



## wwPDB EM Validation Summary Report ⓘ

Feb 23, 2023 – 03:29 pm GMT

PDB ID : 7PIN  
EMDB ID : EMD-13444  
Title : Stacked compact Dunaliella PSII  
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.  
Deposited on : 2021-08-22  
Resolution : 3.60 Å (reported)  
Based on initial model : 6KAC

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

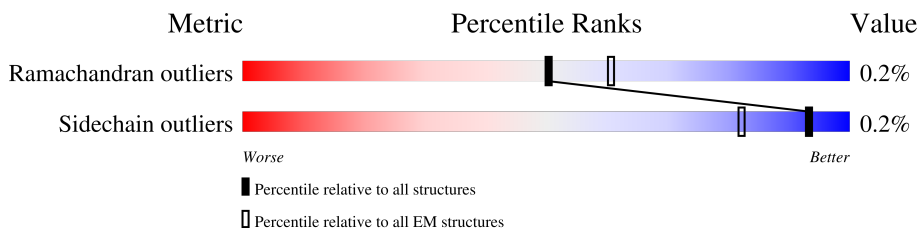
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	336	
1	A1	336	
1	a	336	
1	a1	336	
2	B	484	
2	B1	484	
2	b	484	
2	b1	484	
3	V	32	

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Mol	Chain	Length	Quality of chain
3	V1	32	69% 100%
3	v	32	84% 100%
3	v1	32	94% 97%
4	C	449	55% 100%
4	C1	449	42% 100%
4	c	449	55% 100%
4	c1	449	66% 99%
5	D	348	63% 99%
5	D1	348	63% 100%
5	d	348	61% 99%
5	d1	348	75% 99%
6	E	76	92% 100%
6	E1	76	50% 100%
6	e	76	93% 99%
6	e1	76	76% 100%
7	F	31	74% 100%
7	F1	31	58% 100%
7	f	31	90% 100%
7	f1	31	71% 100%
8	H	67	84% 97%
8	H1	67	78% 99%
8	h	67	88% 99%
8	h1	67	84% 100%
9	I	35	57% 100%
9	I1	35	71% 100%

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Mol	Chain	Length	Quality of chain
9	i	35	60% 100%
9	i1	35	74% 100%
10	J	36	89% 100%
10	J1	36	81% 100%
10	j	36	86% 97%
10	j1	36	81% 100%
11	K	37	81% 97%
11	K1	37	41% 100%
11	k	37	76% 100%
11	k1	37	73% 100%
12	L	38	71% 100%
12	L1	38	79% 97%
12	l	38	74% 97%
13	M	31	87% 100%
13	M1	31	84% 100%
13	m	31	84% 100%
13	m1	31	77% 100%
14	O	238	92% 98%
14	O1	238	67% 98%
14	o	238	94% 98%
14	o1	238	72% 97%
15	P	187	100% 99%
15	P1	187	98% 100%
15	p	187	100% 99%
15	p1	187	99% 100%

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Mol	Chain	Length	Quality of chain
16	T	30	83% 97%
16	T1	30	83% 93% 7%
16	t	30	90% 100%
16	t1	30	80% 100%
17	W	44	95% 100%
17	W1	44	75% 100%
17	w	44	86% 100%
17	w1	44	82% 100%
18	X	30	97% 100%
18	X1	30	57% 100%
18	x	30	100% 100%
18	x1	30	83% 100%
19	Z	61	90% 100%
19	Z1	61	52% 98%
19	z	61	87% 100%
19	z1	61	84% 100%
20	N	222	94% 98%
20	N1	222	37% 99%
20	n	222	89% 99%
20	n1	222	55% 98%
21	G	221	99% 100%
21	G1	221	43% 99%
21	g	221	97% 100%
21	g1	221	62% 100%
22	R	196	97% 99%

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Mol	Chain	Length	Quality of chain
22	R1	196	78% 99%
22	r	196	98% 99%
22	r1	196	78% 99%
23	S	243	88% 99%
23	S1	243	42% 99%
23	s	243	90% 98%
23	s1	243	75% 98%
24	Y	222	83% 99%
24	Y1	222	39% 99%
24	y	222	83% 99%
24	y1	222	66% 100%
25	U	27	96% 96%
25	U1	27	81% 100%
25	u	27	100% 96%
25	u1	27	96% 100%

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
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-
29	CLA	A	410	X	-	-	-
29	CLA	A1	405	X	-	-	-
29	CLA	A1	406	X	-	-	-
29	CLA	A1	407	X	-	-	-
29	CLA	A1	410	X	-	-	-
29	CLA	B	602	X	-	-	-
29	CLA	B	603	X	-	-	-
29	CLA	B	604	X	-	-	-
29	CLA	B	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	606	X	-	-	-
29	CLA	B	607	X	-	-	-
29	CLA	B	608	X	-	-	-
29	CLA	B	609	X	-	-	-
29	CLA	B	610	X	-	-	-
29	CLA	B	611	X	-	-	-
29	CLA	B	612	X	-	-	-
29	CLA	B	613	X	-	-	-
29	CLA	B	614	X	-	-	-
29	CLA	B	615	X	-	-	-
29	CLA	B	616	X	-	-	-
29	CLA	B	617	X	-	-	-
29	CLA	B1	602	X	-	-	-
29	CLA	B1	603	X	-	-	-
29	CLA	B1	604	X	-	-	-
29	CLA	B1	605	X	-	-	-
29	CLA	B1	606	X	-	-	-
29	CLA	B1	607	X	-	-	-
29	CLA	B1	608	X	-	-	-
29	CLA	B1	609	X	-	-	-
29	CLA	B1	610	X	-	-	-
29	CLA	B1	611	X	-	-	-
29	CLA	B1	612	X	-	-	-
29	CLA	B1	613	X	-	-	-
29	CLA	B1	614	X	-	-	-
29	CLA	B1	615	X	-	-	-
29	CLA	B1	616	X	-	-	-
29	CLA	B1	617	X	-	-	-
29	CLA	C	501	X	-	-	-
29	CLA	C	502	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	504	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	506	X	-	-	-
29	CLA	C	507	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	C1	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	C1	502	X	-	-	-
29	CLA	C1	503	X	-	-	-
29	CLA	C1	504	X	-	-	-
29	CLA	C1	505	X	-	-	-
29	CLA	C1	506	X	-	-	-
29	CLA	C1	507	X	-	-	-
29	CLA	C1	508	X	-	-	-
29	CLA	C1	509	X	-	-	-
29	CLA	C1	510	X	-	-	-
29	CLA	C1	511	X	-	-	-
29	CLA	C1	512	X	-	-	-
29	CLA	C1	513	X	-	-	-
29	CLA	D	402	X	-	-	-
29	CLA	D	403	X	-	-	-
29	CLA	D1	402	X	-	-	-
29	CLA	D1	403	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	G1	602	X	-	-	-
29	CLA	G1	603	X	-	-	-
29	CLA	G1	604	X	-	-	-
29	CLA	G1	610	X	-	-	-
29	CLA	G1	611	X	-	-	-
29	CLA	G1	612	X	-	-	-
29	CLA	G1	613	X	-	-	-
29	CLA	G1	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	N1	602	X	-	-	-
29	CLA	N1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	N1	604	X	-	-	-
29	CLA	N1	610	X	-	-	-
29	CLA	N1	611	X	-	-	-
29	CLA	N1	612	X	-	-	-
29	CLA	N1	613	X	-	-	-
29	CLA	N1	614	X	-	-	-
29	CLA	R	602	X	-	-	-
29	CLA	R	603	X	-	-	-
29	CLA	R	604	X	-	-	-
29	CLA	R	608	X	-	-	-
29	CLA	R	609	X	-	-	-
29	CLA	R	610	X	-	-	-
29	CLA	R	612	X	-	-	-
29	CLA	R1	602	X	-	-	-
29	CLA	R1	603	X	-	-	-
29	CLA	R1	604	X	-	-	-
29	CLA	R1	608	X	-	-	-
29	CLA	R1	609	X	-	-	-
29	CLA	R1	610	X	-	-	-
29	CLA	R1	612	X	-	-	-
29	CLA	S	602	X	-	-	-
29	CLA	S	603	X	-	-	-
29	CLA	S	604	X	-	-	-
29	CLA	S	605	X	-	-	-
29	CLA	S	609	X	-	-	-
29	CLA	S	610	X	-	-	-
29	CLA	S	611	X	-	-	-
29	CLA	S	612	X	-	-	-
29	CLA	S	613	X	-	-	-
29	CLA	S	614	X	-	-	-
29	CLA	S	617	X	-	-	-
29	CLA	S1	602	X	-	-	-
29	CLA	S1	603	X	-	-	-
29	CLA	S1	604	X	-	-	-
29	CLA	S1	605	X	-	-	-
29	CLA	S1	609	X	-	-	-
29	CLA	S1	610	X	-	-	-
29	CLA	S1	611	X	-	-	-
29	CLA	S1	612	X	-	-	-
29	CLA	S1	613	X	-	-	-
29	CLA	S1	614	X	-	-	-
29	CLA	S1	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	Y	602	X	-	-	-
29	CLA	Y	603	X	-	-	-
29	CLA	Y	604	X	-	-	-
29	CLA	Y	608	X	-	-	-
29	CLA	Y	610	X	-	-	-
29	CLA	Y	611	X	-	-	-
29	CLA	Y	612	X	-	-	-
29	CLA	Y	613	X	-	-	-
29	CLA	Y	614	X	-	-	-
29	CLA	Y1	602	X	-	-	-
29	CLA	Y1	603	X	-	-	-
29	CLA	Y1	604	X	-	-	-
29	CLA	Y1	608	X	-	-	-
29	CLA	Y1	610	X	-	-	-
29	CLA	Y1	611	X	-	-	-
29	CLA	Y1	612	X	-	-	-
29	CLA	Y1	613	X	-	-	-
29	CLA	Y1	614	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	a	406	X	-	-	-
29	CLA	a	407	X	-	-	-
29	CLA	a	410	X	-	-	-
29	CLA	a1	405	X	-	-	-
29	CLA	a1	406	X	-	-	-
29	CLA	a1	407	X	-	-	-
29	CLA	a1	410	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	605	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	609	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	b	612	X	-	-	-
29	CLA	b	613	X	-	-	-
29	CLA	b	614	X	-	-	-
29	CLA	b	615	X	-	-	-
29	CLA	b	616	X	-	-	-
29	CLA	b	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	b1	602	X	-	-	-
29	CLA	b1	603	X	-	-	-
29	CLA	b1	604	X	-	-	-
29	CLA	b1	605	X	-	-	-
29	CLA	b1	606	X	-	-	-
29	CLA	b1	607	X	-	-	-
29	CLA	b1	608	X	-	-	-
29	CLA	b1	609	X	-	-	-
29	CLA	b1	610	X	-	-	-
29	CLA	b1	611	X	-	-	-
29	CLA	b1	612	X	-	-	-
29	CLA	b1	613	X	-	-	-
29	CLA	b1	614	X	-	-	-
29	CLA	b1	615	X	-	-	-
29	CLA	b1	616	X	-	-	-
29	CLA	b1	617	X	-	-	-
29	CLA	c	501	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	503	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	506	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-
29	CLA	c	511	X	-	-	-
29	CLA	c	512	X	-	-	-
29	CLA	c	513	X	-	-	-
29	CLA	c1	501	X	-	-	-
29	CLA	c1	502	X	-	-	-
29	CLA	c1	503	X	-	-	-
29	CLA	c1	504	X	-	-	-
29	CLA	c1	505	X	-	-	-
29	CLA	c1	506	X	-	-	-
29	CLA	c1	507	X	-	-	-
29	CLA	c1	508	X	-	-	-
29	CLA	c1	509	X	-	-	-
29	CLA	c1	510	X	-	-	-
29	CLA	c1	511	X	-	-	-
29	CLA	c1	512	X	-	-	-
29	CLA	c1	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	d	402	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	d1	402	X	-	-	-
29	CLA	d1	403	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	612	X	-	-	-
29	CLA	g	613	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	g1	602	X	-	-	-
29	CLA	g1	603	X	-	-	-
29	CLA	g1	604	X	-	-	-
29	CLA	g1	610	X	-	-	-
29	CLA	g1	611	X	-	-	-
29	CLA	g1	612	X	-	-	-
29	CLA	g1	613	X	-	-	-
29	CLA	g1	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	612	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	n	614	X	-	-	-
29	CLA	n1	602	X	-	-	-
29	CLA	n1	603	X	-	-	-
29	CLA	n1	604	X	-	-	-
29	CLA	n1	610	X	-	-	-
29	CLA	n1	611	X	-	-	-
29	CLA	n1	612	X	-	-	-
29	CLA	n1	613	X	-	-	-
29	CLA	n1	614	X	-	-	-
29	CLA	r	602	X	-	-	-
29	CLA	r	603	X	-	-	-
29	CLA	r	604	X	-	-	-
29	CLA	r	608	X	-	-	-
29	CLA	r	609	X	-	-	-
29	CLA	r	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	r	612	X	-	-	-
29	CLA	r1	602	X	-	-	-
29	CLA	r1	603	X	-	-	-
29	CLA	r1	604	X	-	-	-
29	CLA	r1	608	X	-	-	-
29	CLA	r1	609	X	-	-	-
29	CLA	r1	610	X	-	-	-
29	CLA	r1	612	X	-	-	-
29	CLA	s	602	X	-	-	-
29	CLA	s	603	X	-	-	-
29	CLA	s	604	X	-	-	-
29	CLA	s	605	X	-	-	-
29	CLA	s	609	X	-	-	-
29	CLA	s	610	X	-	-	-
29	CLA	s	611	X	-	-	-
29	CLA	s	612	X	-	-	-
29	CLA	s	613	X	-	-	-
29	CLA	s	614	X	-	-	-
29	CLA	s	617	X	-	-	-
29	CLA	s1	602	X	-	-	-
29	CLA	s1	603	X	-	-	-
29	CLA	s1	604	X	-	-	-
29	CLA	s1	605	X	-	-	-
29	CLA	s1	609	X	-	-	-
29	CLA	s1	610	X	-	-	-
29	CLA	s1	611	X	-	-	-
29	CLA	s1	612	X	-	-	-
29	CLA	s1	613	X	-	-	-
29	CLA	s1	614	X	-	-	-
29	CLA	s1	617	X	-	-	-
29	CLA	y	602	X	-	-	-
29	CLA	y	603	X	-	-	-
29	CLA	y	604	X	-	-	-
29	CLA	y	608	X	-	-	-
29	CLA	y	610	X	-	-	-
29	CLA	y	611	X	-	-	-
29	CLA	y	612	X	-	-	-
29	CLA	y	613	X	-	-	-
29	CLA	y	614	X	-	-	-
29	CLA	y1	602	X	-	-	-
29	CLA	y1	603	X	-	-	-
29	CLA	y1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	y1	608	X	-	-	-
29	CLA	y1	610	X	-	-	-
29	CLA	y1	611	X	-	-	-
29	CLA	y1	612	X	-	-	-
29	CLA	y1	613	X	-	-	-
29	CLA	y1	614	X	-	-	-
36	C7Z	B	620	X	-	-	-
36	C7Z	B1	620	X	-	-	-
36	C7Z	b	620	X	-	-	-
36	C7Z	b1	620	X	-	-	-
41	LMK	C	527	X	-	-	-
41	LMK	C1	527	X	-	-	-
41	LMK	c	527	X	-	-	-
41	LMK	c1	527	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	H1	101	X	-	-	-
45	RRX	h	101	X	-	-	-
45	RRX	h1	101	X	-	-	-
48	CHL	G	601	X	-	-	-
48	CHL	G	605	X	-	-	-
48	CHL	G	606	X	-	-	-
48	CHL	G	607	X	-	-	-
48	CHL	G	608	X	-	-	-
48	CHL	G	609	X	-	-	-
48	CHL	G1	601	X	-	-	-
48	CHL	G1	605	X	-	-	-
48	CHL	G1	606	X	-	-	-
48	CHL	G1	607	X	-	-	-
48	CHL	G1	608	X	-	-	-
48	CHL	G1	609	X	-	-	-
48	CHL	N	601	X	-	-	-
48	CHL	N	605	X	-	-	-
48	CHL	N	606	X	-	-	-
48	CHL	N	607	X	-	-	-
48	CHL	N	608	X	-	-	-
48	CHL	N	609	X	-	-	-
48	CHL	N1	601	X	-	-	-
48	CHL	N1	605	X	-	-	-
48	CHL	N1	606	X	-	-	-
48	CHL	N1	607	X	-	-	-
48	CHL	N1	608	X	-	-	-
48	CHL	N1	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	R	606	X	-	-	-
48	CHL	R	607	X	-	-	-
48	CHL	R1	606	X	-	-	-
48	CHL	R1	607	X	-	-	-
48	CHL	S	601	X	-	-	-
48	CHL	S	606	X	-	-	-
48	CHL	S	607	X	-	-	-
48	CHL	S	608	X	-	-	-
48	CHL	S1	601	X	-	-	-
48	CHL	S1	606	X	-	-	-
48	CHL	S1	607	X	-	-	-
48	CHL	S1	608	X	-	-	-
48	CHL	Y	601	X	-	-	-
48	CHL	Y	605	X	-	-	-
48	CHL	Y	606	X	-	-	-
48	CHL	Y	607	X	-	-	-
48	CHL	Y	609	X	-	-	-
48	CHL	Y1	601	X	-	-	-
48	CHL	Y1	605	X	-	-	-
48	CHL	Y1	606	X	-	-	-
48	CHL	Y1	607	X	-	-	-
48	CHL	Y1	609	X	-	-	-
48	CHL	g	601	X	-	-	-
48	CHL	g	605	X	-	-	-
48	CHL	g	606	X	-	-	-
48	CHL	g	607	X	-	-	-
48	CHL	g	608	X	-	-	-
48	CHL	g	609	X	-	-	-
48	CHL	g1	601	X	-	-	-
48	CHL	g1	605	X	-	-	-
48	CHL	g1	606	X	-	-	-
48	CHL	g1	607	X	-	-	-
48	CHL	g1	608	X	-	-	-
48	CHL	g1	609	X	-	-	-
48	CHL	n	601	X	-	-	-
48	CHL	n	605	X	-	-	-
48	CHL	n	606	X	-	-	-
48	CHL	n	607	X	-	-	-
48	CHL	n	608	X	-	-	-
48	CHL	n	609	X	-	-	-
48	CHL	n1	601	X	-	-	-
48	CHL	n1	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	n1	606	X	-	-	-
48	CHL	n1	607	X	-	-	-
48	CHL	n1	608	X	-	-	-
48	CHL	n1	609	X	-	-	-
48	CHL	r	606	X	-	-	-
48	CHL	r	607	X	-	-	-
48	CHL	r1	606	X	-	-	-
48	CHL	r1	607	X	-	-	-
48	CHL	s	601	X	-	-	-
48	CHL	s	606	X	-	-	-
48	CHL	s	607	X	-	-	-
48	CHL	s	608	X	-	-	-
48	CHL	s1	601	X	-	-	-
48	CHL	s1	606	X	-	-	-
48	CHL	s1	607	X	-	-	-
48	CHL	s1	608	X	-	-	-
48	CHL	y	601	X	-	-	-
48	CHL	y	605	X	-	-	-
48	CHL	y	606	X	-	-	-
48	CHL	y	607	X	-	-	-
48	CHL	y	609	X	-	-	-
48	CHL	y1	601	X	-	-	-
48	CHL	y1	605	X	-	-	-
48	CHL	y1	606	X	-	-	-
48	CHL	y1	607	X	-	-	-
48	CHL	y1	609	X	-	-	-
49	LUT	G	621	X	-	-	-
49	LUT	R	620	X	-	-	-
49	LUT	n1	621	X	-	-	-
50	XAT	G	622	X	-	-	-
50	XAT	G1	622	X	-	-	-
50	XAT	N	622	X	-	-	-
50	XAT	N1	622	X	-	-	-
50	XAT	Y1	622	X	-	-	-
50	XAT	g	622	X	-	-	-
50	XAT	g1	622	X	-	-	-
50	XAT	n	622	X	-	-	-
50	XAT	r	621	X	-	-	-
50	XAT	r1	621	X	-	-	-
51	NEX	g	623	X	-	-	-
51	NEX	g1	623	X	-	-	-
53	ERG	R	626	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	ERG	R1	626	X	-	-	-
53	ERG	r	626	X	-	-	-
53	ERG	r1	626	X	-	-	-

## 2 Entry composition i

There are 55 unique types of molecules in this entry. The entry contains 152240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	336	2638	1721	432	468	17	1	0
1	a	336	2638	1721	432	468	17	1	0
1	A1	336	2638	1721	432	468	17	1	0
1	a1	336	2638	1721	432	468	17	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	484	3783	2480	630	663	10	0	0
2	b	484	3783	2480	630	663	10	0	0
2	B1	484	3783	2480	630	663	10	0	0
2	b1	484	3783	2480	630	663	10	0	0

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	V	32	227	152	37	38	0	0
3	v	32	227	152	37	38	0	0
3	V1	32	227	152	37	38	0	0
3	v1	32	227	152	37	38	0	0

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	C1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	D1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		
6	E1	76	Total	C	N	O	0	0
			621	404	102	115		
6	e1	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	F1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	f1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	H1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

- Molecule 10 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		
10	j	36	Total	C	N	O	0	0
			266	183	40	43		
10	J1	36	Total	C	N	O	0	0
			266	183	40	43		
10	j1	36	Total	C	N	O	0	0
			266	183	40	43		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	L1	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		
13	M1	31	Total	C	N	O	0	0
			234	159	33	42		
13	m1	31	Total	C	N	O	0	0
			234	159	33	42		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	O1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	x1	30	201	132	32	37	0	0

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	61	457	312	68	76	1	0	0
19	z	61	457	312	68	76	1	0	0
19	Z1	61	457	312	68	76	1	0	0
19	z1	61	457	312	68	76	1	0	0

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	222	1703	1100	277	321	5	0	0
20	n	222	1703	1100	277	321	5	0	0
20	N1	222	1703	1100	277	321	5	0	0
20	n1	222	1703	1100	277	321	5	0	0

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	221	1680	1085	271	321	3	0	0
21	g	221	1680	1085	271	321	3	0	0
21	G1	221	1680	1085	271	321	3	0	0
21	g1	221	1680	1085	271	321	3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7
G1	180	ALA	PRO	conflict	UNP A1XKU7
g1	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
22	R	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

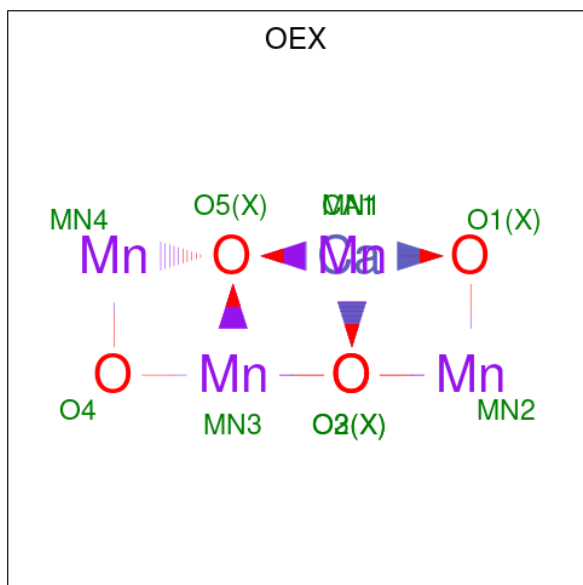
- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	U1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	A1	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	a1	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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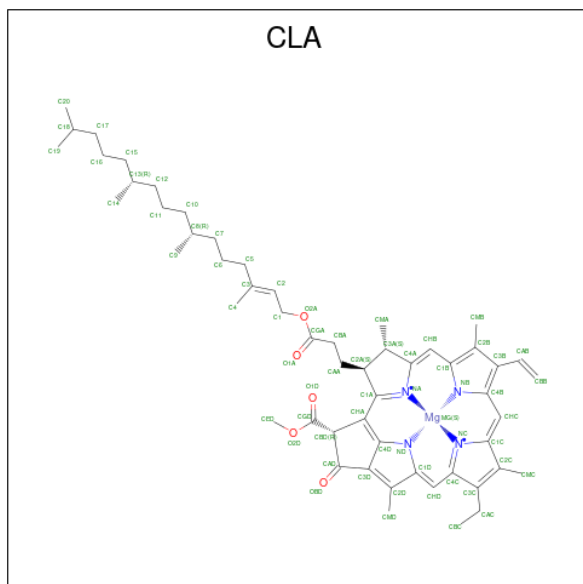
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Mol	Chain	Residues	Atoms	AltConf
27	A1	1	Total Fe 1 1	0
27	a1	1	Total Fe 1 1	0

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
28	A	2	Total Cl 2 2	0
28	a	2	Total Cl 2 2	0
28	A1	2	Total Cl 2 2	0
28	a1	2	Total Cl 2 2	0

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C Mg N O 65 55 1 4 5	0
29	A	1	Total C Mg N O 65 55 1 4 5	0
29	A	1	Total C Mg N O 50 40 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	A	1	60	50	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	B	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	C	1	65	55	1	4	5	0
29	D	1	65	55	1	4	5	0
29	D	1	65	55	1	4	5	0
29	N	1	65	55	1	4	5	0
29	N	1	65	55	1	4	5	0
29	N	1	65	55	1	4	5	0
29	N	1	65	55	1	4	5	0
29	N	1	49	39	1	4	5	0
29	N	1	45	35	1	4	5	0
29	N	1	65	55	1	4	5	0
29	N	1	49	39	1	4	5	0
29	G	1	65	55	1	4	5	0
29	G	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	G	1	49	39	1	4	5	0
29	G	1	65	55	1	4	5	0
29	G	1	65	55	1	4	5	0
29	G	1	43	35	1	4	3	0
29	G	1	65	55	1	4	5	0
29	G	1	49	39	1	4	5	0
29	R	1	60	50	1	4	5	0
29	R	1	60	50	1	4	5	0
29	R	1	49	39	1	4	5	0
29	R	1	60	50	1	4	5	0
29	R	1	60	50	1	4	5	0
29	R	1	60	50	1	4	5	0
29	R	1	60	50	1	4	5	0
29	R	1	60	50	1	4	5	0
29	S	1	60	50	1	4	5	0
29	S	1	65	55	1	4	5	0
29	S	1	55	45	1	4	5	0
29	S	1	50	40	1	4	5	0
29	S	1	60	50	1	4	5	0
29	S	1	65	55	1	4	5	0
29	S	1	65	55	1	4	5	0
29	S	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	S	1	55	45	1	4	5	0
29	S	1	55	45	1	4	5	0
29	S	1	50	40	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	50	40	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	Y	1	65	55	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	65	55	1	4	5	0
29	a	1	49	39	1	4	5	0
29	a	1	60	50	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	b	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	c	1	65	55	1	4	5	0
29	d	1	65	55	1	4	5	0
29	d	1	65	55	1	4	5	0
29	n	1	65	55	1	4	5	0
29	n	1	65	55	1	4	5	0
29	n	1	65	55	1	4	5	0
29	n	1	65	55	1	4	5	0
29	n	1	49	39	1	4	5	0
29	n	1	45	35	1	4	5	0
29	n	1	65	55	1	4	5	0
29	n	1	49	39	1	4	5	0
29	g	1	65	55	1	4	5	0
29	g	1	65	55	1	4	5	0
29	g	1	49	39	1	4	5	0
29	g	1	65	55	1	4	5	0
29	g	1	65	55	1	4	5	0
29	g	1	43	35	1	4	3	0
29	g	1	65	55	1	4	5	0
29	g	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	r	1	60	50	1	4	5	0
29	r	1	60	50	1	4	5	0
29	r	1	49	39	1	4	5	0
29	r	1	60	50	1	4	5	0
29	r	1	60	50	1	4	5	0
29	r	1	60	50	1	4	5	0
29	r	1	60	50	1	4	5	0
29	r	1	60	50	1	4	5	0
29	s	1	60	50	1	4	5	0
29	s	1	65	55	1	4	5	0
29	s	1	55	45	1	4	5	0
29	s	1	50	40	1	4	5	0
29	s	1	60	50	1	4	5	0
29	s	1	65	55	1	4	5	0
29	s	1	65	55	1	4	5	0
29	s	1	45	35	1	4	5	0
29	s	1	55	45	1	4	5	0
29	s	1	55	45	1	4	5	0
29	s	1	50	40	1	4	5	0
29	y	1	65	55	1	4	5	0
29	y	1	65	55	1	4	5	0
29	y	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	B1	1	65	55	1	4	5	0
29	B1	1	65	55	1	4	5	0
29	B1	1	65	55	1	4	5	0
29	B1	1	65	55	1	4	5	0
29	B1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	C1	1	65	55	1	4	5	0
29	D1	1	65	55	1	4	5	0
29	D1	1	65	55	1	4	5	0
29	N1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	N1	1	65	55	1	4	5	0
29	N1	1	65	55	1	4	5	0
29	N1	1	65	55	1	4	5	0
29	N1	1	49	39	1	4	5	0
29	N1	1	45	35	1	4	5	0
29	N1	1	65	55	1	4	5	0
29	N1	1	49	39	1	4	5	0
29	G1	1	65	55	1	4	5	0
29	G1	1	65	55	1	4	5	0
29	G1	1	49	39	1	4	5	0
29	G1	1	65	55	1	4	5	0
29	G1	1	65	55	1	4	5	0
29	G1	1	43	35	1	4	3	0
29	G1	1	65	55	1	4	5	0
29	G1	1	49	39	1	4	5	0
29	R1	1	60	50	1	4	5	0
29	R1	1	60	50	1	4	5	0
29	R1	1	49	39	1	4	5	0
29	R1	1	60	50	1	4	5	0
29	R1	1	60	50	1	4	5	0
29	R1	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	R1	1	60	50	1	4	5	0
29	S1	1	60	50	1	4	5	0
29	S1	1	65	55	1	4	5	0
29	S1	1	55	45	1	4	5	0
29	S1	1	50	40	1	4	5	0
29	S1	1	60	50	1	4	5	0
29	S1	1	65	55	1	4	5	0
29	S1	1	65	55	1	4	5	0
29	S1	1	45	35	1	4	5	0
29	S1	1	55	45	1	4	5	0
29	S1	1	55	45	1	4	5	0
29	S1	1	50	40	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	50	40	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	65	55	1	4	5	0
29	Y1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	a1	1	65	55	1	4	5	0
29	a1	1	65	55	1	4	5	0
29	a1	1	49	39	1	4	5	0
29	a1	1	60	50	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	b1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	c1	1	65	55	1	4	5	0
29	d1	1	65	55	1	4	5	0
29	d1	1	65	55	1	4	5	0
29	n1	1	65	55	1	4	5	0
29	n1	1	65	55	1	4	5	0
29	n1	1	65	55	1	4	5	0
29	n1	1	65	55	1	4	5	0
29	n1	1	49	39	1	4	5	0
29	n1	1	45	35	1	4	5	0
29	n1	1	65	55	1	4	5	0

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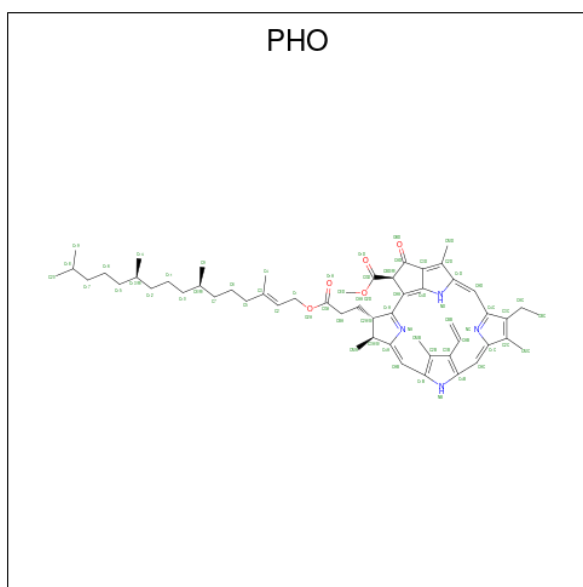
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	n1	1	49	39	1	4	5	0
29	g1	1	65	55	1	4	5	0
29	g1	1	65	55	1	4	5	0
29	g1	1	49	39	1	4	5	0
29	g1	1	65	55	1	4	5	0
29	g1	1	65	55	1	4	5	0
29	g1	1	43	35	1	4	3	0
29	g1	1	65	55	1	4	5	0
29	g1	1	49	39	1	4	5	0
29	r1	1	60	50	1	4	5	0
29	r1	1	60	50	1	4	5	0
29	r1	1	49	39	1	4	5	0
29	r1	1	60	50	1	4	5	0
29	r1	1	60	50	1	4	5	0
29	r1	1	60	50	1	4	5	0
29	r1	1	60	50	1	4	5	0
29	s1	1	60	50	1	4	5	0
29	s1	1	65	55	1	4	5	0
29	s1	1	55	45	1	4	5	0
29	s1	1	50	40	1	4	5	0
29	s1	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
29	s1	1	65	55	1	4	5	0
29	s1	1	65	55	1	4	5	0
29	s1	1	45	35	1	4	5	0
29	s1	1	55	45	1	4	5	0
29	s1	1	55	45	1	4	5	0
29	s1	1	50	40	1	4	5	0
29	y1	1	65	55	1	4	5	0
29	y1	1	65	55	1	4	5	0
29	y1	1	65	55	1	4	5	0
29	y1	1	50	40	1	4	5	0
29	y1	1	65	55	1	4	5	0
29	y1	1	65	55	1	4	5	0
29	y1	1	65	55	1	4	5	0
29	y1	1	65	55	1	4	5	0
29	y1	1	65	55	1	4	5	0

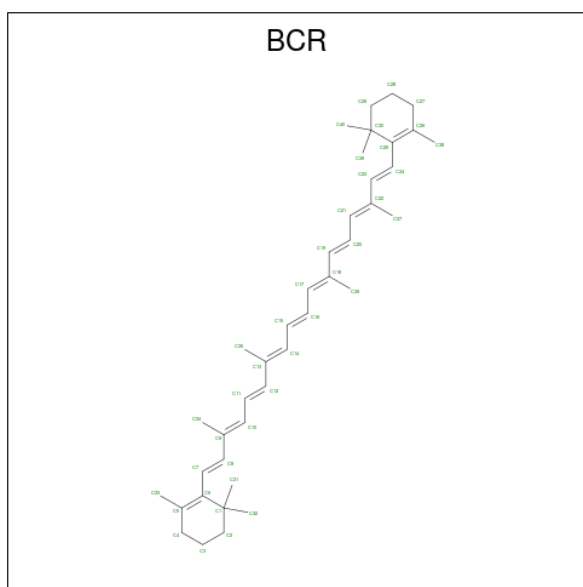
- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	A1	1	Total	C	N	O	0
			64	55	4	5	
30	A1	1	Total	C	N	O	0
			64	55	4	5	
30	a1	1	Total	C	N	O	0
			64	55	4	5	
30	a1	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).





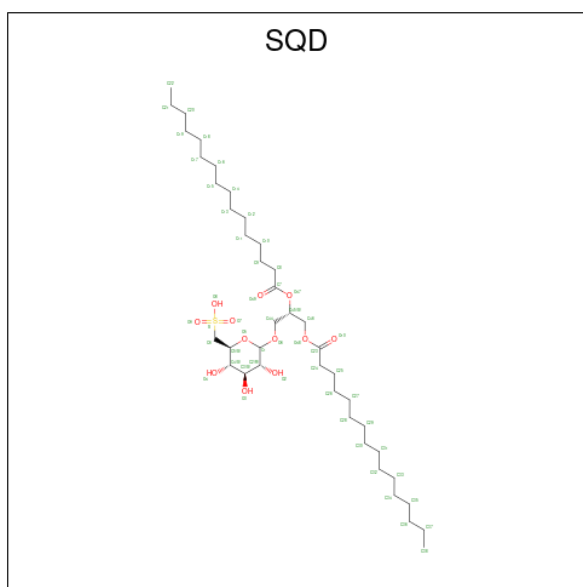
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	A1	1	Total C 40 40	0
31	B1	1	Total C 40 40	0
31	B1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	D1	1	Total C 40 40	0
31	a1	1	Total C 40 40	0
31	b1	1	Total C 40 40	0
31	b1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	d1	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



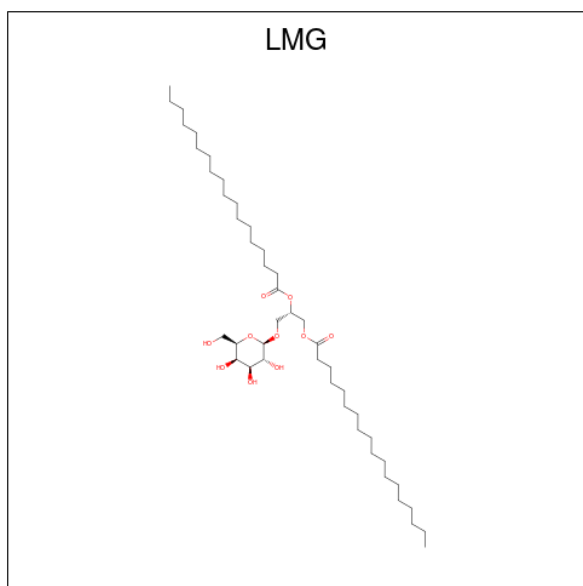
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	A	1	51	38	12	1	0
32	B	1	42	29	12	1	0
32	B	1	54	41	12	1	0
32	C	1	54	41	12	1	0
32	M	1	42	29	12	1	0
32	a	1	51	38	12	1	0
32	b	1	42	29	12	1	0
32	b	1	54	41	12	1	0
32	c	1	54	41	12	1	0
32	m	1	42	29	12	1	0
32	A1	1	51	38	12	1	0
32	B1	1	42	29	12	1	0
32	B1	1	54	41	12	1	0
32	C1	1	54	41	12	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	M1	1	Total 42	C 29	O 12	S 1	0
32	a1	1	Total 51	C 38	O 12	S 1	0
32	b1	1	Total 42	C 29	O 12	S 1	0
32	b1	1	Total 54	C 41	O 12	S 1	0
32	c1	1	Total 54	C 41	O 12	S 1	0
32	m1	1	Total 42	C 29	O 12	S 1	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	A	1	Total 48	C 38	O 10	0
33	B	1	Total 44	C 34	O 10	0
33	C	1	Total 51	C 41	O 10	0
33	C	1	Total 55	C 45	O 10	0
33	D	1	Total 46	C 36	O 10	0

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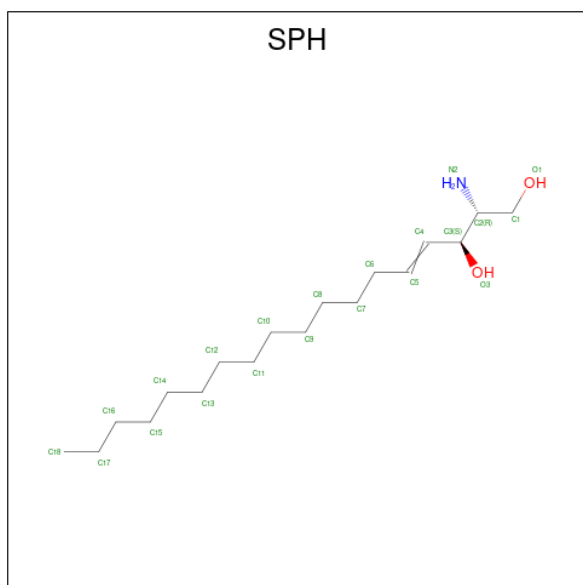
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	H	1	48	38	10	0
33	W	1	39	29	10	0
33	a	1	48	38	10	0
33	b	1	44	34	10	0
33	c	1	51	41	10	0
33	c	1	55	45	10	0
33	d	1	46	36	10	0
33	h	1	48	38	10	0
33	w	1	39	29	10	0
33	A1	1	48	38	10	0
33	B1	1	44	34	10	0
33	C1	1	51	41	10	0
33	C1	1	55	45	10	0
33	D1	1	46	36	10	0
33	H1	1	48	38	10	0
33	W1	1	39	29	10	0
33	a1	1	48	38	10	0
33	b1	1	44	34	10	0
33	c1	1	51	41	10	0
33	c1	1	55	45	10	0
33	d1	1	46	36	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	h1	1	48	38	10	0
33	w1	1	39	29	10	0

- Molecule 34 is SPHINGOSINE (three-letter code: SPH) (formula:  $C_{18}H_{37}NO_2$ ).

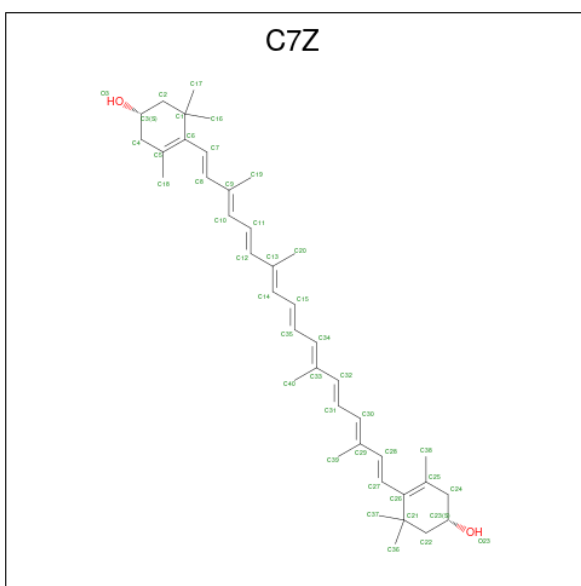


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
34	A	1	21	18	1	2	0
34	Y	1	21	18	1	2	0
34	a	1	21	18	1	2	0
34	y	1	21	18	1	2	0
34	A1	1	21	18	1	2	0
34	Y1	1	21	18	1	2	0
34	a1	1	21	18	1	2	0
34	y1	1	21	18	1	2	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

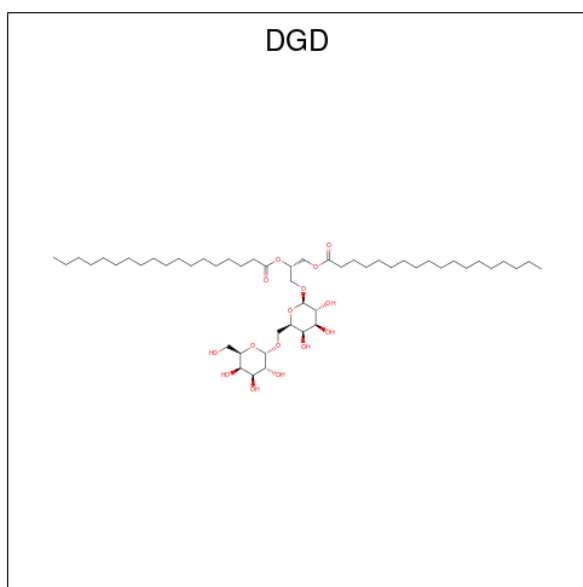
Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Na	0
			1	1	
35	a	1	Total	Na	0
			1	1	
35	A1	1	Total	Na	0
			1	1	
35	a1	1	Total	Na	0
			1	1	

- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]oc tadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	
36	B1	1	Total	C	O	0
			42	40	2	
36	b1	1	Total	C	O	0
			42	40	2	

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	B	1	43	28	15	0
37	C	1	55	40	15	0
37	C	1	62	47	15	0
37	C	1	59	44	15	0
37	b	1	43	28	15	0
37	c	1	55	40	15	0
37	c	1	62	47	15	0
37	c	1	59	44	15	0
37	B1	1	43	28	15	0
37	C1	1	55	40	15	0
37	C1	1	62	47	15	0
37	C1	1	59	44	15	0
37	b1	1	43	28	15	0
37	c1	1	55	40	15	0

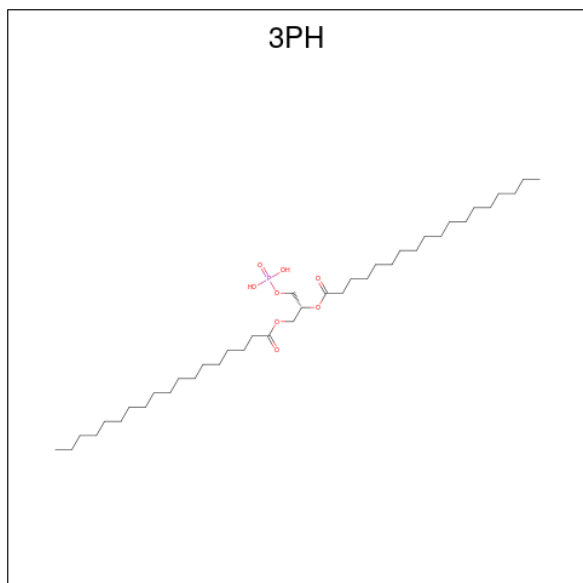
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
37	c1	1	62	47	15	0
37	c1	1	59	44	15	0

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



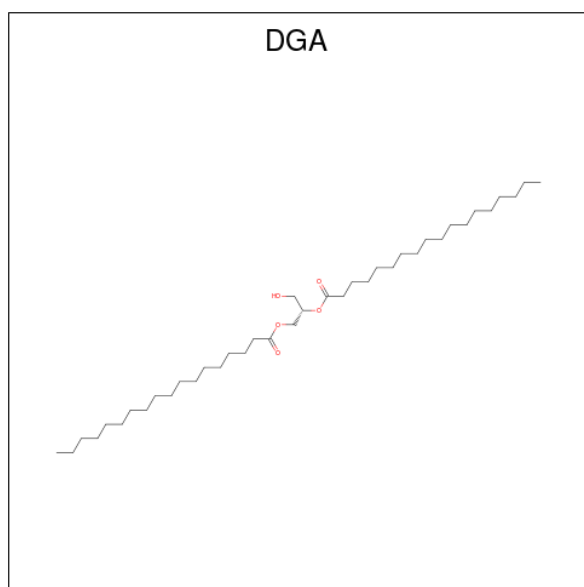
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
38	B	1	48	39	8	1	0
38	T	1	48	39	8	1	0
38	S	1	48	39	8	1	0
38	b	1	48	39	8	1	0
38	t	1	48	39	8	1	0
38	s	1	48	39	8	1	0
38	B1	1	48	39	8	1	0
38	T1	1	48	39	8	1	0
38	S1	1	48	39	8	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
38	b1	1	48	39	8	1	0
38	t1	1	48	39	8	1	0
38	s1	1	48	39	8	1	0

- Molecule 39 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



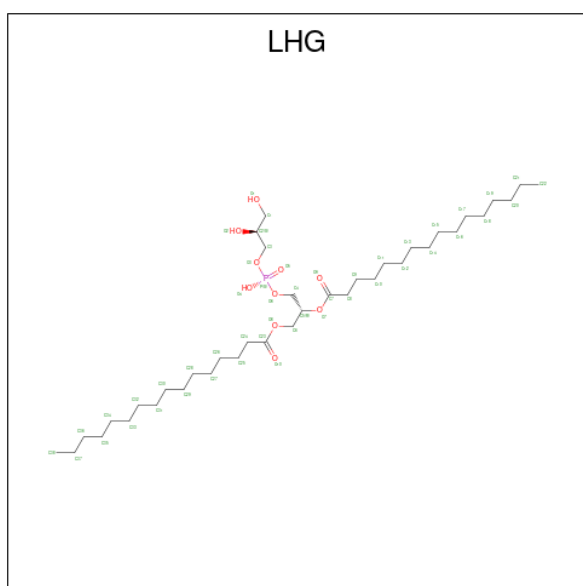
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	B	1	44	39	5	0
39	C	1	44	39	5	0
39	J	1	29	24	5	0
39	b	1	44	39	5	0
39	c	1	44	39	5	0
39	j	1	29	24	5	0
39	B1	1	44	39	5	0
39	C1	1	44	39	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	J1	1	29	24	5	0
39	b1	1	44	39	5	0
39	c1	1	44	39	5	0
39	j1	1	29	24	5	0

- Molecule 40 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	C	1	47	36	10	1	0
40	D	1	44	33	10	1	0
40	D	1	49	38	10	1	0
40	D	1	39	28	10	1	0
40	L	1	49	38	10	1	0
40	N	1	49	38	10	1	0
40	G	1	49	38	10	1	0

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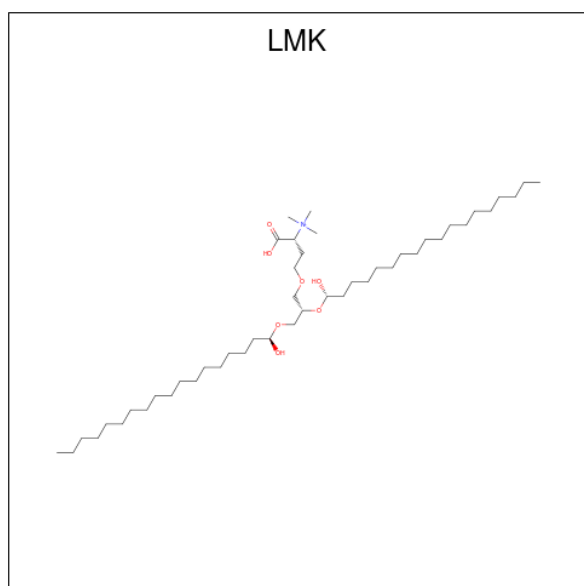
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	S	1	45	34	10	1	0
40	Y	1	49	38	10	1	0
40	c	1	47	36	10	1	0
40	d	1	44	33	10	1	0
40	d	1	49	38	10	1	0
40	d	1	39	28	10	1	0
40	l	1	49	38	10	1	0
40	n	1	49	38	10	1	0
40	g	1	49	38	10	1	0
40	s	1	45	34	10	1	0
40	y	1	49	38	10	1	0
40	C1	1	47	36	10	1	0
40	D1	1	44	33	10	1	0
40	D1	1	49	38	10	1	0
40	D1	1	39	28	10	1	0
40	L1	1	49	38	10	1	0
40	N1	1	49	38	10	1	0
40	G1	1	49	38	10	1	0
40	S1	1	45	34	10	1	0
40	Y1	1	49	38	10	1	0
40	c1	1	47	36	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
40	d1	1	Total 44	C 33	O 10	P 1	0
40	d1	1	Total 49	C 38	O 10	P 1	0
40	d1	1	Total 39	C 28	O 10	P 1	0
40	n1	1	Total 49	C 38	O 10	P 1	0
40	g1	1	Total 49	C 38	O 10	P 1	0
40	s1	1	Total 45	C 34	O 10	P 1	0
40	y1	1	Total 49	C 38	O 10	P 1	0

- Molecule 41 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxido-nyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (three-letter code: LMK) (formula: C<sub>46</sub>H<sub>94</sub>NO<sub>7</sub>).



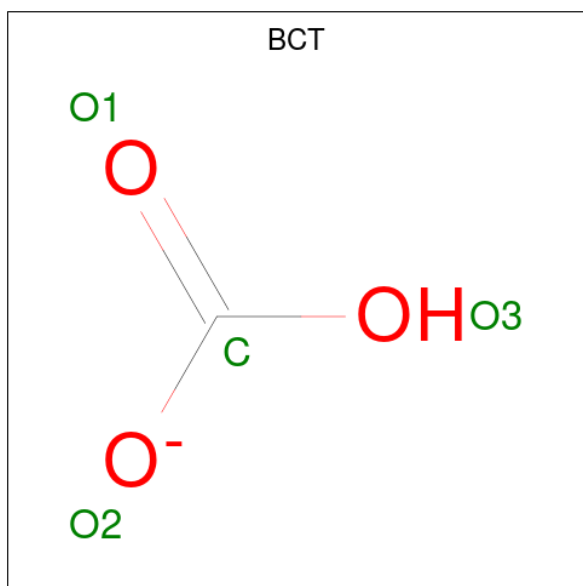
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
41	C	1	Total 40	C 32	N 1	O 7	0
41	c	1	Total 40	C 32	N 1	O 7	0
41	C1	1	Total 40	C 32	N 1	O 7	0

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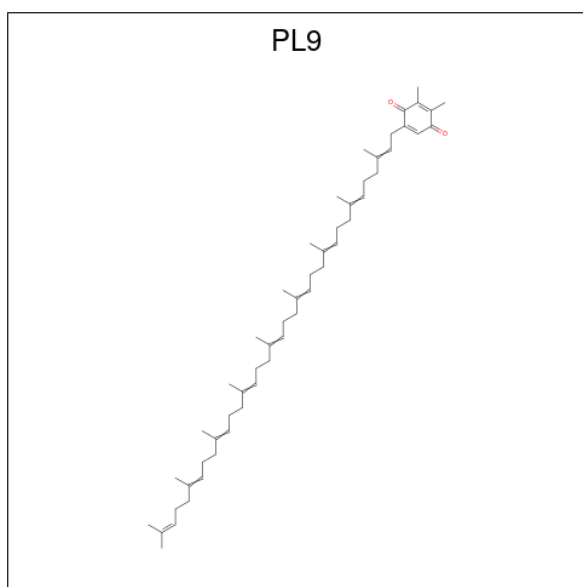
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
41	c1	1	40	32	1	7	0

- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



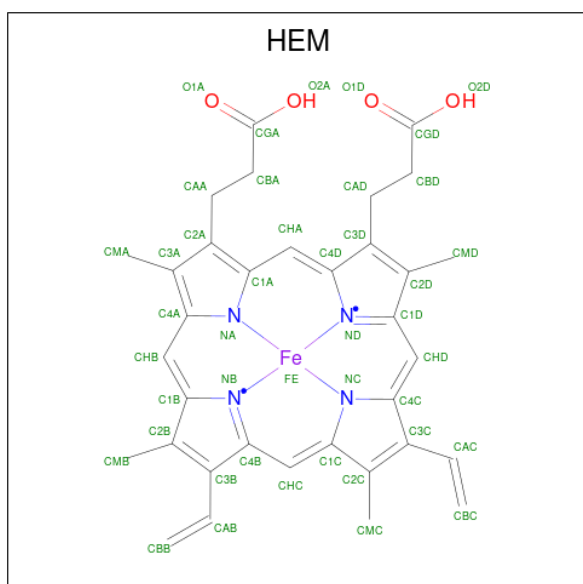
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	D	1	4	1	3	0
42	d	1	4	1	3	0
42	D1	1	4	1	3	0
42	d1	1	4	1	3	0

- Molecule 43 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



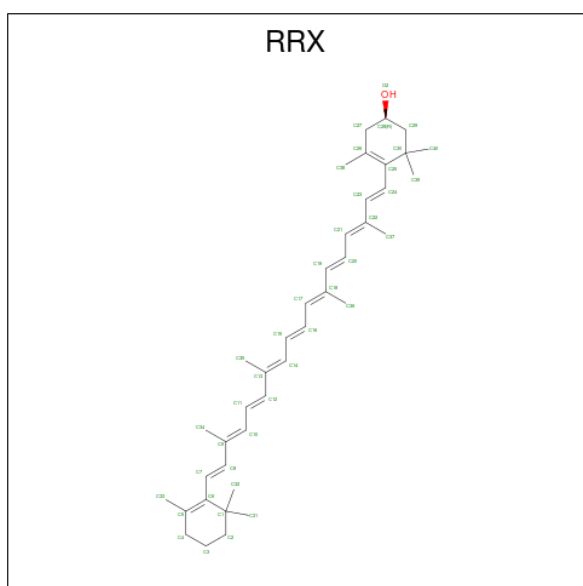
Mol	Chain	Residues	Atoms			AltConf
43	D	1	Total	C	O	0
			55	53	2	
43	d	1	Total	C	O	0
			55	53	2	
43	D1	1	Total	C	O	0
			55	53	2	
43	d1	1	Total	C	O	0
			55	53	2	

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				AltConf	
44	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	F1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms		AltConf
45	H	1	Total	C O	0
			41	40 1	
45	h	1	Total	C O	0
			41	40 1	
45	H1	1	Total	C O	0
			41	40 1	
45	h1	1	Total	C O	0
			41	40 1	

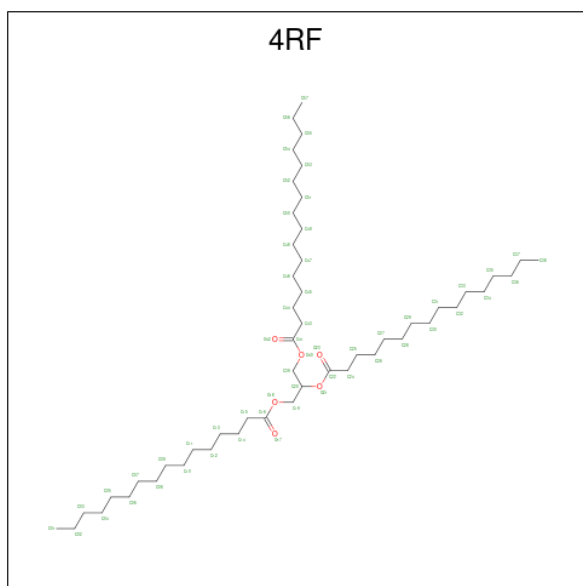
- Molecule 46 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	C	O	0
			6	3	3	
46	I1	1	Total	C	O	0
			6	3	3	

- Molecule 47 is Tripalmitoylglycerol (three-letter code: 4RF) (formula:  $C_{51}H_{98}O_6$ ).



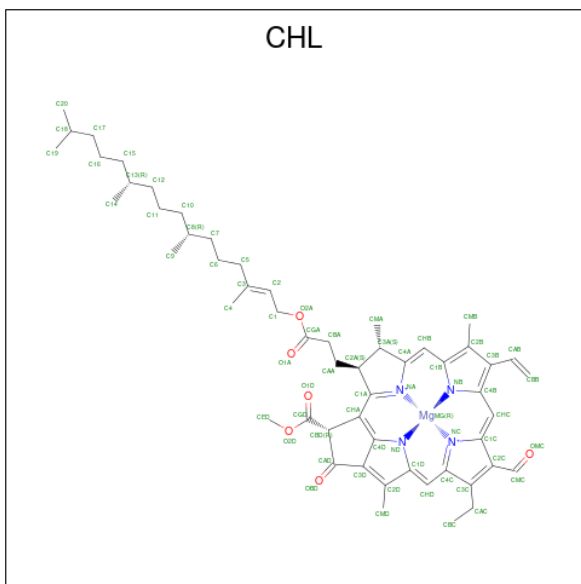
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	C	O	0
			57	51	6	
47	K	1	Total	C	O	0
			57	51	6	

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Mol	Chain	Residues	Atoms			AltConf
47	i	1	Total	C	O	0
			57	51	6	
47	k	1	Total	C	O	0
			57	51	6	
47	I1	1	Total	C	O	0
			57	51	6	
47	K1	1	Total	C	O	0
			57	51	6	
47	i1	1	Total	C	O	0
			57	51	6	
47	k1	1	Total	C	O	0
			57	51	6	

- Molecule 48 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



Mol	Chain	Residues	Atoms				AltConf	
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	N	1	66	55	1	4	6	0
48	G	1	66	55	1	4	6	0
48	G	1	48	37	1	4	6	0
48	G	1	50	39	1	4	6	0
48	G	1	66	55	1	4	6	0
48	G	1	44	35	1	4	4	0
48	G	1	66	55	1	4	6	0
48	R	1	44	35	1	4	4	0
48	R	1	50	39	1	4	6	0
48	S	1	46	35	1	4	6	0
48	S	1	44	35	1	4	4	0
48	S	1	43	34	1	4	4	0
48	S	1	61	50	1	4	6	0
48	Y	1	66	55	1	4	6	0
48	Y	1	46	35	1	4	6	0
48	Y	1	66	55	1	4	6	0
48	Y	1	66	55	1	4	6	0
48	Y	1	66	55	1	4	6	0
48	n	1	66	55	1	4	6	0
48	n	1	66	55	1	4	6	0
48	n	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	n	1	66	55	1	4	6	0
48	n	1	50	39	1	4	6	0
48	n	1	66	55	1	4	6	0
48	g	1	66	55	1	4	6	0
48	g	1	48	37	1	4	6	0
48	g	1	50	39	1	4	6	0
48	g	1	66	55	1	4	6	0
48	g	1	44	35	1	4	4	0
48	g	1	66	55	1	4	6	0
48	r	1	44	35	1	4	4	0
48	r	1	50	39	1	4	6	0
48	s	1	46	35	1	4	6	0
48	s	1	44	35	1	4	4	0
48	s	1	43	34	1	4	4	0
48	s	1	61	50	1	4	6	0
48	y	1	66	55	1	4	6	0
48	y	1	46	35	1	4	6	0
48	y	1	66	55	1	4	6	0
48	y	1	66	55	1	4	6	0
48	y	1	66	55	1	4	6	0
48	N1	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	N1	1	66	55	1	4	6	0
48	N1	1	66	55	1	4	6	0
48	N1	1	66	55	1	4	6	0
48	N1	1	50	39	1	4	6	0
48	N1	1	66	55	1	4	6	0
48	G1	1	66	55	1	4	6	0
48	G1	1	48	37	1	4	6	0
48	G1	1	50	39	1	4	6	0
48	G1	1	66	55	1	4	6	0
48	G1	1	44	35	1	4	4	0
48	G1	1	66	55	1	4	6	0
48	R1	1	44	35	1	4	4	0
48	R1	1	50	39	1	4	6	0
48	S1	1	46	35	1	4	6	0
48	S1	1	44	35	1	4	4	0
48	S1	1	43	34	1	4	4	0
48	S1	1	61	50	1	4	6	0
48	Y1	1	66	55	1	4	6	0
48	Y1	1	46	35	1	4	6	0
48	Y1	1	66	55	1	4	6	0
48	Y1	1	66	55	1	4	6	0

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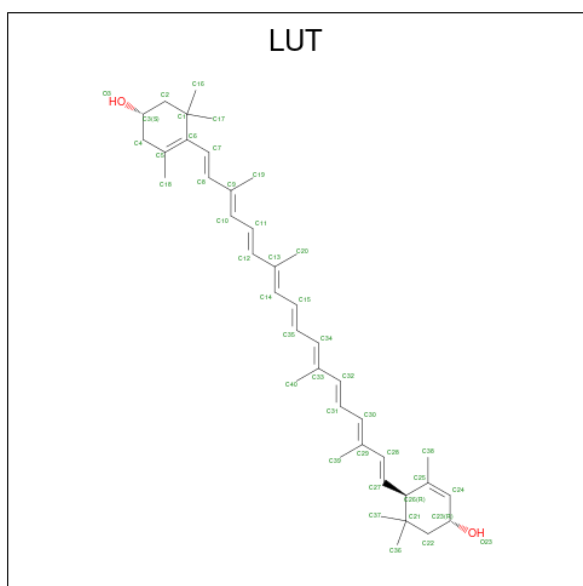
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	Y1	1	66	55	1	4	6	0
48	n1	1	66	55	1	4	6	0
48	n1	1	66	55	1	4	6	0
48	n1	1	66	55	1	4	6	0
48	n1	1	66	55	1	4	6	0
48	n1	1	50	39	1	4	6	0
48	n1	1	66	55	1	4	6	0
48	g1	1	66	55	1	4	6	0
48	g1	1	48	37	1	4	6	0
48	g1	1	50	39	1	4	6	0
48	g1	1	66	55	1	4	6	0
48	g1	1	44	35	1	4	4	0
48	g1	1	66	55	1	4	6	0
48	r1	1	44	35	1	4	4	0
48	r1	1	50	39	1	4	6	0
48	s1	1	46	35	1	4	6	0
48	s1	1	44	35	1	4	4	0
48	s1	1	43	34	1	4	4	0
48	s1	1	61	50	1	4	6	0
48	y1	1	66	55	1	4	6	0
48	y1	1	46	35	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 49 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
49	N	1	Total	C	O	0
			42	40	2	
49	N	1	Total	C	O	0
			42	40	2	
49	G	1	Total	C	O	0
			42	40	2	
49	G	1	Total	C	O	0
			42	40	2	
49	R	1	Total	C	O	0
			42	40	2	
49	S	1	Total	C	O	0
			42	40	2	
49	S	1	Total	C	O	0
			42	40	2	
49	Y	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
49	Y	1	42	40	2	0
49	n	1	42	40	2	0
49	n	1	42	40	2	0
49	g	1	42	40	2	0
49	g	1	42	40	2	0
49	r	1	42	40	2	0
49	s	1	42	40	2	0
49	s	1	42	40	2	0
49	y	1	42	40	2	0
49	y	1	42	40	2	0
49	N1	1	42	40	2	0
49	N1	1	42	40	2	0
49	G1	1	42	40	2	0
49	G1	1	42	40	2	0
49	R1	1	42	40	2	0
49	S1	1	42	40	2	0
49	S1	1	42	40	2	0
49	Y1	1	42	40	2	0
49	Y1	1	42	40	2	0
49	n1	1	42	40	2	0
49	n1	1	42	40	2	0

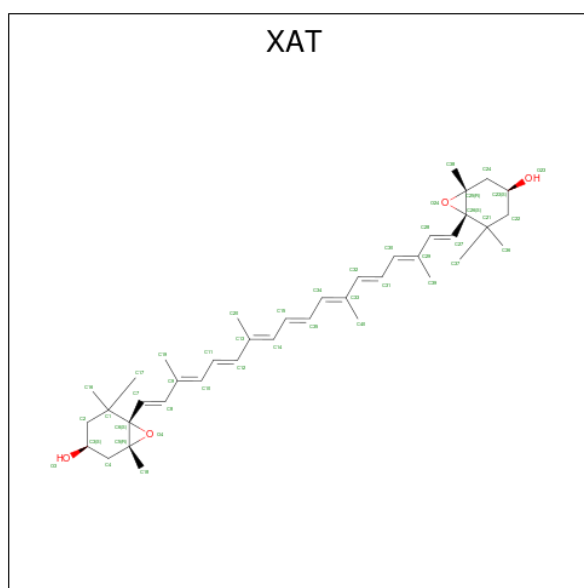
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Mol	Chain	Residues	Atoms			AltConf
49	g1	1	Total	C	O	0
			42	40	2	
49	g1	1	Total	C	O	0
			42	40	2	
49	r1	1	Total	C	O	0
			42	40	2	
49	s1	1	Total	C	O	0
			42	40	2	
49	s1	1	Total	C	O	0
			42	40	2	
49	y1	1	Total	C	O	0
			42	40	2	
49	y1	1	Total	C	O	0
			42	40	2	

- Molecule 50 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 (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



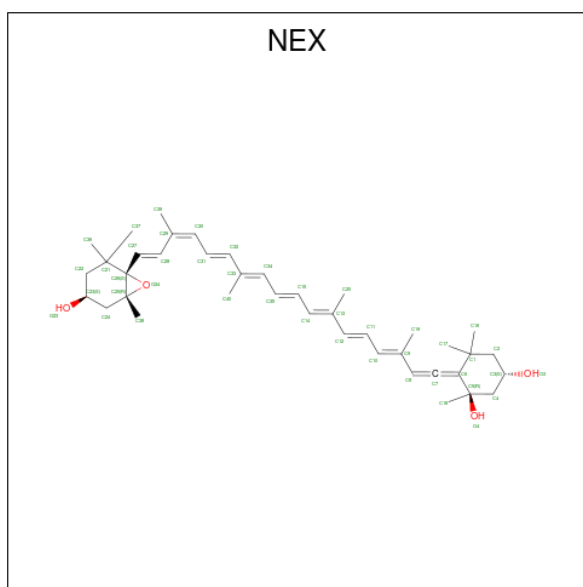
Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			44	40	4	
50	G	1	Total	C	O	0
			44	40	4	
50	R	1	Total	C	O	0
			44	40	4	
50	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	n	1	44	40	4	0
50	g	1	44	40	4	0
50	r	1	44	40	4	0
50	y	1	44	40	4	0
50	N1	1	44	40	4	0
50	G1	1	44	40	4	0
50	R1	1	44	40	4	0
50	Y1	1	44	40	4	0
50	n1	1	44	40	4	0
50	g1	1	44	40	4	0
50	r1	1	44	40	4	0
50	y1	1	44	40	4	0

- Molecule 51 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 (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



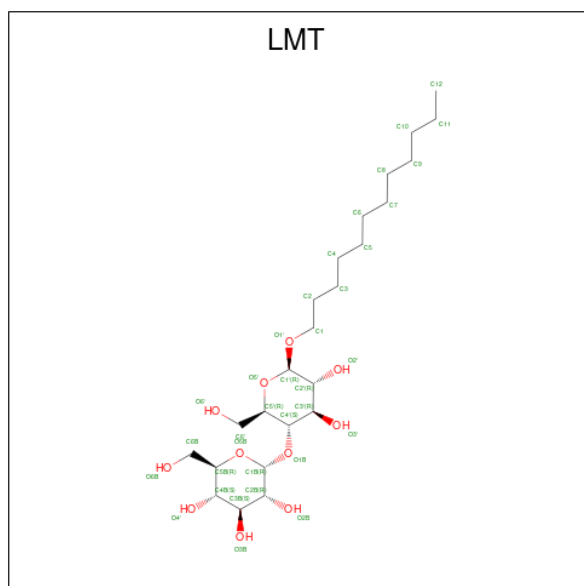
Mol	Chain	Residues	Atoms			AltConf
51	N	1	Total	C	O	0
			44	40	4	
51	G	1	Total	C	O	0
			44	40	4	
51	R	1	Total	C	O	0
			44	40	4	
51	S	1	Total	C	O	0
			44	40	4	
51	Y	1	Total	C	O	0
			44	40	4	
51	n	1	Total	C	O	0
			44	40	4	
51	g	1	Total	C	O	0
			44	40	4	
51	r	1	Total	C	O	0
			44	40	4	
51	s	1	Total	C	O	0
			44	40	4	
51	y	1	Total	C	O	0
			44	40	4	
51	N1	1	Total	C	O	0
			44	40	4	
51	G1	1	Total	C	O	0
			44	40	4	
51	R1	1	Total	C	O	0
			44	40	4	
51	S1	1	Total	C	O	0
			44	40	4	

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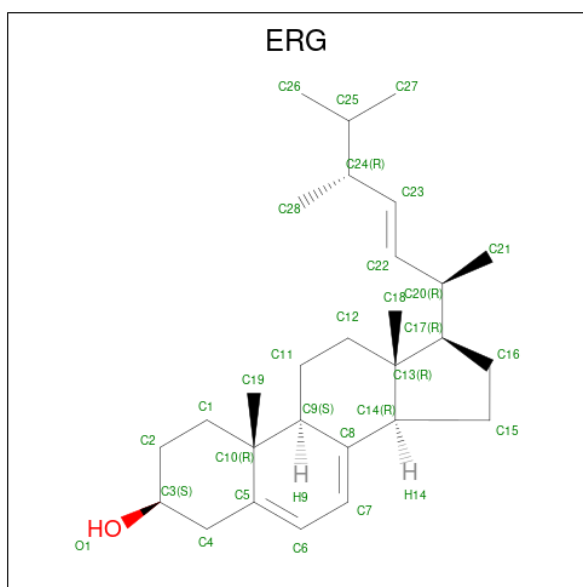
Mol	Chain	Residues	Atoms			AltConf
51	Y1	1	Total	C	O	0
			44	40	4	
51	n1	1	Total	C	O	0
			44	40	4	
51	g1	1	Total	C	O	0
			44	40	4	
51	r1	1	Total	C	O	0
			44	40	4	
51	s1	1	Total	C	O	0
			44	40	4	
51	y1	1	Total	C	O	0
			44	40	4	

- Molecule 52 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



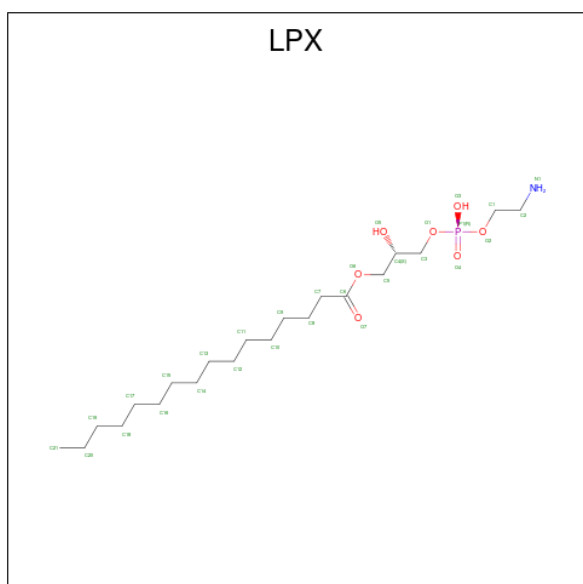
Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			35	24	11	
52	r	1	Total	C	O	0
			35	24	11	
52	R1	1	Total	C	O	0
			35	24	11	
52	r1	1	Total	C	O	0
			35	24	11	

- Molecule 53 is ERGOSTEROL (three-letter code: ERG) (formula:  $C_{28}H_{44}O$ ).



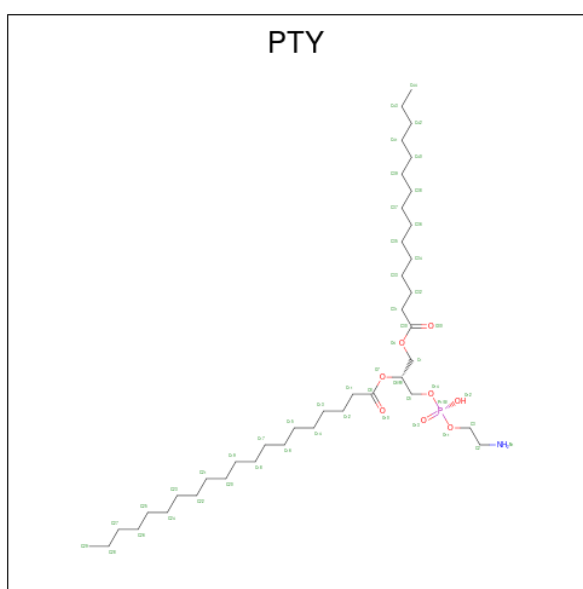
Mol	Chain	Residues	Atoms			AltConf
53	R	1	Total	C	O	0
			29	28	1	
53	r	1	Total	C	O	0
			29	28	1	
53	R1	1	Total	C	O	0
			29	28	1	
53	r1	1	Total	C	O	0
			29	28	1	

- Molecule 54 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C<sub>21</sub>H<sub>44</sub>NO<sub>7</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	S	1	Total 30	C 21	N 1	O 7	P 1	0
54	s	1	Total 30	C 21	N 1	O 7	P 1	0
54	S1	1	Total 30	C 21	N 1	O 7	P 1	0
54	s1	1	Total 30	C 21	N 1	O 7	P 1	0

- Molecule 55 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	Y	1	Total 50	C 40	N 1	O 8	P 1	0
55	Y	1	Total 19	C 9	N 1	O 8	P 1	0
55	y	1	Total 50	C 40	N 1	O 8	P 1	0
55	y	1	Total 19	C 9	N 1	O 8	P 1	0
55	Y1	1	Total 50	C 40	N 1	O 8	P 1	0
55	Y1	1	Total 19	C 9	N 1	O 8	P 1	0
55	y1	1	Total 50	C 40	N 1	O 8	P 1	0

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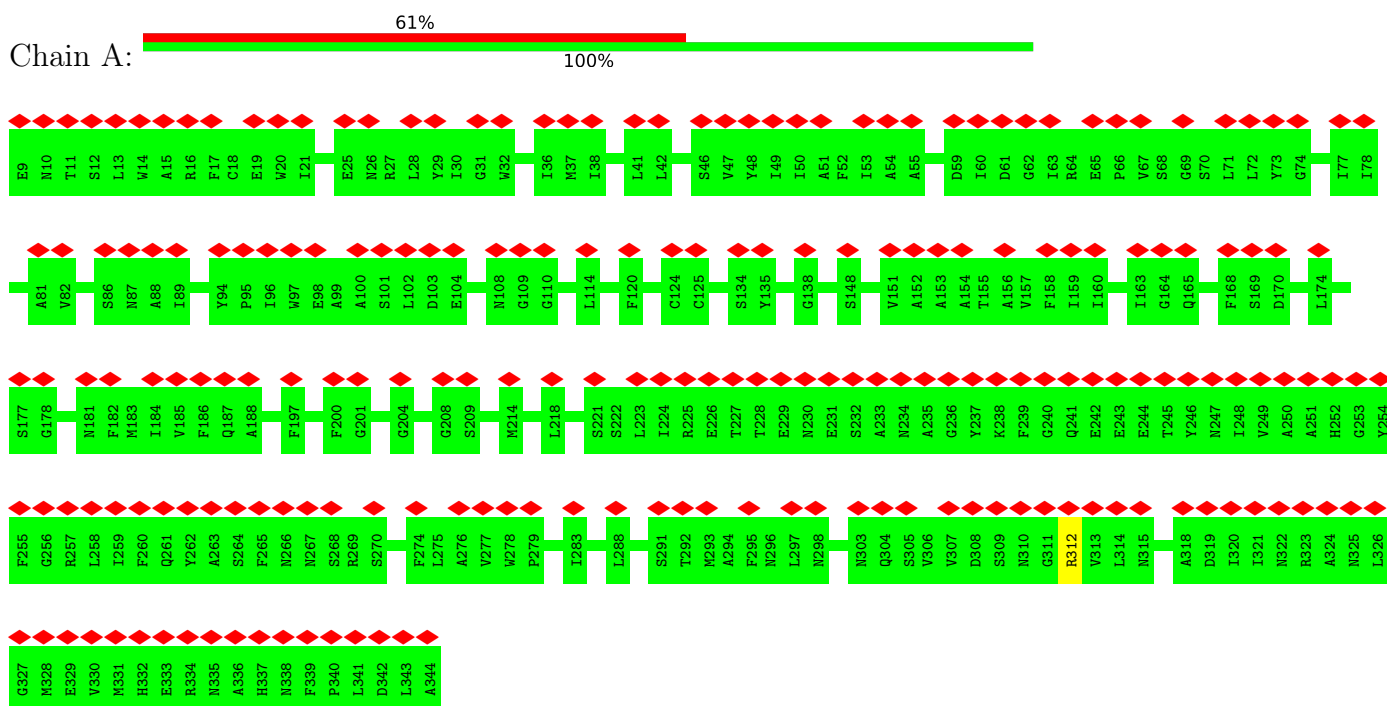
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	y1	1	19	9	1	8	1	0

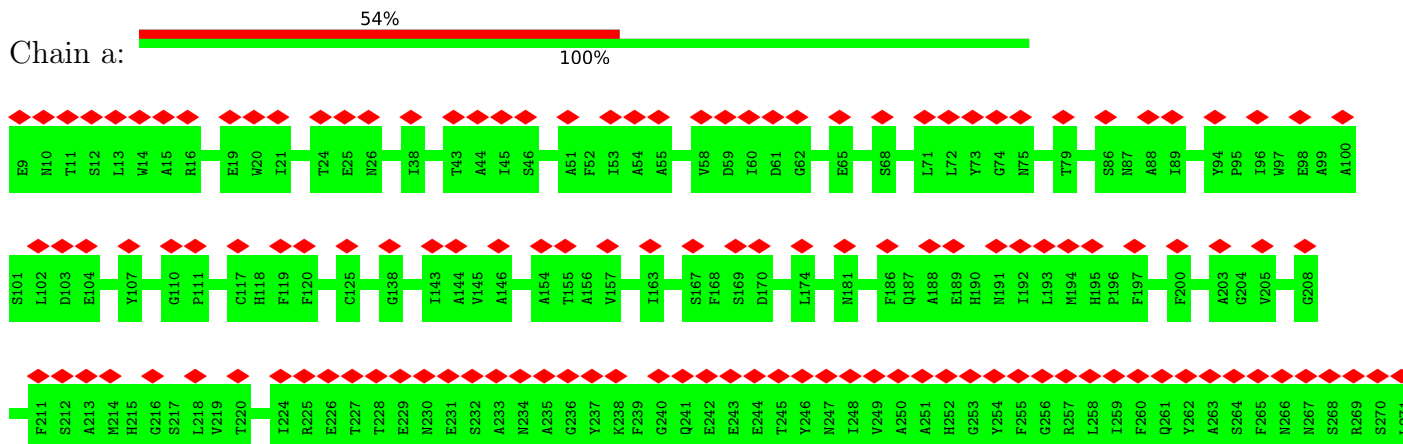
### 3 Residue-property plots

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

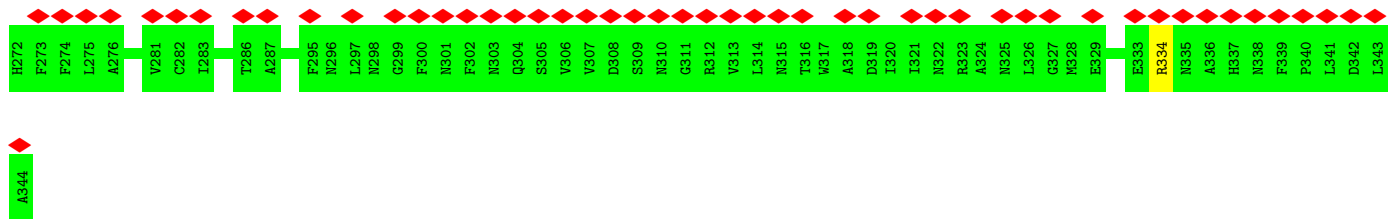
- Molecule 1: Photosystem II protein D1



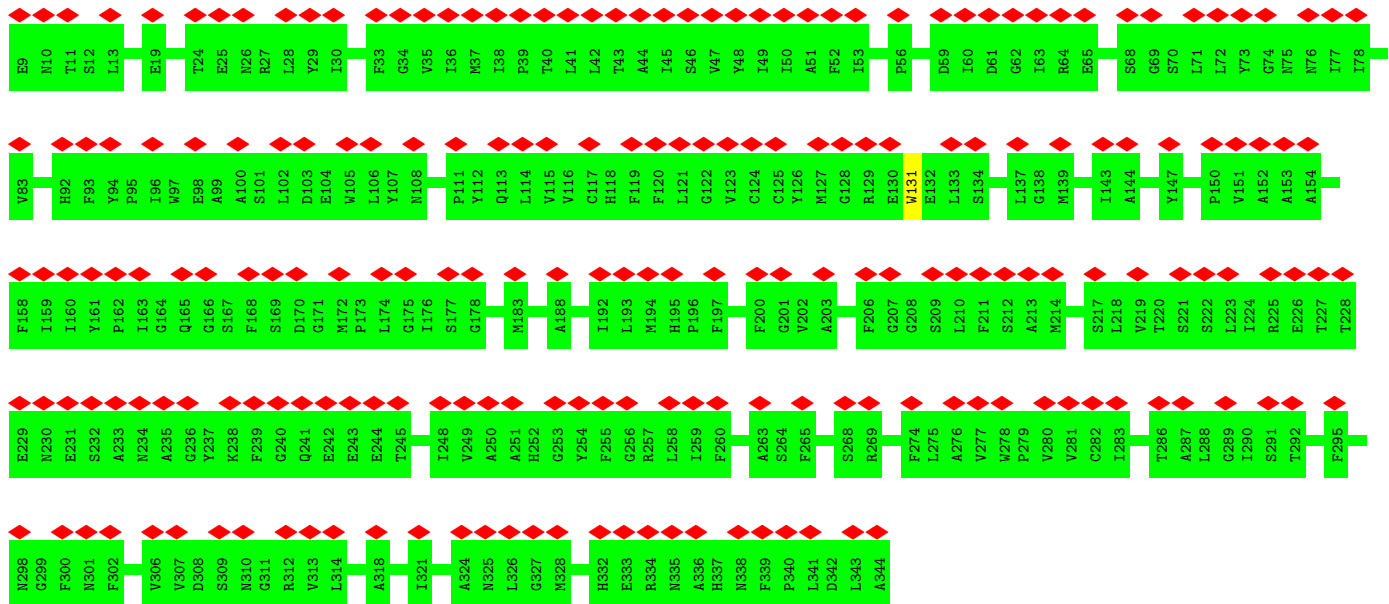
- Molecule 1: Photosystem II protein D1



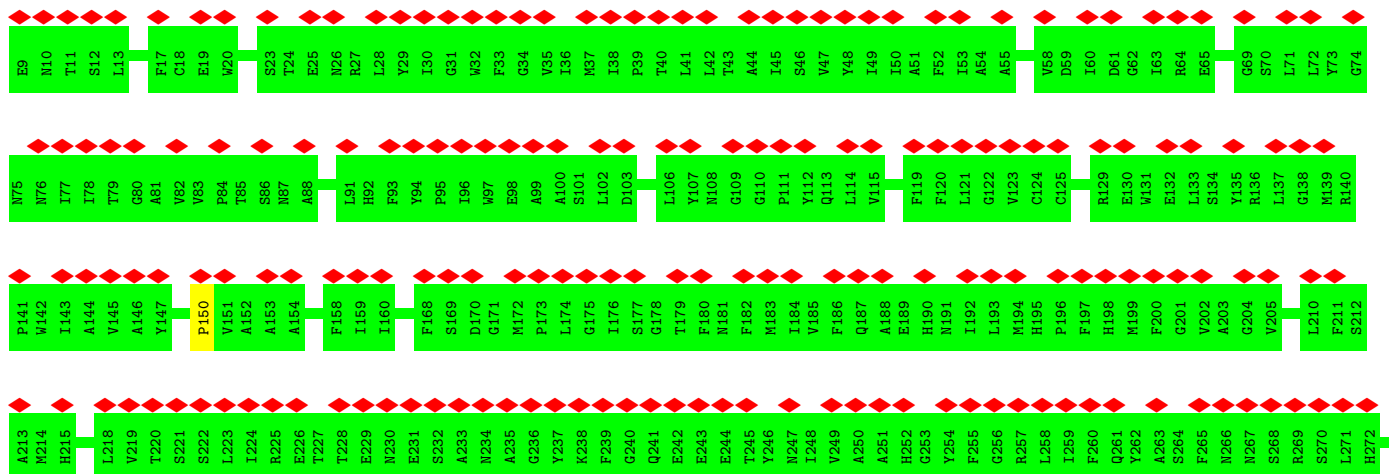


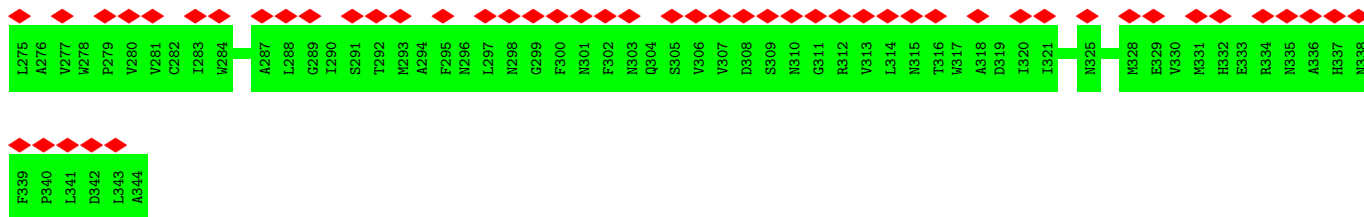


• Molecule 1: Photosystem II protein D1

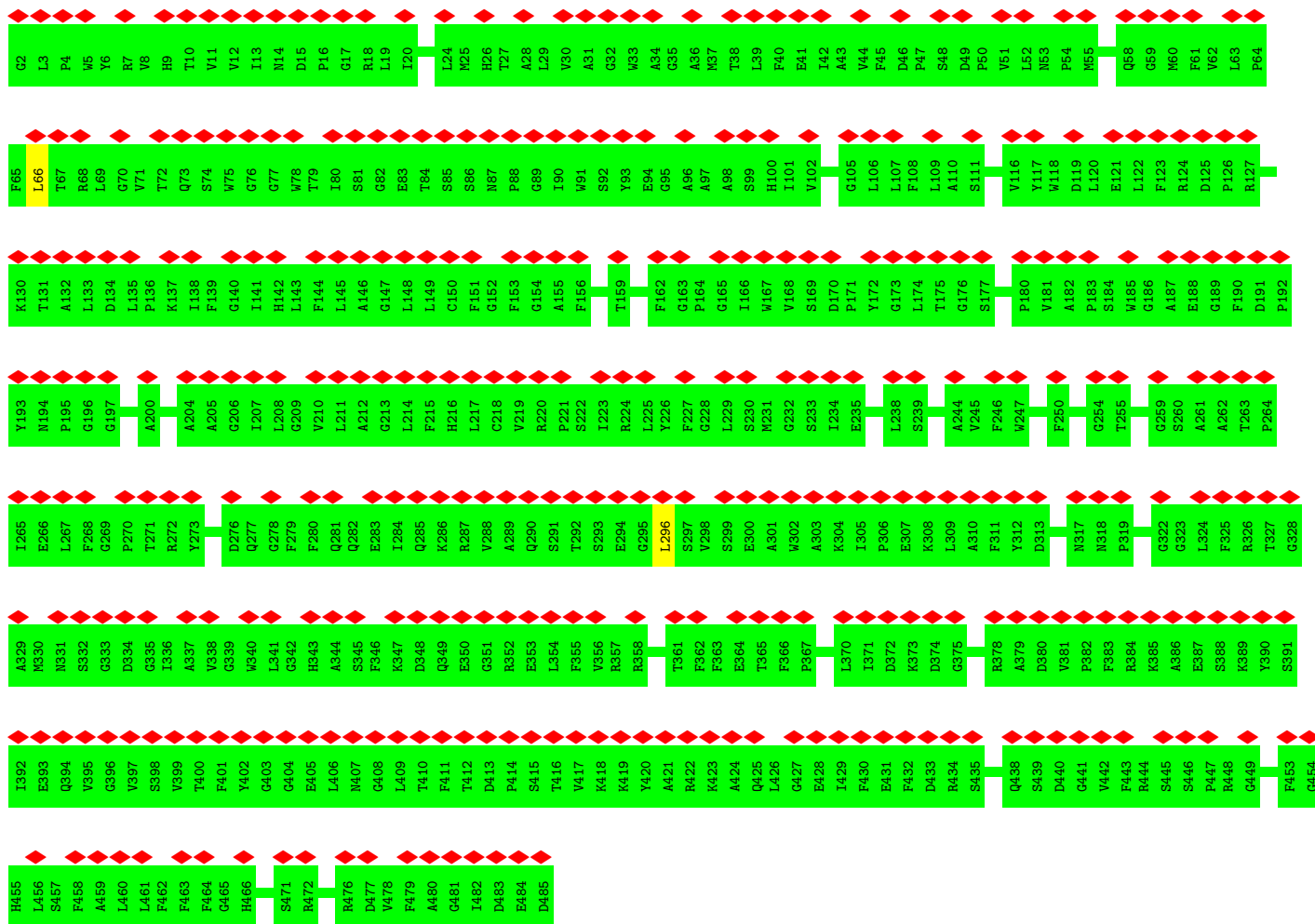
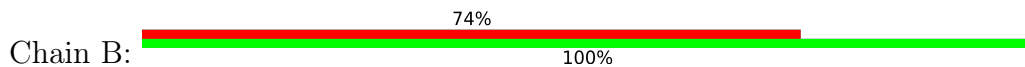


• Molecule 1: Photosystem II protein D1

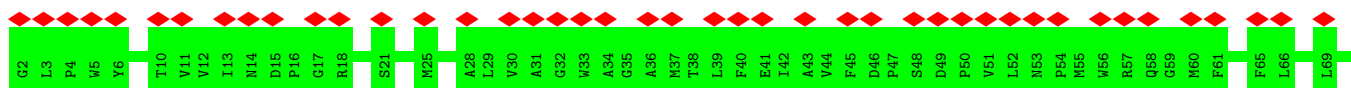


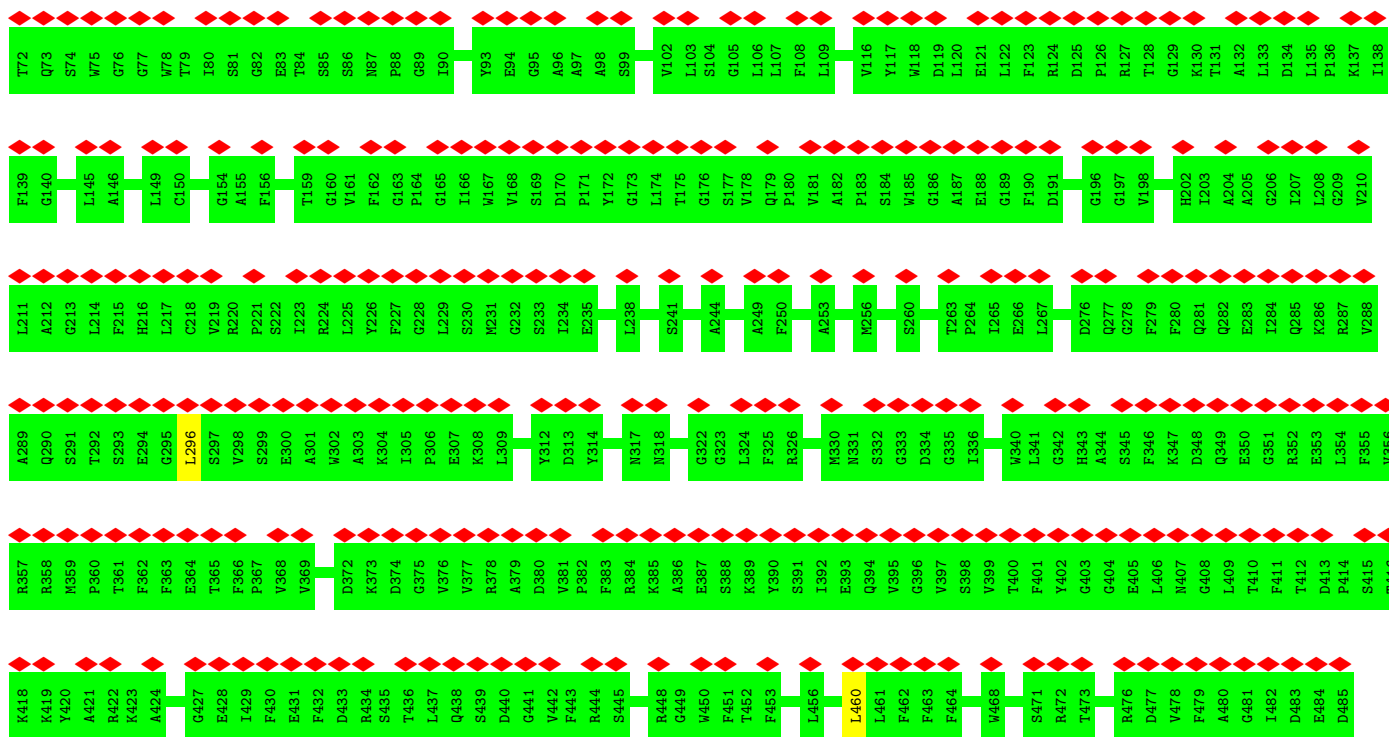


• Molecule 2: Photosystem II CP47 reaction center protein

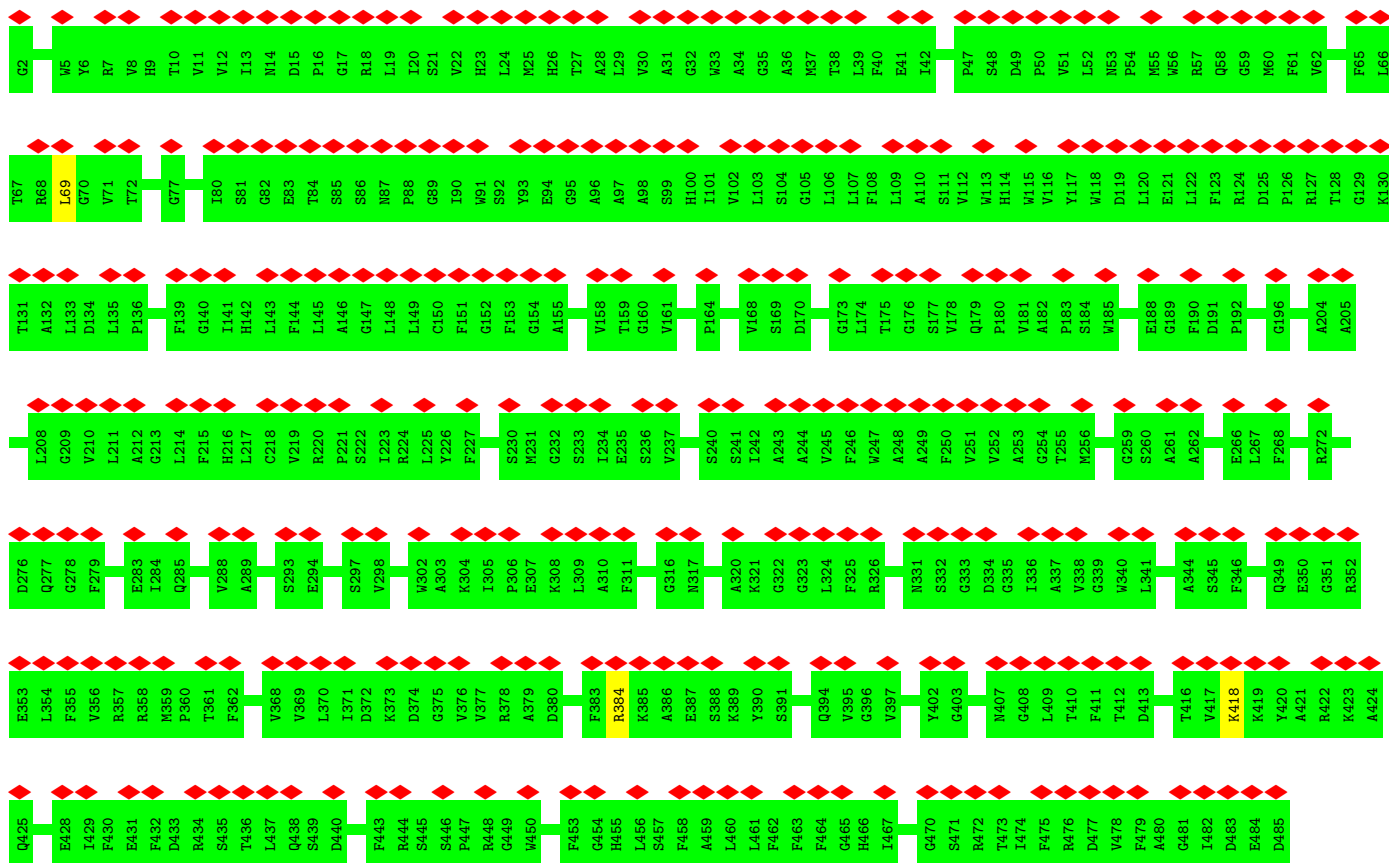


• Molecule 2: Photosystem II CP47 reaction center protein

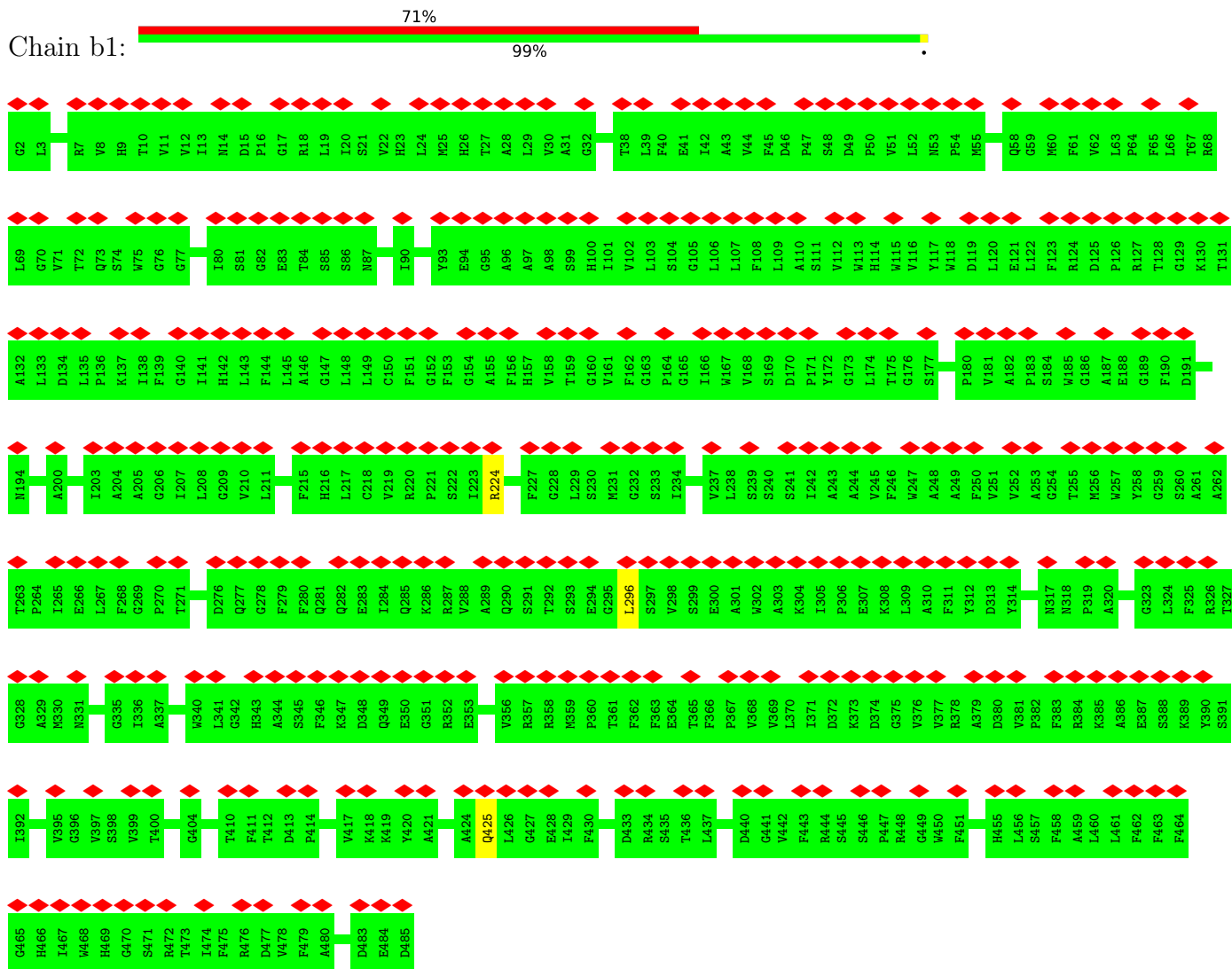




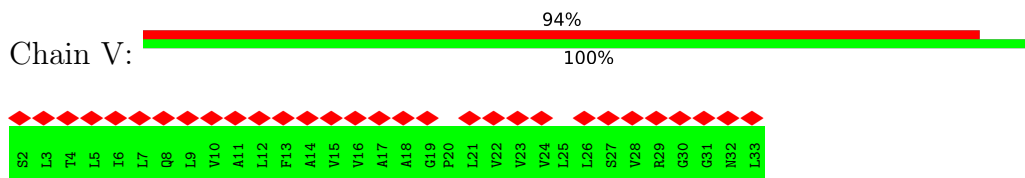
• Molecule 2: Photosystem II CP47 reaction center protein



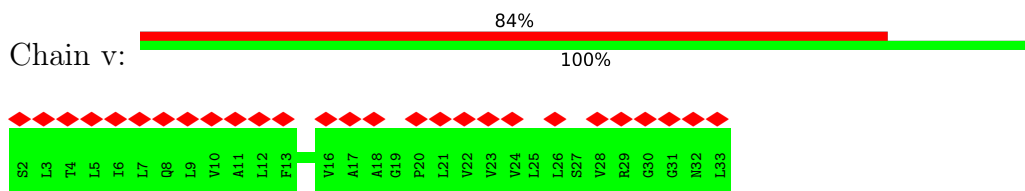
• Molecule 2: Photosystem II CP47 reaction center protein



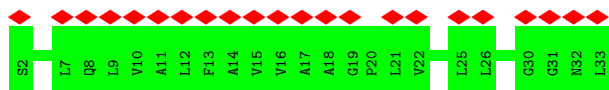
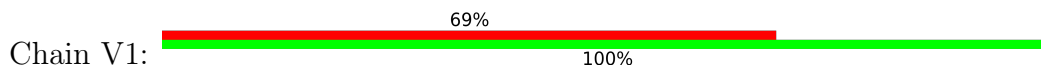
• Molecule 3: Photosystem II reaction center protein Ycf12



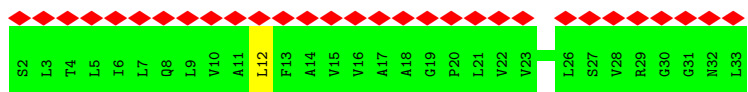
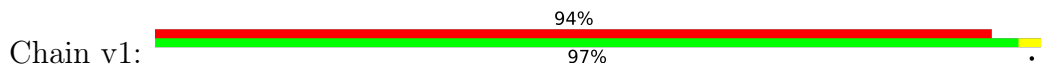
• Molecule 3: Photosystem II reaction center protein Ycf12



• Molecule 3: Photosystem II reaction center protein Ycf12



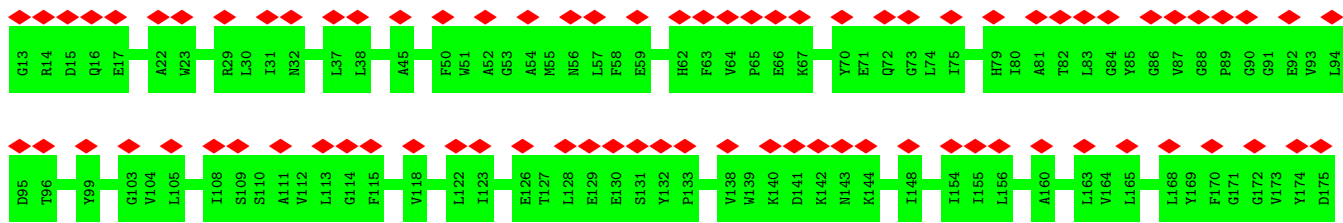
• Molecule 3: Photosystem II reaction center protein Ycf12

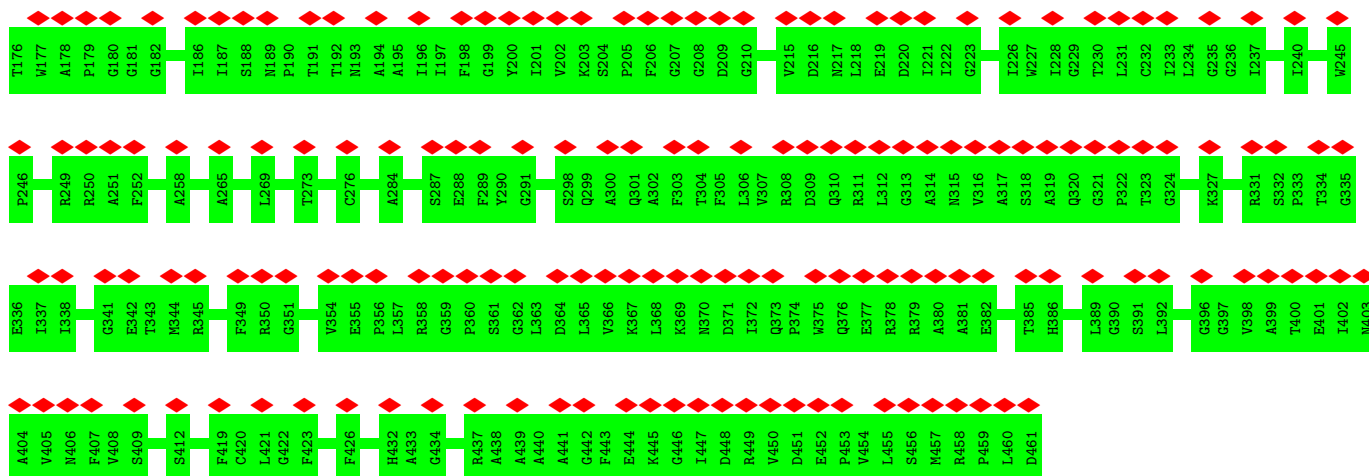


• Molecule 4: Photosystem II CP43 reaction center protein

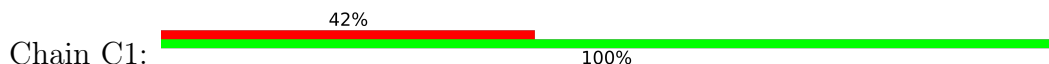


• Molecule 4: Photosystem II CP43 reaction center protein

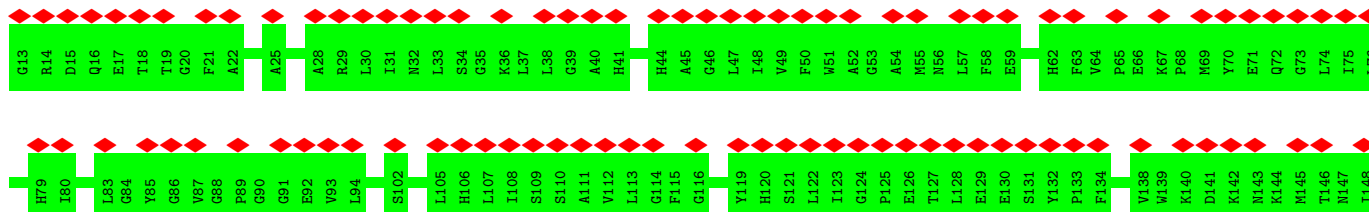


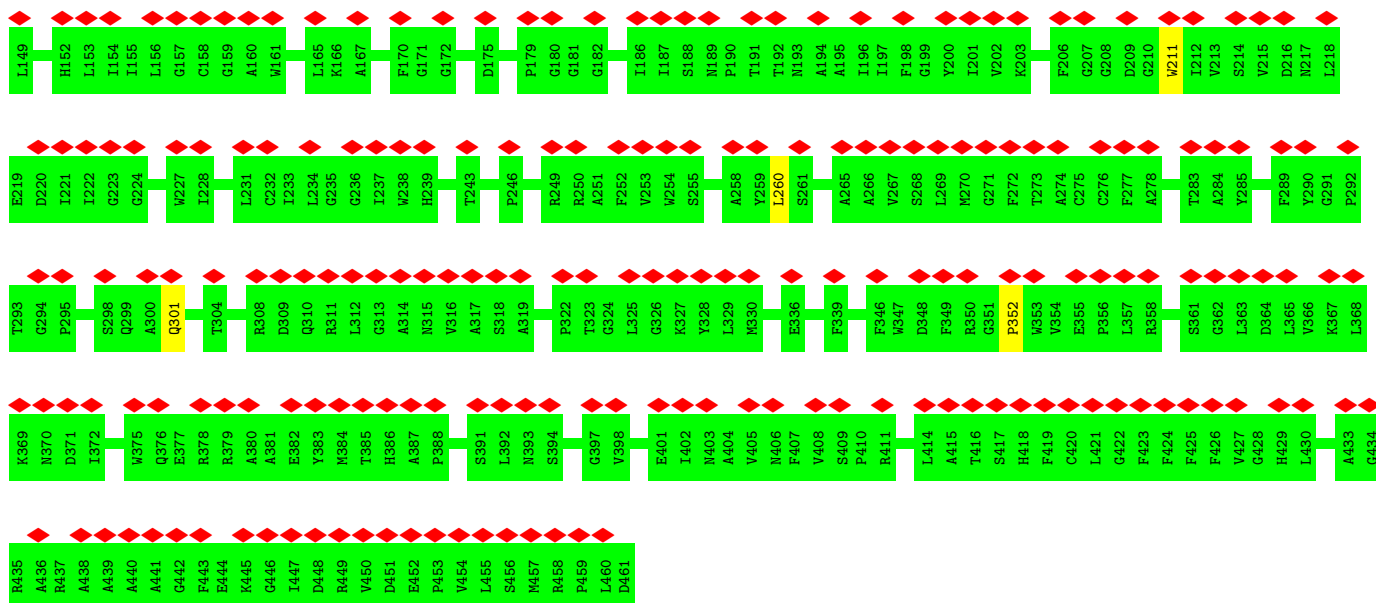


• Molecule 4: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II CP43 reaction center protein

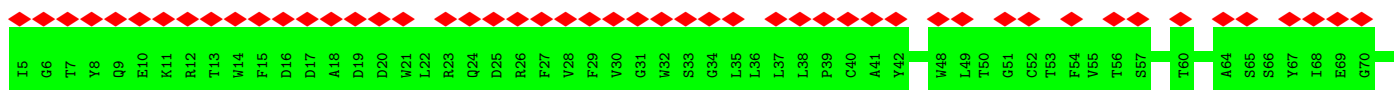


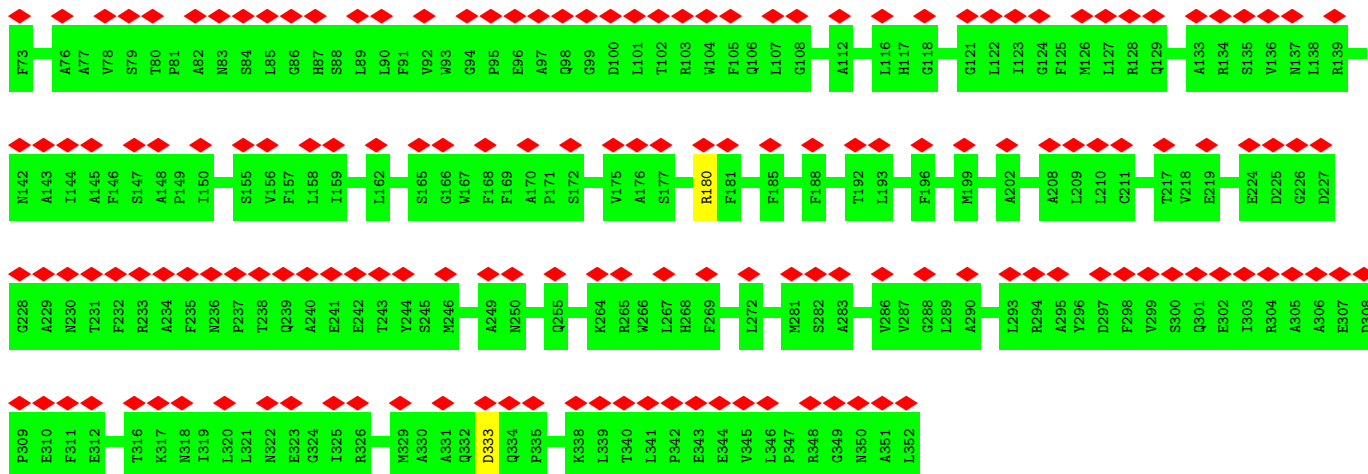


• Molecule 5: Photosystem II D2 protein



• Molecule 5: Photosystem II D2 protein

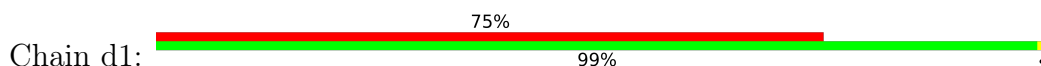




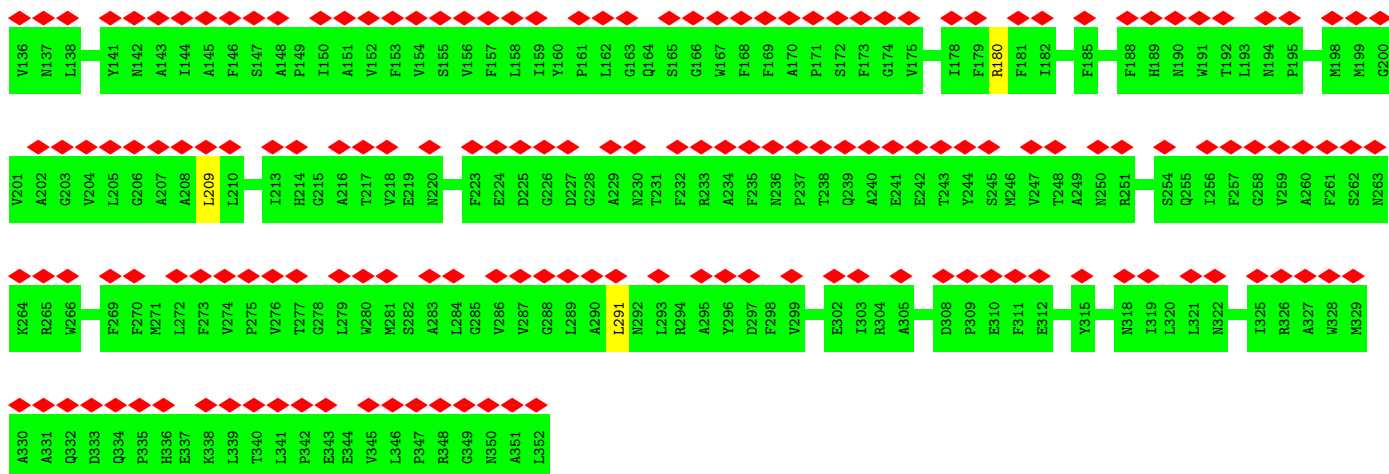
• Molecule 5: Photosystem II D2 protein



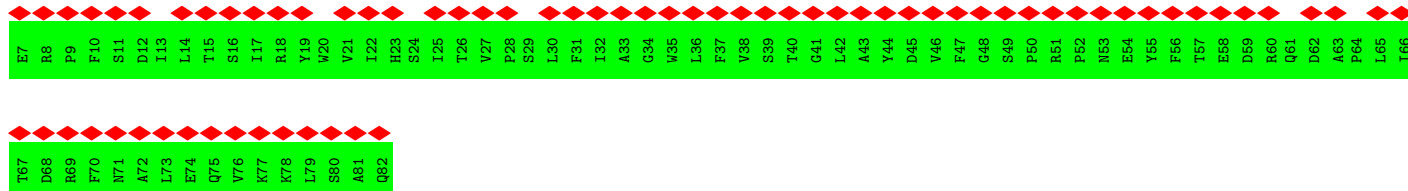
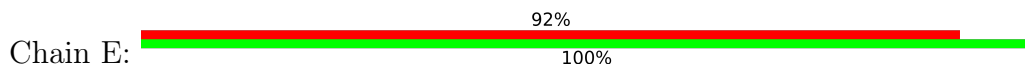
• Molecule 5: Photosystem II D2 protein



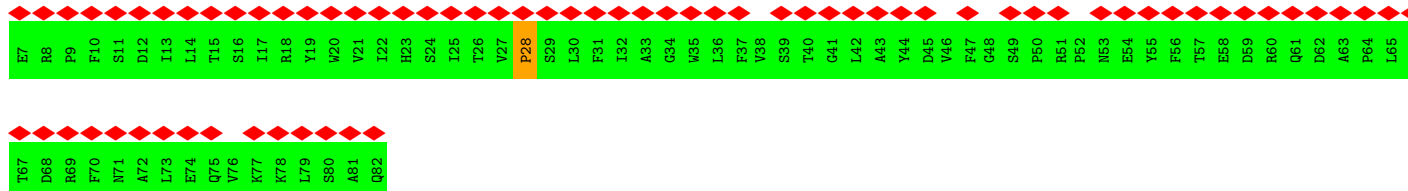




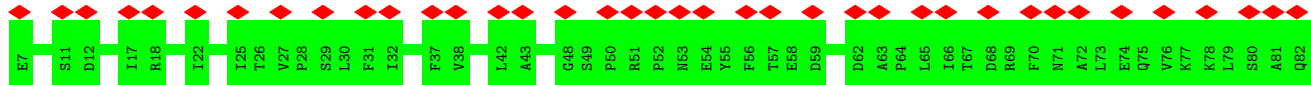
• Molecule 6: Cytochrome b559 subunit alpha



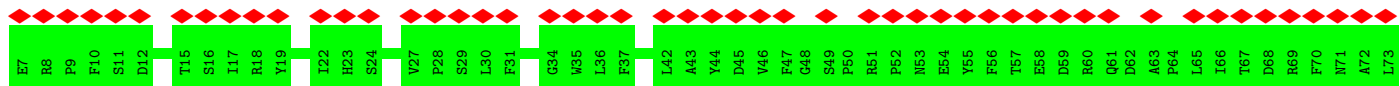
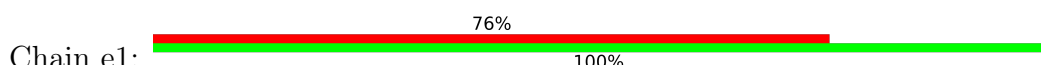
• Molecule 6: Cytochrome b559 subunit alpha

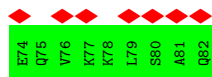


• Molecule 6: Cytochrome b559 subunit alpha

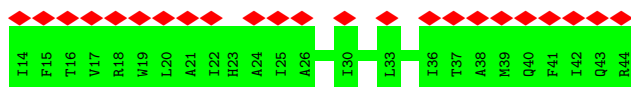
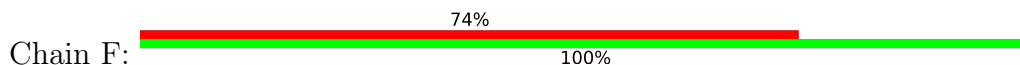


• Molecule 6: Cytochrome b559 subunit alpha

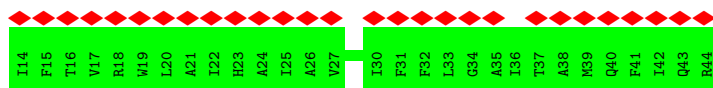
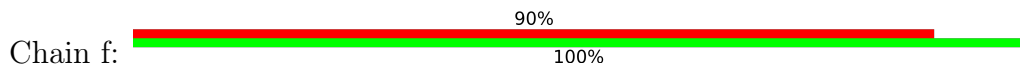




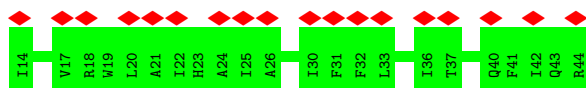
• Molecule 7: Cytochrome b559 subunit beta



• Molecule 7: Cytochrome b559 subunit beta



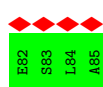
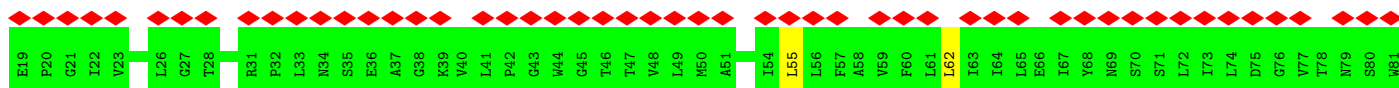
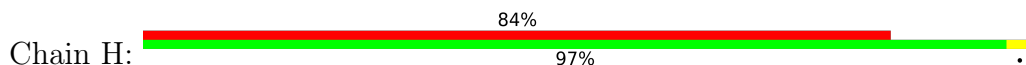
• Molecule 7: Cytochrome b559 subunit beta



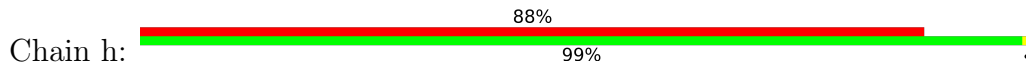
• Molecule 7: Cytochrome b559 subunit beta

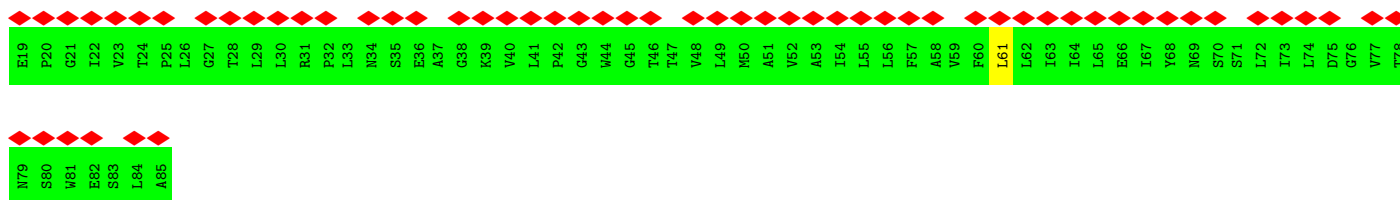


• Molecule 8: Photosystem II reaction center protein H

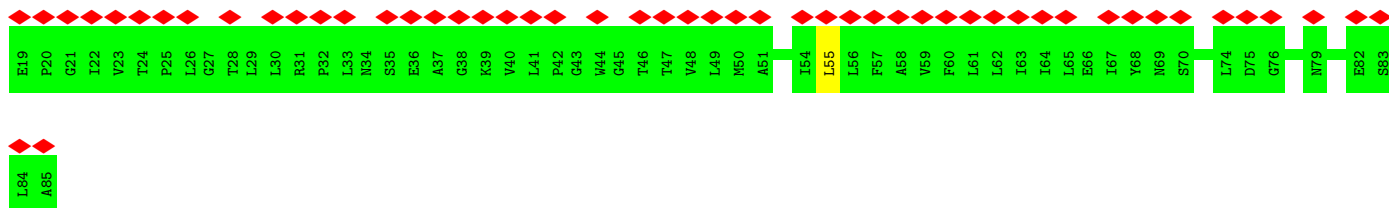
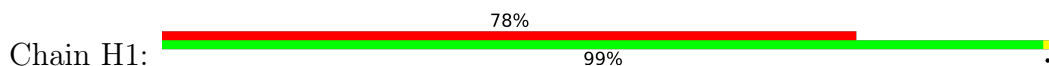


• Molecule 8: Photosystem II reaction center protein H

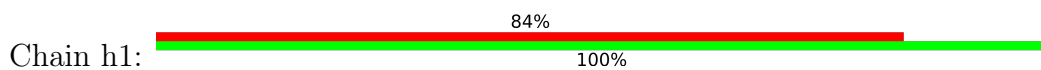




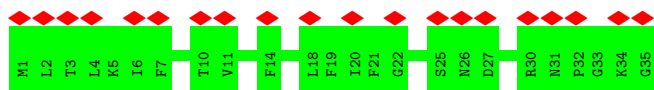
• Molecule 8: Photosystem II reaction center protein H



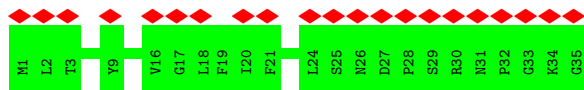
• Molecule 8: Photosystem II reaction center protein H



• Molecule 9: Photosystem II reaction center protein I

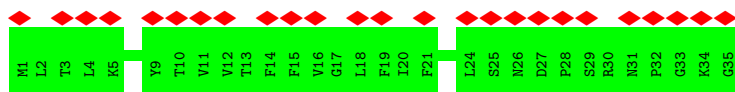


• Molecule 9: Photosystem II reaction center protein I

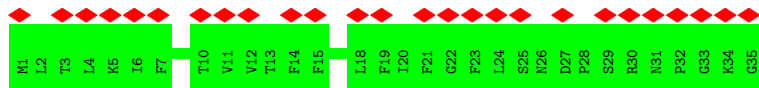
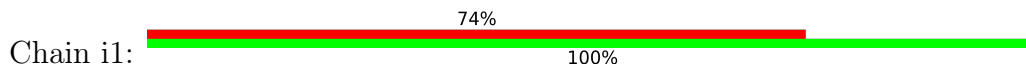


• Molecule 9: Photosystem II reaction center protein I

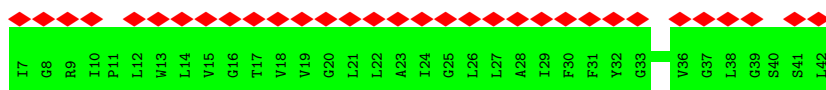
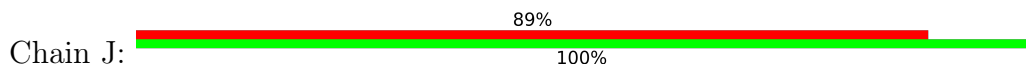




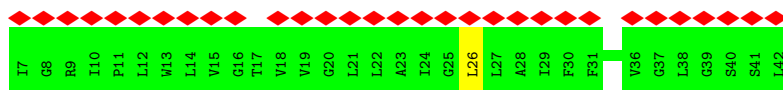
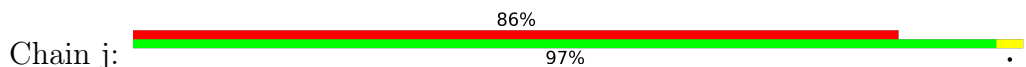
• Molecule 9: Photosystem II reaction center protein I



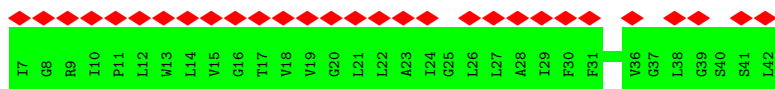
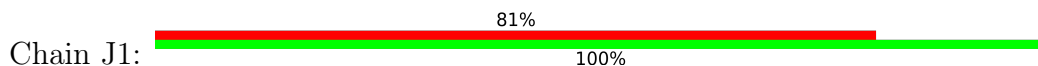
• Molecule 10: PsbJ



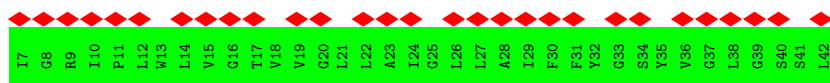
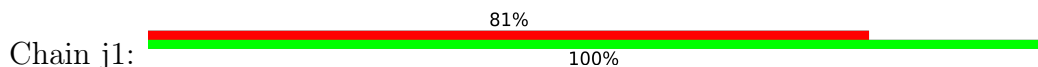
• Molecule 10: PsbJ



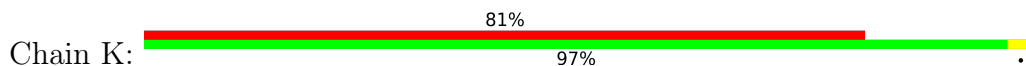
• Molecule 10: PsbJ



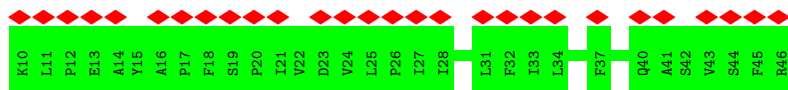
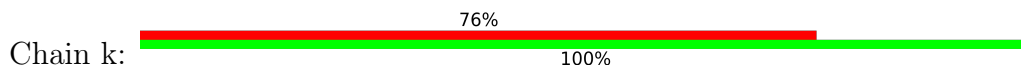
• Molecule 10: PsbJ



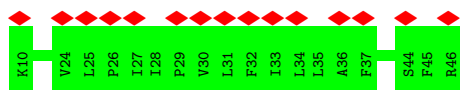
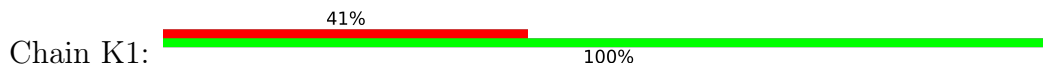
• Molecule 11: Photosystem II reaction center protein K



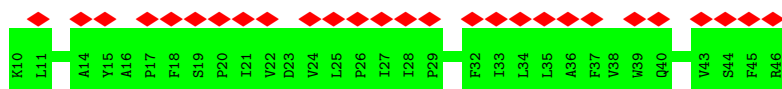
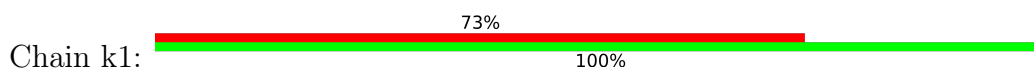
• Molecule 11: Photosystem II reaction center protein K



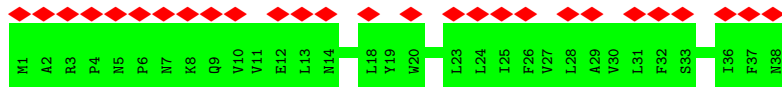
• Molecule 11: Photosystem II reaction center protein K



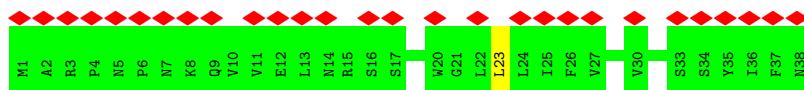
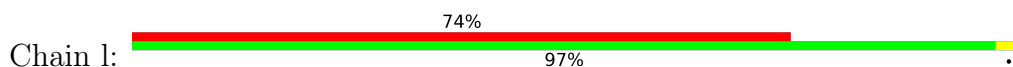
• Molecule 11: Photosystem II reaction center protein K



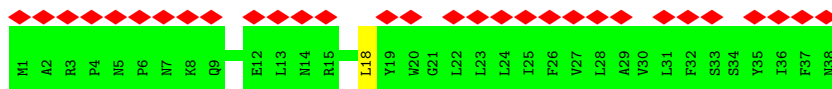
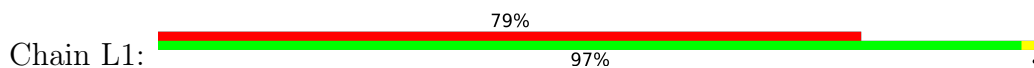
• Molecule 12: Photosystem II reaction center protein L



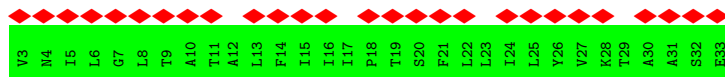
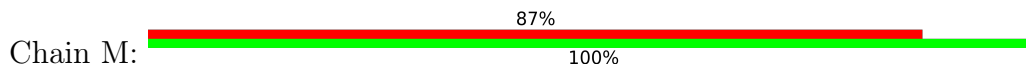
• Molecule 12: Photosystem II reaction center protein L



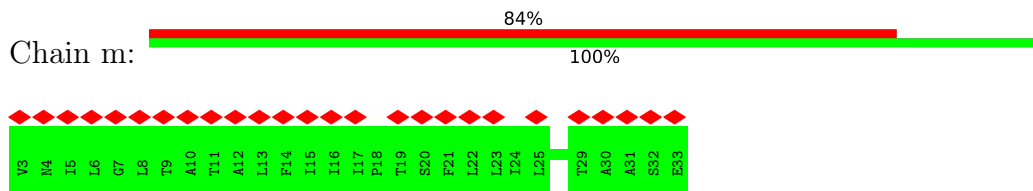
• Molecule 12: Photosystem II reaction center protein L



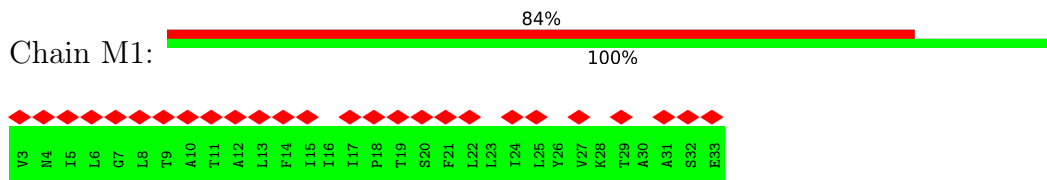
• Molecule 13: PsbM



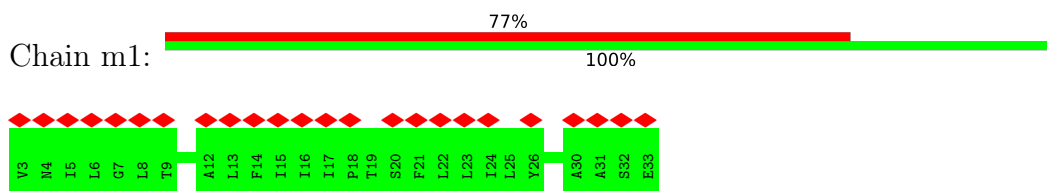
• Molecule 13: PsbM



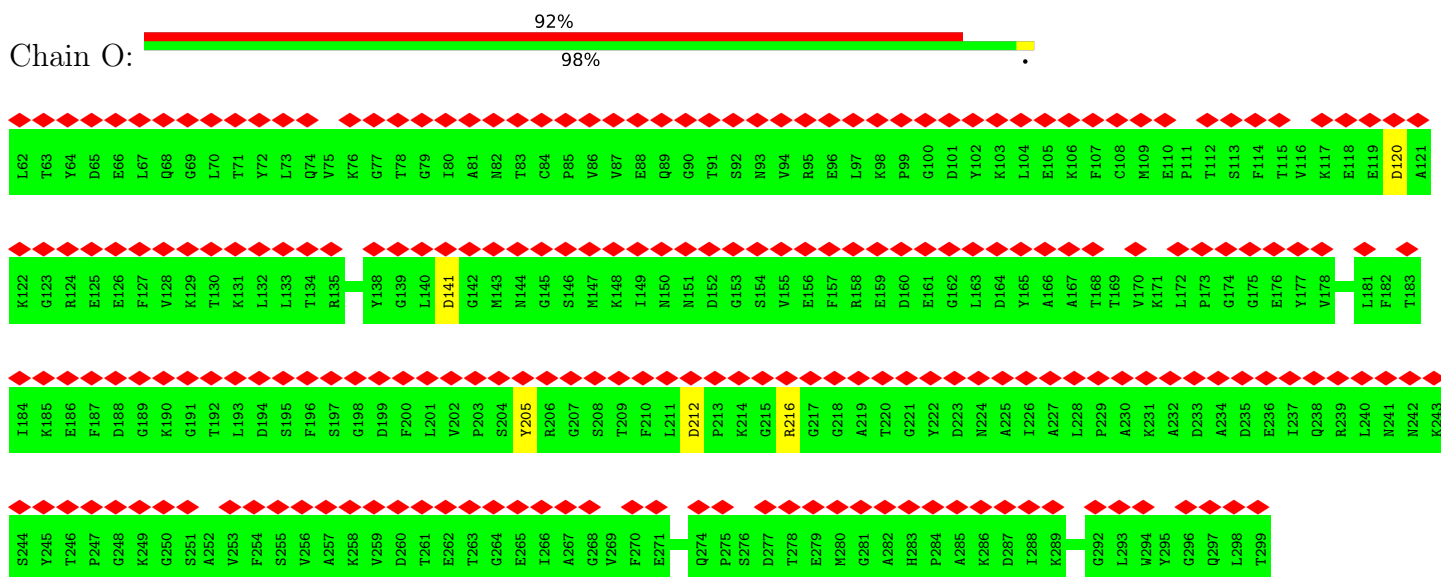
• Molecule 13: PsbM



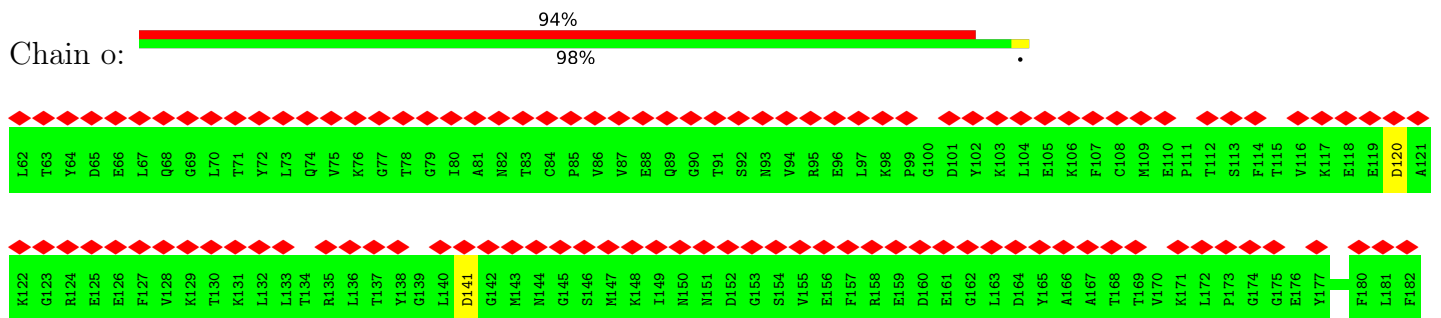
• Molecule 13: PsbM

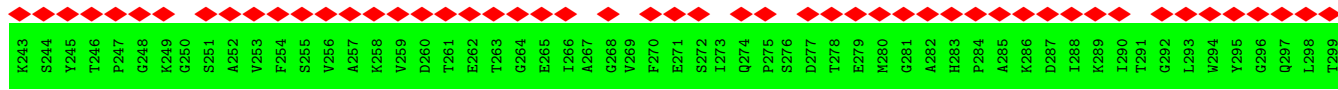
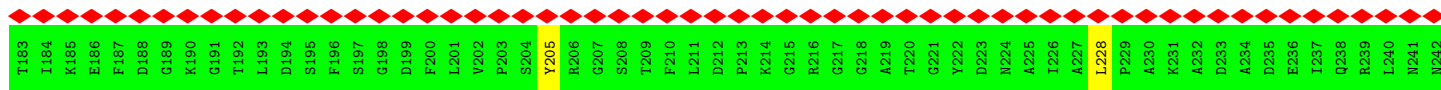


• Molecule 14: PsbO

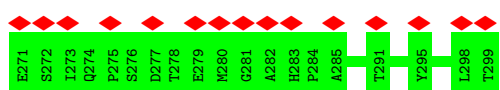
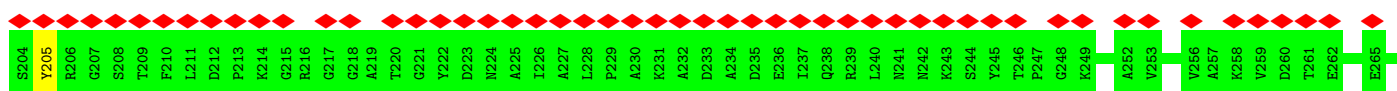
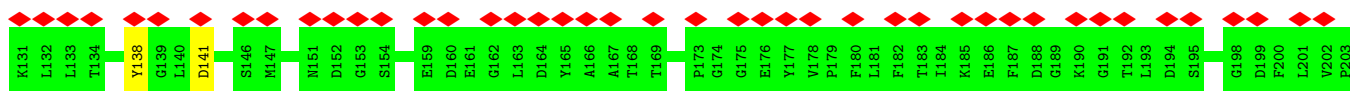
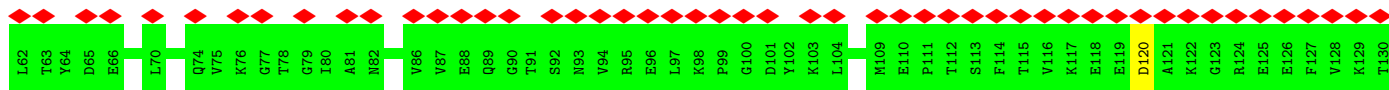


• Molecule 14: PsbO

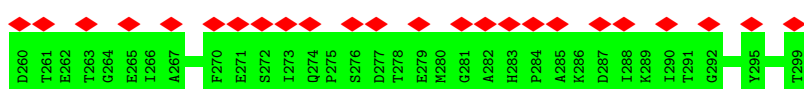
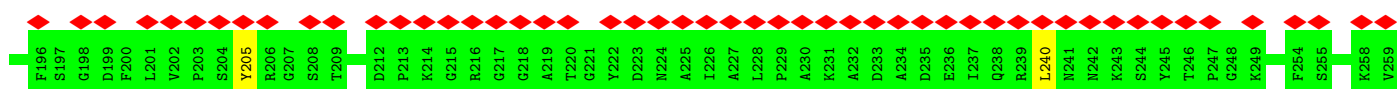
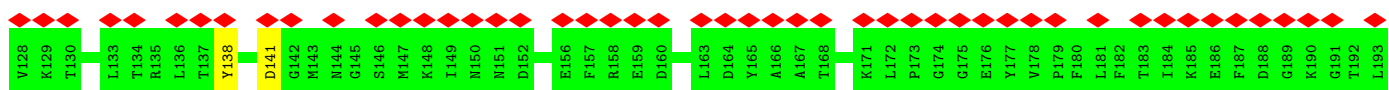
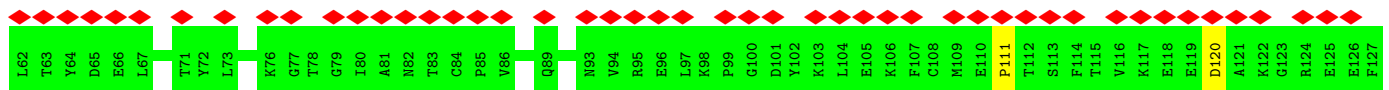




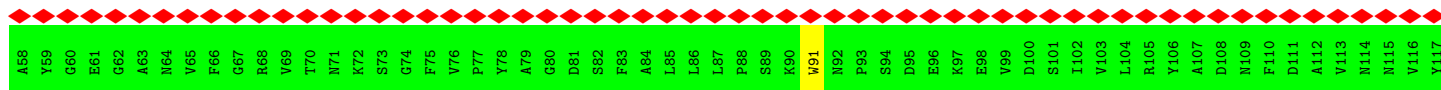
• Molecule 14: PsbO

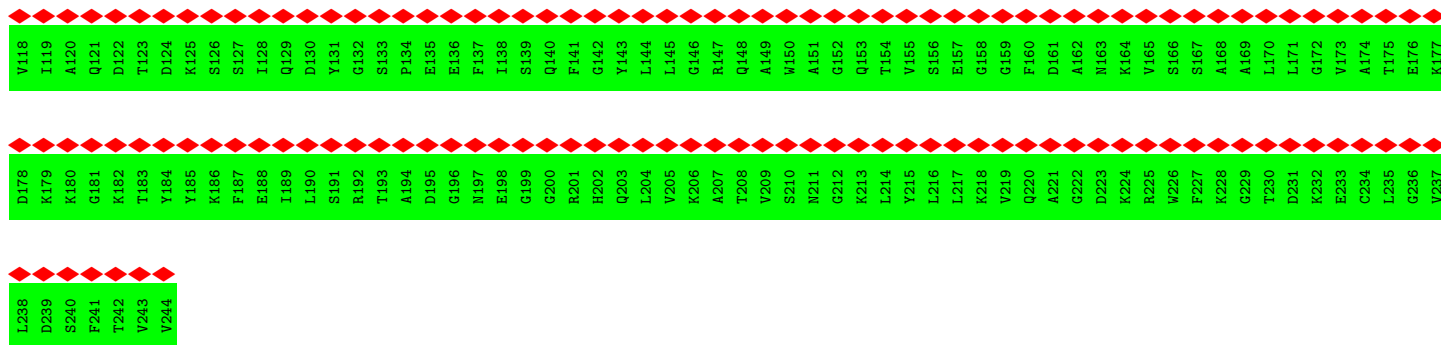


• Molecule 14: PsbO

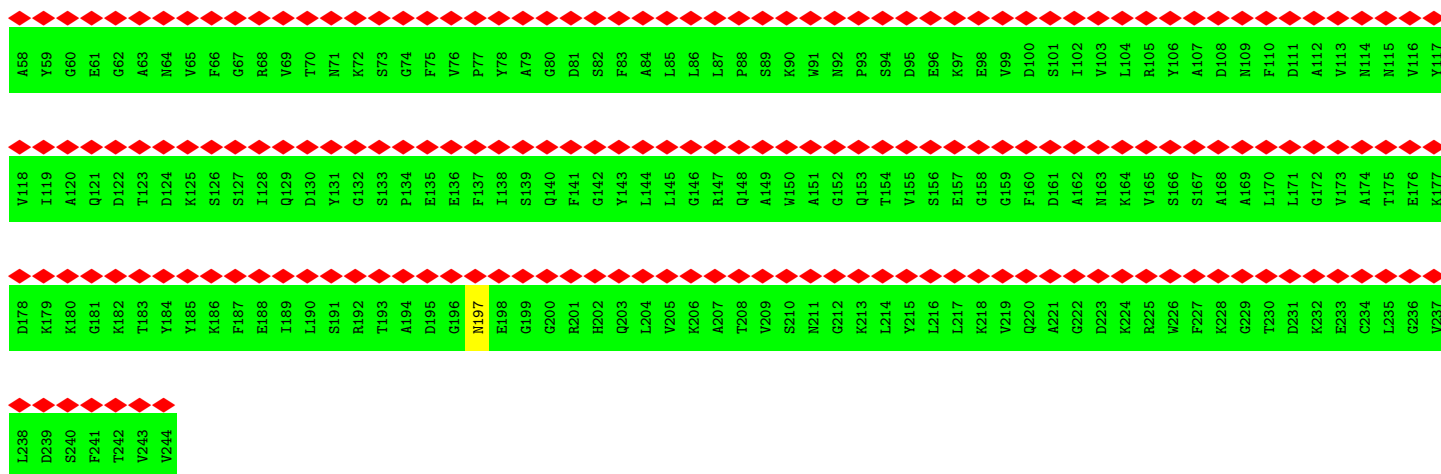


• Molecule 15: PsbP

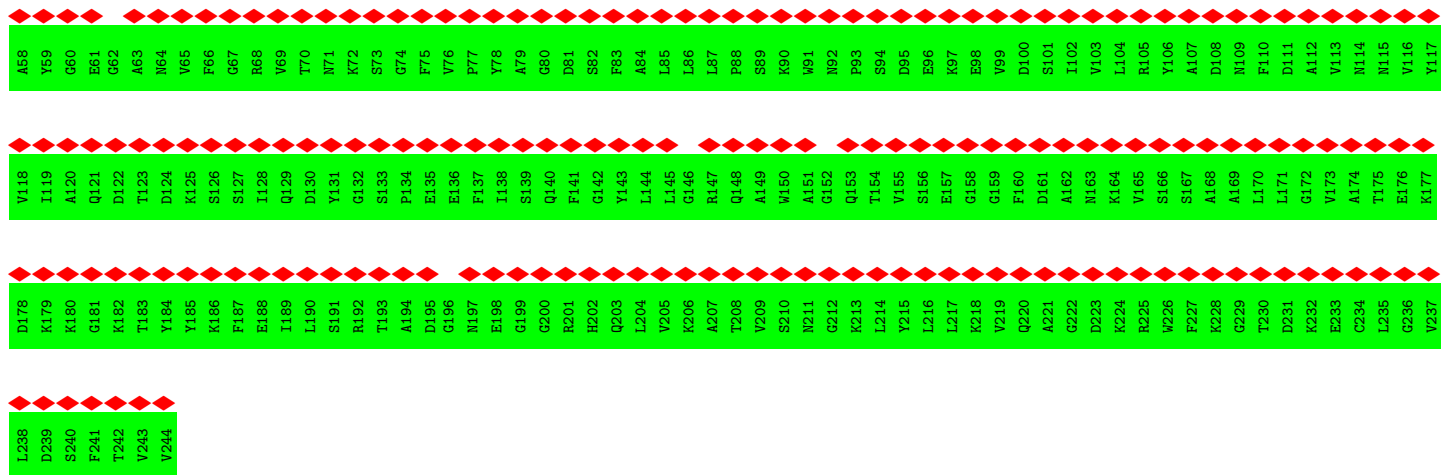




• Molecule 15: PsbP

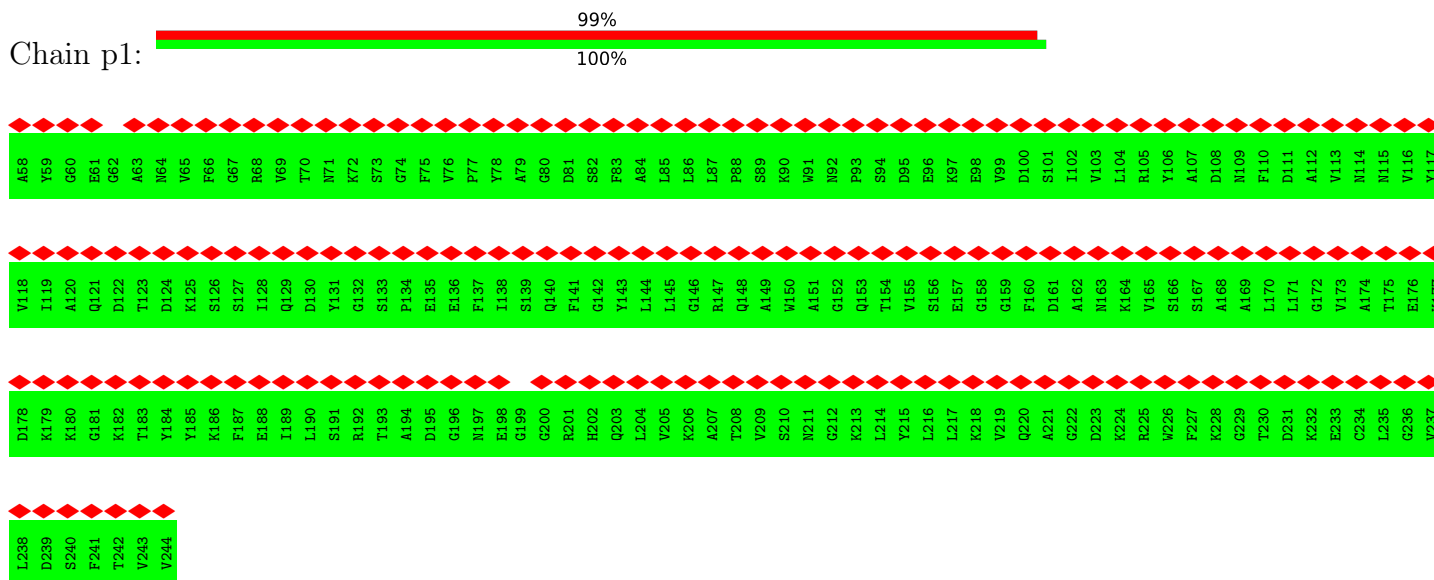


• Molecule 15: PsbP

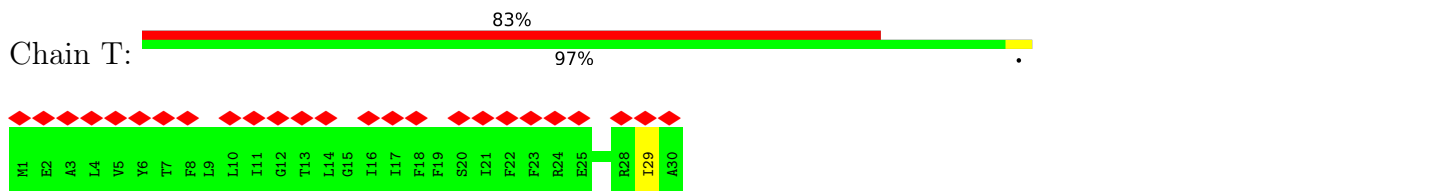


• Molecule 15: PsbP

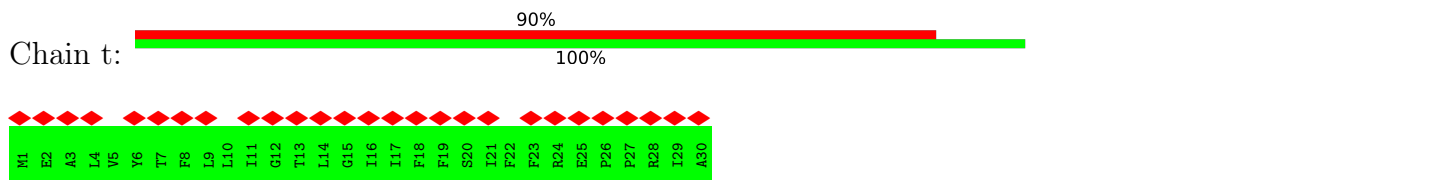




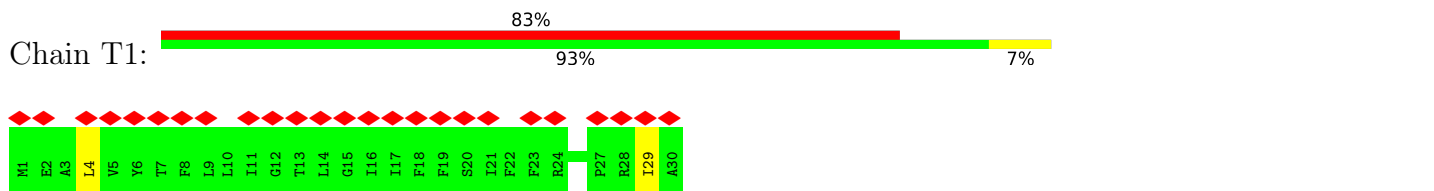
• Molecule 16: Photosystem II reaction center protein T



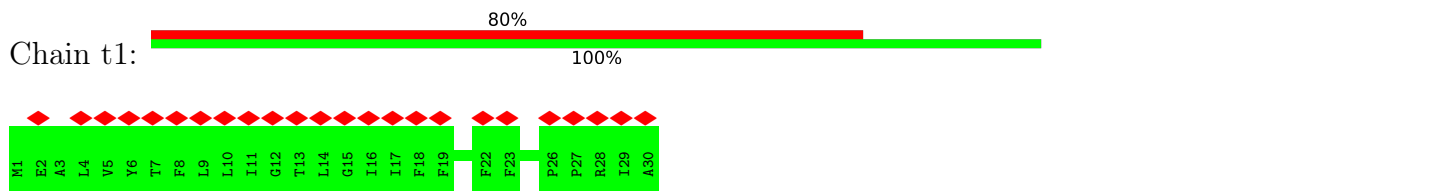
• Molecule 16: Photosystem II reaction center protein T



• Molecule 16: Photosystem II reaction center protein T



• Molecule 16: Photosystem II reaction center protein T

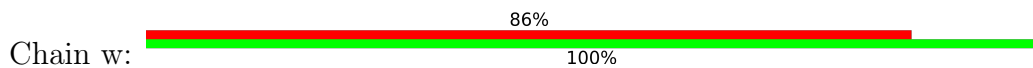


• Molecule 17: PsbW

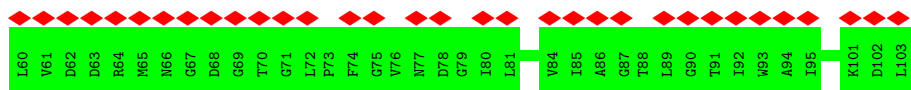
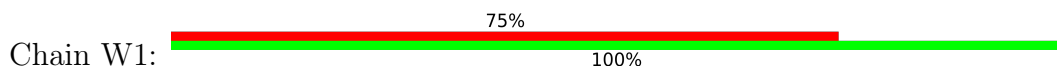




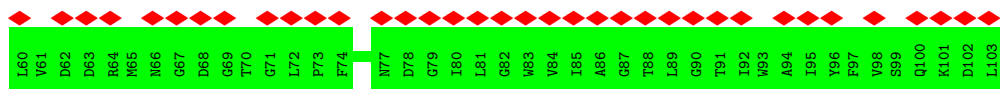
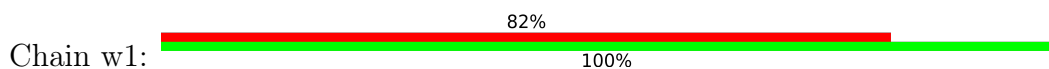
• Molecule 17: PsbW



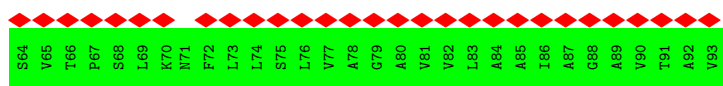
• Molecule 17: PsbW



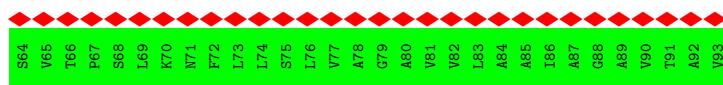
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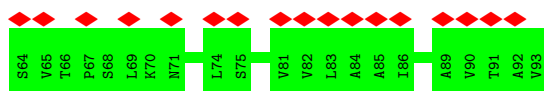
• Molecule 18: PsbX



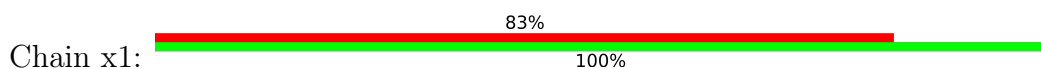
• Molecule 18: PsbX

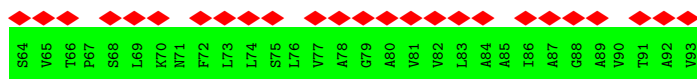


• Molecule 18: PsbX

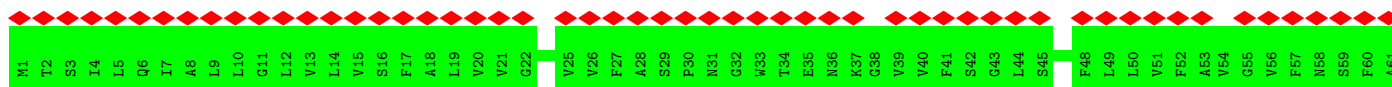


• Molecule 18: PsbX

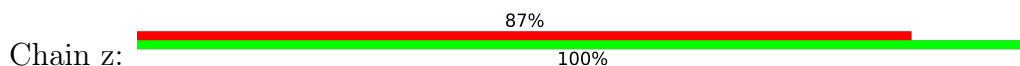




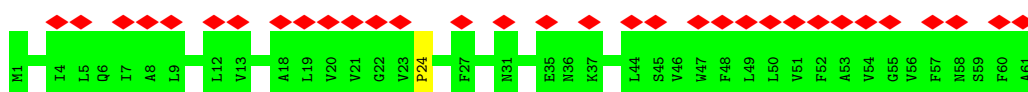
• Molecule 19: Photosystem II reaction center protein Z



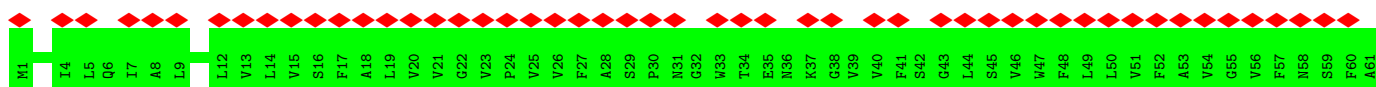
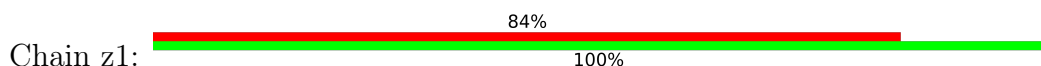
• Molecule 19: Photosystem II reaction center protein Z



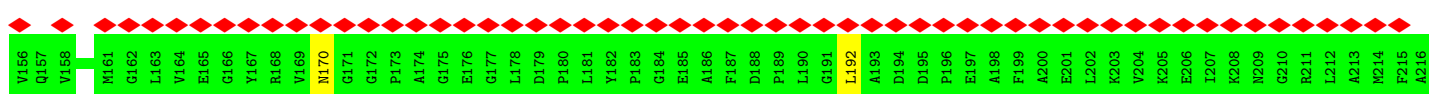
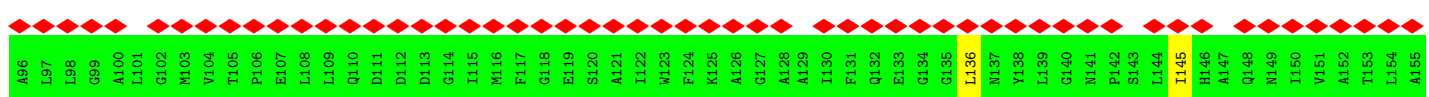
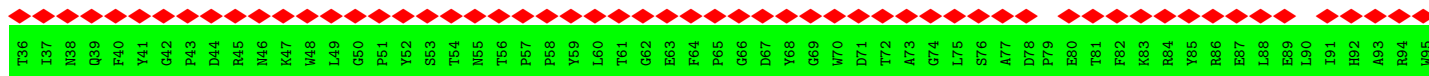
• Molecule 19: Photosystem II reaction center protein Z

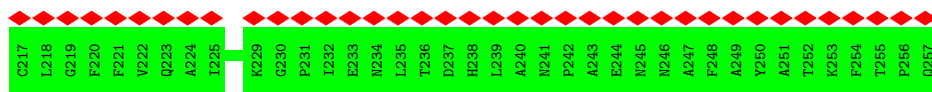


• Molecule 19: Photosystem II reaction center protein Z

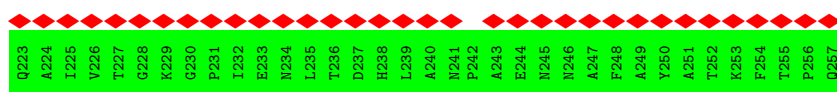
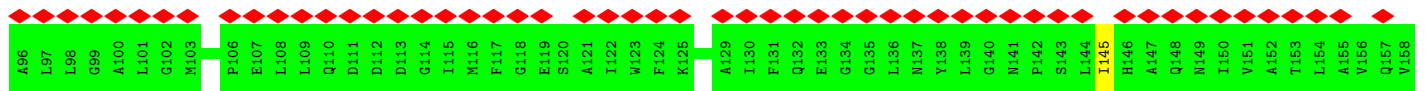
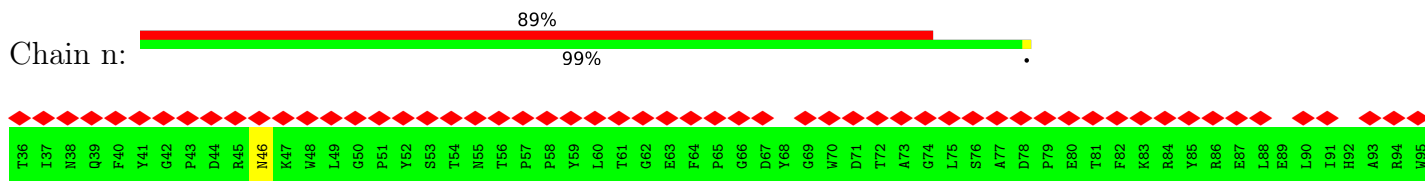


• Molecule 20: LHCII M3

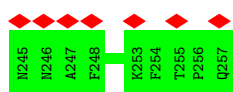
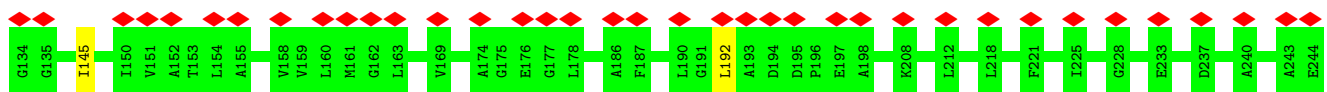
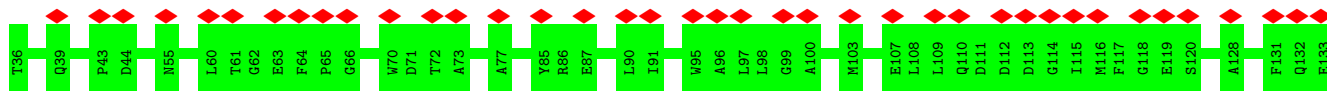




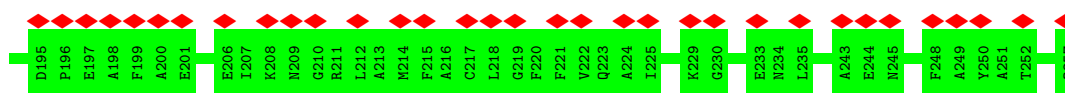
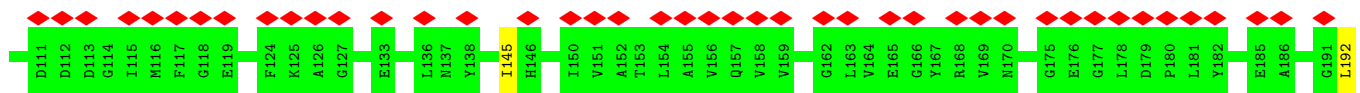
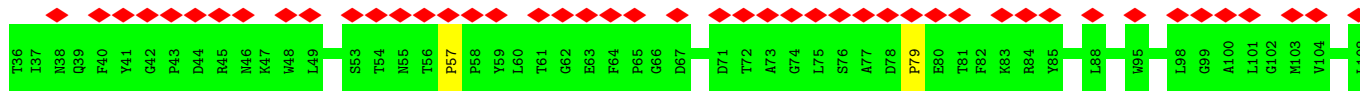
• Molecule 20: LHCII M3



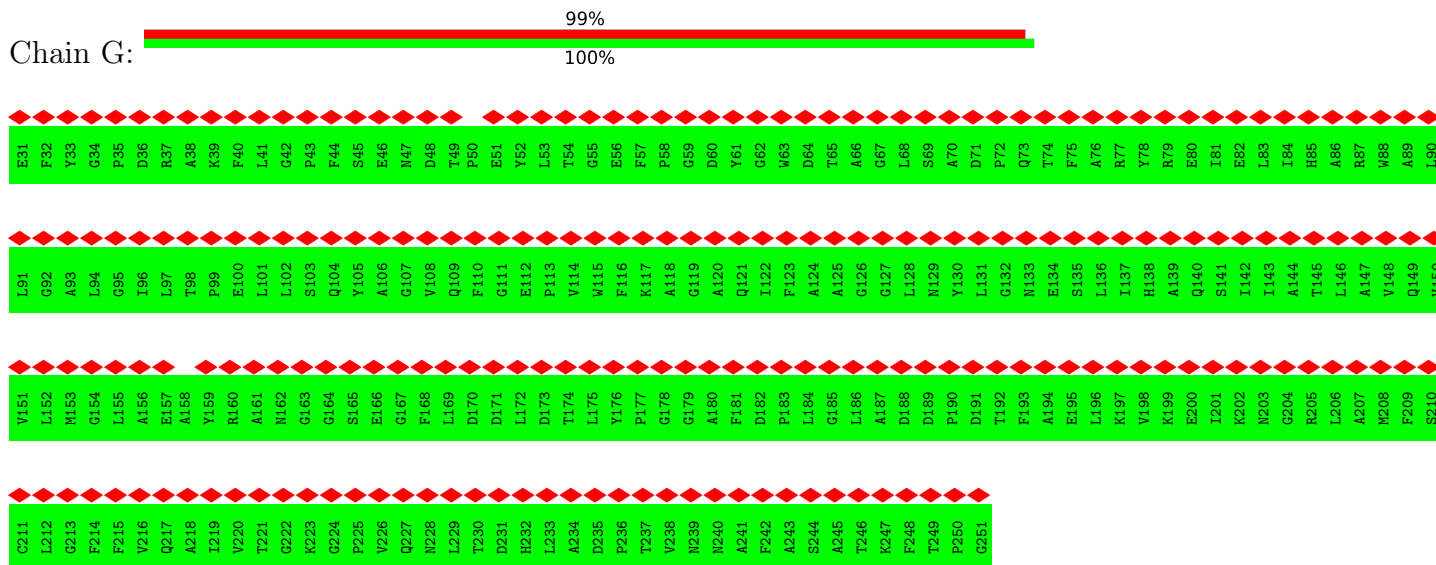
• Molecule 20: LHCII M3



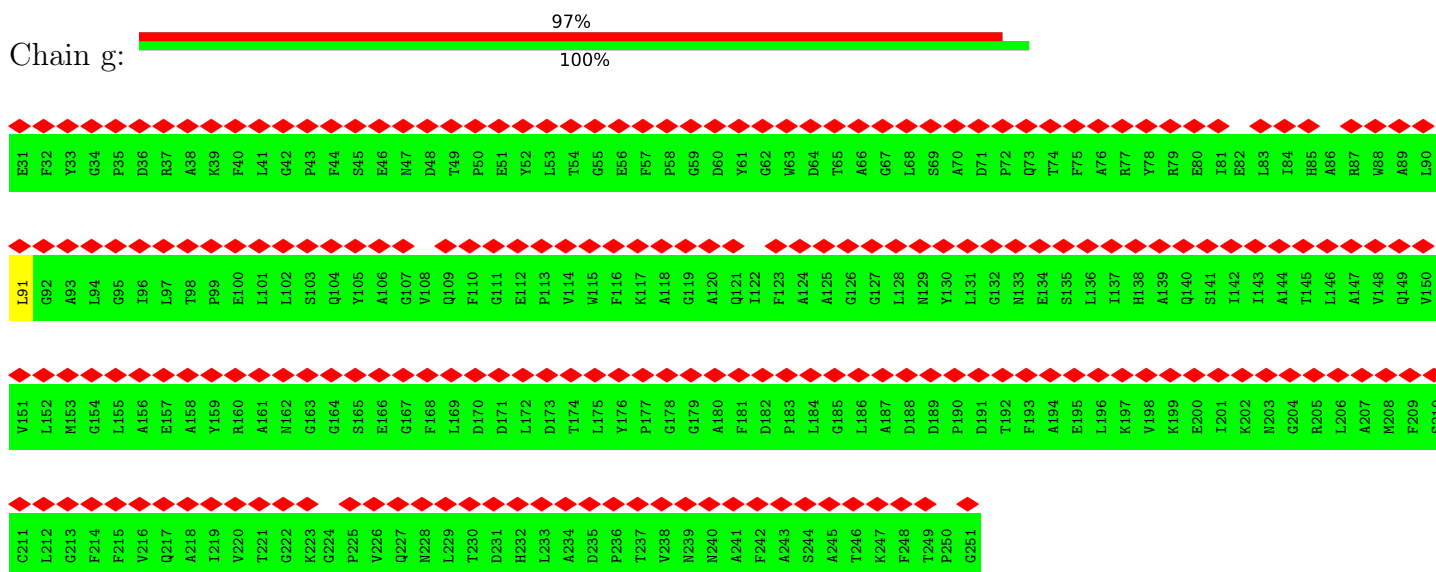
• Molecule 20: LHCII M3



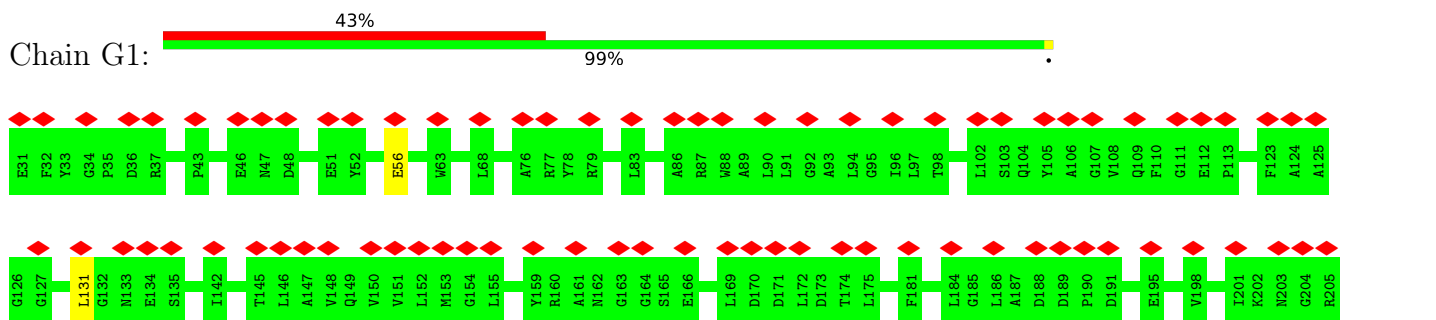
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

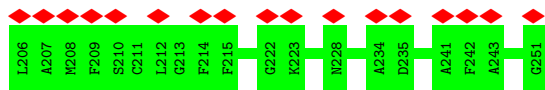


• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

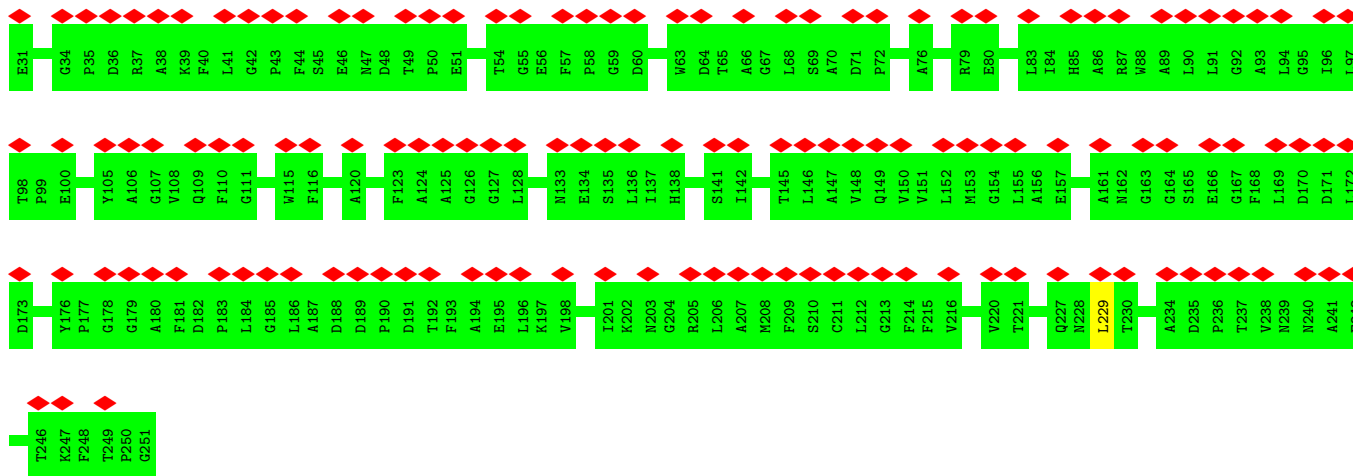


• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

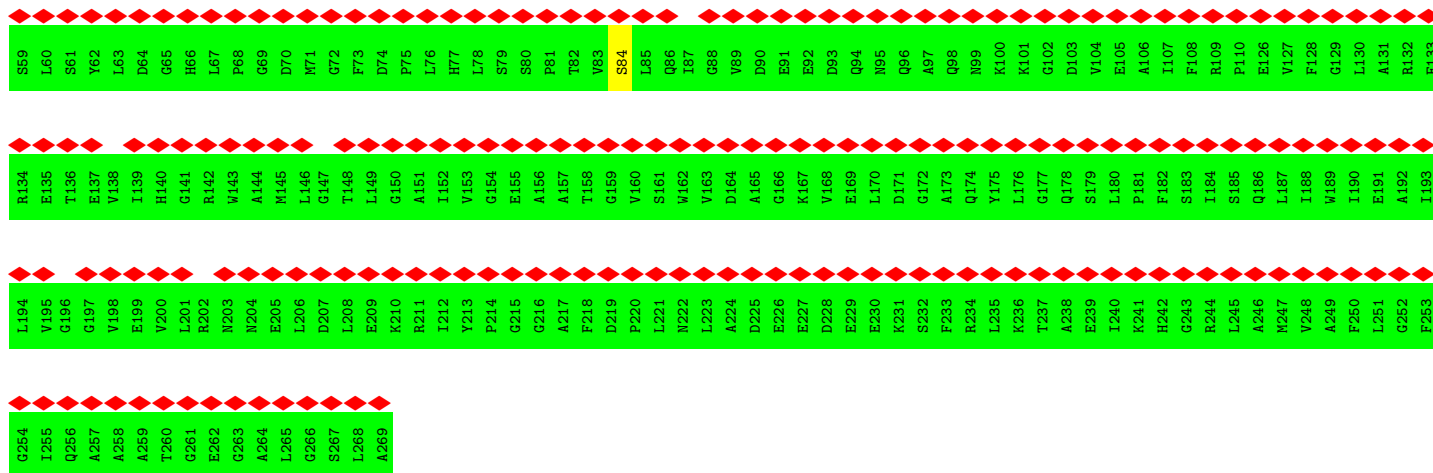




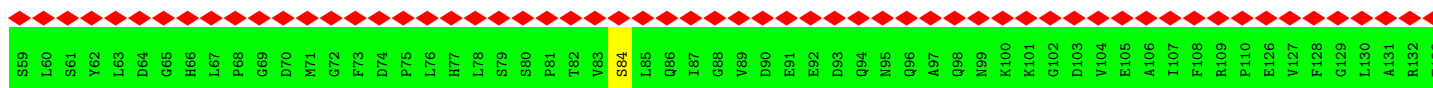
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

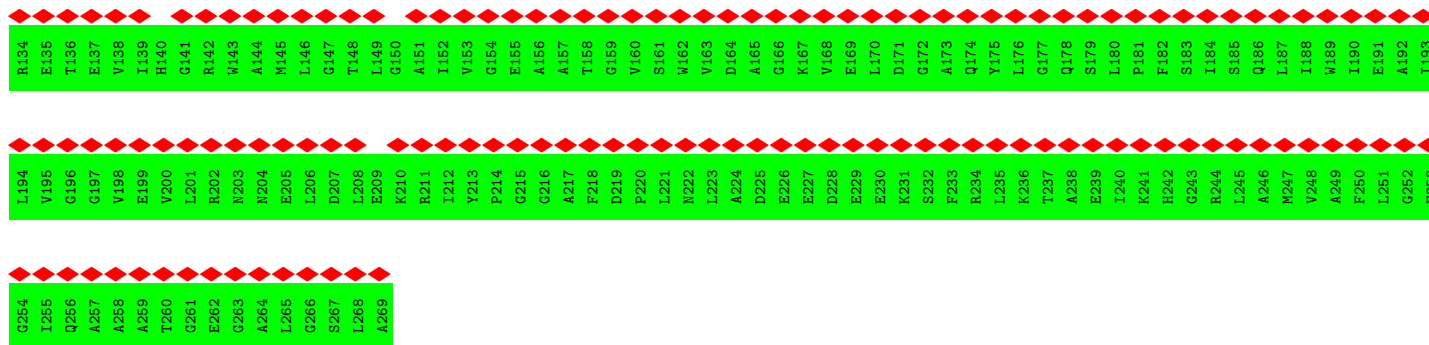


• Molecule 22: CP29

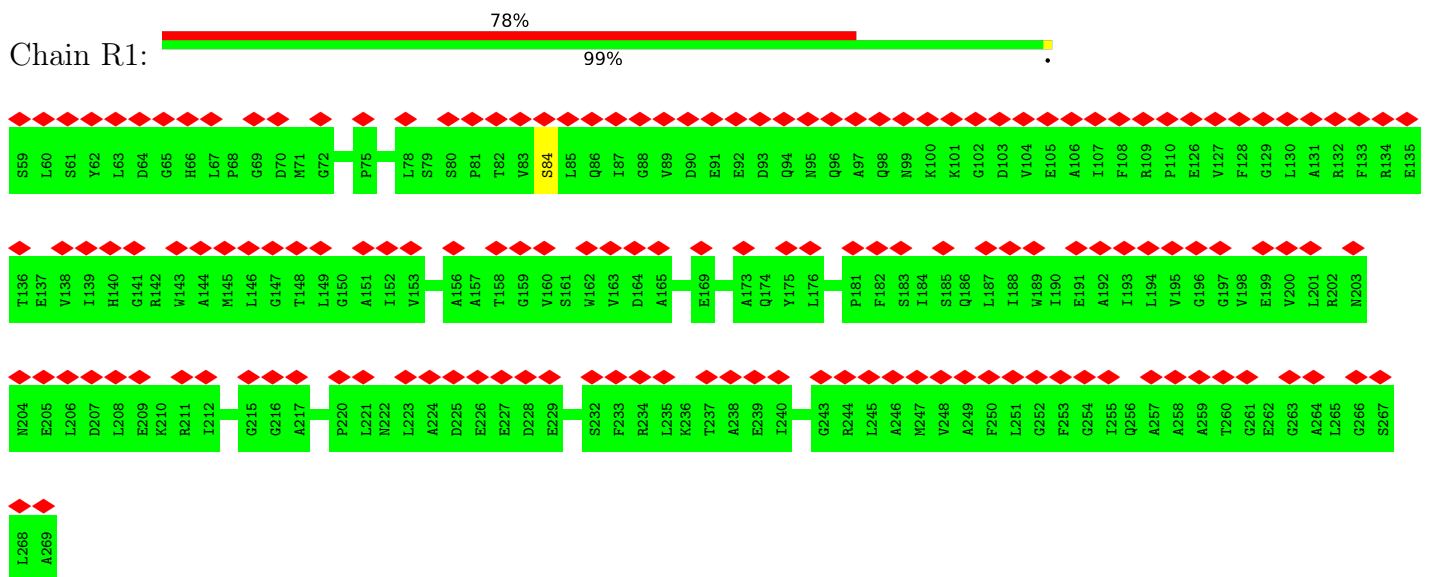


• Molecule 22: CP29





• Molecule 22: CP29

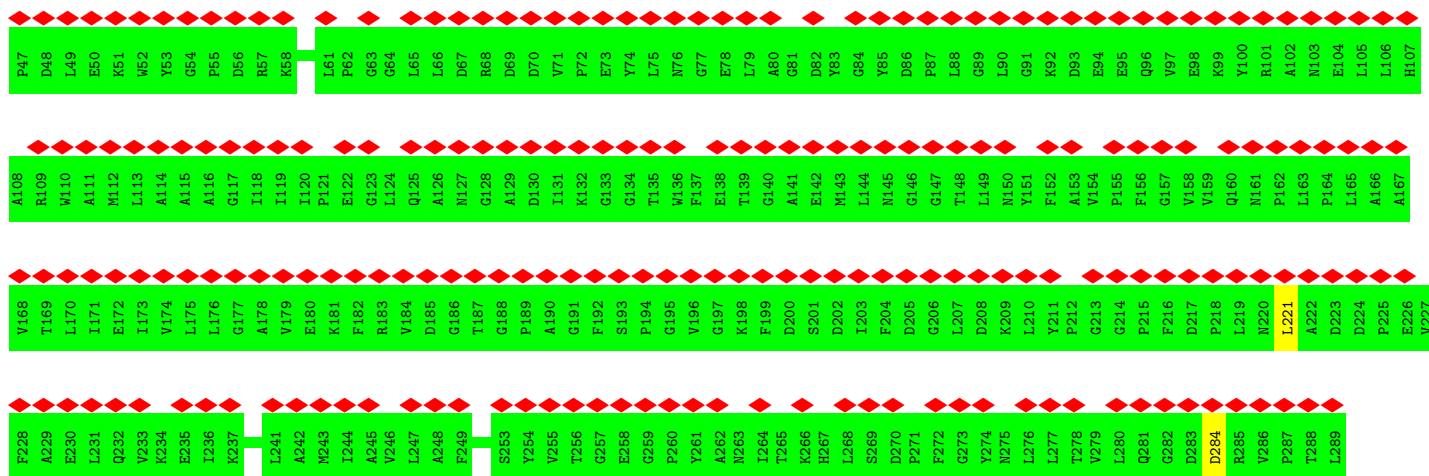


• Molecule 22: CP29

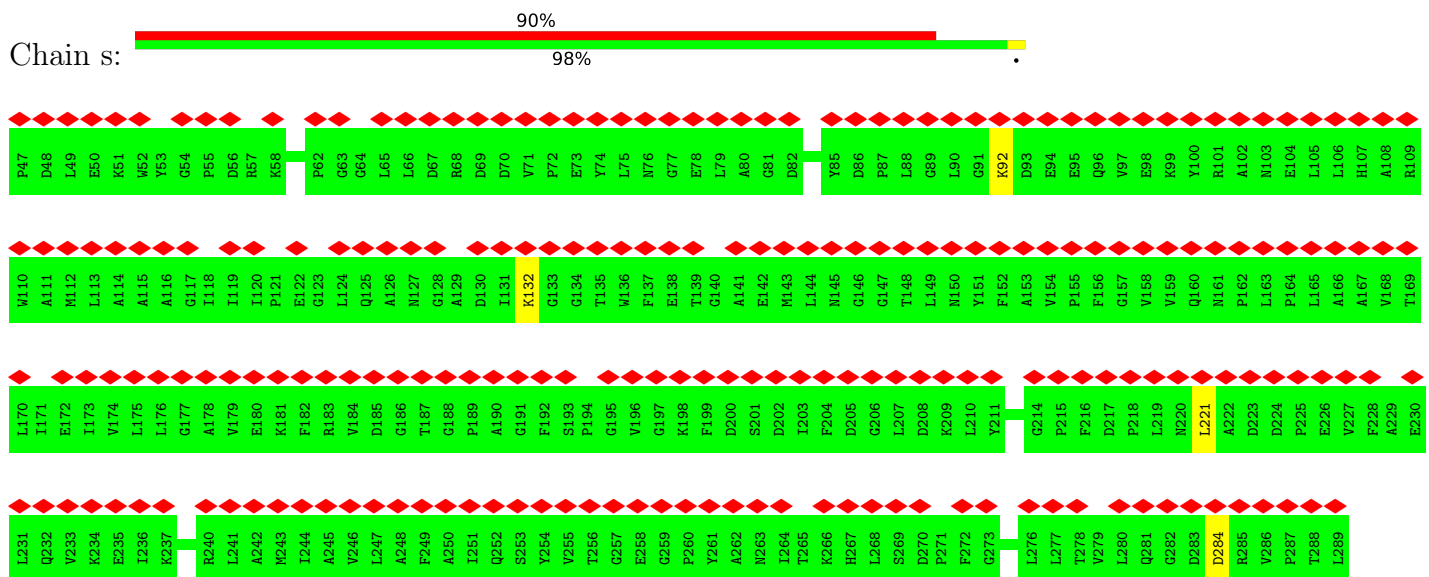


• Molecule 23: CP26

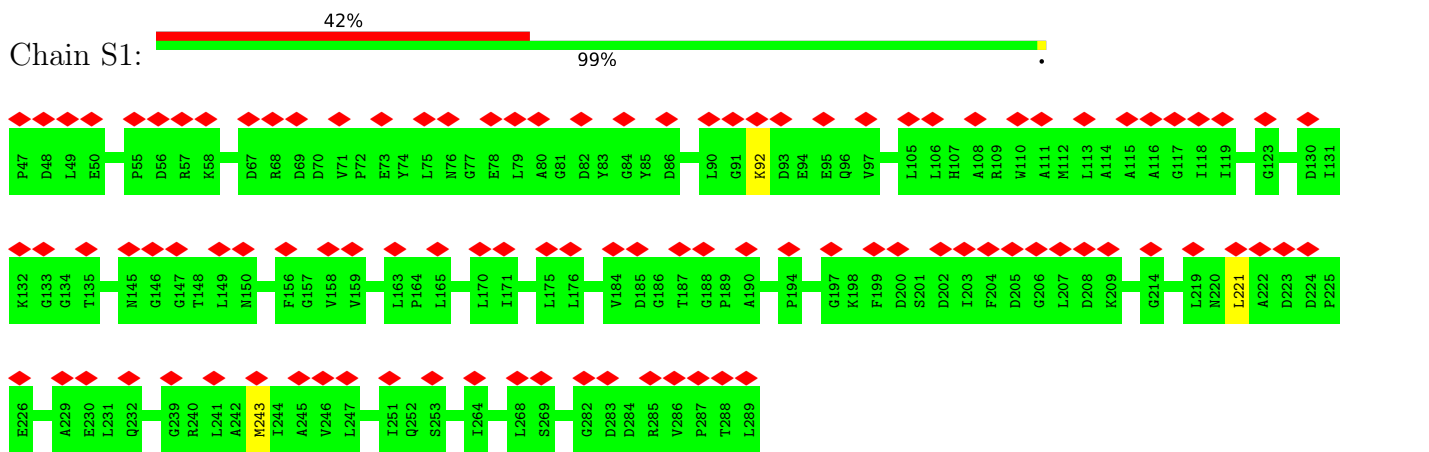




• Molecule 23: CP26



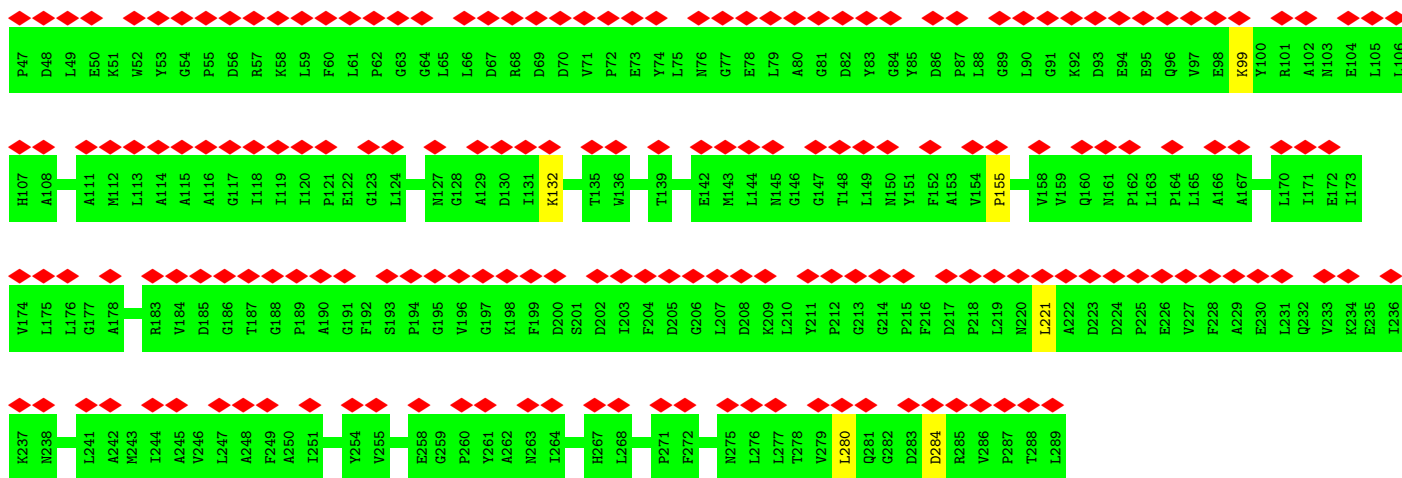
• Molecule 23: CP26



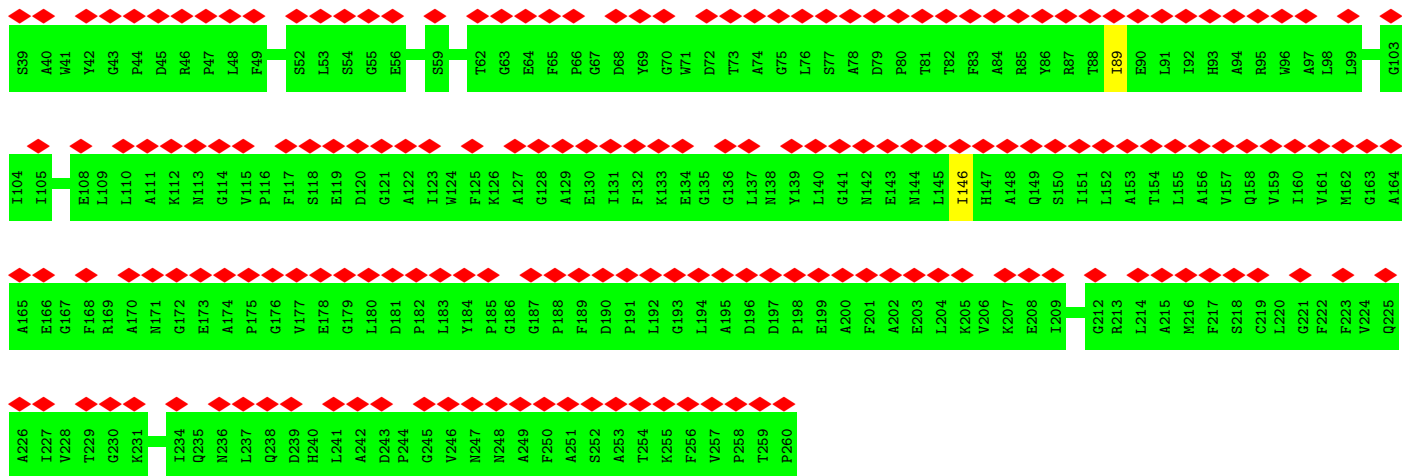
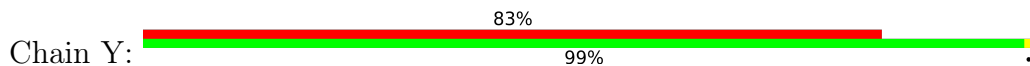
• Molecule 23: CP26



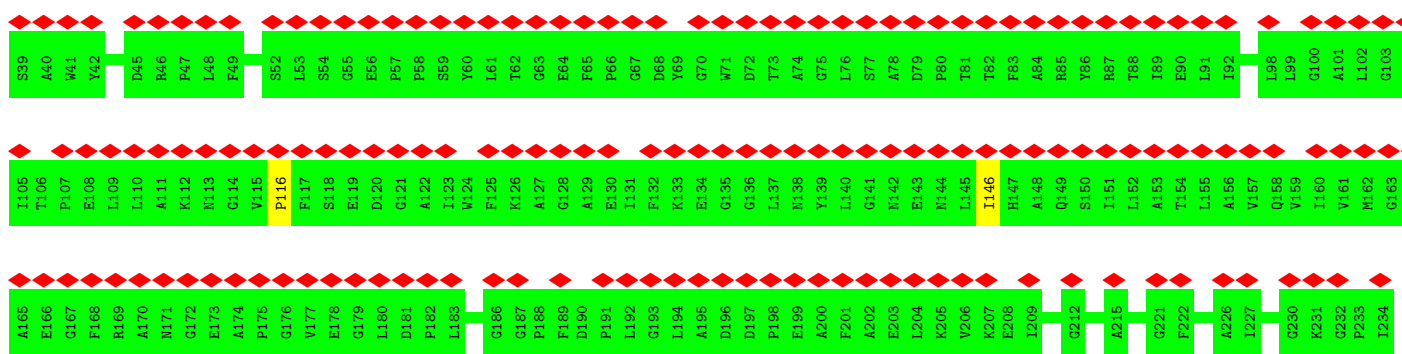
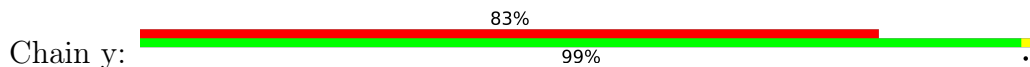


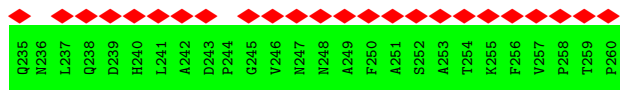


• Molecule 24: LHCII M1

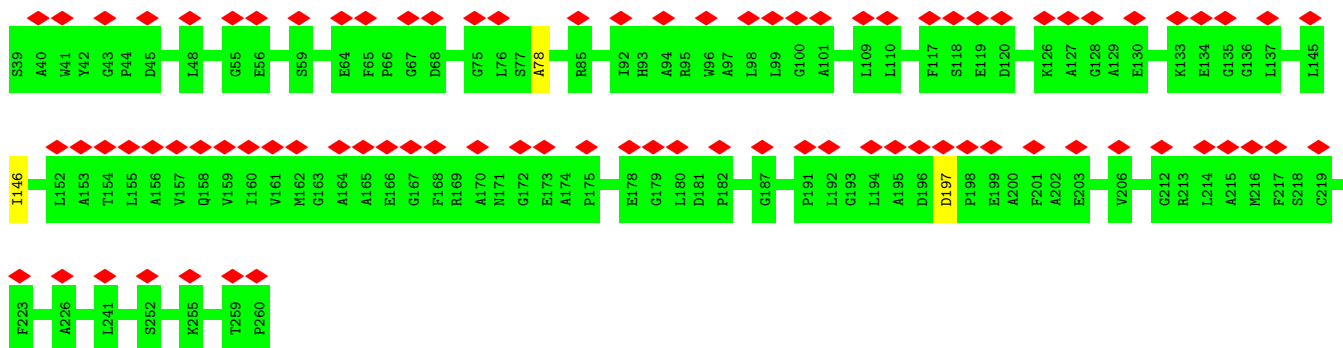


• Molecule 24: LHCII M1

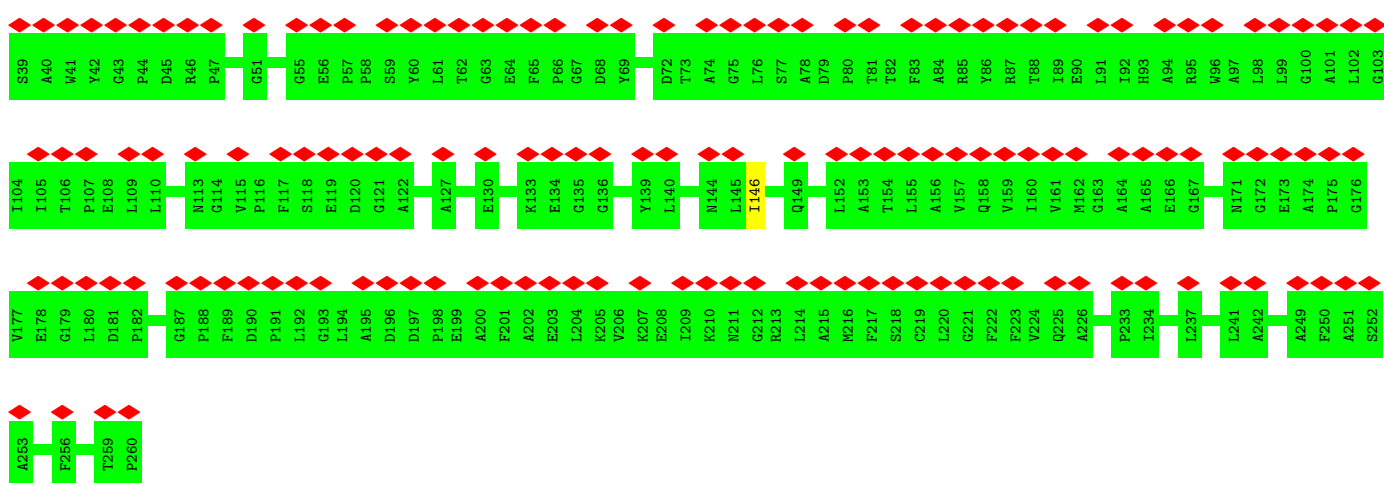




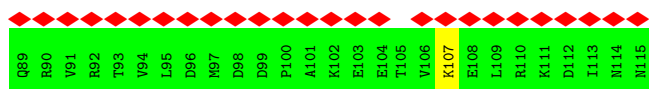
• Molecule 24: LHCII M1



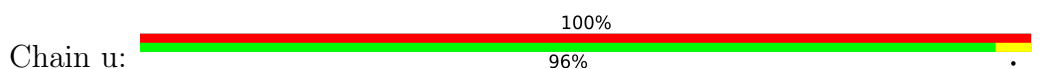
• Molecule 24: LHCII M1

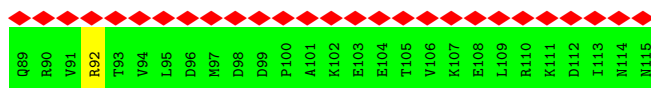


• Molecule 25: PsbU

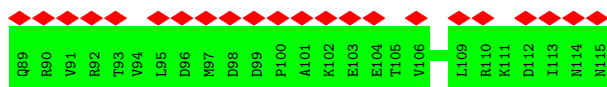
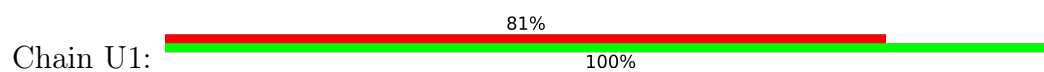


• Molecule 25: PsbU

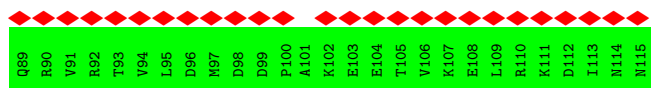




- Molecule 25: PsbU



- Molecule 25: PsbU



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.036	Depositor
Map size ( $\text{\AA}$ )	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.96, 0.96, 0.96	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DGA, GOL, SEP, CLA, FE2, ERG, CL, LHG, LMK, SQD, C7Z, OEX, NA, PHO, LPX, DGD, NEX, PTY, LMT, 3PH, RRX, SPH, LUT, XAT, CHL, BCT, PL9, HEM, 4RF, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/2723	0.60	0/3715
1	A1	0.36	0/2723	0.61	0/3715
1	a	0.41	0/2723	0.61	0/3715
1	a1	0.36	0/2723	0.65	2/3715 (0.1%)
2	B	0.40	0/3912	0.63	2/5327 (0.0%)
2	B1	0.35	0/3912	0.61	1/5327 (0.0%)
2	b	0.39	0/3912	0.61	2/5327 (0.0%)
2	b1	0.33	0/3912	0.60	1/5327 (0.0%)
3	V	0.34	0/228	0.67	0/311
3	V1	0.26	0/228	0.54	0/311
3	v	0.30	0/228	0.66	0/311
3	v1	0.29	0/228	0.76	1/311 (0.3%)
4	C	0.46	2/3602 (0.1%)	0.70	4/4913 (0.1%)
4	C1	0.34	0/3602	0.59	0/4913
4	c	0.39	0/3602	0.59	0/4913
4	c1	0.40	2/3602 (0.1%)	0.67	4/4913 (0.1%)
5	D	0.45	1/2860 (0.0%)	0.64	2/3899 (0.1%)
5	D1	0.36	0/2860	0.62	2/3899 (0.1%)
5	d	0.41	0/2860	0.61	1/3899 (0.0%)
5	d1	0.36	0/2860	0.65	2/3899 (0.1%)
6	E	0.34	0/639	0.59	0/870
6	E1	0.33	0/639	0.63	0/870
6	e	0.55	1/639 (0.2%)	0.85	3/870 (0.3%)
6	e1	0.30	0/639	0.59	0/870
7	F	0.33	0/259	0.56	0/351
7	F1	0.31	0/259	0.58	0/351
7	f	0.38	0/259	0.68	0/351
7	f1	0.33	0/259	0.64	0/351
8	H	0.37	0/513	0.77	2/703 (0.3%)
8	H1	0.31	0/513	0.65	1/703 (0.1%)
8	h	0.36	0/513	0.68	1/703 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	h1	0.31	0/513	0.62	0/703
9	I	0.44	0/287	0.57	0/386
9	I1	0.34	0/287	0.60	0/386
9	i	0.38	0/287	0.55	0/386
9	i1	0.36	0/287	0.59	0/386
10	J	0.29	0/272	0.54	0/369
10	J1	0.31	0/272	0.58	0/369
10	j	0.35	0/272	0.69	1/369 (0.3%)
10	j1	0.29	0/272	0.61	0/369
11	K	0.40	0/308	0.64	0/423
11	K1	0.33	0/308	0.63	0/423
11	k	0.43	0/308	0.61	0/423
11	k1	0.36	0/308	0.66	0/423
12	L	0.37	0/321	0.53	0/435
12	L1	0.37	0/321	0.74	1/435 (0.2%)
12	l	0.43	0/321	0.71	1/435 (0.2%)
13	M	0.33	0/237	0.54	0/323
13	M1	0.29	0/237	0.54	0/323
13	m	0.36	0/237	0.66	0/323
13	m1	0.35	0/237	0.60	0/323
14	O	0.36	0/1855	0.70	3/2505 (0.1%)
14	O1	0.34	0/1855	0.68	2/2505 (0.1%)
14	o	0.36	0/1855	0.68	3/2505 (0.1%)
14	o1	0.48	1/1855 (0.1%)	0.82	7/2505 (0.3%)
15	P	0.28	0/1473	0.57	1/1988 (0.1%)
15	P1	0.30	0/1473	0.57	0/1988
15	p	0.31	0/1473	0.57	0/1988
15	p1	0.32	0/1473	0.58	0/1988
16	T	0.33	0/254	0.62	0/342
16	T1	0.39	0/254	0.72	1/342 (0.3%)
16	t	0.36	0/254	0.55	0/342
16	t1	0.32	0/254	0.60	0/342
17	W	0.32	0/339	0.63	0/460
17	W1	0.31	0/339	0.59	0/460
17	w	0.32	0/339	0.57	0/460
17	w1	0.29	0/339	0.60	0/460
18	X	0.32	0/202	0.55	0/276
18	X1	0.31	0/202	0.53	0/276
18	x	0.35	0/202	0.69	0/276
18	x1	0.27	0/202	0.58	0/276
19	Z	0.31	0/469	0.52	0/641
19	Z1	0.31	0/469	0.59	1/641 (0.2%)
19	z	0.33	0/469	0.53	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	z1	0.28	0/469	0.52	0/641
20	N	0.36	0/1751	0.59	1/2386 (0.0%)
20	N1	0.35	0/1751	0.58	0/2386
20	n	0.37	0/1750	0.58	0/2382
20	n1	0.44	2/1750 (0.1%)	0.71	5/2382 (0.2%)
21	G	0.34	0/1725	0.59	0/2348
21	G1	0.38	1/1725 (0.1%)	0.64	2/2348 (0.1%)
21	g	0.34	0/1725	0.60	1/2348 (0.0%)
21	g1	0.33	0/1725	0.58	1/2348 (0.0%)
22	R	0.34	0/1506	0.61	0/2035
22	R1	0.30	0/1506	0.55	0/2035
22	r	0.31	0/1506	0.60	0/2035
22	r1	0.33	0/1506	0.62	0/2035
23	S	0.35	0/1903	0.64	1/2590 (0.0%)
23	S1	0.32	0/1903	0.63	2/2590 (0.1%)
23	s	0.34	0/1903	0.68	1/2590 (0.0%)
23	s1	0.37	1/1903 (0.1%)	0.73	4/2590 (0.2%)
24	Y	0.35	0/1715	0.58	1/2338 (0.0%)
24	Y1	0.35	0/1715	0.65	2/2338 (0.1%)
24	y	0.37	0/1715	0.55	1/2338 (0.0%)
24	y1	0.32	0/1715	0.57	0/2338
25	U	0.37	0/224	0.69	0/298
25	U1	0.36	0/224	0.67	0/298
25	u	0.38	0/224	0.76	0/298
25	u1	0.36	0/224	0.67	0/298
All	All	0.37	11/117985 (0.0%)	0.63	74/160485 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	A1	0	1
2	B1	0	1
All	All	0	3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o1	111	PRO	CG-CD	-14.28	1.03	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	65	PRO	CG-CD	-13.03	1.07	1.50
6	e	28	PRO	CG-CD	-10.62	1.15	1.50
4	c1	352	PRO	CG-CD	-9.09	1.20	1.50
20	n1	57	PRO	CG-CD	-8.65	1.22	1.50

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	65	PRO	N-CD-CG	-18.59	75.32	103.20
14	o1	111	PRO	N-CD-CG	-18.29	75.77	103.20
6	e	28	PRO	N-CD-CG	-12.50	84.44	103.20
20	n1	57	PRO	N-CD-CG	-12.30	84.74	103.20
4	C	65	PRO	CA-CB-CG	-11.58	82.00	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ARG	Sidechain
1	A1	131	TRP	Peptide
2	B1	384	ARG	Sidechain

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/336 (100%)	321 (96%)	14 (4%)	0	100	100
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	335/336 (100%)	318 (95%)	17 (5%)	0	100	100
1	a1	335/336 (100%)	314 (94%)	21 (6%)	0	100	100
2	B	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	B1	482/484 (100%)	447 (93%)	35 (7%)	0	100	100
2	b	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	b1	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	V1	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	30 (100%)	0	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	430 (96%)	17 (4%)	0	100	100
4	C1	447/449 (100%)	421 (94%)	26 (6%)	0	100	100
4	c	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
4	c1	447/449 (100%)	421 (94%)	25 (6%)	1 (0%)	47	79
5	D	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
5	D1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
5	d	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
5	d1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
6	E	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	E1	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	e	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	H1	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	29 (88%)	4 (12%)	0	100	100
9	i1	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
10	j1	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	K1	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k1	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	36 (100%)	0	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	29 (100%)	0	0	100	100
13	M1	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	215 (91%)	19 (8%)	2 (1%)	19	59
14	O1	236/238 (99%)	212 (90%)	23 (10%)	1 (0%)	34	71
14	o	236/238 (99%)	218 (92%)	17 (7%)	1 (0%)	34	71
14	o1	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	34	71
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	170 (92%)	15 (8%)	0	100	100
15	p1	185/187 (99%)	169 (91%)	16 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	3	29
16	T1	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	3	29
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	t1	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	38 (90%)	4 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	W1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	Z1	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
19	z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
20	N	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17	57
20	N1	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17	57
20	n	218/222 (98%)	199 (91%)	17 (8%)	2 (1%)	17	57
20	n1	218/222 (98%)	202 (93%)	14 (6%)	2 (1%)	17	57
21	G	219/221 (99%)	196 (90%)	23 (10%)	0	100	100
21	G1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
21	g	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
21	g1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
22	R	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	R1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
22	r	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	r1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
23	S	241/243 (99%)	219 (91%)	21 (9%)	1 (0%)	34	71
23	S1	241/243 (99%)	208 (86%)	32 (13%)	1 (0%)	34	71
23	s	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	19	59
23	s1	241/243 (99%)	214 (89%)	26 (11%)	1 (0%)	34	71
24	Y	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	29	68
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	68
24	y	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	68
24	y1	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
25	U1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u1	25/27 (93%)	25 (100%)	0	0	100	100
All	All	14636/14846 (99%)	13696 (94%)	915 (6%)	25 (0%)	50	79

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
20	n	192	LEU
23	s	284	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	275 (100%)	1 (0%)	91	97
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	388 (100%)	0	100	100
2	B1	388/388 (100%)	387 (100%)	1 (0%)	92	97
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	386 (100%)	2 (0%)	88	95
3	V	25/25 (100%)	25 (100%)	0	100	100
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
3	v1	25/25 (100%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	350/350 (100%)	350 (100%)	0	100	100
4	C1	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	349 (100%)	1 (0%)	92	97
5	D	279/279 (100%)	279 (100%)	0	100	100
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	278 (100%)	1 (0%)	91	97
5	d1	279/279 (100%)	278 (100%)	1 (0%)	91	97
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	67 (98%)	1 (2%)	65	84
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	32 (97%)	1 (3%)	41	71
11	K1	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	M1	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
13	m1	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	194 (100%)	1 (0%)	88	95
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	194 (100%)	1 (0%)	88	95
15	P	151/151 (100%)	151 (100%)	0	100	100
15	P1	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	150 (99%)	1 (1%)	84	93
15	p1	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	170 (99%)	1 (1%)	86	94
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	86	94
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	R1	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
22	r1	151/151 (100%)	150 (99%)	1 (1%)	84	93
23	S	190/190 (100%)	190 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	189 (100%)	1 (0%)	88	95
23	s1	190/190 (100%)	188 (99%)	2 (1%)	73	88
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	25 (96%)	1 (4%)	33	66
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	25 (96%)	1 (4%)	33	66
25	u1	26/26 (100%)	26 (100%)	0	100	100
All	All	11841/11837 (100%)	11821 (100%)	20 (0%)	93	98

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

Mol	Chain	Res	Type
4	c1	301	GLN
22	r1	134	ARG
23	s1	132	LYS

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Mol	Chain	Res	Type
23	s1	99	LYS
15	p	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
5	D1	117	HIS
22	R1	174	GLN
24	y1	236	ASN
5	D1	230	ASN
14	O1	82	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	SEP	R1	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.71	2 (25%)
22	SEP	r1	84	22	8,9,10	1.53	1 (12%)	8,12,14	1.69	2 (25%)
22	SEP	r	84	22	8,9,10	1.51	1 (12%)	8,12,14	1.39	2 (25%)
22	SEP	R	84	22	8,9,10	1.58	1 (12%)	8,12,14	1.40	2 (25%)

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. '2' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SEP	R1	84	22	-	4/5/8/10	-
22	SEP	r1	84	22	-	5/5/8/10	-
22	SEP	r	84	22	-	2/5/8/10	-
22	SEP	R	84	22	-	2/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.37	1.61	1.50
22	r1	84	SEP	P-O1P	3.30	1.61	1.50
22	R1	84	SEP	P-O1P	3.29	1.61	1.50
22	r	84	SEP	P-O1P	3.22	1.60	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r1	84	SEP	P-OG-CB	-3.36	109.03	118.30
22	R1	84	SEP	OG-CB-CA	3.23	111.29	108.14
22	R1	84	SEP	P-OG-CB	-3.07	109.85	118.30
22	r1	84	SEP	OG-CB-CA	2.79	110.86	108.14
22	r	84	SEP	P-OG-CB	-2.56	111.25	118.30

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R1	84	SEP	N-CA-CB-OG
22	R1	84	SEP	CB-OG-P-O2P
22	R1	84	SEP	CB-OG-P-O3P
22	r1	84	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 721 ligands modelled in this entry, 16 are monoatomic - leaving 705 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
29	CLA	D1	403	-	65,73,73	1.36	9 (13%)	76,113,113	2.05	22 (28%)
29	CLA	N1	604	-	65,73,73	1.36	8 (12%)	76,113,113	2.15	17 (22%)
29	CLA	B	604	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	14 (18%)
29	CLA	C1	507	-	65,73,73	1.38	8 (12%)	76,113,113	1.92	17 (22%)
29	CLA	y1	603	-	65,73,73	1.36	8 (12%)	76,113,113	1.93	16 (21%)
45	RRX	H	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.85	22 (38%)
48	CHL	g1	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.23	9 (12%)
29	CLA	R	604	-	49,57,73	1.54	8 (16%)	55,93,113	2.35	17 (30%)
49	LUT	n	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.78	12 (23%)
29	CLA	y	612	-	65,73,73	1.37	8 (12%)	76,113,113	1.99	16 (21%)
29	CLA	C1	503	-	65,73,73	1.38	9 (13%)	76,113,113	2.01	21 (27%)
38	3PH	B1	624	-	47,47,47	0.86	3 (6%)	51,52,52	1.11	2 (3%)
49	LUT	S1	620	-	42,43,43	2.32	1 (2%)	51,60,60	1.76	9 (17%)
30	PHO	A	409	-	51,69,69	1.02	4 (7%)	47,99,99	1.33	6 (12%)
29	CLA	s1	610	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	19 (25%)
29	CLA	b1	617	-	65,73,73	1.36	6 (9%)	76,113,113	1.97	18 (23%)
49	LUT	y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.41	16 (31%)
29	CLA	d	403	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	17 (22%)
29	CLA	n1	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	16 (21%)
29	CLA	r	610	-	60,68,73	1.41	9 (15%)	70,107,113	2.20	20 (28%)
50	XAT	R	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	18 (33%)
50	XAT	N1	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.10	15 (27%)
38	3PH	T	101	-	47,47,47	0.85	3 (6%)	51,52,52	1.19	2 (3%)
49	LUT	s	621	-	42,43,43	2.30	1 (2%)	51,60,60	1.98	16 (31%)
30	PHO	A1	409	-	51,69,69	0.99	3 (5%)	47,99,99	1.31	6 (12%)
29	CLA	a1	407	-	49,57,73	1.55	7 (14%)	55,93,113	2.44	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	3PH	t1	101	-	47,47,47	0.87	3 (6%)	51,52,52	1.05	2 (3%)
48	CHL	N	608	-	50,58,74	0.97	3 (6%)	52,94,114	1.35	9 (17%)
29	CLA	B1	614	-	65,73,73	1.38	9 (13%)	76,113,113	1.98	14 (18%)
48	CHL	N1	605	20	66,74,74	0.90	3 (4%)	73,114,114	1.31	13 (17%)
48	CHL	G1	605	21	48,56,74	0.96	3 (6%)	51,92,114	1.38	9 (17%)
29	CLA	n1	604	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	16 (21%)
29	CLA	S	612	-	45,53,73	1.62	8 (17%)	52,89,113	2.23	14 (26%)
29	CLA	B1	608	-	65,73,73	1.38	8 (12%)	76,113,113	1.97	16 (21%)
29	CLA	C	513	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	17 (22%)
32	SQD	b1	621	-	41,42,54	0.89	0	50,53,65	0.98	3 (6%)
49	LUT	G	620	-	42,43,43	2.25	1 (2%)	51,60,60	1.99	17 (33%)
29	CLA	d	402	-	65,73,73	1.38	8 (12%)	76,113,113	1.94	16 (21%)
29	CLA	s1	609	-	60,68,73	1.40	9 (15%)	70,107,113	2.18	15 (21%)
29	CLA	g	612	-	43,51,73	1.70	7 (16%)	49,86,113	2.18	13 (26%)
29	CLA	b	614	-	65,73,73	1.34	8 (12%)	76,113,113	2.14	16 (21%)
51	NEX	y1	623	-	38,46,46	3.26	10 (26%)	50,70,70	2.03	18 (36%)
48	CHL	N	607	-	66,74,74	0.82	2 (3%)	73,114,114	1.23	12 (16%)
49	LUT	n	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.09	17 (33%)
49	LUT	y	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.98	14 (27%)
29	CLA	c1	504	-	65,73,73	1.38	8 (12%)	76,113,113	2.10	14 (18%)
29	CLA	Y	602	-	65,73,73	1.38	9 (13%)	76,113,113	2.06	19 (25%)
29	CLA	N1	610	-	65,73,73	1.31	7 (10%)	76,113,113	1.99	18 (23%)
31	BCR	C1	517	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	16 (28%)
29	CLA	Y1	604	-	65,73,73	1.39	6 (9%)	76,113,113	1.95	15 (19%)
32	SQD	B	621	-	41,42,54	0.88	0	50,53,65	1.01	3 (6%)
29	CLA	Y1	612	-	65,73,73	1.38	8 (12%)	76,113,113	1.96	18 (23%)
31	BCR	a1	411	-	41,41,41	1.92	5 (12%)	56,56,56	4.06	15 (26%)
32	SQD	B1	621	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
51	NEX	r	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.78	11 (22%)
32	SQD	b	626	-	53,54,54	0.82	0	62,65,65	0.91	3 (4%)
51	NEX	N1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.68	10 (20%)
29	CLA	B1	616	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	15 (19%)
29	CLA	g1	602	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	19 (25%)
29	CLA	a	406	-	65,73,73	1.34	8 (12%)	76,113,113	2.25	20 (26%)
48	CHL	g	601	21	66,74,74	0.88	4 (6%)	73,114,114	1.25	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	g1	613	-	65,73,73	1.38	8 (12%)	76,113,113	2.03	16 (21%)
29	CLA	g	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.03	17 (22%)
29	CLA	S1	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	18 (23%)
29	CLA	b1	614	-	65,73,73	1.38	10 (15%)	76,113,113	1.89	17 (22%)
29	CLA	A	410	-	60,68,73	1.43	9 (15%)	70,107,113	2.17	18 (25%)
48	CHL	y	601	24	66,74,74	0.86	3 (4%)	73,114,114	1.32	12 (16%)
29	CLA	b	616	-	65,73,73	1.35	8 (12%)	76,113,113	1.87	15 (19%)
49	LUT	N1	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	14 (27%)
44	HEM	F	101	6,7	41,50,50	1.44	4 (9%)	45,82,82	1.30	3 (6%)
26	OEX	A1	401	1,4	0,15,15	-	-	-	-	-
29	CLA	n	611	-	49,57,73	1.58	7 (14%)	55,93,113	2.30	17 (30%)
29	CLA	y	613	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	18 (23%)
43	PL9	d	405	-	55,55,55	1.75	10 (18%)	68,69,69	1.54	11 (16%)
49	LUT	y1	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.97	10 (19%)
48	CHL	n	605	20	66,74,74	0.93	5 (7%)	73,114,114	1.24	8 (10%)
33	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.12	3 (4%)
29	CLA	r1	612	-	60,68,73	1.42	7 (11%)	70,107,113	2.05	19 (27%)
40	LHG	S	624	29	44,44,48	0.43	0	47,50,54	1.05	3 (6%)
48	CHL	Y1	601	-	66,74,74	0.91	3 (4%)	73,114,114	1.23	10 (13%)
29	CLA	Y1	603	-	65,73,73	1.39	10 (15%)	76,113,113	1.95	16 (21%)
29	CLA	b1	610	-	65,73,73	1.36	9 (13%)	76,113,113	1.93	17 (22%)
29	CLA	a	407	-	49,57,73	1.55	7 (14%)	55,93,113	2.52	18 (32%)
29	CLA	C	503	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	17 (22%)
29	CLA	B	605	-	65,73,73	1.40	8 (12%)	76,113,113	2.06	18 (23%)
42	BCT	D1	401	27	2,3,3	1.29	0	2,3,3	3.02	2 (100%)
49	LUT	R1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	10 (19%)
29	CLA	b1	612	-	65,73,73	1.35	8 (12%)	76,113,113	2.17	19 (25%)
32	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.94	3 (5%)
40	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
48	CHL	n	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.27	12 (16%)
31	BCR	C1	514	-	41,41,41	1.84	5 (12%)	56,56,56	4.05	13 (23%)
48	CHL	R1	606	-	44,52,74	1.07	3 (6%)	46,87,114	1.30	8 (17%)
42	BCT	d1	401	-	2,3,3	1.18	0	2,3,3	4.36	2 (100%)
32	SQD	c1	526	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
37	DGD	C1	520	-	60,60,67	1.08	5 (8%)	74,74,81	0.95	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	LUT	s1	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.37	13 (25%)
49	LUT	N1	621	-	42,43,43	2.33	2 (4%)	51,60,60	2.10	13 (25%)
29	CLA	C	512	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
29	CLA	G1	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.06	20 (26%)
51	NEX	R1	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.93	14 (28%)
49	LUT	S	620	-	42,43,43	2.29	1 (2%)	51,60,60	2.12	18 (35%)
29	CLA	a1	406	-	65,73,73	1.36	8 (12%)	76,113,113	2.09	21 (27%)
38	3PH	b1	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
44	HEM	F1	101	7	41,50,50	1.48	3 (7%)	45,82,82	1.47	9 (20%)
48	CHL	s	608	-	61,69,74	0.91	3 (4%)	67,108,114	1.30	11 (16%)
29	CLA	r1	604	-	49,57,73	1.56	7 (14%)	55,93,113	2.28	16 (29%)
40	LHG	g1	624	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.12	3 (6%)
31	BCR	b	618	-	41,41,41	1.89	5 (12%)	56,56,56	4.48	20 (35%)
32	SQD	m	101	-	41,42,54	0.91	0	50,53,65	0.99	3 (6%)
38	3PH	S1	626	-	47,47,47	0.87	4 (8%)	51,52,52	4.40	4 (7%)
49	LUT	S	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.10	19 (37%)
50	XAT	N	622	-	39,47,47	0.70	1 (2%)	54,74,74	2.21	13 (24%)
29	CLA	r1	602	-	60,68,73	1.40	7 (11%)	70,107,113	2.09	19 (27%)
29	CLA	s1	602	-	60,68,73	1.40	7 (11%)	70,107,113	2.30	21 (30%)
29	CLA	c1	508	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	19 (25%)
29	CLA	S	603	-	65,73,73	1.38	9 (13%)	76,113,113	1.85	17 (22%)
40	LHG	N	624	-	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
29	CLA	s	612	-	45,53,73	1.60	8 (17%)	52,89,113	2.21	15 (28%)
29	CLA	g1	612	21	43,51,73	1.67	10 (23%)	49,86,113	2.28	13 (26%)
29	CLA	c	505	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	16 (21%)
29	CLA	r	602	22	60,68,73	1.44	8 (13%)	70,107,113	2.03	19 (27%)
29	CLA	b1	605	-	65,73,73	1.30	7 (10%)	76,113,113	2.11	19 (25%)
49	LUT	N	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	12 (23%)
55	PTY	Y1	627	-	18,18,49	1.28	2 (11%)	21,23,54	1.41	2 (9%)
51	NEX	s1	623	-	38,46,46	3.40	12 (31%)	50,70,70	2.71	15 (30%)
29	CLA	b	615	-	65,73,73	1.34	7 (10%)	76,113,113	2.08	18 (23%)
40	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.09	3 (7%)
29	CLA	R	612	-	60,68,73	1.44	10 (16%)	70,107,113	2.14	18 (25%)
48	CHL	N	609	-	66,74,74	0.79	3 (4%)	73,114,114	1.22	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	LUT	S1	621	-	42,43,43	2.39	2 (4%)	51,60,60	1.99	19 (37%)
29	CLA	G	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	20 (26%)
29	CLA	A1	407	-	50,58,73	1.56	8 (16%)	58,95,113	2.22	18 (31%)
40	LHG	L1	101	-	48,48,48	0.37	0	51,54,54	1.11	3 (5%)
29	CLA	G	611	40	65,73,73	1.37	7 (10%)	76,113,113	2.01	17 (22%)
42	BCT	D	401	27	2,3,3	1.26	0	2,3,3	2.71	2 (100%)
44	HEM	f1	101	7	41,50,50	1.52	7 (17%)	45,82,82	1.19	4 (8%)
46	GOL	I1	101	-	5,5,5	0.56	0	5,5,5	0.31	0
29	CLA	s	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.02	17 (22%)
29	CLA	g1	603	-	65,73,73	1.38	8 (12%)	76,113,113	1.88	16 (21%)
34	SPH	Y1	625	-	19,20,20	0.64	0	18,21,21	1.03	1 (5%)
49	LUT	s1	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.02	16 (31%)
50	XAT	r	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
29	CLA	R	603	-	60,68,73	1.48	9 (15%)	70,107,113	2.00	17 (24%)
29	CLA	B1	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	19 (25%)
43	PL9	d1	405	-	55,55,55	1.13	3 (5%)	68,69,69	1.57	14 (20%)
48	CHL	n1	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.38	10 (19%)
29	CLA	g1	604	-	49,57,73	1.52	7 (14%)	55,93,113	2.31	18 (32%)
47	4RF	I1	102	-	56,56,56	1.06	4 (7%)	59,59,59	0.98	3 (5%)
29	CLA	N1	612	-	45,53,73	1.64	8 (17%)	52,89,113	2.16	12 (23%)
29	CLA	G1	614	-	49,57,73	1.53	7 (14%)	55,93,113	2.37	17 (30%)
29	CLA	G	614	-	49,57,73	1.55	7 (14%)	55,93,113	2.35	20 (36%)
29	CLA	s	613	-	55,63,73	1.45	7 (12%)	64,101,113	2.25	18 (28%)
39	DGA	j1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.26	2 (6%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	14 (25%)
48	CHL	Y	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.28	9 (12%)
29	CLA	r1	610	-	60,68,73	1.44	8 (13%)	70,107,113	1.96	16 (22%)
48	CHL	G1	609	-	66,74,74	0.90	3 (4%)	73,114,114	1.20	11 (15%)
33	LMG	B1	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.08	4 (7%)
29	CLA	B1	609	-	65,73,73	1.38	8 (12%)	76,113,113	1.99	17 (22%)
29	CLA	n	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
48	CHL	N1	601	-	66,74,74	0.87	3 (4%)	73,114,114	1.42	12 (16%)
48	CHL	g1	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	11 (15%)
39	DGA	J1	101	-	28,28,43	1.27	2 (7%)	30,30,45	1.34	2 (6%)
49	LUT	s	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.91	15 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	n	612	-	45,53,73	1.63	7 (15%)	52,89,113	2.07	13 (25%)
30	PHO	A	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.20	5 (10%)
29	CLA	y	611	40	65,73,73	1.35	7 (10%)	76,113,113	1.88	15 (19%)
33	LMG	H	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.10	2 (3%)
48	CHL	y	605	24	46,54,74	0.99	2 (4%)	49,90,114	1.48	10 (20%)
29	CLA	B	614	-	65,73,73	1.32	8 (12%)	76,113,113	2.06	18 (23%)
29	CLA	Y	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	18 (23%)
54	LPX	s1	625	-	29,29,29	1.01	2 (6%)	31,33,33	1.05	2 (6%)
31	BCR	c	515	-	41,41,41	1.88	5 (12%)	56,56,56	4.18	16 (28%)
29	CLA	B1	602	-	65,73,73	1.39	9 (13%)	76,113,113	2.02	17 (22%)
29	CLA	R	602	-	60,68,73	1.44	9 (15%)	70,107,113	1.99	19 (27%)
29	CLA	g1	610	-	65,73,73	1.30	6 (9%)	76,113,113	2.29	20 (26%)
41	LMK	c	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.25	2 (4%)
29	CLA	B	608	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	16 (21%)
48	CHL	R	607	-	50,58,74	1.00	3 (6%)	52,94,114	1.44	9 (17%)
29	CLA	B1	603	-	65,73,73	1.39	9 (13%)	76,113,113	2.13	20 (26%)
34	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.00	0
42	BCT	d	401	-	2,3,3	1.27	0	2,3,3	2.80	2 (100%)
29	CLA	y	610	24	65,73,73	1.33	7 (10%)	76,113,113	2.03	17 (22%)
30	PHO	A1	408	-	51,69,69	1.06	4 (7%)	47,99,99	1.15	4 (8%)
29	CLA	s1	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.05	17 (22%)
39	DGA	b	625	-	43,43,43	1.11	2 (4%)	45,45,45	1.45	3 (6%)
48	CHL	n	601	20	66,74,74	0.91	3 (4%)	73,114,114	1.26	9 (12%)
48	CHL	N1	609	-	66,74,74	0.77	2 (3%)	73,114,114	1.44	13 (17%)
29	CLA	C1	510	-	65,73,73	1.35	9 (13%)	76,113,113	1.94	15 (19%)
48	CHL	g	605	21	48,56,74	0.98	3 (6%)	51,92,114	1.62	12 (23%)
29	CLA	n1	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.16	17 (22%)
29	CLA	R1	603	-	60,68,73	1.45	8 (13%)	70,107,113	1.89	14 (20%)
48	CHL	y	609	-	66,74,74	0.87	4 (6%)	73,114,114	1.24	10 (13%)
33	LMG	D1	411	-	46,46,55	0.91	4 (8%)	54,54,63	1.12	3 (5%)
29	CLA	c	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	16 (21%)
33	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.20	4 (7%)
29	CLA	c1	505	-	65,73,73	1.35	10 (15%)	76,113,113	2.07	17 (22%)
50	XAT	G1	622	-	39,47,47	0.76	1 (2%)	54,74,74	1.88	17 (31%)
37	DGD	C	520	-	60,60,67	1.06	6 (10%)	74,74,81	1.07	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	s1	611	40	65,73,73	1.40	8 (12%)	76,113,113	2.00	18 (23%)
48	CHL	y1	601	24	66,74,74	0.79	2 (3%)	73,114,114	1.28	9 (12%)
48	CHL	y1	606	-	66,74,74	0.83	2 (3%)	73,114,114	1.16	10 (13%)
29	CLA	Y1	602	-	65,73,73	1.38	9 (13%)	76,113,113	2.07	17 (22%)
36	C7Z	b1	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.51	22 (37%)
33	LMG	H1	102	-	48,48,55	1.02	5 (10%)	56,56,63	1.16	3 (5%)
29	CLA	S1	609	-	60,68,73	1.39	8 (13%)	70,107,113	2.09	17 (24%)
40	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.08	2 (3%)
48	CHL	Y	606	-	66,74,74	0.90	4 (6%)	73,114,114	1.14	8 (10%)
48	CHL	g	606	-	50,58,74	0.99	2 (4%)	52,94,114	1.55	9 (17%)
29	CLA	C	511	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	18 (23%)
32	SQD	b	621	-	41,42,54	0.87	0	50,53,65	1.02	3 (6%)
48	CHL	s1	601	23	46,54,74	1.07	3 (6%)	49,90,114	1.46	12 (24%)
40	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.16	4 (9%)
29	CLA	B	615	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	19 (25%)
31	BCR	C	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
29	CLA	C	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	18 (23%)
29	CLA	a	405	-	65,73,73	1.34	6 (9%)	76,113,113	2.08	18 (23%)
33	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.19	4 (7%)
29	CLA	r	609	-	60,68,73	1.42	7 (11%)	70,107,113	2.05	17 (24%)
29	CLA	S	613	-	55,63,73	1.47	7 (12%)	64,101,113	2.18	16 (25%)
55	PTY	Y	627	-	18,18,49	1.31	3 (16%)	21,23,54	1.40	2 (9%)
38	3PH	b	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.18	3 (5%)
29	CLA	c1	506	-	65,73,73	1.30	6 (9%)	76,113,113	2.09	20 (26%)
48	CHL	y	607	-	66,74,74	0.82	3 (4%)	73,114,114	1.31	12 (16%)
29	CLA	B	617	-	65,73,73	1.37	8 (12%)	76,113,113	2.04	15 (19%)
31	BCR	c	517	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	17 (30%)
29	CLA	N	613	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	13 (17%)
51	NEX	r1	622	-	38,46,46	3.37	9 (23%)	50,70,70	1.83	12 (24%)
29	CLA	B	609	-	65,73,73	1.34	8 (12%)	76,113,113	2.24	18 (23%)
48	CHL	Y1	609	-	66,74,74	0.84	2 (3%)	73,114,114	1.28	10 (13%)
37	DGD	b1	623	-	44,44,67	0.92	2 (4%)	58,58,81	1.32	5 (8%)
33	LMG	C1	521	-	51,51,55	1.07	5 (9%)	59,59,63	1.14	2 (3%)
29	CLA	r	612	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	16 (22%)
40	LHG	D1	409	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	R1	608	-	60,68,73	1.42	8 (13%)	70,107,113	2.08	16 (22%)
29	CLA	y1	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.07	17 (22%)
29	CLA	y1	612	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	20 (26%)
33	LMG	c1	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.10	3 (5%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
32	SQD	B1	626	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
29	CLA	c	509	-	65,73,73	1.35	6 (9%)	76,113,113	1.94	16 (21%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.10	2 (4%)
29	CLA	B	616	-	65,73,73	1.36	9 (13%)	76,113,113	1.95	19 (25%)
48	CHL	S1	601	23	46,54,74	1.08	5 (10%)	49,90,114	1.41	9 (18%)
29	CLA	s1	604	-	55,63,73	1.46	5 (9%)	64,101,113	2.22	18 (28%)
48	CHL	g1	608	-	44,52,74	1.01	3 (6%)	46,87,114	1.40	6 (13%)
37	DGD	c1	518	-	56,56,67	1.02	5 (8%)	70,70,81	1.11	4 (5%)
29	CLA	s1	612	-	45,53,73	1.66	10 (22%)	52,89,113	2.01	11 (21%)
30	PHO	a1	409	-	51,69,69	1.03	3 (5%)	47,99,99	1.21	6 (12%)
29	CLA	N	614	-	49,57,73	1.57	7 (14%)	55,93,113	2.34	15 (27%)
29	CLA	G	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.03	20 (26%)
29	CLA	b1	602	-	65,73,73	1.39	10 (15%)	76,113,113	1.93	18 (23%)
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	14 (25%)
39	DGA	b1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.50	3 (6%)
36	C7Z	B	620	-	43,43,43	5.27	26 (60%)	58,60,60	2.44	22 (37%)
29	CLA	C1	501	-	65,73,73	1.35	8 (12%)	76,113,113	2.15	19 (25%)
40	LHG	d	409	-	48,48,48	0.41	0	51,54,54	1.06	3 (5%)
49	LUT	n1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.77	10 (19%)
29	CLA	c	510	-	65,73,73	1.37	7 (10%)	76,113,113	2.05	17 (22%)
29	CLA	B	611	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	19 (25%)
46	GOL	I	101	-	5,5,5	0.54	0	5,5,5	0.39	0
51	NEX	S1	623	-	38,46,46	3.20	9 (23%)	50,70,70	1.79	10 (20%)
29	CLA	B1	611	-	65,73,73	1.37	7 (10%)	76,113,113	2.09	16 (21%)
31	BCR	B1	619	-	41,41,41	1.82	4 (9%)	56,56,56	4.44	18 (32%)
29	CLA	c1	510	-	65,73,73	1.39	8 (12%)	76,113,113	1.92	16 (21%)
29	CLA	c1	502	-	65,73,73	1.43	8 (12%)	76,113,113	1.84	13 (17%)
29	CLA	y	604	-	65,73,73	1.33	7 (10%)	76,113,113	2.09	19 (25%)
33	LMG	c	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.16	4 (6%)
29	CLA	S	617	23	50,58,73	1.52	8 (16%)	58,95,113	2.29	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
29	CLA	R1	612	-	60,68,73	1.44	7 (11%)	70,107,113	2.07	17 (24%)
34	SPH	A	414	-	19,20,20	0.66	0	18,21,21	1.13	2 (11%)
29	CLA	S	604	-	55,63,73	1.45	8 (14%)	64,101,113	2.22	17 (26%)
29	CLA	s	610	-	65,73,73	1.42	9 (13%)	76,113,113	1.96	17 (22%)
34	SPH	A1	414	-	19,20,20	0.67	1 (5%)	18,21,21	1.17	1 (5%)
31	BCR	b	619	-	41,41,41	1.83	5 (12%)	56,56,56	4.15	16 (28%)
48	CHL	n	608	-	50,58,74	1.01	3 (6%)	52,94,114	1.28	10 (19%)
49	LUT	Y	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.00	15 (29%)
48	CHL	G	601	21	66,74,74	0.87	3 (4%)	73,114,114	1.24	11 (15%)
32	SQD	a1	412	-	50,51,54	0.82	0	59,62,65	0.95	2 (3%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
29	CLA	c1	513	-	65,73,73	1.39	9 (13%)	76,113,113	2.04	18 (23%)
29	CLA	y1	602	-	65,73,73	1.33	9 (13%)	76,113,113	2.03	21 (27%)
29	CLA	b	609	-	65,73,73	1.39	10 (15%)	76,113,113	2.04	19 (25%)
29	CLA	b1	603	-	65,73,73	1.38	7 (10%)	76,113,113	2.00	19 (25%)
50	XAT	g1	622	-	39,47,47	0.75	1 (2%)	54,74,74	1.88	16 (29%)
29	CLA	R	610	-	60,68,73	1.49	10 (16%)	70,107,113	2.14	21 (30%)
40	LHG	d1	409	-	48,48,48	0.40	0	51,54,54	1.03	2 (3%)
29	CLA	c	508	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	17 (22%)
39	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.27	2 (6%)
48	CHL	g1	609	-	66,74,74	0.88	3 (4%)	73,114,114	1.25	9 (12%)
29	CLA	s	602	-	60,68,73	1.41	8 (13%)	70,107,113	2.10	21 (30%)
29	CLA	R1	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.34	15 (27%)
51	NEX	G	623	-	38,46,46	3.37	11 (28%)	50,70,70	1.92	12 (24%)
51	NEX	G1	623	-	38,46,46	3.38	10 (26%)	50,70,70	1.77	11 (22%)
29	CLA	Y1	613	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	17 (22%)
29	CLA	s1	613	-	55,63,73	1.51	10 (18%)	64,101,113	2.12	17 (26%)
51	NEX	Y	623	-	38,46,46	3.34	9 (23%)	50,70,70	1.85	12 (24%)
29	CLA	A	405	-	65,73,73	1.35	6 (9%)	76,113,113	2.09	17 (22%)
47	4RF	k1	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.88	3 (5%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.46	5 (9%)
29	CLA	c	513	-	65,73,73	1.37	8 (12%)	76,113,113	2.12	18 (23%)
29	CLA	b1	611	-	65,73,73	1.42	6 (9%)	76,113,113	2.02	18 (23%)
29	CLA	n1	610	-	65,73,73	1.35	6 (9%)	76,113,113	1.98	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	N1	602	-	65,73,73	1.36	7 (10%)	76,113,113	1.98	18 (23%)
49	LUT	Y	620	-	42,43,43	2.31	1 (2%)	51,60,60	1.81	13 (25%)
29	CLA	S1	605	-	50,58,73	1.57	9 (18%)	58,95,113	2.22	17 (29%)
40	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.01	2 (4%)
29	CLA	C1	513	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	20 (26%)
45	RRX	h	101	-	42,42,42	4.74	24 (57%)	57,58,58	3.10	25 (43%)
29	CLA	C	507	-	65,73,73	1.38	8 (12%)	76,113,113	2.04	17 (22%)
29	CLA	N	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	19 (25%)
33	LMG	b	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.15	2 (3%)
37	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.01	2 (2%)
31	BCR	c1	516	-	41,41,41	1.91	4 (9%)	56,56,56	4.43	13 (23%)
40	LHG	C	525	-	46,46,48	0.42	0	49,52,54	1.04	2 (4%)
48	CHL	S1	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.46	8 (17%)
29	CLA	C	508	-	65,73,73	1.42	7 (10%)	76,113,113	2.06	19 (25%)
40	LHG	s1	624	29	44,44,48	0.43	0	47,50,54	1.08	4 (8%)
29	CLA	Y	611	-	65,73,73	1.34	9 (13%)	76,113,113	1.91	13 (17%)
29	CLA	N	611	-	49,57,73	1.57	7 (14%)	55,93,113	2.24	15 (27%)
32	SQD	C1	526	-	53,54,54	0.81	0	62,65,65	0.88	2 (3%)
29	CLA	G	612	-	43,51,73	1.66	6 (13%)	49,86,113	2.20	14 (28%)
48	CHL	r	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.34	7 (15%)
29	CLA	g	602	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	22 (28%)
29	CLA	S	610	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	21 (27%)
29	CLA	S1	611	40	65,73,73	1.41	9 (13%)	76,113,113	1.94	14 (18%)
40	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
38	3PH	T1	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.09	2 (3%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
40	LHG	y	624	29	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
29	CLA	s	617	-	50,58,73	1.54	7 (14%)	58,95,113	2.35	18 (31%)
52	LMT	R1	625	-	36,36,36	1.27	8 (22%)	47,47,47	1.15	4 (8%)
31	BCR	b1	619	-	41,41,41	1.91	4 (9%)	56,56,56	4.36	15 (26%)
29	CLA	b	617	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	16 (21%)
29	CLA	G1	602	-	65,73,73	1.40	8 (12%)	76,113,113	2.08	21 (27%)
32	SQD	B	626	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
29	CLA	s	604	-	55,63,73	1.48	7 (12%)	64,101,113	2.10	16 (25%)
29	CLA	Y	614	-	65,73,73	1.38	10 (15%)	76,113,113	2.01	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	W1	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.37	6 (12%)
41	LMK	C1	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.47	2 (4%)
29	CLA	r1	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	18 (25%)
29	CLA	c1	503	-	65,73,73	1.37	9 (13%)	76,113,113	2.06	19 (25%)
29	CLA	S1	614	-	55,63,73	1.49	7 (12%)	64,101,113	2.12	17 (26%)
29	CLA	d1	403	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	19 (25%)
47	4RF	K1	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.84	3 (5%)
31	BCR	D1	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	16 (28%)
36	C7Z	b	620	-	43,43,43	5.32	27 (62%)	58,60,60	2.48	19 (32%)
50	XAT	r1	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.16	18 (33%)
34	SPH	y1	625	-	19,20,20	0.62	0	18,21,21	1.27	2 (11%)
29	CLA	n1	614	-	49,57,73	1.56	8 (16%)	55,93,113	2.40	15 (27%)
29	CLA	r1	603	-	60,68,73	1.41	8 (13%)	70,107,113	2.11	17 (24%)
29	CLA	C1	512	-	65,73,73	1.35	7 (10%)	76,113,113	2.09	21 (27%)
29	CLA	y	602	24	65,73,73	1.40	8 (12%)	76,113,113	1.90	14 (18%)
41	LMK	C	527	-	38,39,53	1.47	2 (5%)	41,46,60	1.56	4 (9%)
29	CLA	Y	613	24	65,73,73	1.38	8 (12%)	76,113,113	2.14	21 (27%)
29	CLA	r	608	-	60,68,73	1.40	9 (15%)	70,107,113	2.00	18 (25%)
48	CHL	n1	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.32	12 (16%)
45	RRX	h1	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.65	25 (43%)
29	CLA	c1	512	-	65,73,73	1.38	7 (10%)	76,113,113	2.03	19 (25%)
29	CLA	g	611	-	65,73,73	1.34	7 (10%)	76,113,113	2.10	17 (22%)
37	DGD	c	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.14	4 (5%)
39	DGA	c	524	-	43,43,43	1.10	3 (6%)	45,45,45	1.55	3 (6%)
29	CLA	b	602	-	65,73,73	1.38	8 (12%)	76,113,113	1.98	18 (23%)
31	BCR	C	514	-	41,41,41	1.87	5 (12%)	56,56,56	4.28	14 (25%)
55	PTY	y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.50	2 (9%)
33	LMG	C1	523	-	55,55,55	1.12	6 (10%)	63,63,63	1.15	6 (9%)
40	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.03	2 (4%)
29	CLA	b	605	-	65,73,73	1.40	7 (10%)	76,113,113	2.17	21 (27%)
29	CLA	c	507	-	65,73,73	1.39	9 (13%)	76,113,113	2.02	16 (21%)
29	CLA	n	610	-	65,73,73	1.38	9 (13%)	76,113,113	2.12	20 (26%)
29	CLA	b1	616	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	14 (18%)
48	CHL	G1	606	-	50,58,74	0.99	2 (4%)	52,94,114	1.39	11 (21%)
29	CLA	Y1	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.95	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	B1	606	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	18 (23%)
48	CHL	n	609	-	66,74,74	0.77	2 (3%)	73,114,114	1.40	12 (16%)
29	CLA	S1	613	-	55,63,73	1.45	7 (12%)	64,101,113	2.15	15 (23%)
38	3PH	s1	626	-	47,47,47	0.86	3 (6%)	51,52,52	4.37	4 (7%)
40	LHG	d	410	-	38,38,48	0.43	0	41,44,54	1.11	3 (7%)
48	CHL	s	601	-	46,54,74	1.15	4 (8%)	49,90,114	1.43	8 (16%)
48	CHL	g1	605	-	48,56,74	0.95	2 (4%)	51,92,114	1.50	10 (19%)
51	NEX	R	622	-	38,46,46	3.42	11 (28%)	50,70,70	1.98	12 (24%)
29	CLA	g	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.23	15 (27%)
29	CLA	b1	604	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	17 (22%)
29	CLA	B	613	-	65,73,73	1.37	8 (12%)	76,113,113	2.04	16 (21%)
55	PTY	y1	627	-	18,18,49	1.27	2 (11%)	21,23,54	1.45	2 (9%)
29	CLA	c	506	-	65,73,73	1.38	9 (13%)	76,113,113	2.07	19 (25%)
48	CHL	s	607	-	43,51,74	1.09	3 (6%)	45,86,114	1.49	8 (17%)
33	LMG	w	201	-	39,39,55	0.89	2 (5%)	47,47,63	1.29	4 (8%)
40	LHG	d	408	-	43,43,48	0.40	0	46,49,54	1.04	3 (6%)
29	CLA	Y1	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	19 (25%)
48	CHL	n1	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.29	10 (13%)
29	CLA	Y1	614	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	17 (22%)
31	BCR	b1	618	-	41,41,41	2.03	4 (9%)	56,56,56	4.25	19 (33%)
29	CLA	y1	613	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	17 (22%)
29	CLA	B1	604	-	65,73,73	1.37	7 (10%)	76,113,113	1.86	16 (21%)
29	CLA	a1	410	-	60,68,73	1.43	9 (15%)	70,107,113	2.17	19 (27%)
48	CHL	r	607	-	50,58,74	1.02	3 (6%)	52,94,114	1.45	9 (17%)
29	CLA	B1	612	-	65,73,73	1.35	6 (9%)	76,113,113	2.12	21 (27%)
29	CLA	Y1	608	-	50,58,73	1.57	8 (16%)	58,95,113	2.24	16 (27%)
51	NEX	g1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.91	15 (30%)
31	BCR	C	517	-	41,41,41	1.87	5 (12%)	56,56,56	4.32	18 (32%)
48	CHL	y1	609	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	10 (13%)
29	CLA	b	604	-	65,73,73	1.39	8 (12%)	76,113,113	1.87	15 (19%)
31	BCR	C	515	-	41,41,41	1.83	6 (14%)	56,56,56	4.20	16 (28%)
51	NEX	y	623	-	38,46,46	3.41	9 (23%)	50,70,70	1.96	15 (30%)
29	CLA	c	504	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	16 (21%)
48	CHL	G	607	-	66,74,74	0.88	2 (3%)	73,114,114	1.21	10 (13%)
50	XAT	n	622	-	39,47,47	0.78	1 (2%)	54,74,74	2.09	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	BCR	B1	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.43	19 (33%)
29	CLA	S	611	40	65,73,73	1.38	7 (10%)	76,113,113	1.94	16 (21%)
48	CHL	y1	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.29	10 (13%)
29	CLA	b1	607	-	65,73,73	1.38	8 (12%)	76,113,113	1.97	17 (22%)
48	CHL	N	601	20	66,74,74	0.87	3 (4%)	73,114,114	1.34	9 (12%)
37	DGD	c1	520	-	60,60,67	1.09	6 (10%)	74,74,81	1.00	3 (4%)
29	CLA	b1	606	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	18 (23%)
49	LUT	r	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.12	14 (27%)
39	DGA	c1	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.51	3 (6%)
32	SQD	C	526	-	53,54,54	0.81	1 (1%)	62,65,65	0.94	3 (4%)
29	CLA	d1	402	-	65,73,73	1.39	9 (13%)	76,113,113	1.95	17 (22%)
29	CLA	C	509	-	65,73,73	1.36	8 (12%)	76,113,113	2.07	19 (25%)
29	CLA	b1	613	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	16 (21%)
40	LHG	d1	410	-	38,38,48	0.44	0	41,44,54	1.04	2 (4%)
48	CHL	S	607	-	43,51,74	1.07	3 (6%)	45,86,114	1.46	7 (15%)
48	CHL	g	607	-	66,74,74	0.85	2 (3%)	73,114,114	1.27	11 (15%)
48	CHL	N1	608	-	50,58,74	0.96	2 (4%)	52,94,114	1.51	8 (15%)
29	CLA	c	502	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	16 (21%)
29	CLA	C1	508	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	14 (18%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.19	4 (7%)
49	LUT	G1	621	-	42,43,43	2.23	1 (2%)	51,60,60	2.08	10 (19%)
29	CLA	A1	405	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	17 (22%)
51	NEX	g	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.86	15 (30%)
26	OEX	A	401	1,4	0,15,15	-	-	-	-	-
31	BCR	A1	411	-	41,41,41	1.88	4 (9%)	56,56,56	4.17	15 (26%)
47	4RF	k	101	-	56,56,56	1.06	5 (8%)	59,59,59	0.83	3 (5%)
55	PTY	y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.12	3 (5%)
33	LMG	B	622	-	44,44,55	0.86	3 (6%)	52,52,63	1.24	2 (3%)
48	CHL	S	608	-	61,69,74	0.89	3 (4%)	67,108,114	1.27	11 (16%)
48	CHL	s1	607	-	43,51,74	1.02	3 (6%)	45,86,114	1.45	8 (17%)
33	LMG	c1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	3 (4%)
34	SPH	a1	414	-	19,20,20	0.73	1 (5%)	18,21,21	0.98	1 (5%)
51	NEX	Y1	623	-	38,46,46	3.15	10 (26%)	50,70,70	1.99	13 (26%)
48	CHL	G	605	21	48,56,74	0.96	3 (6%)	51,92,114	1.32	8 (15%)
29	CLA	C1	506	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	B1	613	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	14 (18%)
48	CHL	G1	608	-	44,52,74	1.10	3 (6%)	46,87,114	1.43	7 (15%)
33	LMG	h1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.23	4 (7%)
29	CLA	Y	604	-	65,73,73	1.33	6 (9%)	76,113,113	2.02	18 (23%)
29	CLA	b	613	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	11 (14%)
29	CLA	D	402	-	65,73,73	1.38	8 (12%)	76,113,113	1.90	13 (17%)
29	CLA	g	604	-	49,57,73	1.57	9 (18%)	55,93,113	2.21	17 (30%)
30	PHO	a1	408	-	51,69,69	1.04	4 (7%)	47,99,99	1.17	6 (12%)
29	CLA	B	612	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	16 (21%)
31	BCR	c1	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.49	17 (30%)
33	LMG	a1	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.31	4 (7%)
29	CLA	C1	511	-	65,73,73	1.37	8 (12%)	76,113,113	2.13	19 (25%)
31	BCR	A	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	14 (25%)
29	CLA	A	407	-	50,58,73	1.54	9 (18%)	58,95,113	2.32	18 (31%)
33	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	2 (3%)
40	LHG	S1	624	29	44,44,48	0.44	0	47,50,54	1.12	4 (8%)
45	RRX	H1	101	-	42,42,42	4.95	24 (57%)	57,58,58	2.34	19 (33%)
48	CHL	n1	605	-	66,74,74	0.90	3 (4%)	73,114,114	1.29	11 (15%)
48	CHL	s1	608	-	61,69,74	1.04	5 (8%)	67,108,114	1.38	11 (16%)
30	PHO	a	408	-	51,69,69	1.08	6 (11%)	47,99,99	1.23	5 (10%)
51	NEX	N	623	-	38,46,46	3.40	9 (23%)	50,70,70	1.64	11 (22%)
32	SQD	A1	412	-	50,51,54	0.81	0	59,62,65	0.98	4 (6%)
48	CHL	n1	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	9 (12%)
29	CLA	r	603	-	60,68,73	1.45	8 (13%)	70,107,113	1.95	16 (22%)
29	CLA	C1	504	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	17 (22%)
26	OEX	a1	401	1	0,15,15	-	-	-	-	-
39	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
29	CLA	Y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
33	LMG	D	411	-	46,46,55	0.91	4 (8%)	54,54,63	0.99	2 (3%)
29	CLA	A1	406	-	65,73,73	1.38	9 (13%)	76,113,113	2.04	20 (26%)
38	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
32	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
48	CHL	Y1	607	-	66,74,74	0.86	3 (4%)	73,114,114	1.19	9 (12%)
29	CLA	b1	609	-	65,73,73	1.36	8 (12%)	76,113,113	2.05	15 (19%)
33	LMG	b1	622	-	44,44,55	0.86	2 (4%)	52,52,63	1.17	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	Y	608	-	50,58,73	1.54	9 (18%)	58,95,113	2.29	17 (29%)
29	CLA	S1	602	23	60,68,73	1.39	9 (15%)	70,107,113	2.13	17 (24%)
29	CLA	B	603	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	17 (22%)
37	DGD	C1	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.07	6 (8%)
40	LHG	y1	624	29	48,48,48	0.41	0	51,54,54	0.98	2 (3%)
41	LMK	c1	527	-	38,39,53	1.51	3 (7%)	41,46,60	1.24	2 (4%)
29	CLA	c1	501	-	65,73,73	1.38	8 (12%)	76,113,113	2.05	18 (23%)
50	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.77	16 (29%)
50	XAT	y1	622	-	39,47,47	0.74	1 (2%)	54,74,74	3.88	20 (37%)
51	NEX	n1	623	-	38,46,46	3.26	9 (23%)	50,70,70	1.71	11 (22%)
29	CLA	N1	614	-	49,57,73	1.54	7 (14%)	55,93,113	2.33	17 (30%)
29	CLA	g1	614	-	49,57,73	1.61	10 (20%)	55,93,113	2.31	17 (30%)
48	CHL	S1	607	-	43,51,74	1.01	2 (4%)	45,86,114	1.53	9 (20%)
37	DGD	c	520	-	60,60,67	1.05	4 (6%)	74,74,81	1.03	3 (4%)
29	CLA	Y	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.14	18 (23%)
29	CLA	N1	603	-	65,73,73	1.37	7 (10%)	76,113,113	2.10	22 (28%)
40	LHG	s	624	29	44,44,48	0.43	0	47,50,54	1.13	3 (6%)
40	LHG	G	624	29	48,48,48	0.37	0	51,54,54	1.06	3 (5%)
48	CHL	Y1	606	-	66,74,74	0.90	4 (6%)	73,114,114	1.25	10 (13%)
48	CHL	r1	607	-	50,58,74	0.99	3 (6%)	52,94,114	1.64	12 (23%)
48	CHL	r1	606	-	44,52,74	1.10	3 (6%)	46,87,114	1.12	4 (8%)
37	DGD	C1	519	-	63,63,67	1.10	7 (11%)	77,77,81	1.05	3 (3%)
50	XAT	n1	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.04	14 (25%)
29	CLA	S1	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	16 (21%)
49	LUT	n1	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.13	18 (35%)
29	CLA	n	602	-	65,73,73	1.43	8 (12%)	76,113,113	1.92	19 (25%)
29	CLA	S	609	-	60,68,73	1.43	8 (13%)	70,107,113	1.98	16 (22%)
29	CLA	G	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.10	21 (27%)
50	XAT	y	622	-	39,47,47	0.73	1 (2%)	54,74,74	3.68	19 (35%)
48	CHL	g	608	-	44,52,74	1.07	3 (6%)	46,87,114	1.47	12 (26%)
29	CLA	G1	604	-	49,57,73	1.57	7 (14%)	55,93,113	2.34	18 (32%)
29	CLA	y1	610	24	65,73,73	1.39	9 (13%)	76,113,113	2.02	21 (27%)
43	PL9	D1	405	-	55,55,55	1.18	5 (9%)	68,69,69	1.72	15 (22%)
29	CLA	G1	612	-	43,51,73	1.71	9 (20%)	49,86,113	2.15	12 (24%)
31	BCR	C1	516	-	41,41,41	1.89	4 (9%)	56,56,56	4.66	17 (30%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	LUT	R	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.03	17 (33%)
53	ERG	r	626	-	31,32,32	7.80	18 (58%)	47,50,50	3.01	16 (34%)
47	4RF	i	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.93	3 (5%)
29	CLA	y	603	-	65,73,73	1.39	10 (15%)	76,113,113	2.10	16 (21%)
38	3PH	S	626	-	47,47,47	0.87	2 (4%)	51,52,52	4.41	4 (7%)
51	NEX	S	623	-	38,46,46	3.42	10 (26%)	50,70,70	1.71	12 (24%)
29	CLA	y1	608	-	50,58,73	1.55	10 (20%)	58,95,113	2.21	17 (29%)
49	LUT	g1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.33	14 (27%)
29	CLA	D	403	-	65,73,73	1.35	9 (13%)	76,113,113	2.08	19 (25%)
31	BCR	C1	515	-	41,41,41	1.93	4 (9%)	56,56,56	3.77	16 (28%)
29	CLA	n1	612	-	45,53,73	1.67	9 (20%)	52,89,113	2.05	13 (25%)
49	LUT	N	620	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	15 (29%)
48	CHL	N	606	-	66,74,74	0.96	3 (4%)	73,114,114	1.21	13 (17%)
48	CHL	N1	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.28	11 (15%)
29	CLA	G1	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
31	BCR	c1	517	-	41,41,41	1.91	5 (12%)	56,56,56	4.37	19 (33%)
36	C7Z	B1	620	-	43,43,43	5.38	26 (60%)	58,60,60	2.39	22 (37%)
33	LMG	w1	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.17	3 (6%)
54	LPX	s	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
31	BCR	c1	515	-	41,41,41	1.91	4 (9%)	56,56,56	4.38	13 (23%)
40	LHG	g	624	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
29	CLA	s	605	-	50,58,73	1.57	8 (16%)	58,95,113	2.30	16 (27%)
50	XAT	g	622	-	39,47,47	0.80	1 (2%)	54,74,74	2.22	16 (29%)
49	LUT	g	621	-	42,43,43	2.37	2 (4%)	51,60,60	1.91	12 (23%)
29	CLA	r1	608	-	60,68,73	1.45	7 (11%)	70,107,113	2.03	16 (22%)
38	3PH	s	626	-	47,47,47	0.87	3 (6%)	51,52,52	4.40	4 (7%)
50	XAT	R1	621	-	39,47,47	0.68	1 (2%)	54,74,74	1.91	18 (33%)
55	PTY	y1	626	-	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
31	BCR	B	619	-	41,41,41	1.85	4 (9%)	56,56,56	3.81	21 (37%)
55	PTY	Y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.02	2 (3%)
29	CLA	A1	410	-	60,68,73	1.40	7 (11%)	70,107,113	2.13	20 (28%)
40	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
33	LMG	h	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.22	4 (7%)
32	SQD	M	101	-	41,42,54	0.90	0	50,53,65	0.98	3 (6%)
50	XAT	Y1	622	-	39,47,47	0.69	1 (2%)	54,74,74	3.83	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	B	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	17 (22%)
30	PHO	a	409	-	51,69,69	0.97	3 (5%)	47,99,99	1.38	8 (17%)
49	LUT	Y1	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.33	13 (25%)
29	CLA	c1	509	-	65,73,73	1.37	8 (12%)	76,113,113	1.82	16 (21%)
48	CHL	S	601	23	46,54,74	1.21	5 (10%)	49,90,114	1.37	9 (18%)
52	LMT	r1	625	-	36,36,36	1.18	4 (11%)	47,47,47	1.08	4 (8%)
48	CHL	N	605	20	66,74,74	0.92	4 (6%)	73,114,114	1.24	11 (15%)
29	CLA	B1	605	-	65,73,73	1.34	8 (12%)	76,113,113	2.06	18 (23%)
29	CLA	C1	502	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	17 (22%)
29	CLA	C1	505	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	17 (22%)
29	CLA	R1	610	-	60,68,73	1.43	9 (15%)	70,107,113	2.28	18 (25%)
29	CLA	n1	611	-	49,57,73	1.57	7 (14%)	55,93,113	2.29	15 (27%)
29	CLA	b	611	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
53	ERG	R1	626	-	31,32,32	7.67	19 (61%)	47,50,50	2.83	19 (40%)
49	LUT	G1	620	-	42,43,43	2.26	1 (2%)	51,60,60	1.86	13 (25%)
48	CHL	G1	601	21	66,74,74	0.89	3 (4%)	73,114,114	1.33	13 (17%)
37	DGD	C	519	-	63,63,67	1.13	7 (11%)	77,77,81	1.01	2 (2%)
43	PL9	D	405	-	55,55,55	1.56	5 (9%)	68,69,69	1.47	12 (17%)
48	CHL	G1	607	-	66,74,74	0.87	2 (3%)	73,114,114	1.16	8 (10%)
29	CLA	B1	610	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	14 (18%)
31	BCR	d1	404	-	41,41,41	1.88	4 (9%)	56,56,56	4.27	22 (39%)
29	CLA	g	613	-	65,73,73	1.33	7 (10%)	76,113,113	2.04	18 (23%)
39	DGA	C1	524	-	43,43,43	1.17	3 (6%)	45,45,45	1.54	4 (8%)
29	CLA	S	602	-	60,68,73	1.45	8 (13%)	70,107,113	2.17	18 (25%)
52	LMT	R	625	-	36,36,36	1.22	6 (16%)	47,47,47	1.14	3 (6%)
49	LUT	g	620	-	42,43,43	2.32	1 (2%)	51,60,60	2.16	16 (31%)
47	4RF	K	101	-	56,56,56	1.08	3 (5%)	59,59,59	0.91	3 (5%)
29	CLA	A	406	-	65,73,73	1.32	7 (10%)	76,113,113	2.12	17 (22%)
29	CLA	b	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	20 (26%)
29	CLA	G	610	21	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
29	CLA	b	610	-	65,73,73	1.32	7 (10%)	76,113,113	2.03	17 (22%)
29	CLA	b	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.11	17 (22%)
29	CLA	s1	617	-	50,58,73	1.51	8 (16%)	58,95,113	2.27	19 (32%)
34	SPH	y	625	-	19,20,20	0.61	0	18,21,21	1.21	2 (11%)
33	LMG	d1	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	DGD	B1	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.21	6 (10%)
29	CLA	c	511	4	65,73,73	1.36	8 (12%)	76,113,113	2.01	19 (25%)
31	BCR	D	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	16 (28%)
29	CLA	s	609	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	15 (21%)
29	CLA	C1	509	-	65,73,73	1.34	8 (12%)	76,113,113	2.07	17 (22%)
29	CLA	b	608	-	65,73,73	1.32	7 (10%)	76,113,113	2.02	17 (22%)
29	CLA	b	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.04	18 (23%)
39	DGA	B1	625	-	43,43,43	1.14	3 (6%)	45,45,45	1.46	3 (6%)
31	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.24	12 (21%)
37	DGD	C	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.95	2 (2%)
29	CLA	r	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.37	13 (23%)
32	SQD	m1	101	-	41,42,54	0.88	0	50,53,65	0.99	3 (6%)
29	CLA	R	609	-	60,68,73	1.45	8 (13%)	70,107,113	4.48	18 (25%)
32	SQD	b1	626	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
29	CLA	G	604	-	49,57,73	1.58	8 (16%)	55,93,113	2.28	18 (32%)
29	CLA	a	410	-	60,68,73	1.39	9 (15%)	70,107,113	2.17	18 (25%)
49	LUT	Y1	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.87	14 (27%)
29	CLA	n	614	-	49,57,73	1.56	9 (18%)	55,93,113	2.36	20 (36%)
54	LPX	S	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
29	CLA	G1	611	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	15 (19%)
49	LUT	r1	620	-	42,43,43	2.36	2 (4%)	51,60,60	2.32	15 (29%)
29	CLA	y1	611	40	65,73,73	1.34	8 (12%)	76,113,113	2.05	17 (22%)
48	CHL	n	606	-	66,74,74	0.92	4 (6%)	73,114,114	1.25	12 (16%)
48	CHL	Y1	605	-	46,54,74	0.97	2 (4%)	49,90,114	1.40	7 (14%)
29	CLA	C	506	-	65,73,73	1.43	8 (12%)	76,113,113	2.05	18 (23%)
29	CLA	S	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.14	16 (25%)
29	CLA	N	602	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	21 (27%)
29	CLA	b	612	-	65,73,73	1.37	8 (12%)	76,113,113	2.10	17 (22%)
29	CLA	S	605	23	50,58,73	1.59	9 (18%)	58,95,113	2.42	16 (27%)
29	CLA	c	503	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	21 (27%)
48	CHL	Y	601	24	66,74,74	0.91	3 (4%)	73,114,114	1.21	9 (12%)
29	CLA	S1	617	23	50,58,73	1.54	8 (16%)	58,95,113	2.32	19 (32%)
29	CLA	C	502	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	15 (19%)
29	CLA	c1	507	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	20 (26%)
29	CLA	y1	614	-	65,73,73	1.40	9 (13%)	76,113,113	1.90	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	CHL	S1	608	-	61,69,74	0.84	2 (3%)	67,108,114	1.33	13 (19%)
50	XAT	G	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.11	15 (27%)
29	CLA	N1	611	-	49,57,73	1.59	8 (16%)	55,93,113	2.29	16 (29%)
29	CLA	a1	405	-	65,73,73	1.30	6 (9%)	76,113,113	2.12	19 (25%)
44	HEM	f	101	6,7	41,50,50	1.45	4 (9%)	45,82,82	1.35	6 (13%)
29	CLA	N	610	-	65,73,73	1.36	7 (10%)	76,113,113	2.07	18 (23%)
29	CLA	B	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.14	17 (22%)
33	LMG	A1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.20	5 (8%)
39	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.50	3 (6%)
51	NEX	s	623	-	38,46,46	3.52	11 (28%)	50,70,70	2.12	14 (28%)
29	CLA	C	504	-	65,73,73	1.34	8 (12%)	76,113,113	1.96	13 (17%)
29	CLA	R1	609	-	60,68,73	1.40	9 (15%)	70,107,113	4.53	19 (27%)
48	CHL	Y	609	-	66,74,74	0.91	4 (6%)	73,114,114	1.43	14 (19%)
54	LPX	S1	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
39	DGA	B	625	-	43,43,43	1.09	2 (4%)	45,45,45	1.52	3 (6%)
29	CLA	B	602	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	15 (19%)
29	CLA	B1	617	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	16 (21%)
48	CHL	g	609	-	66,74,74	0.91	3 (4%)	73,114,114	1.25	8 (10%)
48	CHL	n1	606	-	66,74,74	0.86	4 (6%)	73,114,114	1.23	11 (15%)
33	LMG	W	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.21	4 (8%)
29	CLA	y	614	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	18 (23%)
29	CLA	D1	402	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	18 (23%)
34	SPH	a	414	-	19,20,20	0.70	1 (5%)	18,21,21	1.10	1 (5%)
40	LHG	d1	408	-	43,43,48	0.40	0	46,49,54	1.05	2 (4%)
48	CHL	G	609	21	66,74,74	0.90	3 (4%)	73,114,114	1.18	12 (16%)
48	CHL	G	608	-	44,52,74	1.08	3 (6%)	46,87,114	1.41	7 (15%)
49	LUT	g1	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.93	11 (21%)
29	CLA	N1	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
29	CLA	C	510	-	65,73,73	1.37	7 (10%)	76,113,113	1.97	18 (23%)
31	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.32	18 (32%)
40	LHG	Y1	624	-	48,48,48	0.40	0	51,54,54	1.11	4 (7%)
47	4RF	i1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.92	3 (5%)
38	3PH	t	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.19	2 (3%)
48	CHL	G	606	-	50,58,74	1.08	3 (6%)	52,94,114	1.45	11 (21%)
29	CLA	R	608	-	60,68,73	1.46	10 (16%)	70,107,113	2.07	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	s	611	40	65,73,73	1.37	8 (12%)	76,113,113	1.91	13 (17%)
37	DGD	B	623	-	44,44,67	0.89	1 (2%)	58,58,81	1.36	6 (10%)
29	CLA	N	612	-	45,53,73	1.66	9 (20%)	52,89,113	2.05	12 (23%)
48	CHL	S	606	-	44,52,74	1.10	3 (6%)	46,87,114	1.48	10 (21%)
29	CLA	B1	615	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	19 (25%)
33	LMG	C	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.19	3 (5%)
29	CLA	C	505	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	16 (21%)
26	OEX	a	401	1,4	0,15,15	-	-	-	-	-
29	CLA	S1	604	-	55,63,73	1.49	9 (16%)	64,101,113	2.20	18 (28%)
29	CLA	S1	612	-	45,53,73	1.59	6 (13%)	52,89,113	2.18	15 (28%)
48	CHL	N1	606	-	66,74,74	0.94	4 (6%)	73,114,114	1.11	8 (10%)
53	ERG	R	626	-	31,32,32	7.79	18 (58%)	47,50,50	3.10	19 (40%)
52	LMT	r	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.16	3 (6%)
47	4RF	I	102	-	56,56,56	1.05	4 (7%)	59,59,59	0.97	3 (5%)
29	CLA	g	610	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	20 (26%)
29	CLA	s	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.12	15 (23%)
29	CLA	n	613	-	65,73,73	1.36	6 (9%)	76,113,113	2.12	18 (23%)
29	CLA	s1	614	-	55,63,73	1.49	10 (18%)	64,101,113	2.16	16 (25%)
29	CLA	N	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.07	18 (23%)
29	CLA	b1	608	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	19 (25%)
29	CLA	s1	605	-	50,58,73	1.60	11 (22%)	58,95,113	2.28	18 (31%)
29	CLA	g1	611	-	65,73,73	1.37	8 (12%)	76,113,113	1.88	16 (21%)
48	CHL	R1	607	-	50,58,74	0.94	2 (4%)	52,94,114	1.37	9 (17%)
48	CHL	y1	605	24	46,54,74	1.03	3 (6%)	49,90,114	1.31	8 (16%)
32	SQD	M1	101	-	41,42,54	0.90	0	50,53,65	0.97	2 (4%)
29	CLA	G1	613	-	65,73,73	1.32	7 (10%)	76,113,113	2.19	21 (27%)
37	DGD	b	623	-	44,44,67	0.89	2 (4%)	58,58,81	1.26	6 (10%)
48	CHL	s1	606	-	44,52,74	0.95	2 (4%)	46,87,114	1.40	8 (17%)
48	CHL	s	606	-	44,52,74	1.04	3 (6%)	46,87,114	1.46	7 (15%)
48	CHL	g1	606	-	50,58,74	1.06	4 (8%)	52,94,114	1.28	9 (17%)
37	DGD	c1	519	-	63,63,67	1.14	6 (9%)	77,77,81	1.04	3 (3%)
49	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	15 (29%)
53	ERG	r1	626	-	31,32,32	7.77	19 (61%)	47,50,50	2.72	18 (38%)
29	CLA	R1	602	-	60,68,73	1.45	9 (15%)	70,107,113	2.05	17 (24%)
40	LHG	C1	525	-	46,46,48	0.39	0	49,52,54	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	n	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	20 (26%)
29	CLA	y	608	-	50,58,73	1.57	9 (18%)	58,95,113	2.25	17 (29%)
48	CHL	R	606	-	44,52,74	1.20	4 (9%)	46,87,114	1.30	7 (15%)
40	LHG	n1	624	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
29	CLA	B	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
29	CLA	c1	511	-	65,73,73	1.36	7 (10%)	76,113,113	2.06	17 (22%)
48	CHL	y	606	-	66,74,74	0.91	4 (6%)	73,114,114	1.21	10 (13%)
29	CLA	b1	615	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	16 (21%)
48	CHL	Y	605	24	46,54,74	1.07	3 (6%)	49,90,114	1.51	10 (20%)
51	NEX	n	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.66	11 (22%)
49	LUT	G	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	12 (23%)
55	PTY	Y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.04	2 (3%)
29	CLA	c	512	-	65,73,73	1.39	9 (13%)	76,113,113	2.00	19 (25%)
29	CLA	n1	602	20	65,73,73	1.31	8 (12%)	76,113,113	2.04	20 (26%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	D1	403	-	1/1/15/20	17/37/115/115	-
29	CLA	N1	604	-	1/1/15/20	18/37/115/115	-
29	CLA	B	604	-	1/1/15/20	16/37/115/115	-
29	CLA	C1	507	-	1/1/15/20	14/37/115/115	-
29	CLA	y1	603	-	1/1/15/20	18/37/115/115	-
45	RRX	H	101	-	1/1/11/25	7/29/65/65	0/2/2/2
48	CHL	g1	607	-	4/4/20/26	7/39/137/137	-
29	CLA	R	604	-	1/1/11/20	10/18/96/115	-
49	LUT	n	621	-	-	2/29/67/67	0/2/2/2
29	CLA	y	612	-	1/1/15/20	17/37/115/115	-
29	CLA	C1	503	-	1/1/15/20	19/37/115/115	-
38	3PH	B1	624	-	-	27/49/49/49	-
49	LUT	S1	620	-	-	4/29/67/67	0/2/2/2
30	PHO	A	409	-	-	14/37/103/103	0/5/6/6
29	CLA	s1	610	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b1	617	-	1/1/15/20	14/37/115/115	-
49	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
29	CLA	d	403	-	1/1/15/20	16/37/115/115	-
29	CLA	n1	603	-	1/1/15/20	14/37/115/115	-
29	CLA	r	610	-	1/1/14/20	11/31/109/115	-
50	XAT	R	621	-	-	2/31/93/93	0/4/4/4
50	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
38	3PH	T	101	-	-	26/49/49/49	-
49	LUT	s	621	-	-	3/29/67/67	0/2/2/2
30	PHO	A1	409	-	-	11/37/103/103	0/5/6/6
29	CLA	a1	407	-	1/1/11/20	7/18/96/115	-
48	CHL	N	608	-	3/3/16/26	3/20/118/137	-
38	3PH	t1	101	-	-	30/49/49/49	-
29	CLA	B1	614	-	1/1/15/20	14/37/115/115	-
48	CHL	N1	605	20	4/4/20/26	9/39/137/137	-
48	CHL	G1	605	21	4/4/16/26	4/18/116/137	-
29	CLA	n1	604	-	1/1/15/20	14/37/115/115	-
29	CLA	S	612	-	1/1/11/20	6/13/91/115	-
29	CLA	B1	608	-	1/1/15/20	26/37/115/115	-
29	CLA	C	513	-	1/1/15/20	20/37/115/115	-
32	SQD	b1	621	-	-	17/37/57/69	0/1/1/1
49	LUT	G	620	-	-	3/29/67/67	0/2/2/2
29	CLA	d	402	-	1/1/15/20	13/37/115/115	-
29	CLA	s1	609	-	1/1/14/20	17/31/109/115	-
29	CLA	g	612	-	1/1/10/20	6/11/89/115	-
29	CLA	b	614	-	1/1/15/20	13/37/115/115	-
51	NEX	y1	623	-	-	10/27/83/83	0/3/3/3
48	CHL	N	607	-	4/4/20/26	7/39/137/137	-
49	LUT	n	620	-	-	3/29/67/67	0/2/2/2
49	LUT	y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	c1	504	-	1/1/15/20	19/37/115/115	-
29	CLA	Y	602	-	1/1/15/20	18/37/115/115	-
29	CLA	N1	610	-	1/1/15/20	21/37/115/115	-
31	BCR	C1	517	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y1	604	-	1/1/15/20	13/37/115/115	-
32	SQD	B	621	-	-	20/37/57/69	0/1/1/1
29	CLA	Y1	612	-	1/1/15/20	18/37/115/115	-
31	BCR	a1	411	-	-	6/29/63/63	0/2/2/2
32	SQD	B1	621	-	-	11/37/57/69	0/1/1/1
51	NEX	r	622	-	-	9/27/83/83	0/3/3/3
32	SQD	b	626	-	-	17/49/69/69	0/1/1/1
51	NEX	N1	623	-	-	6/27/83/83	0/3/3/3
29	CLA	B1	616	-	1/1/15/20	18/37/115/115	-
29	CLA	g1	602	-	1/1/15/20	19/37/115/115	-
29	CLA	a	406	-	1/1/15/20	17/37/115/115	-
48	CHL	g	601	21	4/4/20/26	16/39/137/137	-
29	CLA	g1	613	-	1/1/15/20	22/37/115/115	-
29	CLA	g	603	-	1/1/15/20	21/37/115/115	-
29	CLA	S1	610	-	1/1/15/20	22/37/115/115	-
29	CLA	b1	614	-	1/1/15/20	10/37/115/115	-
29	CLA	A	410	-	1/1/14/20	14/31/109/115	-
48	CHL	y	601	24	4/4/20/26	9/39/137/137	-
29	CLA	b	616	-	1/1/15/20	15/37/115/115	-
49	LUT	N1	620	-	-	8/29/67/67	0/2/2/2
44	HEM	F	101	6,7	-	1/12/54/54	-
29	CLA	n	611	-	1/1/11/20	8/18/96/115	-
29	CLA	y	613	-	1/1/15/20	24/37/115/115	-
43	PL9	d	405	-	-	9/53/73/73	0/1/1/1
49	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
48	CHL	n	605	20	4/4/20/26	8/39/137/137	-
33	LMG	c	523	-	-	21/50/70/70	0/1/1/1
29	CLA	r1	612	-	1/1/14/20	16/31/109/115	-
40	LHG	S	624	29	-	27/49/49/53	-
48	CHL	Y1	601	-	4/4/20/26	7/39/137/137	-
29	CLA	Y1	603	-	1/1/15/20	14/37/115/115	-
29	CLA	b1	610	-	1/1/15/20	19/37/115/115	-
29	CLA	a	407	-	1/1/11/20	7/18/96/115	-
29	CLA	C	503	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	605	-	1/1/15/20	19/37/115/115	-
49	LUT	R1	620	-	-	9/29/67/67	0/2/2/2
29	CLA	b1	612	-	1/1/15/20	18/37/115/115	-
32	SQD	A	412	-	-	24/46/66/69	0/1/1/1
40	LHG	N1	624	-	-	34/53/53/53	-
48	CHL	n	607	-	4/4/20/26	8/39/137/137	-
48	CHL	R1	606	-	3/3/15/26	4/13/111/137	-
31	BCR	C1	514	-	-	12/29/63/63	0/2/2/2
32	SQD	c1	526	-	-	22/49/69/69	0/1/1/1
37	DGD	C1	520	-	-	16/48/88/95	0/2/2/2
49	LUT	s1	621	-	-	5/29/67/67	0/2/2/2
49	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
29	CLA	C	512	-	1/1/15/20	15/37/115/115	-
29	CLA	G1	610	-	1/1/15/20	15/37/115/115	-
51	NEX	R1	622	-	-	14/27/83/83	0/3/3/3
49	LUT	S	620	-	-	3/29/67/67	0/2/2/2
29	CLA	a1	406	-	1/1/15/20	16/37/115/115	-
38	3PH	b1	624	-	-	24/49/49/49	-
44	HEM	F1	101	7	-	1/12/54/54	-
48	CHL	s	608	-	4/4/19/26	5/33/131/137	-
29	CLA	r1	604	-	1/1/11/20	10/18/96/115	-
40	LHG	g1	624	-	-	35/53/53/53	-
40	LHG	c	525	-	-	30/51/51/53	-
31	BCR	b	618	-	-	9/29/63/63	0/2/2/2
32	SQD	m	101	-	-	20/37/57/69	0/1/1/1
38	3PH	S1	626	-	-	30/49/49/49	-
49	LUT	S	621	-	-	4/29/67/67	0/2/2/2
50	XAT	N	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	r1	602	-	1/1/14/20	11/31/109/115	-
29	CLA	s1	602	-	1/1/14/20	13/31/109/115	-
29	CLA	c1	508	-	1/1/15/20	12/37/115/115	-
29	CLA	S	603	-	1/1/15/20	17/37/115/115	-
40	LHG	N	624	-	-	31/53/53/53	-
29	CLA	s	612	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	g1	612	21	1/1/10/20	4/11/89/115	-
29	CLA	c	505	-	1/1/15/20	19/37/115/115	-
29	CLA	r	602	22	1/1/14/20	14/31/109/115	-
29	CLA	b1	605	-	1/1/15/20	18/37/115/115	-
49	LUT	N	621	-	-	4/29/67/67	0/2/2/2
55	PTY	Y1	627	-	-	12/20/20/53	-
51	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
29	CLA	b	615	-	1/1/15/20	19/37/115/115	-
40	LHG	D1	410	-	-	25/43/43/53	-
29	CLA	R	612	-	1/1/14/20	10/31/109/115	-
48	CHL	N	609	-	4/4/20/26	11/39/137/137	-
49	LUT	S1	621	-	-	7/29/67/67	0/2/2/2
29	CLA	G	613	-	1/1/15/20	19/37/115/115	-
29	CLA	A1	407	-	1/1/12/20	9/19/97/115	-
40	LHG	L1	101	-	-	36/53/53/53	-
29	CLA	G	611	40	1/1/15/20	17/37/115/115	-
44	HEM	f1	101	7	-	2/12/54/54	-
46	GOL	I1	101	-	-	2/4/4/4	-
49	LUT	s1	620	-	-	6/29/67/67	0/2/2/2
29	CLA	s	603	-	1/1/15/20	15/37/115/115	-
29	CLA	g1	603	-	1/1/15/20	18/37/115/115	-
34	SPH	Y1	625	-	-	9/21/21/21	-
50	XAT	r	621	-	2/2/12/26	2/31/93/93	0/4/4/4
29	CLA	R	603	-	1/1/14/20	16/31/109/115	-
29	CLA	B1	607	-	1/1/15/20	14/37/115/115	-
48	CHL	n1	608	-	3/3/16/26	8/20/118/137	-
43	PL9	d1	405	-	-	20/53/73/73	0/1/1/1
29	CLA	g1	604	-	1/1/11/20	9/18/96/115	-
47	4RF	I1	102	-	-	24/59/59/59	-
29	CLA	N1	612	-	1/1/11/20	4/13/91/115	-
29	CLA	G1	614	-	1/1/11/20	8/18/96/115	-
29	CLA	G	614	-	1/1/11/20	10/18/96/115	-
29	CLA	s	613	-	1/1/13/20	9/25/103/115	-
39	DGA	j1	101	-	-	20/30/30/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	c	514	-	-	14/29/63/63	0/2/2/2
48	CHL	Y	607	-	4/4/20/26	6/39/137/137	-
29	CLA	r1	610	-	1/1/14/20	13/31/109/115	-
48	CHL	G1	609	-	4/4/20/26	10/39/137/137	-
33	LMG	B1	622	-	-	19/39/59/70	0/1/1/1
29	CLA	B1	609	-	1/1/15/20	15/37/115/115	-
29	CLA	n	604	-	1/1/15/20	13/37/115/115	-
48	CHL	N1	601	-	4/4/20/26	9/39/137/137	-
48	CHL	g1	601	-	4/4/20/26	12/39/137/137	-
39	DGA	J1	101	-	-	15/30/30/45	-
49	LUT	s	620	-	-	1/29/67/67	0/2/2/2
29	CLA	n	612	-	1/1/11/20	5/13/91/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
29	CLA	y	611	40	1/1/15/20	16/37/115/115	-
33	LMG	H	102	-	-	14/43/63/70	0/1/1/1
48	CHL	y	605	24	3/3/16/26	3/15/113/137	-
29	CLA	B	614	-	1/1/15/20	14/37/115/115	-
29	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
54	LPX	s1	625	-	-	18/31/31/31	-
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2
29	CLA	B1	602	-	1/1/15/20	24/37/115/115	-
29	CLA	R	602	-	1/1/14/20	11/31/109/115	-
29	CLA	g1	610	-	1/1/15/20	18/37/115/115	-
41	LMK	c	527	-	2/2/6/6	13/46/46/60	-
29	CLA	B	608	-	1/1/15/20	27/37/115/115	-
48	CHL	R	607	-	3/3/16/26	7/20/118/137	-
29	CLA	B1	603	-	1/1/15/20	21/37/115/115	-
34	SPH	Y	625	-	-	10/21/21/21	-
29	CLA	y	610	24	1/1/15/20	13/37/115/115	-
48	CHL	N1	609	-	4/4/20/26	10/39/137/137	-
29	CLA	s1	603	-	1/1/15/20	15/37/115/115	-
30	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
48	CHL	n	601	20	4/4/20/26	4/39/137/137	-
39	DGA	b	625	-	-	26/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C1	510	-	1/1/15/20	17/37/115/115	-
48	CHL	g	605	21	4/4/16/26	5/18/116/137	-
29	CLA	n1	613	-	1/1/15/20	20/37/115/115	-
29	CLA	R1	603	-	1/1/14/20	17/31/109/115	-
48	CHL	y	609	-	4/4/20/26	6/39/137/137	-
33	LMG	D1	411	-	-	10/41/61/70	0/1/1/1
29	CLA	c	501	-	1/1/15/20	19/37/115/115	-
33	LMG	A	413	-	-	15/43/63/70	0/1/1/1
29	CLA	c1	505	-	1/1/15/20	16/37/115/115	-
50	XAT	G1	622	-	1/1/12/26	2/31/93/93	0/4/4/4
48	CHL	y1	601	24	4/4/20/26	5/39/137/137	-
29	CLA	s1	611	40	1/1/15/20	20/37/115/115	-
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
48	CHL	y1	606	-	4/4/20/26	6/39/137/137	-
29	CLA	Y1	602	-	1/1/15/20	20/37/115/115	-
36	C7Z	b1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
33	LMG	H1	102	-	-	17/43/63/70	0/1/1/1
29	CLA	S1	609	-	1/1/14/20	10/31/109/115	-
48	CHL	Y	606	-	4/4/20/26	7/39/137/137	-
40	LHG	n	624	-	-	35/53/53/53	-
48	CHL	g	606	-	3/3/16/26	4/20/118/137	-
29	CLA	C	511	-	1/1/15/20	14/37/115/115	-
32	SQD	b	621	-	-	19/37/57/69	0/1/1/1
48	CHL	s1	601	23	3/3/16/26	4/15/113/137	-
40	LHG	D	410	-	-	26/43/43/53	-
29	CLA	B	615	-	1/1/15/20	15/37/115/115	-
31	BCR	C	516	-	-	13/29/63/63	0/2/2/2
29	CLA	C	501	-	1/1/15/20	18/37/115/115	-
29	CLA	a	405	-	1/1/15/20	15/37/115/115	-
33	LMG	d	411	-	-	19/41/61/70	0/1/1/1
29	CLA	r	609	-	1/1/14/20	12/31/109/115	-
29	CLA	S	613	-	1/1/13/20	12/25/103/115	-
55	PTY	Y	627	-	-	15/20/20/53	-
48	CHL	y	607	-	4/4/20/26	9/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c1	506	-	1/1/15/20	16/37/115/115	-
38	3PH	b	624	-	-	23/49/49/49	-
29	CLA	B	617	-	1/1/15/20	17/37/115/115	-
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	N	613	-	1/1/15/20	17/37/115/115	-
51	NEX	r1	622	-	-	8/27/83/83	0/3/3/3
29	CLA	B	609	-	1/1/15/20	12/37/115/115	-
48	CHL	Y1	609	-	4/4/20/26	8/39/137/137	-
37	DGD	b1	623	-	-	14/32/72/95	0/2/2/2
33	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
29	CLA	r	612	-	1/1/14/20	14/31/109/115	-
40	LHG	D1	409	-	-	31/53/53/53	-
29	CLA	R1	608	-	1/1/14/20	11/31/109/115	-
29	CLA	y1	604	-	1/1/15/20	13/37/115/115	-
29	CLA	y1	612	-	1/1/15/20	17/37/115/115	-
33	LMG	c1	521	-	-	14/46/66/70	0/1/1/1
32	SQD	a	412	-	-	14/46/66/69	0/1/1/1
32	SQD	B1	626	-	-	17/49/69/69	0/1/1/1
29	CLA	c	509	-	1/1/15/20	16/37/115/115	-
48	CHL	S1	601	23	3/3/16/26	3/15/113/137	-
29	CLA	B	616	-	1/1/15/20	7/37/115/115	-
40	LHG	D	408	-	-	23/48/48/53	-
29	CLA	s1	604	-	1/1/13/20	8/25/103/115	-
48	CHL	g1	608	-	3/3/15/26	1/13/111/137	-
37	DGD	c1	518	-	-	14/44/84/95	0/2/2/2
29	CLA	s1	612	-	1/1/11/20	6/13/91/115	-
30	PHO	a1	409	-	-	12/37/103/103	0/5/6/6
29	CLA	N	614	-	1/1/11/20	5/18/96/115	-
29	CLA	G	603	-	1/1/15/20	14/37/115/115	-
29	CLA	b1	602	-	1/1/15/20	22/37/115/115	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
39	DGA	b1	625	-	-	22/45/45/45	-
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	C1	501	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LHG	d	409	-	-	26/53/53/53	-
49	LUT	n1	620	-	-	5/29/67/67	0/2/2/2
29	CLA	c	510	-	1/1/15/20	14/37/115/115	-
29	CLA	B	611	-	1/1/15/20	13/37/115/115	-
46	GOL	I	101	-	-	2/4/4/4	-
51	NEX	S1	623	-	-	4/27/83/83	0/3/3/3
29	CLA	B1	611	-	1/1/15/20	13/37/115/115	-
31	BCR	B1	619	-	-	6/29/63/63	0/2/2/2
29	CLA	c1	510	-	1/1/15/20	12/37/115/115	-
29	CLA	c1	502	-	1/1/15/20	16/37/115/115	-
29	CLA	y	604	-	1/1/15/20	15/37/115/115	-
33	LMG	c	521	-	-	14/46/66/70	0/1/1/1
29	CLA	S	617	23	1/1/12/20	7/19/97/115	-
40	LHG	Y	624	-	-	29/53/53/53	-
29	CLA	R1	612	-	1/1/14/20	19/31/109/115	-
34	SPH	A	414	-	-	12/21/21/21	-
29	CLA	S	604	-	1/1/13/20	9/25/103/115	-
29	CLA	s	610	-	1/1/15/20	18/37/115/115	-
34	SPH	A1	414	-	-	16/21/21/21	-
31	BCR	b	619	-	-	6/29/63/63	0/2/2/2
48	CHL	n	608	-	3/3/16/26	6/20/118/137	-
49	LUT	Y	621	-	-	4/29/67/67	0/2/2/2
48	CHL	G	601	21	4/4/20/26	11/39/137/137	-
32	SQD	a1	412	-	-	19/46/66/69	0/1/1/1
40	LHG	D	409	-	-	25/53/53/53	-
29	CLA	c1	513	-	1/1/15/20	23/37/115/115	-
29	CLA	y1	602	-	1/1/15/20	15/37/115/115	-
29	CLA	b	609	-	1/1/15/20	13/37/115/115	-
29	CLA	b1	603	-	1/1/15/20	19/37/115/115	-
50	XAT	g1	622	-	1/1/12/26	7/31/93/93	0/4/4/4
29	CLA	R	610	-	1/1/14/20	14/31/109/115	-
40	LHG	d1	409	-	-	30/53/53/53	-
29	CLA	c	508	-	1/1/15/20	12/37/115/115	-
39	DGA	J	101	-	-	12/30/30/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	g1	609	-	4/4/20/26	7/39/137/137	-
29	CLA	s	602	-	1/1/14/20	16/31/109/115	-
29	CLA	R1	604	-	1/1/11/20	10/18/96/115	-
51	NEX	G	623	-	-	5/27/83/83	0/3/3/3
51	NEX	G1	623	-	-	12/27/83/83	0/3/3/3
29	CLA	Y1	613	-	1/1/15/20	19/37/115/115	-
29	CLA	s1	613	-	1/1/13/20	11/25/103/115	-
51	NEX	Y	623	-	-	7/27/83/83	0/3/3/3
29	CLA	A	405	-	1/1/15/20	14/37/115/115	-
47	4RF	k1	101	-	-	37/59/59/59	-
40	LHG	L	101	-	-	38/53/53/53	-
29	CLA	c	513	-	1/1/15/20	23/37/115/115	-
29	CLA	b1	611	-	1/1/15/20	10/37/115/115	-
29	CLA	n1	610	-	1/1/15/20	20/37/115/115	-
29	CLA	N1	602	-	1/1/15/20	17/37/115/115	-
49	LUT	Y	620	-	-	5/29/67/67	0/2/2/2
29	CLA	S1	605	-	1/1/12/20	8/19/97/115	-
40	LHG	c1	525	-	-	33/51/51/53	-
29	CLA	C1	513	-	1/1/15/20	16/37/115/115	-
45	RRX	h	101	-	1/1/11/25	4/29/65/65	0/2/2/2
29	CLA	C	507	-	1/1/15/20	14/37/115/115	-
29	CLA	N	604	-	1/1/15/20	19/37/115/115	-
33	LMG	b	622	-	-	17/39/59/70	0/1/1/1
37	DGD	c	519	-	-	23/51/91/95	0/2/2/2
31	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
40	LHG	C	525	-	-	32/51/51/53	-
48	CHL	S1	606	-	3/3/15/26	2/13/111/137	-
29	CLA	C	508	-	1/1/15/20	12/37/115/115	-
40	LHG	s1	624	29	-	27/49/49/53	-
29	CLA	Y	611	-	1/1/15/20	12/37/115/115	-
29	CLA	N	611	-	1/1/11/20	7/18/96/115	-
32	SQD	C1	526	-	-	25/49/69/69	0/1/1/1
29	CLA	G	612	-	1/1/10/20	5/11/89/115	-
48	CHL	r	606	-	3/3/15/26	3/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	g	602	-	1/1/15/20	22/37/115/115	-
29	CLA	S	610	-	1/1/15/20	20/37/115/115	-
29	CLA	S1	611	40	1/1/15/20	16/37/115/115	-
40	LHG	l	101	-	-	38/53/53/53	-
38	3PH	T1	101	-	-	29/49/49/49	-
31	BCR	d	404	-	-	13/29/63/63	0/2/2/2
40	LHG	y	624	29	-	30/53/53/53	-
29	CLA	s	617	-	1/1/12/20	8/19/97/115	-
52	LMT	R1	625	-	-	10/21/61/61	0/2/2/2
31	BCR	b1	619	-	-	9/29/63/63	0/2/2/2
29	CLA	b	617	-	1/1/15/20	13/37/115/115	-
29	CLA	G1	602	-	1/1/15/20	21/37/115/115	-
32	SQD	B	626	-	-	23/49/69/69	0/1/1/1
29	CLA	s	604	-	1/1/13/20	11/25/103/115	-
29	CLA	Y	614	-	1/1/15/20	17/37/115/115	-
33	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
41	LMK	C1	527	-	2/2/6/6	19/46/46/60	-
29	CLA	r1	609	-	1/1/14/20	17/31/109/115	-
29	CLA	c1	503	-	1/1/15/20	18/37/115/115	-
29	CLA	S1	614	-	1/1/13/20	8/25/103/115	-
29	CLA	d1	403	-	1/1/15/20	12/37/115/115	-
47	4RF	K1	101	-	-	32/59/59/59	-
31	BCR	D1	404	-	-	14/29/63/63	0/2/2/2
36	C7Z	b	620	-	1/1/12/26	13/29/67/67	0/2/2/2
50	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
34	SPH	y1	625	-	-	12/21/21/21	-
29	CLA	n1	614	-	1/1/11/20	9/18/96/115	-
29	CLA	r1	603	-	1/1/14/20	20/31/109/115	-
29	CLA	C1	512	-	1/1/15/20	16/37/115/115	-
29	CLA	y	602	24	1/1/15/20	15/37/115/115	-
41	LMK	C	527	-	2/2/6/6	21/46/46/60	-
29	CLA	Y	613	24	1/1/15/20	22/37/115/115	-
29	CLA	r	608	-	1/1/14/20	17/31/109/115	-
48	CHL	n1	609	-	4/4/20/26	5/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	RRX	h1	101	-	1/1/11/25	10/29/65/65	0/2/2/2
29	CLA	c1	512	-	1/1/15/20	17/37/115/115	-
29	CLA	g	611	-	1/1/15/20	15/37/115/115	-
37	DGD	c	518	-	-	9/44/84/95	0/2/2/2
39	DGA	c	524	-	-	31/45/45/45	-
29	CLA	b	602	-	1/1/15/20	21/37/115/115	-
31	BCR	C	514	-	-	17/29/63/63	0/2/2/2
55	PTY	y	627	-	-	15/20/20/53	-
33	LMG	C1	523	-	-	19/50/70/70	0/1/1/1
40	LHG	D1	408	-	-	26/48/48/53	-
29	CLA	b	605	-	1/1/15/20	19/37/115/115	-
29	CLA	c	507	-	1/1/15/20	15/37/115/115	-
29	CLA	n	610	-	1/1/15/20	18/37/115/115	-
29	CLA	b1	616	-	1/1/15/20	9/37/115/115	-
48	CHL	G1	606	-	3/3/16/26	4/20/118/137	-
29	CLA	Y1	611	-	1/1/15/20	16/37/115/115	-
29	CLA	B1	606	-	1/1/15/20	18/37/115/115	-
48	CHL	n	609	-	4/4/20/26	5/39/137/137	-
29	CLA	S1	613	-	1/1/13/20	9/25/103/115	-
48	CHL	g1	605	-	4/4/16/26	7/18/116/137	-
48	CHL	s	601	-	3/3/16/26	4/15/113/137	-
38	3PH	s1	626	-	-	27/49/49/49	-
40	LHG	d	410	-	-	20/43/43/53	-
51	NEX	R	622	-	-	8/27/83/83	0/3/3/3
29	CLA	g	614	-	1/1/11/20	11/18/96/115	-
29	CLA	b1	604	-	1/1/15/20	18/37/115/115	-
29	CLA	B	613	-	1/1/15/20	18/37/115/115	-
55	PTY	y1	627	-	-	11/20/20/53	-
29	CLA	c	506	-	1/1/15/20	17/37/115/115	-
48	CHL	s	607	-	3/3/15/26	0/12/110/137	-
33	LMG	w	201	-	-	17/34/54/70	0/1/1/1
40	LHG	d	408	-	-	26/48/48/53	-
29	CLA	Y1	610	-	1/1/15/20	12/37/115/115	-
48	CHL	n1	607	-	4/4/20/26	7/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	Y1	614	-	1/1/15/20	14/37/115/115	-
31	BCR	b1	618	-	-	11/29/63/63	0/2/2/2
29	CLA	y1	613	-	1/1/15/20	18/37/115/115	-
29	CLA	B1	604	-	1/1/15/20	14/37/115/115	-
29	CLA	a1	410	-	1/1/14/20	13/31/109/115	-
48	CHL	r	607	-	3/3/16/26	4/20/118/137	-
29	CLA	B1	612	-	1/1/15/20	15/37/115/115	-
29	CLA	Y1	608	-	1/1/12/20	7/19/97/115	-
51	NEX	g1	623	-	1/1/12/25	7/27/83/83	0/3/3/3
48	CHL	y1	609	-	4/4/20/26	8/39/137/137	-
31	BCR	C	517	-	-	13/29/63/63	0/2/2/2
29	CLA	b	604	-	1/1/15/20	14/37/115/115	-
31	BCR	C	515	-	-	9/29/63/63	0/2/2/2
51	NEX	y	623	-	-	6/27/83/83	0/3/3/3
29	CLA	c	504	-	1/1/15/20	18/37/115/115	-
48	CHL	G	607	-	4/4/20/26	11/39/137/137	-
50	XAT	n	622	-	1/1/12/26	4/31/93/93	0/4/4/4
31	BCR	B1	618	-	-	15/29/63/63	0/2/2/2
29	CLA	S	611	40	1/1/15/20	16/37/115/115	-
48	CHL	y1	607	-	4/4/20/26	4/39/137/137	-
29	CLA	b1	607	-	1/1/15/20	12/37/115/115	-
48	CHL	N	601	20	4/4/20/26	5/39/137/137	-
37	DGD	c1	520	-	-	11/48/88/95	0/2/2/2
29	CLA	b1	606	-	1/1/15/20	13/37/115/115	-
49	LUT	r	620	-	-	6/29/67/67	0/2/2/2
39	DGA	c1	524	-	-	28/45/45/45	-
32	SQD	C	526	-	-	23/49/69/69	0/1/1/1
29	CLA	d1	402	-	1/1/15/20	10/37/115/115	-
29	CLA	C	509	-	1/1/15/20	20/37/115/115	-
29	CLA	b1	613	-	1/1/15/20	16/37/115/115	-
48	CHL	S	607	-	3/3/15/26	1/12/110/137	-
40	LHG	d1	410	-	-	33/43/43/53	-
48	CHL	g	607	-	4/4/20/26	10/39/137/137	-
48	CHL	N1	608	-	3/3/16/26	5/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	502	-	1/1/15/20	12/37/115/115	-
29	CLA	C1	508	-	1/1/15/20	13/37/115/115	-
33	LMG	a	413	-	-	20/43/63/70	0/1/1/1
49	LUT	G1	621	-	-	3/29/67/67	0/2/2/2
29	CLA	A1	405	-	1/1/15/20	12/37/115/115	-
51	NEX	g	623	-	1/1/12/25	9/27/83/83	0/3/3/3
31	BCR	A1	411	-	-	9/29/63/63	0/2/2/2
47	4RF	k	101	-	-	31/59/59/59	-
55	PTY	y	626	-	-	27/53/53/53	-
48	CHL	S	608	-	4/4/19/26	7/33/131/137	-
48	CHL	s1	607	-	3/3/15/26	0/12/110/137	-
33	LMG	B	622	-	-	20/39/59/70	0/1/1/1
33	LMG	c1	523	-	-	18/50/70/70	0/1/1/1
34	SPH	a1	414	-	-	10/21/21/21	-
51	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
48	CHL	G	605	21	4/4/16/26	6/18/116/137	-
29	CLA	C1	506	-	1/1/15/20	19/37/115/115	-
29	CLA	B1	613	-	1/1/15/20	19/37/115/115	-
48	CHL	G1	608	-	2/2/15/26	1/13/111/137	-
33	LMG	h1	102	-	-	22/43/63/70	0/1/1/1
29	CLA	Y	604	-	1/1/15/20	17/37/115/115	-
29	CLA	b	613	-	1/1/15/20	19/37/115/115	-
29	CLA	D	402	-	1/1/15/20	19/37/115/115	-
29	CLA	g	604	-	1/1/11/20	7/18/96/115	-
30	PHO	a1	408	-	-	17/37/103/103	0/5/6/6
29	CLA	B	612	-	1/1/15/20	16/37/115/115	-
31	BCR	c1	514	-	-	12/29/63/63	0/2/2/2
33	LMG	a1	413	-	-	20/43/63/70	0/1/1/1
29	CLA	C1	511	-	1/1/15/20	10/37/115/115	-
45	RRX	H1	101	-	1/1/11/25	9/29/65/65	0/2/2/2
29	CLA	A	407	-	1/1/12/20	9/19/97/115	-
31	BCR	A	411	-	-	12/29/63/63	0/2/2/2
48	CHL	n1	605	-	4/4/20/26	7/39/137/137	-
48	CHL	s1	608	-	4/4/19/26	5/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	523	-	-	21/50/70/70	0/1/1/1
40	LHG	S1	624	29	-	32/49/49/53	-
30	PHO	a	408	-	-	12/37/103/103	0/5/6/6
51	NEX	N	623	-	-	4/27/83/83	1/3/3/3
32	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
48	CHL	n1	601	-	4/4/20/26	11/39/137/137	-
29	CLA	r	603	-	1/1/14/20	17/31/109/115	-
29	CLA	C1	504	-	1/1/15/20	18/37/115/115	-
39	DGA	j	101	-	-	20/30/30/45	-
29	CLA	Y	612	-	1/1/15/20	13/37/115/115	-
33	LMG	D	411	-	-	11/41/61/70	0/1/1/1
29	CLA	A1	406	-	1/1/15/20	21/37/115/115	-
38	3PH	B	624	-	-	34/49/49/49	-
32	SQD	c	526	-	-	20/49/69/69	0/1/1/1
48	CHL	Y1	607	-	4/4/20/26	11/39/137/137	-
29	CLA	b1	609	-	1/1/15/20	16/37/115/115	-
33	LMG	b1	622	-	-	19/39/59/70	0/1/1/1
29	CLA	Y	608	-	1/1/12/20	7/19/97/115	-
29	CLA	S1	602	23	1/1/14/20	17/31/109/115	-
29	CLA	B	603	-	1/1/15/20	21/37/115/115	-
37	DGD	C1	518	-	-	12/44/84/95	0/2/2/2
40	LHG	y1	624	29	-	25/53/53/53	-
41	LMK	c1	527	-	2/2/6/6	14/46/46/60	-
29	CLA	c1	501	-	1/1/15/20	17/37/115/115	-
50	XAT	Y	622	-	-	7/31/93/93	0/4/4/4
50	XAT	y1	622	-	-	7/31/93/93	0/4/4/4
51	NEX	n1	623	-	-	5/27/83/83	0/3/3/3
29	CLA	N1	614	-	1/1/11/20	7/18/96/115	-
29	CLA	g1	614	-	1/1/11/20	11/18/96/115	-
48	CHL	S1	607	-	3/3/15/26	1/12/110/137	-
37	DGD	c	520	-	-	9/48/88/95	0/2/2/2
29	CLA	Y	610	-	1/1/15/20	12/37/115/115	-
29	CLA	N1	603	-	1/1/15/20	15/37/115/115	-
40	LHG	s	624	29	-	26/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LHG	G	624	29	-	33/53/53/53	-
48	CHL	Y1	606	-	4/4/20/26	7/39/137/137	-
48	CHL	r1	607	-	3/3/16/26	4/20/118/137	-
48	CHL	r1	606	-	3/3/15/26	4/13/111/137	-
37	DGD	C1	519	-	-	22/51/91/95	0/2/2/2
50	XAT	n1	622	-	-	4/31/93/93	0/4/4/4
29	CLA	S1	603	-	1/1/15/20	12/37/115/115	-
49	LUT	n1	621	-	1/1/12/27	5/29/67/67	0/2/2/2
29	CLA	n	602	-	1/1/15/20	14/37/115/115	-
29	CLA	S	609	-	1/1/14/20	10/31/109/115	-
29	CLA	G	602	-	1/1/15/20	17/37/115/115	-
50	XAT	y	622	-	-	8/31/93/93	0/4/4/4
48	CHL	g	608	-	3/3/15/26	3/13/111/137	-
29	CLA	G1	604	-	1/1/11/20	8/18/96/115	-
29	CLA	y1	610	24	1/1/15/20	13/37/115/115	-
43	PL9	D1	405	-	-	18/53/73/73	0/1/1/1
29	CLA	G1	612	-	1/1/10/20	7/11/89/115	-
31	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
49	LUT	R	620	-	1/1/12/27	2/29/67/67	0/2/2/2
53	ERG	r	626	-	5/5/11/15	8/13/71/71	0/4/4/4
47	4RF	i	101	-	-	31/59/59/59	-
29	CLA	y	603	-	1/1/15/20	18/37/115/115	-
38	3PH	S	626	-	-	24/49/49/49	-
51	NEX	S	623	-	-	8/27/83/83	0/3/3/3
29	CLA	y1	608	-	1/1/12/20	9/19/97/115	-
49	LUT	g1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	D	403	-	1/1/15/20	16/37/115/115	-
31	BCR	C1	515	-	-	12/29/63/63	0/2/2/2
29	CLA	n1	612	-	1/1/11/20	5/13/91/115	-
49	LUT	N	620	-	-	2/29/67/67	0/2/2/2
48	CHL	N	606	-	4/4/20/26	10/39/137/137	-
48	CHL	N1	607	-	4/4/20/26	10/39/137/137	-
29	CLA	G1	603	-	1/1/15/20	23/37/115/115	-
36	C7Z	B1	620	-	1/1/12/26	7/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	c1	517	-	-	9/29/63/63	0/2/2/2
33	LMG	w1	201	-	-	17/34/54/70	0/1/1/1
54	LPX	s	625	-	-	15/31/31/31	-
31	BCR	c1	515	-	-	11/29/63/63	0/2/2/2
40	LHG	g	624	-	-	27/53/53/53	-
29	CLA	s	605	-	1/1/12/20	11/19/97/115	-
50	XAT	g	622	-	2/2/12/26	3/31/93/93	0/4/4/4
49	LUT	g	621	-	-	4/29/67/67	0/2/2/2
29	CLA	r1	608	-	1/1/14/20	16/31/109/115	-
38	3PH	s	626	-	-	22/49/49/49	-
50	XAT	R1	621	-	-	4/31/93/93	0/4/4/4
55	PTY	y1	626	-	-	33/53/53/53	-
31	BCR	B	619	-	-	8/29/63/63	0/2/2/2
55	PTY	Y	626	-	-	31/53/53/53	-
29	CLA	A1	410	-	1/1/14/20	12/31/109/115	-
40	LHG	G1	624	-	-	29/53/53/53	-
33	LMG	h	102	-	-	11/43/63/70	0/1/1/1
32	SQD	M	101	-	-	24/37/57/69	0/1/1/1
50	XAT	Y1	622	-	1/1/12/26	4/31/93/93	0/4/4/4
29	CLA	B	610	-	1/1/15/20	21/37/115/115	-
30	PHO	a	409	-	-	11/37/103/103	0/5/6/6
49	LUT	Y1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	c1	509	-	1/1/15/20	20/37/115/115	-
48	CHL	S	601	23	3/3/16/26	3/15/113/137	-
52	LMT	r1	625	-	-	10/21/61/61	0/2/2/2
48	CHL	N	605	20	4/4/20/26	9/39/137/137	-
29	CLA	B1	605	-	1/1/15/20	15/37/115/115	-
29	CLA	C1	502	-	1/1/15/20	12/37/115/115	-
29	CLA	C1	505	-	1/1/15/20	19/37/115/115	-
29	CLA	R1	610	-	1/1/14/20	17/31/109/115	-
29	CLA	n1	611	-	1/1/11/20	9/18/96/115	-
29	CLA	b	611	-	1/1/15/20	7/37/115/115	-
53	ERG	R1	626	-	5/5/11/15	9/13/71/71	0/4/4/4
49	LUT	G1	620	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	G1	601	21	4/4/20/26	13/39/137/137	-
37	DGD	C	519	-	-	26/51/91/95	0/2/2/2
43	PL9	D	405	-	-	9/53/73/73	0/1/1/1
48	CHL	G1	607	-	4/4/20/26	11/39/137/137	-
29	CLA	B1	610	-	1/1/15/20	23/37/115/115	-
31	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
29	CLA	g	613	-	1/1/15/20	19/37/115/115	-
39	DGA	C1	524	-	-	23/45/45/45	-
29	CLA	S	602	-	1/1/14/20	16/31/109/115	-
52	LMT	R	625	-	-	9/21/61/61	0/2/2/2
49	LUT	g	620	-	-	4/29/67/67	0/2/2/2
47	4RF	K	101	-	-	32/59/59/59	-
29	CLA	A	406	-	1/1/15/20	14/37/115/115	-
29	CLA	b	607	-	1/1/15/20	16/37/115/115	-
29	CLA	G	610	21	1/1/15/20	16/37/115/115	-
29	CLA	b	610	-	1/1/15/20	15/37/115/115	-
29	CLA	b	606	-	1/1/15/20	15/37/115/115	-
29	CLA	s1	617	-	1/1/12/20	11/19/97/115	-
34	SPH	y	625	-	-	8/21/21/21	-
33	LMG	d1	411	-	-	19/41/61/70	0/1/1/1
37	DGD	B1	623	-	-	11/32/72/95	0/2/2/2
29	CLA	c	511	4	1/1/15/20	9/37/115/115	-
31	BCR	D	404	-	-	13/29/63/63	0/2/2/2
29	CLA	s	609	-	1/1/14/20	16/31/109/115	-
29	CLA	C1	509	-	1/1/15/20	10/37/115/115	-
29	CLA	b	608	-	1/1/15/20	28/37/115/115	-
29	CLA	b	603	-	1/1/15/20	21/37/115/115	-
39	DGA	B1	625	-	-	26/45/45/45	-
31	BCR	c	516	-	-	15/29/63/63	0/2/2/2
37	DGD	C	518	-	-	18/44/84/95	0/2/2/2
29	CLA	r	604	-	1/1/11/20	9/18/96/115	-
32	SQD	m1	101	-	-	22/37/57/69	0/1/1/1
29	CLA	R	609	-	1/1/14/20	13/31/109/115	-
32	SQD	b1	626	-	-	26/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	604	-	1/1/11/20	8/18/96/115	-
29	CLA	a	410	-	1/1/14/20	15/31/109/115	-
49	LUT	Y1	620	-	-	8/29/67/67	0/2/2/2
29	CLA	n	614	-	1/1/11/20	4/18/96/115	-
54	LPX	S	625	-	-	14/31/31/31	-
29	CLA	G1	611	-	1/1/15/20	19/37/115/115	-
49	LUT	r1	620	-	-	4/29/67/67	0/2/2/2
29	CLA	y1	611	40	1/1/15/20	19/37/115/115	-
48	CHL	n	606	-	4/4/20/26	7/39/137/137	-
48	CHL	Y1	605	-	3/3/16/26	3/15/113/137	-
29	CLA	C	506	-	1/1/15/20	13/37/115/115	-
29	CLA	S	614	-	1/1/13/20	8/25/103/115	-
29	CLA	N	602	-	1/1/15/20	15/37/115/115	-
29	CLA	b	612	-	1/1/15/20	16/37/115/115	-
29	CLA	S	605	23	1/1/12/20	9/19/97/115	-
29	CLA	c	503	-	1/1/15/20	20/37/115/115	-
48	CHL	Y	601	24	4/4/20/26	7/39/137/137	-
29	CLA	S1	617	23	1/1/12/20	7/19/97/115	-
29	CLA	C	502	-	1/1/15/20	13/37/115/115	-
29	CLA	c1	507	-	1/1/15/20	16/37/115/115	-
29	CLA	y1	614	-	1/1/15/20	16/37/115/115	-
48	CHL	S1	608	-	4/4/19/26	10/33/131/137	-
50	XAT	G	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	N1	611	-	1/1/11/20	10/18/96/115	-
29	CLA	a1	405	-	1/1/15/20	17/37/115/115	-
44	HEM	f	101	6,7	-	1/12/54/54	-
29	CLA	N	610	-	1/1/15/20	19/37/115/115	-
29	CLA	B	606	-	1/1/15/20	20/37/115/115	-
33	LMG	A1	413	-	-	18/43/63/70	0/1/1/1
39	DGA	C	524	-	-	18/45/45/45	-
51	NEX	s	623	-	-	4/27/83/83	0/3/3/3
29	CLA	C	504	-	1/1/15/20	16/37/115/115	-
29	CLA	R1	609	-	1/1/14/20	14/31/109/115	-
48	CHL	Y	609	-	4/4/20/26	6/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	LPX	S1	625	-	-	15/31/31/31	-
48	CHL	g	609	-	4/4/20/26	10/39/137/137	-
29	CLA	B	602	-	1/1/15/20	20/37/115/115	-
29	CLA	B1	617	-	1/1/15/20	16/37/115/115	-
48	CHL	n1	606	-	4/4/20/26	7/39/137/137	-
39	DGA	B	625	-	-	23/45/45/45	-
33	LMG	W	201	-	-	14/34/54/70	0/1/1/1
29	CLA	y	614	-	1/1/15/20	15/37/115/115	-
29	CLA	D1	402	-	1/1/15/20	13/37/115/115	-
34	SPH	a	414	-	-	11/21/21/21	-
40	LHG	d1	408	-	-	30/48/48/53	-
48	CHL	G	609	21	4/4/20/26	10/39/137/137	-
48	CHL	G	608	-	3/3/15/26	1/13/111/137	-
49	LUT	g1	620	-	-	6/29/67/67	0/2/2/2
29	CLA	N1	613	-	1/1/15/20	14/37/115/115	-
29	CLA	C	510	-	1/1/15/20	13/37/115/115	-
31	BCR	B	618	-	-	11/29/63/63	0/2/2/2
40	LHG	Y1	624	-	-	18/53/53/53	-
47	4RF	i1	101	-	-	30/59/59/59	-
38	3PH	t	101	-	-	27/49/49/49	-
48	CHL	G	606	-	3/3/16/26	5/20/118/137	-
29	CLA	R	608	-	1/1/14/20	19/31/109/115	-
29	CLA	s	611	40	1/1/15/20	15/37/115/115	-
37	DGD	B	623	-	-	15/32/72/95	0/2/2/2
29	CLA	N	612	-	1/1/11/20	4/13/91/115	-
48	CHL	S	606	-	3/3/15/26	2/13/111/137	-
29	CLA	B1	615	-	1/1/15/20	14/37/115/115	-
33	LMG	C	521	-	-	16/46/66/70	0/1/1/1
29	CLA	C	505	-	1/1/15/20	16/37/115/115	-
29	CLA	S1	604	-	1/1/13/20	10/25/103/115	-
29	CLA	S1	612	-	1/1/11/20	6/13/91/115	-
48	CHL	N1	606	-	4/4/20/26	12/39/137/137	-
53	ERG	R	626	-	5/5/11/15	6/13/71/71	0/4/4/4
52	LMT	r	625	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	4RF	I	102	-	-	30/59/59/59	-
29	CLA	g	610	-	1/1/15/20	19/37/115/115	-
29	CLA	s	614	-	1/1/13/20	4/25/103/115	-
29	CLA	n	613	-	1/1/15/20	18/37/115/115	-
29	CLA	s1	614	-	1/1/13/20	15/25/103/115	-
29	CLA	N	603	-	1/1/15/20	17/37/115/115	-
29	CLA	b1	608	-	1/1/15/20	25/37/115/115	-
29	CLA	s1	605	-	1/1/12/20	9/19/97/115	-
29	CLA	g1	611	-	1/1/15/20	18/37/115/115	-
48	CHL	R1	607	-	3/3/16/26	4/20/118/137	-
48	CHL	y1	605	24	3/3/16/26	4/15/113/137	-
32	SQD	M1	101	-	-	17/37/57/69	0/1/1/1
29	CLA	G1	613	-	1/1/15/20	15/37/115/115	-
37	DGD	b	623	-	-	13/32/72/95	0/2/2/2
48	CHL	s1	606	-	3/3/15/26	0/13/111/137	-
48	CHL	s	606	-	3/3/15/26	2/13/111/137	-
48	CHL	g1	606	-	3/3/16/26	3/20/118/137	-
37	DGD	c1	519	-	-	24/51/91/95	0/2/2/2
49	LUT	y	620	-	-	4/29/67/67	0/2/2/2
53	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
29	CLA	R1	602	-	1/1/14/20	12/31/109/115	-
40	LHG	C1	525	-	-	30/51/51/53	-
29	CLA	n	603	-	1/1/15/20	23/37/115/115	-
29	CLA	y	608	-	1/1/12/20	10/19/97/115	-
48	CHL	R	606	-	3/3/15/26	1/13/111/137	-
40	LHG	n1	624	-	-	29/53/53/53	-
29	CLA	B	607	-	1/1/15/20	18/37/115/115	-
29	CLA	c1	511	-	1/1/15/20	18/37/115/115	-
48	CHL	y	606	-	4/4/20/26	12/39/137/137	-
29	CLA	b1	615	-	1/1/15/20	17/37/115/115	-
48	CHL	Y	605	24	3/3/16/26	3/15/113/137	-
51	NEX	n	623	-	-	5/27/83/83	1/3/3/3
49	LUT	G	621	-	1/1/12/27	4/29/67/67	0/2/2/2
55	PTY	Y1	626	-	-	26/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	512	-	1/1/15/20	18/37/115/115	-
29	CLA	n1	602	20	1/1/15/20	17/37/115/115	-

The worst 5 of 3829 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	R	626	ERG	C1-C10	-23.16	1.10	1.54
53	r	626	ERG	C1-C10	-22.96	1.10	1.54
53	R1	626	ERG	C1-C10	-22.89	1.10	1.54
53	r1	626	ERG	C1-C10	-22.73	1.11	1.54
53	r	626	ERG	C10-C9	-20.15	1.28	1.55

The worst 5 of 8657 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L	101	LHG	O7-C7-C8	22.97	161.00	111.50
40	l	101	LHG	O7-C7-C8	22.96	160.99	111.50
29	R	609	CLA	C4-C3-C5	-22.39	77.60	115.27
38	S	626	3PH	O21-C21-C22	22.18	159.31	111.50
38	S1	626	3PH	O21-C21-C22	22.13	159.19	111.50

5 of 696 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	A	410	CLA	ND
29	B	602	CLA	ND

5 of 9527 torsion outliers are listed below:

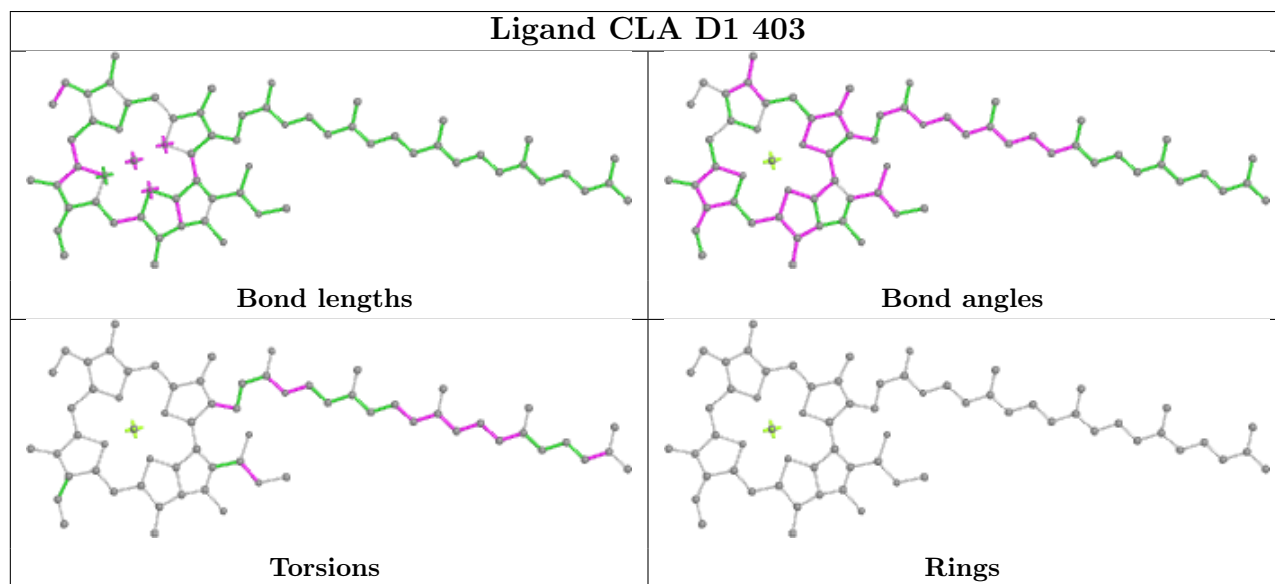
Mol	Chain	Res	Type	Atoms
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C2-C1-O2A-CGA

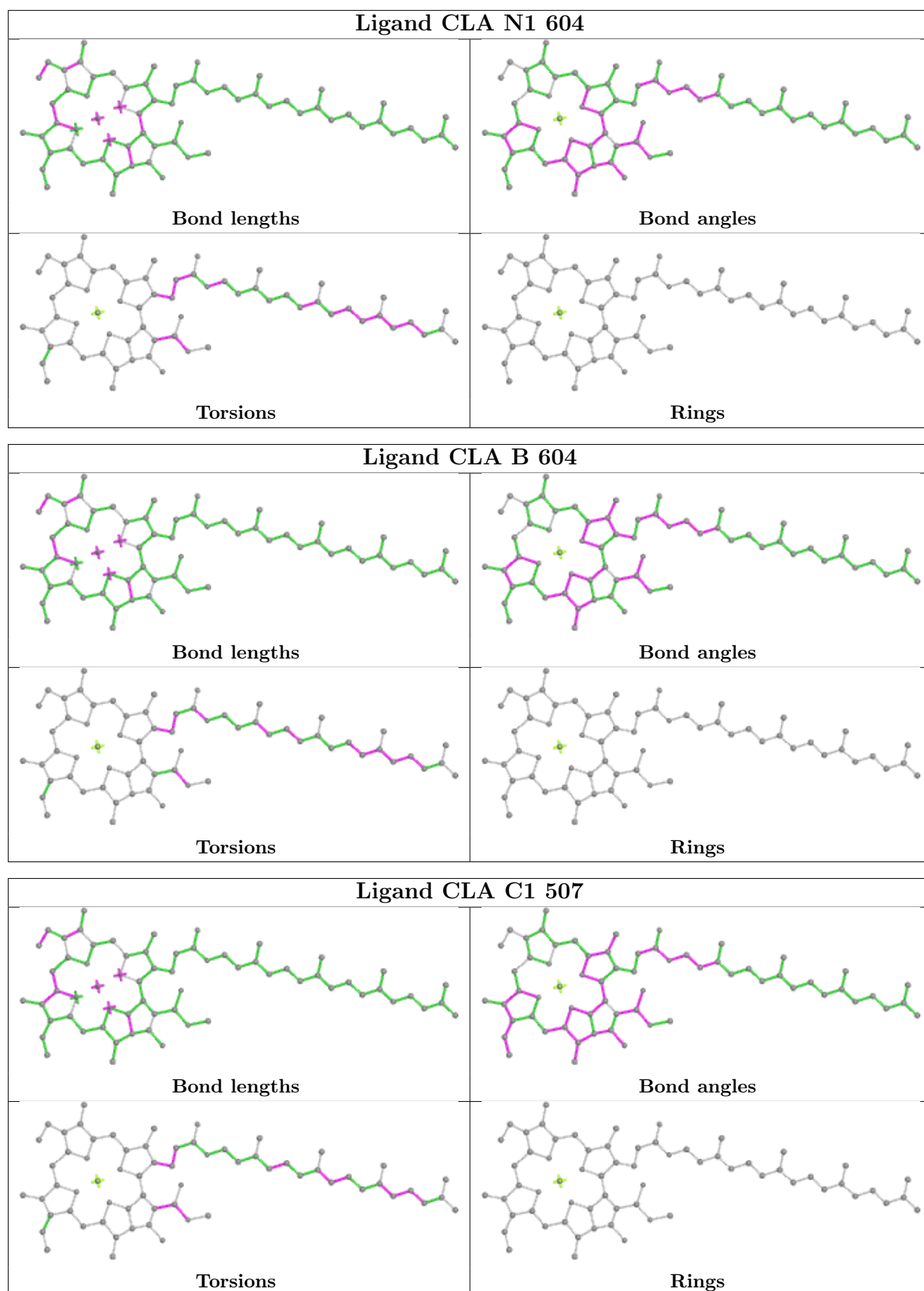
All (2) ring outliers are listed below:

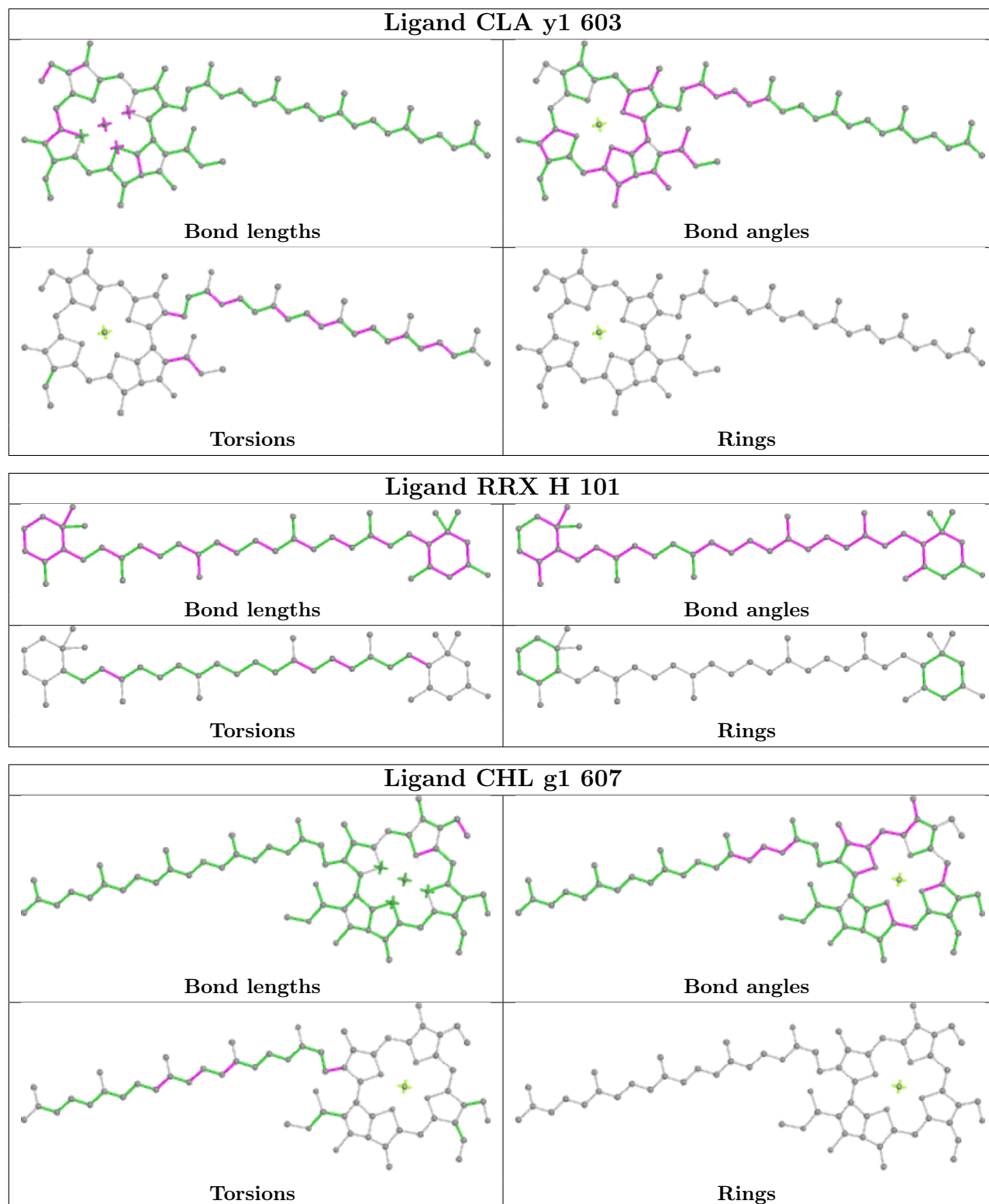
Mol	Chain	Res	Type	Atoms
51	N	623	NEX	C1-C2-C3-C4-C5-C6
51	n	623	NEX	C1-C2-C3-C4-C5-C6

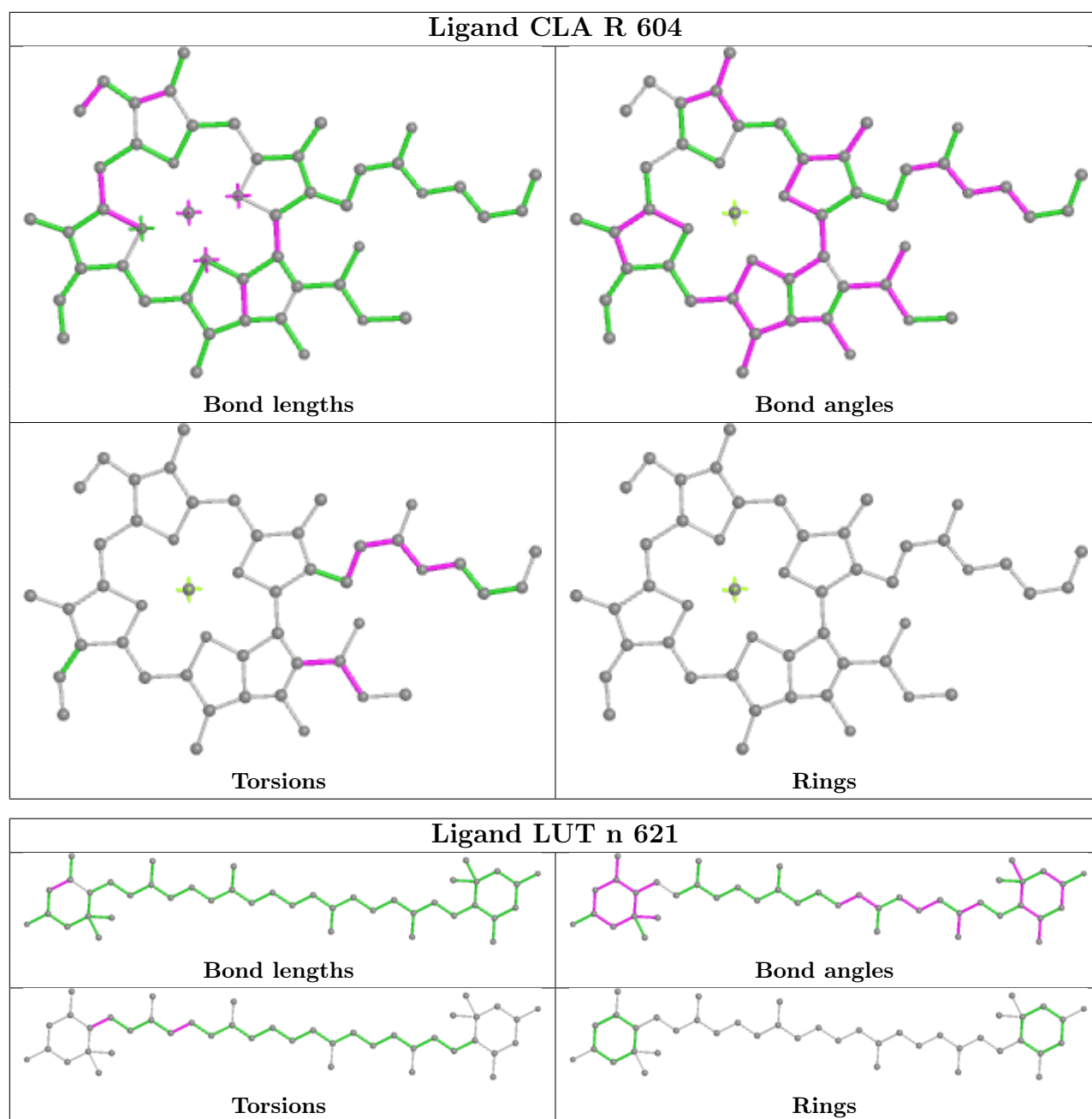
No monomer is involved in short contacts.

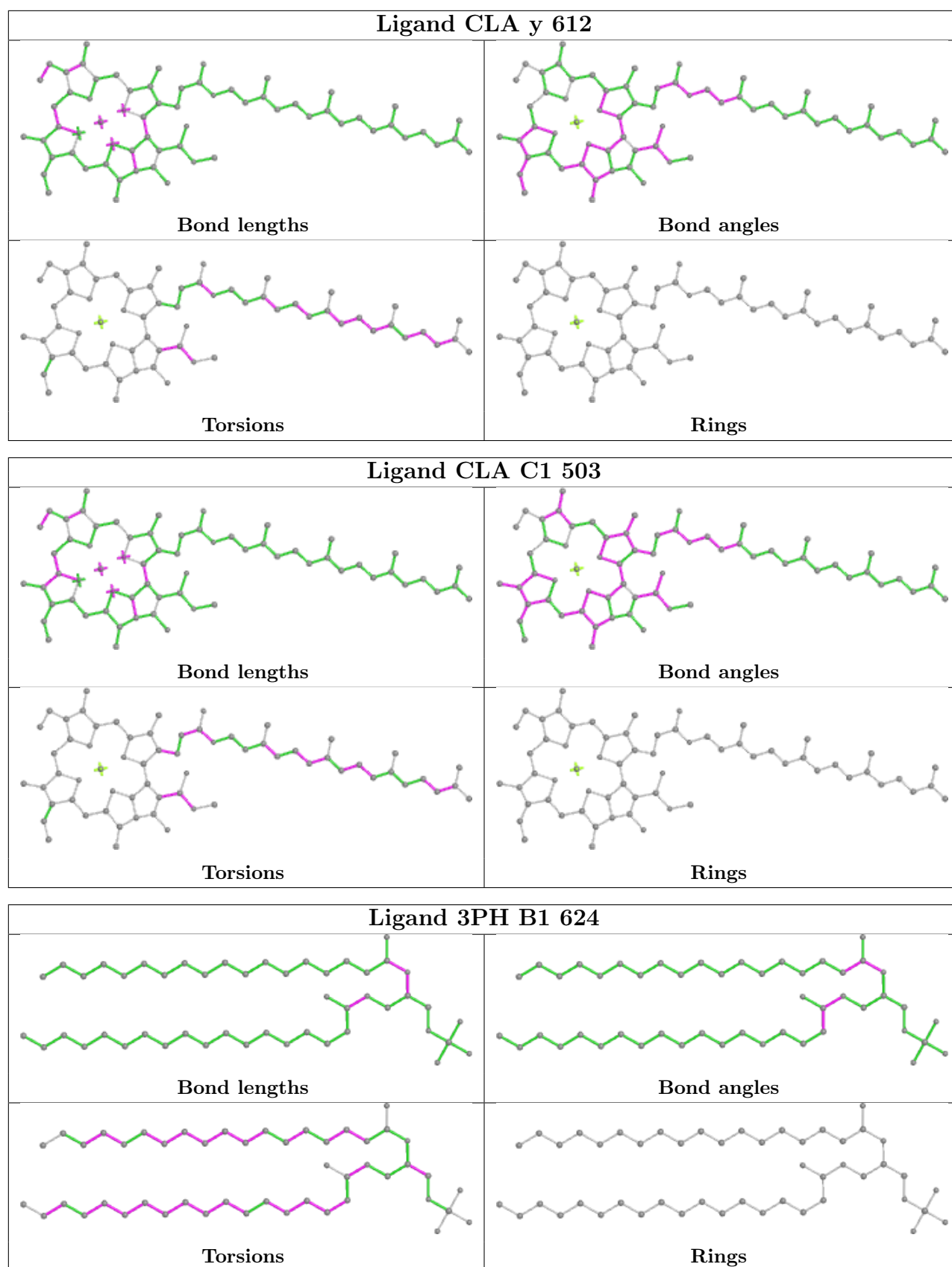
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



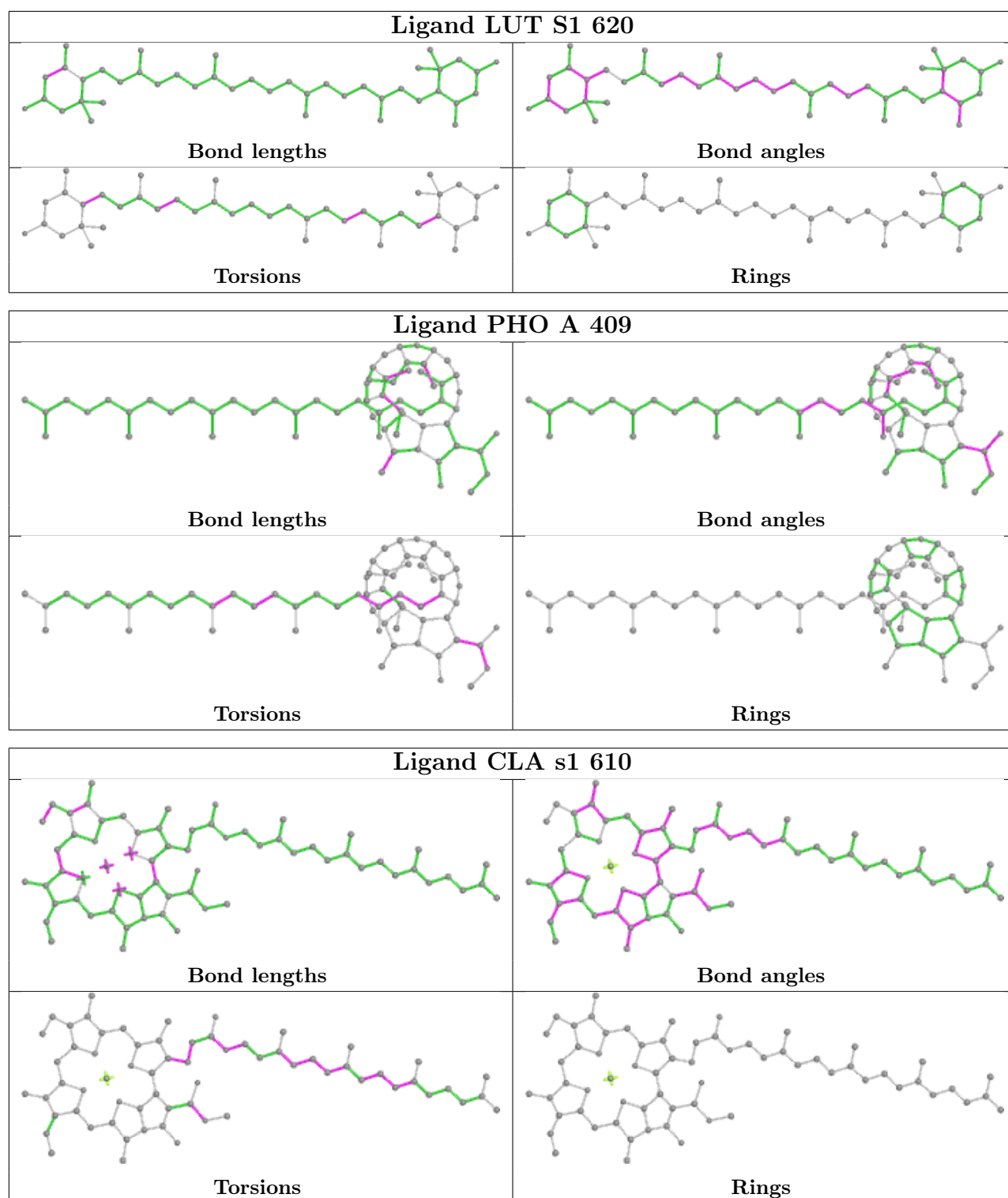


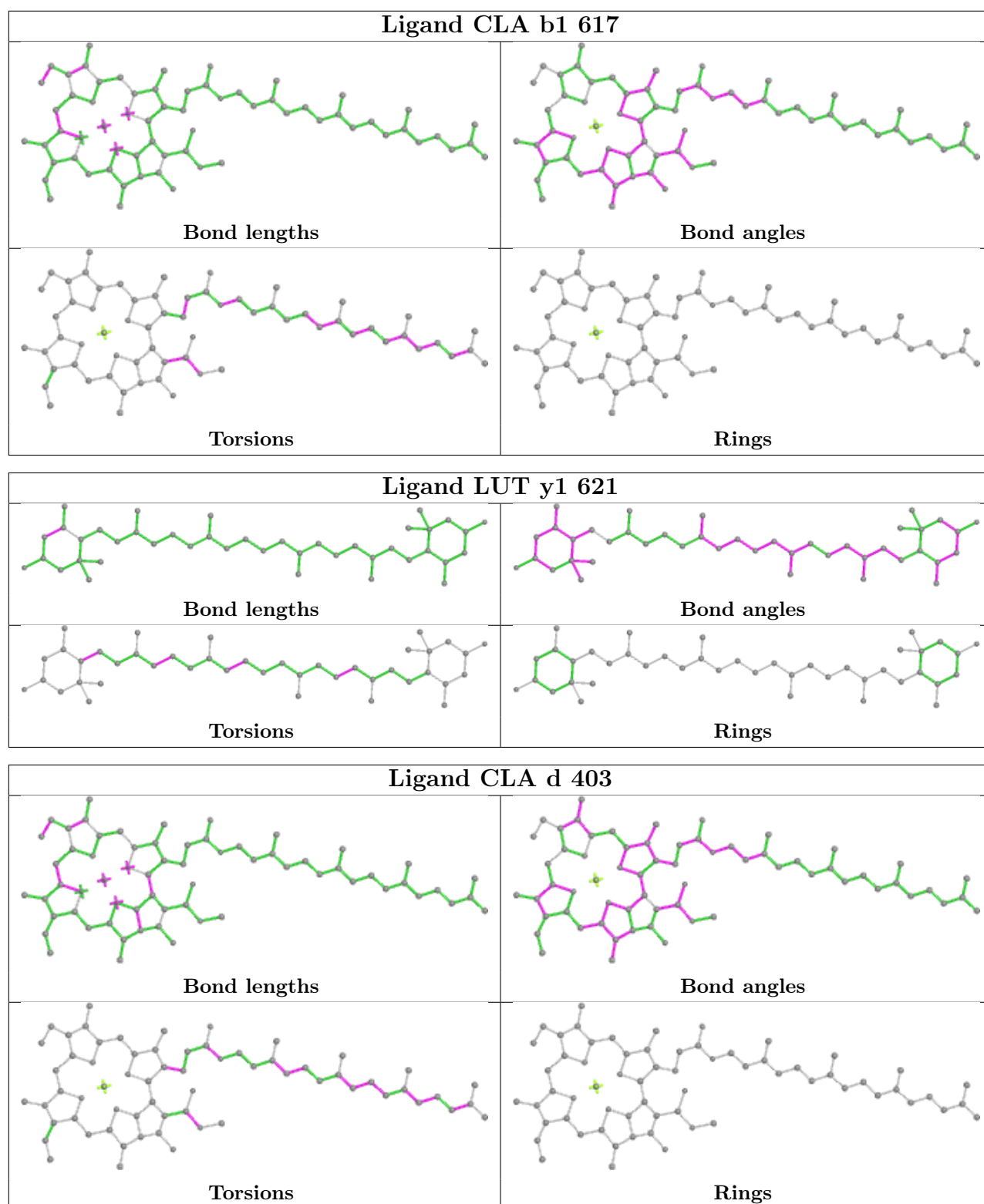


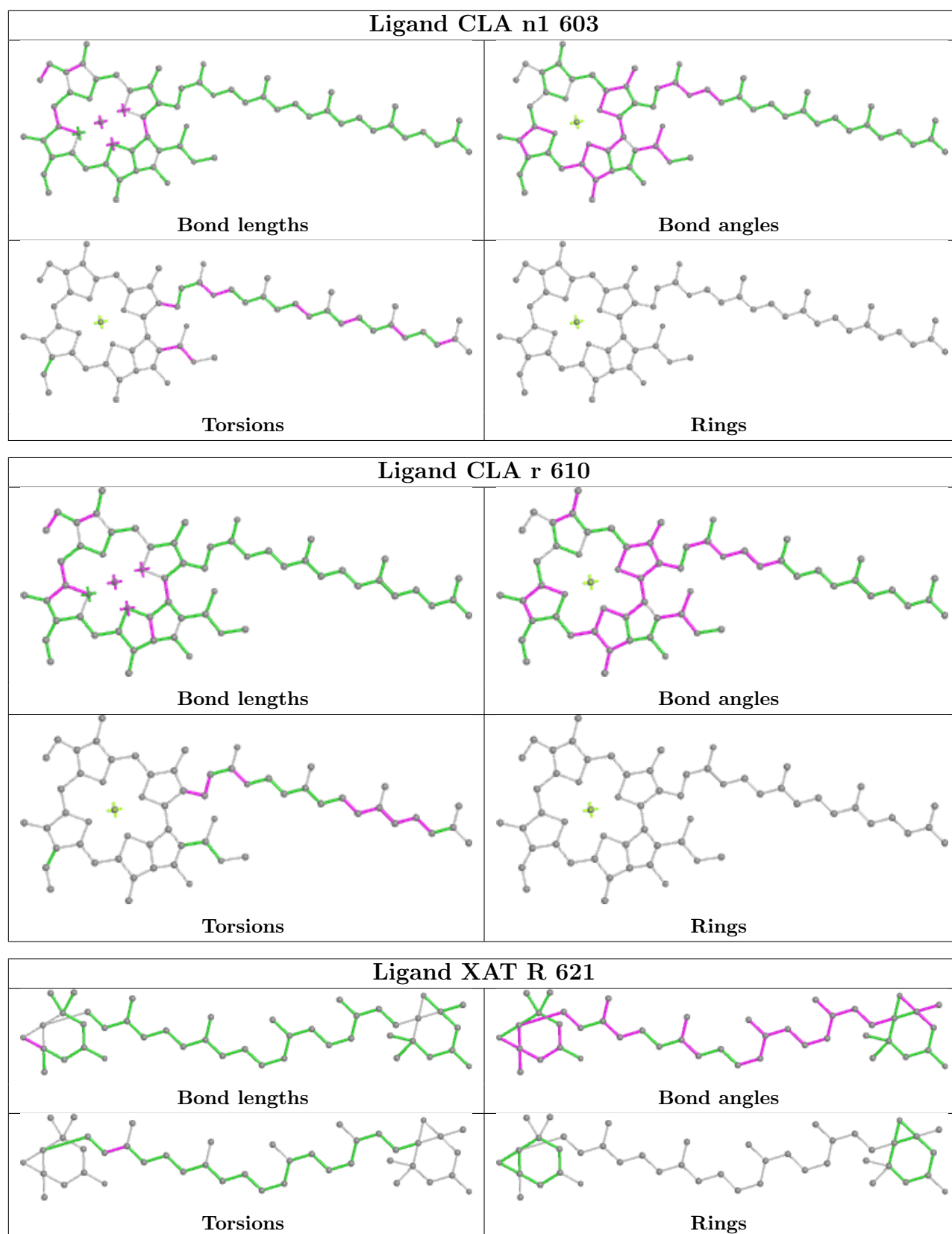


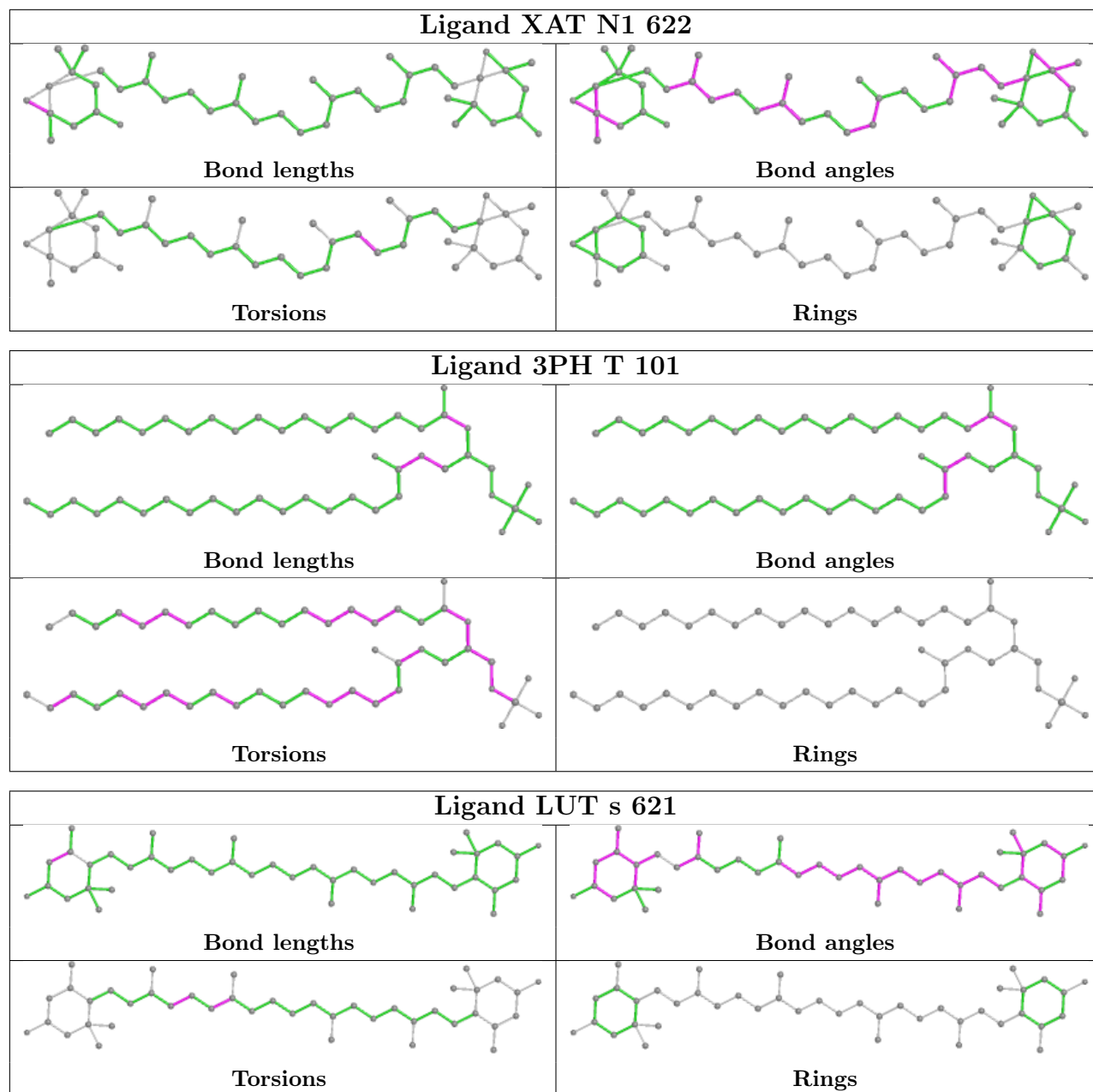


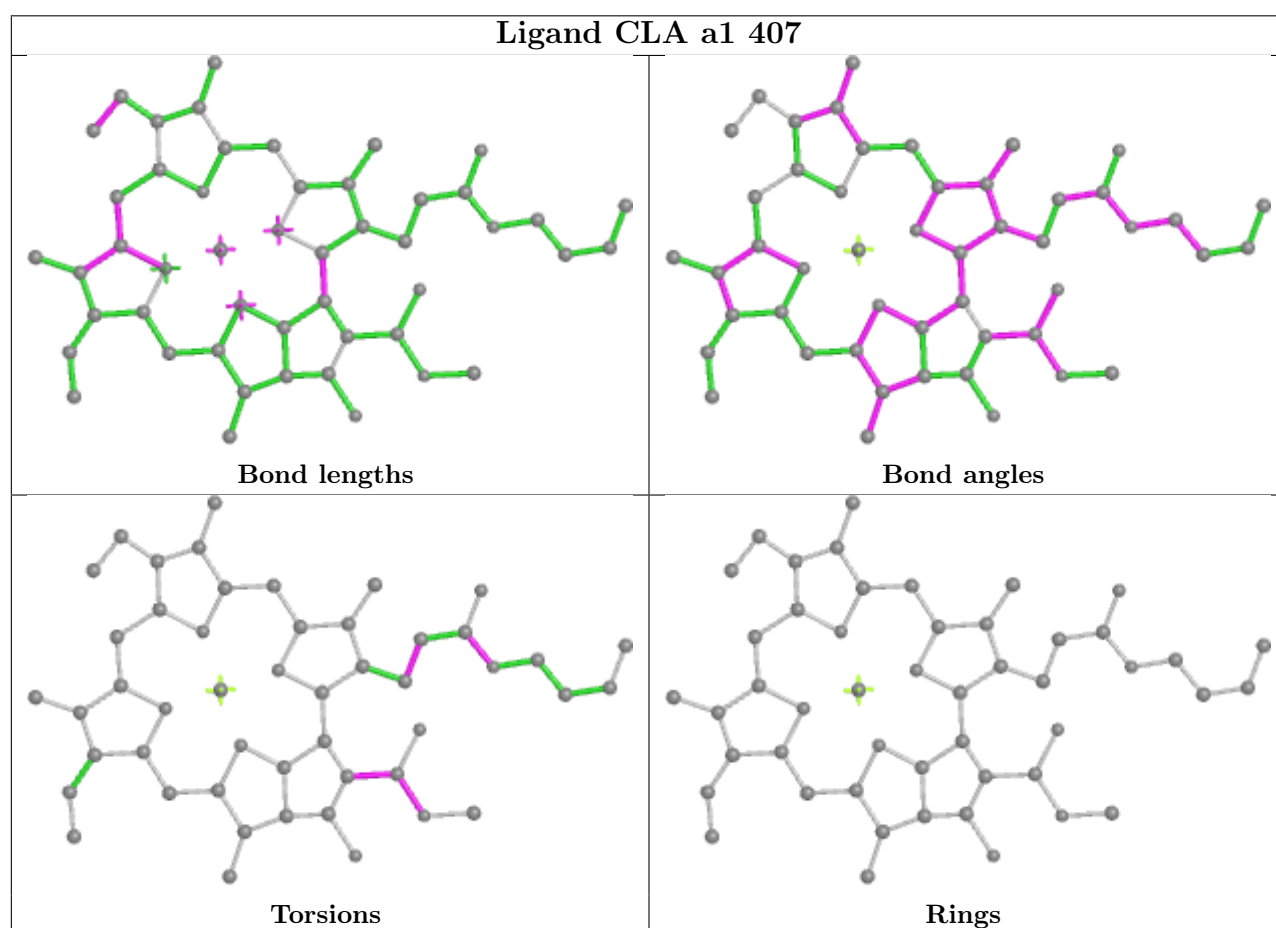
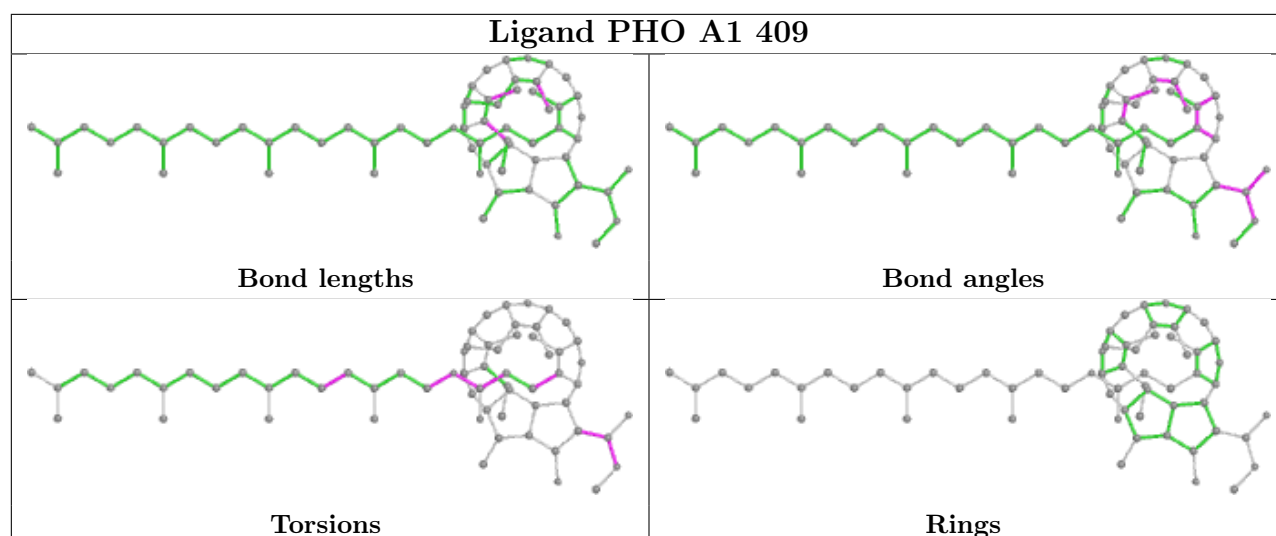


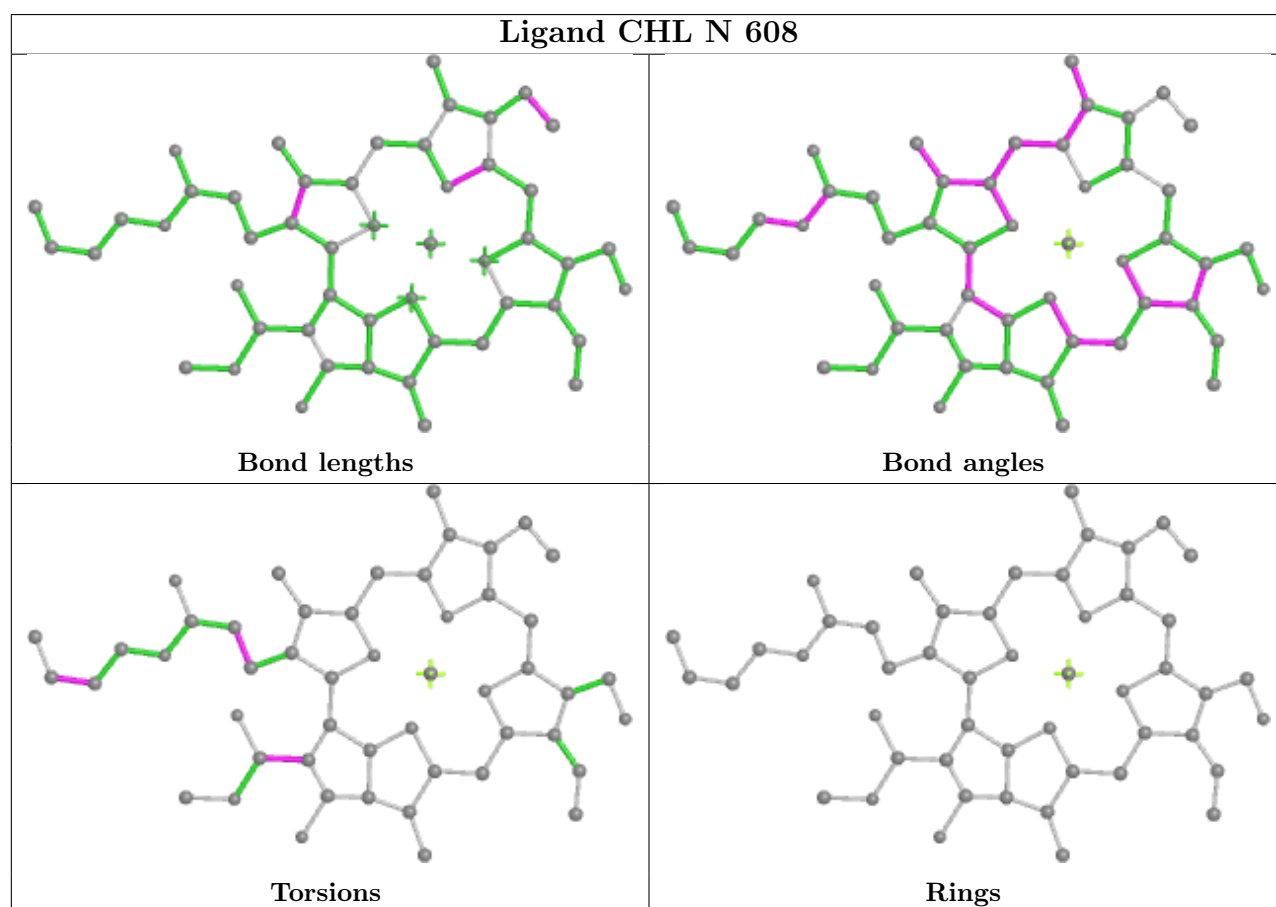
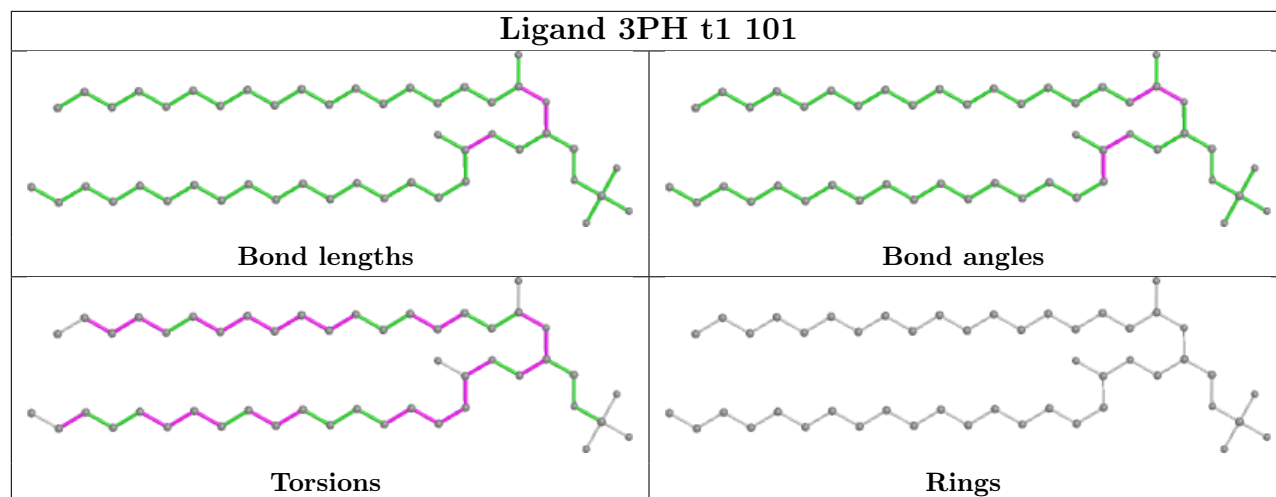


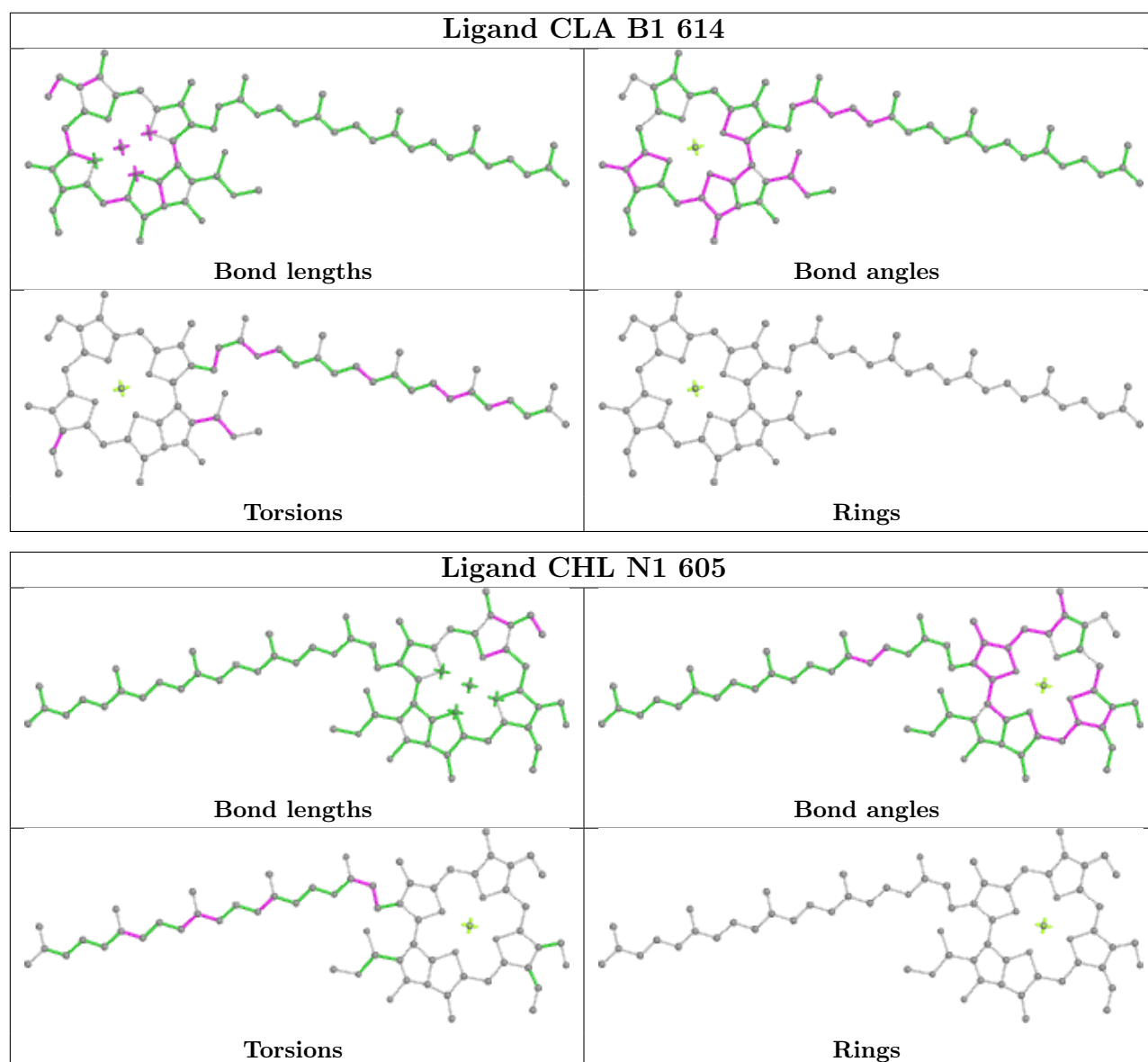


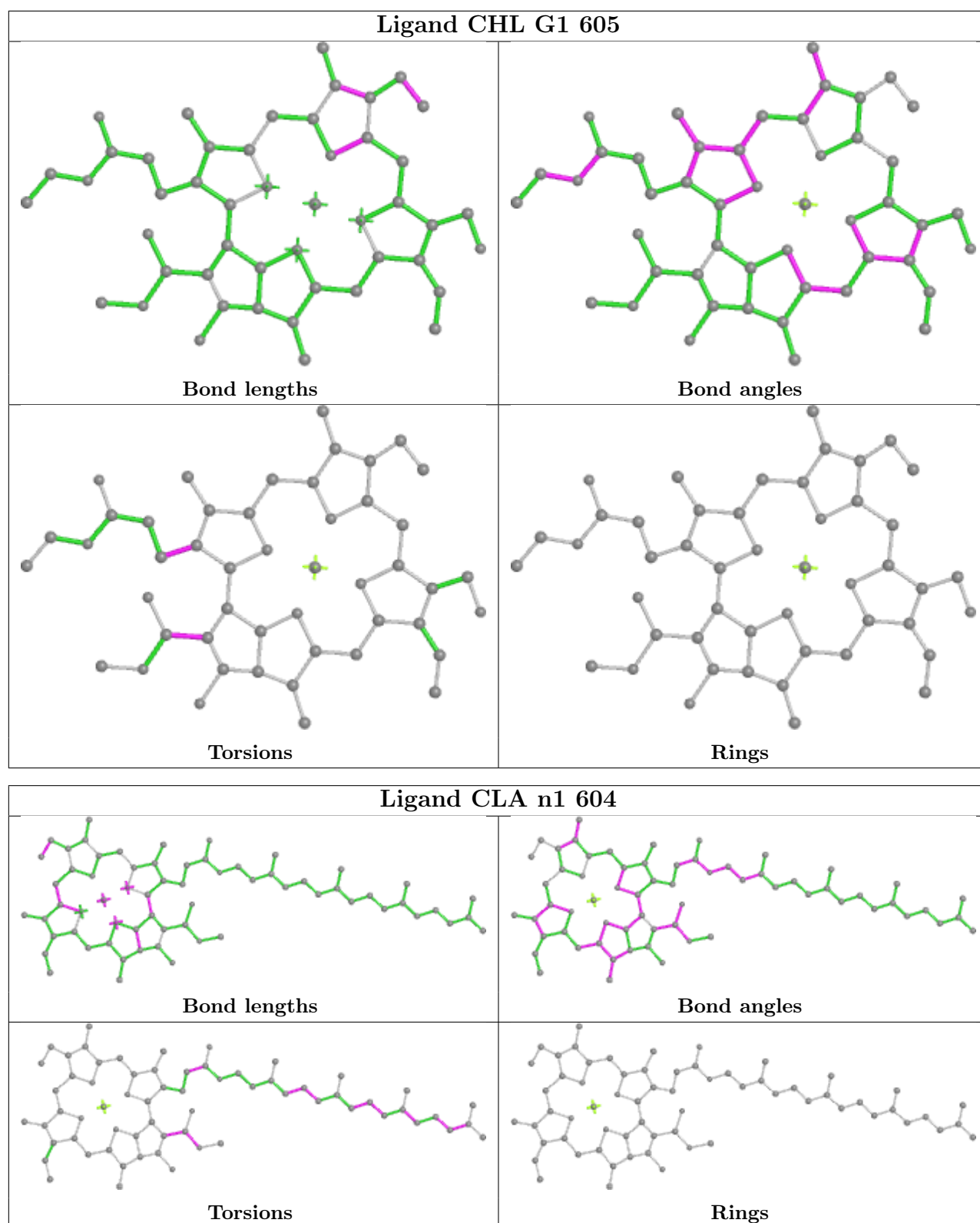




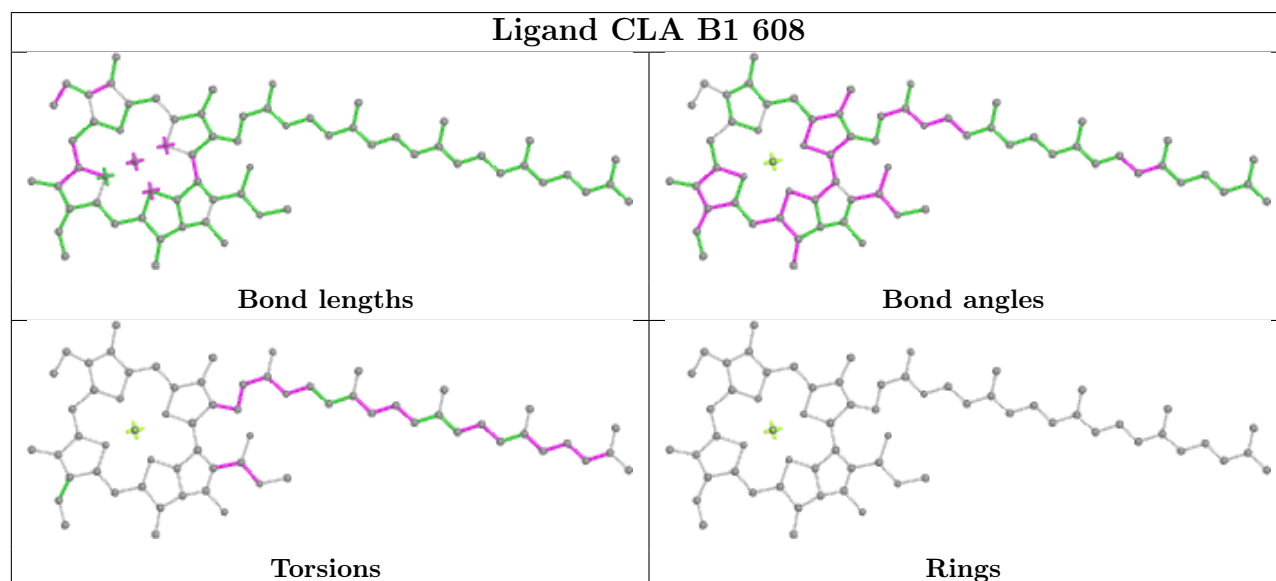
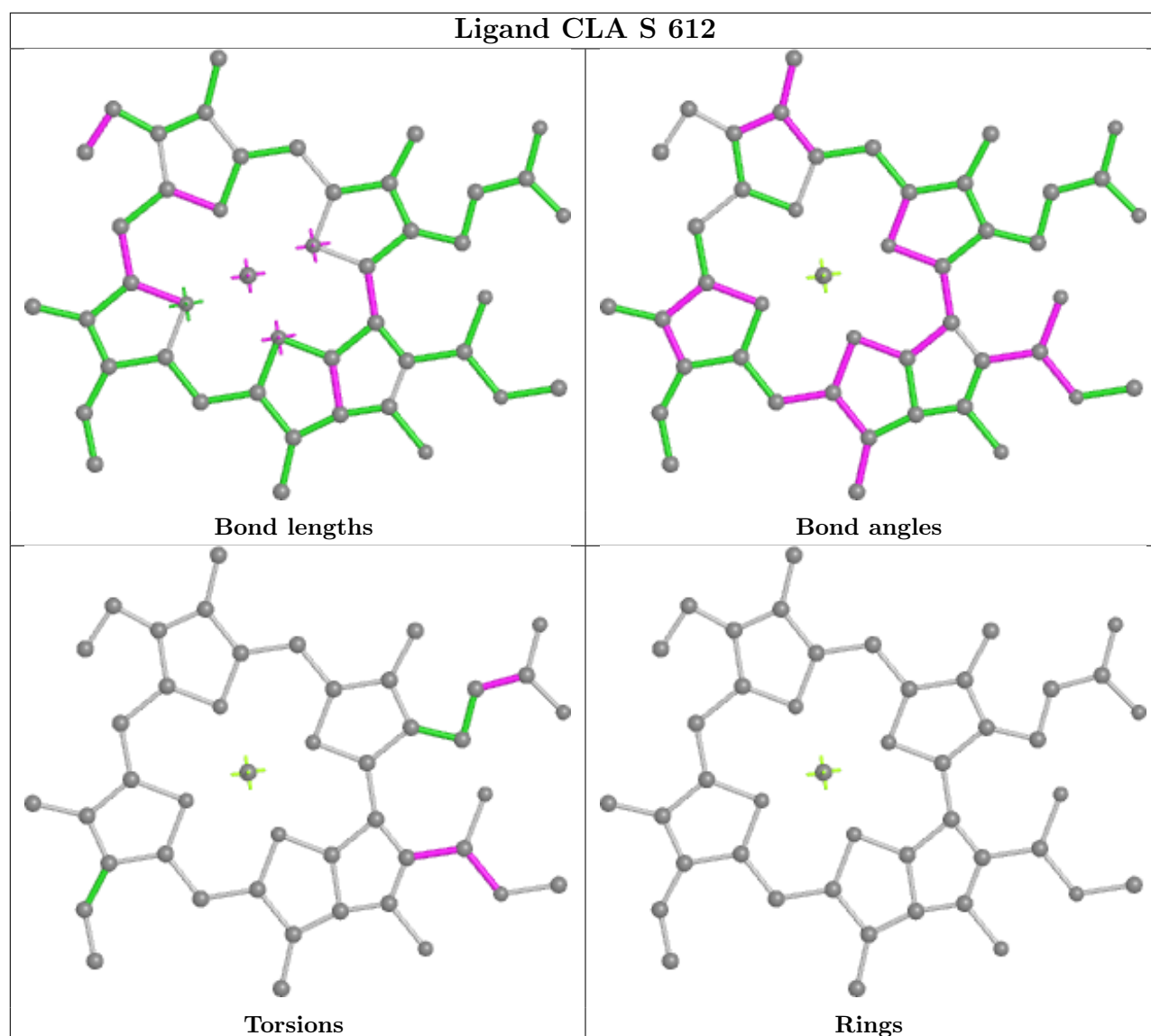


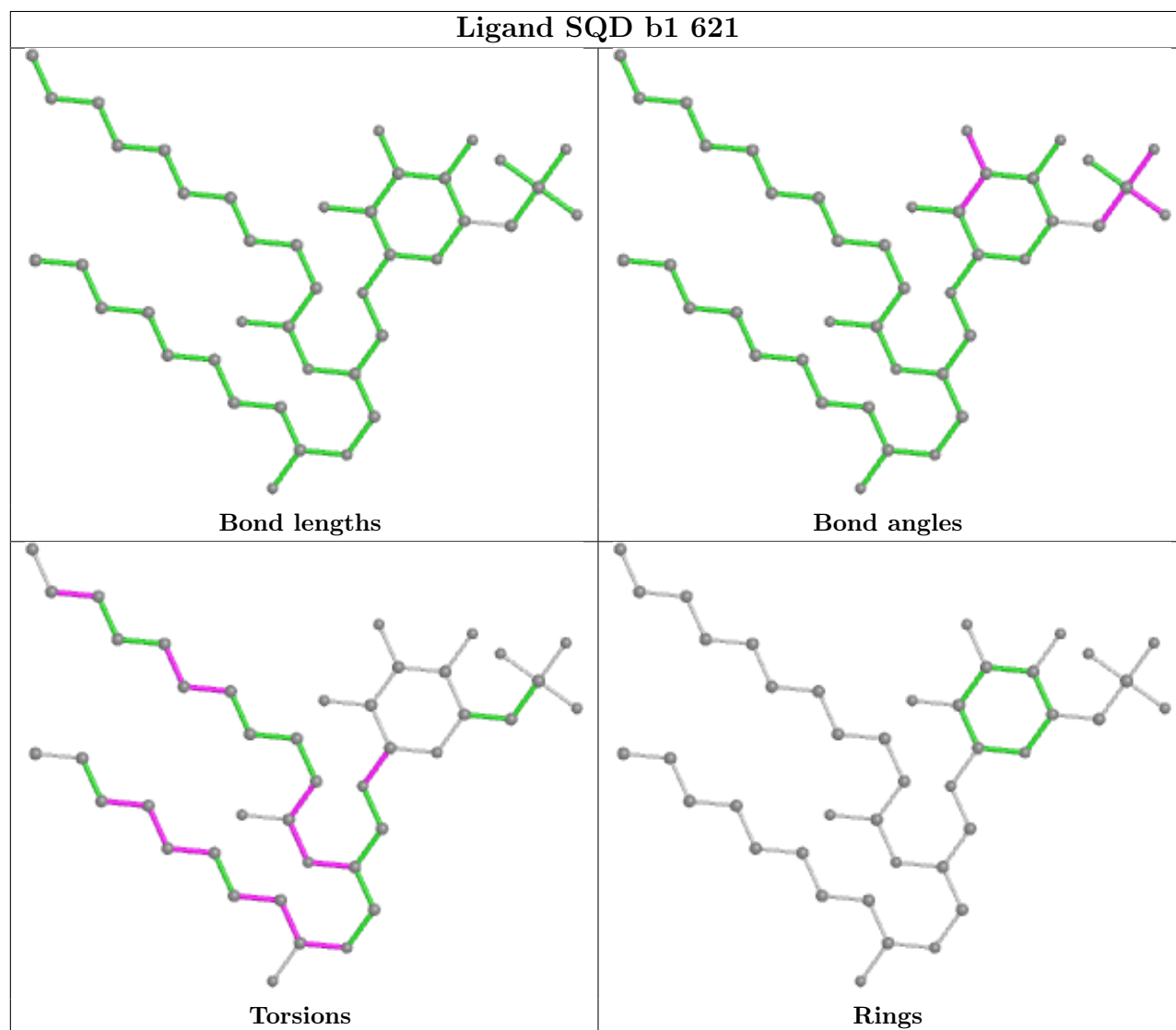
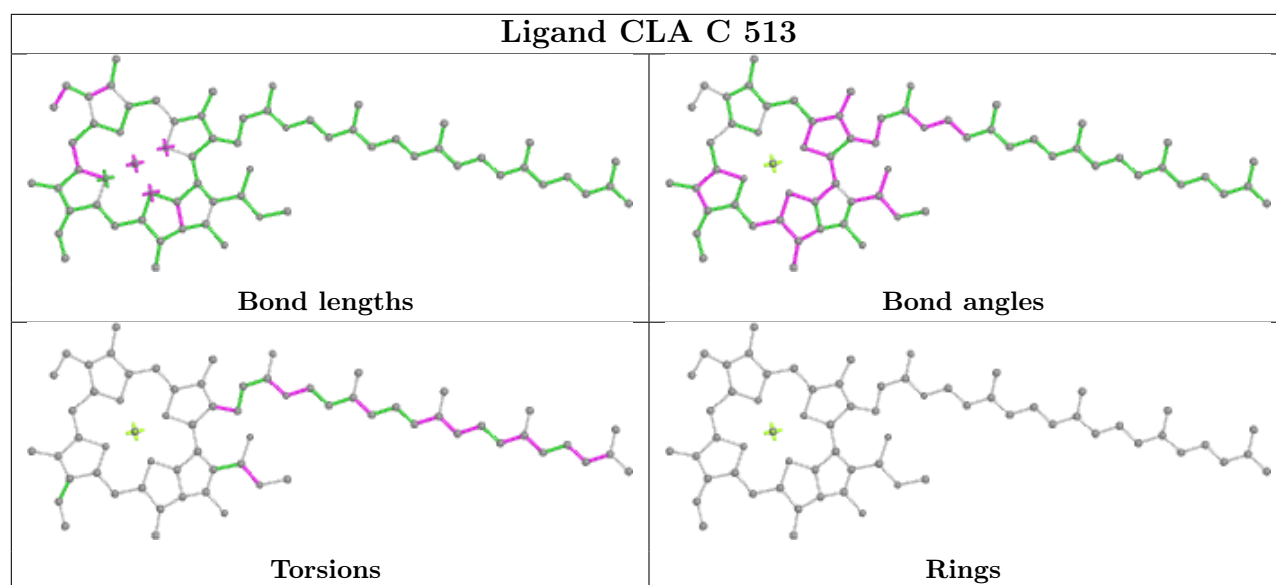


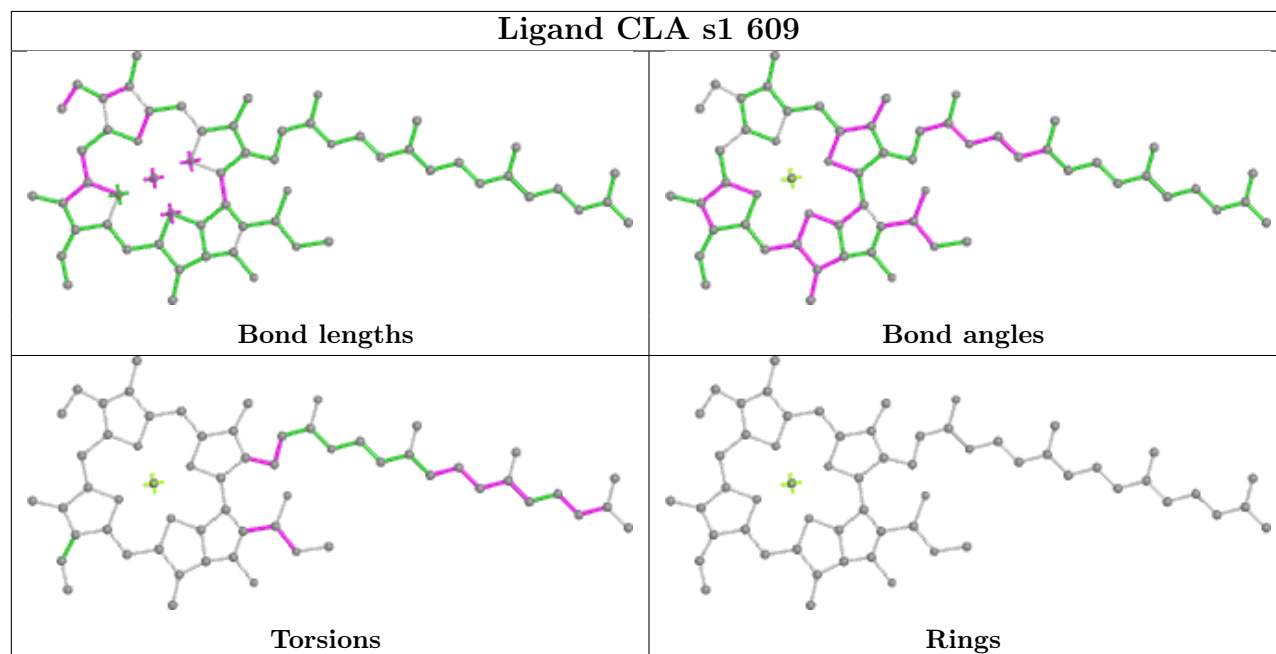
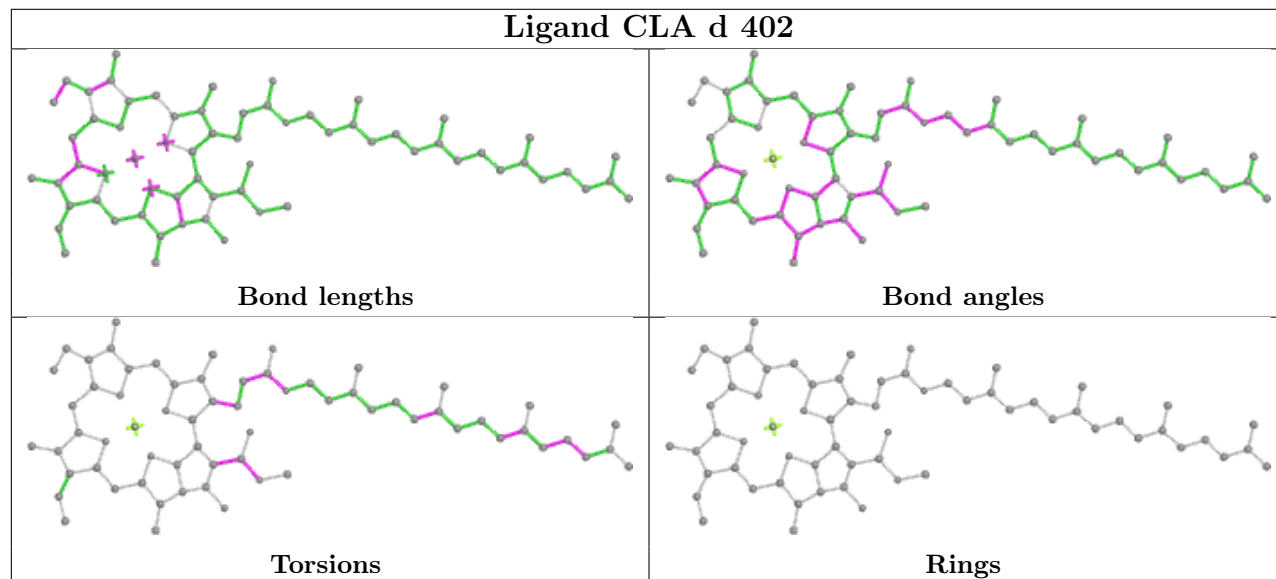
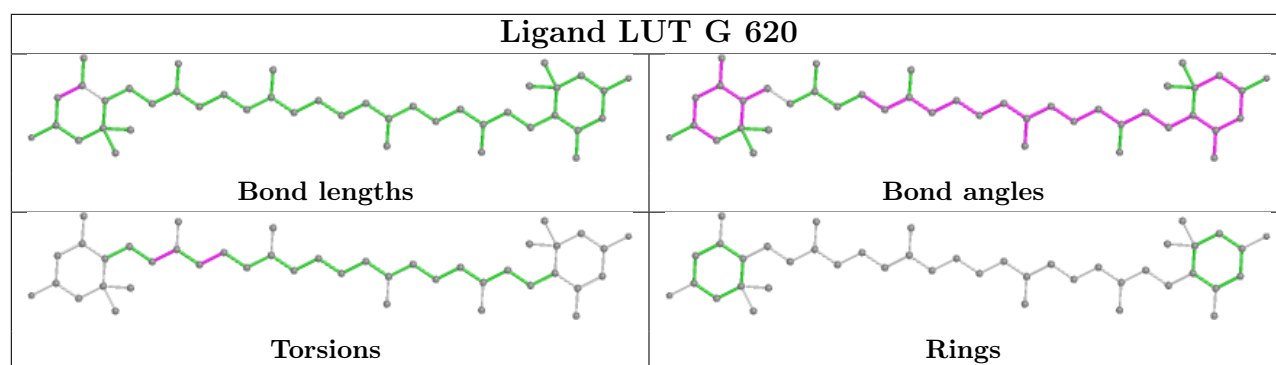


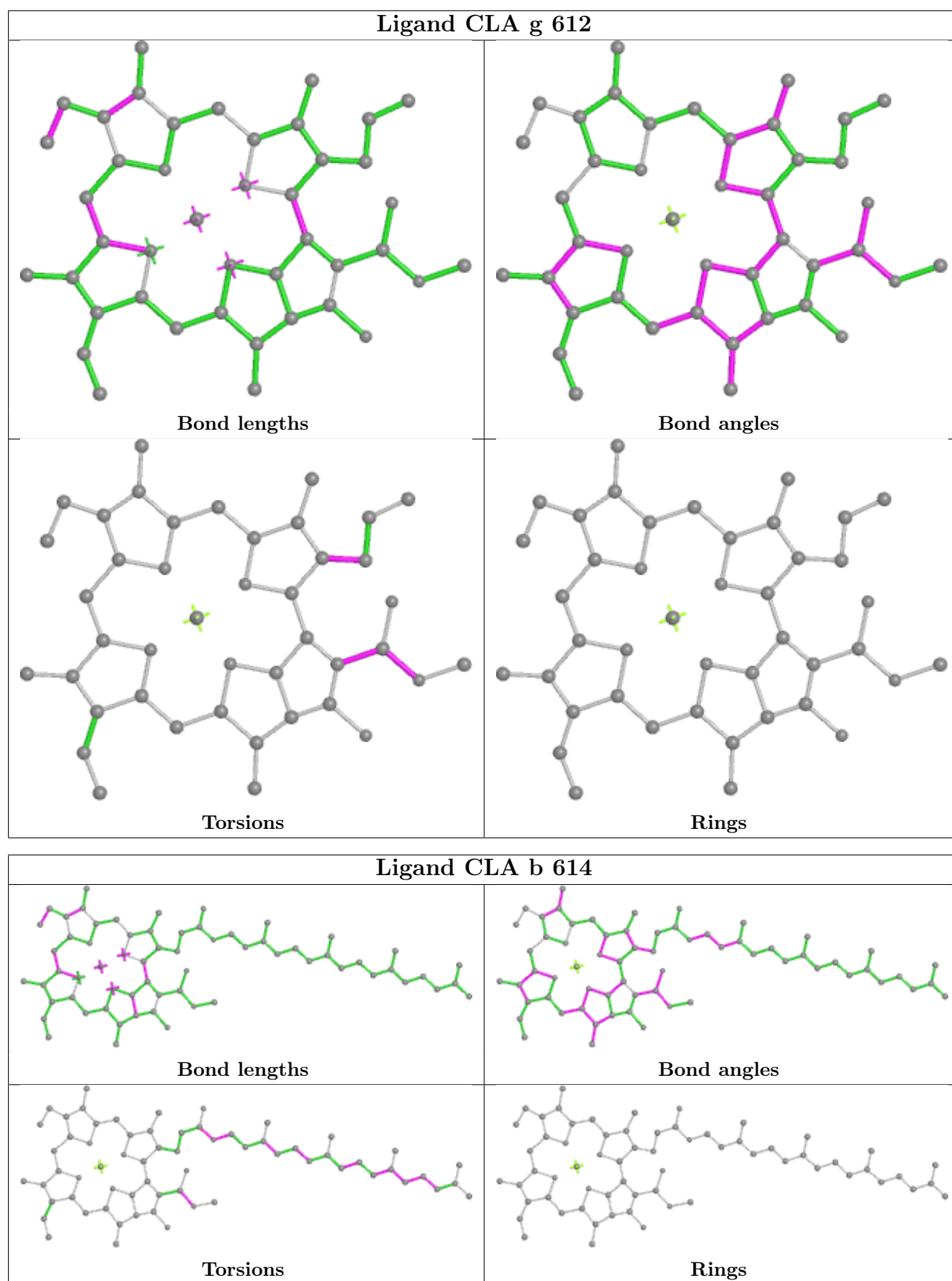


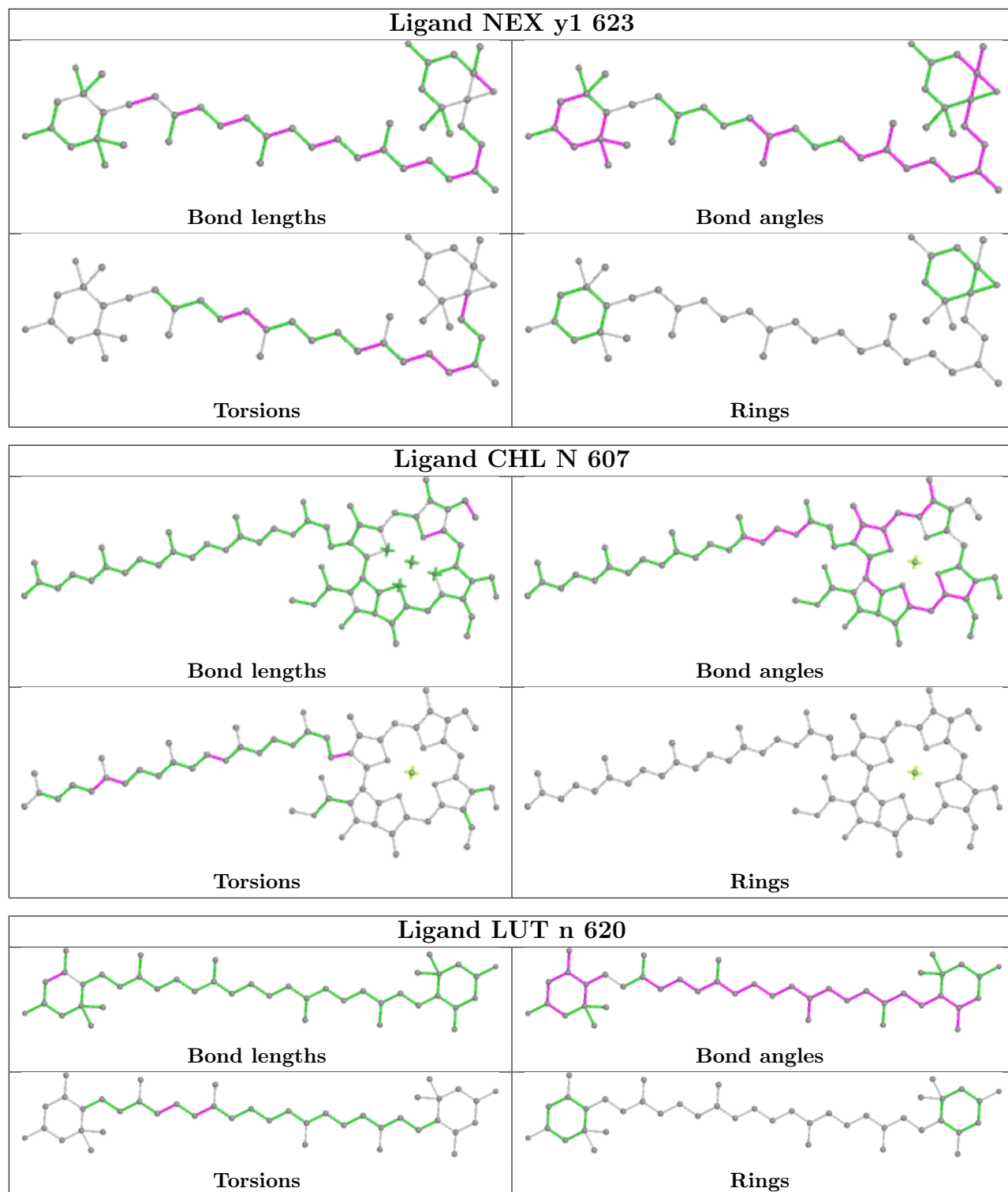


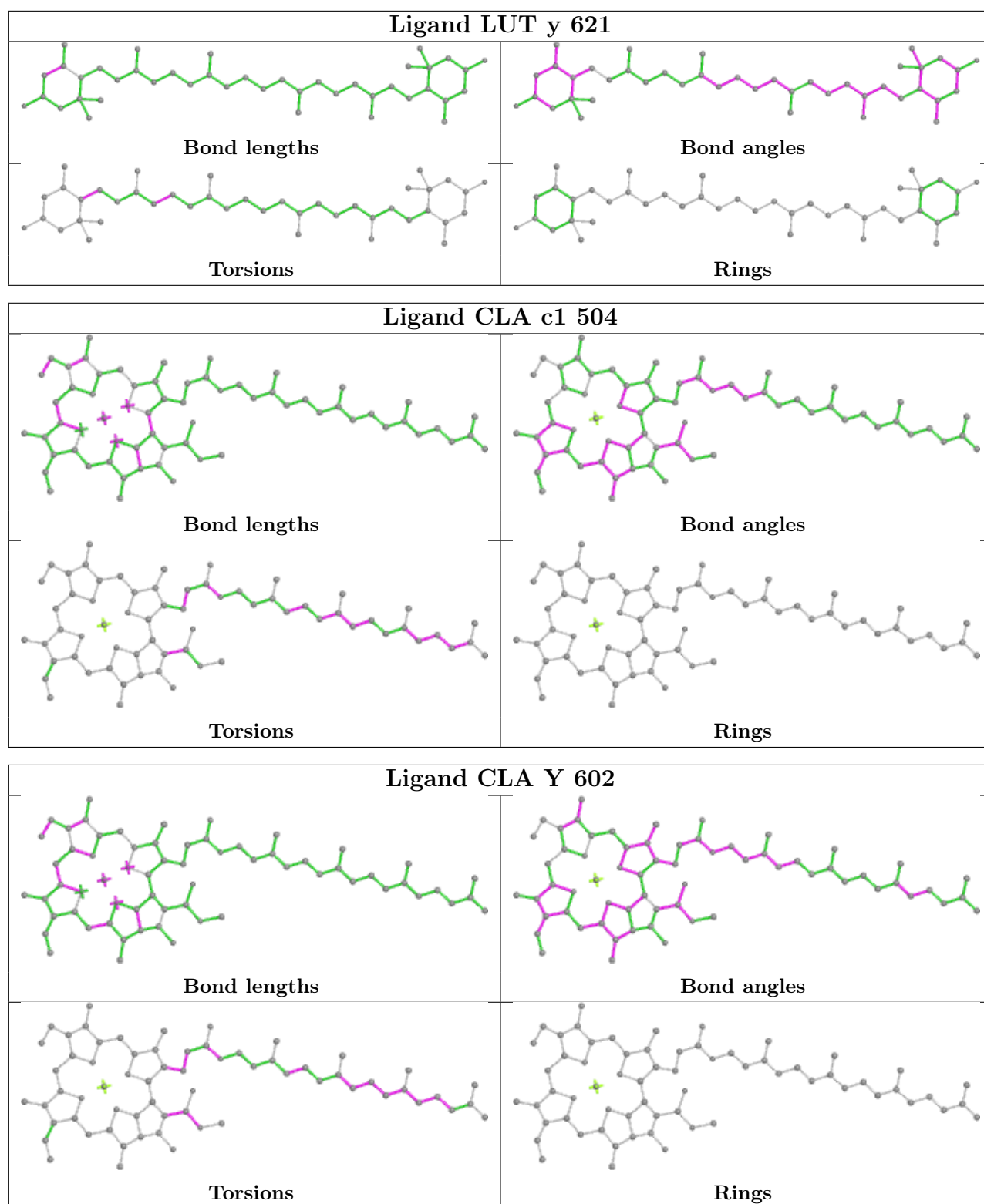


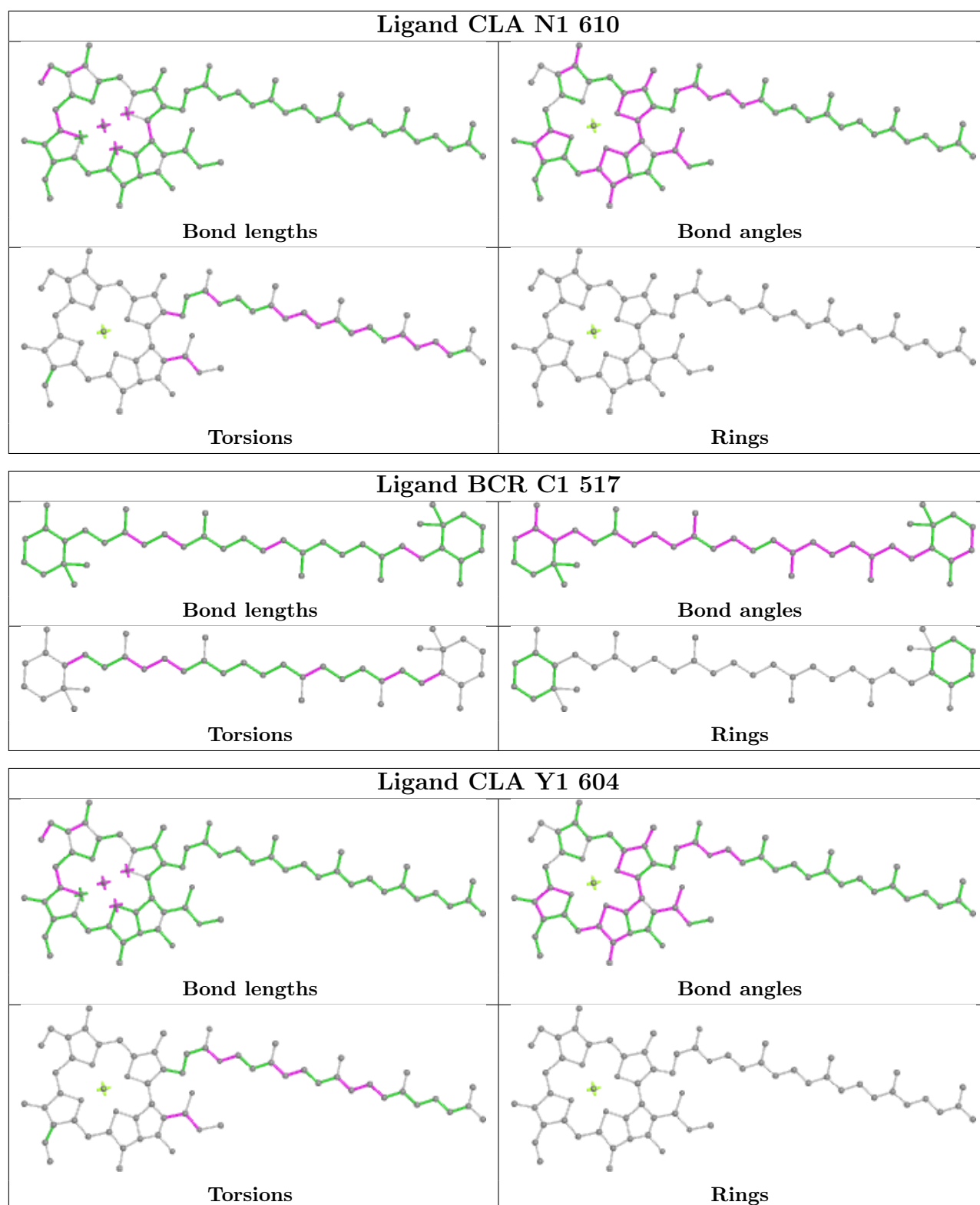


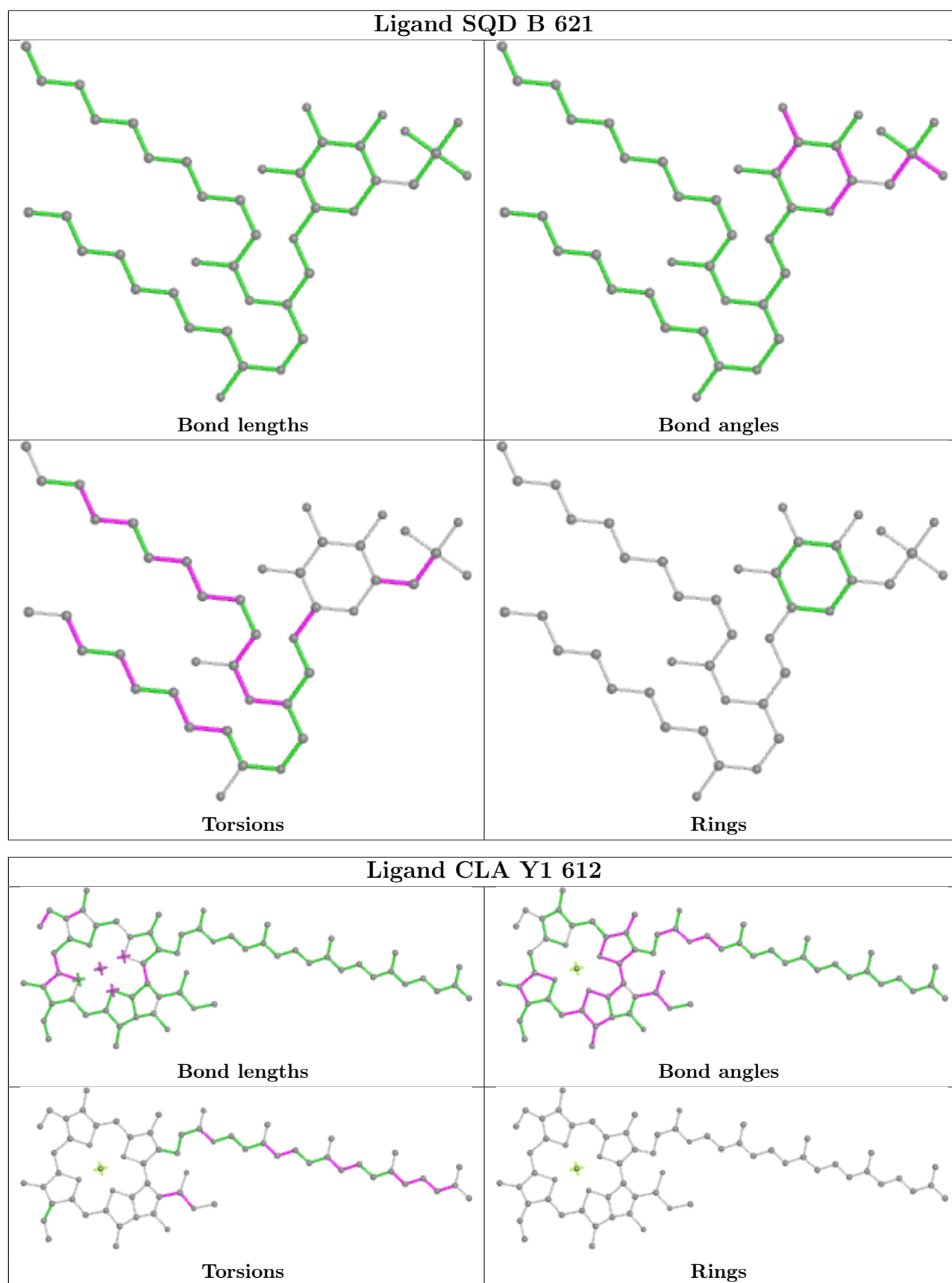




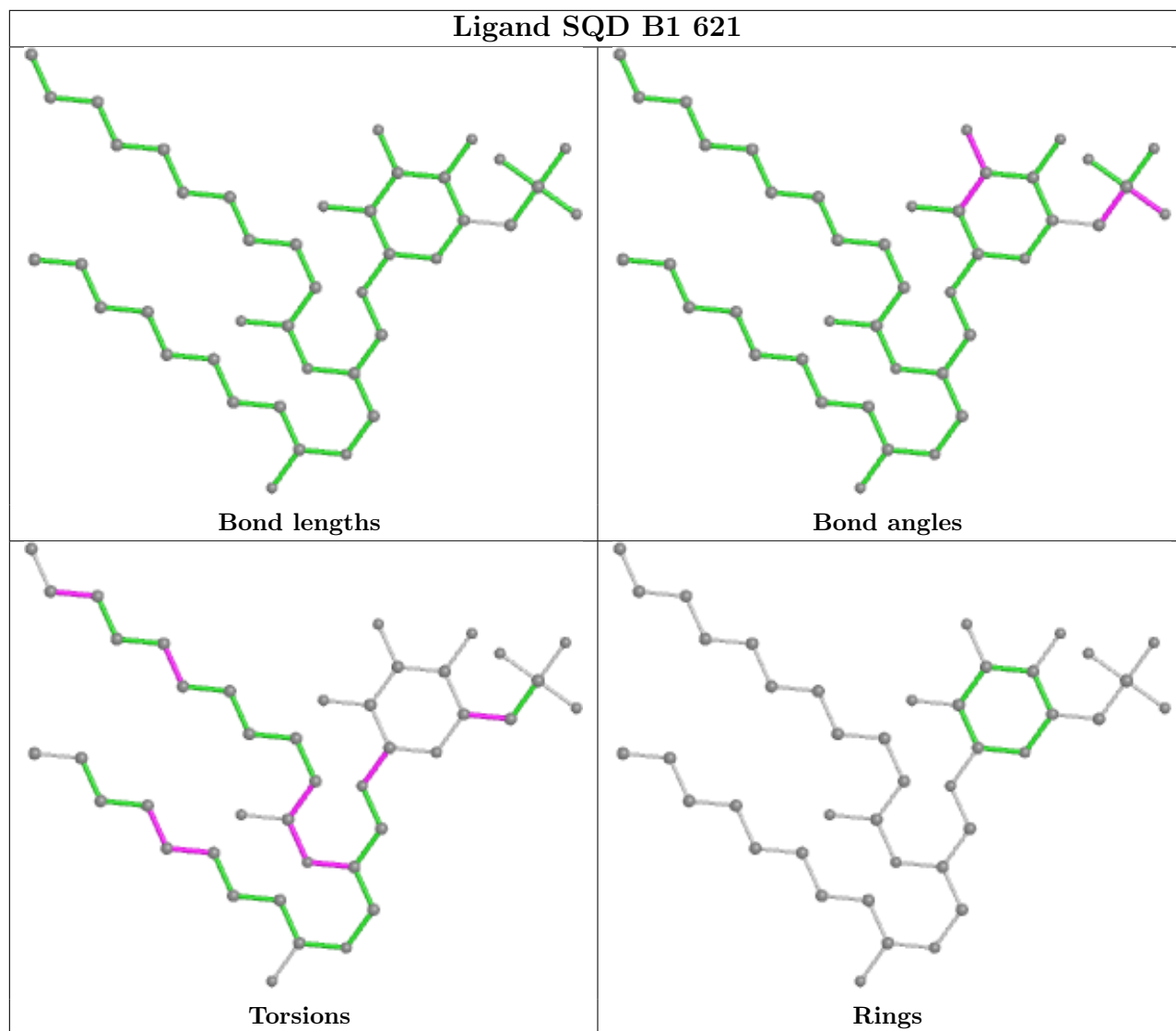
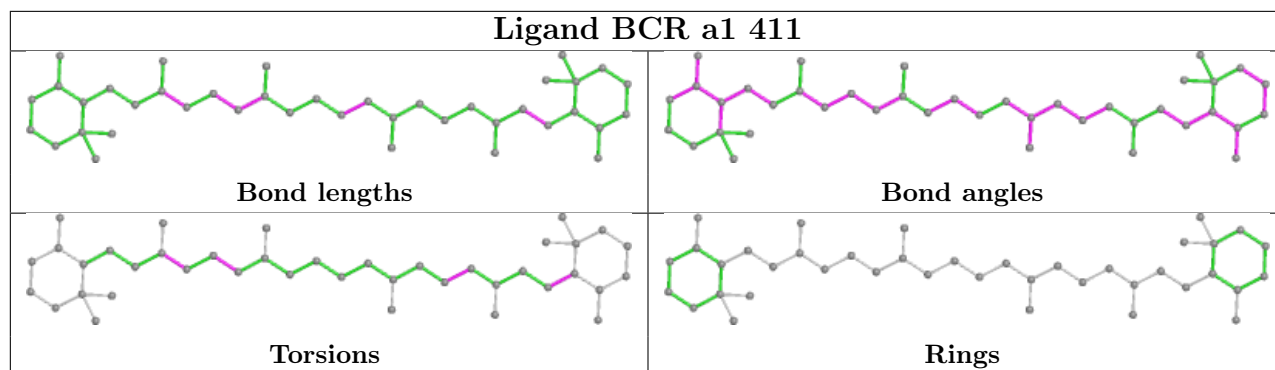


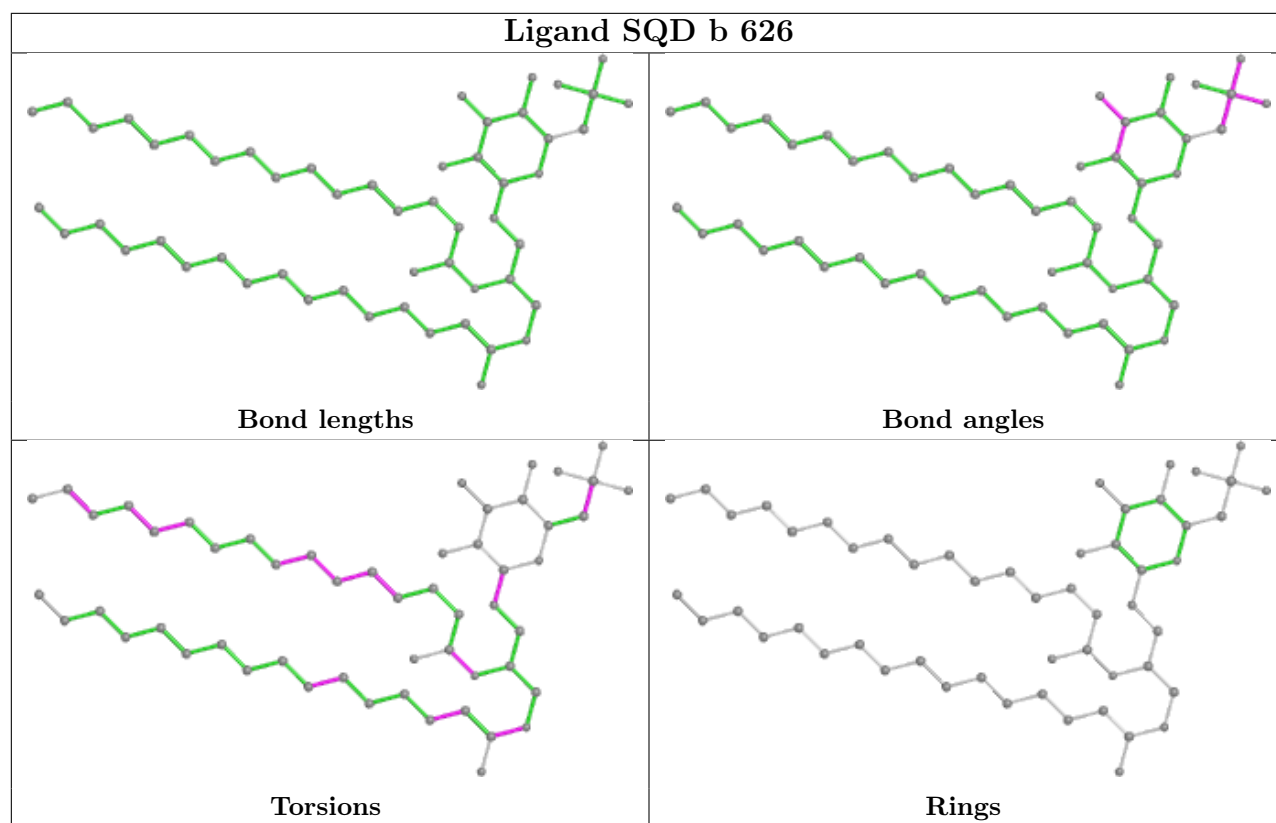
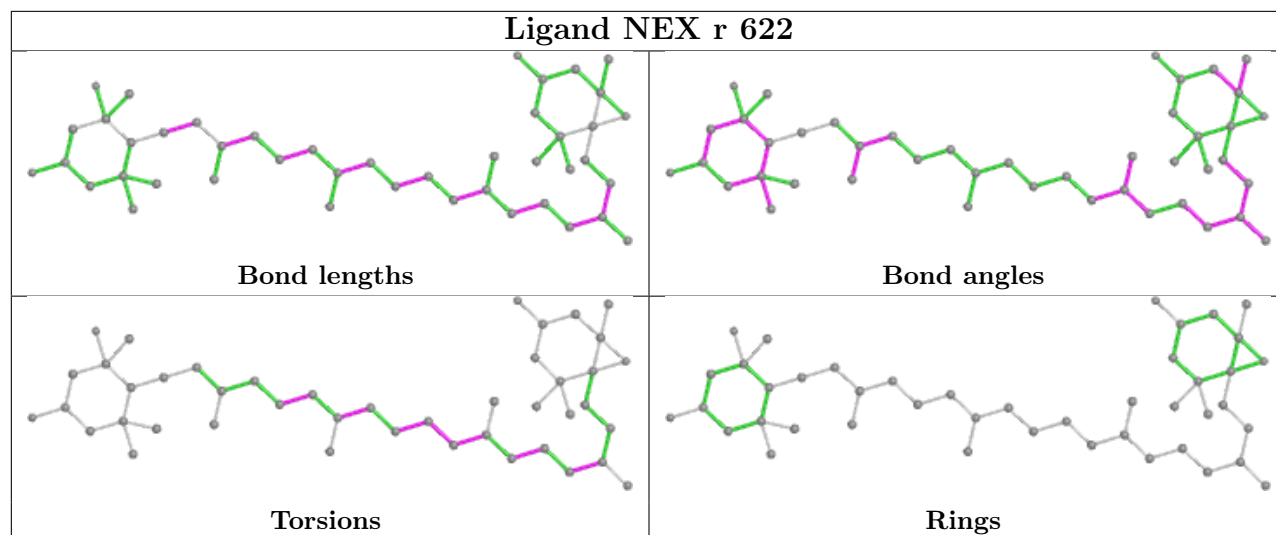


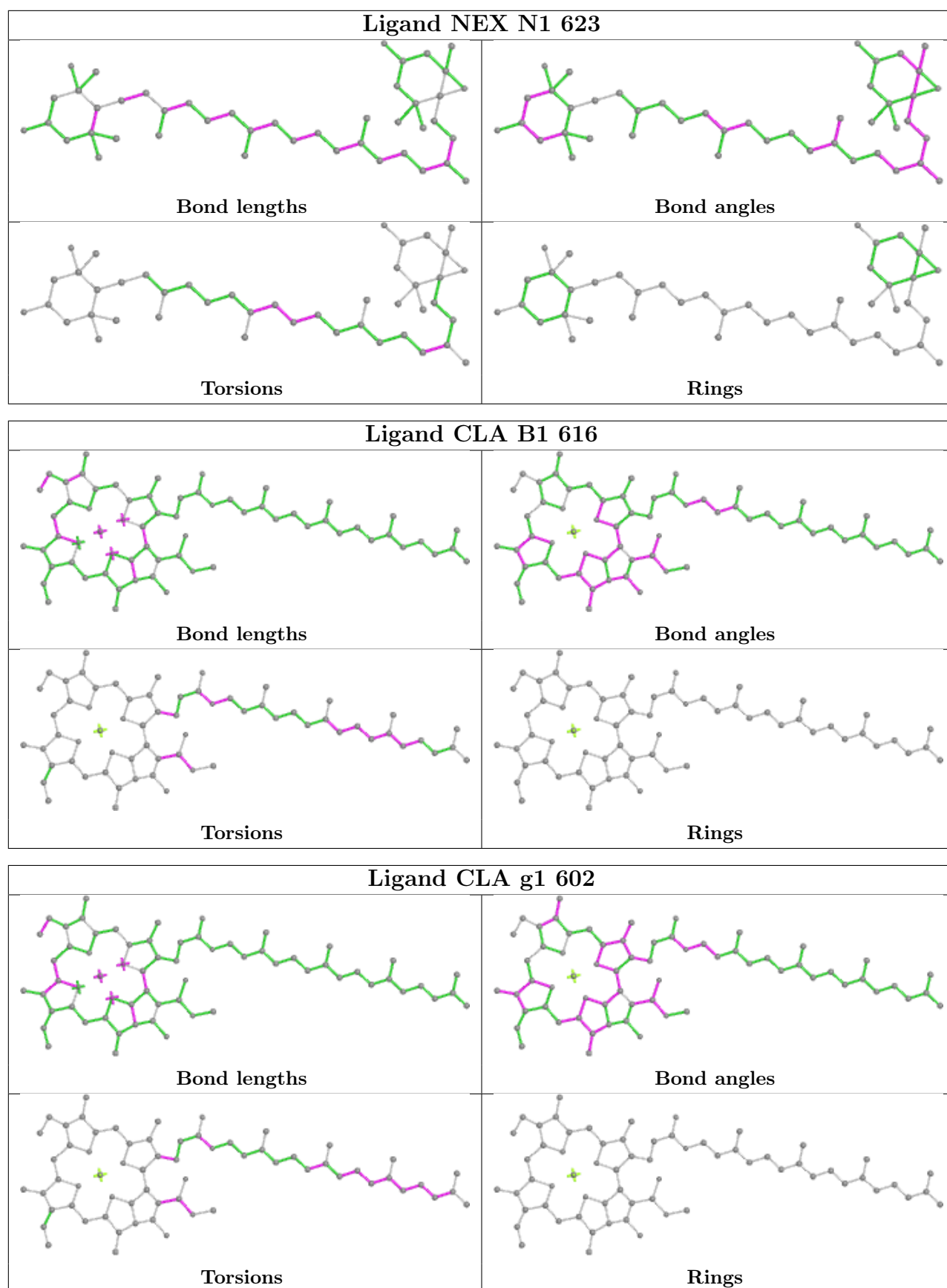


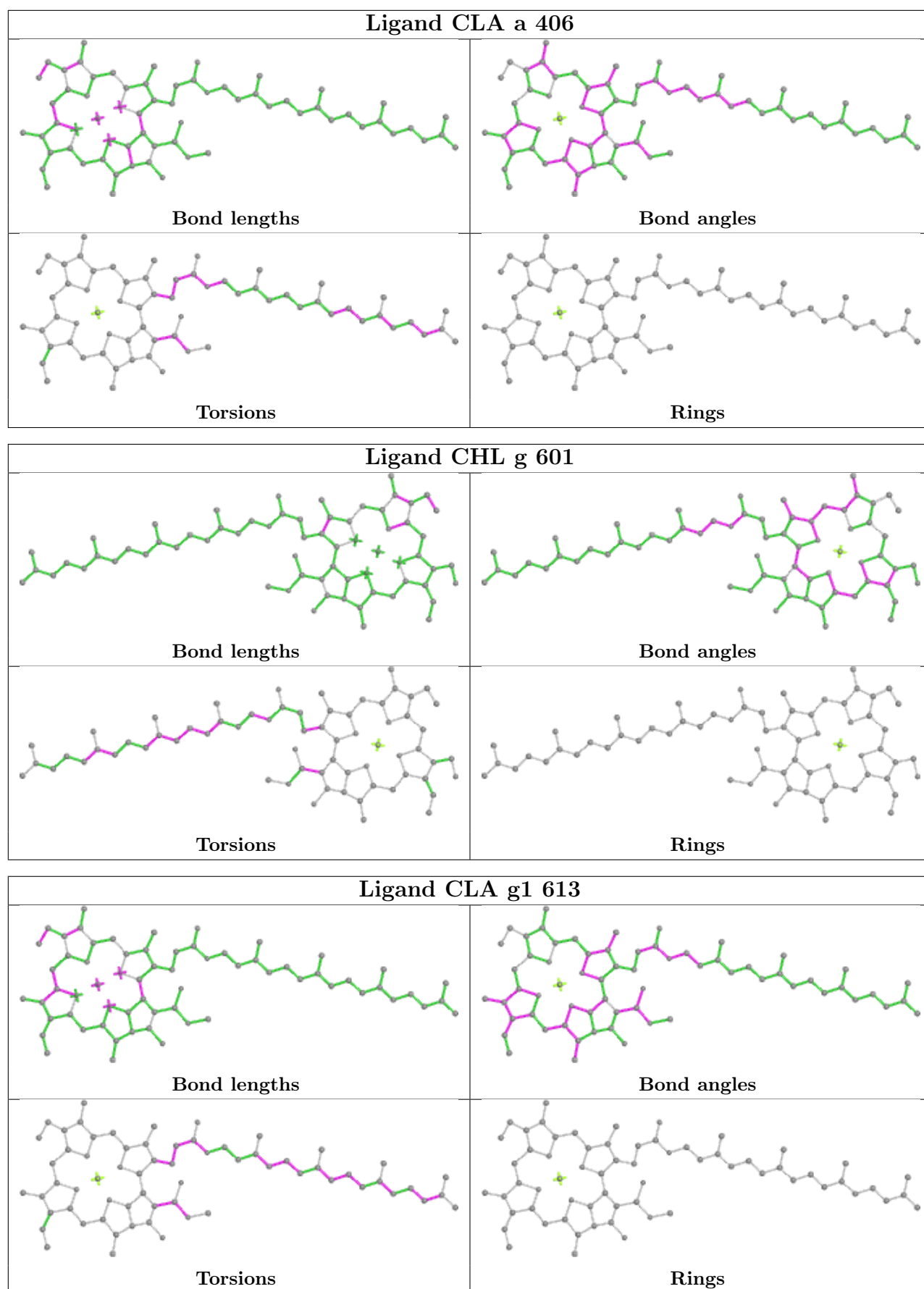


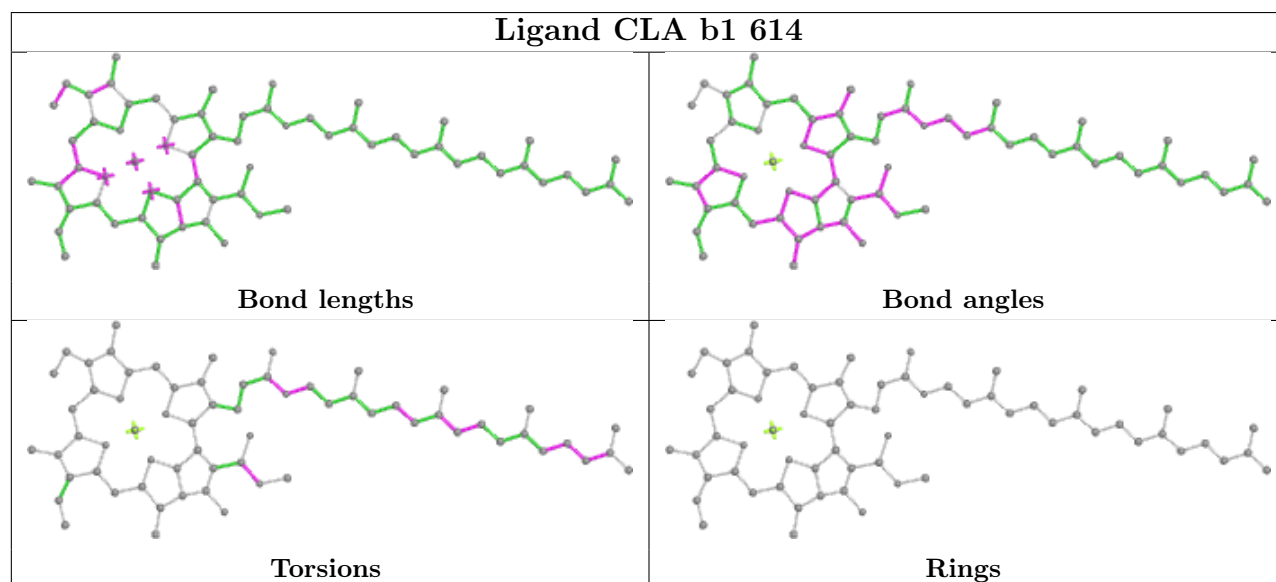
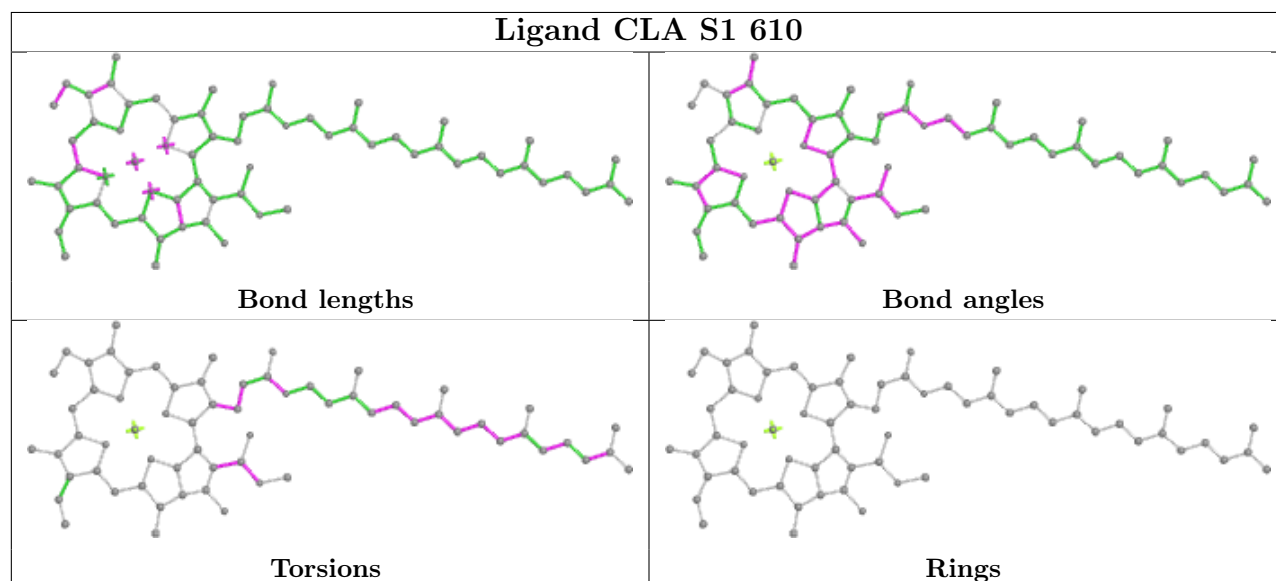
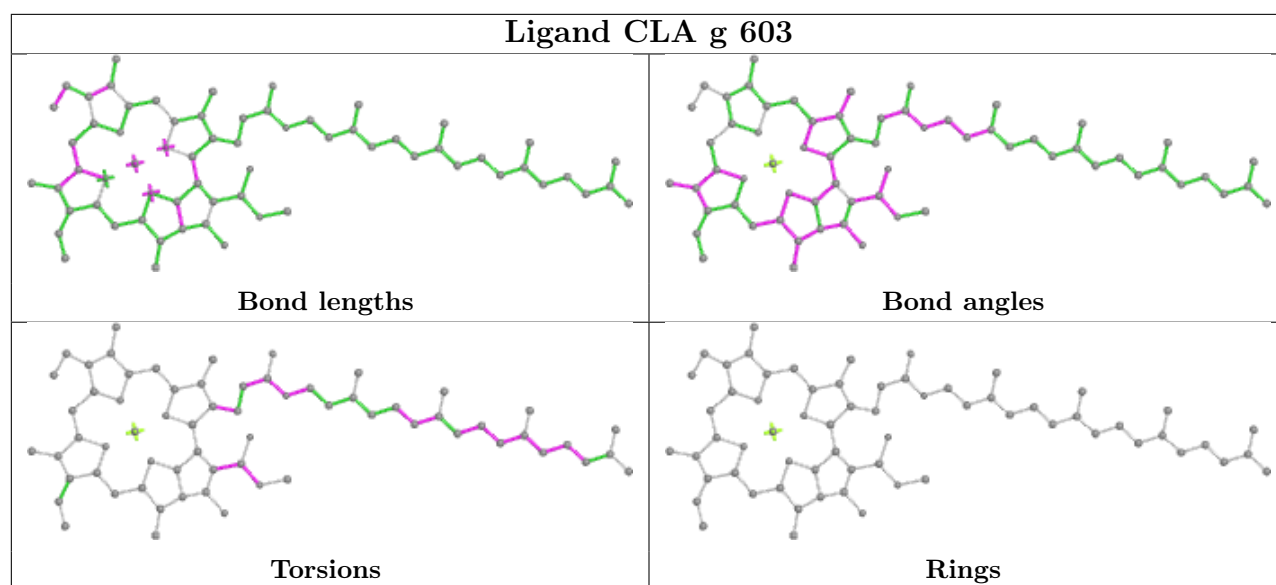


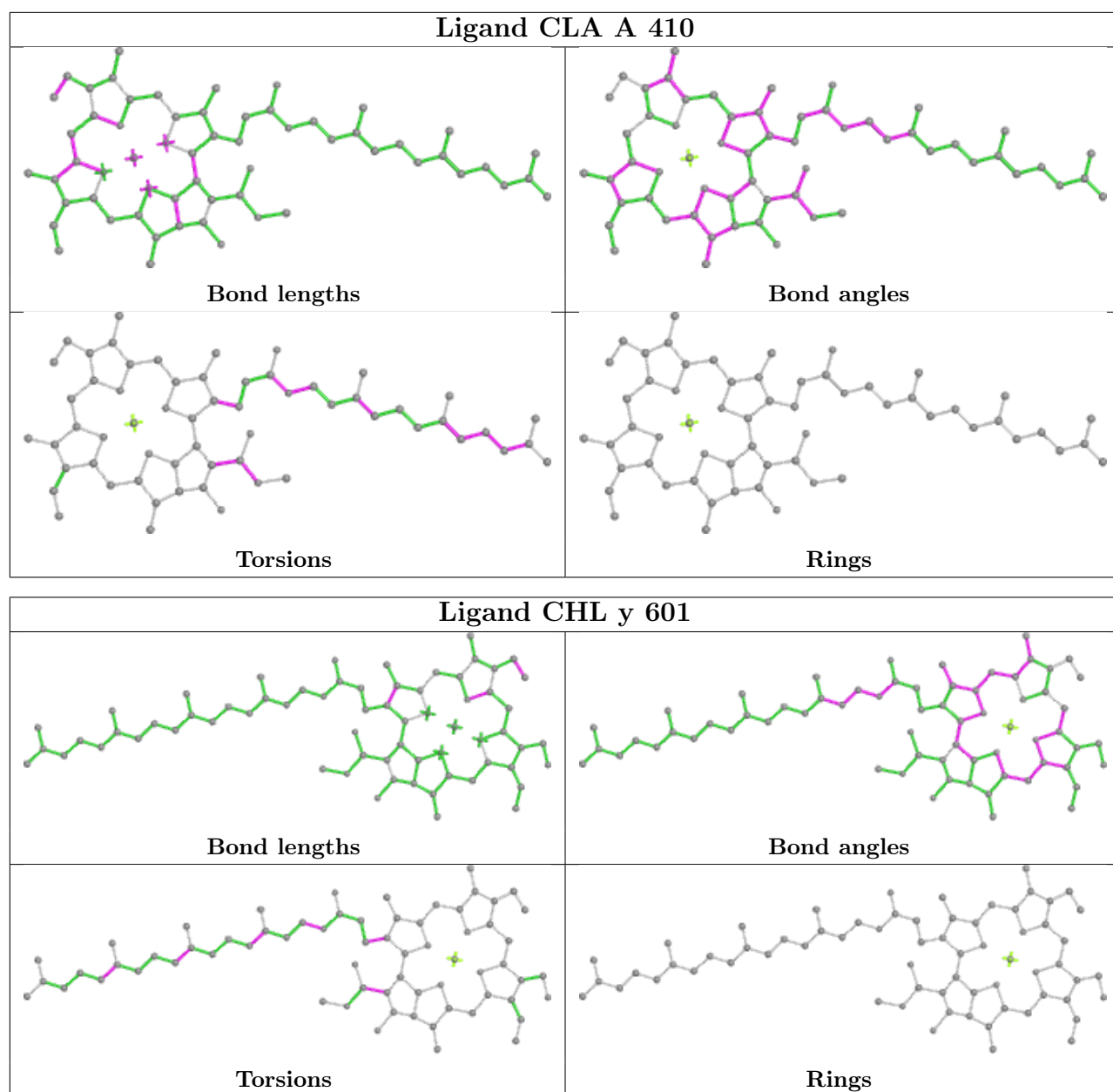


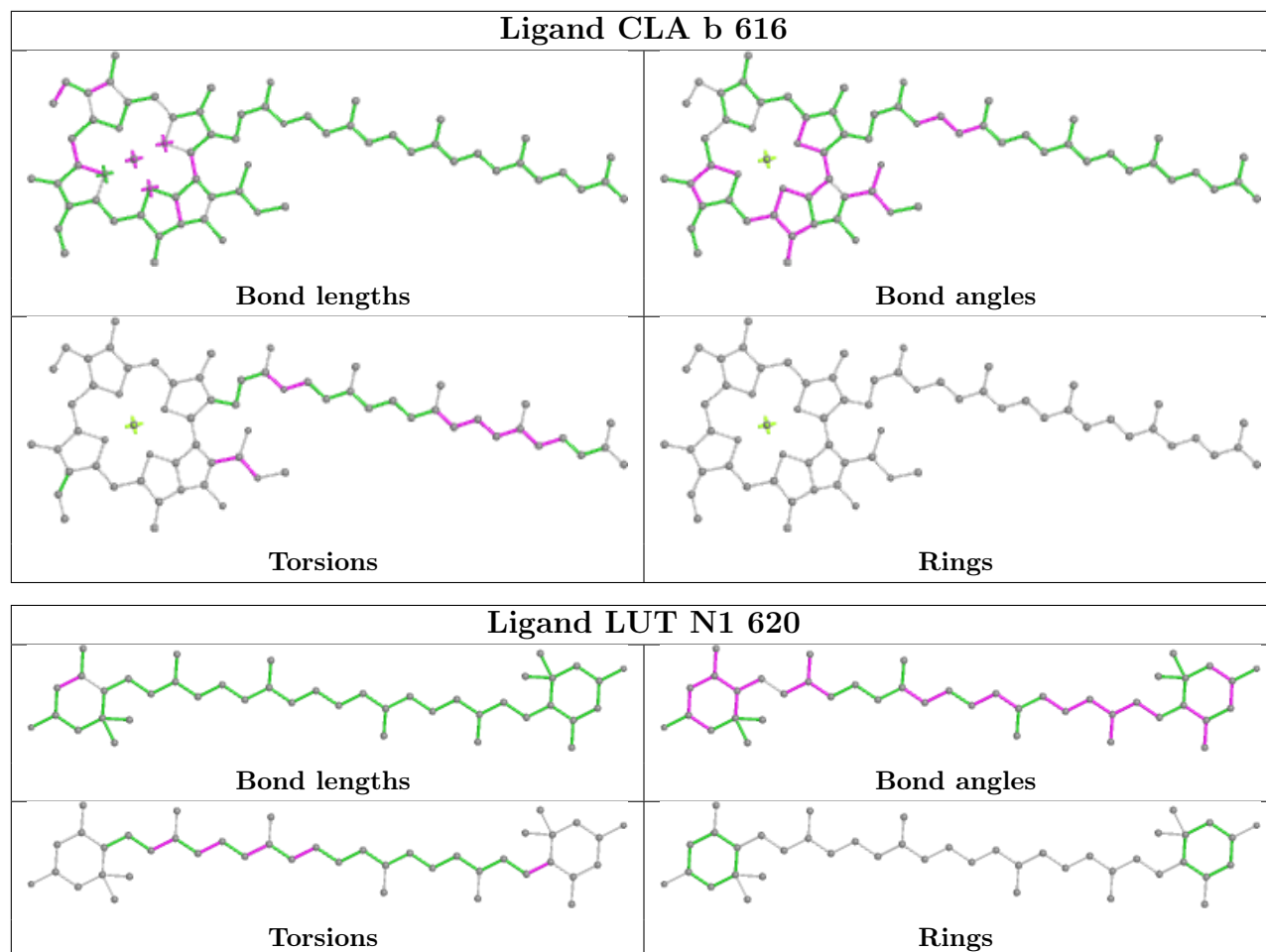


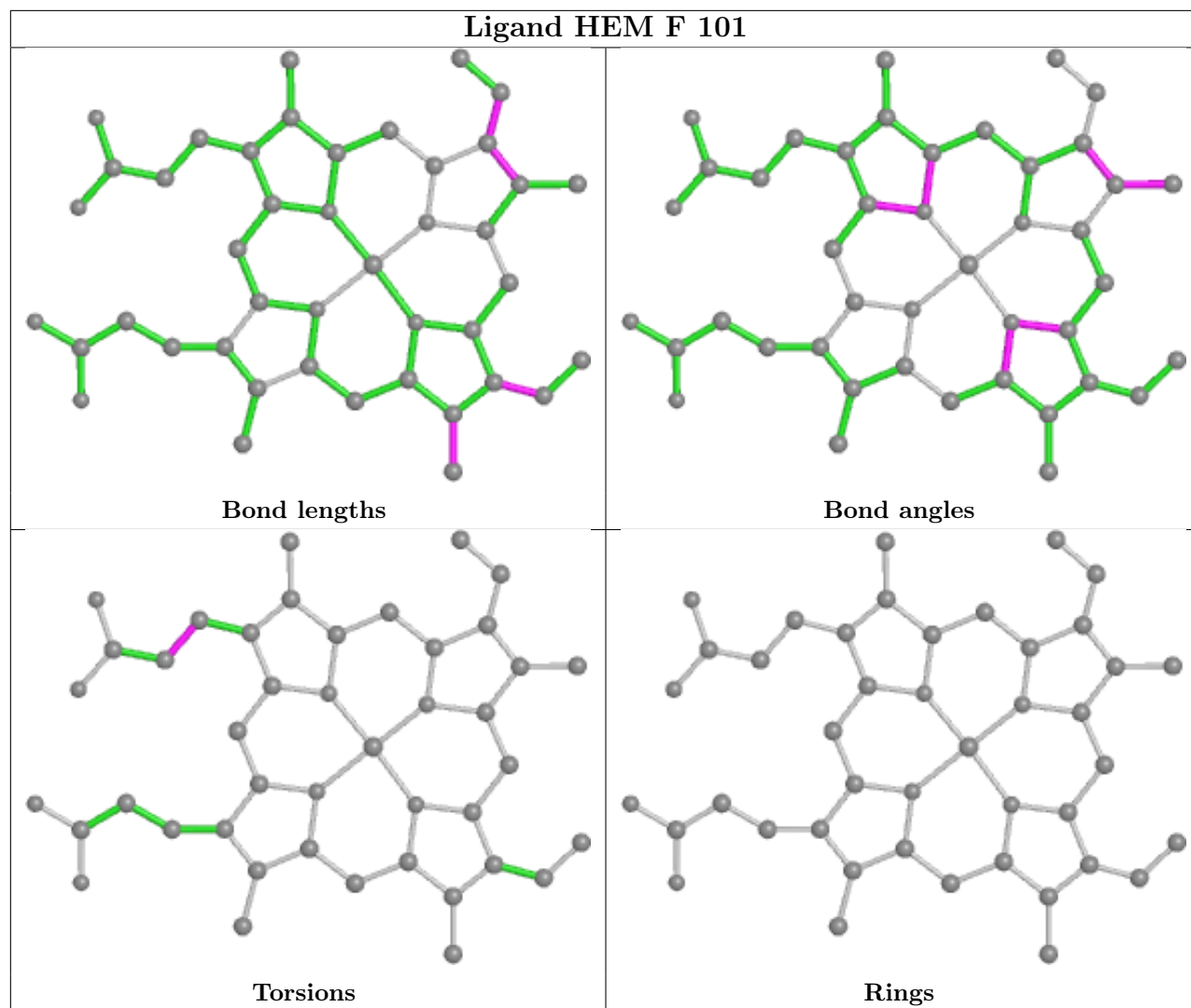




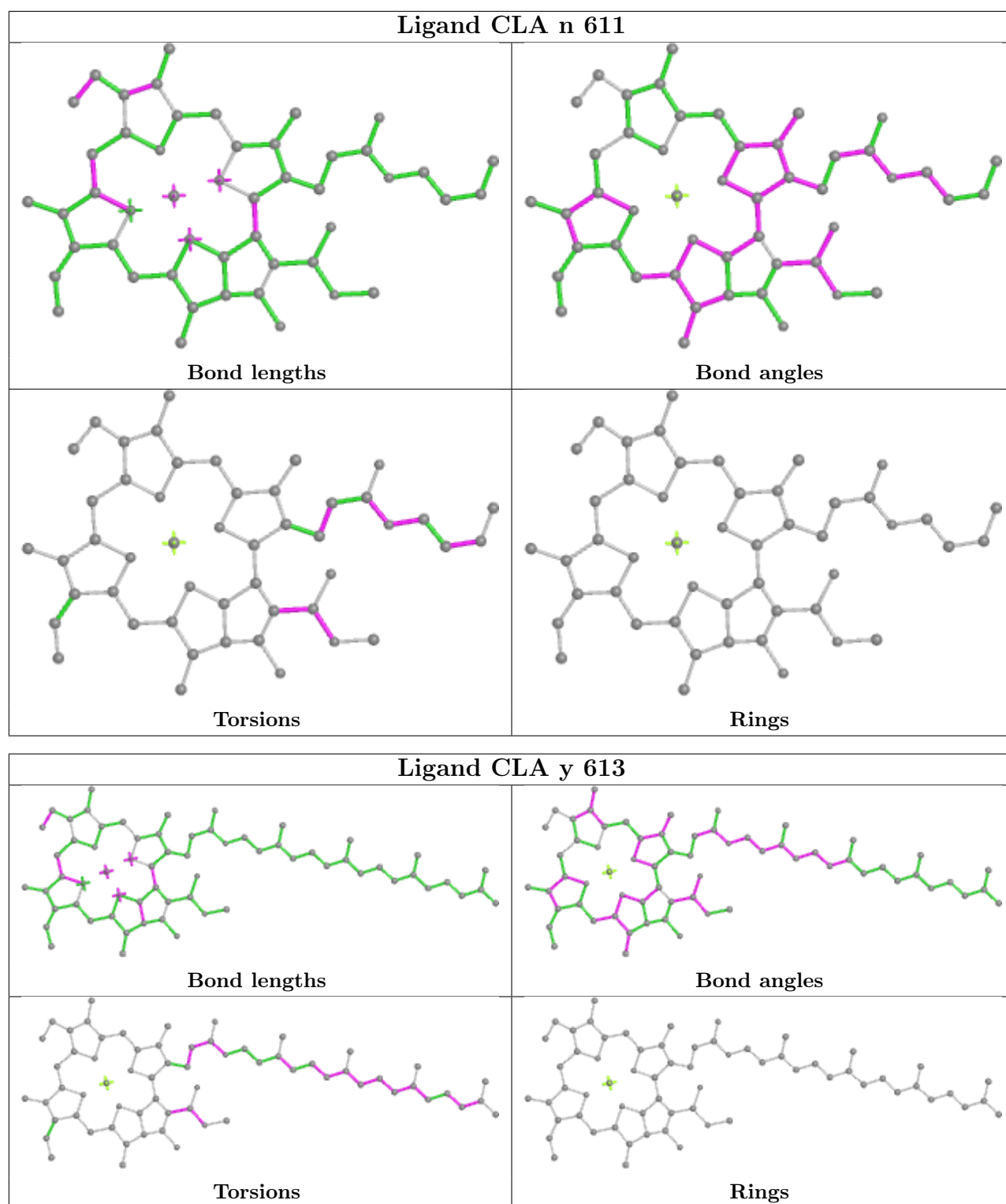


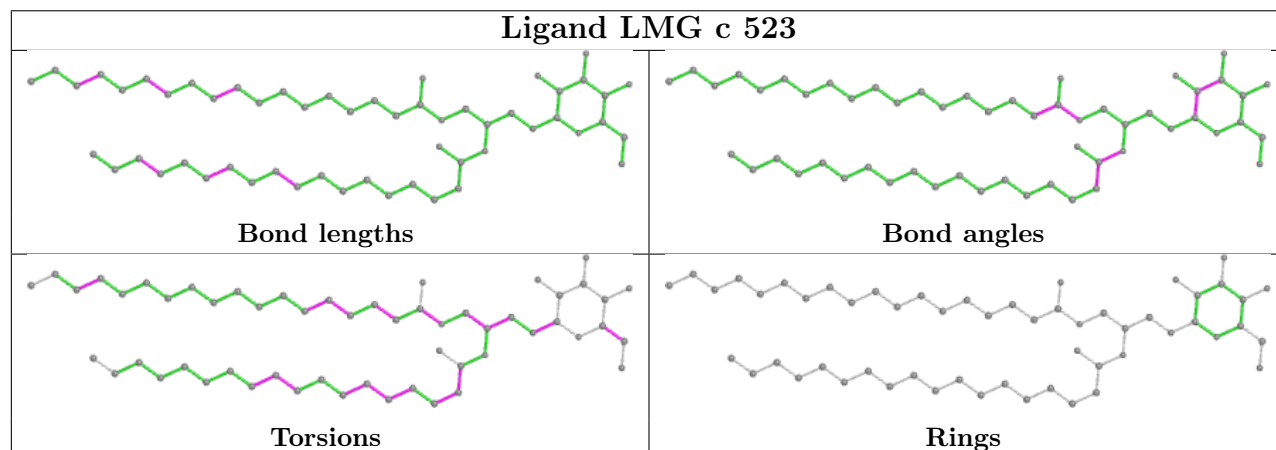
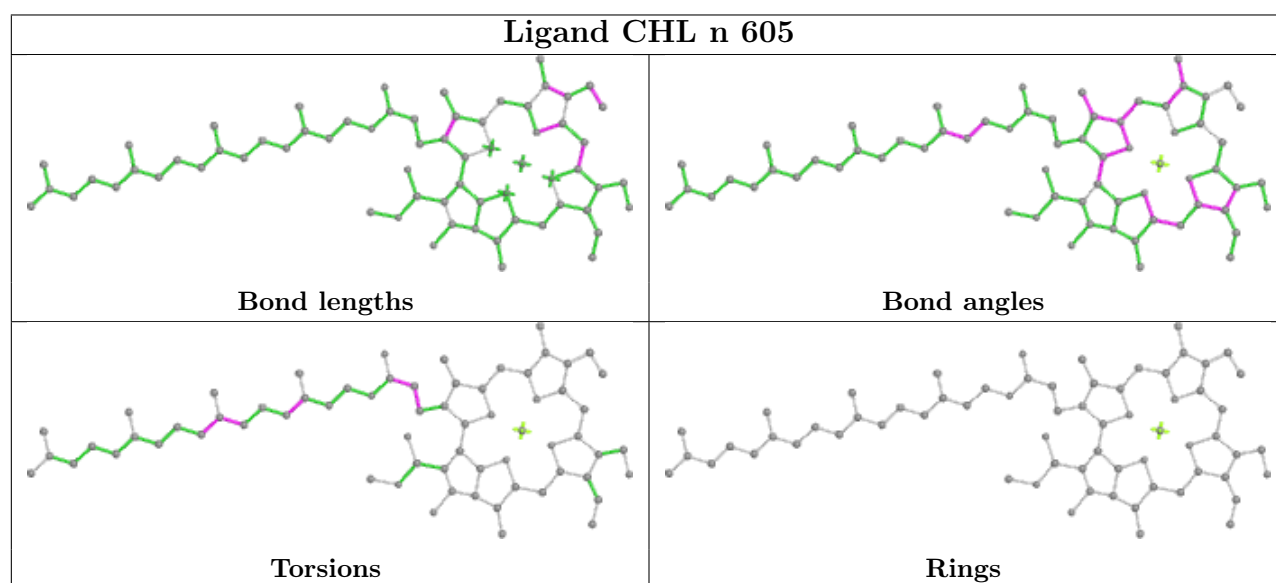
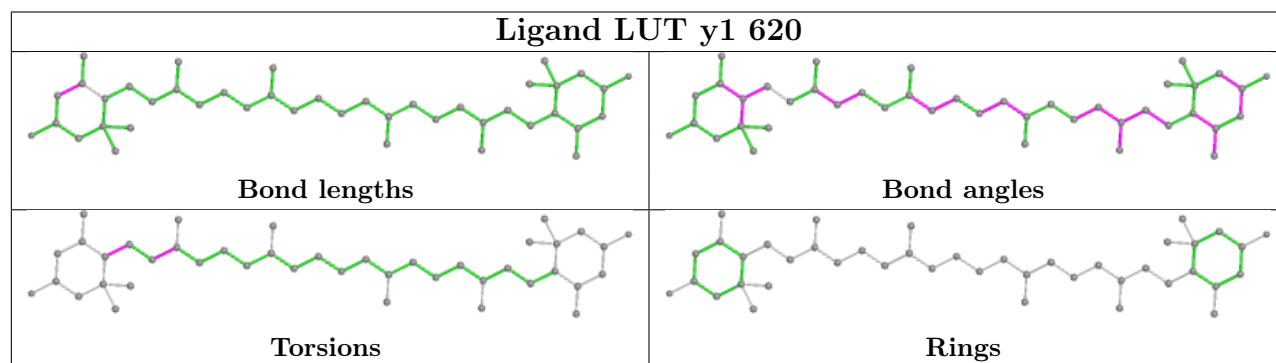
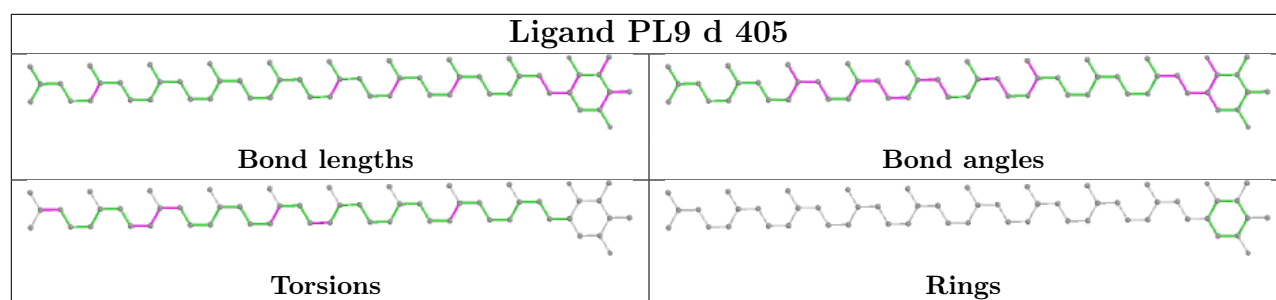


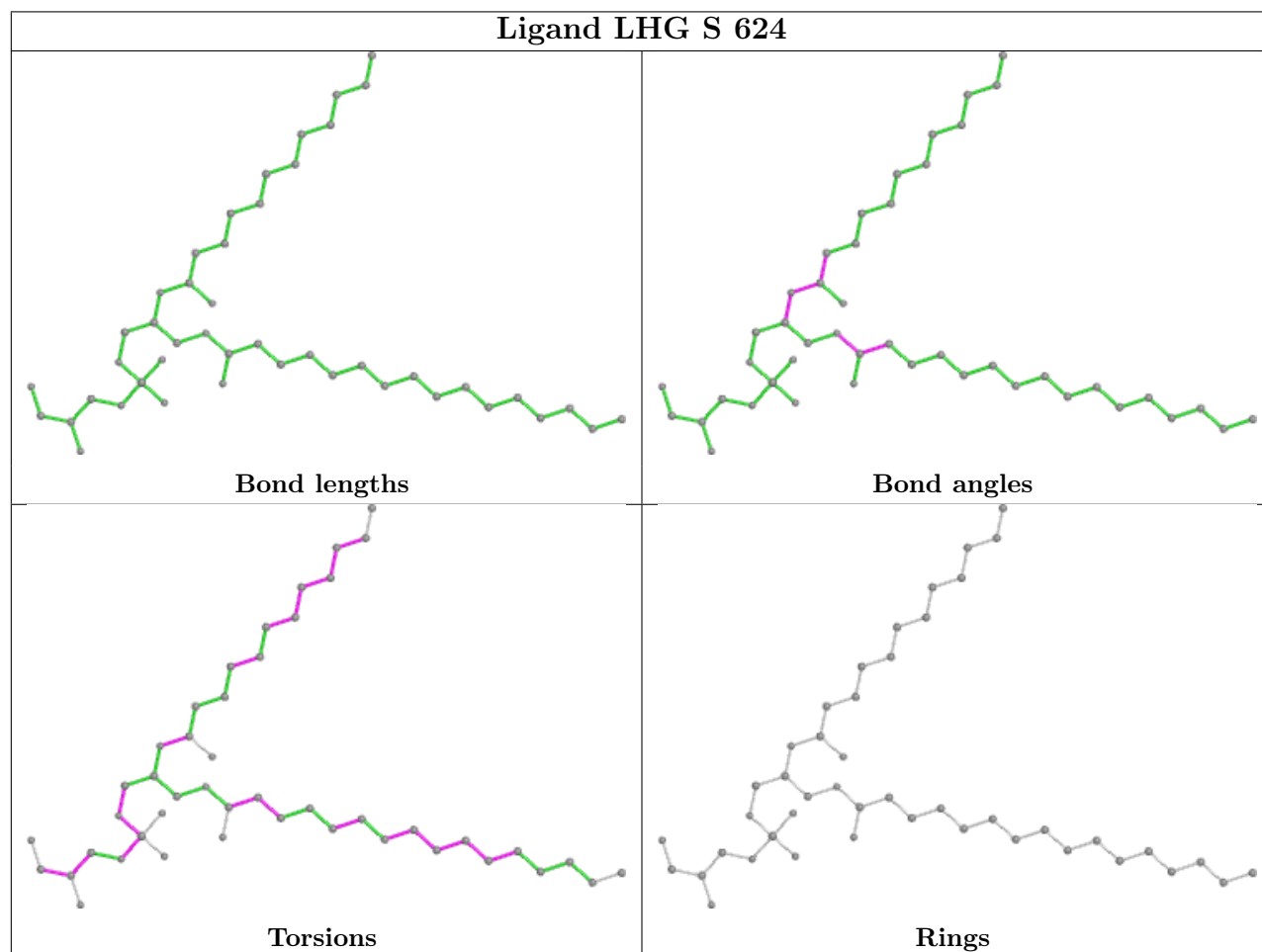
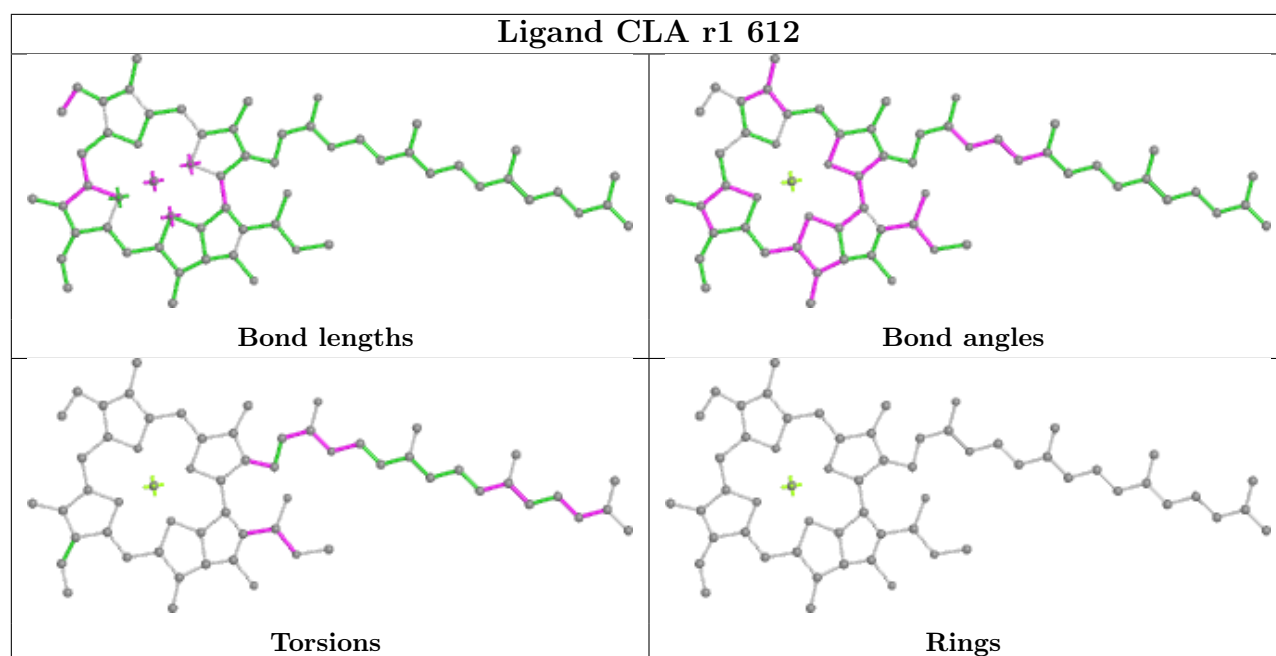


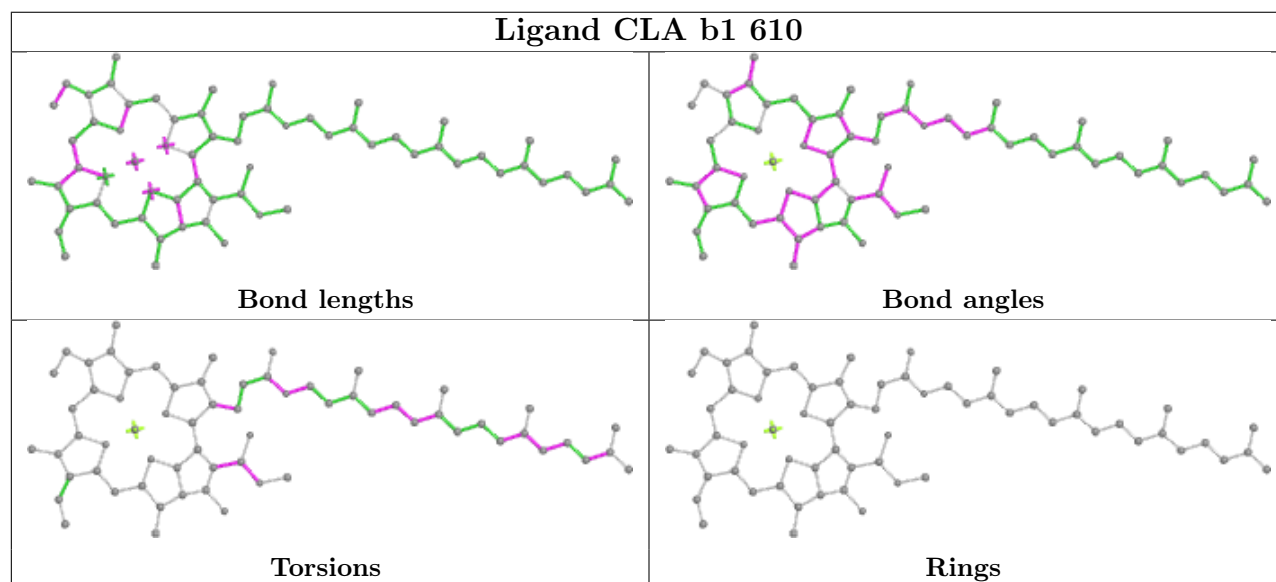
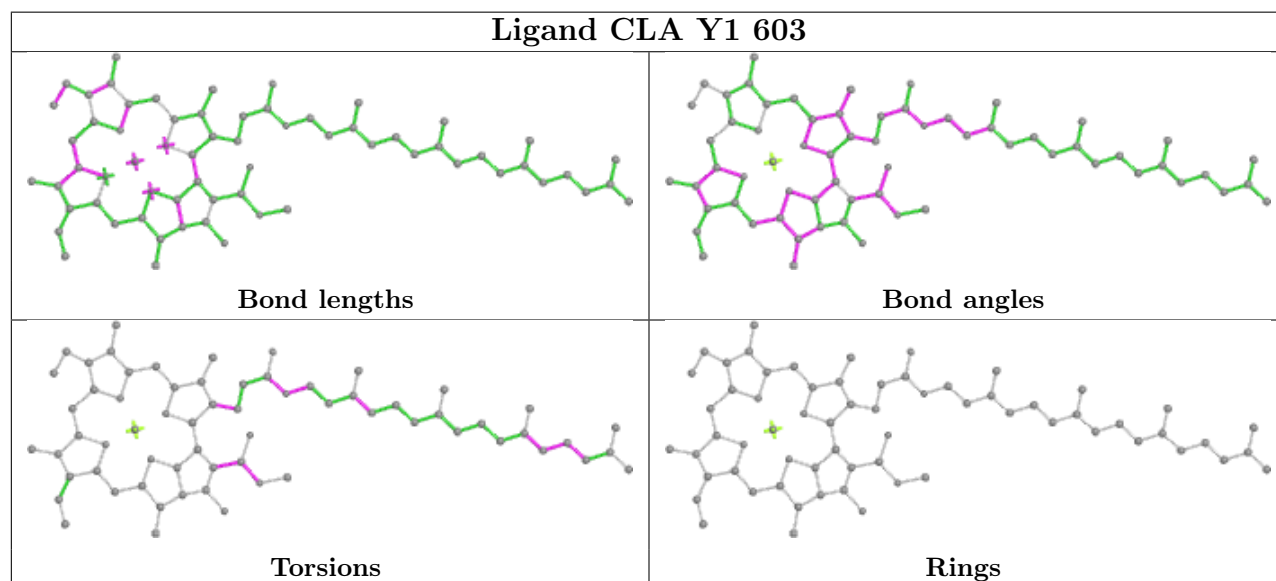
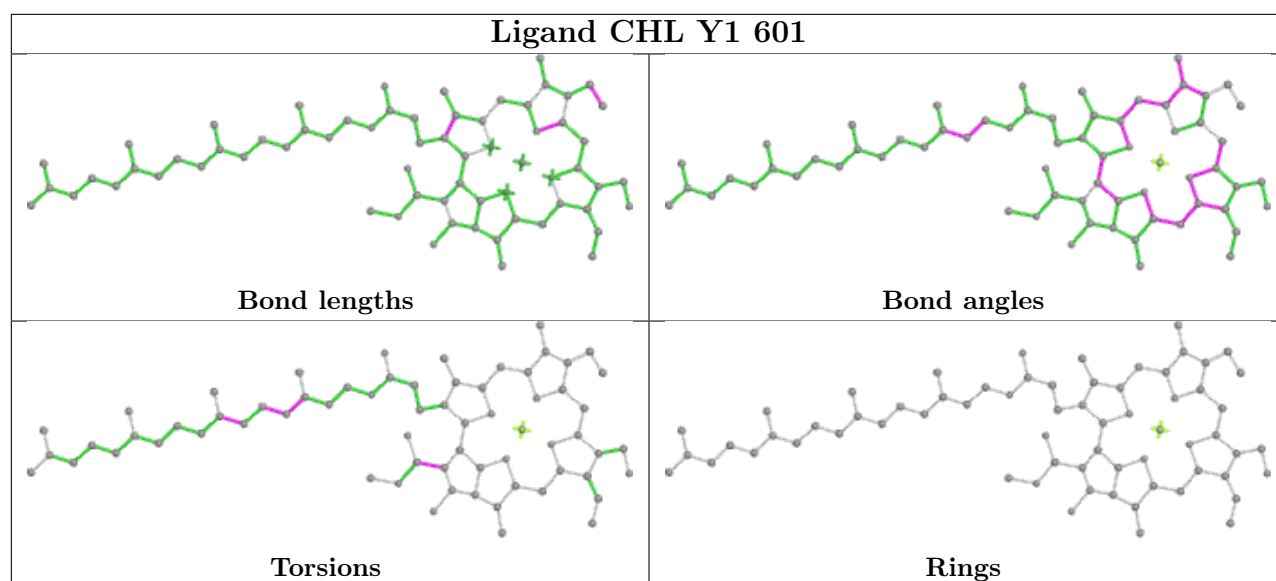


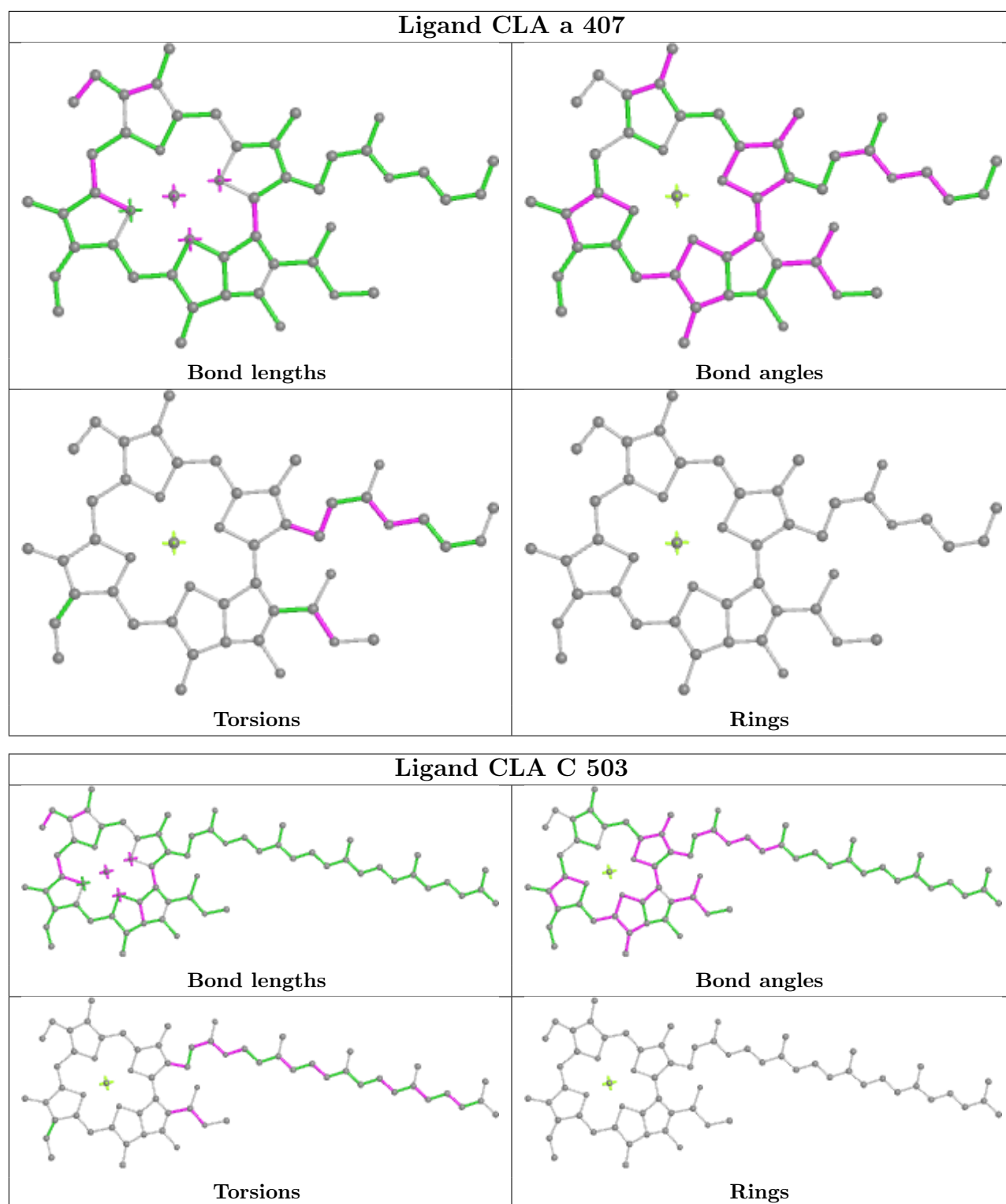


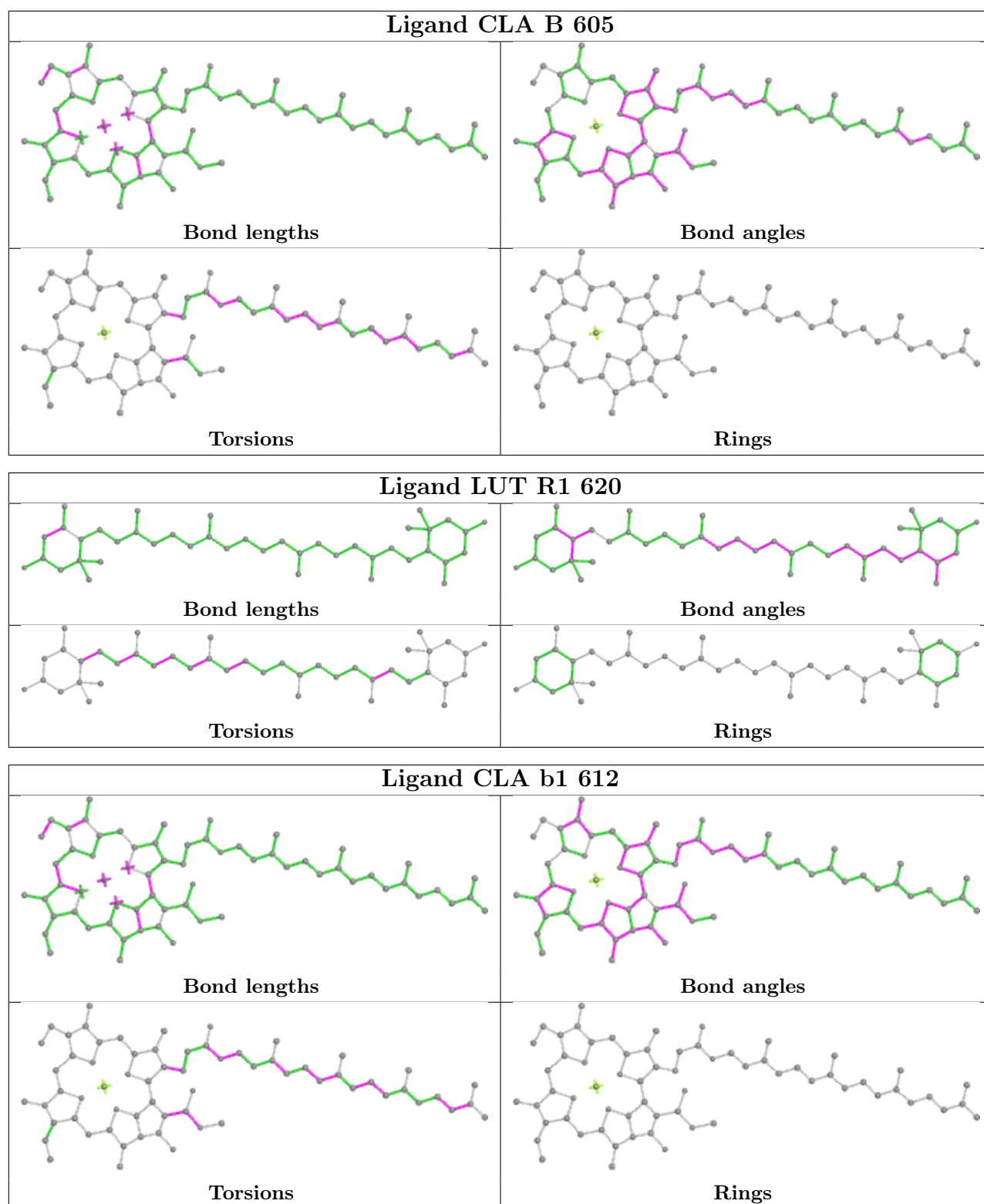


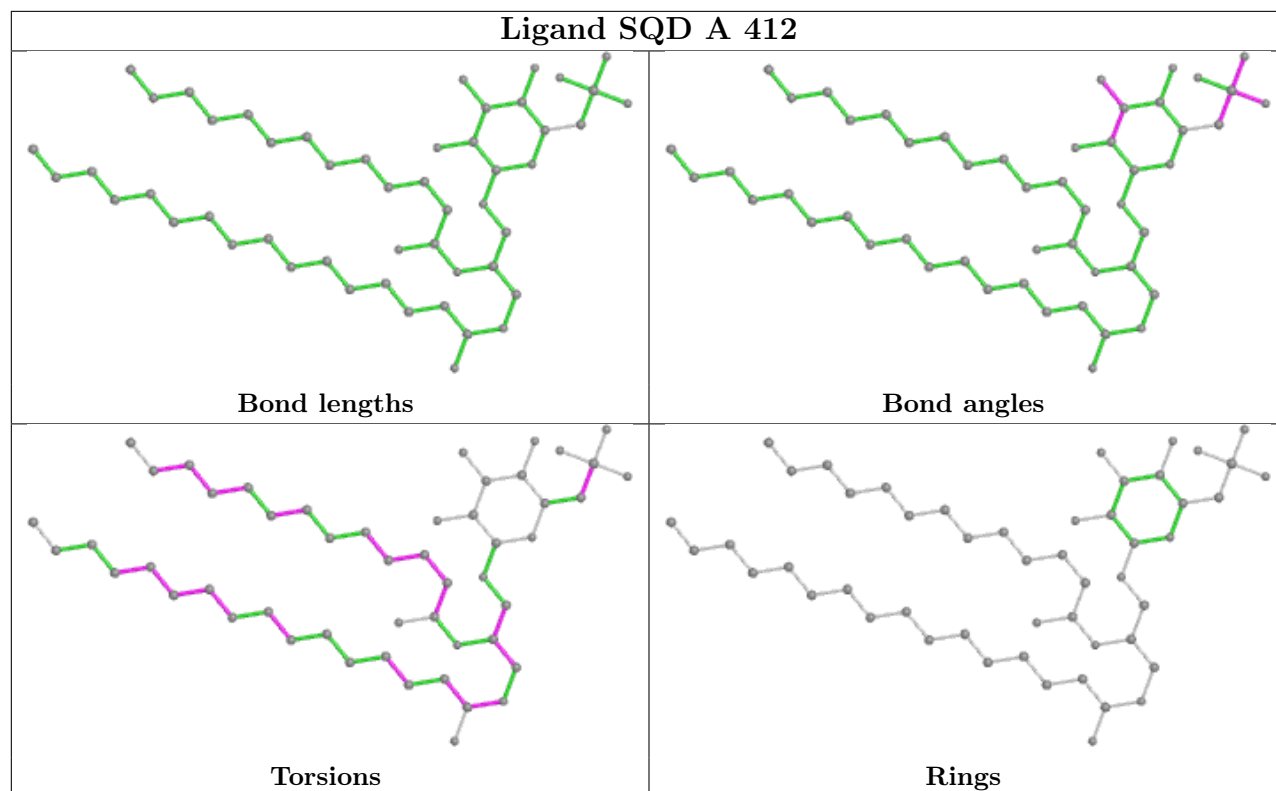


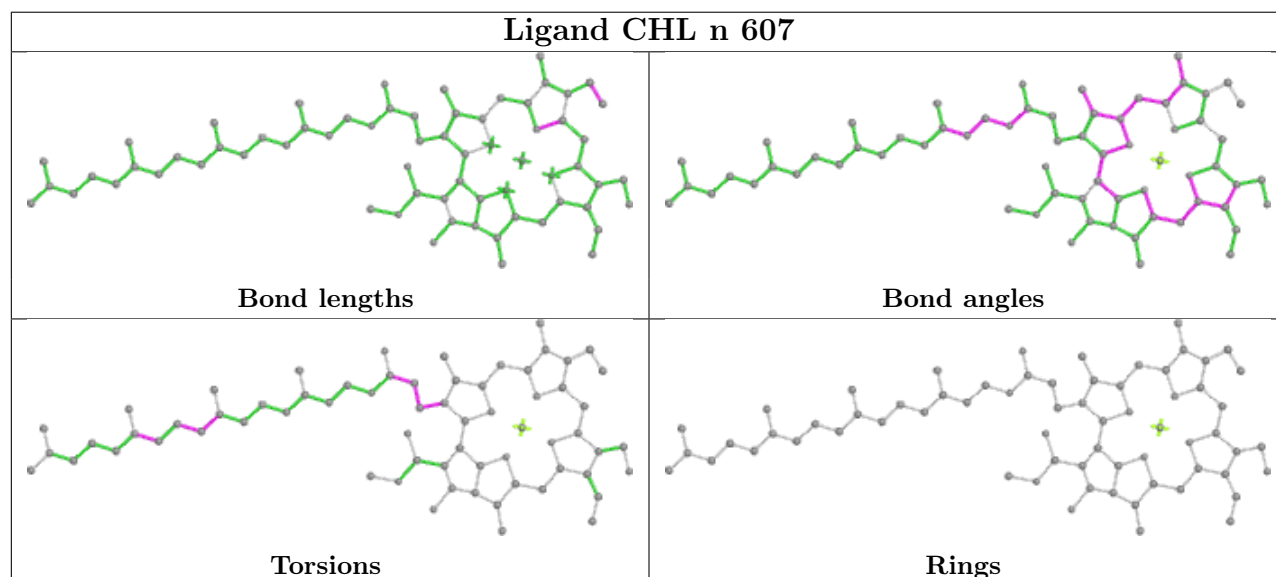
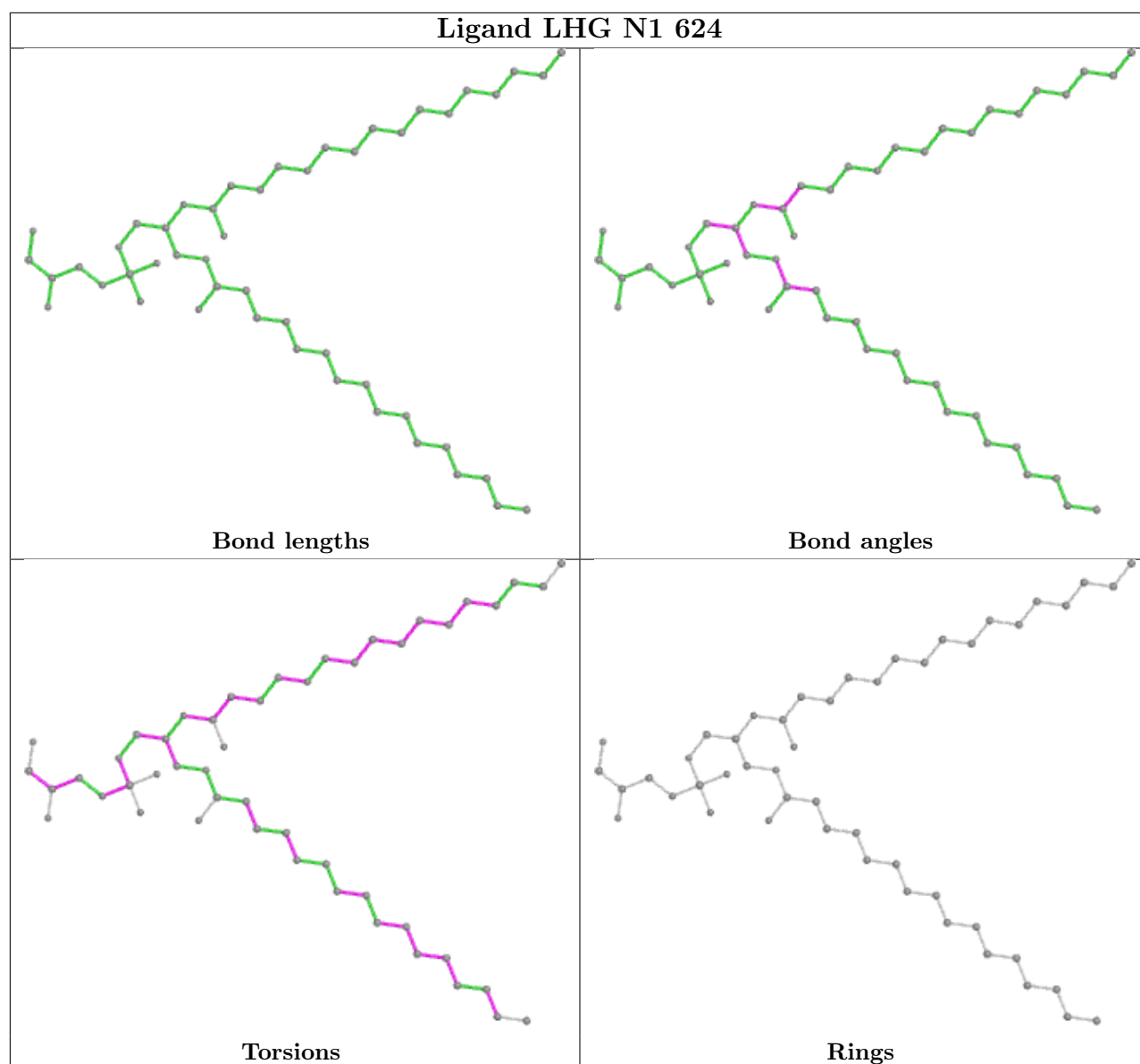




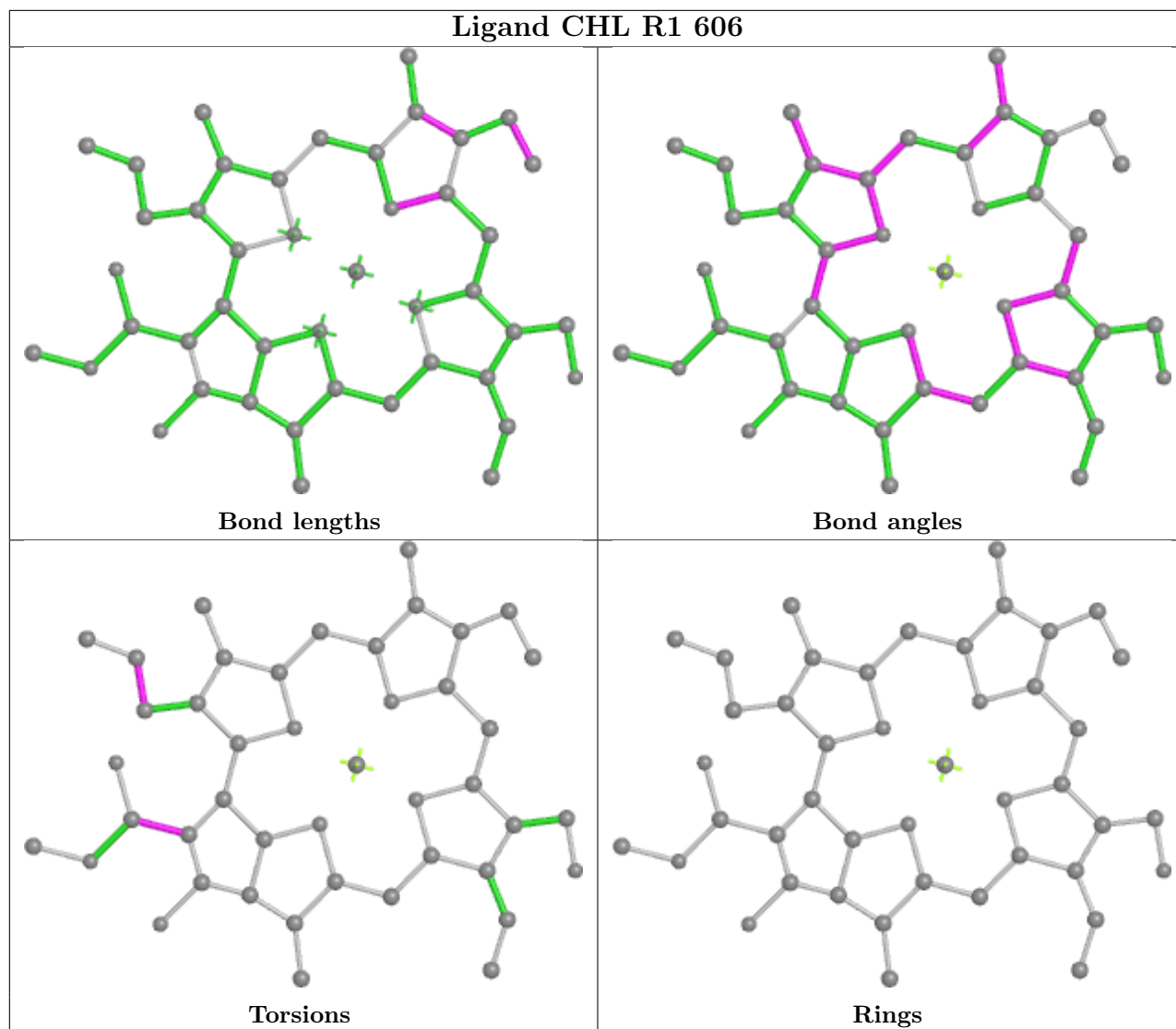
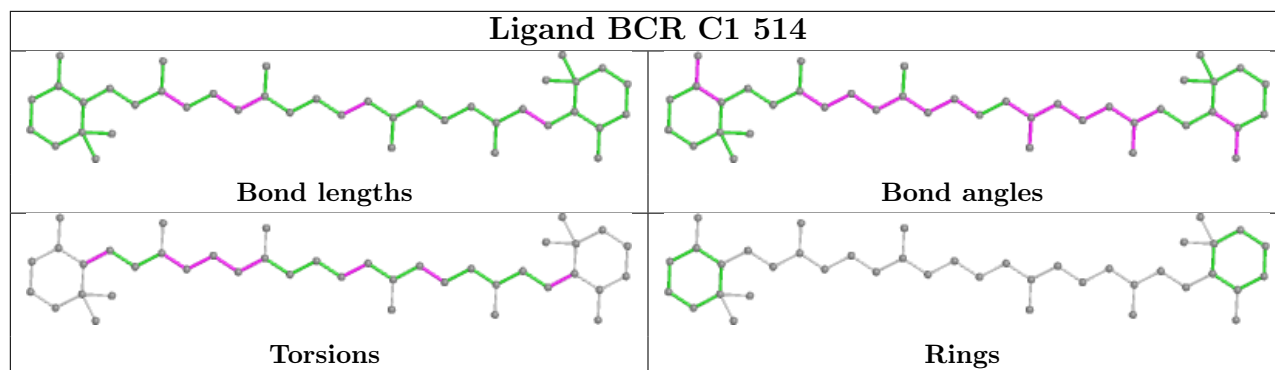


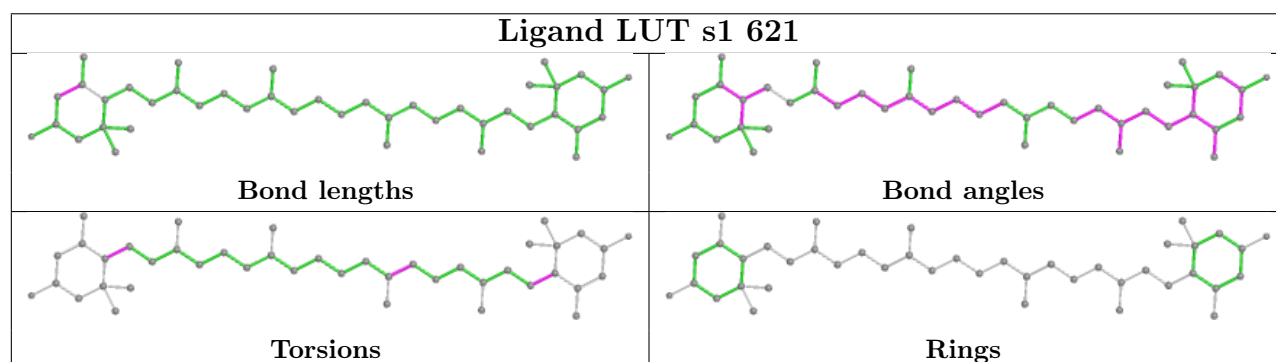
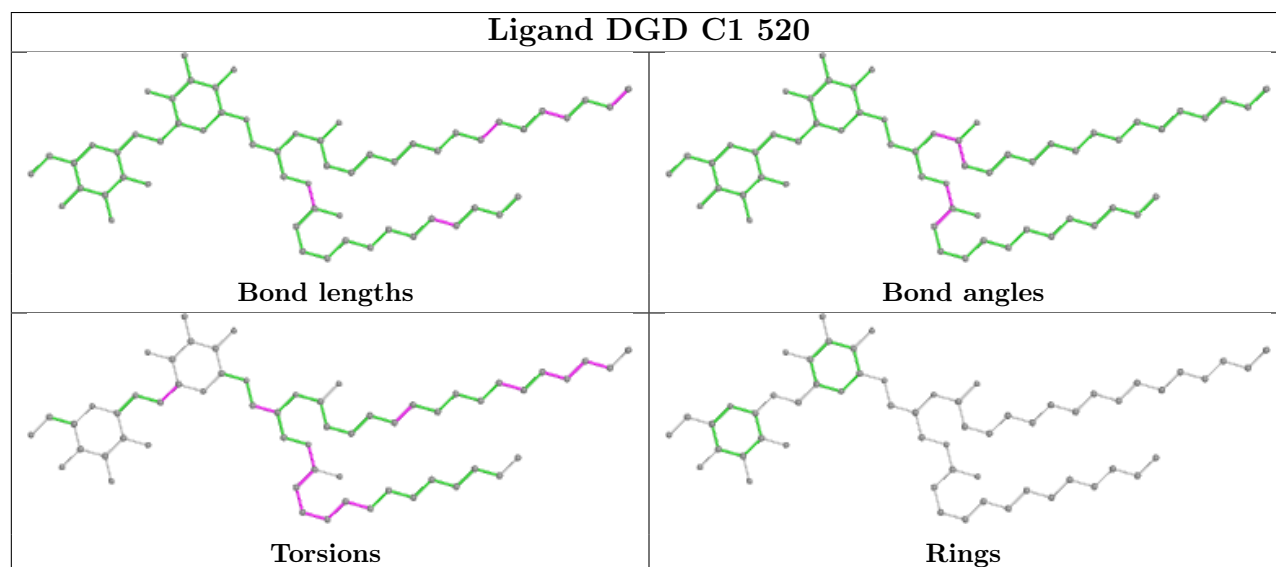
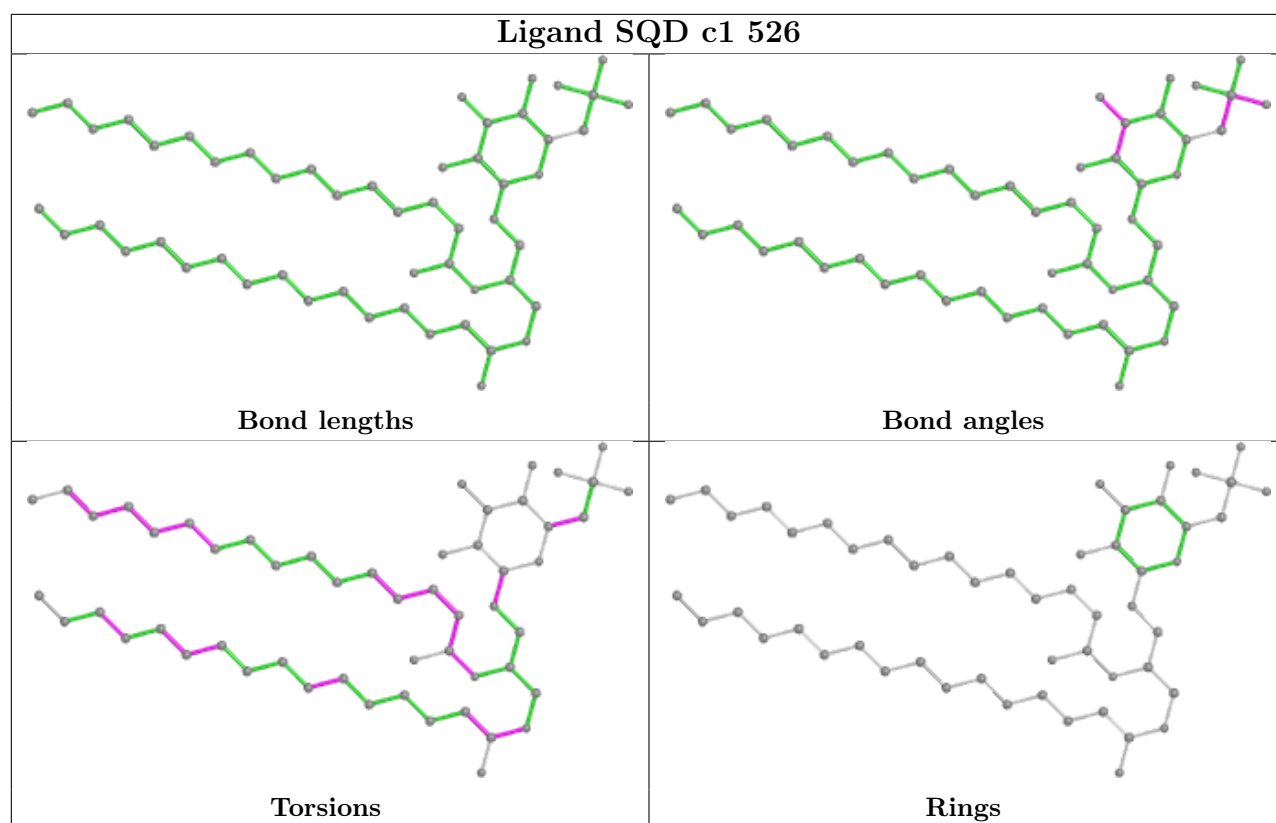


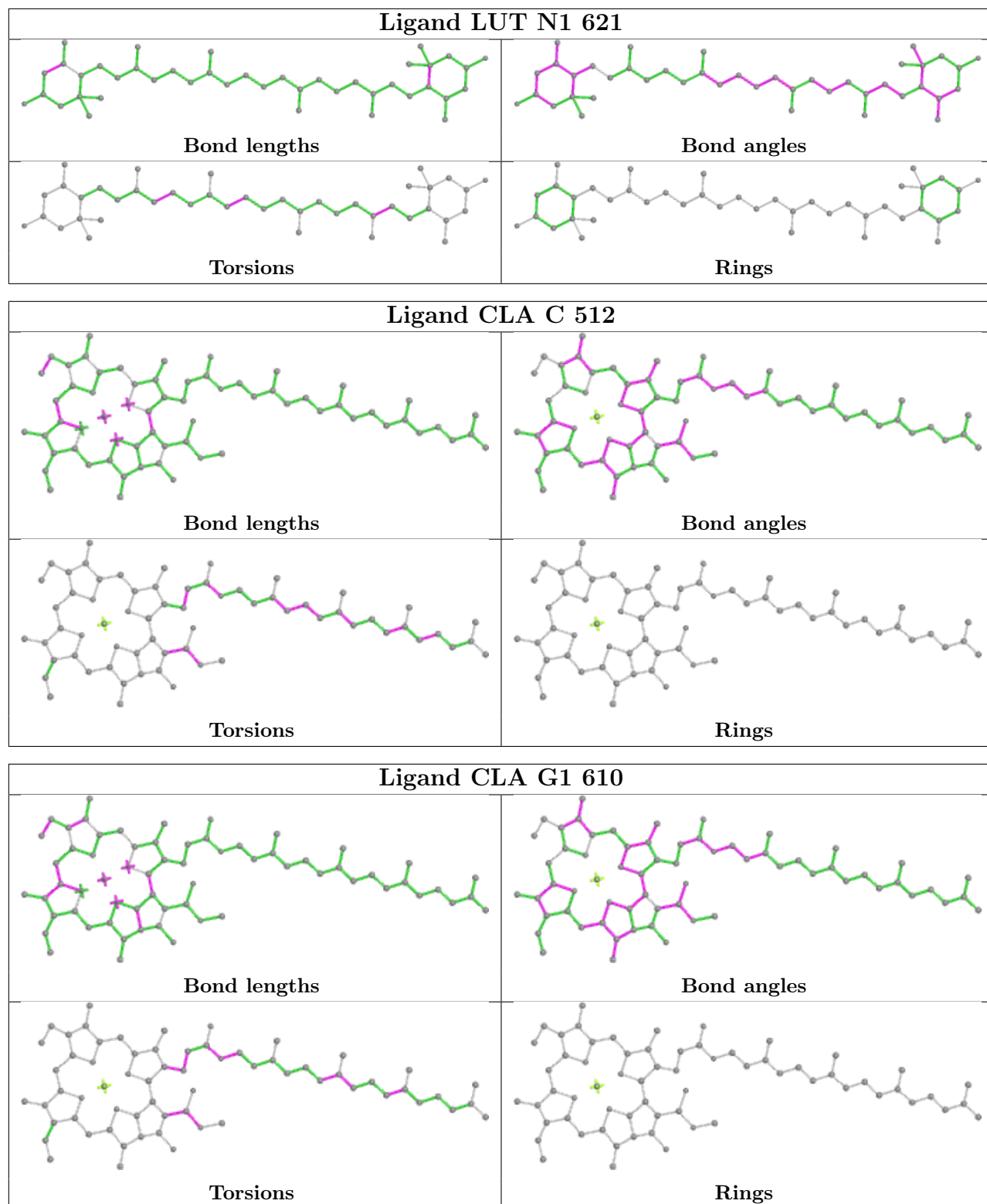


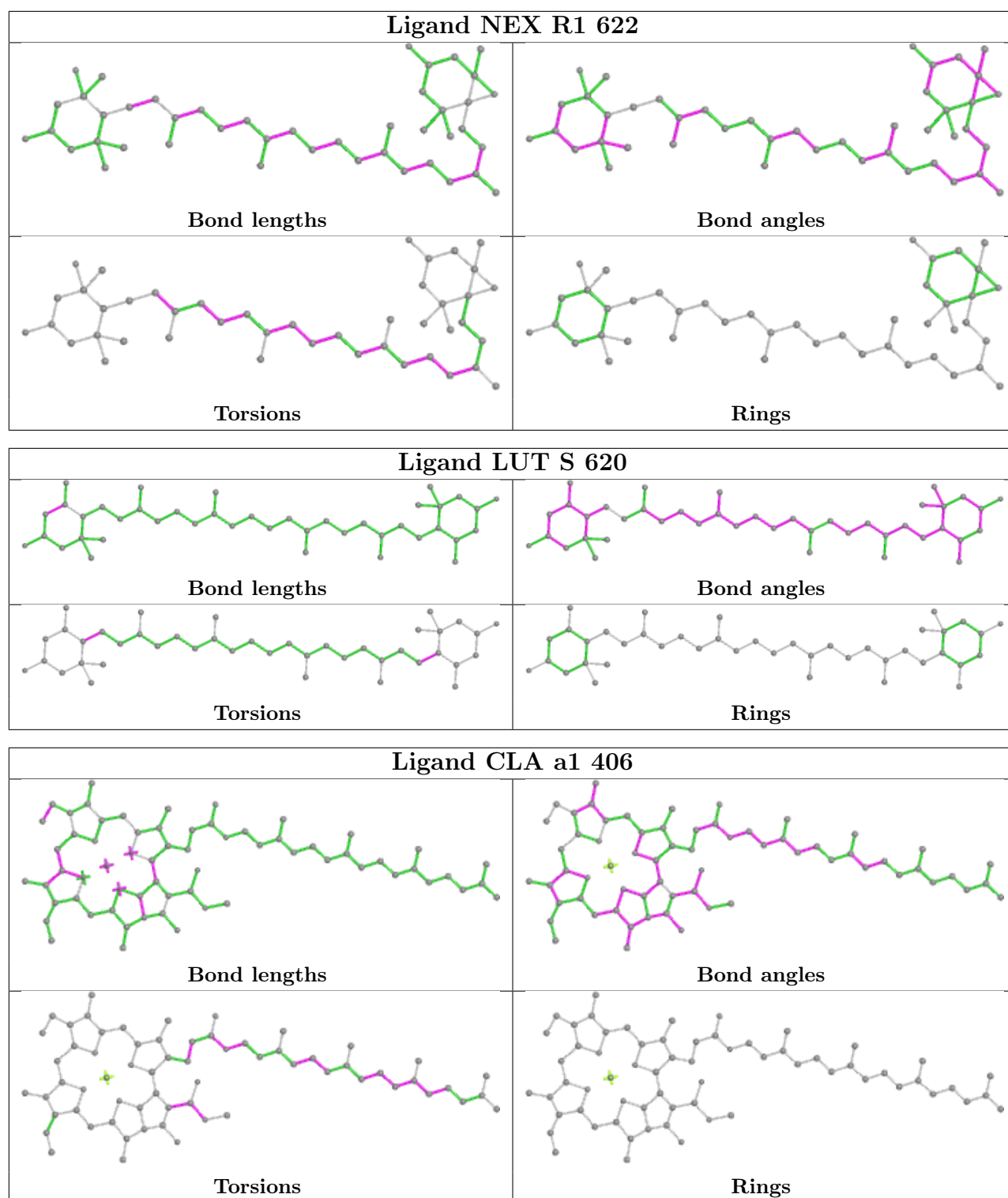


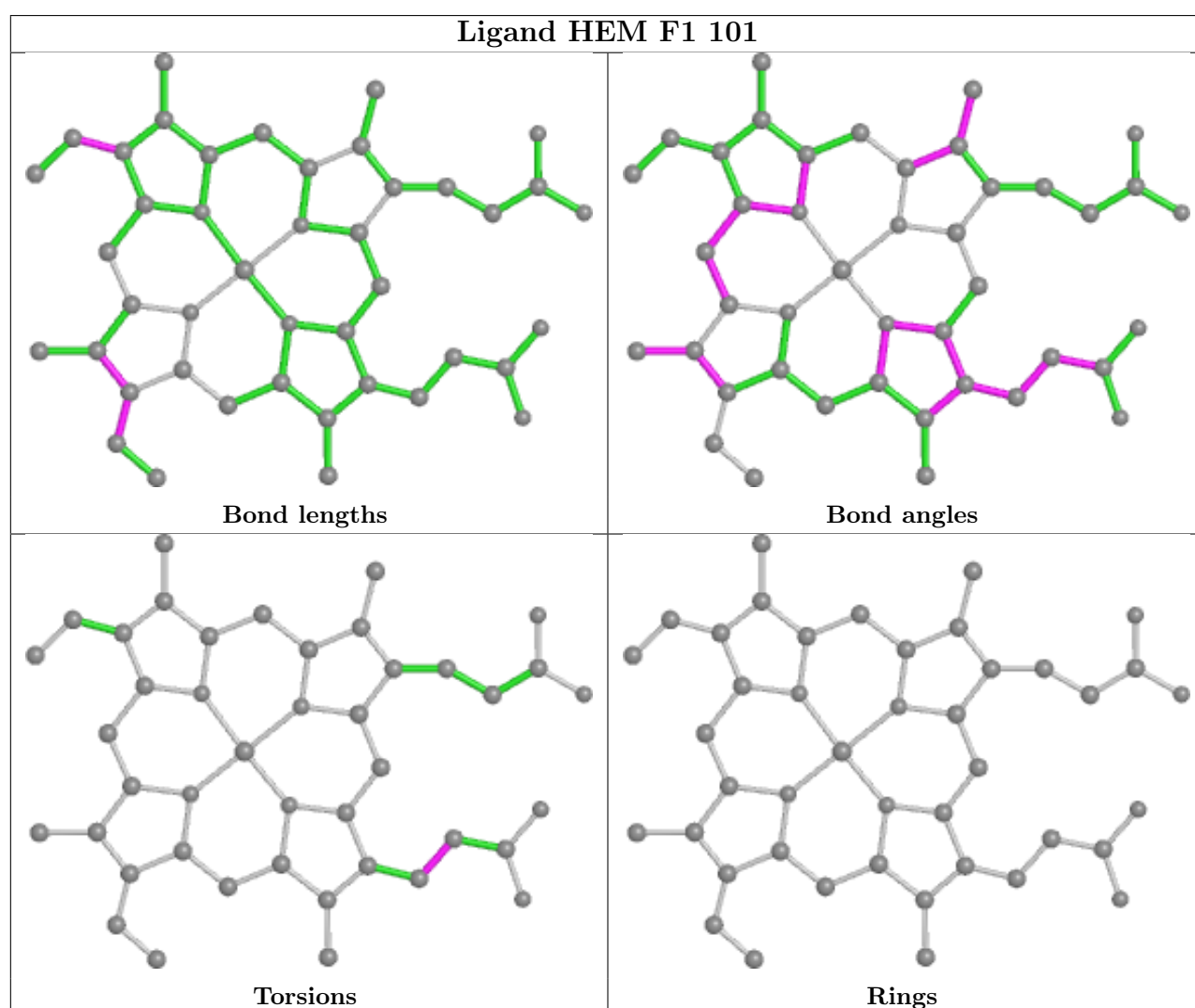
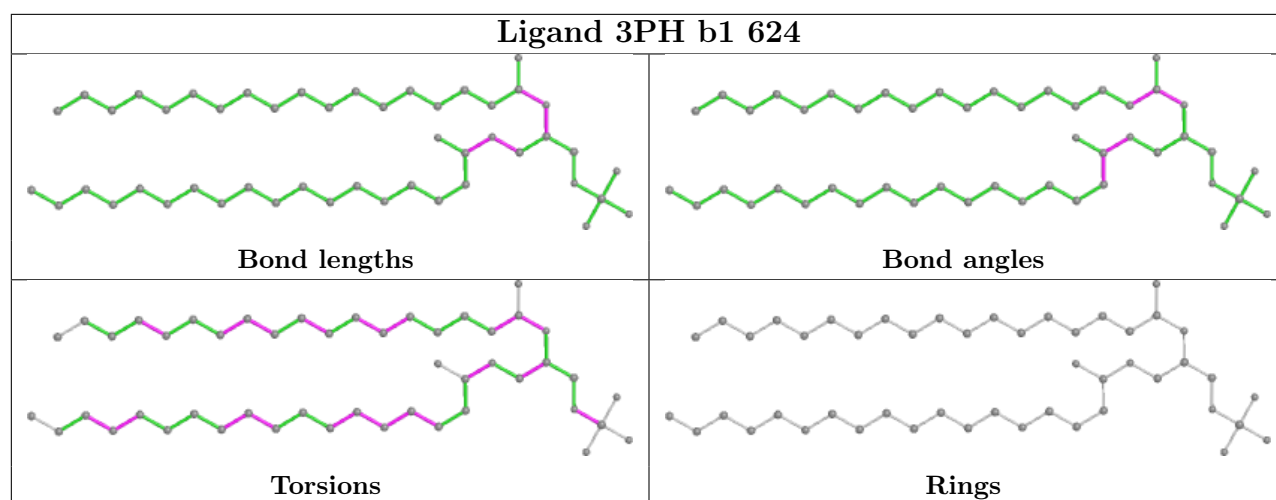


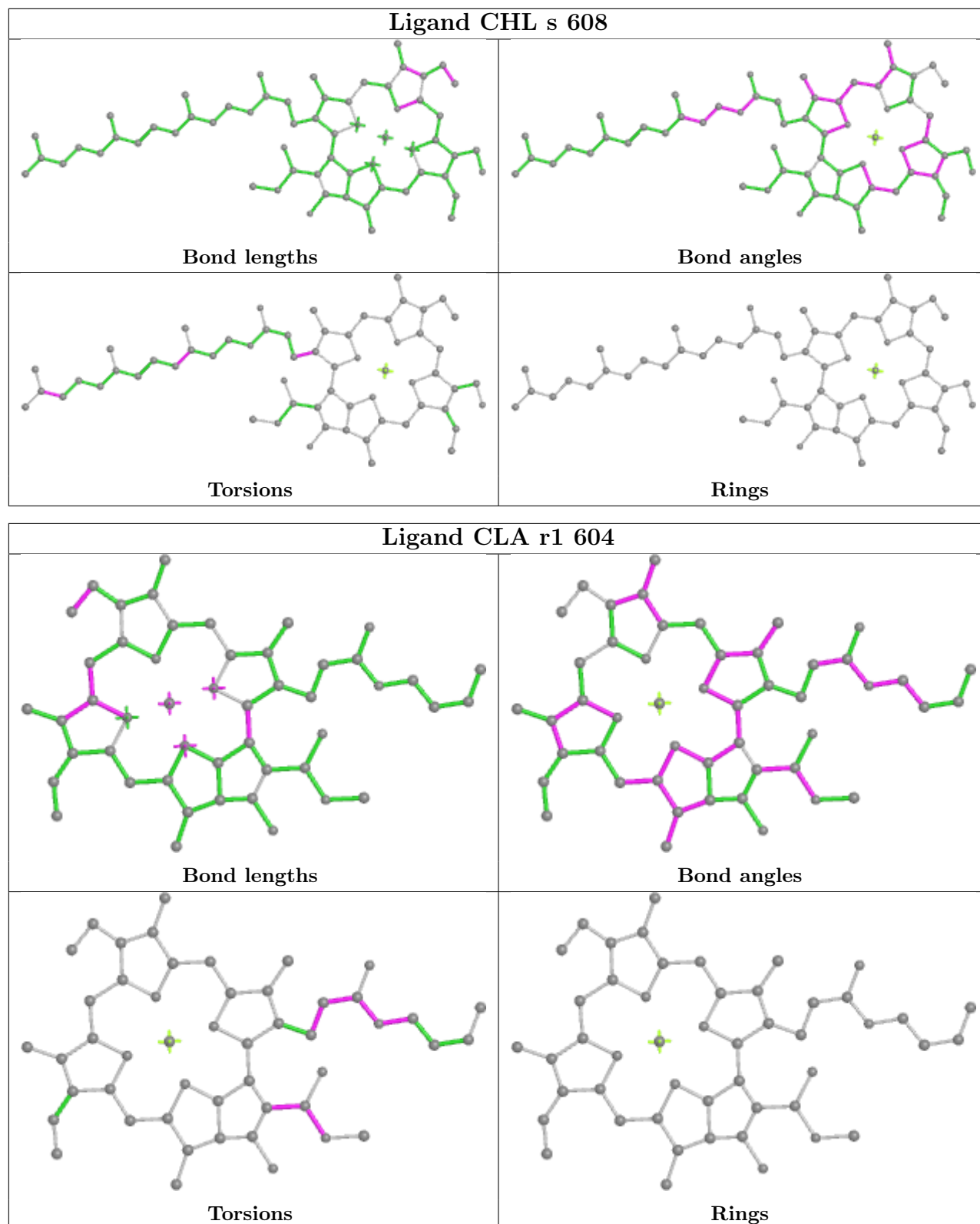


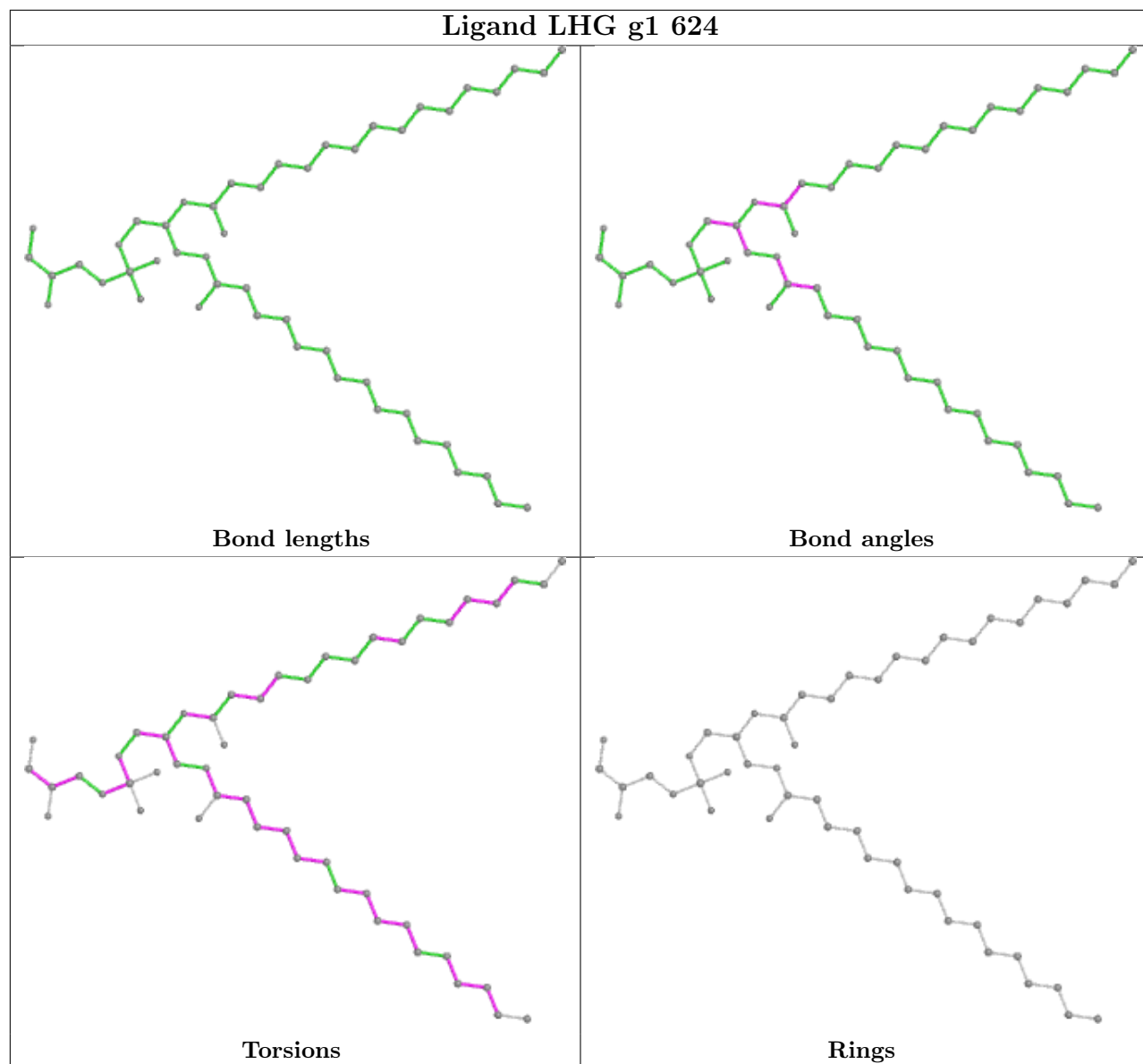


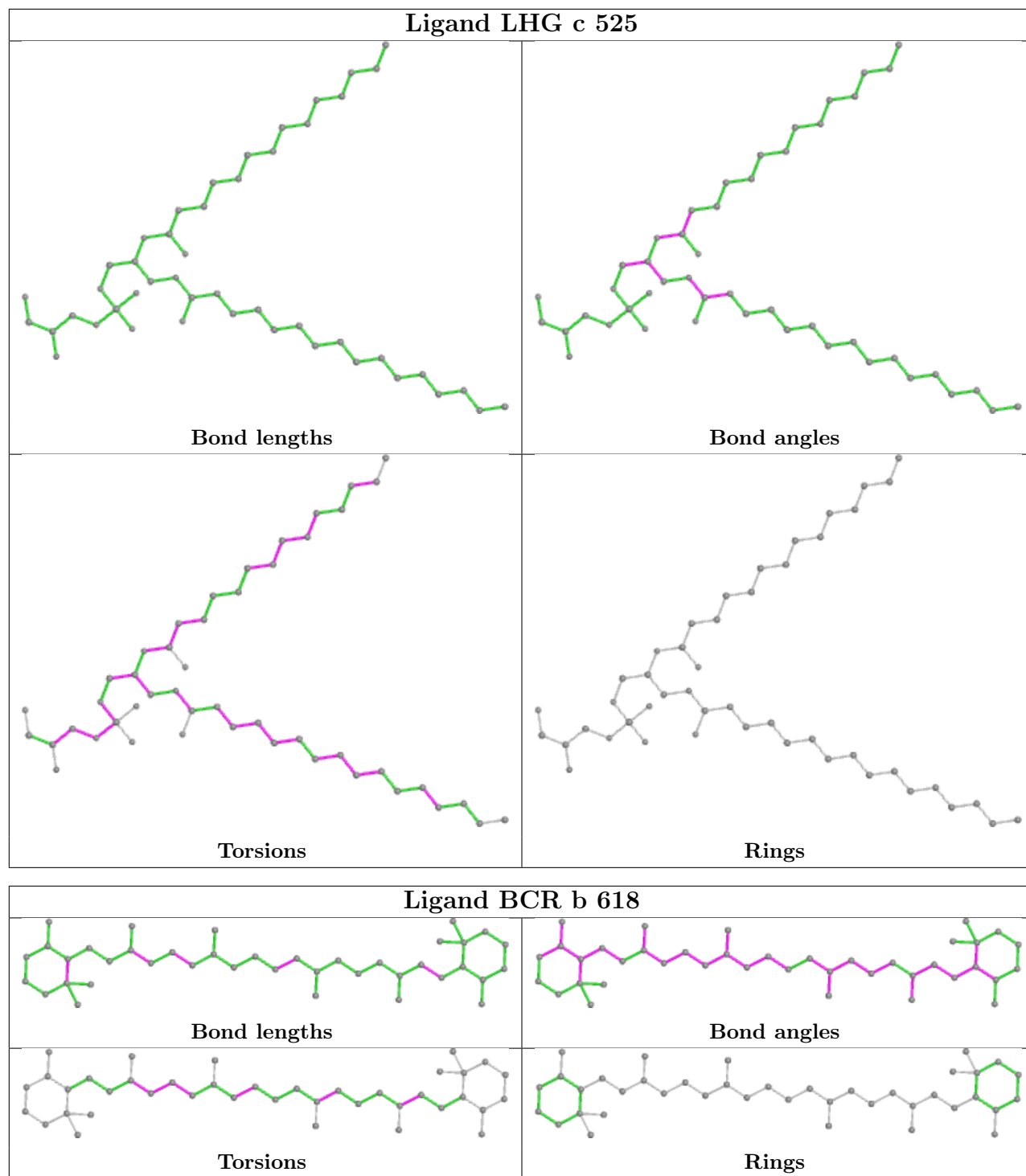




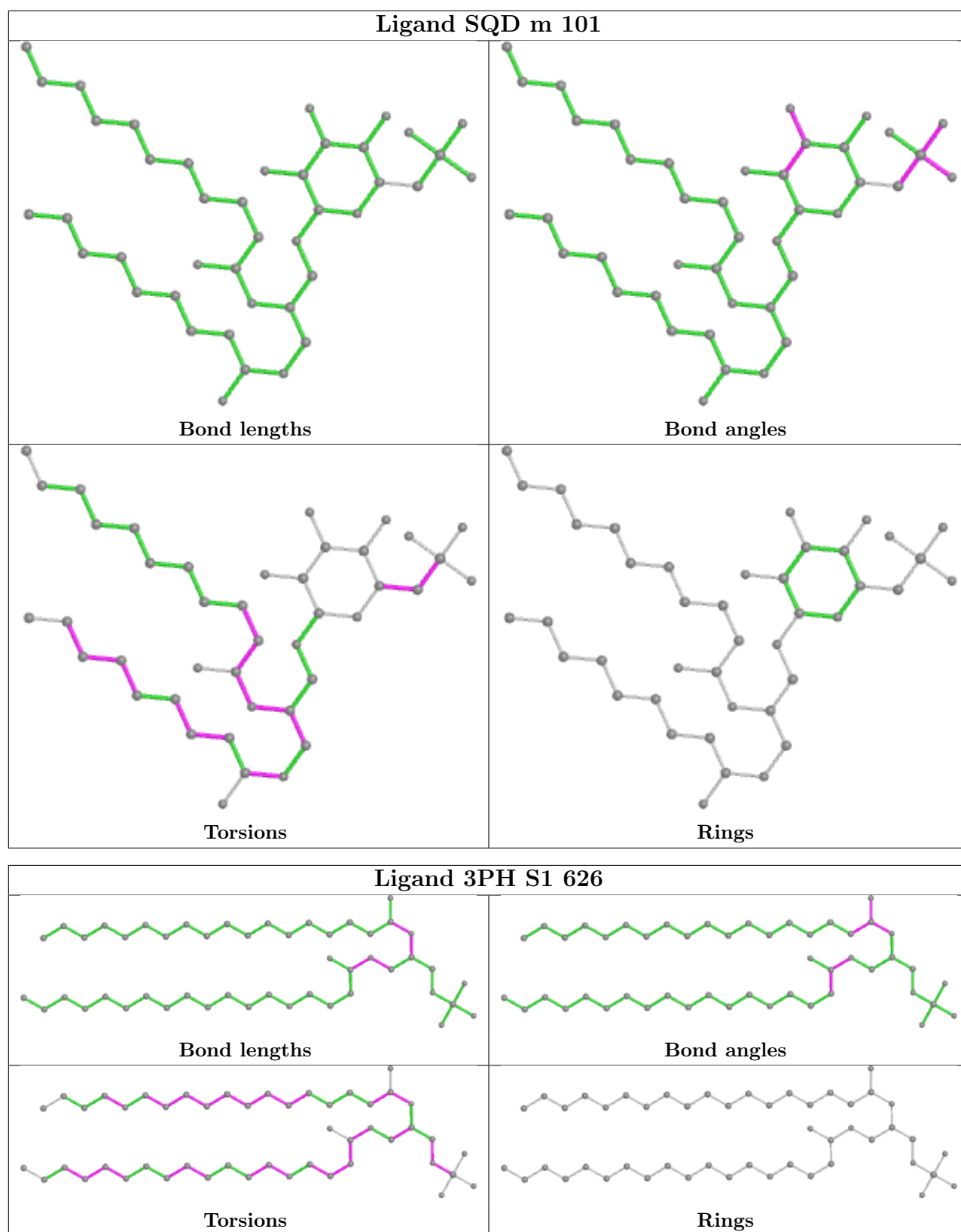


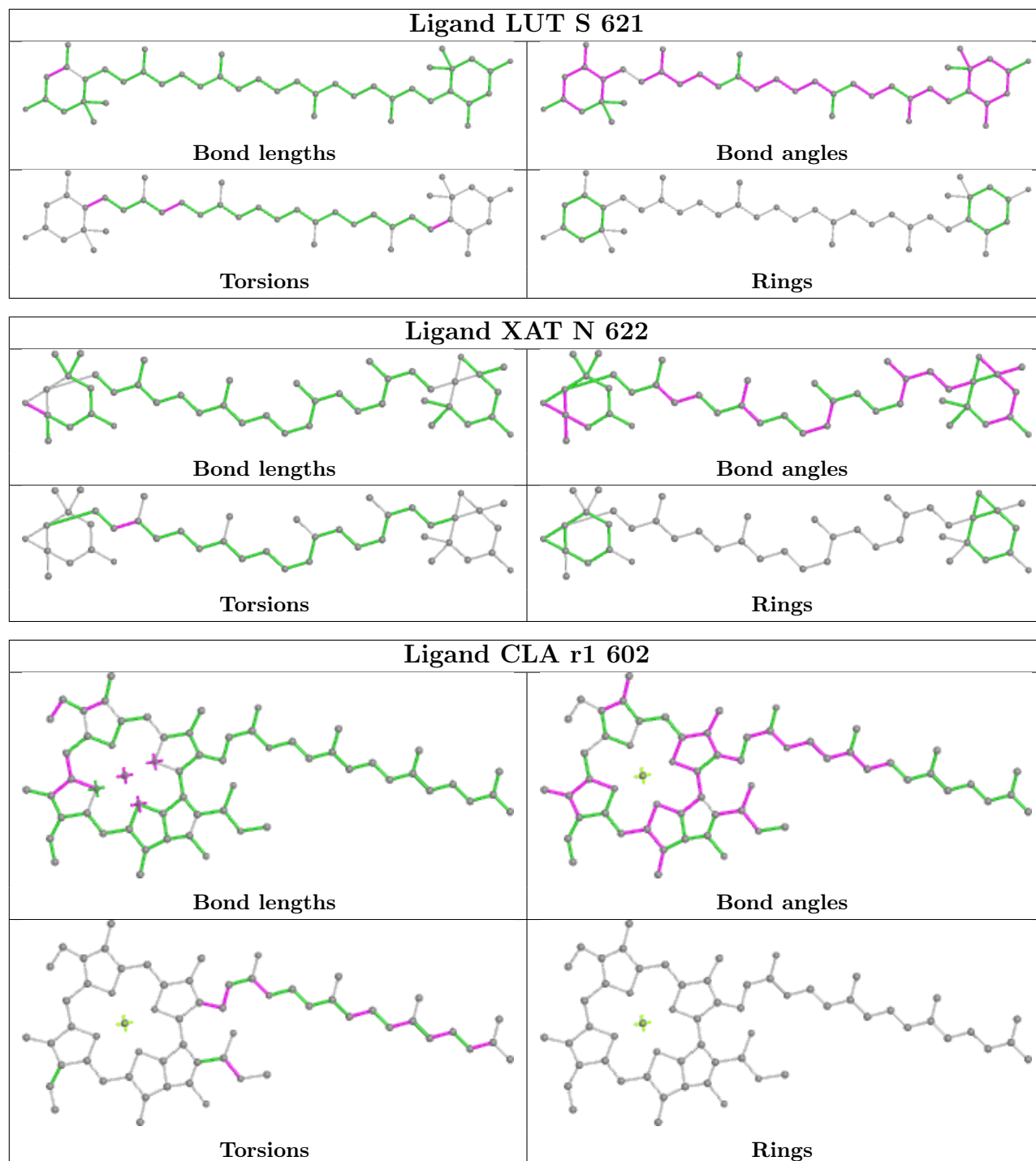


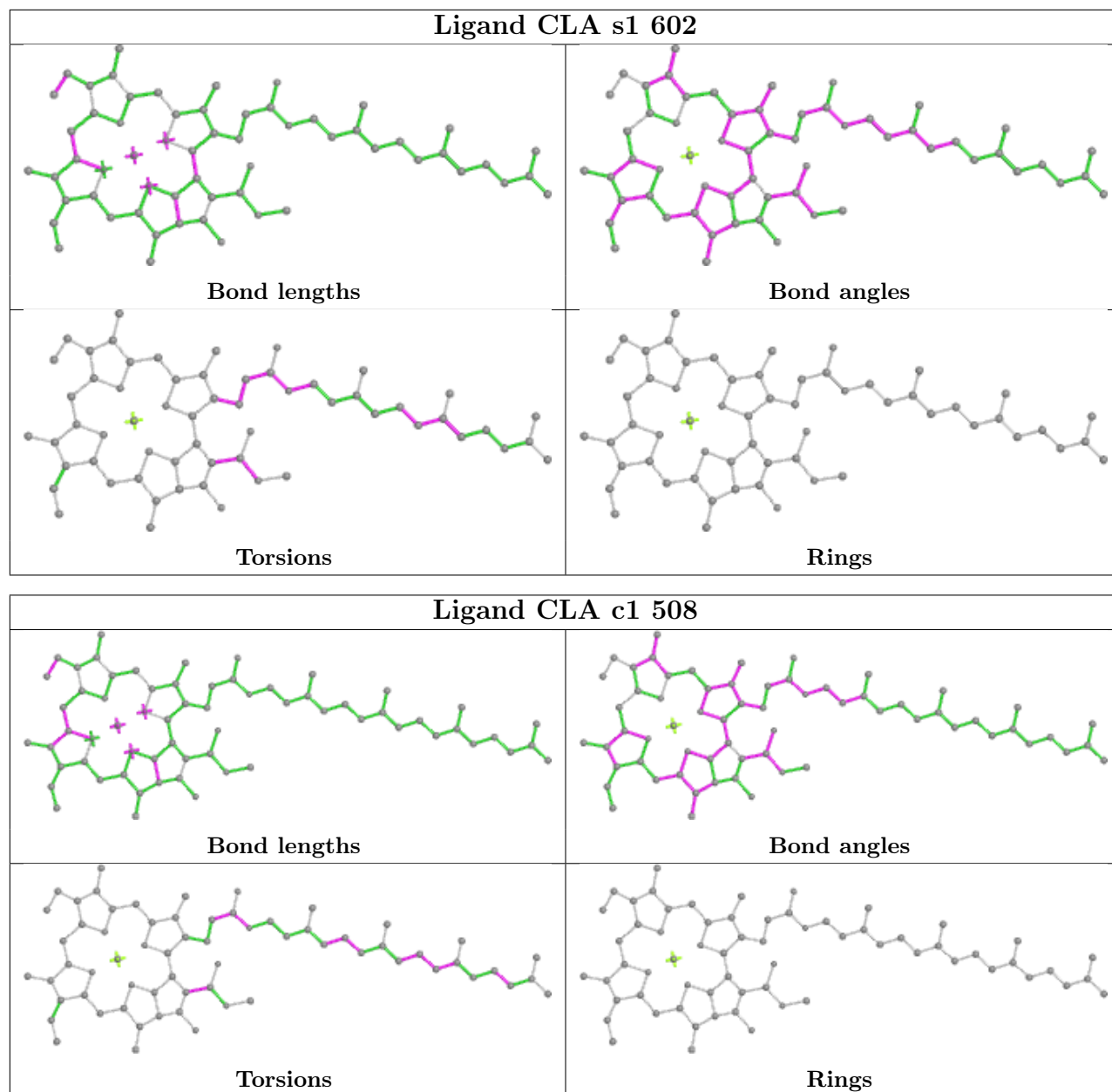


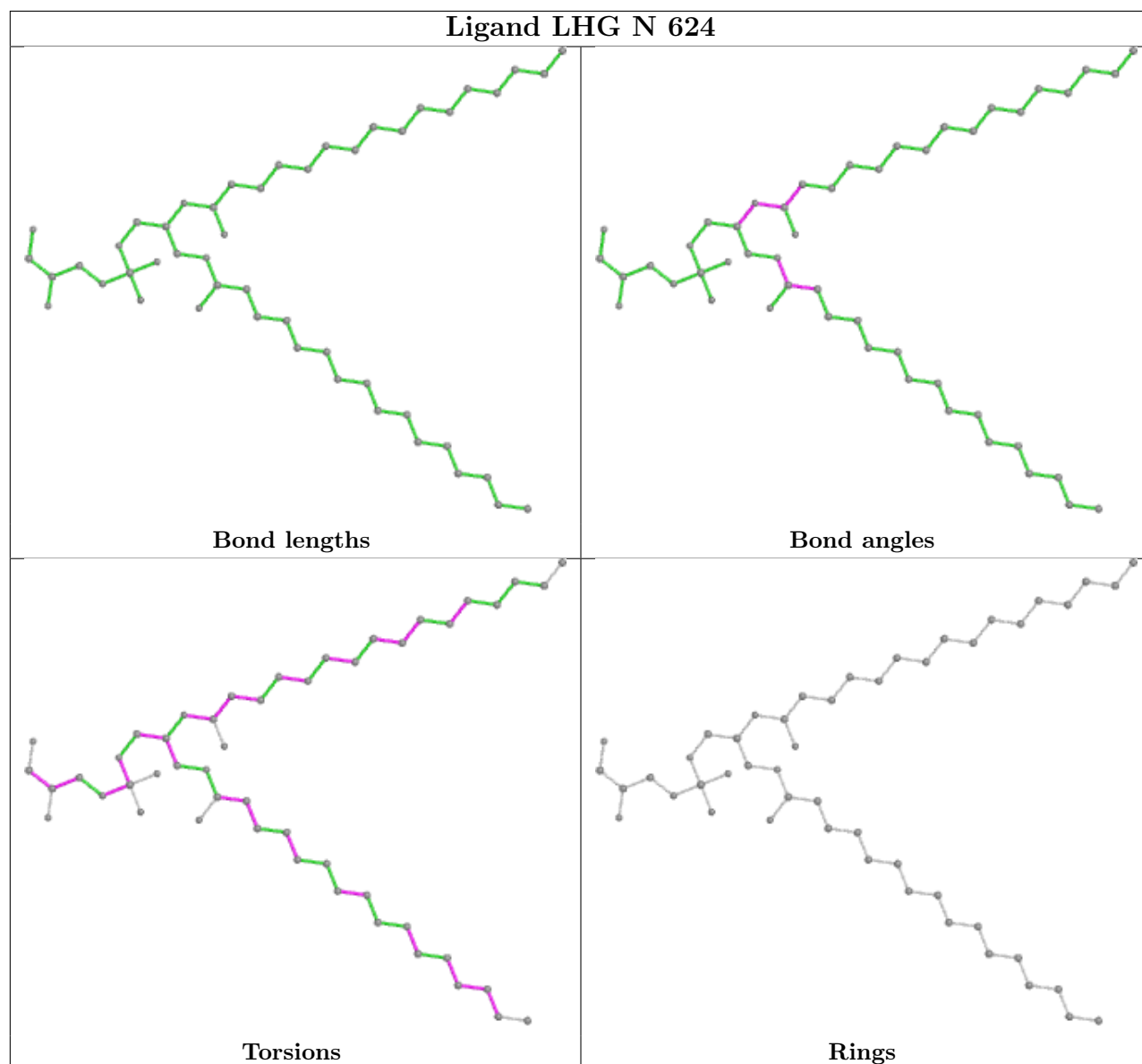
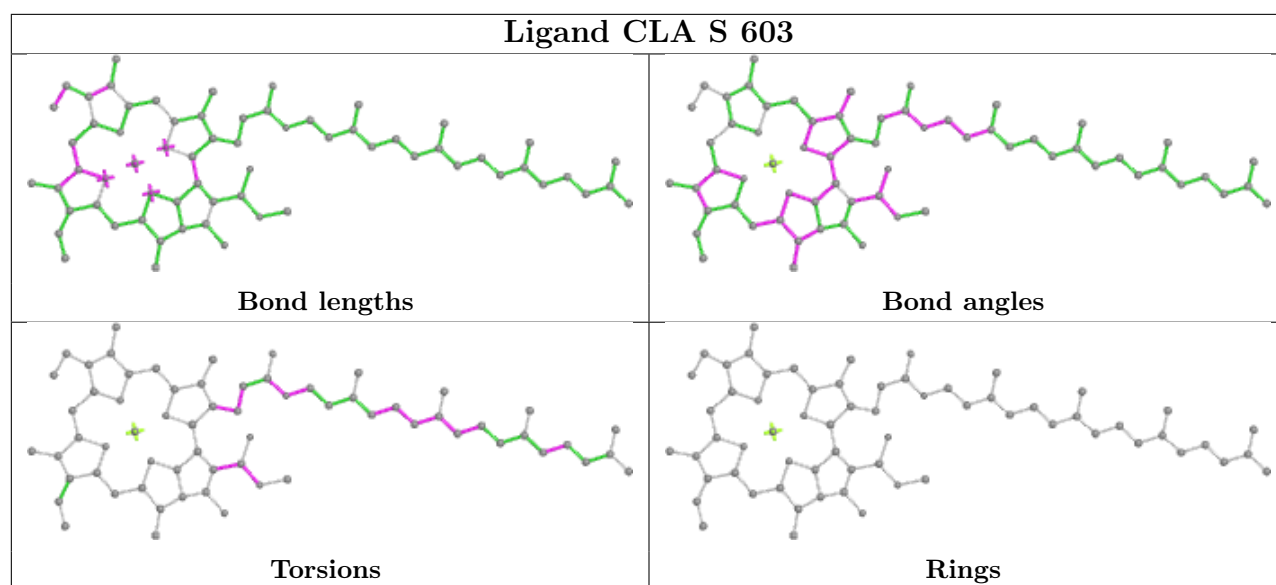


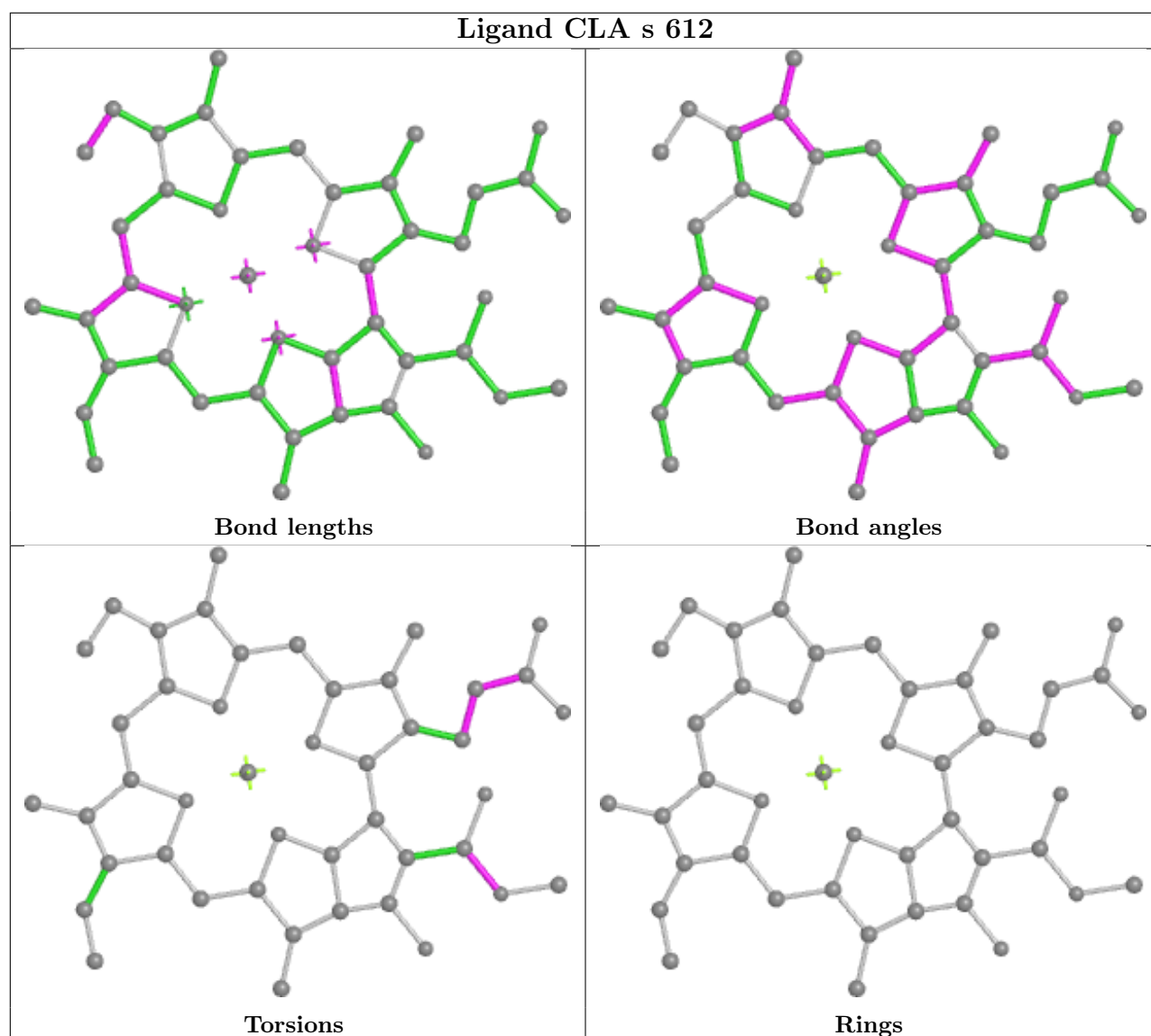


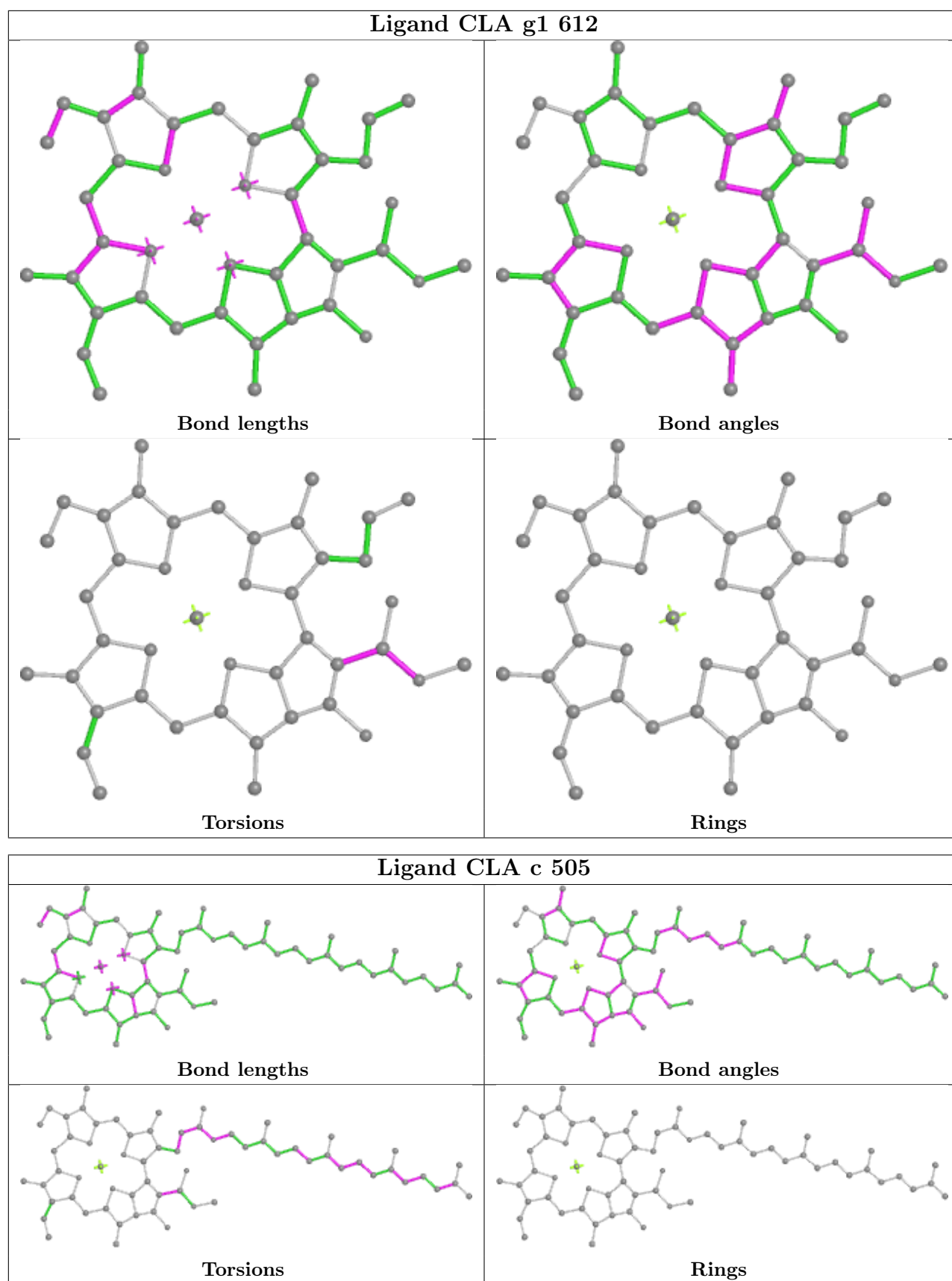


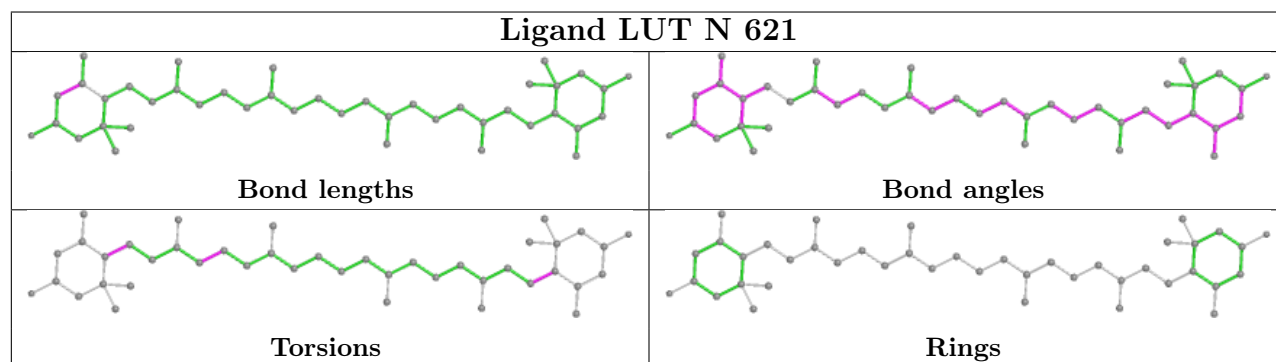
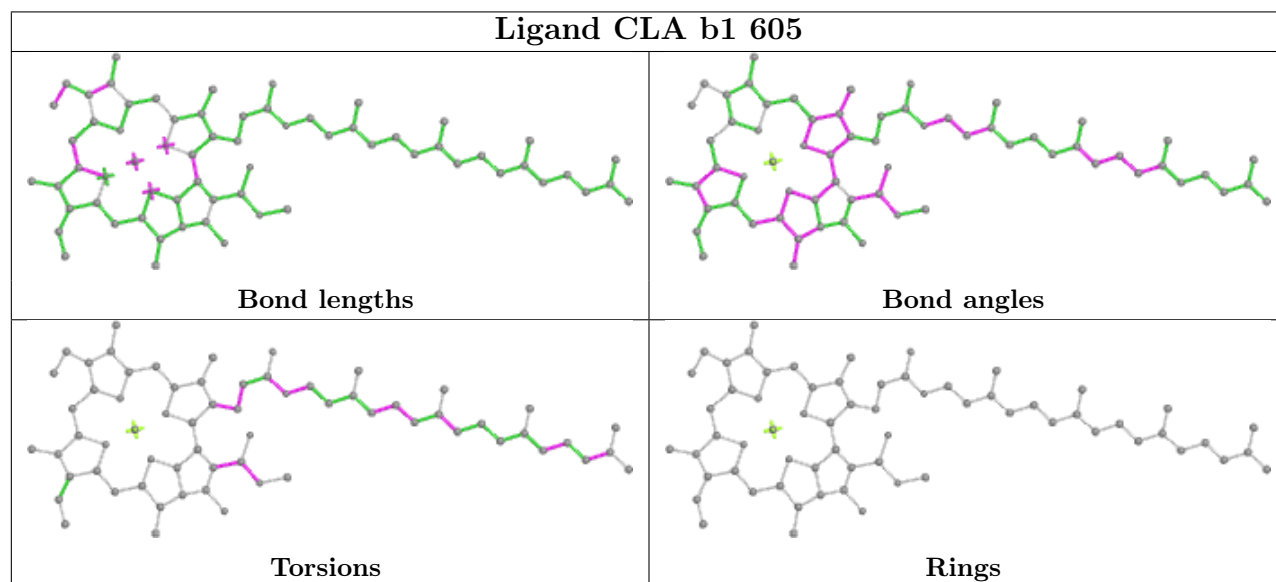
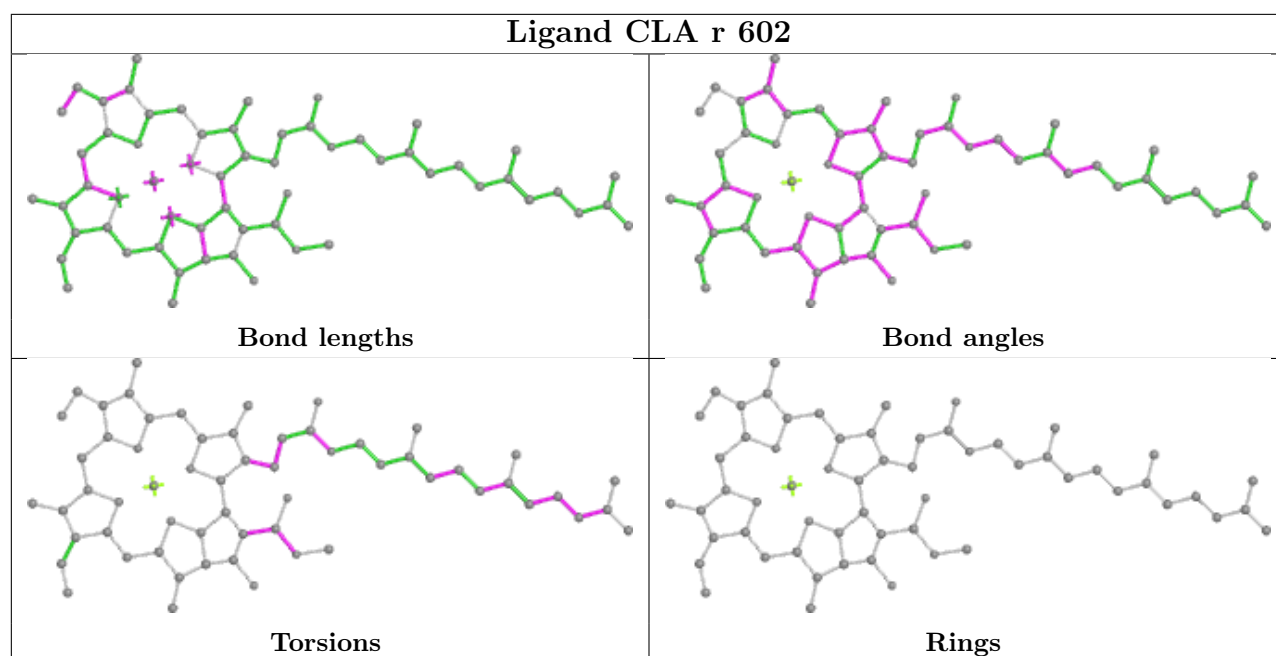


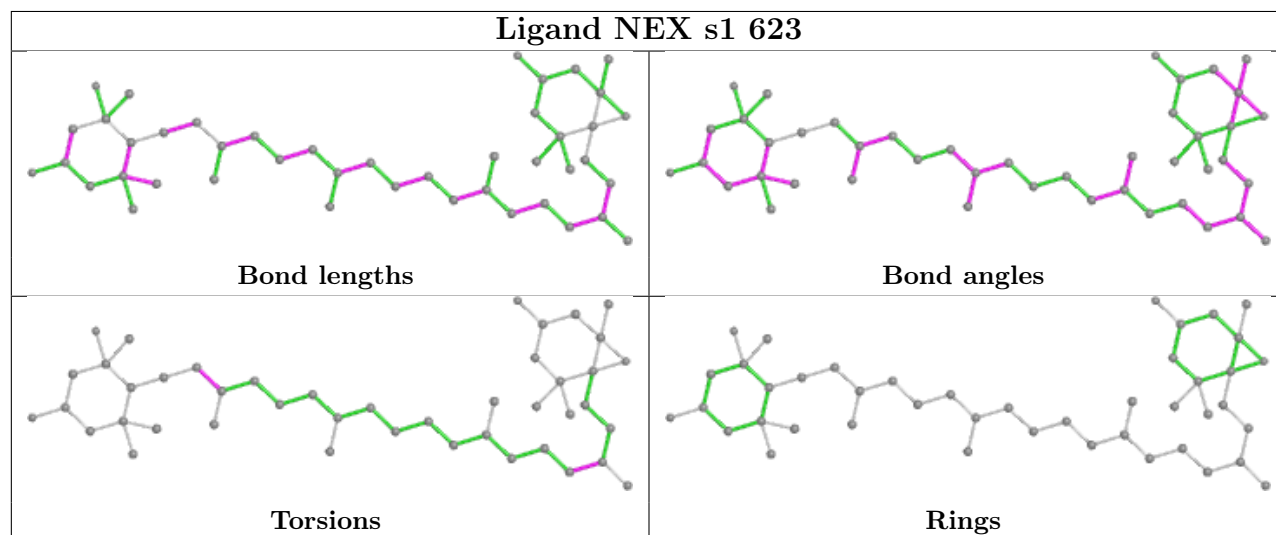
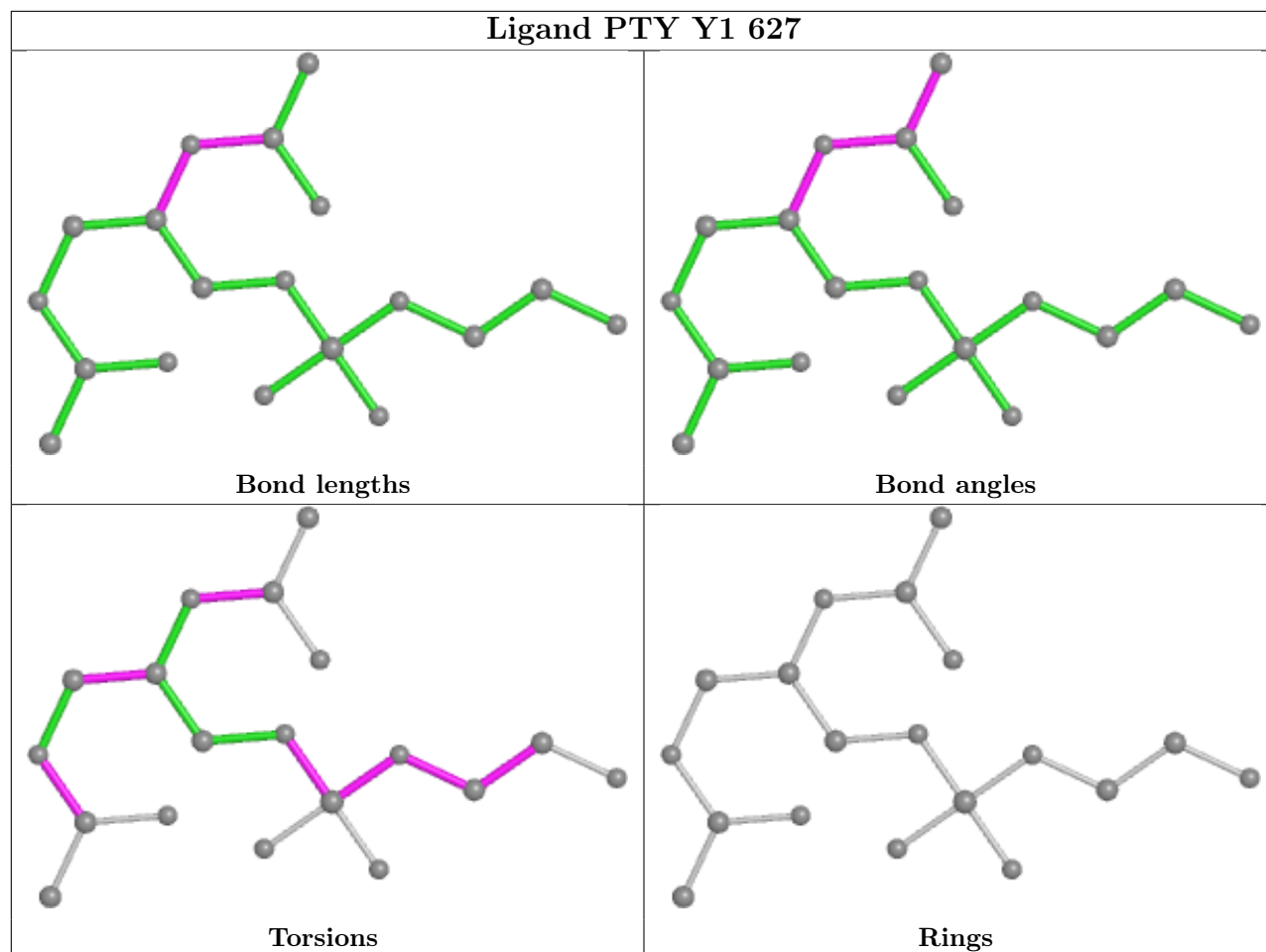




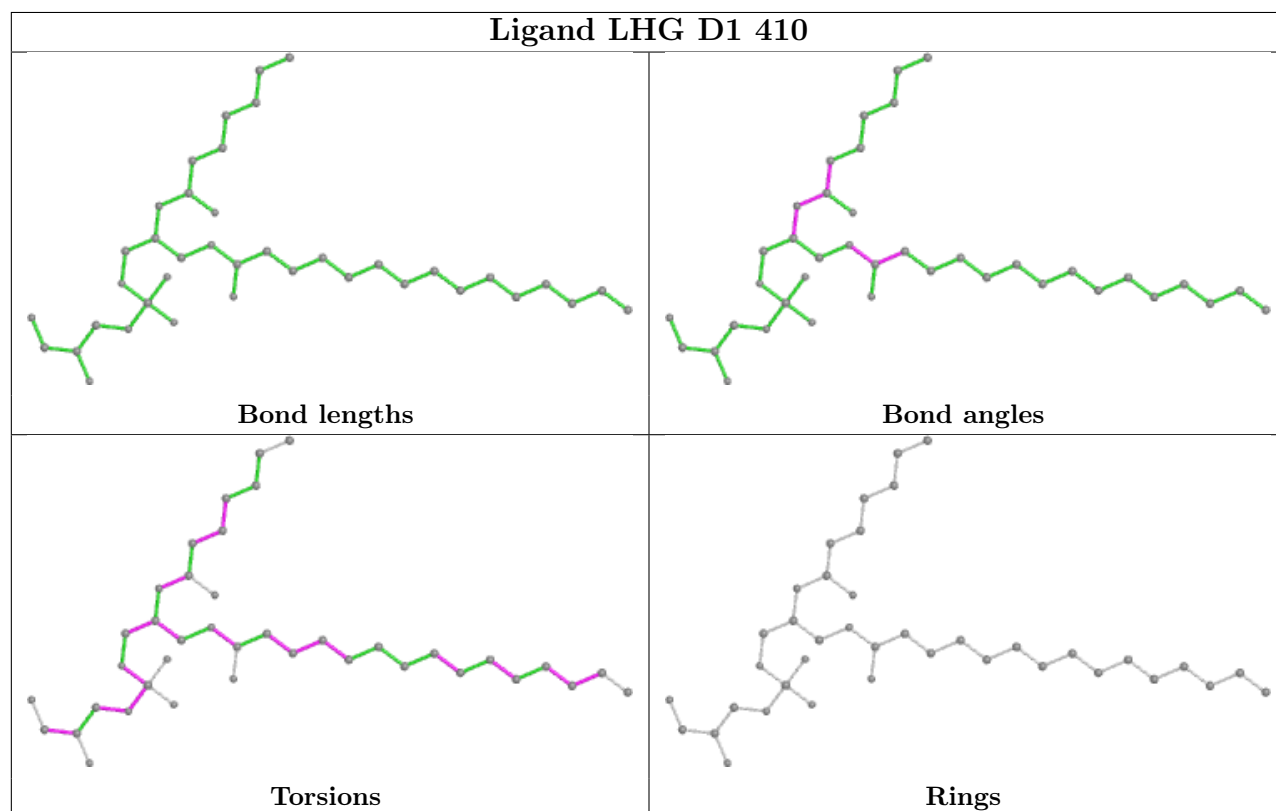
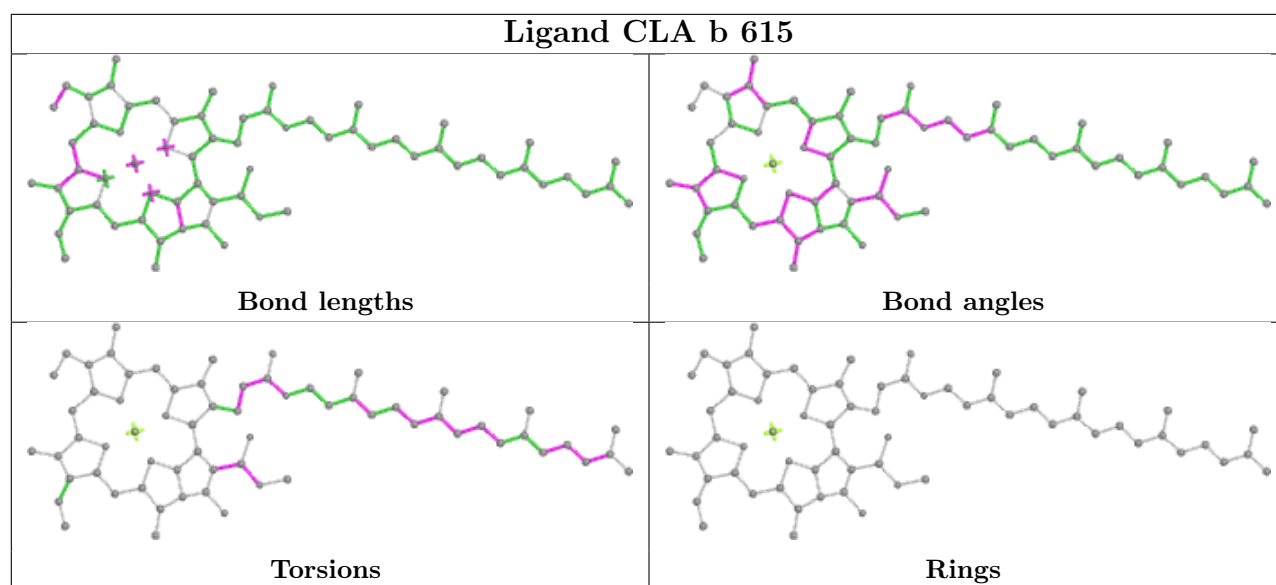


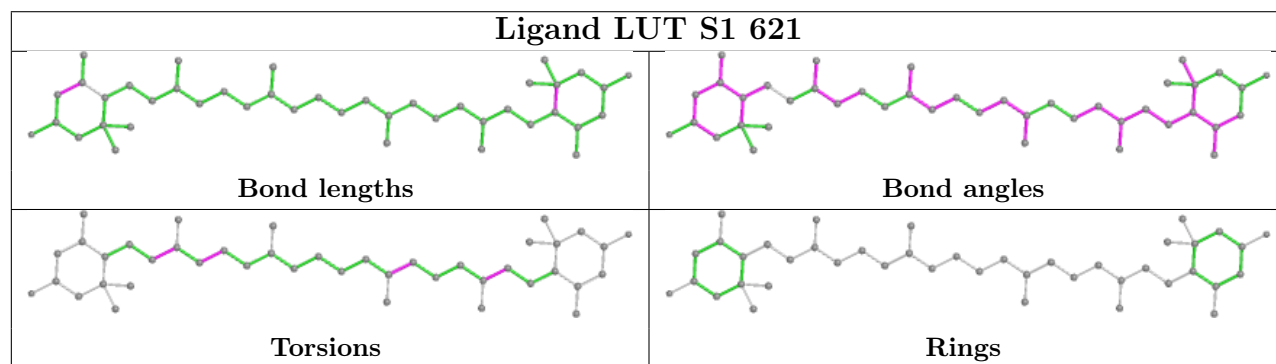
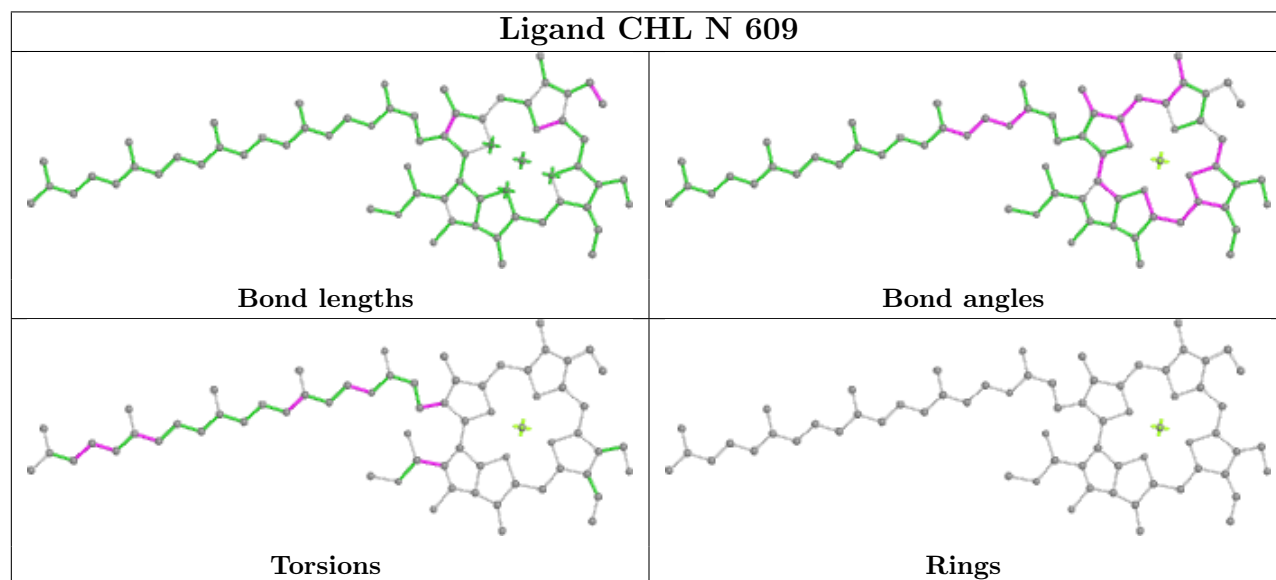
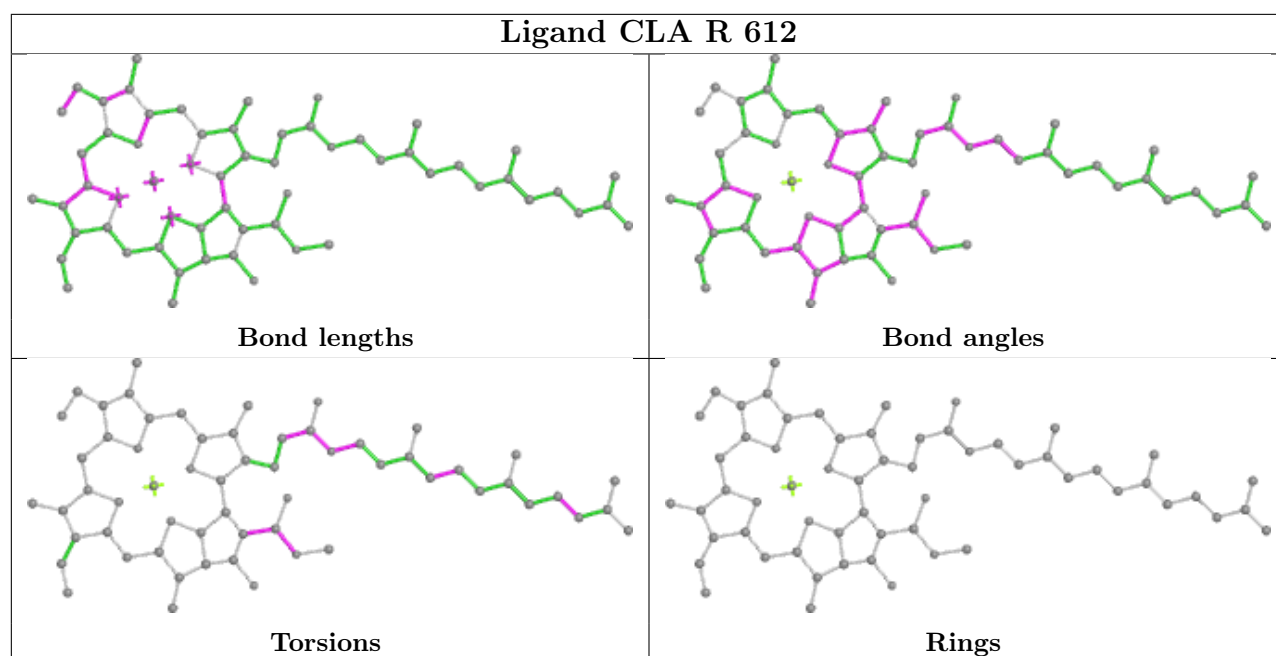


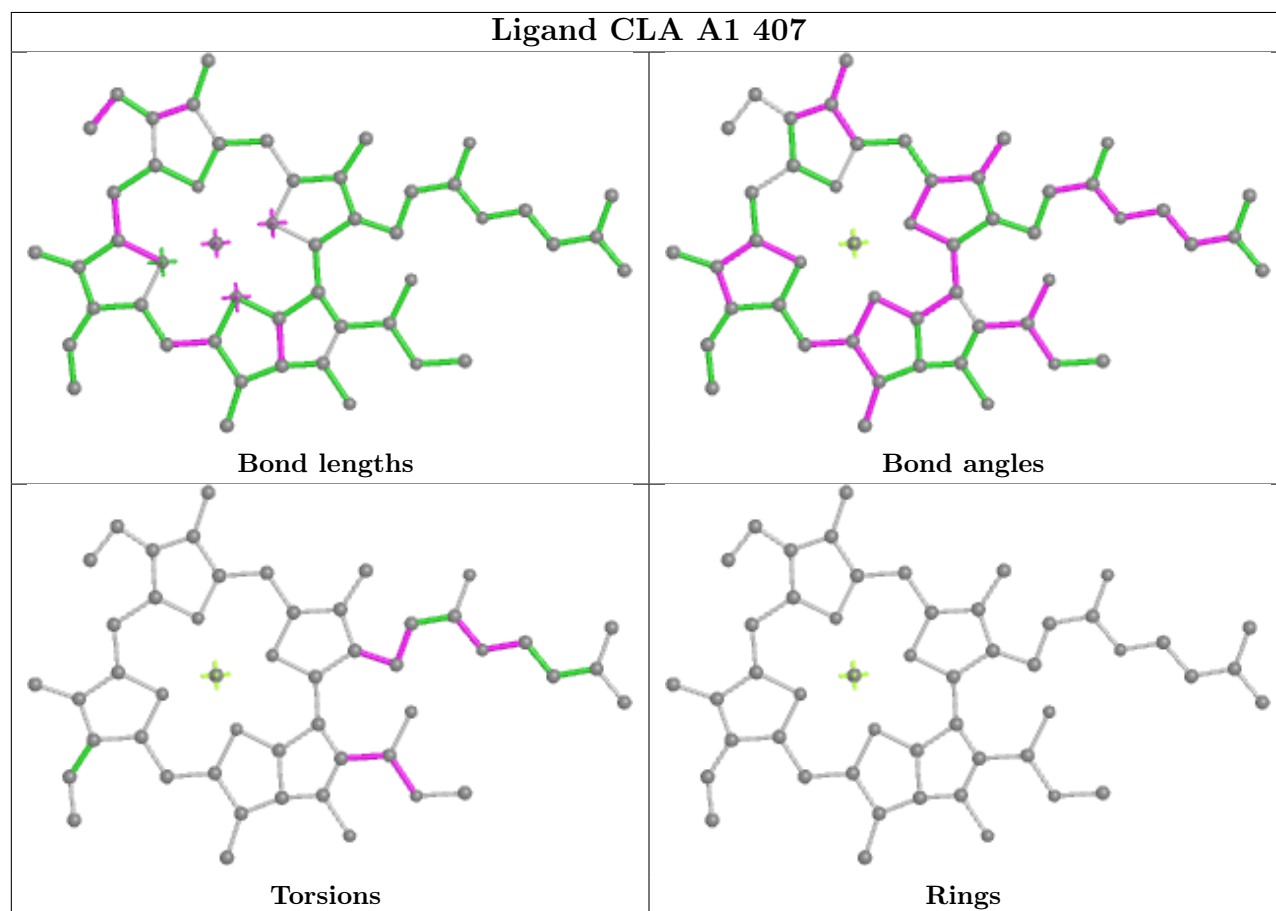
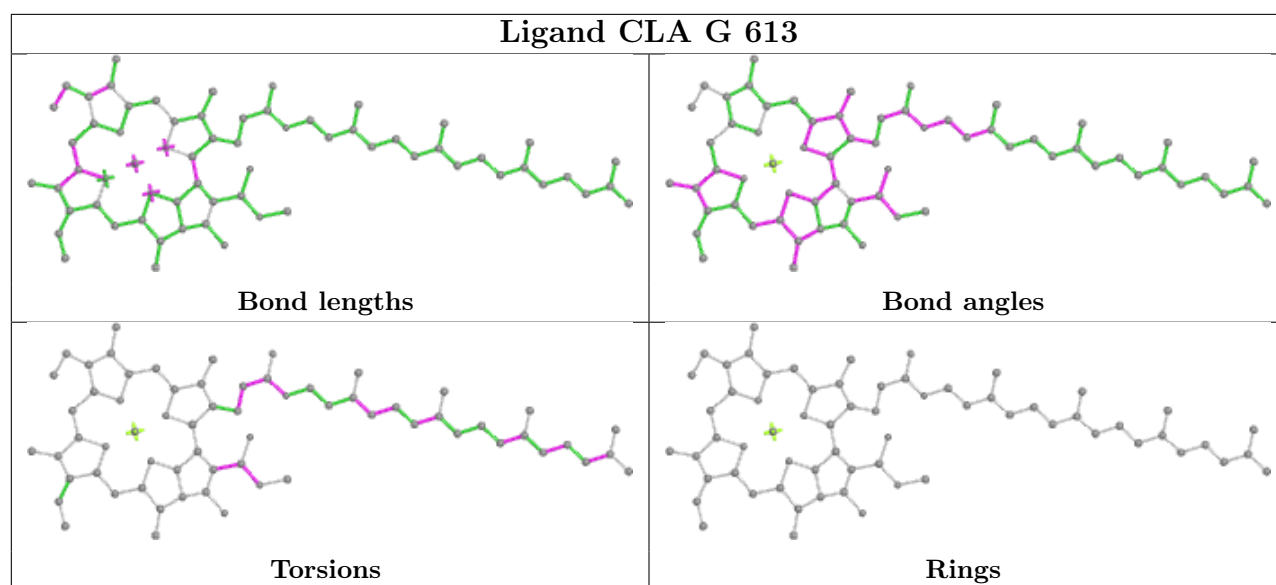


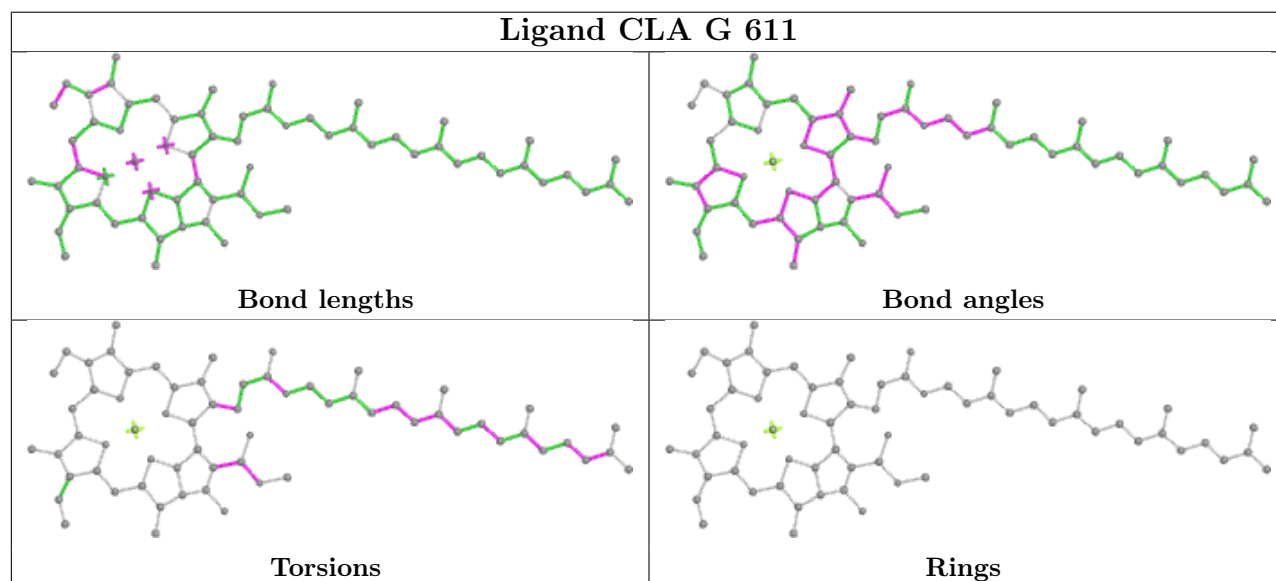
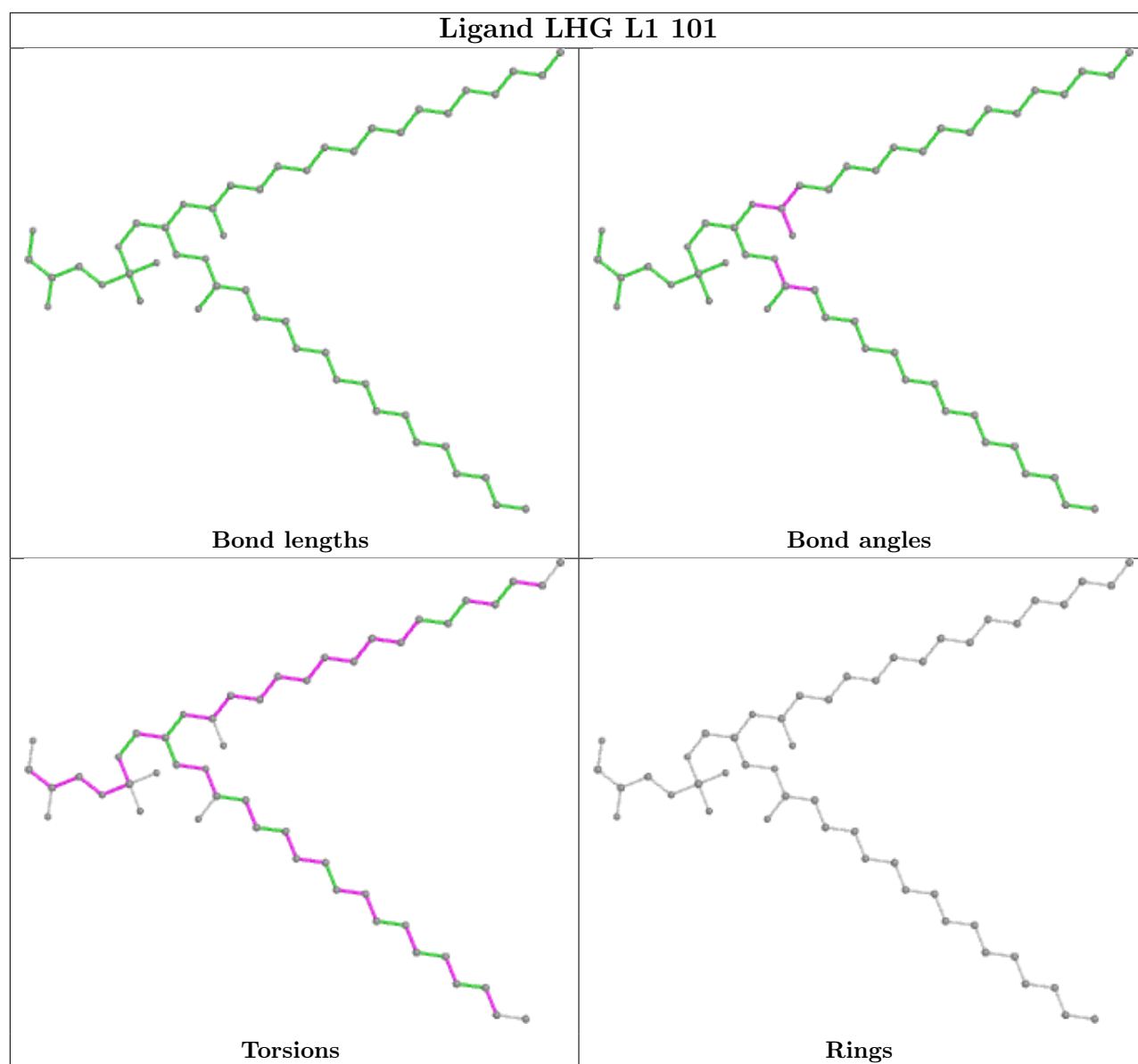


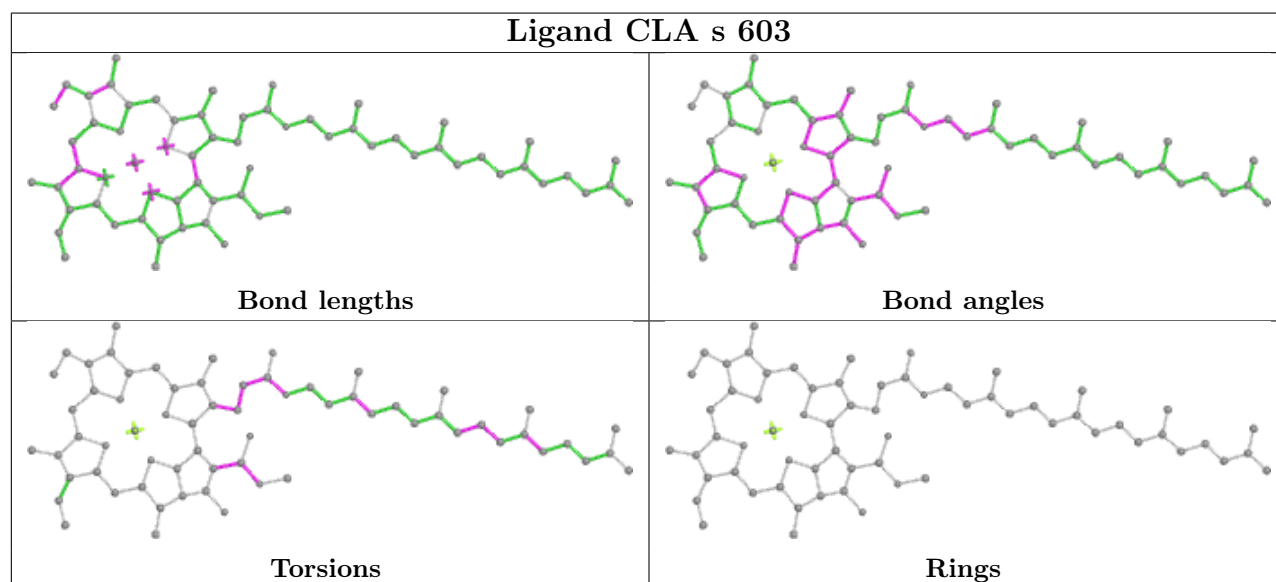
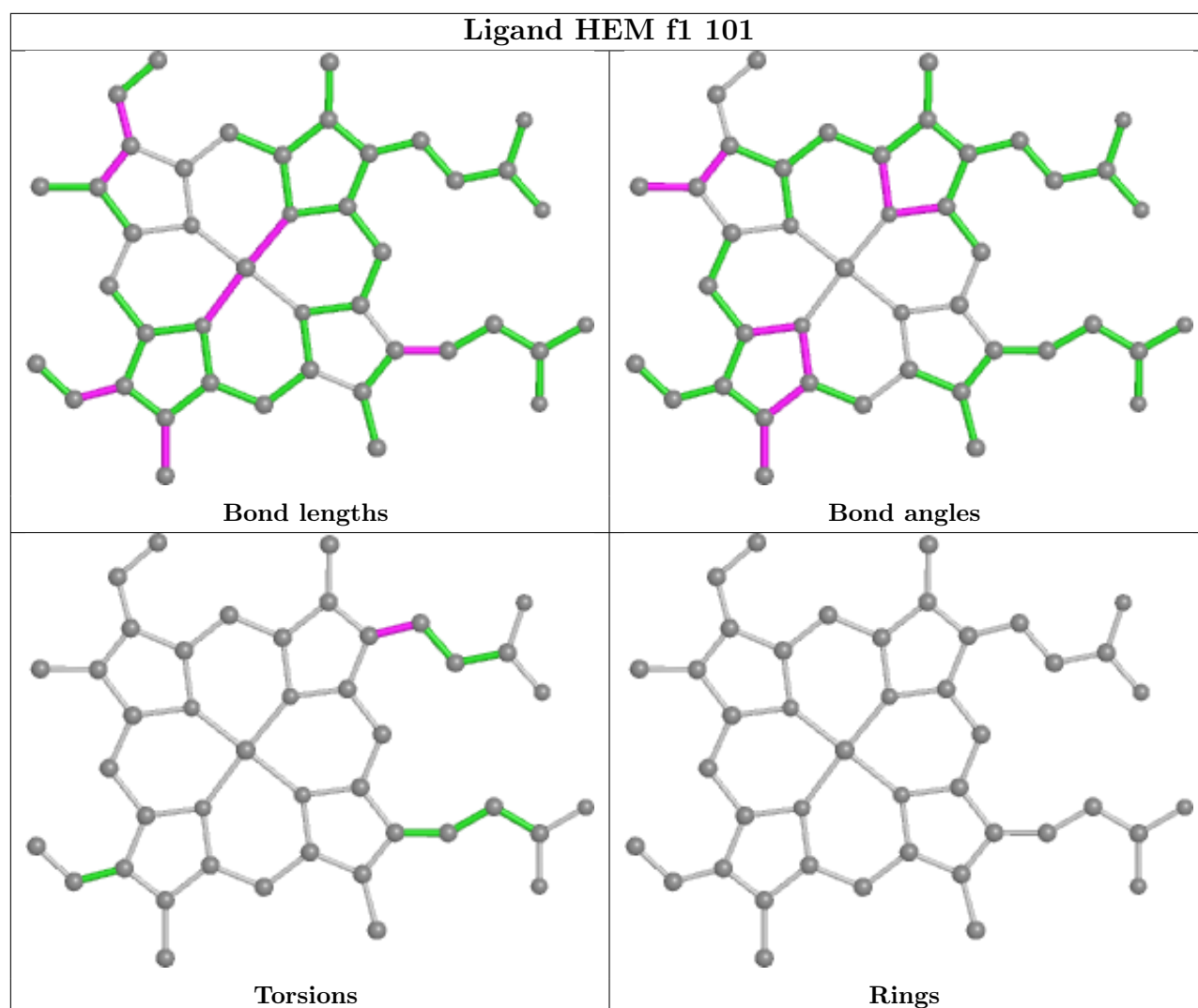


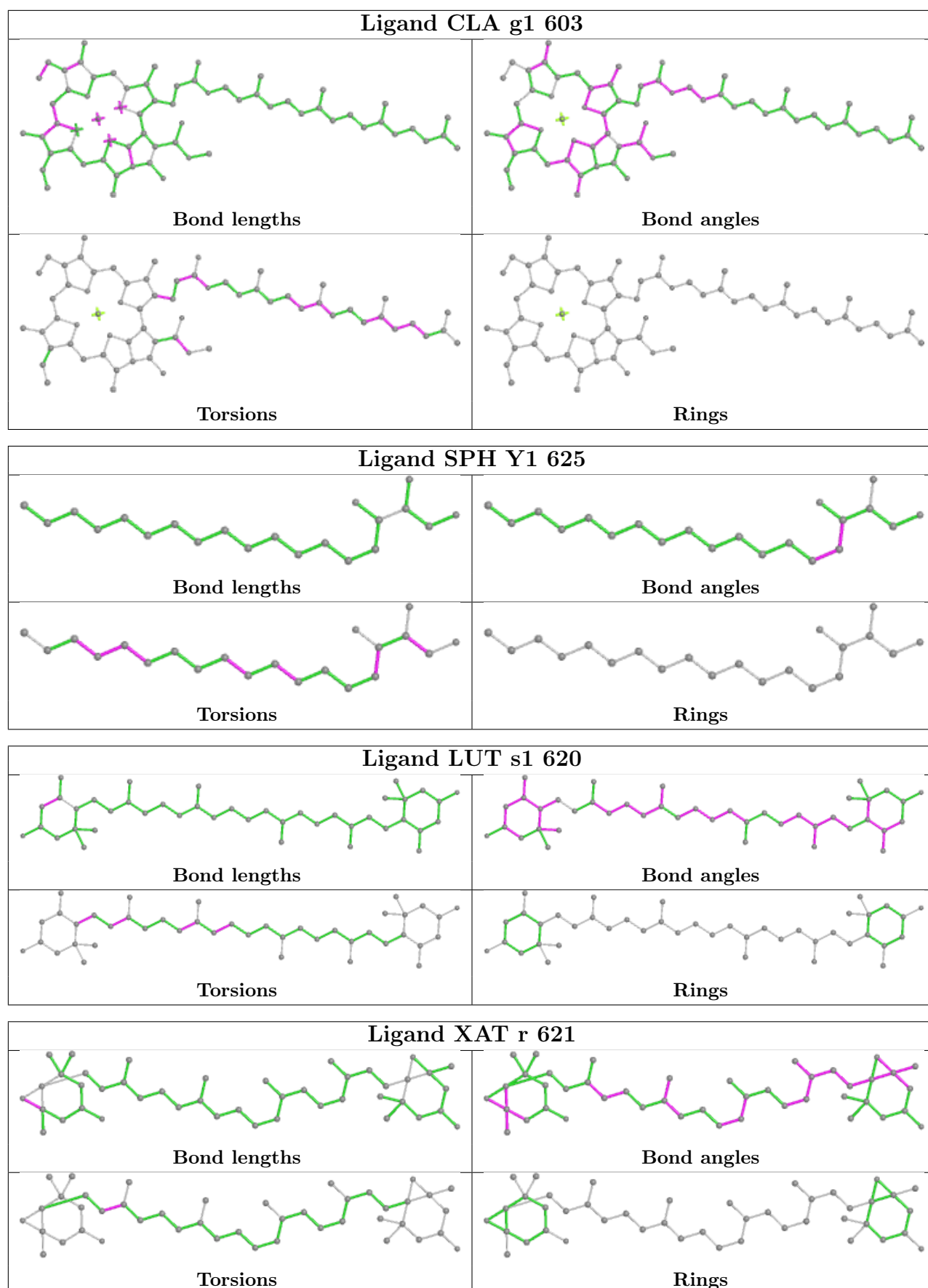


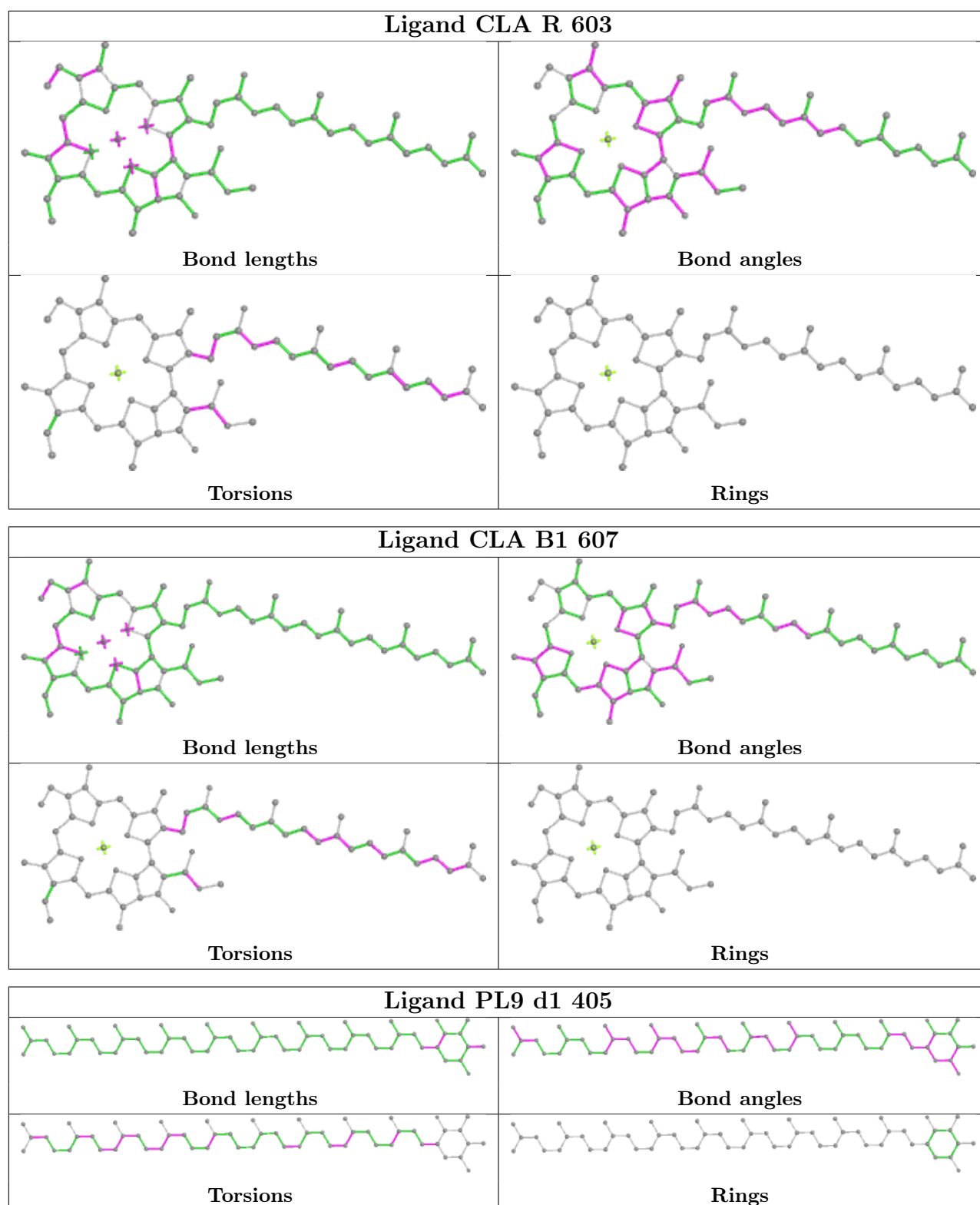


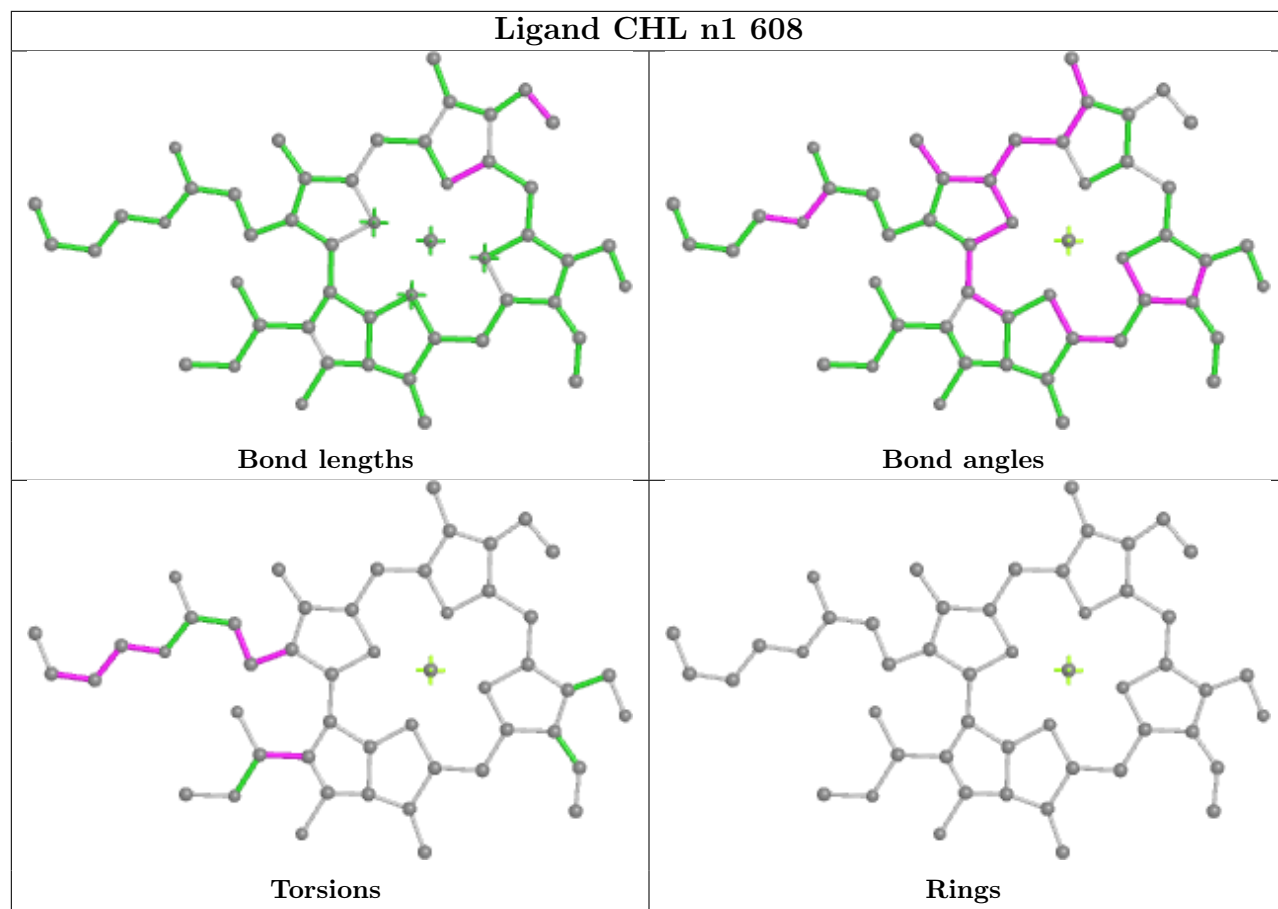




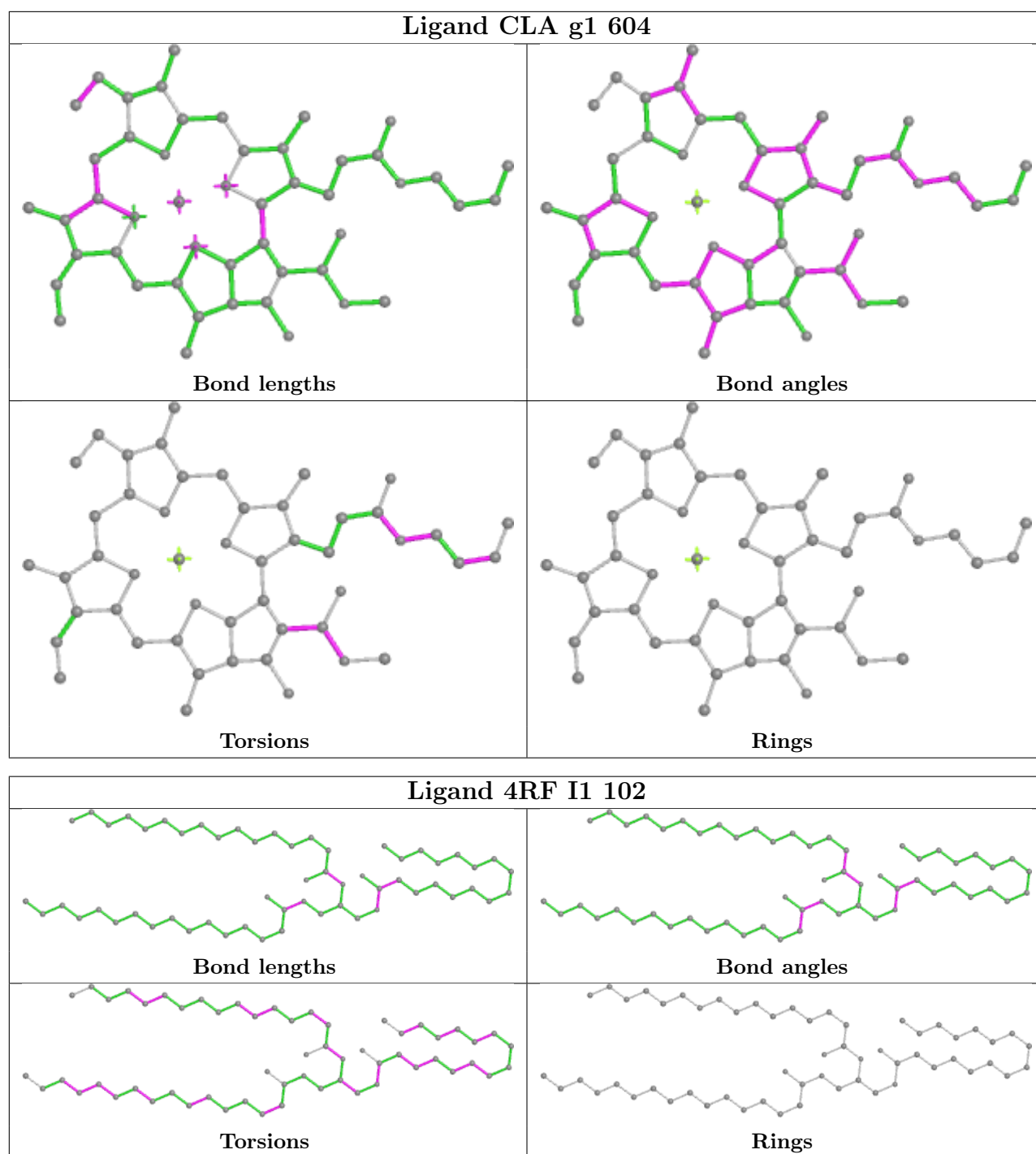


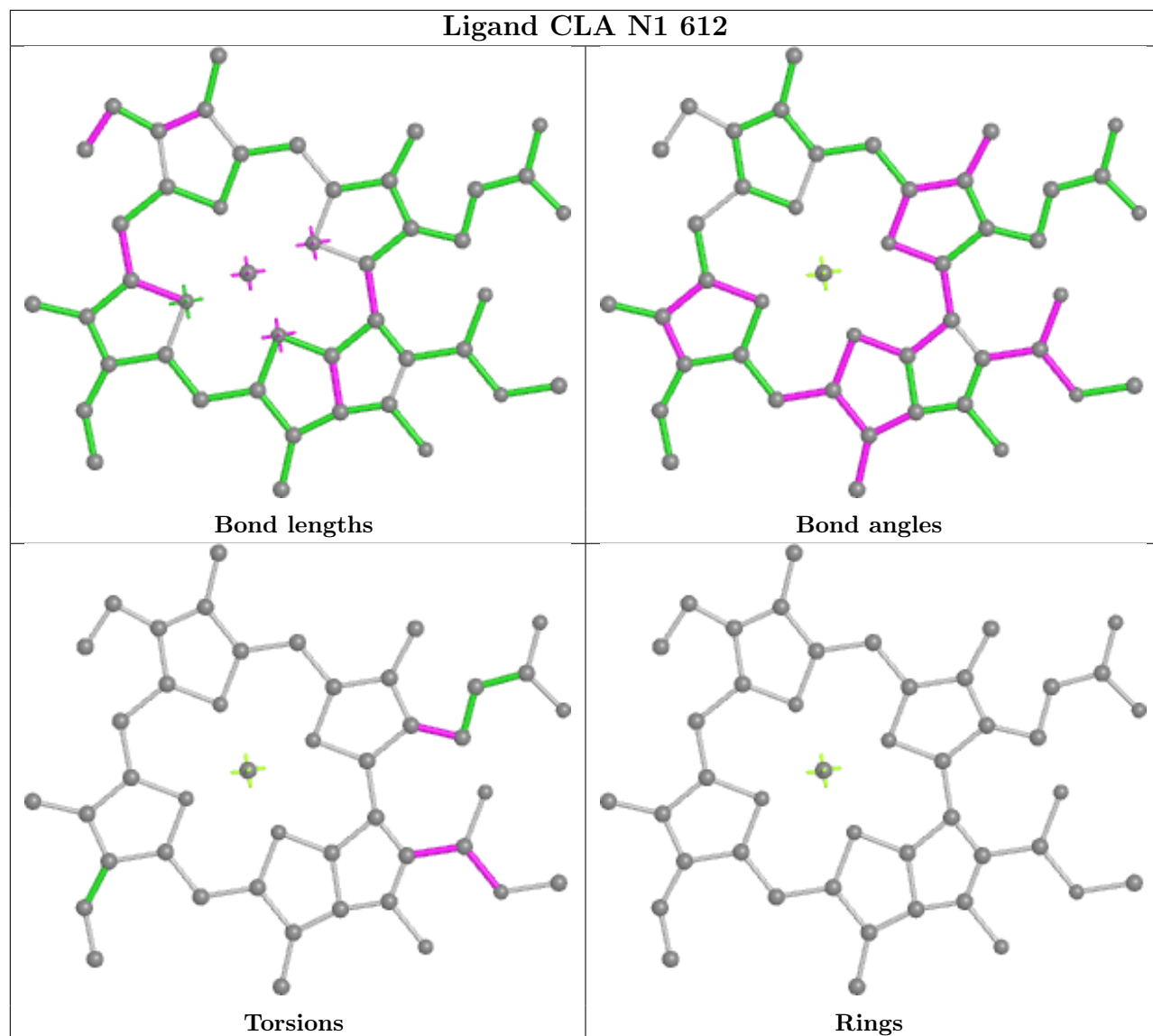


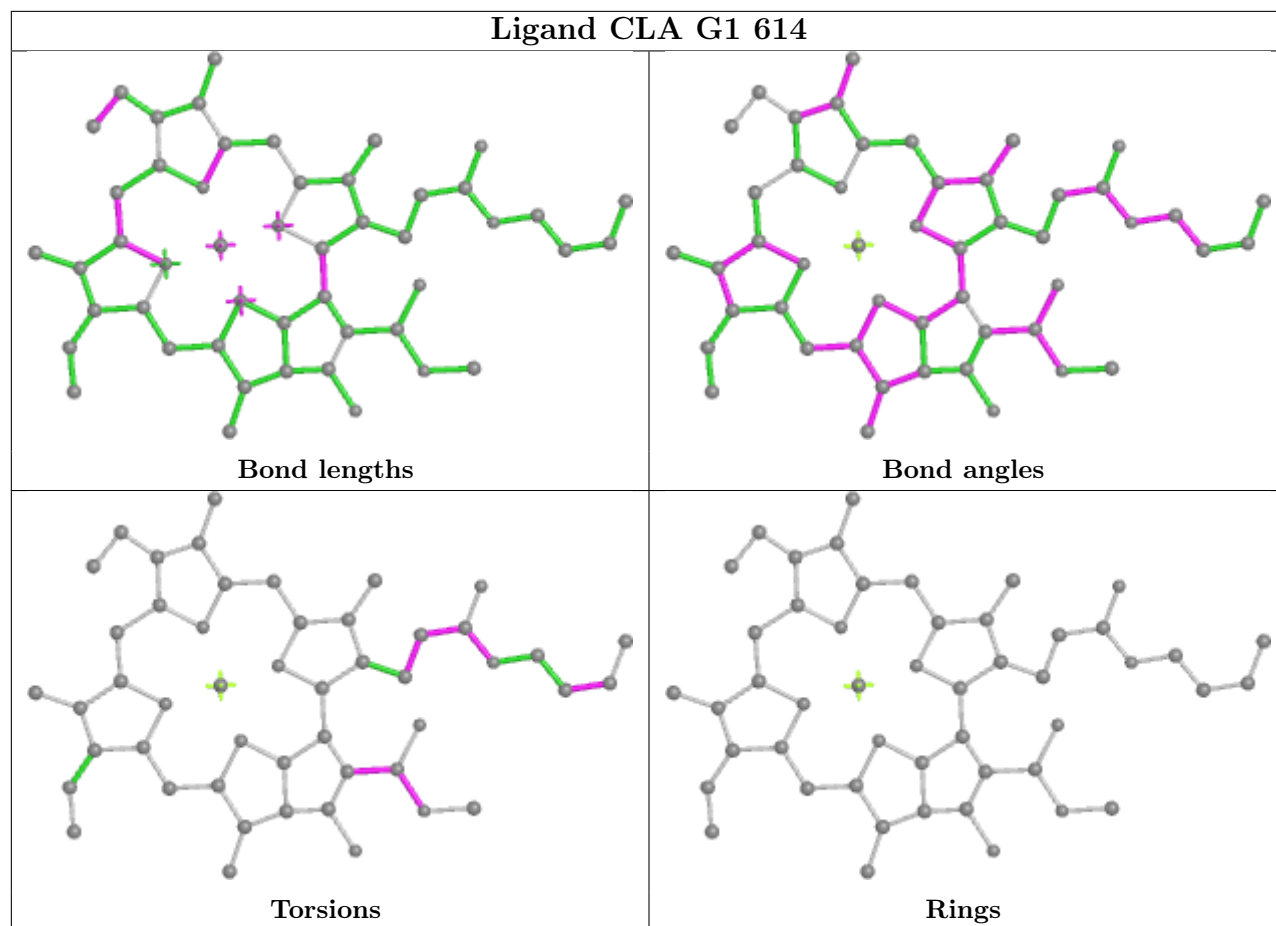


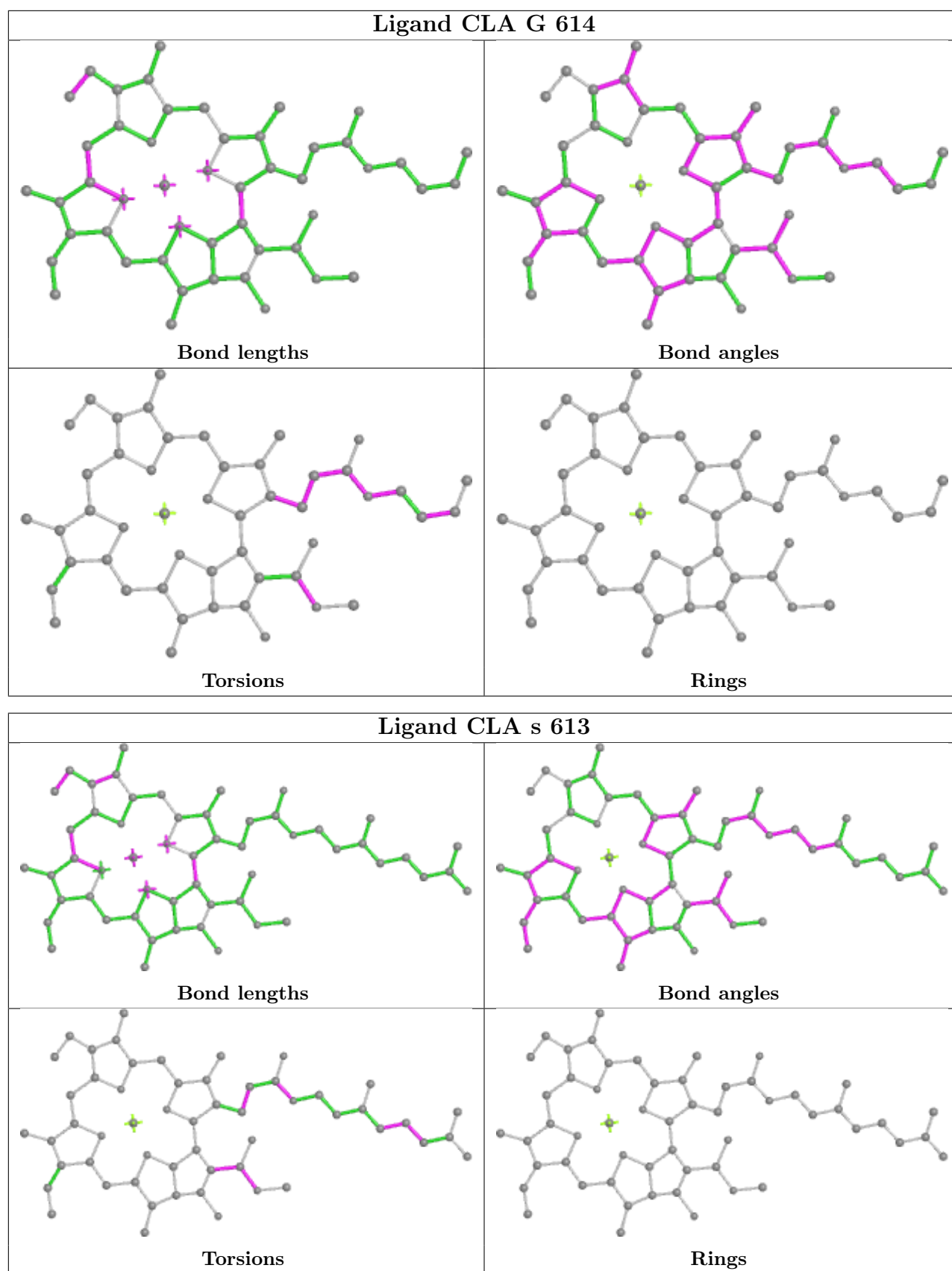


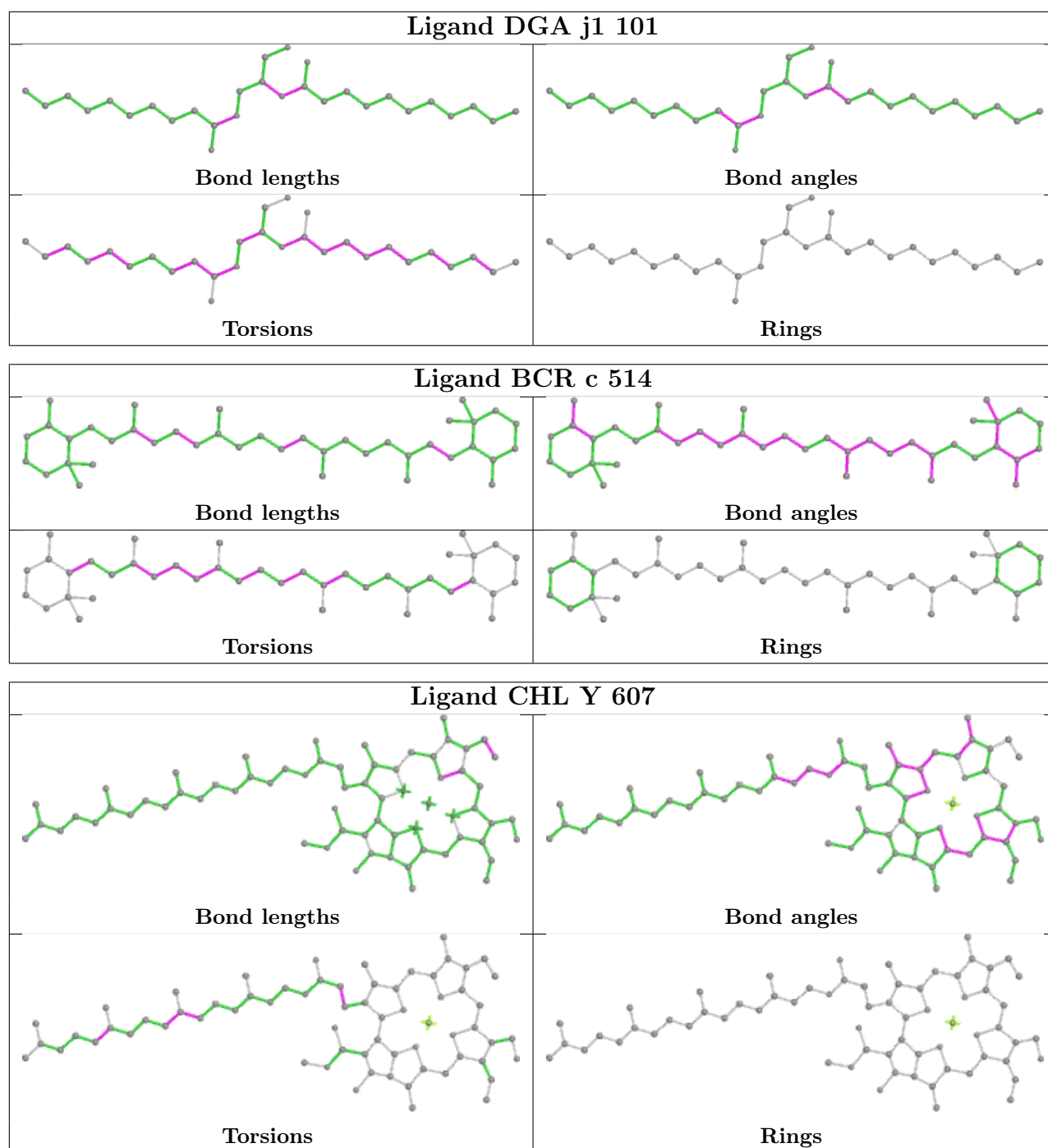


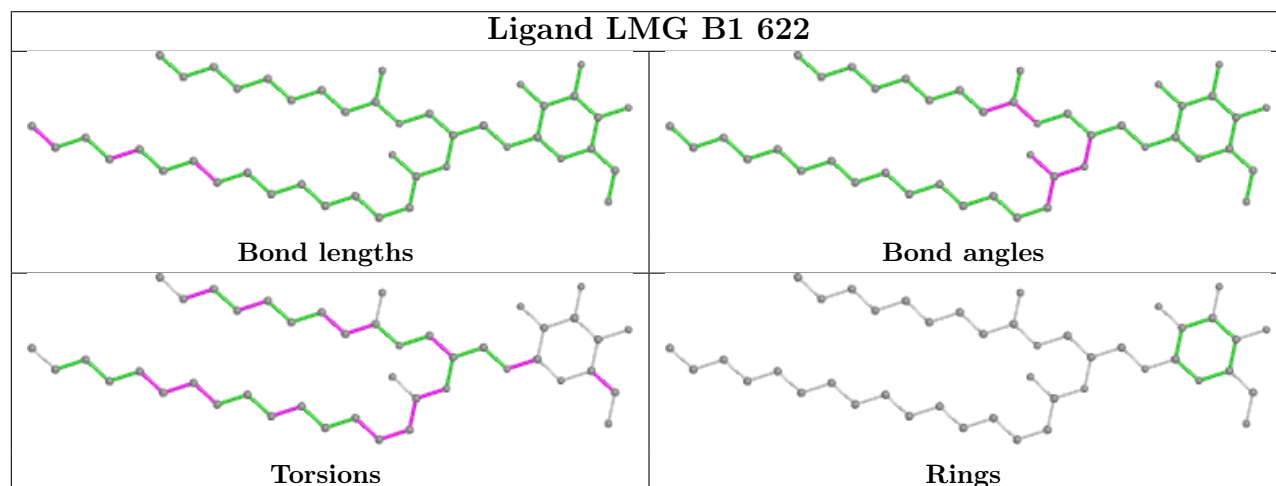
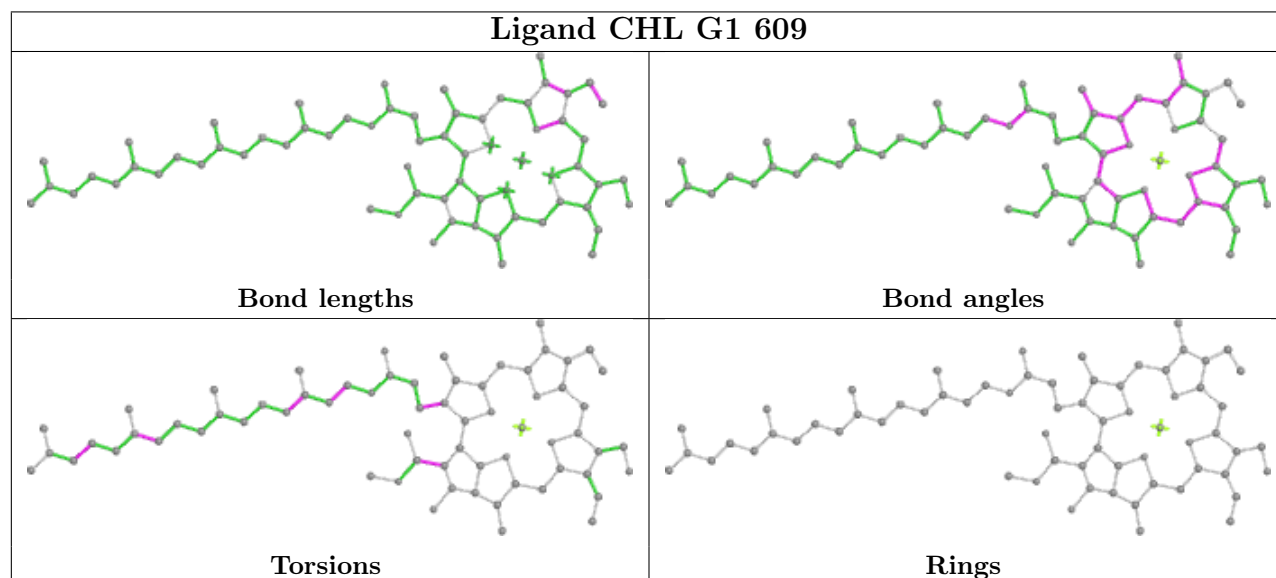
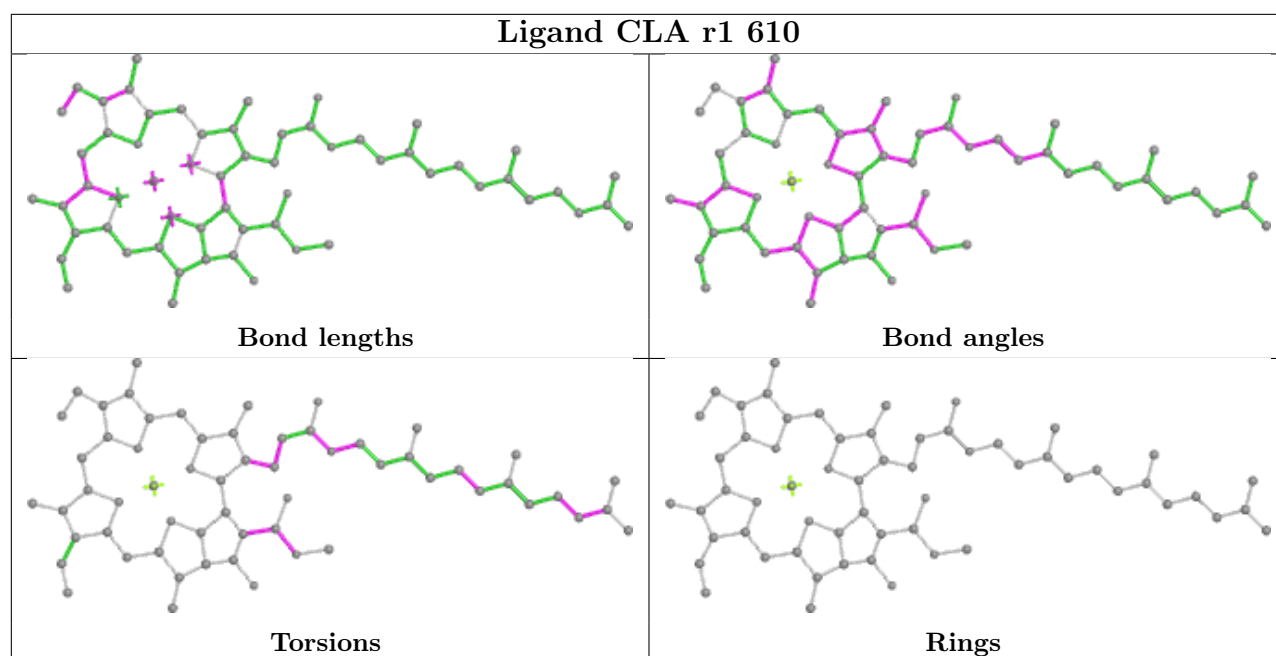


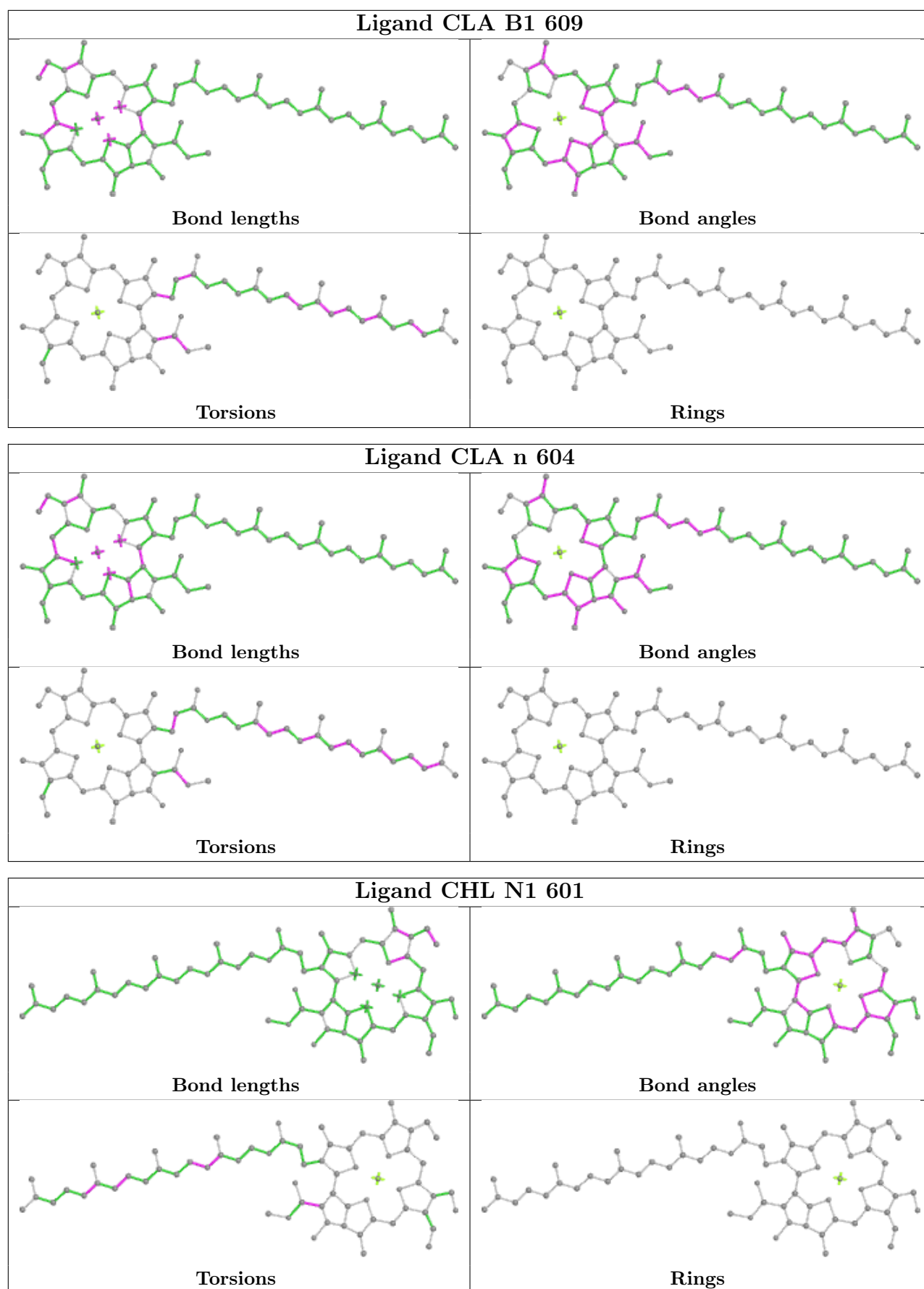


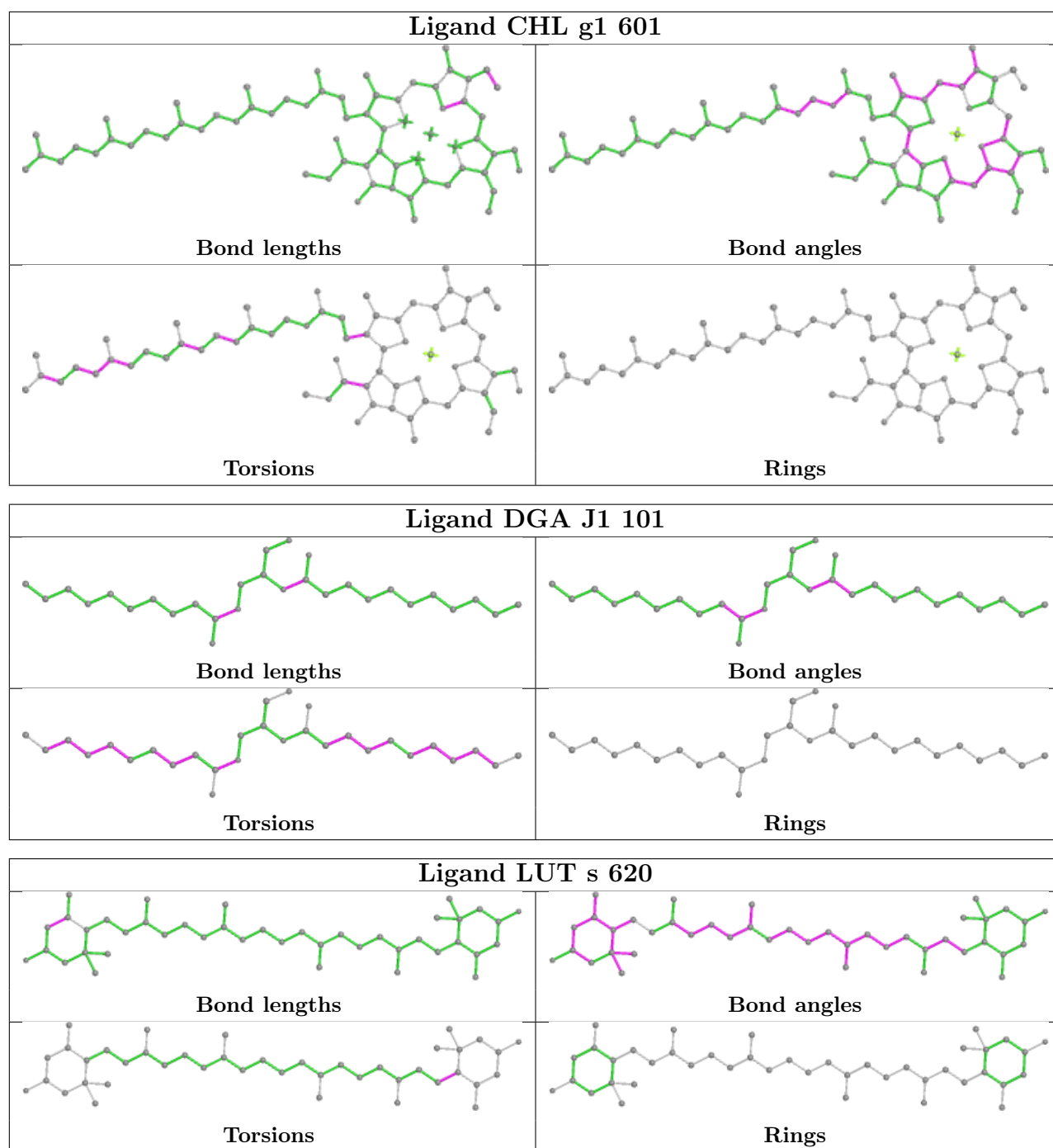




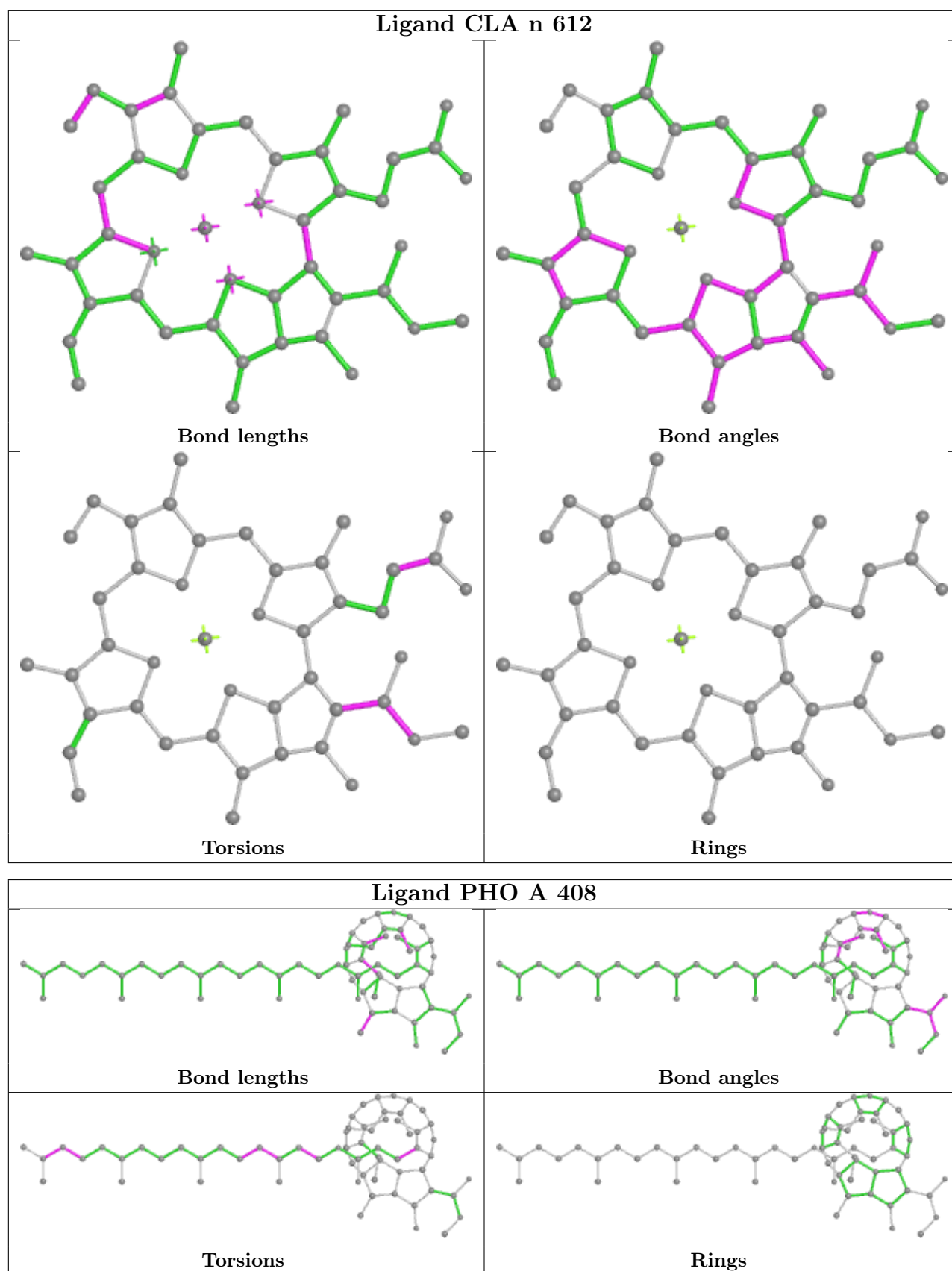


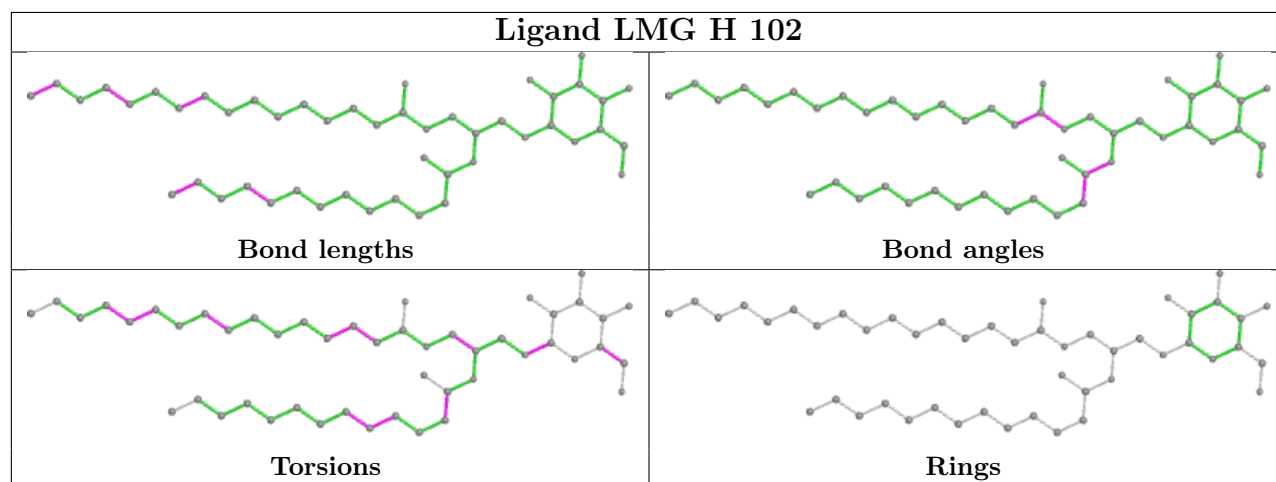
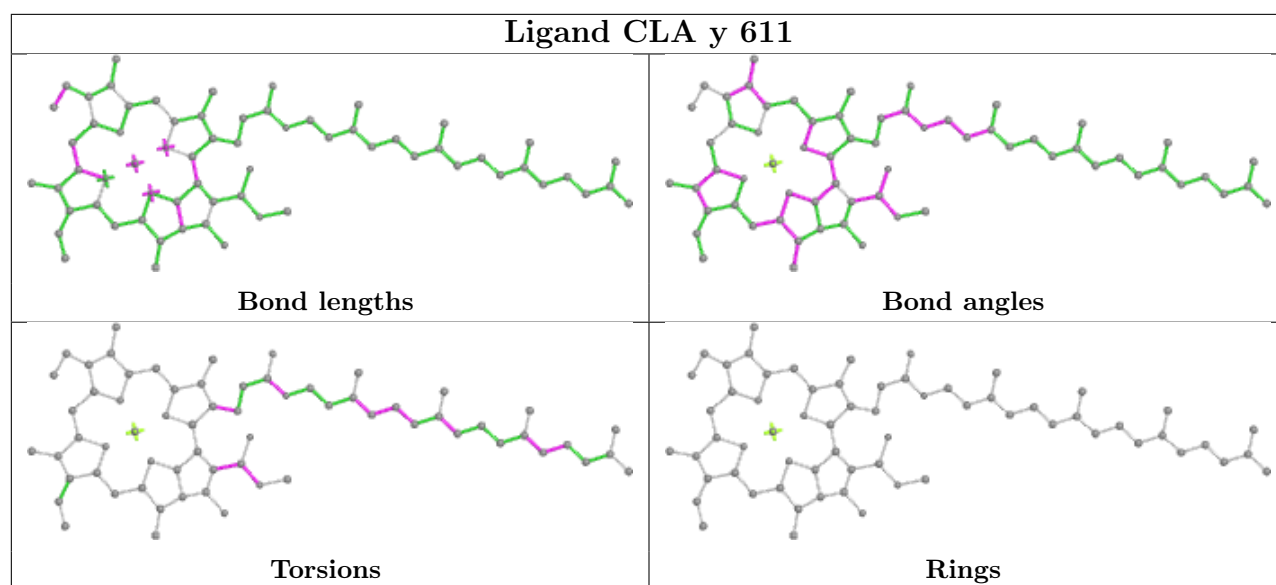


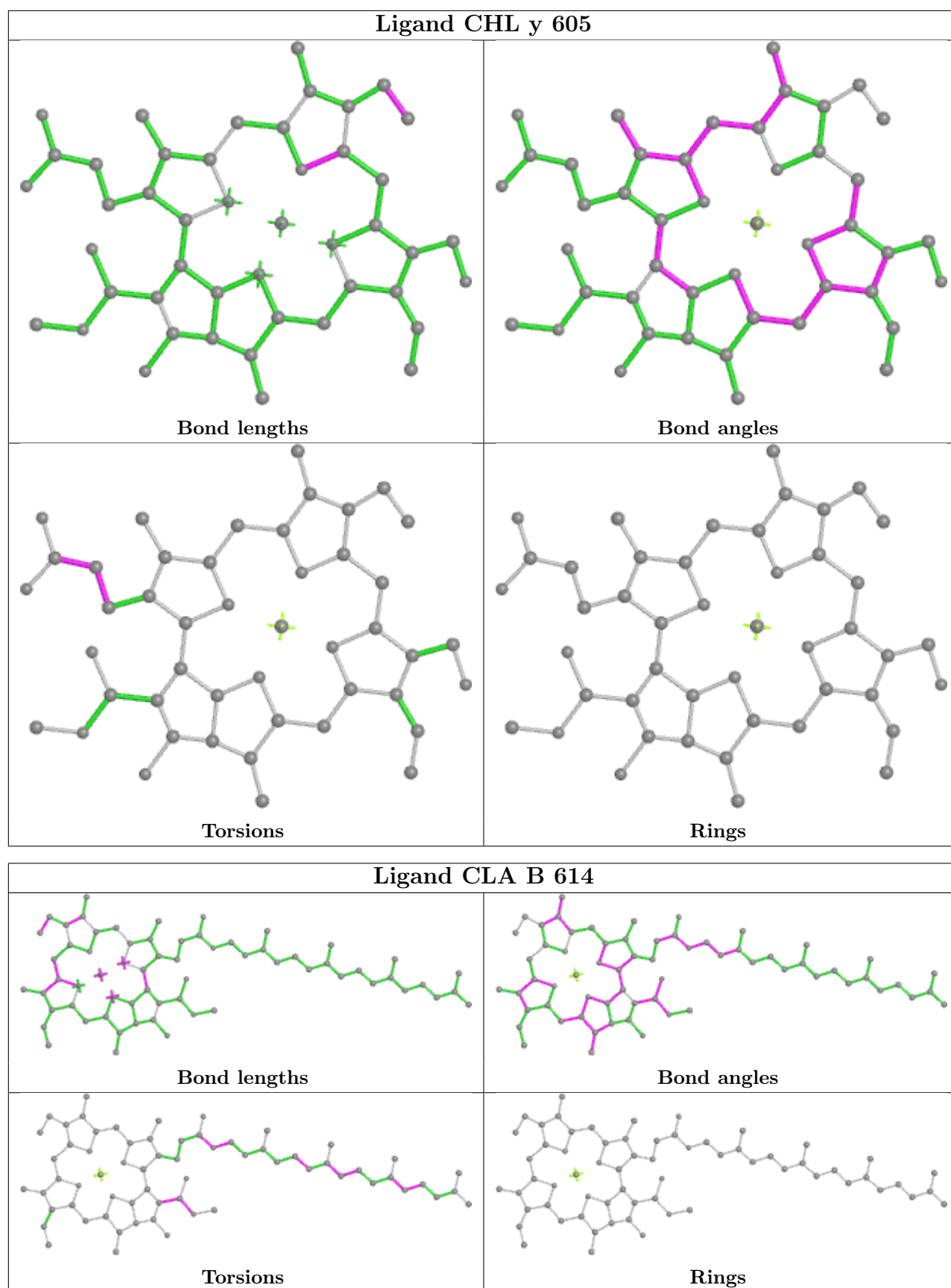


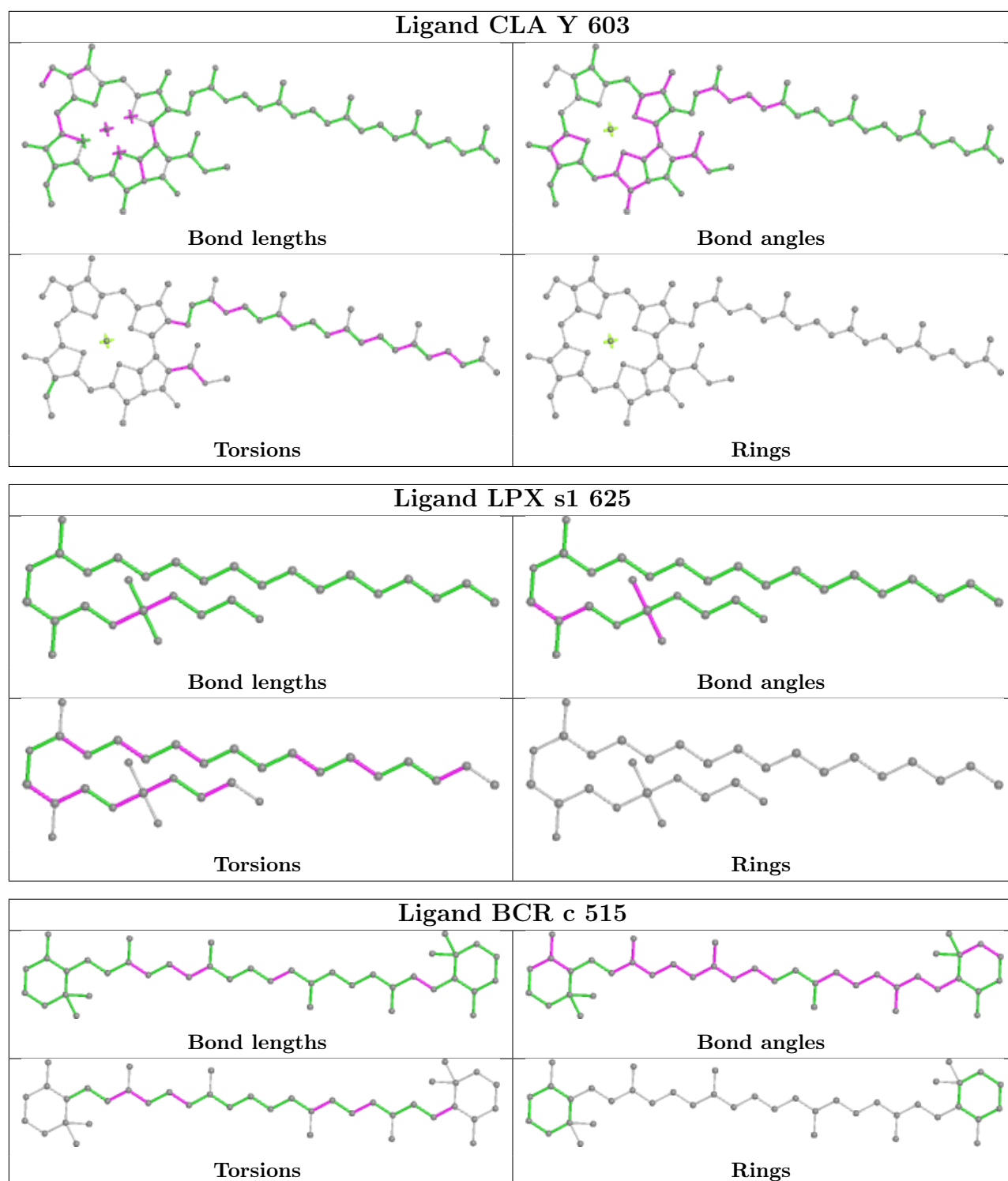


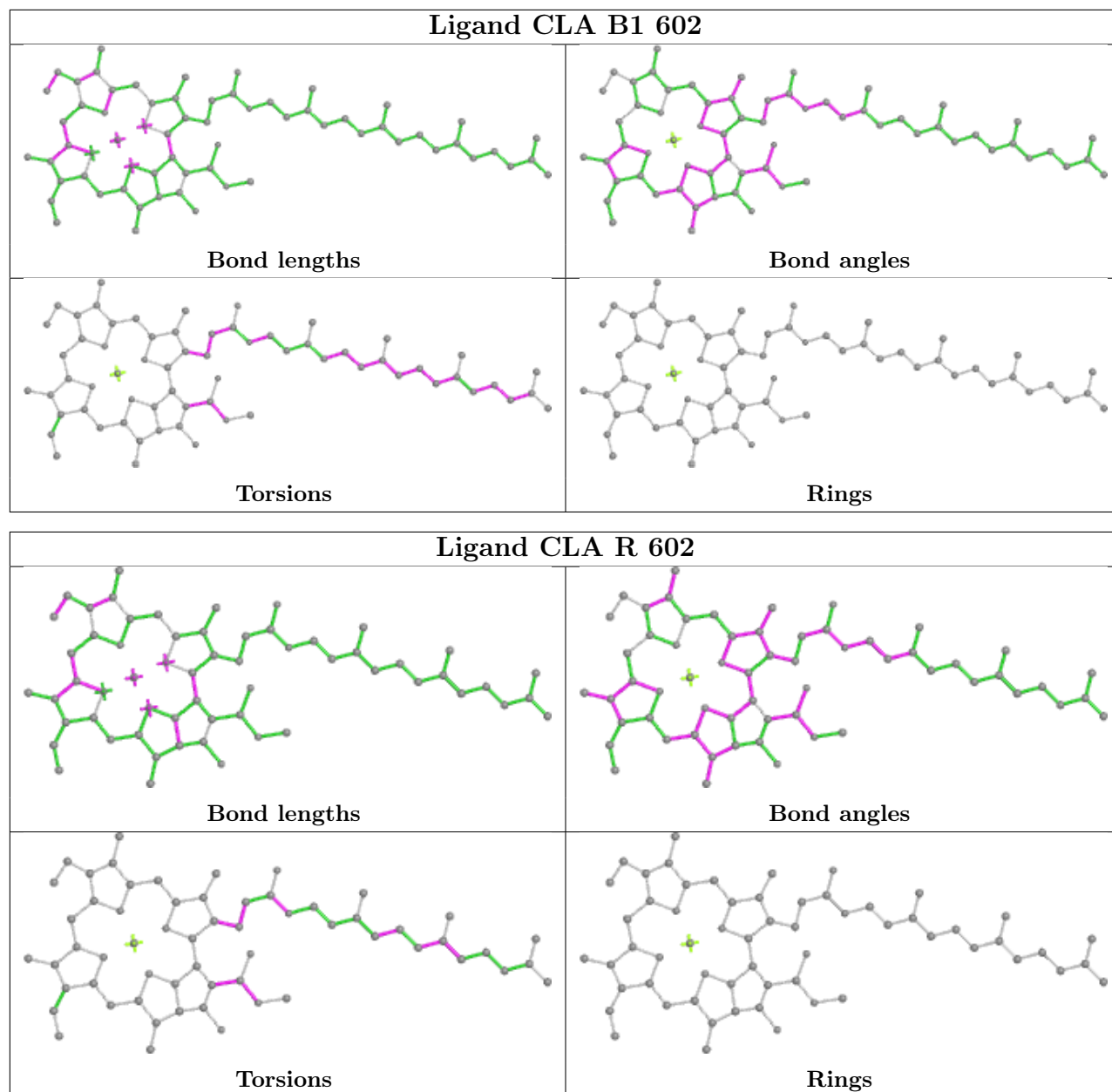


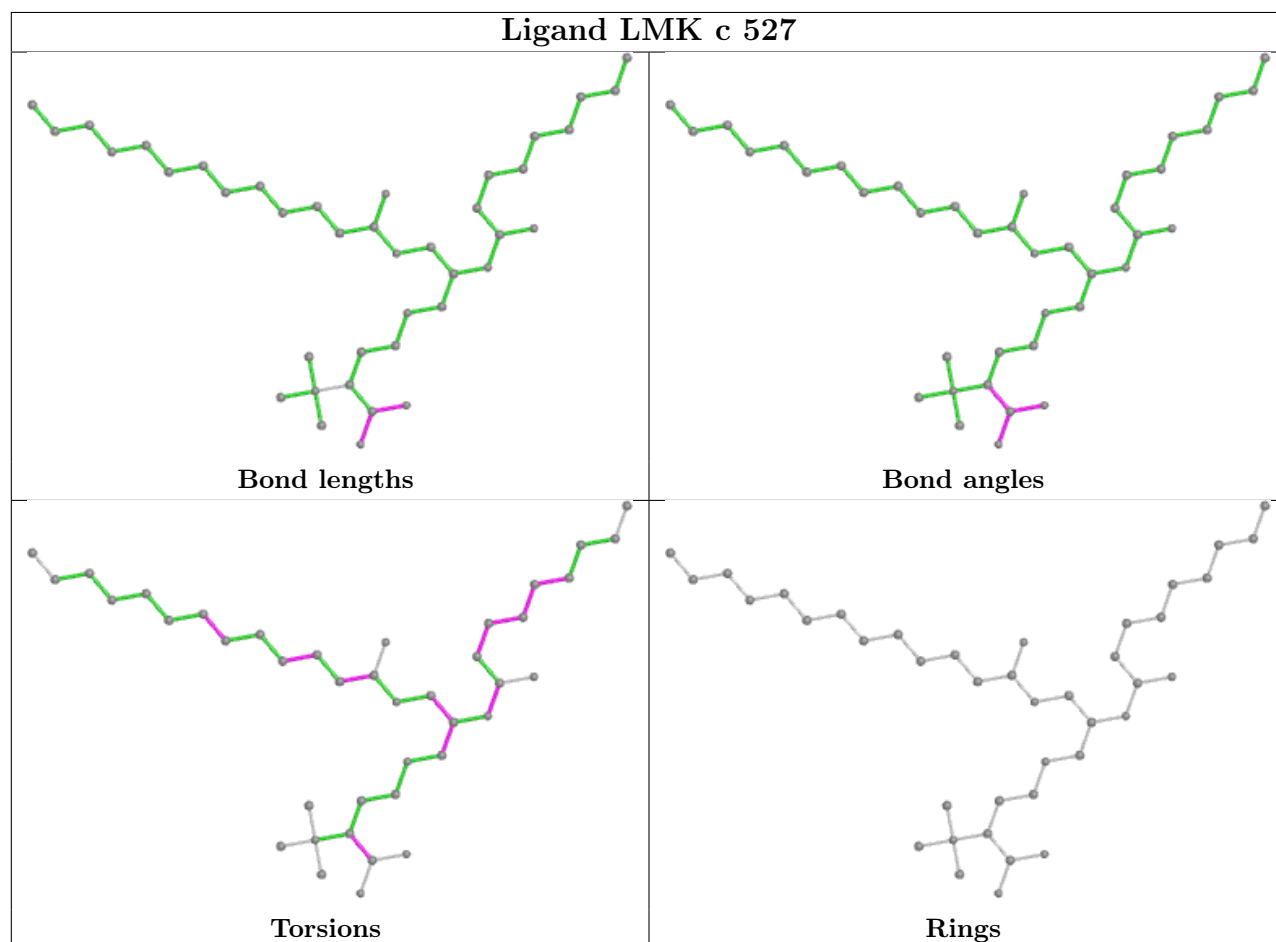
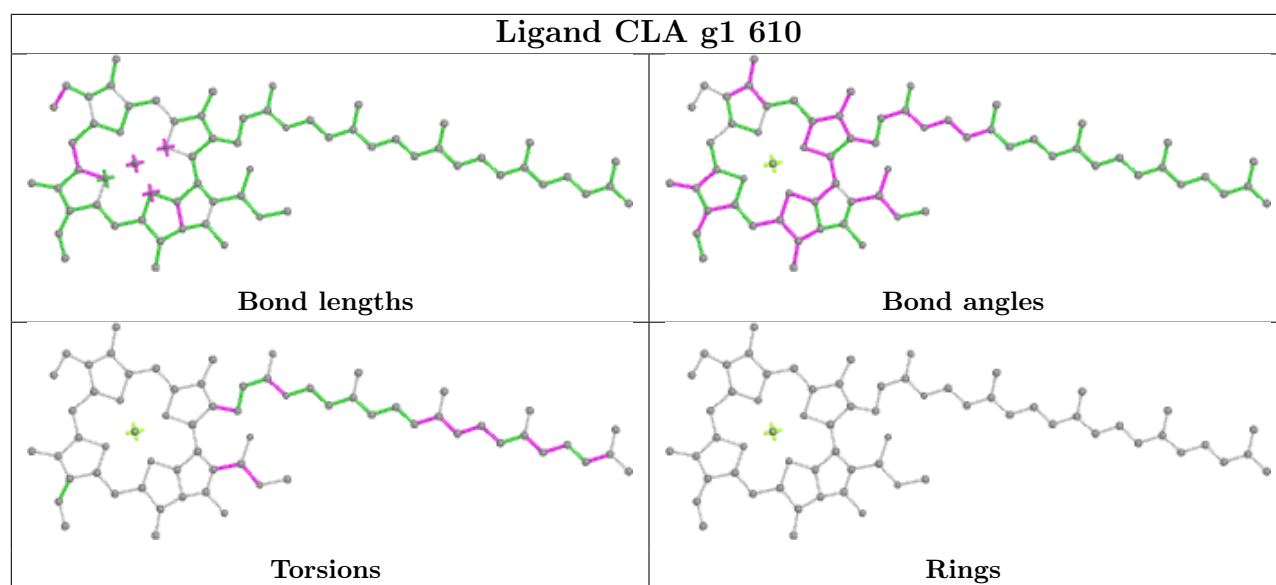


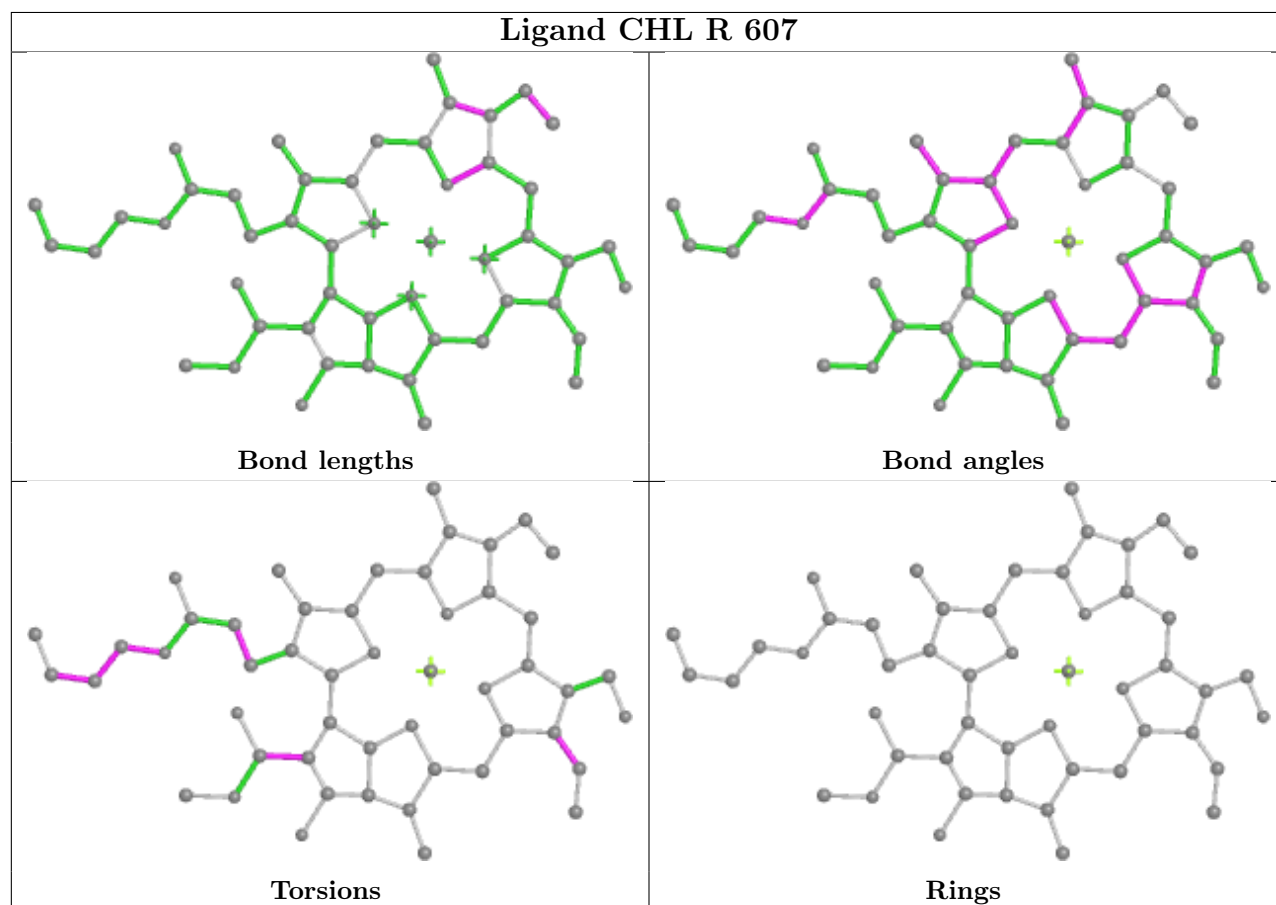
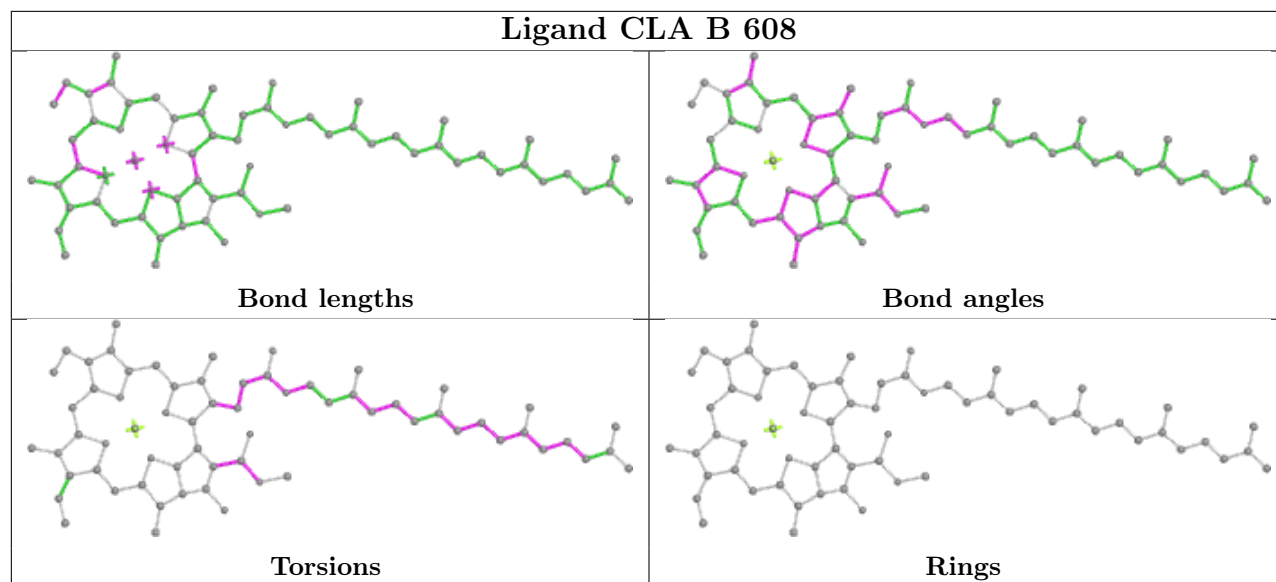


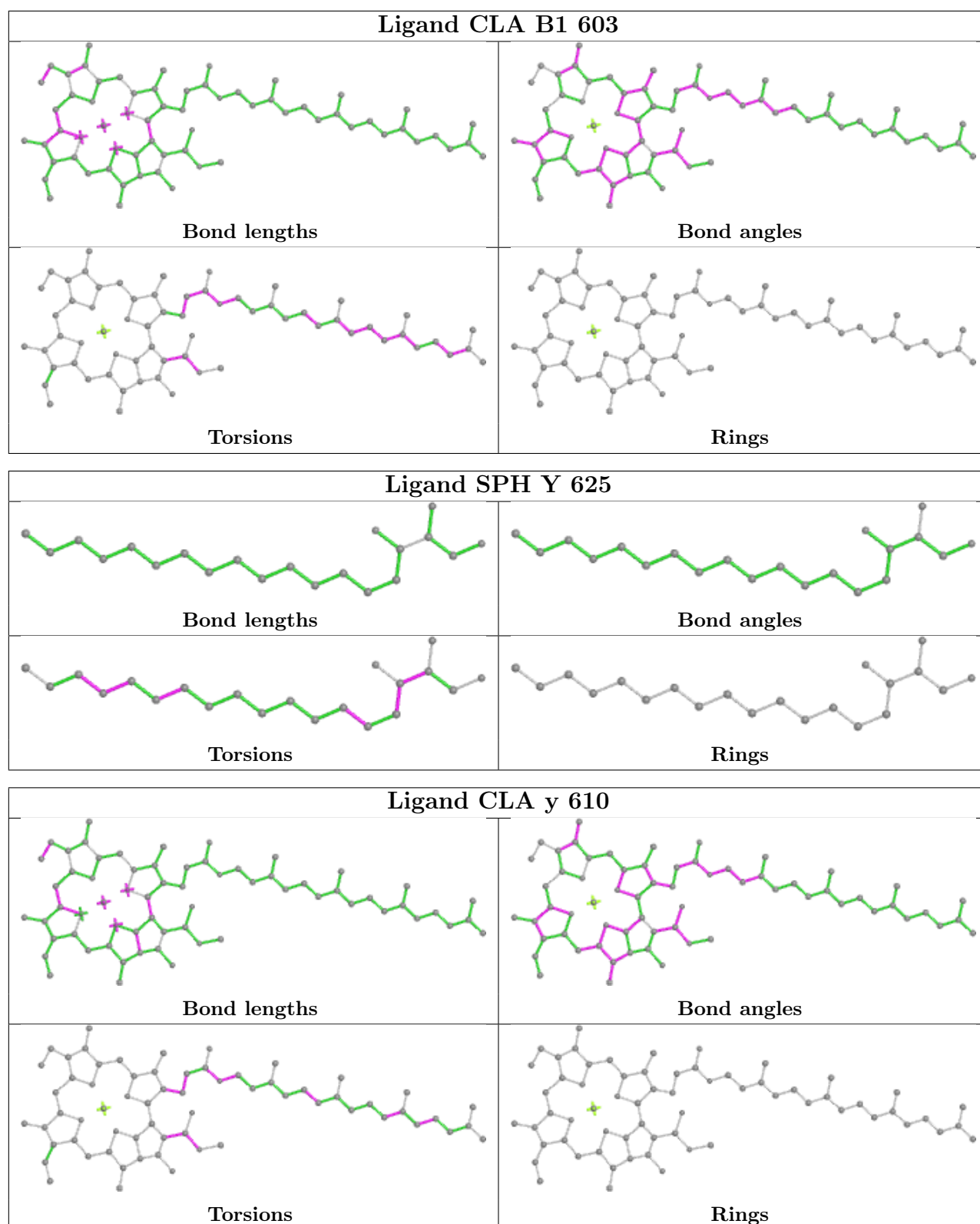




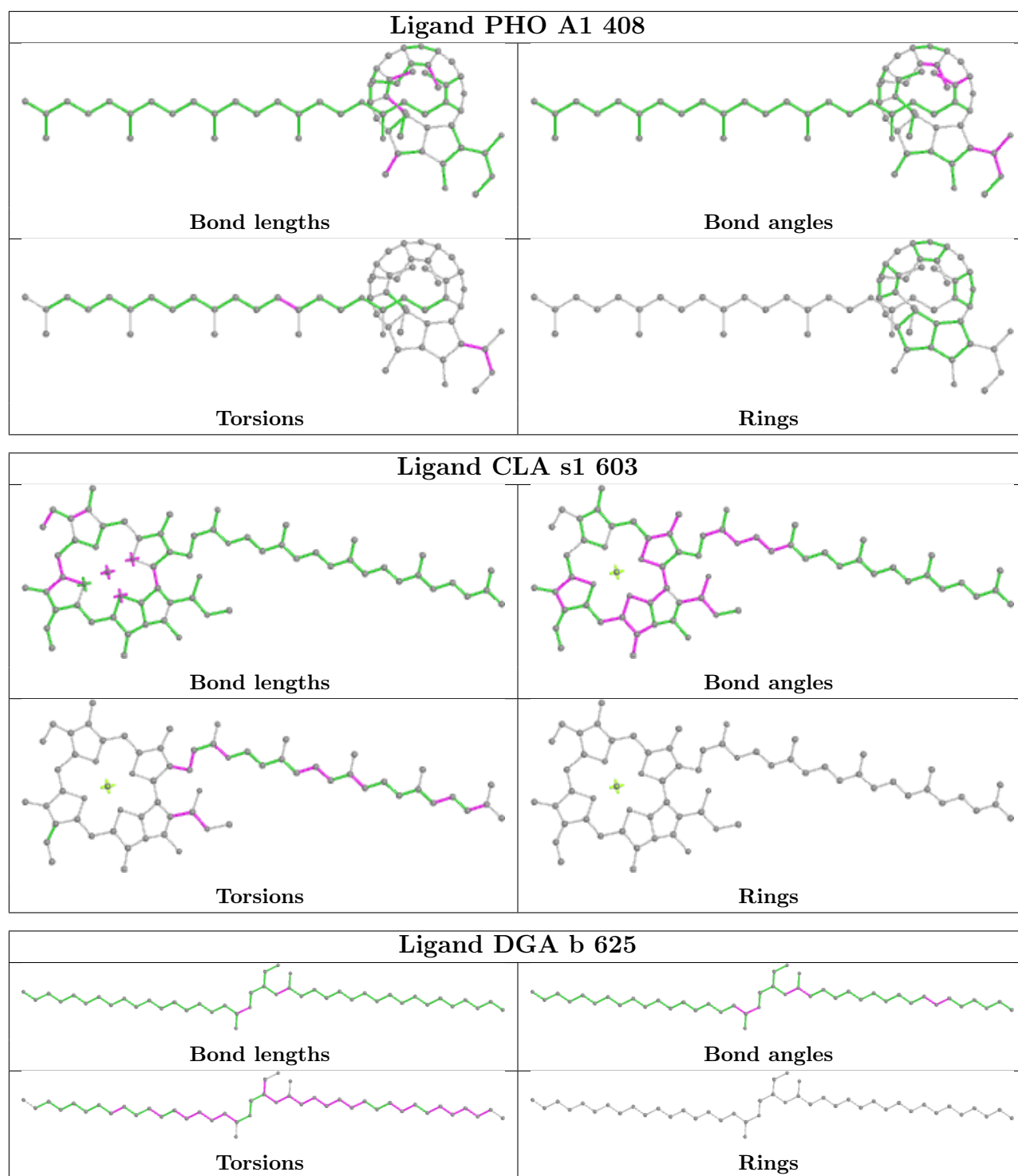


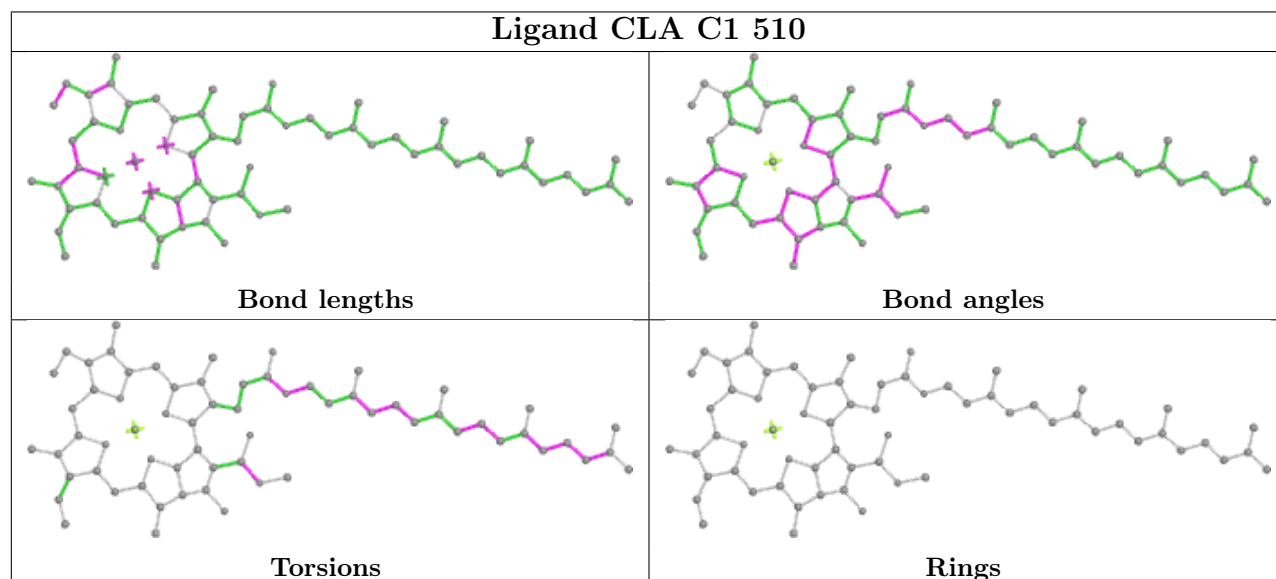
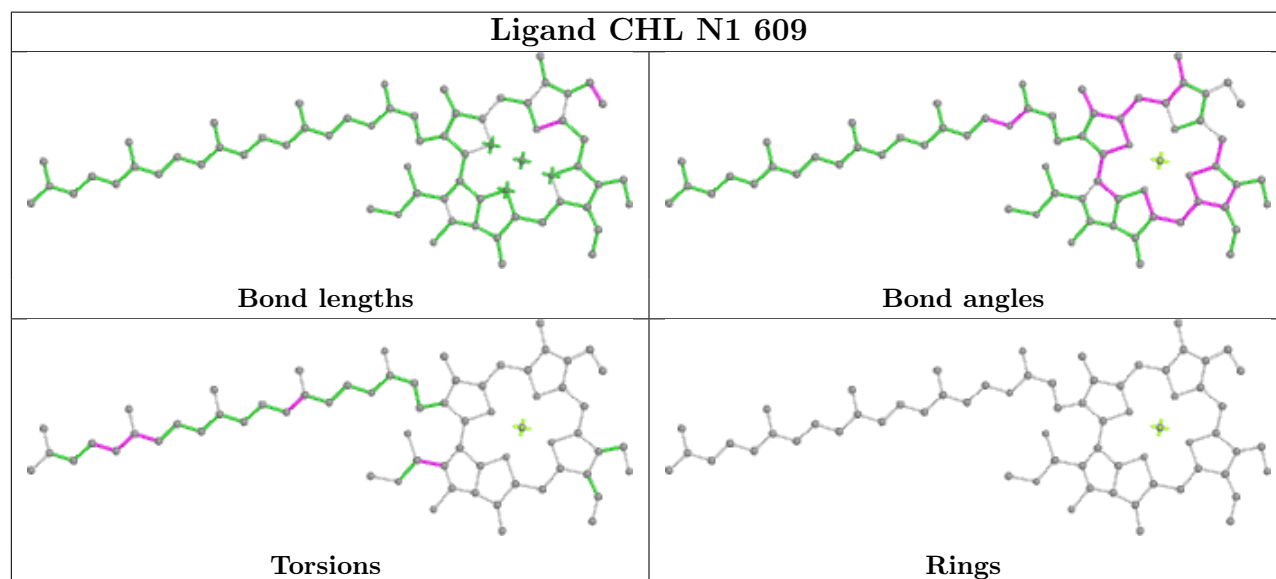
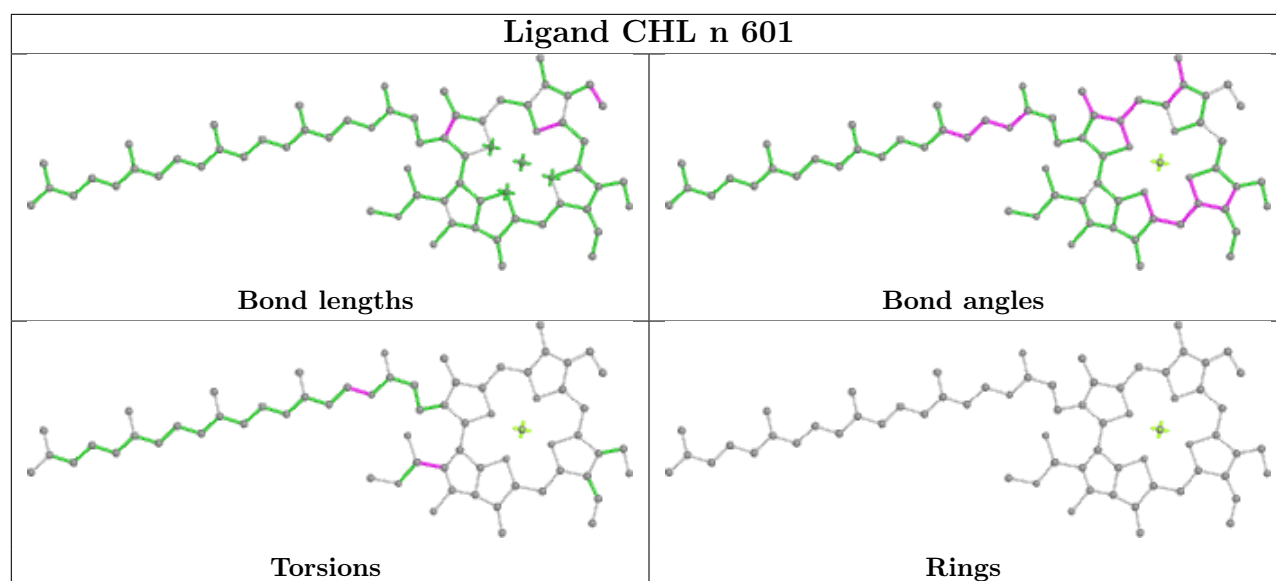


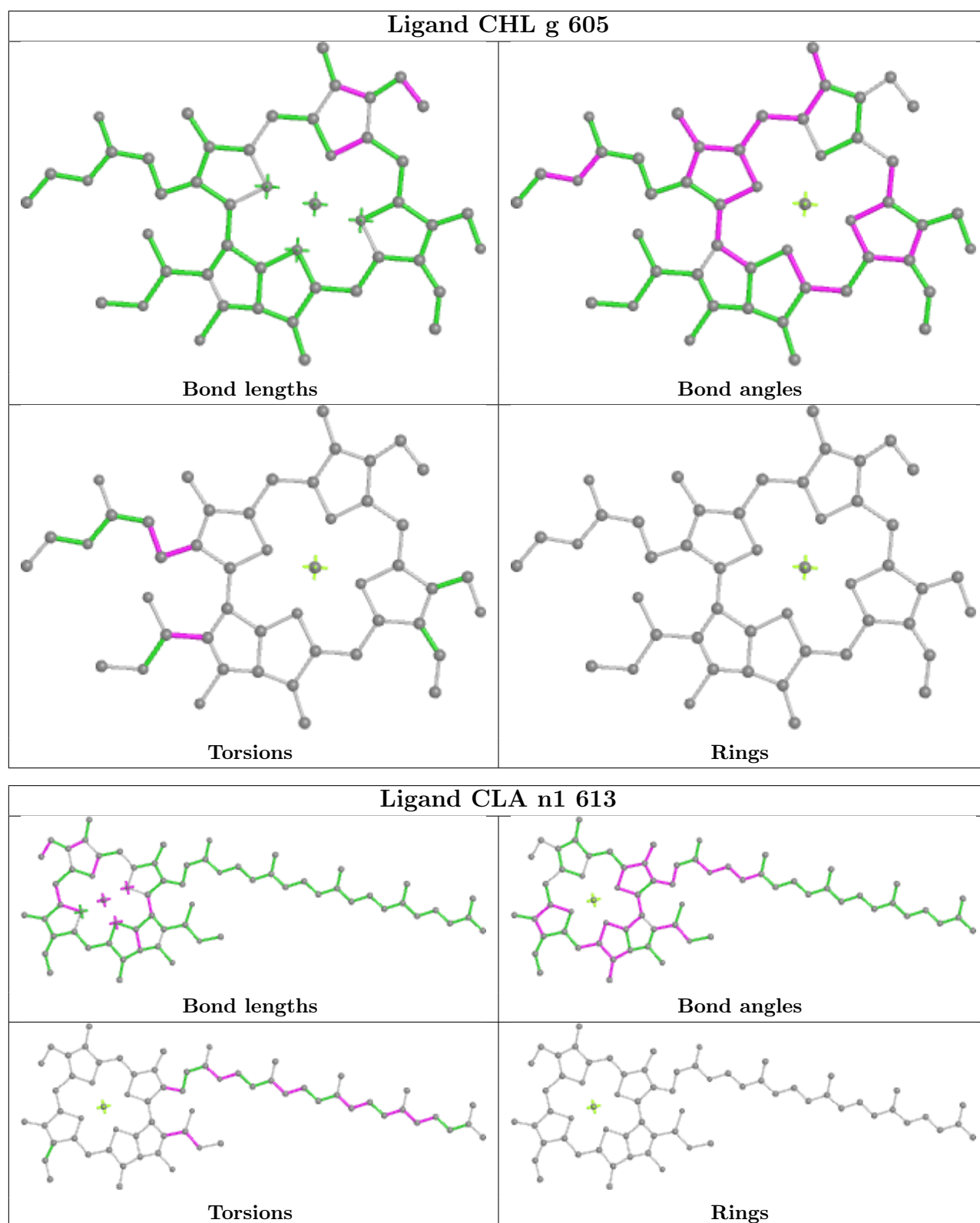


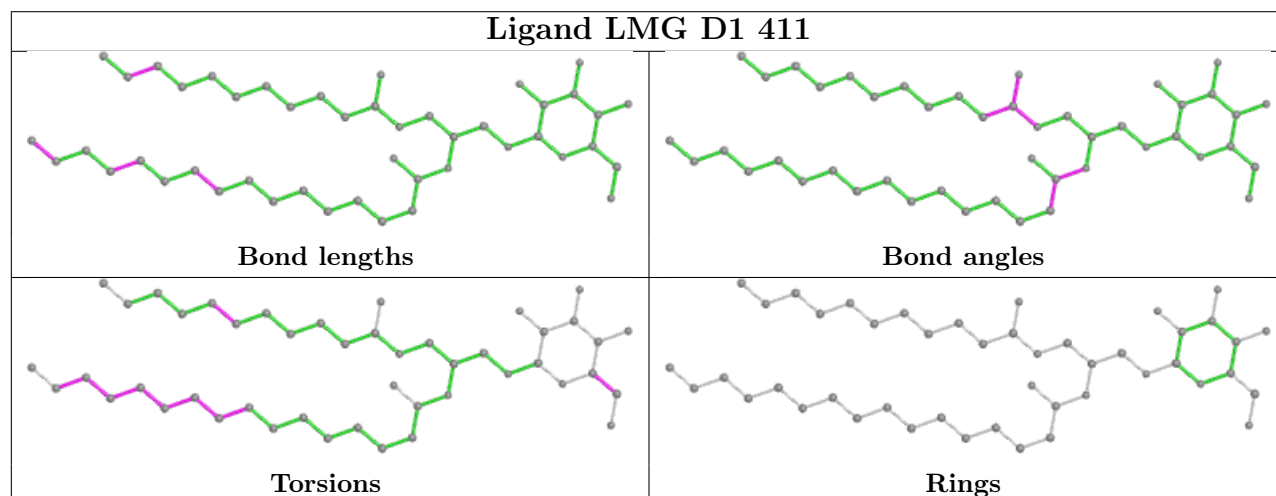
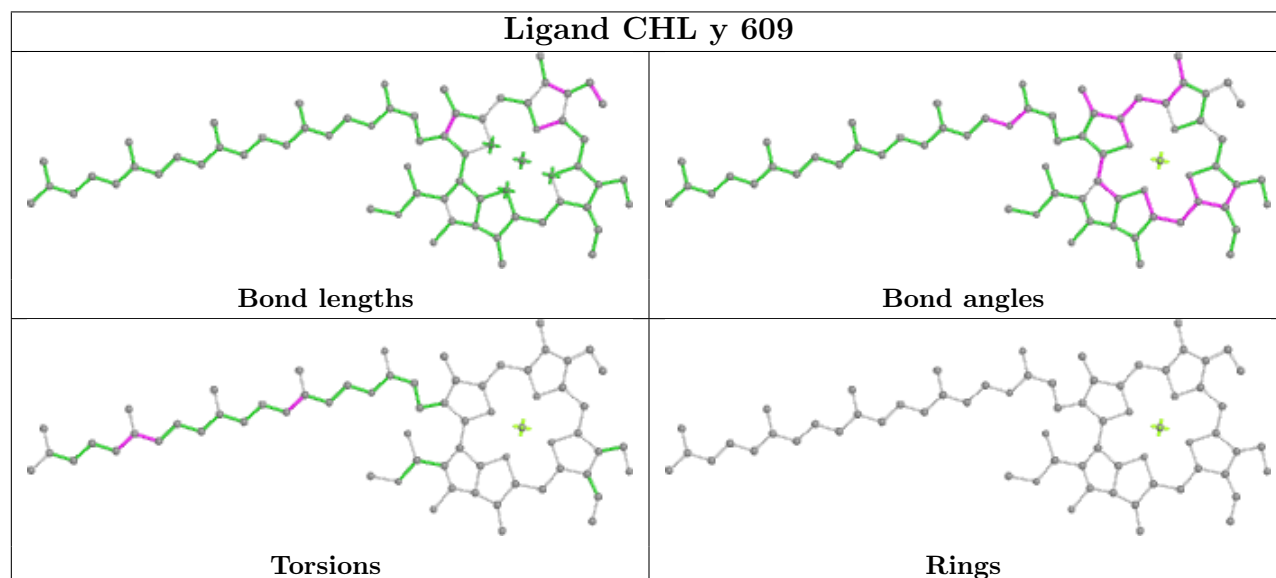
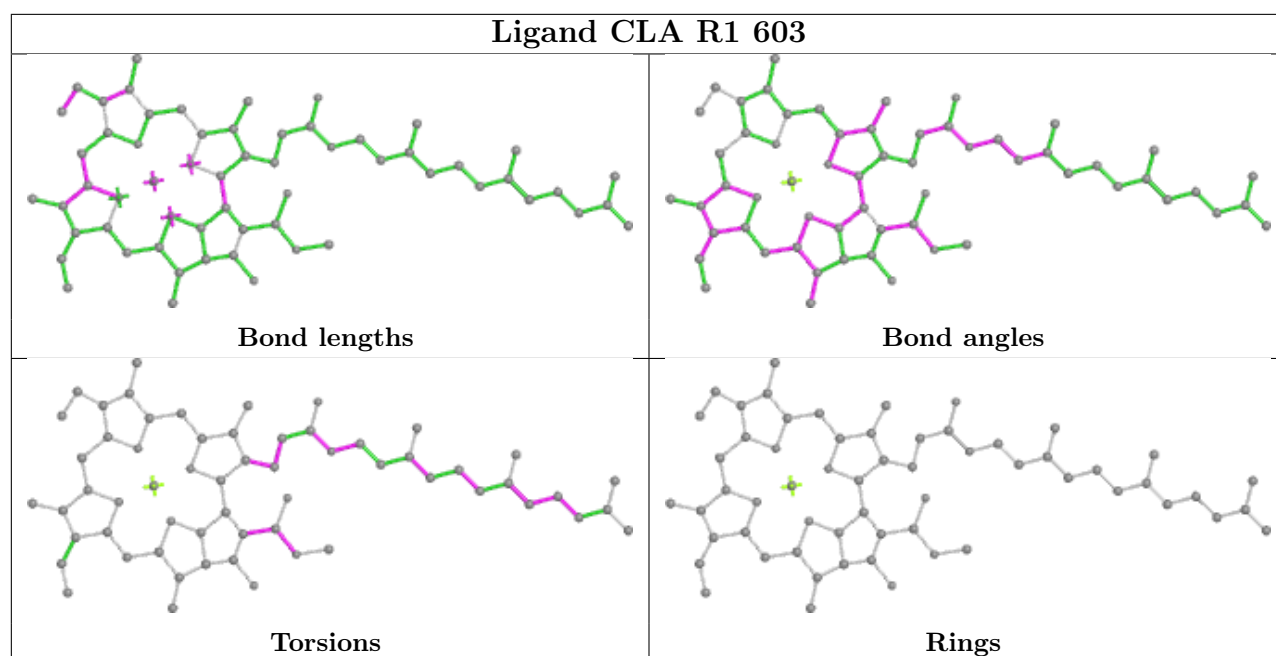


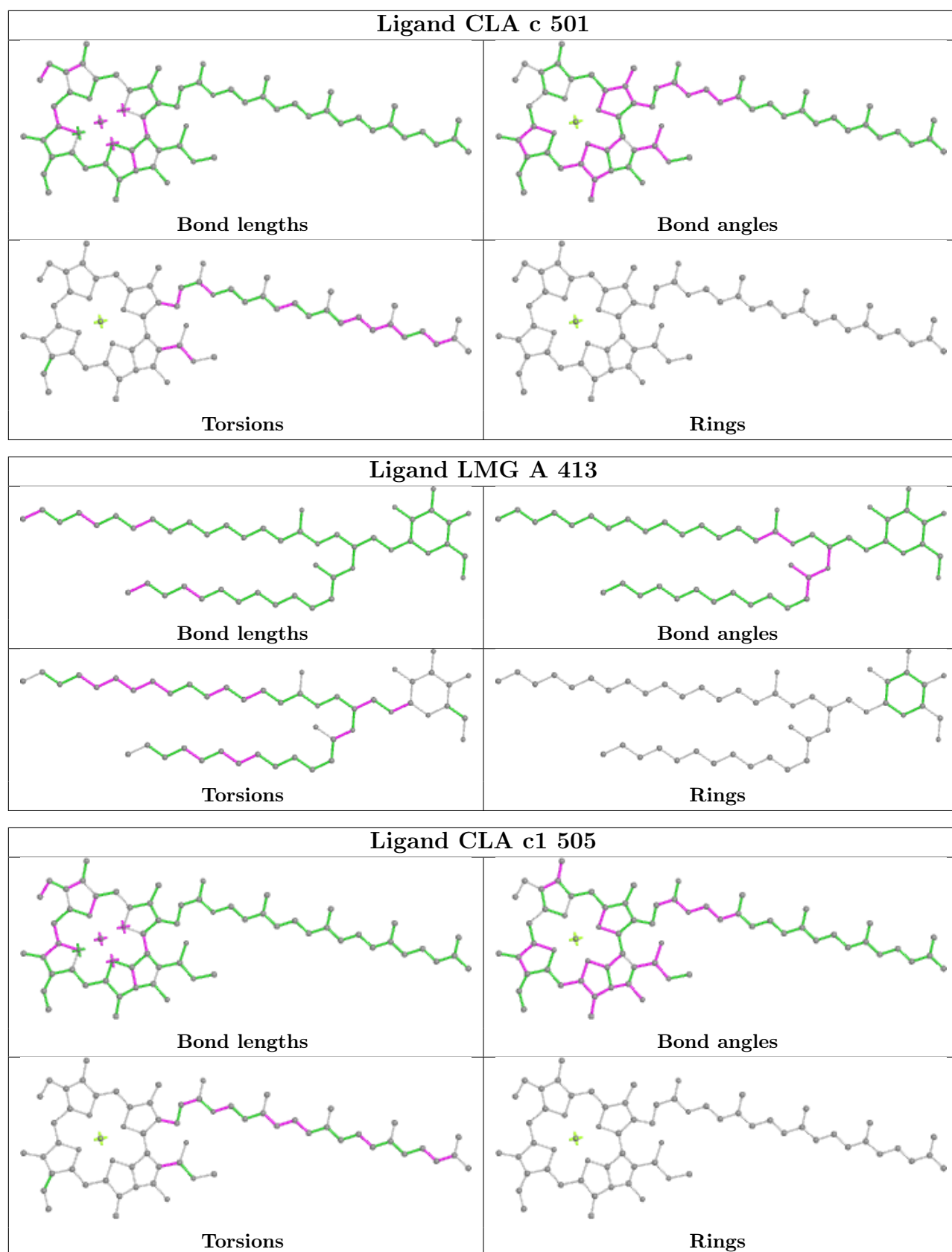


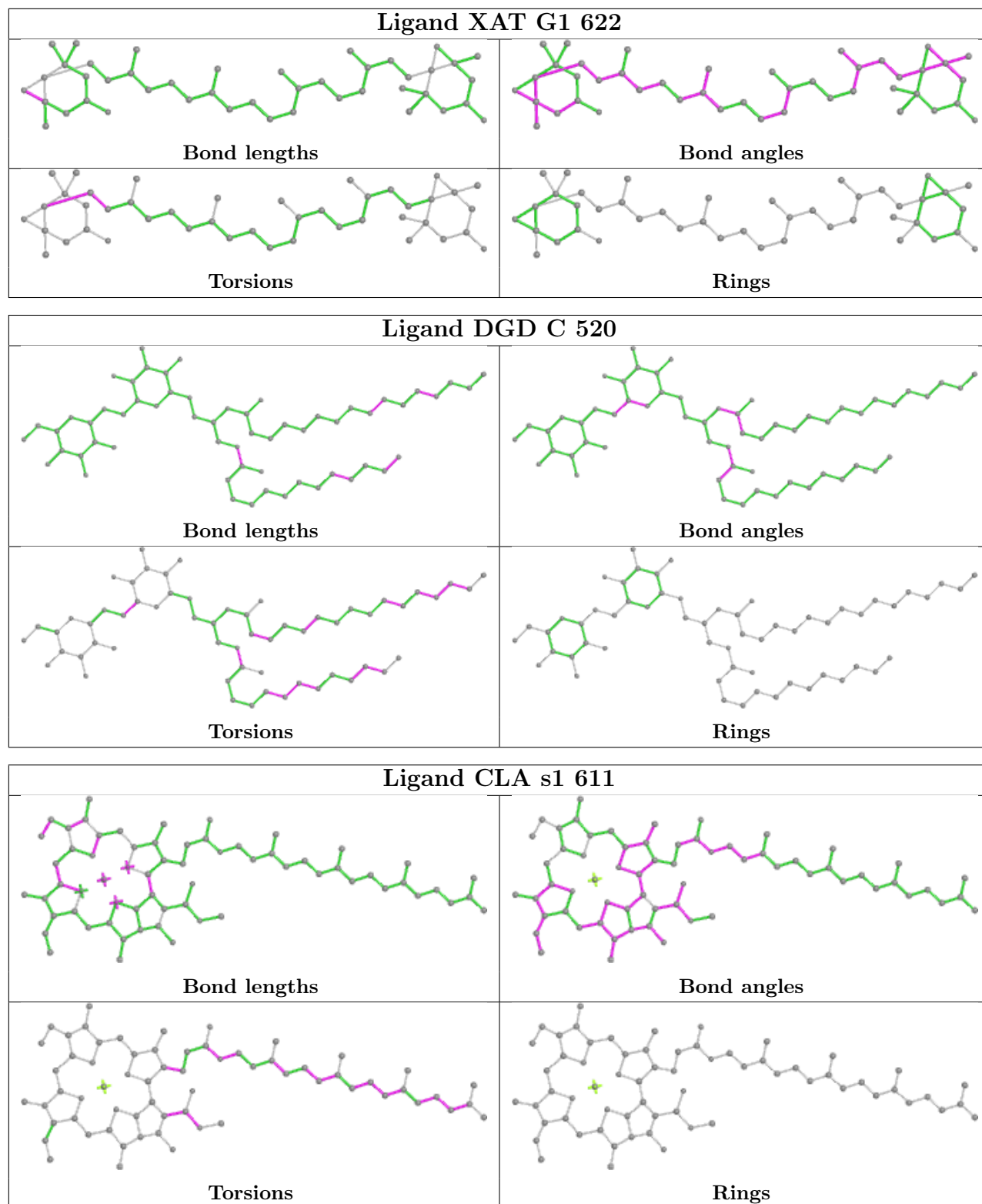


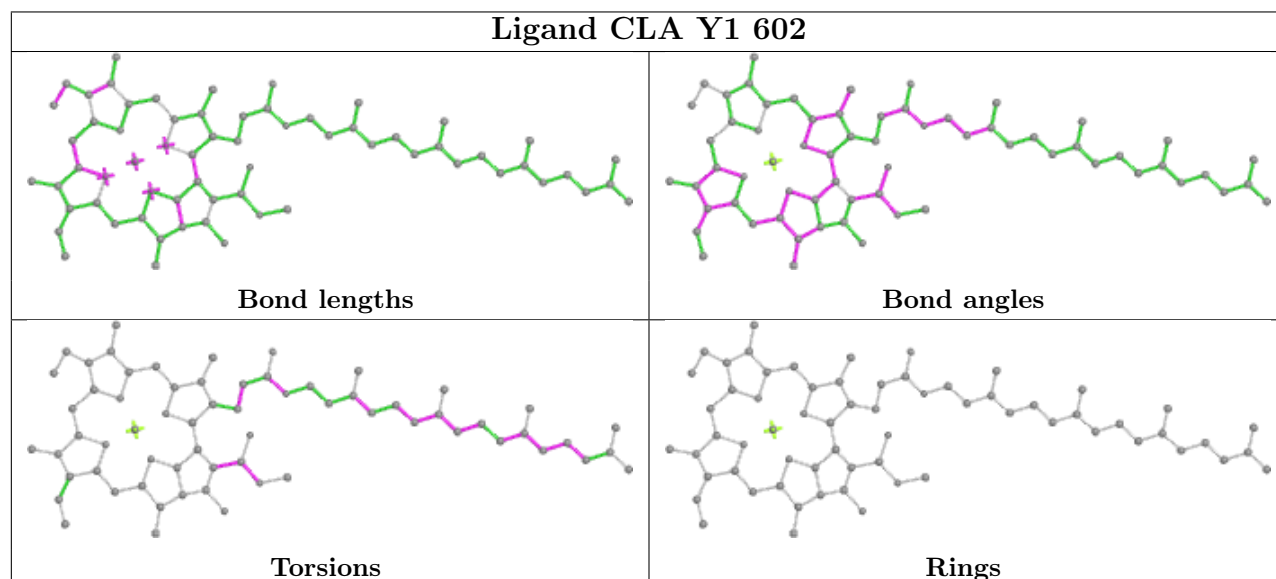
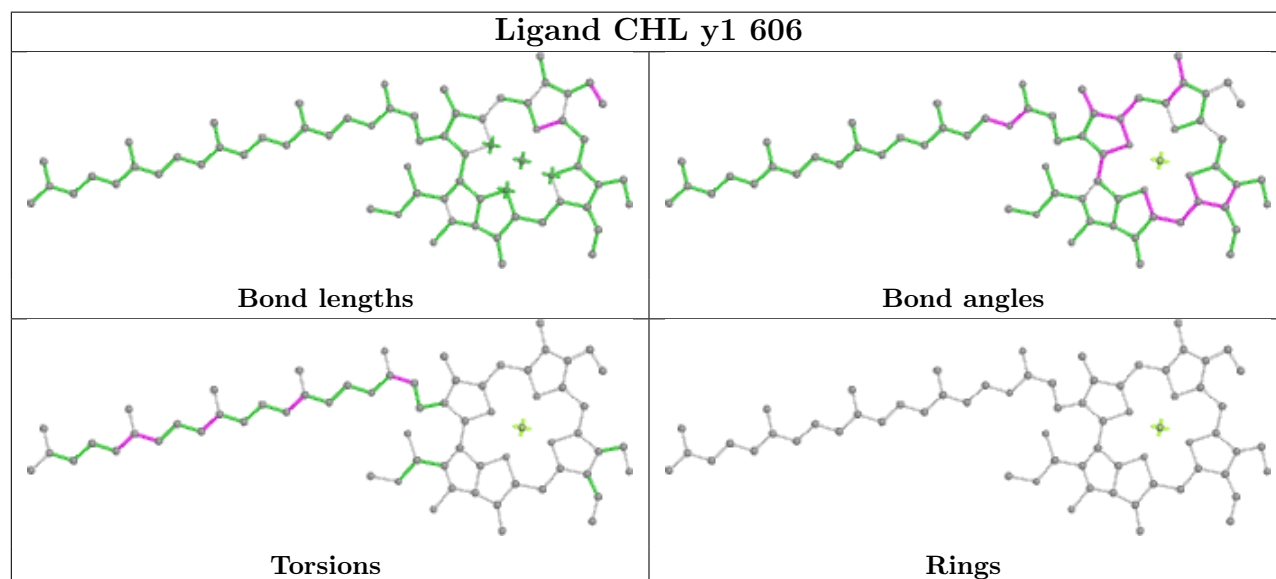
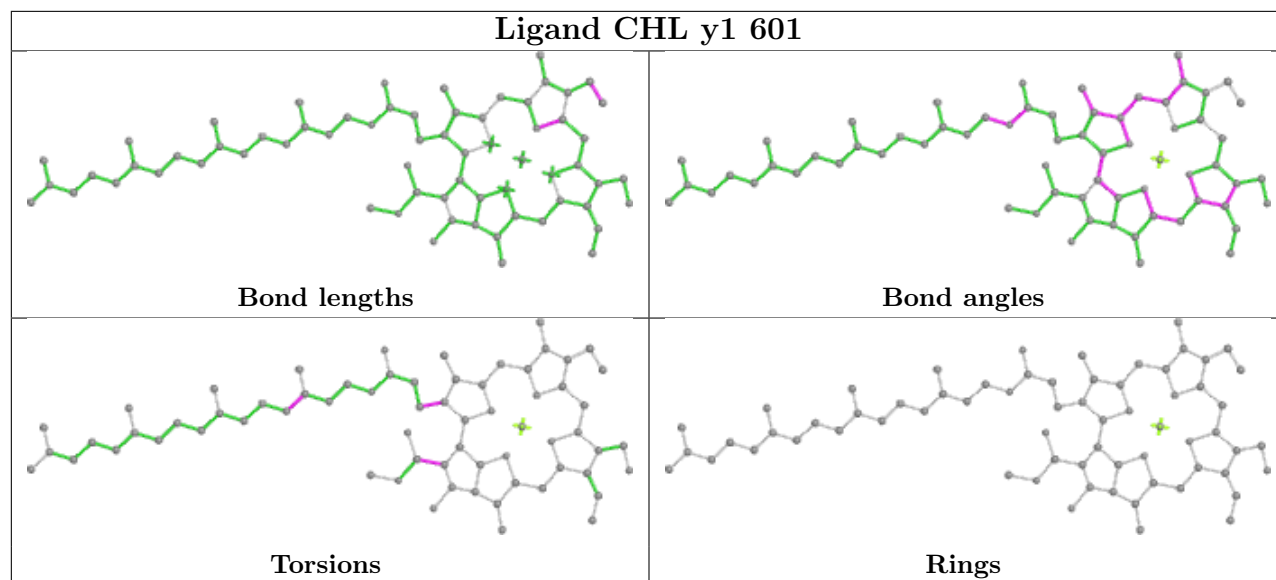


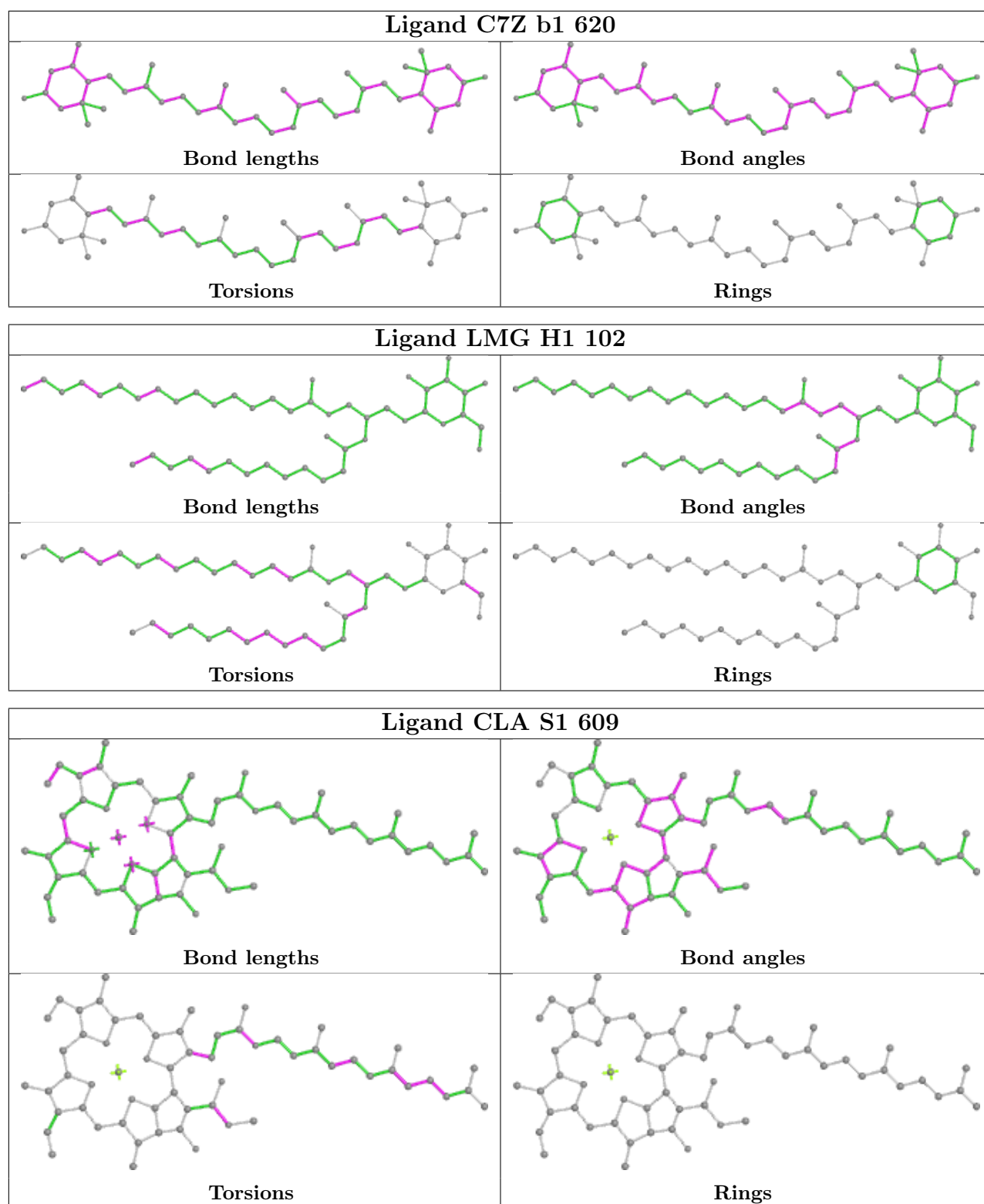




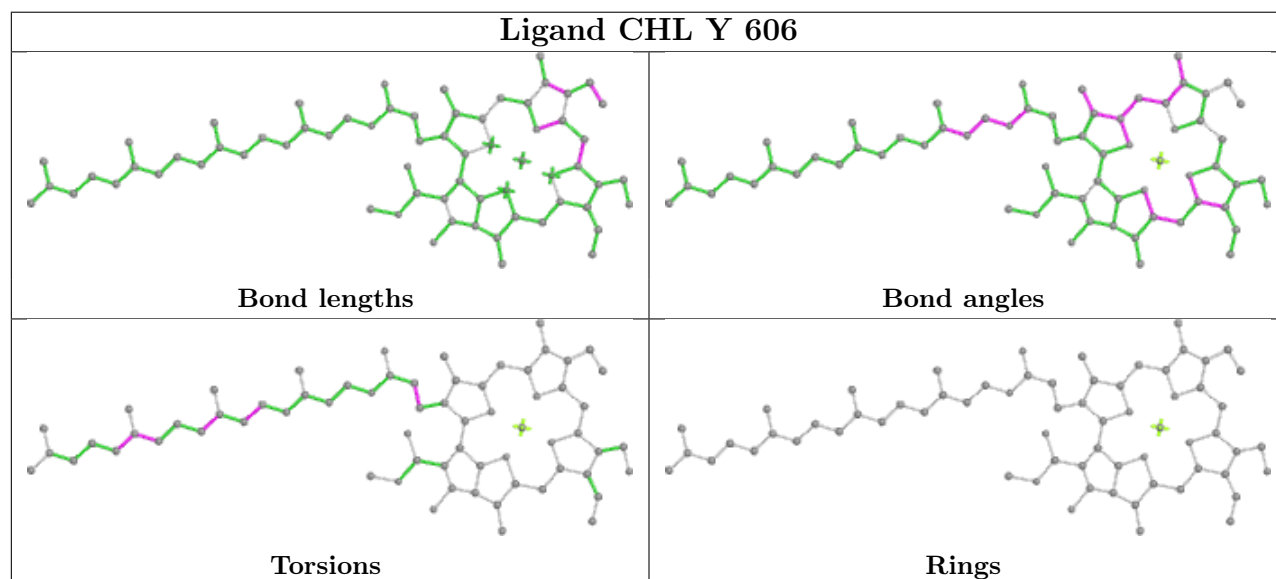
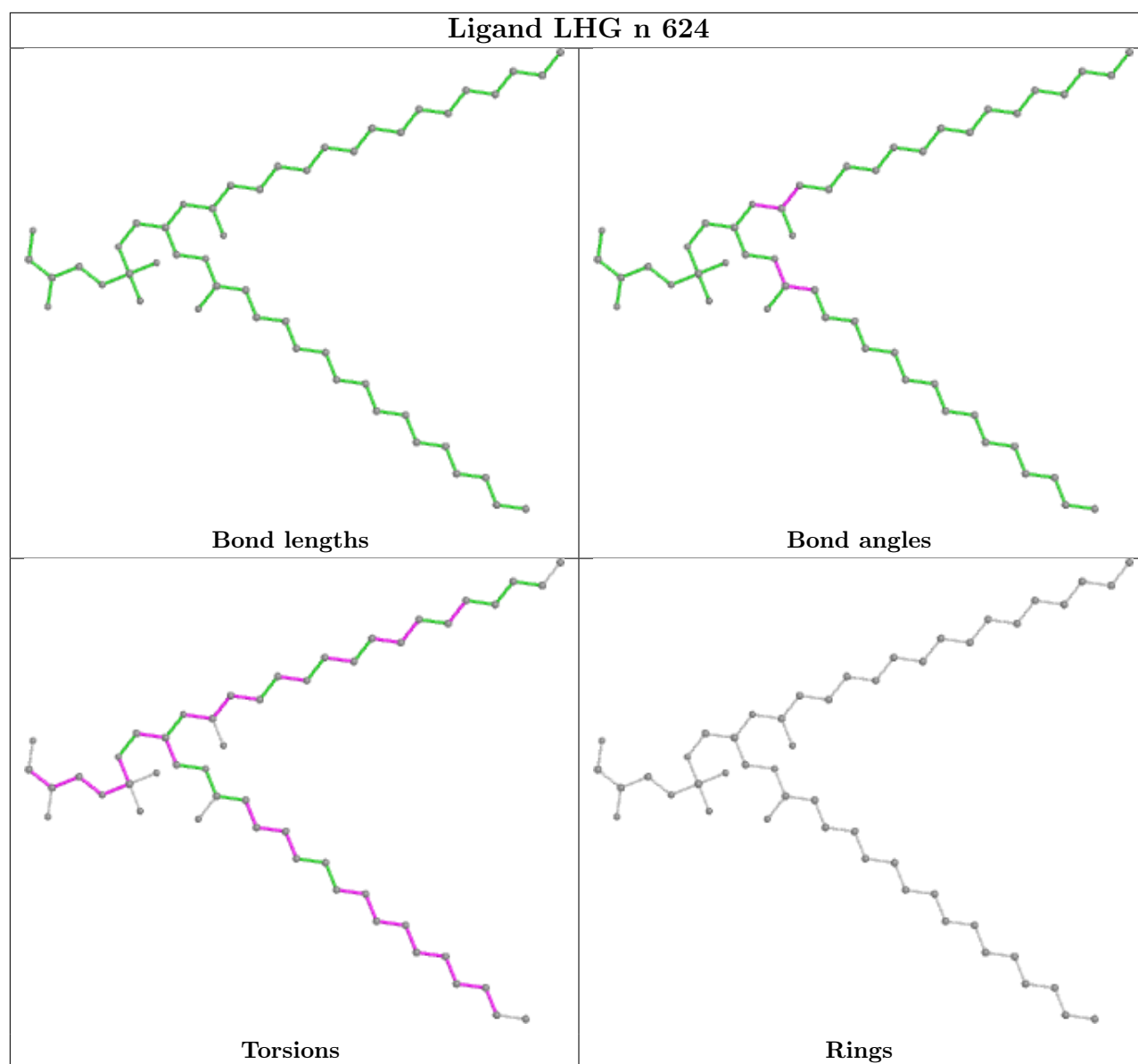


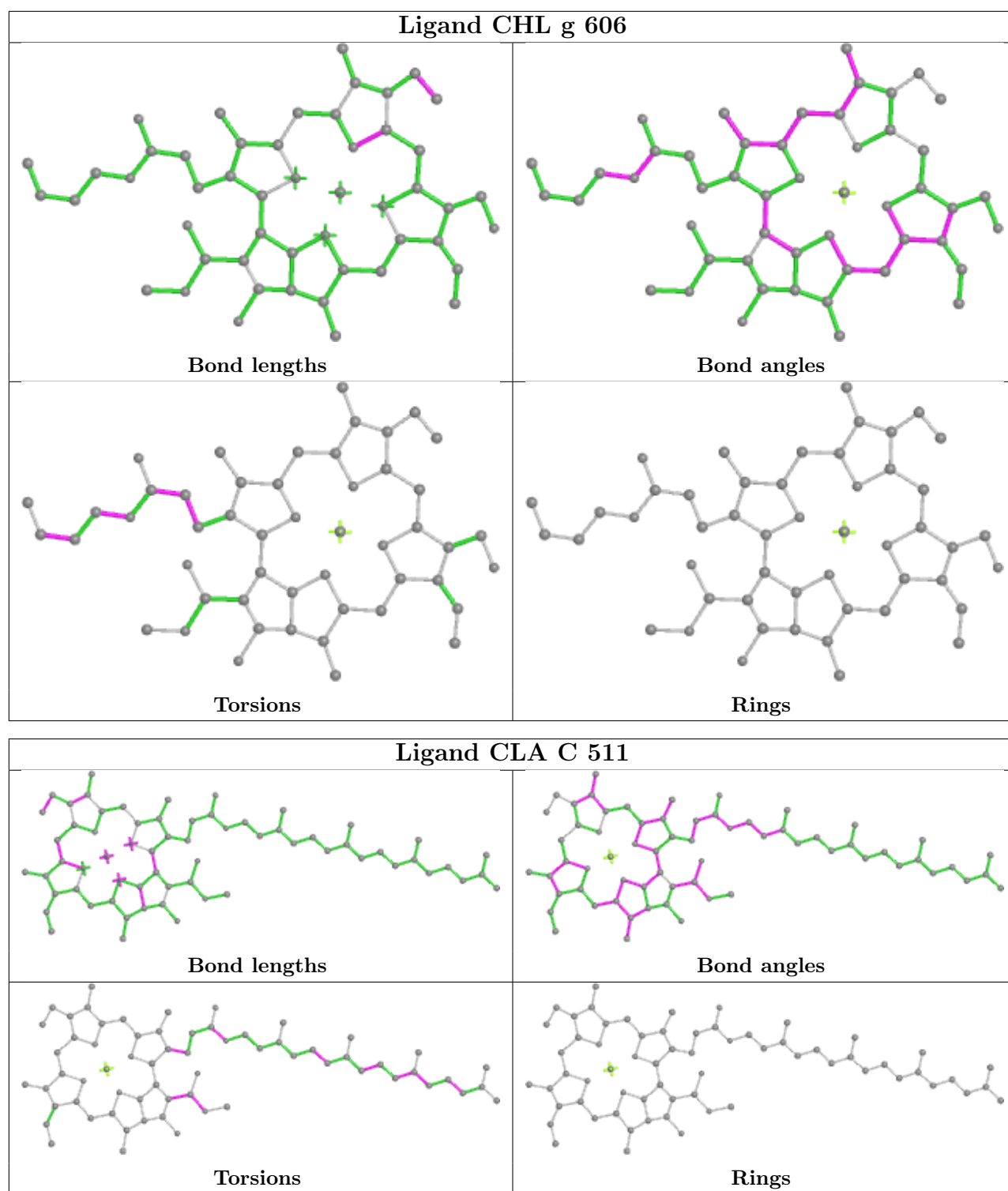


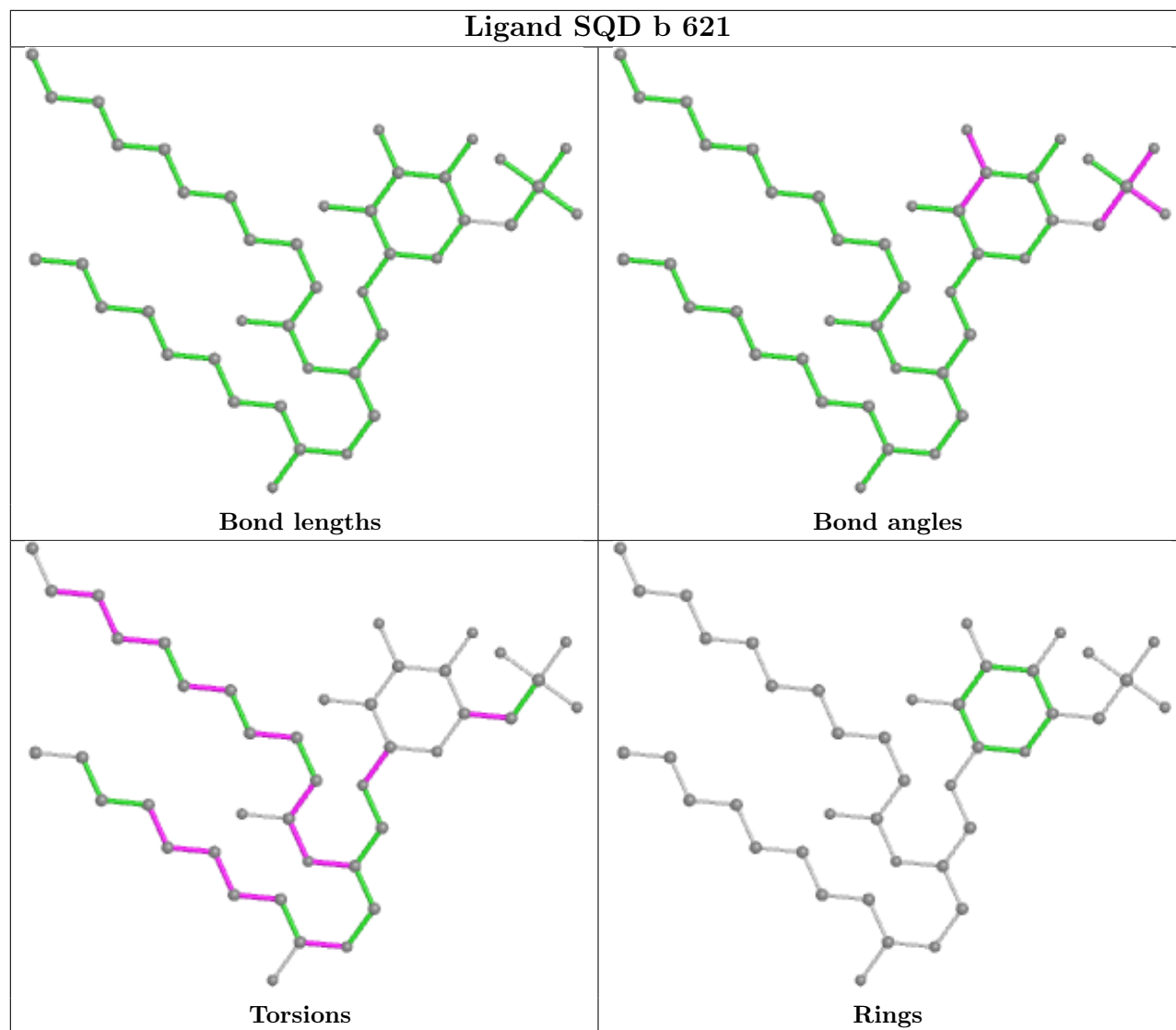


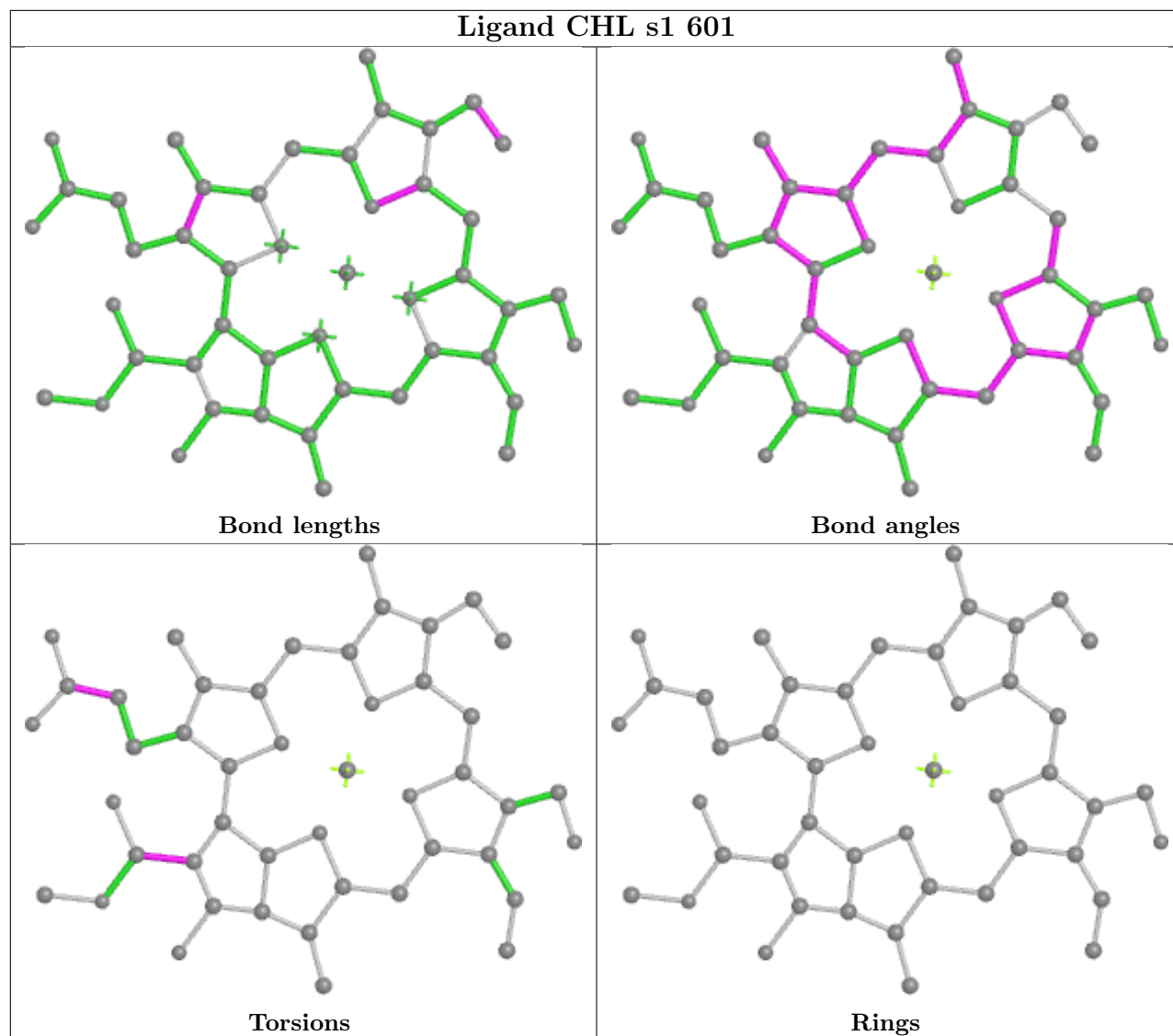


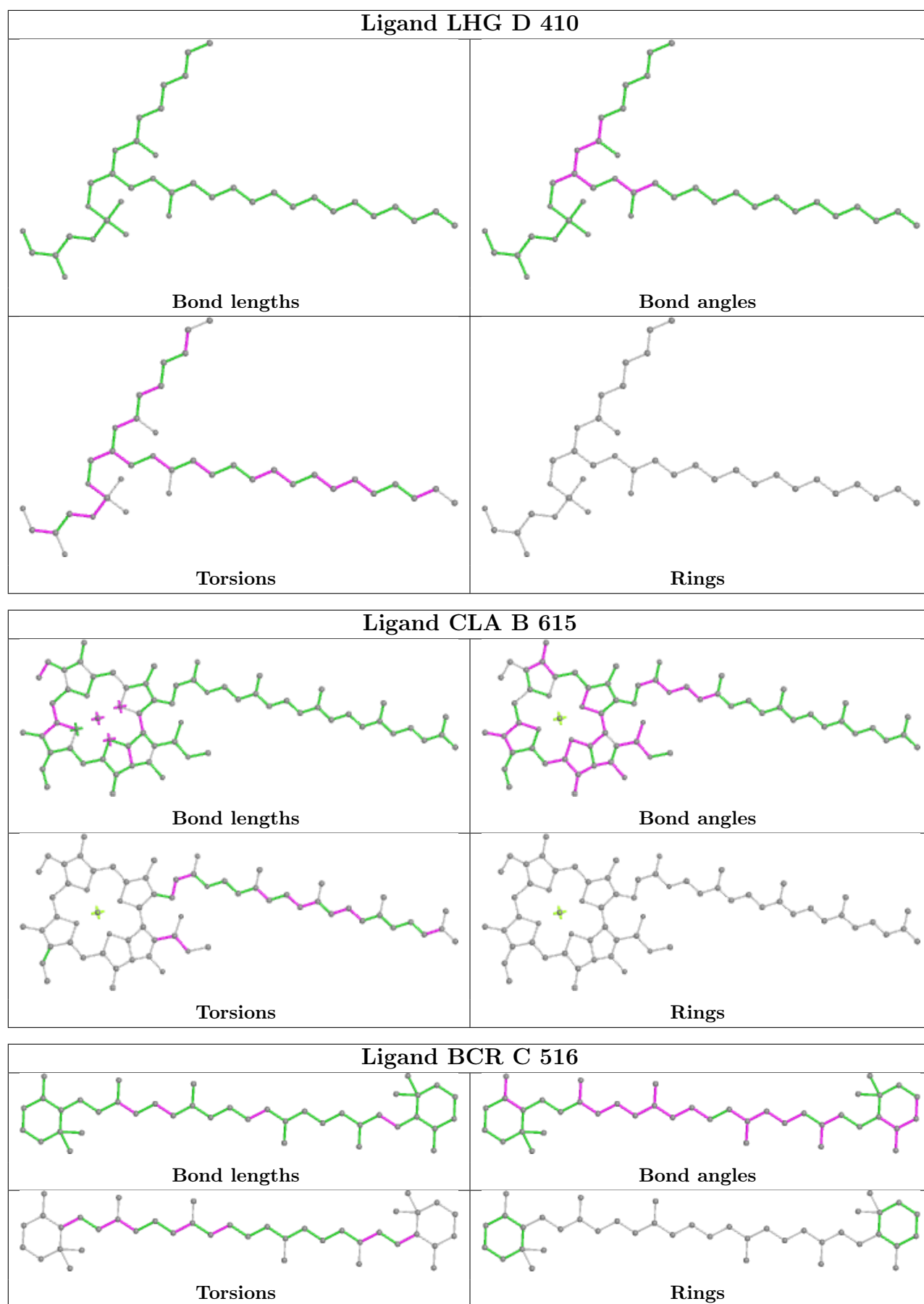


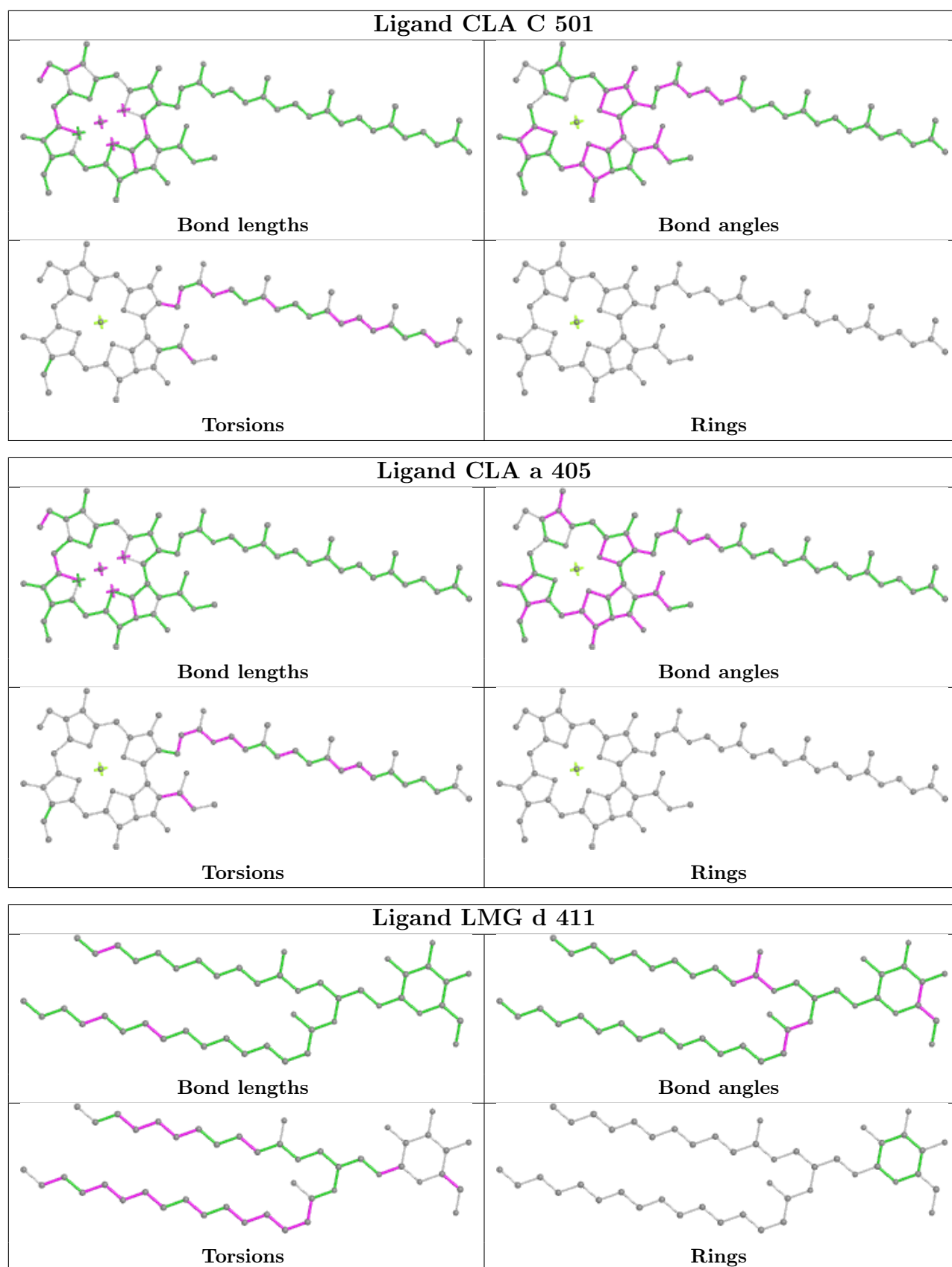


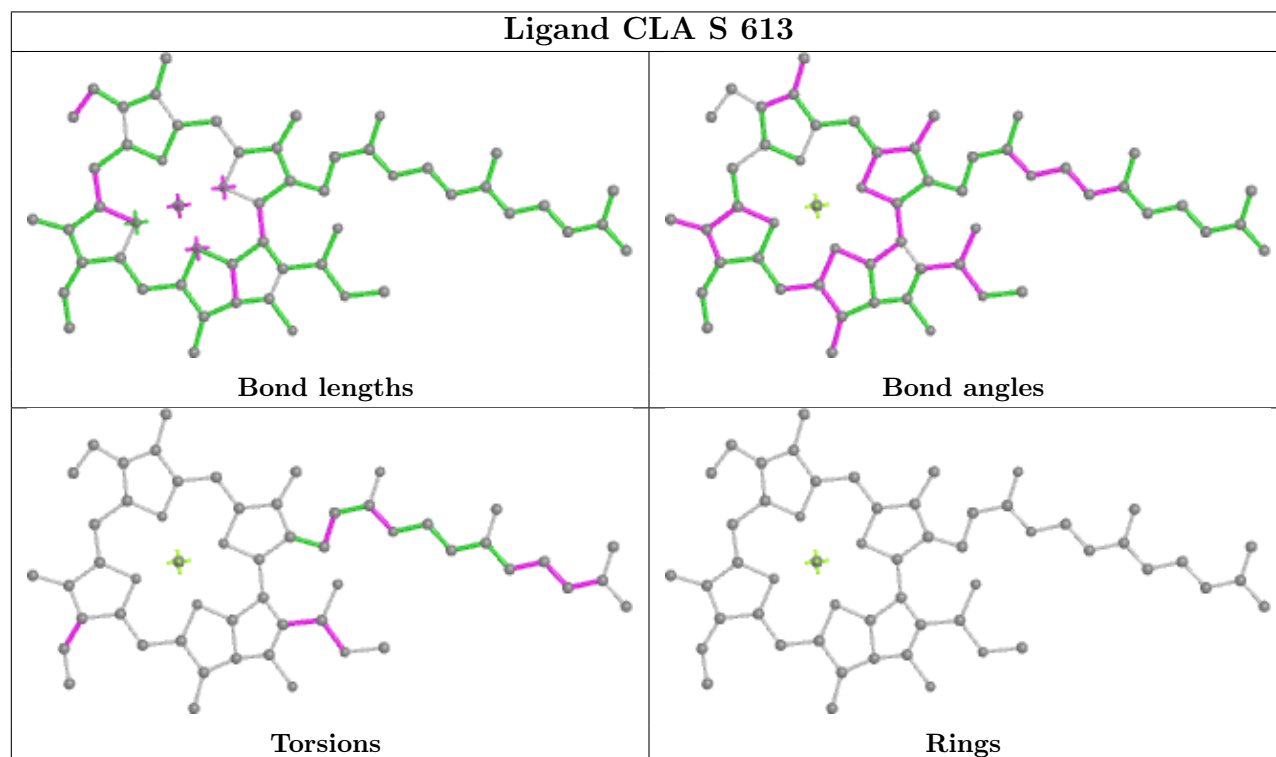
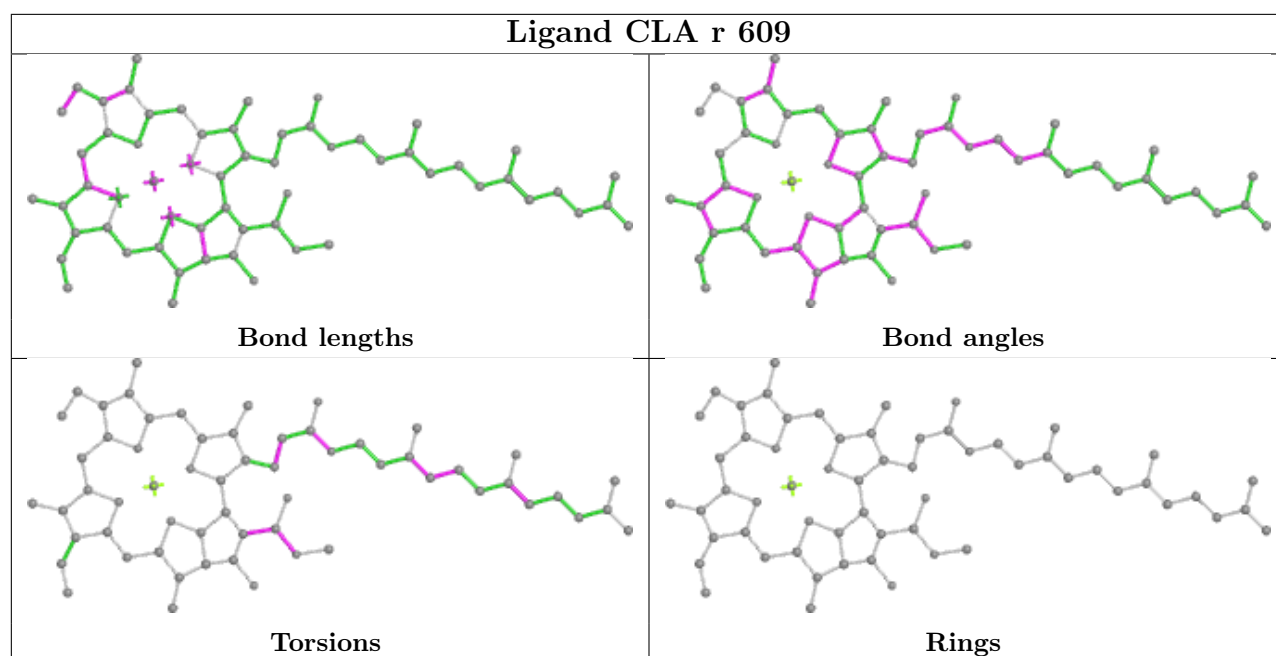


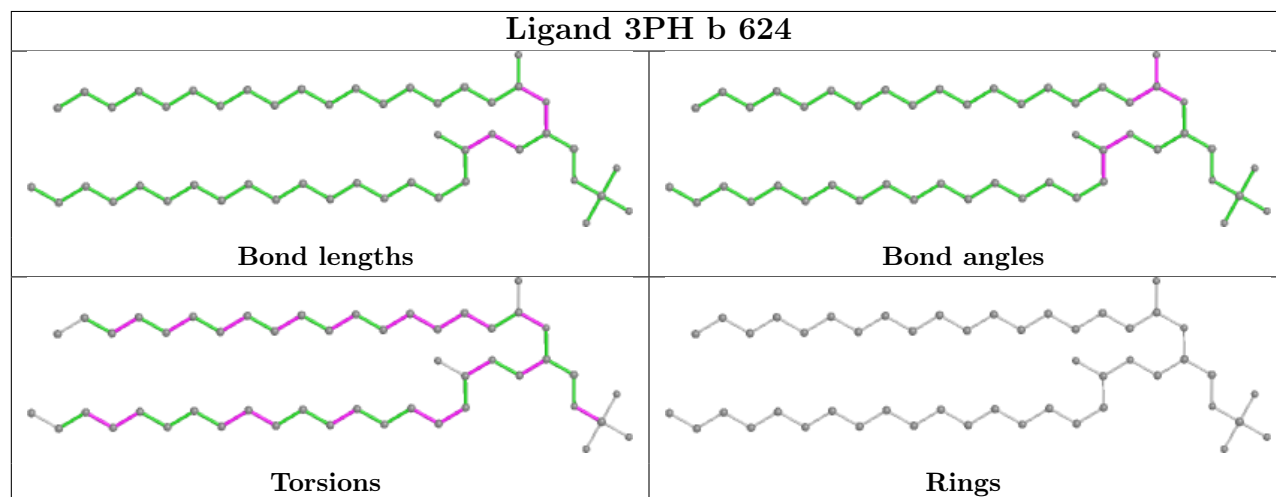
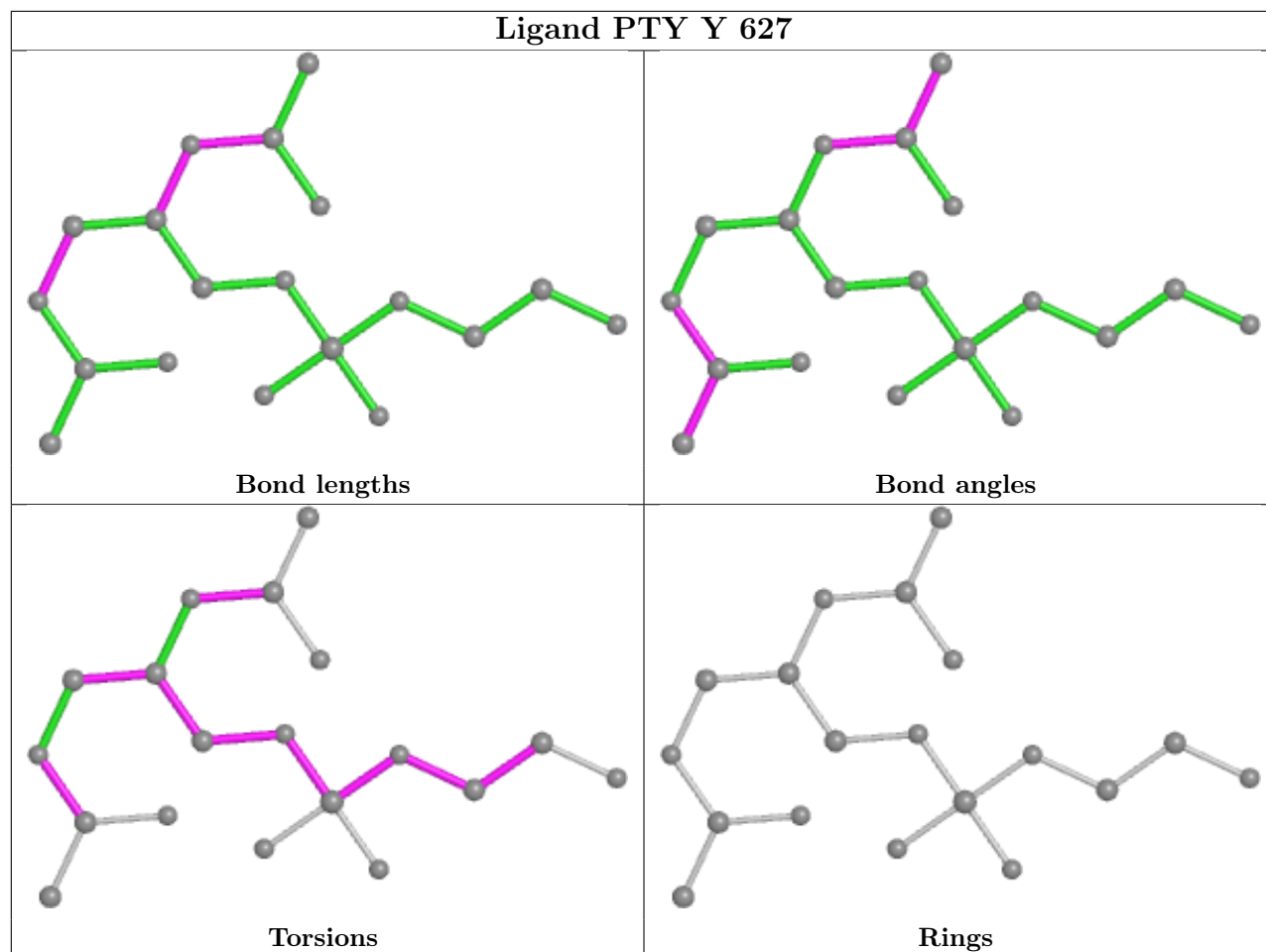




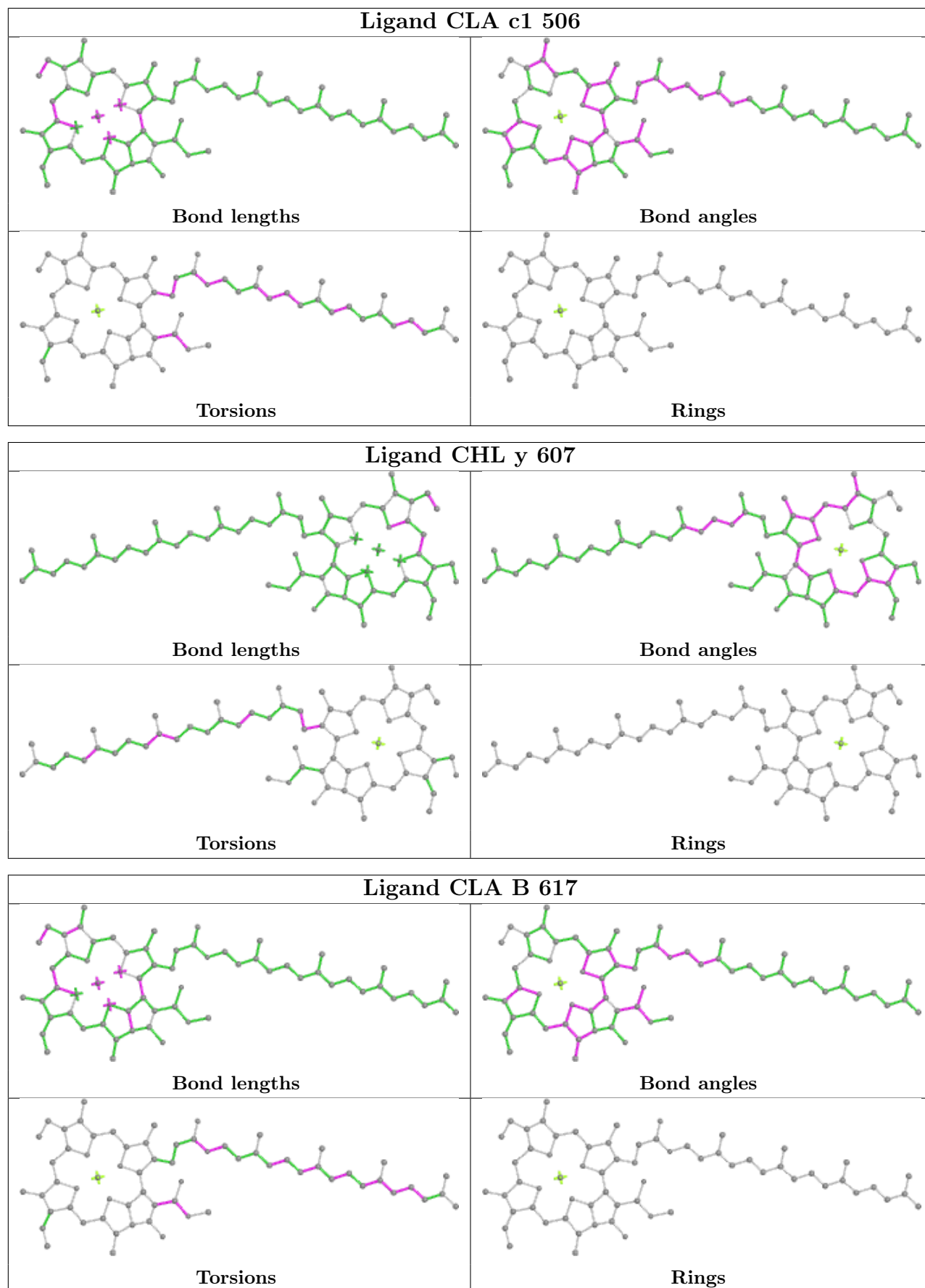


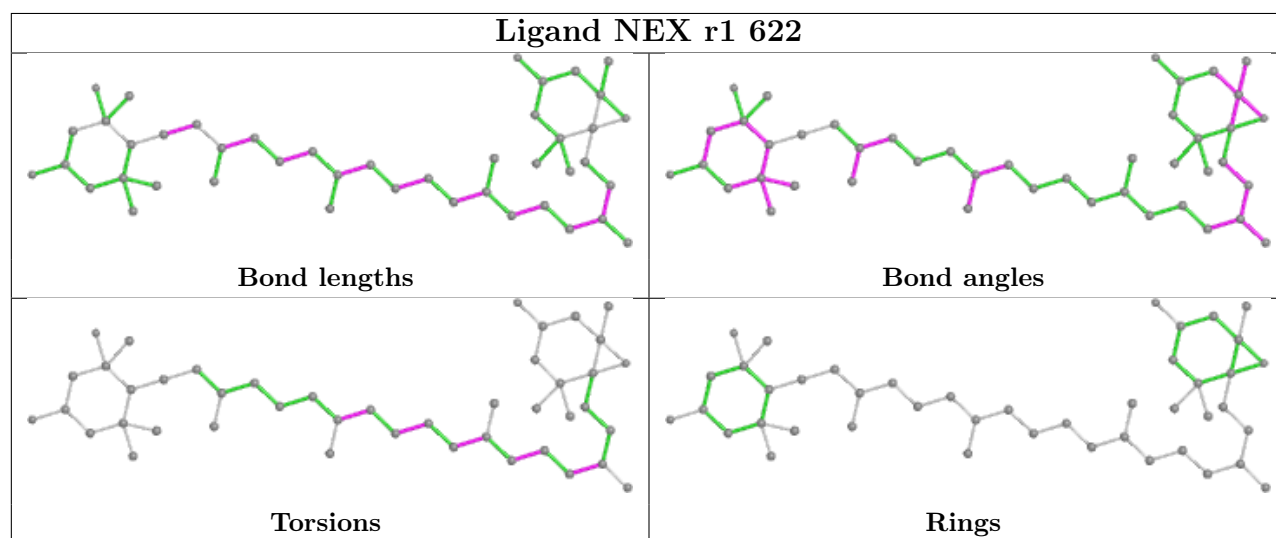
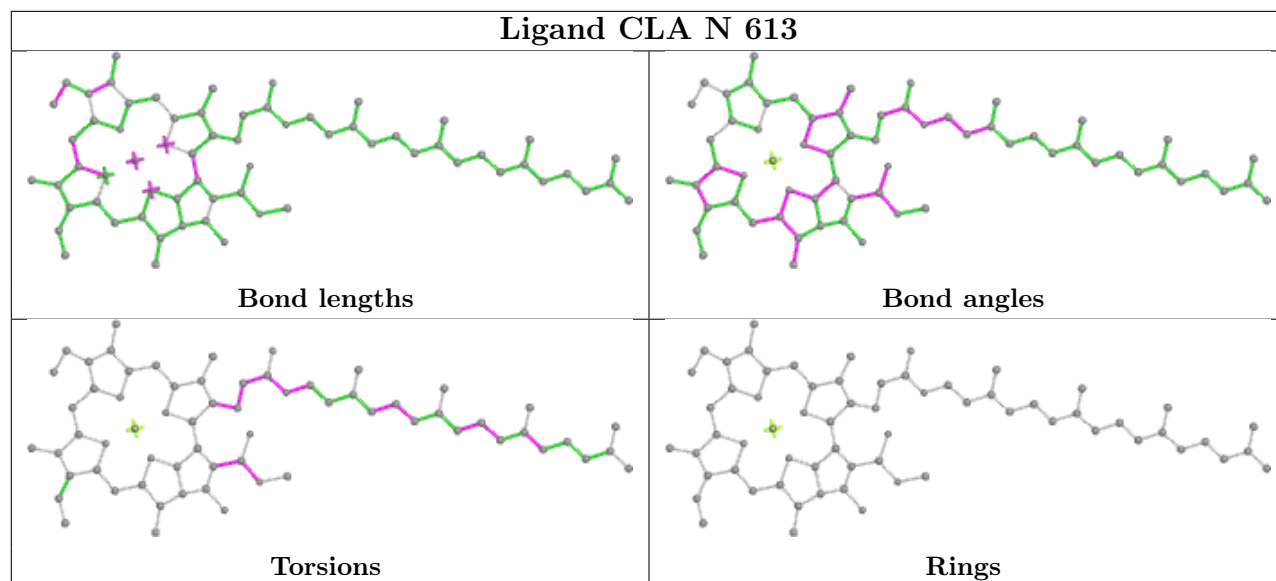
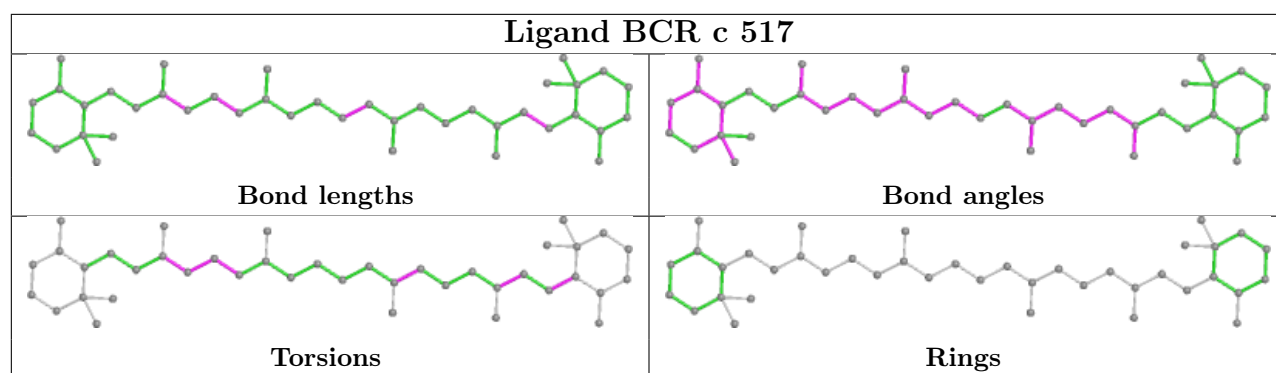


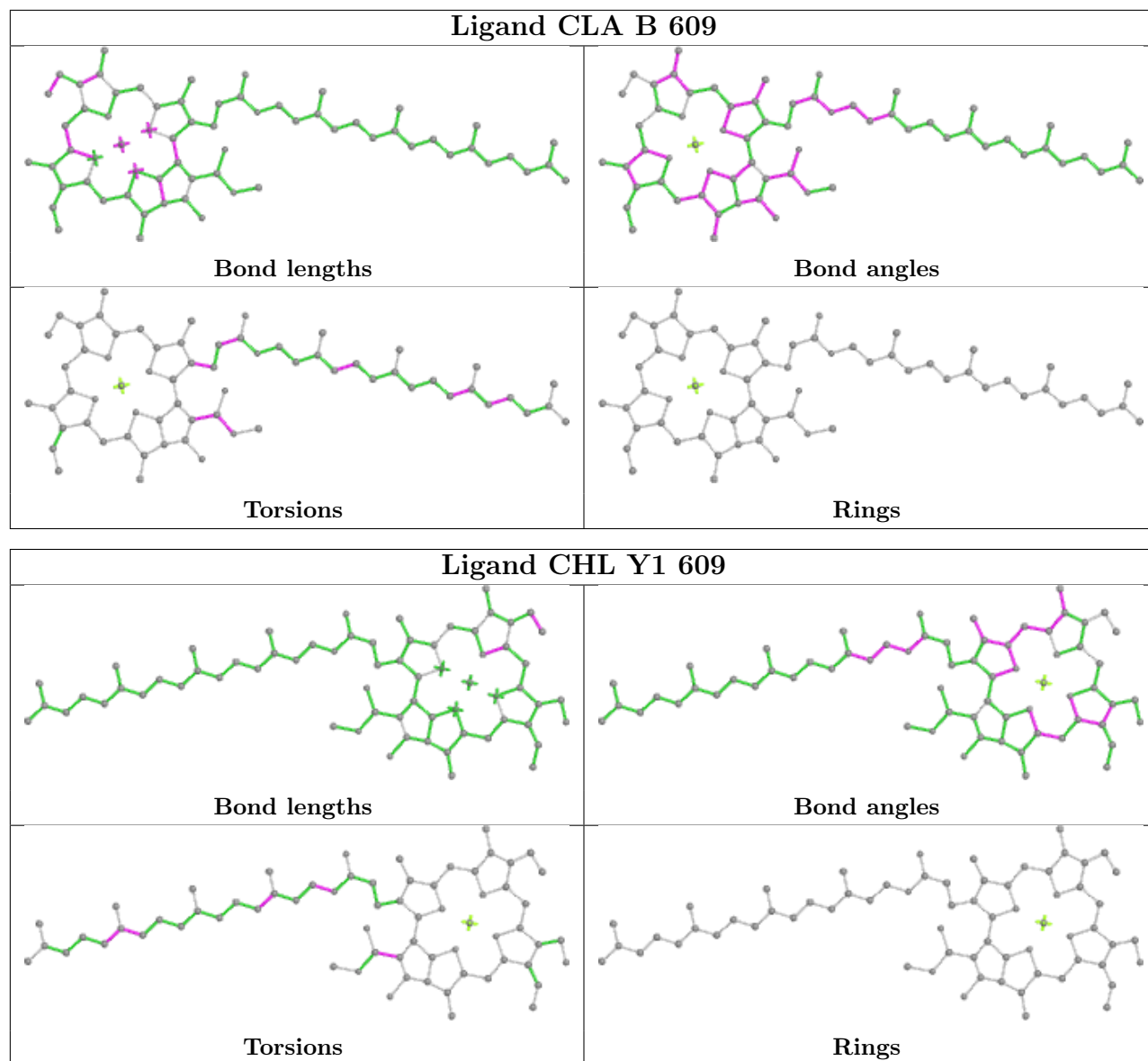


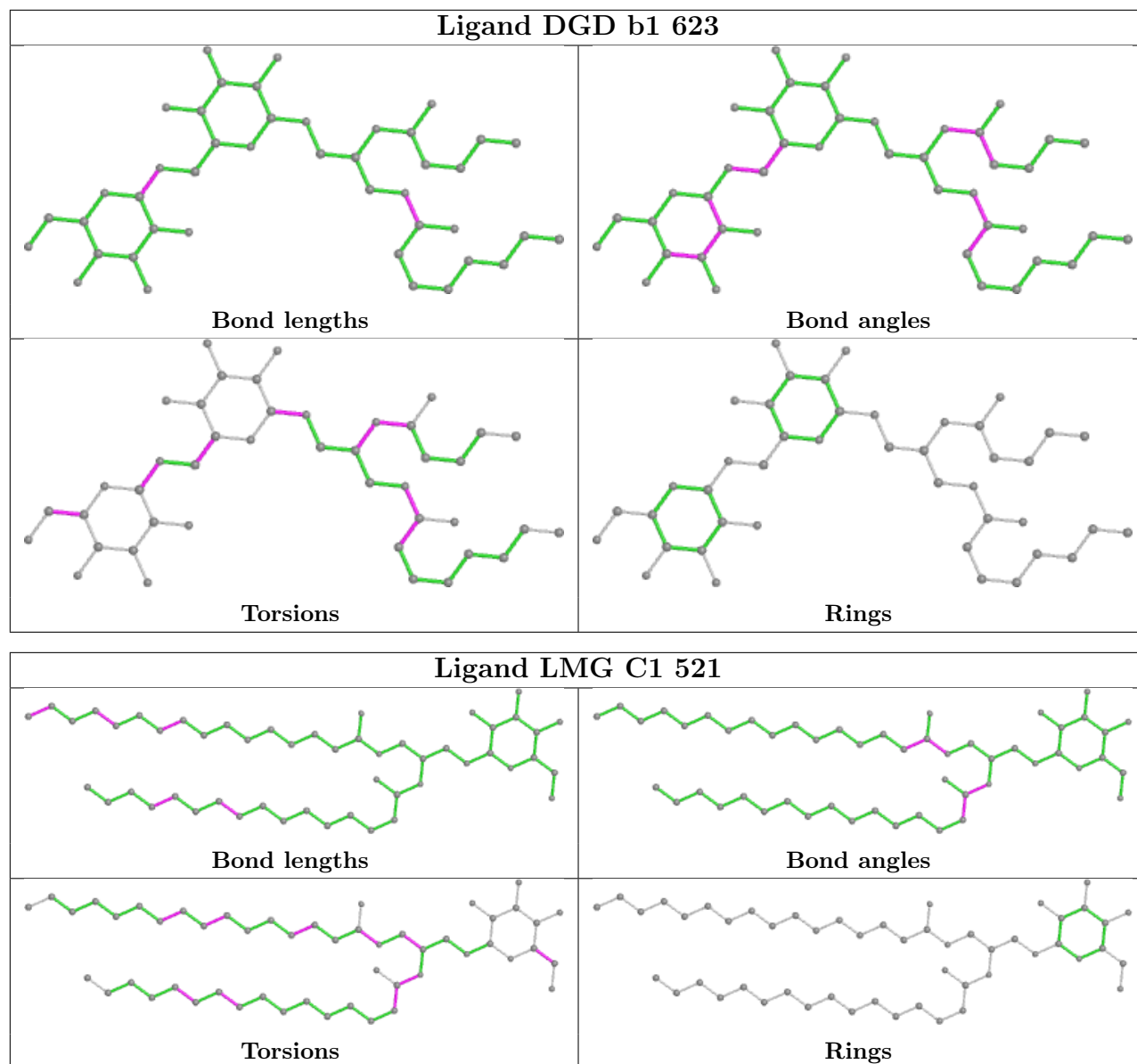


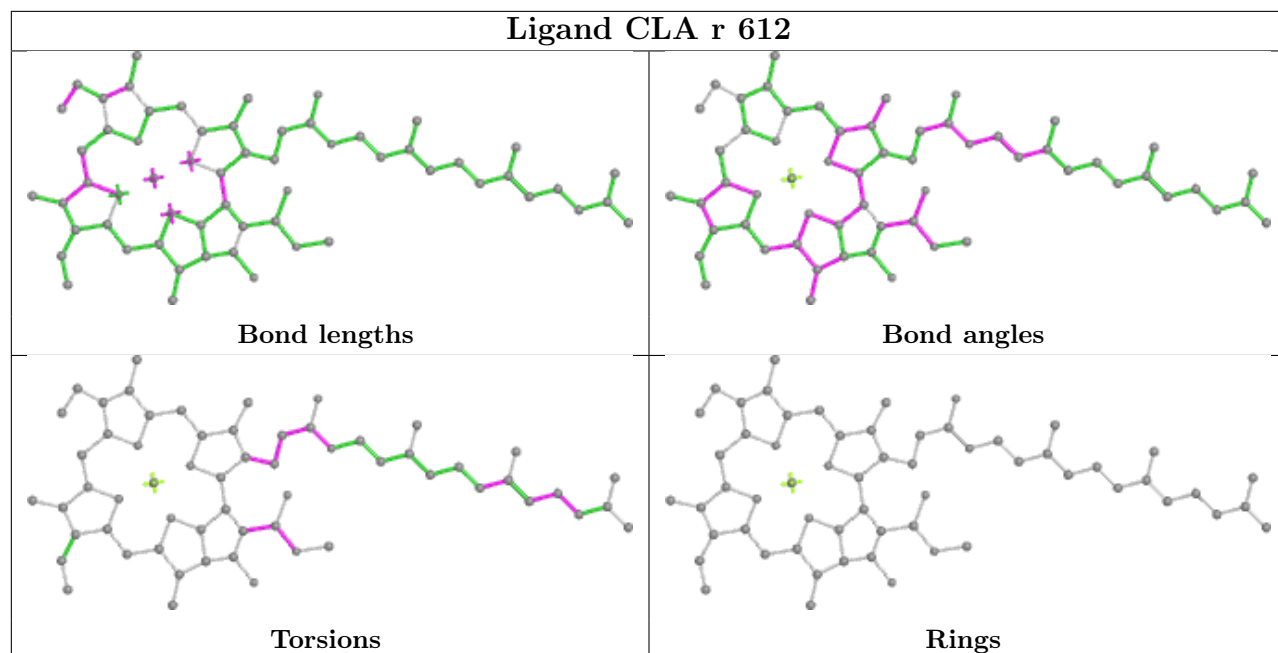


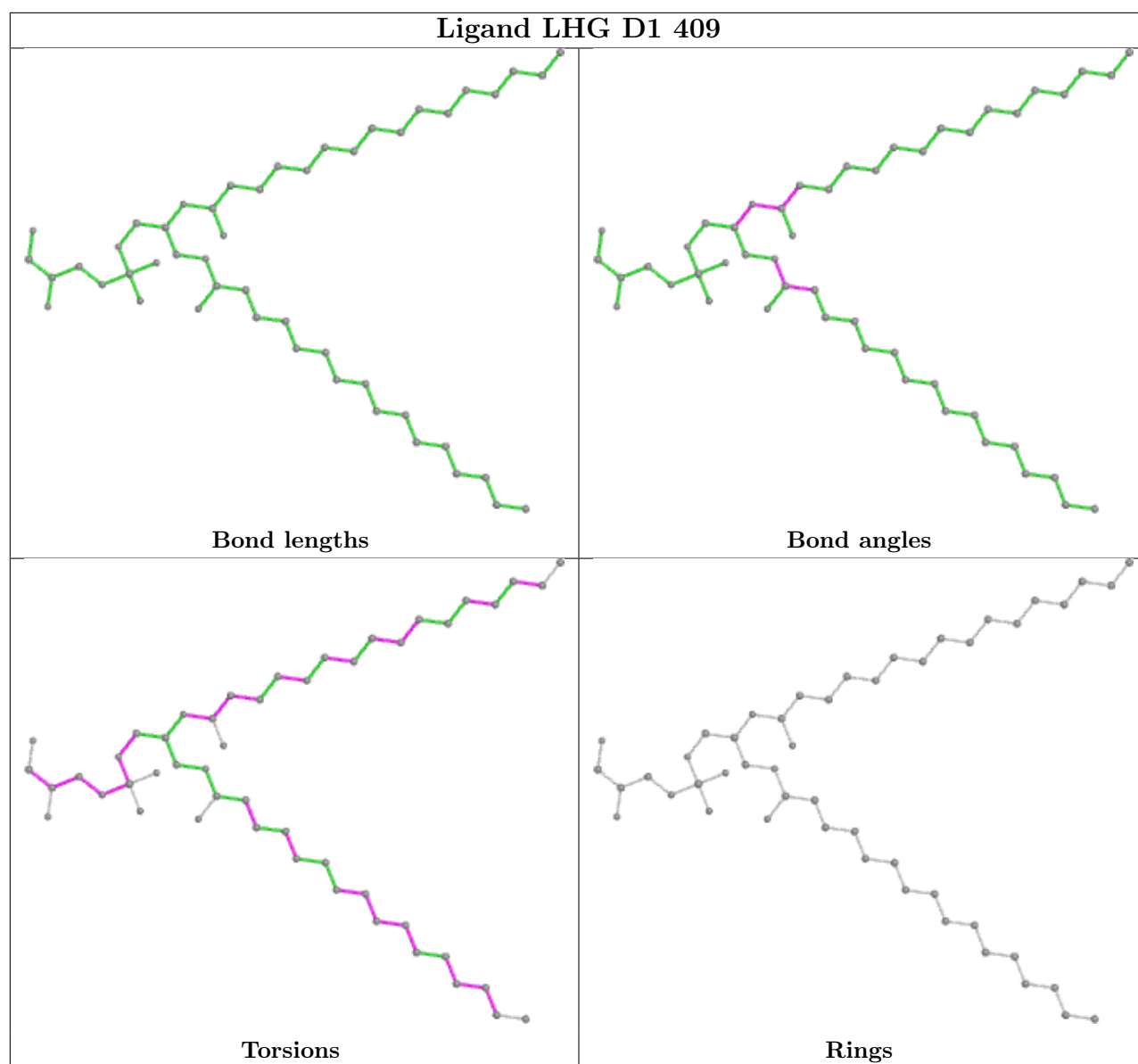


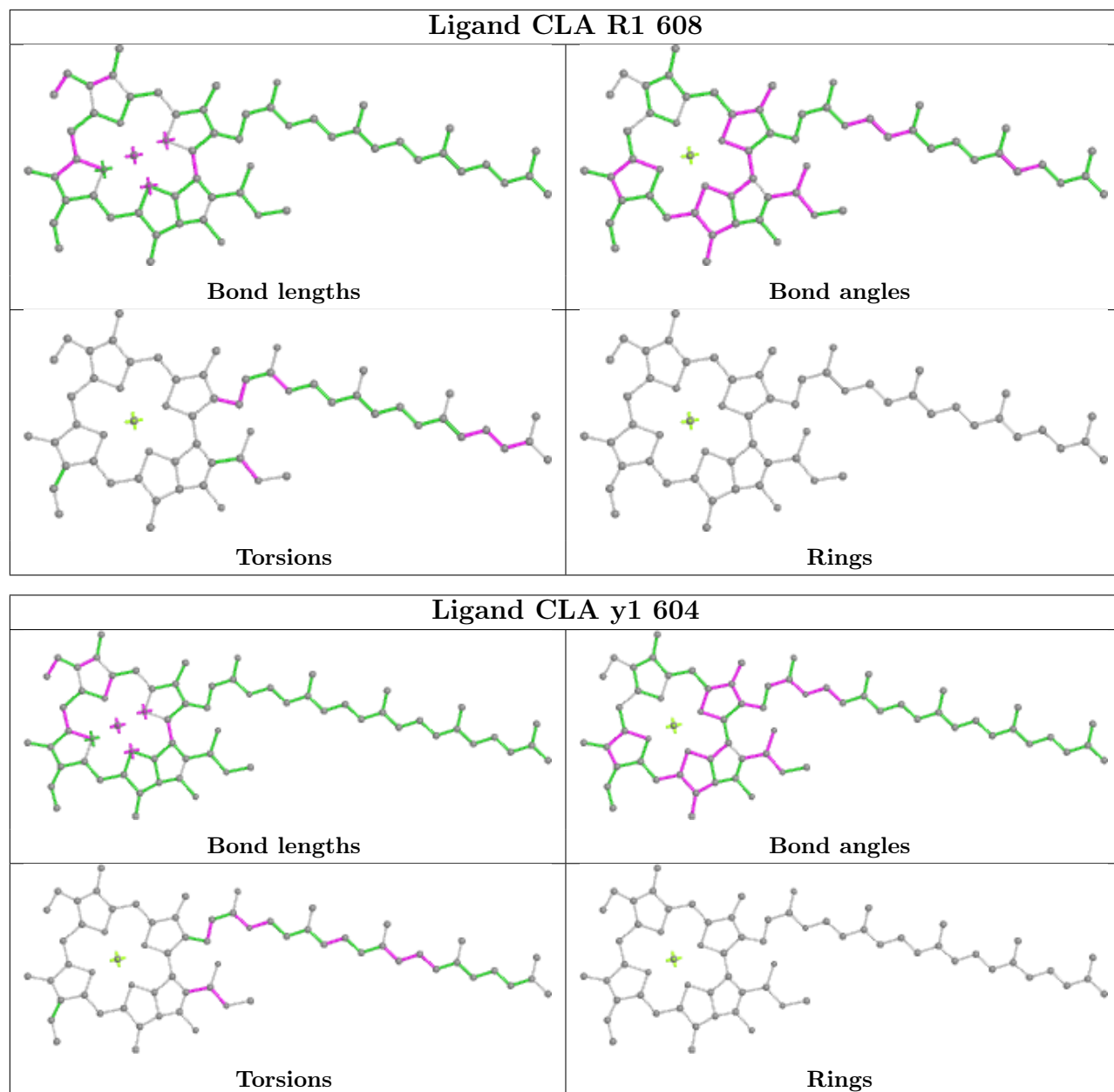


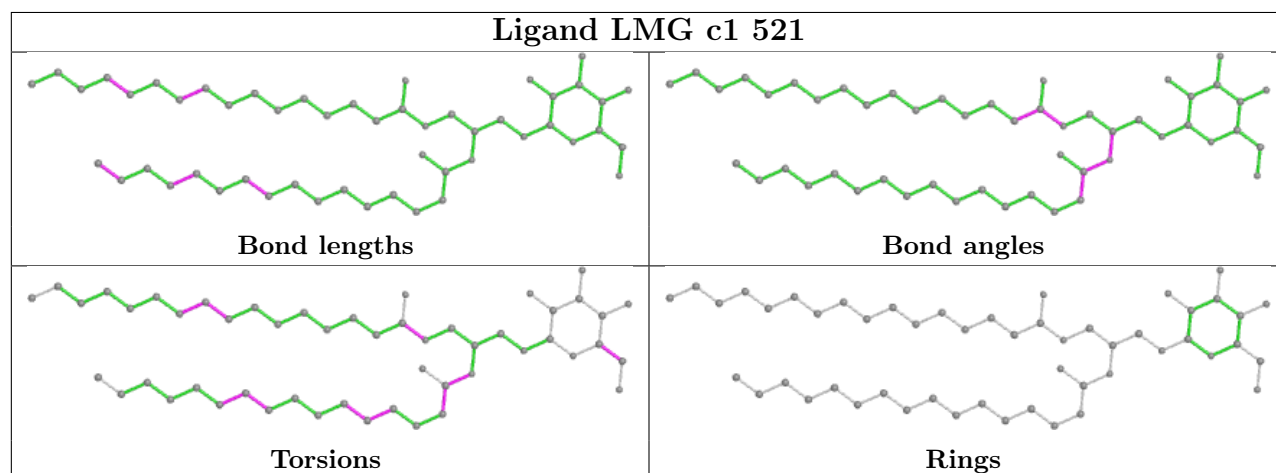
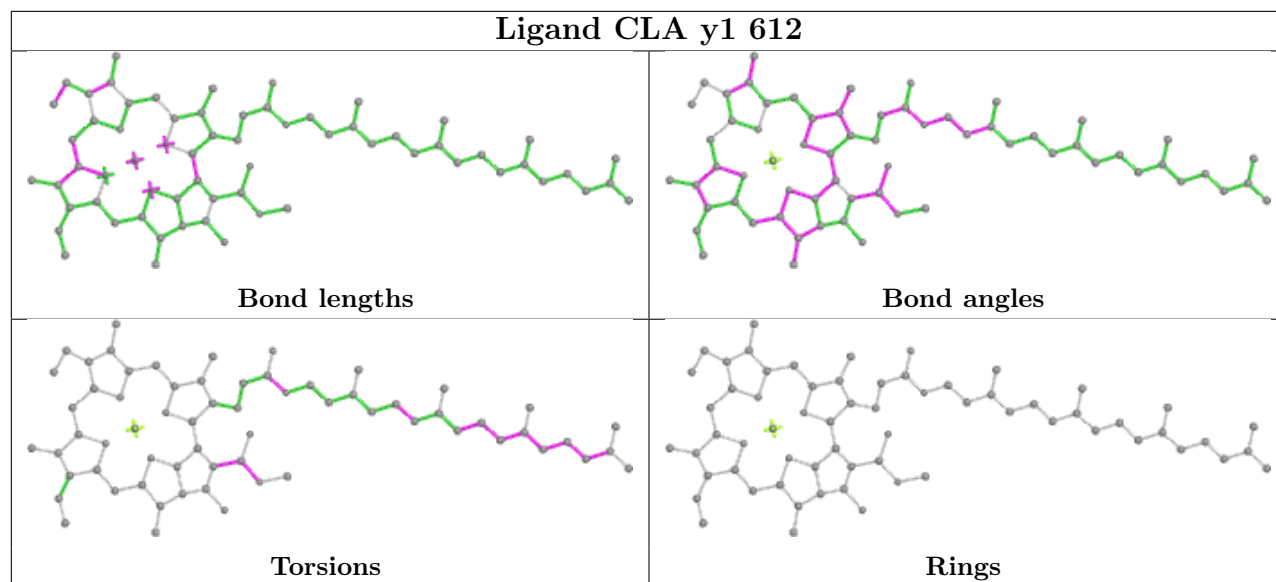




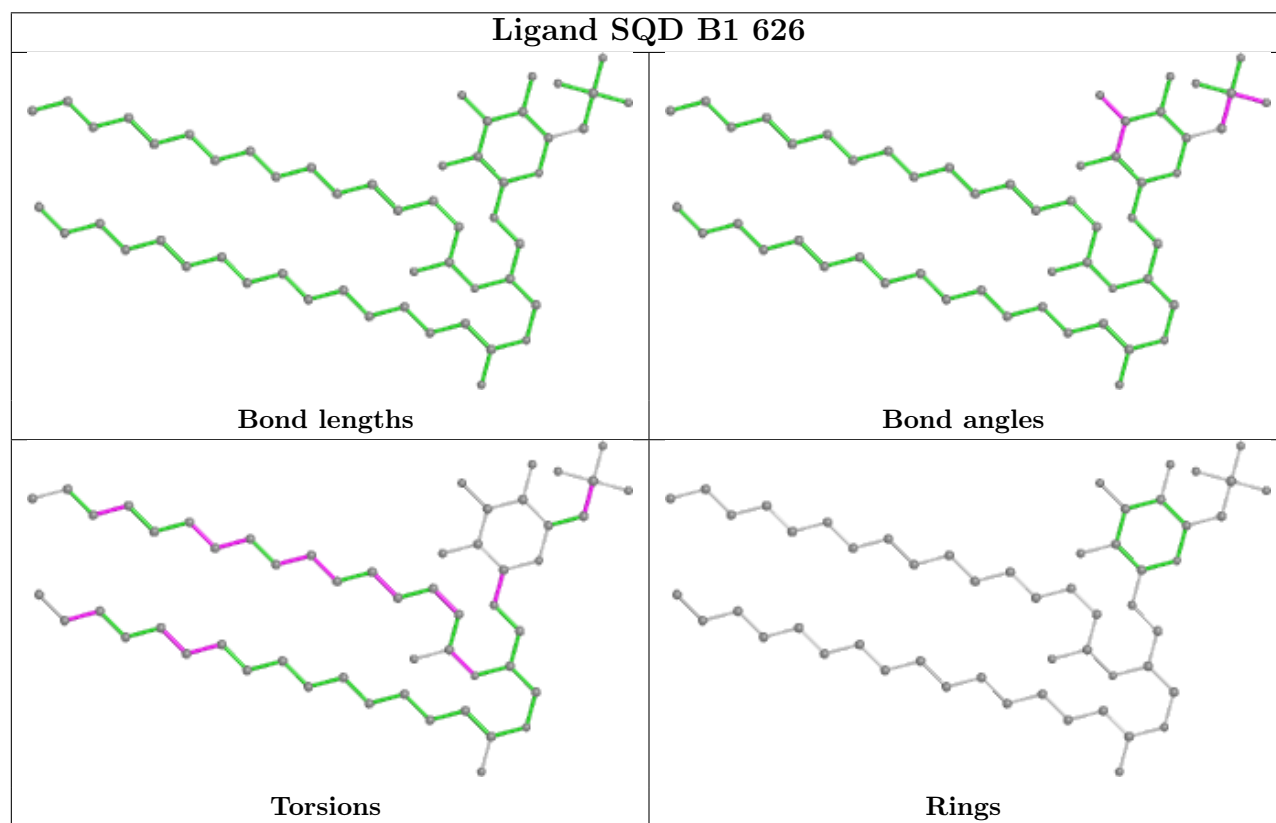
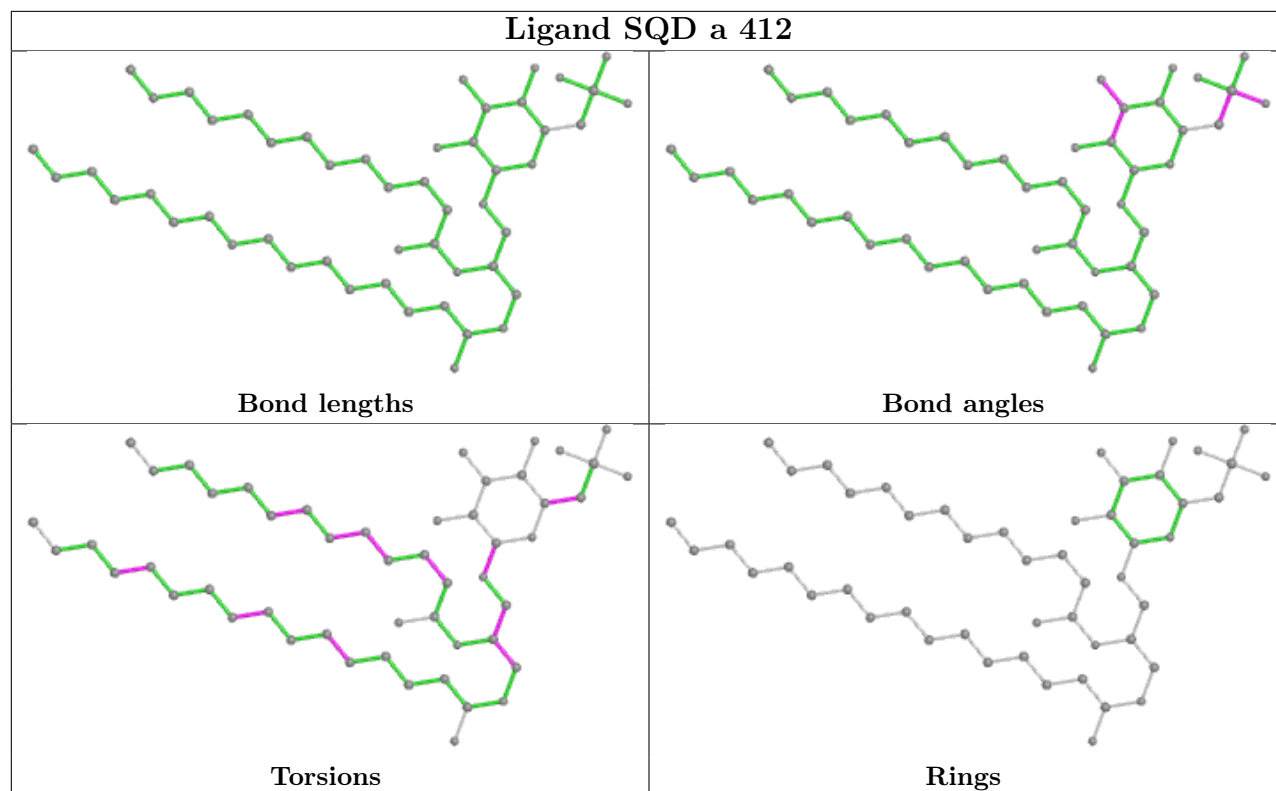


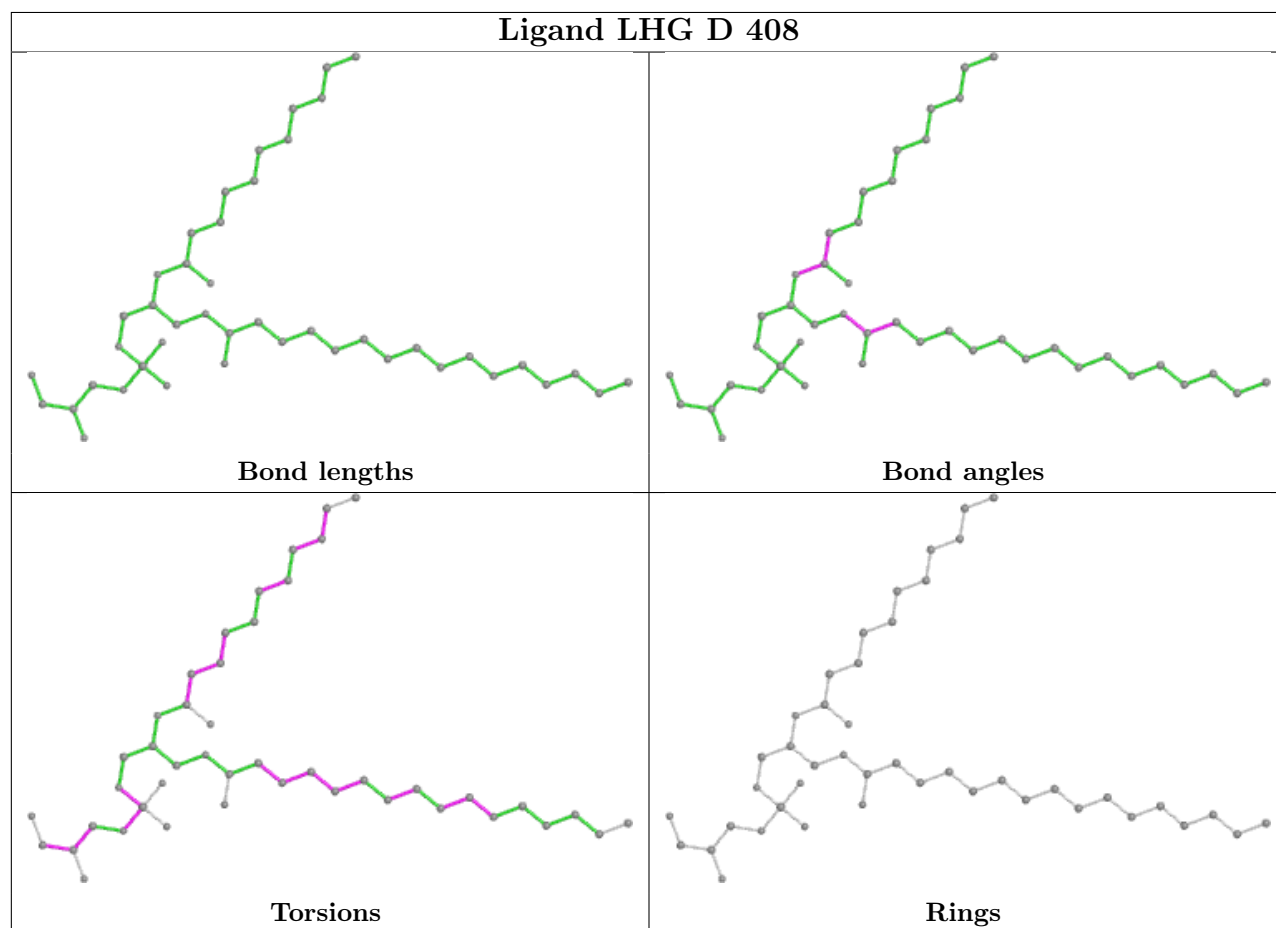
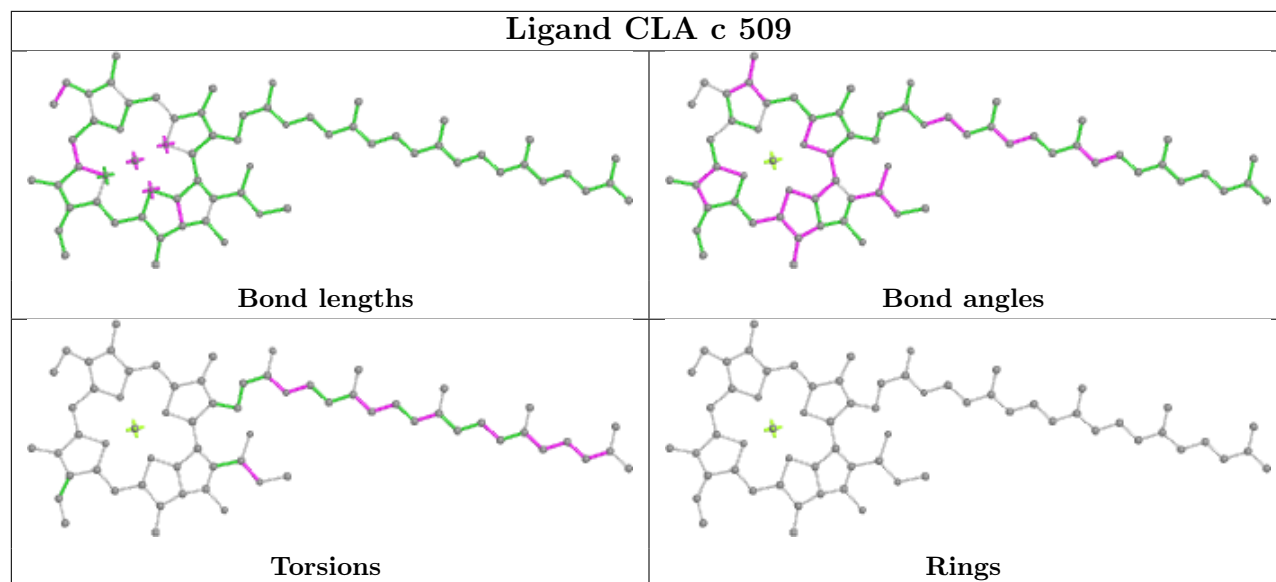


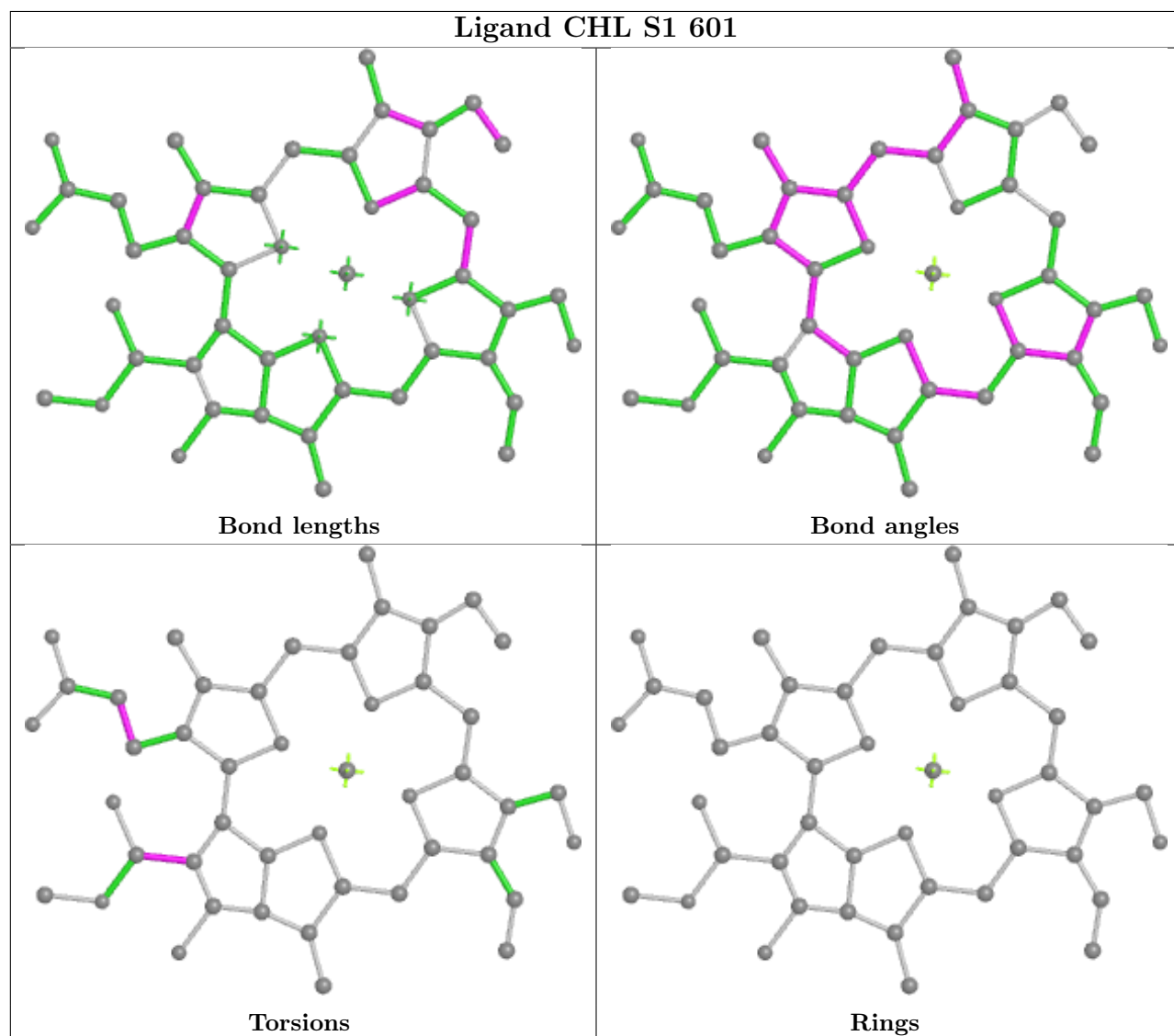
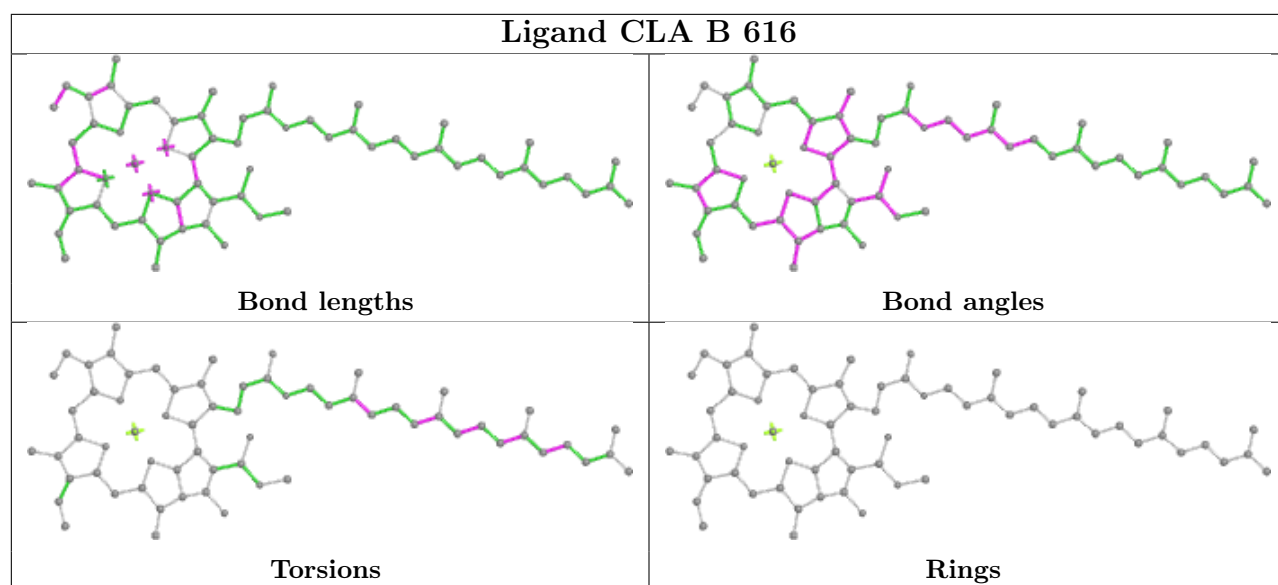


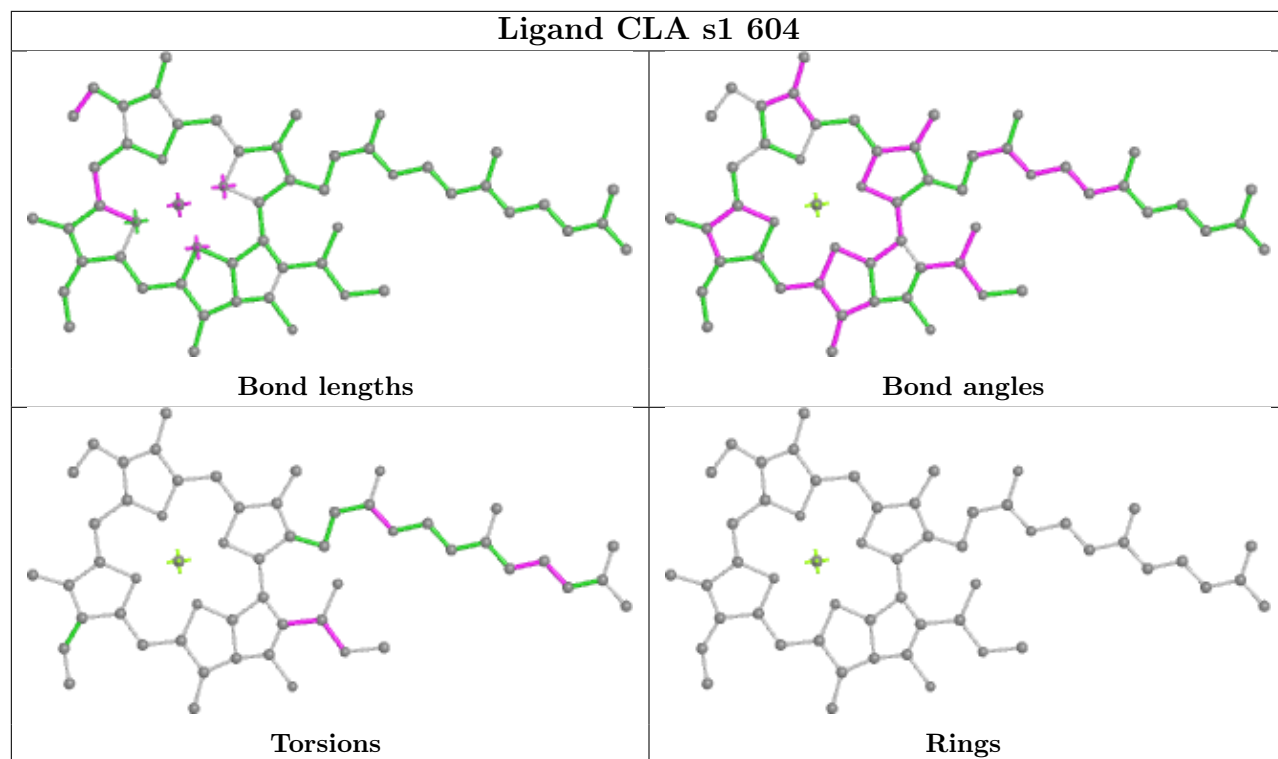


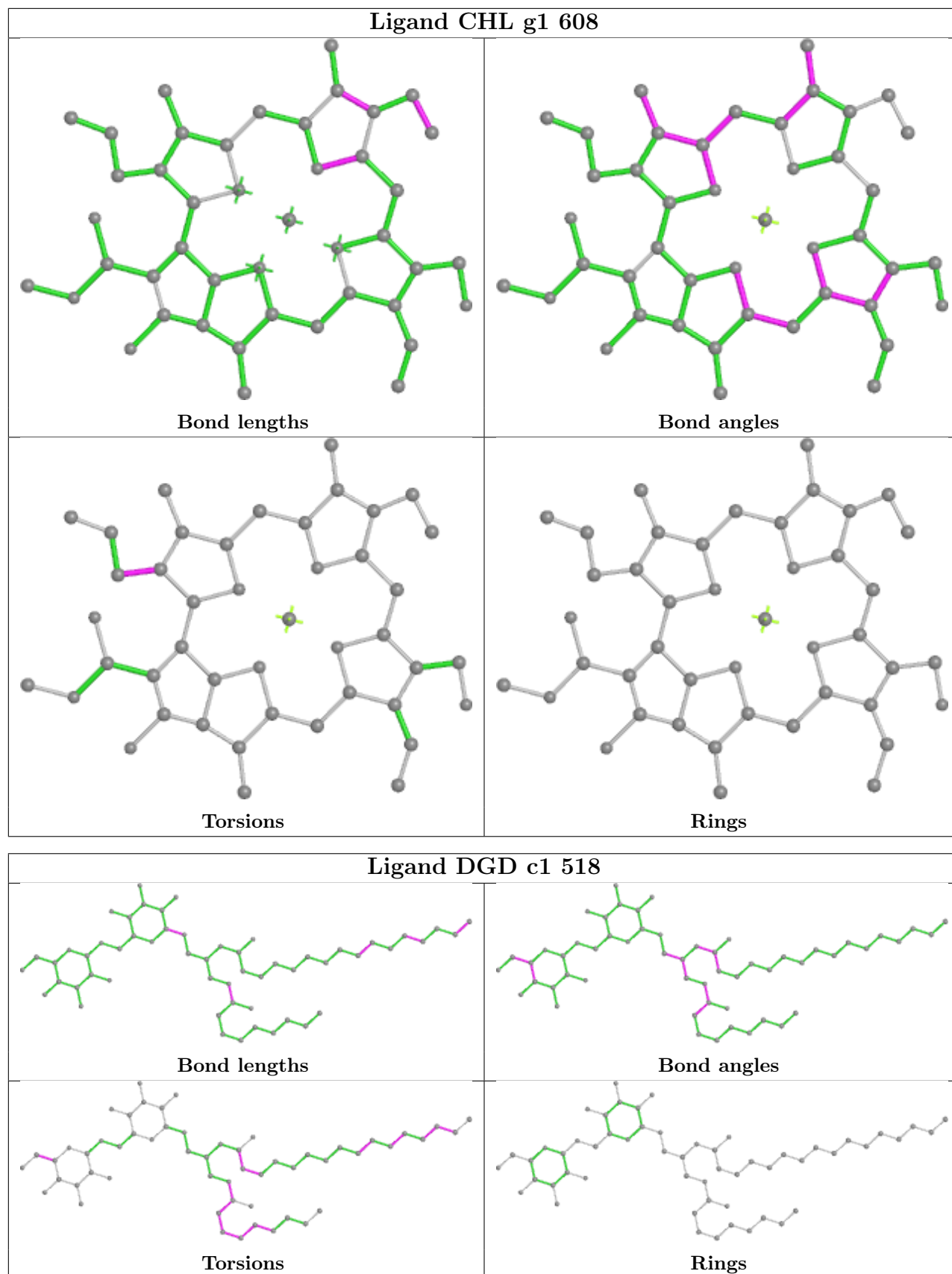


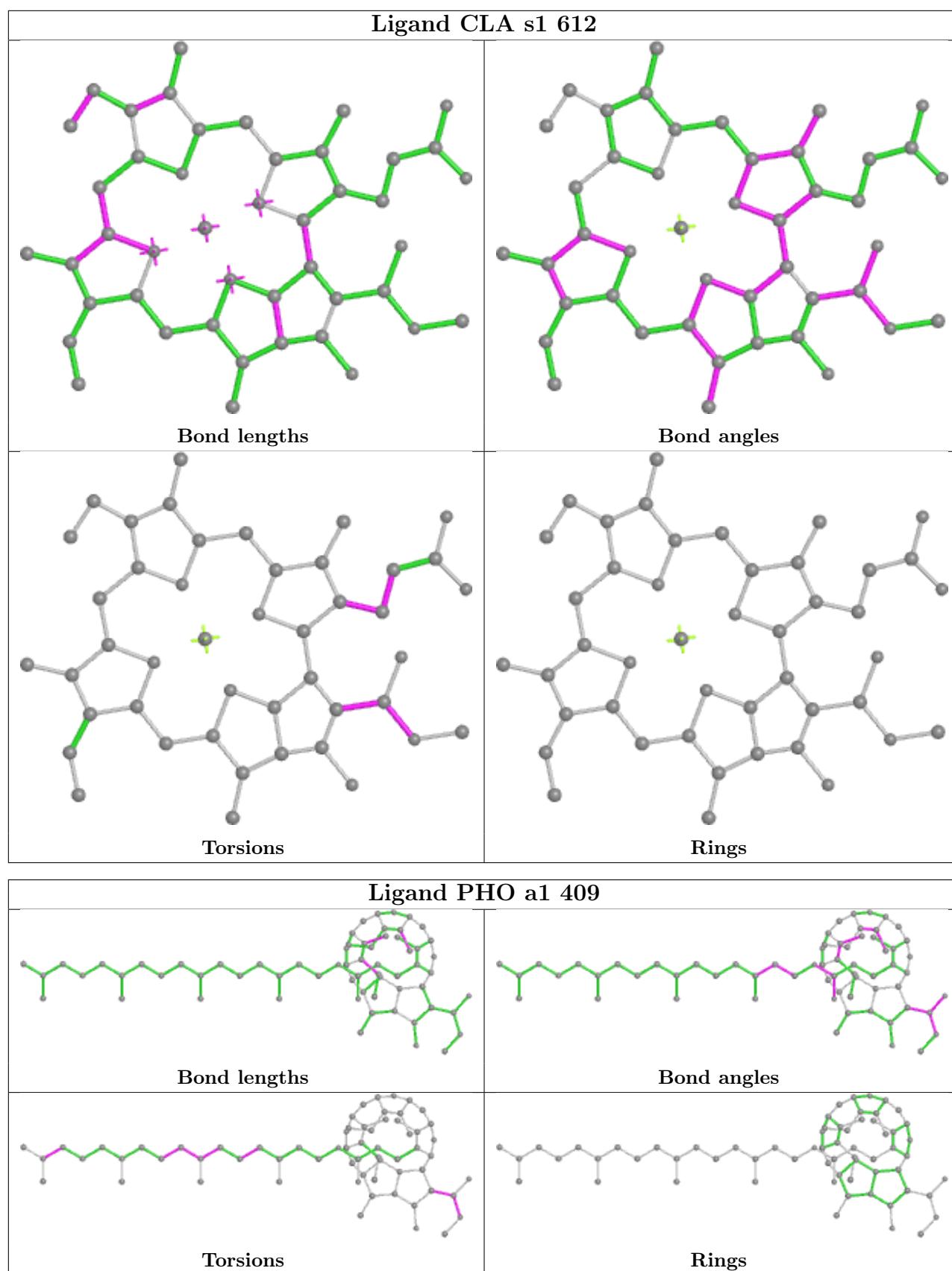


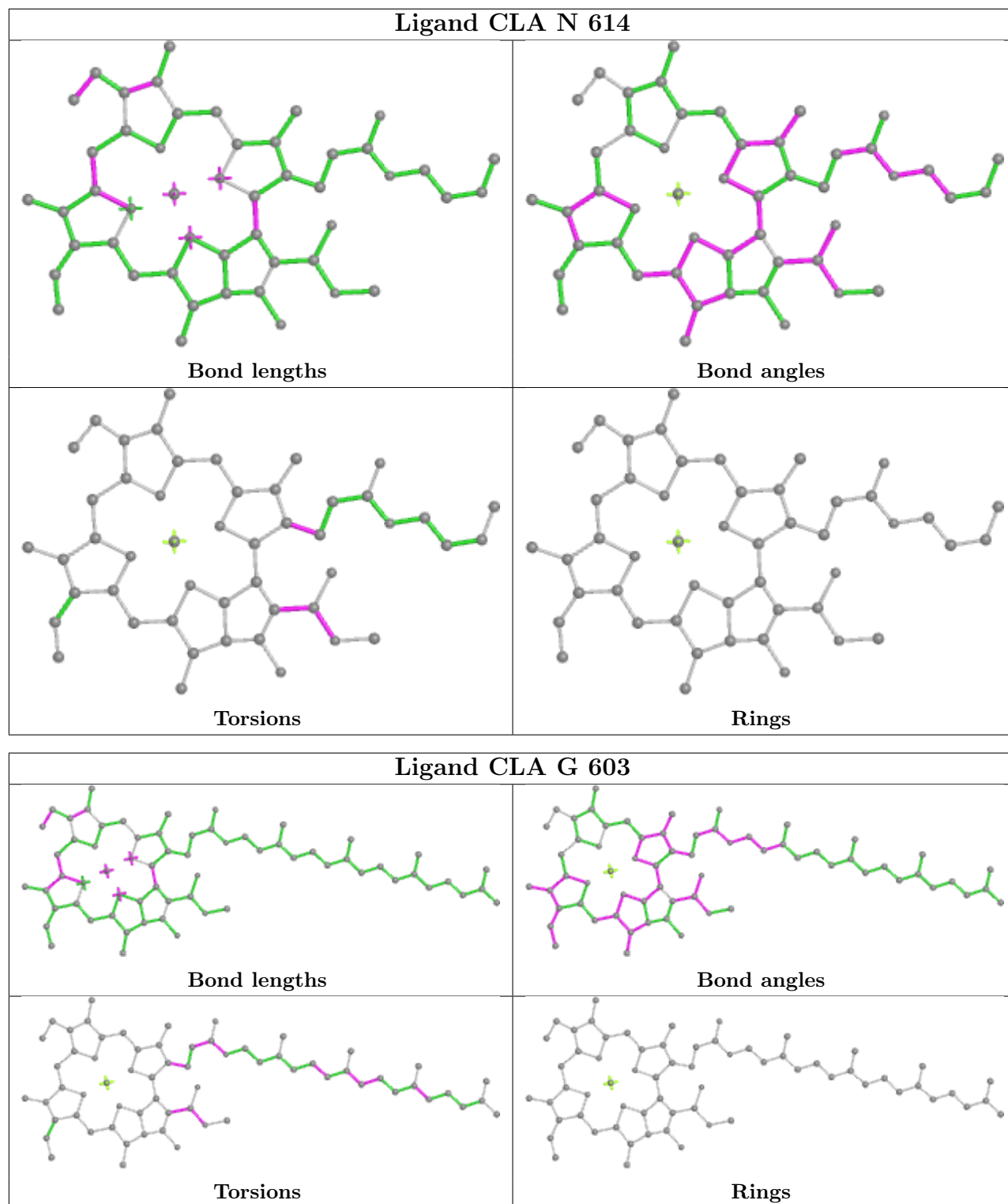


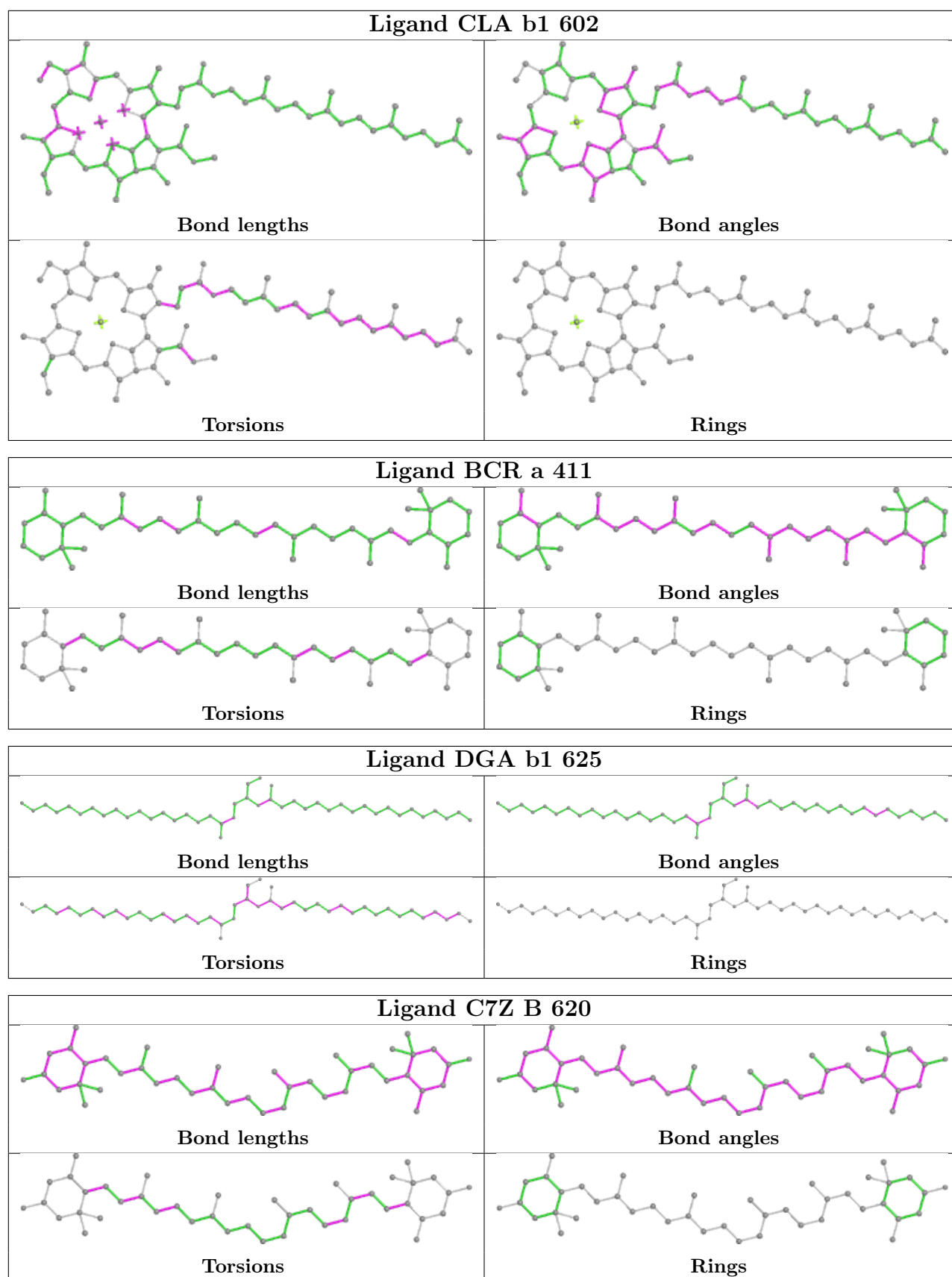




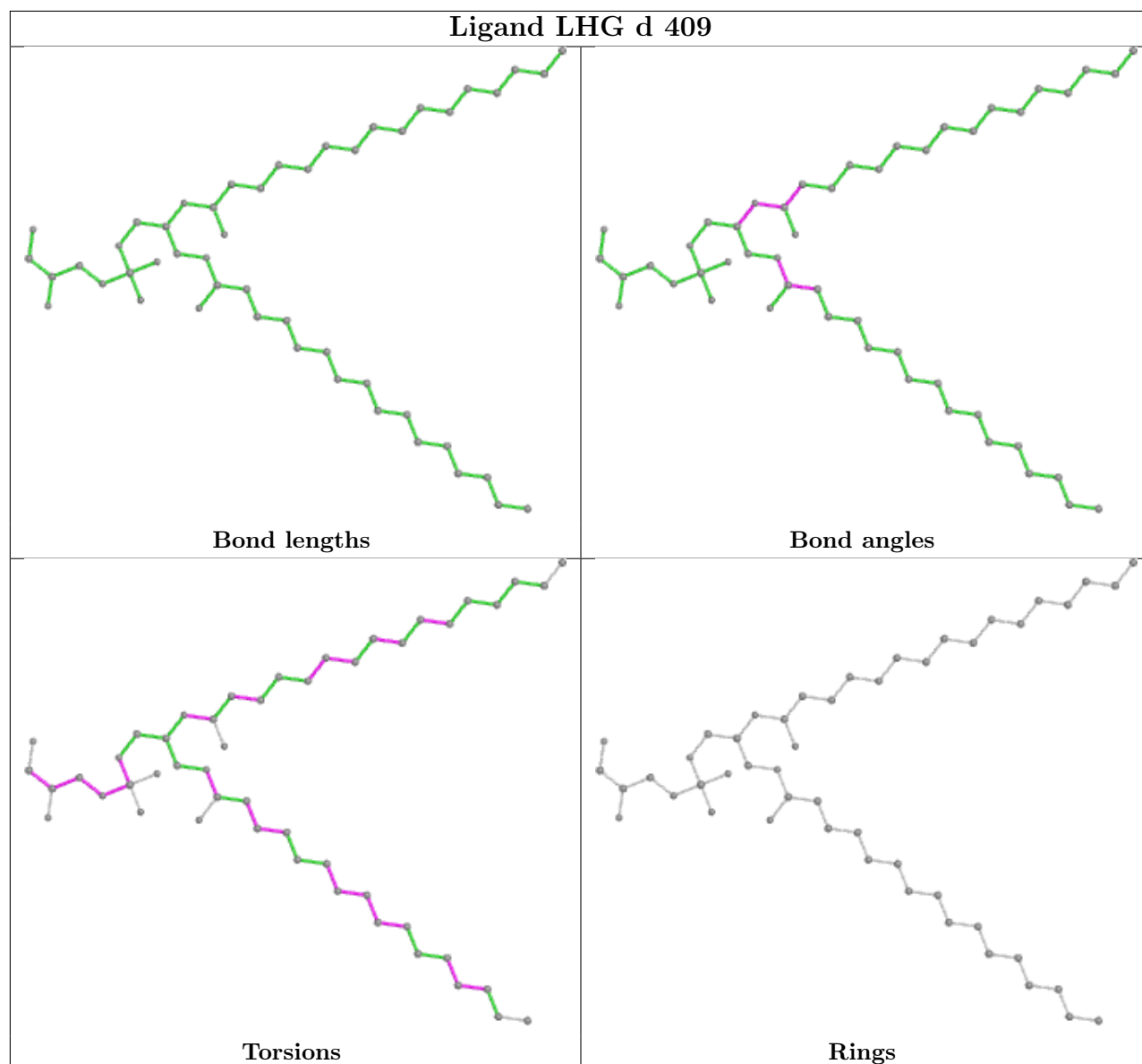
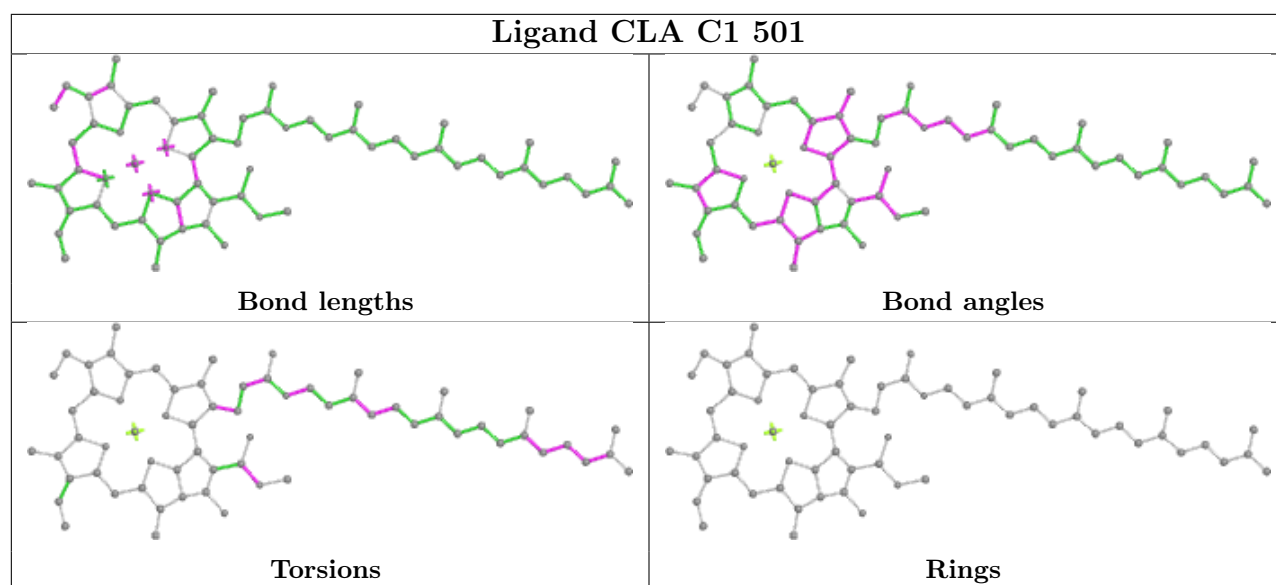


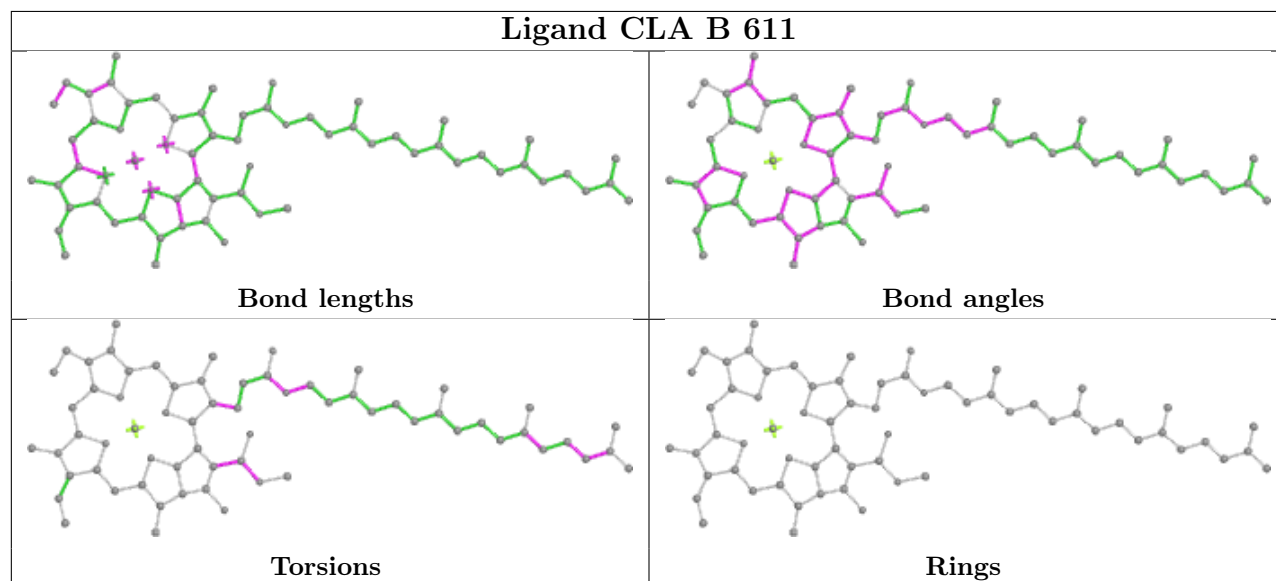
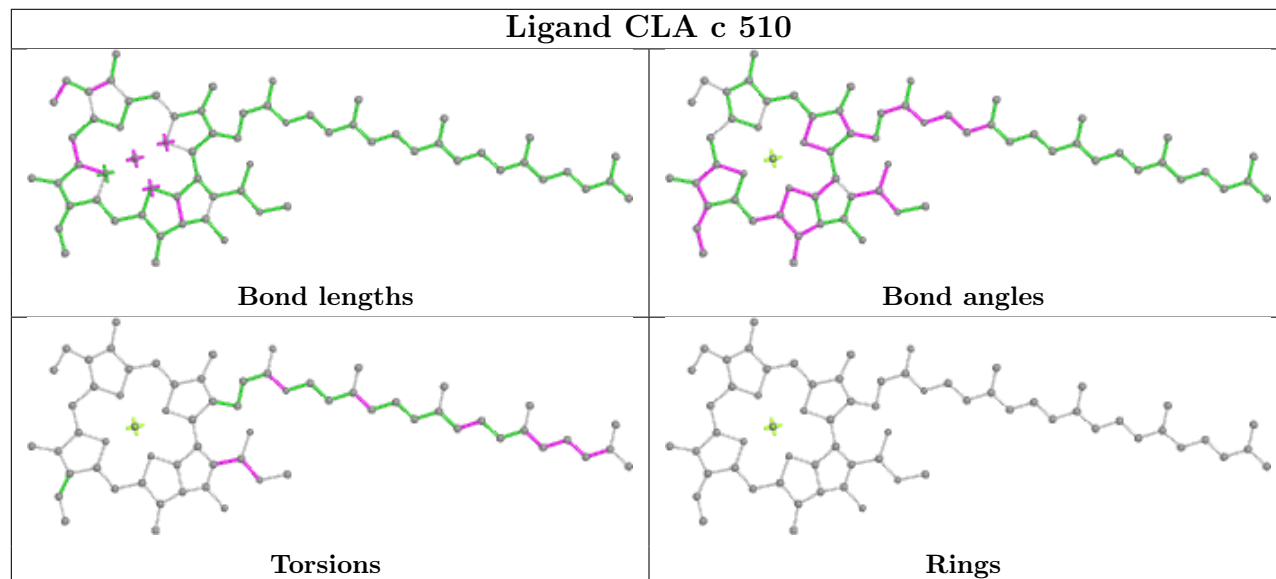
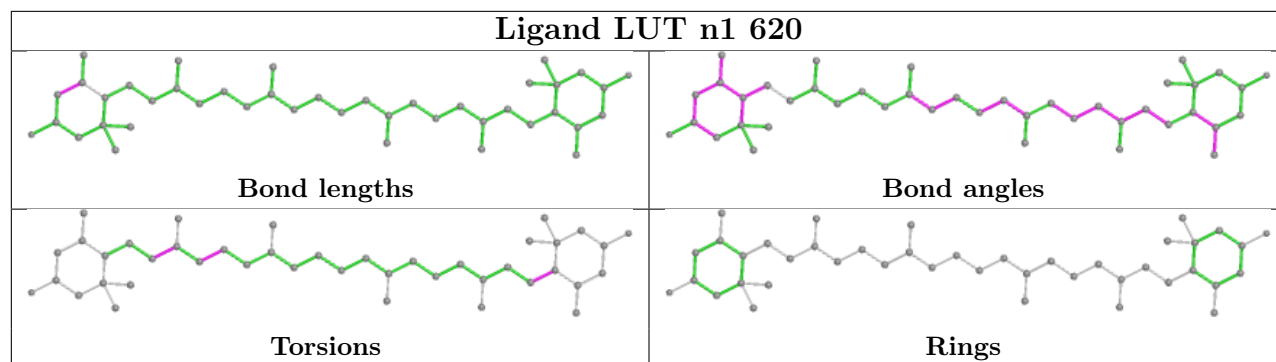


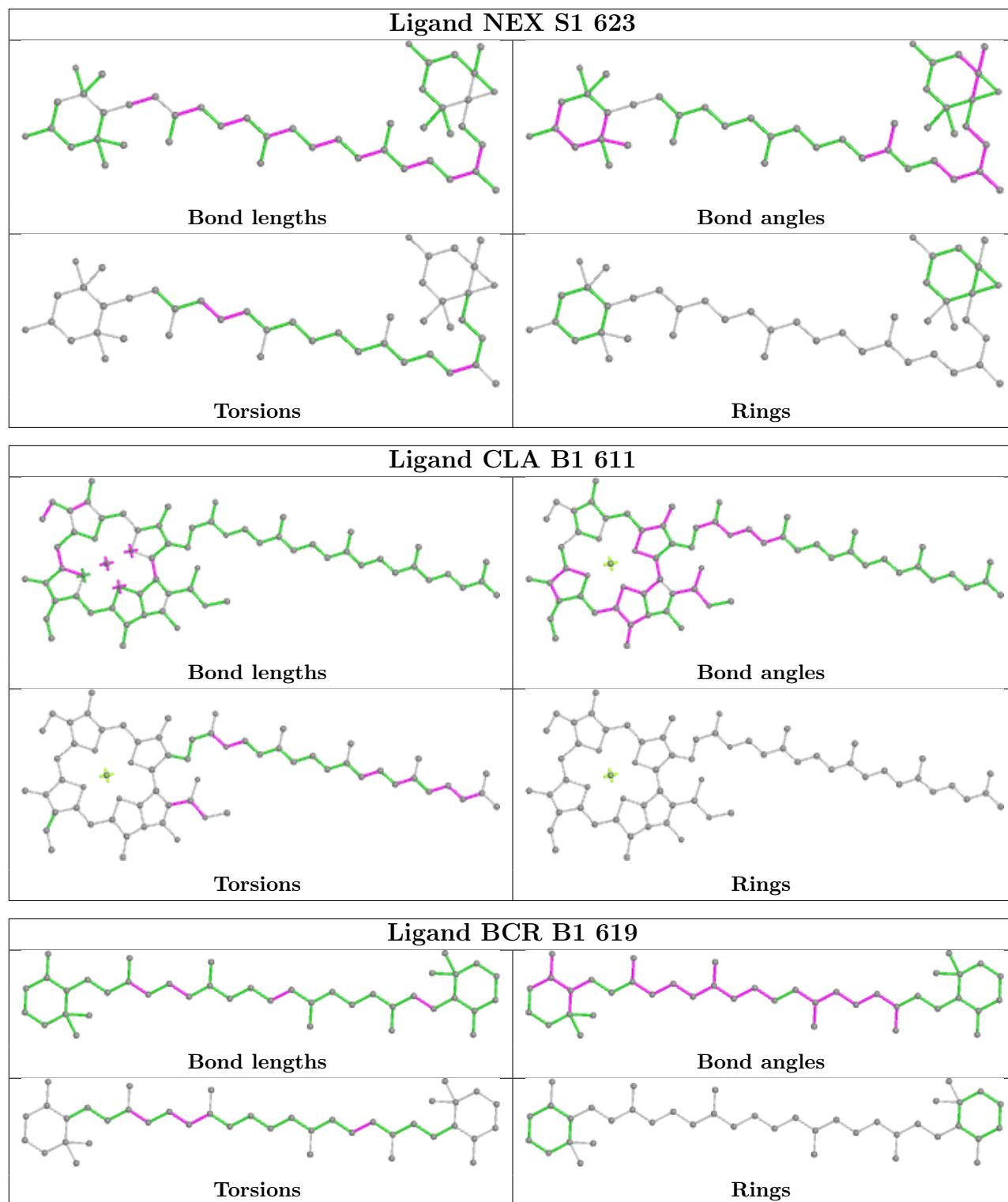


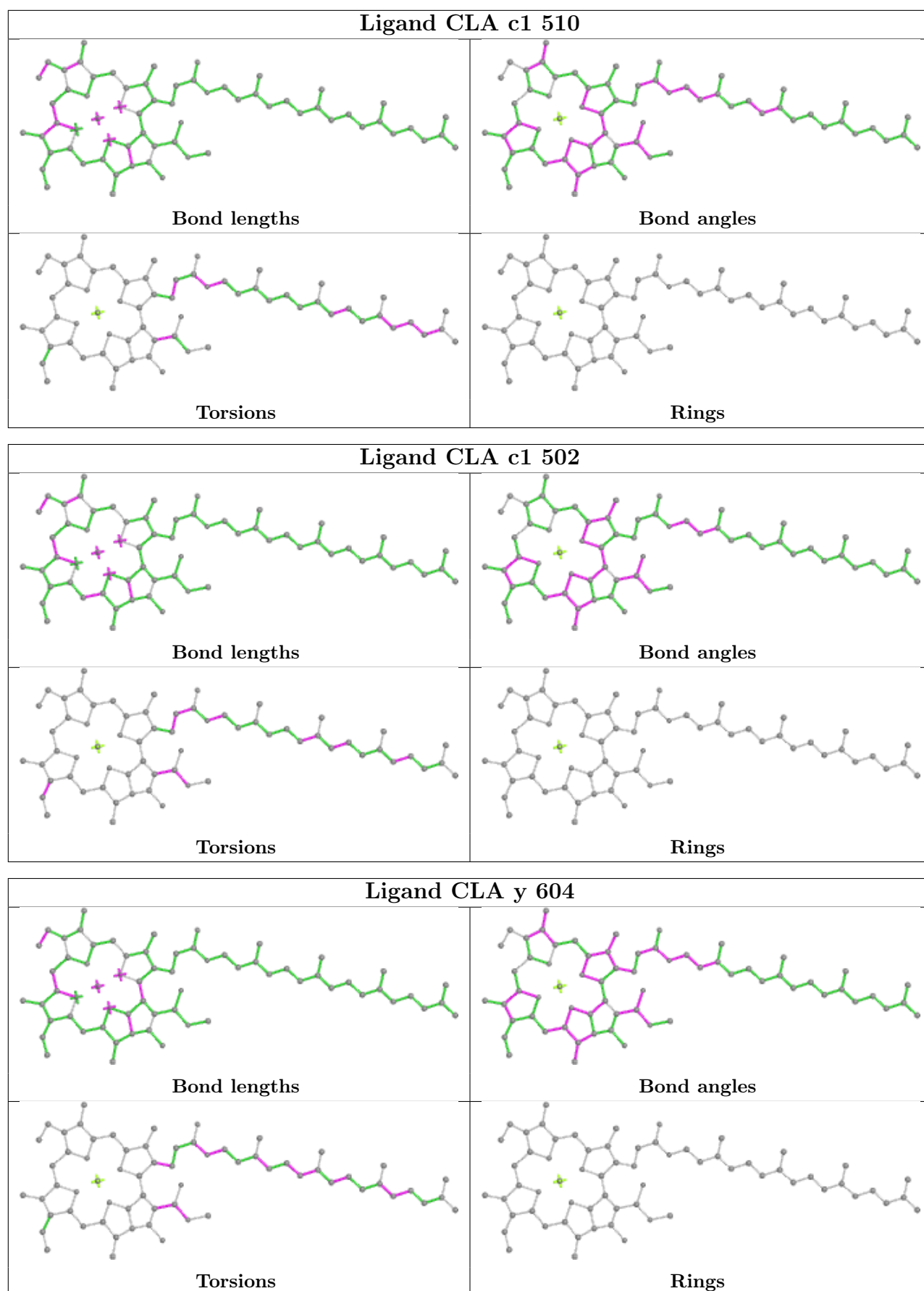


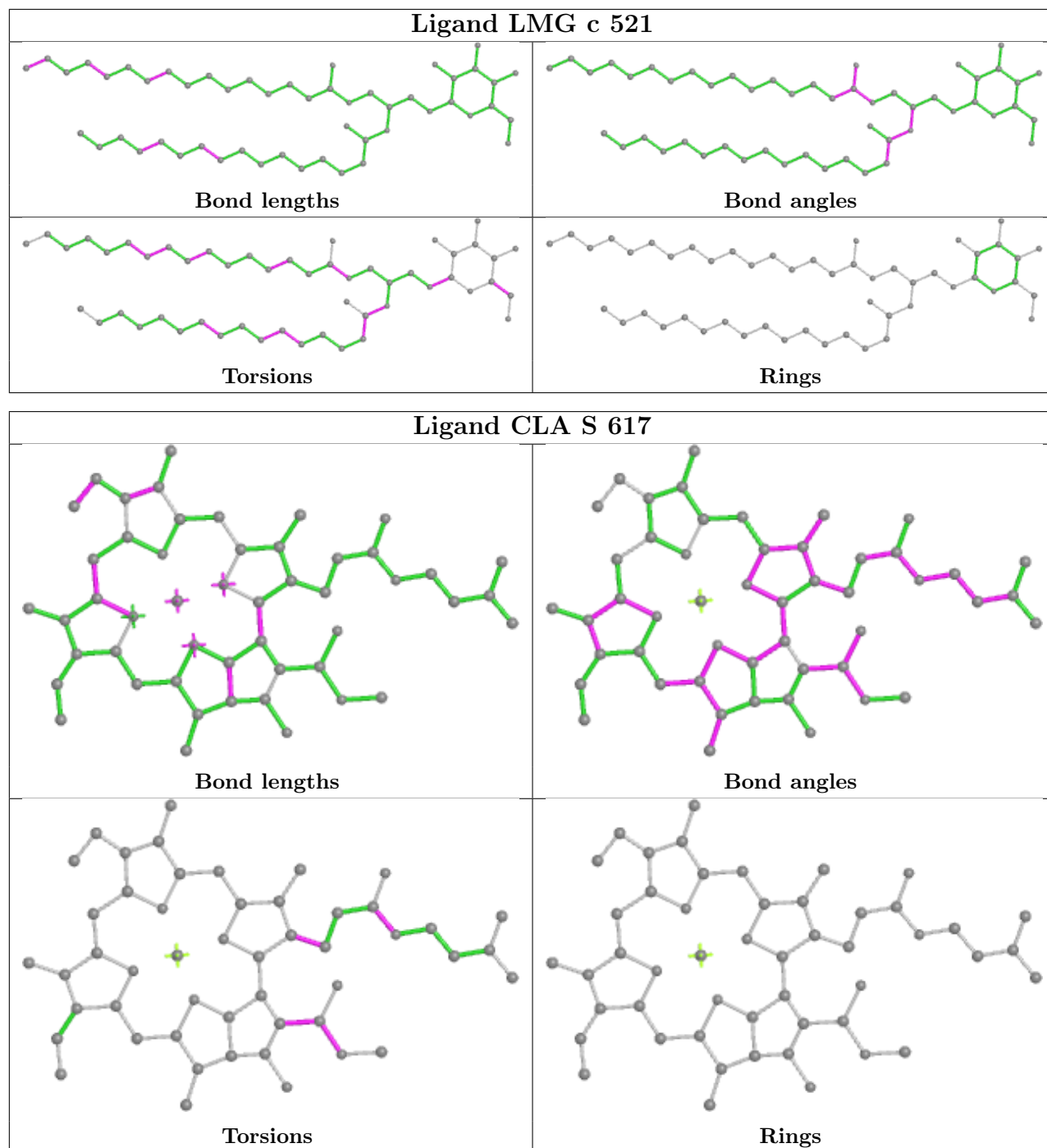


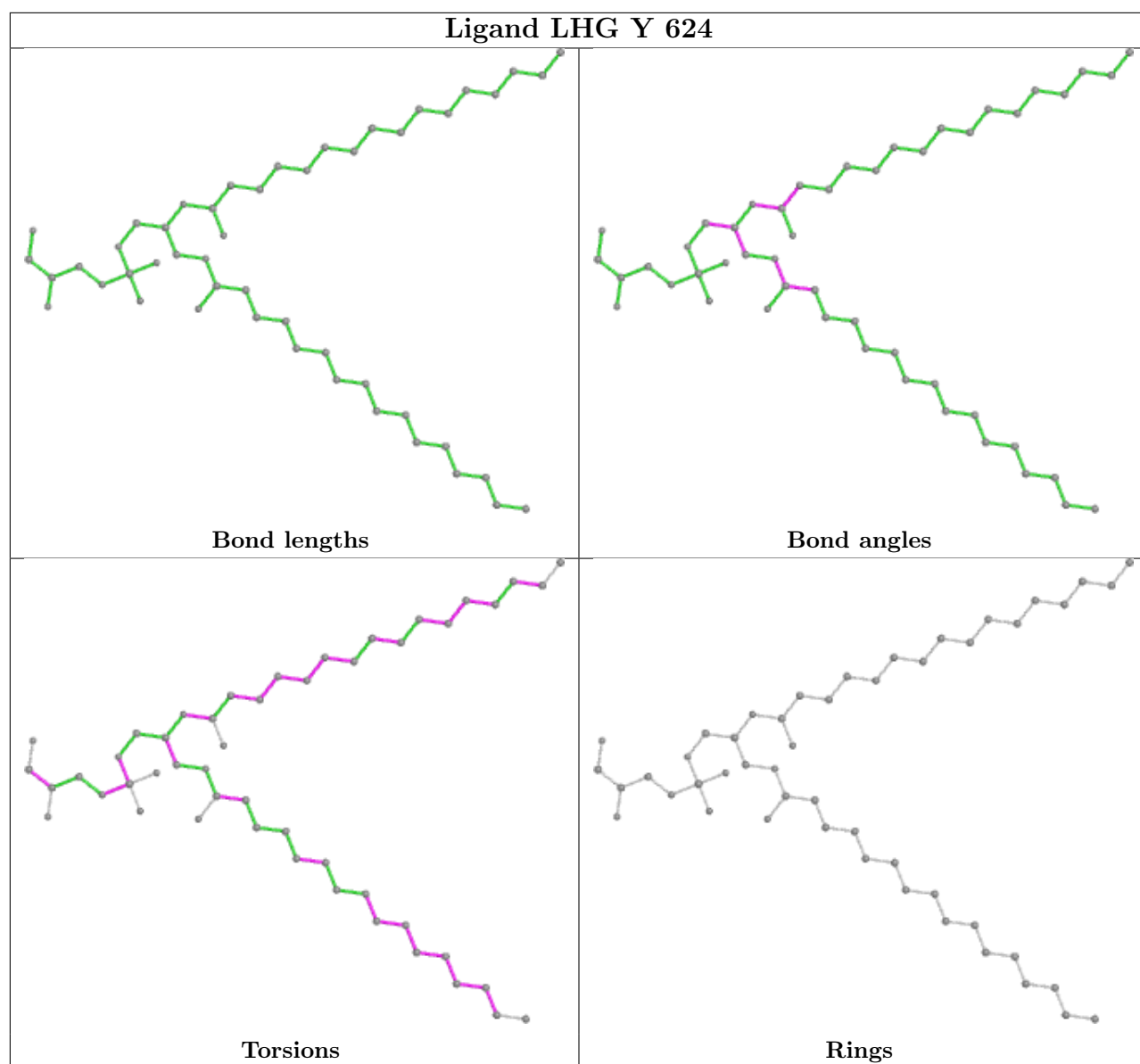


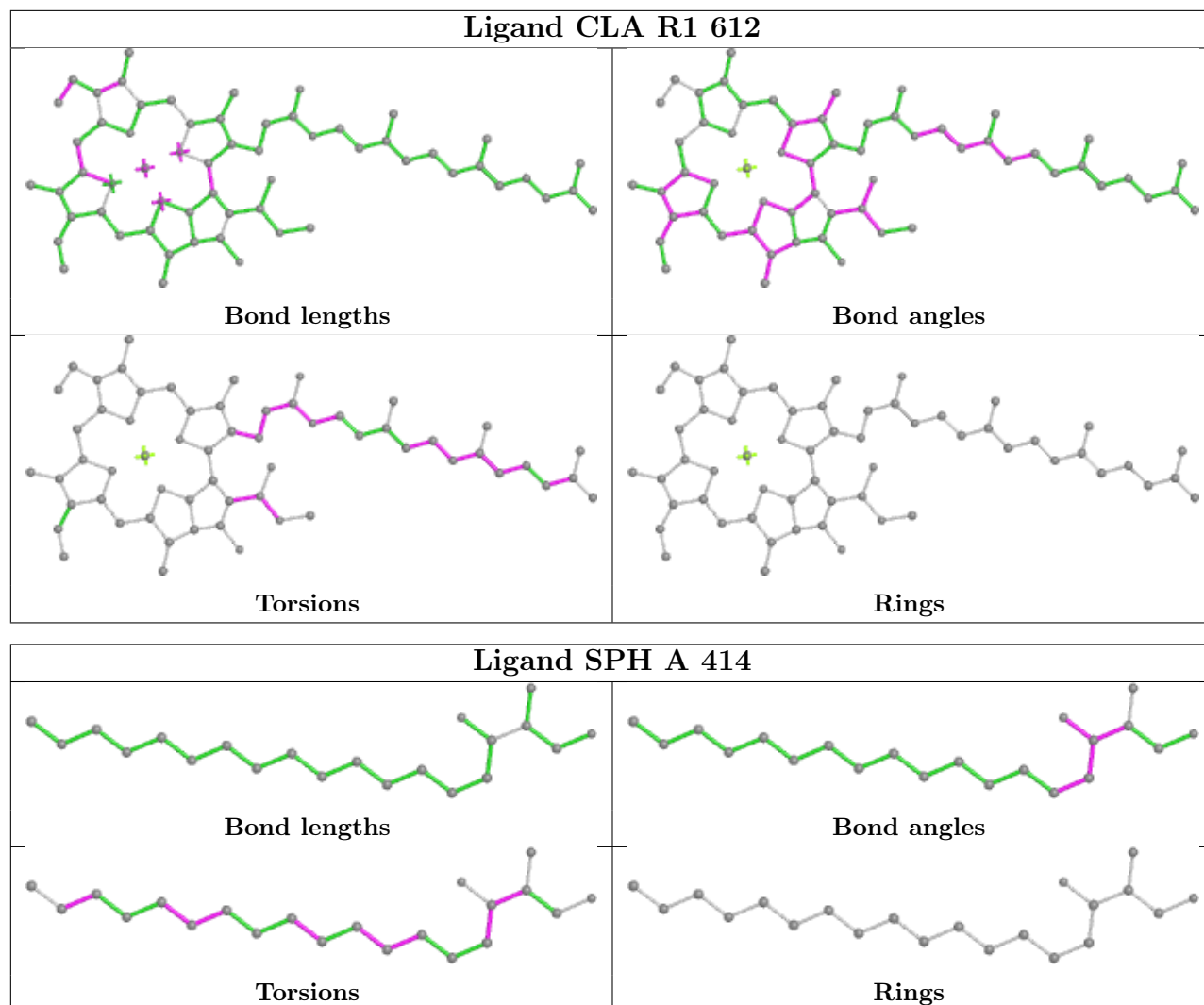


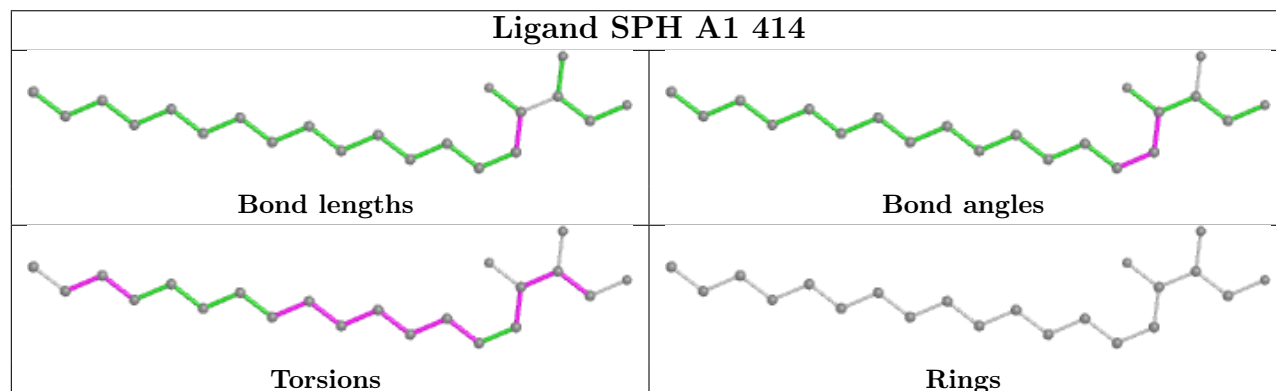
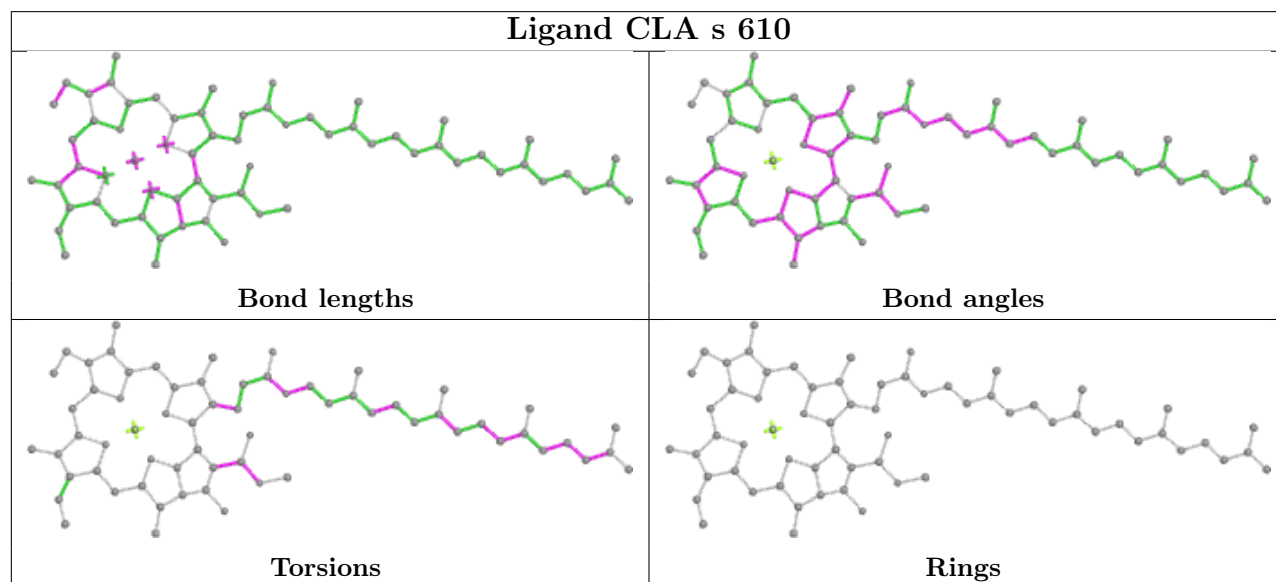
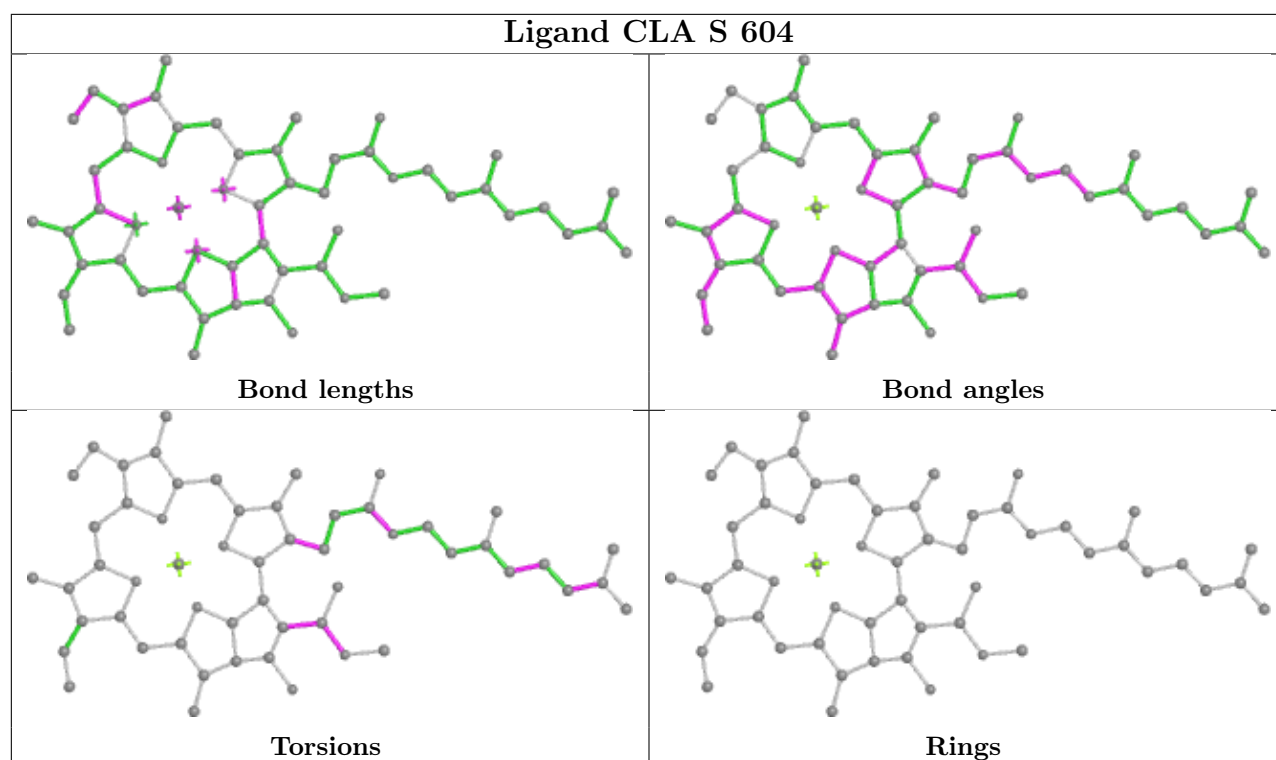




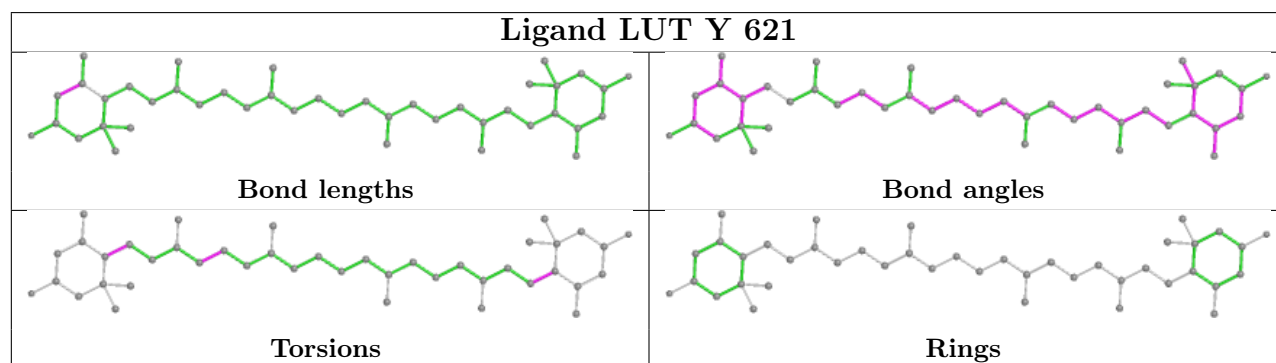
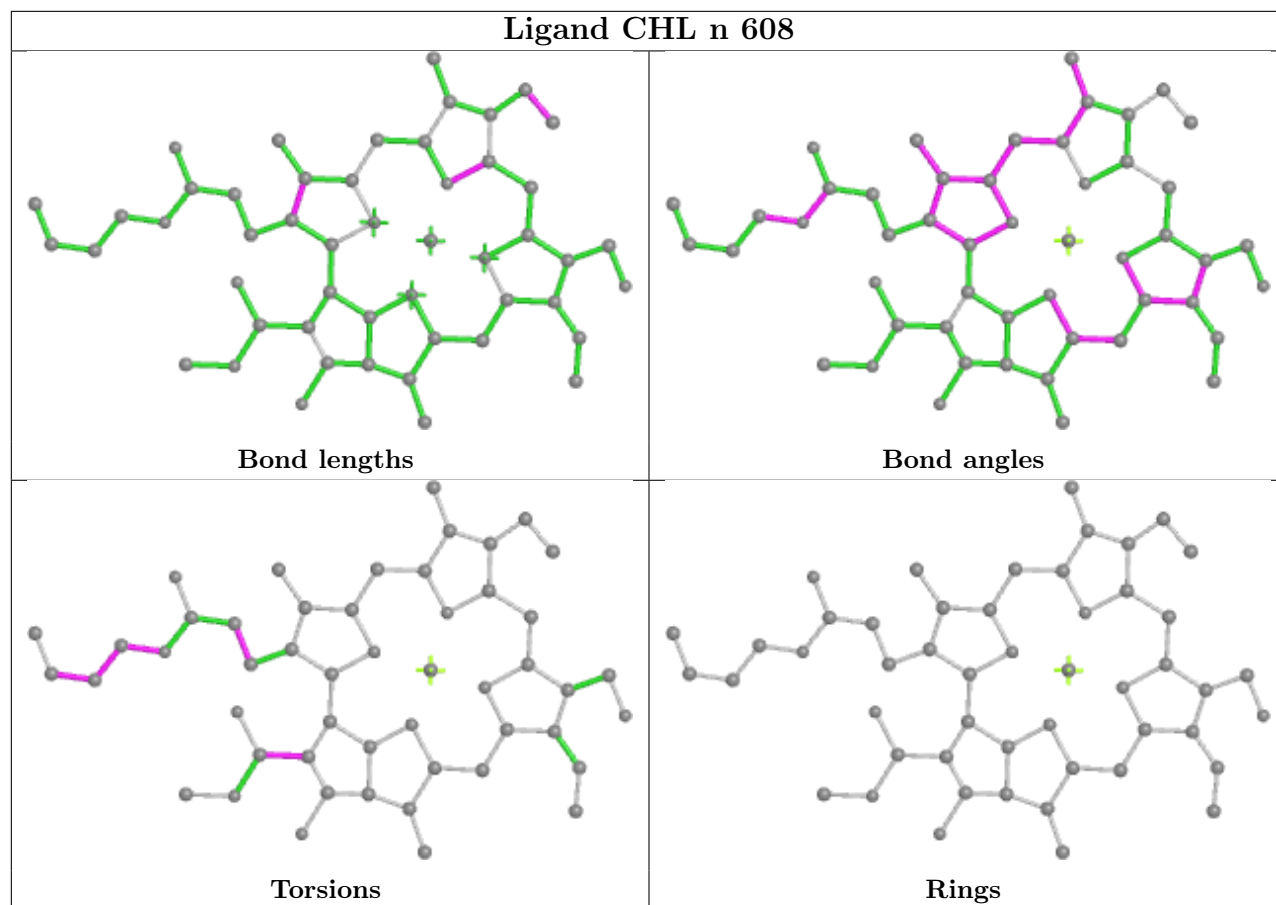
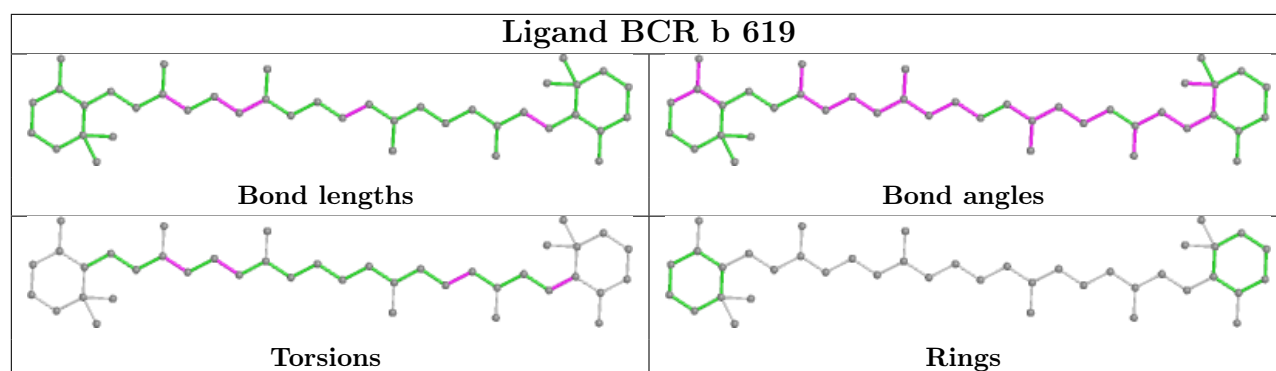


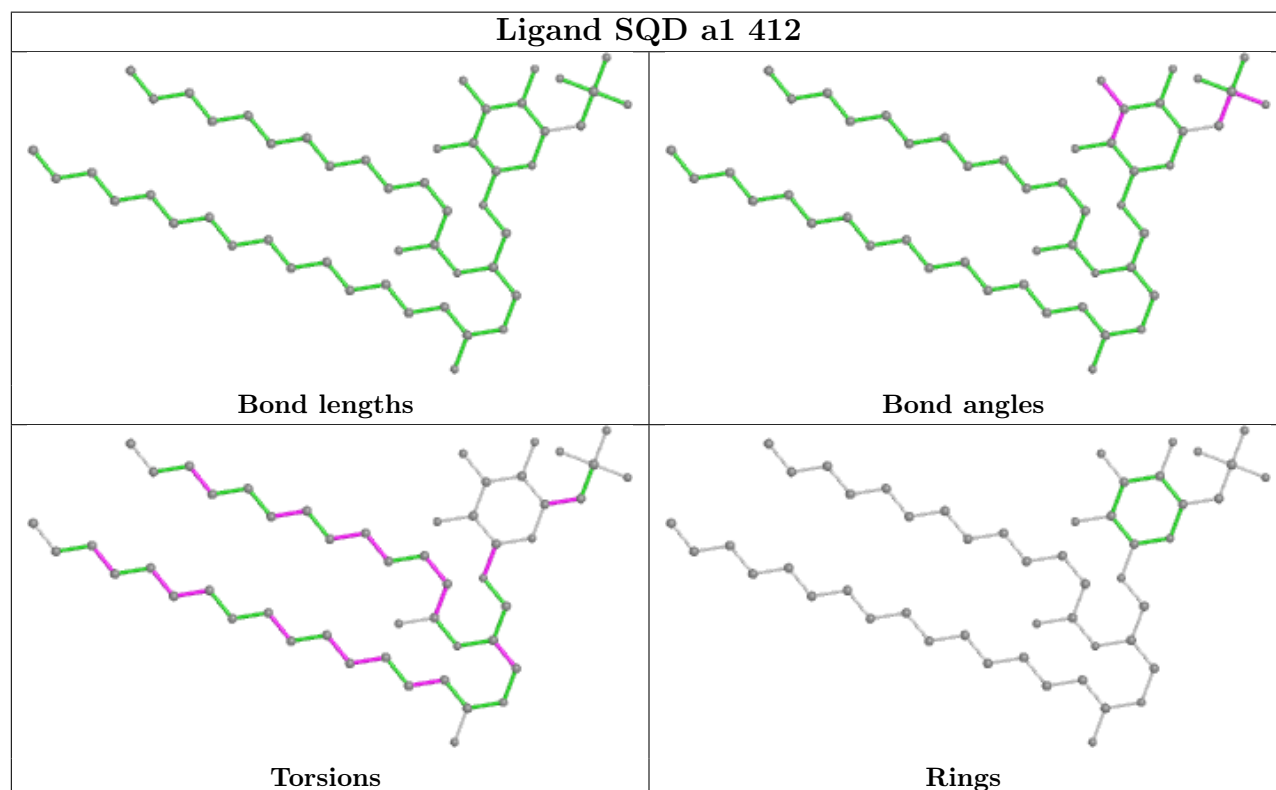
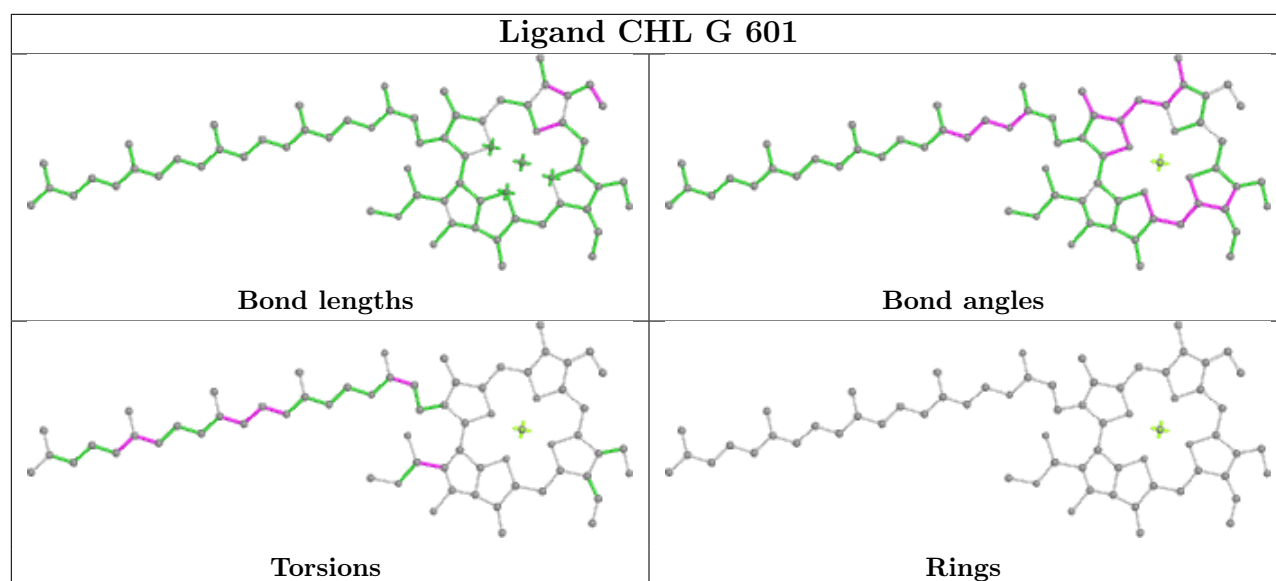


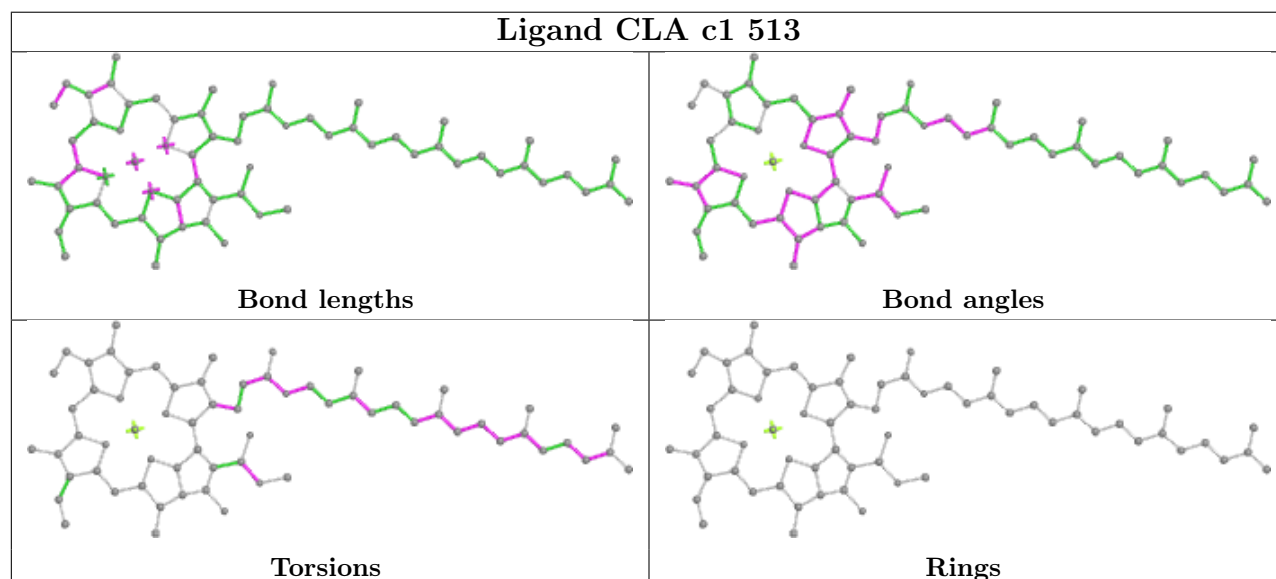
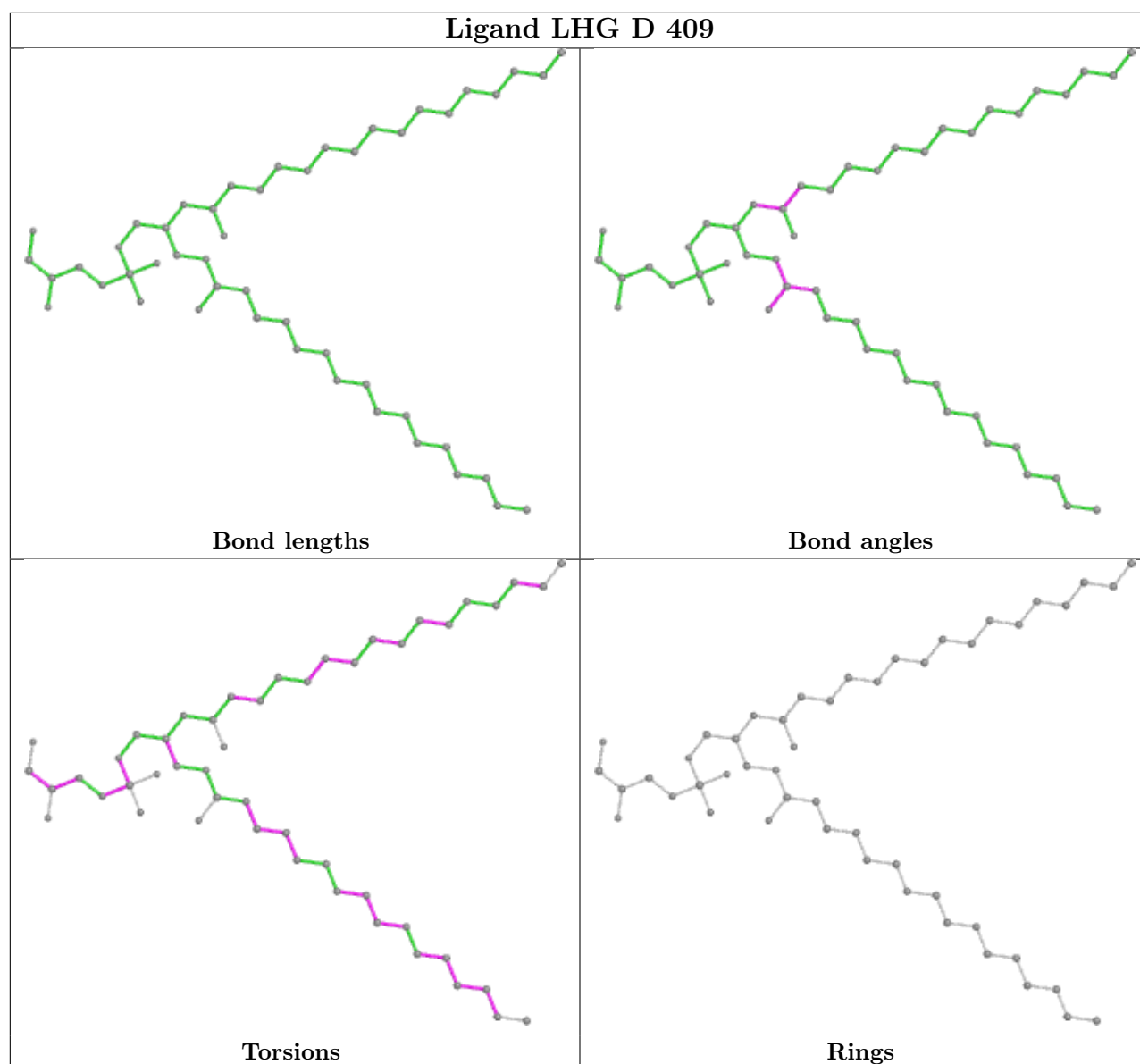


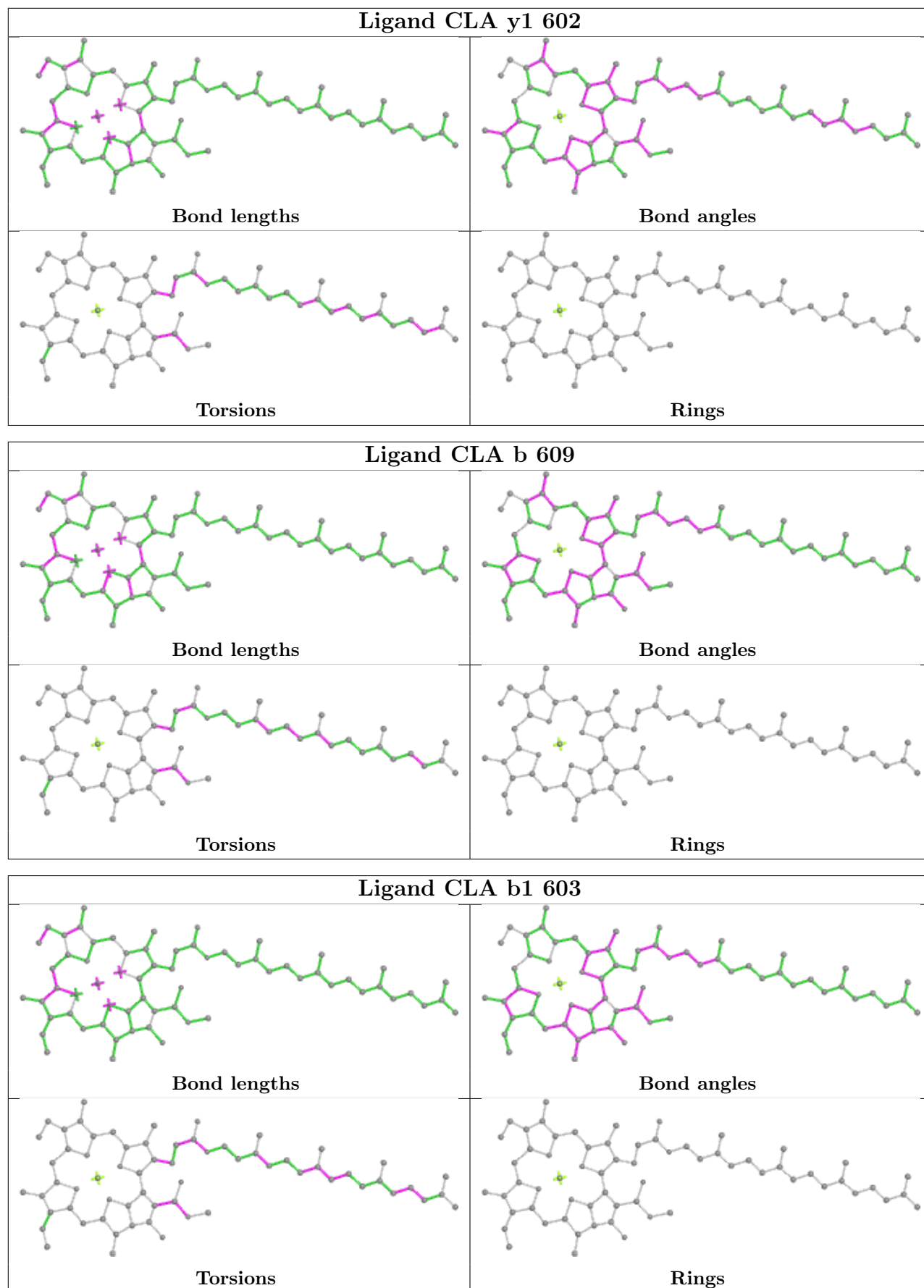


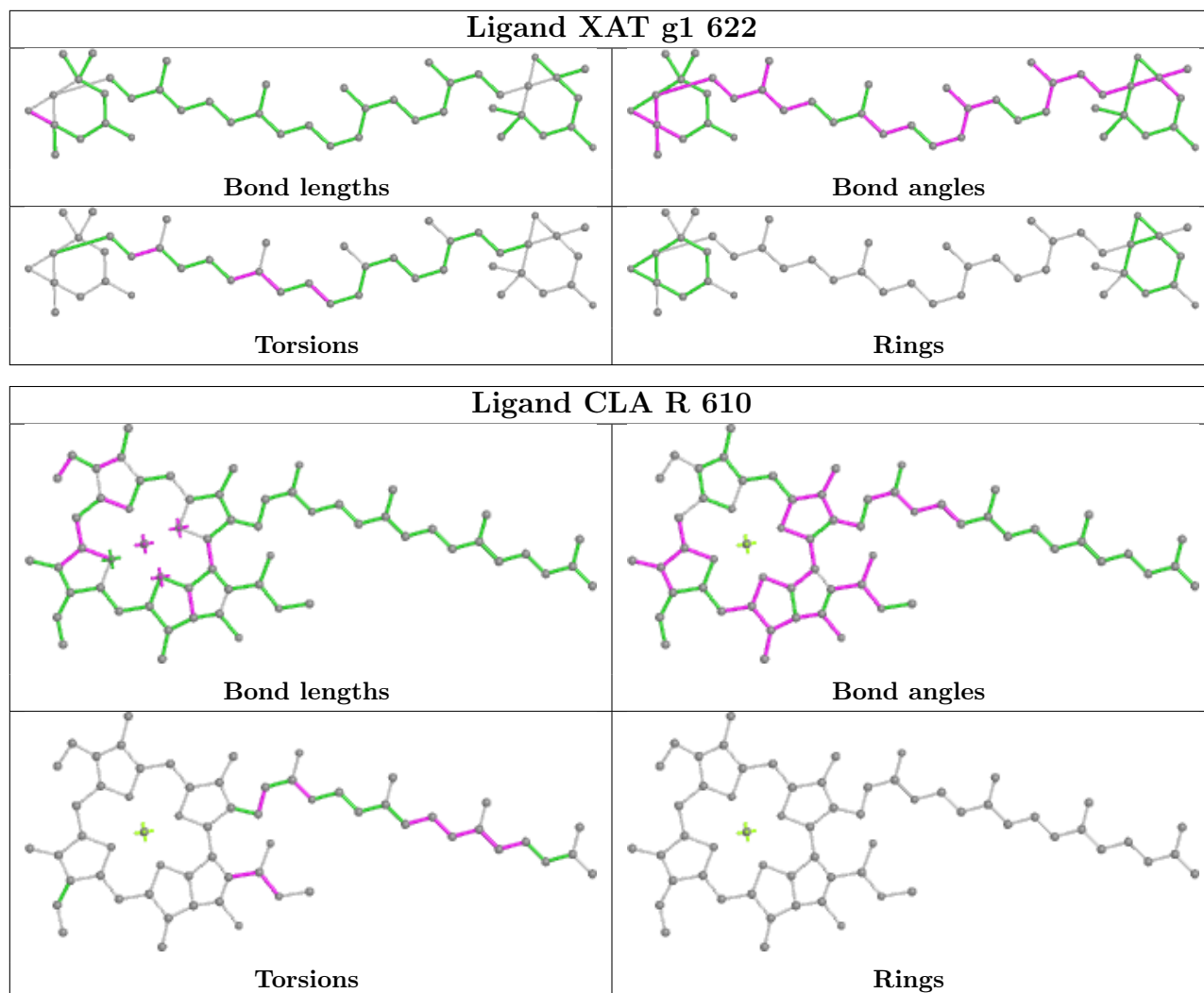


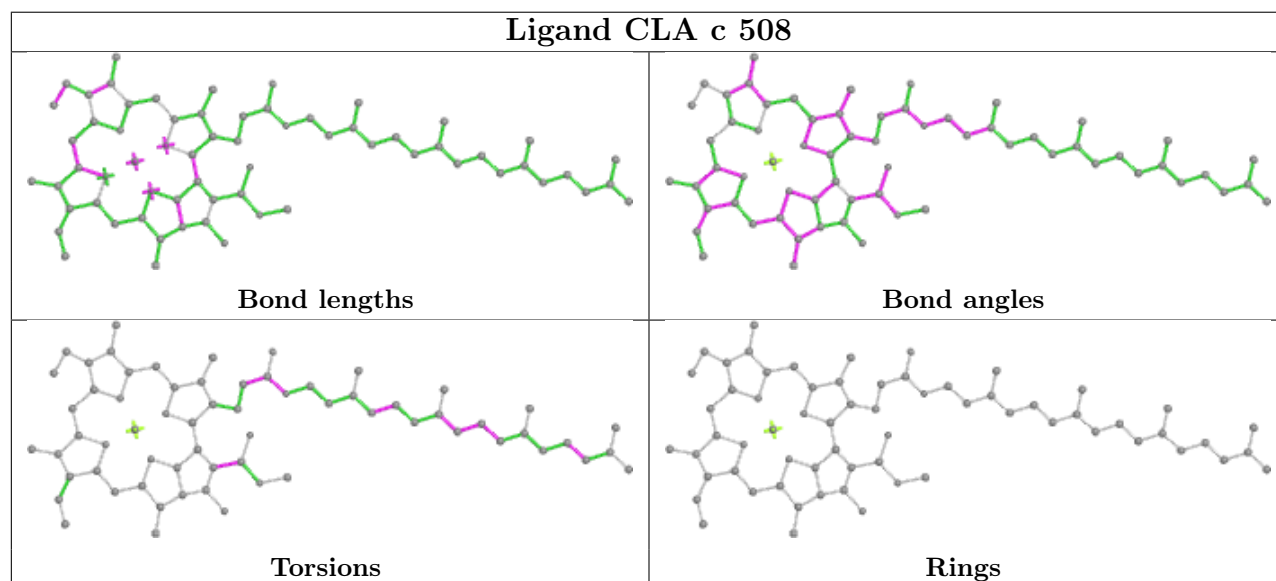
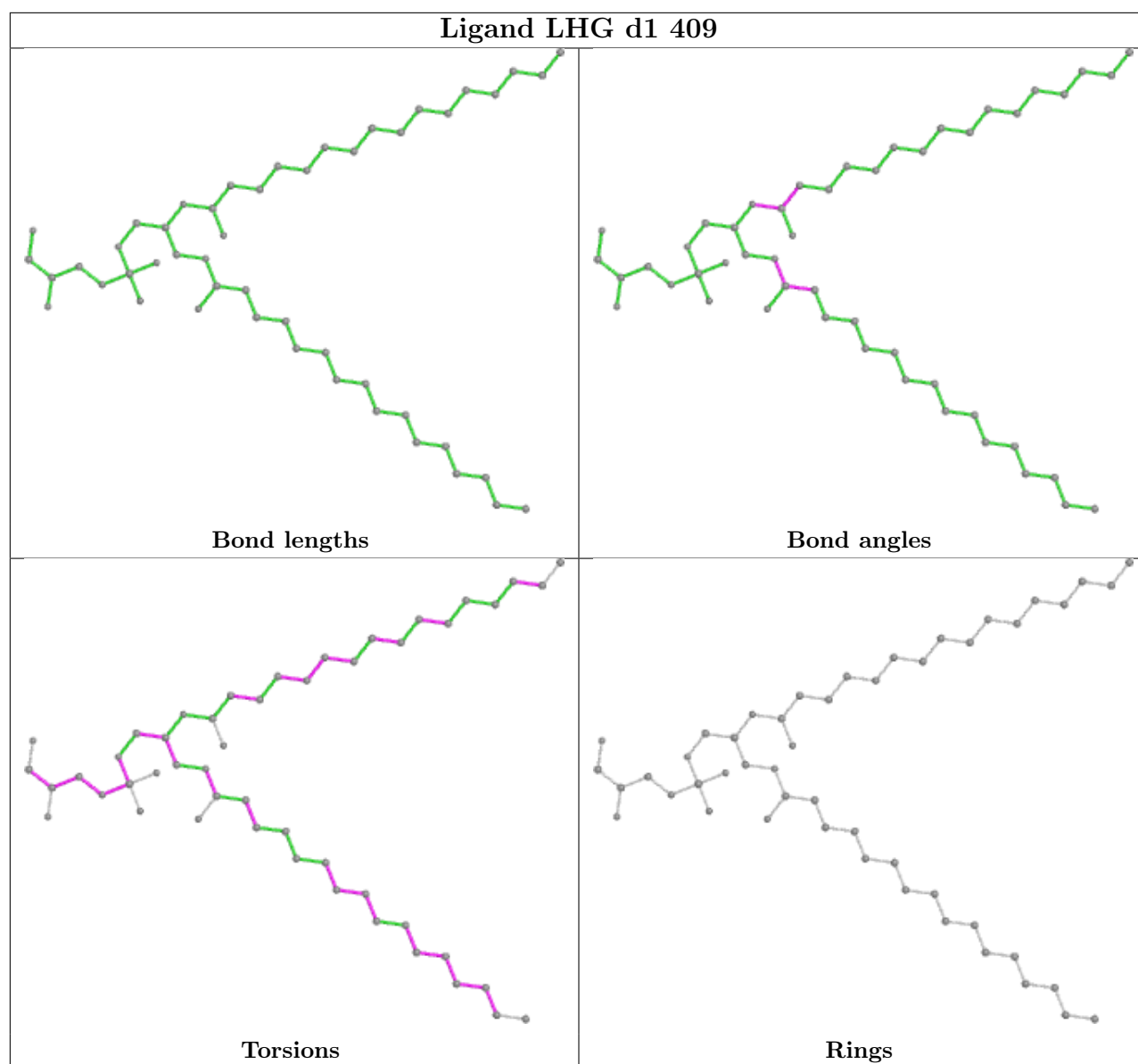


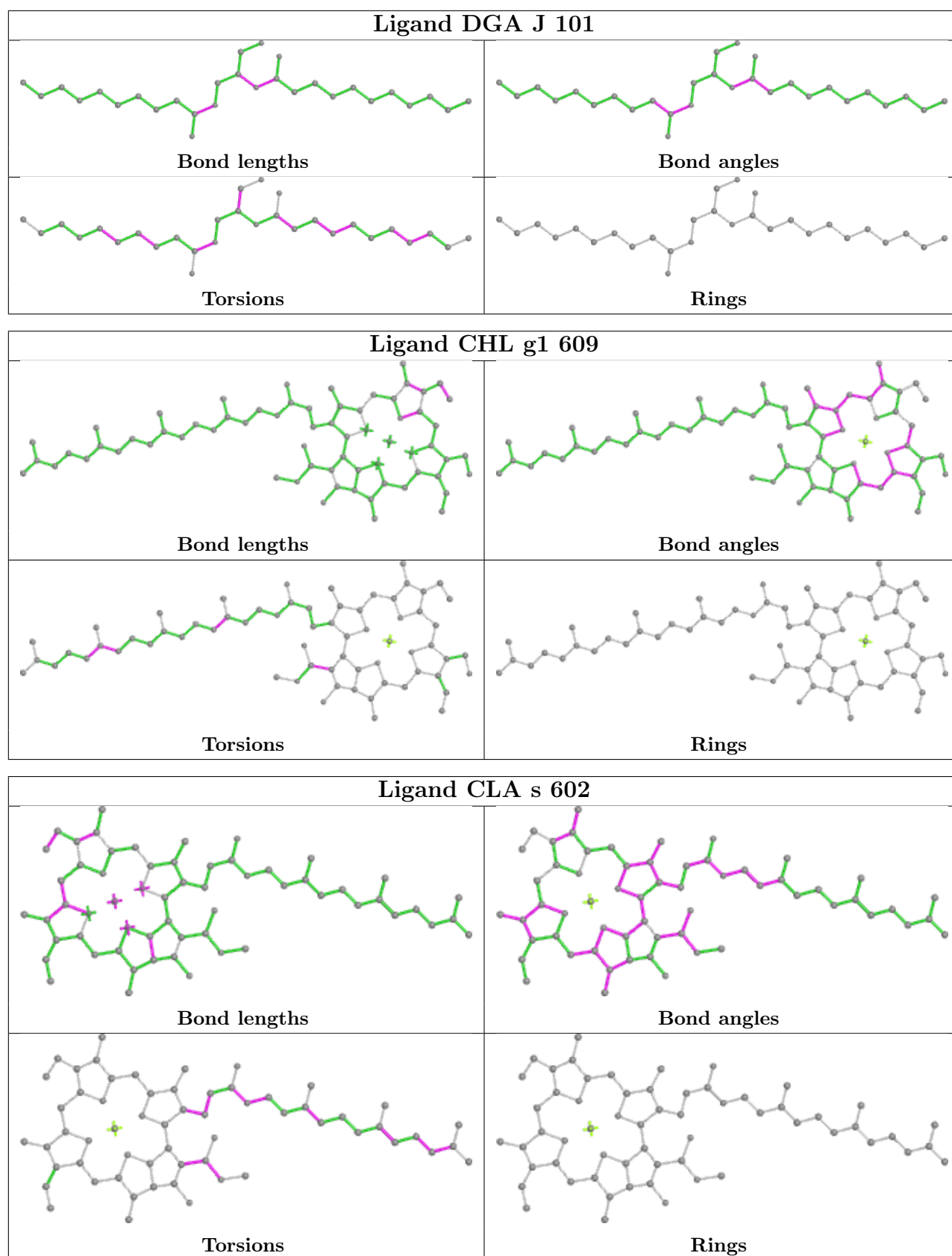


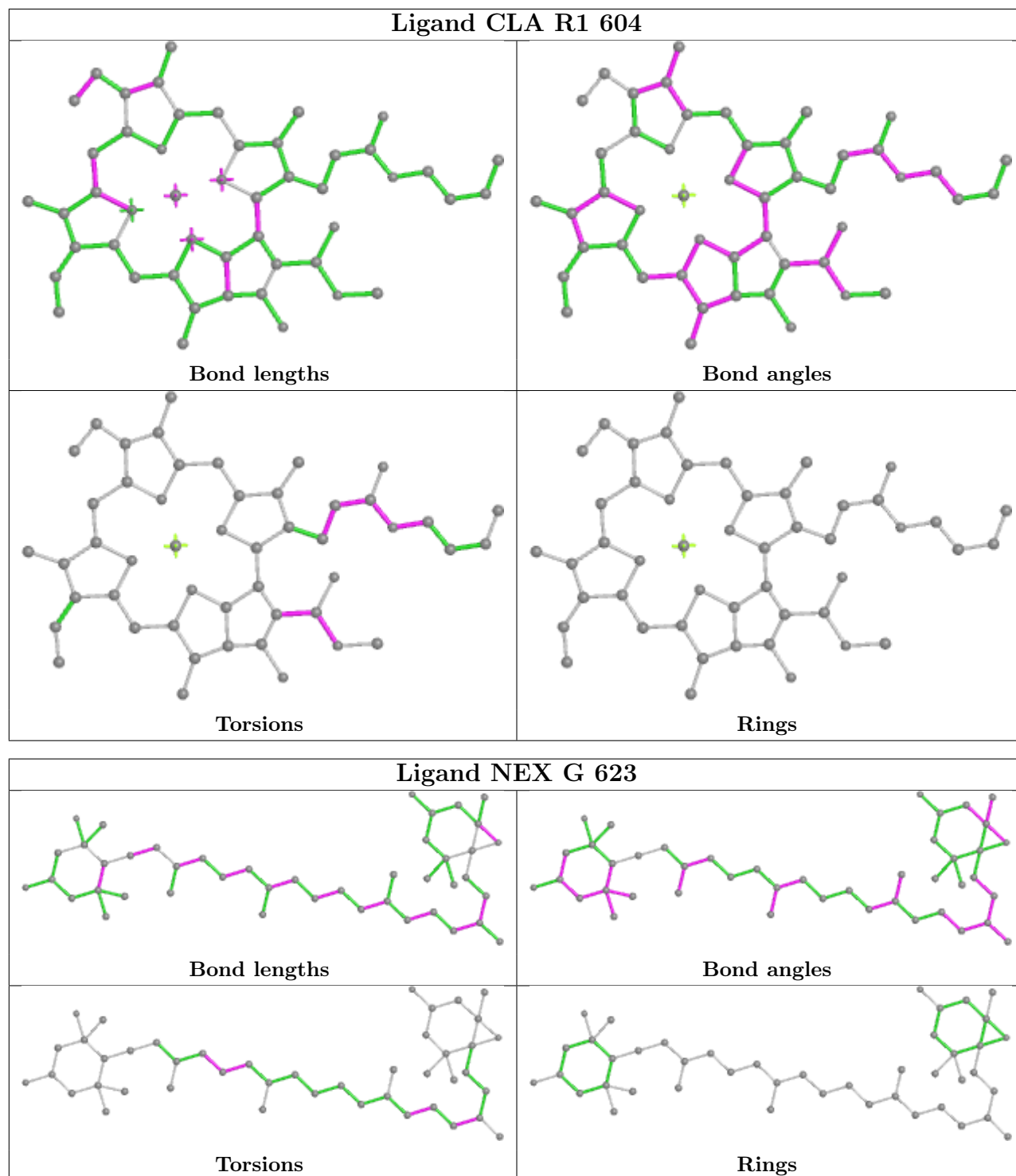




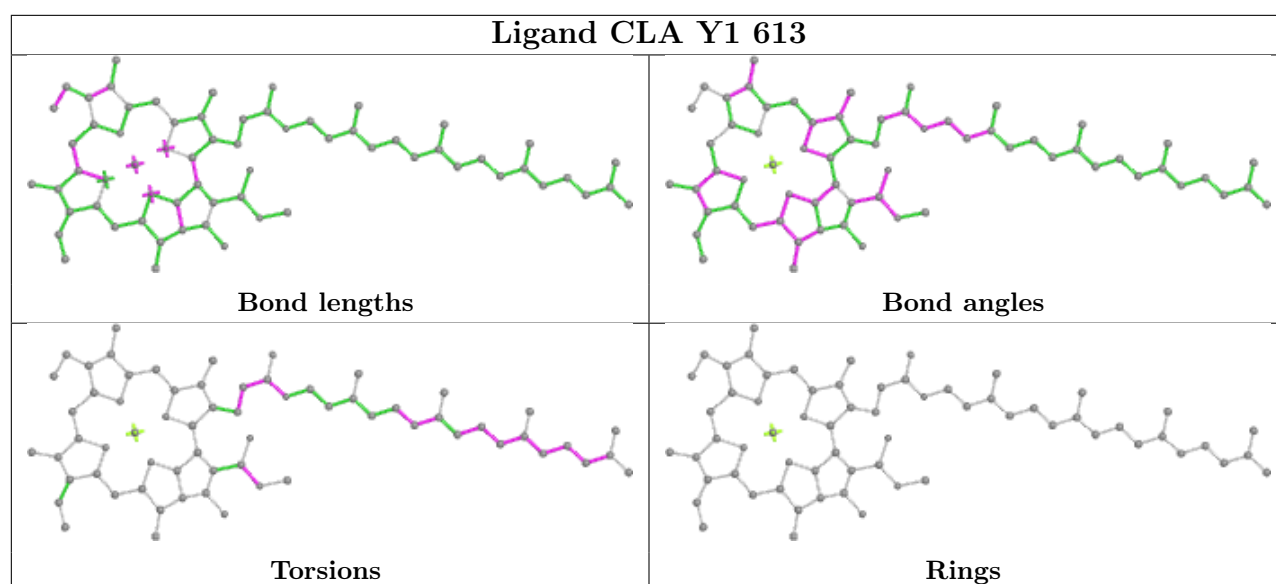
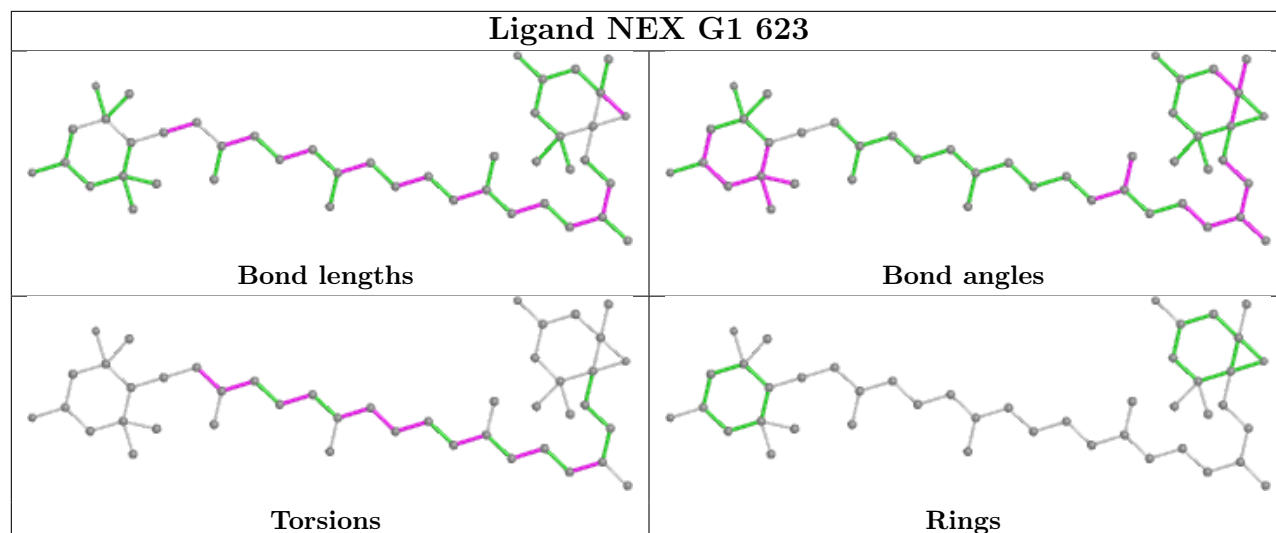


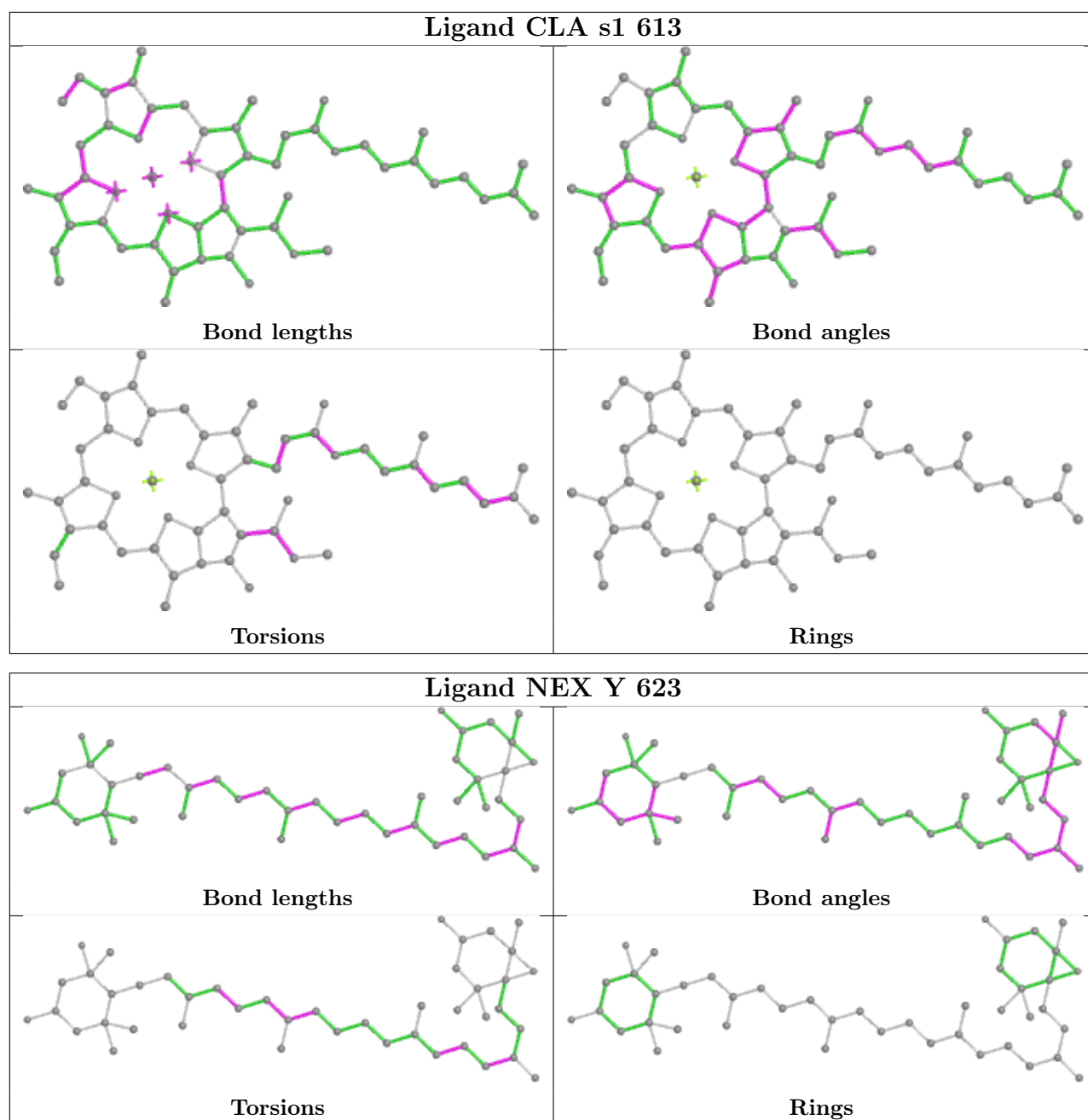


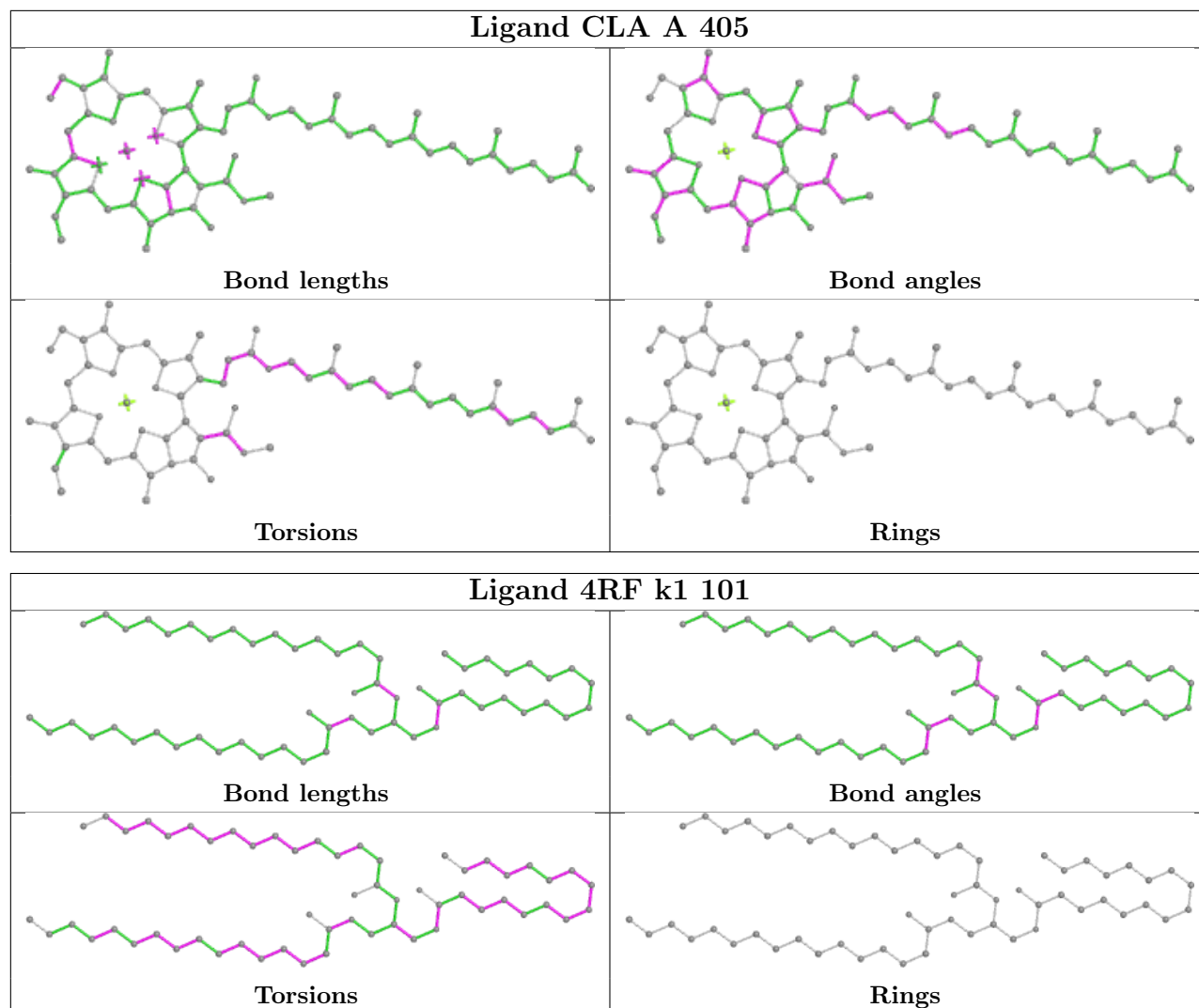


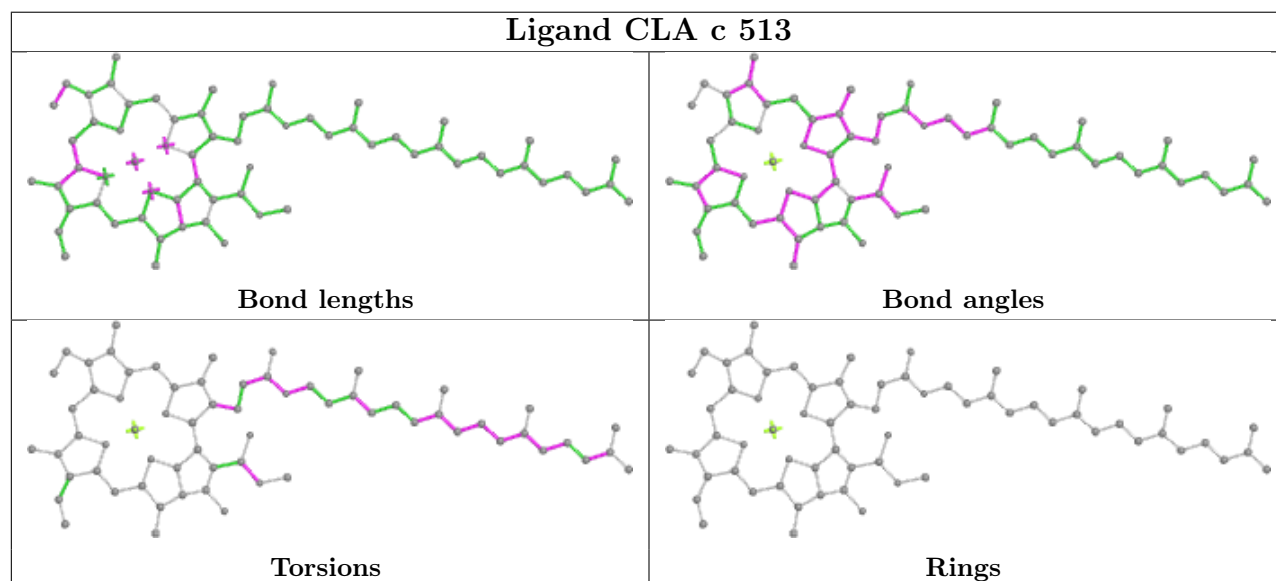
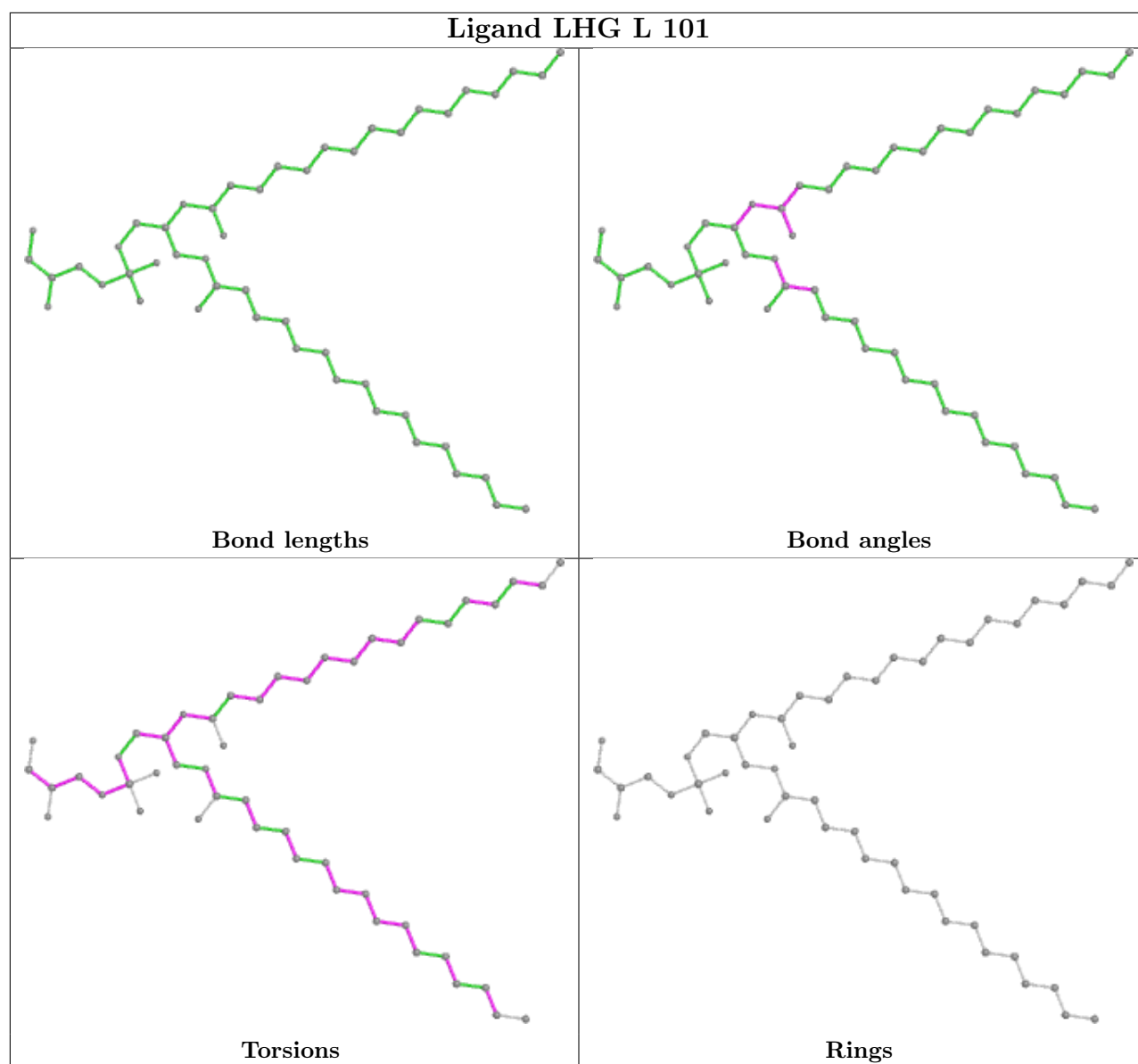


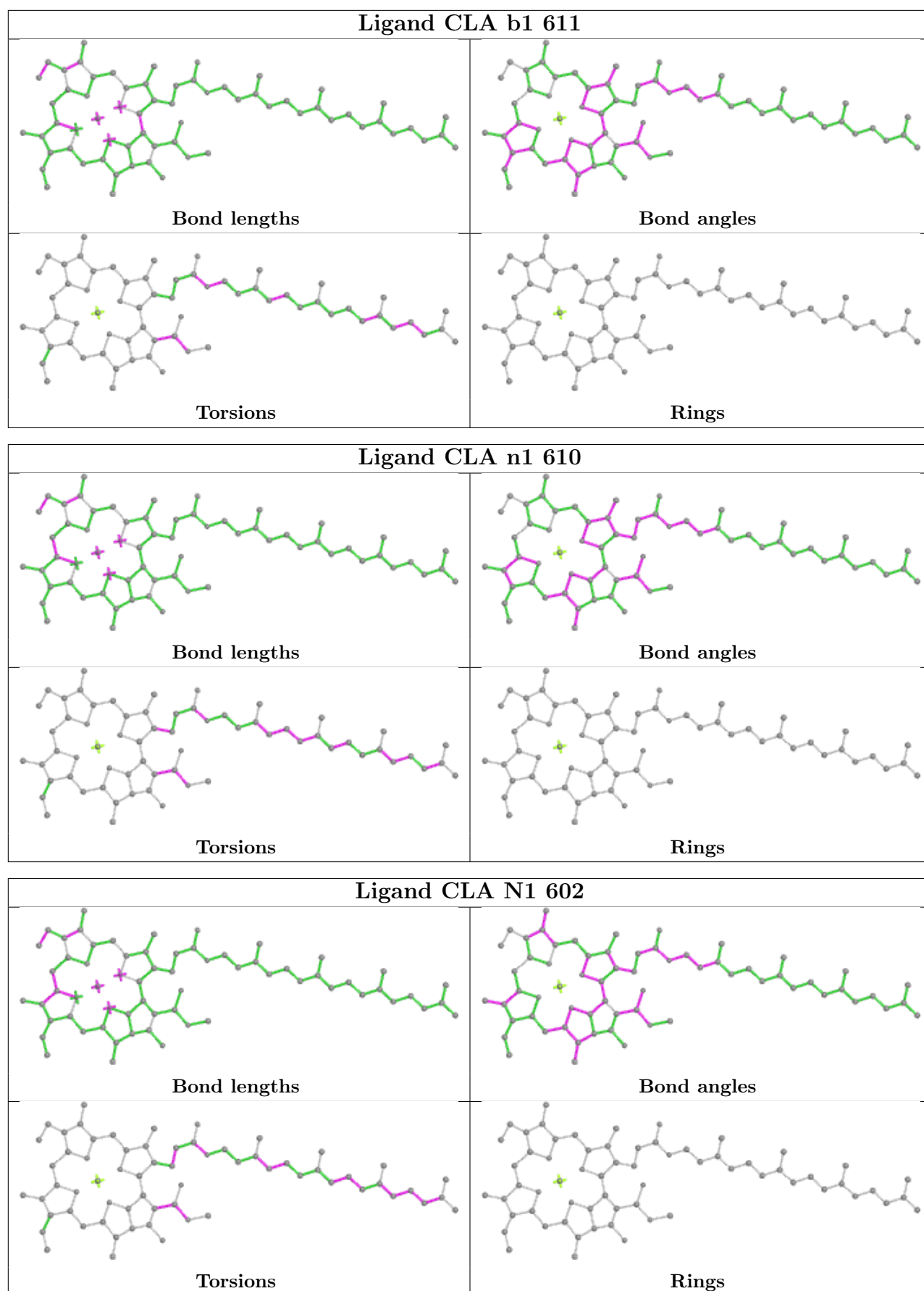


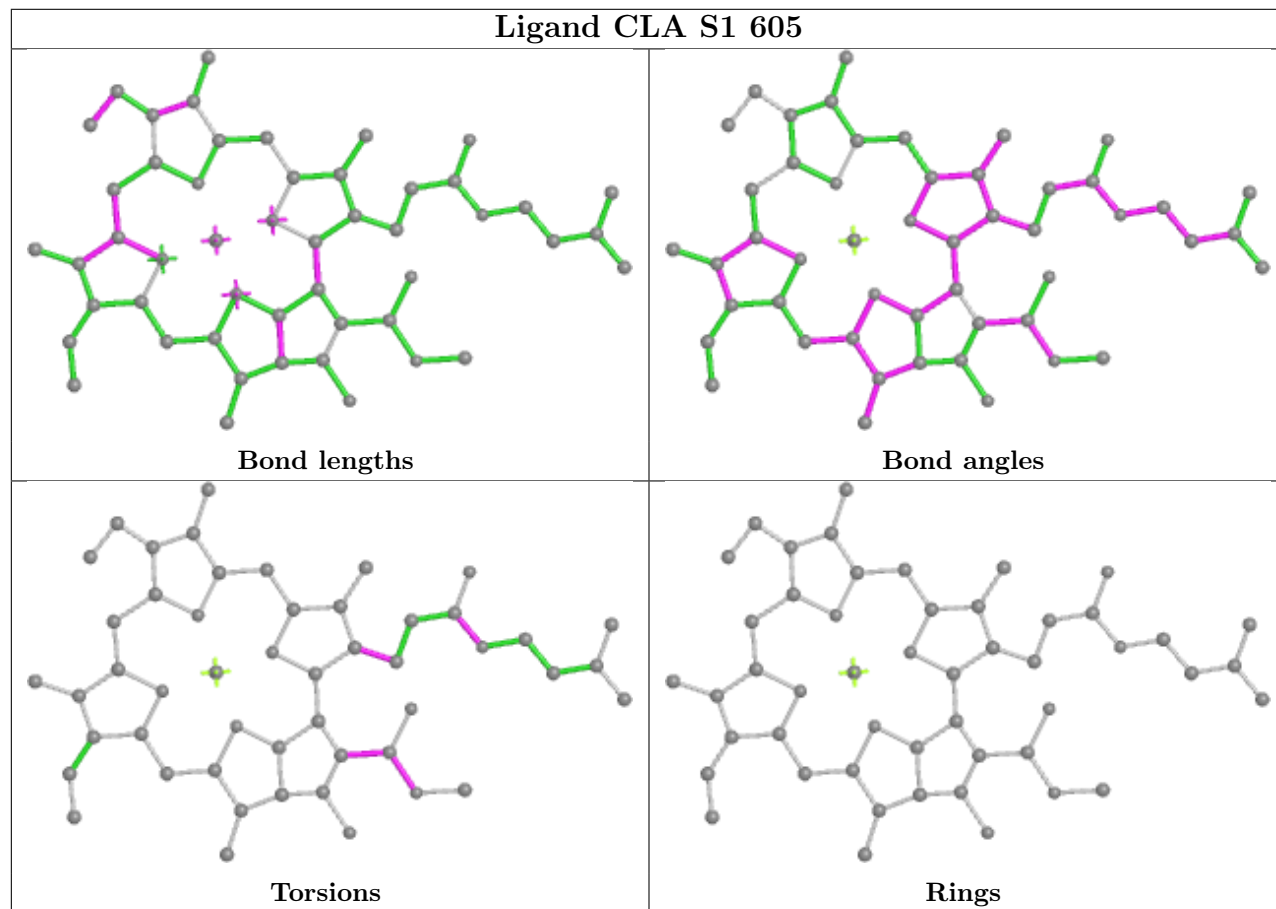
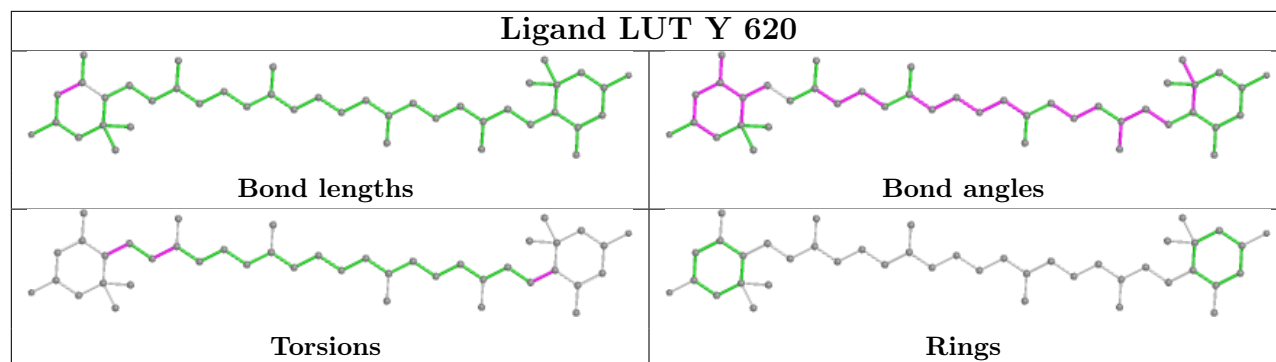


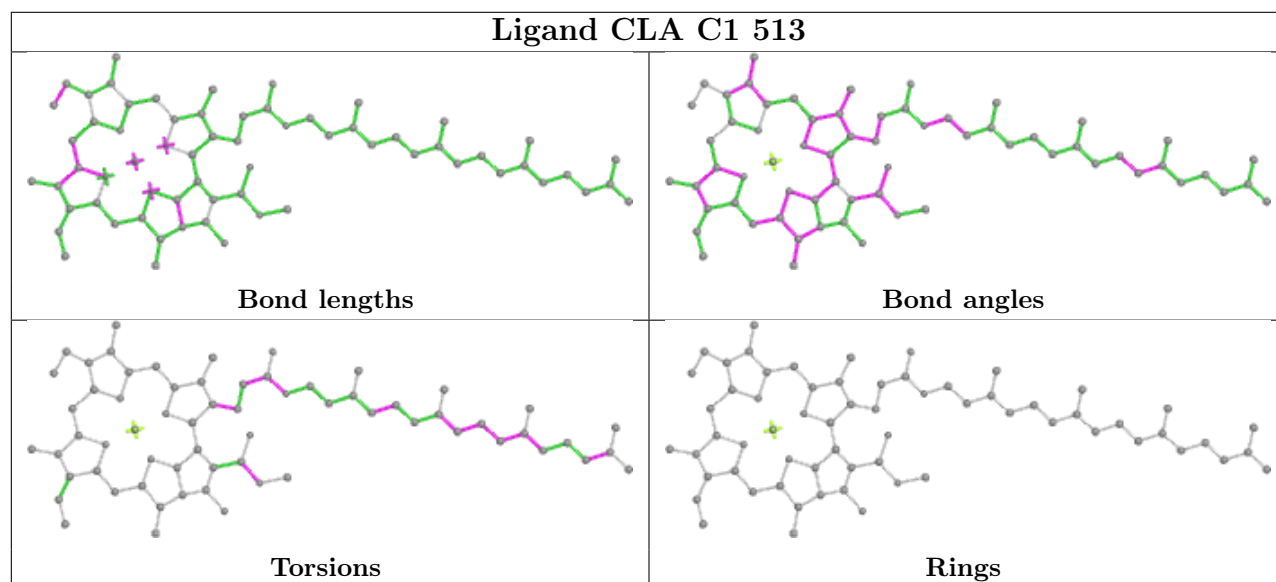
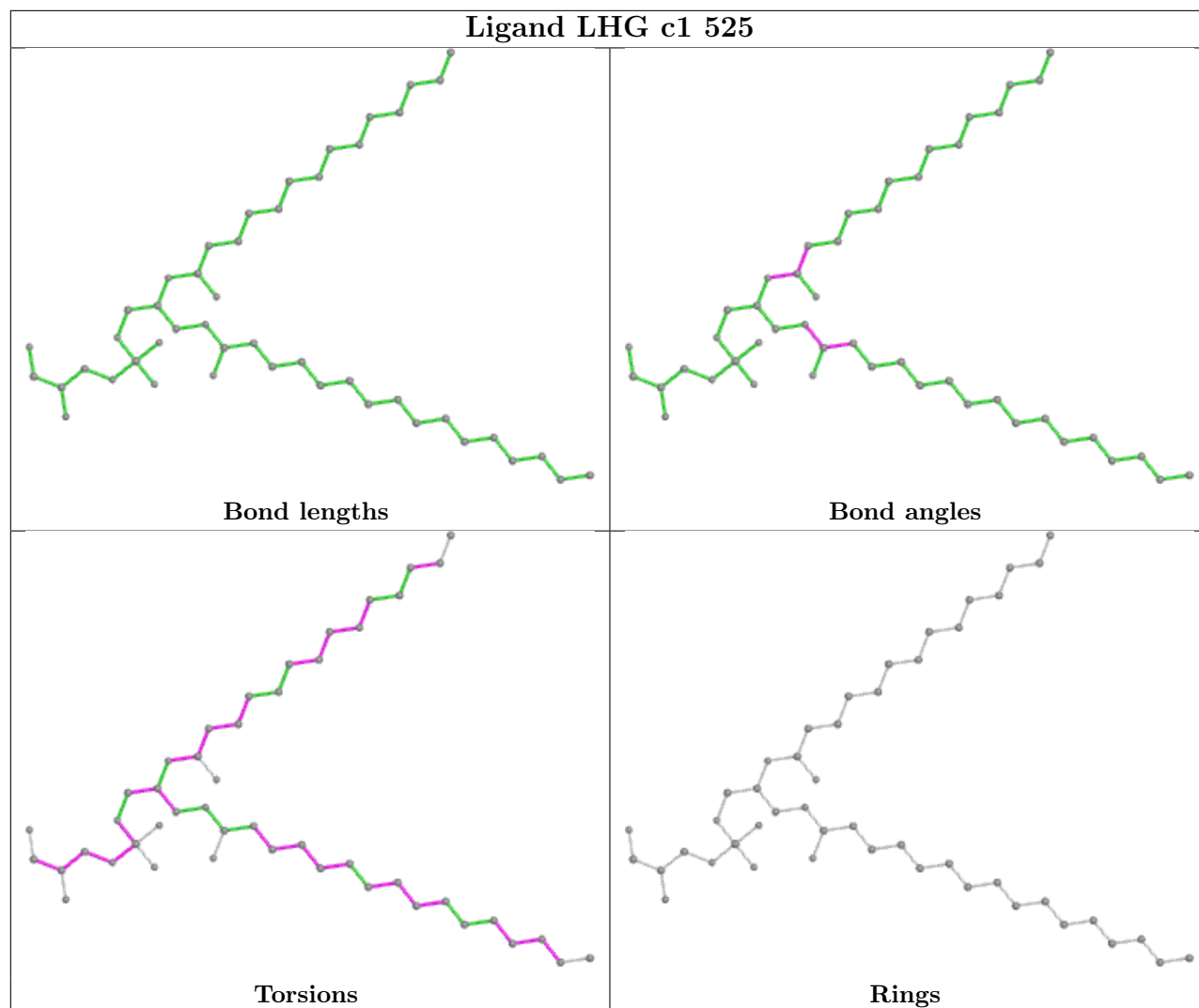


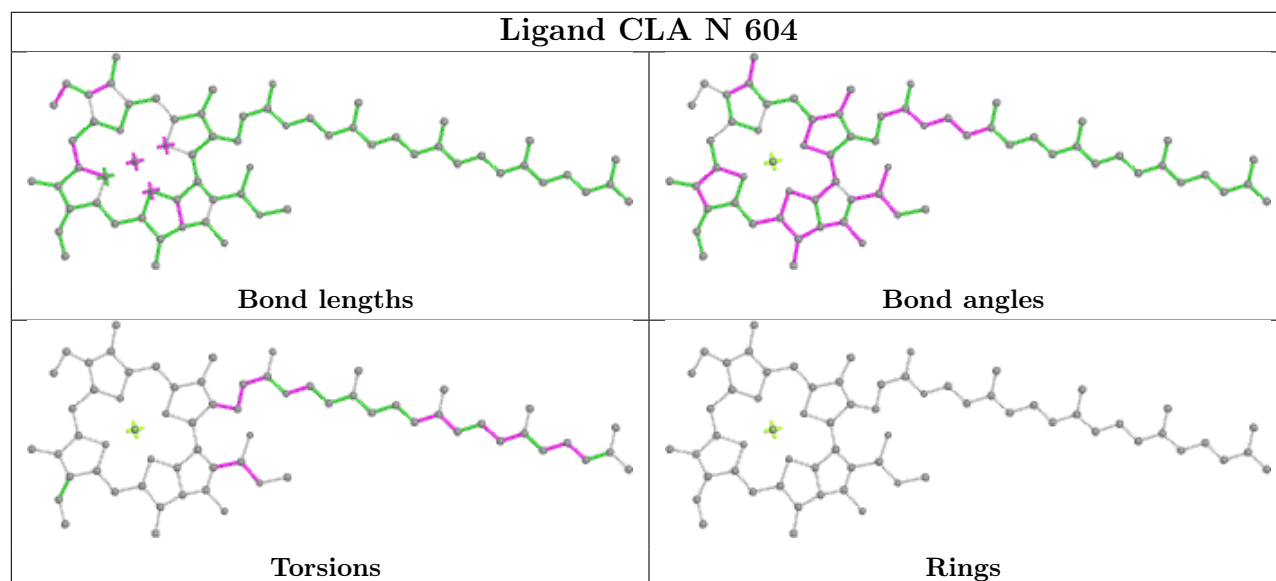
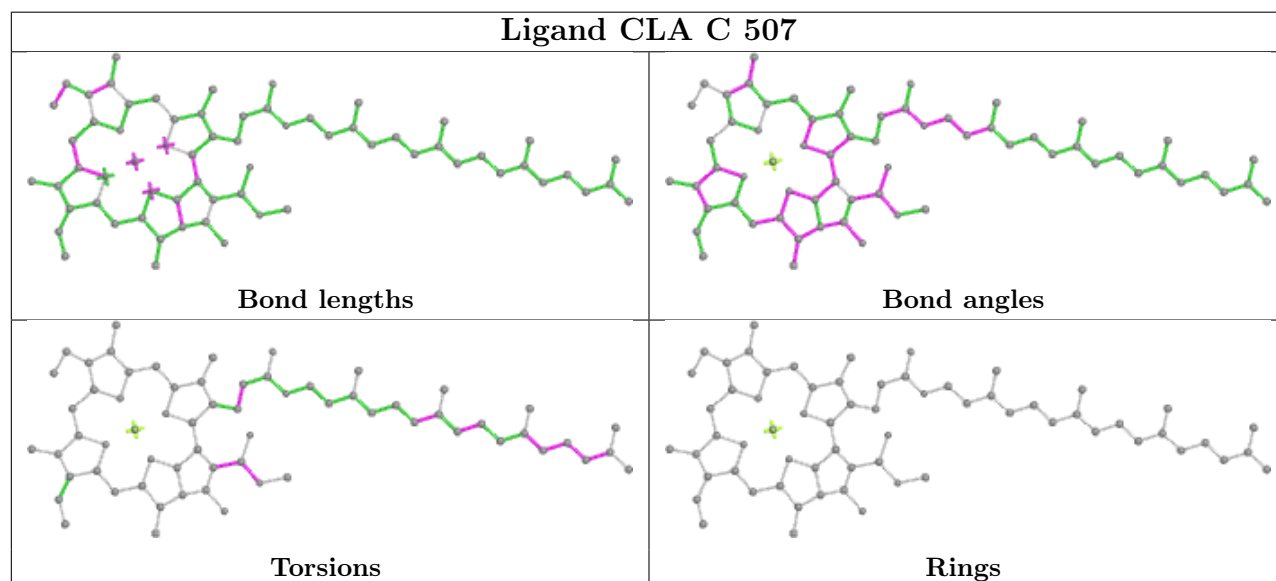
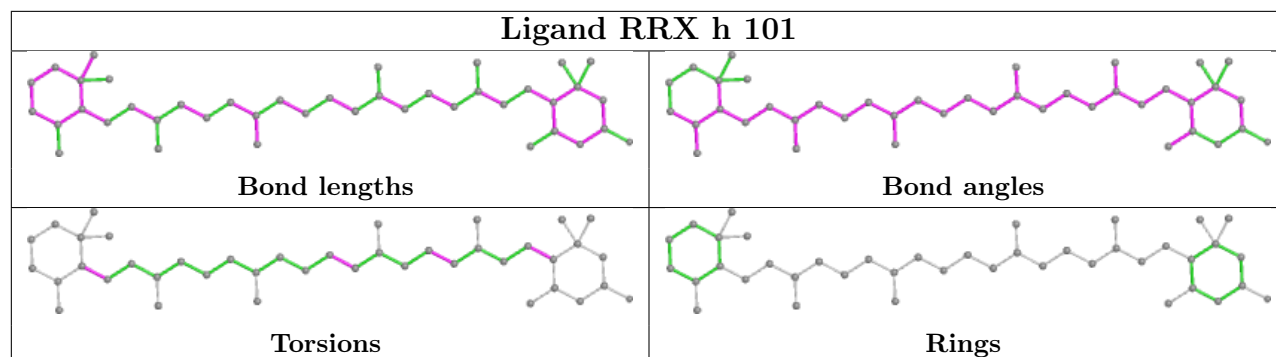




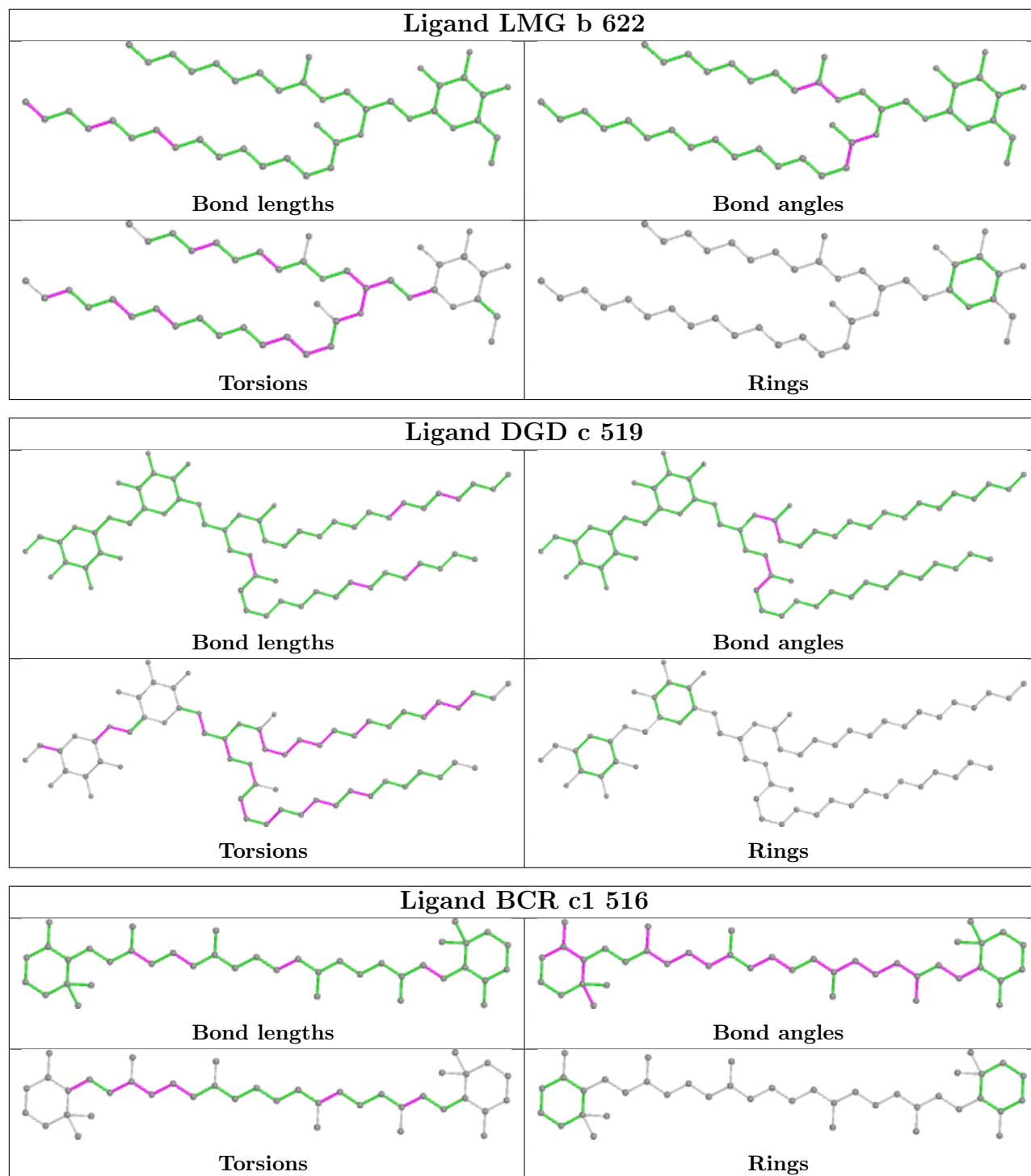


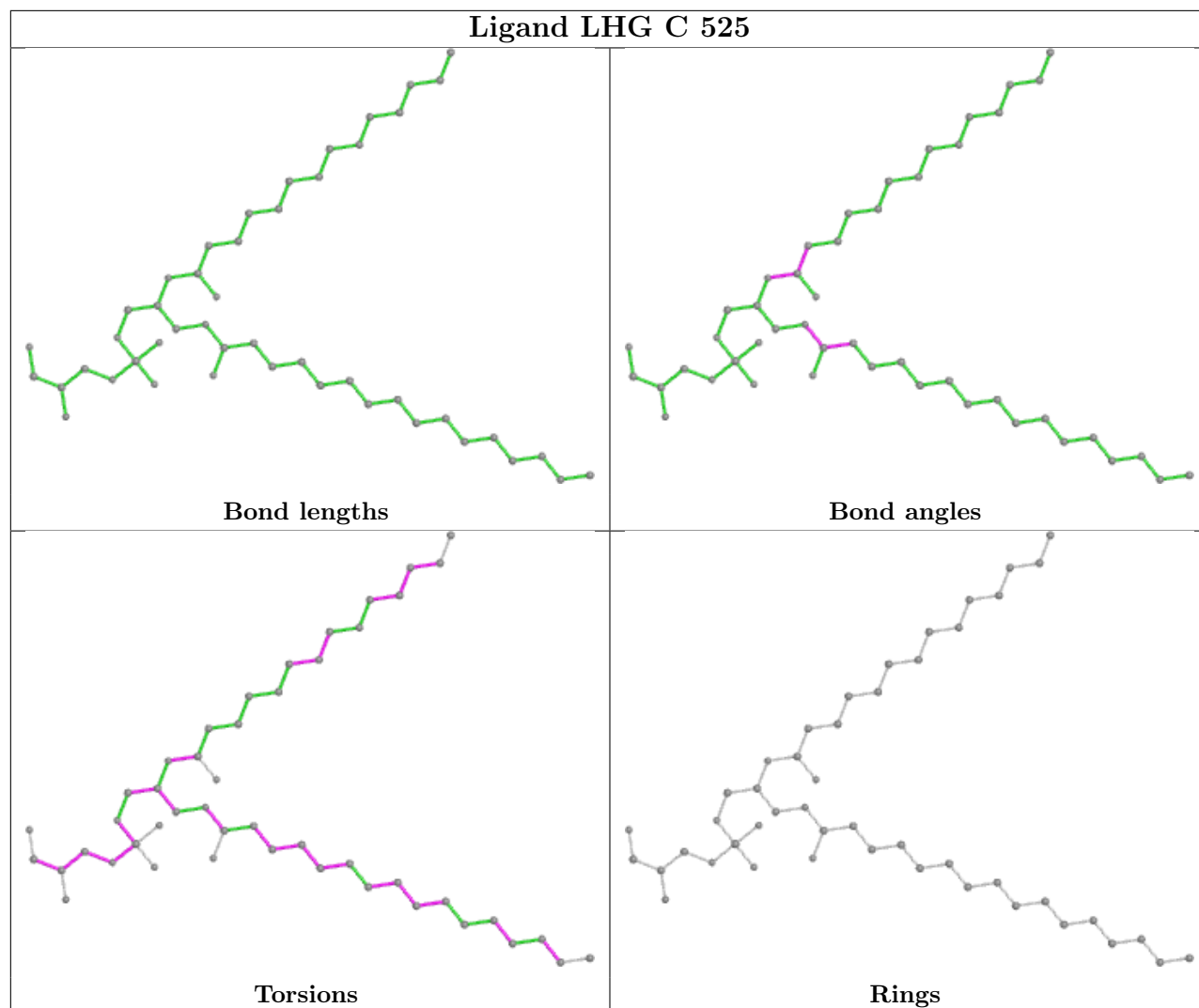


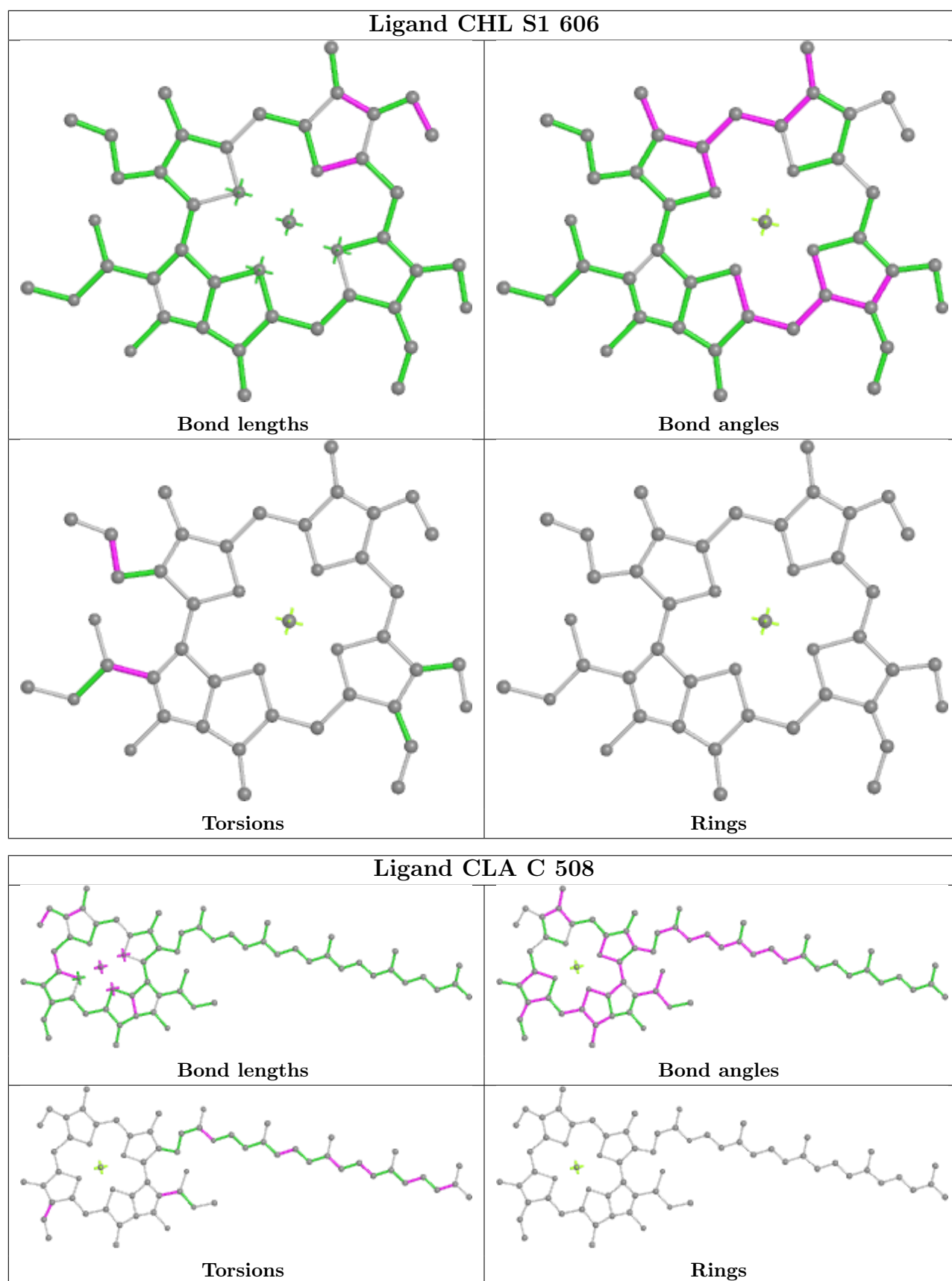


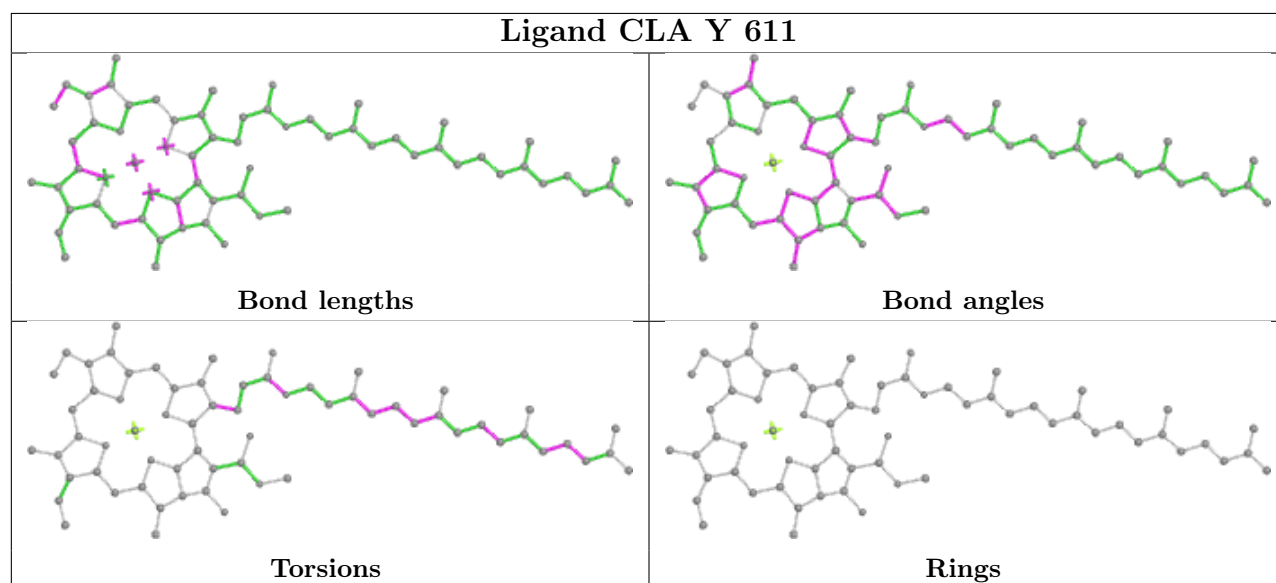
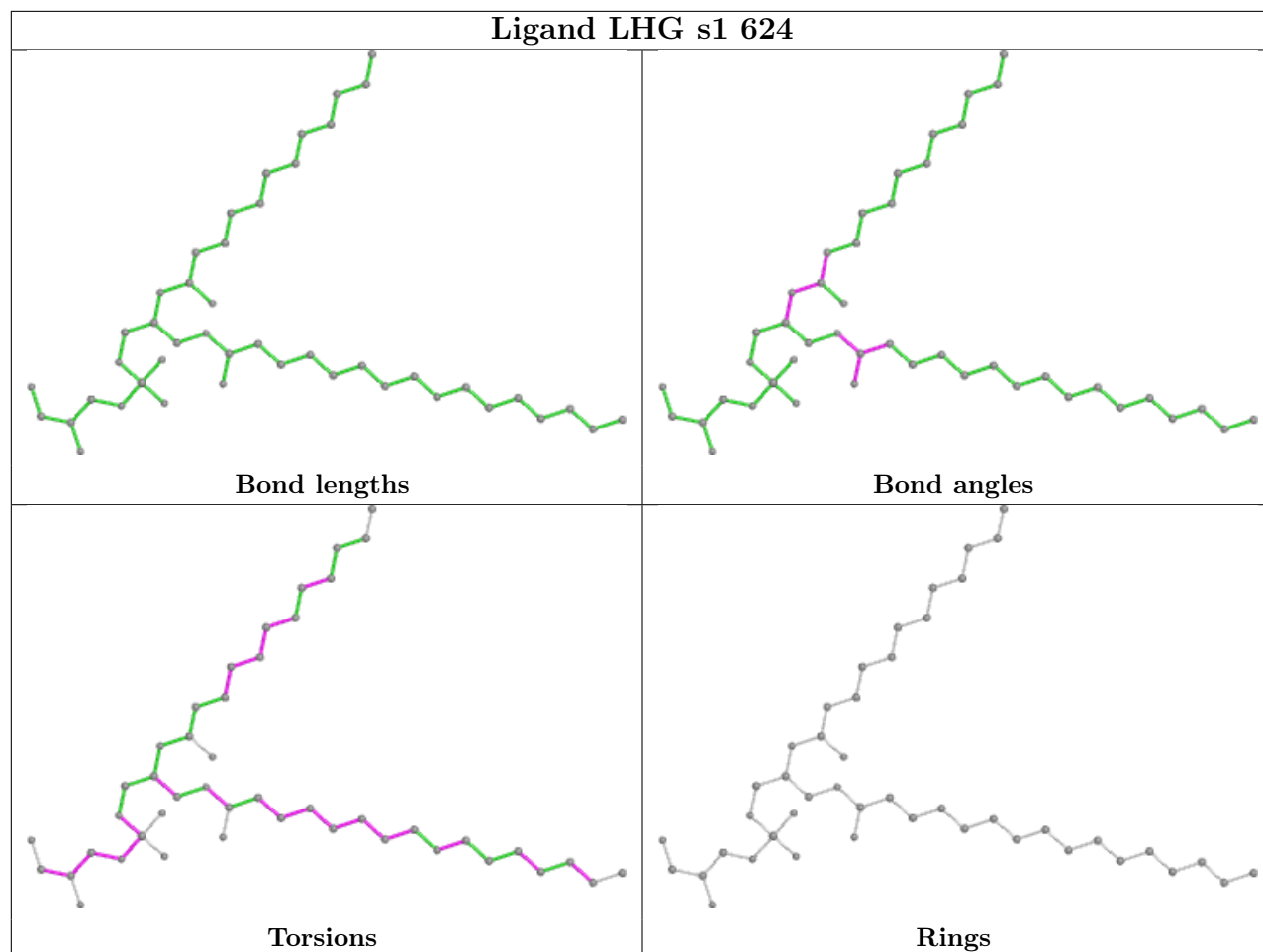


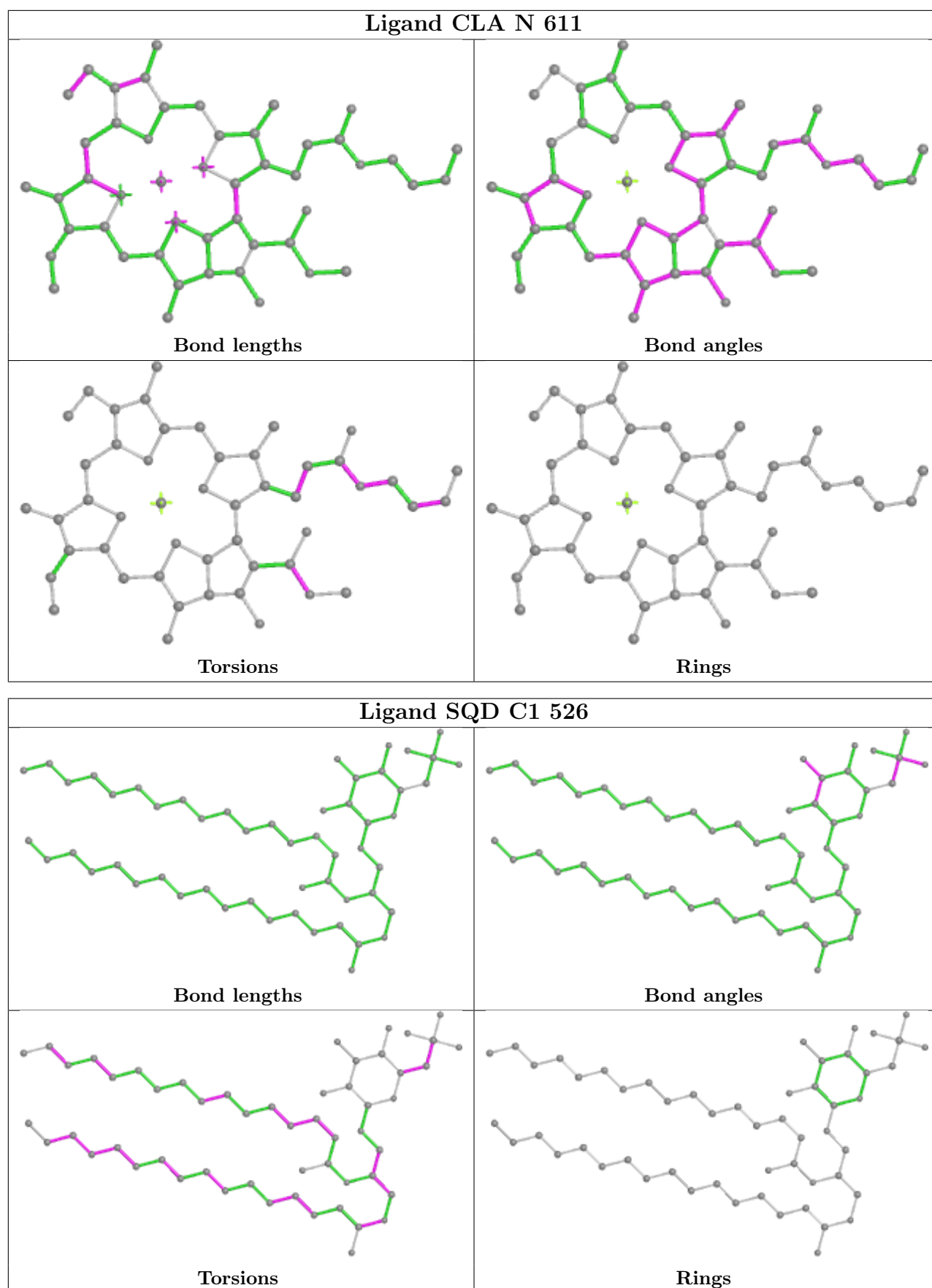


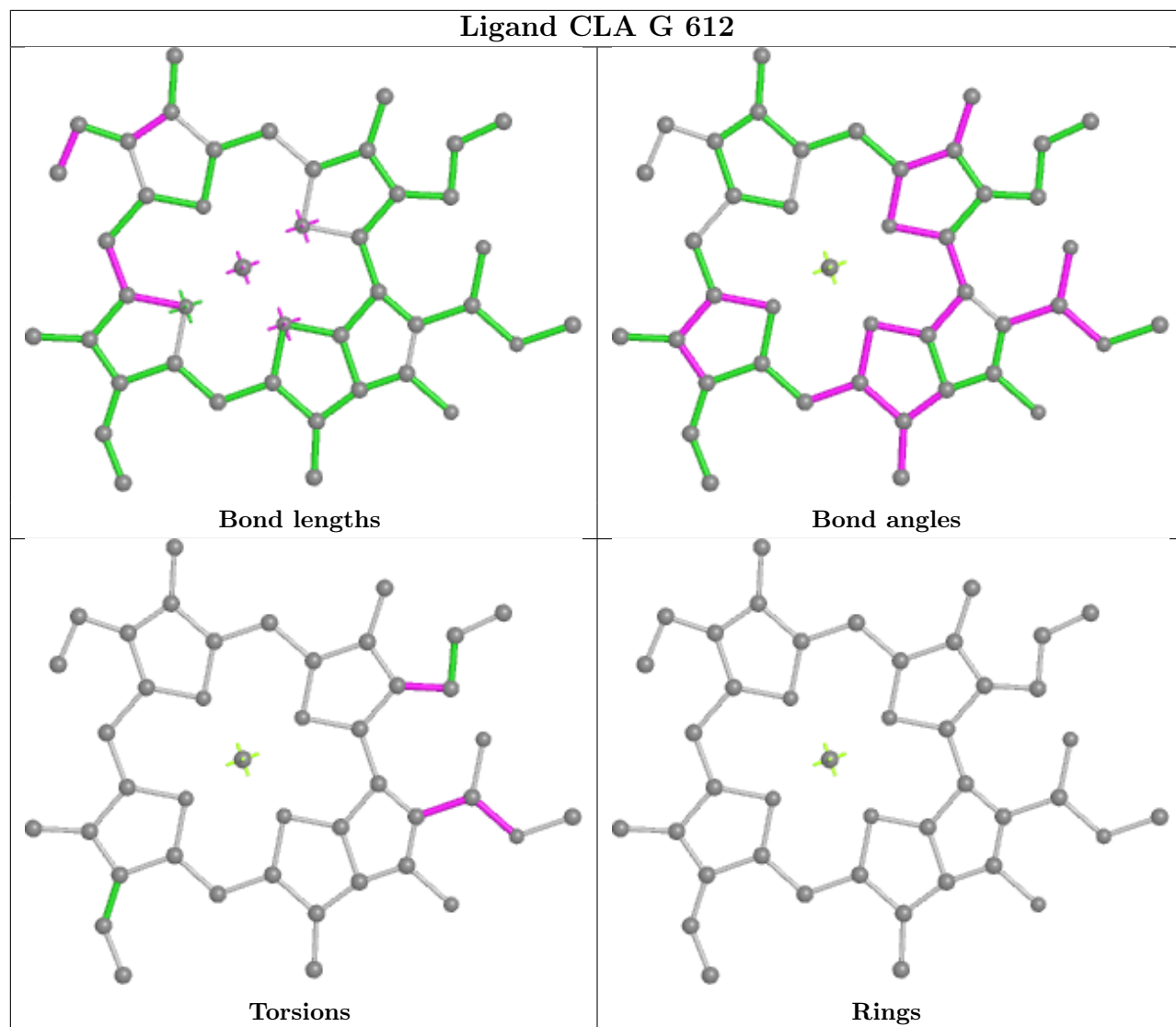


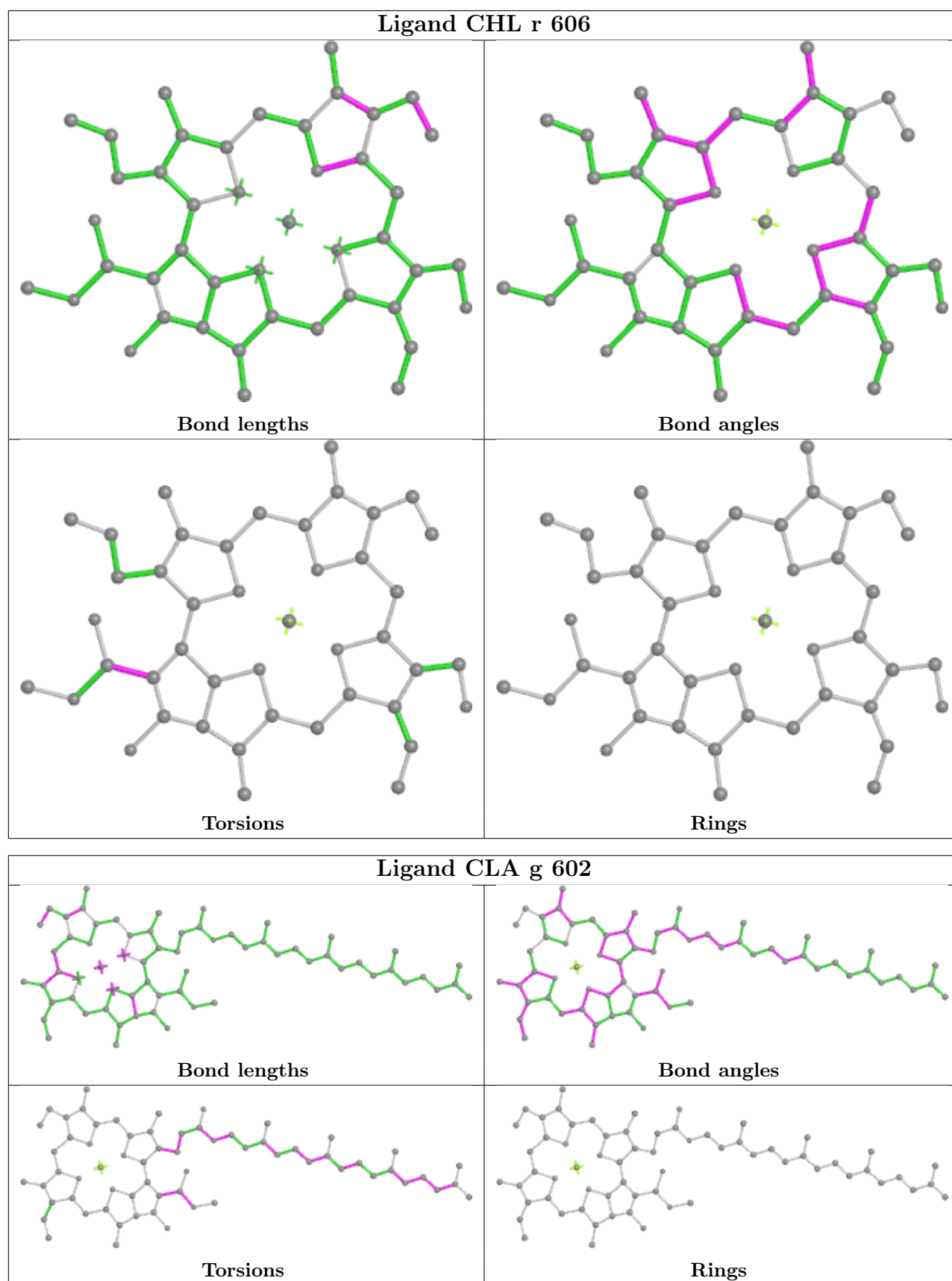


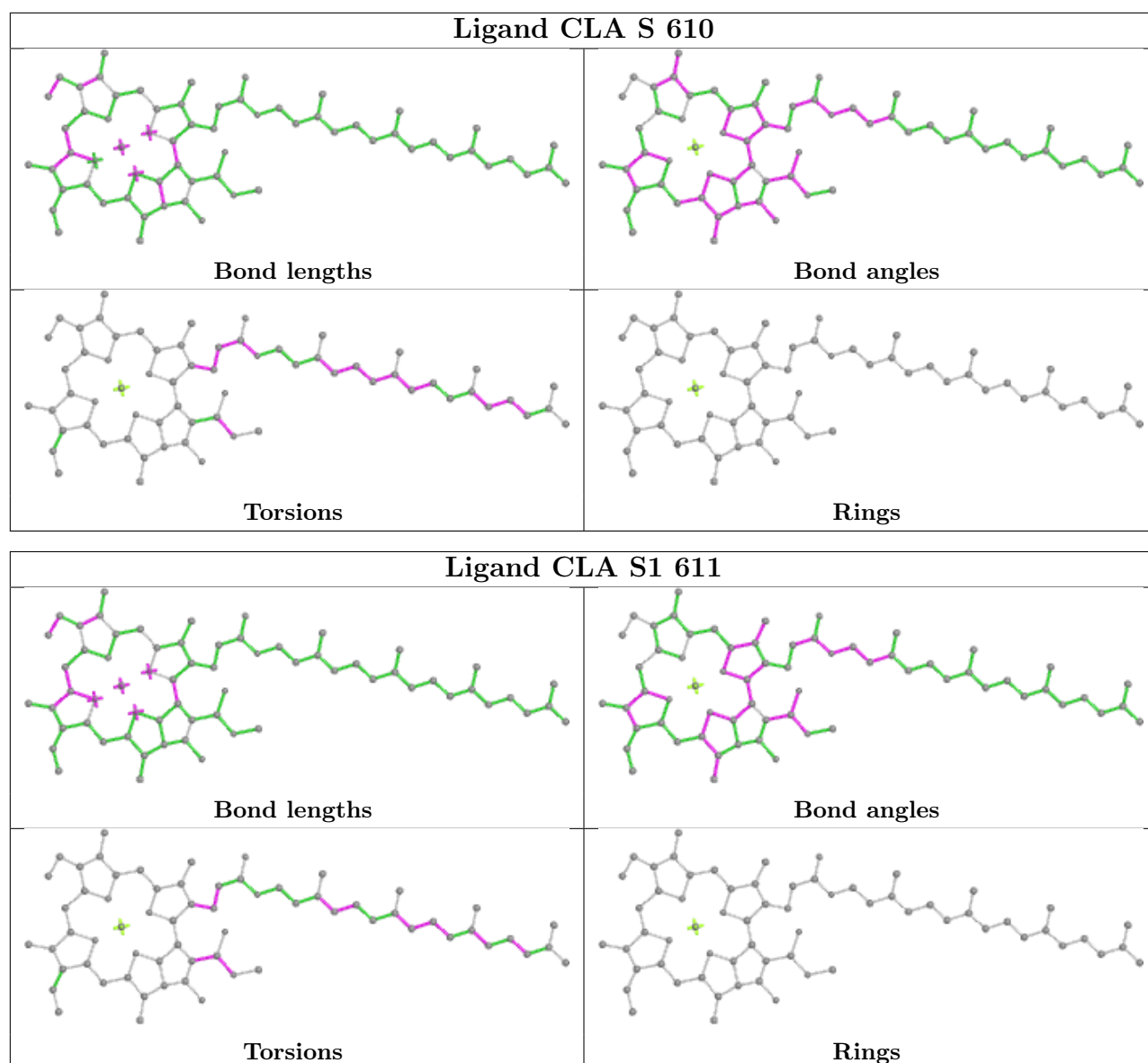




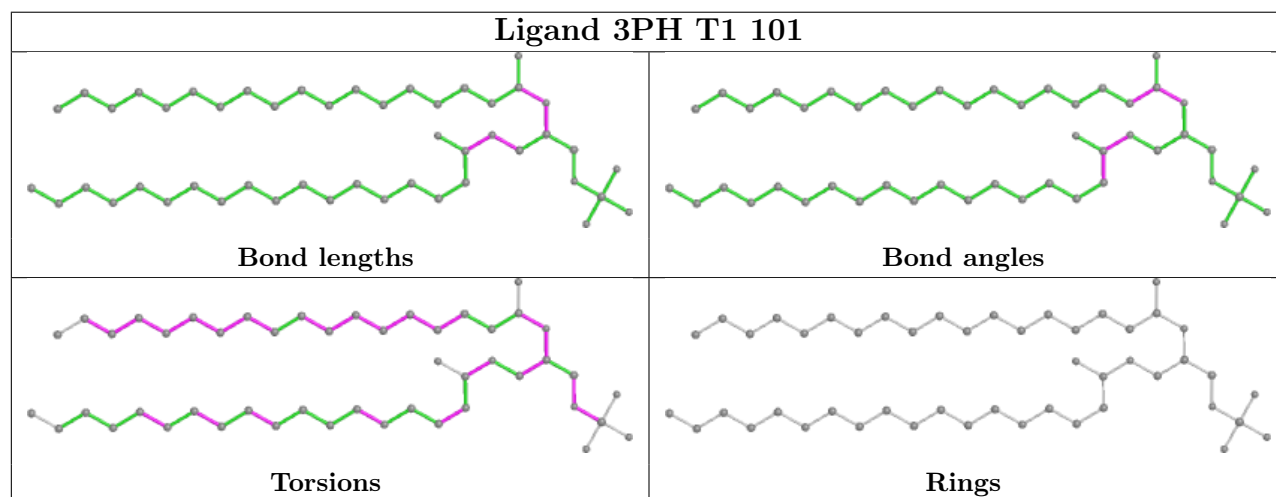
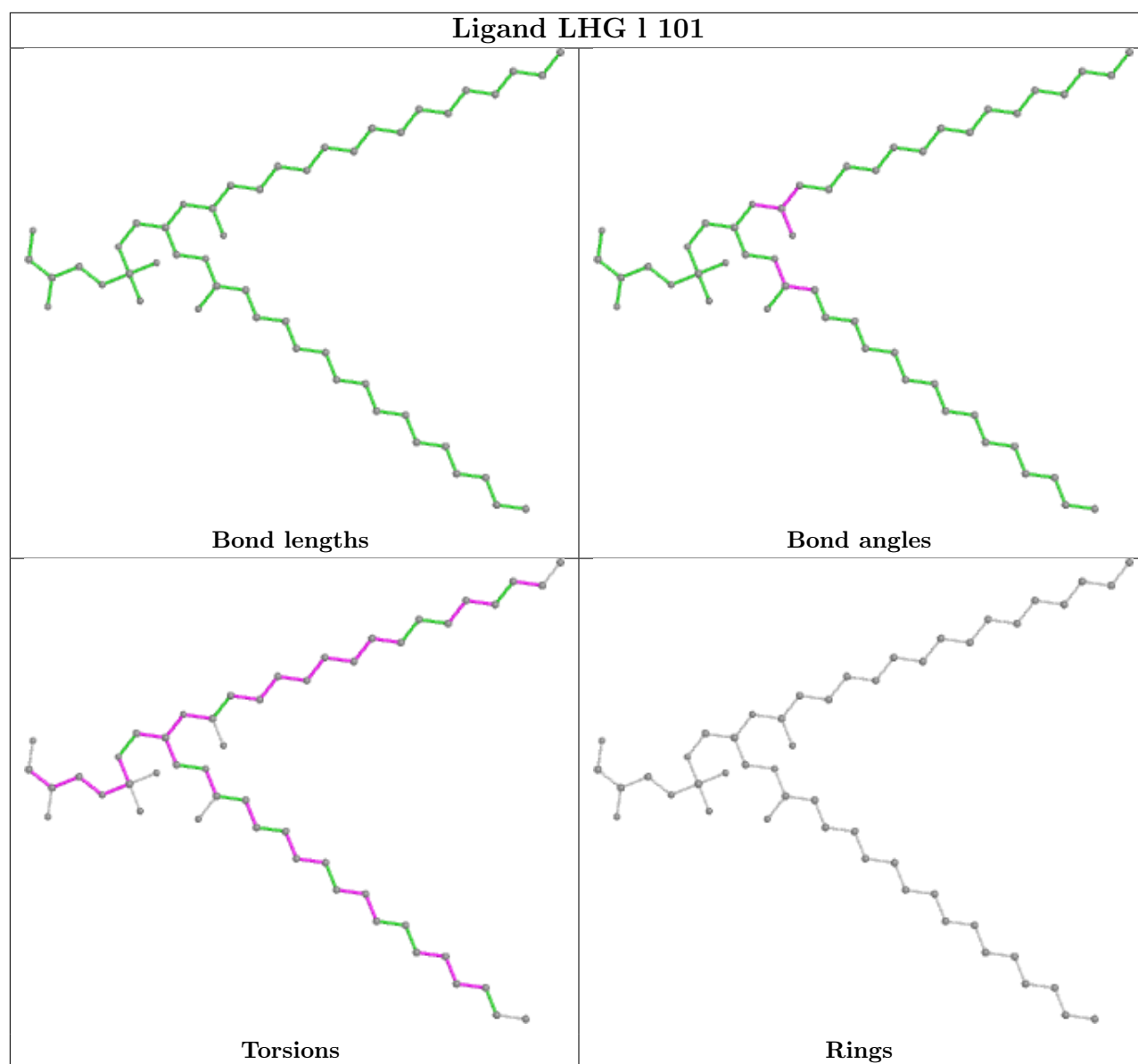


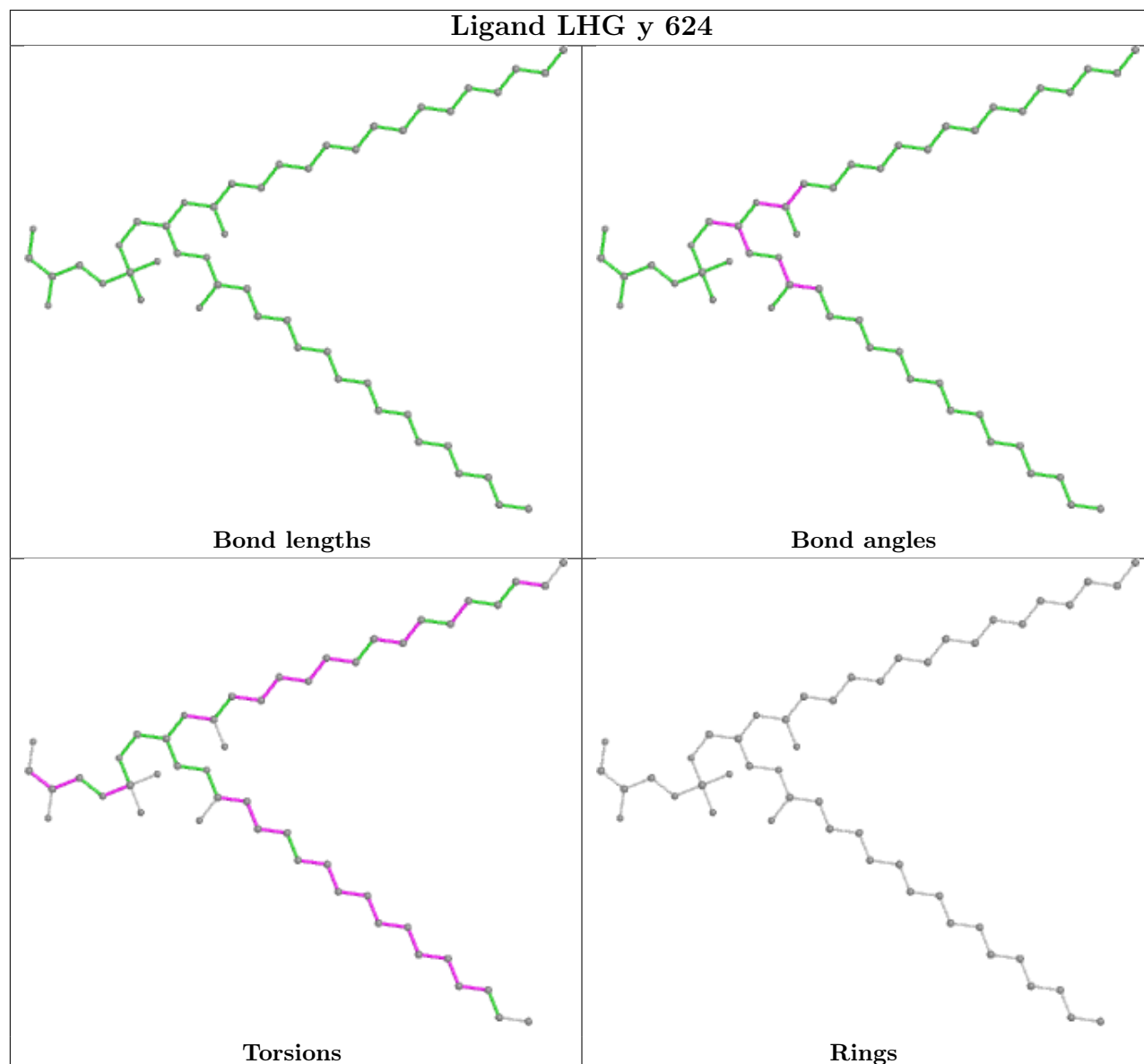
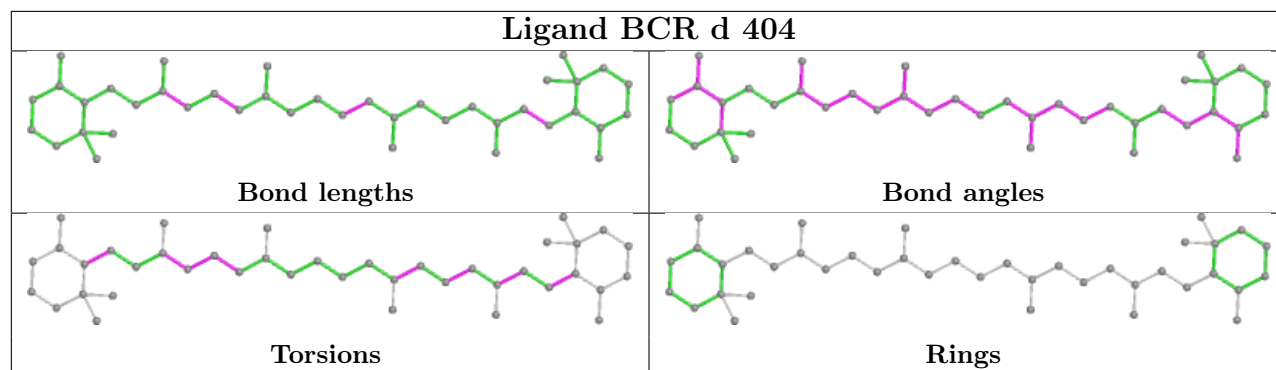


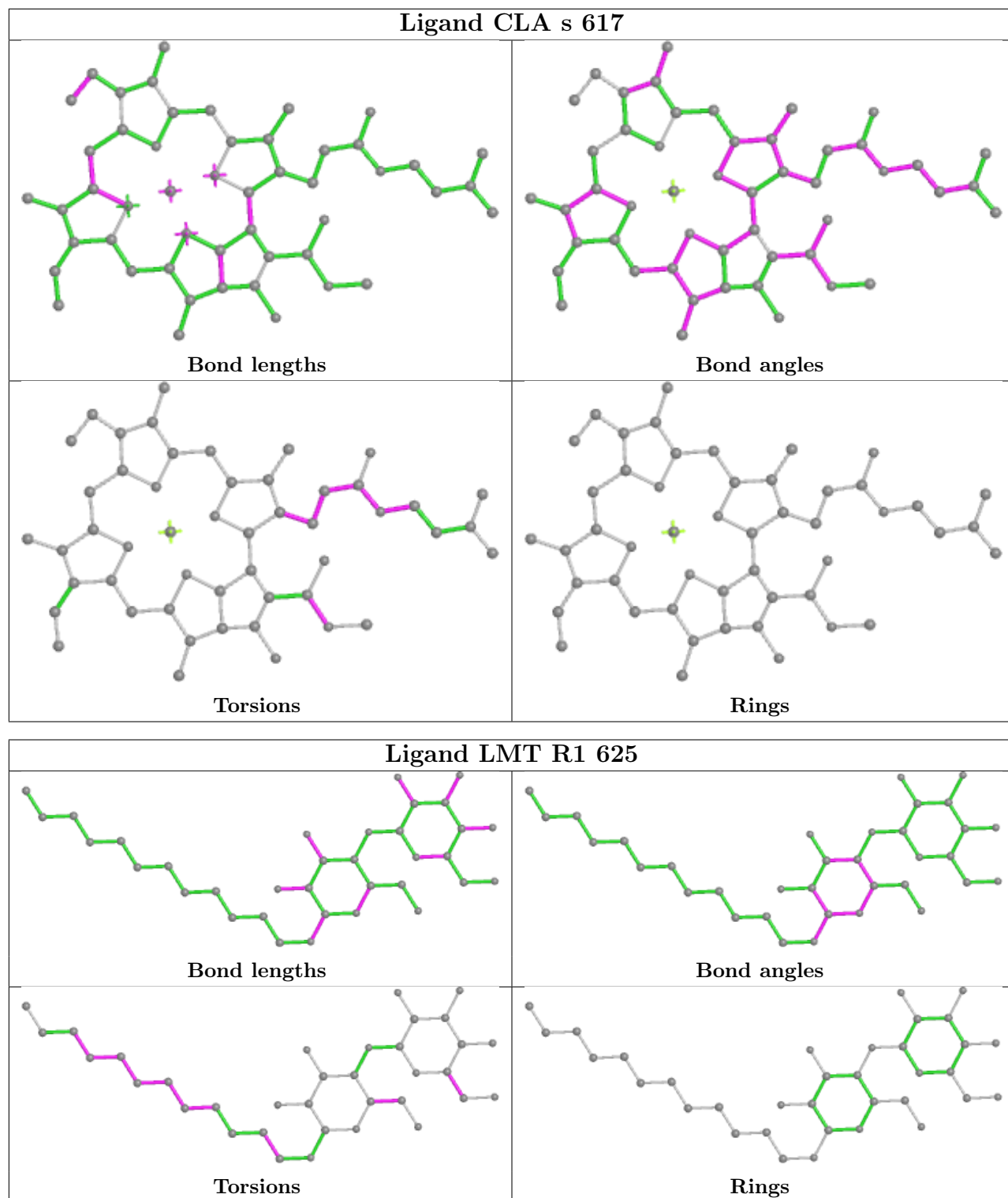


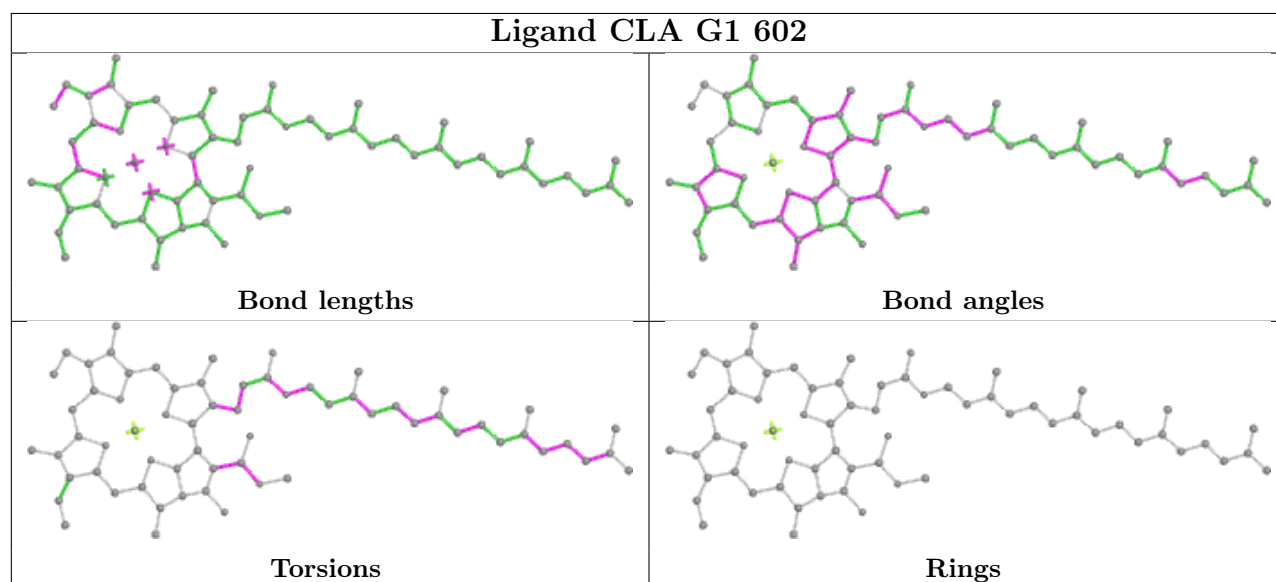
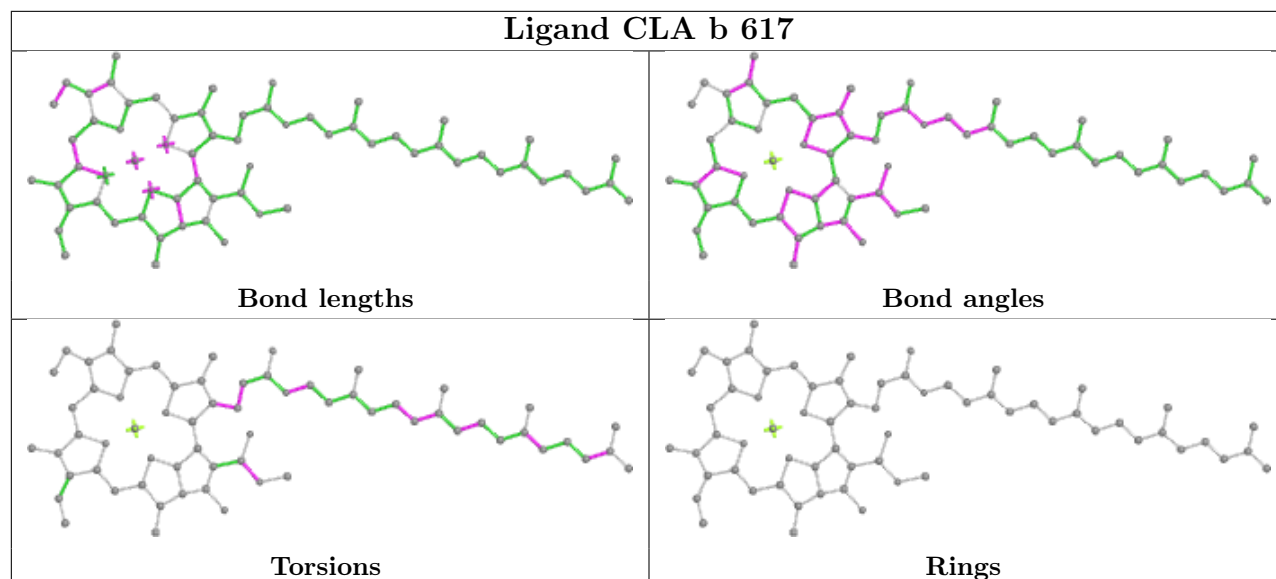
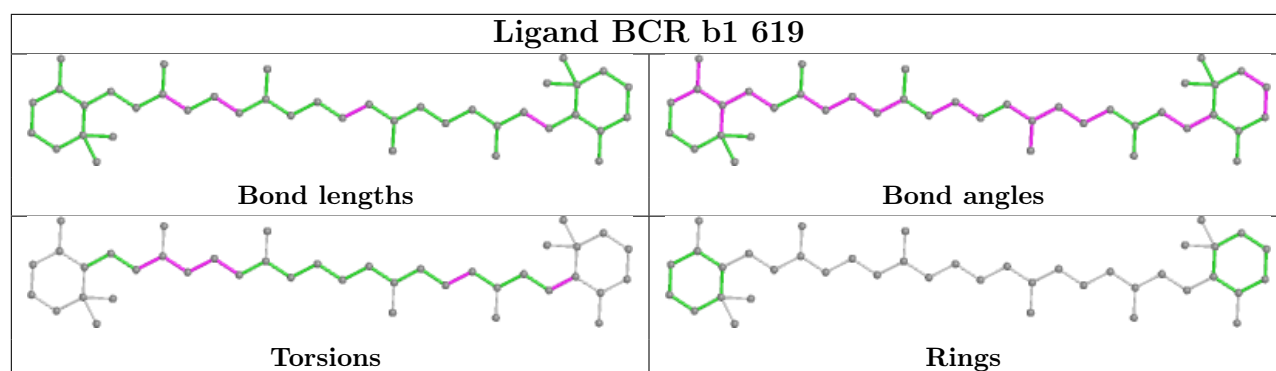


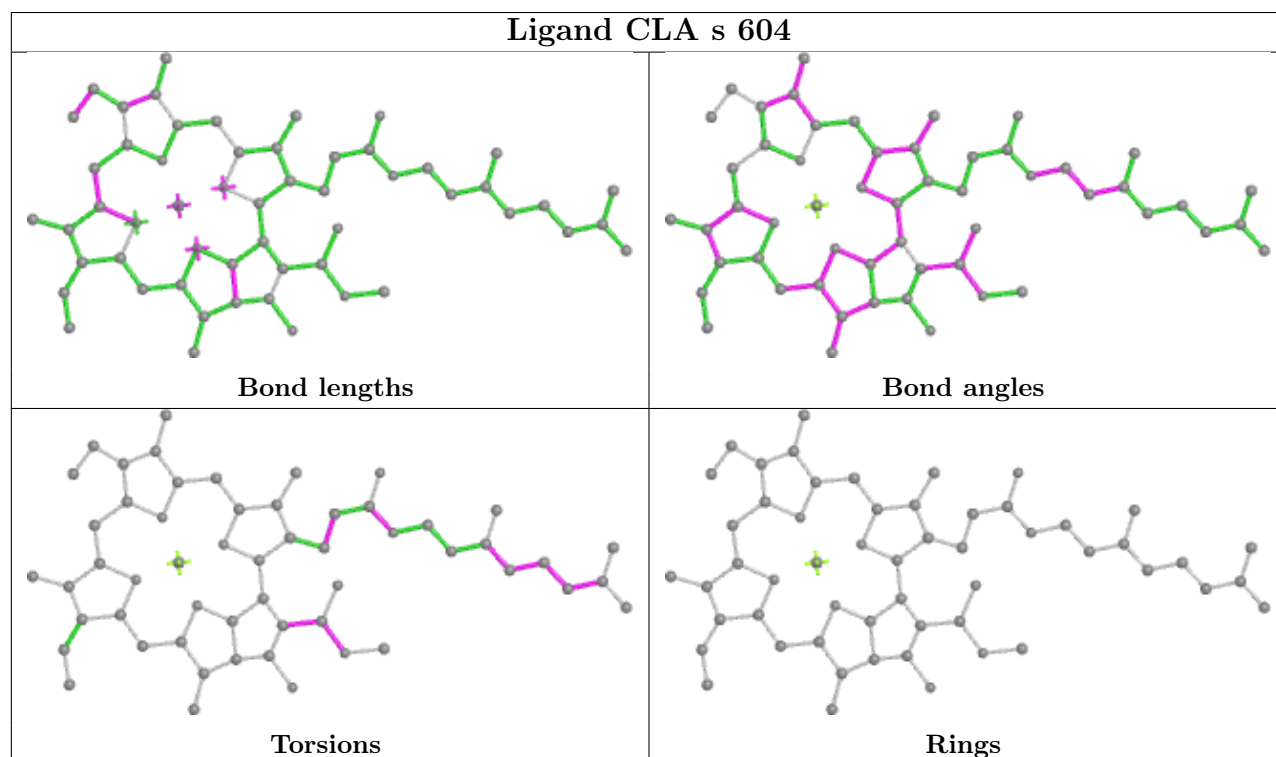
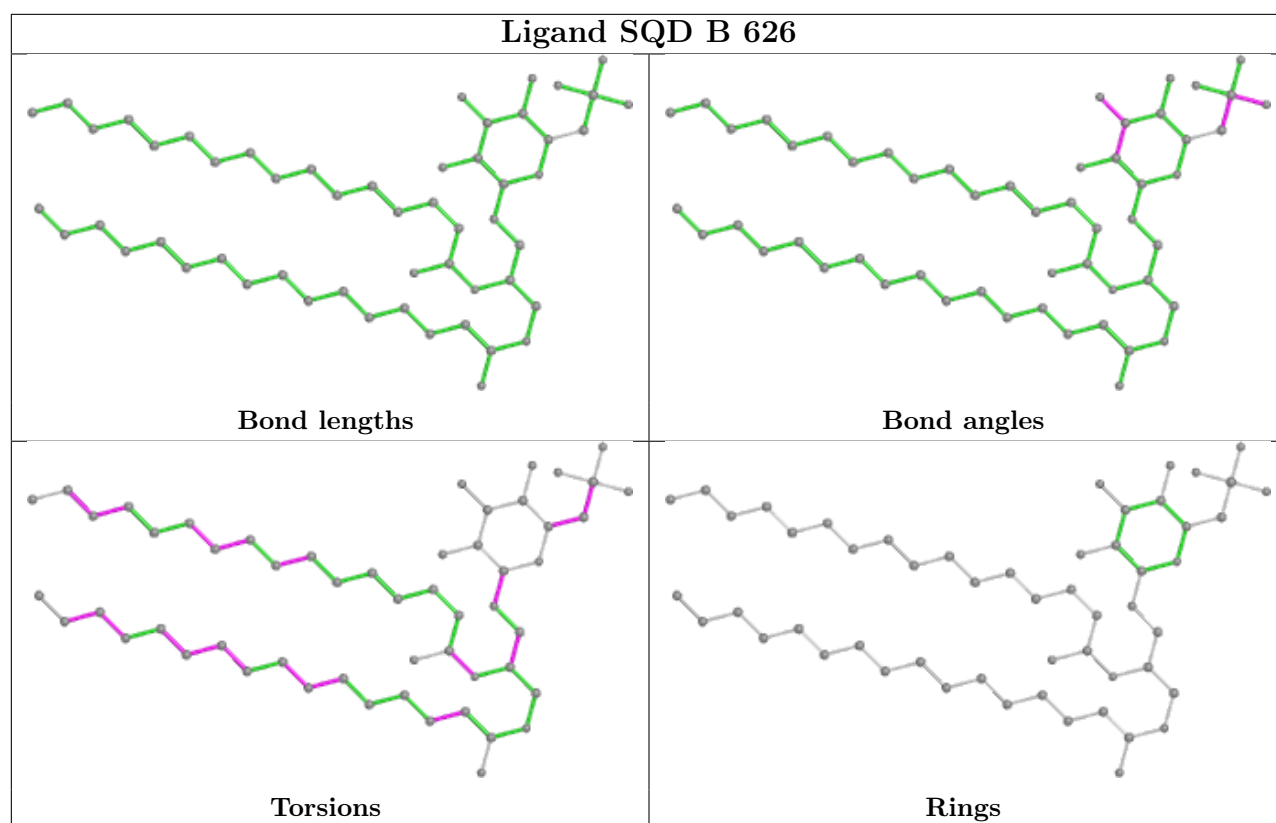


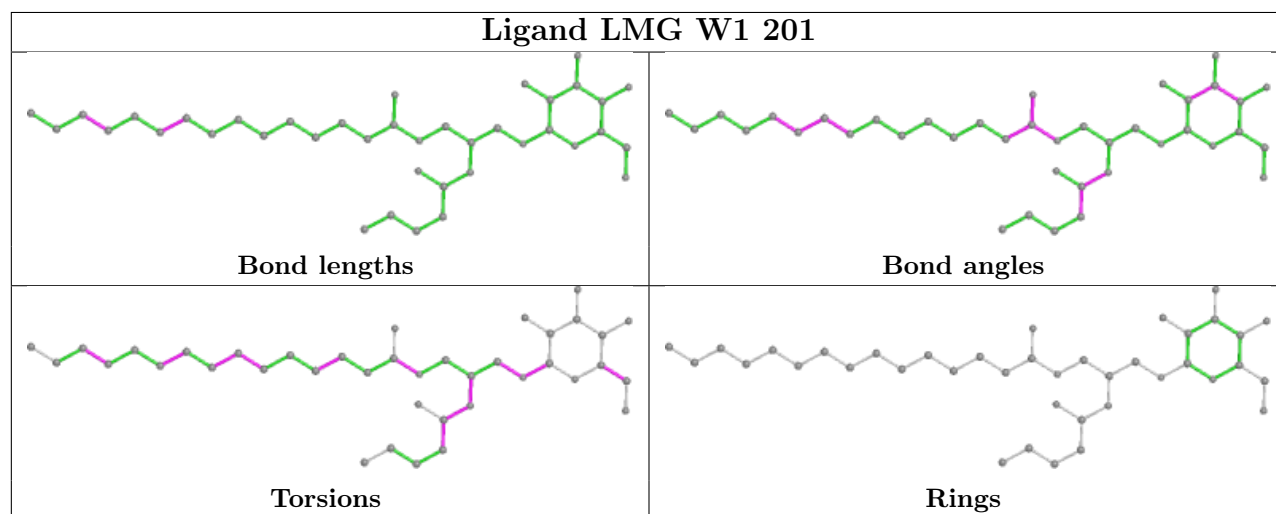
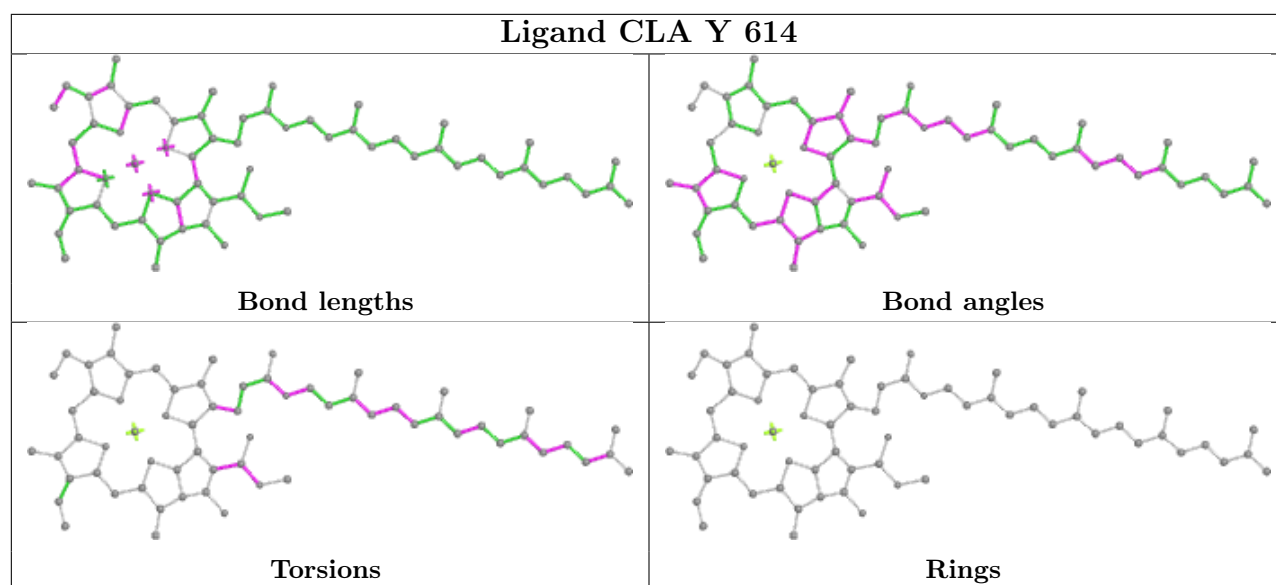


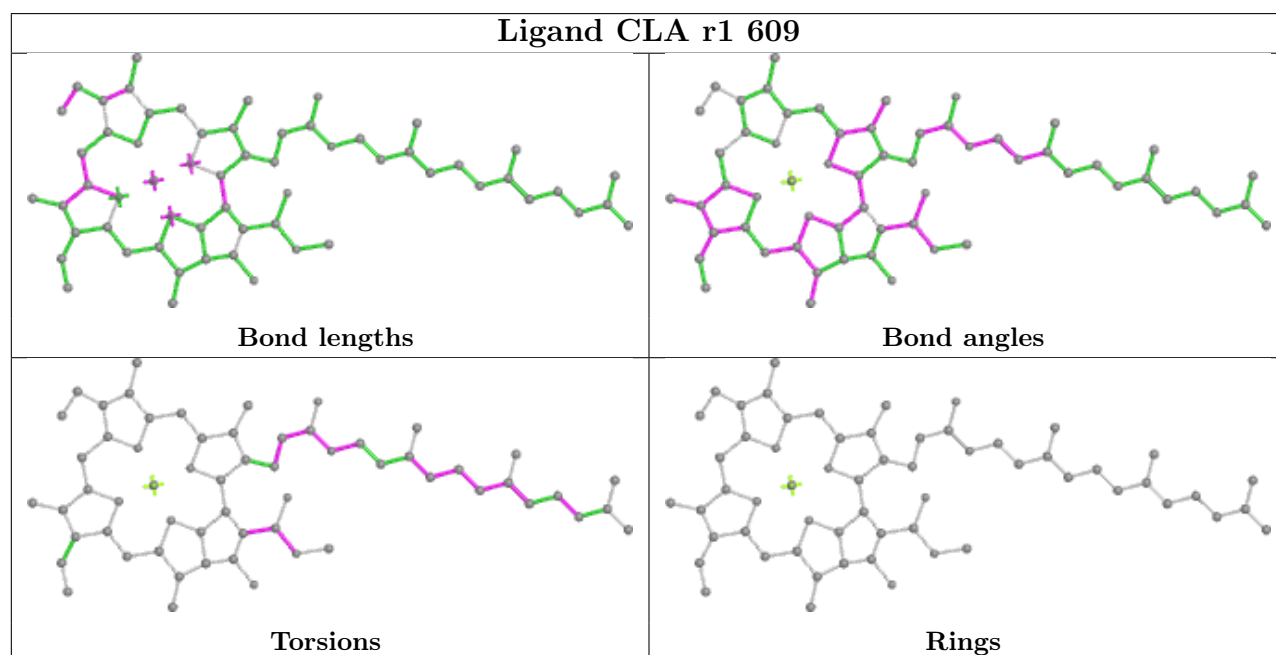
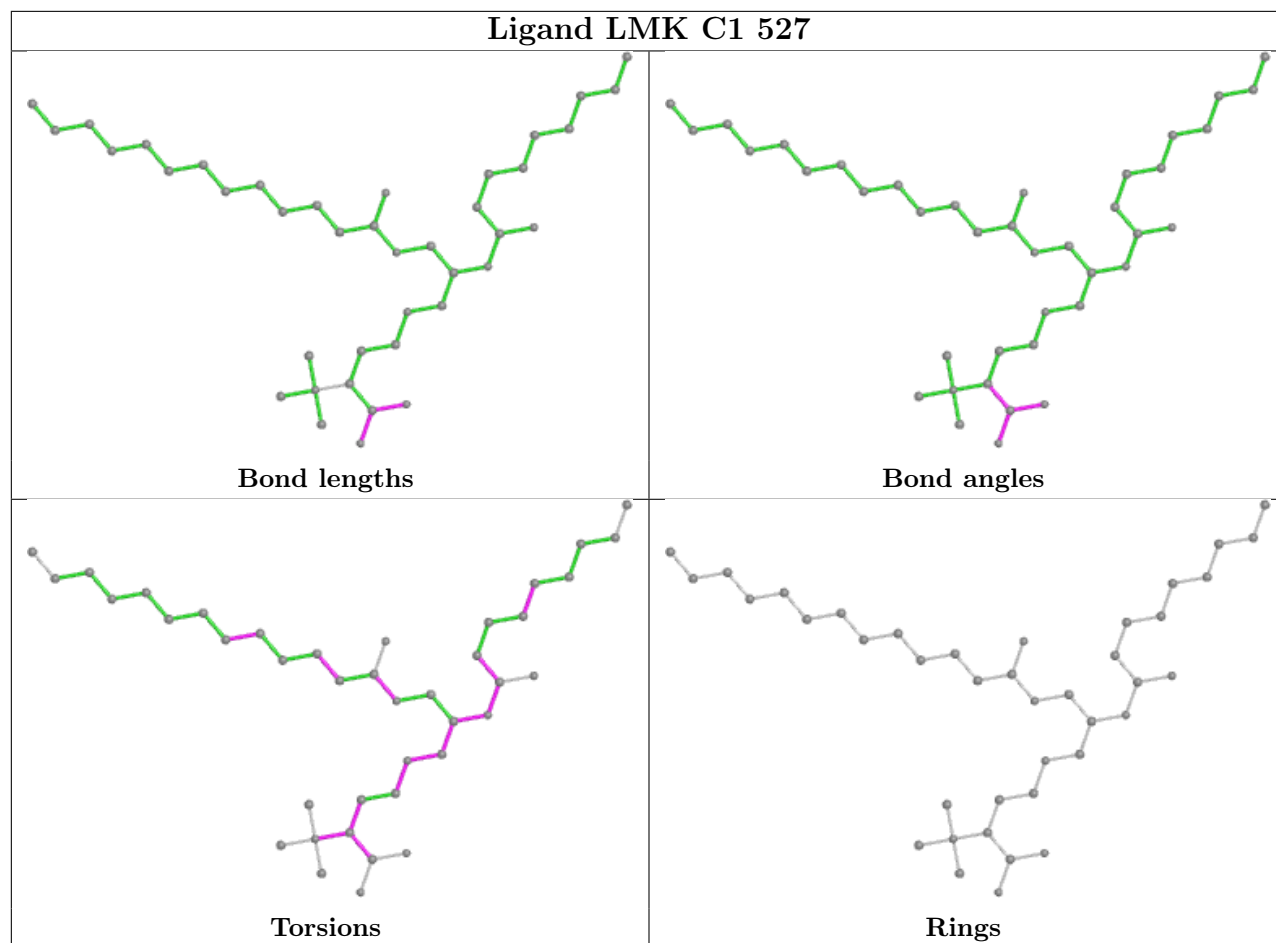


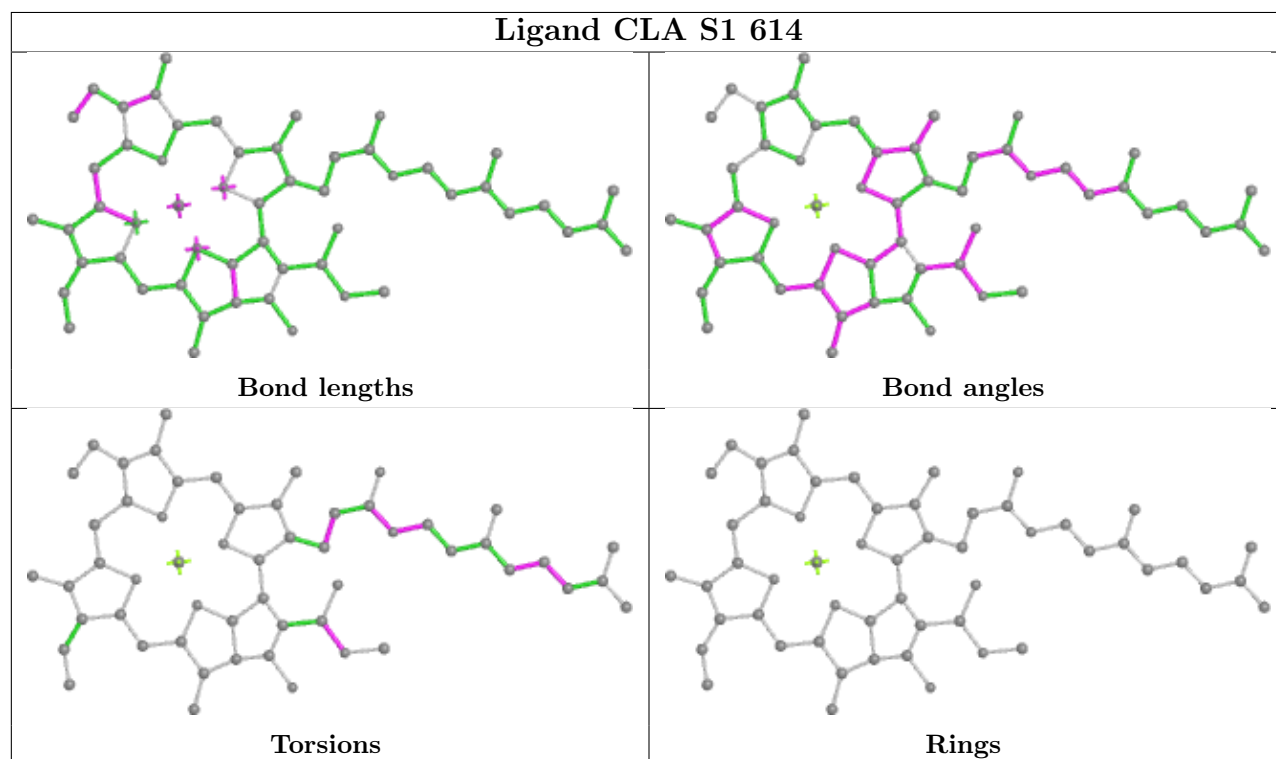
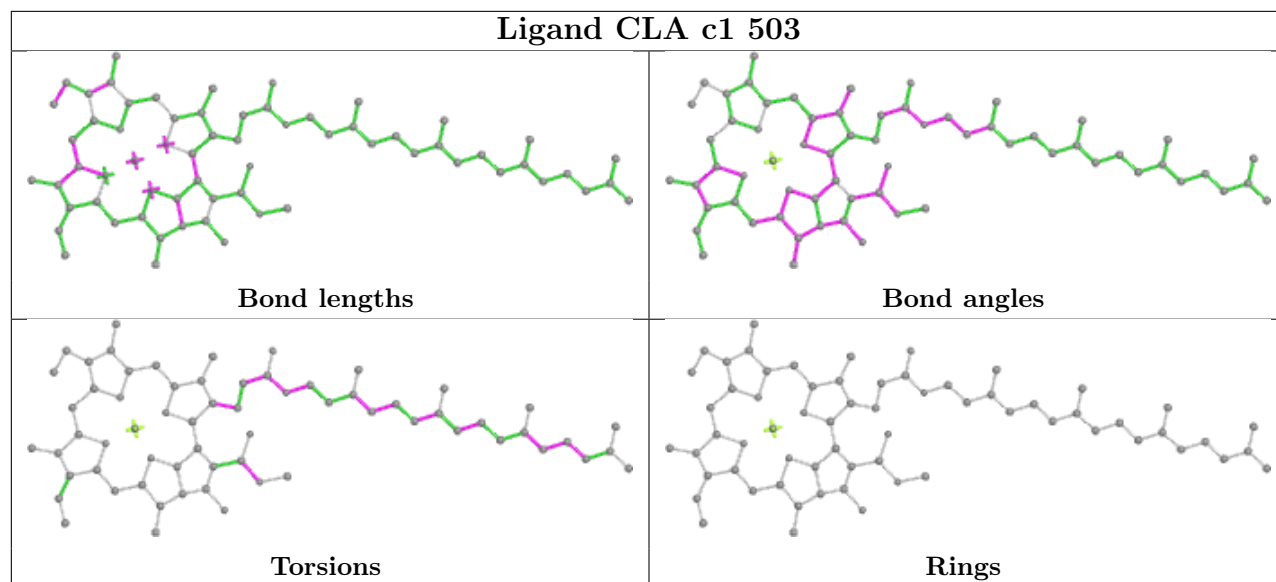




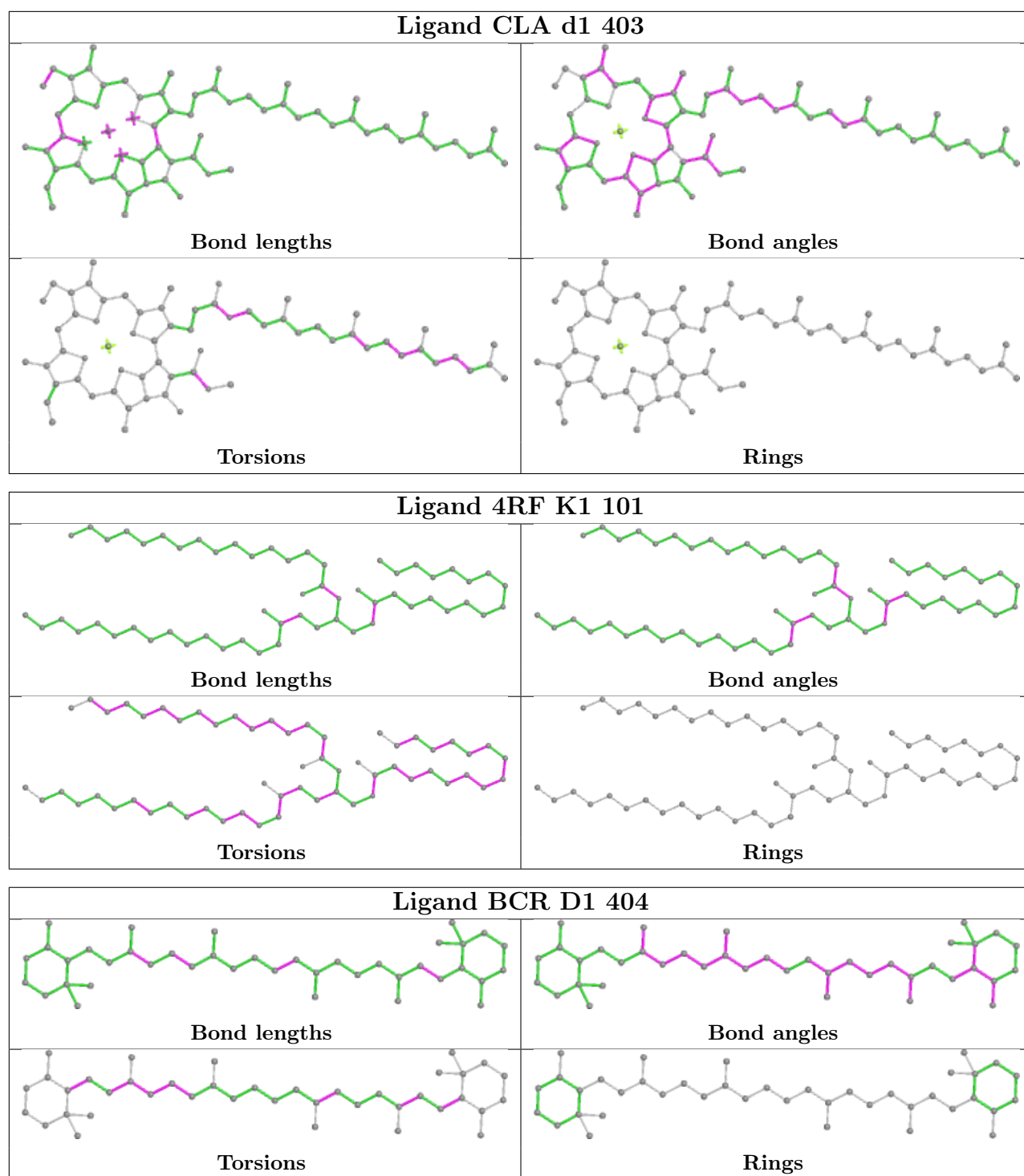


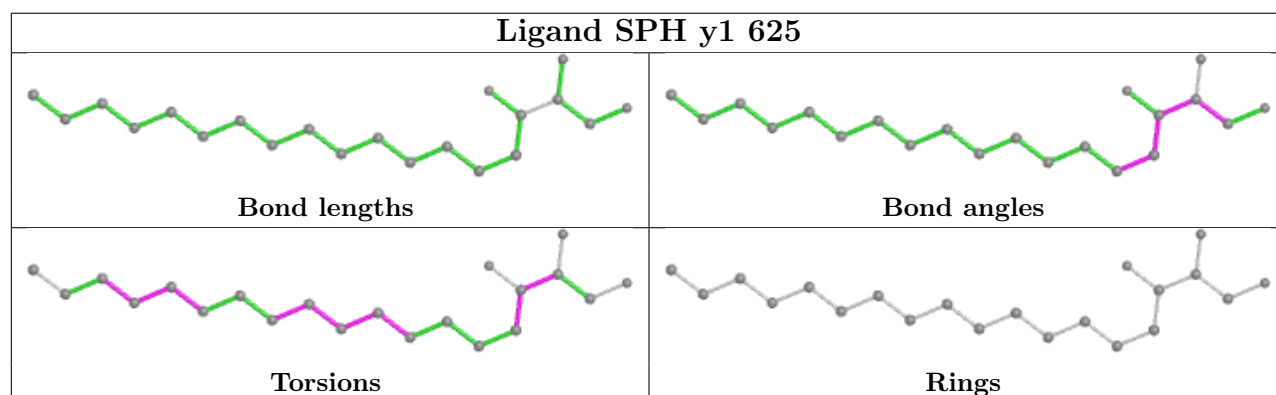
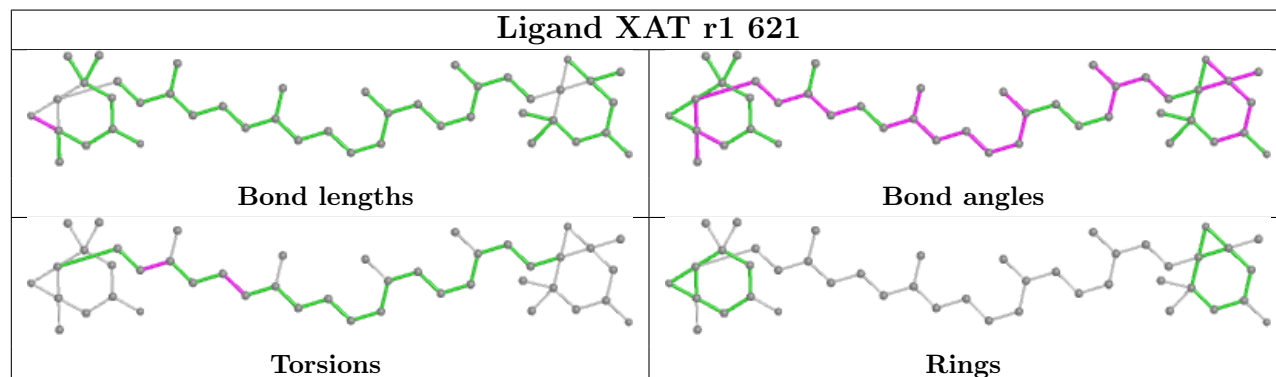
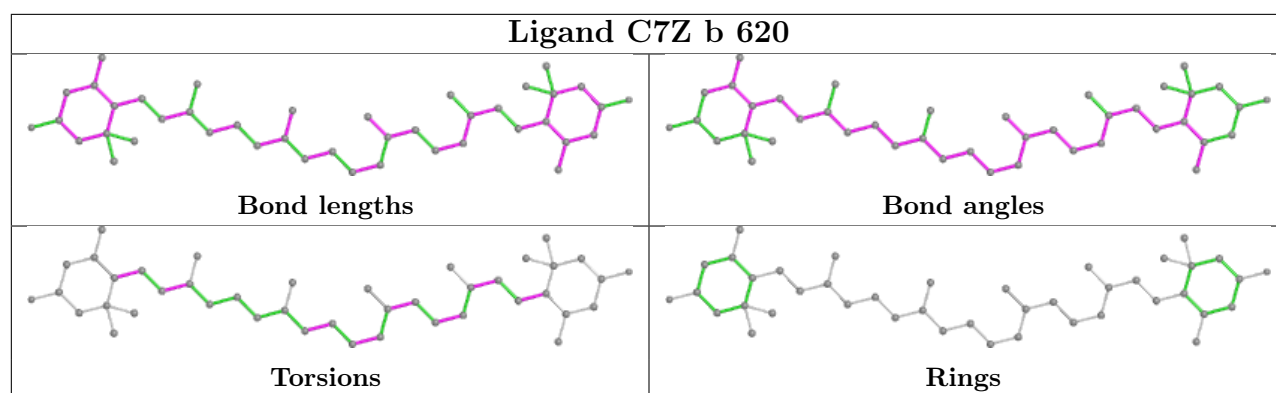


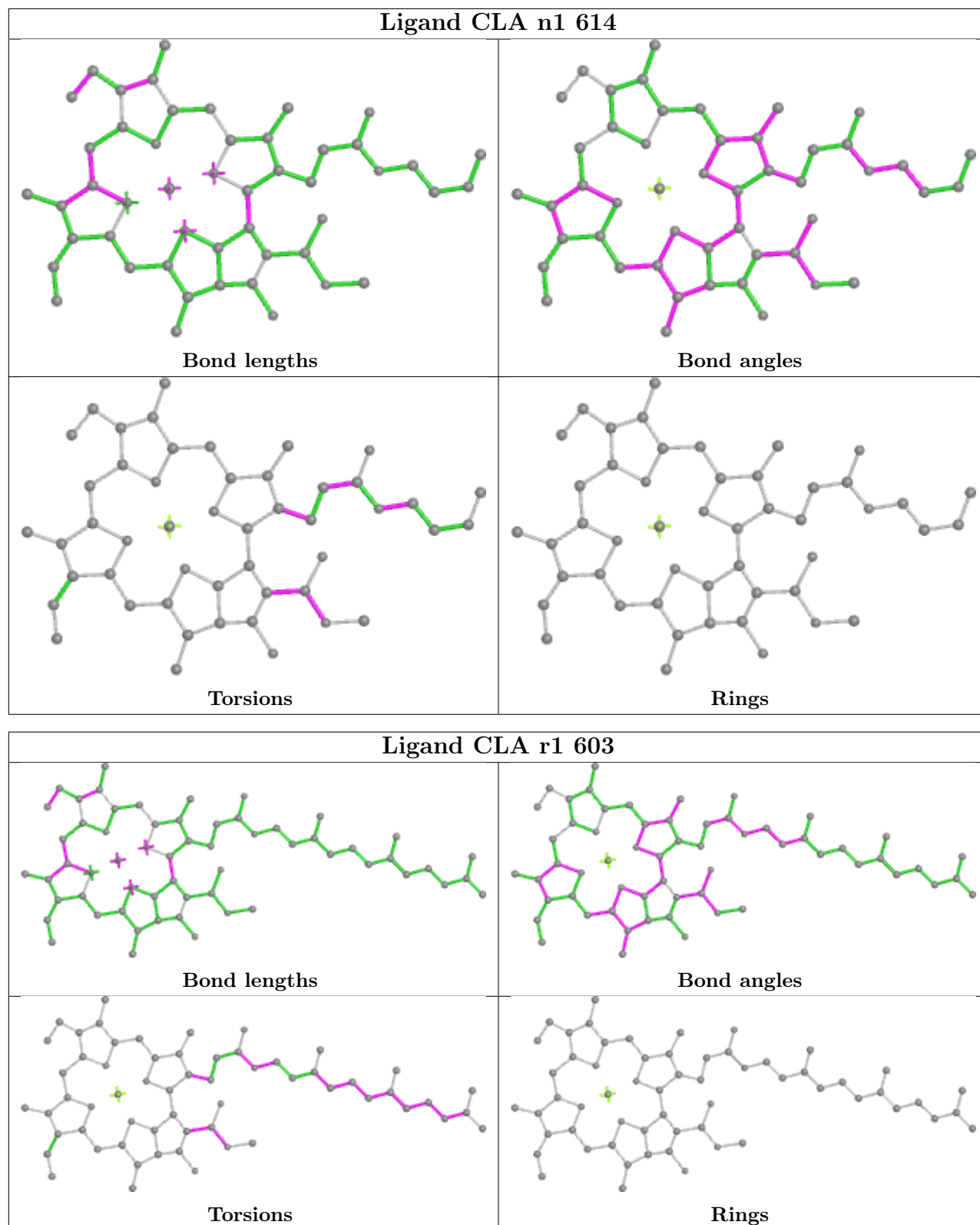


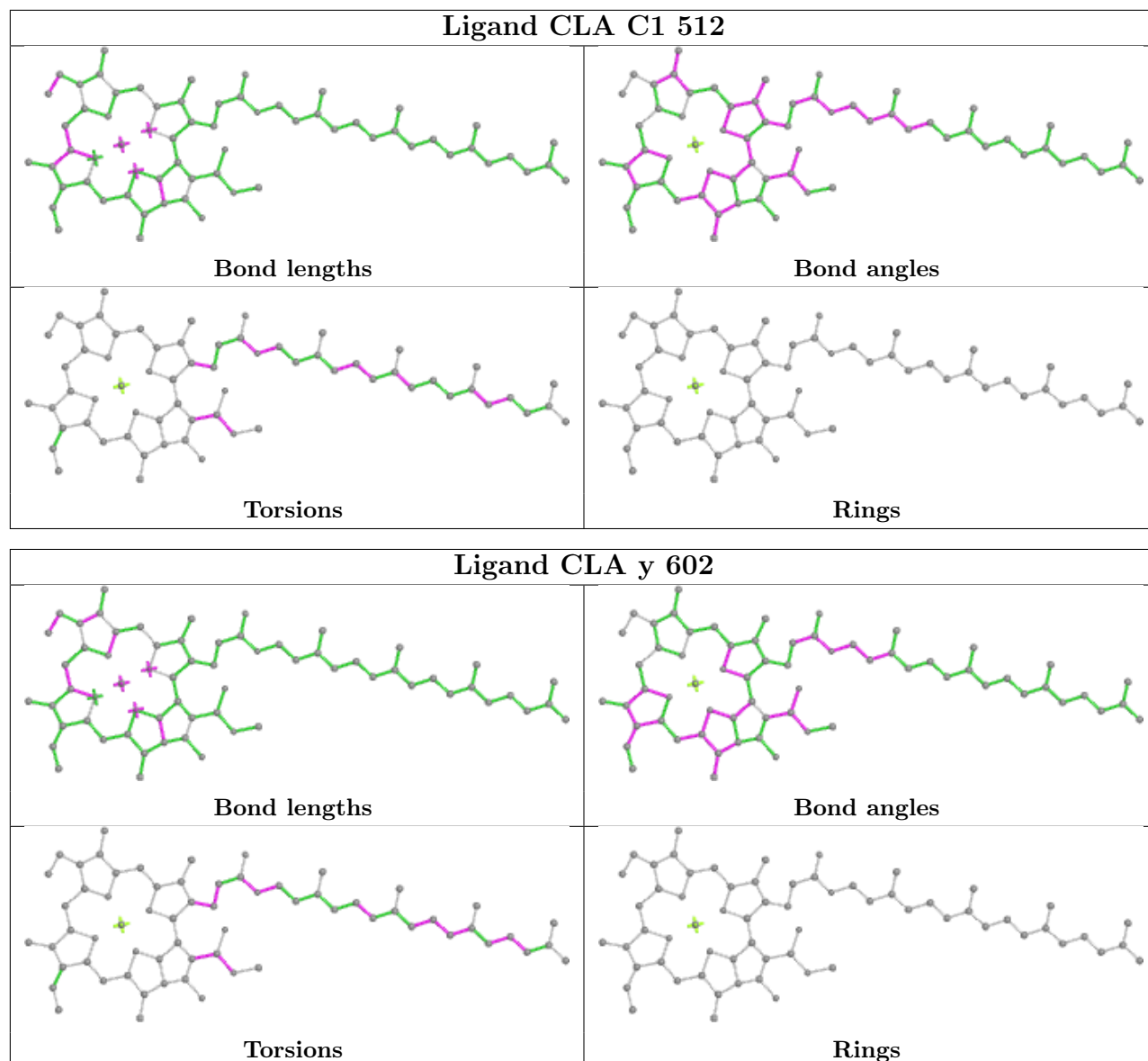


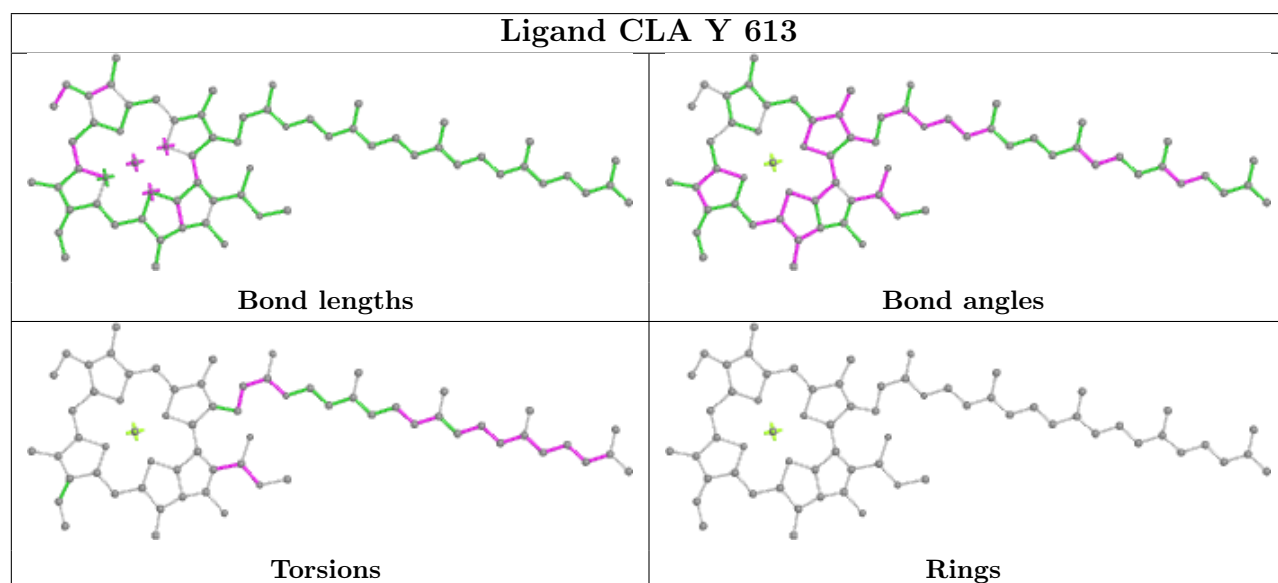
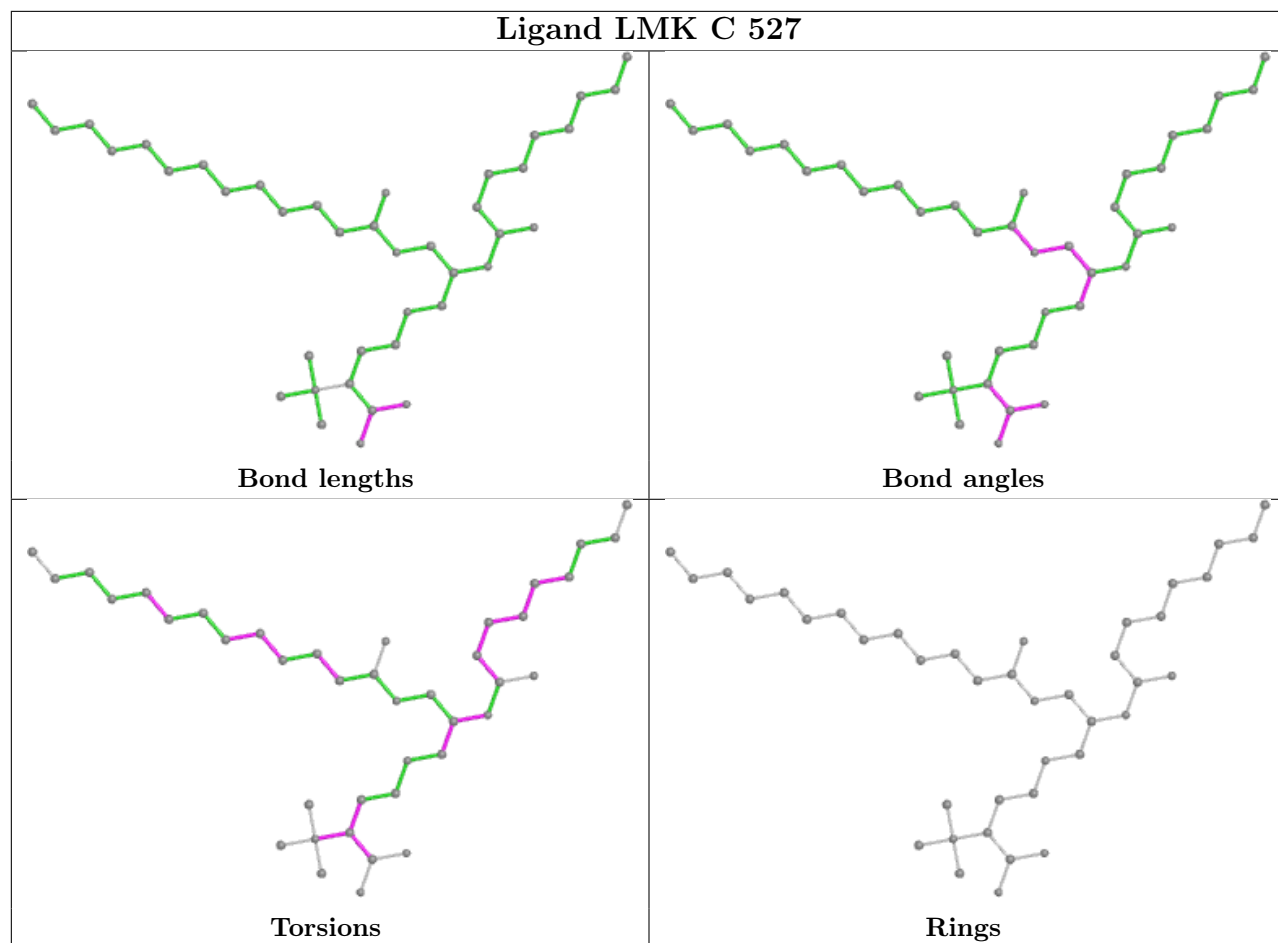


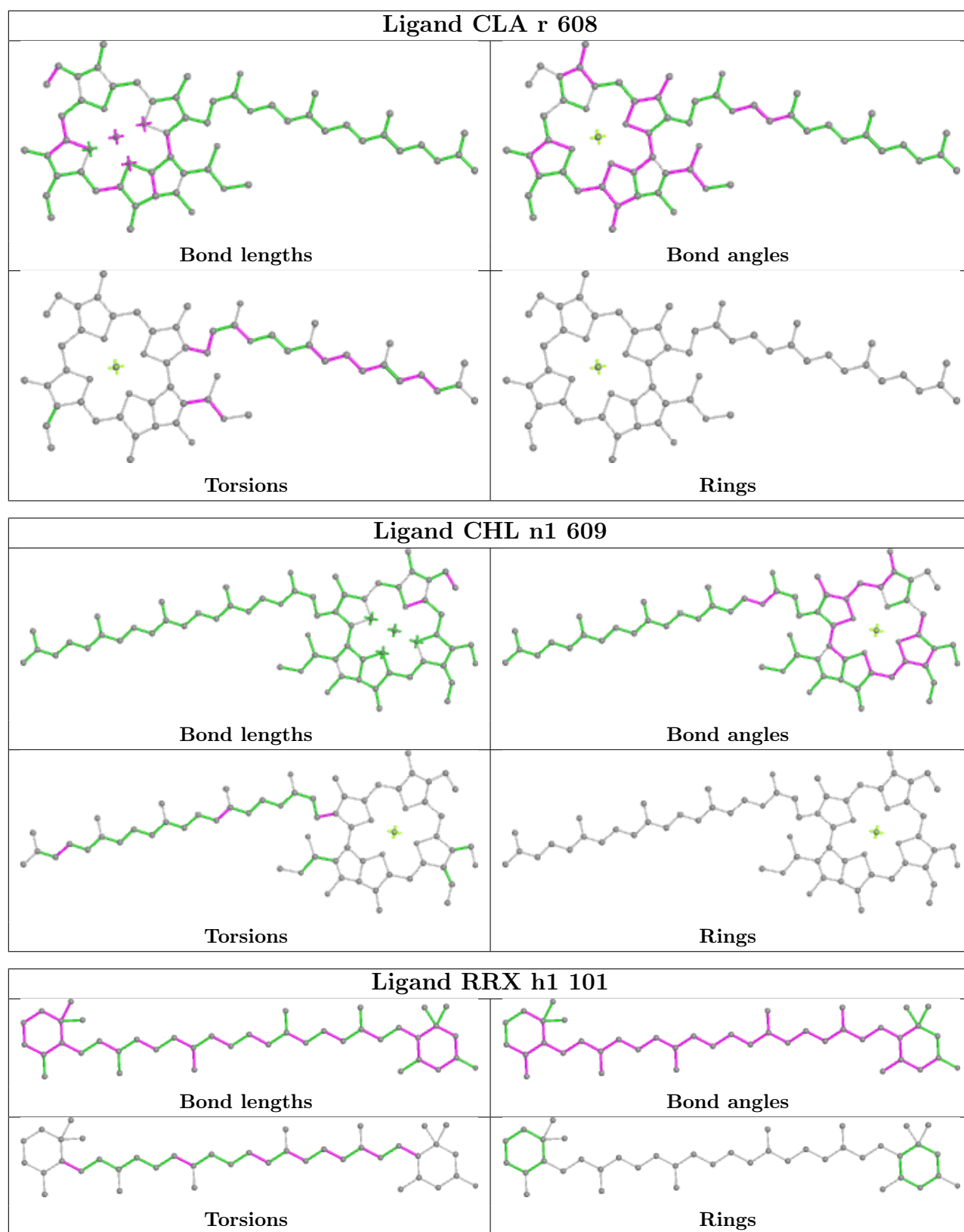


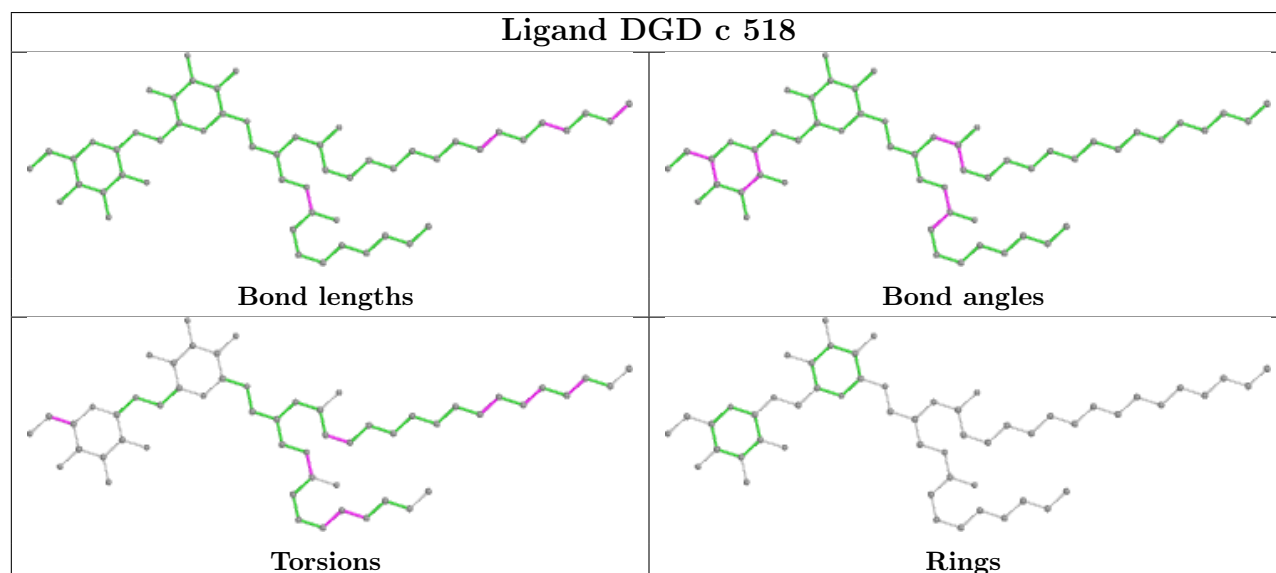
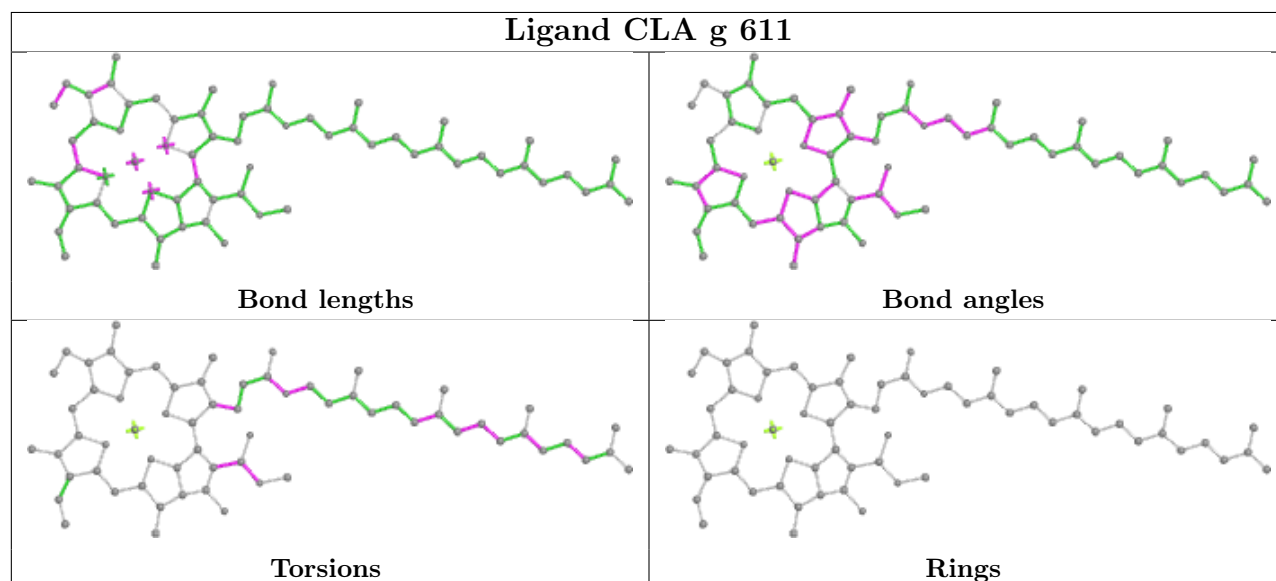
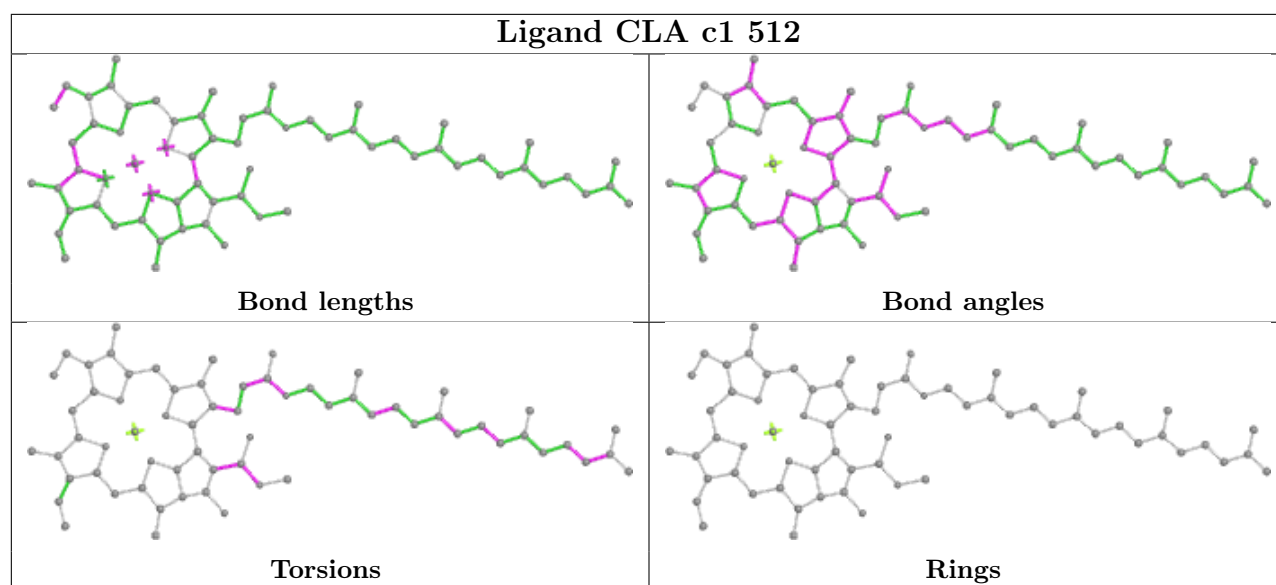


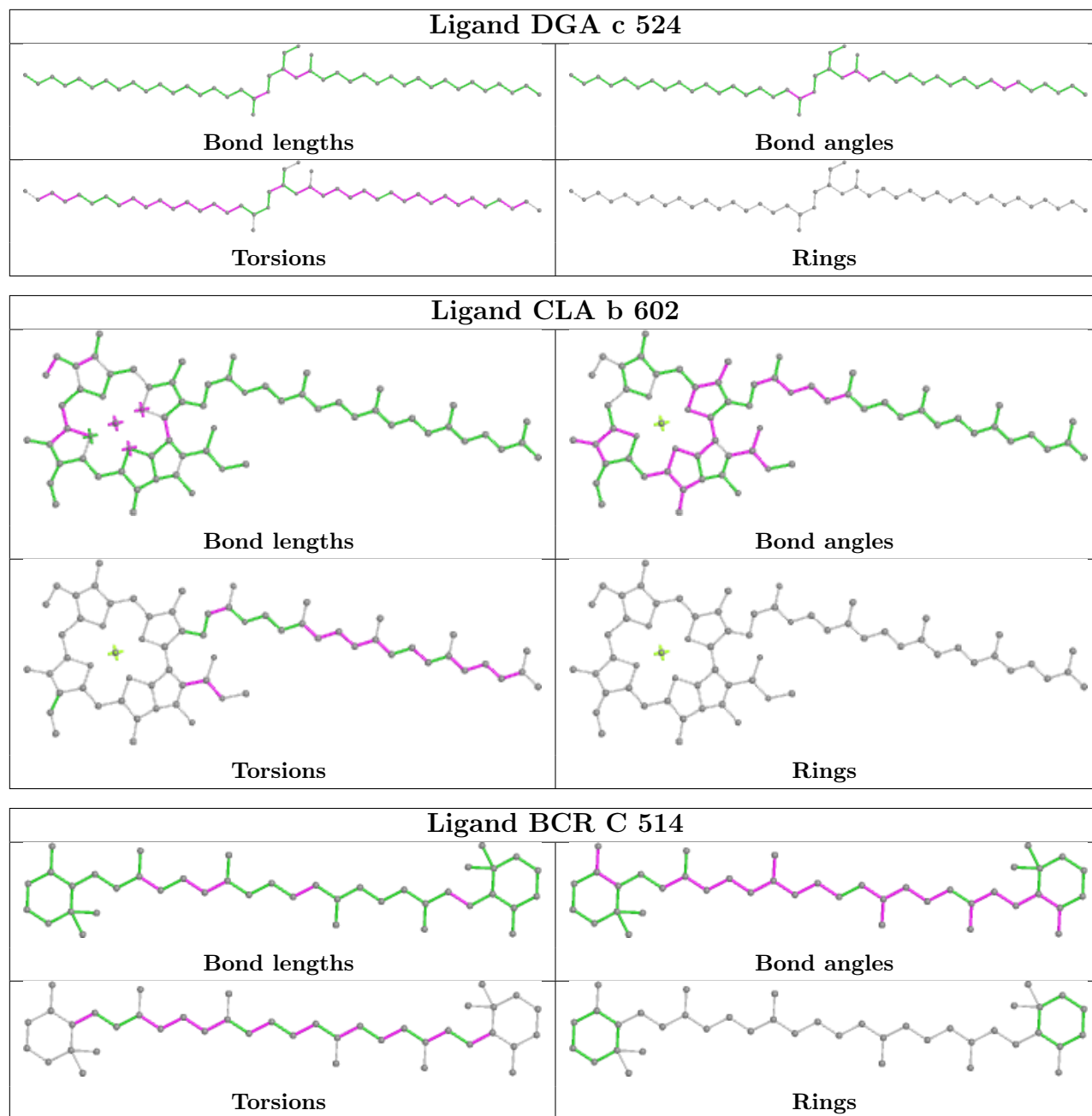




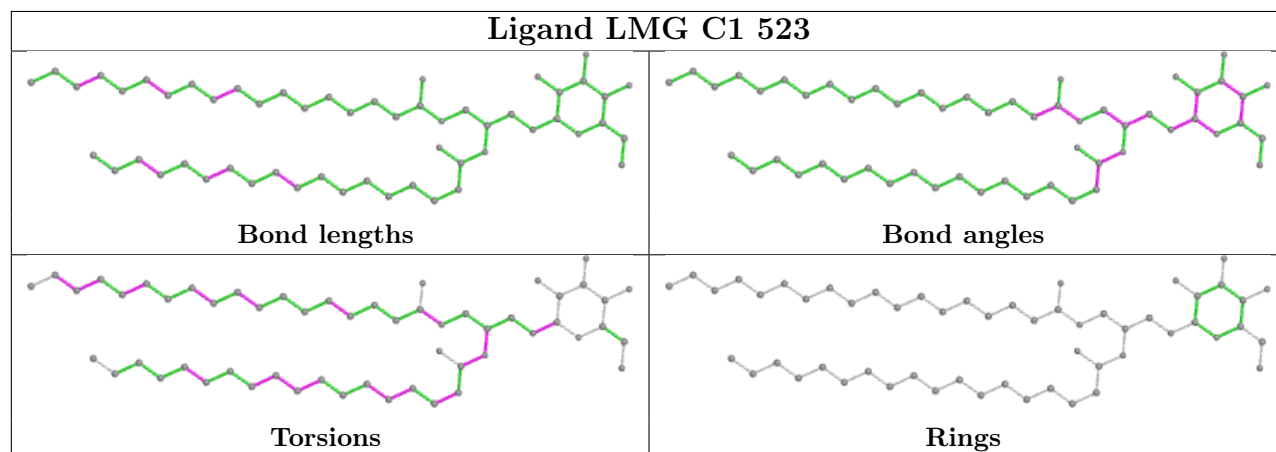
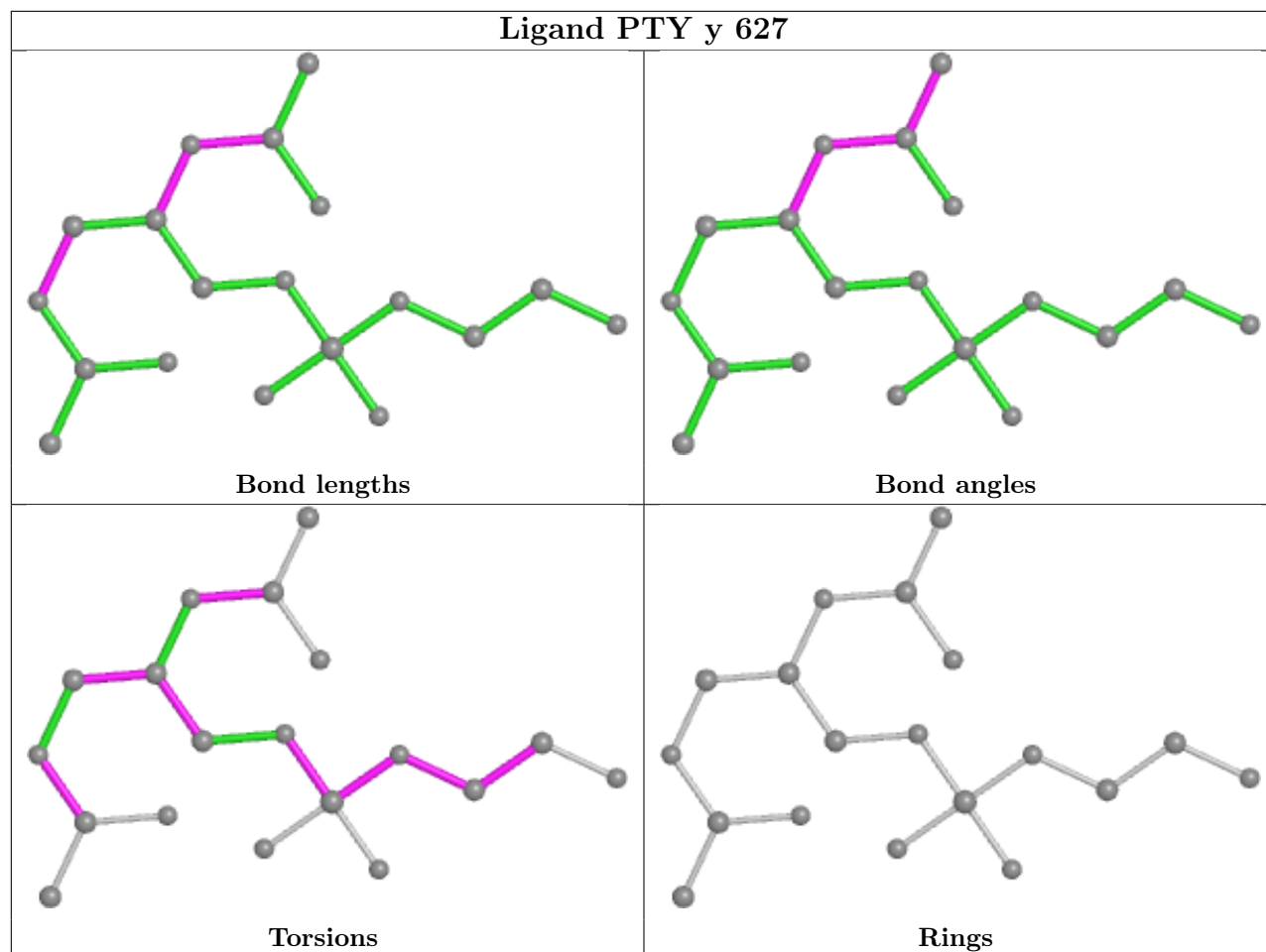


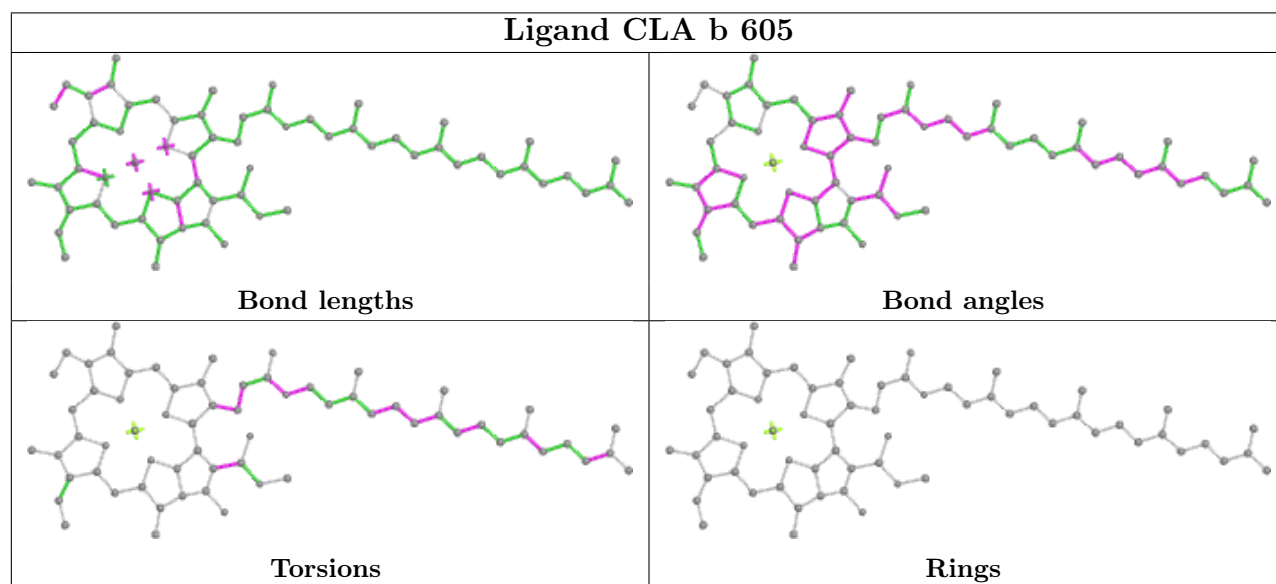
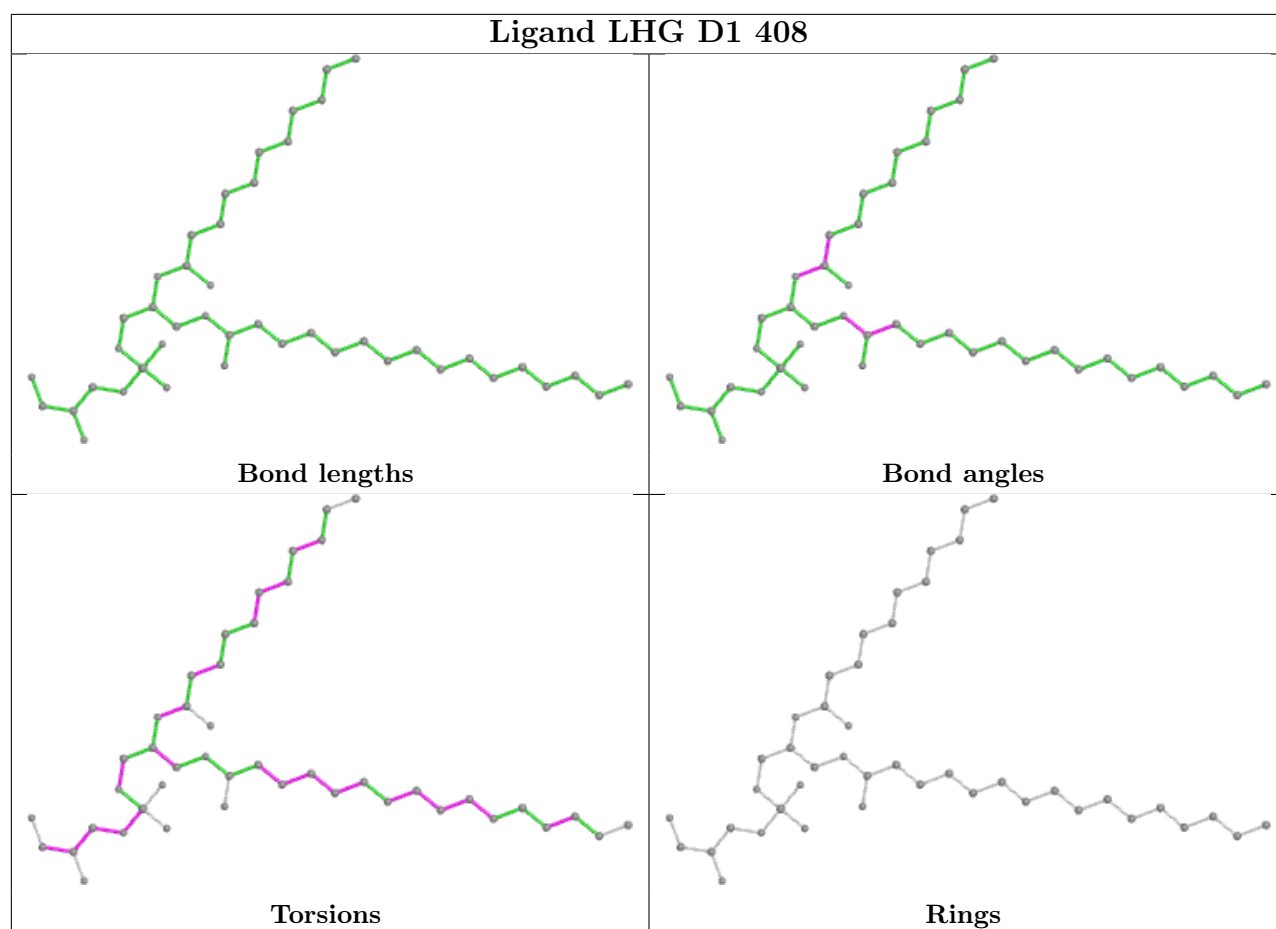


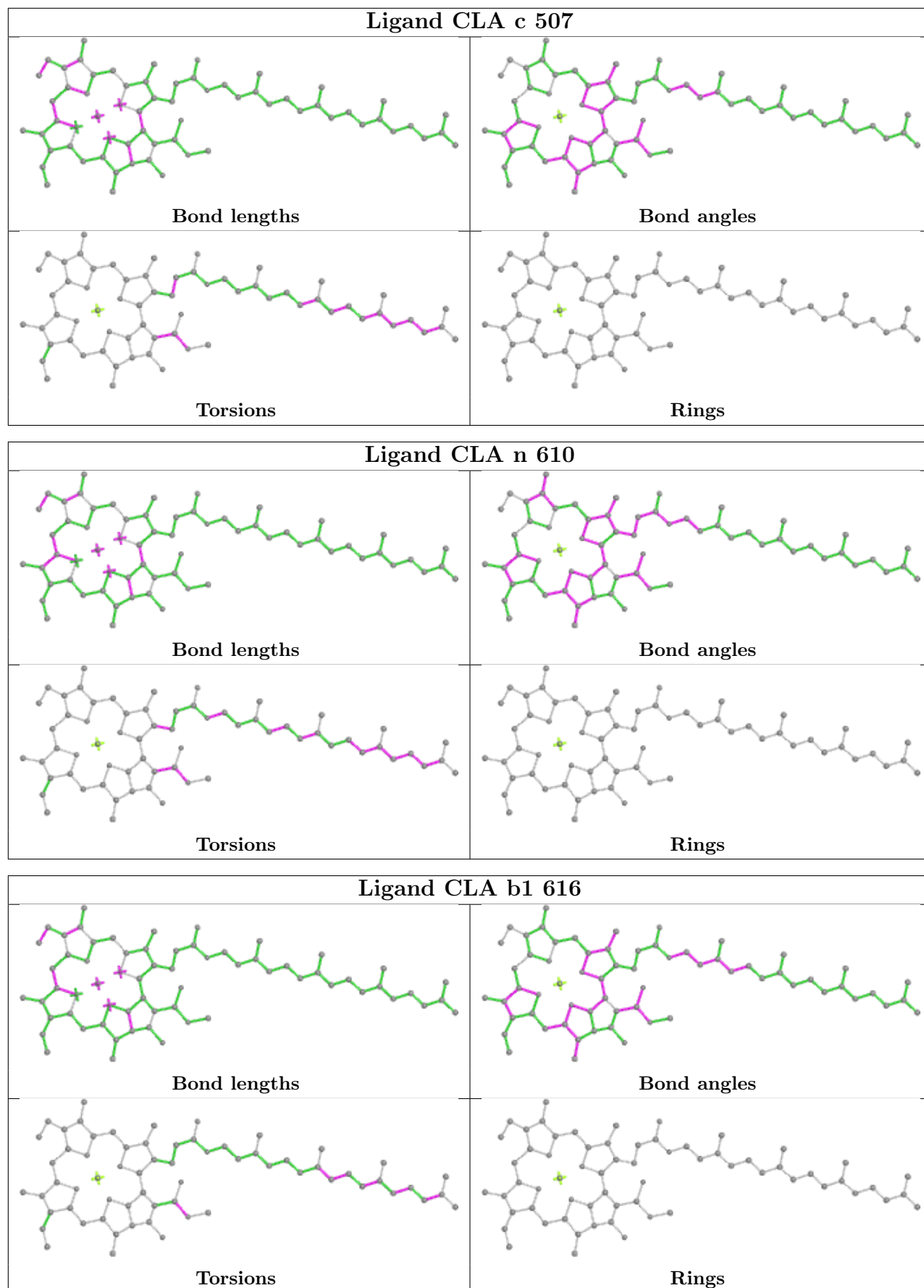


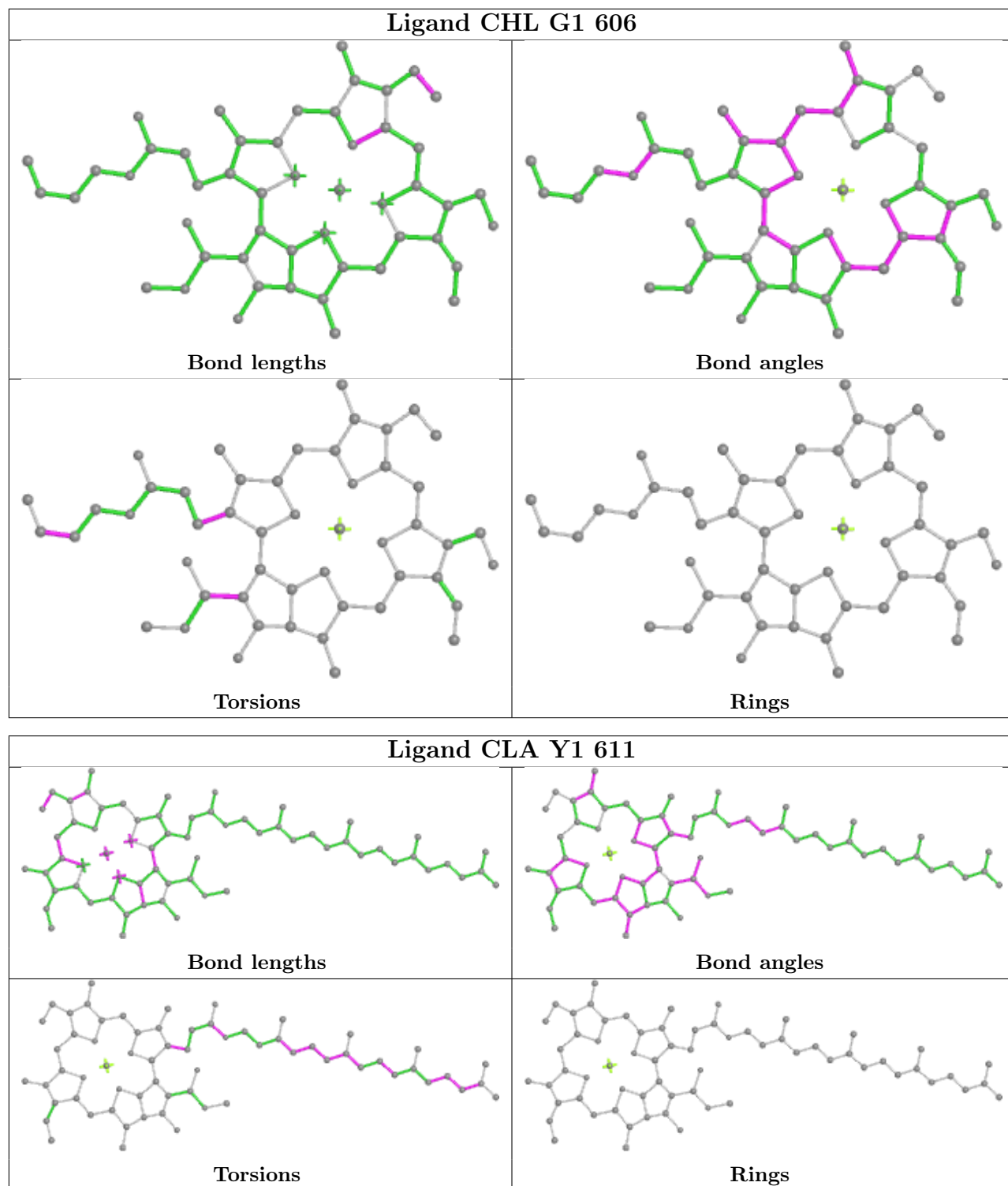


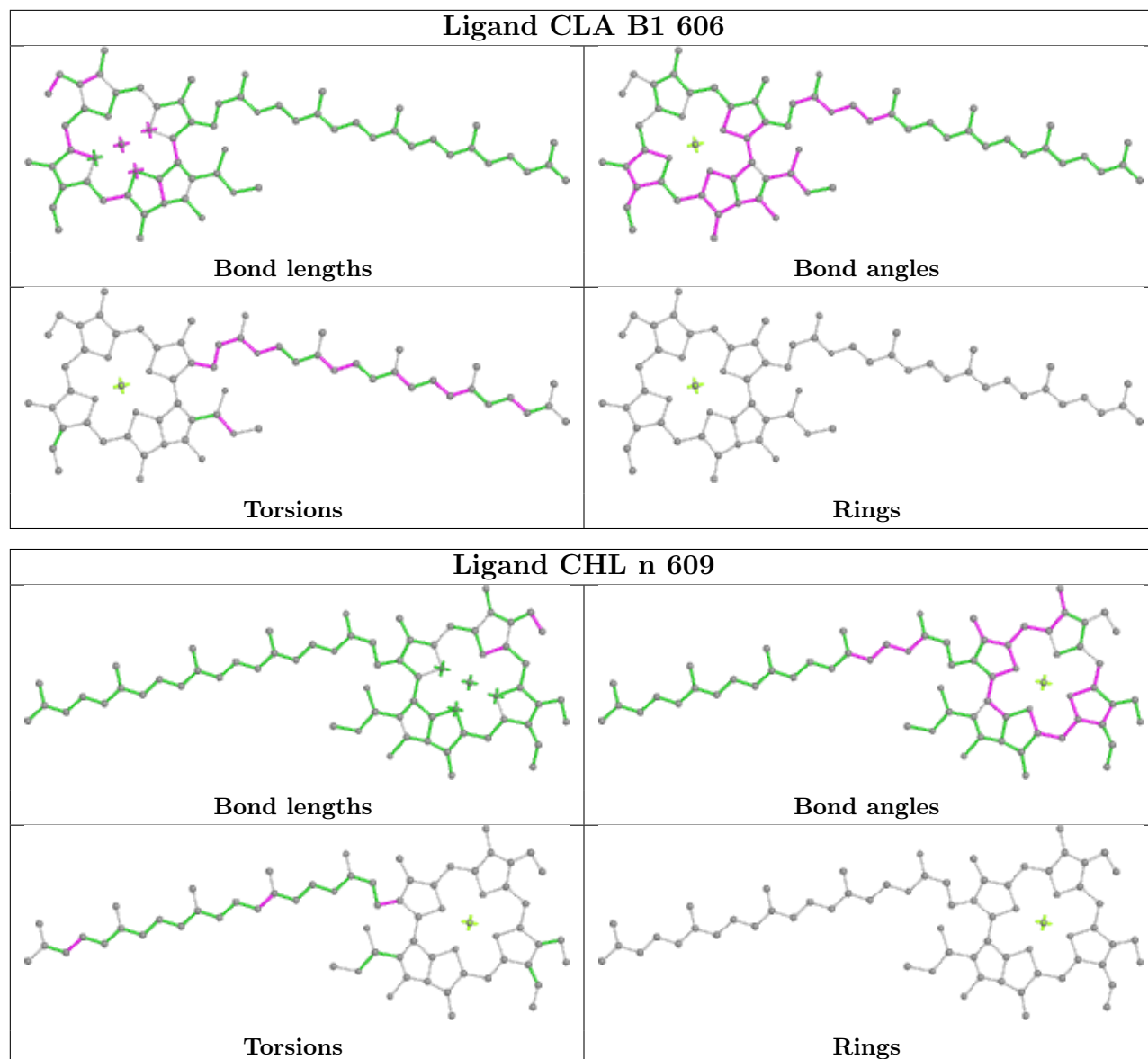


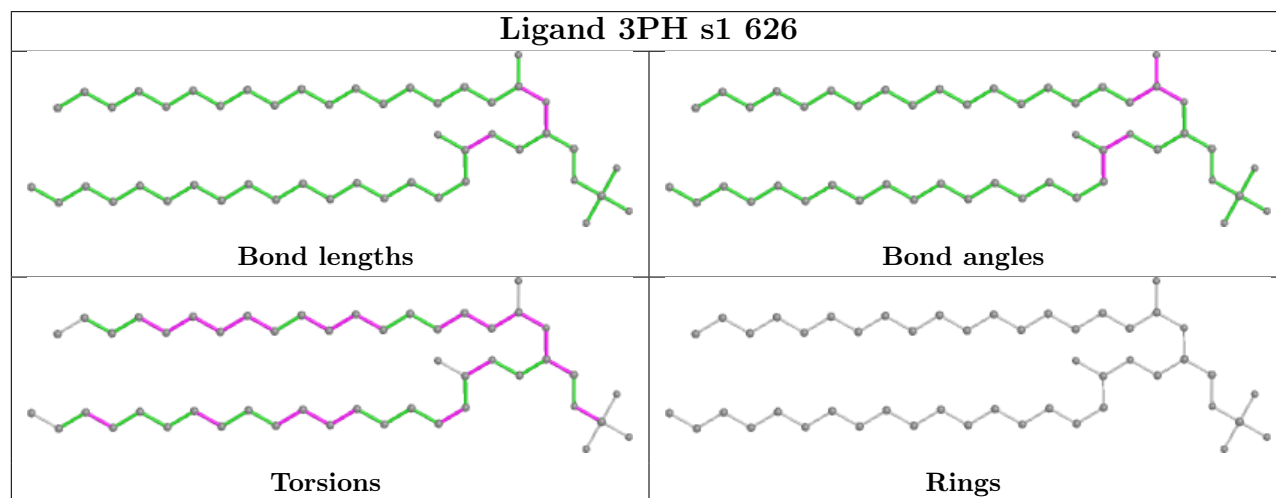
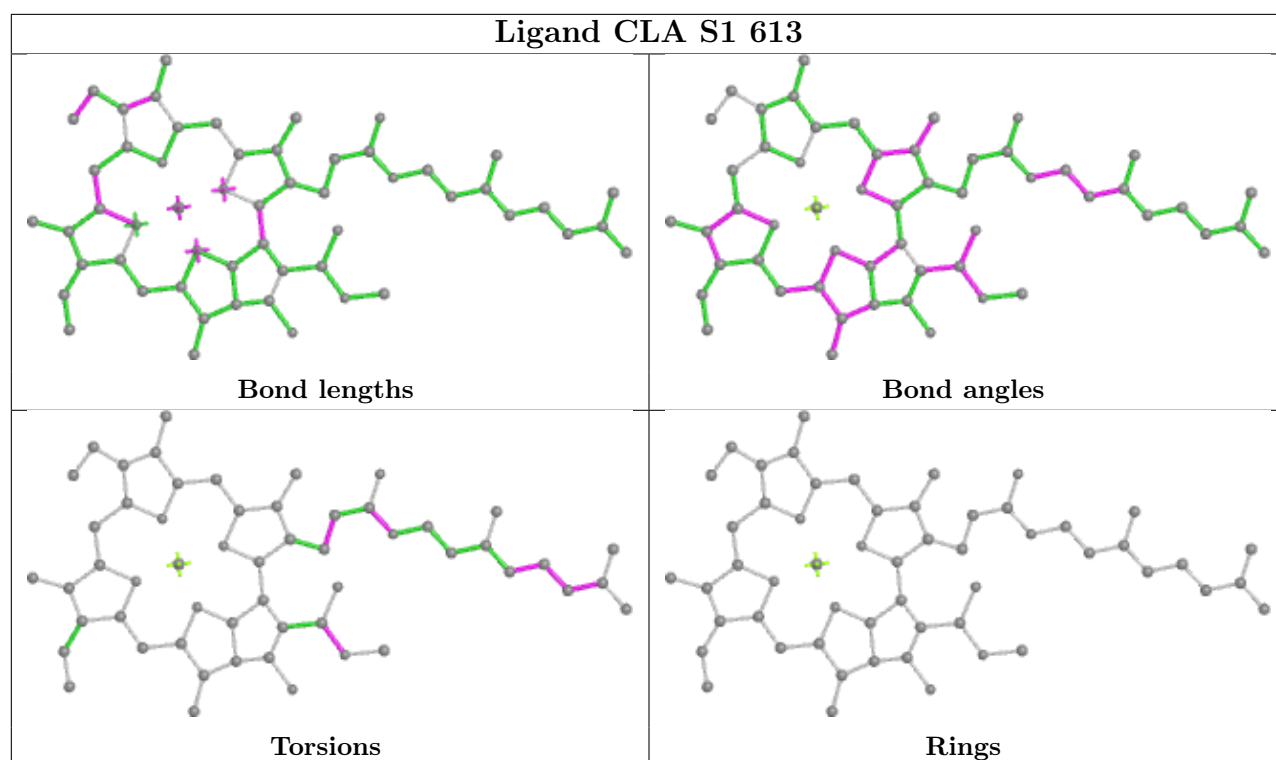


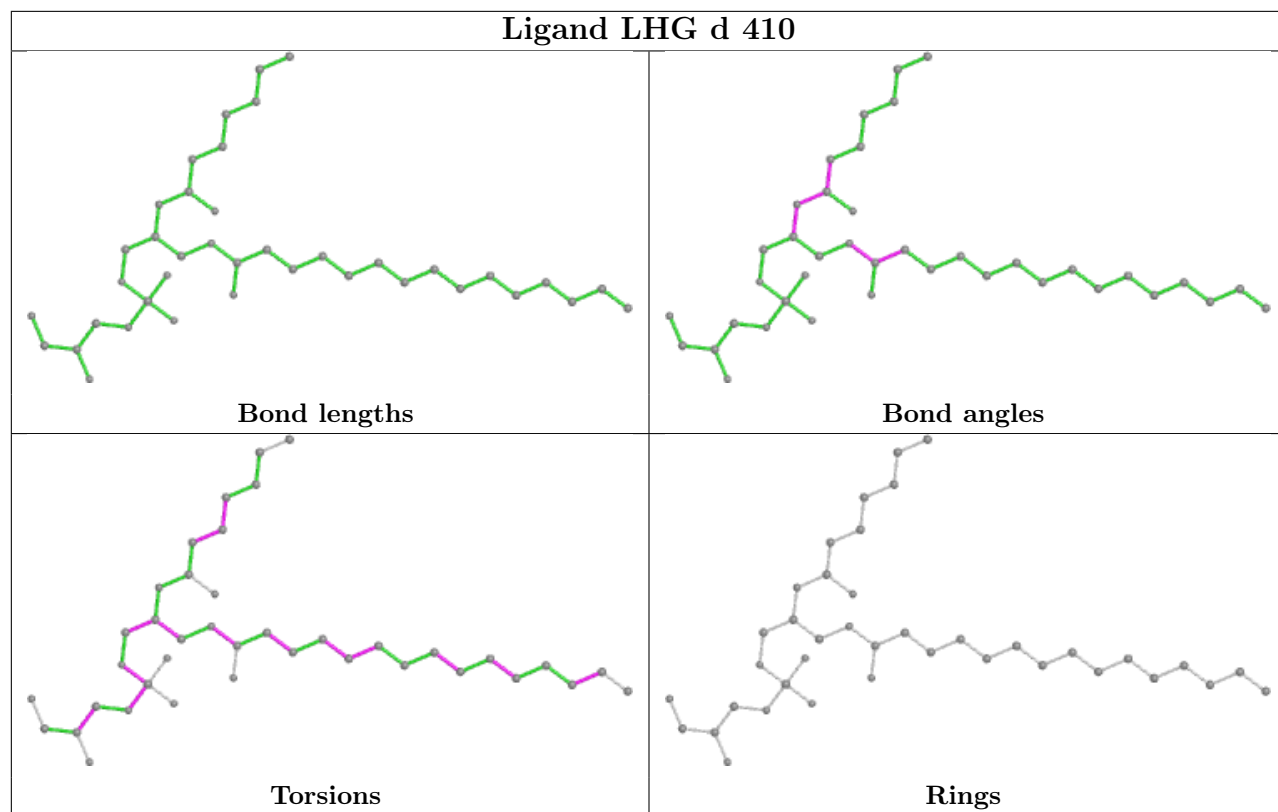


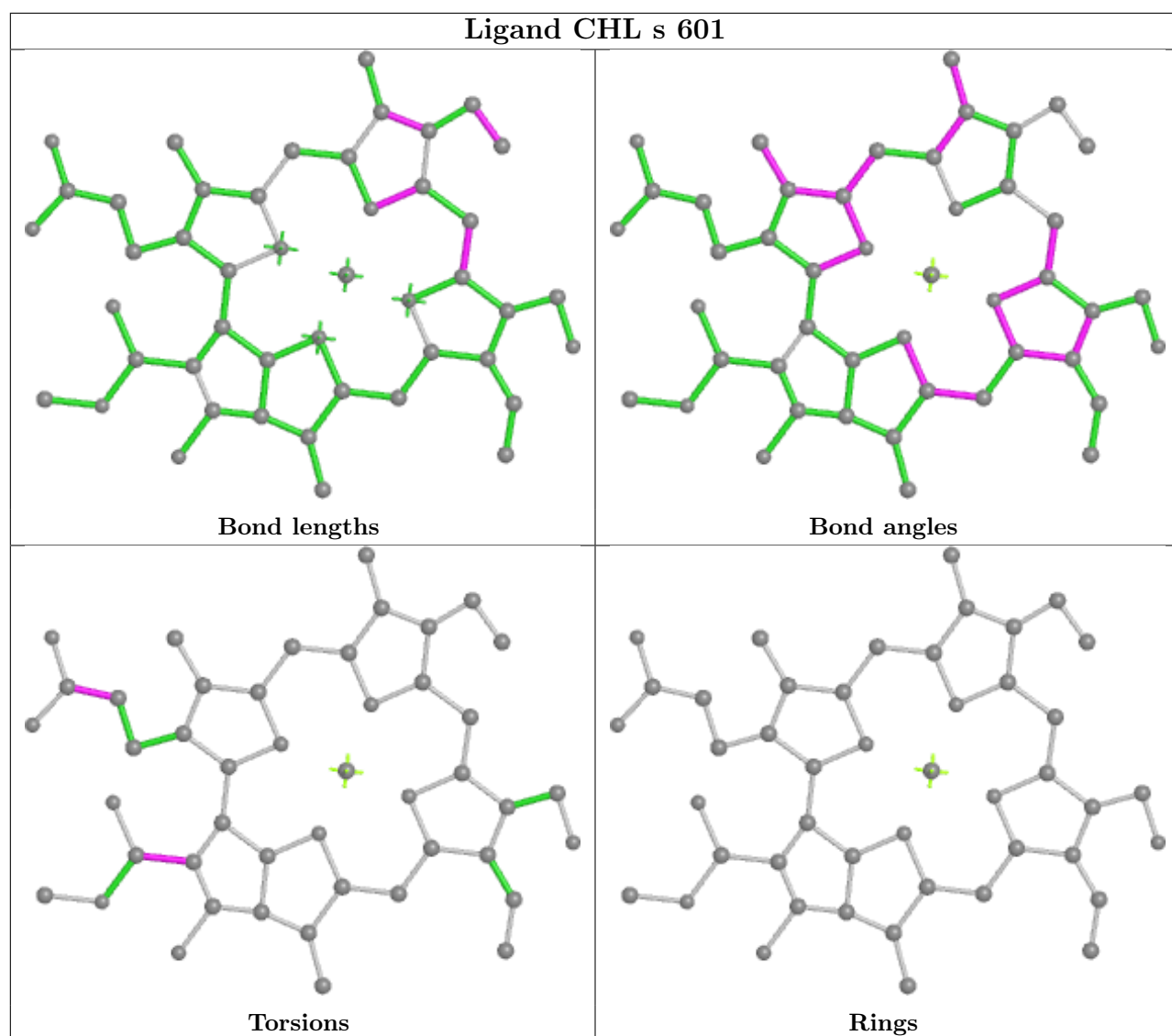




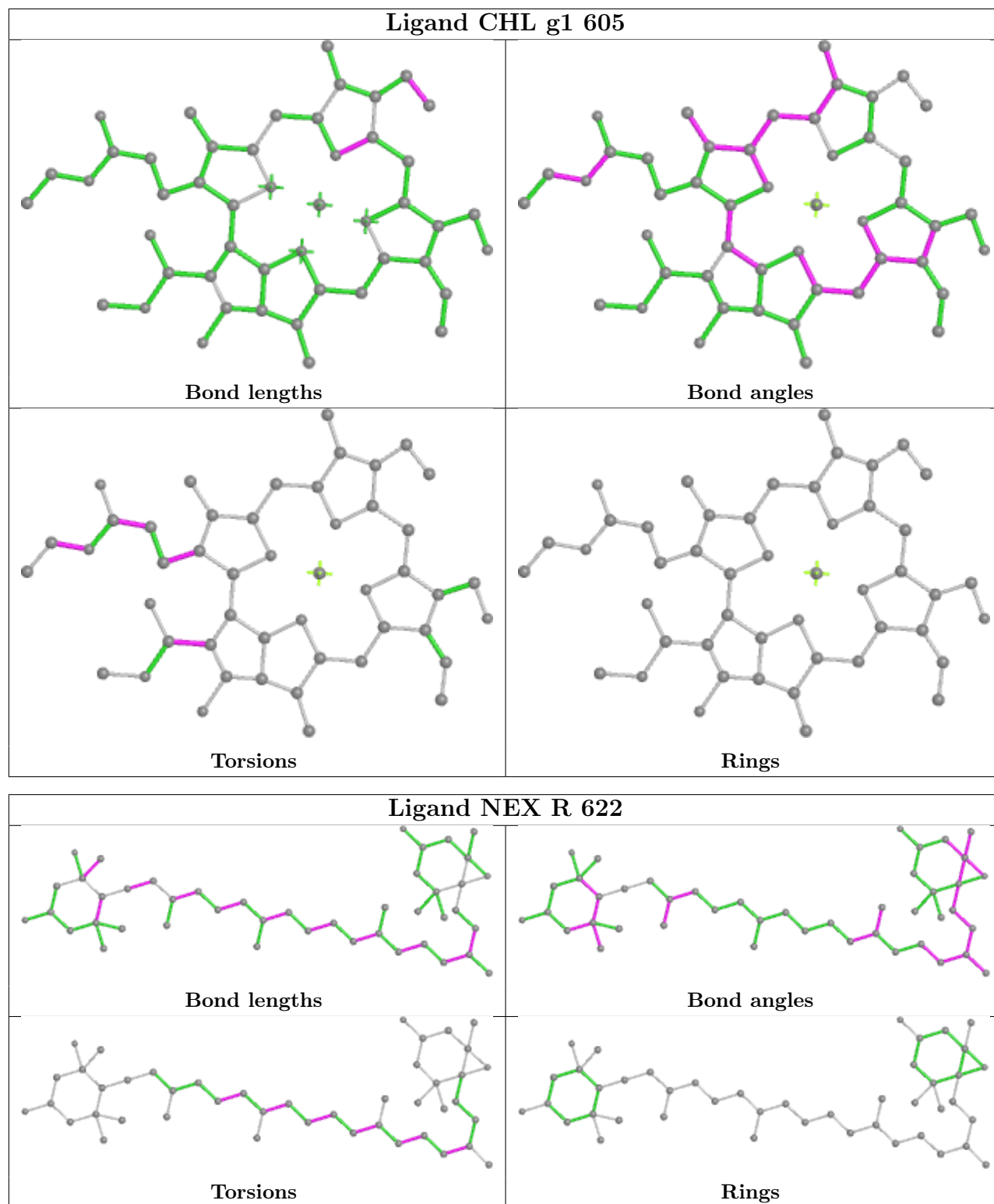


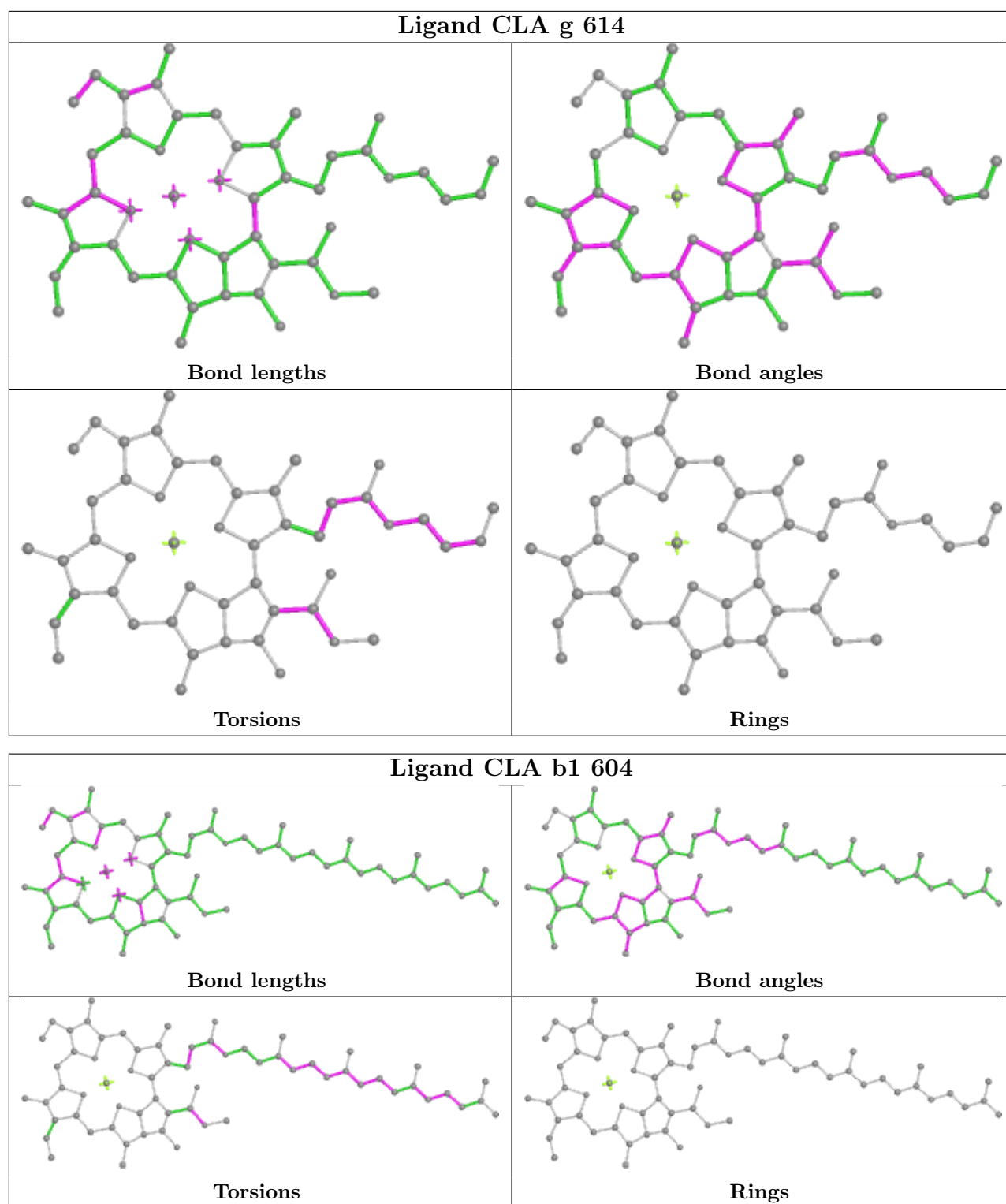


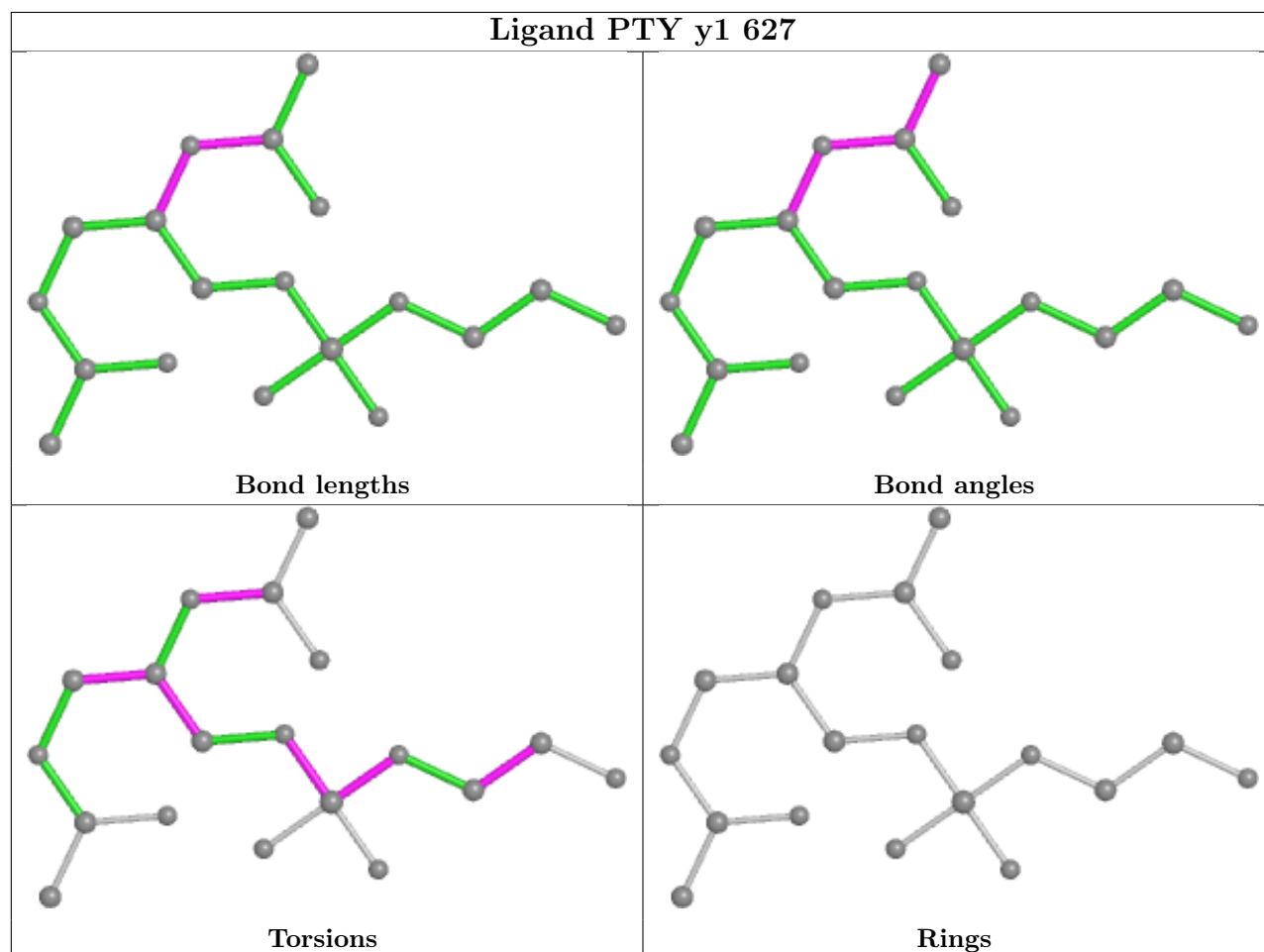
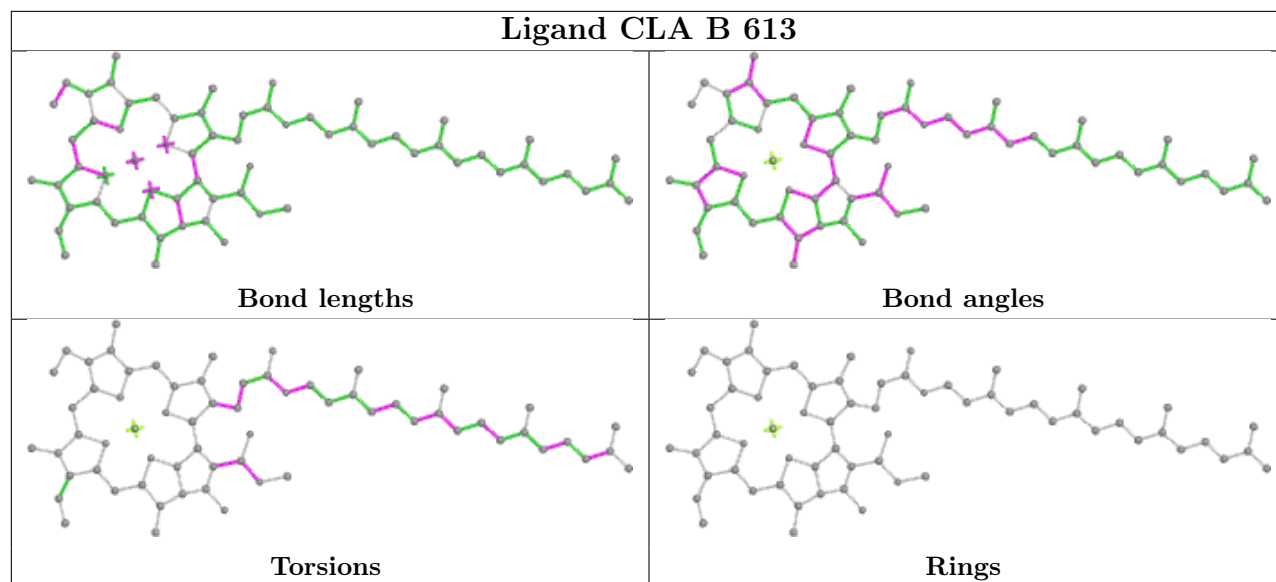


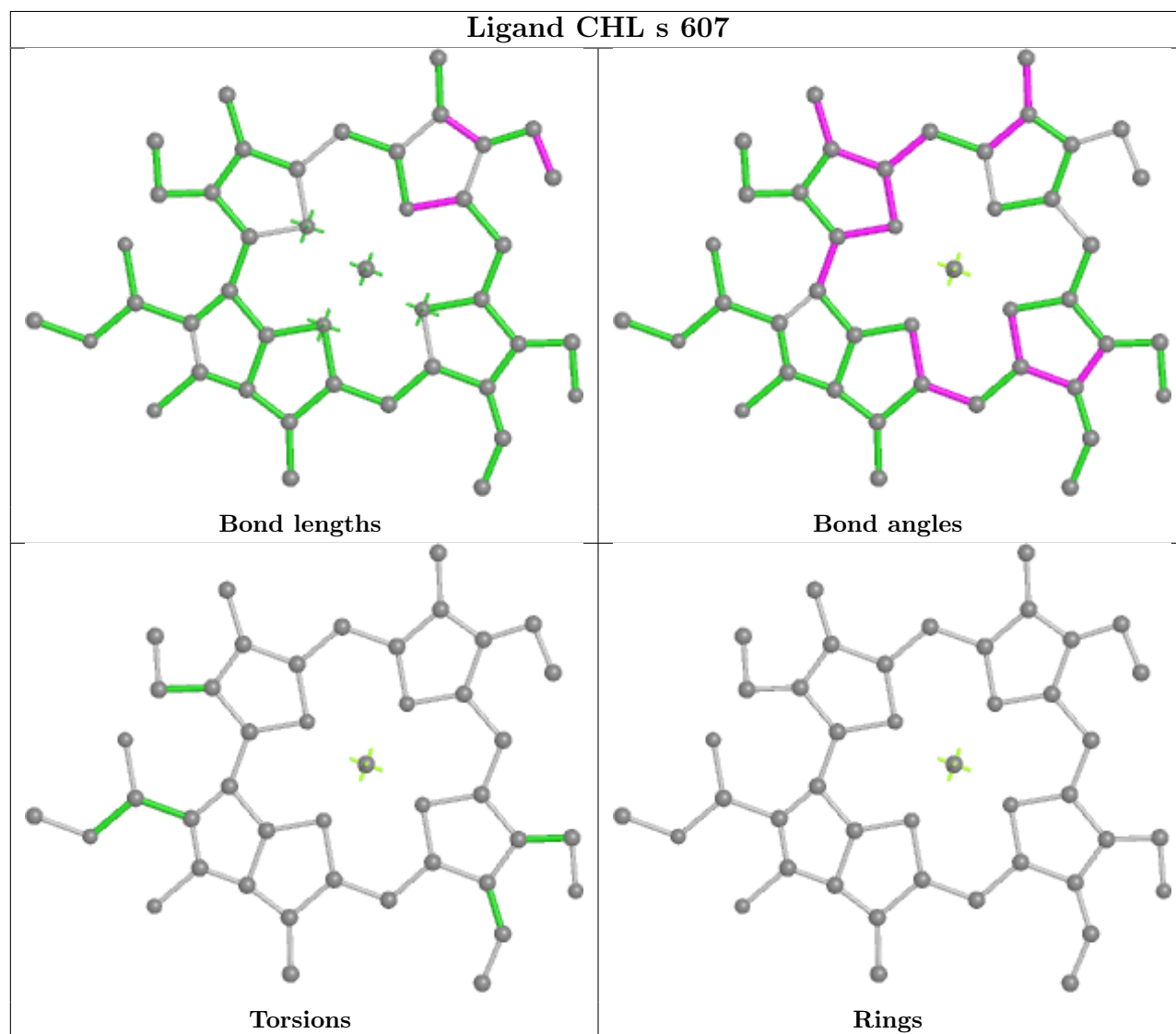
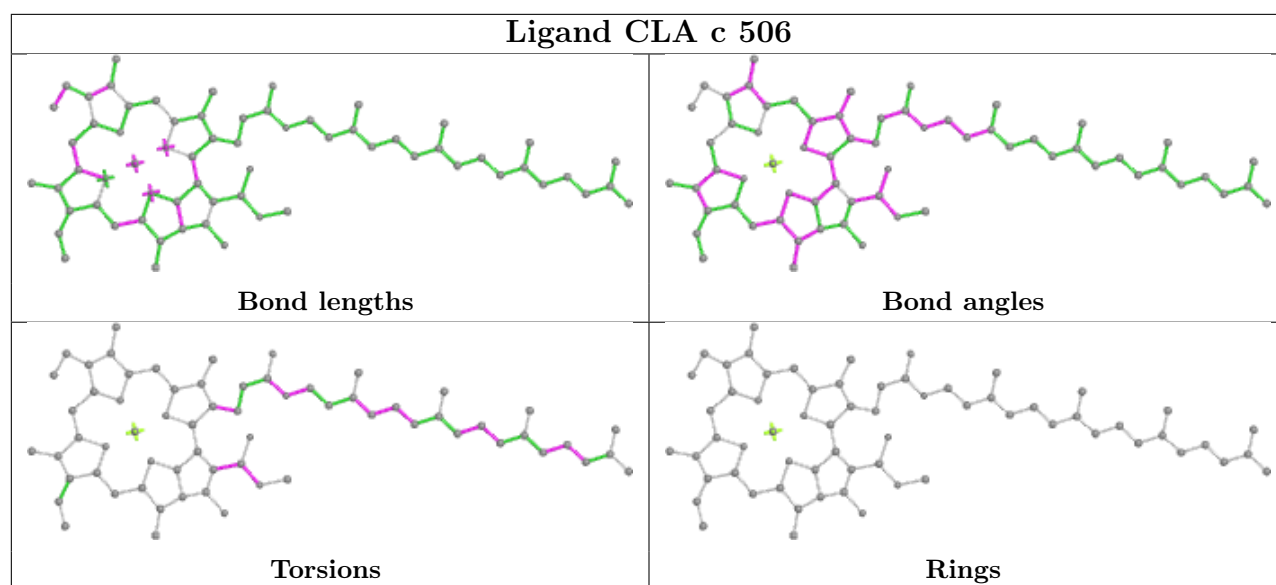


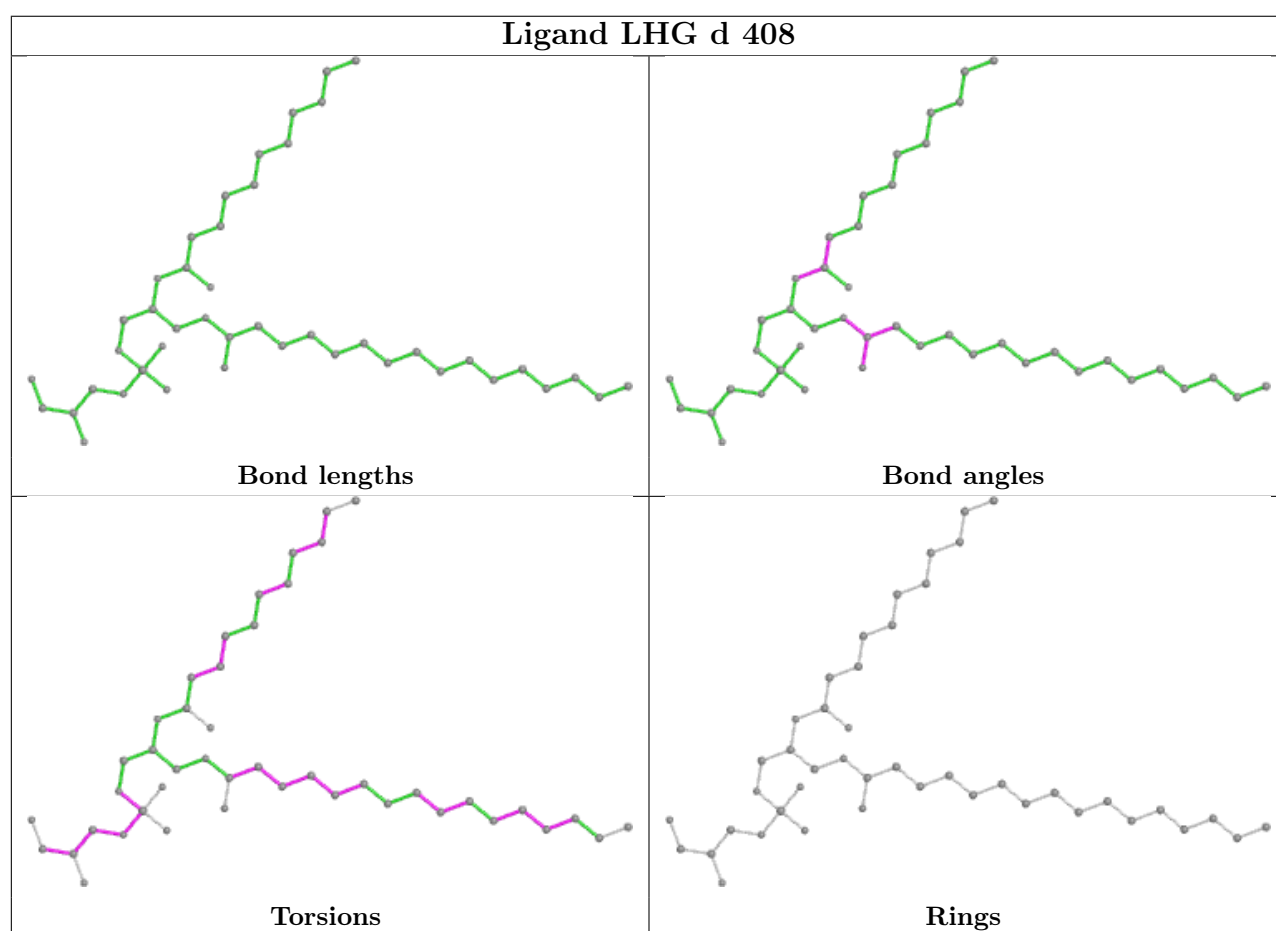
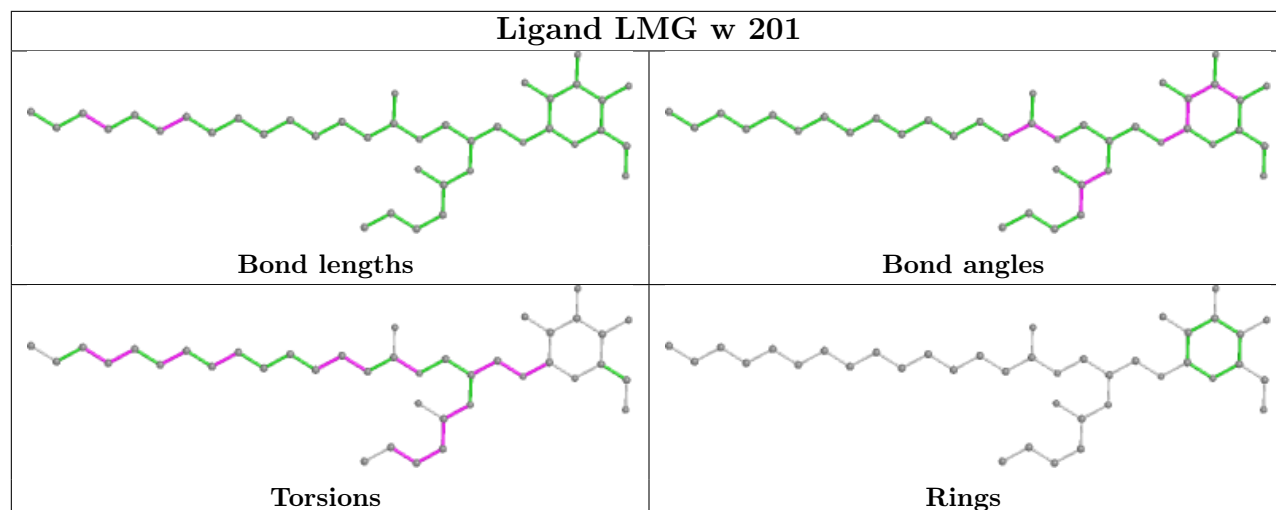


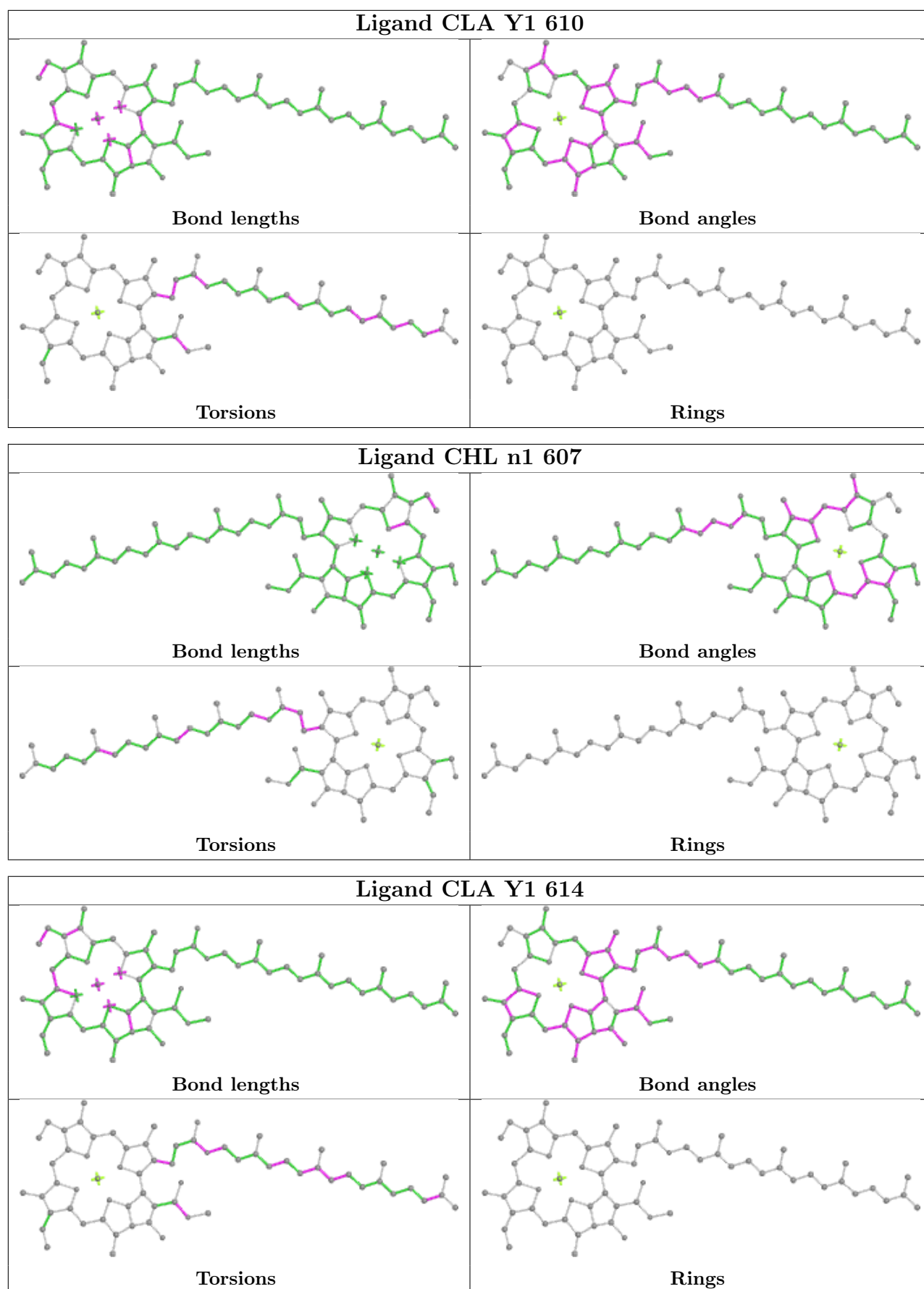


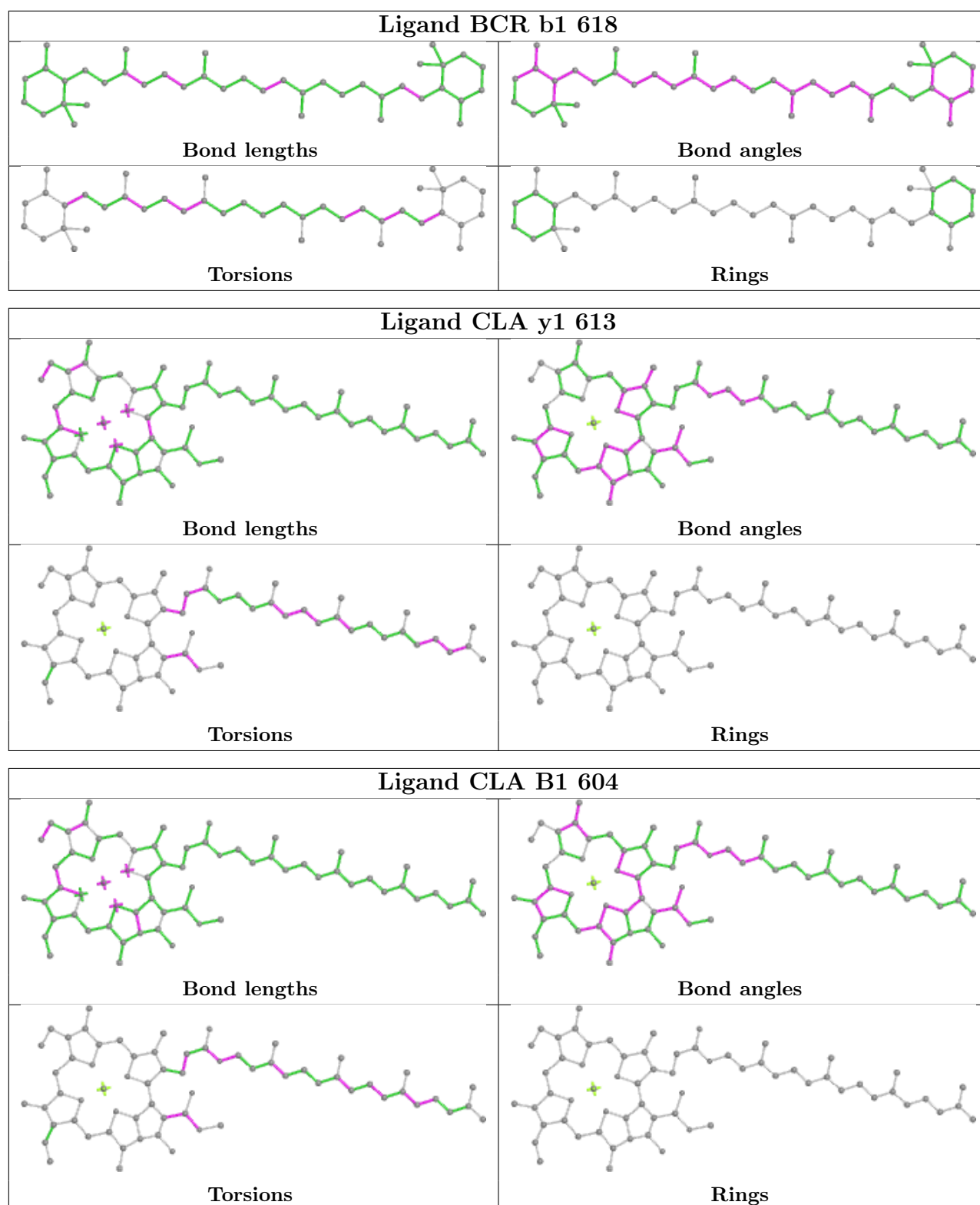


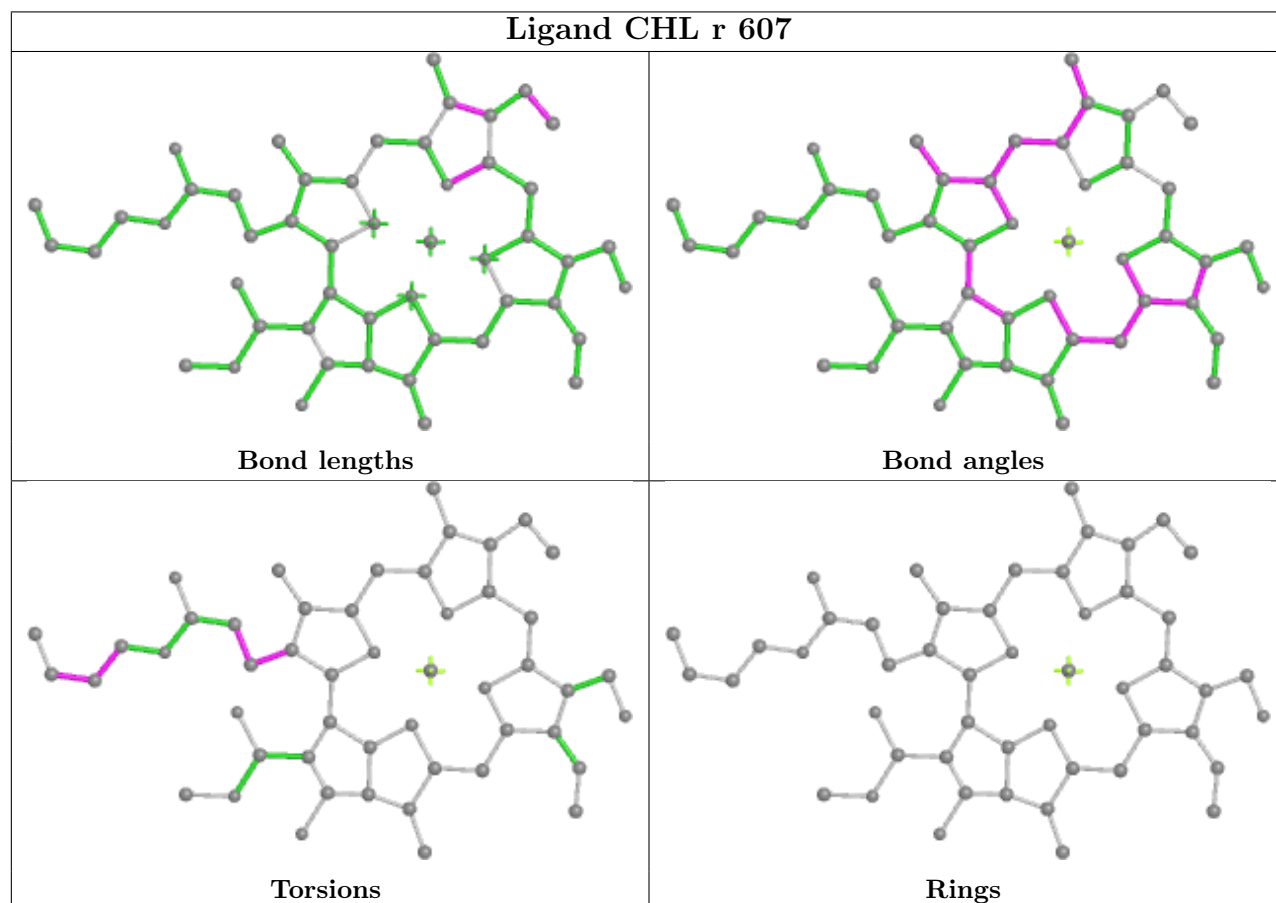
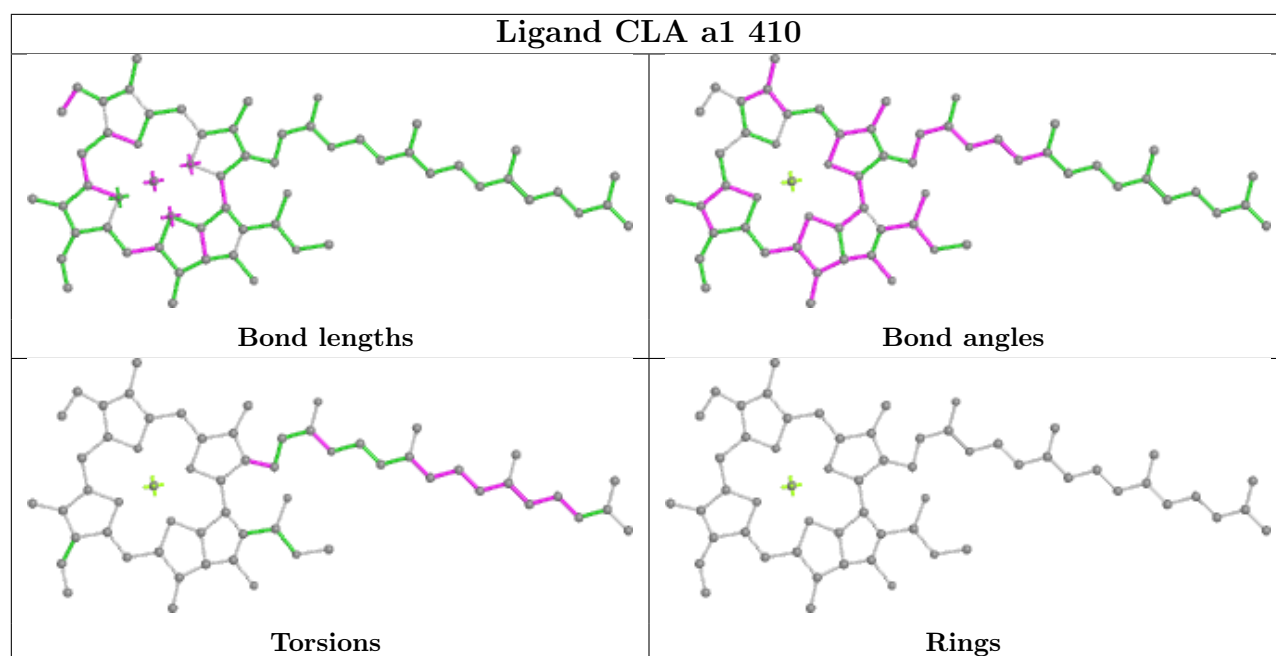




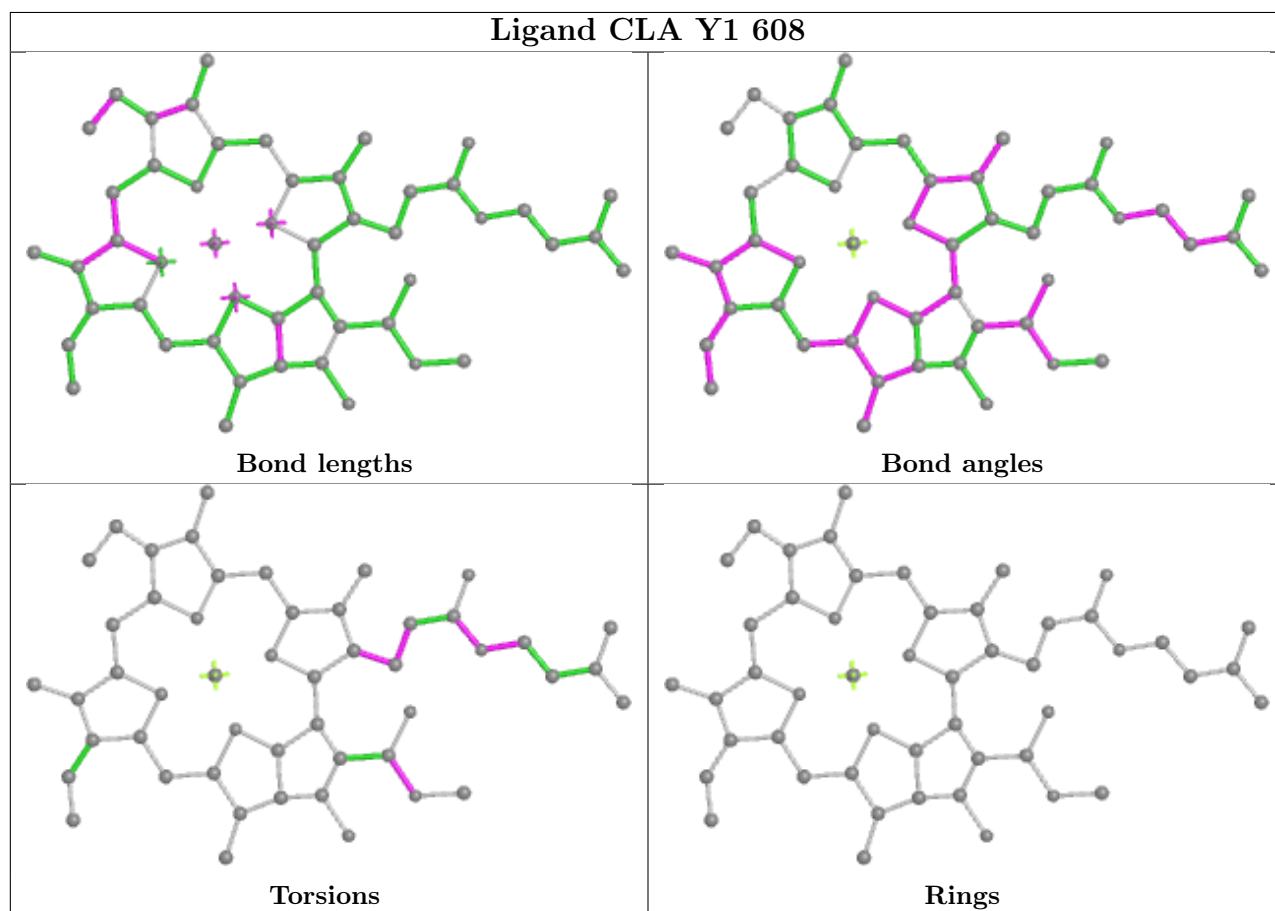
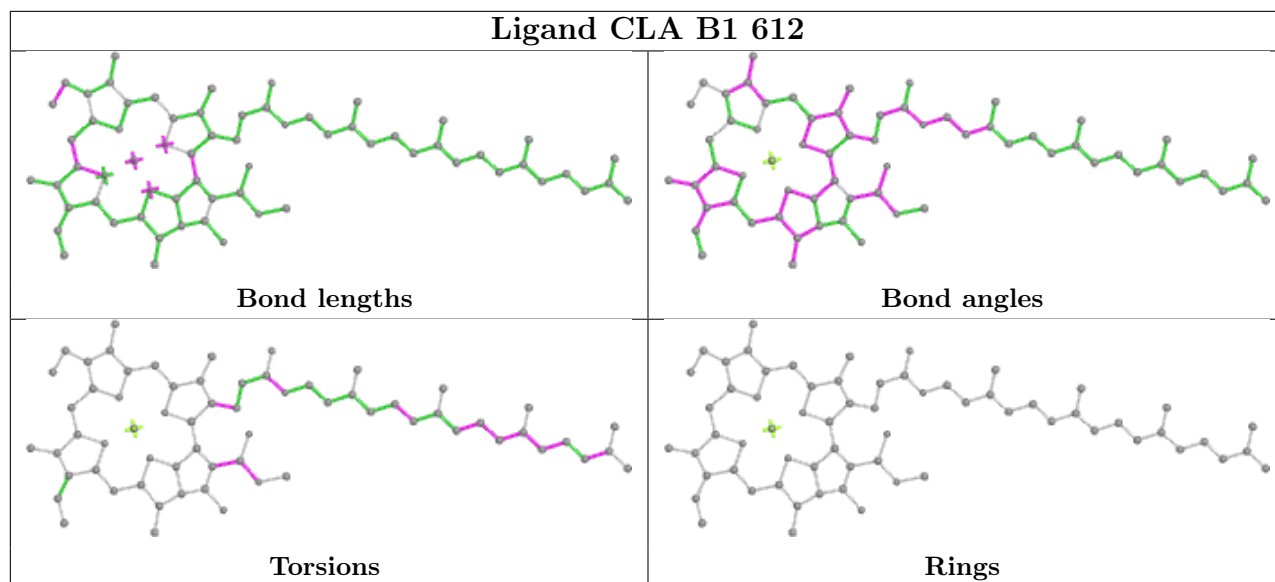


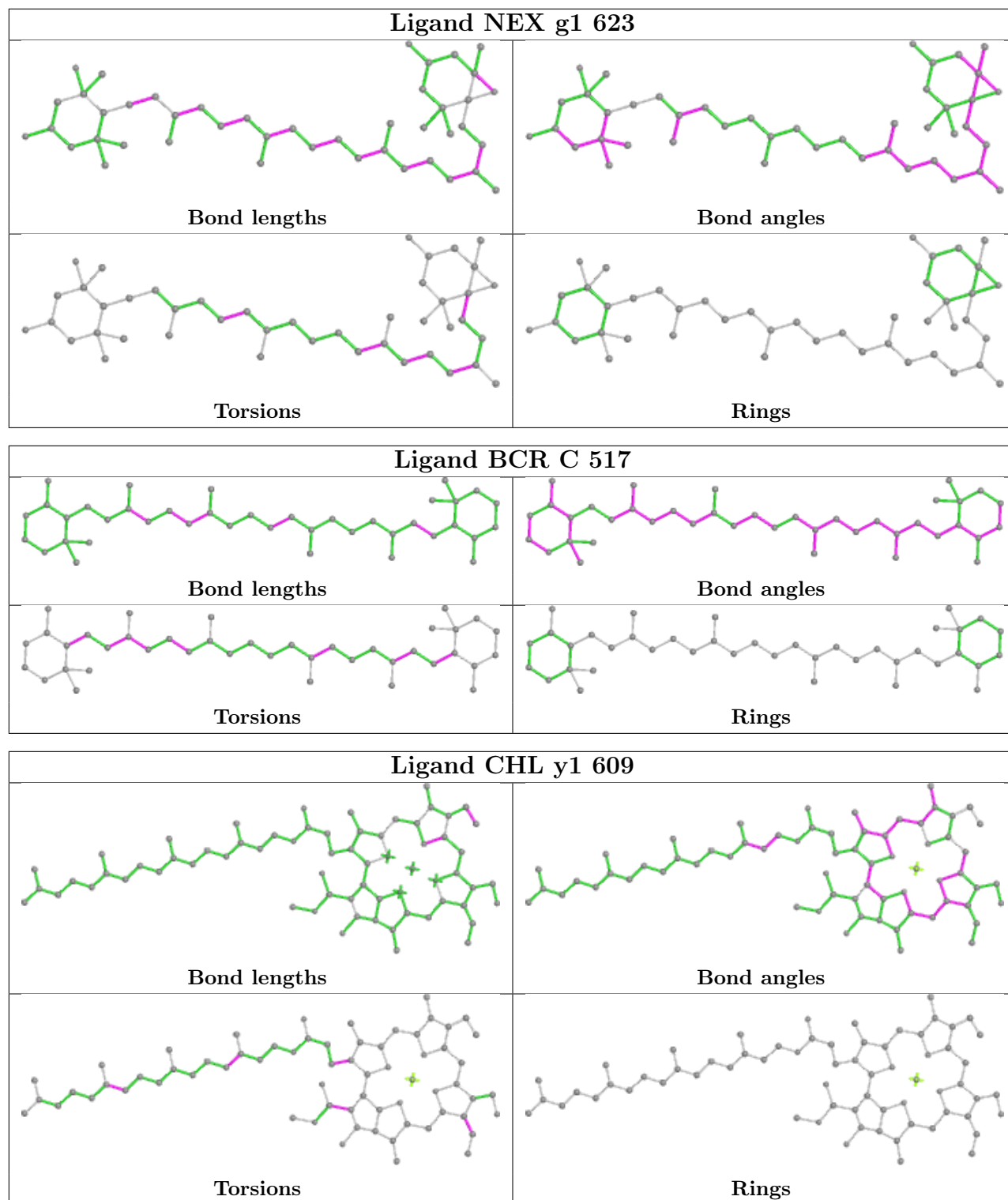


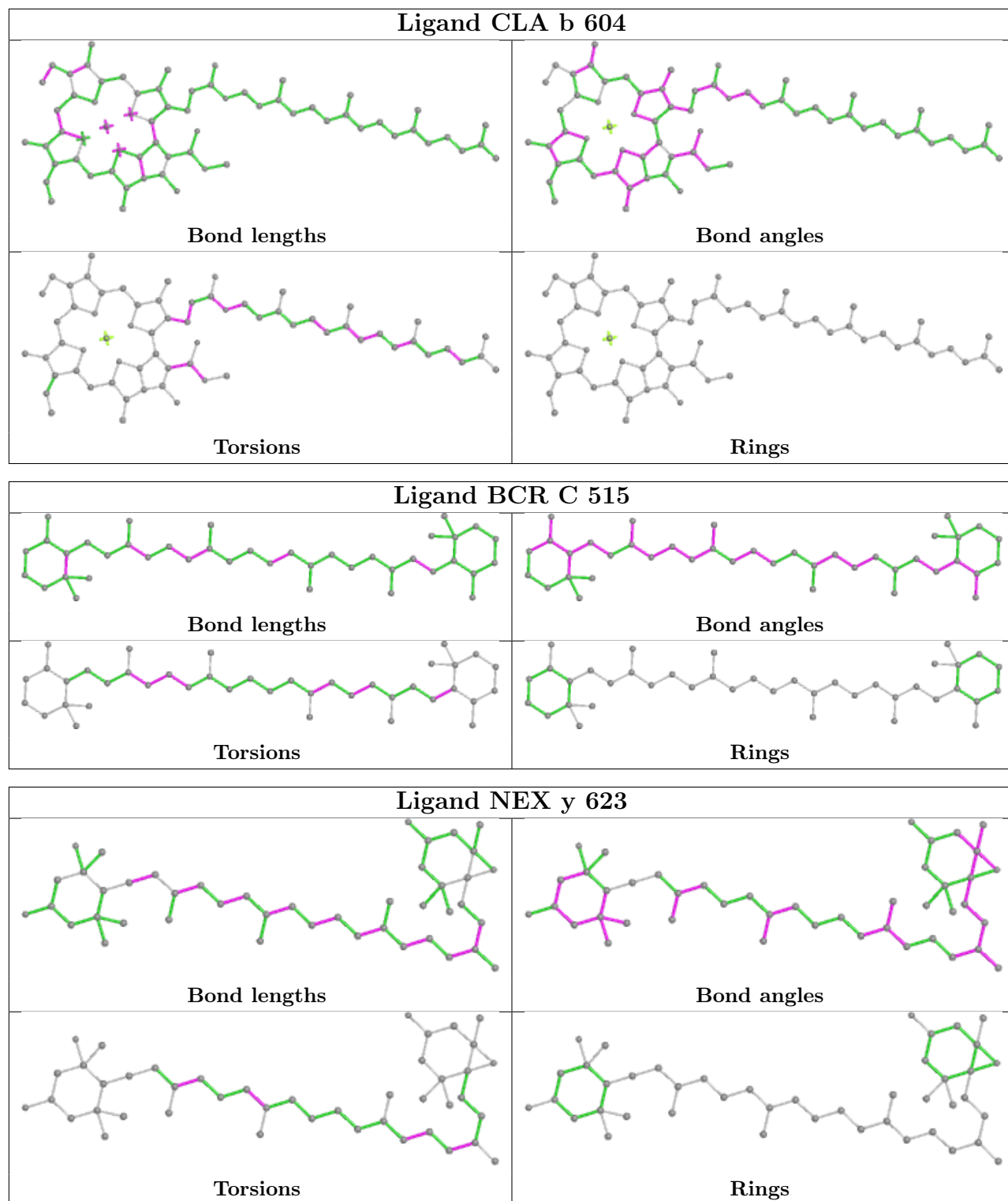


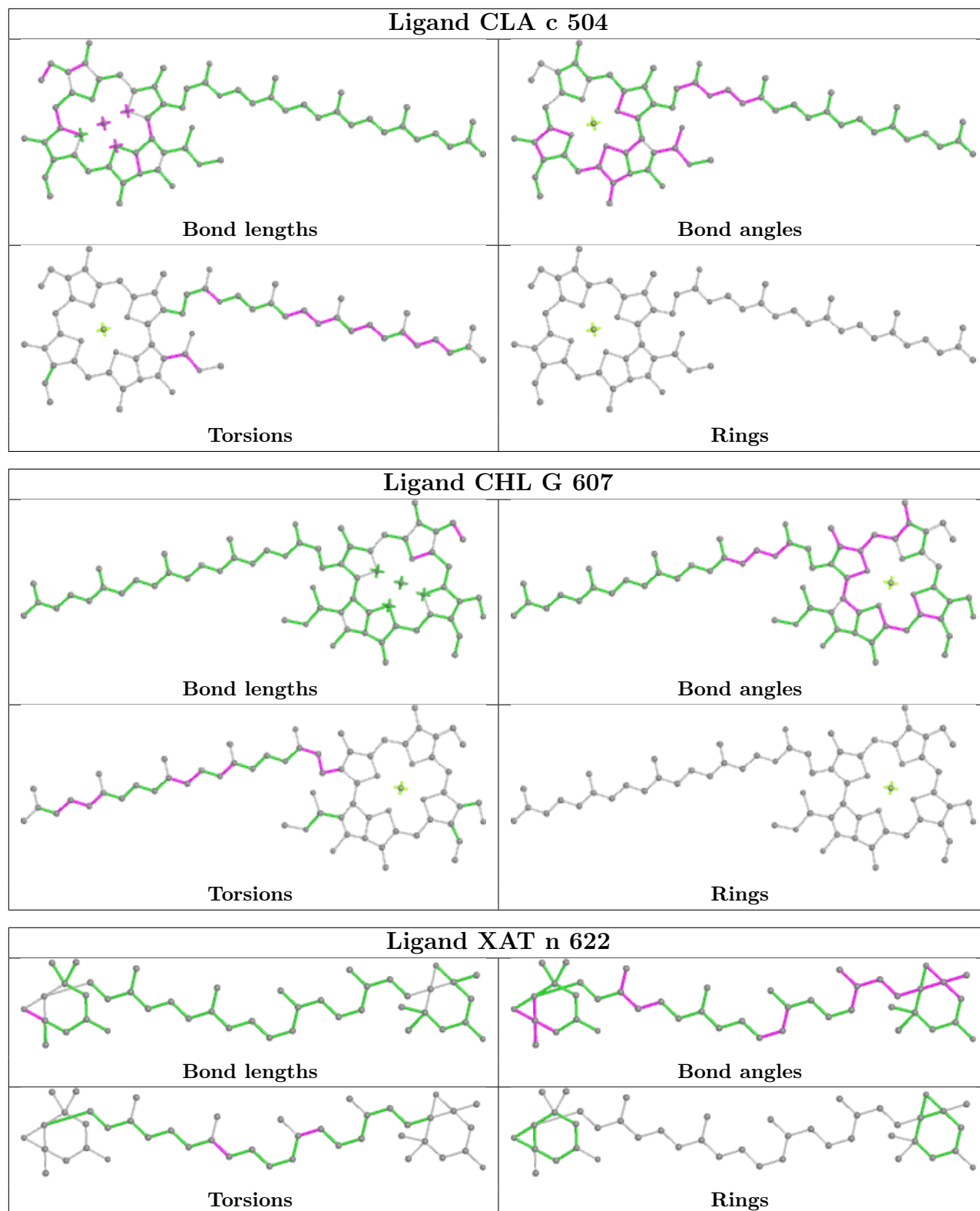


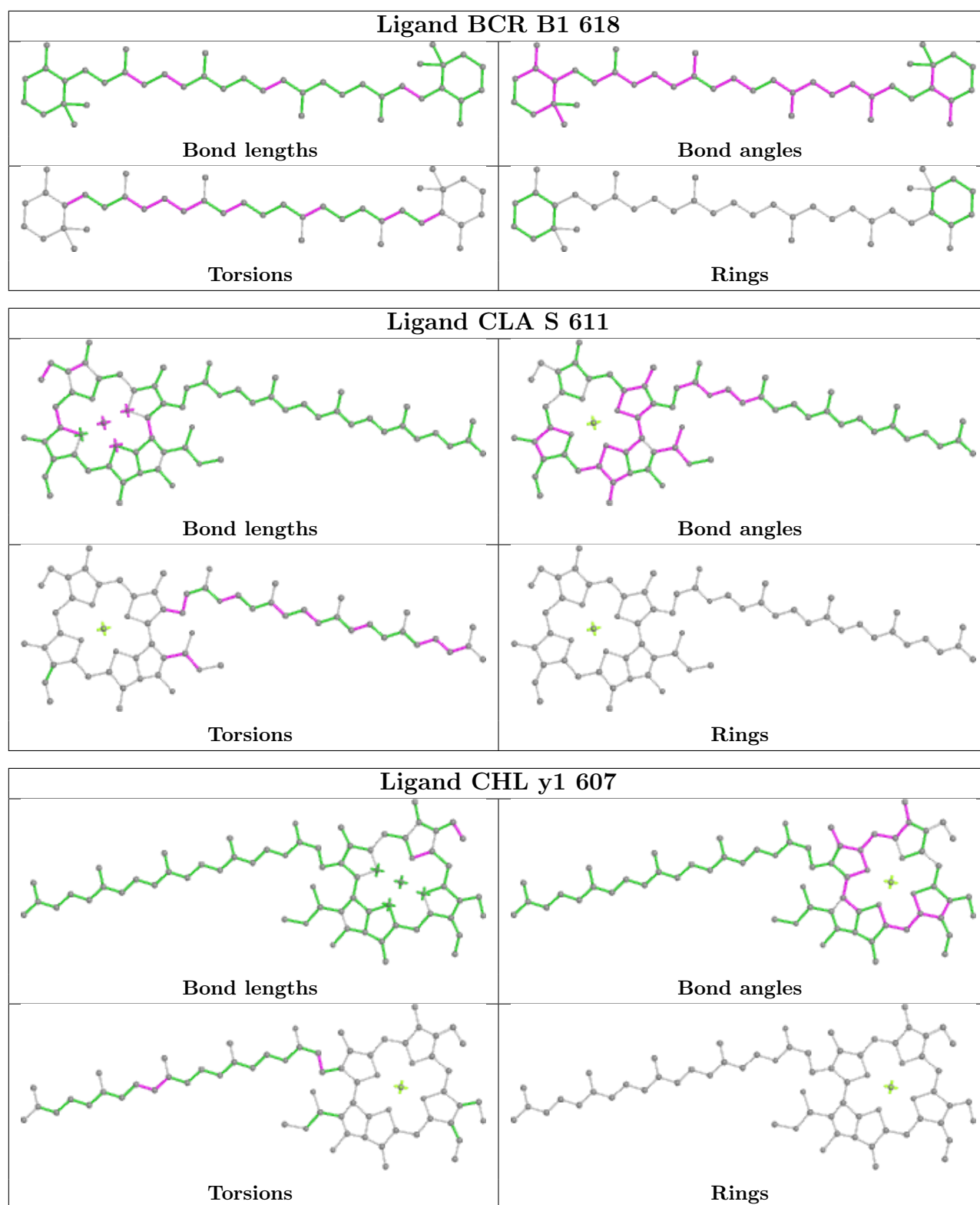


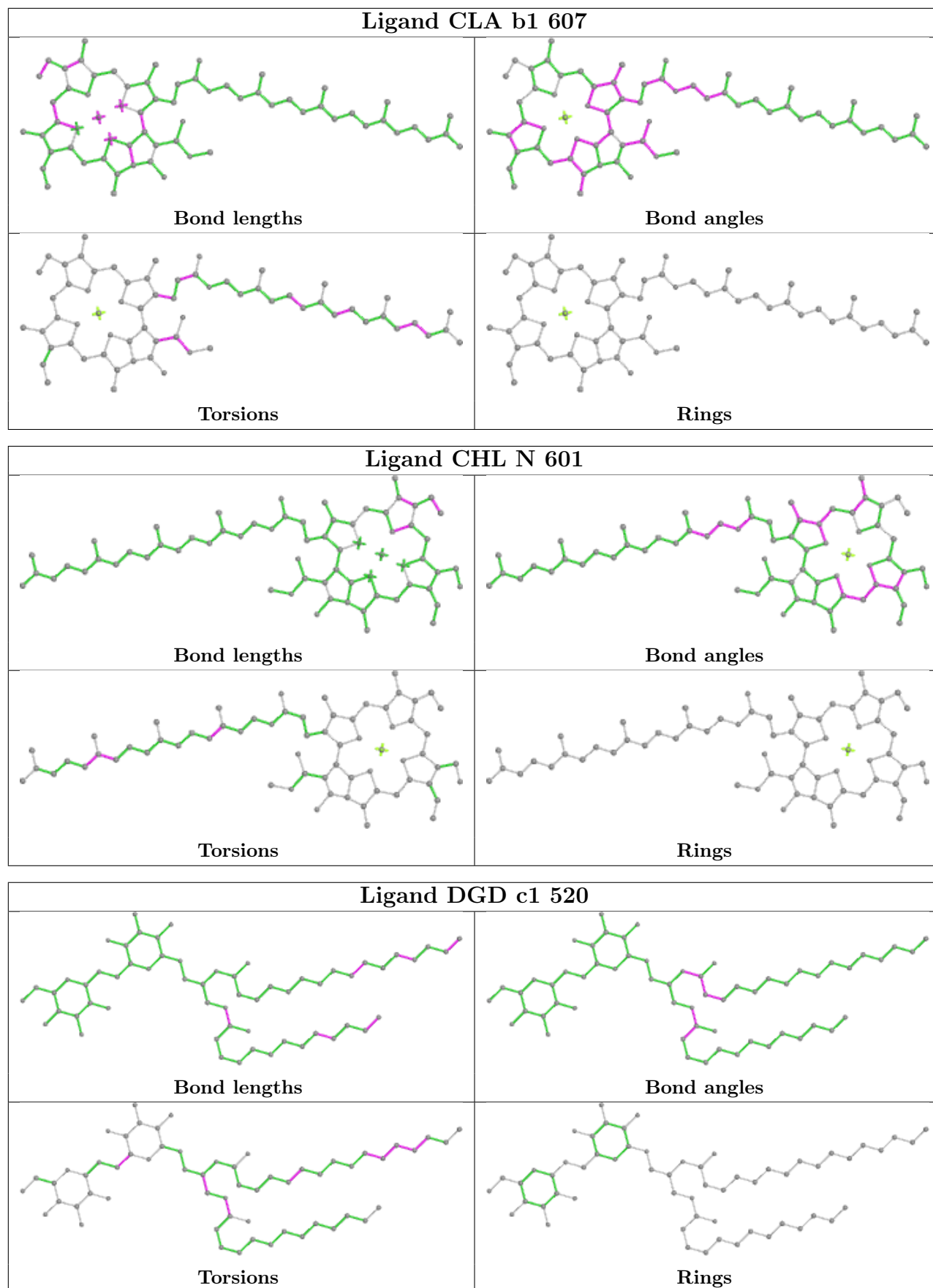


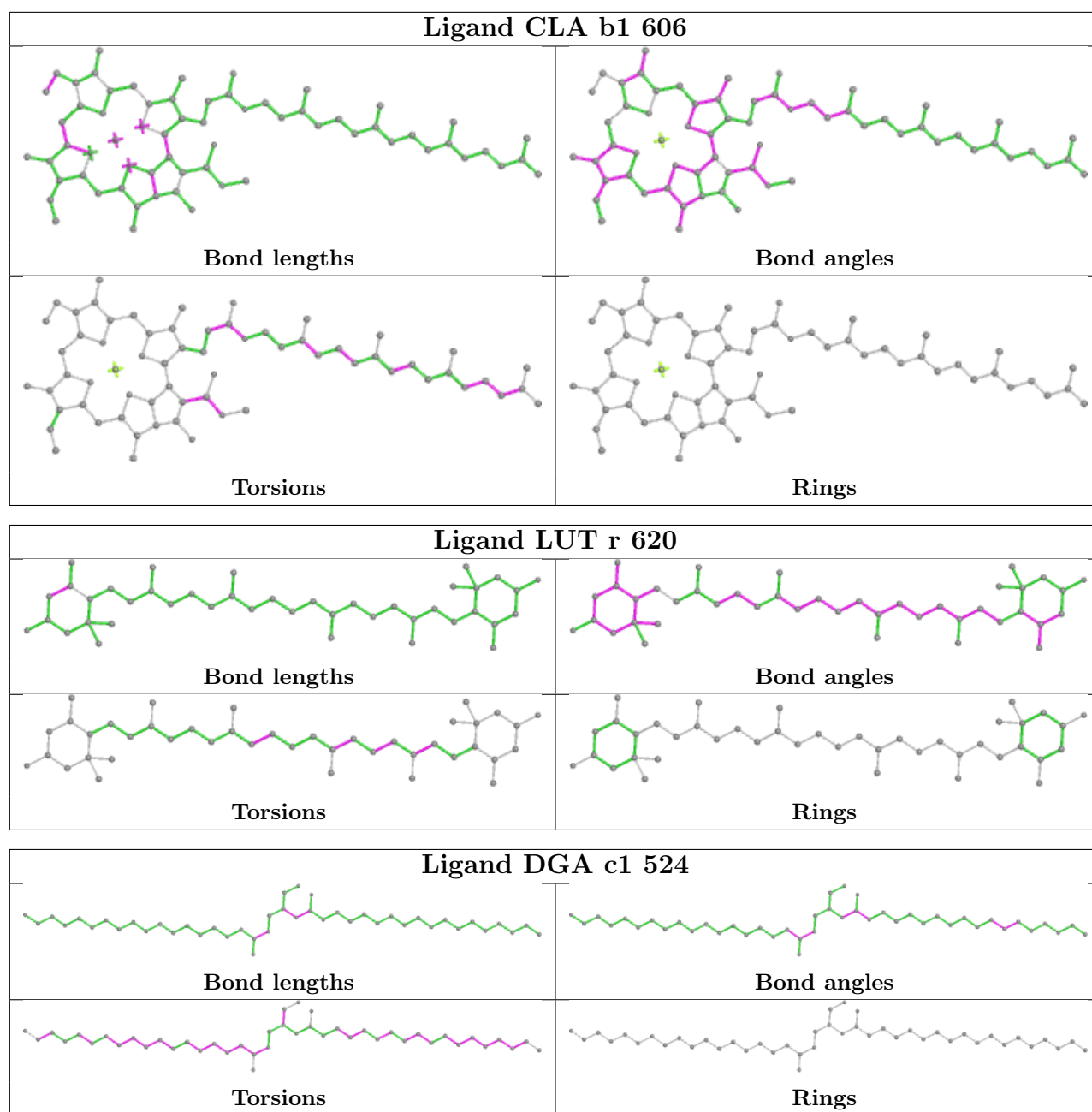


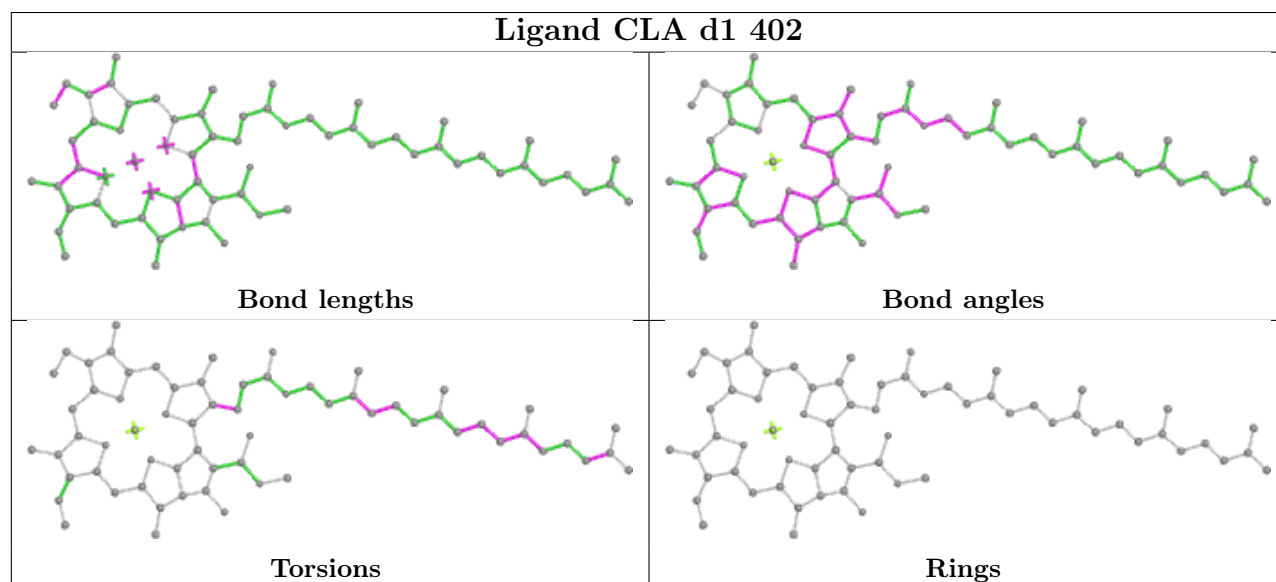
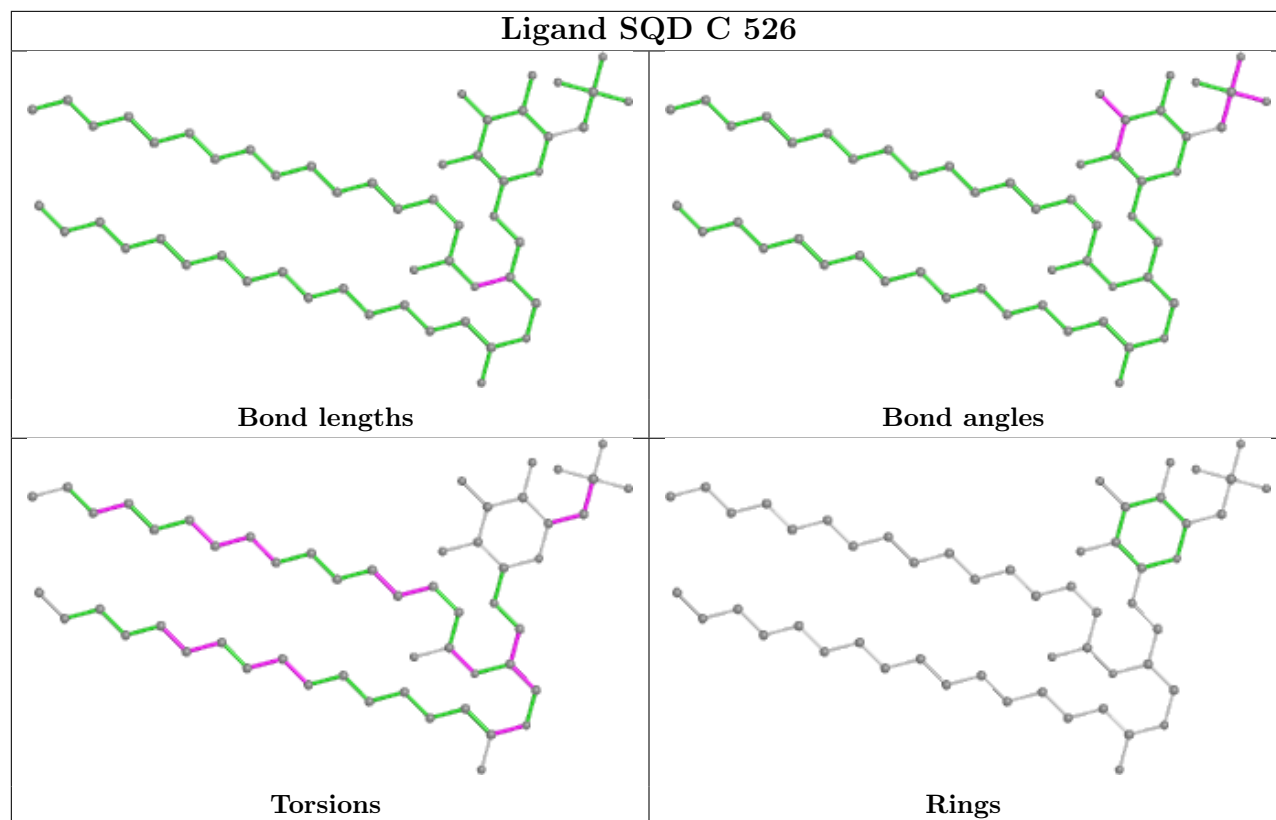




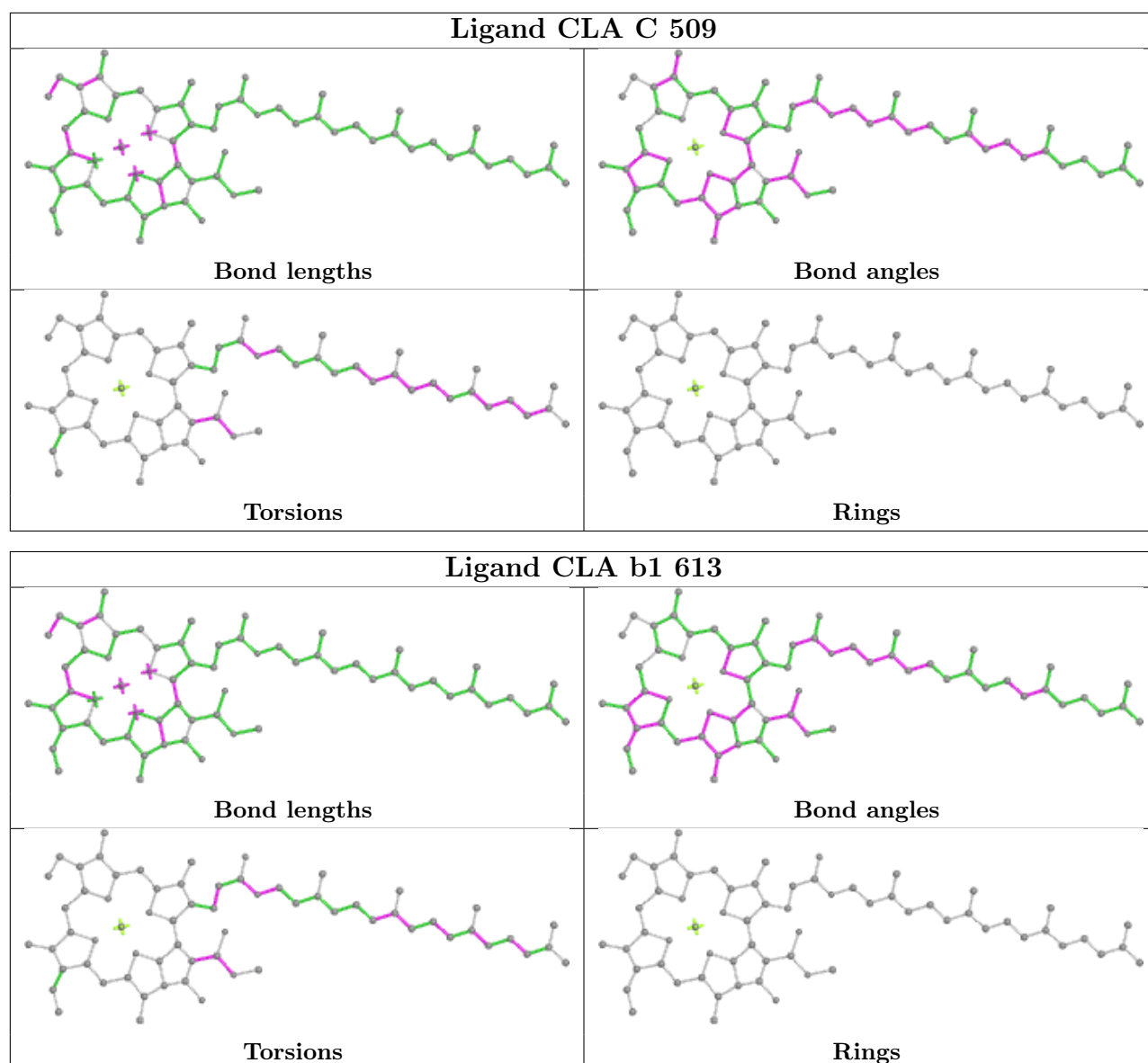


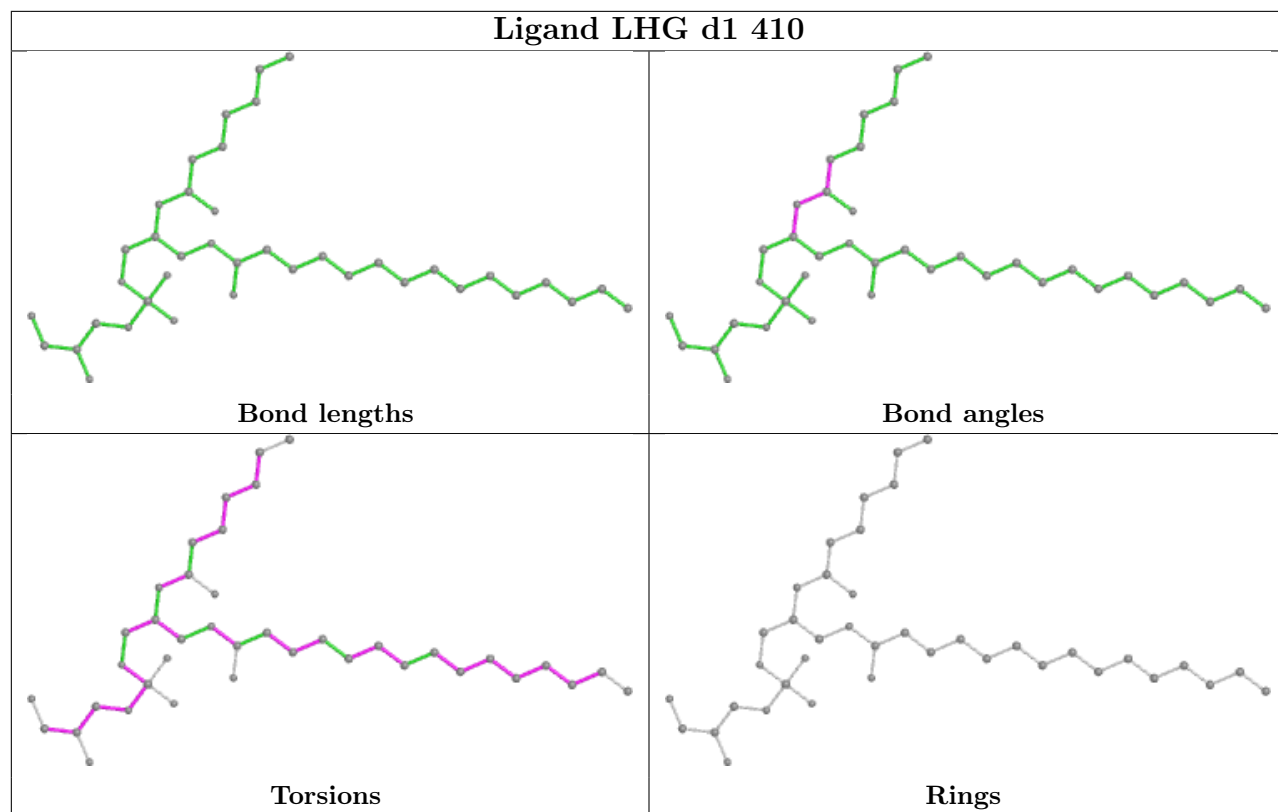


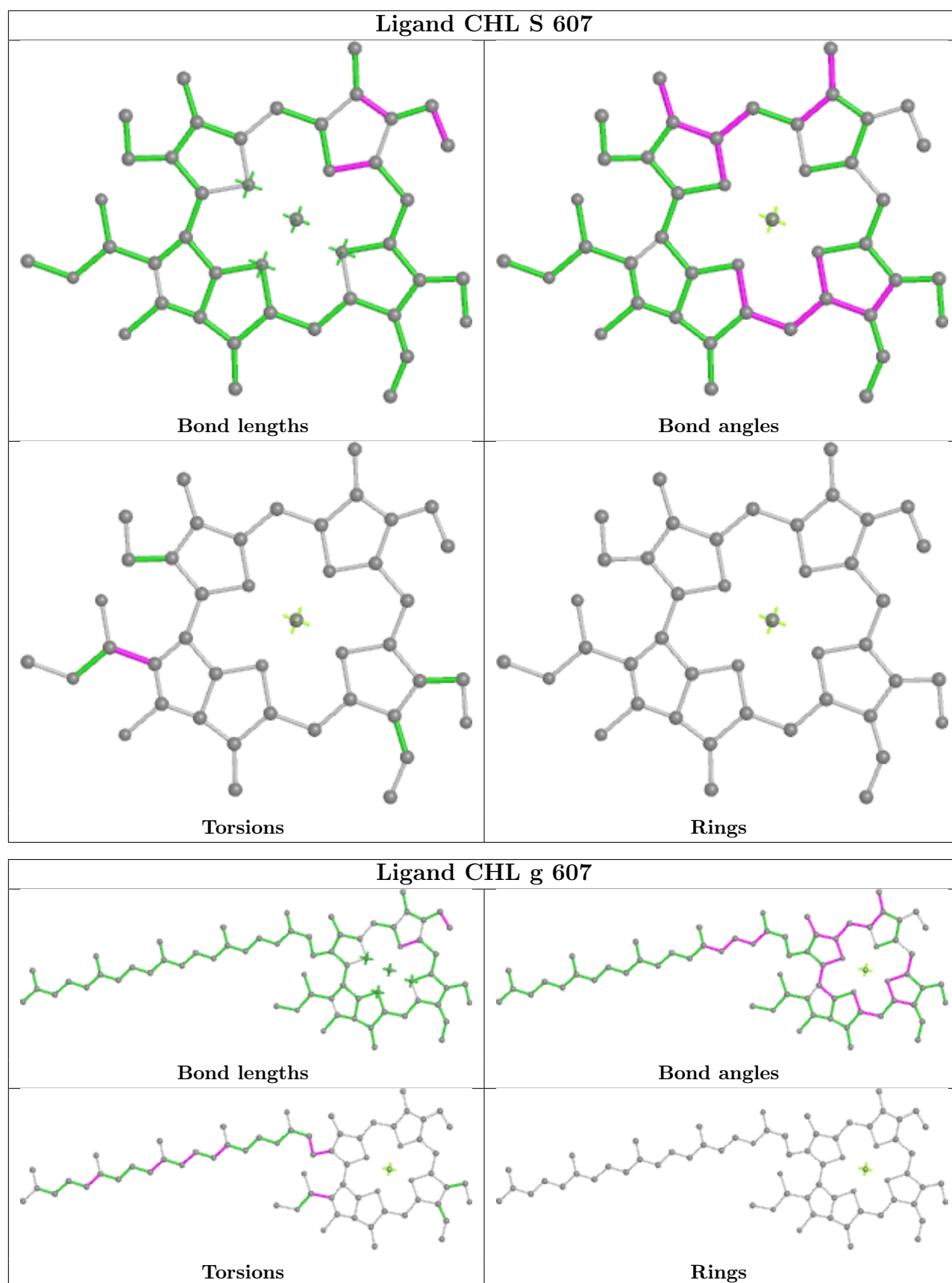


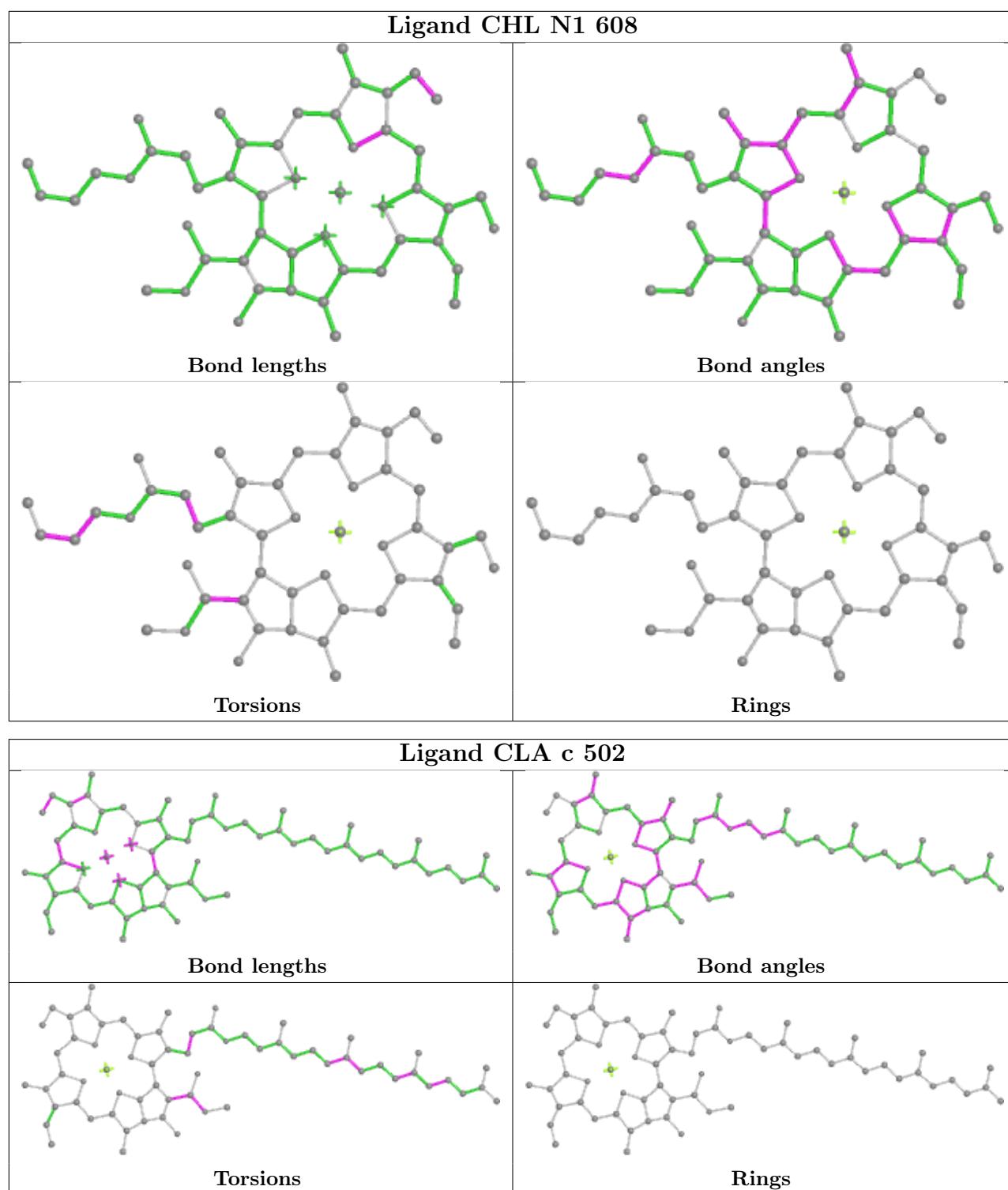


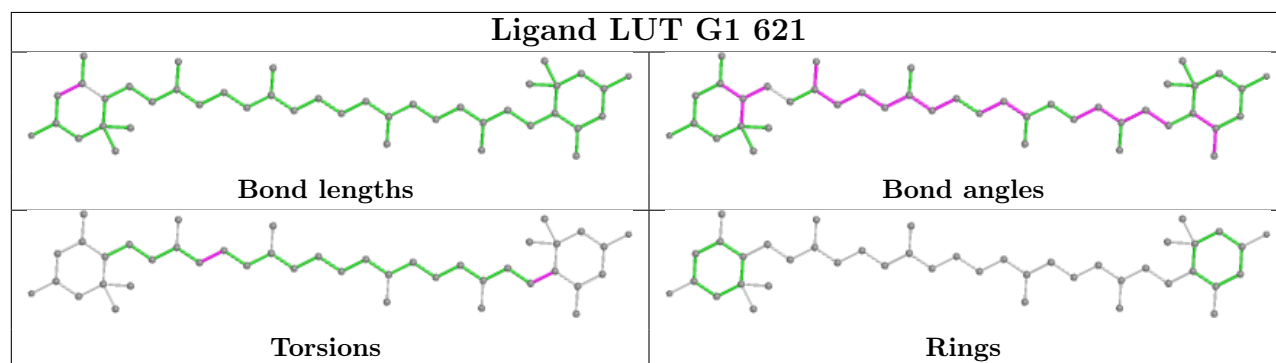
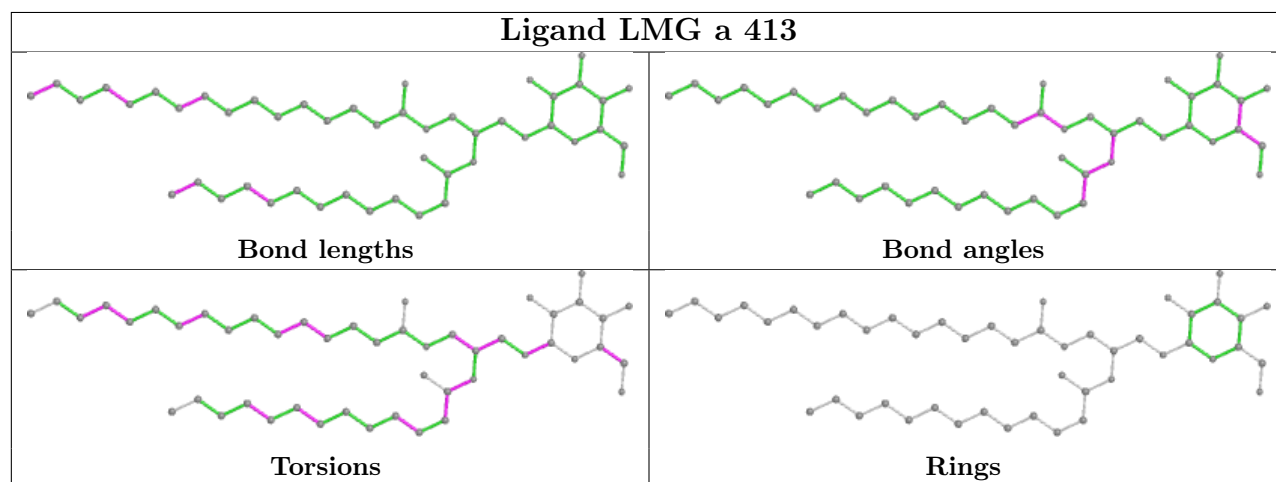
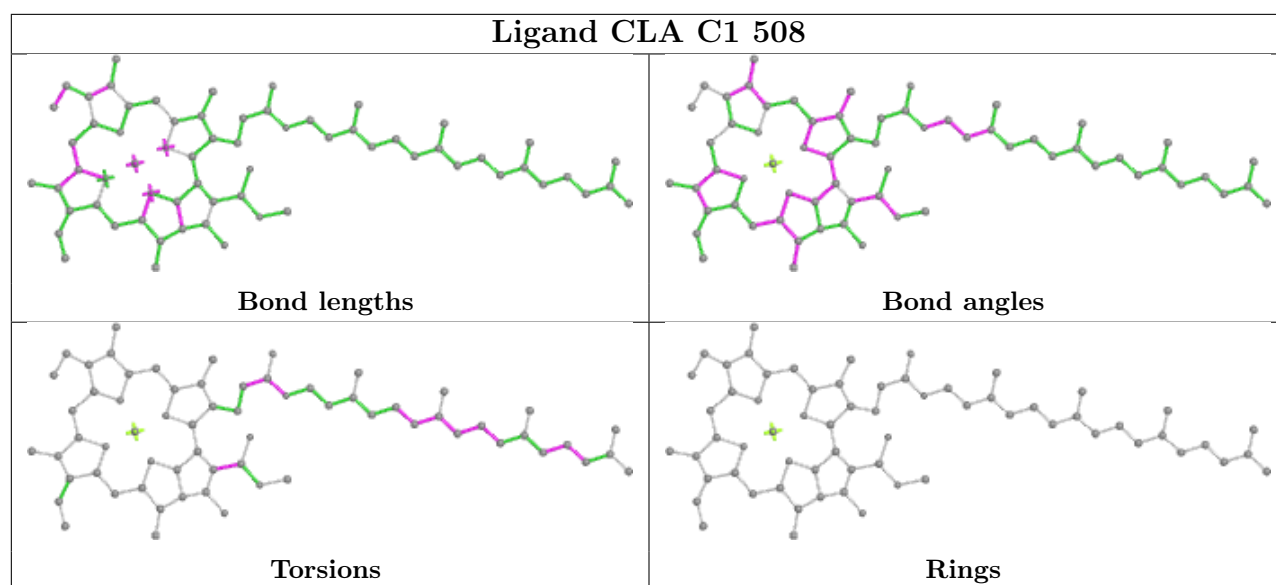


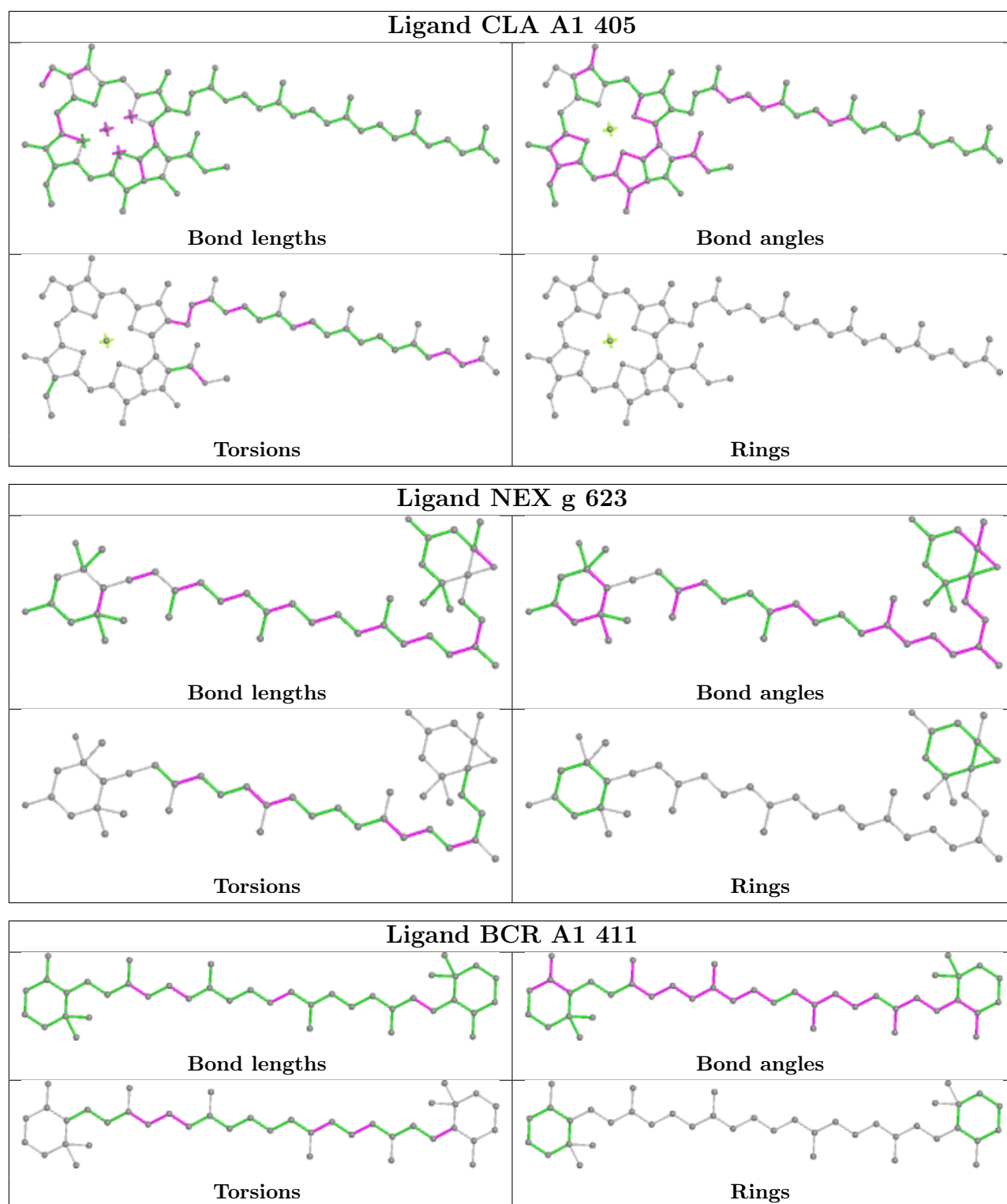


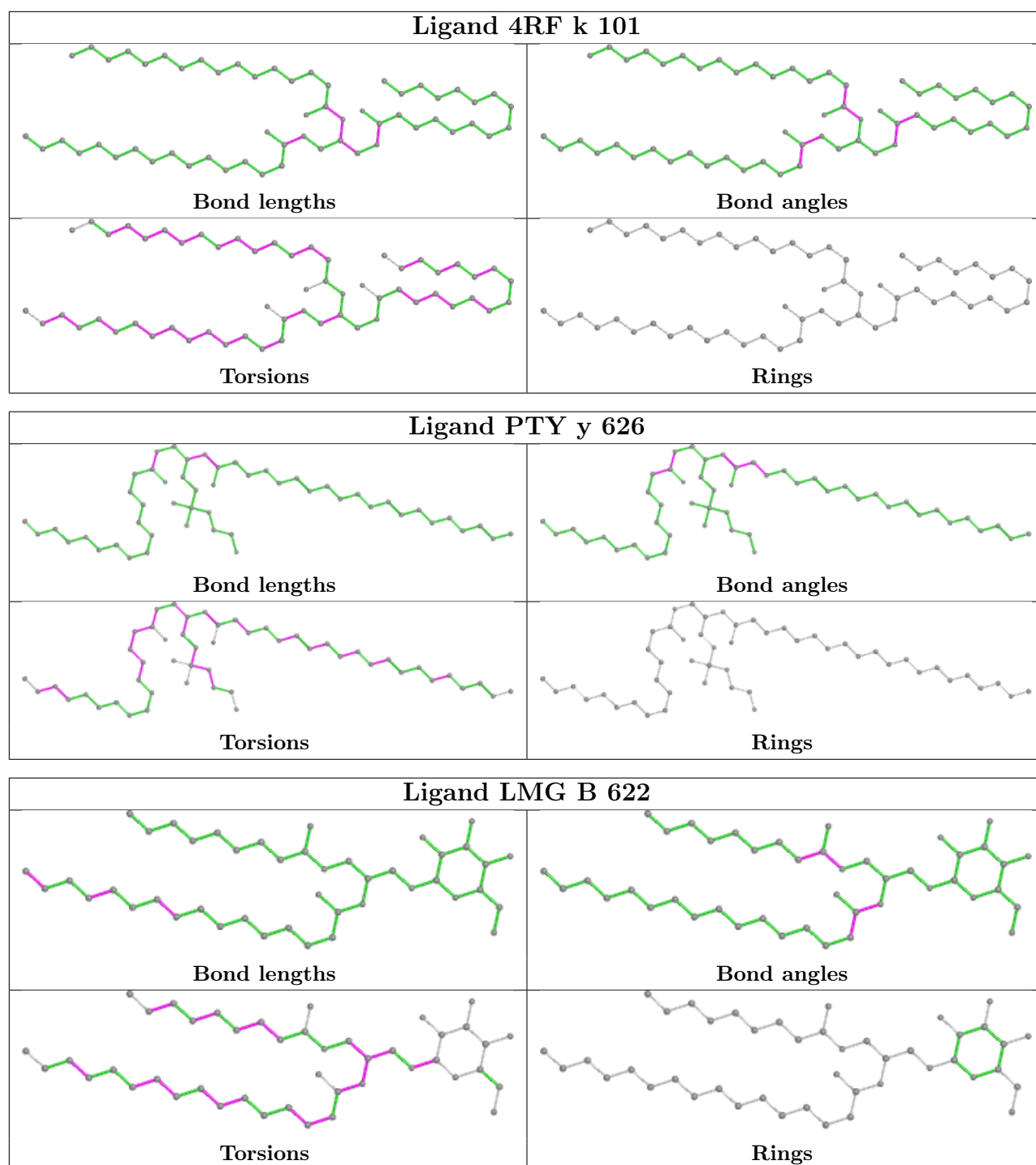


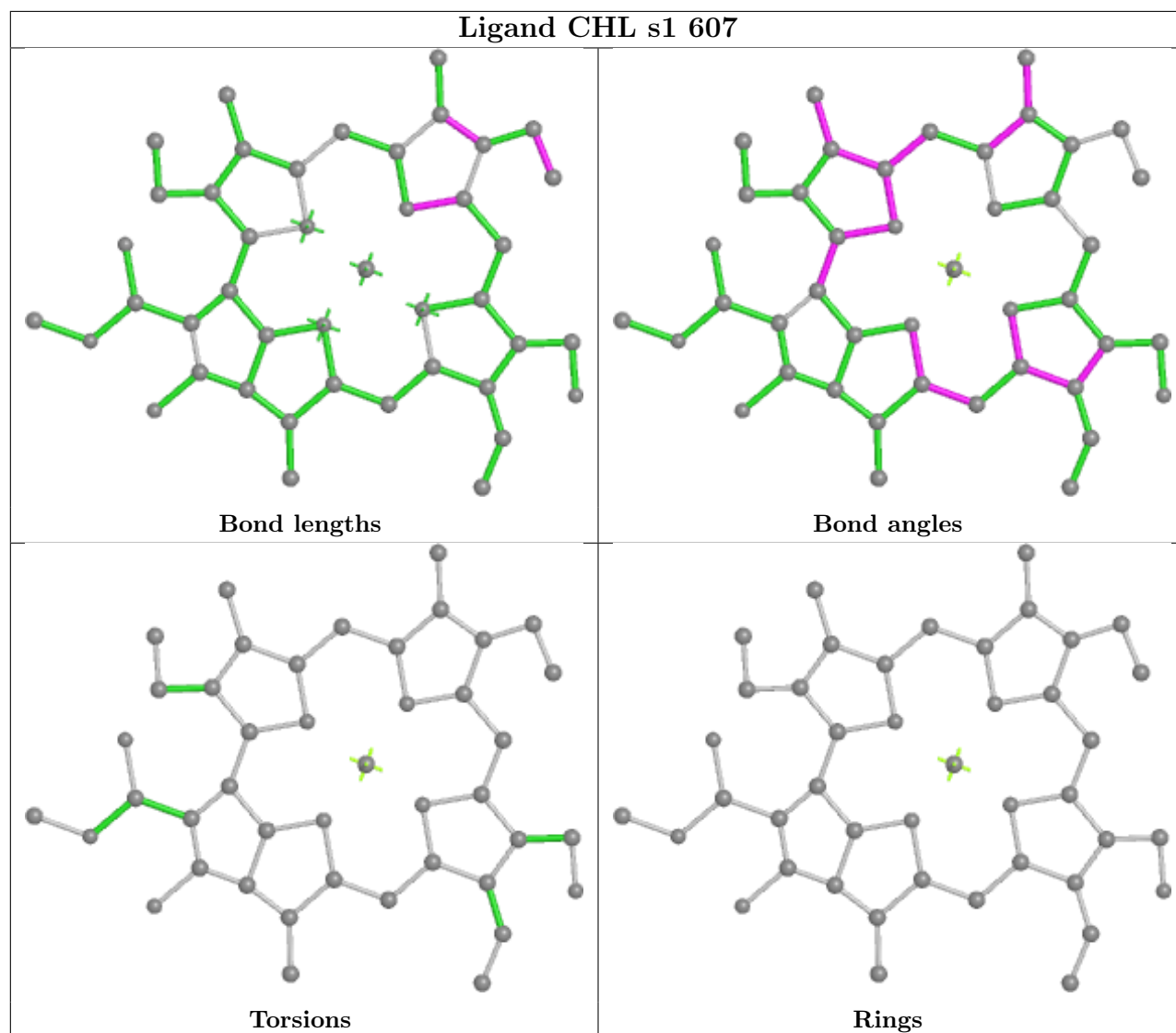
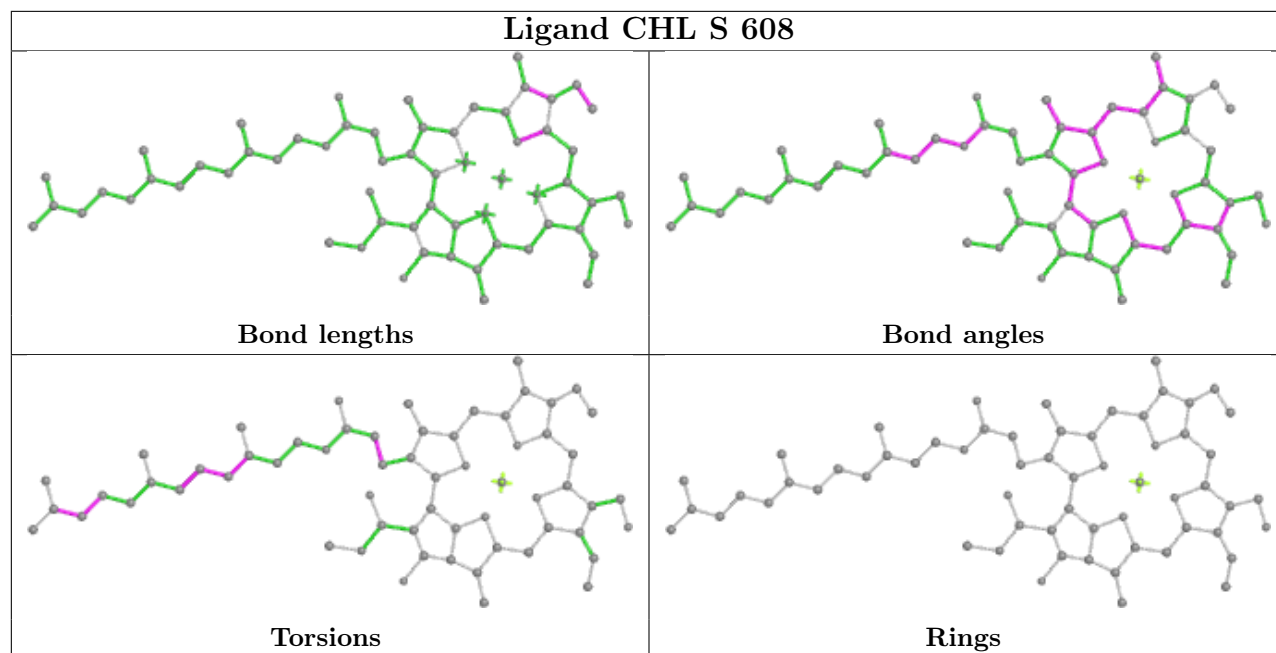




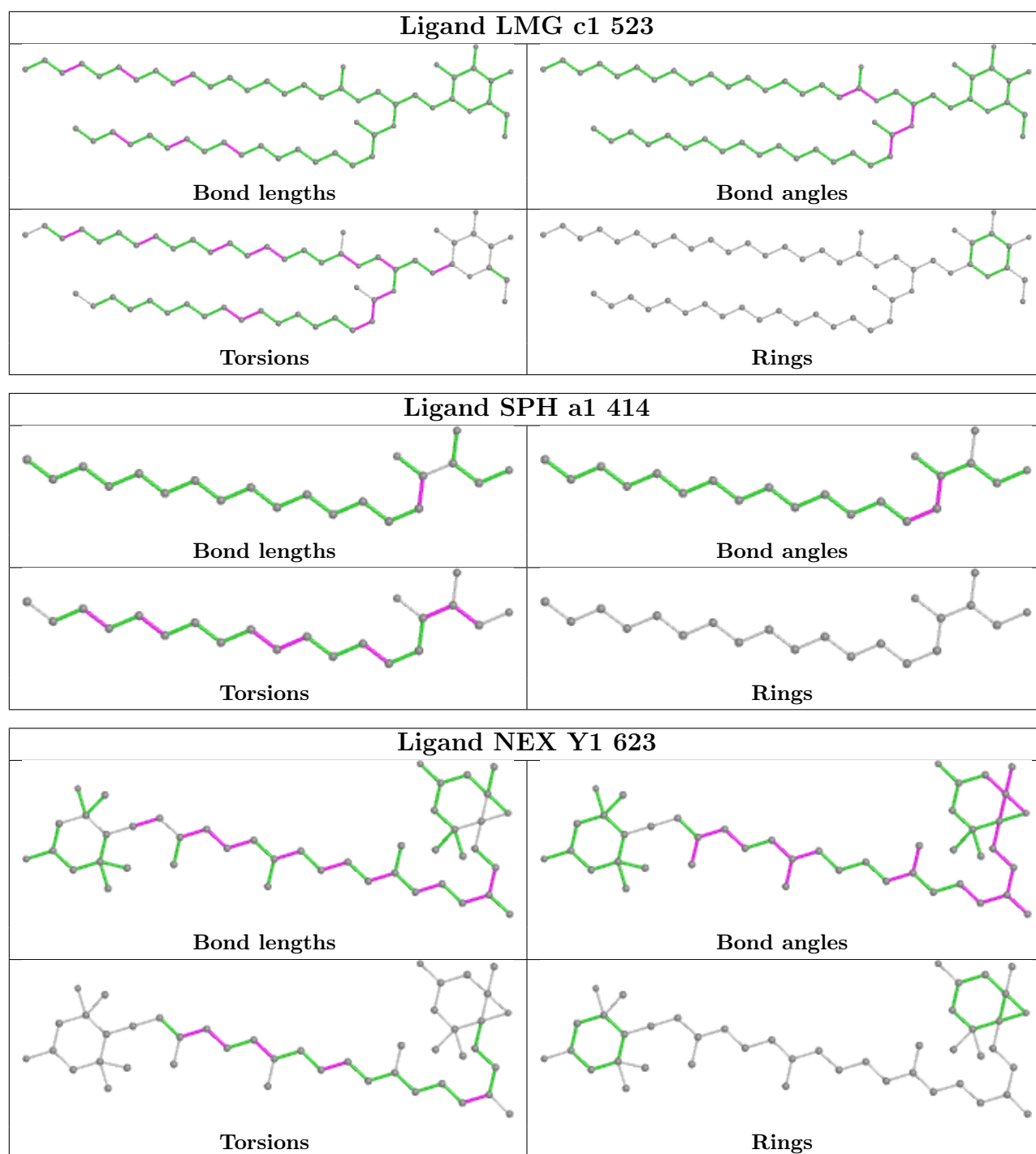


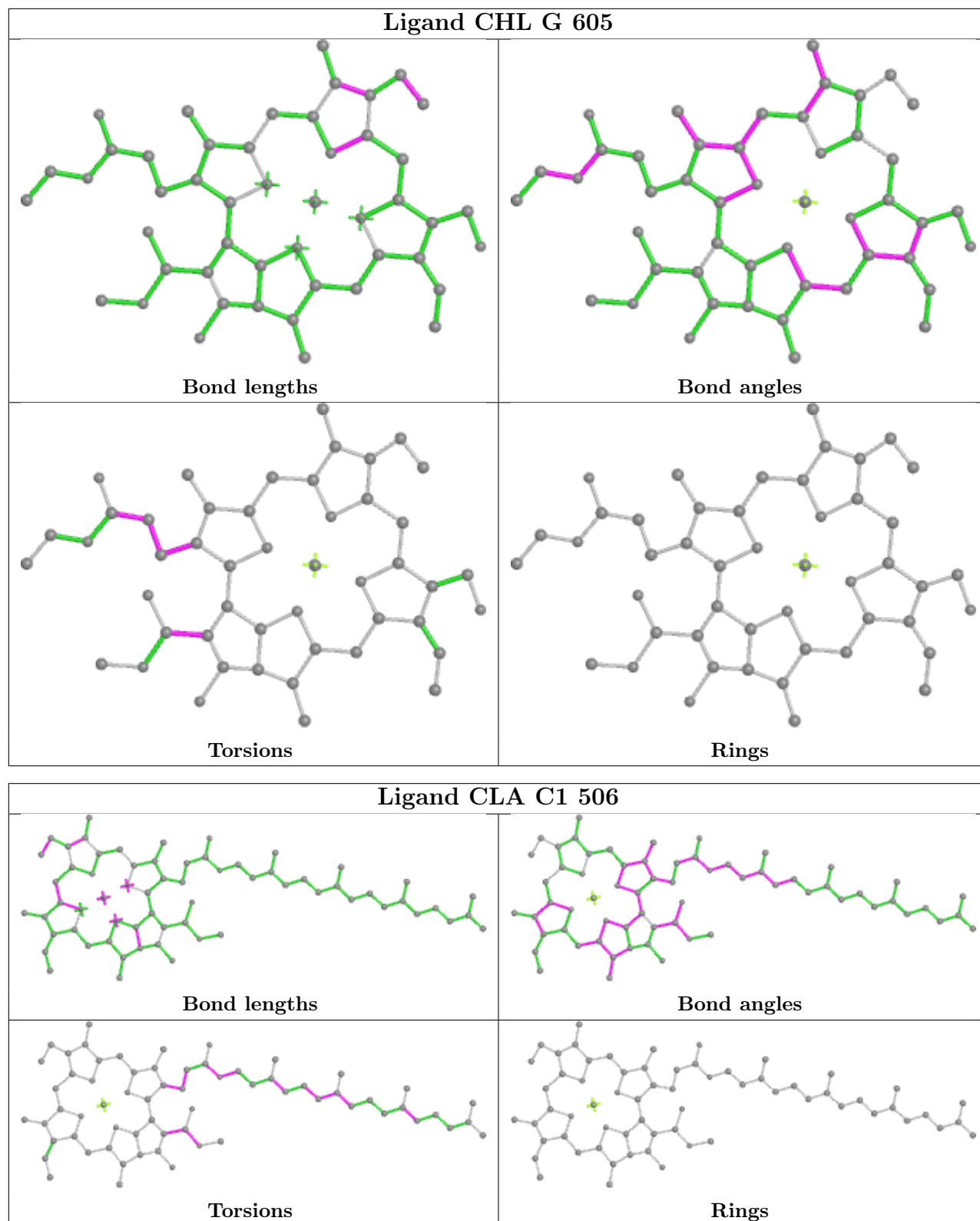


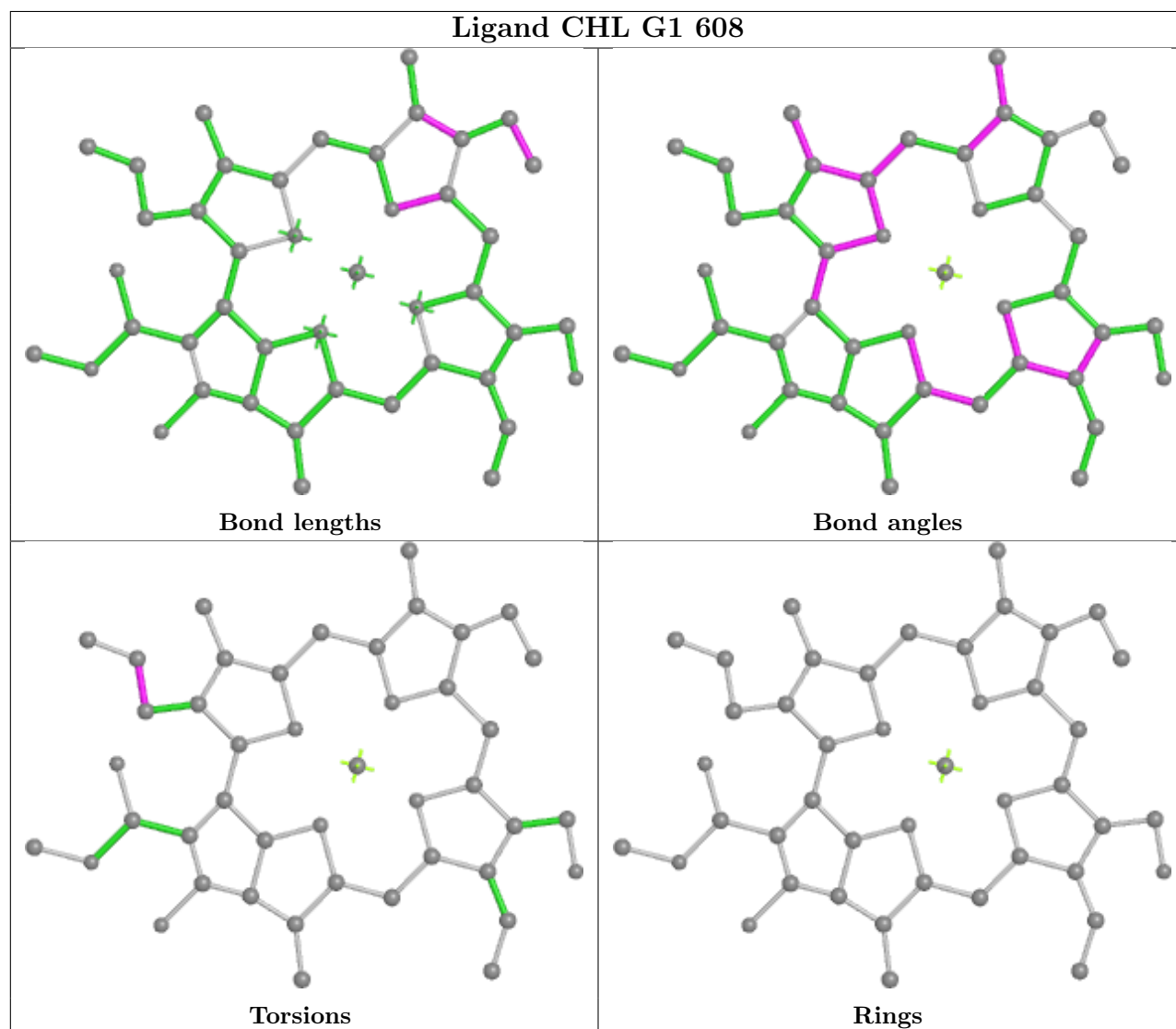
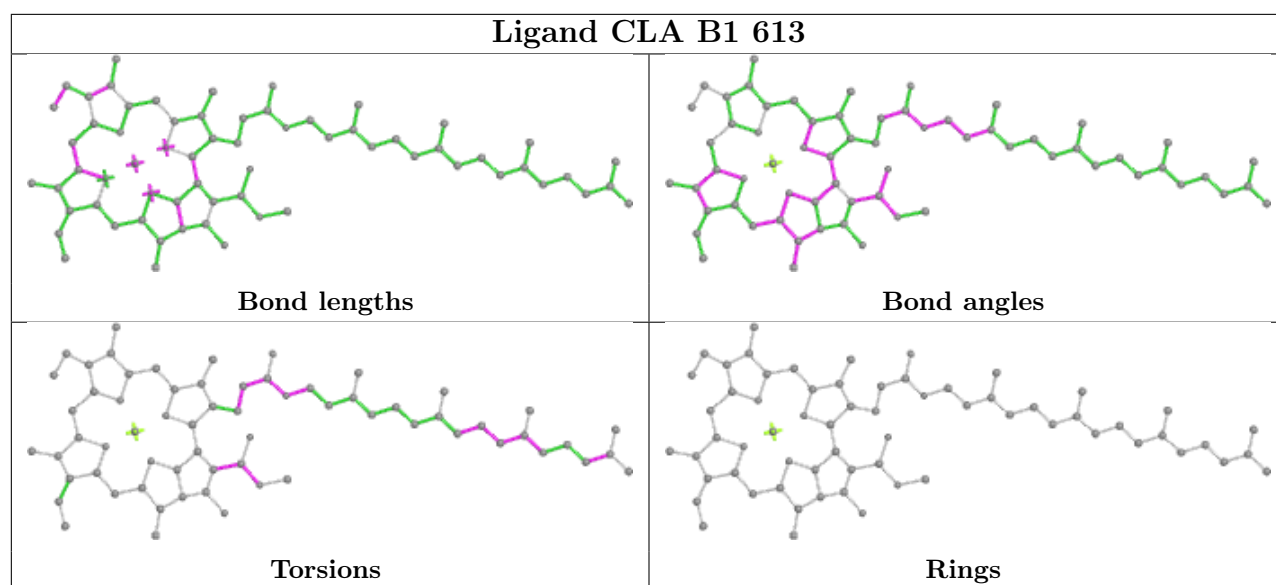


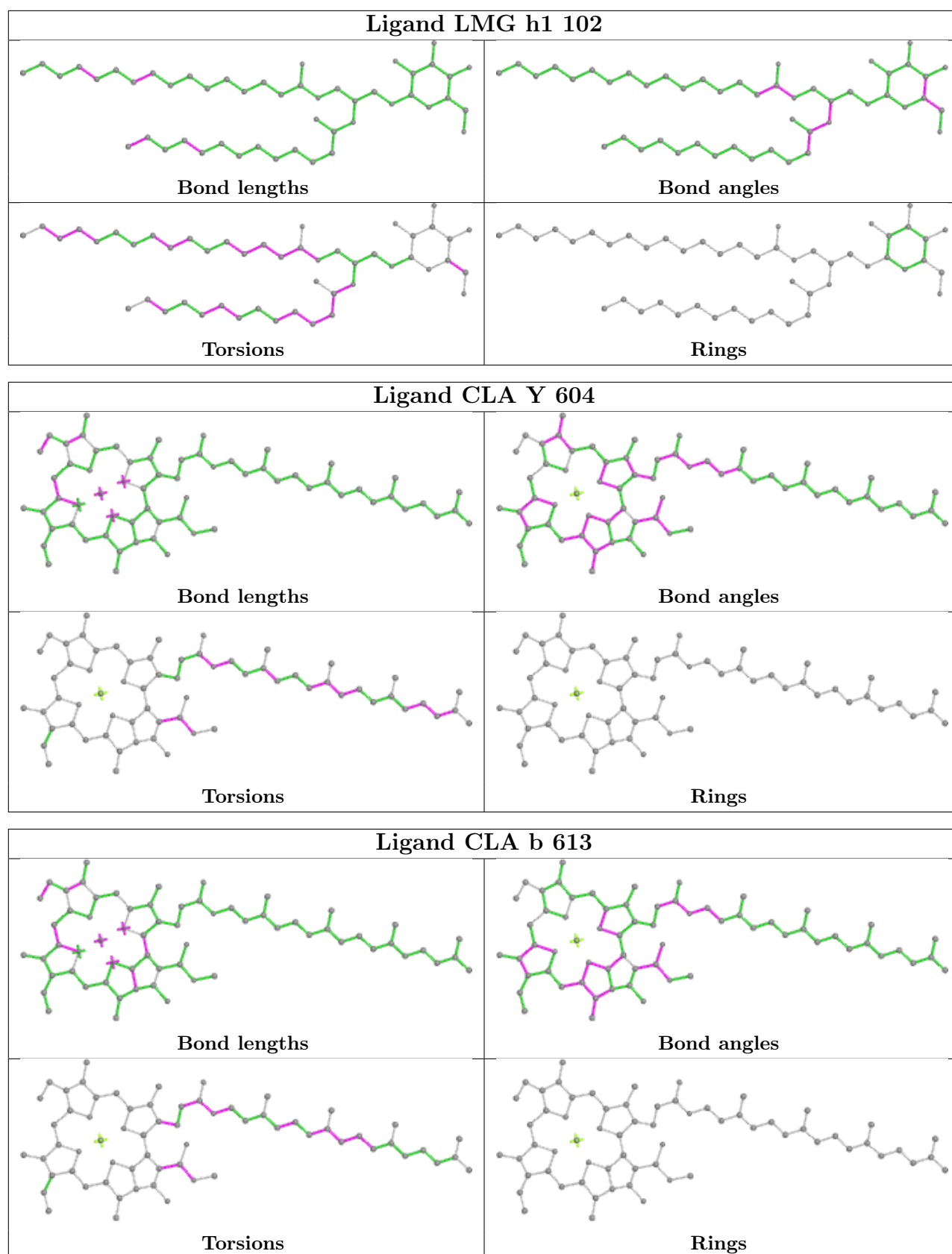


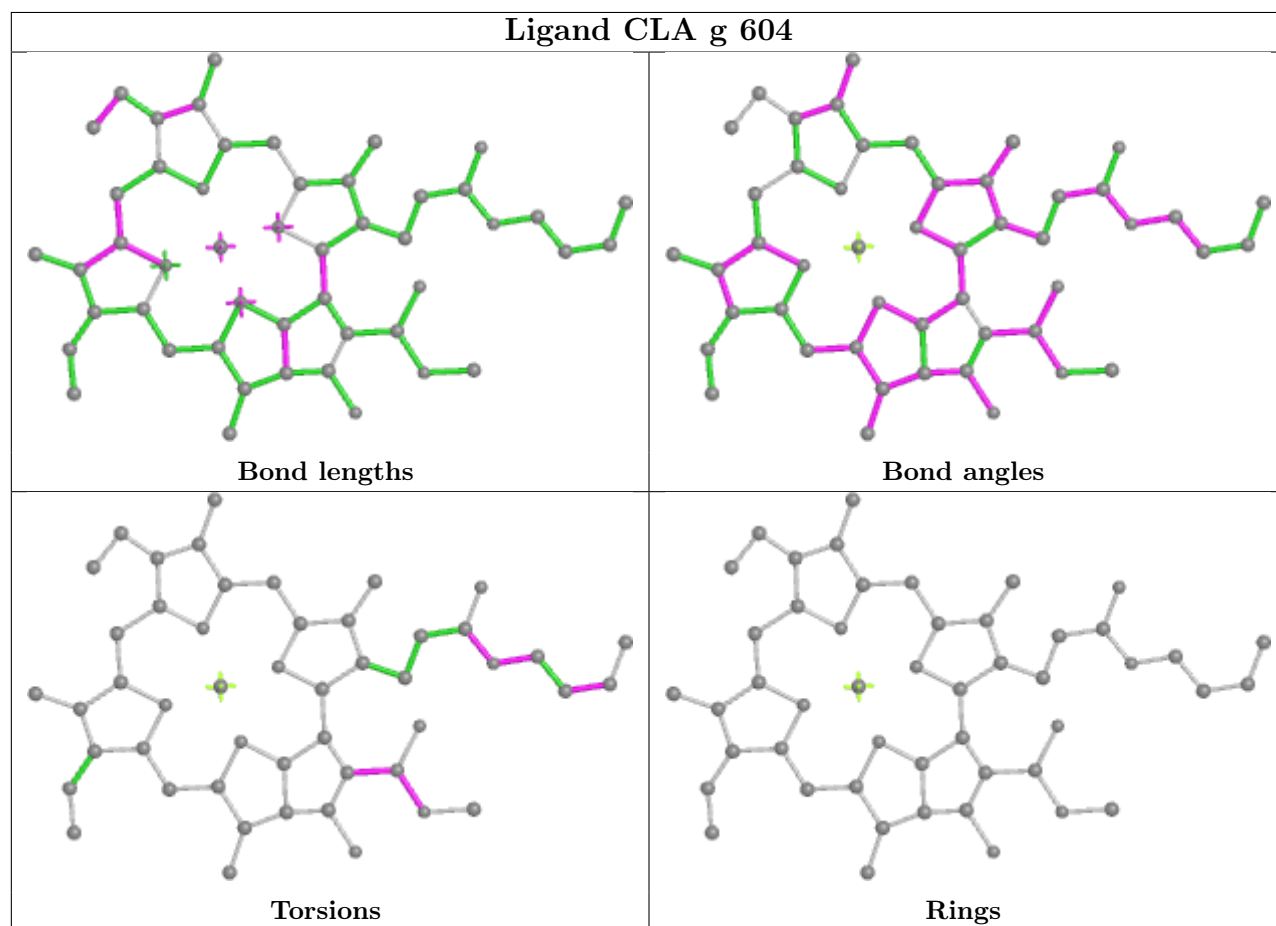
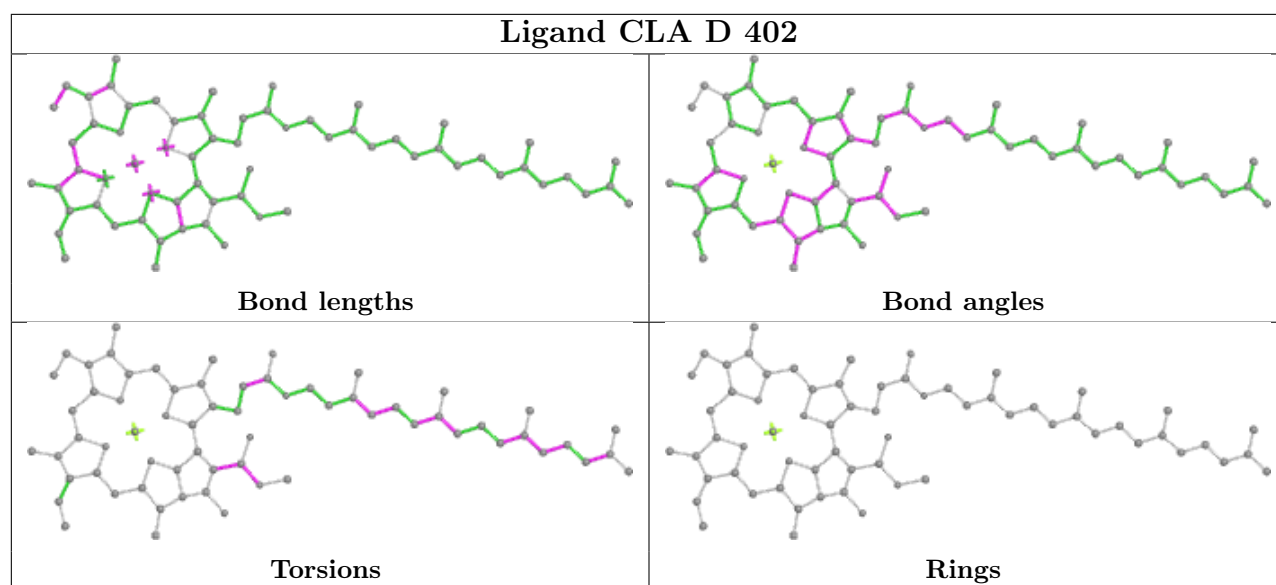


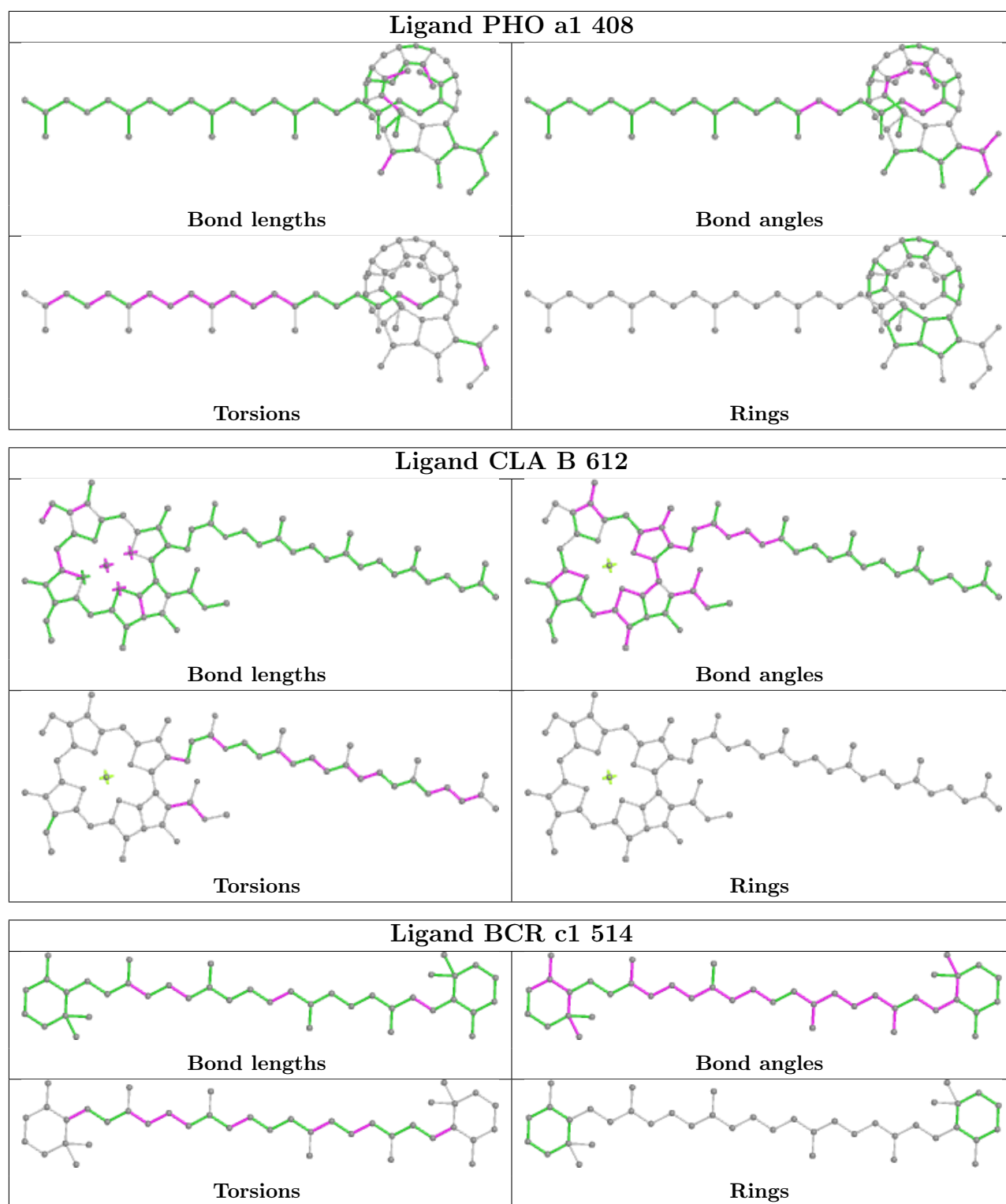


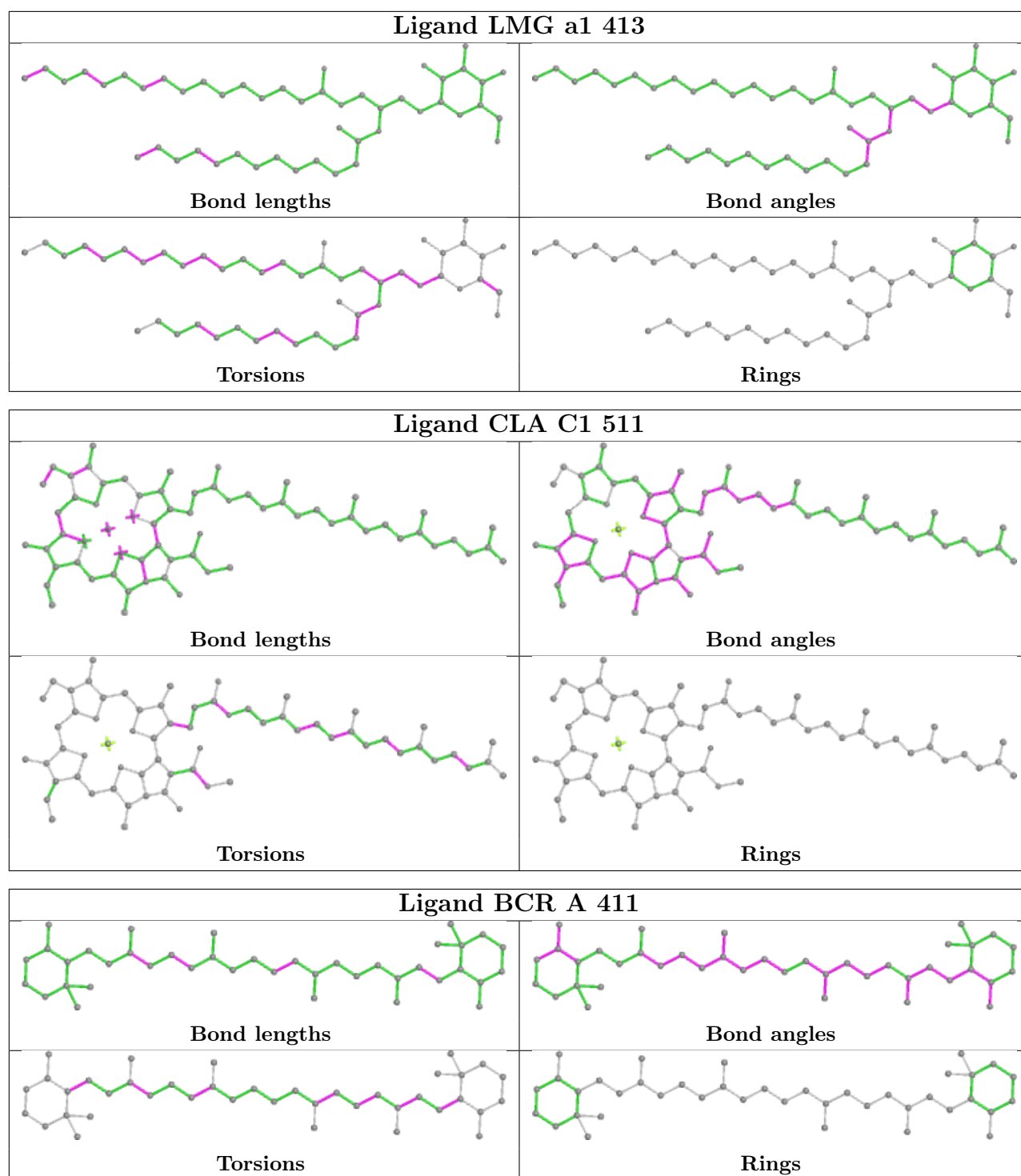


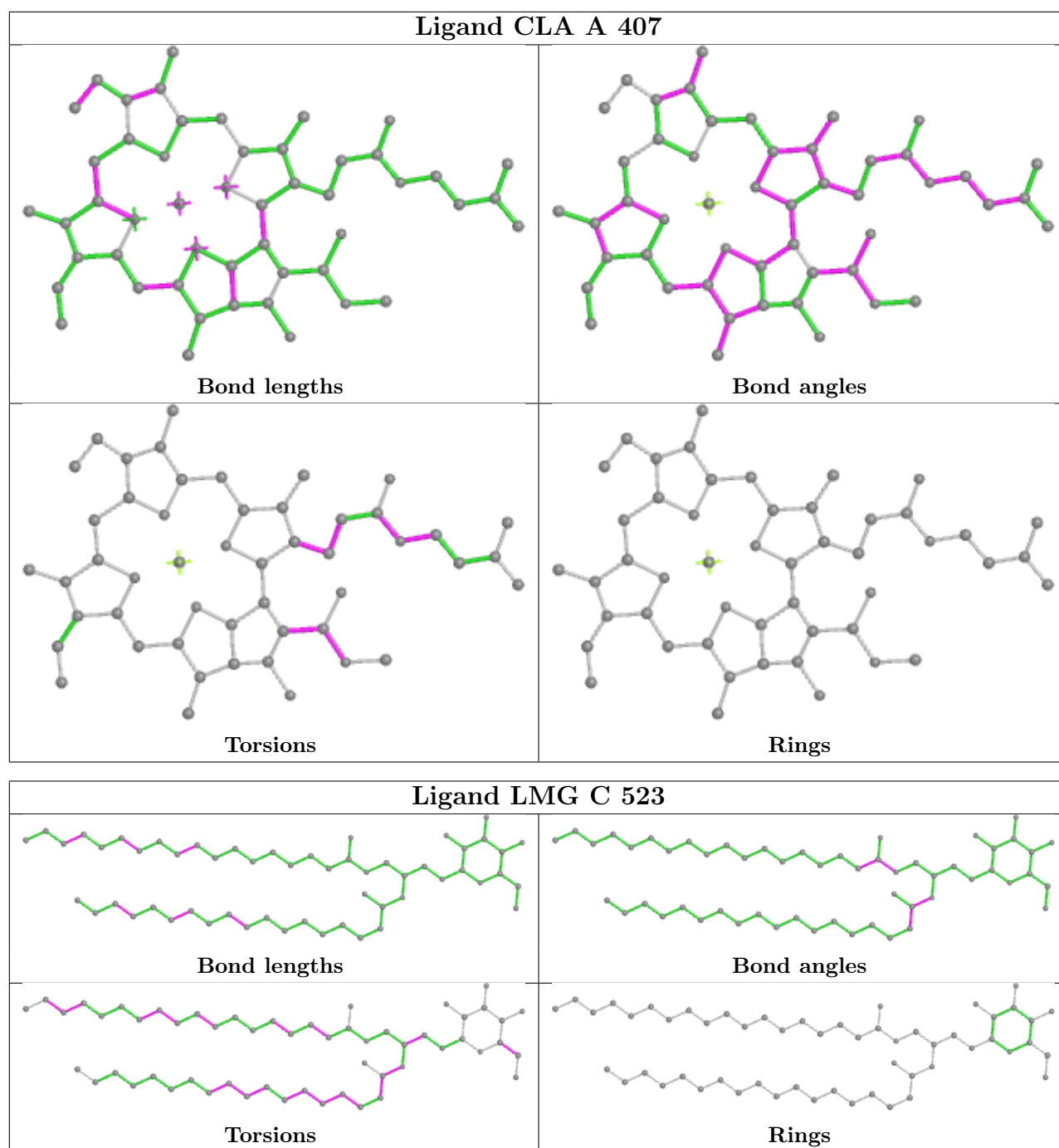




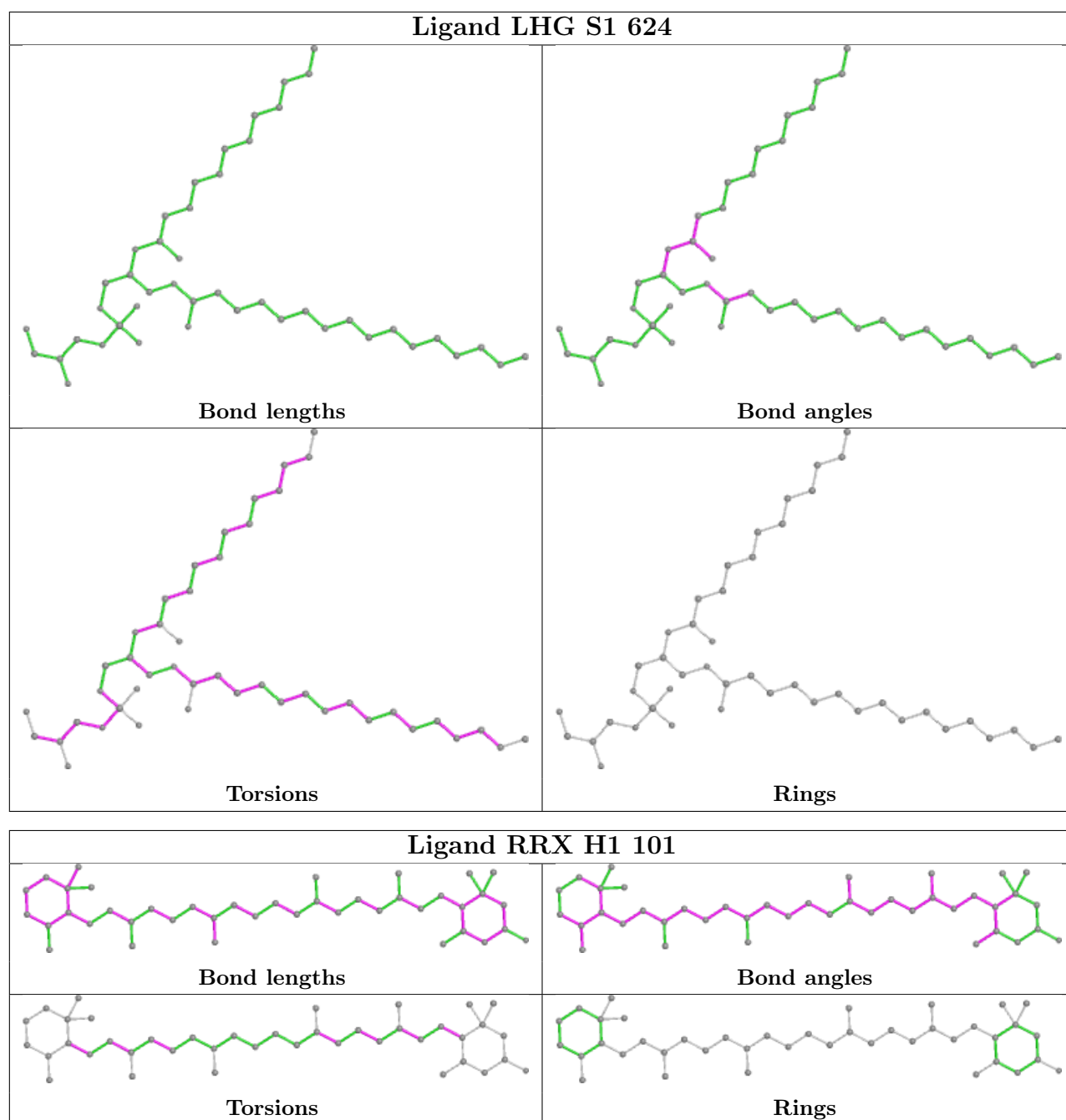


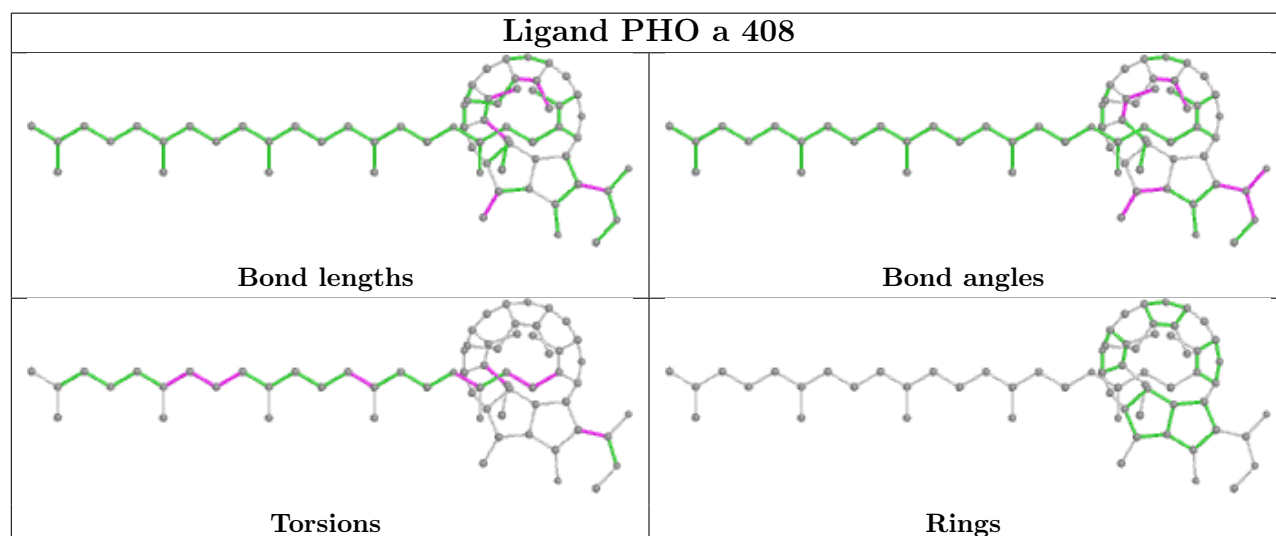
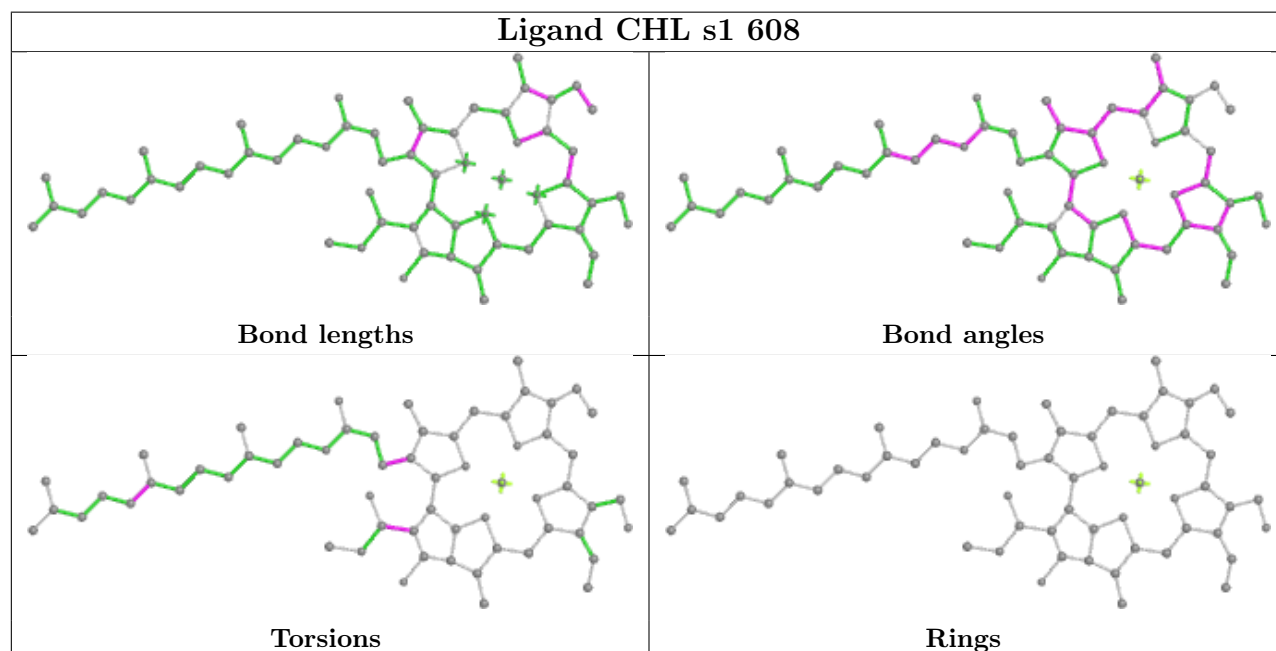
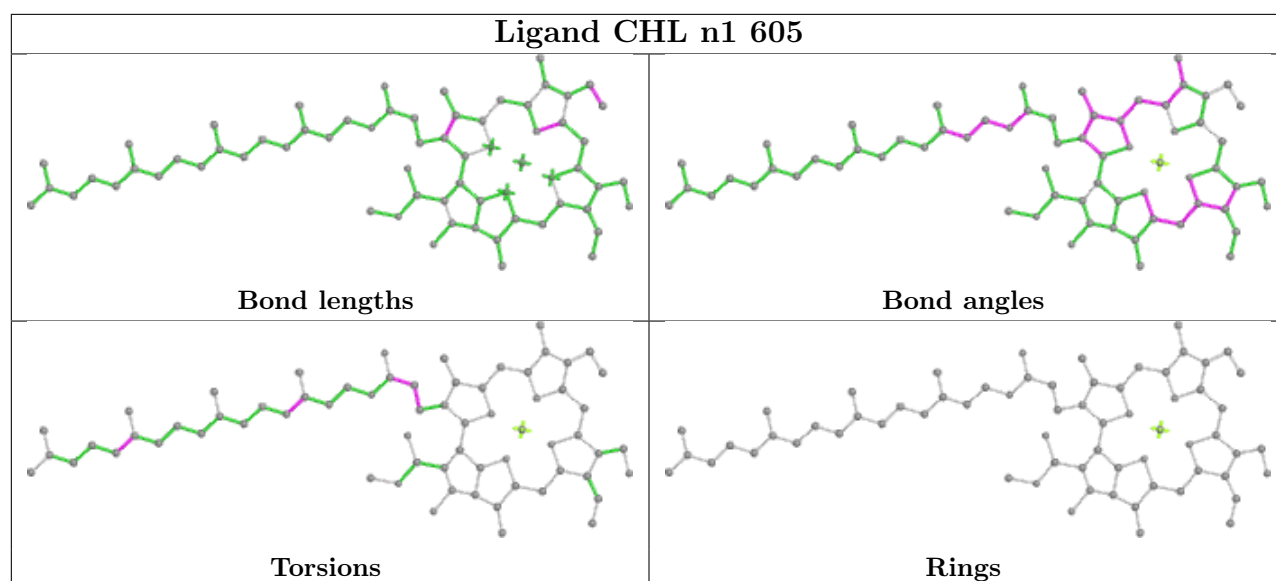


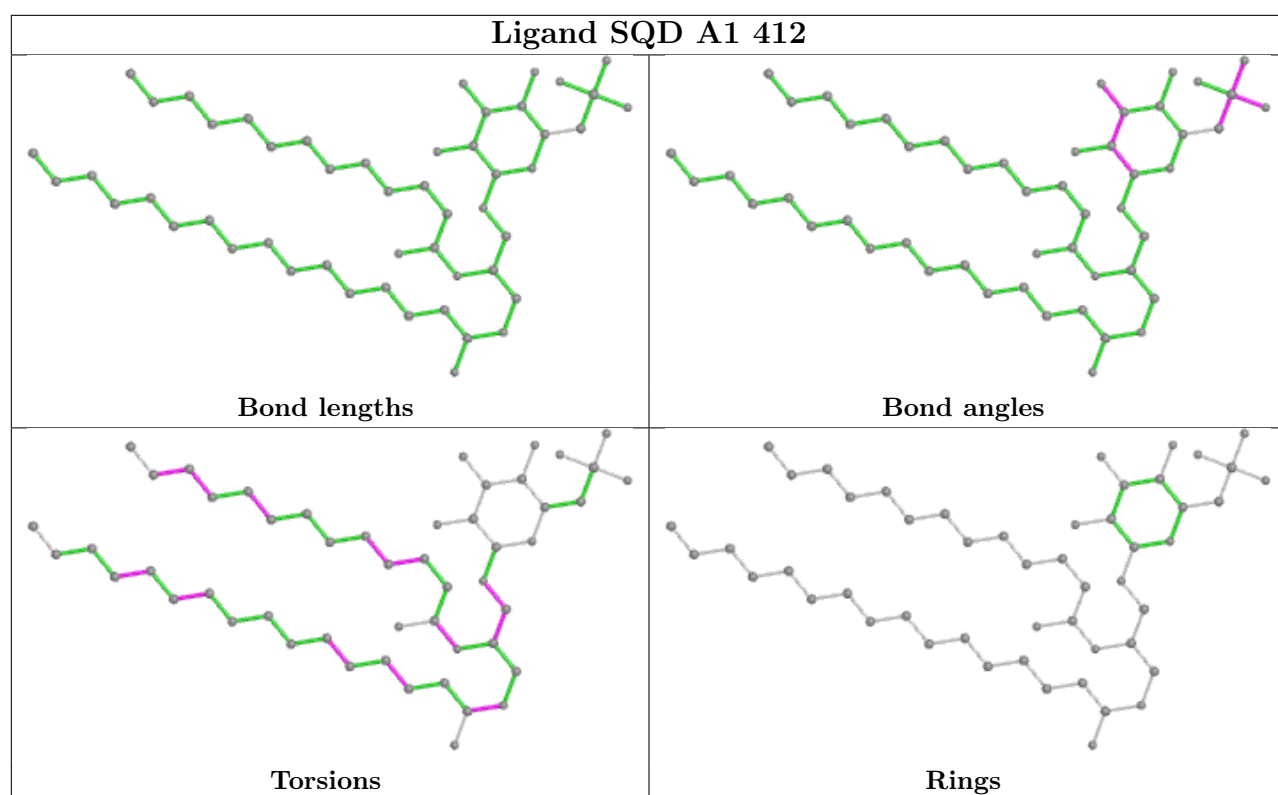
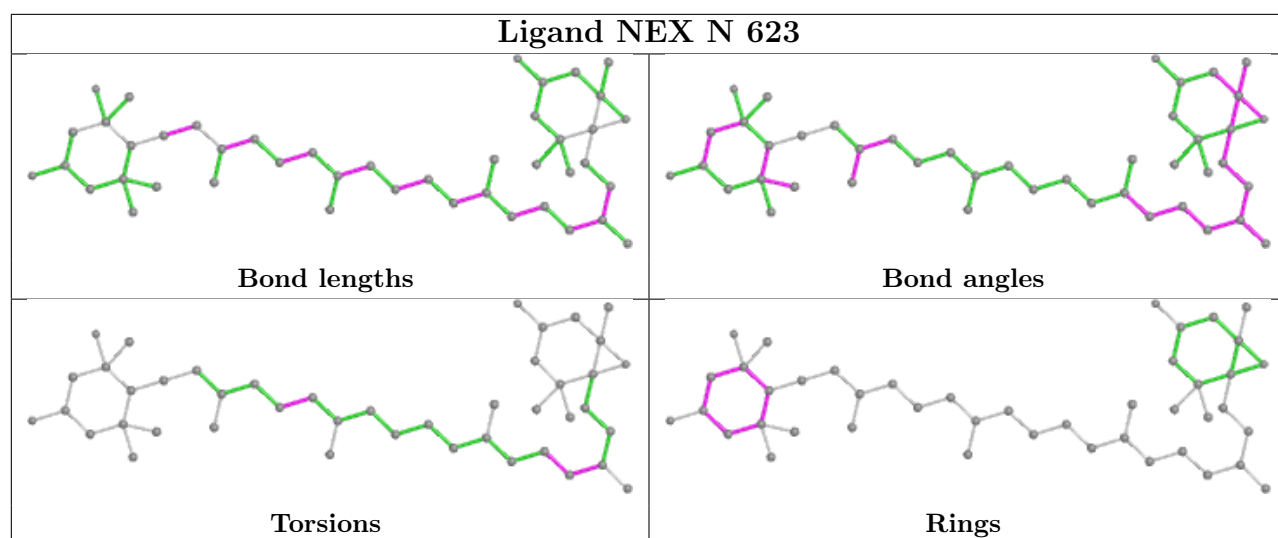


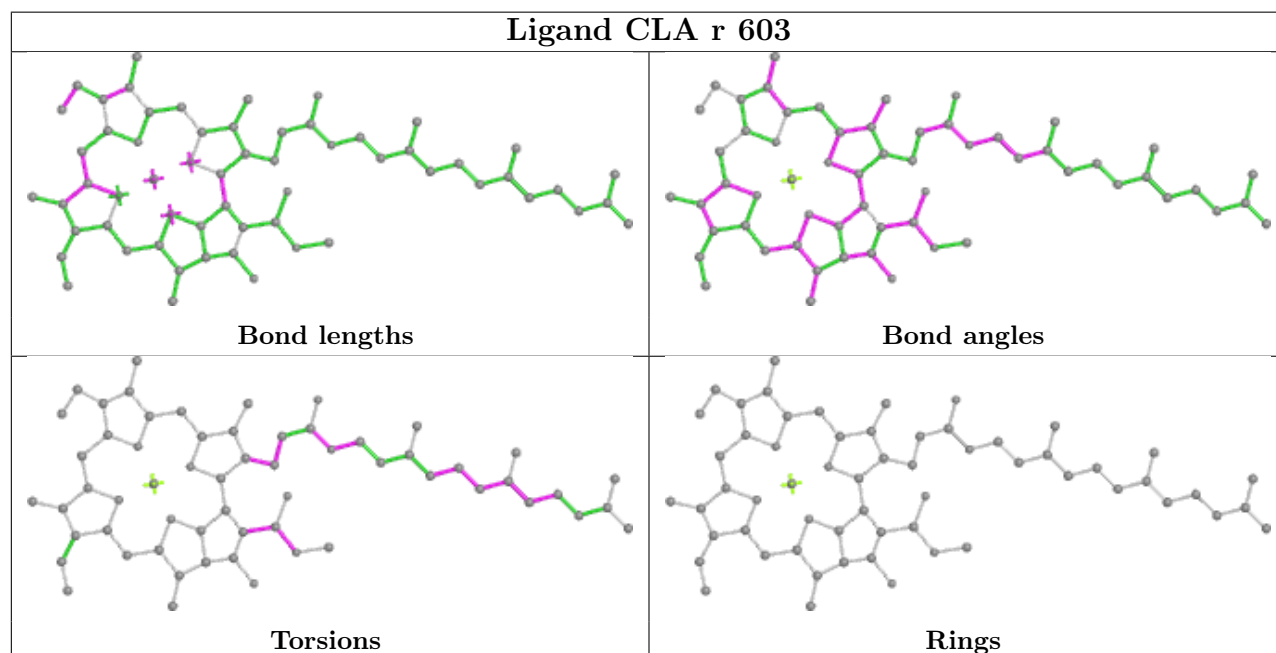
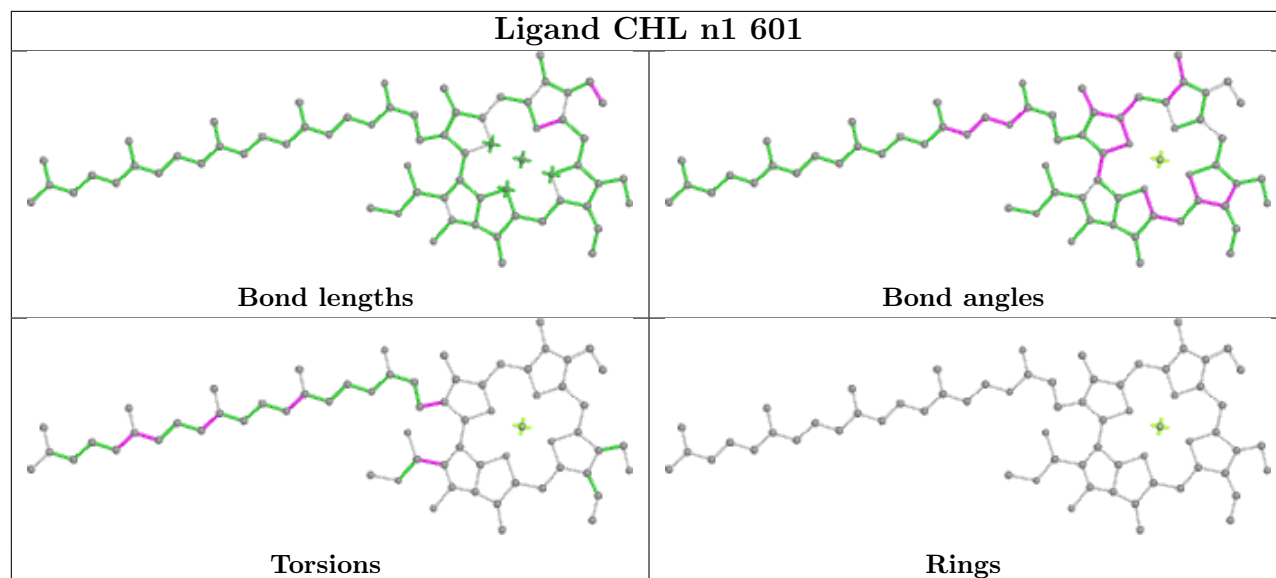


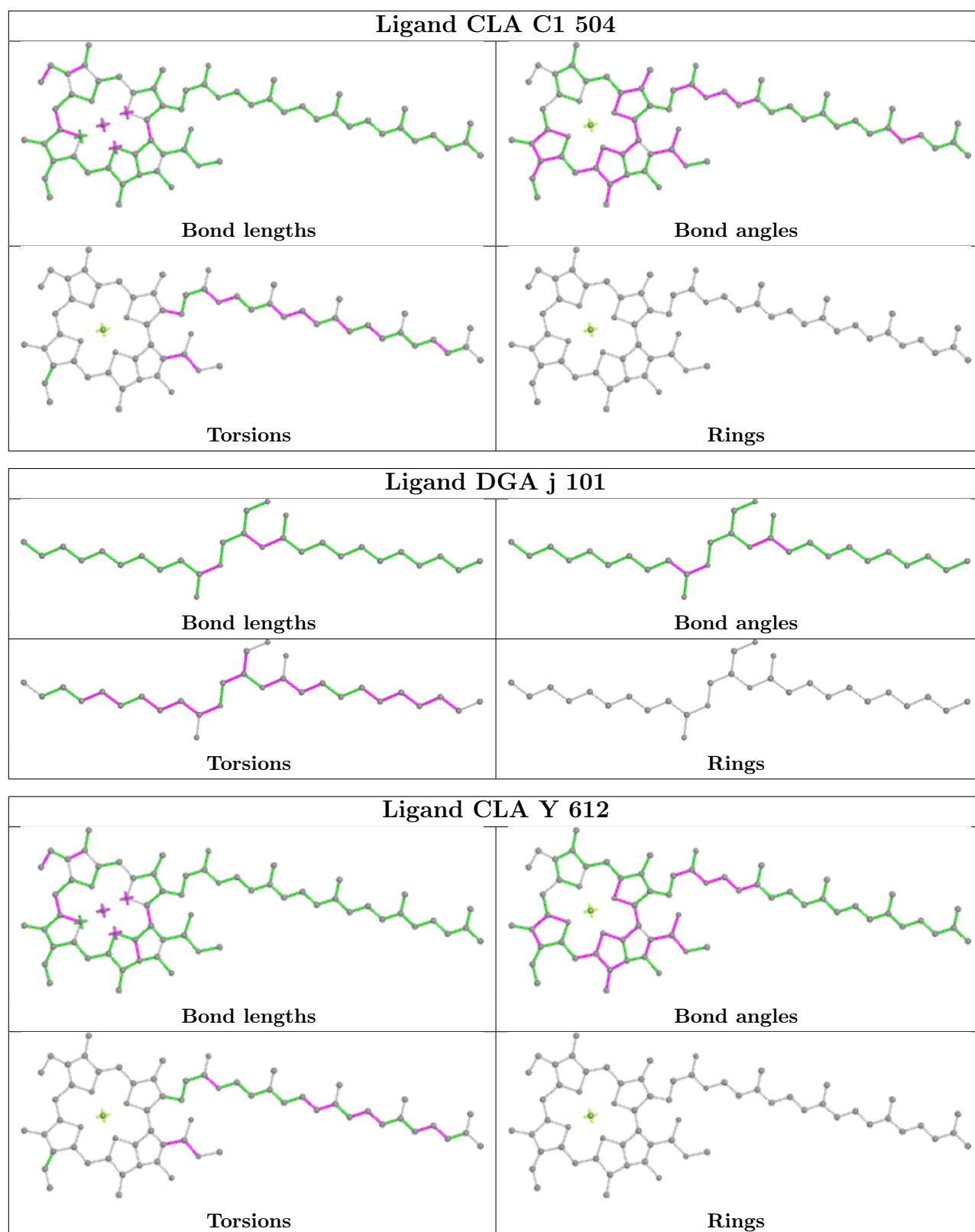


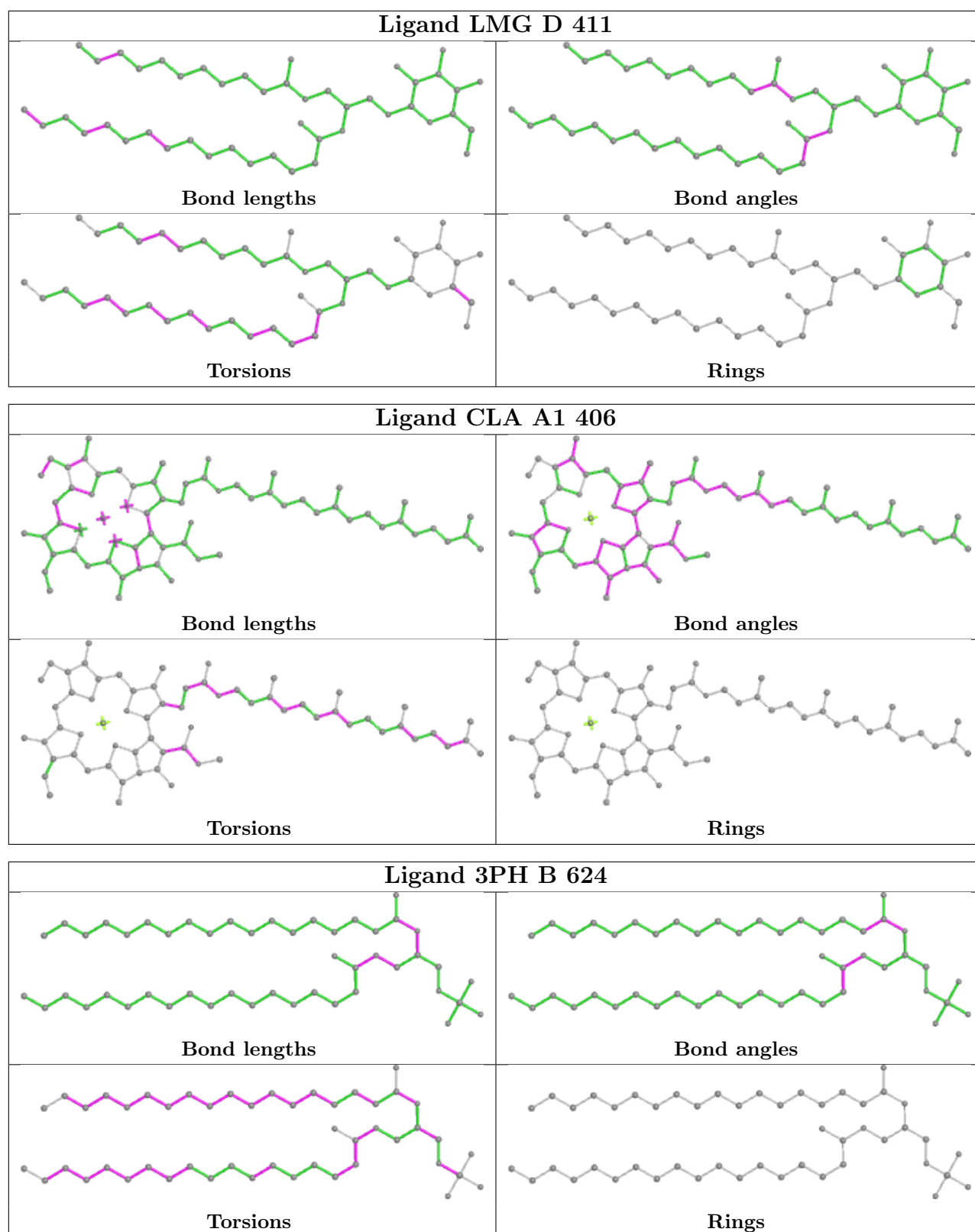


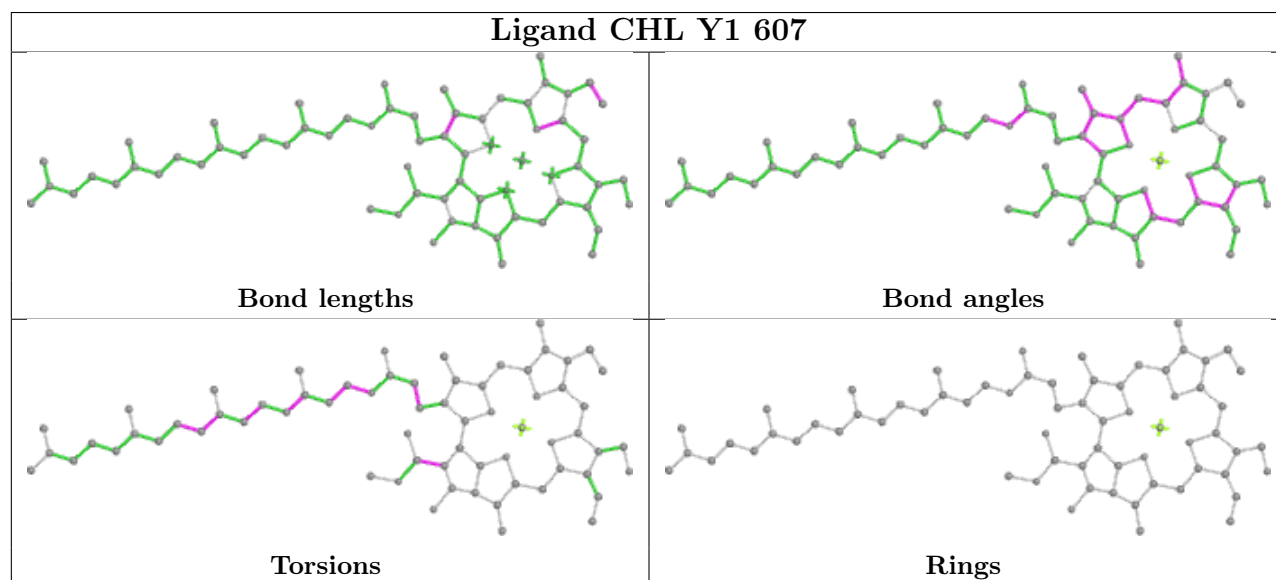
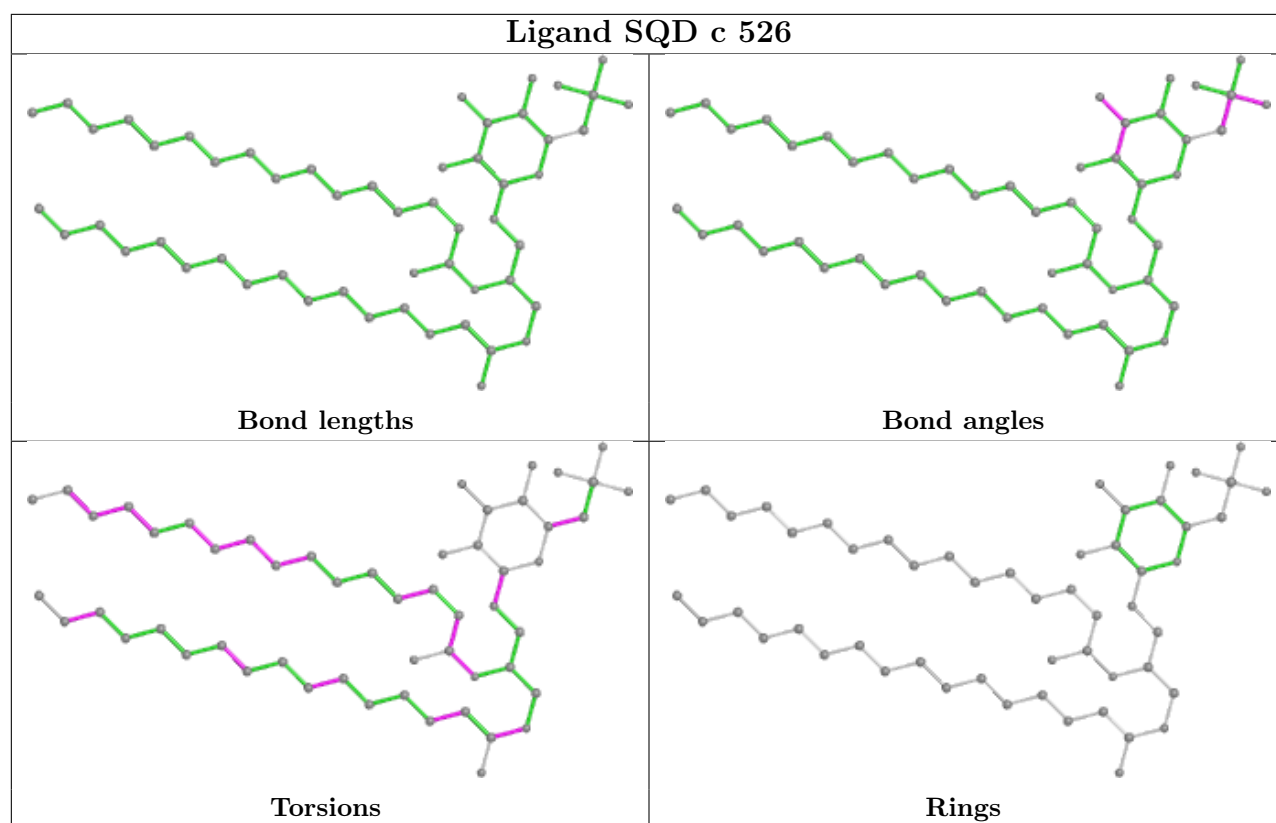


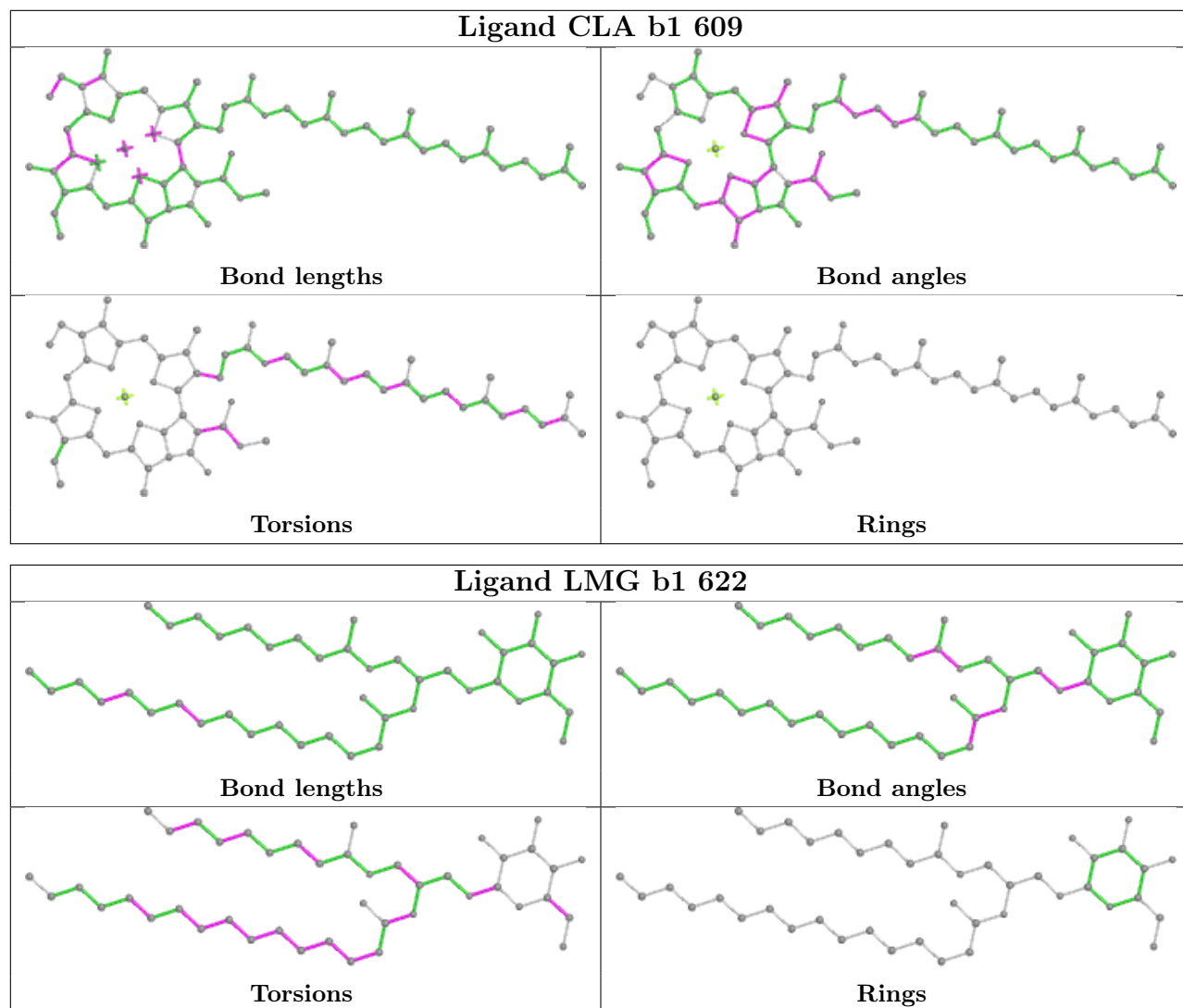




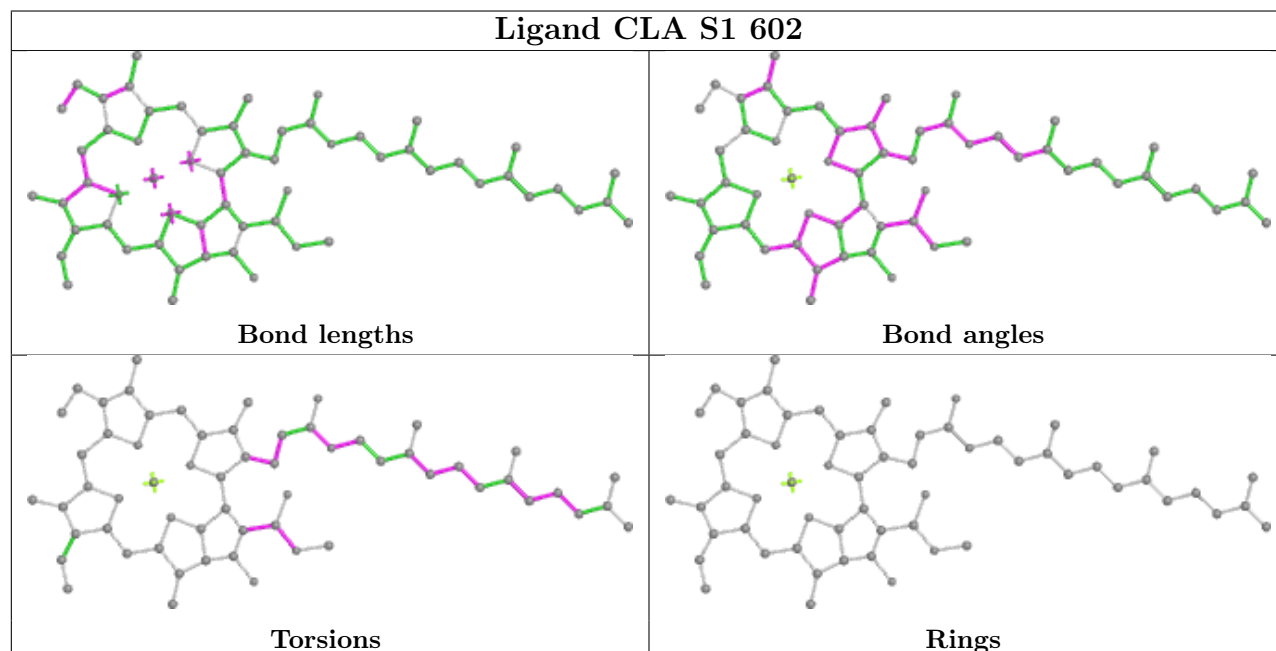
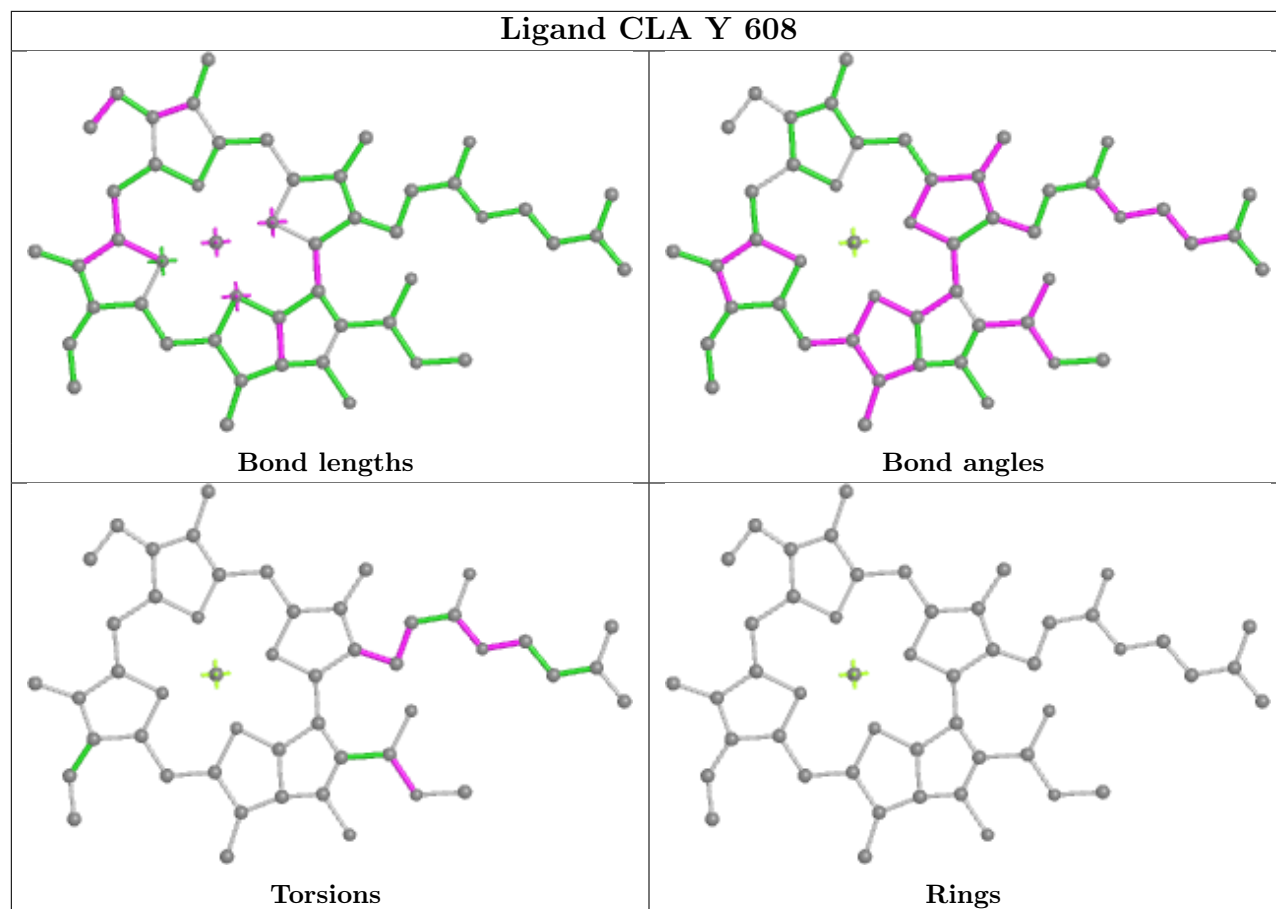


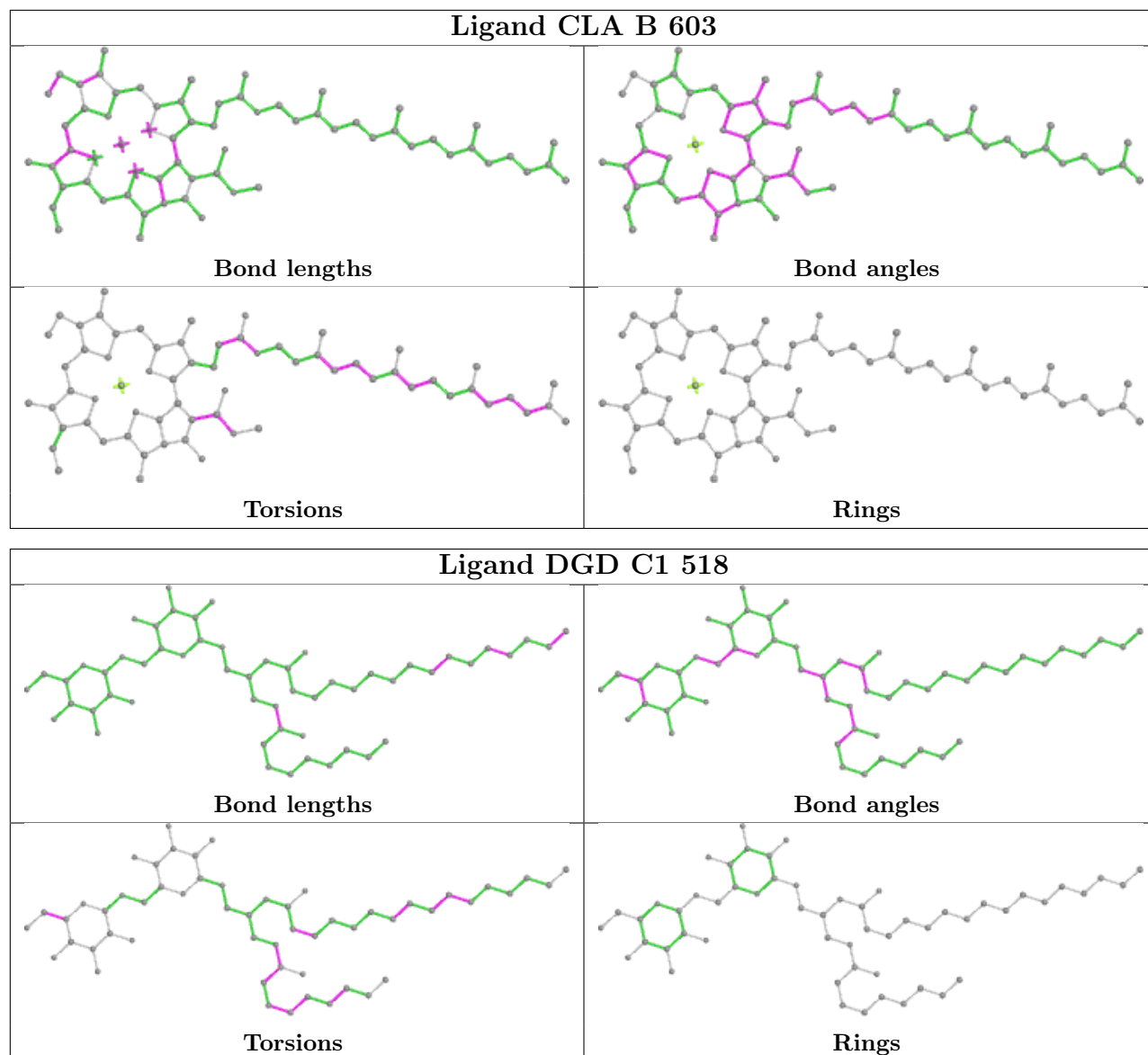


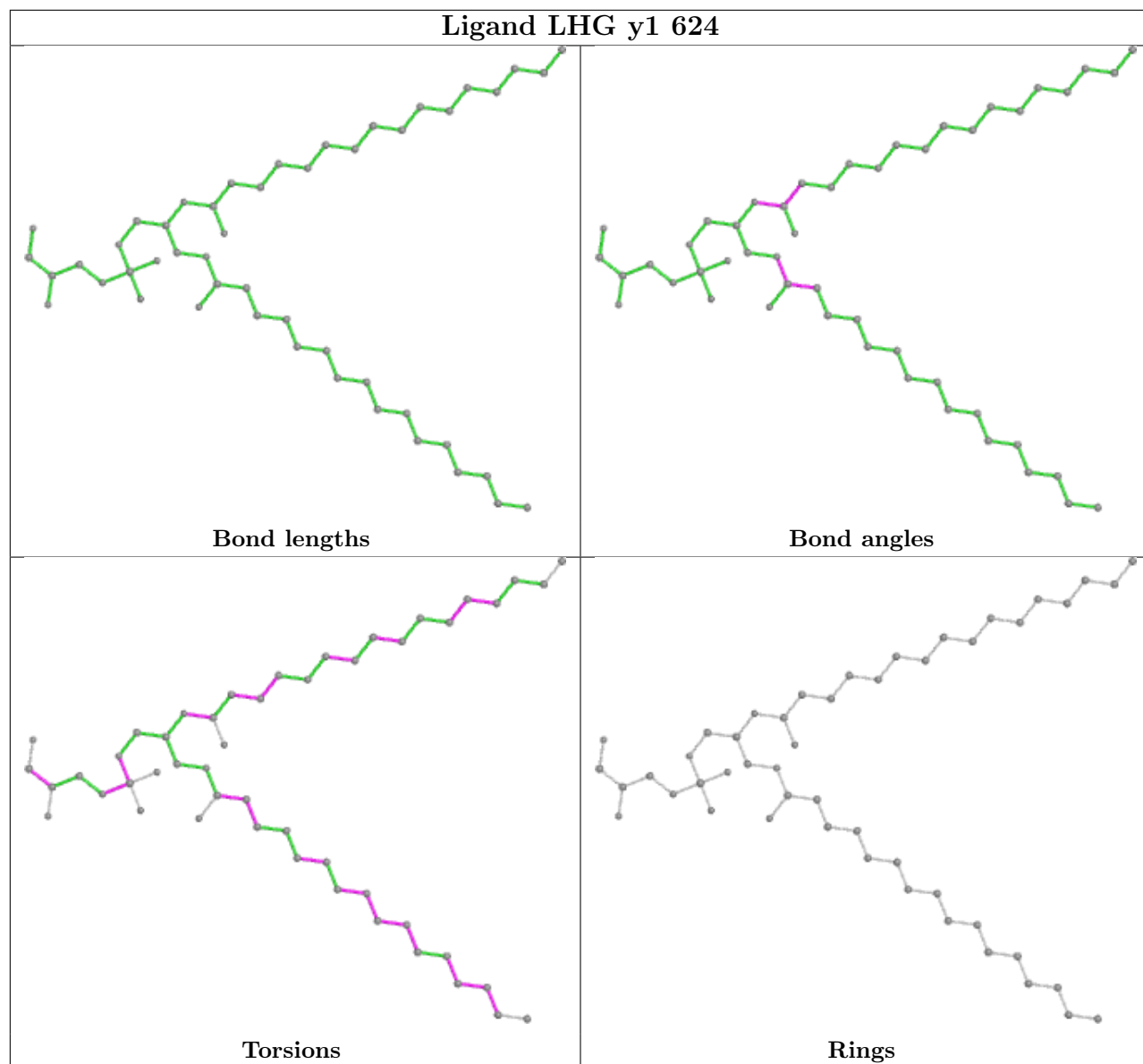


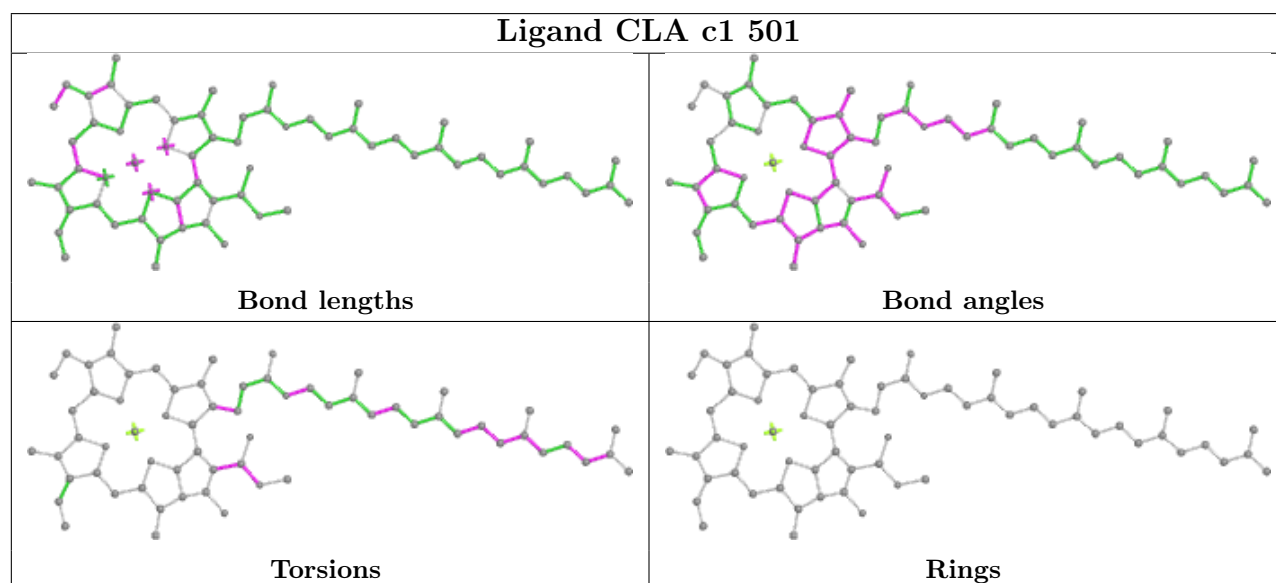
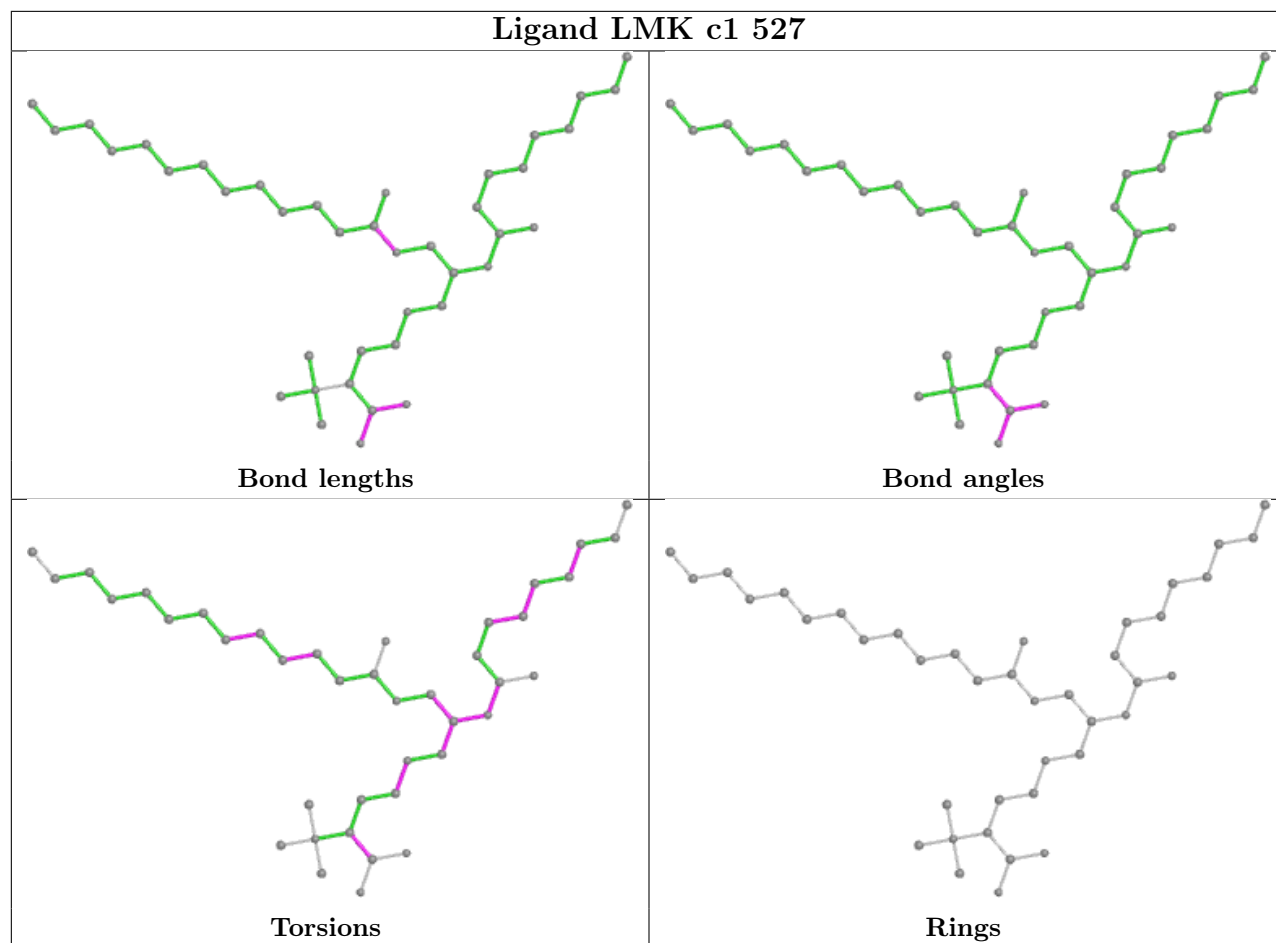


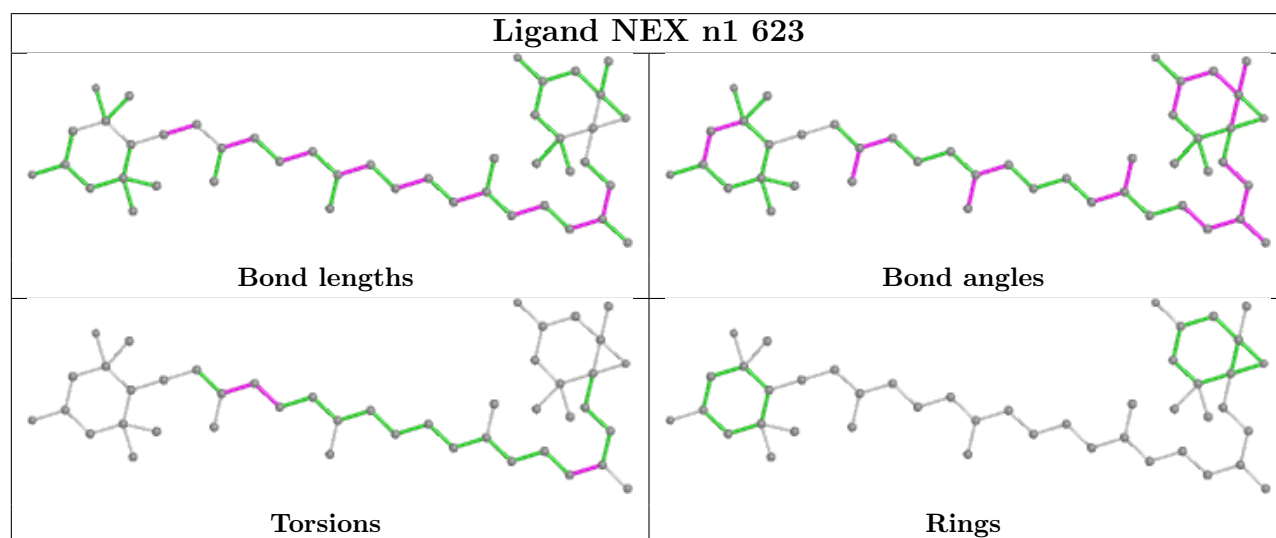
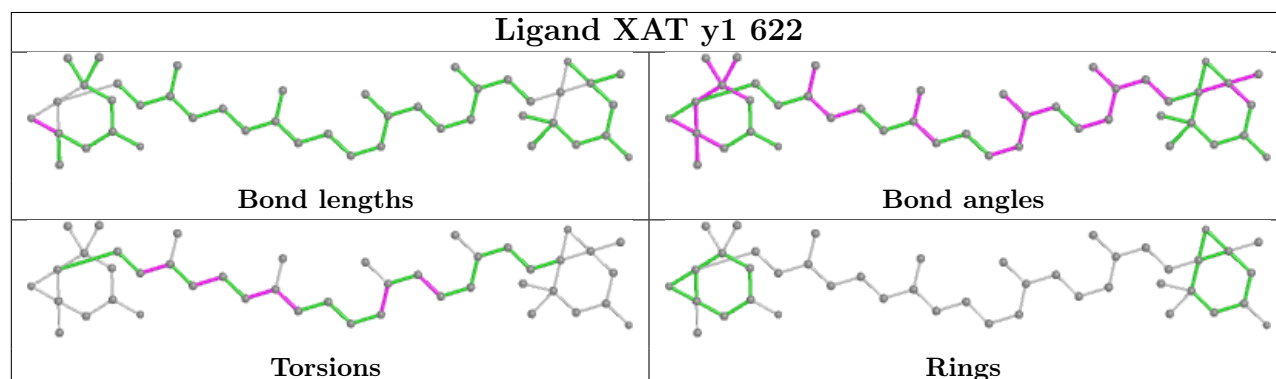
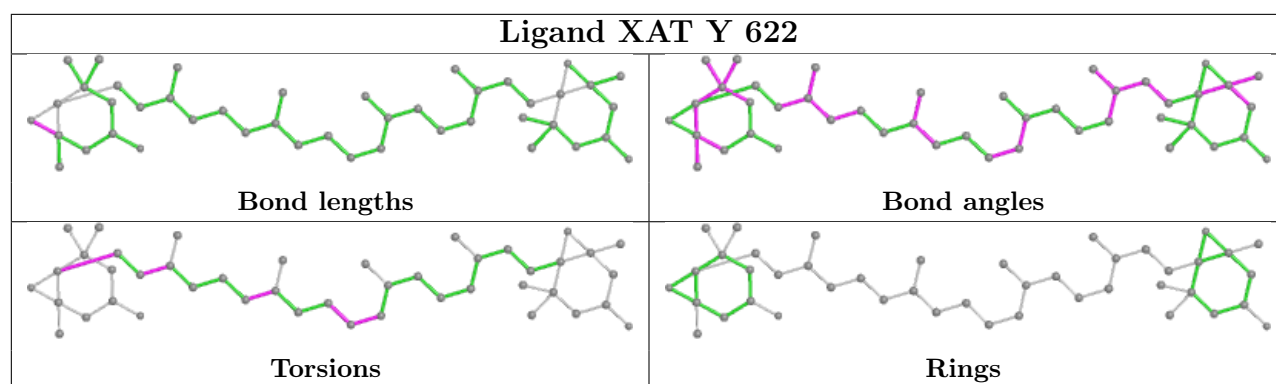


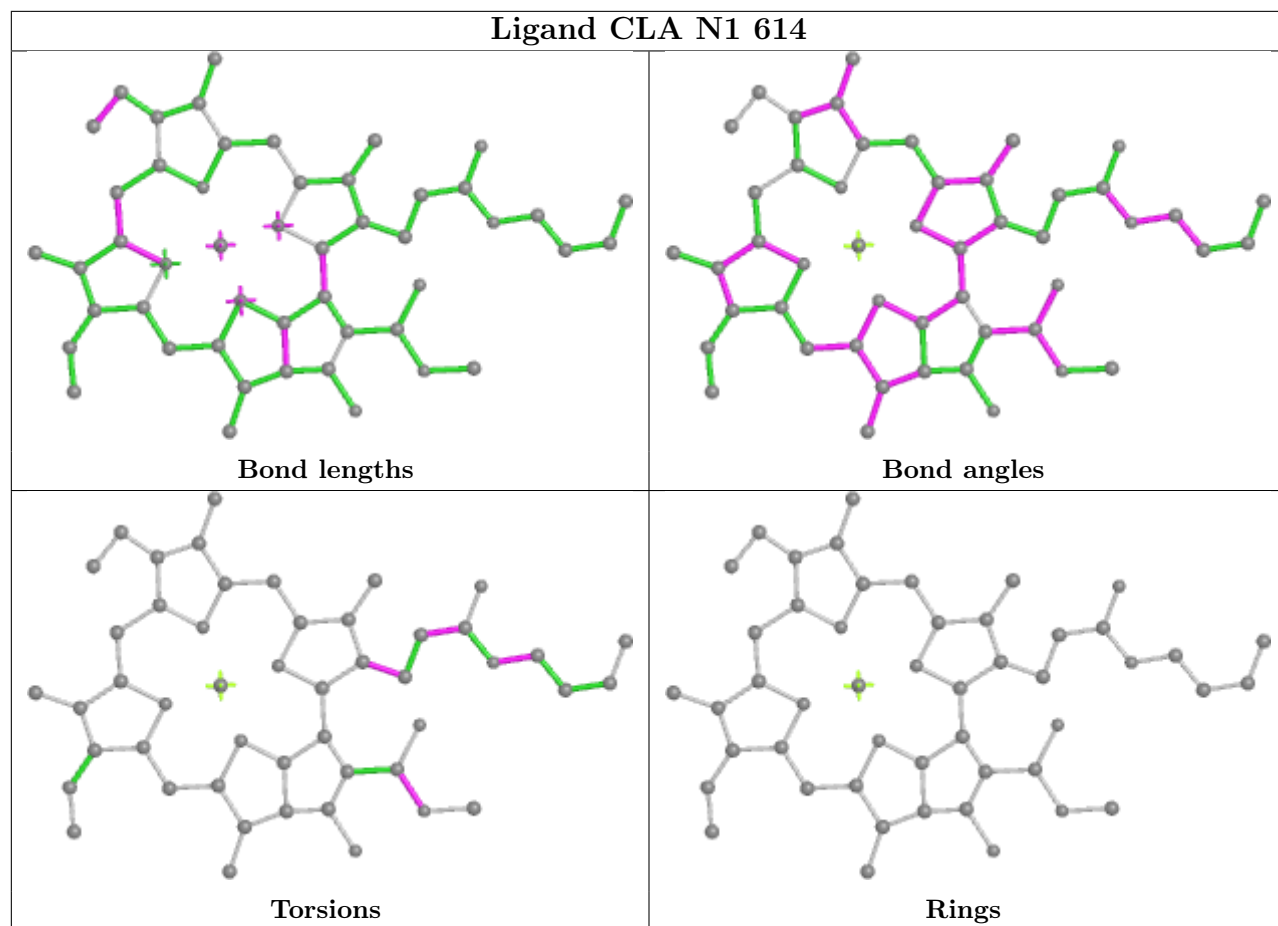


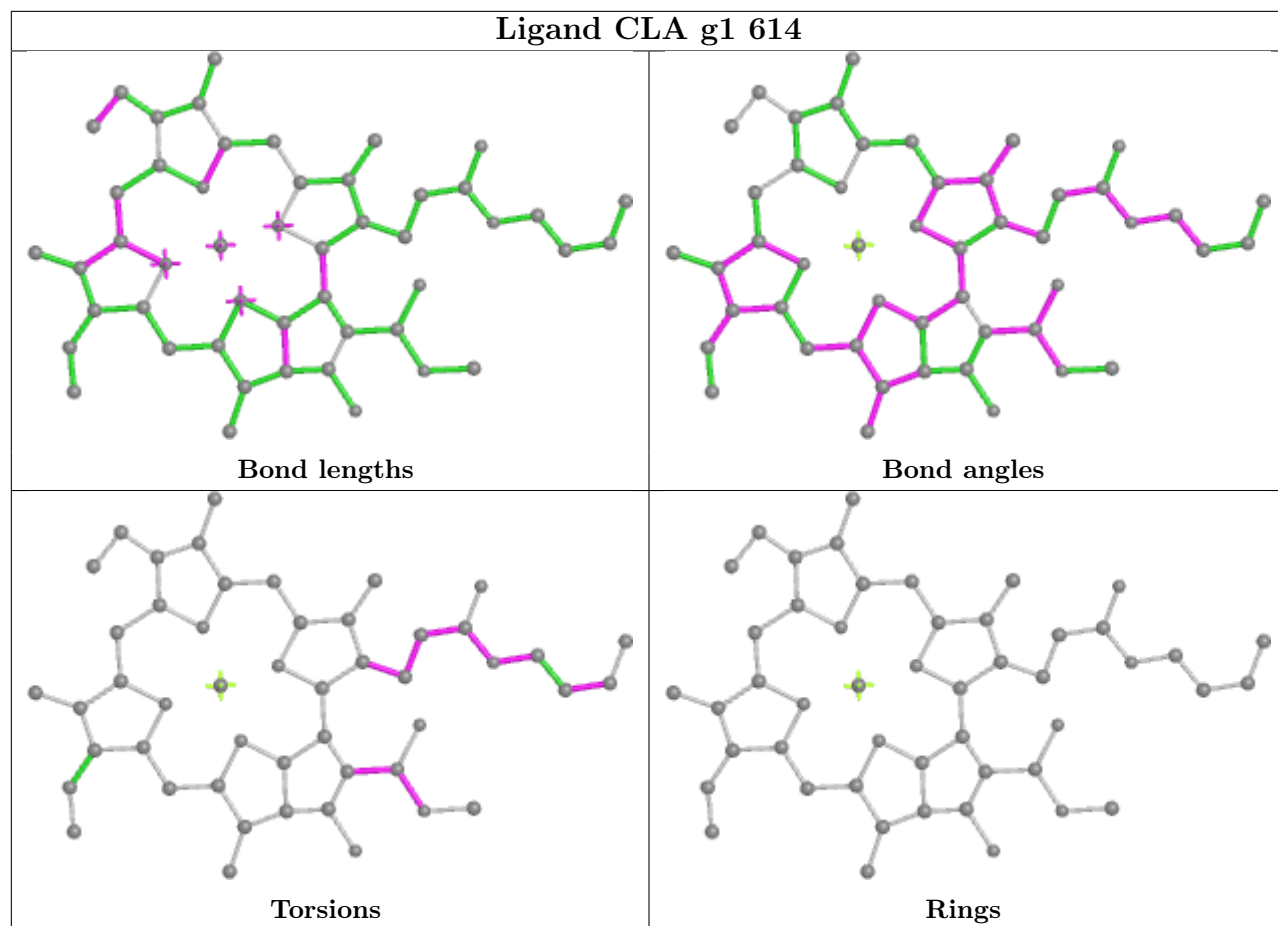


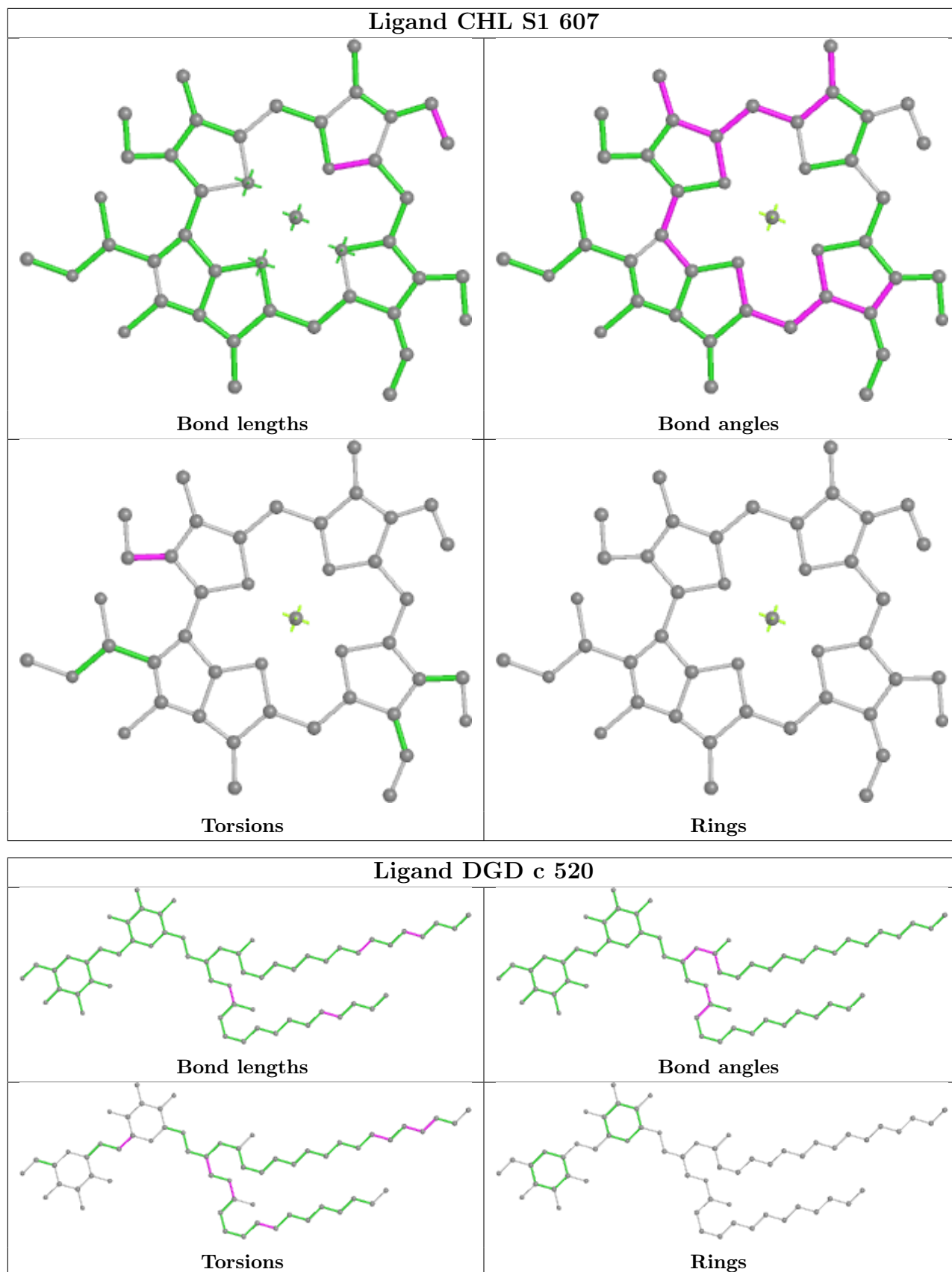




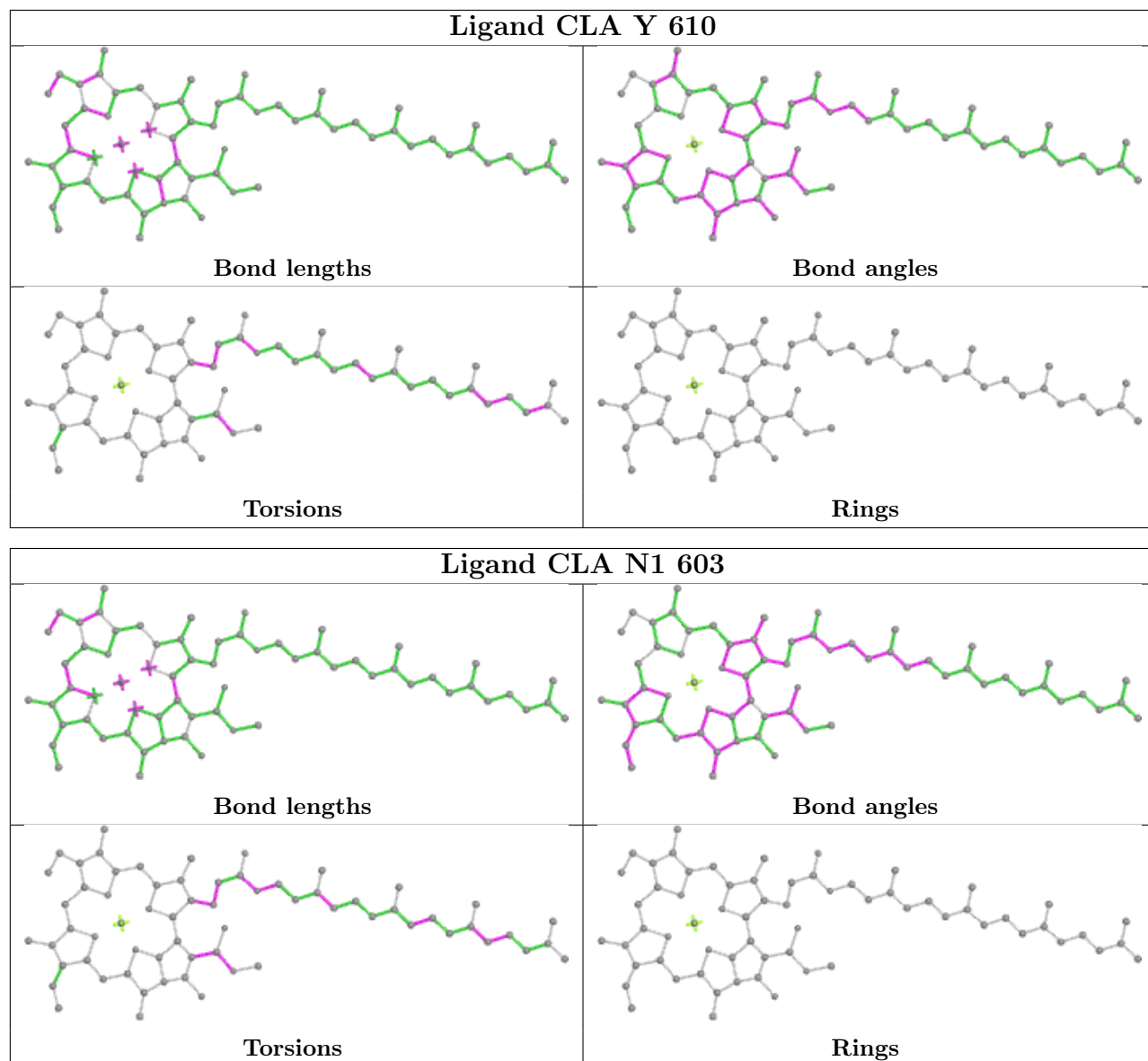


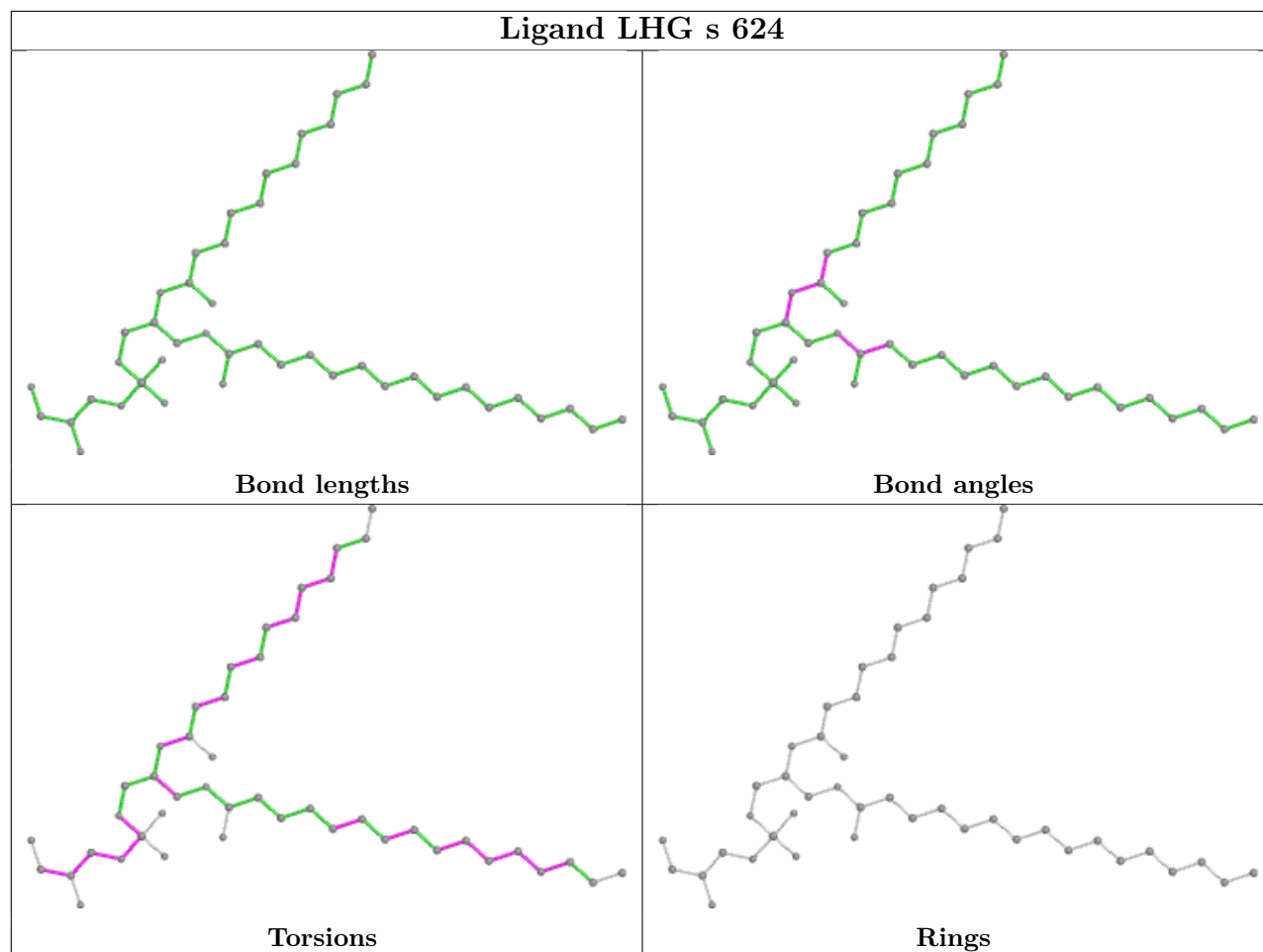


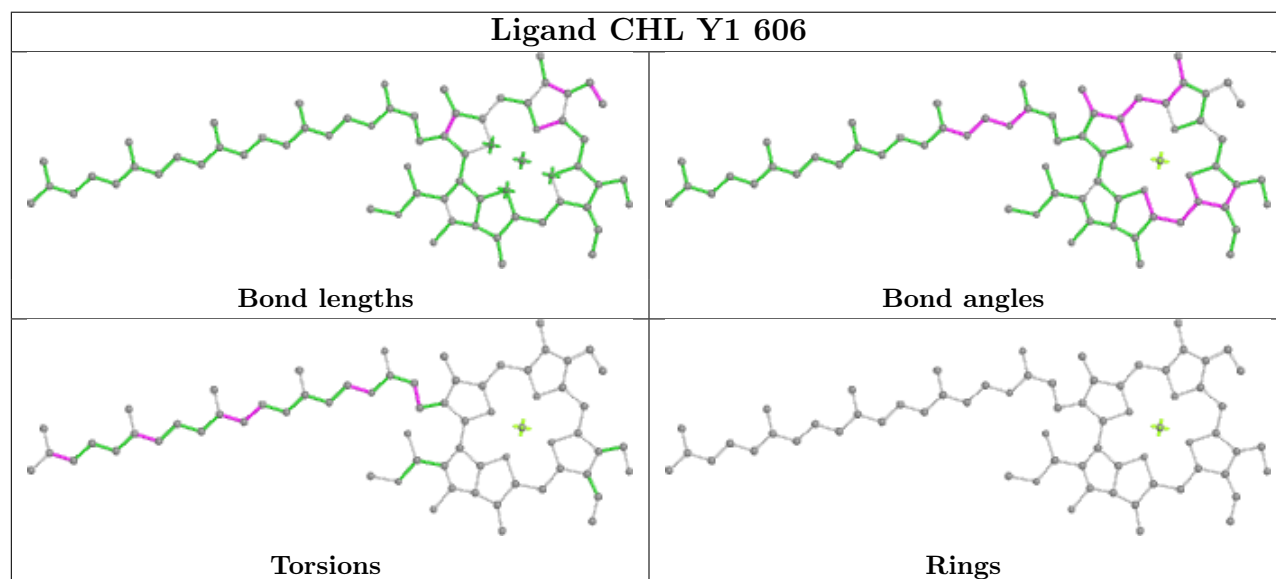
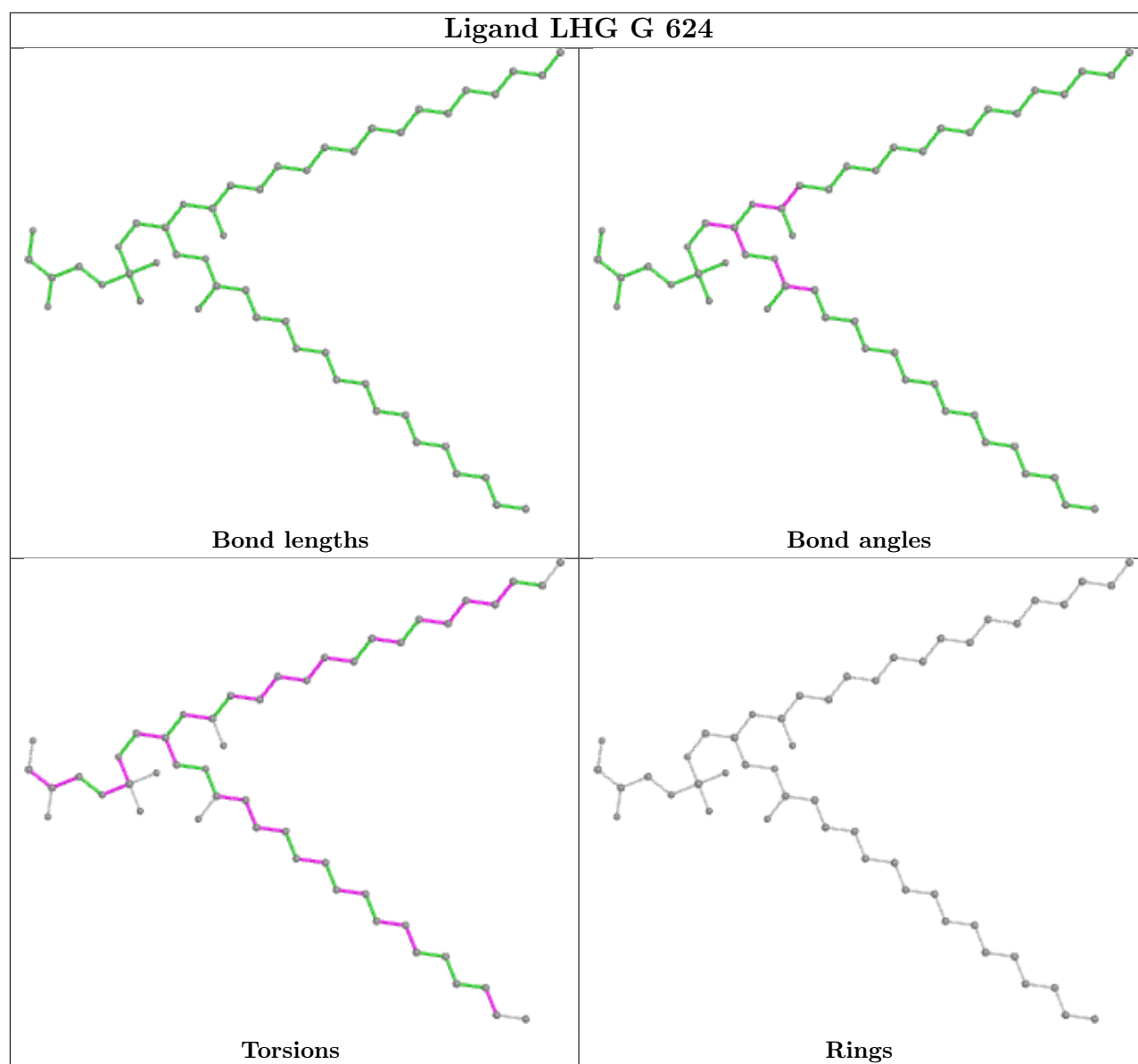


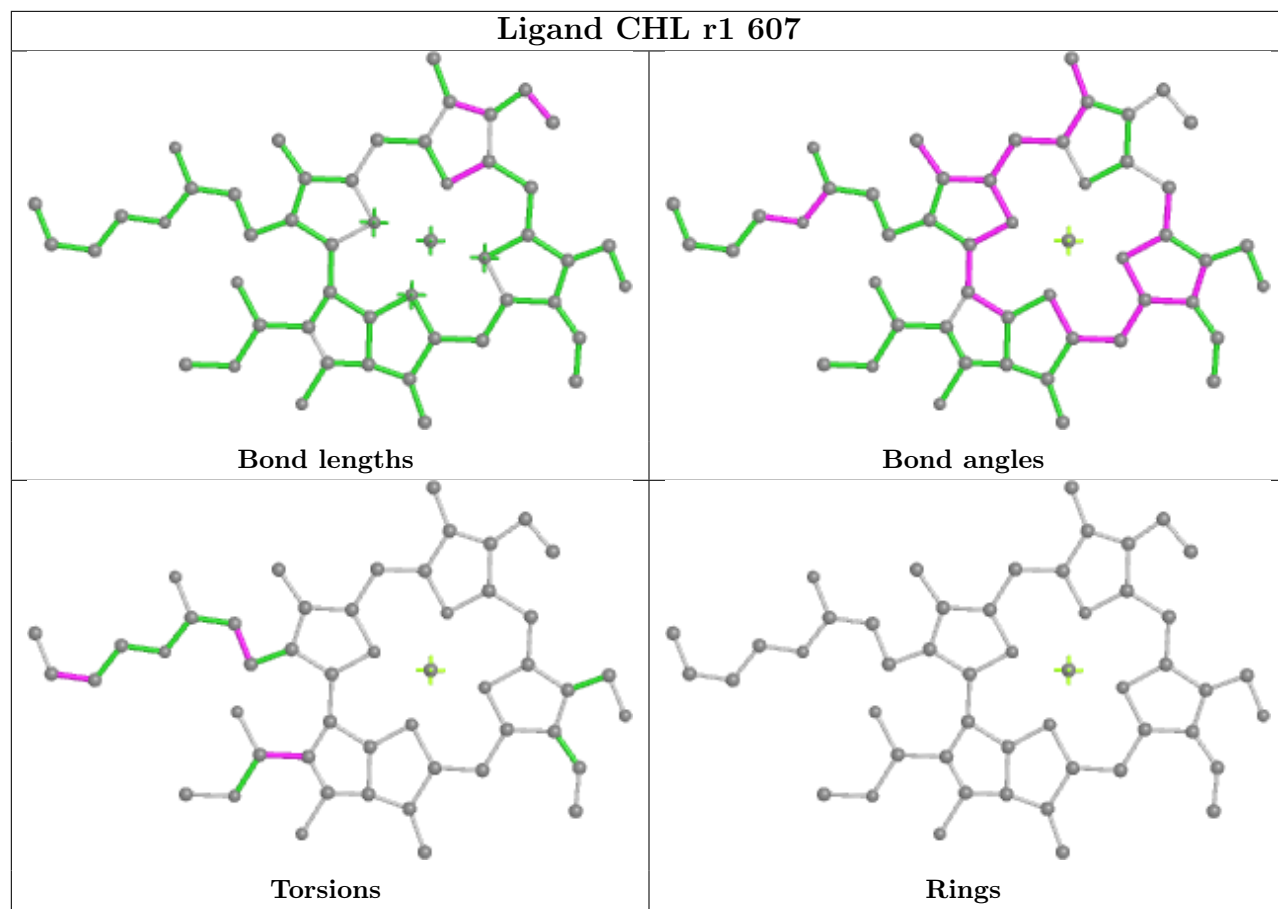


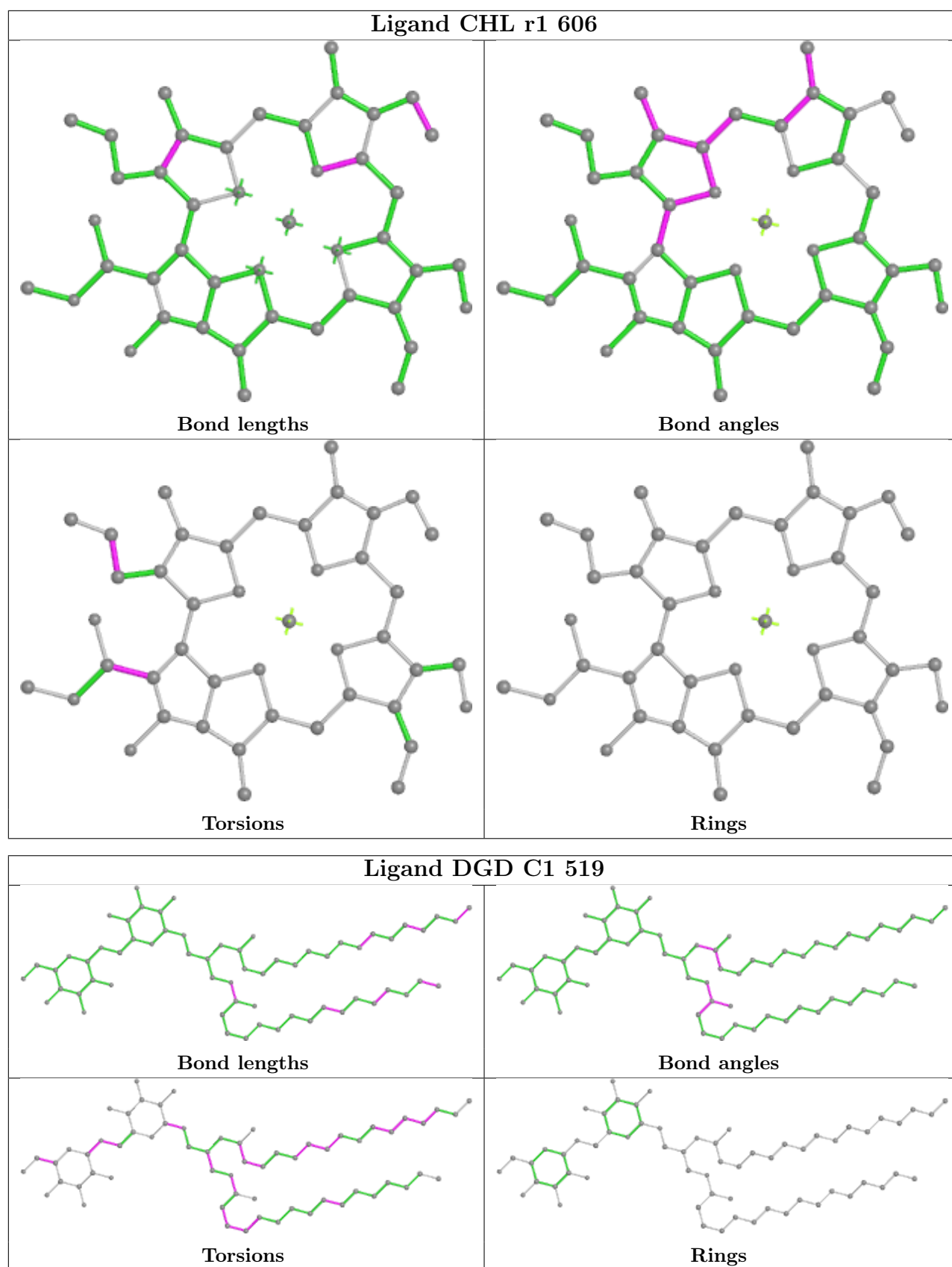


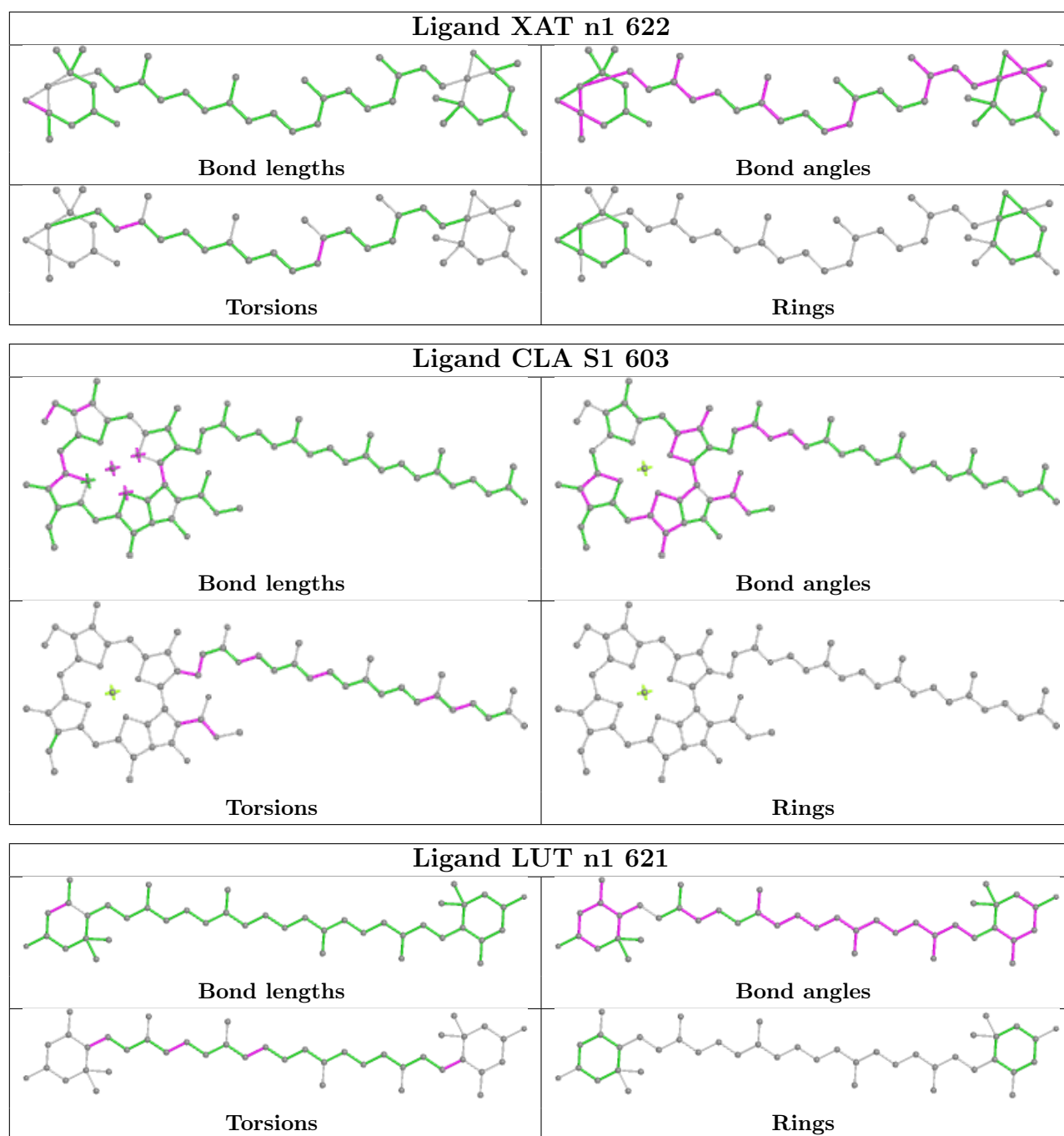


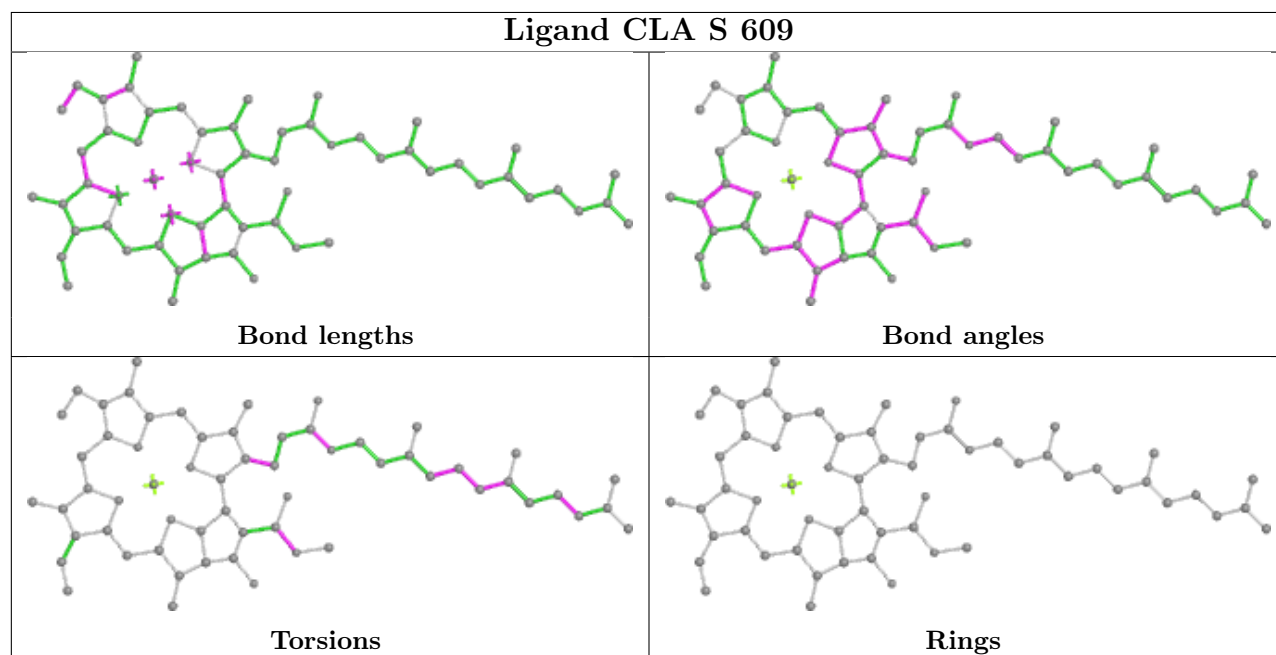
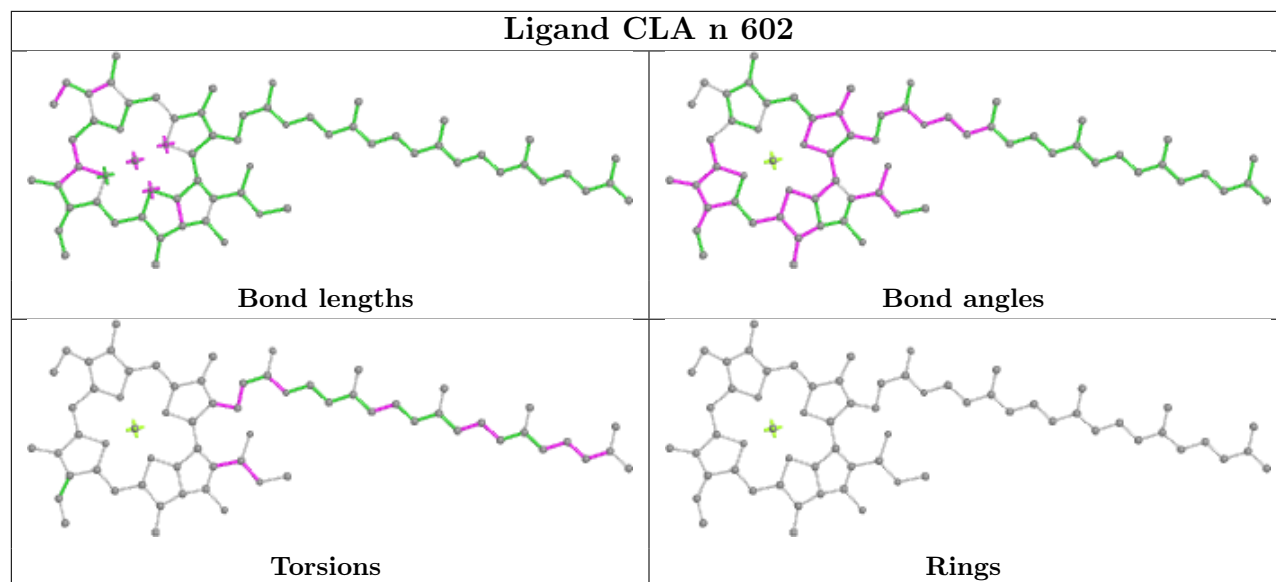


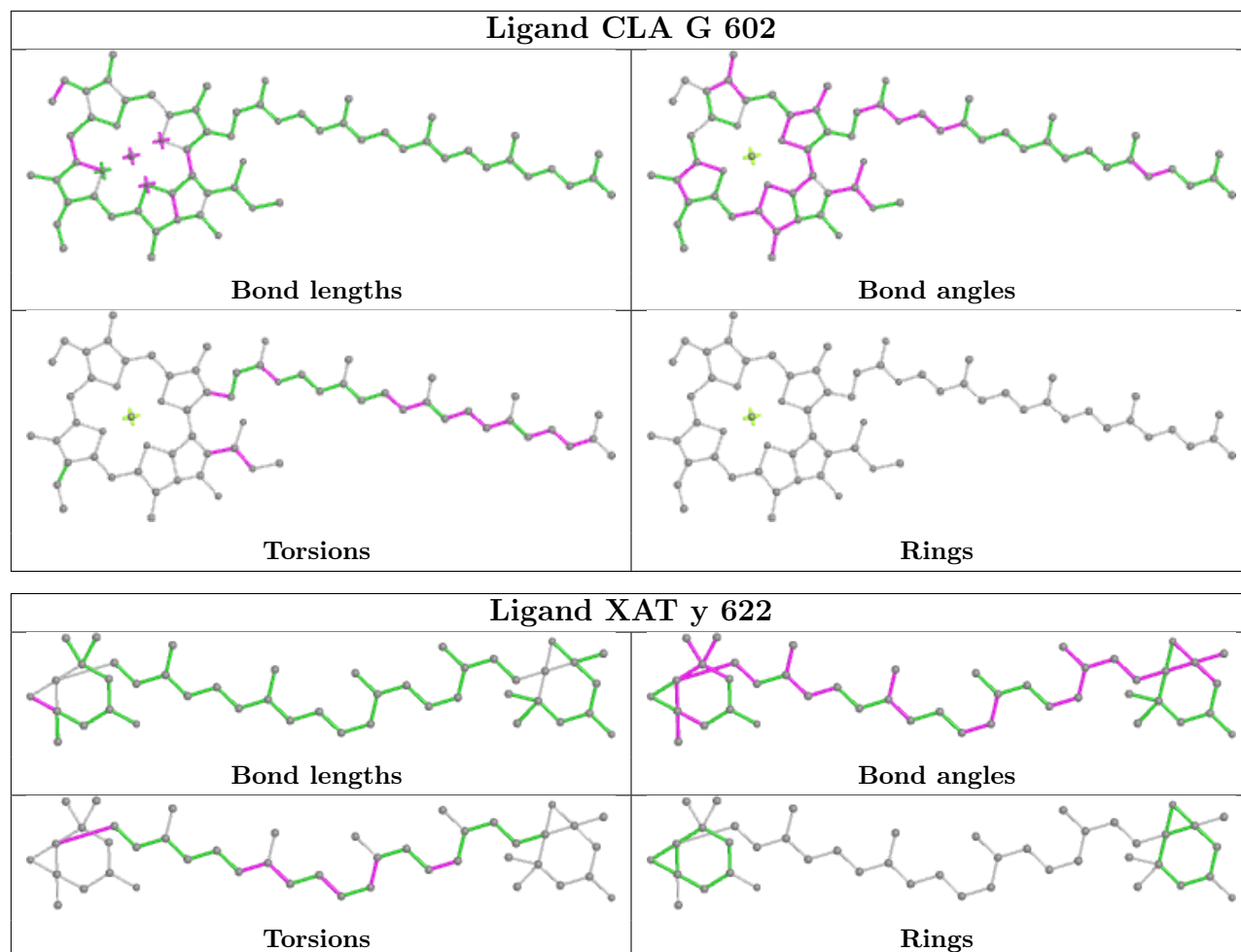




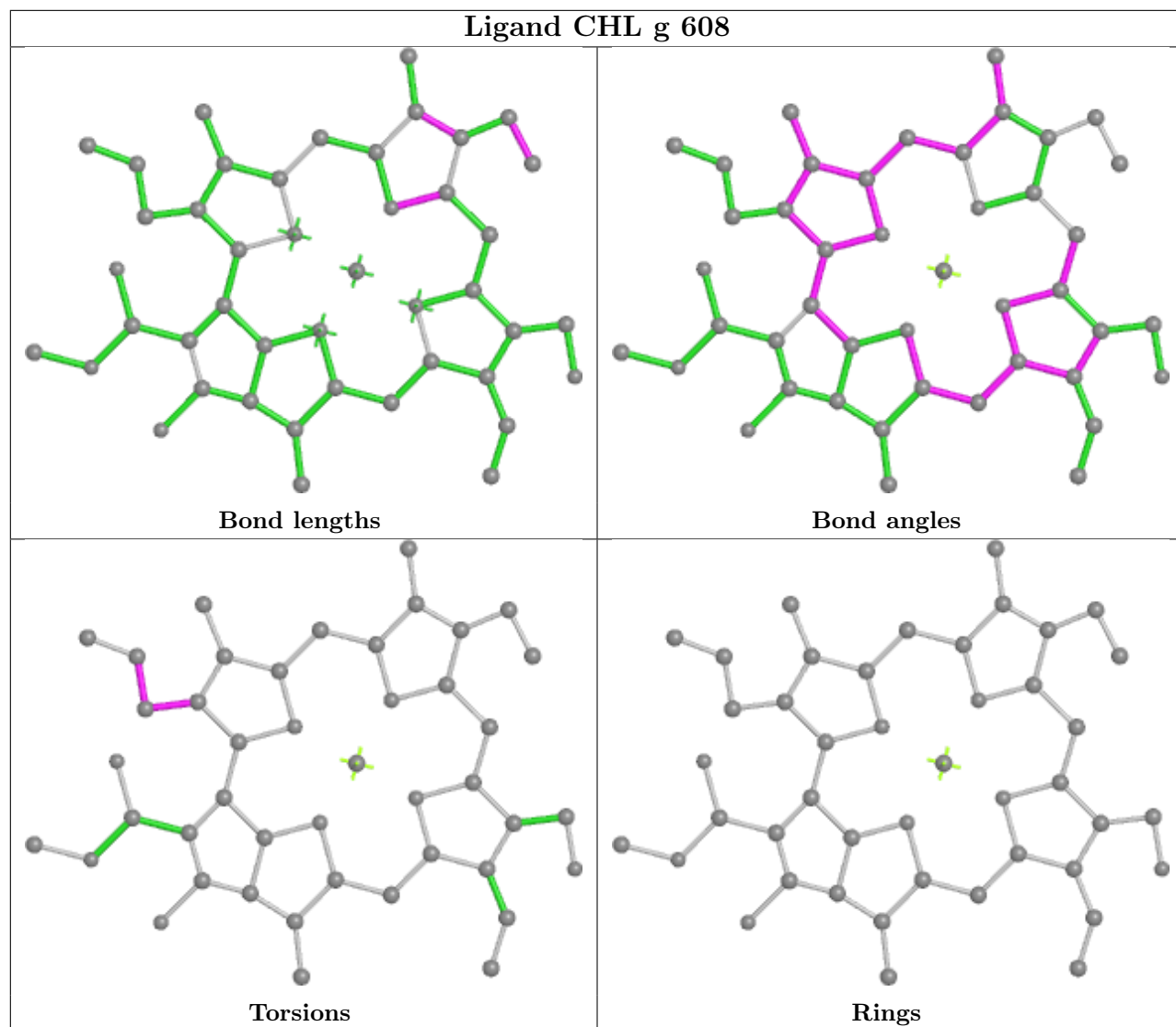


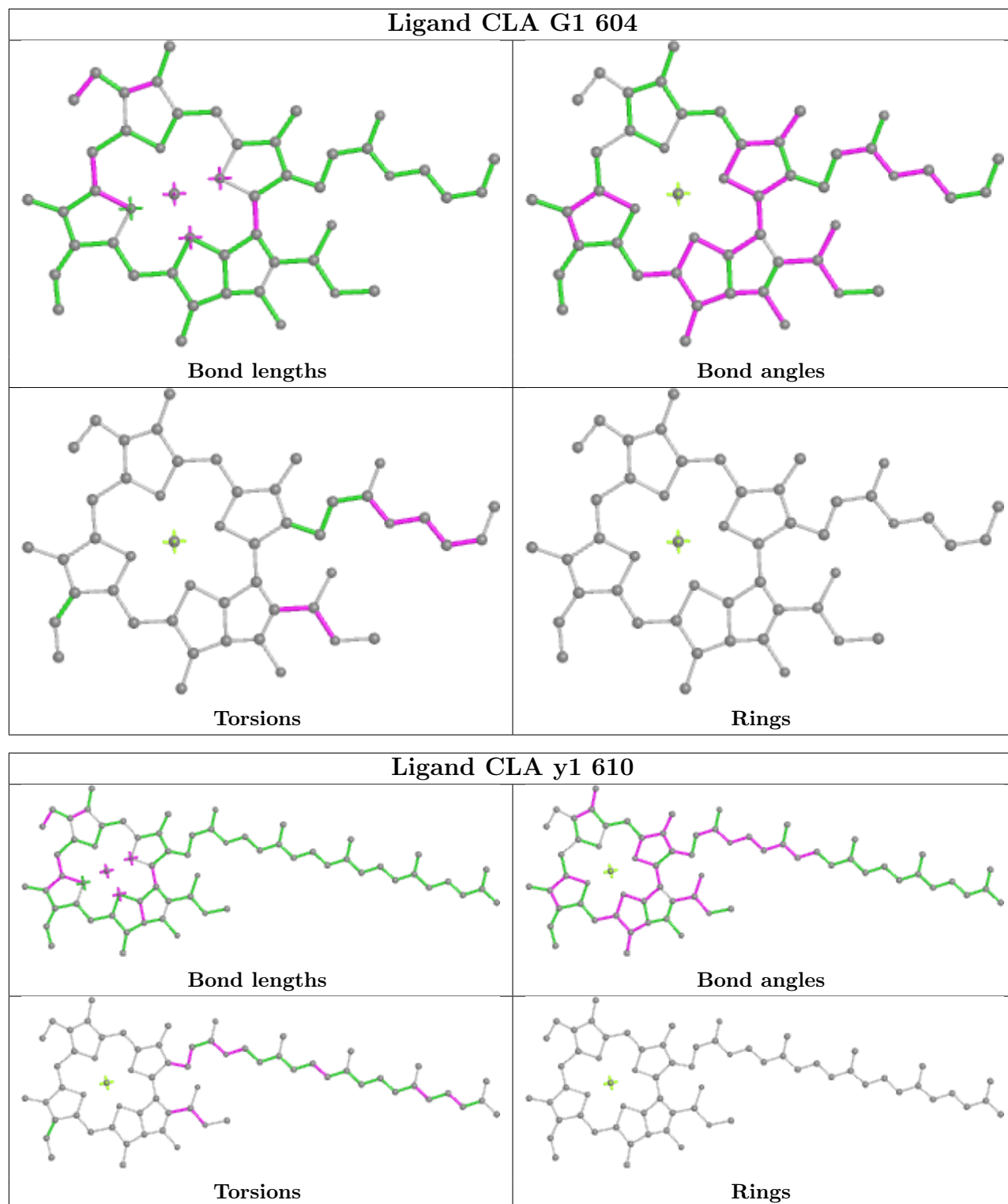


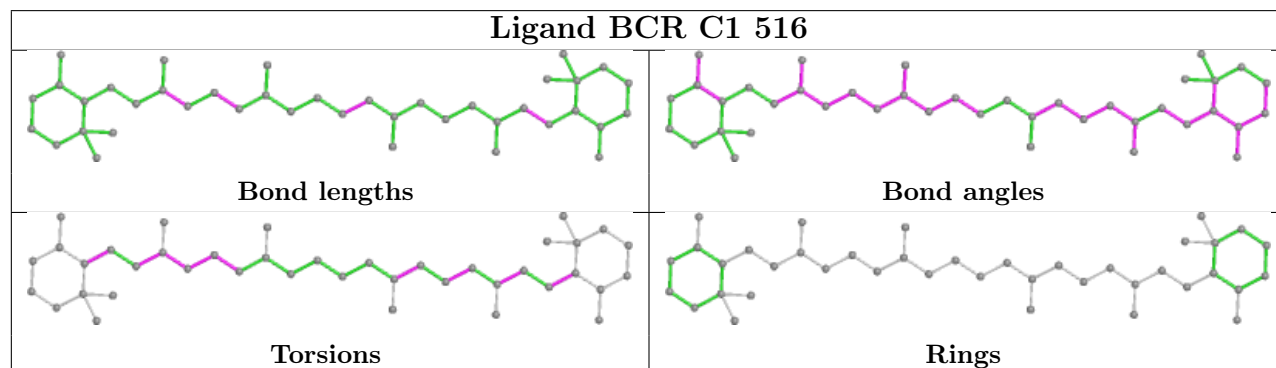
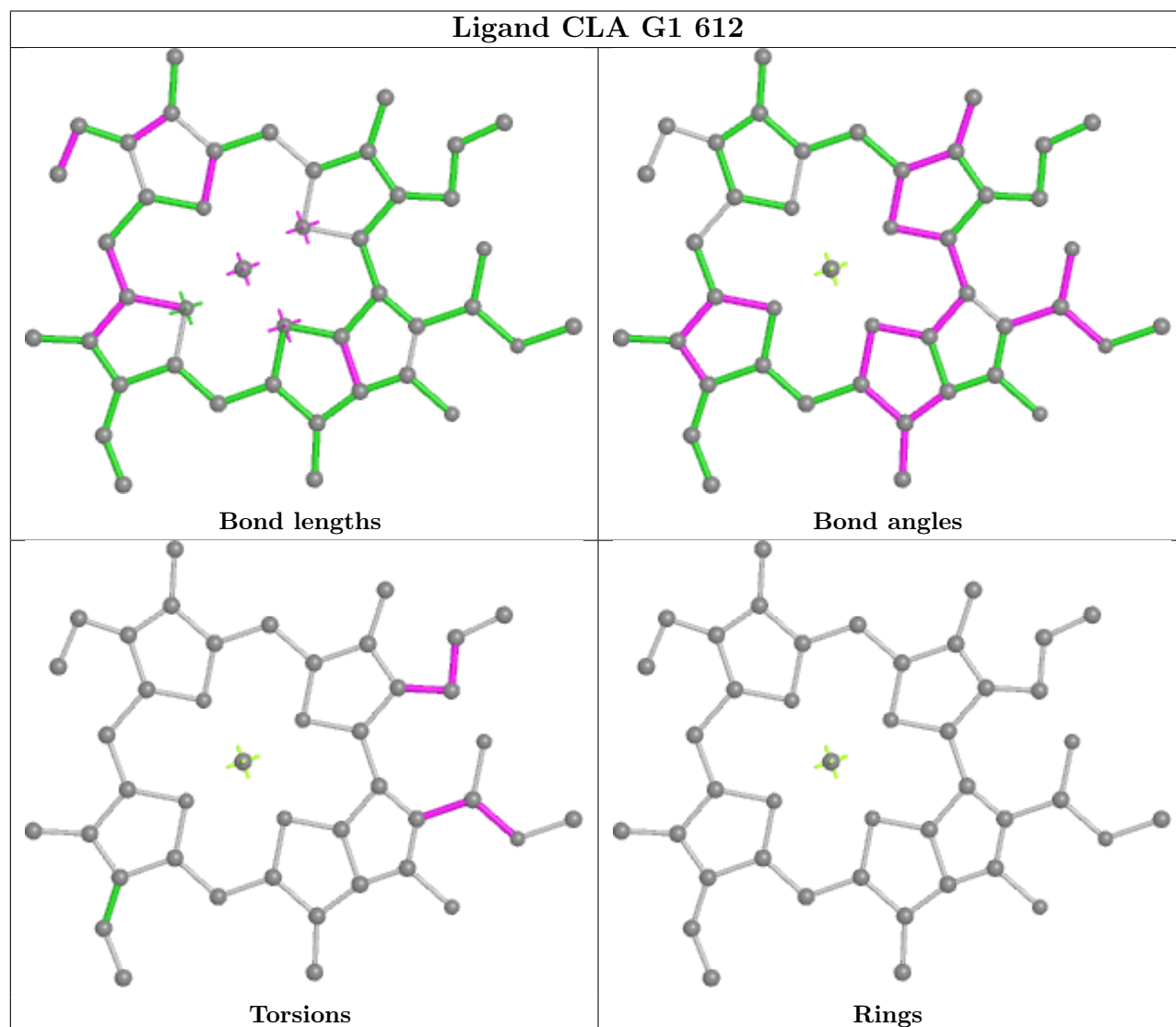
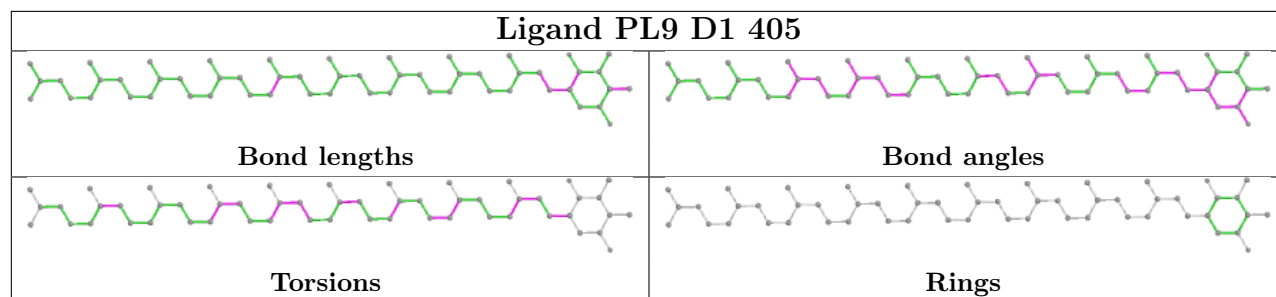


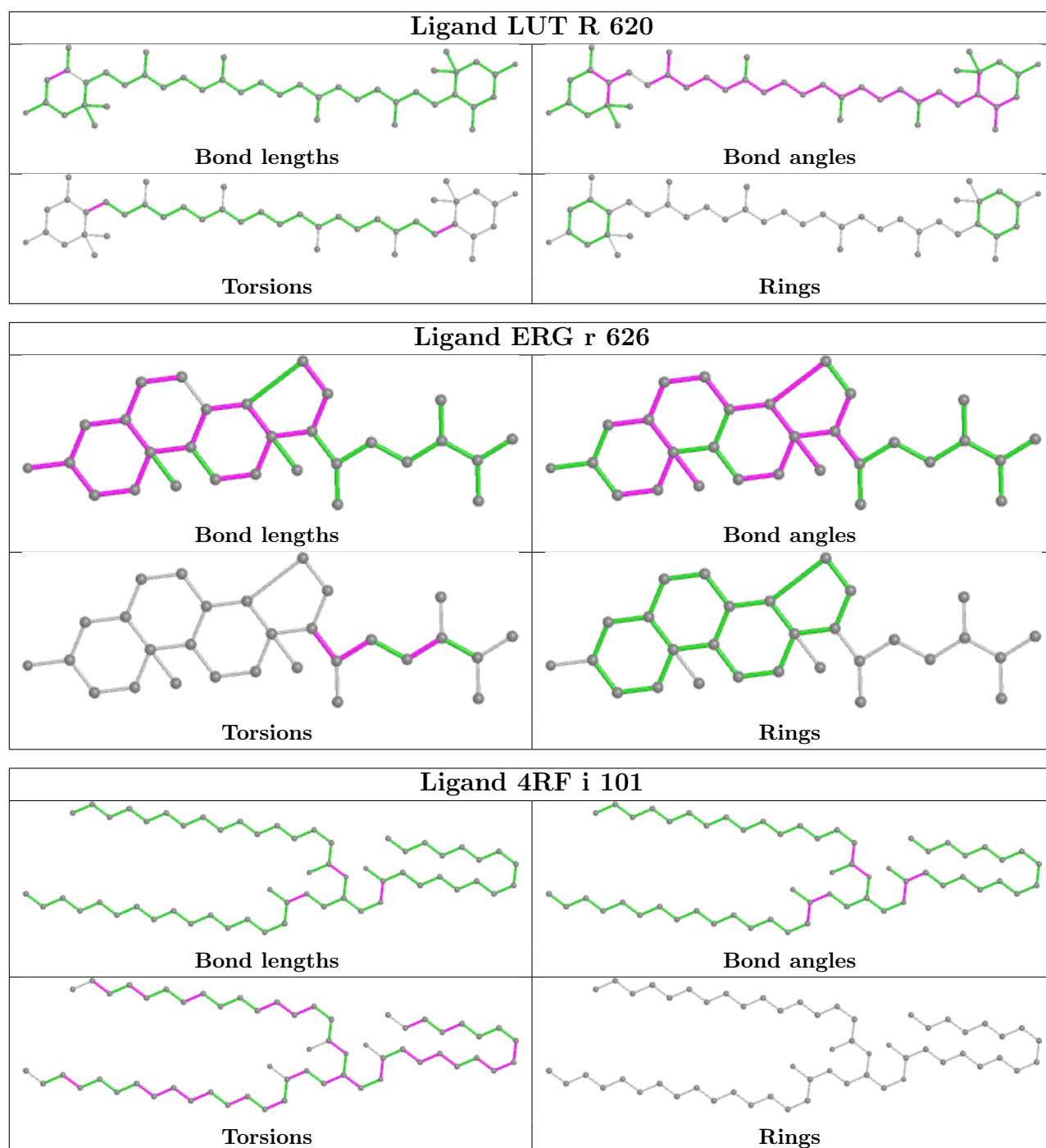


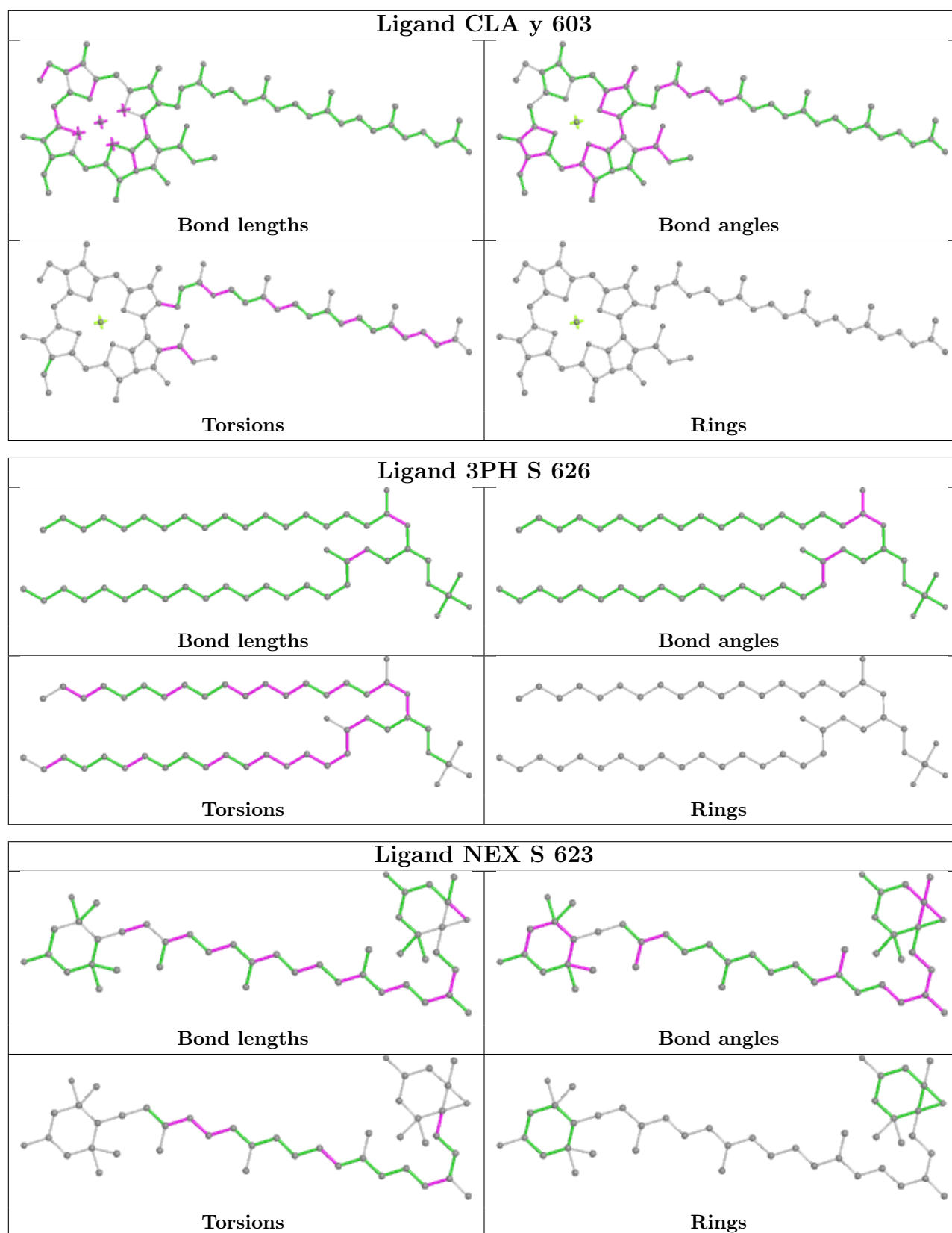


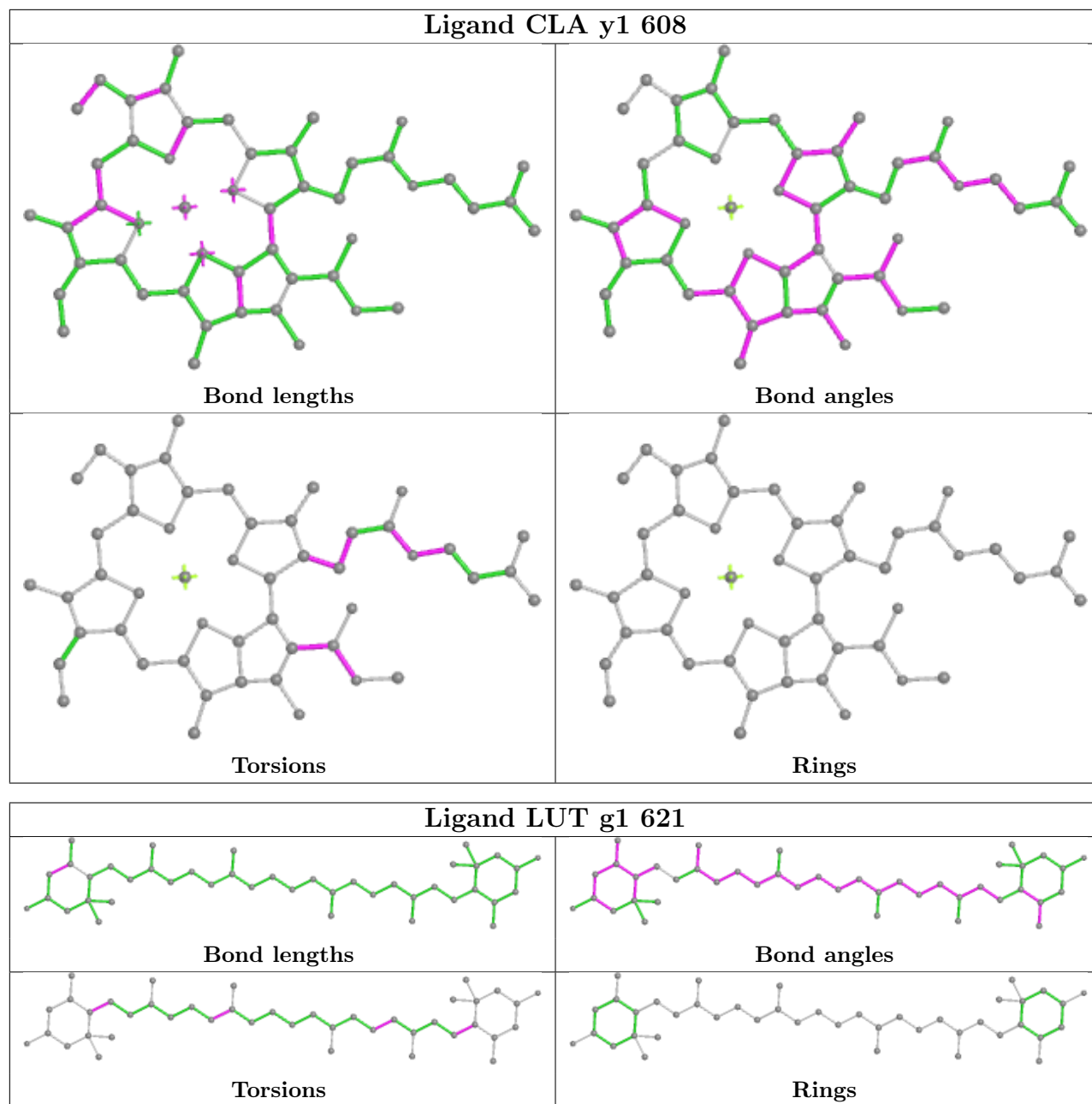


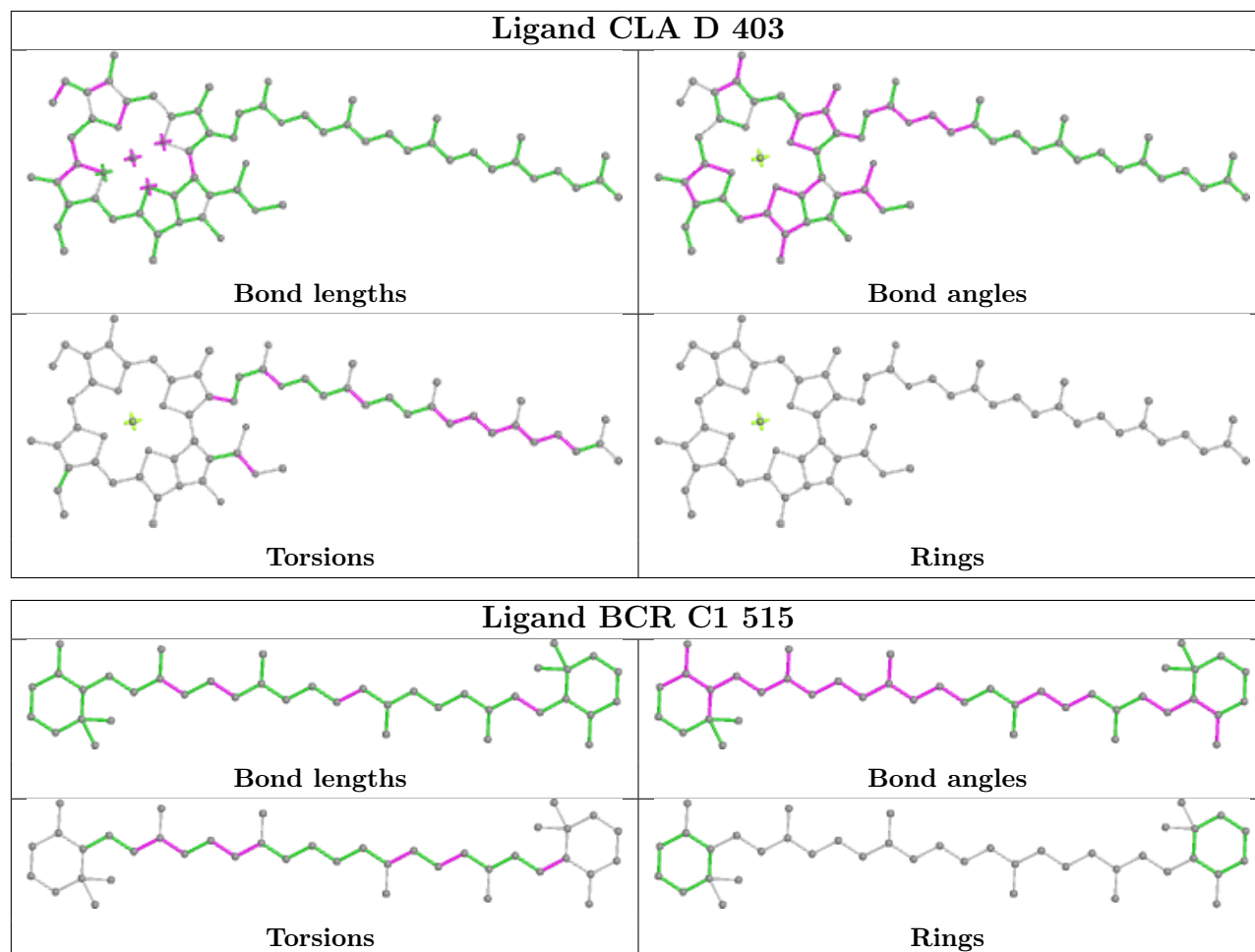


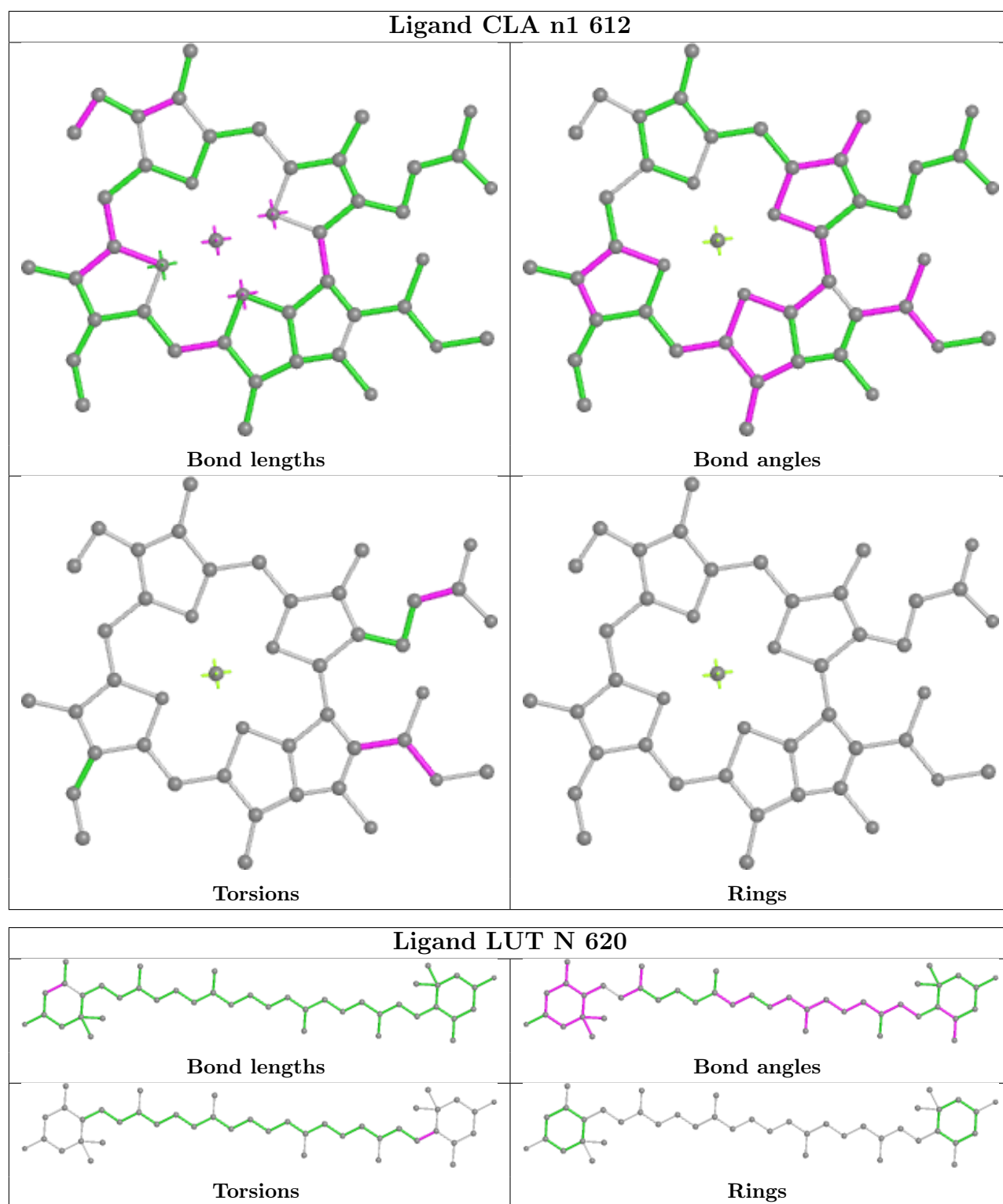




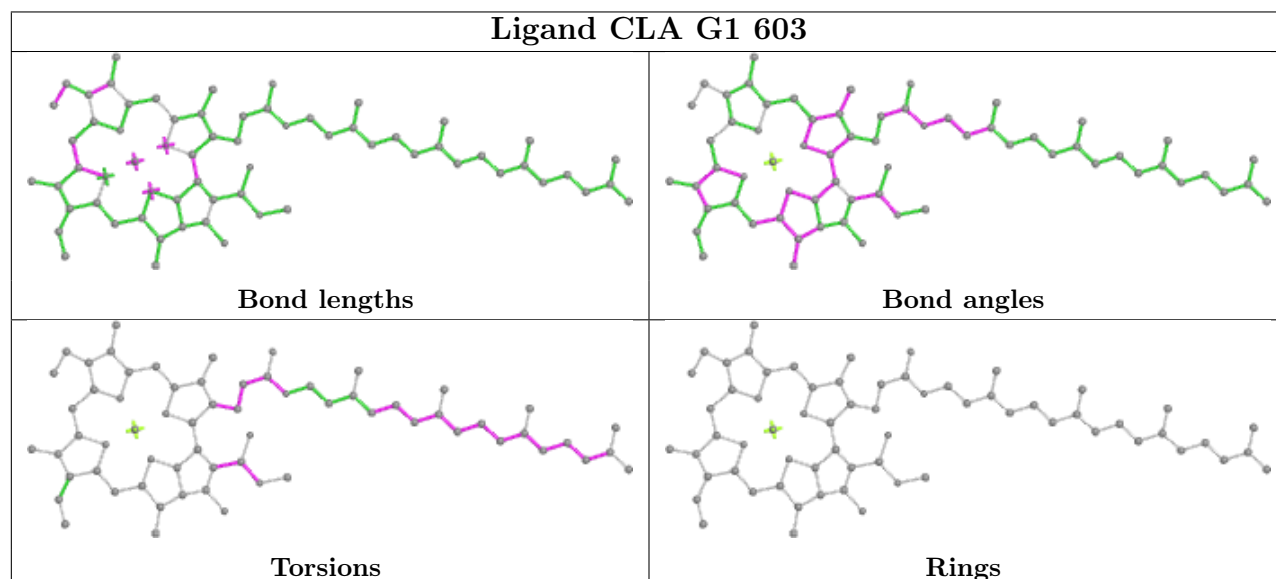
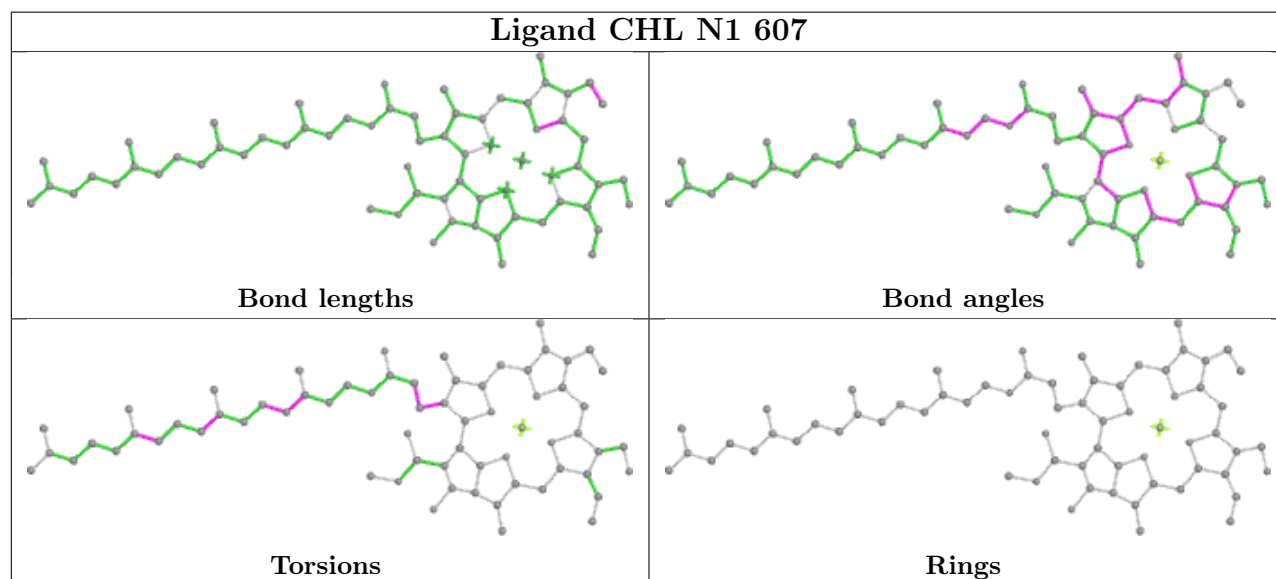
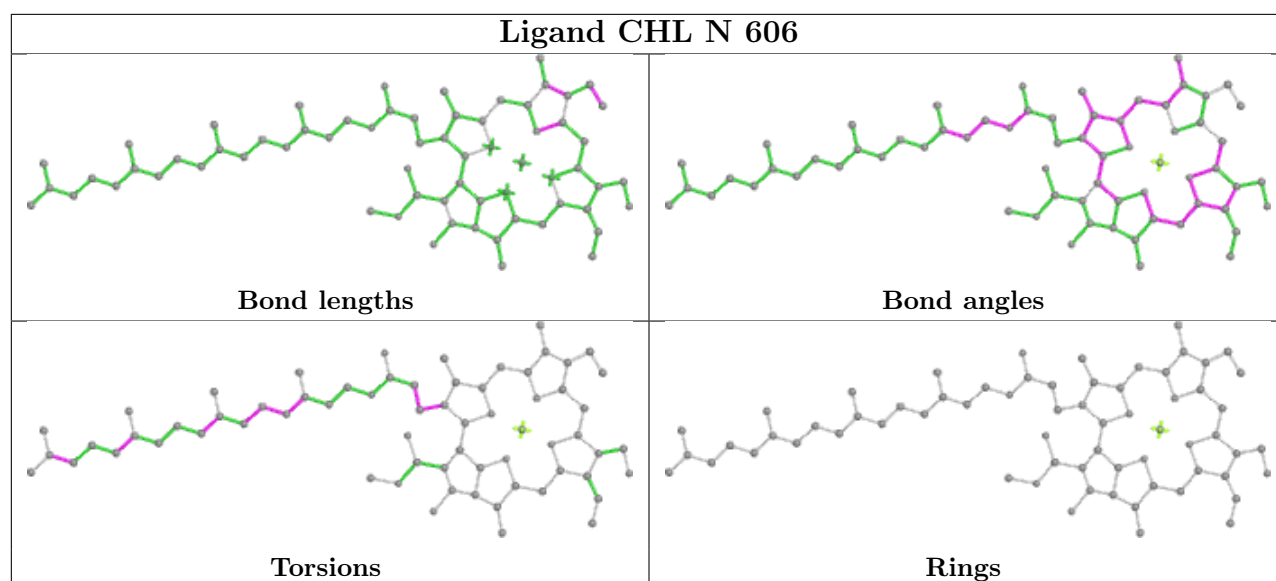


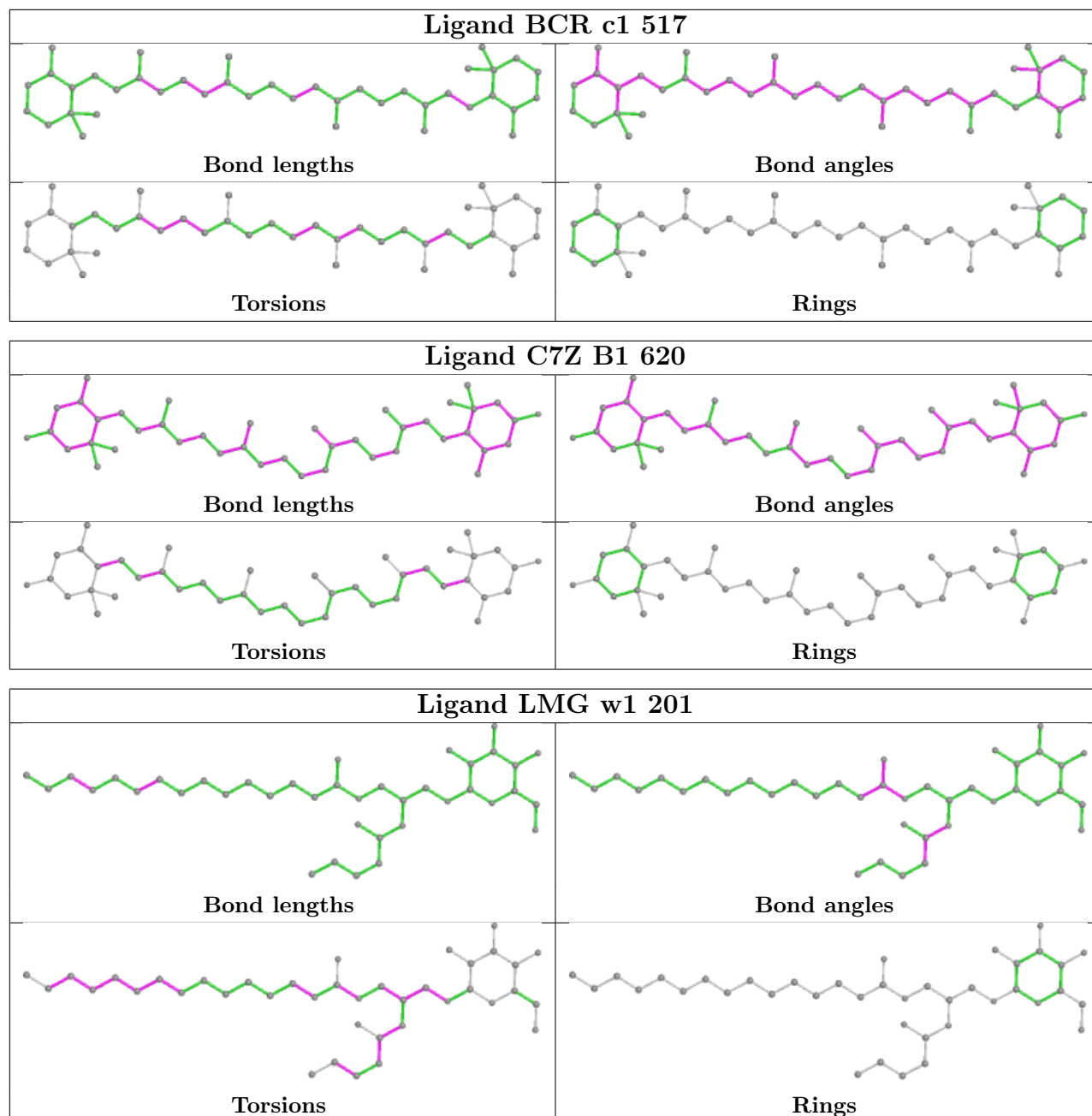


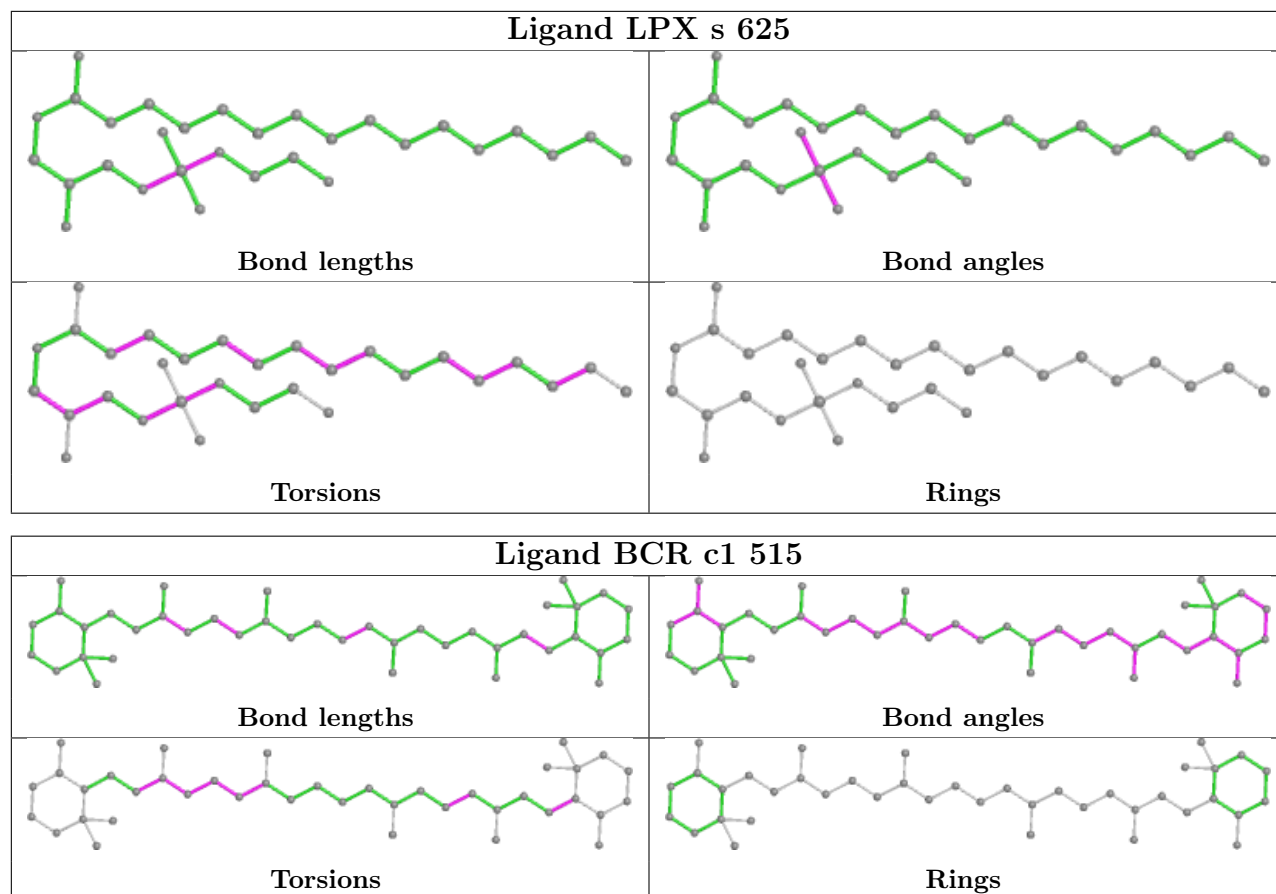


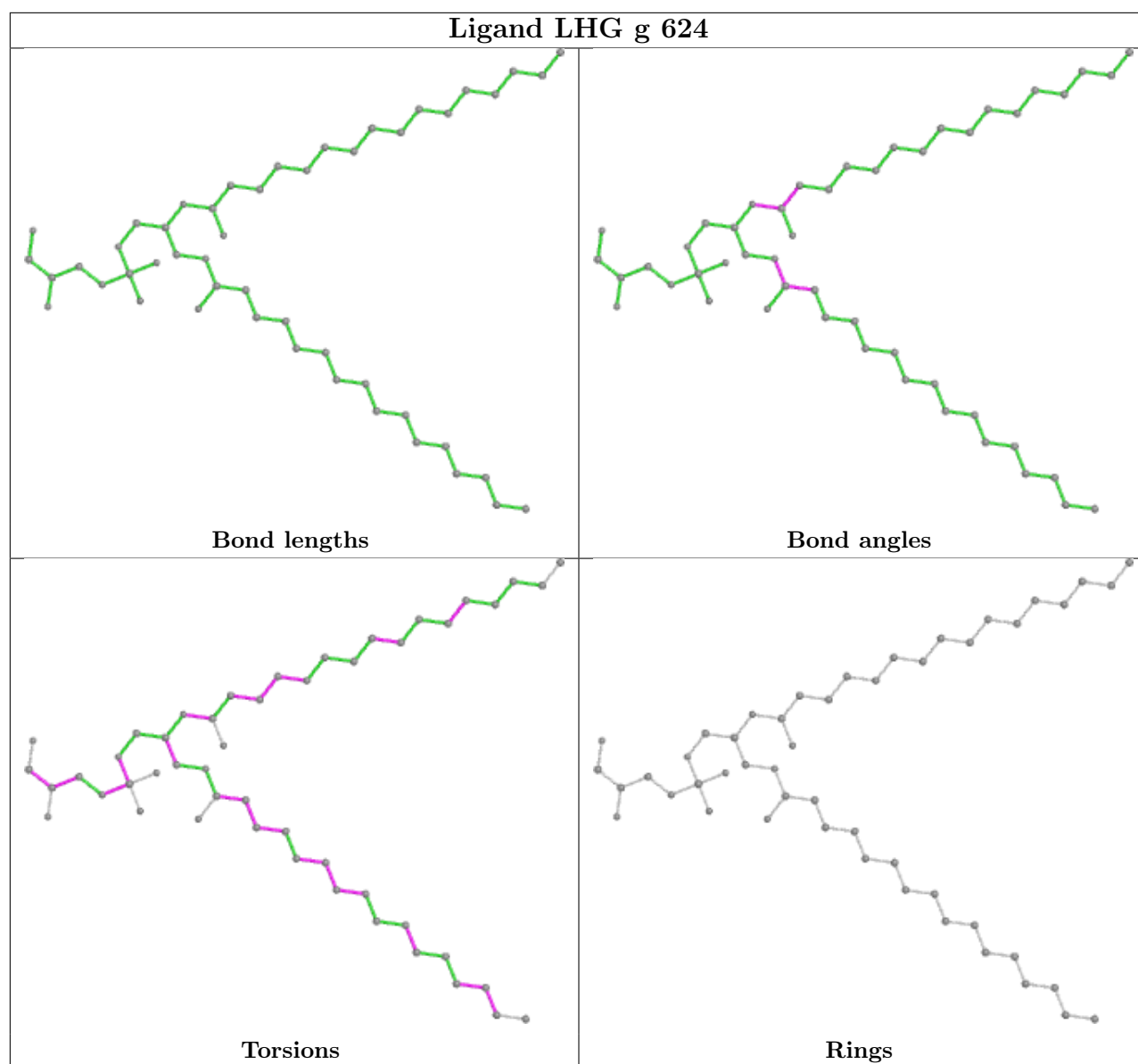


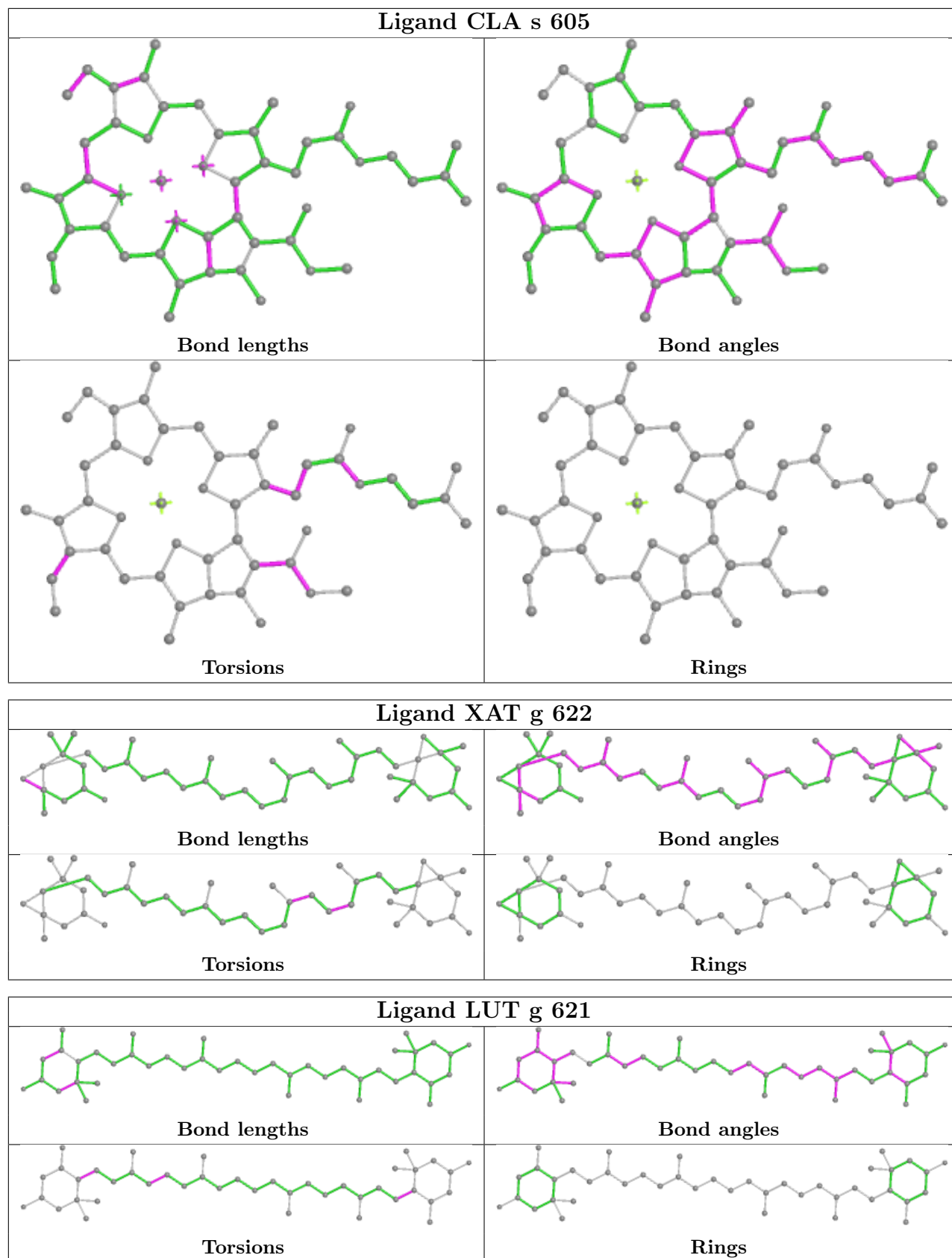


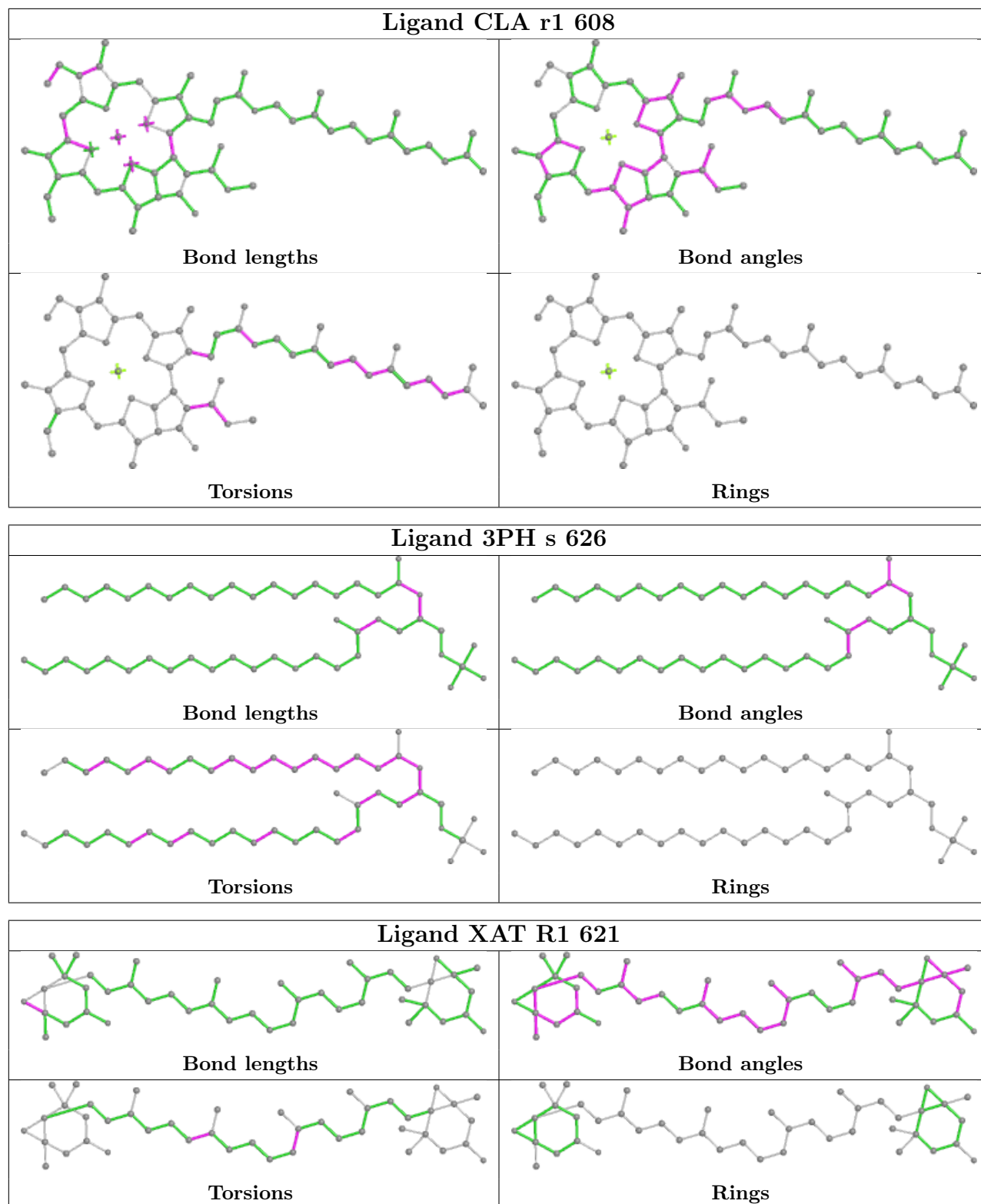


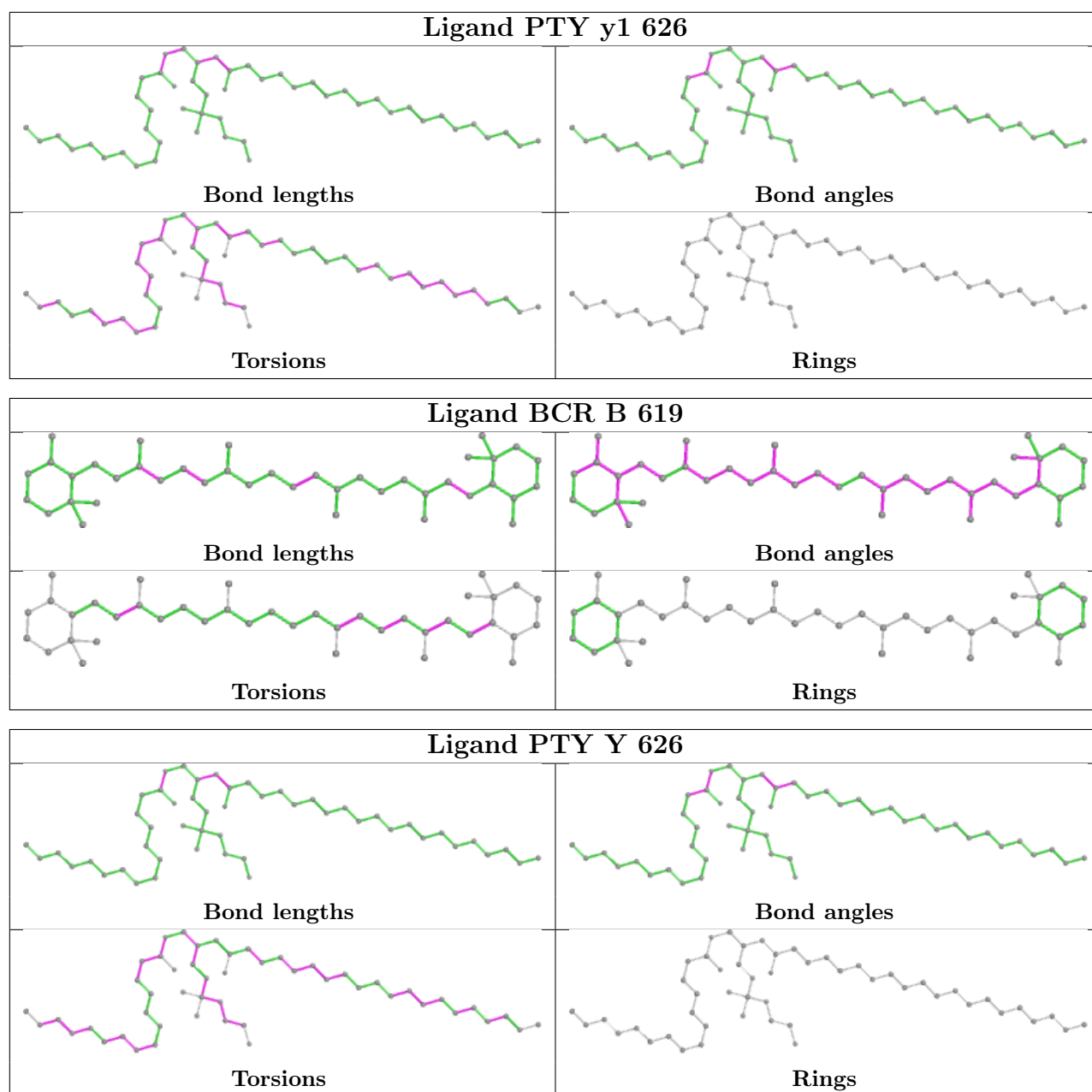


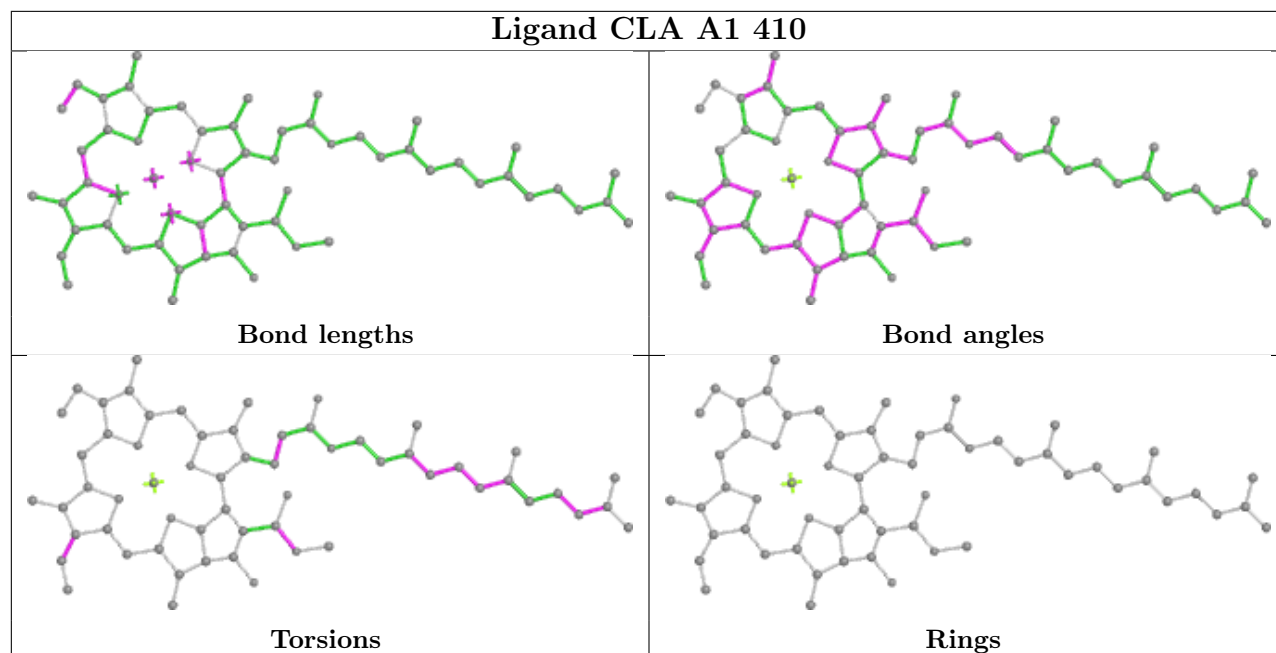




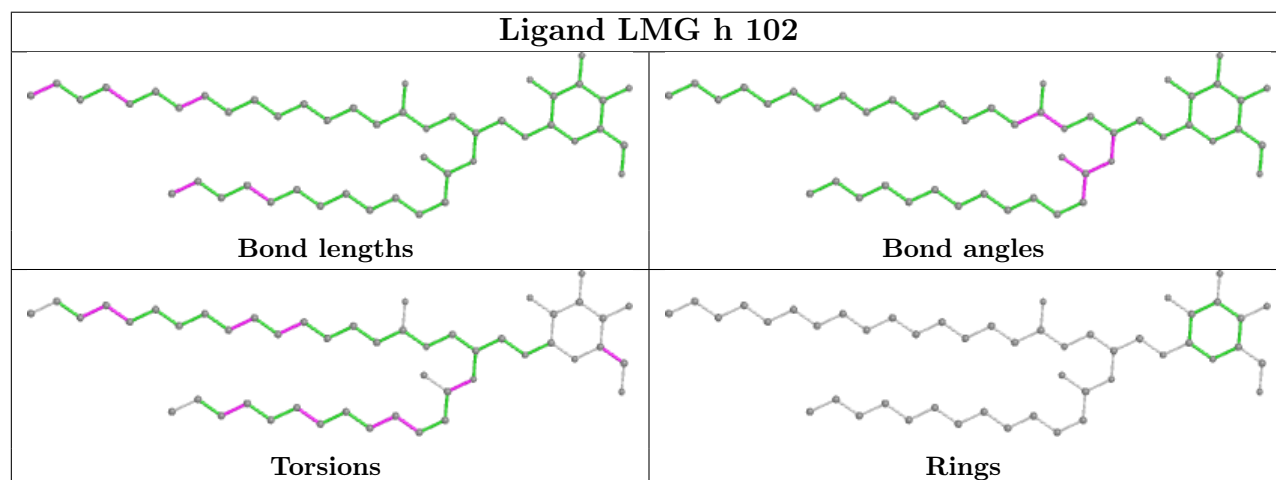
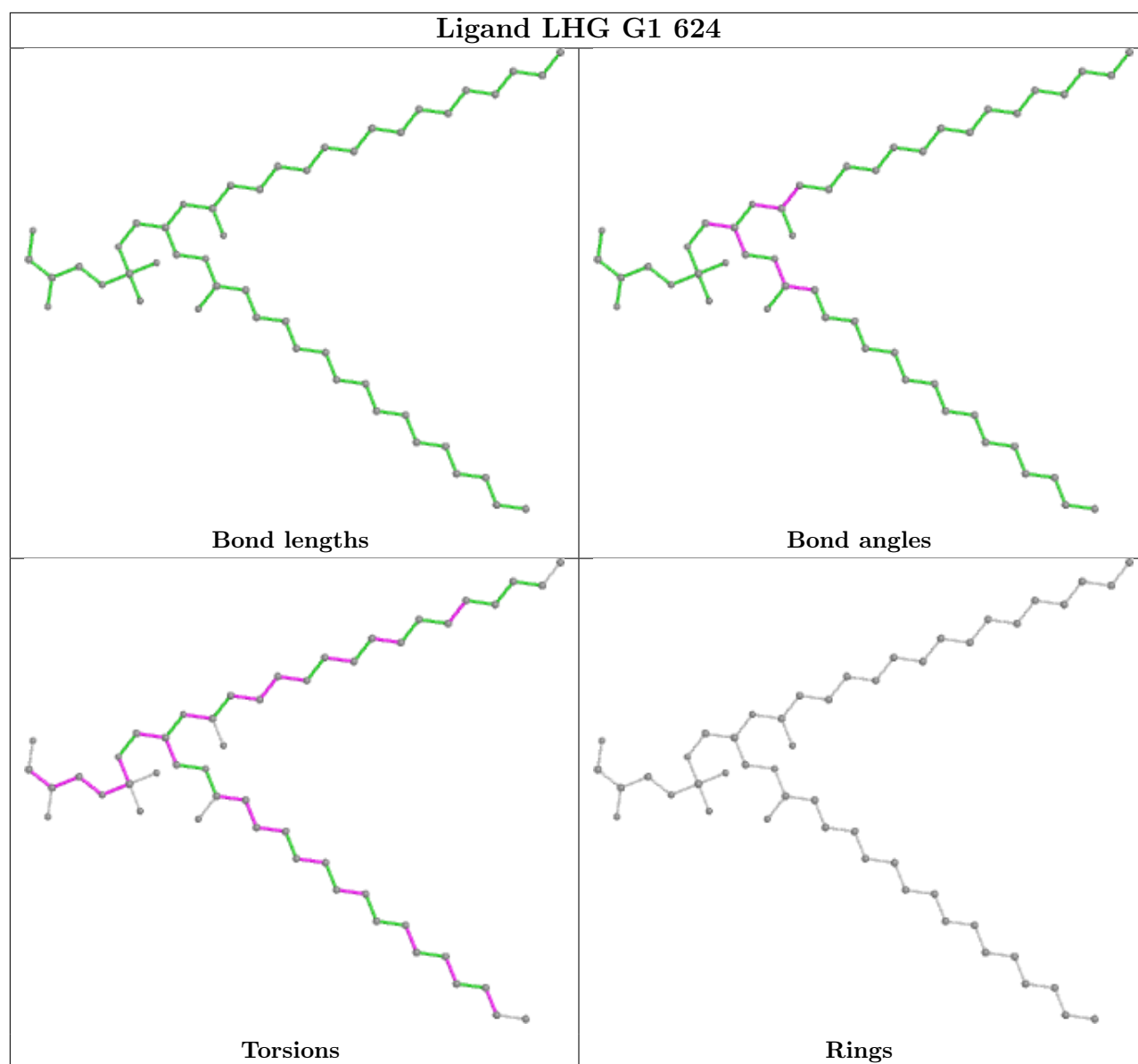


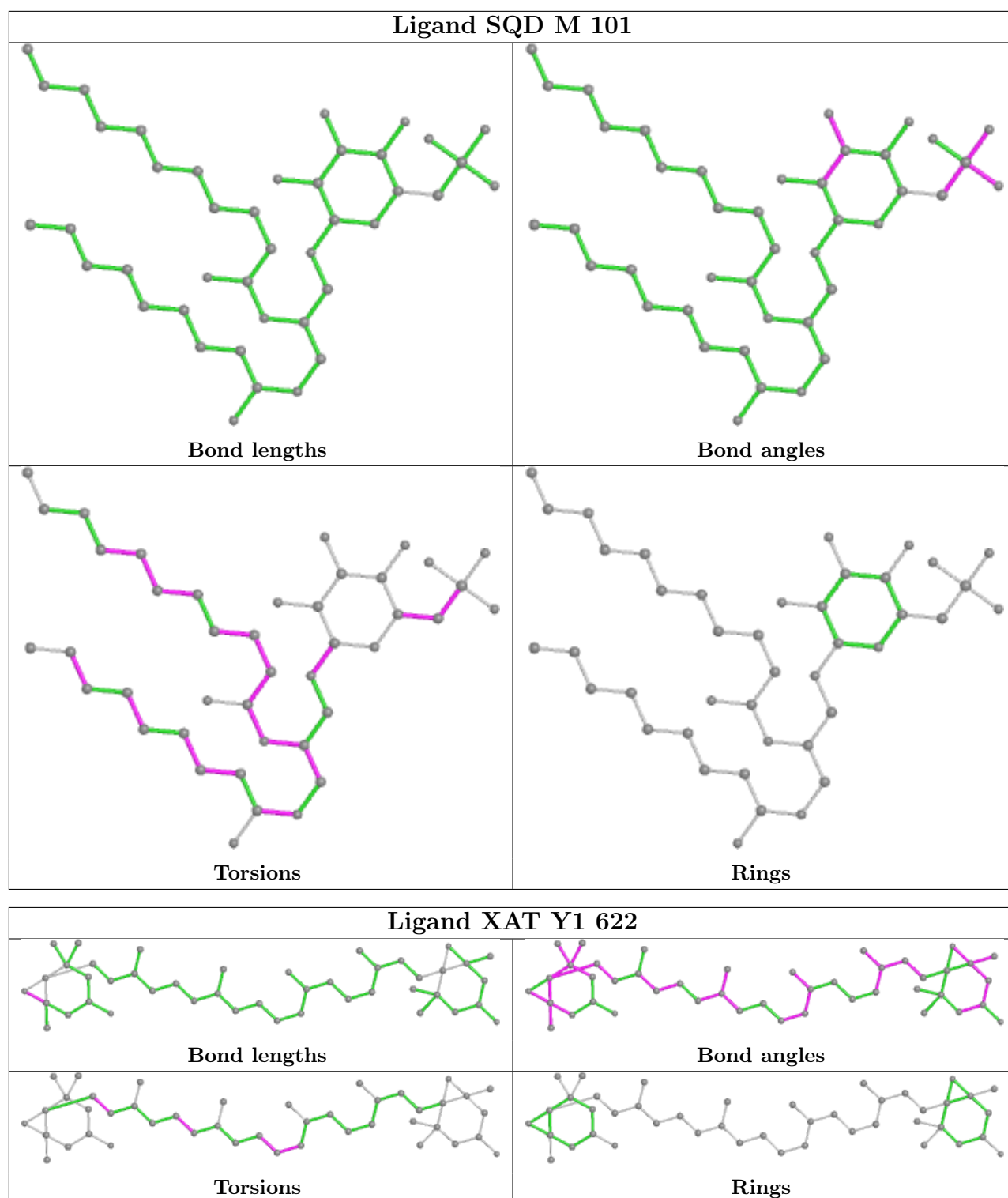


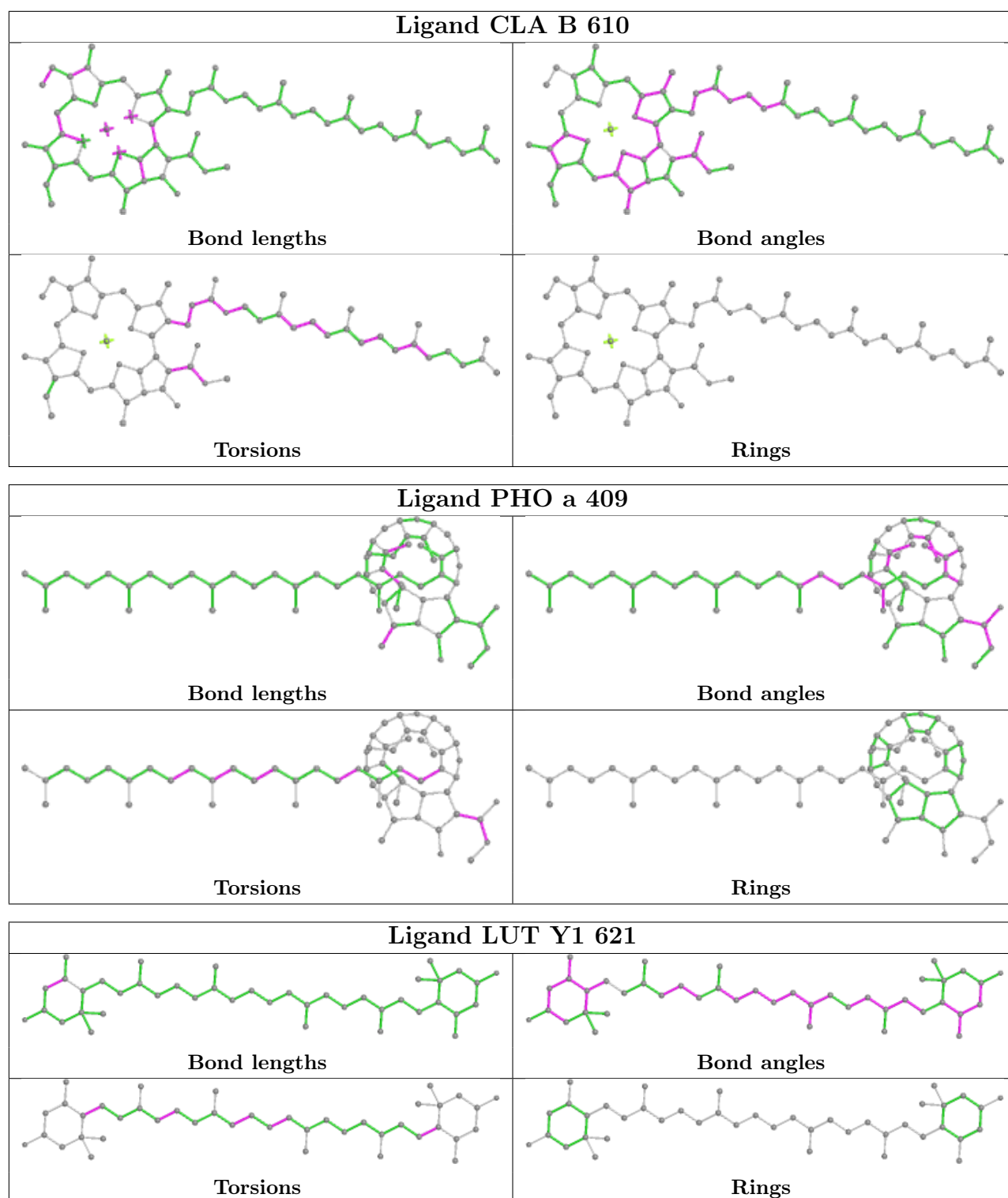


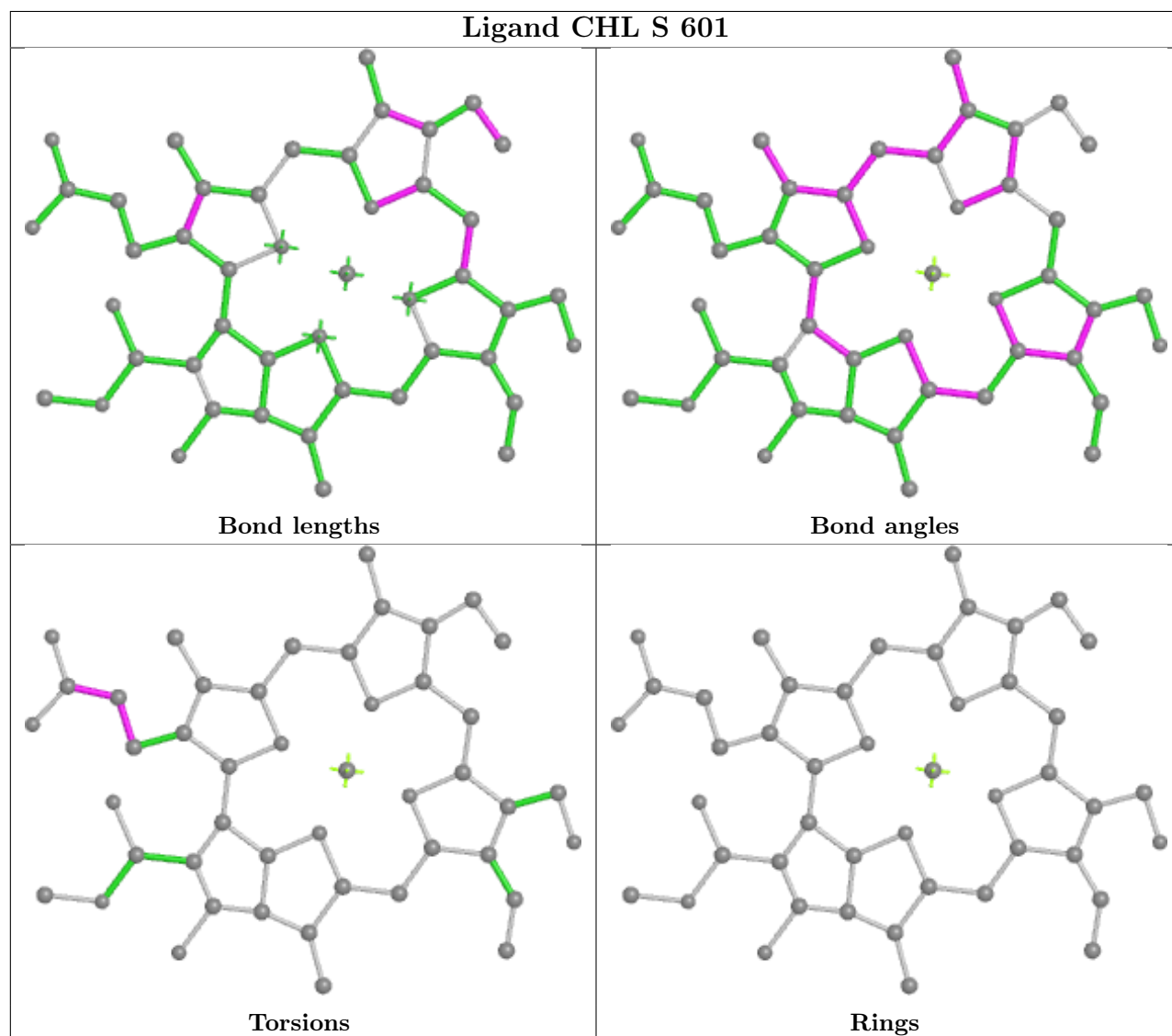
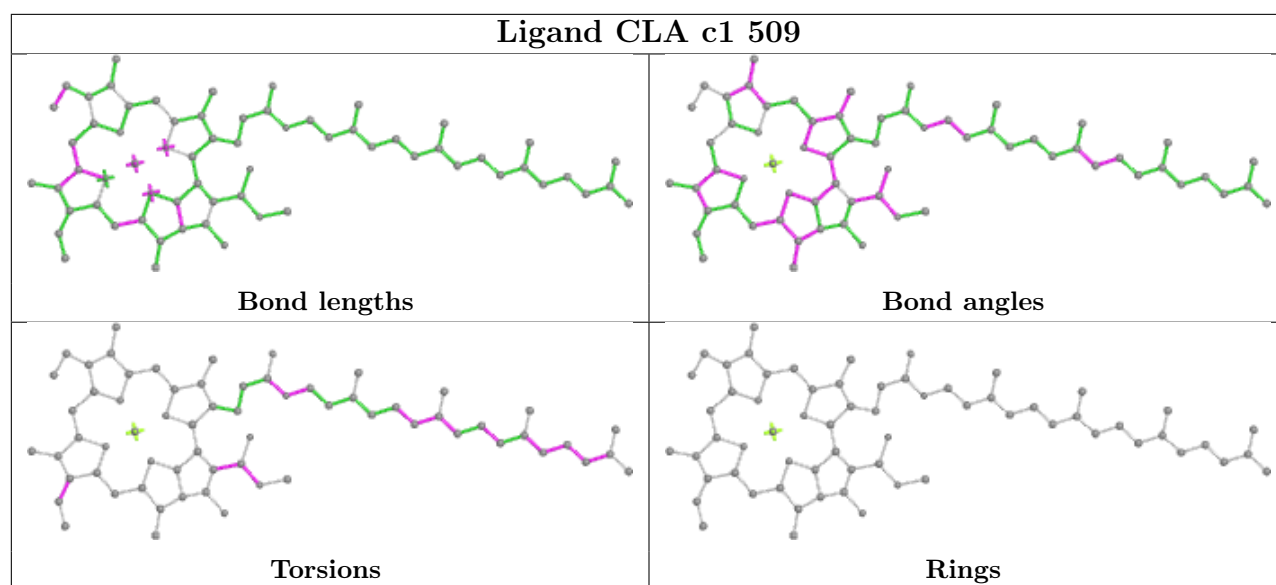


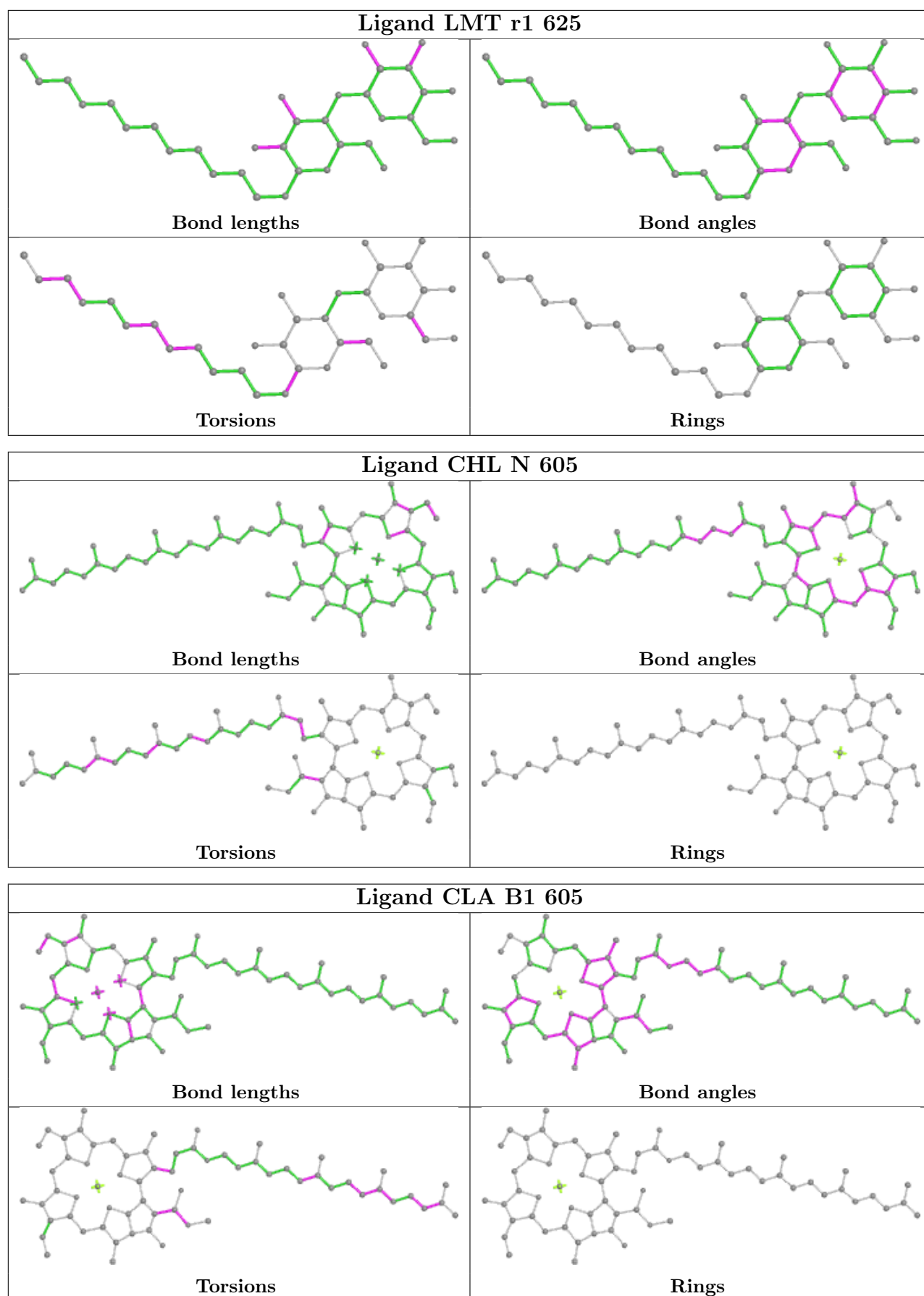


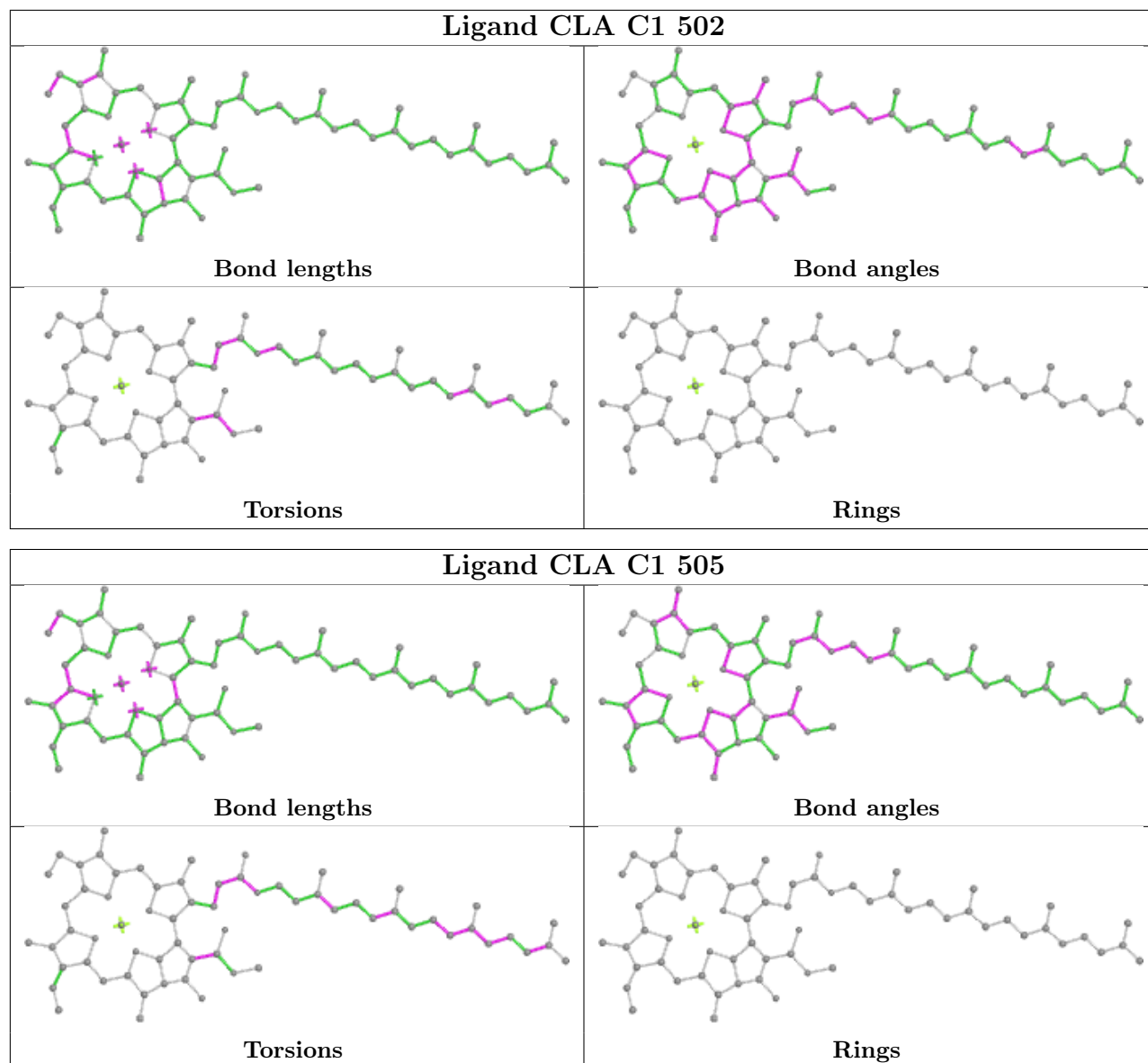


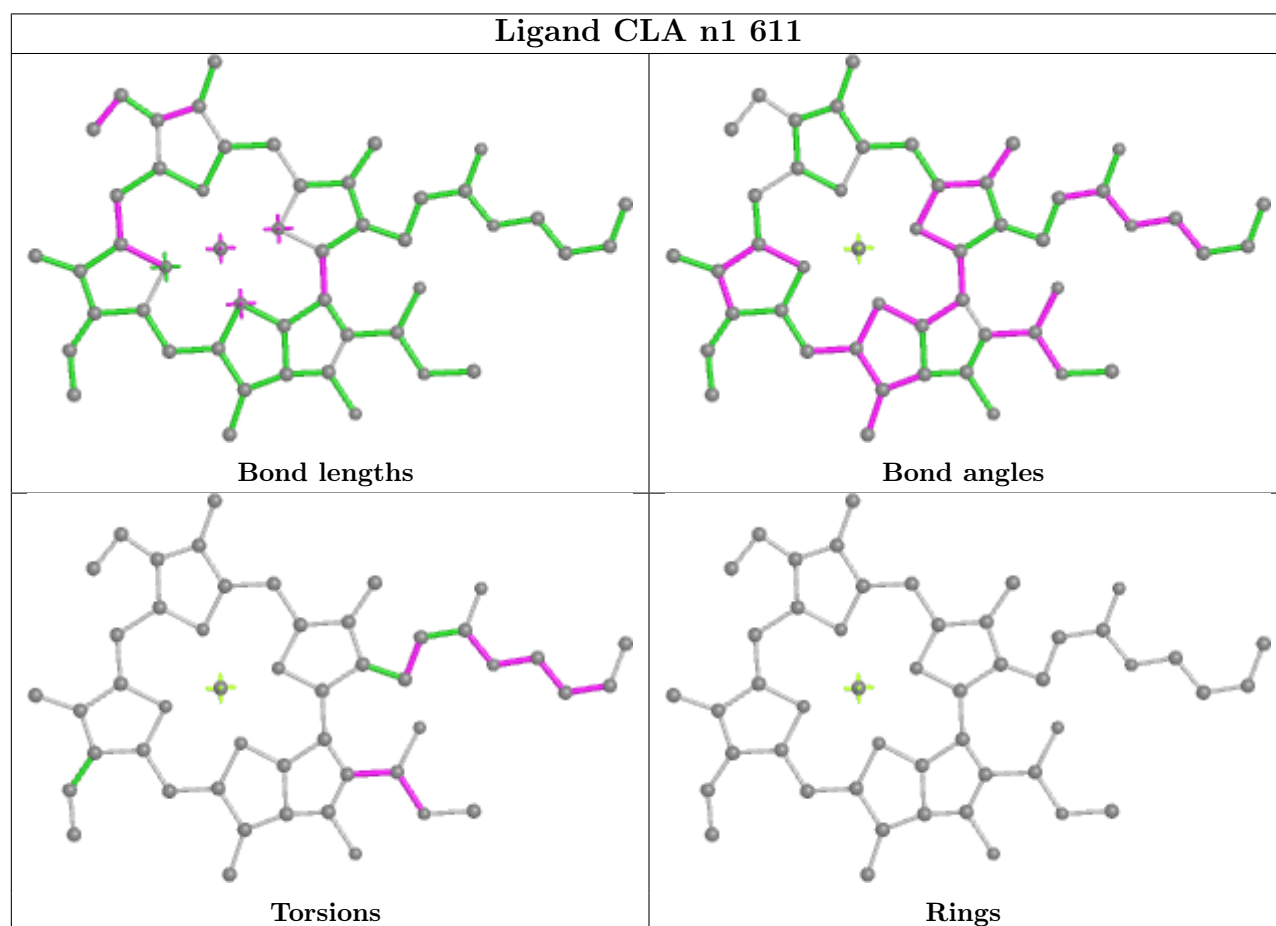
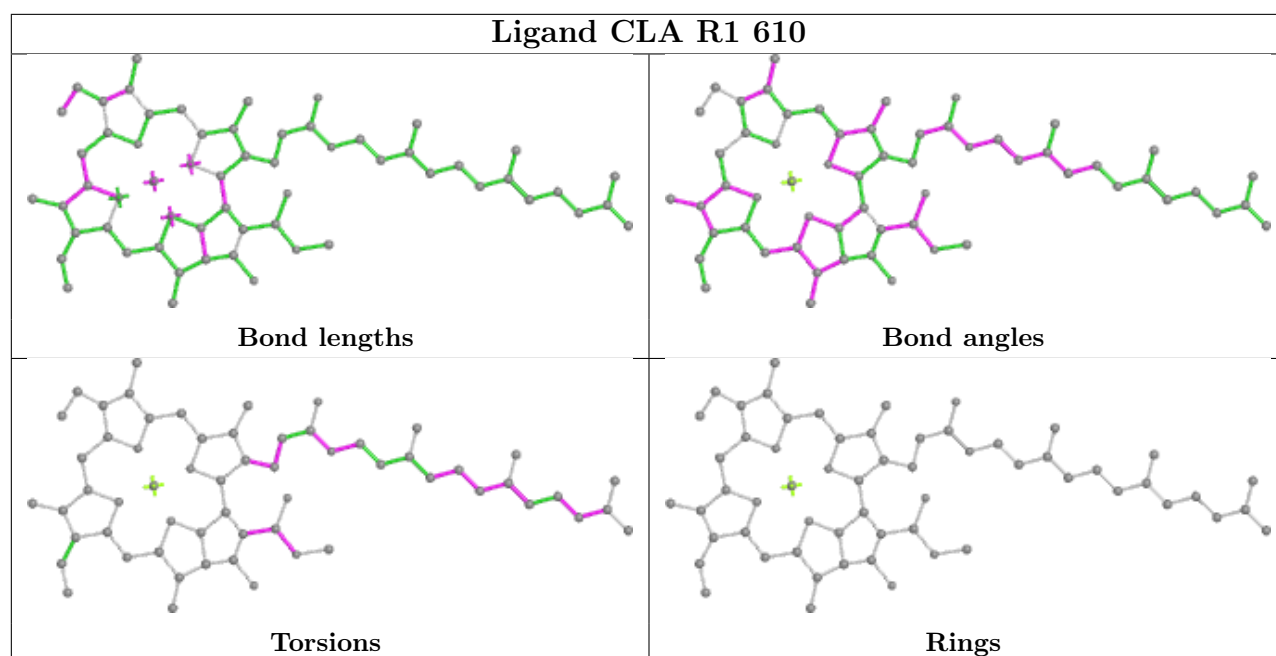


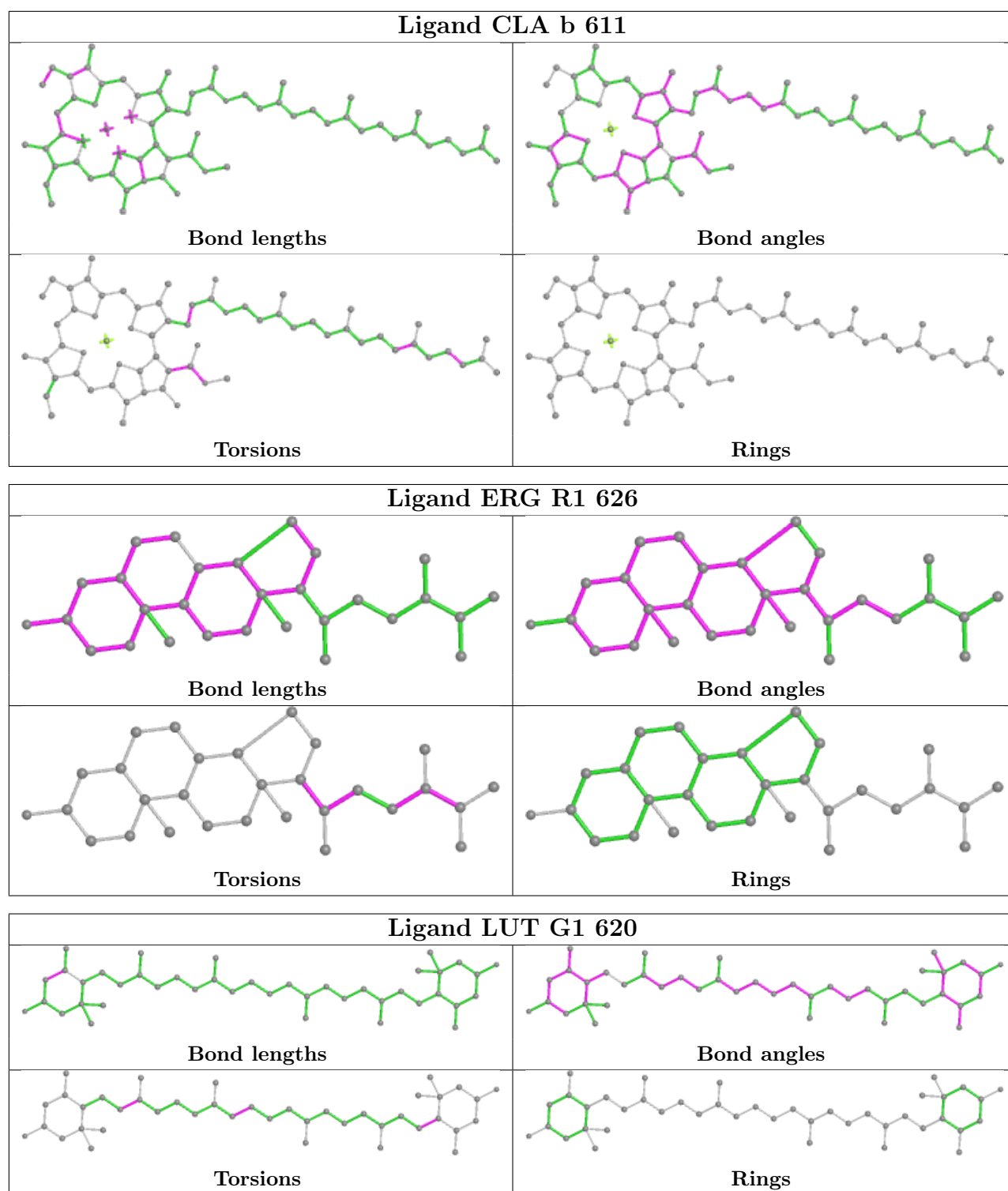




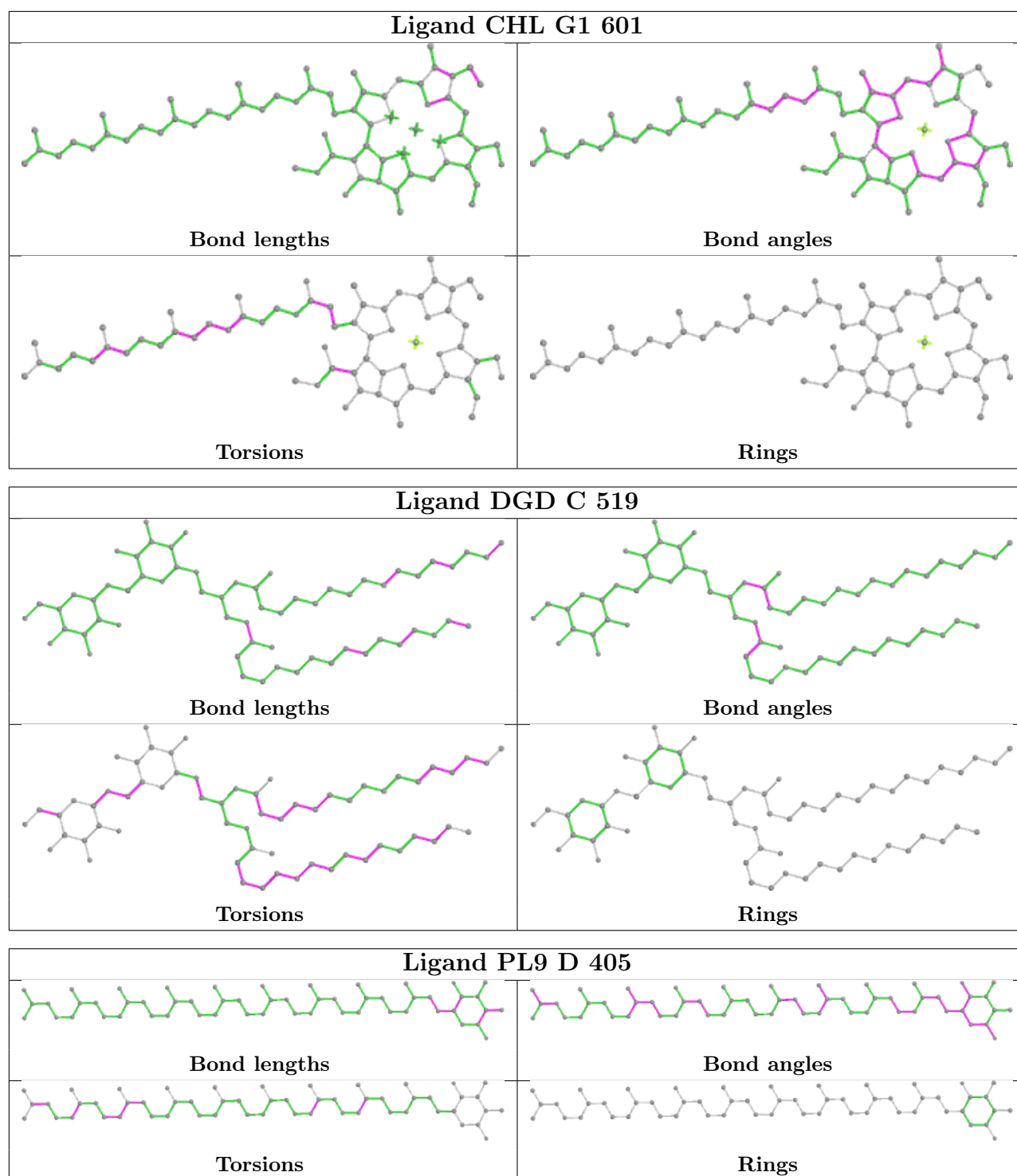


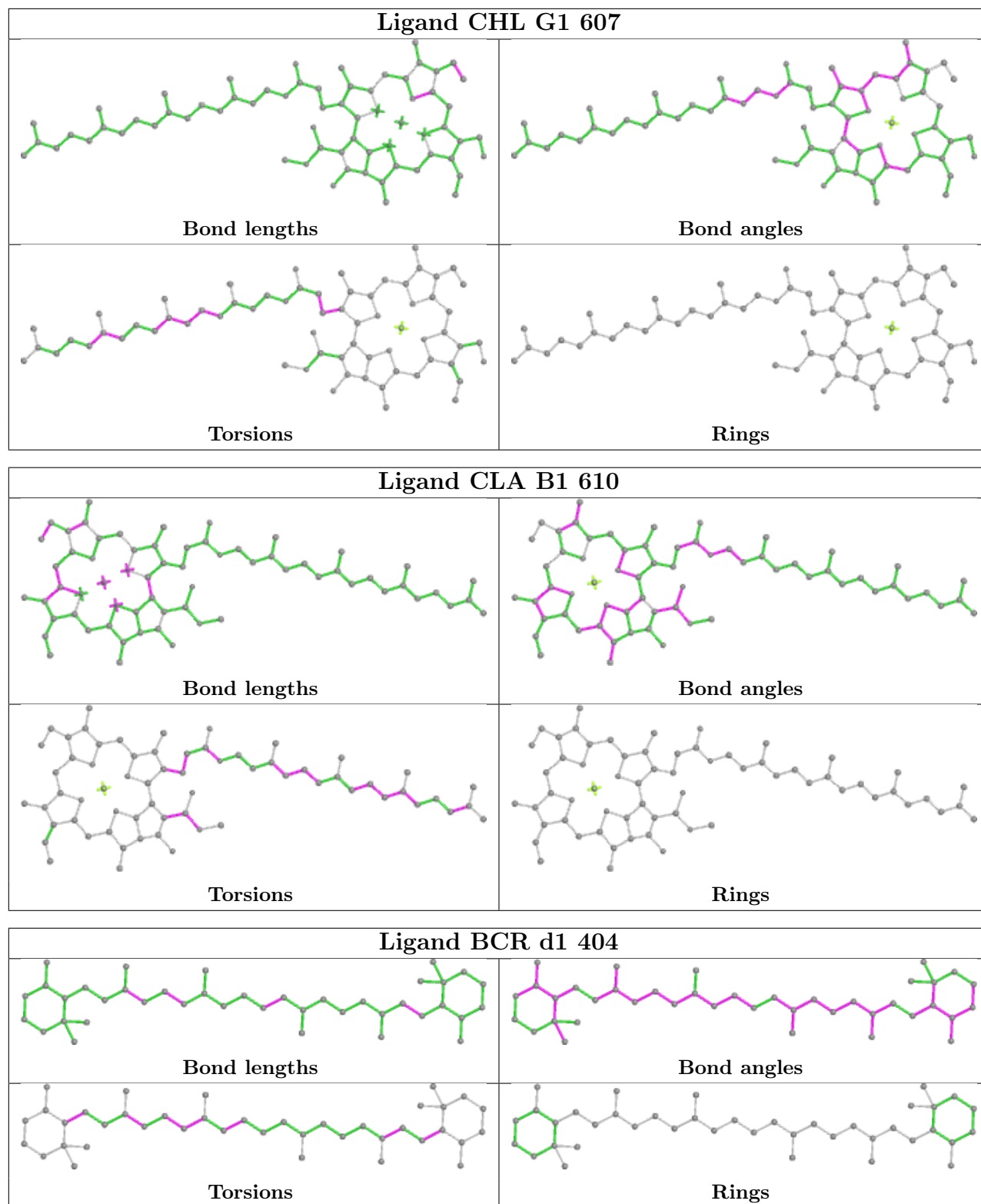


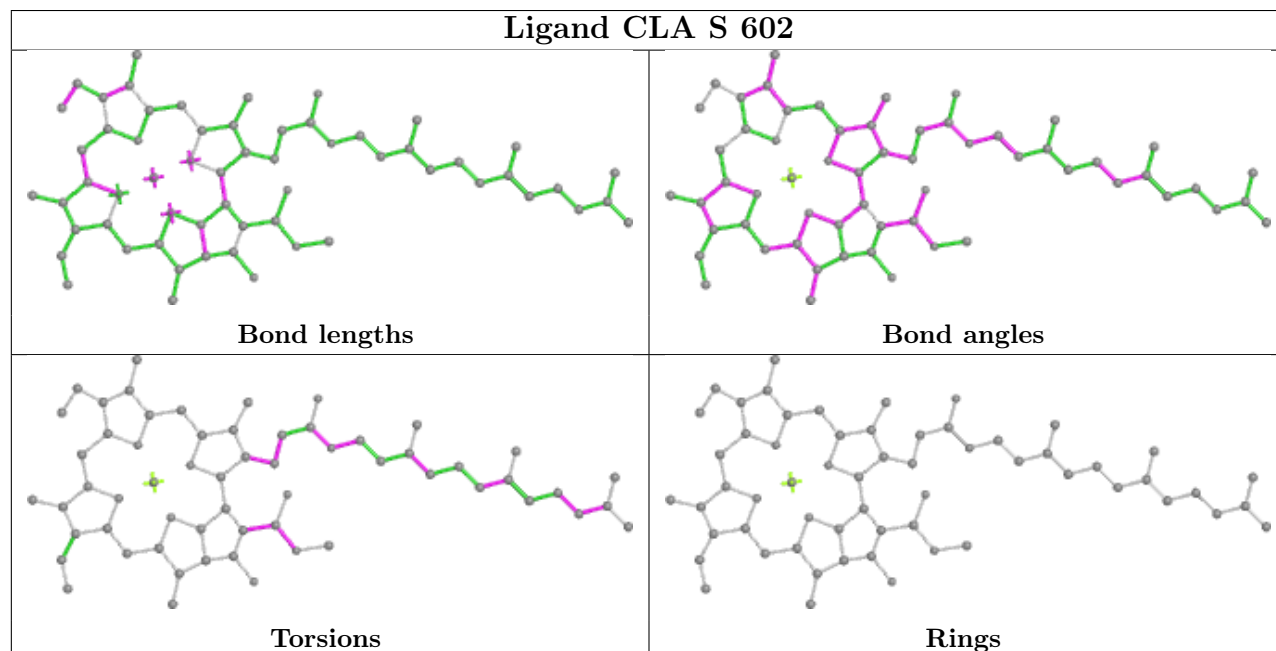
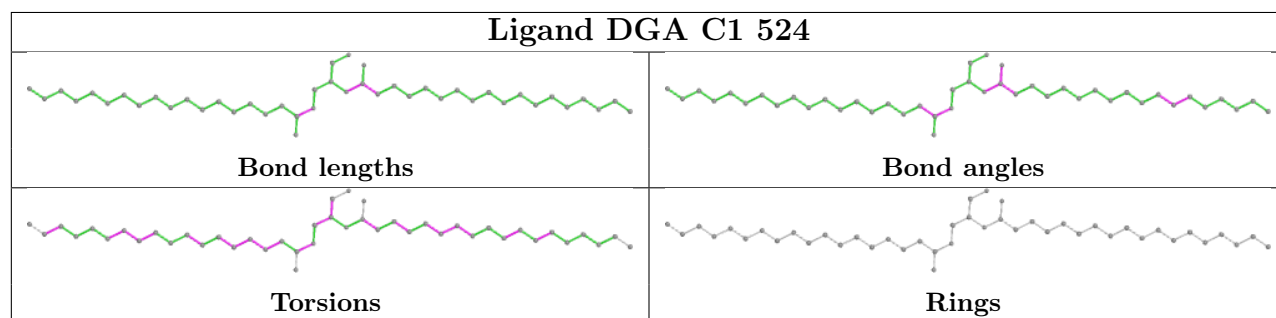
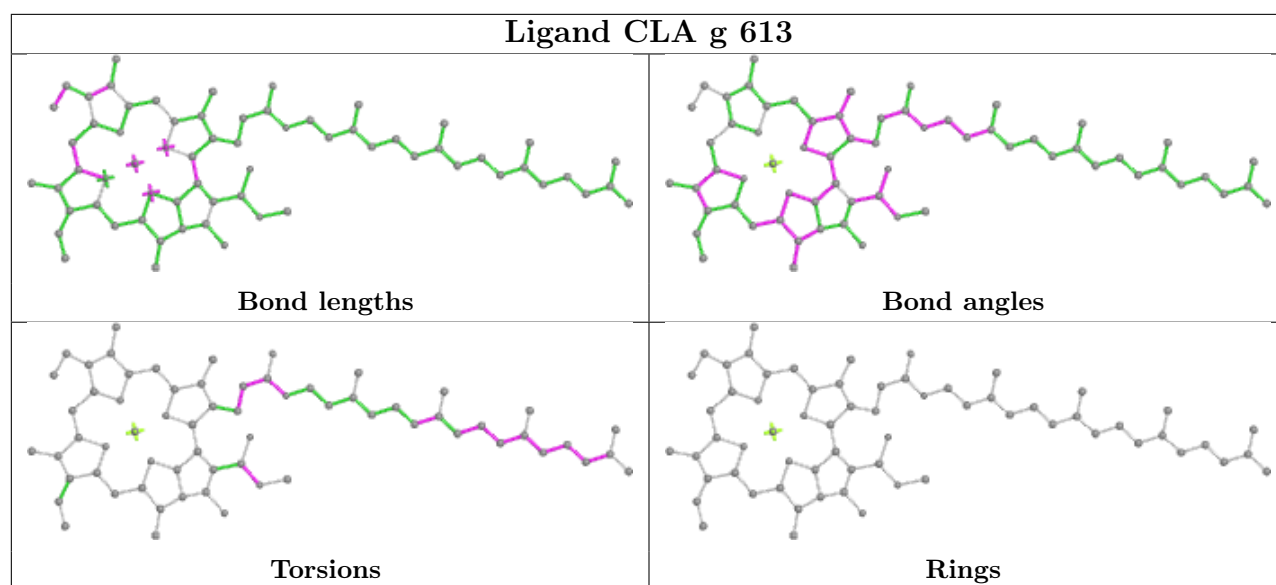


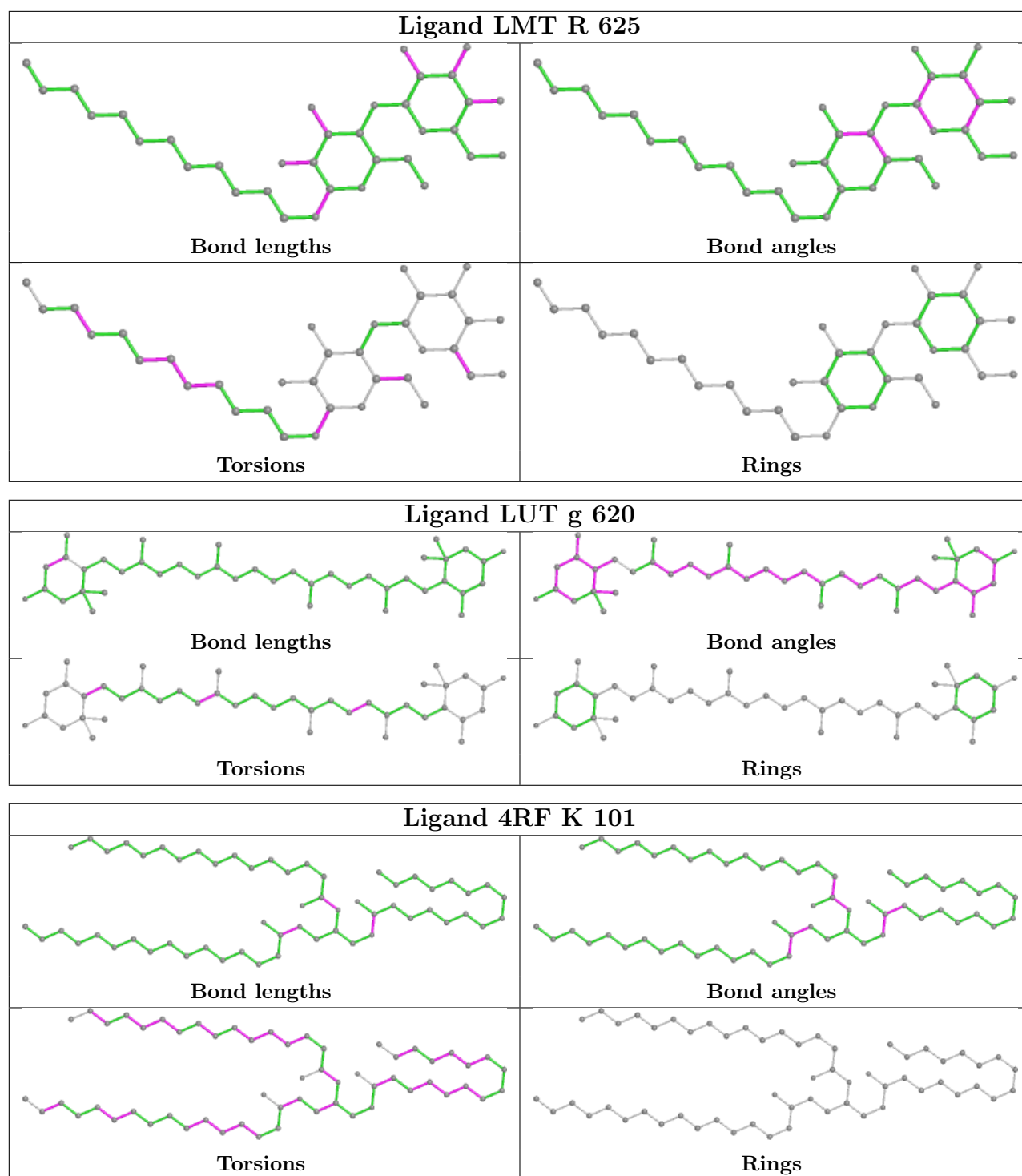


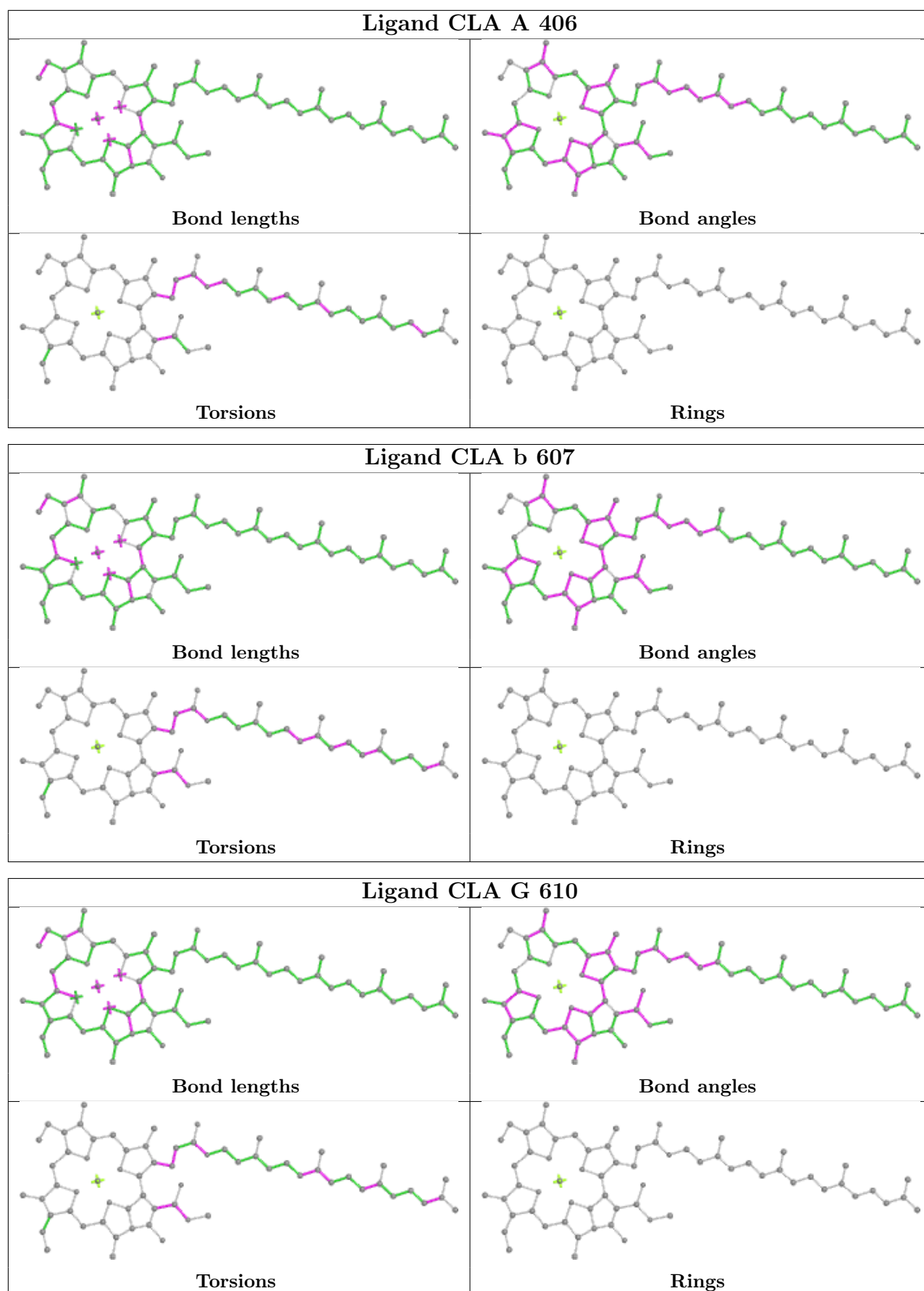


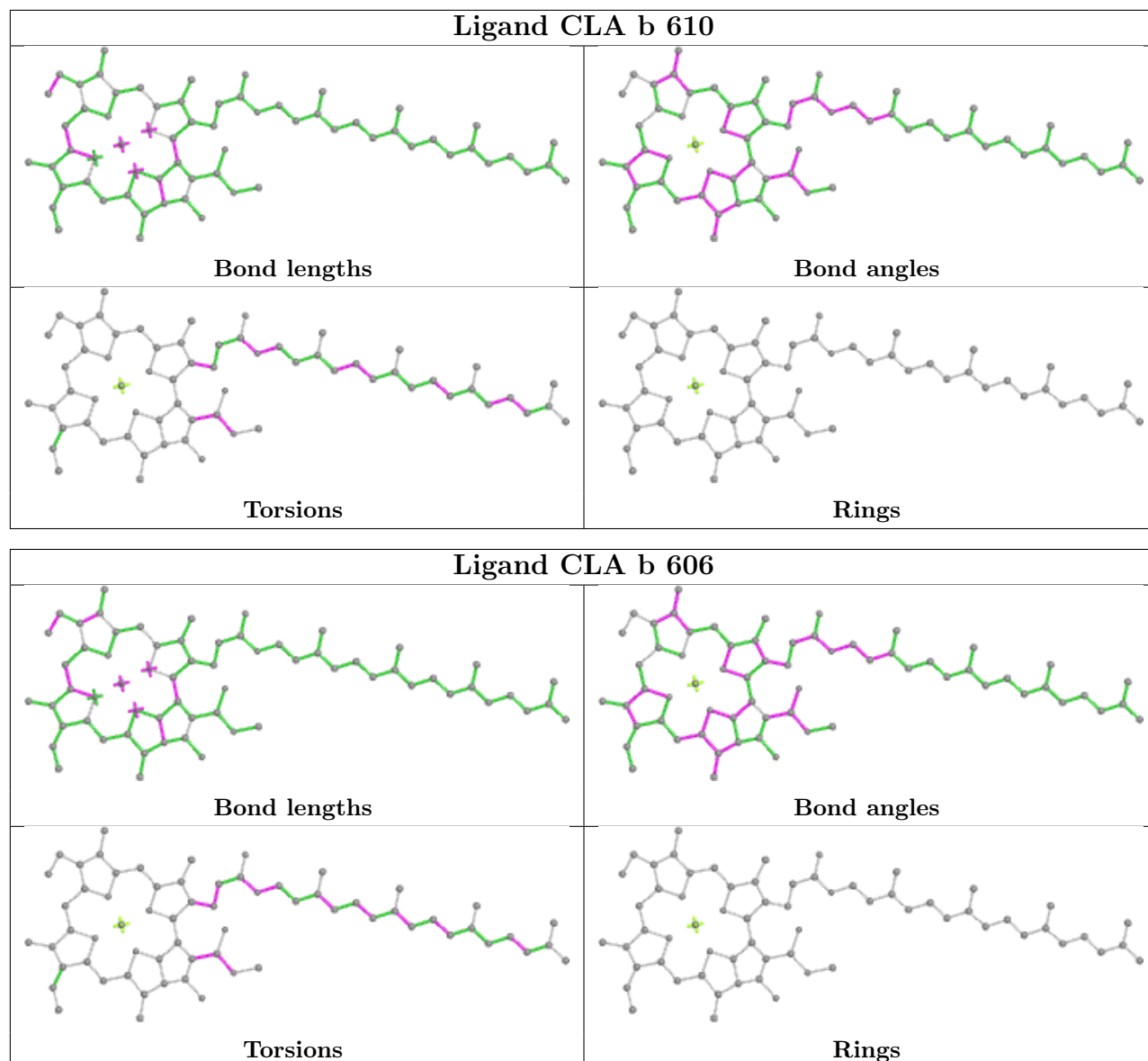


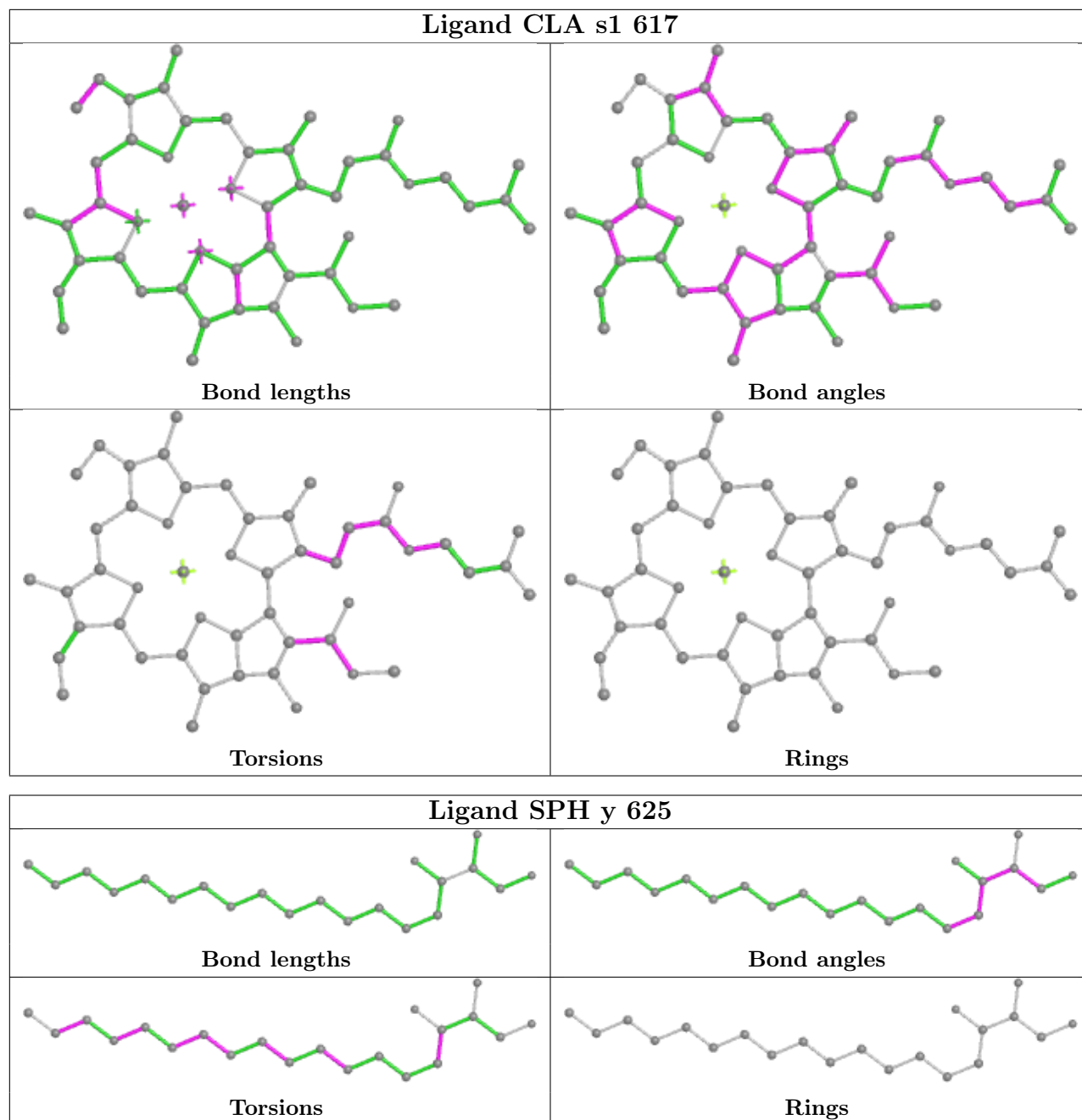


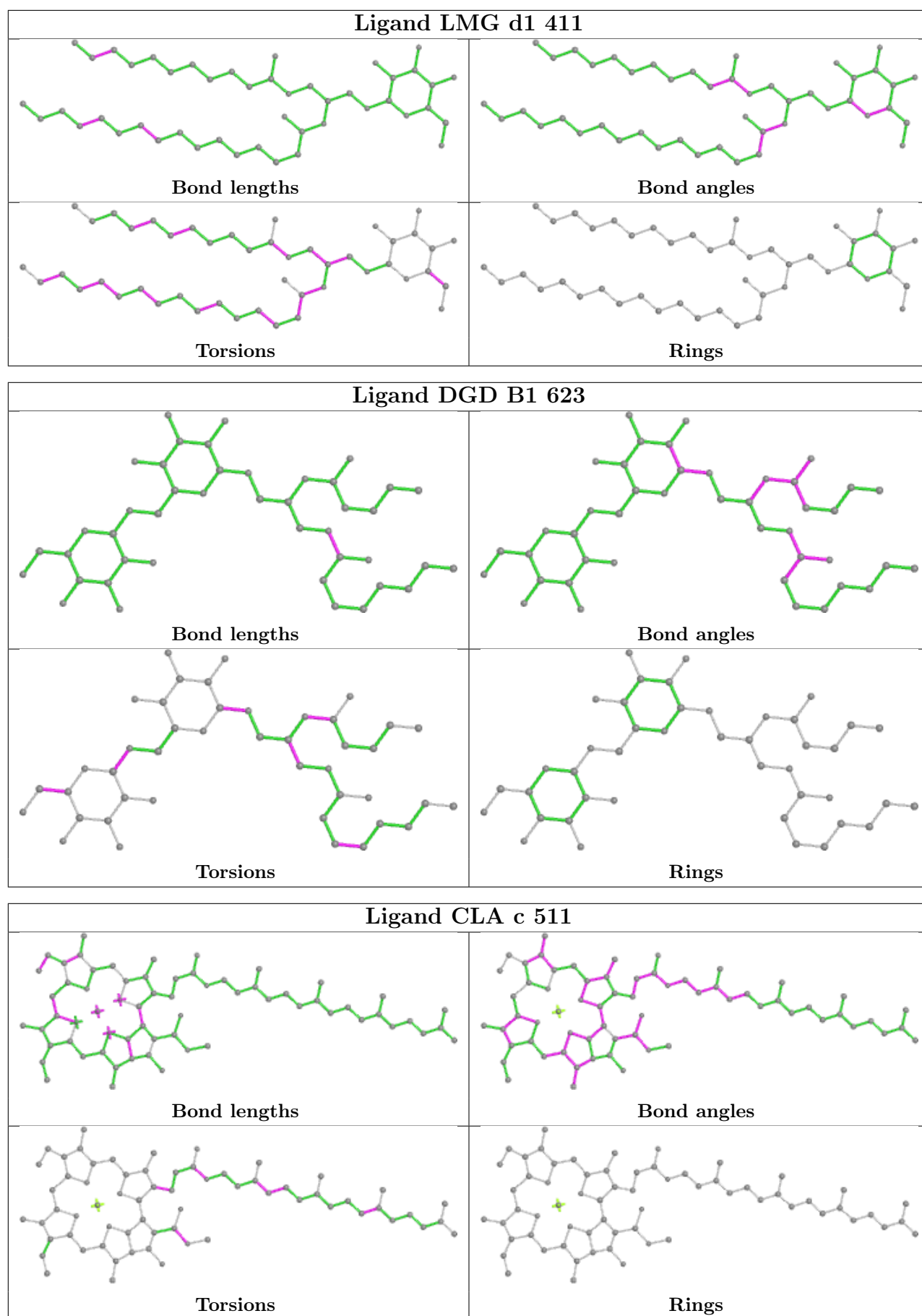




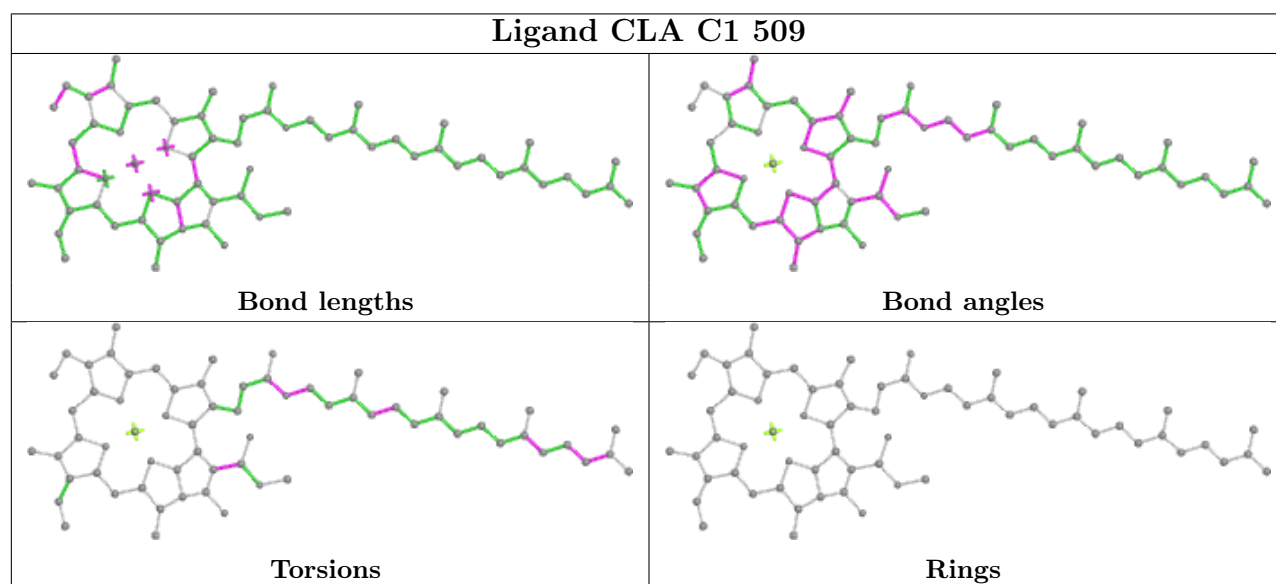
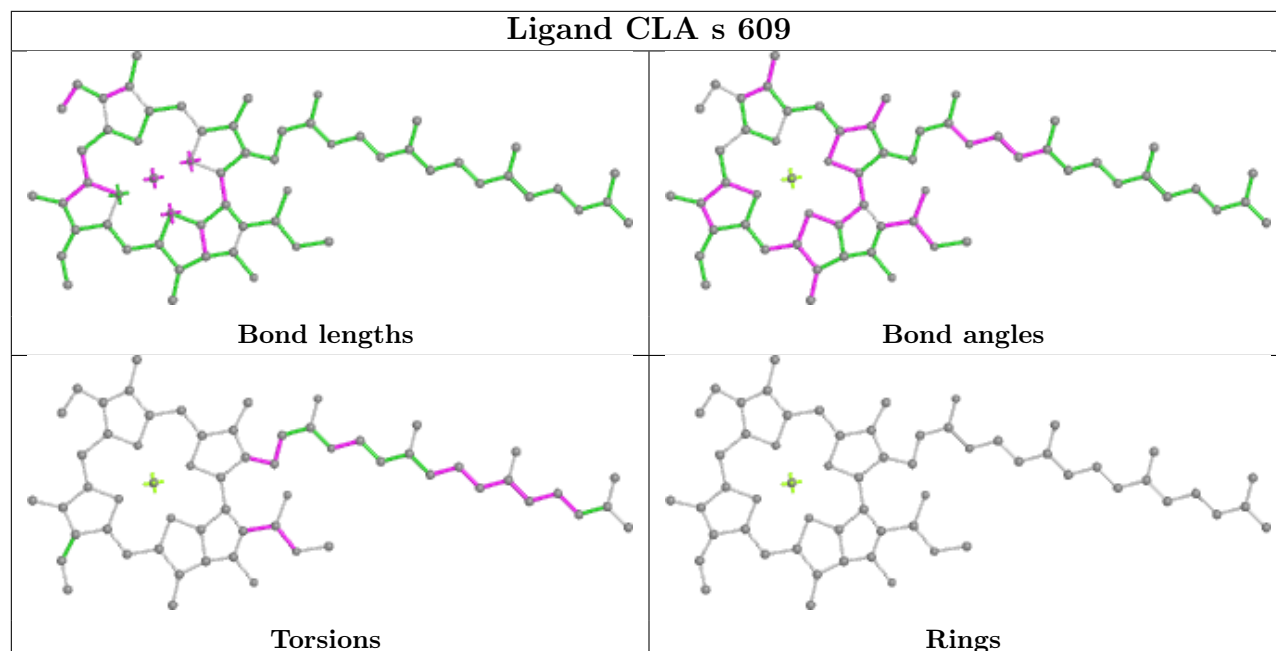
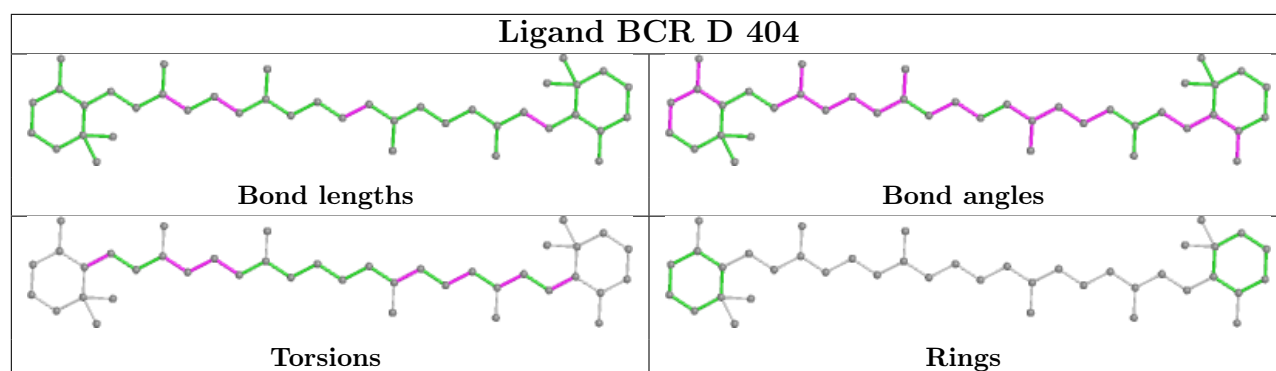


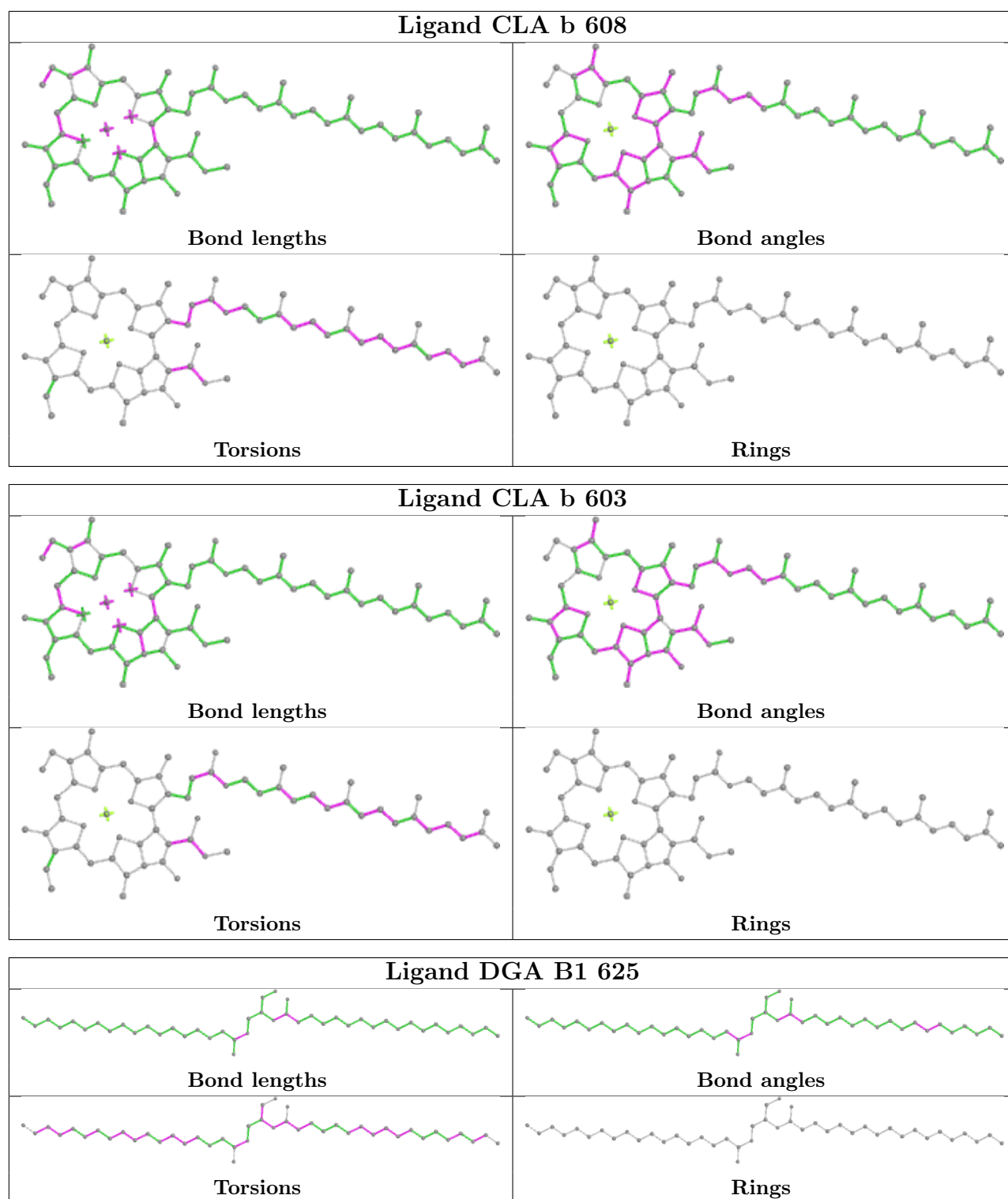


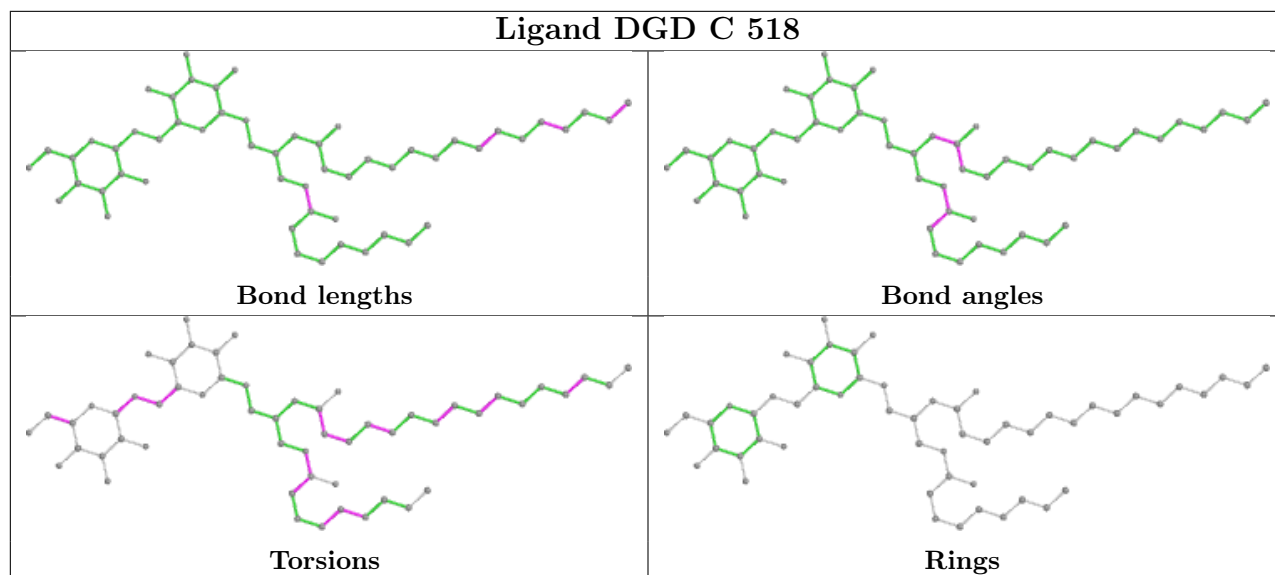
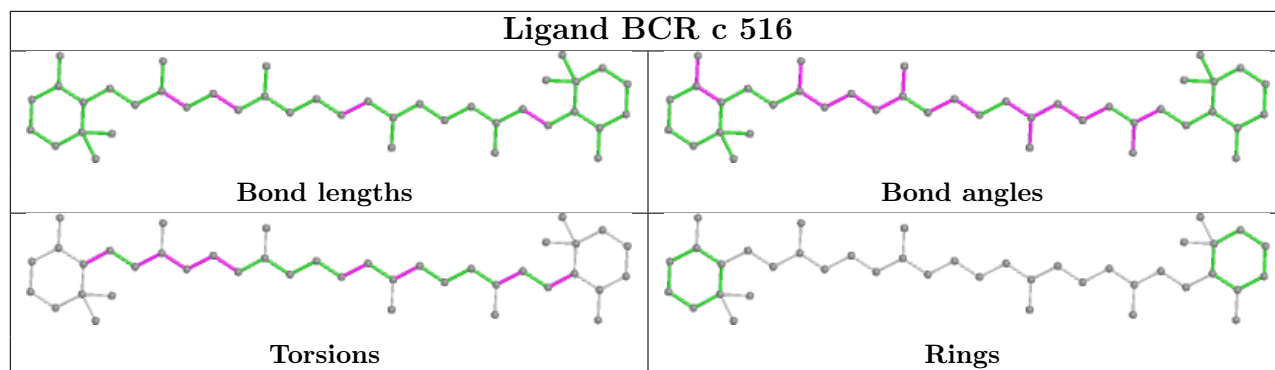


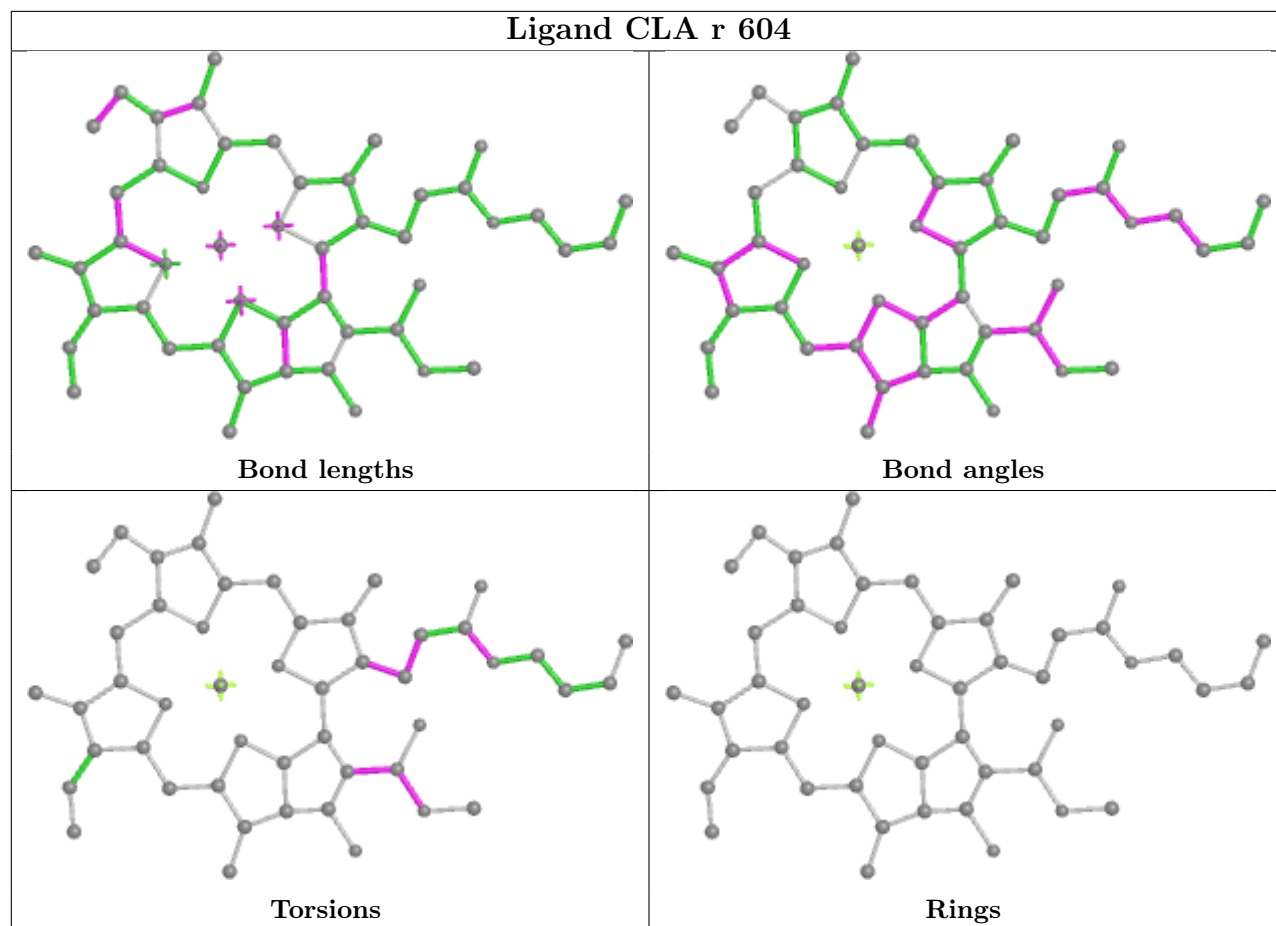


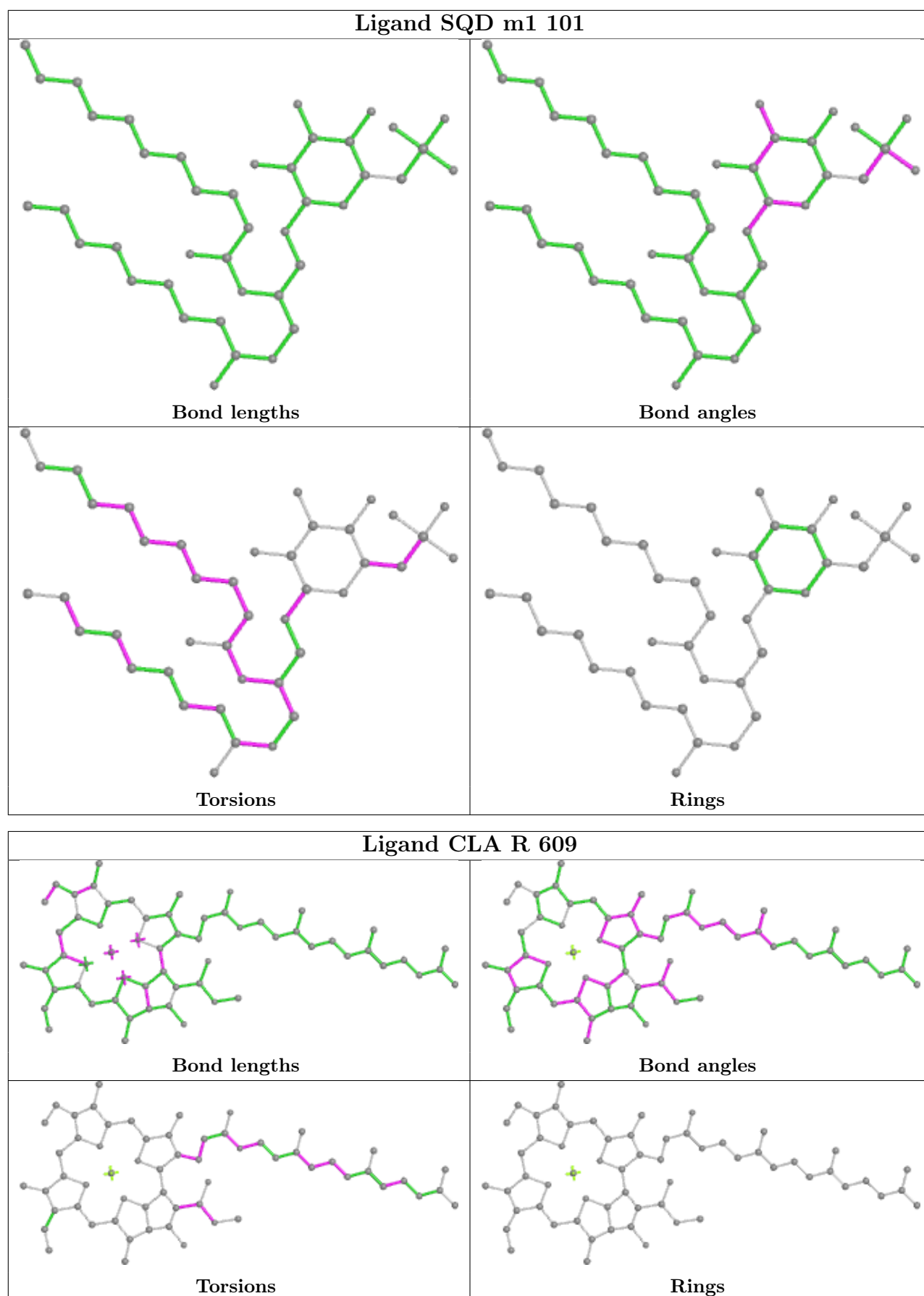


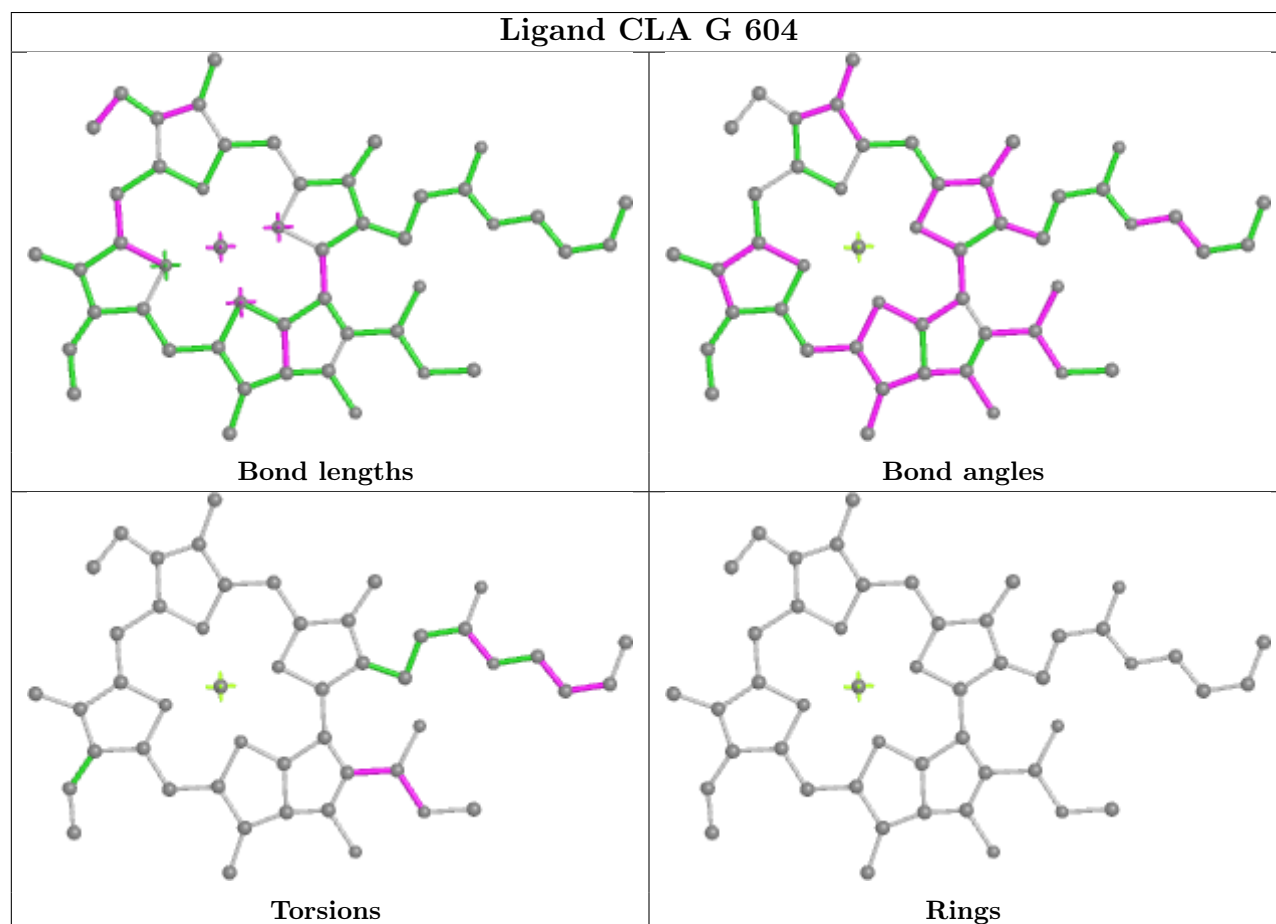
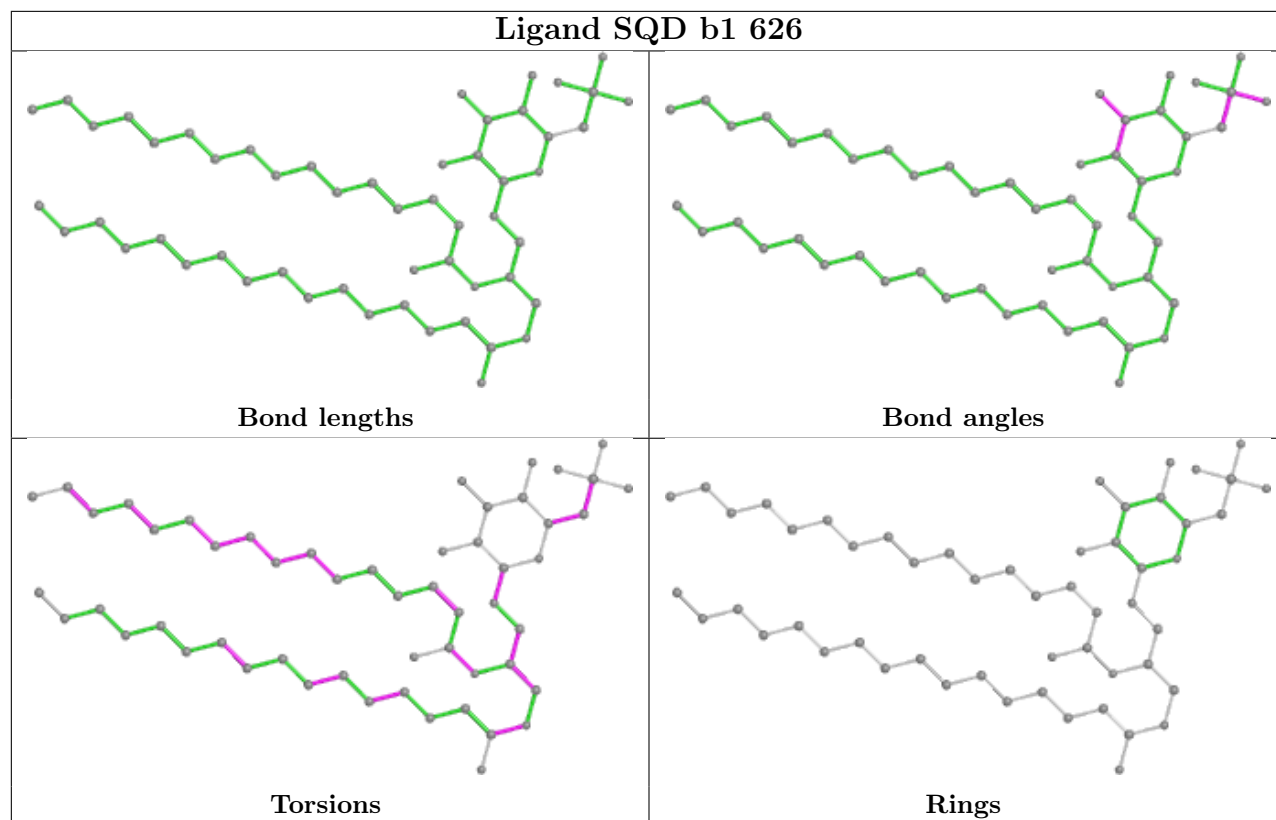


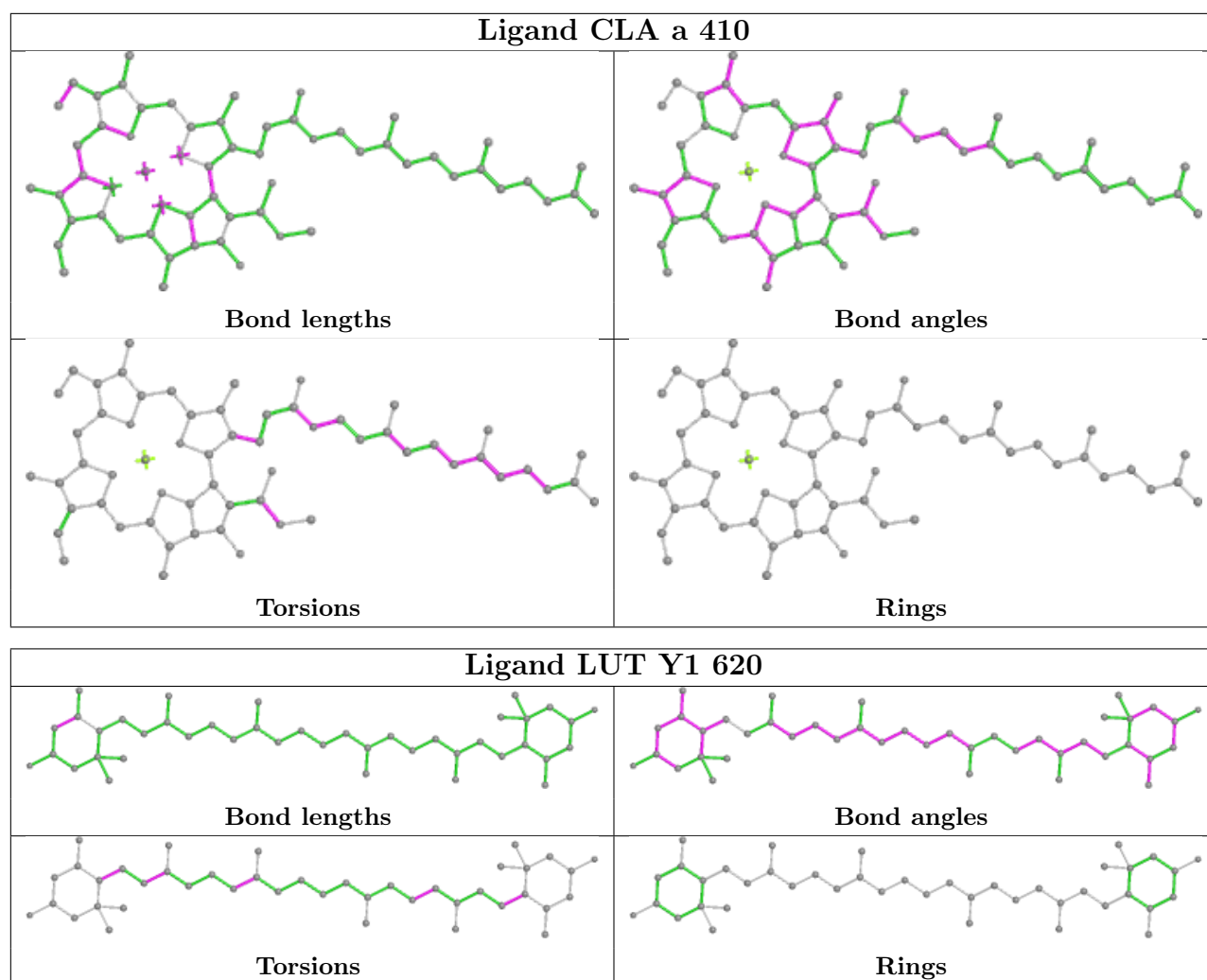


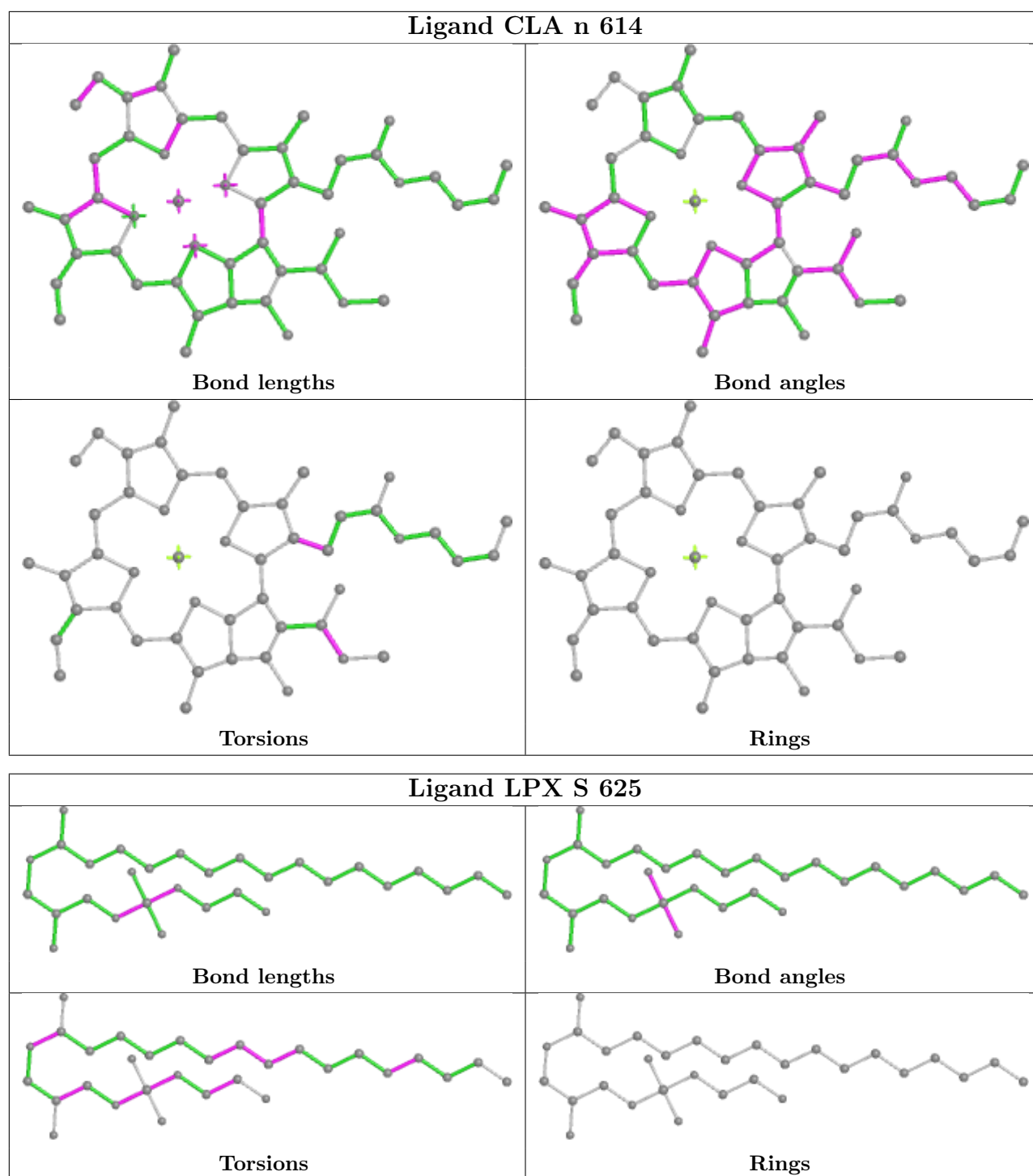




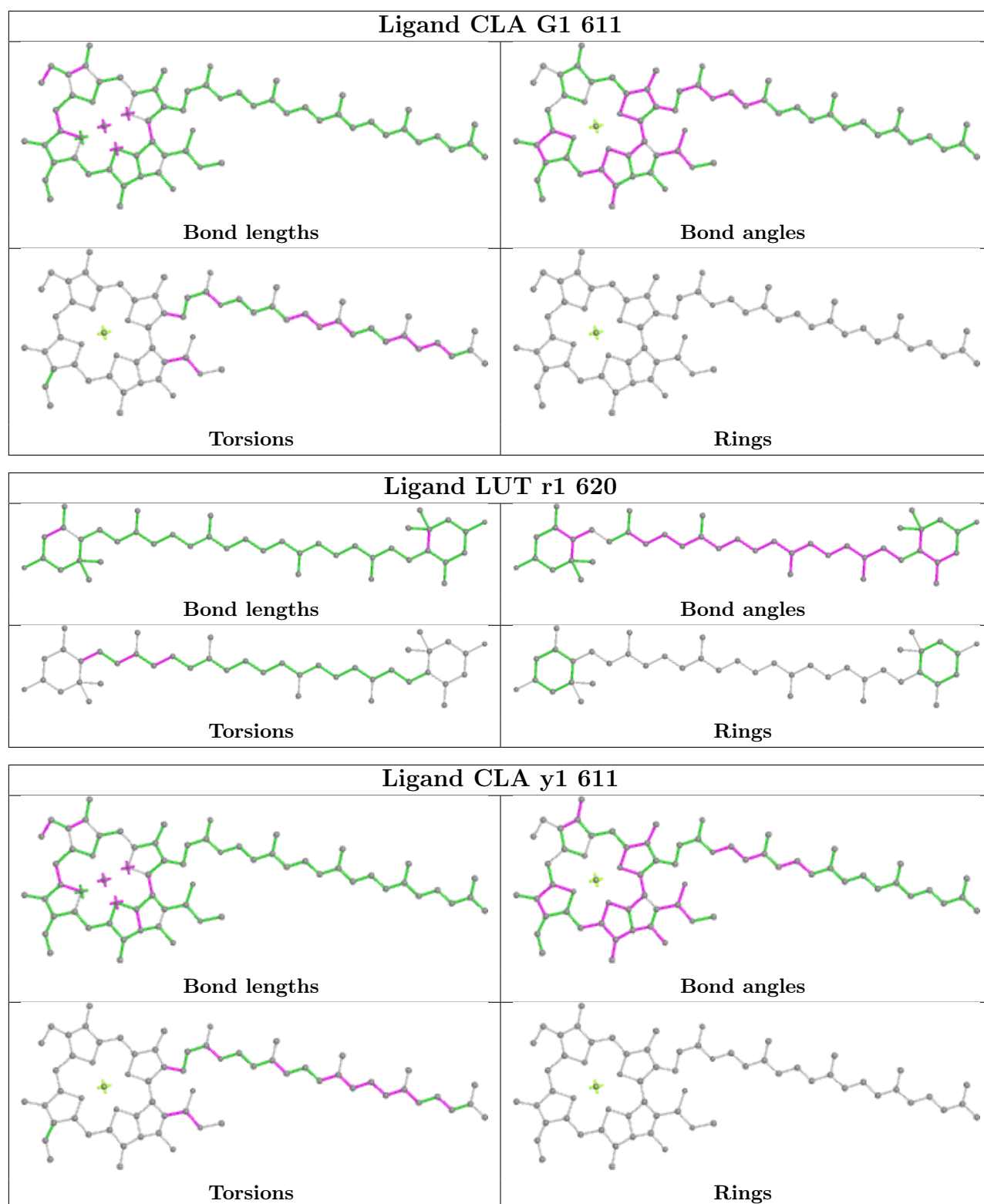


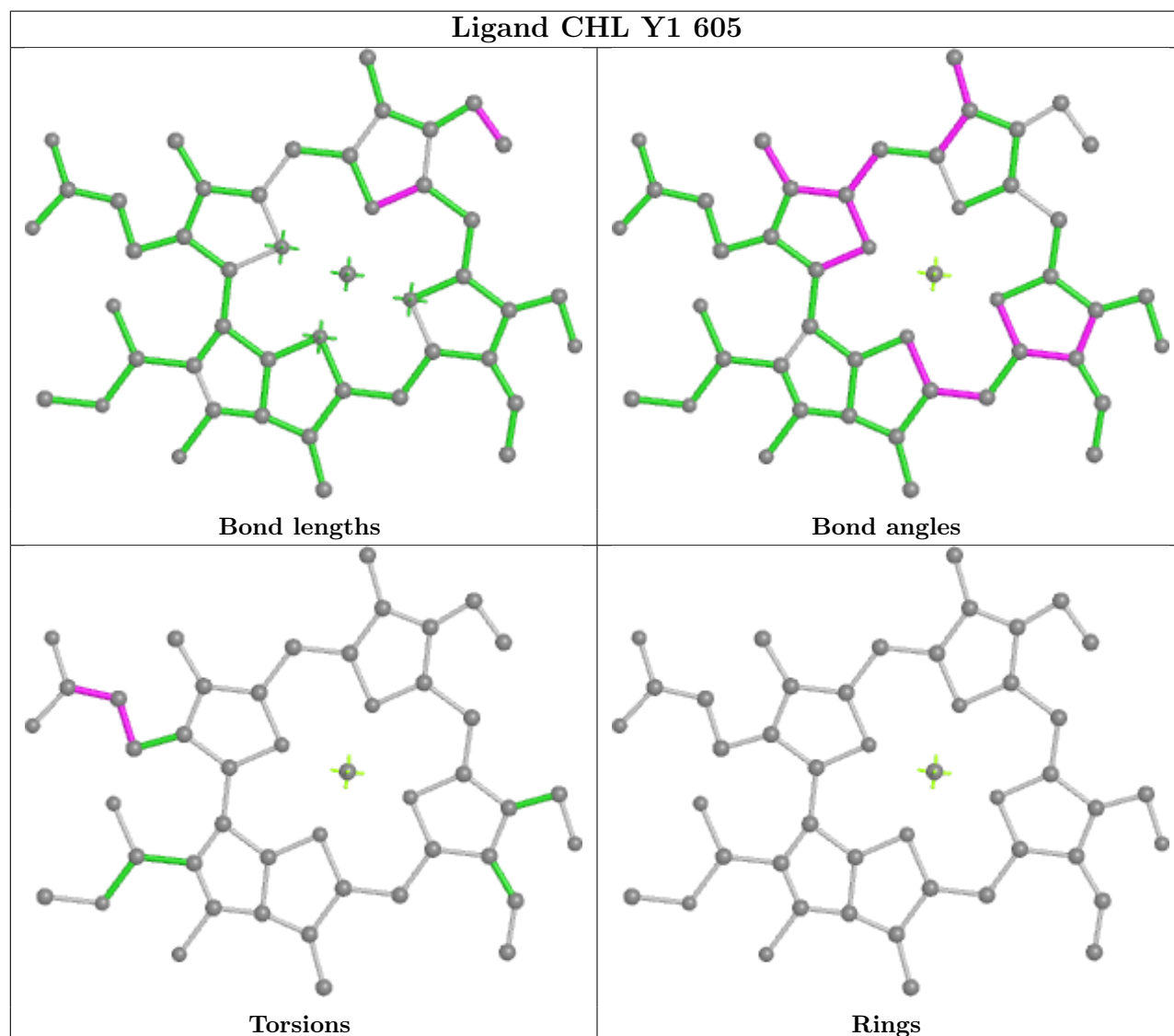
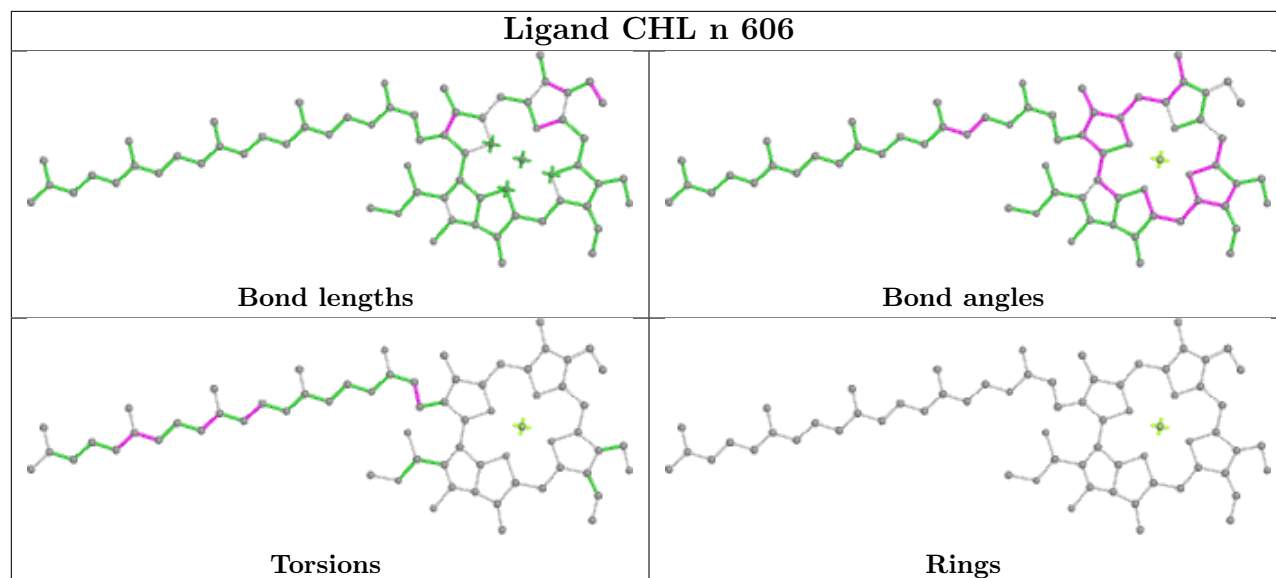


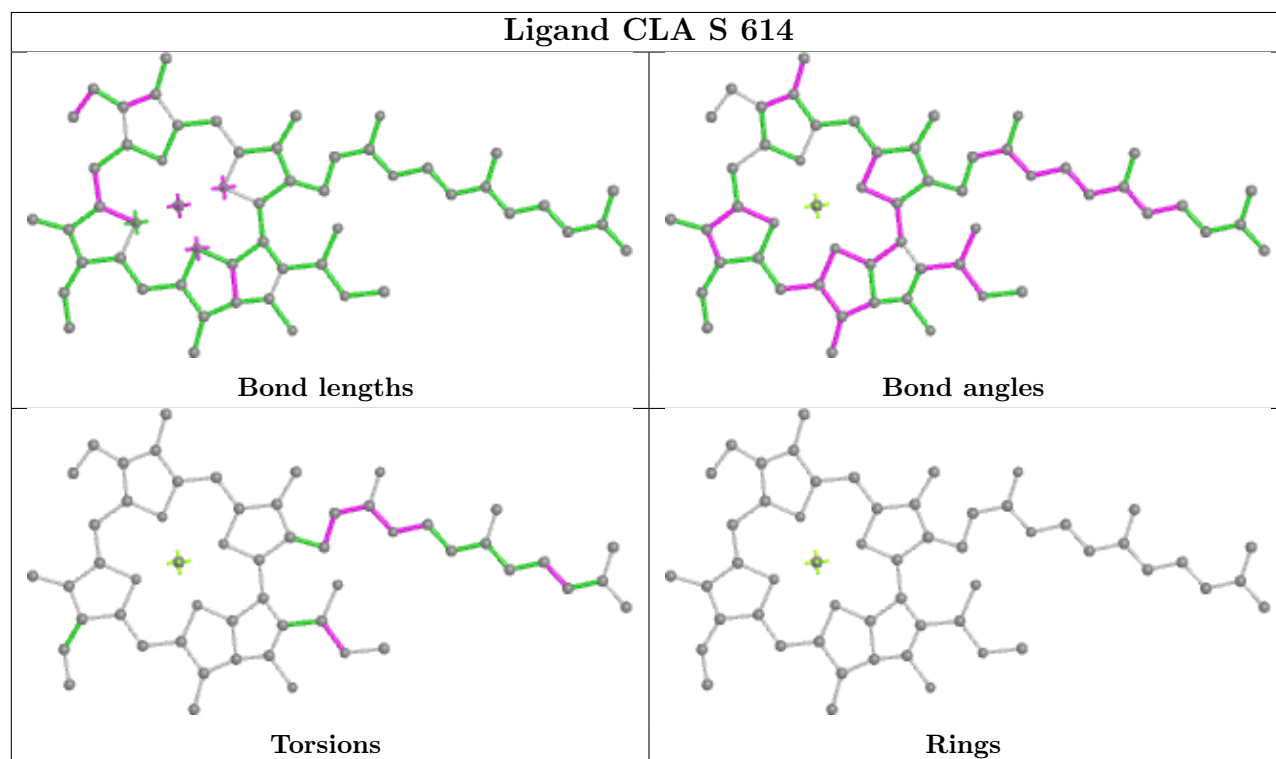
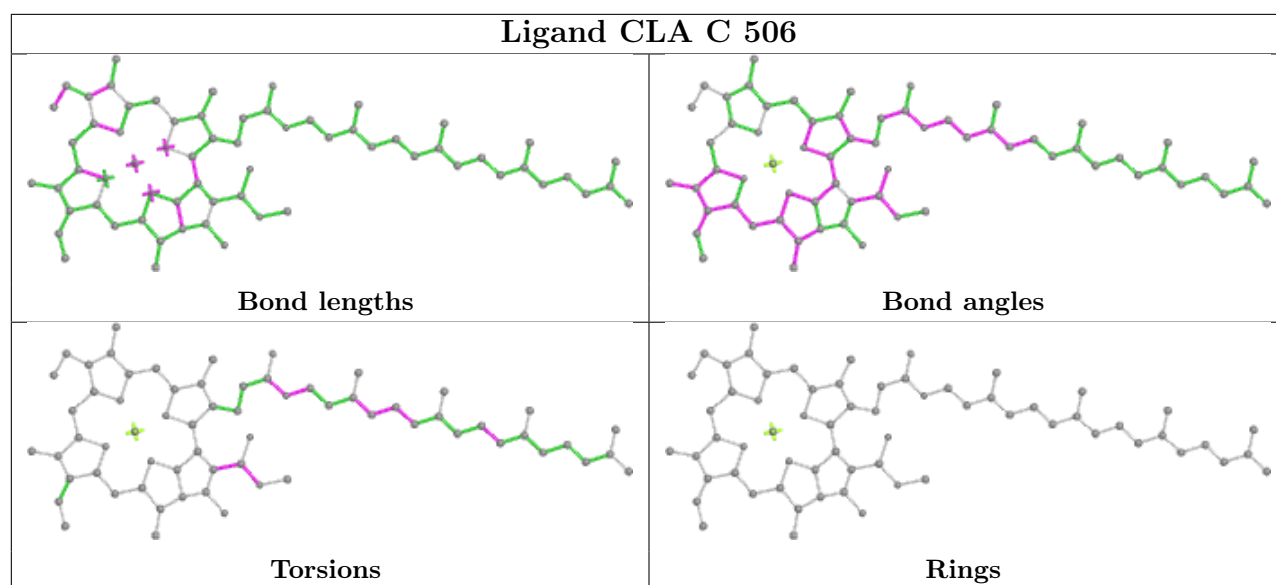


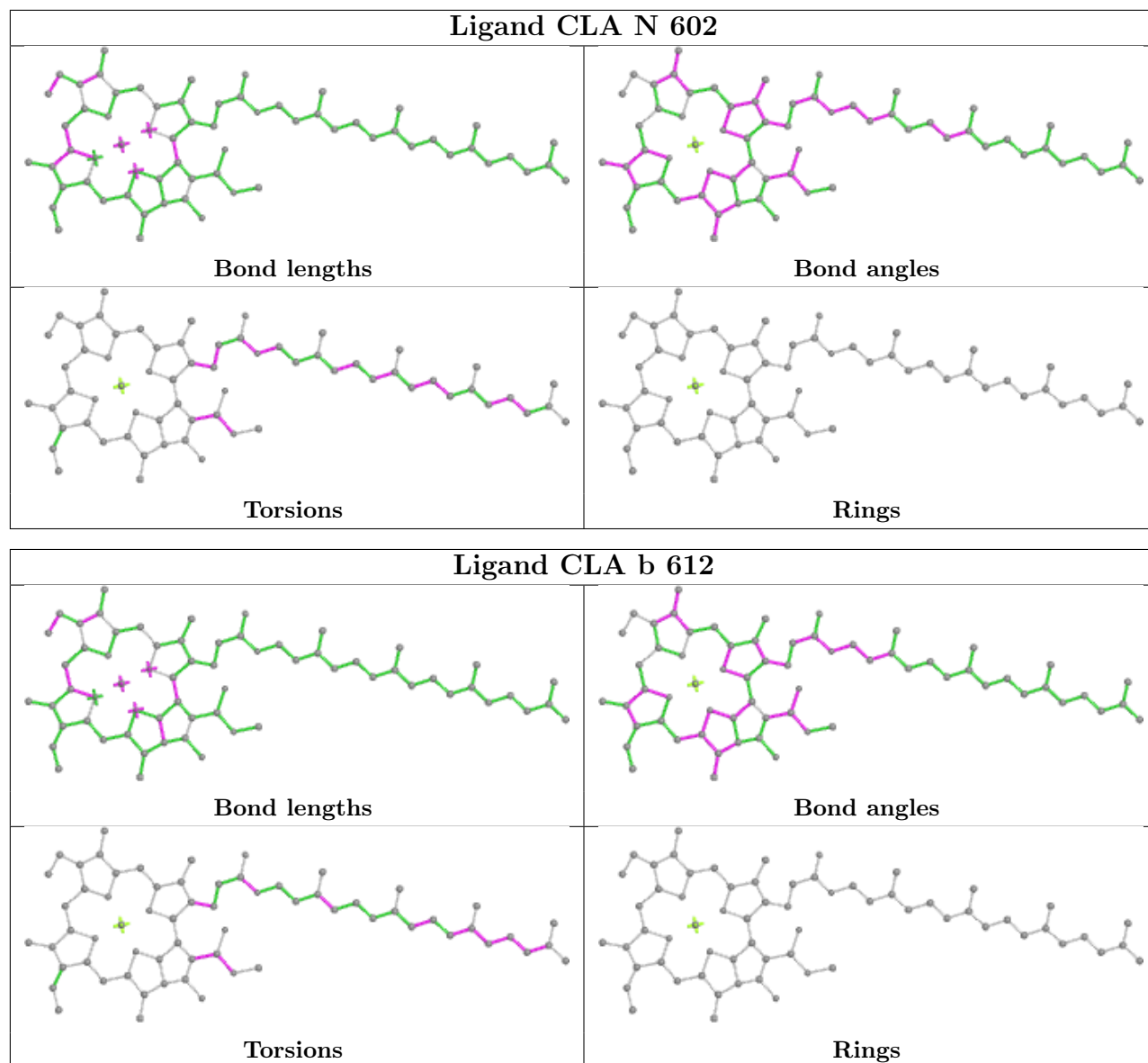


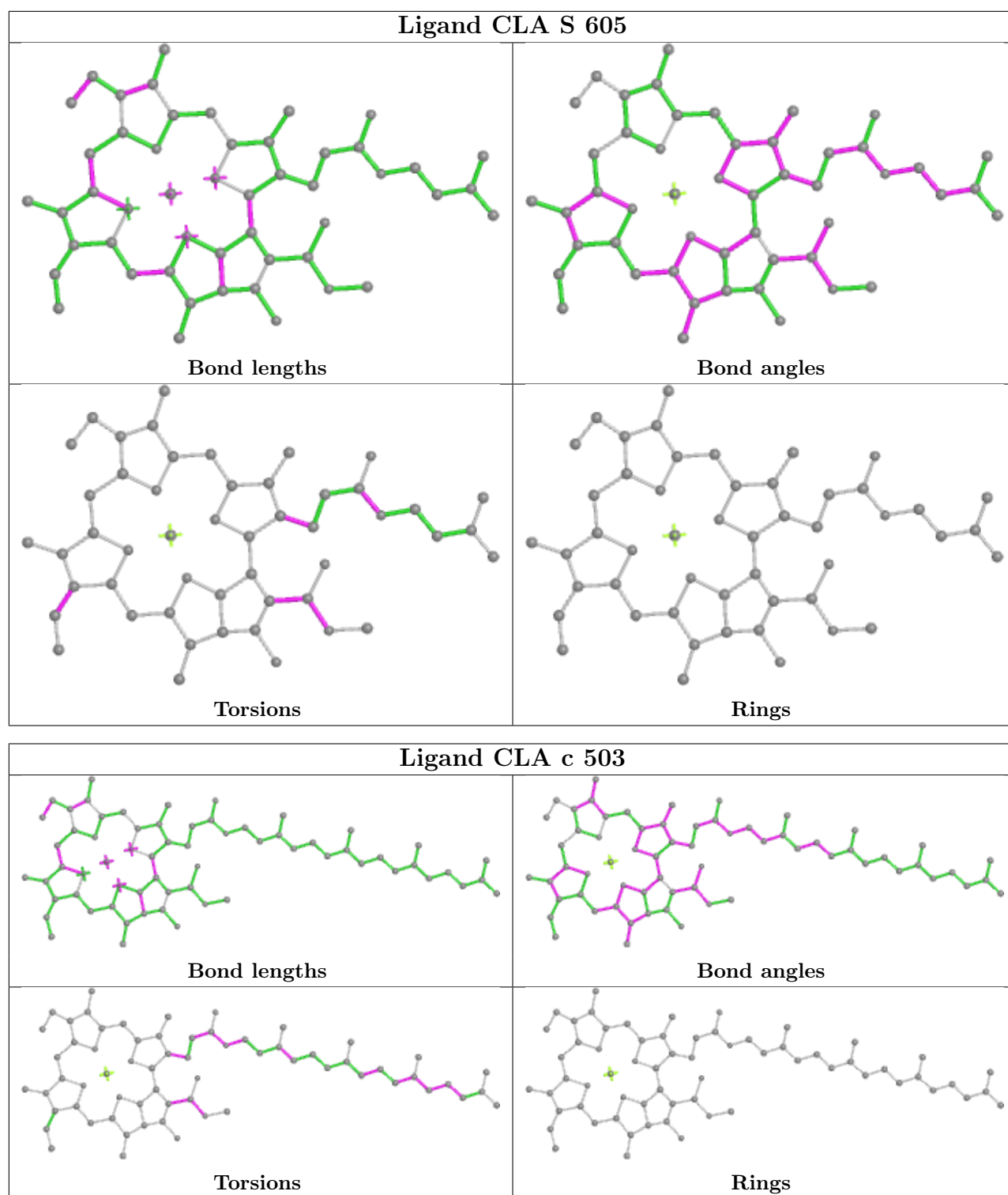


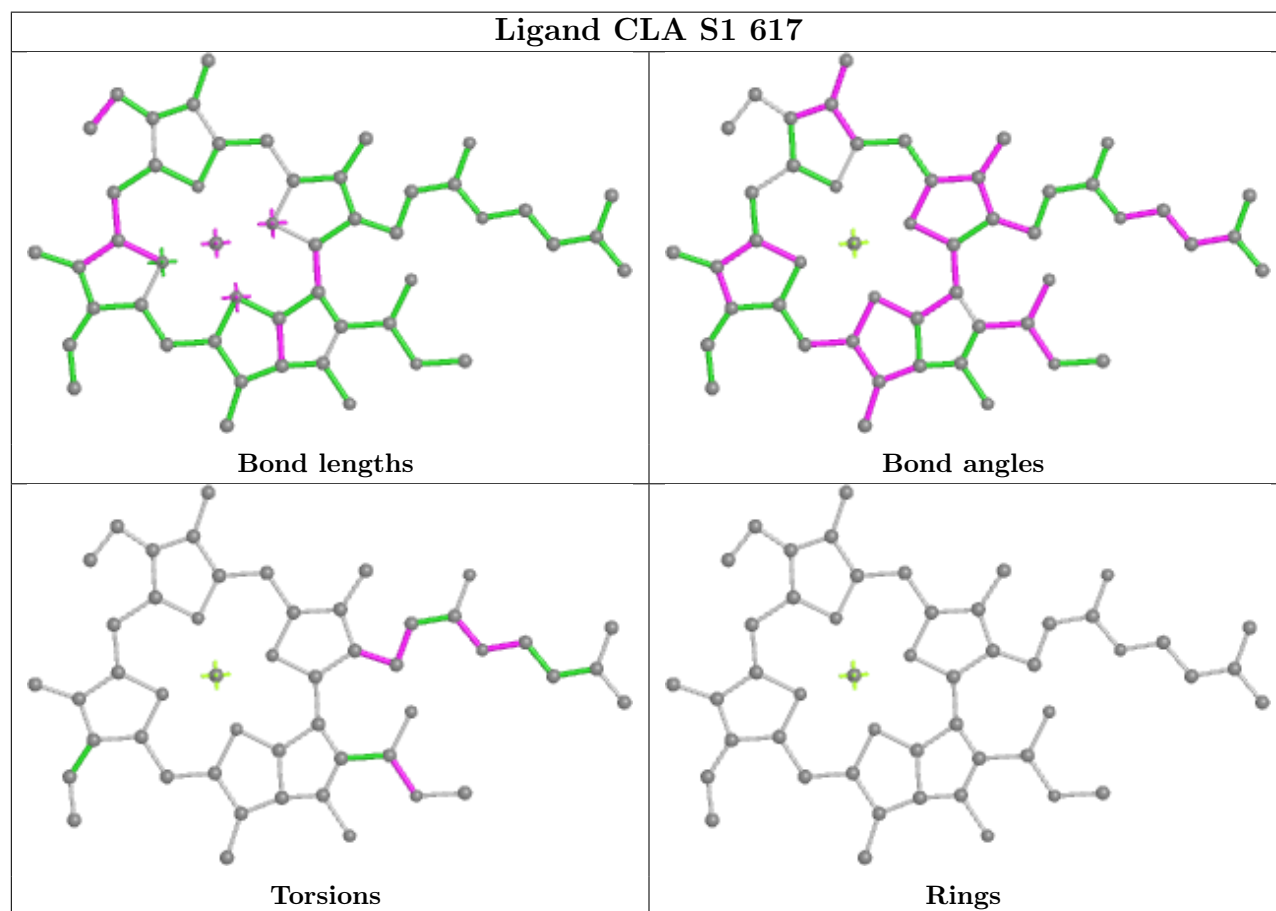
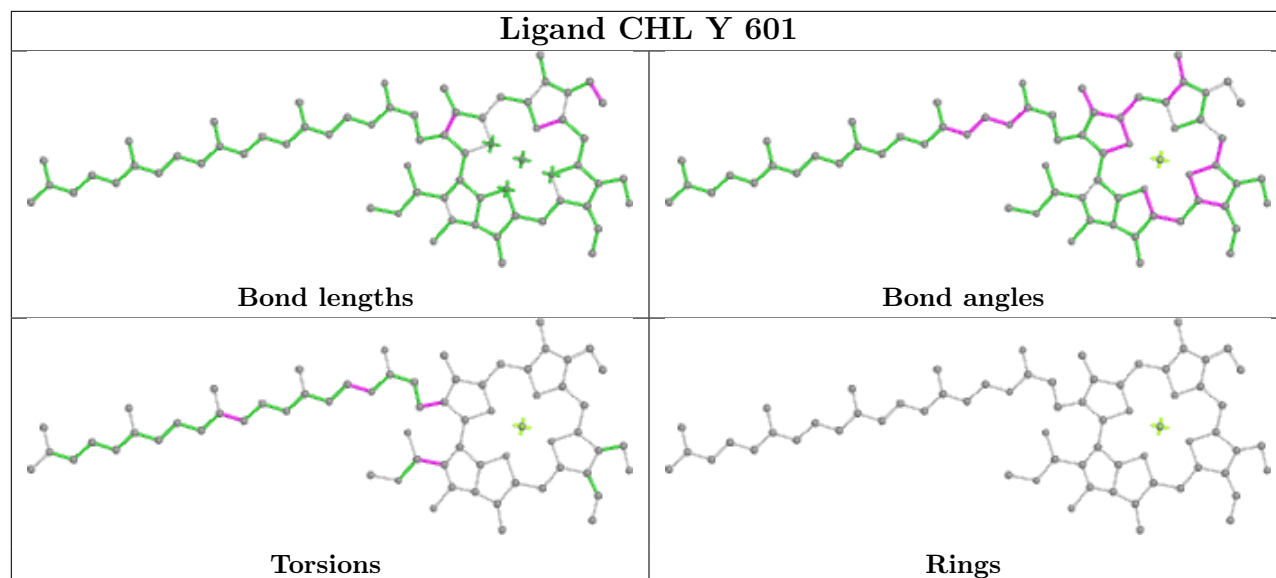


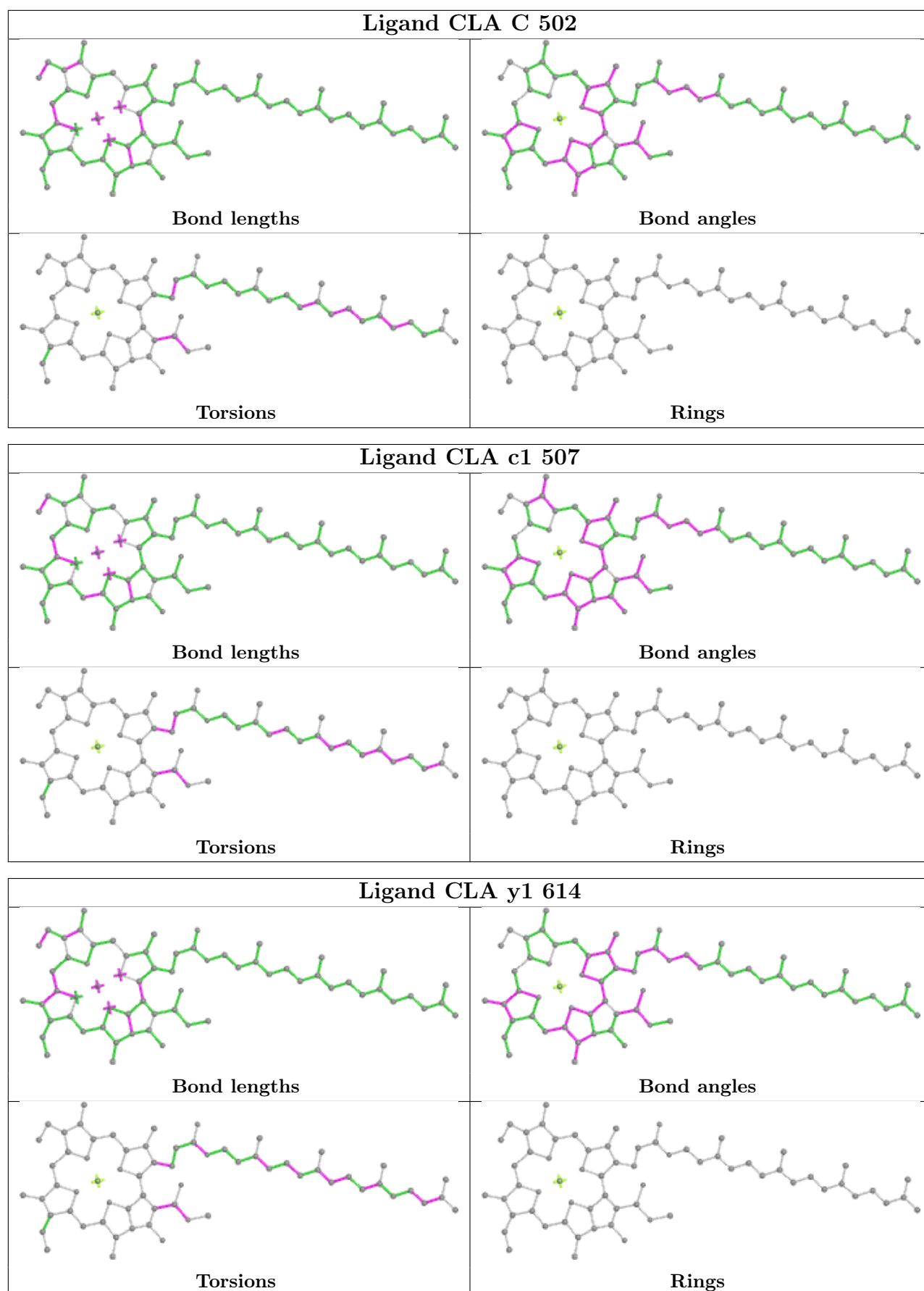


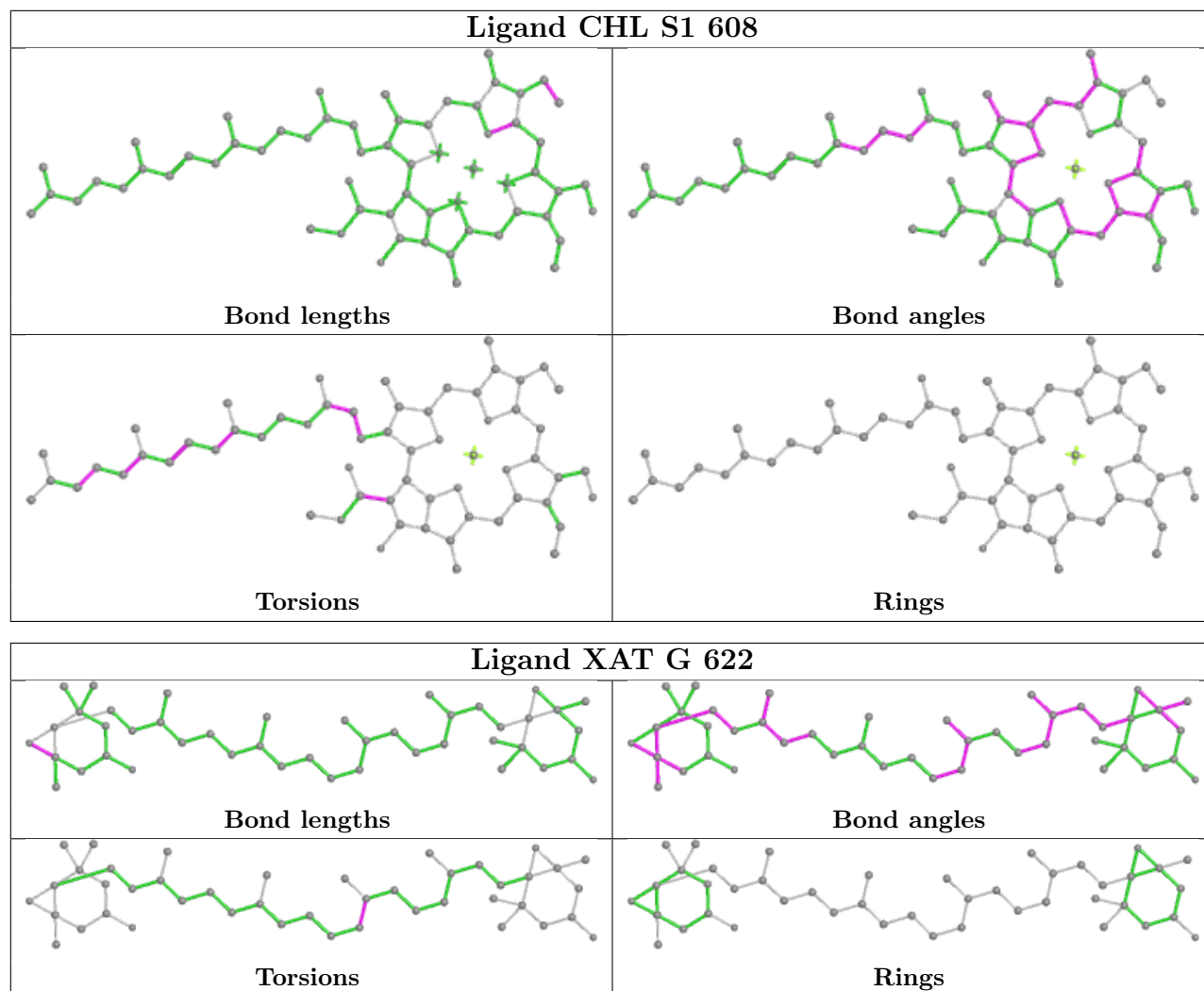




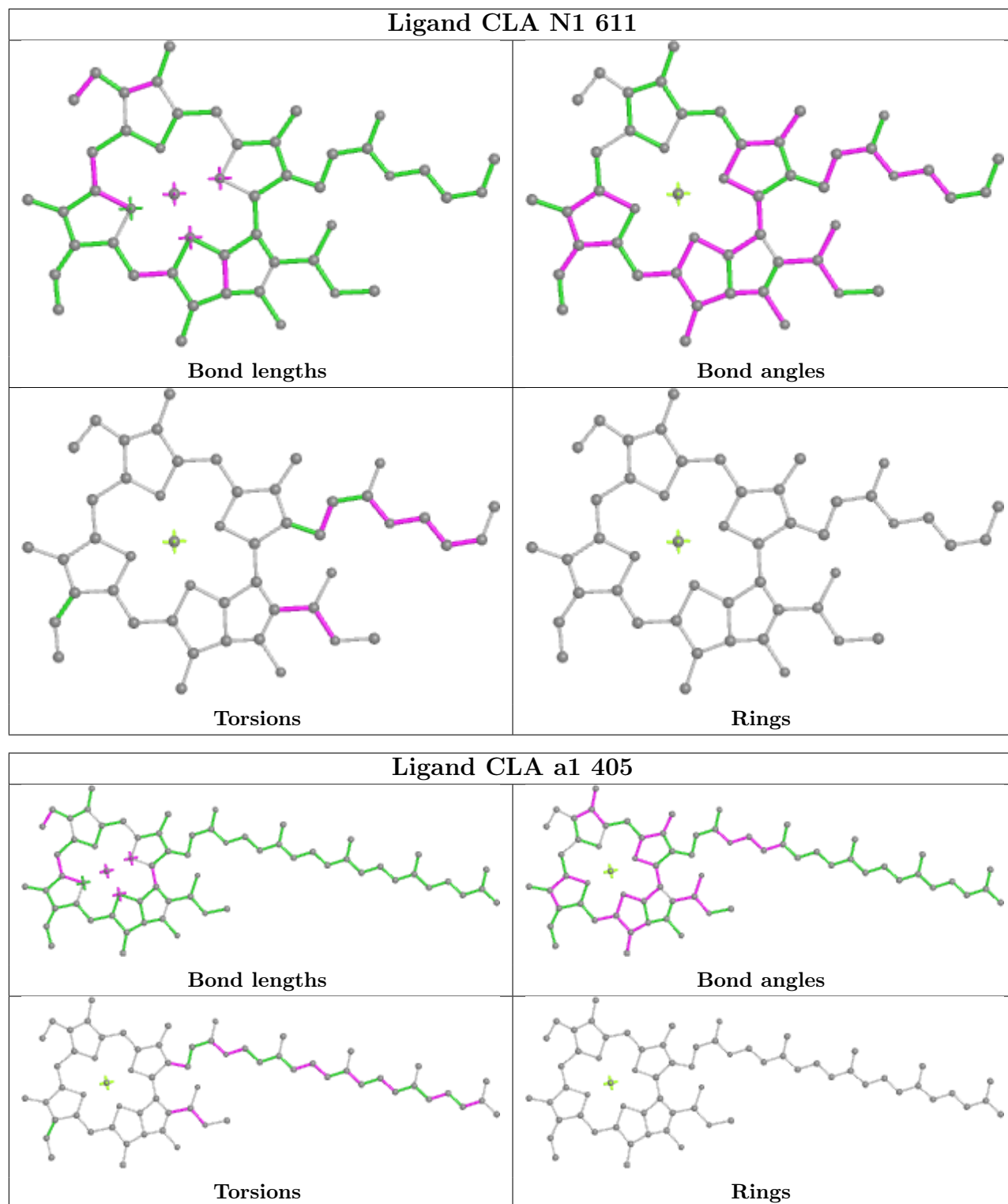


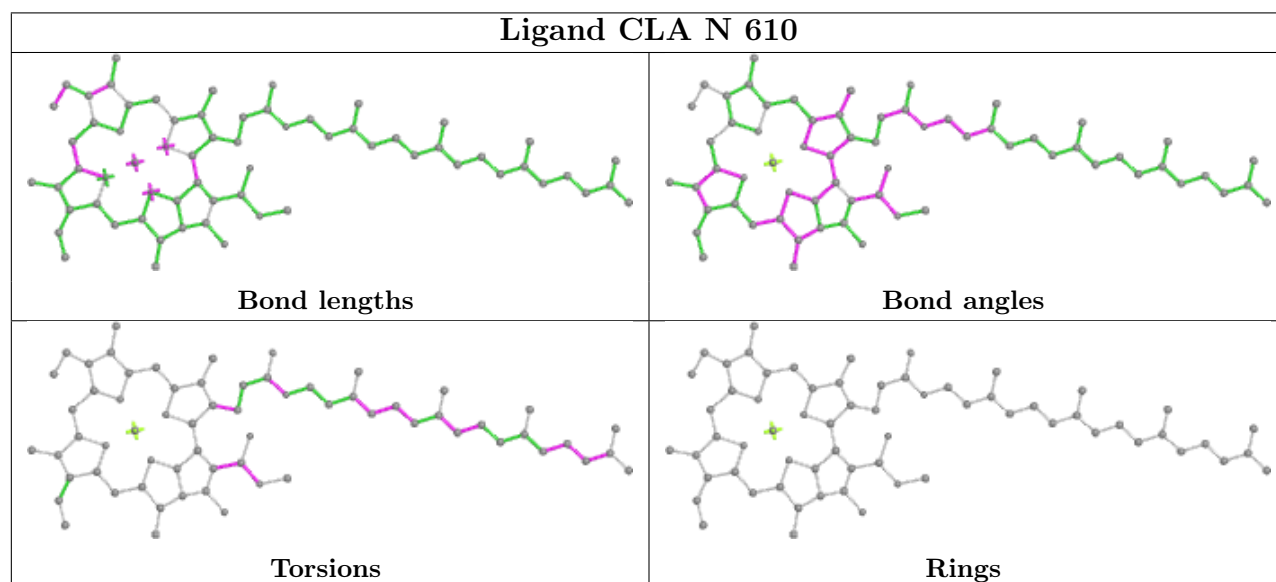
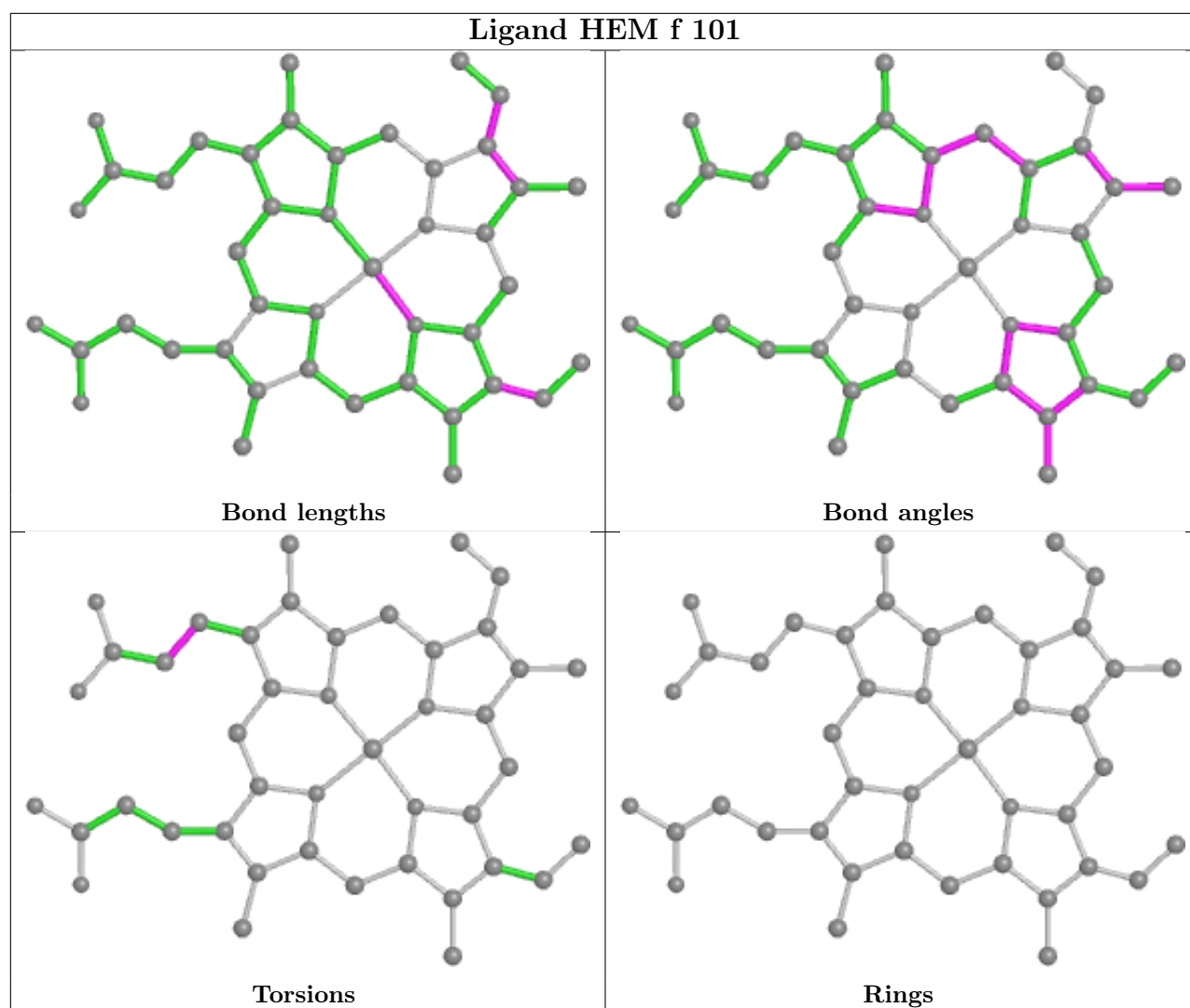


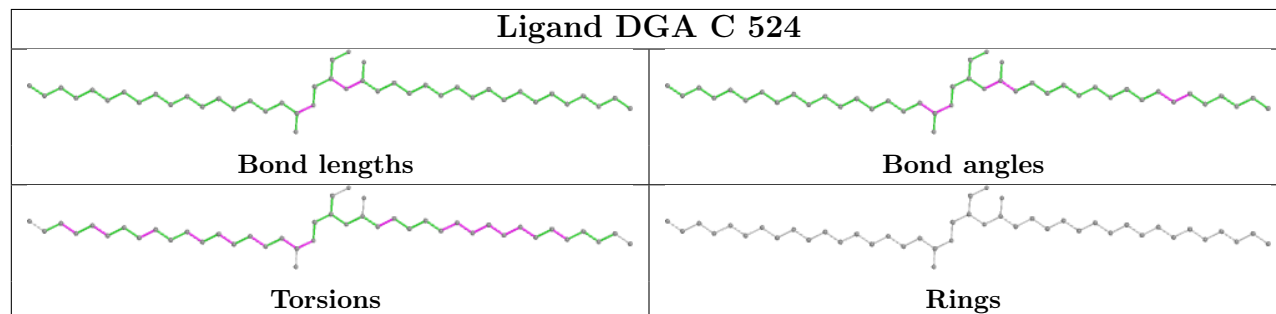
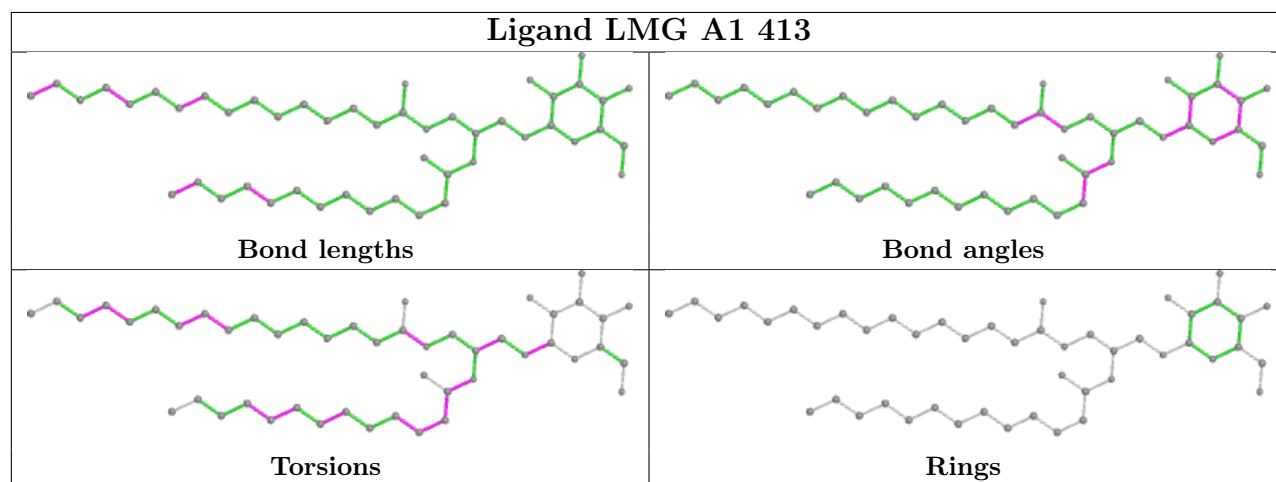
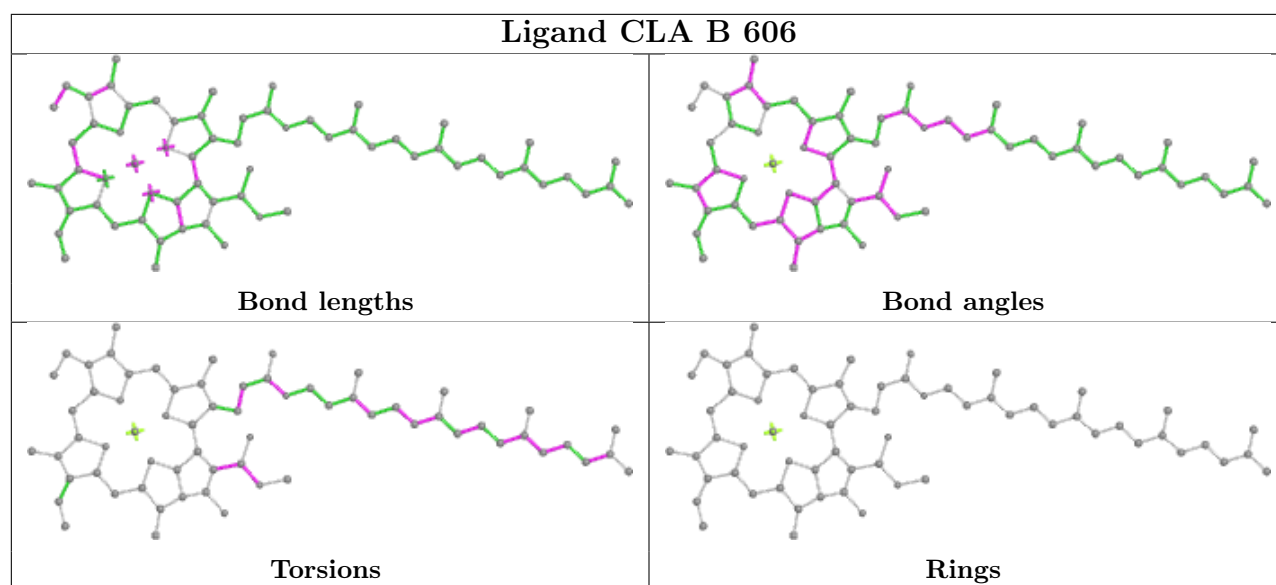


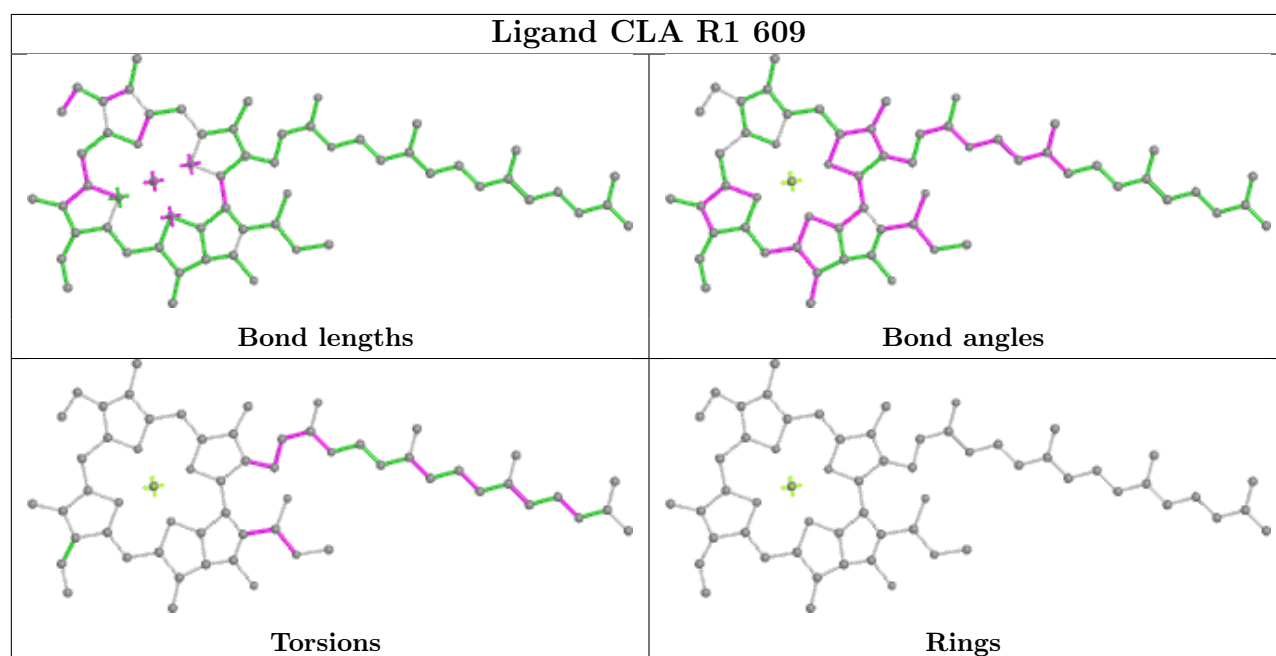
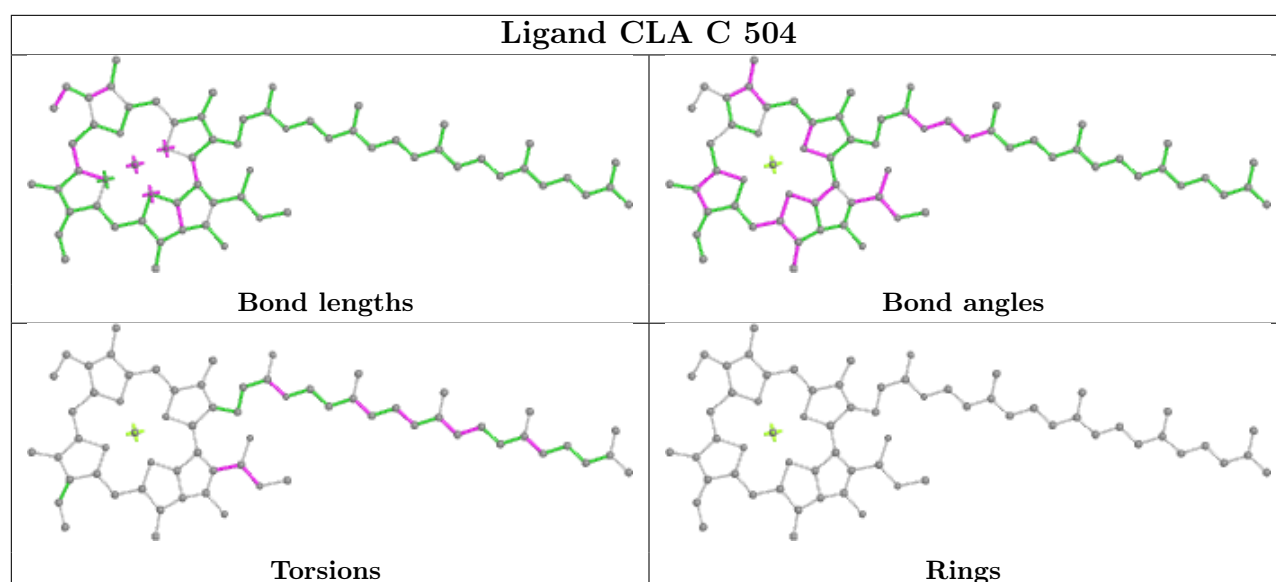
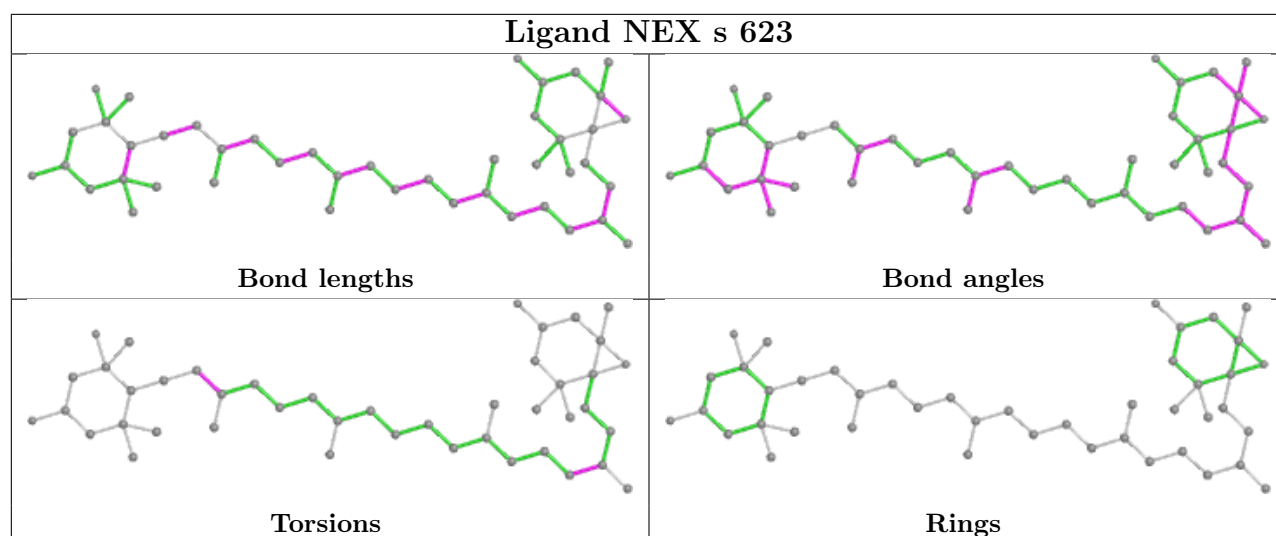


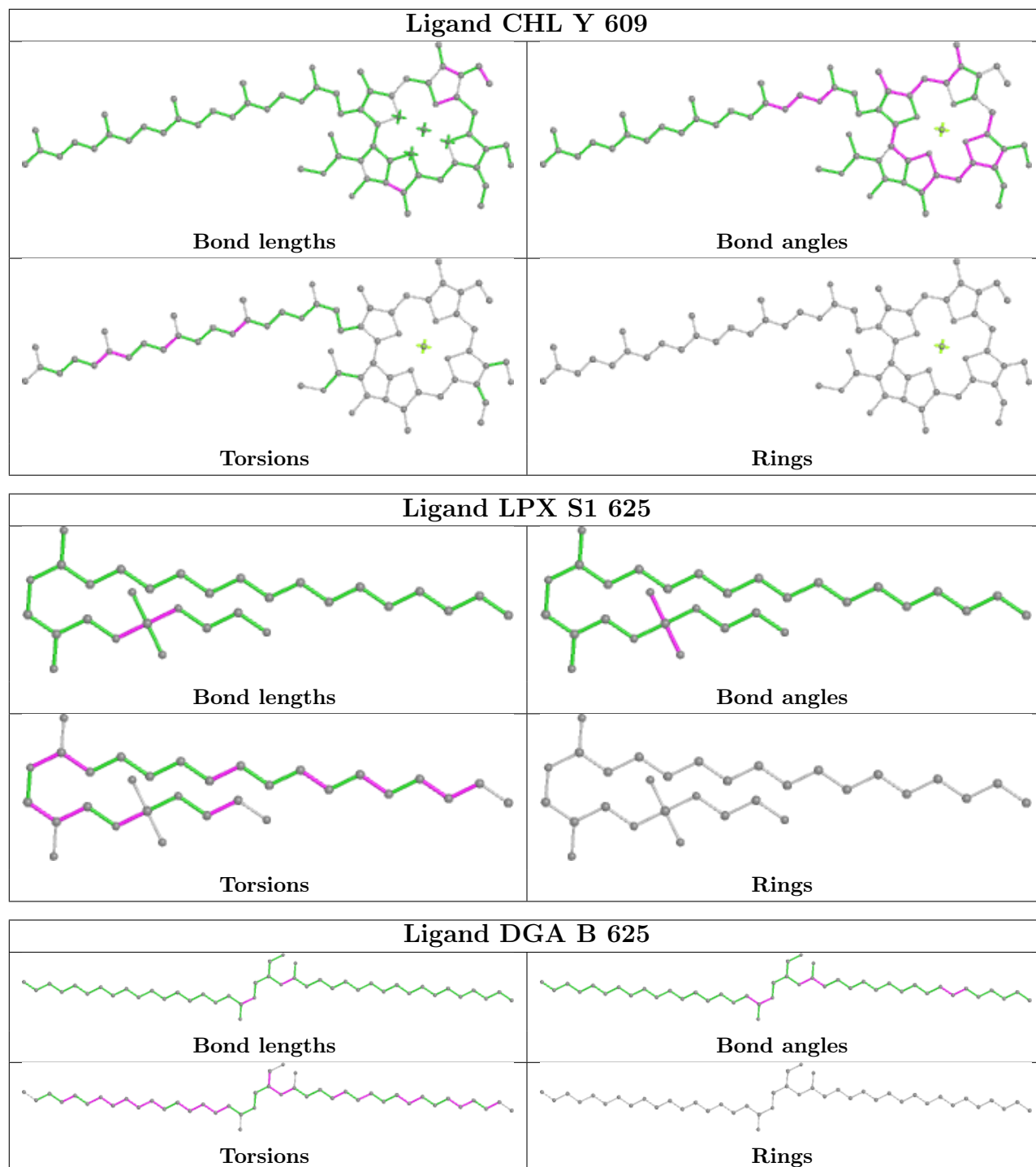


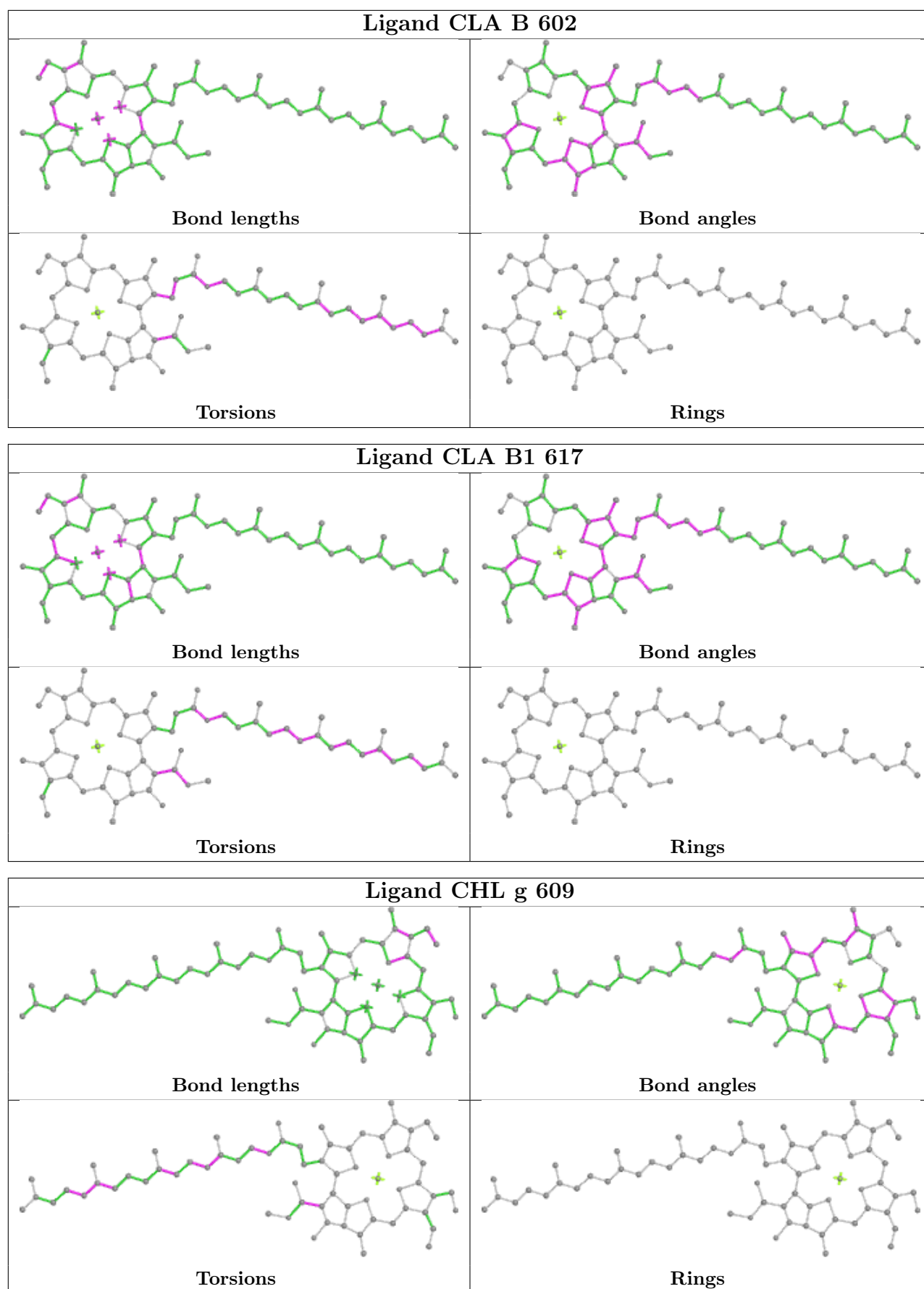


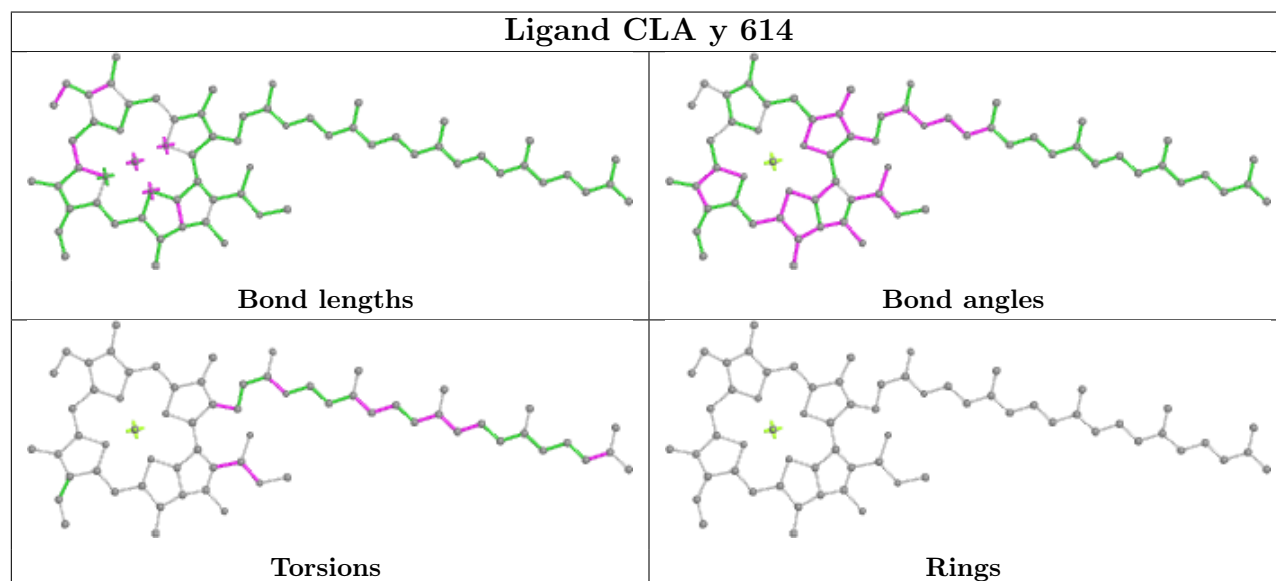
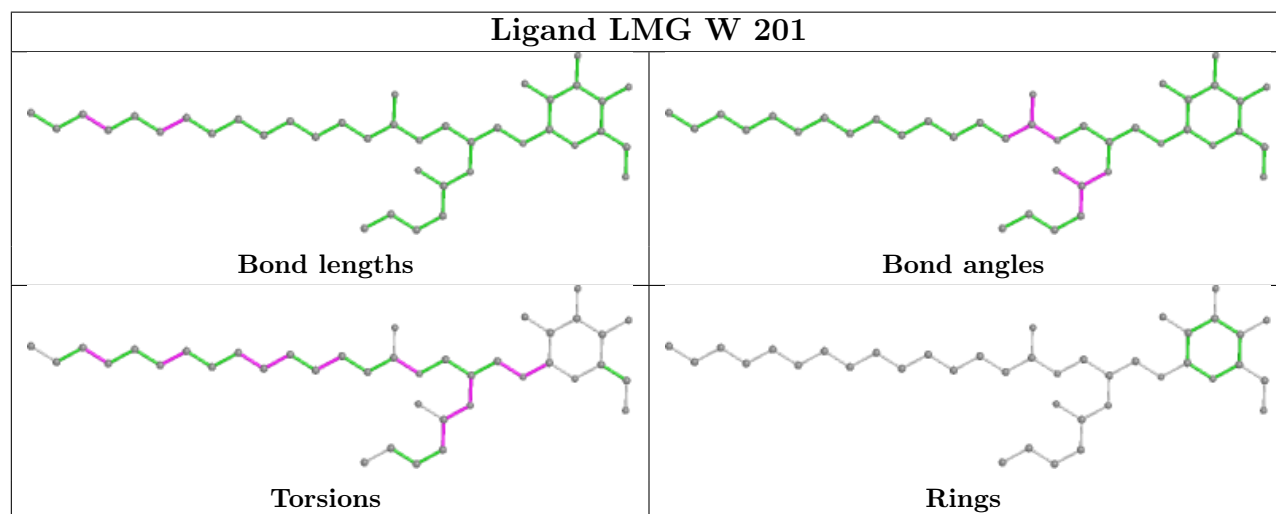
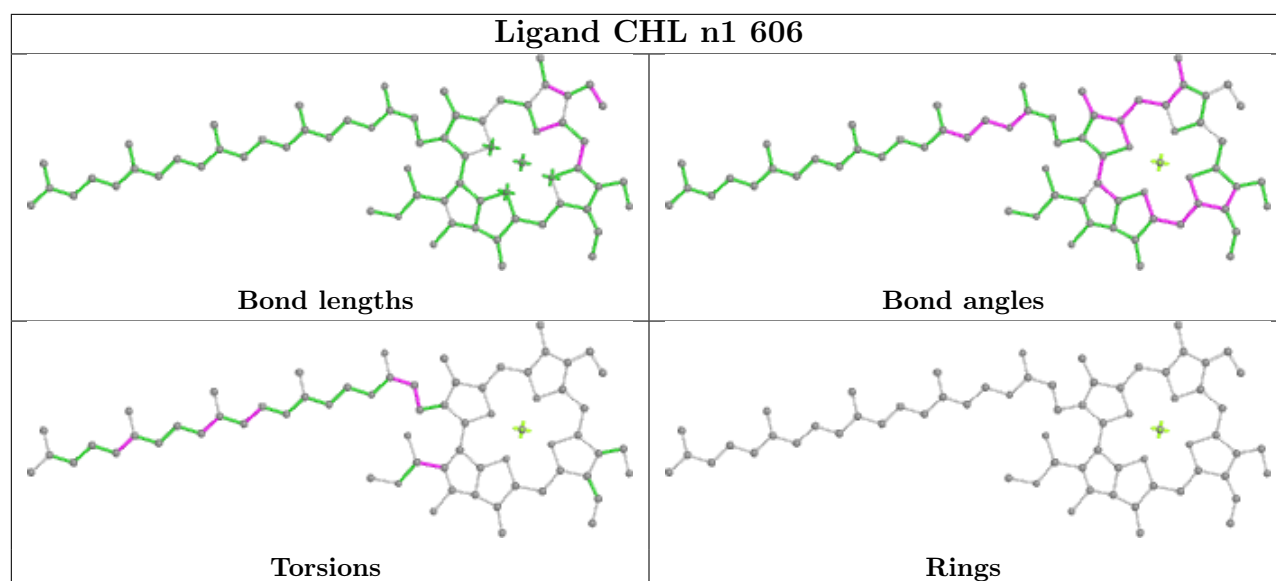


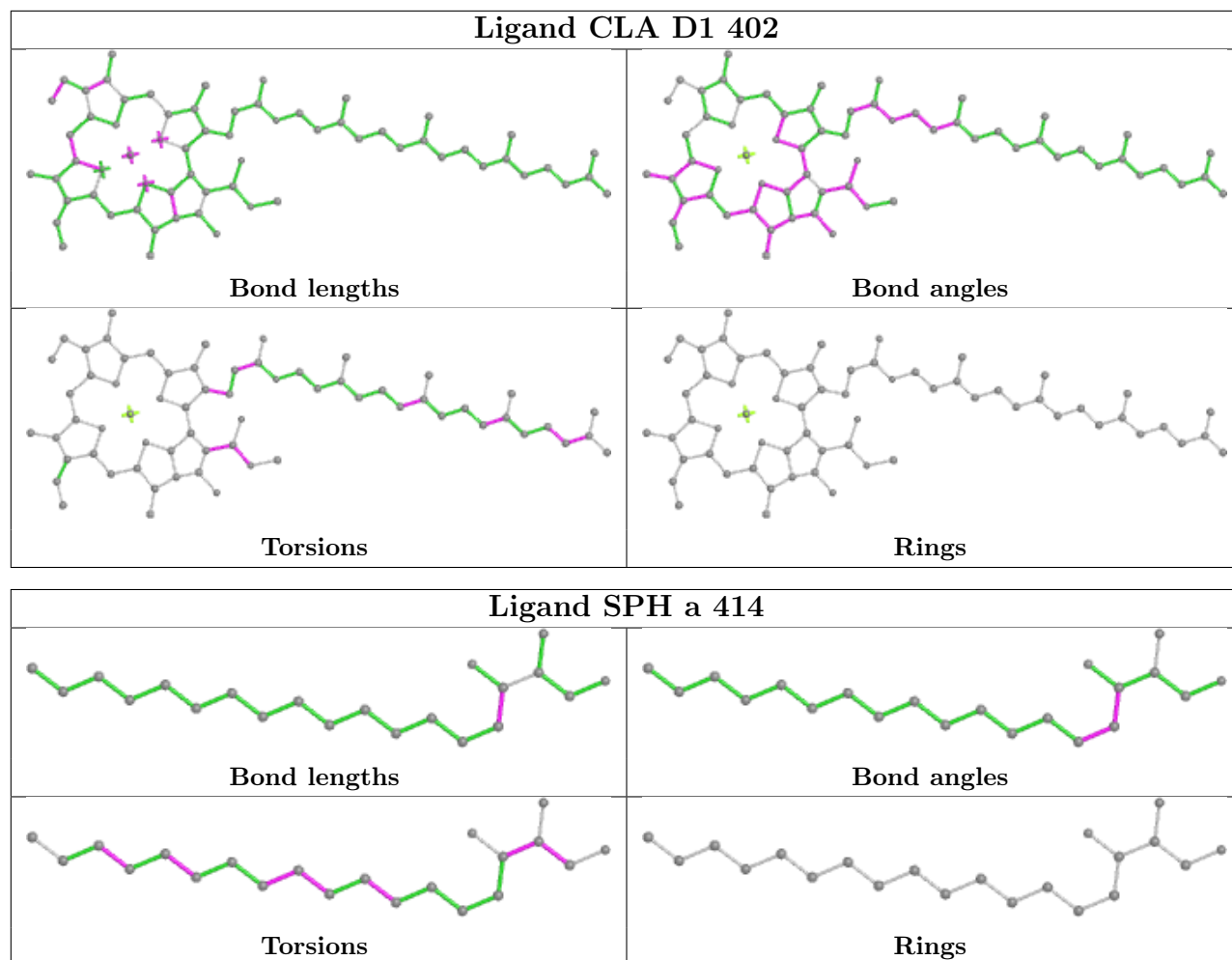




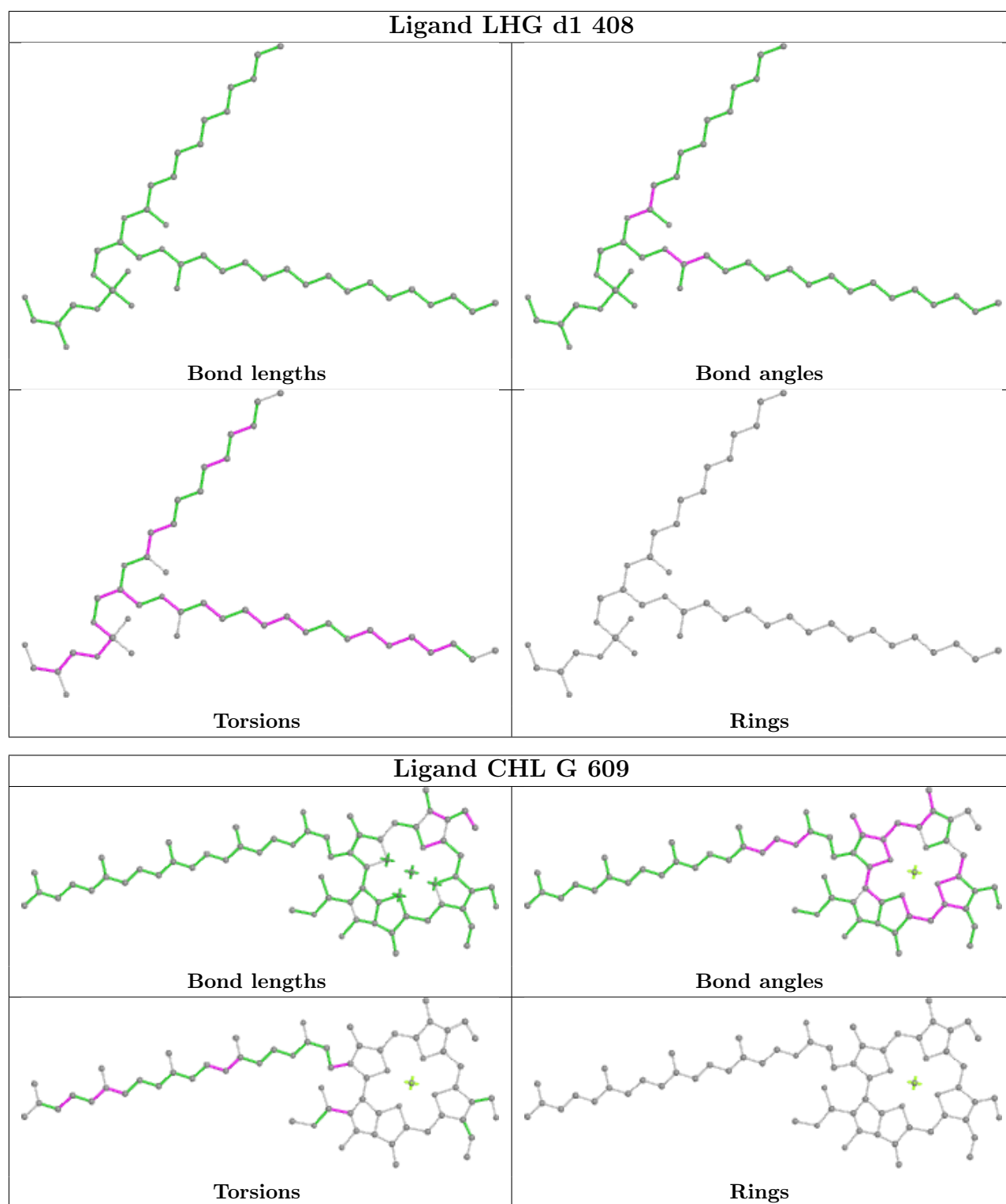


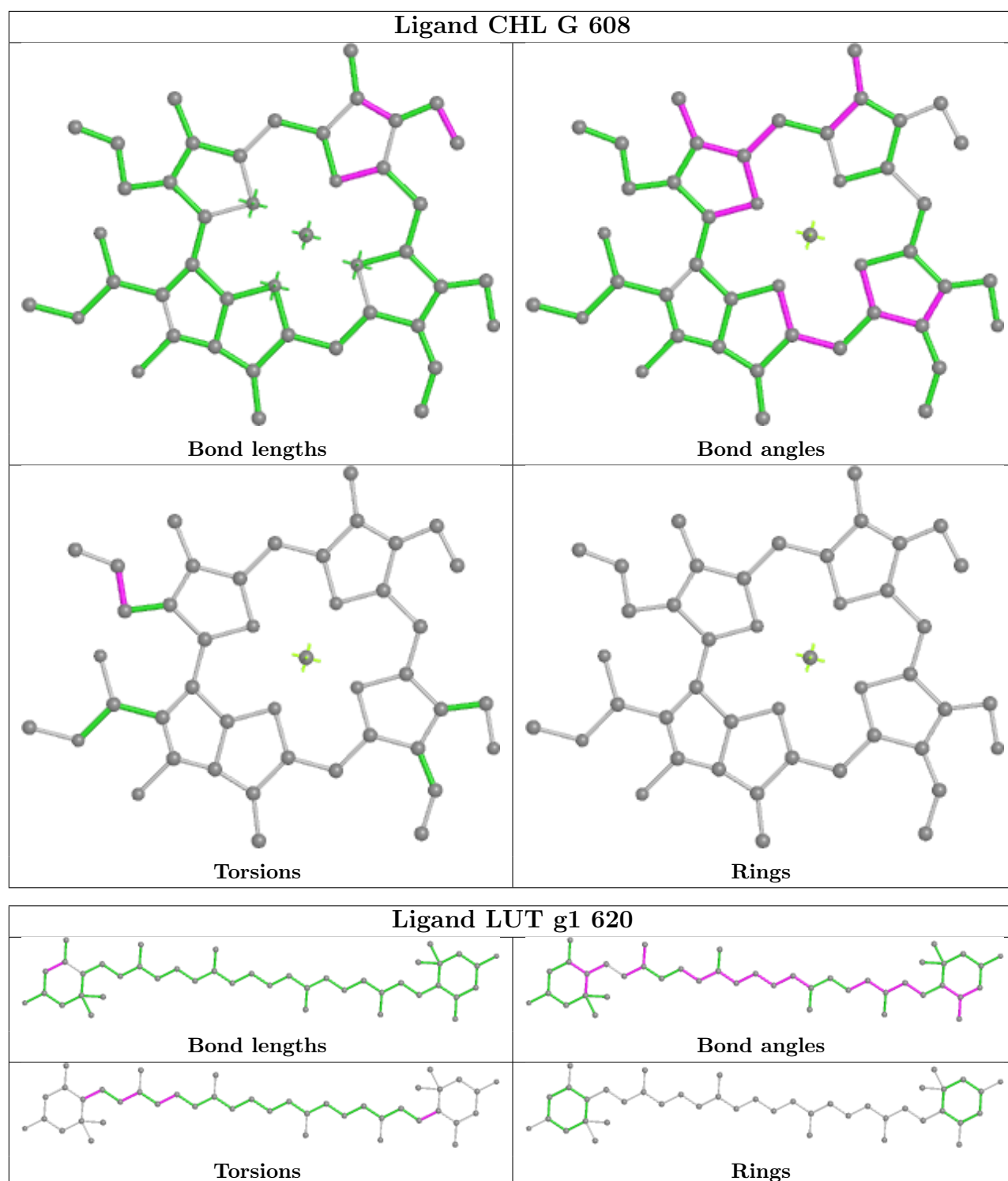


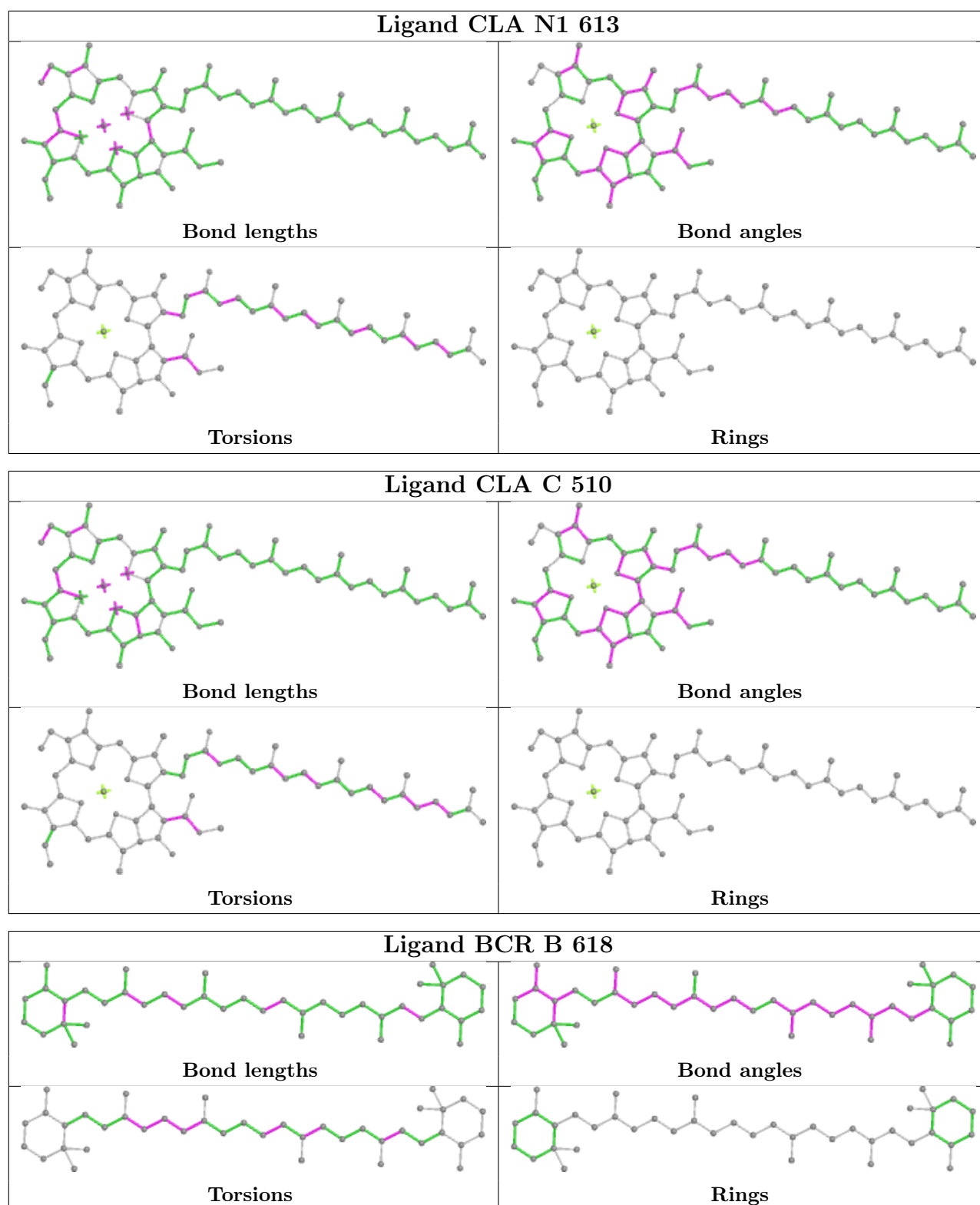


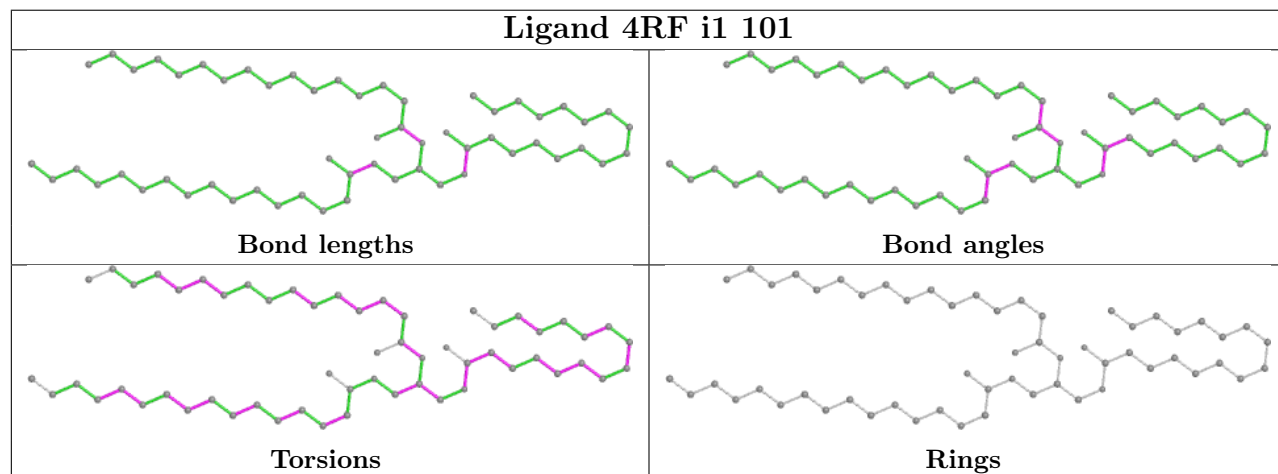
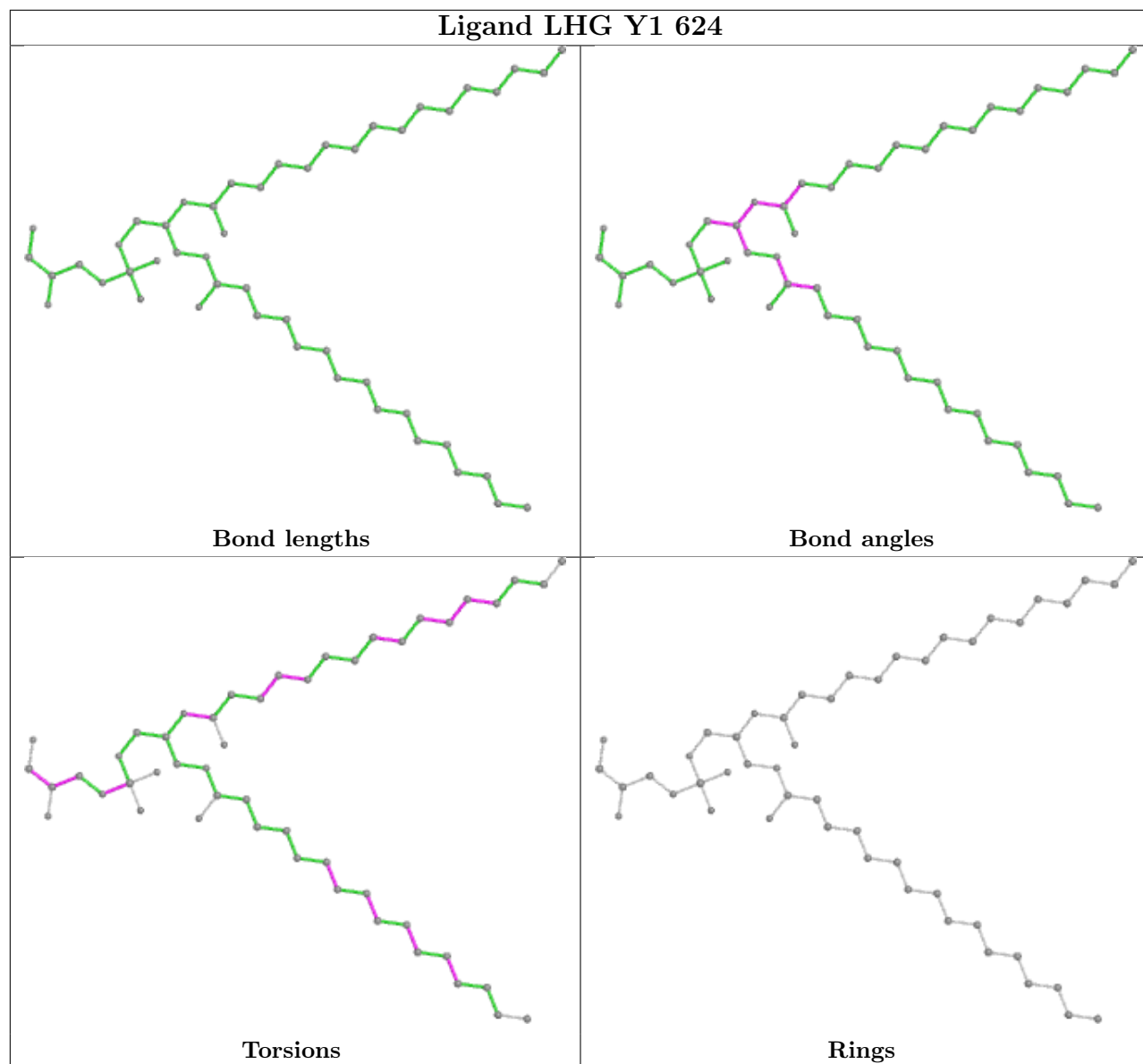


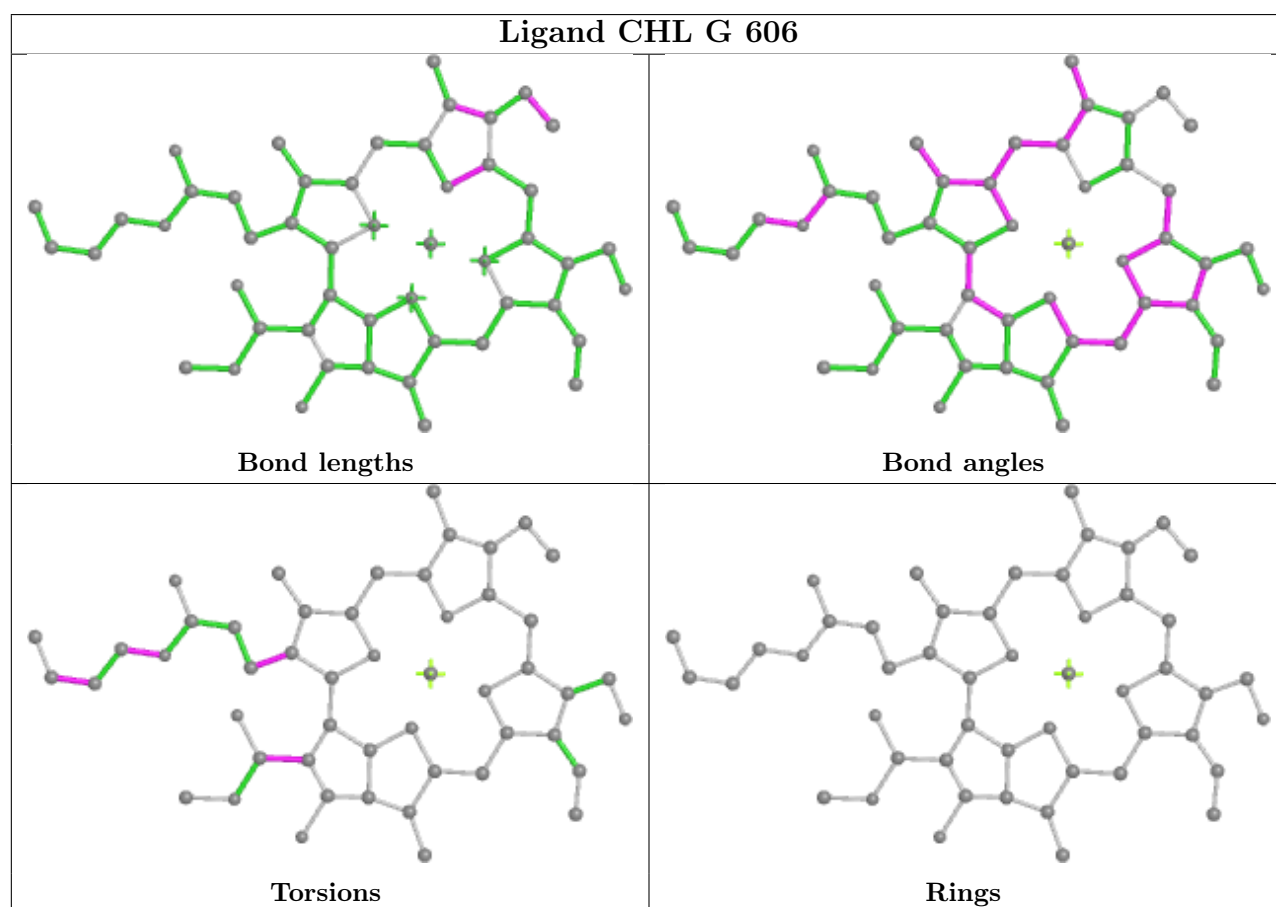
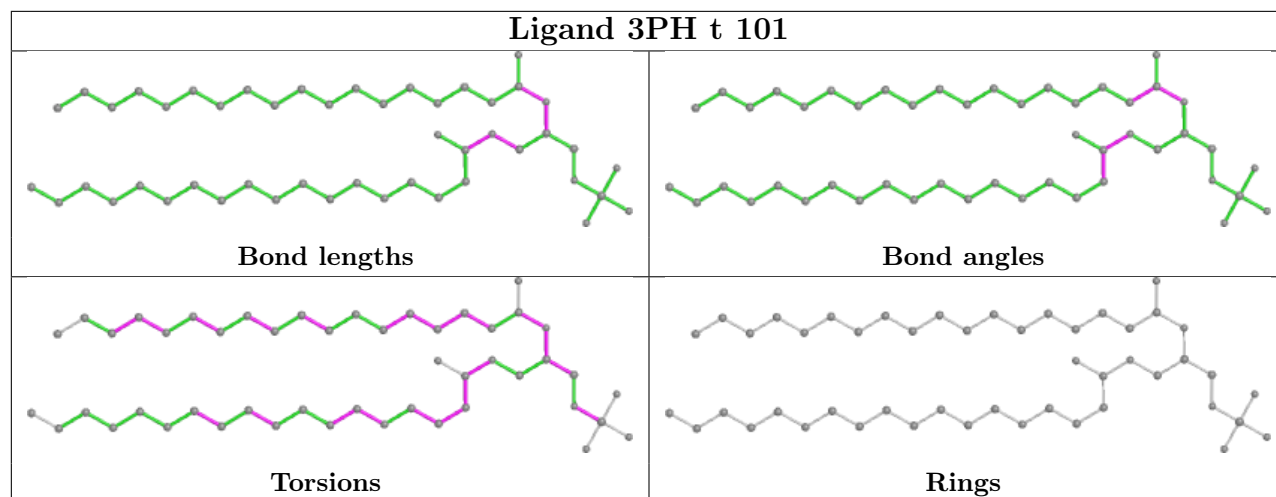


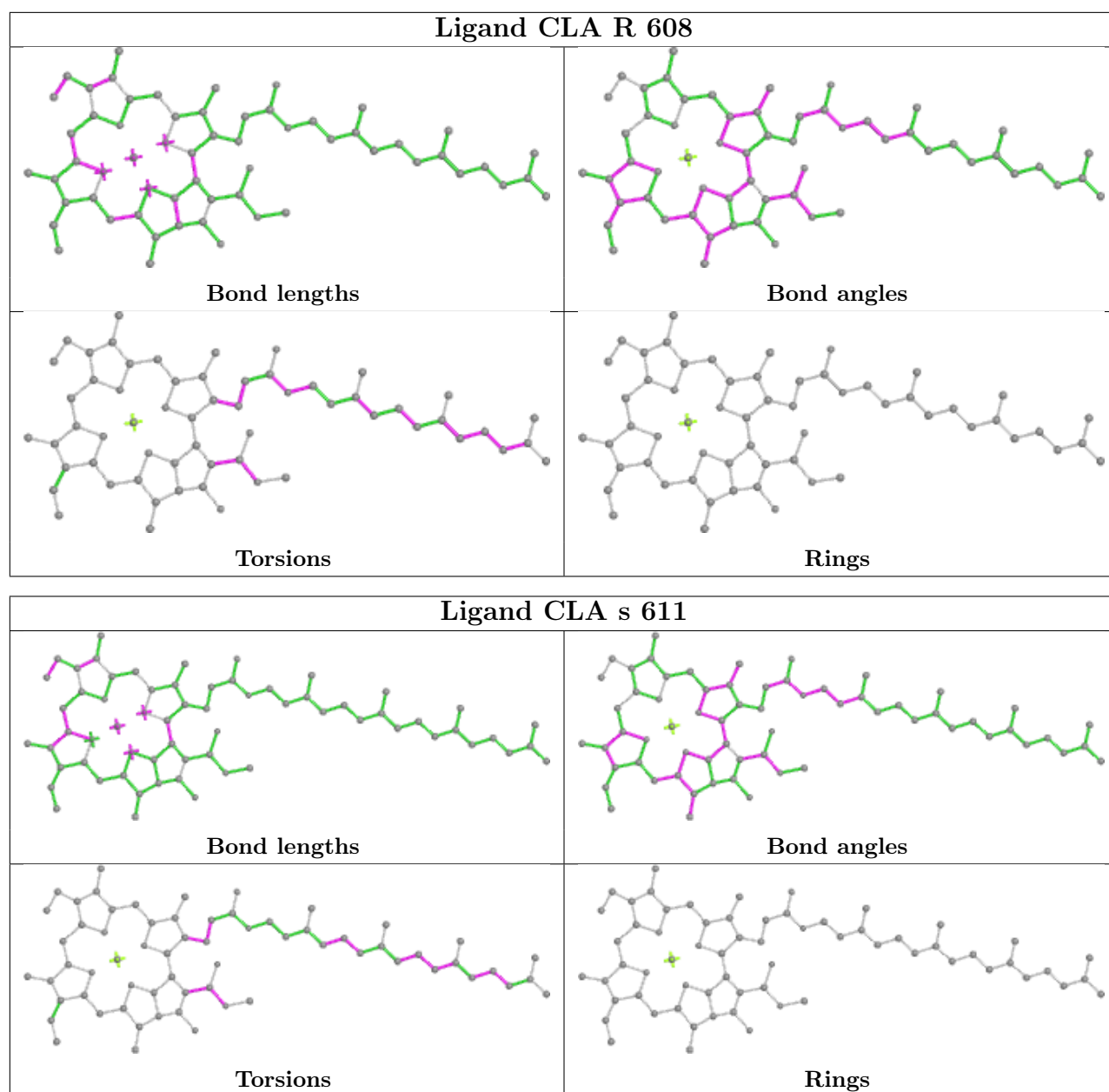


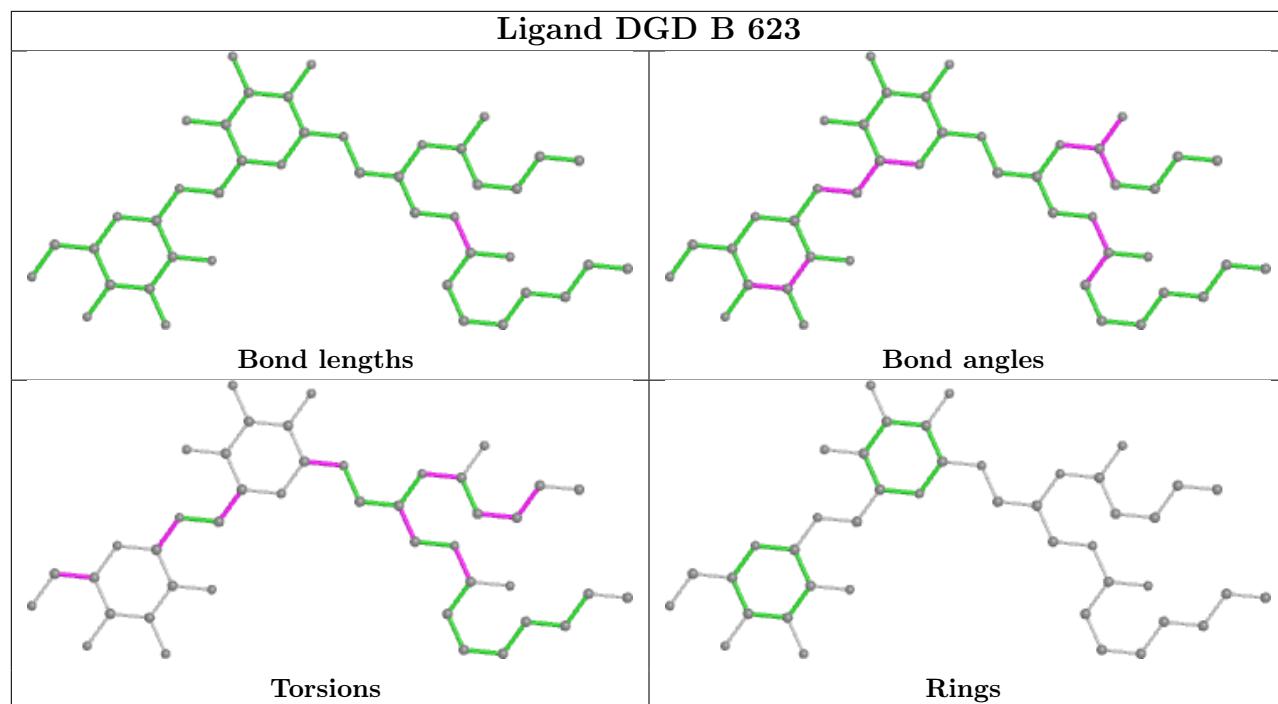


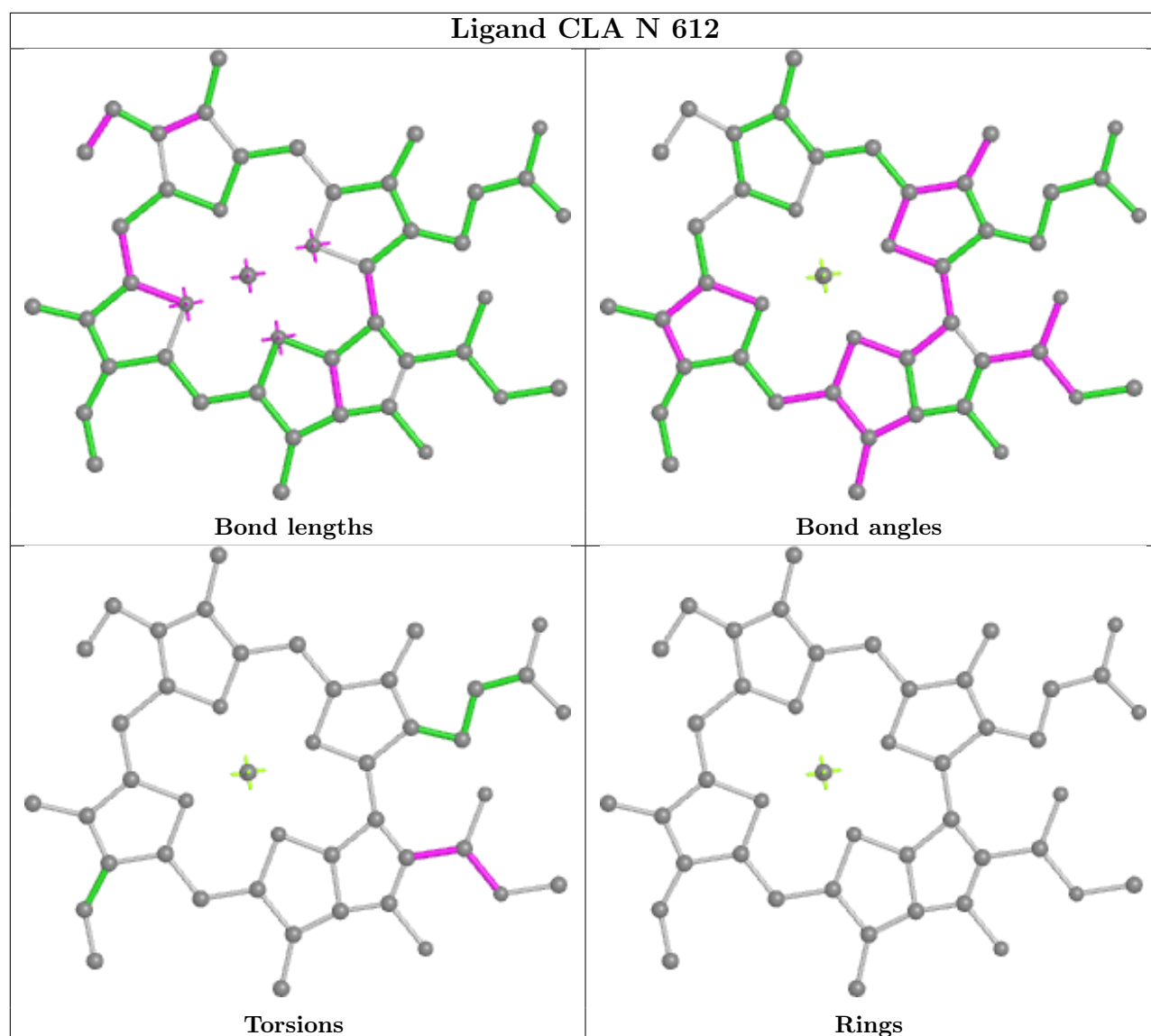




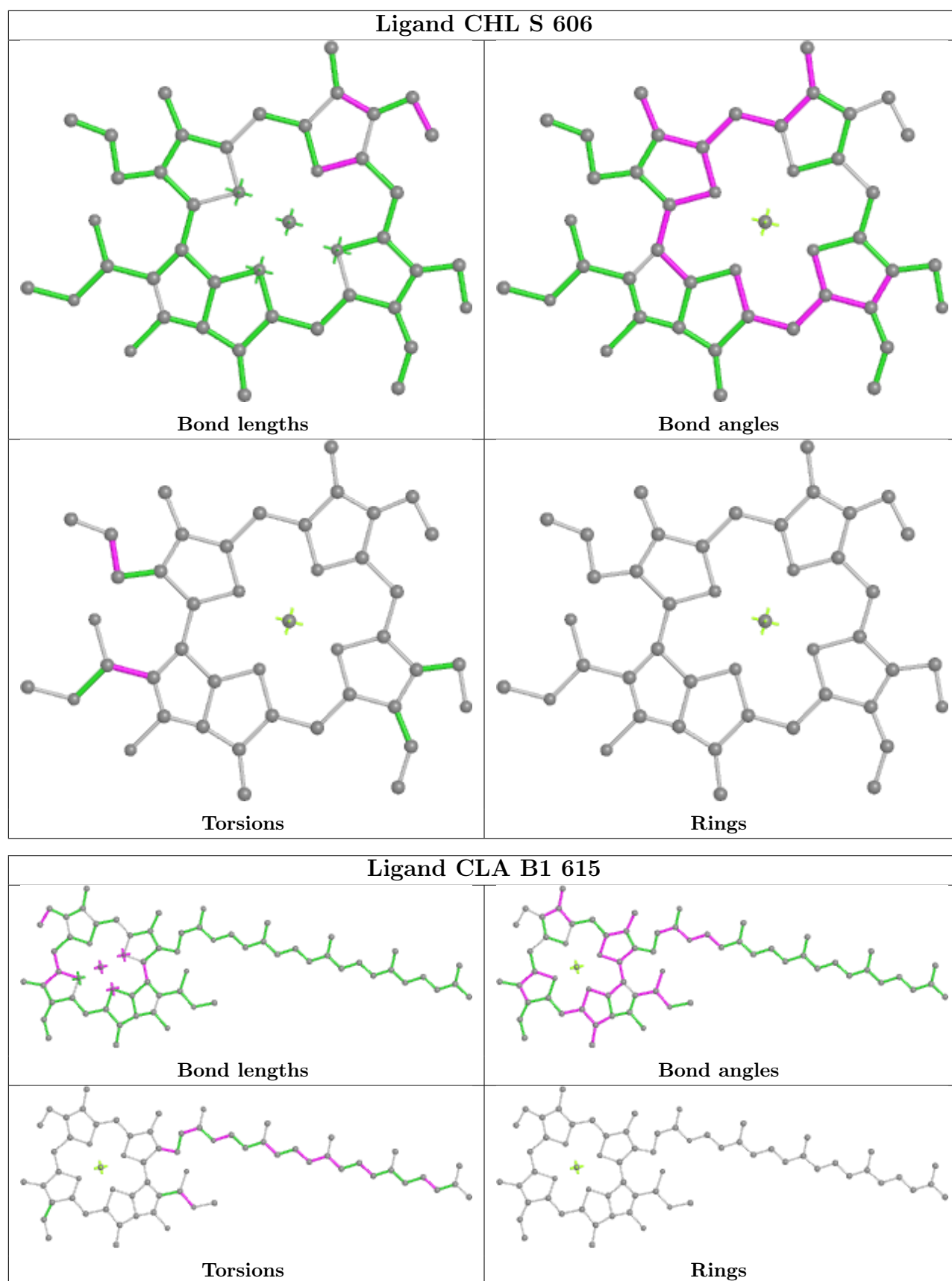


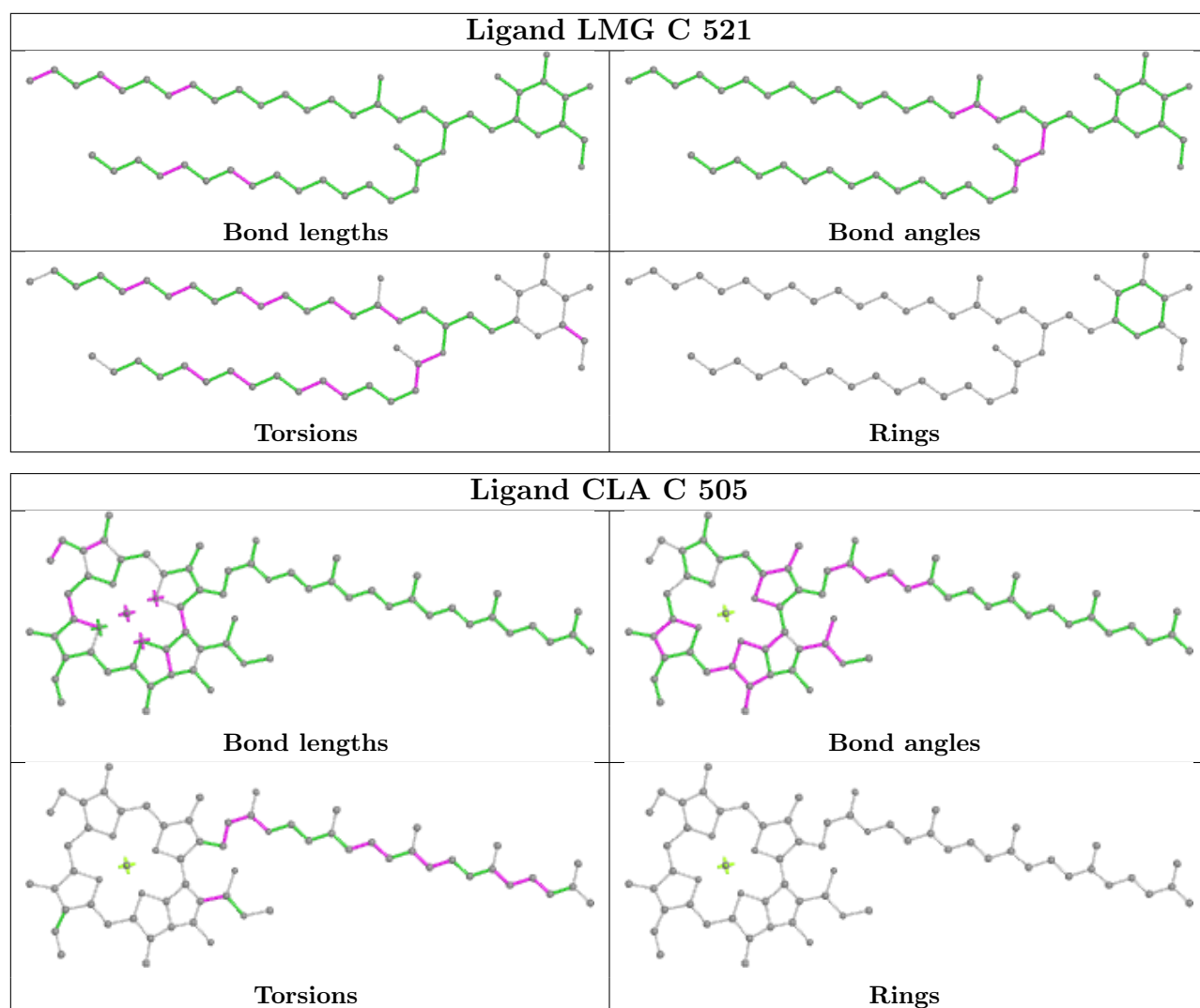


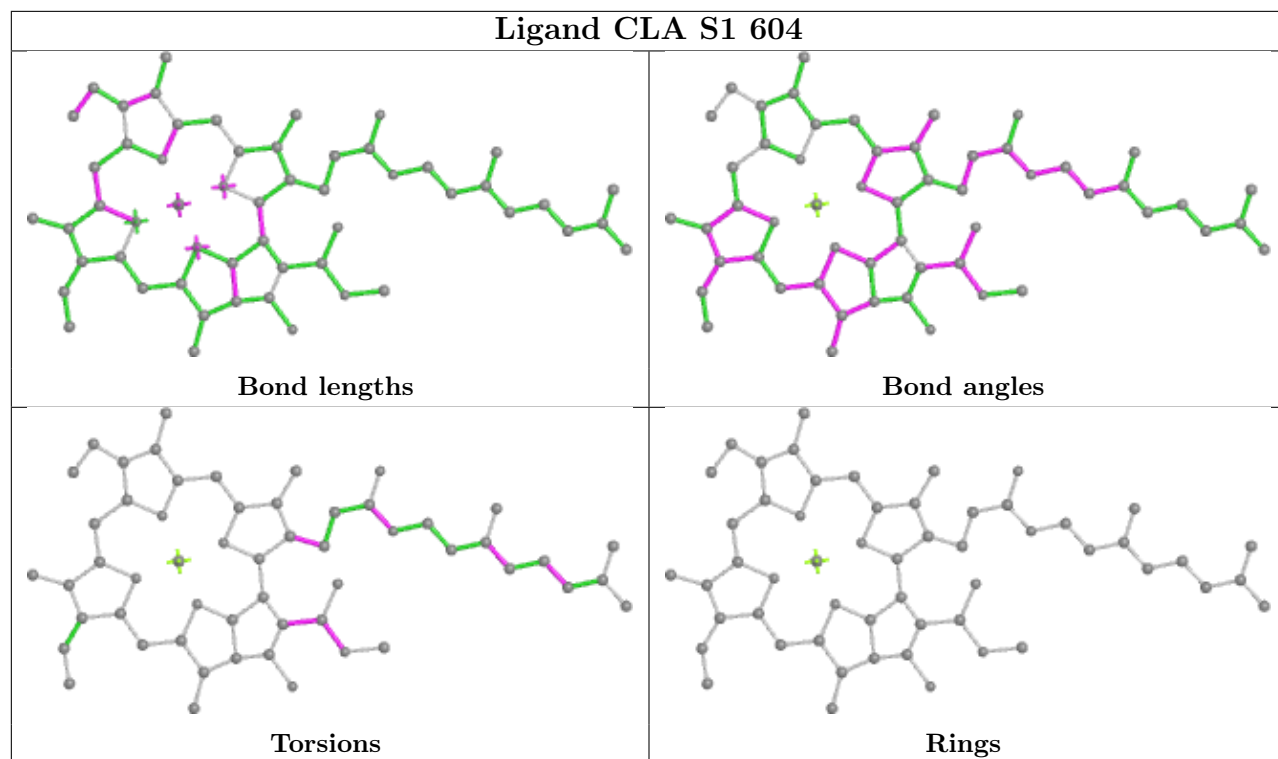


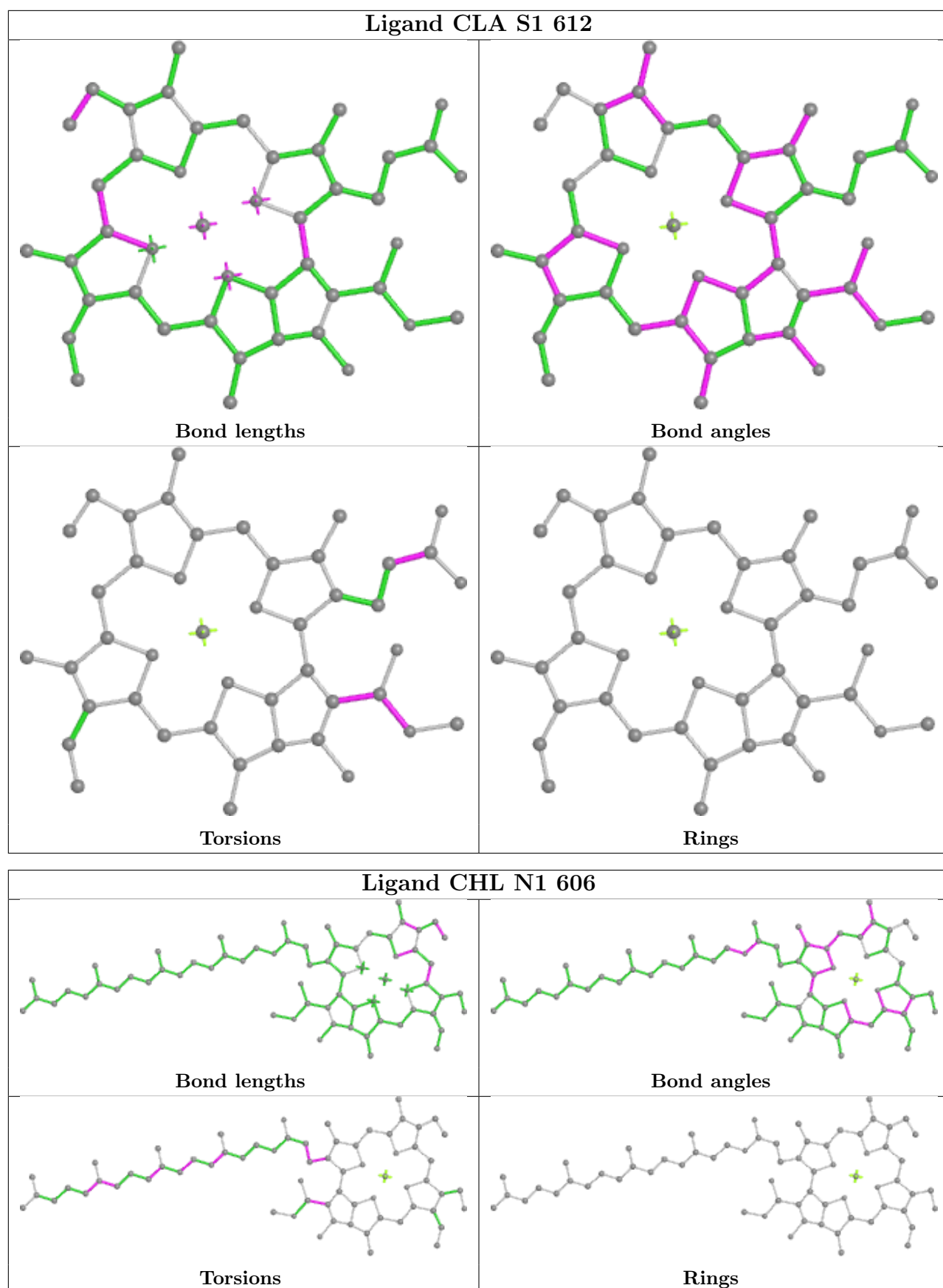


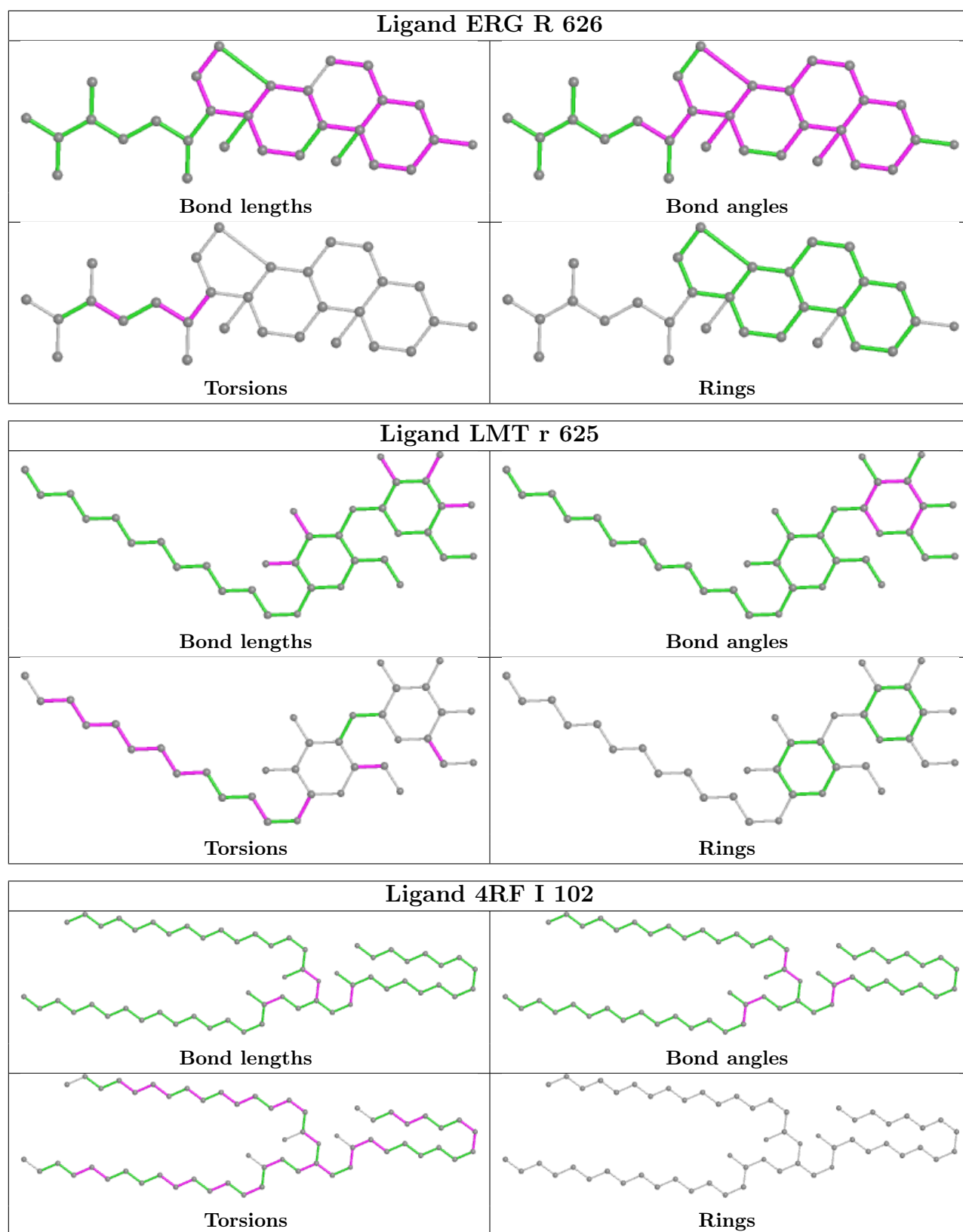


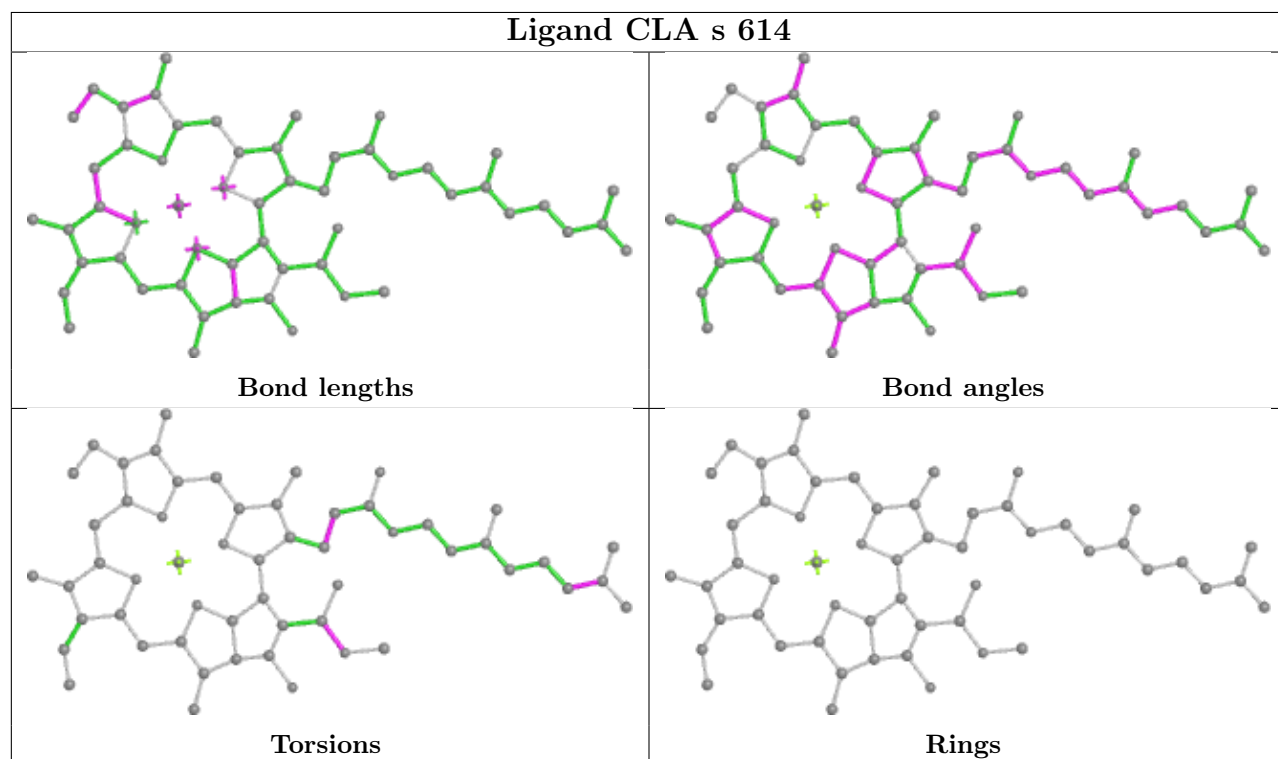
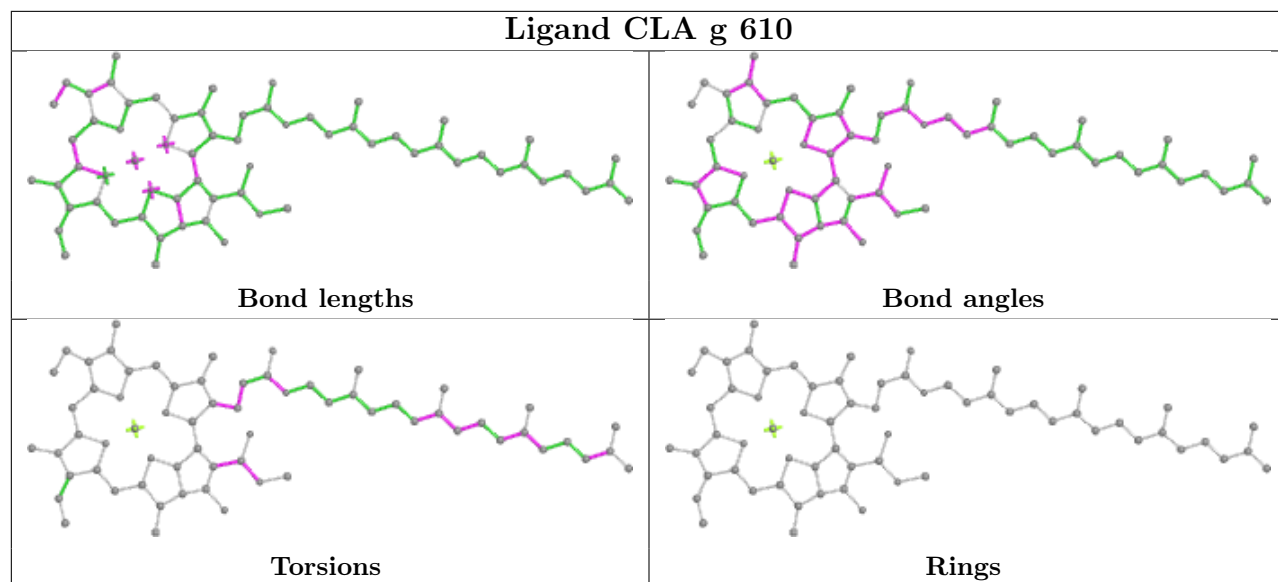


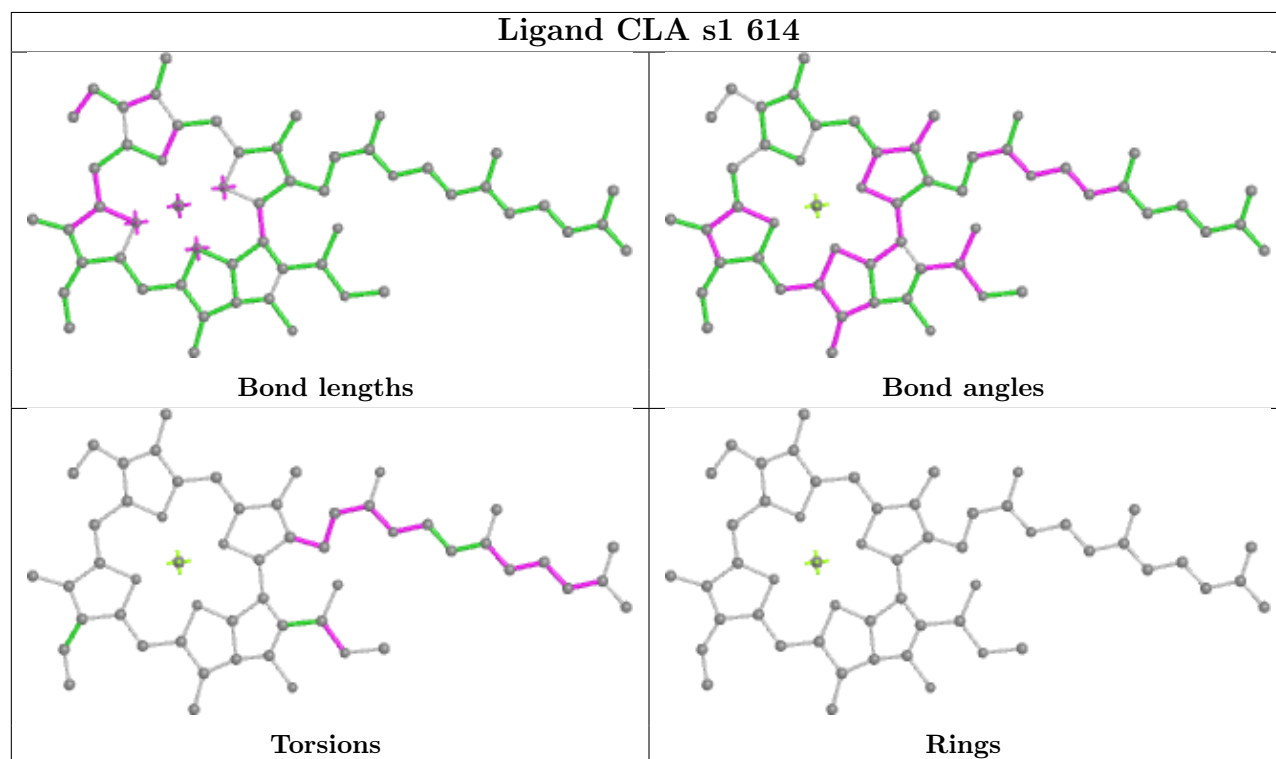
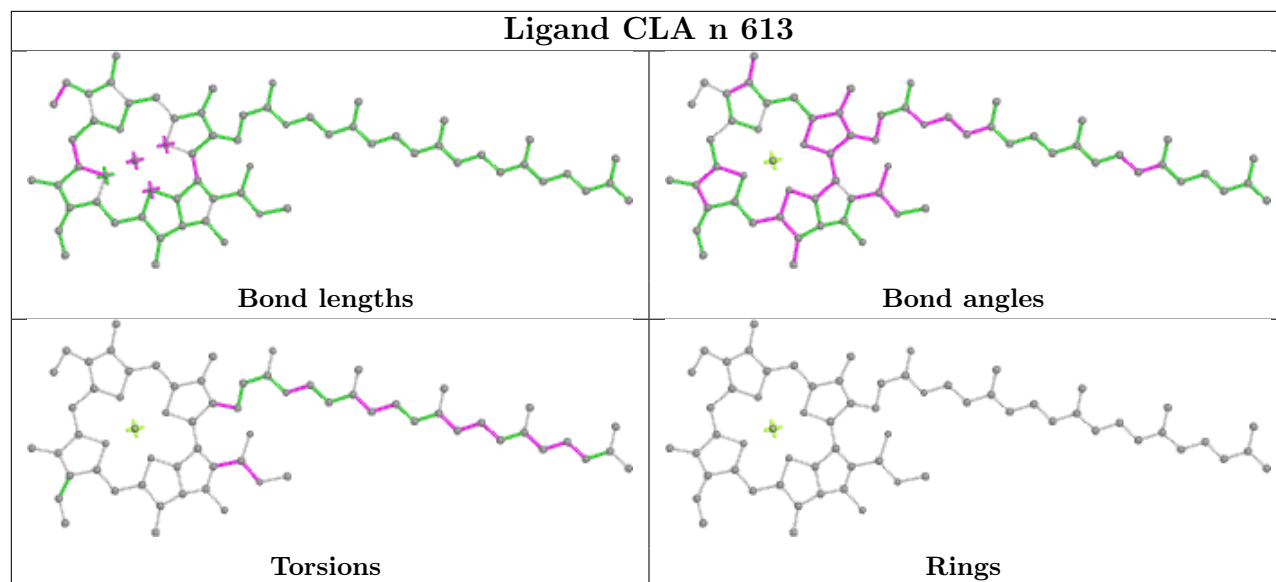


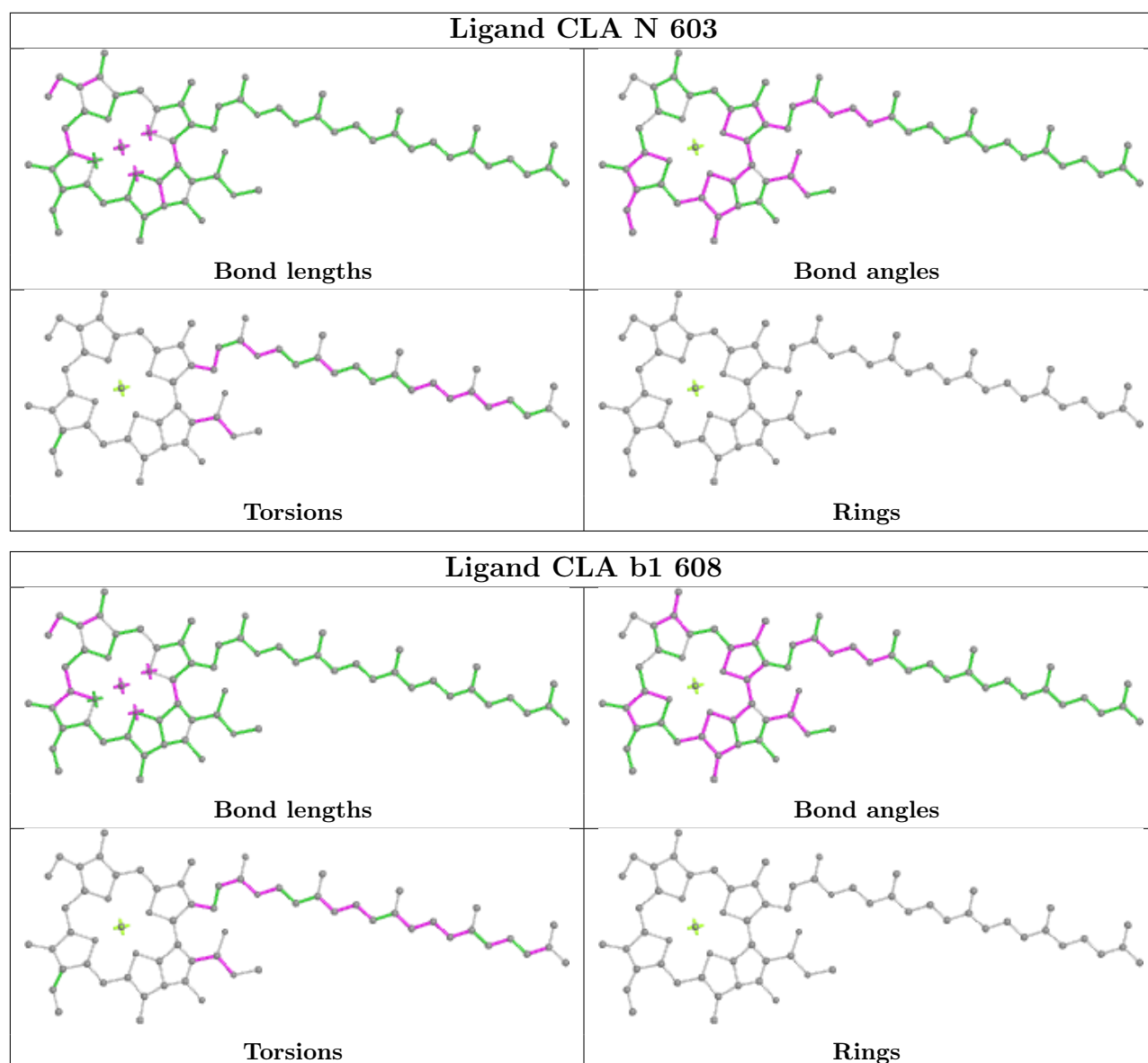




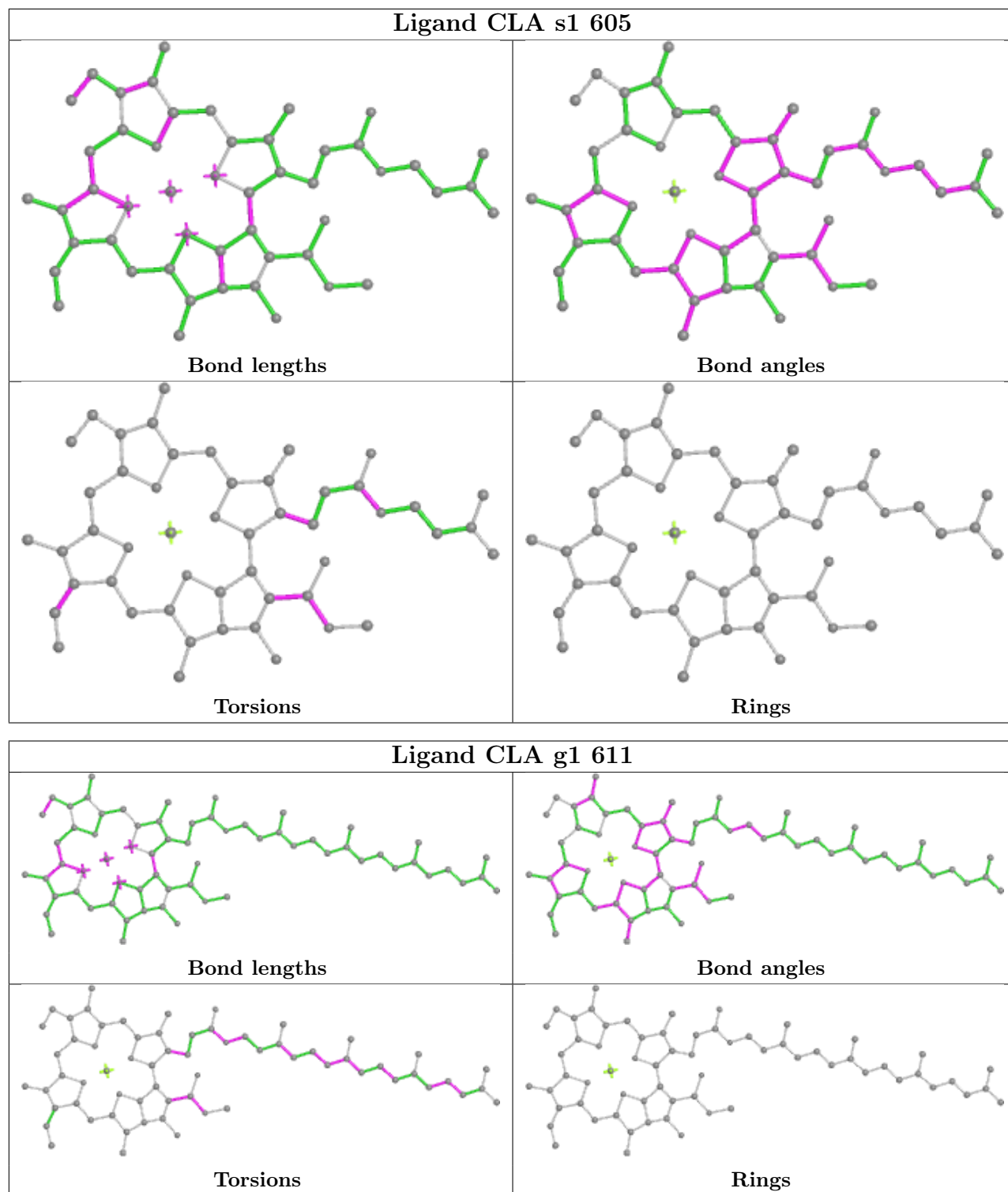


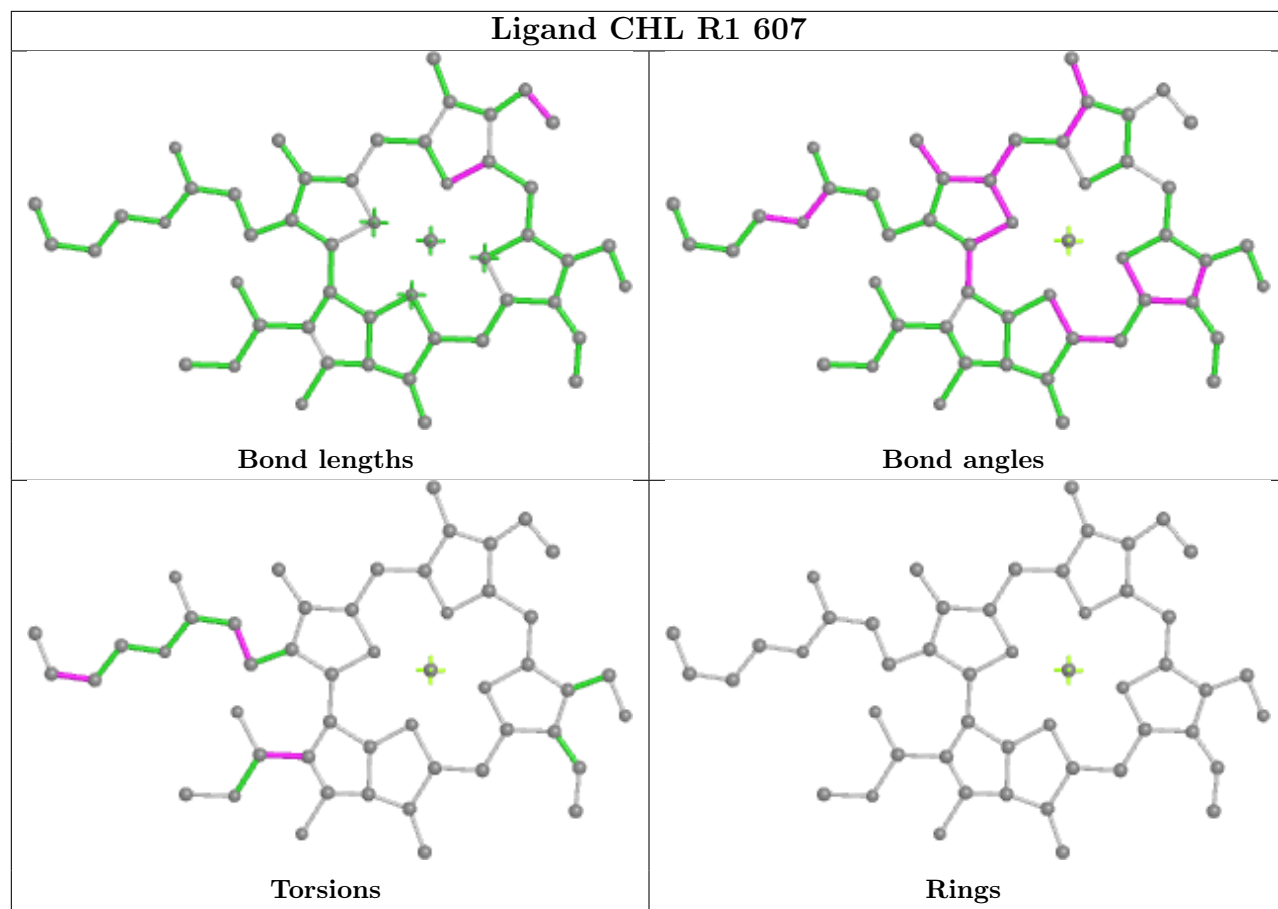


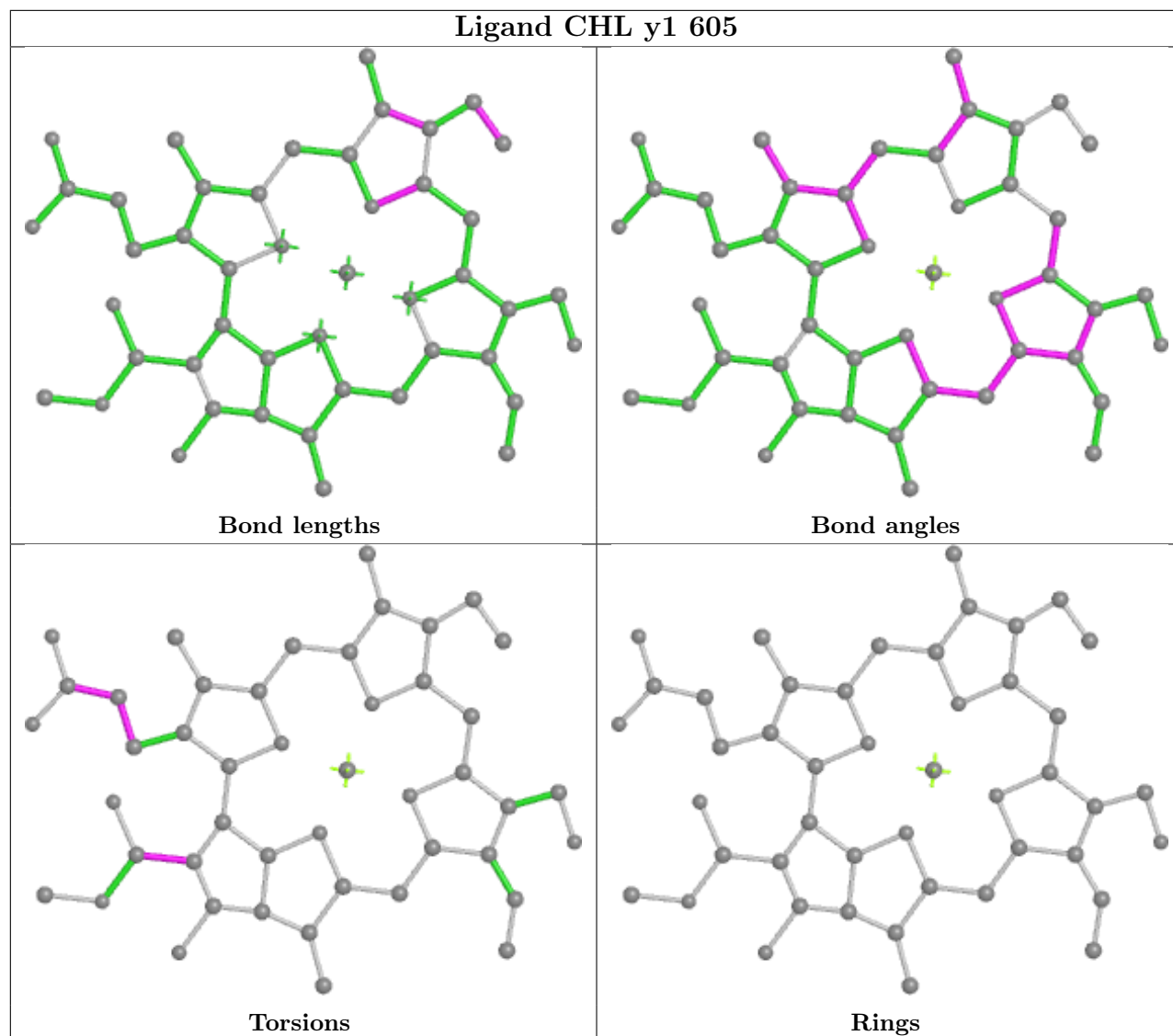


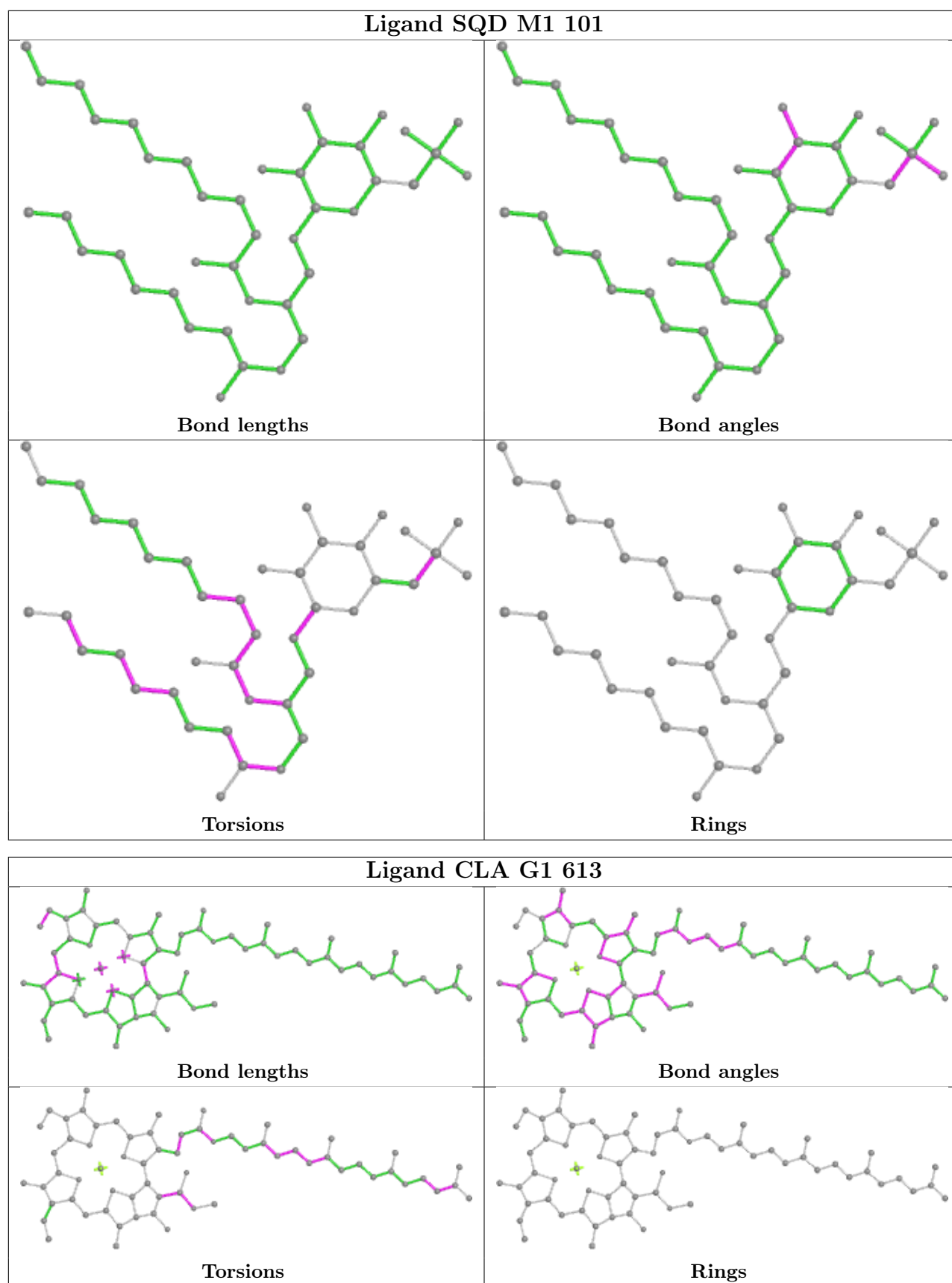


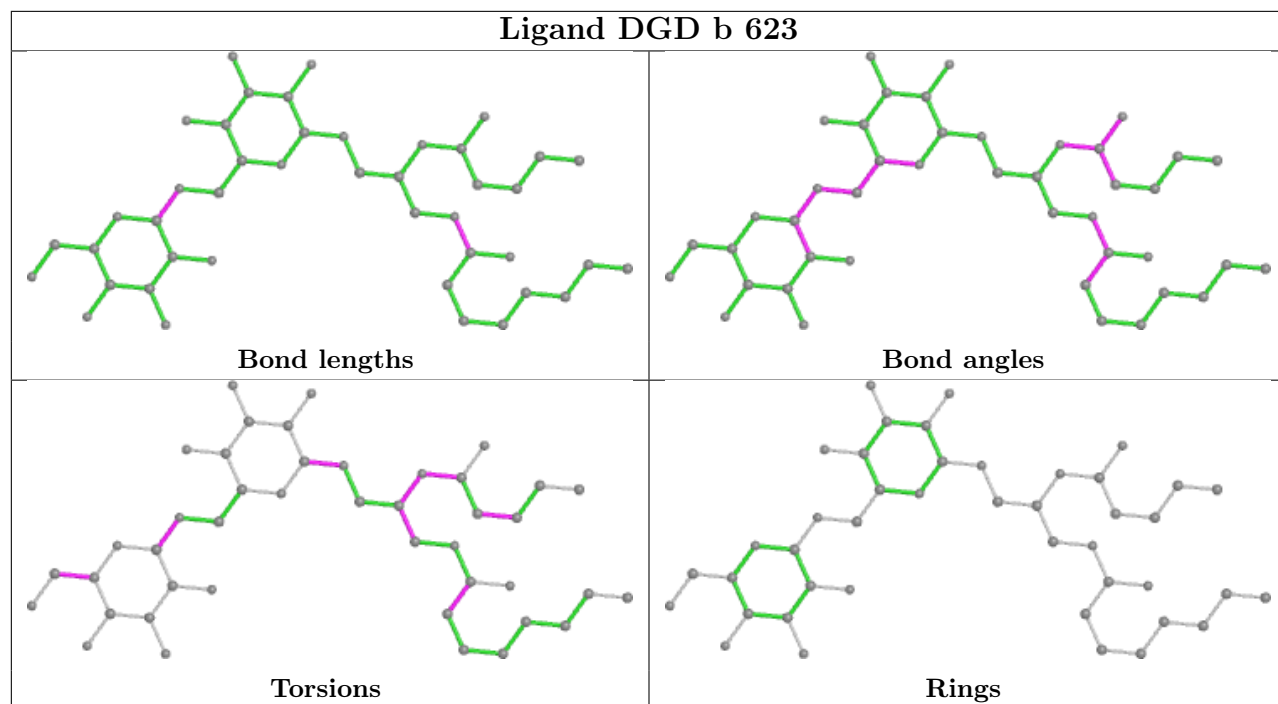


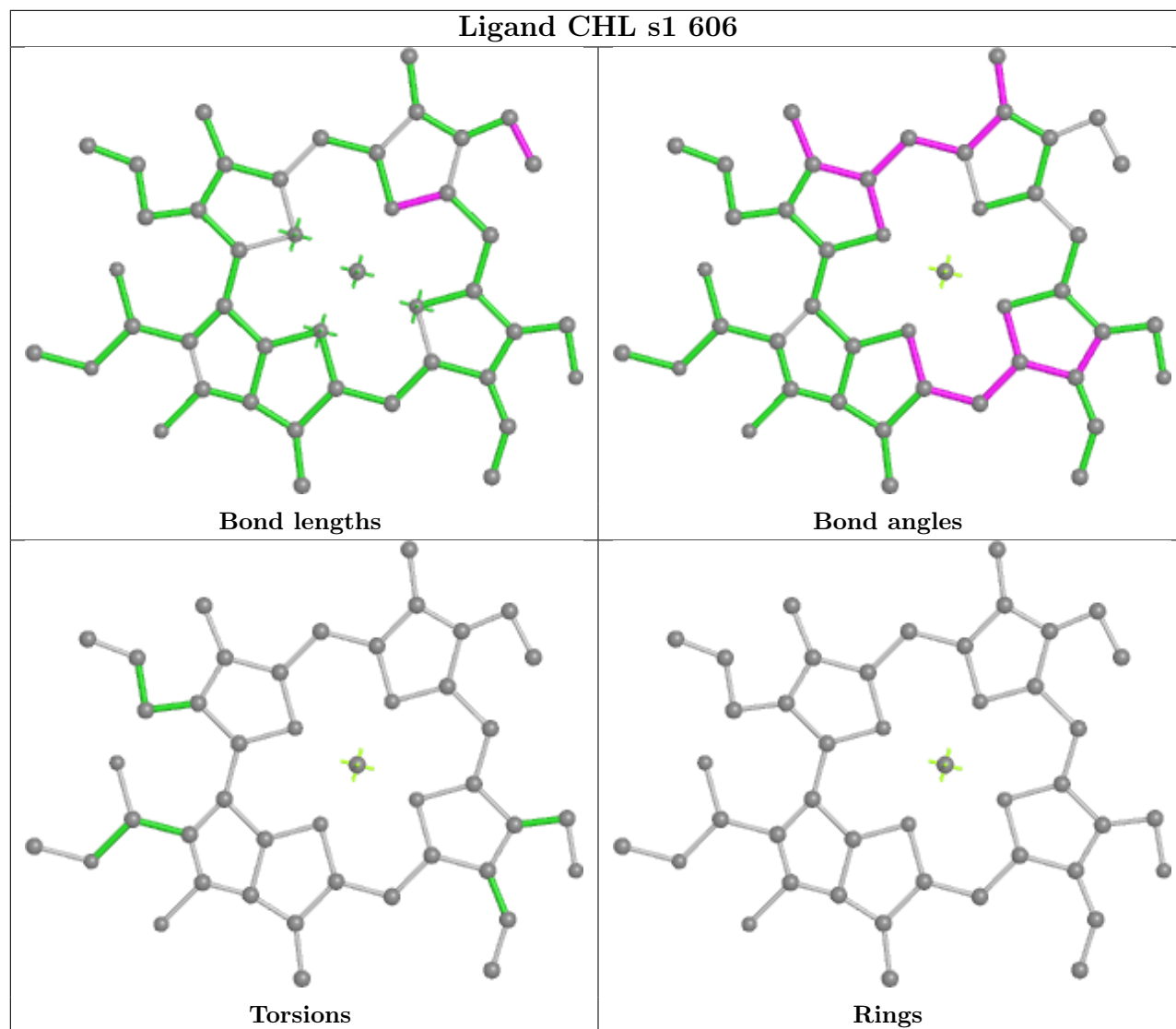


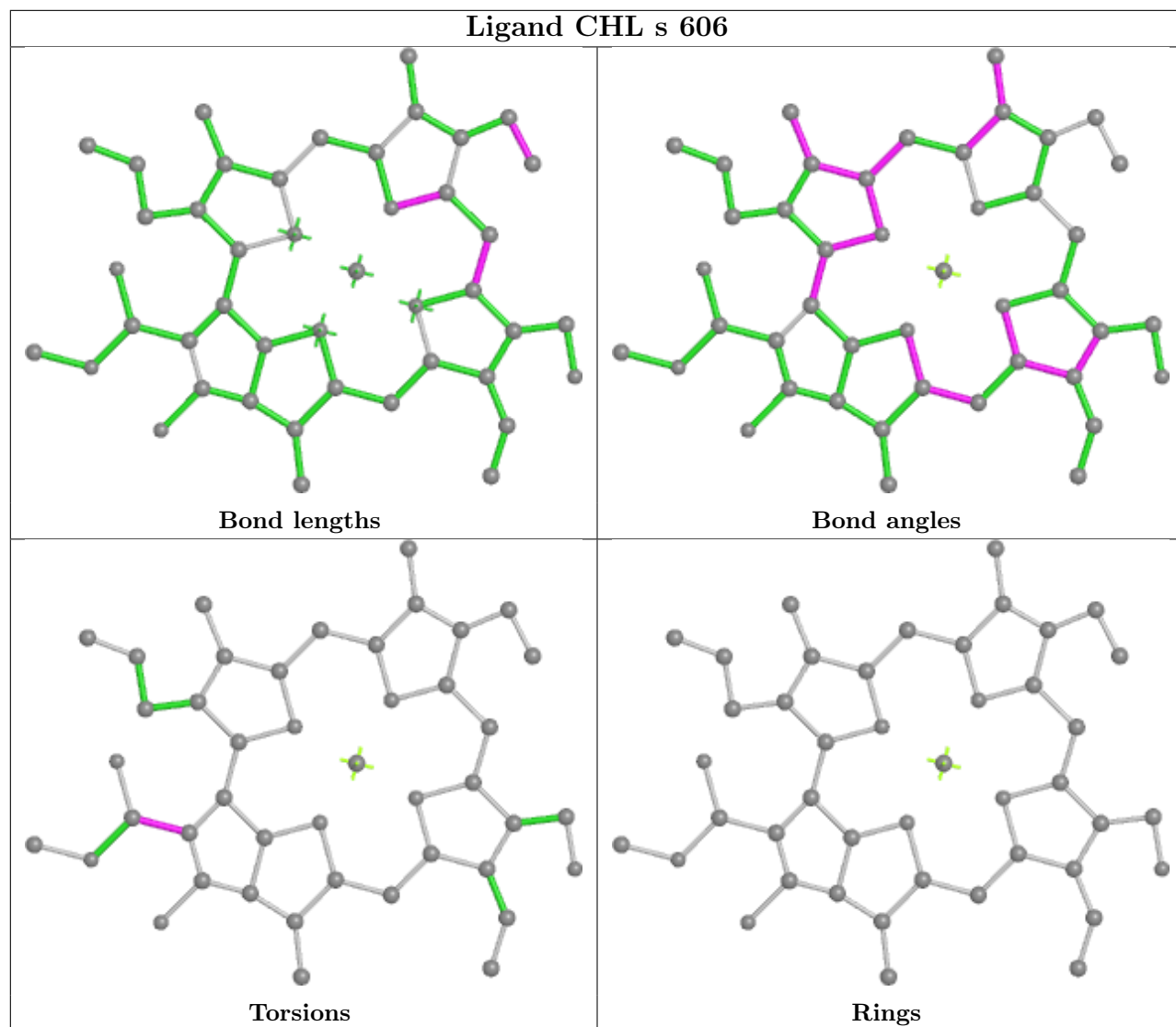


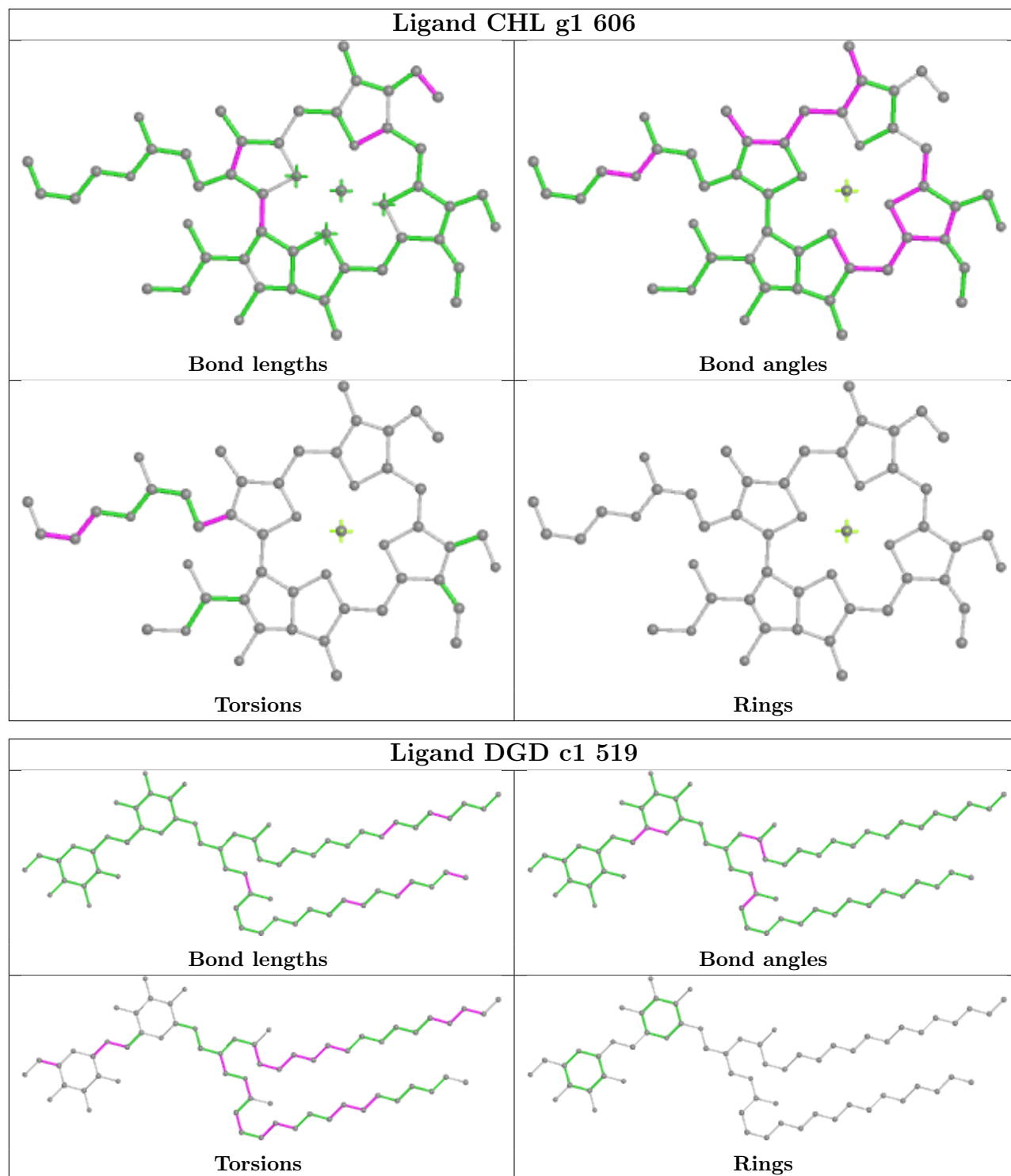




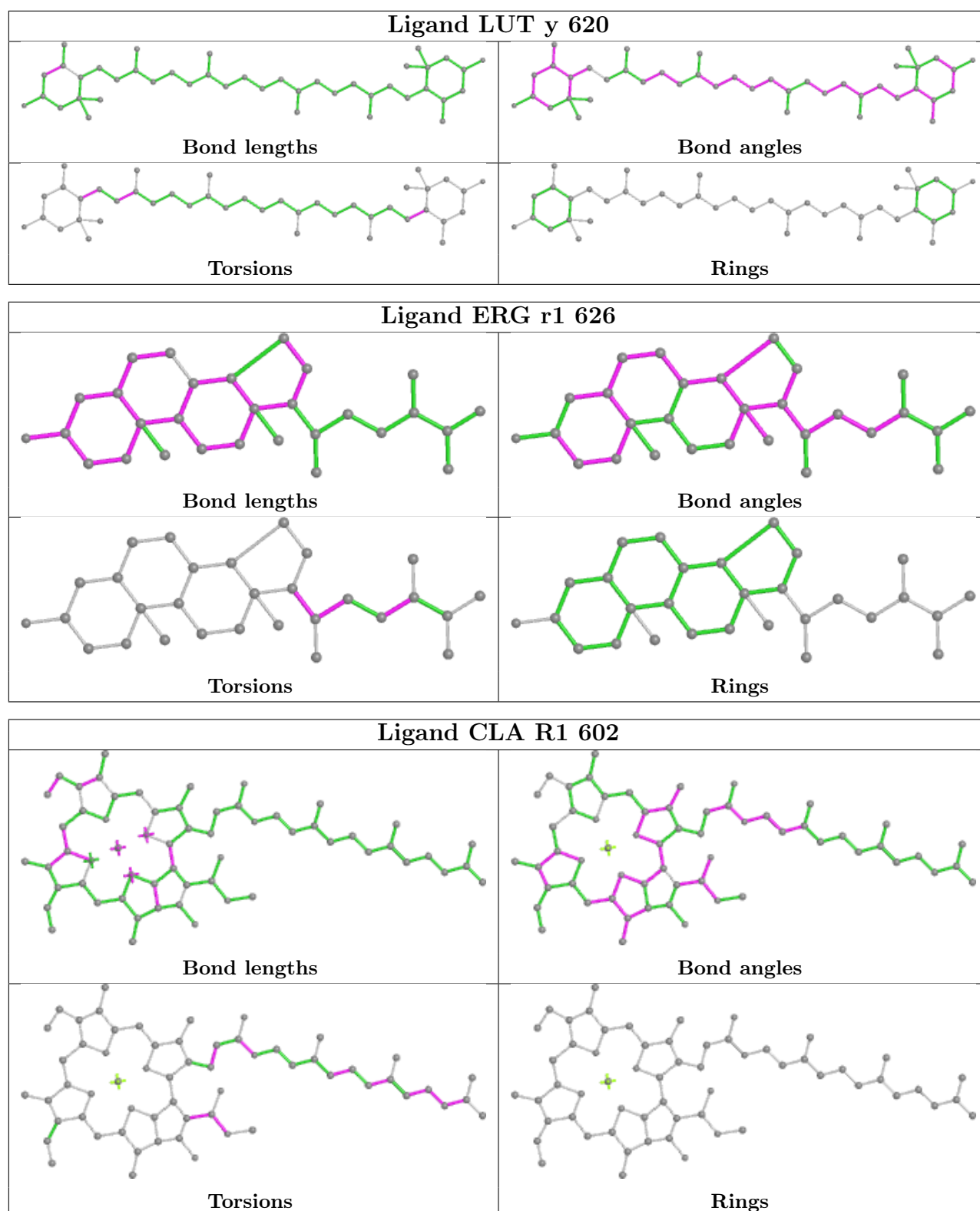


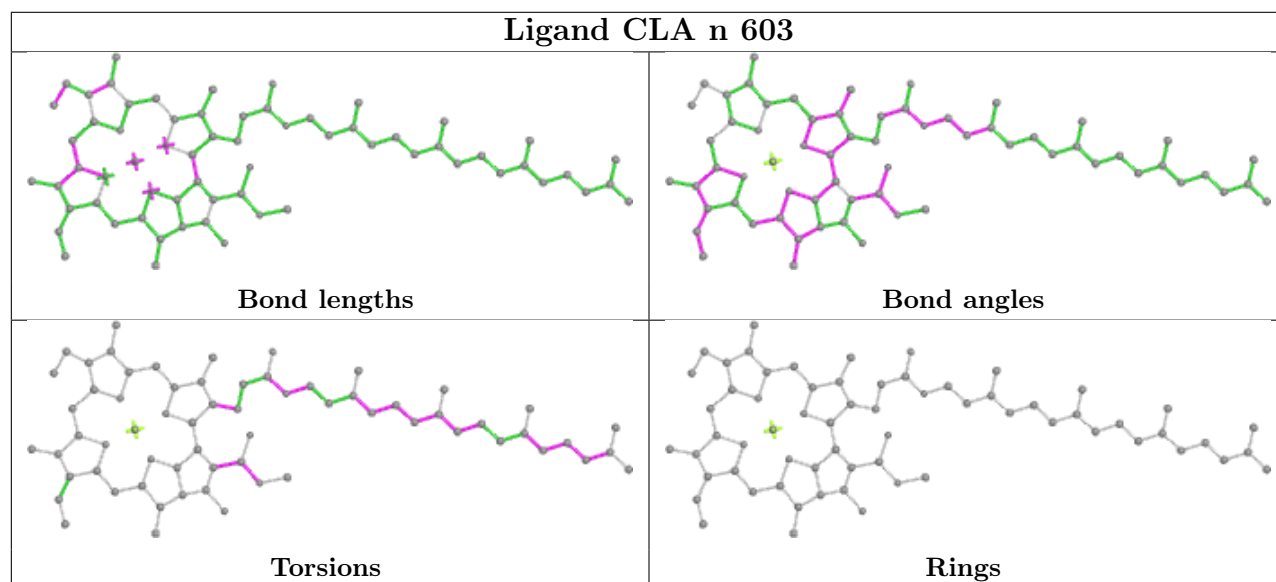
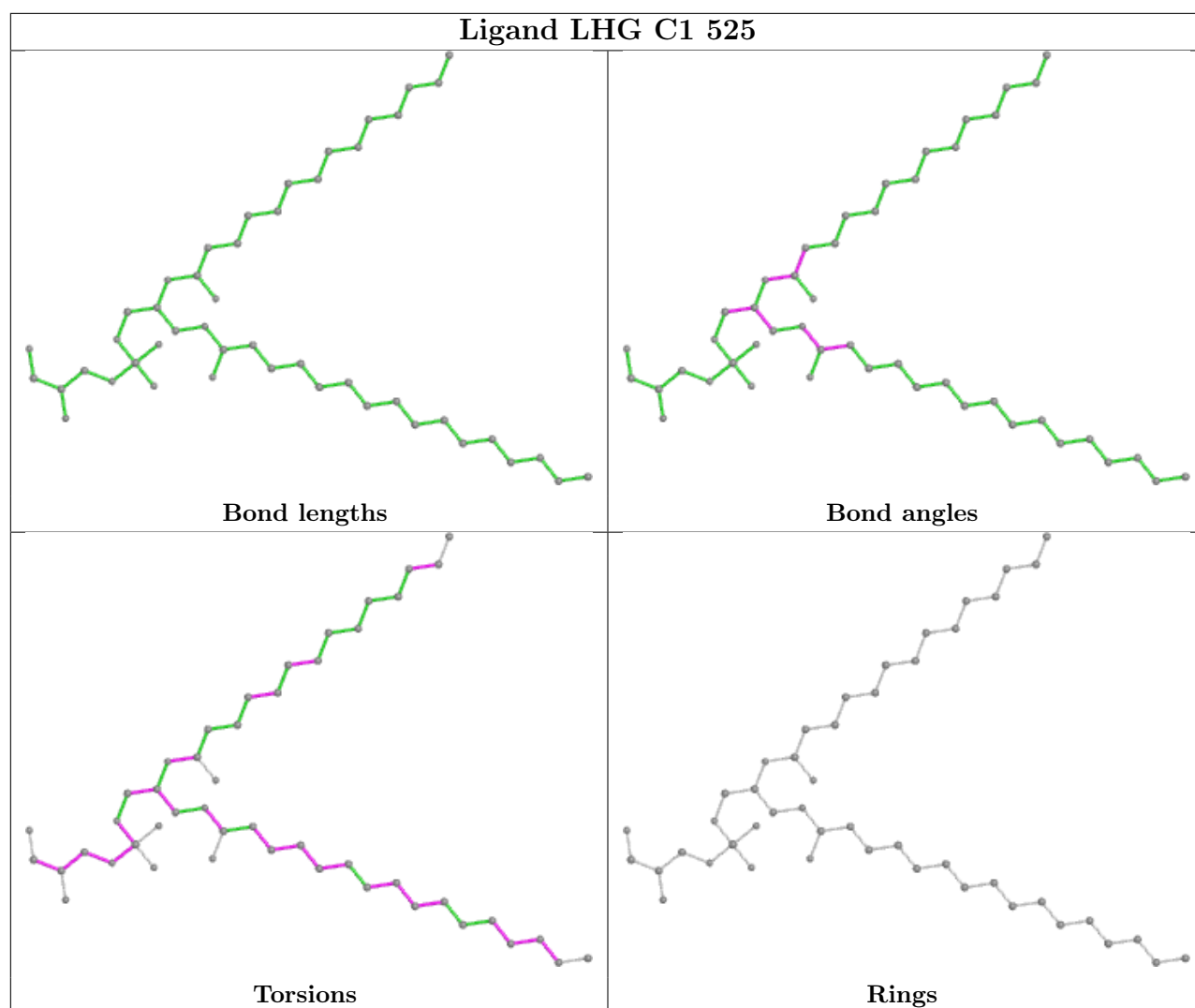


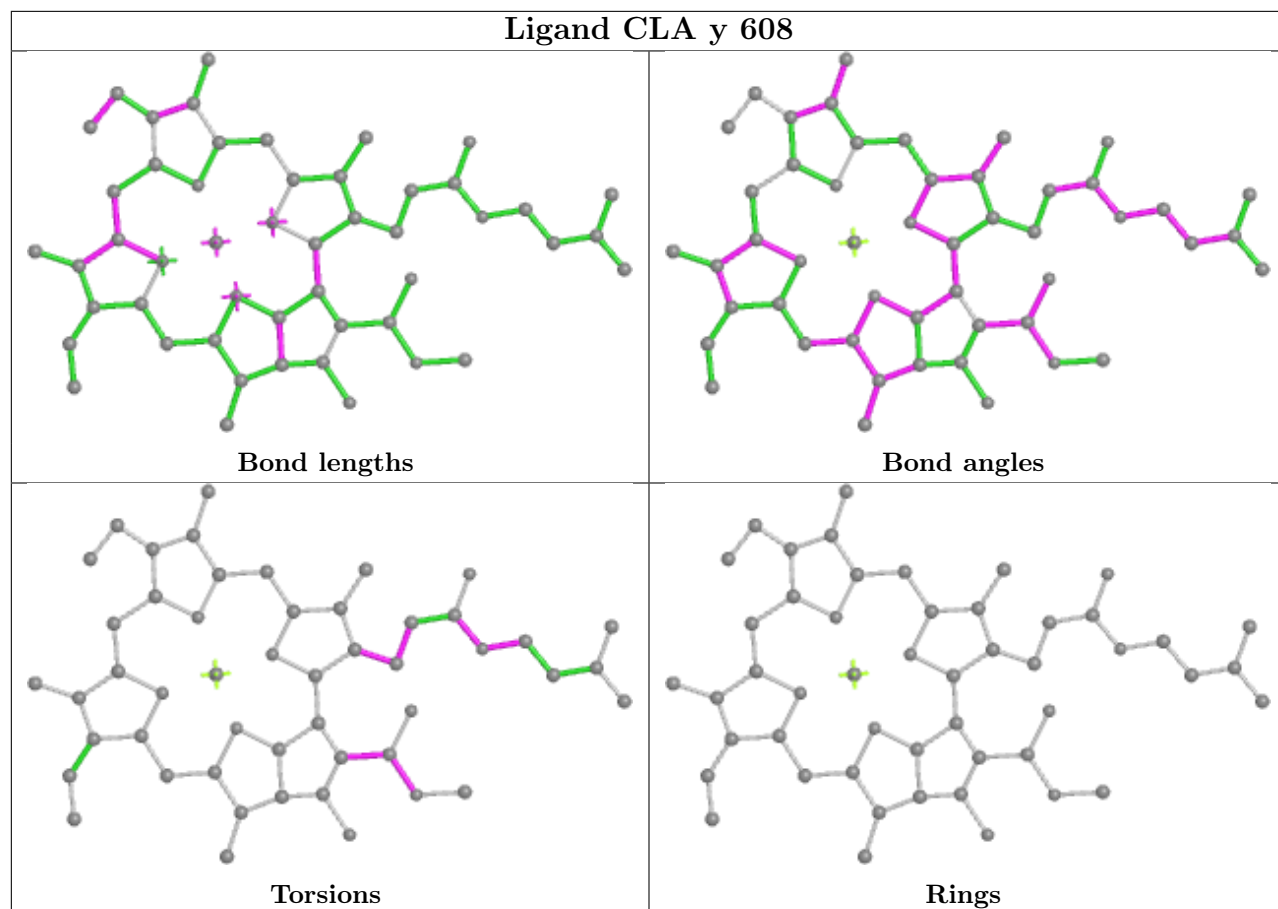


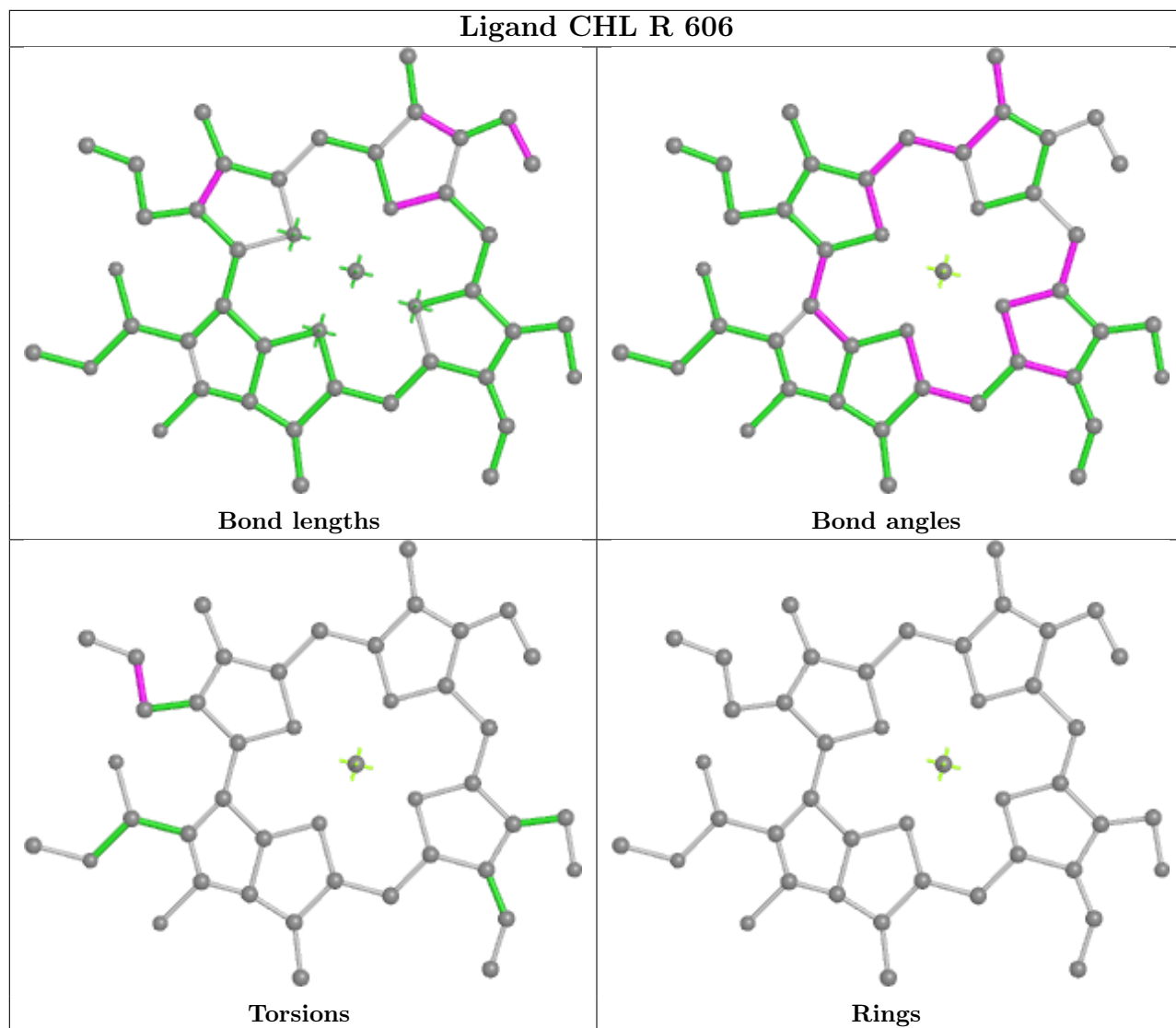


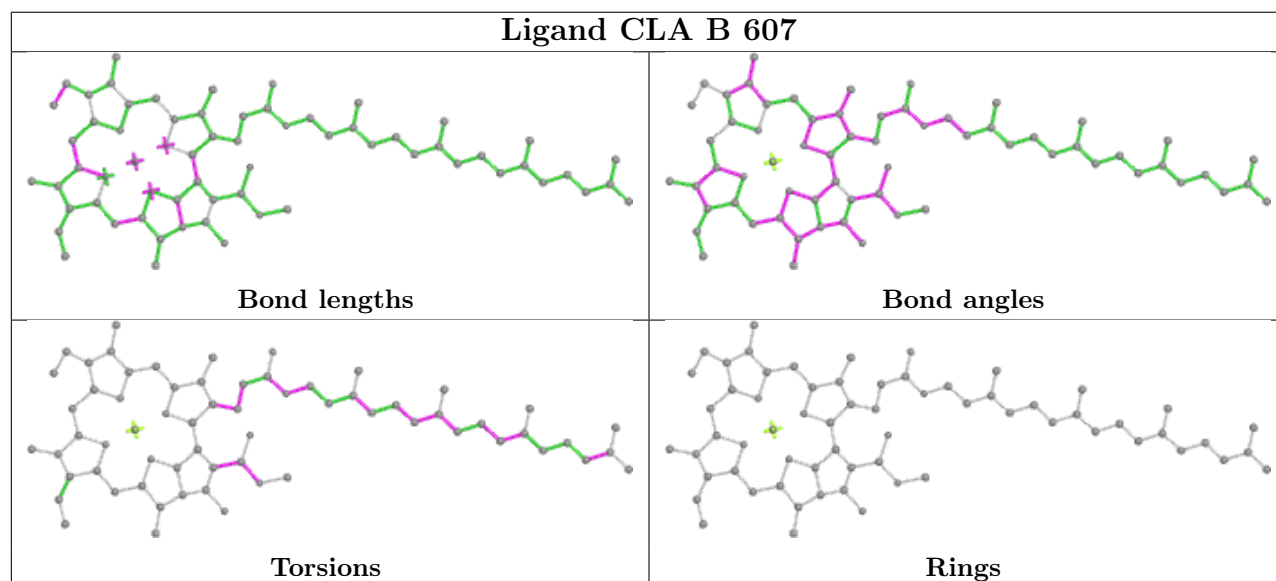
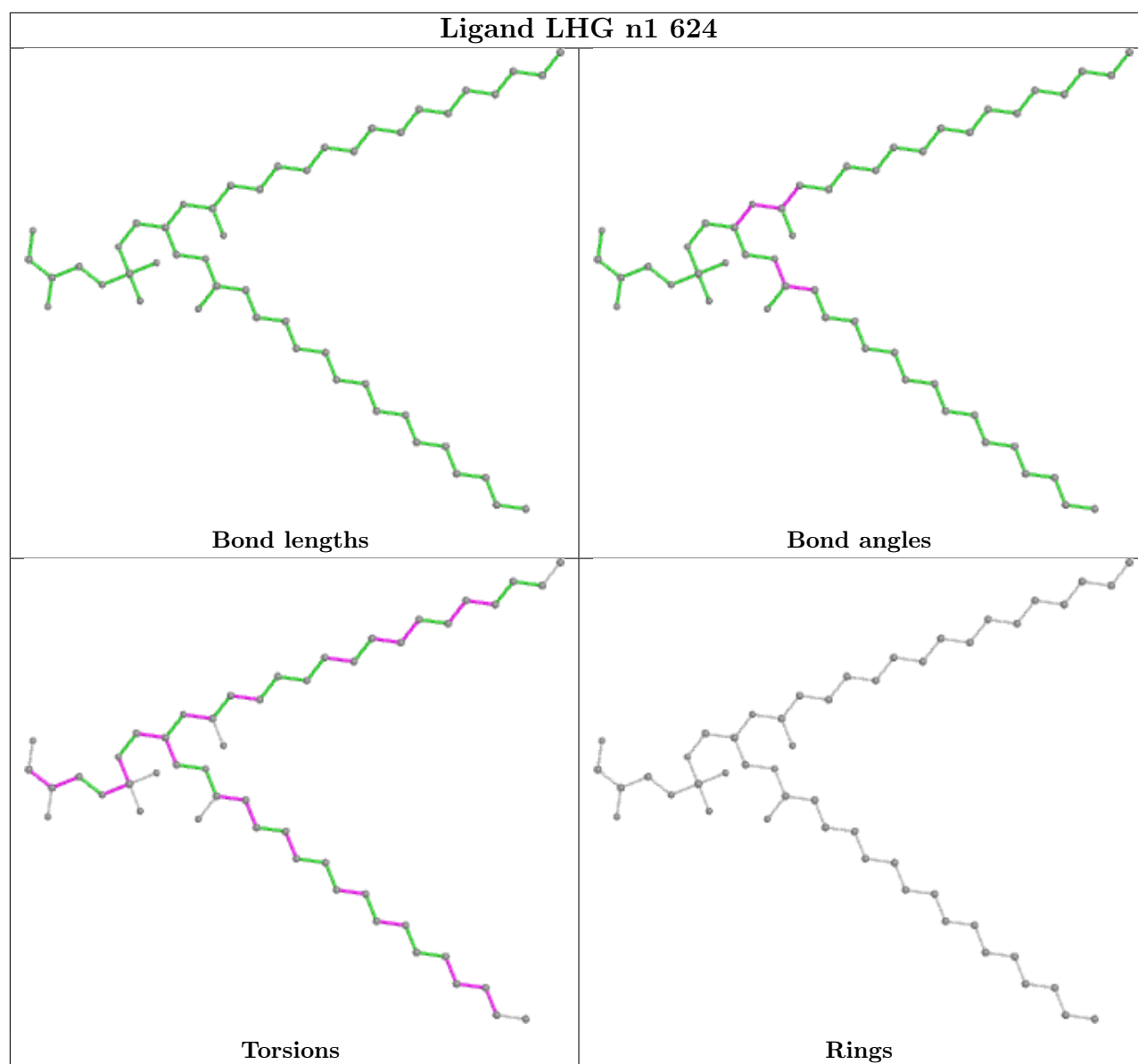


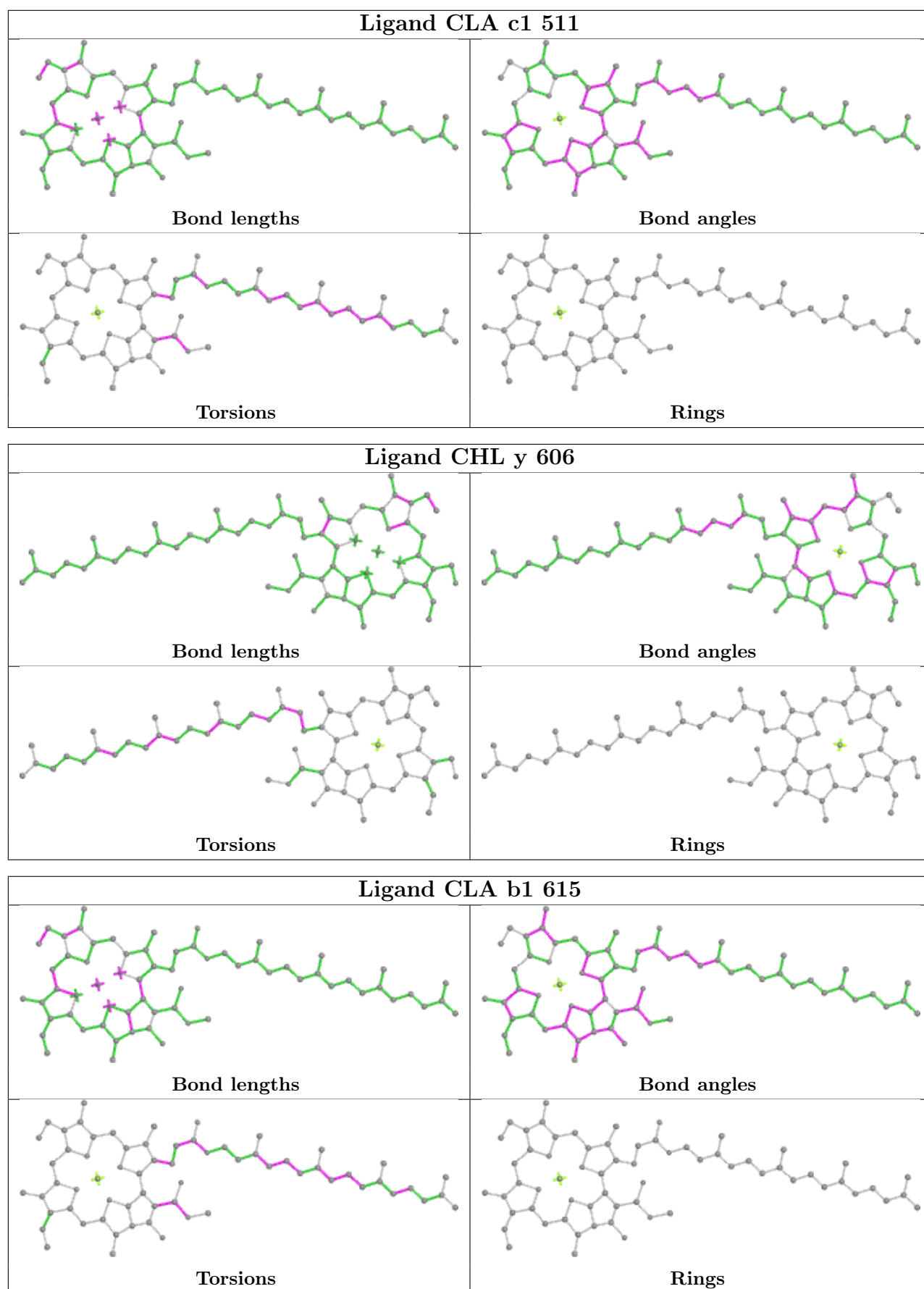


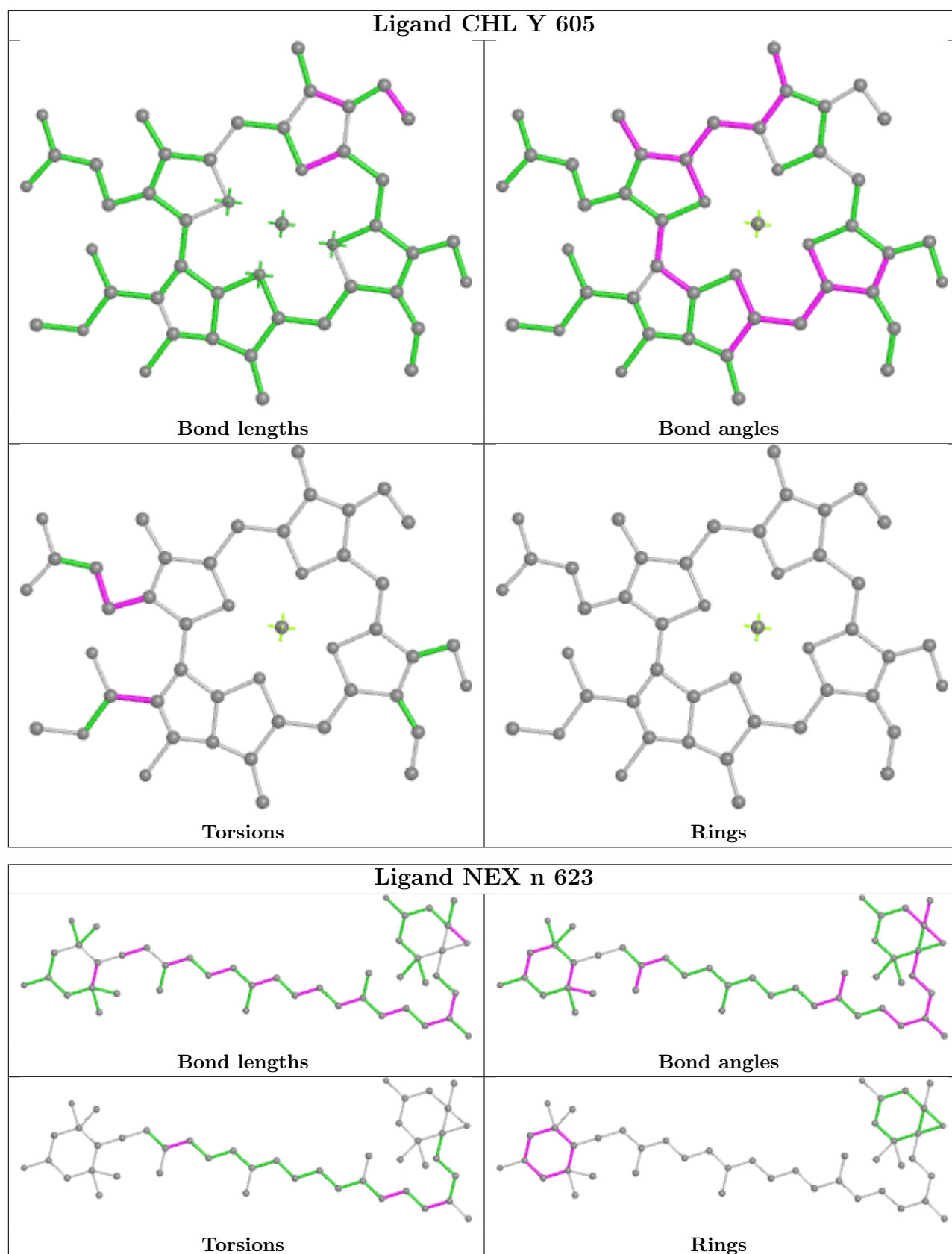


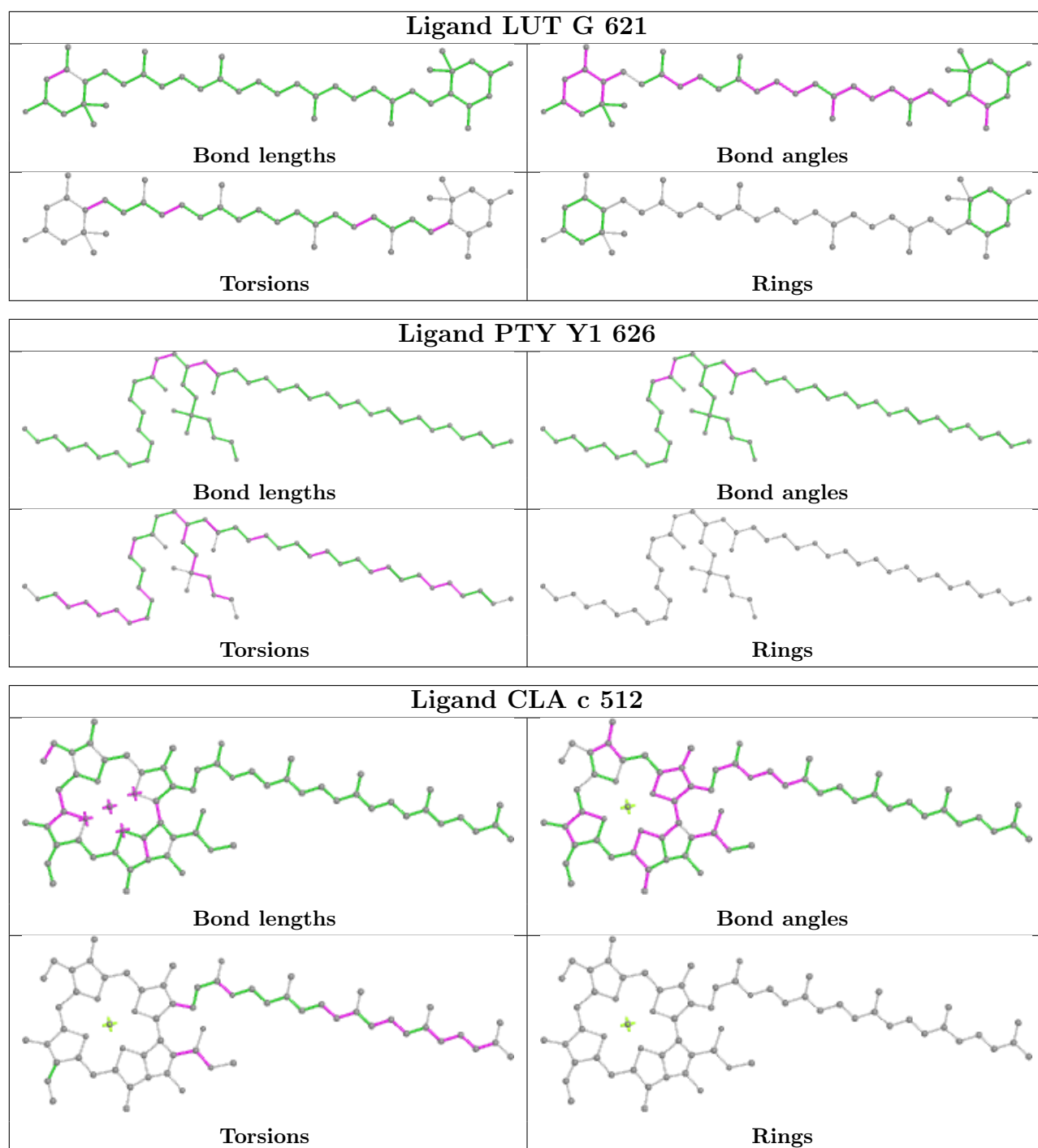




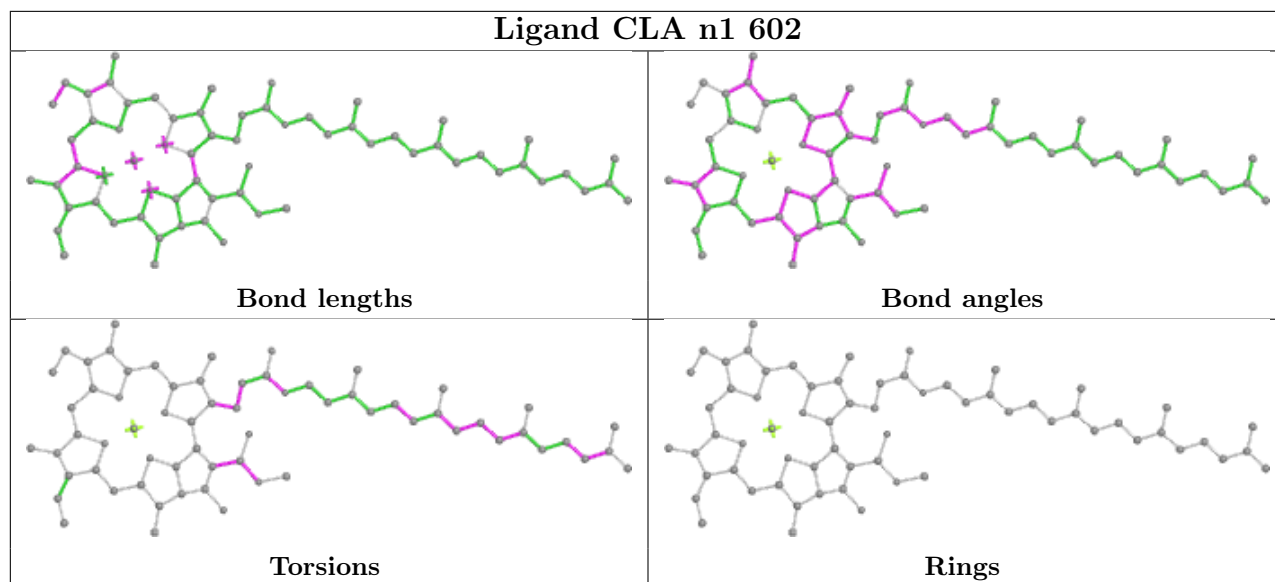












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	r1	1
22	R1	1
22	R	1
20	n1	1
20	n	1
21	G1	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.15
1	r1	110:PRO	C	126:GLU	N	13.08
1	R1	110:PRO	C	126:GLU	N	12.94
1	R	110:PRO	C	126:GLU	N	12.16
1	n1	57:PRO	C	58:PRO	N	3.54

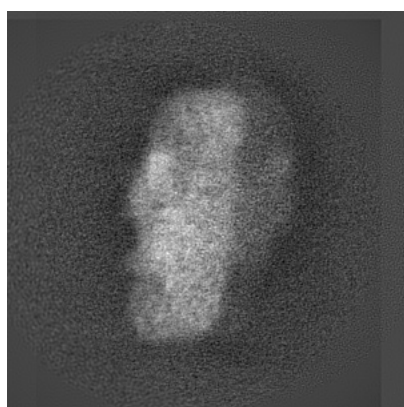
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13444. These allow visual inspection of the internal detail of the map and identification of artifacts.

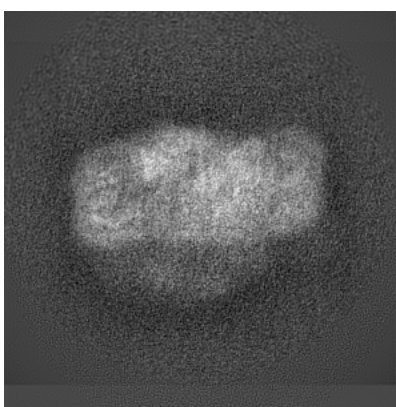
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

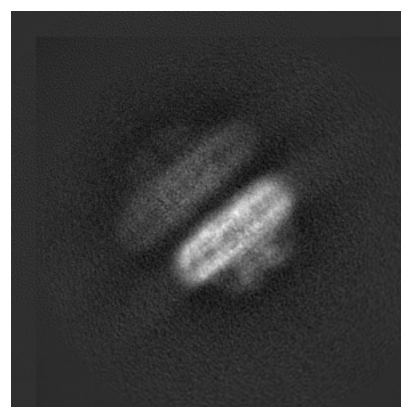
#### 6.1.1 Primary map



X



Y

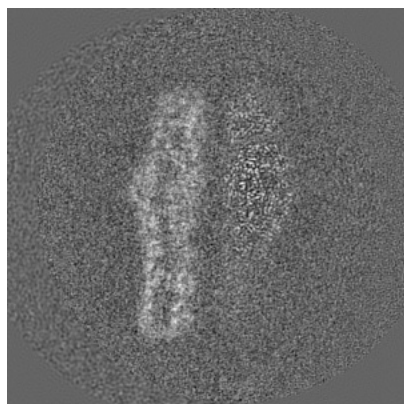


Z

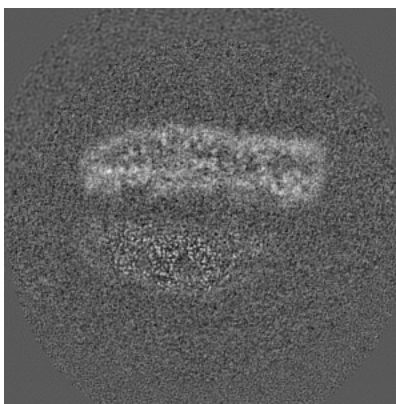
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

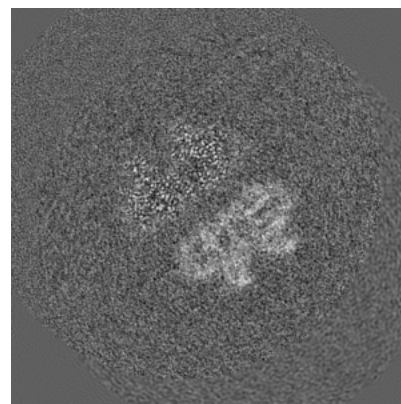
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

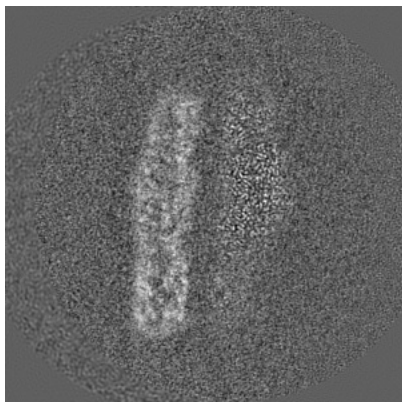


Z Index: 240

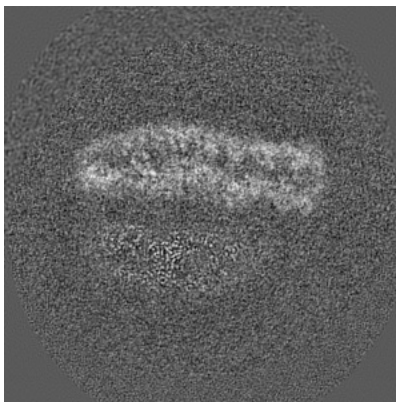
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

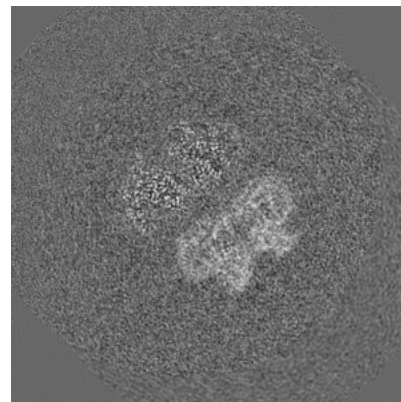
### 6.3.1 Primary map



X Index: 232



Y Index: 233



Z Index: 236

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

## 6.4 Orthogonal surface views [i](#)

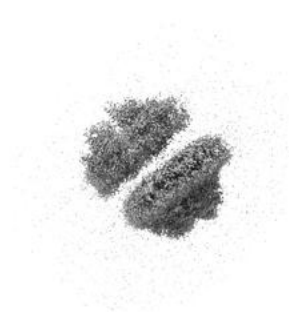
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

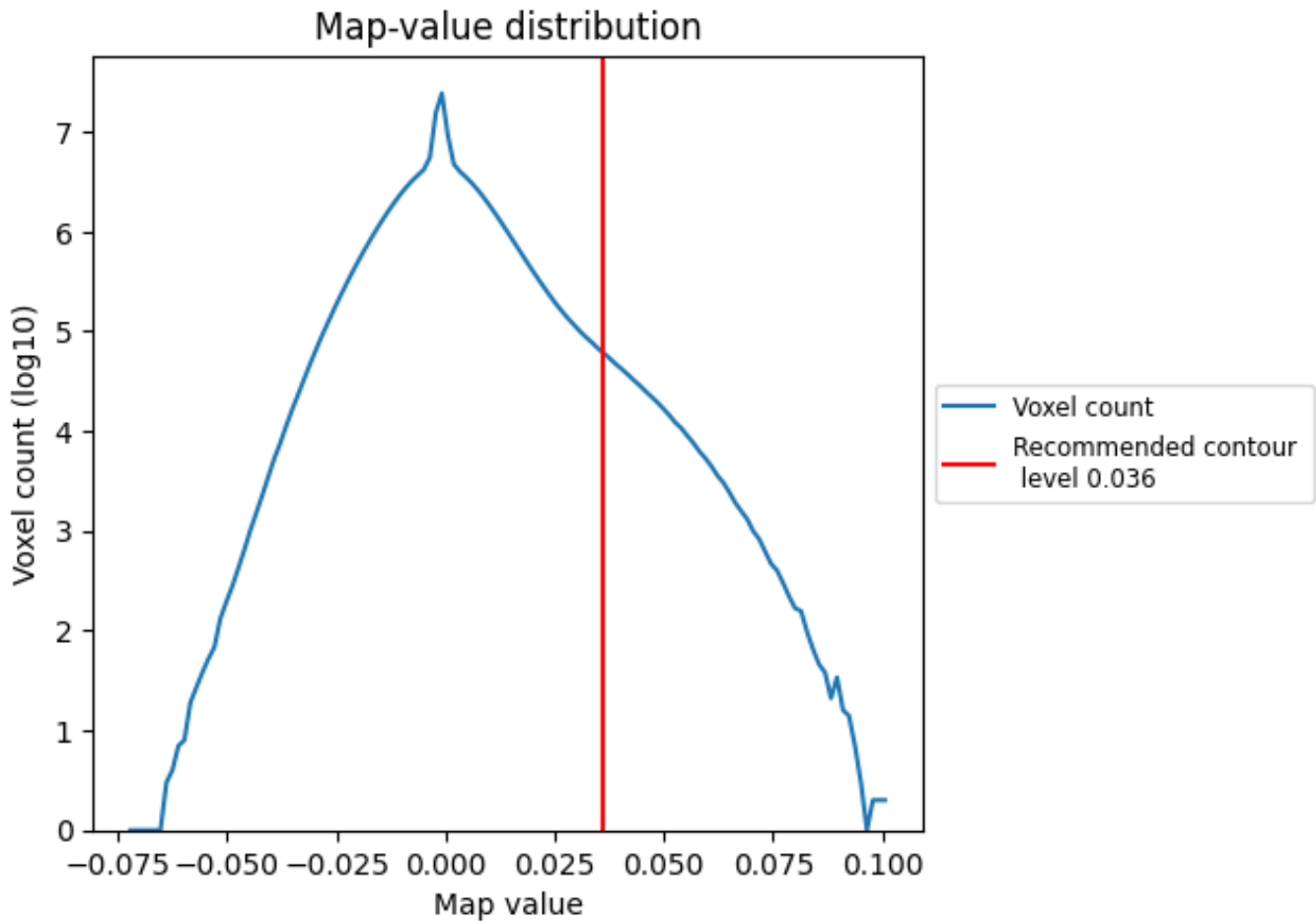
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

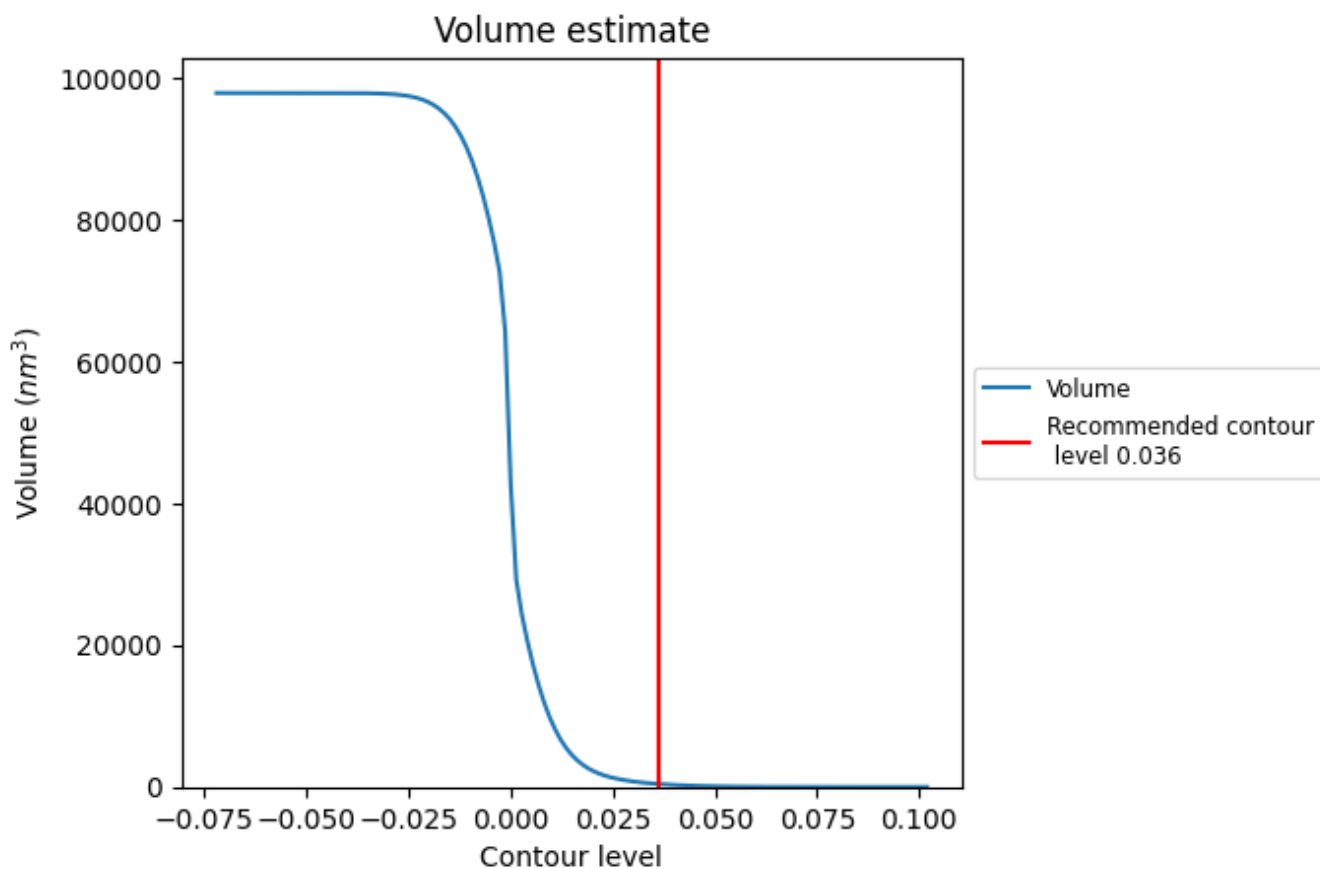
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

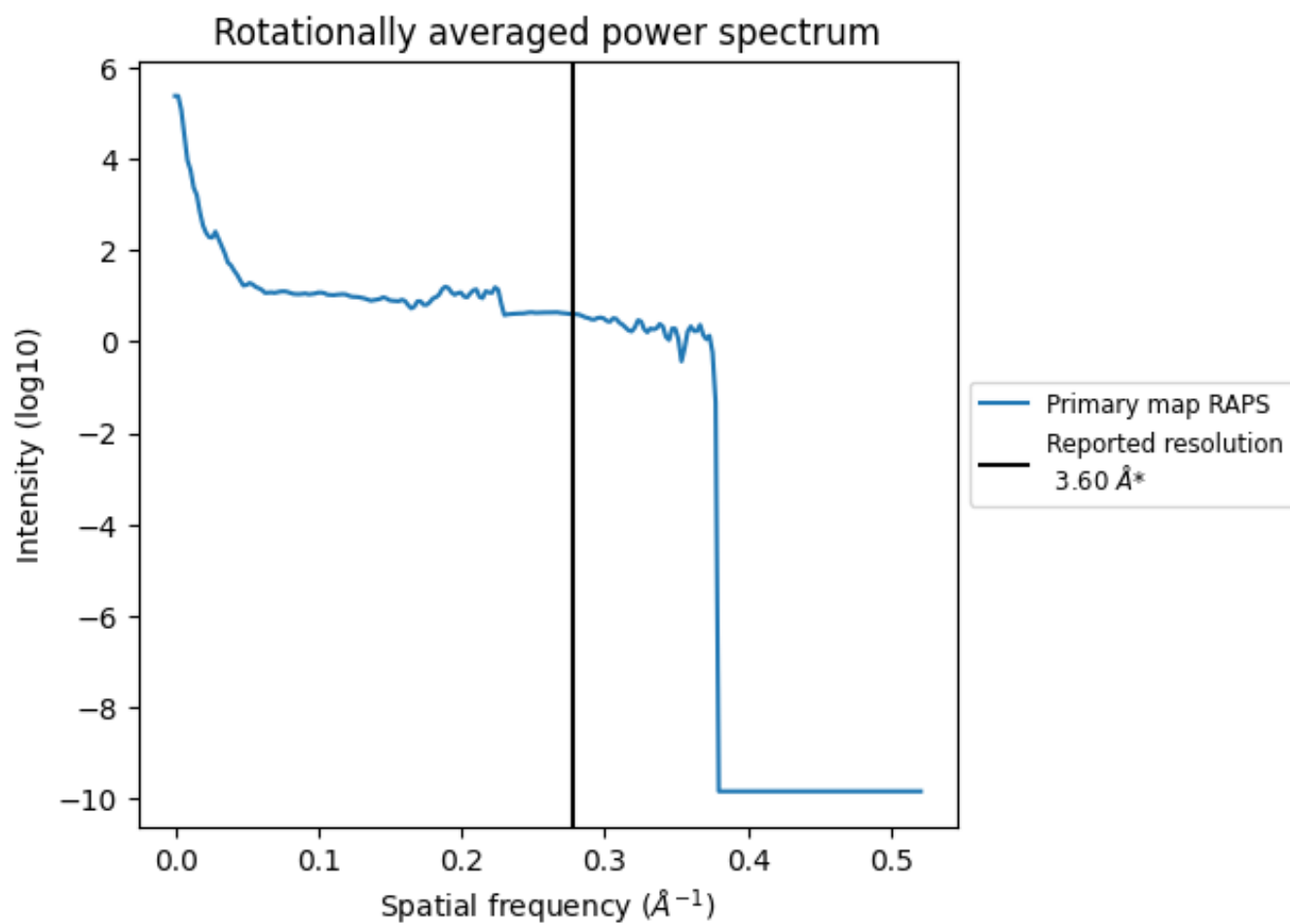
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm<sup>3</sup>; this corresponds to an approximate mass of 387 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)

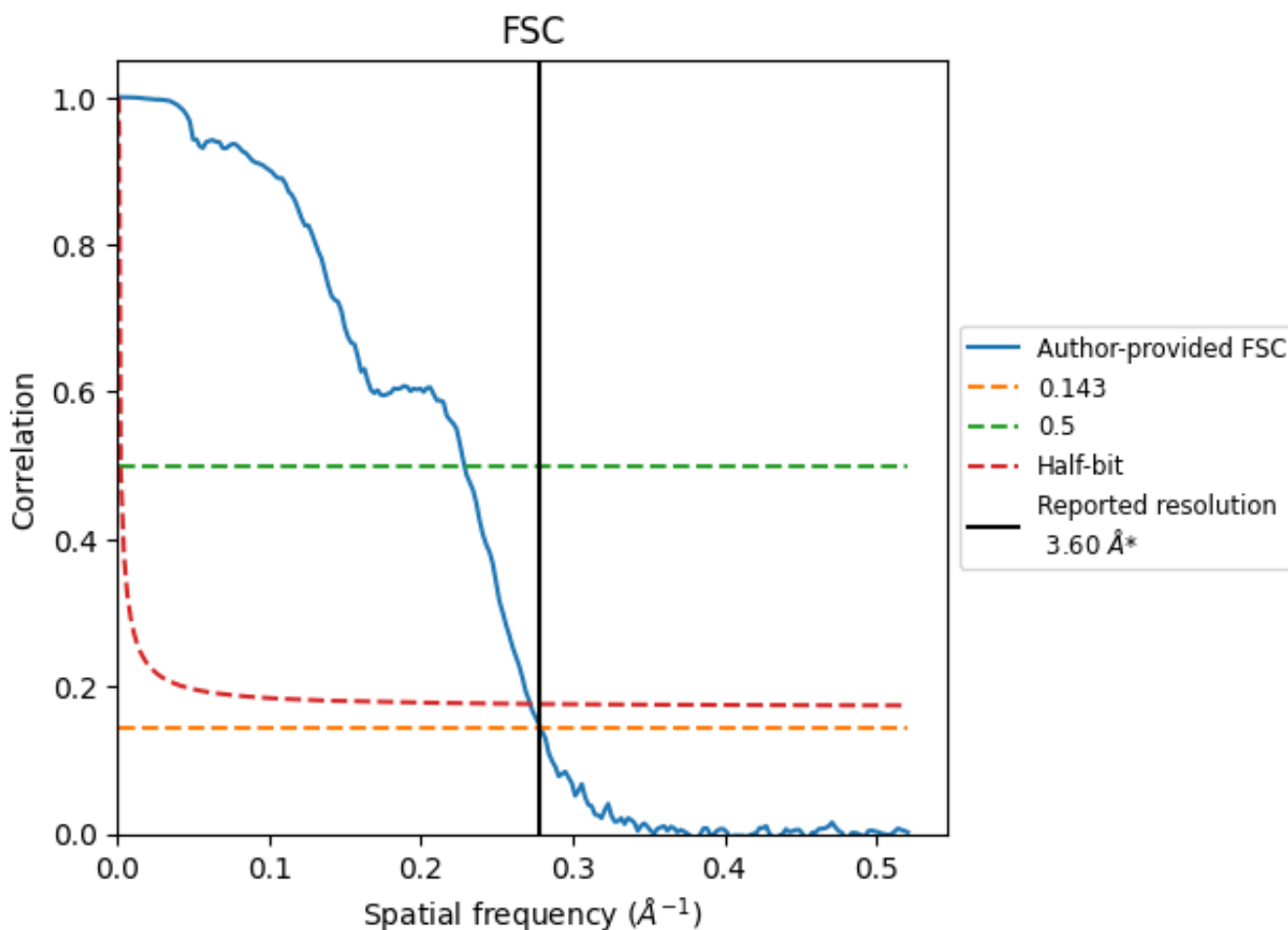


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

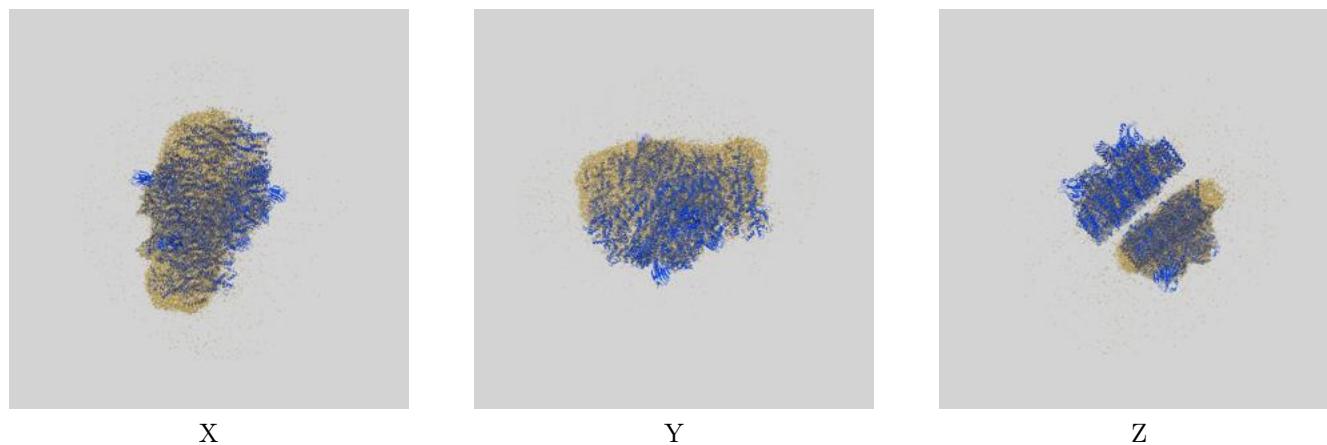
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.37	3.68
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13444 and PDB model 7PIN. Per-residue inclusion information can be found in section [3](#) on page [74](#).

### 9.1 Map-model overlay [i](#)

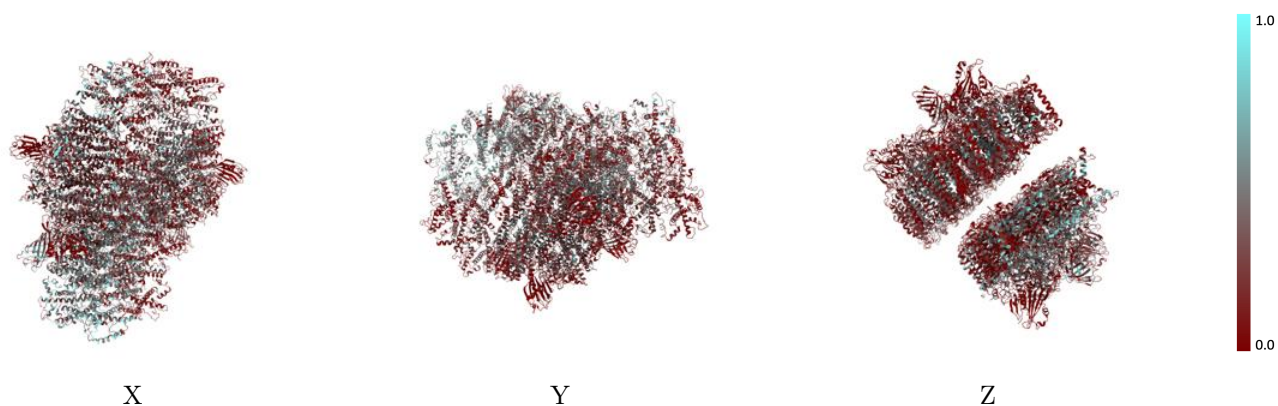


The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

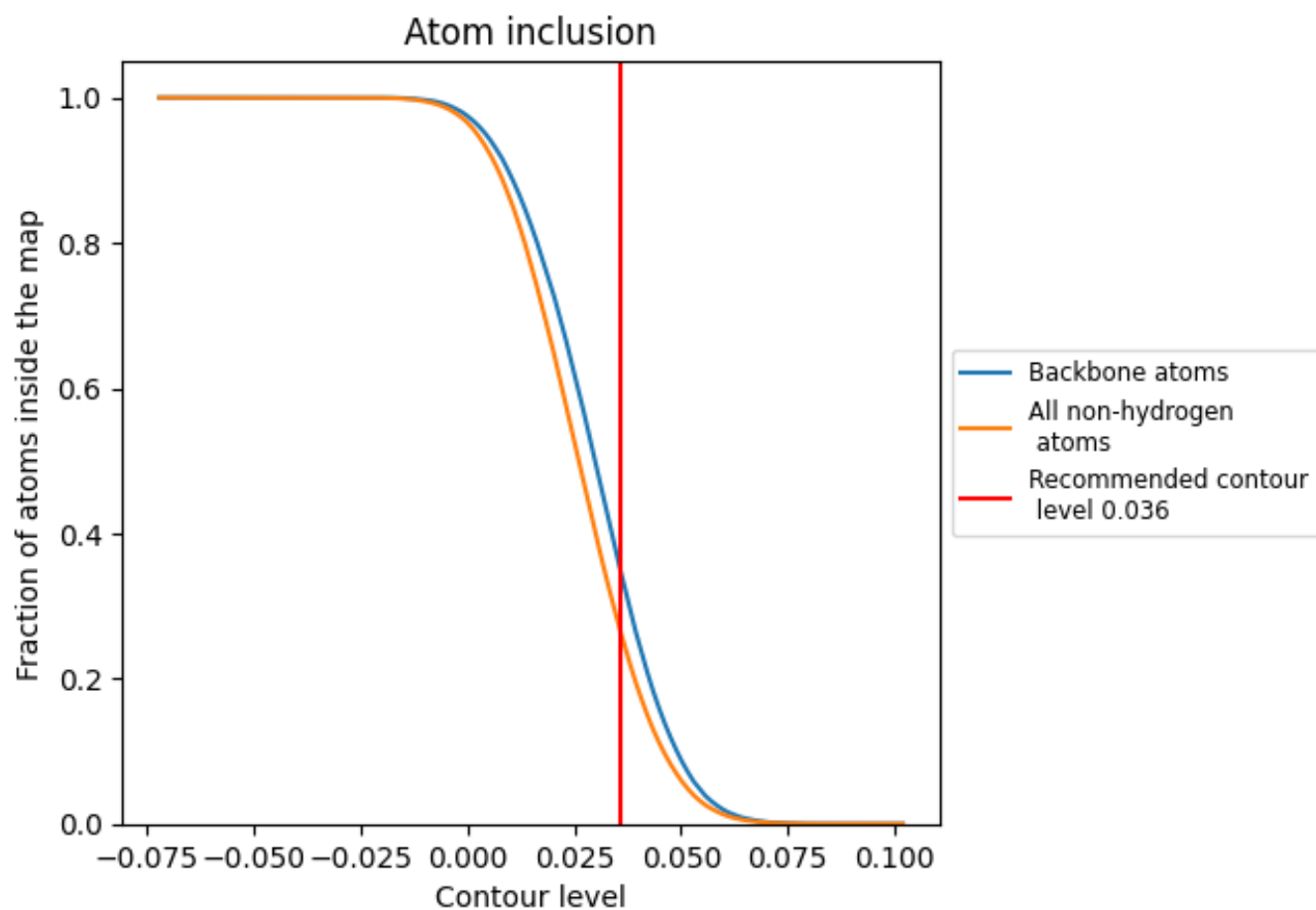
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).




































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 35% of all backbone atoms, 26% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.2617
A	 0.3527
A1	 0.3491
B	 0.2795
B1	 0.2943
C	 0.3493
C1	 0.4041
D	 0.3194
D1	 0.3355
E	 0.1683
E1	 0.3960
F	 0.2273
F1	 0.3846
G	 0.1005
G1	 0.4159
H	 0.2164
H1	 0.2709
I	 0.2714
I1	 0.2802
J	 0.1655
J1	 0.2517
K	 0.2343
K1	 0.3914
L	 0.2817
L1	 0.2225
M	 0.1855
M1	 0.1745
N	 0.1412
N1	 0.4418
O	 0.1148
O1	 0.3025
P	 0.0007
P1	 0.0254
R	 0.0977
R1	 0.2381



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Chain	Atom inclusion
S	0.1777
S1	0.4388
T	0.1701
T1	0.1944
U	0.0826
U1	0.2202
V	0.1467
V1	0.2800
W	0.1421
W1	0.2650
X	0.1294
X1	0.3881
Y	0.2291
Y1	0.4007
Z	0.1714
Z1	0.3890
a	0.3669
a1	0.2622
b	0.2919
b1	0.2543
c	0.3480
c1	0.2839
d	0.3364
d1	0.2314
e	0.1584
e1	0.2261
f	0.1643
f1	0.2727
g	0.0993
g1	0.3063
h	0.2147
h1	0.1891
i	0.2943
i1	0.2432
j	0.2103
j1	0.2069
k	0.2457
k1	0.2371
l	0.2789
m	0.1818
m1	0.2000
n	0.1583

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Chain	Atom inclusion
n1	0.3226
o	0.1070
o1	0.2652
p	0.0007
p1	0.0254
r	0.0911
r1	0.2372
s	0.1794
s1	0.2429
t	0.2153
t1	0.1701
u	0.0367
u1	0.1284
v	0.1689
v1	0.1467
w	0.1639
w1	0.2459
x	0.0846
x1	0.2090
y	0.2245
y1	0.2950
z	0.1692
z1	0.1956