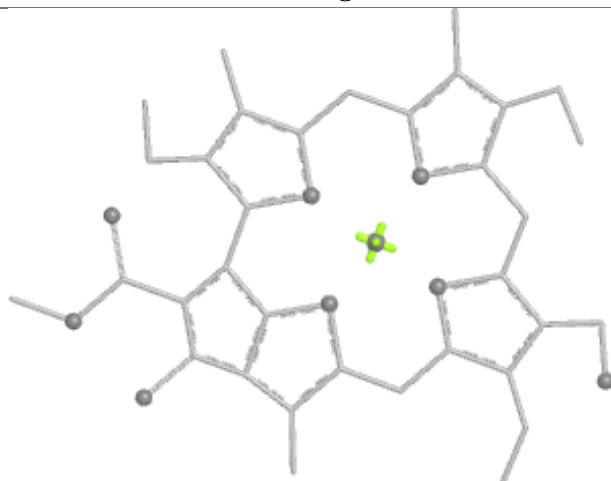
Bond lengths



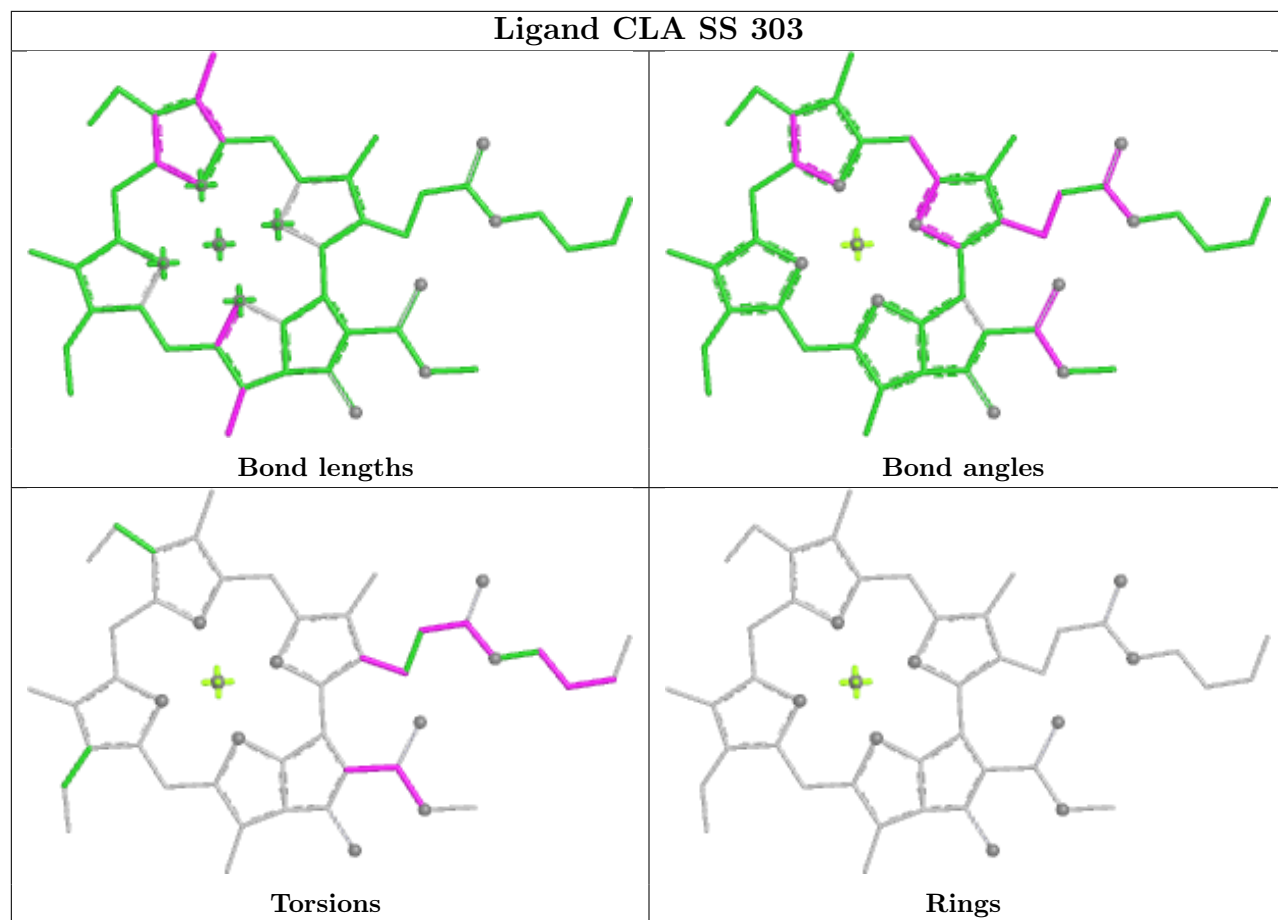
Bond angles



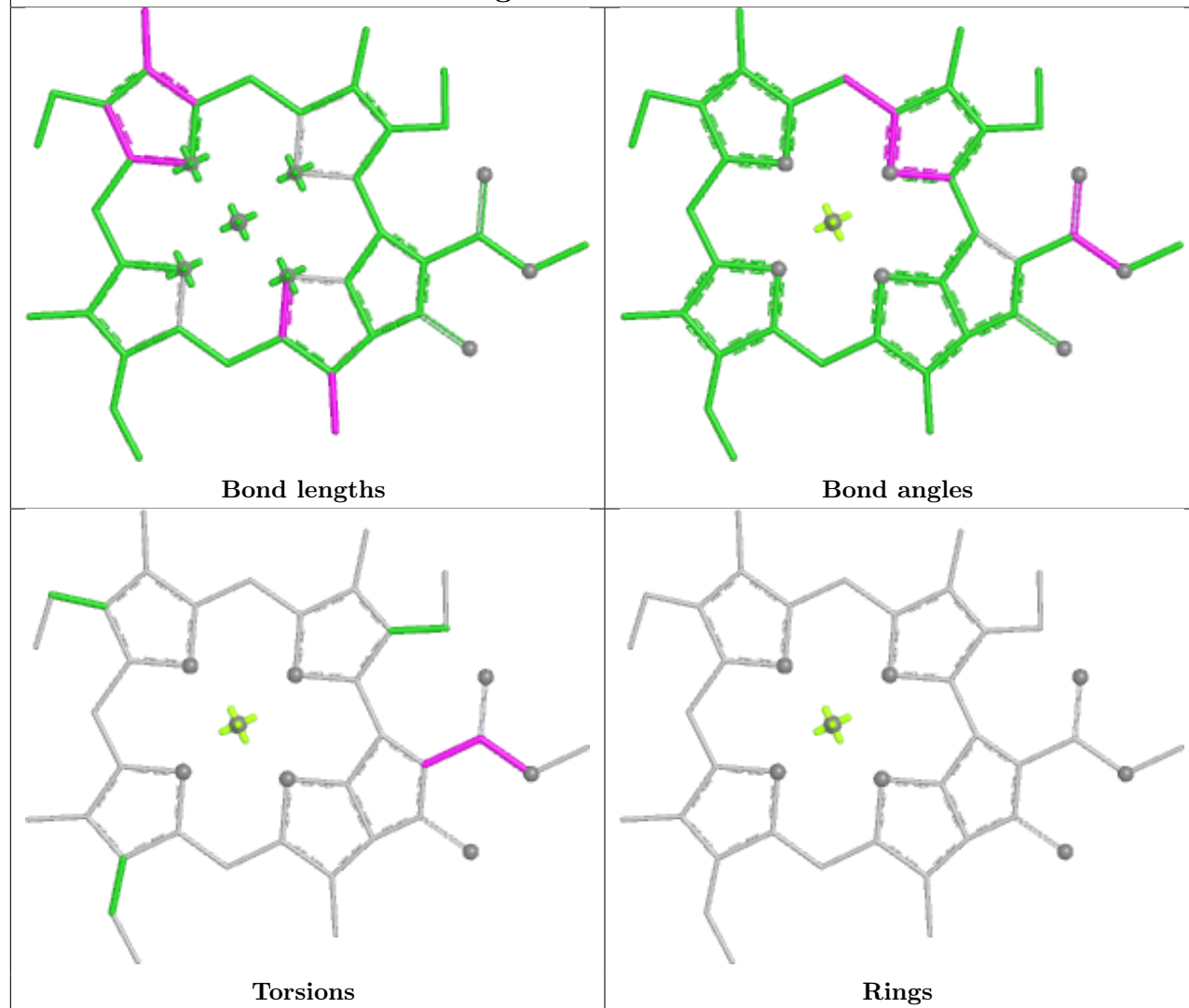
Torsions



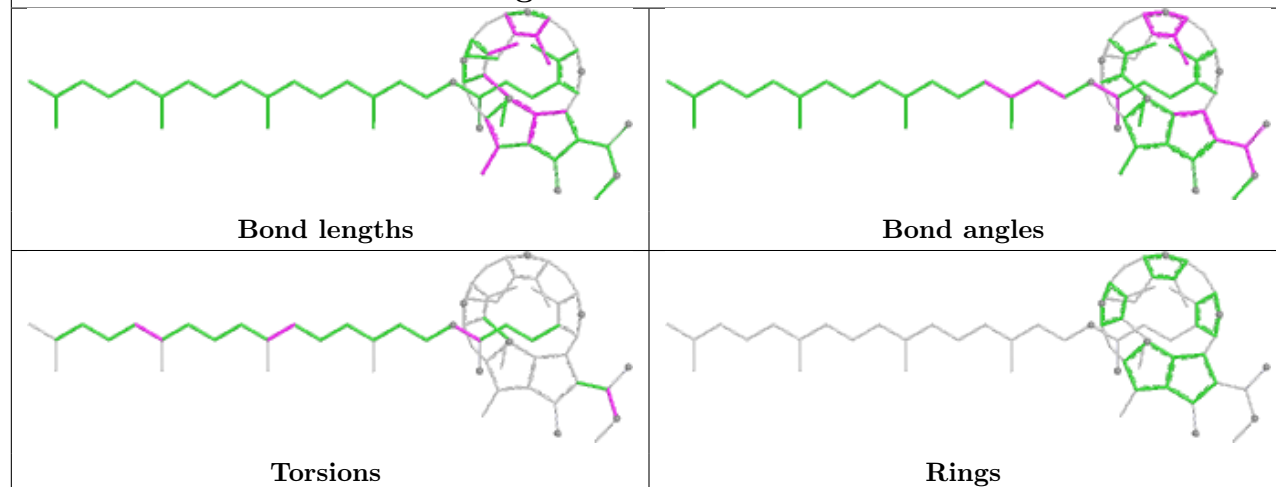
Rings



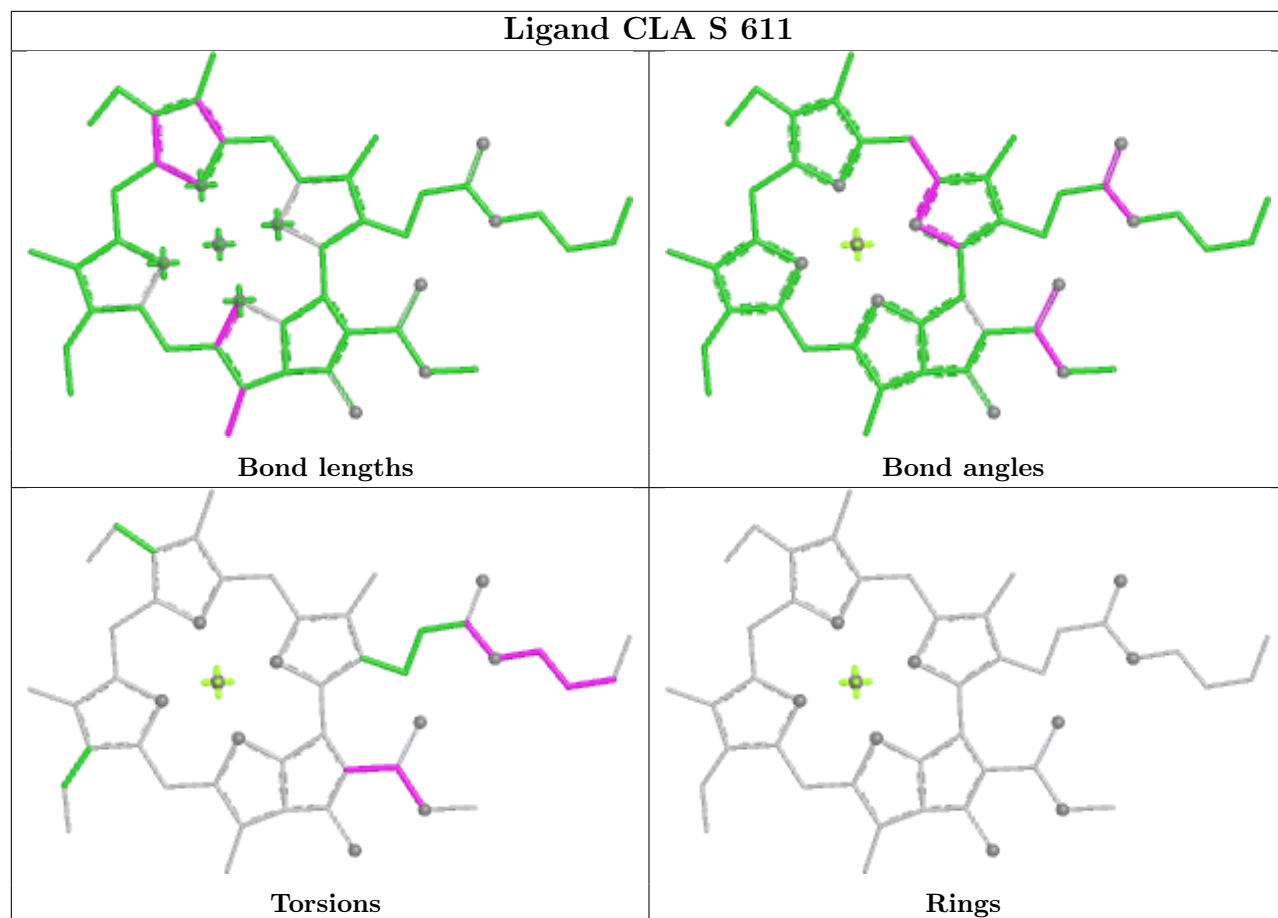
Ligand CLA N 603



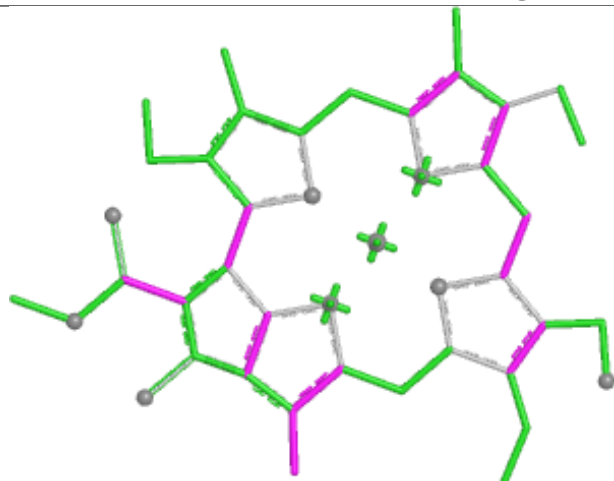
Ligand PHO AA 407



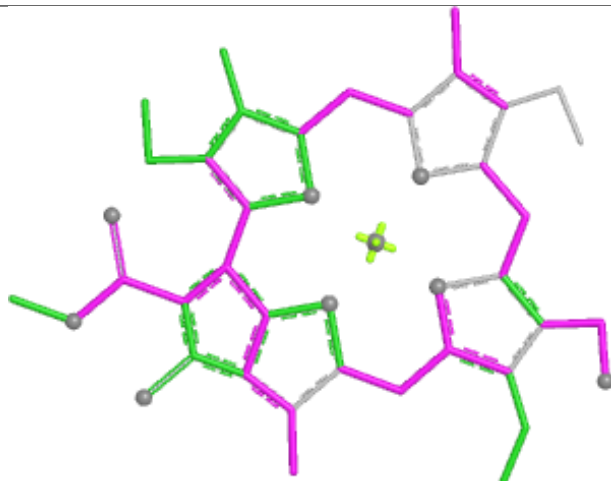
Ligand CLA S 611



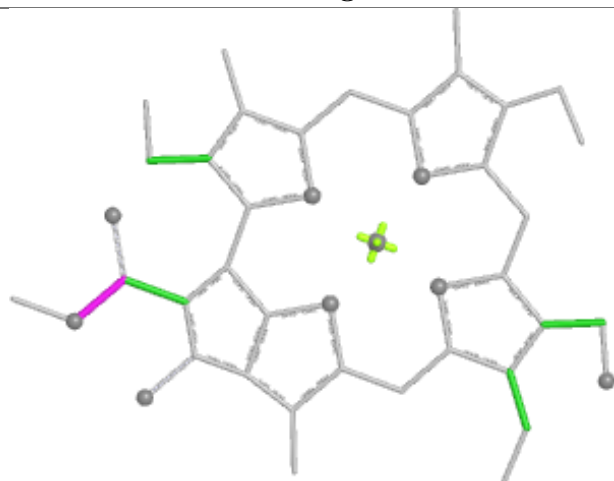
Ligand CHL Y 607



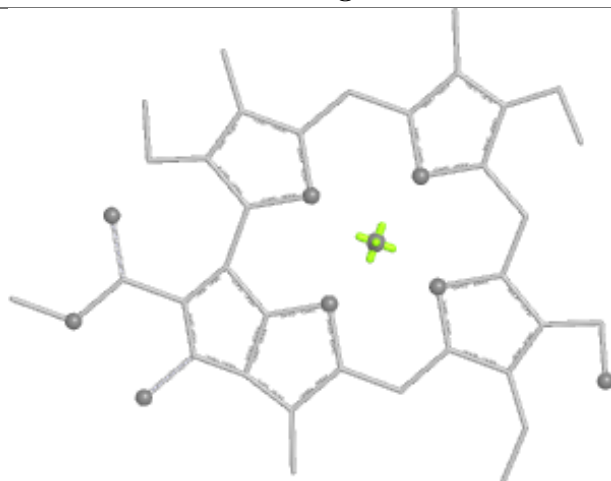
Bond lengths



Bond angles

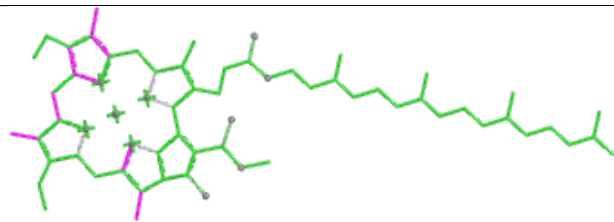


Torsions

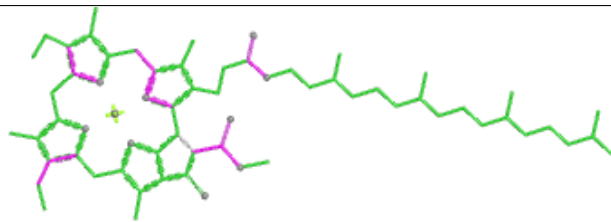


Rings

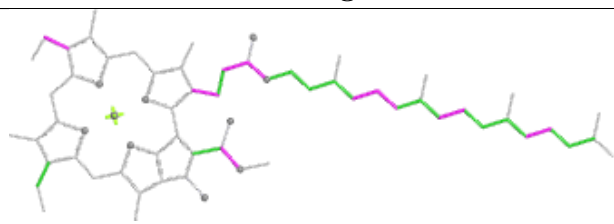
Ligand CLA NN 602



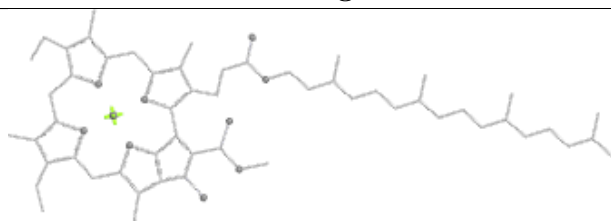
Bond lengths



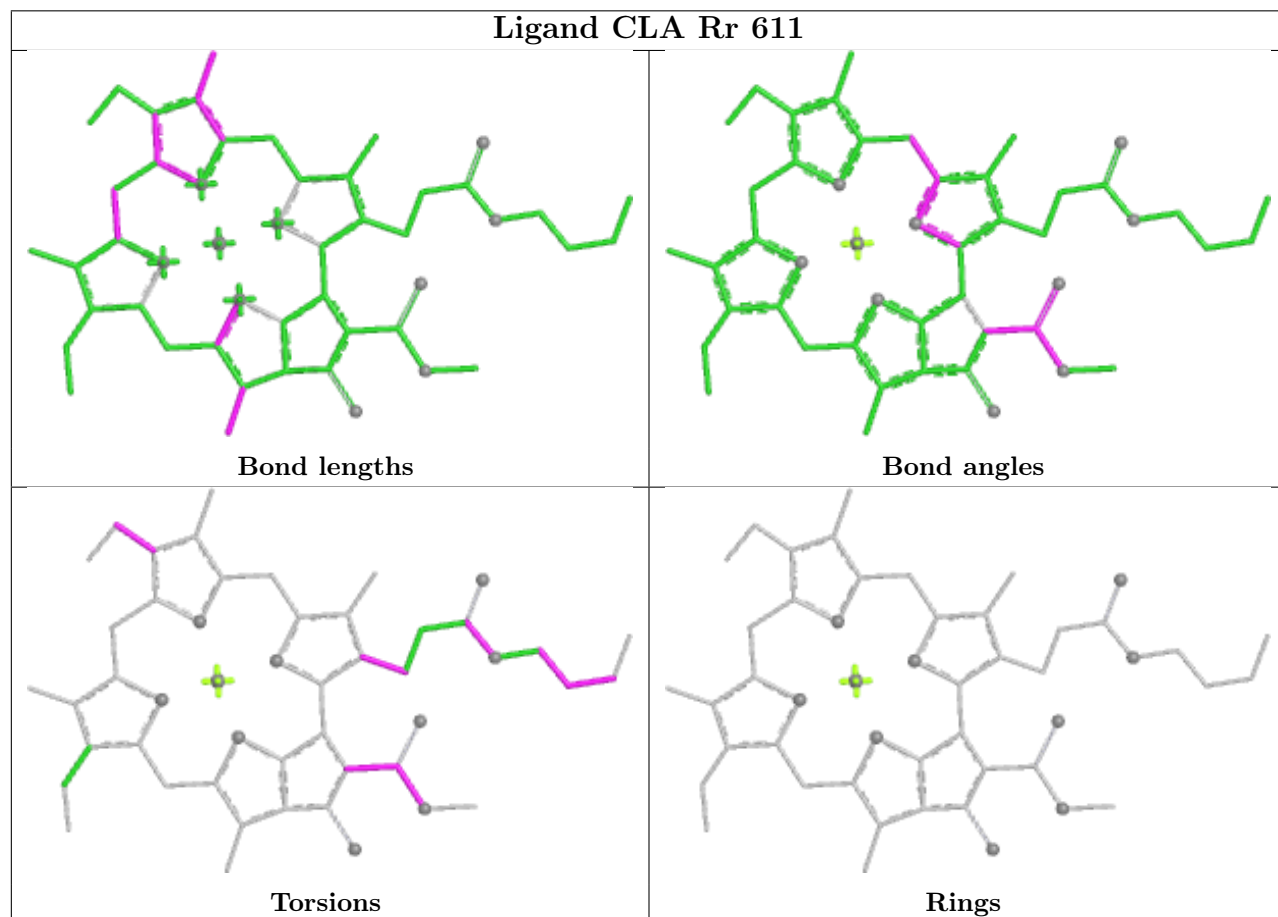
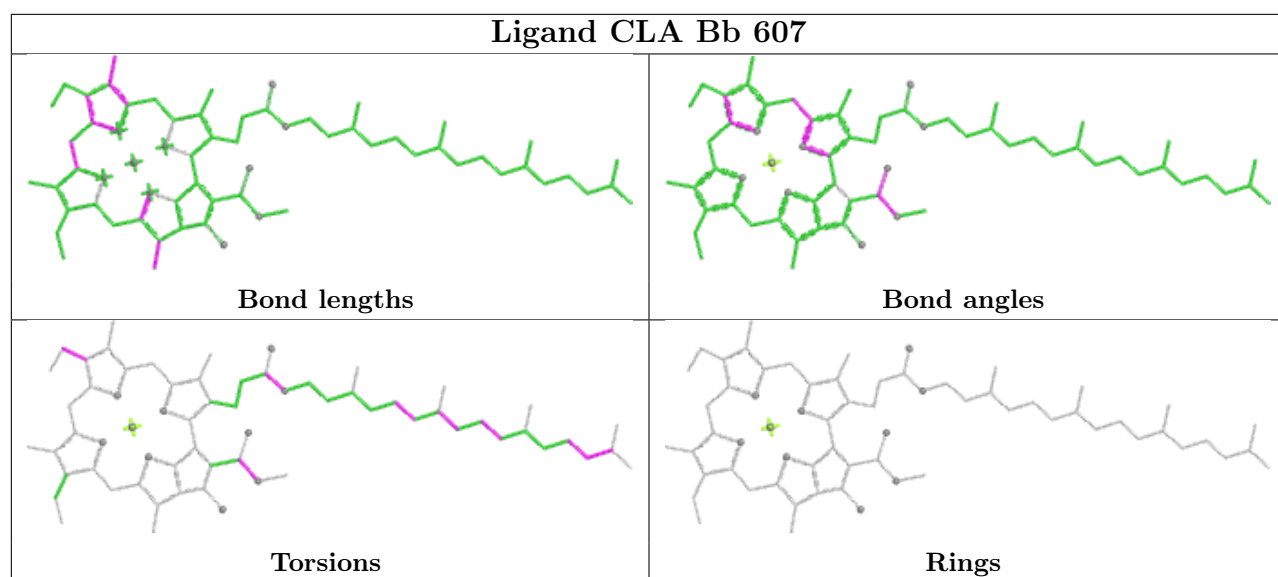
Bond angles

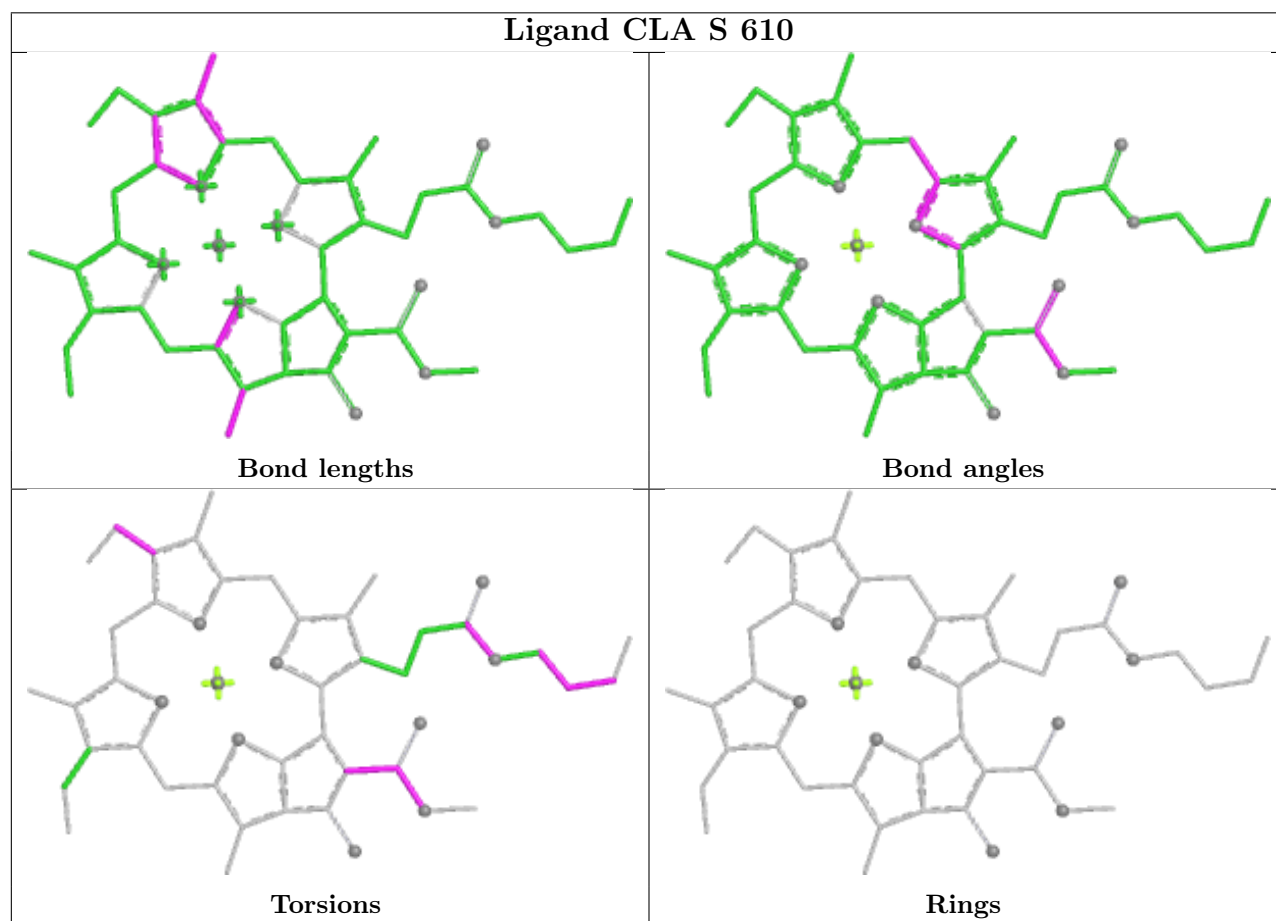
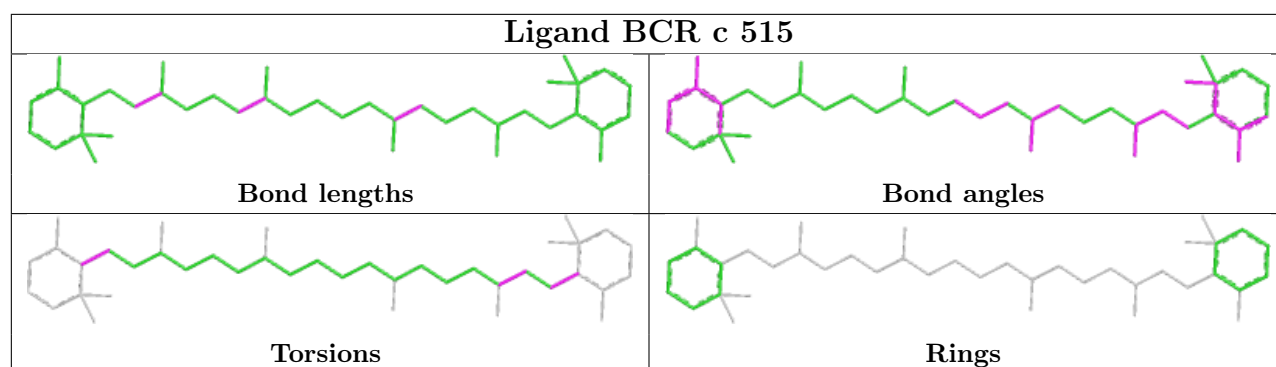


Torsions

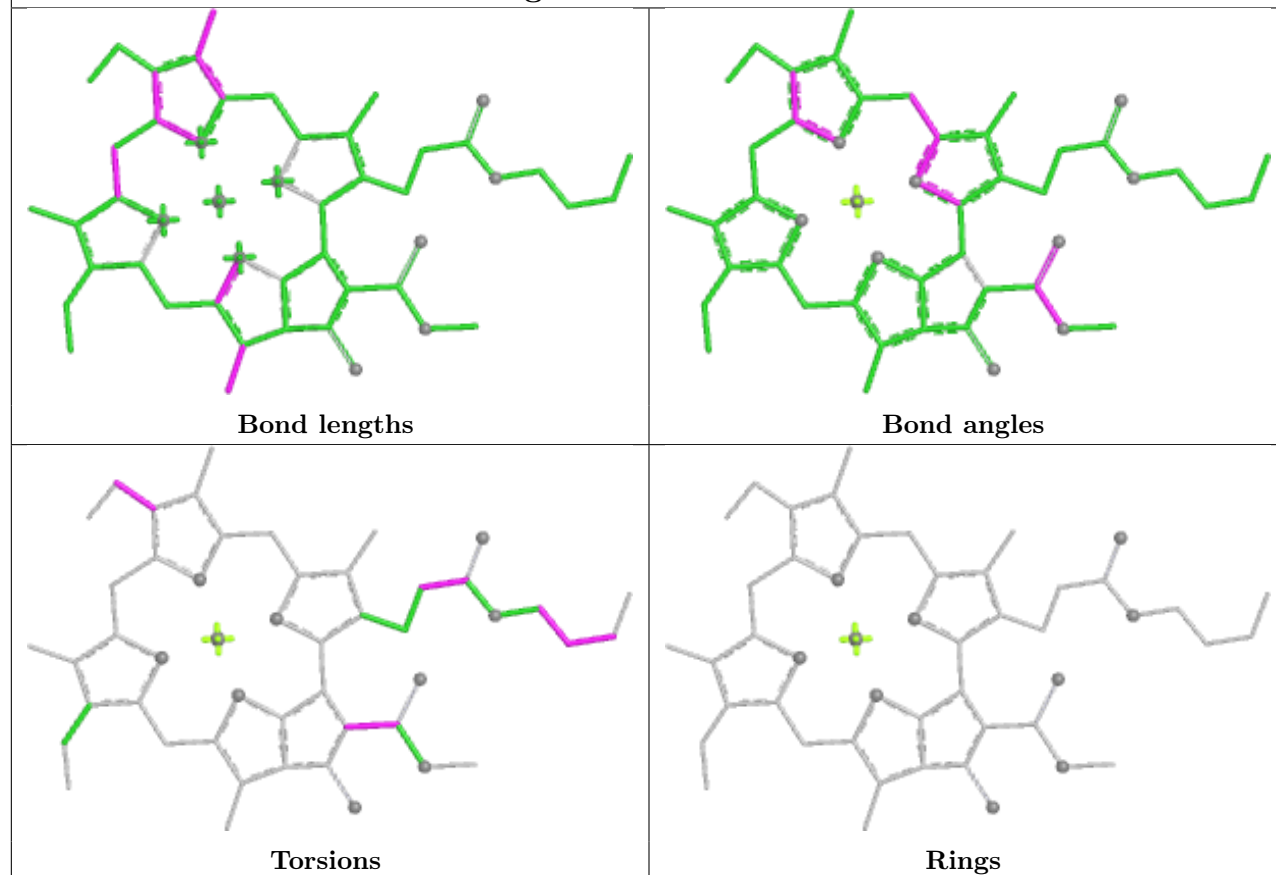


Rings

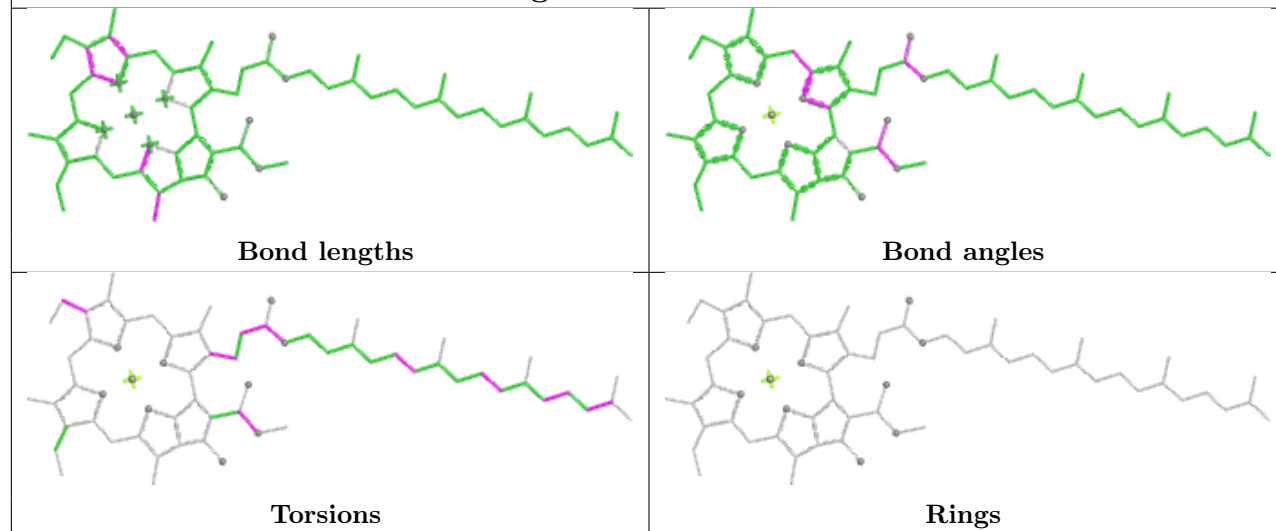


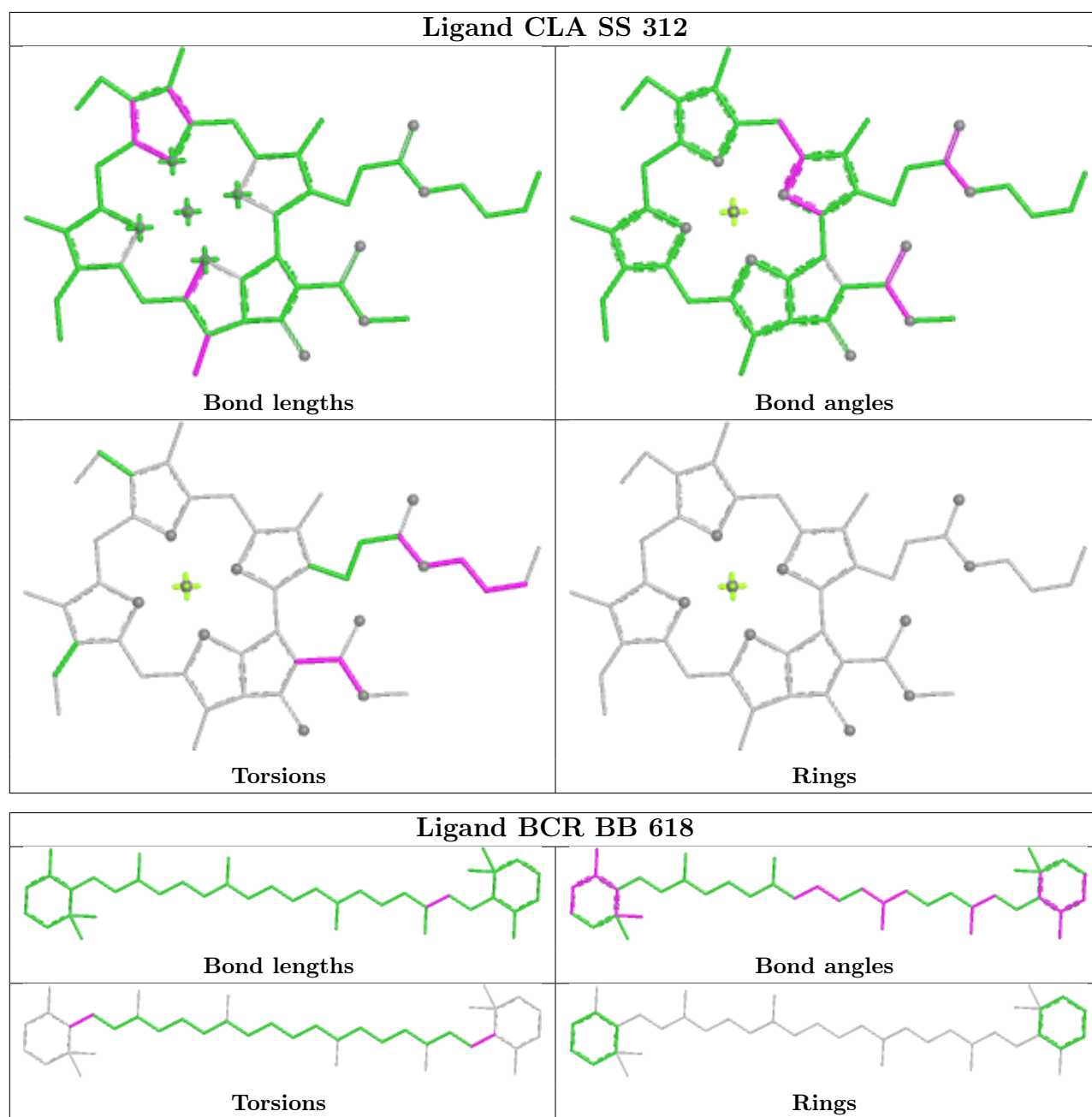


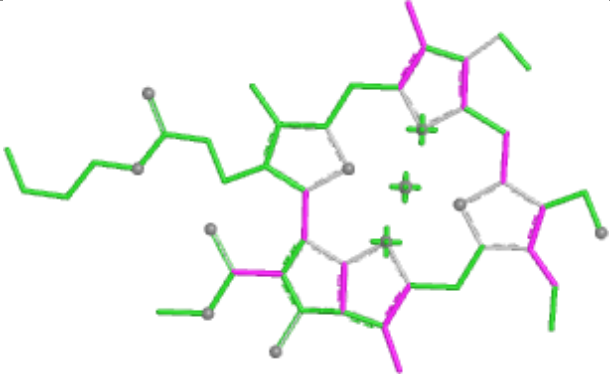
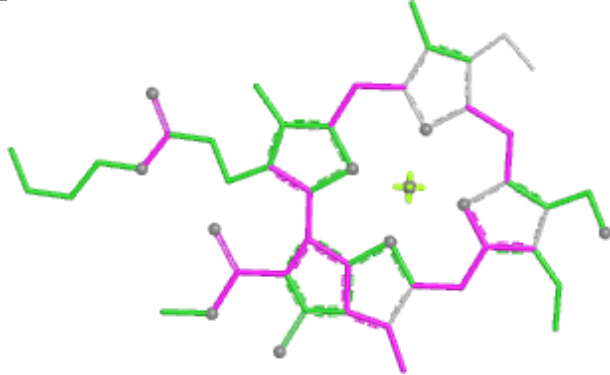
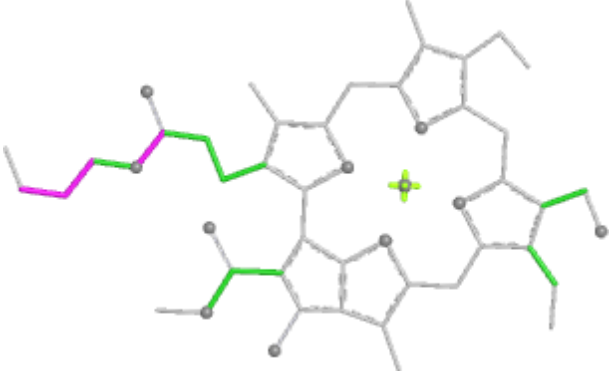
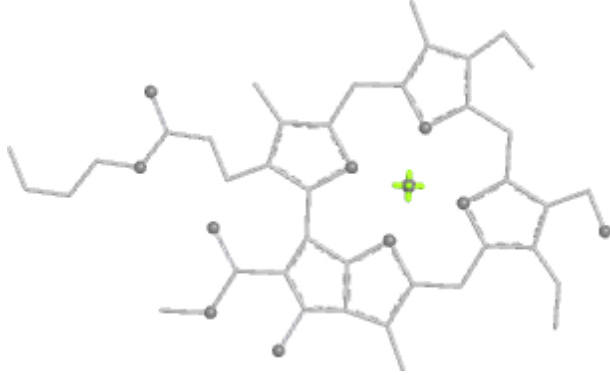
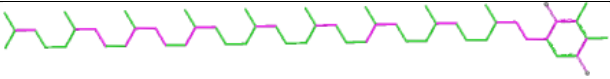
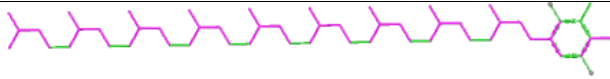
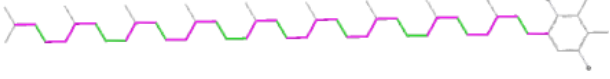
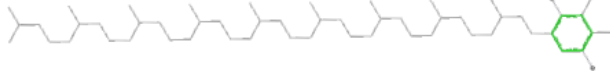
Ligand CLA Rr 603

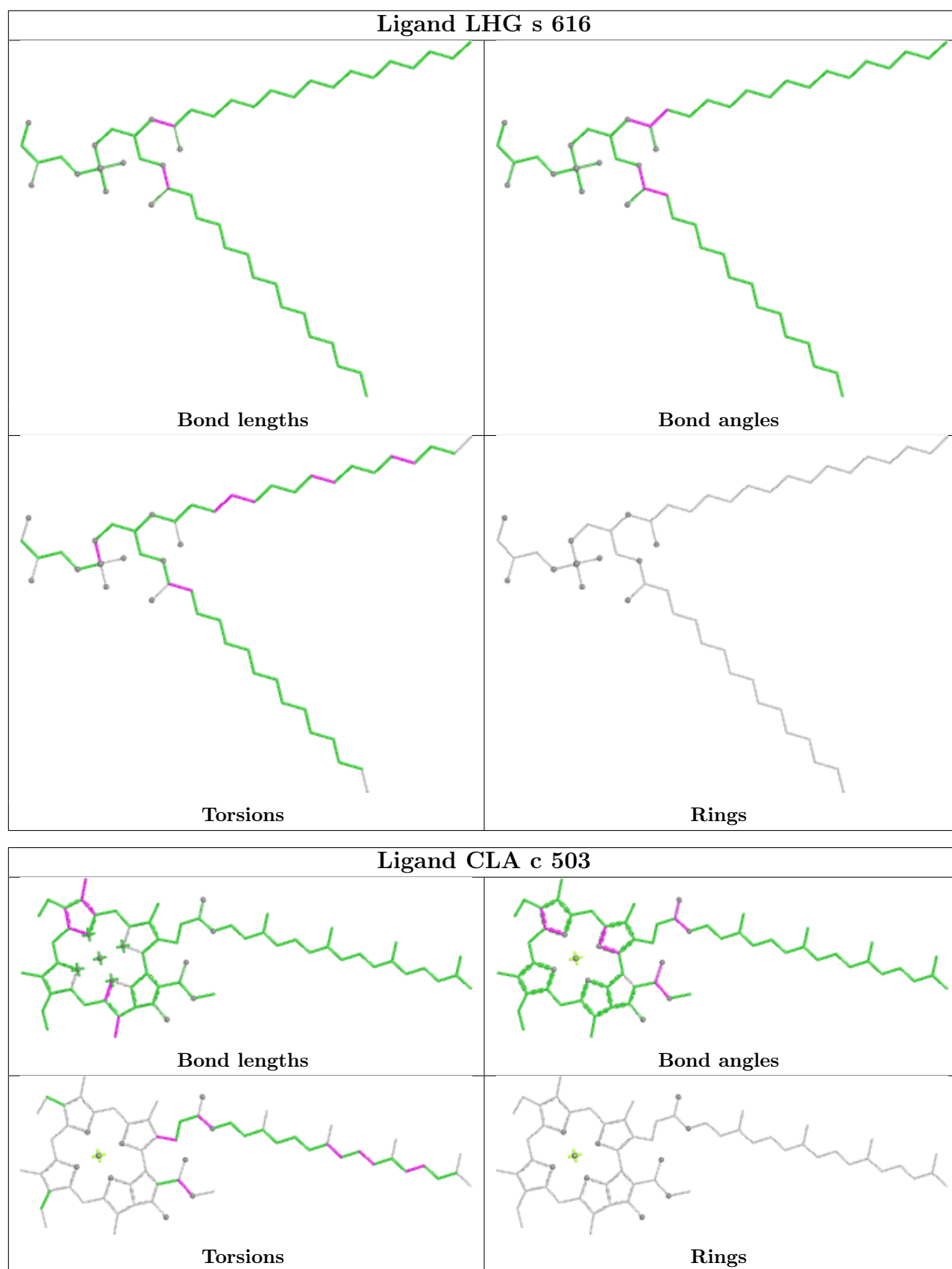


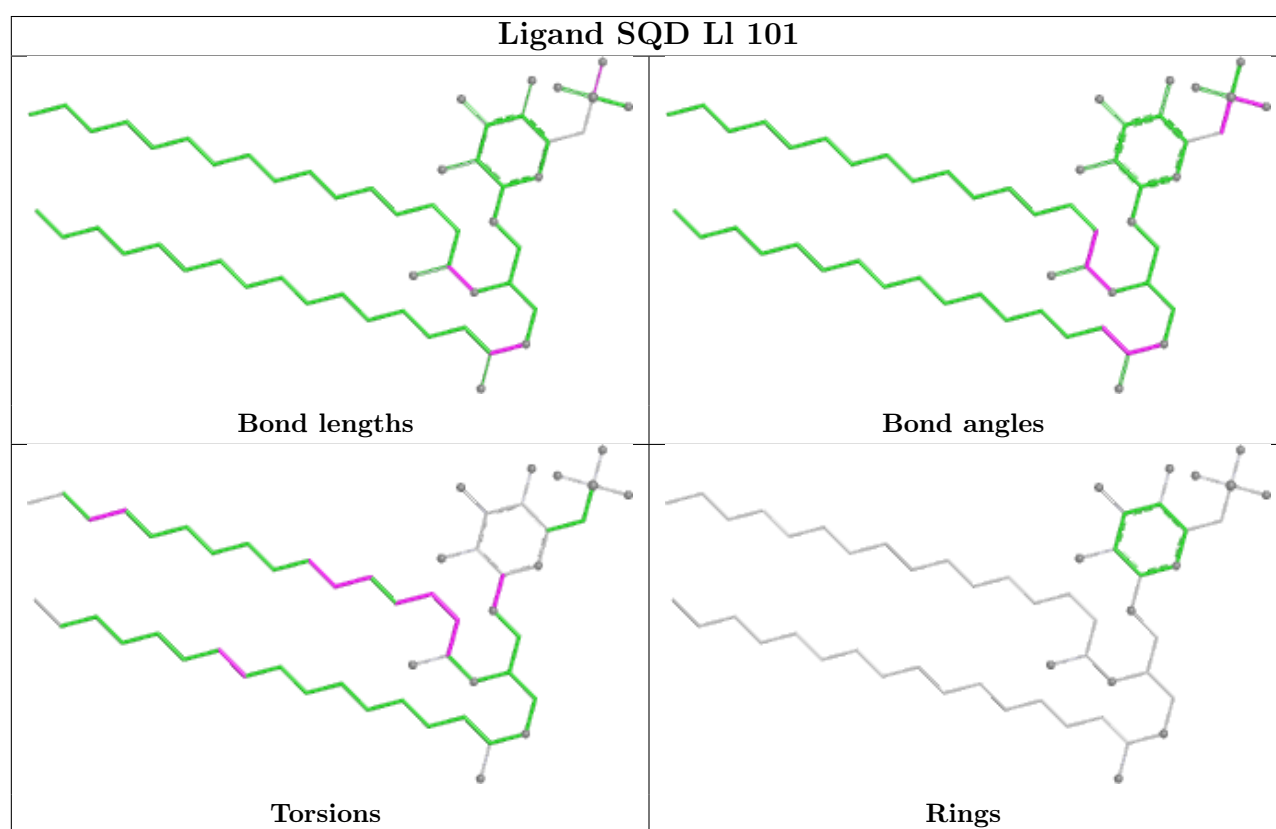
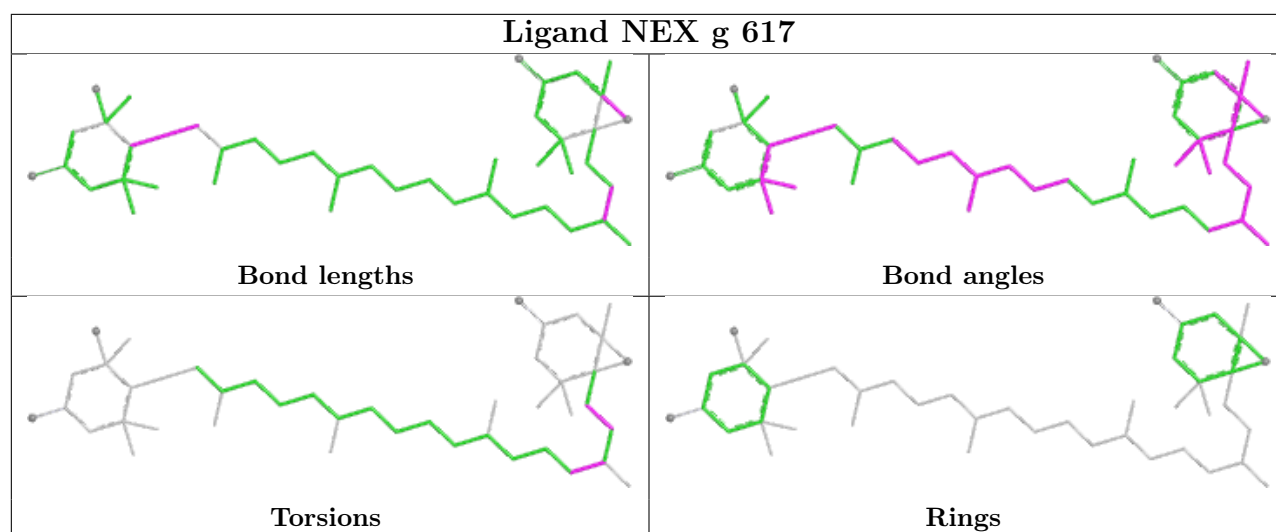
Ligand CLA G 603

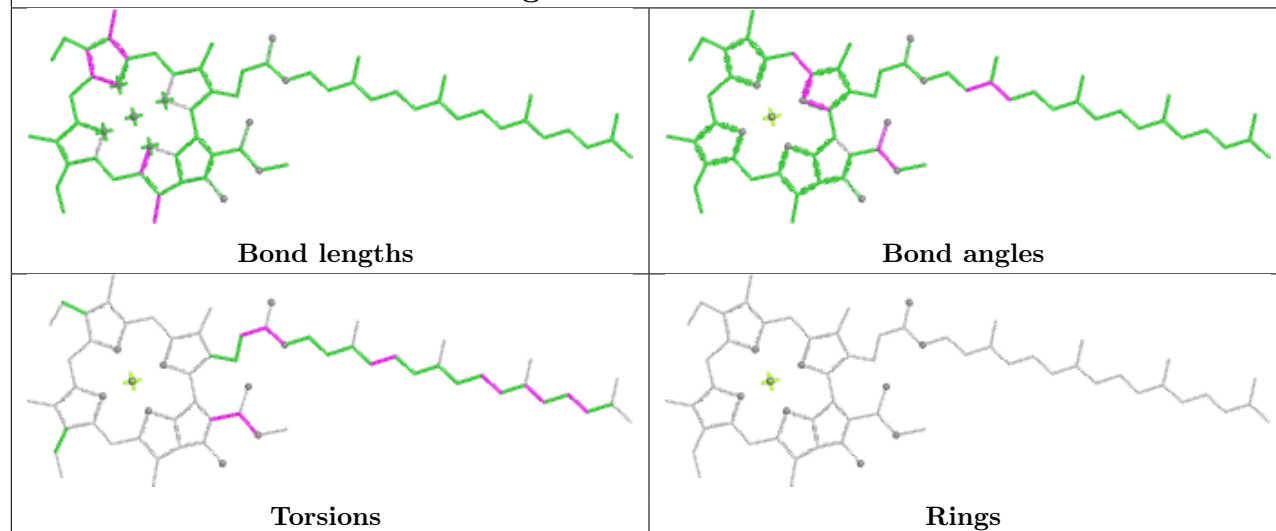
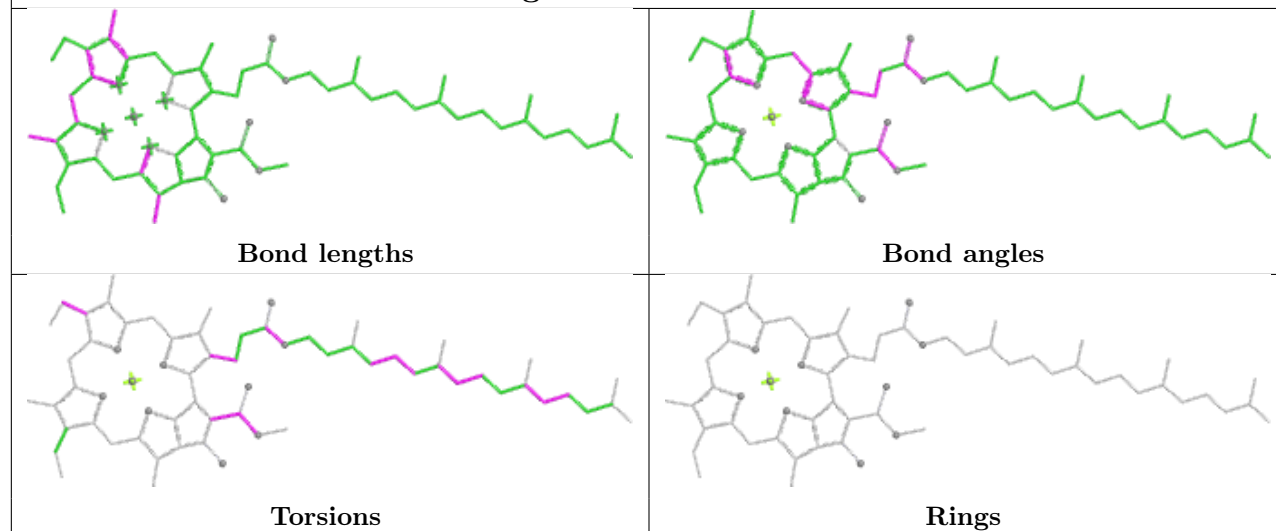


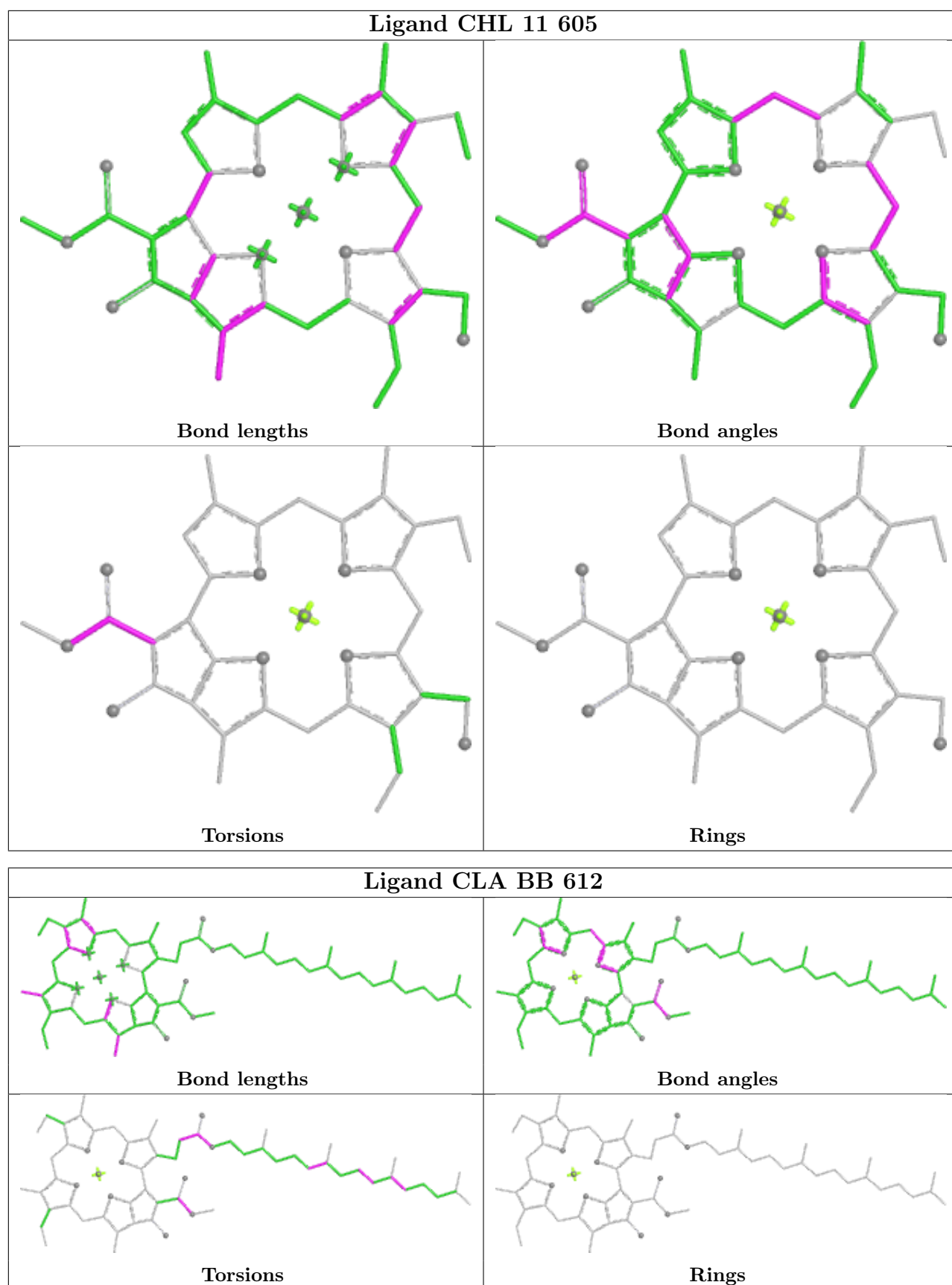


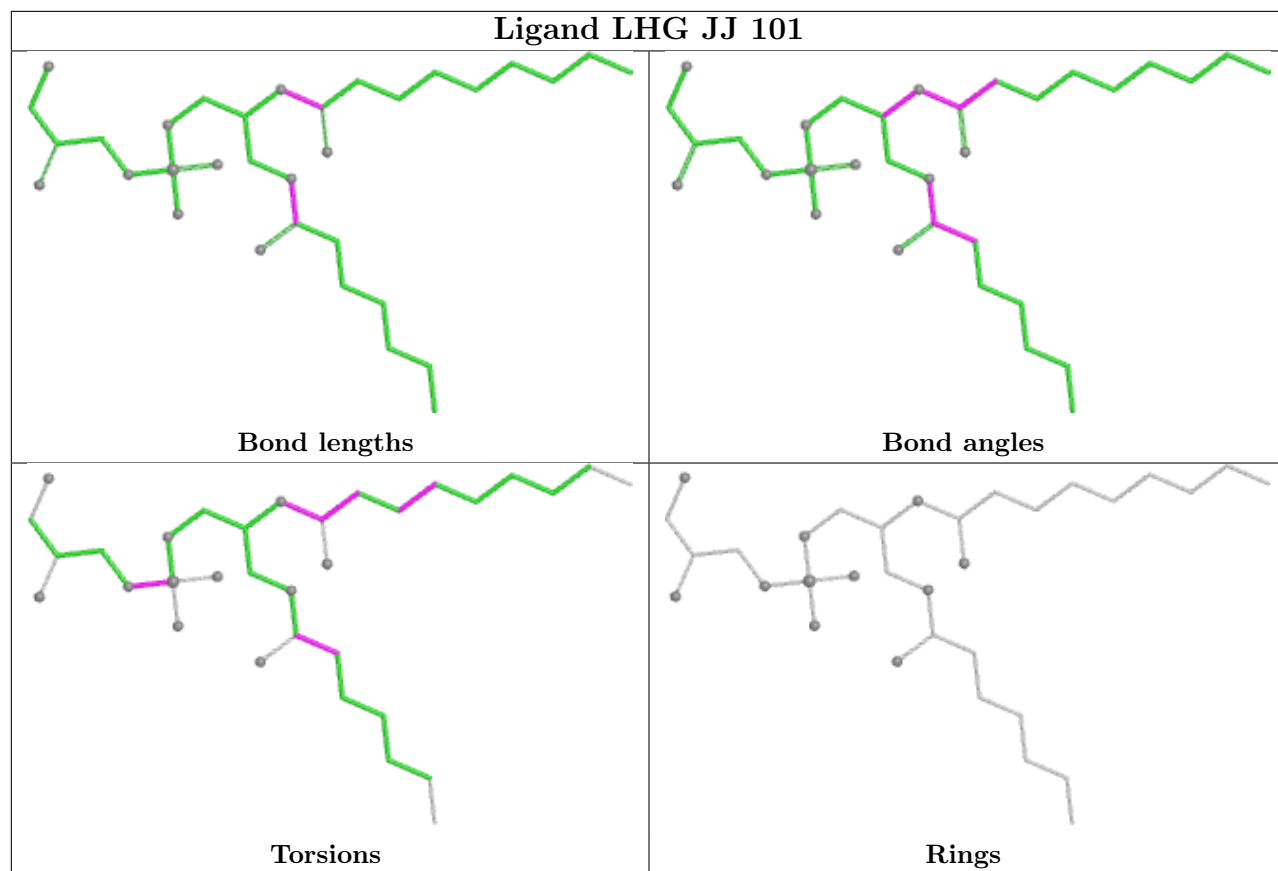
Ligand CHL y 310	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings



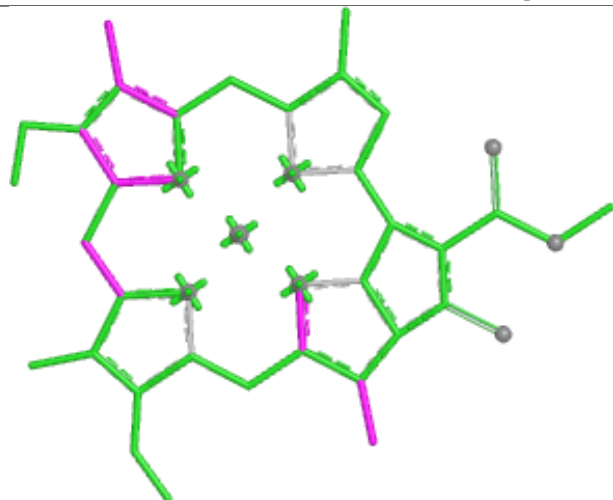


Ligand CLA Bb 605**Ligand CLA Bb 603**

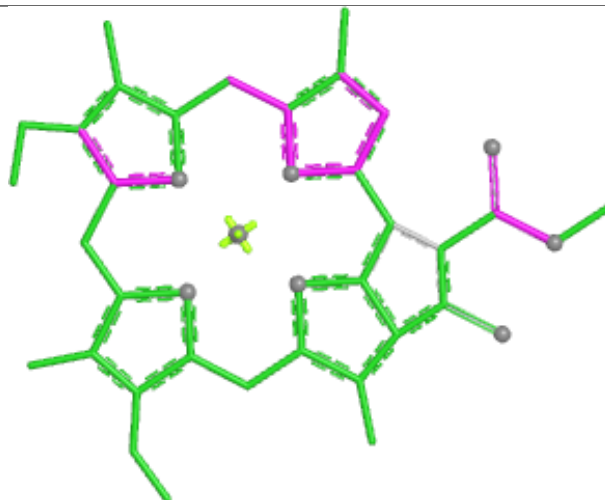




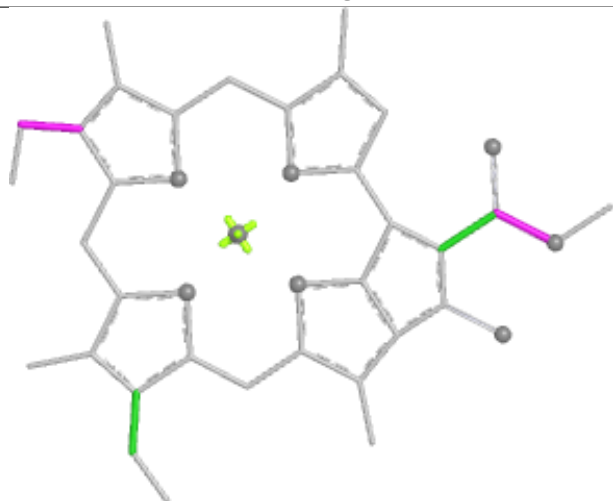
Ligand CLA 1 604



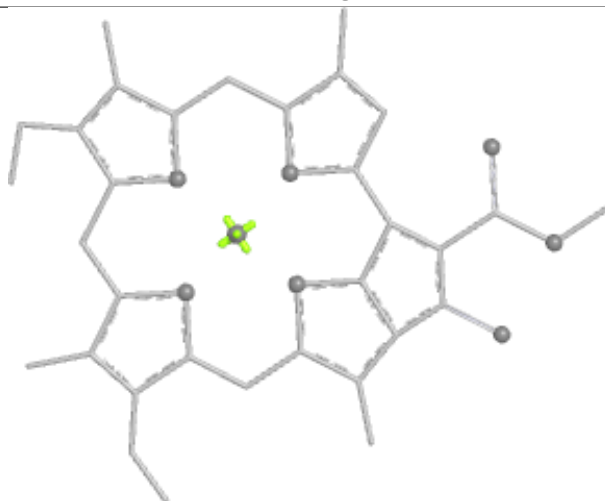
Bond lengths



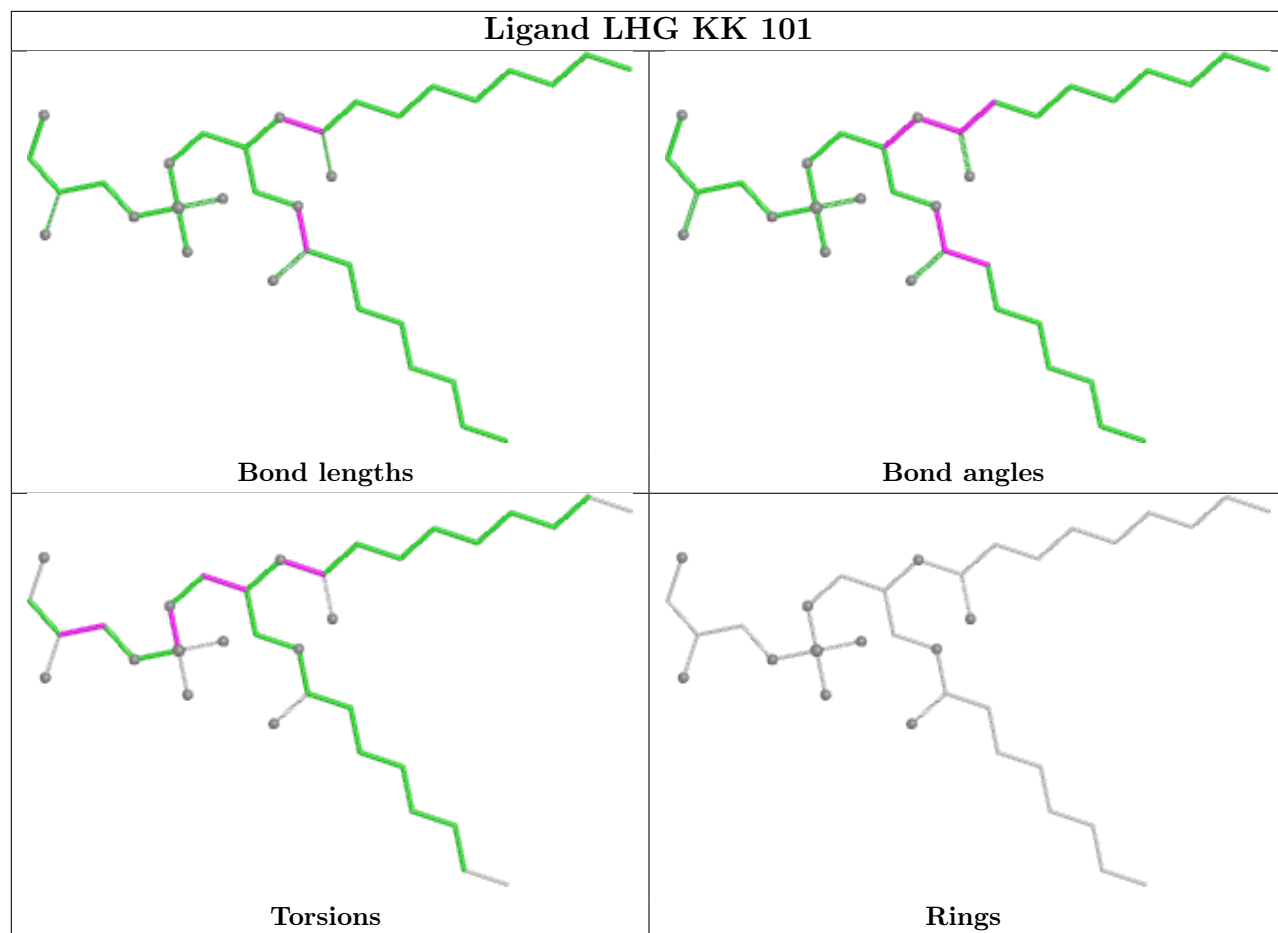
Bond angles



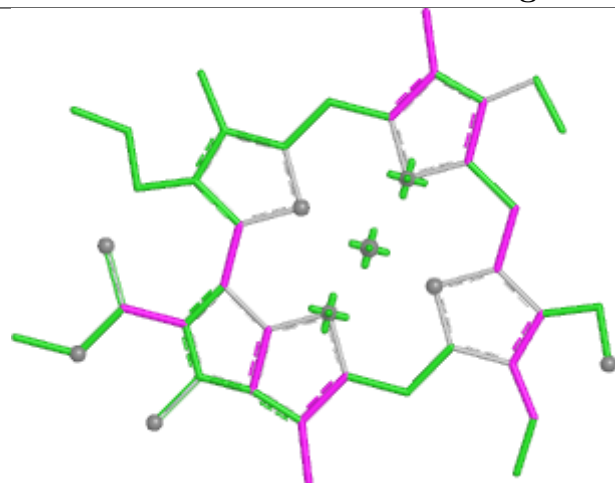
Torsions



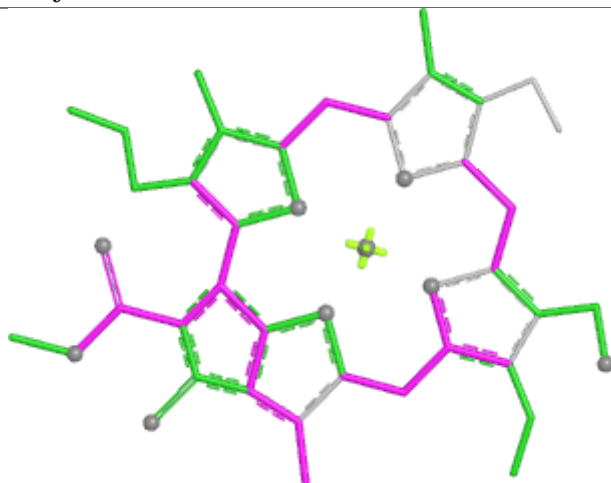
Rings



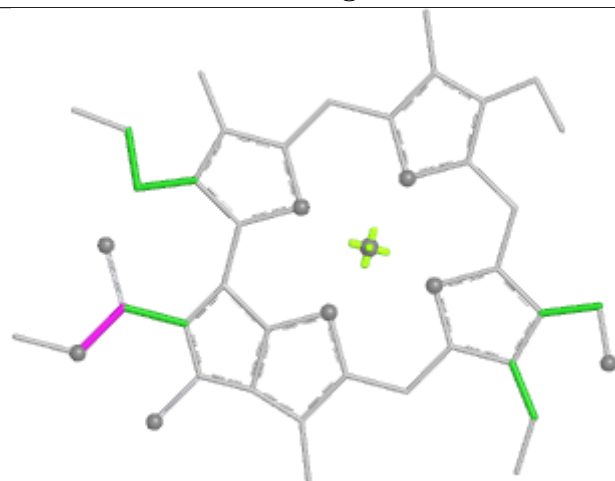
Ligand CHL y 308



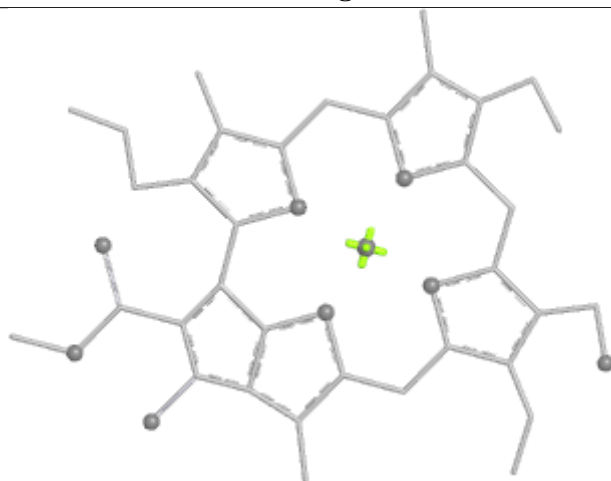
Bond lengths



Bond angles

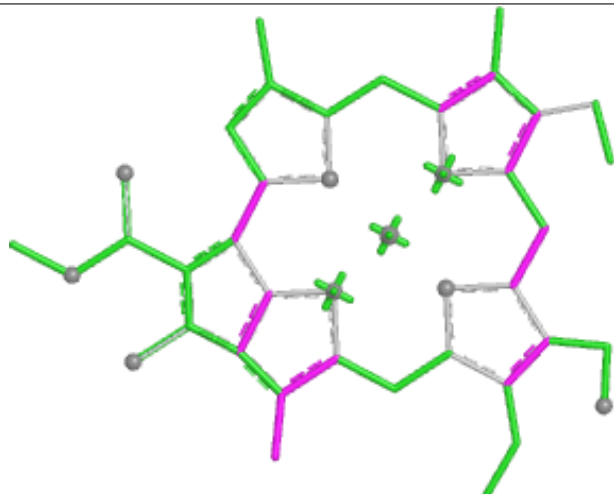


Torsions

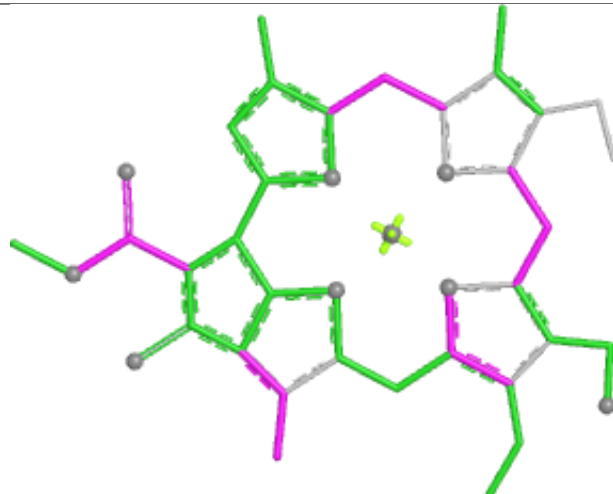


Rings

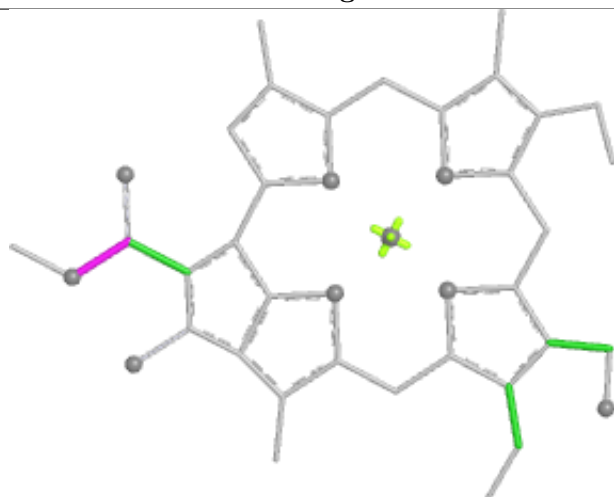
Ligand CHL 1 601



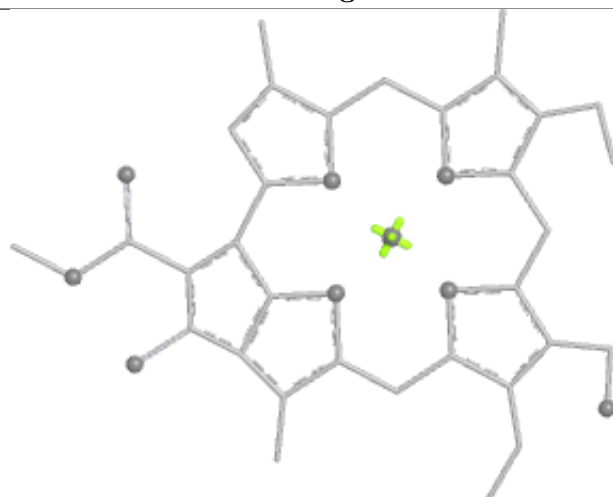
Bond lengths



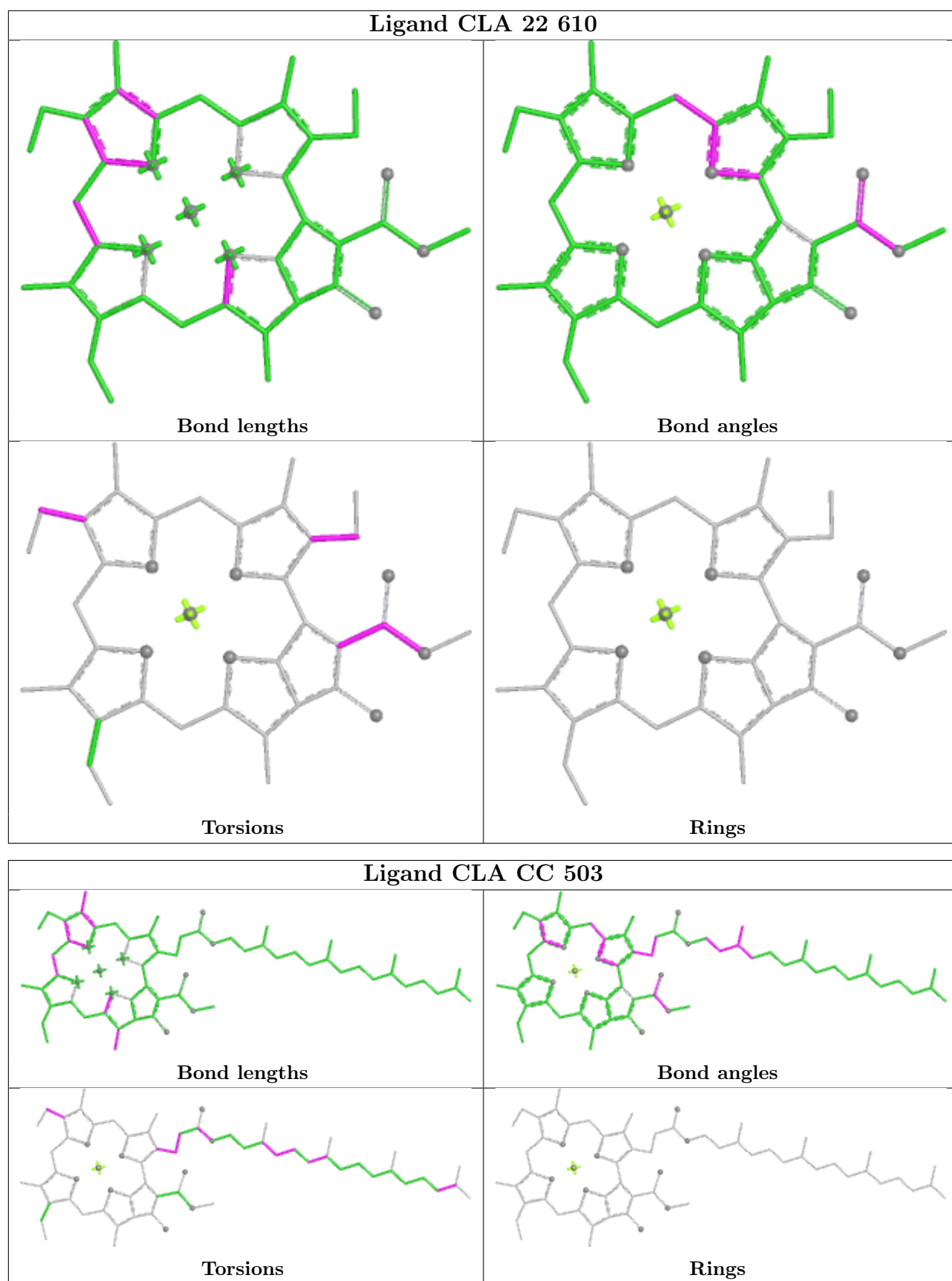
Bond angles

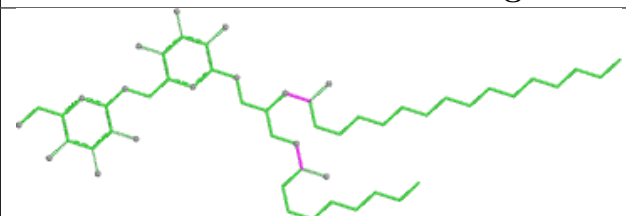
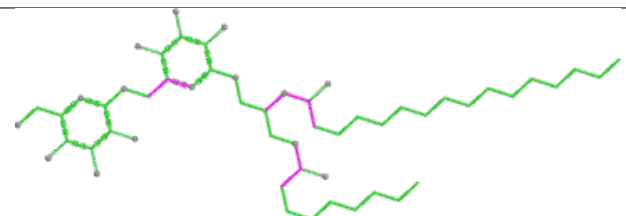
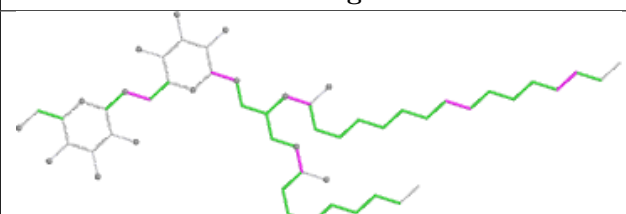
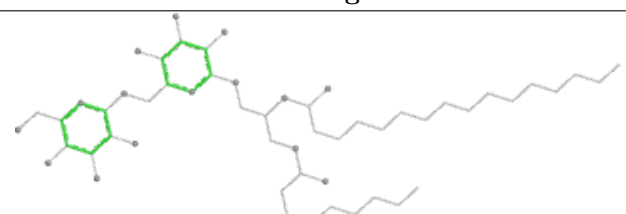


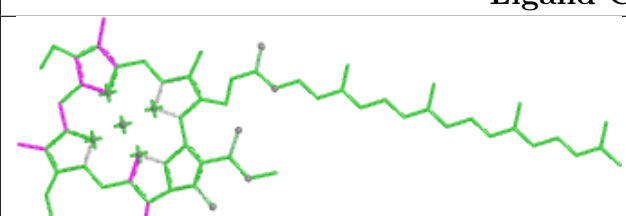
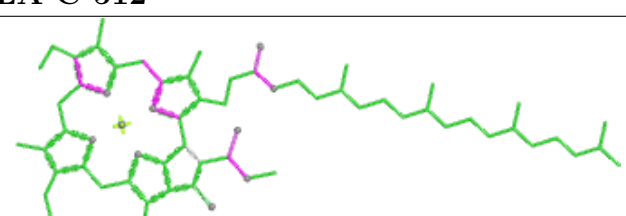
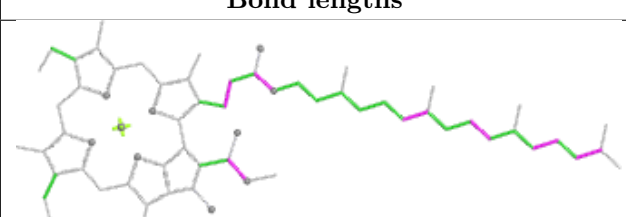
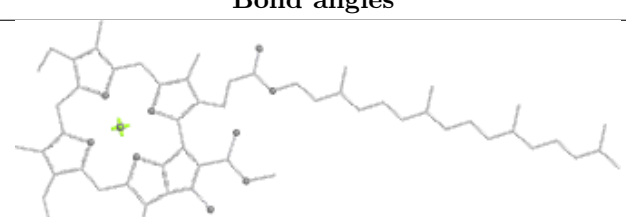
Torsions

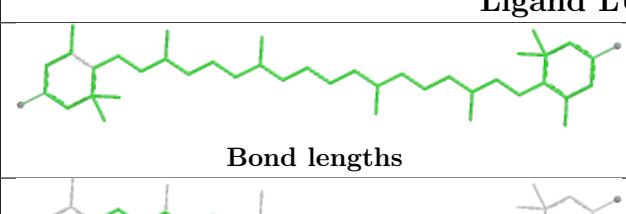
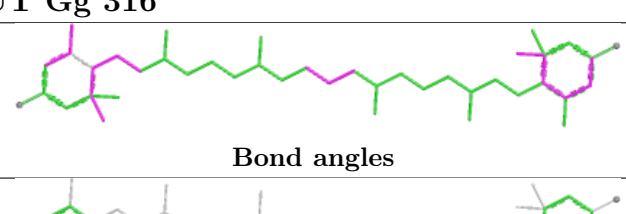


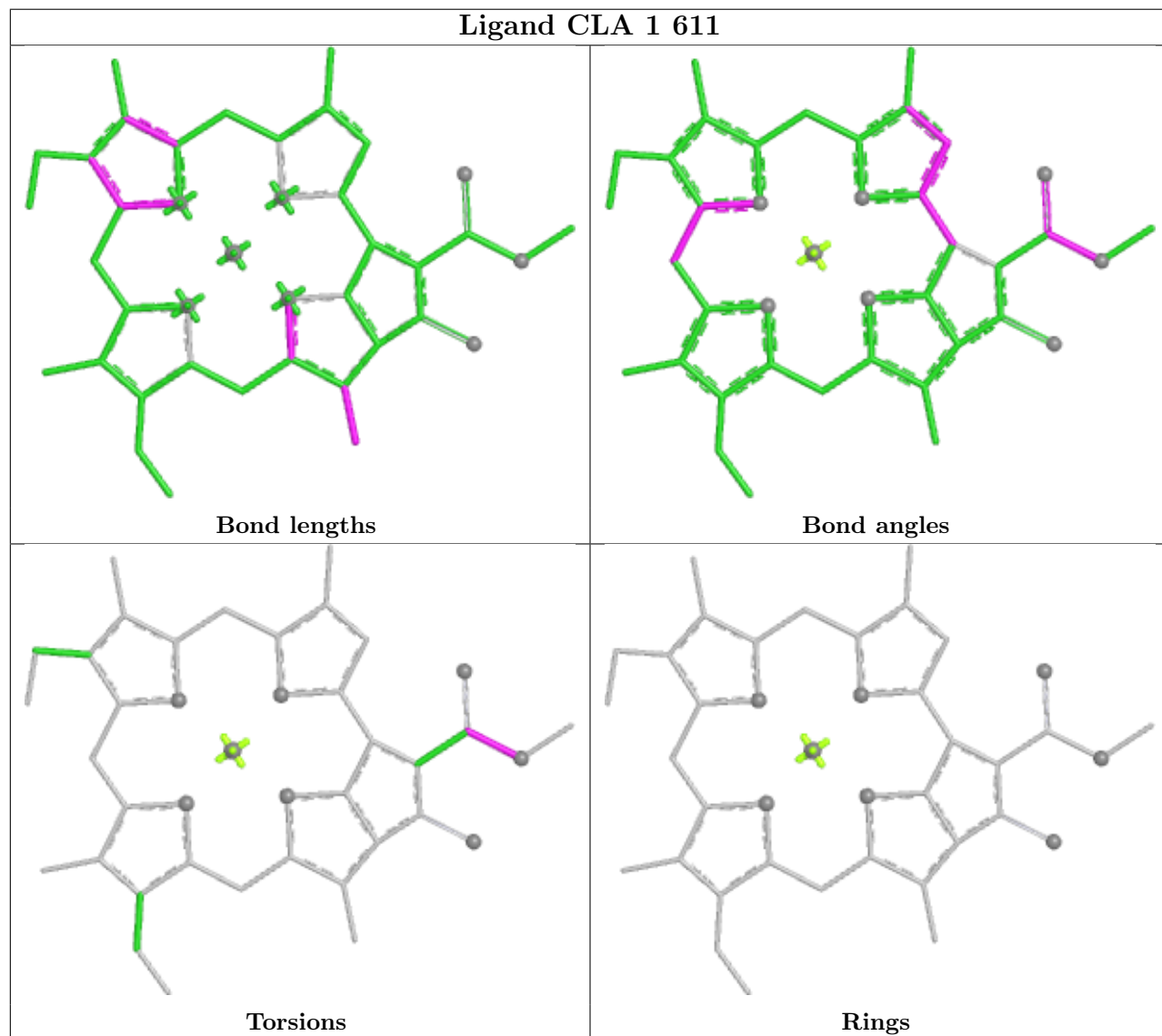
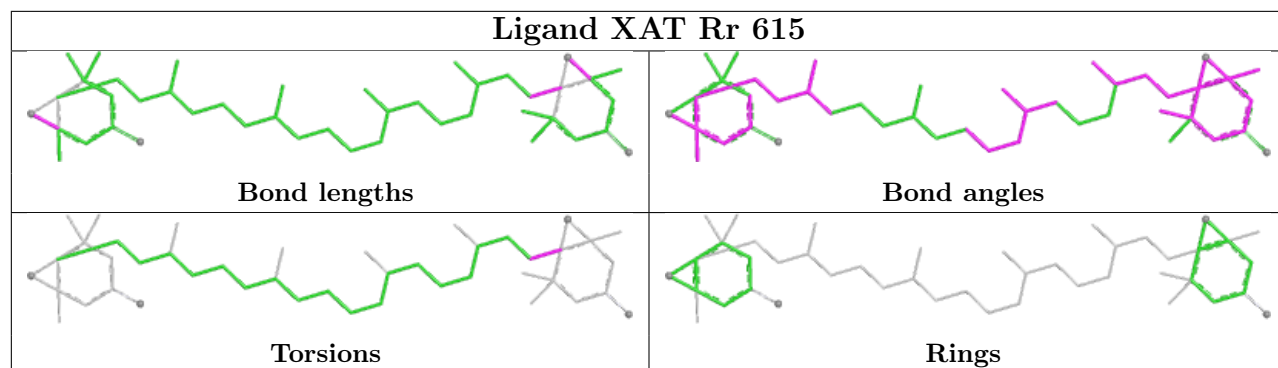
Rings



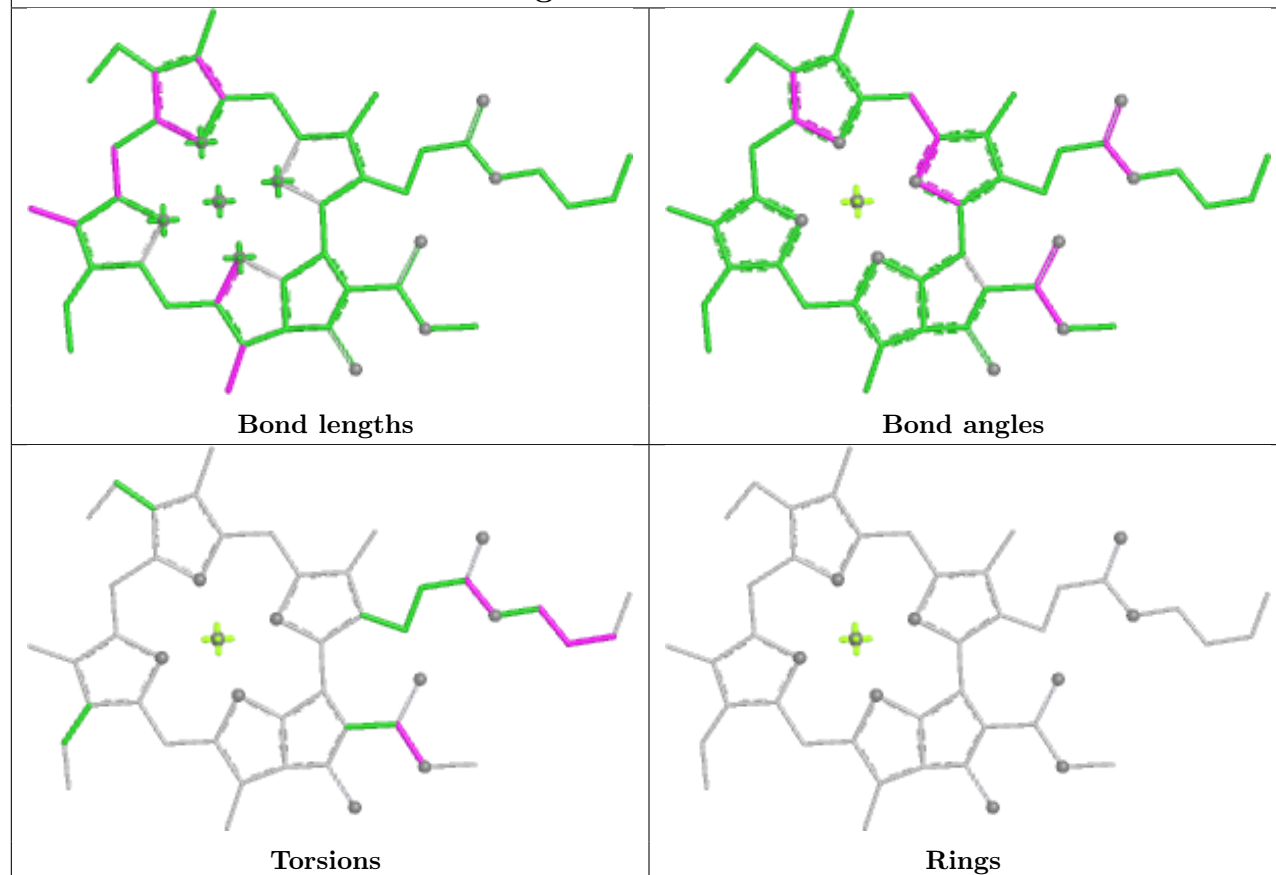
Ligand DGD BB 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

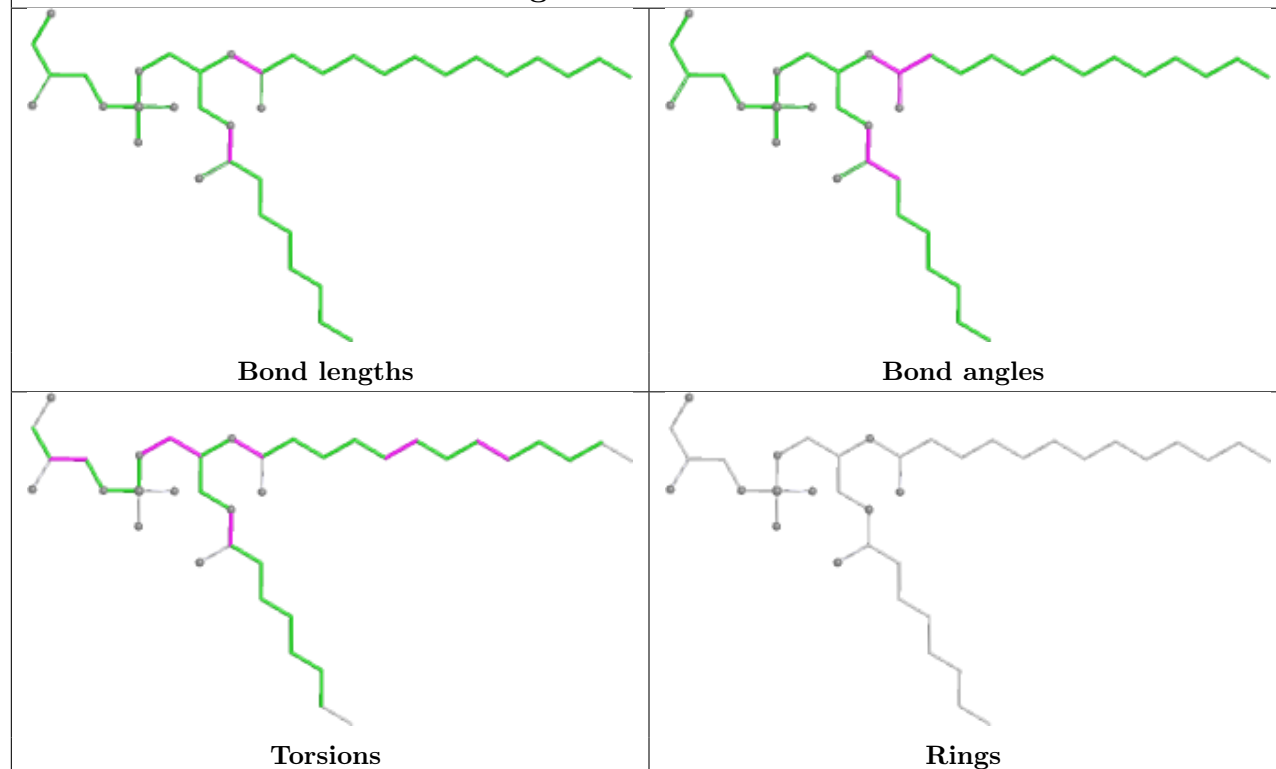
Ligand LUT Gg 316	
	
Bond lengths	Bond angles
	
Torsions	Rings



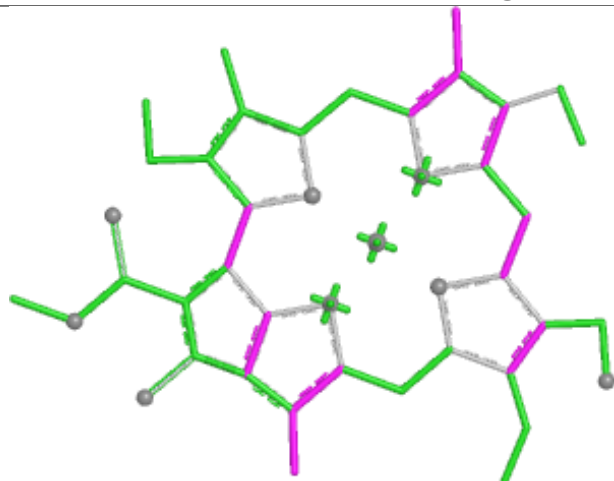
Ligand CLA n 604



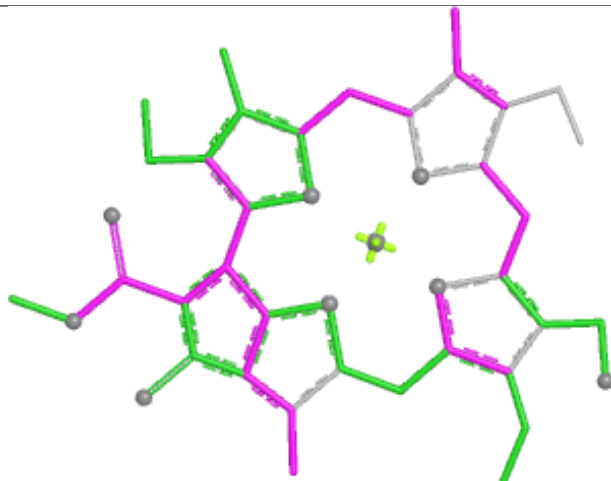
Ligand LHG N 619



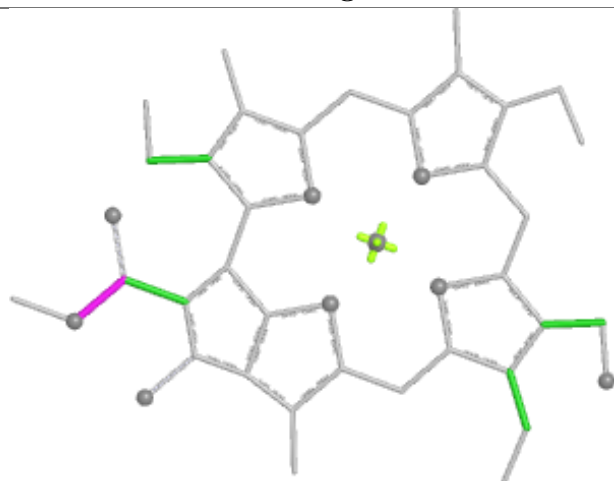
Ligand CHL GG 609



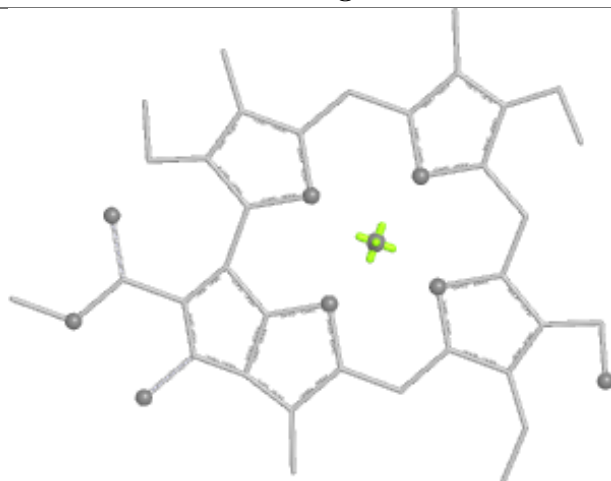
Bond lengths



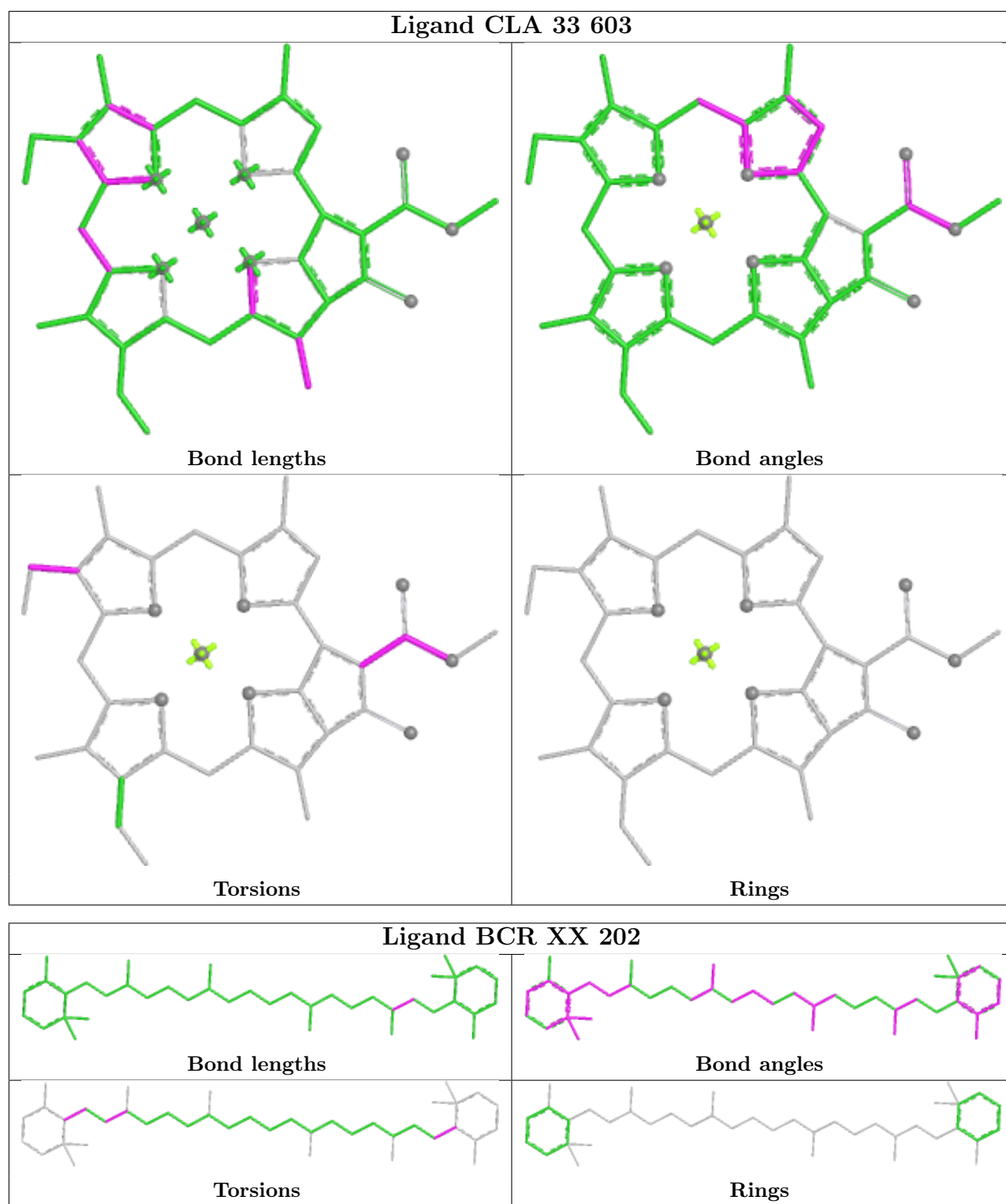
Bond angles



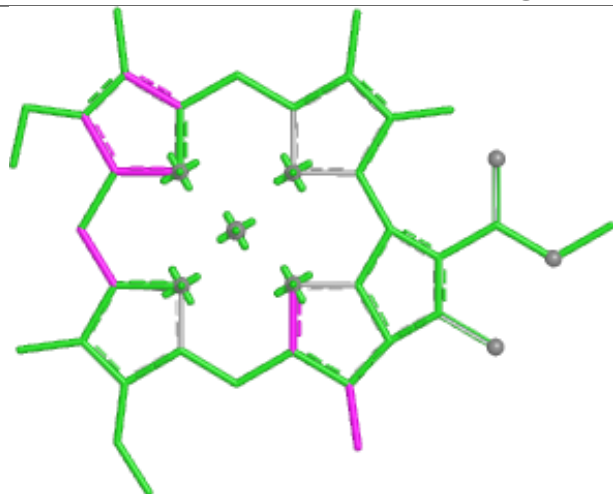
Torsions



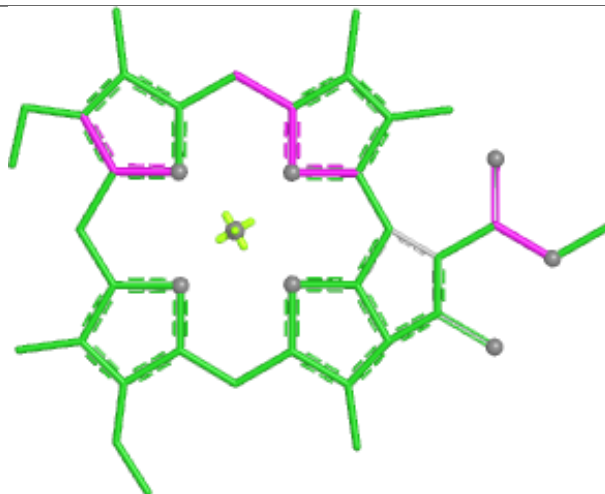
Rings



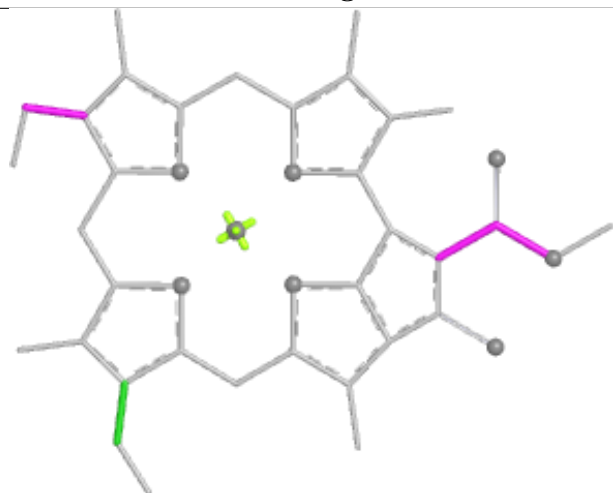
Ligand CLA S 608



Bond lengths



Bond angles

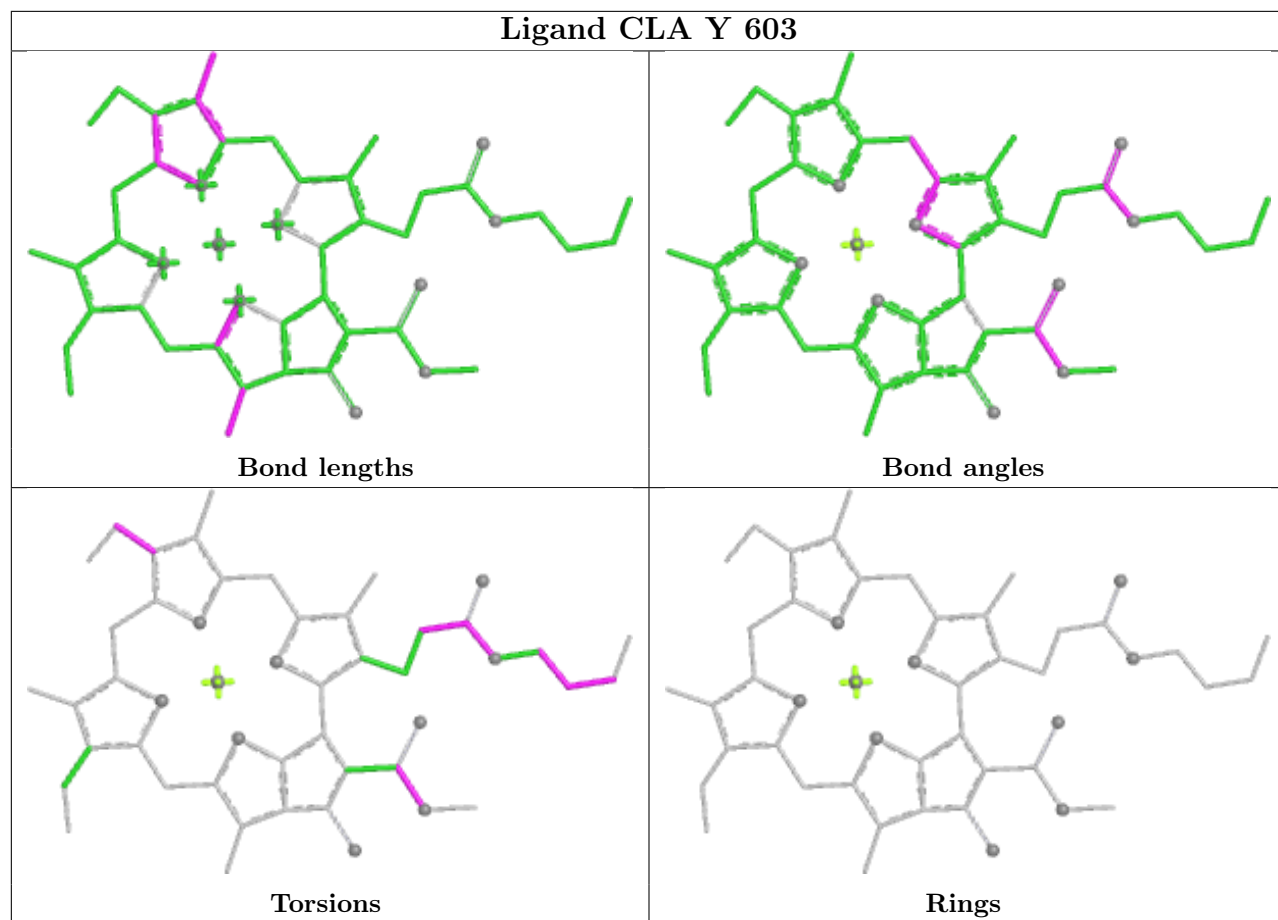


Torsions

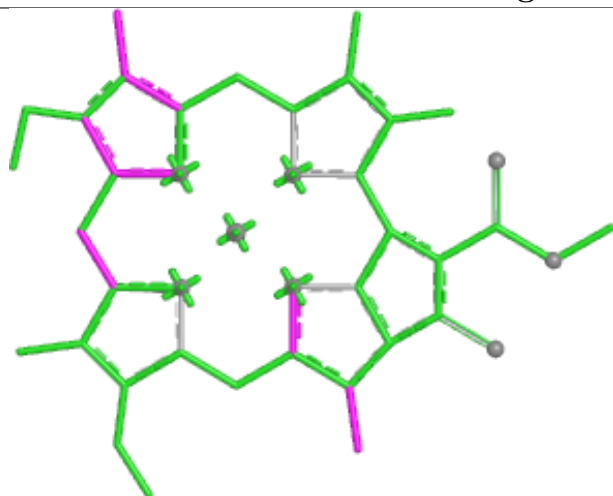


Rings

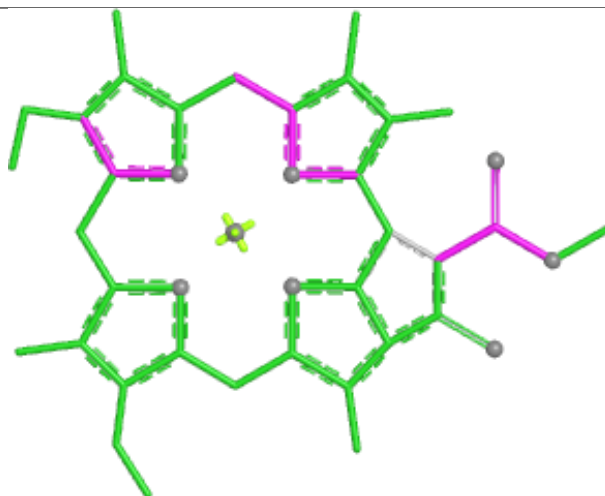
Ligand CLA Y 603



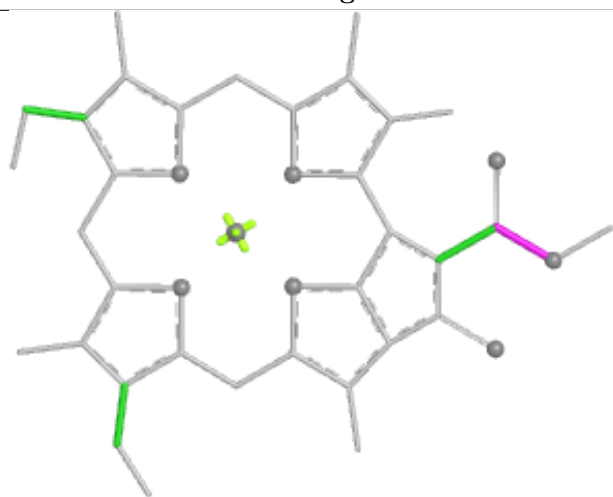
Ligand CLA S 609



Bond lengths



Bond angles

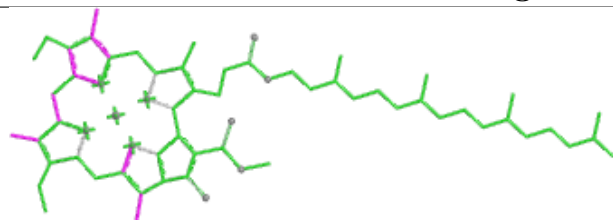


Torsions

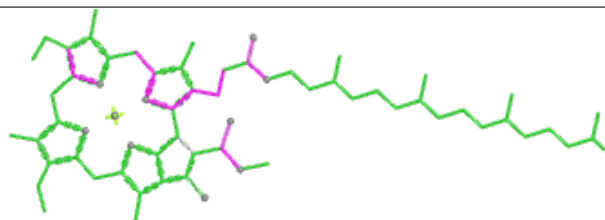


Rings

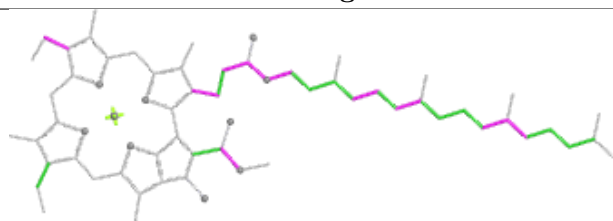
Ligand CLA Y 610



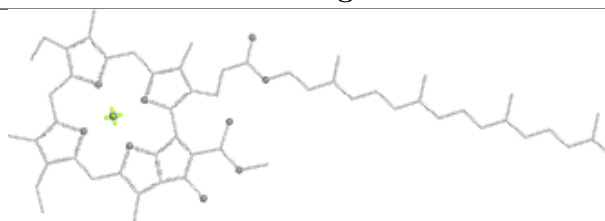
Bond lengths



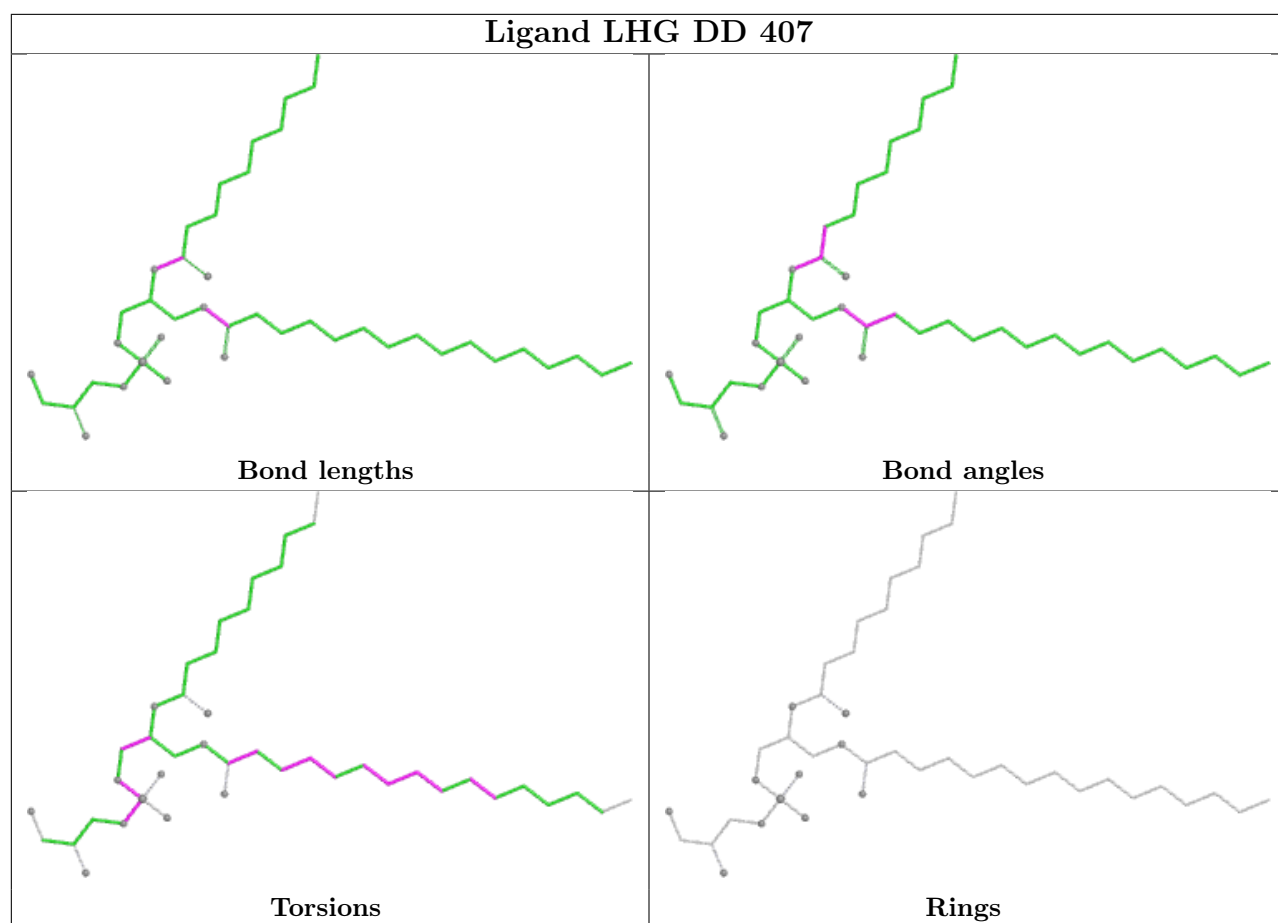
Bond angles



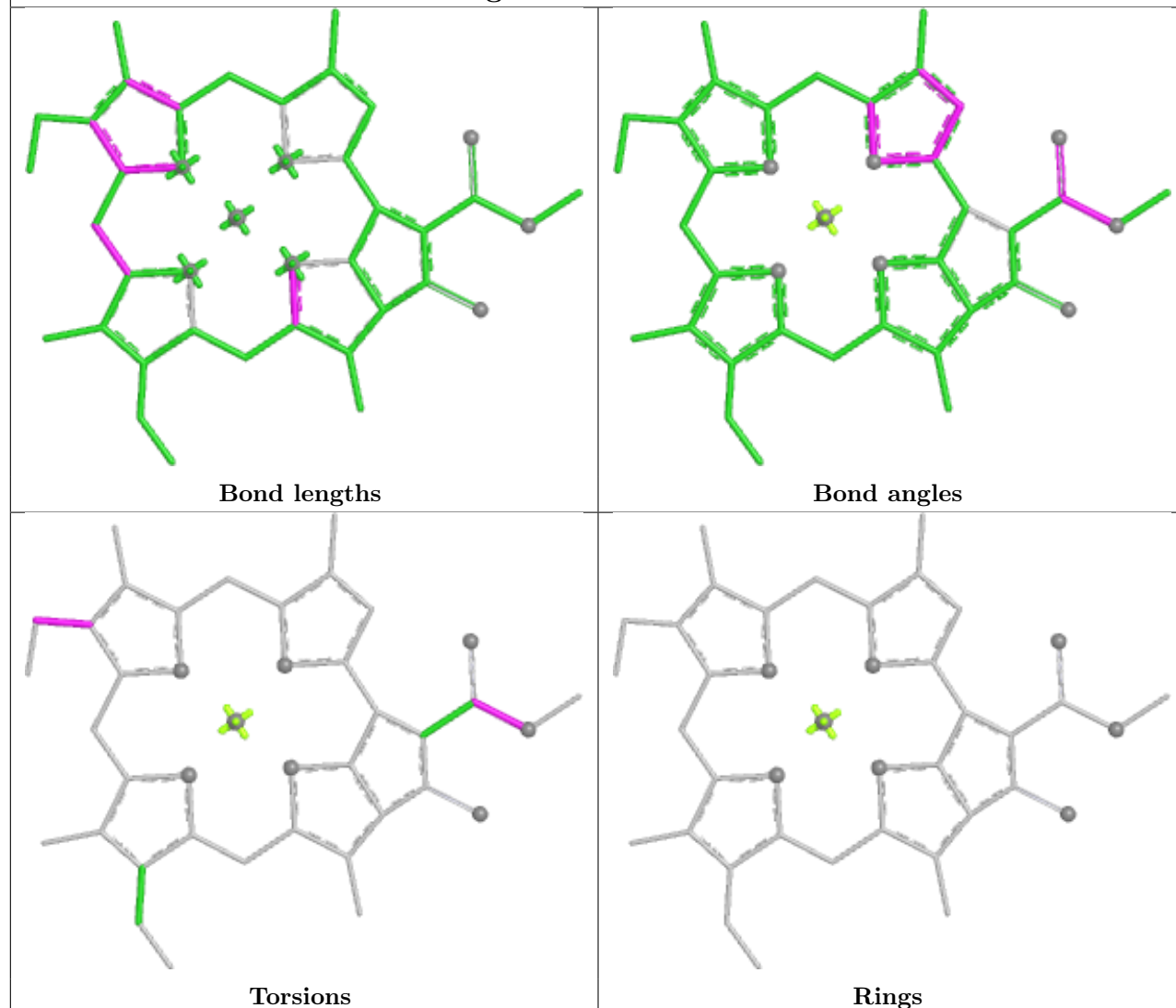
Torsions



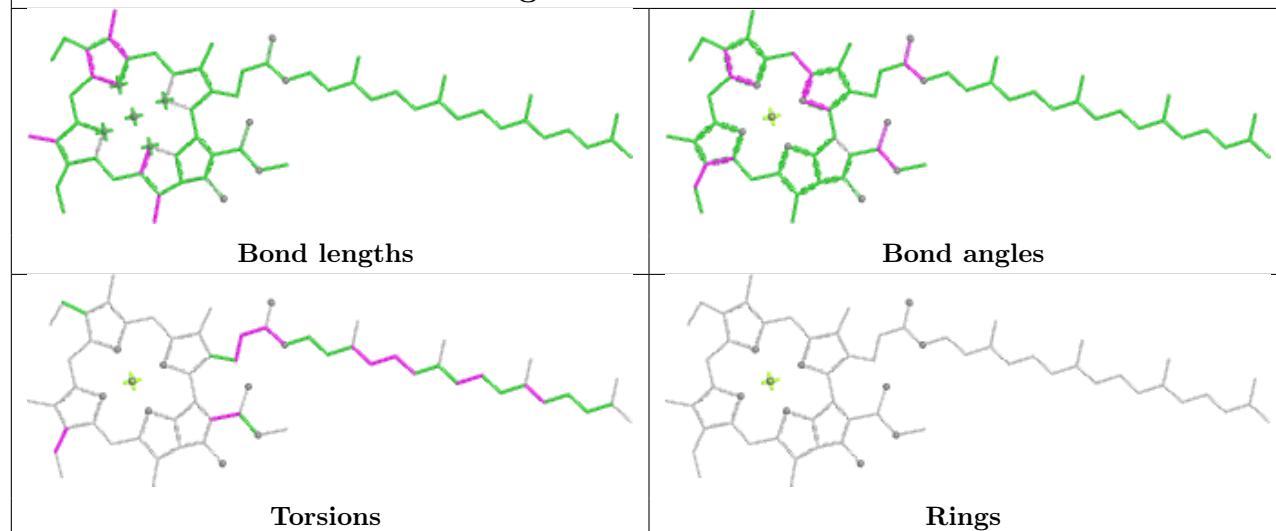
Rings



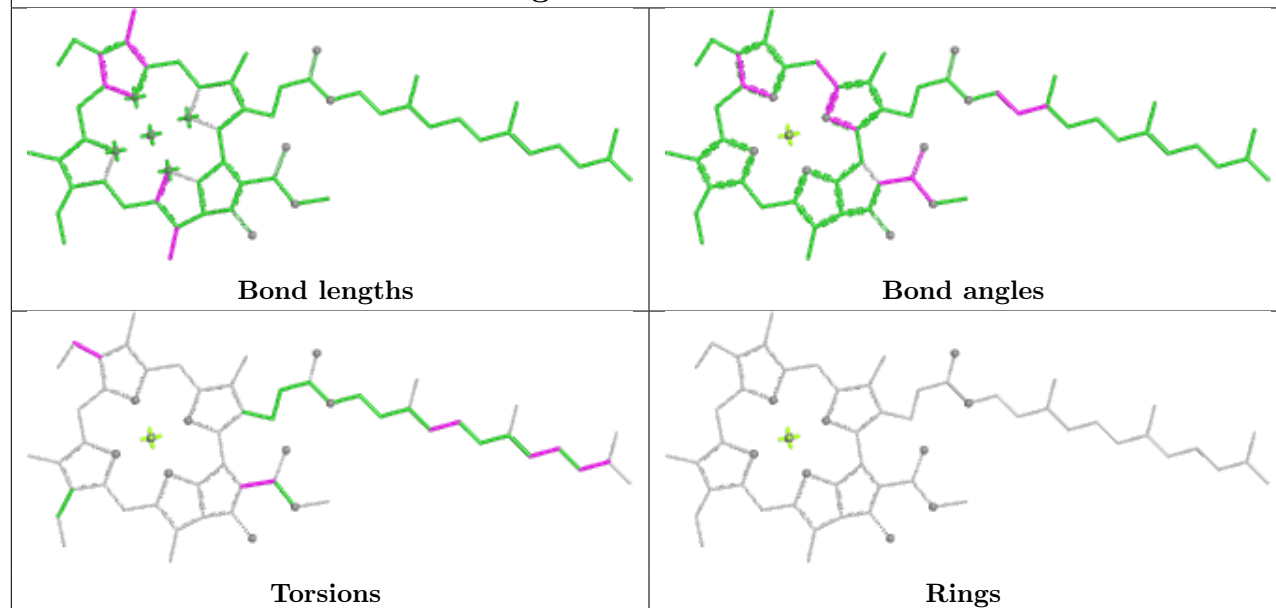
Ligand CLA 11 613



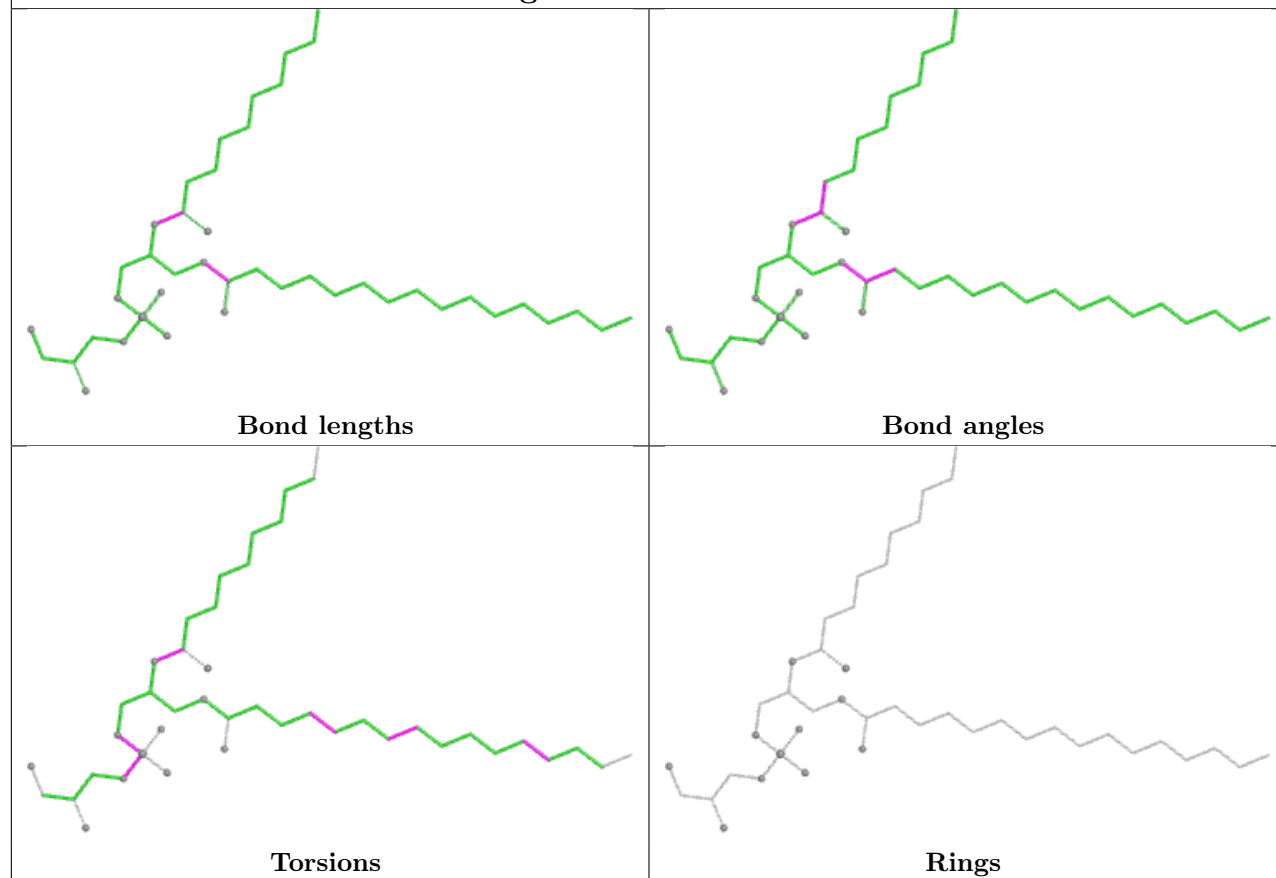
Ligand CLA CC 506

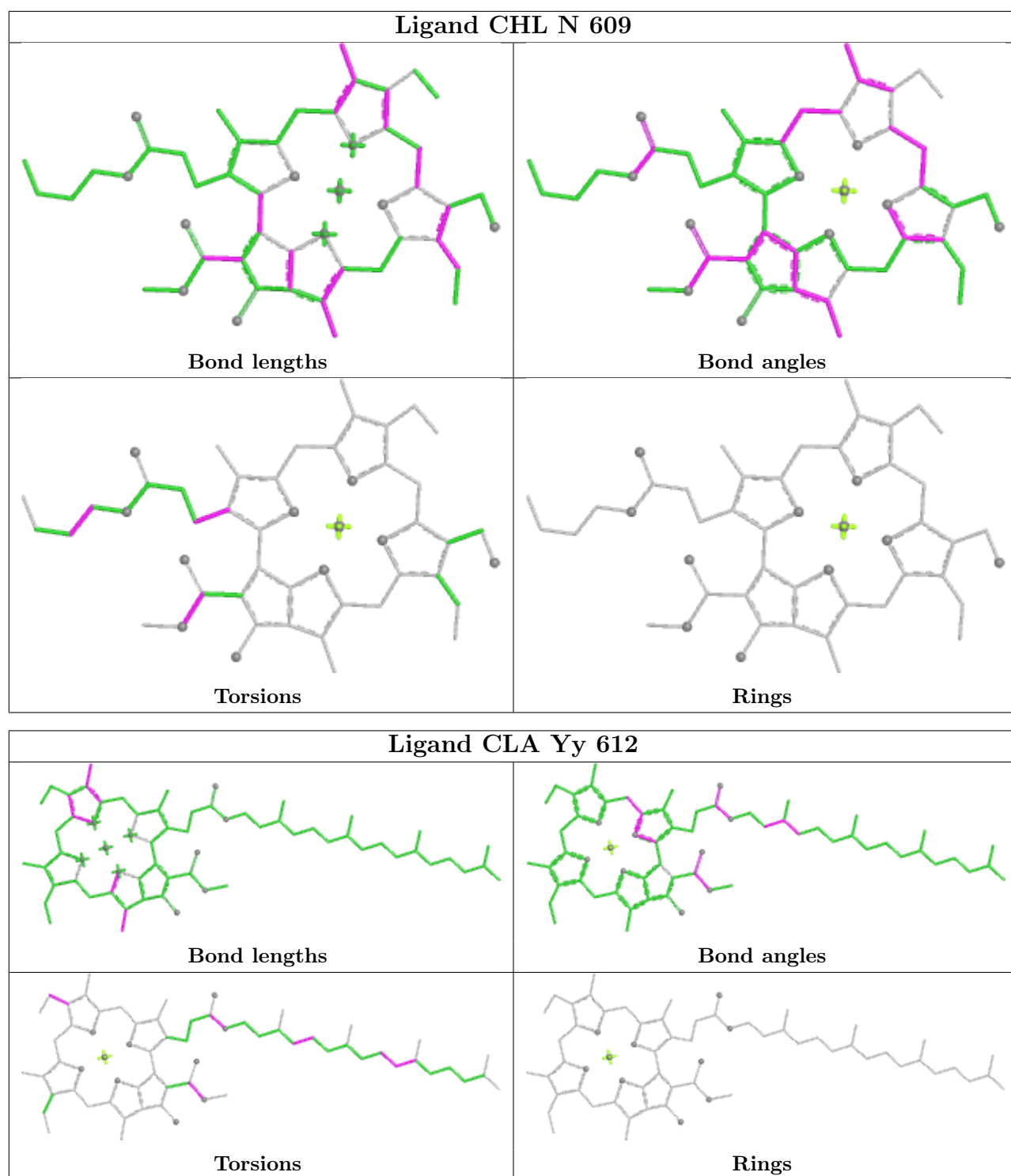


Ligand CLA A 408

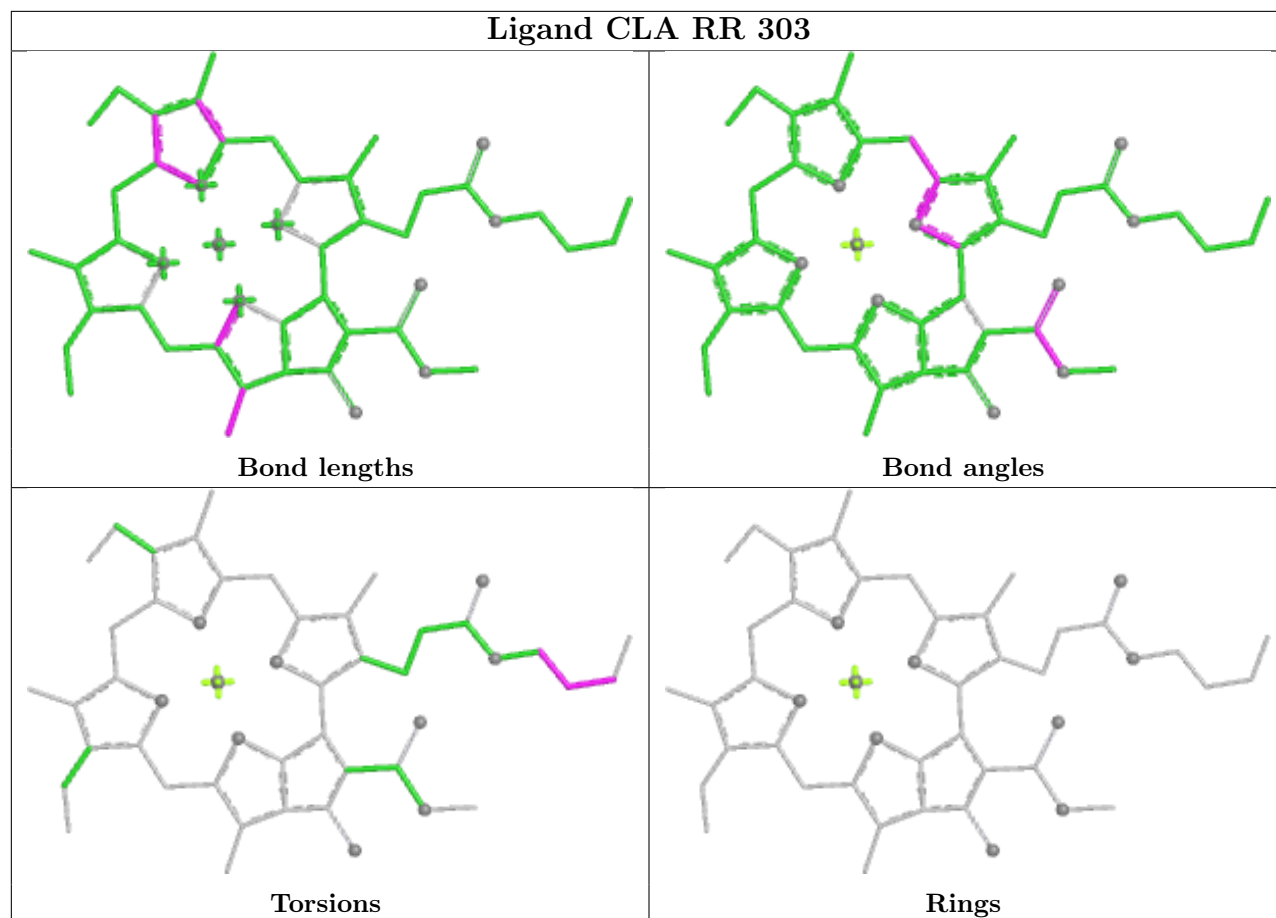


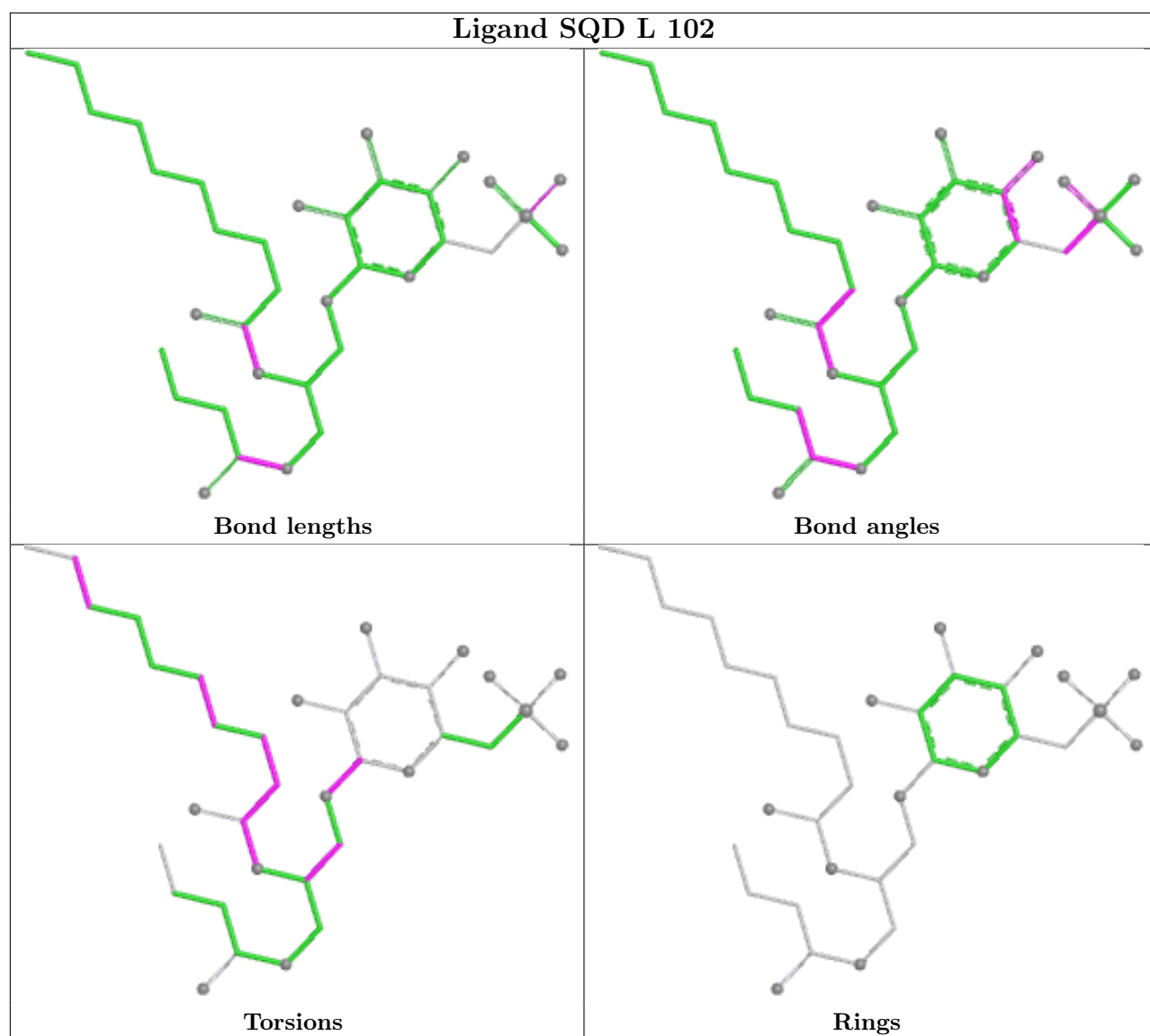
Ligand LHG Dd 405



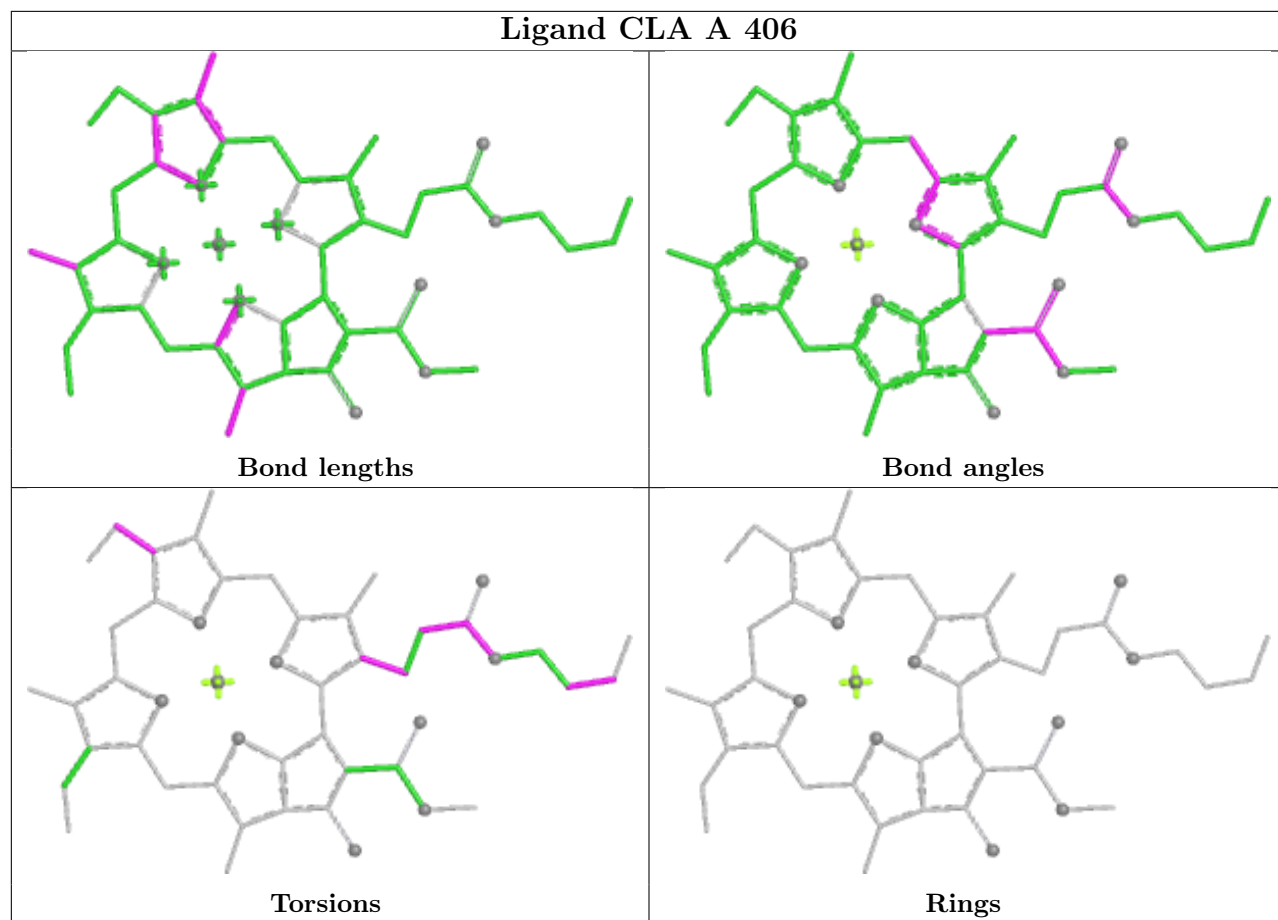


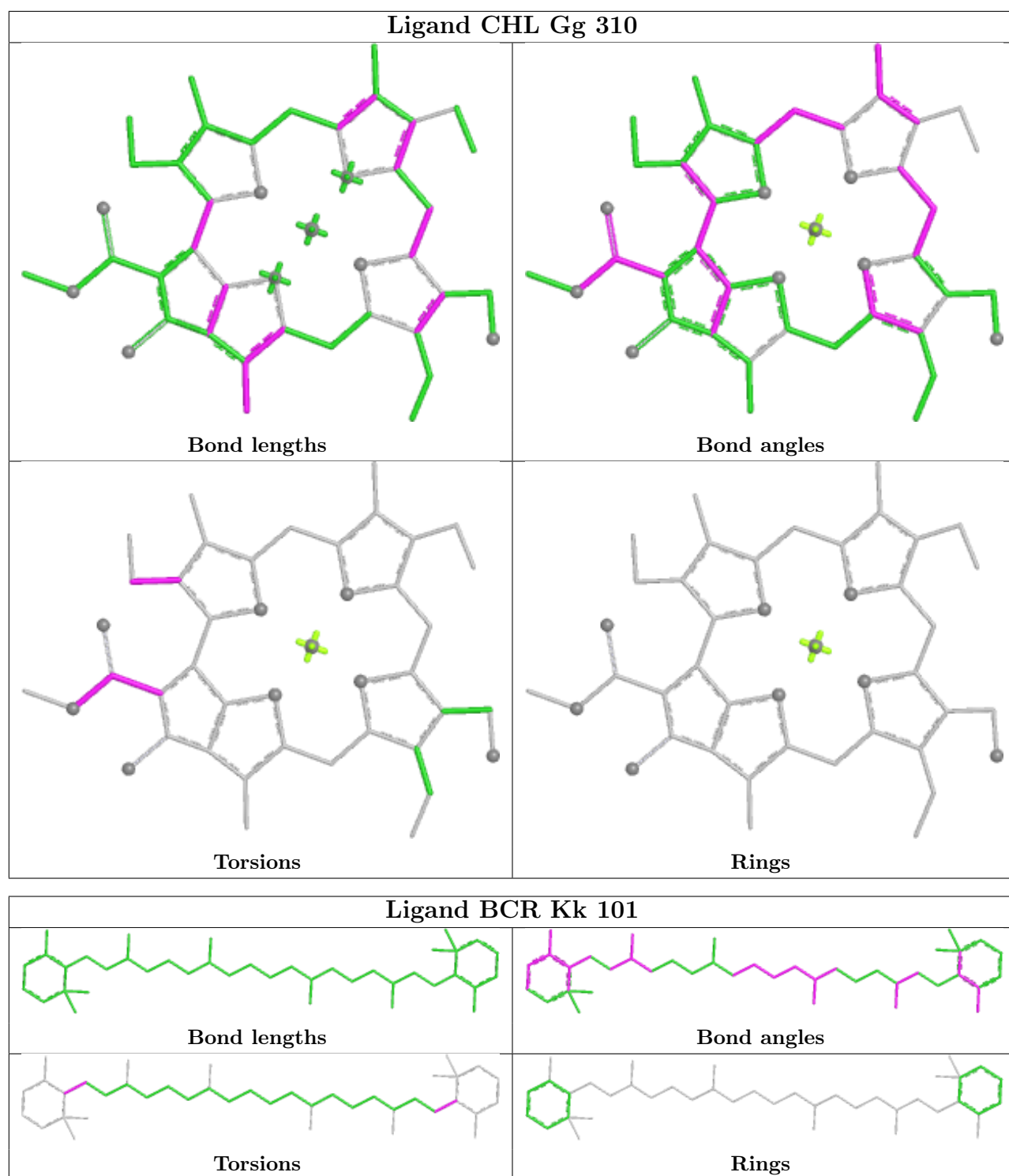
Ligand CLA RR 303



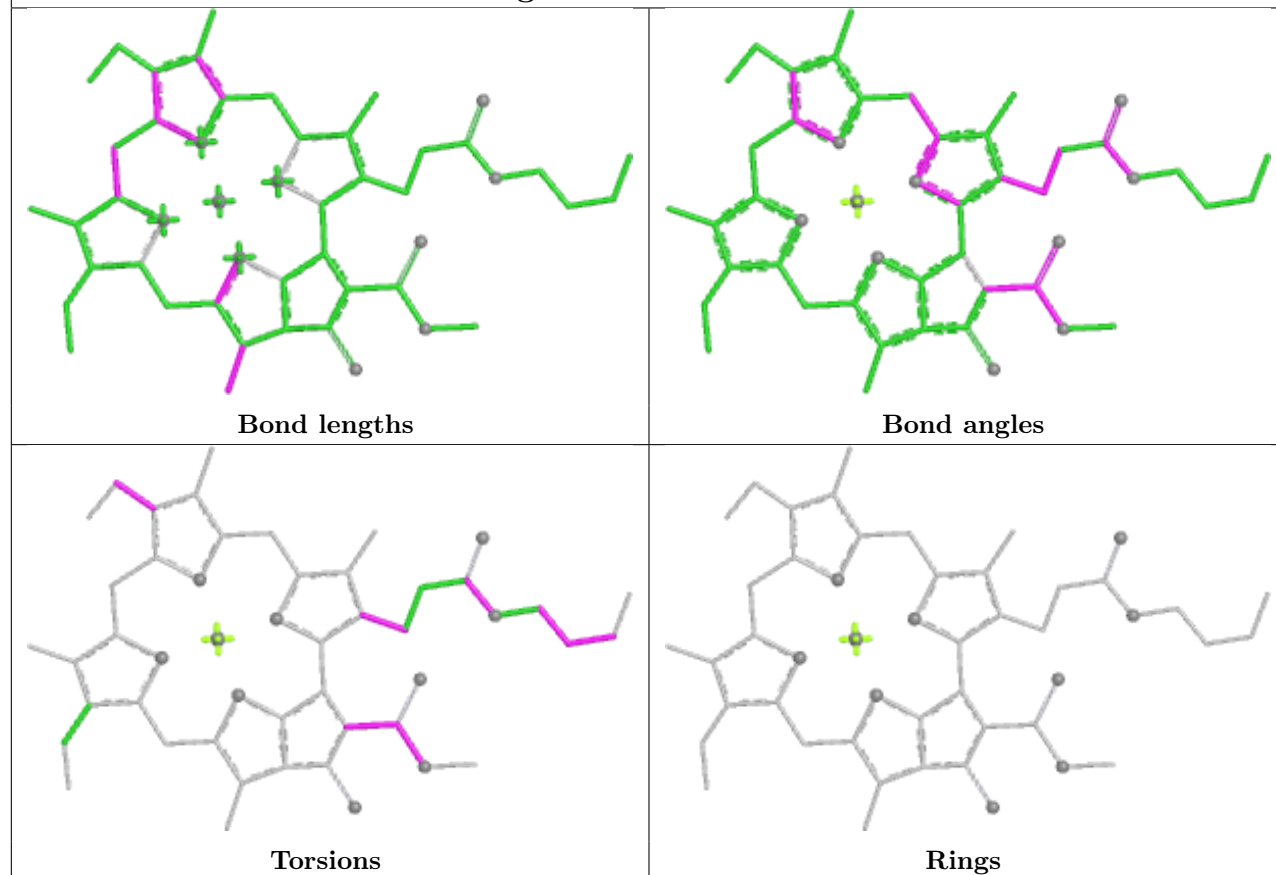


Ligand CLA A 406

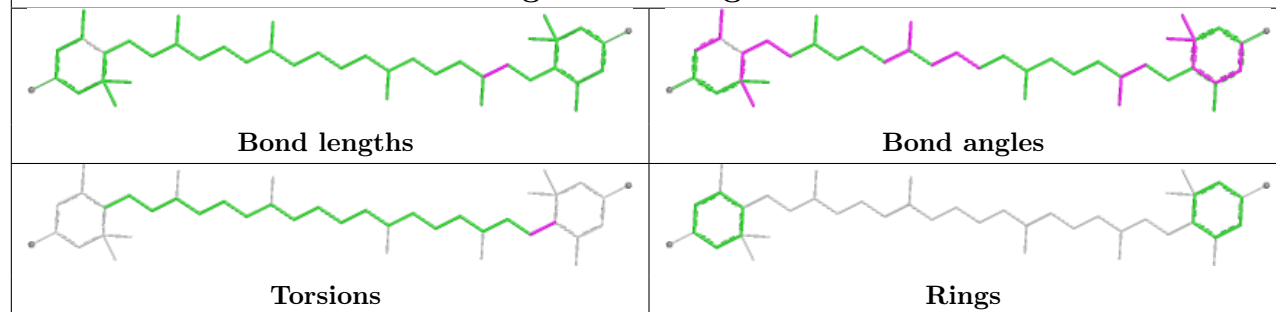


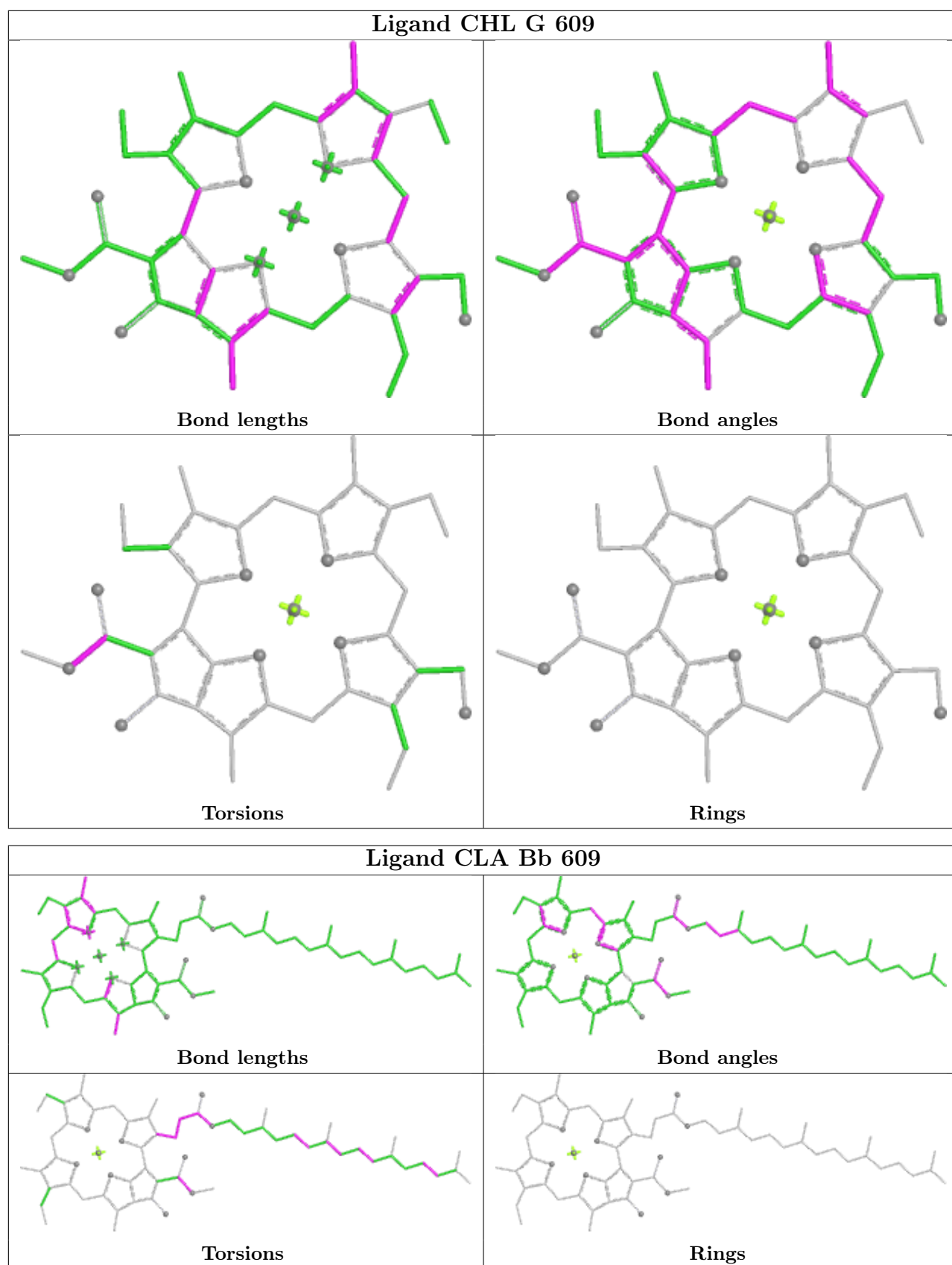


Ligand CLA NN 611

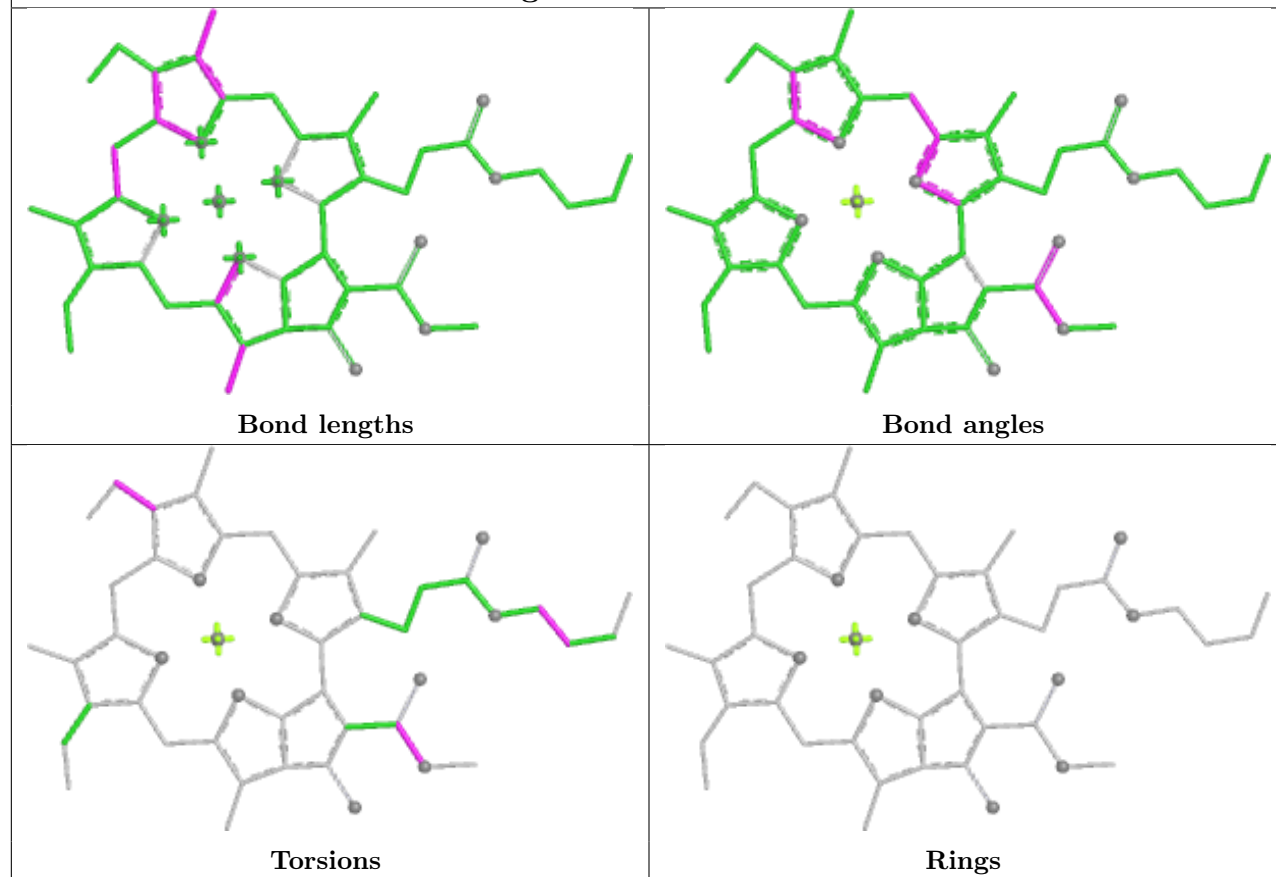


Ligand LUT Gg 317

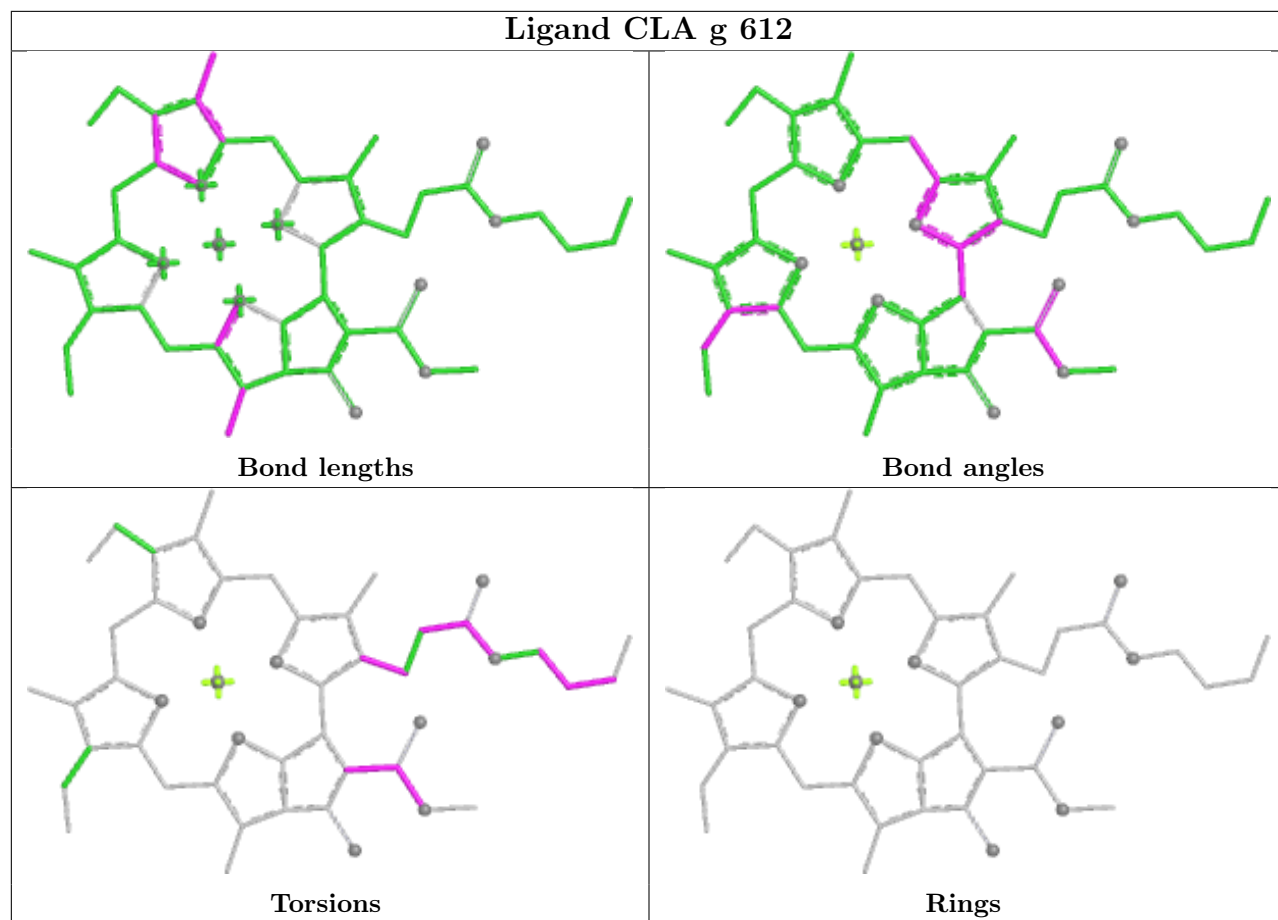




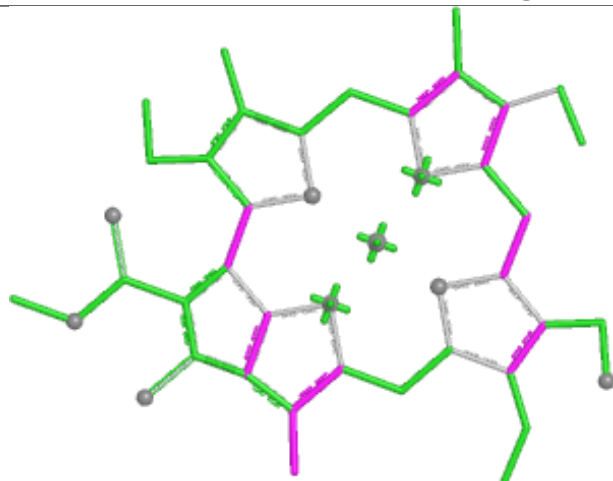
Ligand CLA Nn 302



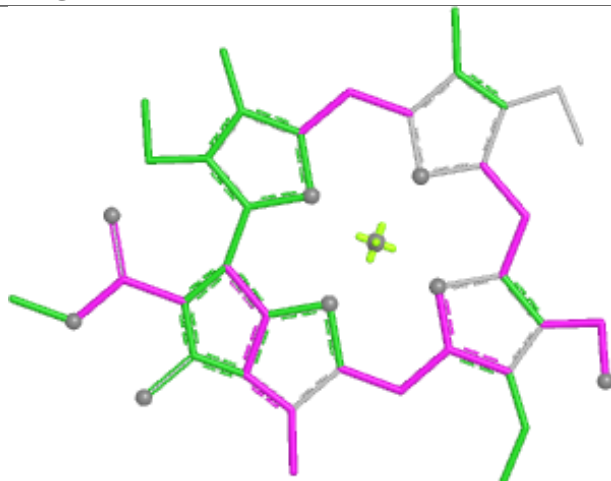
Ligand CLA g 612



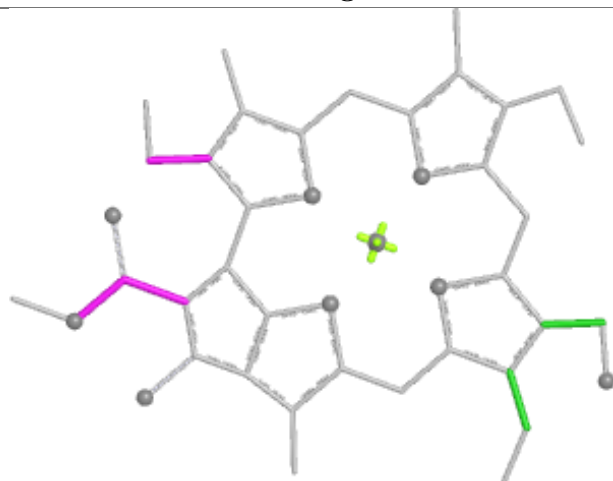
Ligand CHL g 605



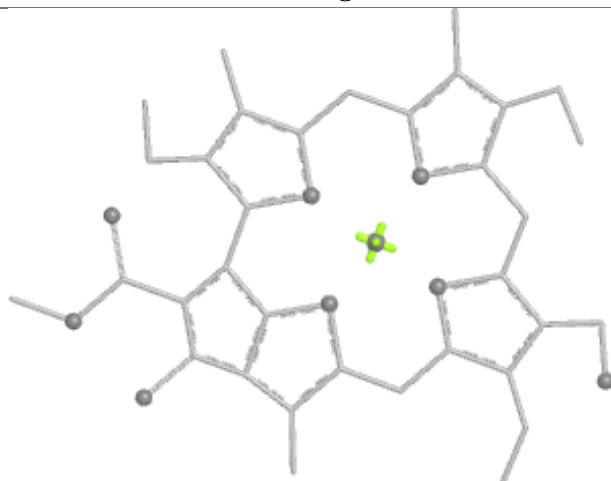
Bond lengths



Bond angles

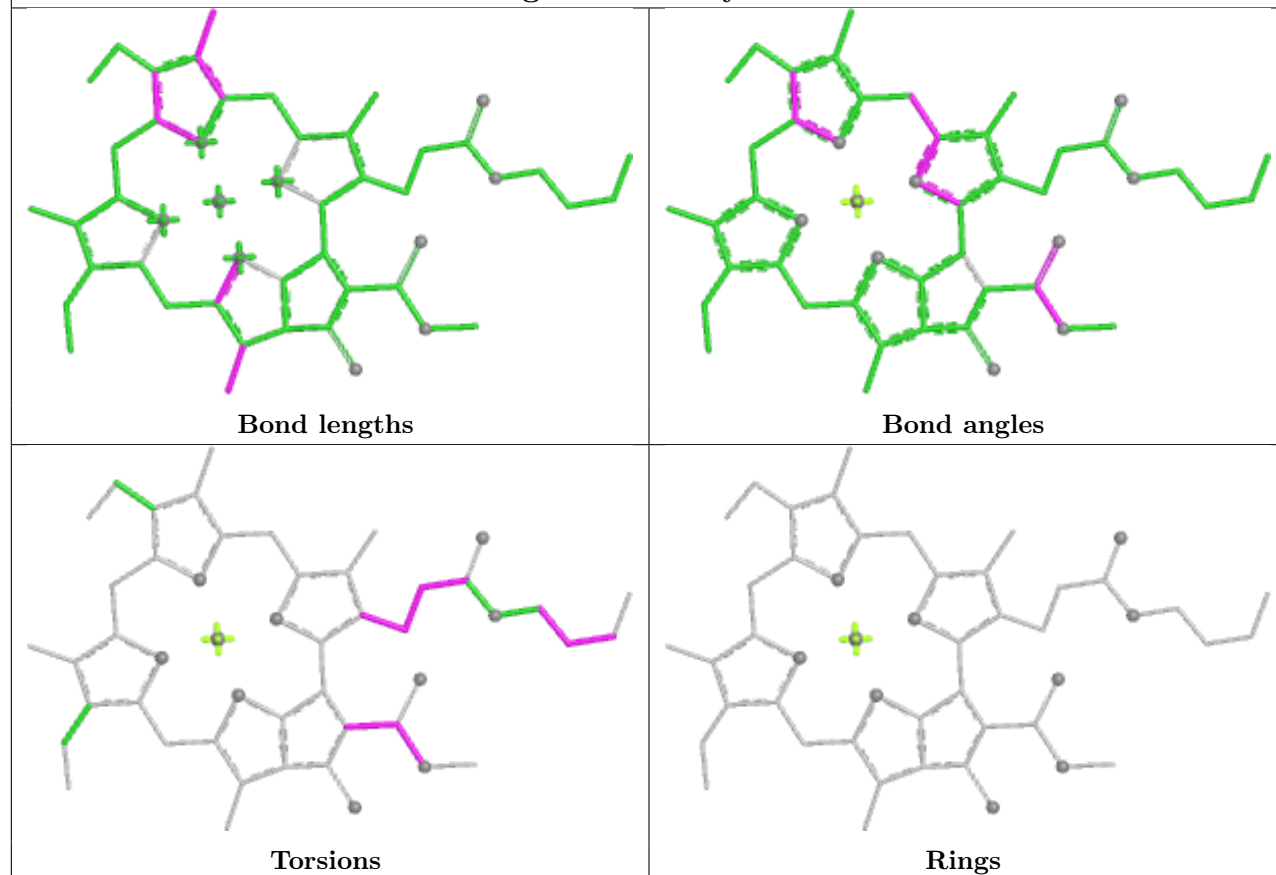


Torsions

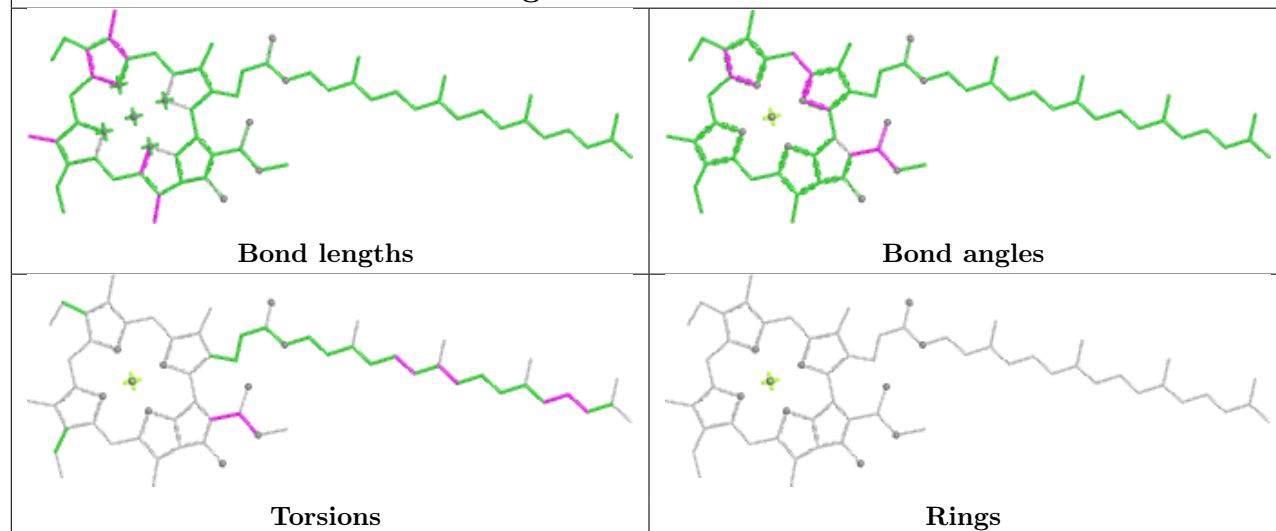


Rings

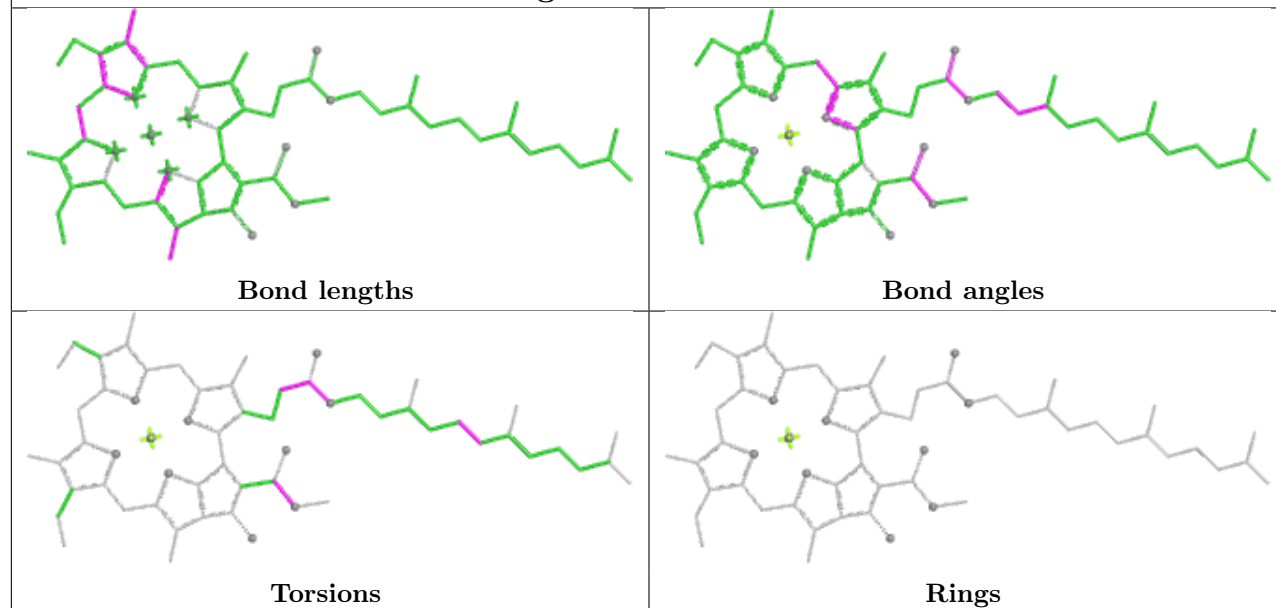
Ligand CLA Yy 604



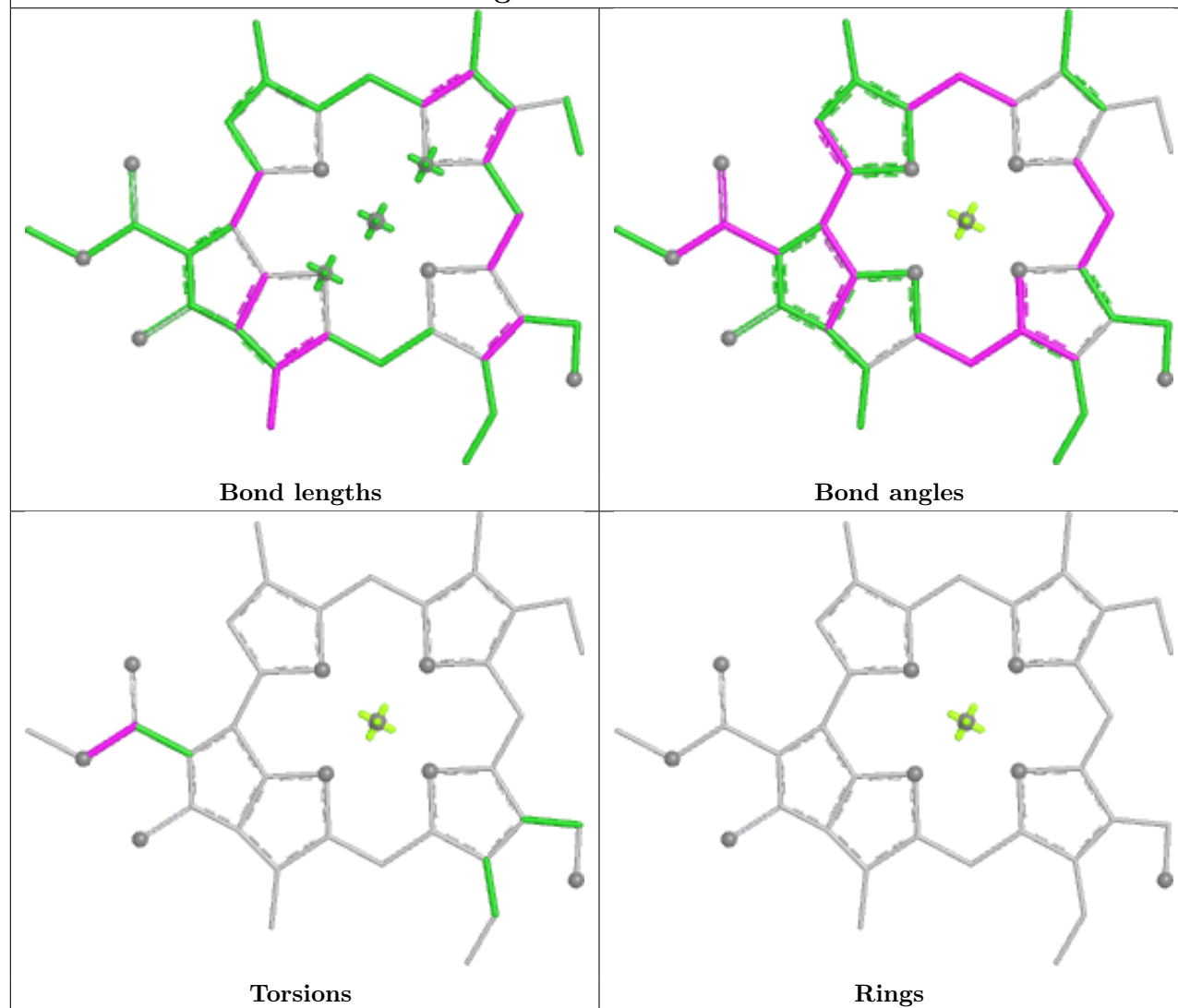
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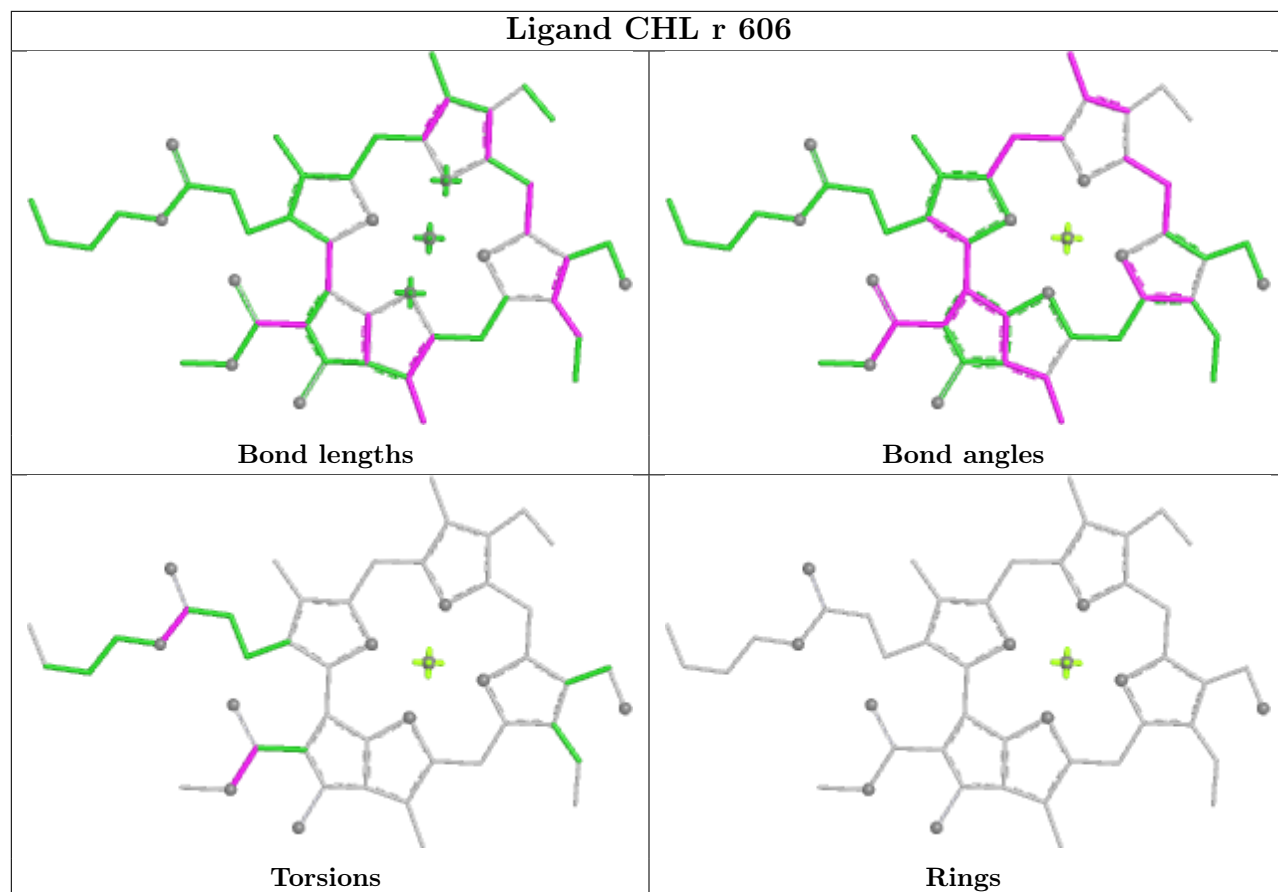


Ligand CLA c 508

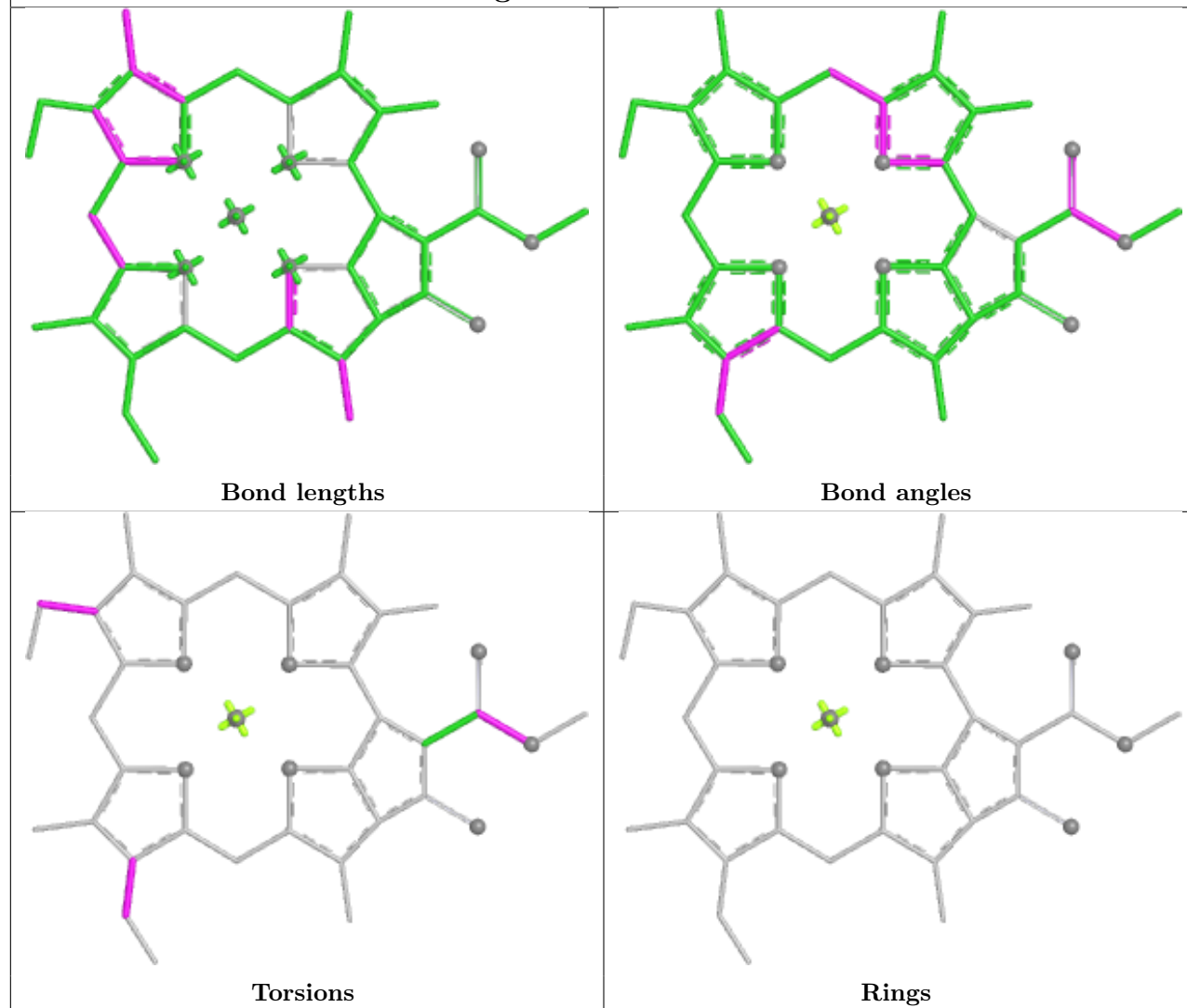


Ligand CHL 2 607

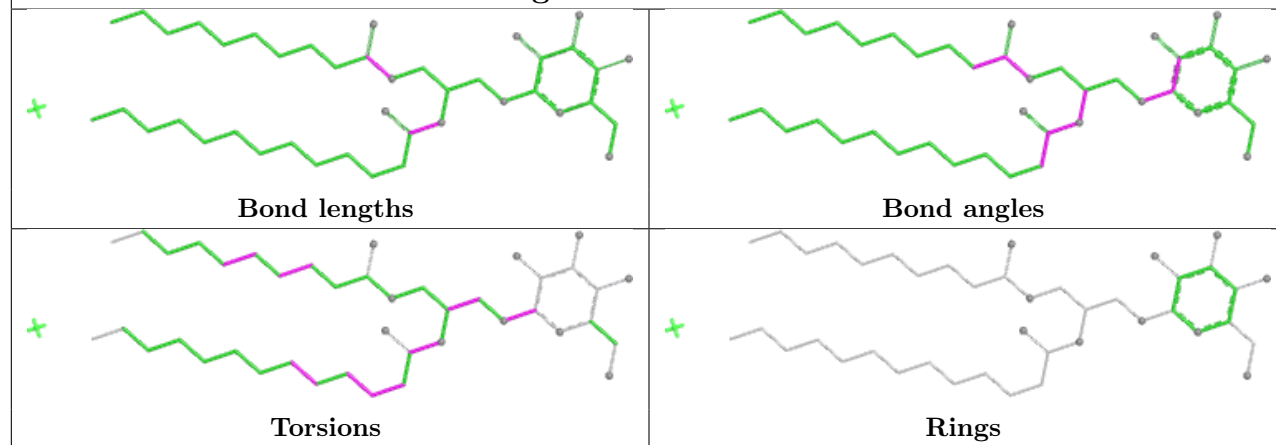




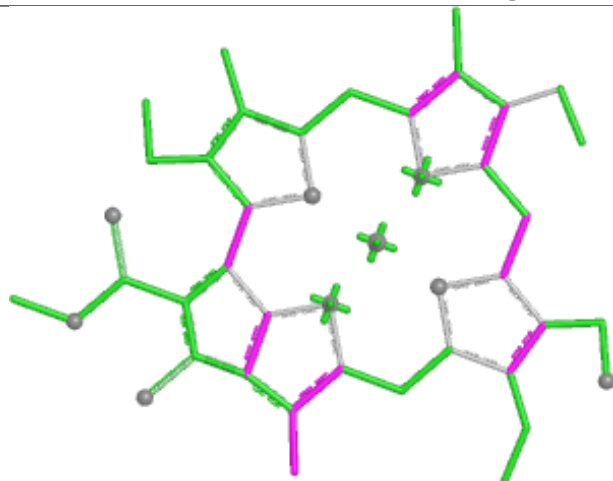
Ligand CLA R 613



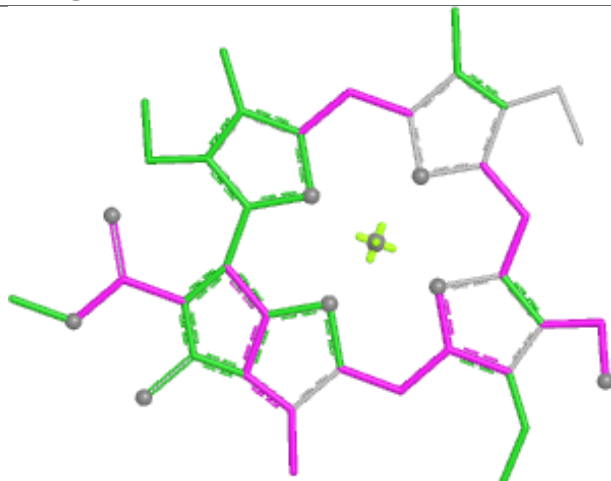
Ligand LMG a 412



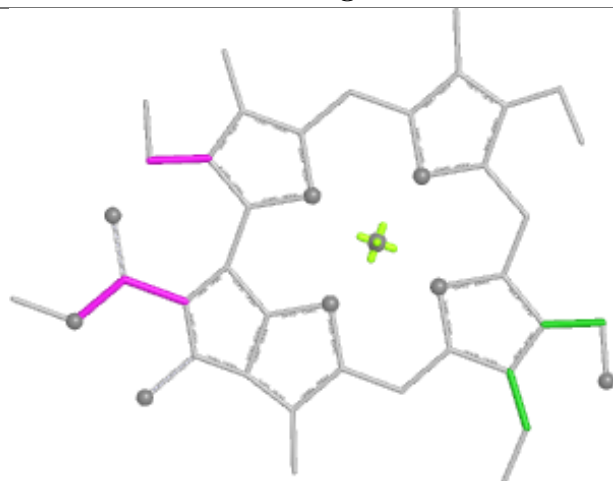
Ligand CHL Gg 306



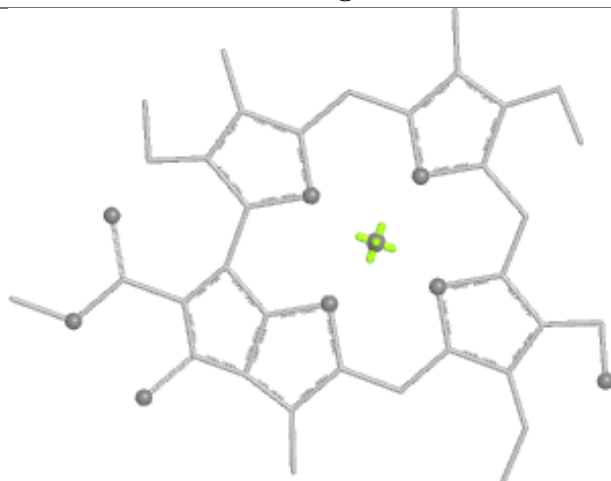
Bond lengths



Bond angles

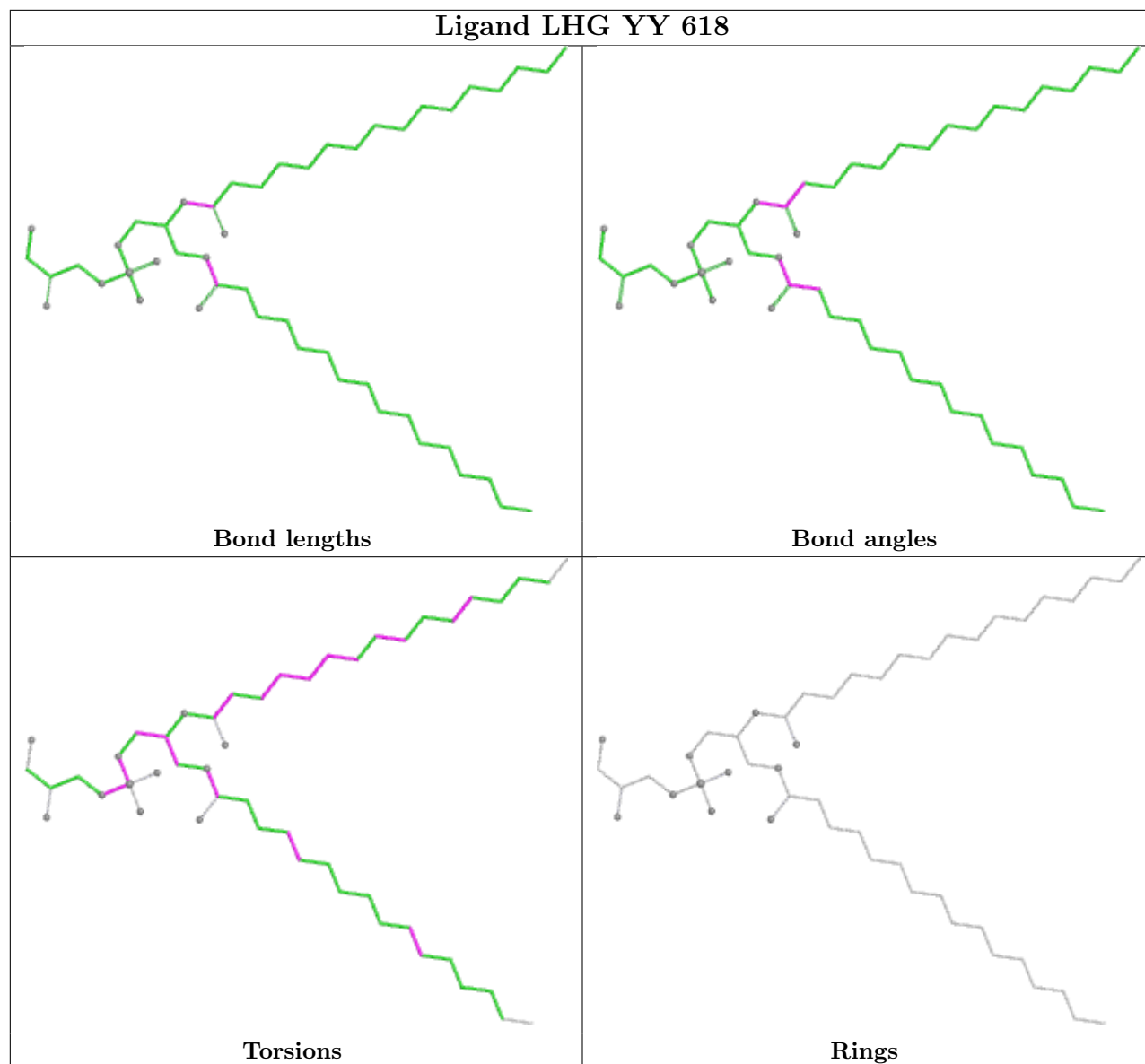


Torsions

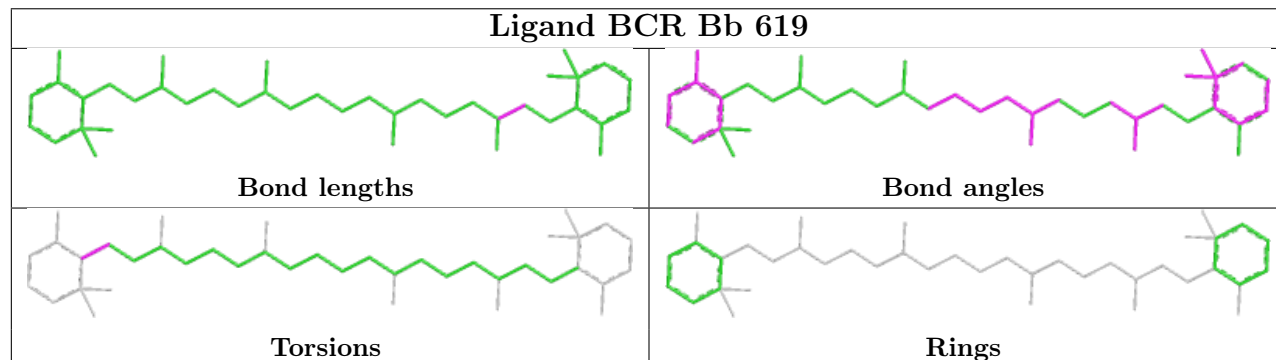


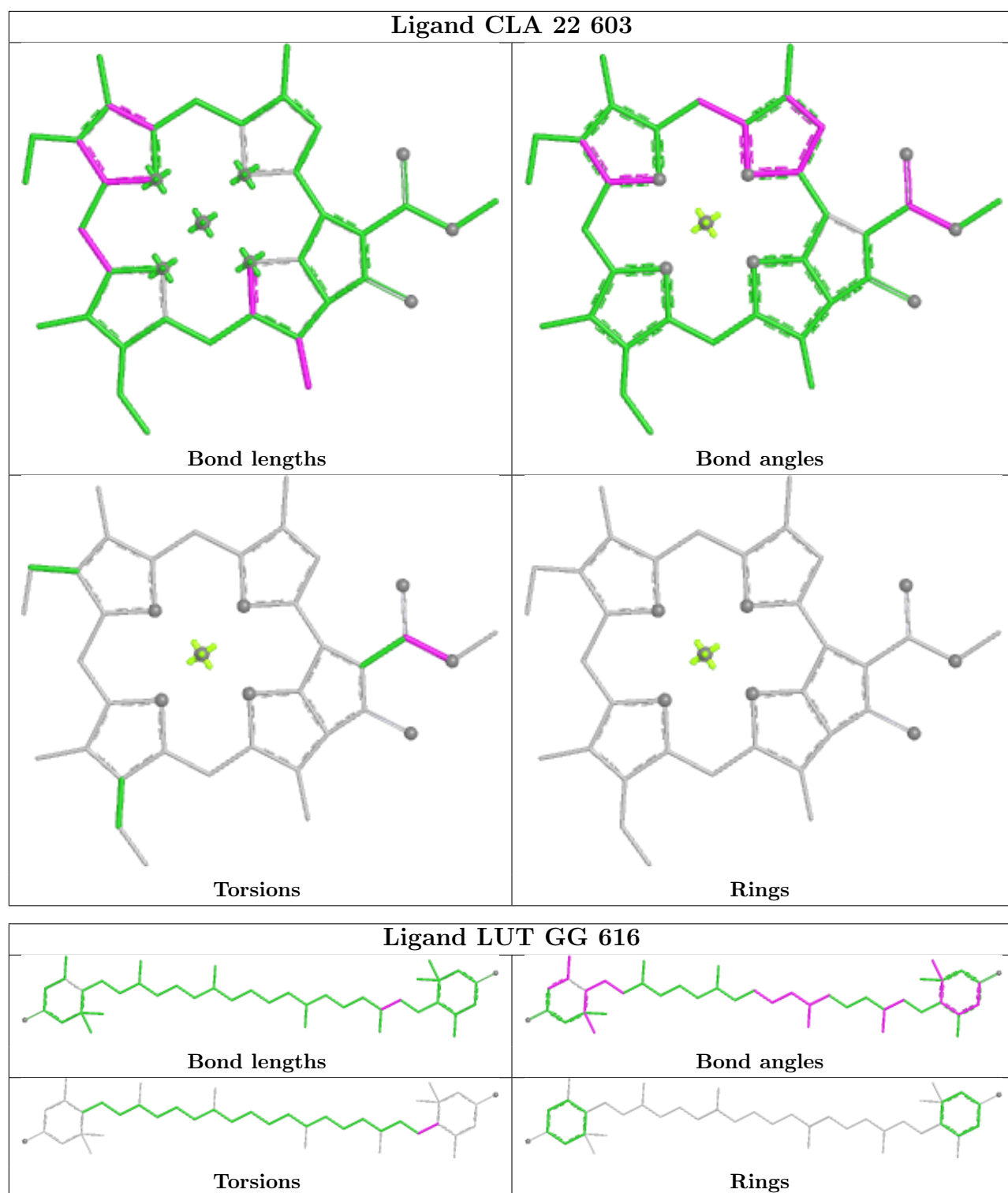
Rings

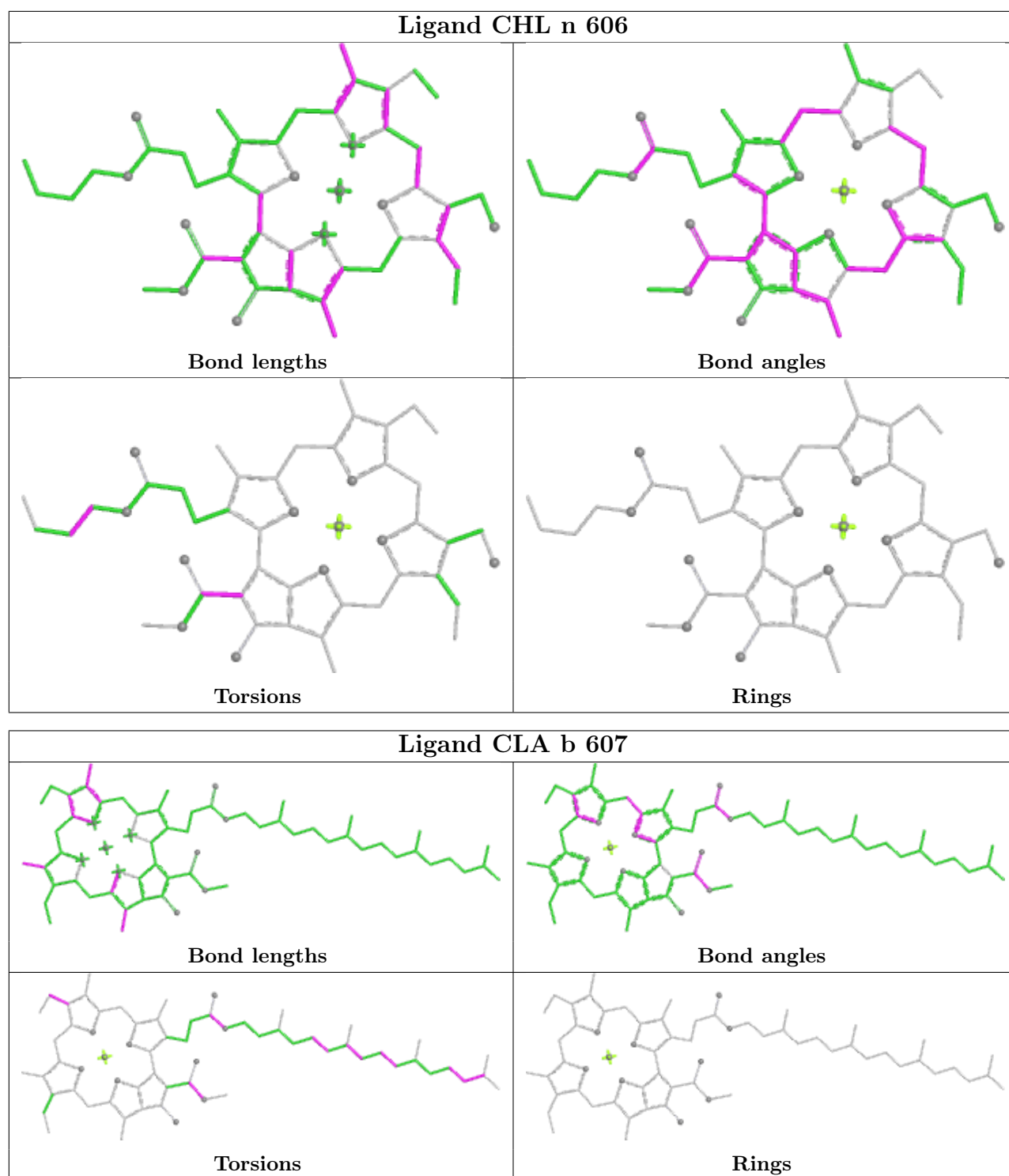
Ligand LHG YY 618

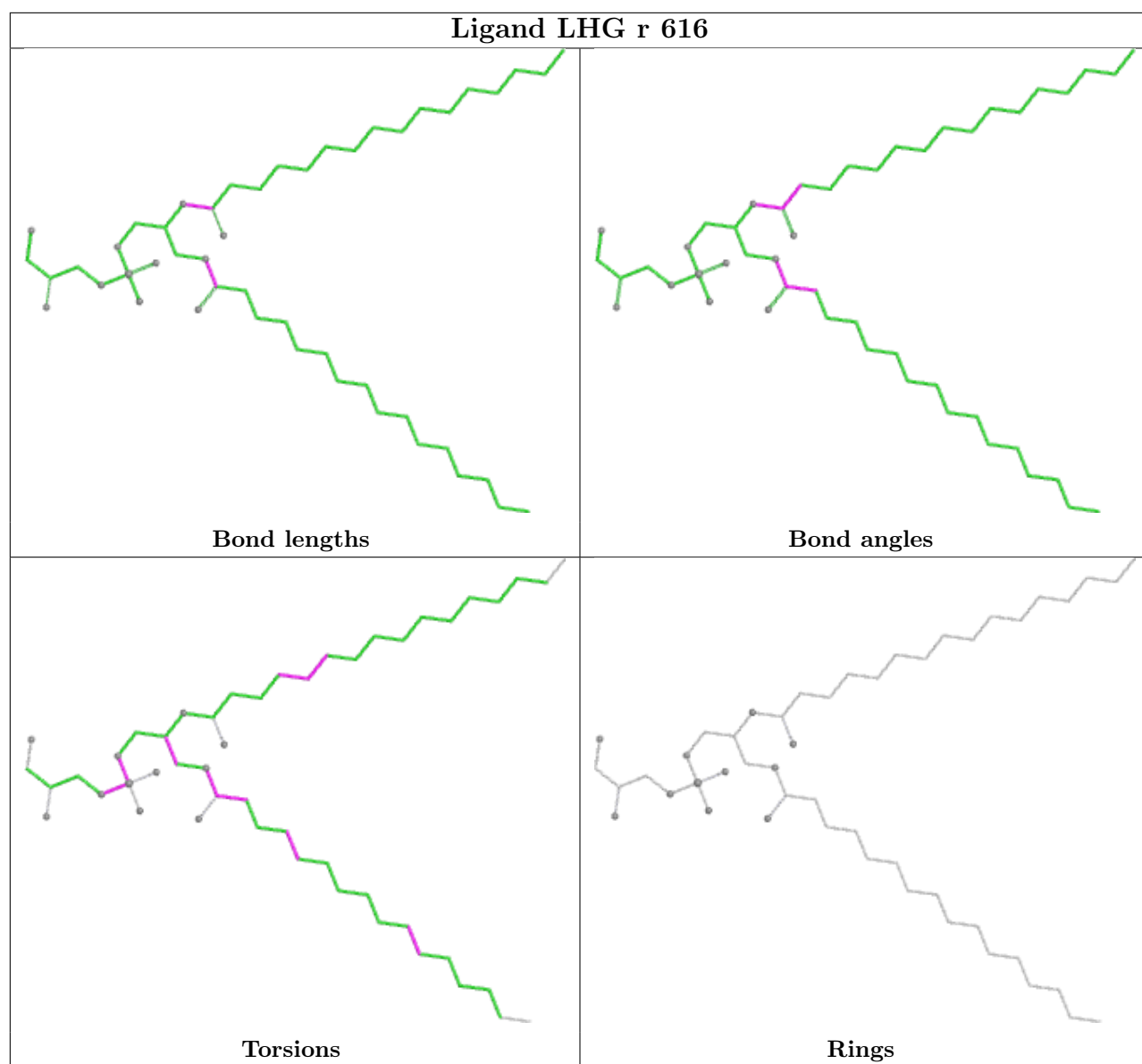


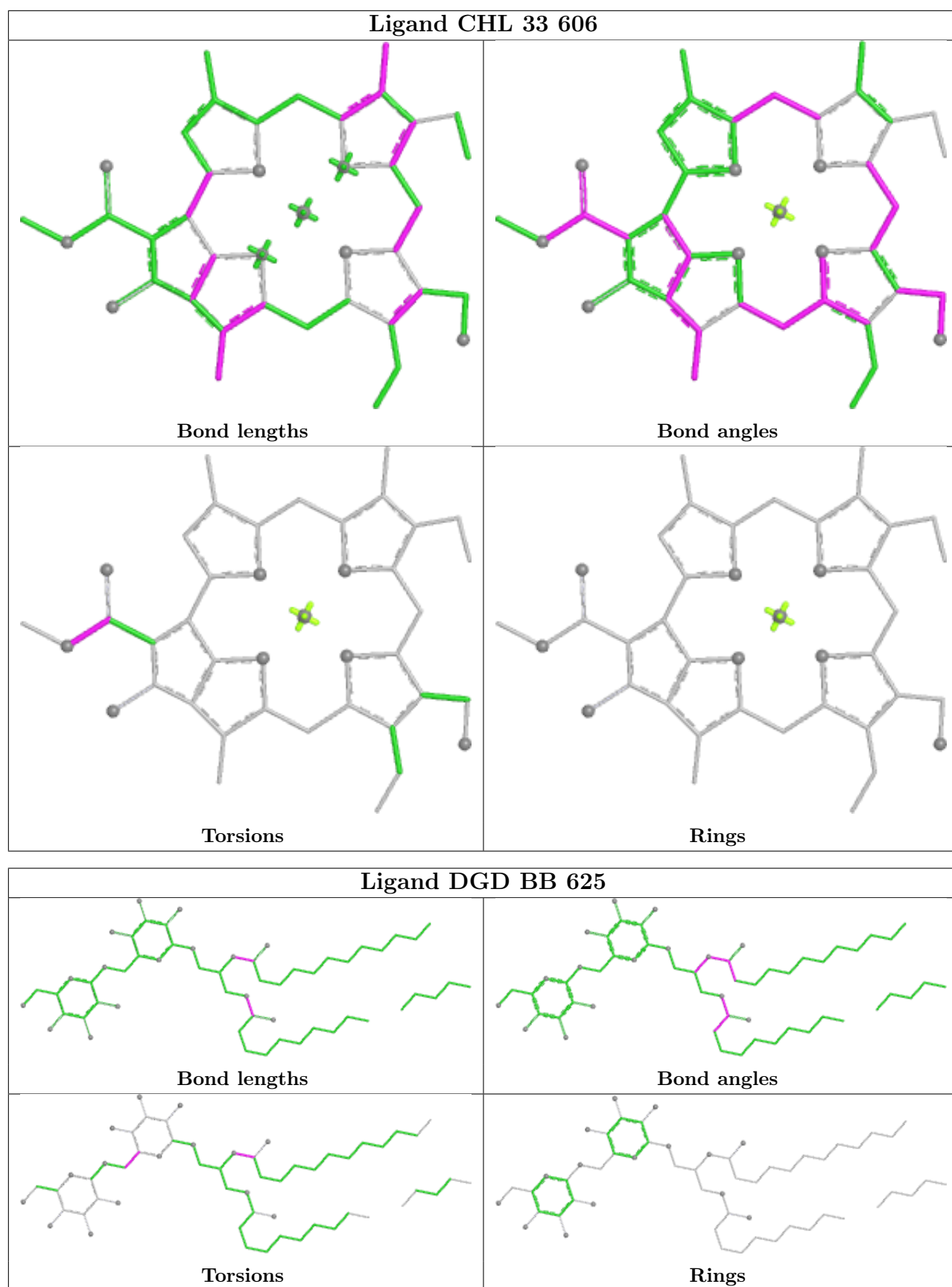
Ligand BCR Bb 619

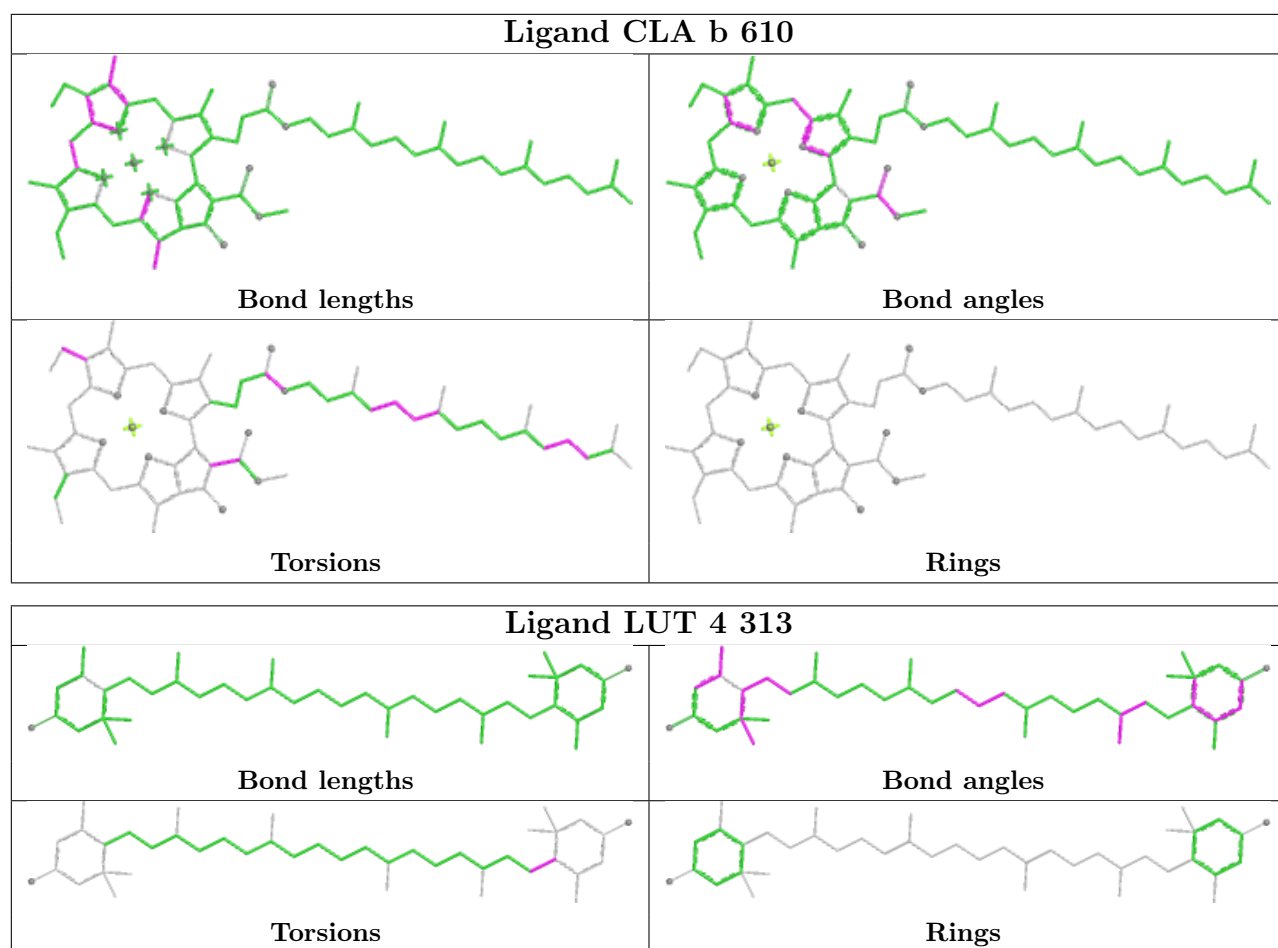




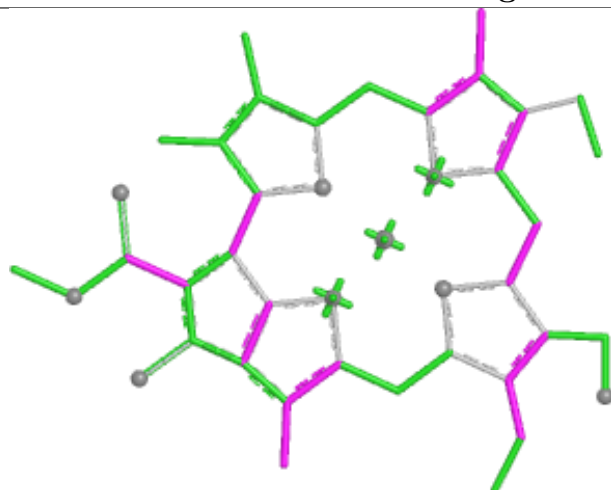




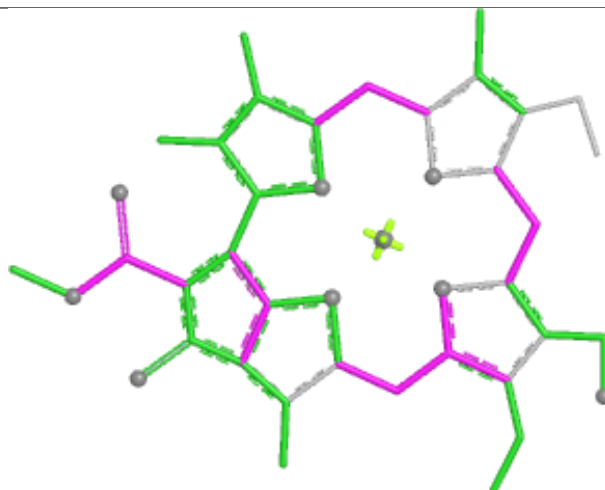




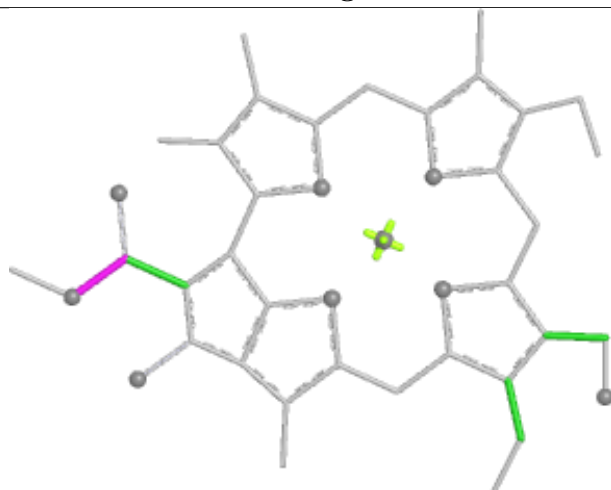
Ligand CHL NN 606



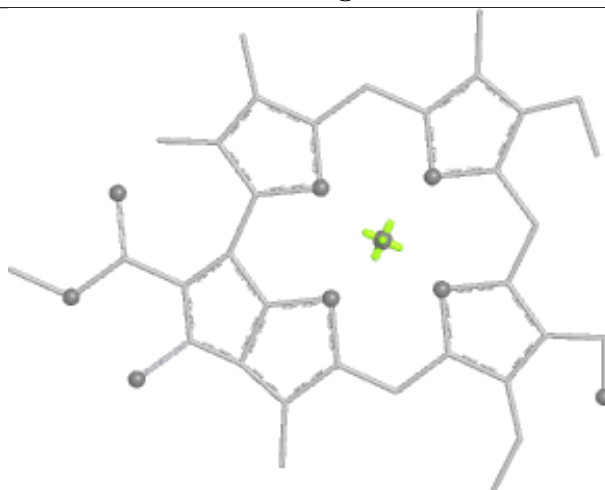
Bond lengths



Bond angles

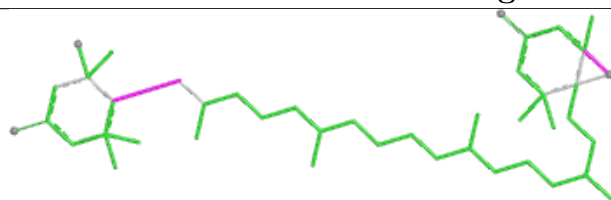


Torsions

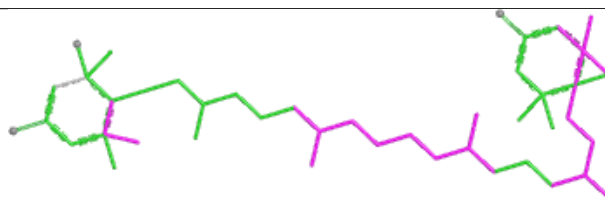


Rings

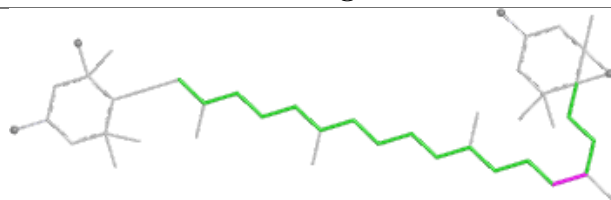
Ligand NEX YY 617



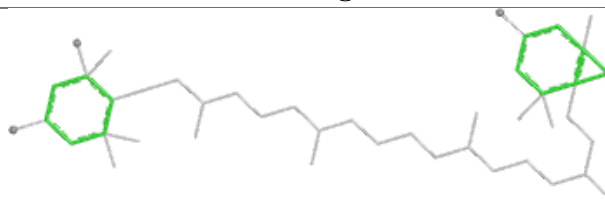
Bond lengths



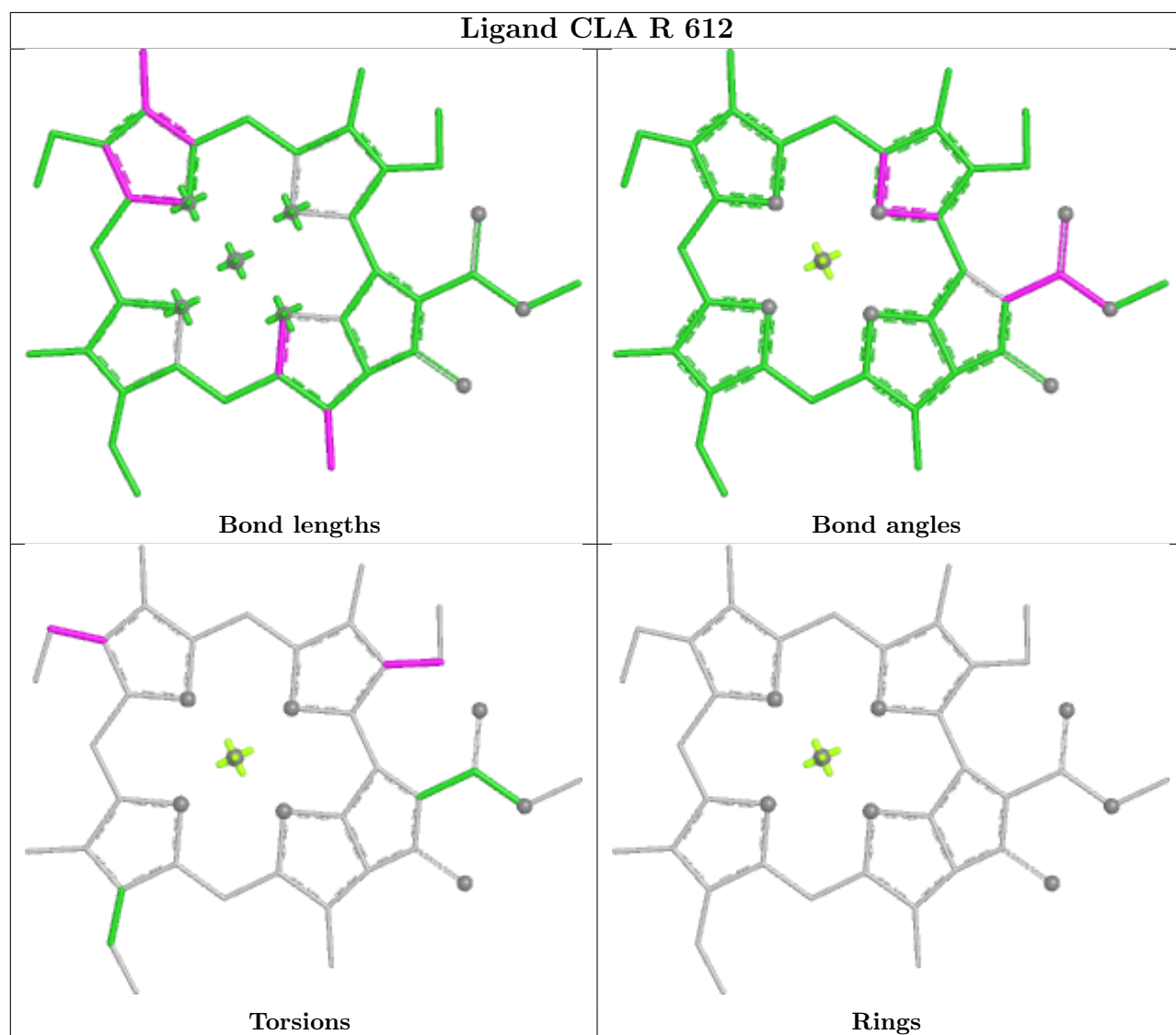
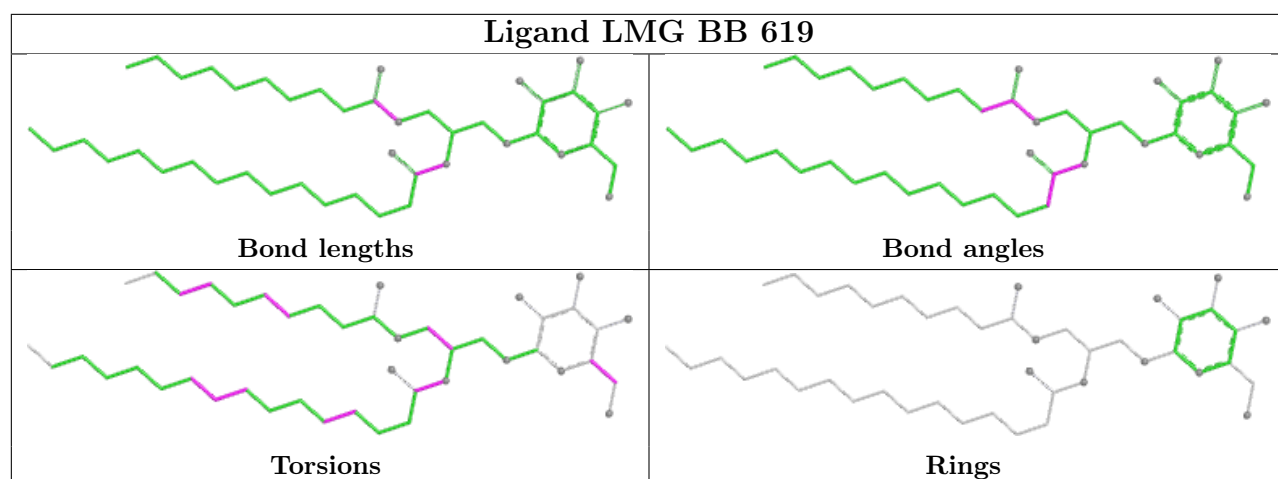
Bond angles

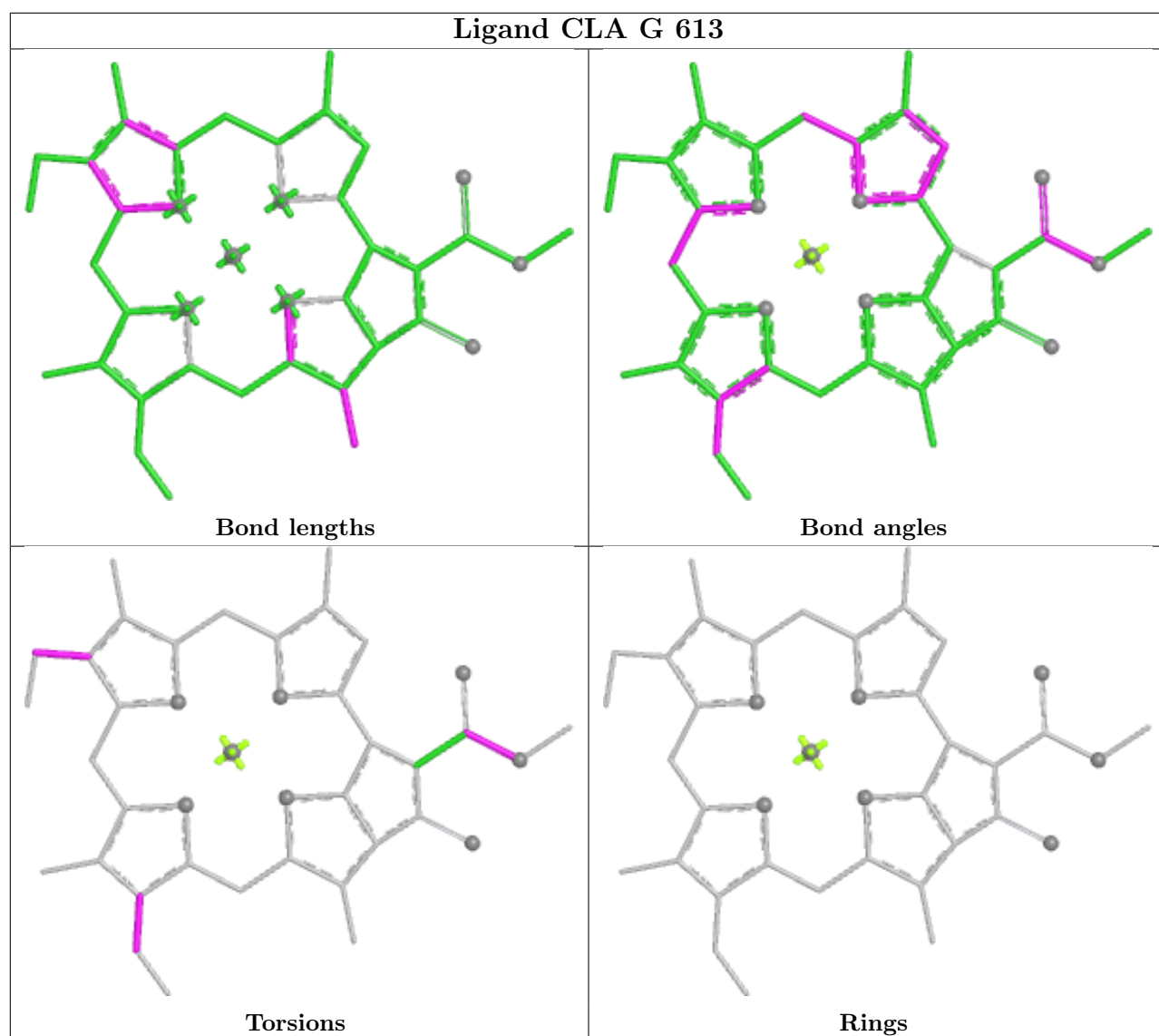


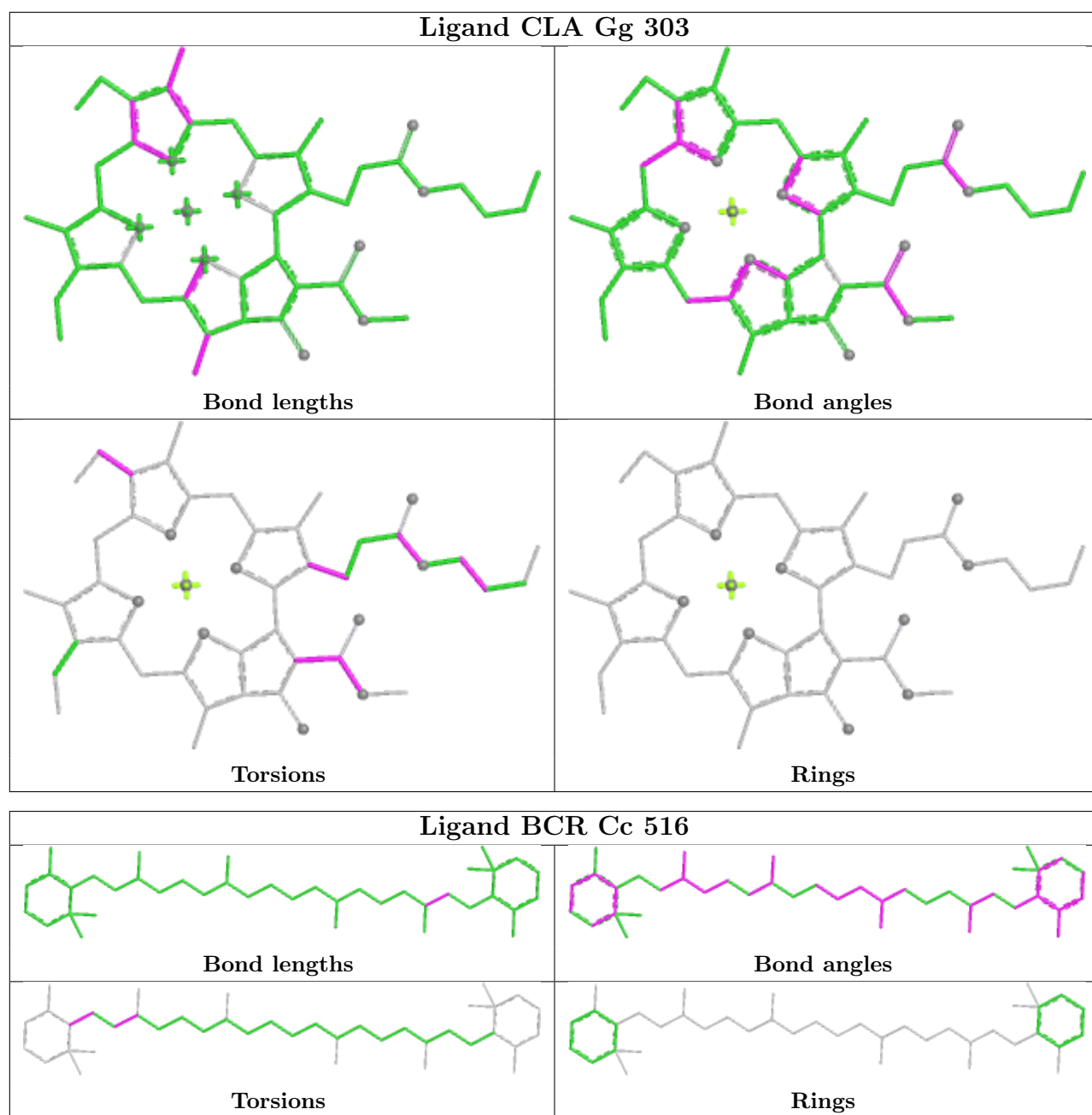
Torsions



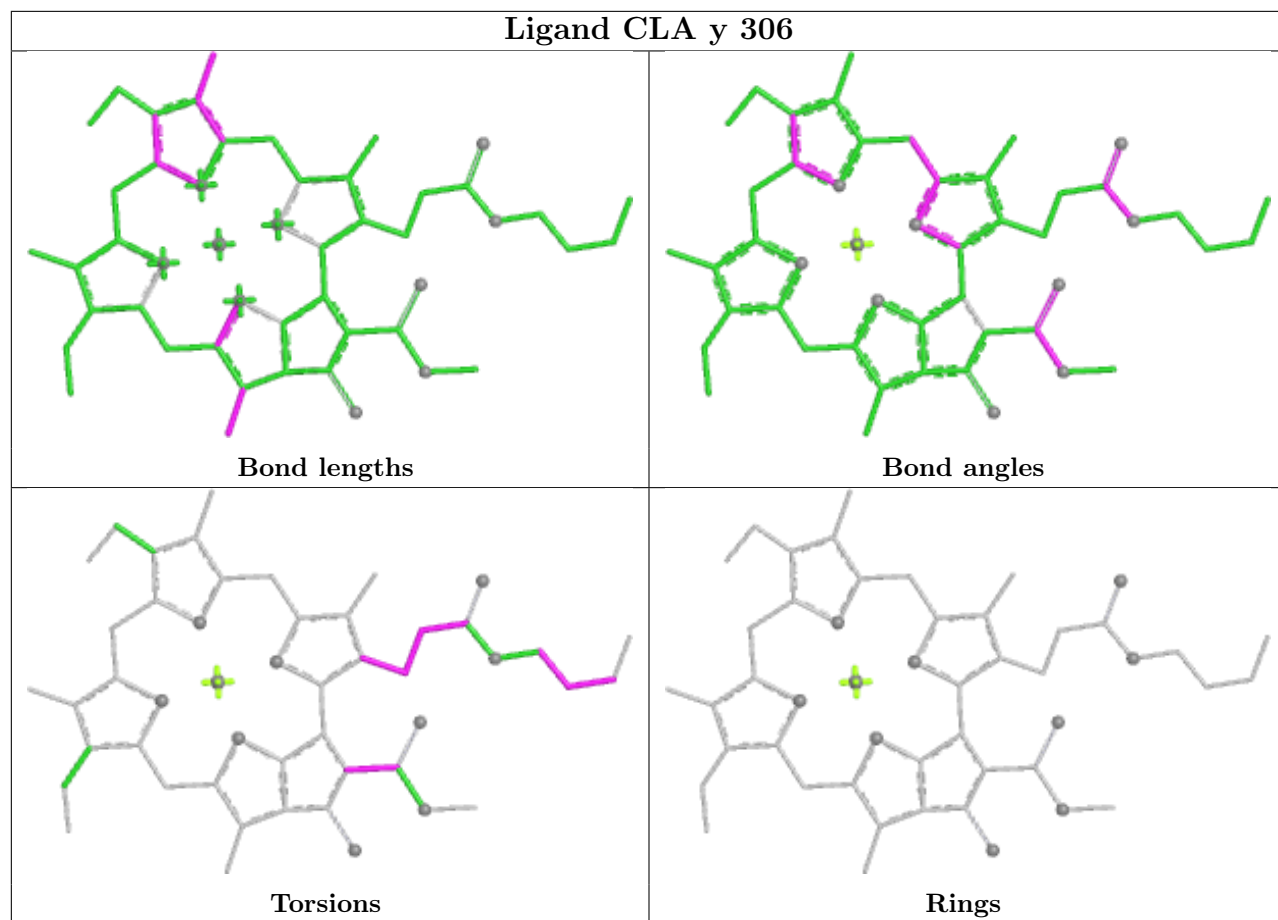
Rings

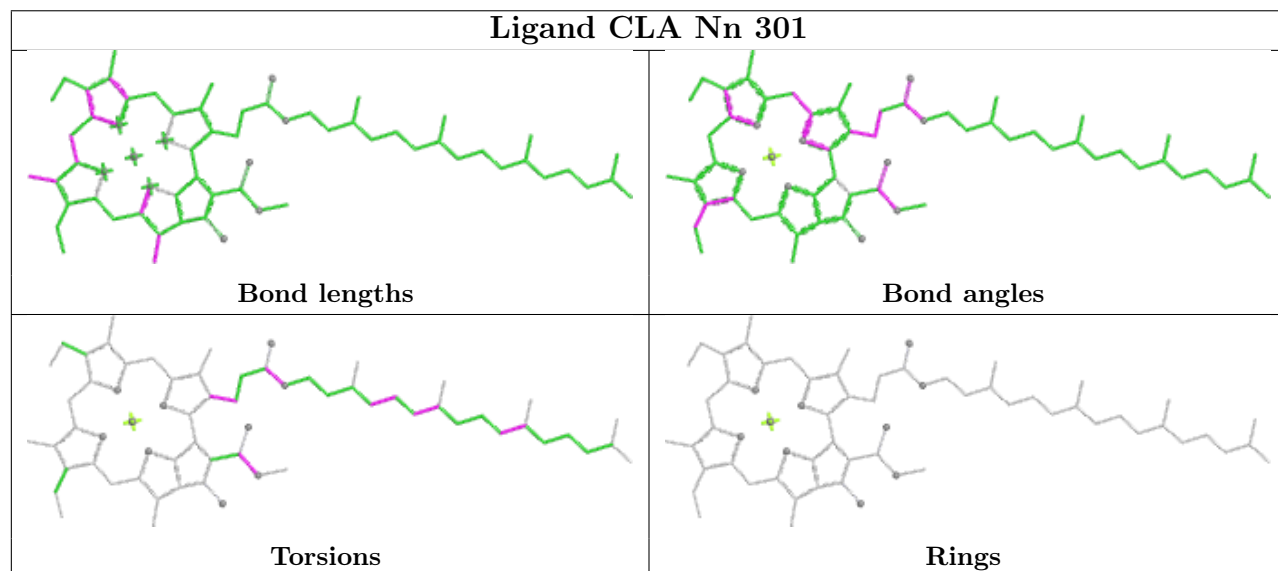
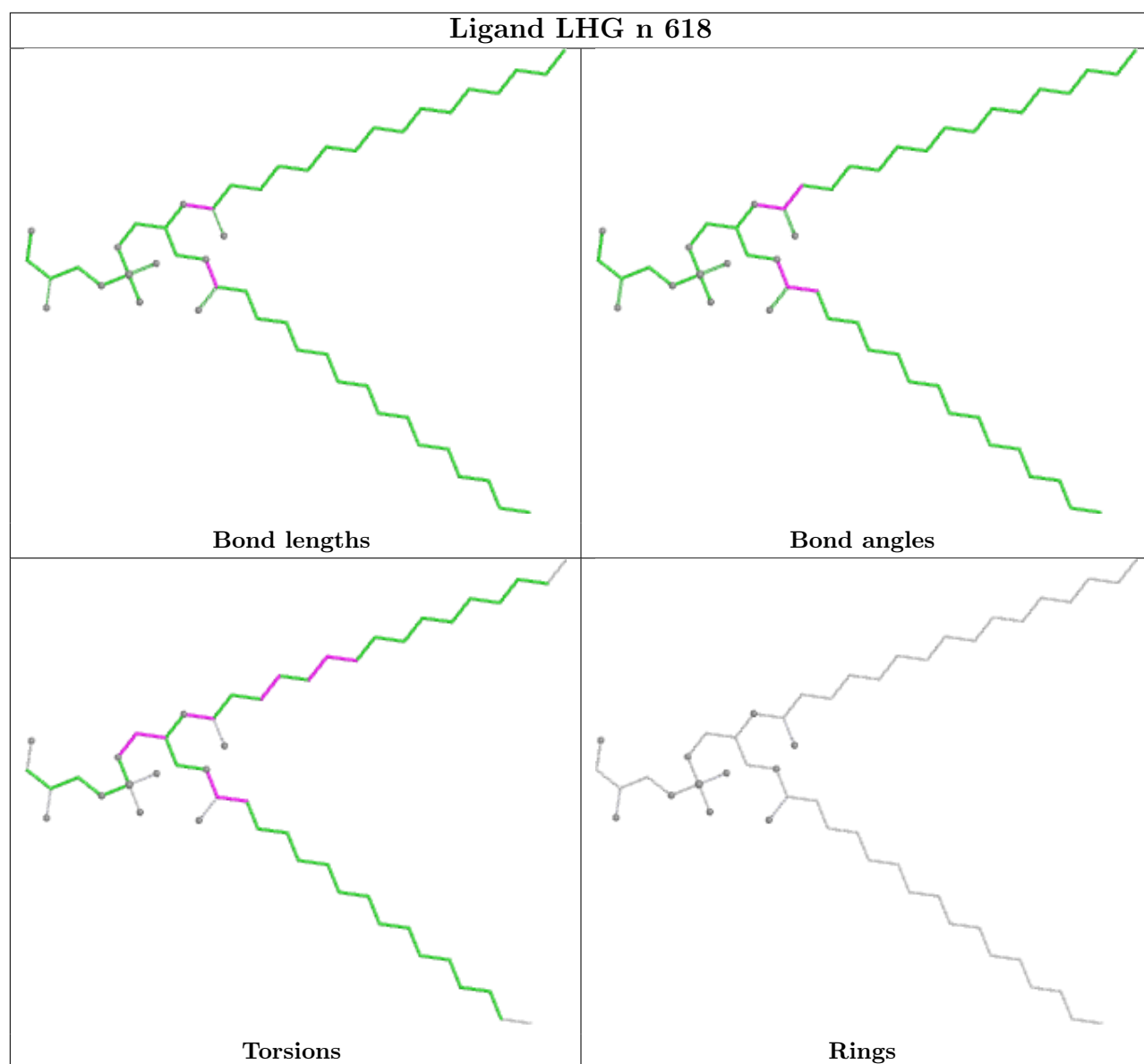


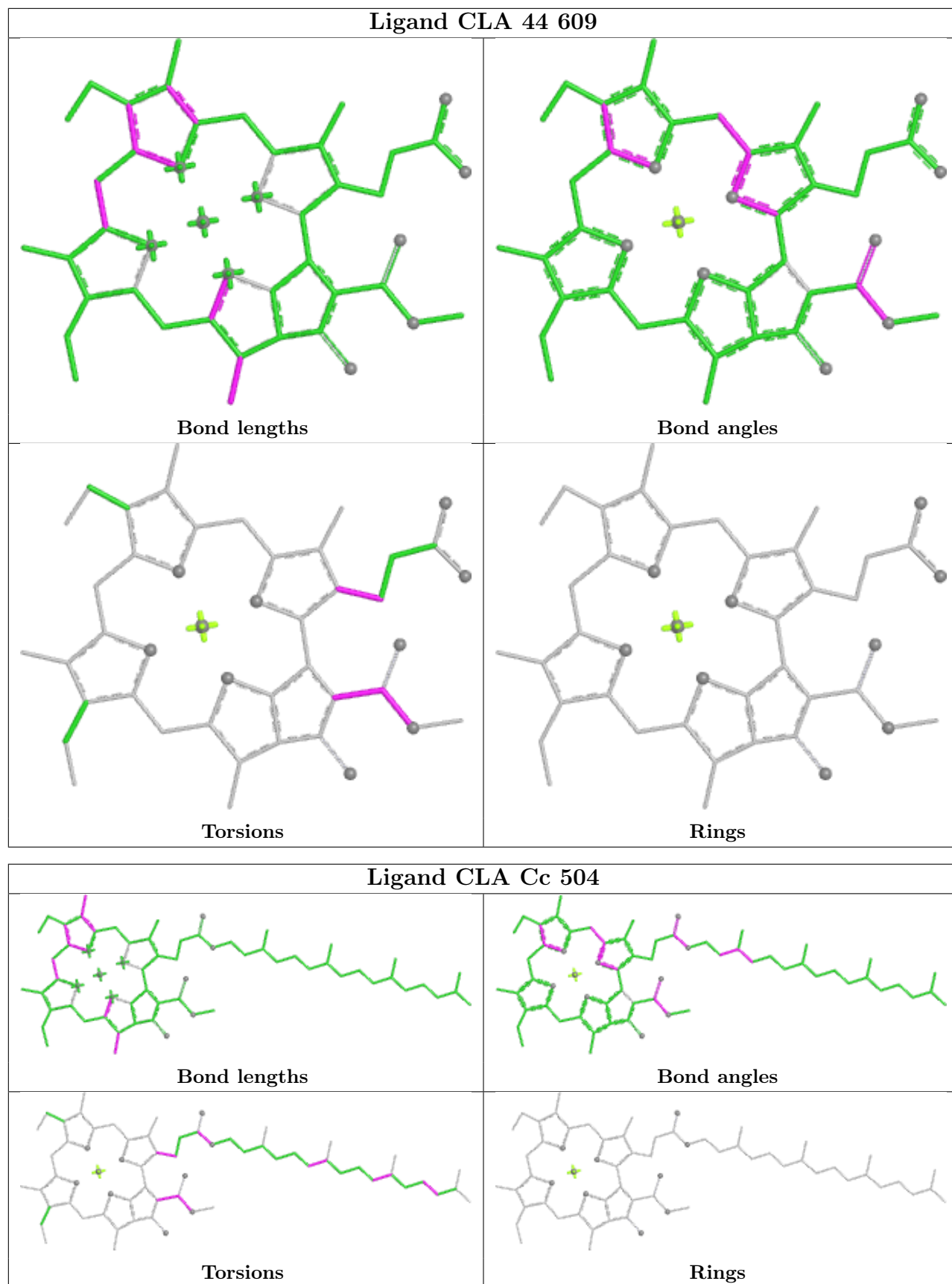


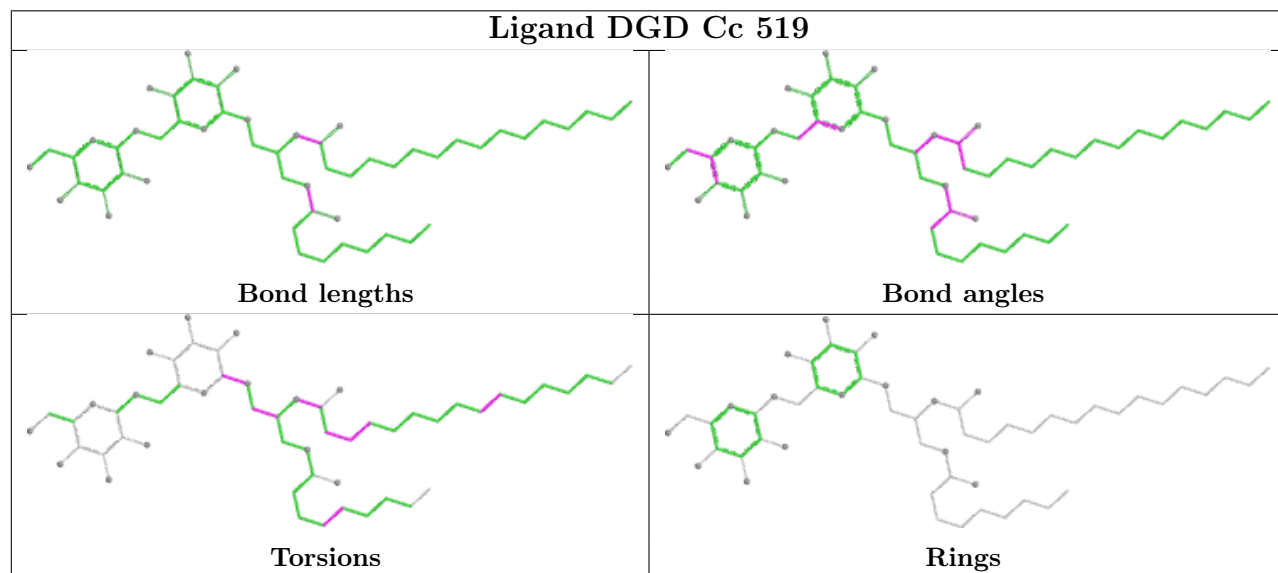
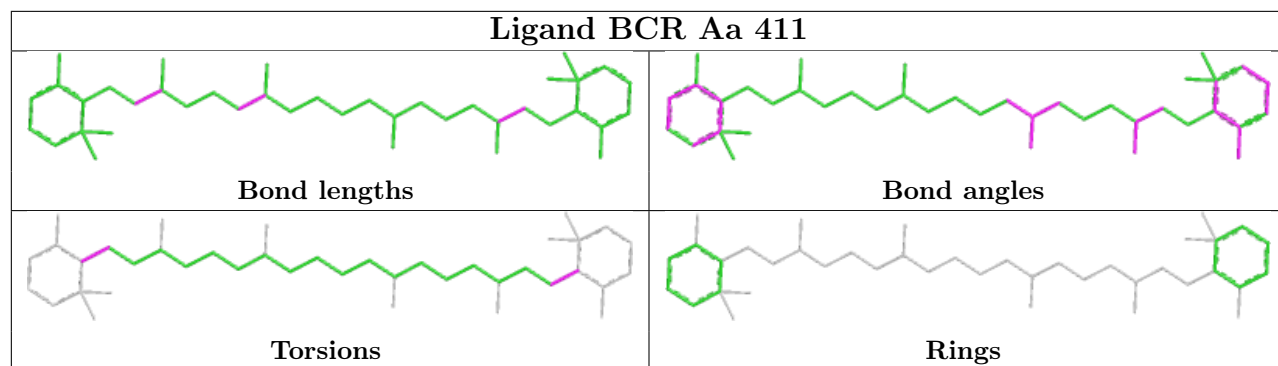


Ligand CLA y 306

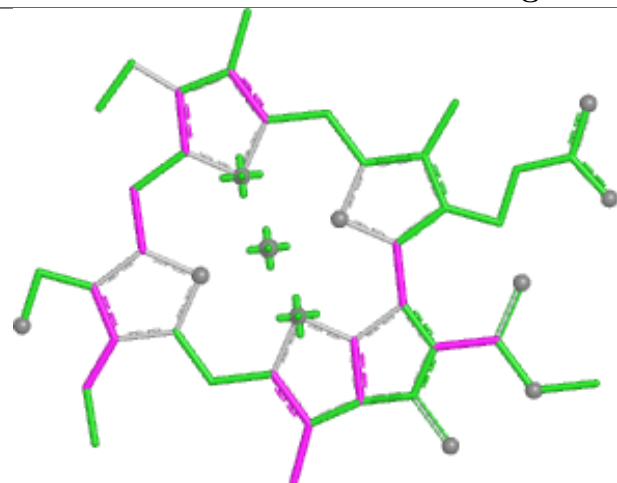




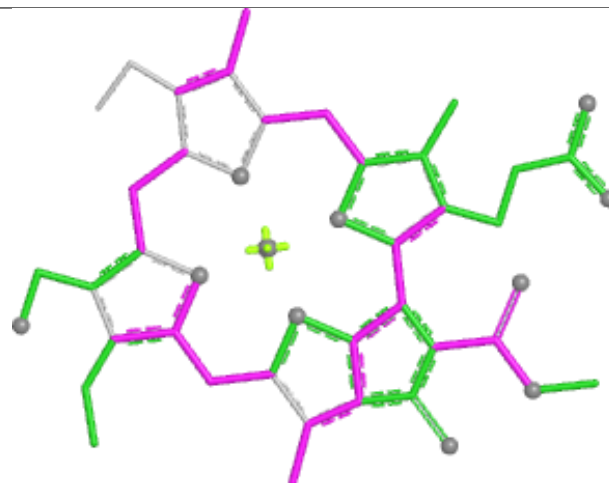




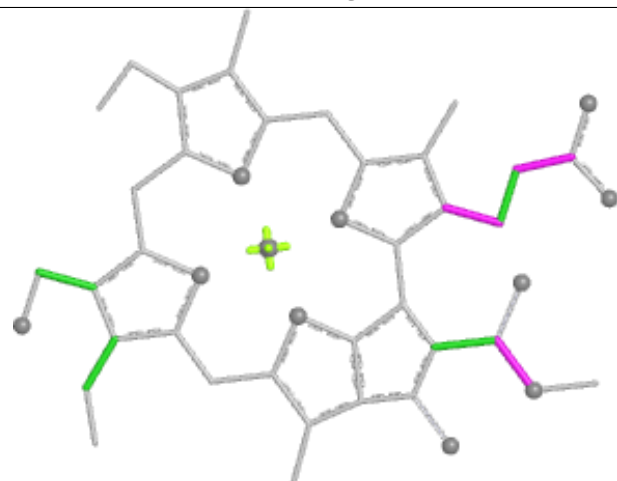
Ligand CHL 4 308



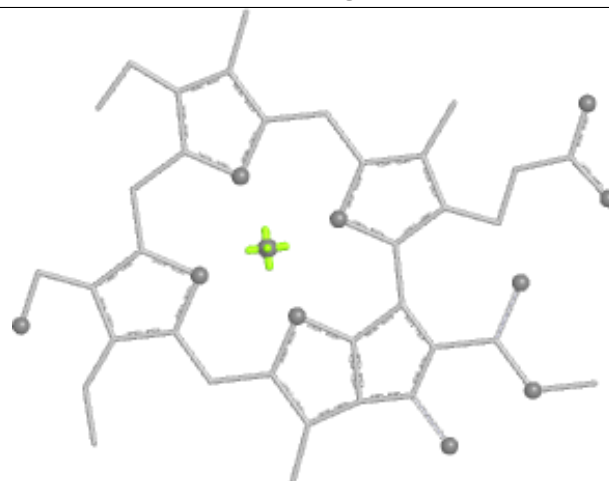
Bond lengths



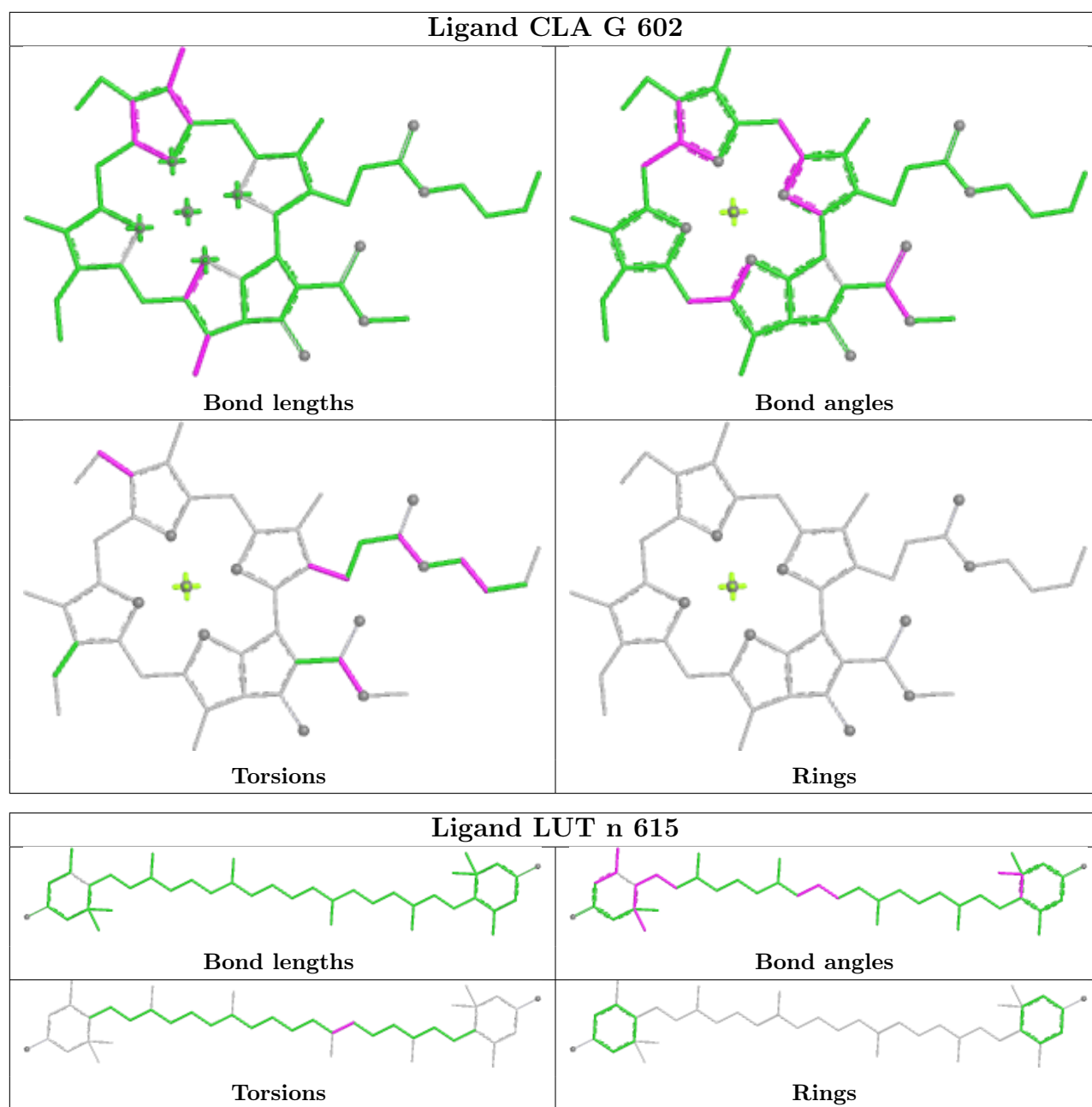
Bond angles

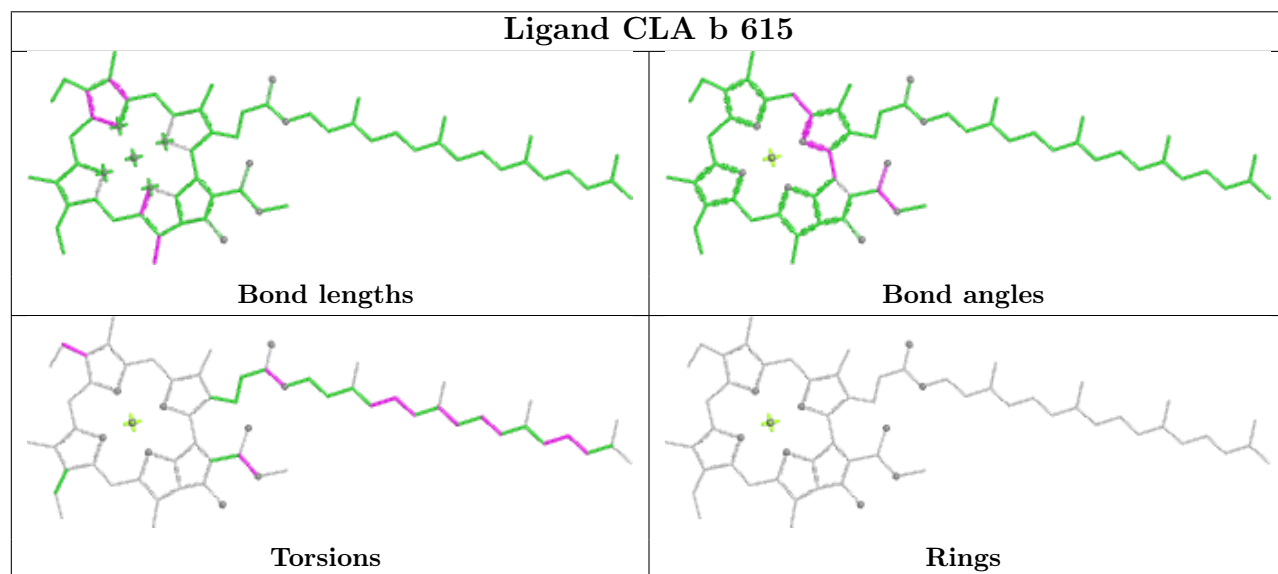
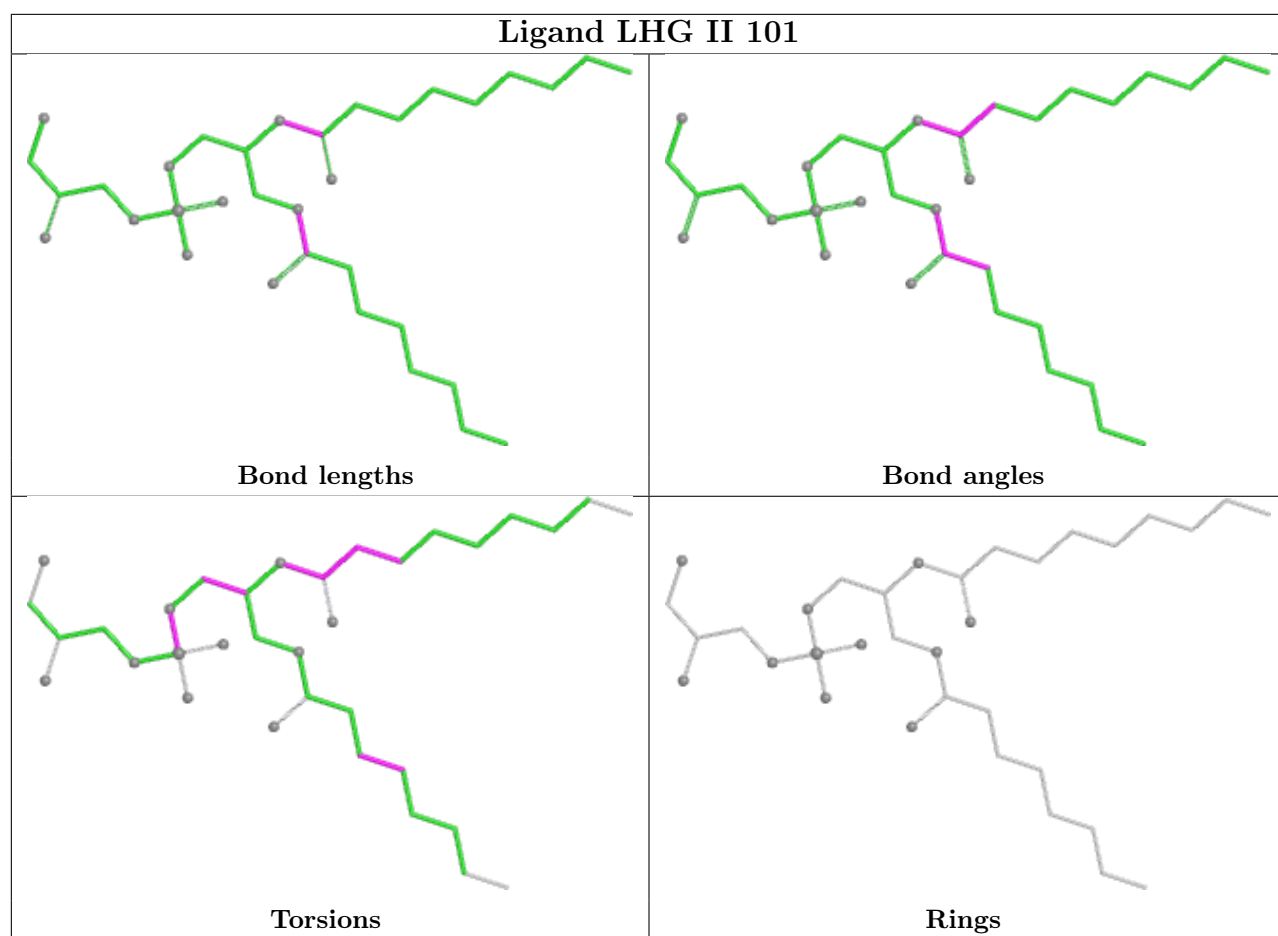


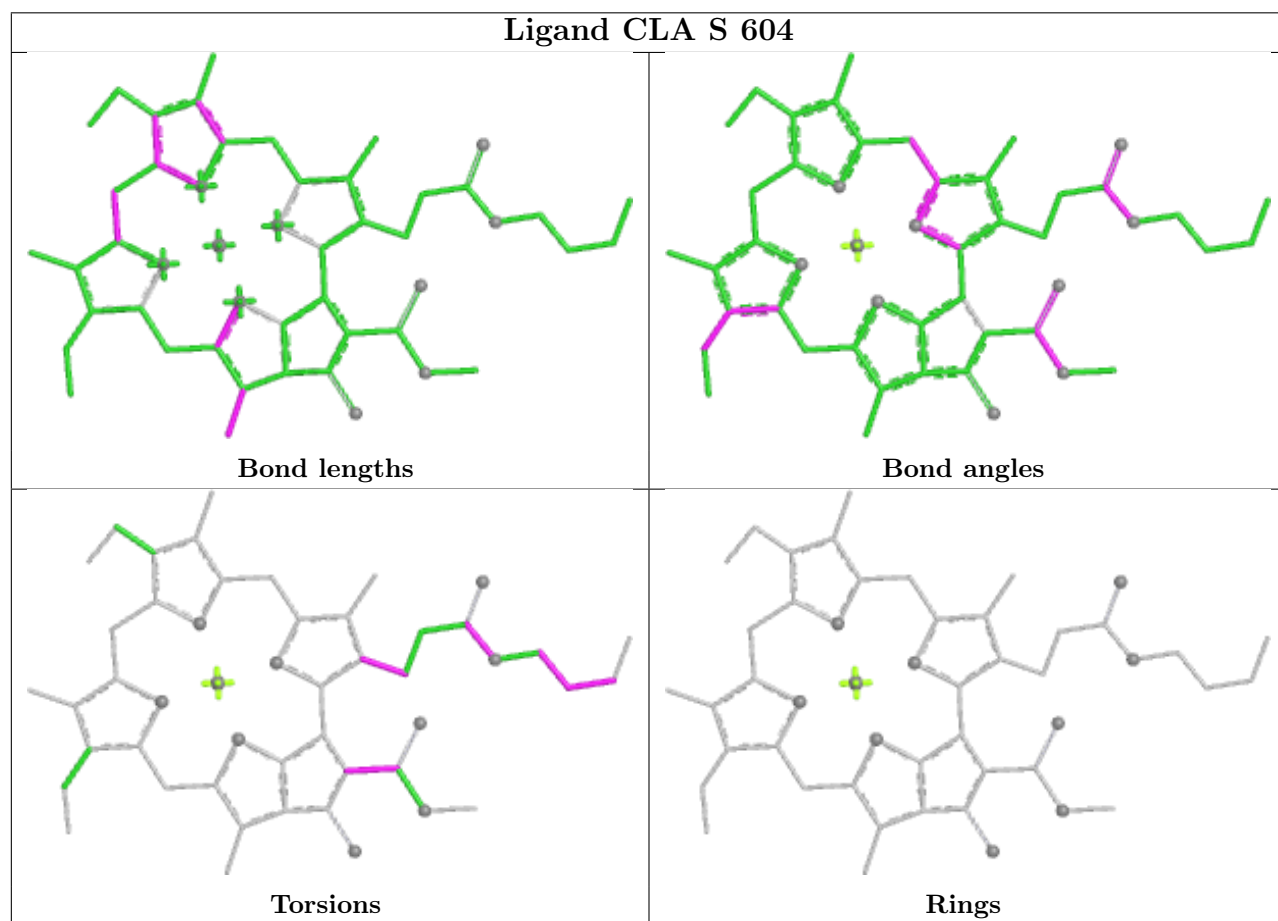
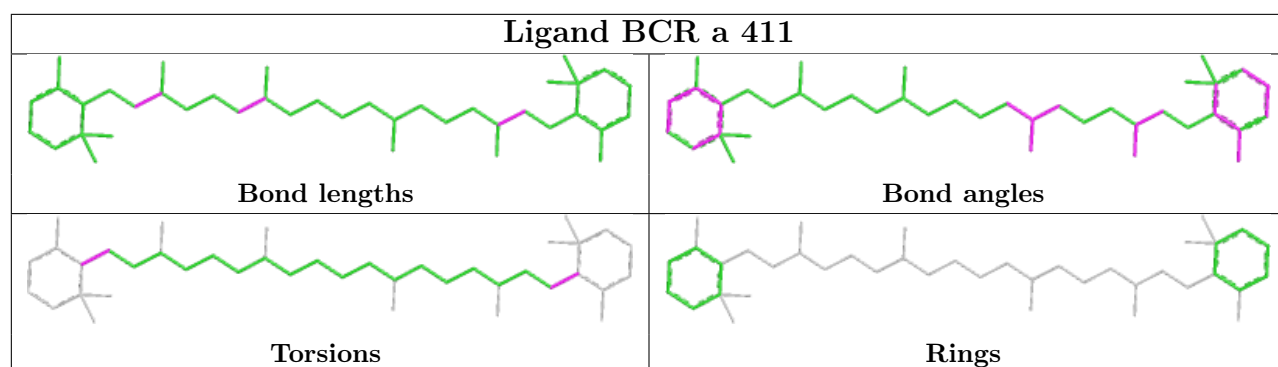
Torsions

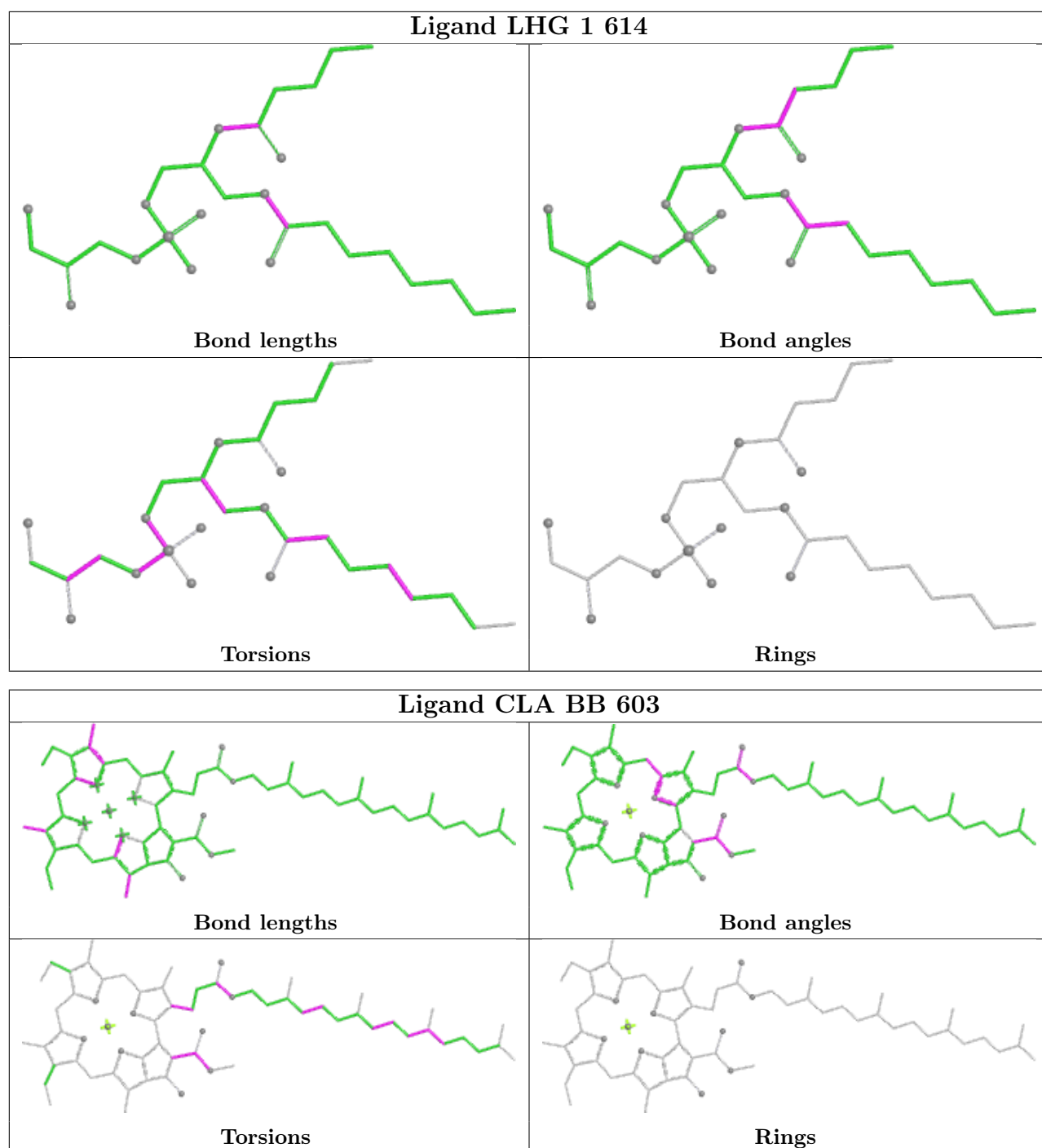


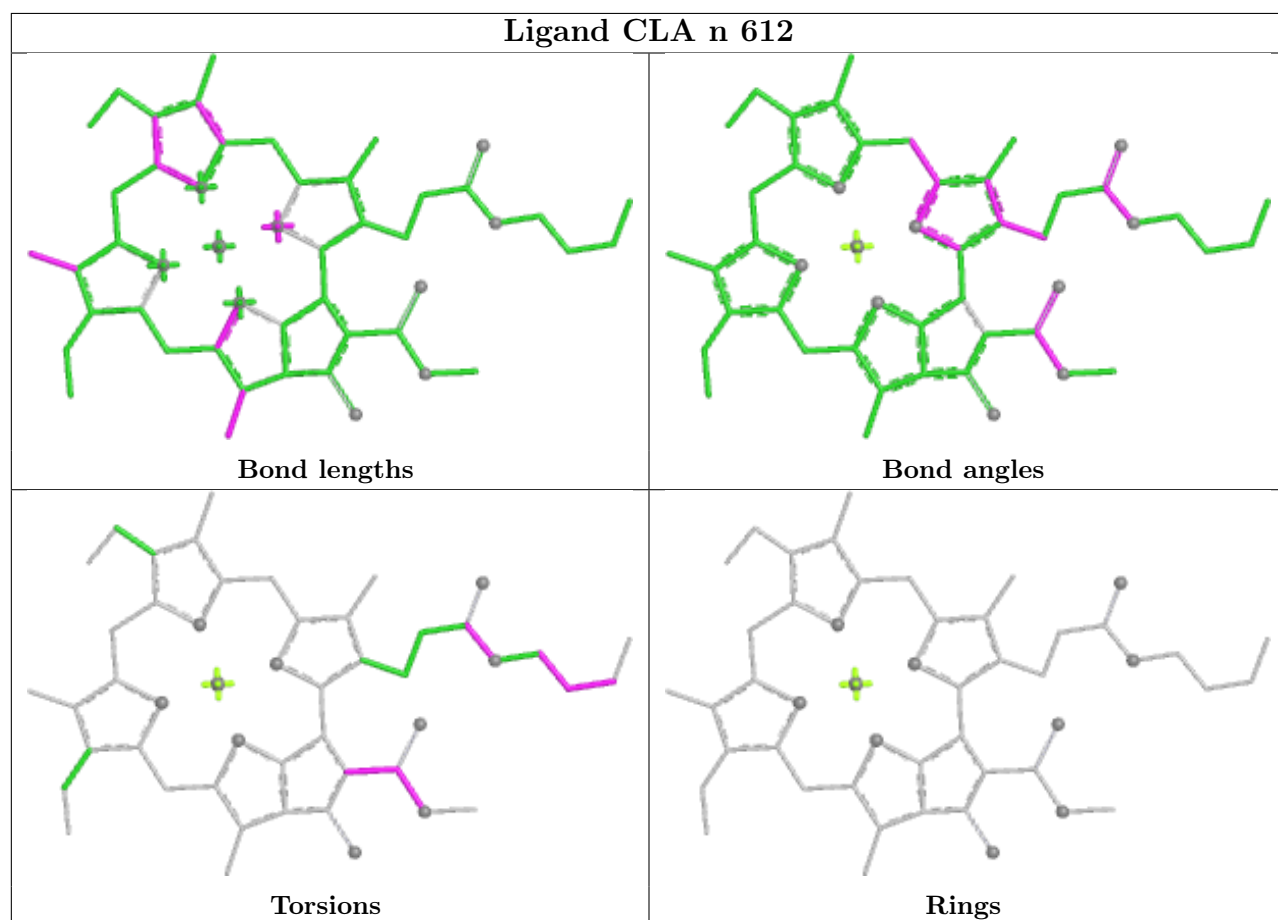
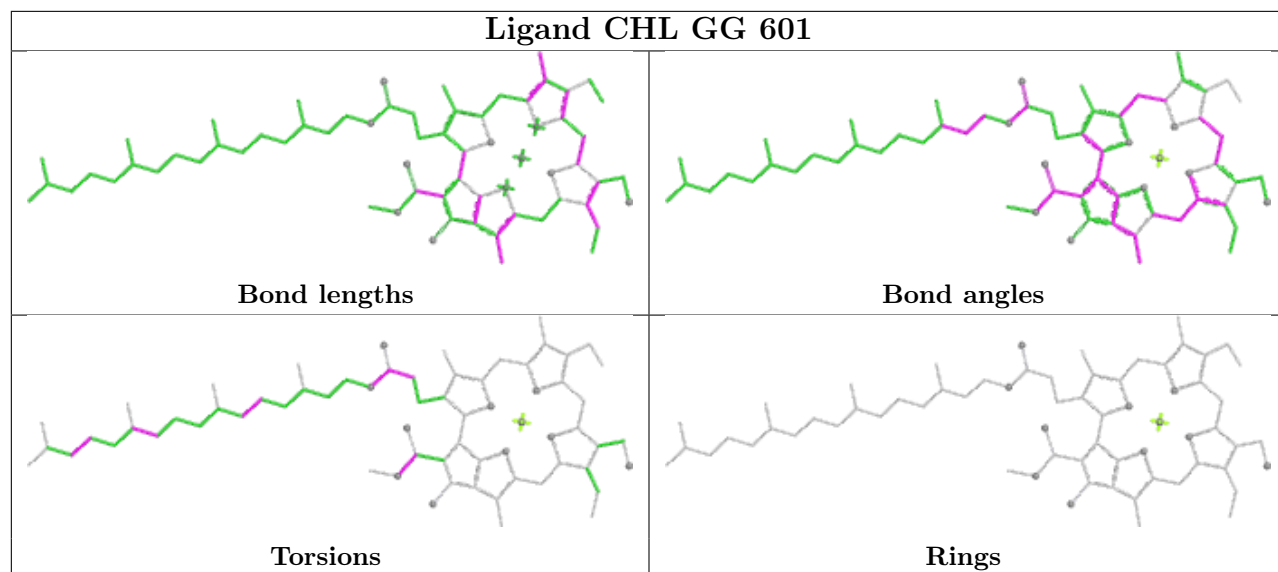
Rings



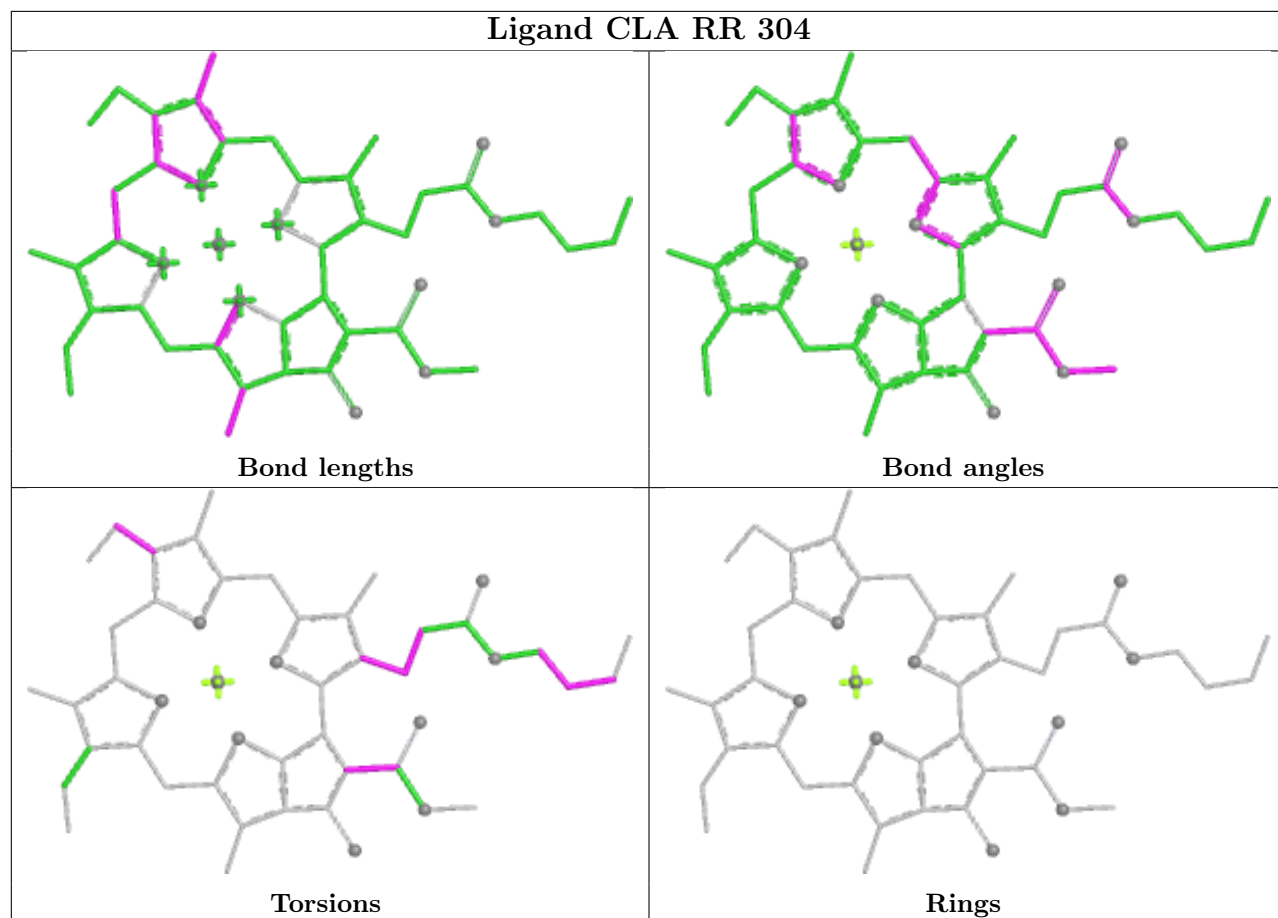


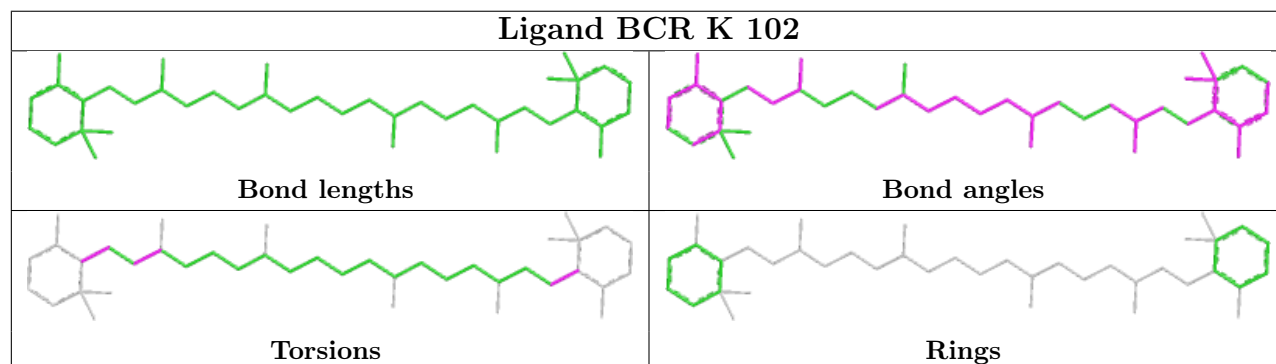
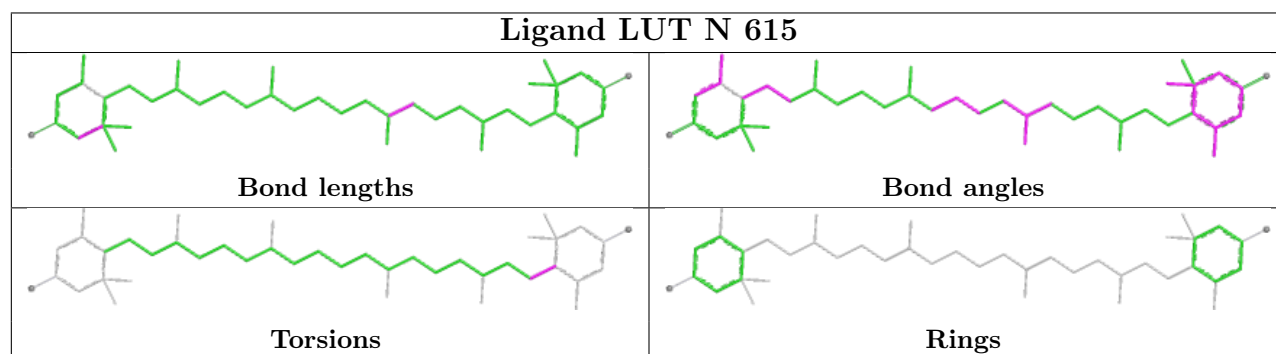
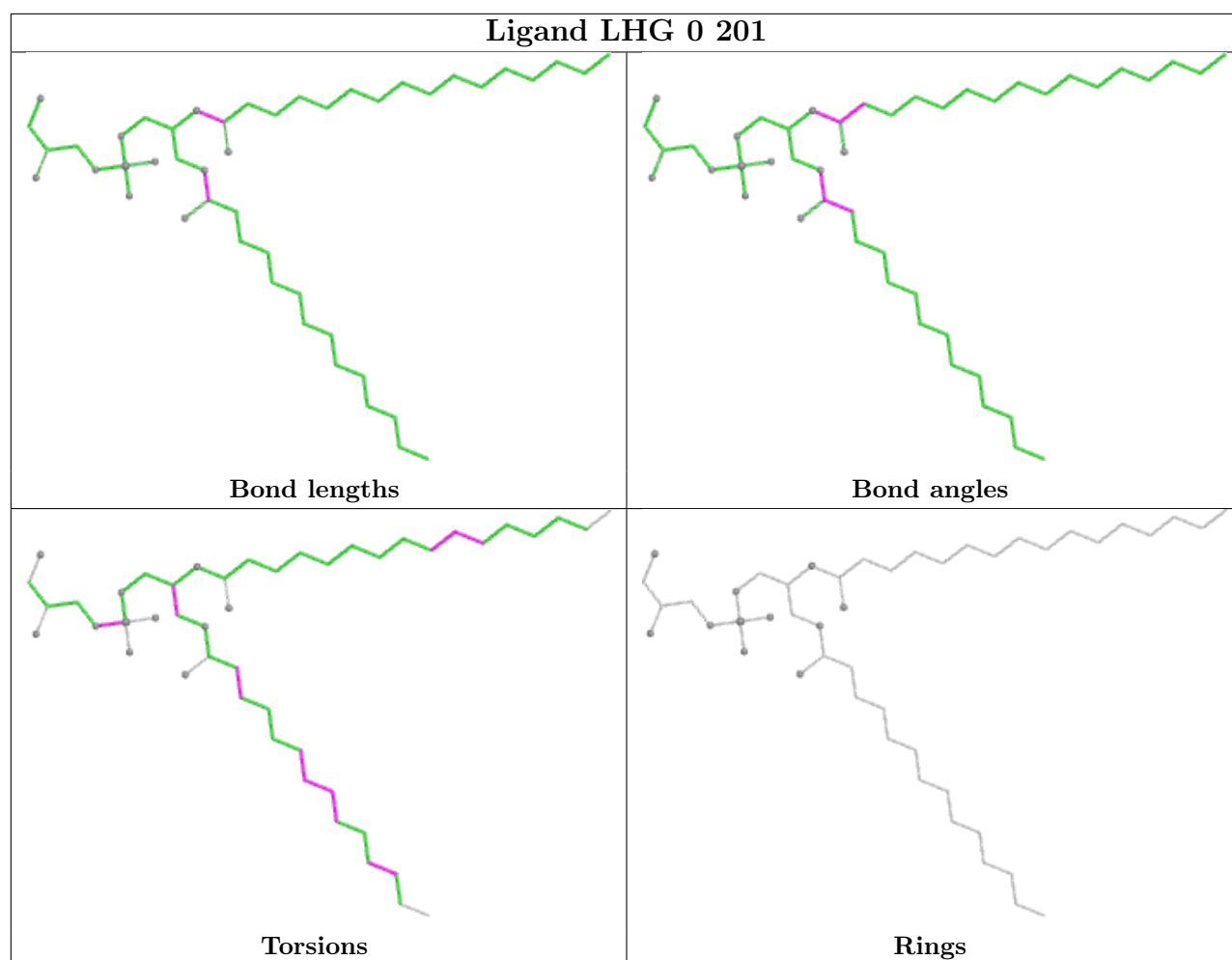




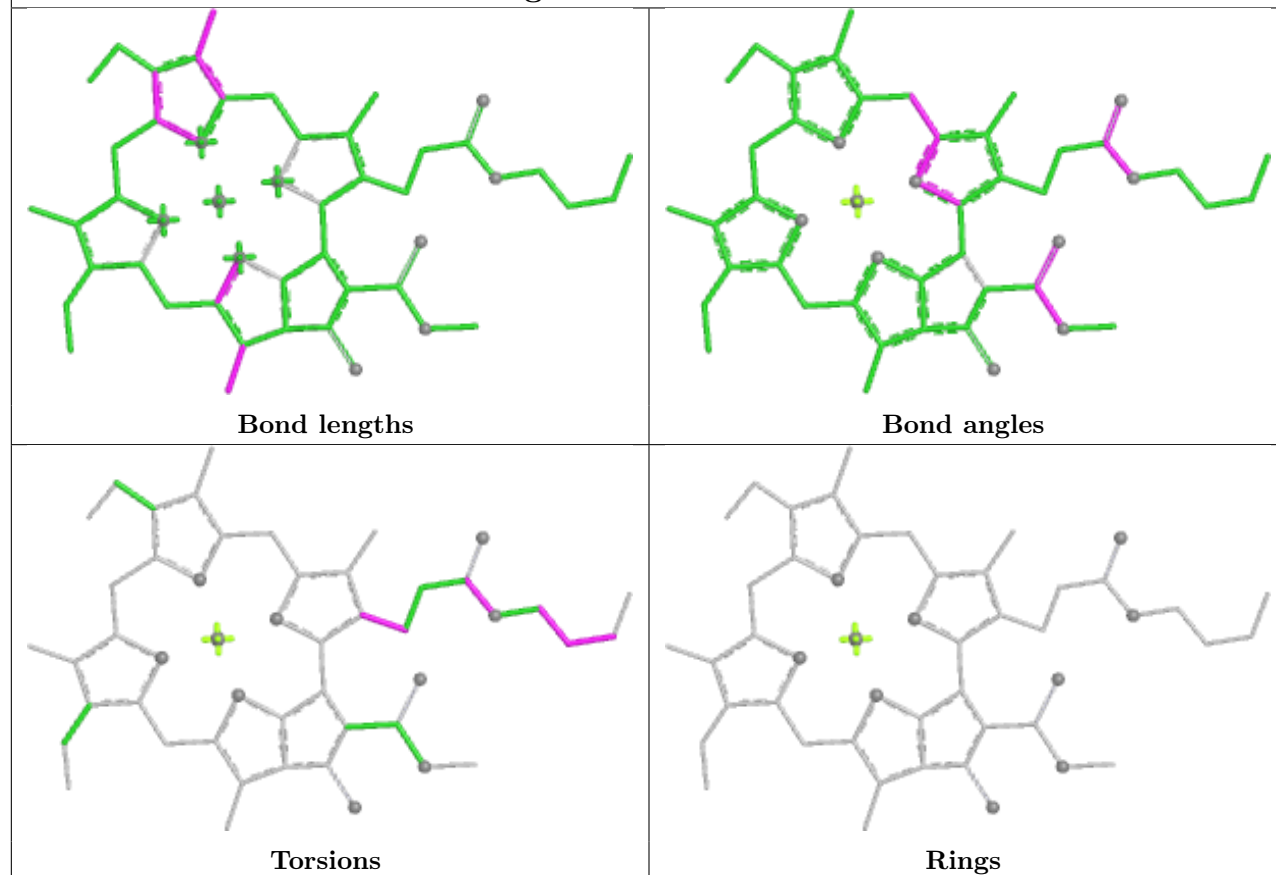


Ligand CLA RR 304

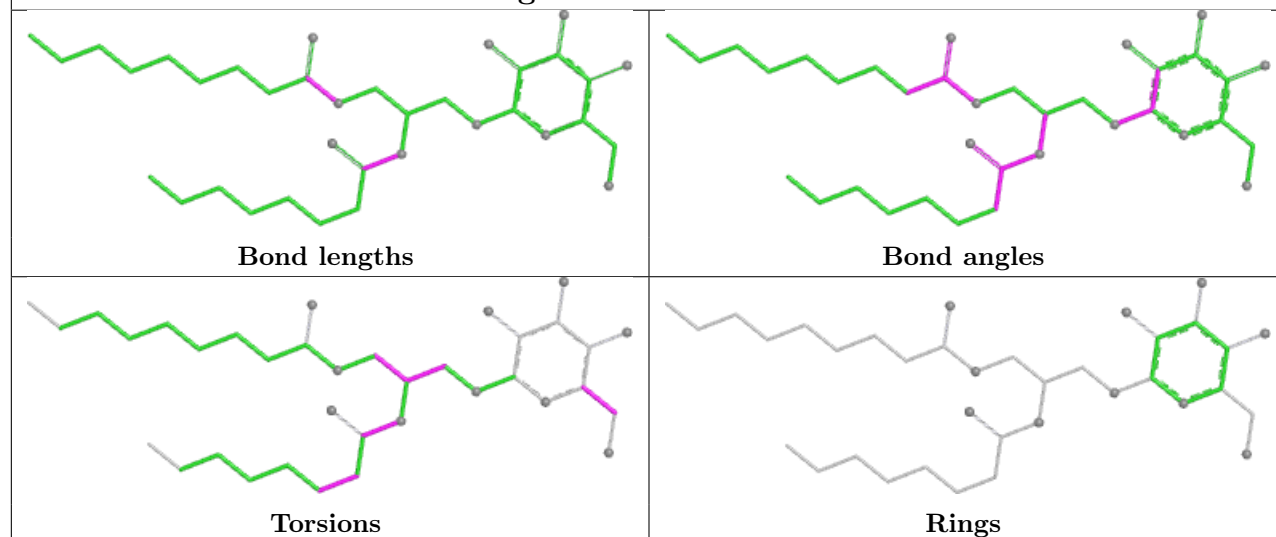


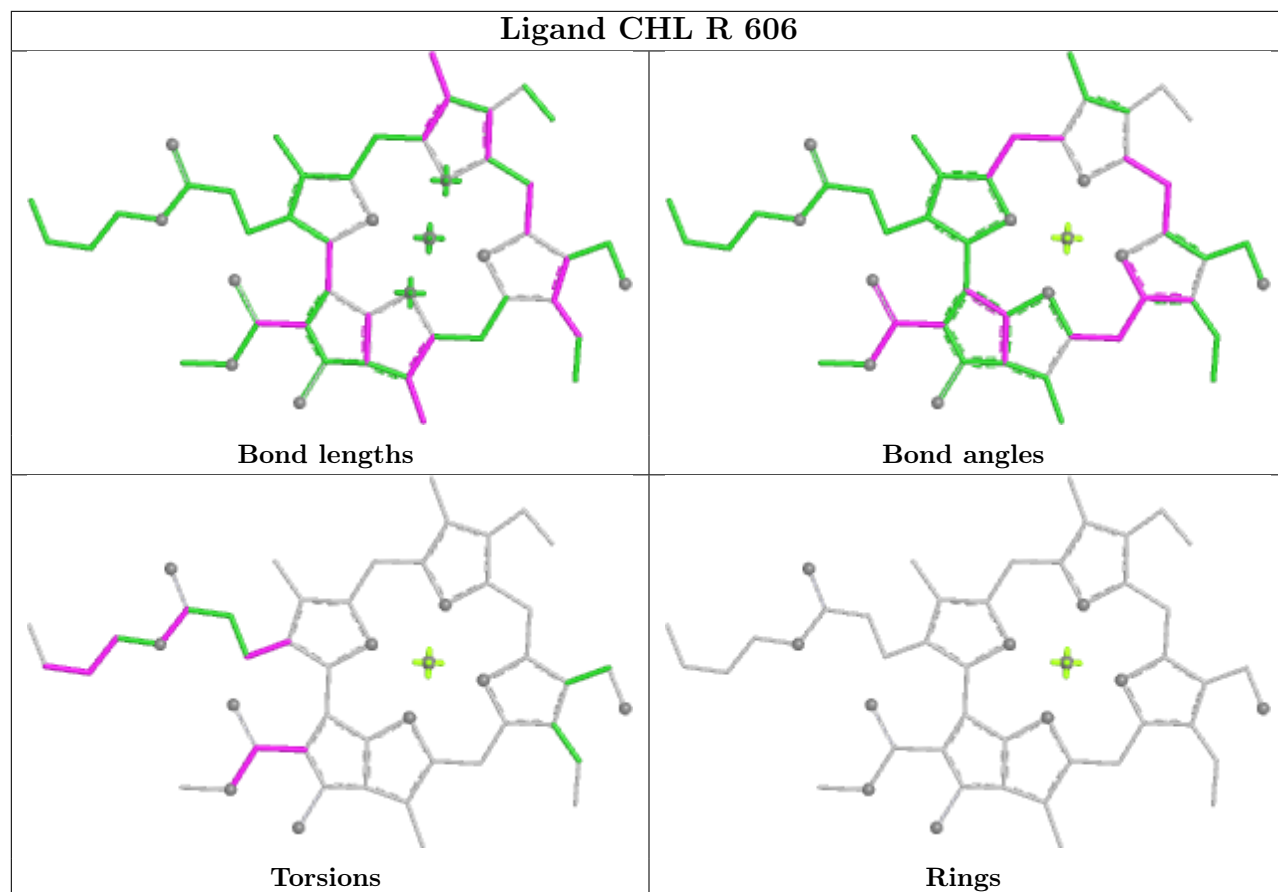


Ligand CLA Rr 612

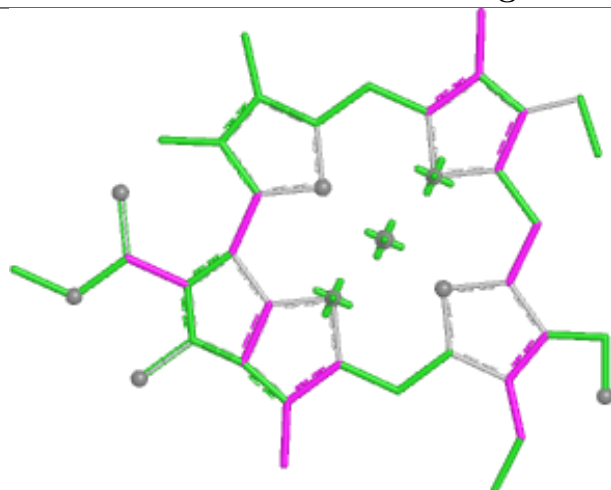


Ligand LMG Bb 621

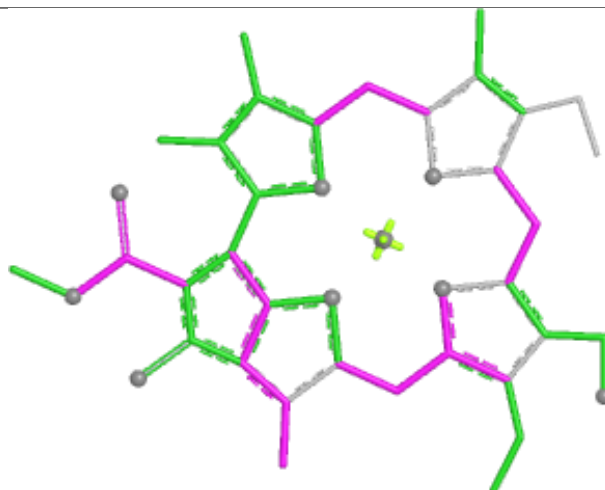




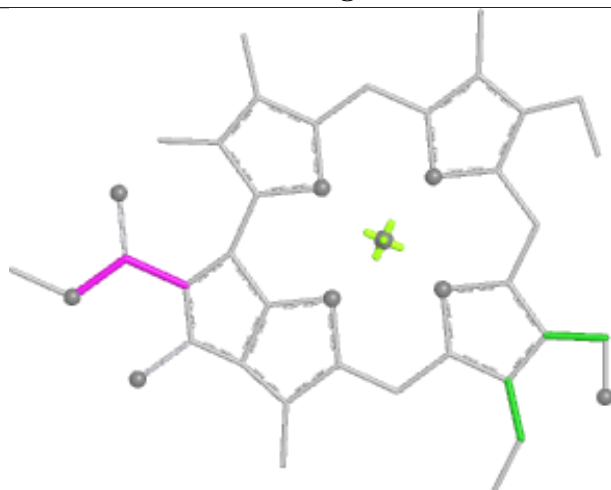
Ligand CHL GG 608



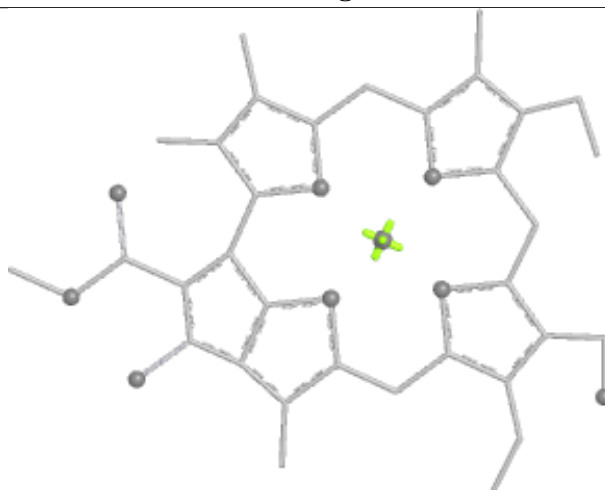
Bond lengths



Bond angles

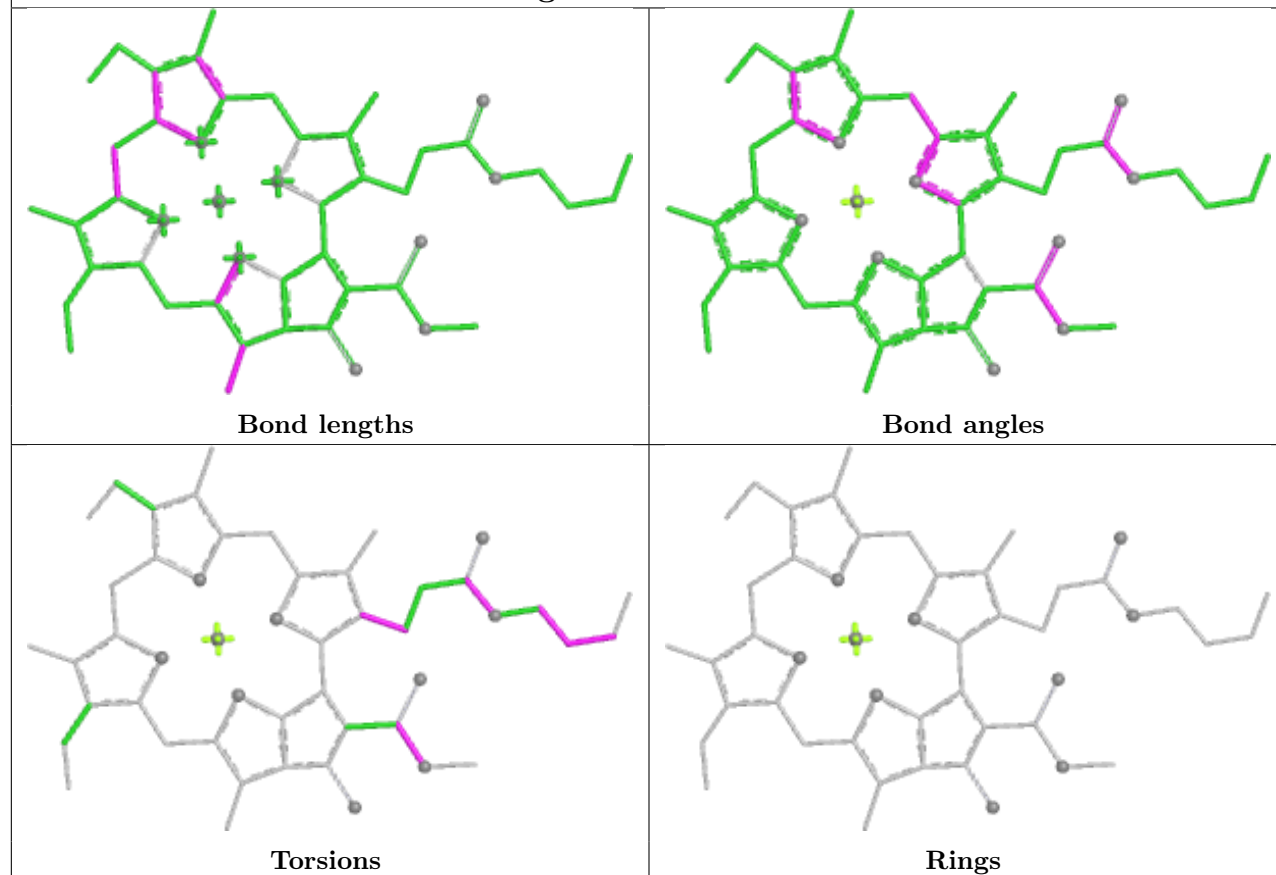


Torsions

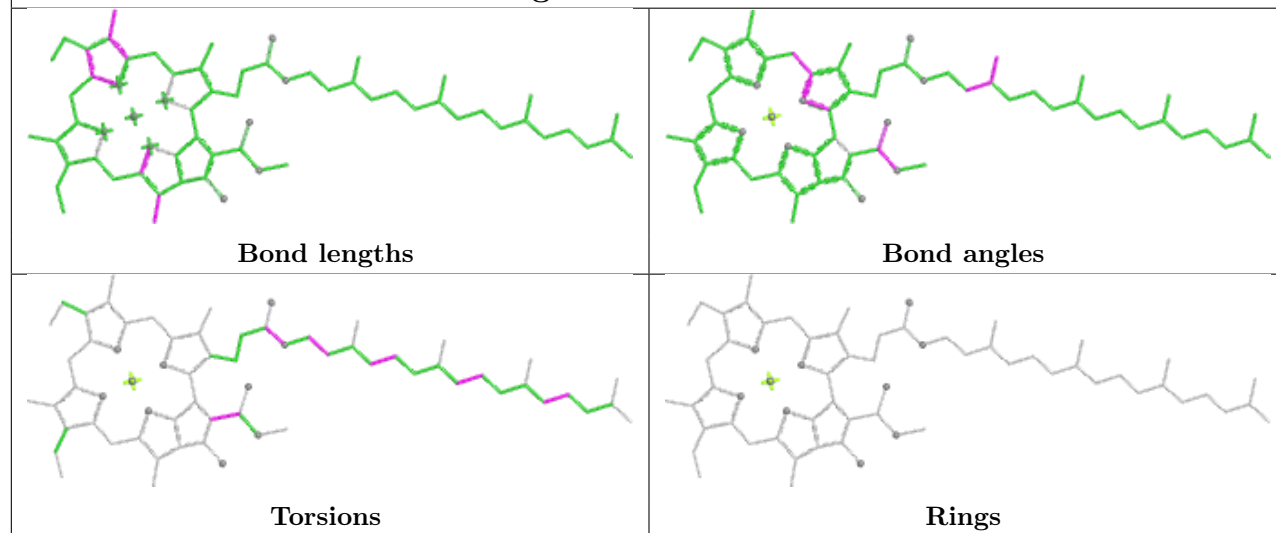


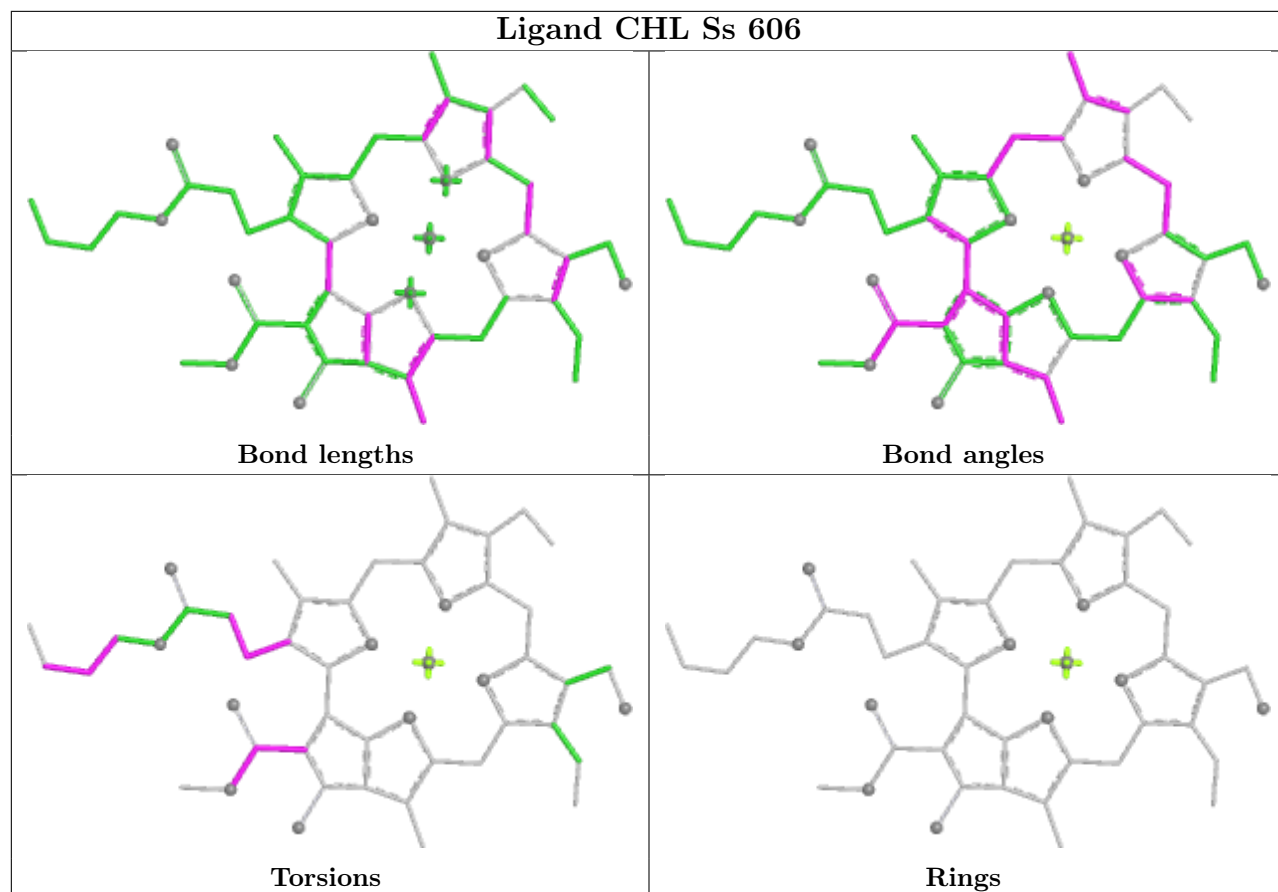
Rings

Ligand CLA s 608

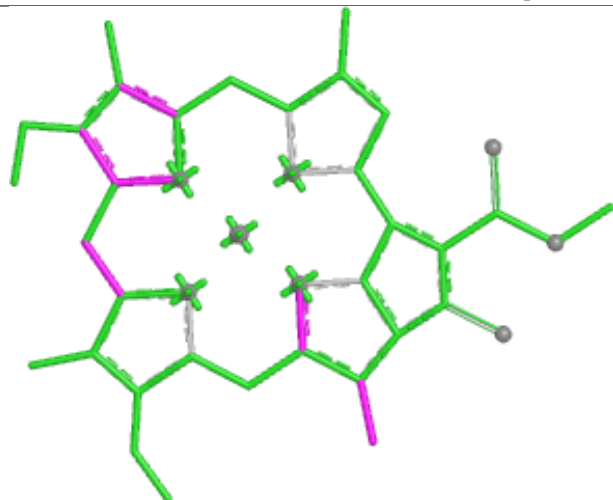


Ligand CLA C 514

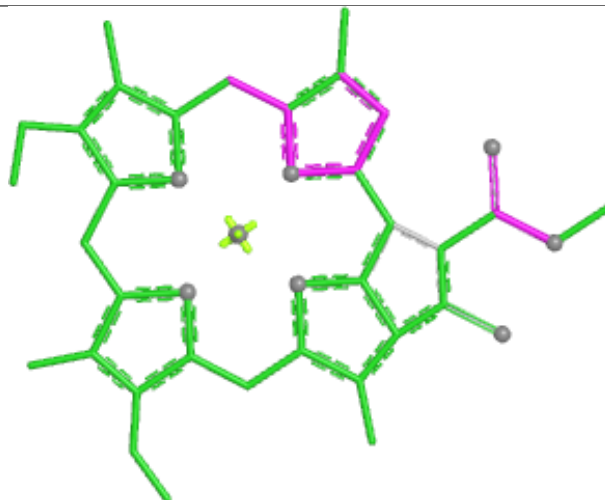




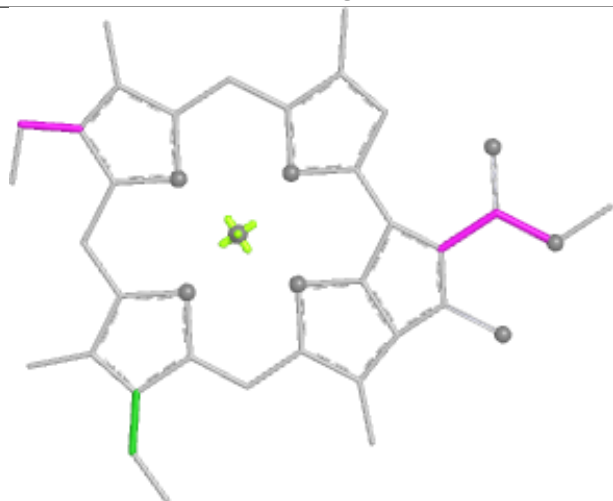
Ligand CLA 3 611



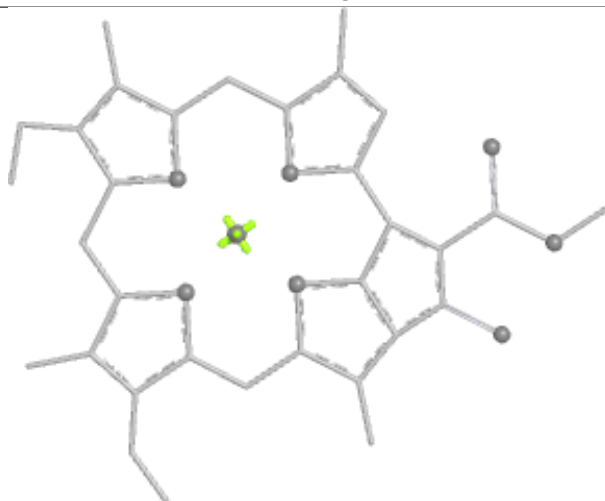
Bond lengths



Bond angles

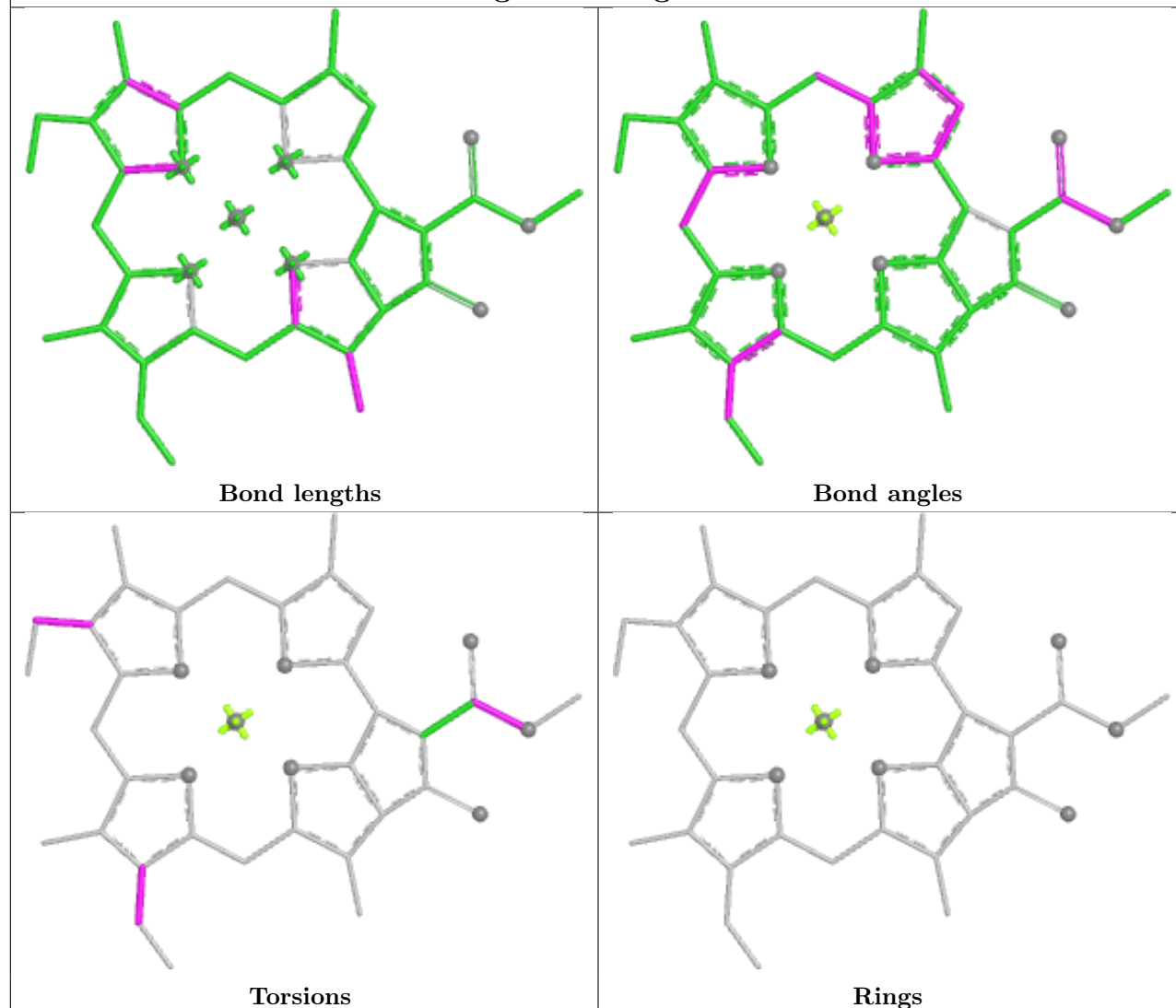


Torsions

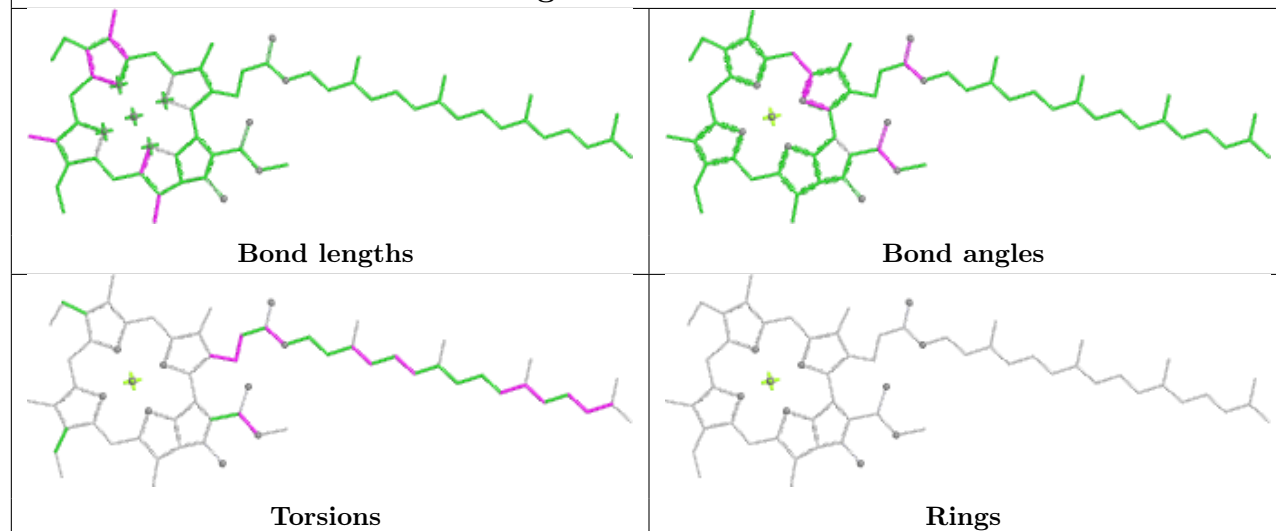


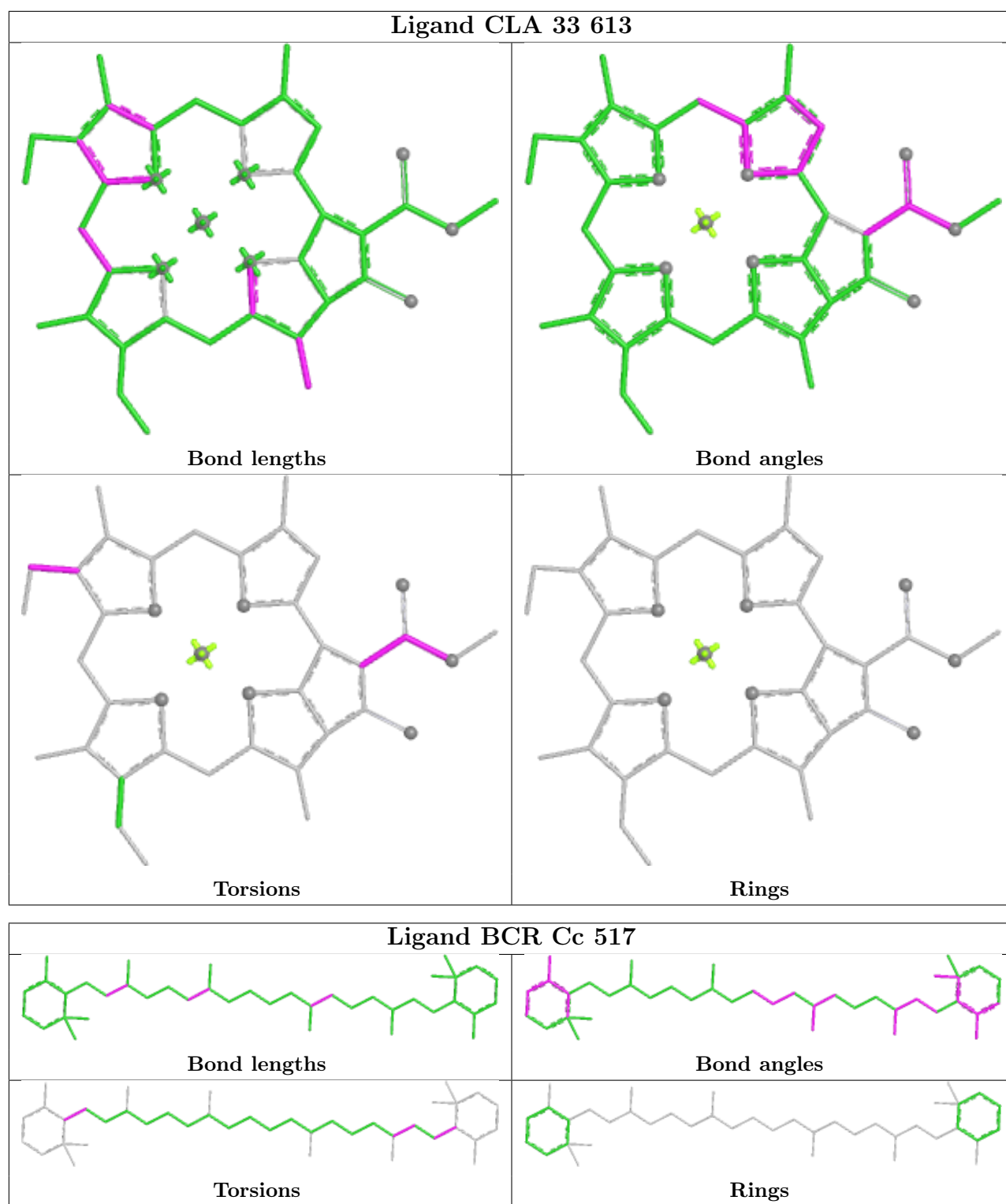
Rings

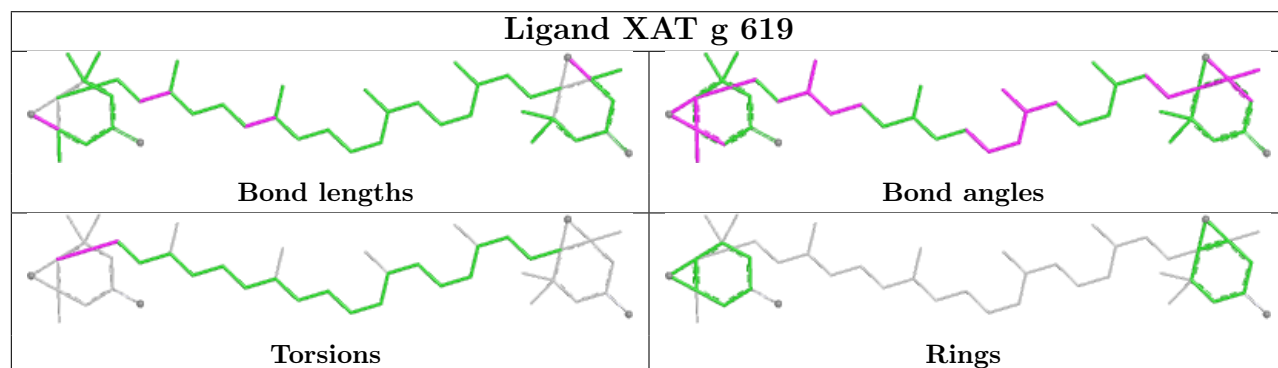
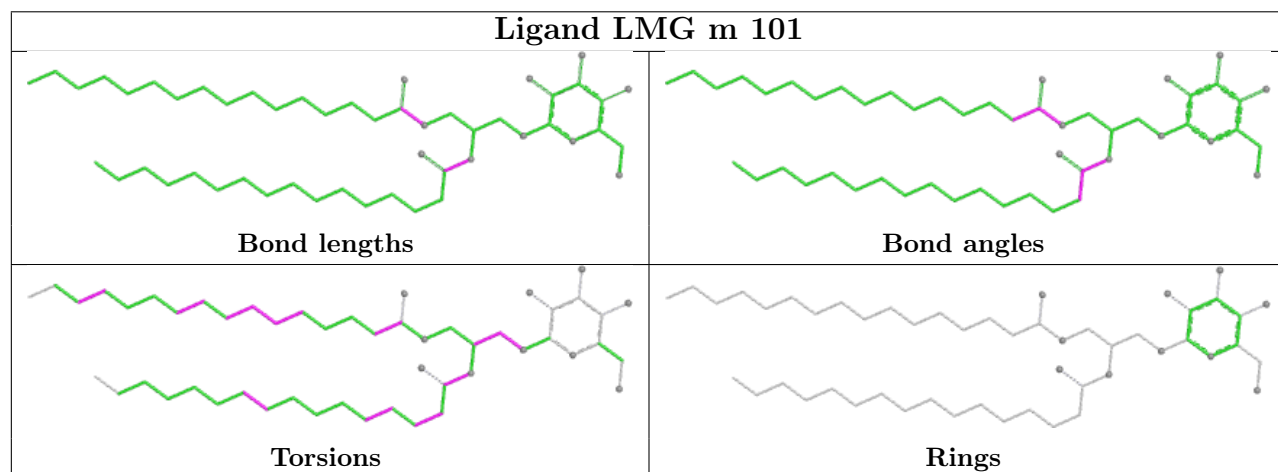
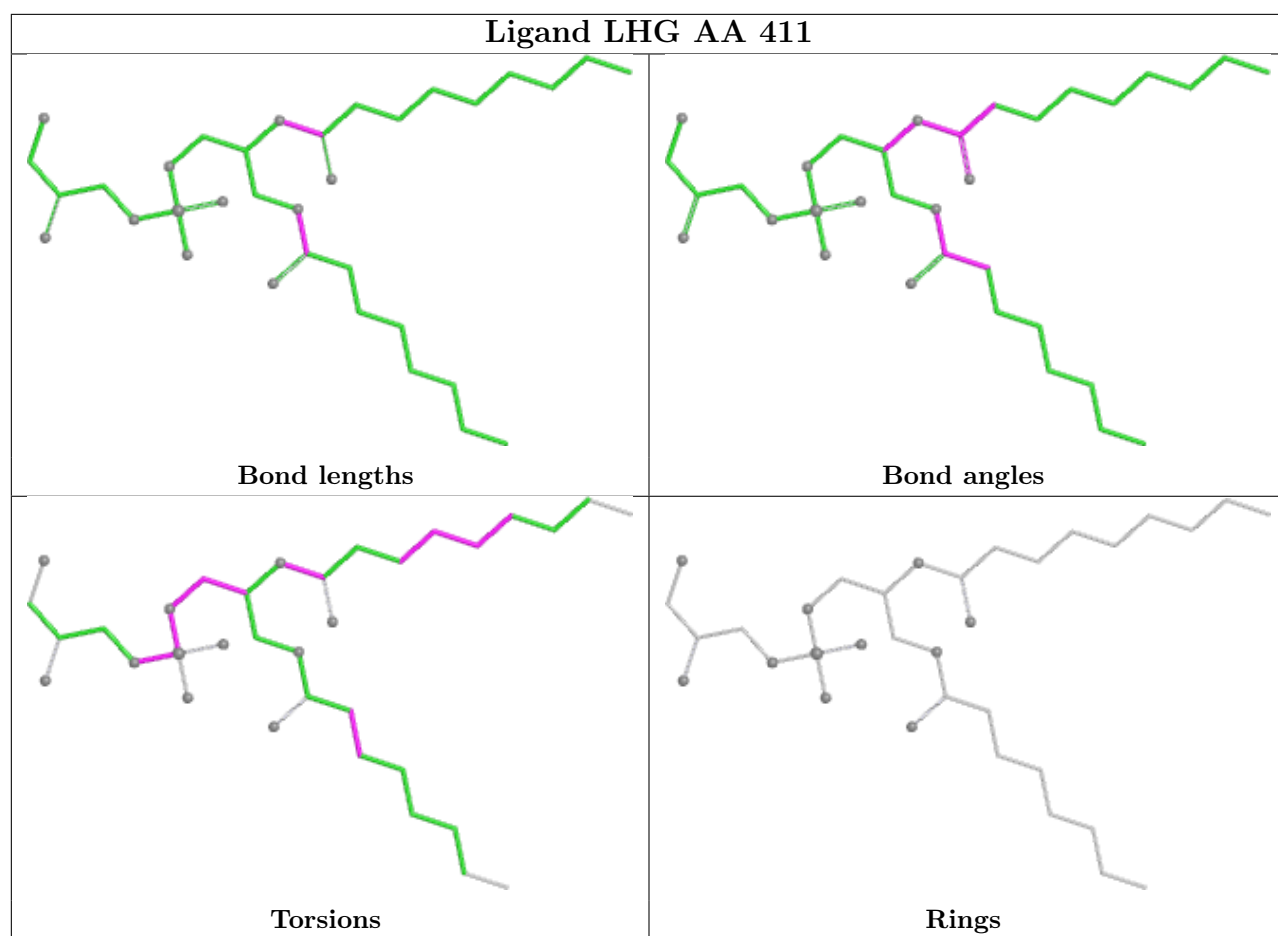
Ligand CLA g 613



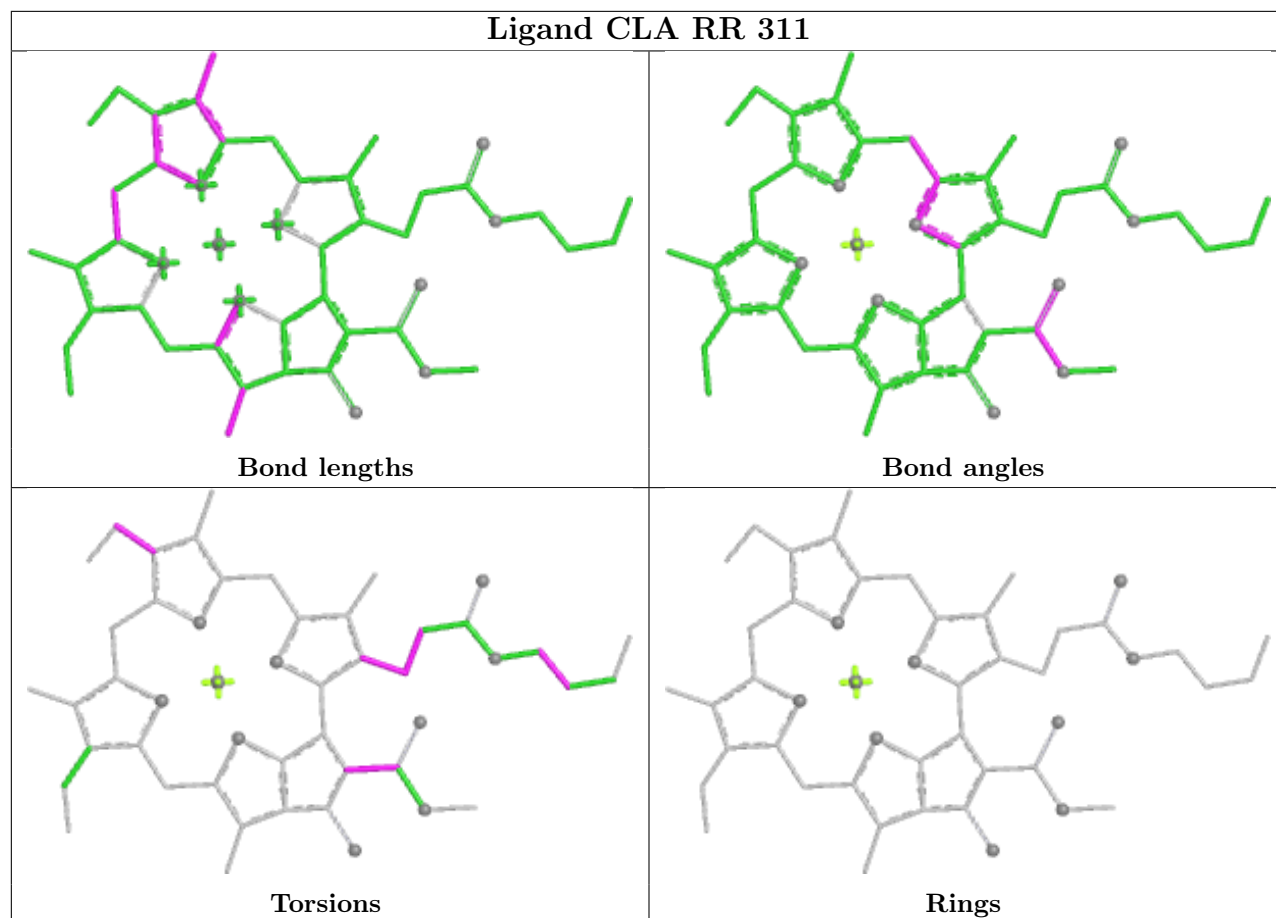
Ligand CLA c 510



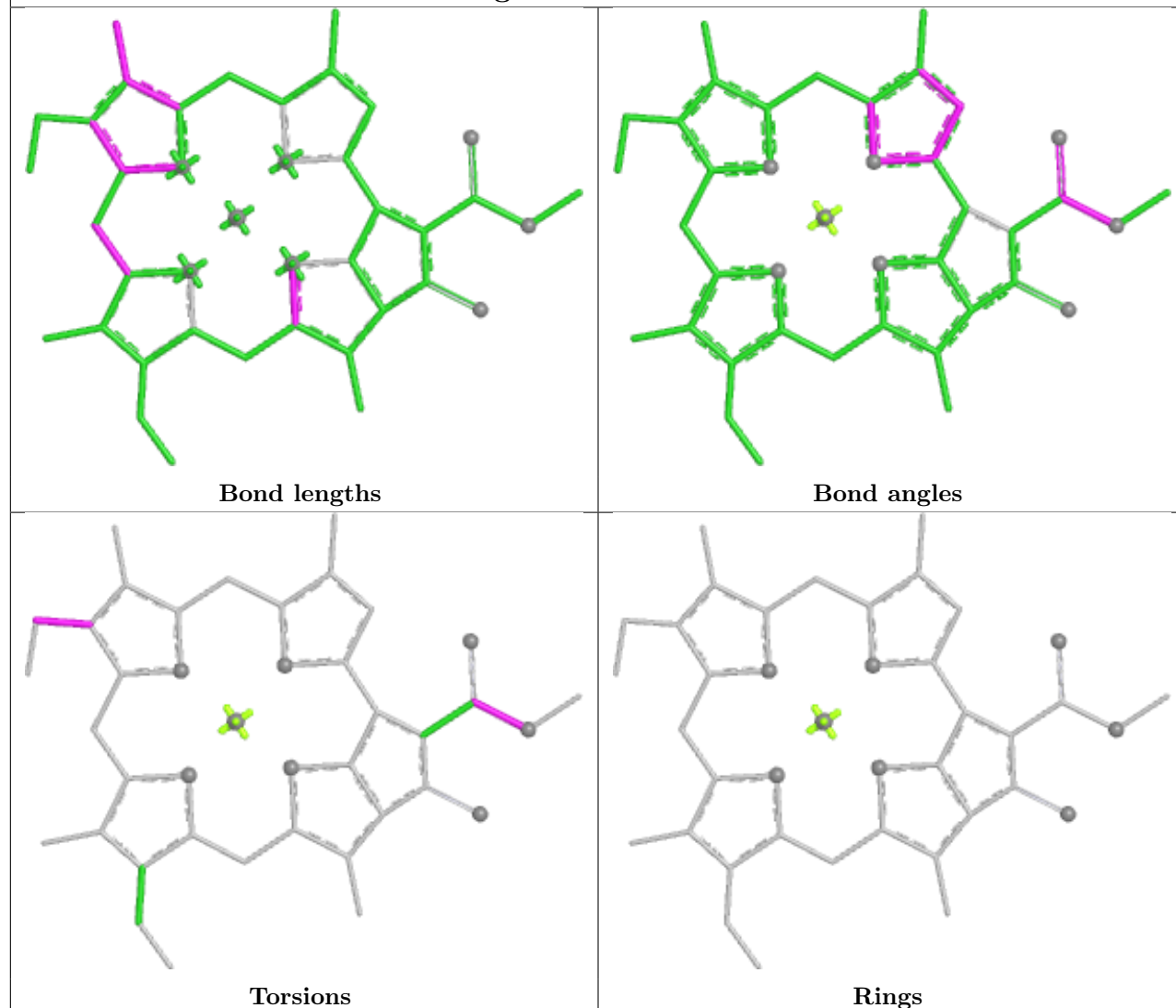




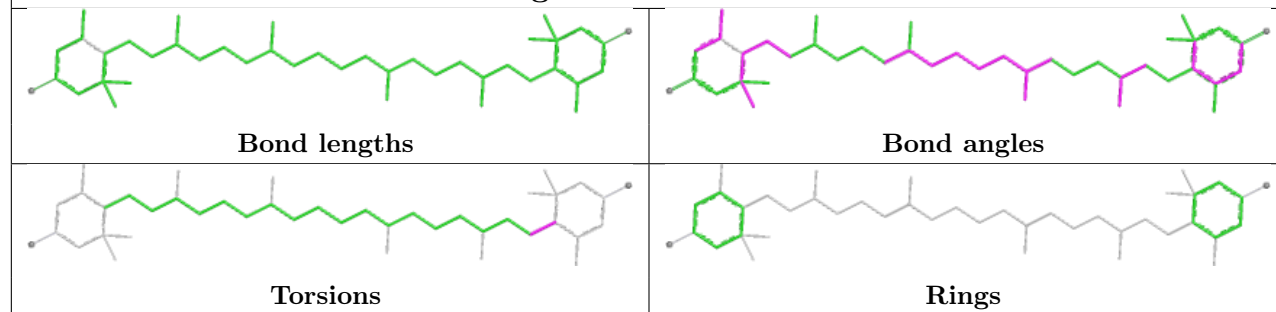
Ligand CLA RR 311

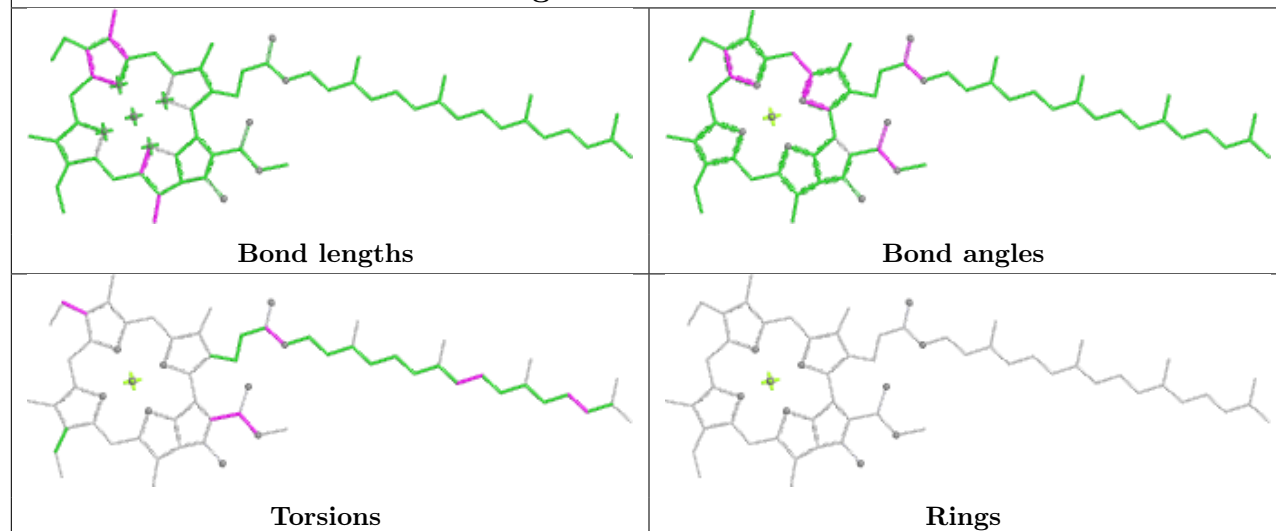
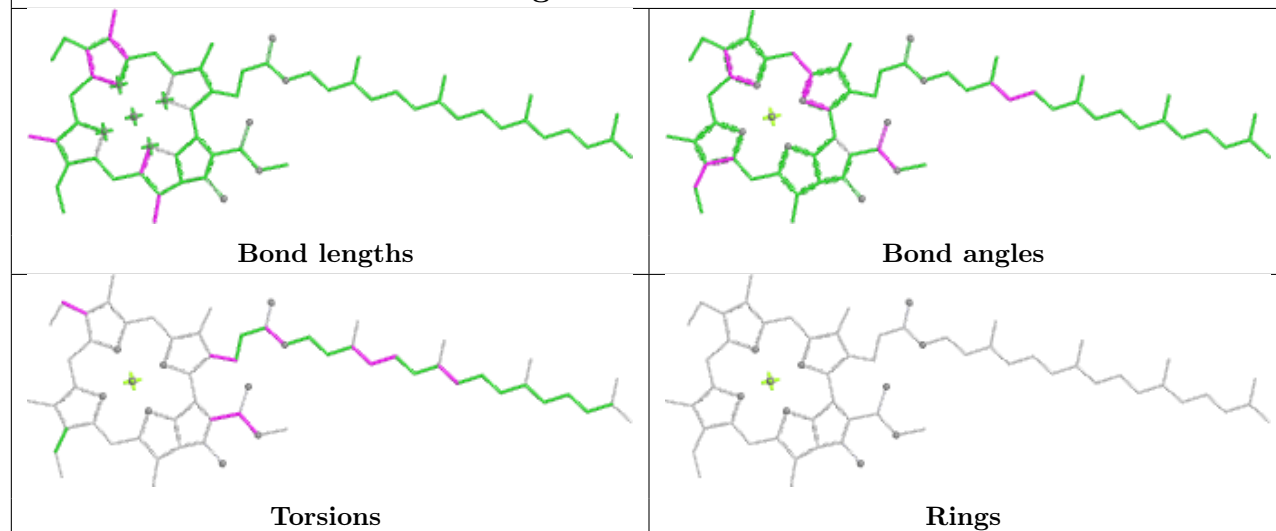


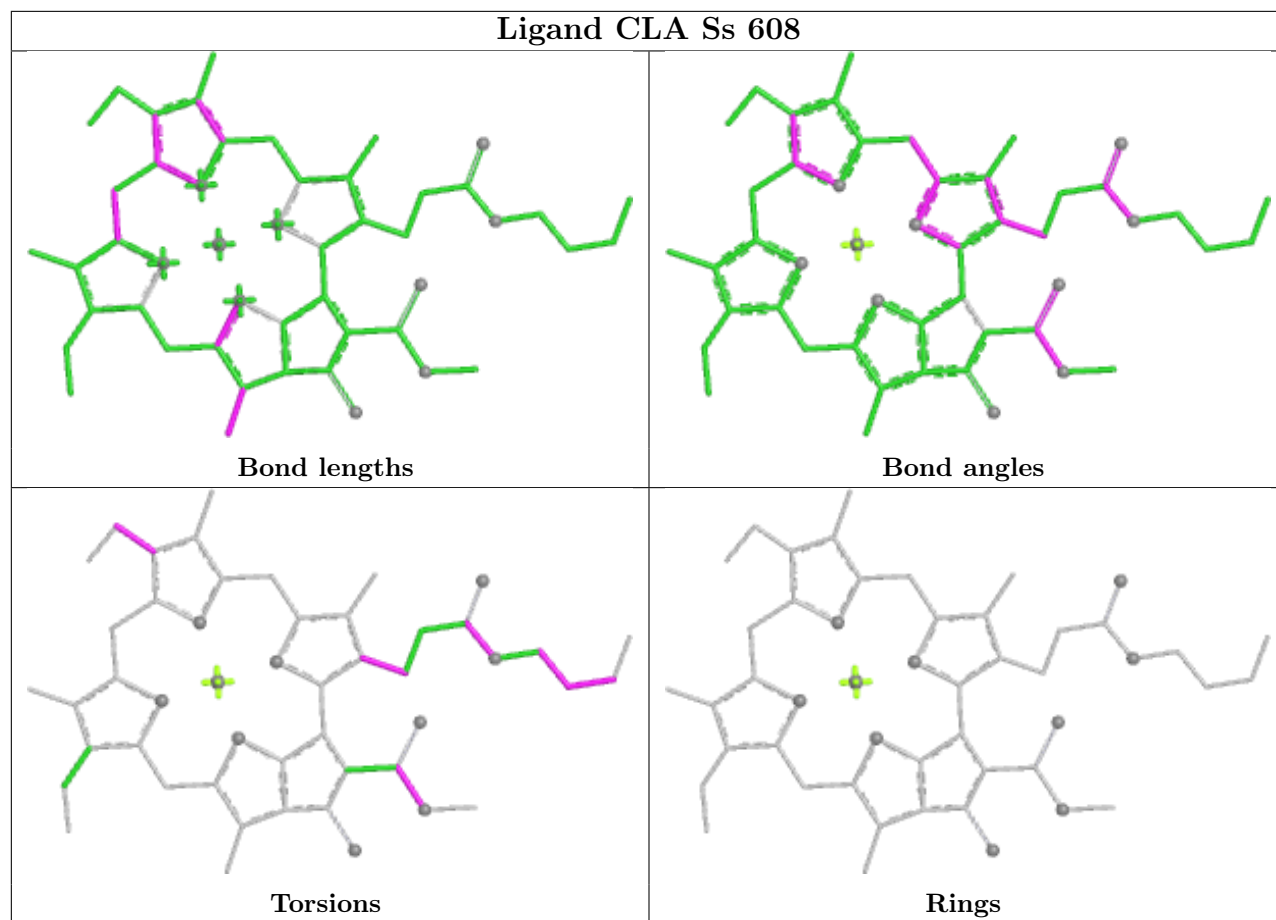
Ligand CLA 3 604



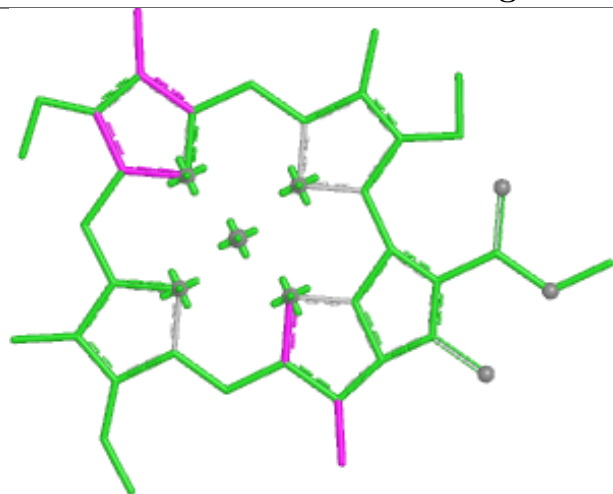
Ligand LUT G 616



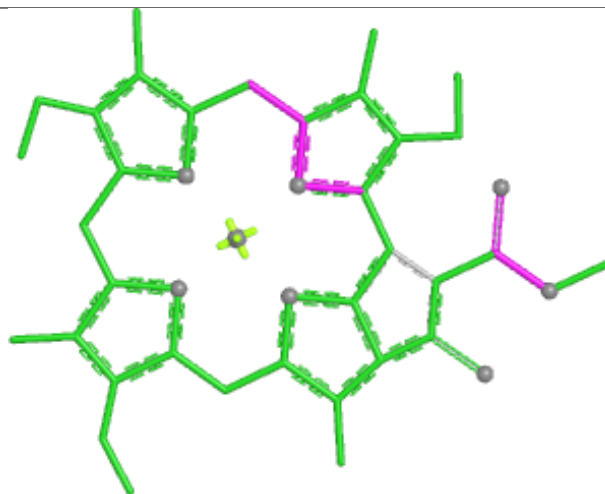
Ligand CLA C 506**Ligand CLA B 621**



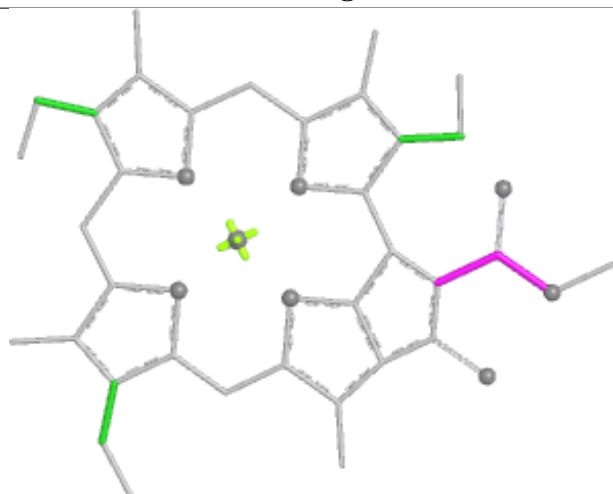
Ligand CLA GG 604



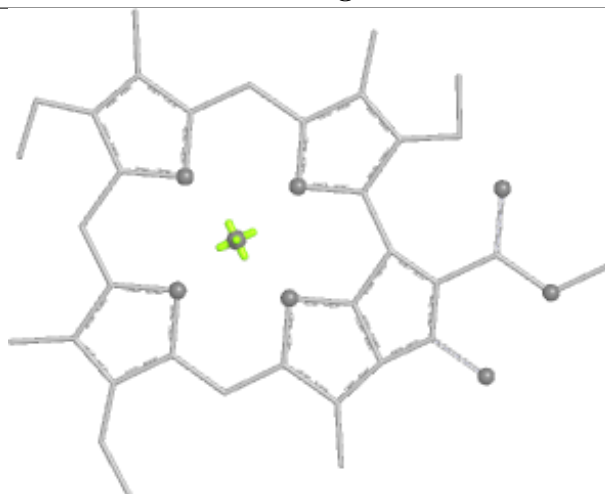
Bond lengths



Bond angles

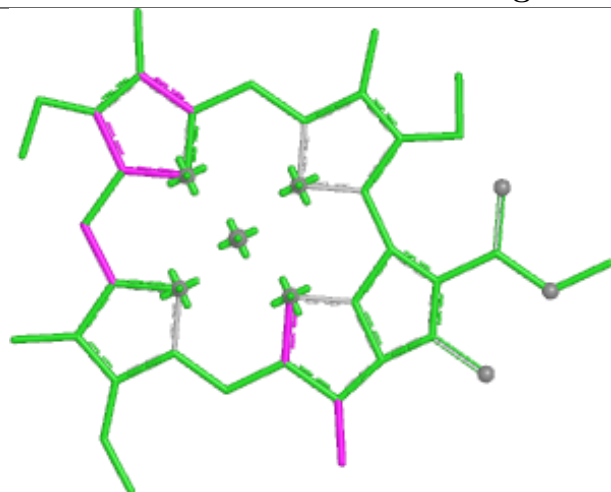


Torsions

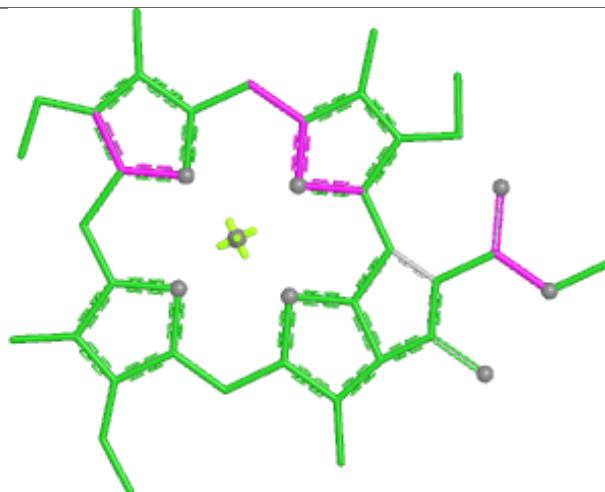


Rings

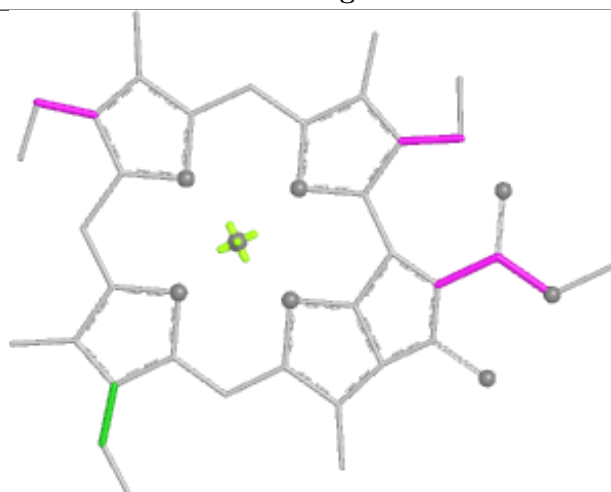
Ligand CLA G 604



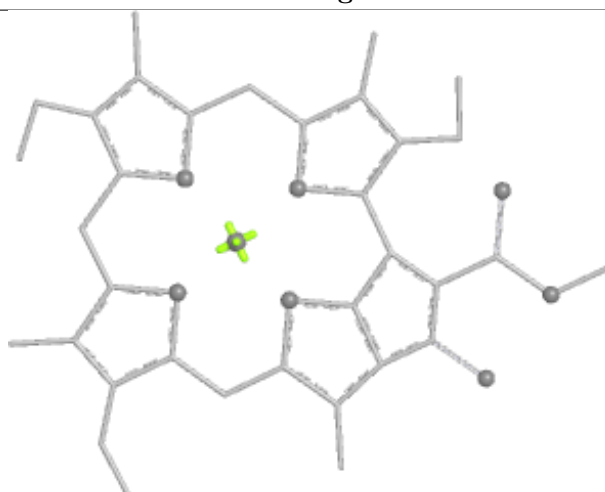
Bond lengths



Bond angles

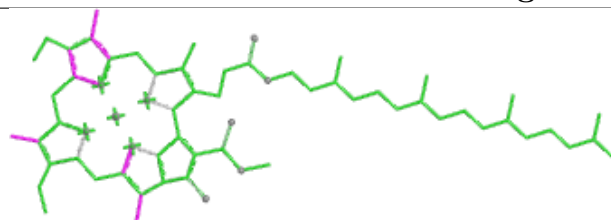


Torsions

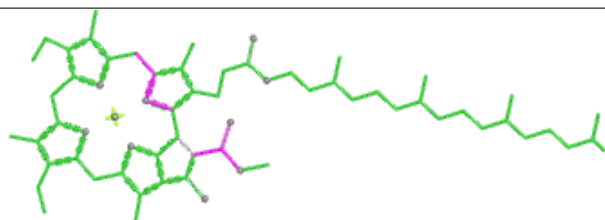


Rings

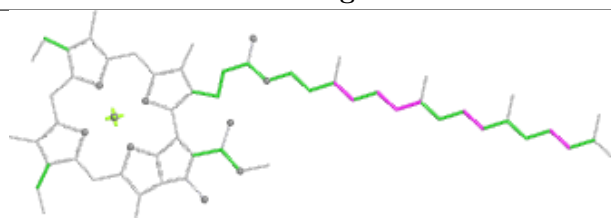
Ligand CLA b 611



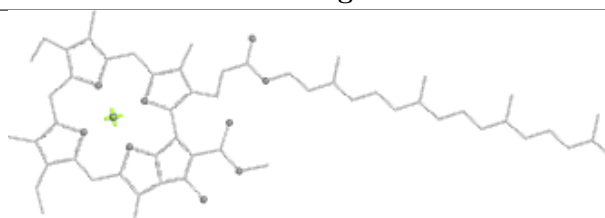
Bond lengths



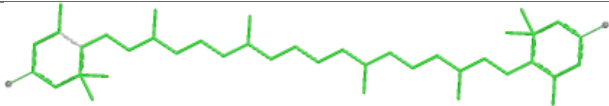
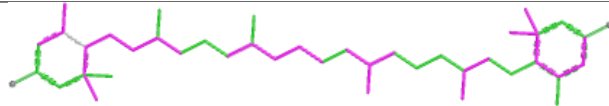
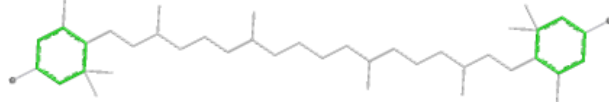
Bond angles

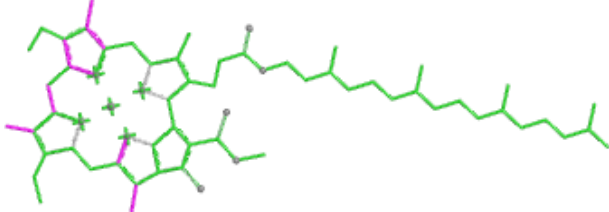
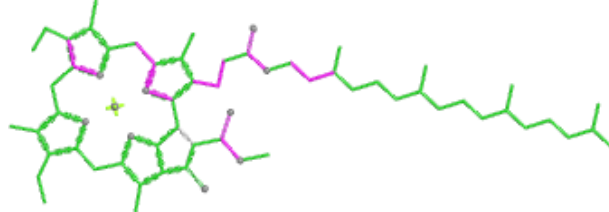
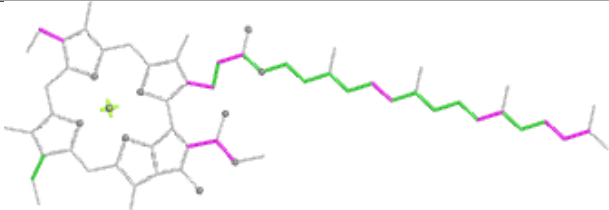
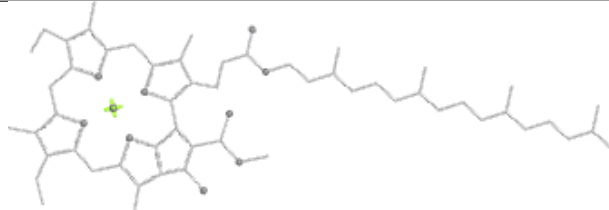


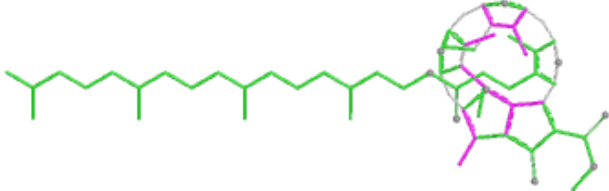
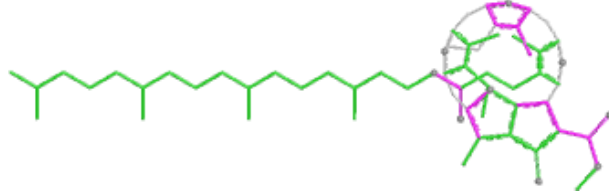
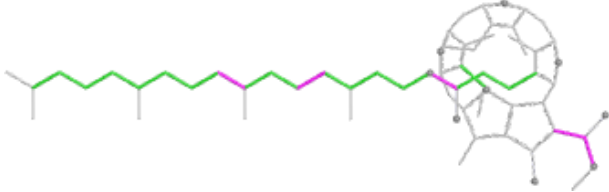
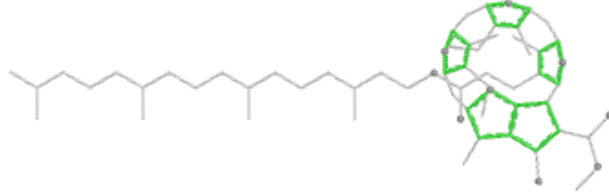
Torsions



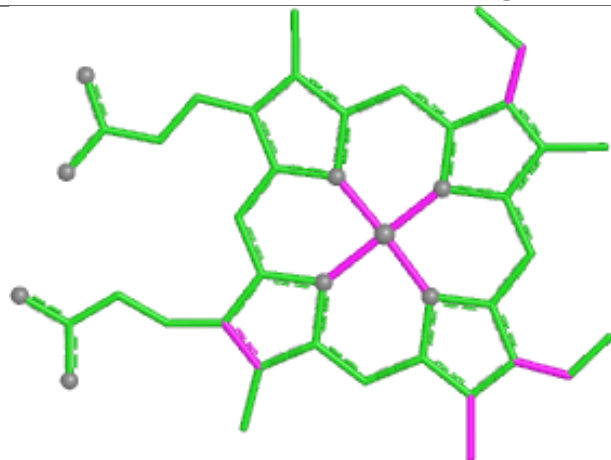
Rings

Ligand LUT R 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

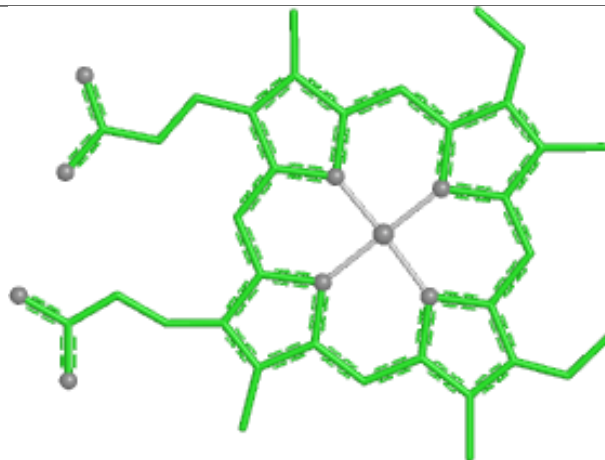
Ligand CLA Bb 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO Aa 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

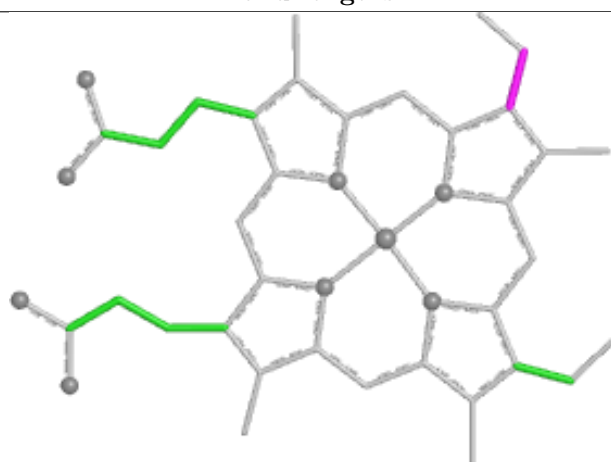
Ligand HEM EE 102



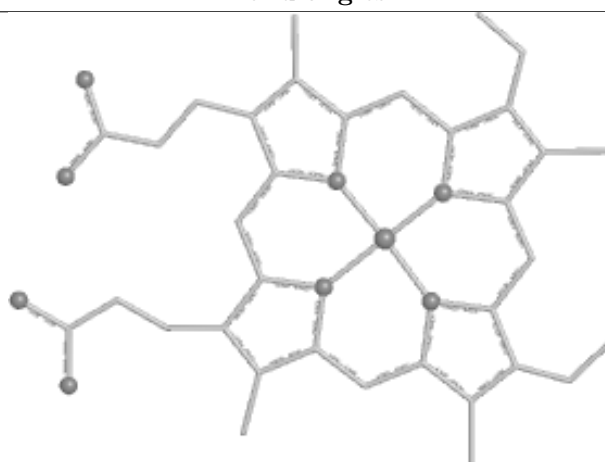
Bond lengths



Bond angles

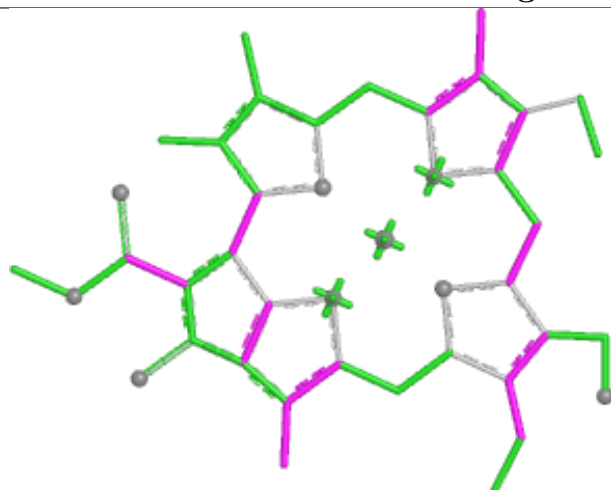


Torsions

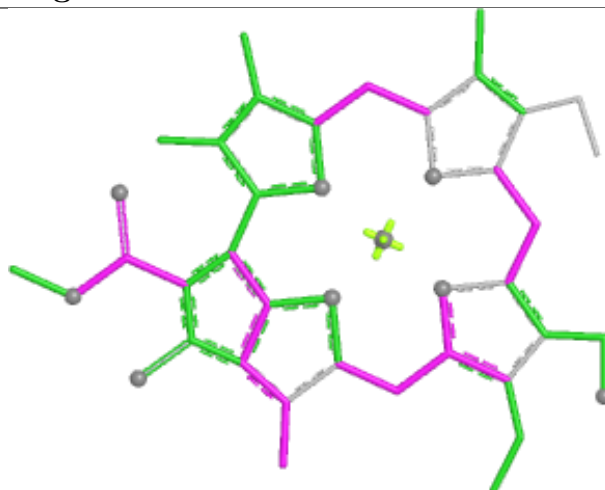


Rings

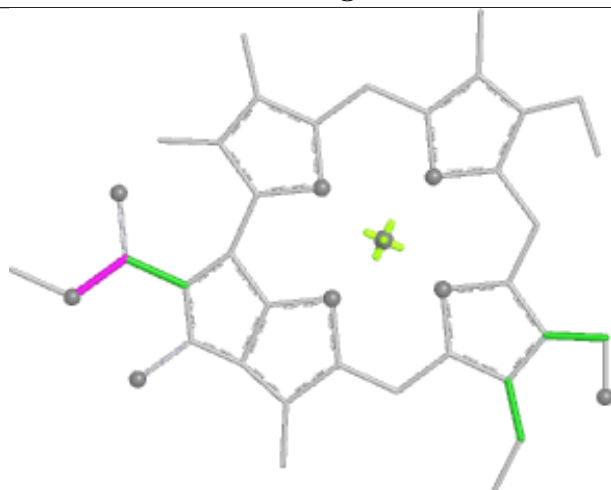
Ligand CHL g 608



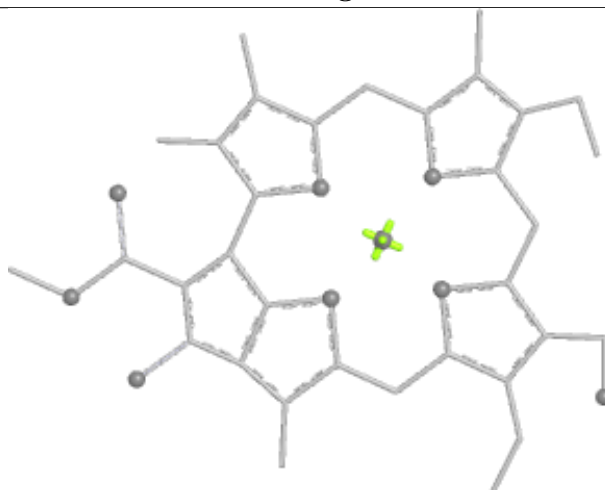
Bond lengths



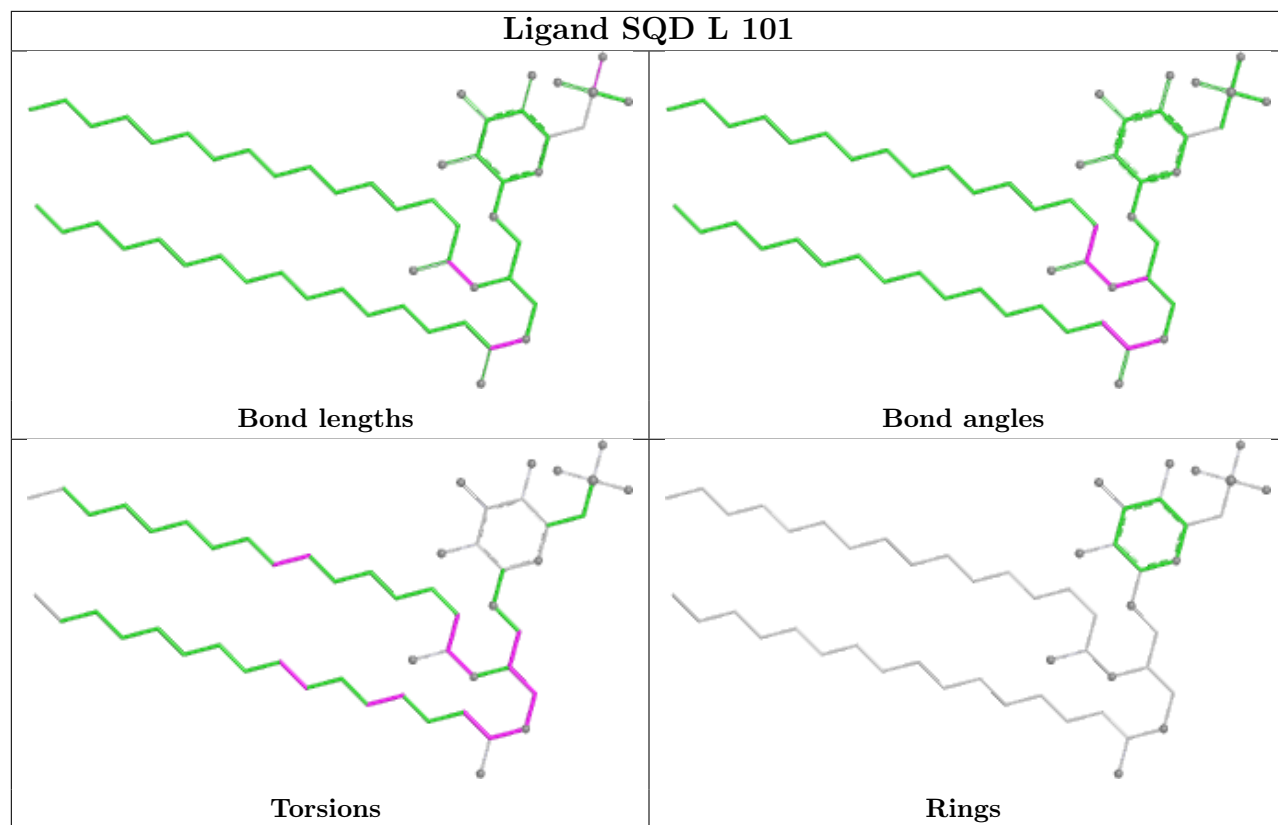
Bond angles

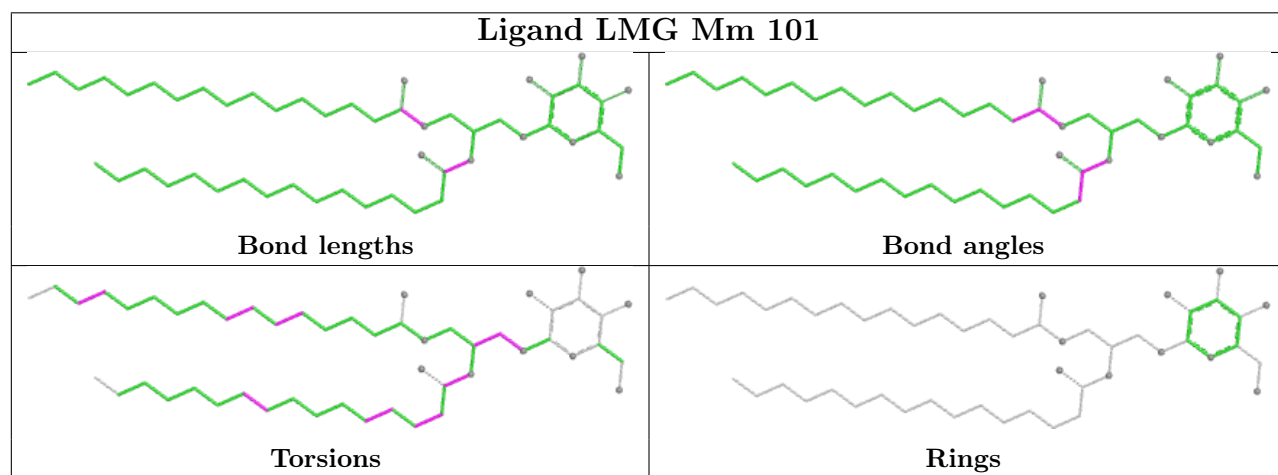
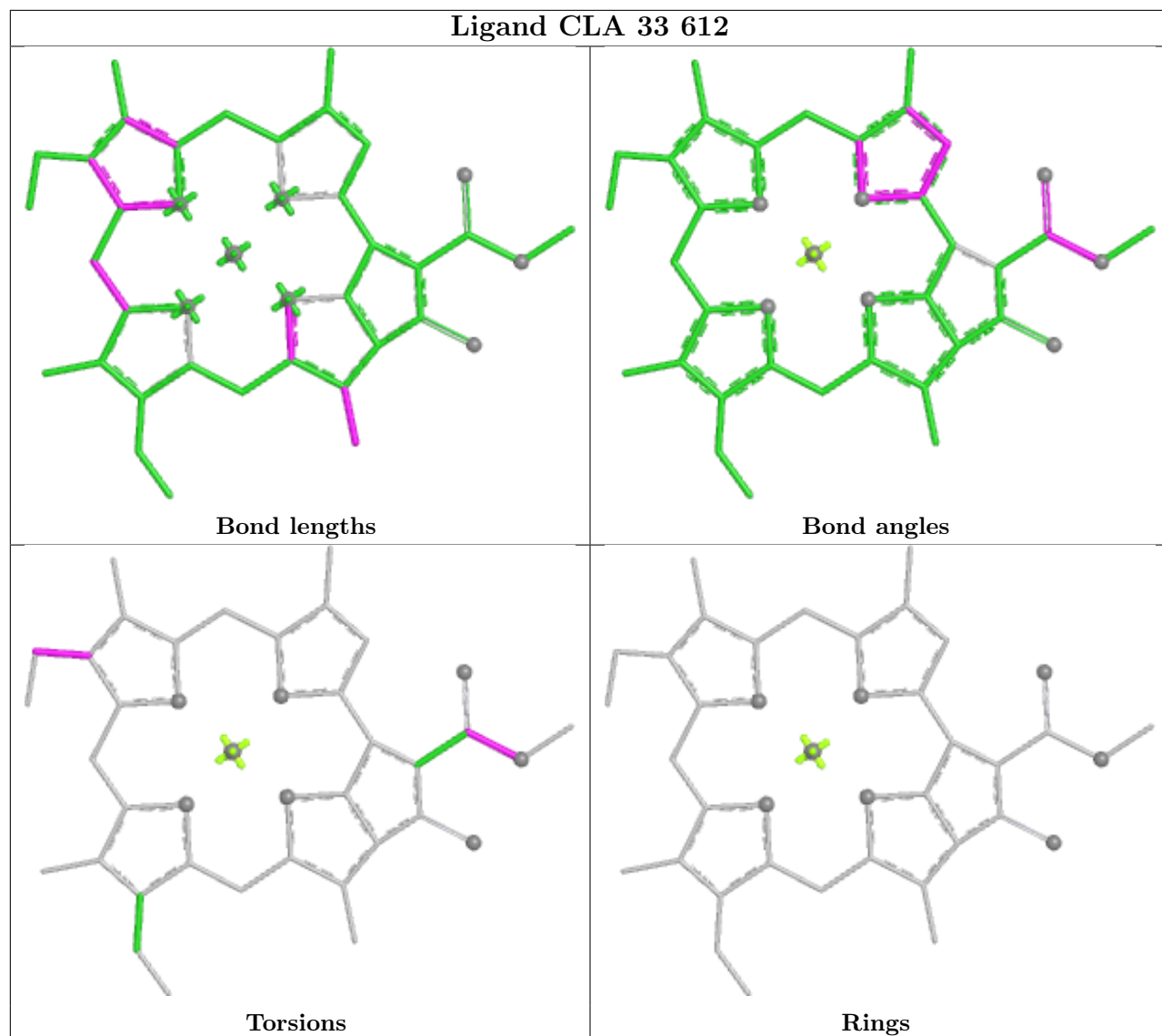


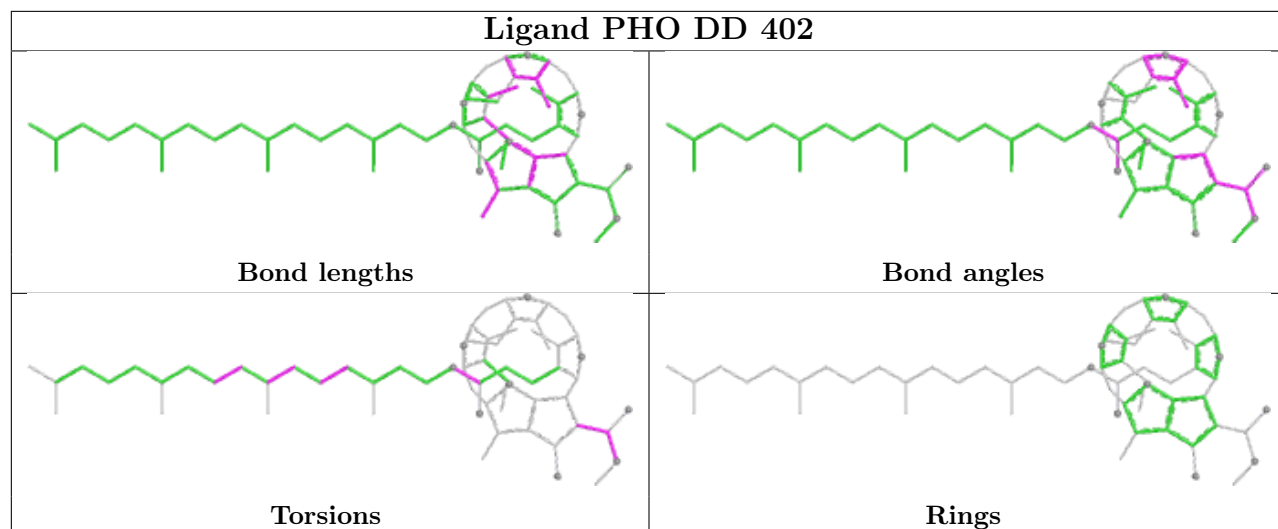
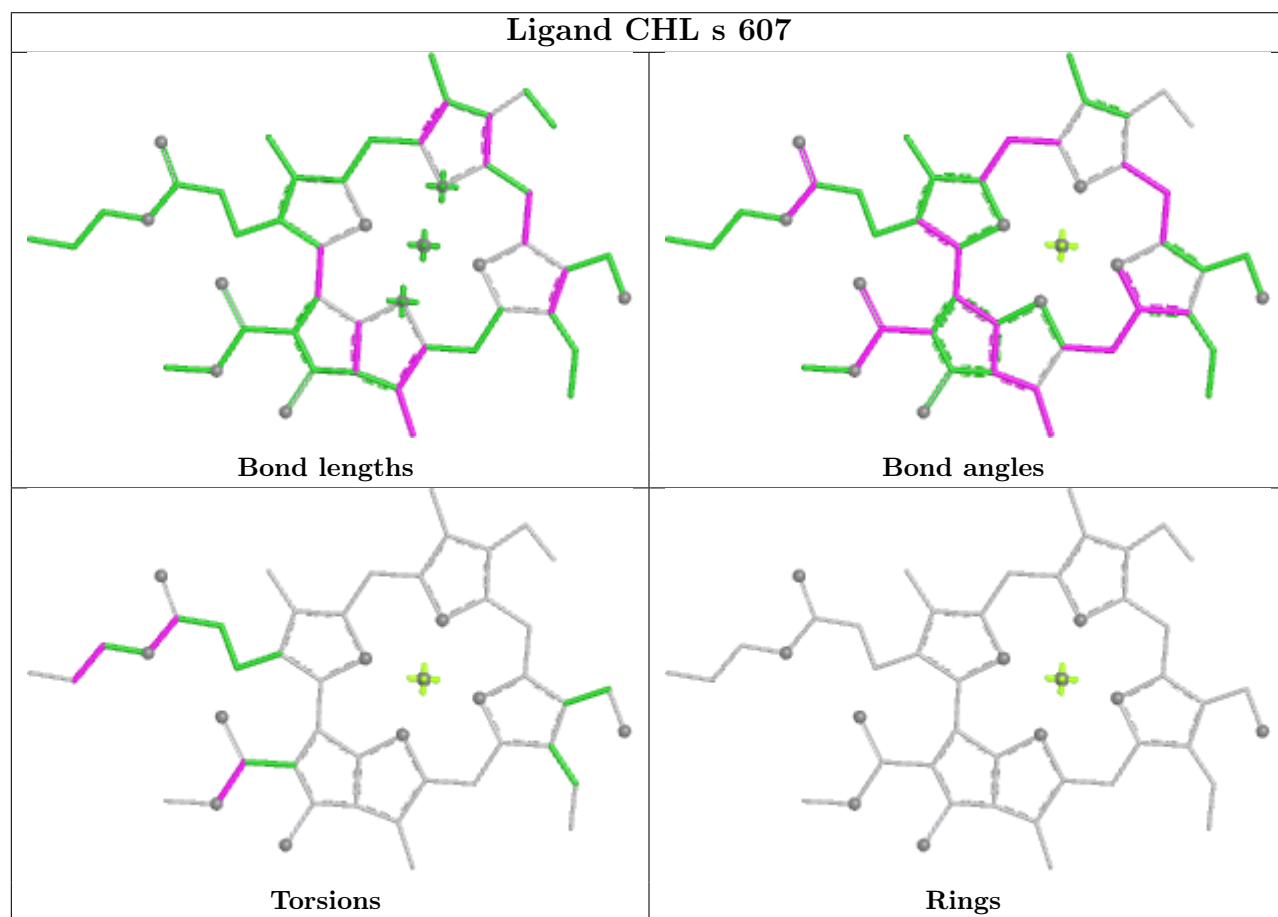
Torsions

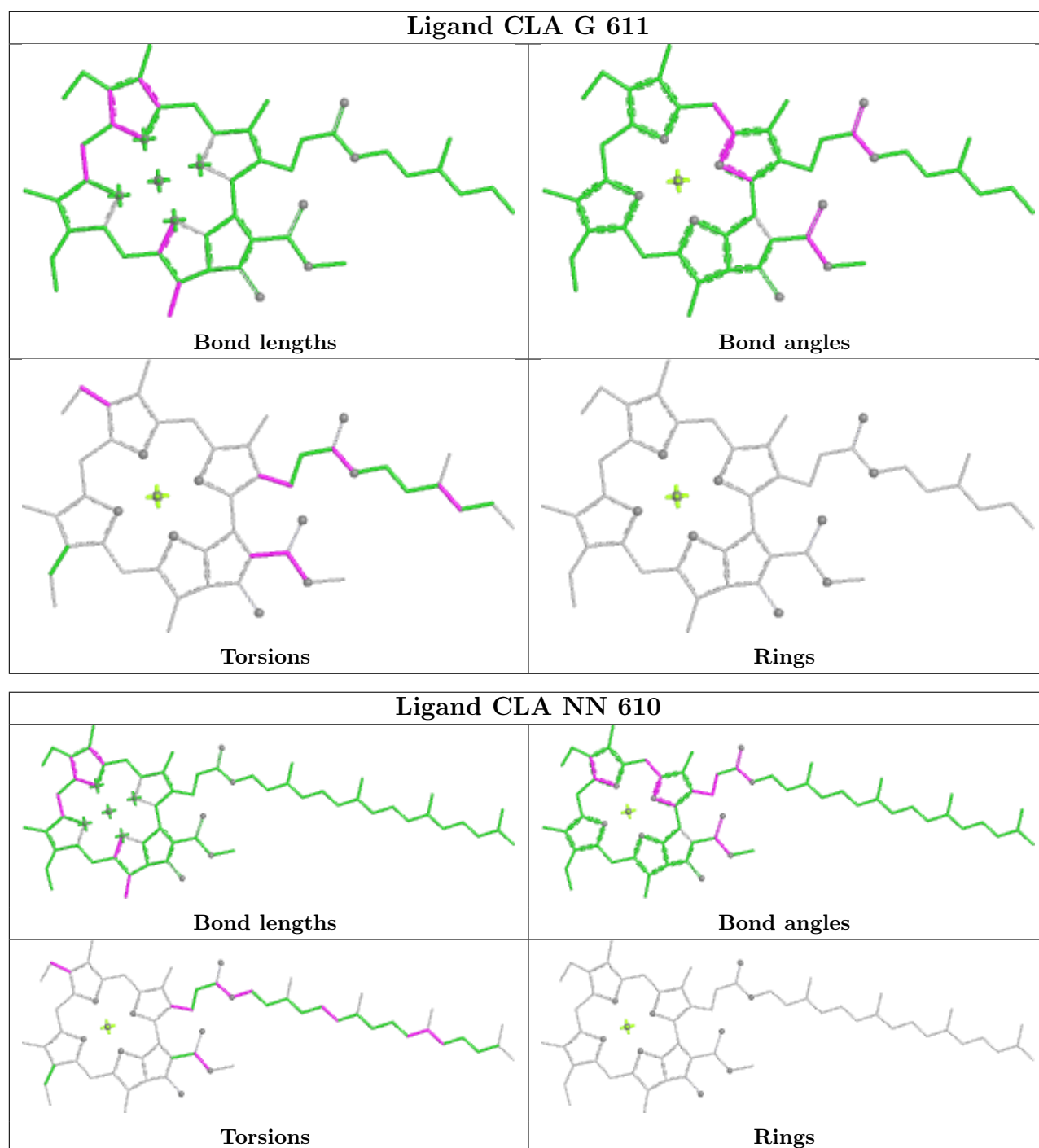


Rings

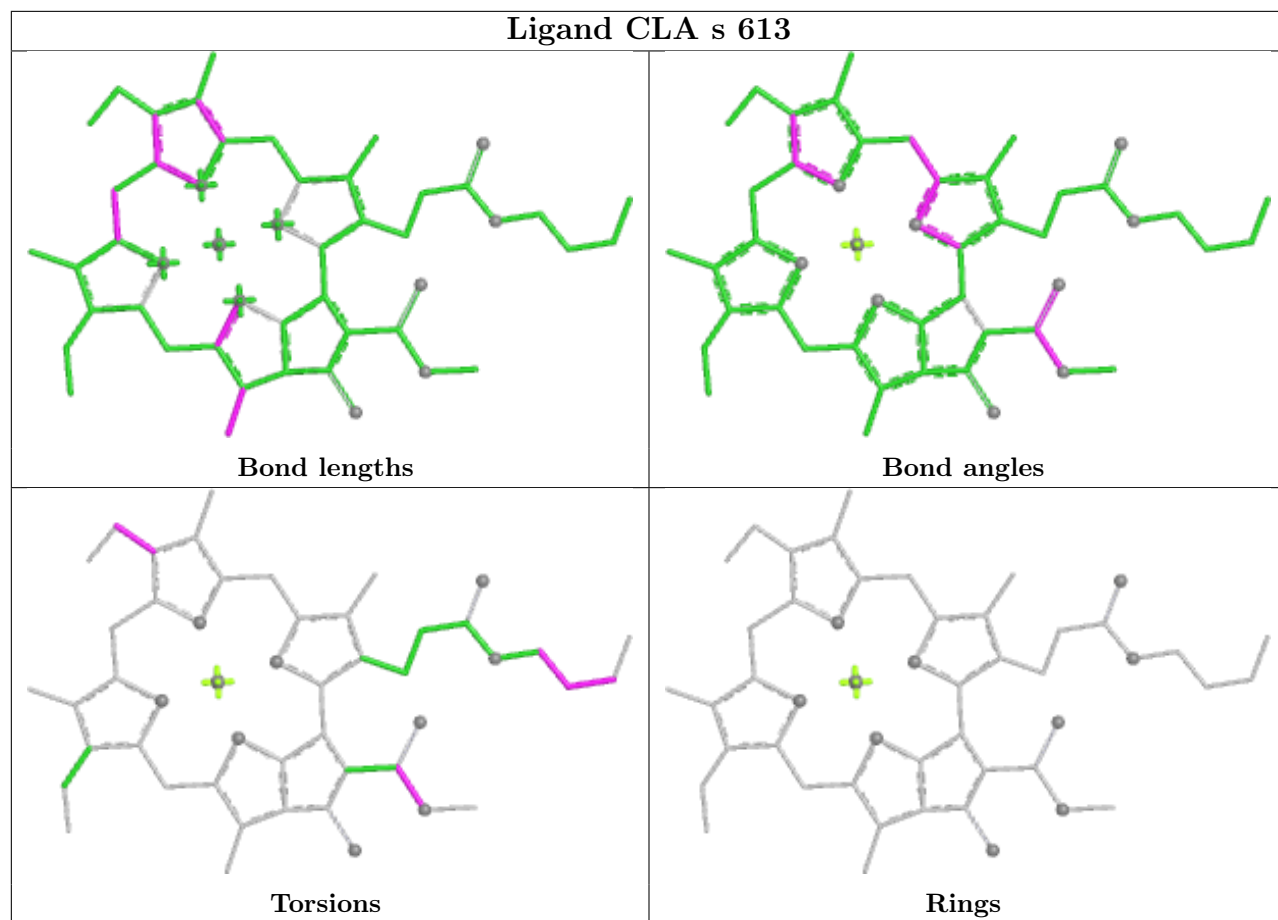


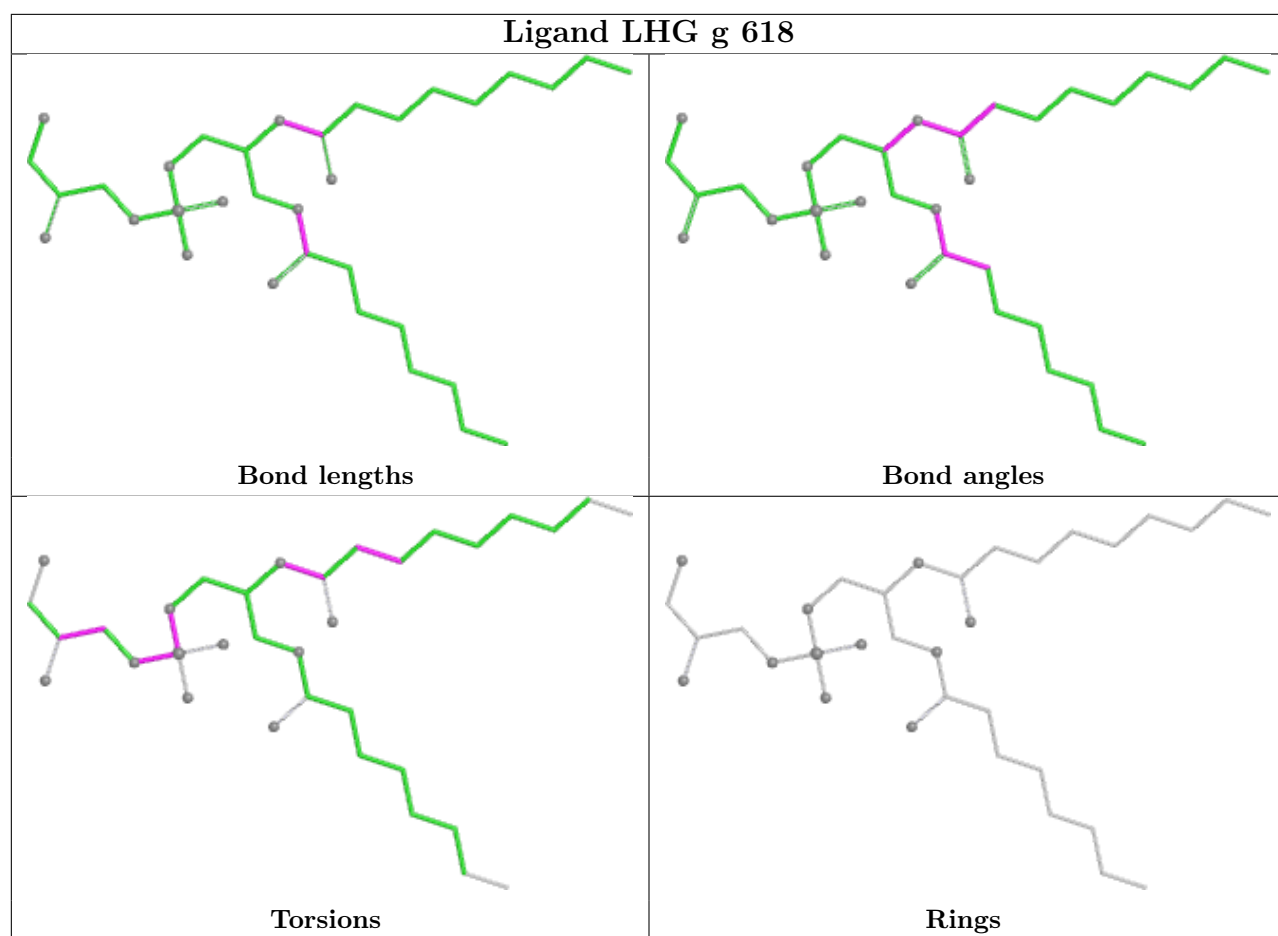


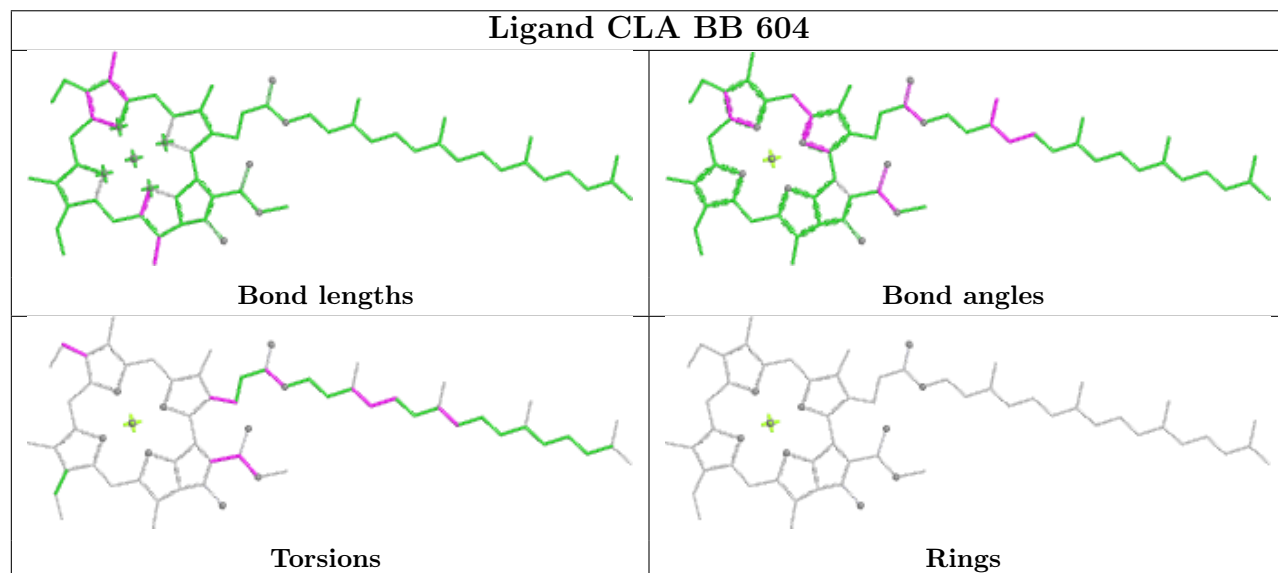
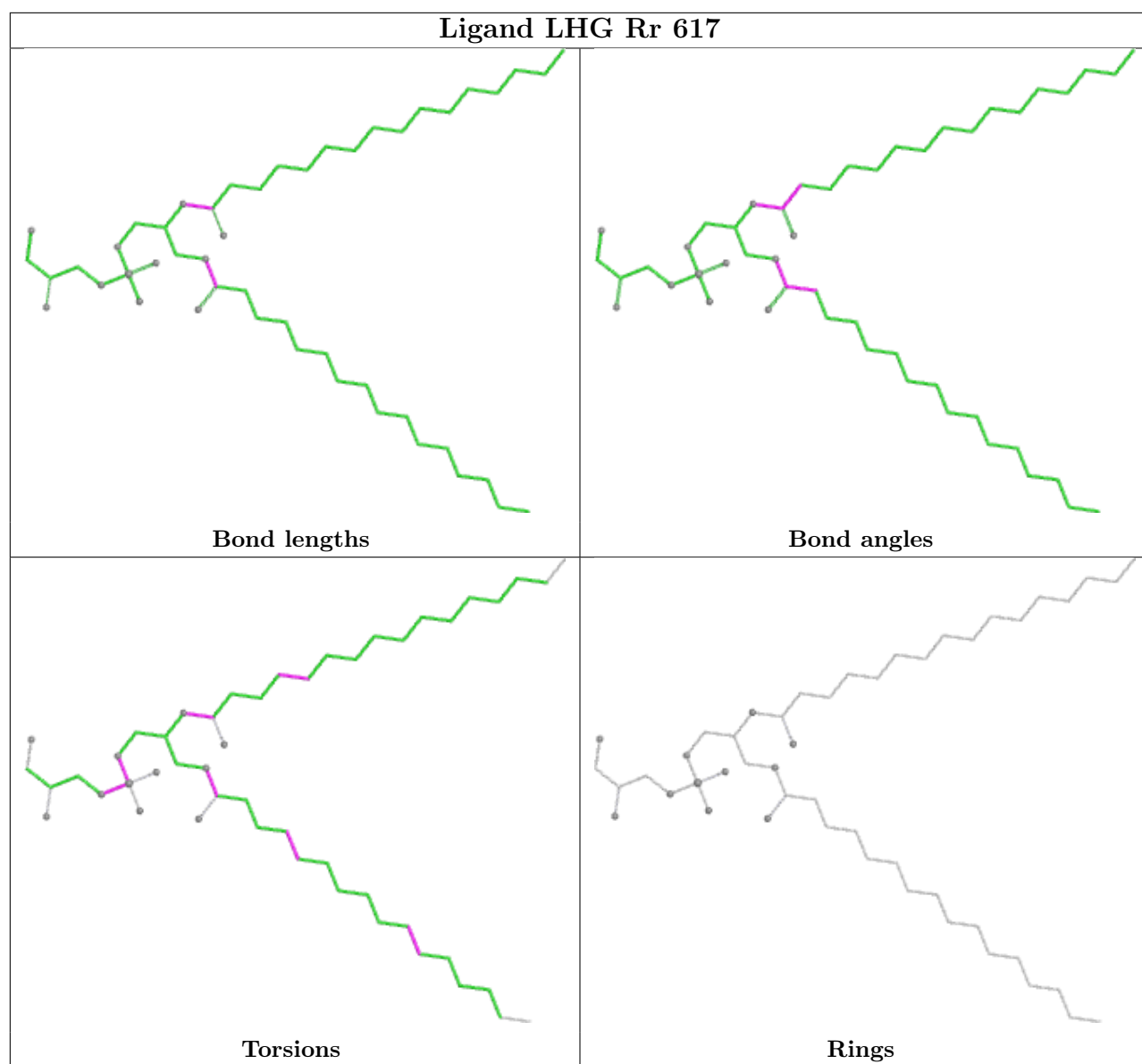
Ligand PHO DD 402**Ligand CHL s 607**

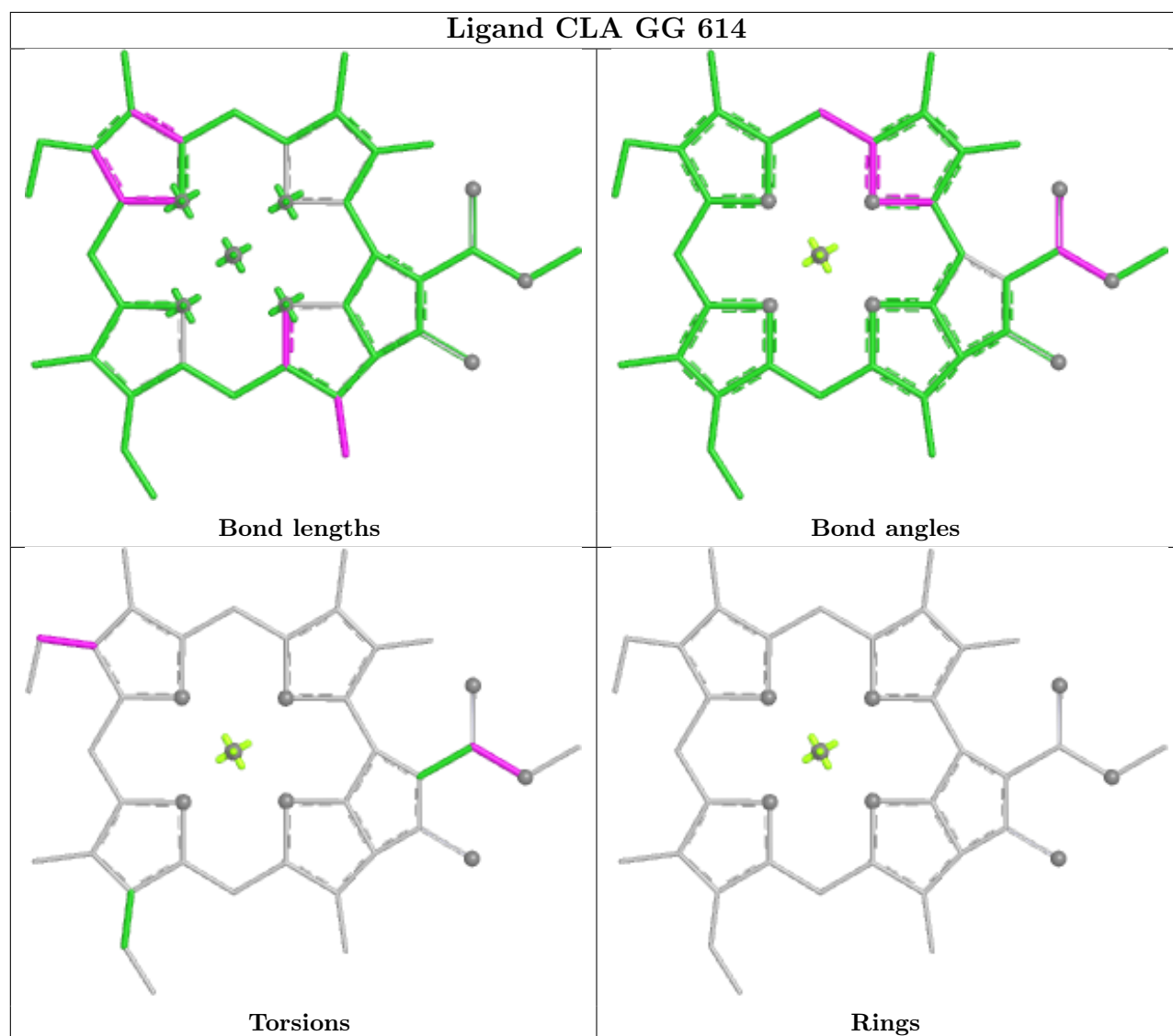
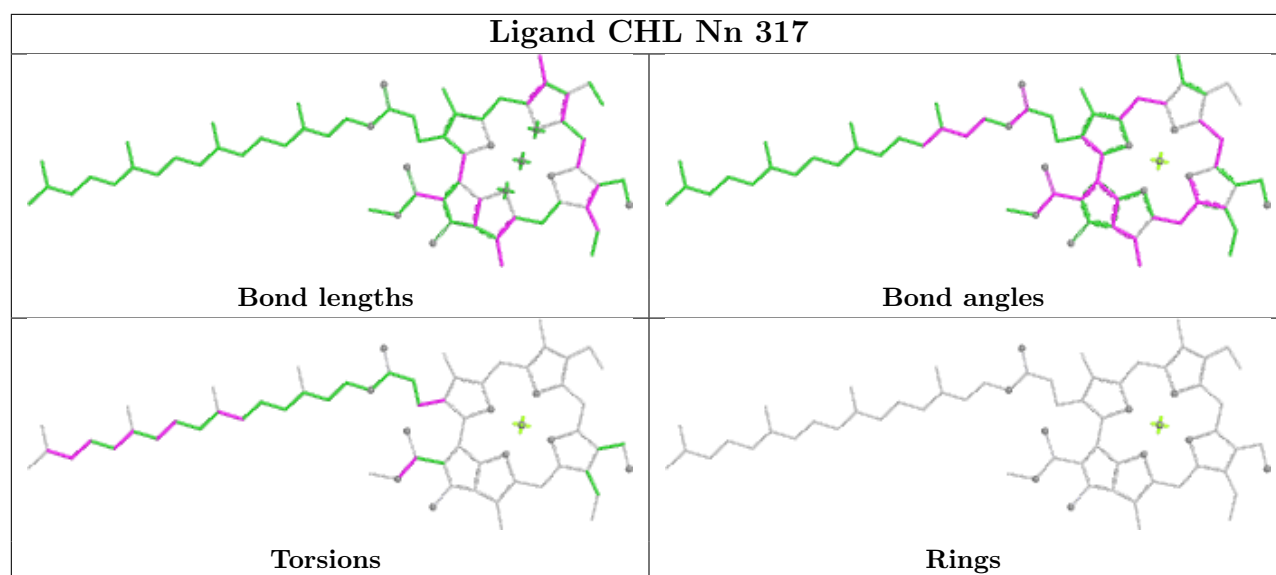


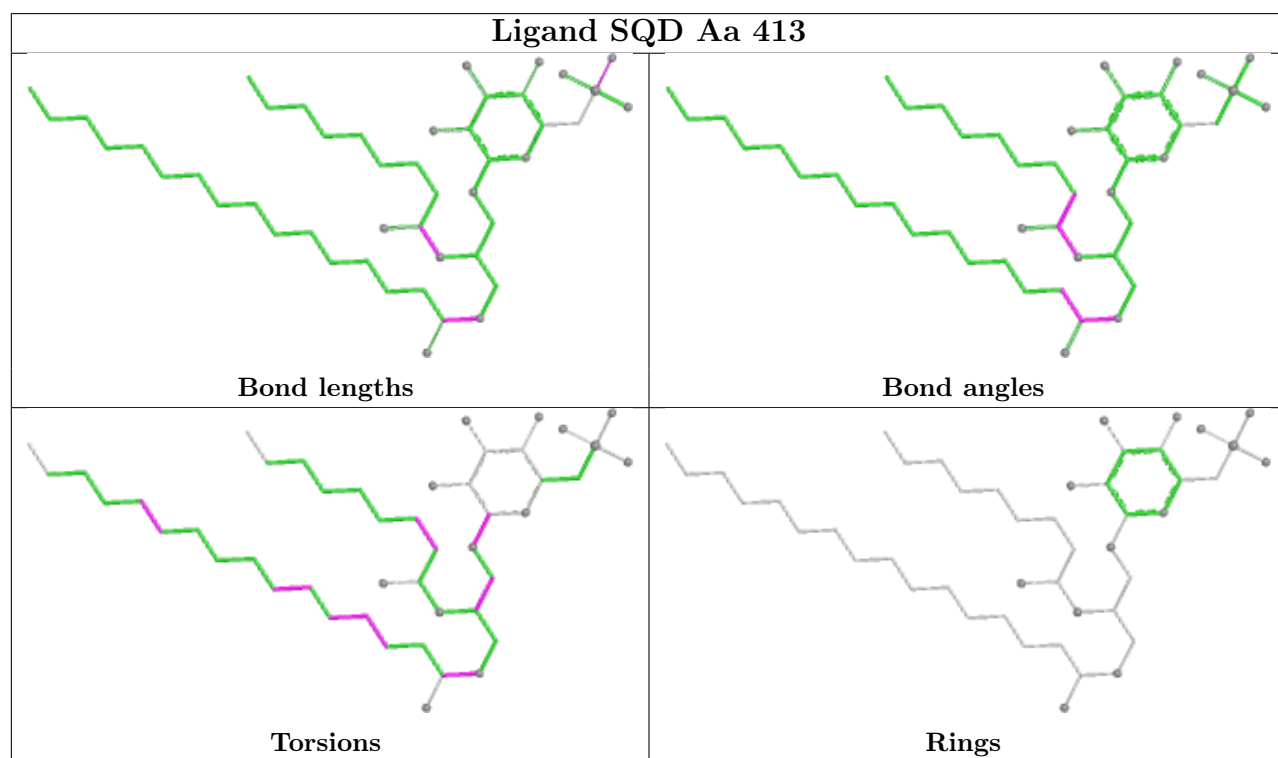
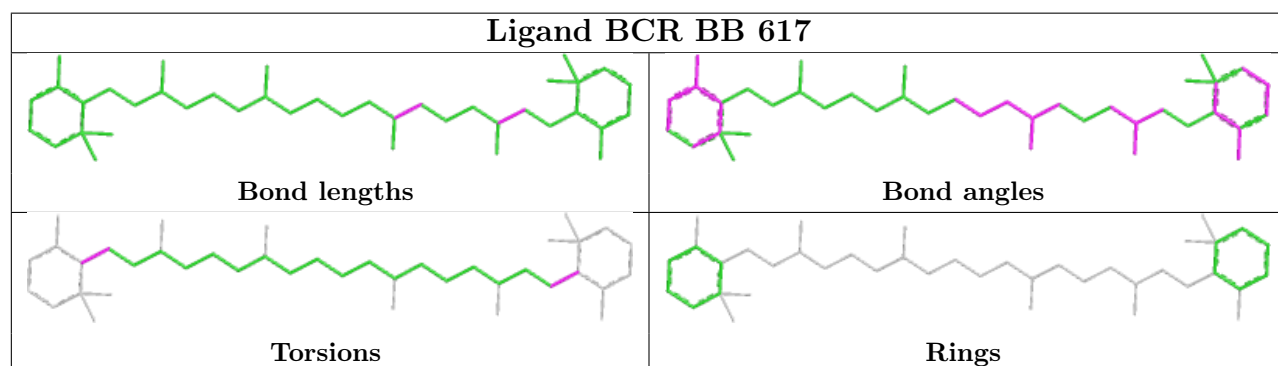
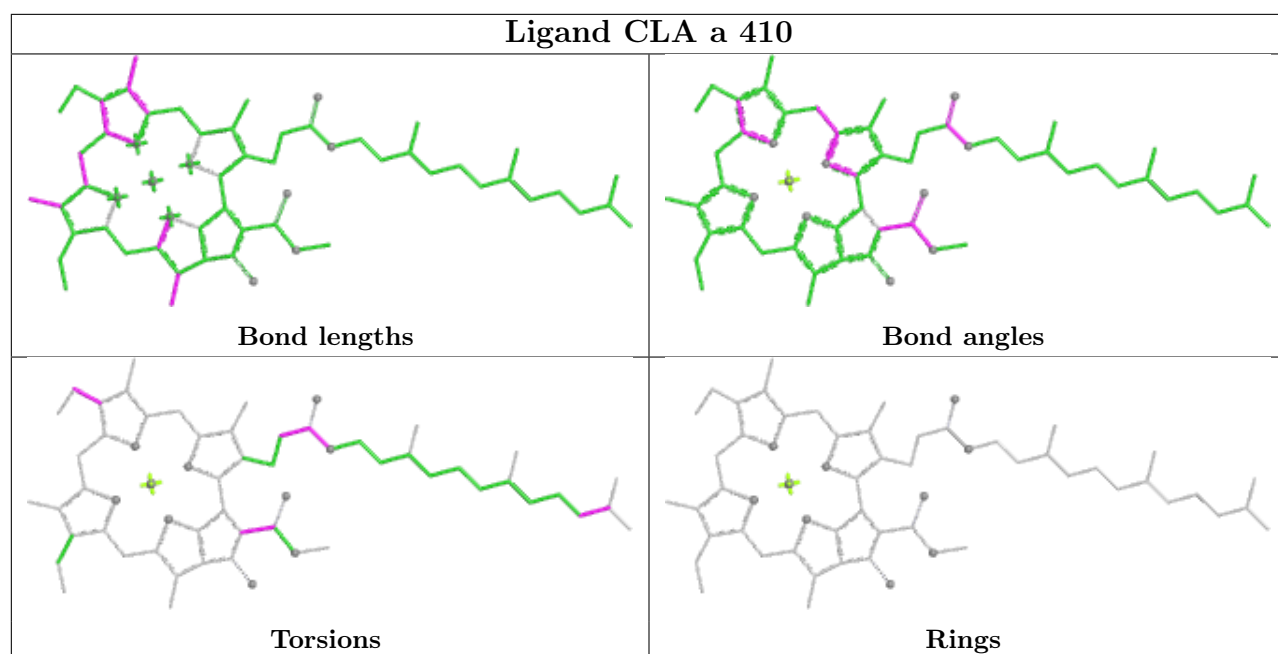
Ligand CLA s 613

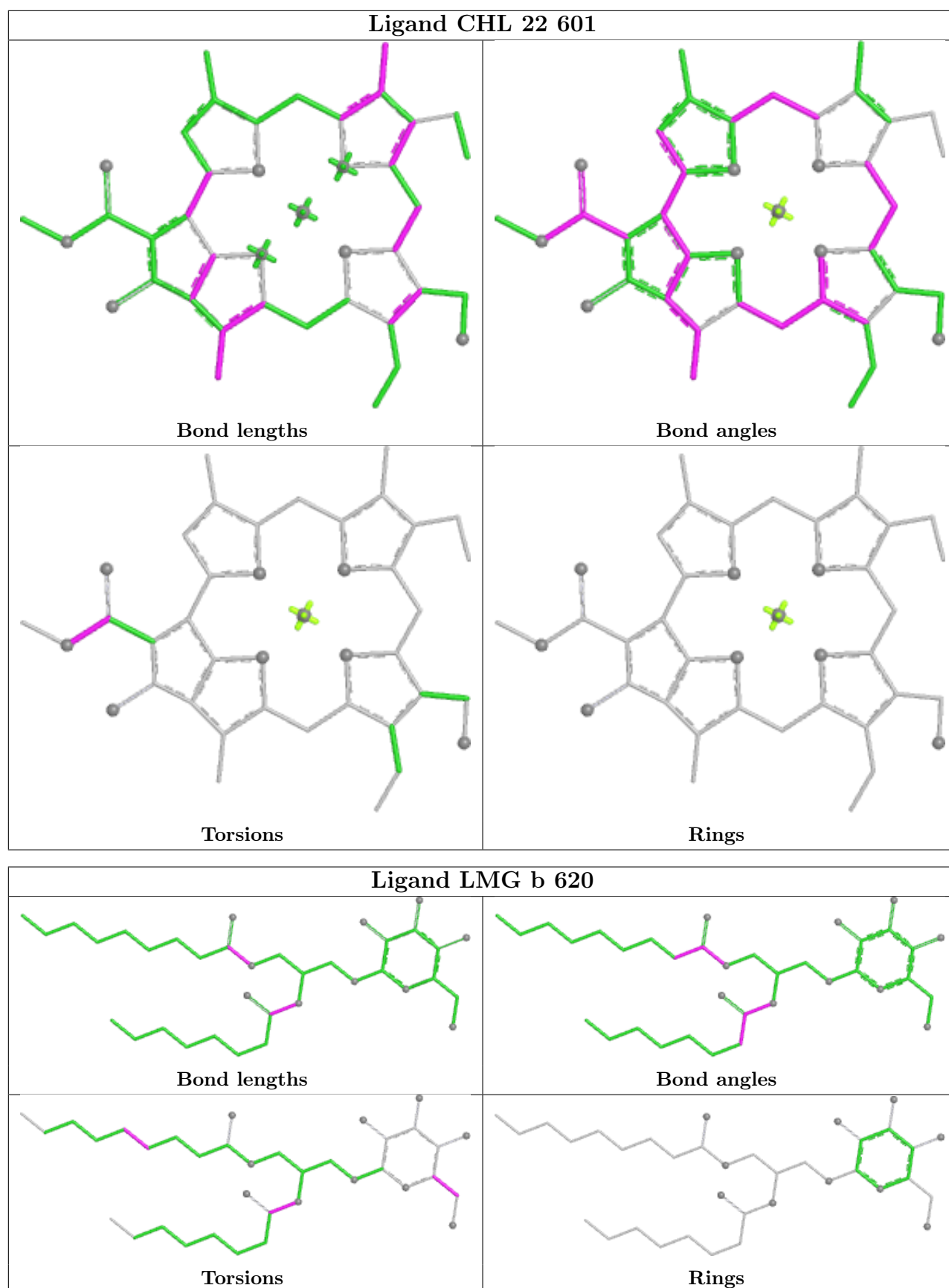


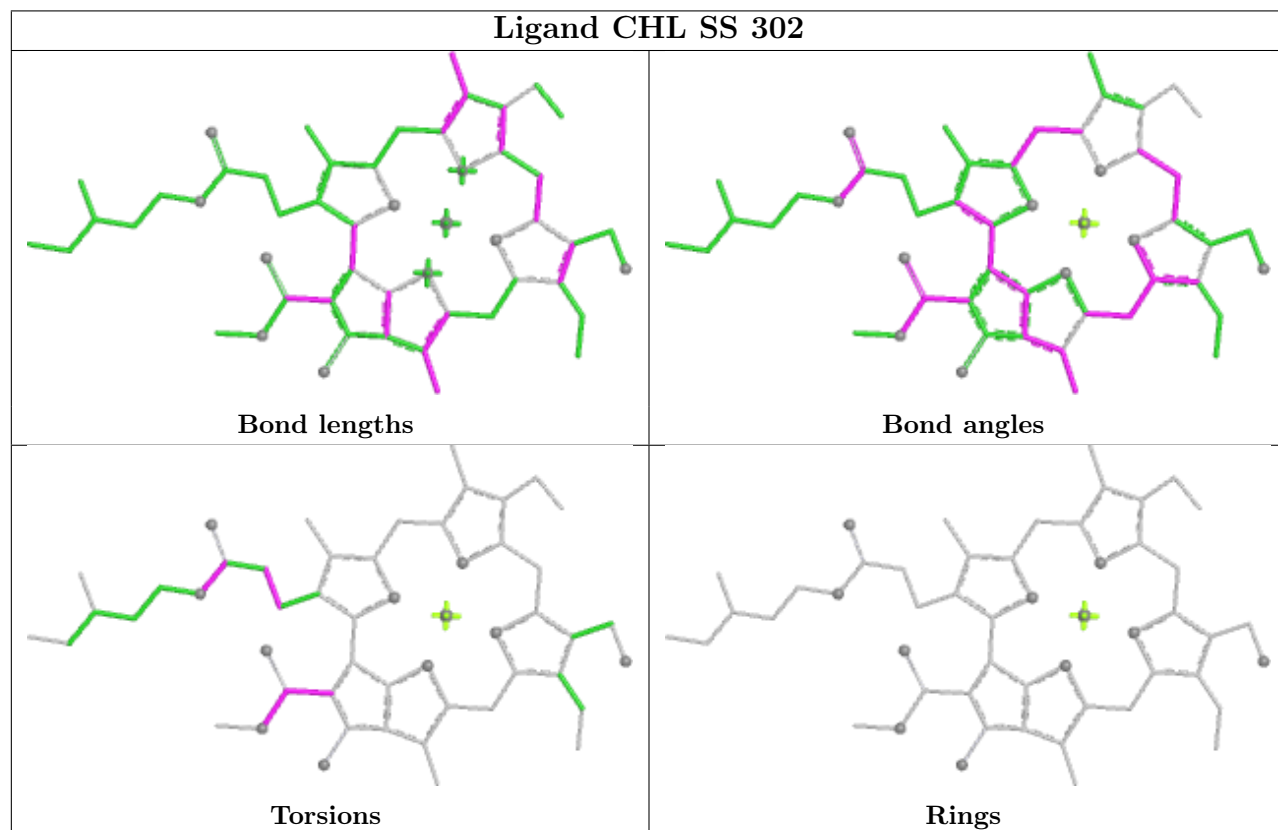
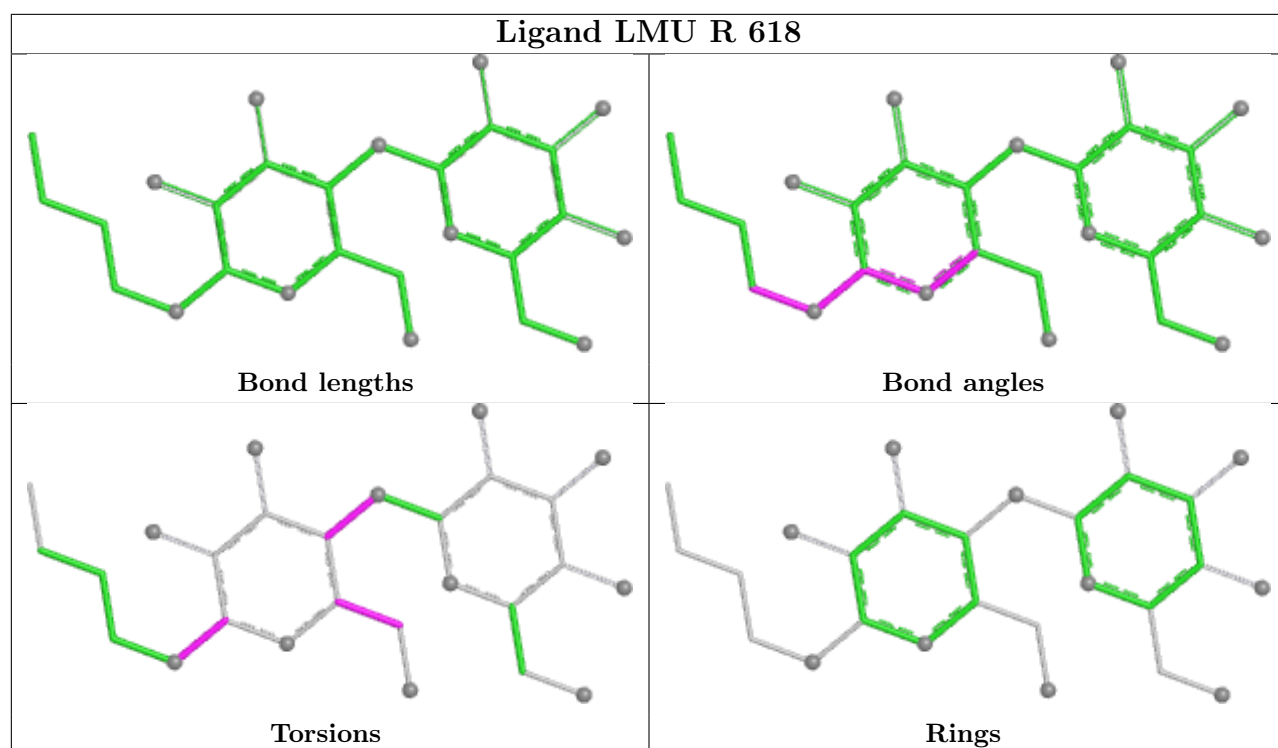




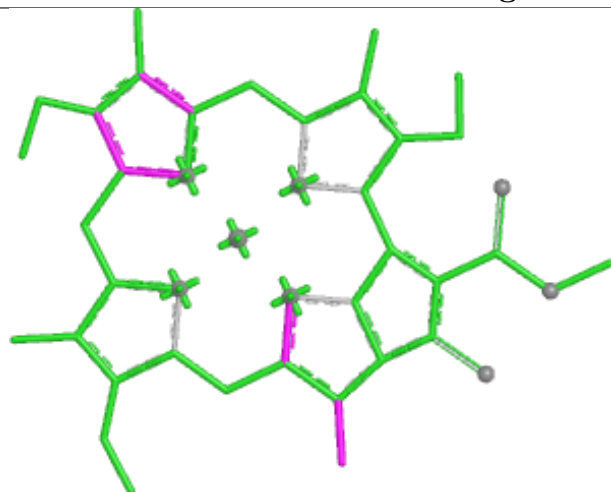




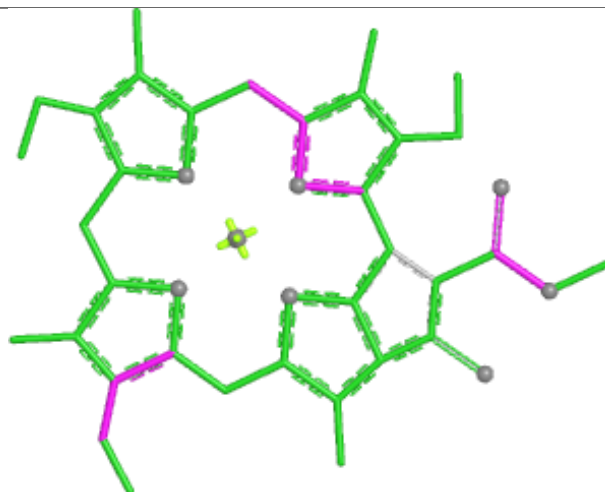




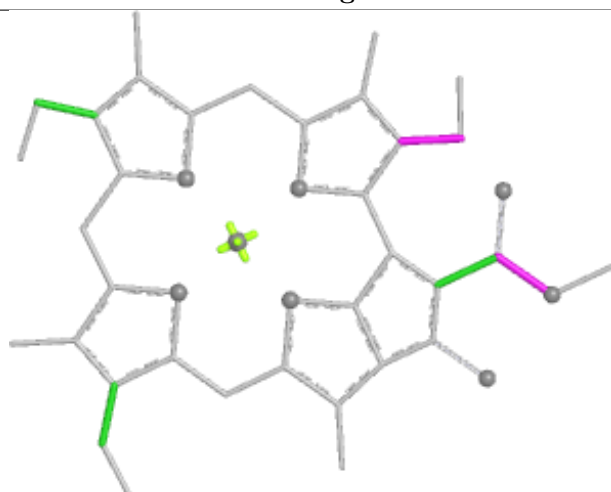
Ligand CLA NN 612



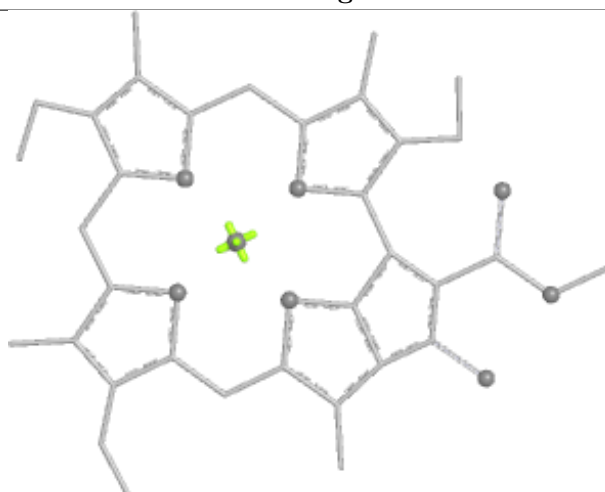
Bond lengths



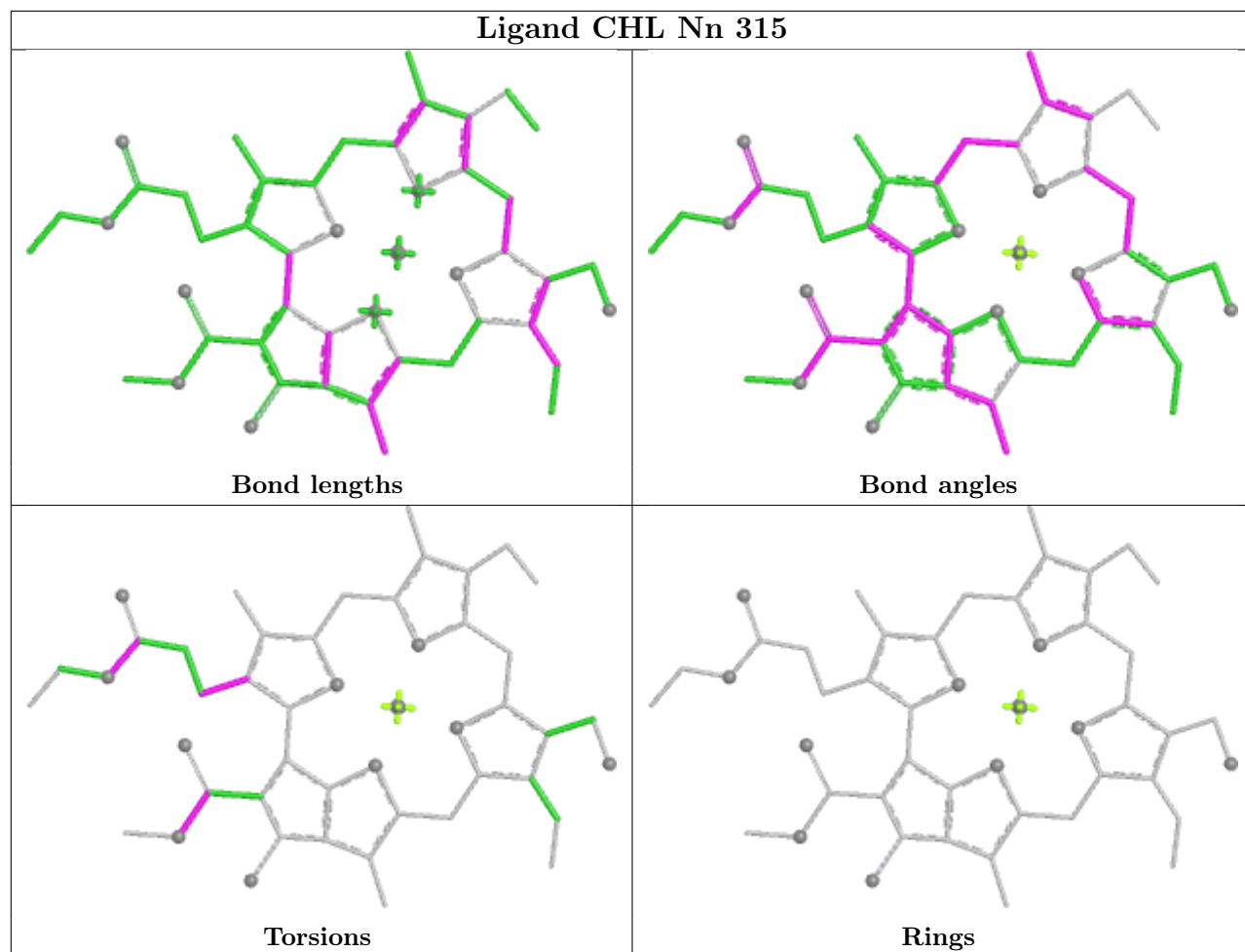
Bond angles

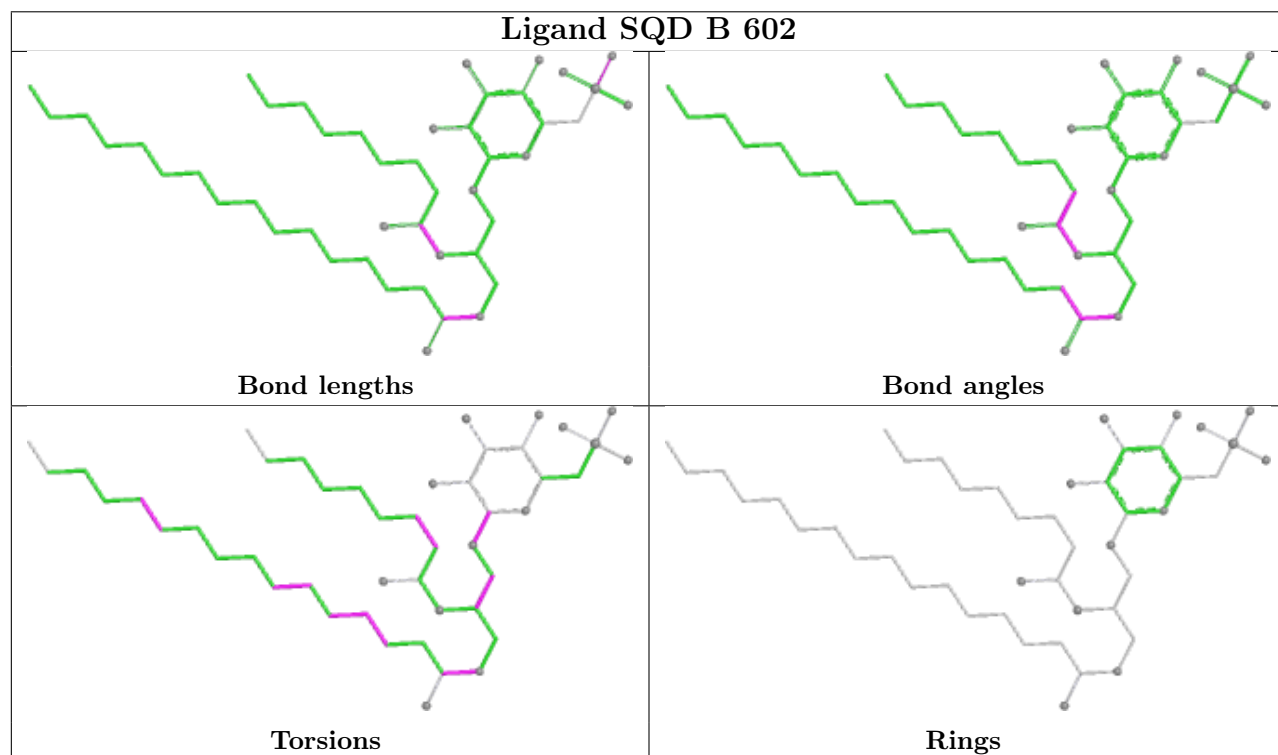
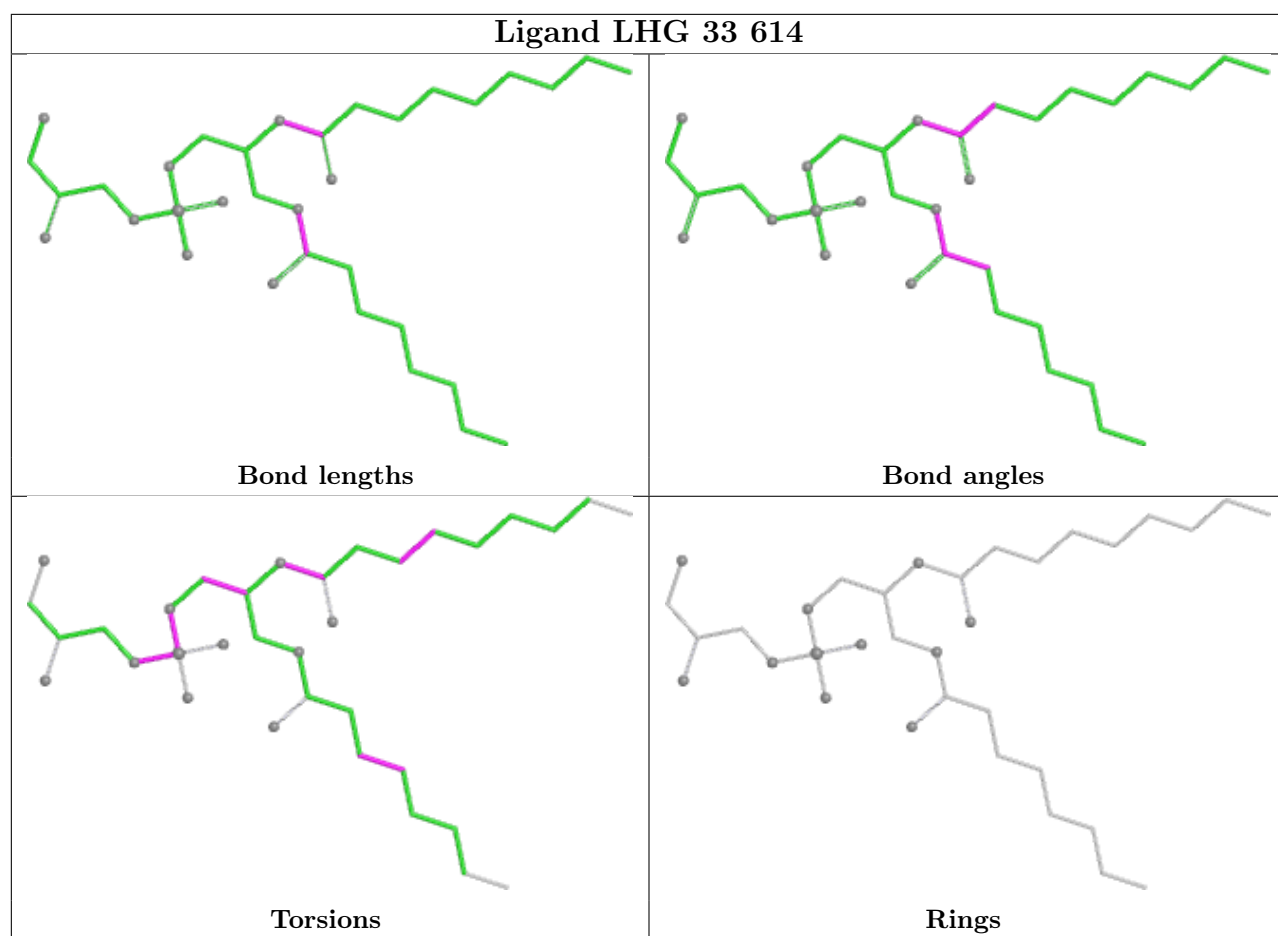


Torsions

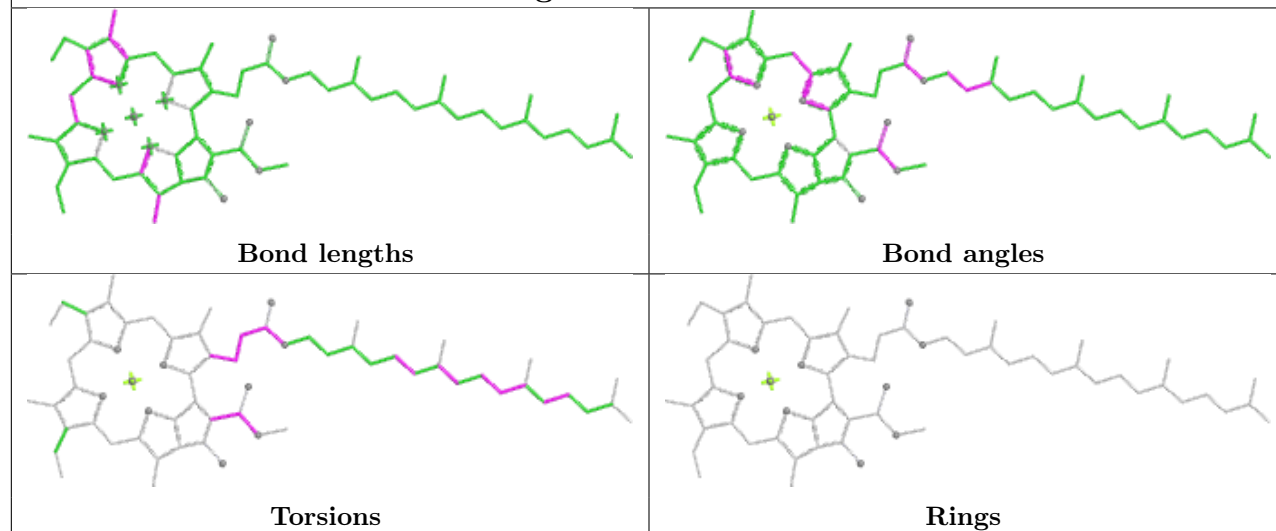


Rings

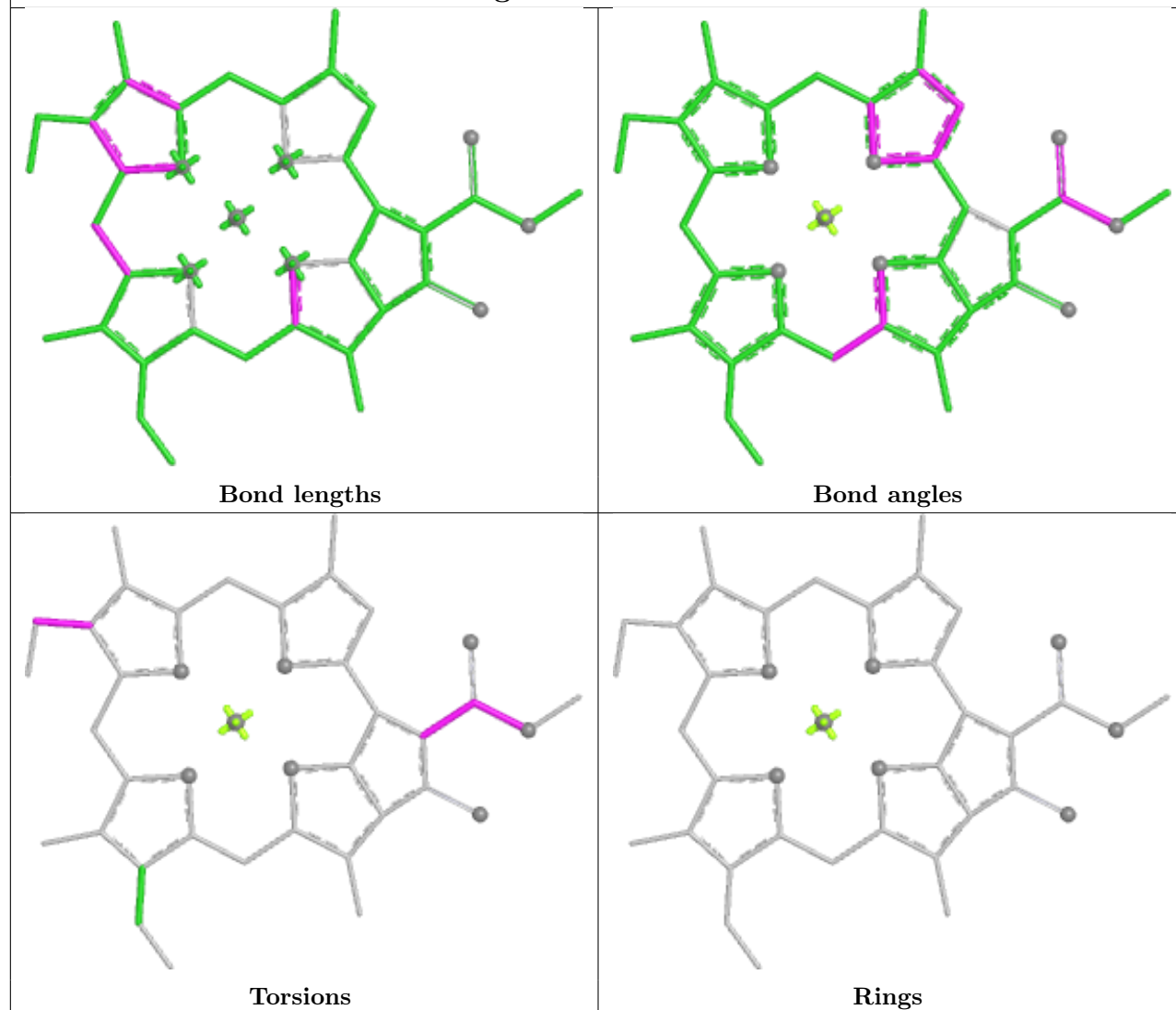




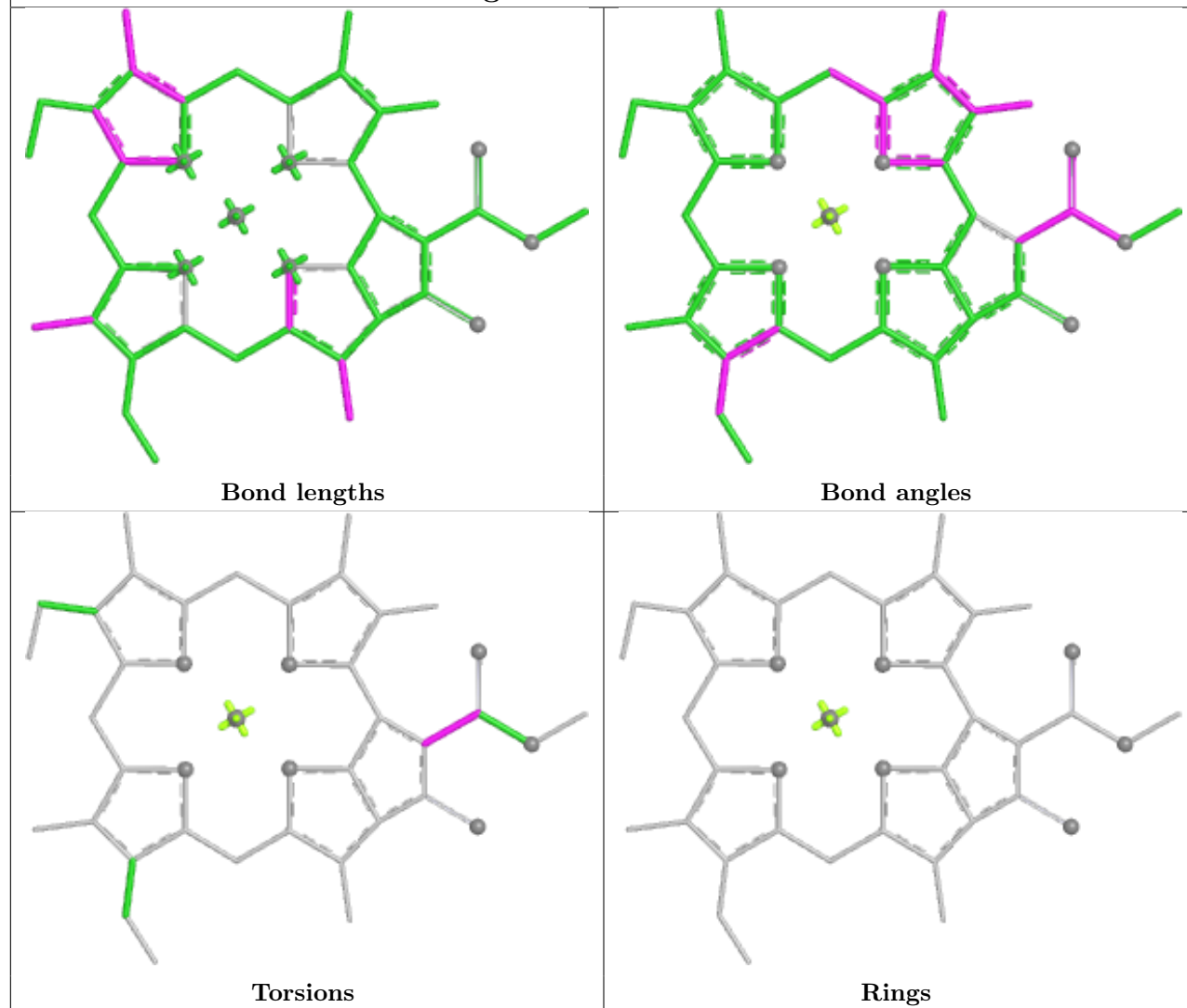
Ligand CLA b 609



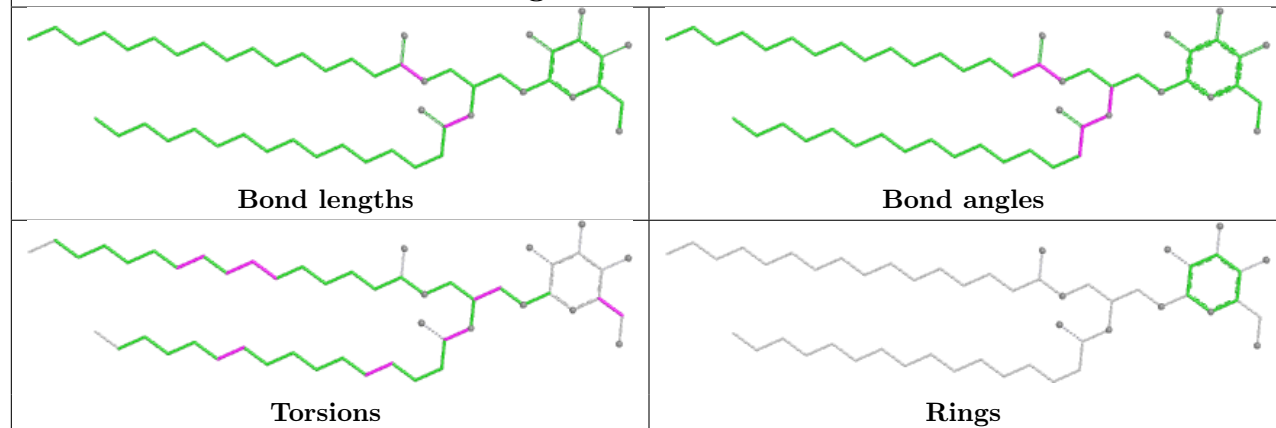
Ligand CLA 2 602



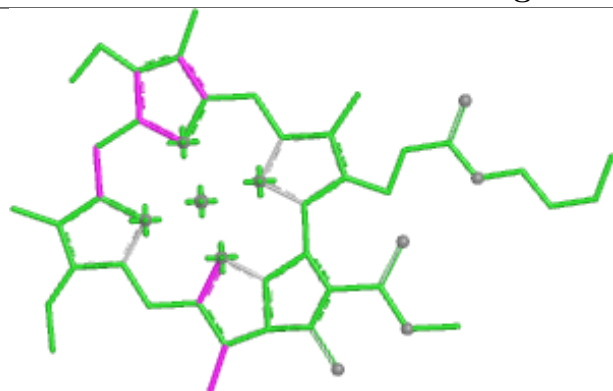
Ligand CLA BB 615



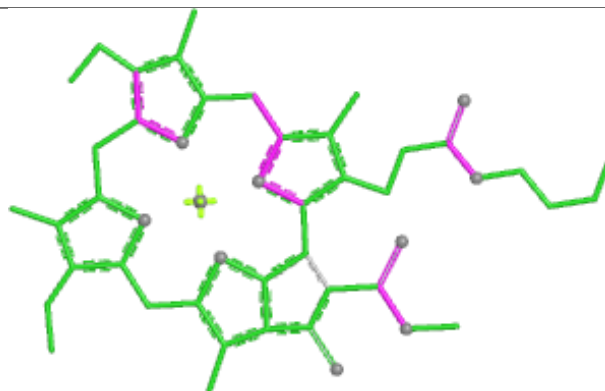
Ligand LMG C 521



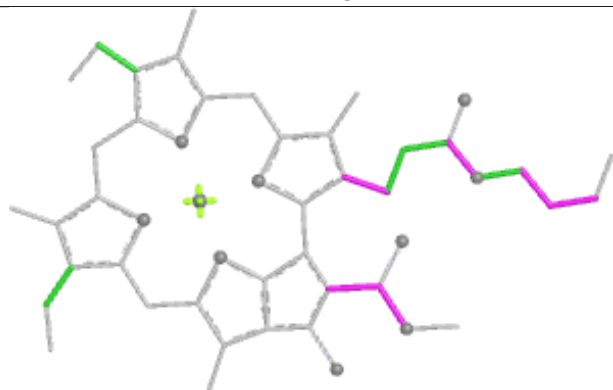
Ligand CLA R 610



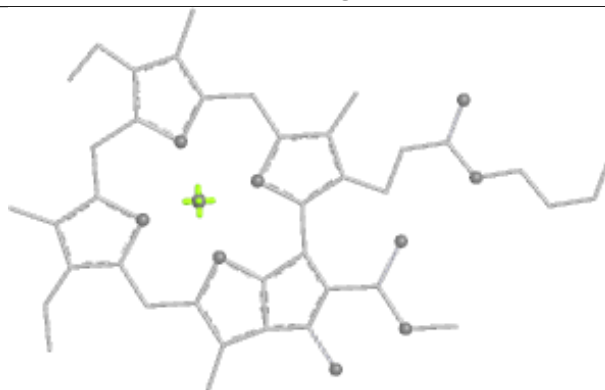
Bond lengths



Bond angles

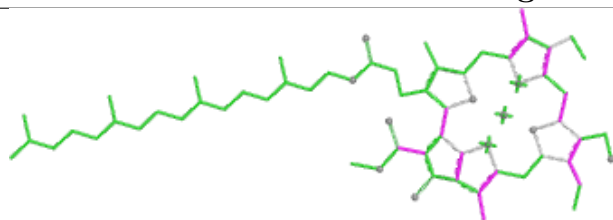


Torsions

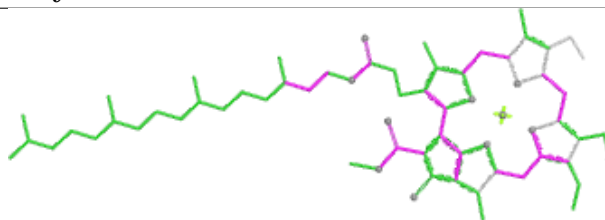


Rings

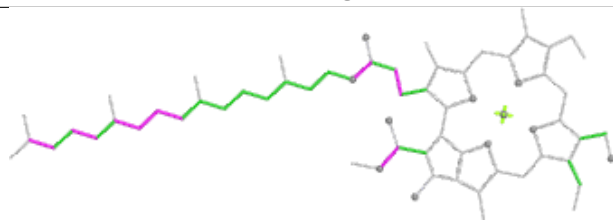
Ligand CHL y 303



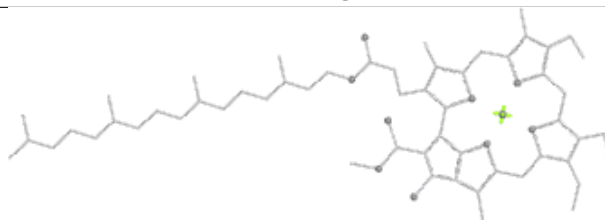
Bond lengths



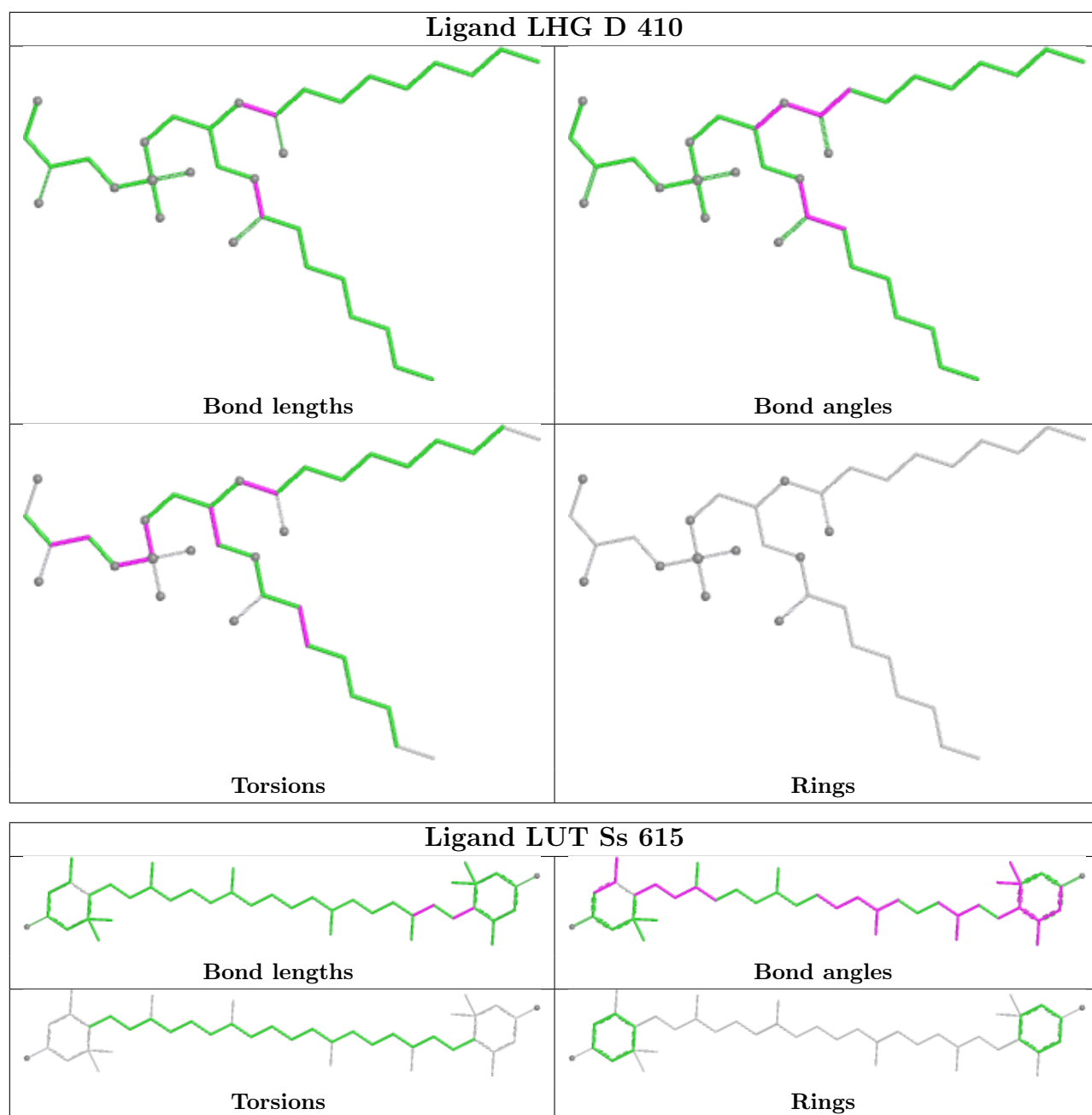
Bond angles

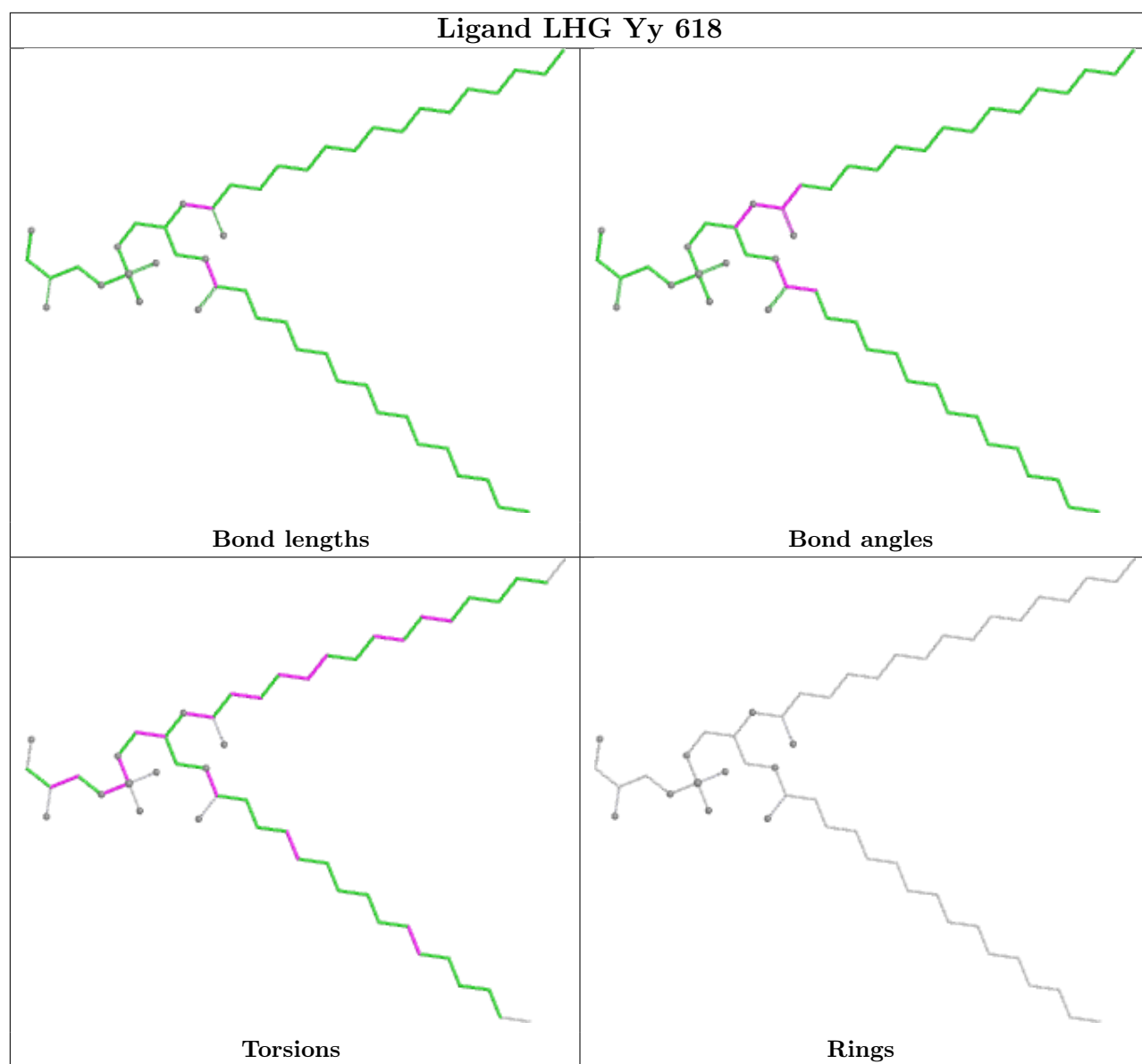


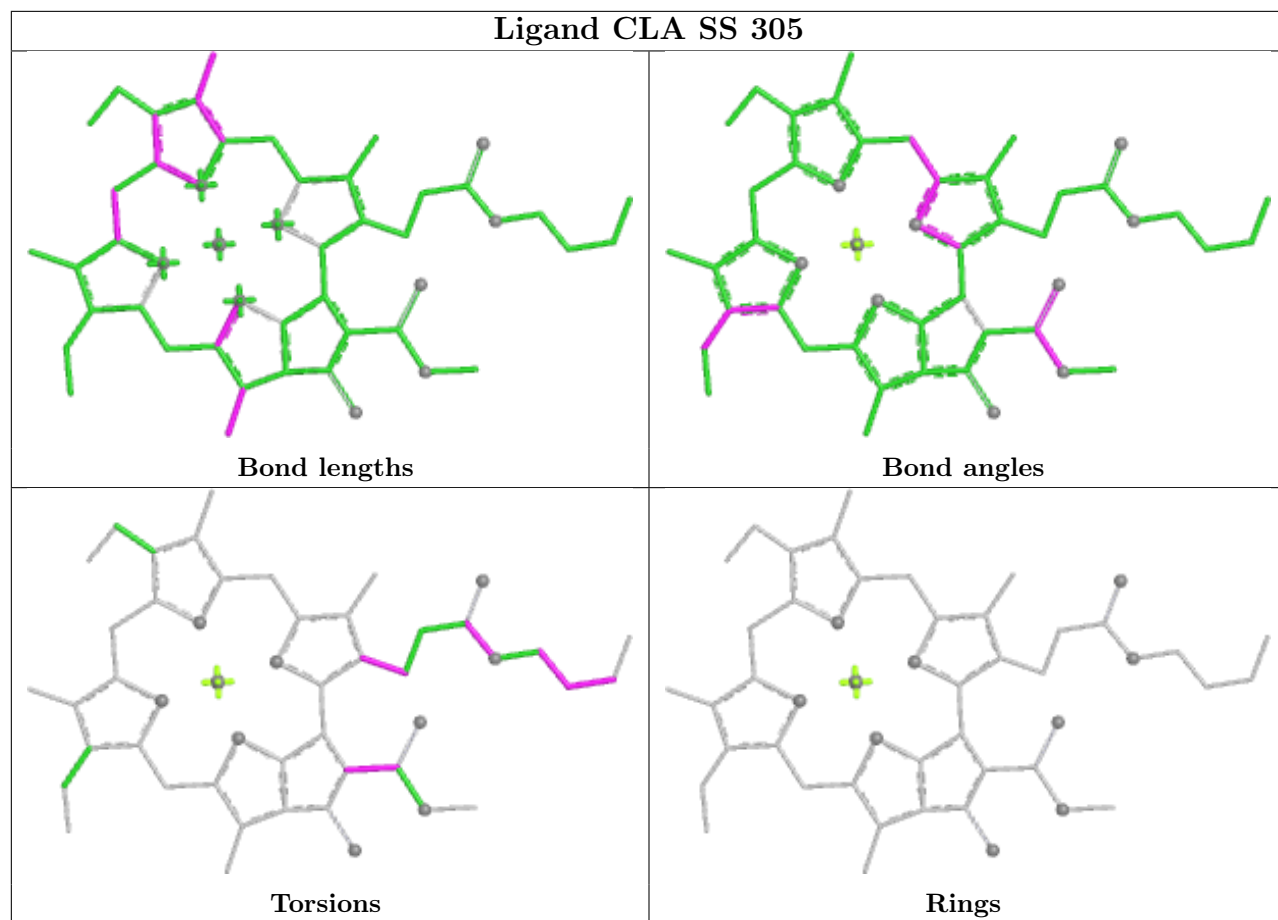
Torsions



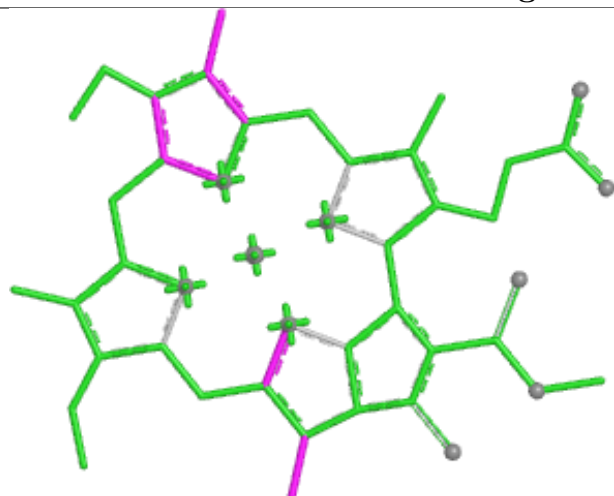
Rings



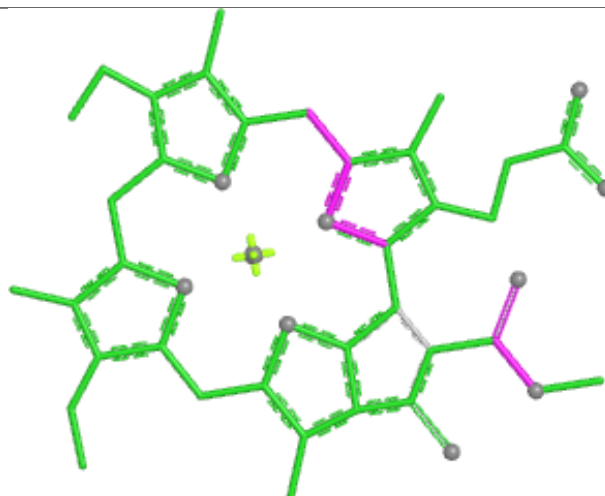




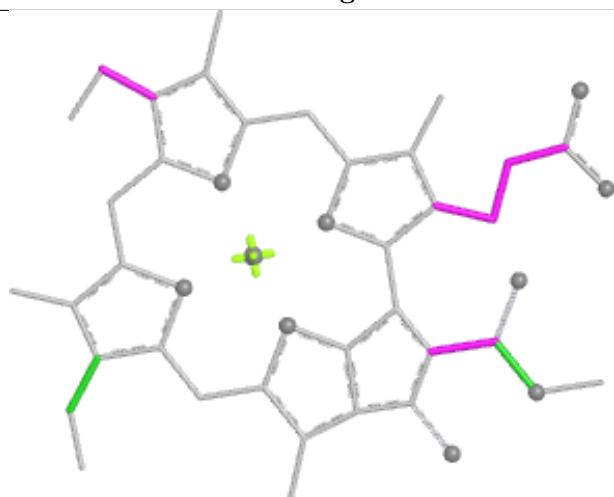
Ligand CLA 4 312



Bond lengths



Bond angles

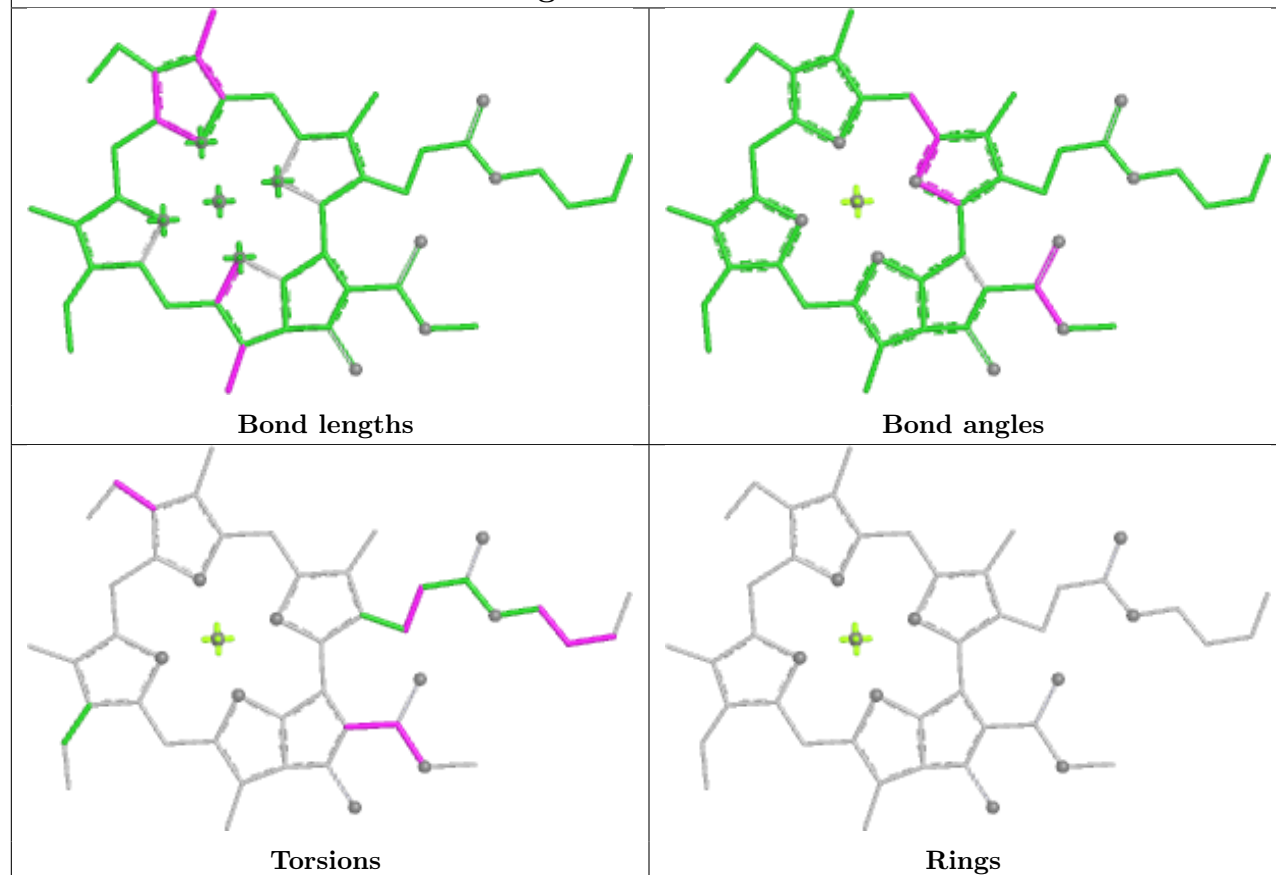


Torsions

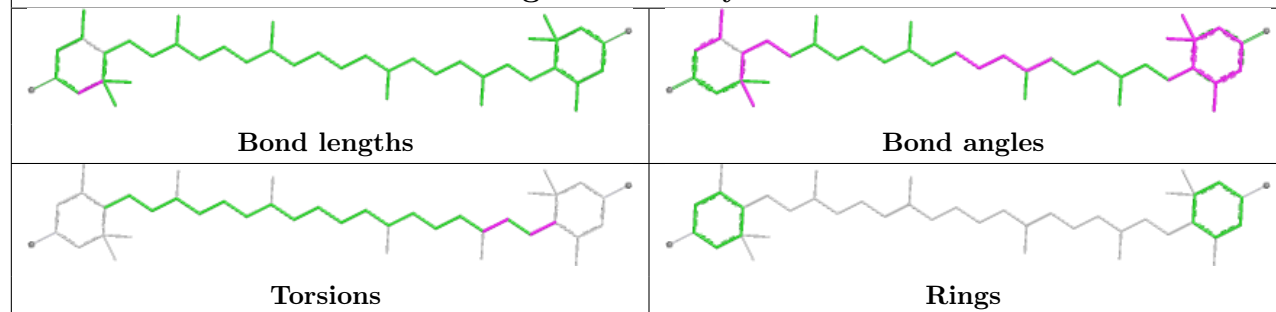


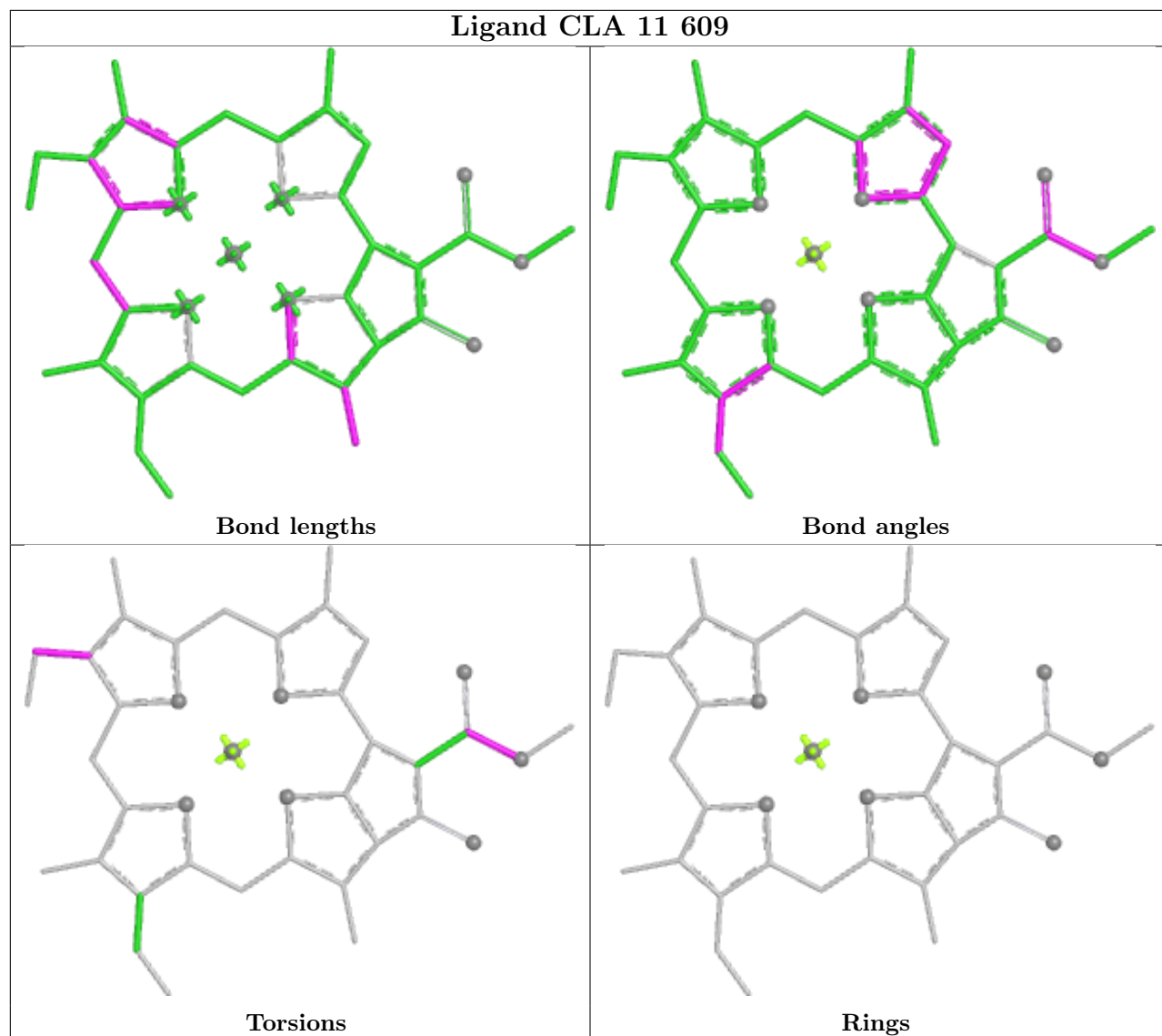
Rings

Ligand CLA s 610

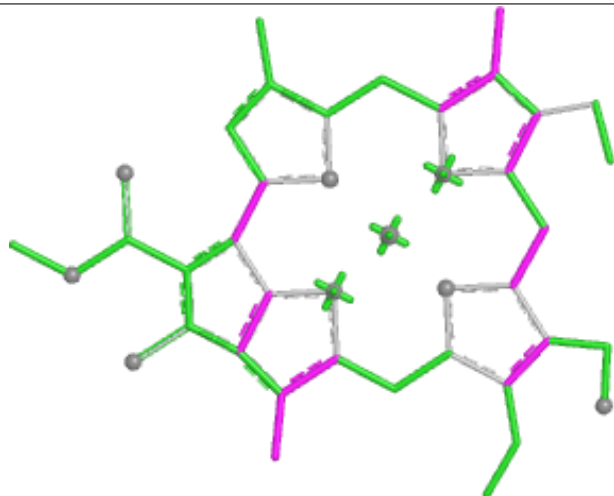


Ligand LUT Yy 615

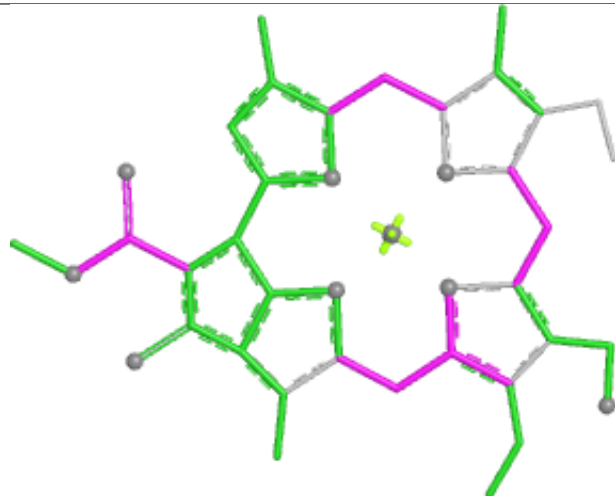




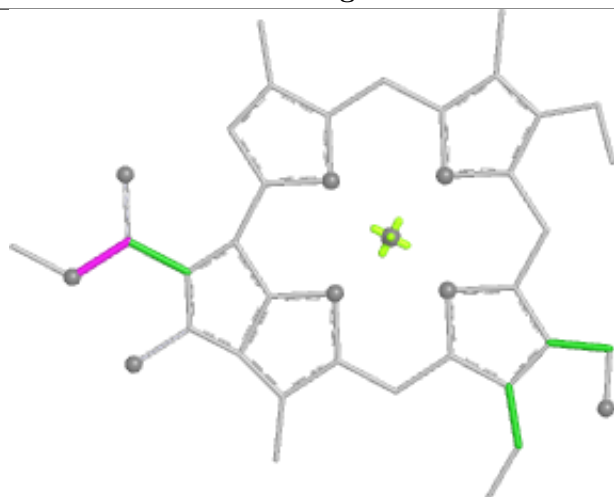
Ligand CHL 2 608



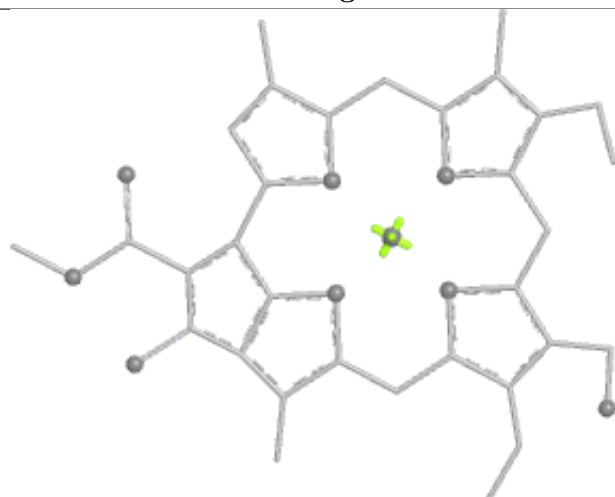
Bond lengths



Bond angles

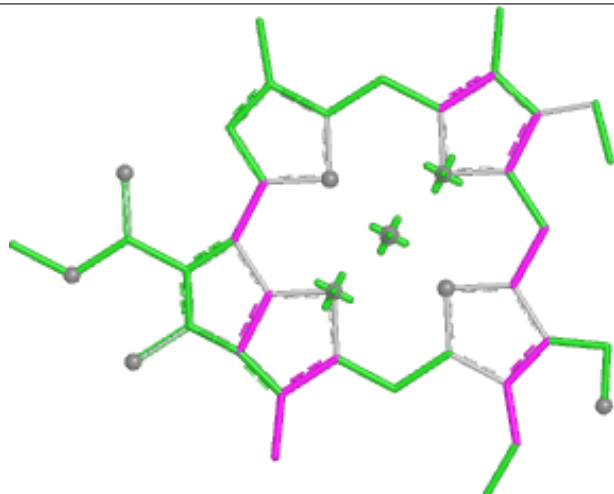


Torsions

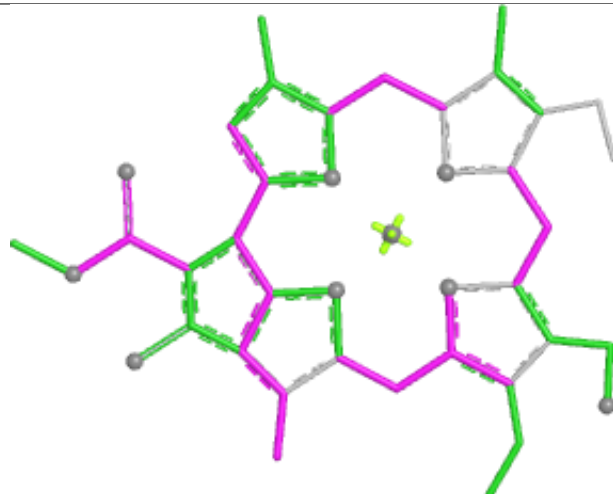


Rings

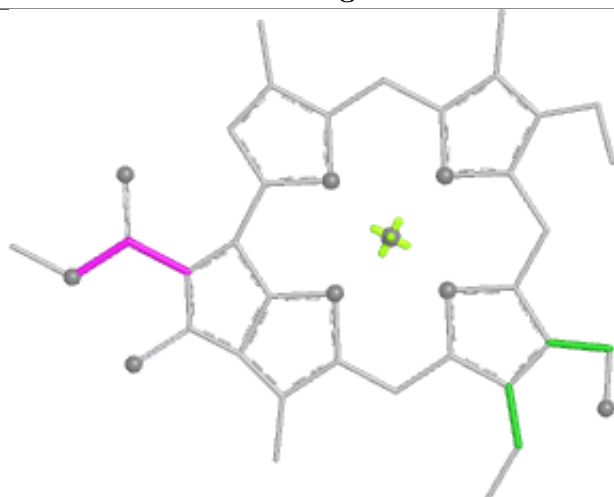
Ligand CHL 3 605



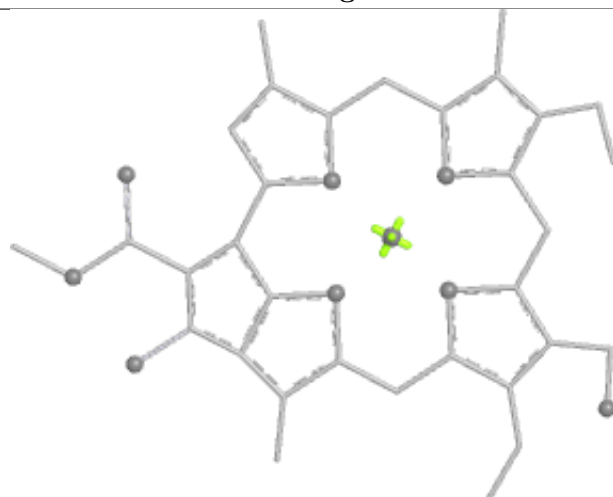
Bond lengths



Bond angles

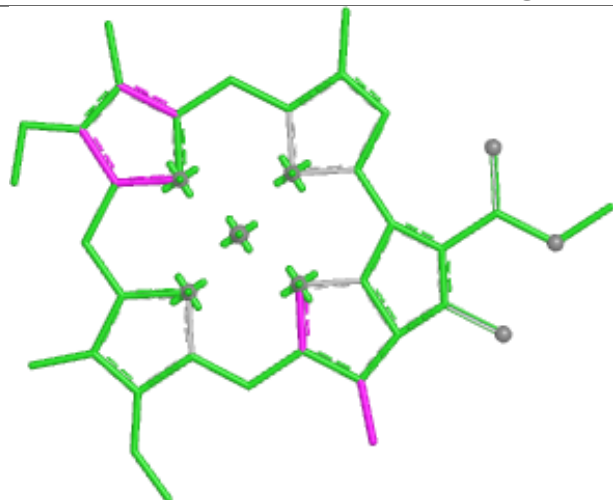


Torsions

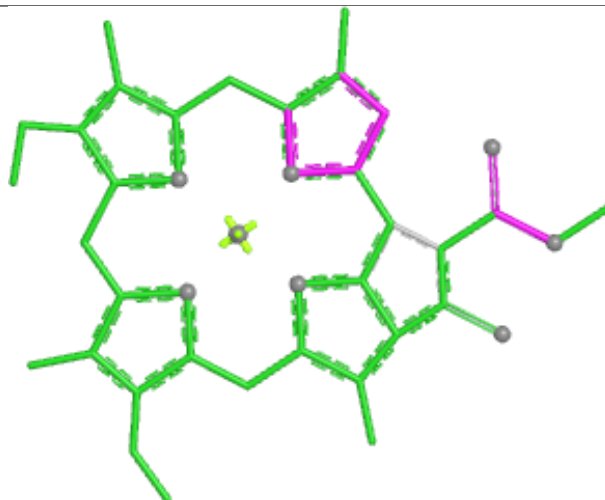


Rings

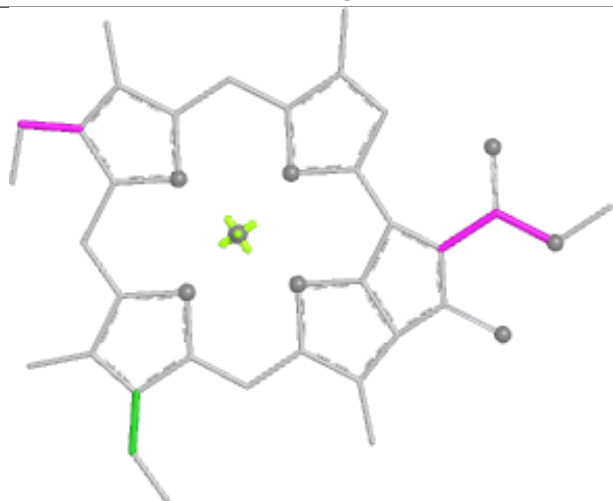
Ligand CLA 1 603



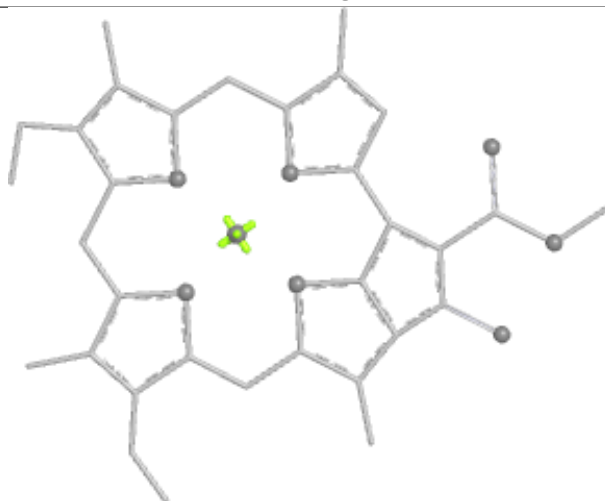
Bond lengths



Bond angles

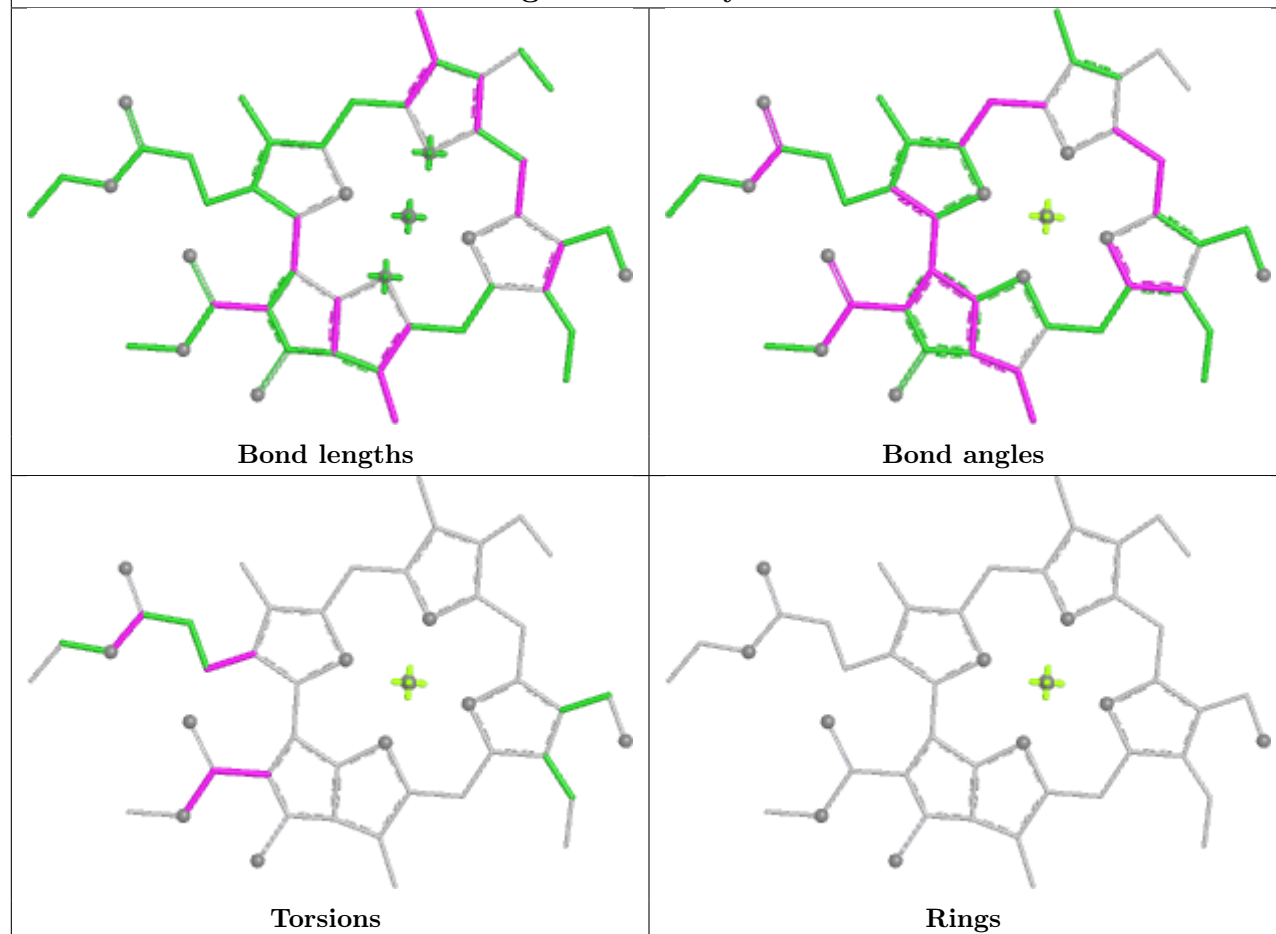


Torsions

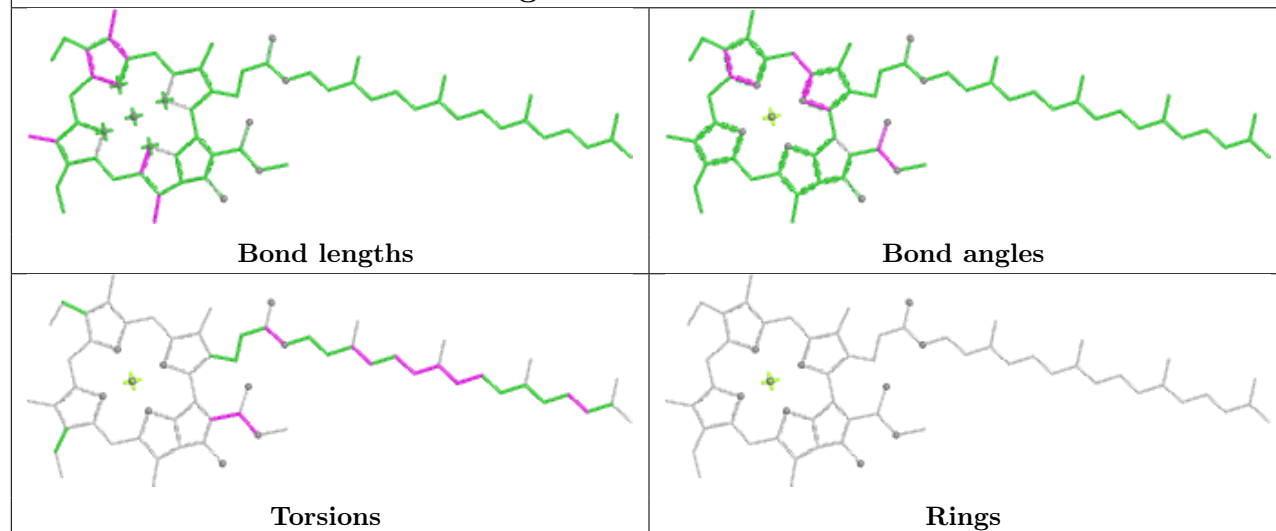


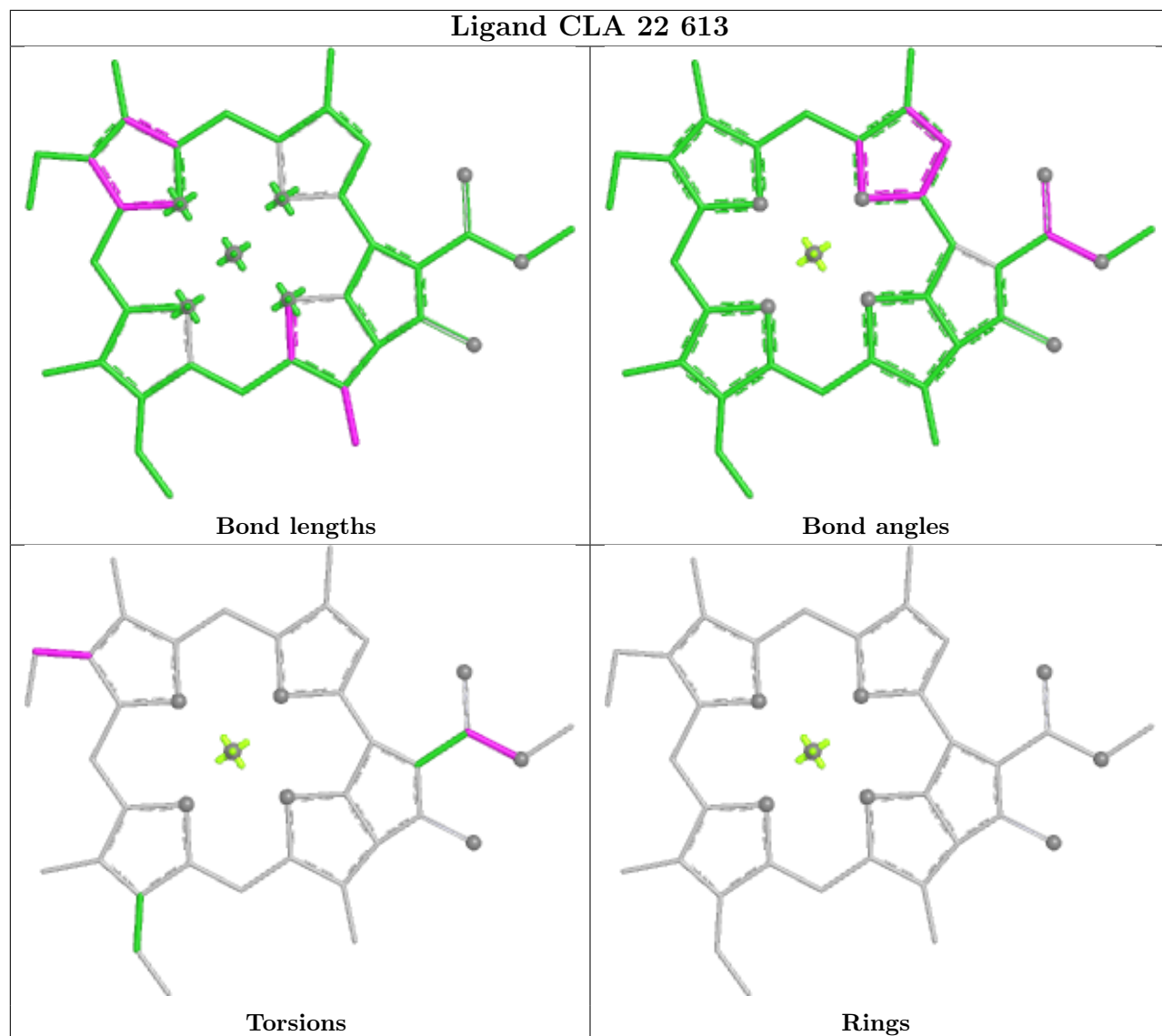
Rings

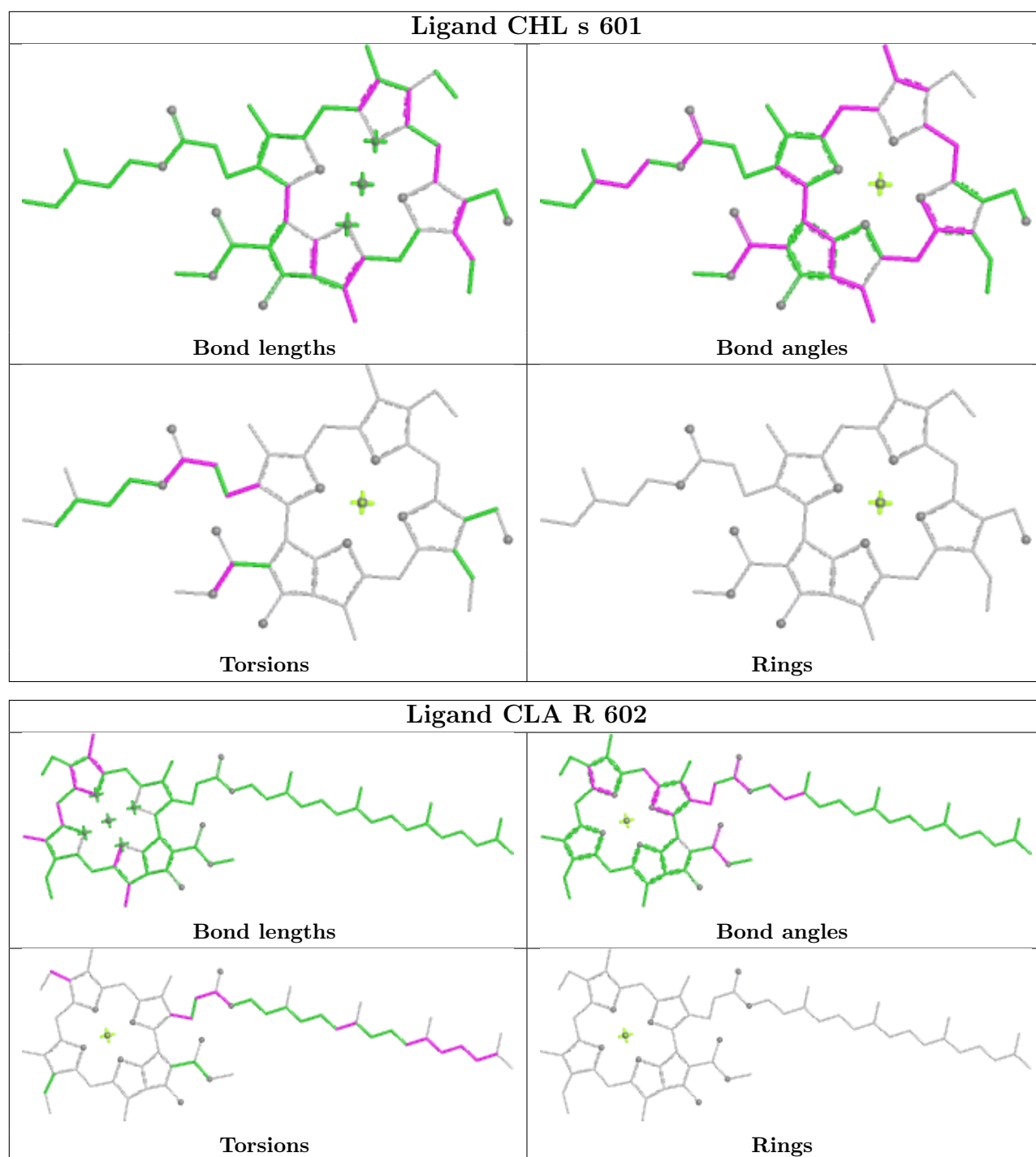
Ligand CHL Yy 605

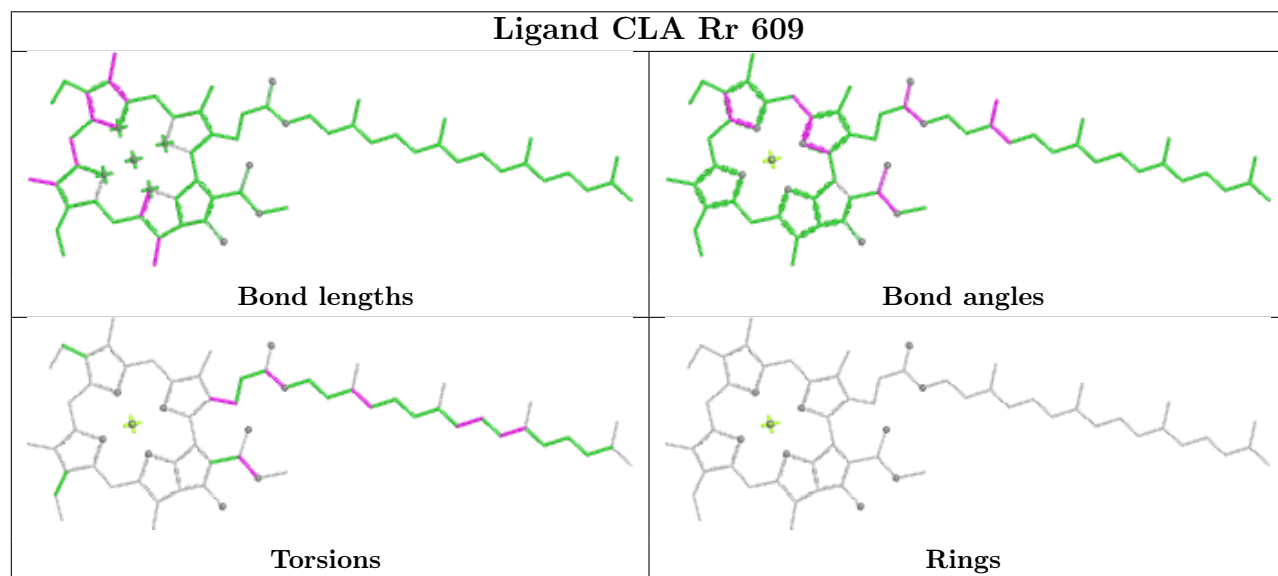
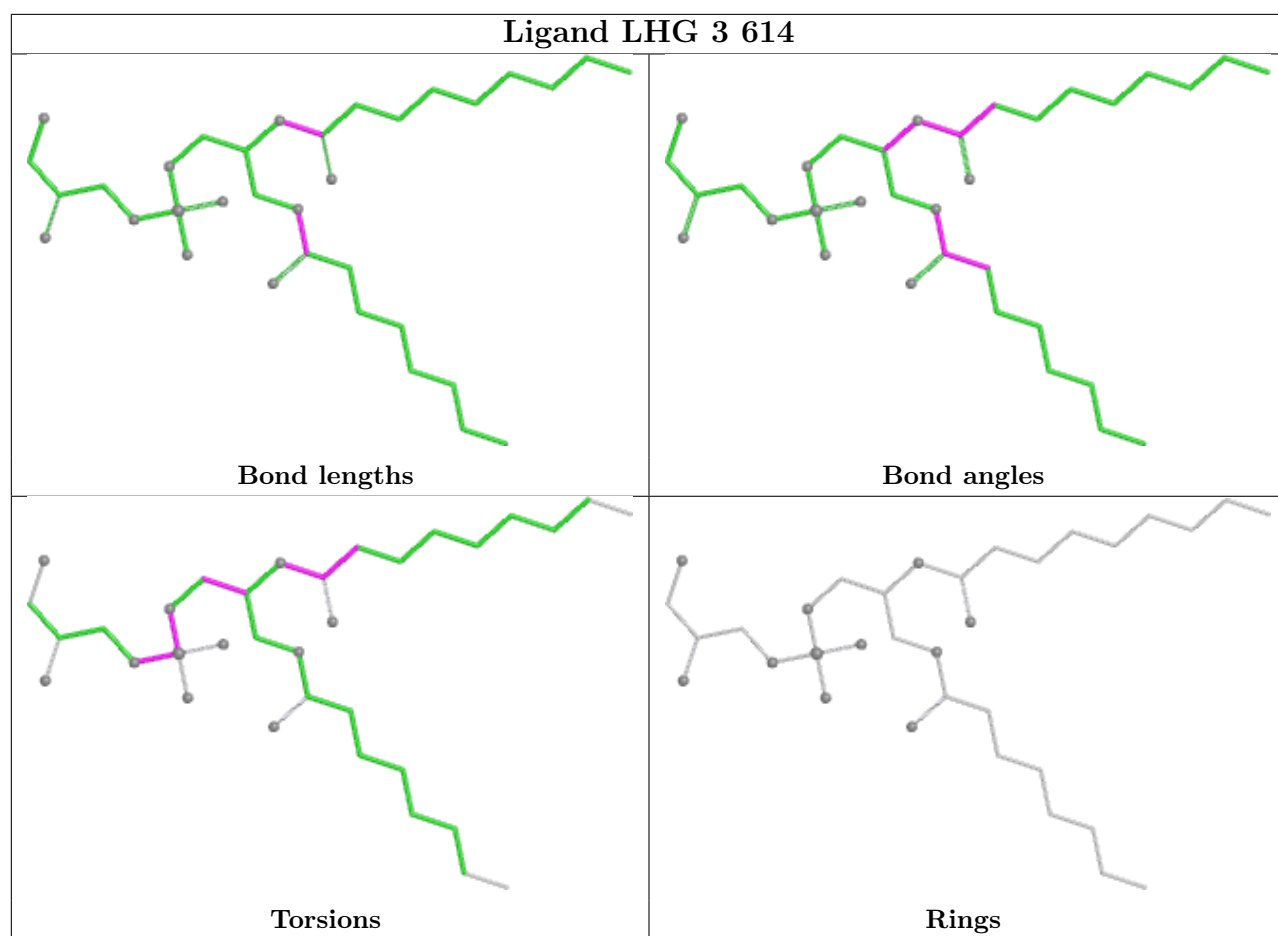


Ligand CLA CC 512

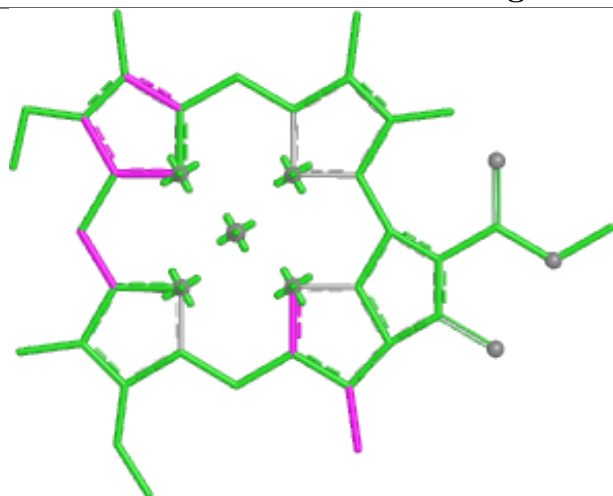




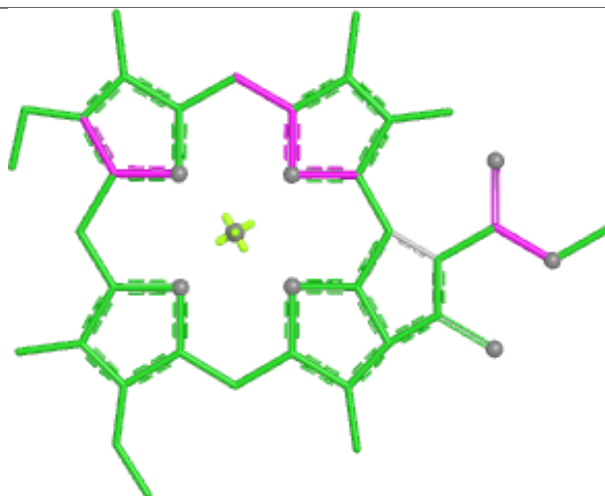




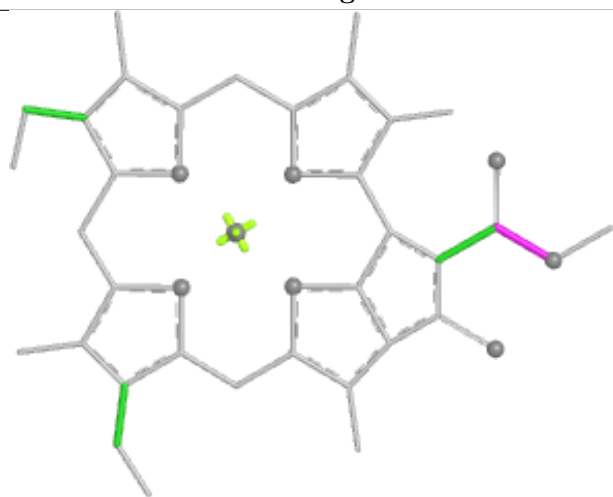
Ligand CLA SS 310



Bond lengths



Bond angles

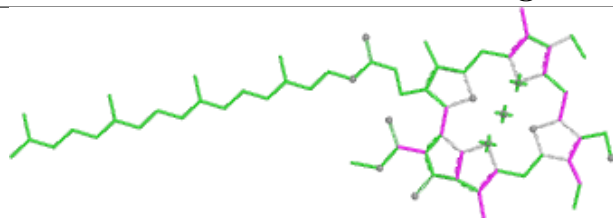


Torsions

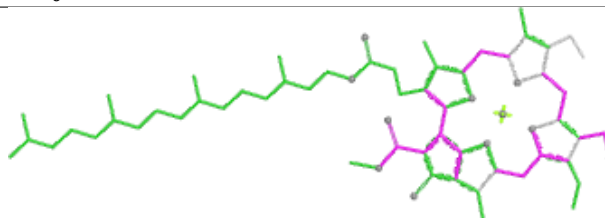


Rings

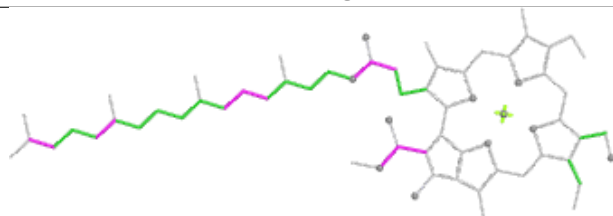
Ligand CHL y 311



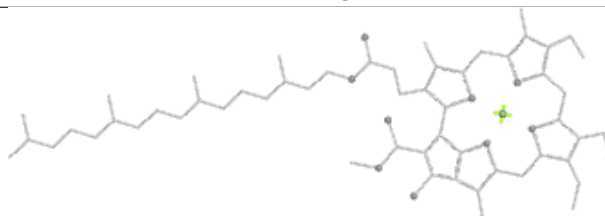
Bond lengths



Bond angles

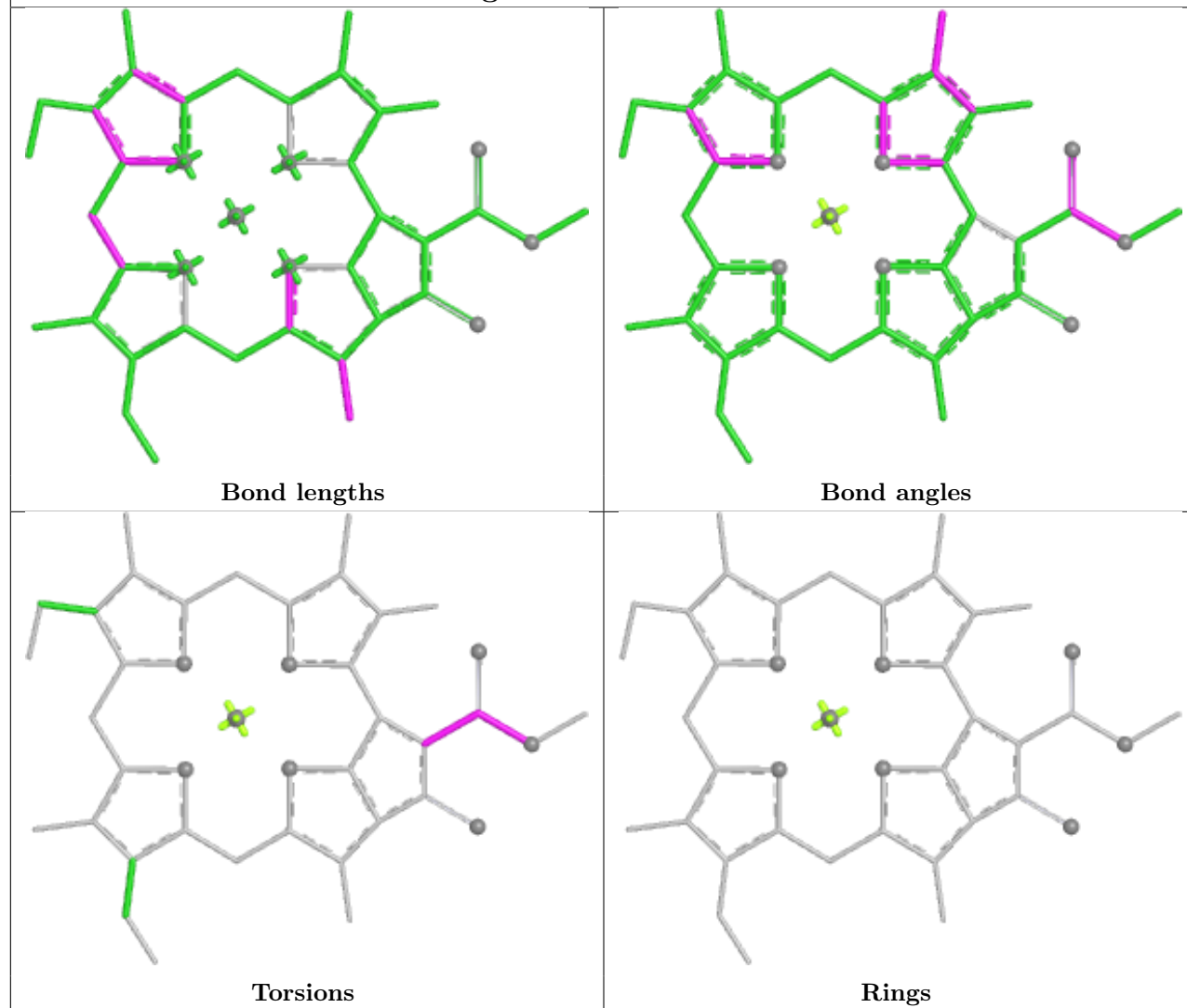


Torsions

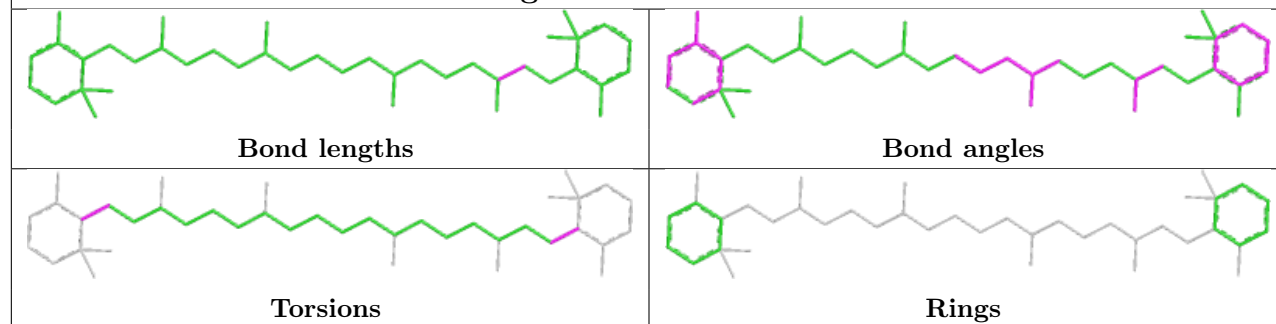


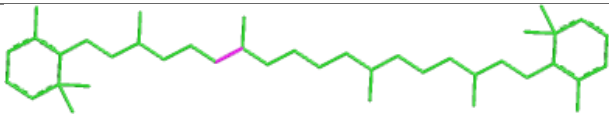
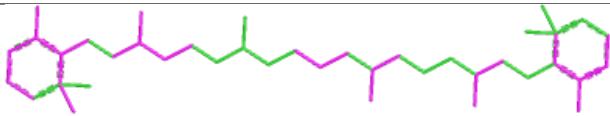
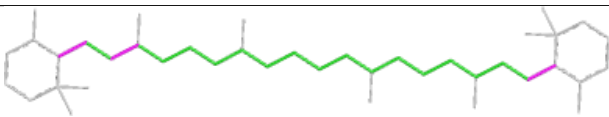
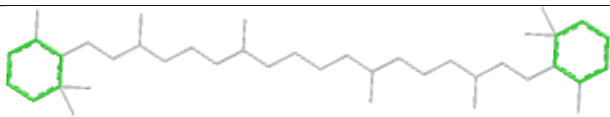
Rings

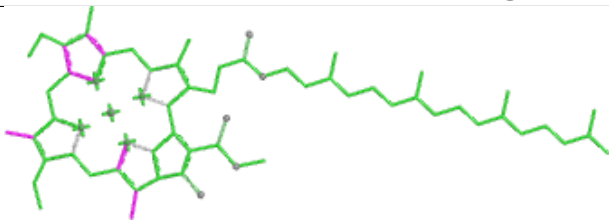
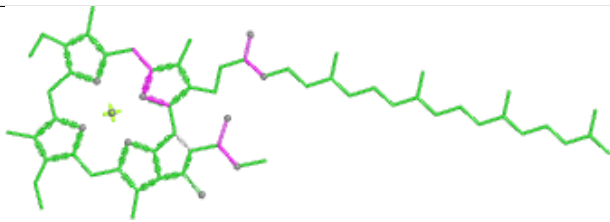
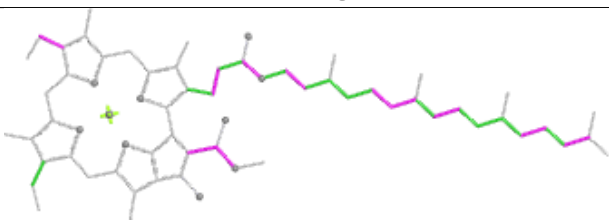
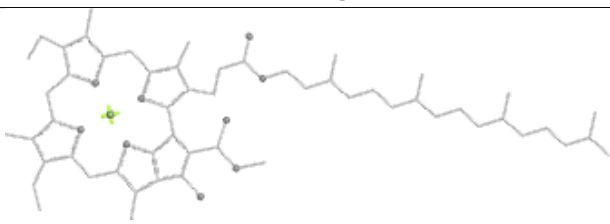
Ligand CLA XX 201

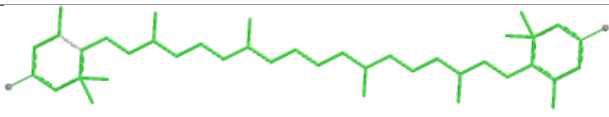
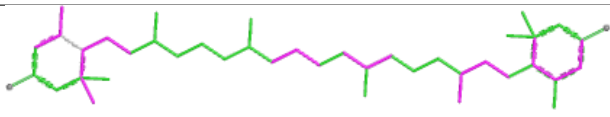
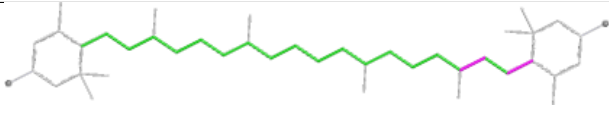
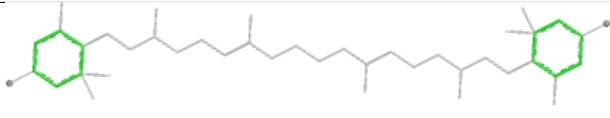


Ligand BCR Bb 618

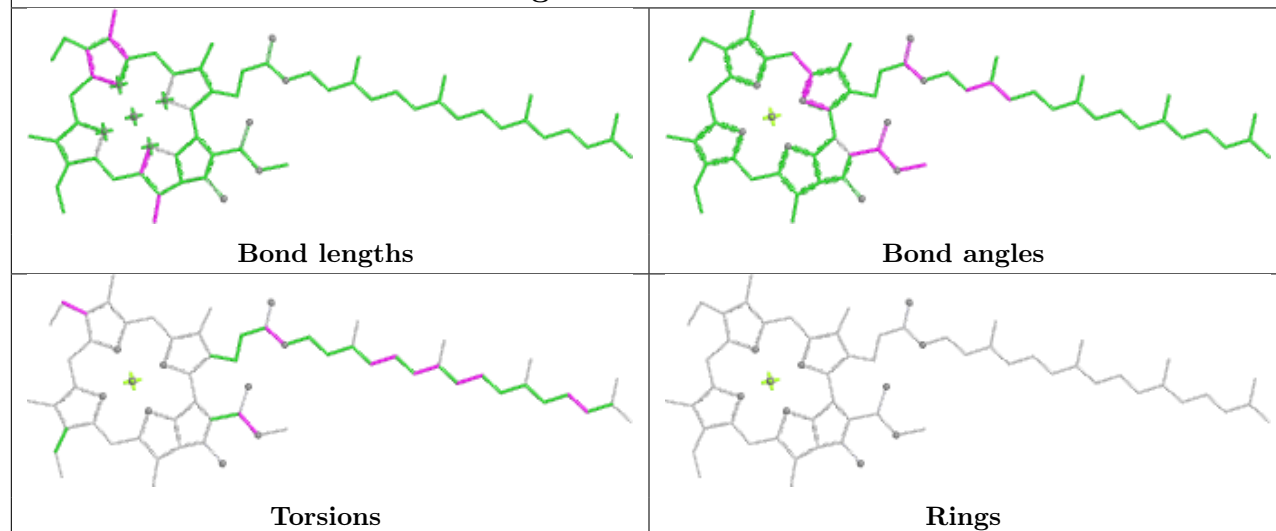


Ligand BCR CC 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

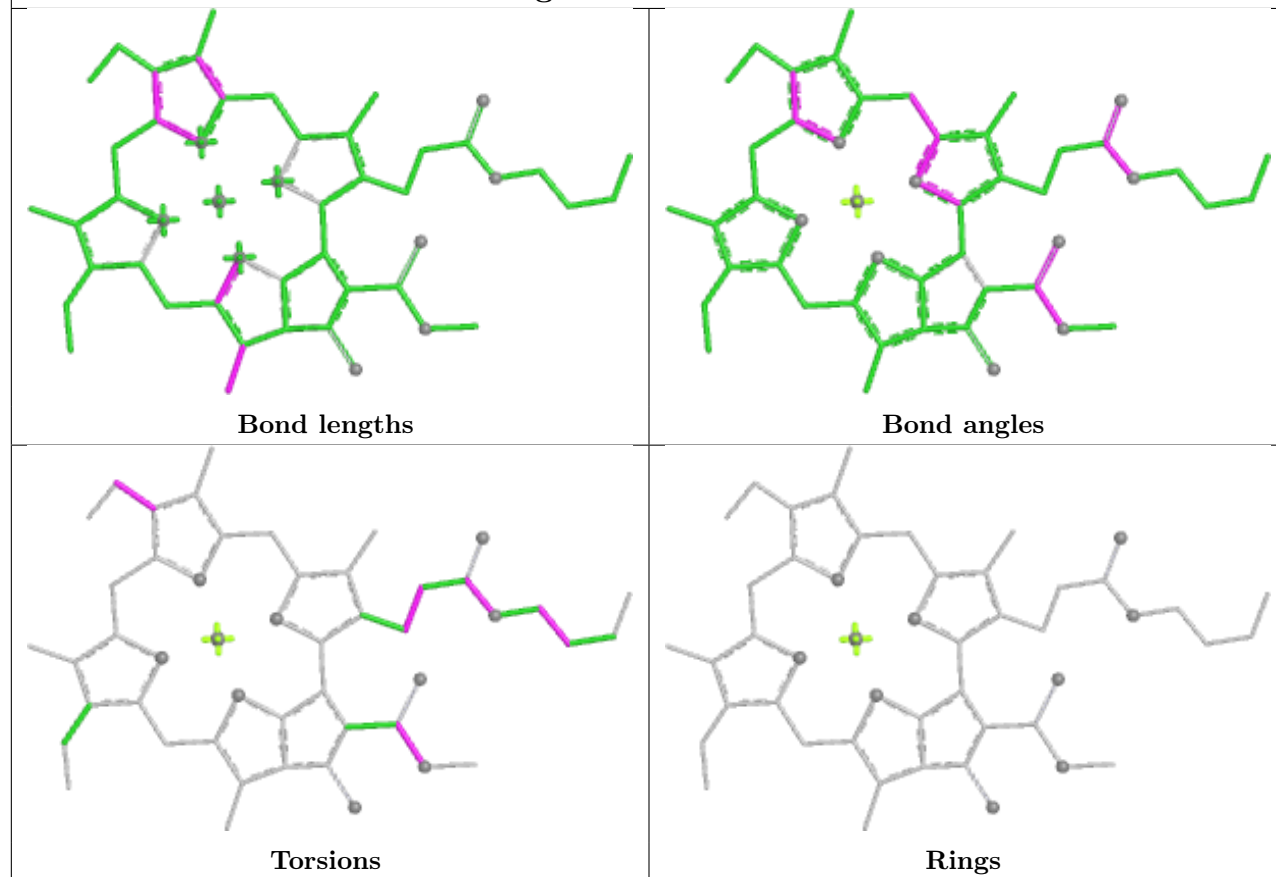
Ligand CLA Cc 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT n 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

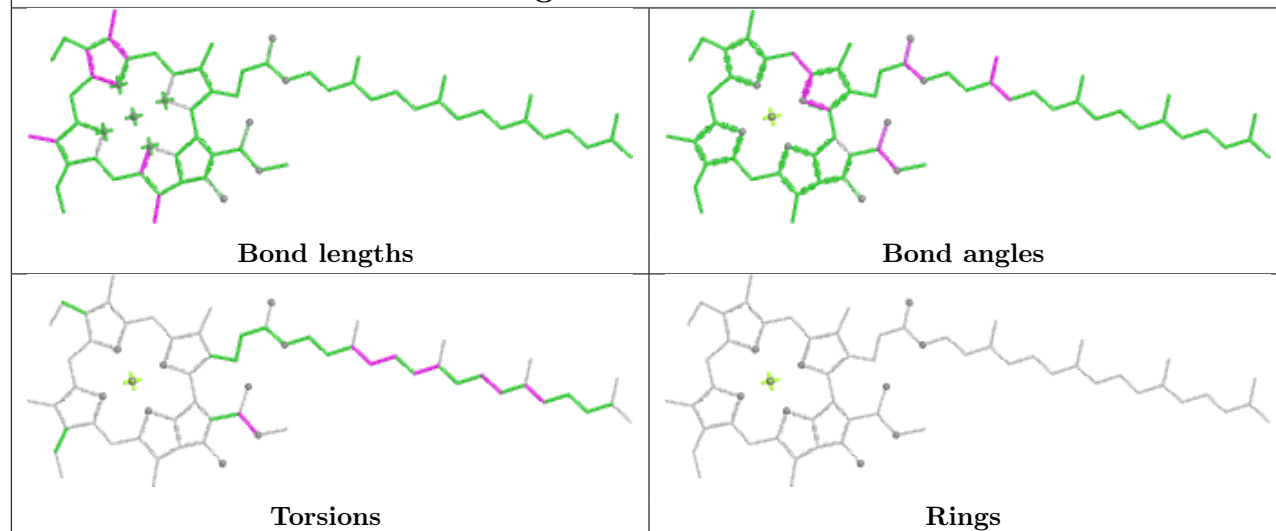
Ligand CLA Y 612



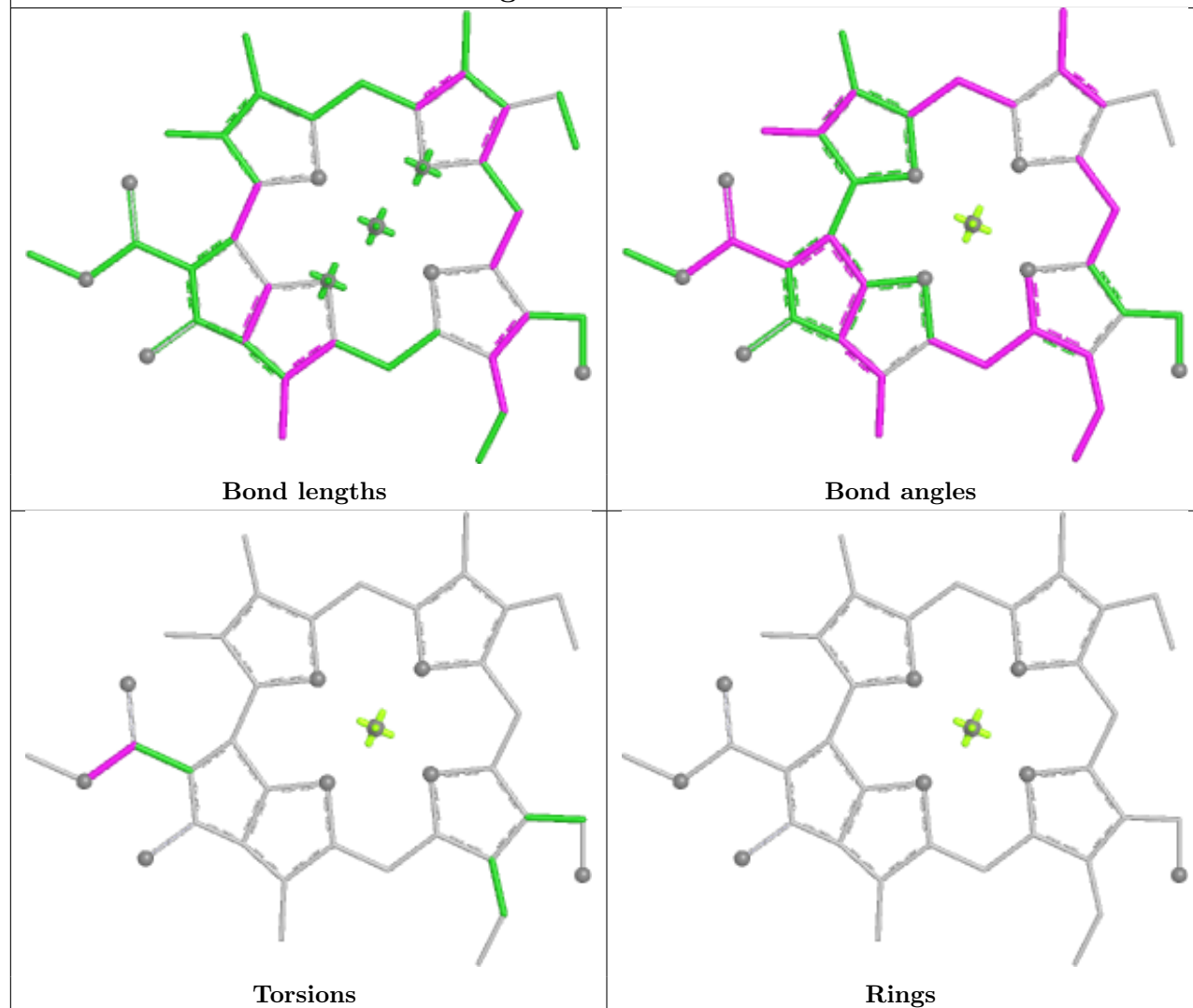
Ligand CLA S 612

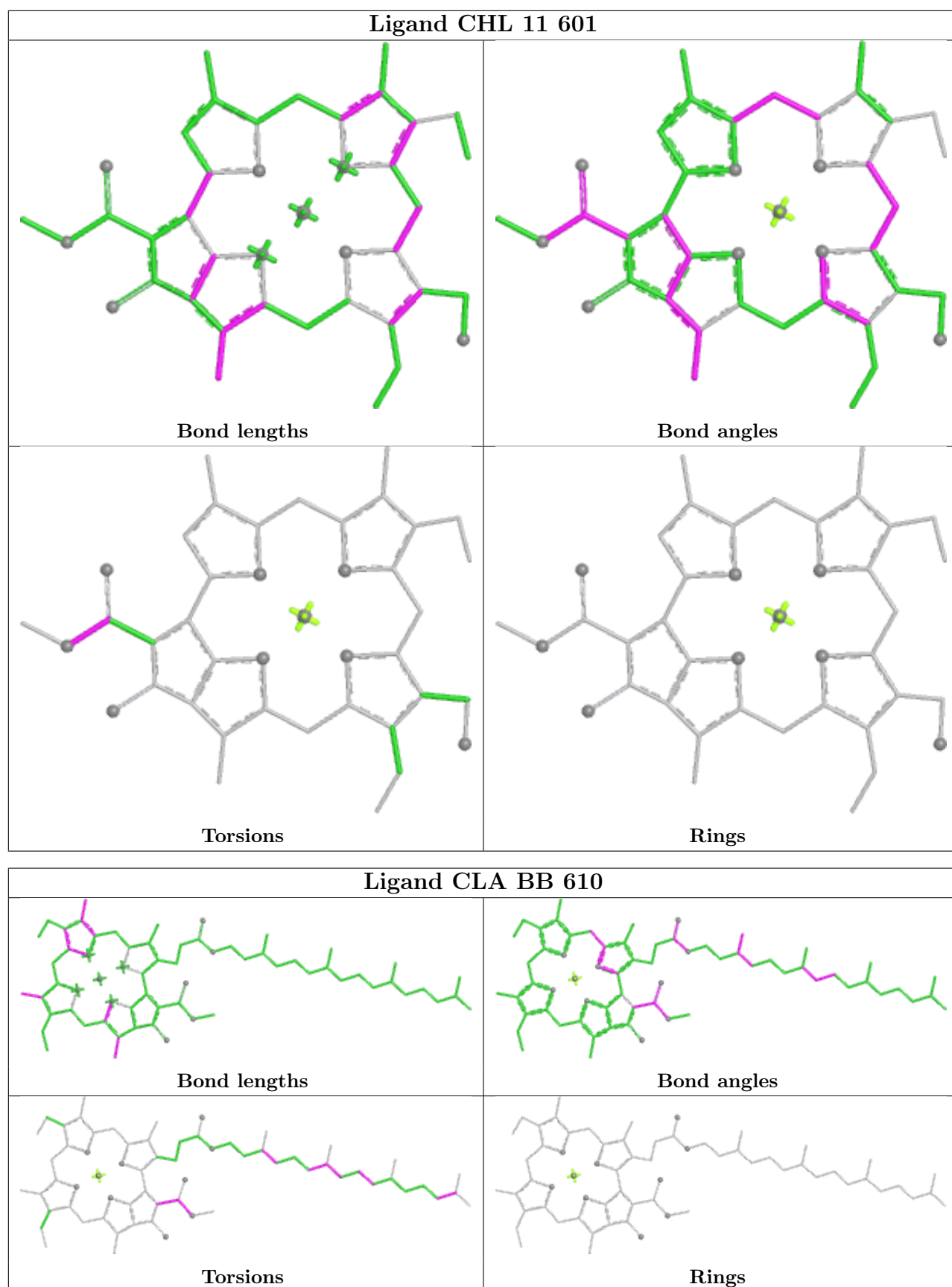


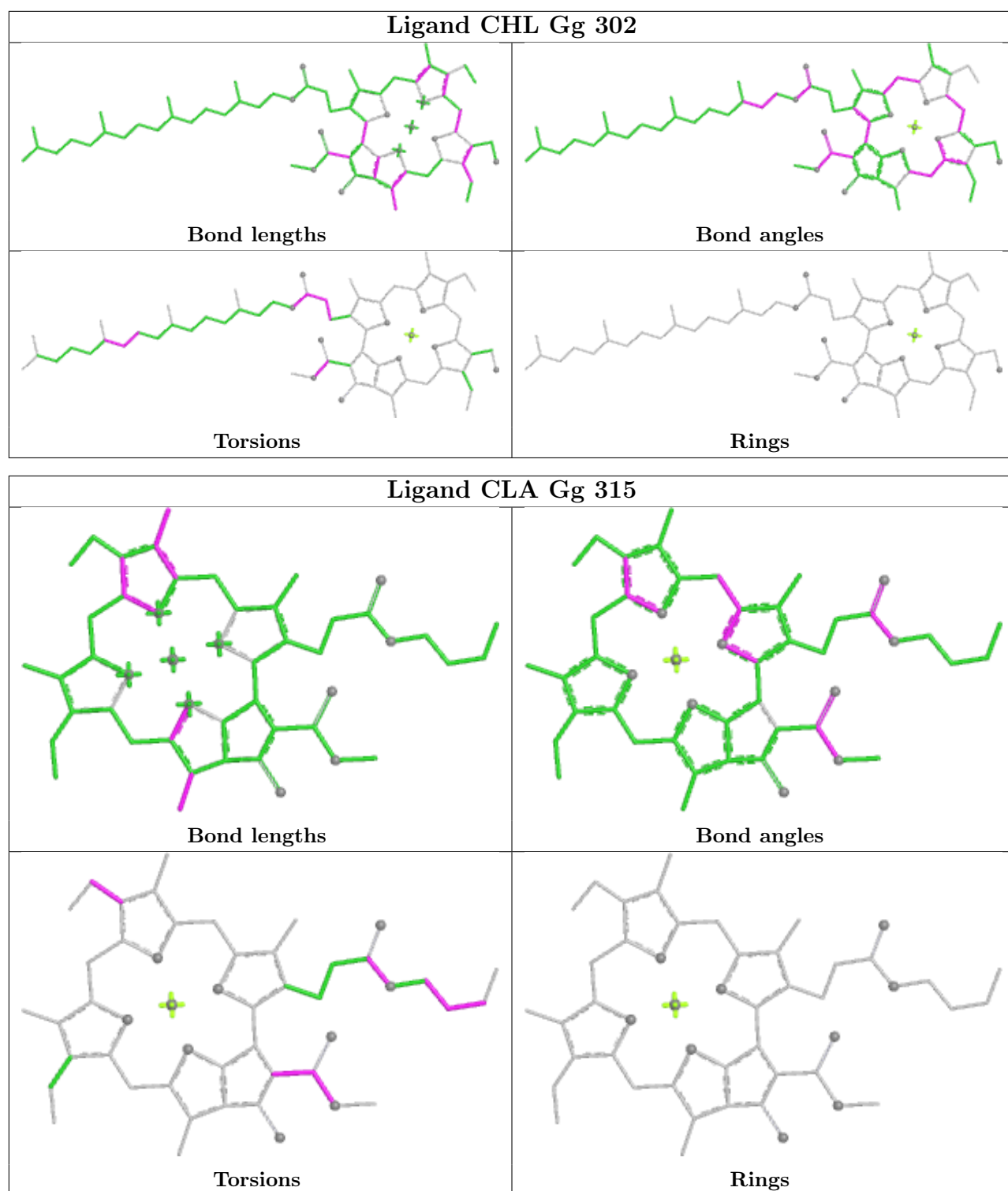
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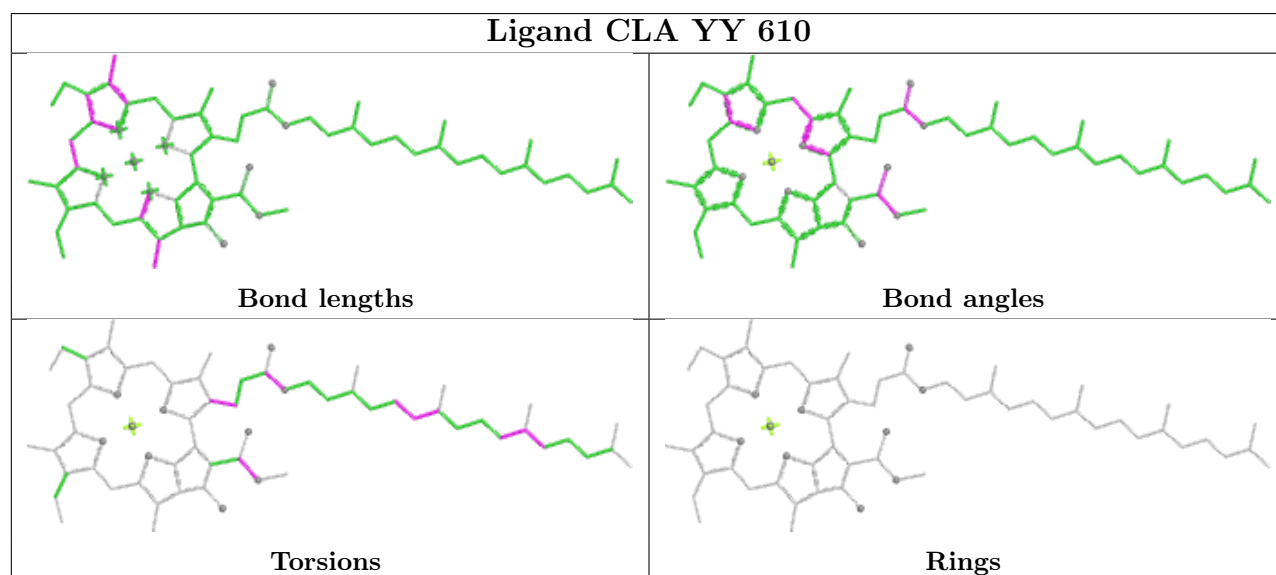
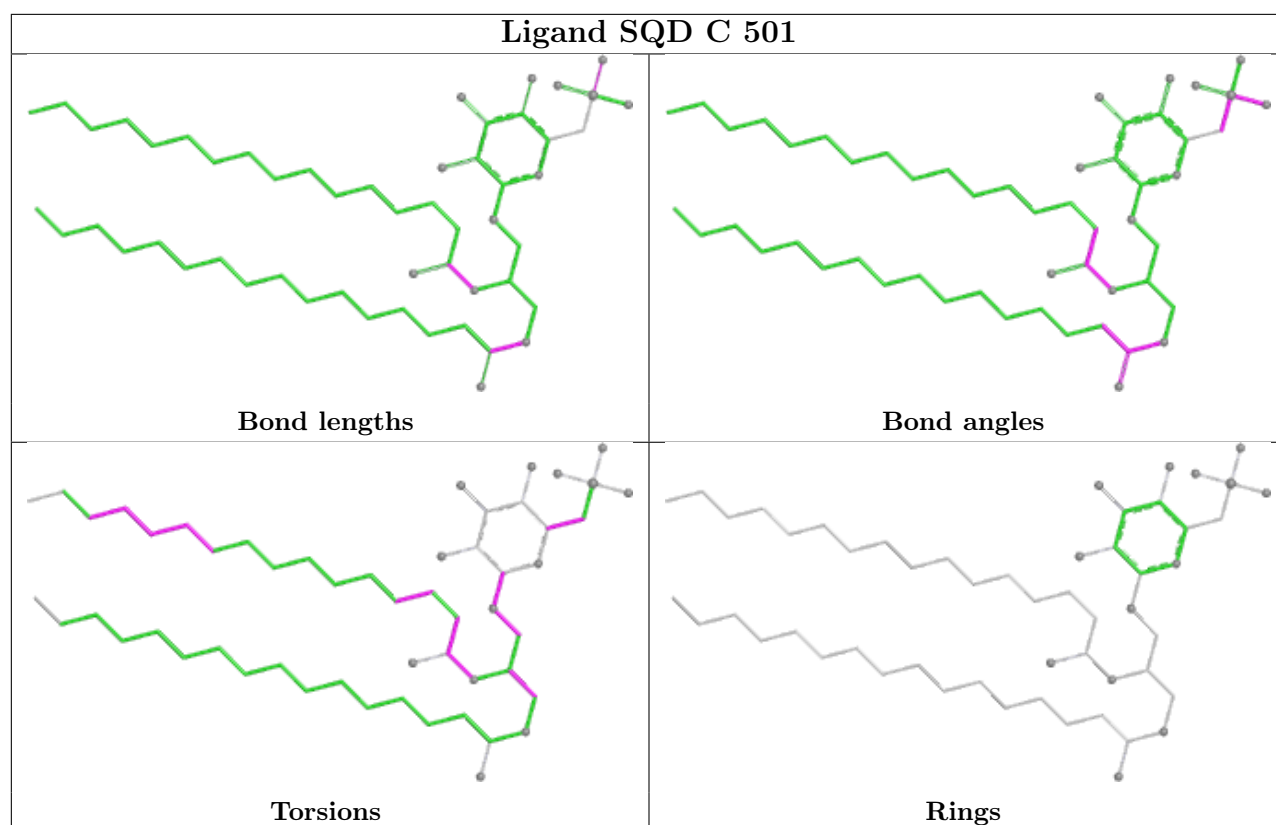


Ligand CHL S 605

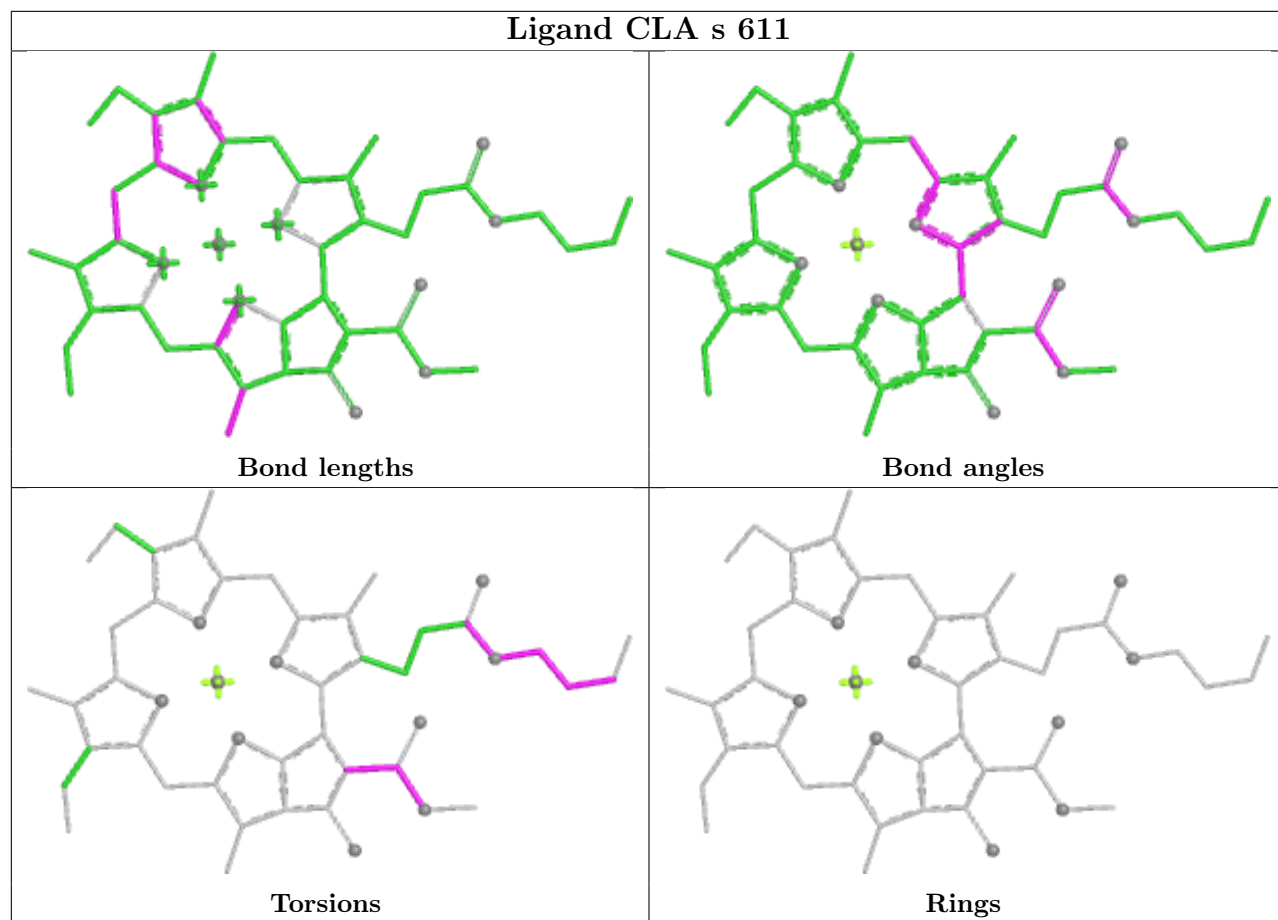


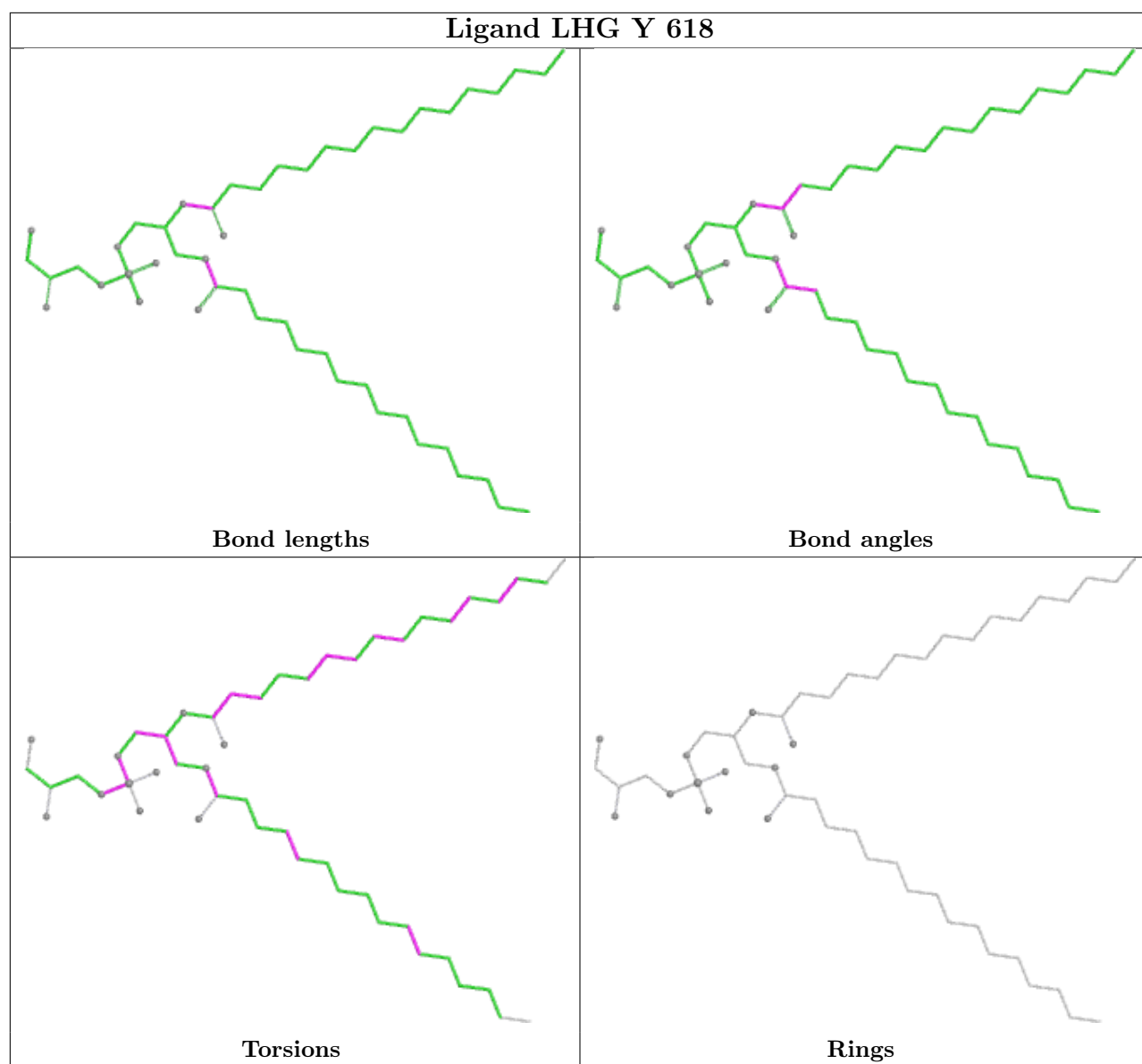




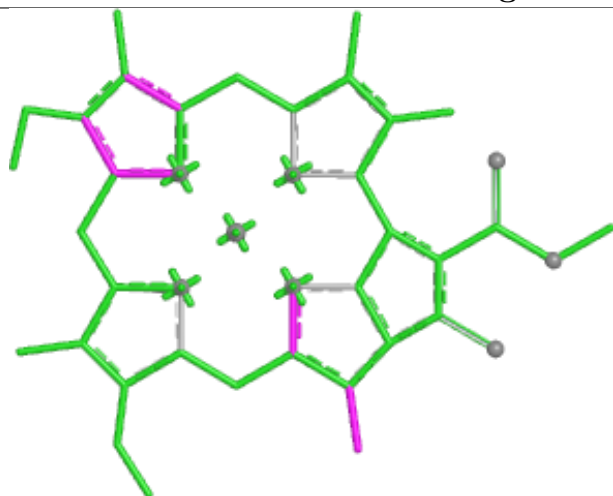


Ligand CLA s 611

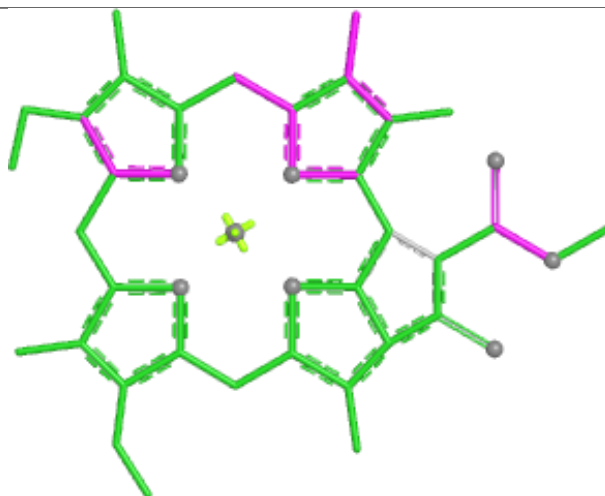




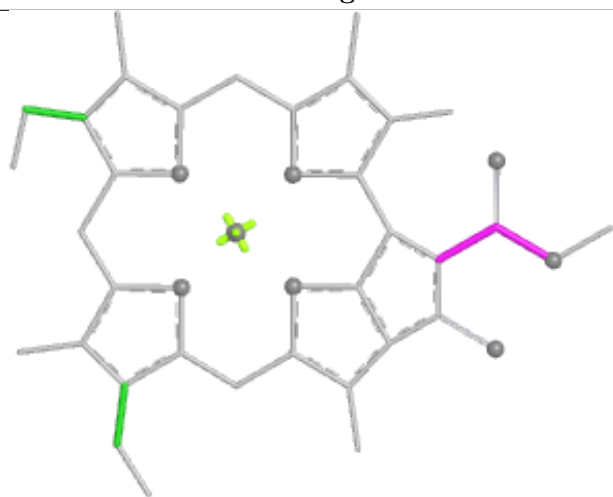
Ligand CLA NN 604



Bond lengths



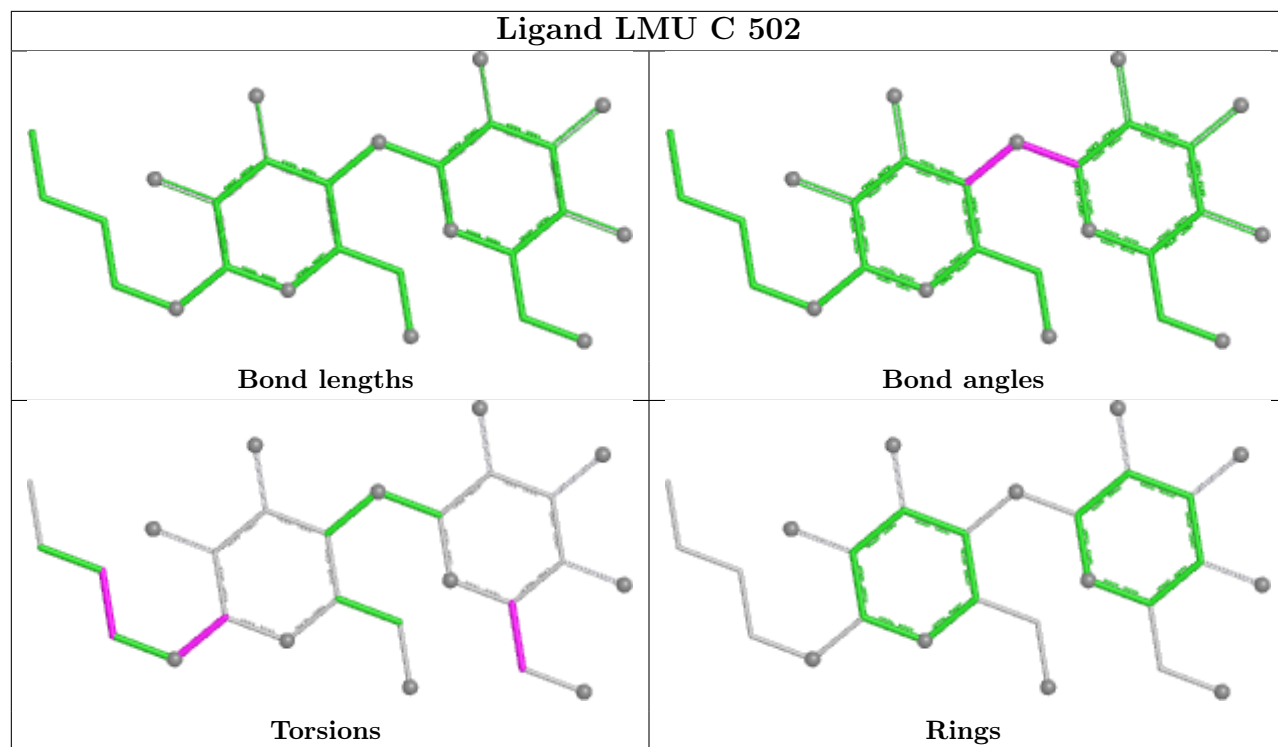
Bond angles

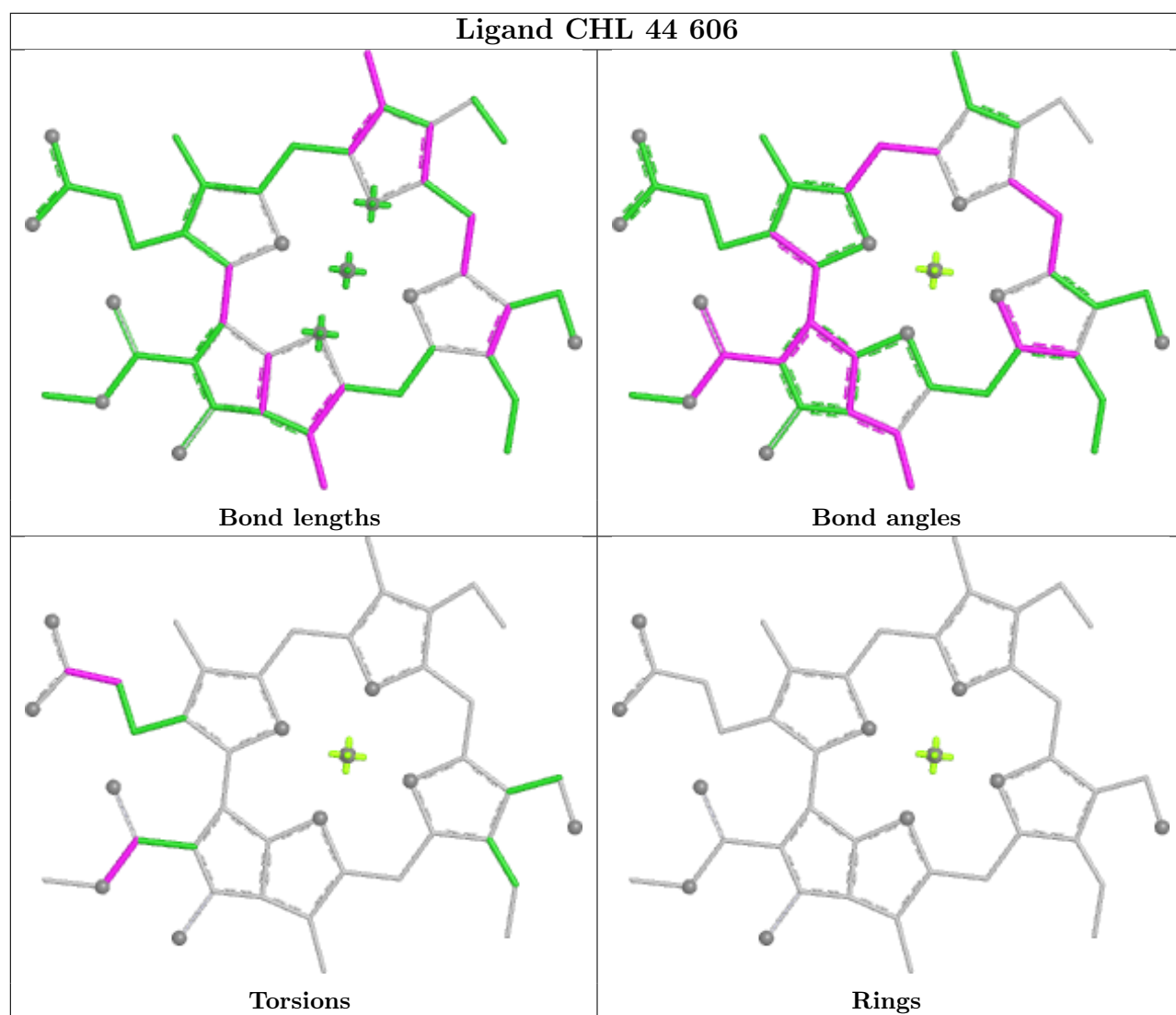


Torsions

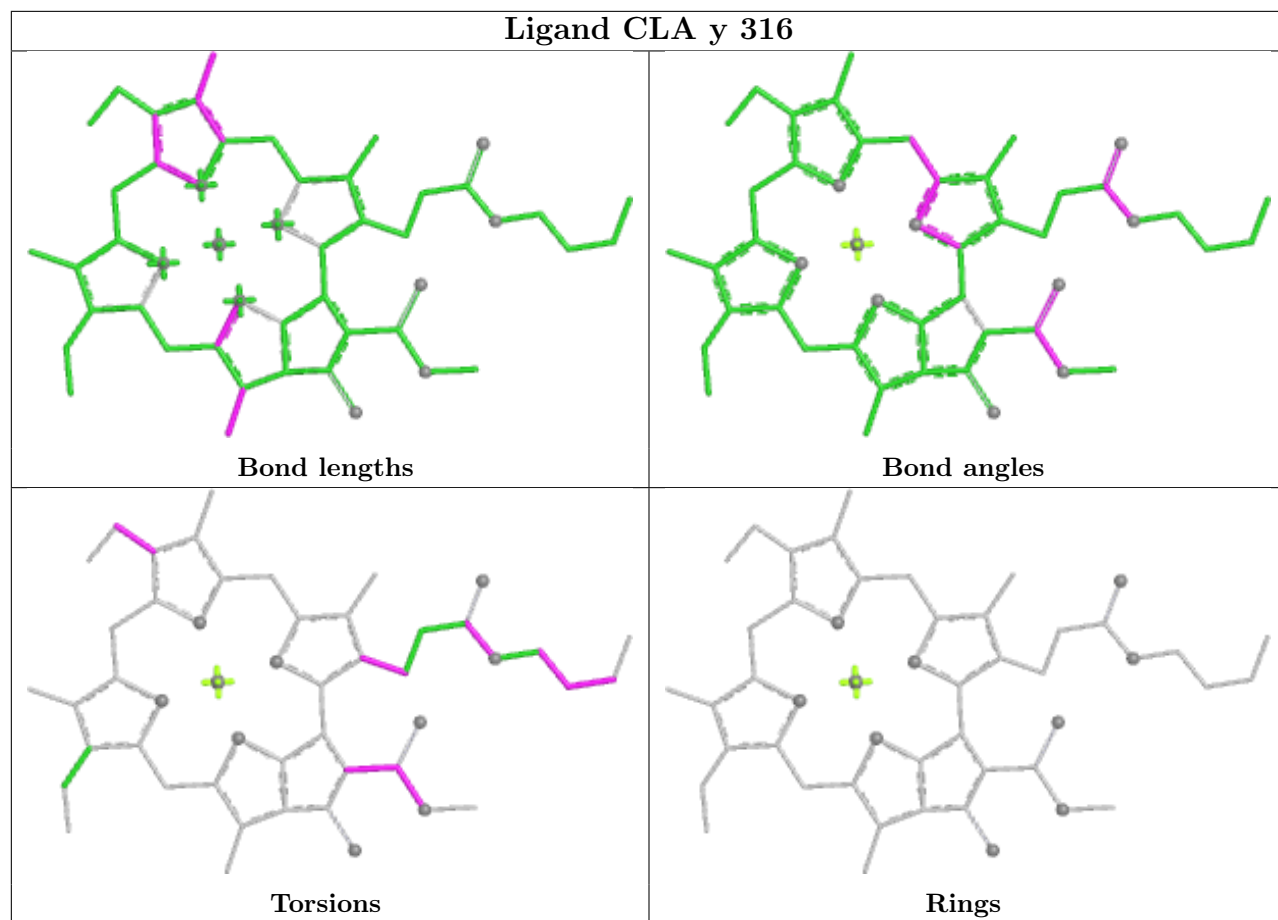


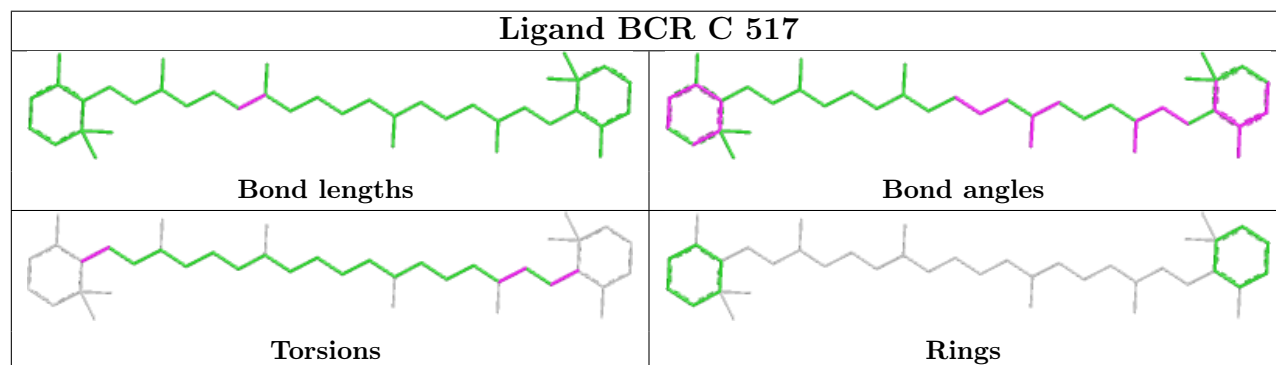
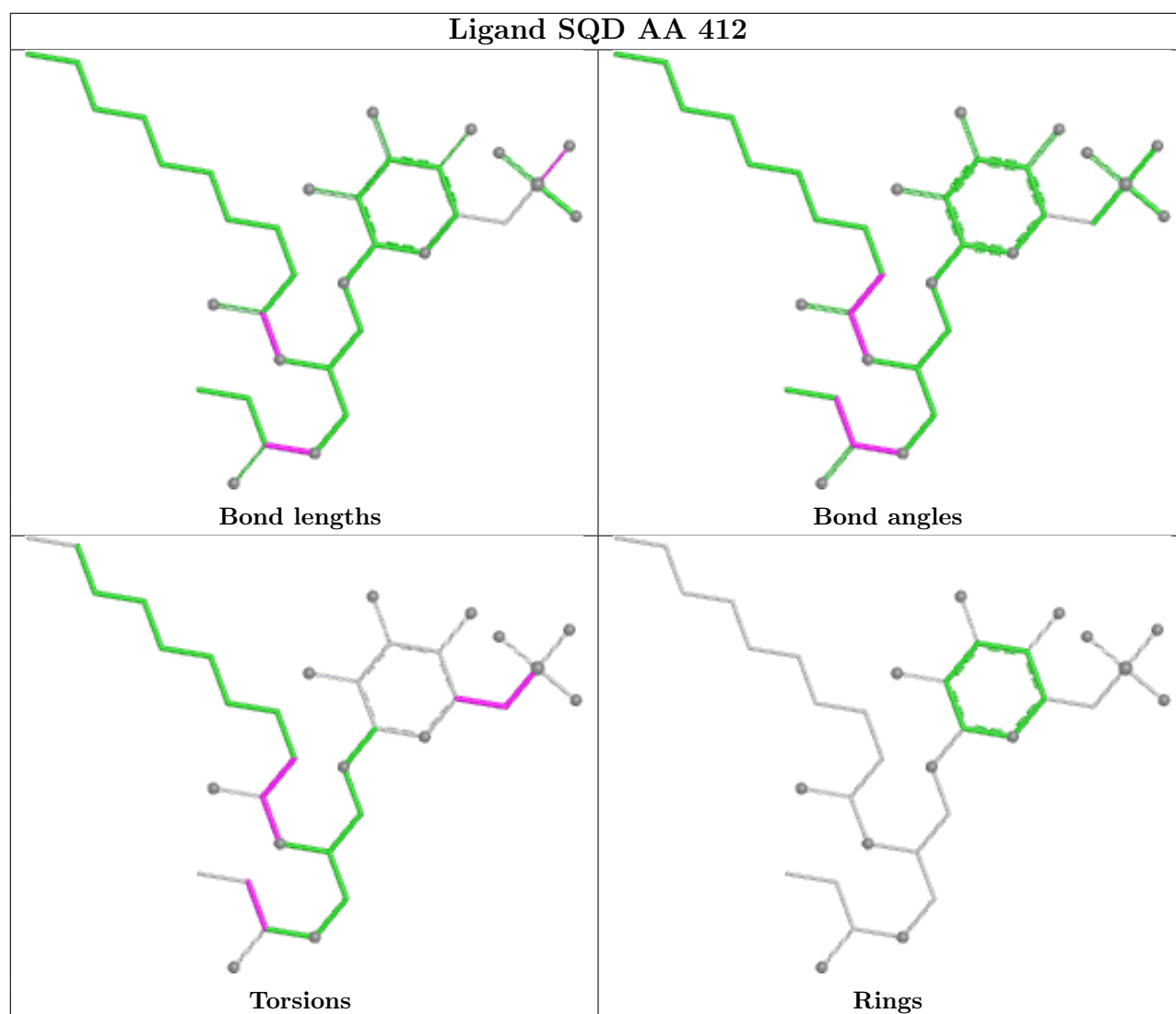
Rings



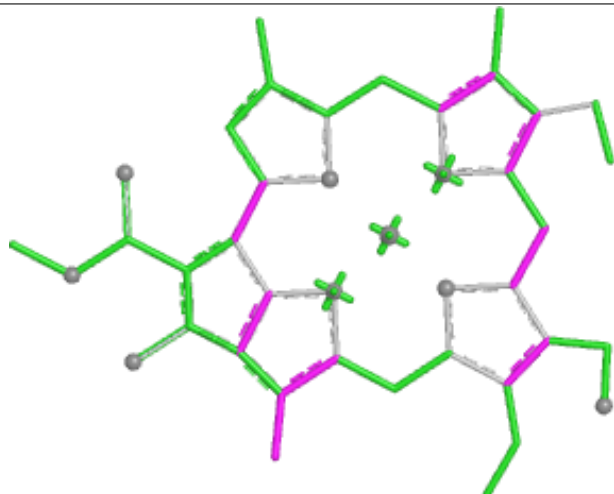


Ligand CLA y 316

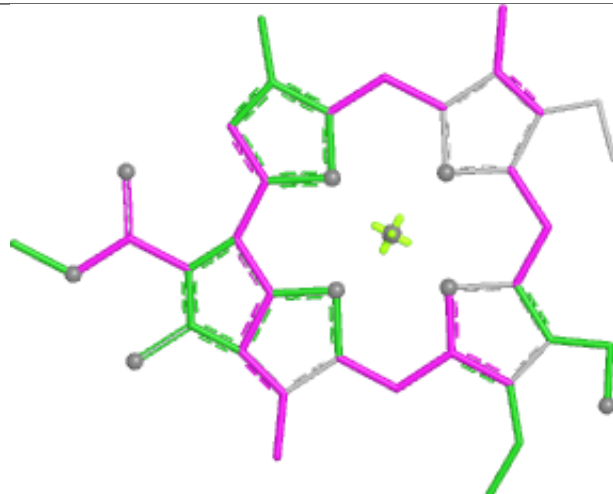




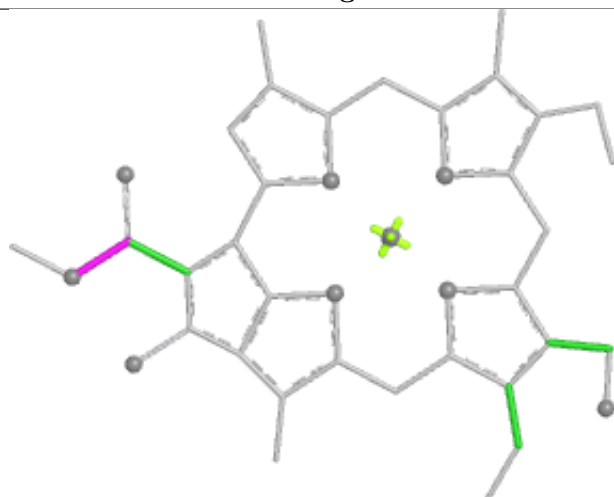
Ligand CHL 2 605



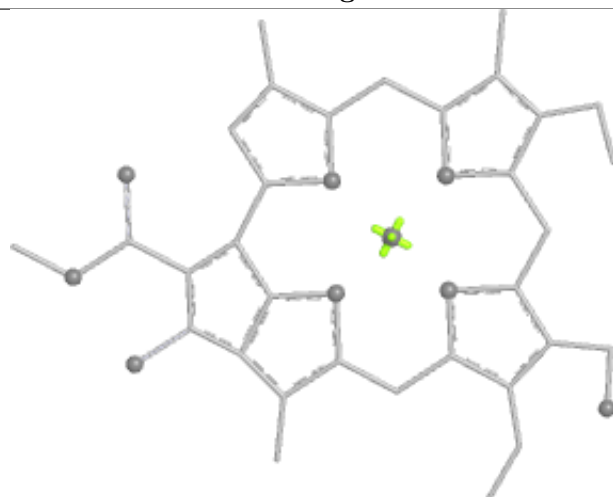
Bond lengths



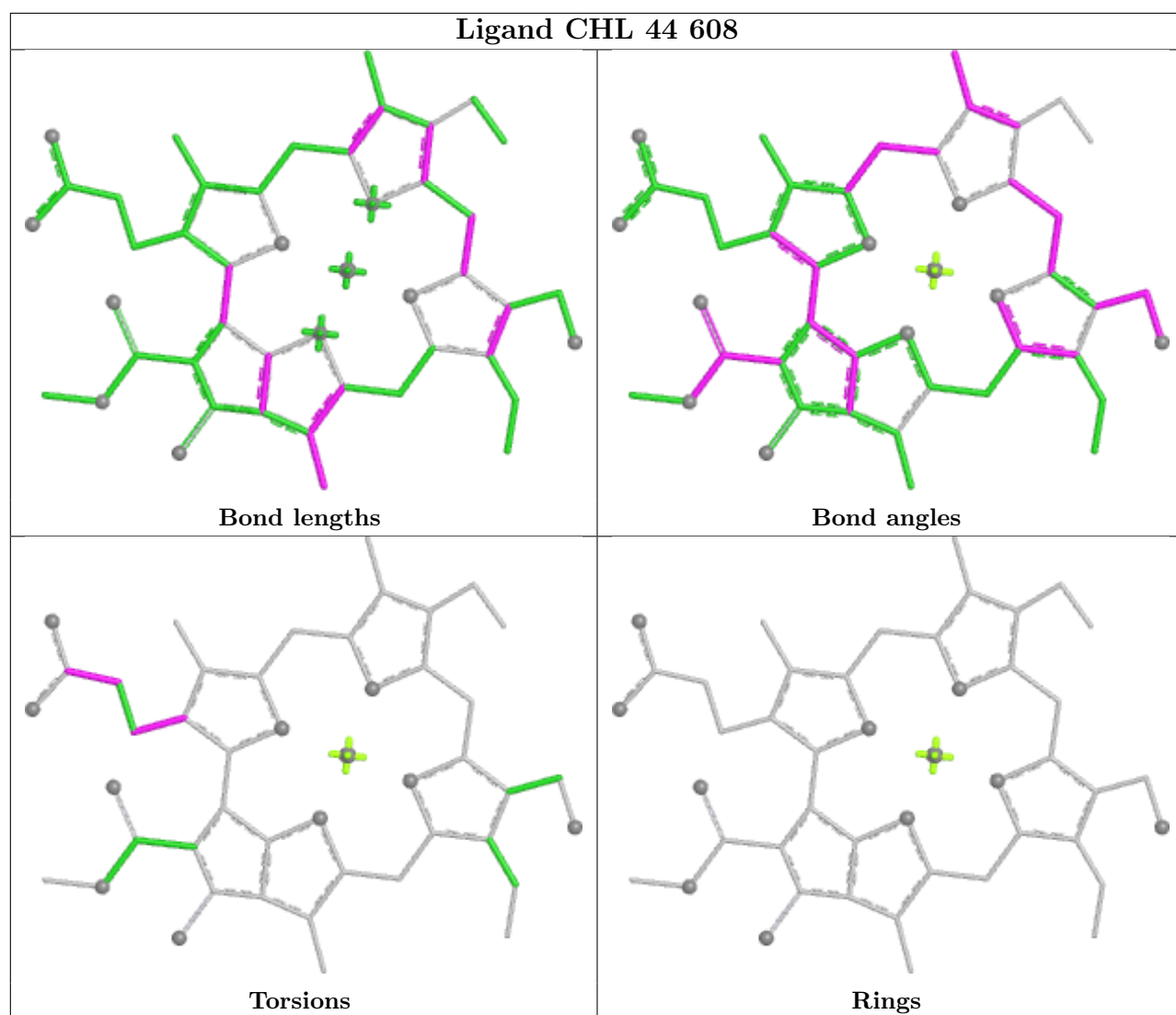
Bond angles

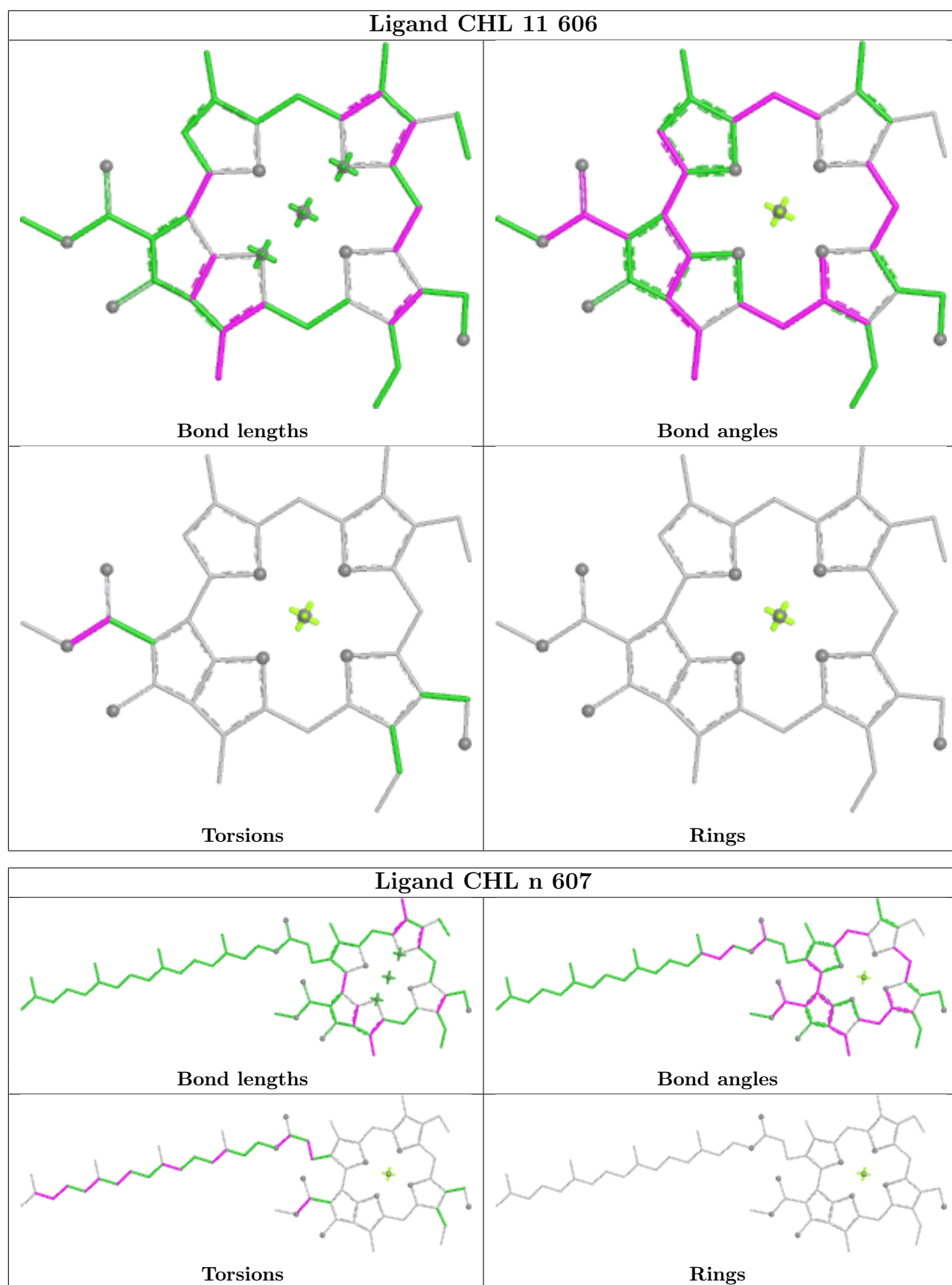


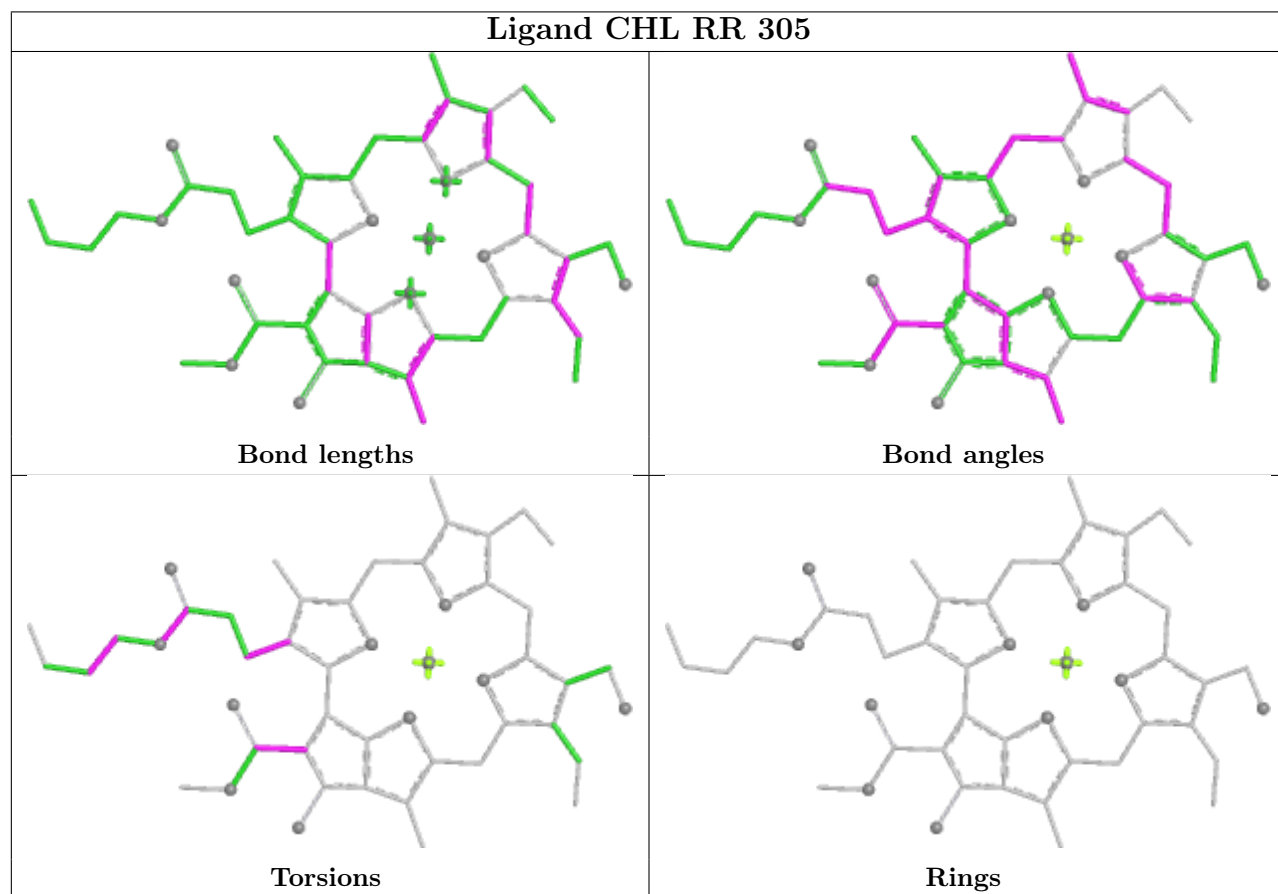
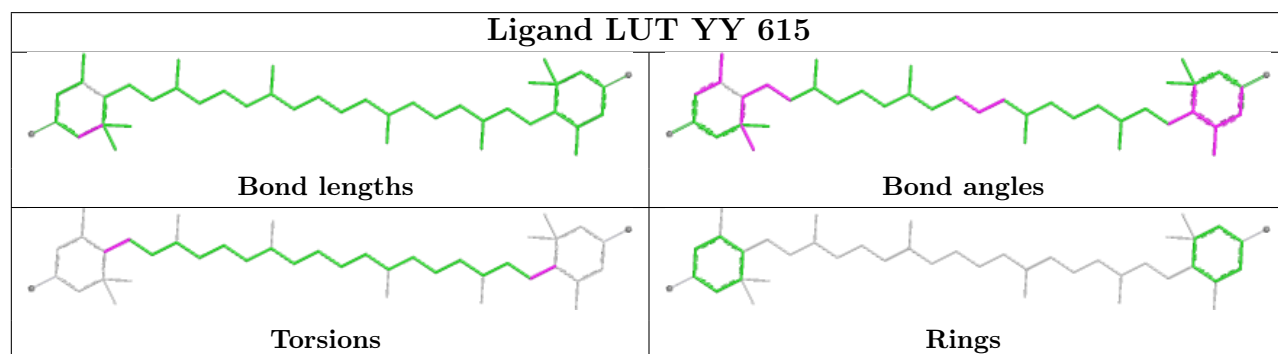
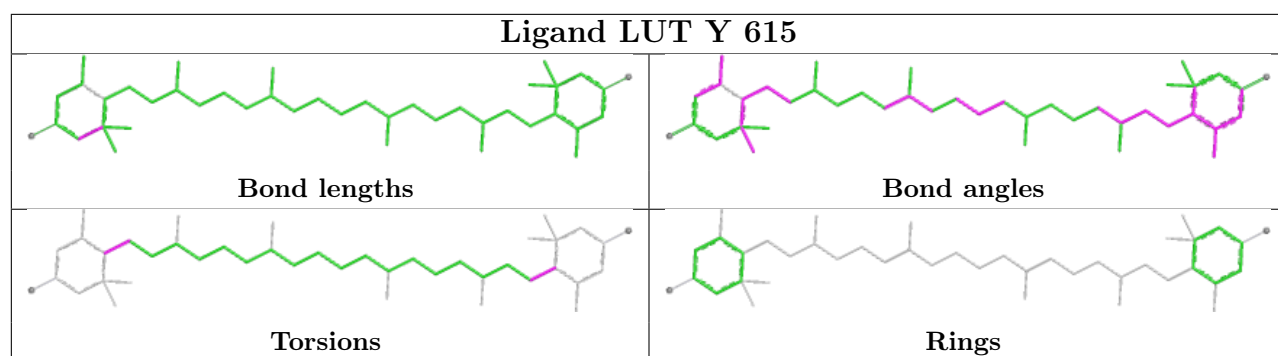
Torsions

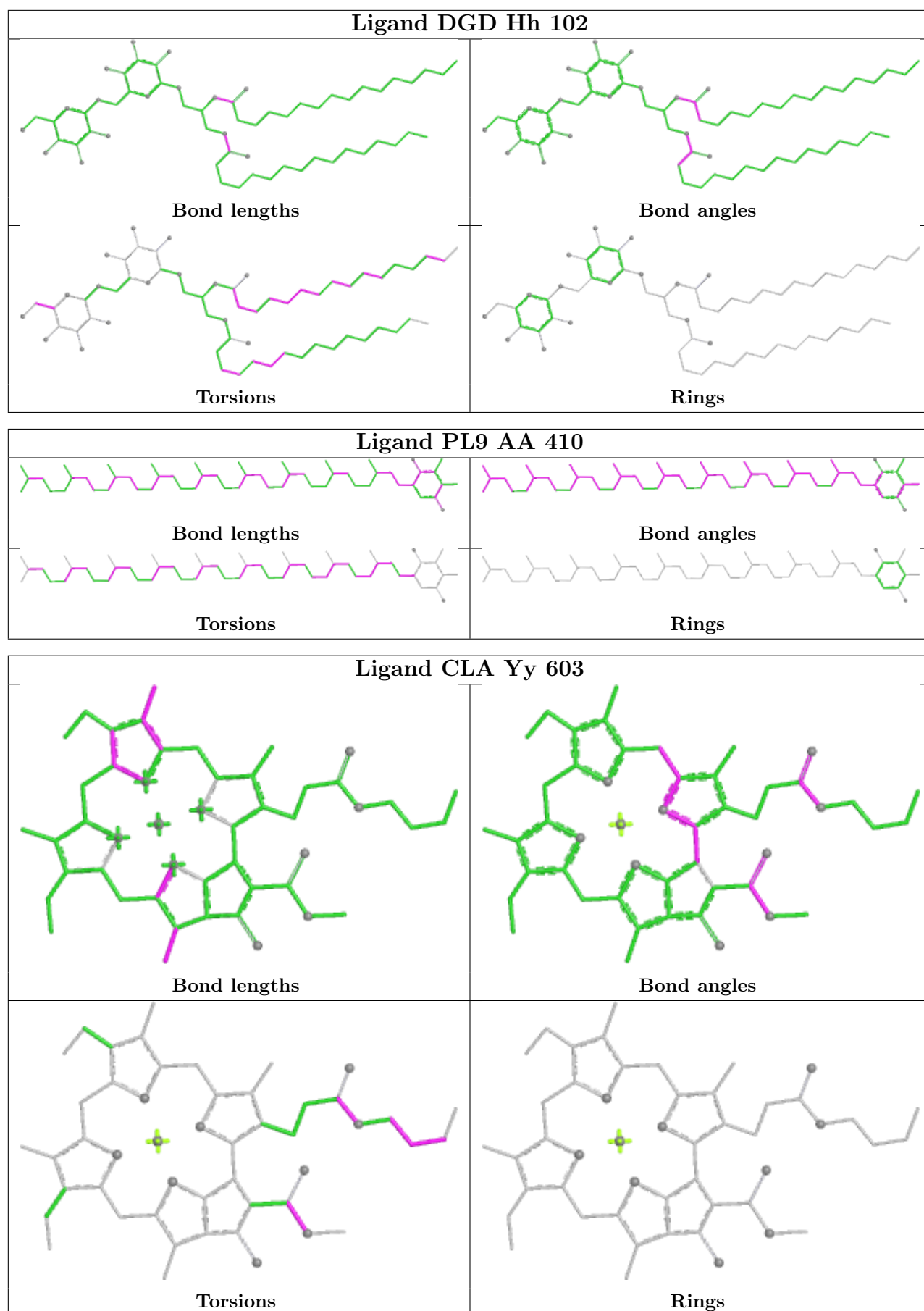


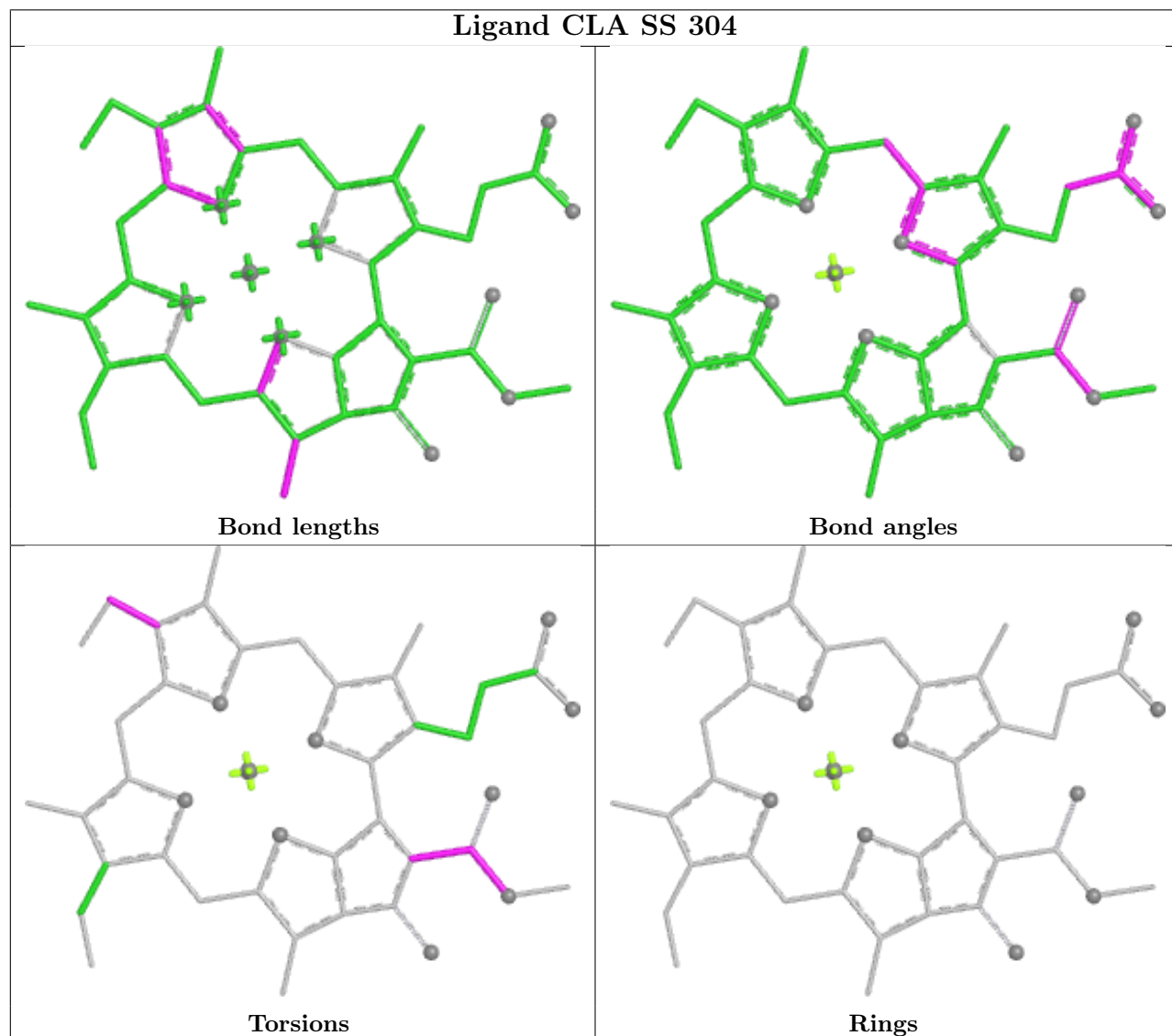
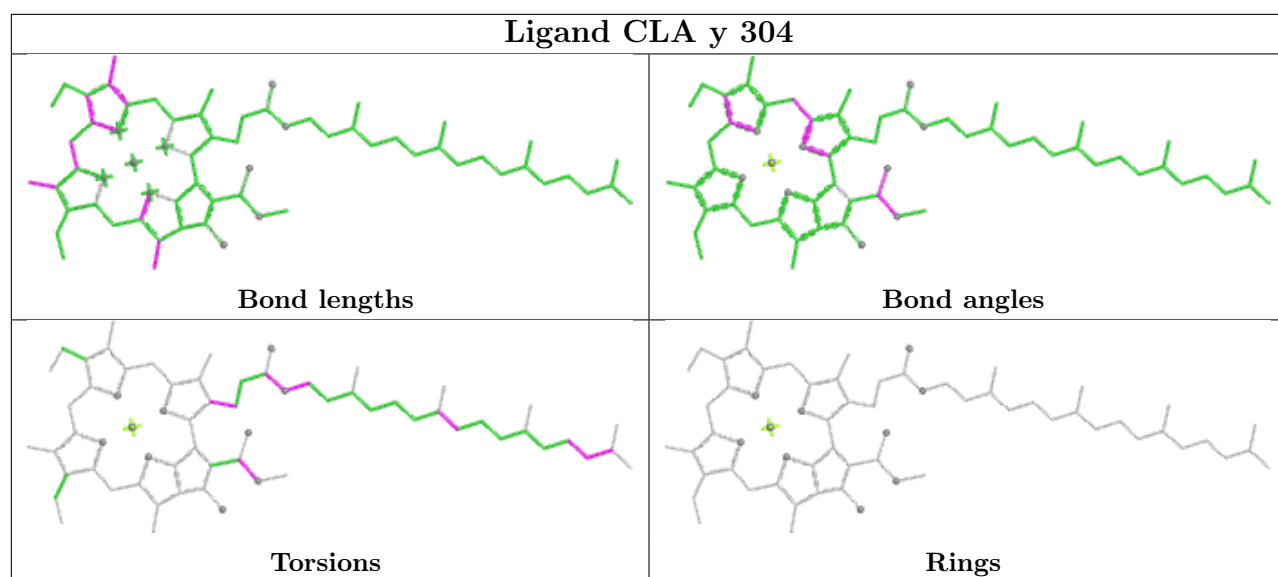
Rings

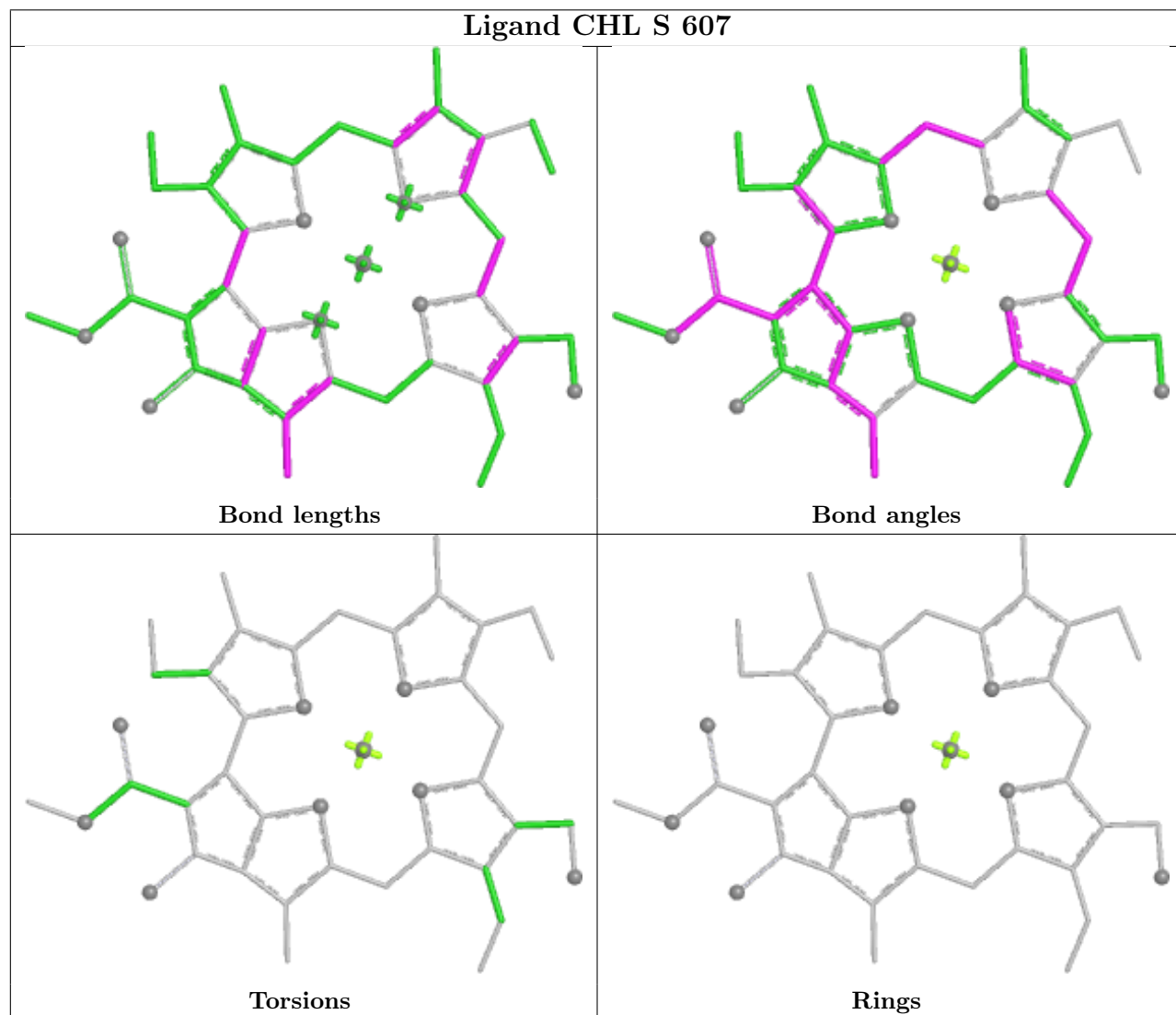
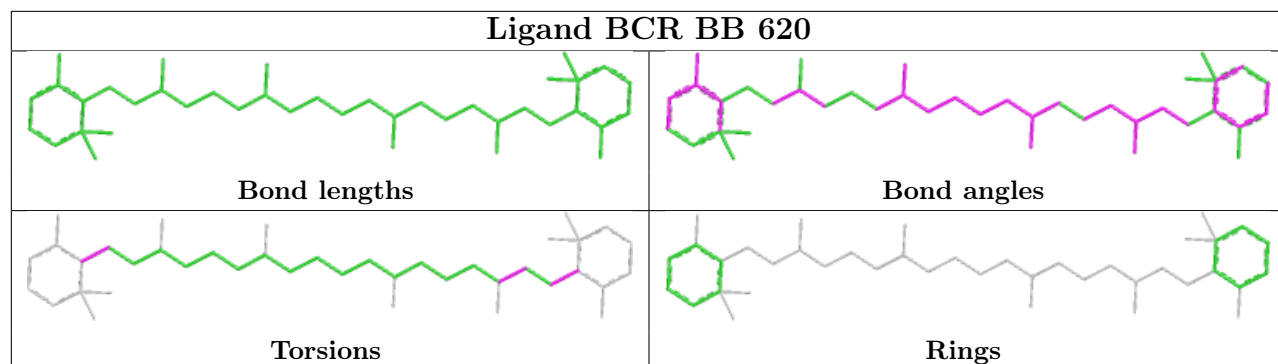


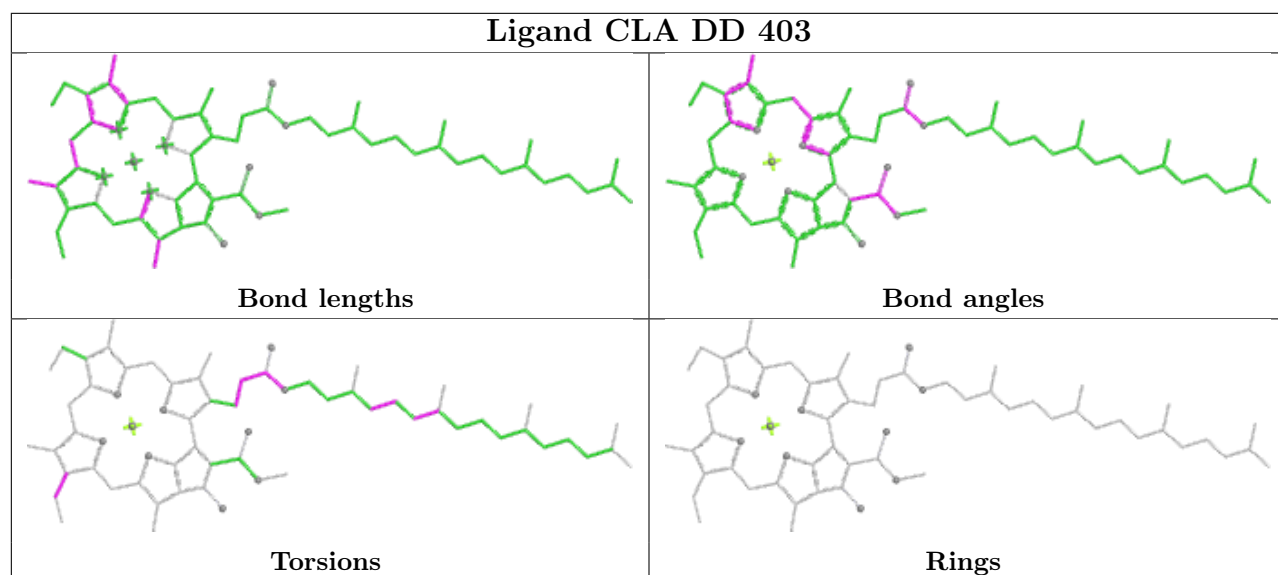
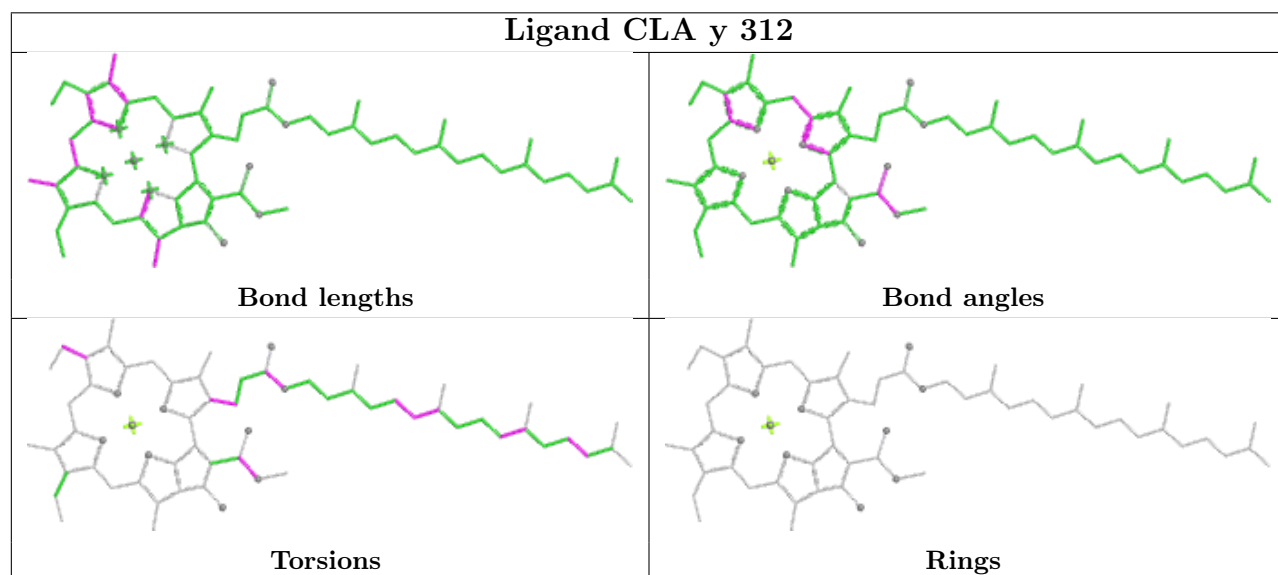
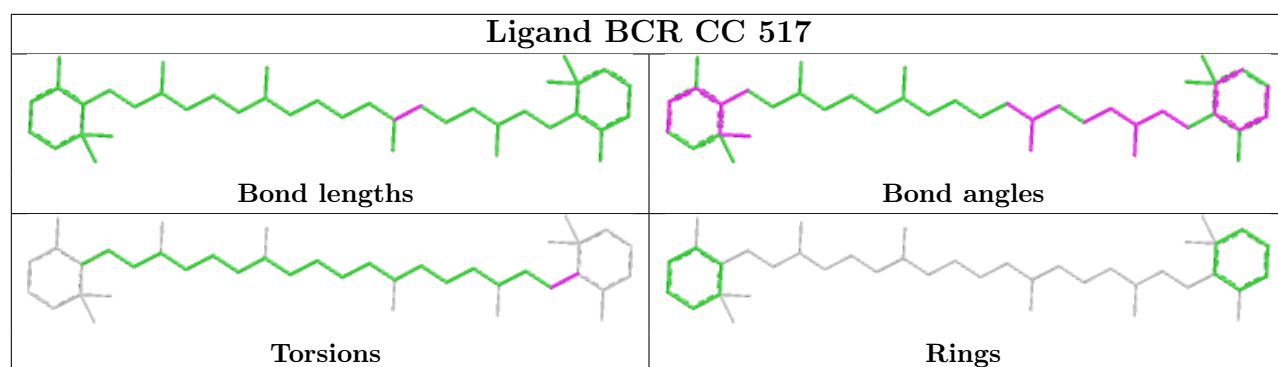




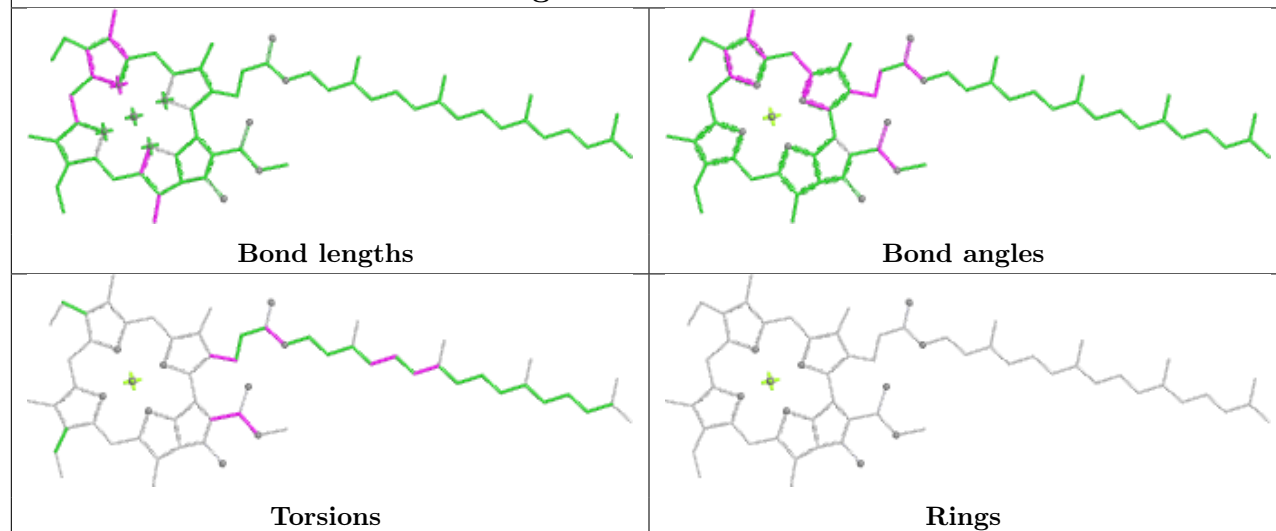




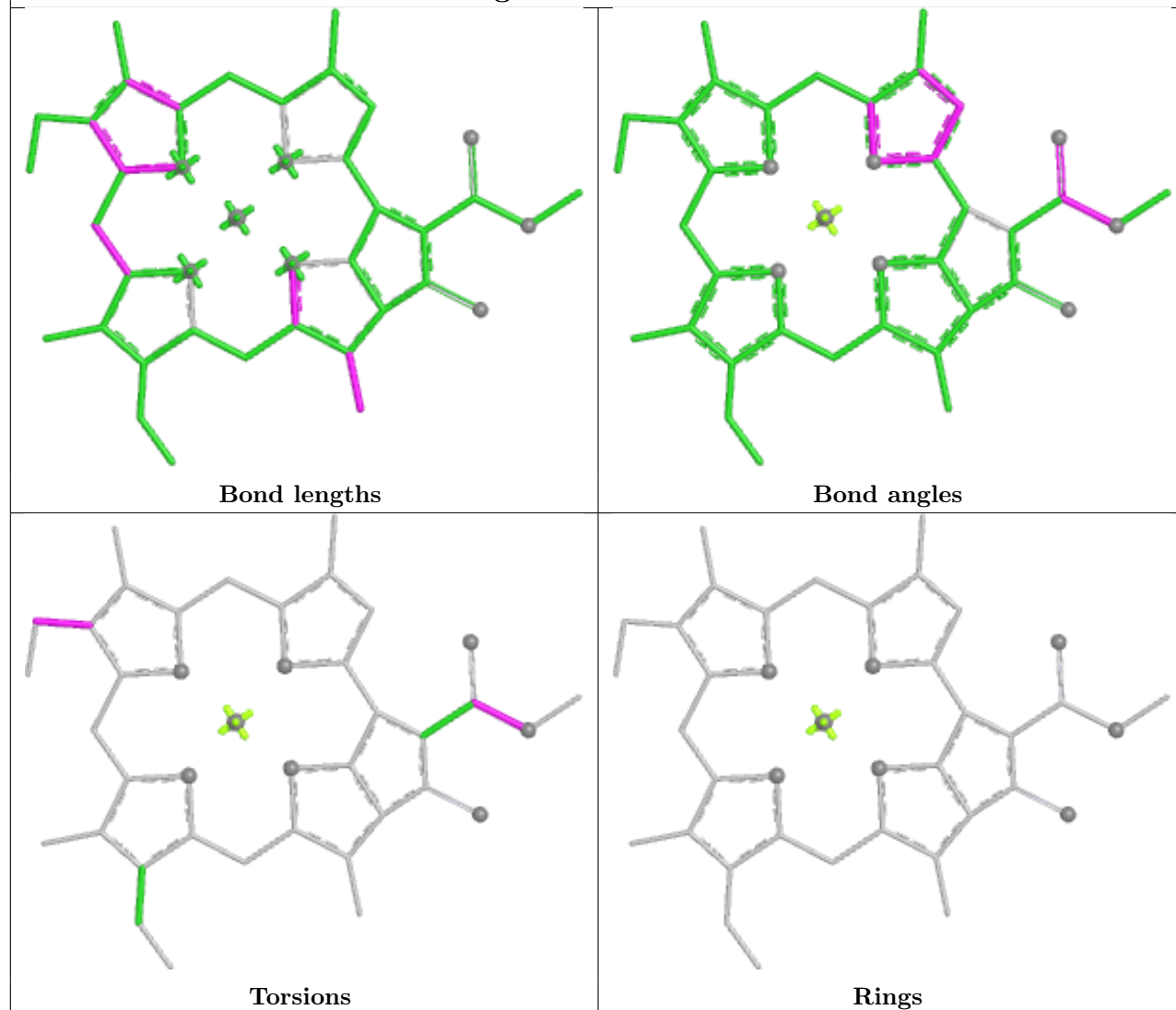


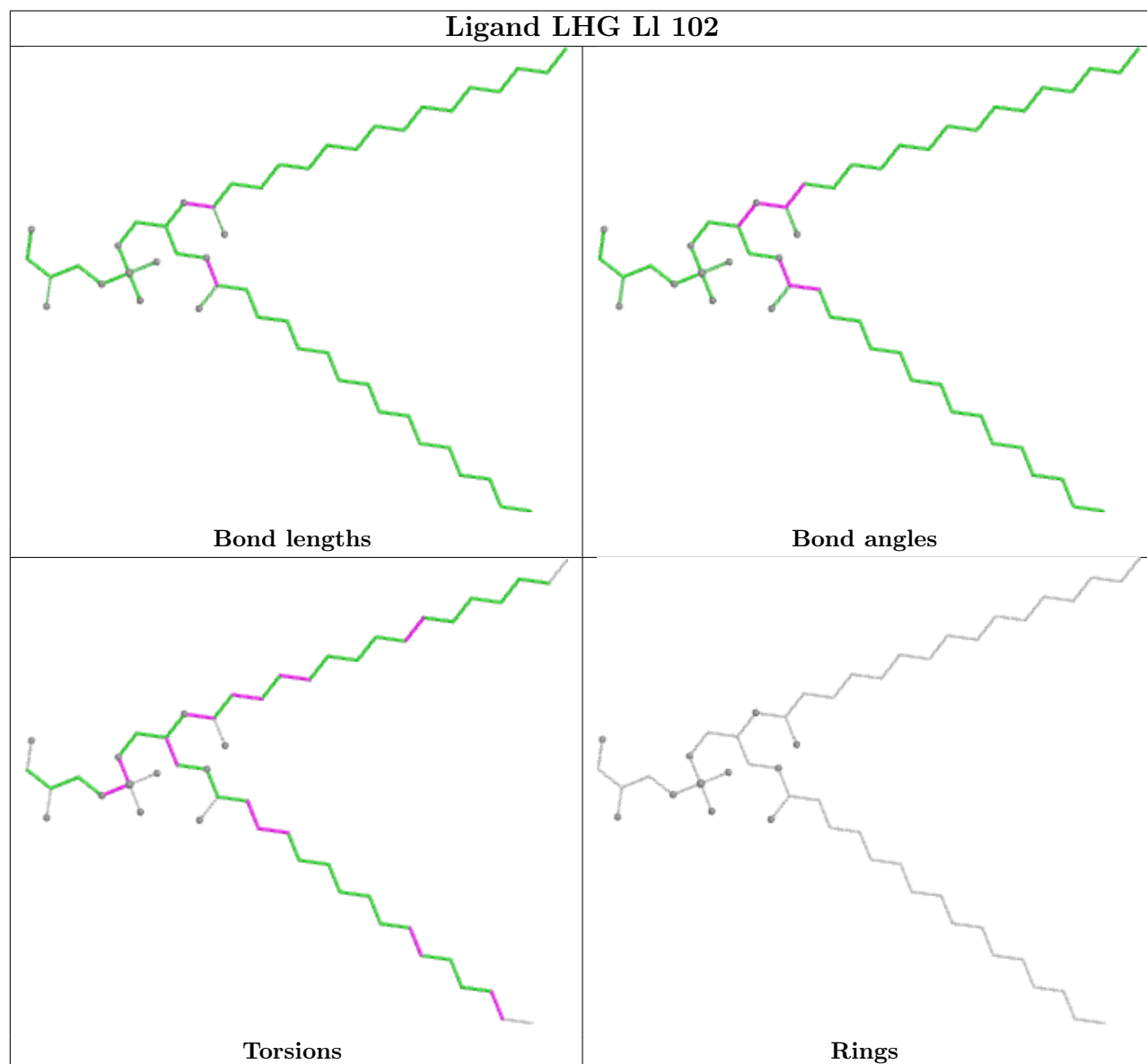
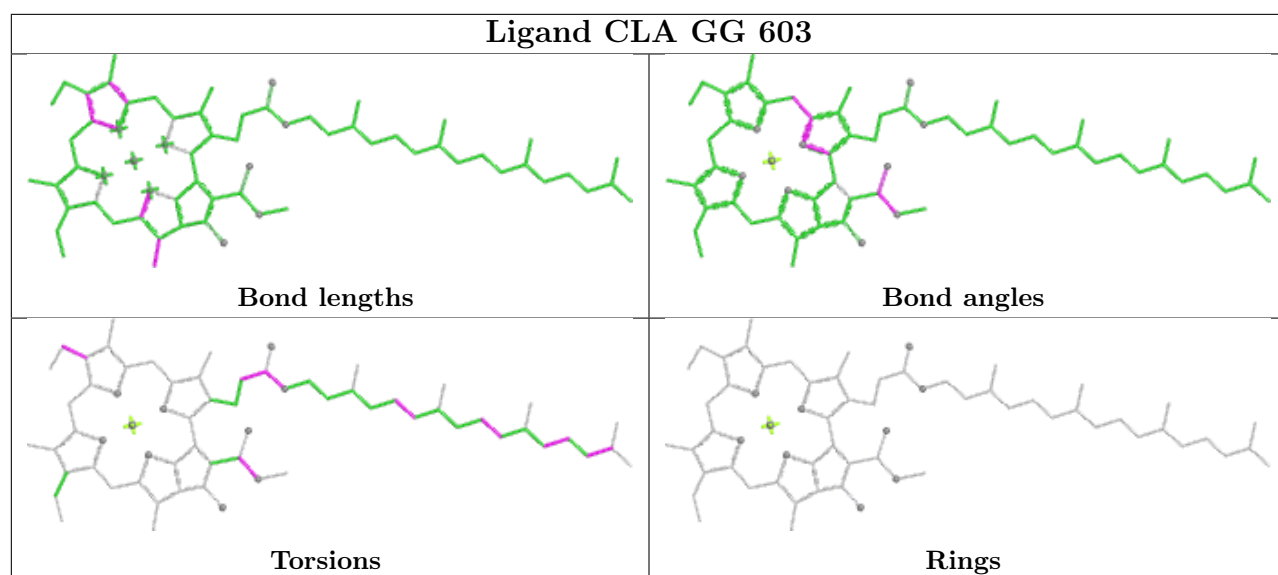


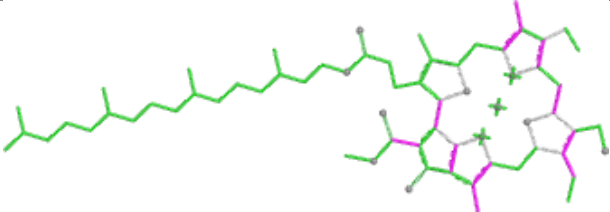
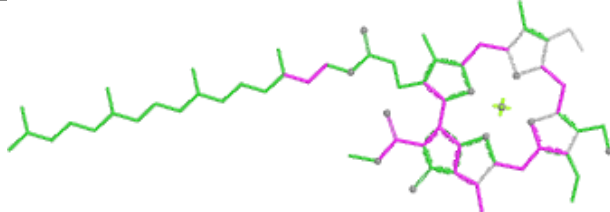
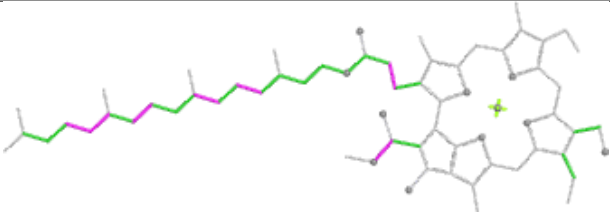
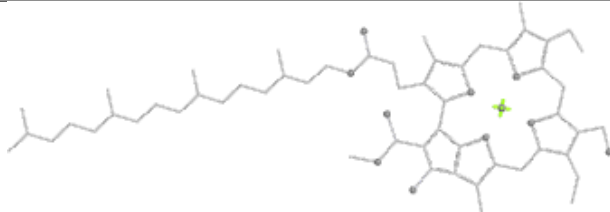
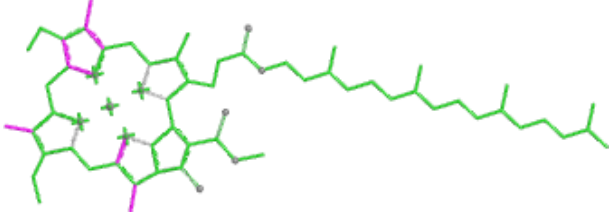
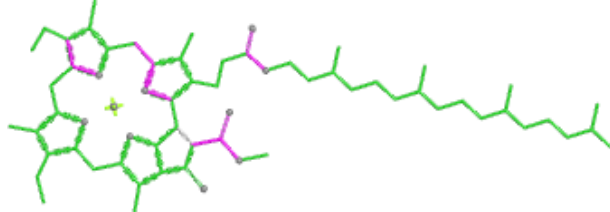
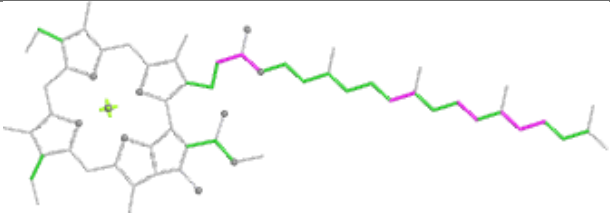
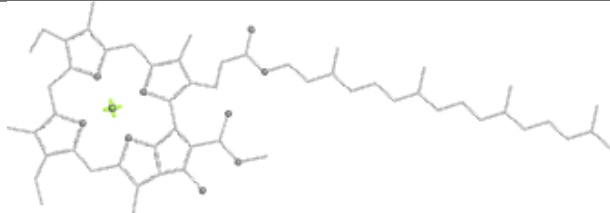
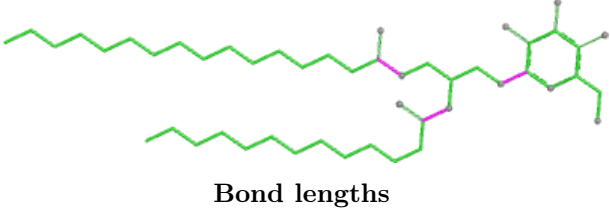
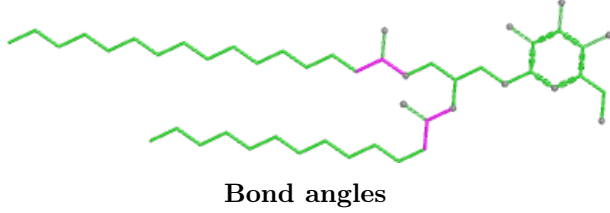
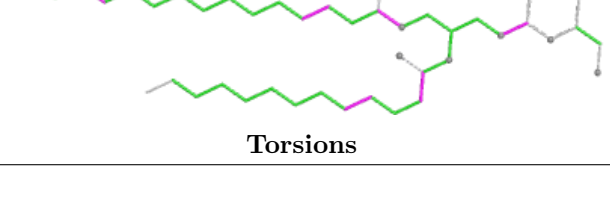
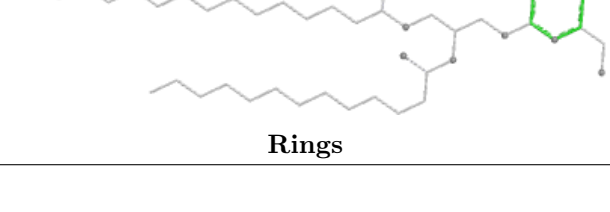
Ligand CLA C 508



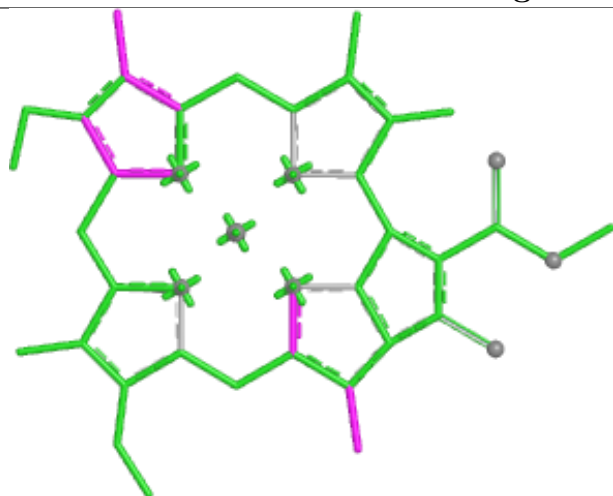
Ligand CLA 3 612



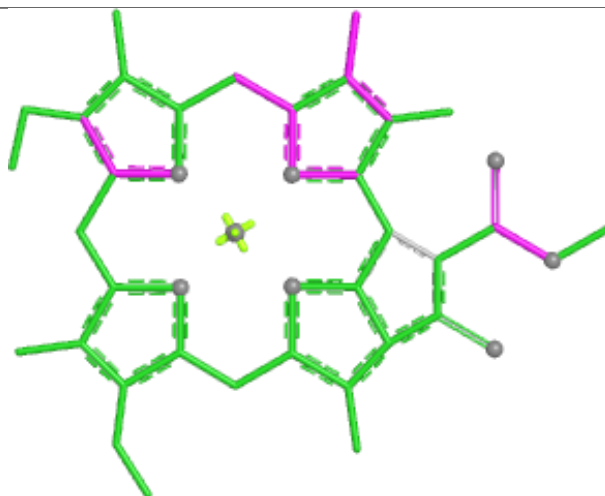


Ligand CHL NN 607	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG WW 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

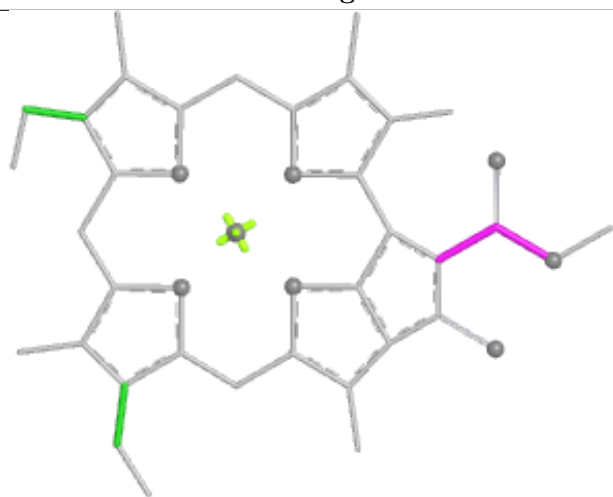
Ligand CLA N 604



Bond lengths



Bond angles

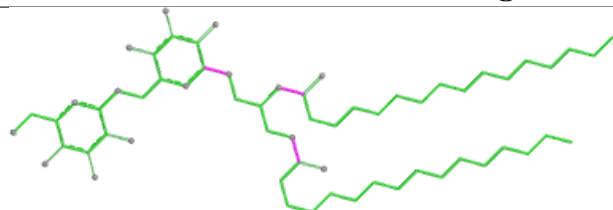


Torsions

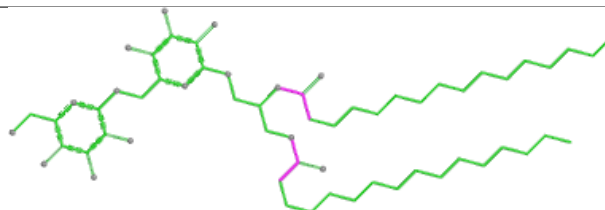


Rings

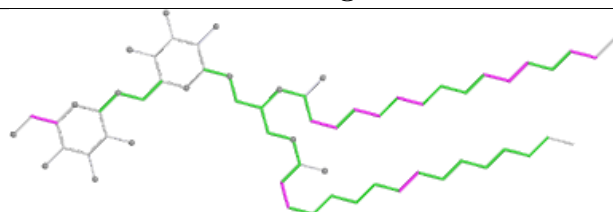
Ligand DGD BB 623



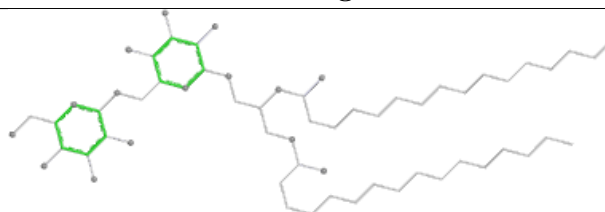
Bond lengths



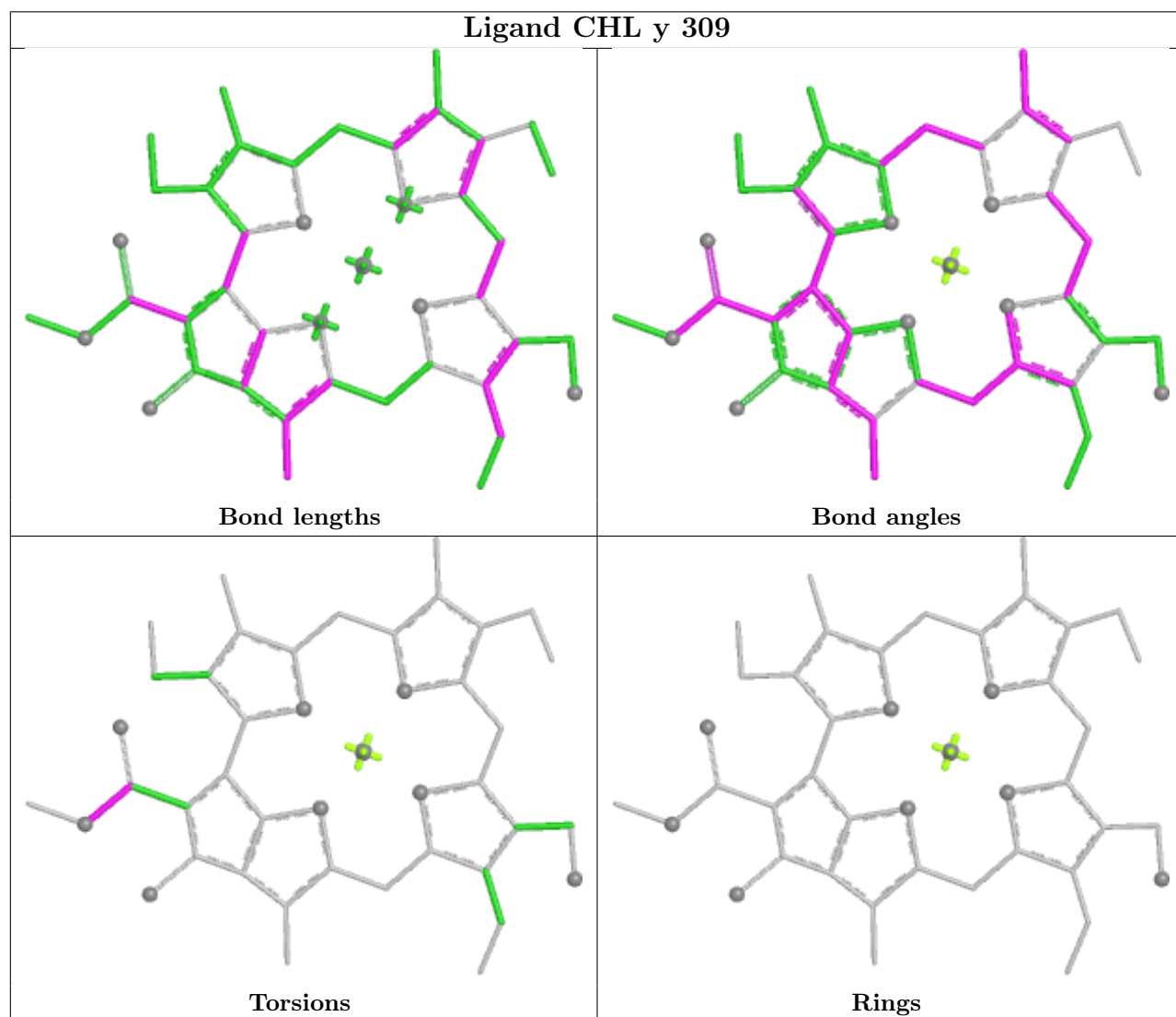
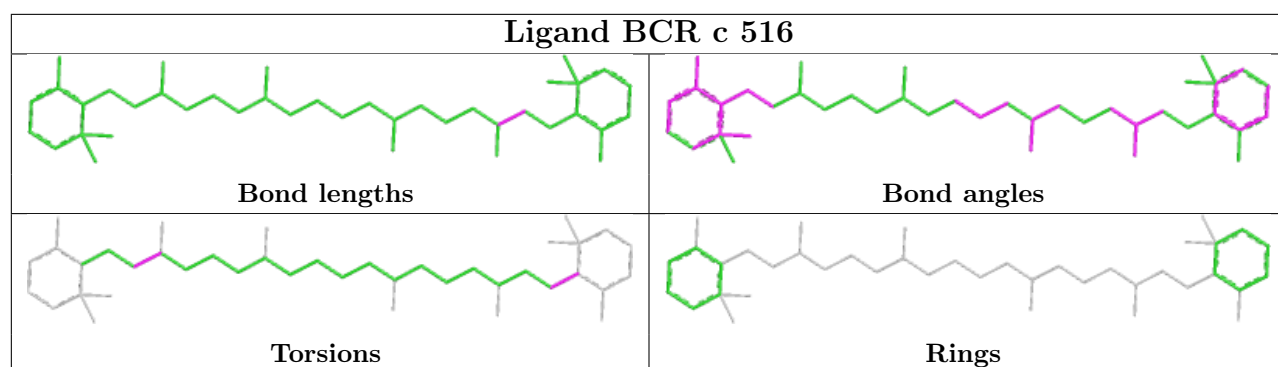
Bond angles

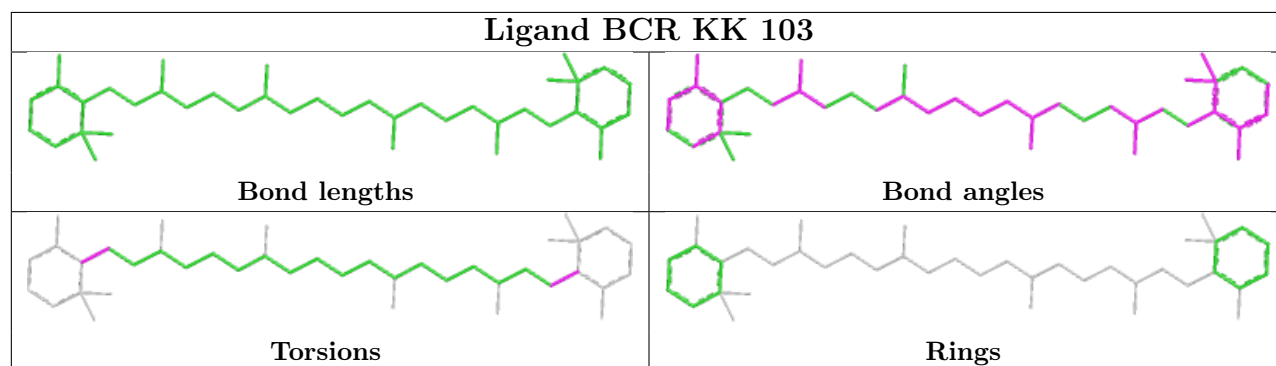
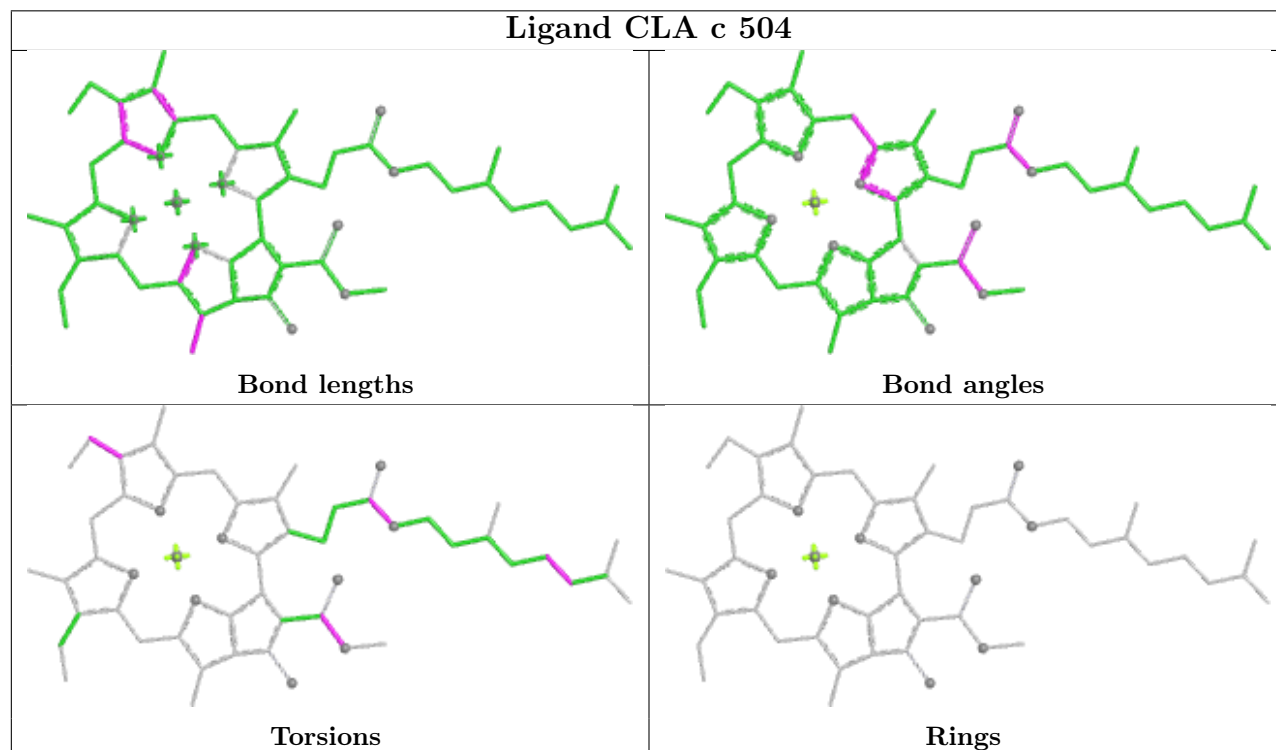
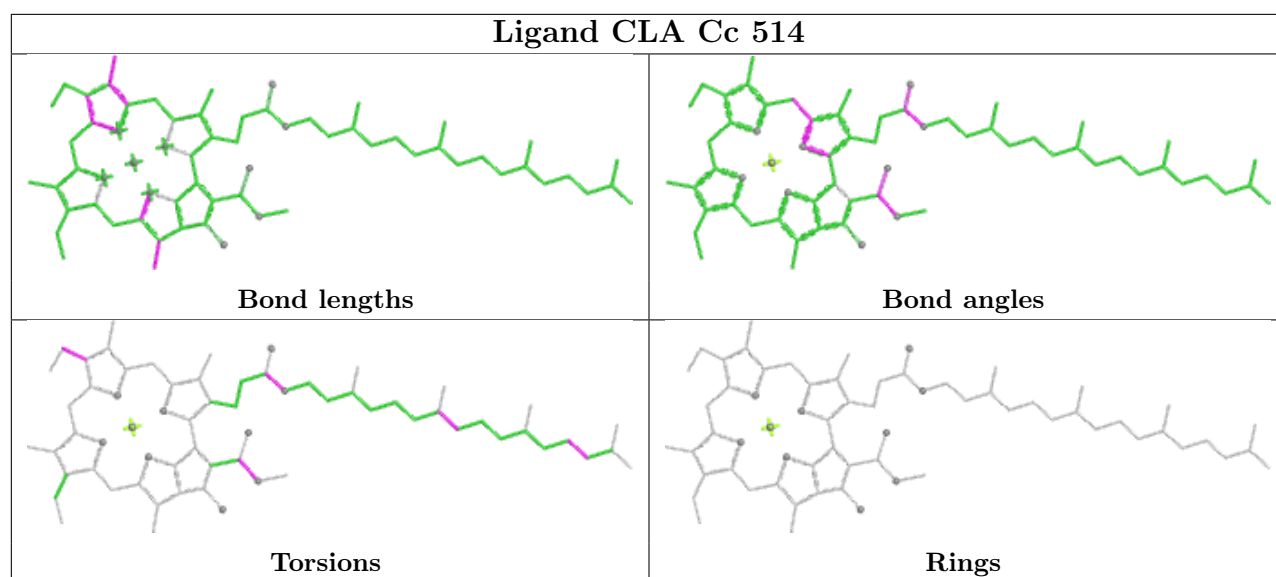


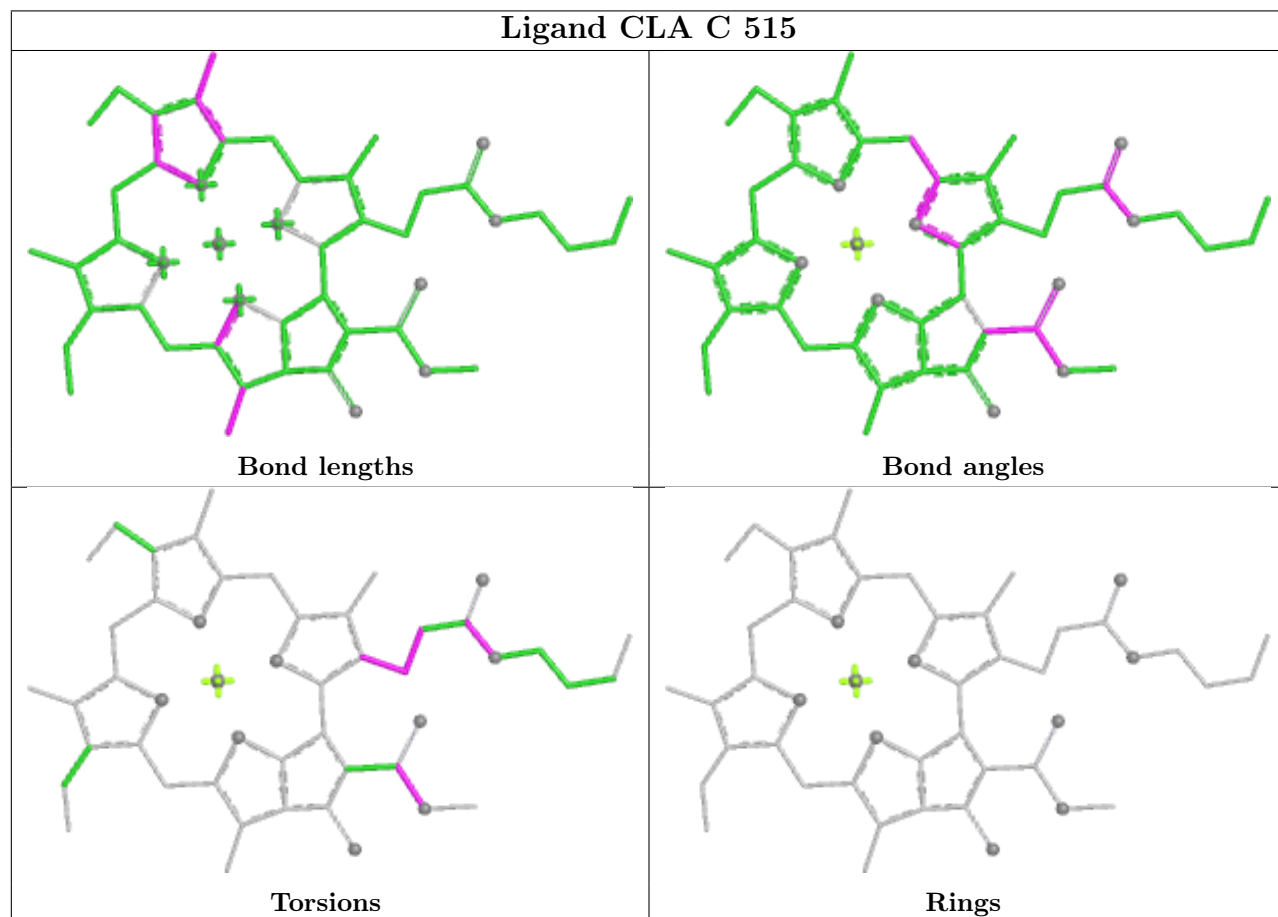
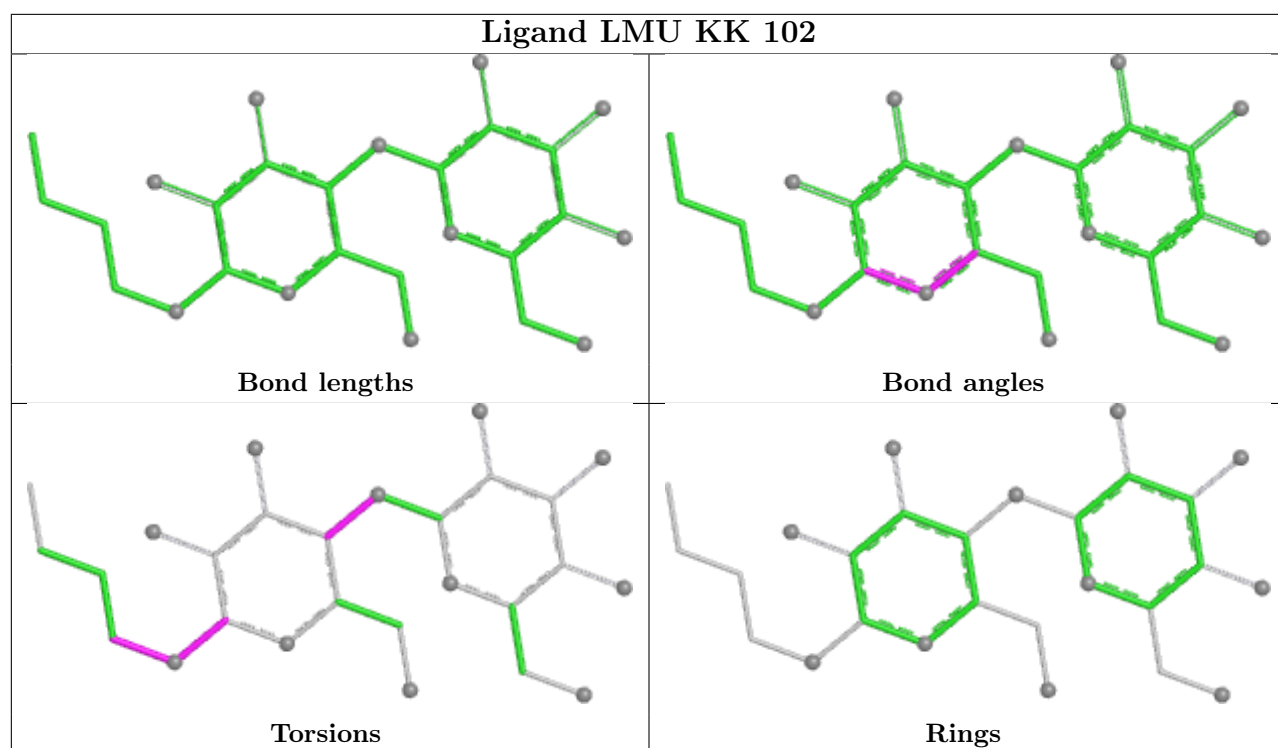
Torsions

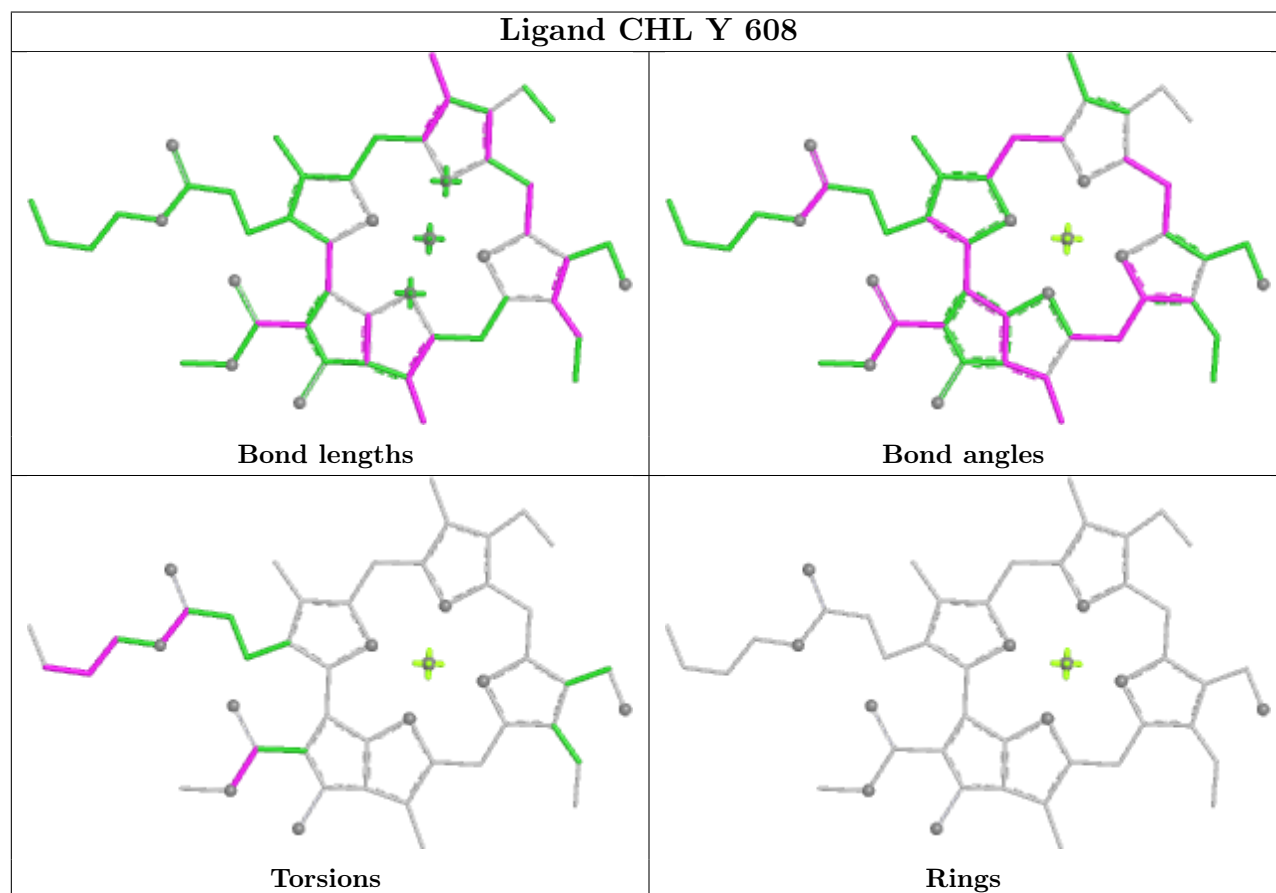
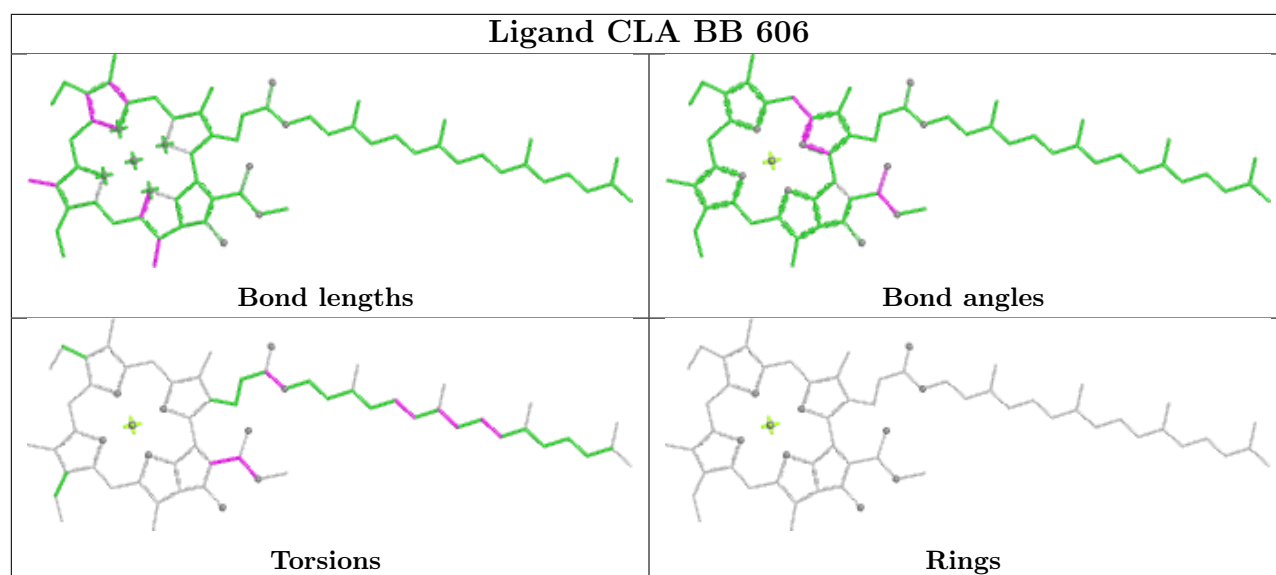


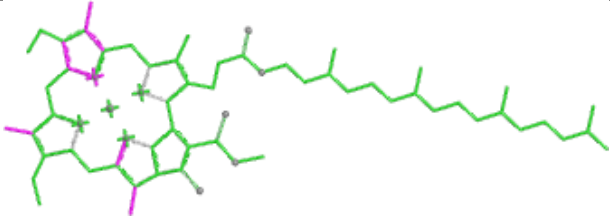
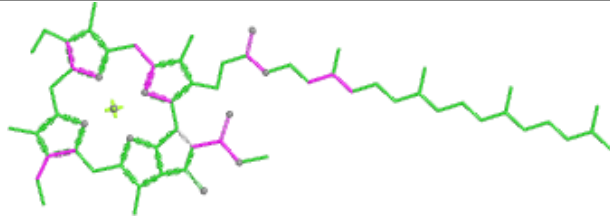
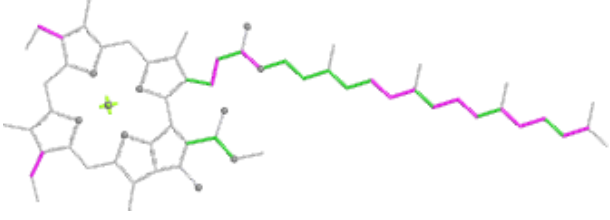
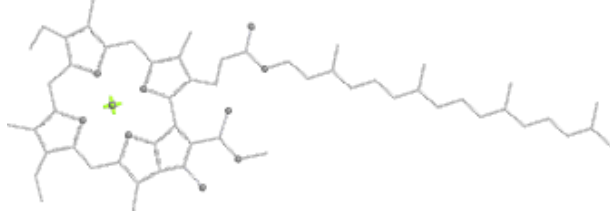
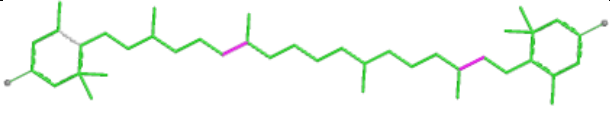
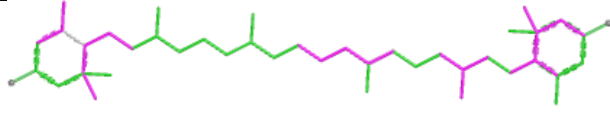
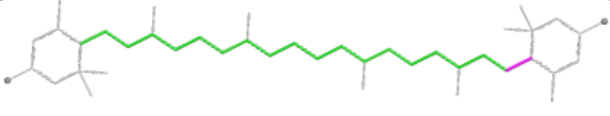
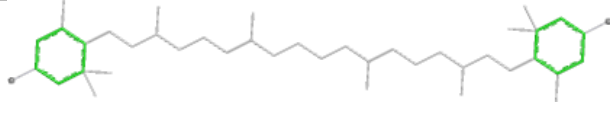
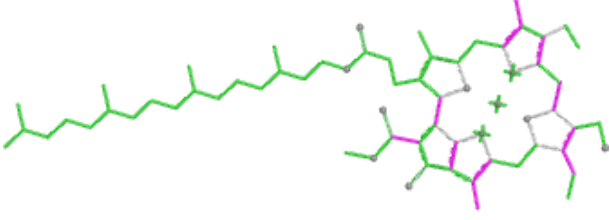
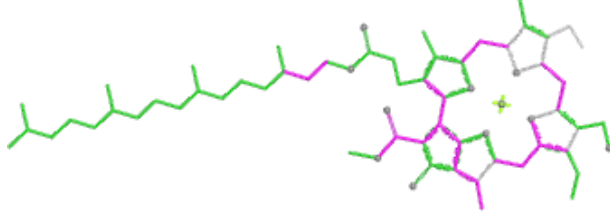
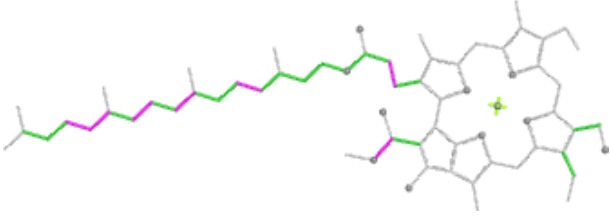
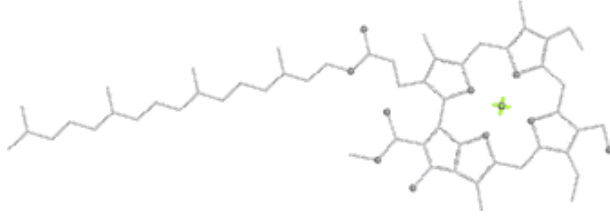
Rings



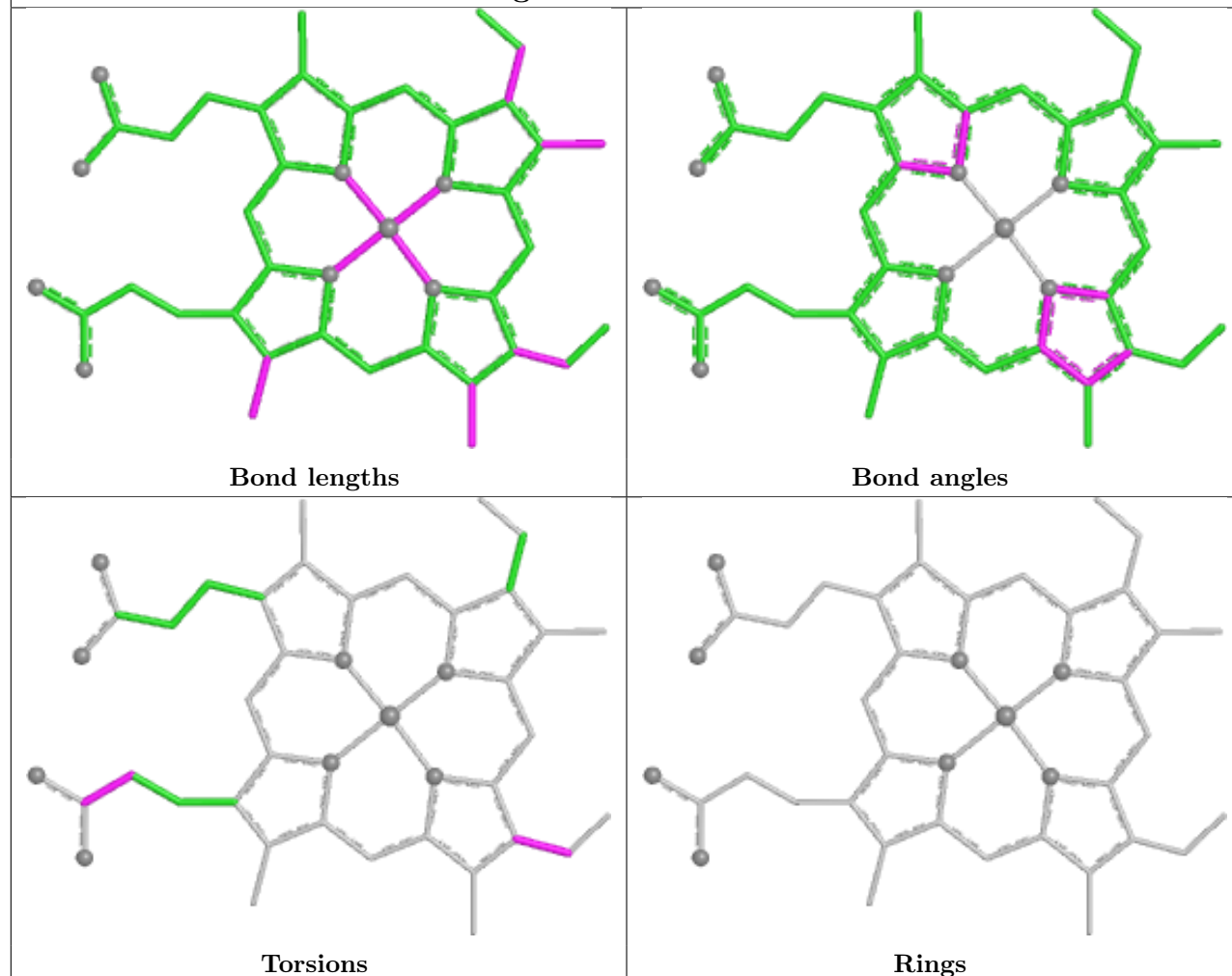




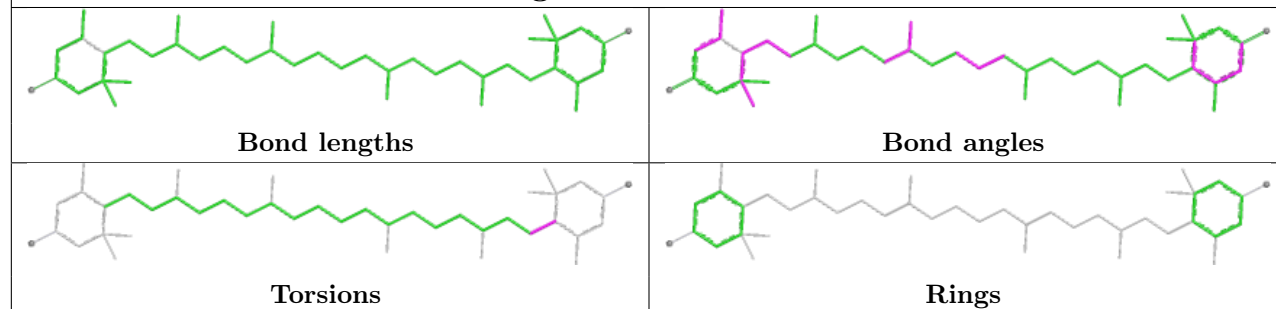


Ligand CLA B 605	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT Ss 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL N 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

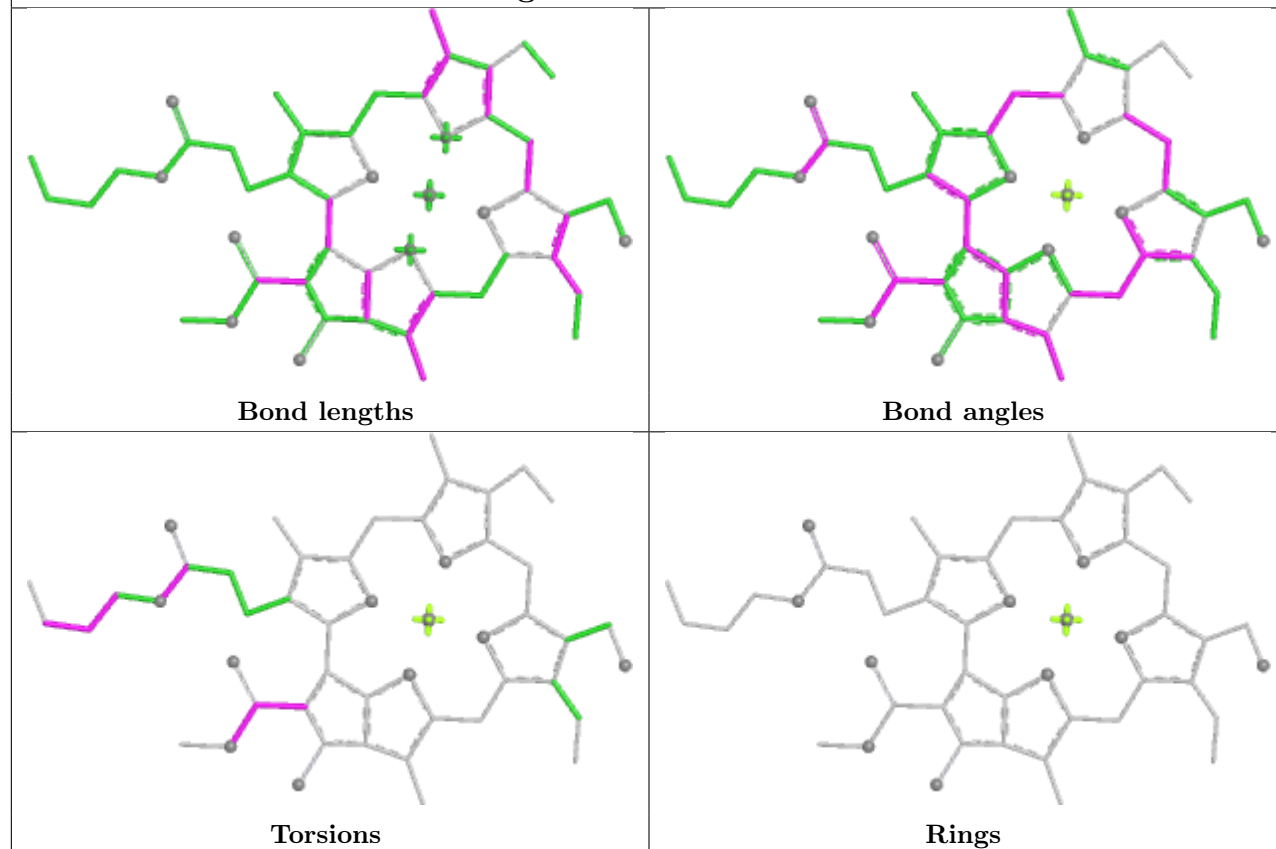
Ligand HEM e 101



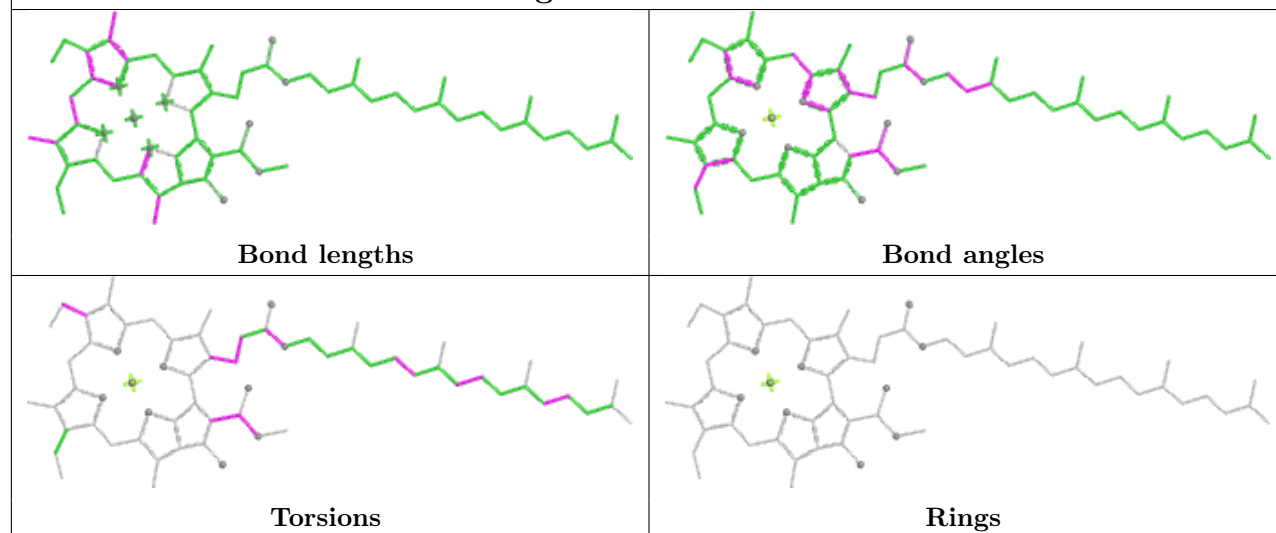
Ligand LUT G 615



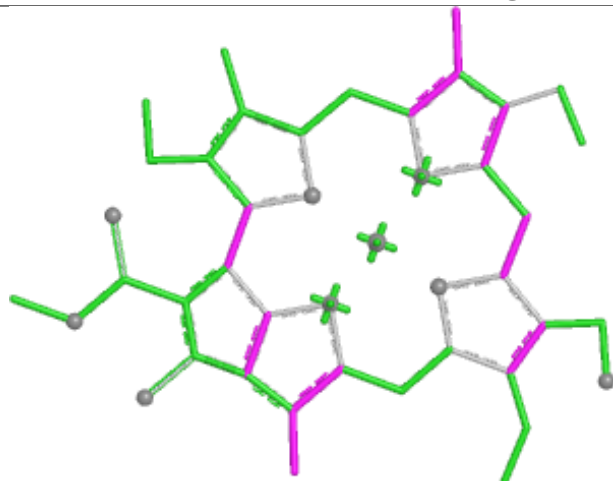
Ligand CHL YY 608



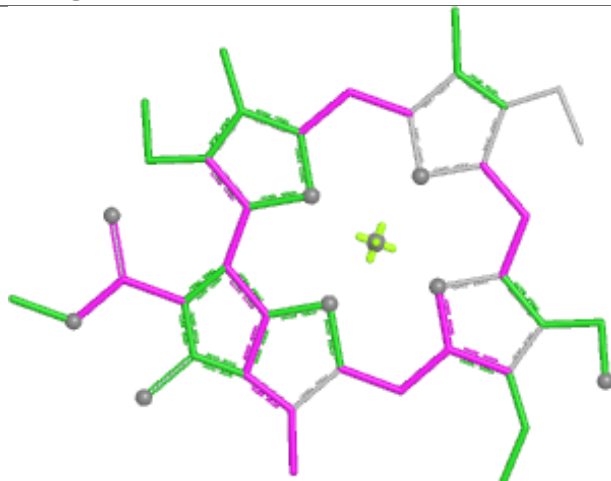
Ligand CLA n 602



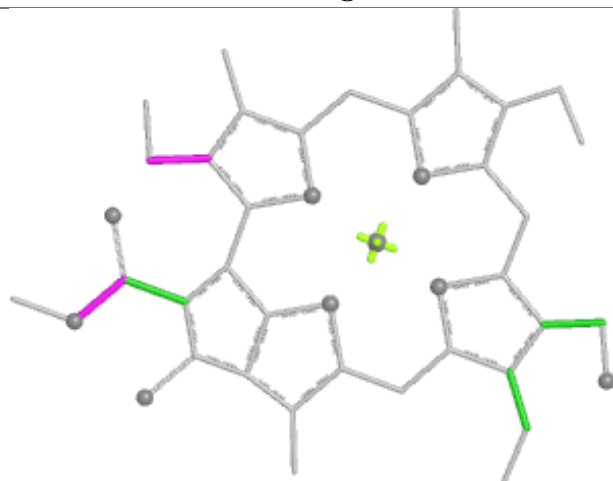
Ligand CHL Gg 307



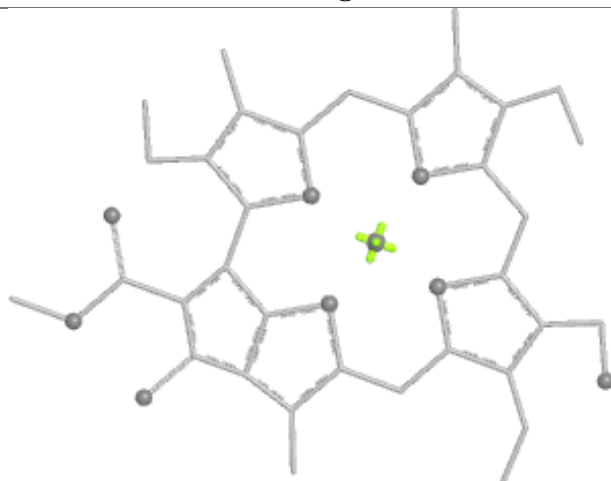
Bond lengths



Bond angles

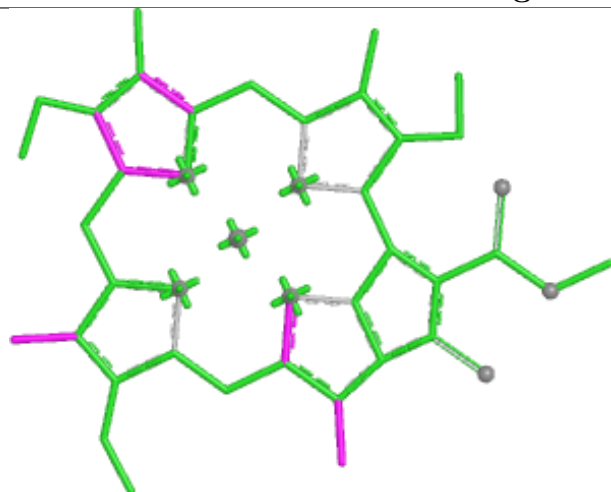


Torsions

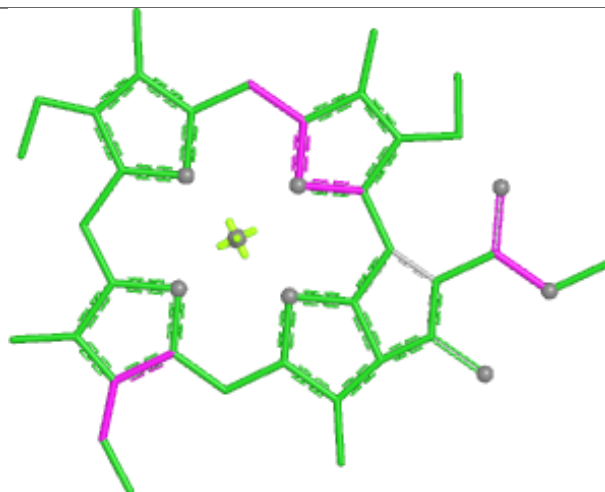


Rings

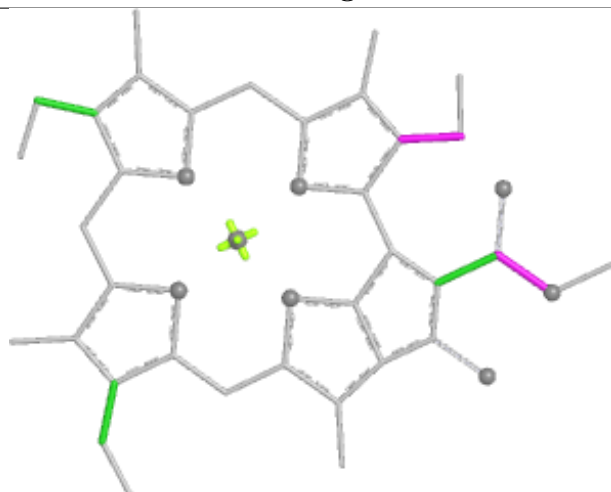
Ligand CLA N 612



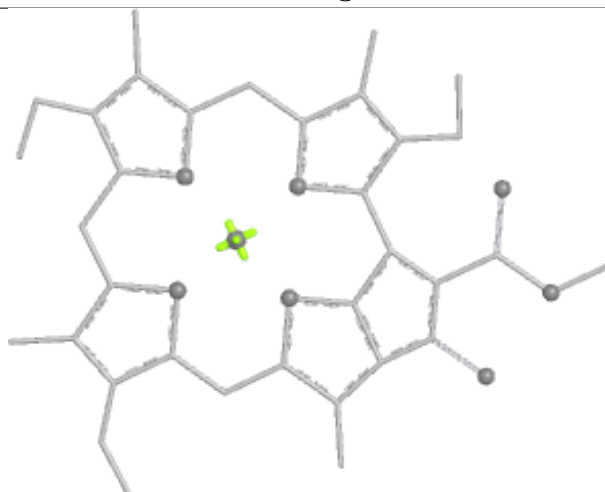
Bond lengths



Bond angles

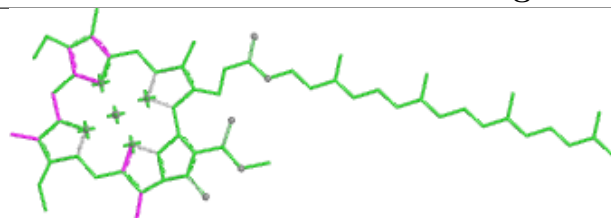


Torsions

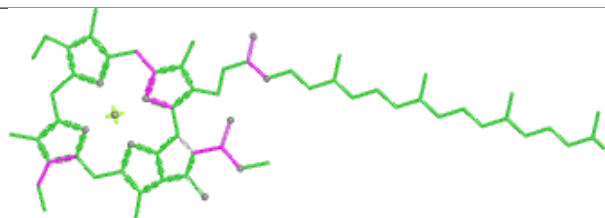


Rings

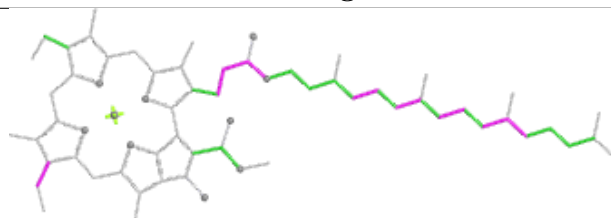
Ligand CLA D 404



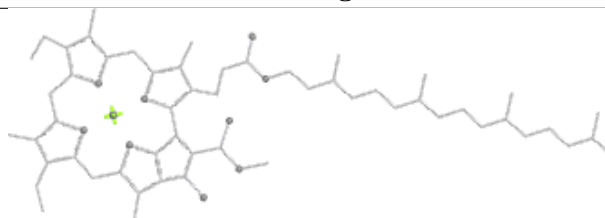
Bond lengths



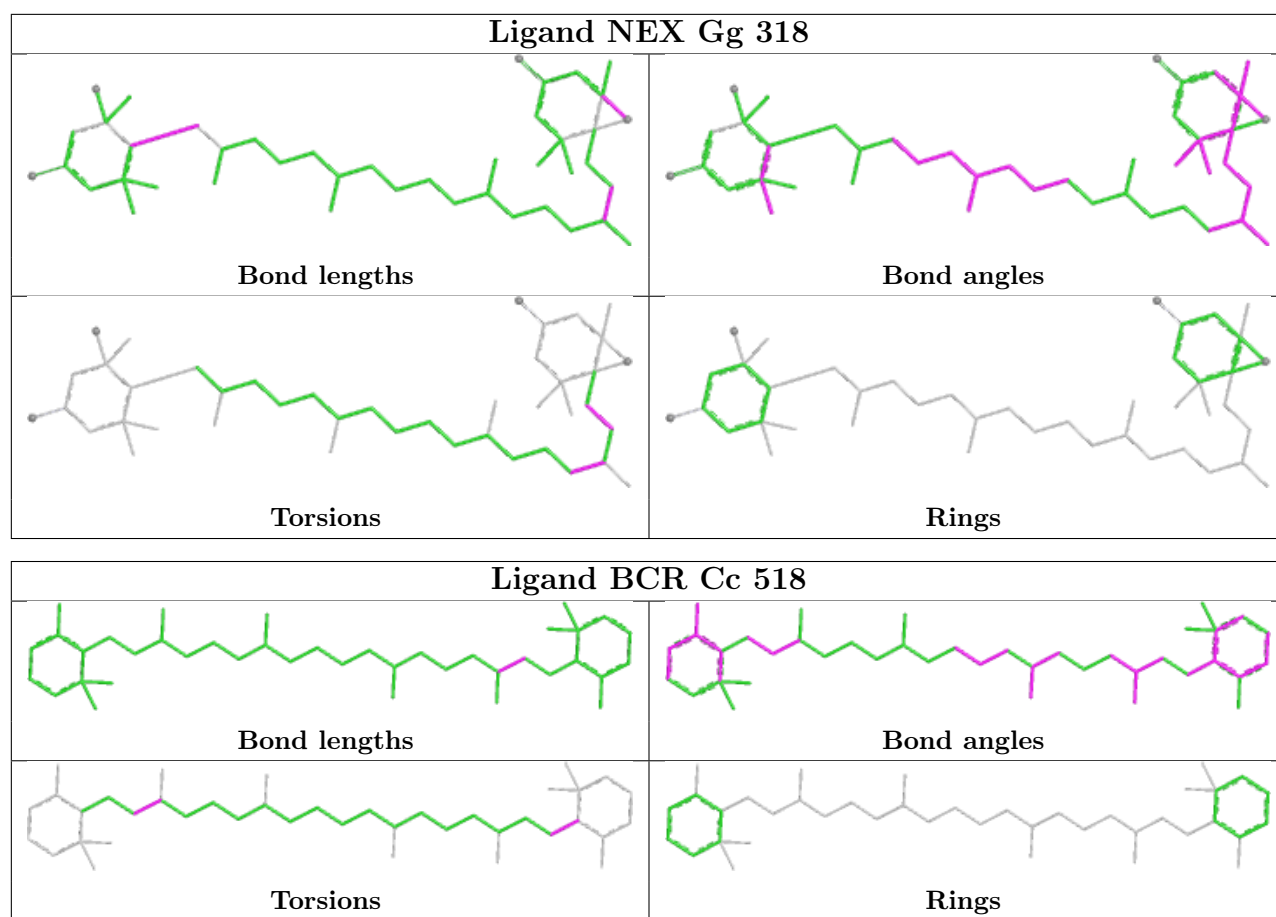
Bond angles

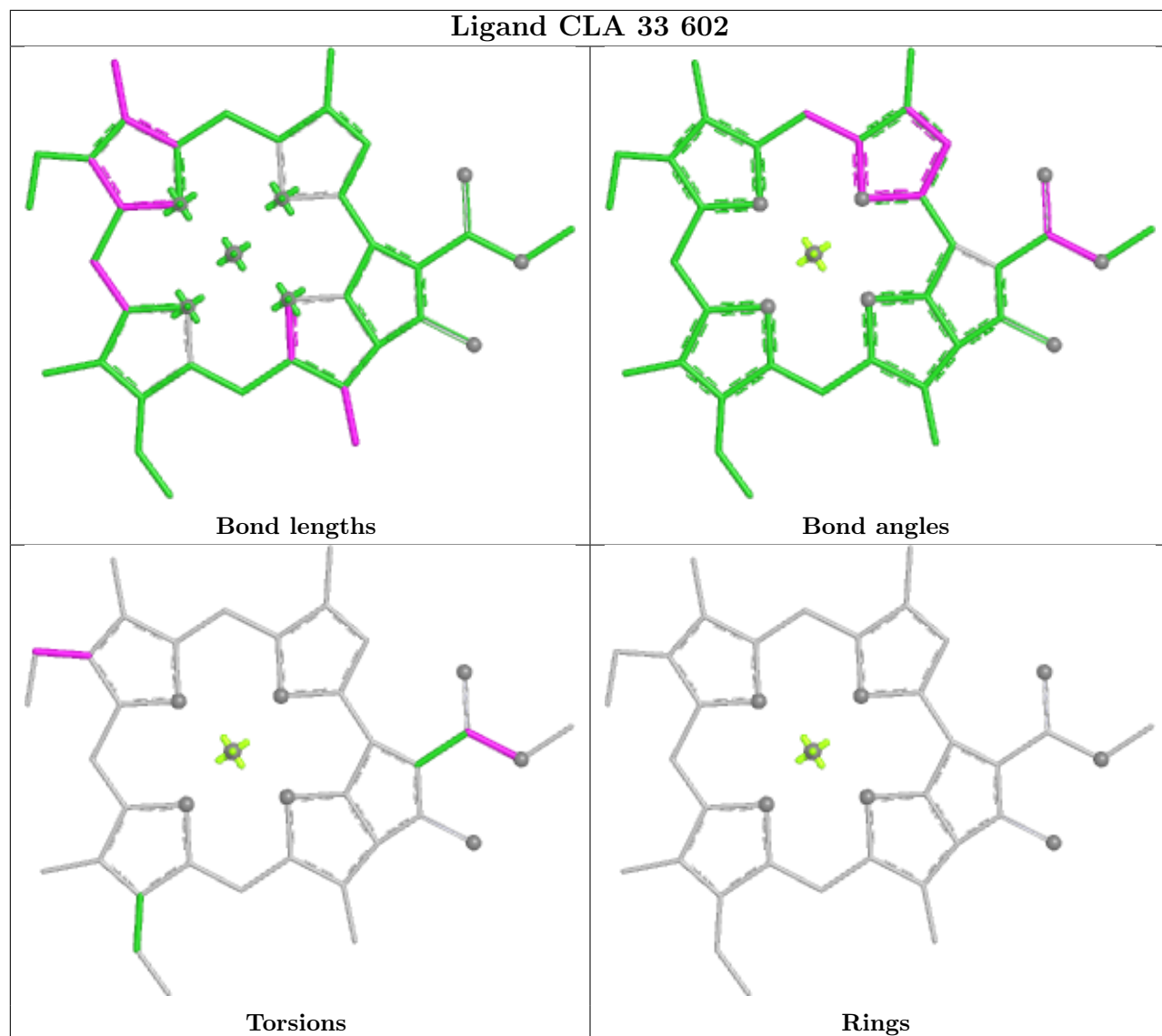


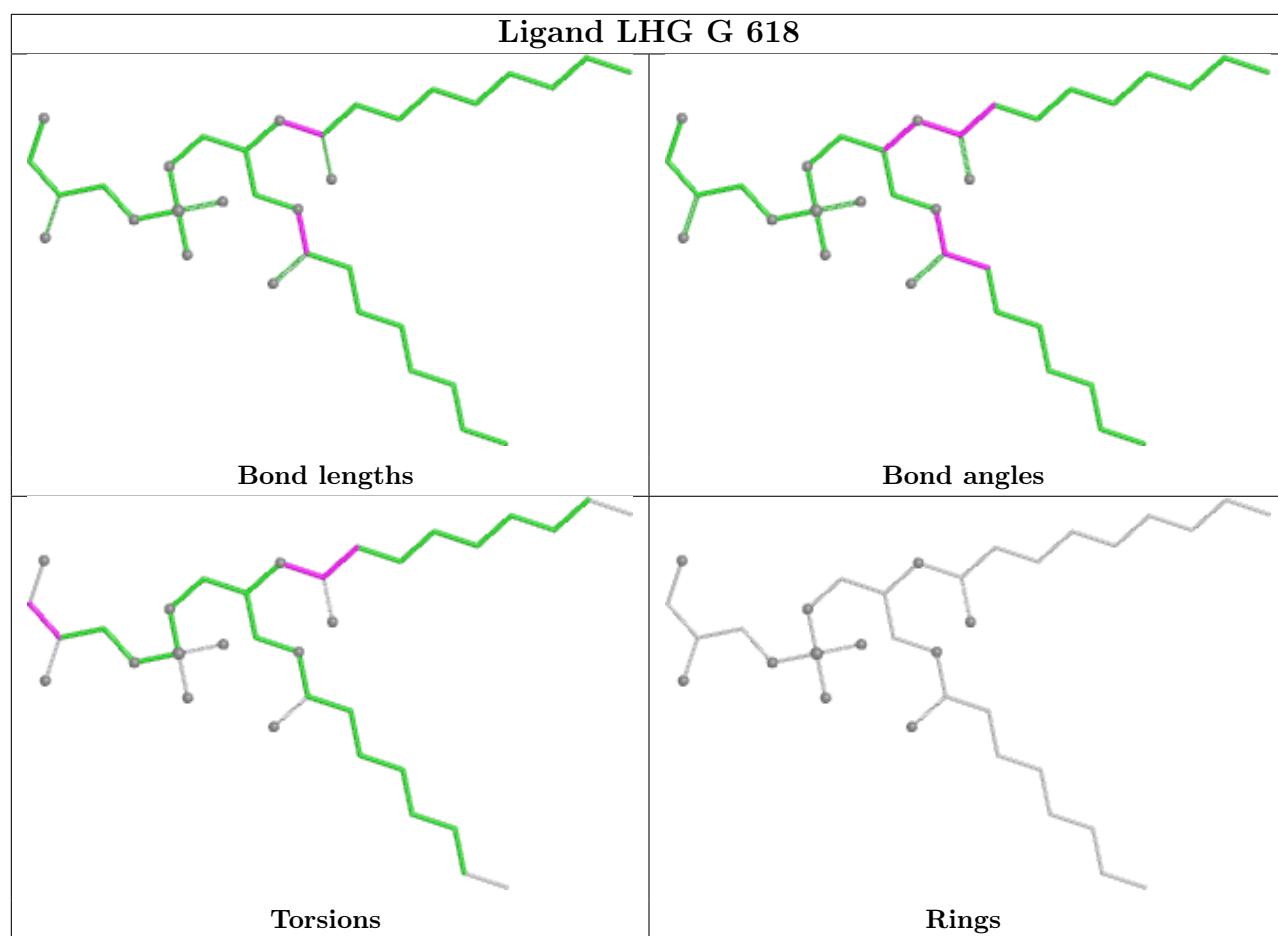
Torsions

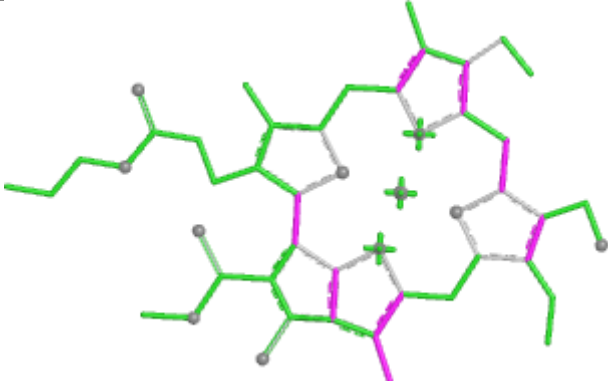
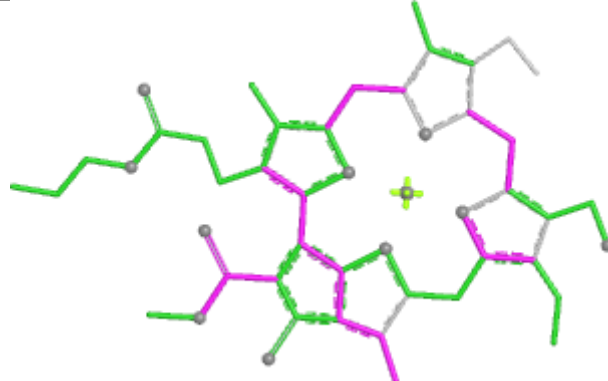
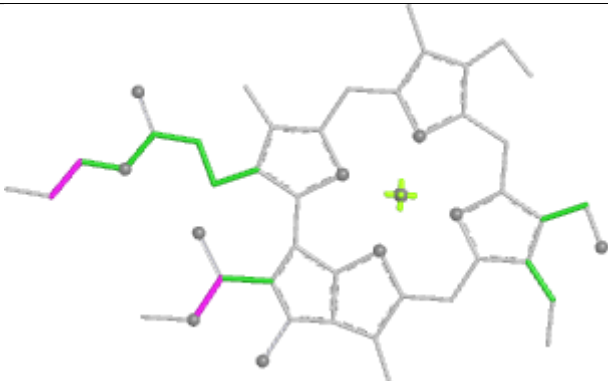
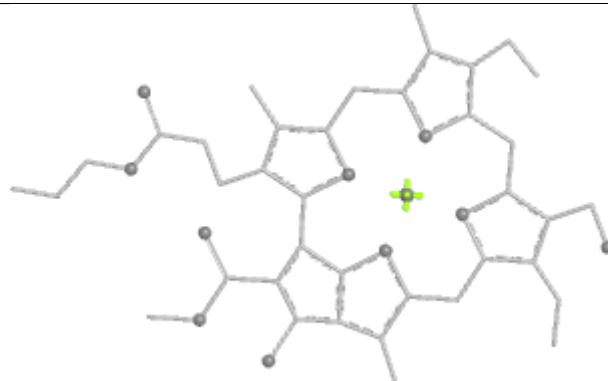


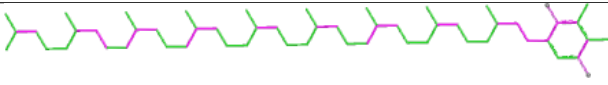
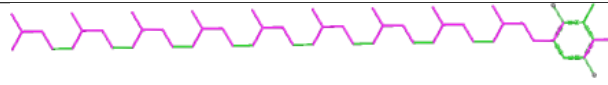
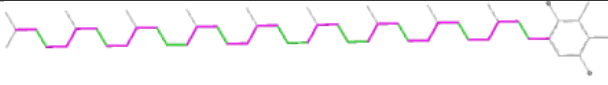
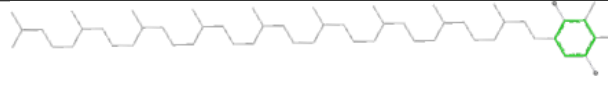
Rings

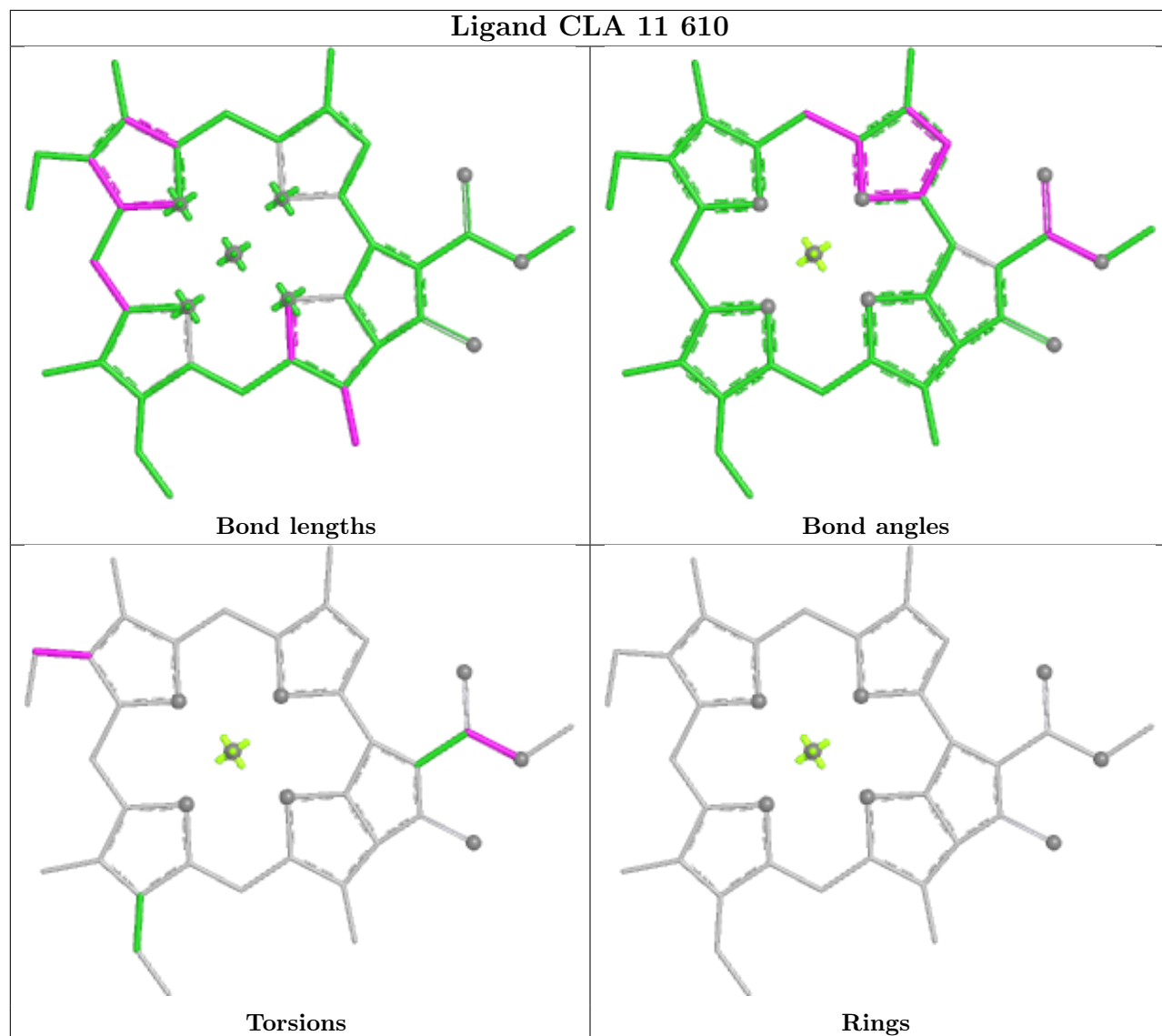


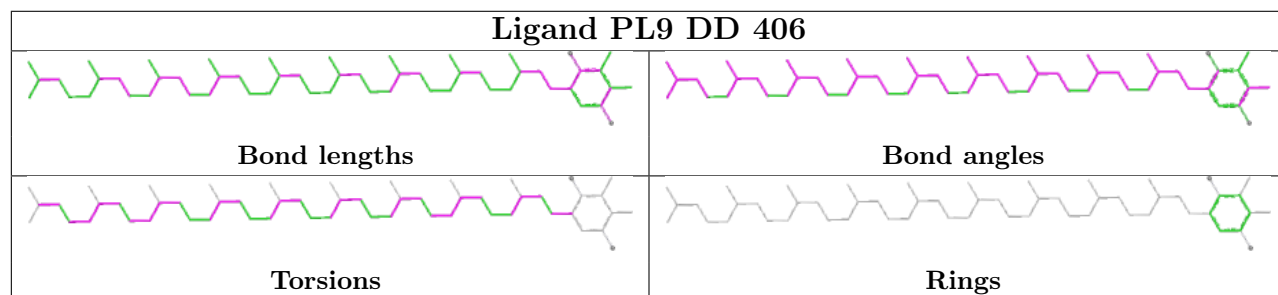
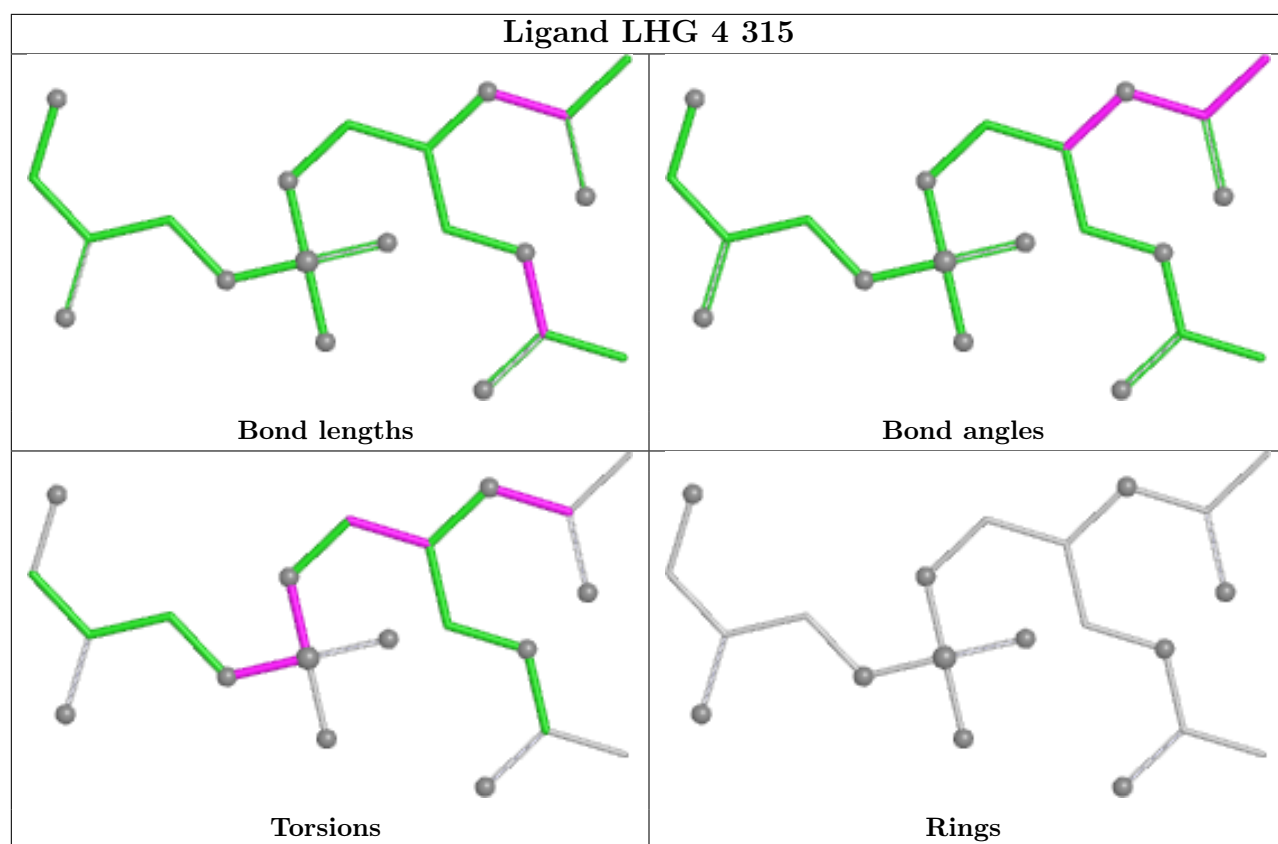


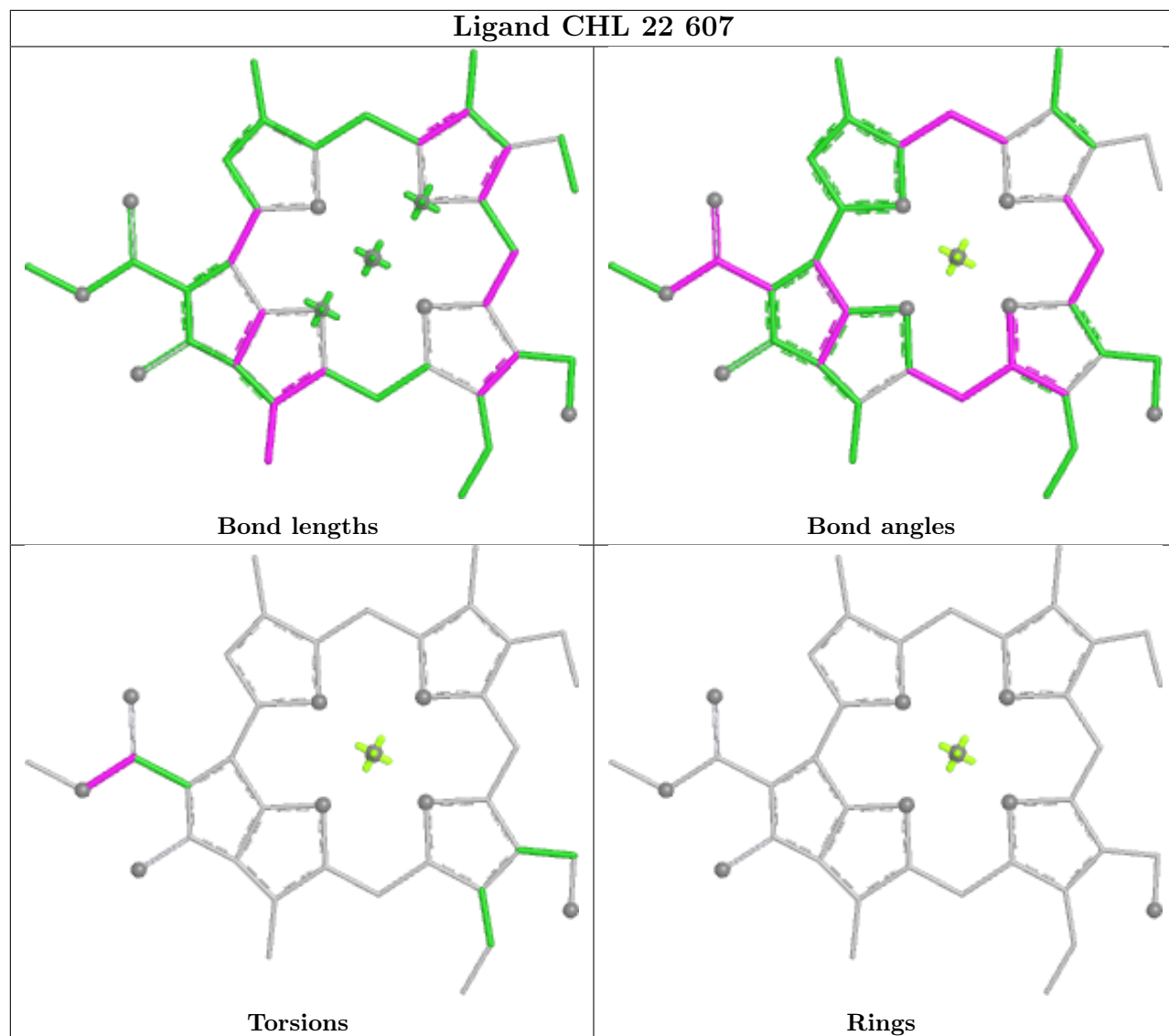


Ligand CHL SS 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

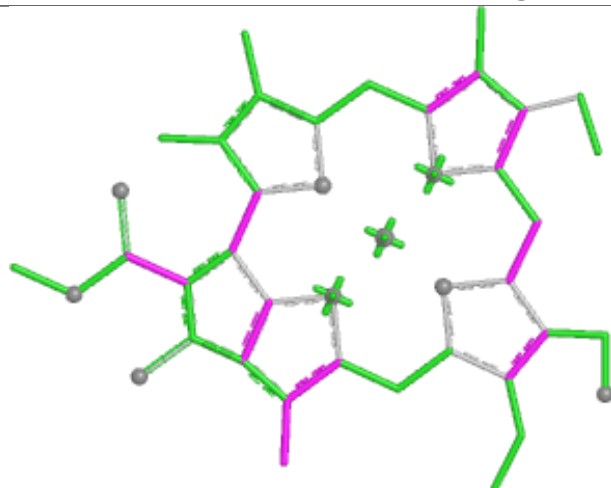
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



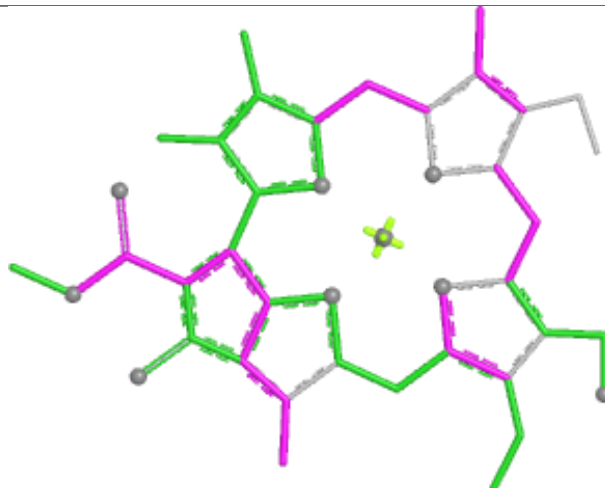




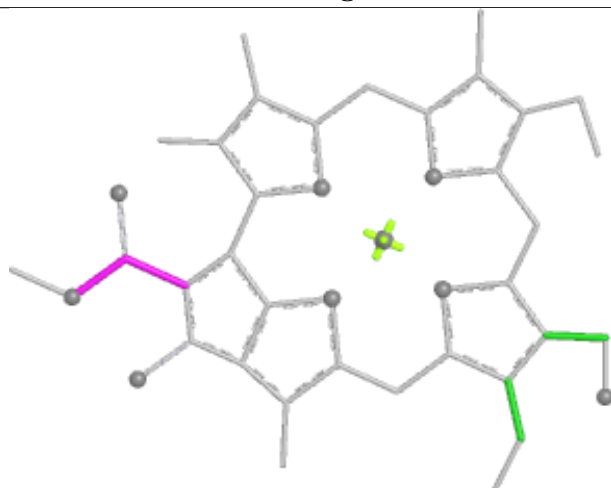
Ligand CHL N 605



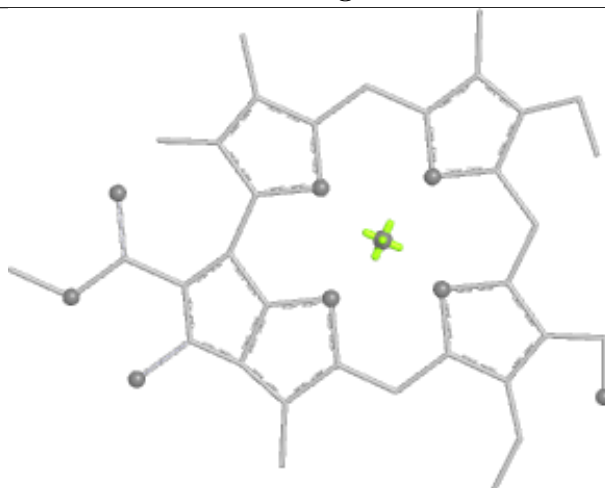
Bond lengths



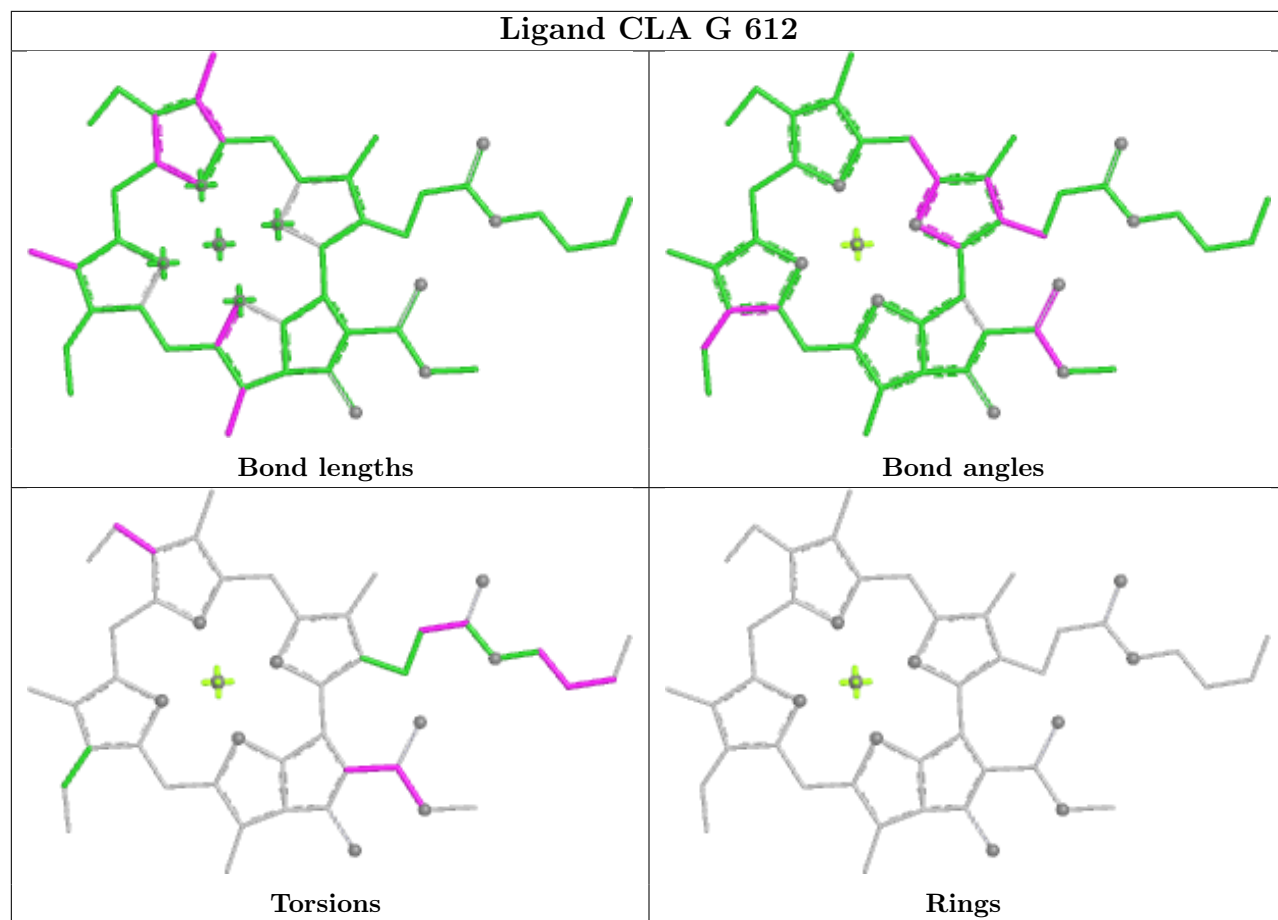
Bond angles



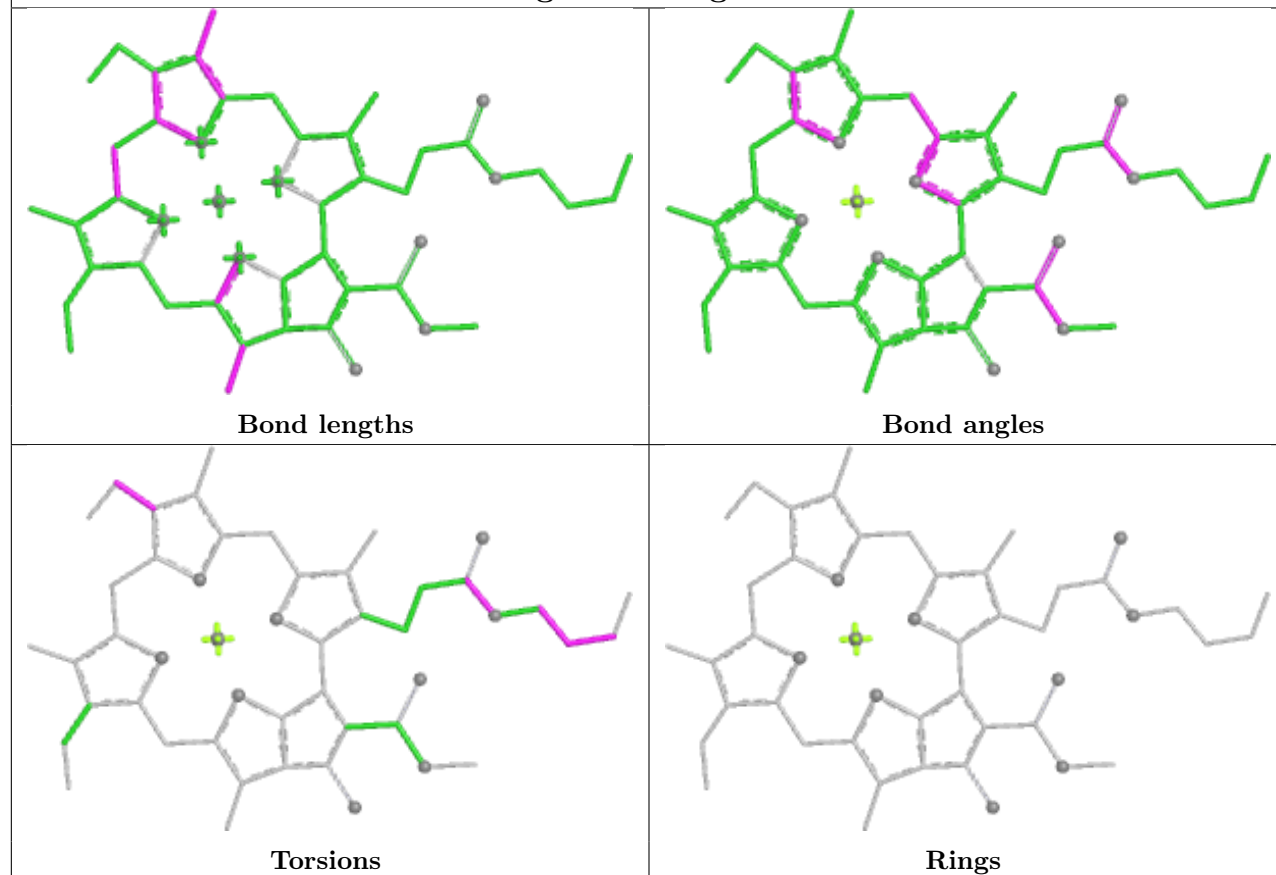
Torsions



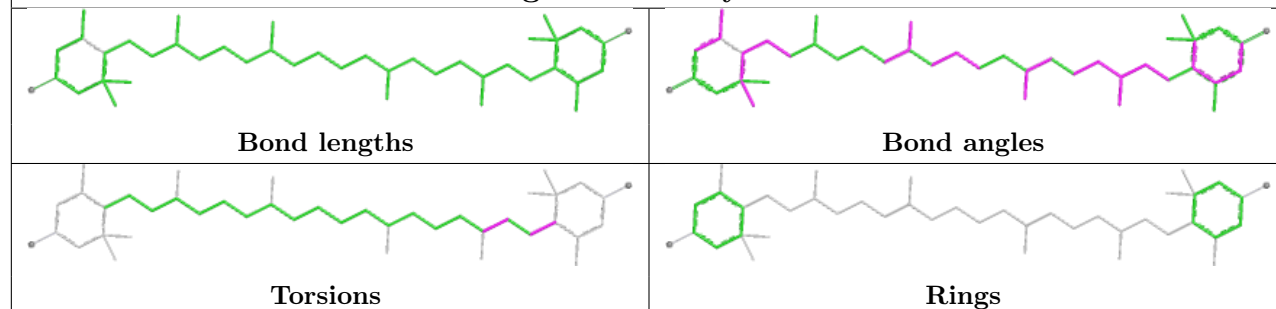
Rings

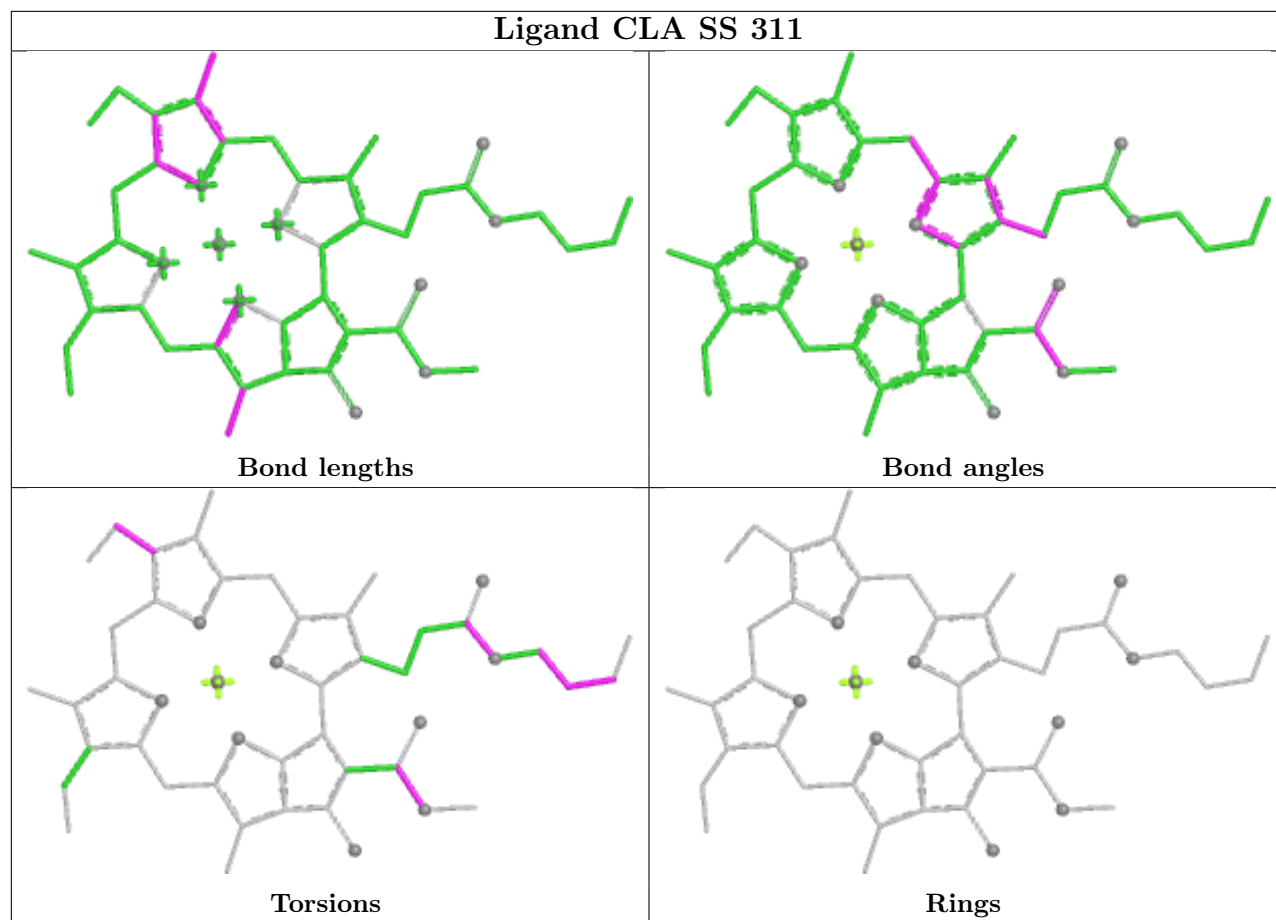


Ligand CLA g 610

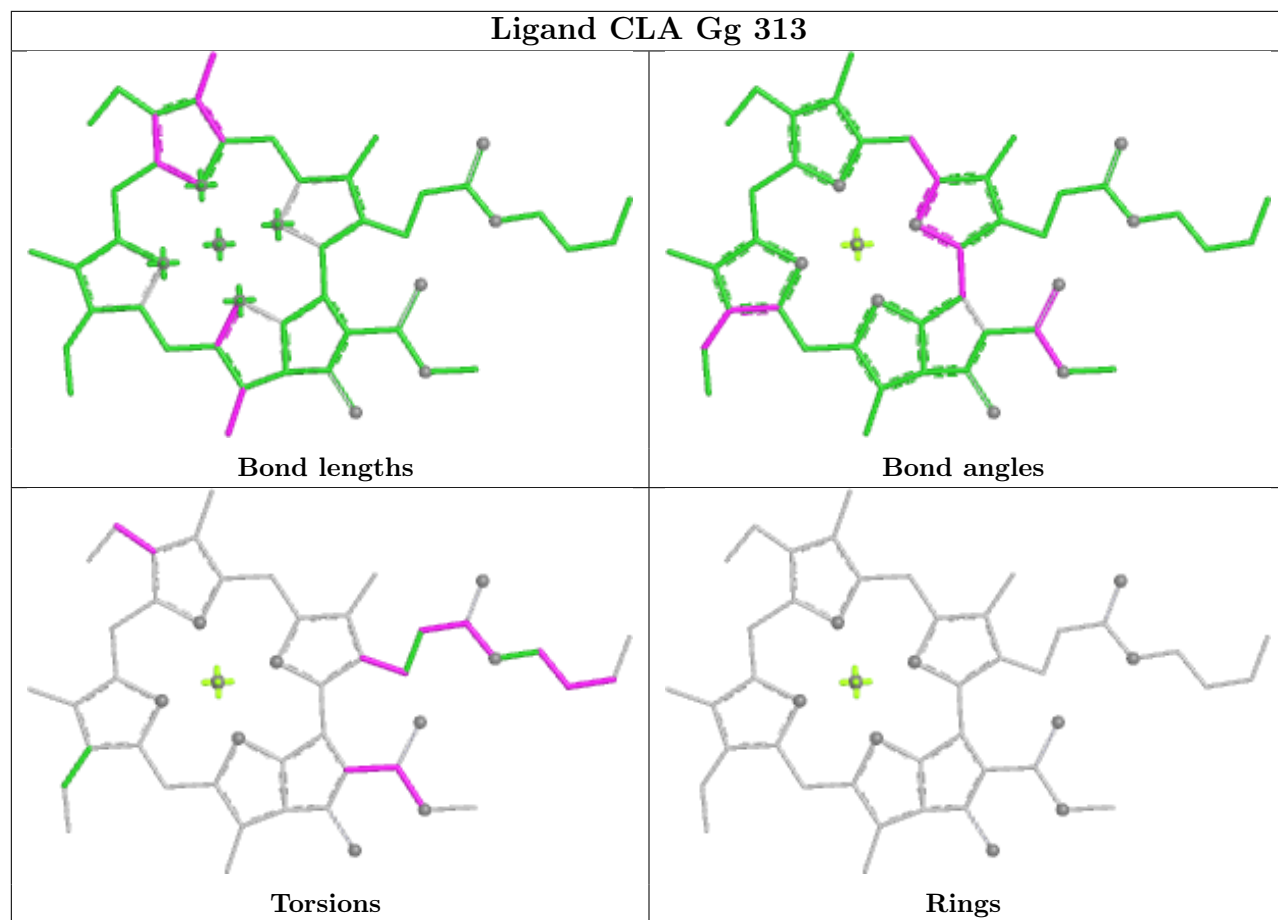


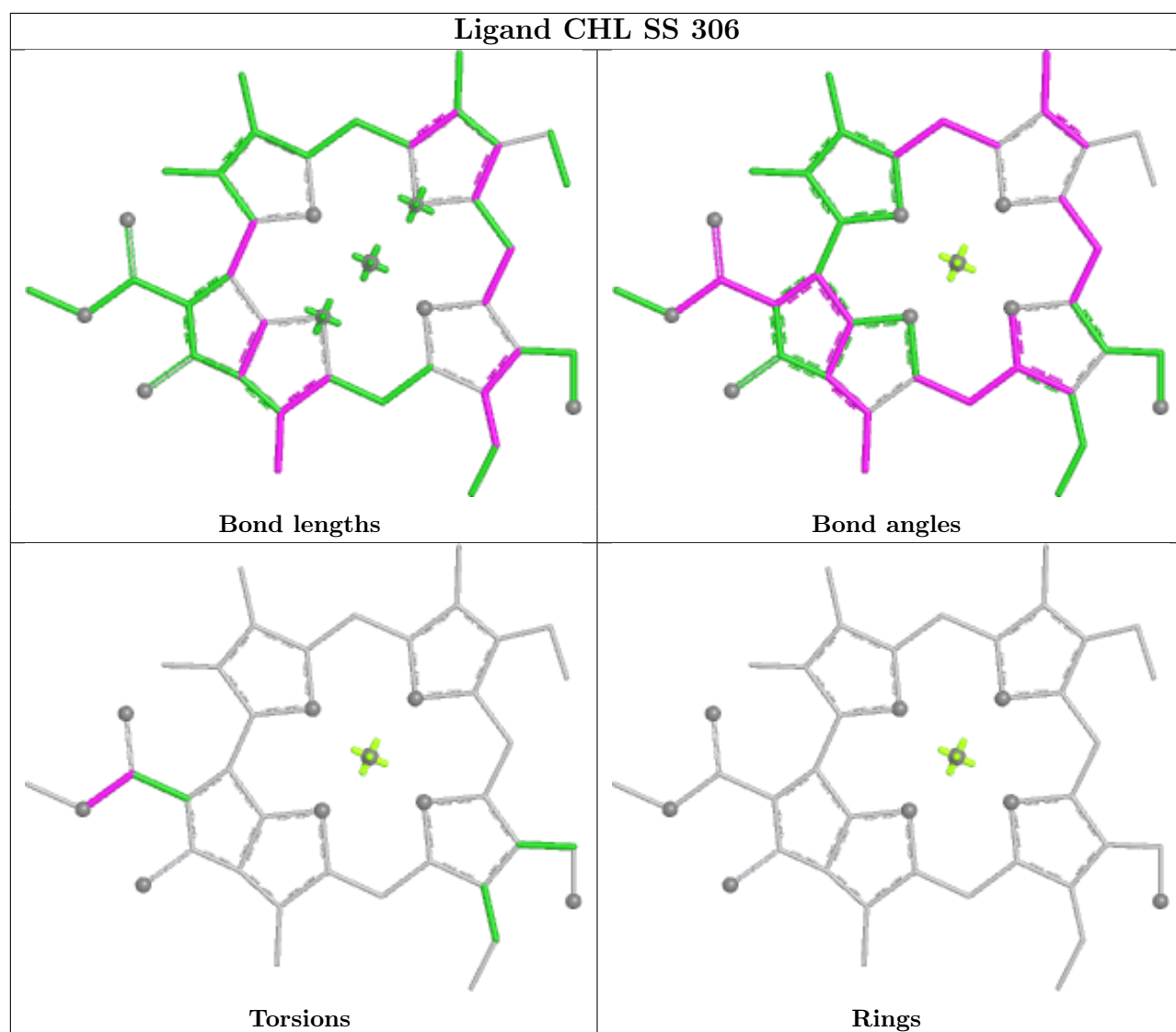
Ligand LUT Yy 616



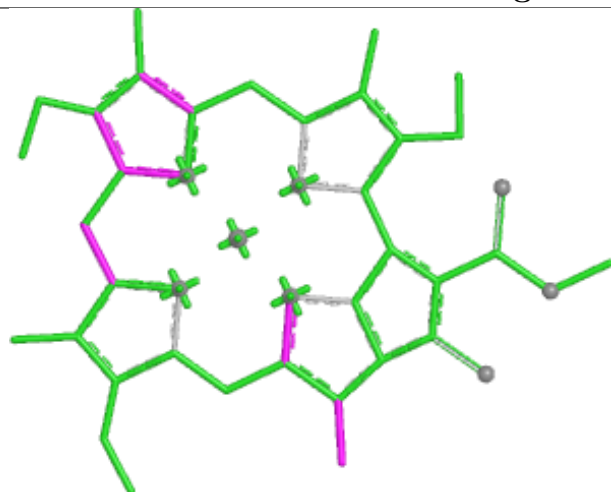


Ligand CLA Gg 313

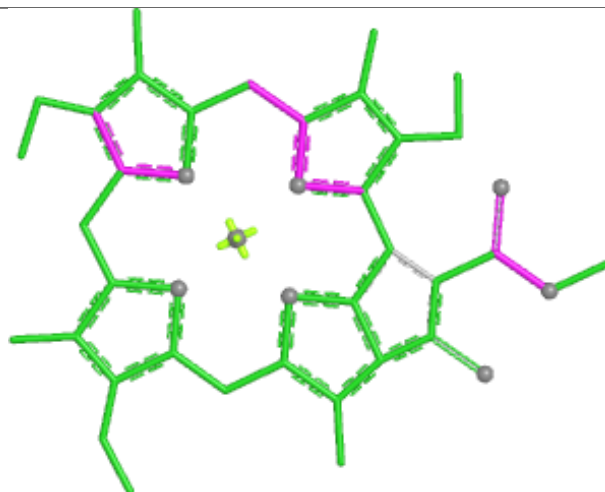




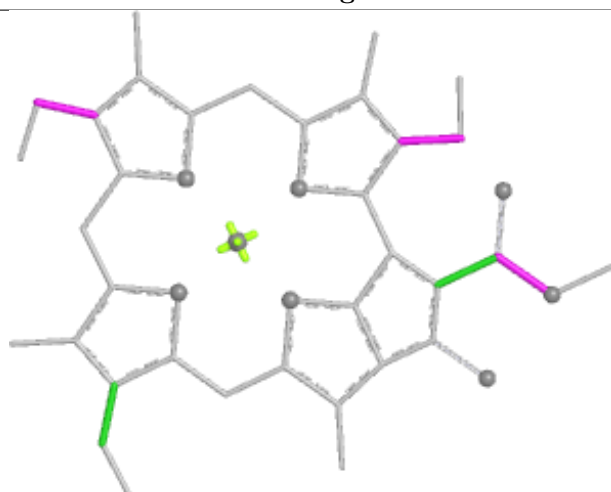
Ligand CLA Y 611



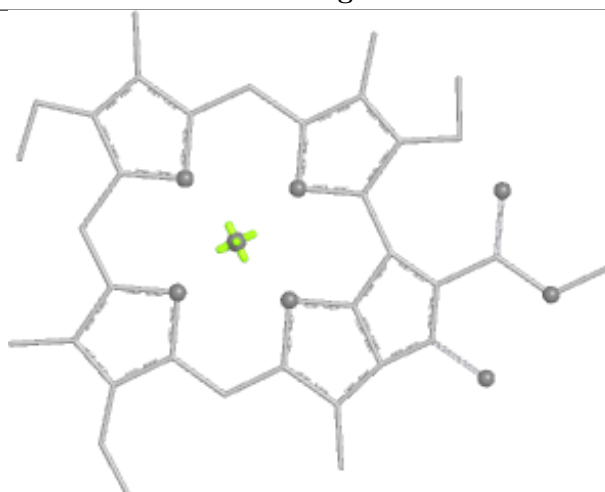
Bond lengths



Bond angles

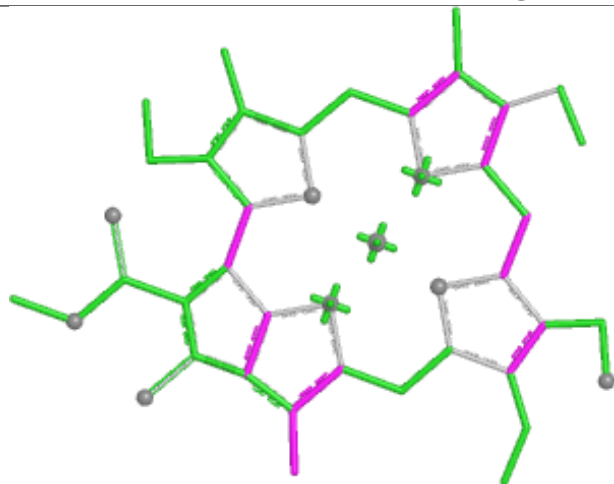


Torsions

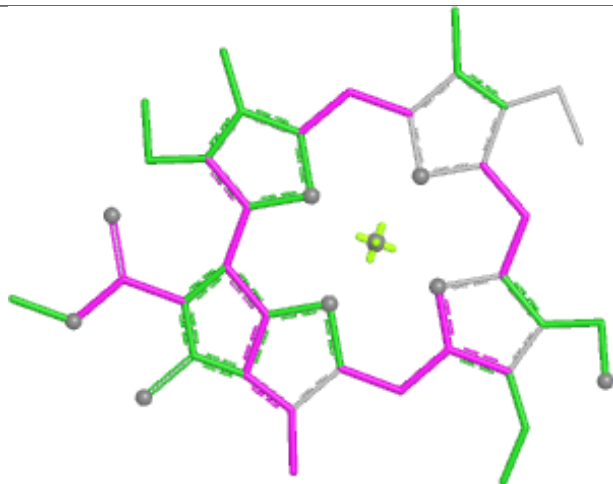


Rings

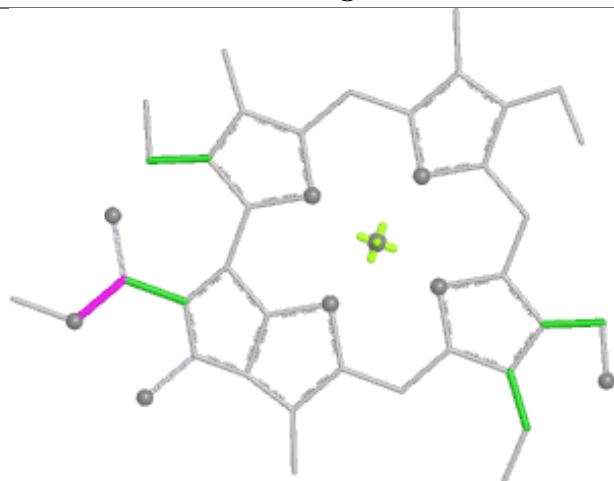
Ligand CHL G 605



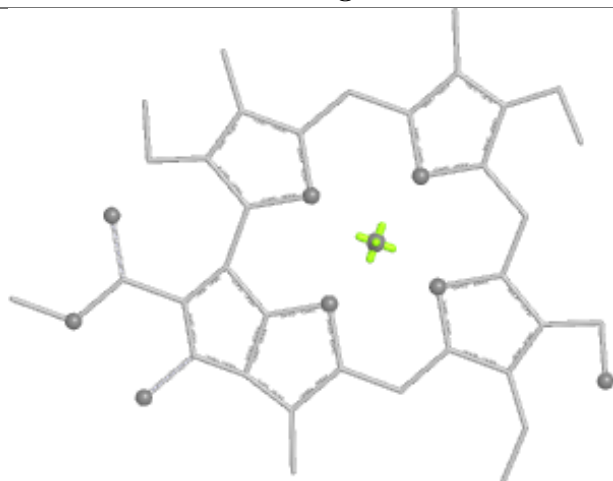
Bond lengths



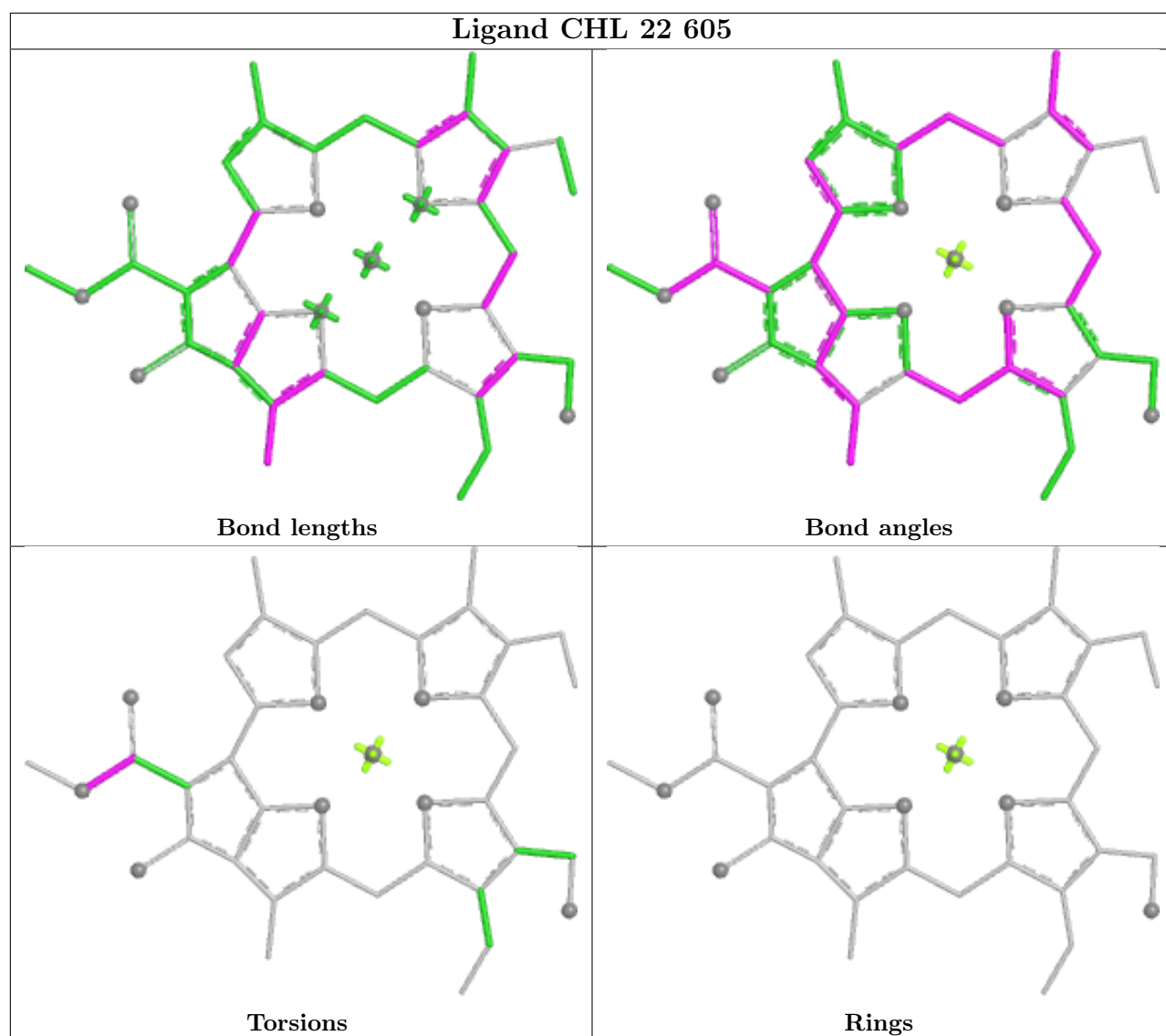
Bond angles

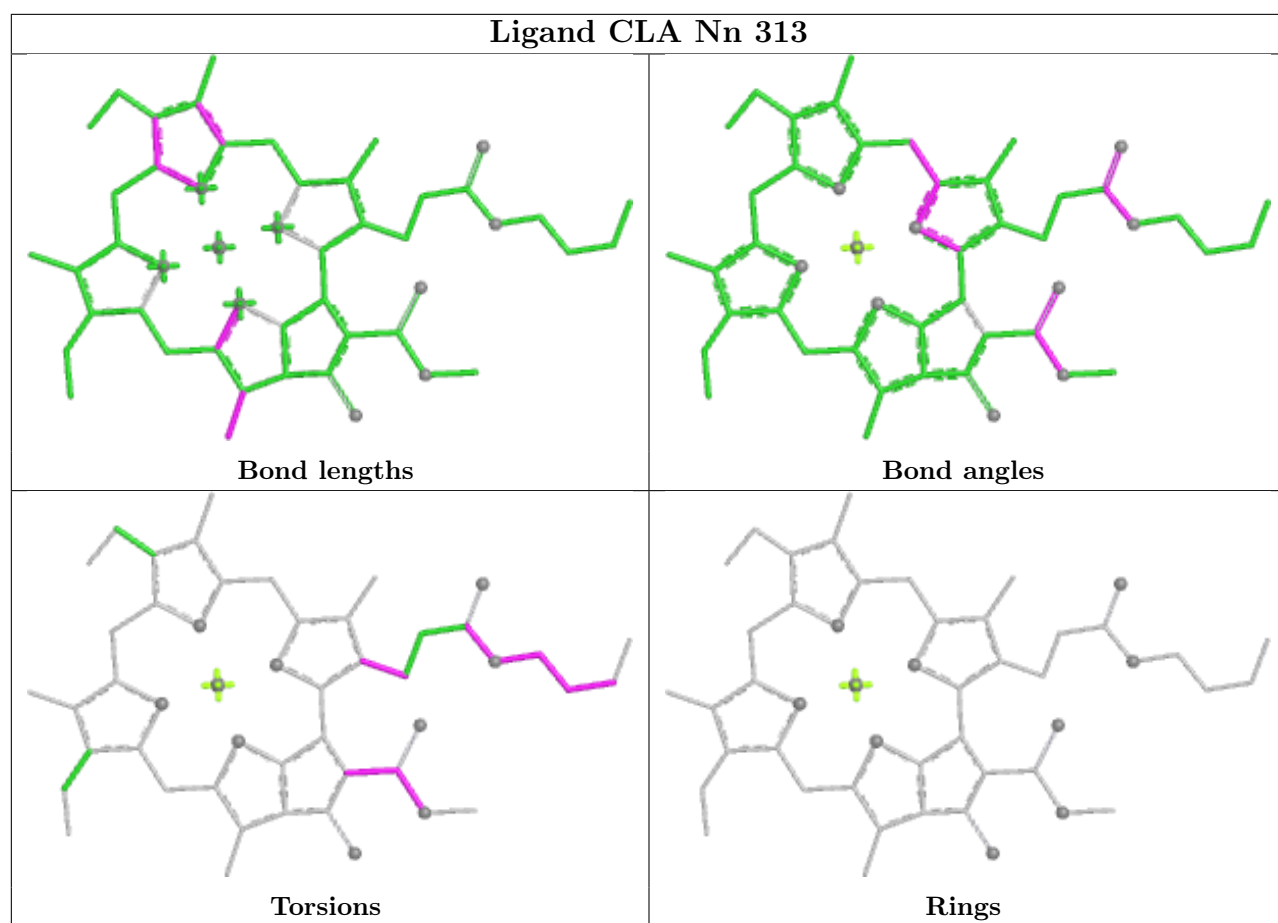


Torsions

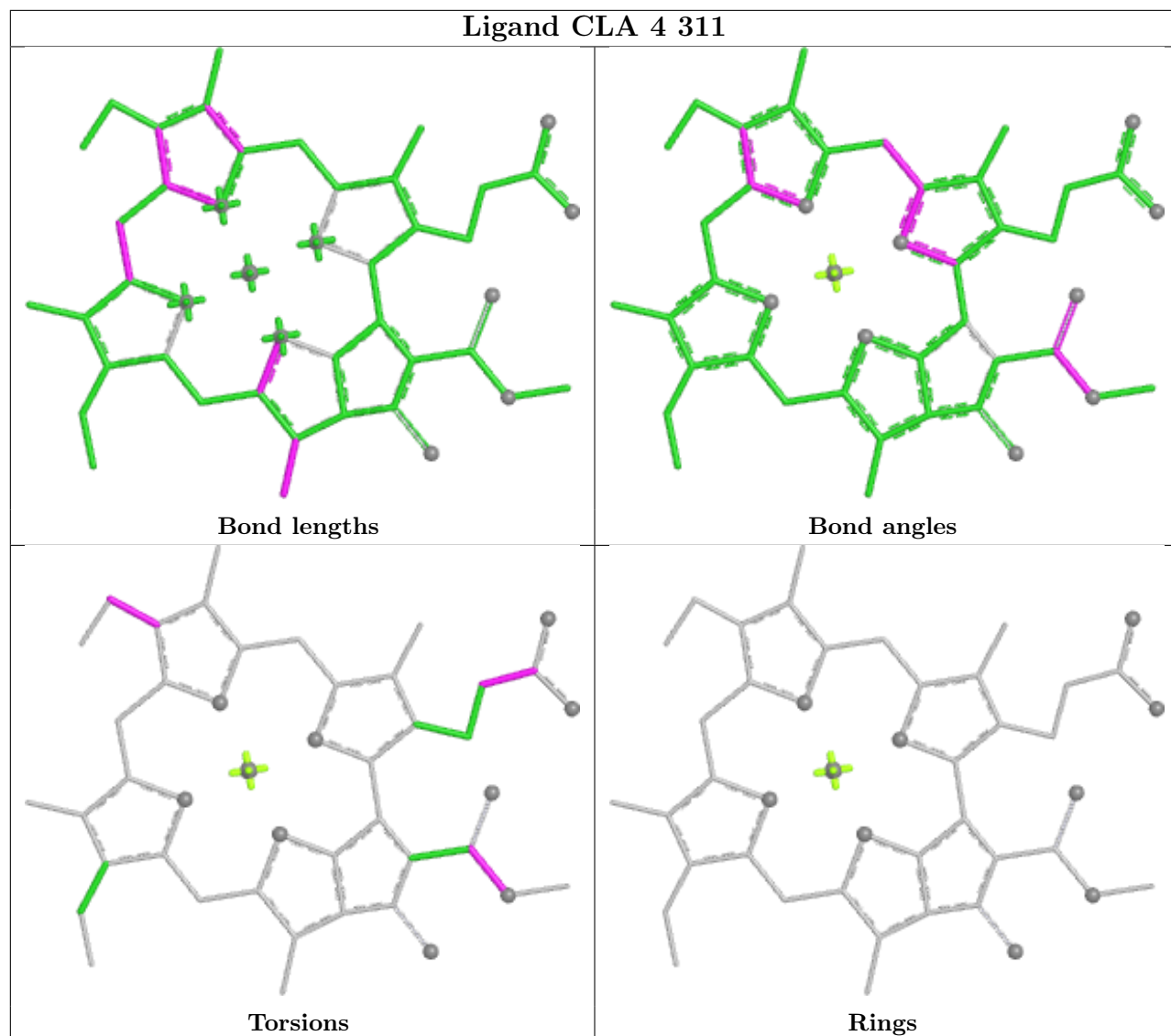


Rings

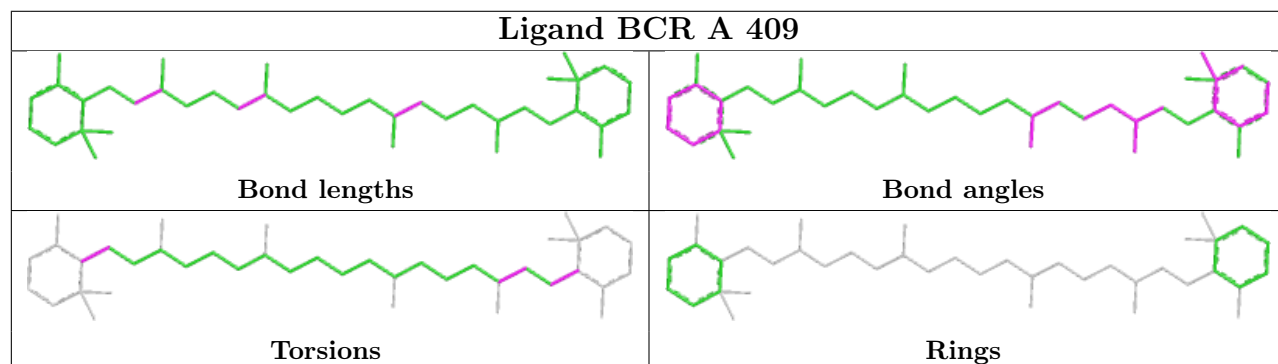


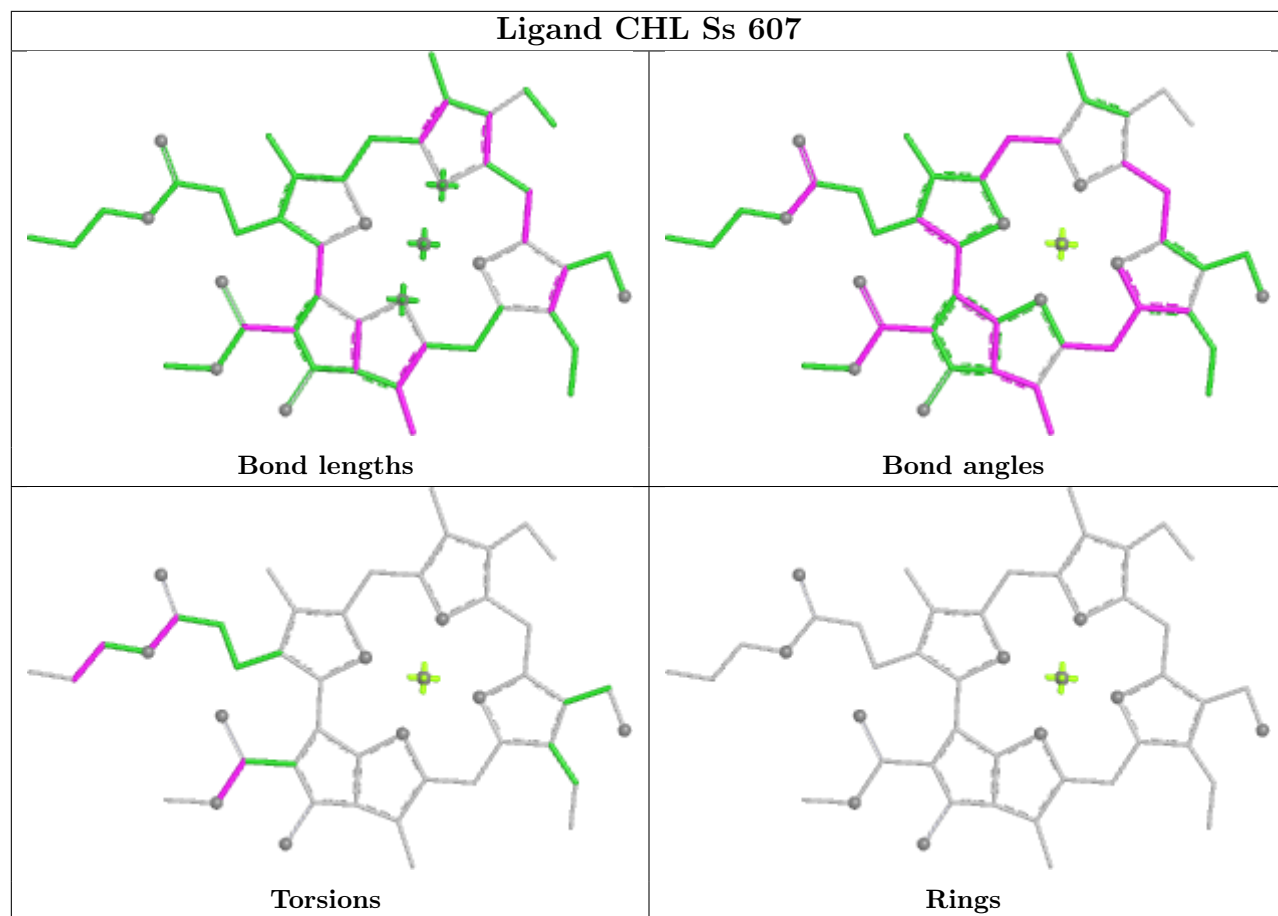


Ligand CLA 4 311

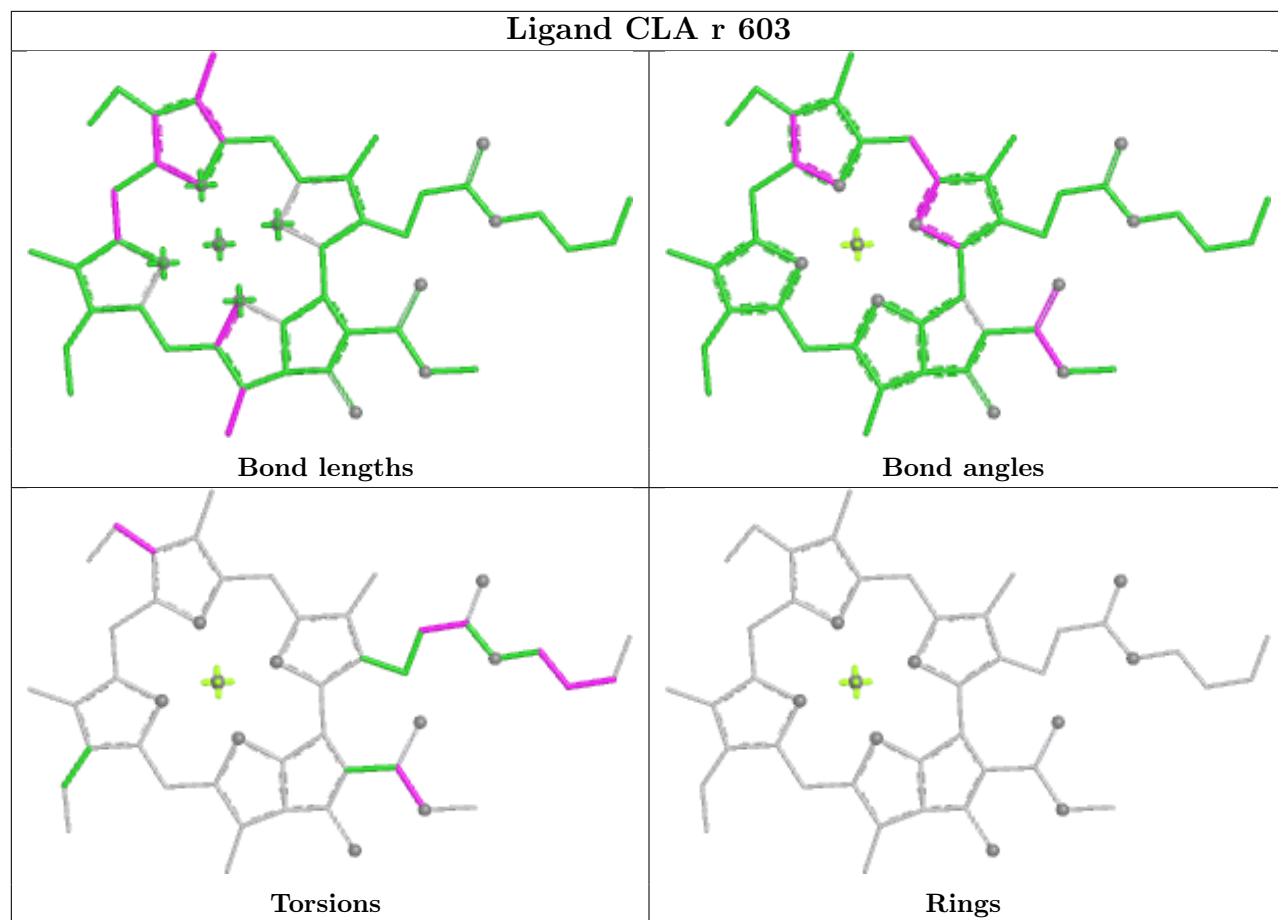


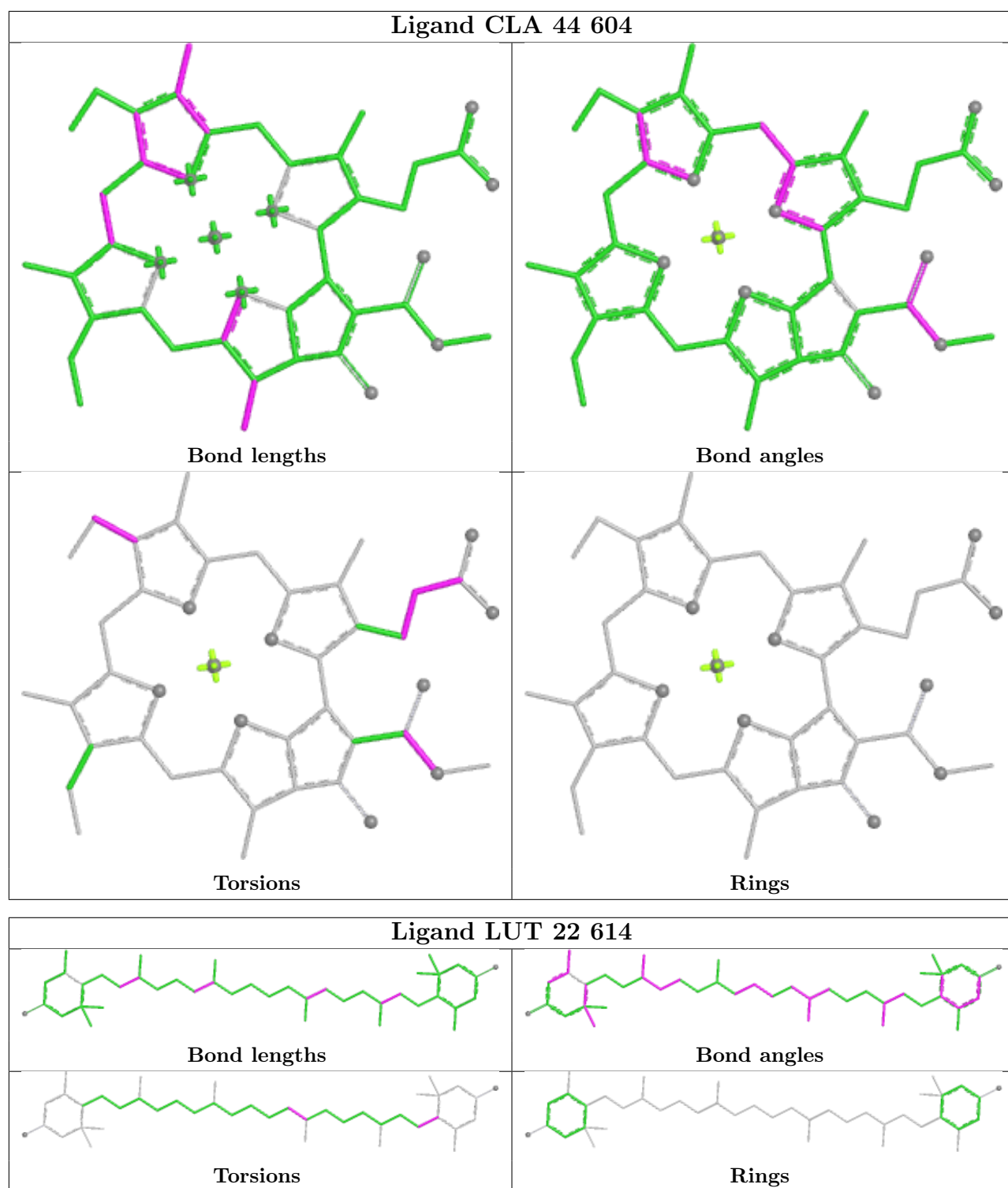
Ligand BCR A 409

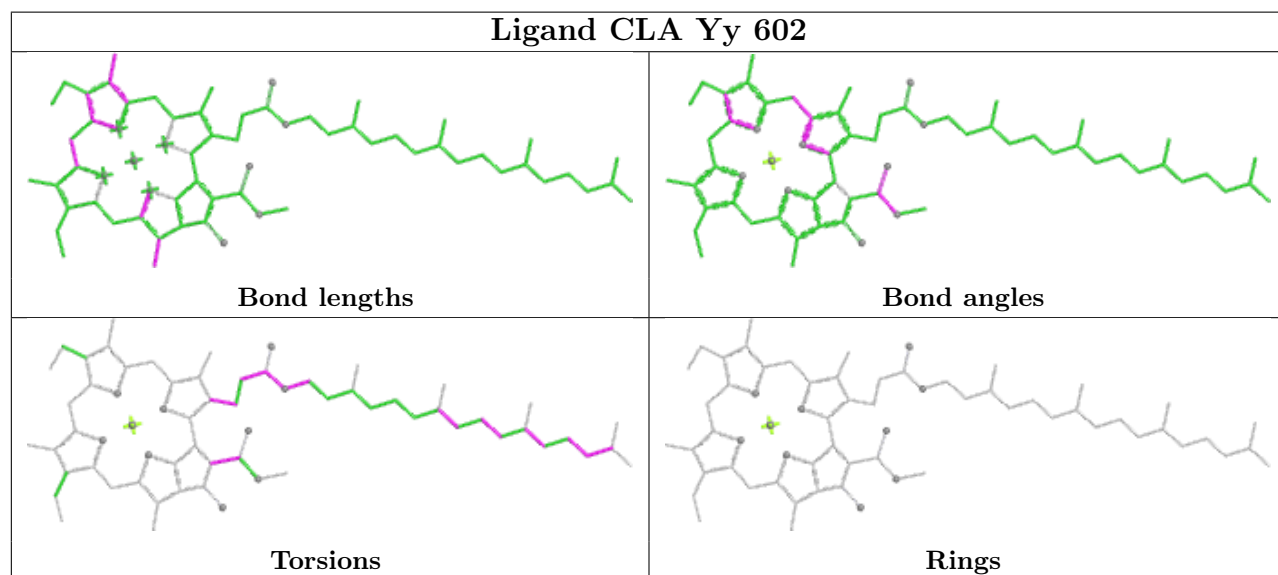
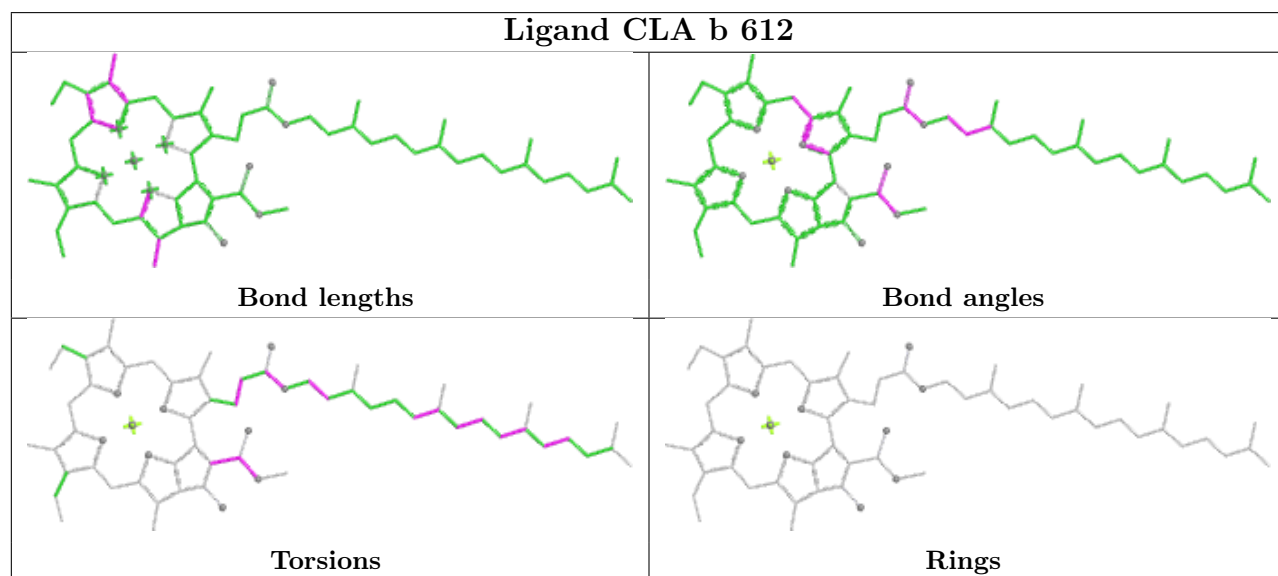
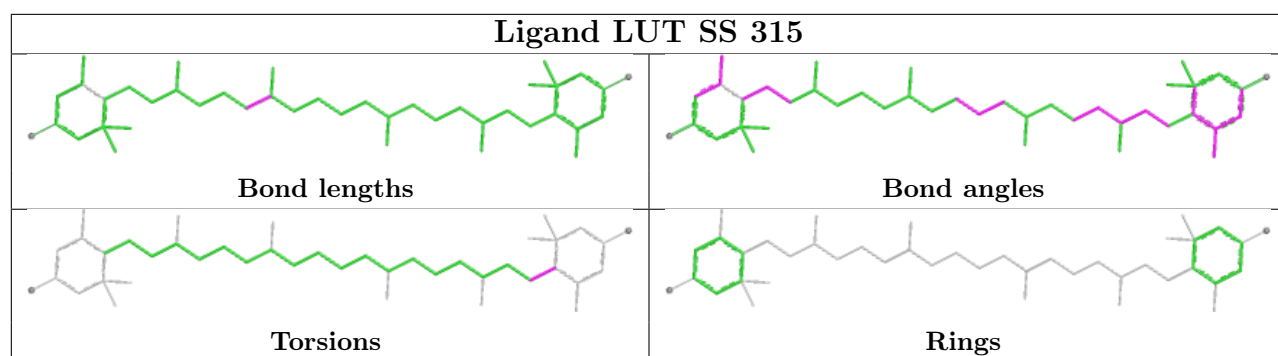


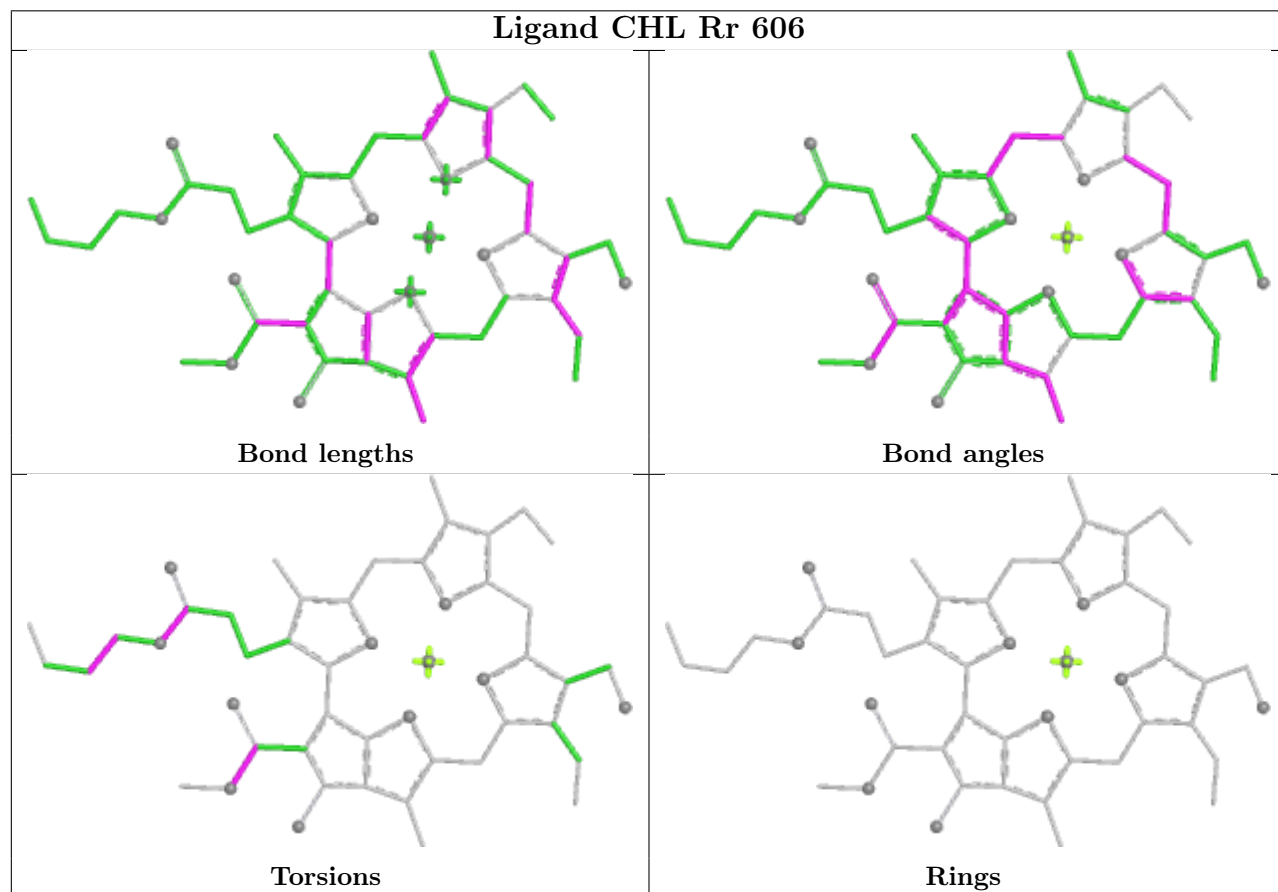
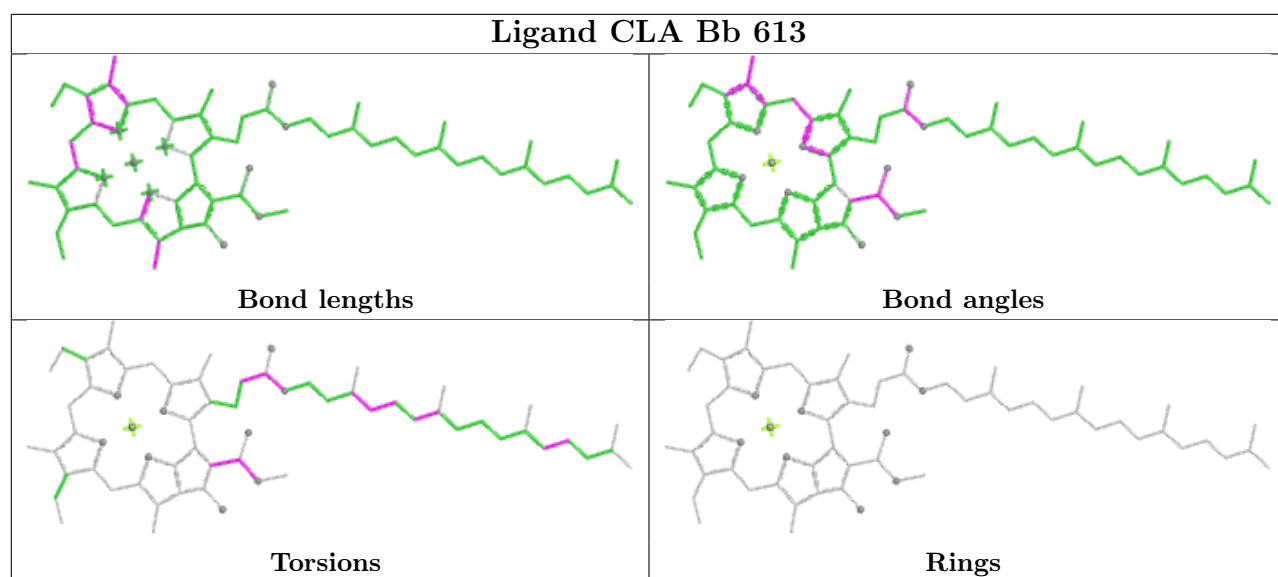


Ligand CLA r 603

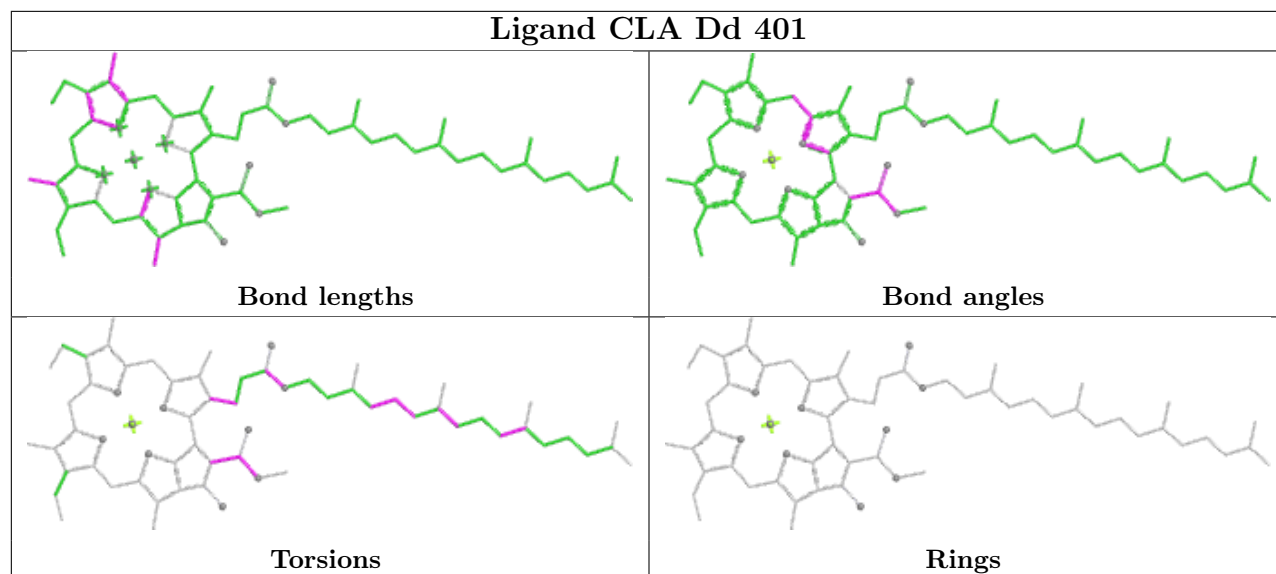




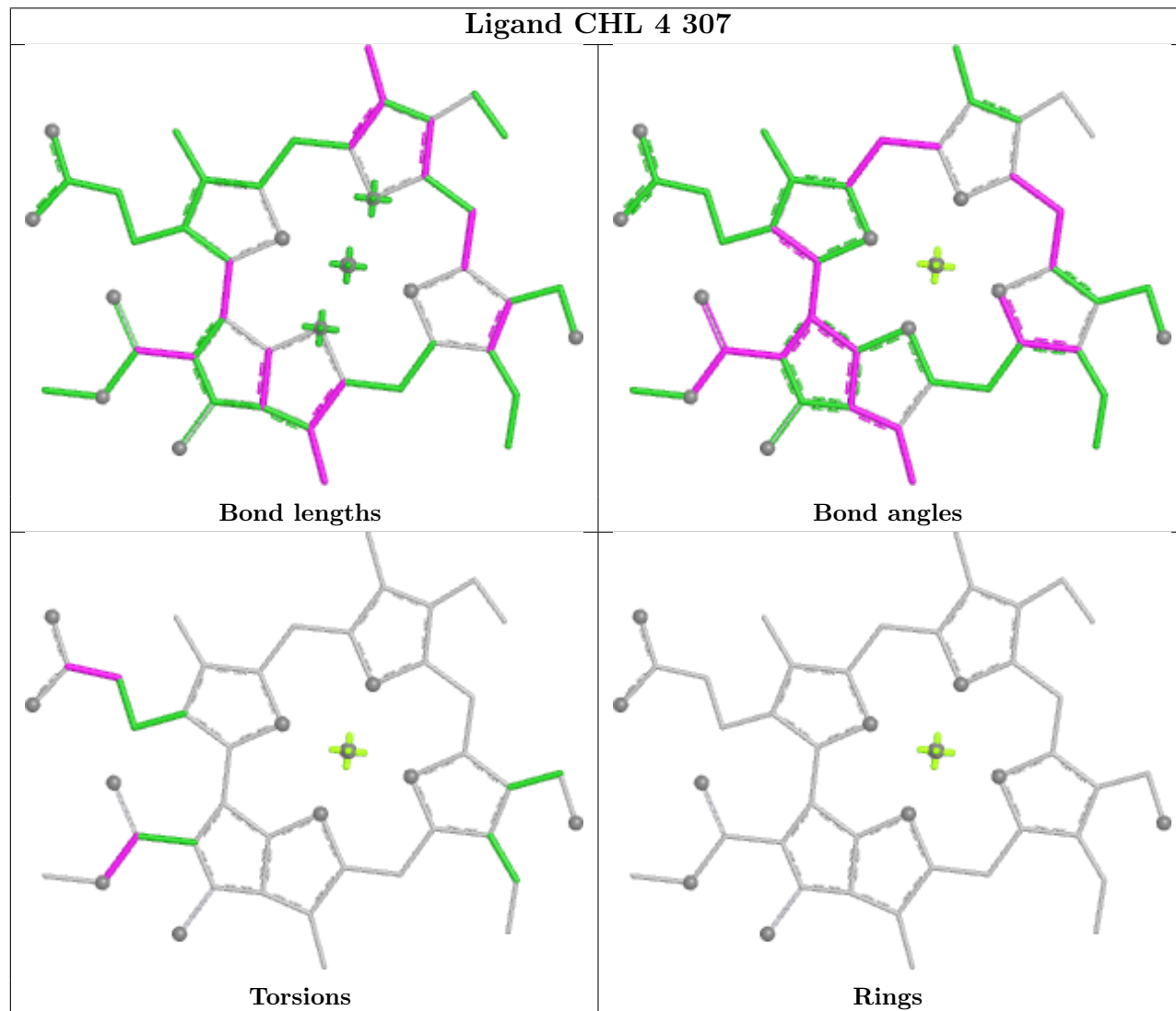


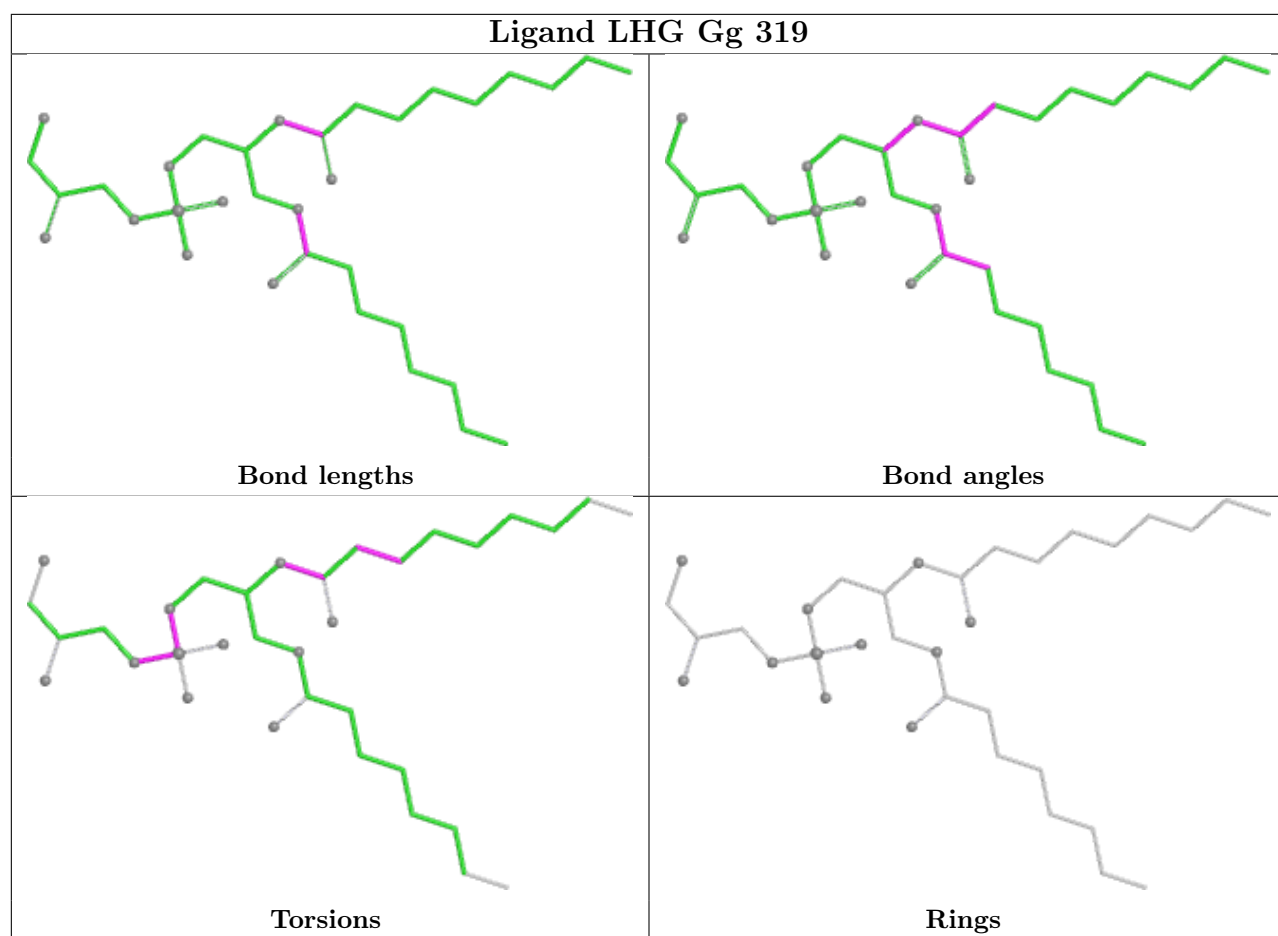


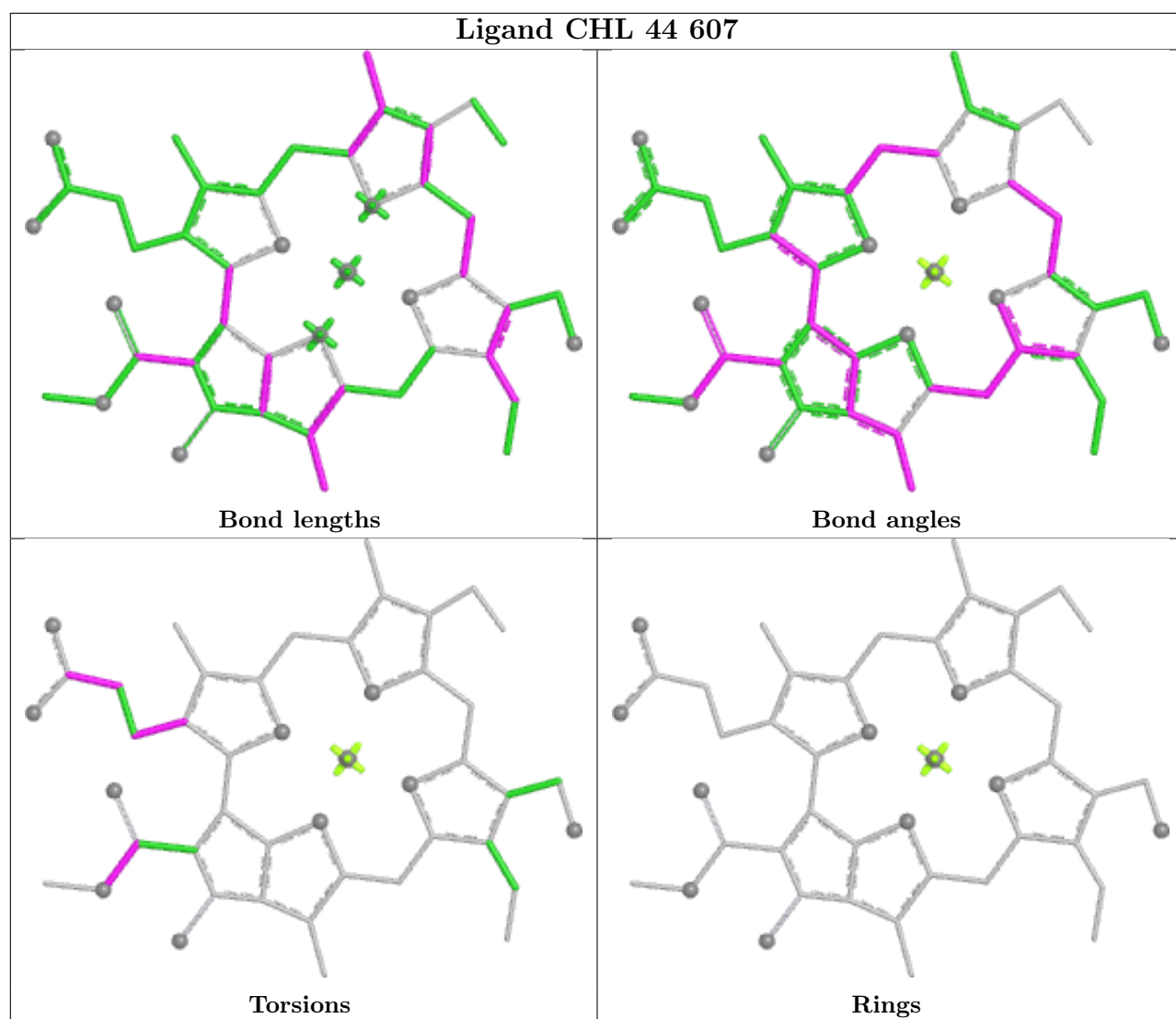
Ligand CLA Dd 401

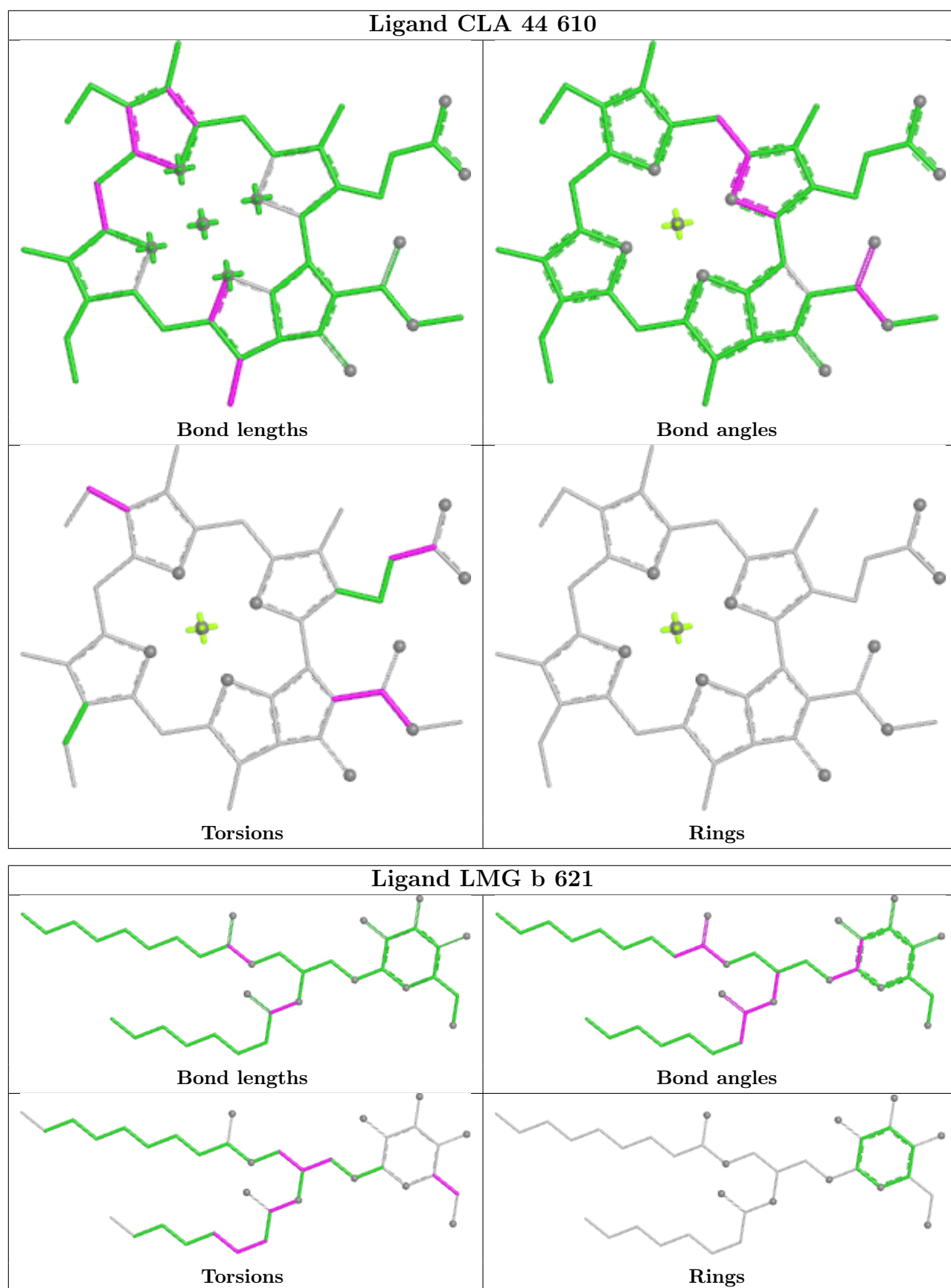


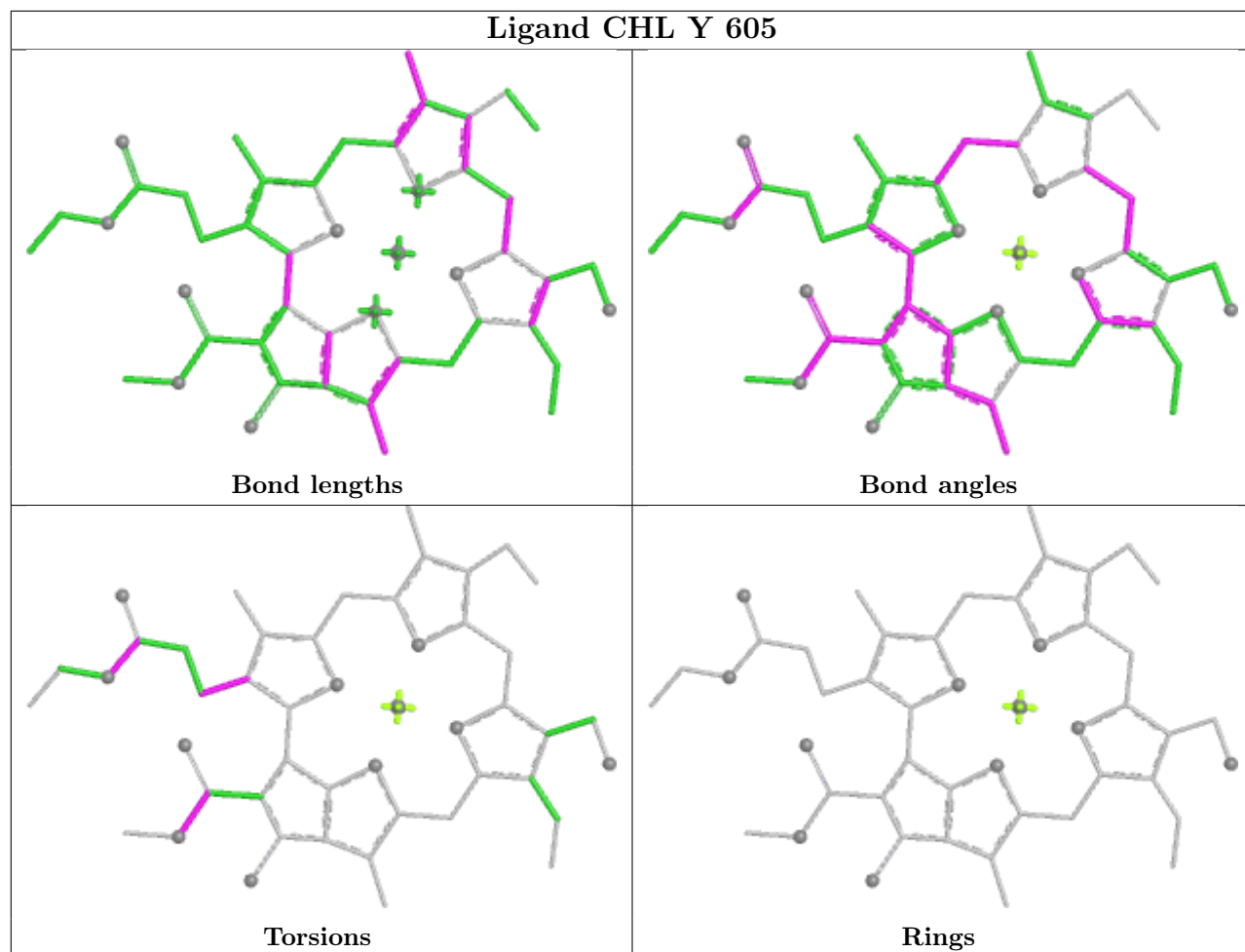
Ligand CHL 4 307



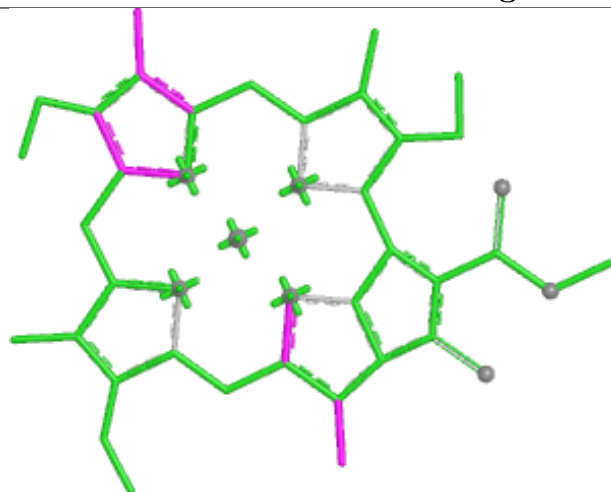




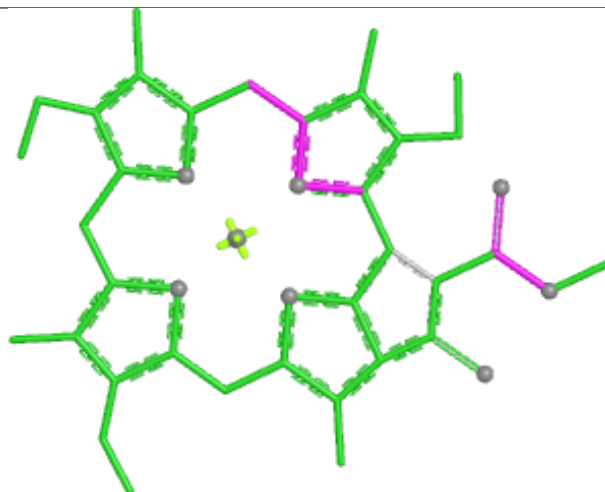




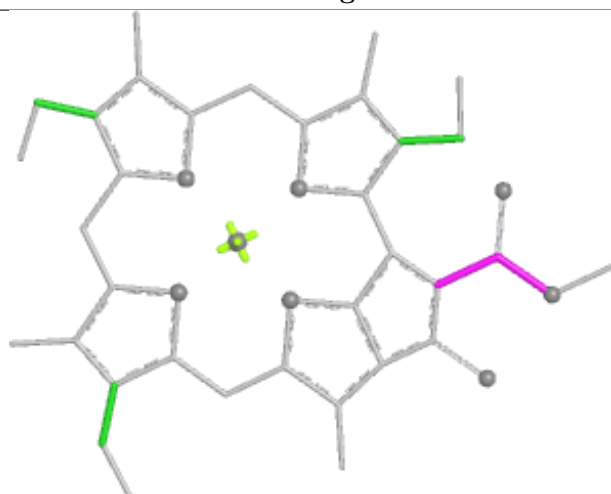
Ligand CLA NN 603



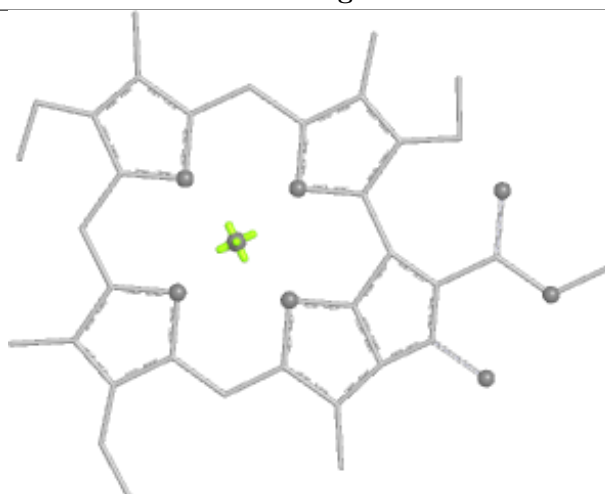
Bond lengths



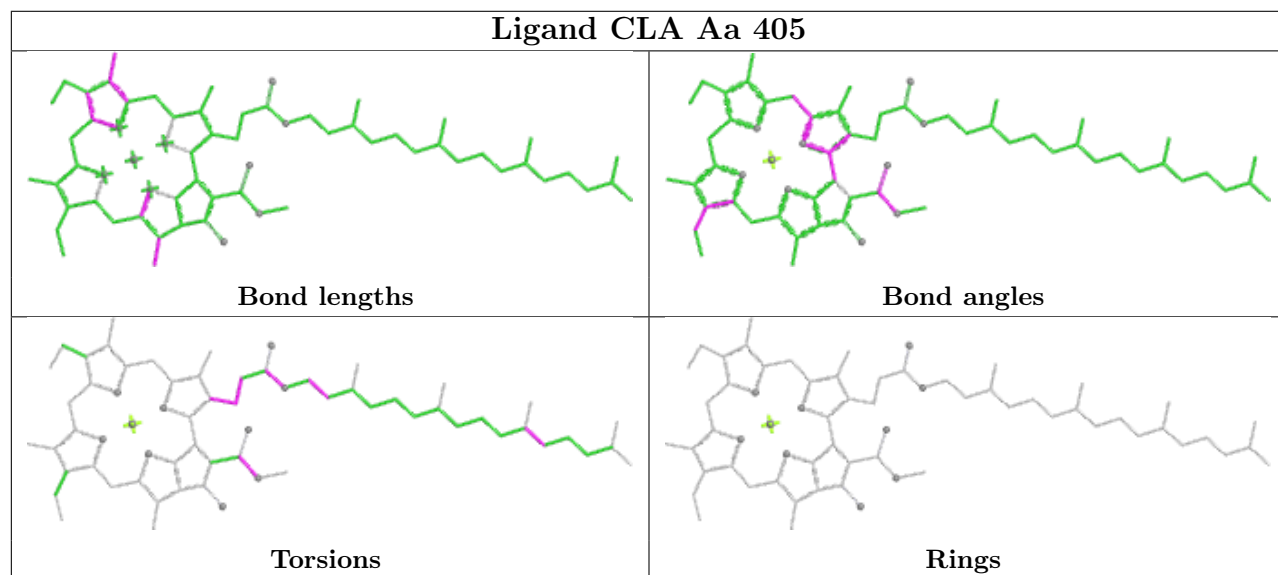
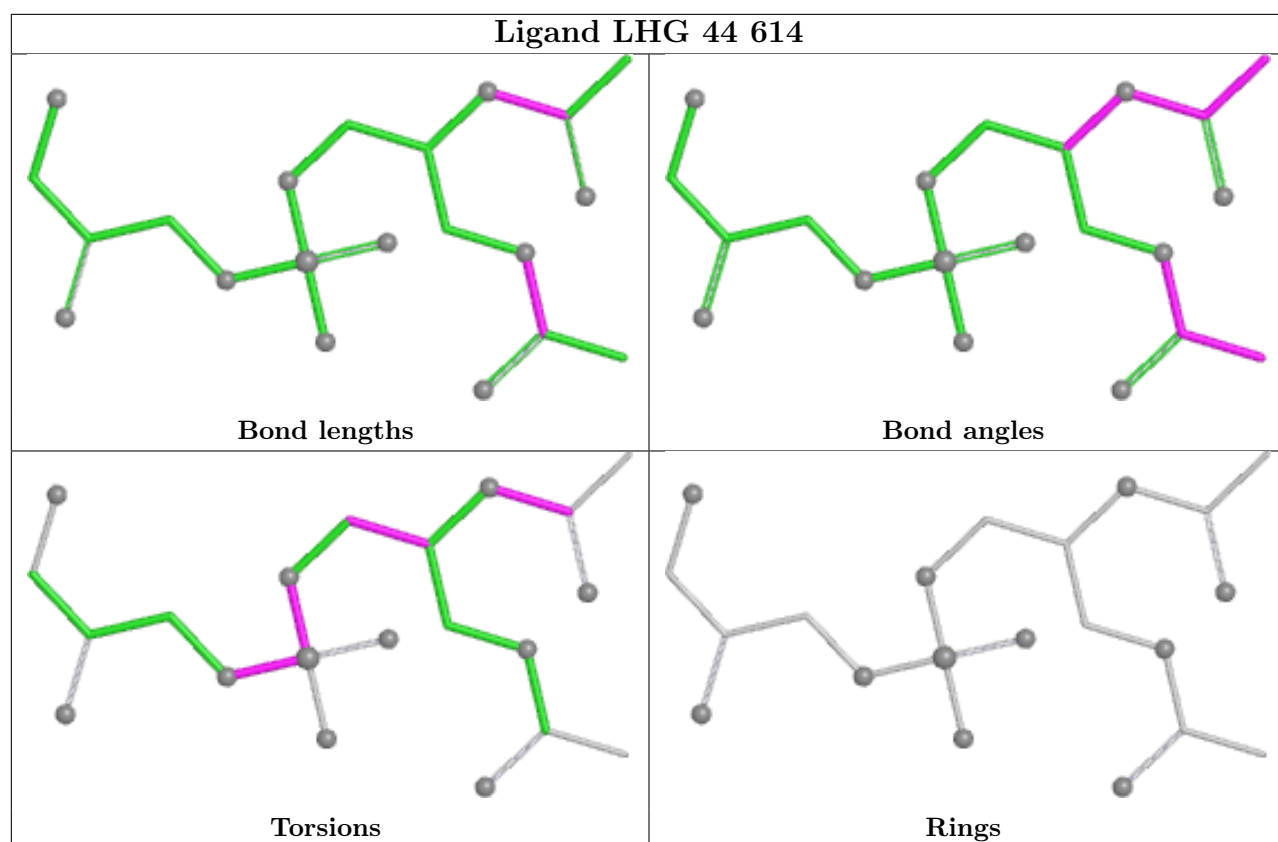
Bond angles

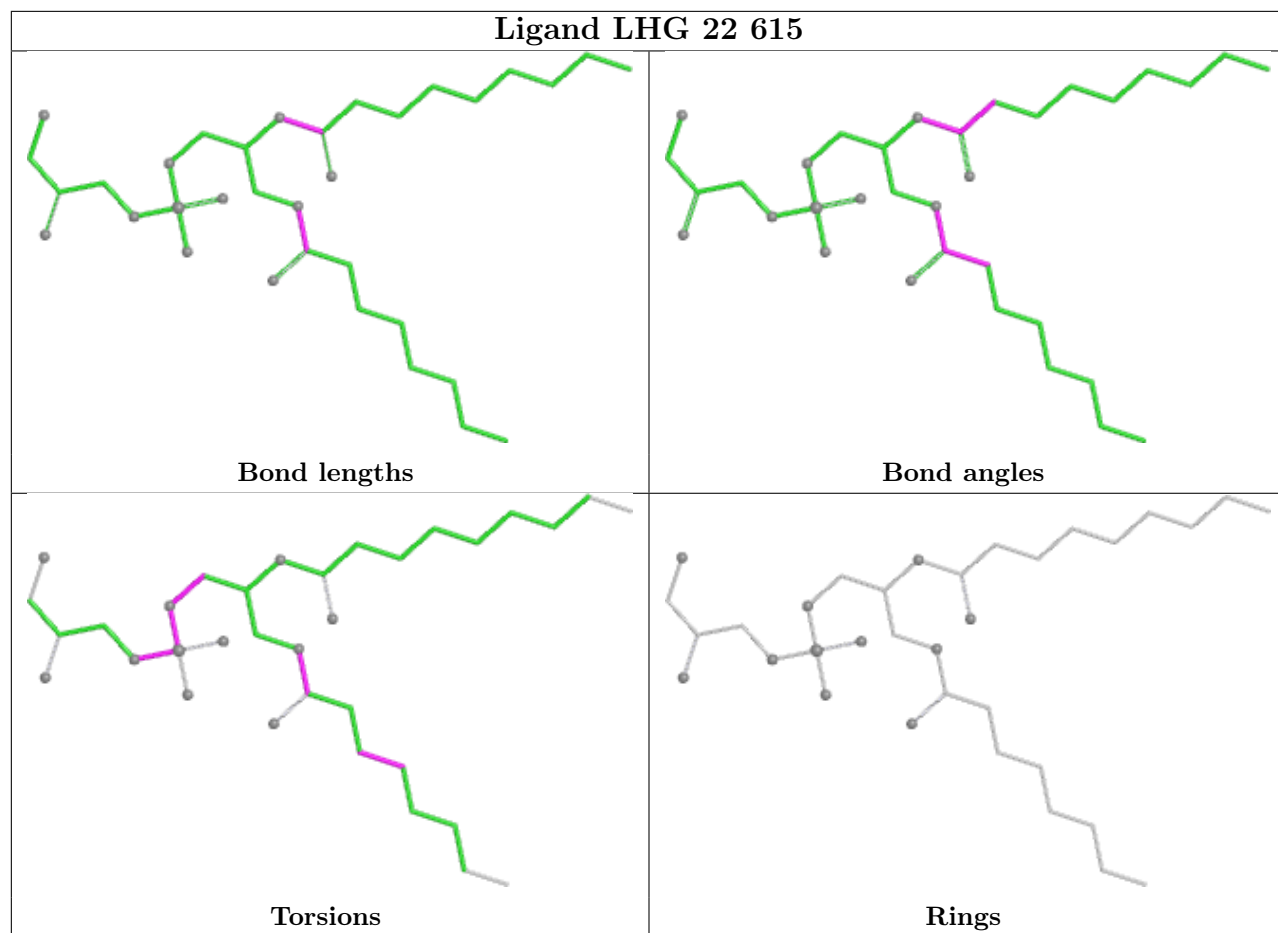


Torsions

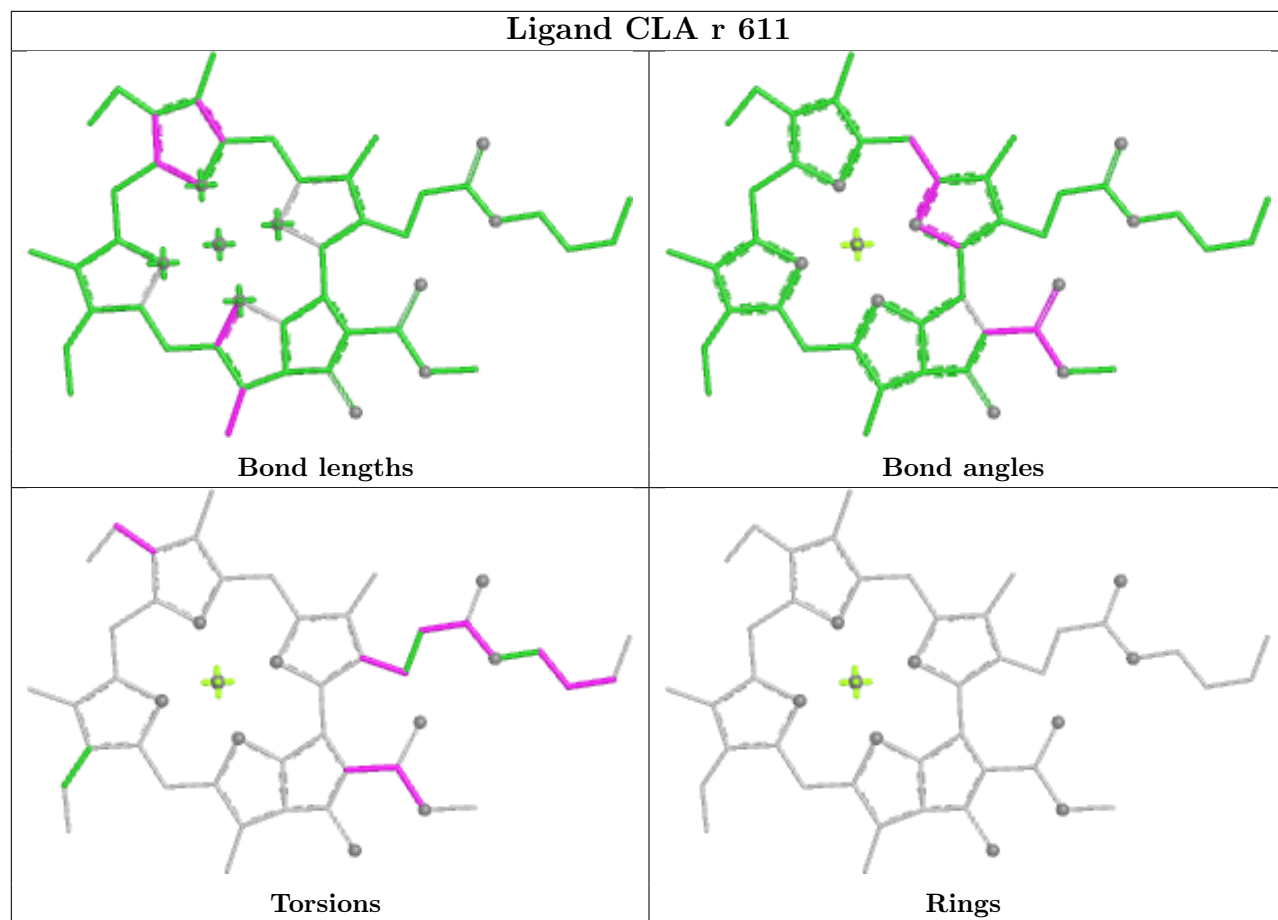


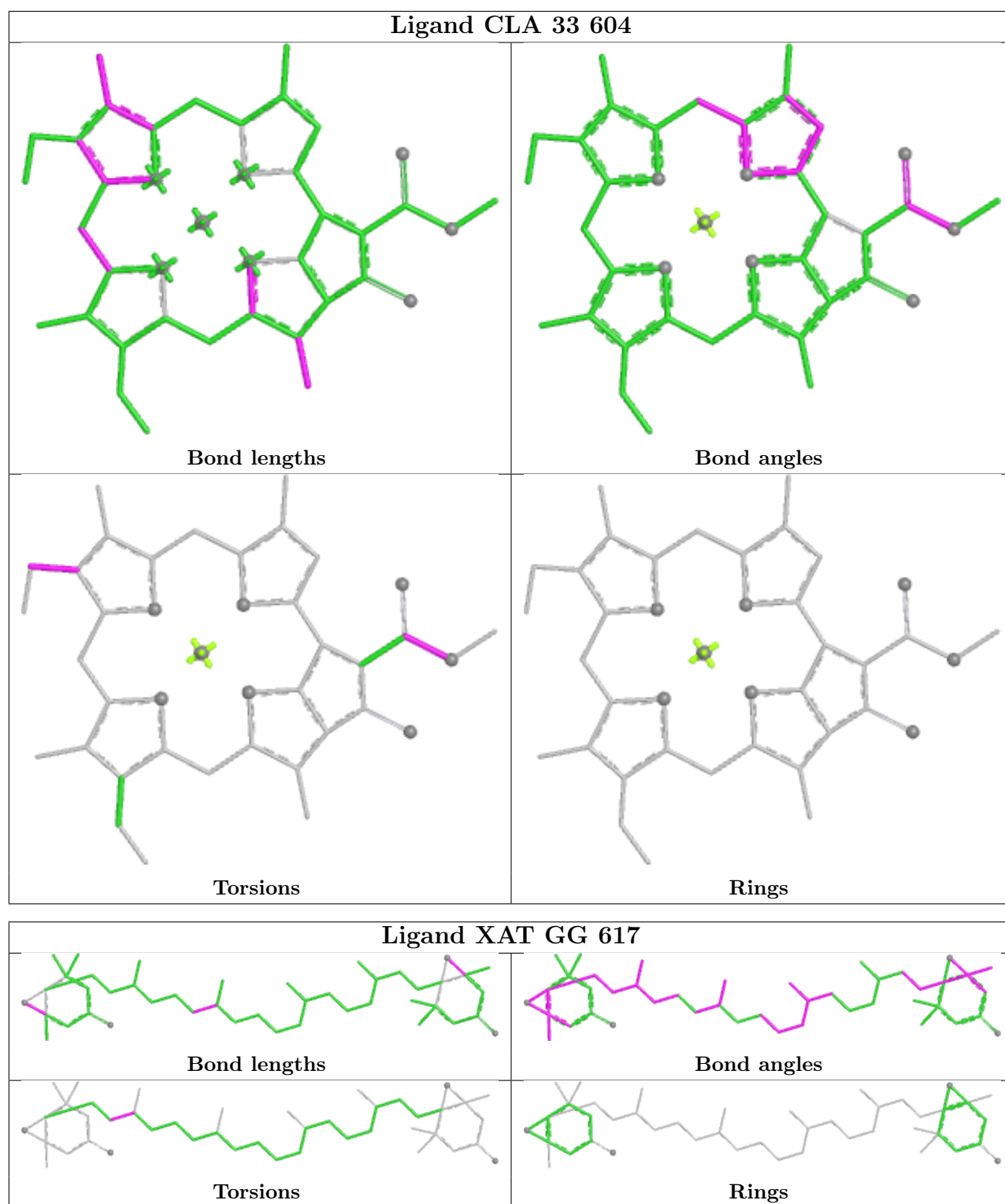
Rings

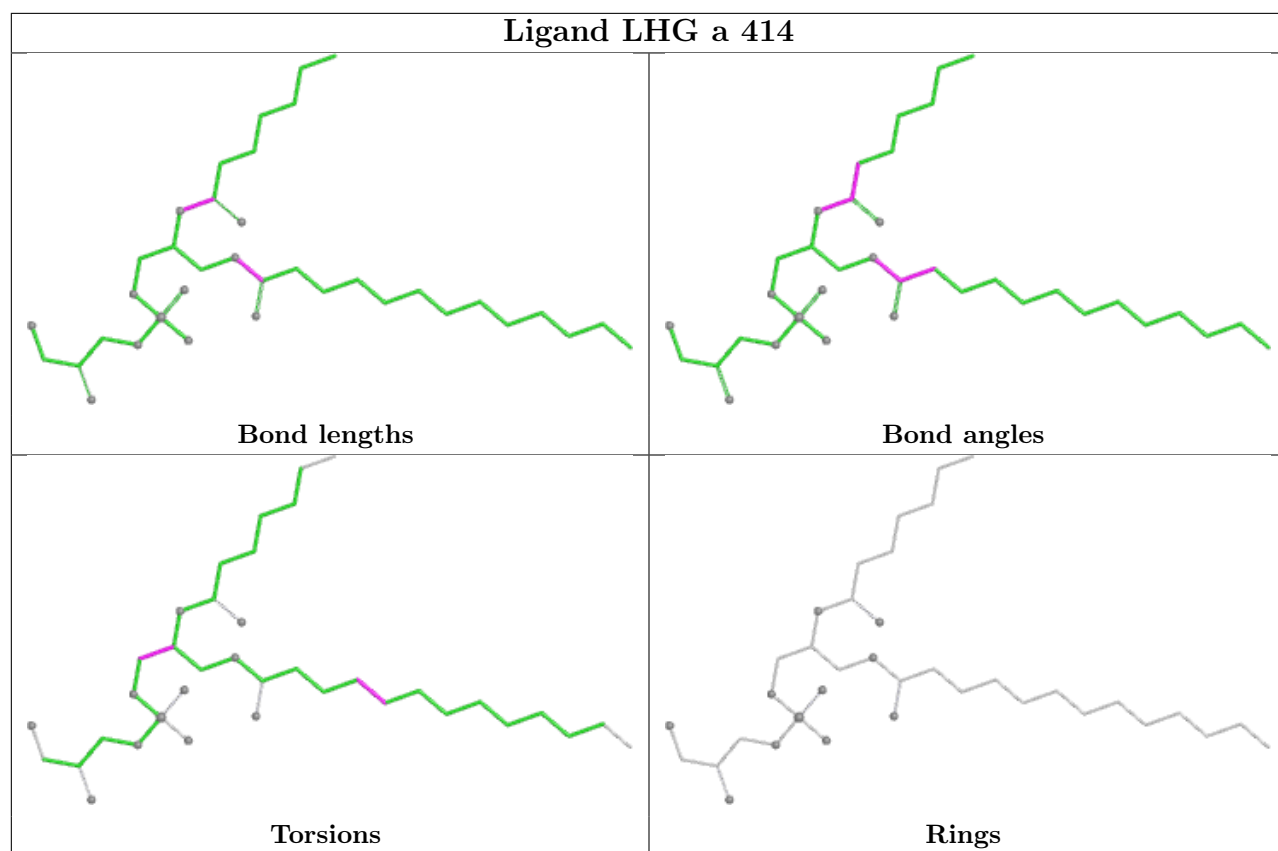
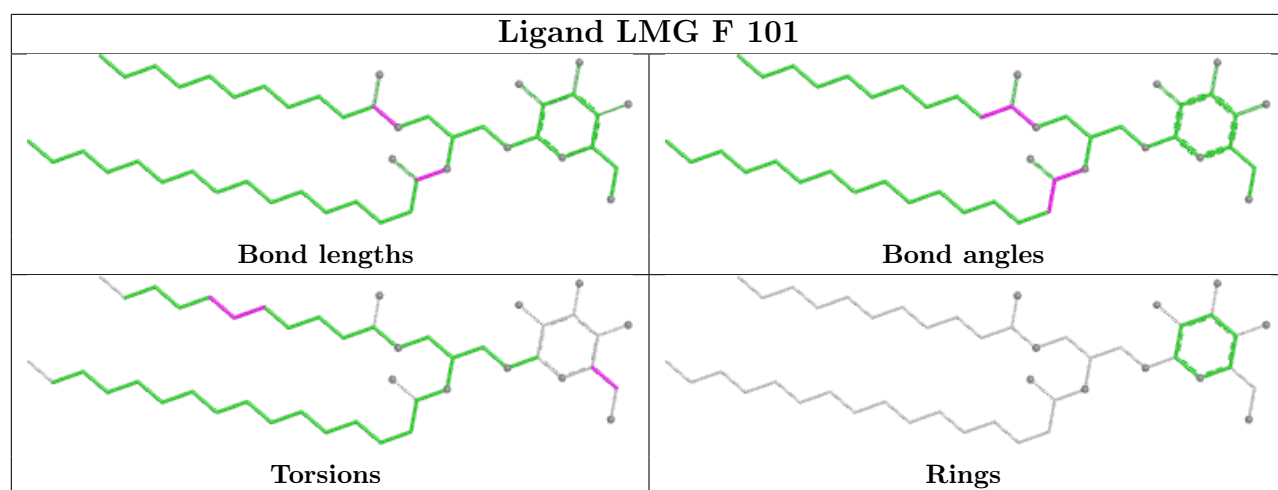




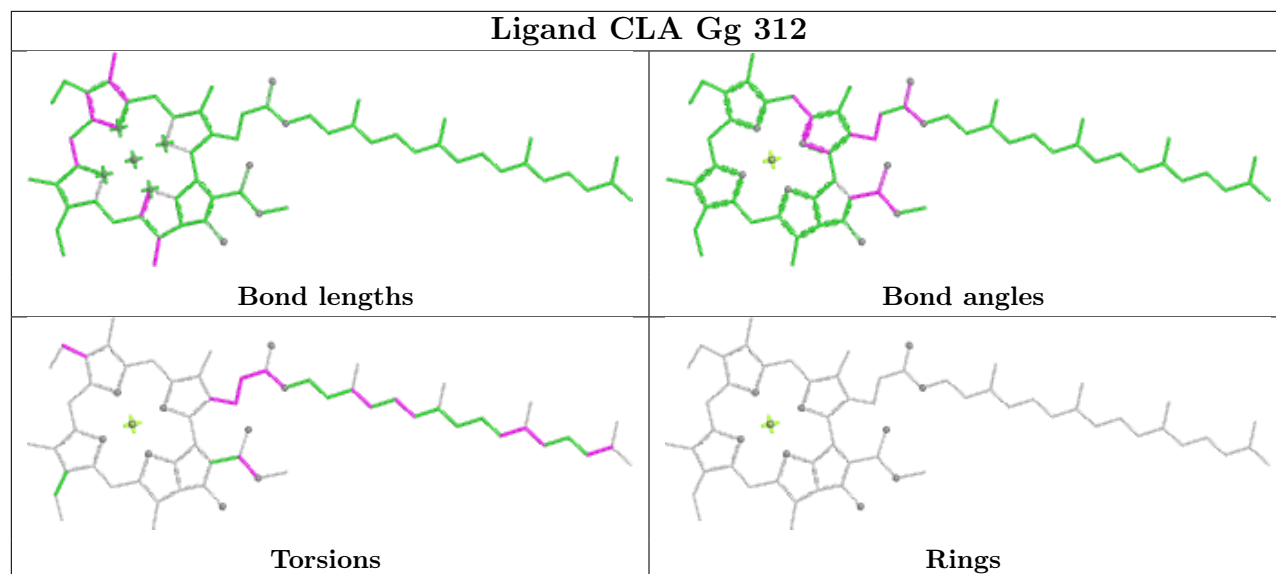
Ligand CLA r 611



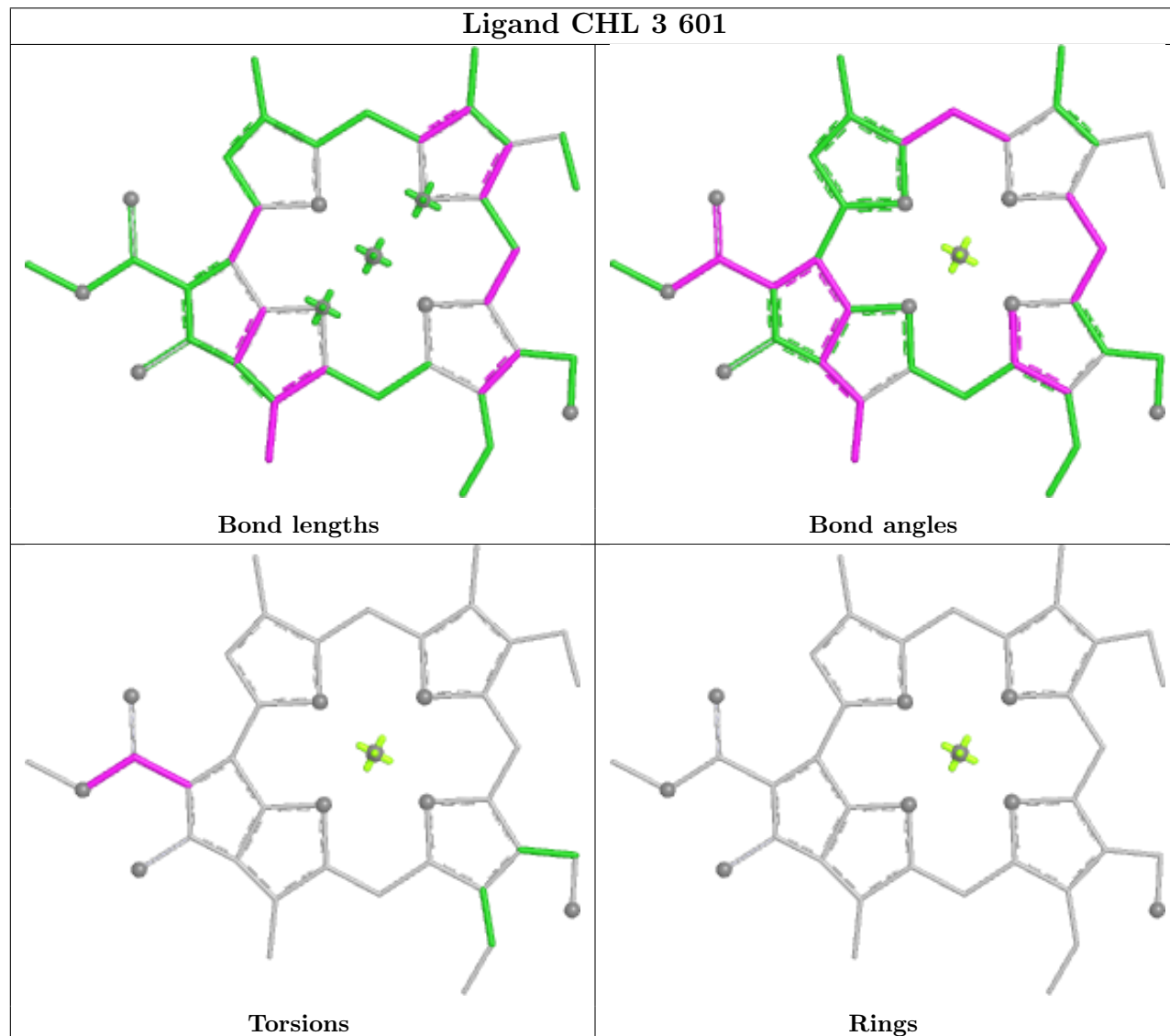


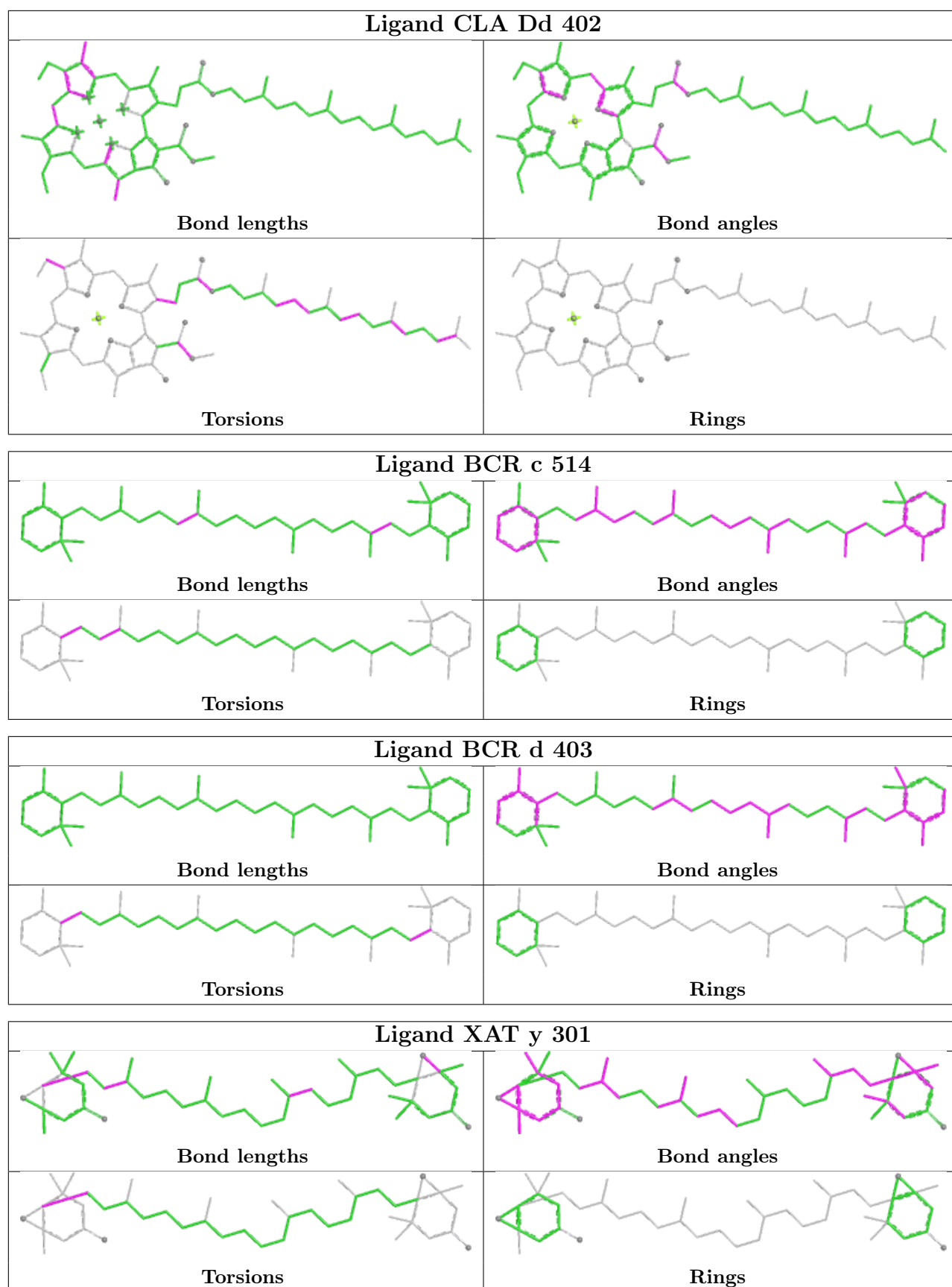


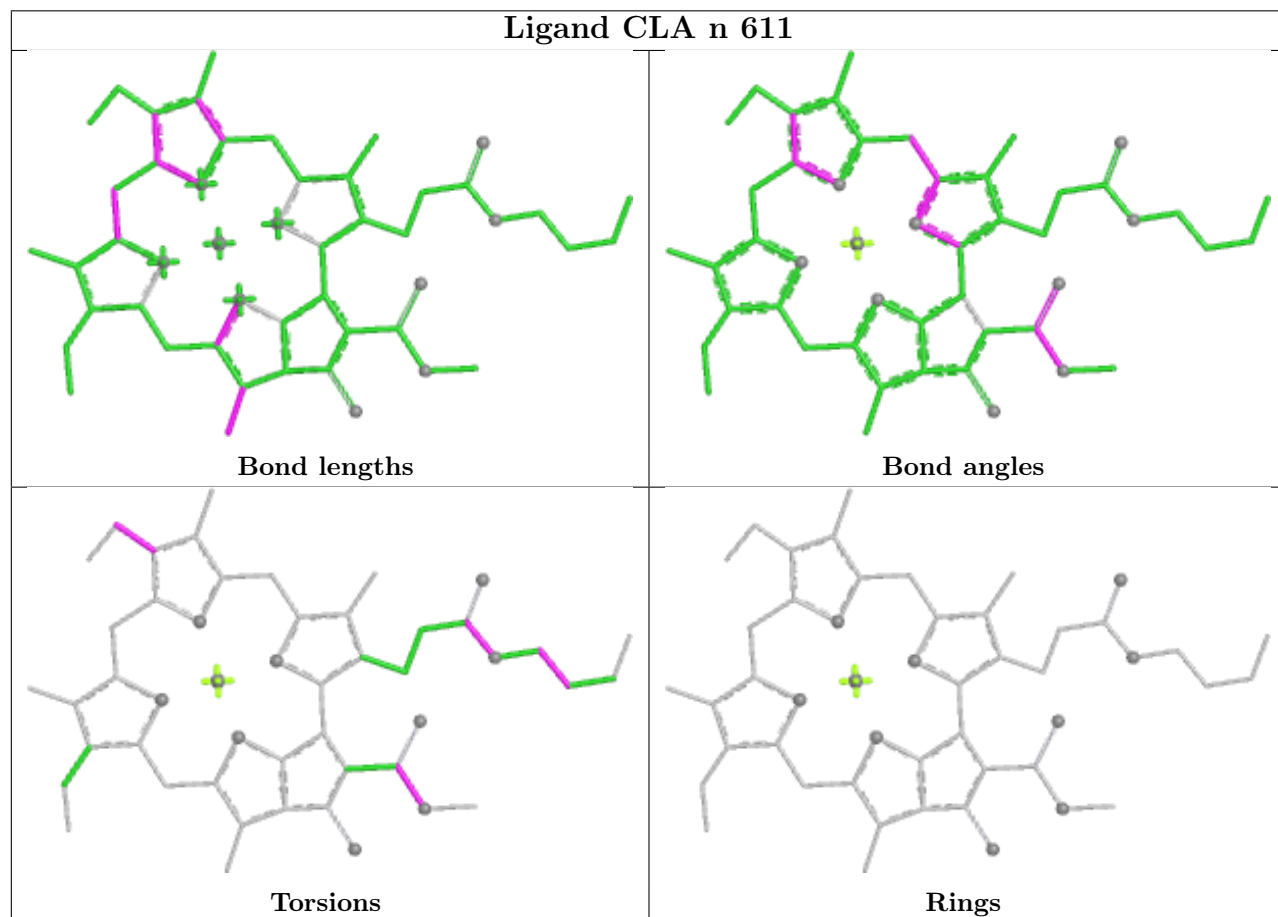
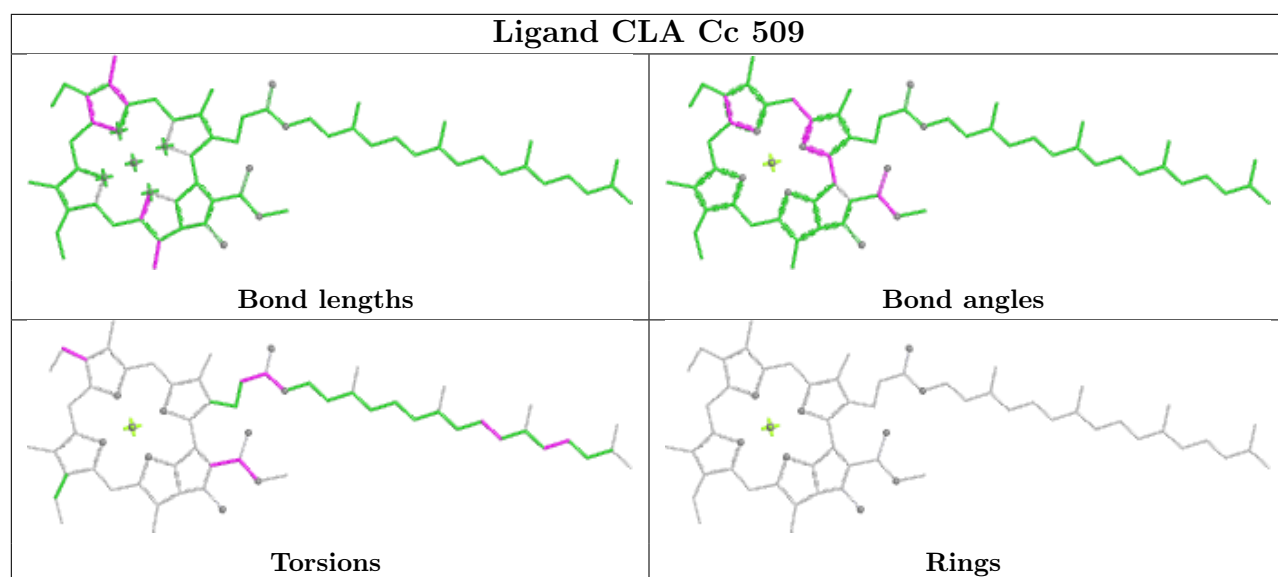
Ligand CLA Gg 312

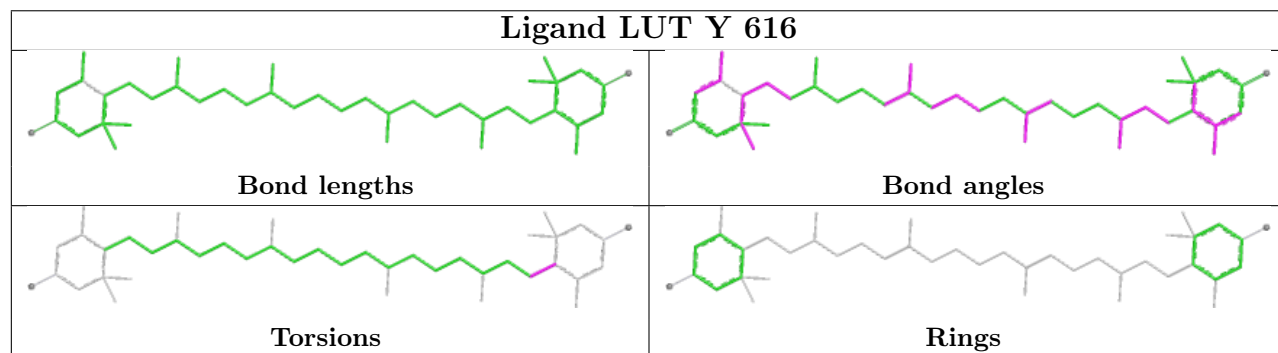
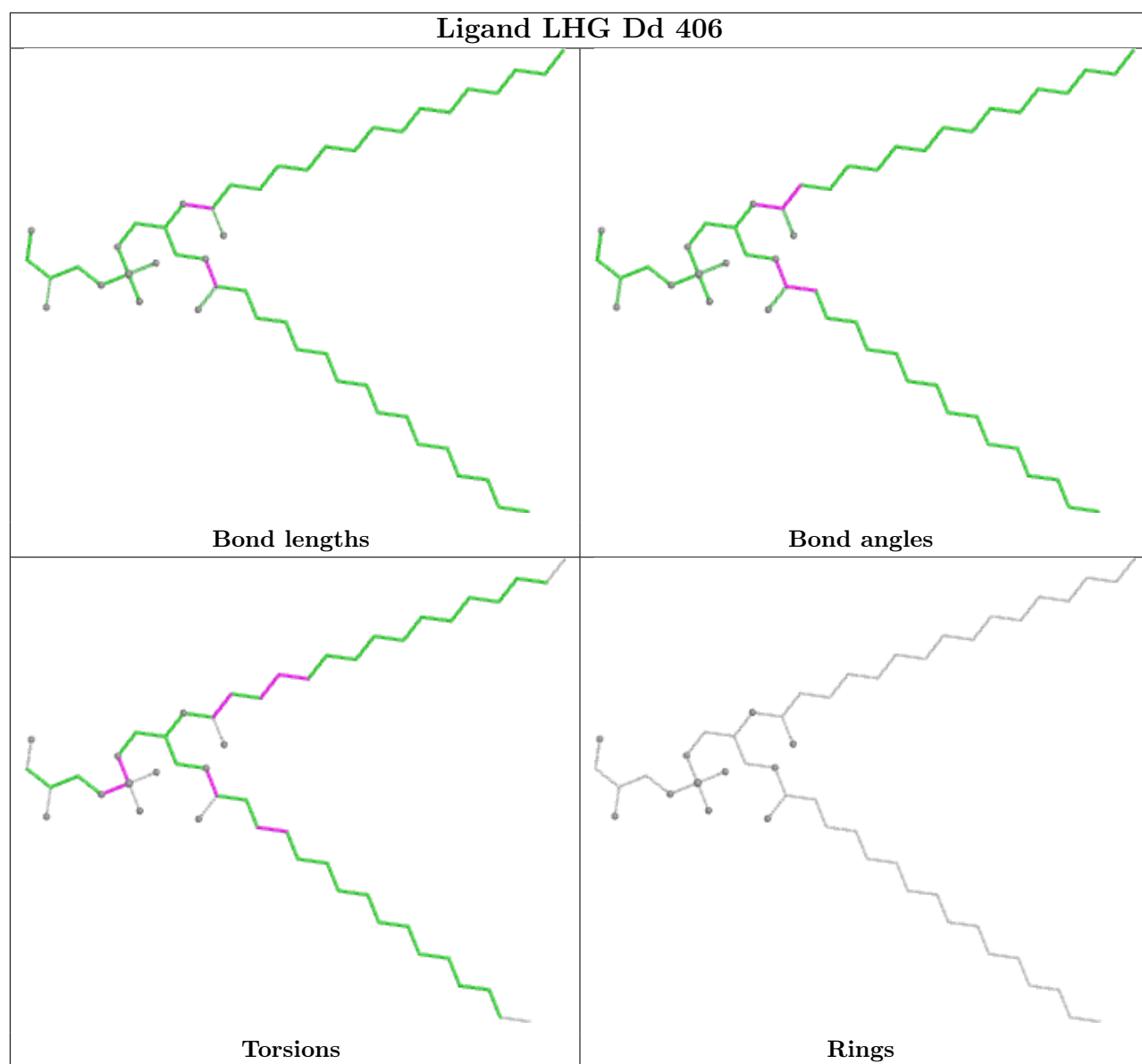


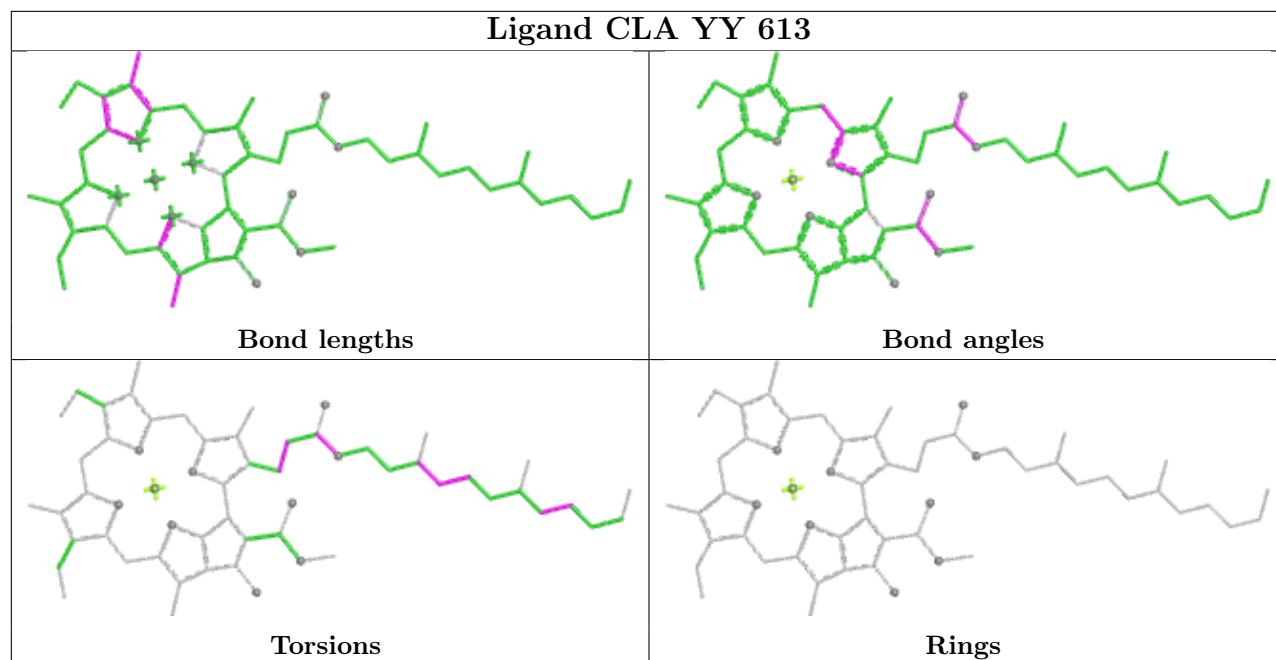
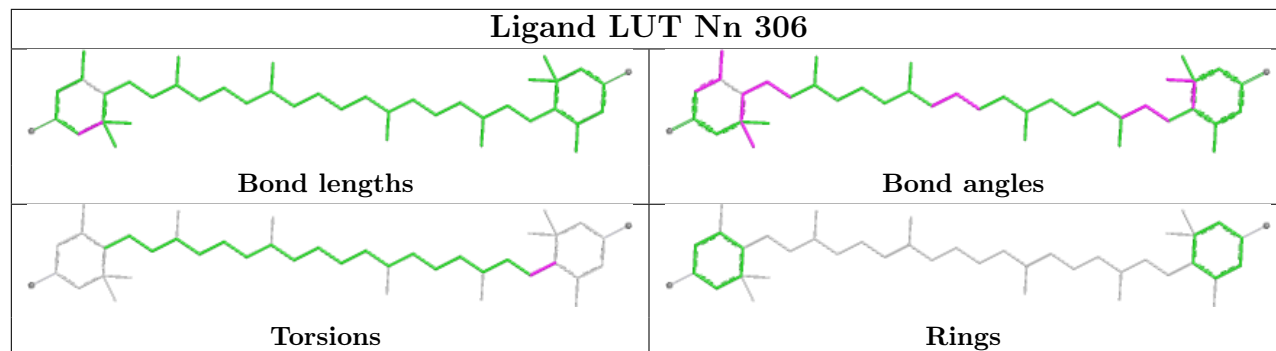
Ligand CHL 3 601



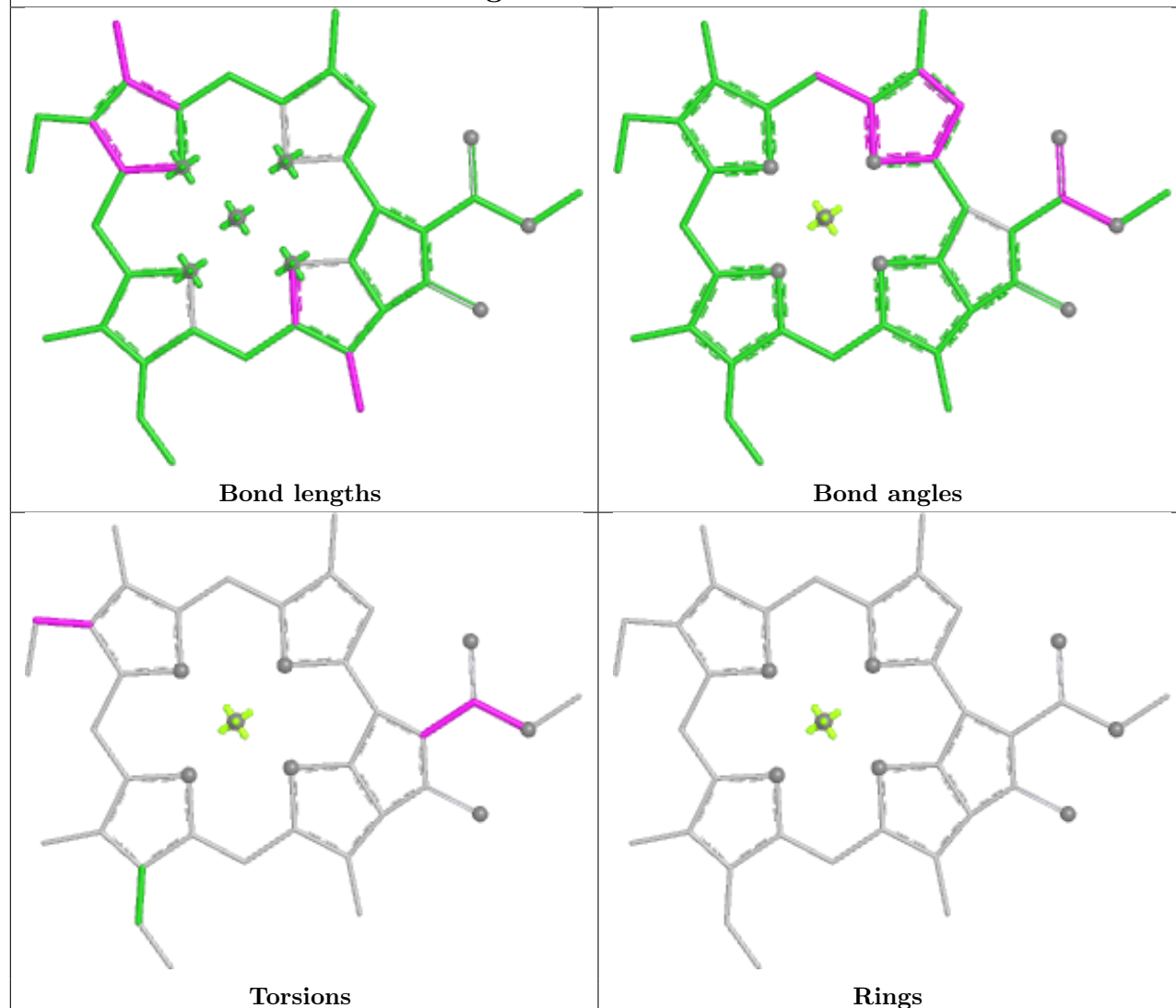




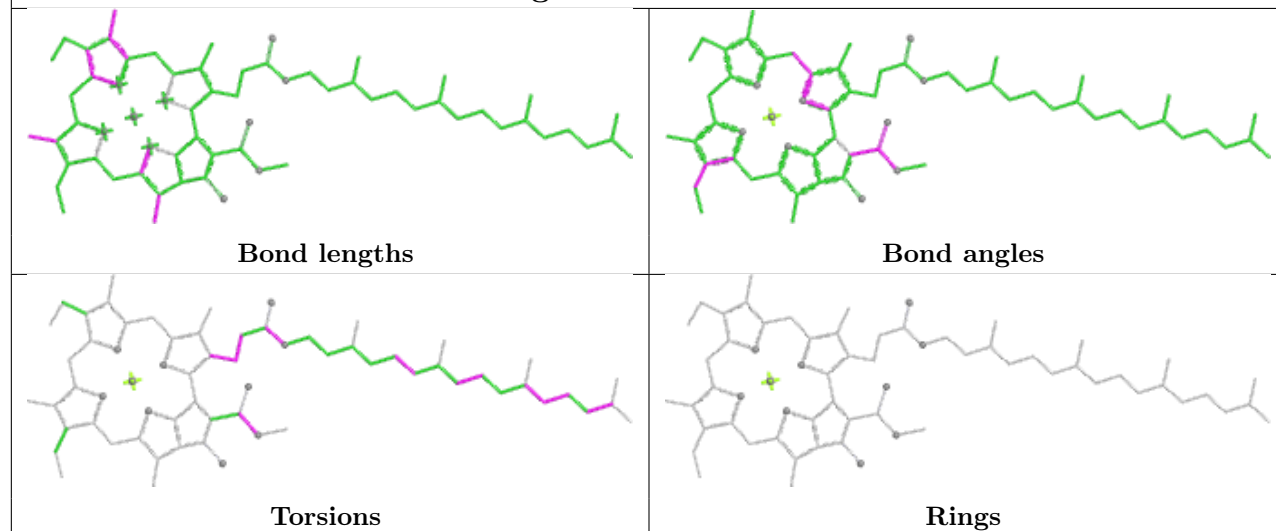


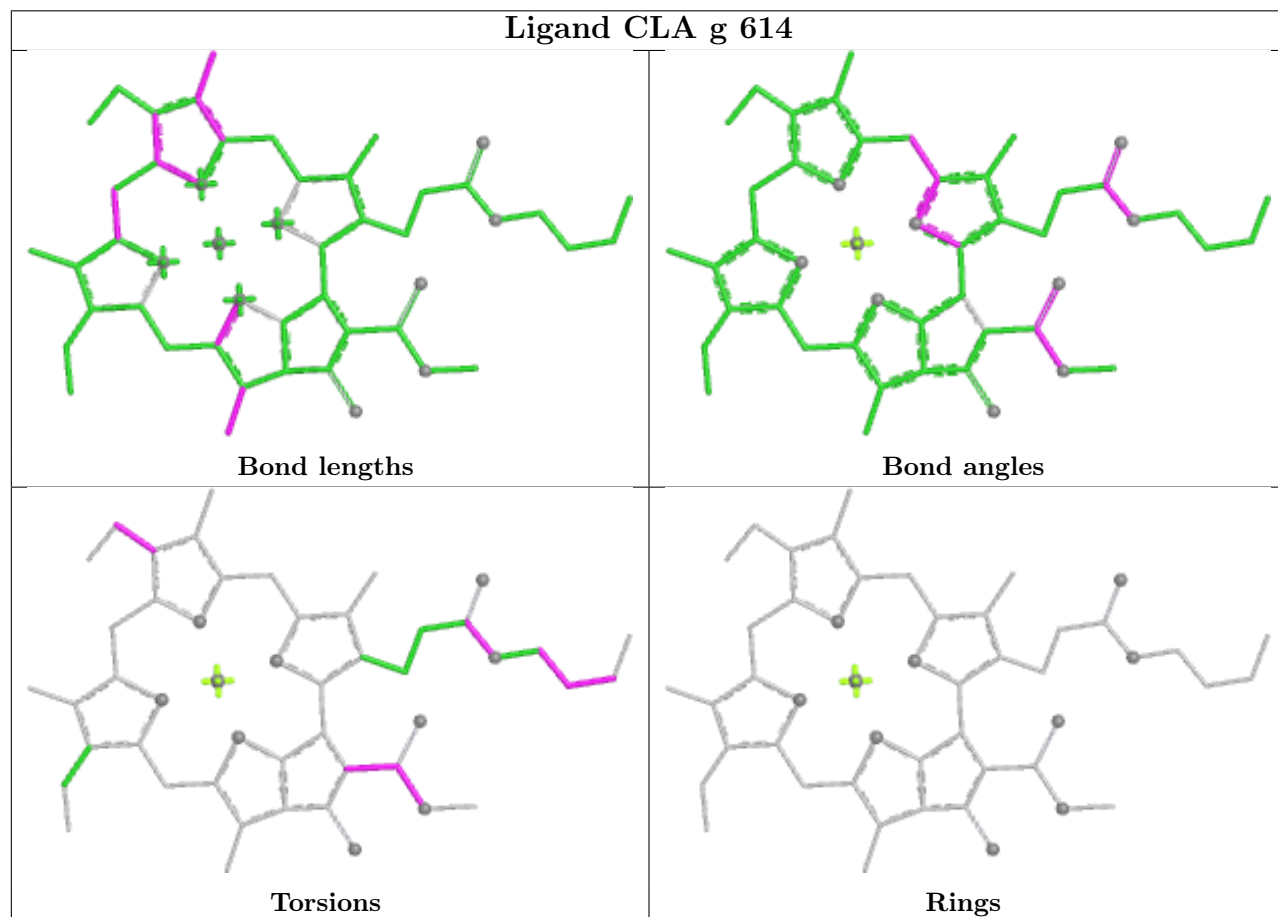
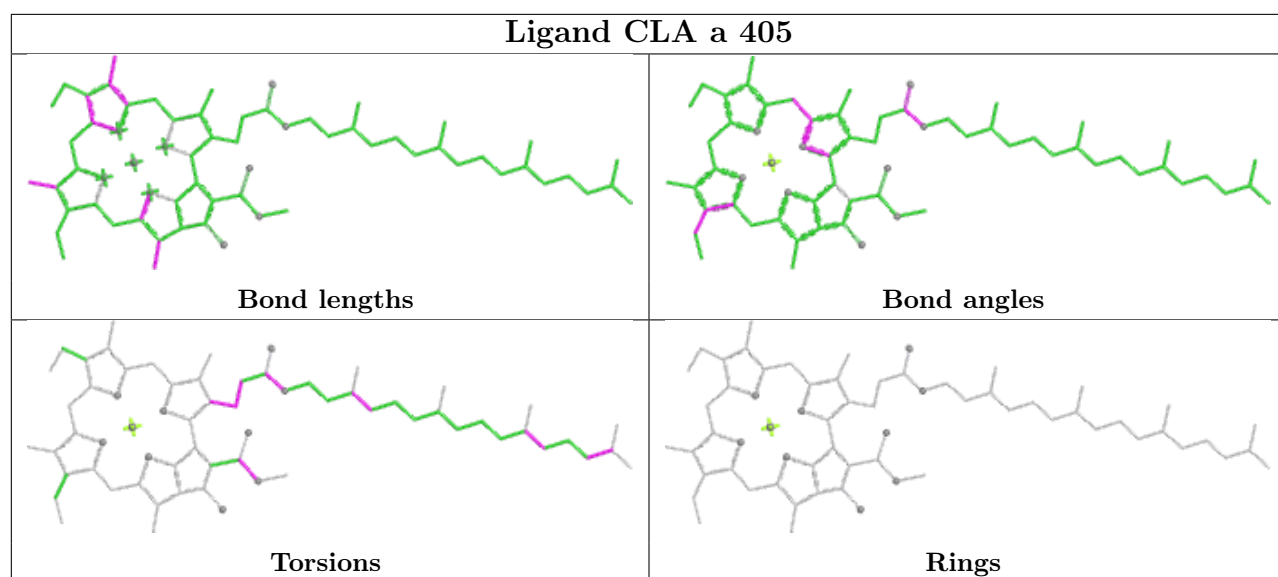
Ligand CLA YY 613**Ligand LUT Nn 306**

Ligand CLA 33 611

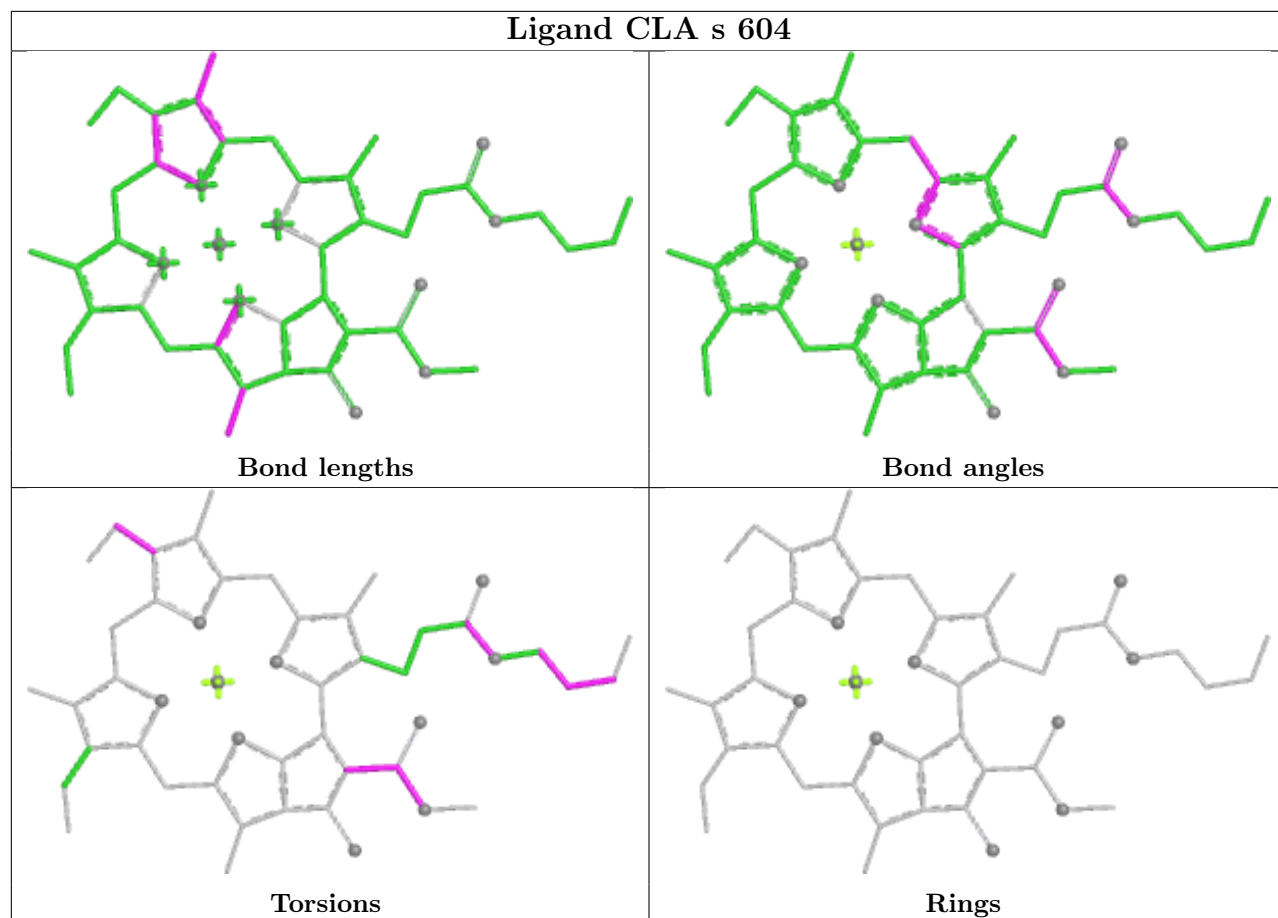


Ligand CLA A 405

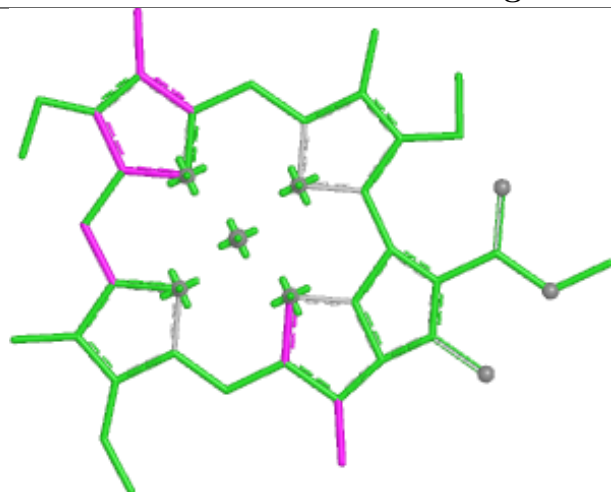




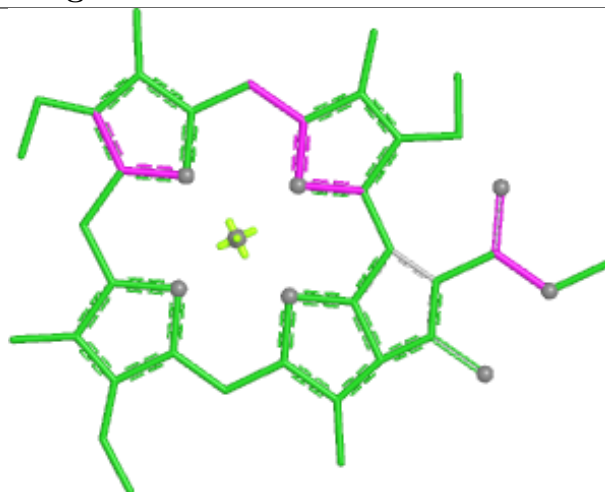
Ligand CLA s 604



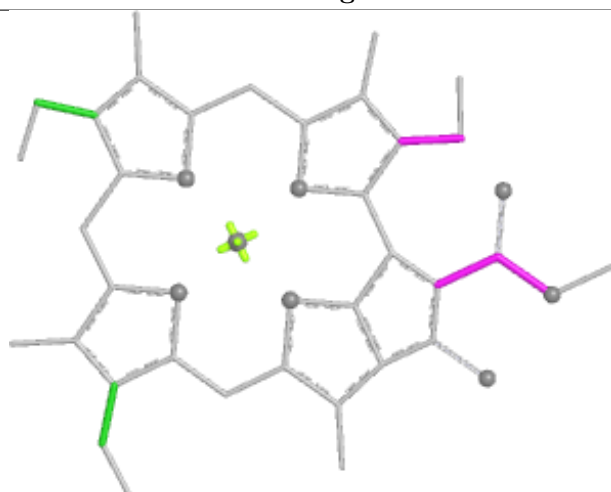
Ligand CLA Gg 305



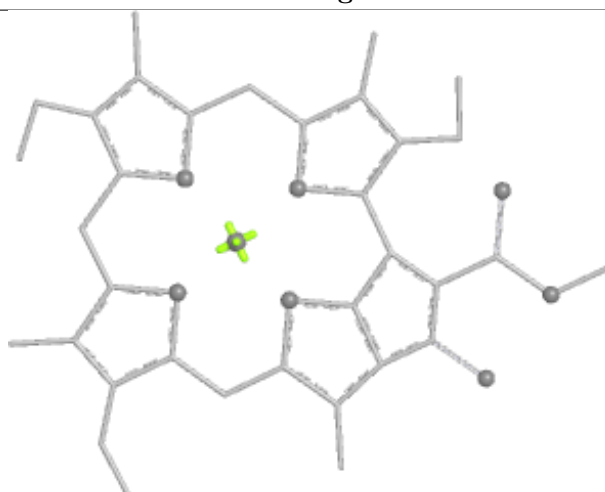
Bond lengths



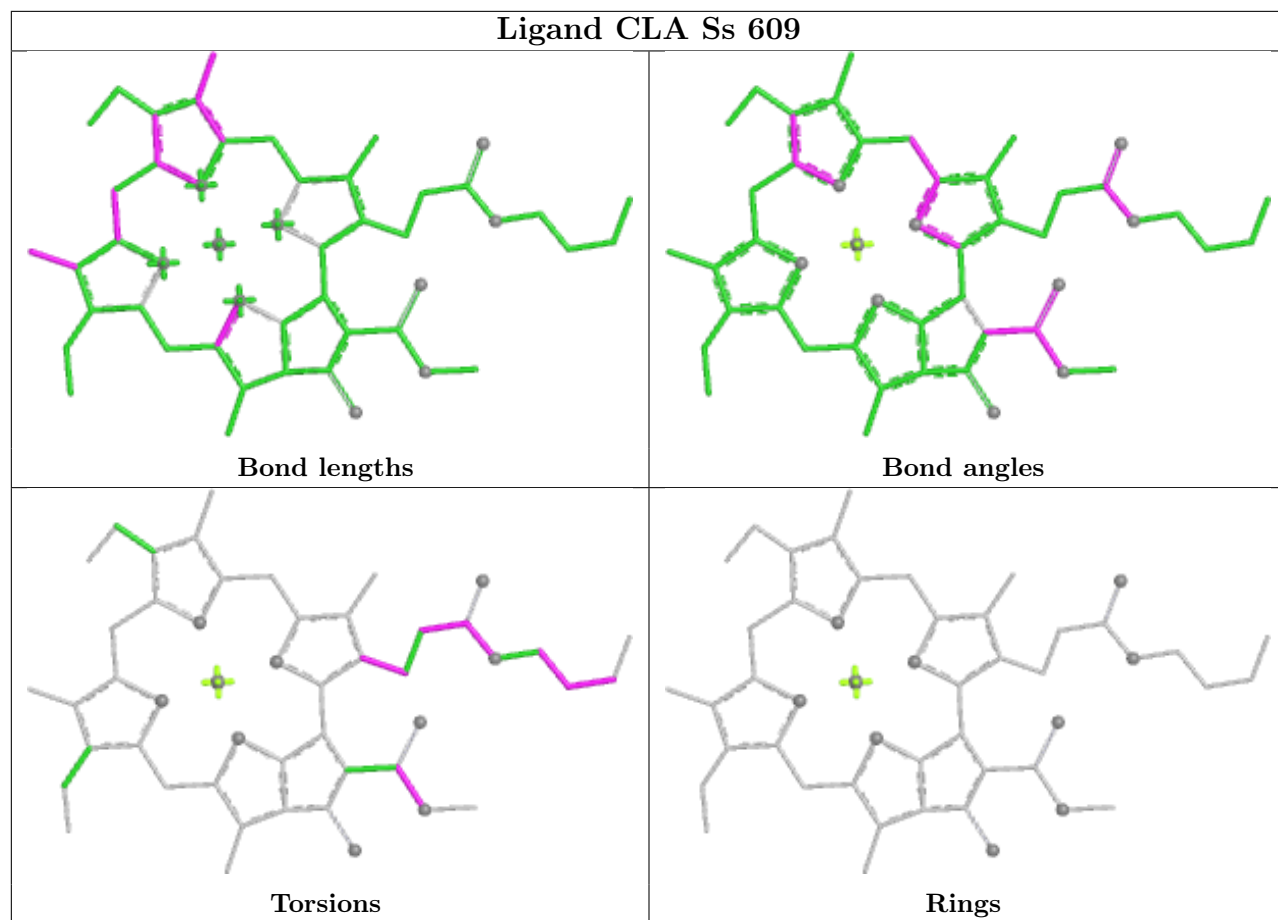
Bond angles



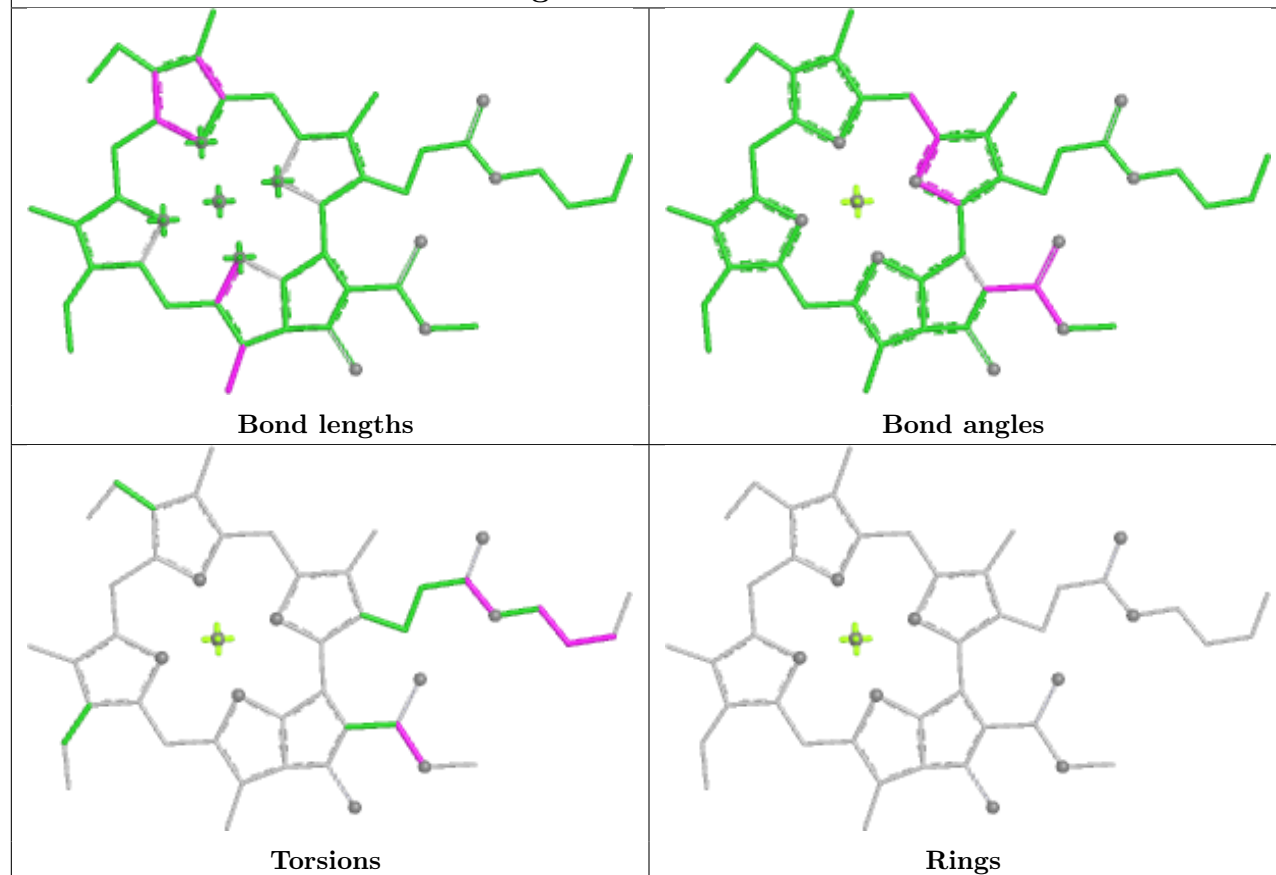
Torsions



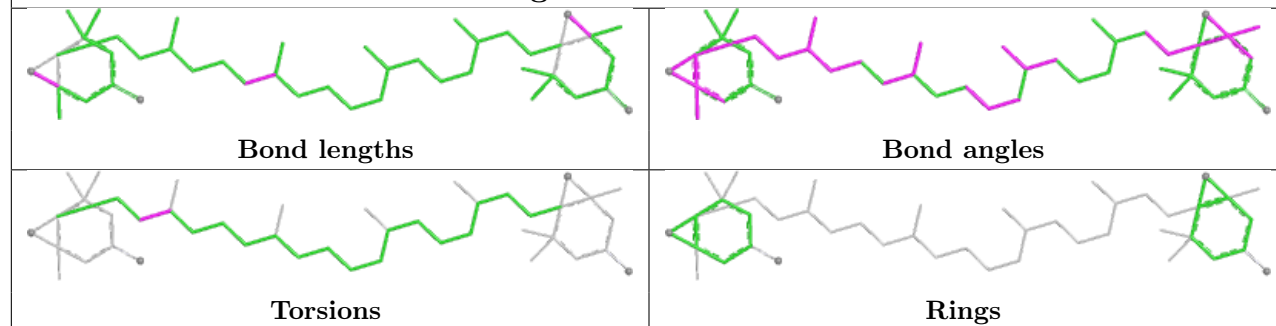
Rings



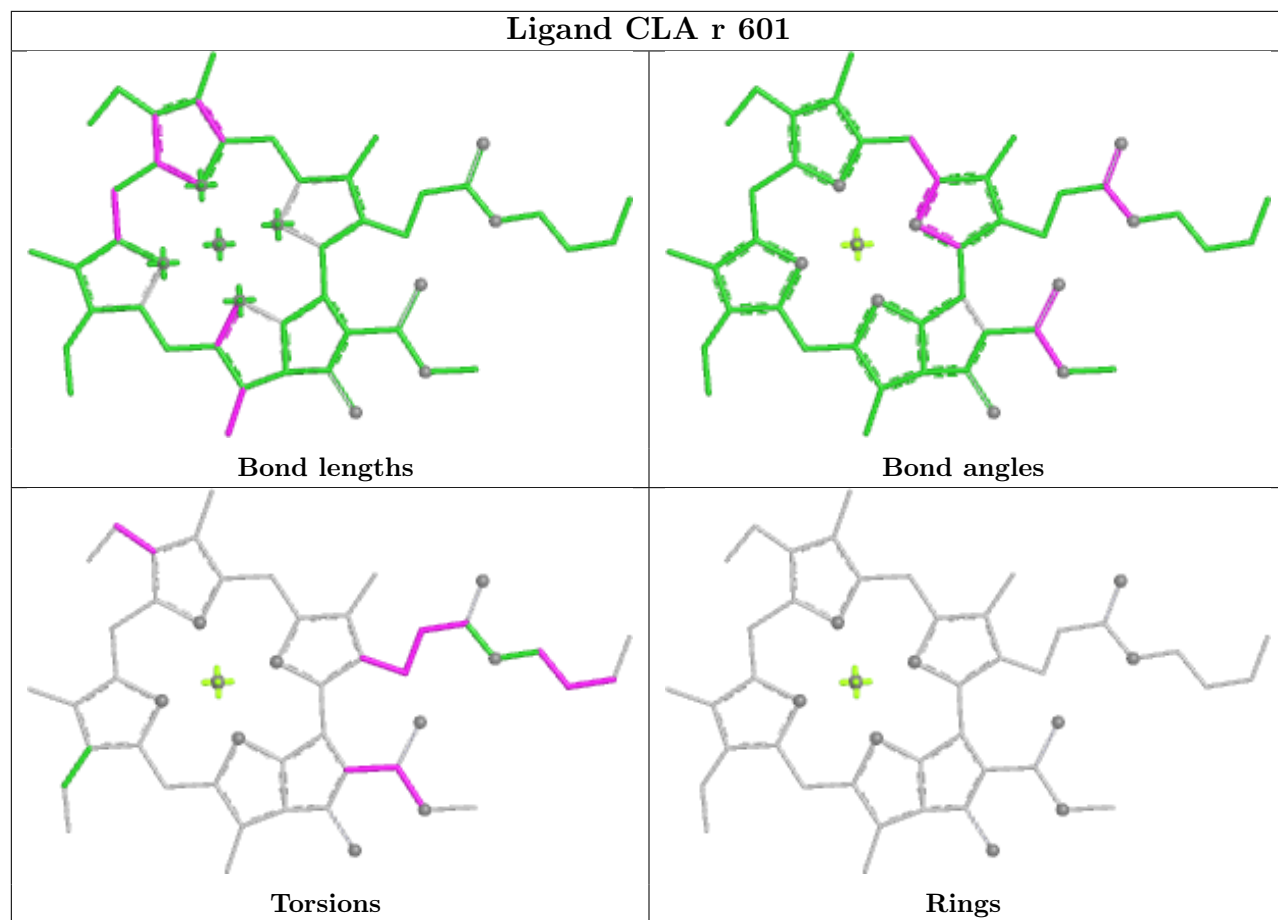
Ligand CLA R 614

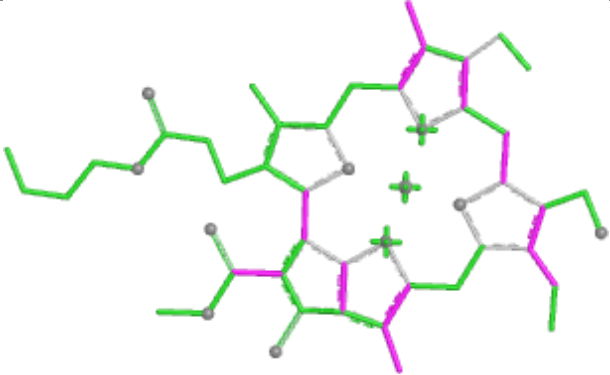
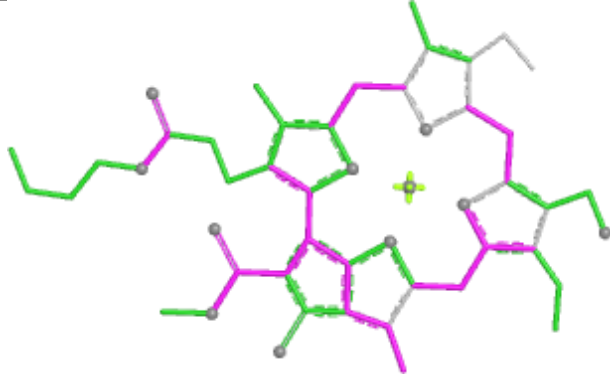
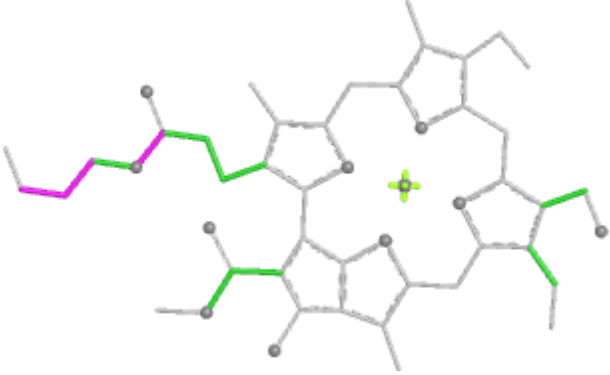
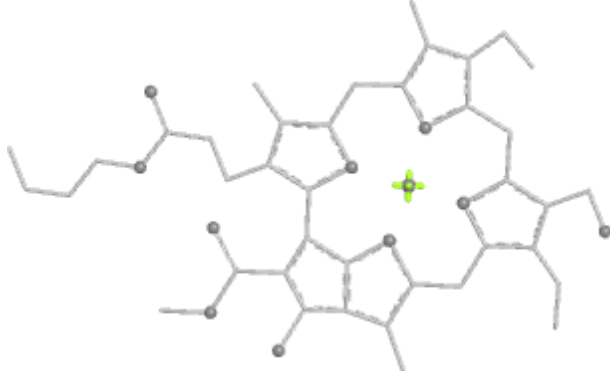


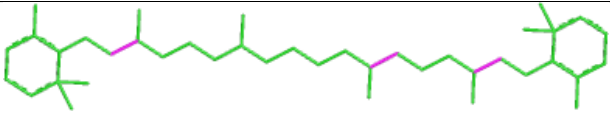
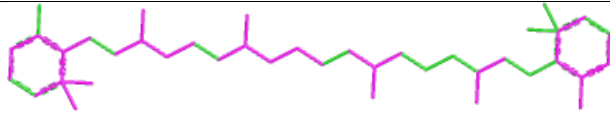
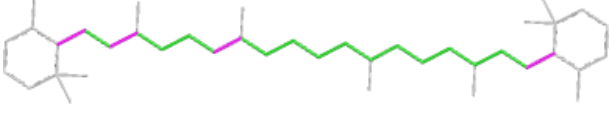
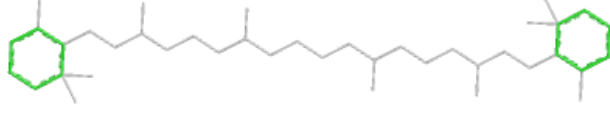
Ligand XAT G 617

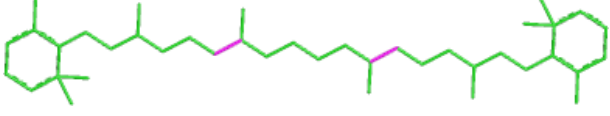
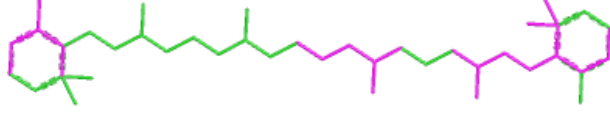
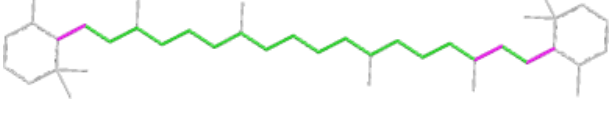
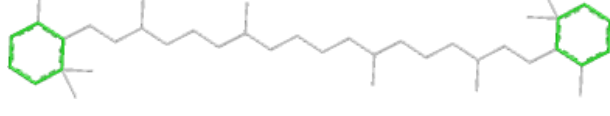


Ligand CLA r 601

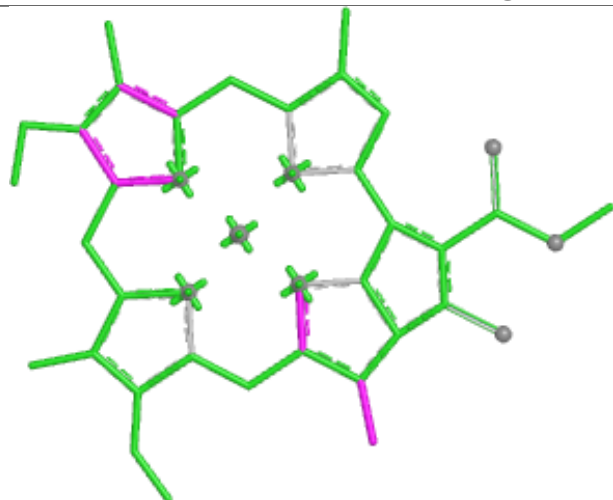


Ligand CHL Yy 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

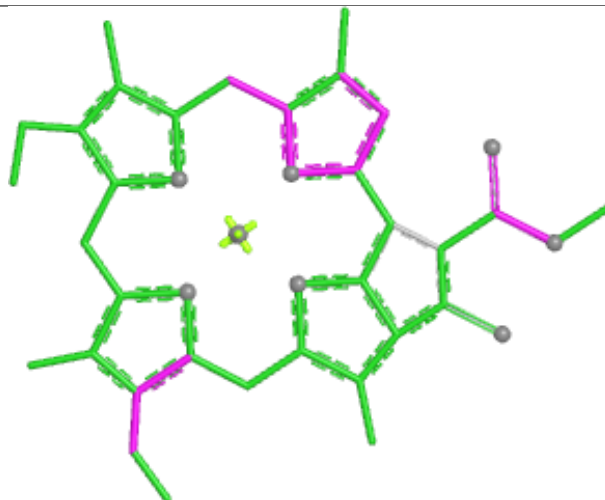
Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Bb 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

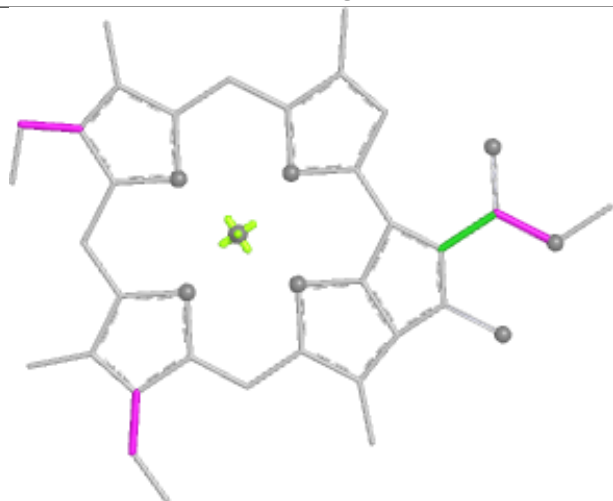
Ligand CLA GG 613



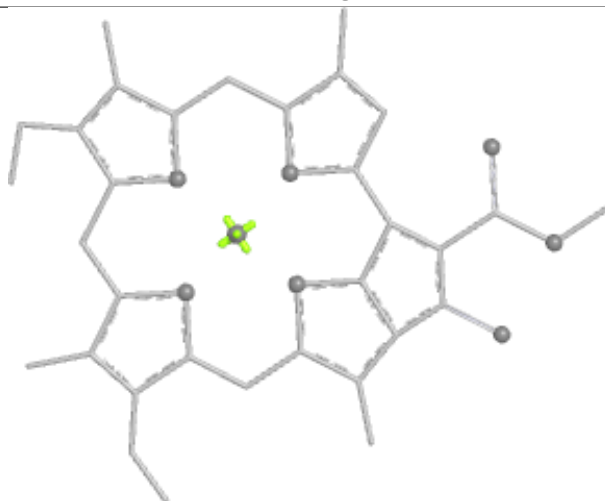
Bond lengths



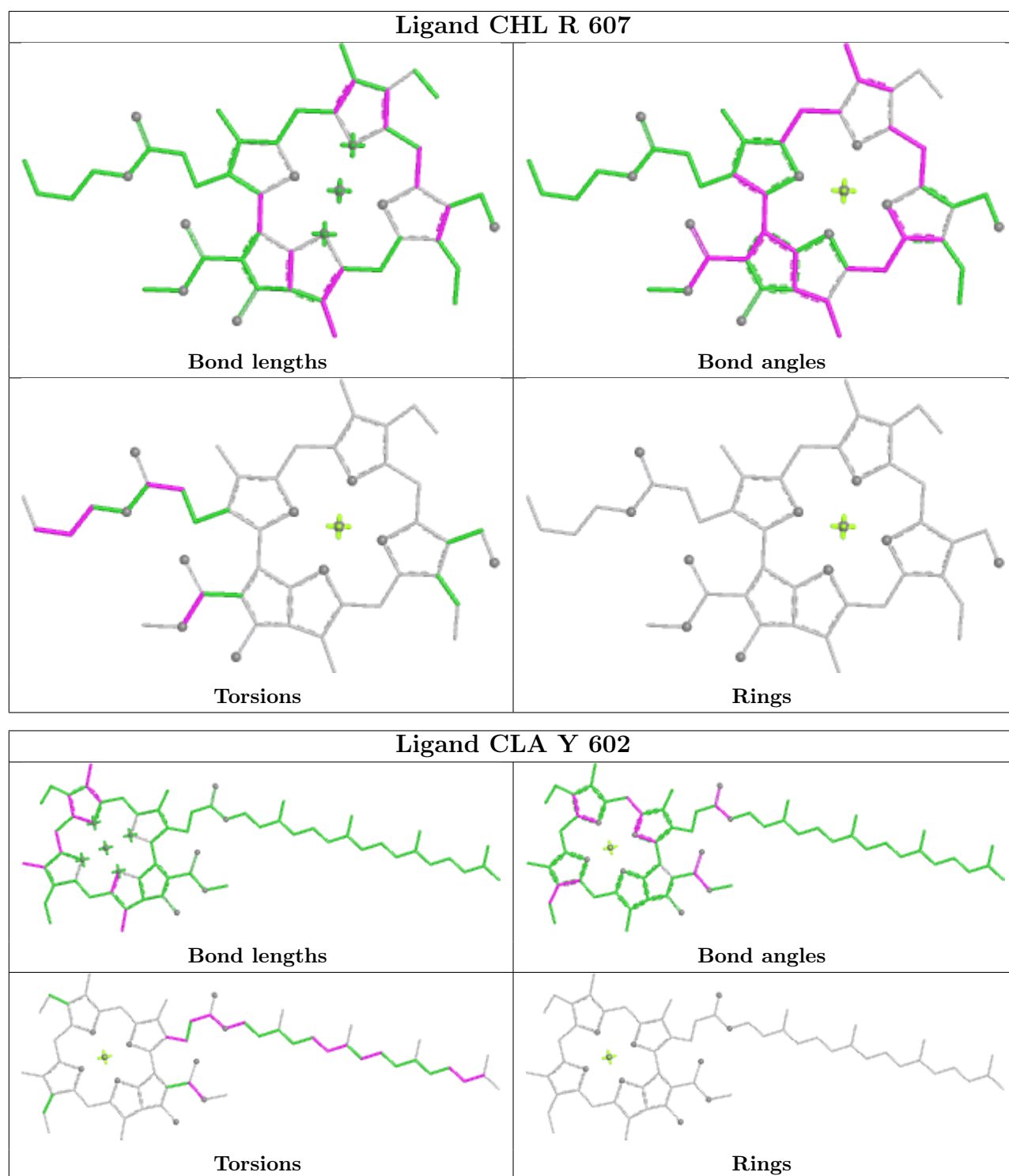
Bond angles



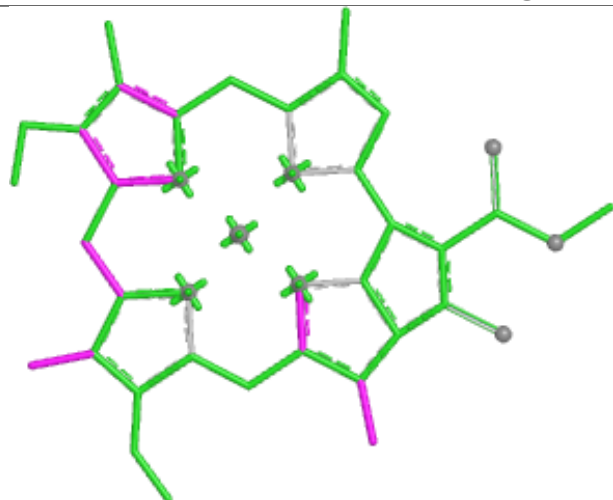
Torsions



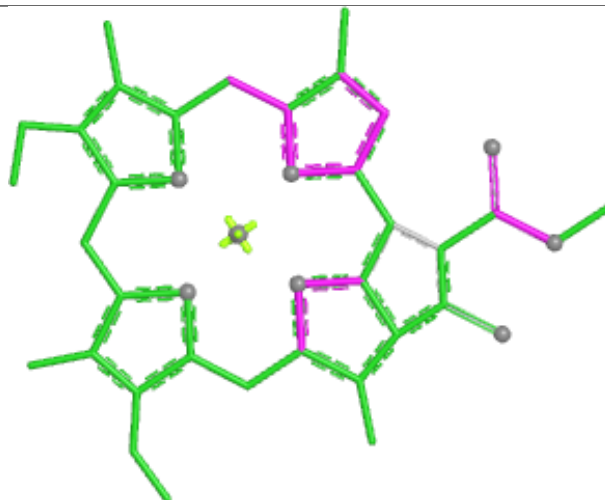
Rings



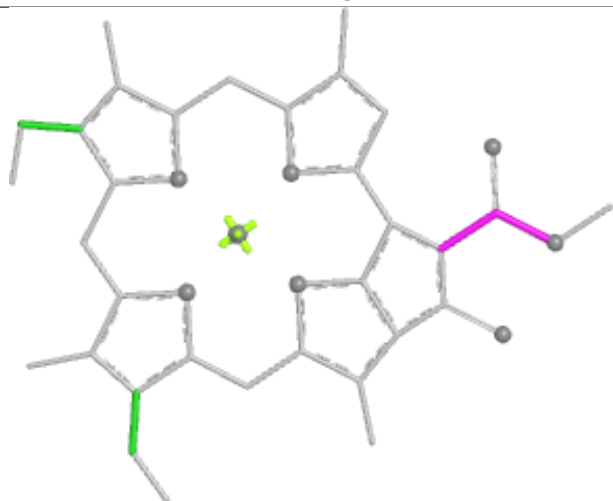
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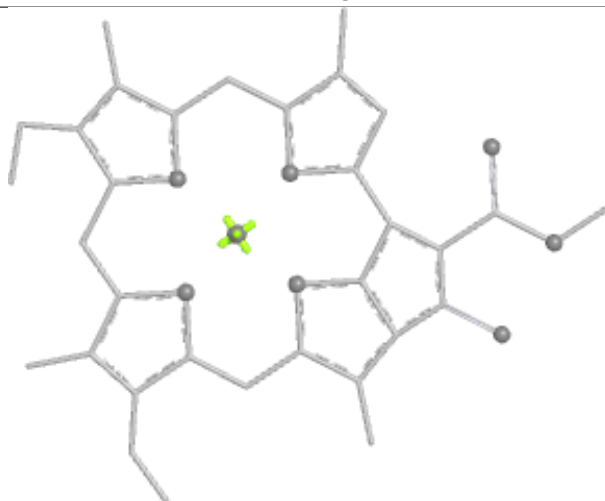
Bond lengths



Bond angles

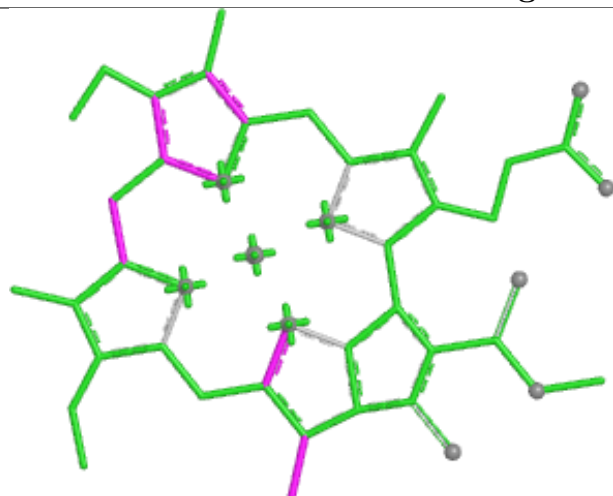


Torsions

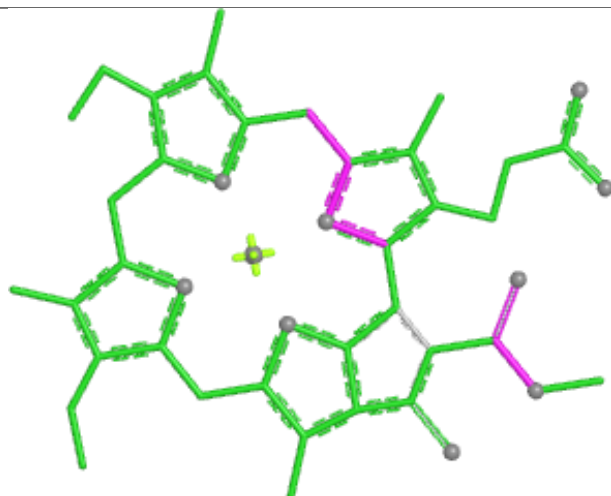


Rings

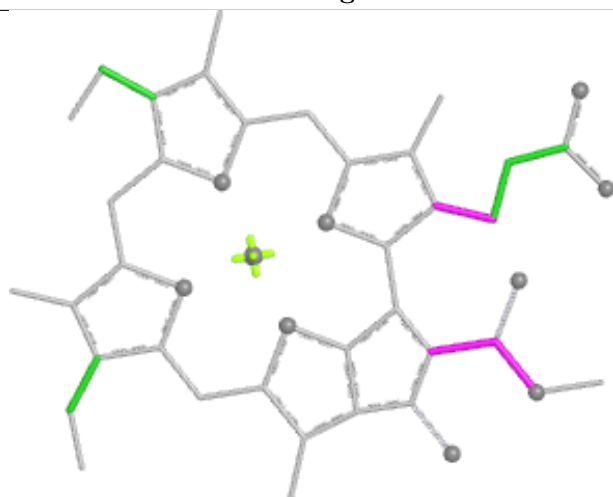
Ligand CLA 4 310



Bond lengths



Bond angles

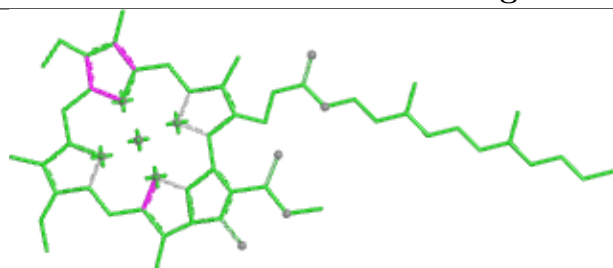


Torsions

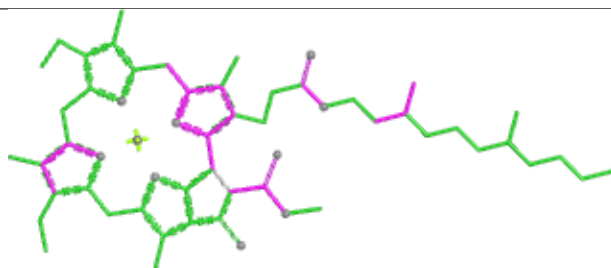


Rings

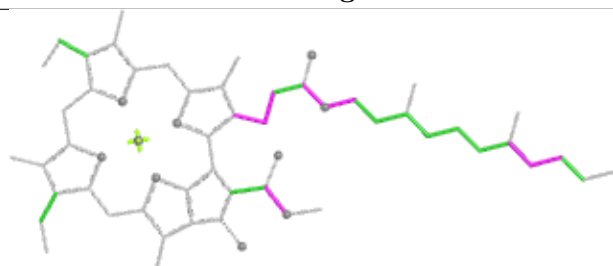
Ligand CLA YY 612



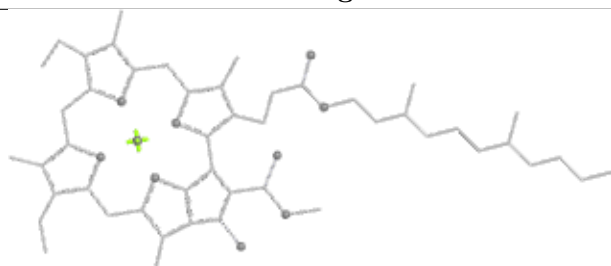
Bond lengths



Bond angles

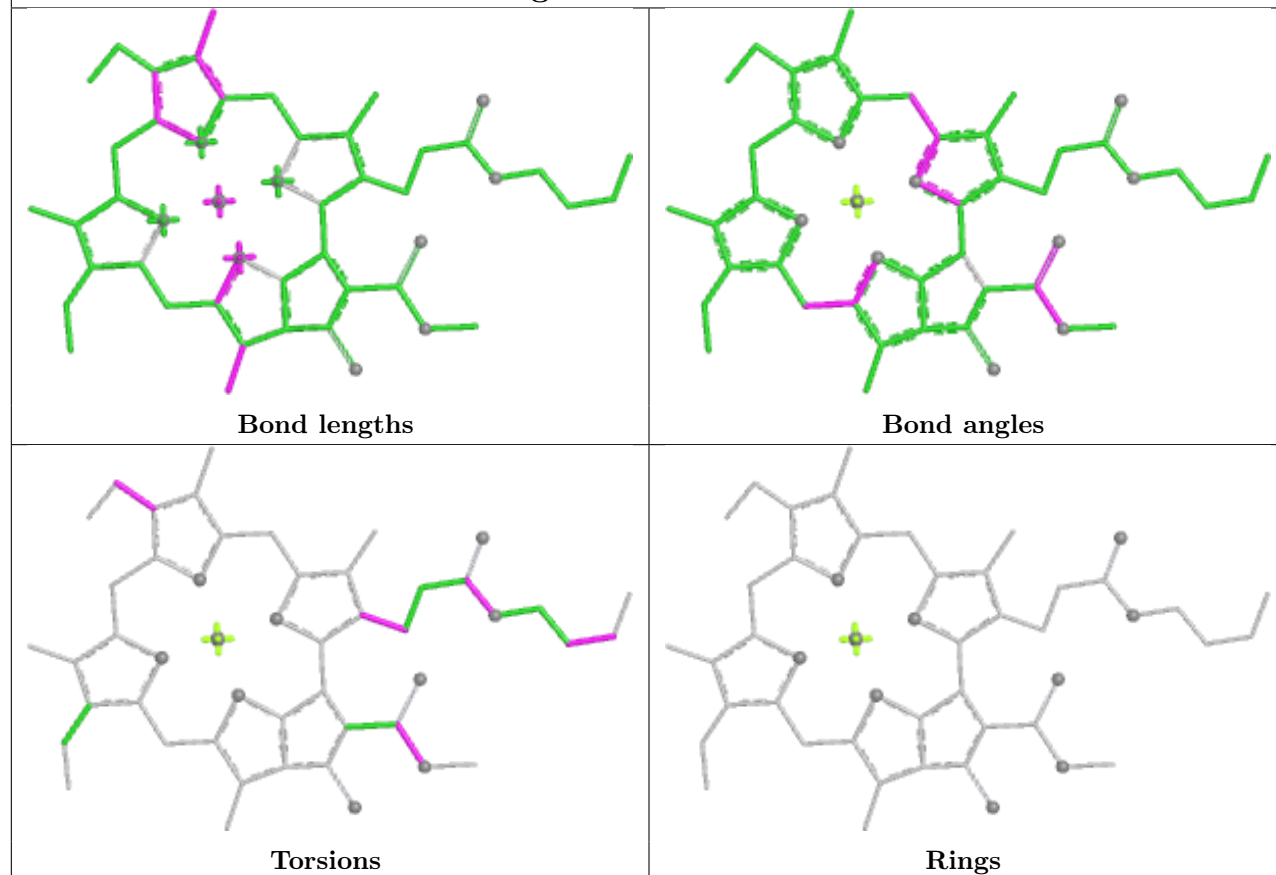


Torsions

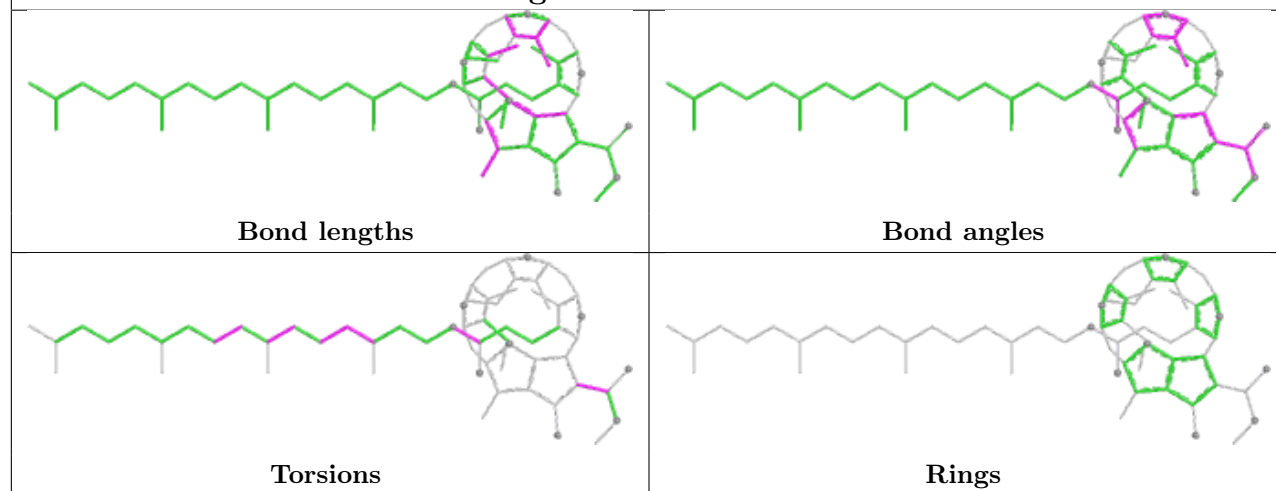


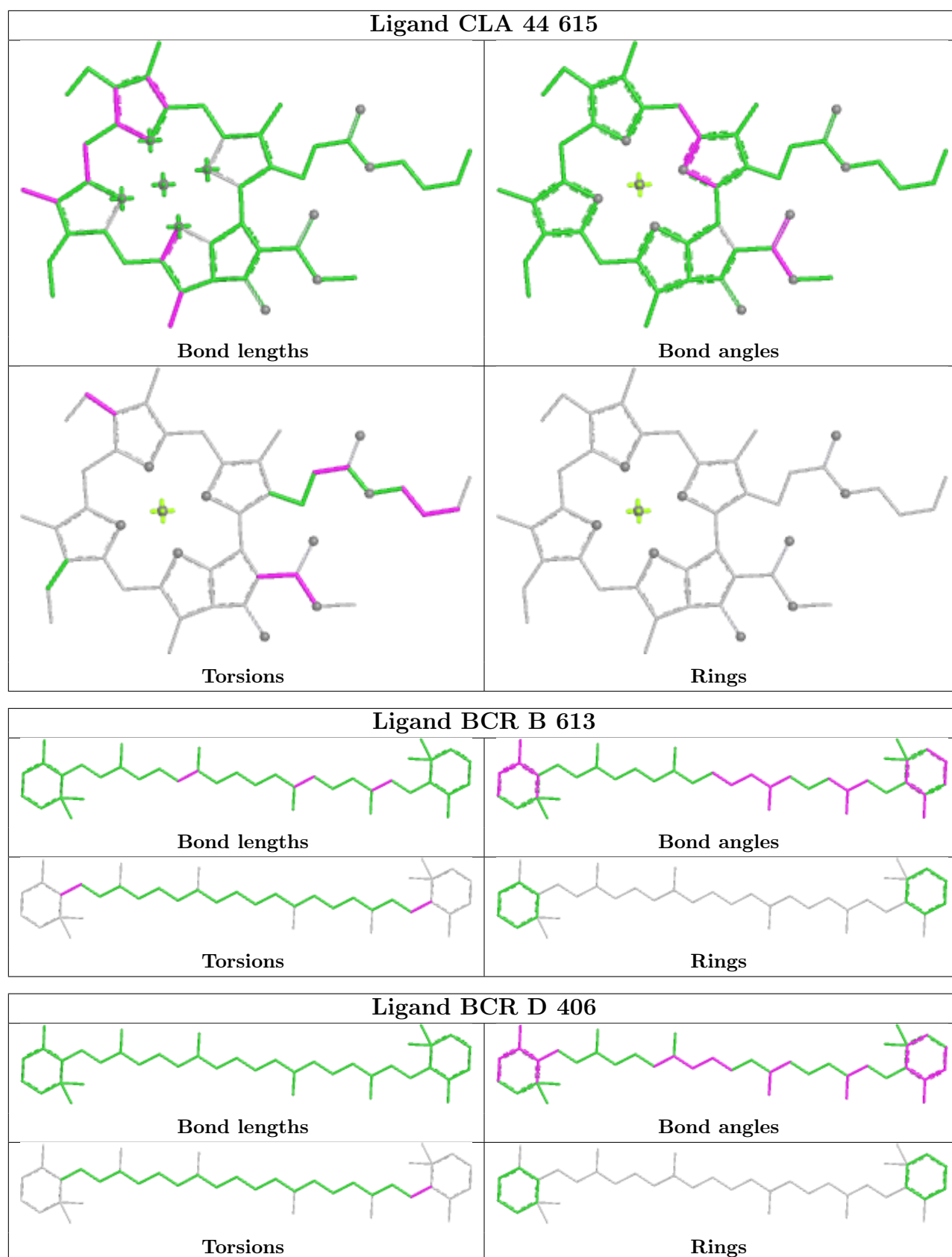
Rings

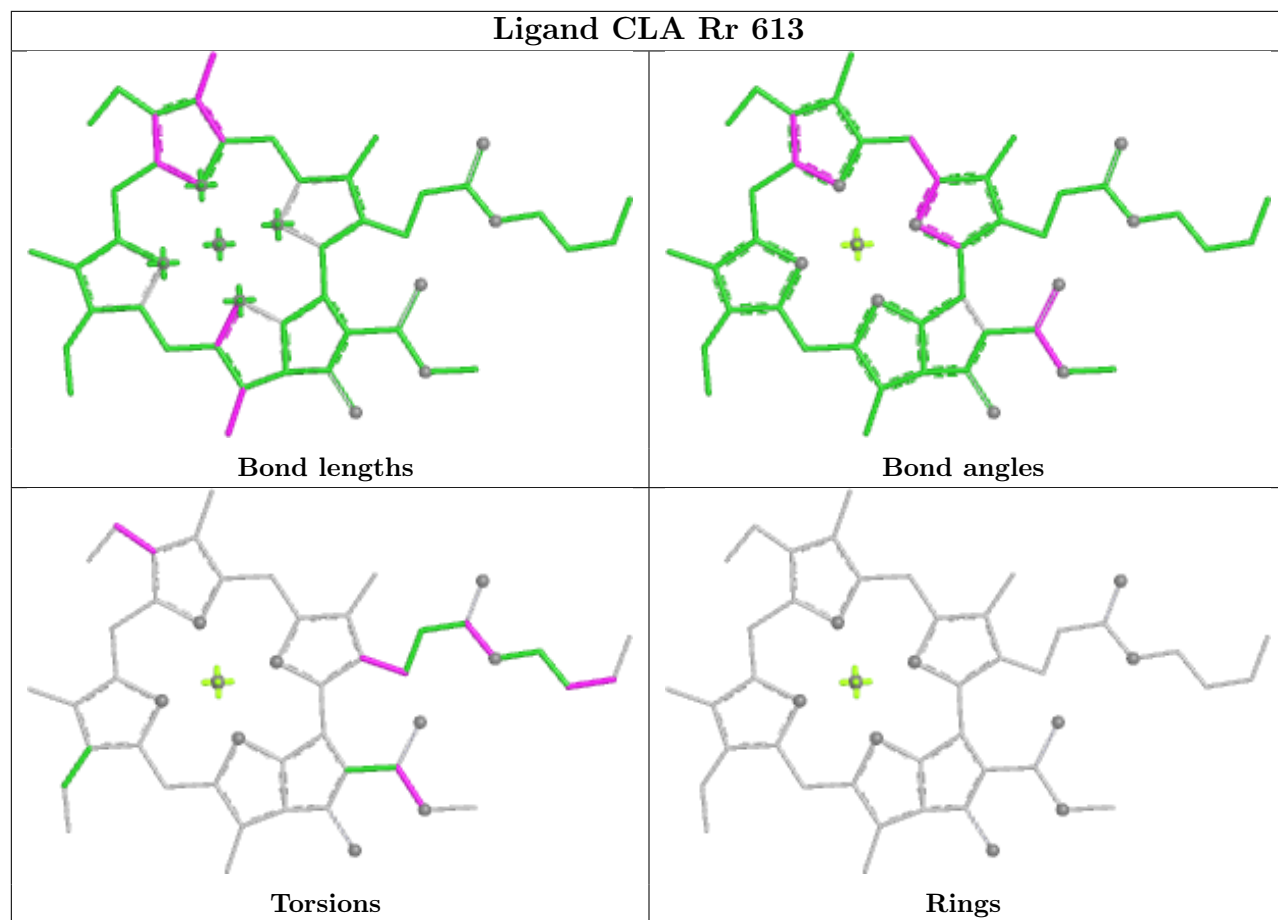
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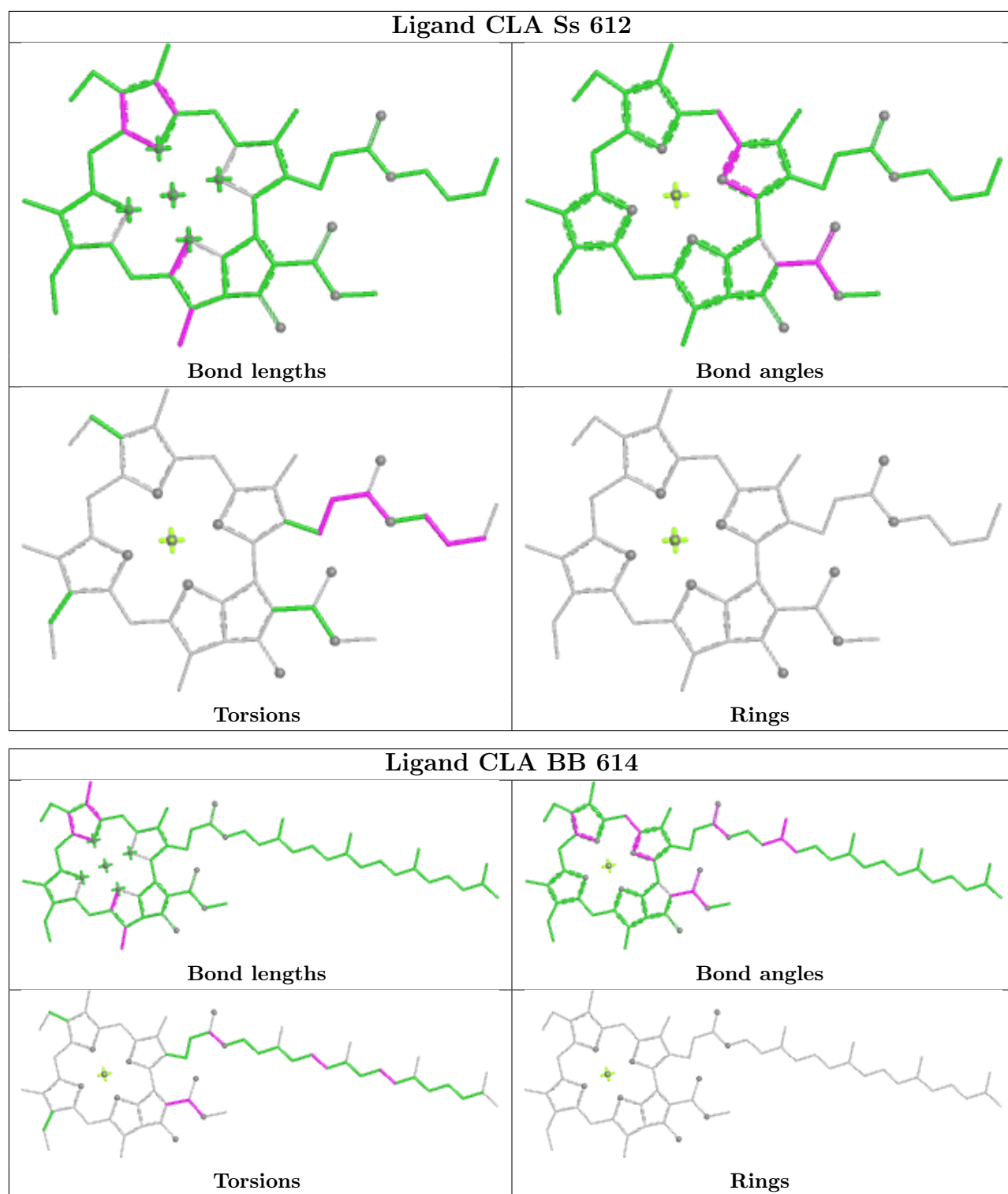


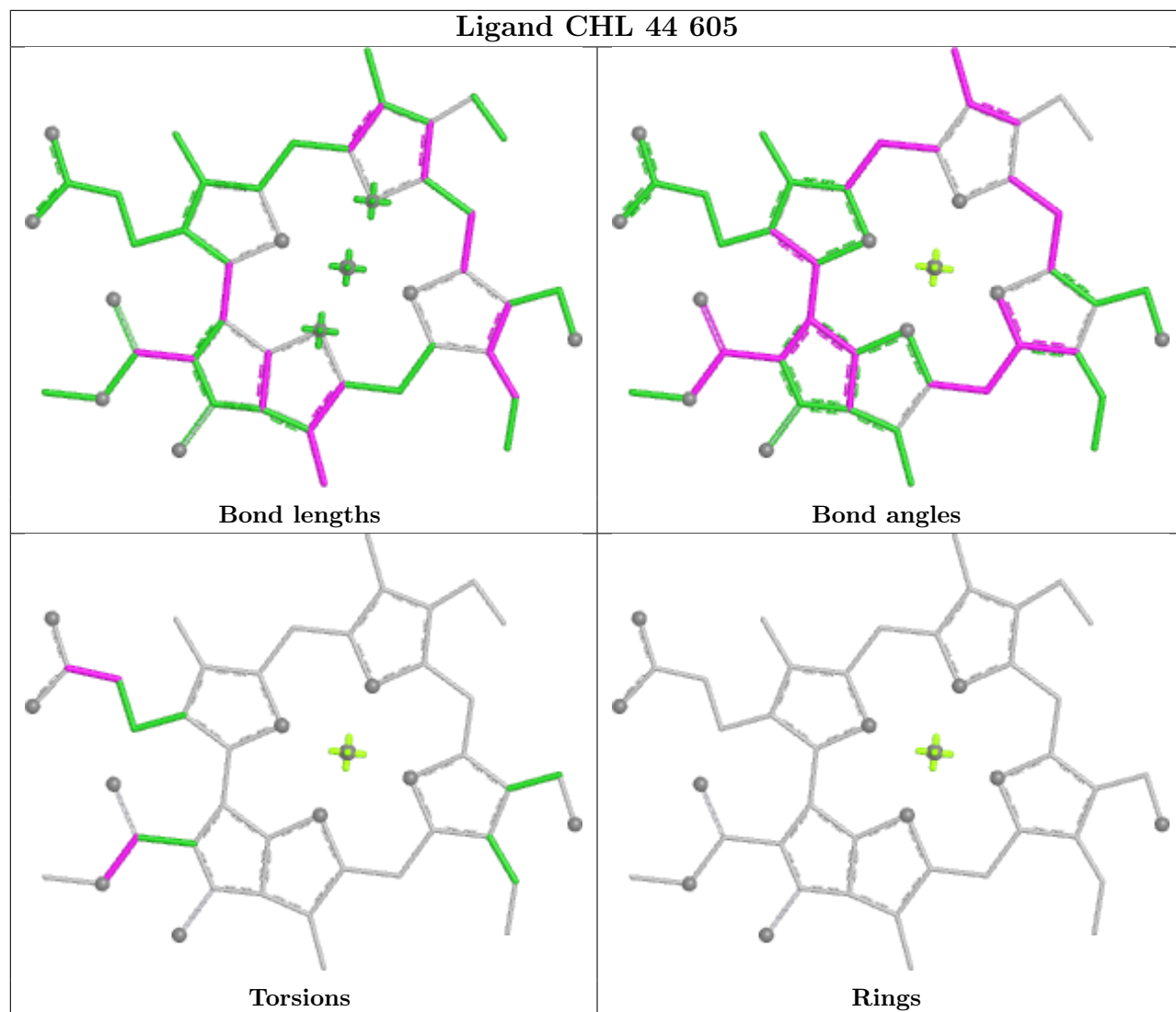
Ligand PHO D 402



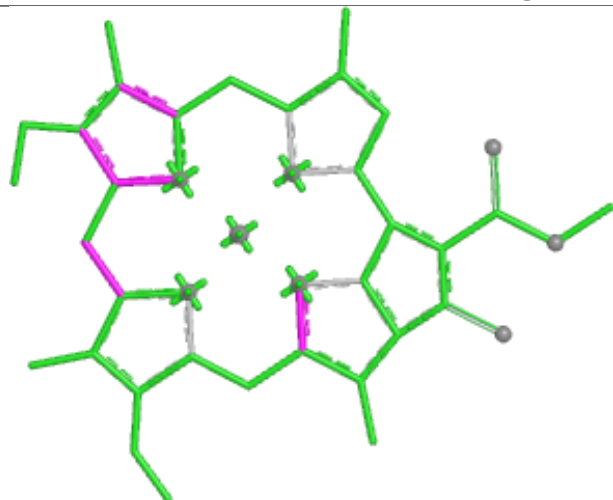




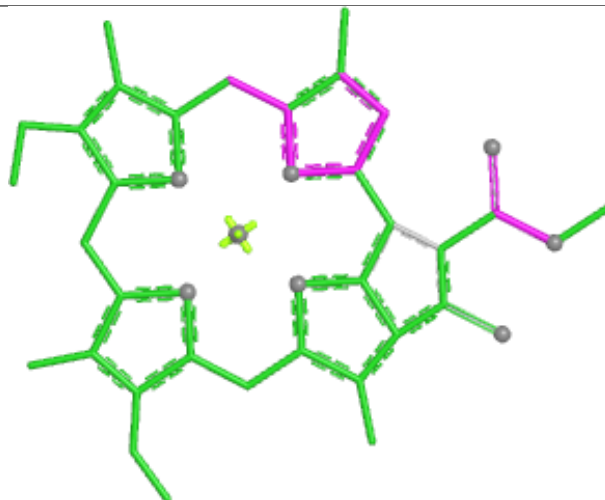




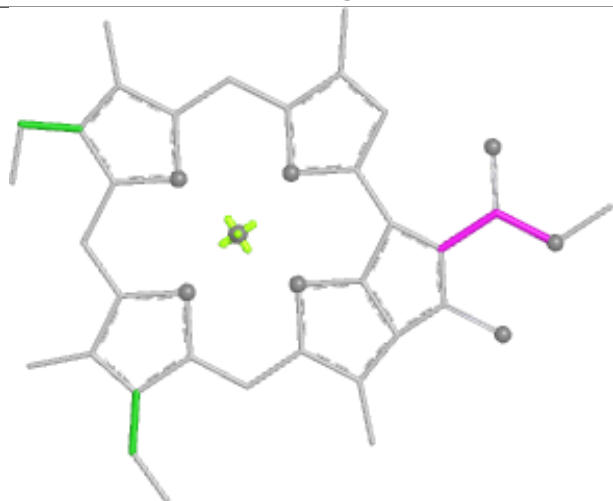
Ligand CLA 2 612



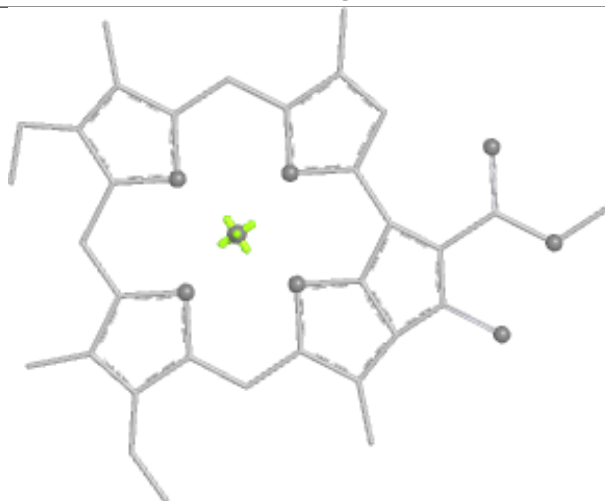
Bond lengths



Bond angles

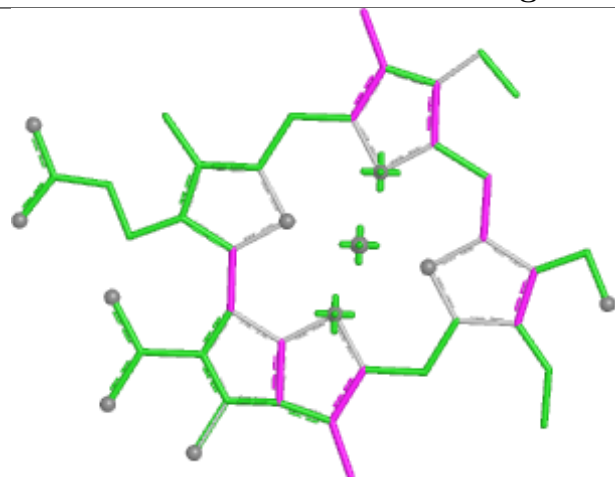


Torsions

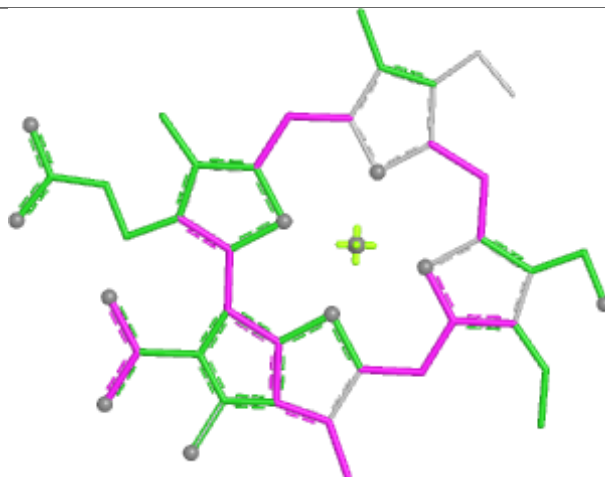


Rings

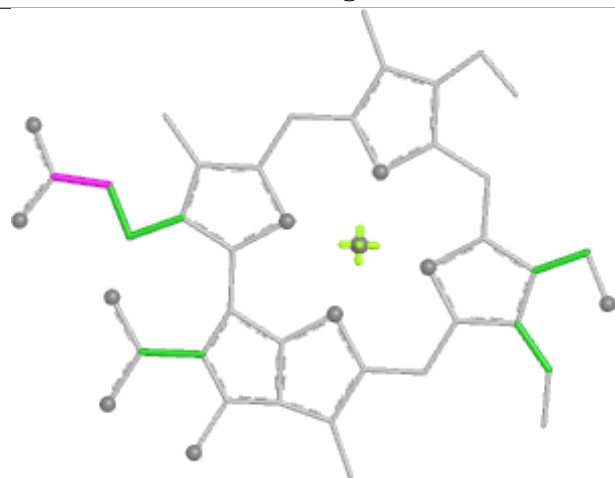
Ligand CHL 4 302



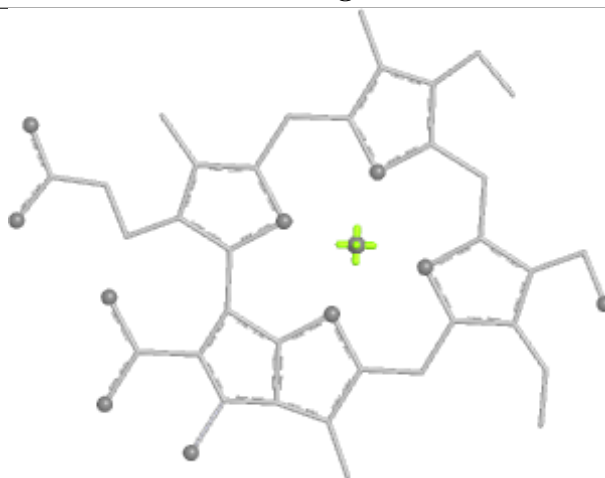
Bond lengths



Bond angles

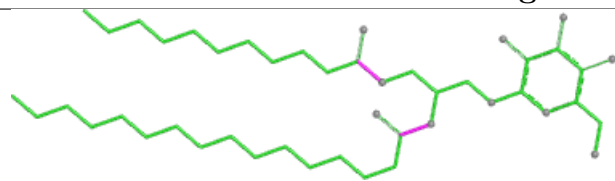


Torsions

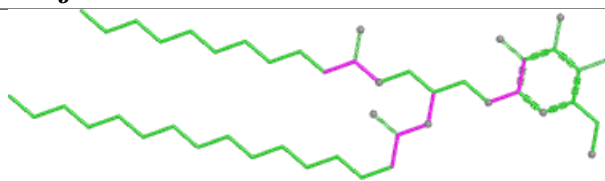


Rings

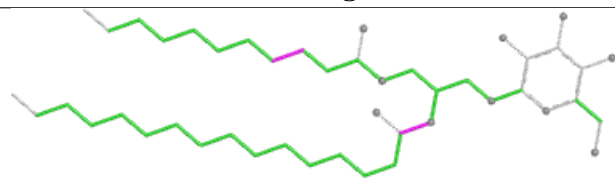
Ligand LMG j 101



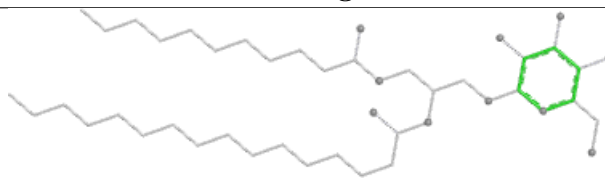
Bond lengths



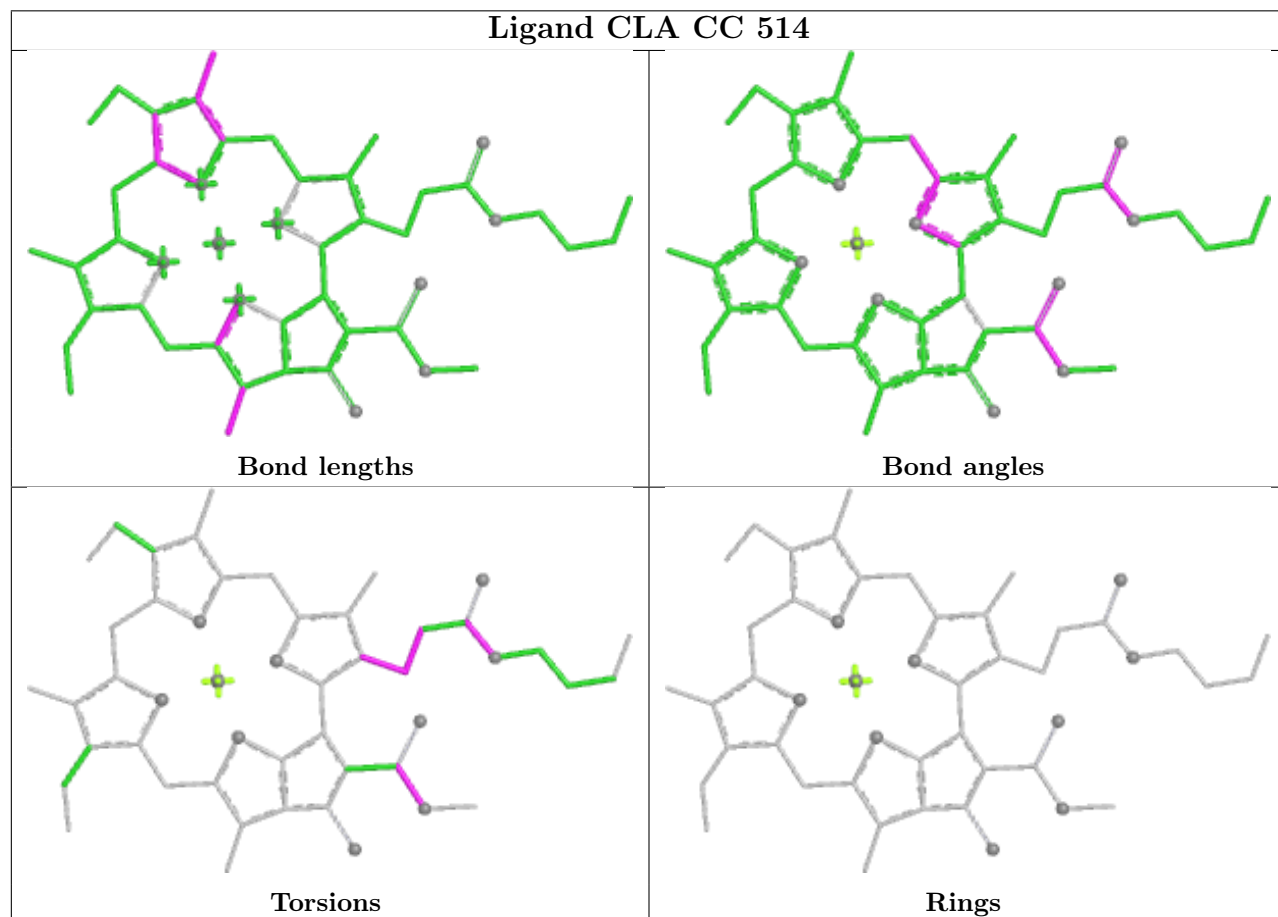
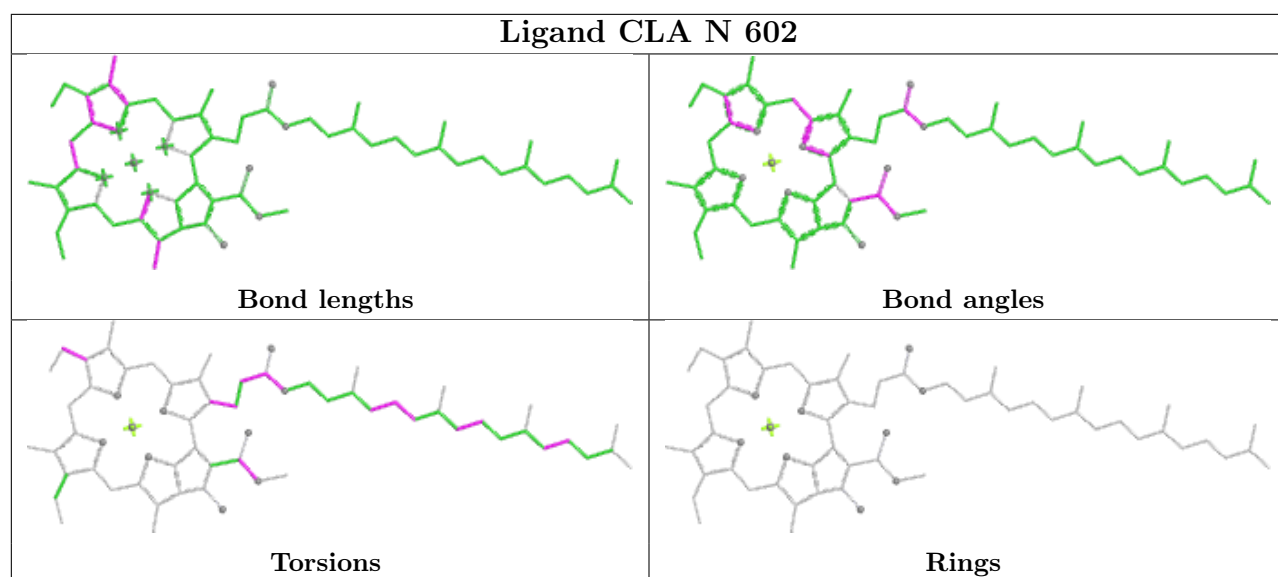
Bond angles

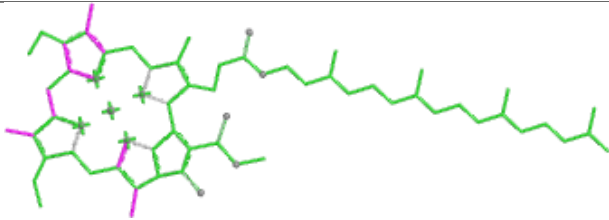
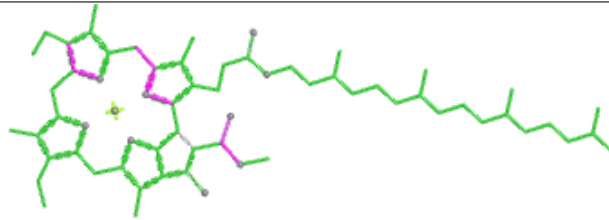
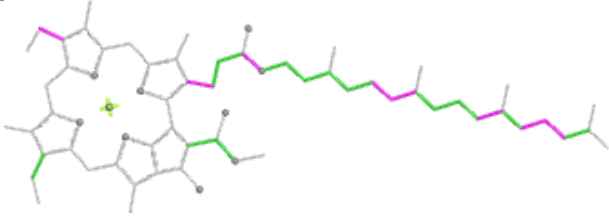
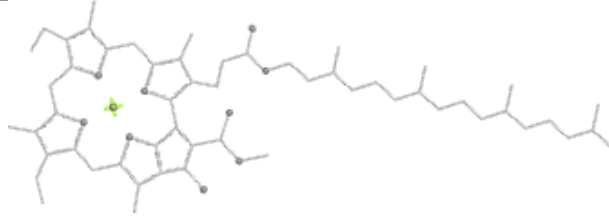


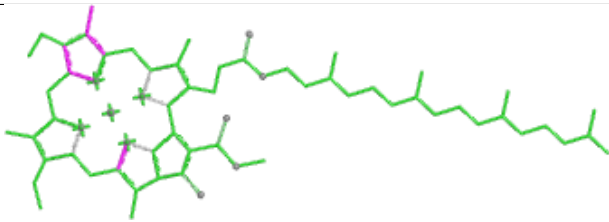
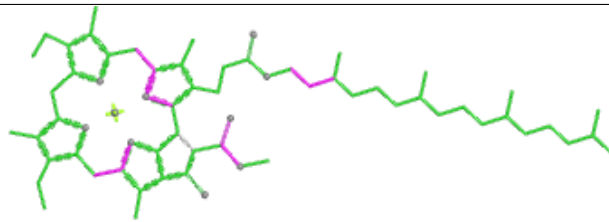
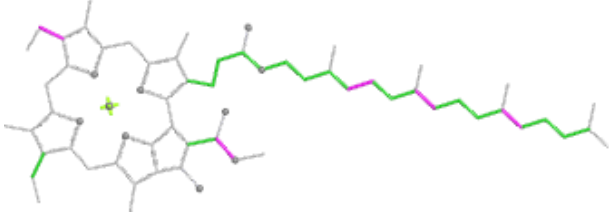
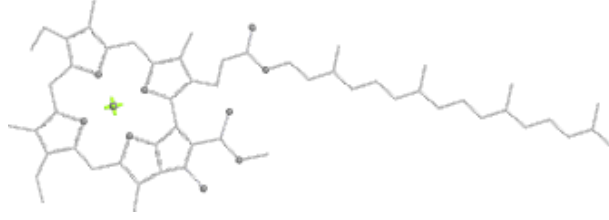
Torsions

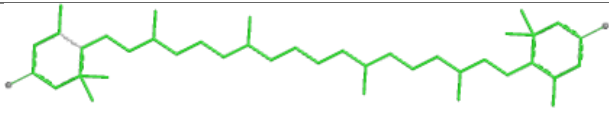
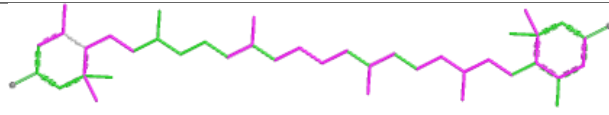
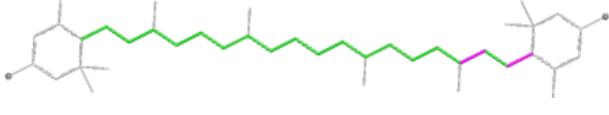
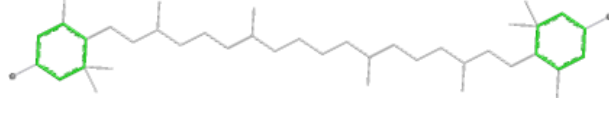


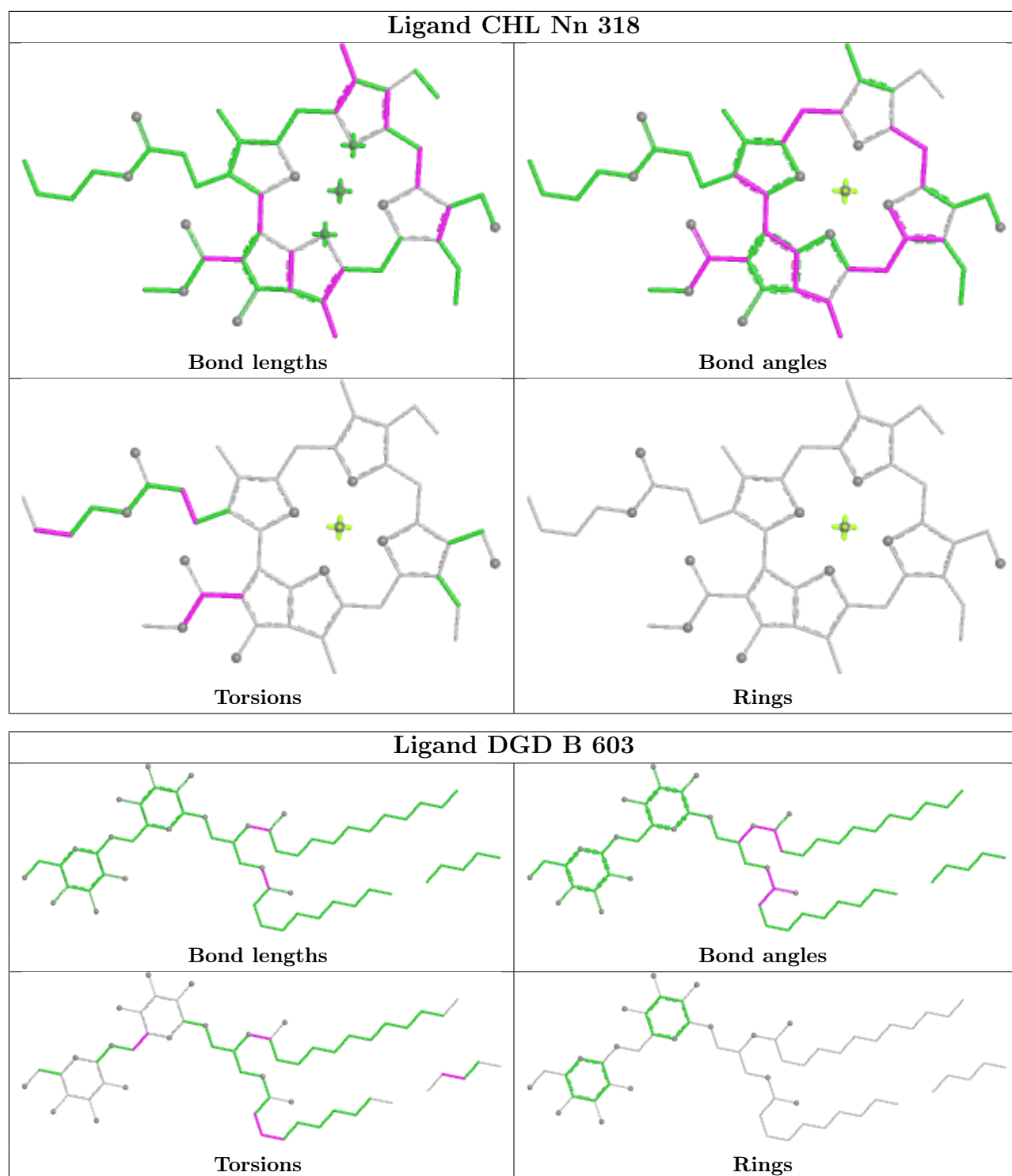
Rings



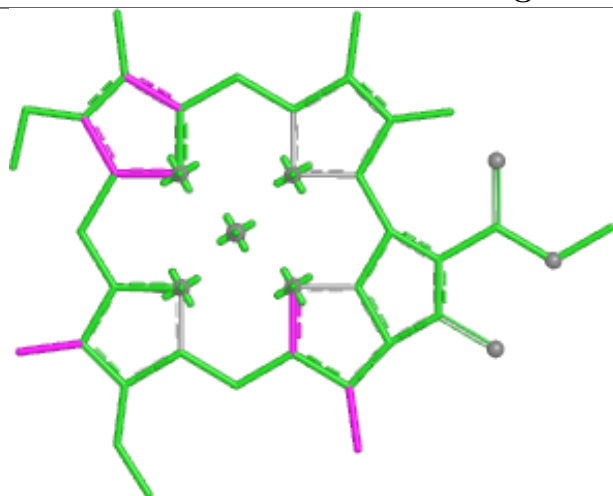
Ligand CLA Yy 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Cc 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

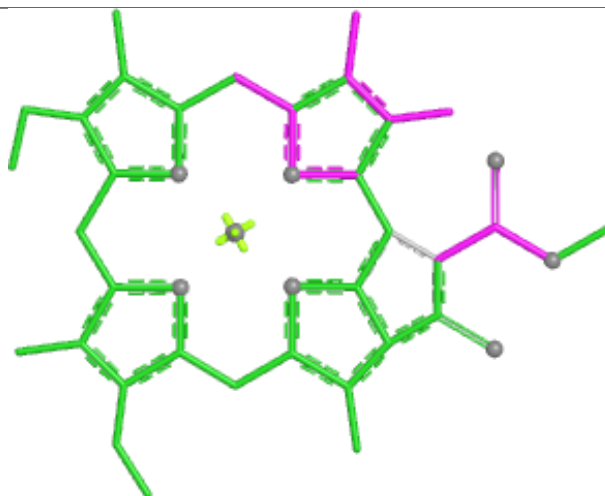
Ligand LUT y 318	
	
Bond lengths	Bond angles
	
Torsions	Rings



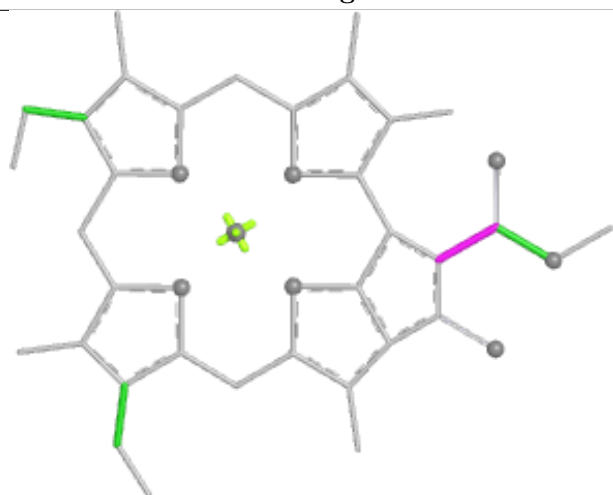
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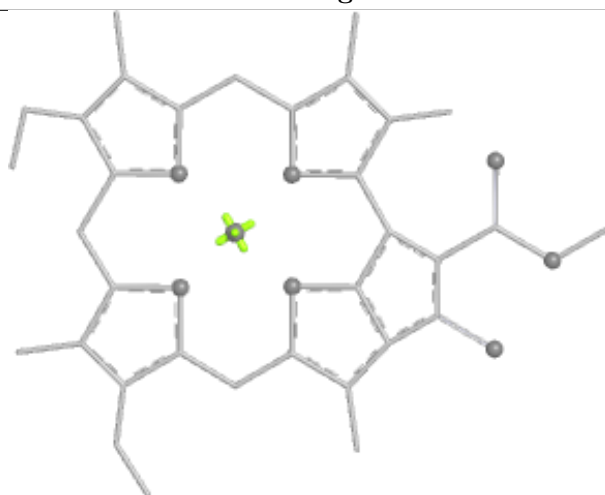
Bond lengths



Bond angles

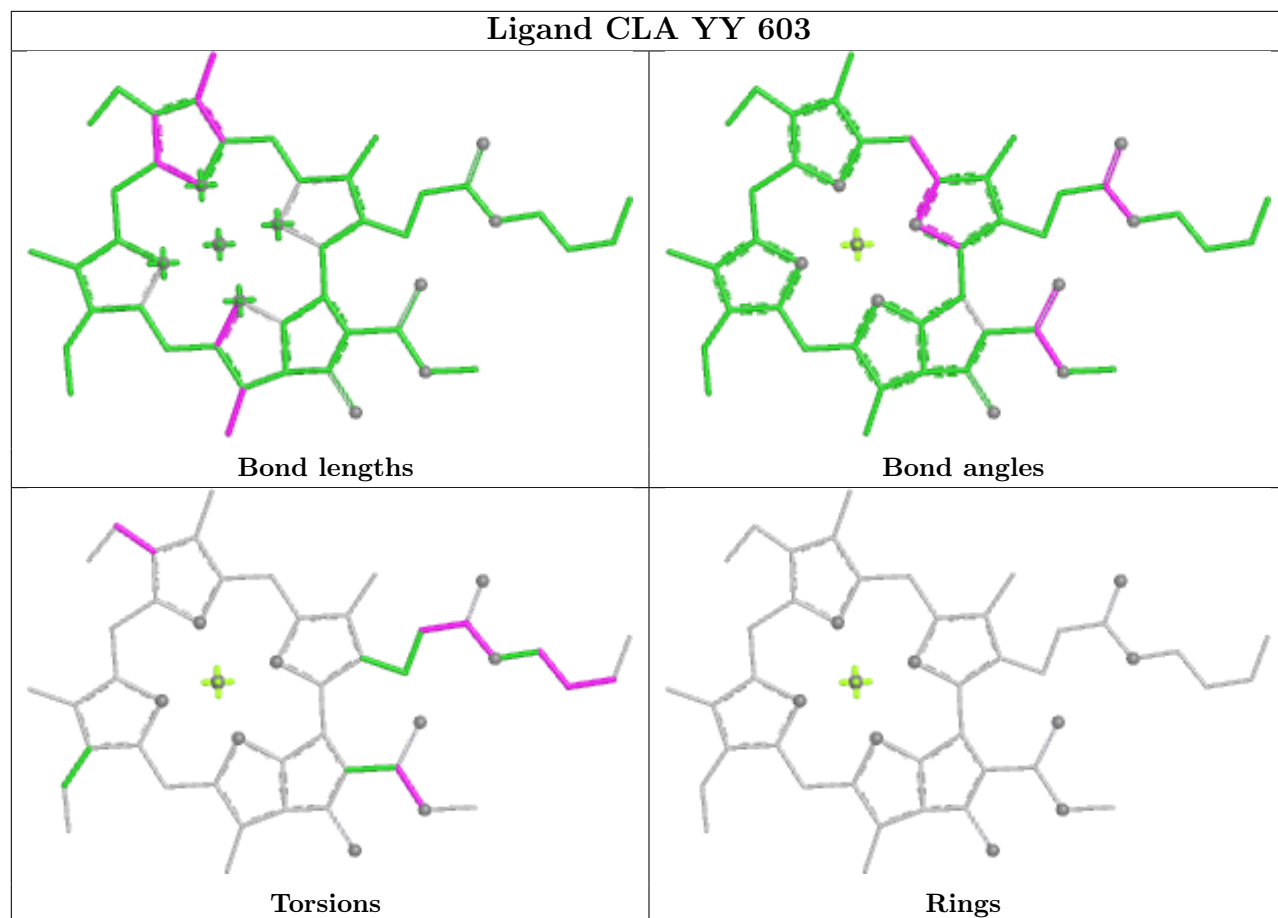


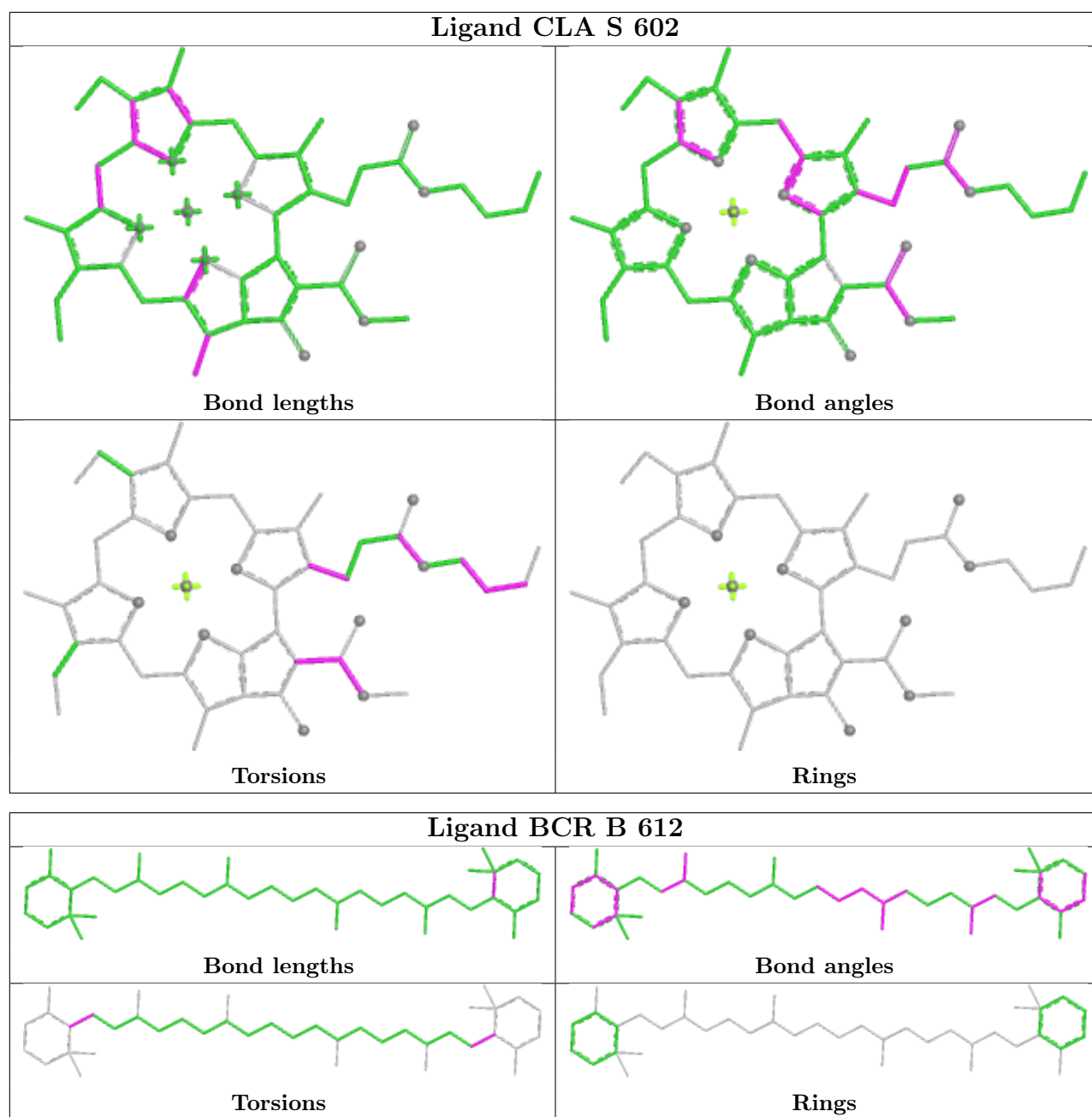
Torsions

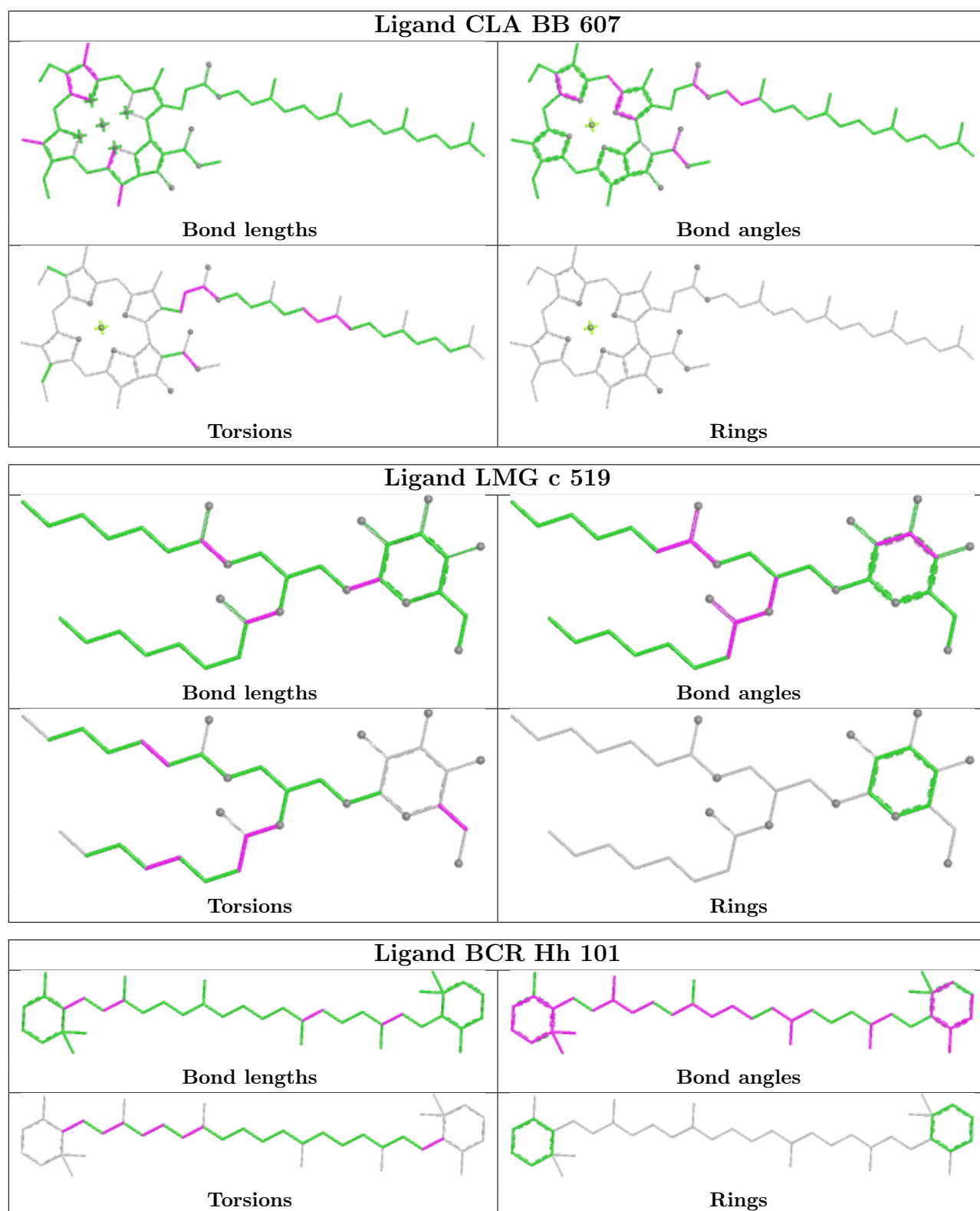


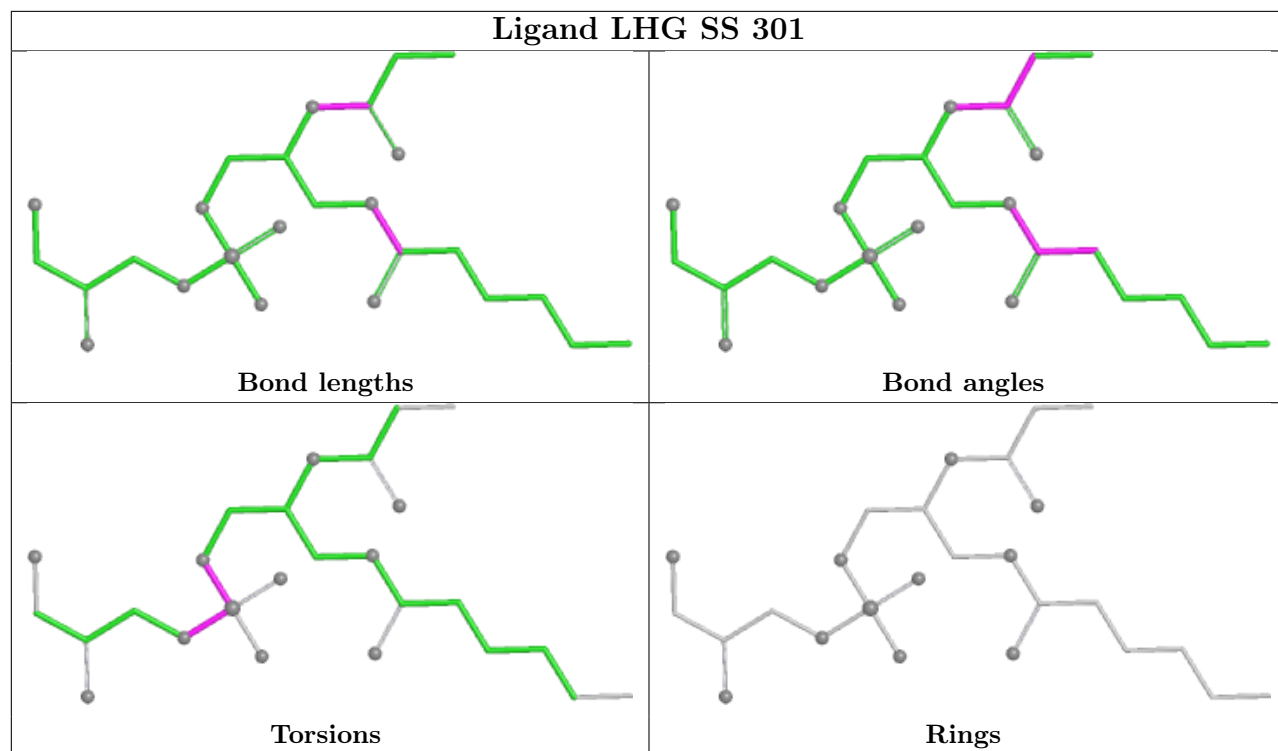
Rings

Ligand CLA YY 603

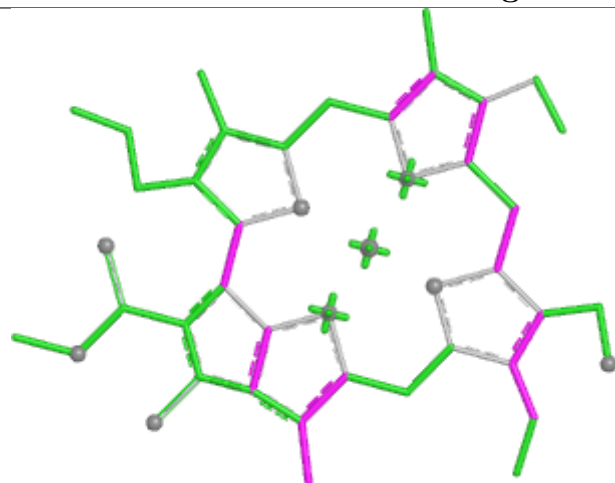




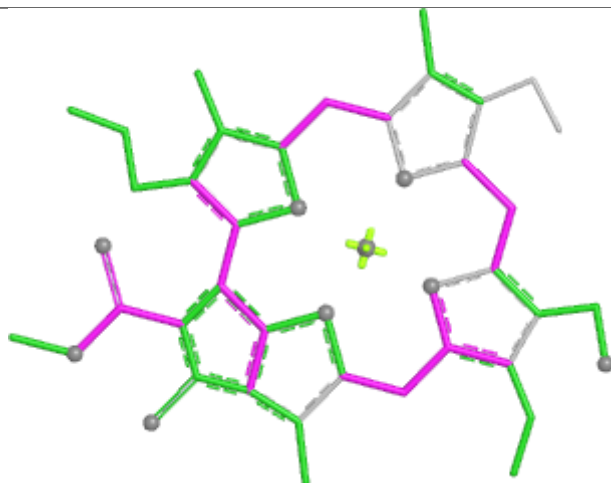




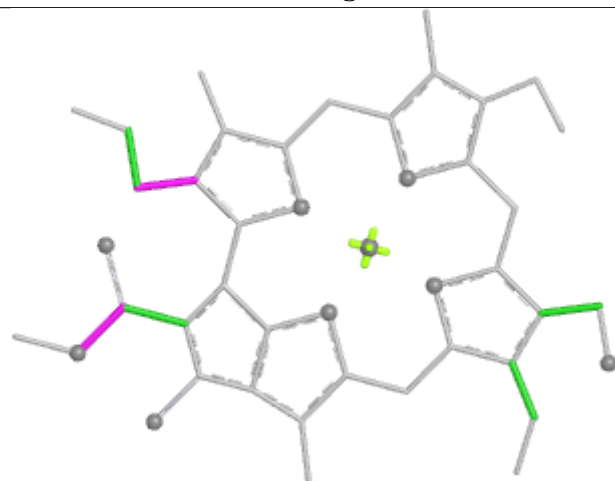
Ligand CHL YY 606



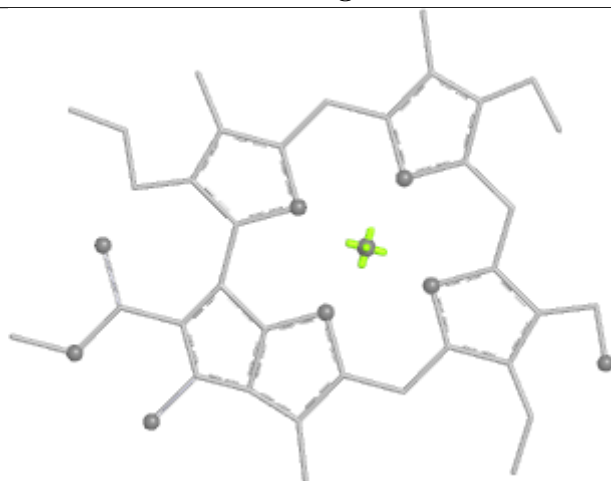
Bond lengths



Bond angles

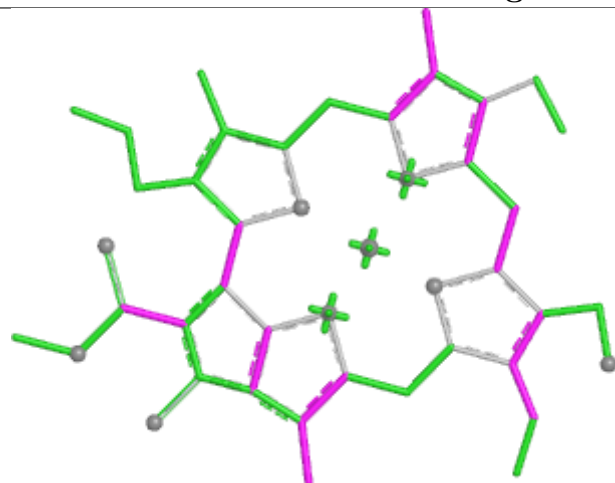


Torsions

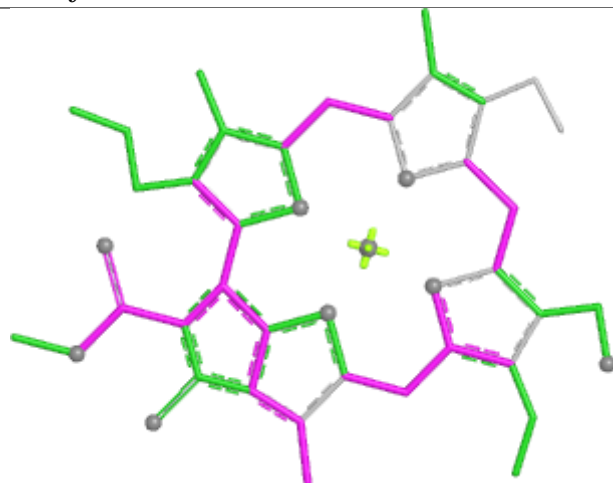


Rings

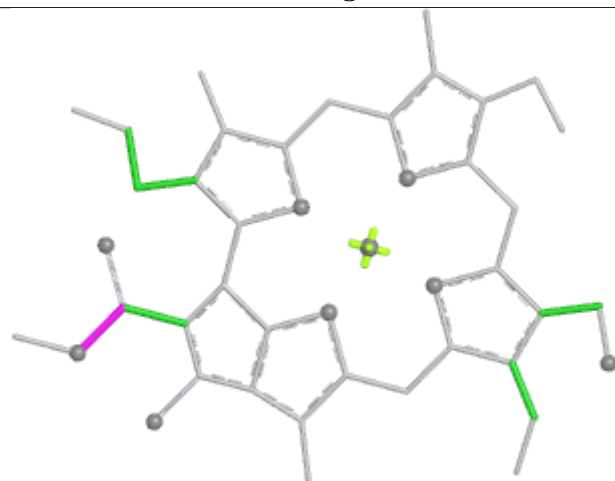
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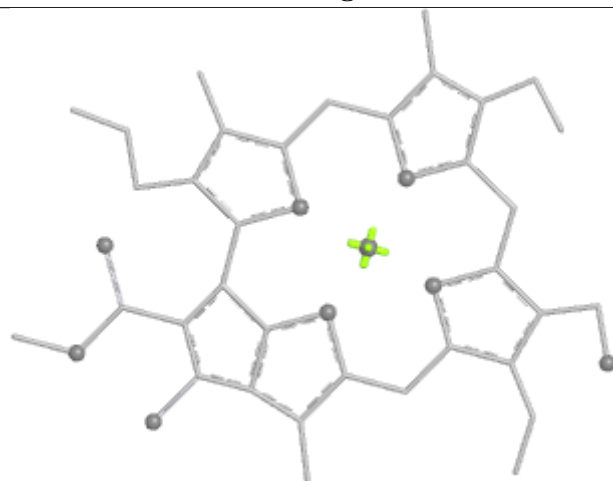
Bond lengths



Bond angles

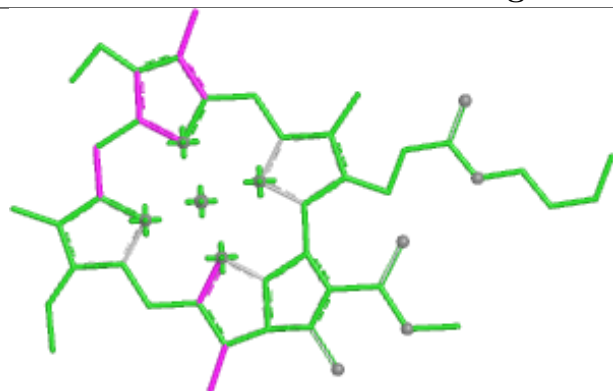


Torsions

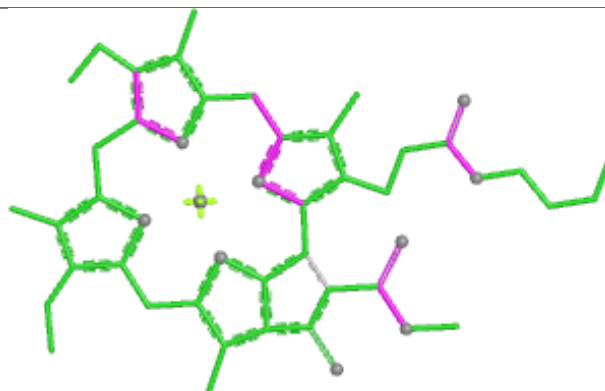


Rings

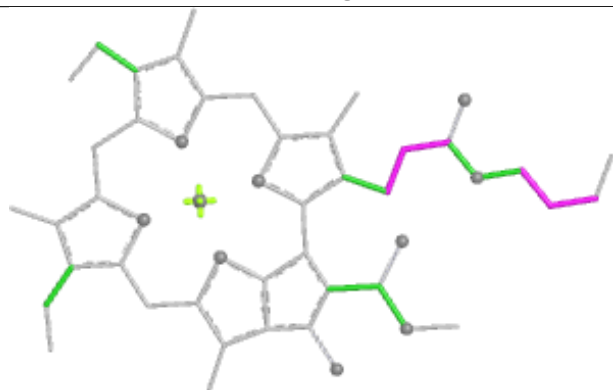
Ligand CLA SS 314



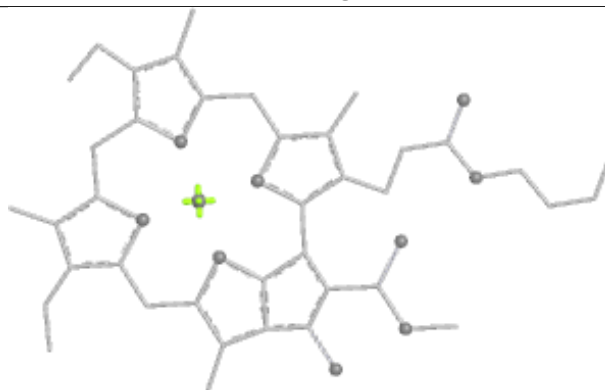
Bond lengths



Bond angles

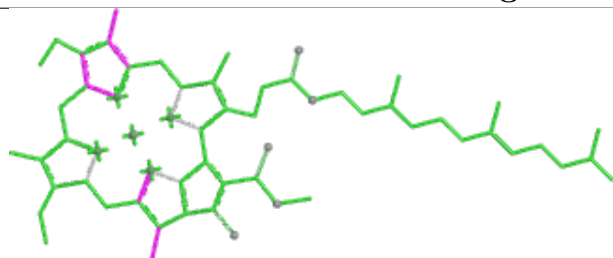


Torsions

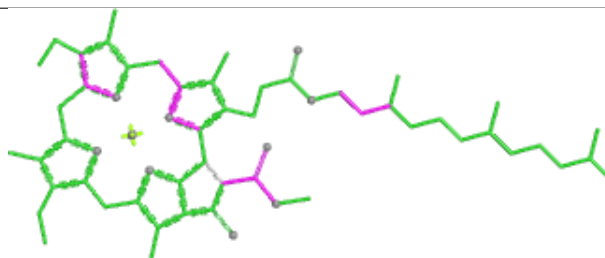


Rings

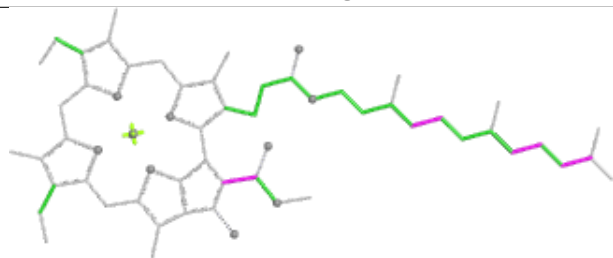
Ligand CLA AA 408



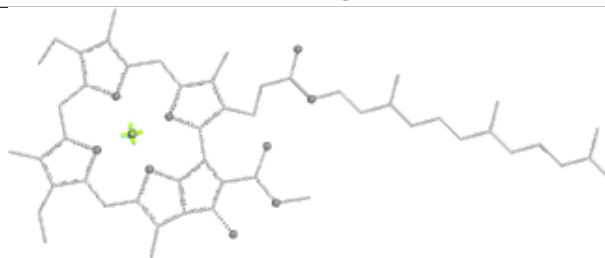
Bond lengths



Bond angles

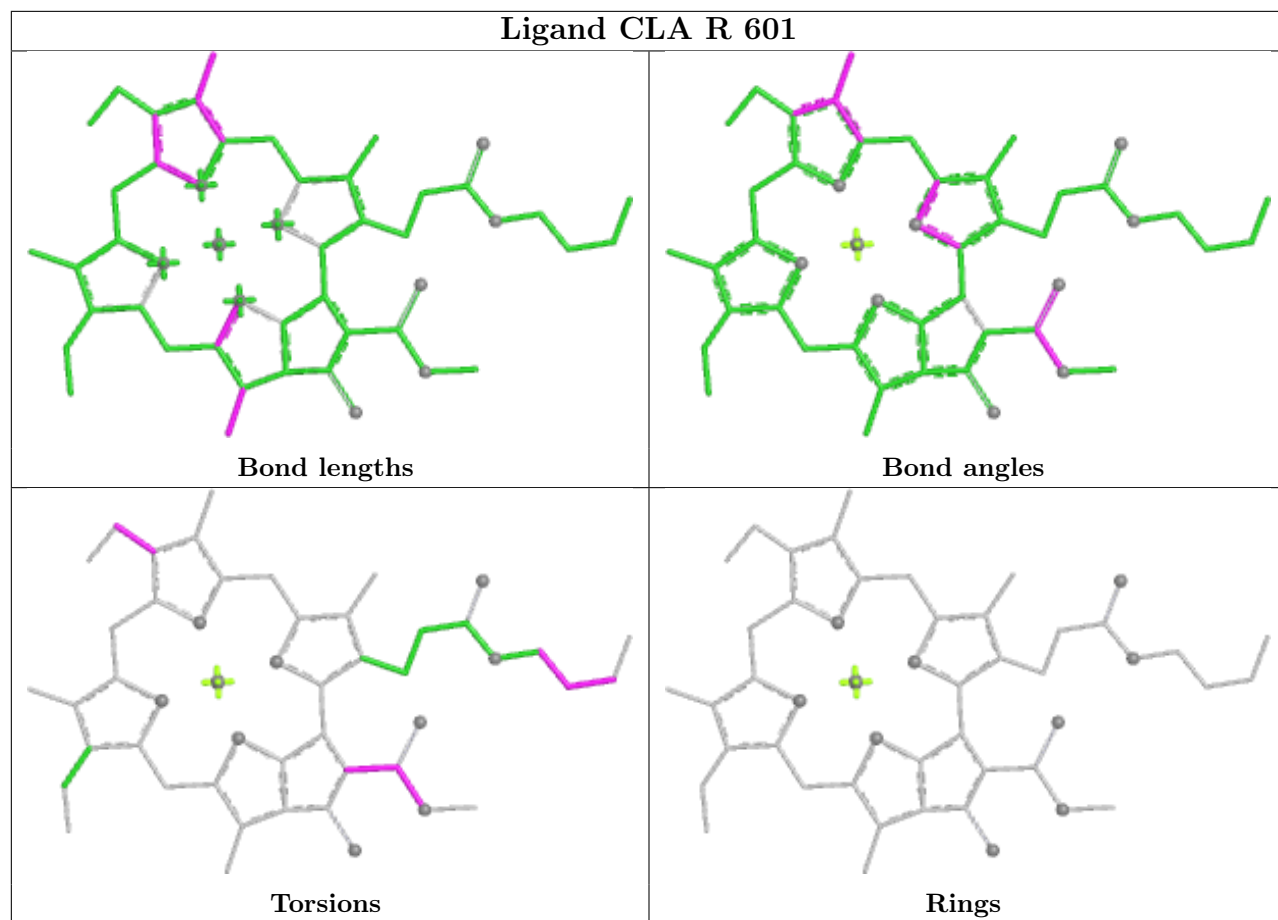


Torsions

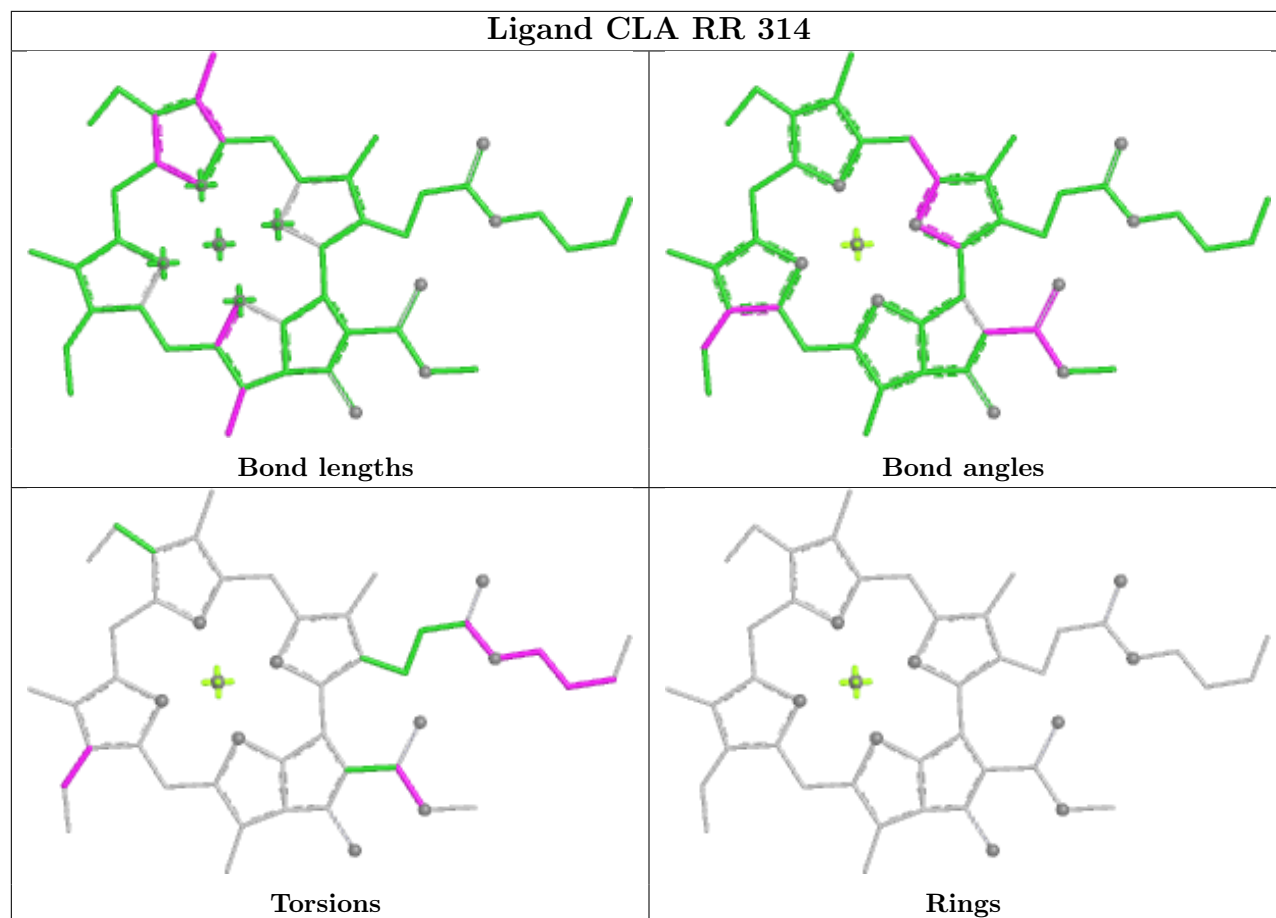


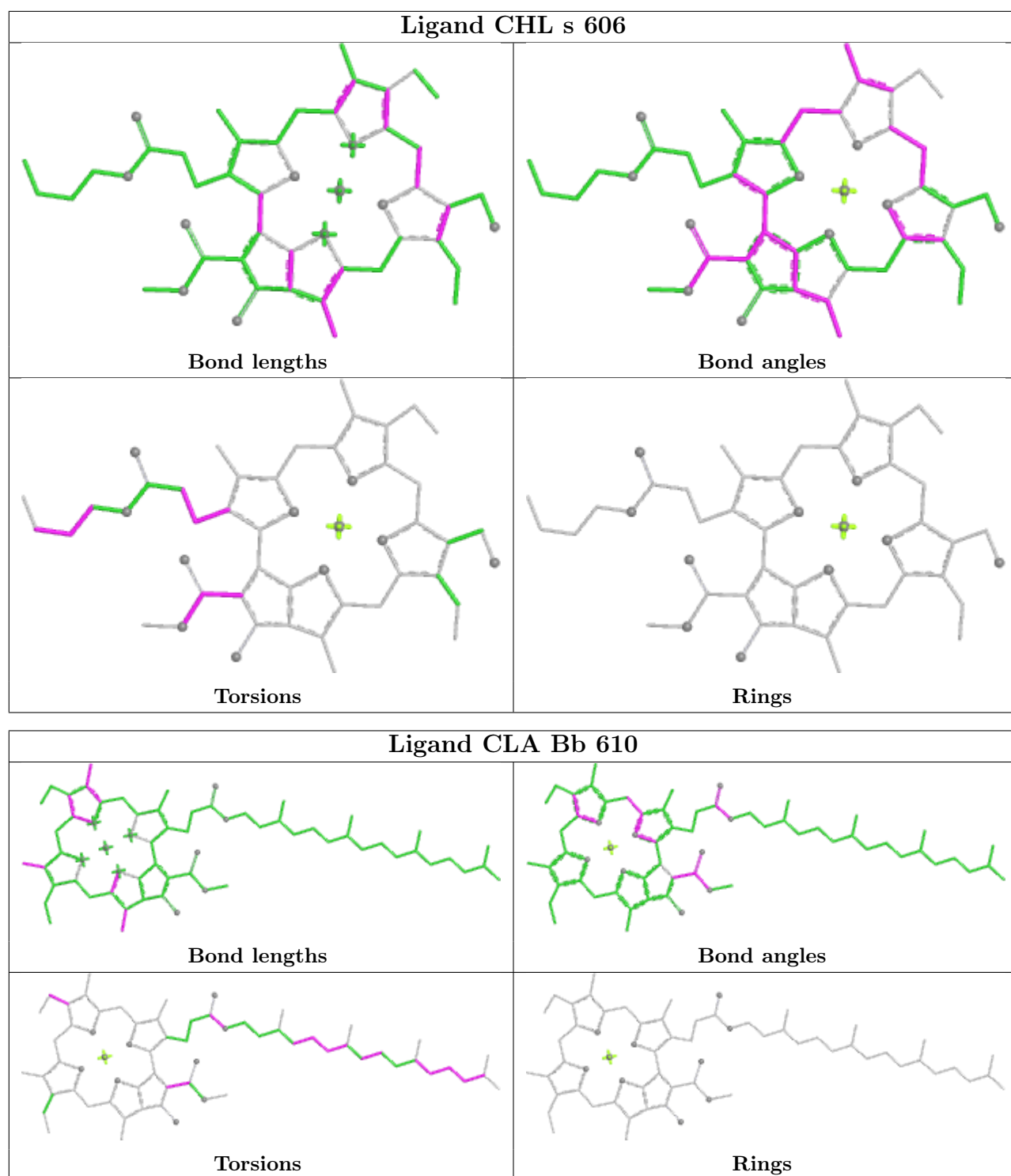
Rings

Ligand CLA R 601

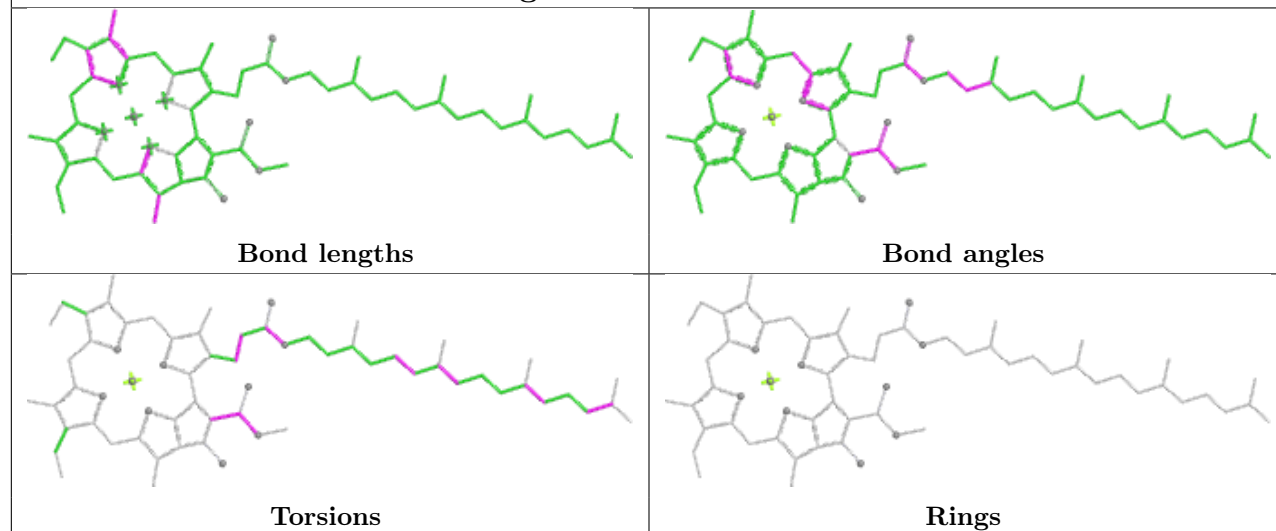


Ligand CLA RR 314

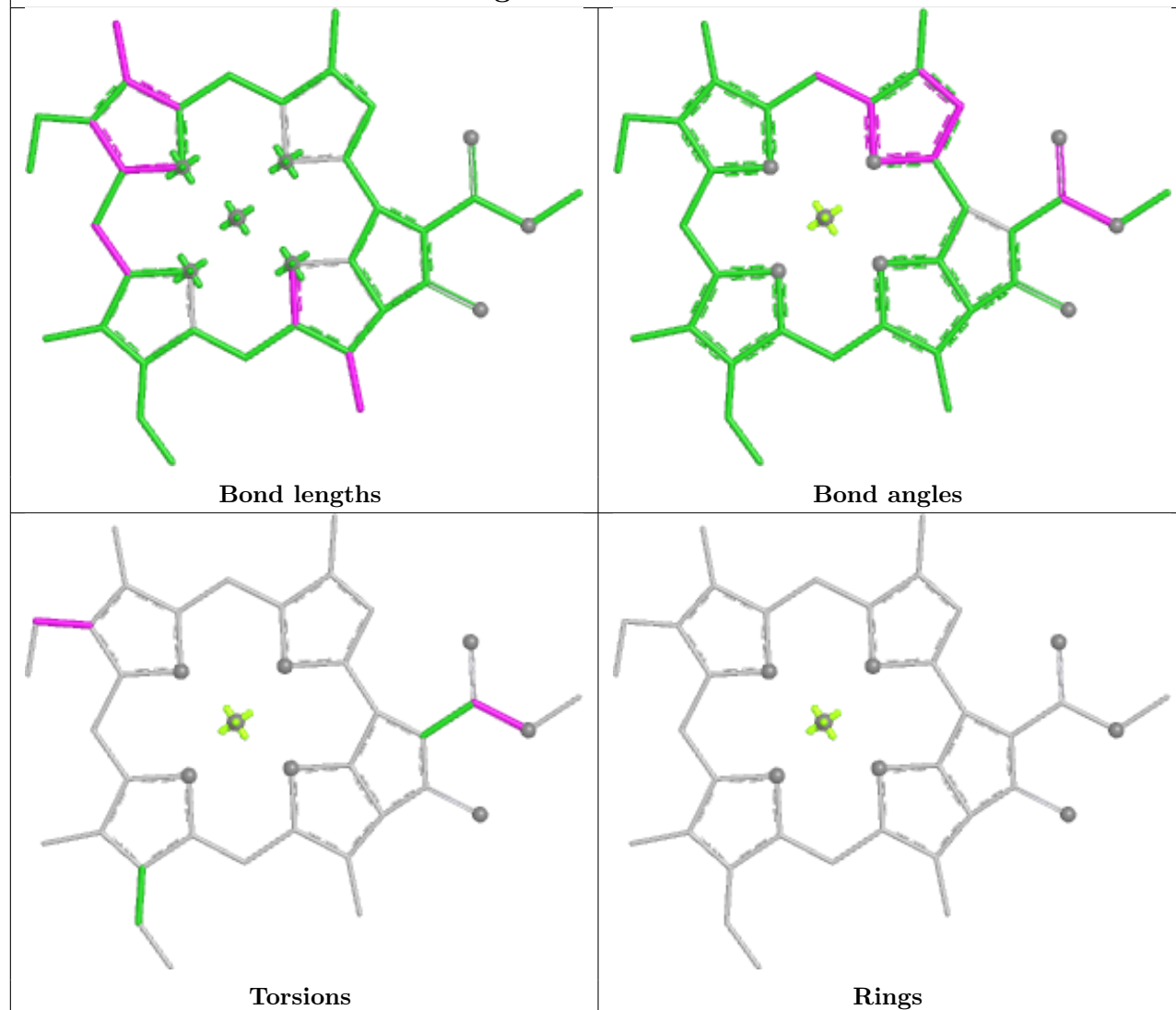




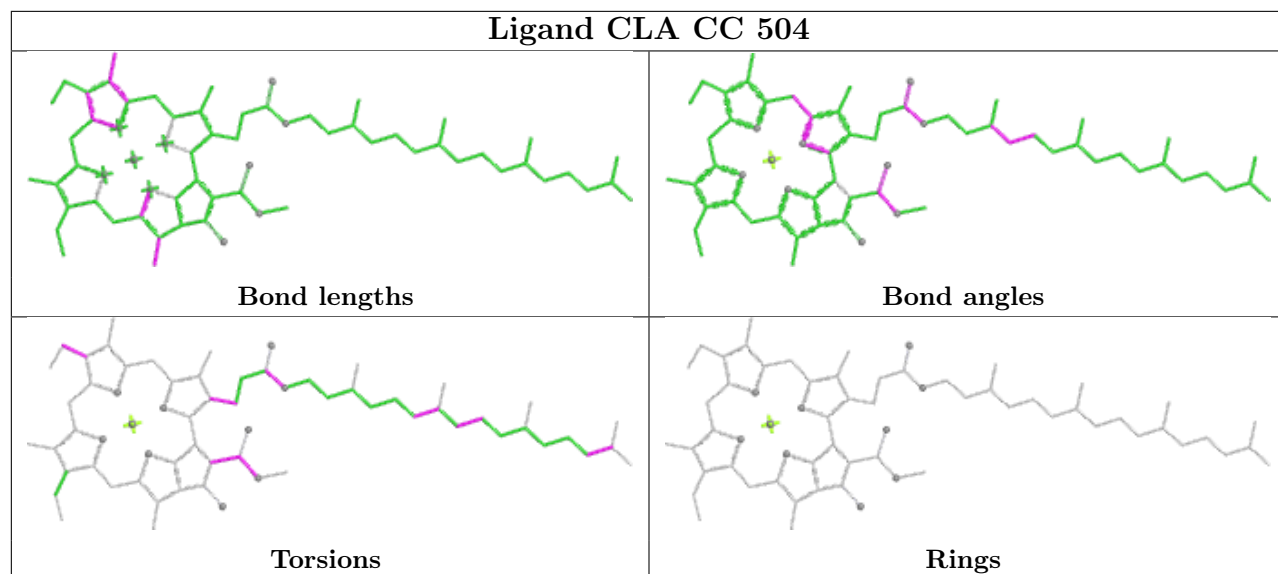
Ligand CLA BB 605



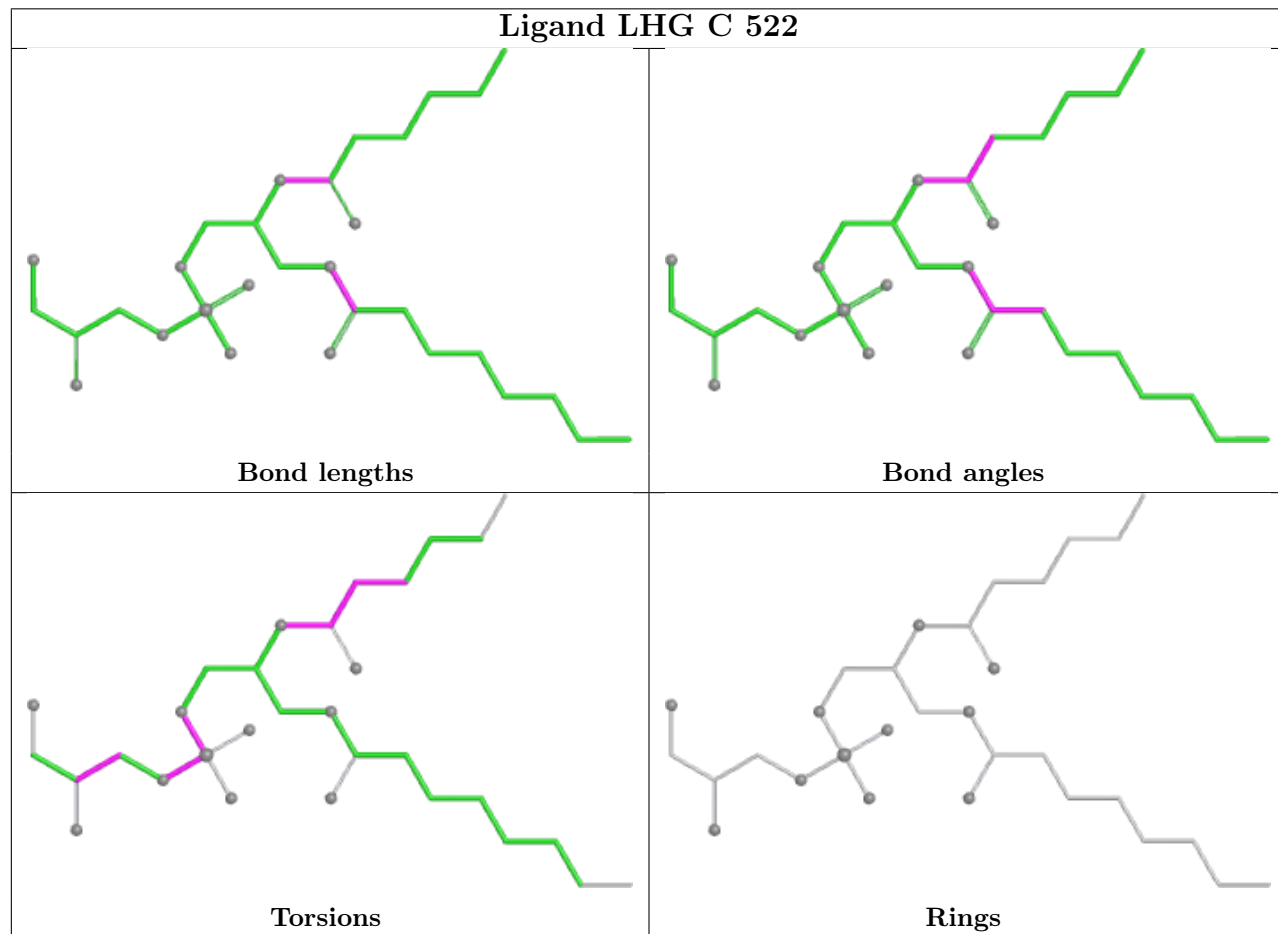
Ligand CLA 2 603

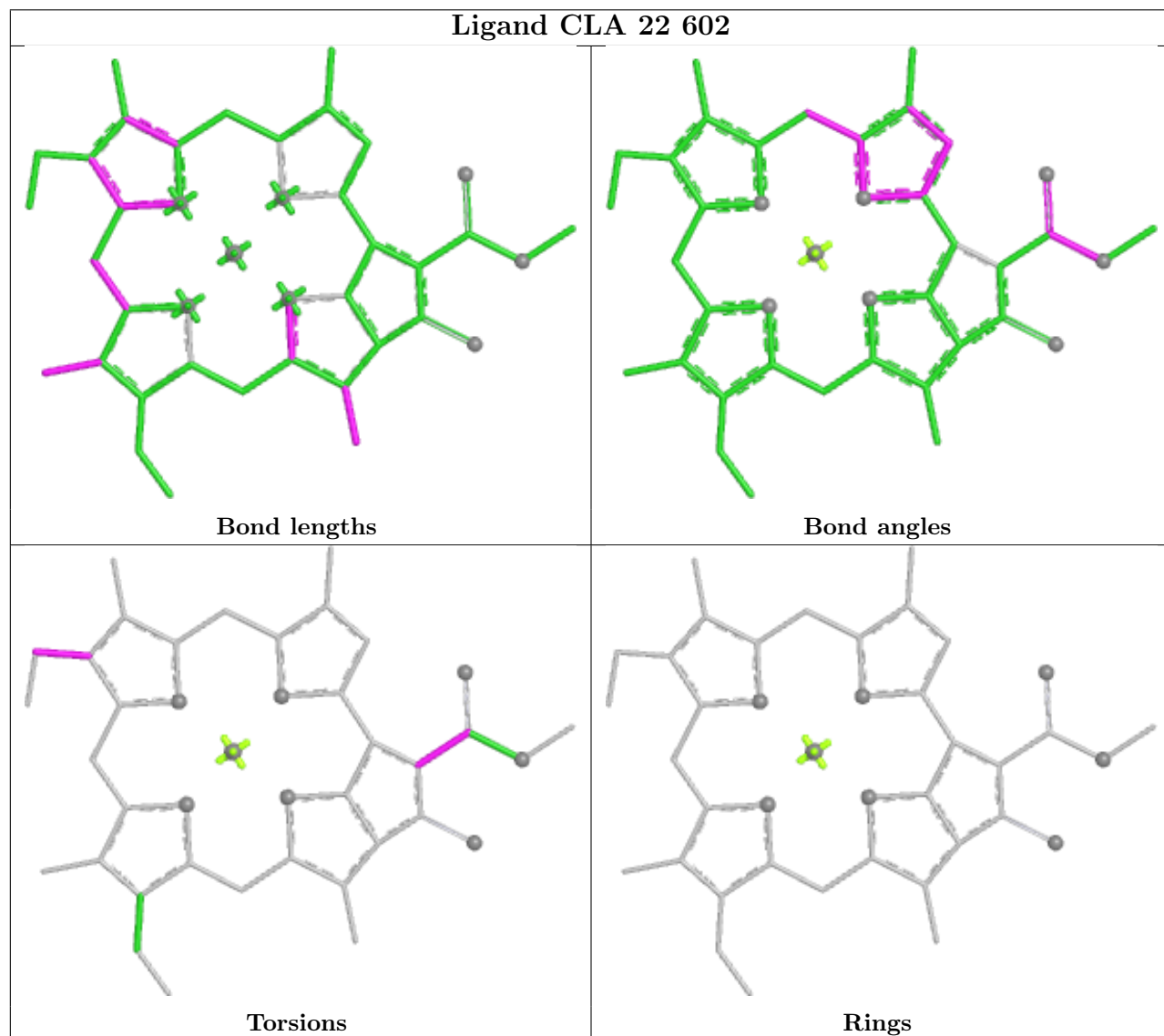
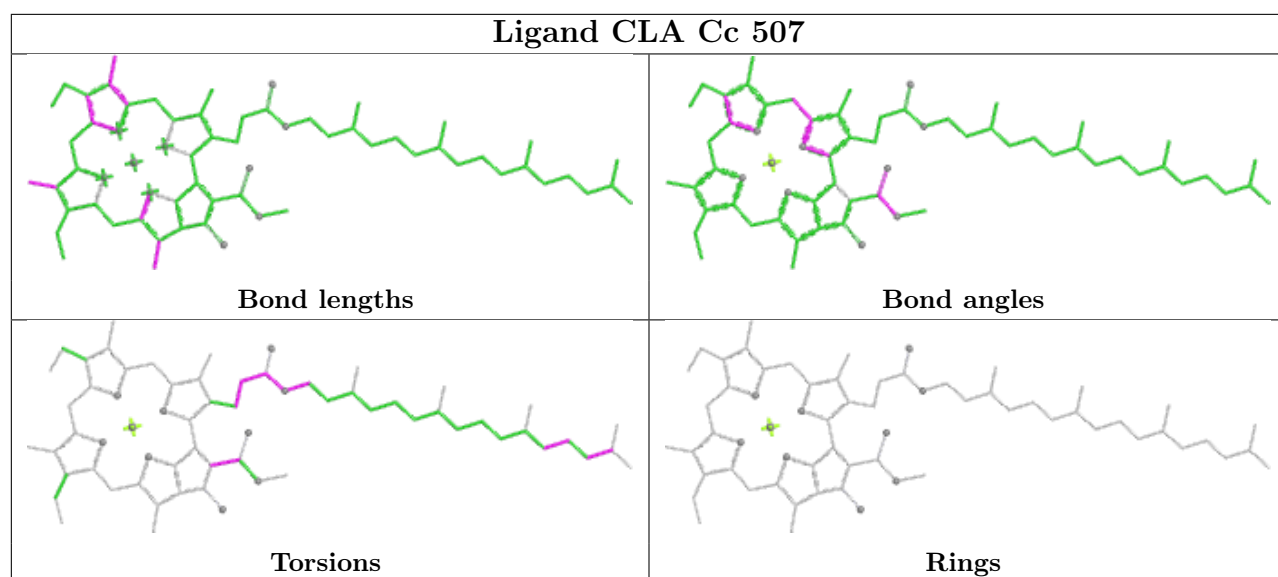


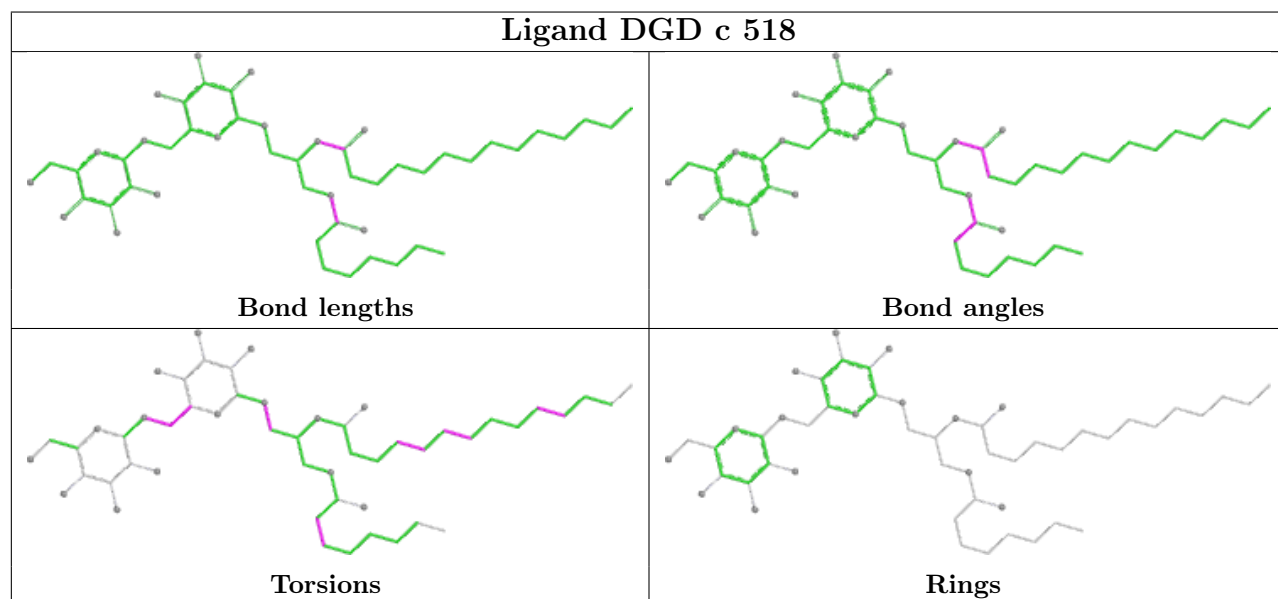
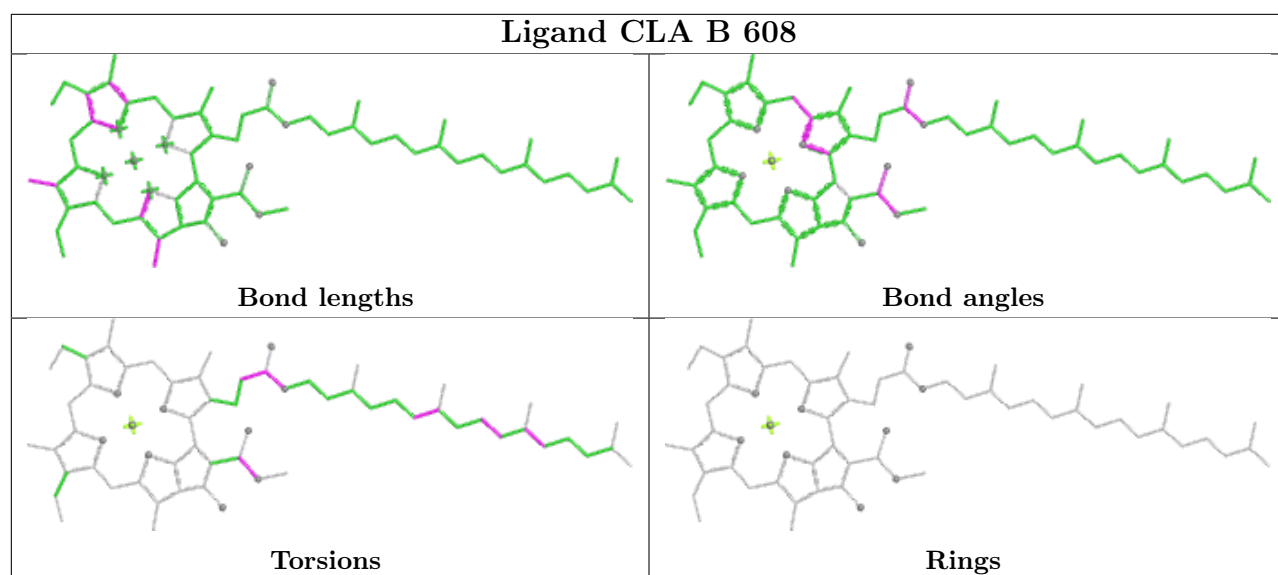
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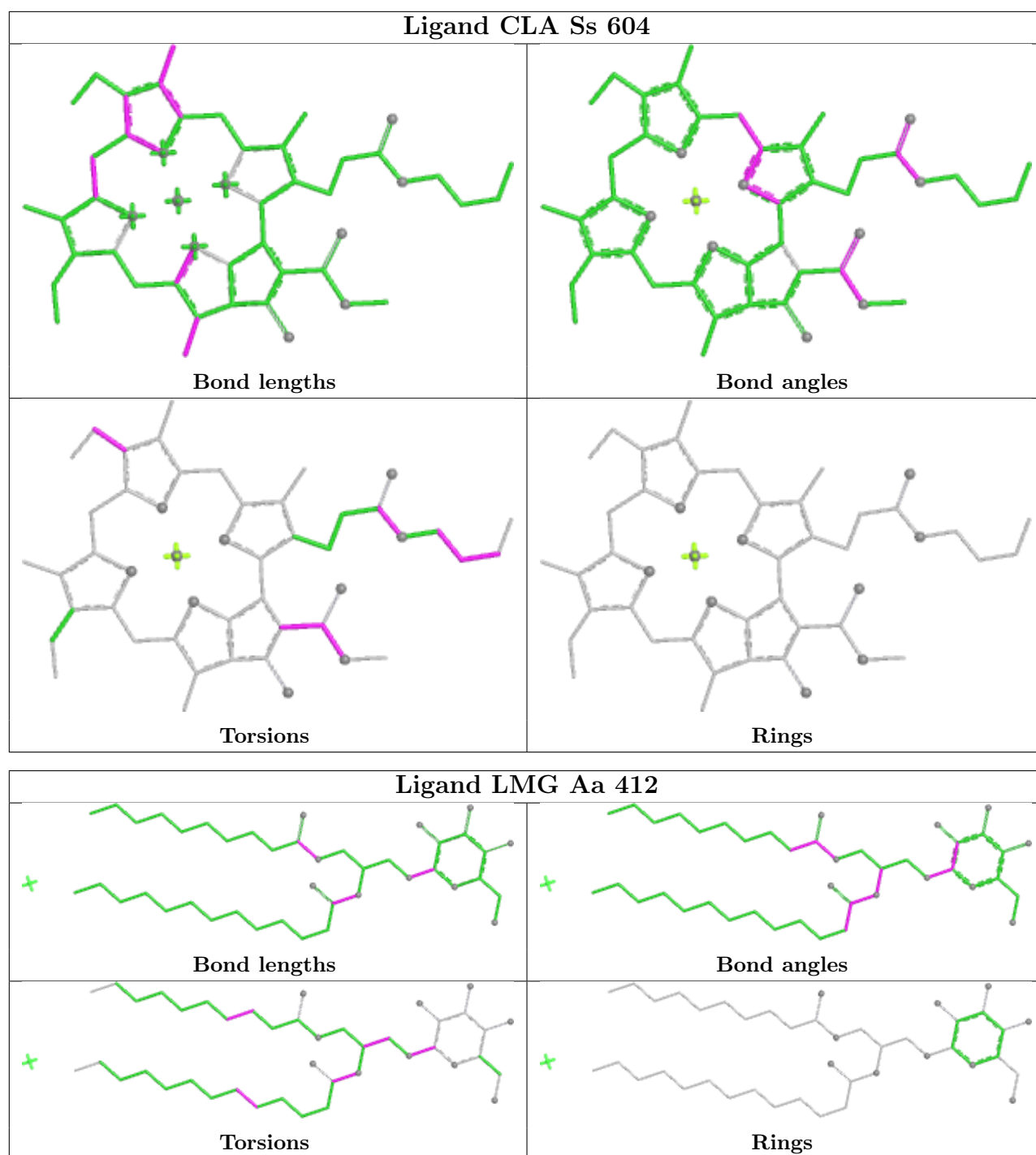


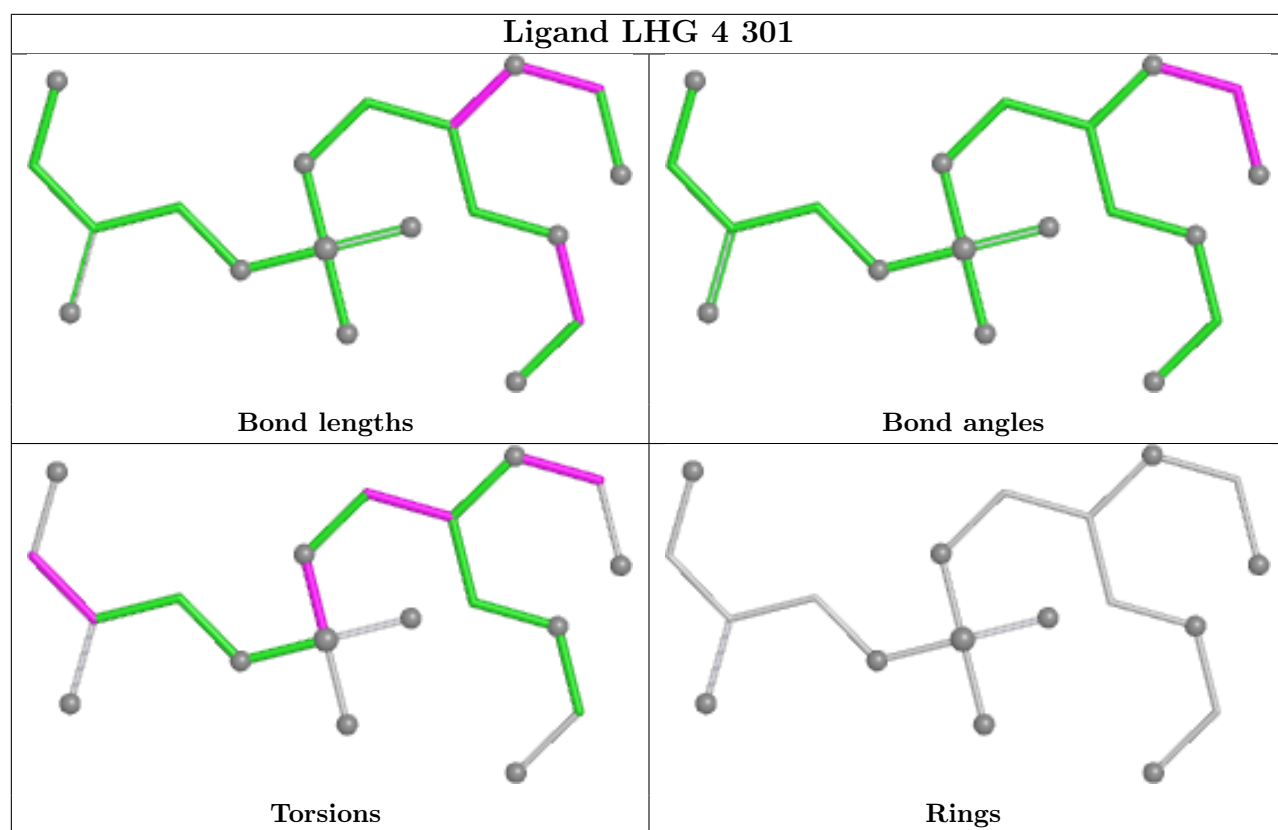
Ligand LHG C 522



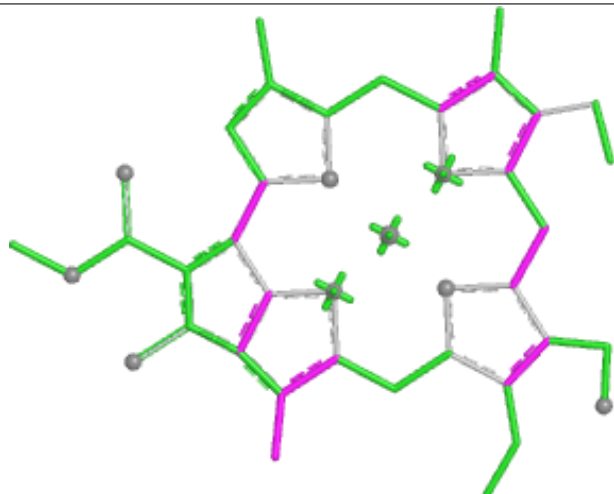




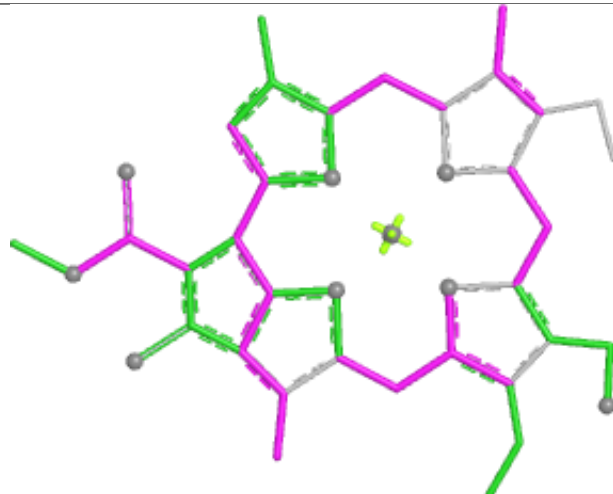




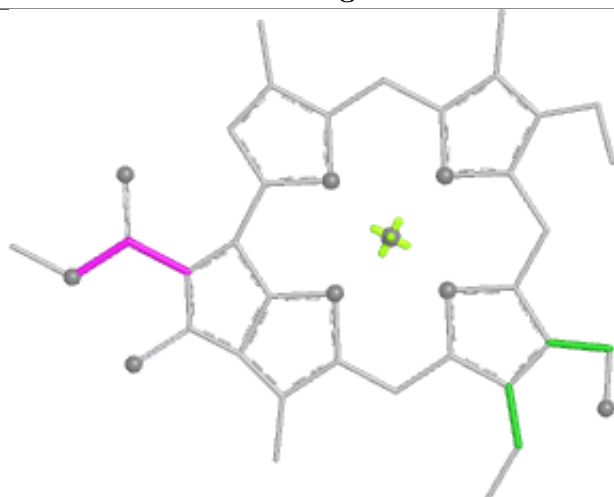
Ligand CHL 1 607



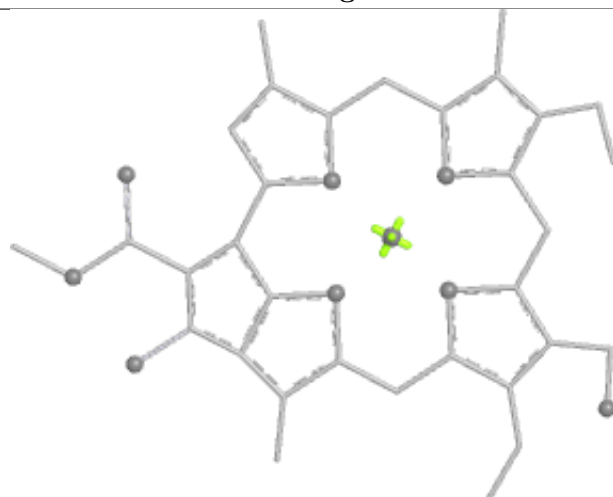
Bond lengths



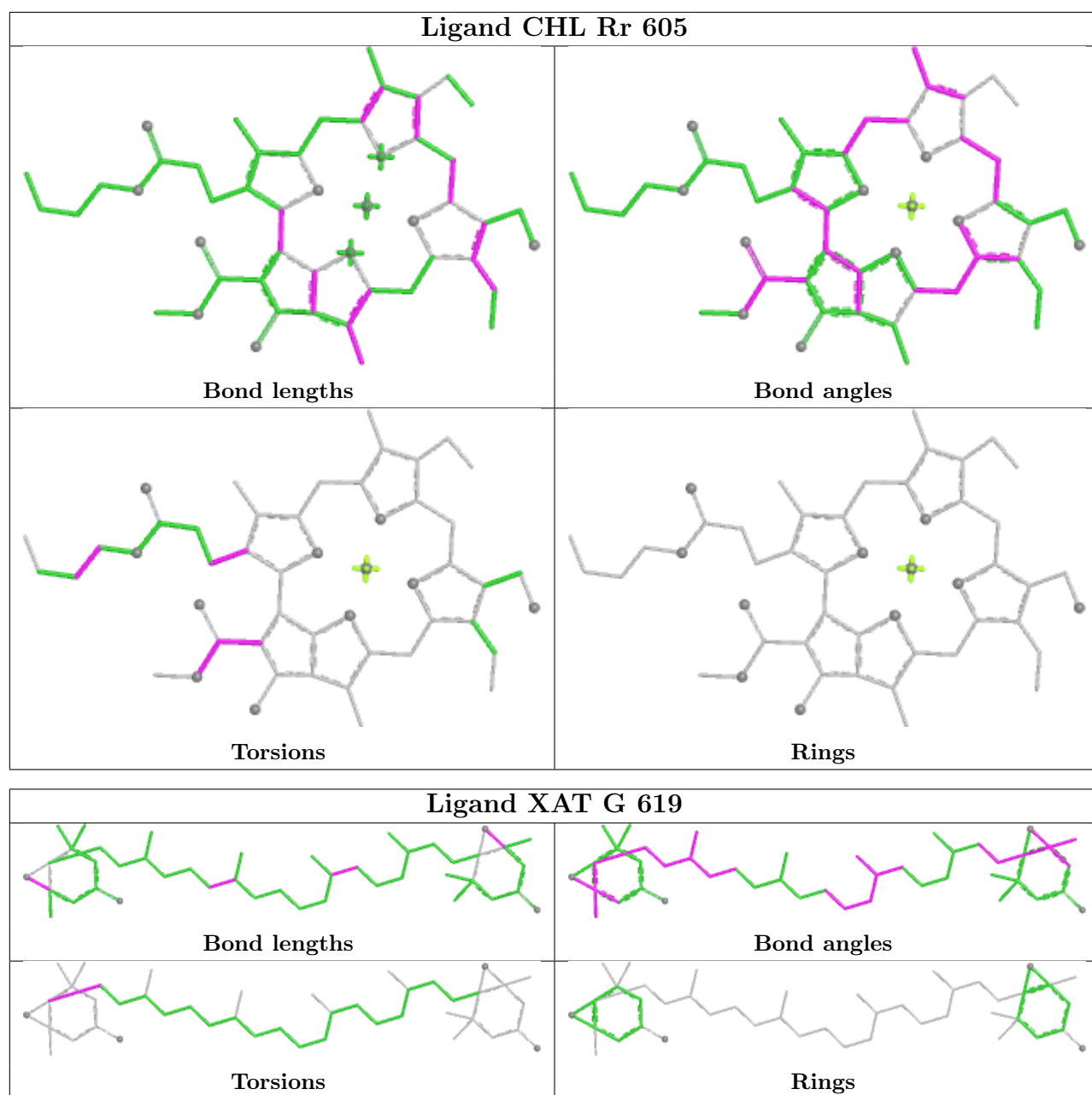
Bond angles



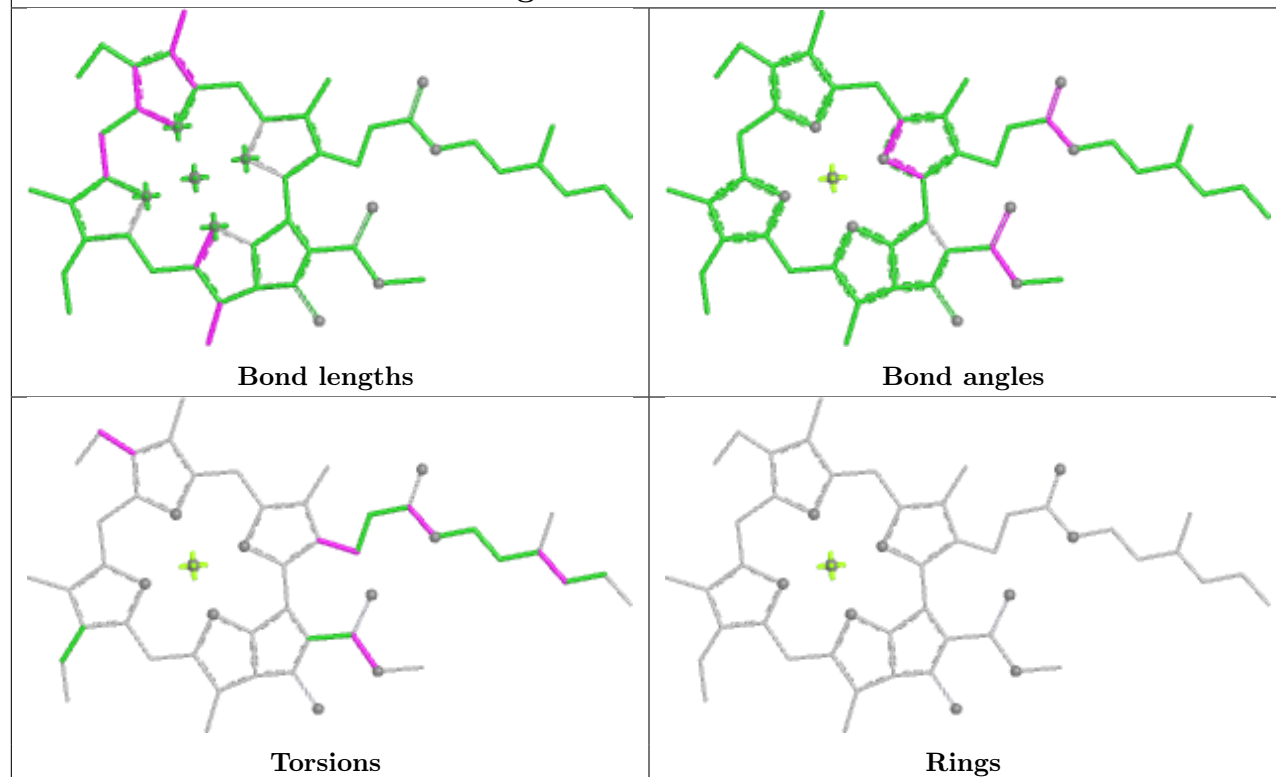
Torsions



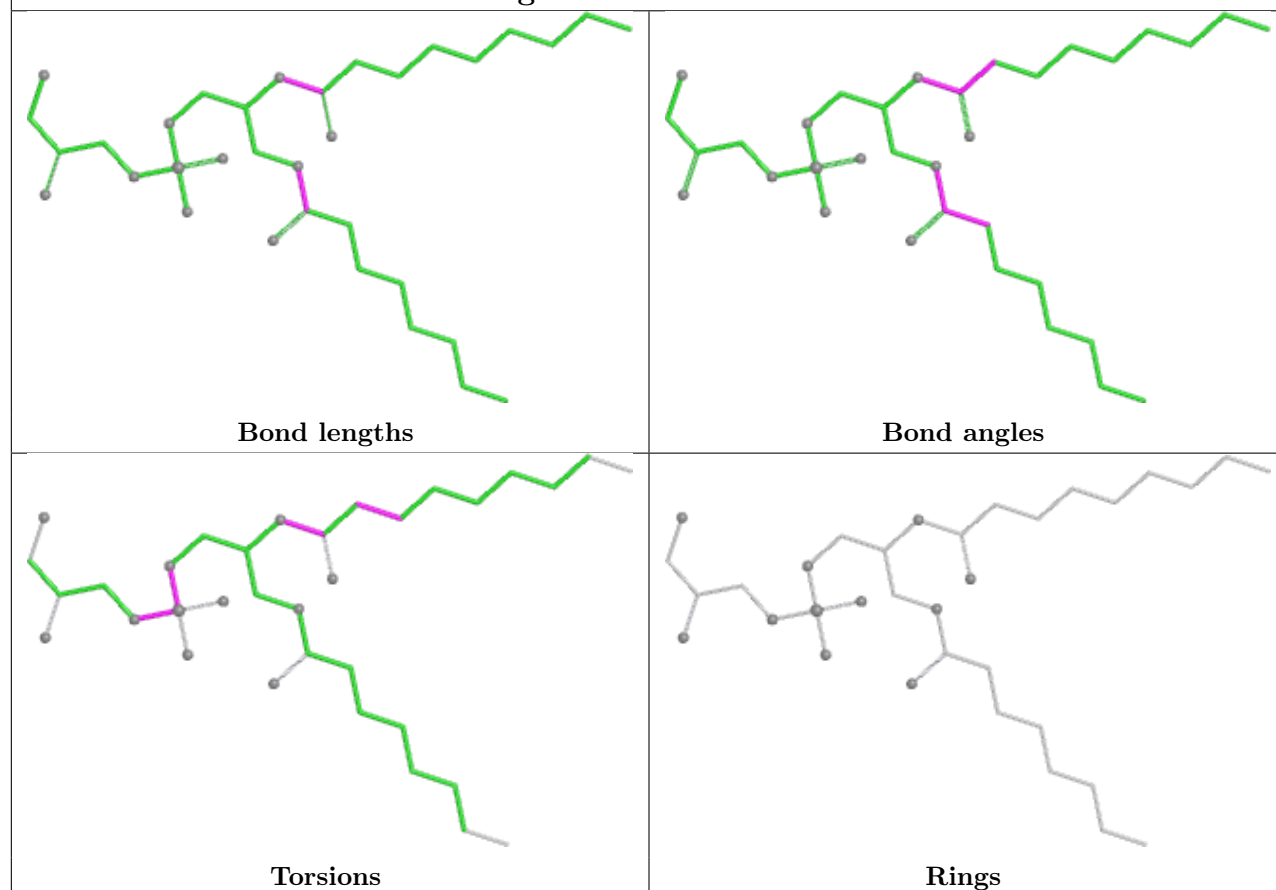
Rings

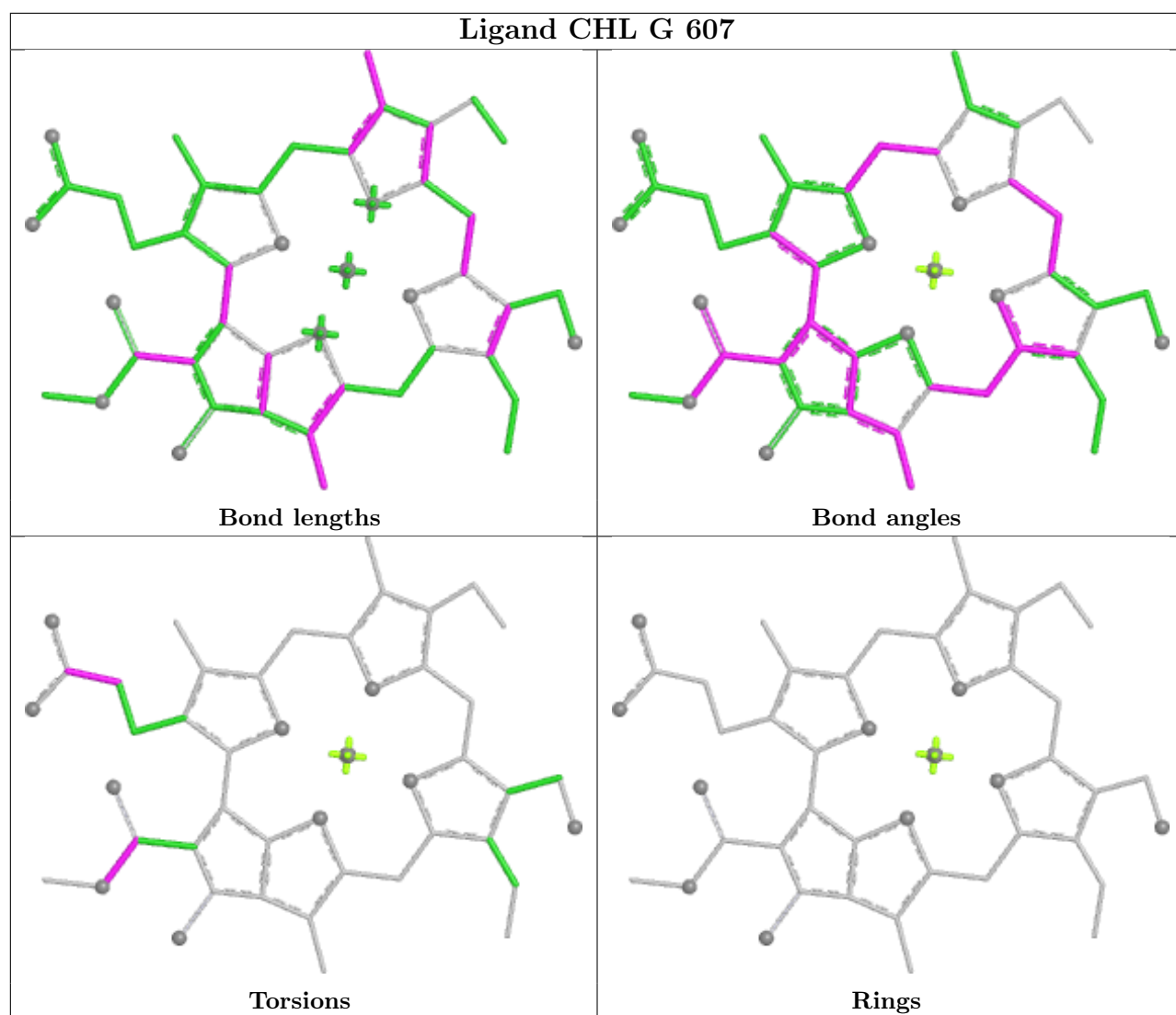


Ligand CLA GG 611

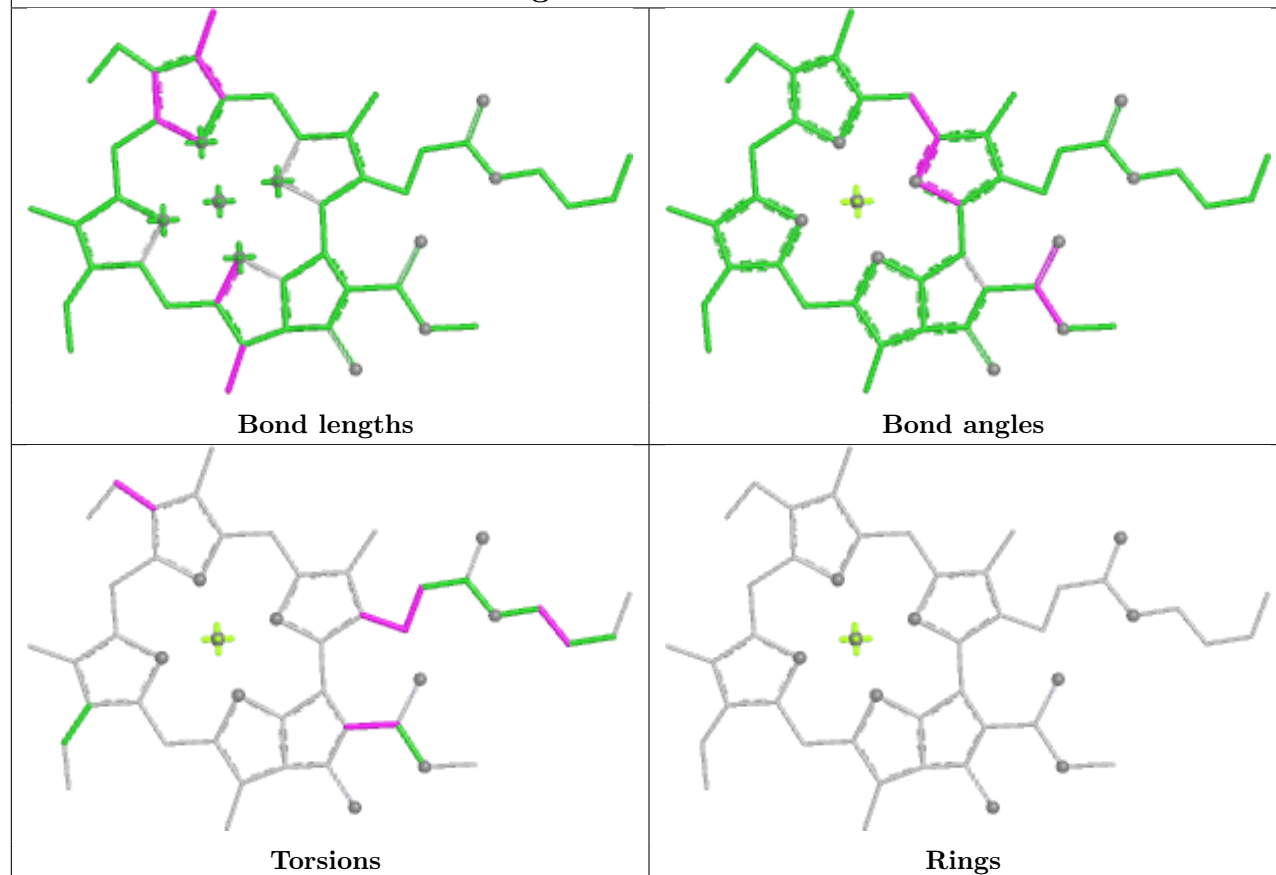


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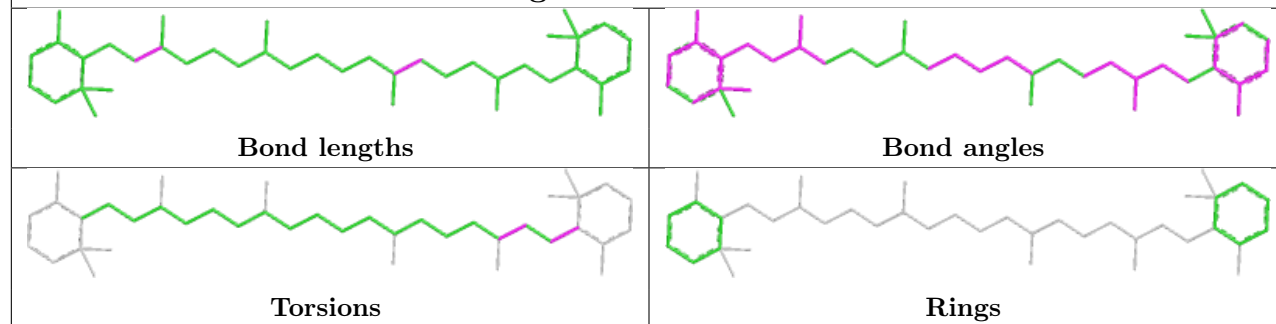


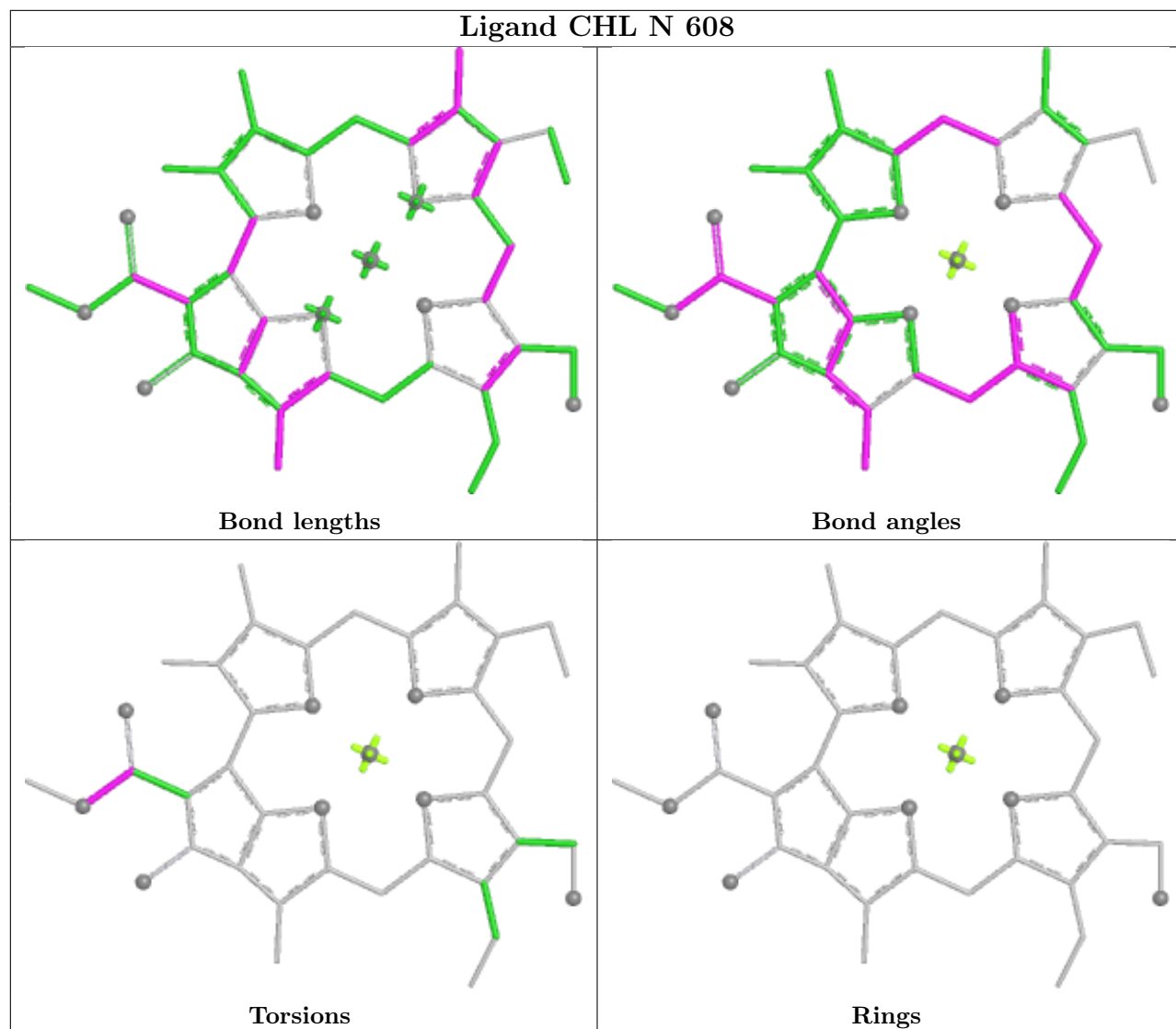


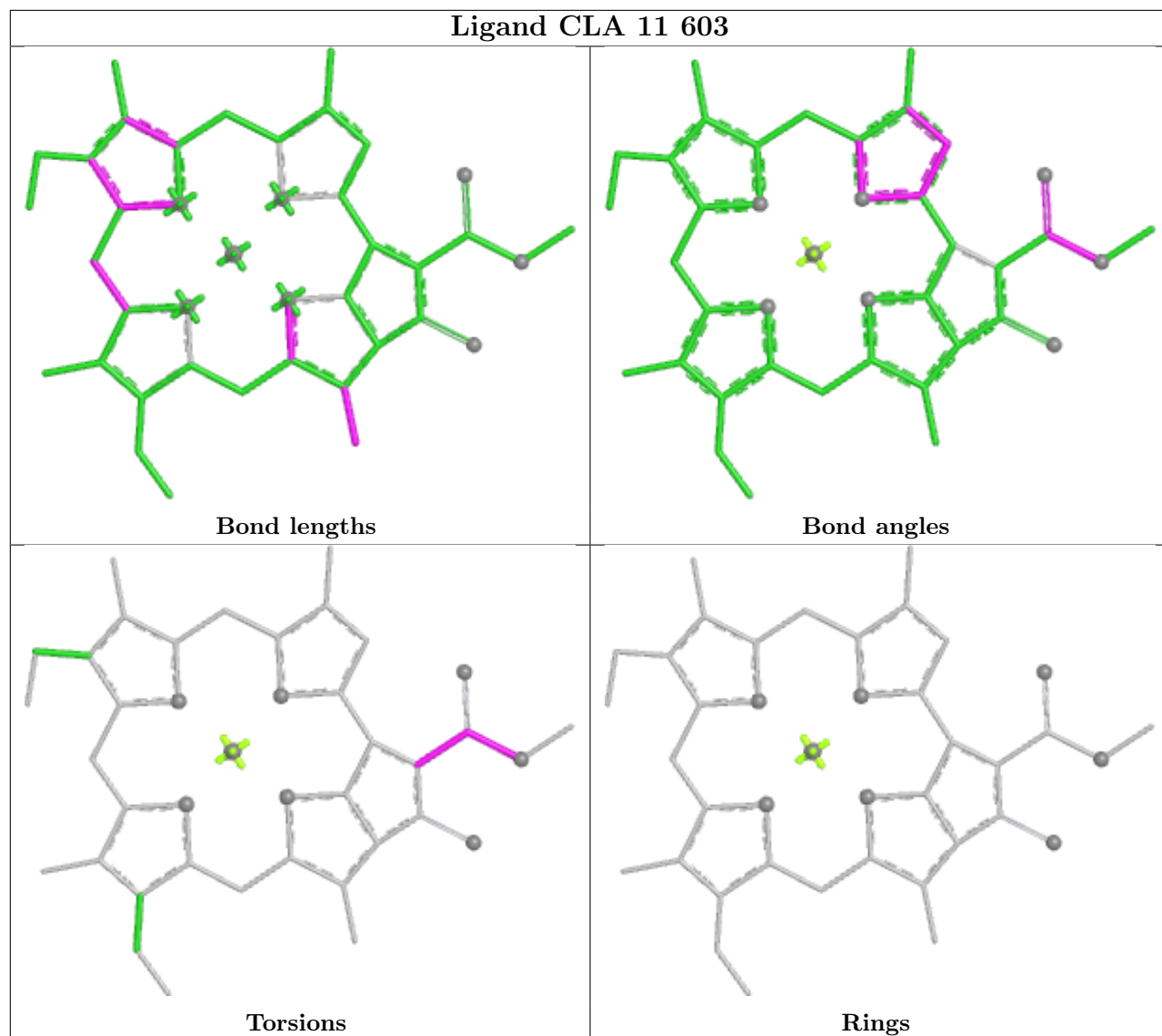
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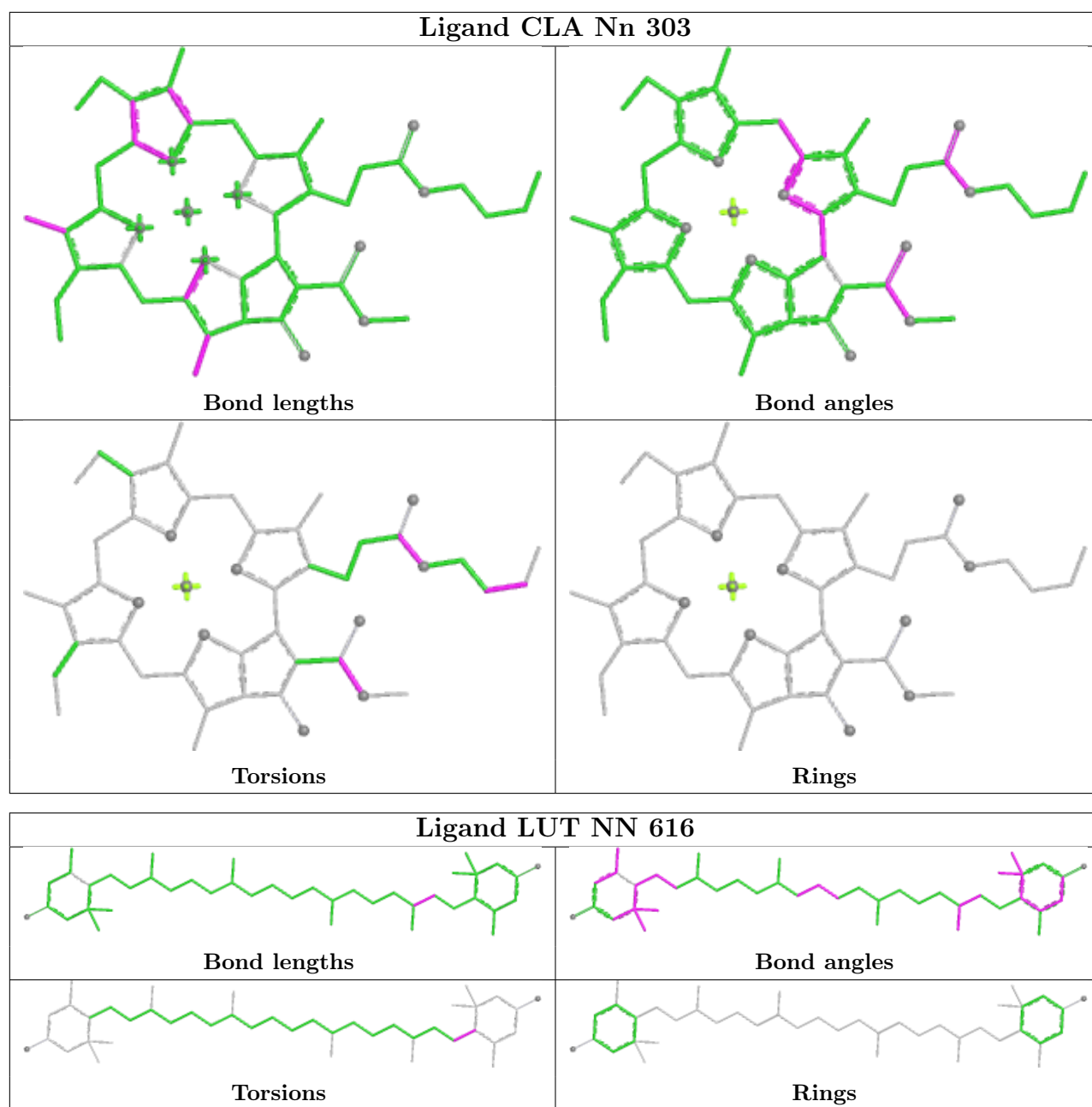


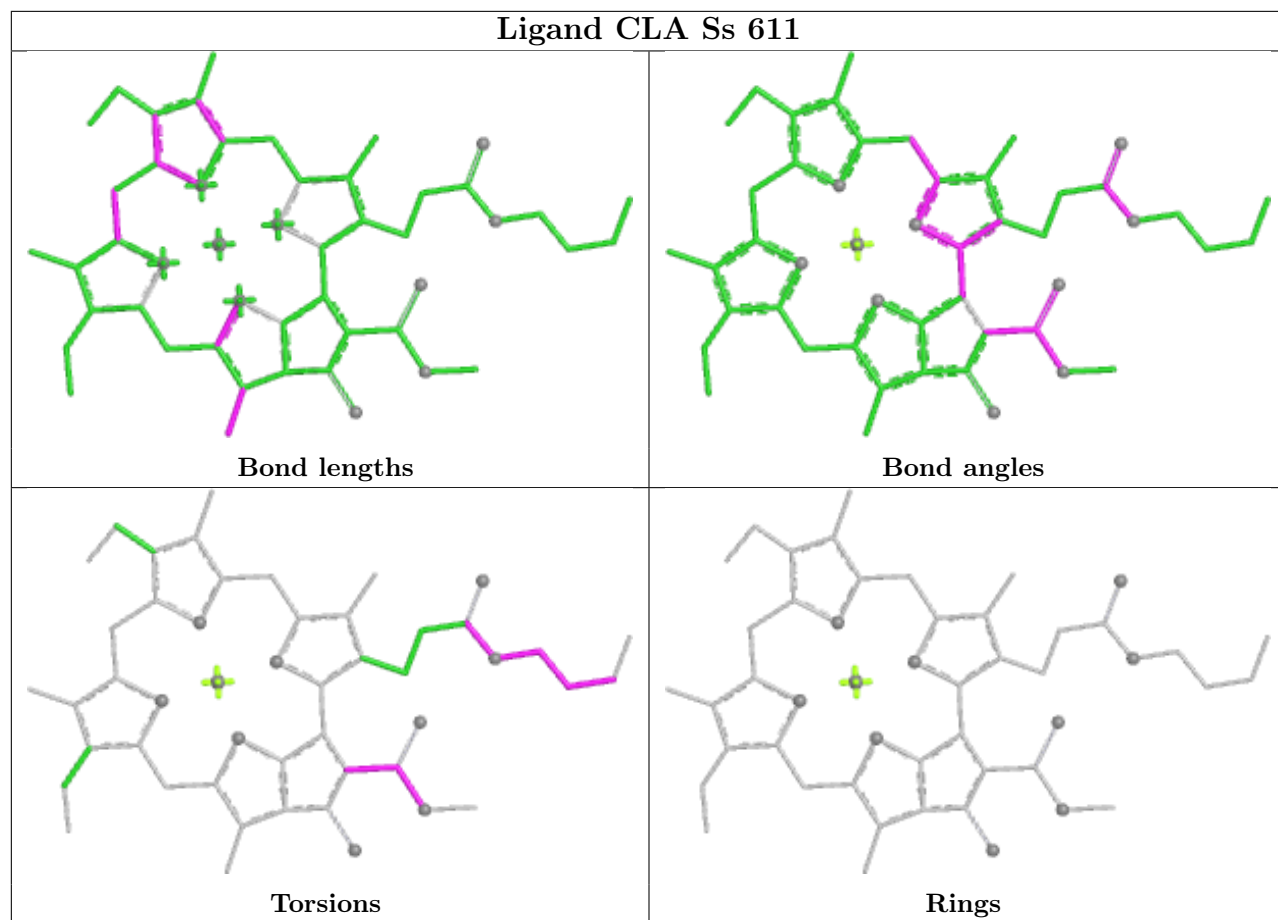
Ligand BCR H 101



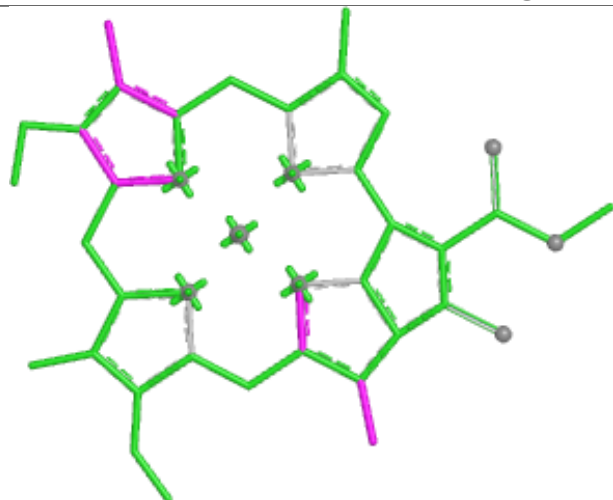




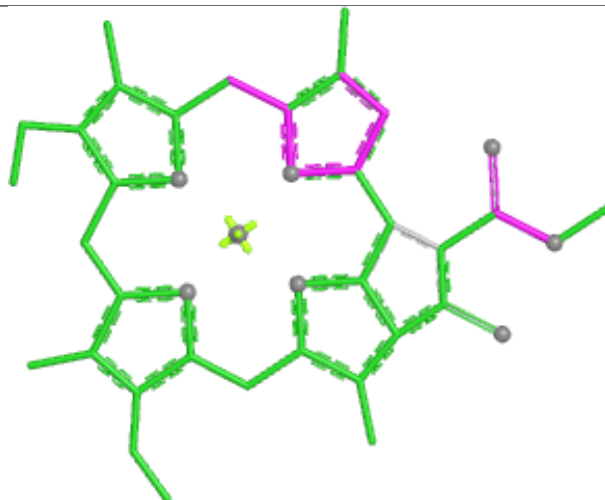




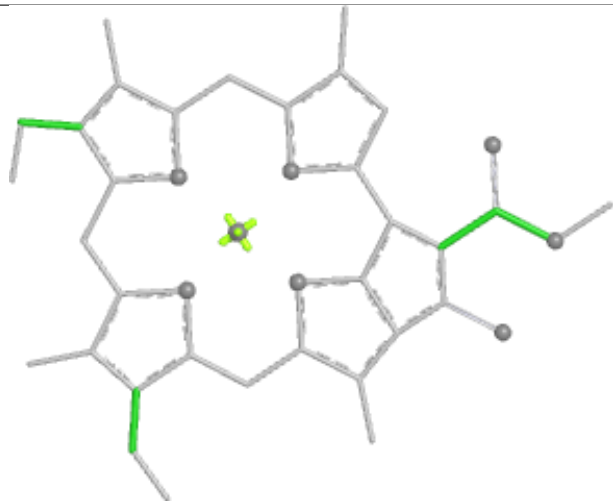
Ligand CLA 1 612



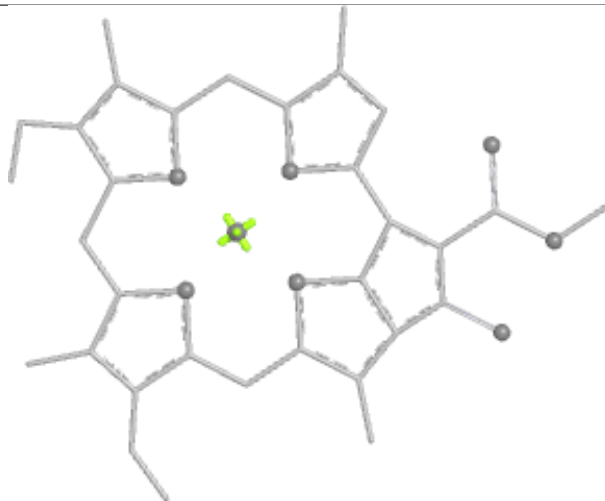
Bond lengths



Bond angles

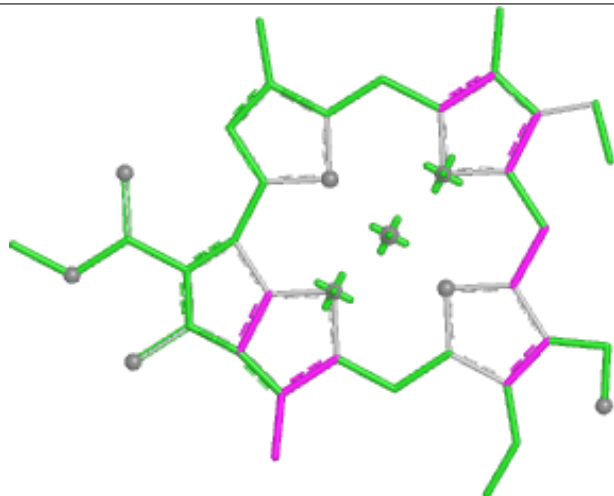


Torsions

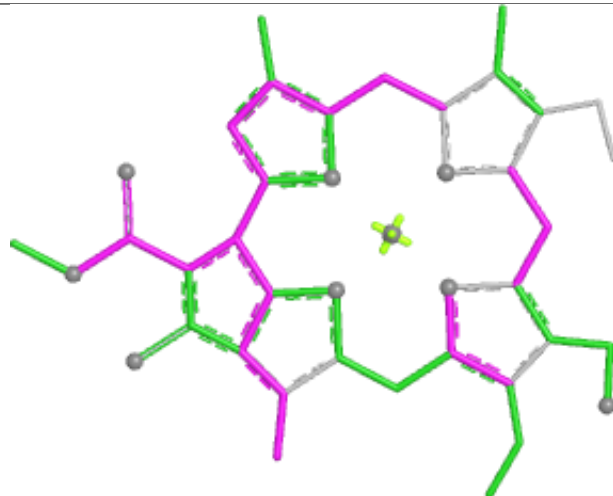


Rings

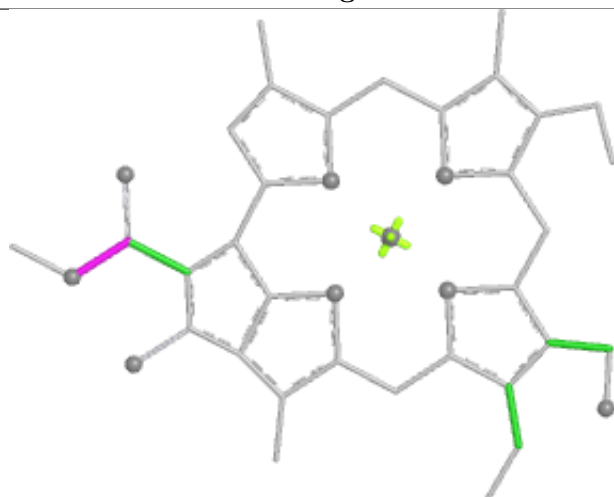
Ligand CHL 1 605



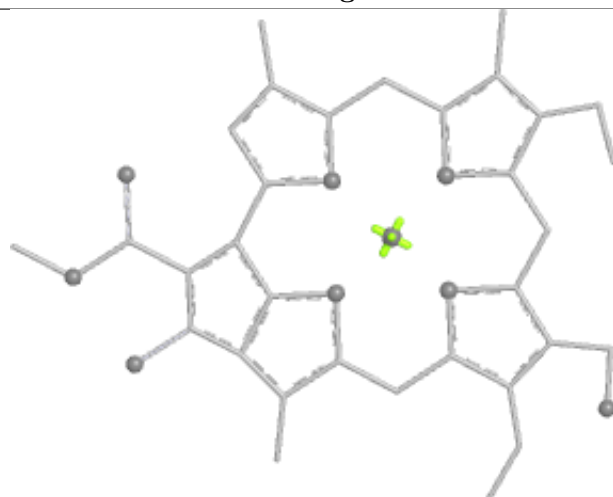
Bond lengths



Bond angles

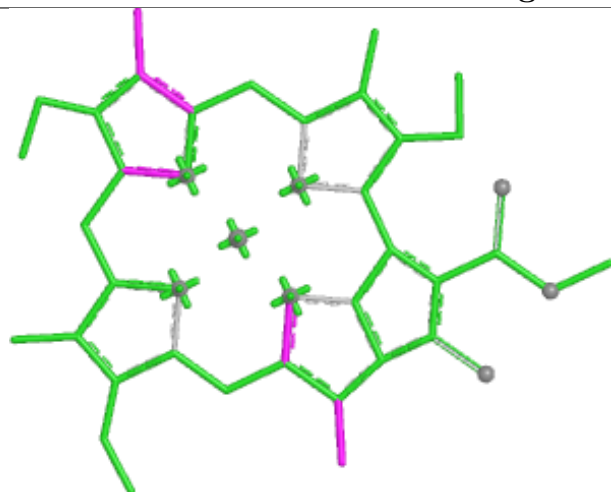


Torsions

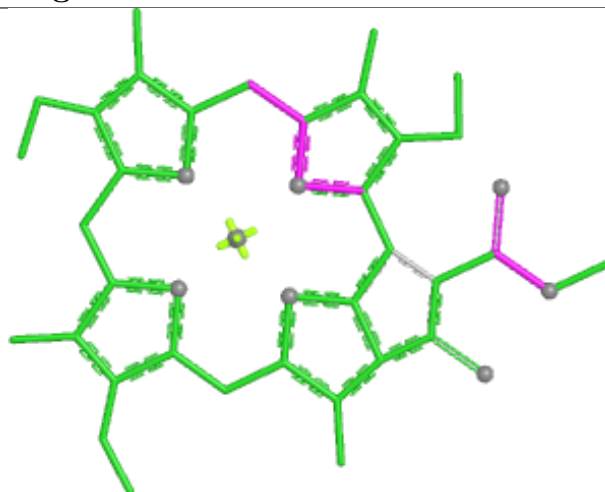


Rings

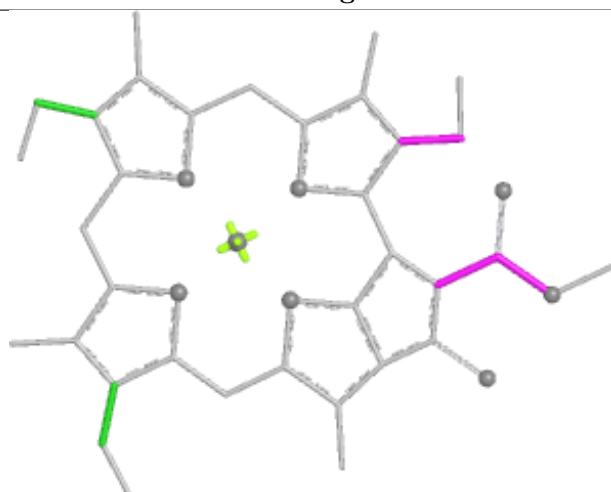
Ligand CLA g 604



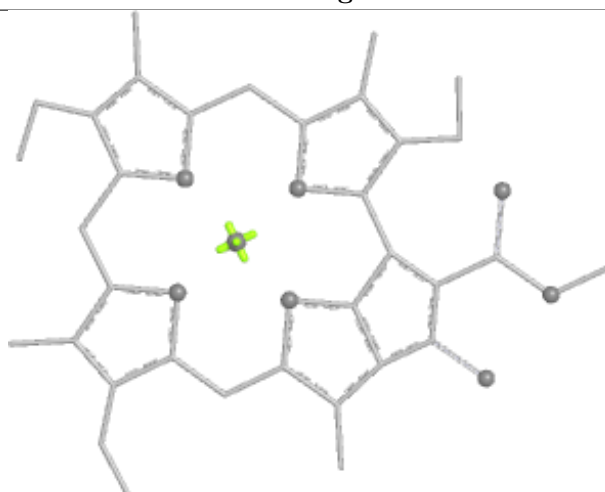
Bond lengths



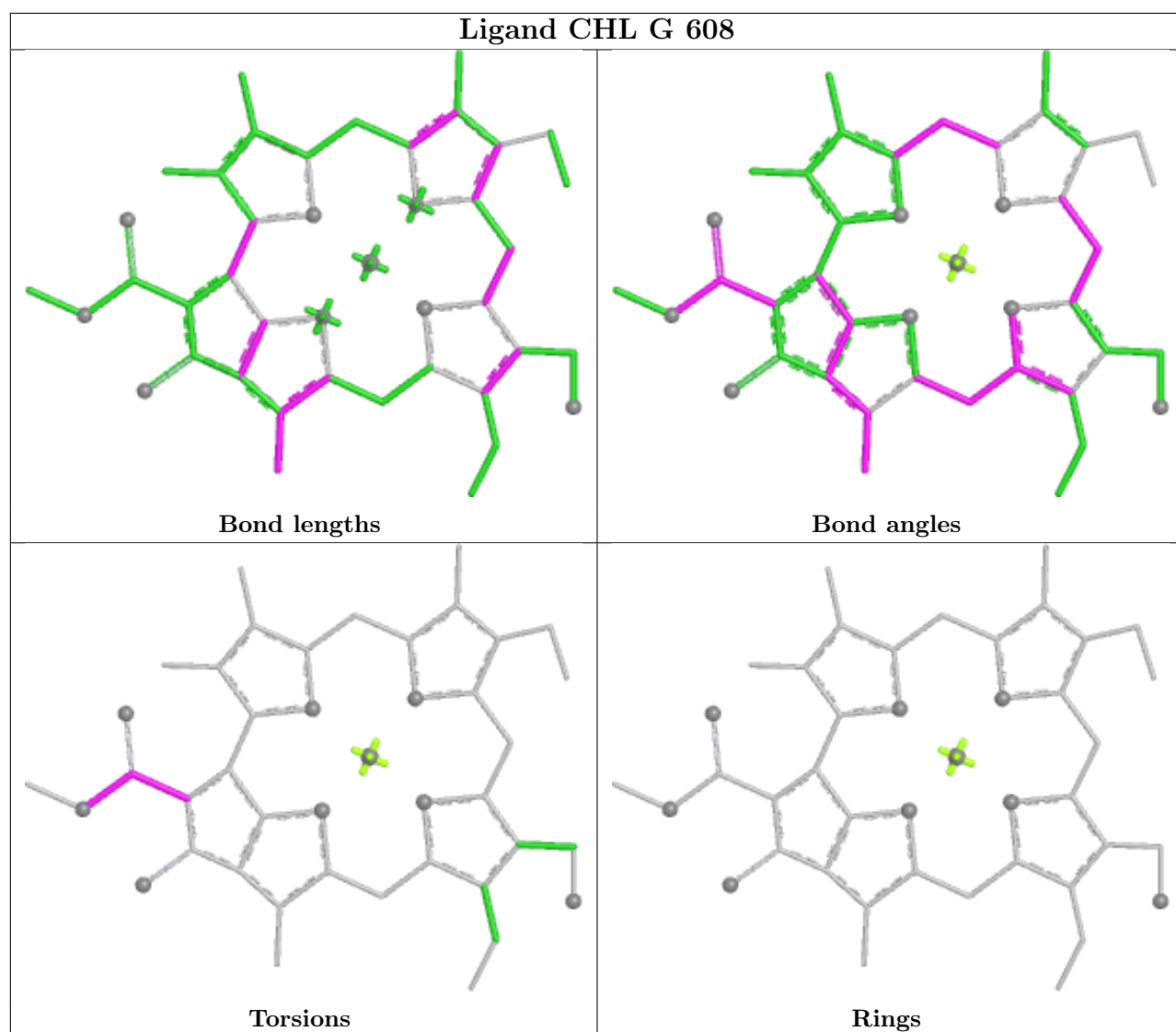
Bond angles



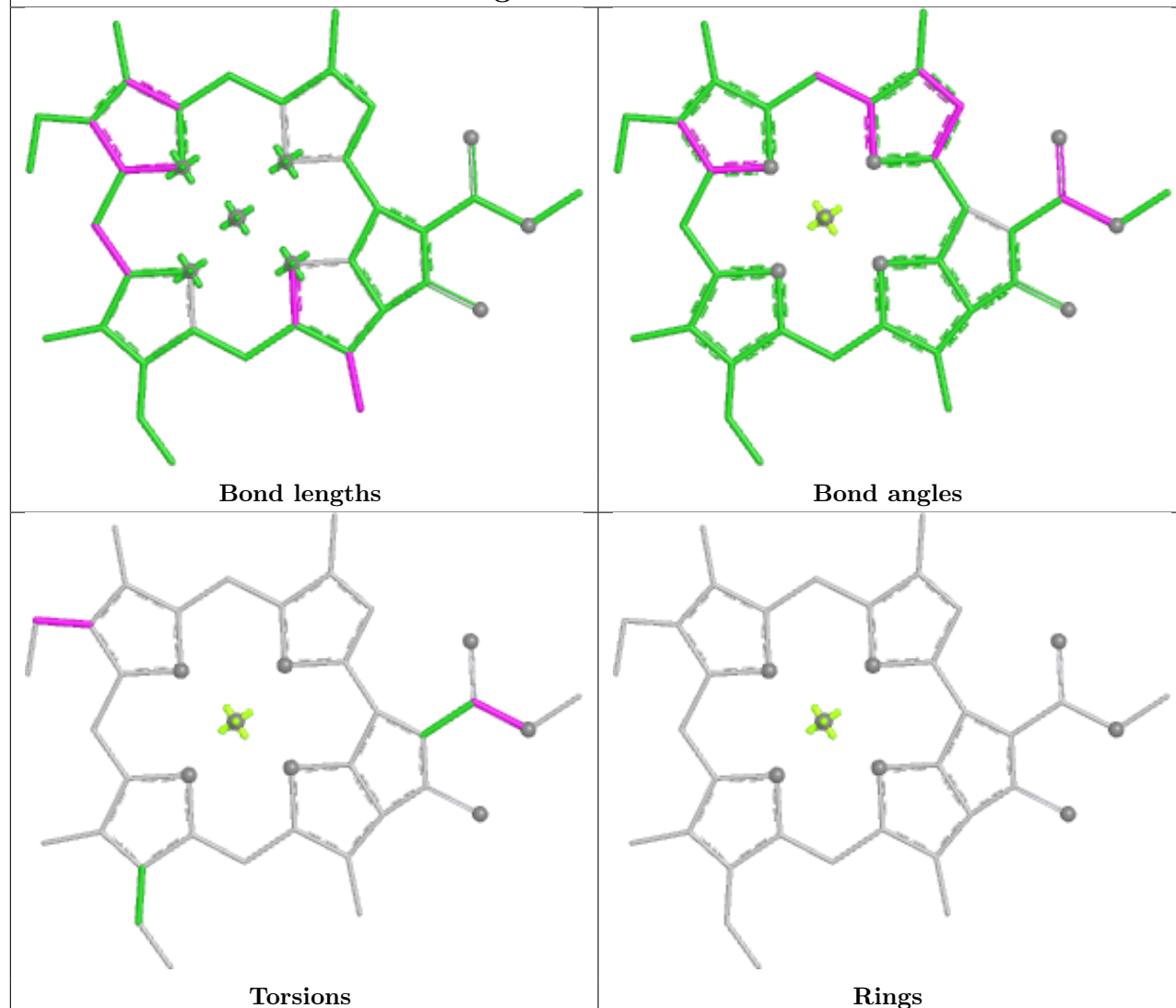
Torsions



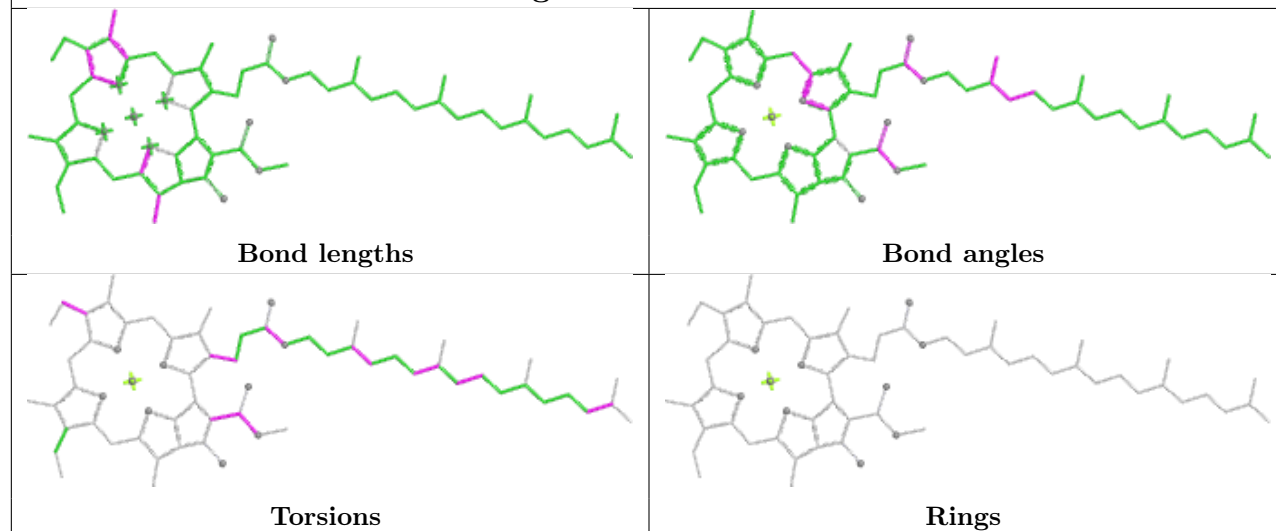
Rings

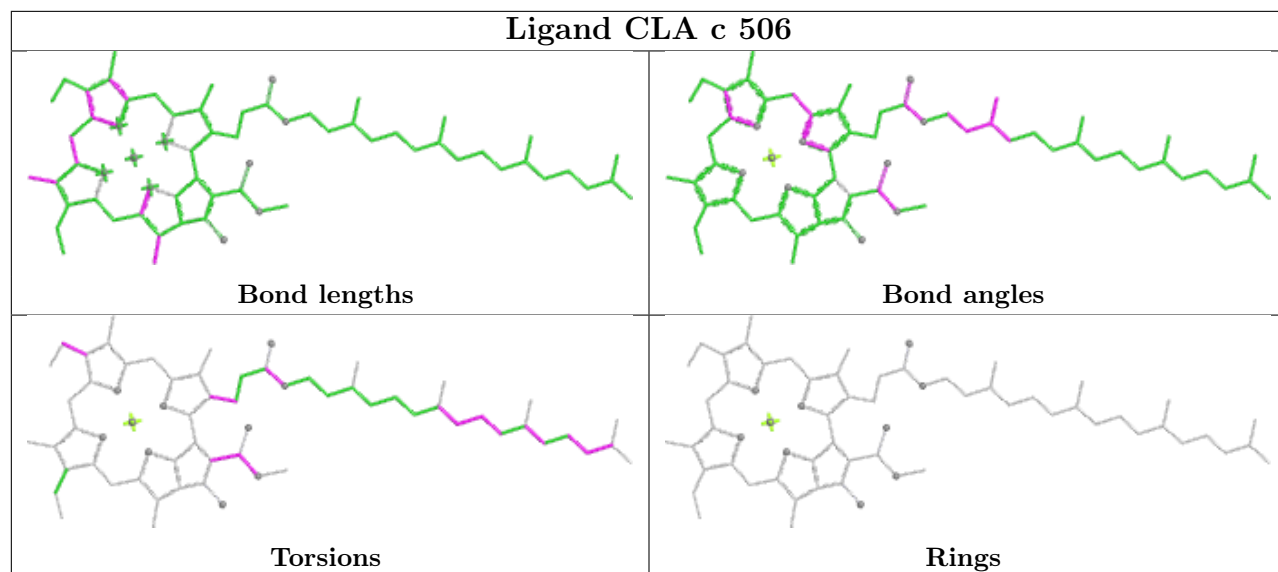
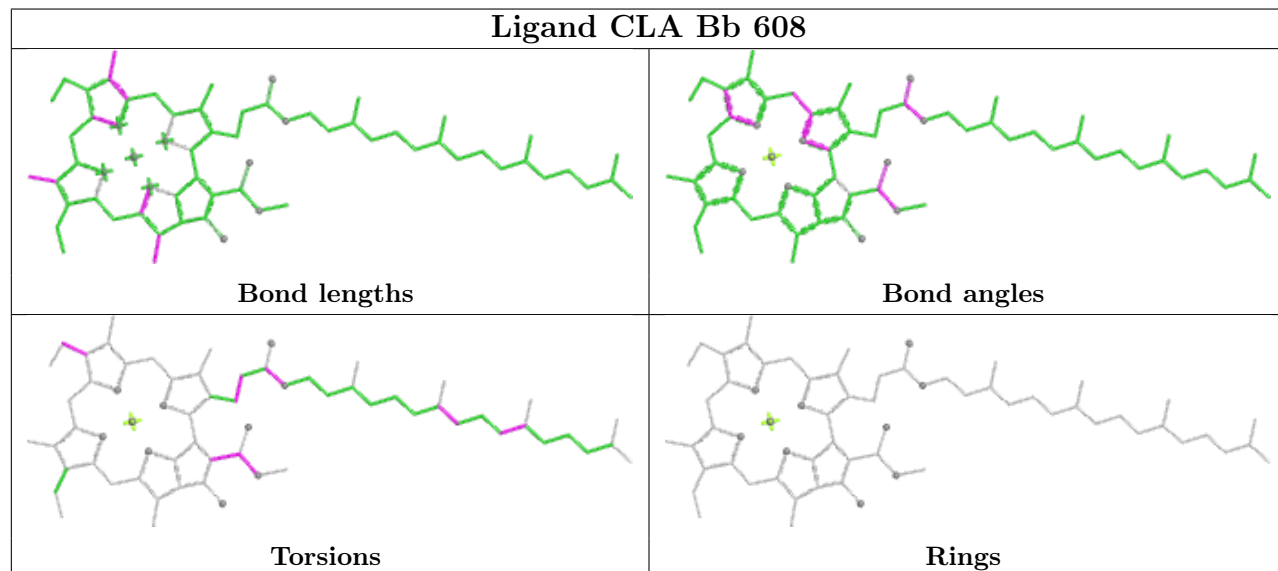


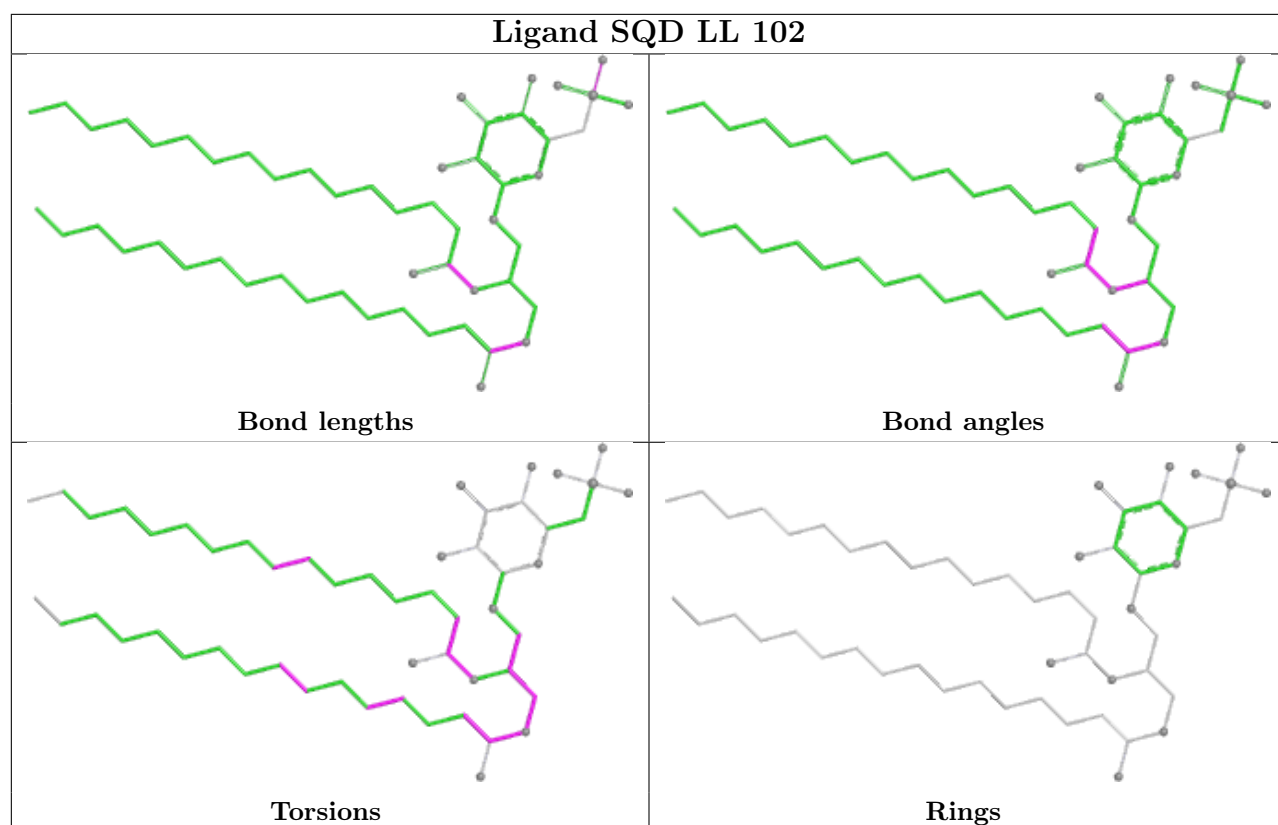
Ligand CLA 2 613

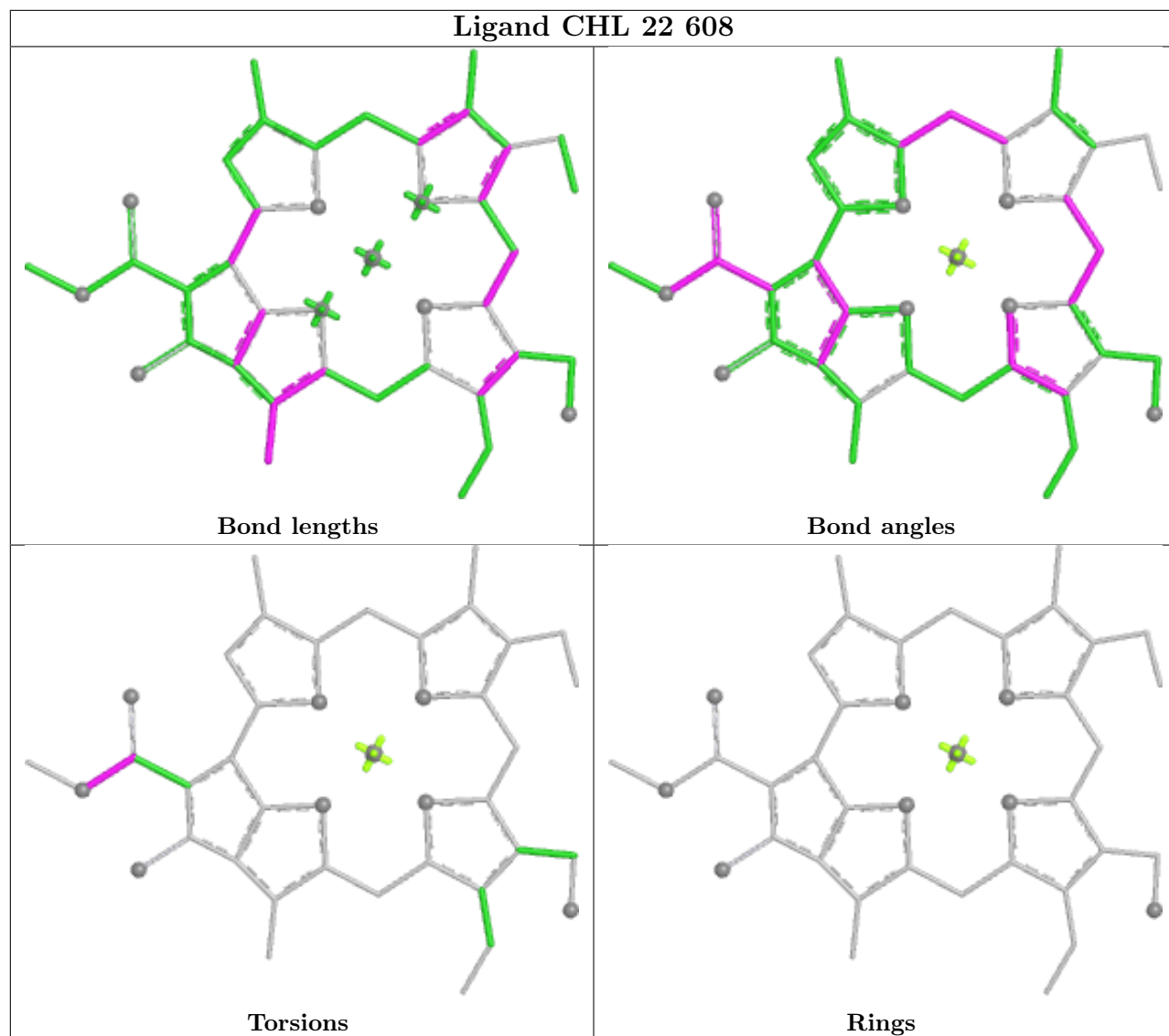


Ligand CLA C 505

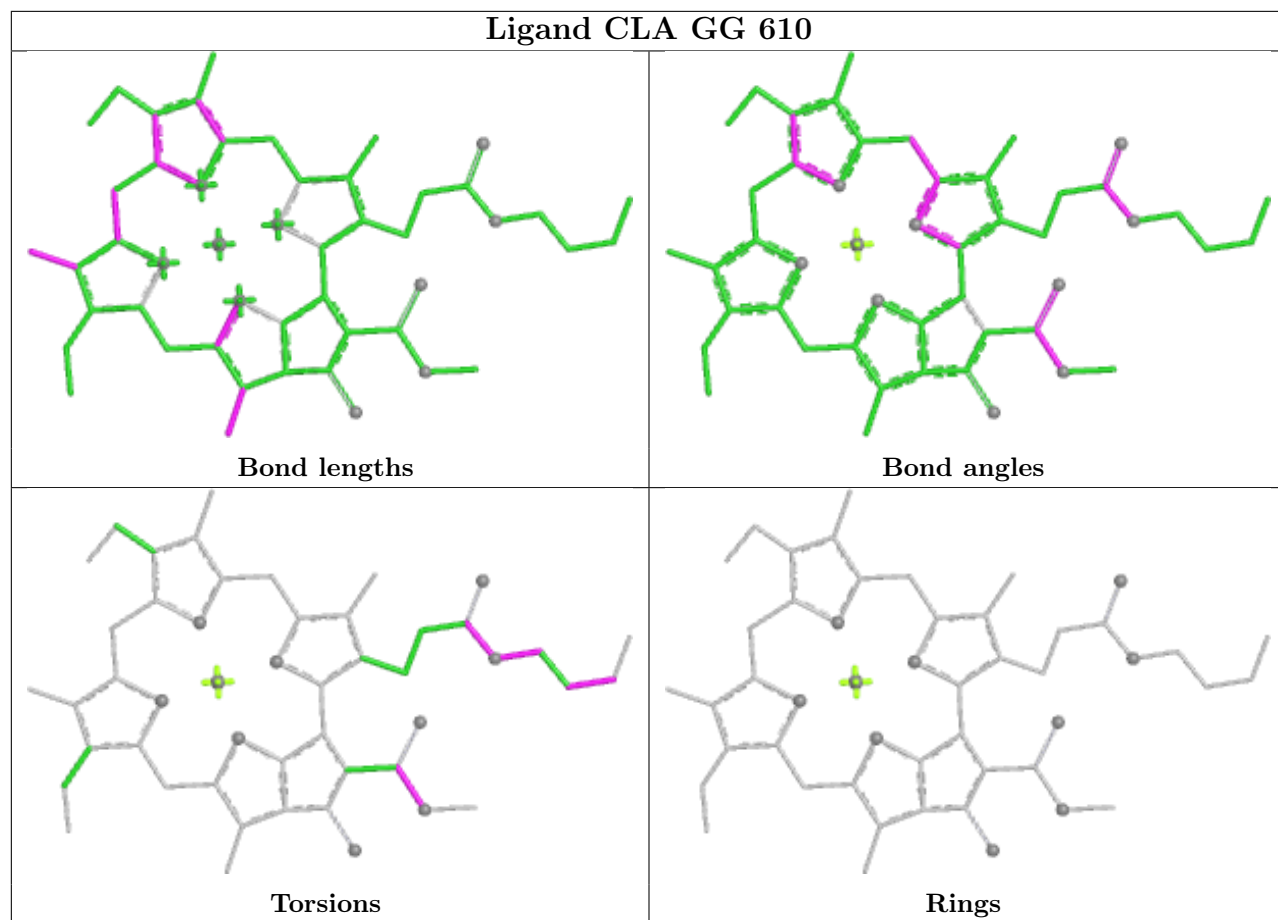


Ligand CLA c 506**Ligand CLA Bb 608**

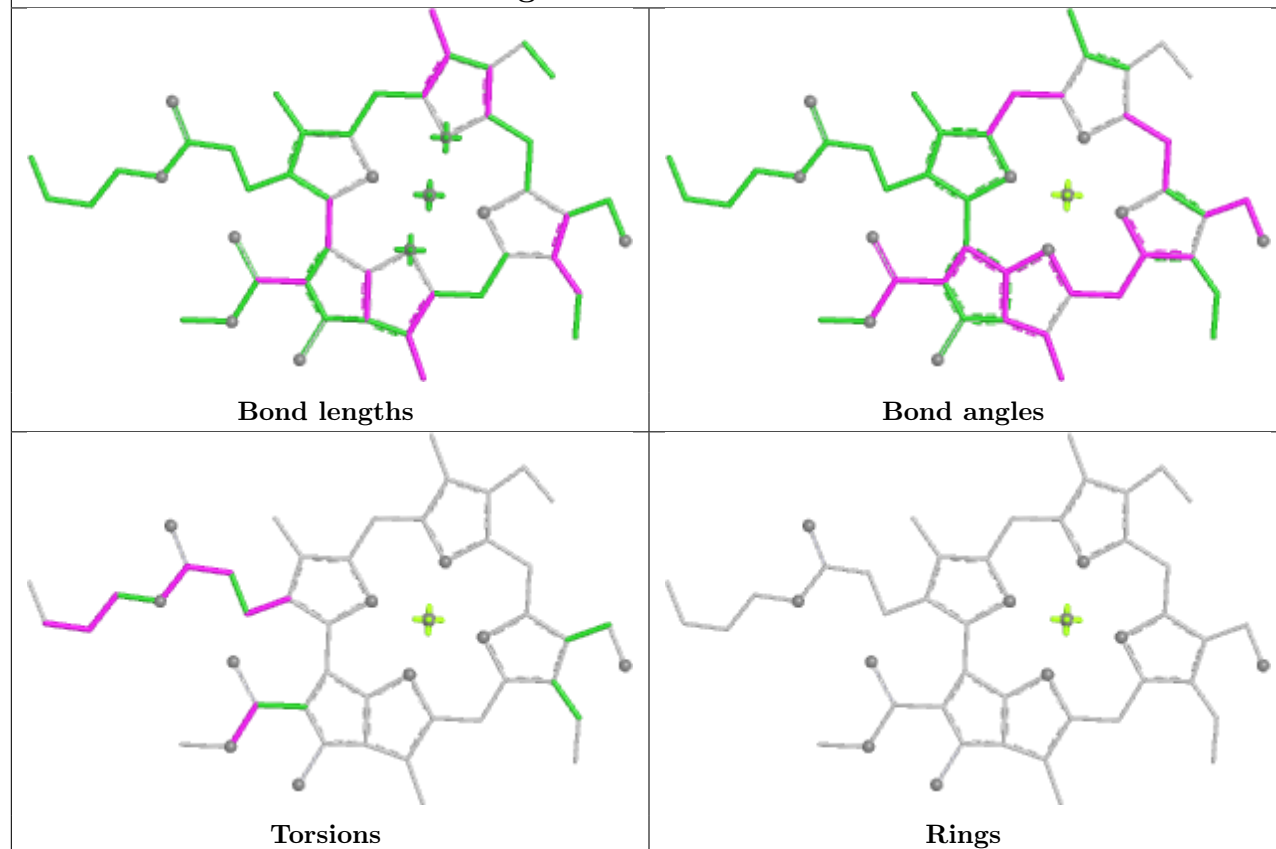




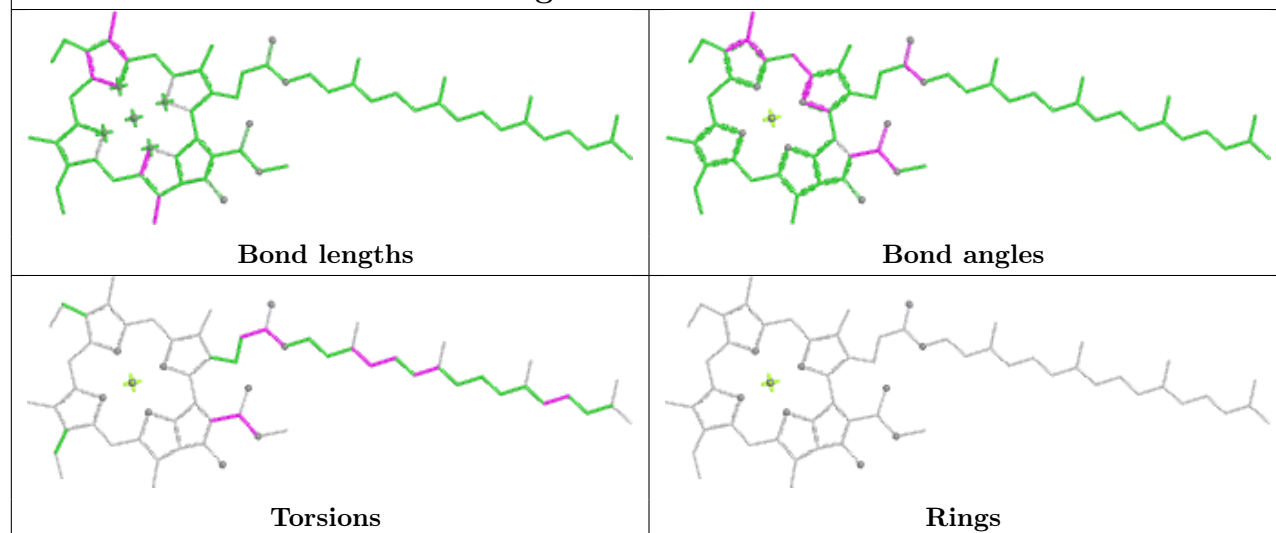
Ligand CLA GG 610



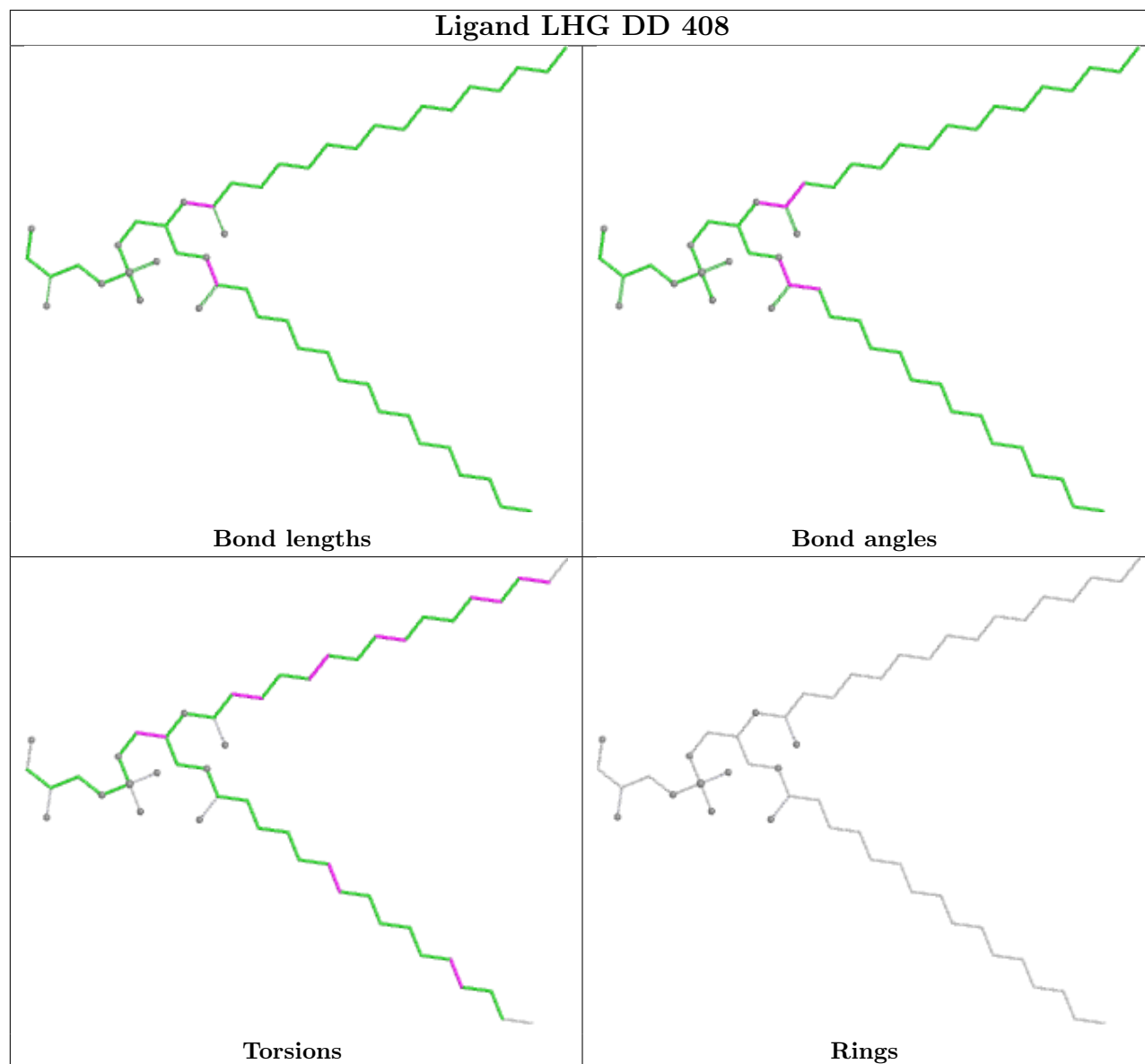
Ligand CHL RR 306



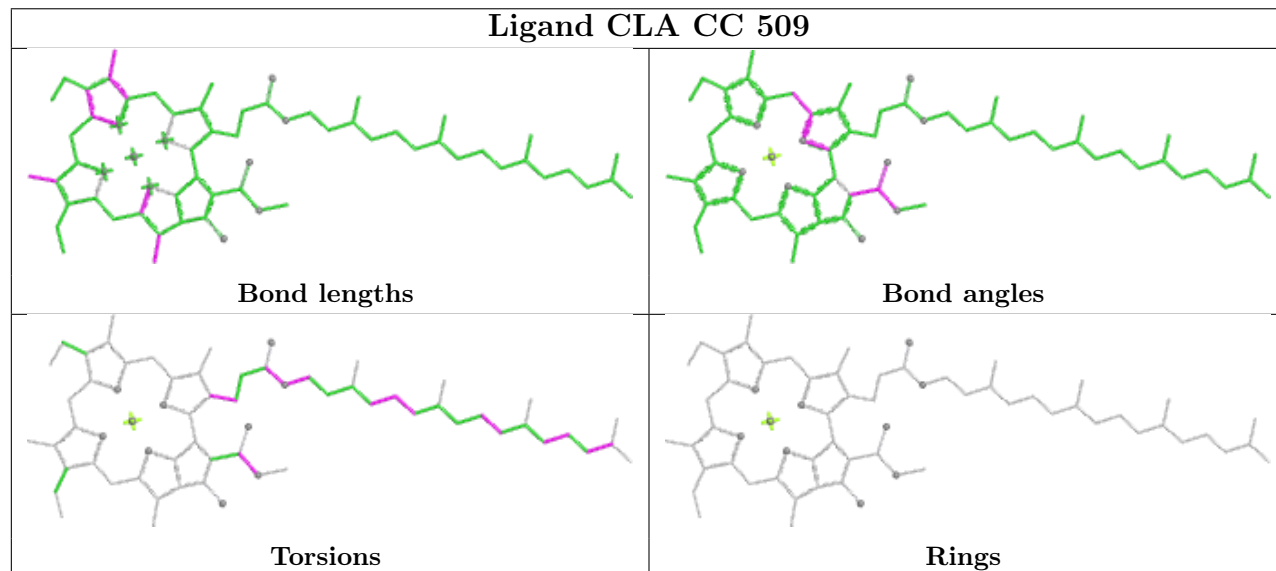
Ligand CLA b 613

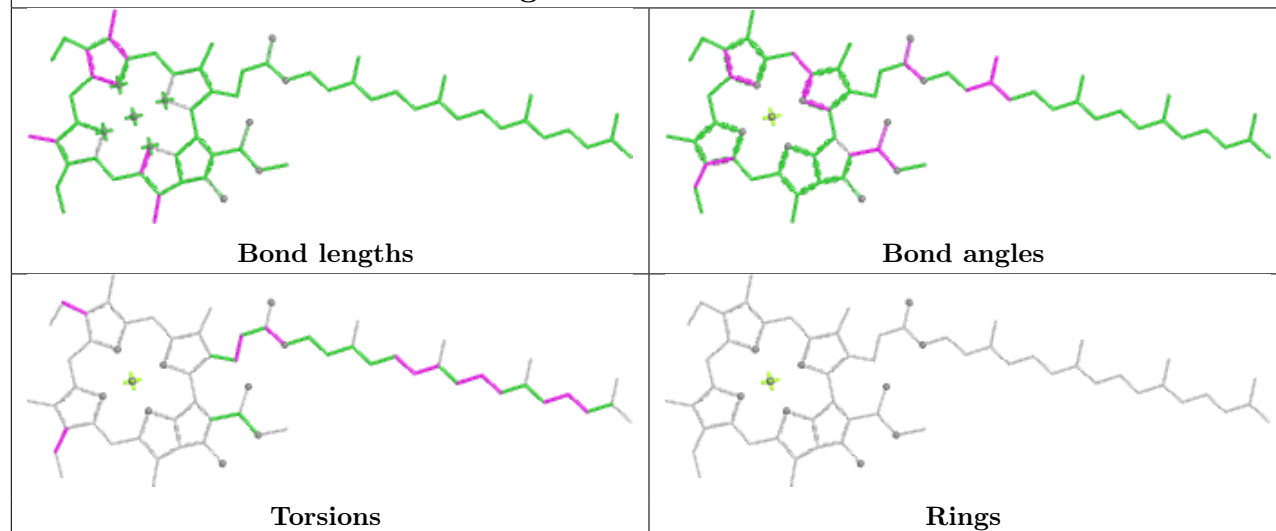
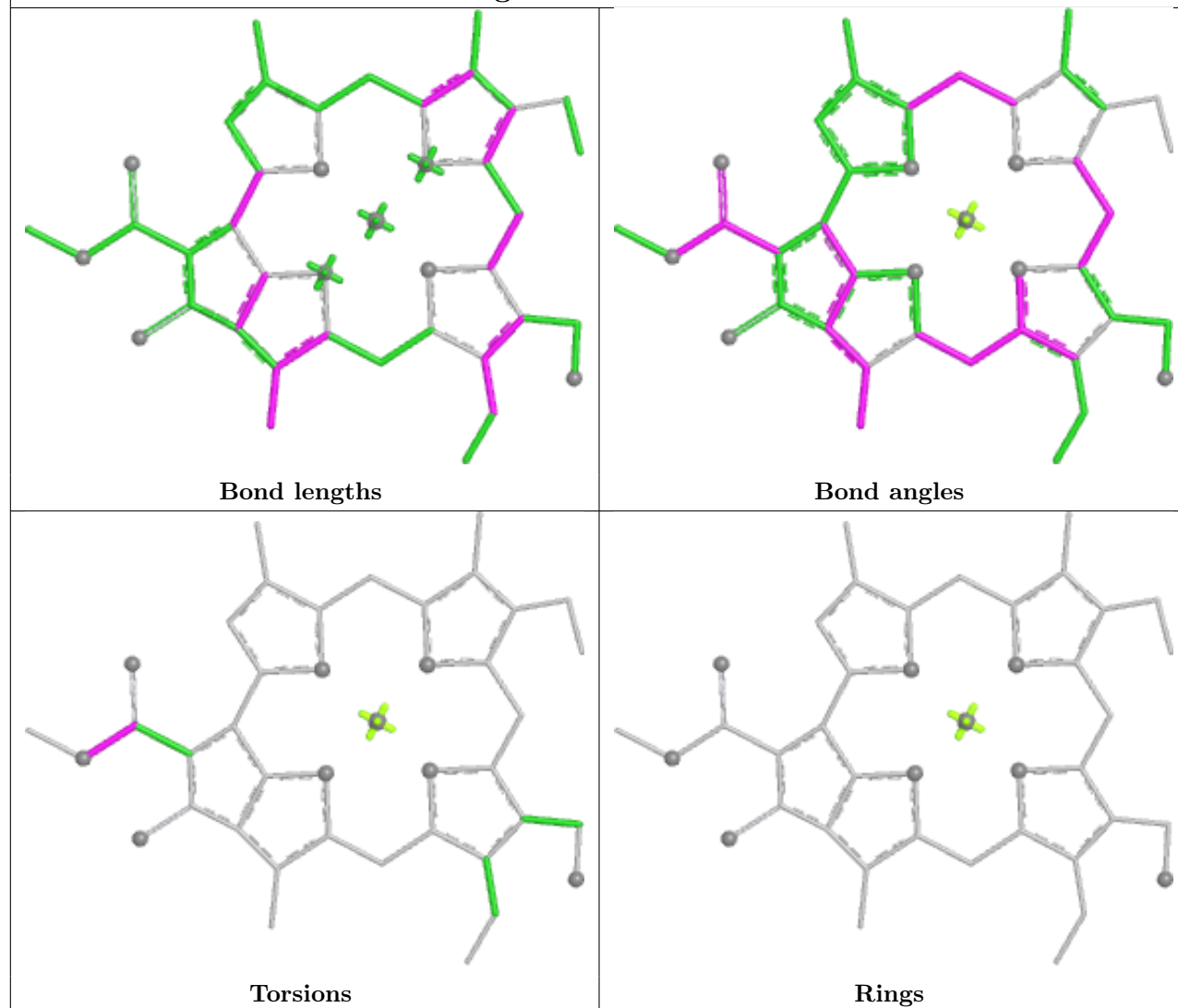


Ligand LHG DD 408

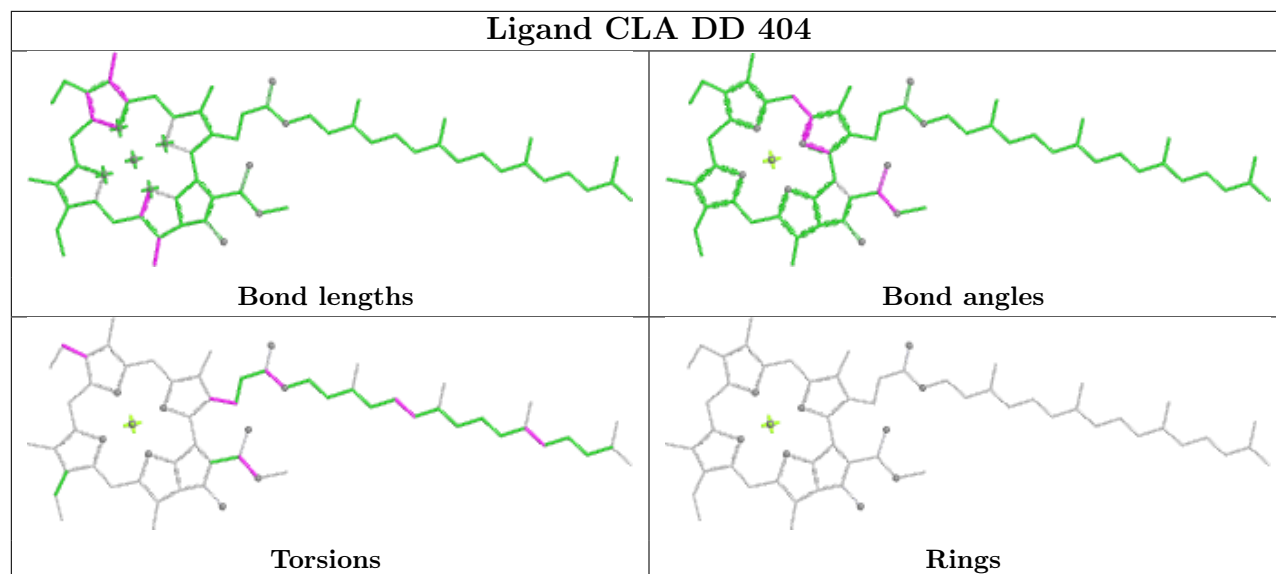


Ligand CLA CC 509

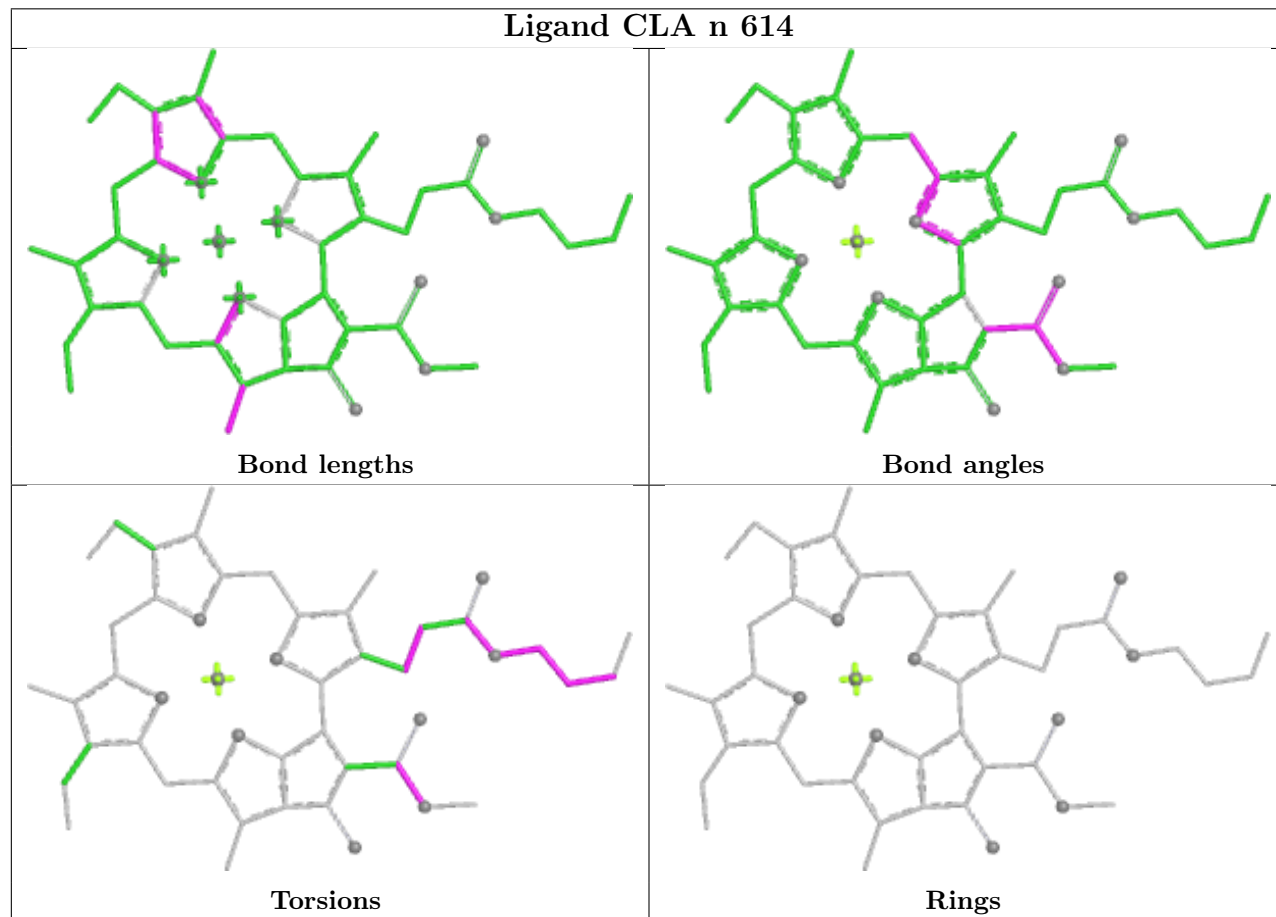


Ligand CLA BB 609**Ligand CHL 3 606**

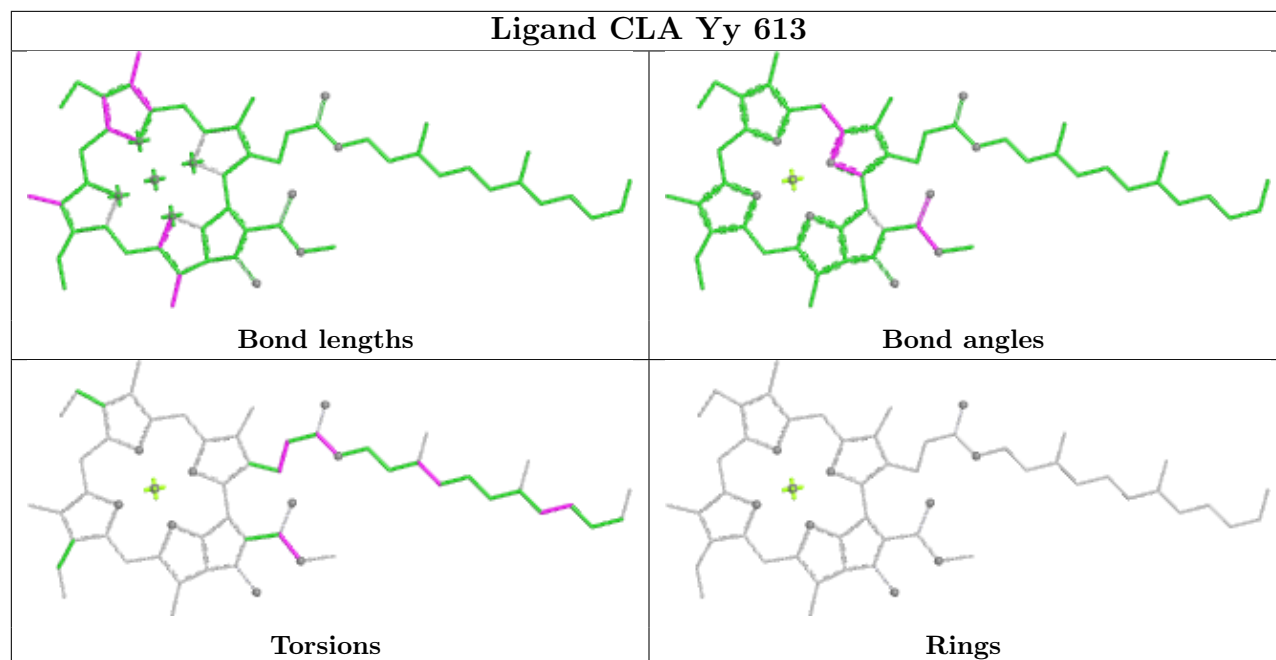
Ligand CLA DD 404



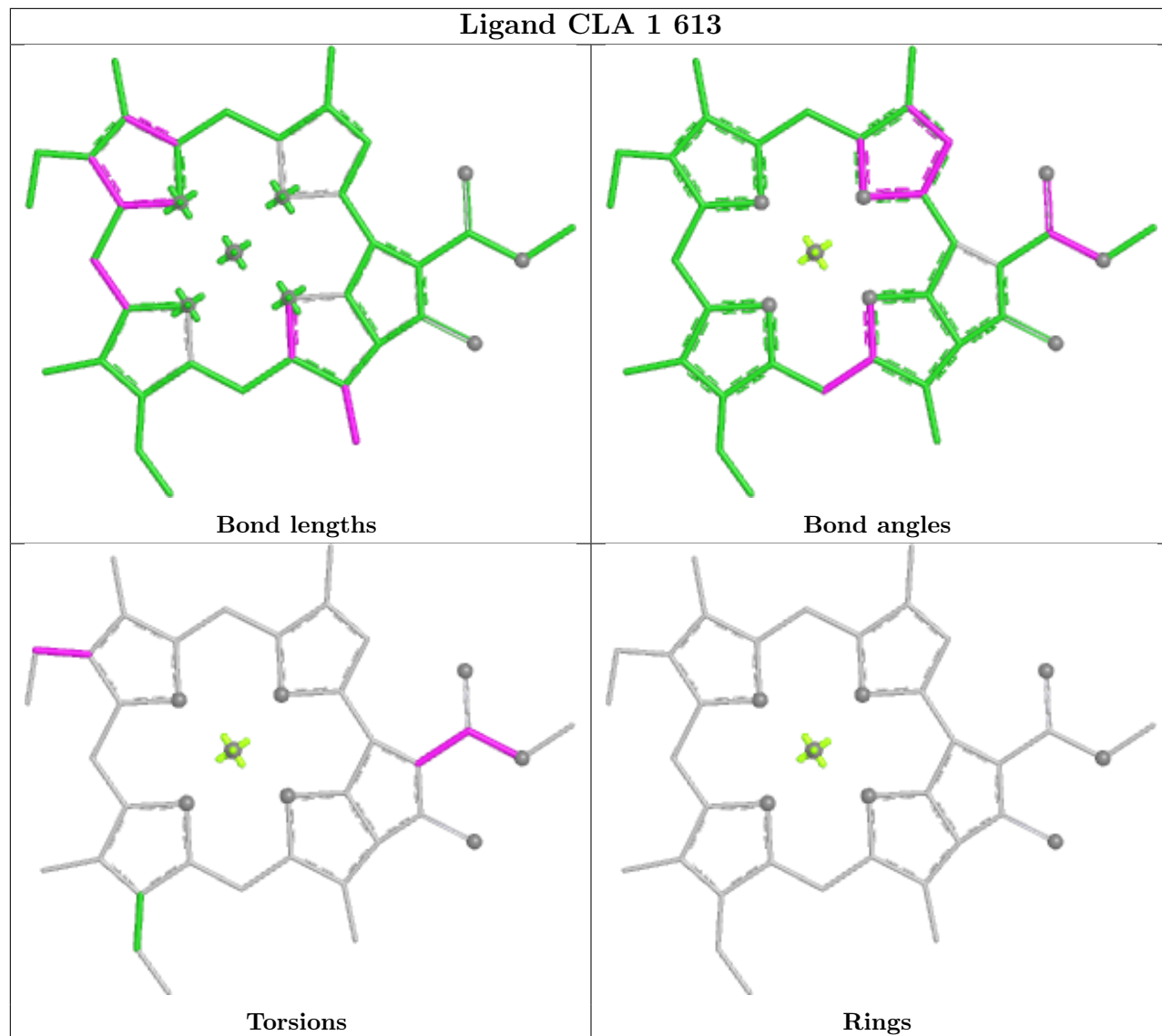
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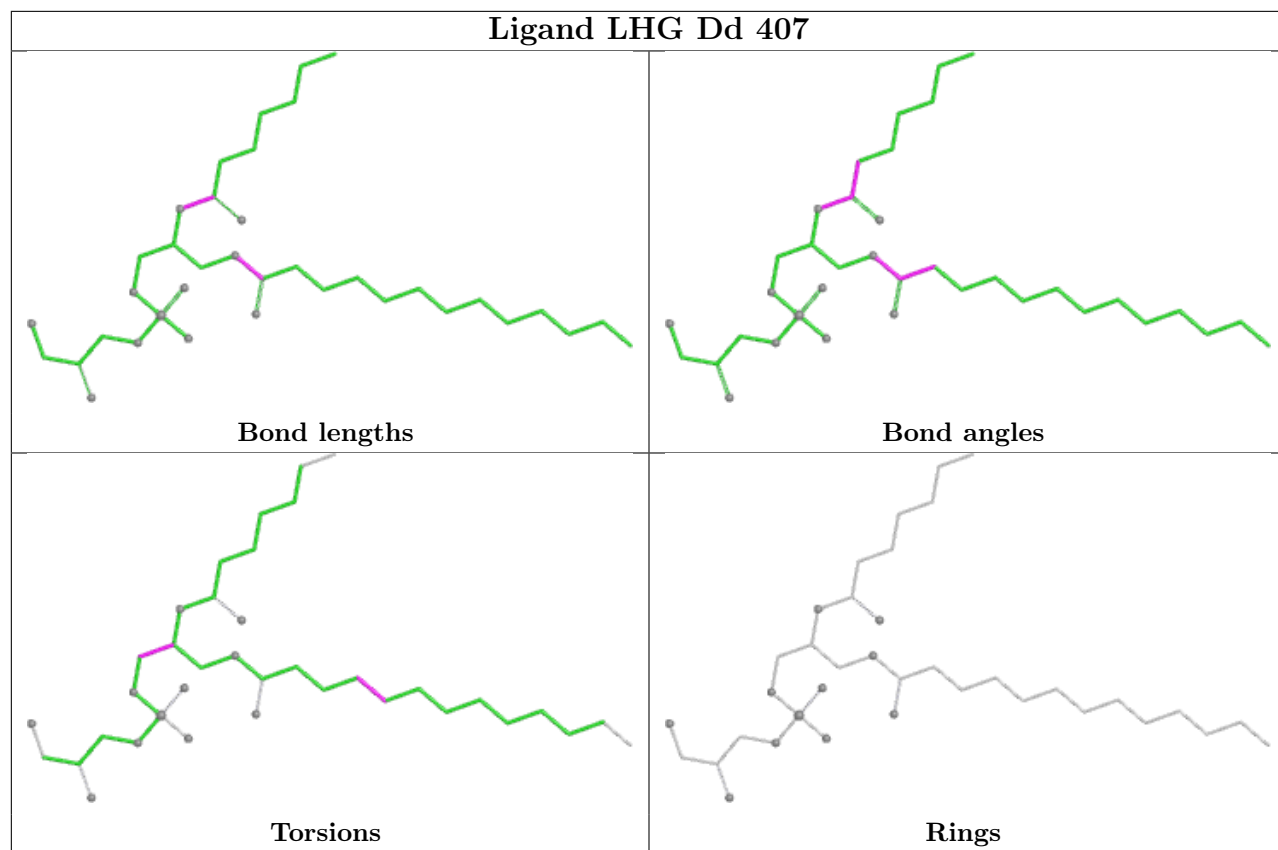


Ligand CLA Yy 613

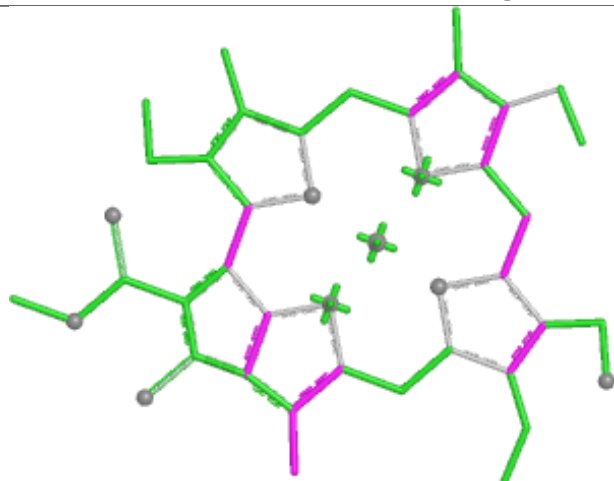


Ligand CLA 1 613

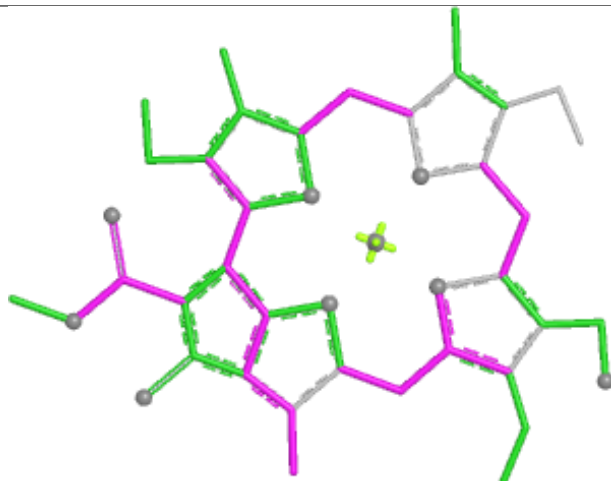




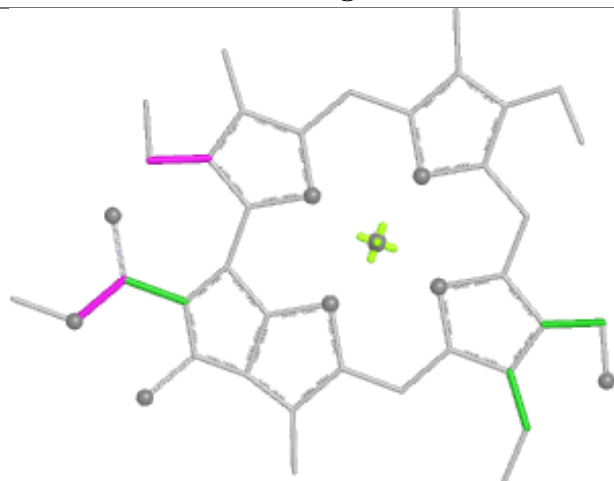
Ligand CHL GG 606



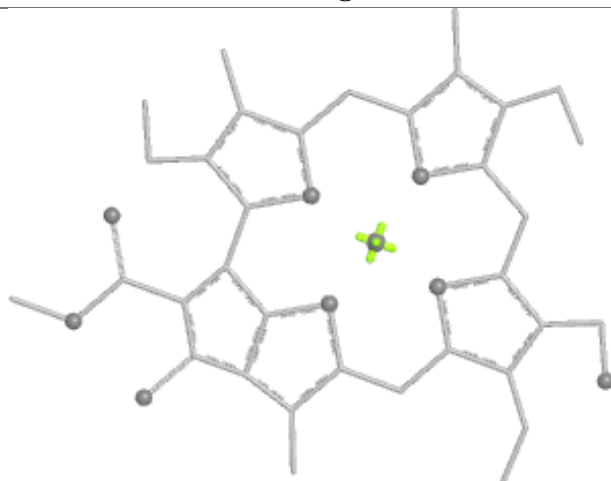
Bond lengths



Bond angles

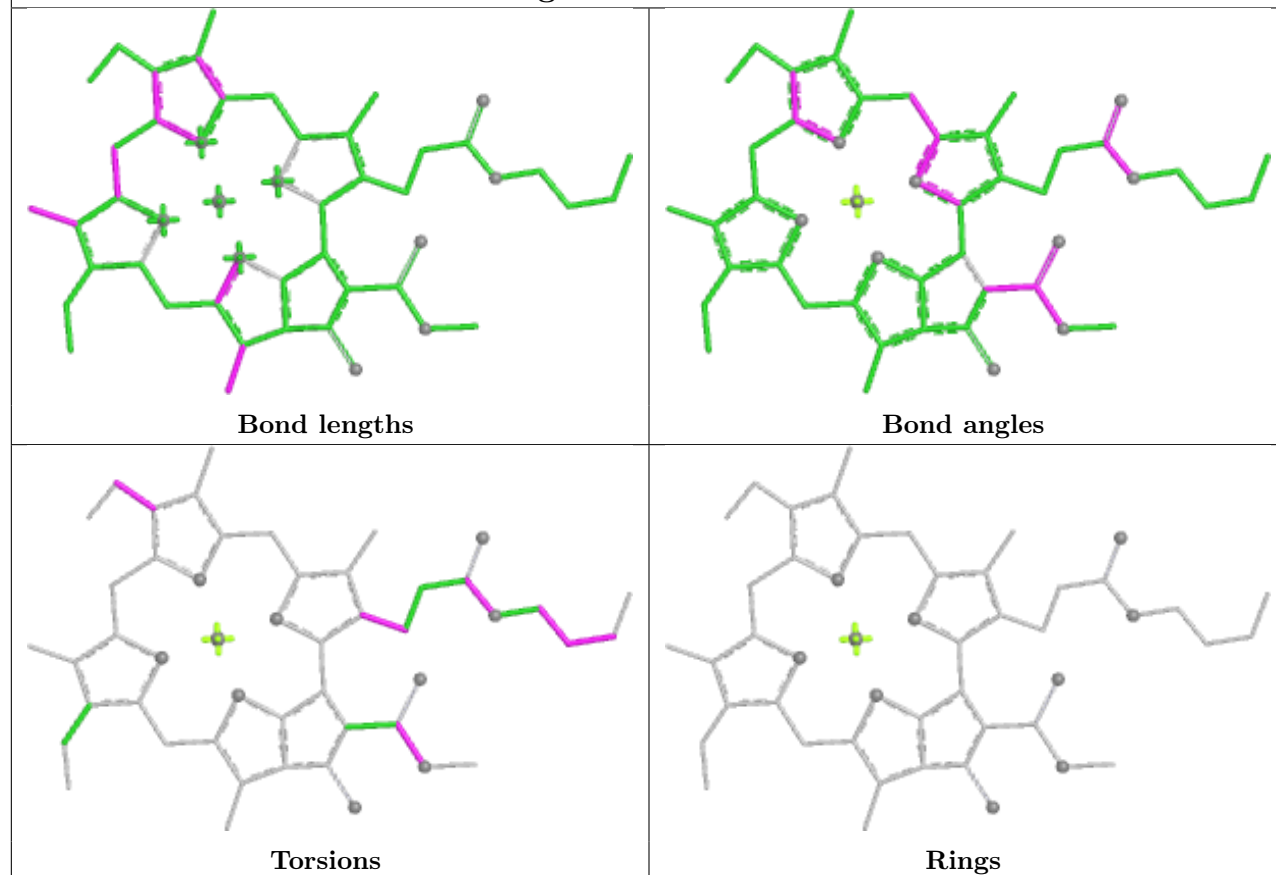


Torsions

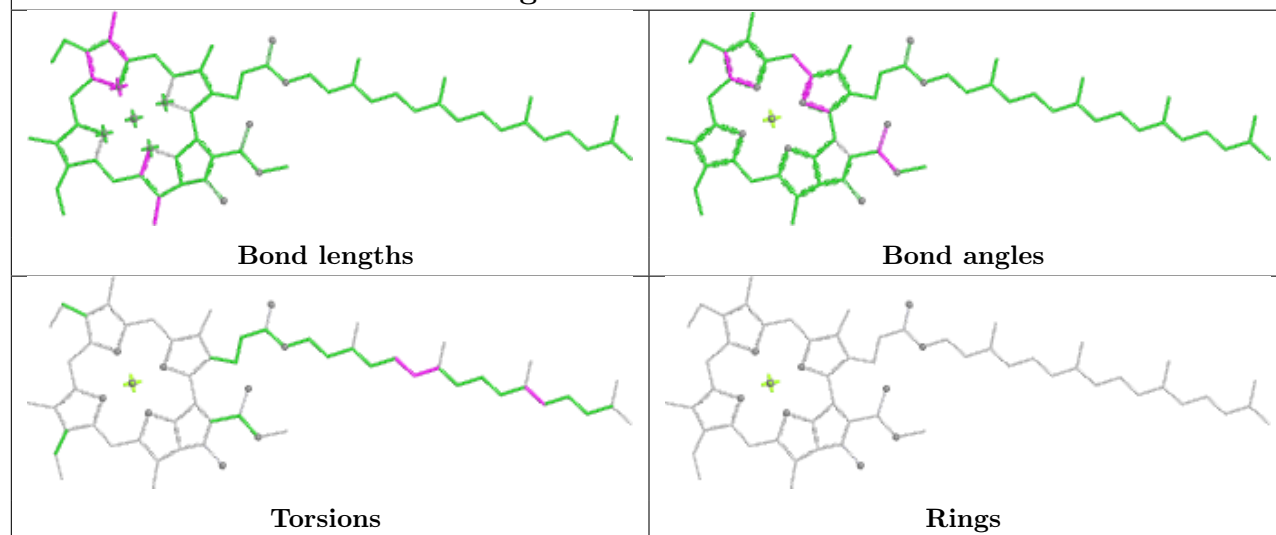


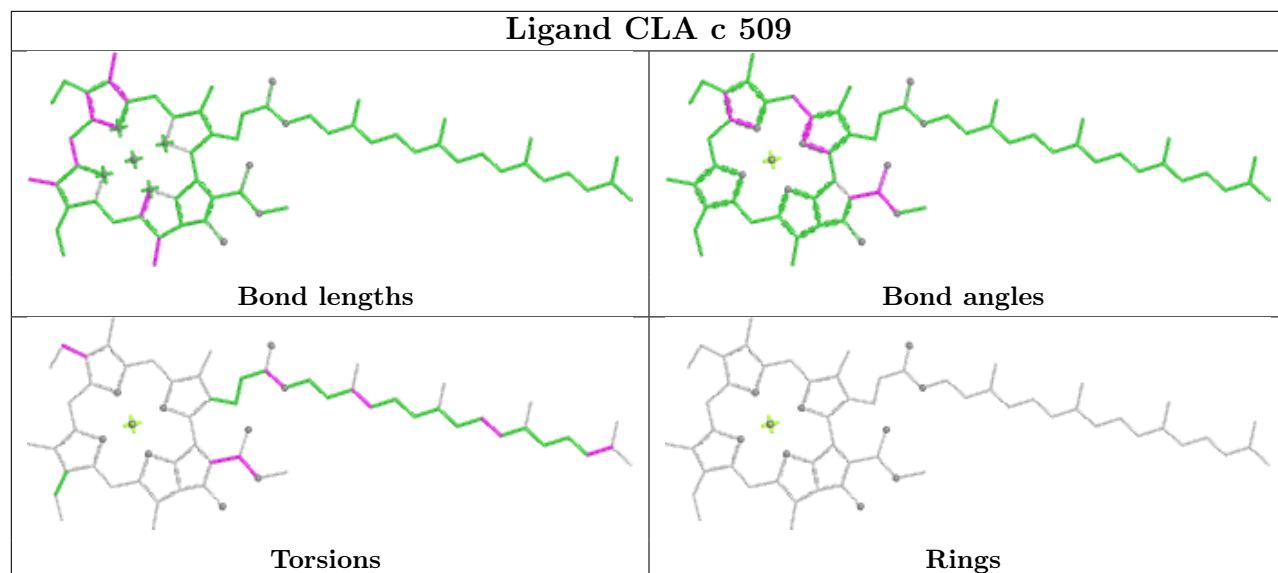
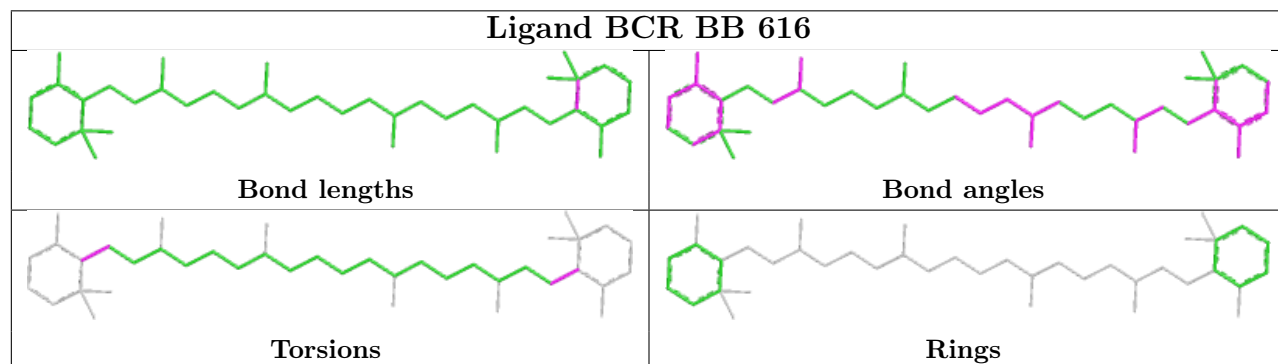
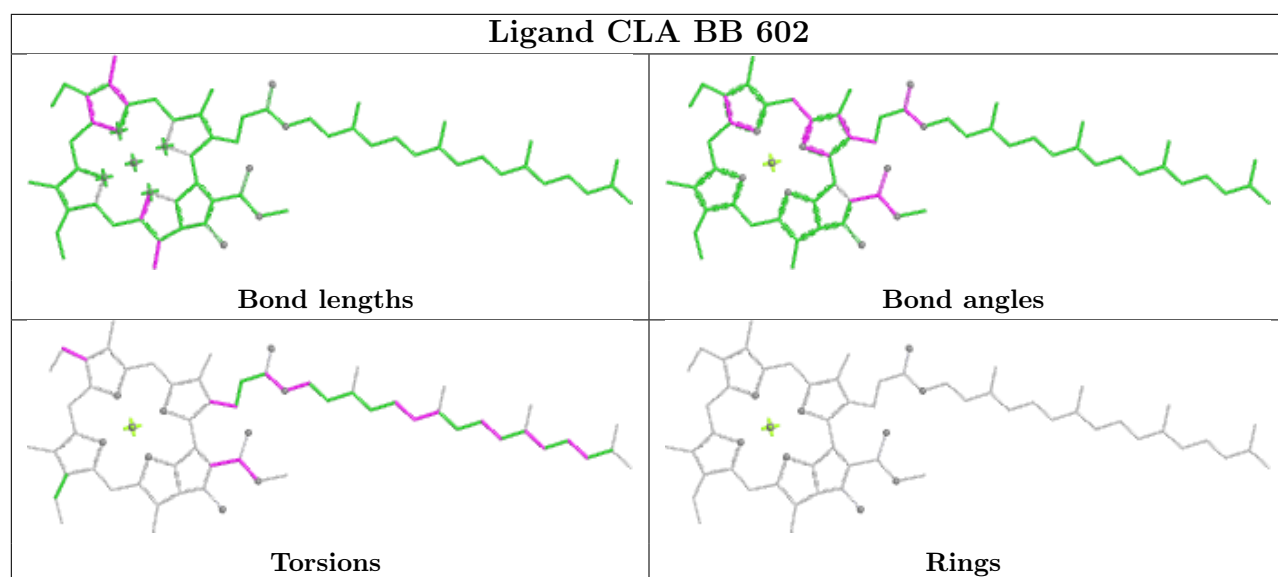
Rings

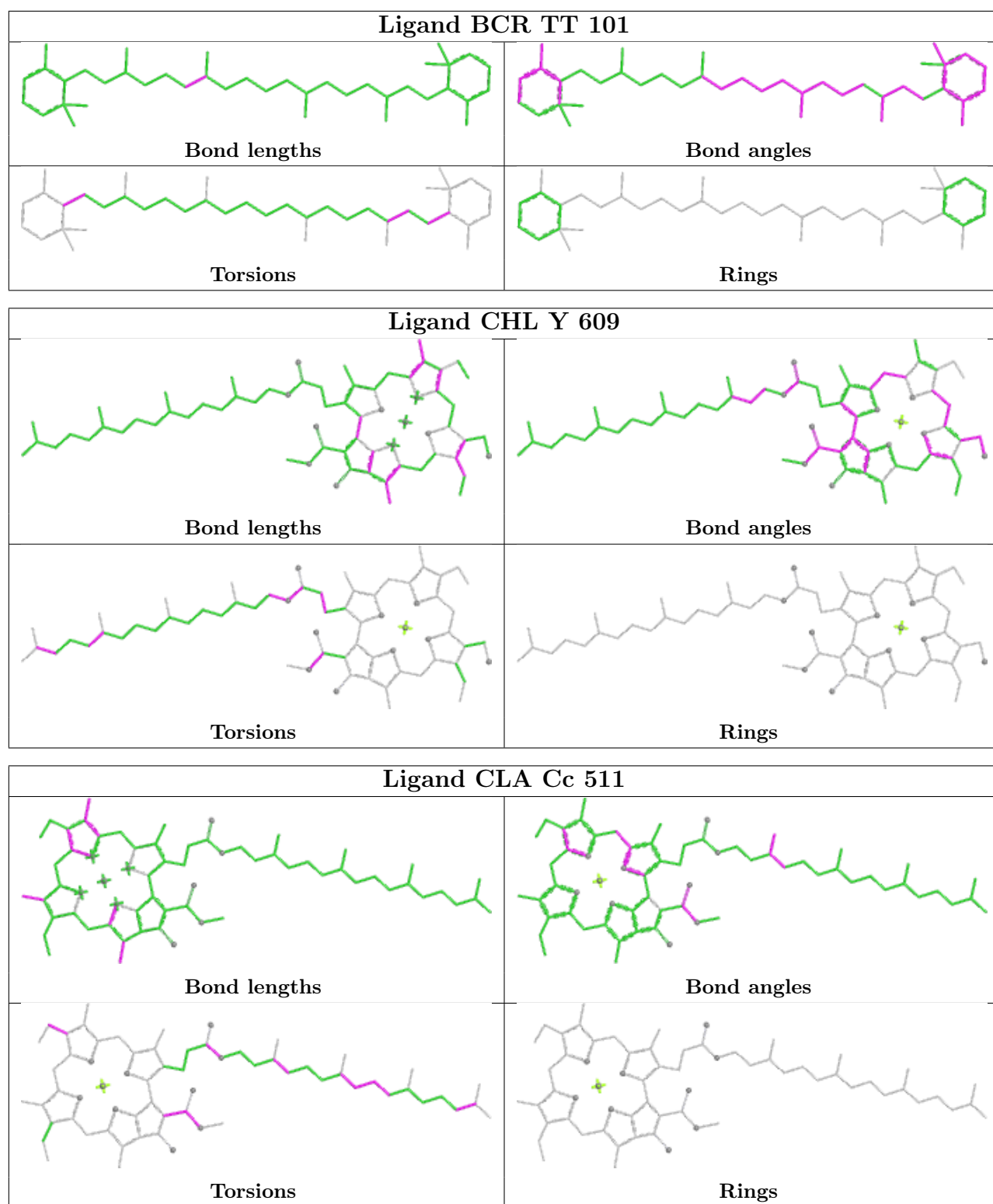
Ligand CLA s 609

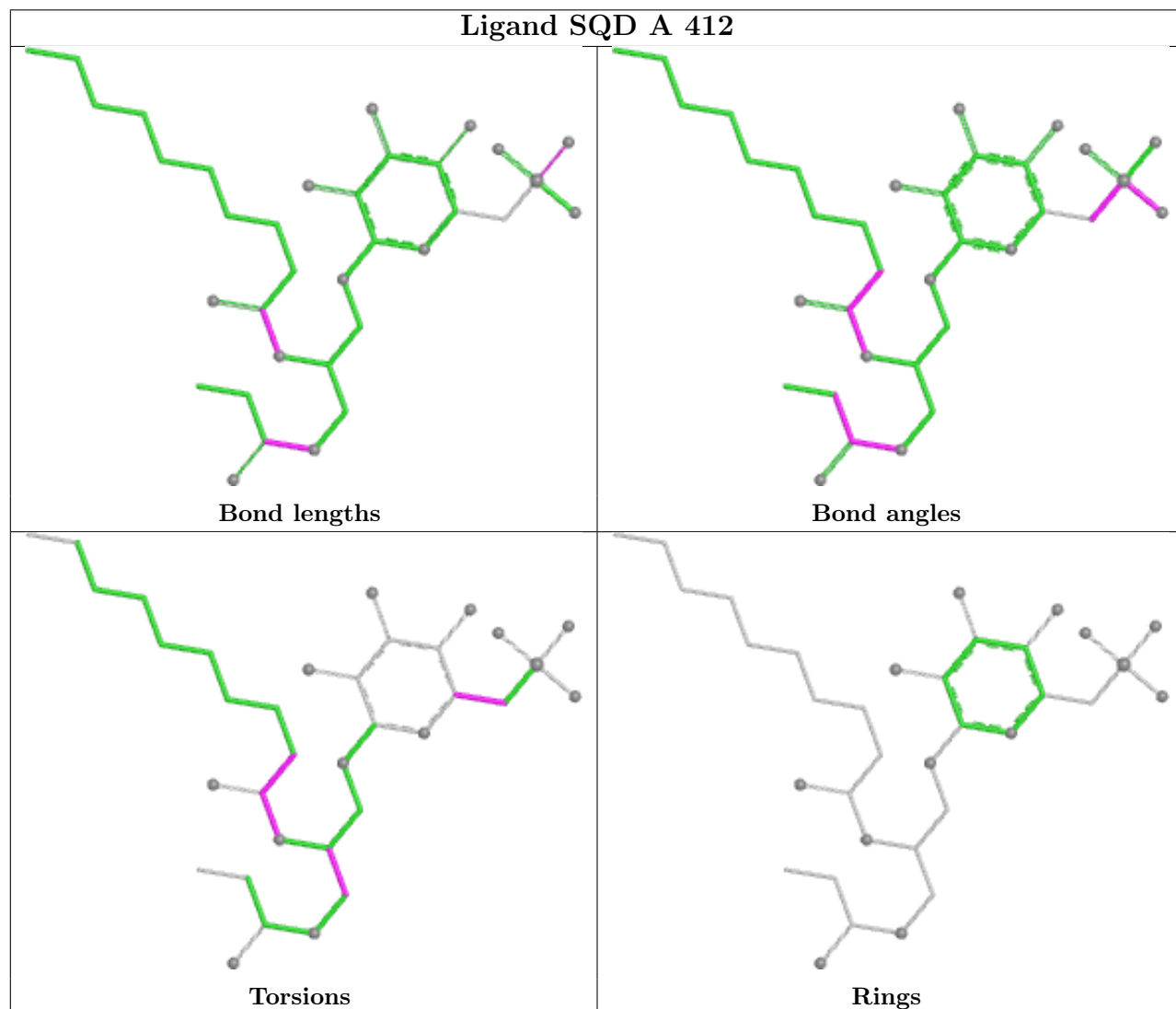
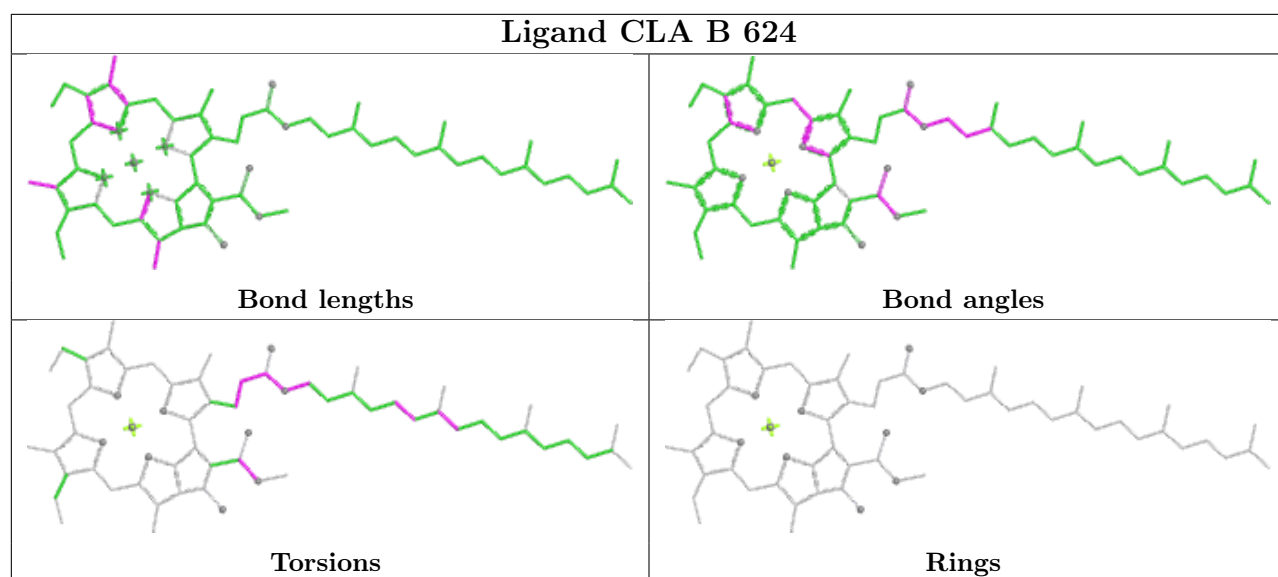


Ligand CLA BB 611

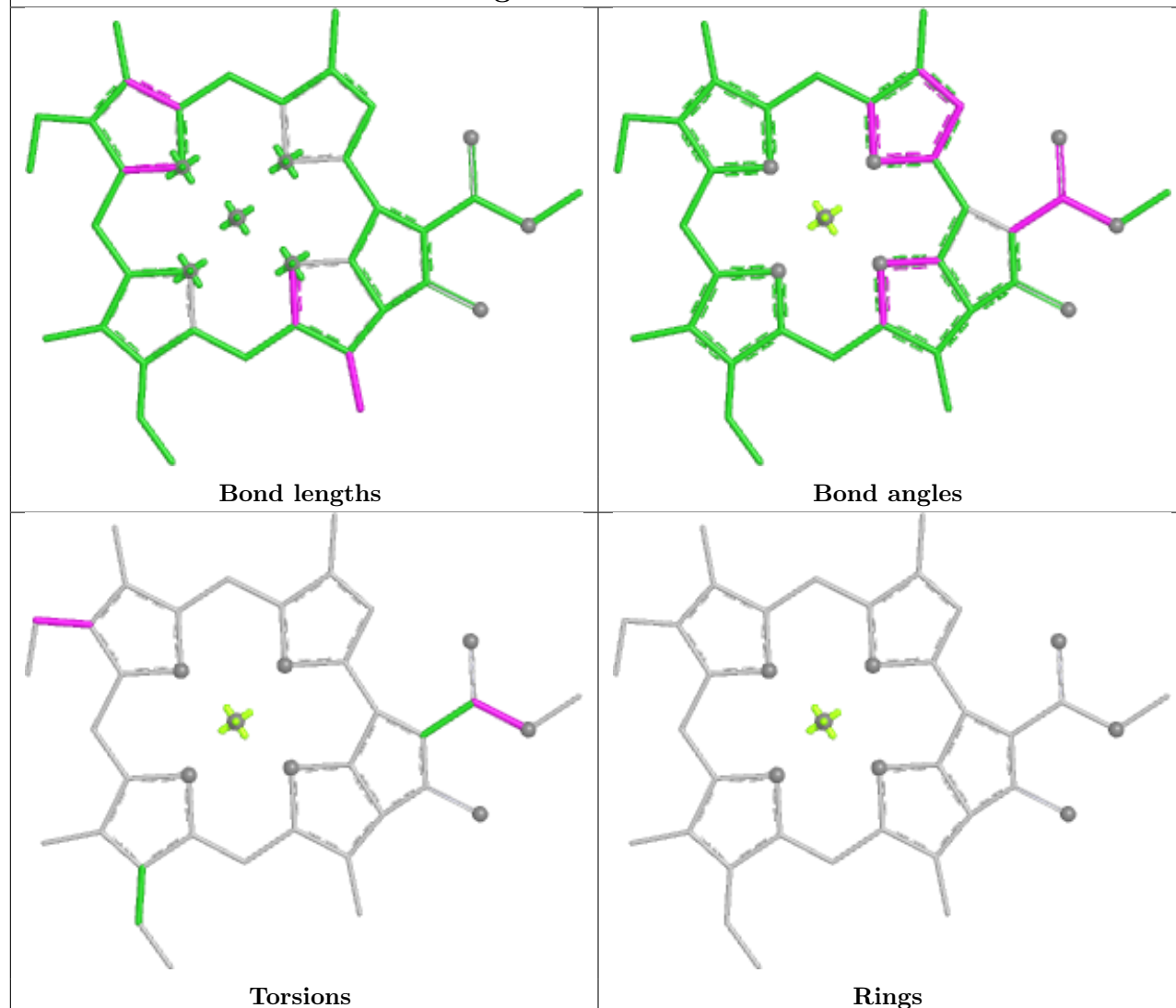




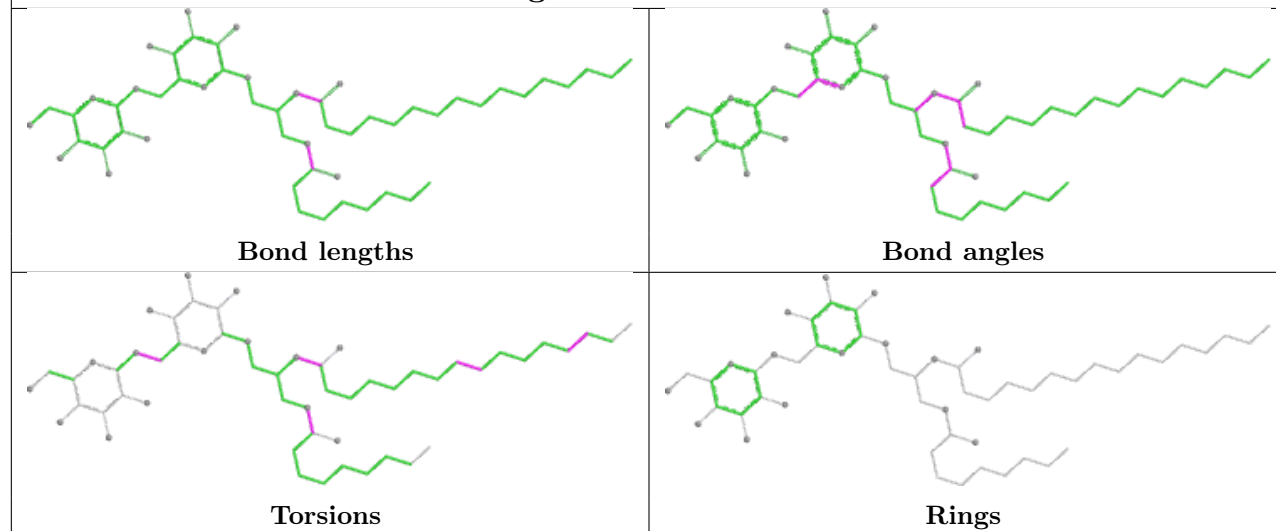


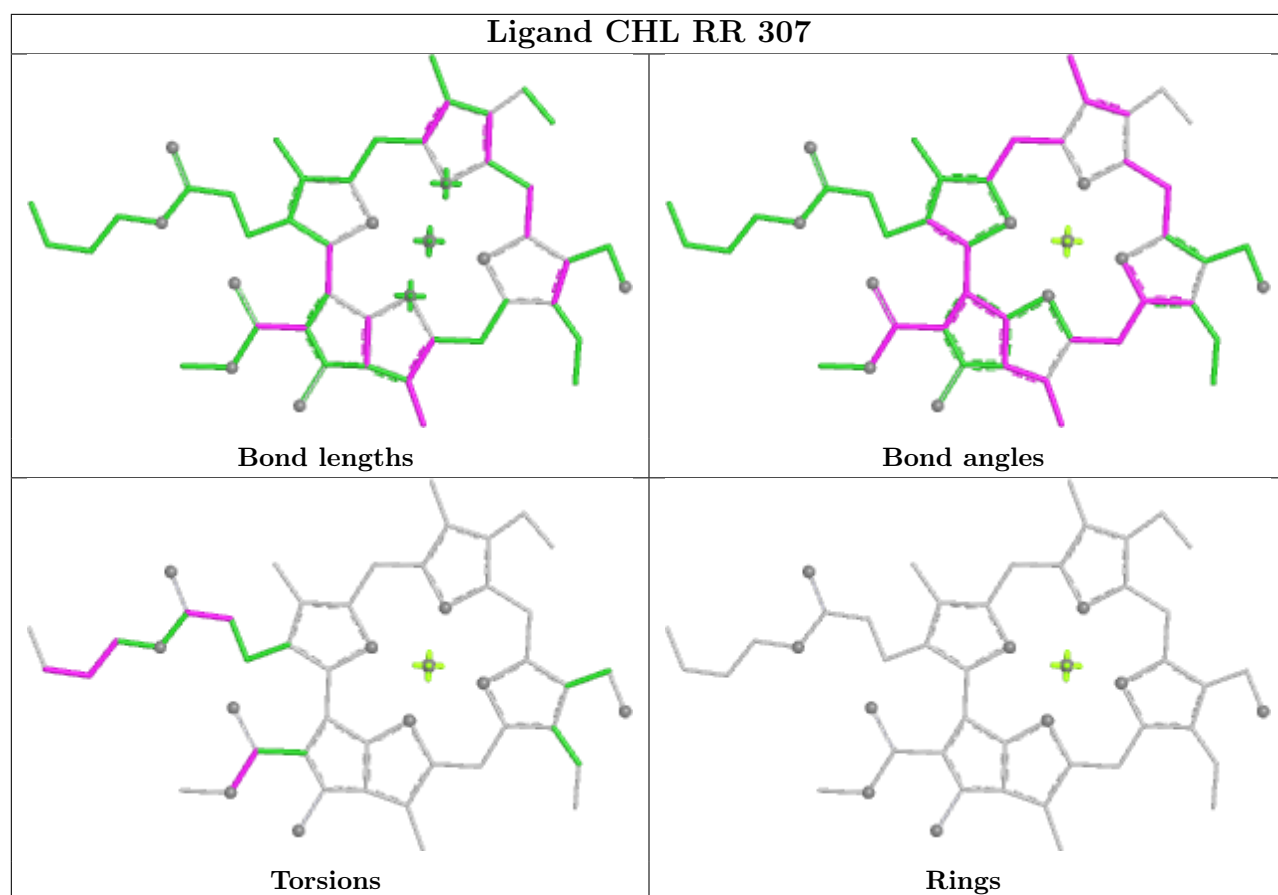


Ligand CLA 1 609

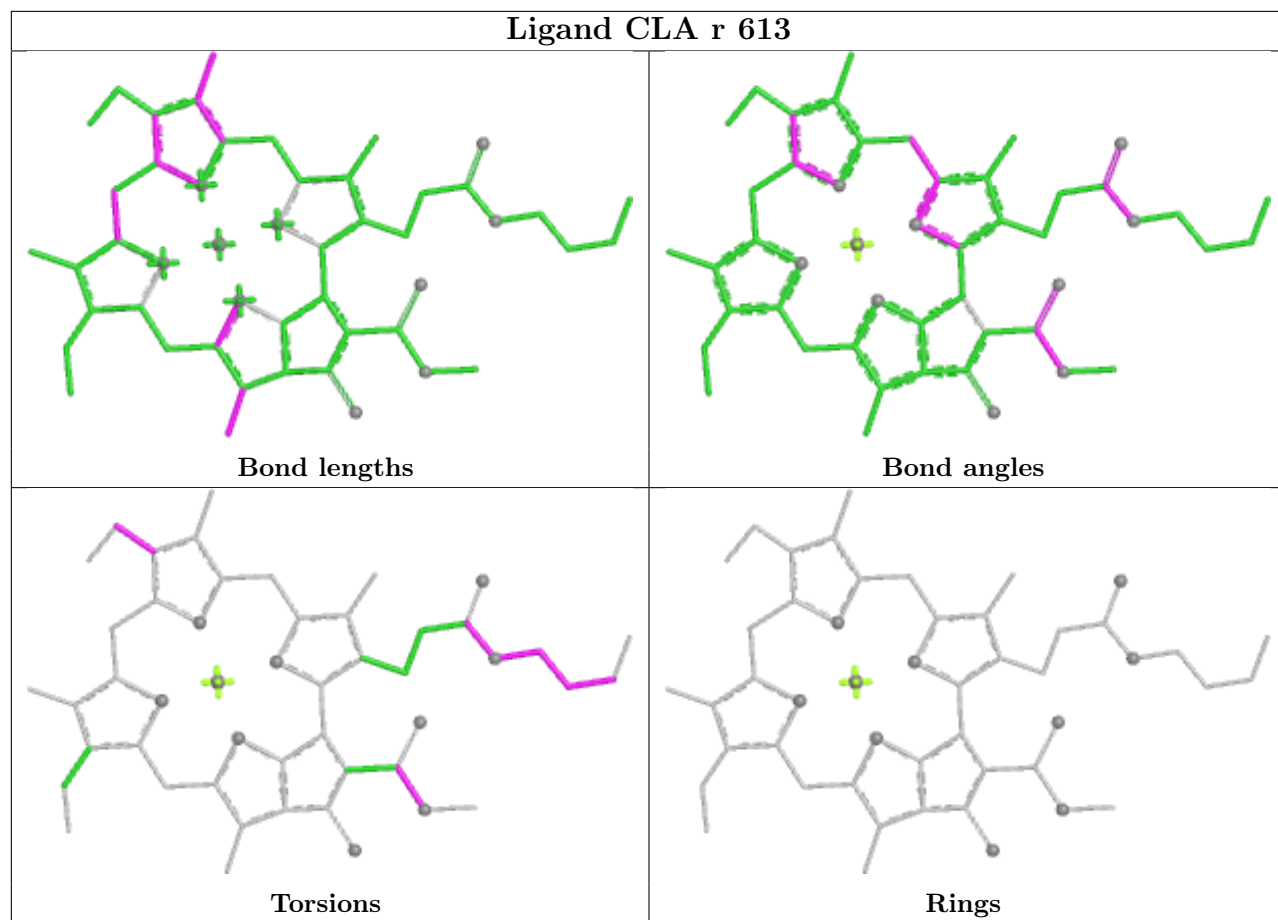


Ligand DGD B 601

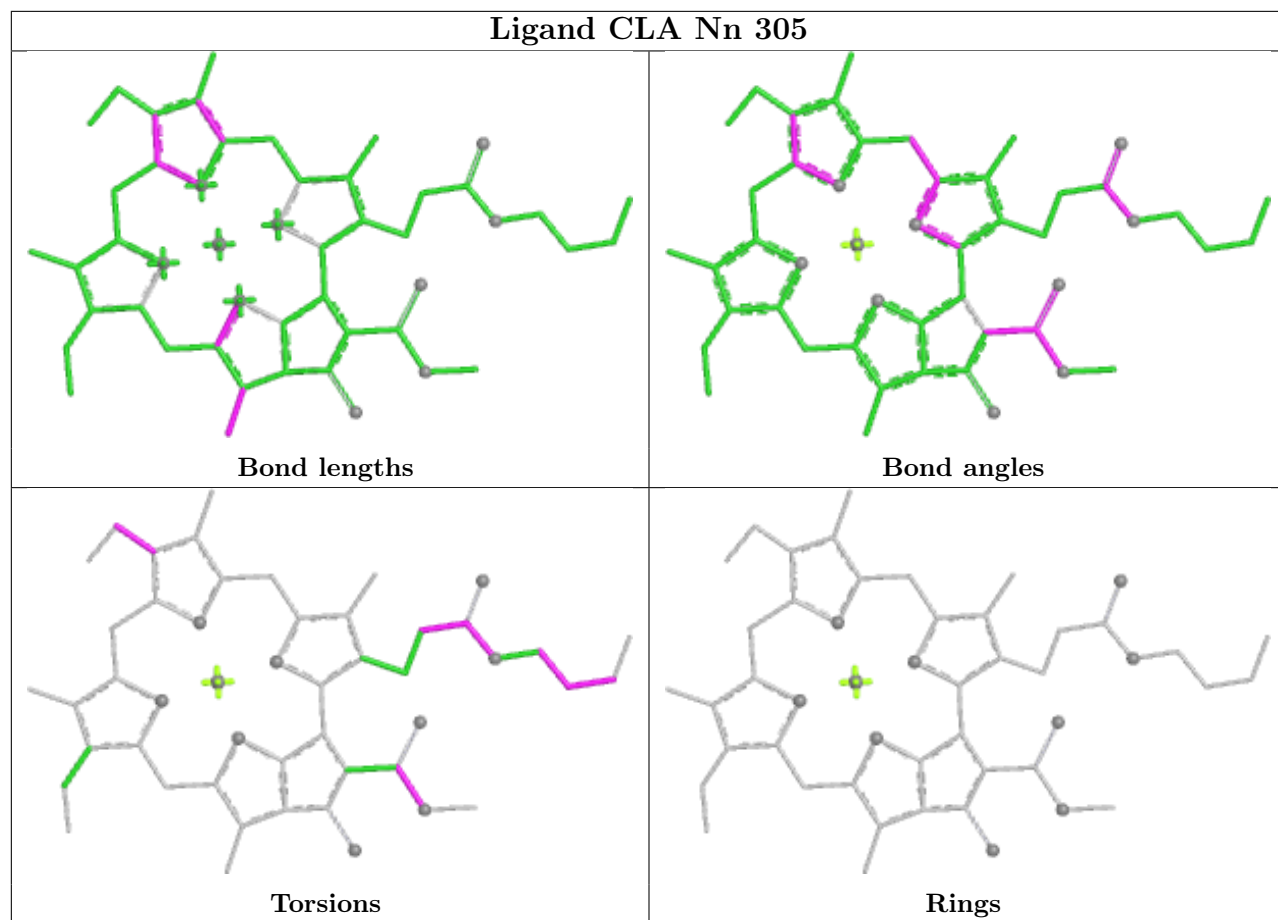


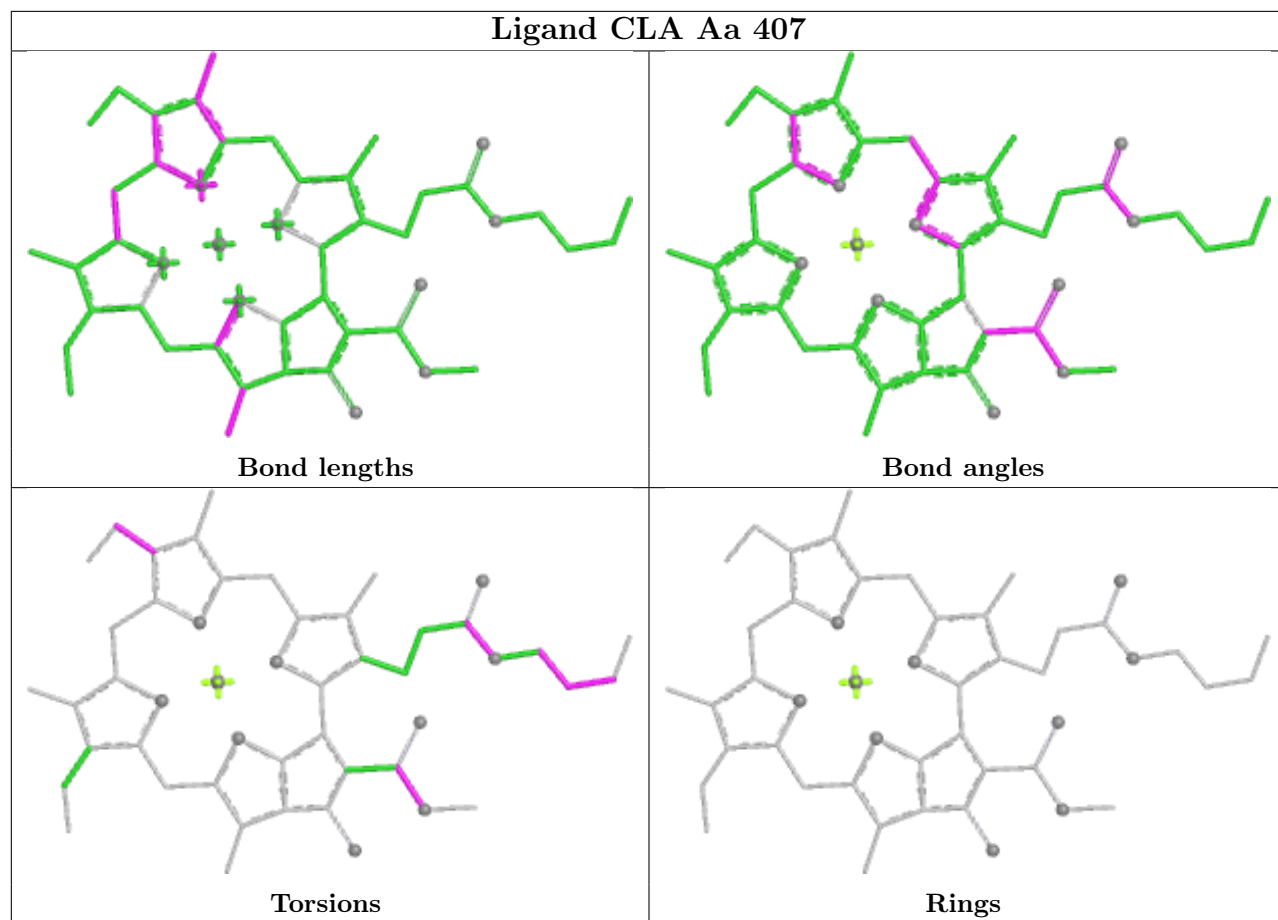


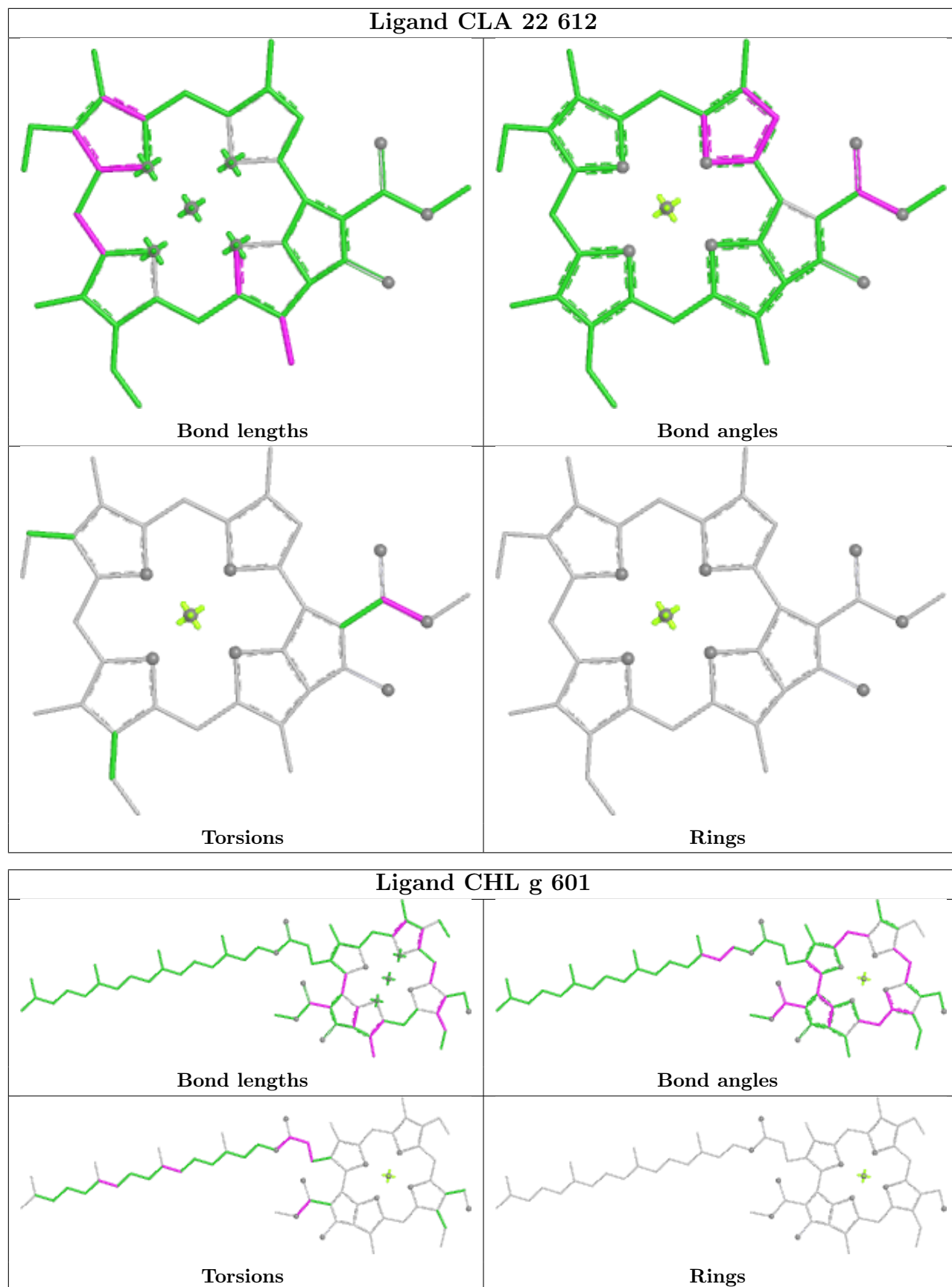
Ligand CLA r 613

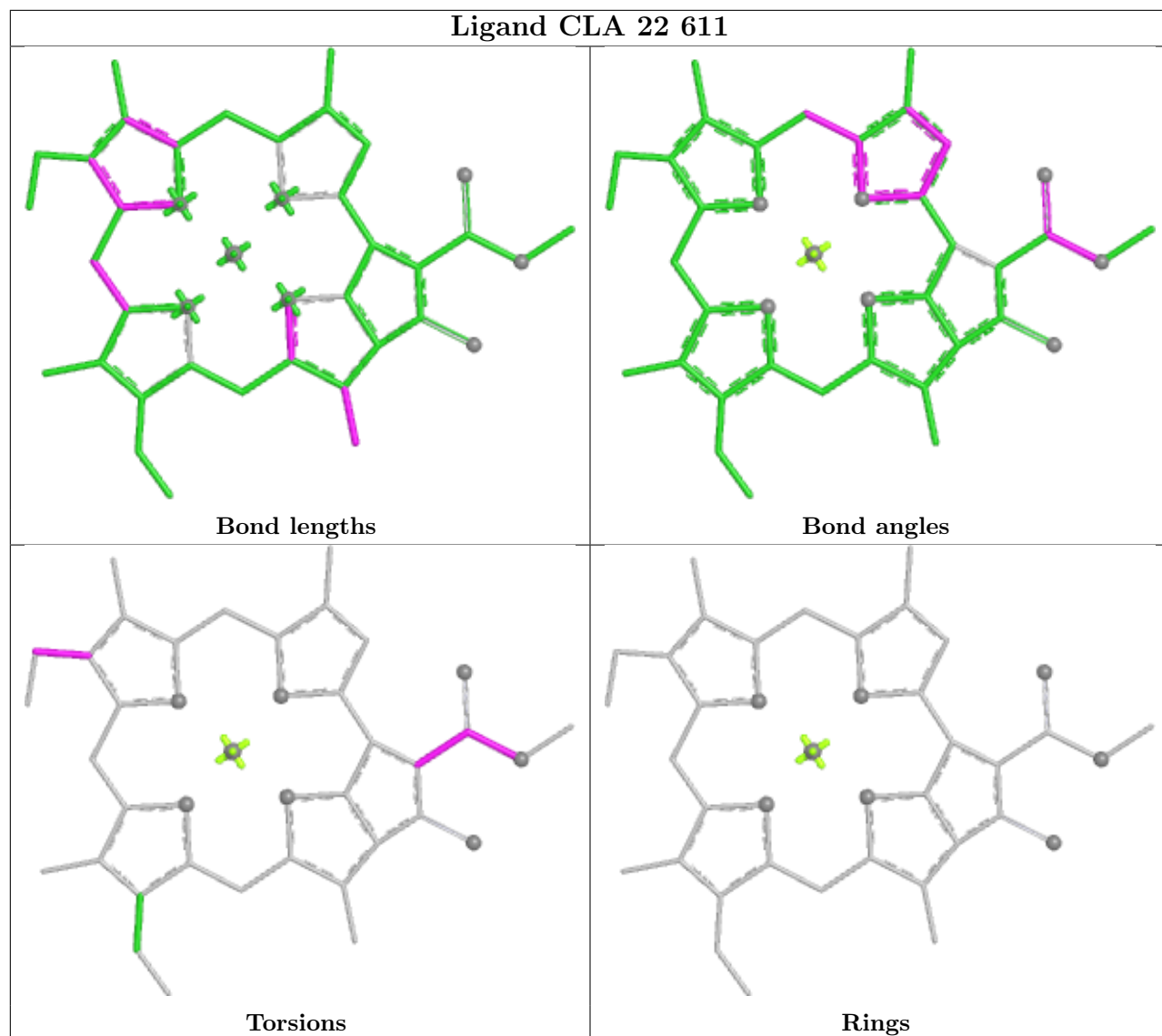


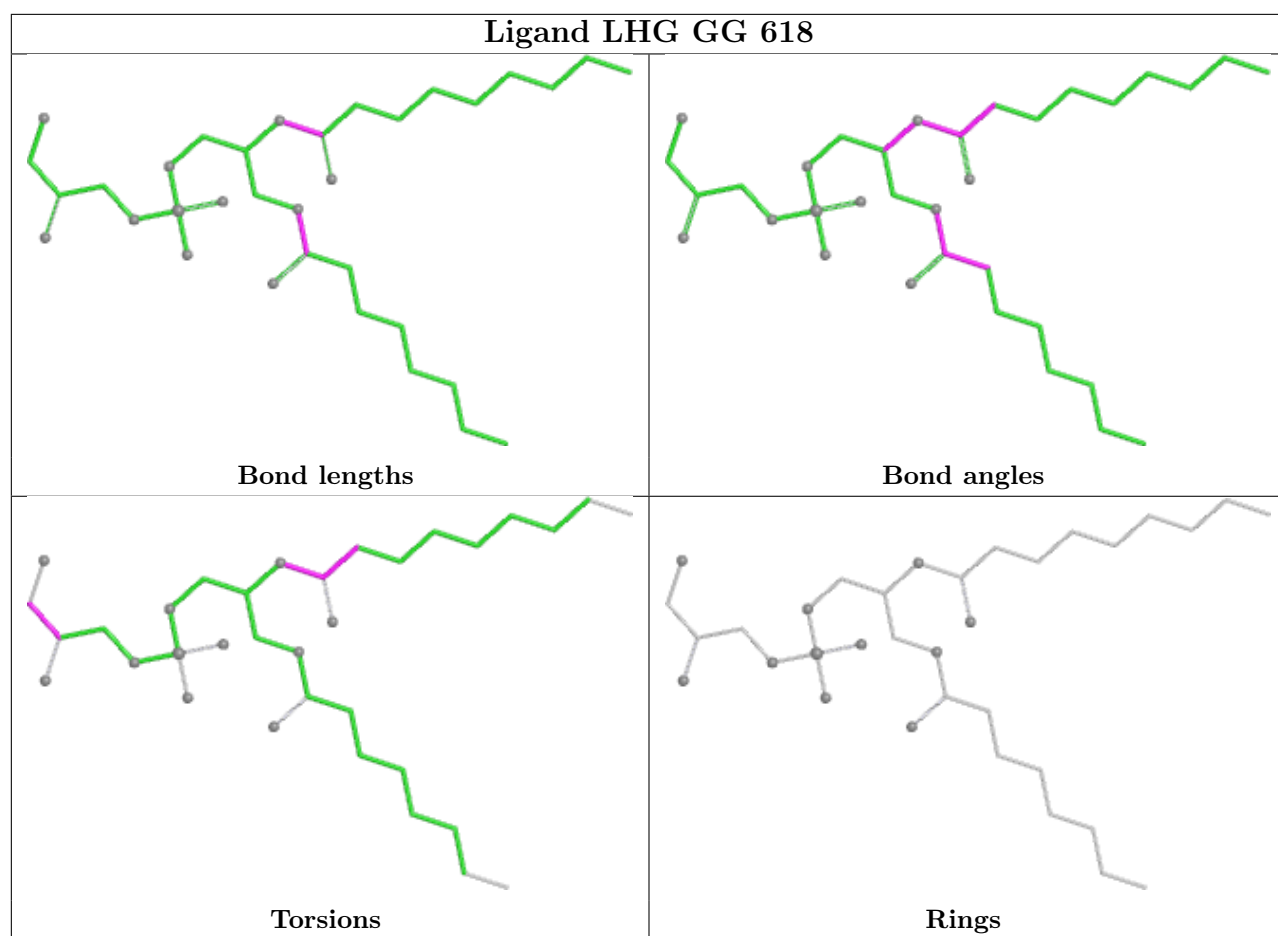
Ligand CLA Nn 305



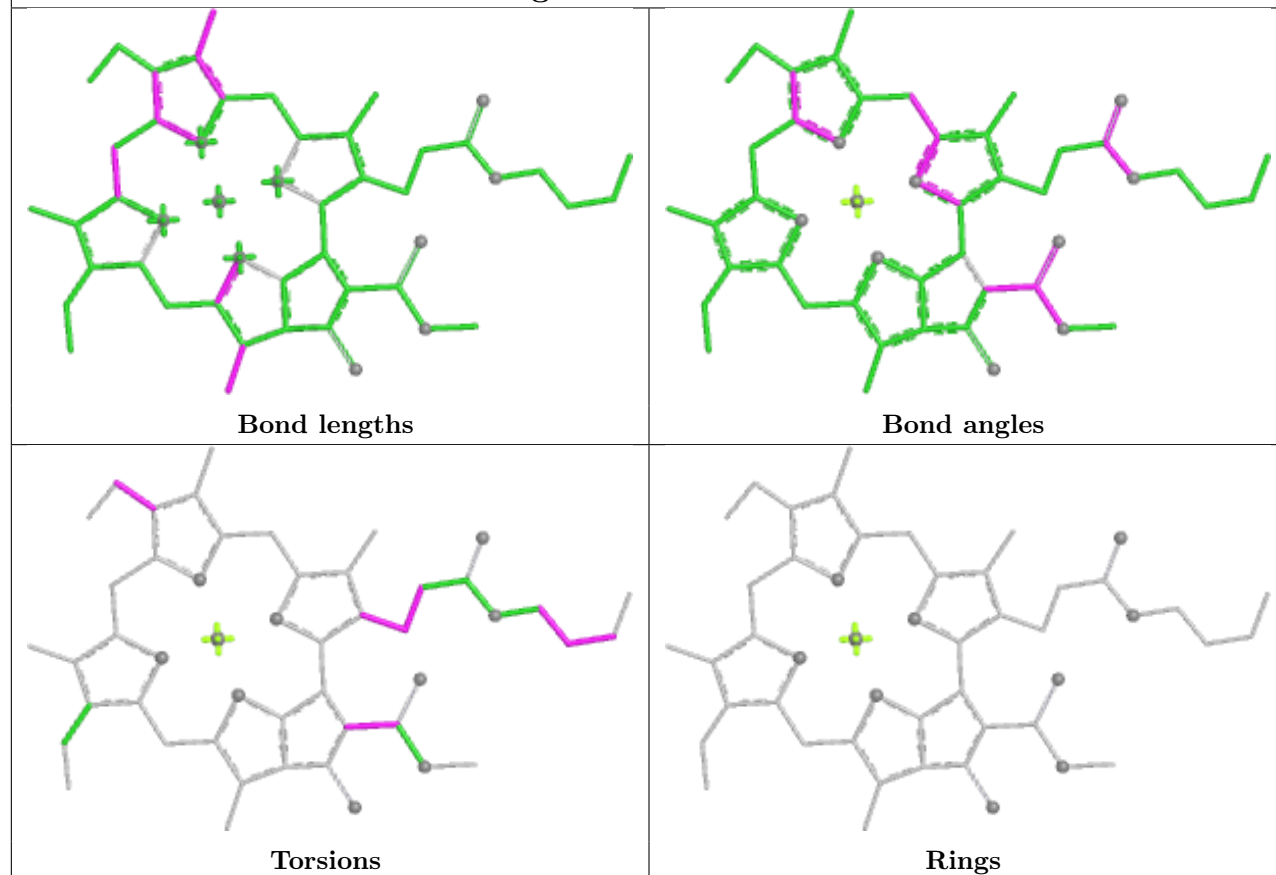




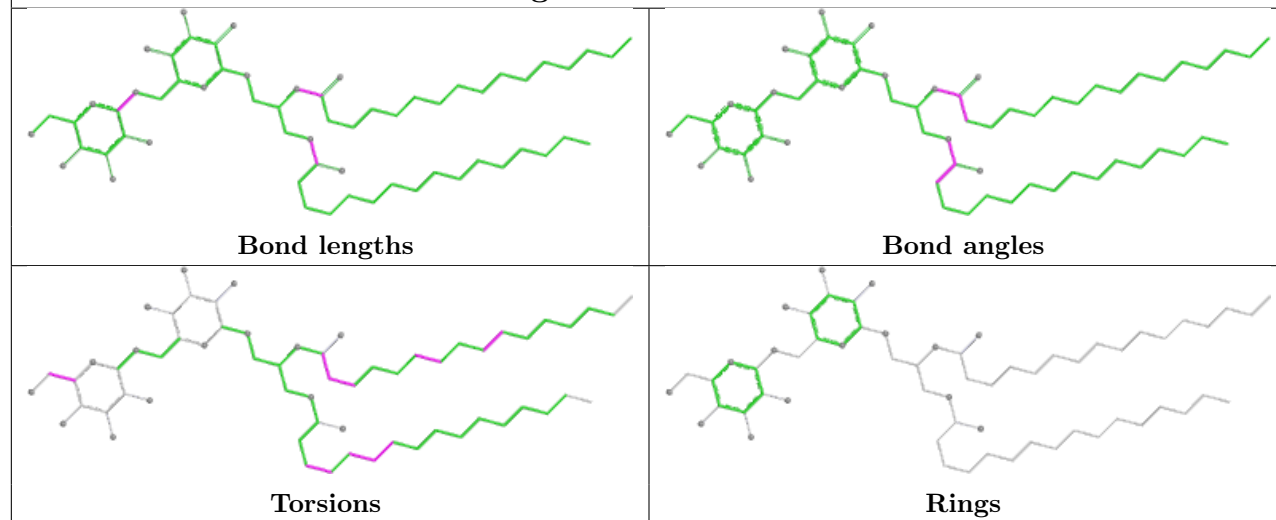




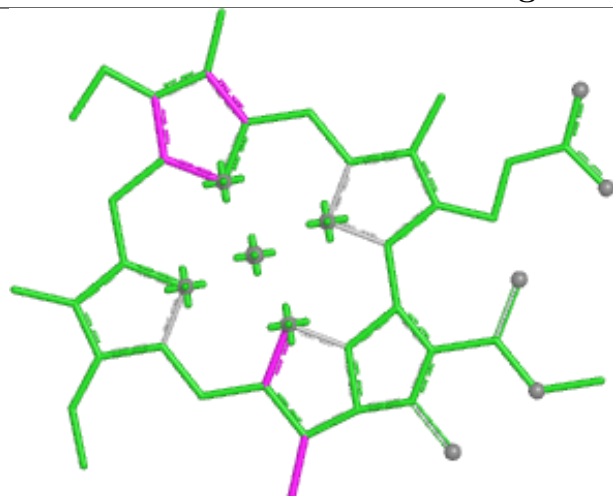
Ligand CLA R 604



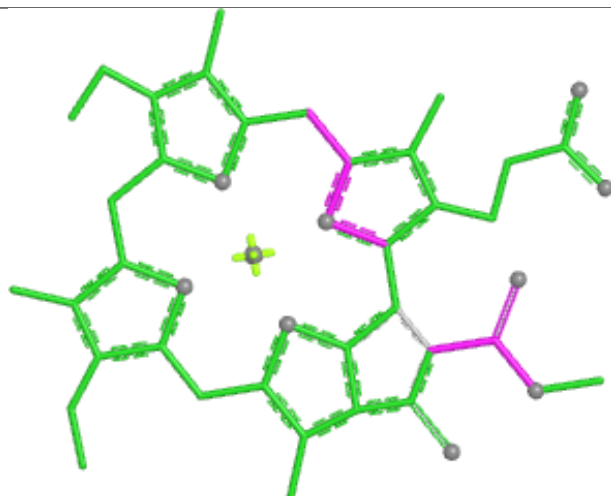
Ligand DGD h 102



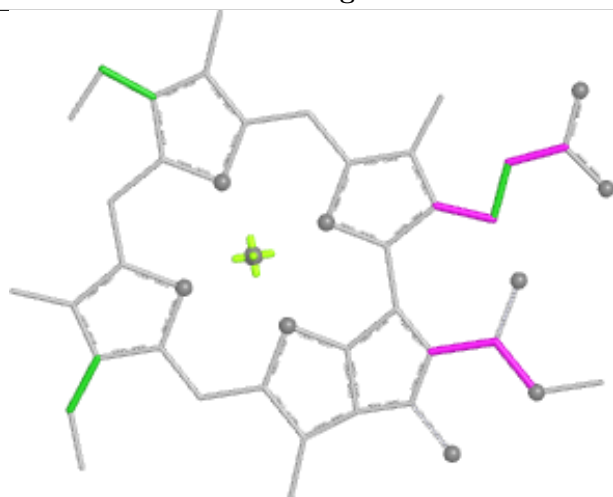
Ligand CLA 4 303



Bond lengths



Bond angles

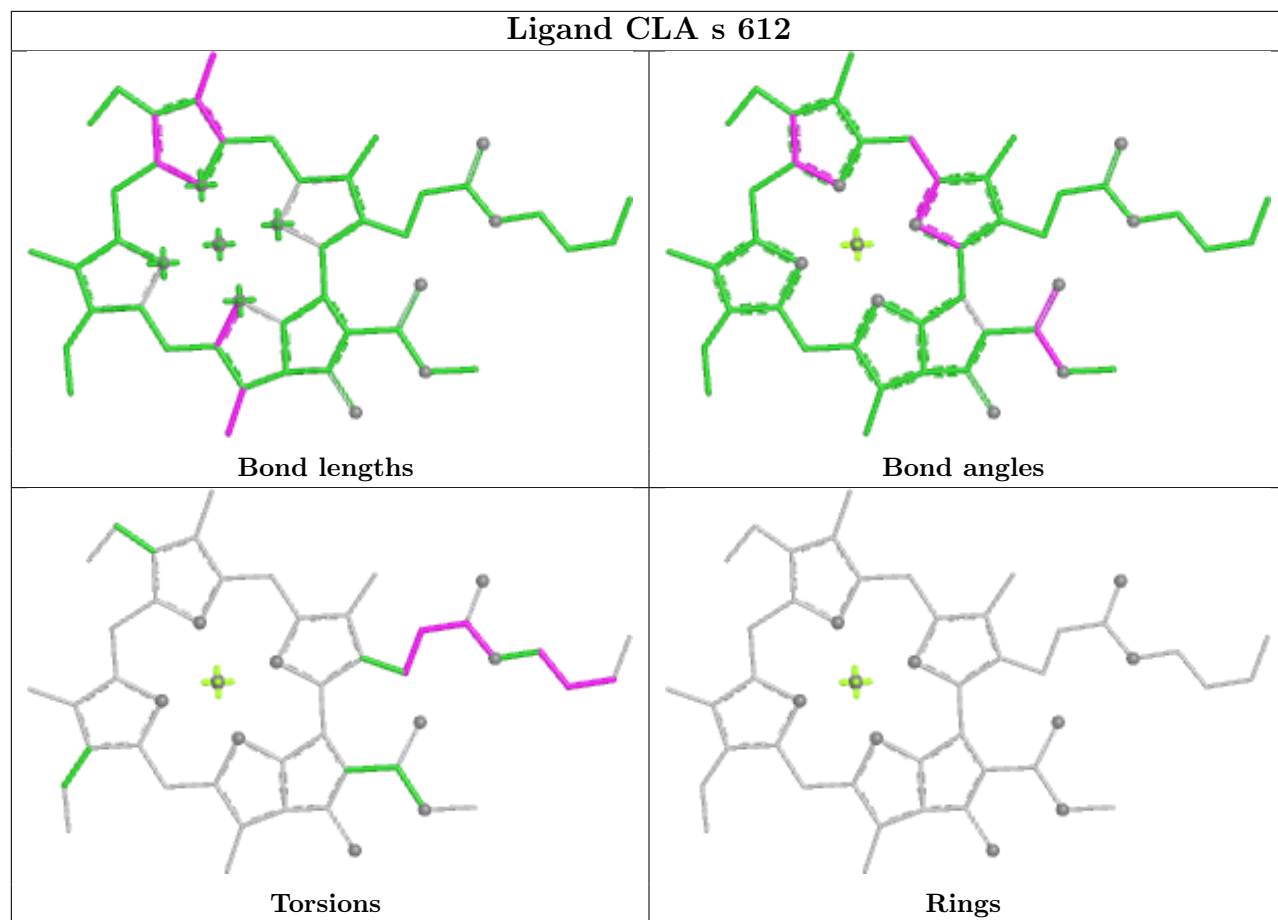


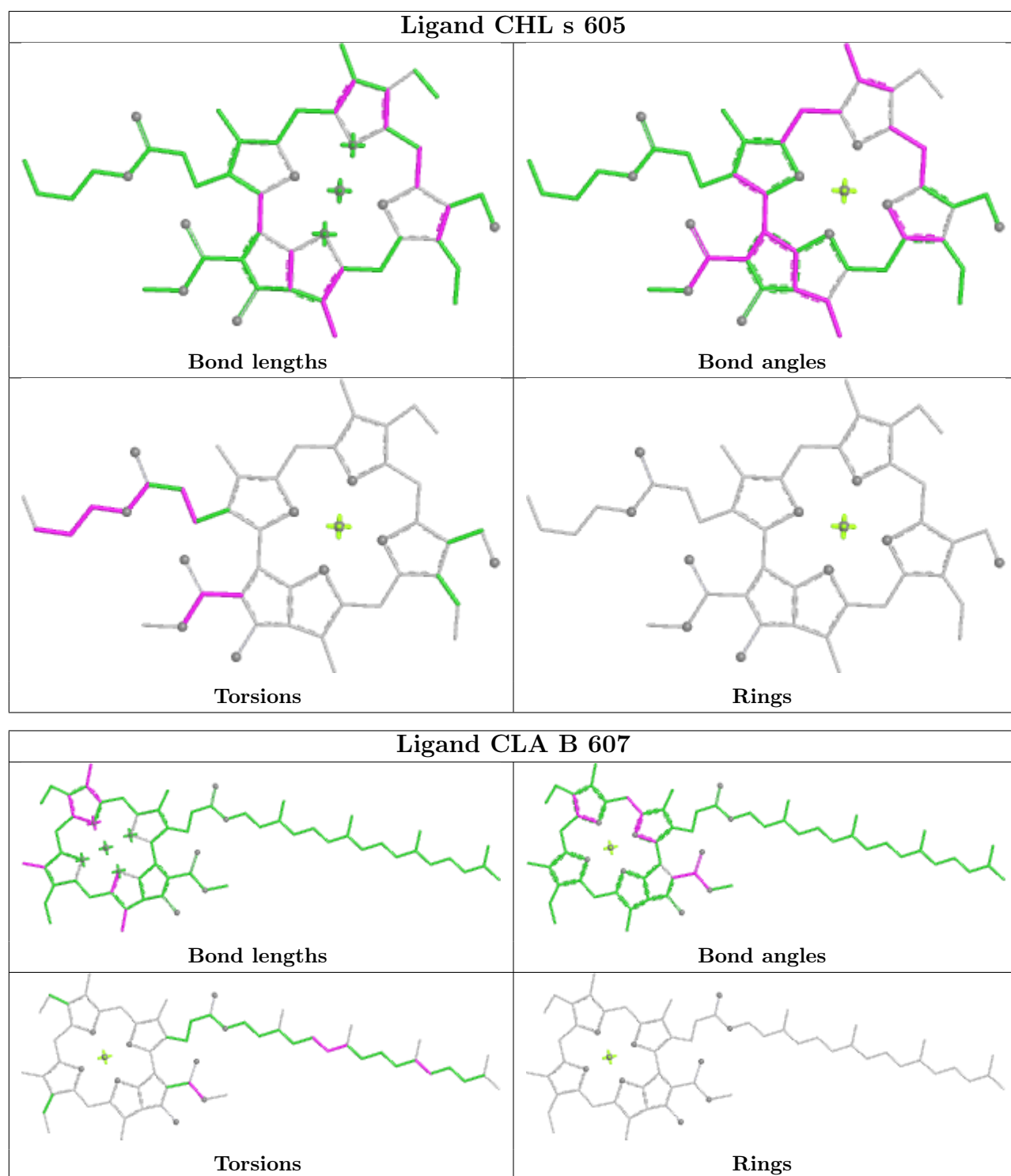
Torsions



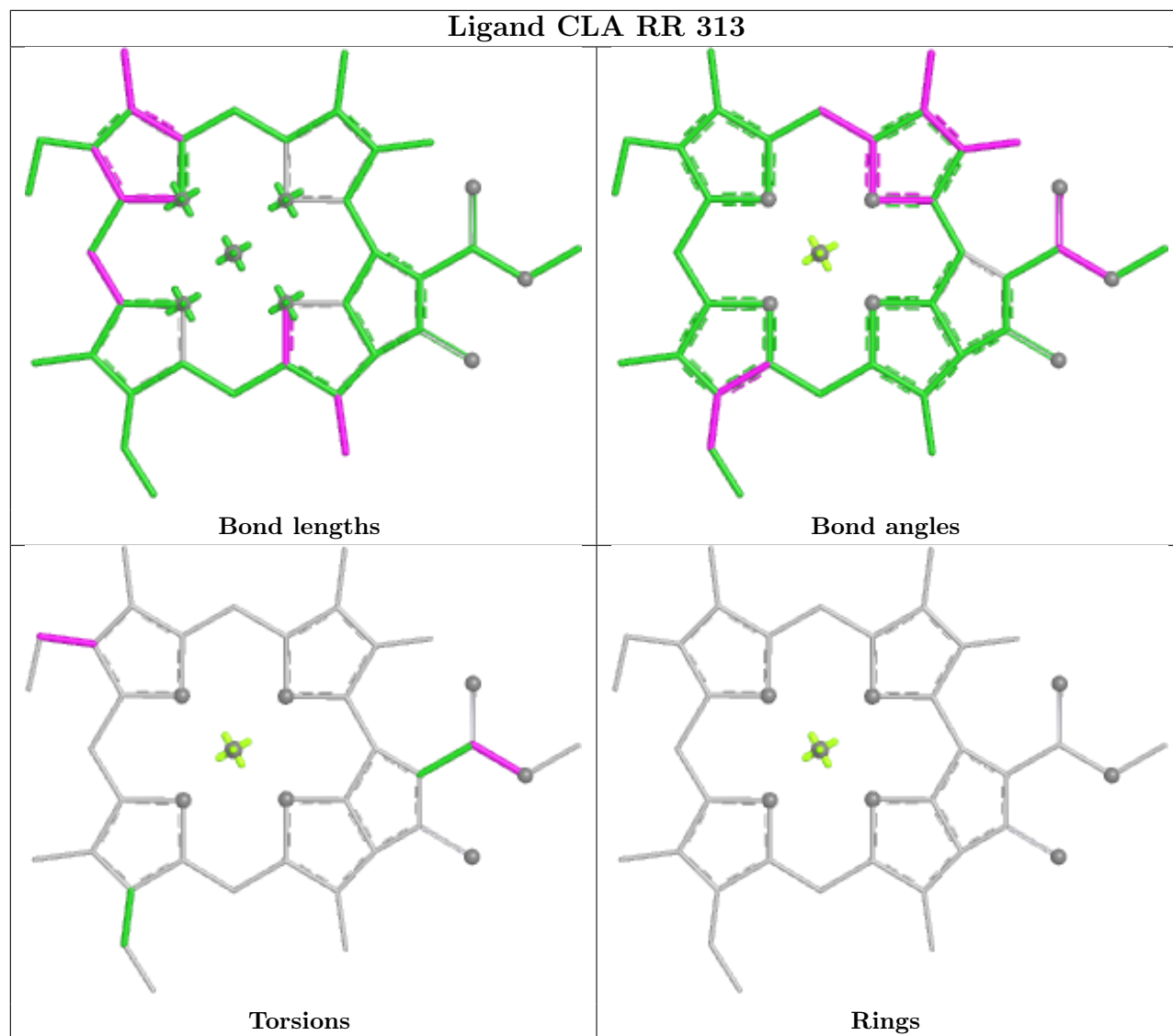
Rings

Ligand CLA s 612

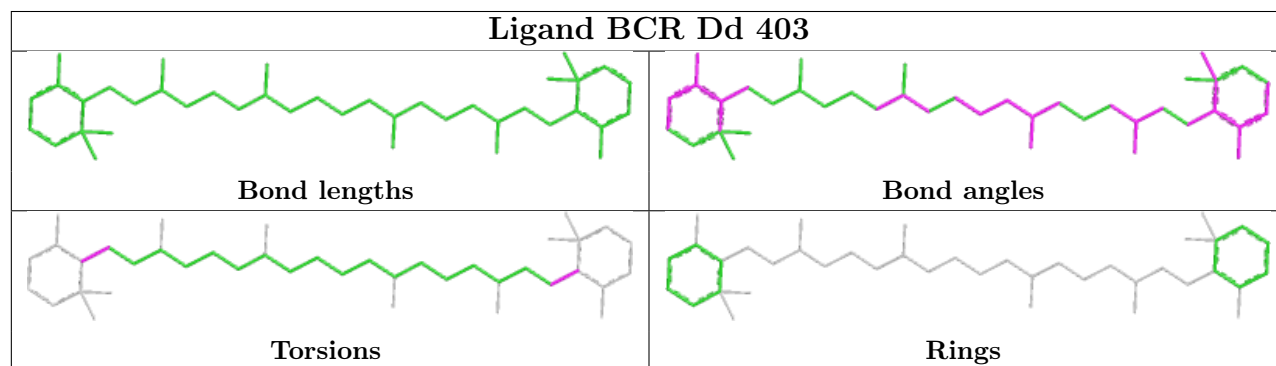


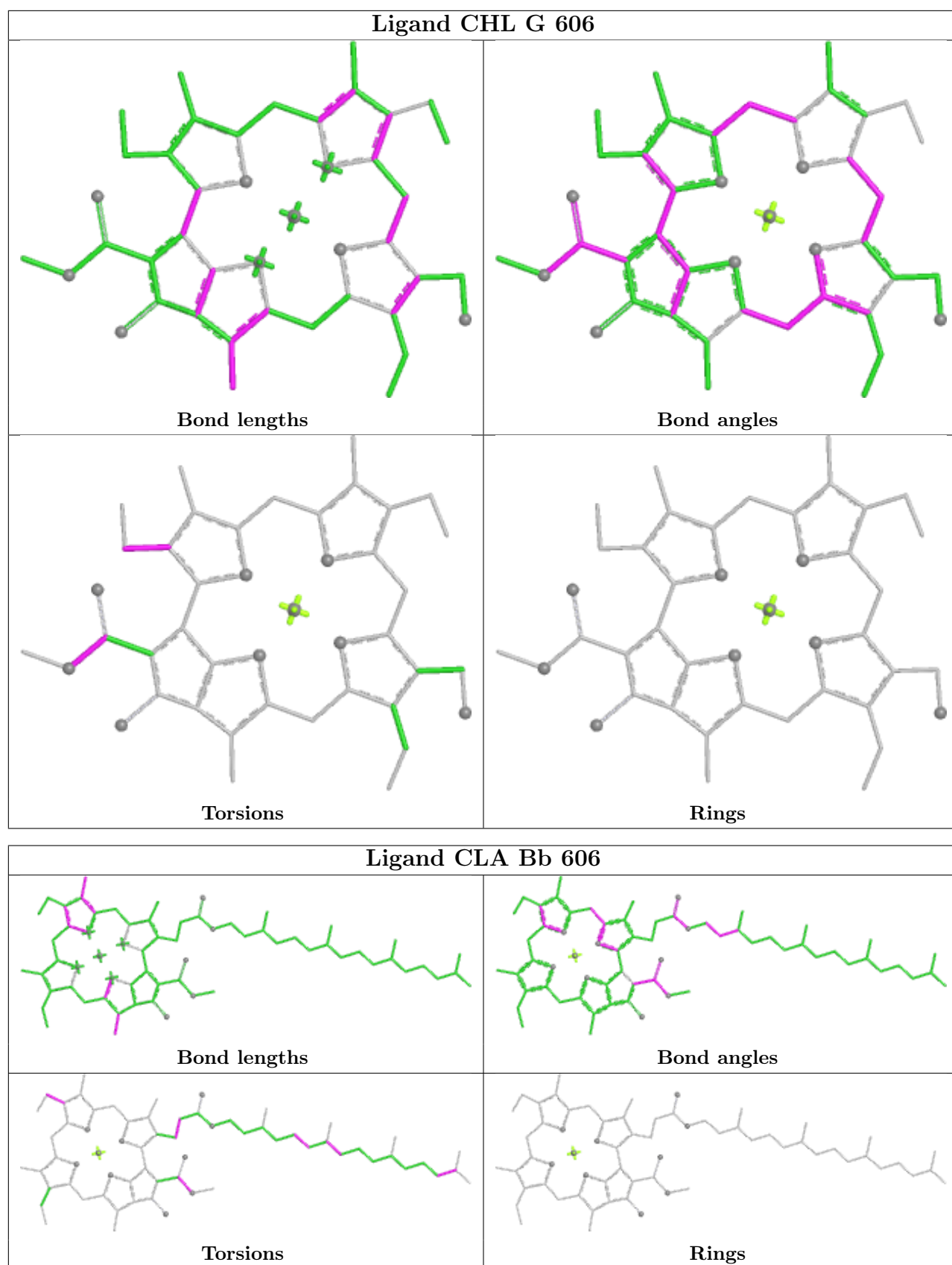


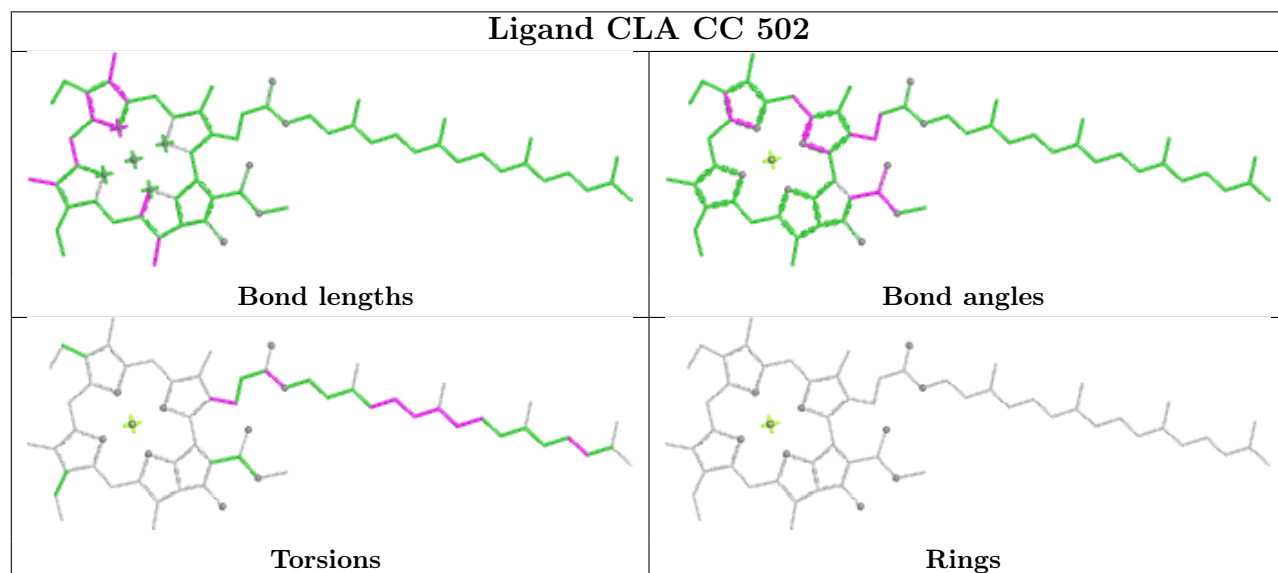
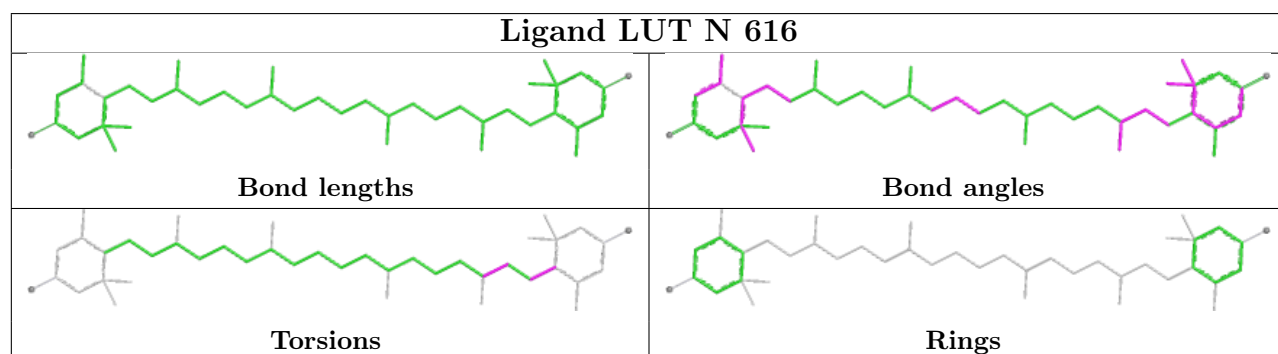
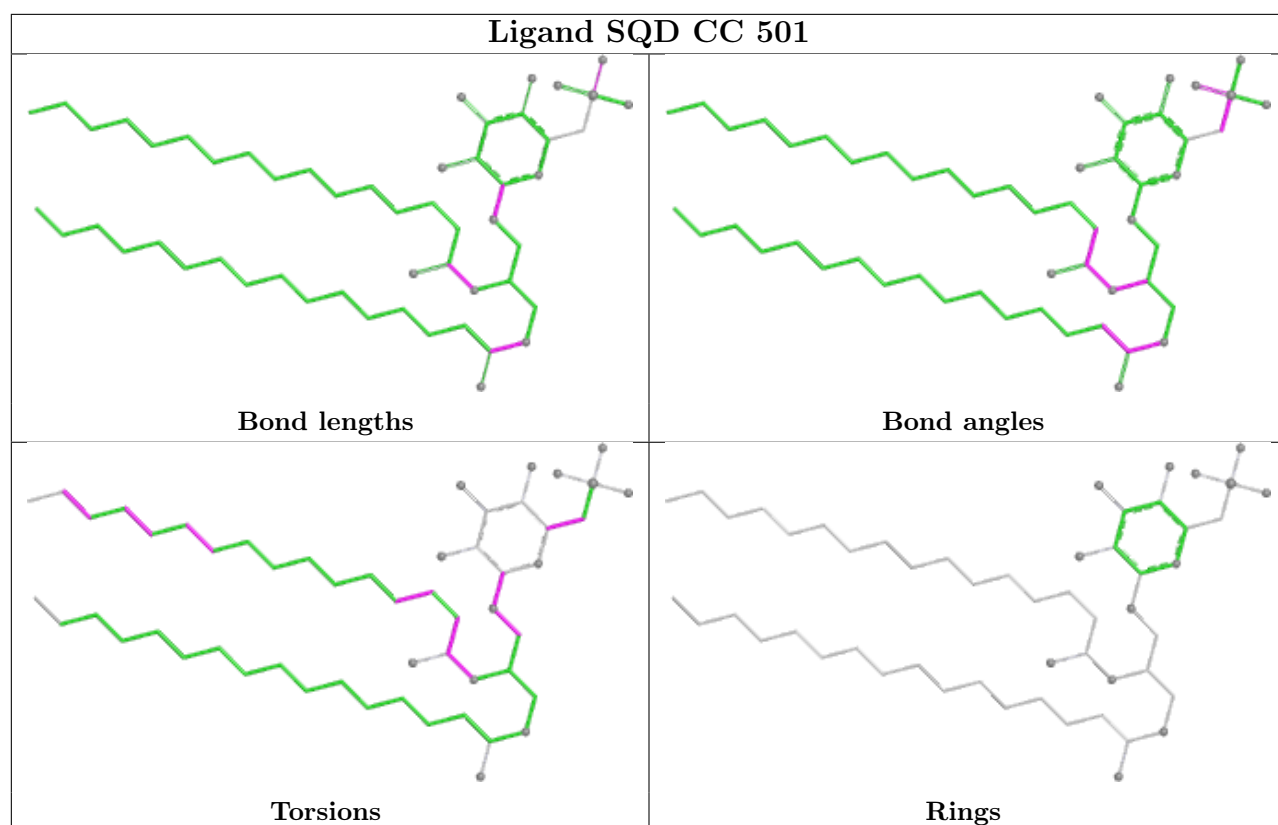
Ligand CLA RR 313



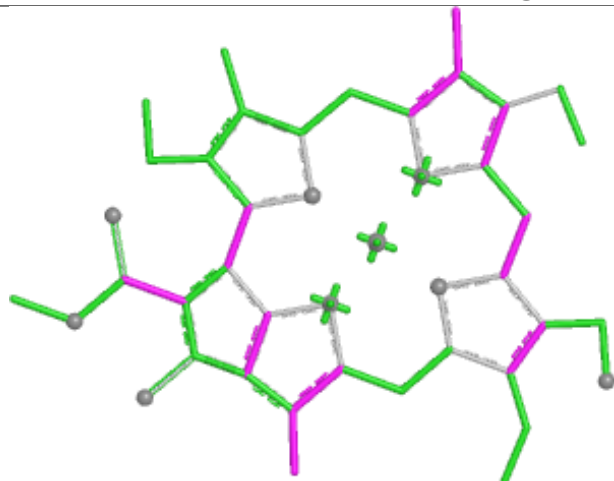
Ligand BCR Dd 403



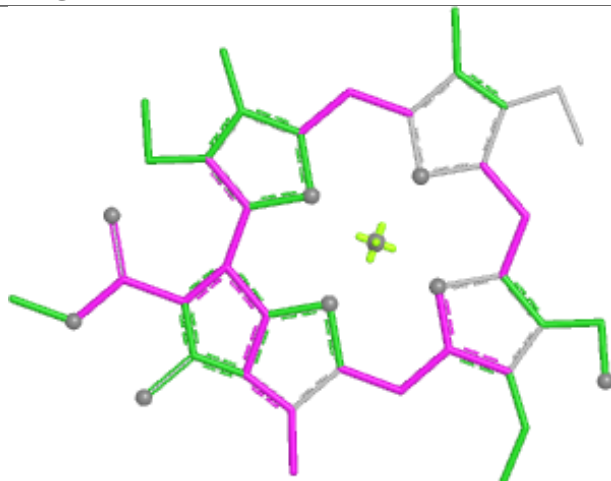




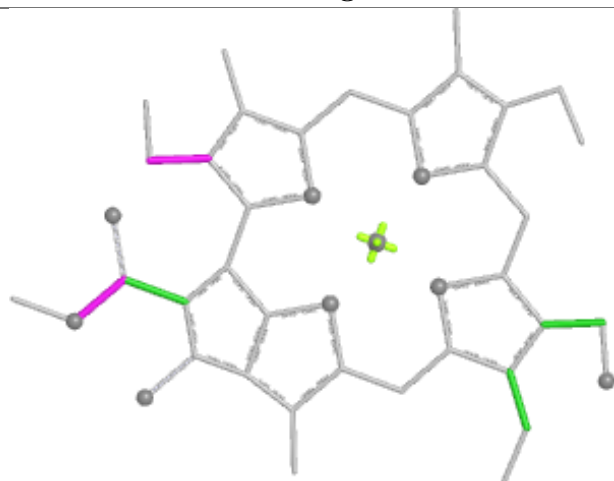
Ligand CHL g 606



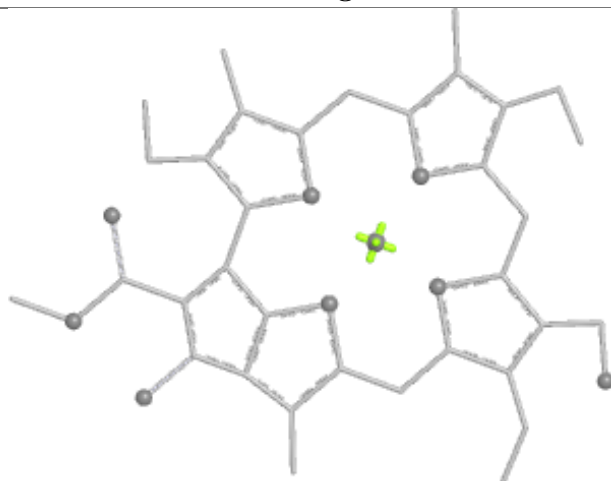
Bond lengths



Bond angles

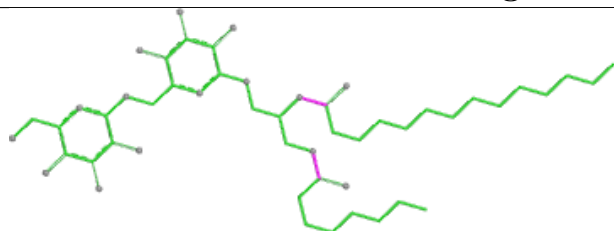


Torsions

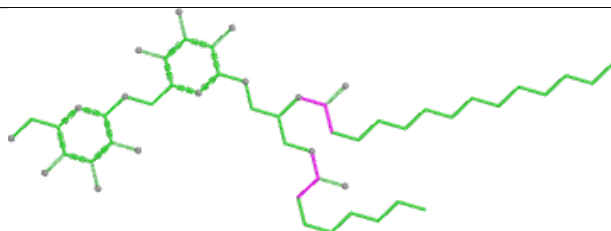


Rings

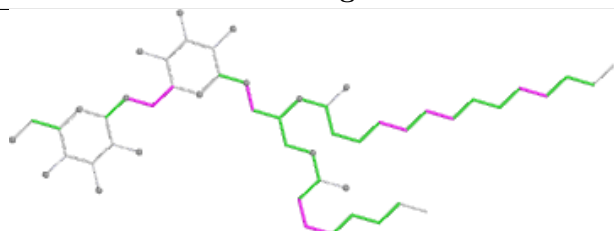
Ligand DGD Cc 520



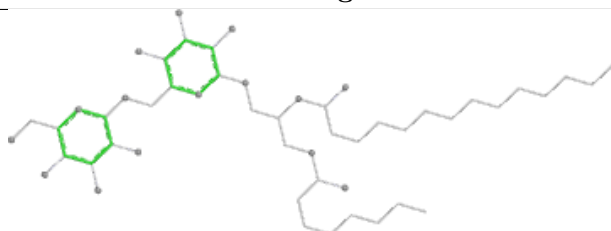
Bond lengths



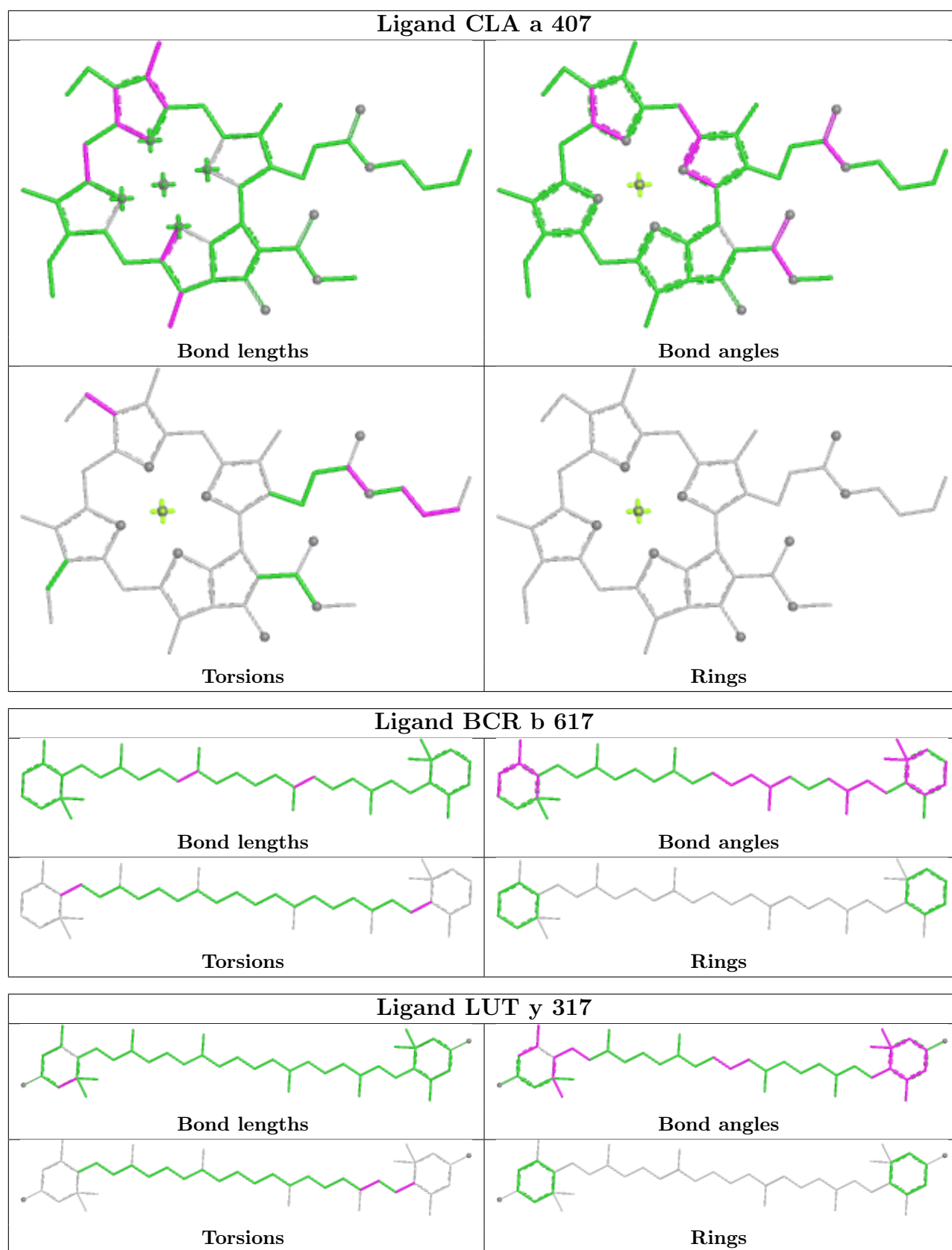
Bond angles

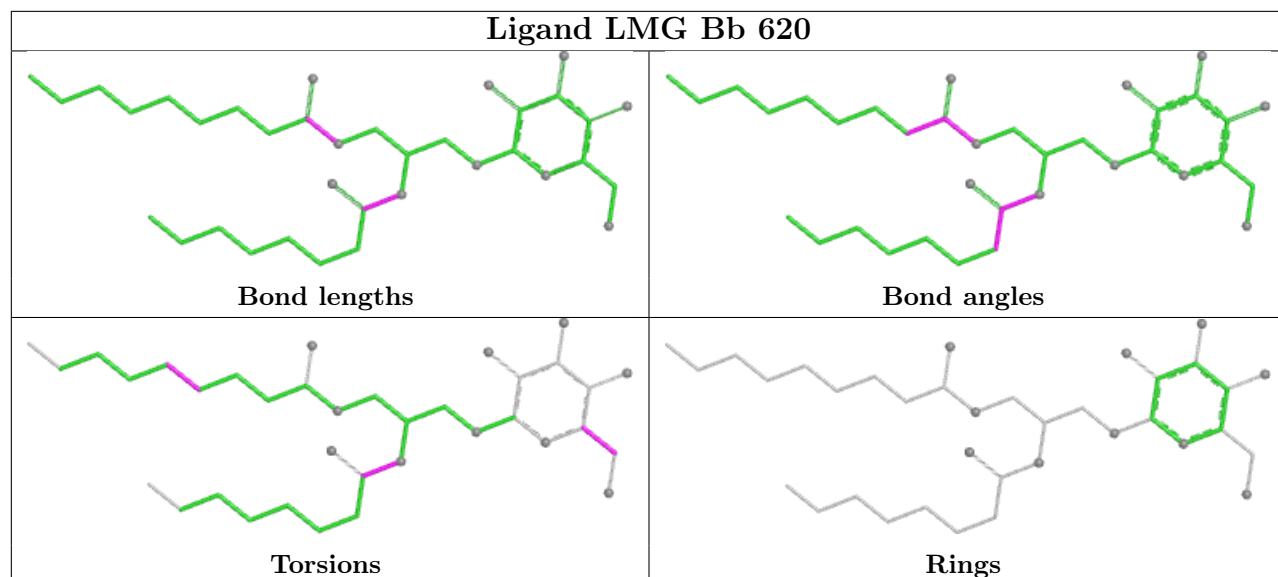
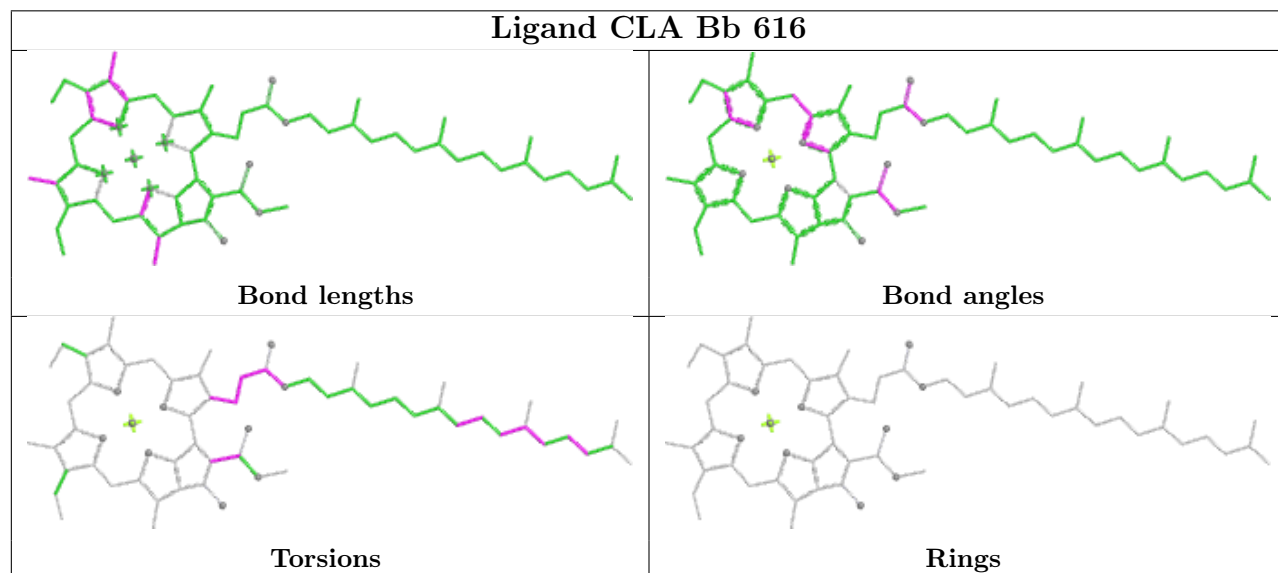
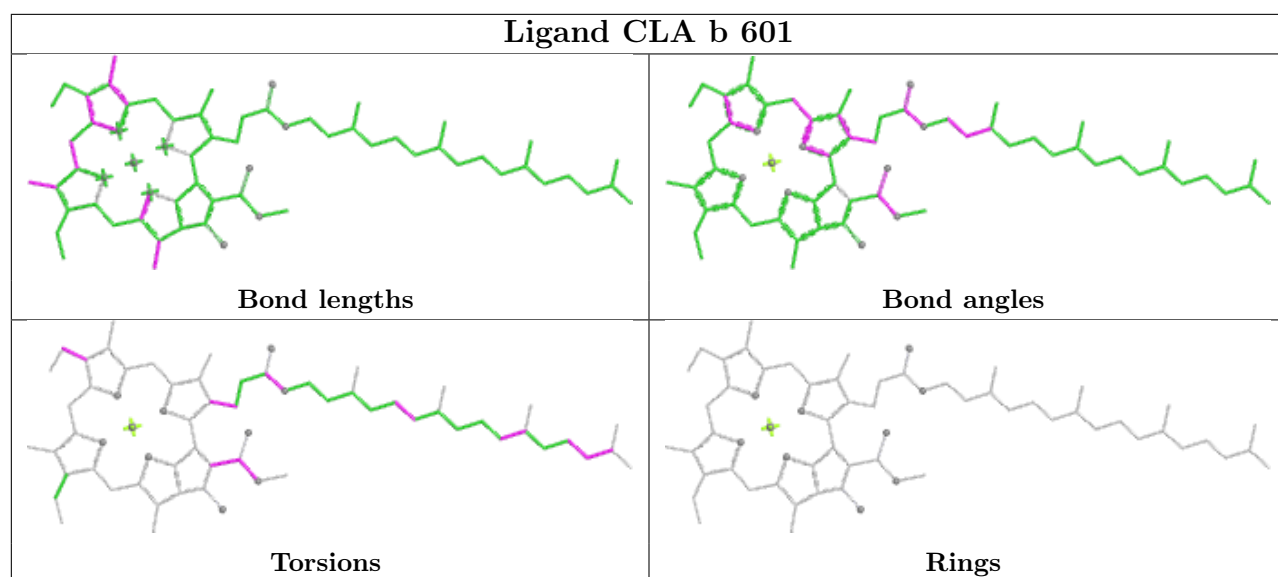


Torsions

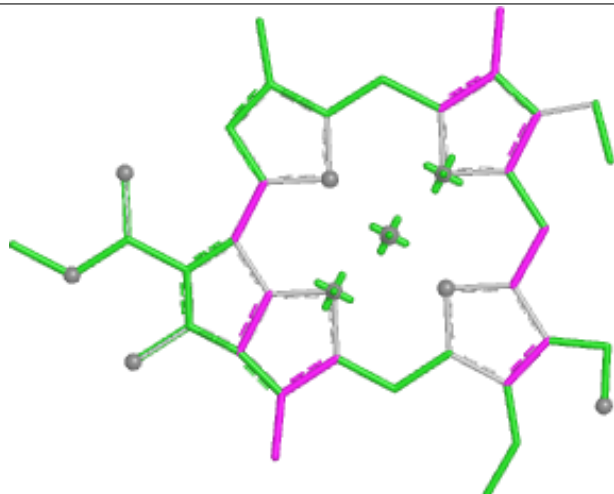


Rings

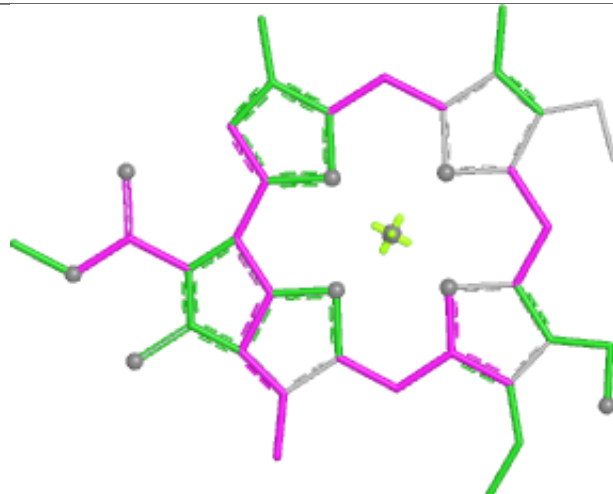




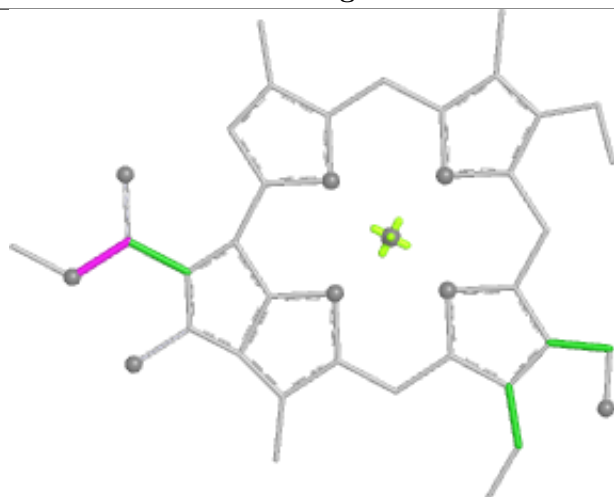
Ligand CHL 2 601



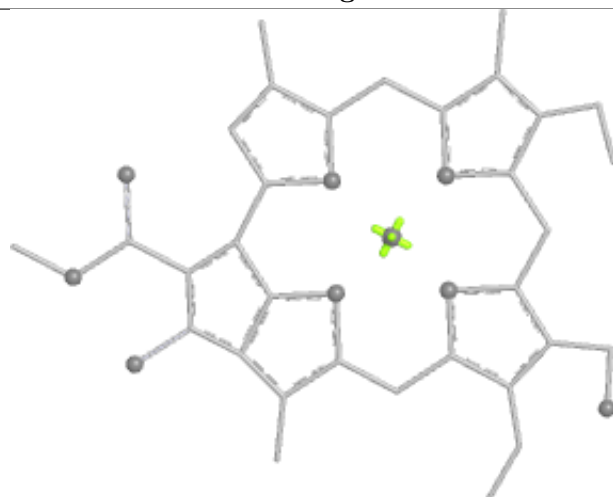
Bond lengths



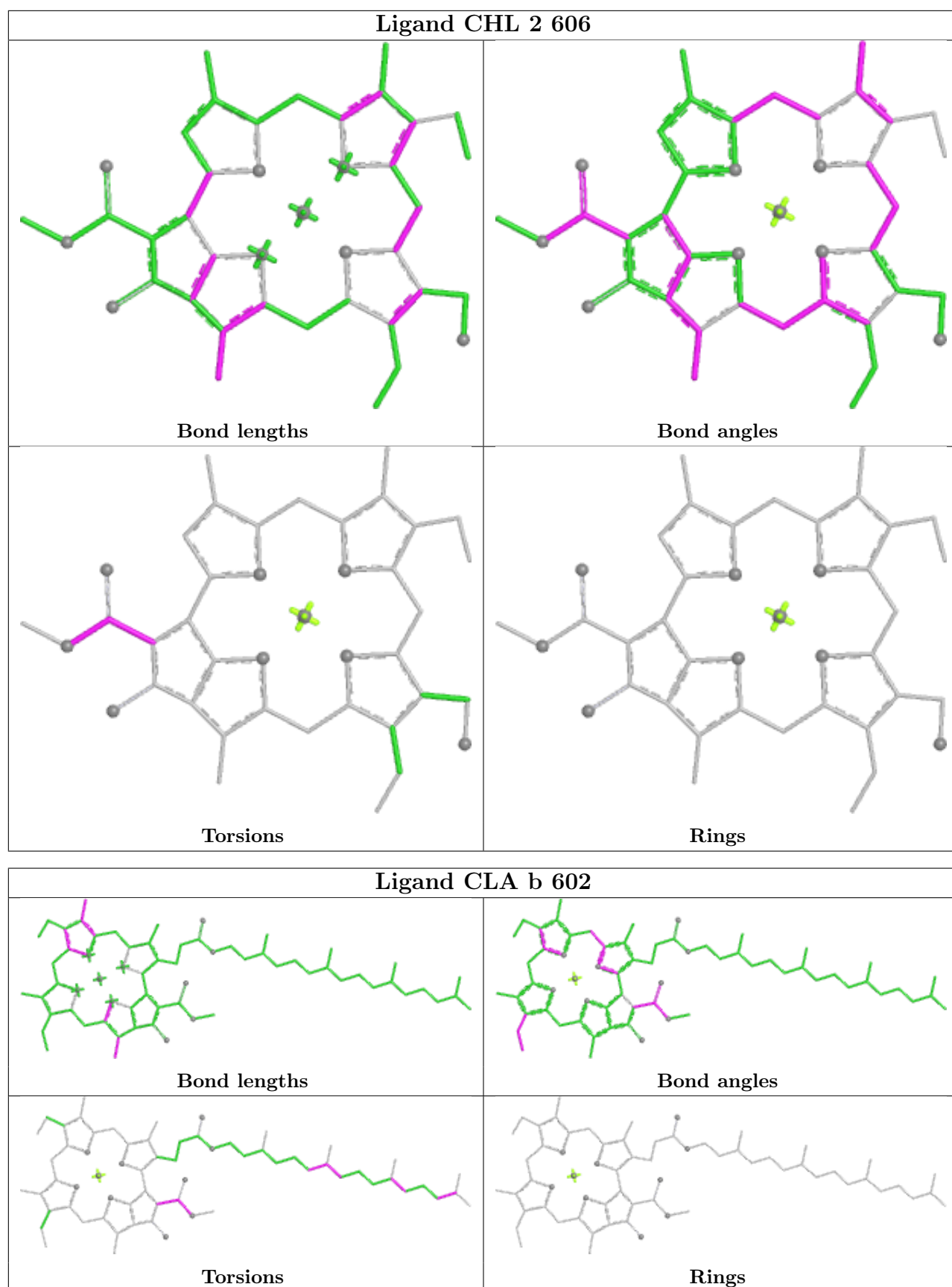
Bond angles

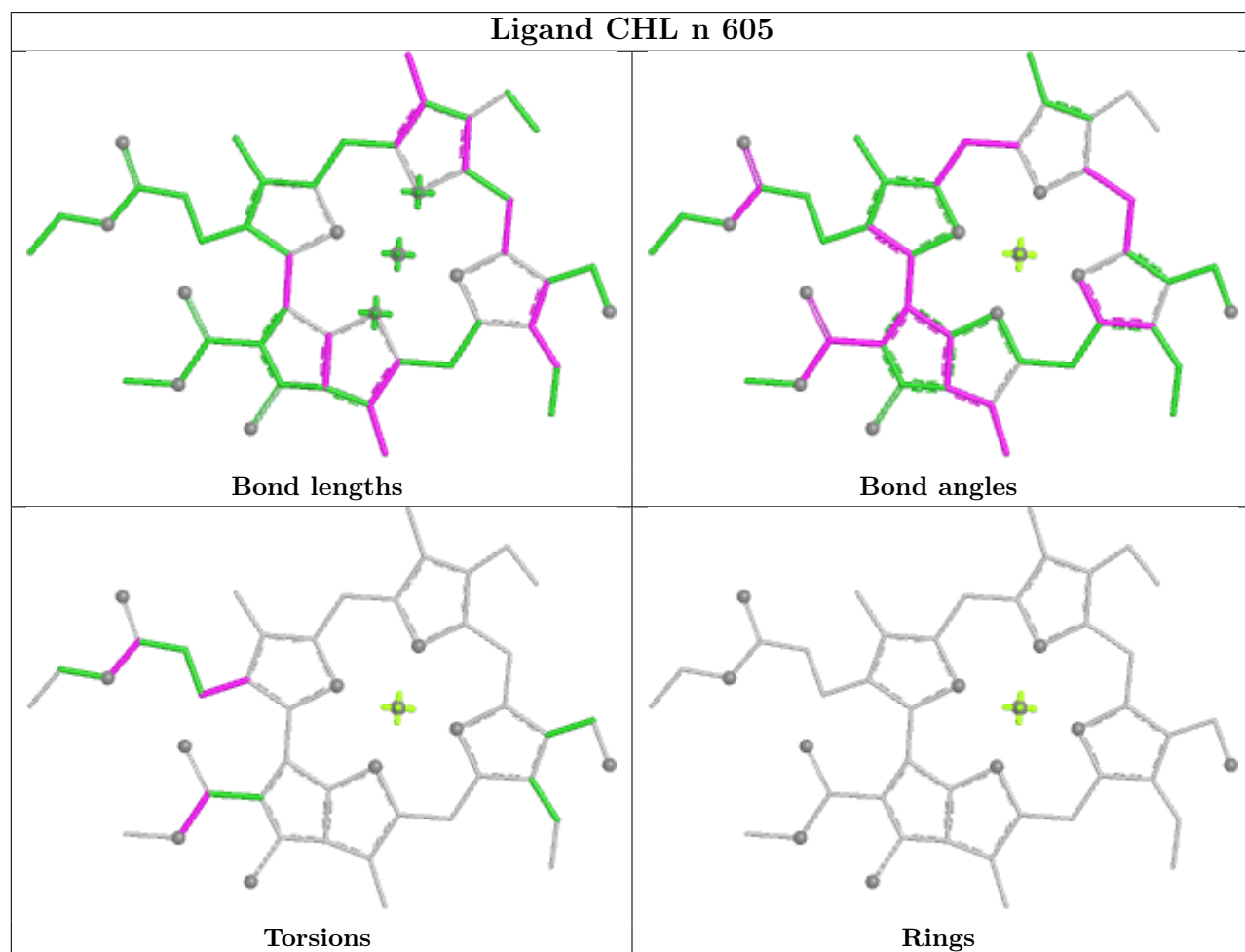
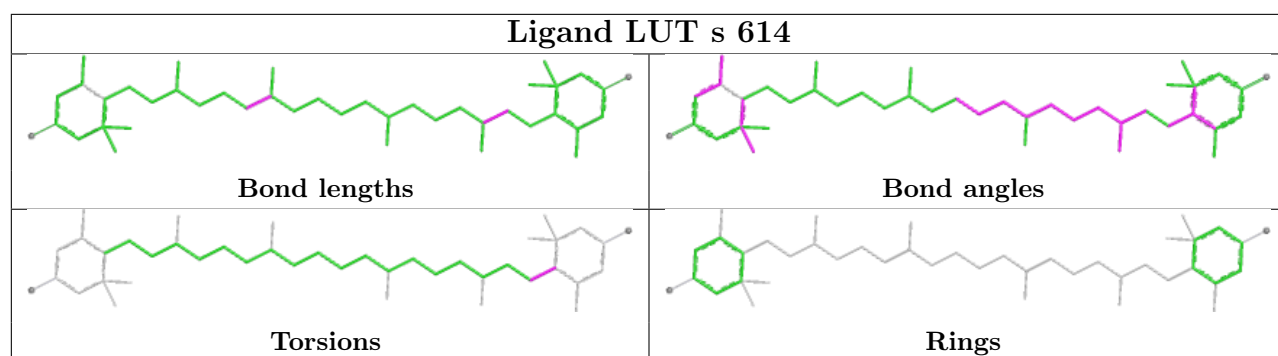


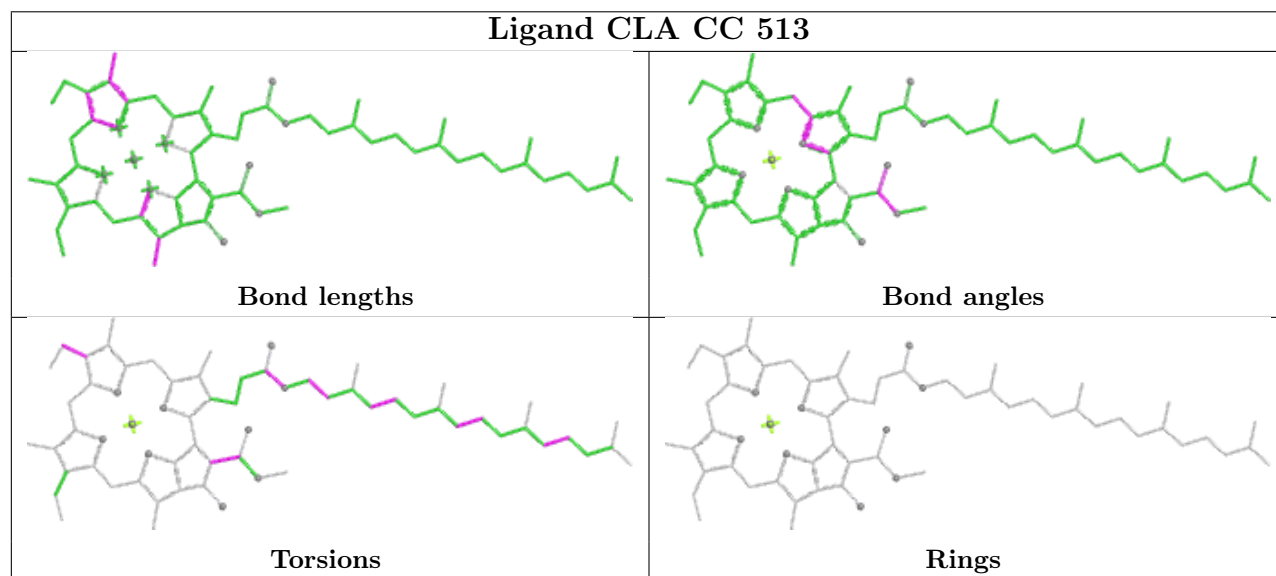
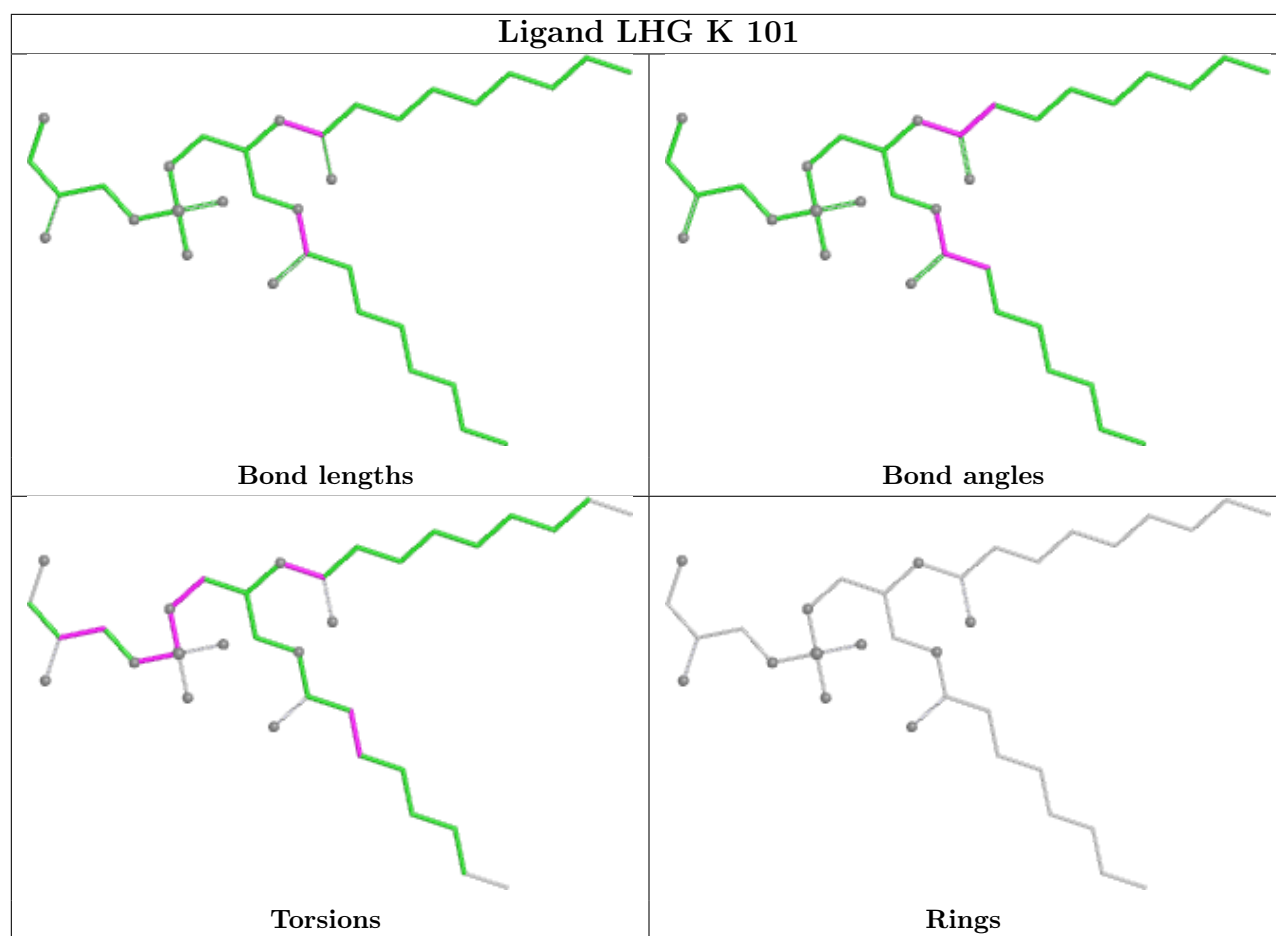
Torsions

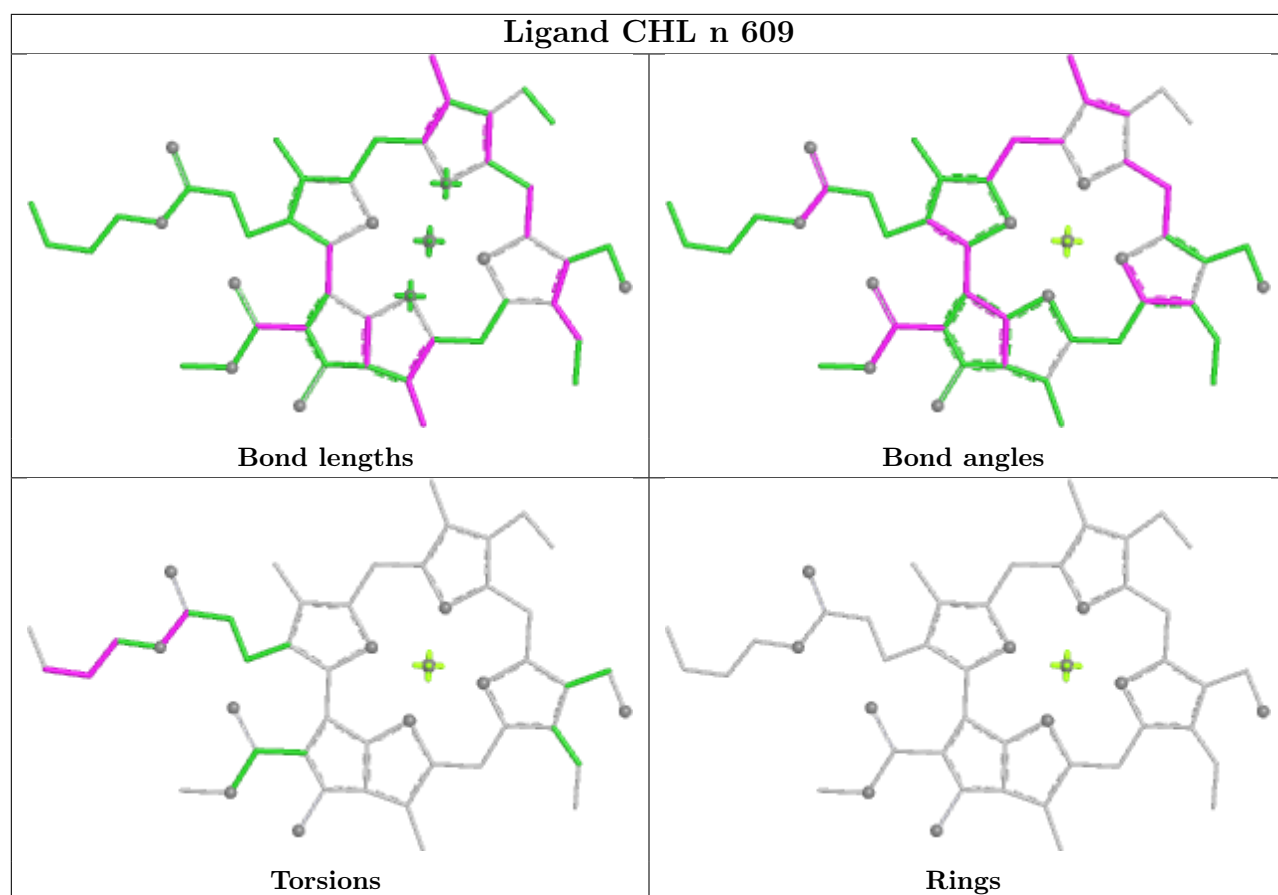


Rings

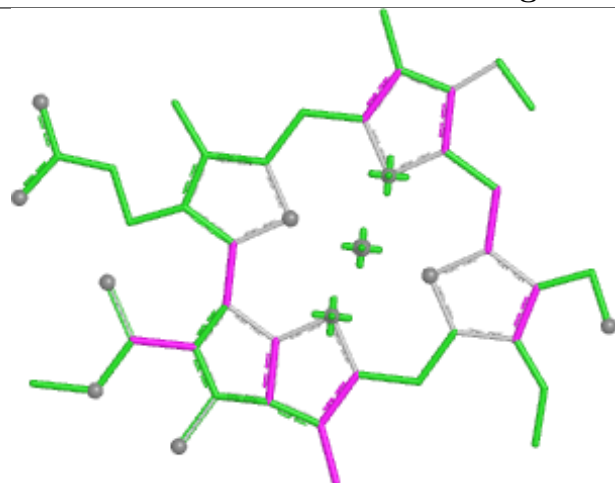




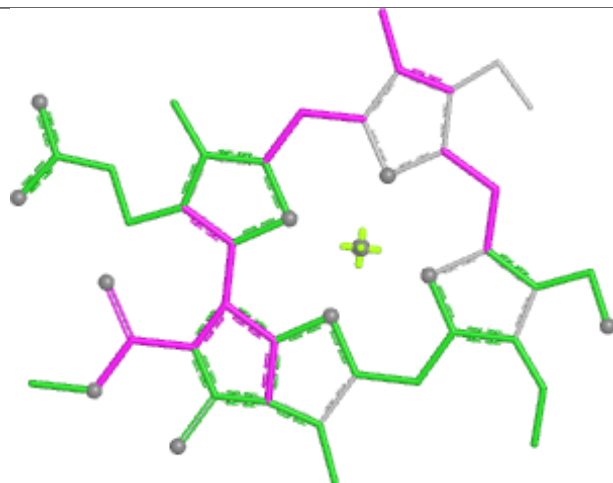




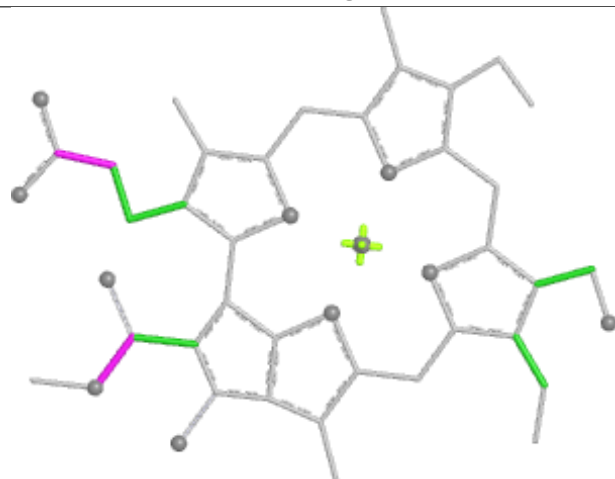
Ligand CHL 4 306



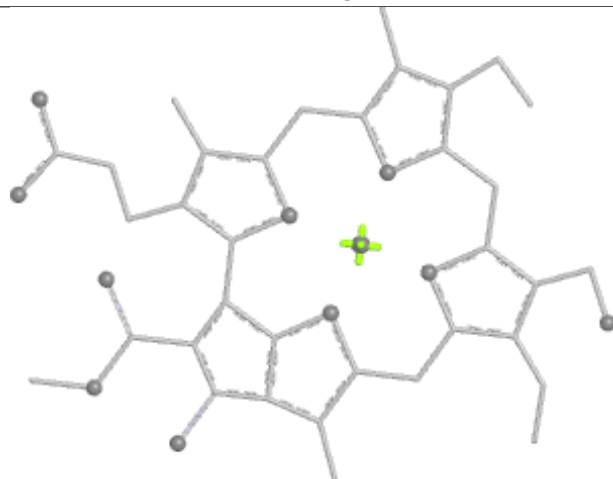
Bond lengths



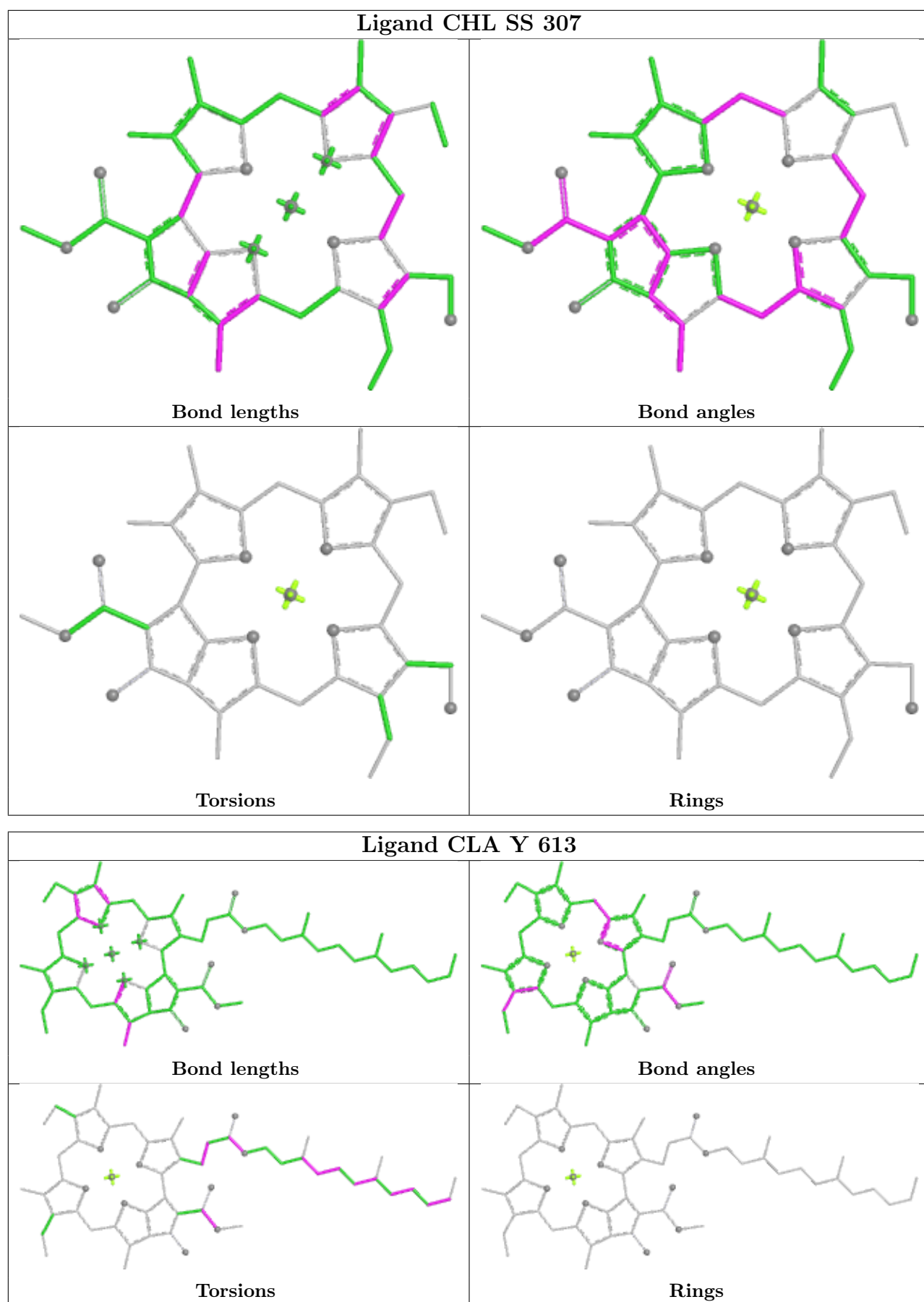
Bond angles

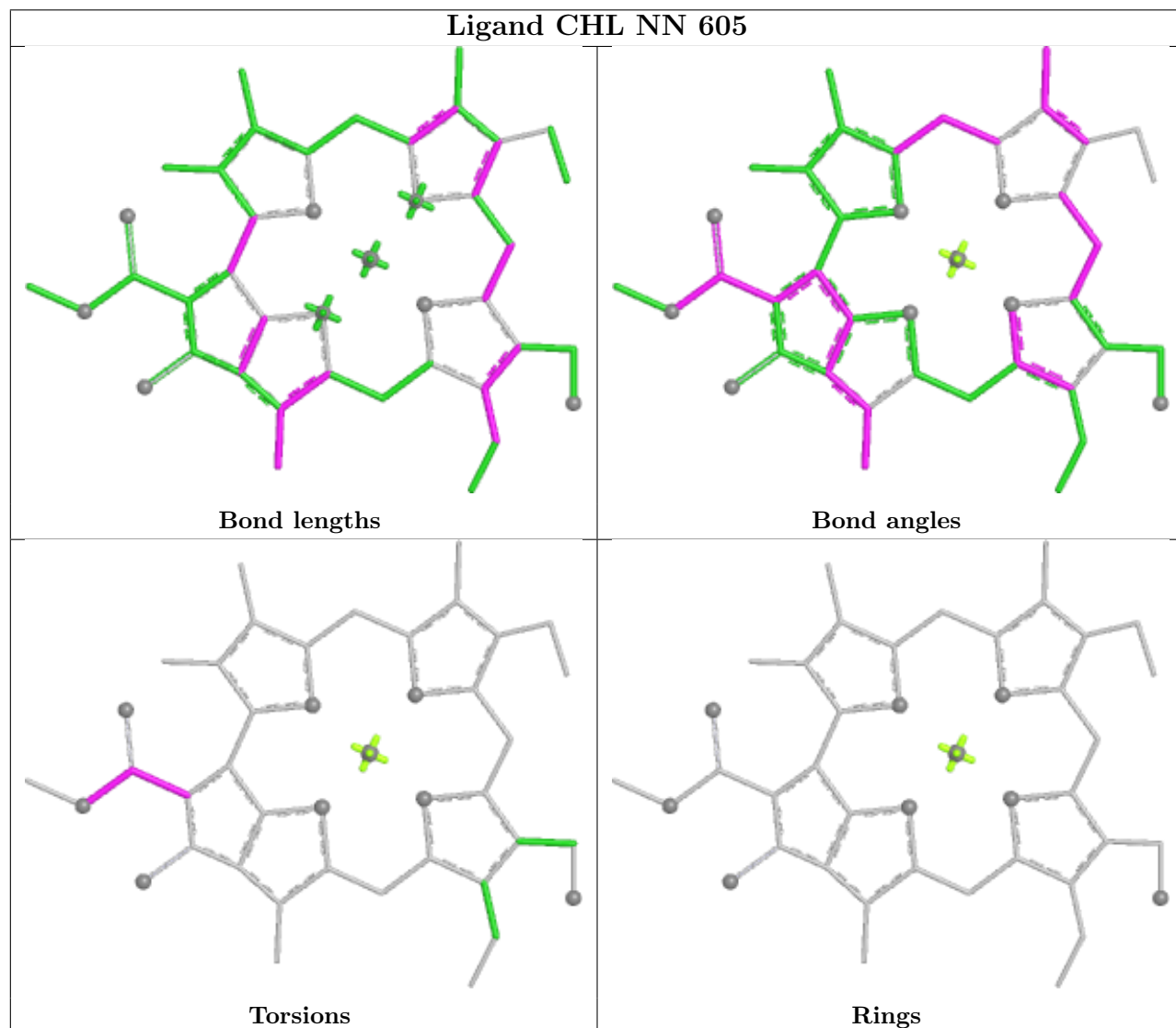
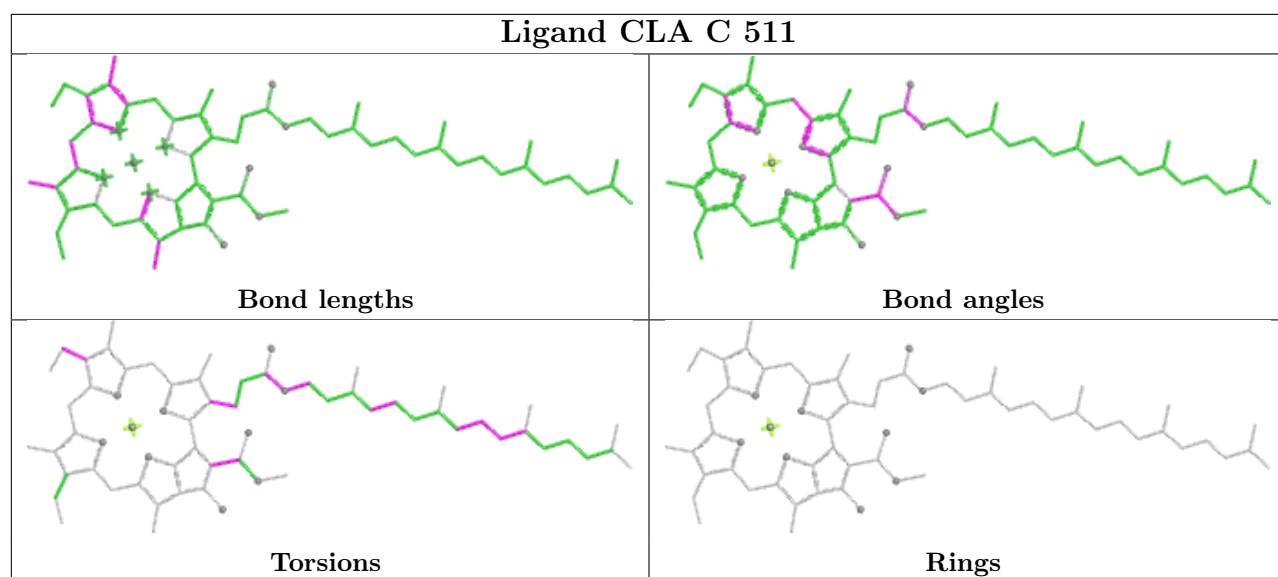


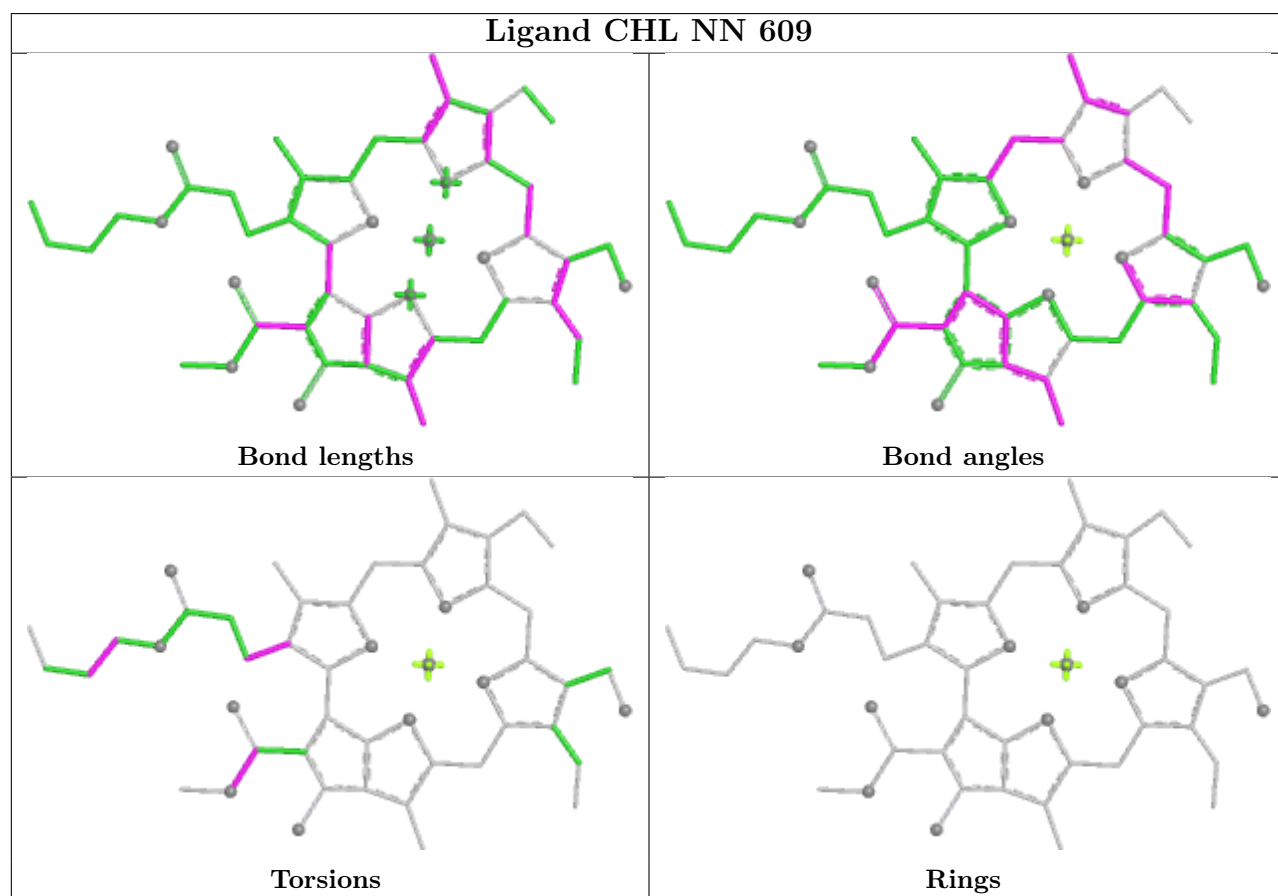
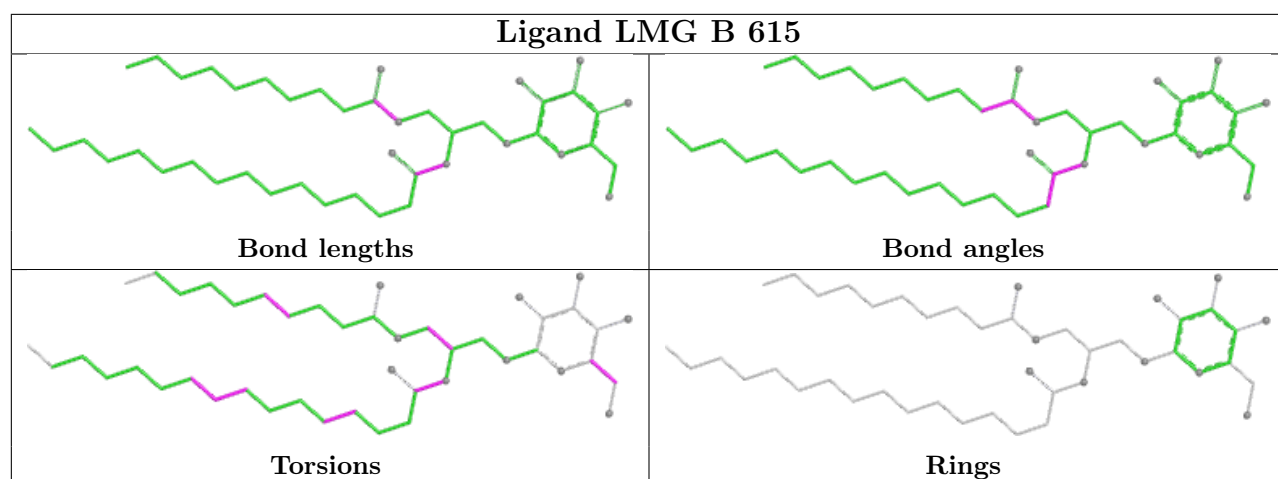
Torsions

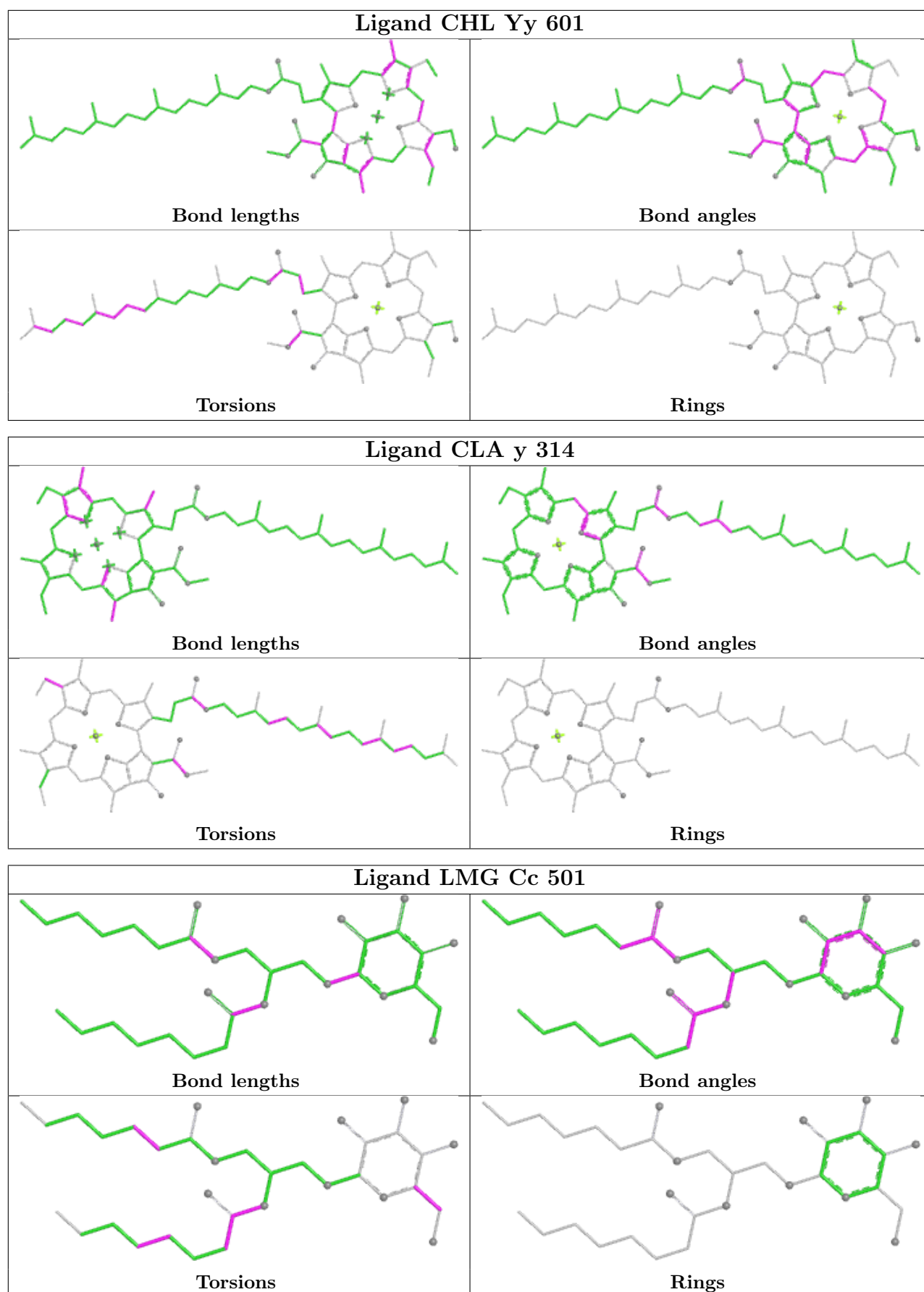


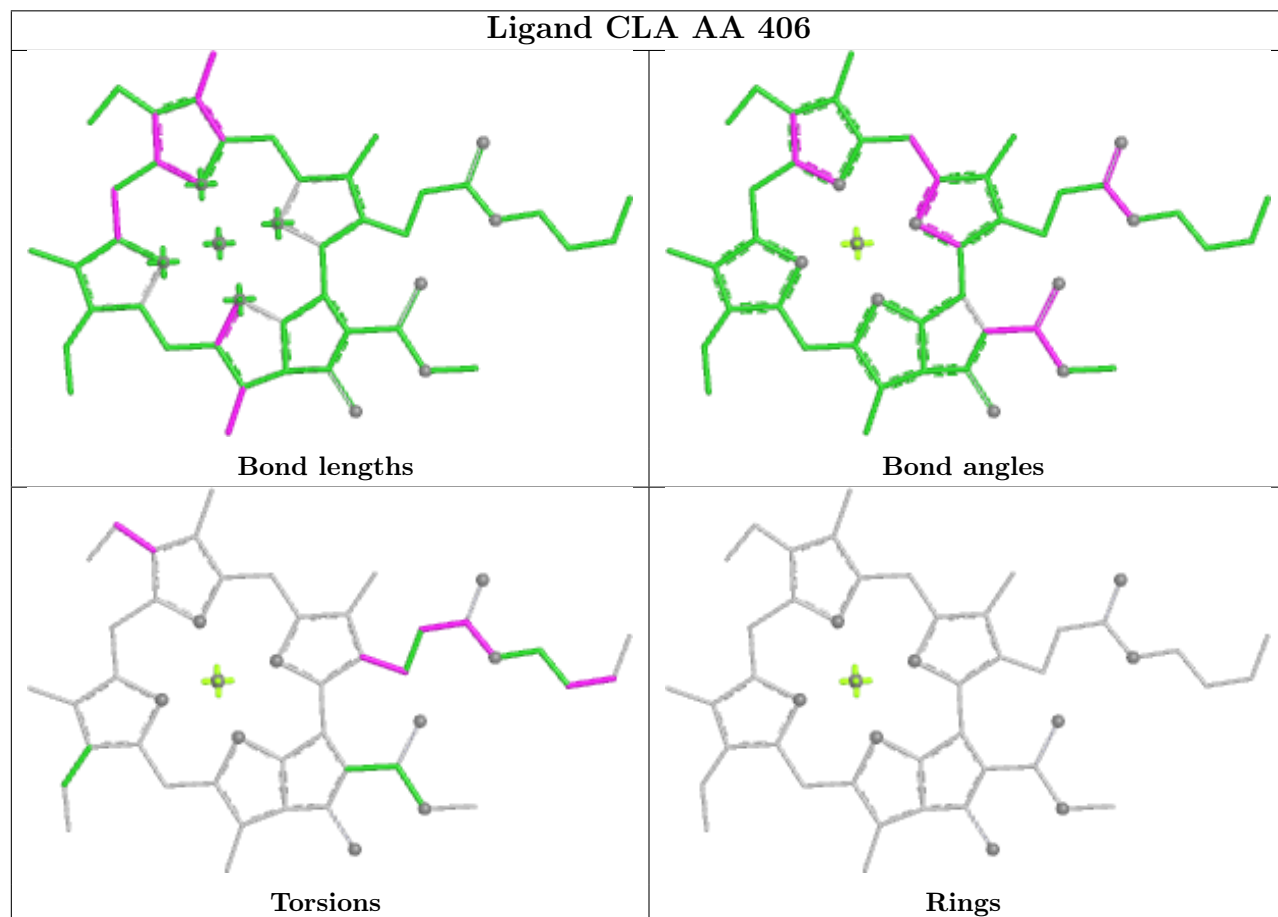
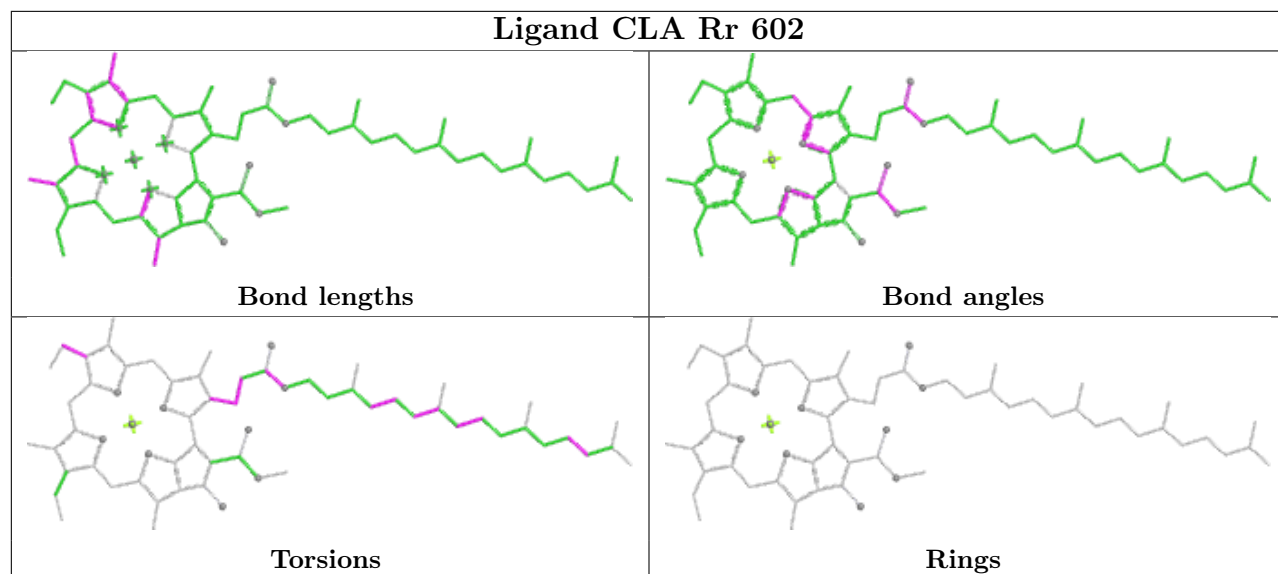
Rings

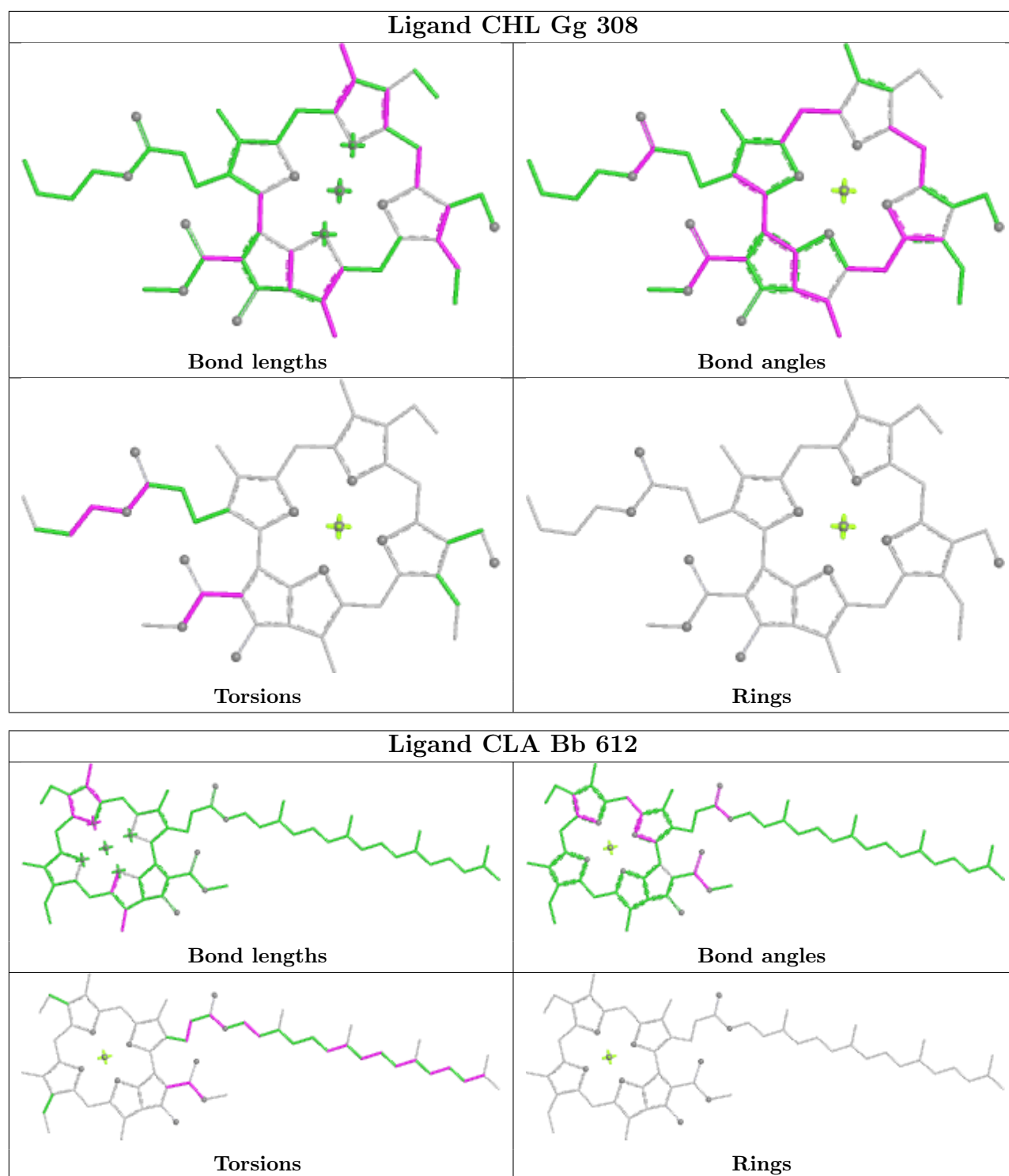


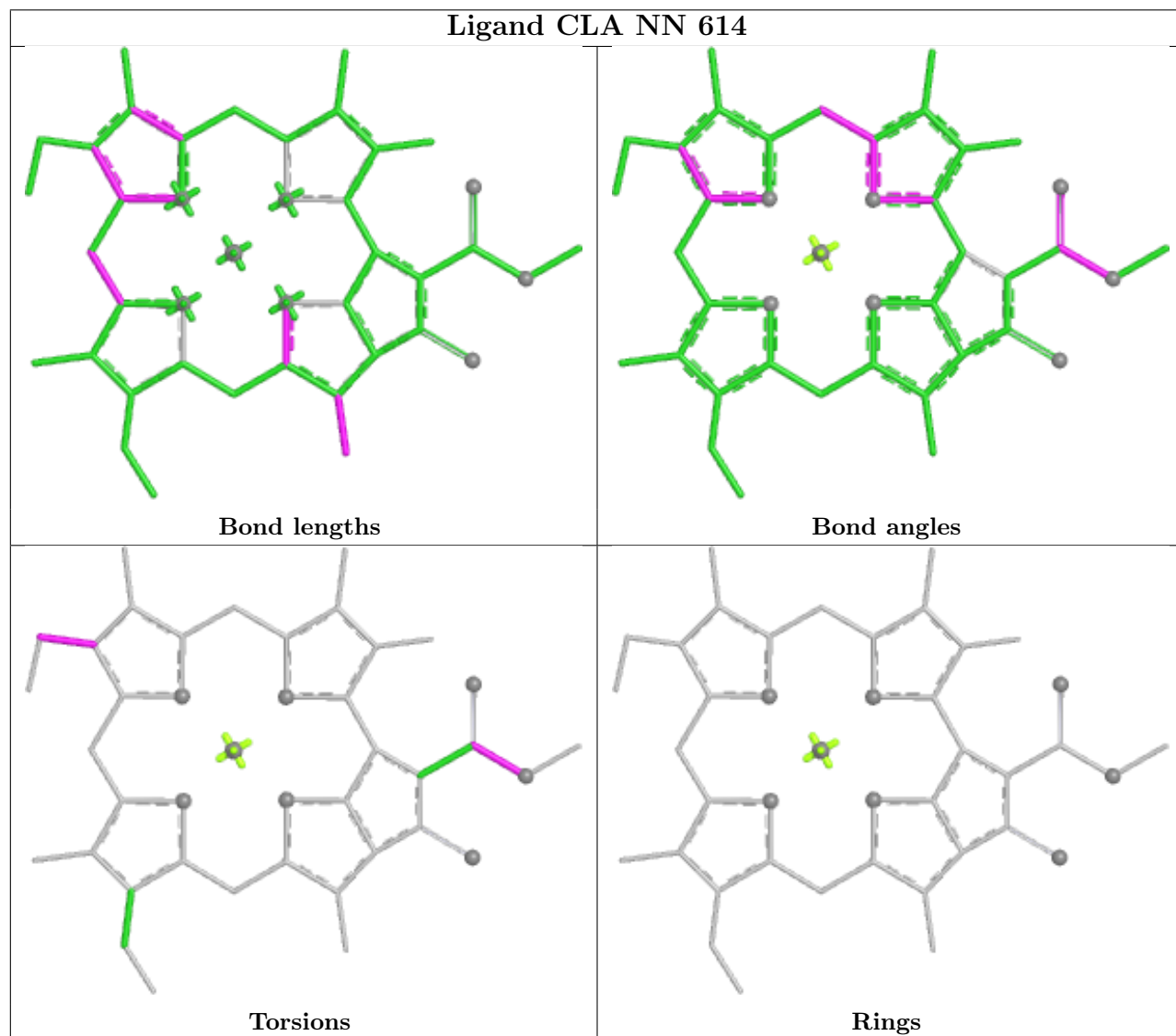
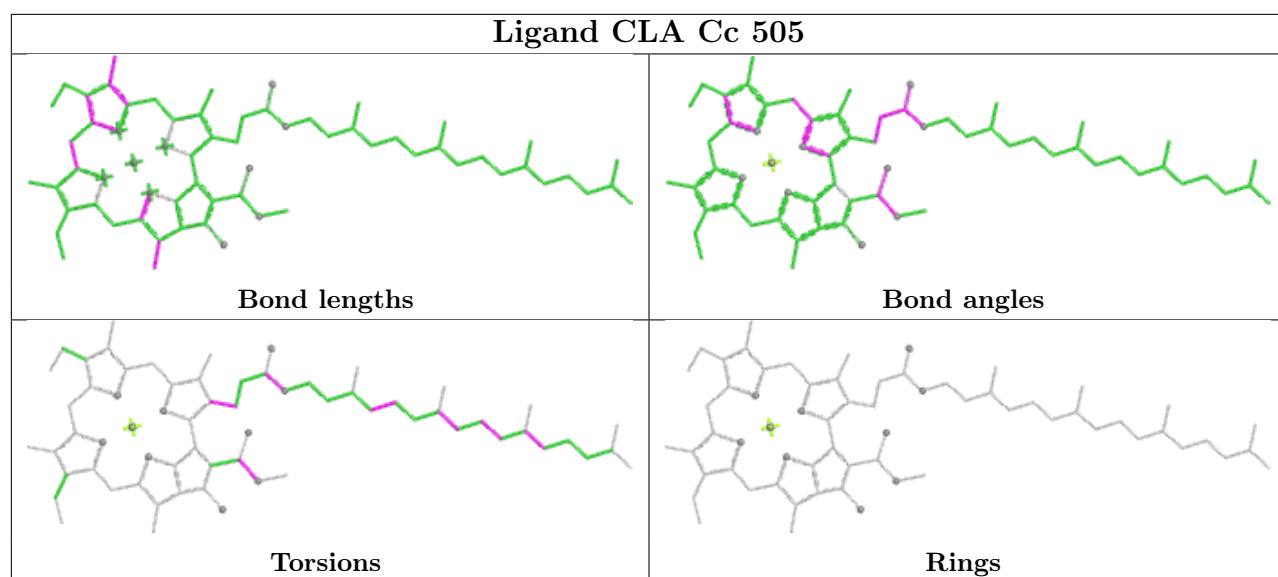




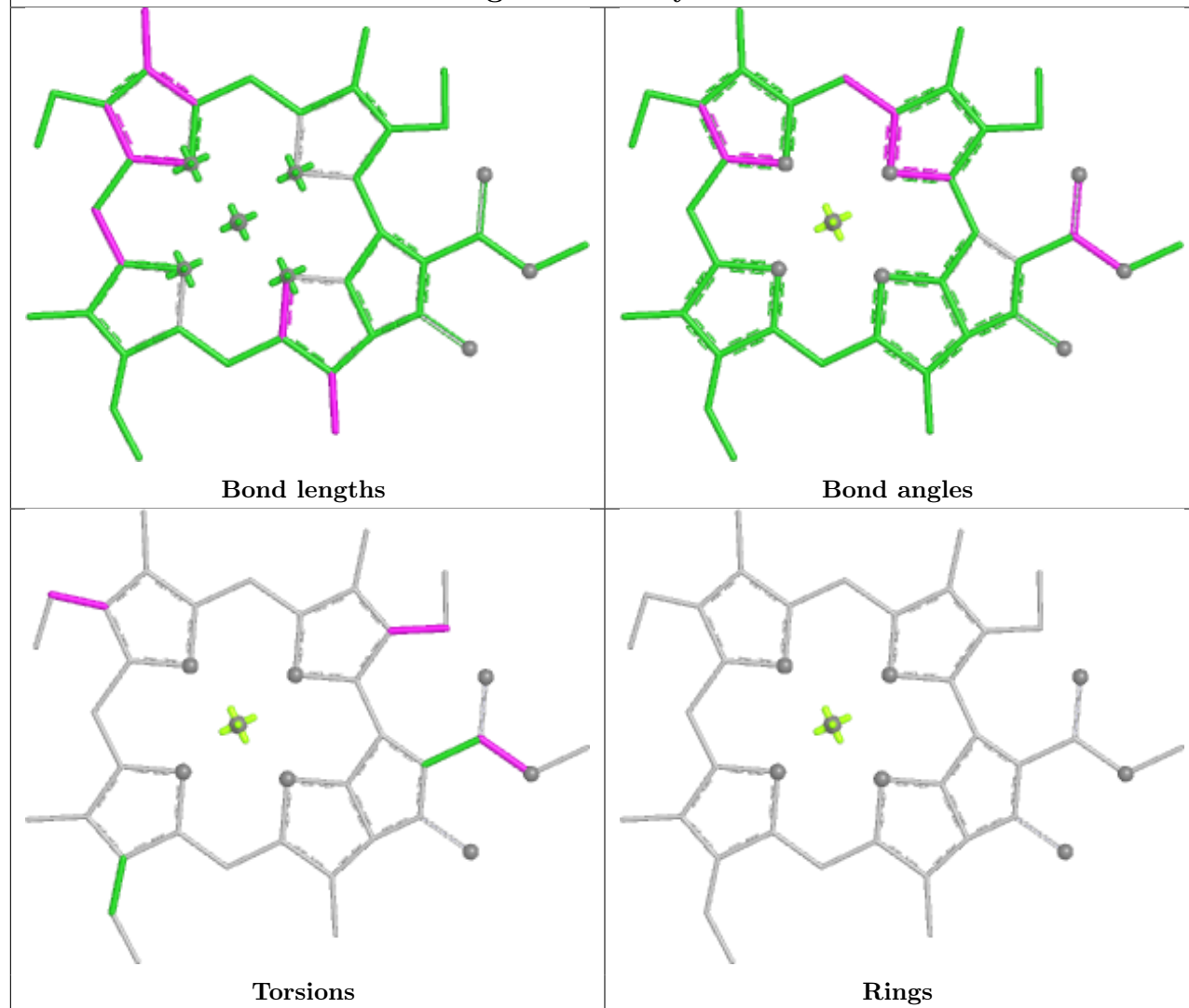




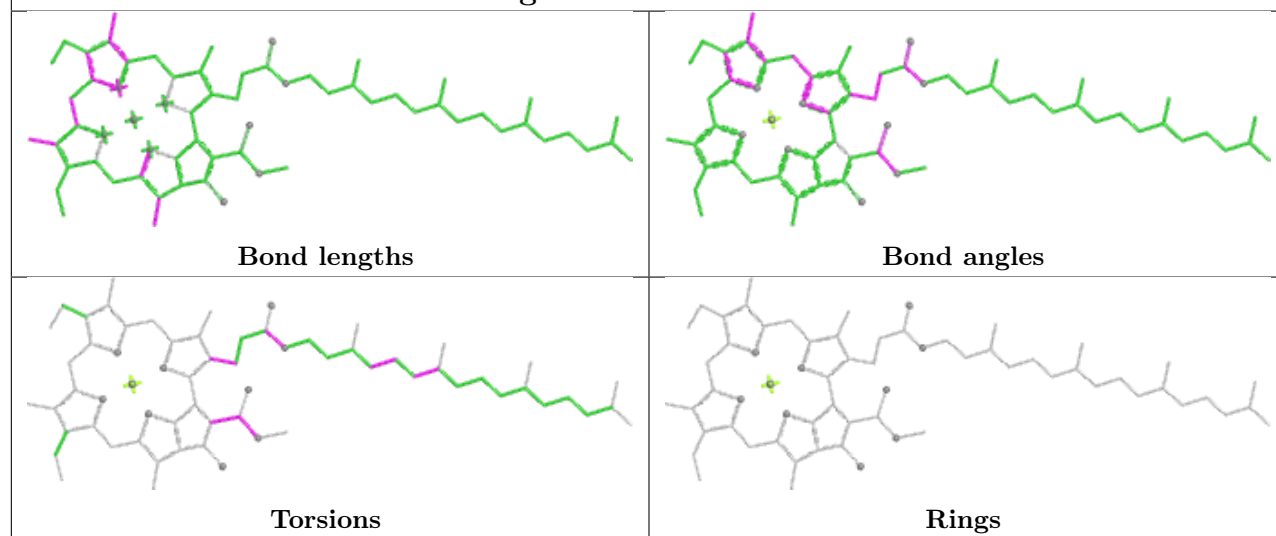


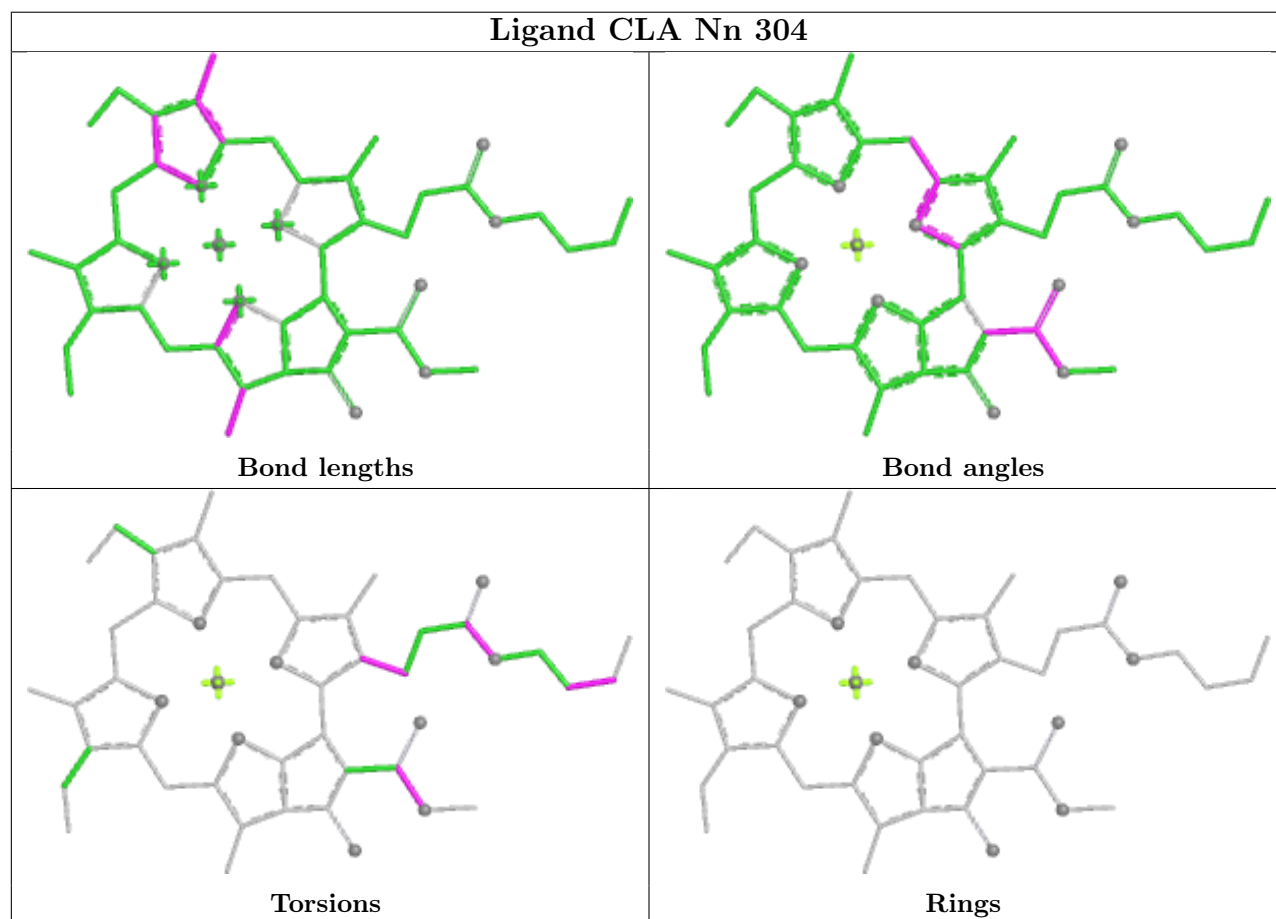
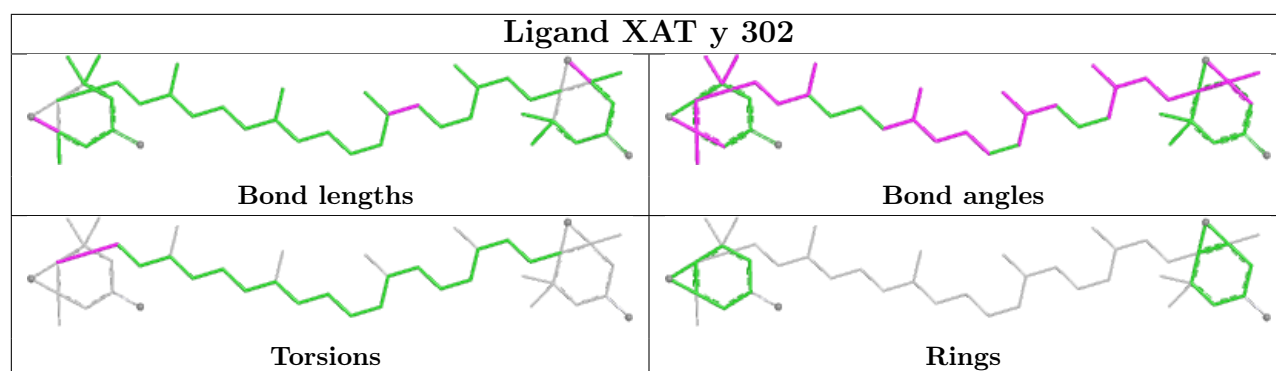


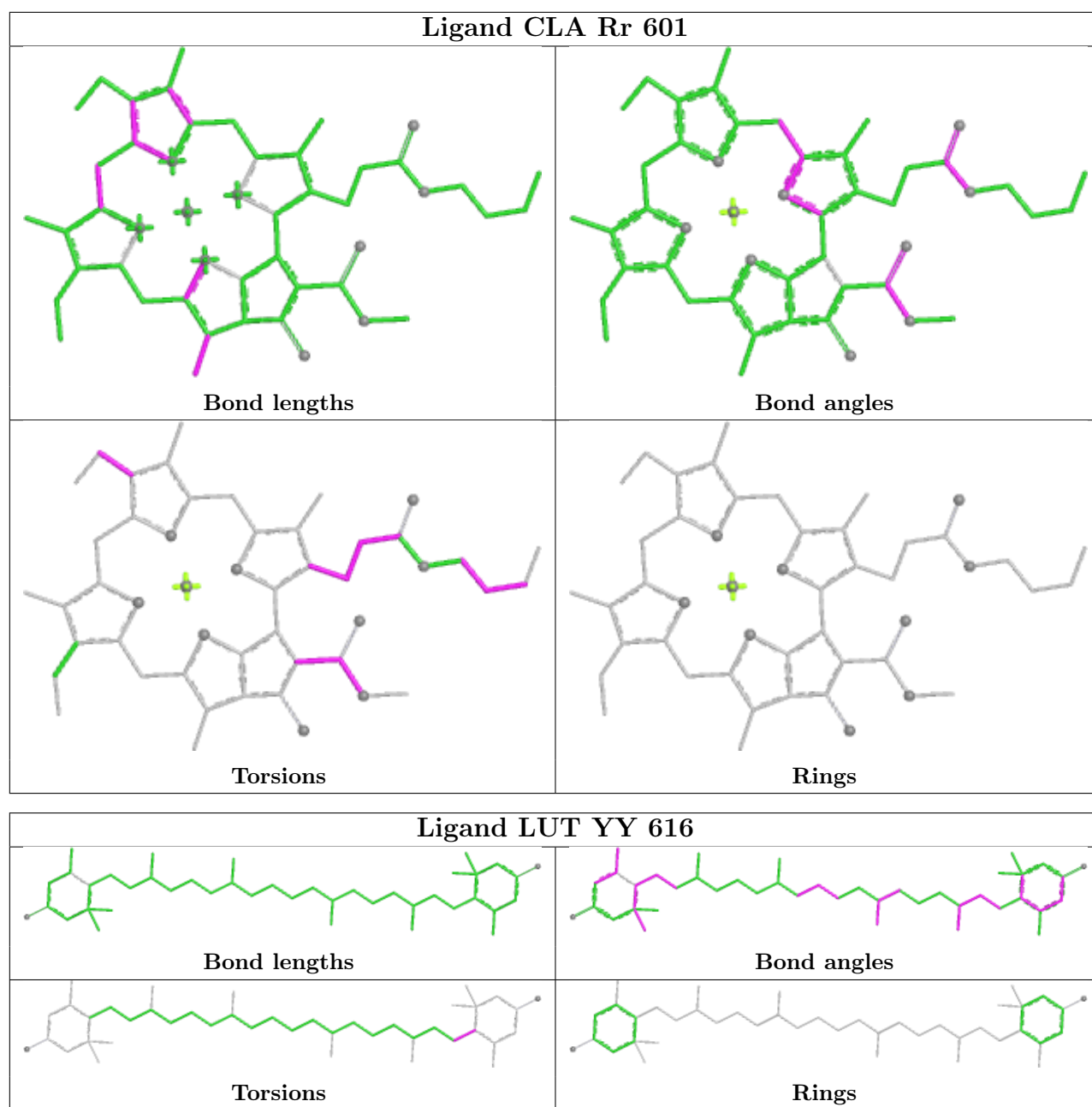
Ligand CLA Yy 611



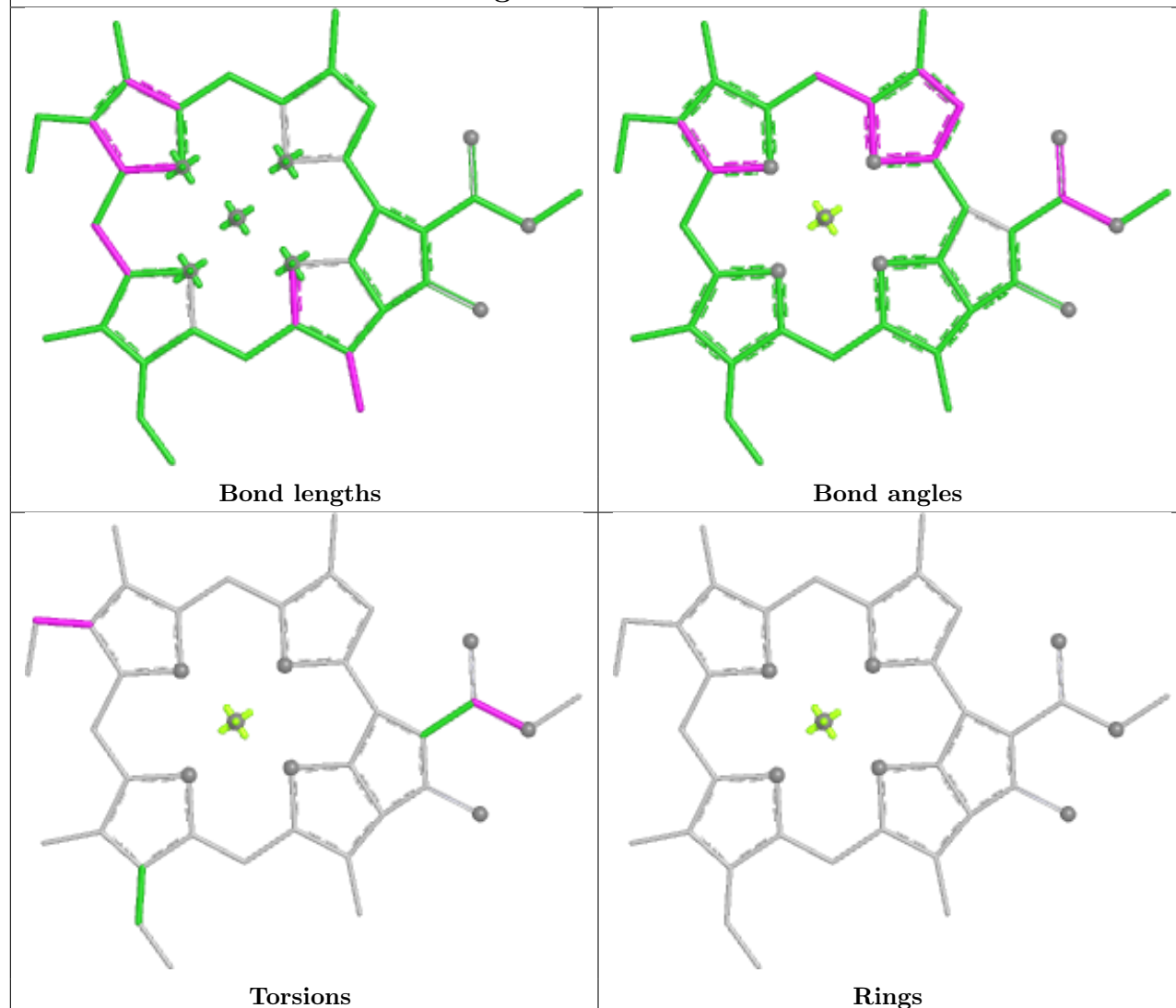
Ligand CLA CC 507



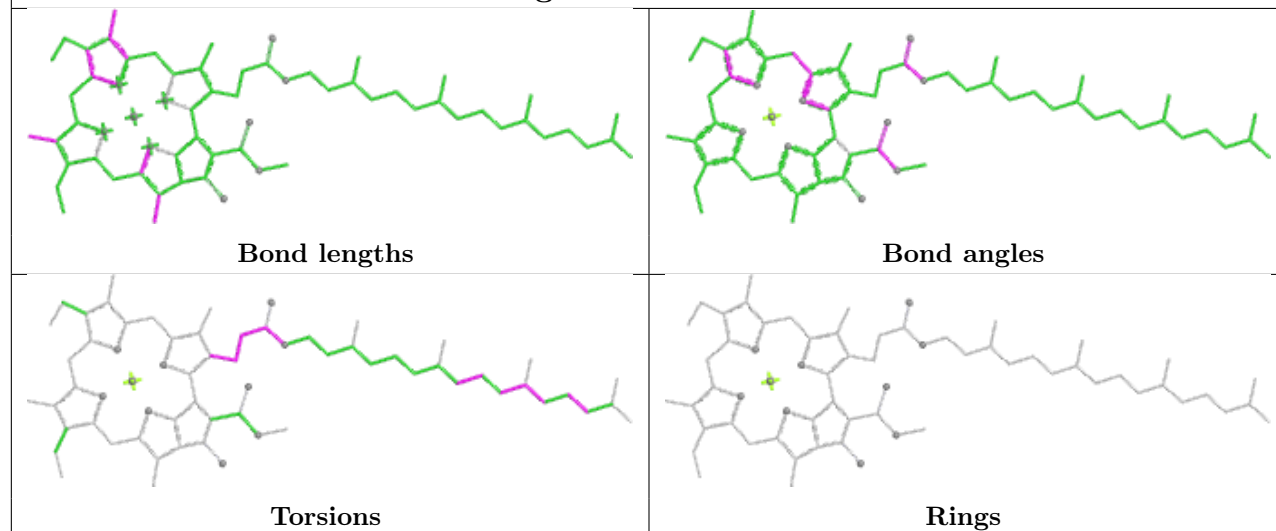


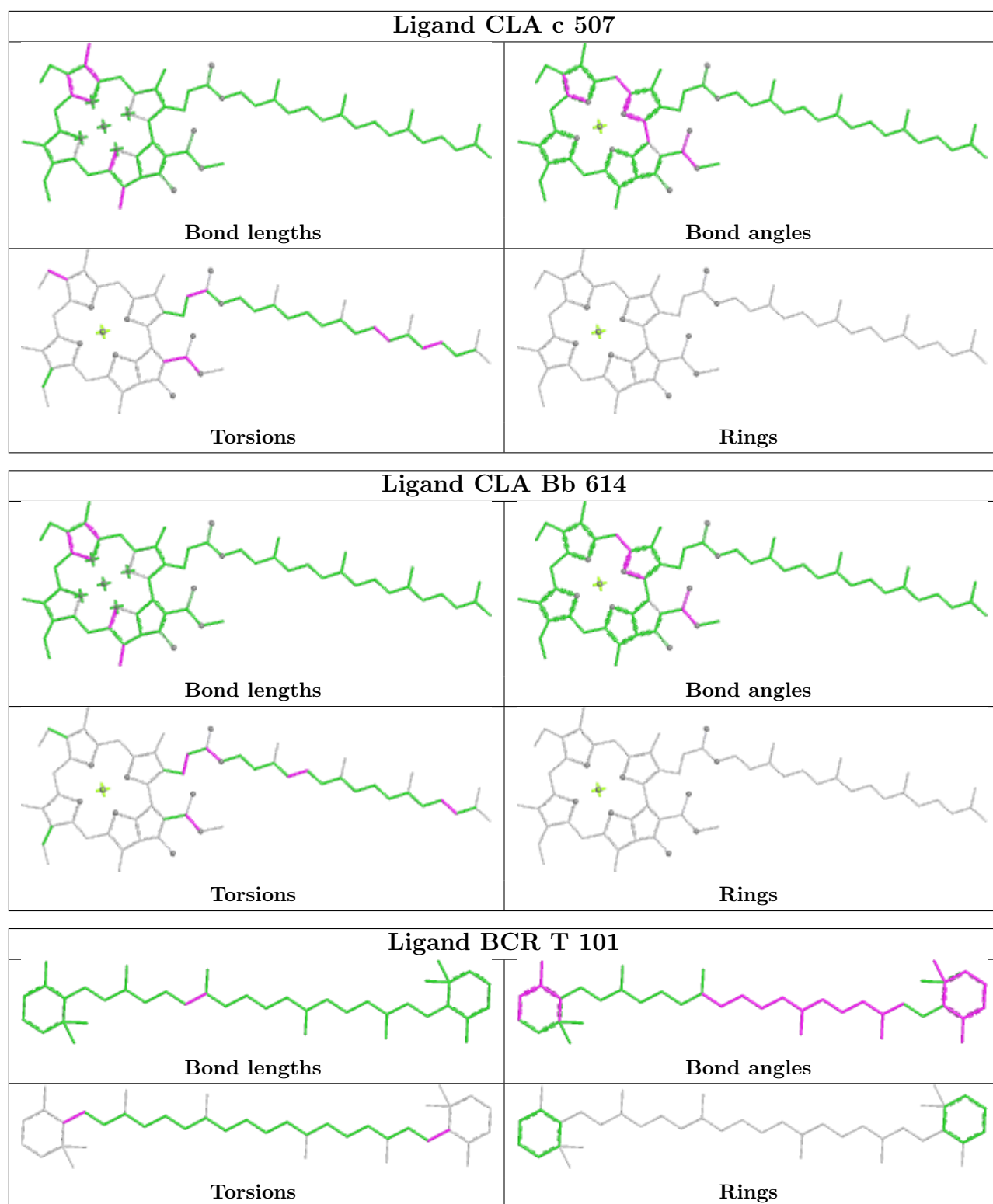


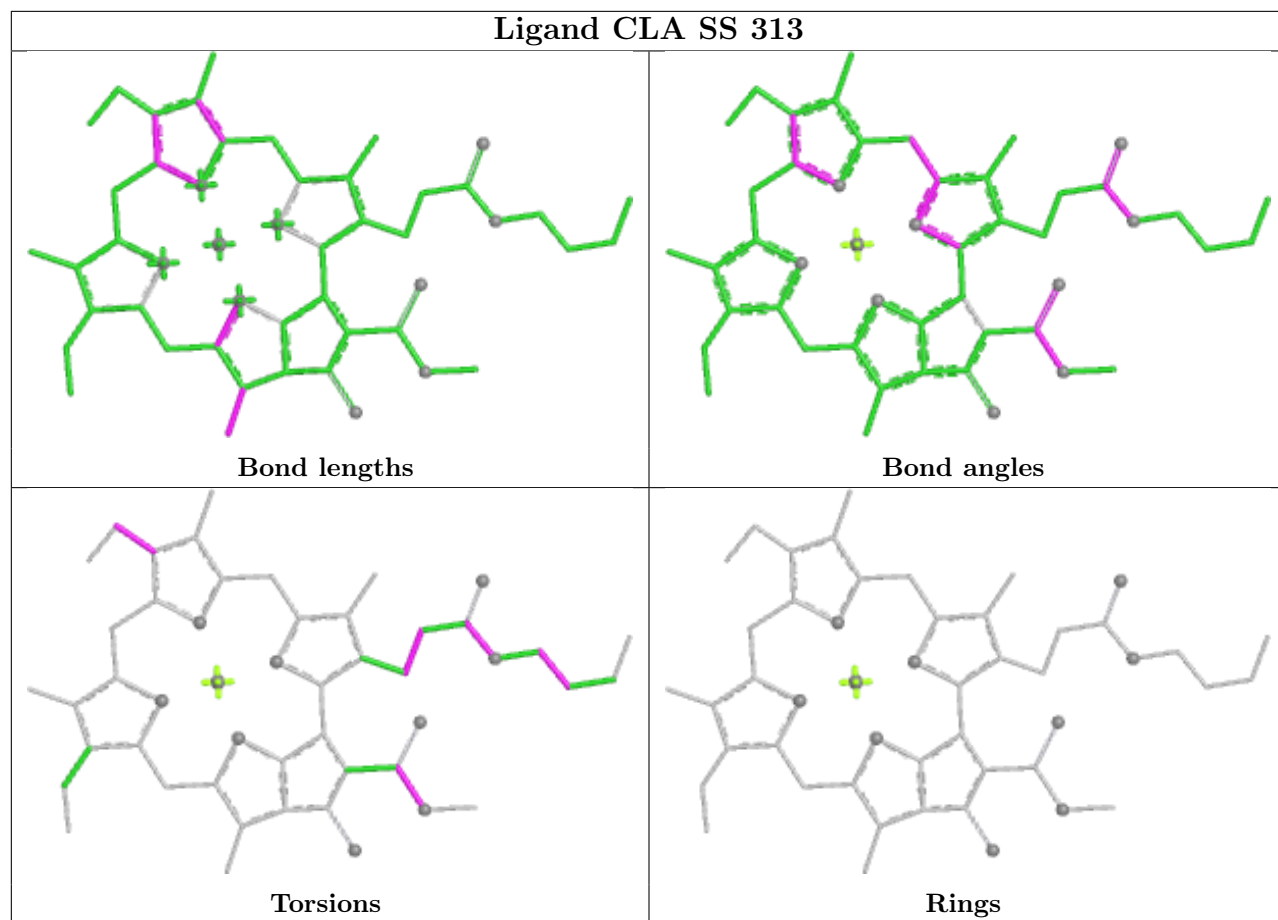
Ligand CLA 2 610



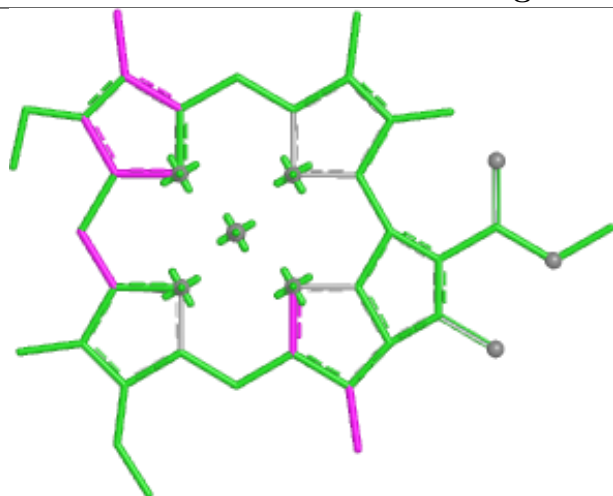
Ligand CLA b 616



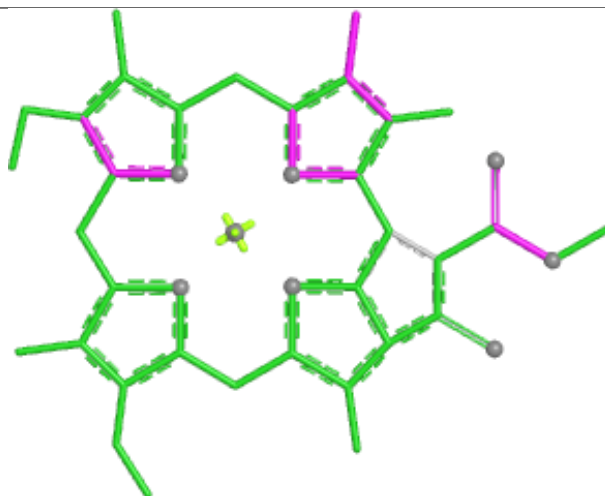




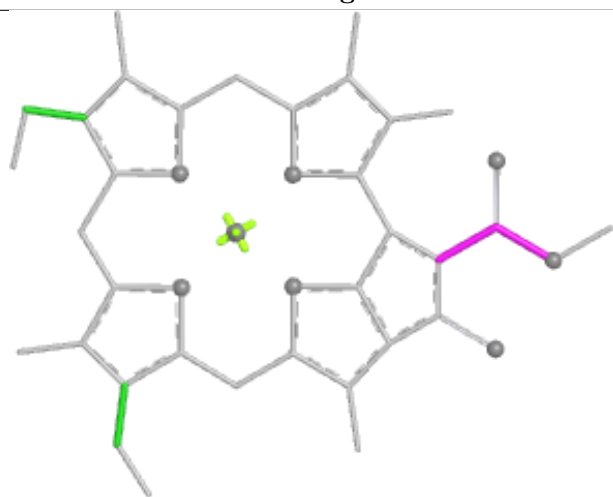
Ligand CLA X 201



Bond lengths



Bond angles

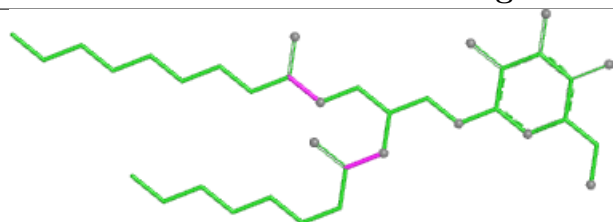


Torsions

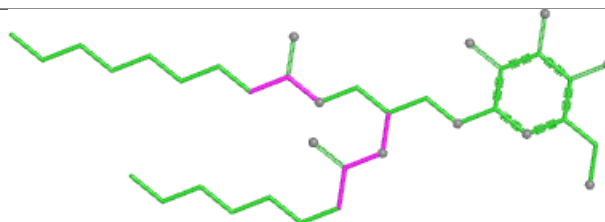


Rings

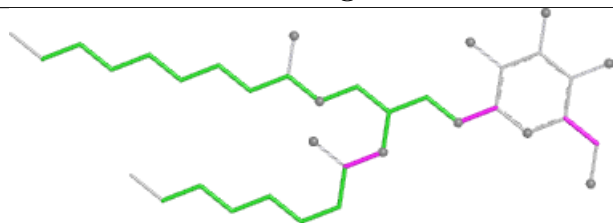
Ligand LMG AA 415



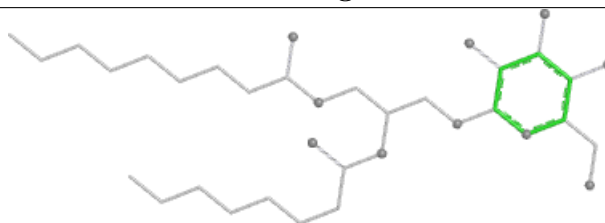
Bond lengths



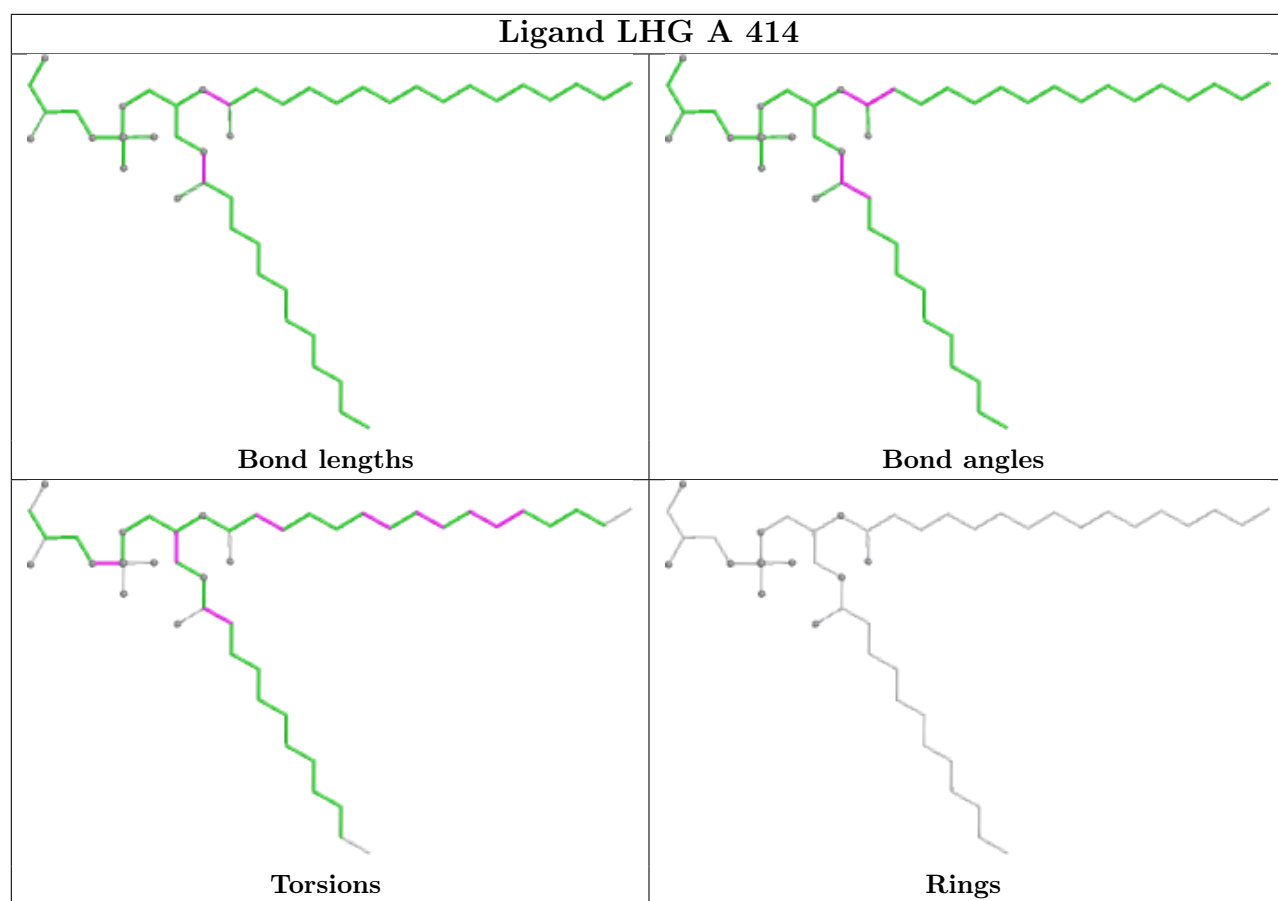
Bond angles

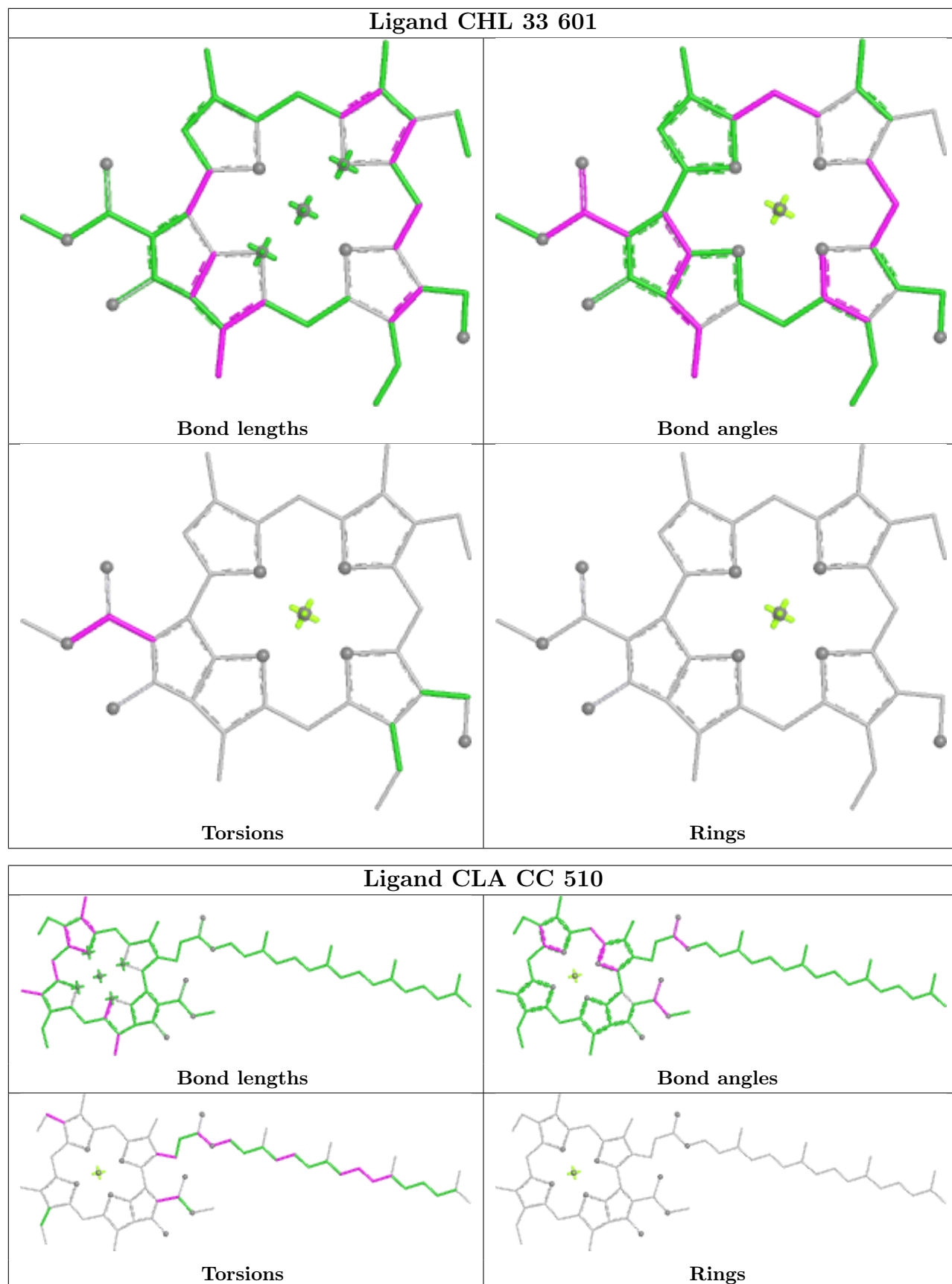


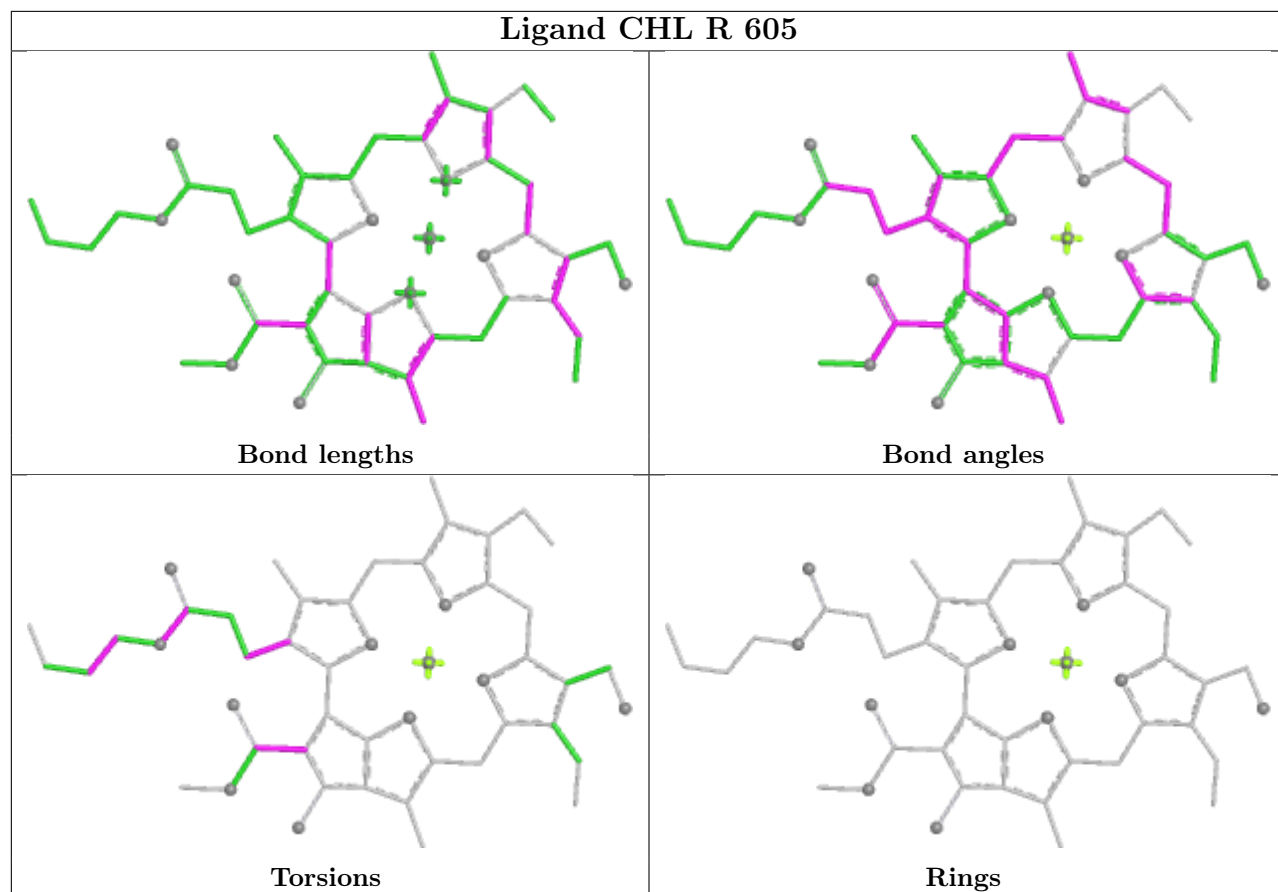
Torsions



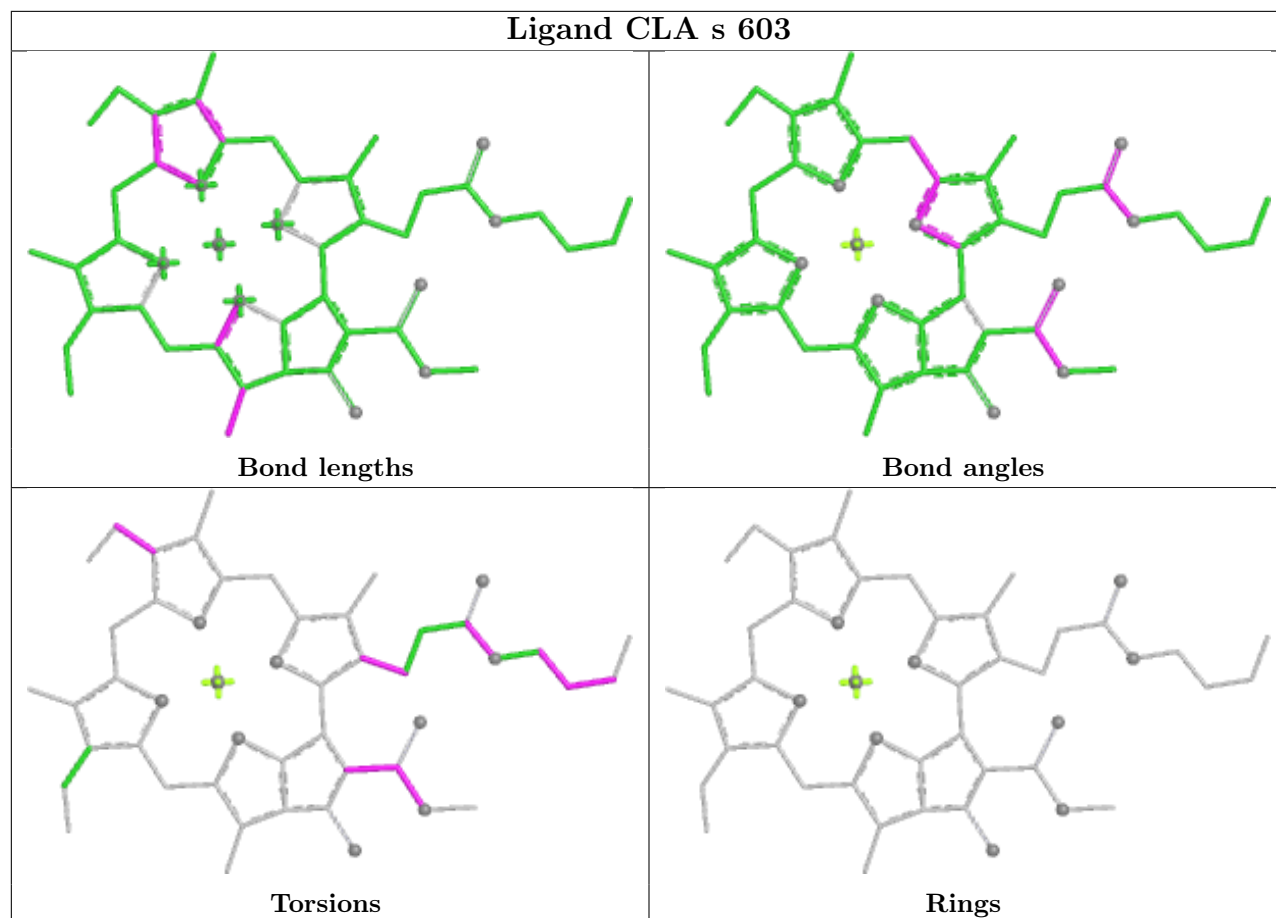
Rings



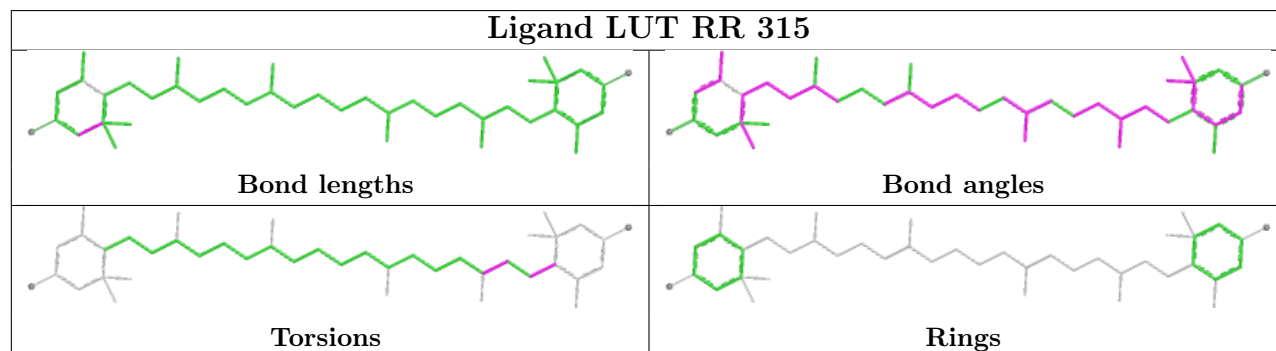


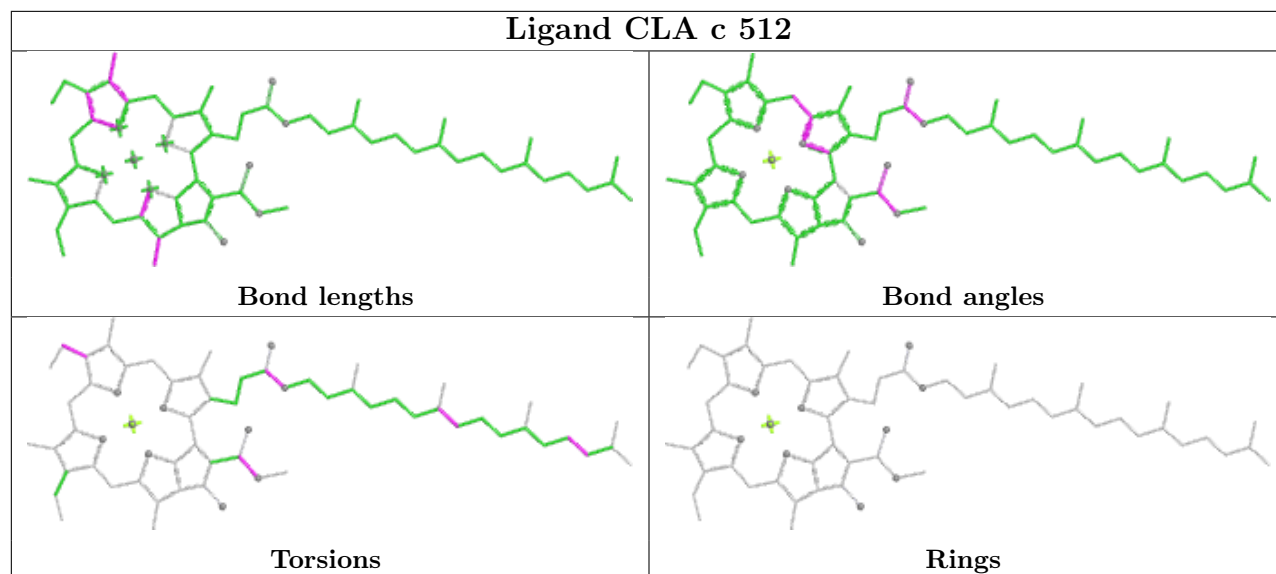
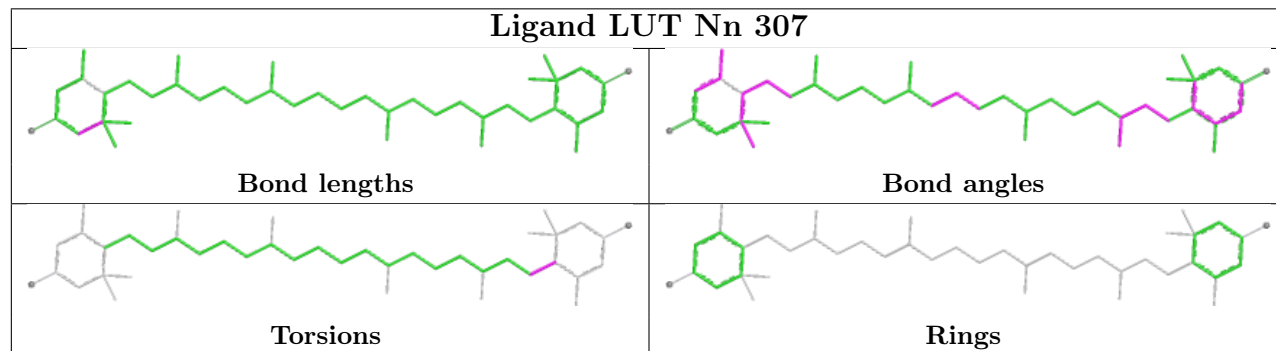
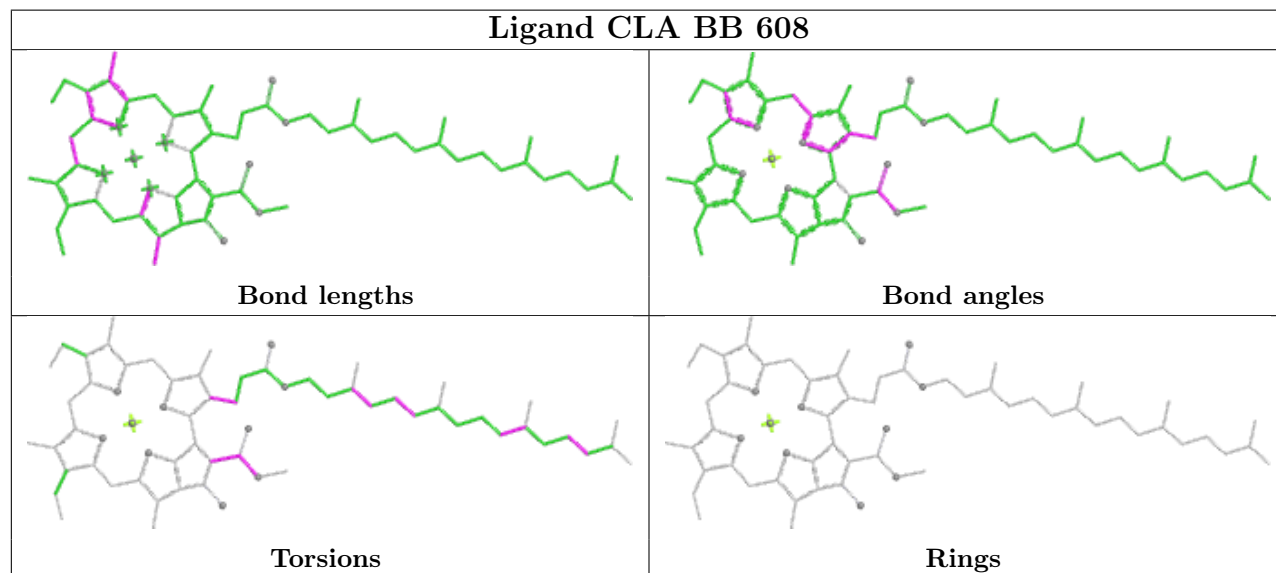


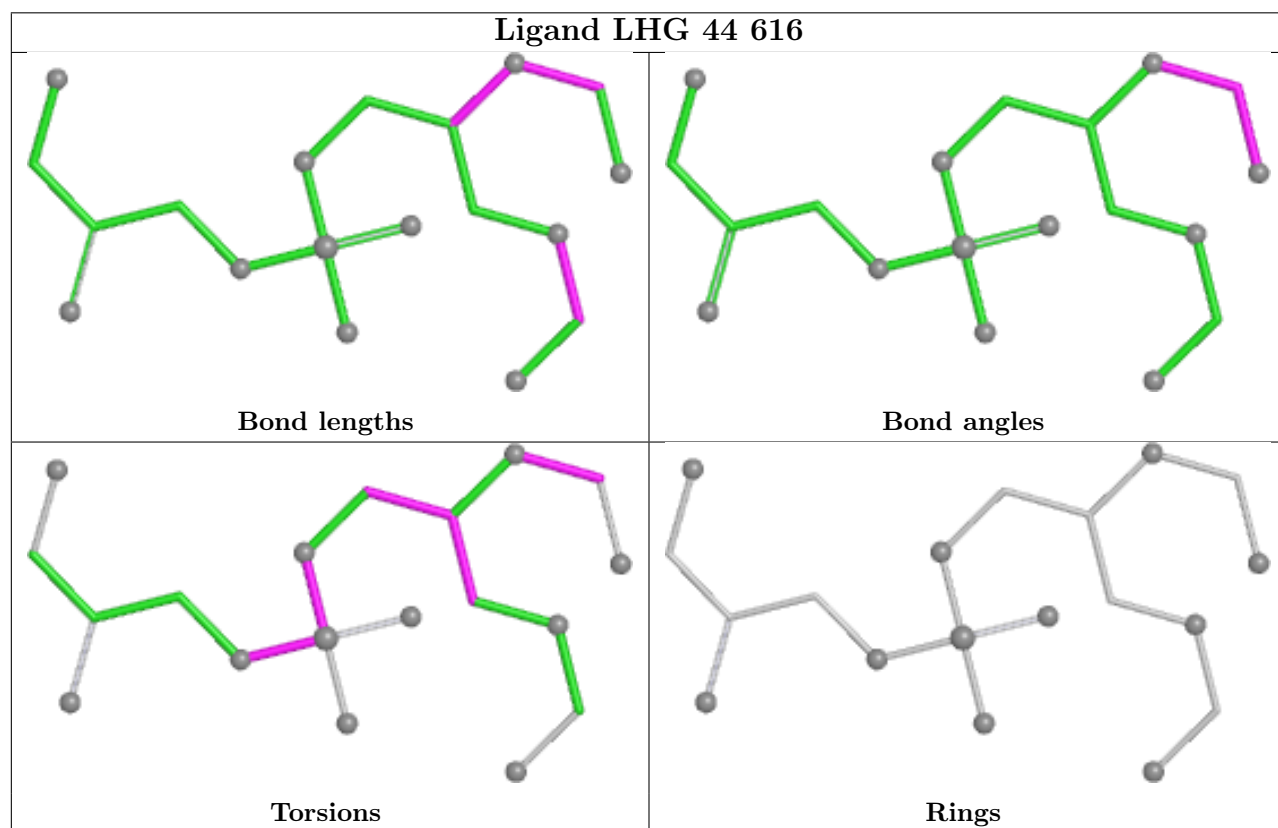
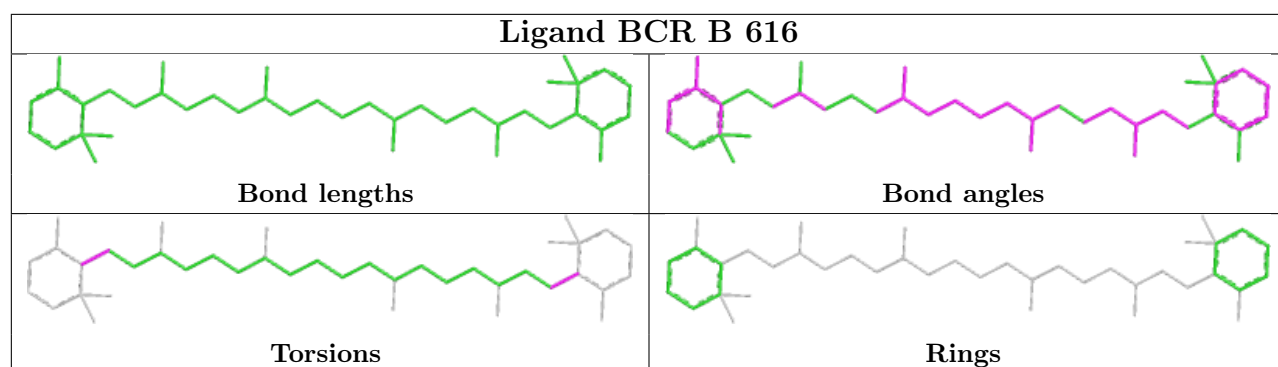
Ligand CLA s 603

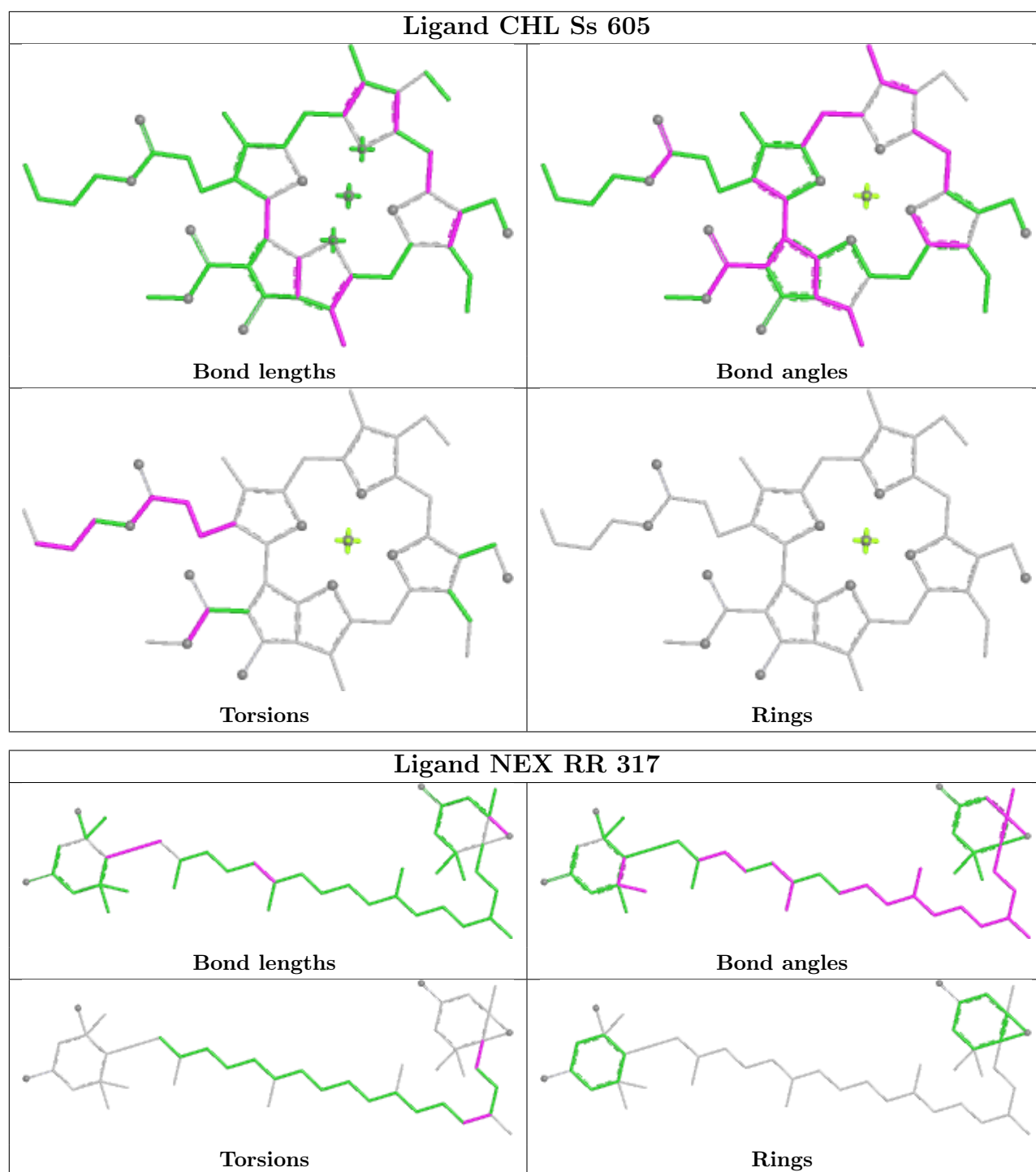


Ligand LUT RR 315

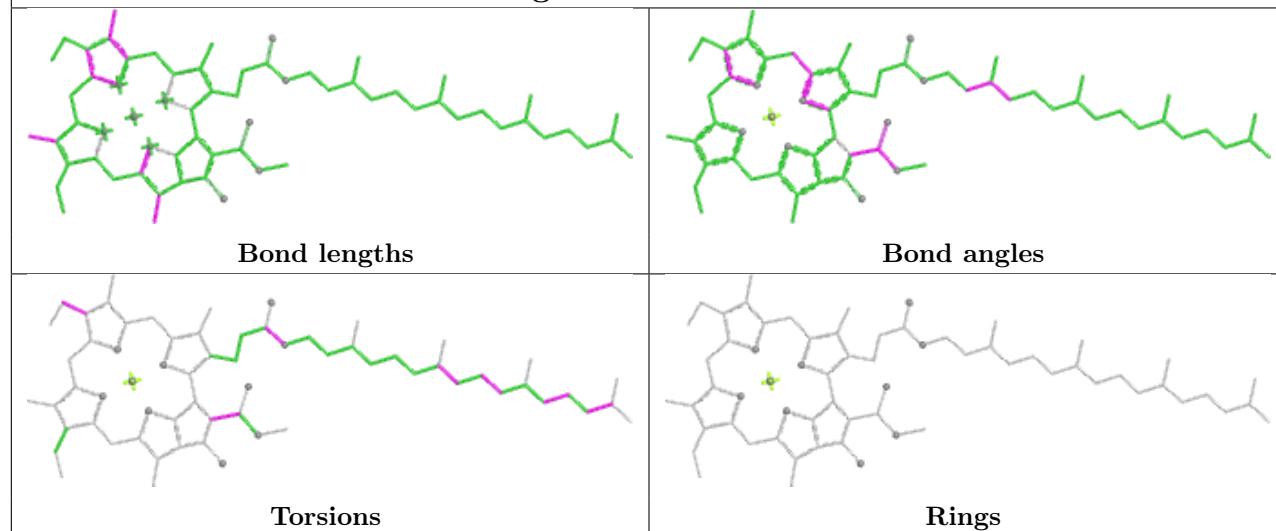


Ligand CLA c 512**Ligand LUT Nn 307****Ligand CLA BB 608**

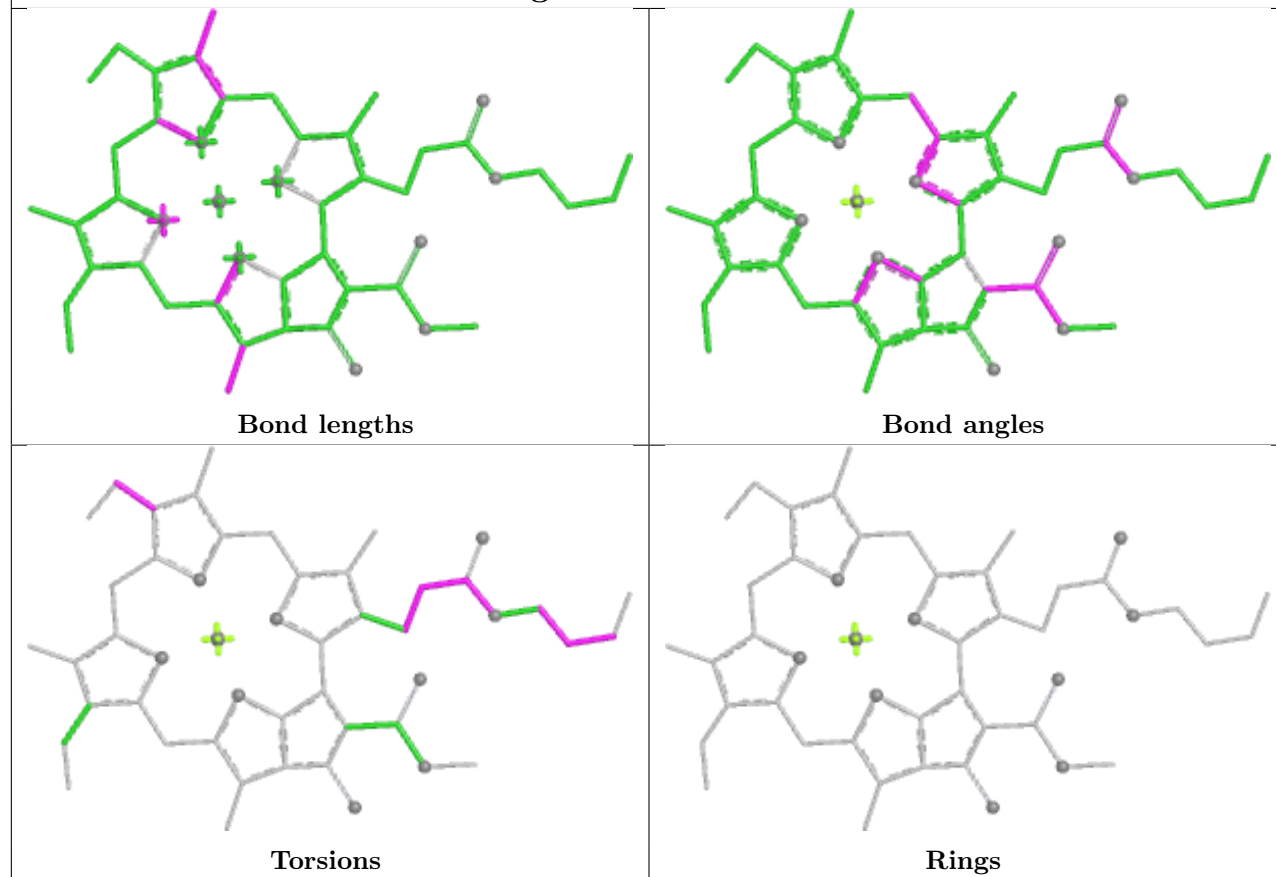


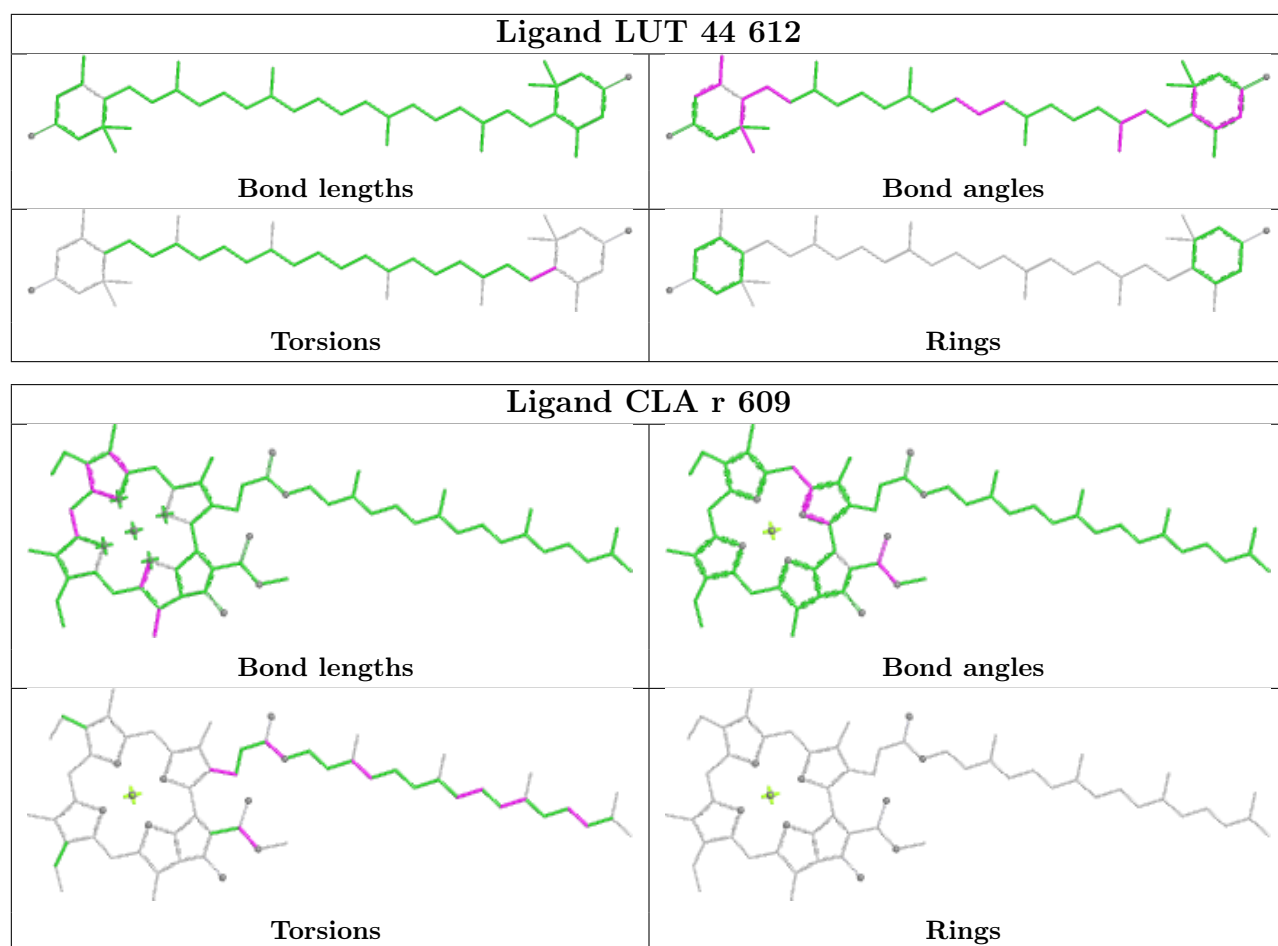


Ligand CLA C 509

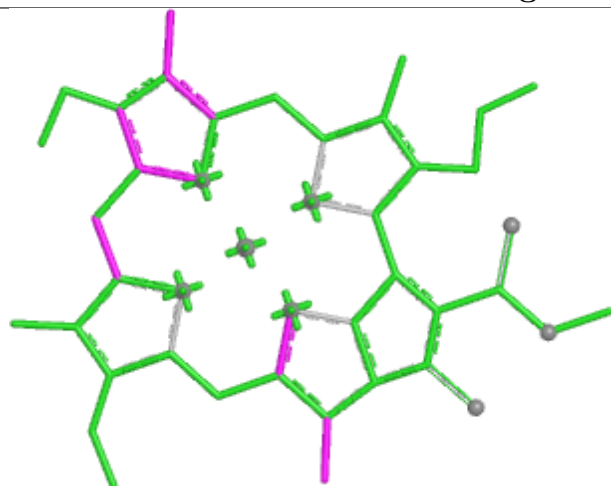


Ligand CLA G 610

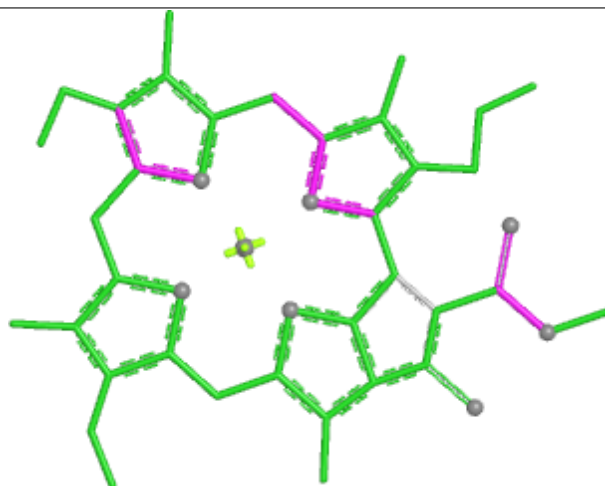




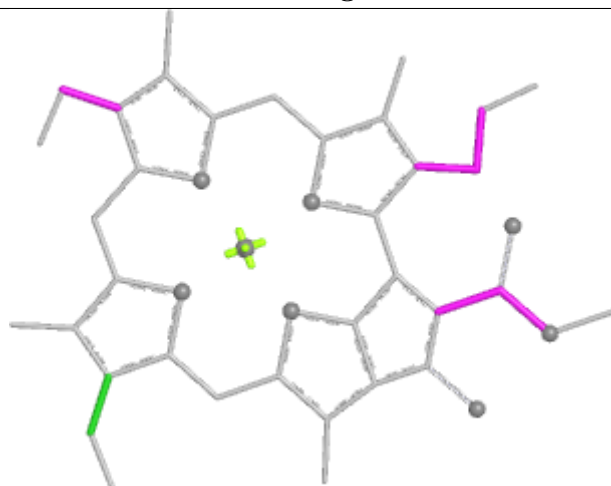
Ligand CLA c 513



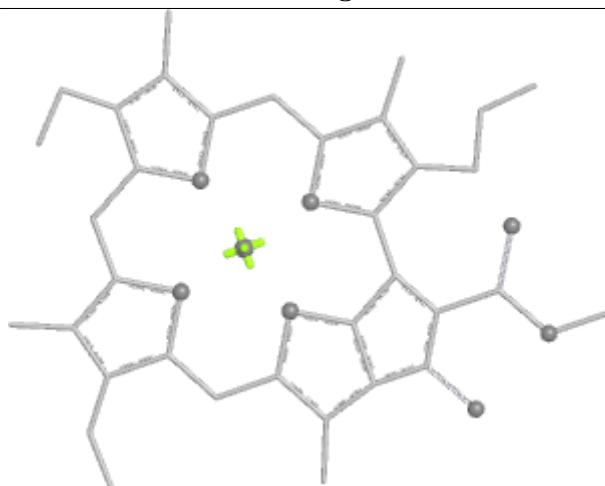
Bond lengths



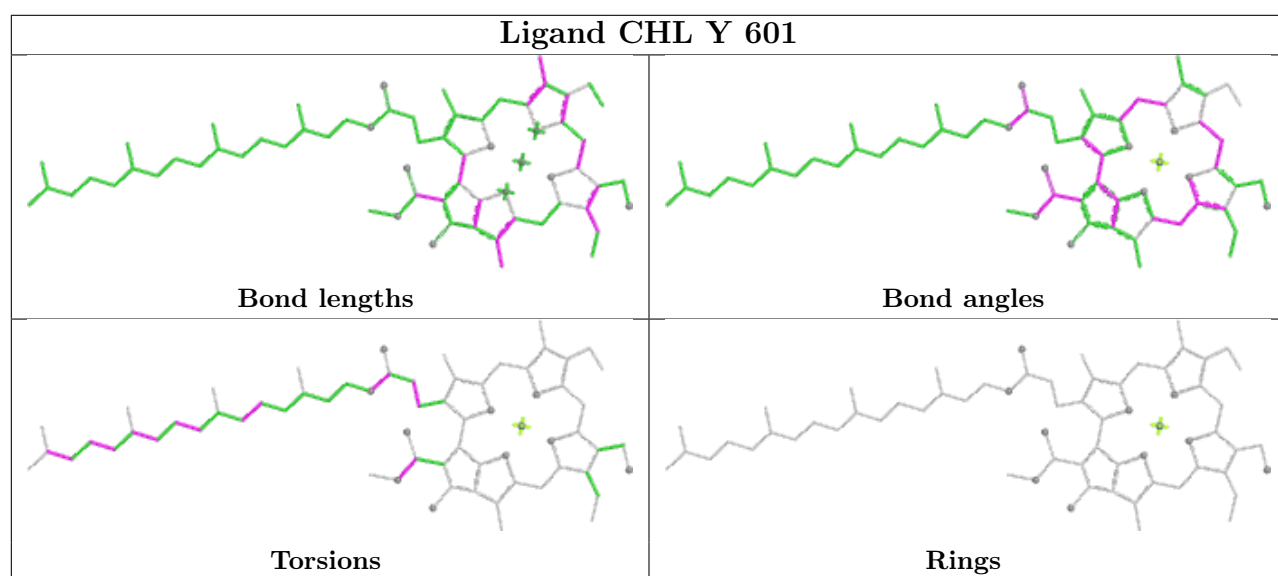
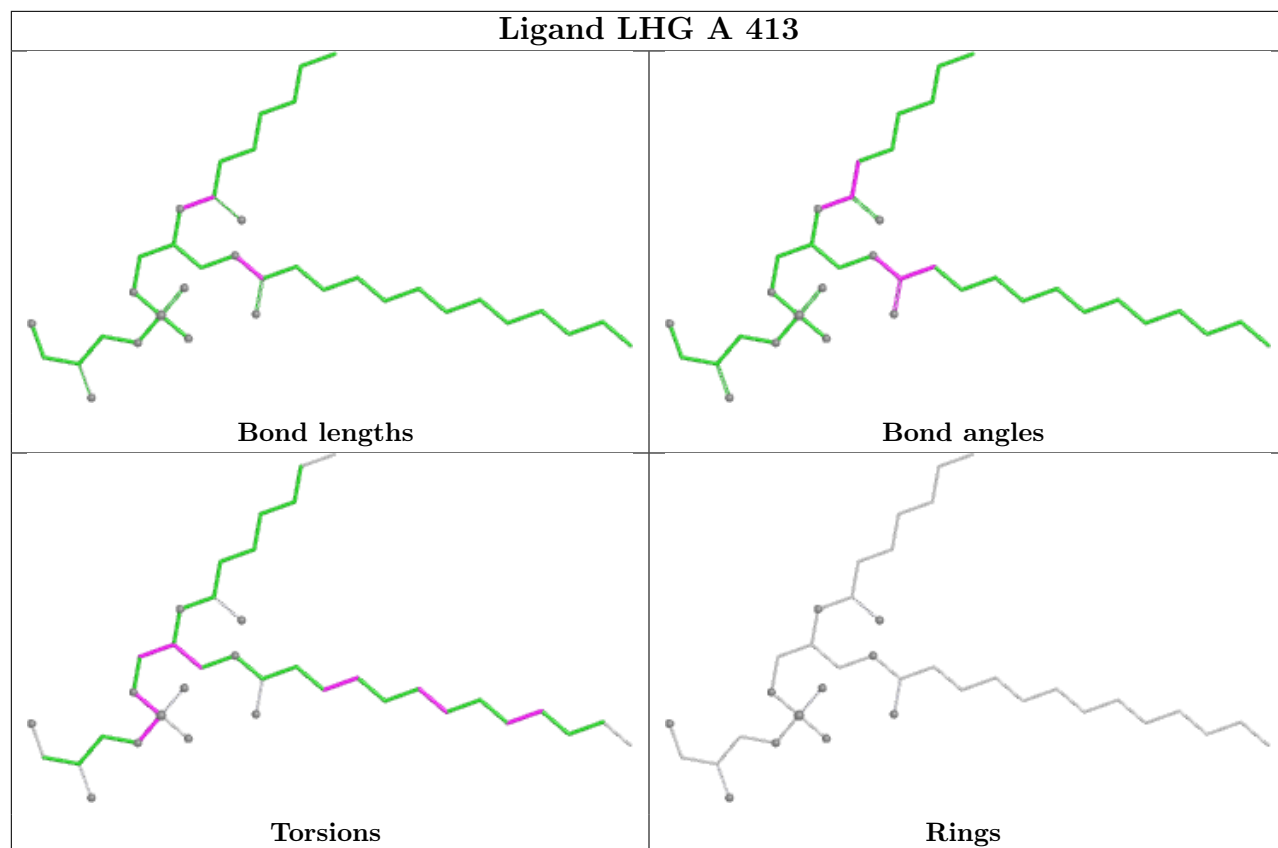
Bond angles



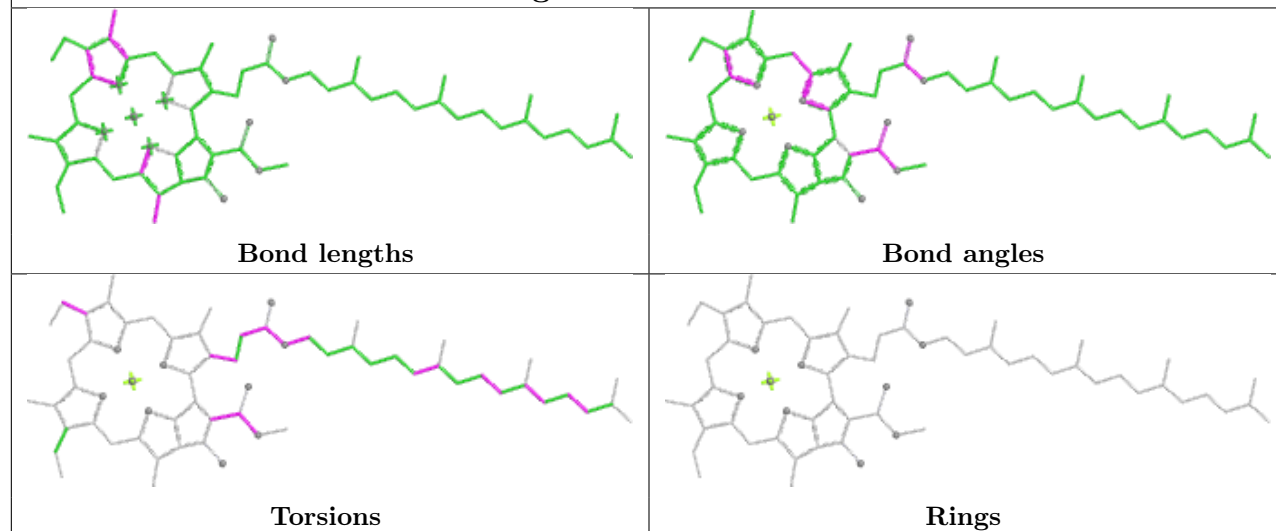
Torsions



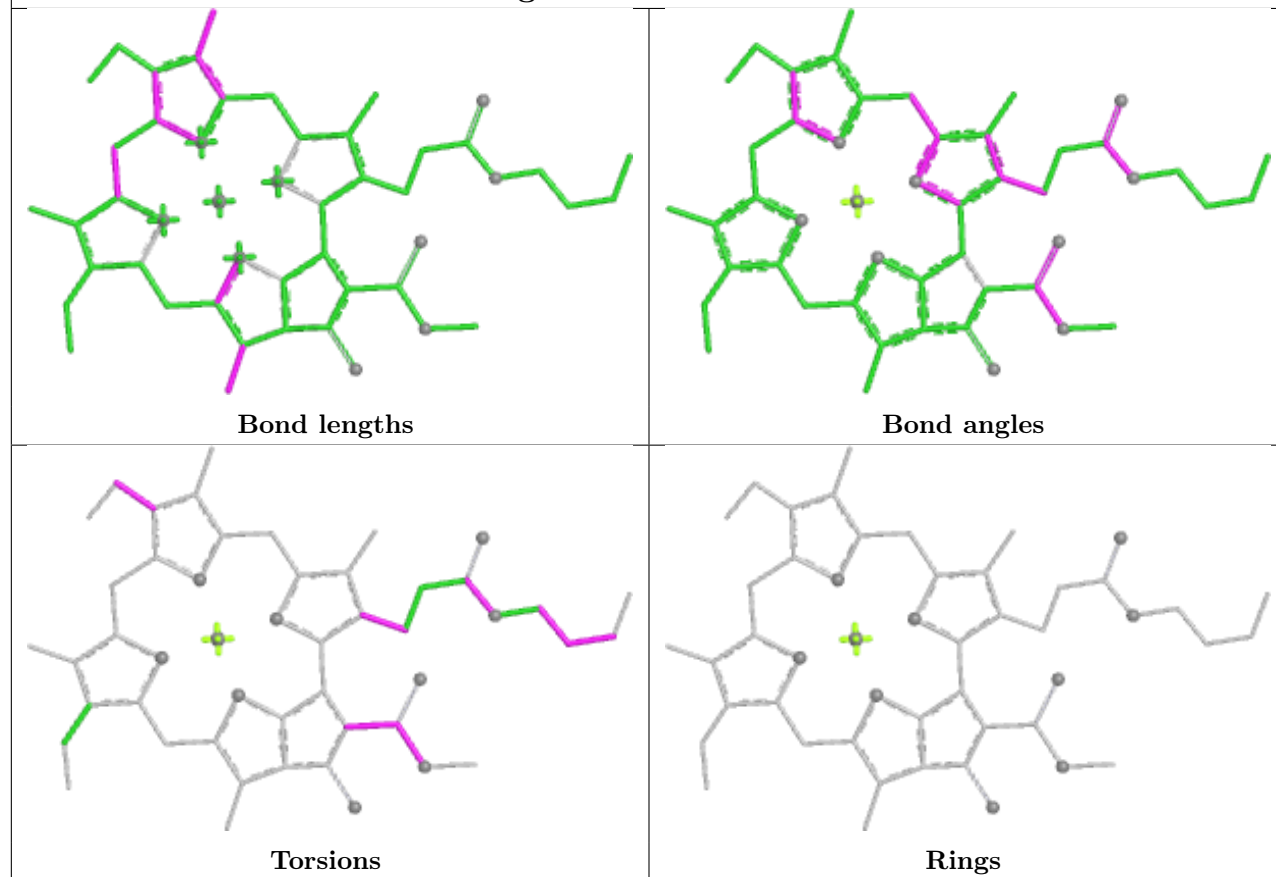
Rings

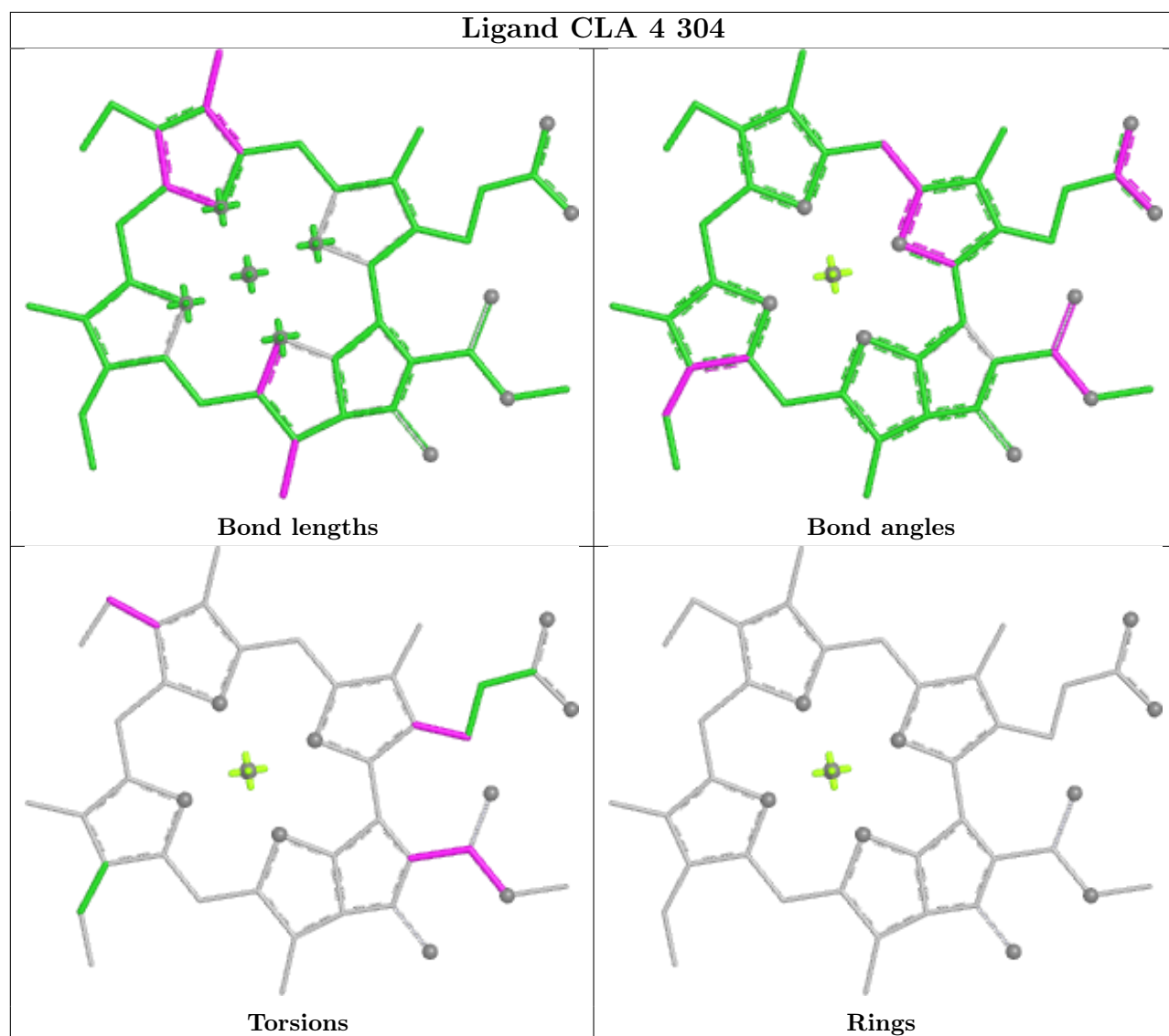
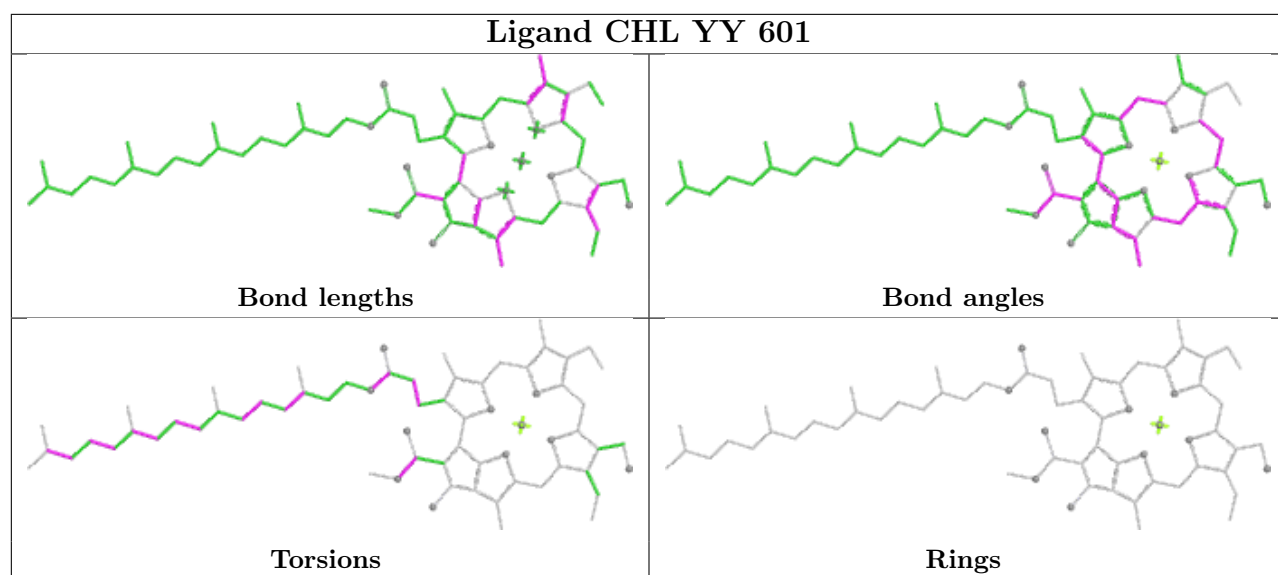


Ligand CLA B 619

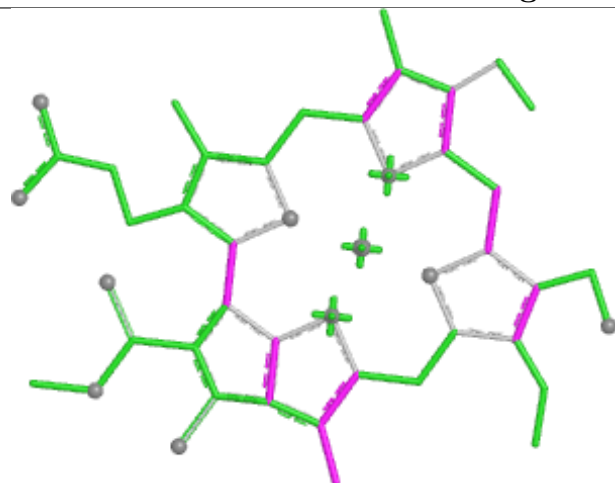


Ligand CLA YY 614

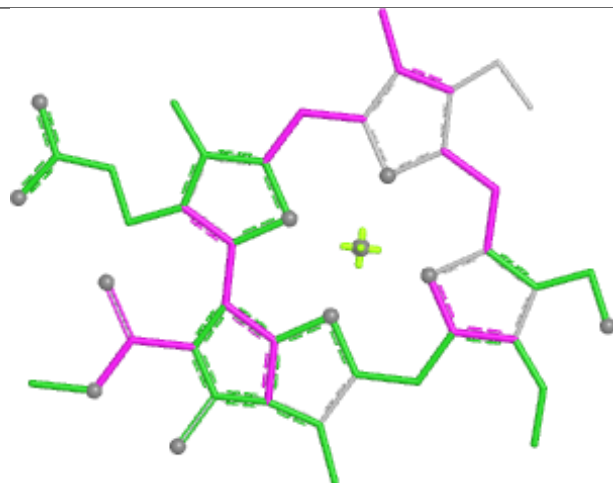




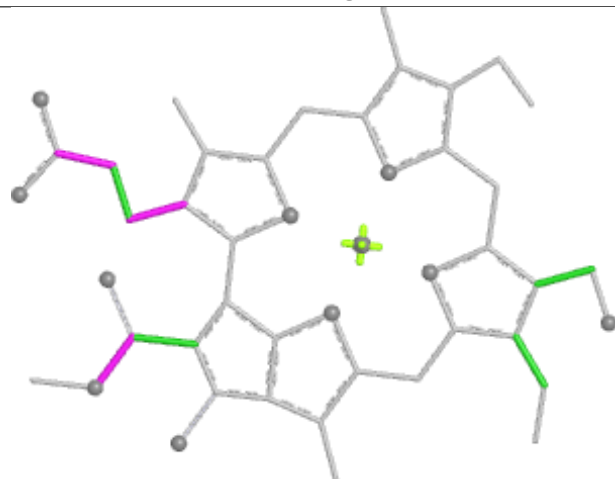
Ligand CHL 4 309



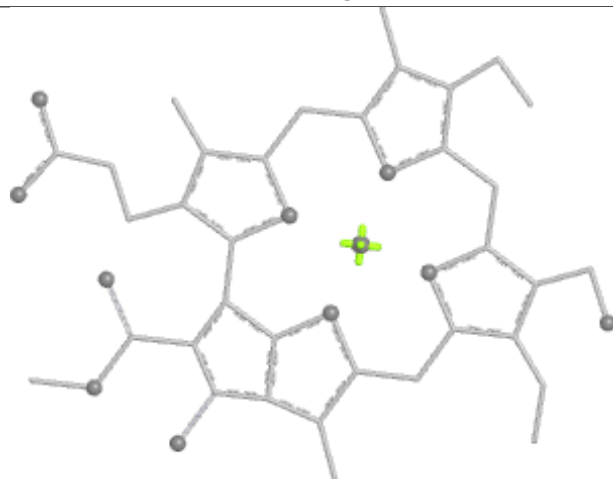
Bond lengths



Bond angles



Torsions

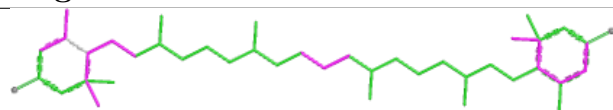


Rings

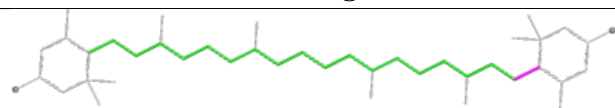
Ligand LUT g 615



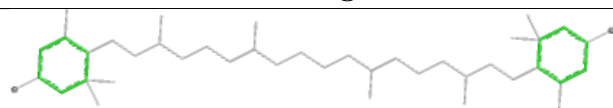
Bond lengths



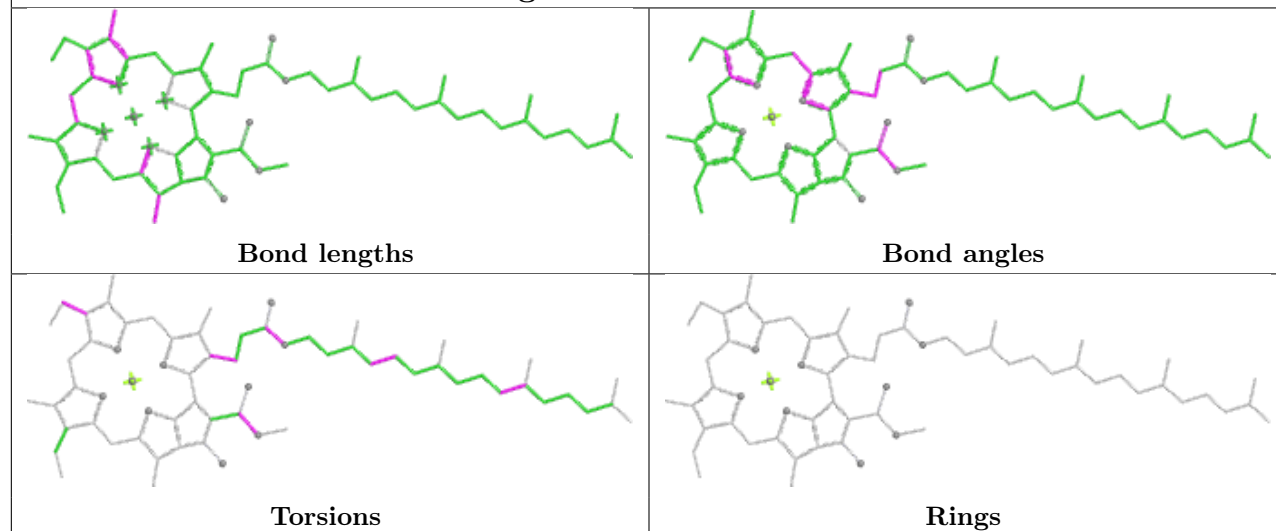
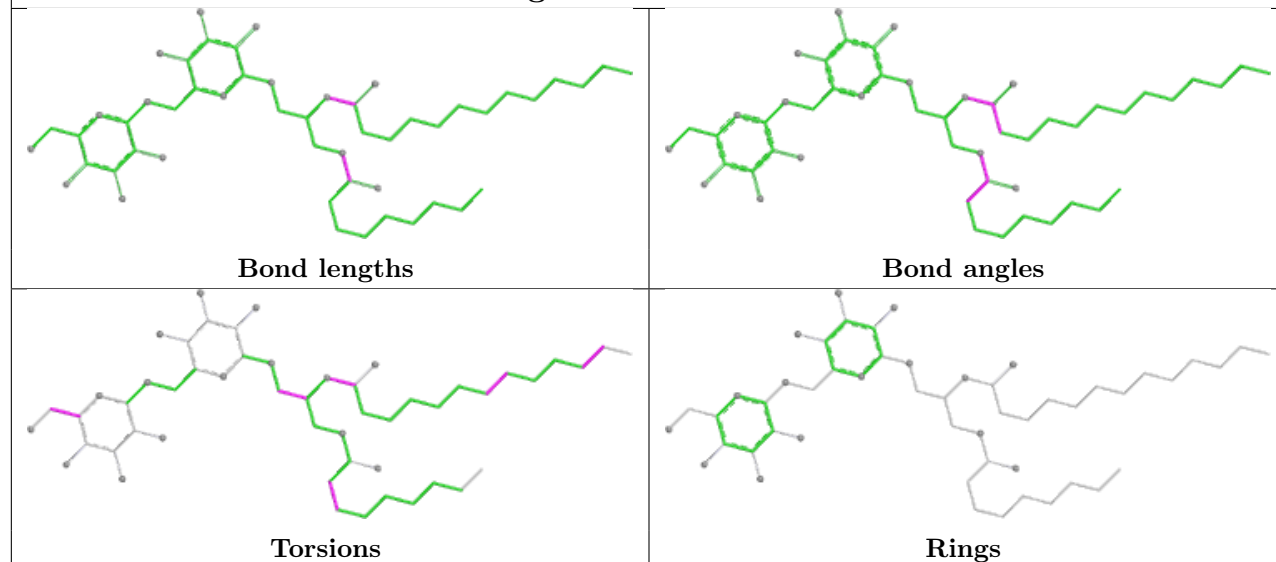
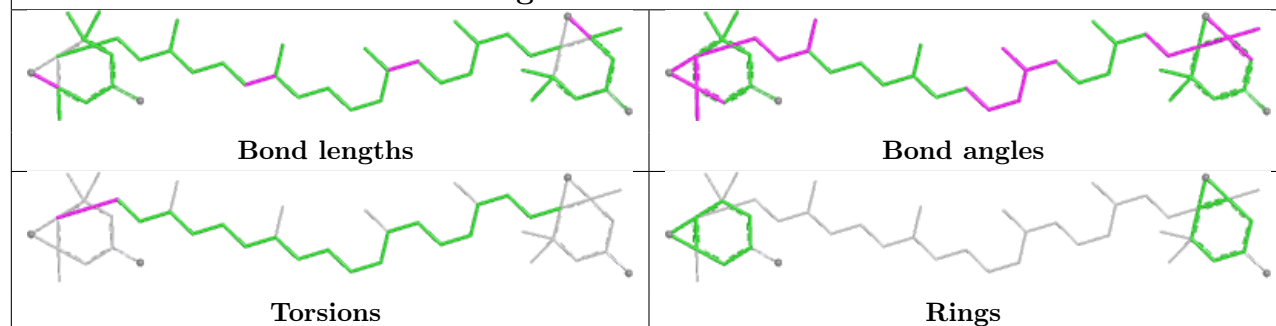
Bond angles

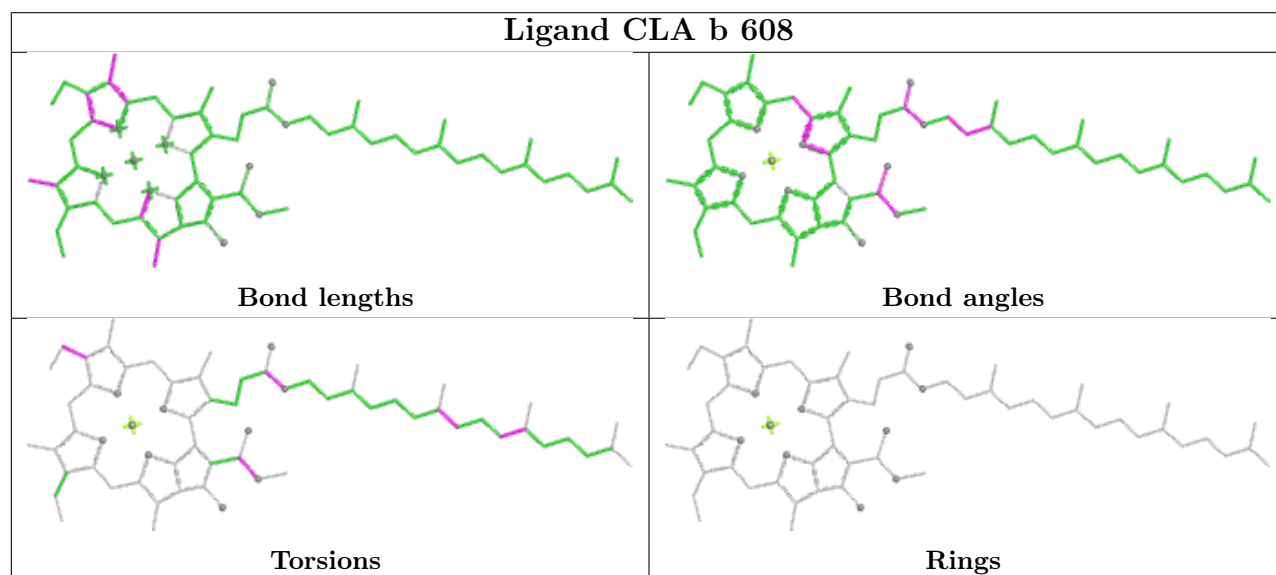
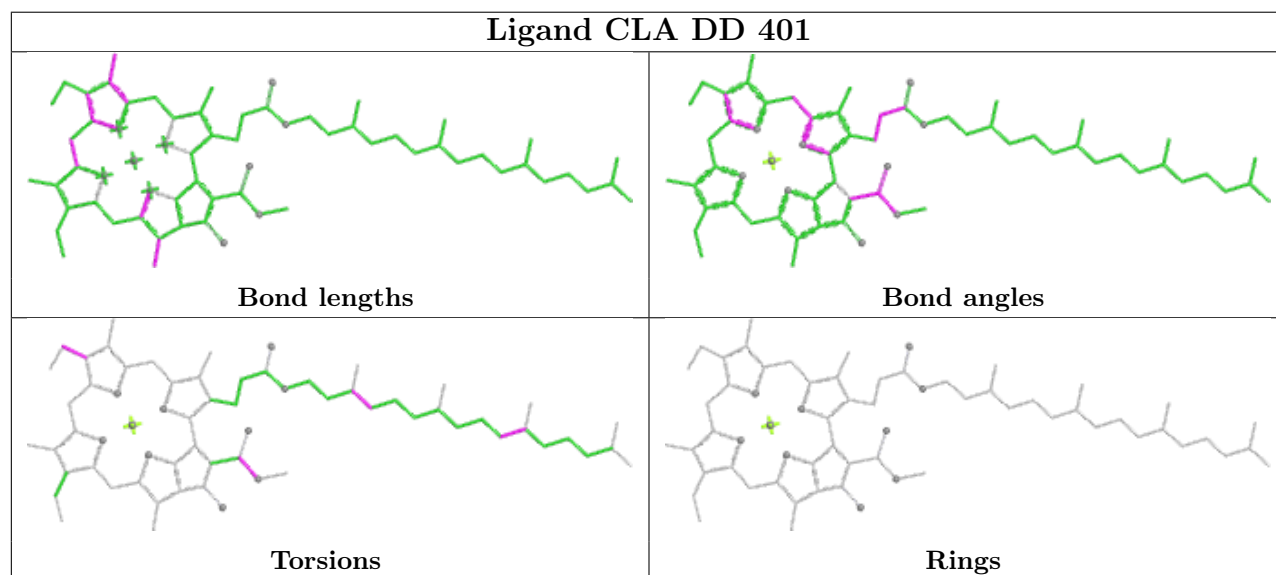
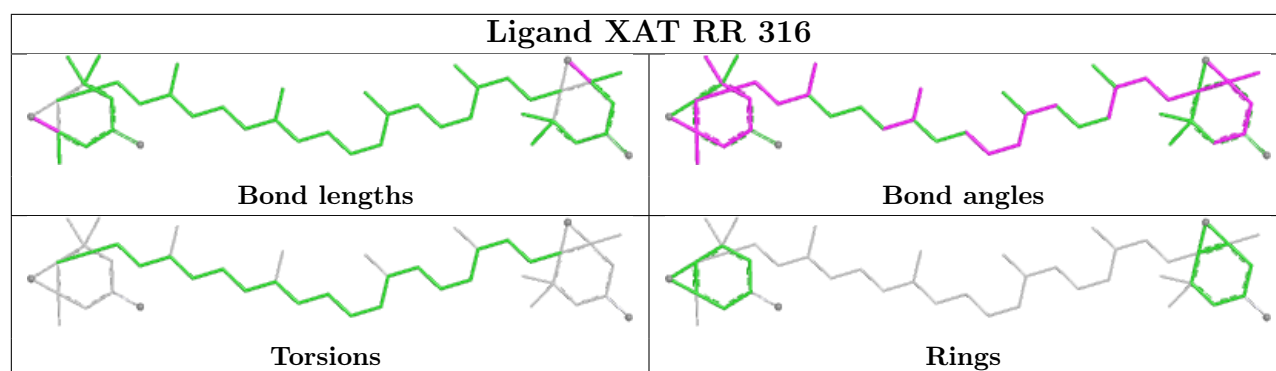


Torsions

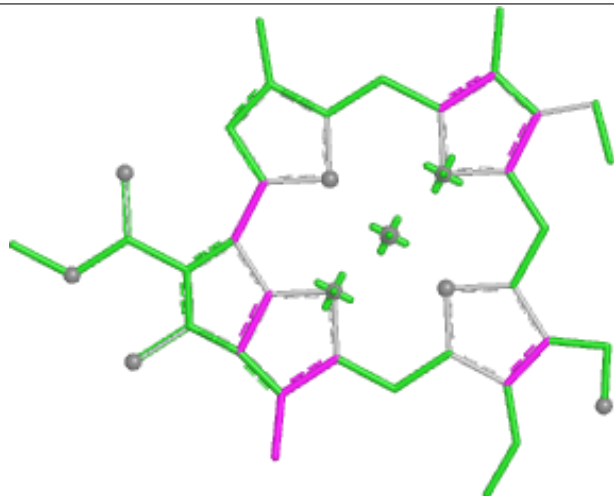


Rings

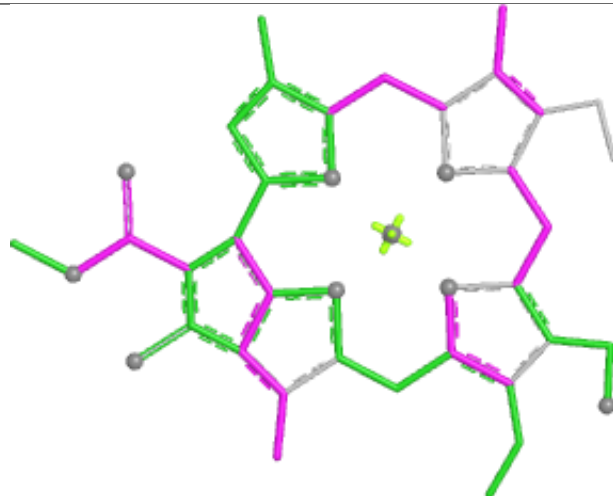
Ligand CLA RR 309**Ligand DGD C 523****Ligand XAT GG 619**



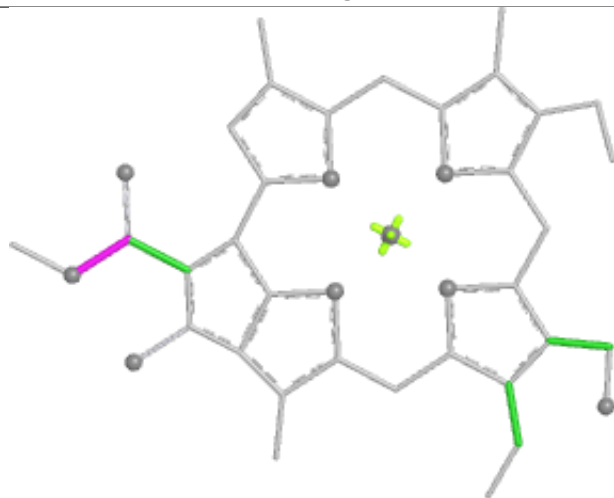
Ligand CHL 1 608



Bond lengths



Bond angles

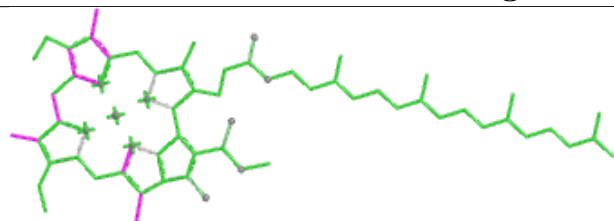


Torsions

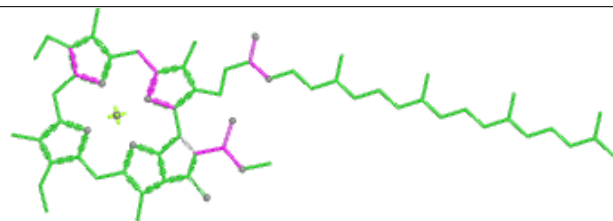


Rings

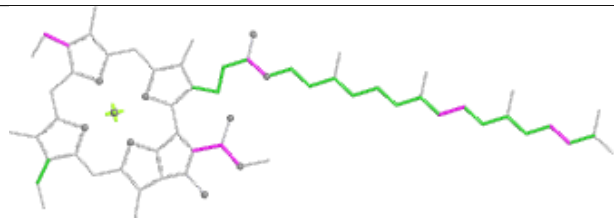
Ligand CLA CC 505



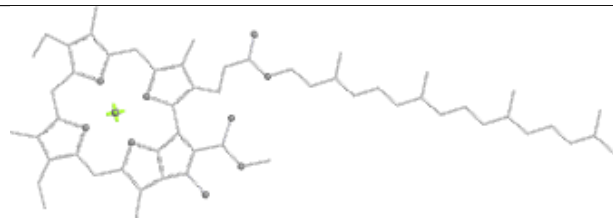
Bond lengths



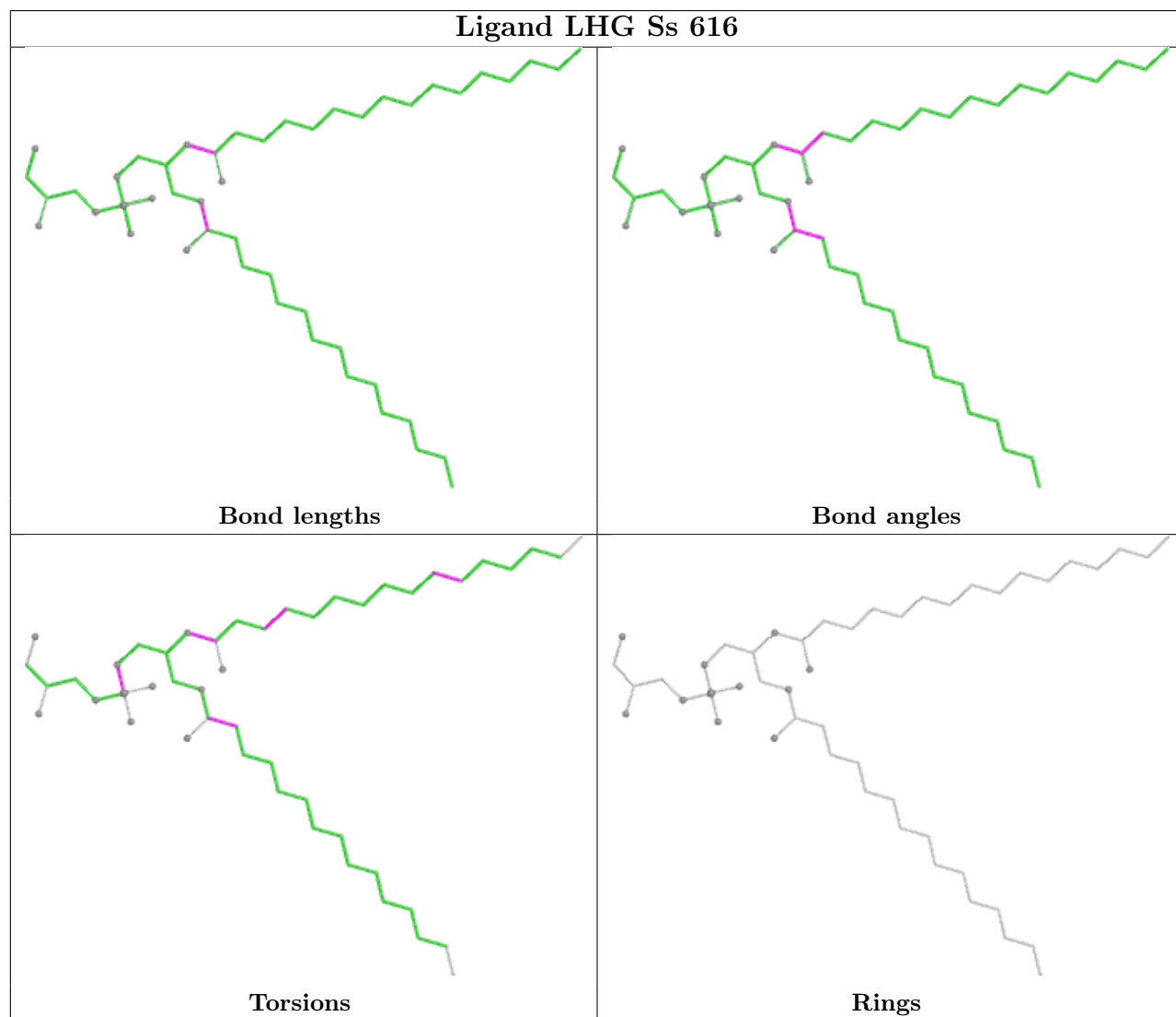
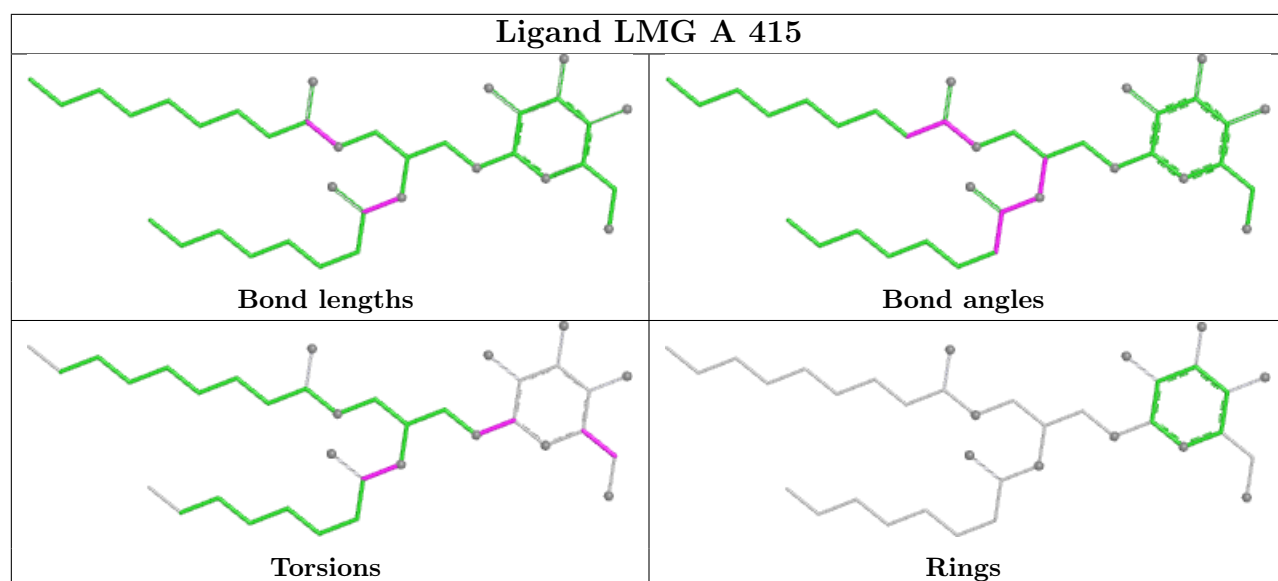
Bond angles

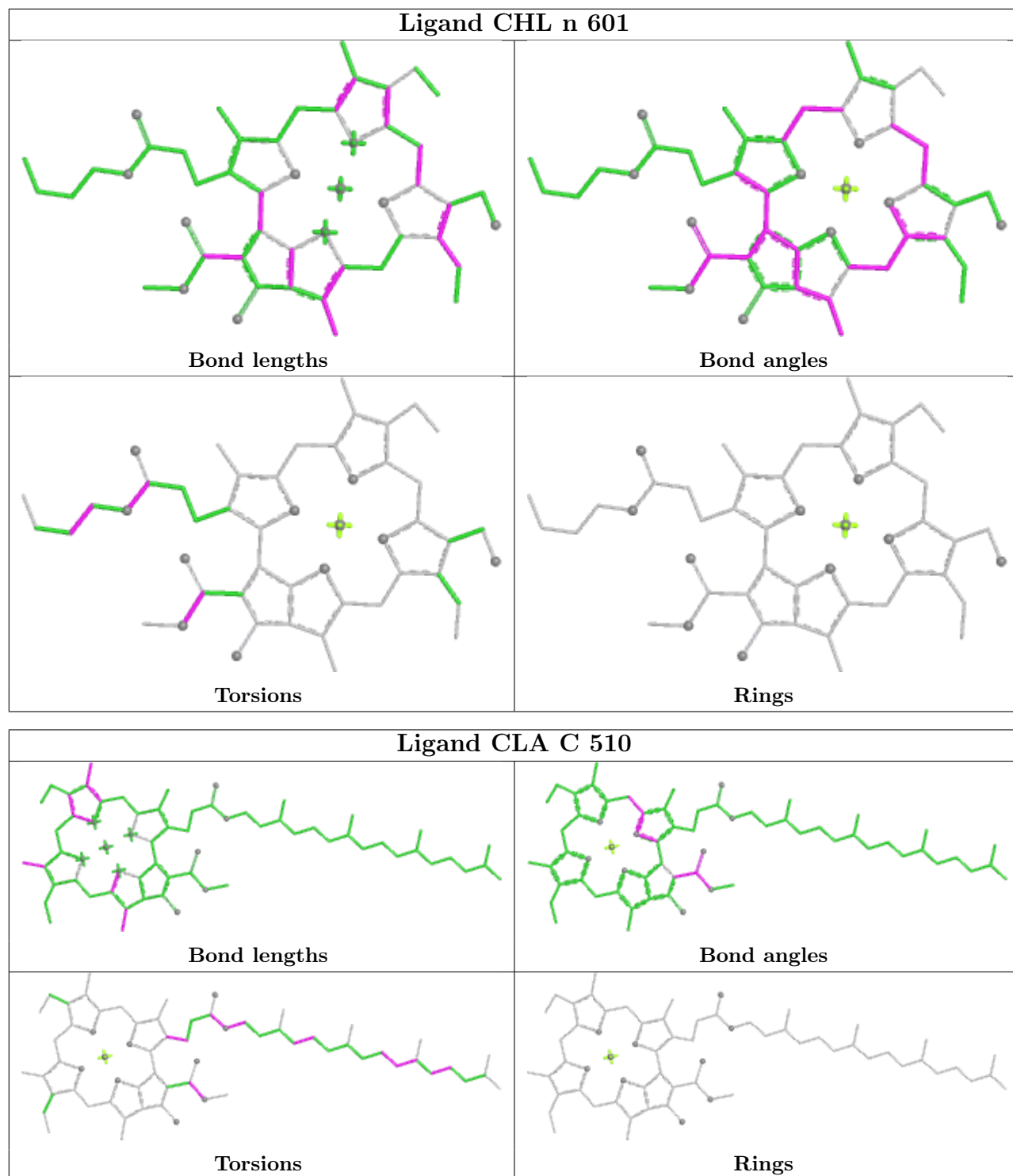


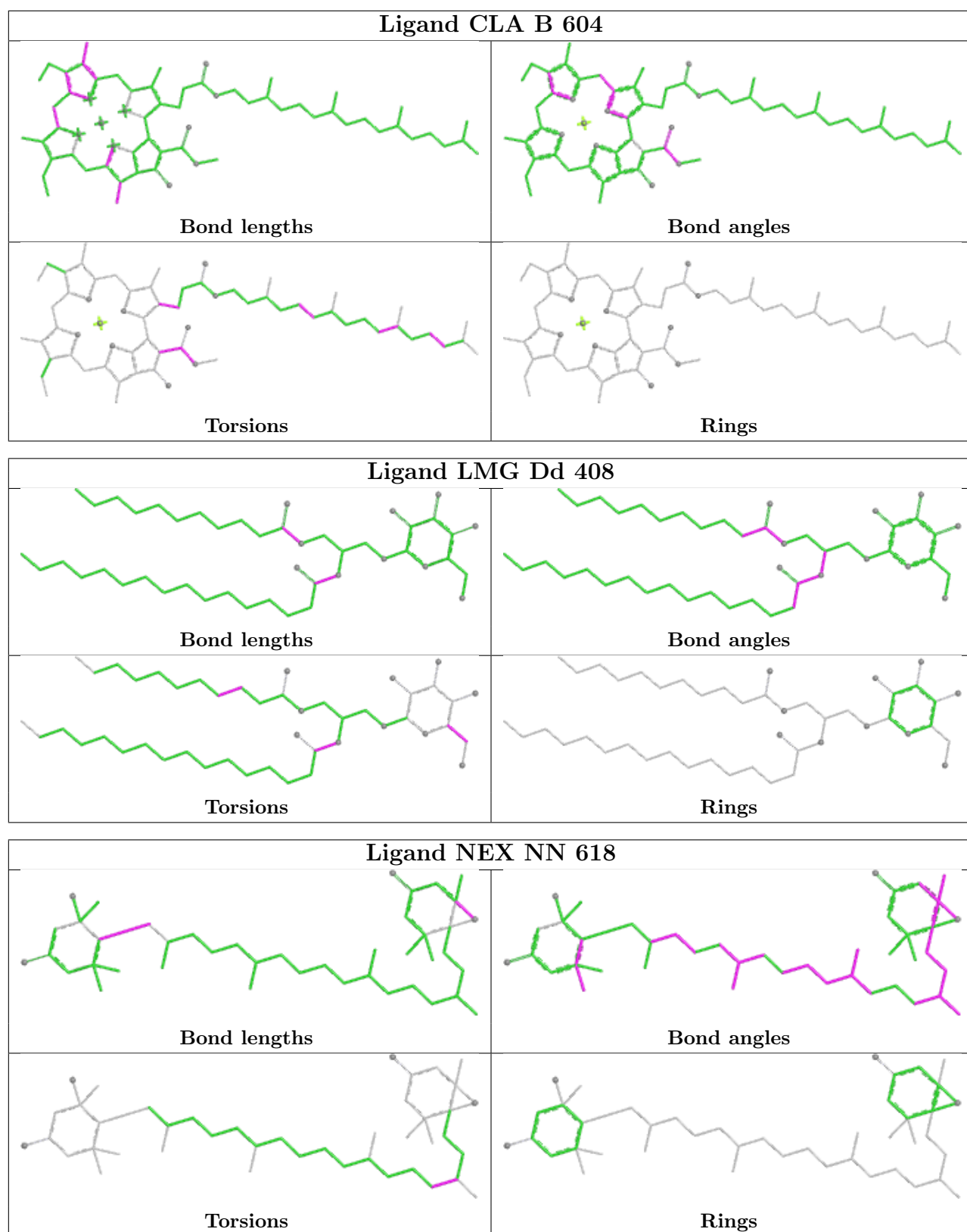
Torsions



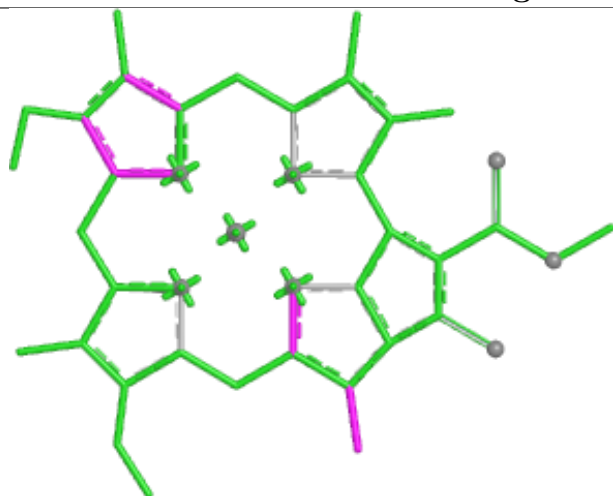
Rings



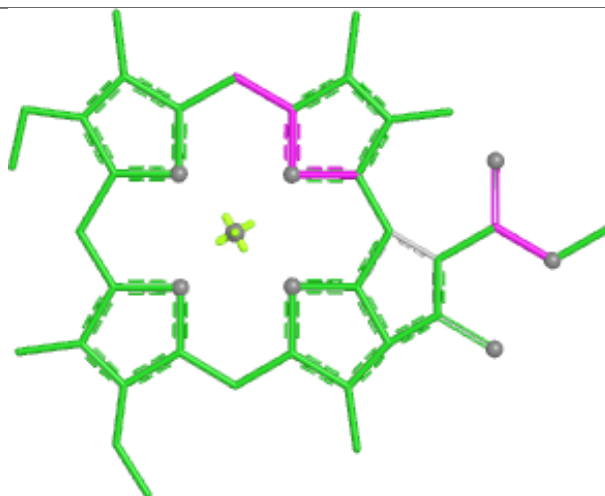




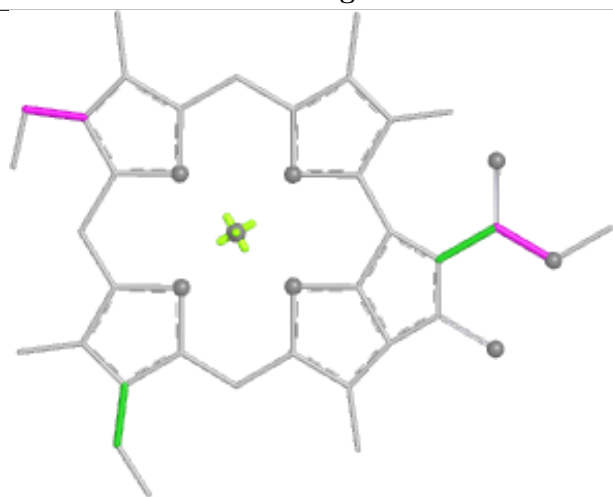
Ligand CLA G 614



Bond lengths



Bond angles

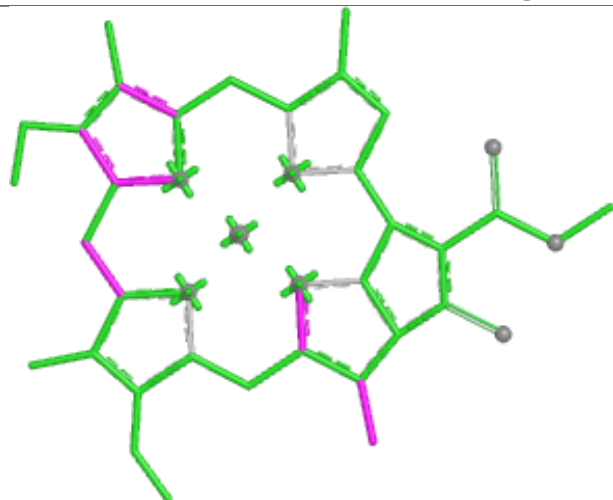


Torsions

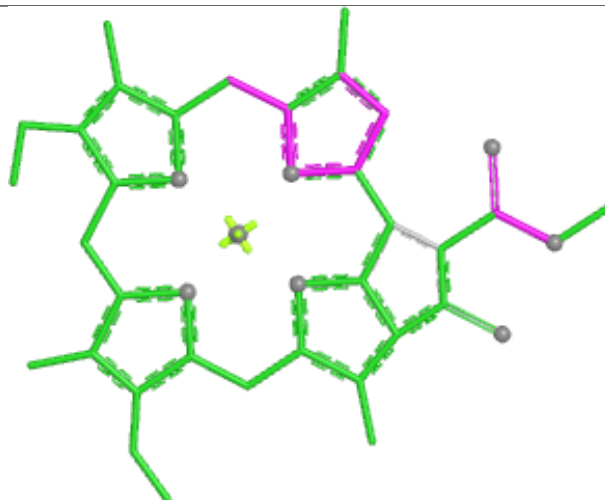


Rings

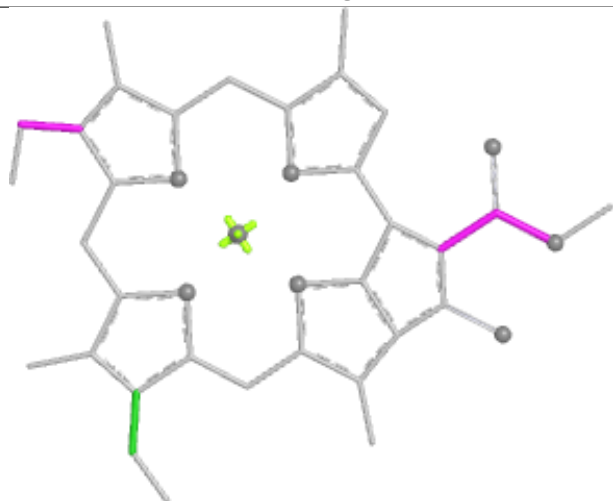
Ligand CLA 3 603



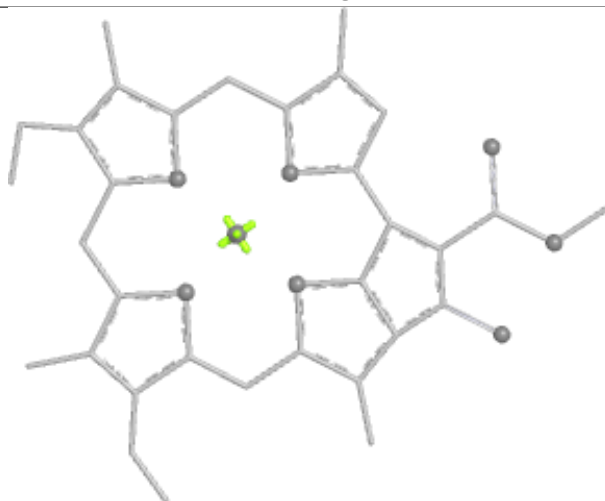
Bond lengths



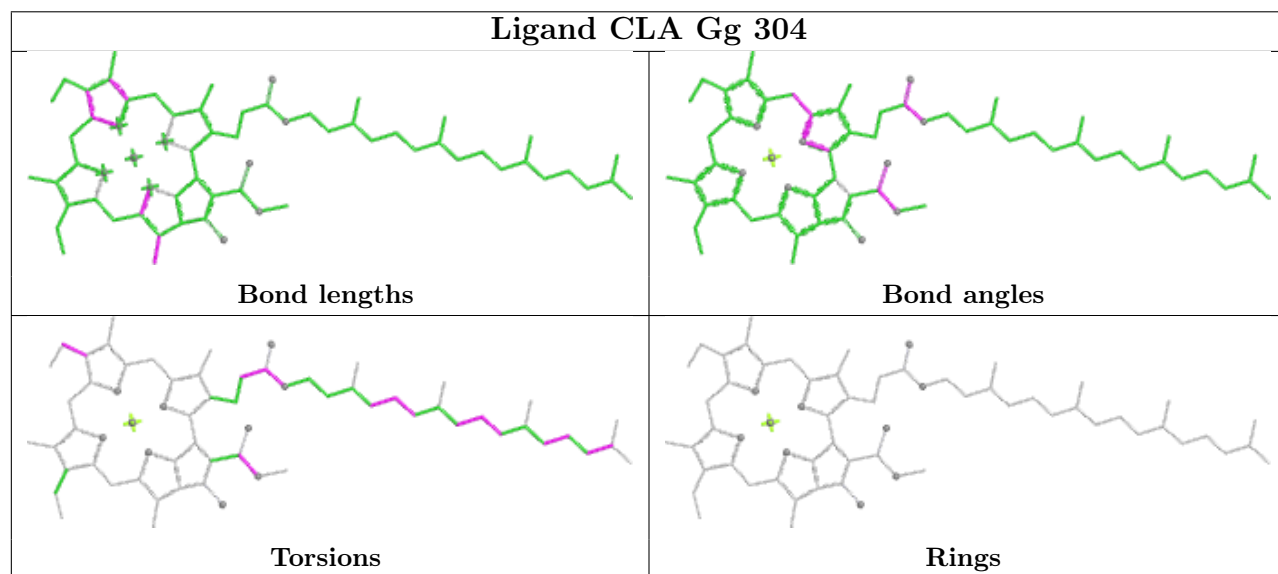
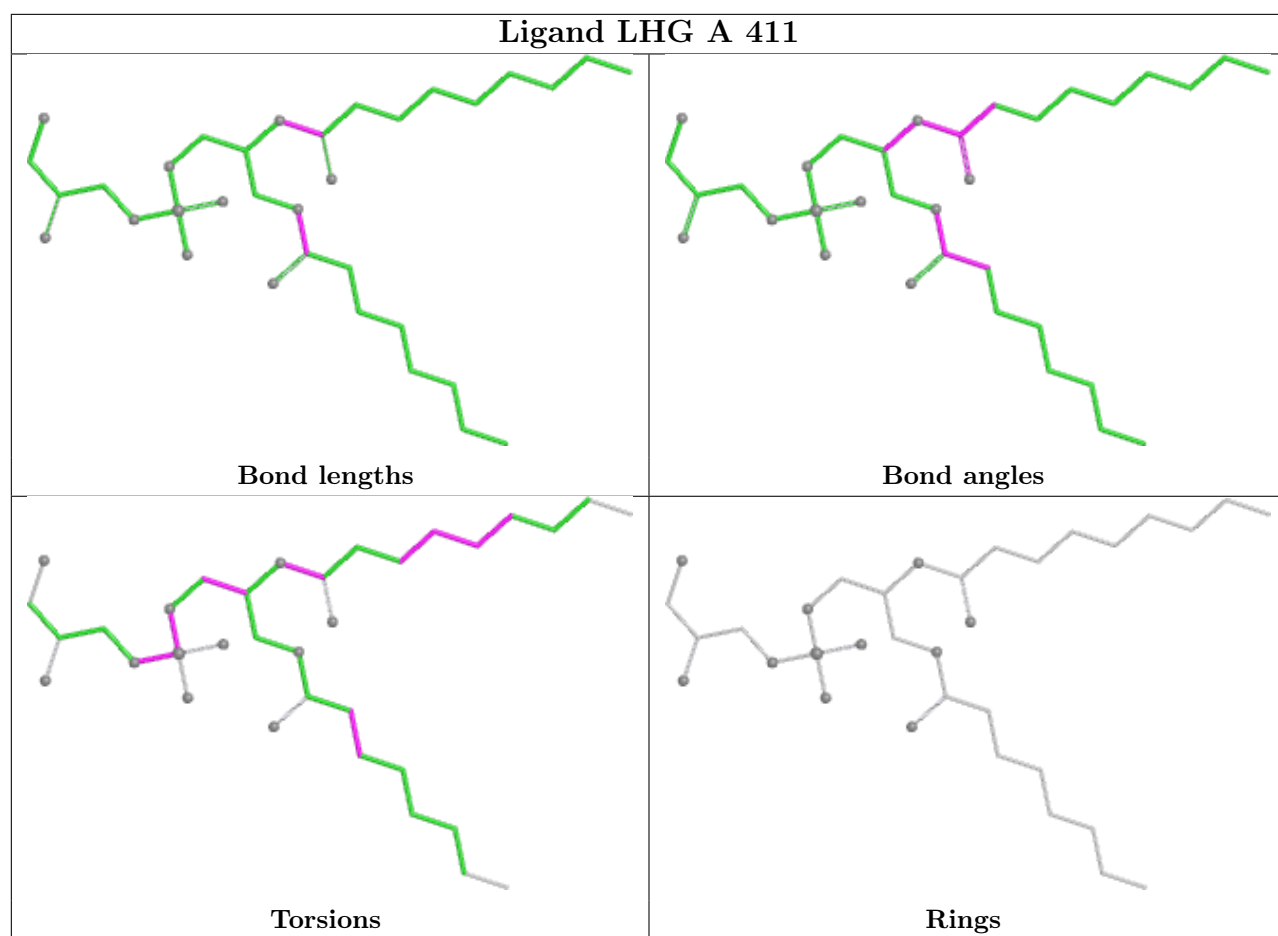
Bond angles

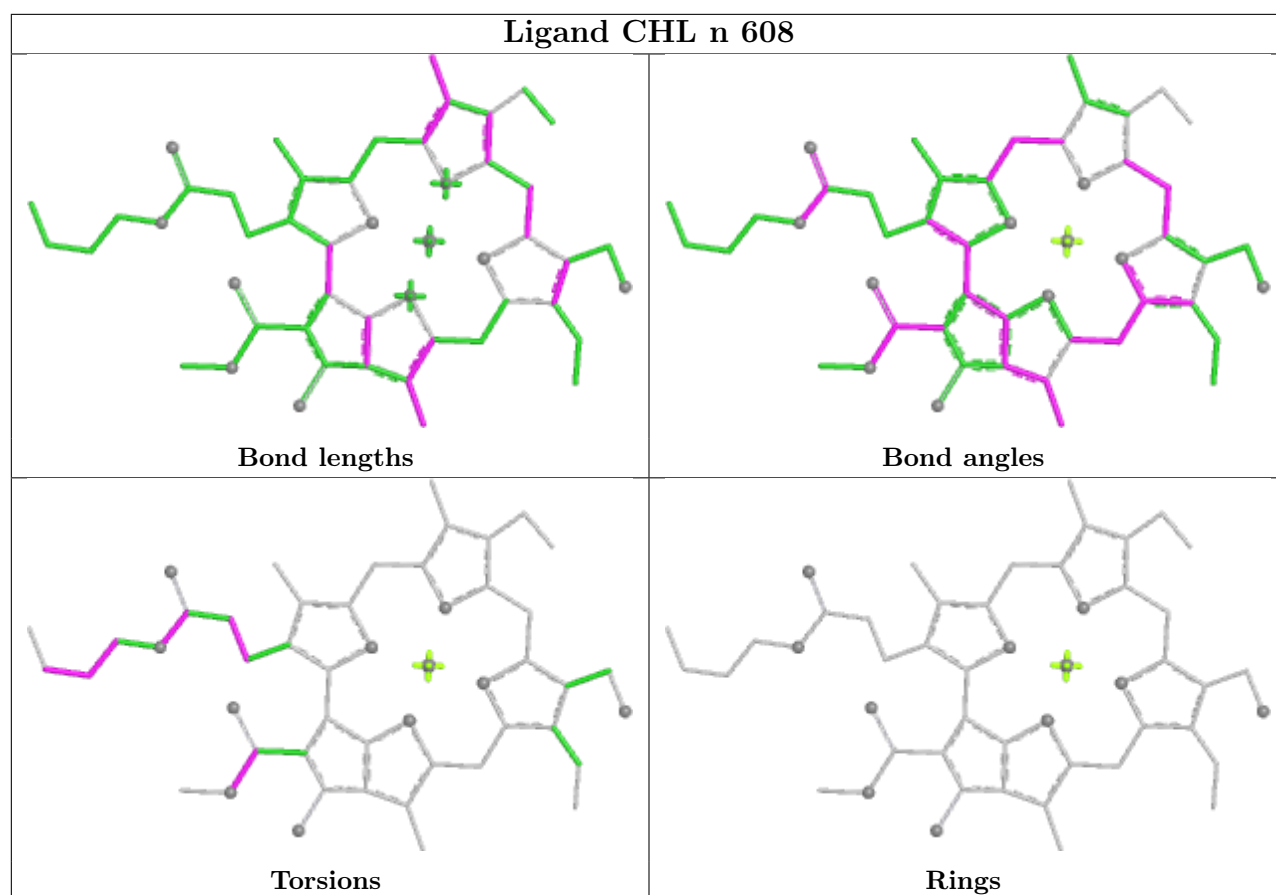


Torsions



Rings





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

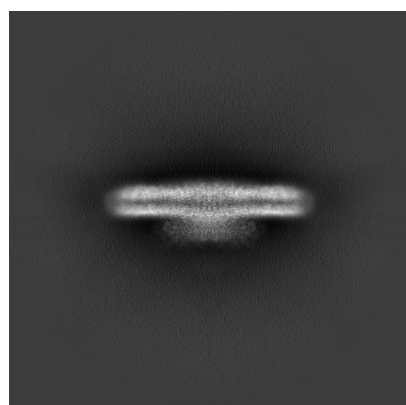
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39860. These allow visual inspection of the internal detail of the map and identification of artifacts.

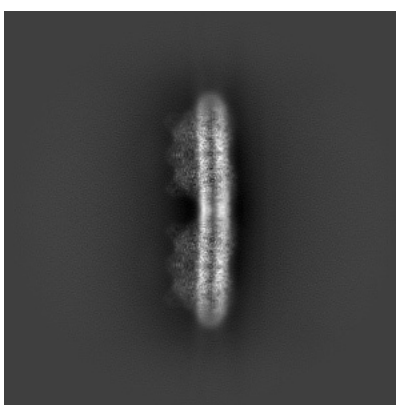
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

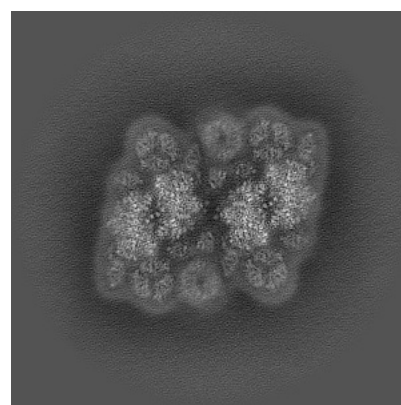
5.1.1 Primary map



X



Y

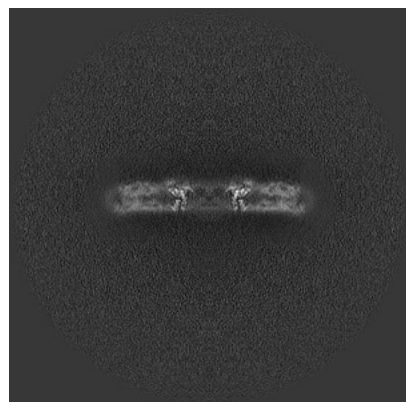


Z

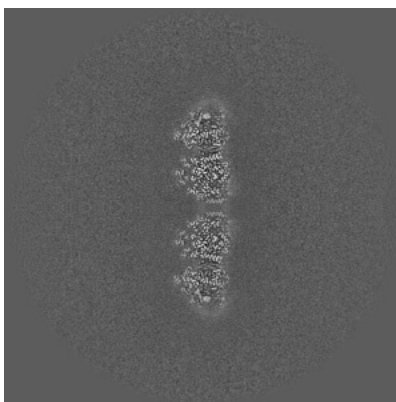
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

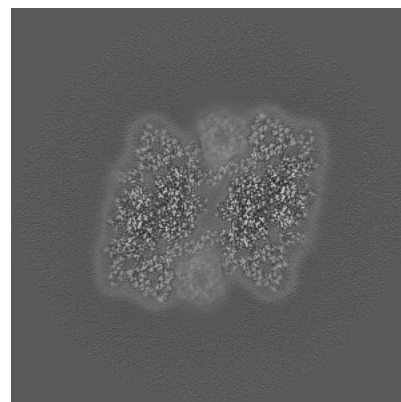
5.2.1 Primary map



X Index: 240



Y Index: 240

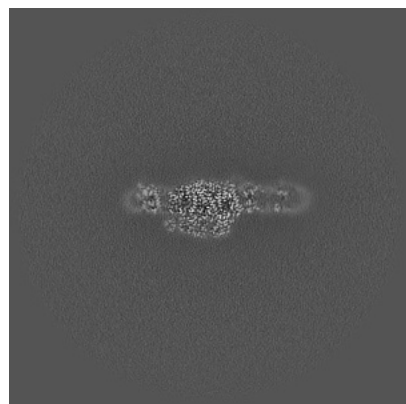


Z Index: 240

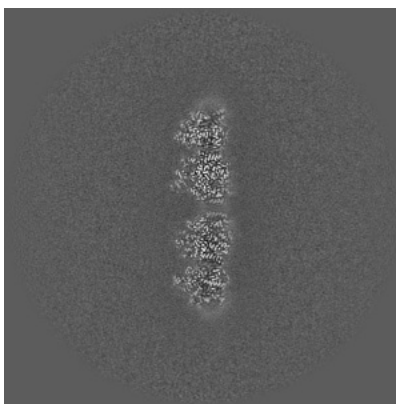
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

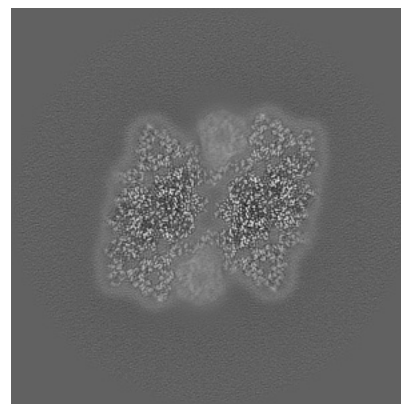
5.3.1 Primary map



X Index: 286



Y Index: 239

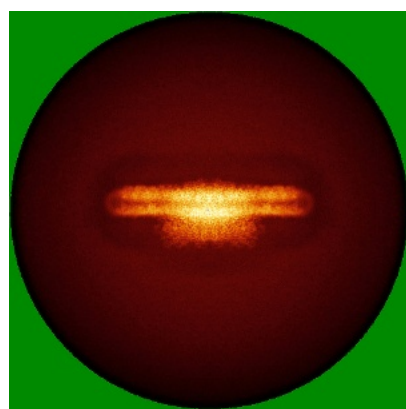


Z Index: 239

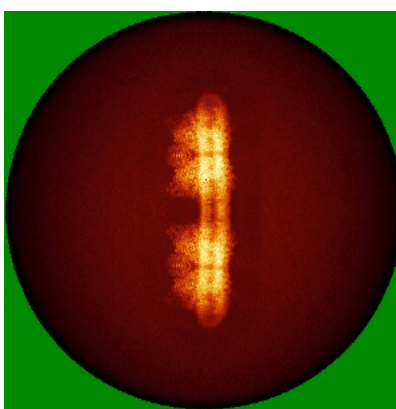
The images above show the largest variance slices of the map in three orthogonal directions.

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

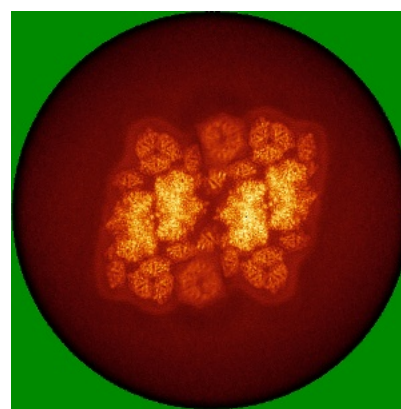
5.4.1 Primary map



X



Y



Z

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

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

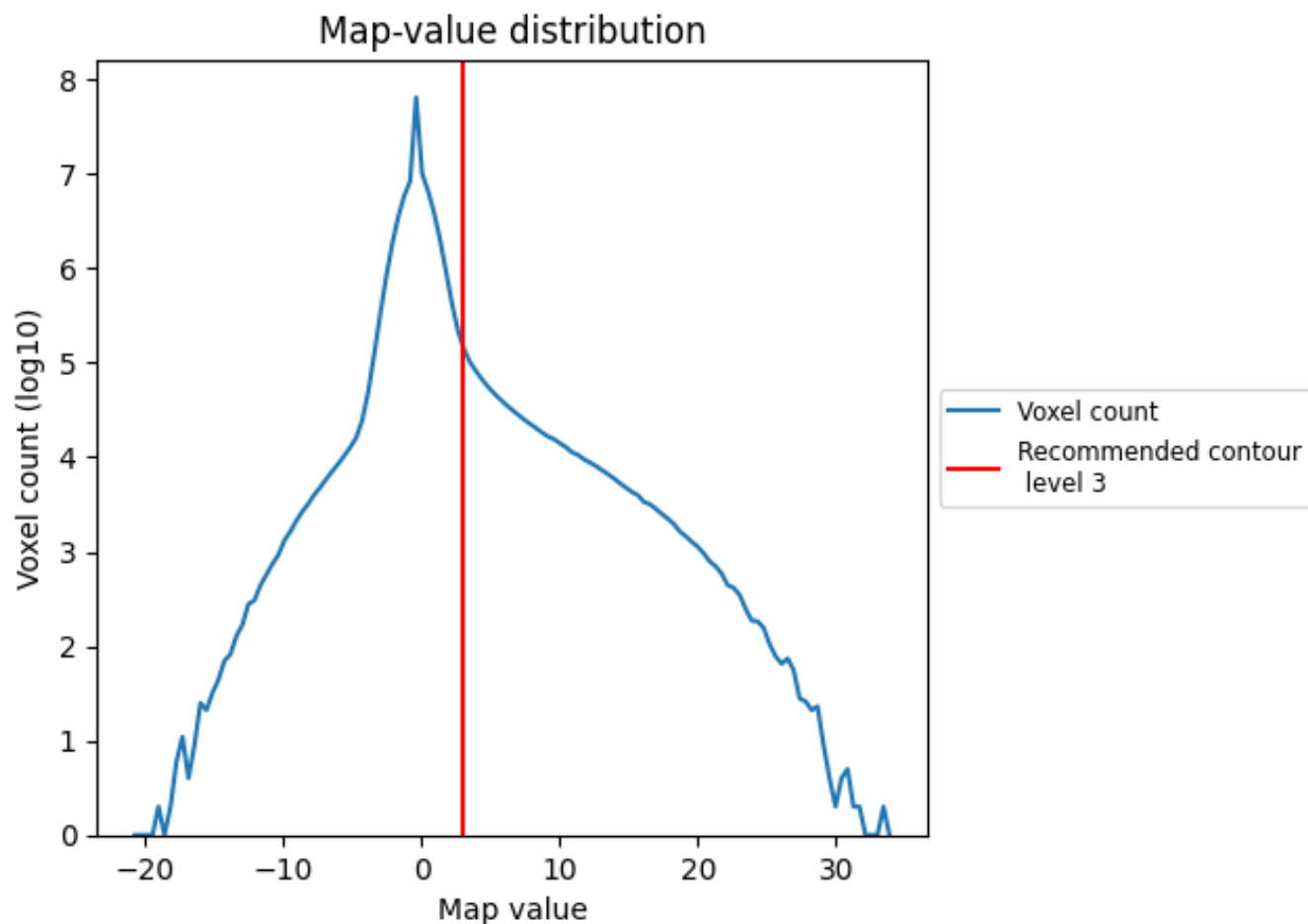
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

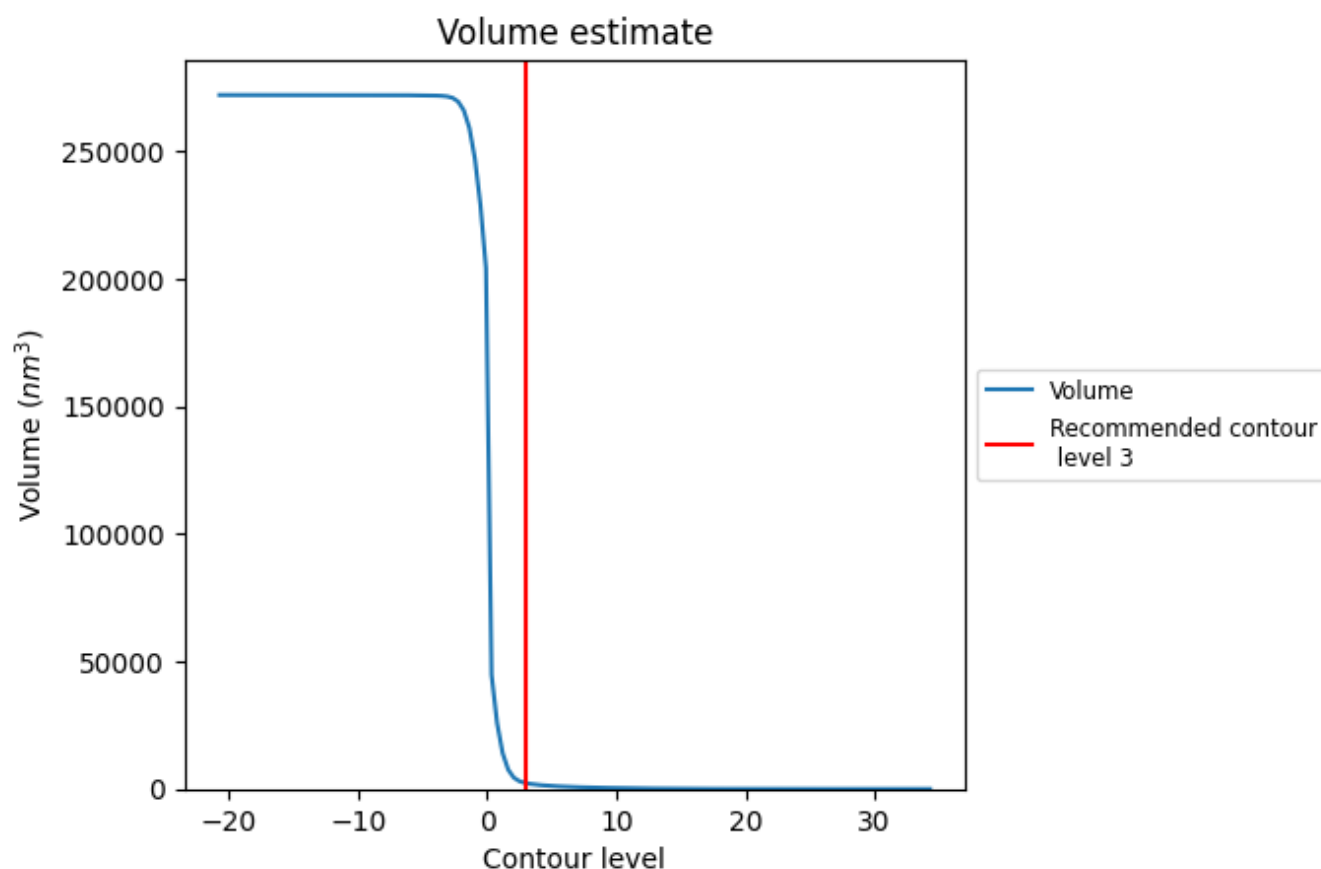
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution [i](#)



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

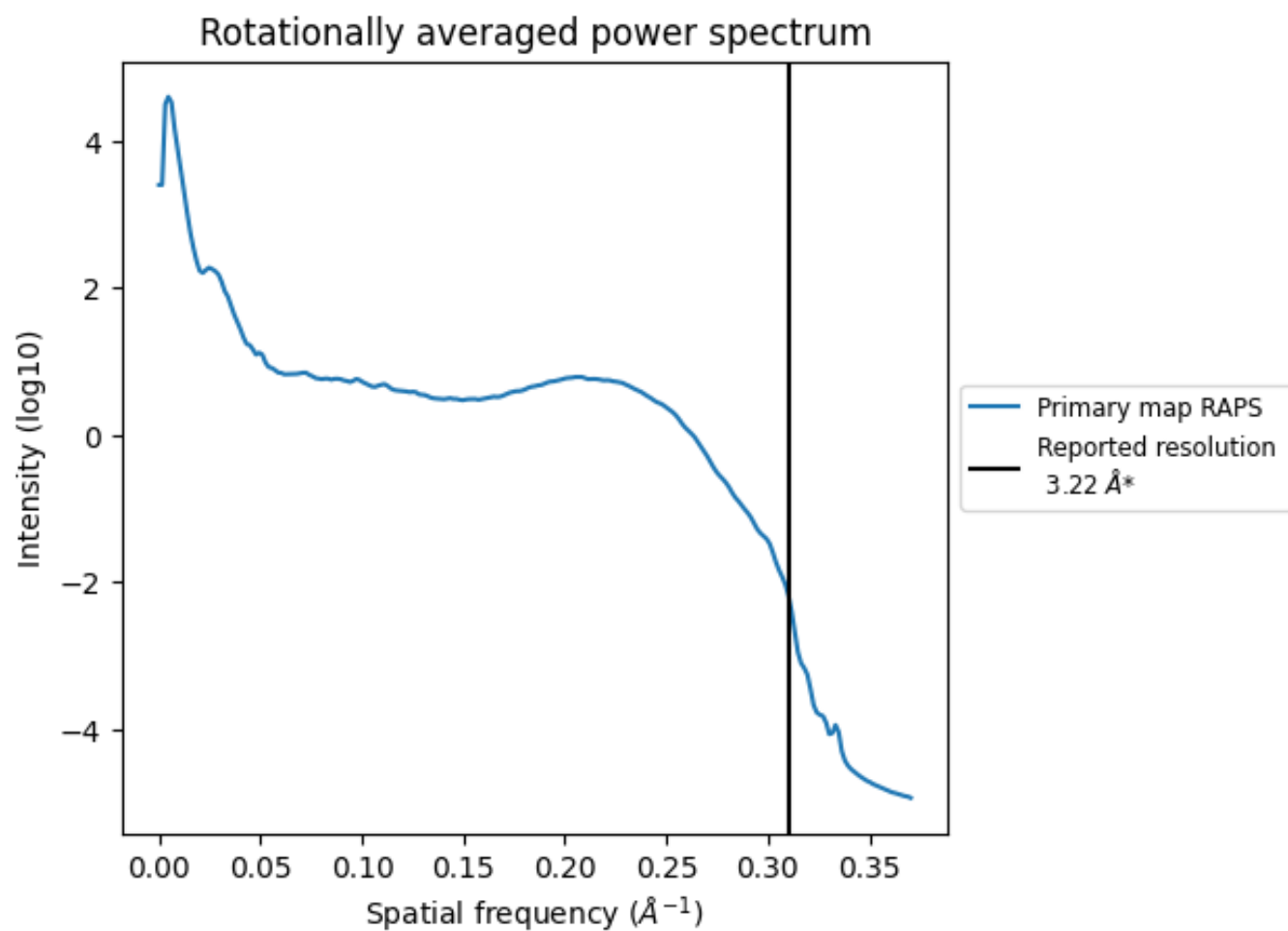
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 2290 nm^3 ; this corresponds to an approximate mass of 2069 kDa.

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

6.3 Rotationally averaged power spectrum ⓘ

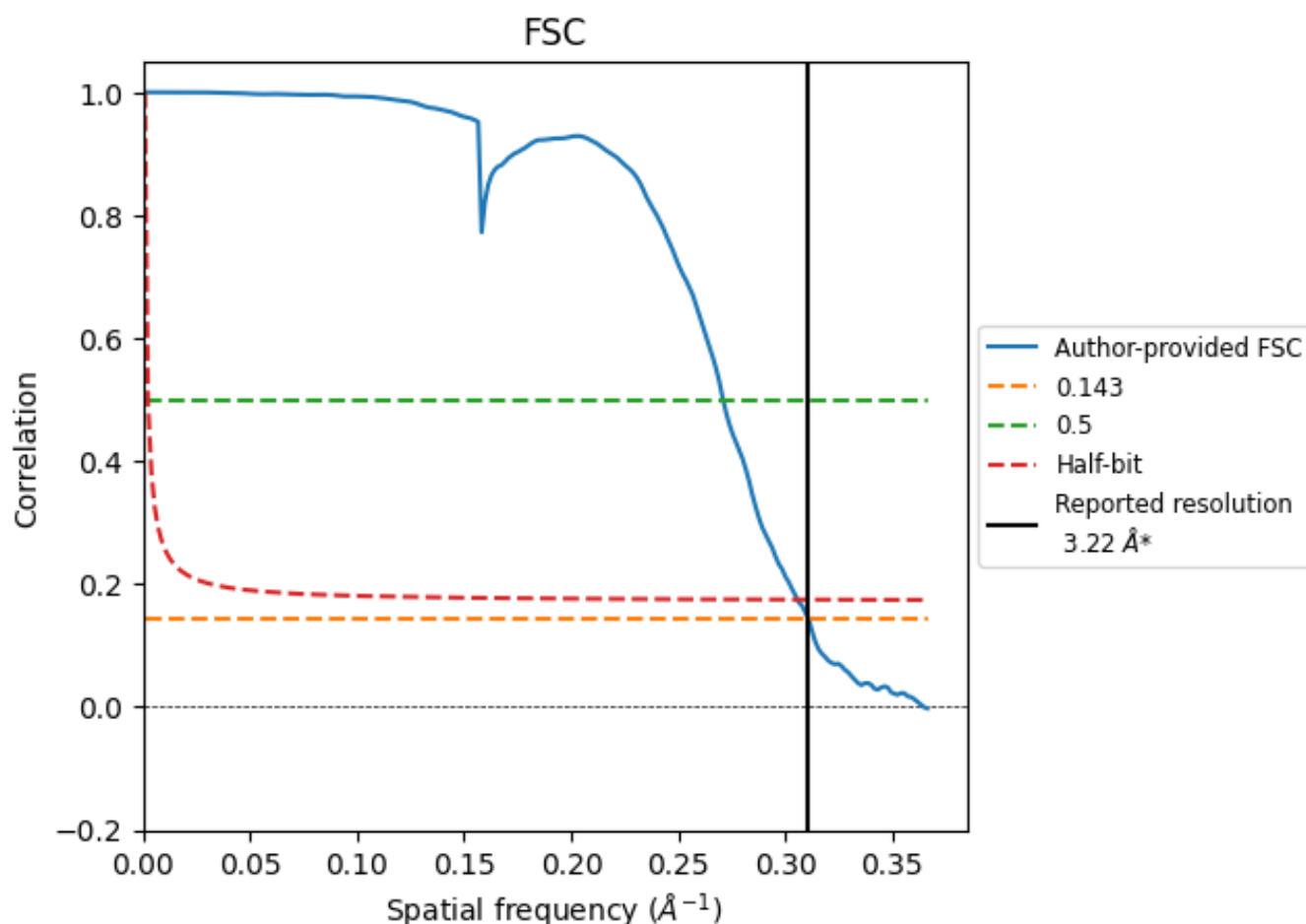


*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

7 Fourier-Shell correlation [i](#)

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

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.311 Å⁻¹

7.2 Resolution estimates [i](#)

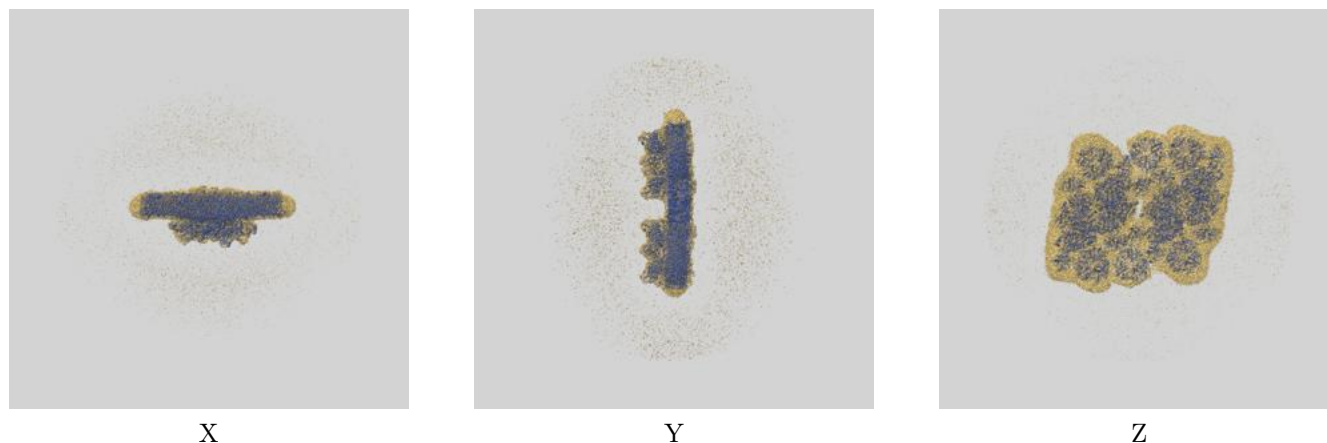
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.22	3.69	3.27
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

8 Map-model fit [i](#)

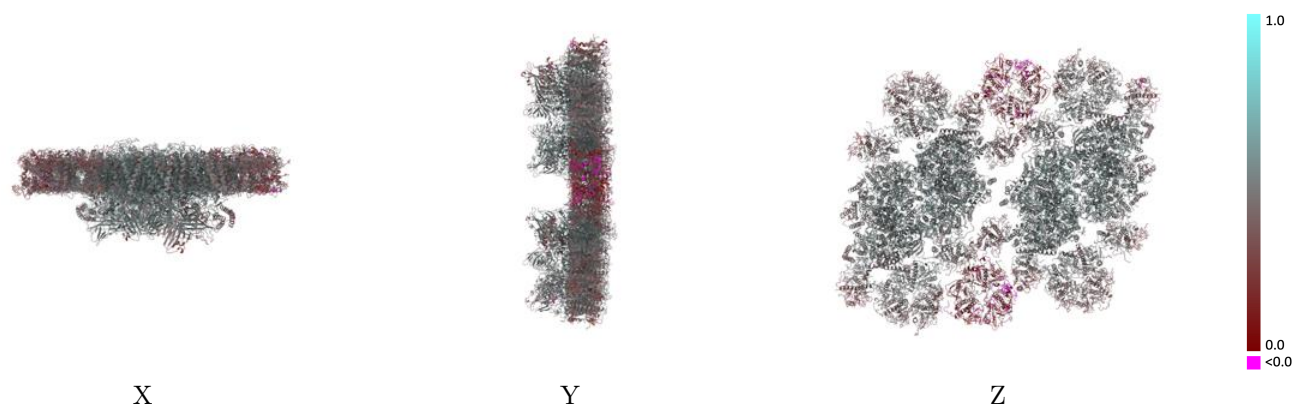
This section contains information regarding the fit between EMDB map EMD-39860 and PDB model 8Z9D. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



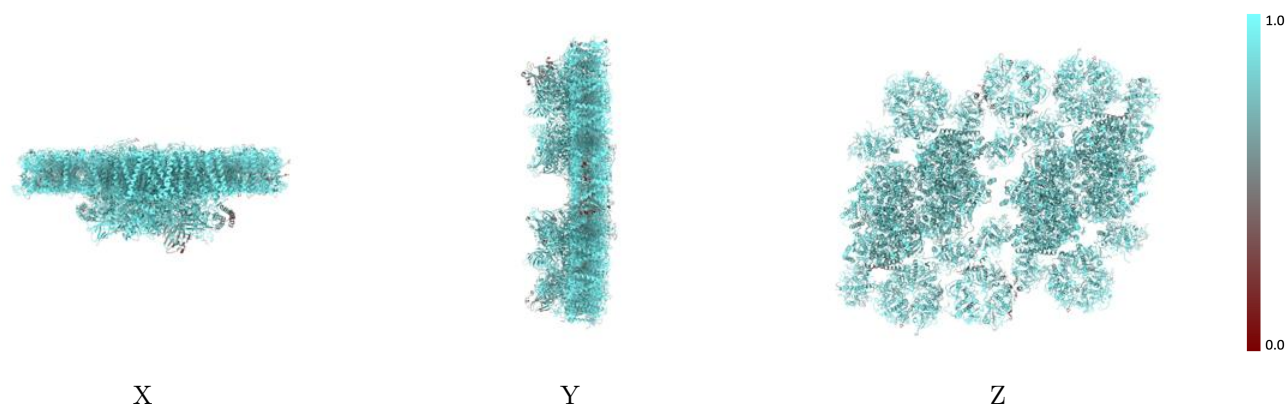
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



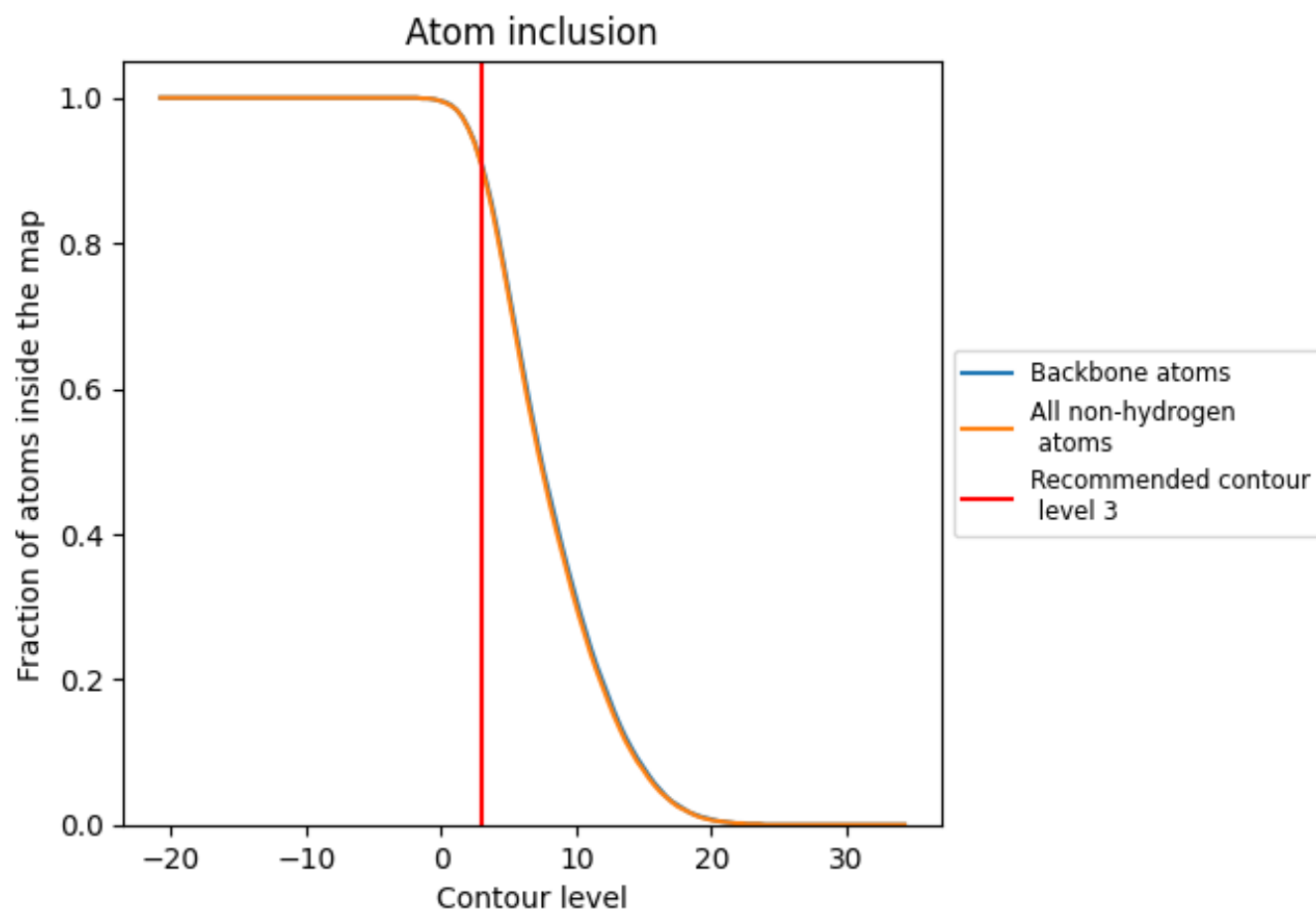
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

8.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.4520
0	 0.7820	 0.4470
00	 0.8280	 0.4610
1	 0.9110	 0.2140
11	 0.9050	 0.2020
2	 0.8440	 0.1600
22	 0.8610	 0.1580
3	 0.8500	 0.2130
33	 0.8750	 0.2150
4	 0.8810	 0.3570
44	 0.8990	 0.3600
5	 0.7560	 0.4260
55	 0.7820	 0.4450
A	 0.9570	 0.5300
AA	 0.9670	 0.5400
Aa	 0.9620	 0.5300
B	 0.9400	 0.5240
BB	 0.9600	 0.5340
Bb	 0.9510	 0.5250
C	 0.9370	 0.5200
CC	 0.9590	 0.5350
Cc	 0.9490	 0.5110
D	 0.9610	 0.5370
DD	 0.9730	 0.5490
Dd	 0.9620	 0.5260
E	 0.9460	 0.5120
EE	 0.9570	 0.5310
Ee	 0.9620	 0.4650
F	 0.9400	 0.5180
FF	 0.9630	 0.5240
Ff	 0.9590	 0.4630
G	 0.8850	 0.3760
GG	 0.8850	 0.3780
Gg	 0.8880	 0.4220
H	 0.9450	 0.5020



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Chain	Atom inclusion	Q-score
HH	 0.9680	 0.5110
Hh	 0.9590	 0.5020
I	 0.9610	 0.5120
II	 0.9360	 0.5160
Ii	 0.9810	 0.5360
J	 0.9140	 0.5180
JJ	 0.9390	 0.5160
Jj	 0.9170	 0.4780
K	 0.9280	 0.5180
KK	 0.9460	 0.5210
Kk	 0.9330	 0.4940
L	 0.9450	 0.5110
LL	 0.9660	 0.5290
Ll	 0.9600	 0.5350
M	 0.9070	 0.4980
MM	 0.9530	 0.5190
Mm	 0.9300	 0.5070
N	 0.9150	 0.4240
NN	 0.9210	 0.4310
Nn	 0.9130	 0.4370
O	 0.9310	 0.4960
OO	 0.9490	 0.5030
Oo	 0.9220	 0.4880
P	 0.8840	 0.4920
PP	 0.9000	 0.4970
Pp	 0.6740	 0.4290
Q	 0.7830	 0.4040
QQ	 0.8270	 0.4370
Qq	 0.6200	 0.3860
R	 0.8940	 0.4400
RR	 0.8960	 0.4460
Rr	 0.8500	 0.4130
S	 0.7940	 0.3810
SS	 0.8480	 0.3780
Ss	 0.8570	 0.3590
T	 0.8830	 0.5030
TT	 0.9150	 0.5170
Tt	 0.9550	 0.5320
U	 0.8820	 0.4630
UU	 0.9210	 0.4980
Uu	 0.9390	 0.4600
W	 0.9390	 0.4990

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Chain	Atom inclusion	Q-score
WW	 0.9440	 0.5110
Ww	 0.9320	 0.4960
X	 0.8750	 0.4520
XX	 0.8870	 0.4570
Xx	 0.9750	 0.4450
Y	 0.9120	 0.4590
YY	 0.9200	 0.4640
Yy	 0.9240	 0.4790
Z	 0.8960	 0.4590
ZZ	 0.9490	 0.4830
Zz	 0.9030	 0.4090
a	 0.9510	 0.5180
b	 0.9400	 0.5140
c	 0.9320	 0.4970
d	 0.9470	 0.5150
e	 0.9380	 0.4520
f	 0.9430	 0.4510
g	 0.8810	 0.4140
h	 0.9510	 0.4950
i	 0.9510	 0.4960
j	 0.8720	 0.4540
k	 0.9070	 0.4750
l	 0.9480	 0.5210
m	 0.9000	 0.4900
n	 0.9050	 0.4240
o	 0.8960	 0.4860
p	 0.6280	 0.4170
q	 0.5550	 0.3560
r	 0.8720	 0.4080
s	 0.8580	 0.3630
t	 0.9260	 0.5160
u	 0.9130	 0.4260
w	 0.9130	 0.4860
x	 0.9370	 0.4280
y	 0.9190	 0.4750
z	 0.8800	 0.3990