



## wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 06:49 AM JST

PDB ID : 7FIX  
EMDB ID : EMD-31605  
Title : Cryo-EM structure of cyanobacterial photosystem I in the presence of ferredoxin and cytochrome c6  
Authors : Li, J.; Kurisu, G.  
Deposited on : 2021-08-01  
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

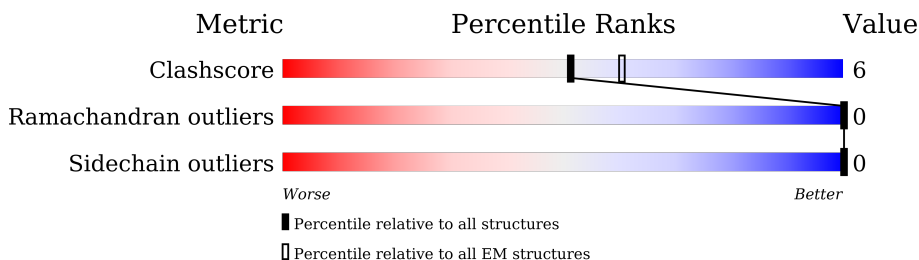
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 1.97 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) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 158937                   | 4297                     |
| 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   | A1    | 755    |                  |
| 1   | A2    | 755    |                  |
| 1   | A3    | 755    |                  |
| 2   | B1    | 741    |                  |
| 2   | B2    | 741    |                  |
| 2   | B3    | 741    |                  |
| 3   | C1    | 81     |                  |
| 3   | C2    | 81     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C3    | 81     | 91% 7%           |
| 4   | D1    | 139    | 94% 6%           |
| 4   | D2    | 139    | 92% 7%           |
| 4   | D3    | 139    | 94% 6%           |
| 5   | E1    | 76     | 87% 9%           |
| 5   | E2    | 76     | 87% 9%           |
| 5   | E3    | 76     | 87% 9%           |
| 6   | F1    | 174    | 74% 7% 19%       |
| 6   | F2    | 174    | 74% 7% 19%       |
| 6   | F3    | 174    | 74% 7% 19%       |
| 7   | I1    | 38     | 84% 16%          |
| 7   | I2    | 38     | 82% 18%          |
| 7   | I3    | 38     | 84% 16%          |
| 8   | J1    | 41     | 83% 17%          |
| 8   | J2    | 41     | 78% 22%          |
| 8   | J3    | 41     | 78% 22%          |
| 9   | K1    | 83     | 90% 5% 5%        |
| 9   | K2    | 83     | 90% 5% 5%        |
| 9   | K3    | 83     | 90% 5% 5%        |
| 10  | L1    | 155    | 90% 8%           |
| 10  | L2    | 155    | 91% 7%           |
| 10  | L3    | 155    | 90% 8%           |
| 11  | M1    | 31     | 100%             |
| 11  | M2    | 31     | 100%             |
| 11  | M3    | 31     | 100%             |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 12  | R1    | 98     |                  |
| 12  | R2    | 98     |                  |
| 12  | R3    | 98     |                  |
| 13  | X1    | 39     |                  |
| 13  | X2    | 39     |                  |
| 13  | X3    | 39     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CL0  | A1    | 801 | X         | -        | -       | -                |
| 14  | CL0  | A2    | 801 | X         | -        | -       | -                |
| 14  | CL0  | A3    | 801 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 802 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 803 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 804 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 805 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 806 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 807 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 808 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 809 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 810 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 811 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 812 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 813 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 814 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 815 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 816 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 817 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 818 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 819 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 820 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 821 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 822 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 823 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 824 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 825 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15  | CLA  | A1    | 826 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 827 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 828 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 829 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 830 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 831 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 832 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 833 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 834 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 835 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 836 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 837 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 838 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 839 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 840 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 841 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 842 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 843 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 844 | X         | -        | -       | -                |
| 15  | CLA  | A1    | 856 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 802 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 803 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 804 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 805 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 806 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 807 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 808 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 809 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 810 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 811 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 812 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 813 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 814 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 815 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 816 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 817 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 818 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 819 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 820 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 821 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 822 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 823 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15  | CLA  | A2    | 824 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 825 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 826 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 827 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 828 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 829 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 830 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 831 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 832 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 833 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 834 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 835 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 836 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 837 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 838 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 839 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 840 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 841 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 842 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 843 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 844 | X         | -        | -       | -                |
| 15  | CLA  | A2    | 856 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 802 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 803 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 804 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 805 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 806 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 807 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 808 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 809 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 810 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 811 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 812 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 813 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 814 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 815 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 816 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 817 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 818 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 819 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 820 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 821 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15  | CLA  | A3    | 822 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 823 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 824 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 825 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 826 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 827 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 828 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 829 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 830 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 831 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 832 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 833 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 834 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 835 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 836 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 837 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 838 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 839 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 840 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 841 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 842 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 843 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 844 | X         | -        | -       | -                |
| 15  | CLA  | A3    | 856 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 801 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 802 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 803 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 804 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 805 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 806 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 807 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 808 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 809 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 810 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 811 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 812 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 813 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 814 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 815 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 816 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 817 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 818 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15  | CLA  | B1    | 819 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 820 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 821 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 822 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 823 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 824 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 825 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 826 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 827 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 828 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 829 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 830 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 831 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 832 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 833 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 834 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 835 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 836 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 837 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 838 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 839 | X         | -        | -       | -                |
| 15  | CLA  | B1    | 849 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 801 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 802 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 803 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 804 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 805 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 806 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 807 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 808 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 809 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 810 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 811 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 812 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 813 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 814 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 815 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 816 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 817 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 818 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 819 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 820 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15  | CLA  | B2    | 821 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 822 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 823 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 824 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 825 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 826 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 827 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 828 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 829 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 830 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 831 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 832 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 833 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 834 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 835 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 836 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 837 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 838 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 839 | X         | -        | -       | -                |
| 15  | CLA  | B2    | 849 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 801 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 802 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 803 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 804 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 805 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 806 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 807 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 808 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 809 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 810 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 811 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 812 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 813 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 814 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 815 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 816 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 817 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 818 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 819 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 820 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 821 | X         | -        | -       | -                |
| 15  | CLA  | B3    | 822 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 15  | CLA  | B3    | 823  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 824  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 825  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 826  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 827  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 828  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 829  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 830  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 831  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 832  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 833  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 834  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 835  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 836  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 837  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 838  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 839  | X         | -        | -       | -                |
| 15  | CLA  | B3    | 849  | X         | -        | -       | -                |
| 15  | CLA  | I1    | 101  | X         | -        | -       | -                |
| 15  | CLA  | I2    | 101  | X         | -        | -       | -                |
| 15  | CLA  | I3    | 101  | X         | -        | -       | -                |
| 15  | CLA  | J1    | 1301 | X         | -        | -       | -                |
| 15  | CLA  | J1    | 1302 | X         | -        | -       | -                |
| 15  | CLA  | J1    | 1303 | X         | -        | -       | -                |
| 15  | CLA  | J1    | 1307 | X         | -        | -       | -                |
| 15  | CLA  | J2    | 1301 | X         | -        | -       | -                |
| 15  | CLA  | J2    | 1302 | X         | -        | -       | -                |
| 15  | CLA  | J2    | 1303 | X         | -        | -       | -                |
| 15  | CLA  | J2    | 1307 | X         | -        | -       | -                |
| 15  | CLA  | J3    | 1301 | X         | -        | -       | -                |
| 15  | CLA  | J3    | 1302 | X         | -        | -       | -                |
| 15  | CLA  | J3    | 1303 | X         | -        | -       | -                |
| 15  | CLA  | J3    | 1307 | X         | -        | -       | -                |
| 15  | CLA  | K1    | 101  | X         | -        | -       | -                |
| 15  | CLA  | K1    | 103  | X         | -        | -       | -                |
| 15  | CLA  | K2    | 101  | X         | -        | -       | -                |
| 15  | CLA  | K2    | 103  | X         | -        | -       | -                |
| 15  | CLA  | K3    | 101  | X         | -        | -       | -                |
| 15  | CLA  | K3    | 103  | X         | -        | -       | -                |
| 15  | CLA  | L1    | 1002 | X         | -        | -       | -                |
| 15  | CLA  | L1    | 1003 | X         | -        | -       | -                |
| 15  | CLA  | L1    | 1004 | X         | -        | -       | -                |

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| <b>Mol</b> | <b>Type</b> | <b>Chain</b> | <b>Res</b> | <b>Chirality</b> | <b>Geometry</b> | <b>Clashes</b> | <b>Electron density</b> |
|------------|-------------|--------------|------------|------------------|-----------------|----------------|-------------------------|
| 15         | CLA         | L2           | 1002       | X                | -               | -              | -                       |
| 15         | CLA         | L2           | 1003       | X                | -               | -              | -                       |
| 15         | CLA         | L2           | 1004       | X                | -               | -              | -                       |
| 15         | CLA         | L3           | 1002       | X                | -               | -              | -                       |
| 15         | CLA         | L3           | 1003       | X                | -               | -              | -                       |
| 15         | CLA         | L3           | 1004       | X                | -               | -              | -                       |
| 15         | CLA         | X1           | 102        | X                | -               | -              | -                       |
| 15         | CLA         | X2           | 102        | X                | -               | -              | -                       |
| 15         | CLA         | X3           | 102        | X                | -               | -              | -                       |

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 73929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 1   | A1    | 745      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5676  | 3708 | 990 | 952 | 26 |         |       |
| 1   | A2    | 745      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5676  | 3708 | 990 | 952 | 26 |         |       |
| 1   | A3    | 745      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5676  | 3708 | 990 | 952 | 26 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 2   | B1    | 740      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5853  | 3853 | 984 | 995 | 21 |         |       |
| 2   | B2    | 740      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5853  | 3853 | 984 | 995 | 21 |         |       |
| 2   | B3    | 740      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5853  | 3853 | 984 | 995 | 21 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | S  |         |       |
| 3   | C1    | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |
| 3   | C2    | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |
| 3   | C3    | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 4   | D1    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1067  | 677 | 185 | 202 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D2    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1067  | 677 | 185 | 202 | 3 |         |       |
| 4   | D3    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1067  | 677 | 185 | 202 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 5   | E1    | 69       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 100 |         |       |
| 5   | E2    | 69       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 100 |         |       |
| 5   | E3    | 69       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 100 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F1    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1038  | 667 | 183 | 184 | 4 |         |       |
| 6   | F2    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1038  | 667 | 183 | 184 | 4 |         |       |
| 6   | F3    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1038  | 667 | 183 | 184 | 4 |         |       |

There are 30 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F1    | -9      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -8      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -7      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -6      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -5      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -4      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -3      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -2      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | -1      | HIS      | -      | expression tag | UNP P0A401 |
| F1    | 0       | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -9      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -8      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -7      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -6      | HIS      | -      | expression tag | UNP P0A401 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F2    | -5      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -4      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -3      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -2      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | -1      | HIS      | -      | expression tag | UNP P0A401 |
| F2    | 0       | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -9      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -8      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -7      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -6      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -5      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -4      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -3      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -2      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | -1      | HIS      | -      | expression tag | UNP P0A401 |
| F3    | 0       | HIS      | -      | expression tag | UNP P0A401 |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | I1    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 301   | 208 | 40 | 48 | 5 |         |       |
| 7   | I2    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 301   | 208 | 40 | 48 | 5 |         |       |
| 7   | I3    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 301   | 208 | 40 | 48 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | J1    | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 337   | 231 | 51 | 53 | 2 |         |       |
| 8   | J2    | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 337   | 231 | 51 | 53 | 2 |         |       |
| 8   | J3    | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 337   | 231 | 51 | 53 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | K1    | 79       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 483   | 306 | 84 | 92 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | K2    | 79       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 483   | 306 | 84 | 92 | 1 |         |       |
| 9   | K3    | 79       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 483   | 306 | 84 | 92 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | L1    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 736 | 180 | 201 | 4 |         |       |
| 10  | L2    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 736 | 180 | 201 | 4 |         |       |
| 10  | L3    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 736 | 180 | 201 | 4 |         |       |

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | M1    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 161 | 36 | 43 | 1 |         |       |
| 11  | M2    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 161 | 36 | 43 | 1 |         |       |
| 11  | M3    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 161 | 36 | 43 | 1 |         |       |

- Molecule 12 is a protein called Ferredoxin-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | R1    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 748   | 463 | 116 | 164 | 5 |         |       |
| 12  | R2    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 748   | 463 | 116 | 164 | 5 |         |       |
| 12  | R3    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 748   | 463 | 116 | 164 | 5 |         |       |

- Molecule 13 is a protein called Photosystem I 4.8K protein.

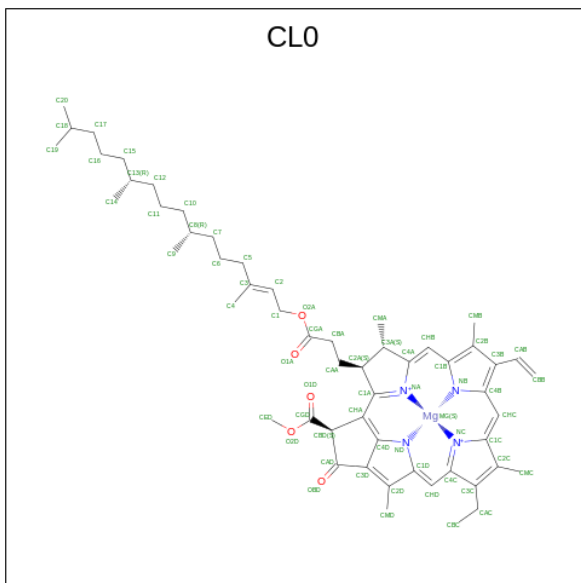
| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 13  | X1    | 28       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 225   | 159 | 33 | 33 |         |       |
| 13  | X2    | 28       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 225   | 159 | 33 | 33 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
|     |       |          | Total | C   | N  | O  |         |       |
| 13  | X3    | 28       | 225   | 159 | 33 | 33 | 0       | 0     |

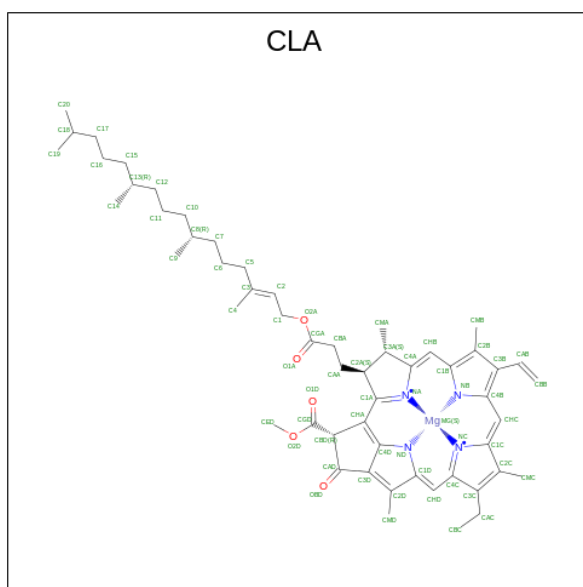
- Molecule 14 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
|     |       |          | Total | C  | Mg | N | O |         |
| 14  | A1    | 1        | 65    | 55 | 1  | 4 | 5 | 0       |
| 14  | A2    | 1        | 65    | 55 | 1  | 4 | 5 | 0       |
| 14  | A3    | 1        | 65    | 55 | 1  | 4 | 5 | 0       |

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |
| 15  | A1    | 1        | Total | C    | Mg | N   | O   | 0       |
|     |       |          | 2328  | 1912 | 44 | 176 | 196 |         |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A1    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B1    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B1    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | I1    | 1        | Total<br>65   | C<br>55   | Mg<br>1  | N<br>4   | O<br>5   | 0       |
| 15  | J1    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J1    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J1    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J1    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | K1    | 1        | Total<br>66   | C<br>54   | Mg<br>2  | N<br>8   | O<br>2   | 0       |
| 15  | K1    | 1        | Total<br>66   | C<br>54   | Mg<br>2  | N<br>8   | O<br>2   | 0       |
| 15  | L1    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | L1    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | L1    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | X1    | 1        | Total<br>40   | C<br>32   | Mg<br>1  | N<br>4   | O<br>3   | 0       |
| 15  | A2    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A2    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A2    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | A2    | 1        | 2328  | 1912 | 44 | 176 | 196 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |

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| Mol | Chain | Residues | Atoms |      |    |     |     | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
|     |       |          | Total | C    | Mg | N   | O   |         |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |
| 15  | B2    | 1        | 1961  | 1600 | 40 | 160 | 161 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B2    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | I2    | 1        | Total<br>65   | C<br>55   | Mg<br>1  | N<br>4   | O<br>5   | 0       |
| 15  | J2    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J2    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 15  | J2    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J2    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | K2    | 1        | Total<br>66   | C<br>54   | Mg<br>2  | N<br>8   | O<br>2   | 0       |
| 15  | K2    | 1        | Total<br>66   | C<br>54   | Mg<br>2  | N<br>8   | O<br>2   | 0       |
| 15  | L2    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | L2    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | L2    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | X2    | 1        | Total<br>40   | C<br>32   | Mg<br>1  | N<br>4   | O<br>3   | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | A3    | 1        | Total<br>2328 | C<br>1912 | Mg<br>44 | N<br>176 | O<br>196 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |

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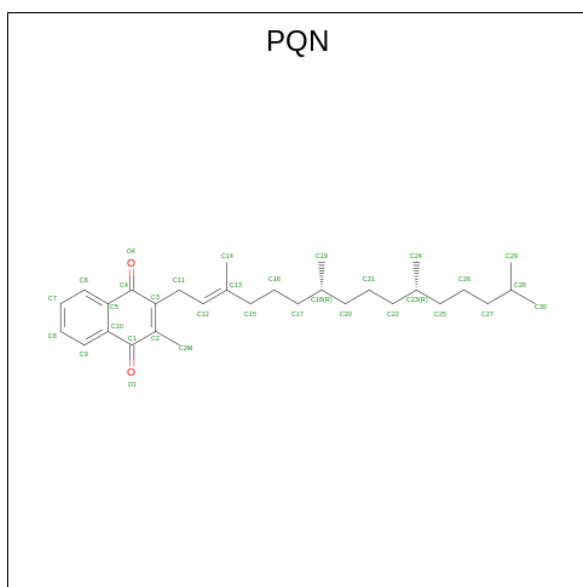
| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
|     |       |          | Total         | C         | Mg       | N        | O        |         |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |

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| Mol | Chain | Residues | Atoms         |           |          |          |          | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | B3    | 1        | Total<br>1961 | C<br>1600 | Mg<br>40 | N<br>160 | O<br>161 | 0       |
| 15  | I3    | 1        | Total<br>65   | C<br>55   | Mg<br>1  | N<br>4   | O<br>5   | 0       |
| 15  | J3    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J3    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J3    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | J3    | 1        | Total<br>143  | C<br>117  | Mg<br>4  | N<br>16  | O<br>6   | 0       |
| 15  | K3    | 1        | Total<br>66   | C<br>54   | Mg<br>2  | N<br>8   | O<br>2   | 0       |
| 15  | K3    | 1        | Total<br>66   | C<br>54   | Mg<br>2  | N<br>8   | O<br>2   | 0       |
| 15  | L3    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | L3    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | L3    | 1        | Total<br>190  | C<br>160  | Mg<br>3  | N<br>12  | O<br>15  | 0       |
| 15  | X3    | 1        | Total<br>40   | C<br>32   | Mg<br>1  | N<br>4   | O<br>3   | 0       |

- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16  | A1    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 16  | B1    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 16  | A2    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 16  | B2    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 16  | A3    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 16  | B3    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

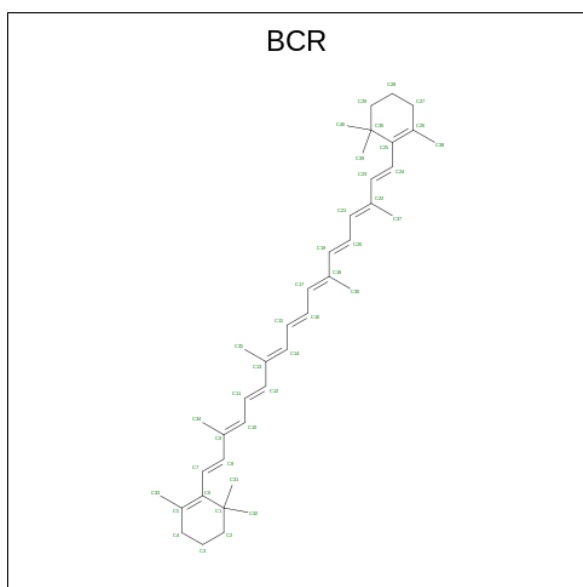
- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | Fe | S |         |
| 17  | A1    | 1        | 8     | 4  | 4 | 0       |
| 17  | C1    | 1        | 16    | 8  | 8 | 0       |
| 17  | C1    | 1        | 16    | 8  | 8 | 0       |
| 17  | A2    | 1        | 8     | 4  | 4 | 0       |
| 17  | C2    | 1        | 16    | 8  | 8 | 0       |
| 17  | C2    | 1        | 16    | 8  | 8 | 0       |
| 17  | A3    | 1        | 8     | 4  | 4 | 0       |
| 17  | C3    | 1        | 16    | 8  | 8 | 0       |
| 17  | C3    | 1        | 16    | 8  | 8 | 0       |

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms              | AltConf |
|-----|-------|----------|--------------------|---------|
| 18  | A1    | 1        | Total C<br>270 270 | 0       |
| 18  | A1    | 1        | Total C<br>270 270 | 0       |
| 18  | A1    | 1        | Total C<br>270 270 | 0       |
| 18  | A1    | 1        | Total C<br>270 270 | 0       |
| 18  | A1    | 1        | Total C<br>270 270 | 0       |
| 18  | A1    | 1        | Total C<br>270 270 | 0       |
| 18  | A1    | 1        | Total C<br>270 270 | 0       |
| 18  | B1    | 1        | Total C<br>255 255 | 0       |
| 18  | B1    | 1        | Total C<br>255 255 | 0       |
| 18  | B1    | 1        | Total C<br>255 255 | 0       |
| 18  | B1    | 1        | Total C<br>255 255 | 0       |
| 18  | B1    | 1        | Total C<br>255 255 | 0       |
| 18  | B1    | 1        | Total C<br>255 255 | 0       |
| 18  | B1    | 1        | Total C<br>255 255 | 0       |

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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 18  | F1    | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | I1    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | I1    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | J1    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | J1    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | J1    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | K1    | 1        | Total<br>25  | C<br>25  | 0       |
| 18  | L1    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | L1    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | L1    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | M1    | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | A2    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A2    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A2    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A2    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A2    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A2    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A2    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | B2    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B2    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B2    | 1        | Total<br>255 | C<br>255 | 0       |

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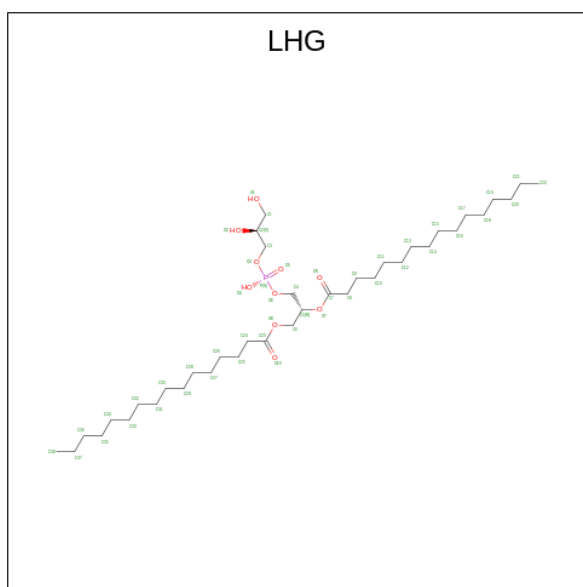
| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 18  | B2    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B2    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B2    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B2    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | F2    | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | I2    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | I2    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | J2    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | J2    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | J2    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | K2    | 1        | Total<br>25  | C<br>25  | 0       |
| 18  | L2    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | L2    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | M2    | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | A3    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A3    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A3    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A3    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A3    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A3    | 1        | Total<br>270 | C<br>270 | 0       |
| 18  | A3    | 1        | Total<br>270 | C<br>270 | 0       |

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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 18  | B3    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B3    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B3    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B3    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B3    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B3    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | B3    | 1        | Total<br>255 | C<br>255 | 0       |
| 18  | F3    | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | I3    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | I3    | 1        | Total<br>80  | C<br>80  | 0       |
| 18  | J3    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | J3    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | J3    | 1        | Total<br>120 | C<br>120 | 0       |
| 18  | K3    | 1        | Total<br>25  | C<br>25  | 0       |
| 18  | L3    | 1        | Total<br>40  | C<br>40  | 0       |
| 18  | M3    | 1        | Total<br>40  | C<br>40  | 0       |

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | AltConf |   |
|-----|-------|----------|-------|----|----|---------|---|
|     |       |          | Total | C  | O  |         | P |
| 19  | A1    | 1        | 82    | 60 | 20 | 2       | 0 |
| 19  | A1    | 1        | 82    | 60 | 20 | 2       | 0 |
| 19  | X1    | 1        | 42    | 31 | 10 | 1       | 0 |
| 19  | A2    | 1        | 82    | 60 | 20 | 2       | 0 |
| 19  | A2    | 1        | 82    | 60 | 20 | 2       | 0 |
| 19  | X2    | 1        | 42    | 31 | 10 | 1       | 0 |
| 19  | A3    | 1        | 82    | 60 | 20 | 2       | 0 |
| 19  | A3    | 1        | 82    | 60 | 20 | 2       | 0 |
| 19  | X3    | 1        | 42    | 31 | 10 | 1       | 0 |

- Molecule 20 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

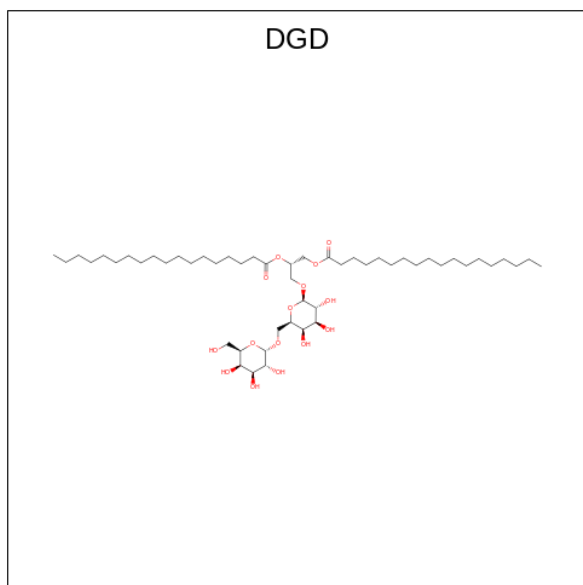
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 20  | A1    | 7        | Total | C  | 0       |
|     |       |          | 97    | 97 |         |
| 20  | I1    | 4        | Total | C  | 0       |
|     |       |          | 61    | 61 |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 20  | L1    | 4        | Total | C  | 0       |
|     |       |          | 64    | 64 |         |
| 20  | M1    | 2        | Total | C  | 0       |
|     |       |          | 32    | 32 |         |
| 20  | A2    | 7        | Total | C  | 0       |
|     |       |          | 97    | 97 |         |
| 20  | I2    | 4        | Total | C  | 0       |
|     |       |          | 61    | 61 |         |
| 20  | L2    | 4        | Total | C  | 0       |
|     |       |          | 64    | 64 |         |
| 20  | M2    | 2        | Total | C  | 0       |
|     |       |          | 32    | 32 |         |
| 20  | A3    | 7        | Total | C  | 0       |
|     |       |          | 97    | 97 |         |
| 20  | I3    | 4        | Total | C  | 0       |
|     |       |          | 61    | 61 |         |
| 20  | L3    | 4        | Total | C  | 0       |
|     |       |          | 64    | 64 |         |
| 20  | M3    | 2        | Total | C  | 0       |
|     |       |          | 32    | 32 |         |

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 21  | B1    | 1        | Total | C  | O  | 0       |
|     |       |          | 66    | 51 | 15 |         |

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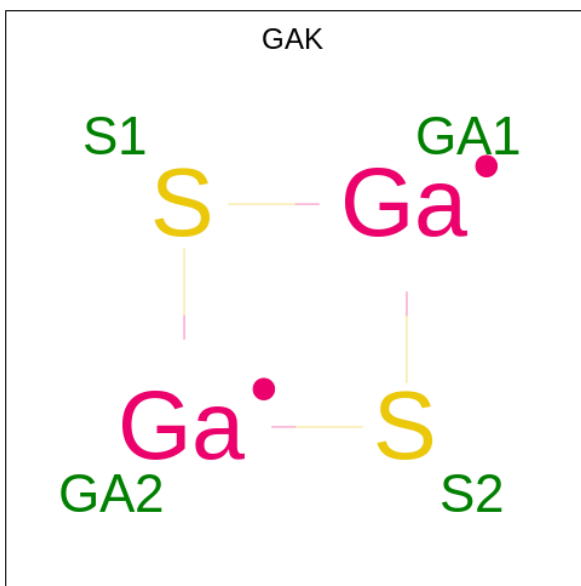
Continued from previous page...

| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
|     |       |          | Total | C  | O  |         |
| 21  | B2    | 1        | 66    | 51 | 15 | 0       |
| 21  | B3    | 1        | 66    | 51 | 15 | 0       |

- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
|     |       |          | Total | Ca |         |
| 22  | L1    | 1        | 1     | 1  | 0       |
| 22  | L2    | 1        | 1     | 1  | 0       |
| 22  | L3    | 1        | 1     | 1  | 0       |

- Molecule 23 is [2Ga-2S] cluster (three-letter code: GAK) (formula: Ga<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | Ga | S |         |
| 23  | R1    | 1        | 4     | 2  | 2 | 0       |
| 23  | R2    | 1        | 4     | 2  | 2 | 0       |
| 23  | R3    | 1        | 4     | 2  | 2 | 0       |

- Molecule 24 is water.

| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 24  | A1    | 26       | Total O<br>26 26 | 0       |
| 24  | B1    | 42       | Total O<br>42 42 | 0       |
| 24  | C1    | 13       | Total O<br>13 13 | 0       |
| 24  | D1    | 7        | Total O<br>7 7   | 0       |
| 24  | E1    | 1        | Total O<br>1 1   | 0       |
| 24  | I1    | 1        | Total O<br>1 1   | 0       |
| 24  | L1    | 22       | Total O<br>22 22 | 0       |
| 24  | R1    | 4        | Total O<br>4 4   | 0       |
| 24  | A2    | 26       | Total O<br>26 26 | 0       |
| 24  | B2    | 42       | Total O<br>42 42 | 0       |
| 24  | C2    | 13       | Total O<br>13 13 | 0       |
| 24  | D2    | 7        | Total O<br>7 7   | 0       |
| 24  | E2    | 1        | Total O<br>1 1   | 0       |
| 24  | I2    | 1        | Total O<br>1 1   | 0       |
| 24  | L2    | 22       | Total O<br>22 22 | 0       |
| 24  | R2    | 4        | Total O<br>4 4   | 0       |
| 24  | A3    | 26       | Total O<br>26 26 | 0       |
| 24  | B3    | 42       | Total O<br>42 42 | 0       |
| 24  | C3    | 13       | Total O<br>13 13 | 0       |
| 24  | D3    | 7        | Total O<br>7 7   | 0       |
| 24  | E3    | 1        | Total O<br>1 1   | 0       |

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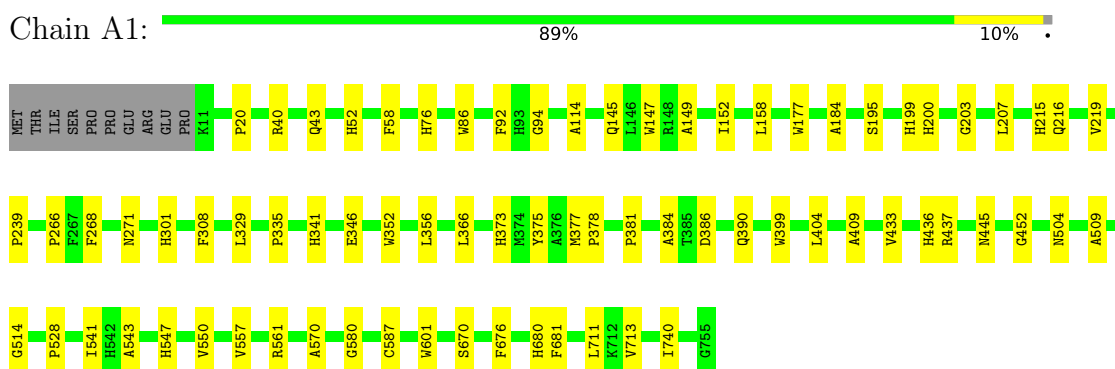
*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Residues</b> | <b>Atoms</b> |         | <b>AltConf</b> |
|------------|--------------|-----------------|--------------|---------|----------------|
| 24         | I3           | 1               | Total<br>1   | O<br>1  | 0              |
| 24         | L3           | 22              | Total<br>22  | O<br>22 | 0              |
| 24         | R3           | 4               | Total<br>4   | O<br>4  | 0              |

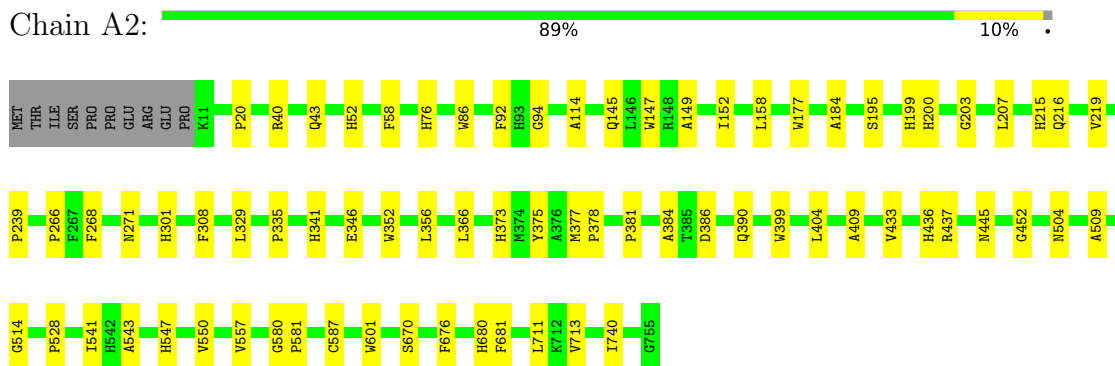
### 3 Residue-property plots

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.

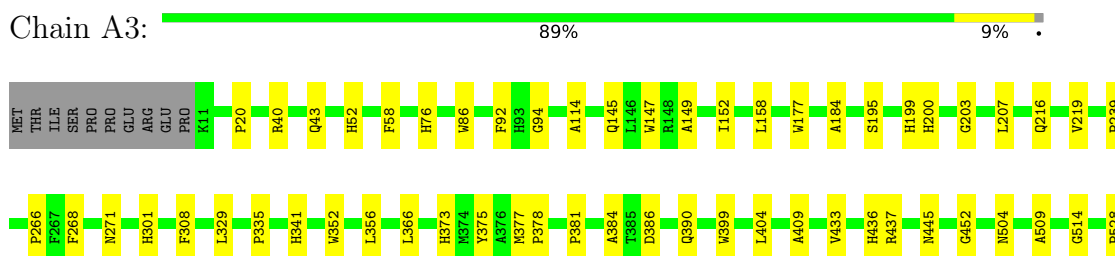
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

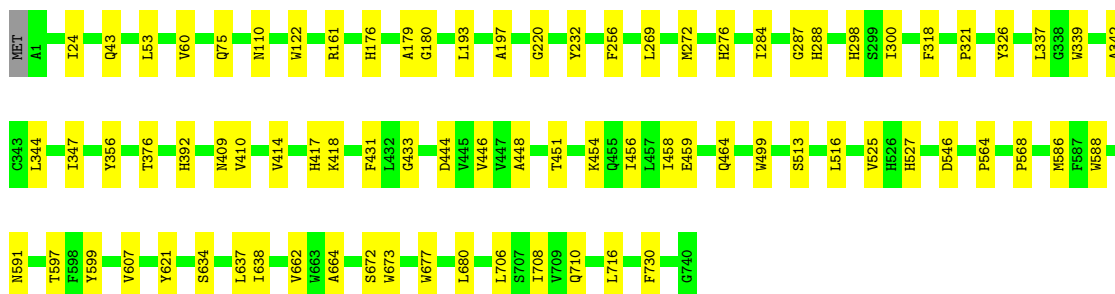


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

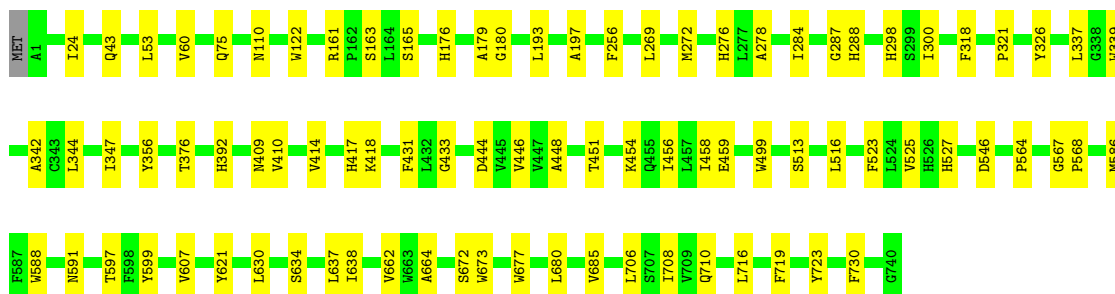
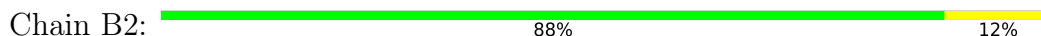




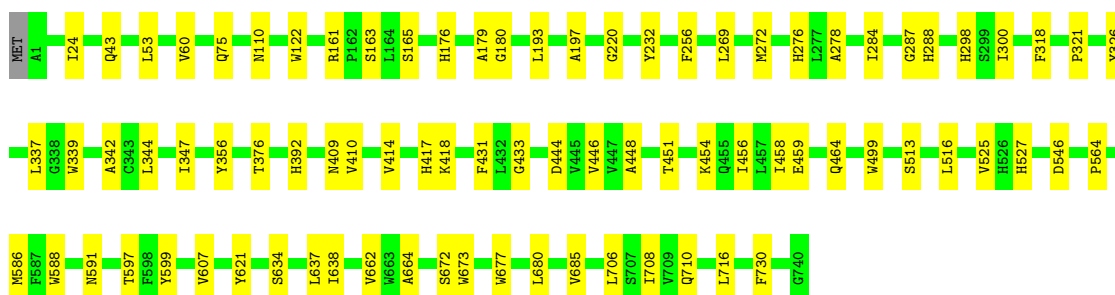
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



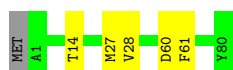
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 3: Photosystem I iron-sulfur center



- Molecule 3: Photosystem I iron-sulfur center

Chain C2:  91% 7%



- Molecule 3: Photosystem I iron-sulfur center

Chain C3:  91% 7%



- Molecule 4: Photosystem I reaction center subunit II

Chain D1:  94% 6%



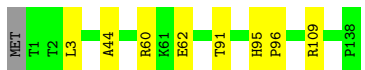
- Molecule 4: Photosystem I reaction center subunit II

Chain D2:  92% 7%




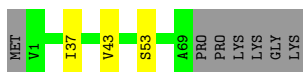
- Molecule 4: Photosystem I reaction center subunit II

Chain D3:  94% 6%




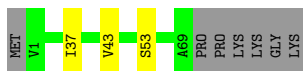
- Molecule 5: Photosystem I reaction center subunit IV

Chain E1:  87% 9%




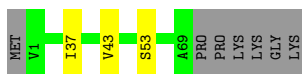
- Molecule 5: Photosystem I reaction center subunit IV

Chain E2:  87% 9%



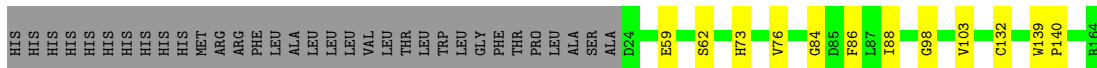
- Molecule 5: Photosystem I reaction center subunit IV

Chain E3:  87% 9%



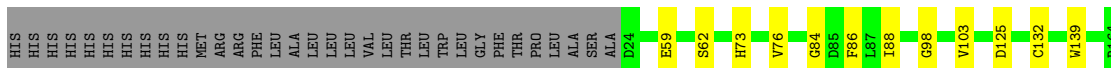
- Molecule 6: Photosystem I reaction center subunit III

Chain F1:  74% 7% 19%



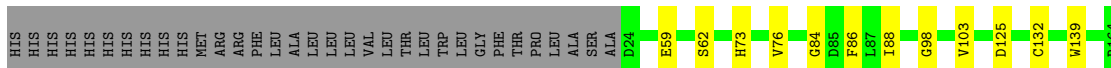
- Molecule 6: Photosystem I reaction center subunit III

Chain F2:  74% 7% 19%




- Molecule 6: Photosystem I reaction center subunit III

Chain F3:  74% 7% 19%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:  84% 16%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain I2:  82% 18%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain I3:  84% 16%




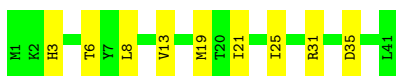
- Molecule 8: Photosystem I reaction center subunit IX

Chain J1:  83% 17%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J2:  78% 22%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J3:  78% 22%




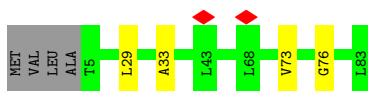
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K1:  90% 5% 5%




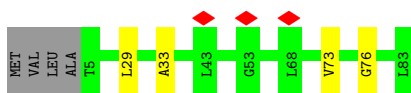
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K2:  90% 5% 5%



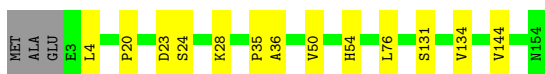
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K3:  90% 5% 5%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L1:  90% 8%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L2:  91% 7%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L3:  90% 8%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M1:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem I reaction center subunit XII

Chain M2:  100%


There are no outlier residues recorded for this chain.

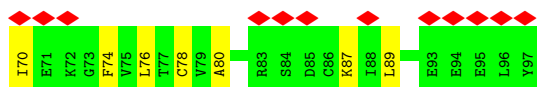
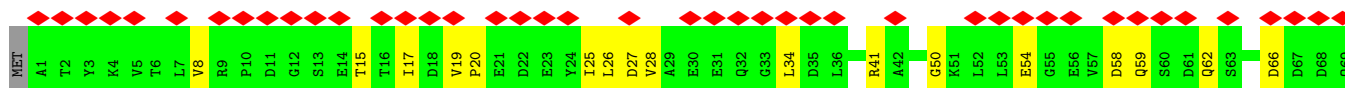
- Molecule 11: Photosystem I reaction center subunit XII

Chain M3:  100%

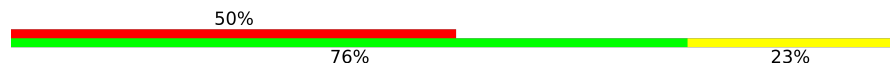
There are no outlier residues recorded for this chain.

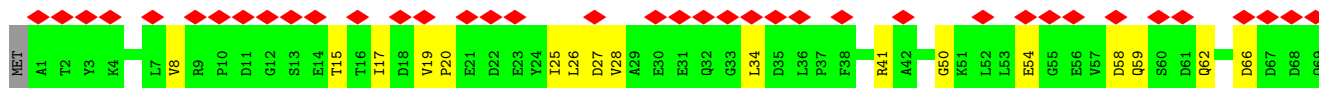
- Molecule 12: Ferredoxin-1

Chain R1:  56% 74% 24%

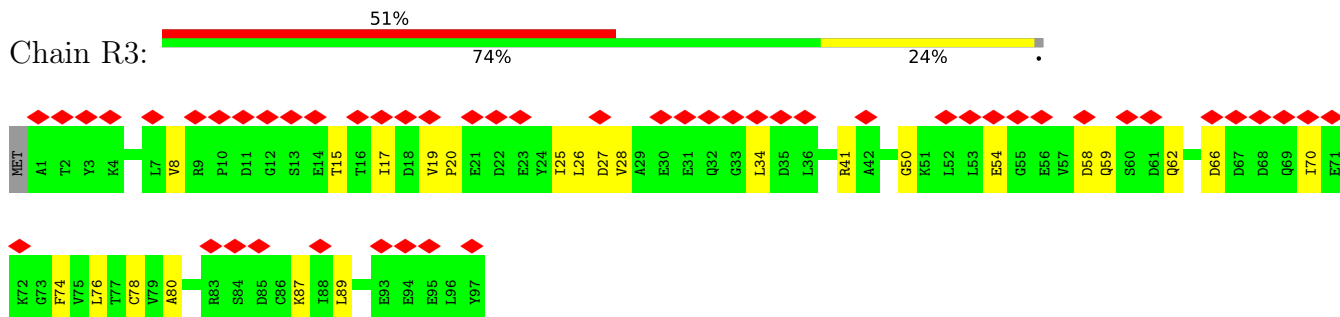


- Molecule 12: Ferredoxin-1

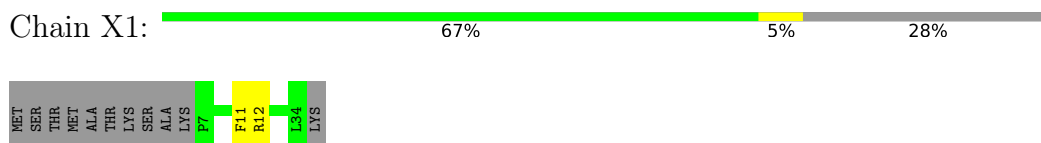
Chain R2:  50% 76% 23%



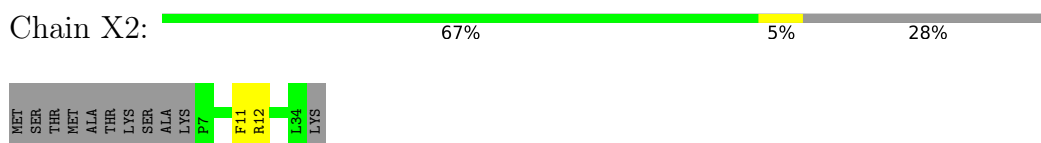
• Molecule 12: Ferredoxin-1



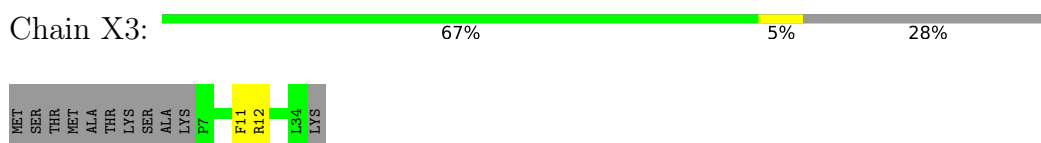
• Molecule 13: Photosystem I 4.8K protein



• Molecule 13: Photosystem I 4.8K protein



• Molecule 13: Photosystem I 4.8K protein





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C3                               | Depositor |
| Number of particles used             | 207142                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | JEOL CRYO ARM 300                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 48                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.090                                   | Depositor |
| Minimum map value                    | -0.024                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.007                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 322.4, 322.4, 322.4                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.806, 0.806, 0.806                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, DGD, CLA, UNL, CA, CL0, GAK, PQN, SF4, LHG

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A1    | 0.26         | 0/5862  | 0.43        | 0/8000  |
| 1   | A2    | 0.26         | 0/5862  | 0.43        | 0/8000  |
| 1   | A3    | 0.26         | 0/5862  | 0.43        | 0/8000  |
| 2   | B1    | 0.26         | 0/6071  | 0.42        | 0/8302  |
| 2   | B2    | 0.26         | 0/6071  | 0.42        | 0/8302  |
| 2   | B3    | 0.26         | 0/6071  | 0.42        | 0/8302  |
| 3   | C1    | 0.25         | 0/608   | 0.51        | 0/824   |
| 3   | C2    | 0.25         | 0/608   | 0.51        | 0/824   |
| 3   | C3    | 0.25         | 0/608   | 0.51        | 0/824   |
| 4   | D1    | 0.26         | 0/1093  | 0.49        | 0/1483  |
| 4   | D2    | 0.26         | 0/1093  | 0.49        | 0/1483  |
| 4   | D3    | 0.26         | 0/1093  | 0.49        | 0/1483  |
| 5   | E1    | 0.26         | 0/544   | 0.47        | 0/741   |
| 5   | E2    | 0.26         | 0/544   | 0.47        | 0/741   |
| 5   | E3    | 0.26         | 0/544   | 0.47        | 0/741   |
| 6   | F1    | 0.24         | 0/1060  | 0.46        | 0/1443  |
| 6   | F2    | 0.24         | 0/1060  | 0.46        | 0/1443  |
| 6   | F3    | 0.24         | 0/1060  | 0.46        | 0/1443  |
| 7   | I1    | 0.26         | 0/312   | 0.41        | 0/425   |
| 7   | I2    | 0.26         | 0/312   | 0.41        | 0/425   |
| 7   | I3    | 0.26         | 0/312   | 0.41        | 0/425   |
| 8   | J1    | 0.27         | 0/349   | 0.45        | 0/476   |
| 8   | J2    | 0.27         | 0/349   | 0.45        | 0/476   |
| 8   | J3    | 0.27         | 0/349   | 0.45        | 0/476   |
| 9   | K1    | 0.25         | 0/490   | 0.40        | 0/674   |
| 9   | K2    | 0.25         | 0/490   | 0.40        | 0/674   |
| 9   | K3    | 0.25         | 0/490   | 0.40        | 0/674   |
| 10  | L1    | 0.26         | 0/1150  | 0.40        | 0/1561  |
| 10  | L2    | 0.26         | 0/1150  | 0.40        | 0/1561  |
| 10  | L3    | 0.26         | 0/1150  | 0.40        | 0/1561  |
| 11  | M1    | 0.24         | 0/244   | 0.41        | 0/332   |
| 11  | M2    | 0.24         | 0/244   | 0.41        | 0/332   |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 11  | M3    | 0.24         | 0/244   | 0.41        | 0/332   |
| 12  | R1    | 0.26         | 0/758   | 0.48        | 0/1029  |
| 12  | R2    | 0.26         | 0/758   | 0.48        | 0/1029  |
| 12  | R3    | 0.26         | 0/758   | 0.48        | 0/1029  |
| 13  | X1    | 0.35         | 0/234   | 0.47        | 0/320   |
| 13  | X2    | 0.35         | 0/234   | 0.47        | 0/320   |
| 13  | X3    | 0.35         | 0/234   | 0.47        | 0/320   |
| All | All   | 0.26         | 0/56325 | 0.44        | 0/76830 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A1    | 5676  | 0        | 5476     | 67      | 0            |
| 1   | A2    | 5676  | 0        | 5476     | 67      | 0            |
| 1   | A3    | 5676  | 0        | 5476     | 64      | 0            |
| 2   | B1    | 5853  | 0        | 5580     | 64      | 0            |
| 2   | B2    | 5853  | 0        | 5580     | 69      | 0            |
| 2   | B3    | 5853  | 0        | 5580     | 68      | 0            |
| 3   | C1    | 598   | 0        | 580      | 3       | 0            |
| 3   | C2    | 598   | 0        | 580      | 4       | 0            |
| 3   | C3    | 598   | 0        | 580      | 4       | 0            |
| 4   | D1    | 1067  | 0        | 1062     | 5       | 0            |
| 4   | D2    | 1067  | 0        | 1062     | 6       | 0            |
| 4   | D3    | 1067  | 0        | 1062     | 5       | 0            |
| 5   | E1    | 532   | 0        | 522      | 4       | 0            |
| 5   | E2    | 532   | 0        | 522      | 4       | 0            |
| 5   | E3    | 532   | 0        | 522      | 4       | 0            |
| 6   | F1    | 1038  | 0        | 1040     | 7       | 0            |
| 6   | F2    | 1038  | 0        | 1040     | 8       | 0            |
| 6   | F3    | 1038  | 0        | 1040     | 8       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | I1    | 301   | 0        | 306      | 5       | 0            |
| 7   | I2    | 301   | 0        | 306      | 6       | 0            |
| 7   | I3    | 301   | 0        | 306      | 5       | 0            |
| 8   | J1    | 337   | 0        | 344      | 7       | 0            |
| 8   | J2    | 337   | 0        | 344      | 8       | 0            |
| 8   | J3    | 337   | 0        | 344      | 8       | 0            |
| 9   | K1    | 483   | 0        | 409      | 3       | 0            |
| 9   | K2    | 483   | 0        | 409      | 3       | 0            |
| 9   | K3    | 483   | 0        | 409      | 3       | 0            |
| 10  | L1    | 1121  | 0        | 1117     | 9       | 0            |
| 10  | L2    | 1121  | 0        | 1117     | 8       | 0            |
| 10  | L3    | 1121  | 0        | 1117     | 9       | 0            |
| 11  | M1    | 241   | 0        | 264      | 0       | 0            |
| 11  | M2    | 241   | 0        | 264      | 0       | 0            |
| 11  | M3    | 241   | 0        | 264      | 0       | 0            |
| 12  | R1    | 748   | 0        | 705      | 16      | 0            |
| 12  | R2    | 748   | 0        | 705      | 15      | 0            |
| 12  | R3    | 748   | 0        | 705      | 16      | 0            |
| 13  | X1    | 225   | 0        | 213      | 3       | 0            |
| 13  | X2    | 225   | 0        | 213      | 3       | 0            |
| 13  | X3    | 225   | 0        | 213      | 2       | 0            |
| 14  | A1    | 65    | 0        | 72       | 4       | 0            |
| 14  | A2    | 65    | 0        | 72       | 2       | 0            |
| 14  | A3    | 65    | 0        | 72       | 2       | 0            |
| 15  | A1    | 2328  | 0        | 2111     | 66      | 0            |
| 15  | A2    | 2328  | 0        | 2111     | 67      | 0            |
| 15  | A3    | 2328  | 0        | 2111     | 65      | 0            |
| 15  | B1    | 1961  | 0        | 1678     | 44      | 0            |
| 15  | B2    | 1961  | 0        | 1678     | 50      | 0            |
| 15  | B3    | 1961  | 0        | 1678     | 49      | 0            |
| 15  | I1    | 65    | 0        | 72       | 3       | 0            |
| 15  | I2    | 65    | 0        | 72       | 3       | 0            |
| 15  | I3    | 65    | 0        | 72       | 3       | 0            |
| 15  | J1    | 143   | 0        | 75       | 0       | 0            |
| 15  | J2    | 143   | 0        | 75       | 1       | 0            |
| 15  | J3    | 143   | 0        | 75       | 1       | 0            |
| 15  | K1    | 66    | 0        | 30       | 2       | 0            |
| 15  | K2    | 66    | 0        | 30       | 2       | 0            |
| 15  | K3    | 66    | 0        | 30       | 2       | 0            |
| 15  | L1    | 190   | 0        | 203      | 9       | 0            |
| 15  | L2    | 190   | 0        | 203      | 7       | 0            |
| 15  | L3    | 190   | 0        | 203      | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15  | X1    | 40    | 0        | 24       | 1       | 0            |
| 15  | X2    | 40    | 0        | 24       | 1       | 0            |
| 15  | X3    | 40    | 0        | 24       | 1       | 0            |
| 16  | A1    | 33    | 0        | 46       | 0       | 0            |
| 16  | A2    | 33    | 0        | 46       | 0       | 0            |
| 16  | A3    | 33    | 0        | 46       | 0       | 0            |
| 16  | B1    | 33    | 0        | 46       | 4       | 0            |
| 16  | B2    | 33    | 0        | 46       | 4       | 0            |
| 16  | B3    | 33    | 0        | 46       | 5       | 0            |
| 17  | A1    | 8     | 0        | 0        | 0       | 0            |
| 17  | A2    | 8     | 0        | 0        | 0       | 0            |
| 17  | A3    | 8     | 0        | 0        | 0       | 0            |
| 17  | C1    | 16    | 0        | 0        | 0       | 0            |
| 17  | C2    | 16    | 0        | 0        | 0       | 0            |
| 17  | C3    | 16    | 0        | 0        | 0       | 0            |
| 18  | A1    | 270   | 0        | 375      | 22      | 0            |
| 18  | A2    | 270   | 0        | 375      | 18      | 0            |
| 18  | A3    | 270   | 0        | 375      | 19      | 0            |
| 18  | B1    | 255   | 0        | 352      | 15      | 0            |
| 18  | B2    | 255   | 0        | 352      | 12      | 0            |
| 18  | B3    | 255   | 0        | 352      | 14      | 0            |
| 18  | F1    | 40    | 0        | 56       | 3       | 0            |
| 18  | F2    | 40    | 0        | 56       | 4       | 0            |
| 18  | F3    | 40    | 0        | 56       | 3       | 0            |
| 18  | I1    | 80    | 0        | 112      | 2       | 0            |
| 18  | I2    | 80    | 0        | 112      | 2       | 0            |
| 18  | I3    | 80    | 0        | 112      | 4       | 0            |
| 18  | J1    | 120   | 0        | 168      | 11      | 0            |
| 18  | J2    | 120   | 0        | 168      | 8       | 0            |
| 18  | J3    | 120   | 0        | 168      | 11      | 0            |
| 18  | K1    | 25    | 0        | 33       | 0       | 0            |
| 18  | K2    | 25    | 0        | 33       | 0       | 0            |
| 18  | K3    | 25    | 0        | 33       | 0       | 0            |
| 18  | L1    | 120   | 0        | 168      | 8       | 0            |
| 18  | L2    | 80    | 0        | 112      | 5       | 0            |
| 18  | L3    | 40    | 0        | 56       | 4       | 0            |
| 18  | M1    | 40    | 0        | 56       | 2       | 0            |
| 18  | M2    | 40    | 0        | 56       | 2       | 0            |
| 18  | M3    | 40    | 0        | 56       | 3       | 0            |
| 19  | A1    | 82    | 0        | 110      | 0       | 0            |
| 19  | A2    | 82    | 0        | 110      | 0       | 0            |
| 19  | A3    | 82    | 0        | 110      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | X1    | 42    | 0        | 57       | 5       | 0            |
| 19  | X2    | 42    | 0        | 57       | 5       | 0            |
| 19  | X3    | 42    | 0        | 57       | 4       | 0            |
| 20  | A1    | 97    | 0        | 0        | 0       | 0            |
| 20  | A2    | 97    | 0        | 0        | 0       | 0            |
| 20  | A3    | 97    | 0        | 0        | 0       | 0            |
| 20  | I1    | 61    | 0        | 0        | 0       | 0            |
| 20  | I2    | 61    | 0        | 0        | 0       | 0            |
| 20  | I3    | 61    | 0        | 0        | 0       | 0            |
| 20  | L1    | 64    | 0        | 0        | 0       | 0            |
| 20  | L2    | 64    | 0        | 0        | 0       | 0            |
| 20  | L3    | 64    | 0        | 0        | 0       | 0            |
| 20  | M1    | 32    | 0        | 0        | 0       | 0            |
| 20  | M2    | 32    | 0        | 0        | 0       | 0            |
| 20  | M3    | 32    | 0        | 0        | 0       | 0            |
| 21  | B1    | 66    | 0        | 96       | 0       | 0            |
| 21  | B2    | 66    | 0        | 96       | 0       | 0            |
| 21  | B3    | 66    | 0        | 96       | 0       | 0            |
| 22  | L1    | 1     | 0        | 0        | 0       | 0            |
| 22  | L2    | 1     | 0        | 0        | 0       | 0            |
| 22  | L3    | 1     | 0        | 0        | 0       | 0            |
| 23  | R1    | 4     | 0        | 0        | 0       | 0            |
| 23  | R2    | 4     | 0        | 0        | 0       | 0            |
| 23  | R3    | 4     | 0        | 0        | 0       | 0            |
| 24  | A1    | 26    | 0        | 0        | 1       | 0            |
| 24  | A2    | 26    | 0        | 0        | 1       | 0            |
| 24  | A3    | 26    | 0        | 0        | 1       | 0            |
| 24  | B1    | 42    | 0        | 0        | 1       | 0            |
| 24  | B2    | 42    | 0        | 0        | 1       | 0            |
| 24  | B3    | 42    | 0        | 0        | 1       | 0            |
| 24  | C1    | 13    | 0        | 0        | 0       | 0            |
| 24  | C2    | 13    | 0        | 0        | 0       | 0            |
| 24  | C3    | 13    | 0        | 0        | 0       | 0            |
| 24  | D1    | 7     | 0        | 0        | 0       | 0            |
| 24  | D2    | 7     | 0        | 0        | 0       | 0            |
| 24  | D3    | 7     | 0        | 0        | 0       | 0            |
| 24  | E1    | 1     | 0        | 0        | 0       | 0            |
| 24  | E2    | 1     | 0        | 0        | 0       | 0            |
| 24  | E3    | 1     | 0        | 0        | 0       | 0            |
| 24  | I1    | 1     | 0        | 0        | 0       | 0            |
| 24  | I2    | 1     | 0        | 0        | 0       | 0            |
| 24  | I3    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | L1    | 22    | 0        | 0        | 0       | 0            |
| 24  | L2    | 22    | 0        | 0        | 0       | 0            |
| 24  | L3    | 22    | 0        | 0        | 0       | 0            |
| 24  | R1    | 4     | 0        | 0        | 0       | 0            |
| 24  | R2    | 4     | 0        | 0        | 0       | 0            |
| 24  | R3    | 4     | 0        | 0        | 0       | 0            |
| All | All   | 73929 | 0        | 70506    | 829     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 829 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:A2:207:LEU:HD11 | 15:A2:820:CLA:HMC1  | 1.72                     | 0.72              |
| 8:J2:31:ARG:HE    | 18:J2:1305:BCR:H312 | 1.55                     | 0.72              |
| 1:A1:207:LEU:HD11 | 15:A1:820:CLA:HMC1  | 1.72                     | 0.71              |
| 1:A3:207:LEU:HD11 | 15:A3:820:CLA:HMC1  | 1.72                     | 0.71              |
| 8:J3:31:ARG:HE    | 18:J3:1305:BCR:H312 | 1.55                     | 0.70              |

There are no symmetry-related clashes.

## 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   | A1    | 743/755 (98%)  | 729 (98%) | 14 (2%) | 0        | 100         | 100 |
| 1   | A2    | 743/755 (98%)  | 729 (98%) | 14 (2%) | 0        | 100         | 100 |
| 1   | A3    | 743/755 (98%)  | 729 (98%) | 14 (2%) | 0        | 100         | 100 |
| 2   | B1    | 738/741 (100%) | 724 (98%) | 14 (2%) | 0        | 100         | 100 |
| 2   | B2    | 738/741 (100%) | 724 (98%) | 14 (2%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 2   | B3    | 738/741 (100%) | 724 (98%) | 14 (2%) | 0        | 100         | 100 |
| 3   | C1    | 78/81 (96%)    | 78 (100%) | 0       | 0        | 100         | 100 |
| 3   | C2    | 78/81 (96%)    | 78 (100%) | 0       | 0        | 100         | 100 |
| 3   | C3    | 78/81 (96%)    | 78 (100%) | 0       | 0        | 100         | 100 |
| 4   | D1    | 136/139 (98%)  | 129 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 4   | D2    | 136/139 (98%)  | 129 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 4   | D3    | 136/139 (98%)  | 129 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 5   | E1    | 67/76 (88%)    | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 5   | E2    | 67/76 (88%)    | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 5   | E3    | 67/76 (88%)    | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 6   | F1    | 139/174 (80%)  | 138 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 6   | F2    | 139/174 (80%)  | 138 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 6   | F3    | 139/174 (80%)  | 138 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 7   | I1    | 36/38 (95%)    | 36 (100%) | 0       | 0        | 100         | 100 |
| 7   | I2    | 36/38 (95%)    | 36 (100%) | 0       | 0        | 100         | 100 |
| 7   | I3    | 36/38 (95%)    | 36 (100%) | 0       | 0        | 100         | 100 |
| 8   | J1    | 39/41 (95%)    | 38 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | J2    | 39/41 (95%)    | 38 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 8   | J3    | 39/41 (95%)    | 38 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 9   | K1    | 77/83 (93%)    | 75 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 9   | K2    | 77/83 (93%)    | 75 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 9   | K3    | 77/83 (93%)    | 75 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 10  | L1    | 150/155 (97%)  | 148 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 10  | L2    | 150/155 (97%)  | 148 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 10  | L3    | 150/155 (97%)  | 148 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 11  | M1    | 29/31 (94%)    | 29 (100%) | 0       | 0        | 100         | 100 |
| 11  | M2    | 29/31 (94%)    | 29 (100%) | 0       | 0        | 100         | 100 |
| 11  | M3    | 29/31 (94%)    | 29 (100%) | 0       | 0        | 100         | 100 |
| 12  | R1    | 95/98 (97%)    | 89 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 12  | R2    | 95/98 (97%)    | 89 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 12  | R3    | 95/98 (97%)    | 89 (94%)  | 6 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 13  | X1    | 26/39 (67%)     | 26 (100%)  | 0        | 0        | 100         | 100 |
| 13  | X2    | 26/39 (67%)     | 26 (100%)  | 0        | 0        | 100         | 100 |
| 13  | X3    | 26/39 (67%)     | 26 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 7059/7353 (96%) | 6912 (98%) | 147 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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   | A1    | 557/603 (92%) | 557 (100%) | 0        | 100         | 100 |
| 1   | A2    | 557/603 (92%) | 557 (100%) | 0        | 100         | 100 |
| 1   | A3    | 557/603 (92%) | 557 (100%) | 0        | 100         | 100 |
| 2   | B1    | 586/598 (98%) | 586 (100%) | 0        | 100         | 100 |
| 2   | B2    | 586/598 (98%) | 586 (100%) | 0        | 100         | 100 |
| 2   | B3    | 586/598 (98%) | 586 (100%) | 0        | 100         | 100 |
| 3   | C1    | 67/68 (98%)   | 67 (100%)  | 0        | 100         | 100 |
| 3   | C2    | 67/68 (98%)   | 67 (100%)  | 0        | 100         | 100 |
| 3   | C3    | 67/68 (98%)   | 67 (100%)  | 0        | 100         | 100 |
| 4   | D1    | 113/116 (97%) | 113 (100%) | 0        | 100         | 100 |
| 4   | D2    | 113/116 (97%) | 113 (100%) | 0        | 100         | 100 |
| 4   | D3    | 113/116 (97%) | 113 (100%) | 0        | 100         | 100 |
| 5   | E1    | 57/65 (88%)   | 57 (100%)  | 0        | 100         | 100 |
| 5   | E2    | 57/65 (88%)   | 57 (100%)  | 0        | 100         | 100 |
| 5   | E3    | 57/65 (88%)   | 57 (100%)  | 0        | 100         | 100 |
| 6   | F1    | 101/138 (73%) | 101 (100%) | 0        | 100         | 100 |
| 6   | F2    | 101/138 (73%) | 101 (100%) | 0        | 100         | 100 |
| 6   | F3    | 101/138 (73%) | 101 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 7   | I1    | 32/32 (100%)    | 32 (100%)   | 0        | 100         | 100 |
| 7   | I2    | 32/32 (100%)    | 32 (100%)   | 0        | 100         | 100 |
| 7   | I3    | 32/32 (100%)    | 32 (100%)   | 0        | 100         | 100 |
| 8   | J1    | 35/36 (97%)     | 35 (100%)   | 0        | 100         | 100 |
| 8   | J2    | 35/36 (97%)     | 35 (100%)   | 0        | 100         | 100 |
| 8   | J3    | 35/36 (97%)     | 35 (100%)   | 0        | 100         | 100 |
| 9   | K1    | 33/61 (54%)     | 33 (100%)   | 0        | 100         | 100 |
| 9   | K2    | 33/61 (54%)     | 33 (100%)   | 0        | 100         | 100 |
| 9   | K3    | 33/61 (54%)     | 33 (100%)   | 0        | 100         | 100 |
| 10  | L1    | 115/120 (96%)   | 115 (100%)  | 0        | 100         | 100 |
| 10  | L2    | 115/120 (96%)   | 115 (100%)  | 0        | 100         | 100 |
| 10  | L3    | 115/120 (96%)   | 115 (100%)  | 0        | 100         | 100 |
| 11  | M1    | 26/26 (100%)    | 26 (100%)   | 0        | 100         | 100 |
| 11  | M2    | 26/26 (100%)    | 26 (100%)   | 0        | 100         | 100 |
| 11  | M3    | 26/26 (100%)    | 26 (100%)   | 0        | 100         | 100 |
| 12  | R1    | 85/86 (99%)     | 85 (100%)   | 0        | 100         | 100 |
| 12  | R2    | 85/86 (99%)     | 85 (100%)   | 0        | 100         | 100 |
| 12  | R3    | 85/86 (99%)     | 85 (100%)   | 0        | 100         | 100 |
| 13  | X1    | 19/31 (61%)     | 19 (100%)   | 0        | 100         | 100 |
| 13  | X2    | 19/31 (61%)     | 19 (100%)   | 0        | 100         | 100 |
| 13  | X3    | 19/31 (61%)     | 19 (100%)   | 0        | 100         | 100 |
| All | All   | 5478/5940 (92%) | 5478 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B2    | 105 | GLN  |
| 1   | A3    | 445 | ASN  |
| 2   | B3    | 105 | GLN  |
| 2   | B1    | 105 | GLN  |
| 1   | A1    | 445 | 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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 444 ligands modelled in this entry, 51 are unknown and 3 are monoatomic - leaving 390 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$ |
| 19  | LHG  | A2    | 853  | -    | 46,46,48     | 0.24 | 0           | 49,52,54    | 0.24 | 0           |
| 18  | BCR  | F2    | 201  | -    | 41,41,41     | 0.11 | 0           | 56,56,56    | 0.28 | 0           |
| 15  | CLA  | A2    | 810  | -    | 37,46,73     | 1.92 | 9 (24%)     | 42,80,113   | 2.09 | 10 (23%)    |
| 17  | SF4  | C1    | 101  | 3    | 0,12,12      | -    | -           | -           | -    | -           |
| 16  | PQN  | B2    | 840  | -    | 34,34,34     | 0.22 | 0           | 42,45,45    | 0.53 | 1 (2%)      |
| 18  | BCR  | B3    | 841  | -    | 41,41,41     | 0.19 | 0           | 56,56,56    | 0.35 | 0           |
| 15  | CLA  | L3    | 1003 | -    | 60,68,73     | 1.31 | 6 (10%)     | 70,107,113  | 1.40 | 11 (15%)    |
| 18  | BCR  | A1    | 848  | -    | 41,41,41     | 0.13 | 0           | 56,56,56    | 0.31 | 0           |
| 15  | CLA  | B3    | 818  | -    | 50,58,73     | 1.43 | 7 (14%)     | 58,95,113   | 1.48 | 9 (15%)     |
| 15  | CLA  | J3    | 1303 | -    | 35,44,73     | 1.73 | 9 (25%)     | 46,78,113   | 1.79 | 11 (23%)    |
| 15  | CLA  | J1    | 1301 | -    | 40,46,73     | 1.71 | 9 (22%)     | 48,79,113   | 1.73 | 12 (25%)    |
| 19  | LHG  | A2    | 854  | -    | 34,34,48     | 0.23 | 0           | 37,40,54    | 0.31 | 0           |
| 15  | CLA  | A1    | 827  | -    | 60,68,73     | 1.33 | 7 (11%)     | 70,107,113  | 1.38 | 6 (8%)      |
| 15  | CLA  | A1    | 807  | -    | 43,52,73     | 1.56 | 7 (16%)     | 49,88,113   | 1.73 | 10 (20%)    |
| 15  | CLA  | B3    | 828  | -    | 41,50,73     | 1.65 | 6 (14%)     | 49,85,113   | 1.66 | 8 (16%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A1    | 840 | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.43 | 9 (11%)  |
| 18  | BCR  | A2    | 849 | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | I2    | 101 | 2    | 65,73,73     | 1.28 | 7 (10%)  | 76,113,113  | 1.27 | 11 (14%) |
| 18  | BCR  | I1    | 102 | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.45 | 0        |
| 15  | CLA  | B3    | 833 | -    | 37,45,73     | 1.74 | 9 (24%)  | 44,78,113   | 1.79 | 10 (22%) |
| 15  | CLA  | B3    | 803 | -    | 54,62,73     | 1.45 | 7 (12%)  | 62,99,113   | 1.37 | 8 (12%)  |
| 18  | BCR  | A3    | 852 | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.38 | 0        |
| 15  | CLA  | A1    | 838 | -    | 55,63,73     | 1.40 | 7 (12%)  | 64,101,113  | 1.40 | 9 (14%)  |
| 18  | BCR  | A2    | 847 | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.33 | 0        |
| 15  | CLA  | A2    | 822 | -    | 45,53,73     | 1.52 | 7 (15%)  | 52,89,113   | 1.65 | 9 (17%)  |
| 15  | CLA  | X2    | 102 | -    | 40,48,73     | 1.73 | 8 (20%)  | 46,83,113   | 1.72 | 13 (28%) |
| 15  | CLA  | B3    | 806 | -    | 50,58,73     | 1.43 | 7 (14%)  | 58,95,113   | 1.46 | 11 (18%) |
| 21  | DGD  | B1    | 848 | -    | 67,67,67     | 0.17 | 0        | 81,81,81    | 0.15 | 0        |
| 15  | CLA  | A2    | 812 | -    | 40,48,73     | 1.69 | 8 (20%)  | 46,83,113   | 1.71 | 9 (19%)  |
| 15  | CLA  | A3    | 821 | -    | 64,72,73     | 1.28 | 7 (10%)  | 75,112,113  | 1.33 | 11 (14%) |
| 15  | CLA  | A3    | 843 | 24   | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.29 | 9 (11%)  |
| 18  | BCR  | B3    | 844 | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.28 | 0        |
| 15  | CLA  | A2    | 817 | -    | 39,46,73     | 1.73 | 10 (25%) | 46,80,113   | 1.76 | 11 (23%) |
| 17  | SF4  | A3    | 846 | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | B2    | 832 | -    | 41,48,73     | 1.65 | 6 (14%)  | 45,82,113   | 1.98 | 9 (20%)  |
| 15  | CLA  | A1    | 832 | -    | 45,53,73     | 1.58 | 6 (13%)  | 52,89,113   | 1.61 | 11 (21%) |
| 15  | CLA  | A3    | 834 | -    | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.33 | 10 (13%) |
| 18  | BCR  | B1    | 847 | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.51 | 0        |
| 15  | CLA  | A3    | 805 | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.32 | 8 (10%)  |
| 15  | CLA  | A3    | 812 | -    | 40,48,73     | 1.70 | 8 (20%)  | 46,83,113   | 1.72 | 9 (19%)  |
| 15  | CLA  | A1    | 817 | -    | 39,46,73     | 1.73 | 10 (25%) | 46,80,113   | 1.76 | 11 (23%) |
| 18  | BCR  | B1    | 842 | -    | 30,30,41     | 0.34 | 0        | 39,39,56    | 0.51 | 0        |
| 15  | CLA  | A3    | 836 | 1    | 41,49,73     | 1.69 | 7 (17%)  | 47,84,113   | 1.67 | 8 (17%)  |
| 15  | CLA  | A2    | 823 | -    | 41,49,73     | 1.68 | 8 (19%)  | 47,84,113   | 1.69 | 8 (17%)  |
| 15  | CLA  | B3    | 829 | -    | 35,43,73     | 1.79 | 8 (22%)  | 41,74,113   | 2.09 | 13 (31%) |
| 19  | LHG  | X2    | 101 | -    | 41,41,48     | 1.01 | 2 (4%)   | 44,47,54    | 1.10 | 2 (4%)   |
| 15  | CLA  | B2    | 826 | -    | 45,53,73     | 1.56 | 7 (15%)  | 52,89,113   | 1.45 | 8 (15%)  |
| 15  | CLA  | X1    | 102 | -    | 40,48,73     | 1.72 | 8 (20%)  | 46,83,113   | 1.72 | 13 (28%) |
| 15  | CLA  | A3    | 841 | 24   | 39,48,73     | 1.72 | 8 (20%)  | 44,83,113   | 1.65 | 10 (22%) |
| 15  | CLA  | A1    | 825 | 24   | 60,68,73     | 1.28 | 6 (10%)  | 70,107,113  | 1.36 | 12 (17%) |
| 15  | CLA  | B1    | 809 | 2    | 65,73,73     | 1.34 | 7 (10%)  | 76,113,113  | 1.27 | 10 (13%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CL0  | A1    | 801  | -    | 65,73,73     | 2.41 | 7 (10%)  | 76,113,113  | 1.19 | 8 (10%)  |
| 15  | CLA  | B1    | 805  | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.31 | 9 (11%)  |
| 15  | CLA  | B2    | 849  | -    | 45,53,73     | 1.60 | 6 (13%)  | 52,89,113   | 1.47 | 8 (15%)  |
| 15  | CLA  | B3    | 808  | -    | 65,73,73     | 1.35 | 7 (10%)  | 76,113,113  | 1.68 | 14 (18%) |
| 15  | CLA  | A1    | 813  | -    | 44,52,73     | 1.47 | 8 (18%)  | 55,88,113   | 1.53 | 10 (18%) |
| 15  | CLA  | B2    | 811  | -    | 45,53,73     | 1.47 | 6 (13%)  | 52,89,113   | 1.48 | 9 (17%)  |
| 15  | CLA  | A2    | 824  | -    | 45,53,73     | 1.51 | 7 (15%)  | 52,89,113   | 1.53 | 9 (17%)  |
| 15  | CLA  | A2    | 828  | -    | 42,50,73     | 1.54 | 7 (16%)  | 48,85,113   | 1.72 | 9 (18%)  |
| 15  | CLA  | A1    | 818  | -    | 50,58,73     | 1.48 | 7 (14%)  | 58,95,113   | 1.54 | 9 (15%)  |
| 16  | PQN  | A3    | 845  | -    | 34,34,34     | 0.24 | 0        | 42,45,45    | 0.46 | 1 (2%)   |
| 15  | CLA  | L2    | 1004 | 24   | 65,73,73     | 1.28 | 7 (10%)  | 76,113,113  | 1.38 | 10 (13%) |
| 18  | BCR  | J2    | 1306 | -    | 41,41,41     | 0.20 | 0        | 56,56,56    | 0.54 | 0        |
| 18  | BCR  | L2    | 1010 | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.33 | 0        |
| 15  | CLA  | A1    | 830  | -    | 65,73,73     | 1.29 | 6 (9%)   | 76,113,113  | 1.28 | 11 (14%) |
| 15  | CLA  | B3    | 816  | -    | 38,46,73     | 1.83 | 9 (23%)  | 40,79,113   | 1.87 | 10 (25%) |
| 15  | CLA  | L1    | 1002 | 10   | 65,73,73     | 1.24 | 7 (10%)  | 76,113,113  | 1.28 | 10 (13%) |
| 15  | CLA  | B2    | 833  | -    | 37,45,73     | 1.73 | 9 (24%)  | 44,78,113   | 1.79 | 10 (22%) |
| 15  | CLA  | A2    | 806  | -    | 65,73,73     | 1.26 | 7 (10%)  | 76,113,113  | 1.28 | 9 (11%)  |
| 15  | CLA  | B2    | 814  | -    | 41,49,73     | 1.68 | 8 (19%)  | 47,84,113   | 1.62 | 8 (17%)  |
| 15  | CLA  | B1    | 830  | -    | 41,49,73     | 1.72 | 8 (19%)  | 47,84,113   | 1.71 | 8 (17%)  |
| 15  | CLA  | B3    | 834  | -    | 37,47,73     | 1.65 | 7 (18%)  | 42,81,113   | 1.79 | 10 (23%) |
| 18  | BCR  | A2    | 852  | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.38 | 0        |
| 15  | CLA  | A3    | 804  | -    | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.38 | 11 (14%) |
| 15  | CLA  | A1    | 844  | -    | 45,53,73     | 1.49 | 7 (15%)  | 52,89,113   | 1.51 | 9 (17%)  |
| 15  | CLA  | B3    | 825  | -    | 65,73,73     | 1.24 | 7 (10%)  | 76,113,113  | 1.27 | 11 (14%) |
| 18  | BCR  | B2    | 846  | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.48 | 0        |
| 15  | CLA  | J1    | 1307 | -    | 34,42,73     | 1.97 | 11 (32%) | 41,73,113   | 2.14 | 12 (29%) |
| 18  | BCR  | J3    | 1304 | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | A1    | 805  | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.32 | 8 (10%)  |
| 15  | CLA  | A2    | 829  | -    | 55,63,73     | 1.35 | 7 (12%)  | 64,101,113  | 1.45 | 10 (15%) |
| 15  | CLA  | A3    | 825  | 24   | 60,68,73     | 1.29 | 7 (11%)  | 70,107,113  | 1.36 | 12 (17%) |
| 17  | SF4  | C2    | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | A3    | 822  | -    | 45,53,73     | 1.52 | 7 (15%)  | 52,89,113   | 1.64 | 9 (17%)  |
| 15  | CLA  | A3    | 818  | -    | 50,58,73     | 1.48 | 7 (14%)  | 58,95,113   | 1.54 | 9 (15%)  |
| 14  | CL0  | A2    | 801  | -    | 65,73,73     | 2.41 | 7 (10%)  | 76,113,113  | 1.18 | 8 (10%)  |
| 15  | CLA  | K3    | 103  | -    | 32,40,73     | 1.80 | 7 (21%)  | 38,70,113   | 2.24 | 13 (34%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | BCR  | F1    | 201  | -    | 41,41,41     | 0.11 | 0        | 56,56,56    | 0.27 | 0        |
| 18  | BCR  | A1    | 855  | -    | 30,30,41     | 0.33 | 0        | 39,39,56    | 0.36 | 0        |
| 17  | SF4  | C3    | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | A1    | 803  | -    | 63,72,73     | 1.31 | 7 (11%)  | 73,112,113  | 1.39 | 9 (12%)  |
| 23  | GAK  | R1    | 101  | 12   | 0,4,4        | -    | -        | -           | -    | -        |
| 15  | CLA  | B2    | 828  | -    | 41,50,73     | 1.66 | 6 (14%)  | 49,85,113   | 1.67 | 8 (16%)  |
| 15  | CLA  | A3    | 844  | -    | 45,53,73     | 1.49 | 7 (15%)  | 52,89,113   | 1.50 | 9 (17%)  |
| 15  | CLA  | A3    | 823  | -    | 41,49,73     | 1.67 | 8 (19%)  | 47,84,113   | 1.69 | 8 (17%)  |
| 15  | CLA  | A1    | 808  | 1    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.31 | 9 (11%)  |
| 15  | CLA  | B2    | 810  | -    | 43,52,73     | 1.55 | 7 (16%)  | 49,88,113   | 1.58 | 9 (18%)  |
| 15  | CLA  | J3    | 1301 | -    | 40,46,73     | 1.71 | 9 (22%)  | 48,79,113   | 1.72 | 12 (25%) |
| 15  | CLA  | B2    | 835  | -    | 46,54,73     | 1.48 | 7 (15%)  | 53,90,113   | 1.61 | 10 (18%) |
| 15  | CLA  | A3    | 807  | -    | 43,52,73     | 1.56 | 7 (16%)  | 49,88,113   | 1.73 | 10 (20%) |
| 18  | BCR  | B2    | 844  | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.28 | 0        |
| 15  | CLA  | B3    | 802  | 24   | 65,73,73     | 1.34 | 6 (9%)   | 76,113,113  | 1.35 | 7 (9%)   |
| 15  | CLA  | B1    | 839  | -    | 65,73,73     | 1.31 | 7 (10%)  | 76,113,113  | 1.27 | 9 (11%)  |
| 15  | CLA  | B2    | 806  | -    | 50,58,73     | 1.43 | 7 (14%)  | 58,95,113   | 1.46 | 10 (17%) |
| 15  | CLA  | A1    | 816  | -    | 41,49,73     | 1.66 | 8 (19%)  | 47,84,113   | 1.70 | 9 (19%)  |
| 15  | CLA  | B2    | 836  | -    | 45,53,73     | 1.55 | 7 (15%)  | 52,89,113   | 1.59 | 9 (17%)  |
| 15  | CLA  | B1    | 807  | -    | 60,68,73     | 1.41 | 6 (10%)  | 70,107,113  | 1.64 | 10 (14%) |
| 15  | CLA  | B1    | 810  | -    | 43,52,73     | 1.55 | 7 (16%)  | 49,88,113   | 1.59 | 9 (18%)  |
| 15  | CLA  | A1    | 834  | -    | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.34 | 10 (13%) |
| 15  | CLA  | B3    | 832  | -    | 41,48,73     | 1.63 | 6 (14%)  | 45,82,113   | 1.97 | 9 (20%)  |
| 15  | CLA  | L3    | 1004 | 24   | 65,73,73     | 1.28 | 7 (10%)  | 76,113,113  | 1.38 | 10 (13%) |
| 19  | LHG  | X3    | 101  | -    | 41,41,48     | 1.01 | 2 (4%)   | 44,47,54    | 1.10 | 2 (4%)   |
| 18  | BCR  | L1    | 1005 | -    | 41,41,41     | 0.23 | 0        | 56,56,56    | 0.47 | 0        |
| 18  | BCR  | M3    | 101  | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.30 | 0        |
| 19  | LHG  | X1    | 101  | -    | 41,41,48     | 1.01 | 2 (4%)   | 44,47,54    | 1.10 | 2 (4%)   |
| 15  | CLA  | B2    | 837  | -    | 41,49,73     | 1.72 | 8 (19%)  | 47,84,113   | 1.67 | 9 (19%)  |
| 18  | BCR  | J1    | 1304 | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | B3    | 826  | -    | 45,53,73     | 1.56 | 7 (15%)  | 52,89,113   | 1.46 | 8 (15%)  |
| 15  | CLA  | A2    | 843  | 24   | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.29 | 9 (11%)  |
| 15  | CLA  | B3    | 835  | -    | 46,54,73     | 1.48 | 7 (15%)  | 53,90,113   | 1.60 | 9 (16%)  |
| 18  | BCR  | A3    | 848  | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.31 | 0        |
| 18  | BCR  | L1    | 1006 | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.33 | 0        |
| 15  | CLA  | A2    | 807  | -    | 43,52,73     | 1.56 | 7 (16%)  | 49,88,113   | 1.73 | 10 (20%) |
| 15  | CLA  | B3    | 849  | -    | 45,53,73     | 1.61 | 6 (13%)  | 52,89,113   | 1.47 | 8 (15%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | B3    | 811  | -    | 45,53,73     | 1.48 | 6 (13%)  | 52,89,113   | 1.49 | 9 (17%)  |
| 18  | BCR  | K3    | 102  | -    | 25,25,41     | 0.37 | 0        | 33,33,56    | 0.41 | 0        |
| 15  | CLA  | B2    | 816  | -    | 38,46,73     | 1.84 | 9 (23%)  | 40,79,113   | 1.88 | 10 (25%) |
| 15  | CLA  | B2    | 801  | -    | 65,73,73     | 1.30 | 6 (9%)   | 76,113,113  | 1.27 | 8 (10%)  |
| 15  | CLA  | B2    | 803  | -    | 54,62,73     | 1.45 | 7 (12%)  | 62,99,113   | 1.36 | 8 (12%)  |
| 15  | CLA  | B3    | 830  | -    | 41,49,73     | 1.72 | 8 (19%)  | 47,84,113   | 1.70 | 8 (17%)  |
| 15  | CLA  | B2    | 824  | 24   | 45,53,73     | 1.54 | 7 (15%)  | 52,89,113   | 1.58 | 8 (15%)  |
| 18  | BCR  | B3    | 842  | -    | 30,30,41     | 0.34 | 0        | 39,39,56    | 0.51 | 0        |
| 15  | CLA  | B3    | 821  | -    | 38,47,73     | 1.72 | 6 (15%)  | 46,80,113   | 2.31 | 12 (26%) |
| 18  | BCR  | B2    | 847  | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.51 | 0        |
| 15  | CLA  | A2    | 804  | -    | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.37 | 10 (13%) |
| 15  | CLA  | A1    | 833  | -    | 65,73,73     | 1.31 | 7 (10%)  | 76,113,113  | 1.33 | 10 (13%) |
| 15  | CLA  | A1    | 829  | -    | 55,63,73     | 1.34 | 7 (12%)  | 64,101,113  | 1.45 | 10 (15%) |
| 18  | BCR  | F3    | 201  | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.27 | 0        |
| 15  | CLA  | B3    | 809  | 2    | 65,73,73     | 1.35 | 7 (10%)  | 76,113,113  | 1.28 | 10 (13%) |
| 15  | CLA  | A2    | 836  | 1    | 41,49,73     | 1.69 | 7 (17%)  | 47,84,113   | 1.67 | 8 (17%)  |
| 18  | BCR  | I3    | 103  | -    | 41,41,41     | 0.18 | 0        | 56,56,56    | 0.35 | 0        |
| 15  | CLA  | B1    | 831  | -    | 41,49,73     | 1.73 | 8 (19%)  | 47,84,113   | 1.74 | 12 (25%) |
| 15  | CLA  | A1    | 820  | -    | 36,46,73     | 1.59 | 8 (22%)  | 45,80,113   | 1.76 | 10 (22%) |
| 15  | CLA  | B1    | 827  | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.26 | 8 (10%)  |
| 18  | BCR  | M2    | 101  | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.30 | 0        |
| 18  | BCR  | A3    | 855  | -    | 30,30,41     | 0.33 | 0        | 39,39,56    | 0.36 | 0        |
| 15  | CLA  | B1    | 836  | -    | 45,53,73     | 1.55 | 7 (15%)  | 52,89,113   | 1.59 | 9 (17%)  |
| 15  | CLA  | B1    | 815  | -    | 36,44,73     | 1.73 | 7 (19%)  | 40,76,113   | 1.83 | 9 (22%)  |
| 17  | SF4  | A1    | 846  | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | A2    | 802  | 24   | 65,73,73     | 1.32 | 7 (10%)  | 76,113,113  | 1.36 | 7 (9%)   |
| 15  | CLA  | A1    | 831  | -    | 50,58,73     | 1.48 | 7 (14%)  | 58,95,113   | 1.63 | 10 (17%) |
| 15  | CLA  | B3    | 814  | -    | 41,49,73     | 1.69 | 8 (19%)  | 47,84,113   | 1.62 | 9 (19%)  |
| 17  | SF4  | C3    | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | B2    | 804  | -    | 55,63,73     | 1.37 | 7 (12%)  | 64,101,113  | 1.38 | 11 (17%) |
| 15  | CLA  | B1    | 838  | 24   | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.30 | 9 (11%)  |
| 18  | BCR  | J2    | 1305 | -    | 41,41,41     | 0.17 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | B1    | 825  | -    | 65,73,73     | 1.24 | 7 (10%)  | 76,113,113  | 1.27 | 11 (14%) |
| 15  | CLA  | A3    | 826  | 24   | 55,63,73     | 1.38 | 6 (10%)  | 64,101,113  | 1.50 | 9 (14%)  |
| 18  | BCR  | B1    | 843  | -    | 25,25,41     | 0.36 | 0        | 33,33,56    | 0.46 | 0        |
| 17  | SF4  | C1    | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | A3    | 802  | 24   | 65,73,73     | 1.32 | 7 (10%)  | 76,113,113  | 1.36 | 7 (9%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A1    | 815  | -    | 37,44,73     | 1.90 | 10 (27%) | 43,76,113   | 1.98 | 10 (23%) |
| 18  | BCR  | B3    | 846  | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.47 | 0        |
| 15  | CLA  | A2    | 811  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.35 | 9 (11%)  |
| 15  | CLA  | A2    | 841  | 24   | 39,48,73     | 1.72 | 8 (20%)  | 44,83,113   | 1.66 | 11 (25%) |
| 15  | CLA  | B2    | 825  | -    | 65,73,73     | 1.24 | 7 (10%)  | 76,113,113  | 1.28 | 11 (14%) |
| 15  | CLA  | B1    | 822  | -    | 39,48,73     | 1.60 | 7 (17%)  | 45,82,113   | 1.66 | 7 (15%)  |
| 15  | CLA  | L1    | 1003 | -    | 60,68,73     | 1.30 | 6 (10%)  | 70,107,113  | 1.40 | 11 (15%) |
| 15  | CLA  | B1    | 804  | -    | 55,63,73     | 1.38 | 7 (12%)  | 64,101,113  | 1.38 | 11 (17%) |
| 18  | BCR  | A1    | 850  | -    | 41,41,41     | 0.11 | 0        | 56,56,56    | 0.30 | 0        |
| 15  | CLA  | B3    | 820  | -    | 36,44,73     | 1.76 | 7 (19%)  | 40,76,113   | 1.89 | 10 (25%) |
| 15  | CLA  | A1    | 811  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.34 | 9 (11%)  |
| 15  | CLA  | B1    | 817  | -    | 50,58,73     | 1.44 | 7 (14%)  | 58,95,113   | 1.55 | 10 (17%) |
| 15  | CLA  | K3    | 101  | -    | 33,42,73     | 1.72 | 5 (15%)  | 35,73,113   | 2.01 | 11 (31%) |
| 17  | SF4  | C2    | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | A3    | 831  | -    | 50,58,73     | 1.48 | 7 (14%)  | 58,95,113   | 1.62 | 10 (17%) |
| 15  | CLA  | B2    | 830  | -    | 41,49,73     | 1.71 | 8 (19%)  | 47,84,113   | 1.71 | 8 (17%)  |
| 15  | CLA  | B3    | 815  | -    | 36,44,73     | 1.74 | 7 (19%)  | 40,76,113   | 1.83 | 9 (22%)  |
| 15  | CLA  | B1    | 818  | -    | 50,58,73     | 1.43 | 7 (14%)  | 58,95,113   | 1.48 | 9 (15%)  |
| 15  | CLA  | A2    | 819  | -    | 58,67,73     | 1.40 | 7 (12%)  | 67,106,113  | 1.64 | 11 (16%) |
| 15  | CLA  | B1    | 824  | 24   | 45,53,73     | 1.54 | 7 (15%)  | 52,89,113   | 1.58 | 8 (15%)  |
| 15  | CLA  | B1    | 828  | -    | 41,50,73     | 1.65 | 6 (14%)  | 49,85,113   | 1.67 | 8 (16%)  |
| 15  | CLA  | A2    | 844  | -    | 45,53,73     | 1.49 | 7 (15%)  | 52,89,113   | 1.52 | 9 (17%)  |
| 15  | CLA  | B1    | 812  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.38 | 12 (15%) |
| 15  | CLA  | A3    | 819  | -    | 58,67,73     | 1.40 | 7 (12%)  | 67,106,113  | 1.64 | 11 (16%) |
| 15  | CLA  | B3    | 810  | -    | 43,52,73     | 1.55 | 7 (16%)  | 49,88,113   | 1.59 | 9 (18%)  |
| 15  | CLA  | K1    | 103  | -    | 32,40,73     | 1.80 | 7 (21%)  | 38,70,113   | 2.23 | 13 (34%) |
| 15  | CLA  | B2    | 838  | 24   | 65,73,73     | 1.26 | 7 (10%)  | 76,113,113  | 1.29 | 9 (11%)  |
| 15  | CLA  | A1    | 802  | 24   | 65,73,73     | 1.32 | 7 (10%)  | 76,113,113  | 1.36 | 7 (9%)   |
| 18  | BCR  | B1    | 841  | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.35 | 0        |
| 15  | CLA  | B1    | 806  | -    | 50,58,73     | 1.43 | 7 (14%)  | 58,95,113   | 1.46 | 10 (17%) |
| 15  | CLA  | A3    | 840  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.43 | 9 (11%)  |
| 15  | CLA  | A3    | 842  | -    | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.29 | 9 (11%)  |
| 15  | CLA  | A3    | 828  | -    | 42,50,73     | 1.54 | 7 (16%)  | 48,85,113   | 1.72 | 9 (18%)  |
| 15  | CLA  | B3    | 837  | -    | 41,49,73     | 1.72 | 8 (19%)  | 47,84,113   | 1.68 | 9 (19%)  |
| 15  | CLA  | A2    | 842  | -    | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.29 | 9 (11%)  |
| 18  | BCR  | B2    | 845  | -    | 41,41,41     | 0.14 | 0        | 56,56,56    | 0.38 | 0        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A3    | 810  | -    | 37,46,73     | 1.92 | 9 (24%)  | 42,80,113   | 2.07 | 10 (23%) |
| 18  | BCR  | B2    | 842  | -    | 30,30,41     | 0.34 | 0        | 39,39,56    | 0.51 | 0        |
| 15  | CLA  | B2    | 809  | 2    | 65,73,73     | 1.34 | 7 (10%)  | 76,113,113  | 1.27 | 10 (13%) |
| 15  | CLA  | B3    | 831  | -    | 41,49,73     | 1.73 | 8 (19%)  | 47,84,113   | 1.74 | 12 (25%) |
| 15  | CLA  | A3    | 803  | -    | 63,72,73     | 1.31 | 7 (11%)  | 73,112,113  | 1.38 | 10 (13%) |
| 18  | BCR  | I2    | 102  | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.45 | 0        |
| 15  | CLA  | A3    | 832  | -    | 45,53,73     | 1.58 | 6 (13%)  | 52,89,113   | 1.61 | 11 (21%) |
| 15  | CLA  | A2    | 832  | -    | 45,53,73     | 1.59 | 6 (13%)  | 52,89,113   | 1.62 | 12 (23%) |
| 15  | CLA  | A2    | 816  | -    | 41,49,73     | 1.66 | 8 (19%)  | 47,84,113   | 1.71 | 9 (19%)  |
| 16  | PQN  | B3    | 840  | -    | 34,34,34     | 0.23 | 0        | 42,45,45    | 0.52 | 1 (2%)   |
| 15  | CLA  | A1    | 843  | 24   | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.29 | 9 (11%)  |
| 15  | CLA  | B3    | 813  | -    | 45,53,73     | 1.53 | 7 (15%)  | 52,89,113   | 1.65 | 10 (19%) |
| 15  | CLA  | A3    | 806  | -    | 65,73,73     | 1.26 | 7 (10%)  | 76,113,113  | 1.29 | 10 (13%) |
| 18  | BCR  | A2    | 848  | -    | 41,41,41     | 0.14 | 0        | 56,56,56    | 0.31 | 0        |
| 18  | BCR  | K2    | 102  | -    | 25,25,41     | 0.37 | 0        | 33,33,56    | 0.41 | 0        |
| 18  | BCR  | I1    | 103  | -    | 41,41,41     | 0.18 | 0        | 56,56,56    | 0.35 | 0        |
| 15  | CLA  | A1    | 814  | -    | 33,41,73     | 1.74 | 9 (27%)  | 43,72,113   | 2.06 | 14 (32%) |
| 15  | CLA  | B3    | 824  | 24   | 45,53,73     | 1.54 | 7 (15%)  | 52,89,113   | 1.58 | 8 (15%)  |
| 18  | BCR  | K1    | 102  | -    | 25,25,41     | 0.37 | 0        | 33,33,56    | 0.41 | 0        |
| 15  | CLA  | B1    | 808  | -    | 65,73,73     | 1.35 | 7 (10%)  | 76,113,113  | 1.68 | 14 (18%) |
| 15  | CLA  | A2    | 808  | 1    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.32 | 9 (11%)  |
| 15  | CLA  | A3    | 829  | -    | 55,63,73     | 1.35 | 7 (12%)  | 64,101,113  | 1.45 | 10 (15%) |
| 15  | CLA  | A2    | 818  | -    | 50,58,73     | 1.48 | 7 (14%)  | 58,95,113   | 1.54 | 9 (15%)  |
| 15  | CLA  | B2    | 839  | -    | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.28 | 9 (11%)  |
| 18  | BCR  | A1    | 851  | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.43 | 0        |
| 19  | LHG  | A1    | 853  | -    | 46,46,48     | 0.24 | 0        | 49,52,54    | 0.24 | 0        |
| 15  | CLA  | B3    | 805  | -    | 65,73,73     | 1.26 | 7 (10%)  | 76,113,113  | 1.31 | 9 (11%)  |
| 15  | CLA  | A1    | 806  | -    | 65,73,73     | 1.26 | 7 (10%)  | 76,113,113  | 1.28 | 10 (13%) |
| 15  | CLA  | B1    | 816  | -    | 38,46,73     | 1.84 | 9 (23%)  | 40,79,113   | 1.87 | 10 (25%) |
| 15  | CLA  | A1    | 835  | -    | 45,53,73     | 1.56 | 6 (13%)  | 52,89,113   | 1.50 | 8 (15%)  |
| 15  | CLA  | B1    | 834  | -    | 37,47,73     | 1.65 | 7 (18%)  | 42,81,113   | 1.79 | 10 (23%) |
| 15  | CLA  | A3    | 816  | -    | 41,49,73     | 1.66 | 8 (19%)  | 47,84,113   | 1.71 | 9 (19%)  |
| 15  | CLA  | A2    | 837  | -    | 50,58,73     | 1.41 | 7 (14%)  | 58,95,113   | 1.53 | 12 (20%) |
| 15  | CLA  | A2    | 856  | -    | 65,73,73     | 1.30 | 6 (9%)   | 76,113,113  | 1.20 | 8 (10%)  |
| 15  | CLA  | J1    | 1302 | 8    | 33,43,73     | 1.68 | 8 (24%)  | 43,76,113   | 1.77 | 10 (23%) |
| 15  | CLA  | A1    | 823  | -    | 41,49,73     | 1.68 | 8 (19%)  | 47,84,113   | 1.70 | 8 (17%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A3    | 814  | -    | 33,41,73     | 1.74 | 9 (27%)  | 43,72,113   | 2.07 | 14 (32%) |
| 15  | CLA  | B3    | 801  | -    | 65,73,73     | 1.30 | 6 (9%)   | 76,113,113  | 1.27 | 8 (10%)  |
| 15  | CLA  | A3    | 824  | -    | 45,53,73     | 1.51 | 7 (15%)  | 52,89,113   | 1.54 | 10 (19%) |
| 18  | BCR  | I2    | 103  | -    | 41,41,41     | 0.18 | 0        | 56,56,56    | 0.35 | 0        |
| 18  | BCR  | L3    | 1005 | -    | 41,41,41     | 0.22 | 0        | 56,56,56    | 0.47 | 0        |
| 15  | CLA  | B2    | 815  | -    | 36,44,73     | 1.73 | 7 (19%)  | 40,76,113   | 1.82 | 9 (22%)  |
| 18  | BCR  | B3    | 847  | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.51 | 0        |
| 18  | BCR  | A1    | 849  | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | B3    | 812  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.38 | 12 (15%) |
| 15  | CLA  | B2    | 829  | -    | 35,43,73     | 1.79 | 8 (22%)  | 41,74,113   | 2.08 | 13 (31%) |
| 15  | CLA  | B3    | 804  | -    | 55,63,73     | 1.37 | 7 (12%)  | 64,101,113  | 1.38 | 11 (17%) |
| 15  | CLA  | B2    | 822  | -    | 39,48,73     | 1.61 | 7 (17%)  | 45,82,113   | 1.67 | 7 (15%)  |
| 15  | CLA  | B2    | 821  | -    | 38,47,73     | 1.72 | 6 (15%)  | 46,80,113   | 2.30 | 12 (26%) |
| 15  | CLA  | K1    | 101  | -    | 33,42,73     | 1.72 | 5 (15%)  | 35,73,113   | 2.00 | 11 (31%) |
| 15  | CLA  | J2    | 1302 | 8    | 33,43,73     | 1.69 | 8 (24%)  | 43,76,113   | 1.78 | 10 (23%) |
| 15  | CLA  | B1    | 833  | -    | 37,45,73     | 1.74 | 9 (24%)  | 44,78,113   | 1.80 | 10 (22%) |
| 18  | BCR  | J1    | 1305 | -    | 41,41,41     | 0.18 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | B1    | 829  | -    | 35,43,73     | 1.79 | 8 (22%)  | 41,74,113   | 2.09 | 13 (31%) |
| 15  | CLA  | J3    | 1302 | 8    | 33,43,73     | 1.69 | 8 (24%)  | 43,76,113   | 1.77 | 9 (20%)  |
| 15  | CLA  | A1    | 837  | -    | 50,58,73     | 1.41 | 7 (14%)  | 58,95,113   | 1.53 | 12 (20%) |
| 15  | CLA  | A1    | 856  | -    | 65,73,73     | 1.30 | 6 (9%)   | 76,113,113  | 1.20 | 8 (10%)  |
| 15  | CLA  | A1    | 822  | -    | 45,53,73     | 1.52 | 7 (15%)  | 52,89,113   | 1.64 | 9 (17%)  |
| 15  | CLA  | L2    | 1002 | 10   | 65,73,73     | 1.24 | 7 (10%)  | 76,113,113  | 1.27 | 10 (13%) |
| 15  | CLA  | A3    | 835  | -    | 45,53,73     | 1.57 | 6 (13%)  | 52,89,113   | 1.51 | 8 (15%)  |
| 15  | CLA  | B2    | 827  | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.27 | 8 (10%)  |
| 15  | CLA  | J2    | 1303 | -    | 35,44,73     | 1.73 | 9 (25%)  | 46,78,113   | 1.78 | 12 (26%) |
| 14  | CL0  | A3    | 801  | -    | 65,73,73     | 2.41 | 7 (10%)  | 76,113,113  | 1.19 | 8 (10%)  |
| 19  | LHG  | A3    | 854  | -    | 34,34,48     | 0.22 | 0        | 37,40,54    | 0.31 | 0        |
| 18  | BCR  | M1    | 101  | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.30 | 0        |
| 15  | CLA  | A2    | 820  | -    | 36,46,73     | 1.59 | 8 (22%)  | 45,80,113   | 1.76 | 10 (22%) |
| 18  | BCR  | B1    | 844  | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.28 | 0        |
| 18  | BCR  | B3    | 845  | -    | 41,41,41     | 0.14 | 0        | 56,56,56    | 0.38 | 0        |
| 15  | CLA  | A3    | 838  | -    | 55,63,73     | 1.40 | 7 (12%)  | 64,101,113  | 1.40 | 9 (14%)  |
| 15  | CLA  | B3    | 817  | -    | 50,58,73     | 1.44 | 7 (14%)  | 58,95,113   | 1.55 | 10 (17%) |
| 18  | BCR  | A3    | 850  | -    | 41,41,41     | 0.12 | 0        | 56,56,56    | 0.30 | 0        |
| 15  | CLA  | B2    | 813  | -    | 45,53,73     | 1.52 | 7 (15%)  | 52,89,113   | 1.64 | 10 (19%) |
| 15  | CLA  | B1    | 802  | 24   | 65,73,73     | 1.34 | 6 (9%)   | 76,113,113  | 1.35 | 7 (9%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | BCR  | A3    | 849  | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | A2    | 825  | 24   | 60,68,73     | 1.28 | 6 (10%)  | 70,107,113  | 1.36 | 12 (17%) |
| 15  | CLA  | L1    | 1004 | 24   | 65,73,73     | 1.28 | 7 (10%)  | 76,113,113  | 1.37 | 10 (13%) |
| 18  | BCR  | A1    | 847  | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.33 | 0        |
| 18  | BCR  | A2    | 855  | -    | 30,30,41     | 0.33 | 0        | 39,39,56    | 0.36 | 0        |
| 15  | CLA  | A1    | 828  | -    | 42,50,73     | 1.54 | 7 (16%)  | 48,85,113   | 1.72 | 9 (18%)  |
| 15  | CLA  | A1    | 812  | -    | 40,48,73     | 1.70 | 8 (20%)  | 46,83,113   | 1.72 | 9 (19%)  |
| 16  | PQN  | B1    | 840  | -    | 34,34,34     | 0.22 | 0        | 42,45,45    | 0.53 | 1 (2%)   |
| 15  | CLA  | B1    | 811  | -    | 45,53,73     | 1.48 | 6 (13%)  | 52,89,113   | 1.49 | 9 (17%)  |
| 15  | CLA  | A2    | 803  | -    | 63,72,73     | 1.31 | 7 (11%)  | 73,112,113  | 1.39 | 9 (12%)  |
| 21  | DGD  | B3    | 848  | -    | 67,67,67     | 0.17 | 0        | 81,81,81    | 0.16 | 0        |
| 15  | CLA  | A2    | 821  | -    | 64,72,73     | 1.28 | 7 (10%)  | 75,112,113  | 1.33 | 11 (14%) |
| 15  | CLA  | A3    | 837  | -    | 50,58,73     | 1.41 | 7 (14%)  | 58,95,113   | 1.53 | 12 (20%) |
| 15  | CLA  | B2    | 805  | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.31 | 9 (11%)  |
| 15  | CLA  | B2    | 819  | -    | 45,53,73     | 1.54 | 7 (15%)  | 52,89,113   | 1.69 | 9 (17%)  |
| 15  | CLA  | B2    | 812  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.38 | 12 (15%) |
| 15  | CLA  | B2    | 817  | -    | 50,58,73     | 1.44 | 7 (14%)  | 58,95,113   | 1.55 | 10 (17%) |
| 23  | GAK  | R3    | 101  | 12   | 0,4,4        | -    | -        | -           | -    | -        |
| 15  | CLA  | B1    | 821  | -    | 38,47,73     | 1.72 | 6 (15%)  | 46,80,113   | 2.30 | 12 (26%) |
| 16  | PQN  | A1    | 845  | -    | 34,34,34     | 0.24 | 0        | 42,45,45    | 0.46 | 1 (2%)   |
| 15  | CLA  | A1    | 826  | 24   | 55,63,73     | 1.38 | 7 (12%)  | 64,101,113  | 1.50 | 9 (14%)  |
| 18  | BCR  | A3    | 847  | -    | 41,41,41     | 0.15 | 0        | 56,56,56    | 0.33 | 0        |
| 15  | CLA  | B2    | 820  | -    | 36,44,73     | 1.76 | 7 (19%)  | 40,76,113   | 1.89 | 10 (25%) |
| 15  | CLA  | B2    | 808  | -    | 65,73,73     | 1.34 | 7 (10%)  | 76,113,113  | 1.68 | 14 (18%) |
| 15  | CLA  | X3    | 102  | -    | 40,48,73     | 1.72 | 8 (20%)  | 46,83,113   | 1.72 | 13 (28%) |
| 15  | CLA  | A3    | 833  | -    | 65,73,73     | 1.31 | 7 (10%)  | 76,113,113  | 1.33 | 10 (13%) |
| 18  | BCR  | A1    | 852  | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.38 | 0        |
| 23  | GAK  | R2    | 101  | 12   | 0,4,4        | -    | -        | -           | -    | -        |
| 18  | BCR  | B2    | 843  | -    | 25,25,41     | 0.36 | 0        | 33,33,56    | 0.46 | 0        |
| 15  | CLA  | A2    | 809  | -    | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.42 | 10 (13%) |
| 15  | CLA  | A1    | 821  | -    | 64,72,73     | 1.28 | 7 (10%)  | 75,112,113  | 1.33 | 11 (14%) |
| 15  | CLA  | A1    | 824  | -    | 45,53,73     | 1.51 | 7 (15%)  | 52,89,113   | 1.53 | 10 (19%) |
| 18  | BCR  | J2    | 1304 | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | A2    | 826  | 24   | 55,63,73     | 1.38 | 7 (12%)  | 64,101,113  | 1.50 | 9 (14%)  |
| 15  | CLA  | A1    | 804  | -    | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.37 | 10 (13%) |
| 15  | CLA  | B3    | 827  | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.27 | 8 (10%)  |
| 19  | LHG  | A3    | 853  | -    | 46,46,48     | 0.24 | 0        | 49,52,54    | 0.24 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | BCR  | A2    | 850  | -    | 41,41,41     | 0.11 | 0        | 56,56,56    | 0.30 | 0        |
| 15  | CLA  | B1    | 819  | -    | 45,53,73     | 1.54 | 7 (15%)  | 52,89,113   | 1.70 | 9 (17%)  |
| 15  | CLA  | B3    | 836  | -    | 45,53,73     | 1.55 | 7 (15%)  | 52,89,113   | 1.59 | 9 (17%)  |
| 15  | CLA  | B2    | 818  | -    | 50,58,73     | 1.43 | 7 (14%)  | 58,95,113   | 1.49 | 9 (15%)  |
| 15  | CLA  | A2    | 830  | -    | 65,73,73     | 1.29 | 6 (9%)   | 76,113,113  | 1.28 | 11 (14%) |
| 15  | CLA  | B1    | 814  | -    | 41,49,73     | 1.68 | 8 (19%)  | 47,84,113   | 1.62 | 9 (19%)  |
| 19  | LHG  | A1    | 854  | -    | 34,34,48     | 0.22 | 0        | 37,40,54    | 0.31 | 0        |
| 18  | BCR  | A3    | 851  | -    | 41,41,41     | 0.13 | 0        | 56,56,56    | 0.43 | 0        |
| 15  | CLA  | A1    | 842  | -    | 65,73,73     | 1.30 | 7 (10%)  | 76,113,113  | 1.30 | 9 (11%)  |
| 15  | CLA  | A3    | 820  | -    | 36,46,73     | 1.59 | 8 (22%)  | 45,80,113   | 1.76 | 10 (22%) |
| 15  | CLA  | K2    | 101  | -    | 33,42,73     | 1.73 | 5 (15%)  | 35,73,113   | 2.00 | 11 (31%) |
| 15  | CLA  | J2    | 1301 | -    | 40,46,73     | 1.71 | 9 (22%)  | 48,79,113   | 1.73 | 12 (25%) |
| 15  | CLA  | B2    | 823  | 2    | 41,49,73     | 1.71 | 8 (19%)  | 47,84,113   | 1.65 | 10 (21%) |
| 15  | CLA  | A2    | 835  | -    | 45,53,73     | 1.56 | 6 (13%)  | 52,89,113   | 1.50 | 8 (15%)  |
| 15  | CLA  | B1    | 826  | -    | 45,53,73     | 1.55 | 7 (15%)  | 52,89,113   | 1.46 | 8 (15%)  |
| 15  | CLA  | A3    | 815  | -    | 37,44,73     | 1.90 | 10 (27%) | 43,76,113   | 1.97 | 10 (23%) |
| 15  | CLA  | A1    | 809  | -    | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.42 | 10 (13%) |
| 15  | CLA  | B1    | 849  | -    | 45,53,73     | 1.60 | 6 (13%)  | 52,89,113   | 1.47 | 8 (15%)  |
| 15  | CLA  | B2    | 834  | -    | 37,47,73     | 1.65 | 7 (18%)  | 42,81,113   | 1.79 | 10 (23%) |
| 21  | DGD  | B2    | 848  | -    | 67,67,67     | 0.18 | 0        | 81,81,81    | 0.16 | 0        |
| 15  | CLA  | B1    | 835  | -    | 46,54,73     | 1.48 | 7 (15%)  | 53,90,113   | 1.60 | 9 (16%)  |
| 15  | CLA  | L3    | 1002 | 10   | 65,73,73     | 1.24 | 7 (10%)  | 76,113,113  | 1.28 | 11 (14%) |
| 15  | CLA  | B3    | 822  | -    | 39,48,73     | 1.60 | 7 (17%)  | 45,82,113   | 1.67 | 7 (15%)  |
| 15  | CLA  | J1    | 1303 | -    | 35,44,73     | 1.72 | 9 (25%)  | 46,78,113   | 1.78 | 12 (26%) |
| 15  | CLA  | J2    | 1307 | -    | 34,42,73     | 1.97 | 11 (32%) | 41,73,113   | 2.14 | 12 (29%) |
| 15  | CLA  | I1    | 101  | 2    | 65,73,73     | 1.28 | 7 (10%)  | 76,113,113  | 1.27 | 11 (14%) |
| 15  | CLA  | B3    | 839  | -    | 65,73,73     | 1.31 | 7 (10%)  | 76,113,113  | 1.27 | 9 (11%)  |
| 18  | BCR  | B2    | 841  | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.35 | 0        |
| 15  | CLA  | J3    | 1307 | -    | 34,42,73     | 1.96 | 11 (32%) | 41,73,113   | 2.15 | 12 (29%) |
| 15  | CLA  | A3    | 811  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.34 | 9 (11%)  |
| 15  | CLA  | L2    | 1003 | -    | 60,68,73     | 1.30 | 6 (10%)  | 70,107,113  | 1.40 | 11 (15%) |
| 15  | CLA  | A3    | 813  | -    | 44,52,73     | 1.47 | 8 (18%)  | 55,88,113   | 1.53 | 11 (20%) |
| 15  | CLA  | B3    | 819  | -    | 45,53,73     | 1.54 | 7 (15%)  | 52,89,113   | 1.70 | 9 (17%)  |
| 15  | CLA  | B3    | 807  | -    | 60,68,73     | 1.41 | 6 (10%)  | 70,107,113  | 1.64 | 10 (14%) |
| 18  | BCR  | L2    | 1005 | -    | 41,41,41     | 0.22 | 0        | 56,56,56    | 0.47 | 0        |
| 15  | CLA  | A3    | 809  | -    | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.42 | 10 (13%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A2    | 839  | -    | 55,63,73     | 1.43 | 7 (12%)  | 64,101,113  | 1.39 | 9 (14%)  |
| 15  | CLA  | A3    | 817  | -    | 39,46,73     | 1.73 | 10 (25%) | 46,80,113   | 1.76 | 11 (23%) |
| 15  | CLA  | B1    | 813  | -    | 45,53,73     | 1.52 | 7 (15%)  | 52,89,113   | 1.65 | 10 (19%) |
| 18  | BCR  | B1    | 845  | -    | 41,41,41     | 0.14 | 0        | 56,56,56    | 0.38 | 0        |
| 18  | BCR  | B1    | 846  | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.48 | 0        |
| 18  | BCR  | J1    | 1306 | -    | 41,41,41     | 0.20 | 0        | 56,56,56    | 0.54 | 0        |
| 15  | CLA  | B2    | 831  | -    | 41,49,73     | 1.73 | 8 (19%)  | 47,84,113   | 1.74 | 12 (25%) |
| 18  | BCR  | L1    | 1011 | -    | 41,41,41     | 0.16 | 0        | 56,56,56    | 0.33 | 0        |
| 18  | BCR  | J3    | 1305 | -    | 41,41,41     | 0.18 | 0        | 56,56,56    | 0.29 | 0        |
| 15  | CLA  | A2    | 805  | -    | 65,73,73     | 1.25 | 7 (10%)  | 76,113,113  | 1.32 | 8 (10%)  |
| 15  | CLA  | A2    | 814  | -    | 33,41,73     | 1.75 | 9 (27%)  | 43,72,113   | 2.06 | 15 (34%) |
| 15  | CLA  | K2    | 103  | -    | 32,40,73     | 1.80 | 7 (21%)  | 38,70,113   | 2.24 | 13 (34%) |
| 15  | CLA  | B1    | 837  | -    | 41,49,73     | 1.73 | 8 (19%)  | 47,84,113   | 1.67 | 9 (19%)  |
| 15  | CLA  | A2    | 834  | -    | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.34 | 11 (14%) |
| 15  | CLA  | B1    | 823  | 2    | 41,49,73     | 1.71 | 8 (19%)  | 47,84,113   | 1.65 | 10 (21%) |
| 15  | CLA  | B1    | 832  | -    | 41,48,73     | 1.64 | 6 (14%)  | 45,82,113   | 1.97 | 9 (20%)  |
| 18  | BCR  | B3    | 843  | -    | 25,25,41     | 0.36 | 0        | 33,33,56    | 0.46 | 0        |
| 15  | CLA  | A3    | 839  | -    | 55,63,73     | 1.43 | 7 (12%)  | 64,101,113  | 1.39 | 9 (14%)  |
| 18  | BCR  | A2    | 851  | -    | 41,41,41     | 0.14 | 0        | 56,56,56    | 0.43 | 0        |
| 18  | BCR  | I3    | 102  | -    | 41,41,41     | 0.19 | 0        | 56,56,56    | 0.45 | 0        |
| 18  | BCR  | J3    | 1306 | -    | 41,41,41     | 0.20 | 0        | 56,56,56    | 0.54 | 0        |
| 15  | CLA  | A2    | 833  | -    | 65,73,73     | 1.32 | 7 (10%)  | 76,113,113  | 1.34 | 10 (13%) |
| 15  | CLA  | B1    | 801  | -    | 65,73,73     | 1.30 | 6 (9%)   | 76,113,113  | 1.27 | 8 (10%)  |
| 15  | CLA  | B1    | 820  | -    | 36,44,73     | 1.76 | 7 (19%)  | 40,76,113   | 1.89 | 10 (25%) |
| 15  | CLA  | A1    | 839  | -    | 55,63,73     | 1.43 | 7 (12%)  | 64,101,113  | 1.39 | 9 (14%)  |
| 15  | CLA  | A1    | 819  | -    | 58,67,73     | 1.40 | 7 (12%)  | 67,106,113  | 1.64 | 11 (16%) |
| 15  | CLA  | A1    | 810  | -    | 37,46,73     | 1.92 | 9 (24%)  | 42,80,113   | 2.08 | 10 (23%) |
| 16  | PQN  | A2    | 845  | -    | 34,34,34     | 0.25 | 0        | 42,45,45    | 0.46 | 1 (2%)   |
| 17  | SF4  | A2    | 846  | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 15  | CLA  | B2    | 802  | 24   | 65,73,73     | 1.35 | 6 (9%)   | 76,113,113  | 1.35 | 7 (9%)   |
| 15  | CLA  | A2    | 831  | -    | 50,58,73     | 1.48 | 7 (14%)  | 58,95,113   | 1.62 | 9 (15%)  |
| 15  | CLA  | B2    | 807  | -    | 60,68,73     | 1.41 | 6 (10%)  | 70,107,113  | 1.64 | 10 (14%) |
| 15  | CLA  | B3    | 838  | 24   | 65,73,73     | 1.27 | 7 (10%)  | 76,113,113  | 1.30 | 9 (11%)  |
| 15  | CLA  | A2    | 827  | -    | 60,68,73     | 1.33 | 7 (11%)  | 70,107,113  | 1.38 | 6 (8%)   |
| 15  | CLA  | I3    | 101  | 2    | 65,73,73     | 1.28 | 7 (10%)  | 76,113,113  | 1.27 | 10 (13%) |
| 15  | CLA  | A2    | 840  | -    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.44 | 10 (13%) |
| 15  | CLA  | A1    | 841  | 24   | 39,48,73     | 1.72 | 8 (20%)  | 44,83,113   | 1.66 | 10 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A3    | 830 | -    | 65,73,73     | 1.29 | 6 (9%)   | 76,113,113  | 1.28 | 11 (14%) |
| 15  | CLA  | A1    | 836 | 1    | 41,49,73     | 1.69 | 7 (17%)  | 47,84,113   | 1.67 | 8 (17%)  |
| 15  | CLA  | A3    | 808 | 1    | 65,73,73     | 1.29 | 7 (10%)  | 76,113,113  | 1.32 | 9 (11%)  |
| 15  | CLA  | A3    | 856 | -    | 65,73,73     | 1.30 | 6 (9%)   | 76,113,113  | 1.20 | 8 (10%)  |
| 15  | CLA  | A2    | 815 | -    | 37,44,73     | 1.89 | 10 (27%) | 43,76,113   | 1.98 | 9 (20%)  |
| 15  | CLA  | B3    | 823 | 2    | 41,49,73     | 1.70 | 8 (19%)  | 47,84,113   | 1.64 | 10 (21%) |
| 15  | CLA  | A2    | 813 | -    | 44,52,73     | 1.47 | 8 (18%)  | 55,88,113   | 1.53 | 11 (20%) |
| 15  | CLA  | B1    | 803 | -    | 54,62,73     | 1.45 | 7 (12%)  | 62,99,113   | 1.36 | 8 (12%)  |
| 15  | CLA  | A3    | 827 | -    | 60,68,73     | 1.33 | 7 (11%)  | 70,107,113  | 1.38 | 6 (8%)   |
| 15  | CLA  | A2    | 838 | -    | 55,63,73     | 1.40 | 7 (12%)  | 64,101,113  | 1.41 | 9 (14%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 19  | LHG  | A2    | 853  | -    | -         | 8/51/51/53   | -       |
| 18  | BCR  | F2    | 201  | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A2    | 810  | -    | 1/1/10/20 | 1/4/82/115   | -       |
| 17  | SF4  | C1    | 101  | 3    | -         | -            | 0/6/5/5 |
| 16  | PQN  | B2    | 840  | -    | -         | 0/23/43/43   | 0/2/2/2 |
| 18  | BCR  | B3    | 841  | -    | -         | 3/29/63/63   | 0/2/2/2 |
| 15  | CLA  | L3    | 1003 | -    | 1/1/14/20 | 3/31/109/115 | -       |
| 18  | BCR  | A1    | 848  | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B3    | 818  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | J3    | 1303 | -    | 1/1/9/20  | -            | -       |
| 15  | CLA  | J1    | 1301 | -    | 1/1/10/20 | 1/8/84/115   | -       |
| 19  | LHG  | A2    | 854  | -    | -         | 8/38/38/53   | -       |
| 15  | CLA  | A1    | 827  | -    | 1/1/14/20 | 9/31/109/115 | -       |
| 15  | CLA  | A1    | 807  | -    | 1/1/11/20 | 7/11/89/115  | -       |
| 15  | CLA  | B3    | 828  | -    | 1/1/10/20 | 4/7/85/115   | -       |
| 15  | CLA  | A1    | 840  | -    | 1/1/15/20 | 5/37/115/115 | -       |
| 18  | BCR  | A2    | 849  | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 15  | CLA  | I2    | 101  | 2    | 1/1/15/20 | 4/37/115/115 | -       |
| 18  | BCR  | I1    | 102  | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B3    | 833  | -    | 1/1/8/20  | 2/4/76/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 15  | CLA  | B3    | 803 | -    | 1/1/12/20 | 3/24/102/115 | -       |
| 18  | BCR  | A3    | 852 | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A1    | 838 | -    | 1/1/13/20 | 8/25/103/115 | -       |
| 18  | BCR  | A2    | 847 | -    | -         | 1/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A2    | 822 | -    | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | X2    | 102 | -    | 1/1/10/20 | 2/6/84/115   | -       |
| 15  | CLA  | B3    | 806 | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 21  | DGD  | B1    | 848 | -    | -         | 8/55/95/95   | 0/2/2/2 |
| 15  | CLA  | A2    | 812 | -    | 1/1/10/20 | 0/6/84/115   | -       |
| 15  | CLA  | A3    | 821 | -    | 1/1/15/20 | 0/35/113/115 | -       |
| 15  | CLA  | A3    | 843 | 24   | 1/1/15/20 | 7/37/115/115 | -       |
| 18  | BCR  | B3    | 844 | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A2    | 817 | -    | 1/1/10/20 | 0/6/82/115   | -       |
| 17  | SF4  | A3    | 846 | 2,1  | -         | -            | 0/6/5/5 |
| 15  | CLA  | B2    | 832 | -    | 1/1/9/20  | 2/8/82/115   | -       |
| 15  | CLA  | A1    | 832 | -    | 1/1/11/20 | 6/13/91/115  | -       |
| 15  | CLA  | A3    | 834 | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 18  | BCR  | B1    | 847 | -    | -         | 6/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A3    | 805 | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | A3    | 812 | -    | 1/1/10/20 | 0/6/84/115   | -       |
| 15  | CLA  | A1    | 817 | -    | 1/1/10/20 | 0/6/82/115   | -       |
| 18  | BCR  | B1    | 842 | -    | -         | 1/24/41/63   | 0/1/1/2 |
| 15  | CLA  | A3    | 836 | 1    | 1/1/10/20 | 2/8/86/115   | -       |
| 15  | CLA  | A2    | 823 | -    | 1/1/10/20 | 2/8/86/115   | -       |
| 15  | CLA  | B3    | 829 | -    | 1/1/6/20  | 0/2/69/115   | -       |
| 19  | LHG  | X2    | 101 | -    | -         | 20/46/46/53  | -       |
| 15  | CLA  | B2    | 826 | -    | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | X1    | 102 | -    | 1/1/10/20 | 2/6/84/115   | -       |
| 15  | CLA  | A3    | 841 | 24   | 1/1/10/20 | 1/6/84/115   | -       |
| 15  | CLA  | A1    | 825 | 24   | 1/1/14/20 | 9/31/109/115 | -       |
| 15  | CLA  | B1    | 809 | 2    | 1/1/15/20 | 4/37/115/115 | -       |
| 14  | CL0  | A1    | 801 | -    | 3/3/20/25 | 4/37/135/135 | -       |
| 15  | CLA  | B1    | 805 | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | B2    | 849 | -    | 1/1/11/20 | 7/13/91/115  | -       |
| 15  | CLA  | B3    | 808 | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 15  | CLA  | A1    | 813 | -    | 1/1/11/20 | 5/13/89/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | B2    | 811  | -    | 1/1/11/20 | 1/13/91/115  | -       |
| 15  | CLA  | A2    | 824  | -    | 1/1/11/20 | 6/13/91/115  | -       |
| 15  | CLA  | A2    | 828  | -    | 1/1/10/20 | 2/10/88/115  | -       |
| 15  | CLA  | A1    | 818  | -    | 1/1/12/20 | 9/19/97/115  | -       |
| 16  | PQN  | A3    | 845  | -    | -         | 0/23/43/43   | 0/2/2/2 |
| 15  | CLA  | L2    | 1004 | 24   | 1/1/15/20 | 4/37/115/115 | -       |
| 18  | BCR  | J2    | 1306 | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 18  | BCR  | L2    | 1010 | -    | -         | 1/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A1    | 830  | -    | 1/1/15/20 | 9/37/115/115 | -       |
| 15  | CLA  | B3    | 816  | -    | 1/1/8/20  | 3/6/76/115   | -       |
| 15  | CLA  | L1    | 1002 | 10   | 1/1/15/20 | 8/37/115/115 | -       |
| 15  | CLA  | B2    | 833  | -    | 1/1/8/20  | 2/4/76/115   | -       |
| 15  | CLA  | A2    | 806  | -    | 1/1/15/20 | 5/37/115/115 | -       |
| 15  | CLA  | B2    | 814  | -    | 1/1/10/20 | 3/8/86/115   | -       |
| 15  | CLA  | B1    | 830  | -    | 1/1/10/20 | 3/8/86/115   | -       |
| 15  | CLA  | B3    | 834  | -    | 1/1/9/20  | 0/6/80/115   | -       |
| 18  | BCR  | A2    | 852  | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A3    | 804  | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | A1    | 844  | -    | 1/1/11/20 | 3/13/91/115  | -       |
| 15  | CLA  | B3    | 825  | -    | 1/1/15/20 | 1/37/115/115 | -       |
| 18  | BCR  | B2    | 846  | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 15  | CLA  | J1    | 1307 | -    | 1/1/8/20  | 0/0/74/115   | -       |
| 18  | BCR  | J3    | 1304 | -    | -         | 3/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A1    | 805  | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | A2    | 829  | -    | 1/1/13/20 | 3/25/103/115 | -       |
| 15  | CLA  | A3    | 825  | 24   | 1/1/14/20 | 9/31/109/115 | -       |
| 17  | SF4  | C2    | 101  | 3    | -         | -            | 0/6/5/5 |
| 15  | CLA  | A3    | 822  | -    | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | A3    | 818  | -    | 1/1/12/20 | 9/19/97/115  | -       |
| 14  | CL0  | A2    | 801  | -    | 3/3/20/25 | 4/37/135/135 | -       |
| 15  | CLA  | K3    | 103  | -    | 1/1/8/20  | -            | -       |
| 18  | BCR  | F1    | 201  | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 18  | BCR  | A1    | 855  | -    | -         | 2/24/41/63   | 0/1/1/2 |
| 17  | SF4  | C3    | 101  | 3    | -         | -            | 0/6/5/5 |
| 15  | CLA  | A1    | 803  | -    | 1/1/15/20 | 3/35/113/115 | -       |
| 23  | GAK  | R1    | 101  | 12   | -         | -            | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | B2    | 828  | -    | 1/1/10/20 | 4/7/85/115   | -       |
| 15  | CLA  | A3    | 844  | -    | 1/1/11/20 | 3/13/91/115  | -       |
| 15  | CLA  | A3    | 823  | -    | 1/1/10/20 | 2/8/86/115   | -       |
| 15  | CLA  | A1    | 808  | 1    | 1/1/15/20 | 3/37/115/115 | -       |
| 15  | CLA  | B2    | 810  | -    | 1/1/11/20 | 0/11/89/115  | -       |
| 15  | CLA  | J3    | 1301 | -    | 1/1/10/20 | 1/8/84/115   | -       |
| 15  | CLA  | B2    | 835  | -    | 1/1/11/20 | 4/15/93/115  | -       |
| 15  | CLA  | A3    | 807  | -    | 1/1/11/20 | 7/11/89/115  | -       |
| 18  | BCR  | B2    | 844  | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B3    | 802  | 24   | 1/1/15/20 | 6/37/115/115 | -       |
| 15  | CLA  | B1    | 839  | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | B2    | 806  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | A1    | 816  | -    | 1/1/10/20 | 0/8/86/115   | -       |
| 15  | CLA  | B2    | 836  | -    | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | B1    | 807  | -    | 1/1/14/20 | 5/31/109/115 | -       |
| 15  | CLA  | B1    | 810  | -    | 1/1/11/20 | 0/11/89/115  | -       |
| 15  | CLA  | A1    | 834  | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | B3    | 832  | -    | 1/1/9/20  | 2/8/82/115   | -       |
| 15  | CLA  | L3    | 1004 | 24   | 1/1/15/20 | 4/37/115/115 | -       |
| 19  | LHG  | X3    | 101  | -    | -         | 20/46/46/53  | -       |
| 18  | BCR  | L1    | 1005 | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 18  | BCR  | M3    | 101  | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 19  | LHG  | X1    | 101  | -    | -         | 20/46/46/53  | -       |
| 15  | CLA  | B2    | 837  | -    | 1/1/10/20 | 5/8/86/115   | -       |
| 18  | BCR  | J1    | 1304 | -    | -         | 3/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B3    | 826  | -    | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | A2    | 843  | 24   | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | B3    | 835  | -    | 1/1/11/20 | 4/15/93/115  | -       |
| 18  | BCR  | A3    | 848  | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 18  | BCR  | L1    | 1006 | -    | -         | 1/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A2    | 807  | -    | 1/1/11/20 | 7/11/89/115  | -       |
| 15  | CLA  | B3    | 849  | -    | 1/1/11/20 | 7/13/91/115  | -       |
| 15  | CLA  | B3    | 811  | -    | 1/1/11/20 | 1/13/91/115  | -       |
| 18  | BCR  | K3    | 102  | -    | -         | 2/18/35/63   | 0/1/1/2 |
| 15  | CLA  | B2    | 816  | -    | 1/1/8/20  | 3/6/76/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 15  | CLA  | B2    | 801  | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 15  | CLA  | B2    | 803  | -    | 1/1/12/20 | 2/24/102/115  | -       |
| 15  | CLA  | B3    | 830  | -    | 1/1/10/20 | 3/8/86/115    | -       |
| 15  | CLA  | B2    | 824  | 24   | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | BCR  | B3    | 842  | -    | -         | 1/24/41/63    | 0/1/1/2 |
| 15  | CLA  | B3    | 821  | -    | 1/1/8/20  | 3/8/79/115    | -       |
| 18  | BCR  | B2    | 847  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 15  | CLA  | A2    | 804  | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 15  | CLA  | A1    | 833  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 15  | CLA  | A1    | 829  | -    | 1/1/13/20 | 3/25/103/115  | -       |
| 18  | BCR  | F3    | 201  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B3    | 809  | 2    | 1/1/15/20 | 4/37/115/115  | -       |
| 15  | CLA  | A2    | 836  | 1    | 1/1/10/20 | 2/8/86/115    | -       |
| 18  | BCR  | I3    | 103  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B1    | 831  | -    | 1/1/10/20 | 1/8/86/115    | -       |
| 15  | CLA  | A1    | 820  | -    | 1/1/9/20  | 1/6/78/115    | -       |
| 15  | CLA  | B1    | 827  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 18  | BCR  | M2    | 101  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 18  | BCR  | A3    | 855  | -    | -         | 2/24/41/63    | 0/1/1/2 |
| 15  | CLA  | B1    | 836  | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 15  | CLA  | B1    | 815  | -    | 1/1/7/20  | 0/2/72/115    | -       |
| 17  | SF4  | A1    | 846  | 2,1  | -         | -             | 0/6/5/5 |
| 15  | CLA  | A2    | 802  | 24   | 1/1/15/20 | 1/37/115/115  | -       |
| 15  | CLA  | A1    | 831  | -    | 1/1/12/20 | 2/19/97/115   | -       |
| 15  | CLA  | B3    | 814  | -    | 1/1/10/20 | 3/8/86/115    | -       |
| 17  | SF4  | C3    | 102  | 3    | -         | -             | 0/6/5/5 |
| 15  | CLA  | B2    | 804  | -    | 1/1/13/20 | 2/25/103/115  | -       |
| 15  | CLA  | B1    | 838  | 24   | 1/1/15/20 | 5/37/115/115  | -       |
| 18  | BCR  | J2    | 1305 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B1    | 825  | -    | 1/1/15/20 | 2/37/115/115  | -       |
| 15  | CLA  | A3    | 826  | 24   | 1/1/13/20 | 5/25/103/115  | -       |
| 18  | BCR  | B1    | 843  | -    | -         | 2/18/35/63    | 0/1/1/2 |
| 17  | SF4  | C1    | 102  | 3    | -         | -             | 0/6/5/5 |
| 15  | CLA  | A3    | 802  | 24   | 1/1/15/20 | 1/37/115/115  | -       |
| 15  | CLA  | A1    | 815  | -    | 1/1/10/20 | 2/6/82/115    | -       |
| 18  | BCR  | B3    | 846  | -    | -         | 0/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | A2    | 811  | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | A2    | 841  | 24   | 1/1/10/20 | 1/6/84/115   | -       |
| 15  | CLA  | B2    | 825  | -    | 1/1/15/20 | 1/37/115/115 | -       |
| 15  | CLA  | B1    | 822  | -    | 1/1/9/20  | 0/8/82/115   | -       |
| 15  | CLA  | L1    | 1003 | -    | 1/1/14/20 | 3/31/109/115 | -       |
| 15  | CLA  | B1    | 804  | -    | 1/1/13/20 | 2/25/103/115 | -       |
| 18  | BCR  | A1    | 850  | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B3    | 820  | -    | 1/1/7/20  | 0/2/72/115   | -       |
| 15  | CLA  | A1    | 811  | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | B1    | 817  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | K3    | 101  | -    | 1/1/7/20  | 0/0/70/115   | -       |
| 17  | SF4  | C2    | 102  | 3    | -         | -            | 0/6/5/5 |
| 15  | CLA  | A3    | 831  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | B2    | 830  | -    | 1/1/10/20 | 3/8/86/115   | -       |
| 15  | CLA  | B3    | 815  | -    | 1/1/7/20  | 0/2/72/115   | -       |
| 15  | CLA  | B1    | 818  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | A2    | 819  | -    | 1/1/14/20 | 2/29/107/115 | -       |
| 15  | CLA  | B1    | 824  | 24   | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | B1    | 828  | -    | 1/1/10/20 | 4/7/85/115   | -       |
| 15  | CLA  | A2    | 844  | -    | 1/1/11/20 | 3/13/91/115  | -       |
| 15  | CLA  | B1    | 812  | -    | 1/1/15/20 | 5/37/115/115 | -       |
| 15  | CLA  | A3    | 819  | -    | 1/1/14/20 | 2/29/107/115 | -       |
| 15  | CLA  | B3    | 810  | -    | 1/1/11/20 | 0/11/89/115  | -       |
| 15  | CLA  | K1    | 103  | -    | 1/1/8/20  | -            | -       |
| 15  | CLA  | B2    | 838  | 24   | 1/1/15/20 | 5/37/115/115 | -       |
| 15  | CLA  | A1    | 802  | 24   | 1/1/15/20 | 1/37/115/115 | -       |
| 18  | BCR  | B1    | 841  | -    | -         | 3/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B1    | 806  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | A3    | 840  | -    | 1/1/15/20 | 5/37/115/115 | -       |
| 15  | CLA  | A3    | 842  | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 15  | CLA  | A3    | 828  | -    | 1/1/10/20 | 2/10/88/115  | -       |
| 15  | CLA  | B3    | 837  | -    | 1/1/10/20 | 5/8/86/115   | -       |
| 15  | CLA  | A2    | 842  | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 18  | BCR  | B2    | 845  | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A3    | 810  | -    | 1/1/10/20 | 1/4/82/115   | -       |
| 18  | BCR  | B2    | 842  | -    | -         | 1/24/41/63   | 0/1/1/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | B2    | 809  | 2    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | B3    | 831  | -    | 1/1/10/20 | 1/8/86/115   | -       |
| 15  | CLA  | A3    | 803  | -    | 1/1/15/20 | 3/35/113/115 | -       |
| 18  | BCR  | I2    | 102  | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A3    | 832  | -    | 1/1/11/20 | 6/13/91/115  | -       |
| 15  | CLA  | A2    | 832  | -    | 1/1/11/20 | 6/13/91/115  | -       |
| 15  | CLA  | A2    | 816  | -    | 1/1/10/20 | 0/8/86/115   | -       |
| 16  | PQN  | B3    | 840  | -    | -         | 0/23/43/43   | 0/2/2/2 |
| 15  | CLA  | A1    | 843  | 24   | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | B3    | 813  | -    | 1/1/11/20 | 7/13/91/115  | -       |
| 15  | CLA  | A3    | 806  | -    | 1/1/15/20 | 5/37/115/115 | -       |
| 18  | BCR  | A2    | 848  | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 18  | BCR  | K2    | 102  | -    | -         | 2/18/35/63   | 0/1/1/2 |
| 18  | BCR  | I1    | 103  | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A1    | 814  | -    | 1/1/6/20  | -            | -       |
| 15  | CLA  | B3    | 824  | 24   | 1/1/11/20 | 2/13/91/115  | -       |
| 18  | BCR  | K1    | 102  | -    | -         | 2/18/35/63   | 0/1/1/2 |
| 15  | CLA  | B1    | 808  | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 15  | CLA  | A2    | 808  | 1    | 1/1/15/20 | 3/37/115/115 | -       |
| 15  | CLA  | A3    | 829  | -    | 1/1/13/20 | 3/25/103/115 | -       |
| 15  | CLA  | A2    | 818  | -    | 1/1/12/20 | 9/19/97/115  | -       |
| 15  | CLA  | B2    | 839  | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 18  | BCR  | A1    | 851  | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 19  | LHG  | A1    | 853  | -    | -         | 8/51/51/53   | -       |
| 15  | CLA  | B3    | 805  | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | A1    | 806  | -    | 1/1/15/20 | 5/37/115/115 | -       |
| 15  | CLA  | B1    | 816  | -    | 1/1/8/20  | 3/6/76/115   | -       |
| 15  | CLA  | A1    | 835  | -    | 1/1/11/20 | 3/13/91/115  | -       |
| 15  | CLA  | B1    | 834  | -    | 1/1/9/20  | 0/6/80/115   | -       |
| 15  | CLA  | A3    | 816  | -    | 1/1/10/20 | 0/8/86/115   | -       |
| 15  | CLA  | A2    | 837  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | A2    | 856  | -    | 1/1/15/20 | 8/37/115/115 | -       |
| 15  | CLA  | J1    | 1302 | 8    | 1/1/8/20  | -            | -       |
| 15  | CLA  | A1    | 823  | -    | 1/1/10/20 | 2/8/86/115   | -       |
| 15  | CLA  | A3    | 814  | -    | 1/1/6/20  | -            | -       |
| 15  | CLA  | B3    | 801  | -    | 1/1/15/20 | 8/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 15  | CLA  | A3    | 824  | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 18  | BCR  | I2    | 103  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 18  | BCR  | L3    | 1005 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B2    | 815  | -    | 1/1/7/20  | 0/2/72/115    | -       |
| 18  | BCR  | B3    | 847  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 18  | BCR  | A1    | 849  | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B3    | 812  | -    | 1/1/15/20 | 5/37/115/115  | -       |
| 15  | CLA  | B2    | 829  | -    | 1/1/6/20  | 0/2/69/115    | -       |
| 15  | CLA  | B3    | 804  | -    | 1/1/13/20 | 2/25/103/115  | -       |
| 15  | CLA  | B2    | 822  | -    | 1/1/9/20  | 0/8/82/115    | -       |
| 15  | CLA  | B2    | 821  | -    | 1/1/8/20  | 3/8/79/115    | -       |
| 15  | CLA  | K1    | 101  | -    | 1/1/7/20  | 0/0/70/115    | -       |
| 15  | CLA  | J2    | 1302 | 8    | 1/1/8/20  | -             | -       |
| 15  | CLA  | B1    | 833  | -    | 1/1/8/20  | 2/4/76/115    | -       |
| 18  | BCR  | J1    | 1305 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B1    | 829  | -    | 1/1/6/20  | 0/2/69/115    | -       |
| 15  | CLA  | J3    | 1302 | 8    | 1/1/8/20  | -             | -       |
| 15  | CLA  | A1    | 837  | -    | 1/1/12/20 | 2/19/97/115   | -       |
| 15  | CLA  | A1    | 856  | -    | 1/1/15/20 | 8/37/115/115  | -       |
| 15  | CLA  | A1    | 822  | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 15  | CLA  | L2    | 1002 | 10   | 1/1/15/20 | 8/37/115/115  | -       |
| 15  | CLA  | A3    | 835  | -    | 1/1/11/20 | 3/13/91/115   | -       |
| 15  | CLA  | B2    | 827  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 15  | CLA  | J2    | 1303 | -    | 1/1/9/20  | -             | -       |
| 14  | CL0  | A3    | 801  | -    | 3/3/20/25 | 4/37/135/135  | -       |
| 19  | LHG  | A3    | 854  | -    | -         | 8/38/38/53    | -       |
| 18  | BCR  | M1    | 101  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 15  | CLA  | A2    | 820  | -    | 1/1/9/20  | 1/6/78/115    | -       |
| 18  | BCR  | B1    | 844  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 18  | BCR  | B3    | 845  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 15  | CLA  | A3    | 838  | -    | 1/1/13/20 | 8/25/103/115  | -       |
| 15  | CLA  | B3    | 817  | -    | 1/1/12/20 | 2/19/97/115   | -       |
| 18  | BCR  | A3    | 850  | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B2    | 813  | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 15  | CLA  | B1    | 802  | 24   | 1/1/15/20 | 6/37/115/115  | -       |
| 18  | BCR  | A3    | 849  | -    | -         | 0/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 15  | CLA  | A2    | 825  | 24   | 1/1/14/20 | 9/31/109/115  | -       |
| 15  | CLA  | L1    | 1004 | 24   | 1/1/15/20 | 4/37/115/115  | -       |
| 18  | BCR  | A1    | 847  | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 18  | BCR  | A2    | 855  | -    | -         | 2/24/41/63    | 0/1/1/2 |
| 15  | CLA  | A1    | 828  | -    | 1/1/10/20 | 2/10/88/115   | -       |
| 15  | CLA  | A1    | 812  | -    | 1/1/10/20 | 0/6/84/115    | -       |
| 16  | PQN  | B1    | 840  | -    | -         | 0/23/43/43    | 0/2/2/2 |
| 15  | CLA  | B1    | 811  | -    | 1/1/11/20 | 1/13/91/115   | -       |
| 15  | CLA  | A2    | 803  | -    | 1/1/15/20 | 3/35/113/115  | -       |
| 21  | DGD  | B3    | 848  | -    | -         | 8/55/95/95    | 0/2/2/2 |
| 15  | CLA  | A2    | 821  | -    | 1/1/15/20 | 0/35/113/115  | -       |
| 15  | CLA  | A3    | 837  | -    | 1/1/12/20 | 2/19/97/115   | -       |
| 15  | CLA  | B2    | 805  | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 15  | CLA  | B2    | 819  | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 15  | CLA  | B2    | 812  | -    | 1/1/15/20 | 5/37/115/115  | -       |
| 15  | CLA  | B2    | 817  | -    | 1/1/12/20 | 2/19/97/115   | -       |
| 23  | GAK  | R3    | 101  | 12   | -         | -             | 0/1/1/1 |
| 15  | CLA  | B1    | 821  | -    | 1/1/8/20  | 3/8/79/115    | -       |
| 16  | PQN  | A1    | 845  | -    | -         | 0/23/43/43    | 0/2/2/2 |
| 15  | CLA  | A1    | 826  | 24   | 1/1/13/20 | 5/25/103/115  | -       |
| 18  | BCR  | A3    | 847  | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 15  | CLA  | B2    | 820  | -    | 1/1/7/20  | 0/2/72/115    | -       |
| 15  | CLA  | B2    | 808  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 15  | CLA  | X3    | 102  | -    | 1/1/10/20 | 2/6/84/115    | -       |
| 15  | CLA  | A3    | 833  | -    | 1/1/15/20 | 6/37/115/115  | -       |
| 18  | BCR  | A1    | 852  | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 23  | GAK  | R2    | 101  | 12   | -         | -             | 0/1/1/1 |
| 18  | BCR  | B2    | 843  | -    | -         | 2/18/35/63    | 0/1/1/2 |
| 15  | CLA  | A2    | 809  | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 15  | CLA  | A1    | 821  | -    | 1/1/15/20 | 0/35/113/115  | -       |
| 15  | CLA  | A1    | 824  | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 18  | BCR  | J2    | 1304 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 15  | CLA  | A2    | 826  | 24   | 1/1/13/20 | 5/25/103/115  | -       |
| 15  | CLA  | A1    | 804  | -    | 1/1/15/20 | 4/37/115/115  | -       |
| 15  | CLA  | B3    | 827  | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 19  | LHG  | A3    | 853  | -    | -         | 8/51/51/53    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 18  | BCR  | A2    | 850  | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B1    | 819  | -    | 1/1/11/20 | 4/13/91/115  | -       |
| 15  | CLA  | B3    | 836  | -    | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | B2    | 818  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | A2    | 830  | -    | 1/1/15/20 | 9/37/115/115 | -       |
| 15  | CLA  | B1    | 814  | -    | 1/1/10/20 | 3/8/86/115   | -       |
| 19  | LHG  | A1    | 854  | -    | -         | 8/38/38/53   | -       |
| 18  | BCR  | A3    | 851  | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A1    | 842  | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 15  | CLA  | A3    | 820  | -    | 1/1/9/20  | 1/6/78/115   | -       |
| 15  | CLA  | K2    | 101  | -    | 1/1/7/20  | 0/0/70/115   | -       |
| 15  | CLA  | J2    | 1301 | -    | 1/1/10/20 | 1/8/84/115   | -       |
| 15  | CLA  | B2    | 823  | 2    | 1/1/10/20 | 2/8/86/115   | -       |
| 15  | CLA  | A2    | 835  | -    | 1/1/11/20 | 3/13/91/115  | -       |
| 15  | CLA  | B1    | 826  | -    | 1/1/11/20 | 2/13/91/115  | -       |
| 15  | CLA  | A3    | 815  | -    | 1/1/10/20 | 2/6/82/115   | -       |
| 15  | CLA  | A1    | 809  | -    | 1/1/15/20 | 9/37/115/115 | -       |
| 15  | CLA  | B1    | 849  | -    | 1/1/11/20 | 7/13/91/115  | -       |
| 15  | CLA  | B2    | 834  | -    | 1/1/9/20  | 0/6/80/115   | -       |
| 21  | DGD  | B2    | 848  | -    | -         | 8/55/95/95   | 0/2/2/2 |
| 15  | CLA  | B1    | 835  | -    | 1/1/11/20 | 4/15/93/115  | -       |
| 15  | CLA  | L3    | 1002 | 10   | 1/1/15/20 | 8/37/115/115 | -       |
| 15  | CLA  | B3    | 822  | -    | 1/1/9/20  | 0/8/82/115   | -       |
| 15  | CLA  | J1    | 1303 | -    | 1/1/9/20  | -            | -       |
| 15  | CLA  | J2    | 1307 | -    | 1/1/8/20  | 0/0/74/115   | -       |
| 15  | CLA  | I1    | 101  | 2    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | B3    | 839  | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 18  | BCR  | B2    | 841  | -    | -         | 3/29/63/63   | 0/2/2/2 |
| 15  | CLA  | J3    | 1307 | -    | 1/1/8/20  | 0/0/74/115   | -       |
| 15  | CLA  | A3    | 811  | -    | 1/1/15/20 | 7/37/115/115 | -       |
| 15  | CLA  | L2    | 1003 | -    | 1/1/14/20 | 3/31/109/115 | -       |
| 15  | CLA  | A3    | 813  | -    | 1/1/11/20 | 5/13/89/115  | -       |
| 15  | CLA  | B3    | 819  | -    | 1/1/11/20 | 4/13/91/115  | -       |
| 15  | CLA  | B3    | 807  | -    | 1/1/14/20 | 5/31/109/115 | -       |
| 18  | BCR  | L2    | 1005 | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A3    | 809  | -    | 1/1/15/20 | 9/37/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | A2    | 839  | -    | 1/1/13/20 | 7/25/103/115 | -       |
| 15  | CLA  | A3    | 817  | -    | 1/1/10/20 | 0/6/82/115   | -       |
| 15  | CLA  | B1    | 813  | -    | 1/1/11/20 | 7/13/91/115  | -       |
| 18  | BCR  | B1    | 845  | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 18  | BCR  | B1    | 846  | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 18  | BCR  | J1    | 1306 | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 15  | CLA  | B2    | 831  | -    | 1/1/10/20 | 1/8/86/115   | -       |
| 18  | BCR  | L1    | 1011 | -    | -         | 1/29/63/63   | 0/2/2/2 |
| 18  | BCR  | J3    | 1305 | -    | -         | 4/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A2    | 805  | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | A2    | 814  | -    | 1/1/6/20  | -            | -       |
| 15  | CLA  | K2    | 103  | -    | 1/1/8/20  | -            | -       |
| 15  | CLA  | B1    | 837  | -    | 1/1/10/20 | 5/8/86/115   | -       |
| 15  | CLA  | A2    | 834  | -    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | B1    | 823  | 2    | 1/1/10/20 | 2/8/86/115   | -       |
| 15  | CLA  | B1    | 832  | -    | 1/1/9/20  | 2/8/82/115   | -       |
| 18  | BCR  | B3    | 843  | -    | -         | 2/18/35/63   | 0/1/1/2 |
| 15  | CLA  | A3    | 839  | -    | 1/1/13/20 | 7/25/103/115 | -       |
| 18  | BCR  | A2    | 851  | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 18  | BCR  | I3    | 102  | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 18  | BCR  | J3    | 1306 | -    | -         | 5/29/63/63   | 0/2/2/2 |
| 15  | CLA  | A2    | 833  | -    | 1/1/15/20 | 6/37/115/115 | -       |
| 15  | CLA  | B1    | 801  | -    | 1/1/15/20 | 8/37/115/115 | -       |
| 15  | CLA  | B1    | 820  | -    | 1/1/7/20  | 0/2/72/115   | -       |
| 15  | CLA  | A1    | 839  | -    | 1/1/13/20 | 7/25/103/115 | -       |
| 15  | CLA  | A1    | 819  | -    | 1/1/14/20 | 2/29/107/115 | -       |
| 15  | CLA  | A1    | 810  | -    | 1/1/10/20 | 1/4/82/115   | -       |
| 16  | PQN  | A2    | 845  | -    | -         | 0/23/43/43   | 0/2/2/2 |
| 17  | SF4  | A2    | 846  | 2,1  | -         | -            | 0/6/5/5 |
| 15  | CLA  | B2    | 802  | 24   | 1/1/15/20 | 6/37/115/115 | -       |
| 15  | CLA  | A2    | 831  | -    | 1/1/12/20 | 2/19/97/115  | -       |
| 15  | CLA  | B2    | 807  | -    | 1/1/14/20 | 5/31/109/115 | -       |
| 15  | CLA  | B3    | 838  | 24   | 1/1/15/20 | 5/37/115/115 | -       |
| 15  | CLA  | A2    | 827  | -    | 1/1/14/20 | 9/31/109/115 | -       |
| 15  | CLA  | I3    | 101  | 2    | 1/1/15/20 | 4/37/115/115 | -       |
| 15  | CLA  | A2    | 840  | -    | 1/1/15/20 | 5/37/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions     | Rings |
|-----|------|-------|-----|------|-----------|--------------|-------|
| 15  | CLA  | A1    | 841 | 24   | 1/1/10/20 | 1/6/84/115   | -     |
| 15  | CLA  | A3    | 830 | -    | 1/1/15/20 | 9/37/115/115 | -     |
| 15  | CLA  | A1    | 836 | 1    | 1/1/10/20 | 2/8/86/115   | -     |
| 15  | CLA  | A3    | 808 | 1    | 1/1/15/20 | 3/37/115/115 | -     |
| 15  | CLA  | A3    | 856 | -    | 1/1/15/20 | 8/37/115/115 | -     |
| 15  | CLA  | A2    | 815 | -    | 1/1/10/20 | 2/6/82/115   | -     |
| 15  | CLA  | B3    | 823 | 2    | 1/1/10/20 | 2/8/86/115   | -     |
| 15  | CLA  | A2    | 813 | -    | 1/1/11/20 | 5/13/89/115  | -     |
| 15  | CLA  | B1    | 803 | -    | 1/1/12/20 | 3/24/102/115 | -     |
| 15  | CLA  | A3    | 827 | -    | 1/1/14/20 | 9/31/109/115 | -     |
| 15  | CLA  | A2    | 838 | -    | 1/1/13/20 | 8/25/103/115 | -     |

The worst 5 of 2082 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 14  | A3    | 801 | CL0  | C4B-NB | 13.40 | 1.47        | 1.35     |
| 14  | A1    | 801 | CL0  | C4B-NB | 13.40 | 1.47        | 1.35     |
| 14  | A2    | 801 | CL0  | C4B-NB | 13.40 | 1.47        | 1.35     |
| 14  | A1    | 801 | CL0  | C1B-NB | 9.41  | 1.43        | 1.35     |
| 14  | A3    | 801 | CL0  | C1B-NB | 9.41  | 1.43        | 1.35     |

The worst 5 of 2818 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 15  | B3    | 821 | CLA  | C4A-NA-C1A | -8.08 | 103.07      | 106.71   |
| 15  | B1    | 821 | CLA  | C4A-NA-C1A | -8.03 | 103.10      | 106.71   |
| 15  | B2    | 821 | CLA  | C4A-NA-C1A | -8.02 | 103.10      | 106.71   |
| 15  | B1    | 808 | CLA  | C4A-NA-C1A | -7.61 | 103.28      | 106.71   |
| 15  | B2    | 808 | CLA  | C4A-NA-C1A | -7.55 | 103.31      | 106.71   |

5 of 294 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | A1    | 801 | CL0  | NA   |
| 14  | A1    | 801 | CL0  | NC   |
| 14  | A1    | 801 | CL0  | ND   |
| 14  | A2    | 801 | CL0  | NA   |
| 14  | A2    | 801 | CL0  | NC   |

5 of 1338 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | A1    | 804 | CLA  | CHA-CBD-CGD-O1D |
| 15  | A1    | 804 | CLA  | CHA-CBD-CGD-O2D |
| 15  | A1    | 805 | CLA  | CHA-CBD-CGD-O1D |
| 15  | A1    | 805 | CLA  | CHA-CBD-CGD-O2D |
| 15  | A1    | 805 | CLA  | CAD-CBD-CGD-O1D |

There are no ring outliers.

276 monomers are involved in 522 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18  | F2    | 201  | BCR  | 4       | 0            |
| 16  | B2    | 840  | PQN  | 4       | 0            |
| 18  | B3    | 841  | BCR  | 3       | 0            |
| 15  | L3    | 1003 | CLA  | 4       | 0            |
| 18  | A1    | 848  | BCR  | 5       | 0            |
| 15  | J3    | 1303 | CLA  | 1       | 0            |
| 15  | A1    | 827  | CLA  | 1       | 0            |
| 15  | A1    | 807  | CLA  | 2       | 0            |
| 15  | A1    | 840  | CLA  | 1       | 0            |
| 18  | A2    | 849  | BCR  | 1       | 0            |
| 15  | I2    | 101  | CLA  | 3       | 0            |
| 18  | I1    | 102  | BCR  | 1       | 0            |
| 15  | B3    | 803  | CLA  | 2       | 0            |
| 18  | A3    | 852  | BCR  | 3       | 0            |
| 15  | A1    | 838  | CLA  | 2       | 0            |
| 18  | A2    | 847  | BCR  | 1       | 0            |
| 15  | X2    | 102  | CLA  | 1       | 0            |
| 15  | A3    | 821  | CLA  | 3       | 0            |
| 15  | A3    | 843  | CLA  | 1       | 0            |
| 18  | B3    | 844  | BCR  | 1       | 0            |
| 15  | B2    | 832  | CLA  | 1       | 0            |
| 15  | A3    | 834  | CLA  | 1       | 0            |
| 15  | A3    | 805  | CLA  | 4       | 0            |
| 18  | B1    | 842  | BCR  | 3       | 0            |
| 15  | A3    | 836  | CLA  | 1       | 0            |
| 19  | X2    | 101  | LHG  | 5       | 0            |
| 15  | B2    | 826  | CLA  | 1       | 0            |
| 15  | X1    | 102  | CLA  | 1       | 0            |
| 15  | A1    | 825  | CLA  | 5       | 0            |
| 15  | B1    | 809  | CLA  | 1       | 0            |
| 14  | A1    | 801  | CL0  | 4       | 0            |
| 15  | B1    | 805  | CLA  | 1       | 0            |
| 15  | B2    | 849  | CLA  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | B3    | 808  | CLA  | 5       | 0            |
| 15  | A1    | 813  | CLA  | 4       | 0            |
| 15  | A2    | 828  | CLA  | 4       | 0            |
| 15  | A1    | 818  | CLA  | 2       | 0            |
| 15  | L2    | 1004 | CLA  | 1       | 0            |
| 18  | J2    | 1306 | BCR  | 2       | 0            |
| 18  | L2    | 1010 | BCR  | 2       | 0            |
| 15  | A1    | 830  | CLA  | 2       | 0            |
| 15  | B3    | 816  | CLA  | 1       | 0            |
| 15  | L1    | 1002 | CLA  | 5       | 0            |
| 15  | A2    | 806  | CLA  | 1       | 0            |
| 18  | A2    | 852  | BCR  | 3       | 0            |
| 15  | A3    | 804  | CLA  | 2       | 0            |
| 18  | B2    | 846  | BCR  | 3       | 0            |
| 18  | J3    | 1304 | BCR  | 2       | 0            |
| 15  | A1    | 805  | CLA  | 4       | 0            |
| 15  | A2    | 829  | CLA  | 4       | 0            |
| 15  | A3    | 825  | CLA  | 5       | 0            |
| 15  | A3    | 818  | CLA  | 3       | 0            |
| 14  | A2    | 801  | CL0  | 2       | 0            |
| 15  | K3    | 103  | CLA  | 2       | 0            |
| 18  | F1    | 201  | BCR  | 3       | 0            |
| 18  | A1    | 855  | BCR  | 1       | 0            |
| 15  | A1    | 803  | CLA  | 2       | 0            |
| 15  | A1    | 808  | CLA  | 2       | 0            |
| 15  | B2    | 810  | CLA  | 1       | 0            |
| 15  | B2    | 835  | CLA  | 1       | 0            |
| 15  | A3    | 807  | CLA  | 2       | 0            |
| 15  | B3    | 802  | CLA  | 5       | 0            |
| 15  | B1    | 839  | CLA  | 3       | 0            |
| 15  | B2    | 836  | CLA  | 2       | 0            |
| 15  | B1    | 807  | CLA  | 2       | 0            |
| 15  | B1    | 810  | CLA  | 1       | 0            |
| 15  | A1    | 834  | CLA  | 1       | 0            |
| 15  | B3    | 832  | CLA  | 1       | 0            |
| 15  | L3    | 1004 | CLA  | 1       | 0            |
| 19  | X3    | 101  | LHG  | 4       | 0            |
| 18  | L1    | 1005 | BCR  | 4       | 0            |
| 18  | M3    | 101  | BCR  | 3       | 0            |
| 19  | X1    | 101  | LHG  | 5       | 0            |
| 15  | B2    | 837  | CLA  | 1       | 0            |
| 18  | J1    | 1304 | BCR  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | B3    | 826  | CLA  | 1       | 0            |
| 15  | A2    | 843  | CLA  | 1       | 0            |
| 15  | B3    | 835  | CLA  | 1       | 0            |
| 18  | A3    | 848  | BCR  | 5       | 0            |
| 18  | L1    | 1006 | BCR  | 2       | 0            |
| 15  | A2    | 807  | CLA  | 2       | 0            |
| 15  | B3    | 849  | CLA  | 2       | 0            |
| 15  | B2    | 816  | CLA  | 1       | 0            |
| 15  | B2    | 801  | CLA  | 4       | 0            |
| 15  | B2    | 803  | CLA  | 2       | 0            |
| 15  | B2    | 824  | CLA  | 1       | 0            |
| 18  | B3    | 842  | BCR  | 3       | 0            |
| 15  | B3    | 821  | CLA  | 1       | 0            |
| 15  | A2    | 804  | CLA  | 2       | 0            |
| 15  | A1    | 833  | CLA  | 3       | 0            |
| 15  | A1    | 829  | CLA  | 4       | 0            |
| 18  | F3    | 201  | BCR  | 3       | 0            |
| 15  | B3    | 809  | CLA  | 1       | 0            |
| 15  | A2    | 836  | CLA  | 1       | 0            |
| 18  | I3    | 103  | BCR  | 2       | 0            |
| 15  | B1    | 831  | CLA  | 1       | 0            |
| 15  | A1    | 820  | CLA  | 1       | 0            |
| 15  | B1    | 827  | CLA  | 4       | 0            |
| 18  | M2    | 101  | BCR  | 2       | 0            |
| 18  | A3    | 855  | BCR  | 1       | 0            |
| 15  | B1    | 836  | CLA  | 2       | 0            |
| 15  | A2    | 802  | CLA  | 5       | 0            |
| 15  | A1    | 831  | CLA  | 2       | 0            |
| 15  | B2    | 804  | CLA  | 1       | 0            |
| 15  | B1    | 838  | CLA  | 3       | 0            |
| 18  | J2    | 1305 | BCR  | 4       | 0            |
| 15  | A3    | 826  | CLA  | 1       | 0            |
| 18  | B1    | 843  | BCR  | 2       | 0            |
| 15  | A3    | 802  | CLA  | 5       | 0            |
| 15  | A1    | 815  | CLA  | 1       | 0            |
| 18  | B3    | 846  | BCR  | 3       | 0            |
| 15  | A2    | 811  | CLA  | 4       | 0            |
| 15  | B1    | 822  | CLA  | 1       | 0            |
| 15  | L1    | 1003 | CLA  | 4       | 0            |
| 15  | B1    | 804  | CLA  | 1       | 0            |
| 18  | A1    | 850  | BCR  | 3       | 0            |
| 15  | B3    | 820  | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 15  | A1    | 811 | CLA  | 4       | 0            |
| 15  | B1    | 817 | CLA  | 1       | 0            |
| 15  | A3    | 831 | CLA  | 2       | 0            |
| 15  | B3    | 815 | CLA  | 1       | 0            |
| 15  | A2    | 819 | CLA  | 6       | 0            |
| 15  | B1    | 812 | CLA  | 4       | 0            |
| 15  | A3    | 819 | CLA  | 5       | 0            |
| 15  | B3    | 810 | CLA  | 1       | 0            |
| 15  | K1    | 103 | CLA  | 2       | 0            |
| 15  | B2    | 838 | CLA  | 3       | 0            |
| 15  | A1    | 802 | CLA  | 4       | 0            |
| 18  | B1    | 841 | BCR  | 4       | 0            |
| 15  | A3    | 840 | CLA  | 1       | 0            |
| 15  | A3    | 842 | CLA  | 4       | 0            |
| 15  | A3    | 828 | CLA  | 4       | 0            |
| 15  | B3    | 837 | CLA  | 1       | 0            |
| 15  | A2    | 842 | CLA  | 4       | 0            |
| 18  | B2    | 845 | BCR  | 1       | 0            |
| 18  | B2    | 842 | BCR  | 2       | 0            |
| 15  | B2    | 809 | CLA  | 2       | 0            |
| 15  | B3    | 831 | CLA  | 1       | 0            |
| 15  | A3    | 803 | CLA  | 2       | 0            |
| 18  | I2    | 102 | BCR  | 1       | 0            |
| 16  | B3    | 840 | PQN  | 5       | 0            |
| 15  | A1    | 843 | CLA  | 1       | 0            |
| 15  | A3    | 806 | CLA  | 1       | 0            |
| 18  | A2    | 848 | BCR  | 5       | 0            |
| 18  | I1    | 103 | BCR  | 1       | 0            |
| 15  | A1    | 814 | CLA  | 1       | 0            |
| 15  | B3    | 824 | CLA  | 1       | 0            |
| 15  | B1    | 808 | CLA  | 4       | 0            |
| 15  | A2    | 808 | CLA  | 2       | 0            |
| 15  | A3    | 829 | CLA  | 3       | 0            |
| 15  | A2    | 818 | CLA  | 3       | 0            |
| 15  | B2    | 839 | CLA  | 3       | 0            |
| 18  | A1    | 851 | BCR  | 5       | 0            |
| 15  | B3    | 805 | CLA  | 2       | 0            |
| 15  | A1    | 806 | CLA  | 1       | 0            |
| 15  | B1    | 816 | CLA  | 1       | 0            |
| 15  | A1    | 835 | CLA  | 1       | 0            |
| 15  | A2    | 837 | CLA  | 1       | 0            |
| 15  | A2    | 856 | CLA  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | B3    | 801  | CLA  | 4       | 0            |
| 18  | I2    | 103  | BCR  | 1       | 0            |
| 18  | L3    | 1005 | BCR  | 4       | 0            |
| 15  | B2    | 815  | CLA  | 1       | 0            |
| 18  | B3    | 847  | BCR  | 1       | 0            |
| 18  | A1    | 849  | BCR  | 3       | 0            |
| 15  | B3    | 812  | CLA  | 4       | 0            |
| 15  | B3    | 804  | CLA  | 1       | 0            |
| 15  | B2    | 822  | CLA  | 1       | 0            |
| 15  | B2    | 821  | CLA  | 1       | 0            |
| 18  | J1    | 1305 | BCR  | 6       | 0            |
| 15  | A1    | 837  | CLA  | 1       | 0            |
| 15  | A1    | 856  | CLA  | 4       | 0            |
| 15  | L2    | 1002 | CLA  | 3       | 0            |
| 15  | A3    | 835  | CLA  | 1       | 0            |
| 15  | B2    | 827  | CLA  | 5       | 0            |
| 15  | J2    | 1303 | CLA  | 1       | 0            |
| 14  | A3    | 801  | CL0  | 2       | 0            |
| 18  | M1    | 101  | BCR  | 2       | 0            |
| 15  | A2    | 820  | CLA  | 1       | 0            |
| 18  | B1    | 844  | BCR  | 1       | 0            |
| 18  | B3    | 845  | BCR  | 1       | 0            |
| 15  | A3    | 838  | CLA  | 2       | 0            |
| 18  | A3    | 850  | BCR  | 3       | 0            |
| 15  | B1    | 802  | CLA  | 5       | 0            |
| 18  | A3    | 849  | BCR  | 3       | 0            |
| 15  | A2    | 825  | CLA  | 5       | 0            |
| 15  | L1    | 1004 | CLA  | 1       | 0            |
| 18  | A1    | 847  | BCR  | 2       | 0            |
| 18  | A2    | 855  | BCR  | 1       | 0            |
| 15  | A1    | 828  | CLA  | 4       | 0            |
| 16  | B1    | 840  | PQN  | 4       | 0            |
| 15  | A2    | 803  | CLA  | 2       | 0            |
| 15  | A2    | 821  | CLA  | 3       | 0            |
| 15  | A3    | 837  | CLA  | 1       | 0            |
| 15  | B2    | 805  | CLA  | 2       | 0            |
| 15  | B2    | 812  | CLA  | 4       | 0            |
| 15  | B1    | 821  | CLA  | 1       | 0            |
| 15  | A1    | 826  | CLA  | 1       | 0            |
| 18  | A3    | 847  | BCR  | 1       | 0            |
| 15  | B2    | 820  | CLA  | 2       | 0            |
| 15  | B2    | 808  | CLA  | 5       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | X3    | 102  | CLA  | 1       | 0            |
| 15  | A3    | 833  | CLA  | 3       | 0            |
| 18  | A1    | 852  | BCR  | 4       | 0            |
| 18  | B2    | 843  | BCR  | 2       | 0            |
| 15  | A2    | 809  | CLA  | 1       | 0            |
| 15  | A1    | 821  | CLA  | 3       | 0            |
| 15  | A1    | 824  | CLA  | 1       | 0            |
| 18  | J2    | 1304 | BCR  | 2       | 0            |
| 15  | A2    | 826  | CLA  | 1       | 0            |
| 15  | A1    | 804  | CLA  | 2       | 0            |
| 15  | B3    | 827  | CLA  | 6       | 0            |
| 18  | A2    | 850  | BCR  | 3       | 0            |
| 15  | B3    | 836  | CLA  | 2       | 0            |
| 15  | A2    | 830  | CLA  | 2       | 0            |
| 18  | A3    | 851  | BCR  | 4       | 0            |
| 15  | A1    | 842  | CLA  | 4       | 0            |
| 15  | A3    | 820  | CLA  | 1       | 0            |
| 15  | B2    | 823  | CLA  | 2       | 0            |
| 15  | A2    | 835  | CLA  | 1       | 0            |
| 15  | B1    | 826  | CLA  | 1       | 0            |
| 15  | A3    | 815  | CLA  | 1       | 0            |
| 15  | A1    | 809  | CLA  | 1       | 0            |
| 15  | B1    | 849  | CLA  | 2       | 0            |
| 15  | B1    | 835  | CLA  | 1       | 0            |
| 15  | L3    | 1002 | CLA  | 4       | 0            |
| 15  | B3    | 822  | CLA  | 1       | 0            |
| 15  | I1    | 101  | CLA  | 3       | 0            |
| 15  | B3    | 839  | CLA  | 3       | 0            |
| 18  | B2    | 841  | BCR  | 4       | 0            |
| 15  | A3    | 811  | CLA  | 4       | 0            |
| 15  | L2    | 1003 | CLA  | 4       | 0            |
| 15  | A3    | 813  | CLA  | 4       | 0            |
| 15  | B3    | 807  | CLA  | 2       | 0            |
| 18  | L2    | 1005 | BCR  | 3       | 0            |
| 15  | A3    | 809  | CLA  | 1       | 0            |
| 15  | A2    | 839  | CLA  | 2       | 0            |
| 18  | B1    | 845  | BCR  | 3       | 0            |
| 18  | B1    | 846  | BCR  | 2       | 0            |
| 18  | J1    | 1306 | BCR  | 3       | 0            |
| 15  | B2    | 831  | CLA  | 1       | 0            |
| 18  | L1    | 1011 | BCR  | 2       | 0            |
| 18  | J3    | 1305 | BCR  | 5       | 0            |

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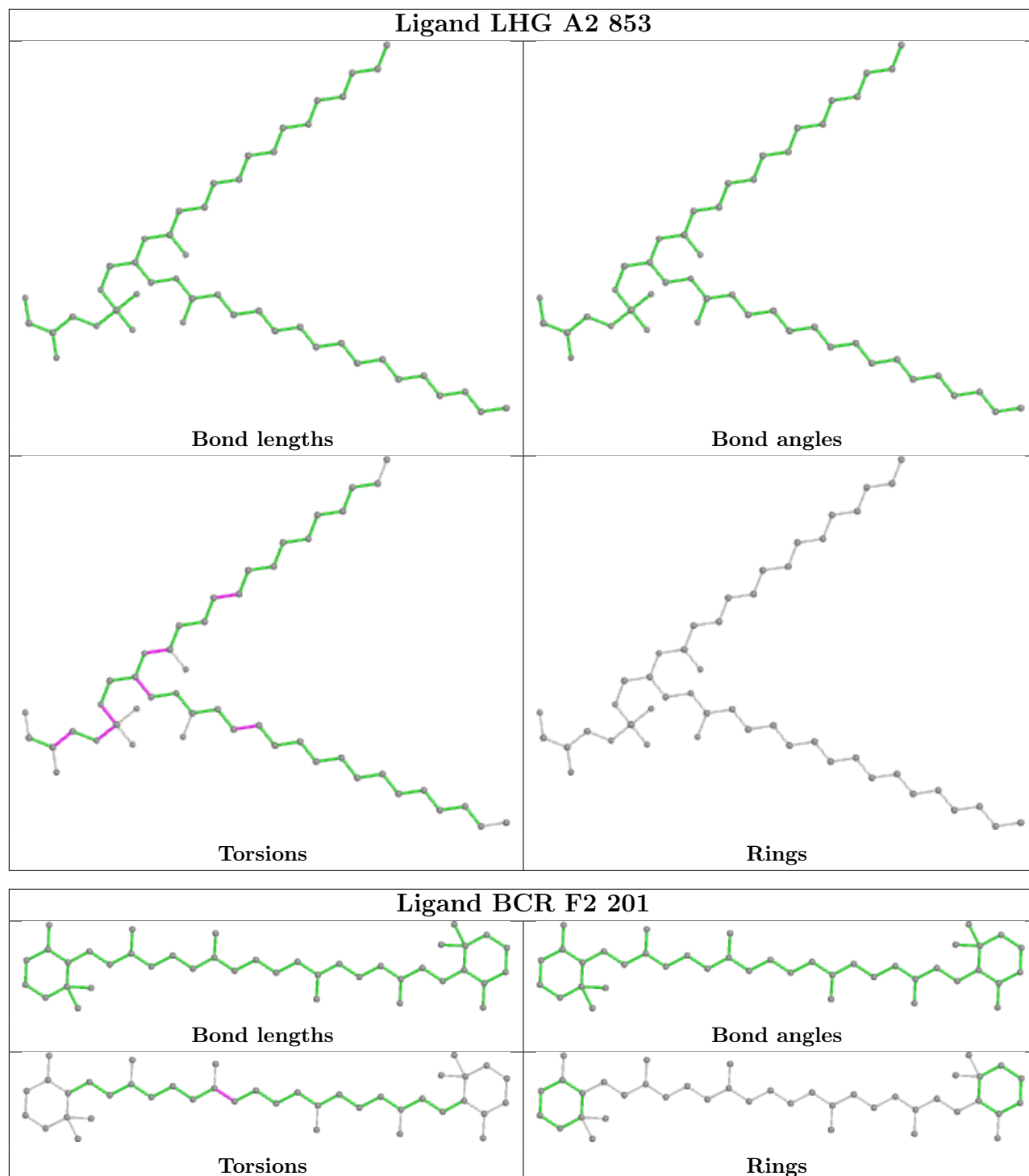
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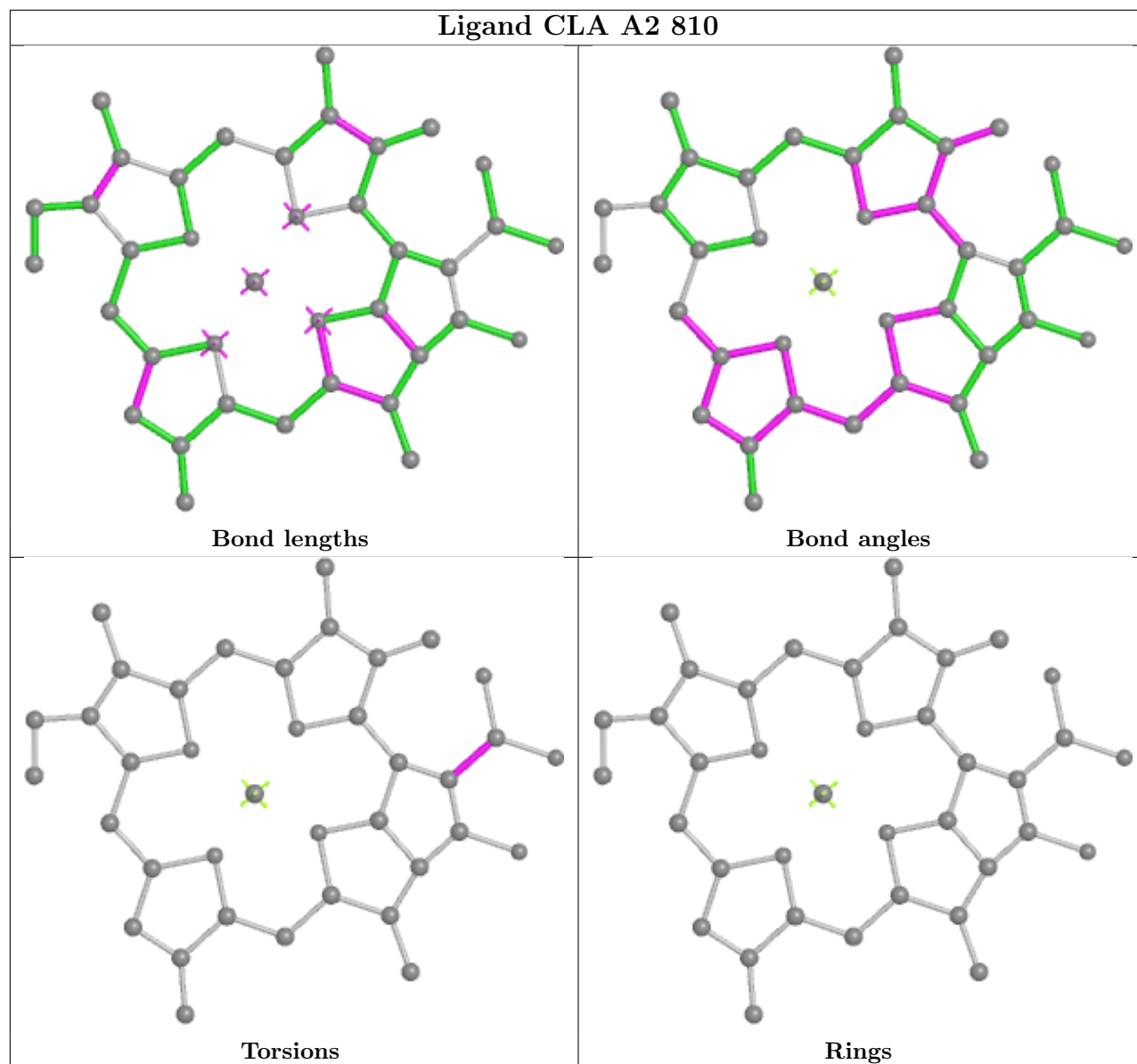
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | A2    | 805  | CLA  | 4       | 0            |
| 15  | A2    | 814  | CLA  | 1       | 0            |
| 15  | K2    | 103  | CLA  | 2       | 0            |
| 15  | A2    | 834  | CLA  | 1       | 0            |
| 15  | B1    | 823  | CLA  | 2       | 0            |
| 15  | B1    | 832  | CLA  | 1       | 0            |
| 18  | B3    | 843  | BCR  | 2       | 0            |
| 15  | A3    | 839  | CLA  | 2       | 0            |
| 18  | A2    | 851  | BCR  | 5       | 0            |
| 18  | I3    | 102  | BCR  | 2       | 0            |
| 18  | J3    | 1306 | BCR  | 4       | 0            |
| 15  | A2    | 833  | CLA  | 3       | 0            |
| 15  | B1    | 801  | CLA  | 4       | 0            |
| 15  | B1    | 820  | CLA  | 1       | 0            |
| 15  | A1    | 839  | CLA  | 2       | 0            |
| 15  | A1    | 819  | CLA  | 6       | 0            |
| 15  | B2    | 802  | CLA  | 5       | 0            |
| 15  | A2    | 831  | CLA  | 2       | 0            |
| 15  | B2    | 807  | CLA  | 2       | 0            |
| 15  | B3    | 838  | CLA  | 3       | 0            |
| 15  | A2    | 827  | CLA  | 1       | 0            |
| 15  | I3    | 101  | CLA  | 3       | 0            |
| 15  | A2    | 840  | CLA  | 1       | 0            |
| 15  | A3    | 830  | CLA  | 2       | 0            |
| 15  | A1    | 836  | CLA  | 1       | 0            |
| 15  | A3    | 808  | CLA  | 2       | 0            |
| 15  | A3    | 856  | CLA  | 4       | 0            |
| 15  | A2    | 815  | CLA  | 1       | 0            |
| 15  | B3    | 823  | CLA  | 2       | 0            |
| 15  | A2    | 813  | CLA  | 4       | 0            |
| 15  | B1    | 803  | CLA  | 2       | 0            |
| 15  | A3    | 827  | CLA  | 1       | 0            |
| 15  | A2    | 838  | CLA  | 2       | 0            |

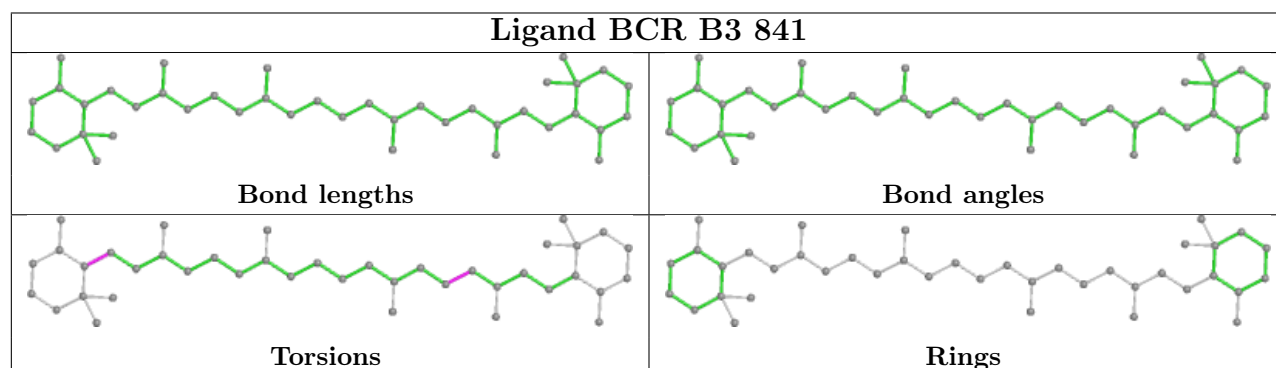
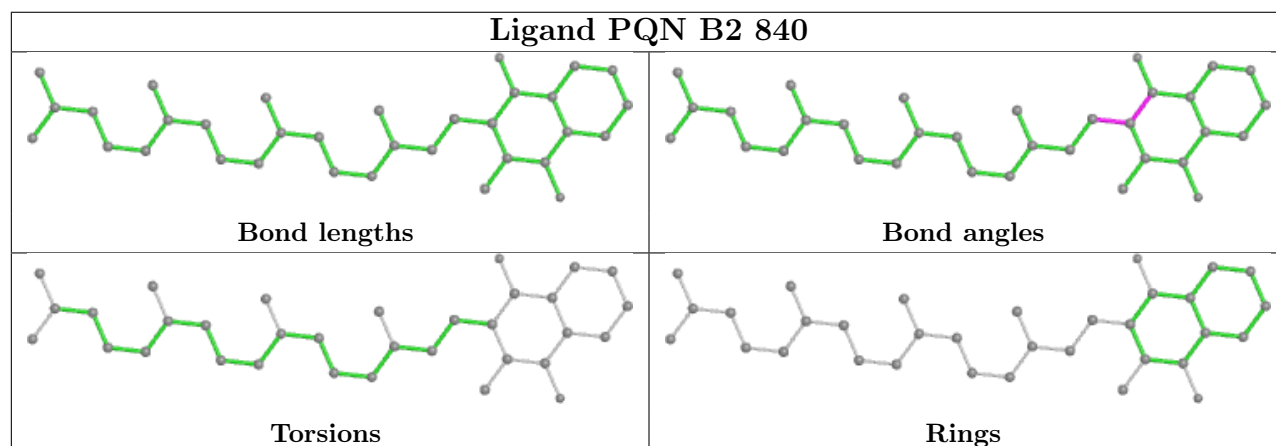
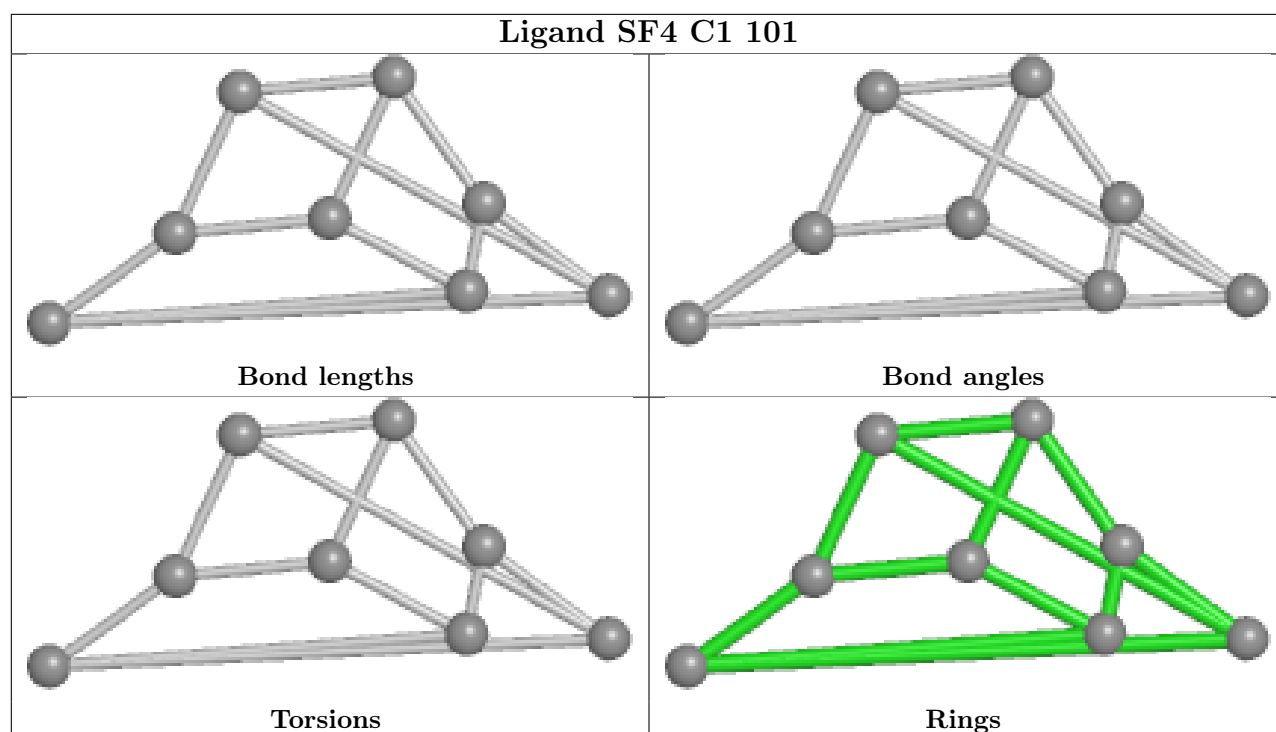
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

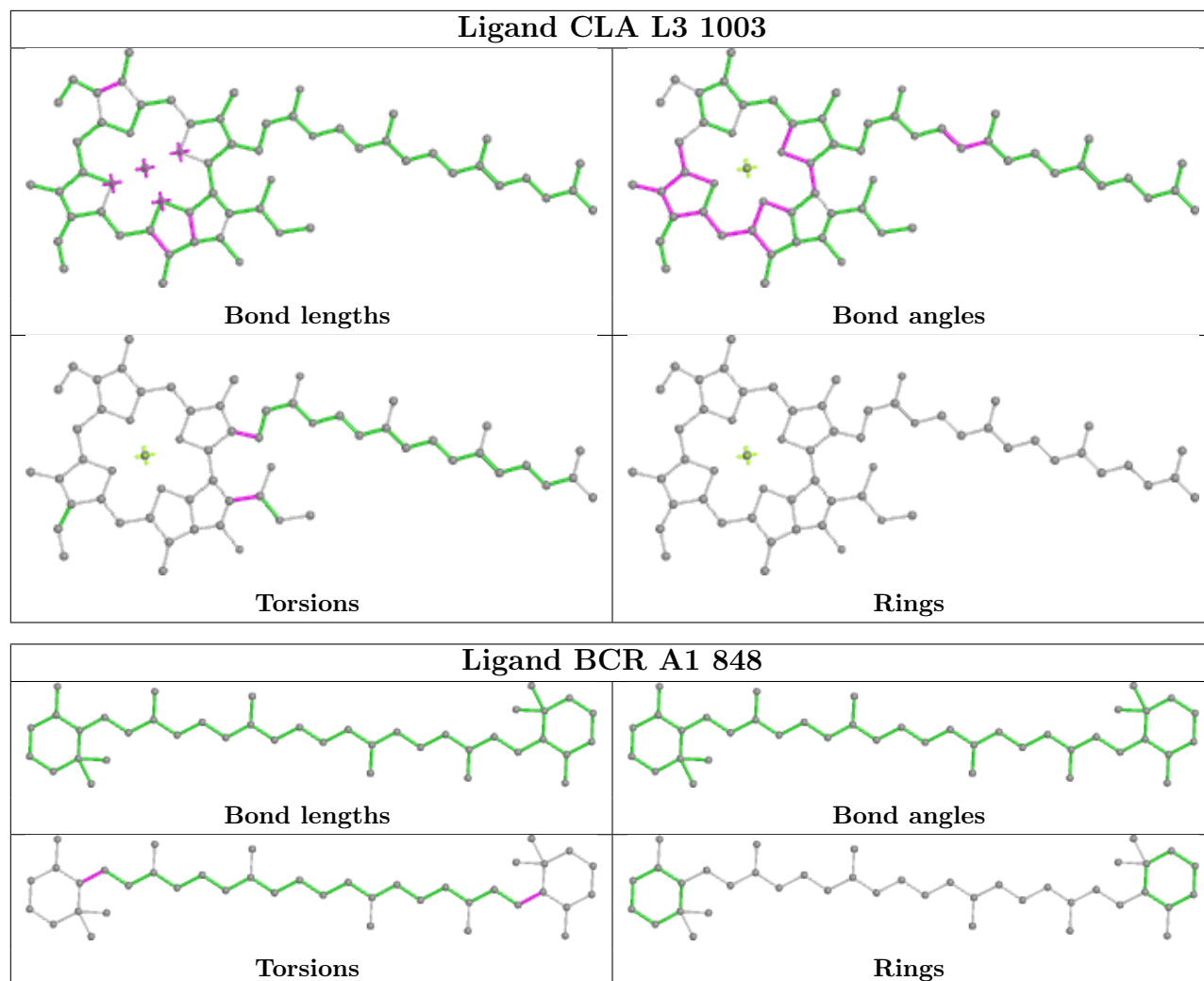


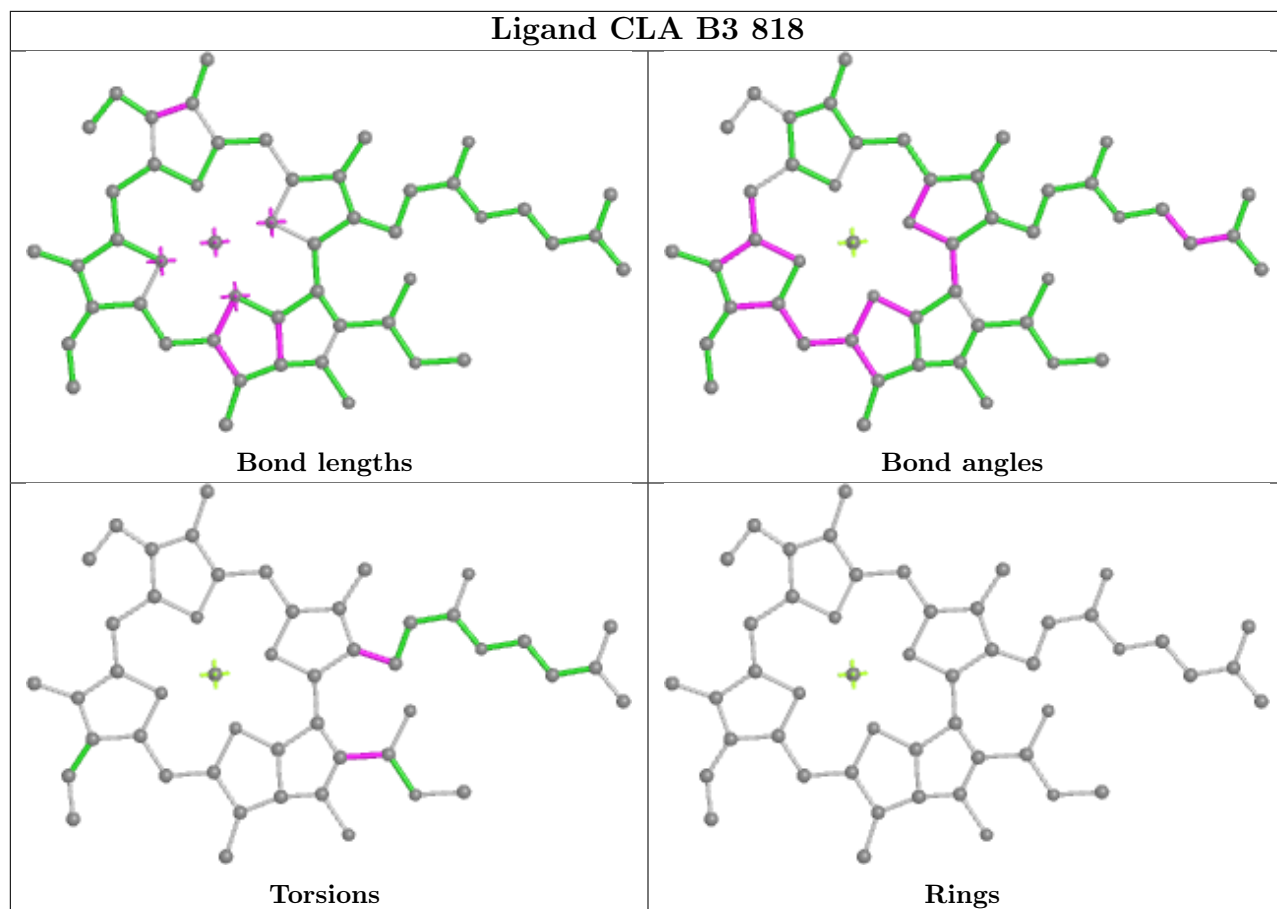
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

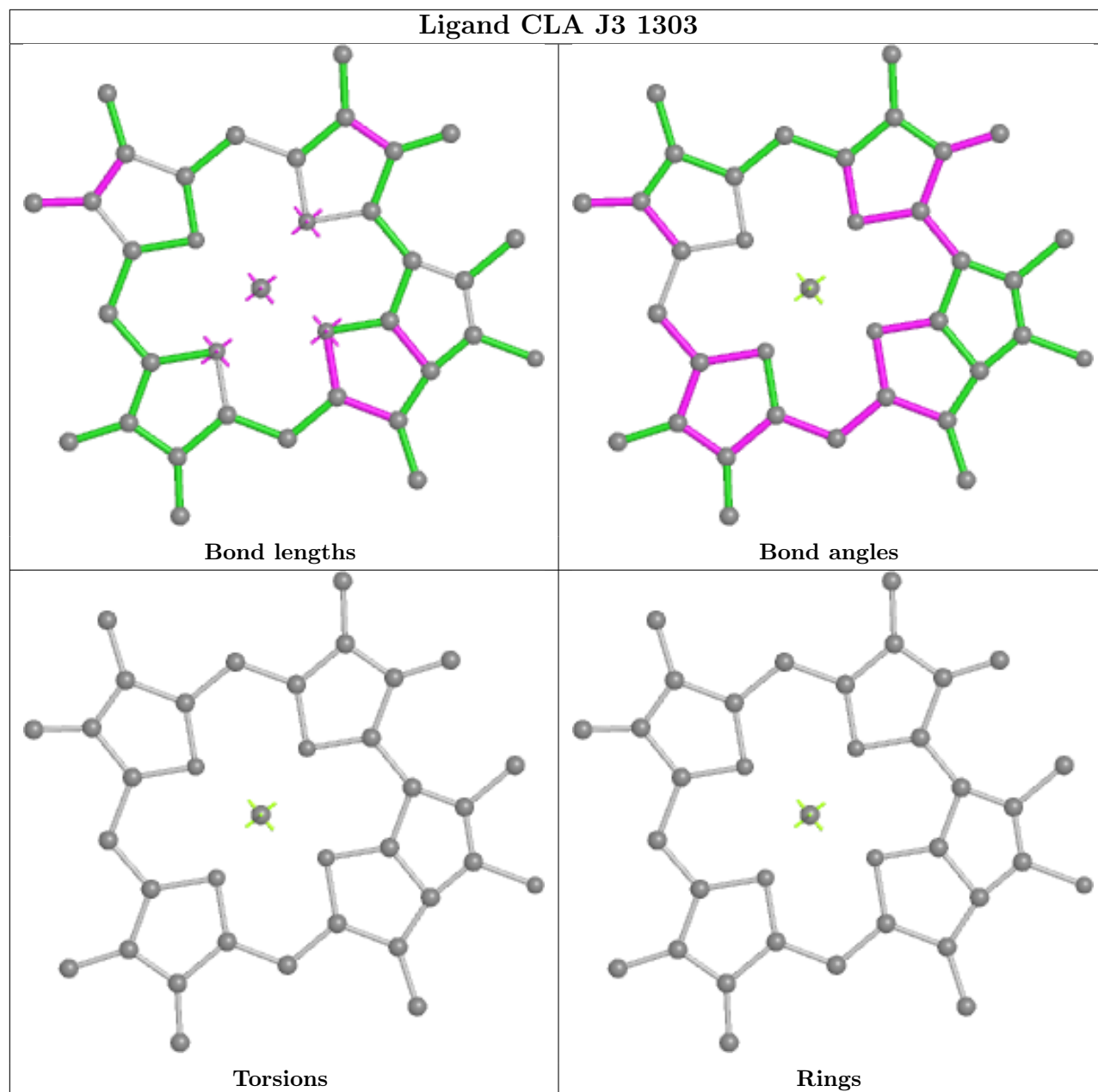


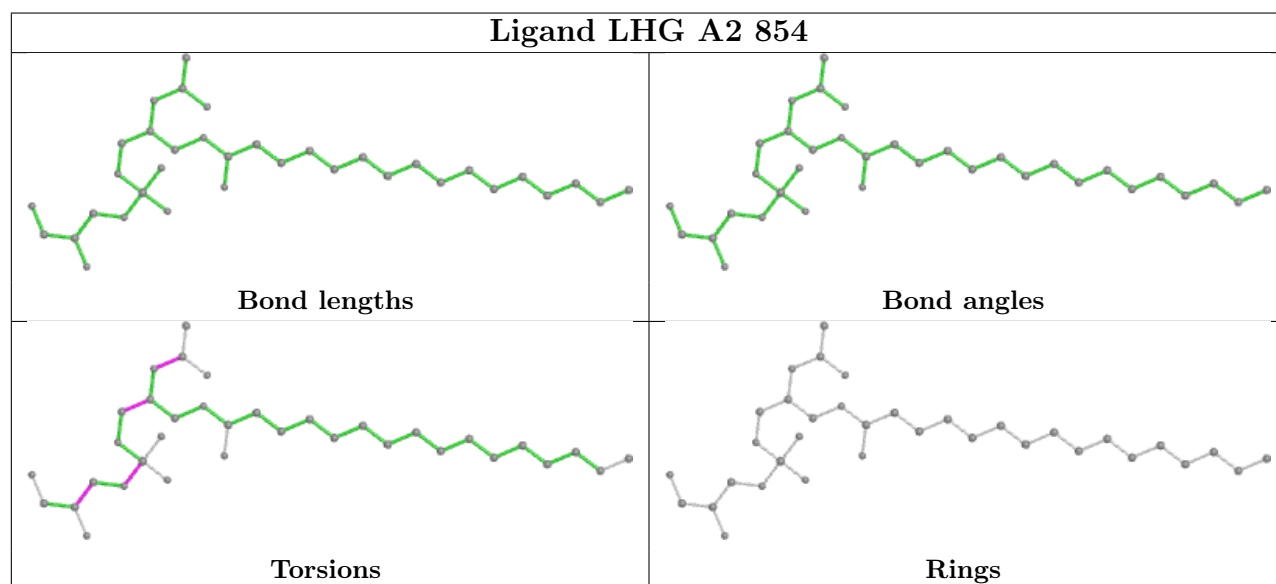
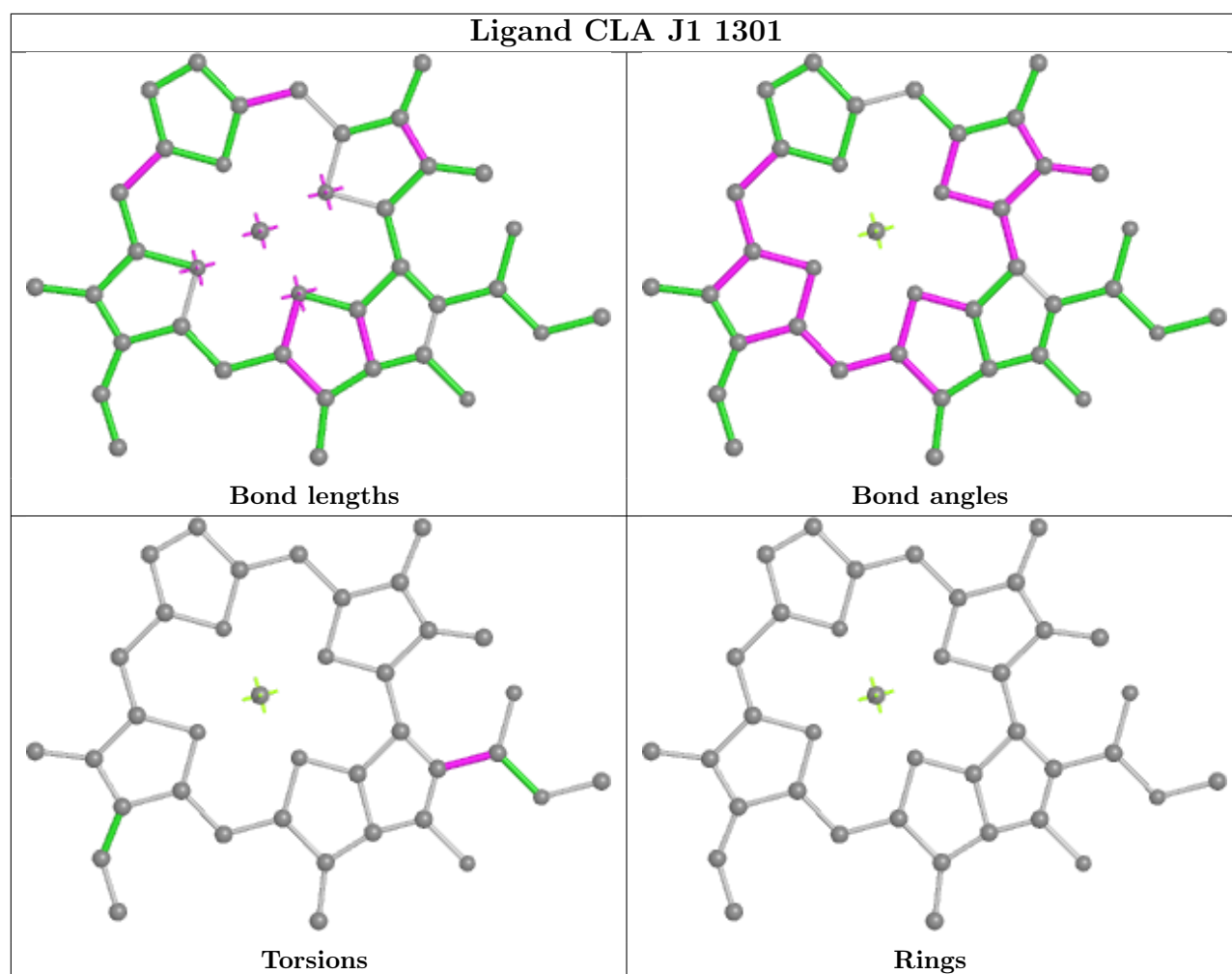


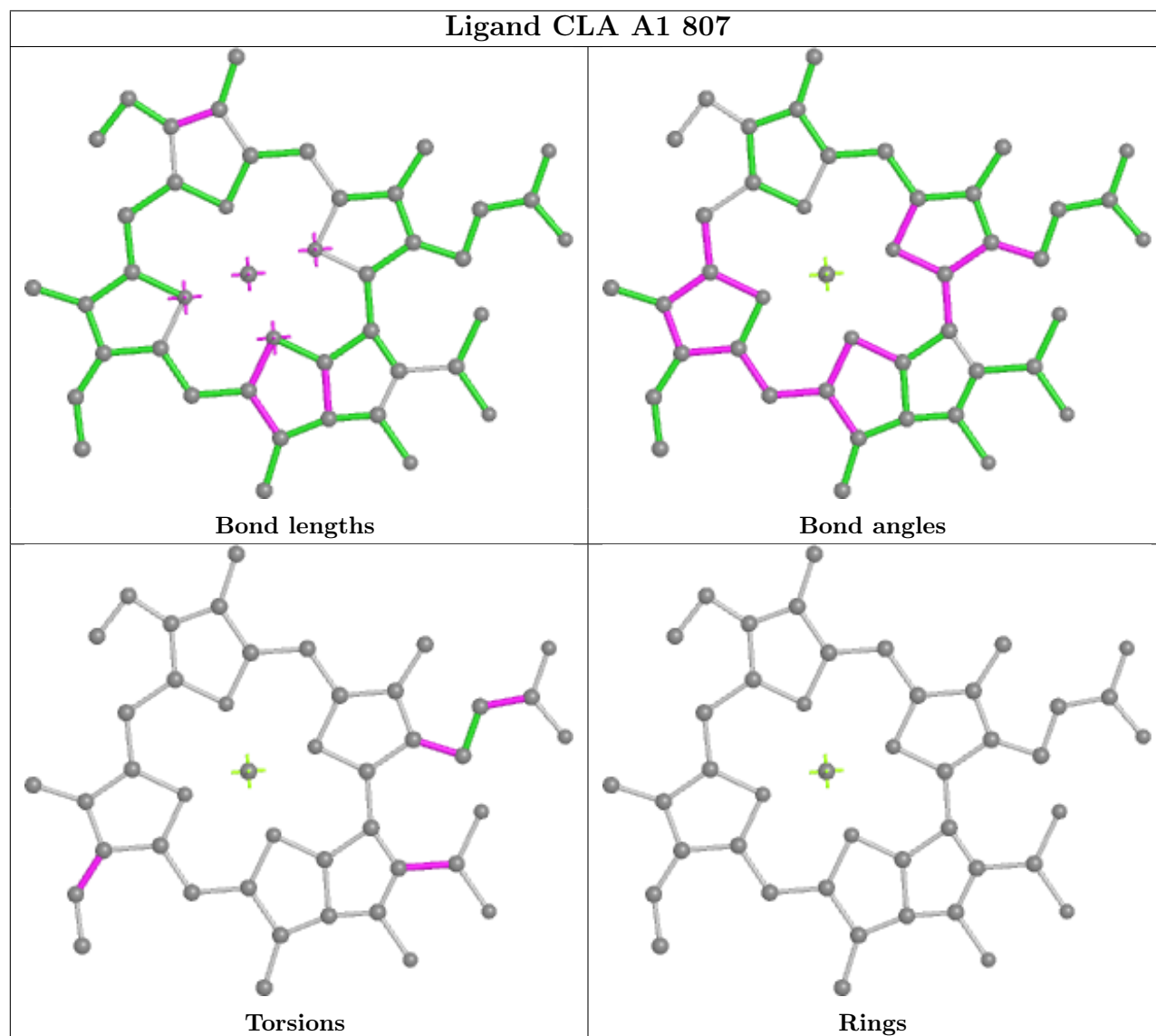
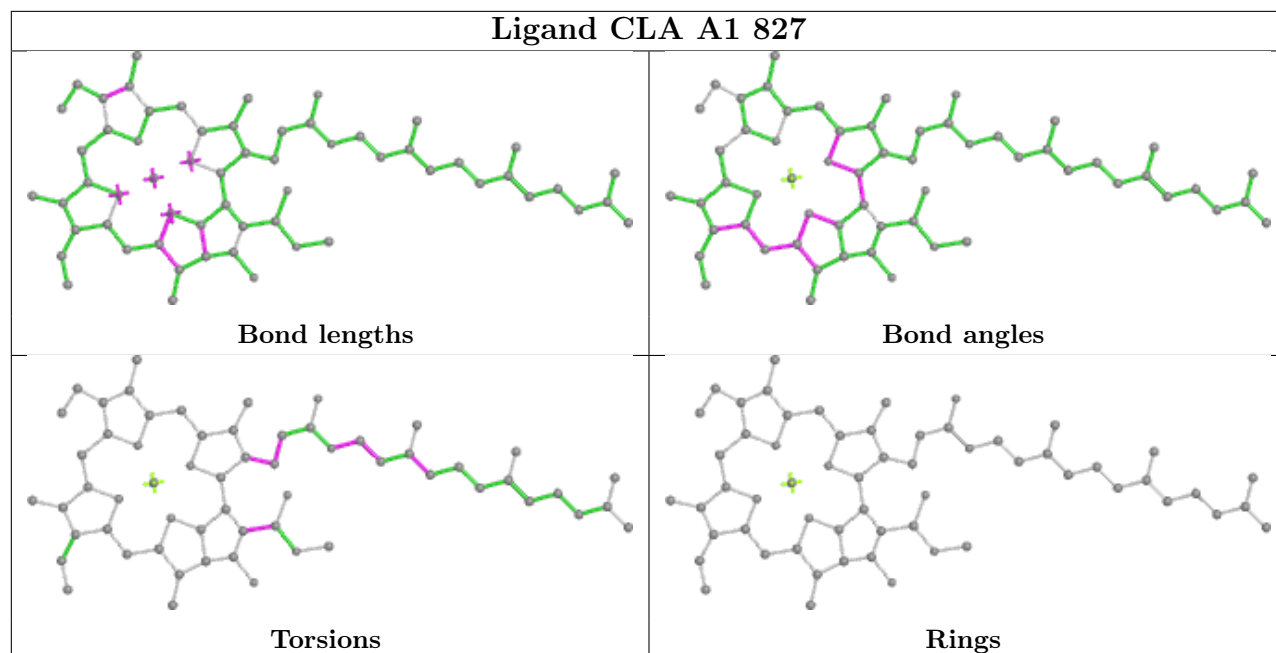




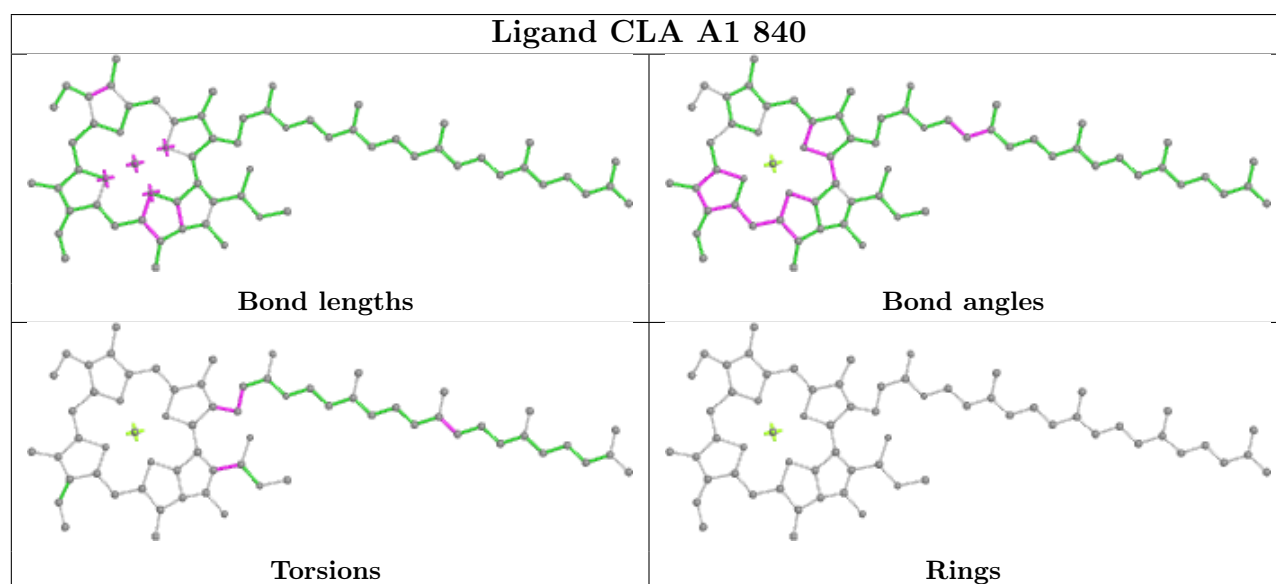
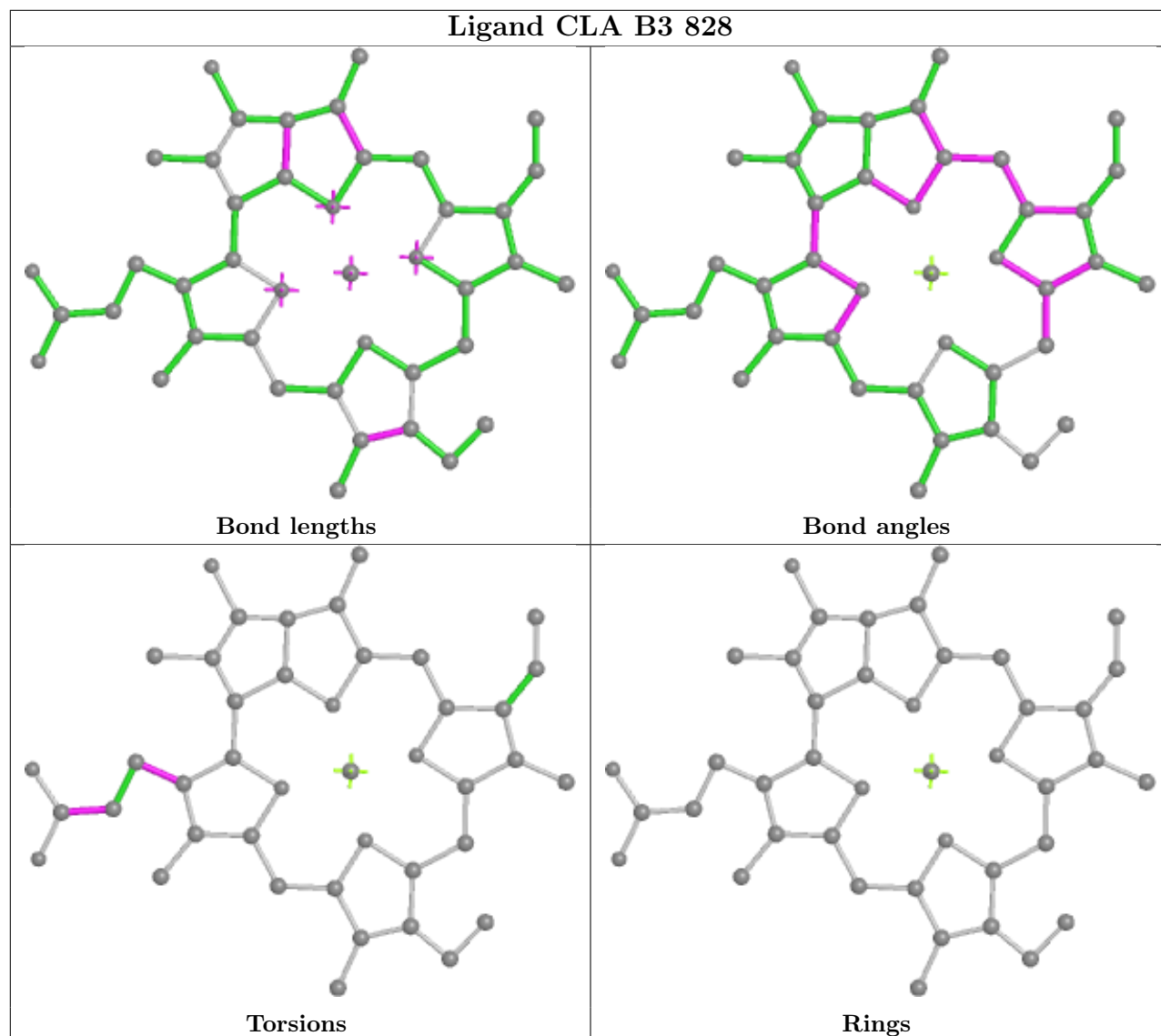


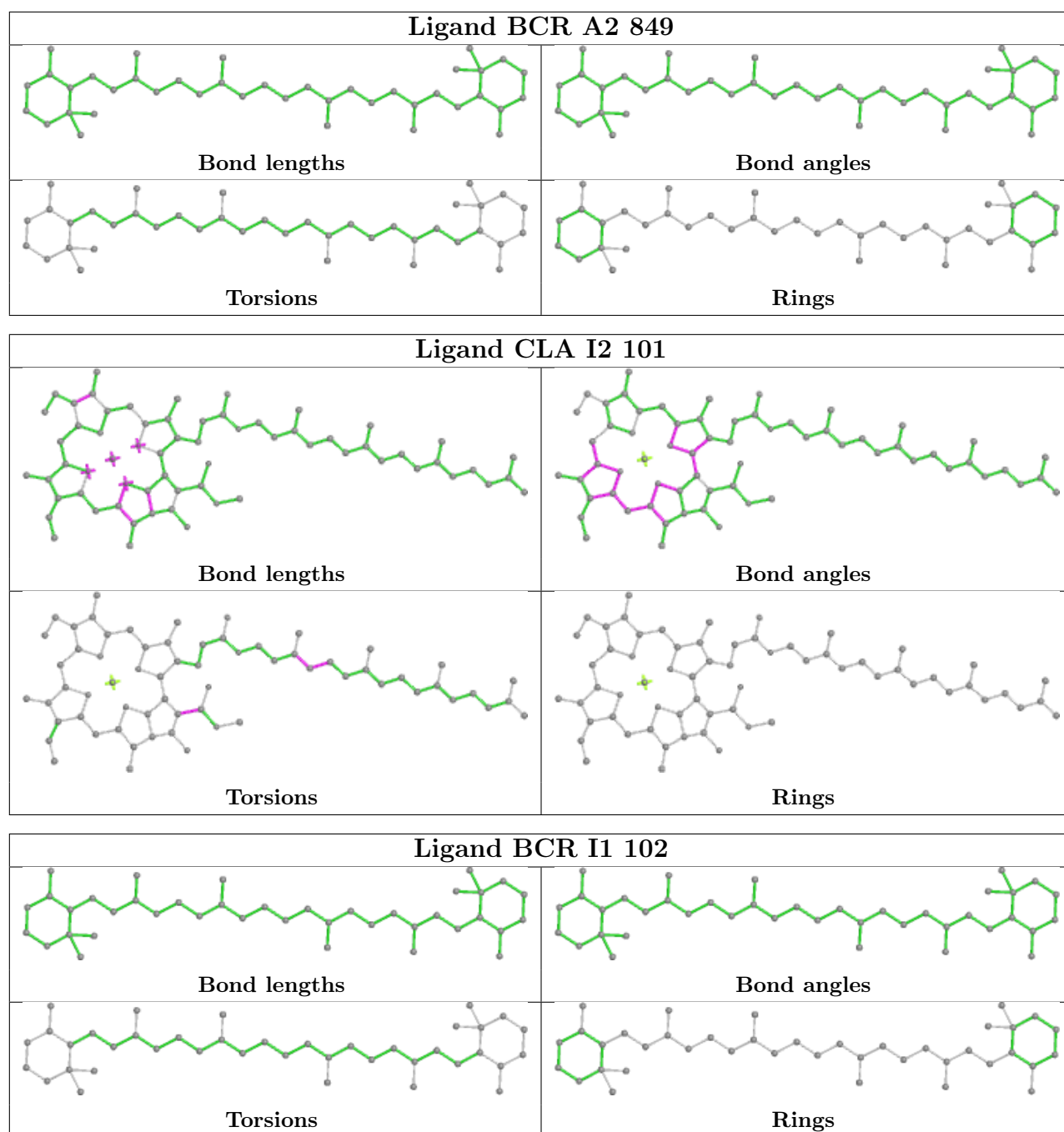


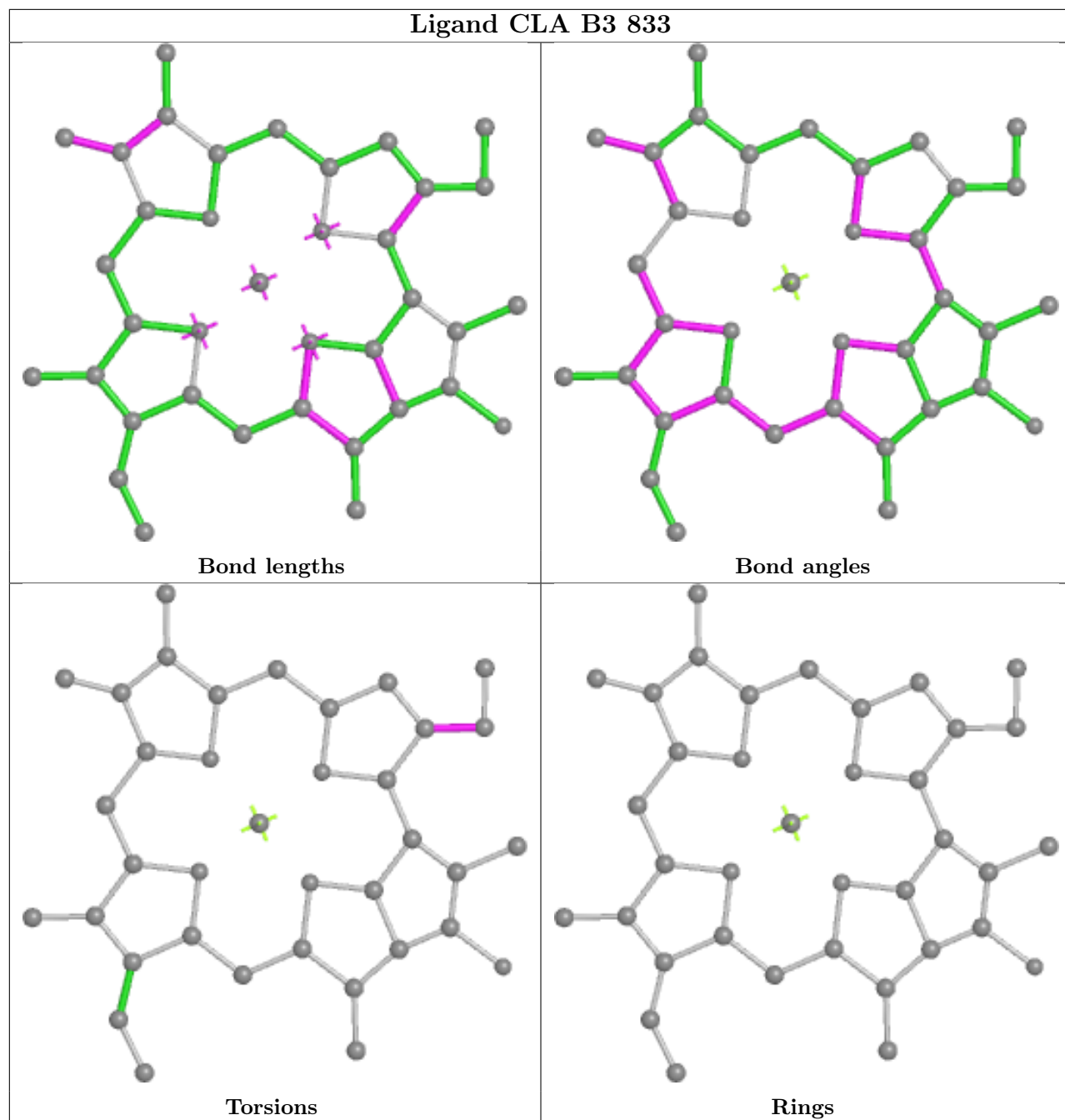


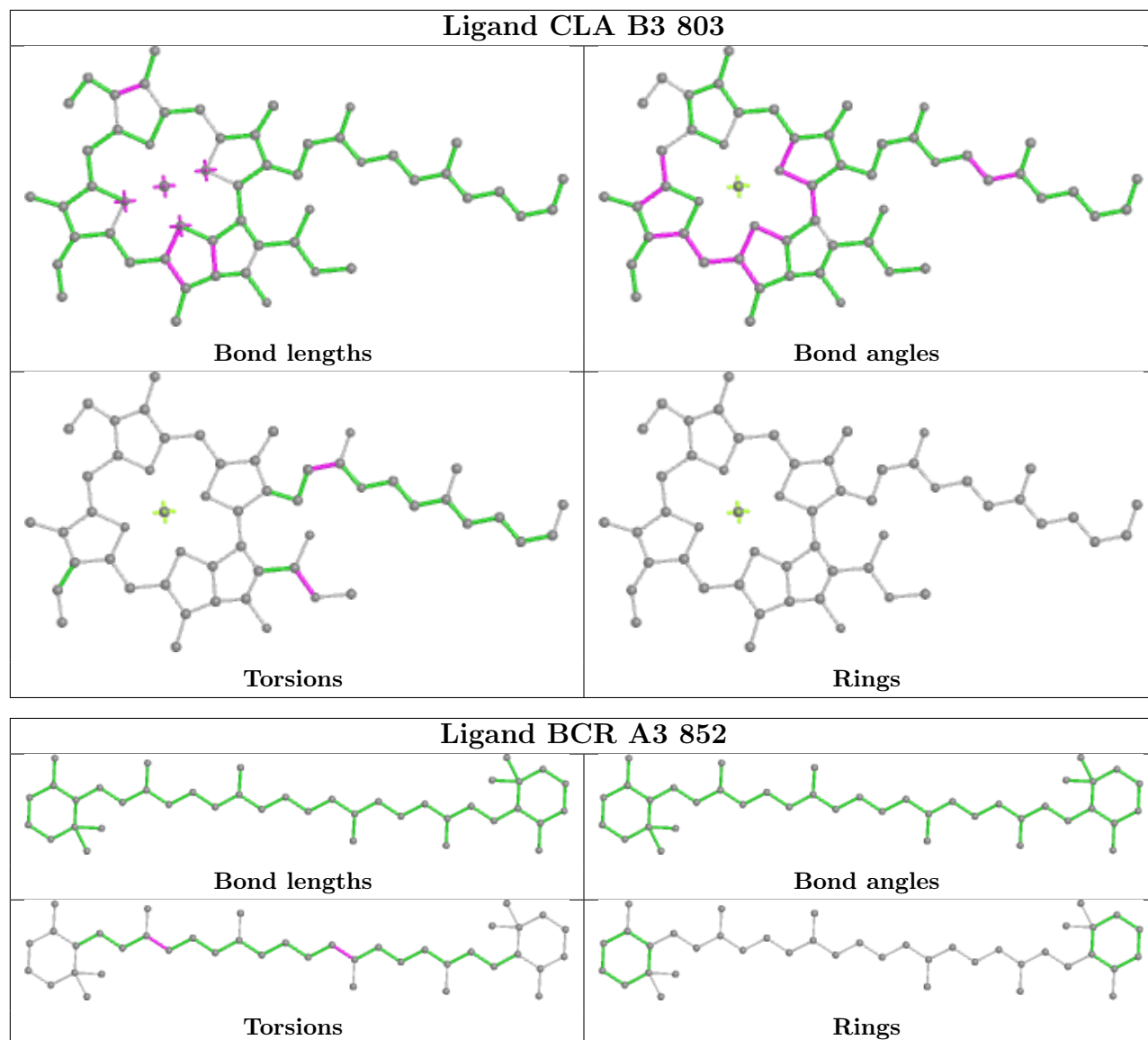


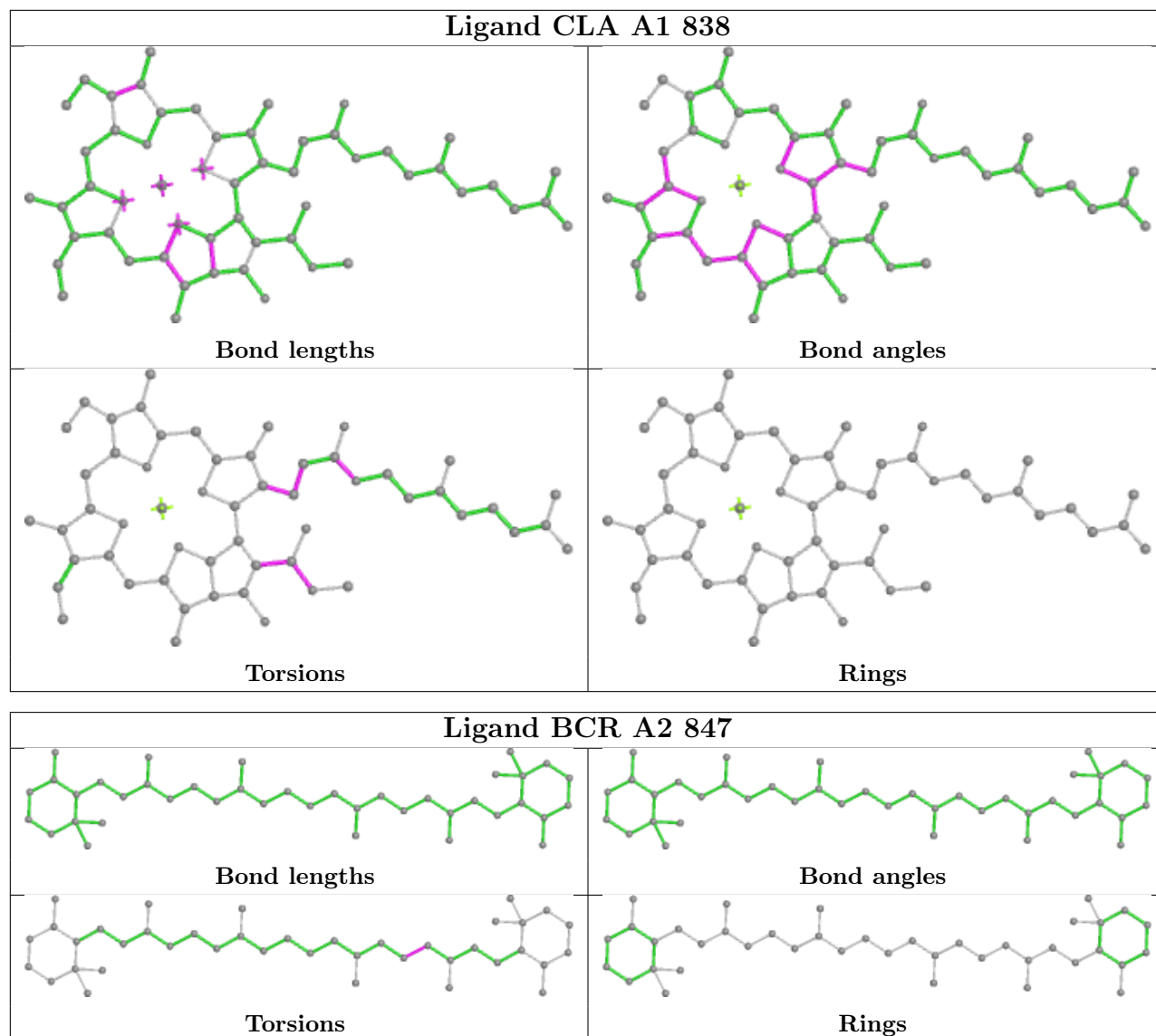


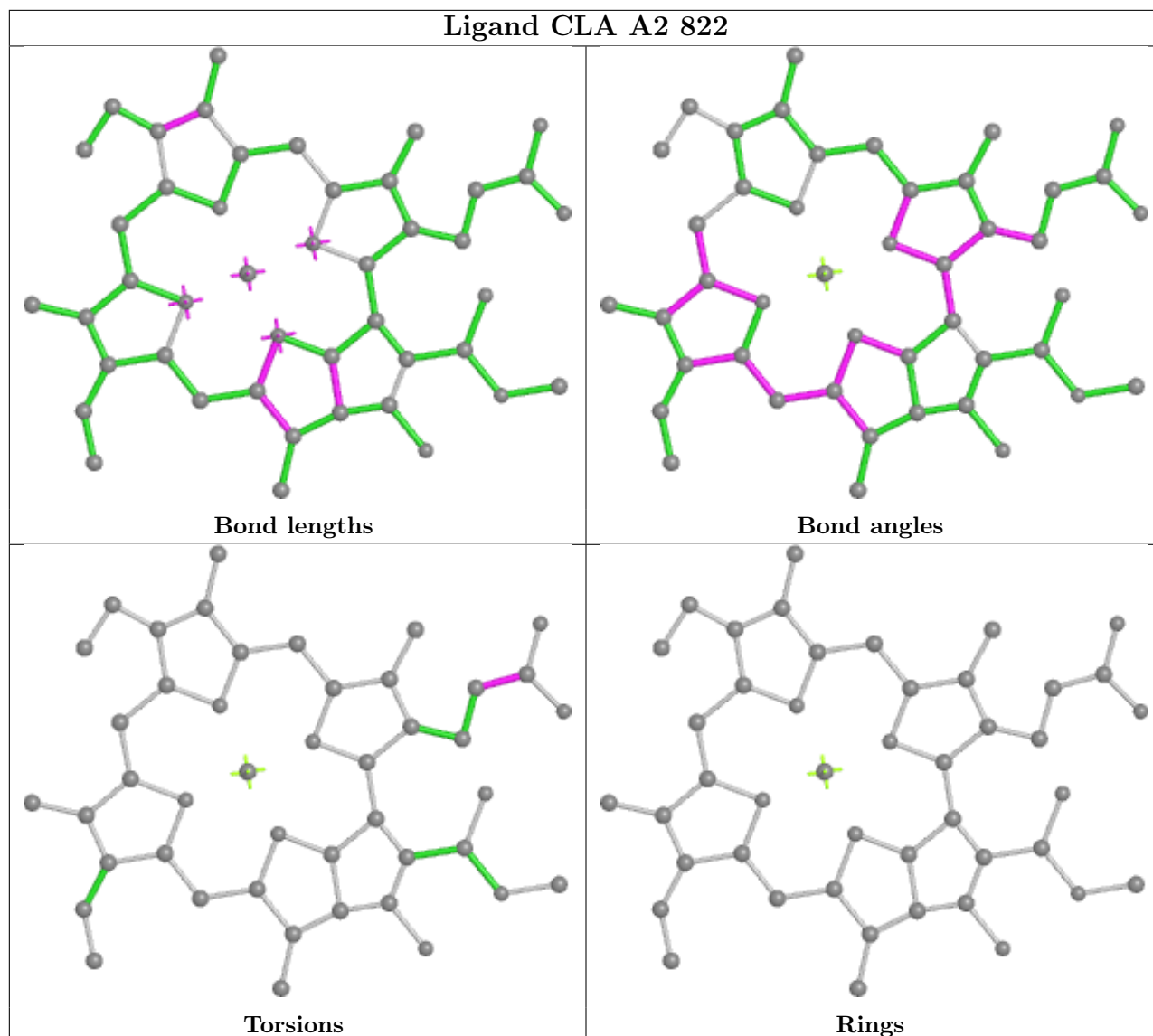


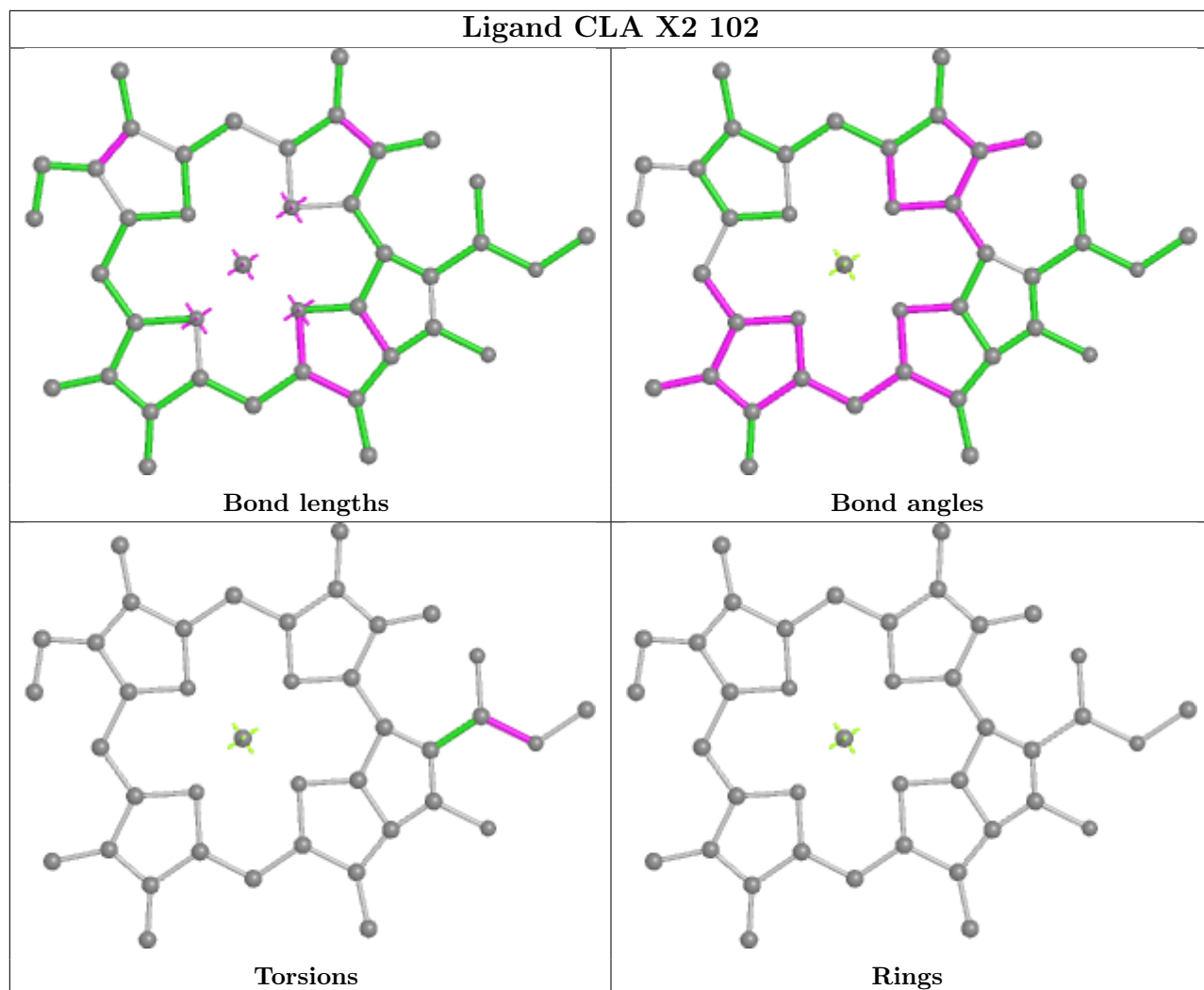


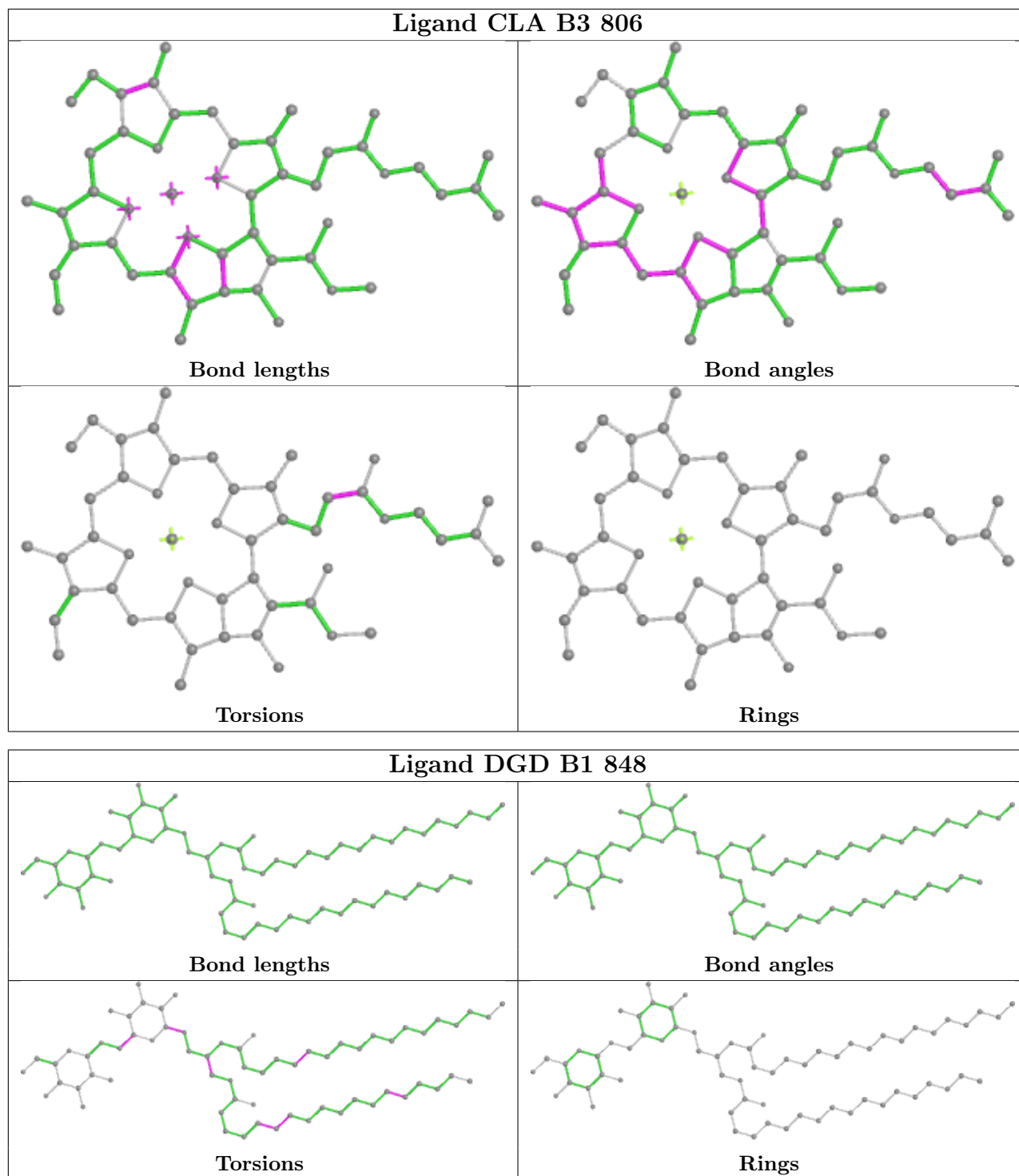




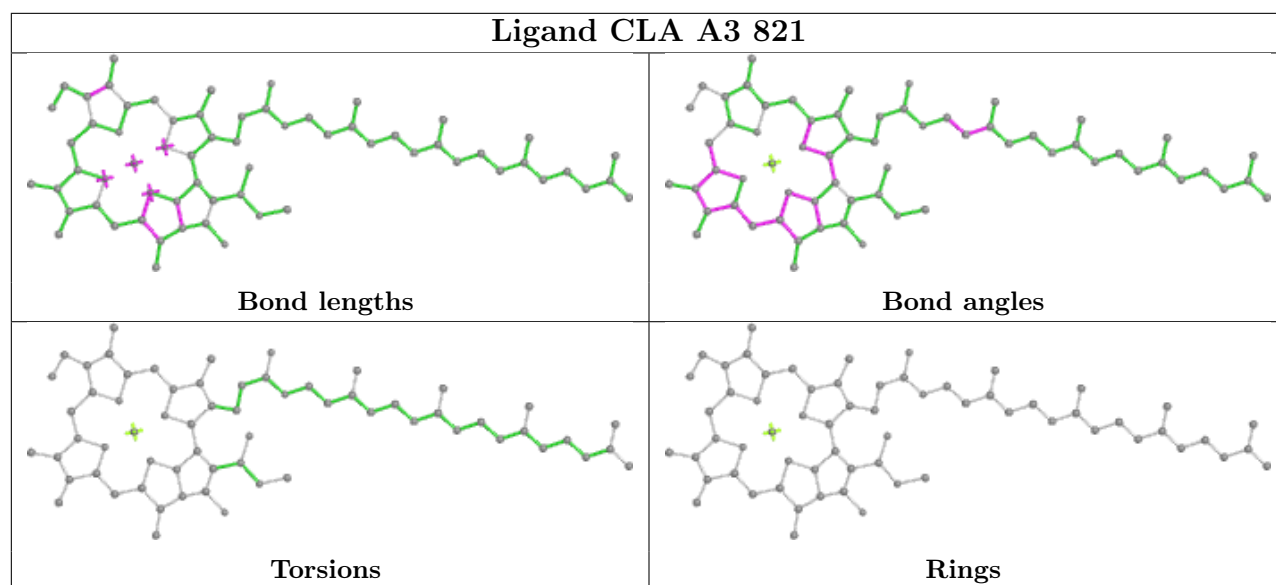
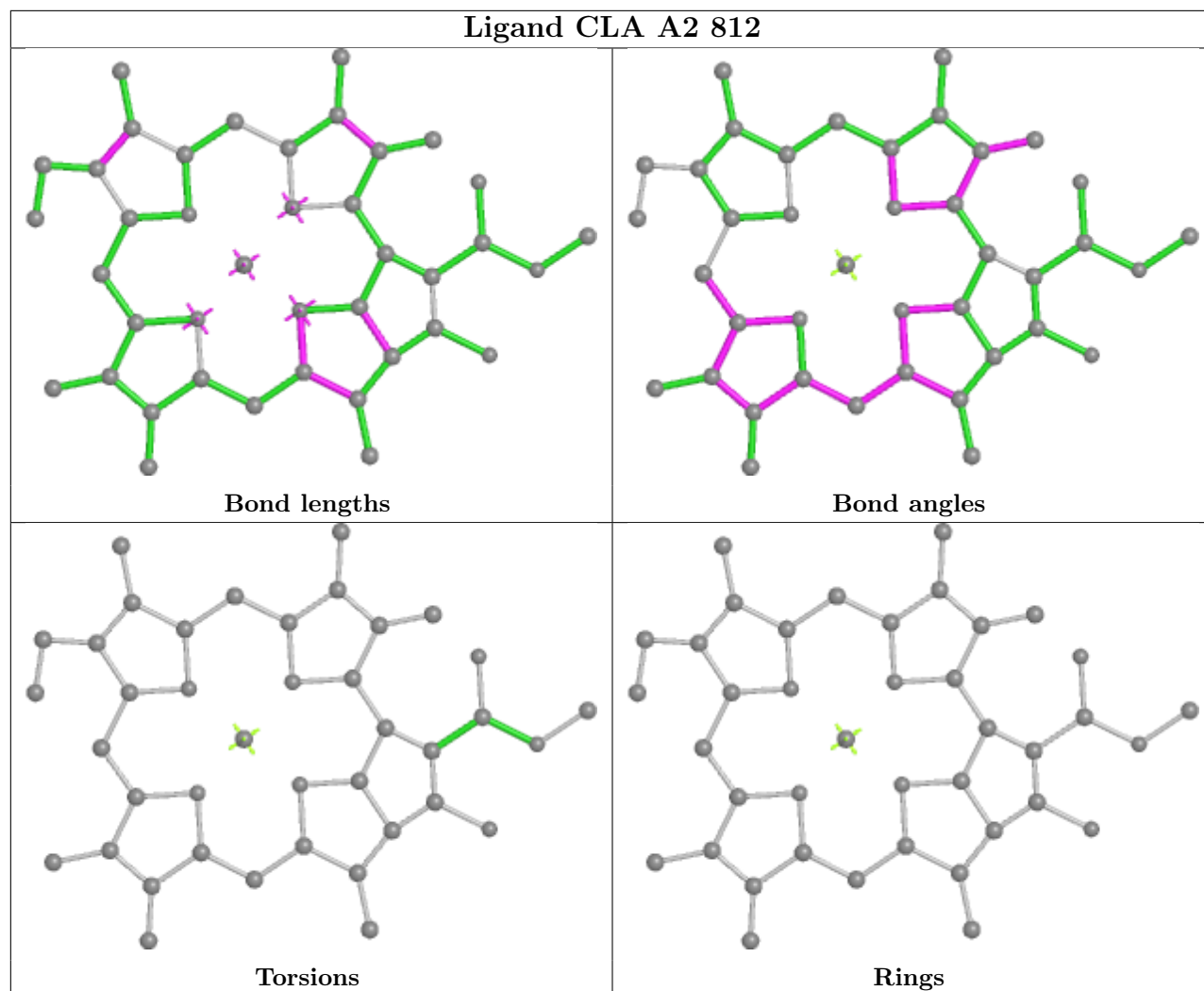


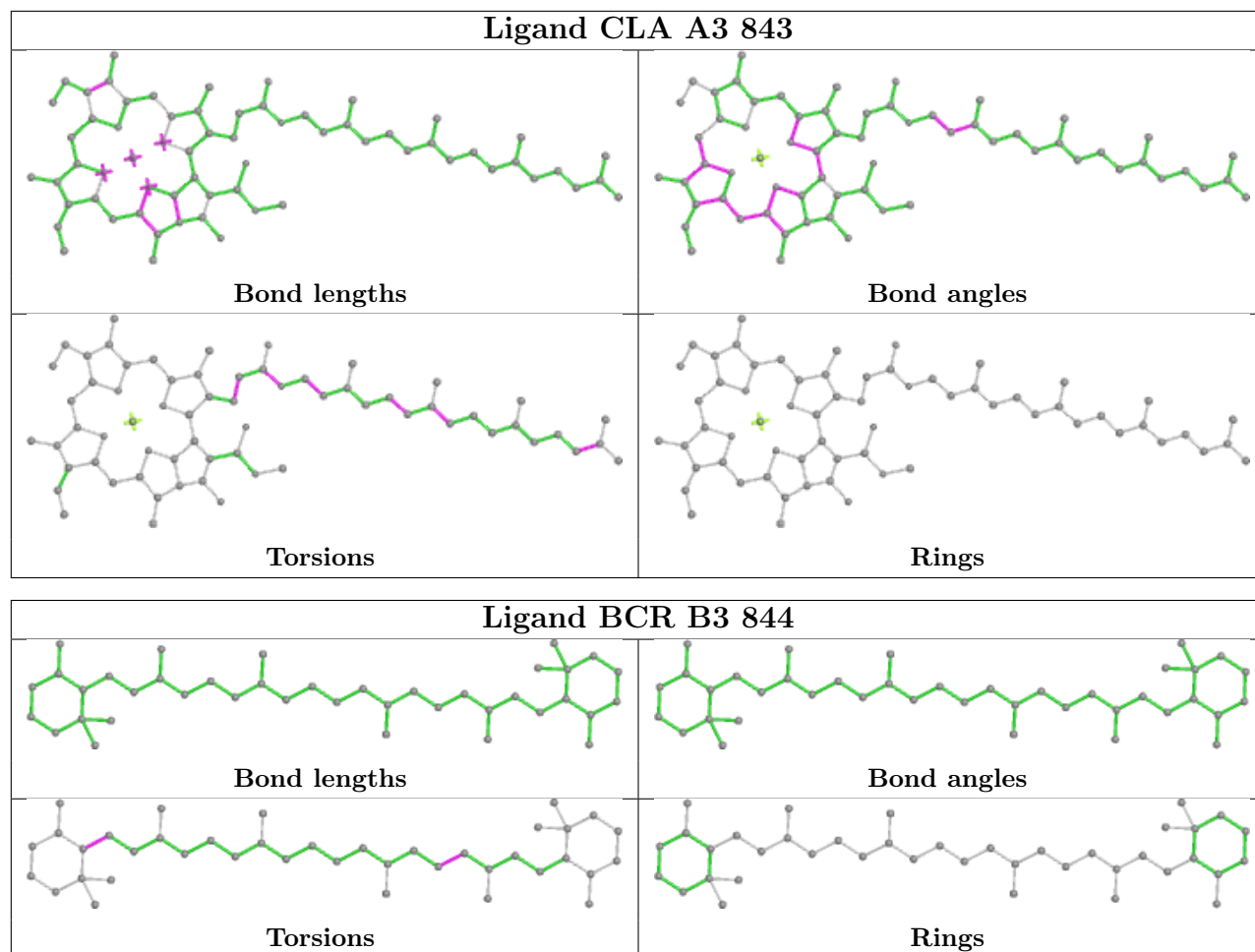


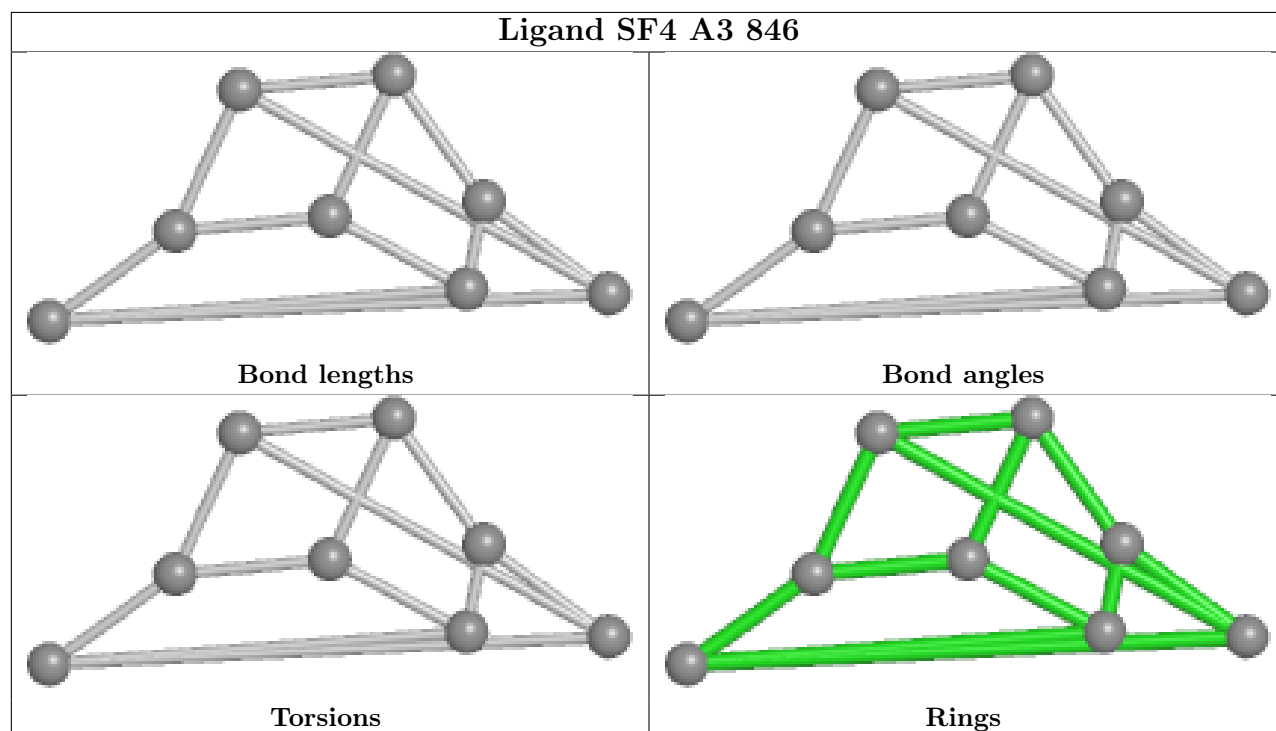
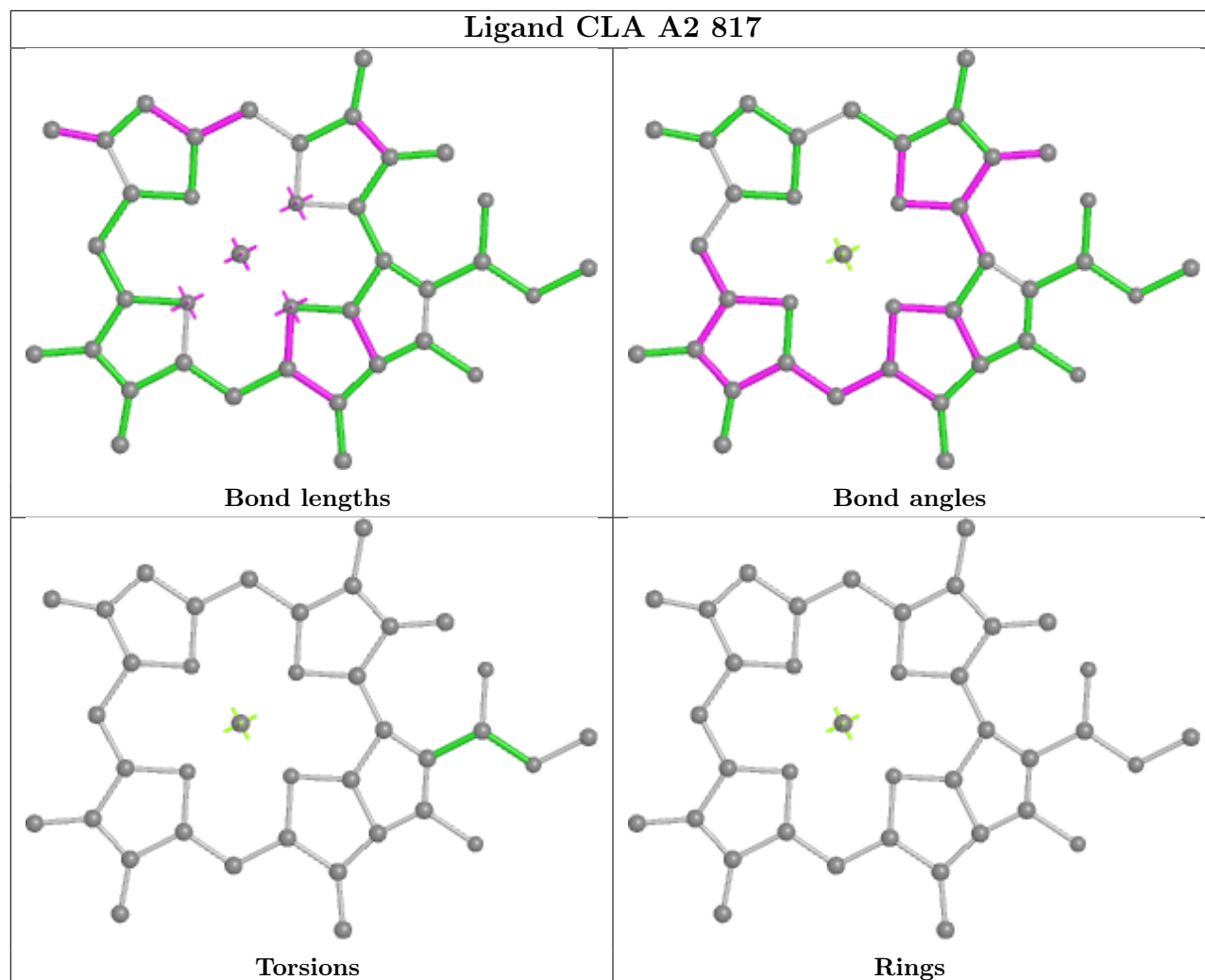


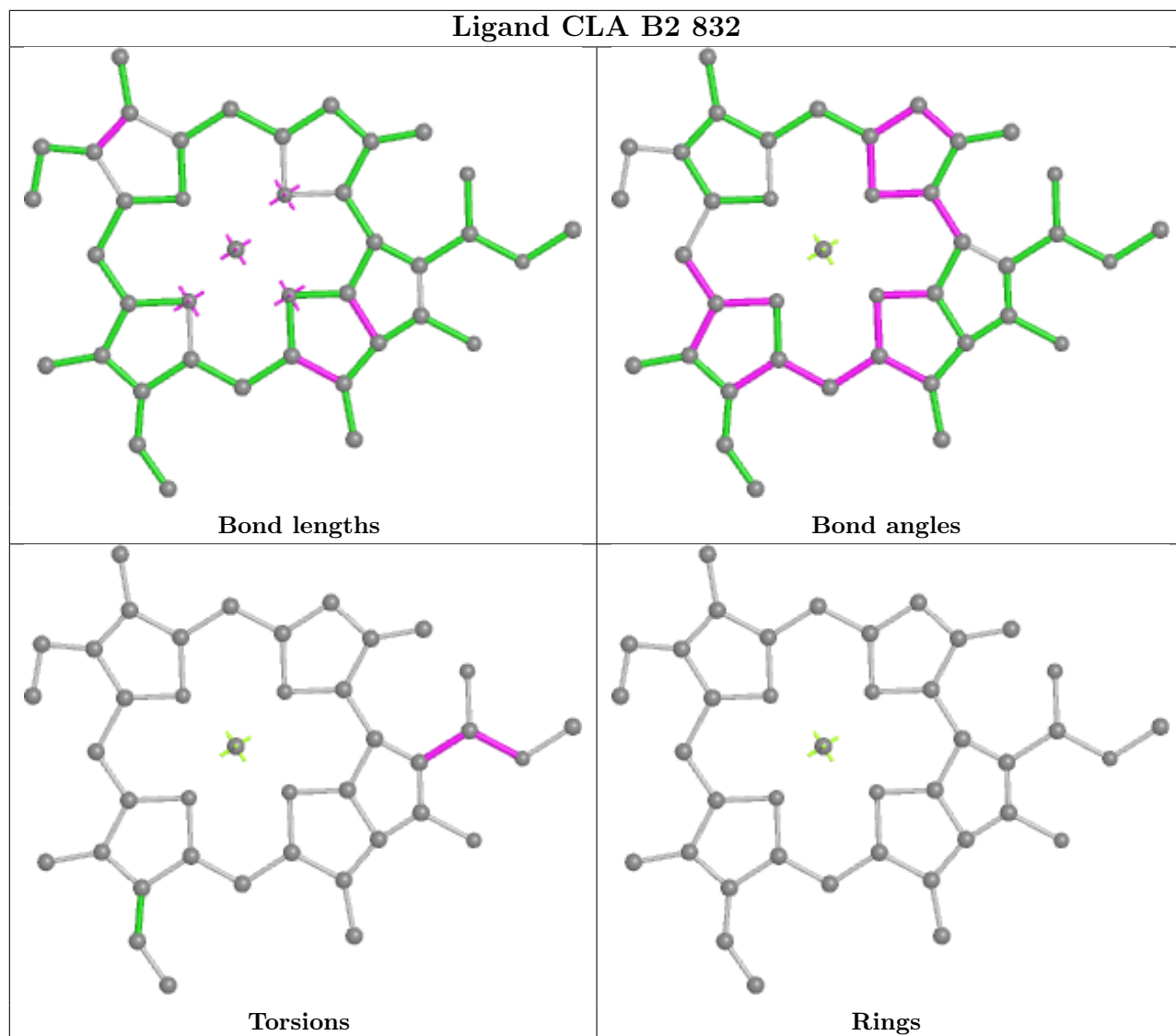


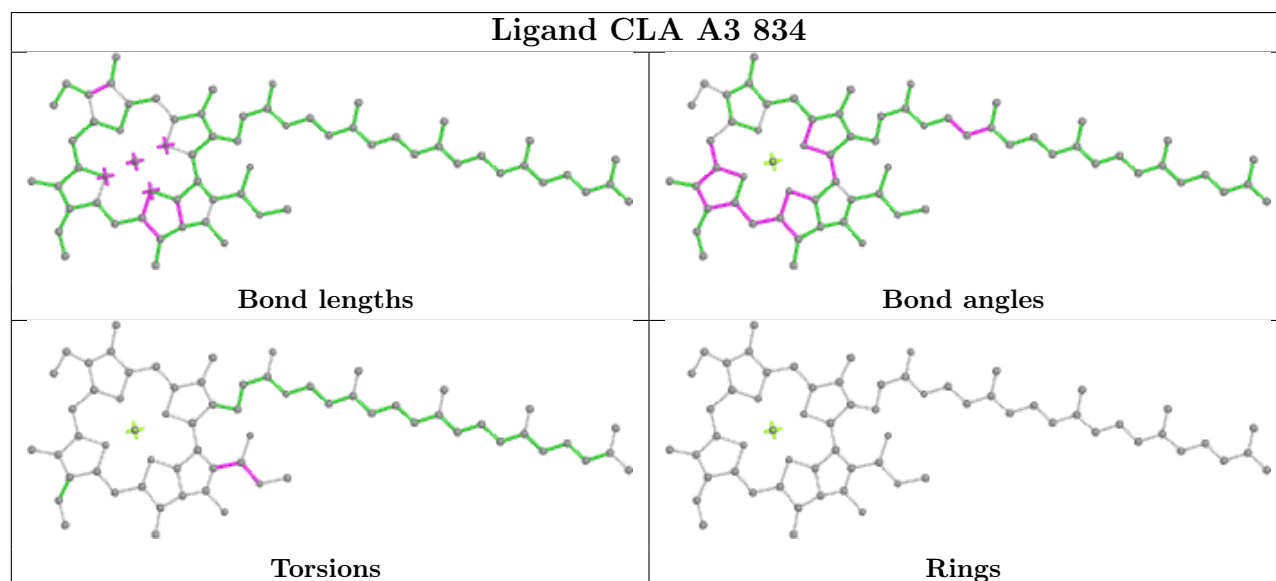
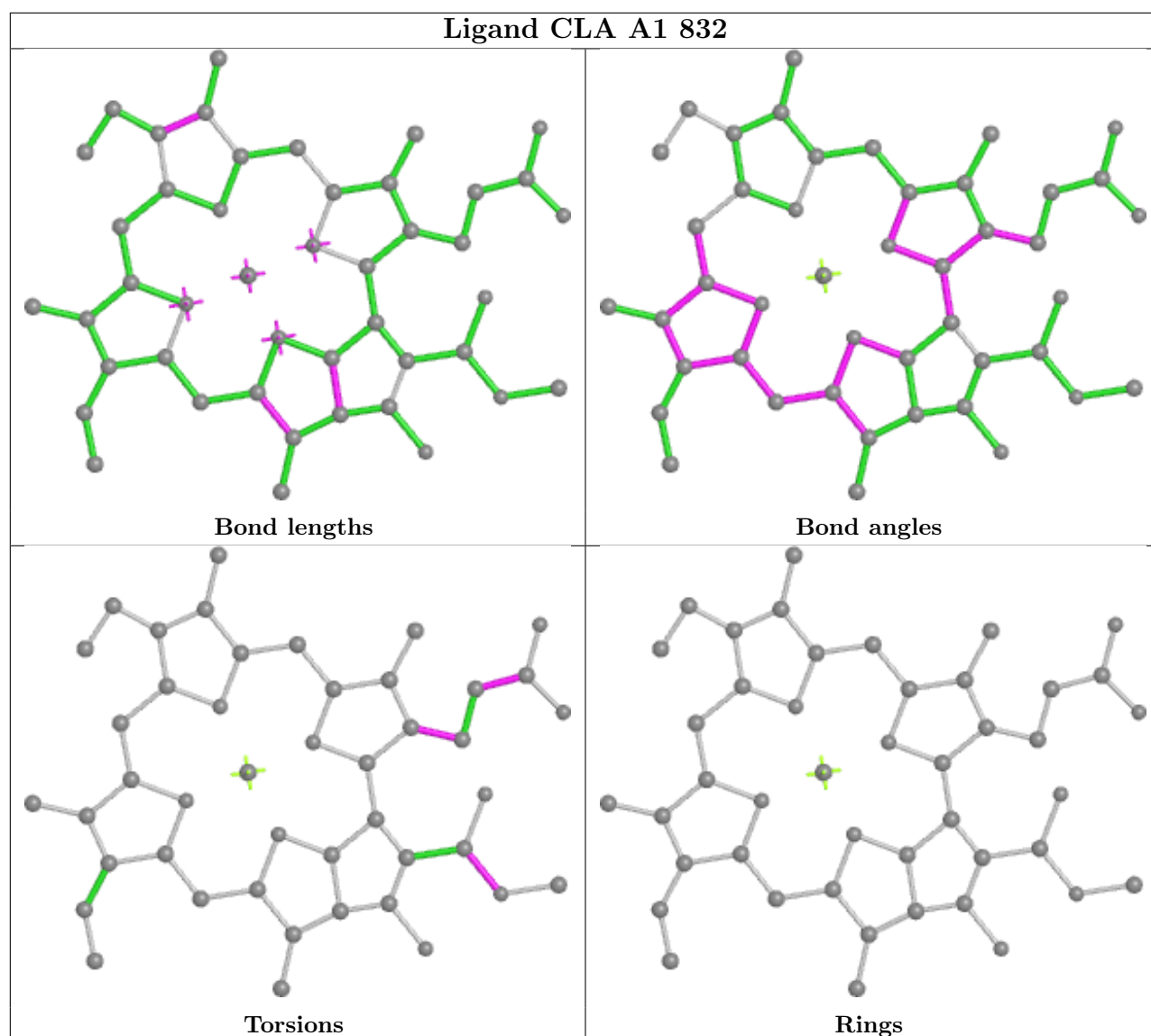


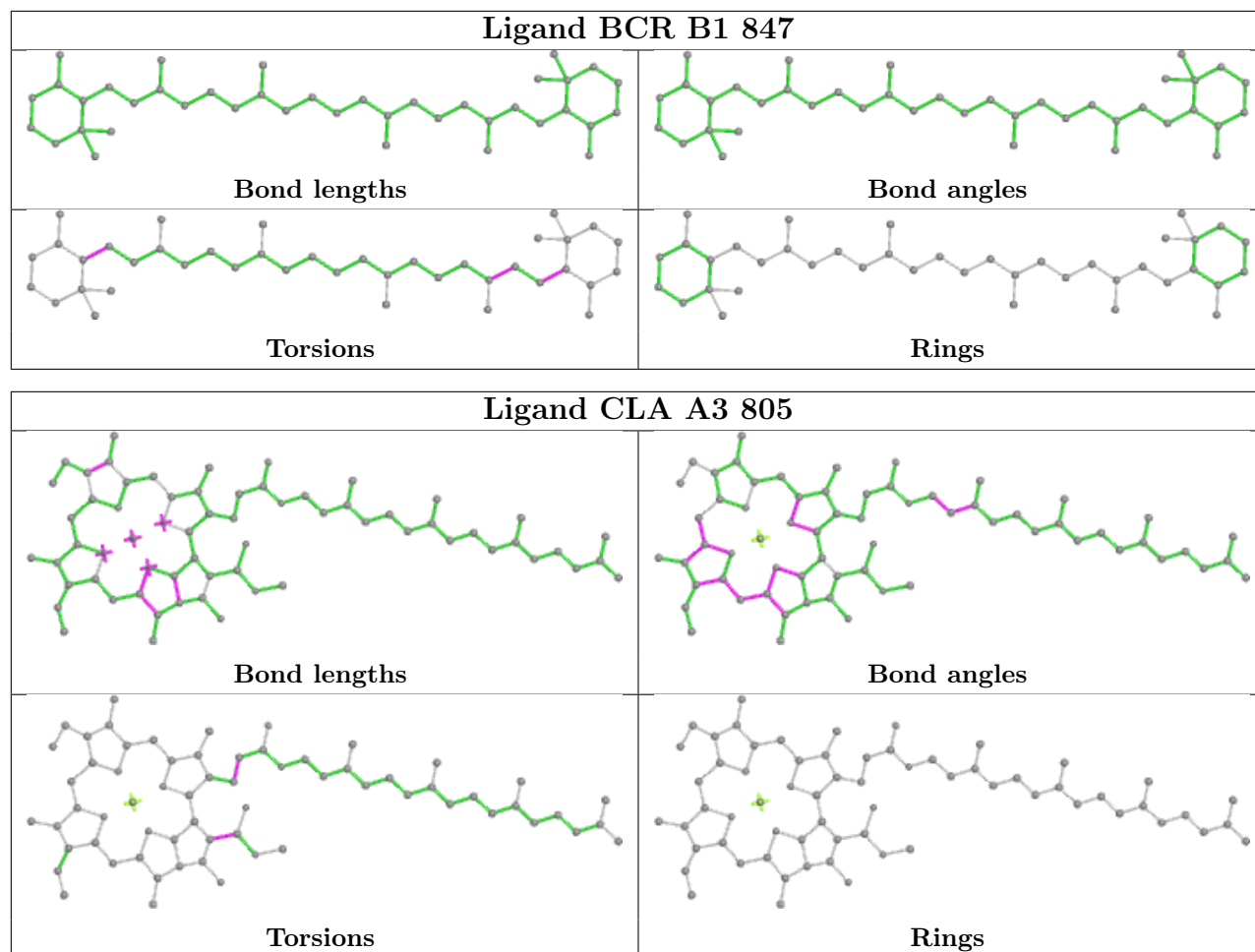


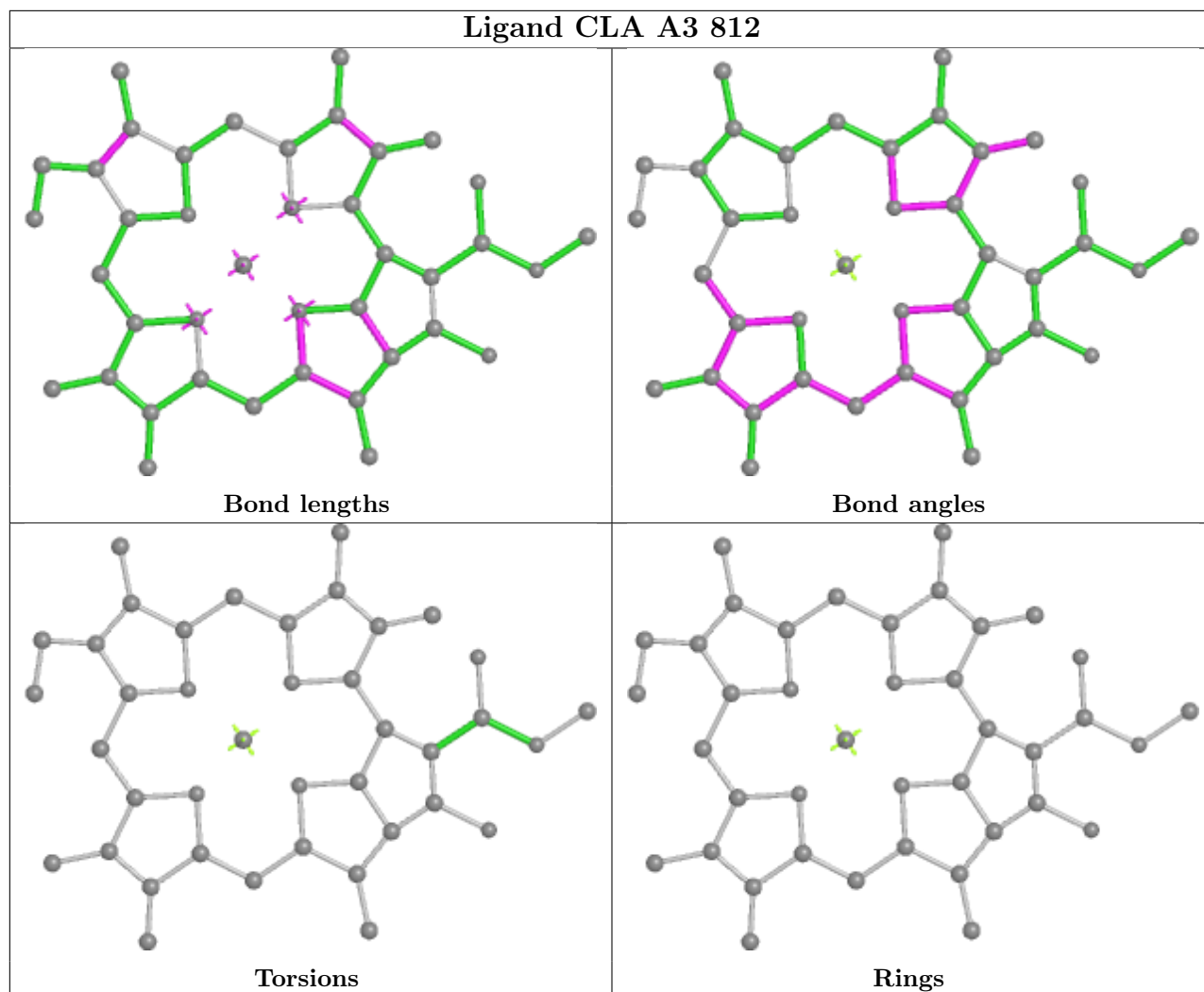


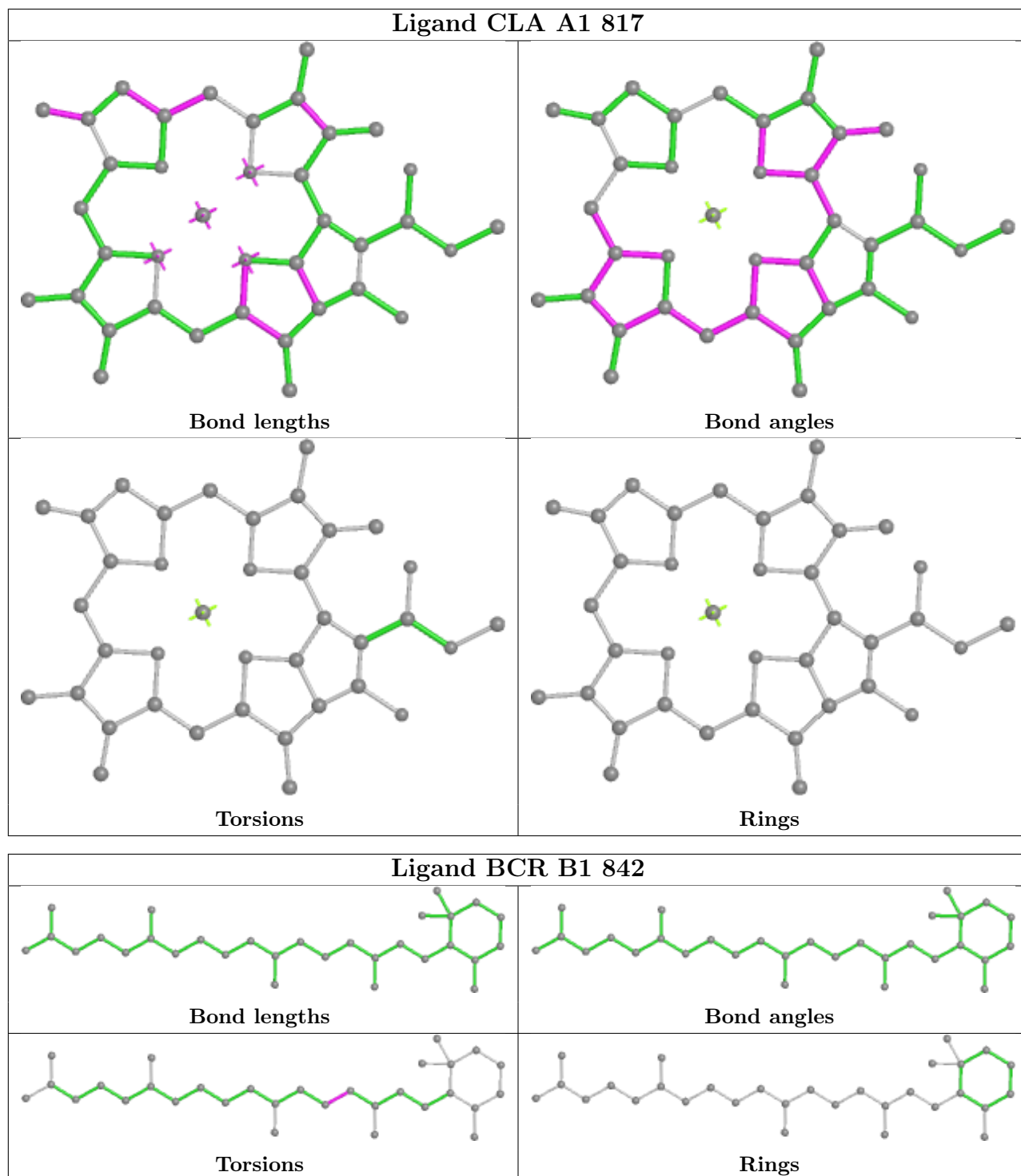




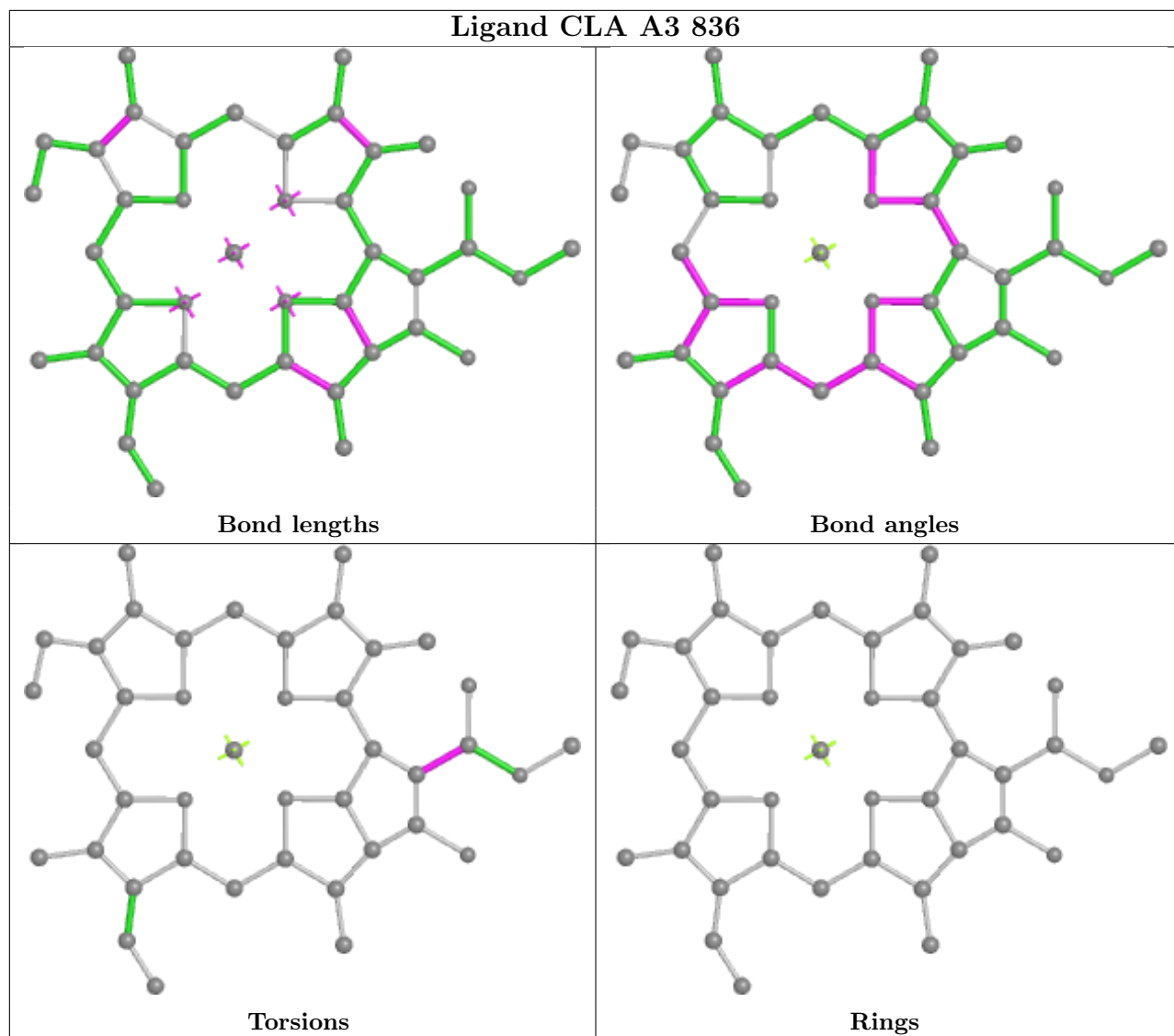


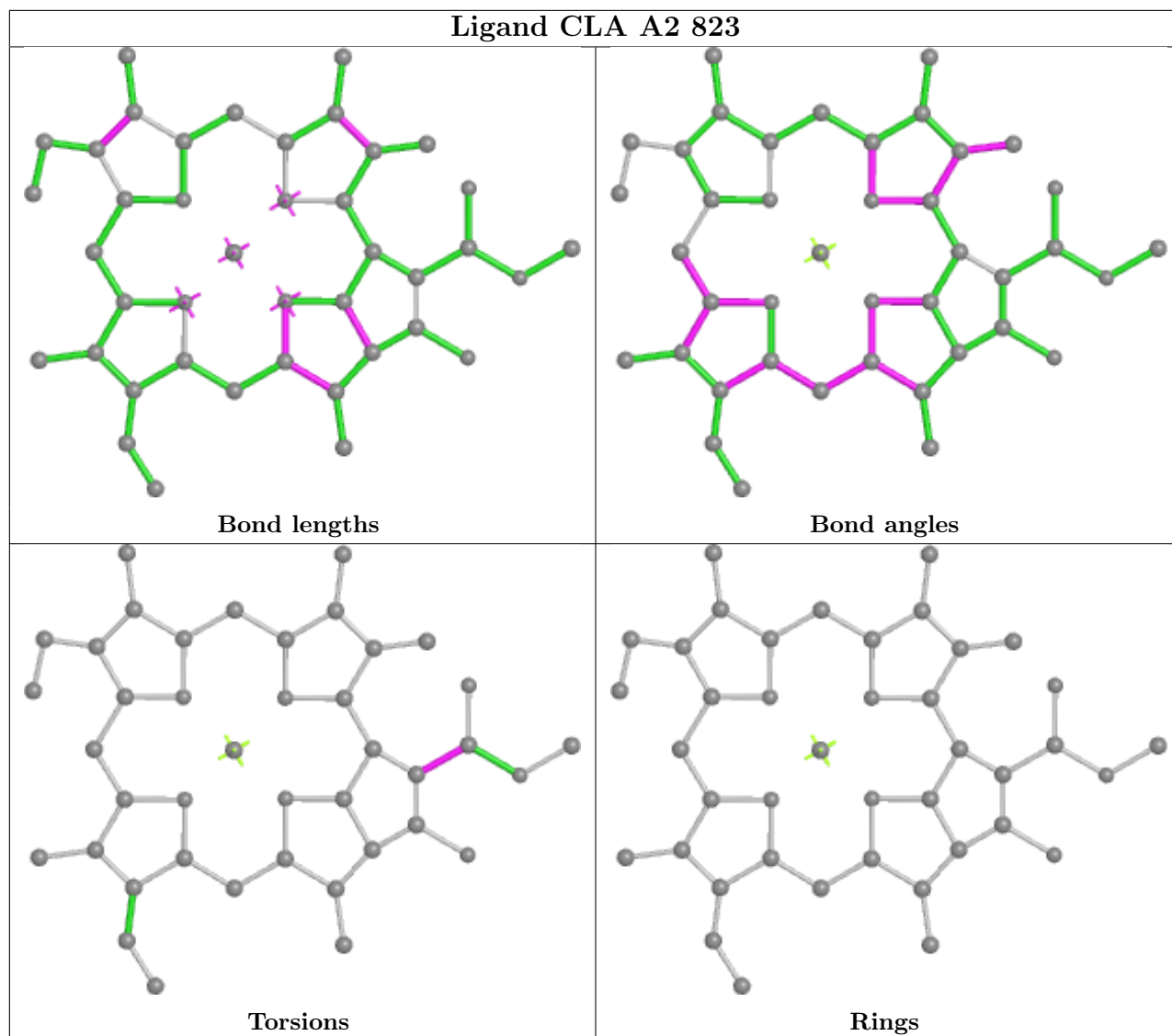


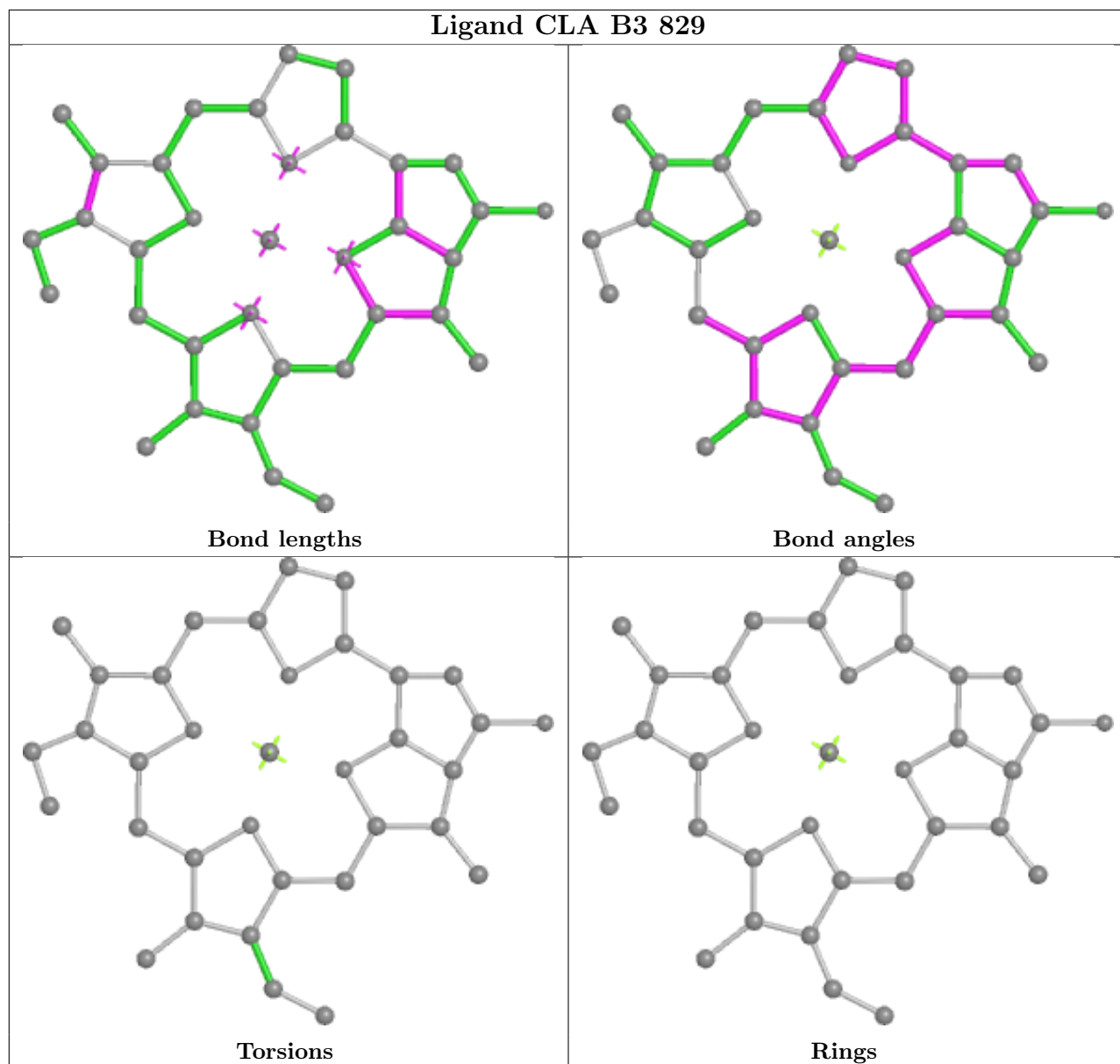


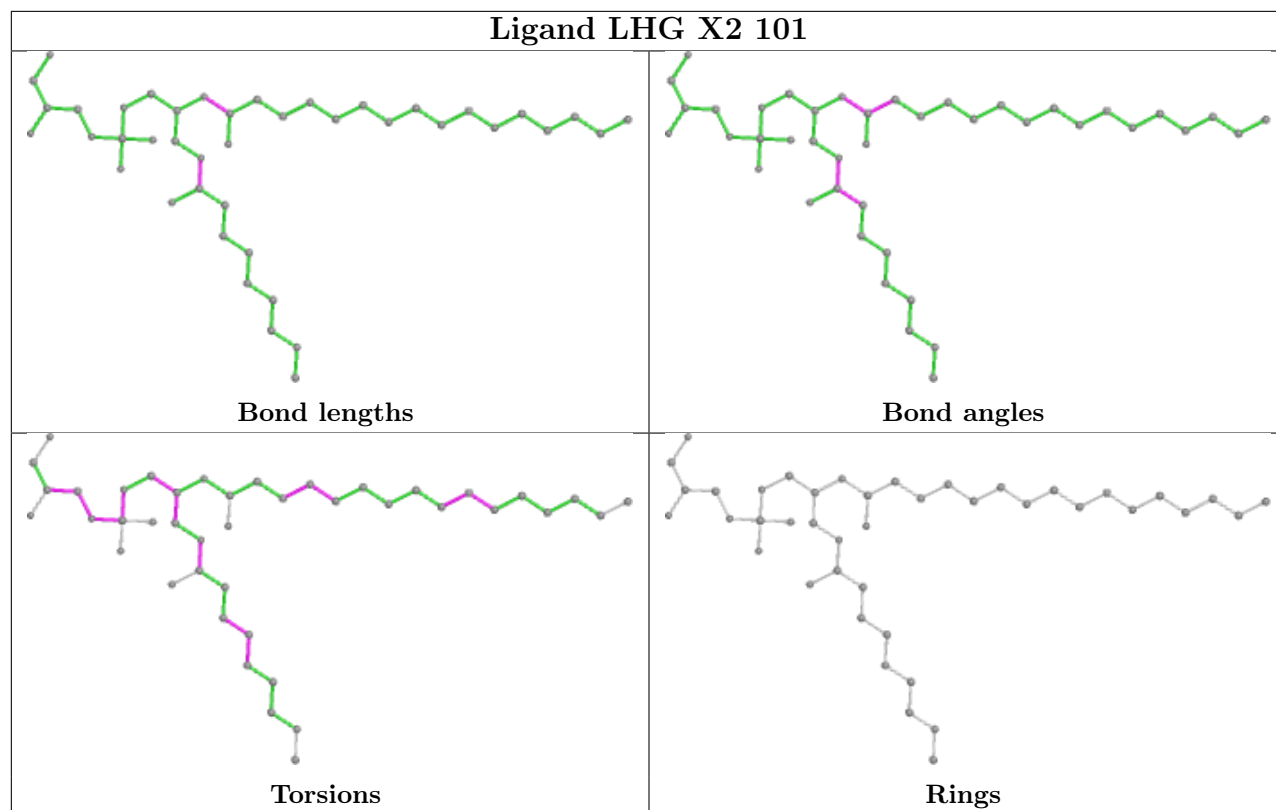


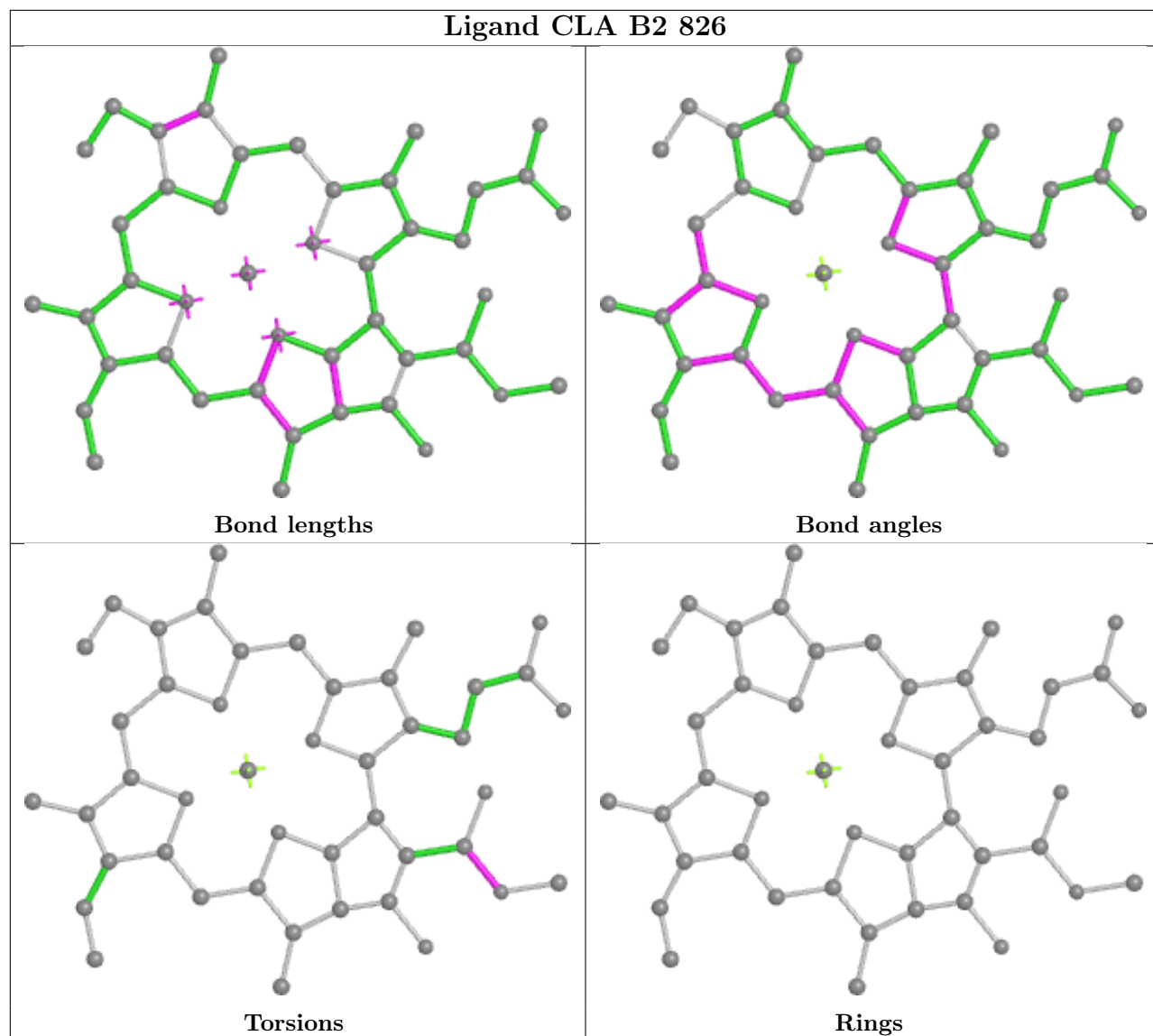


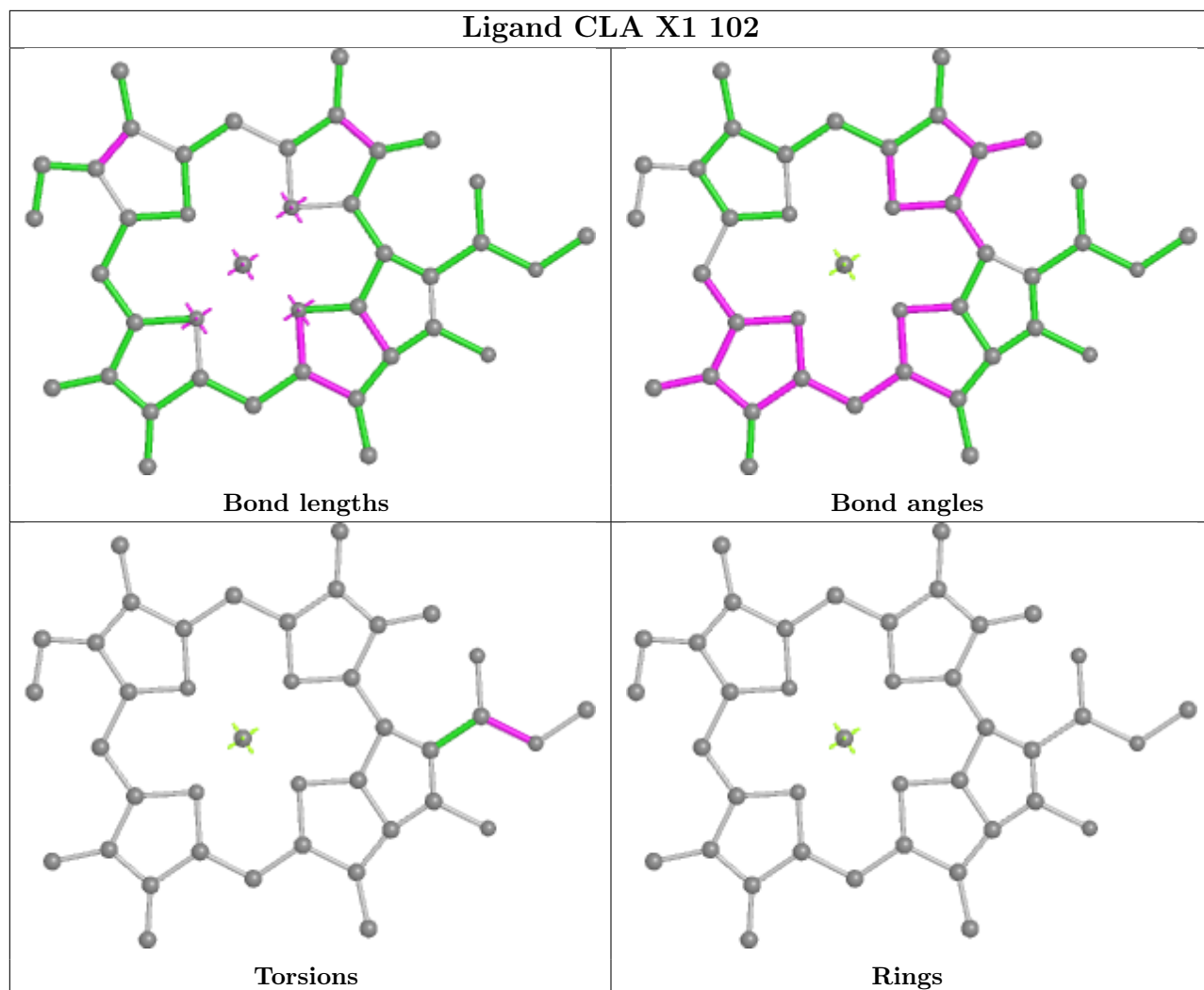


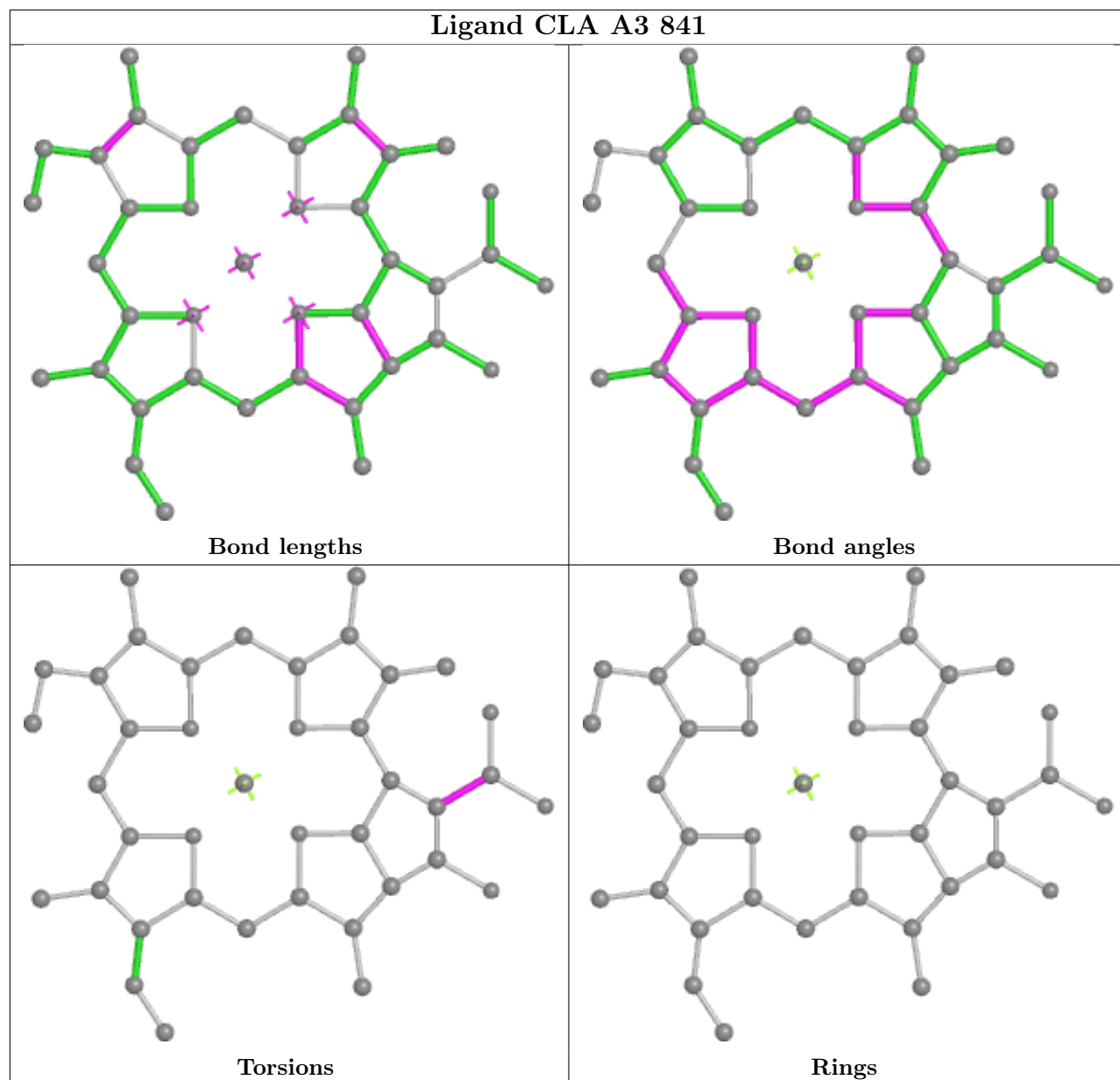


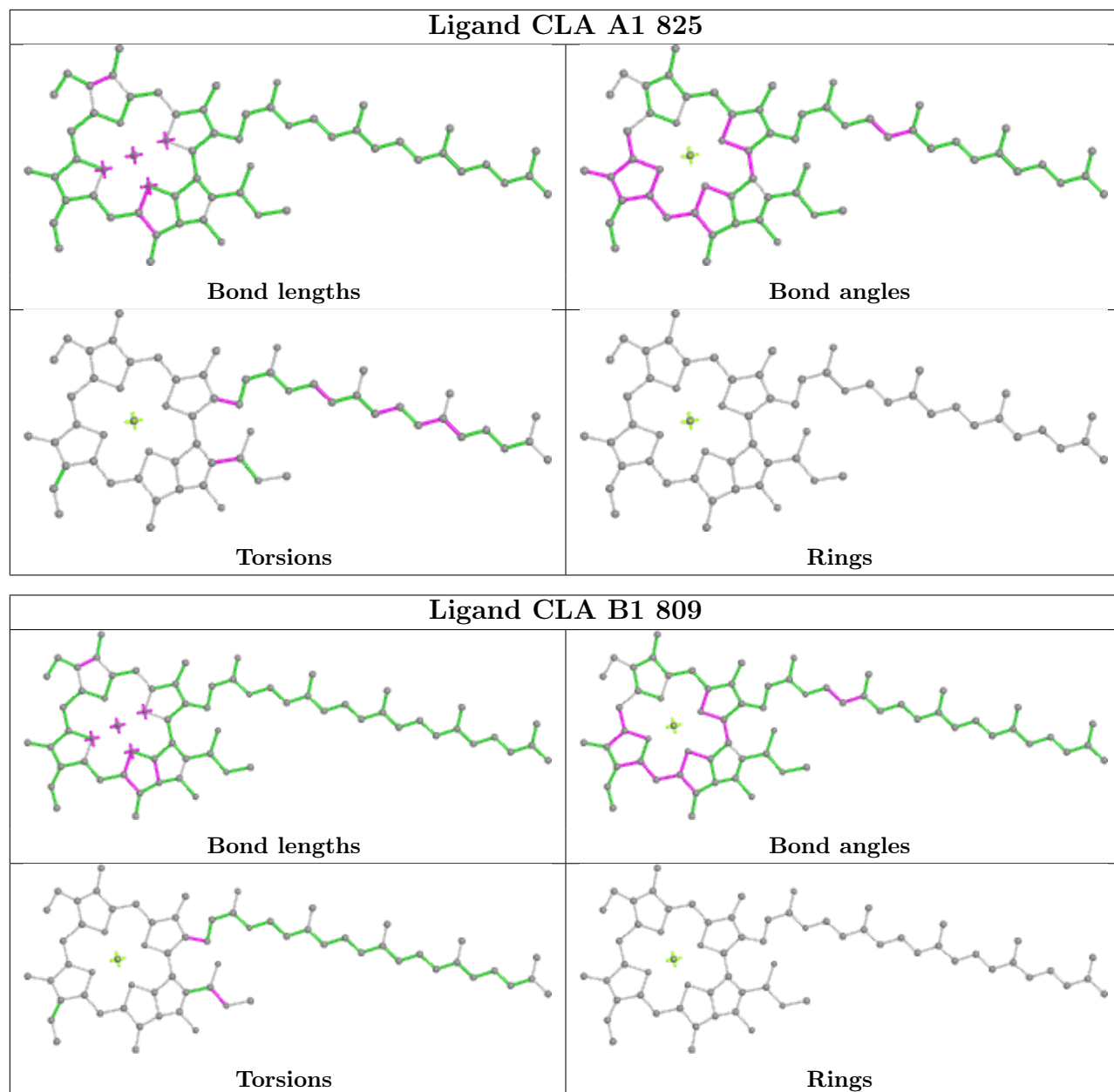




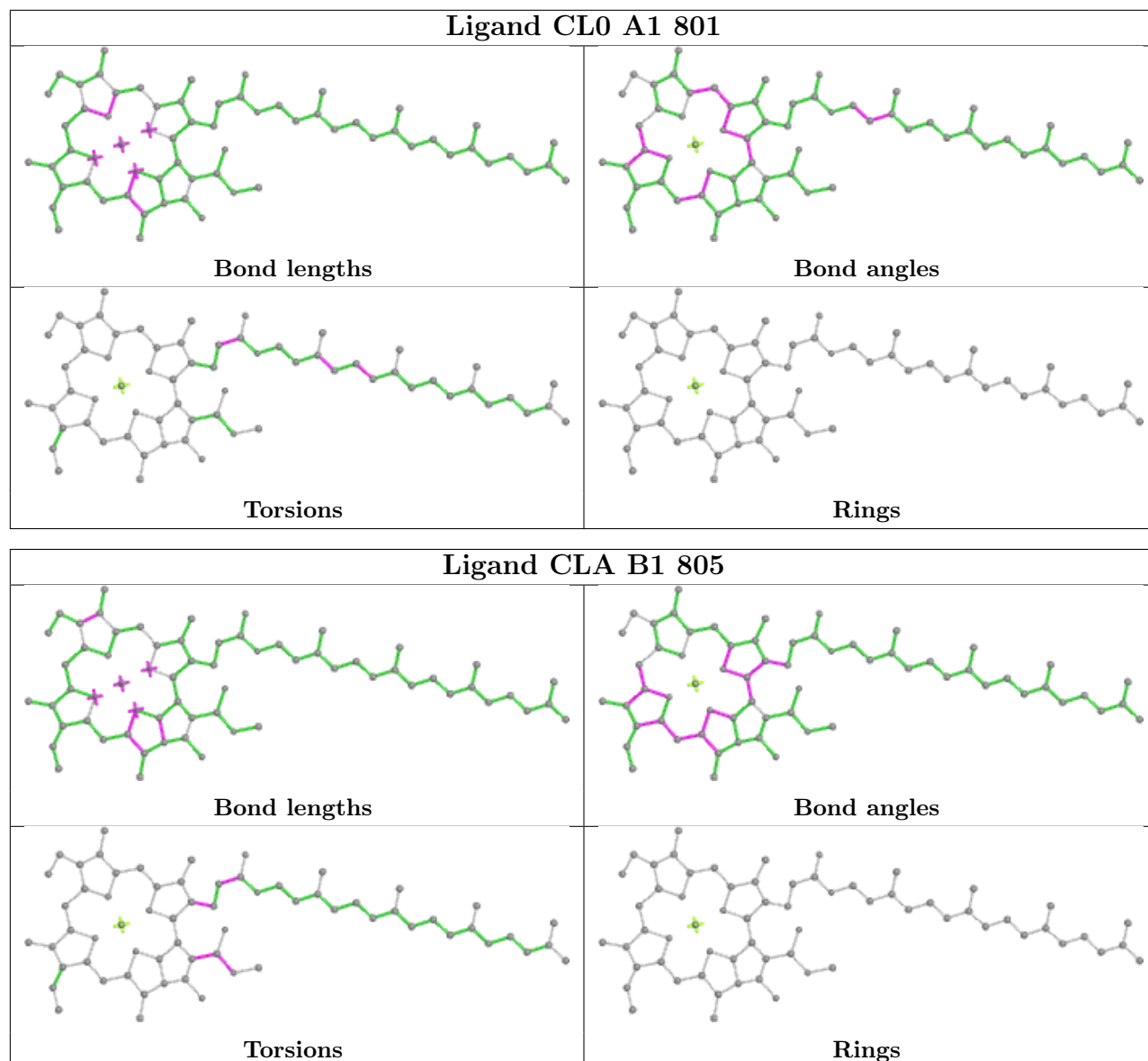


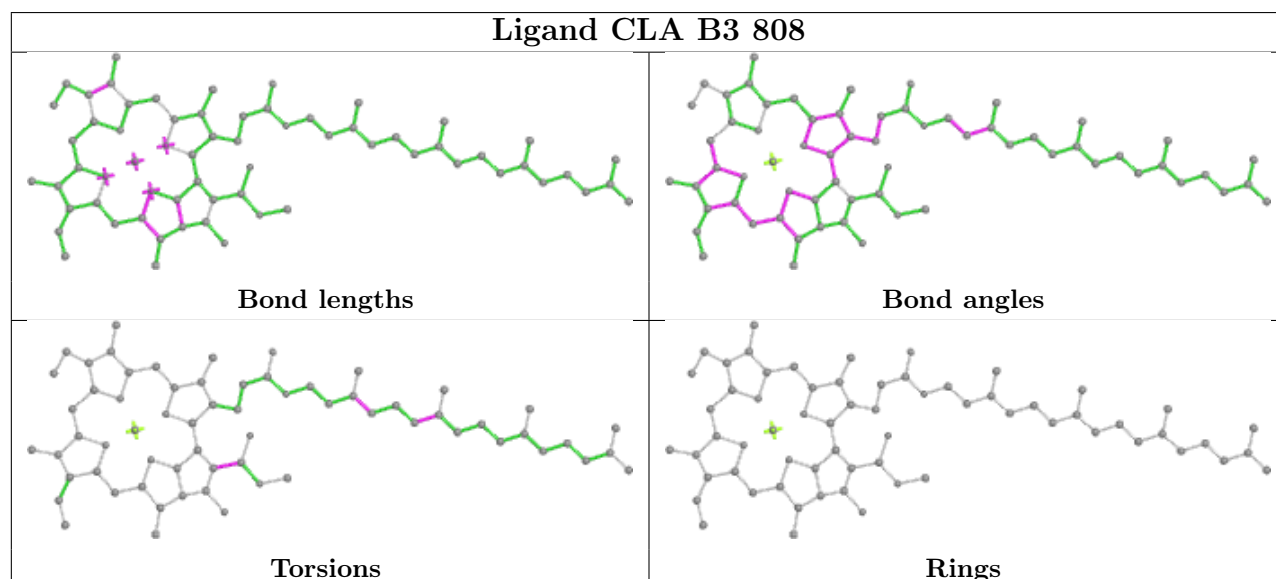
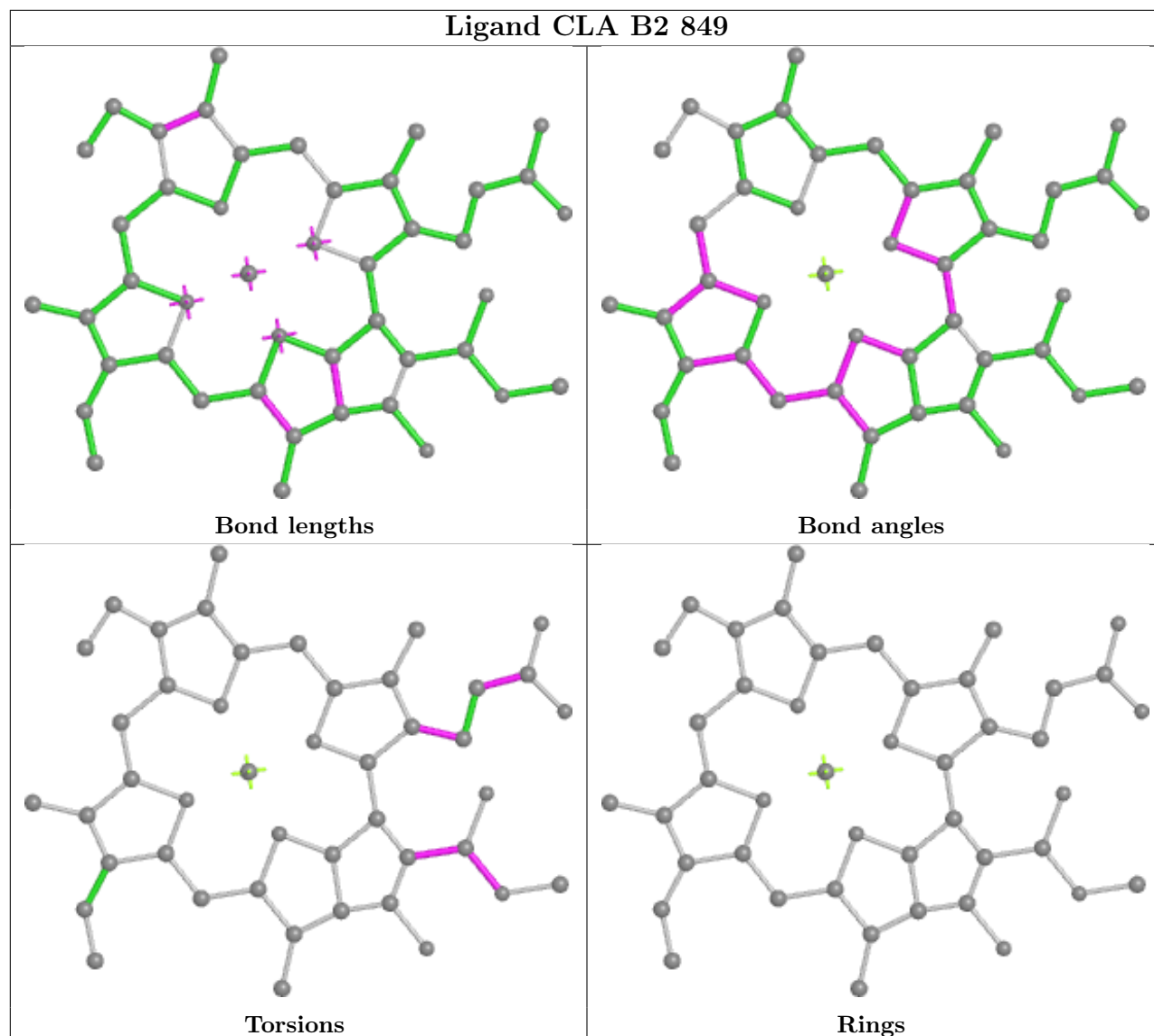


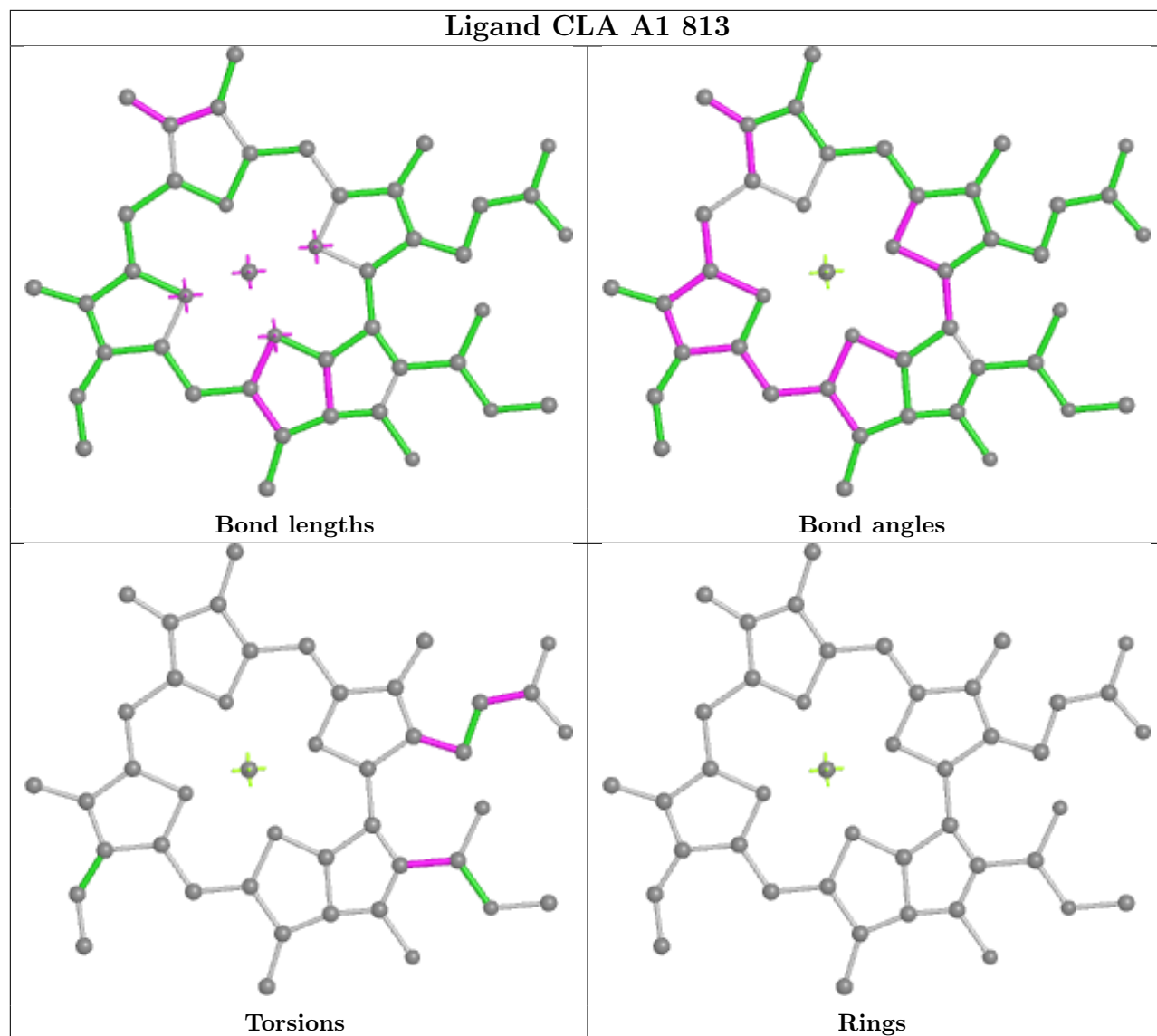


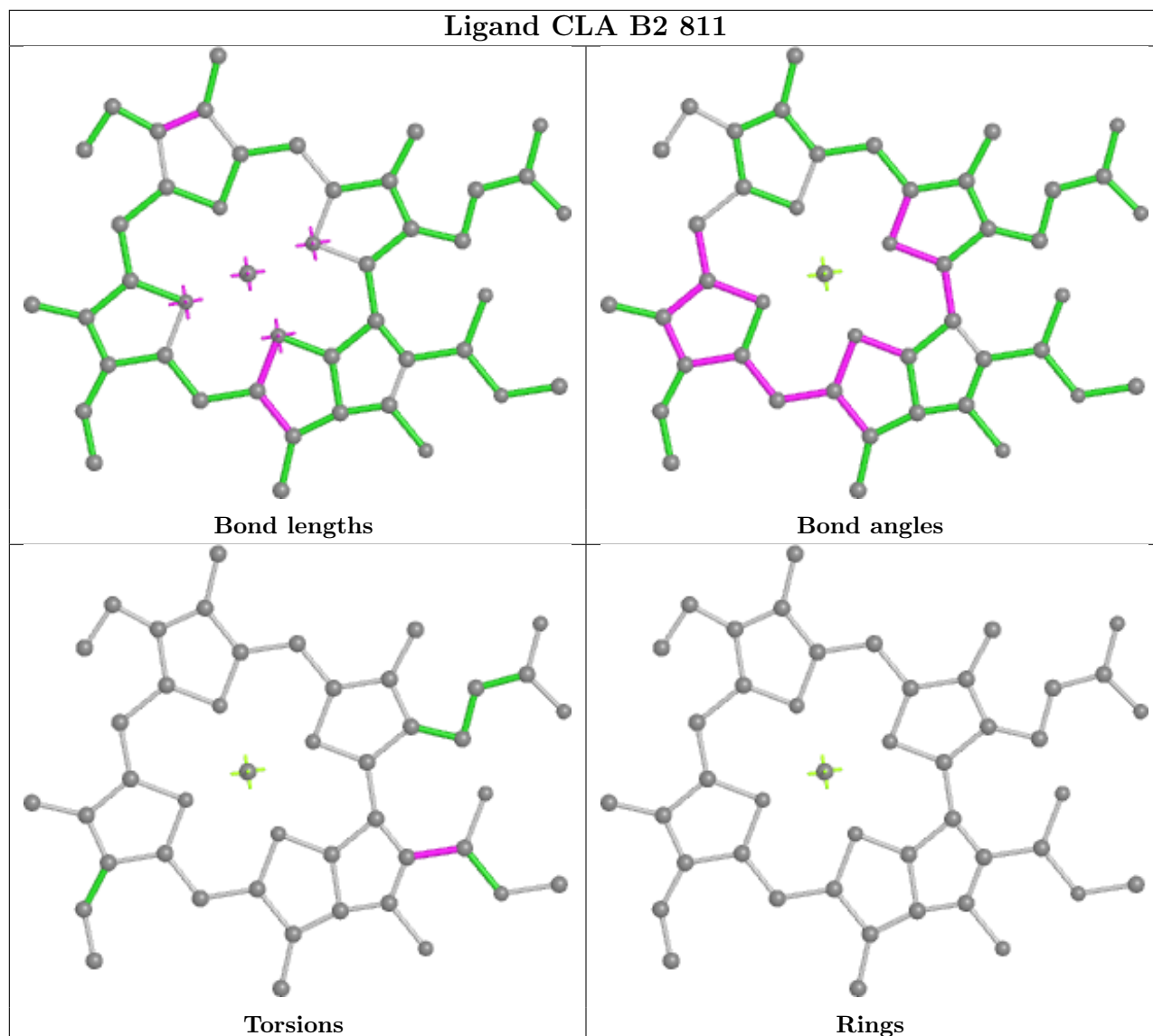


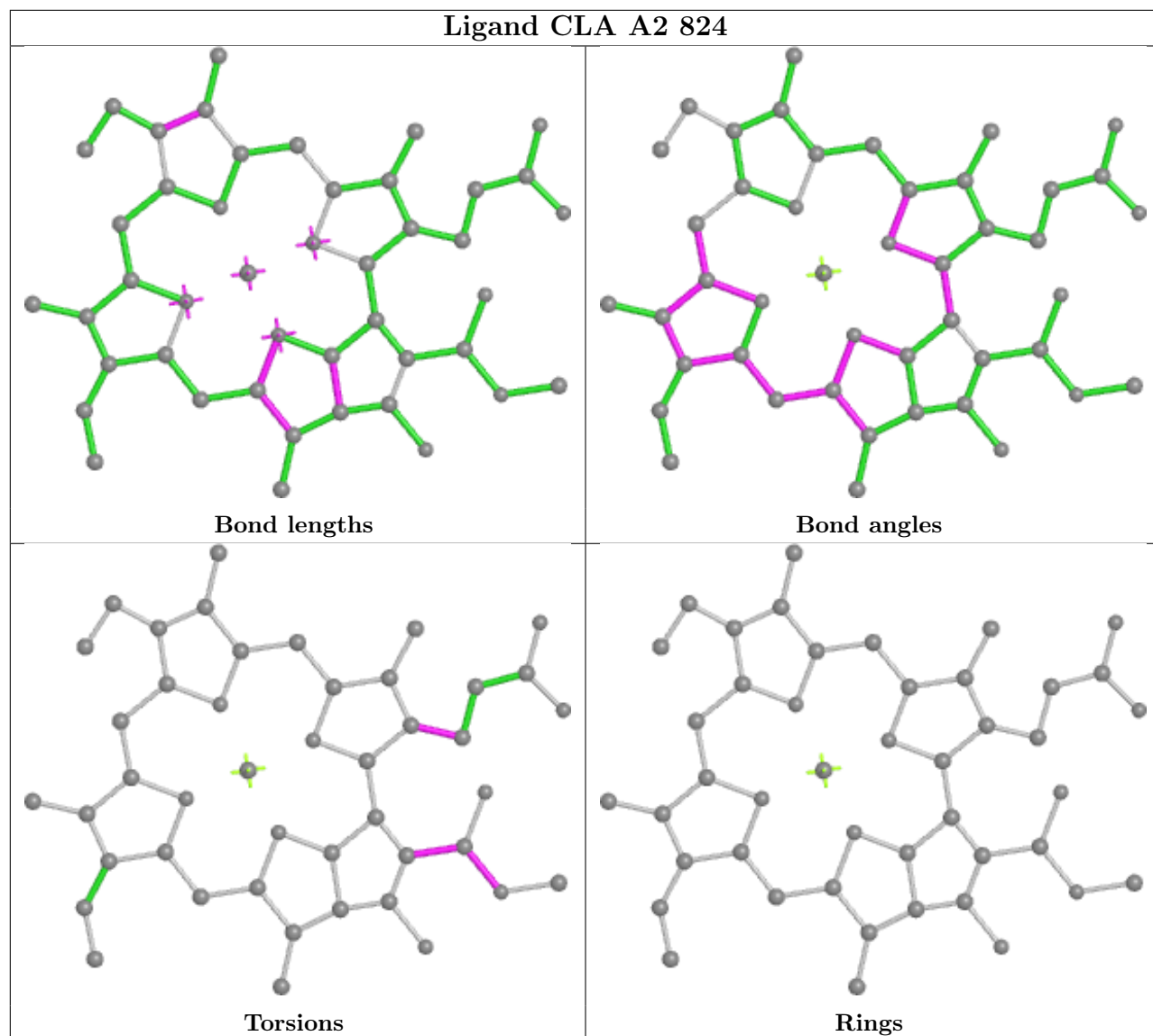


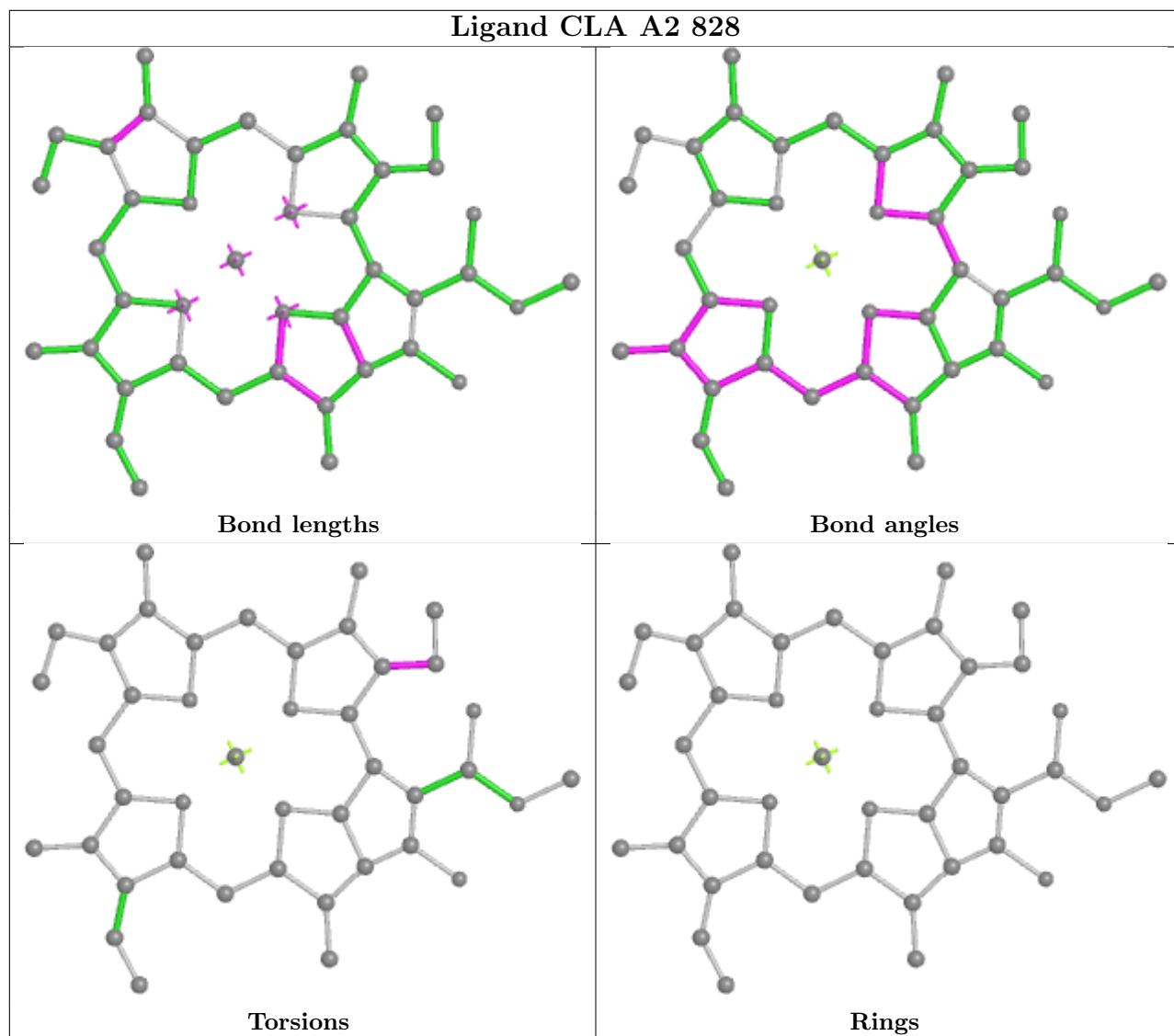


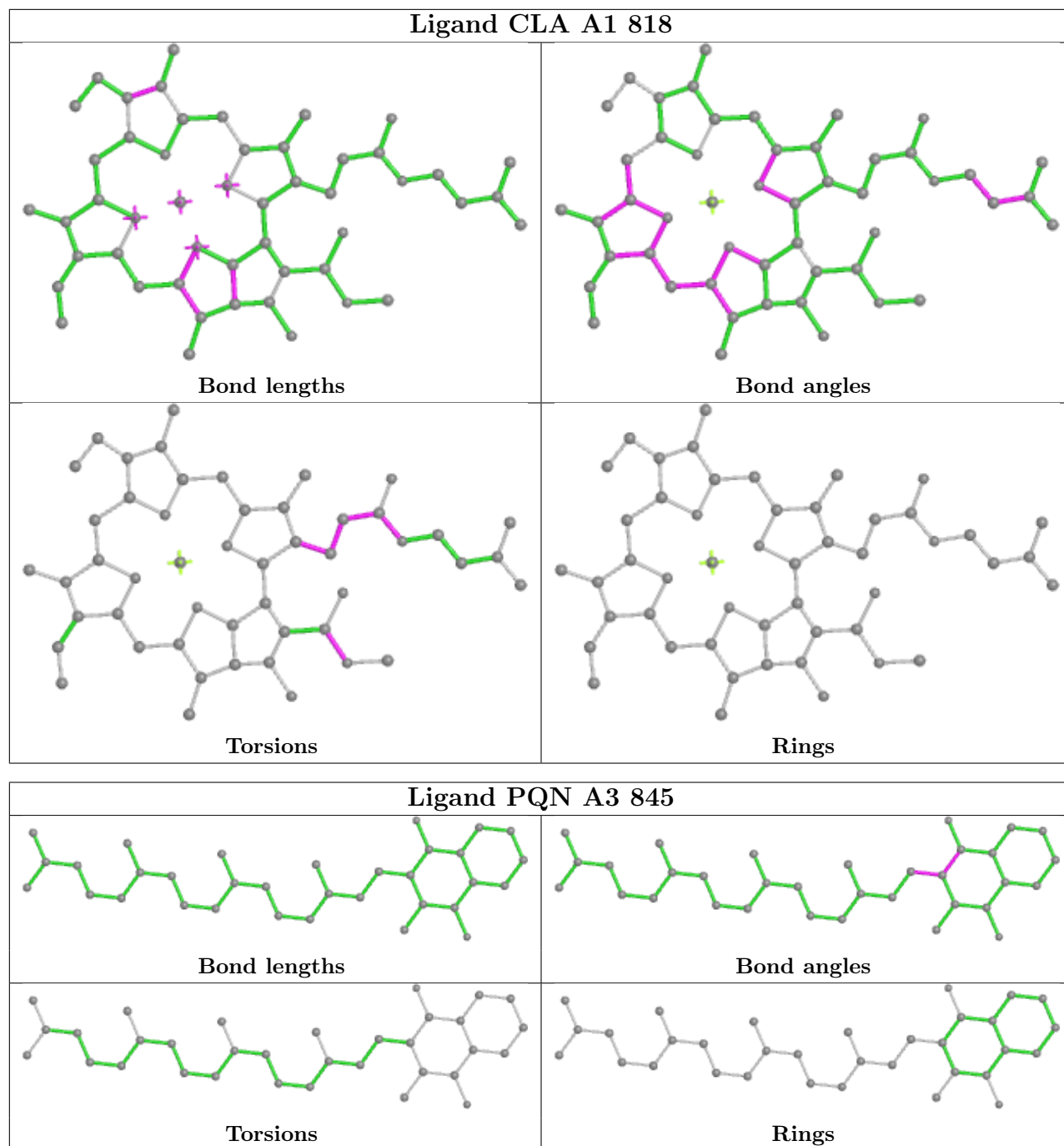


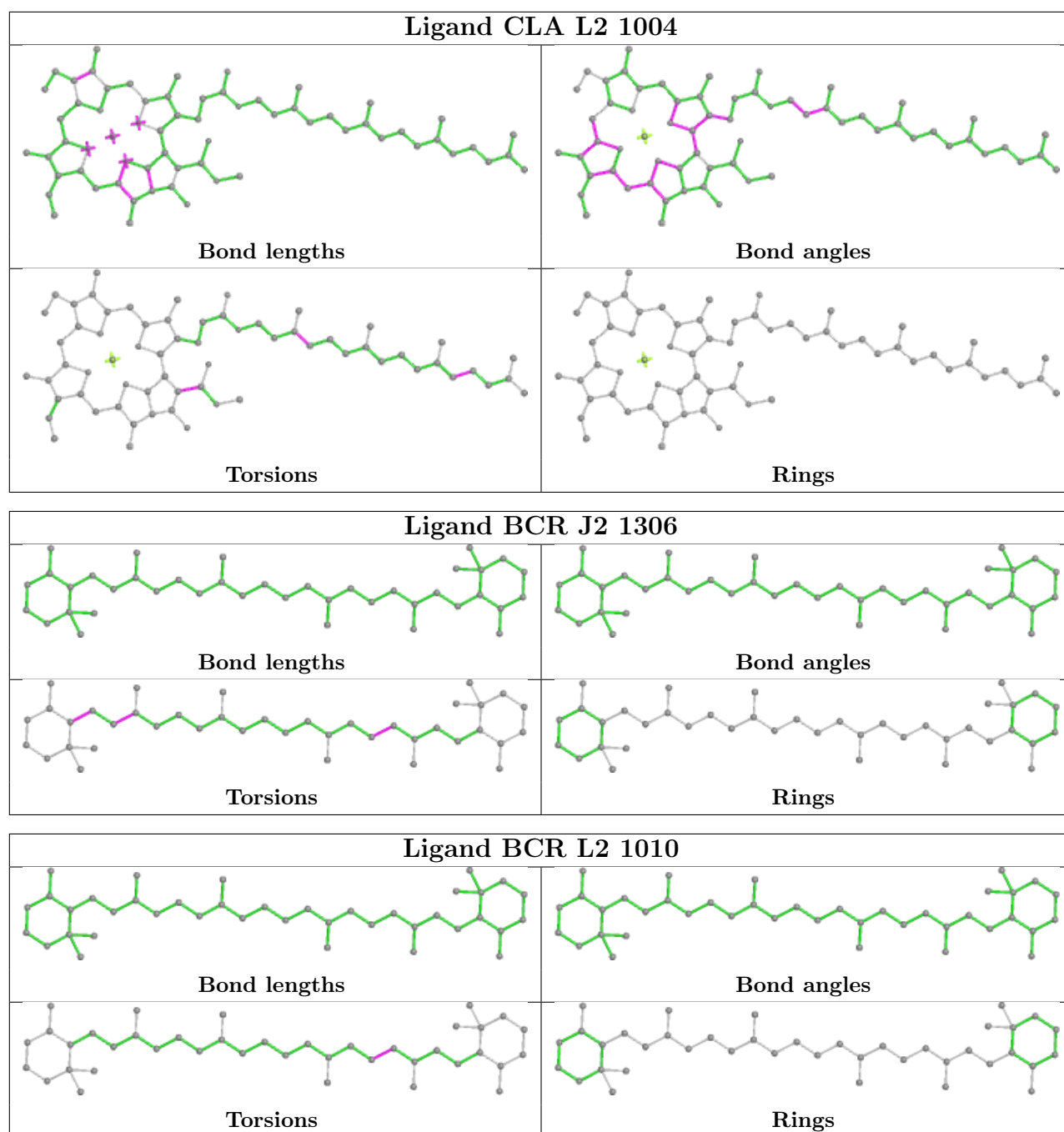




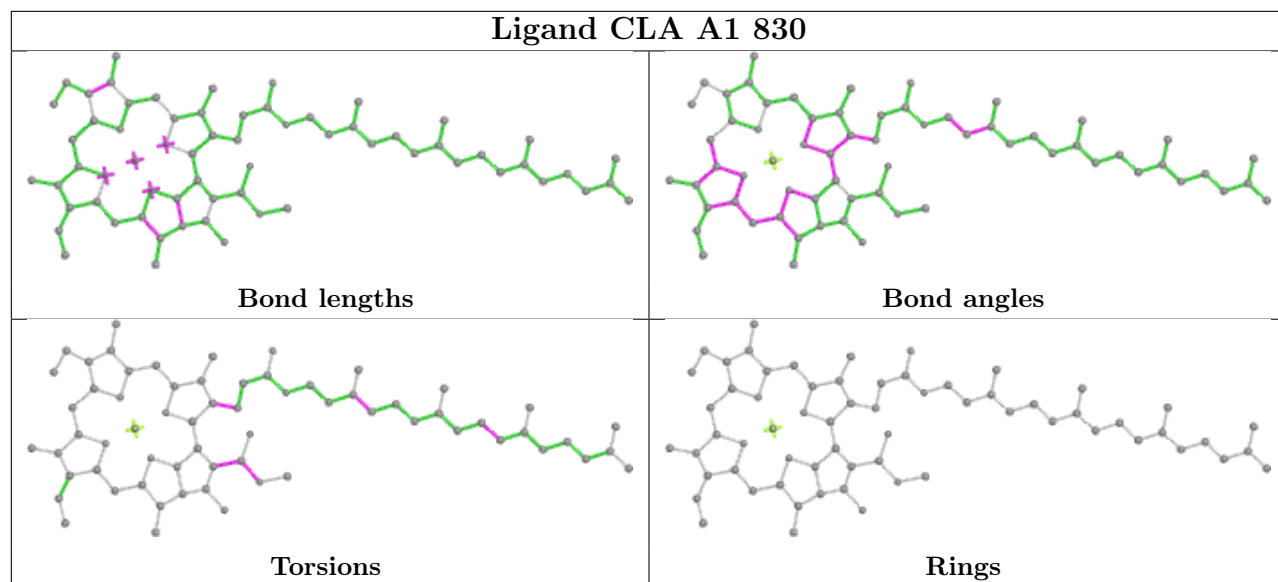


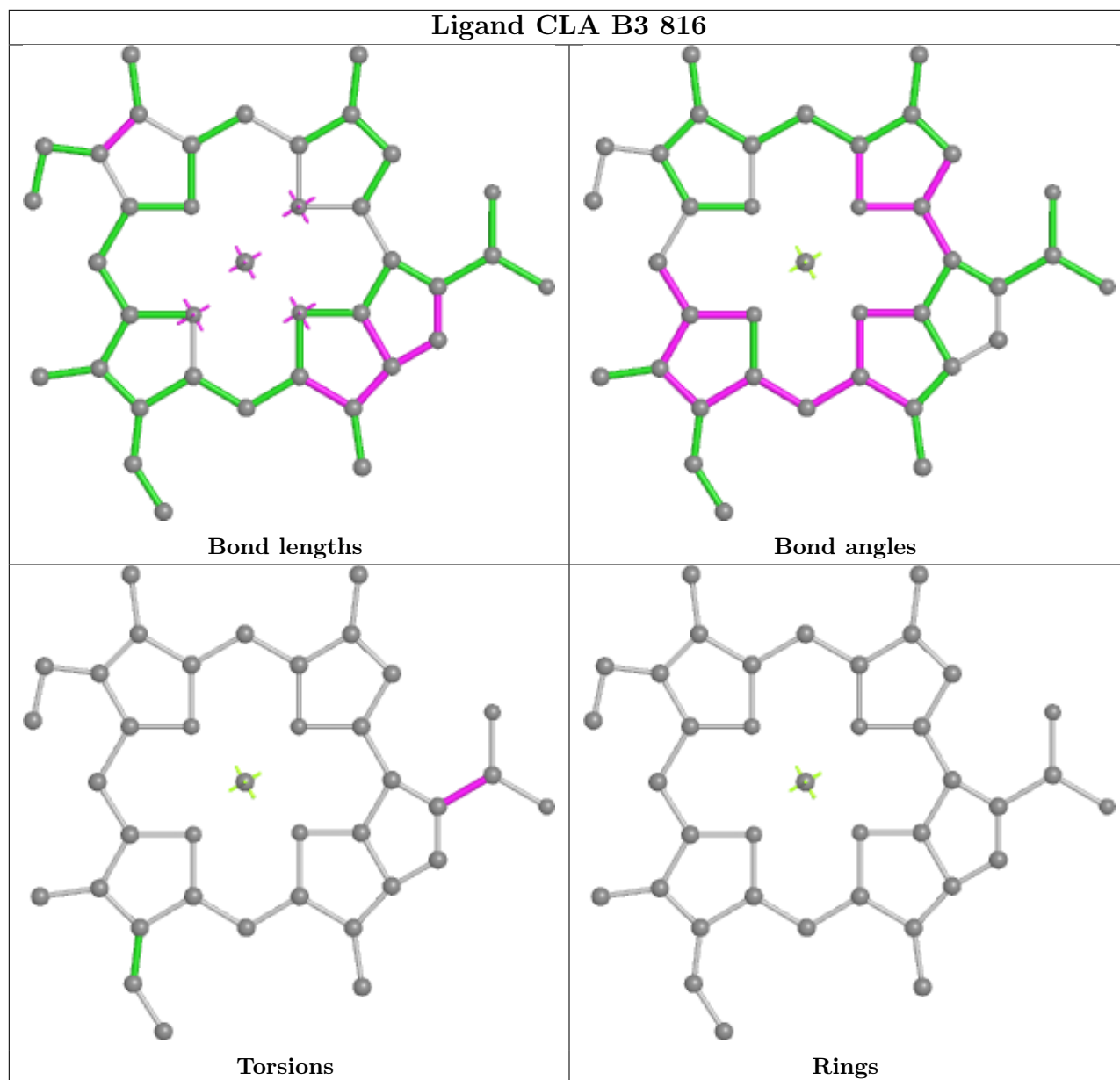


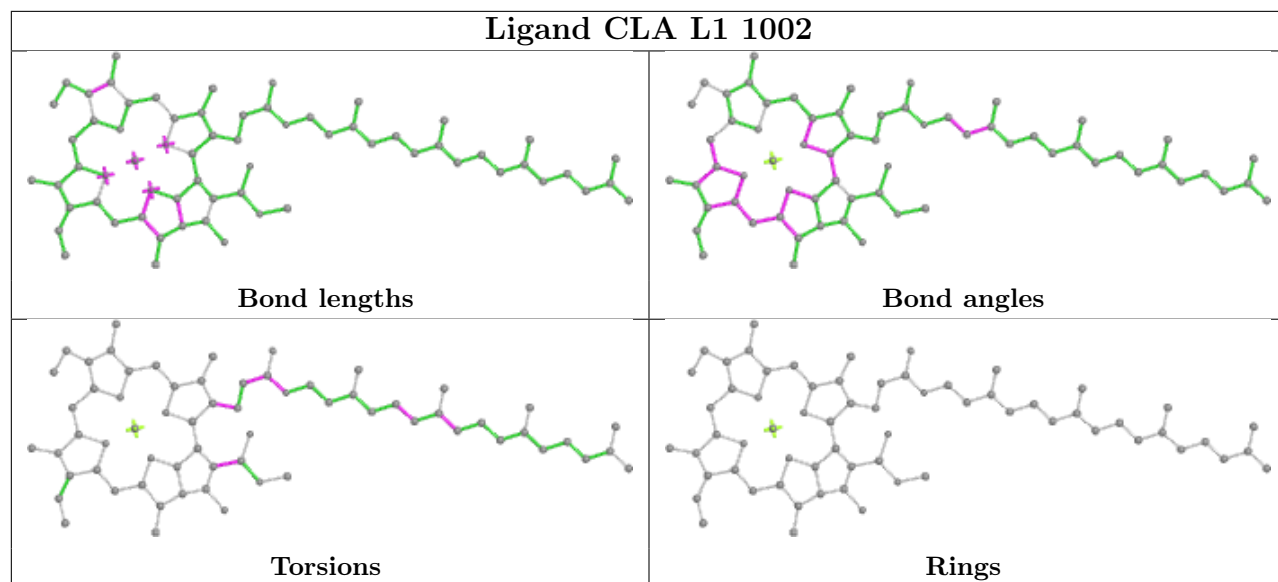


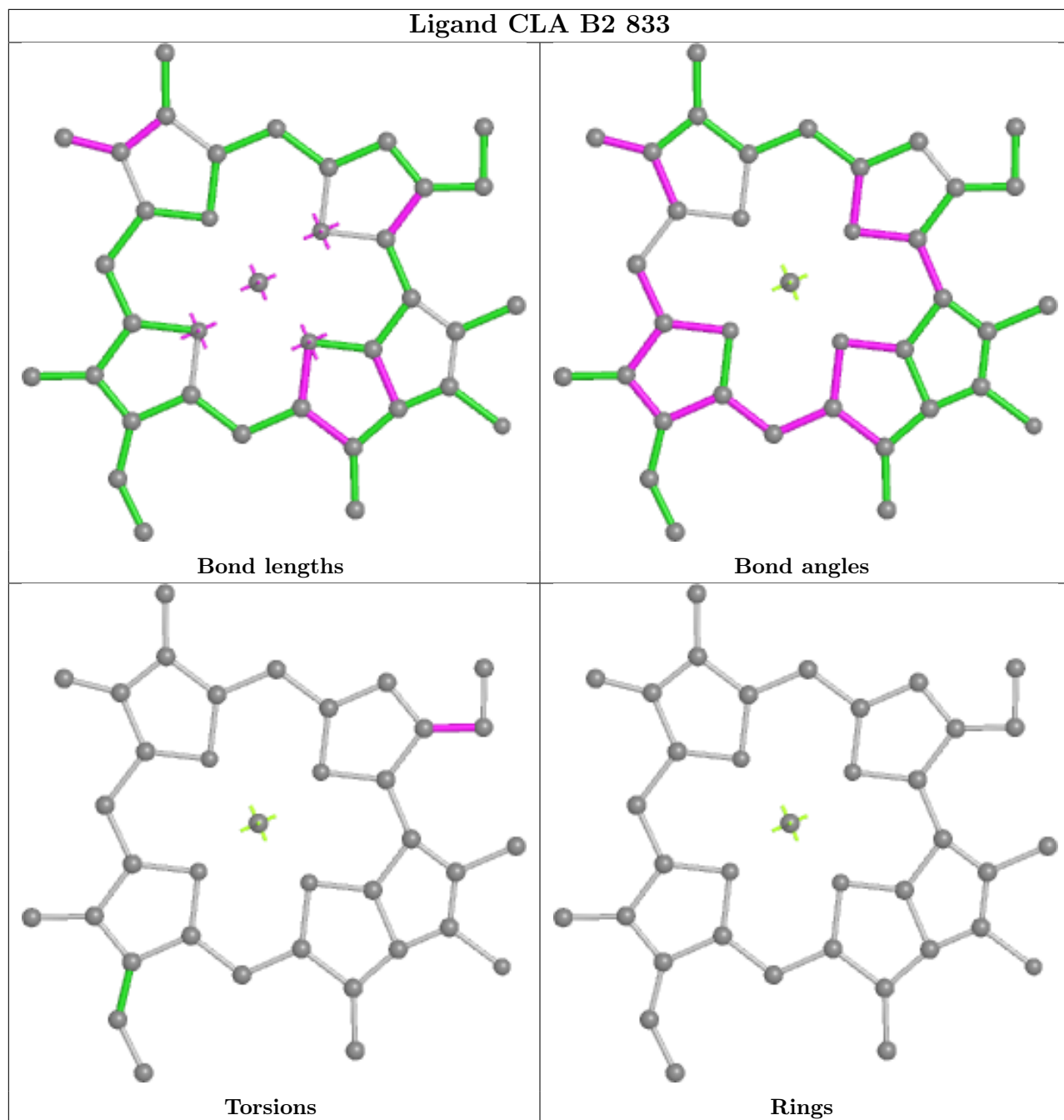


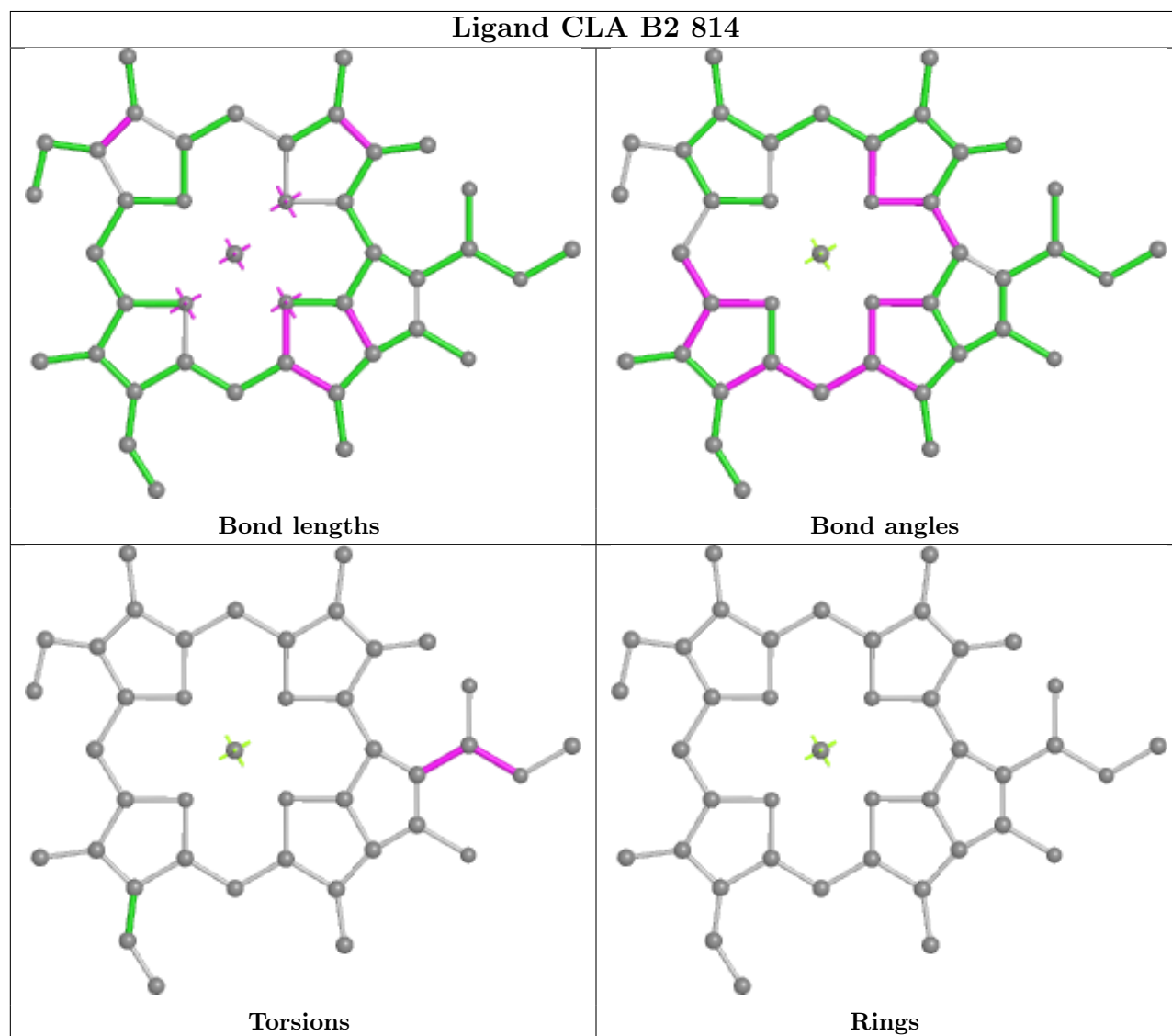
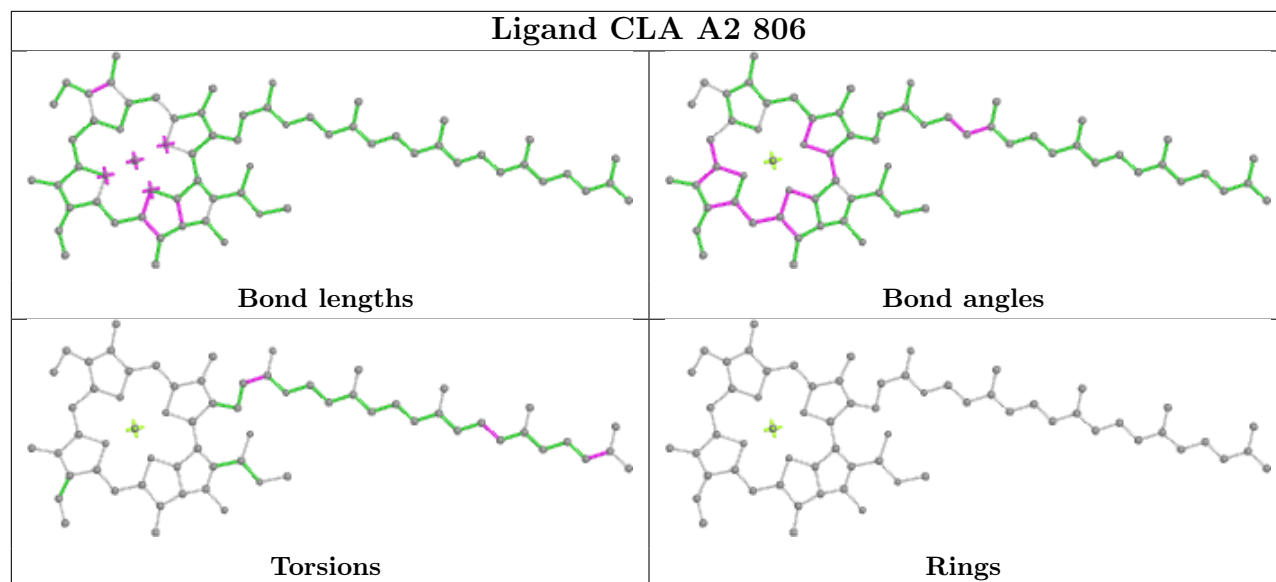


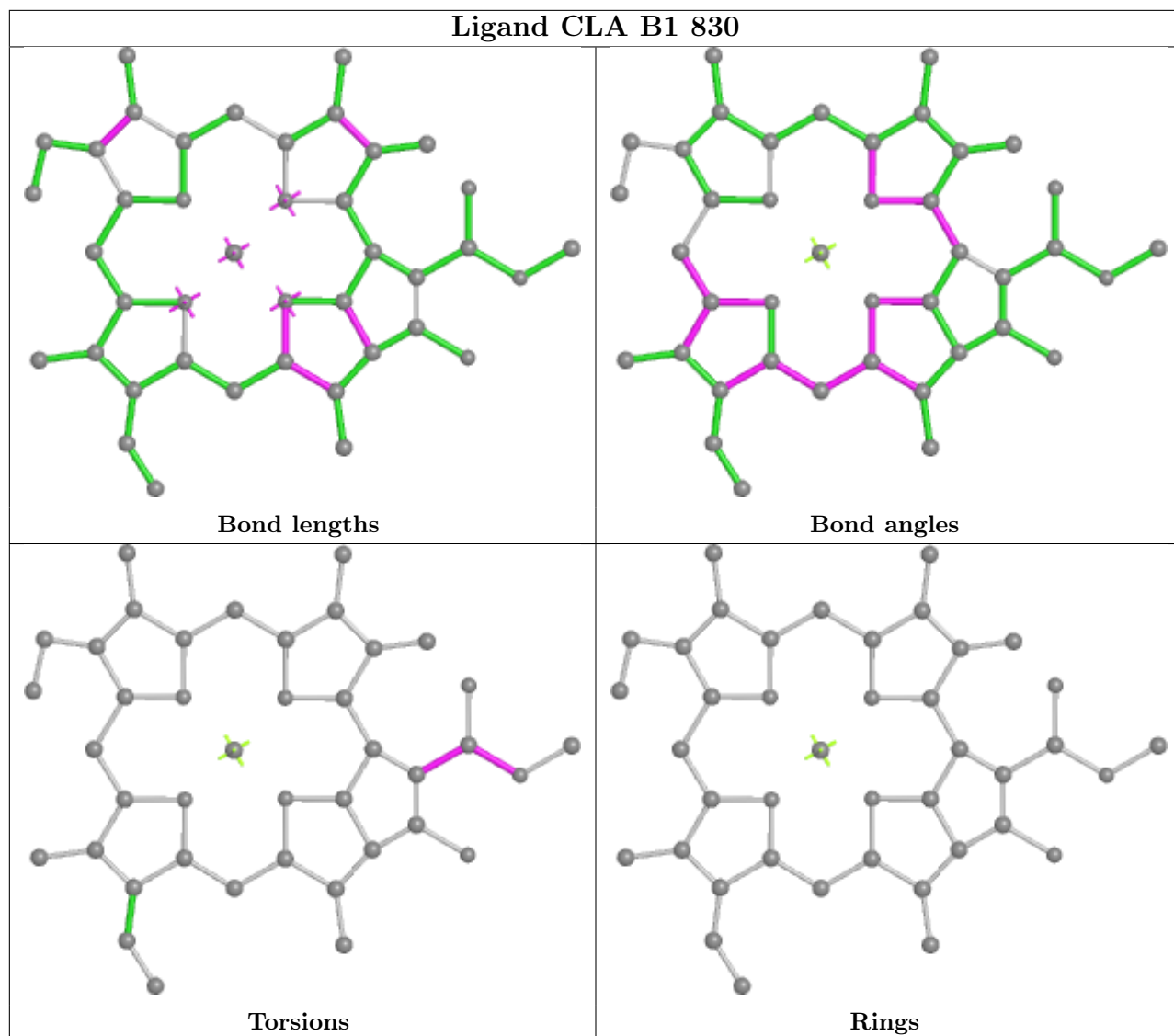


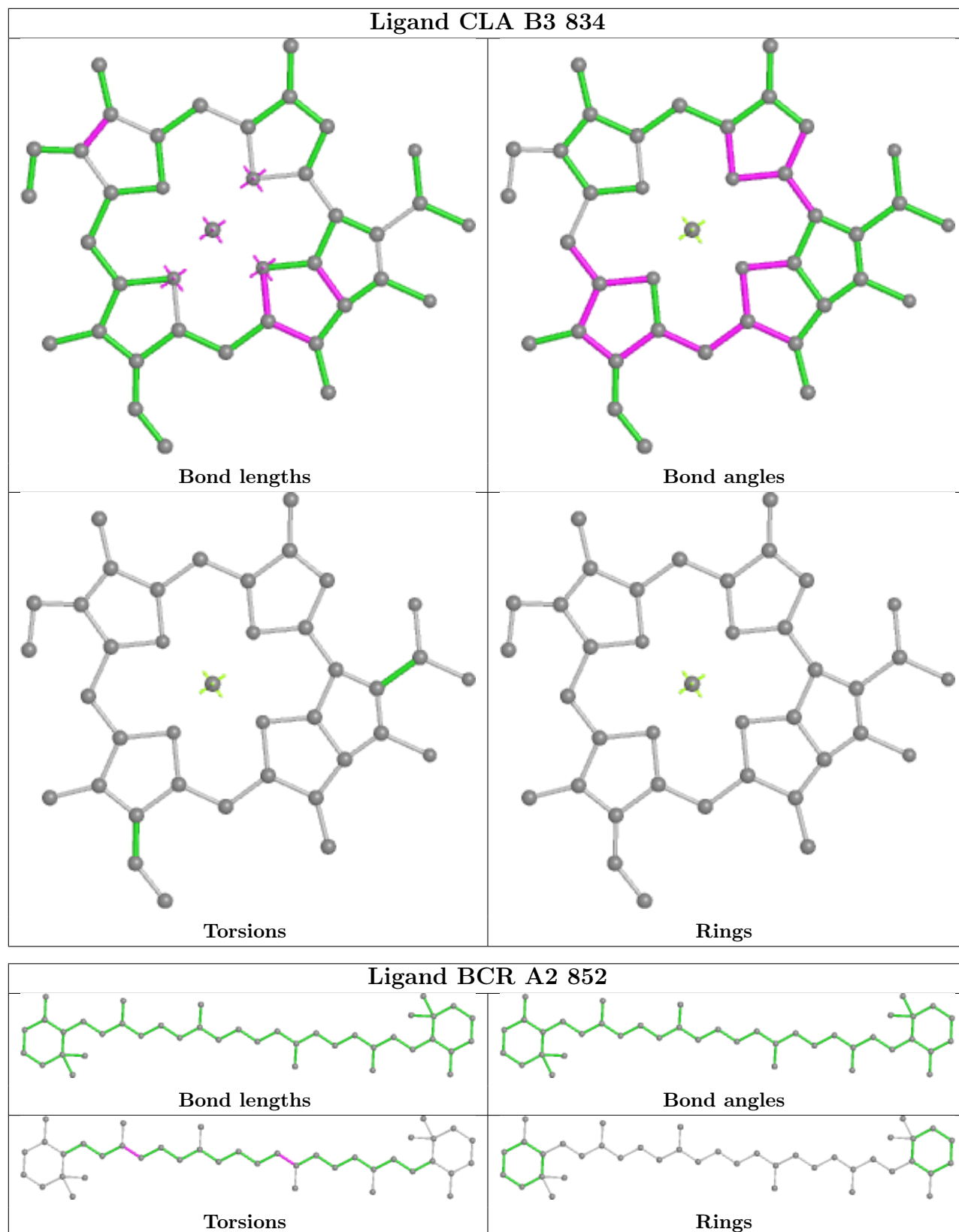


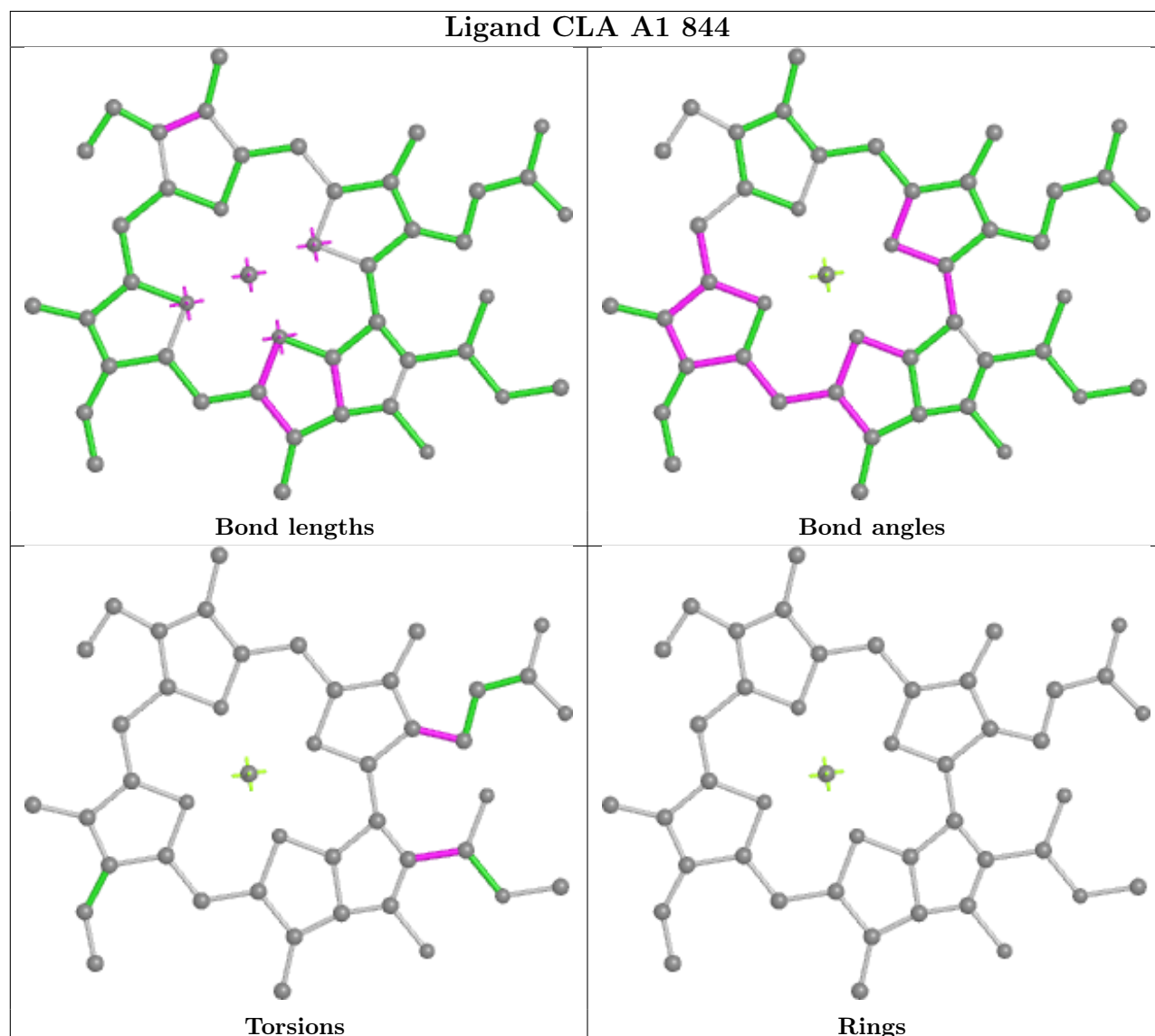
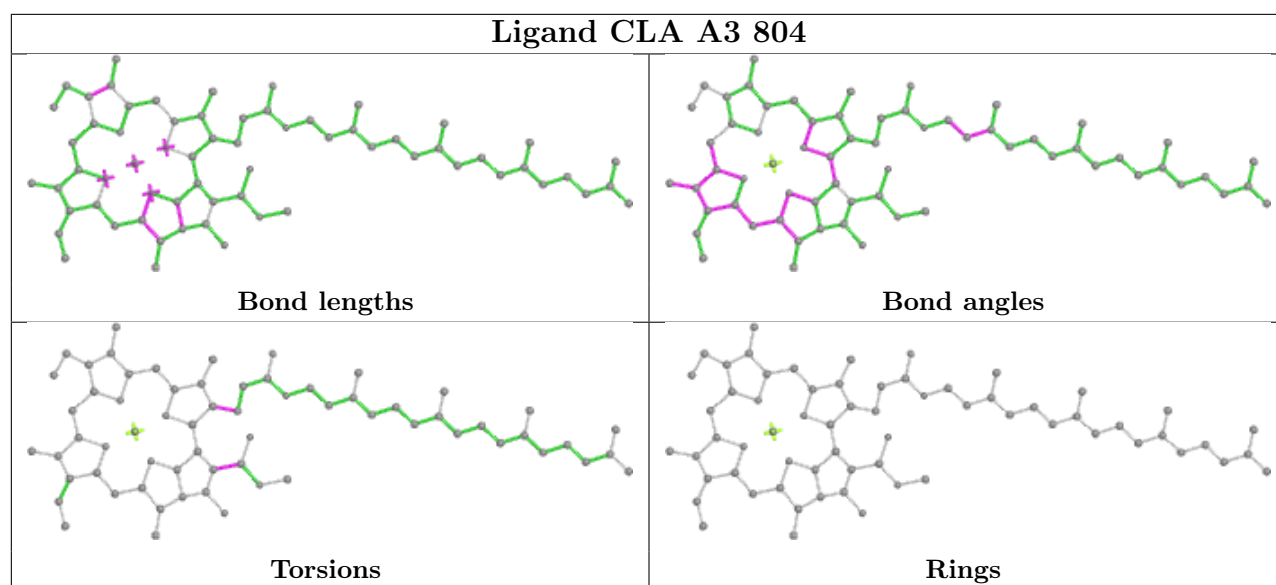




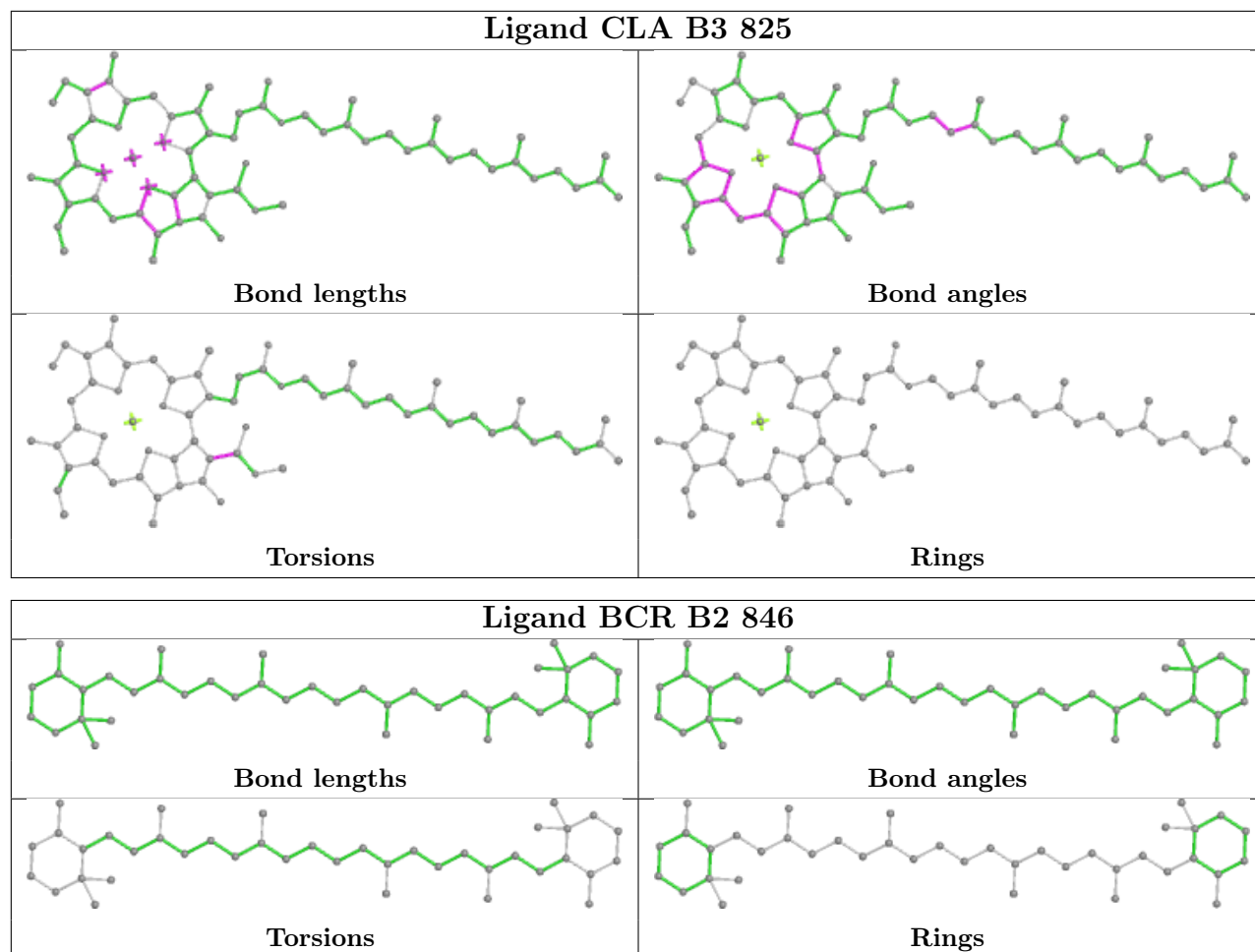


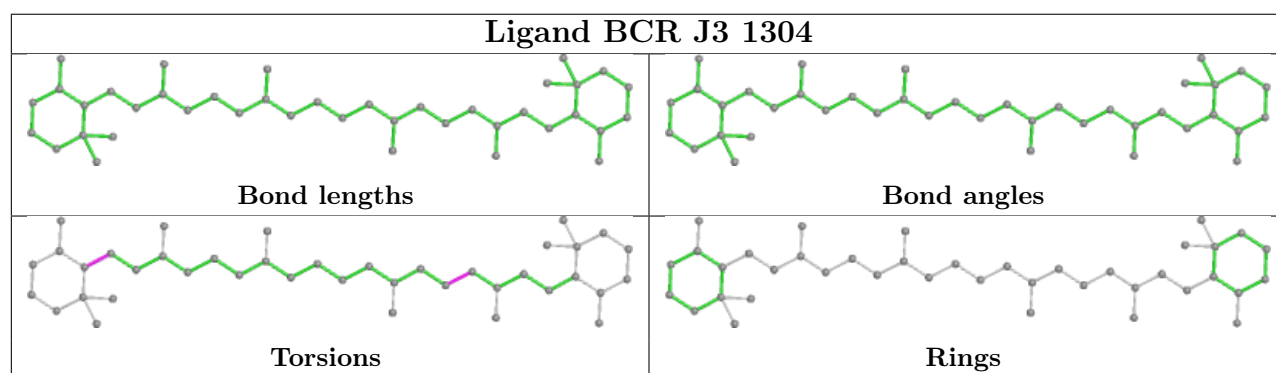
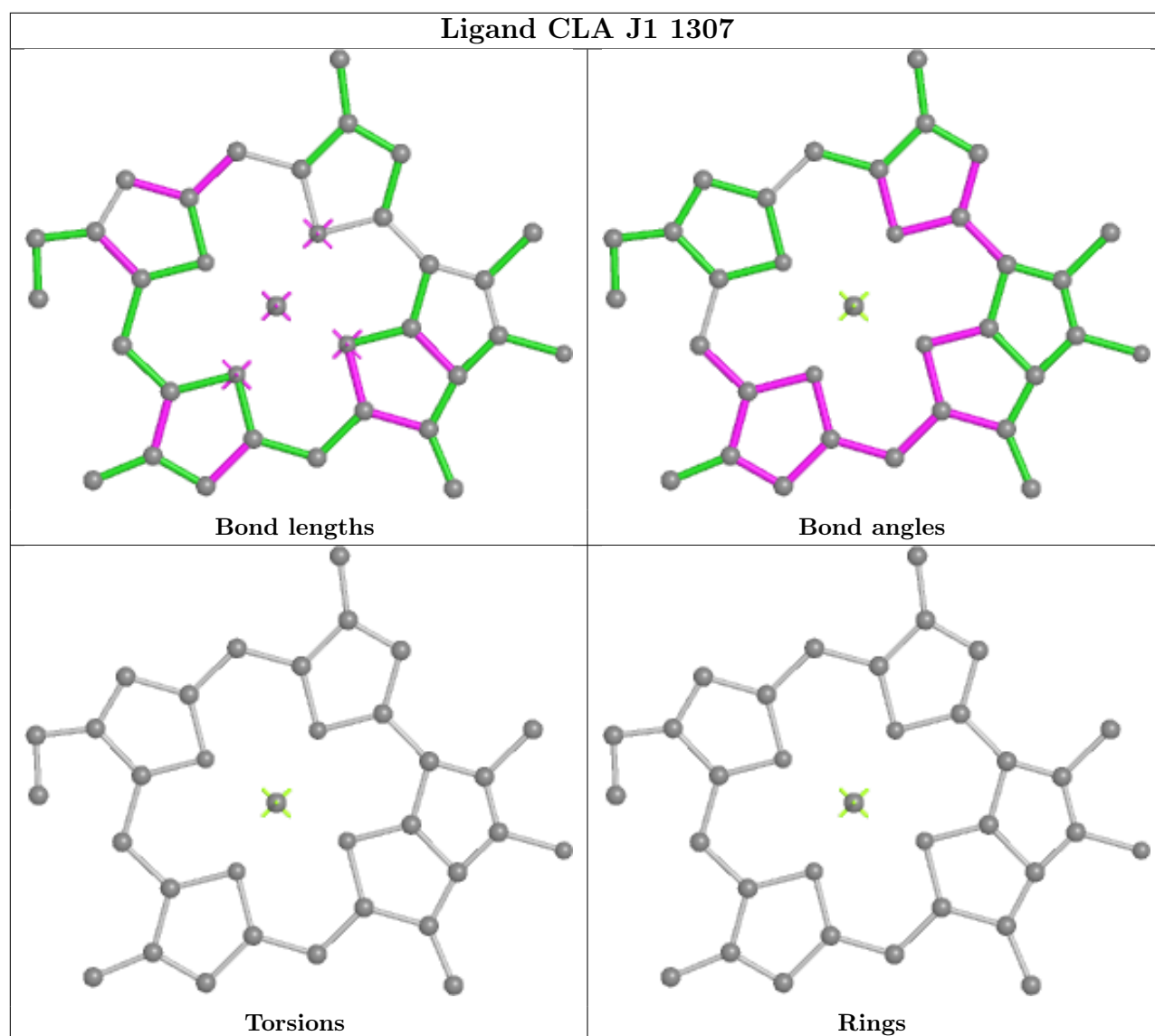


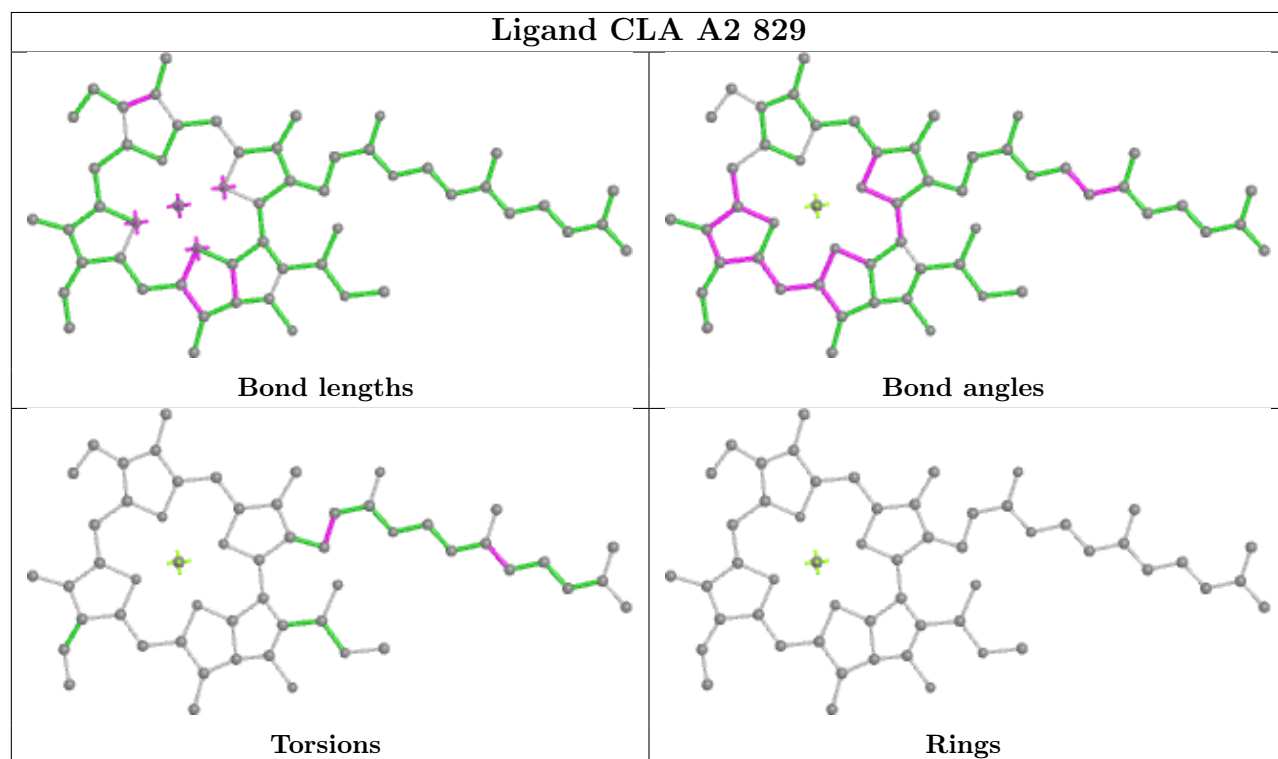
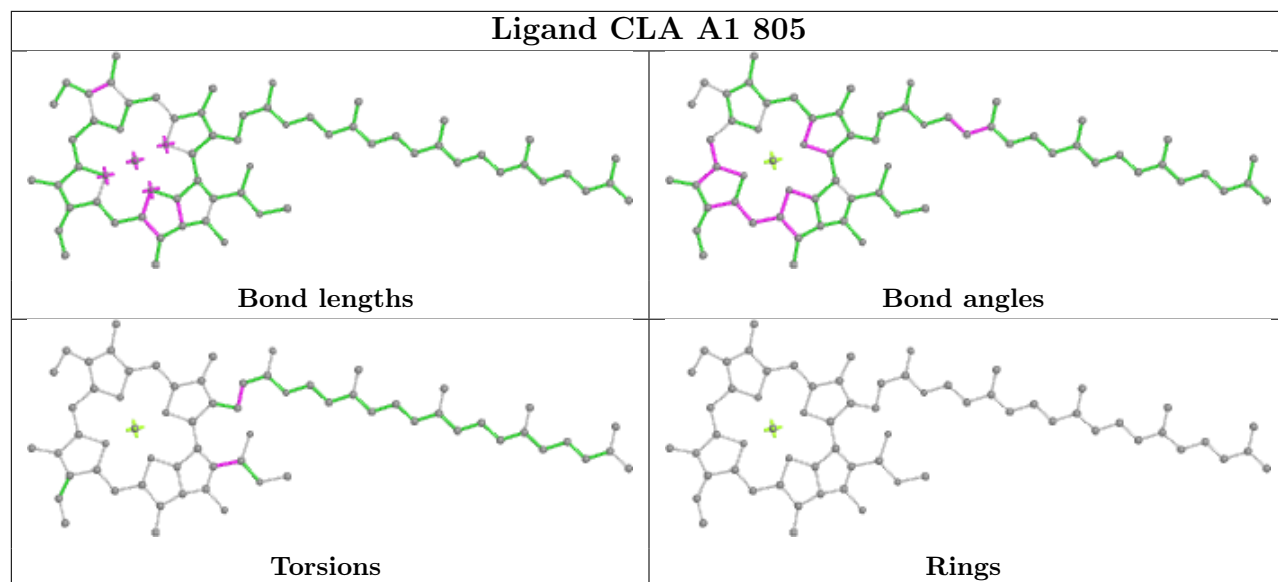


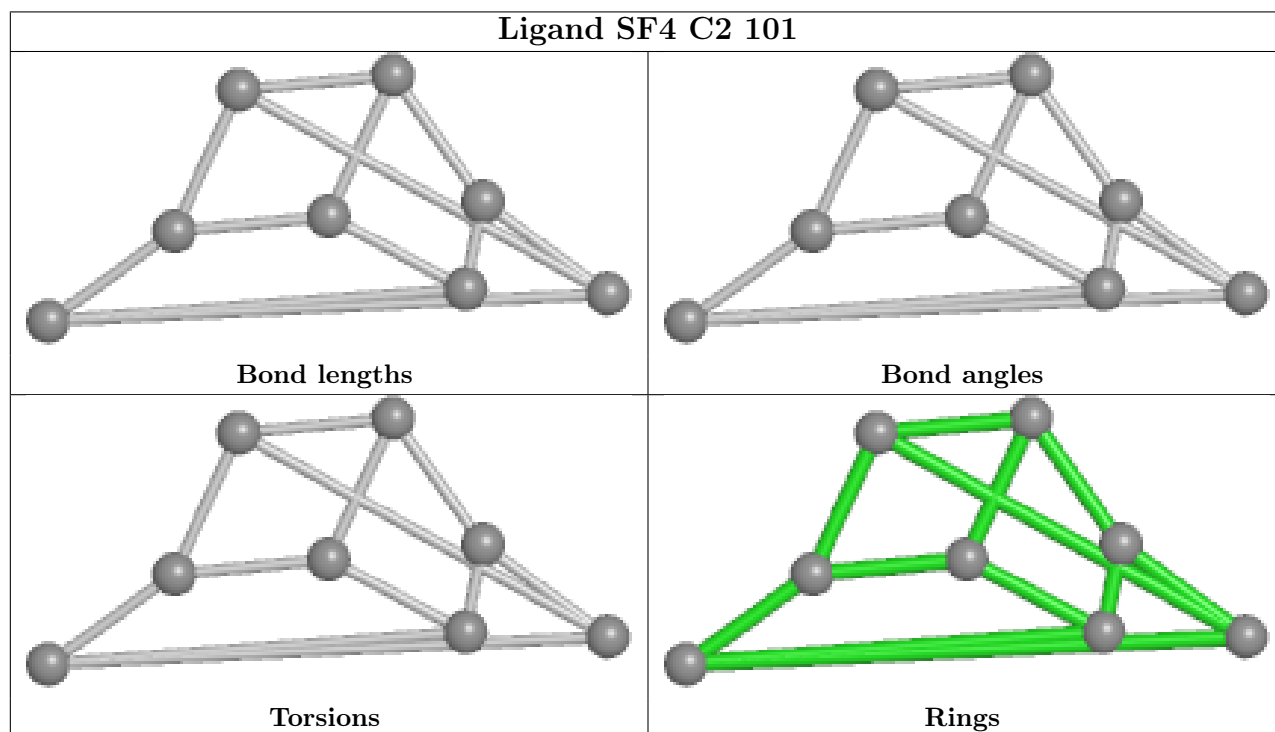
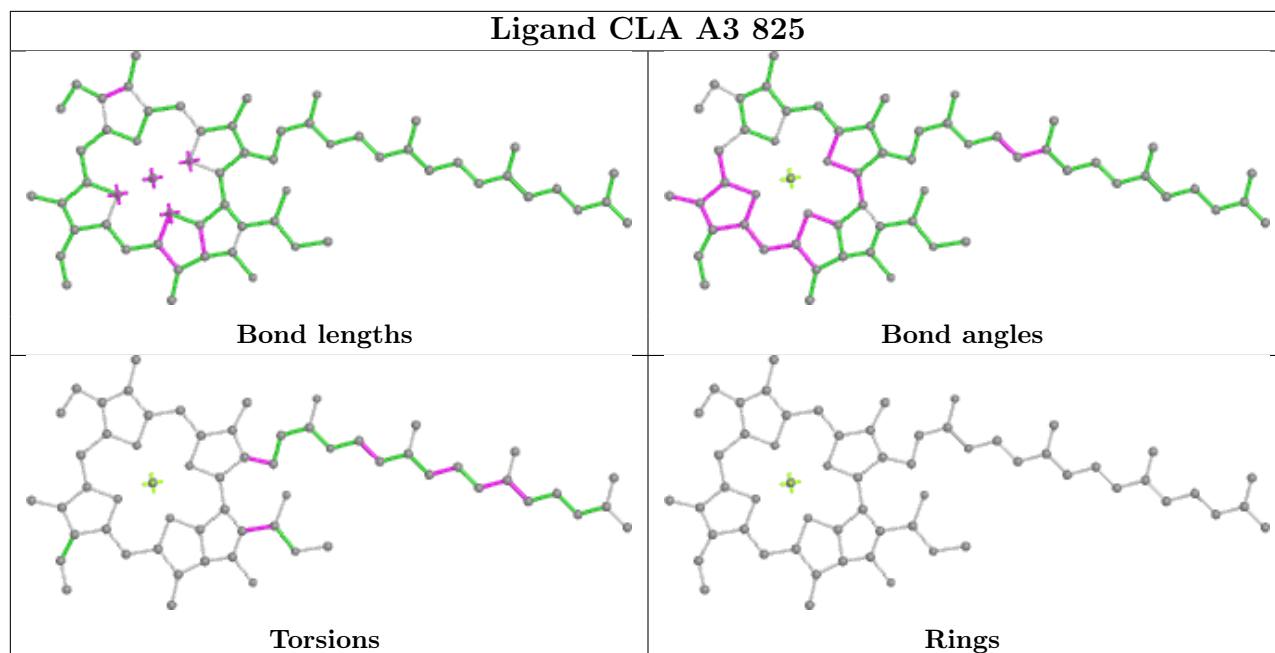


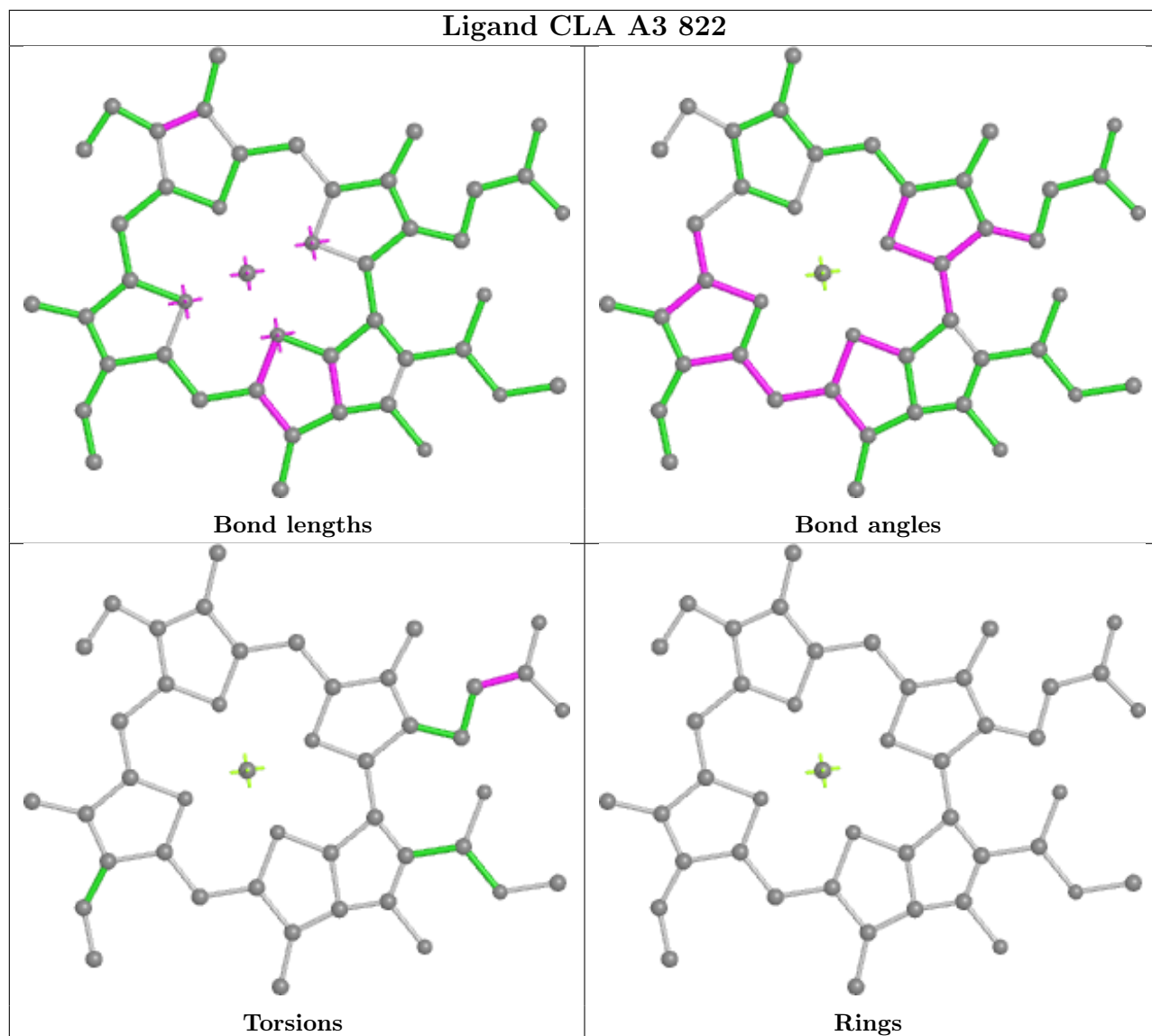


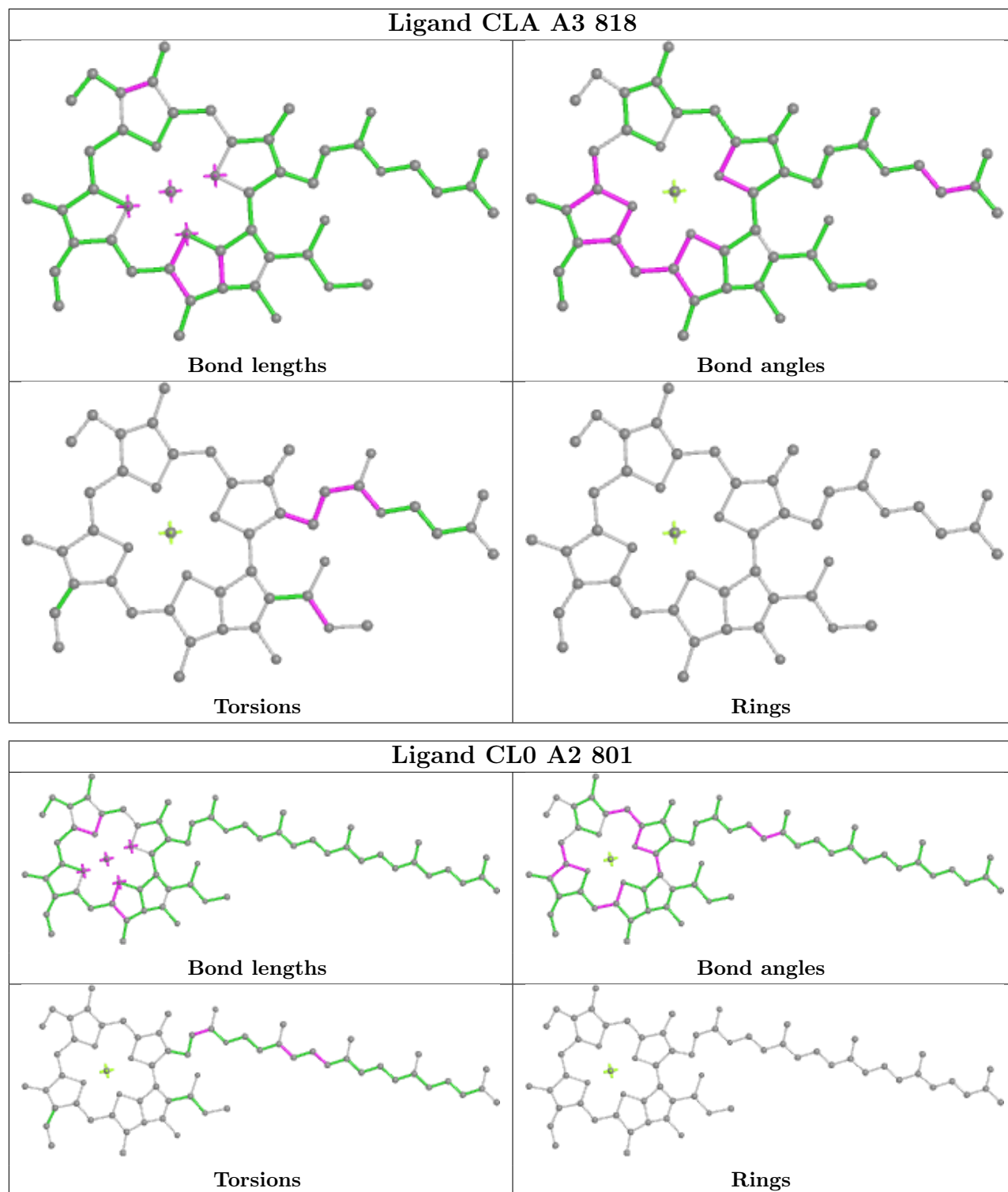


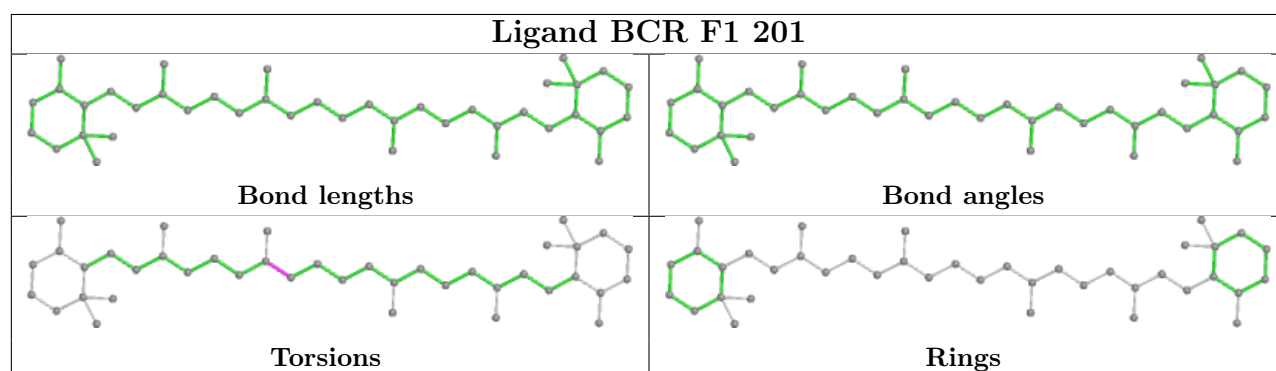
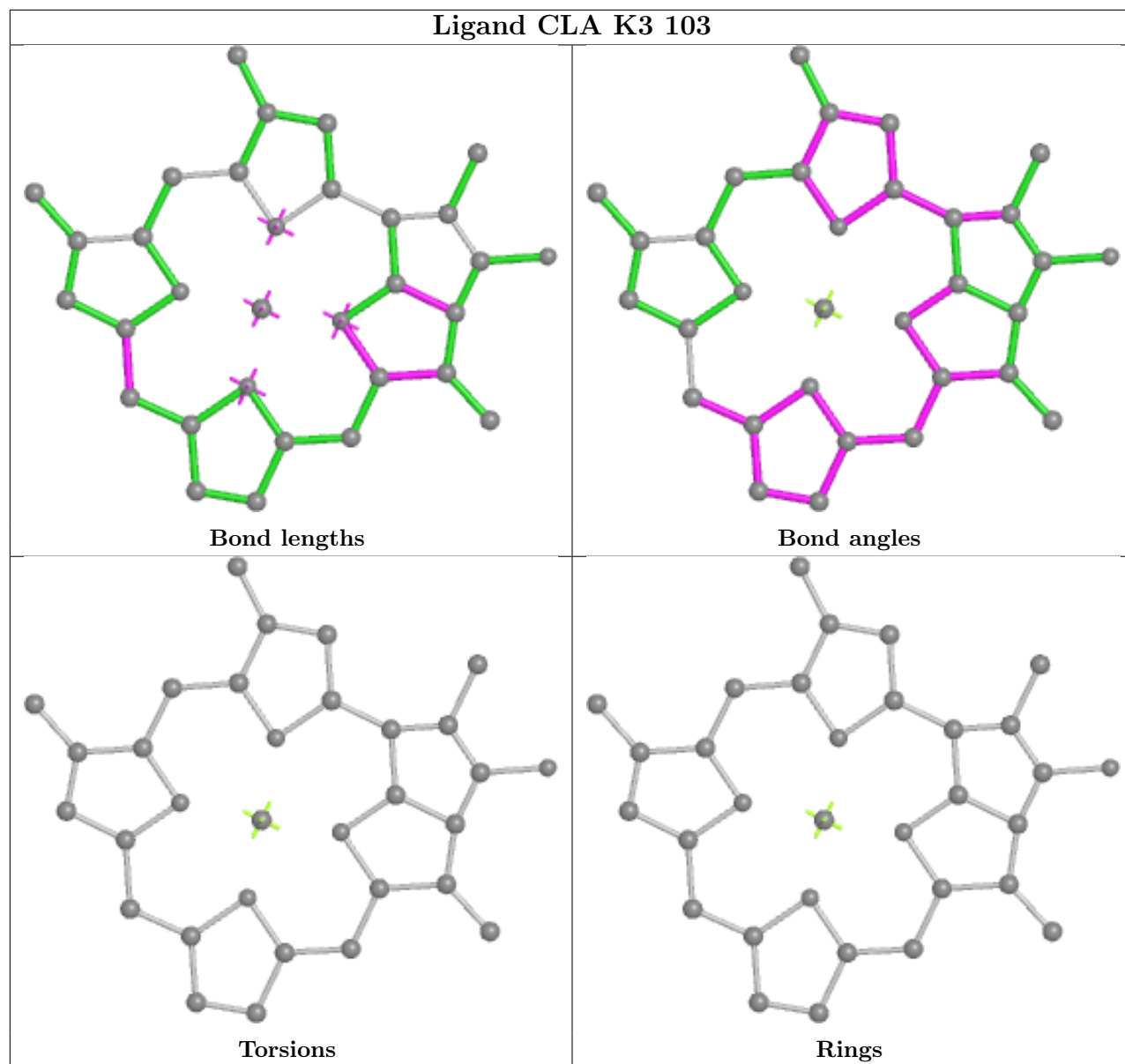


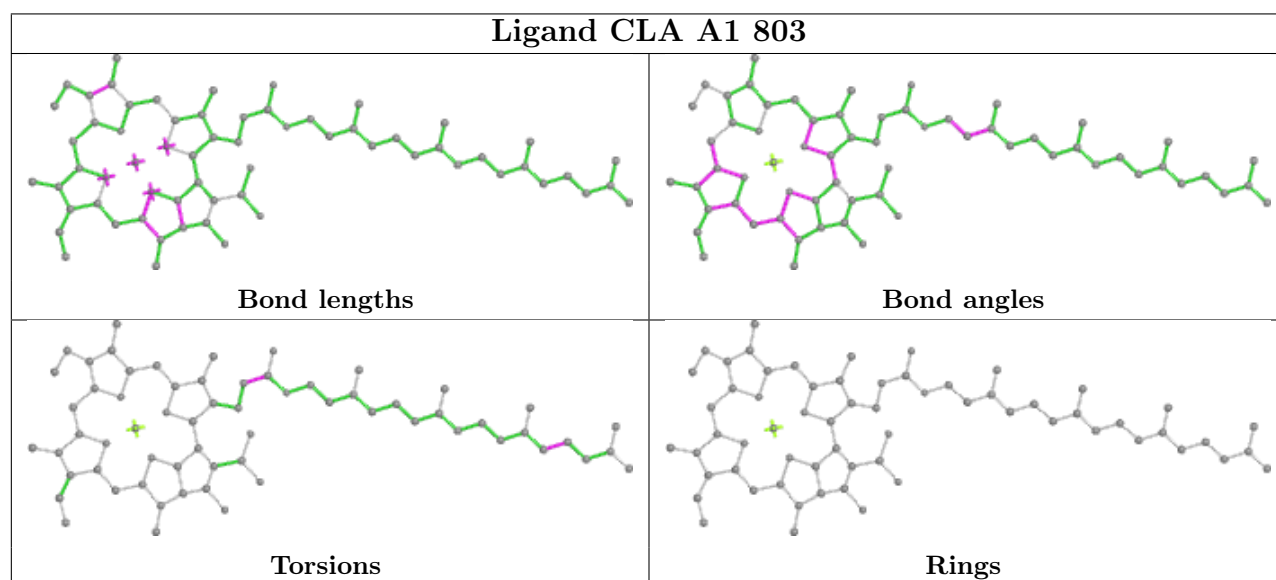
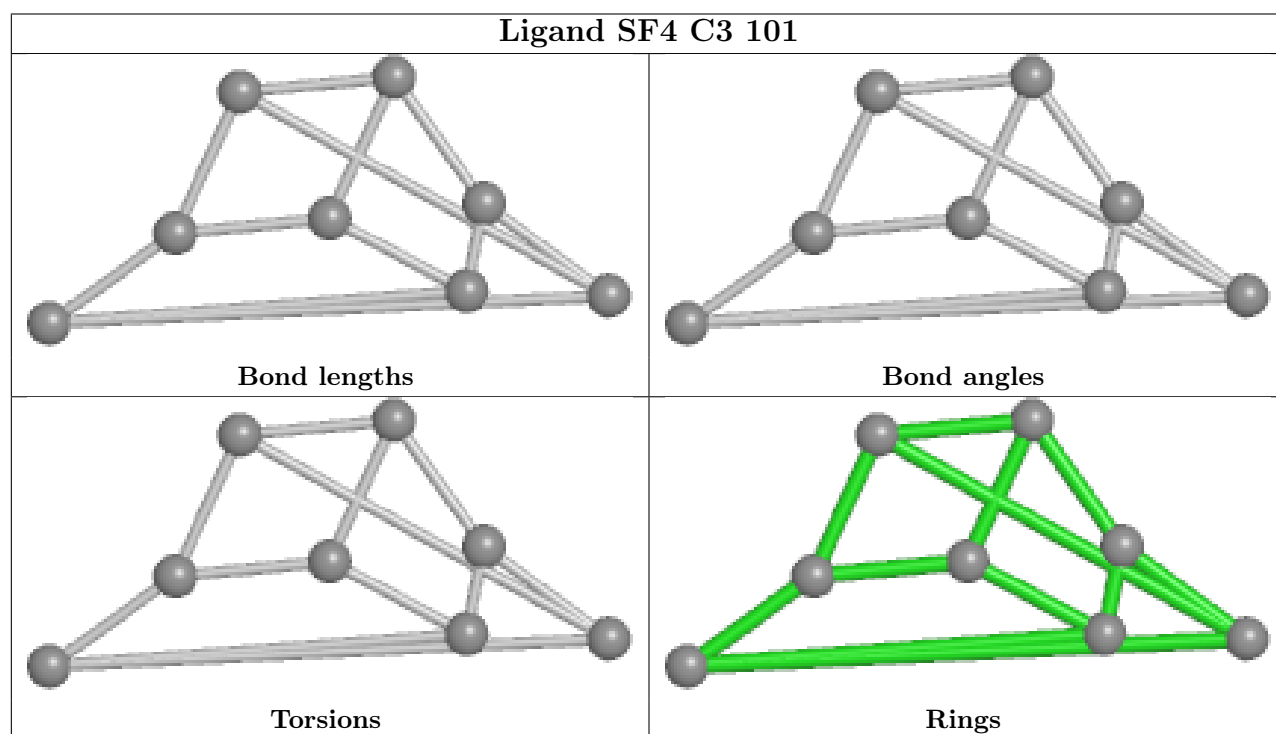
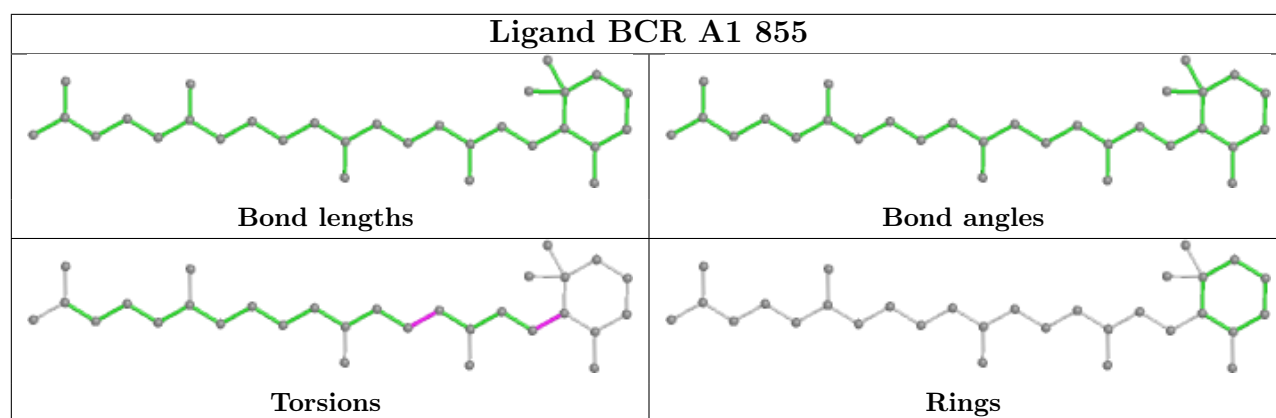




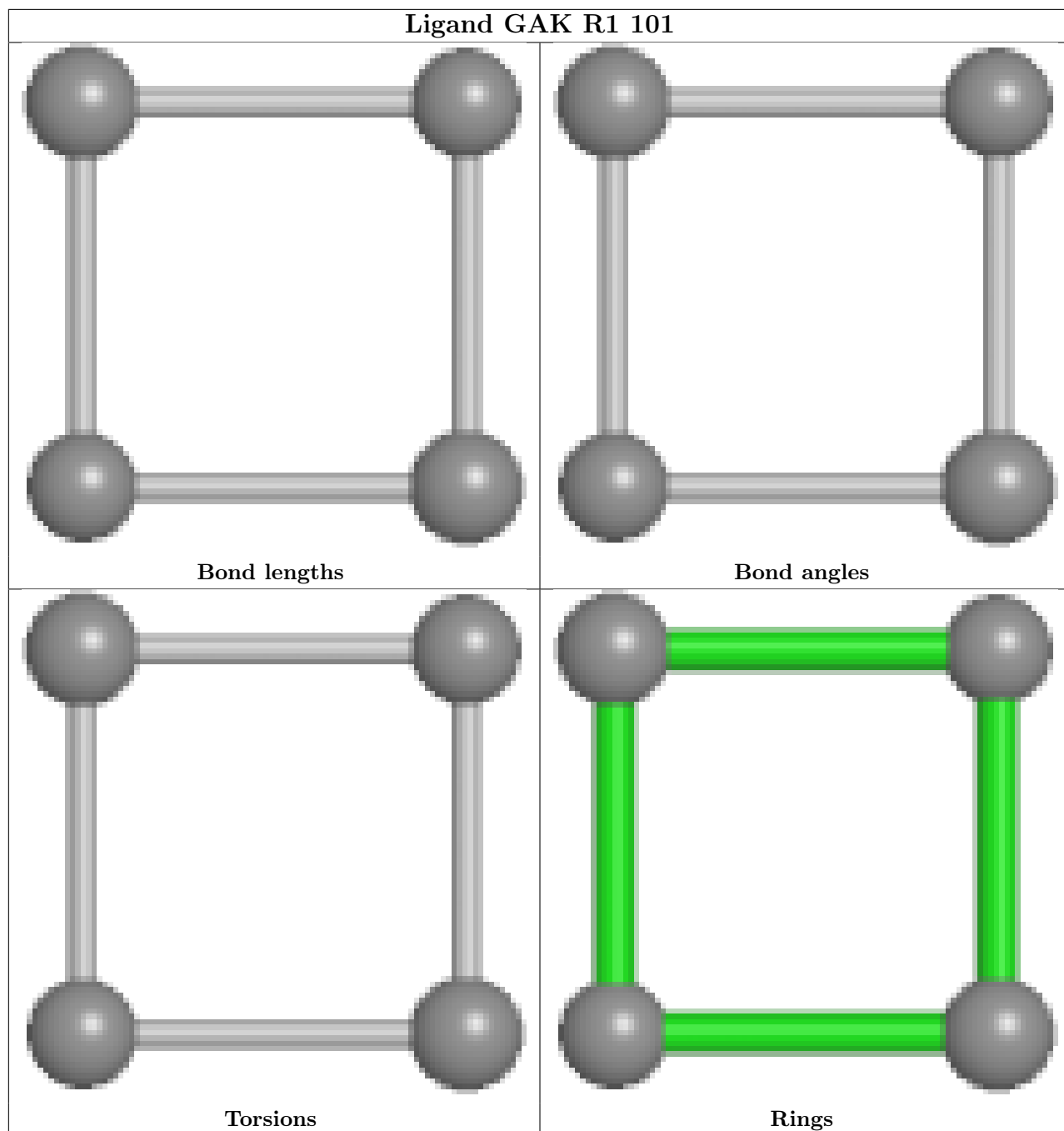


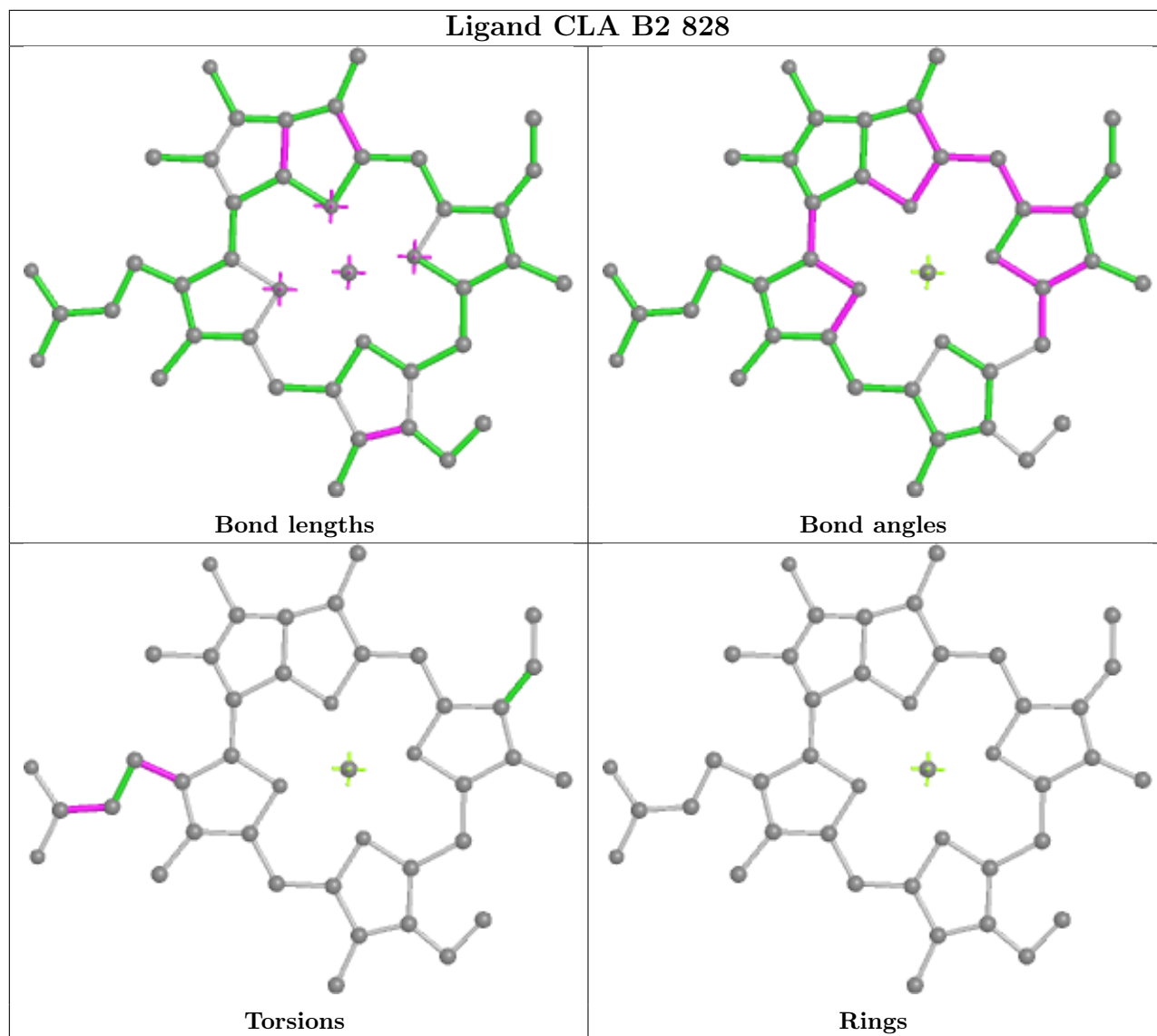


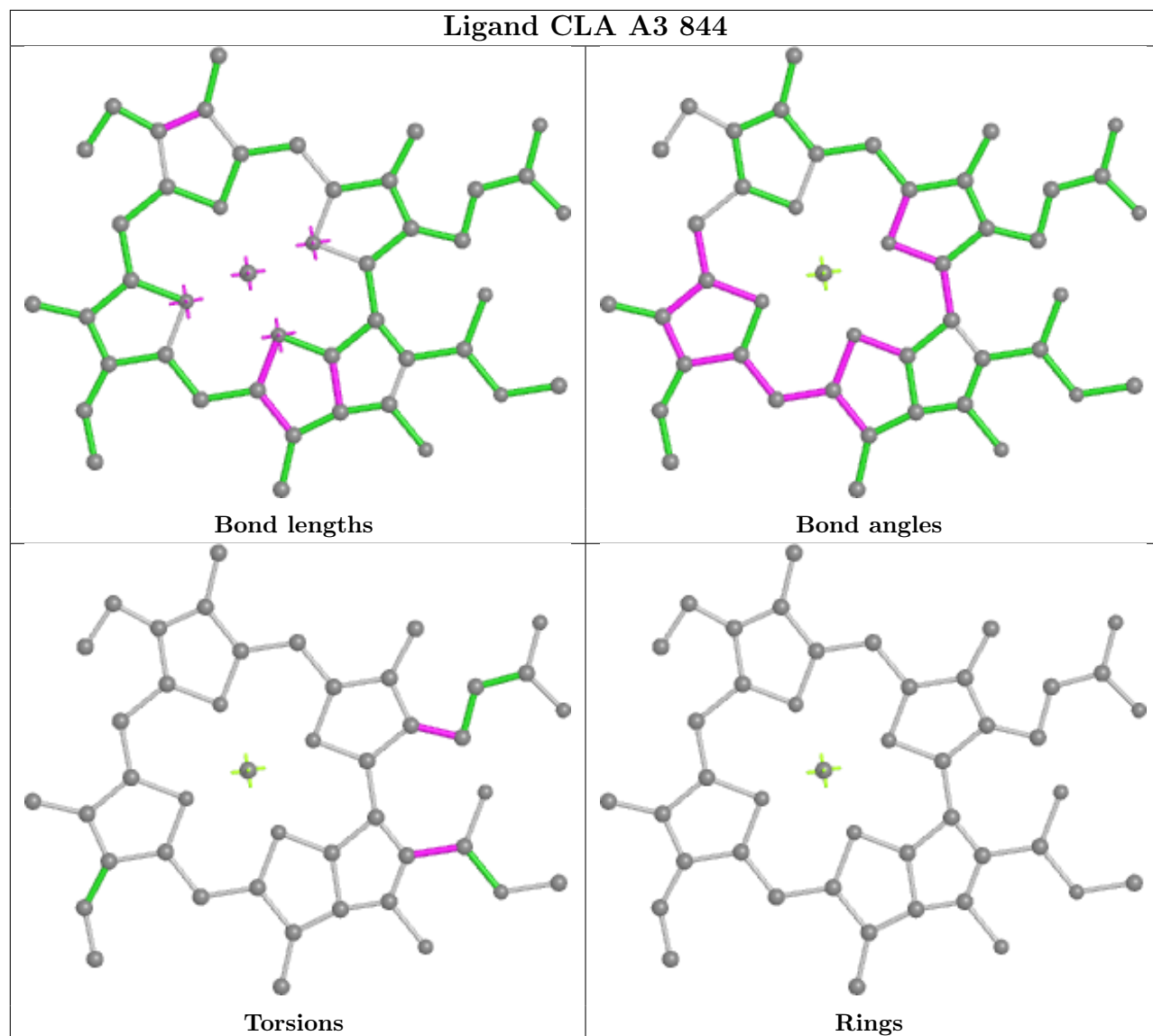


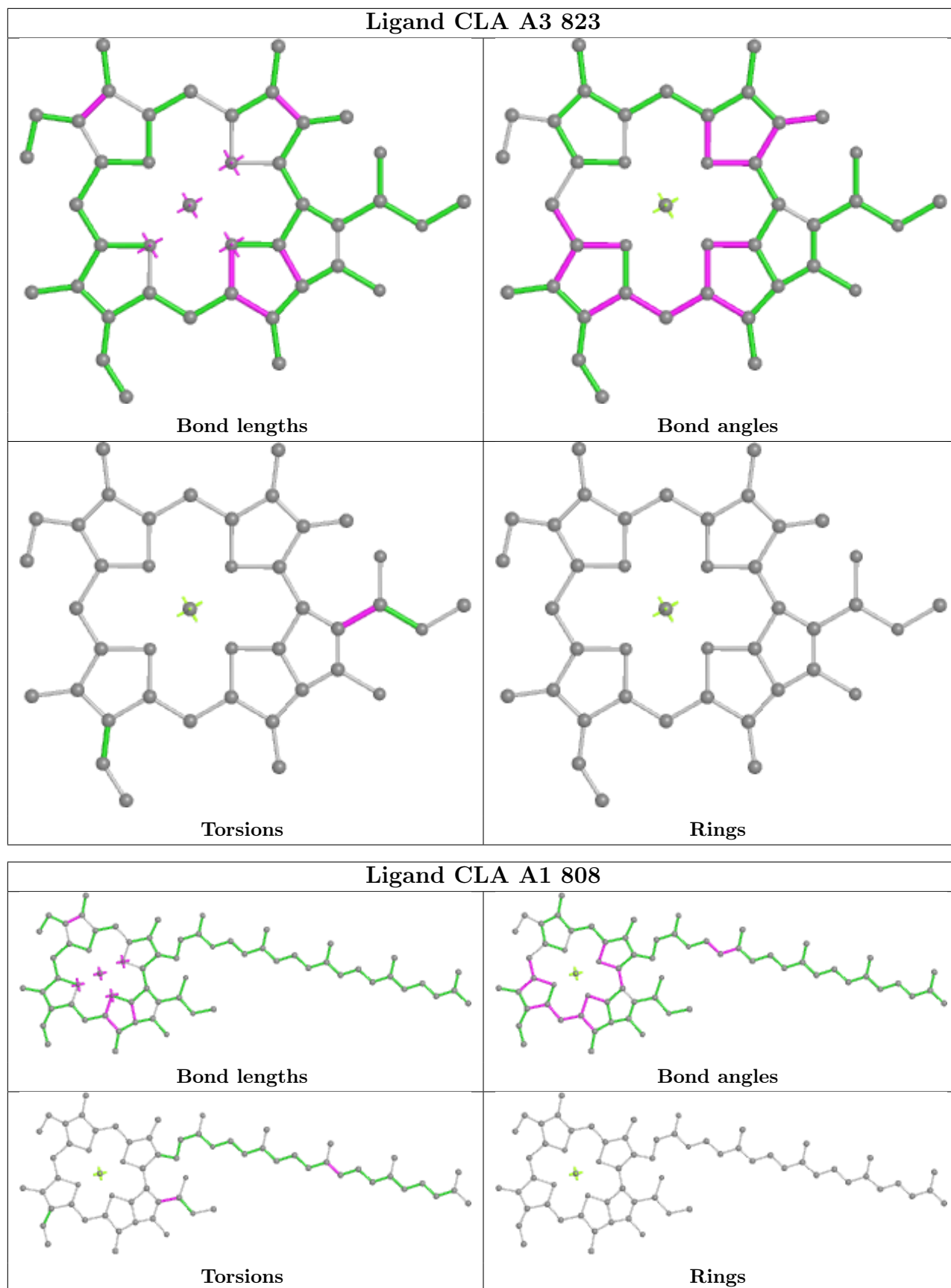


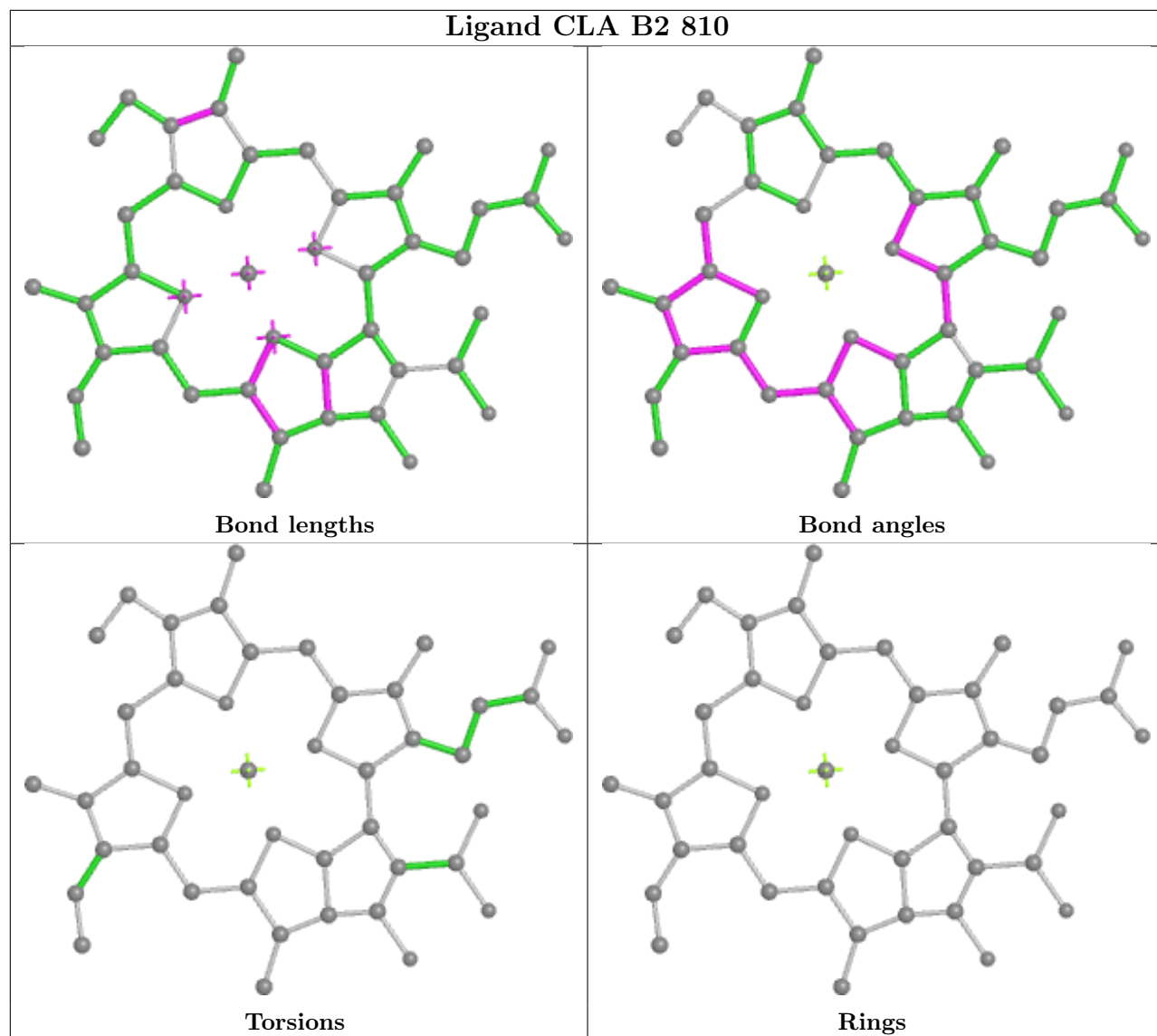


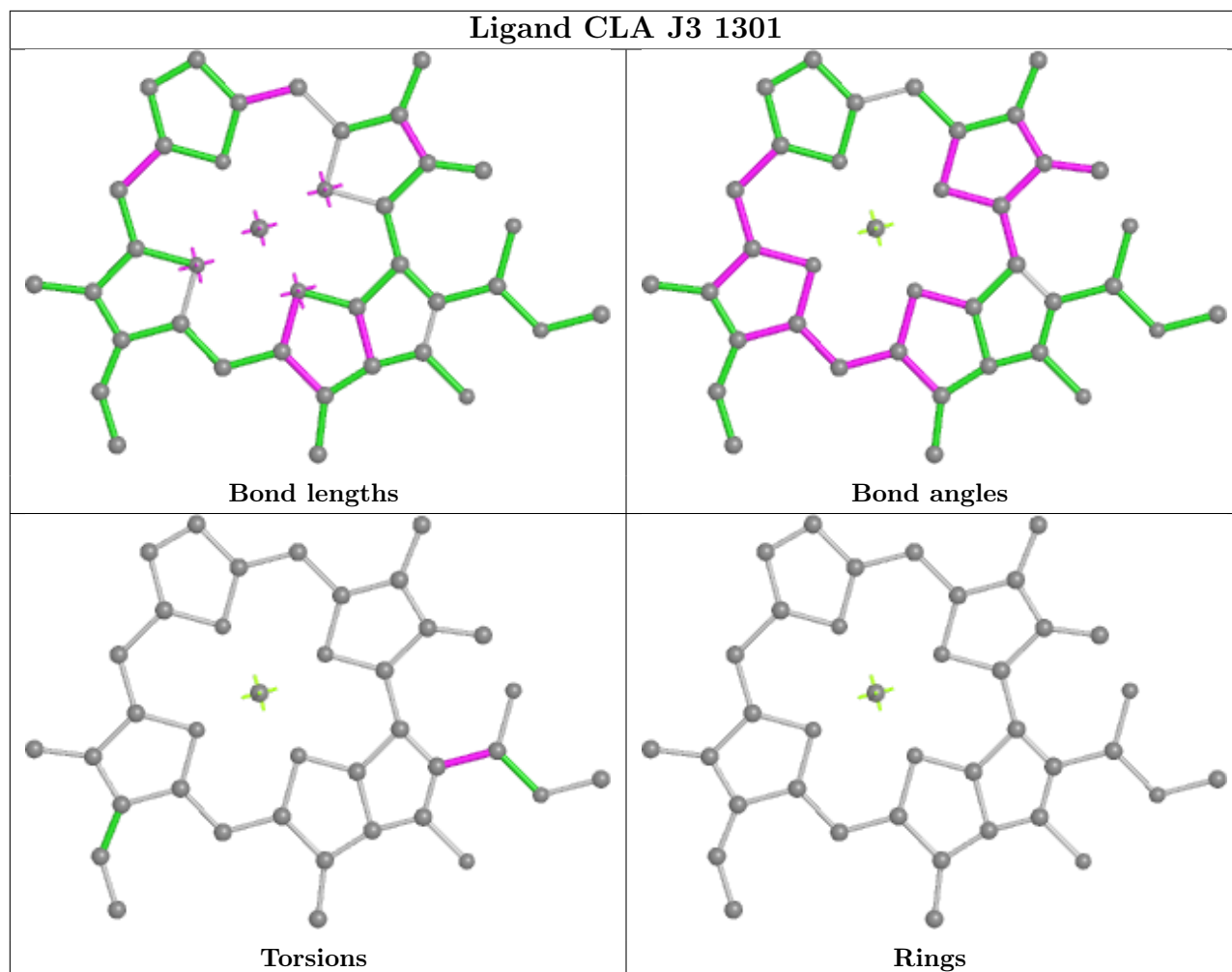


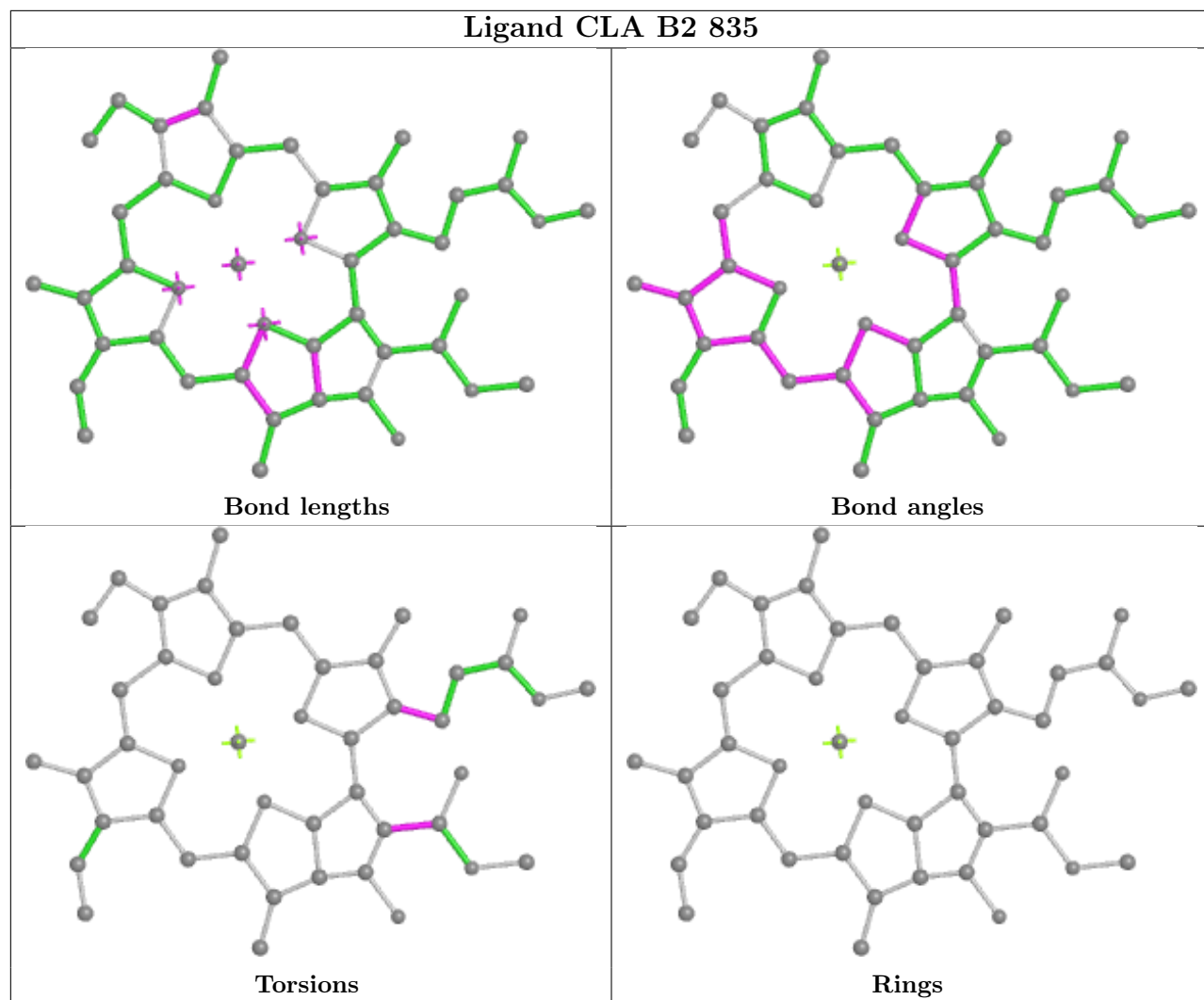


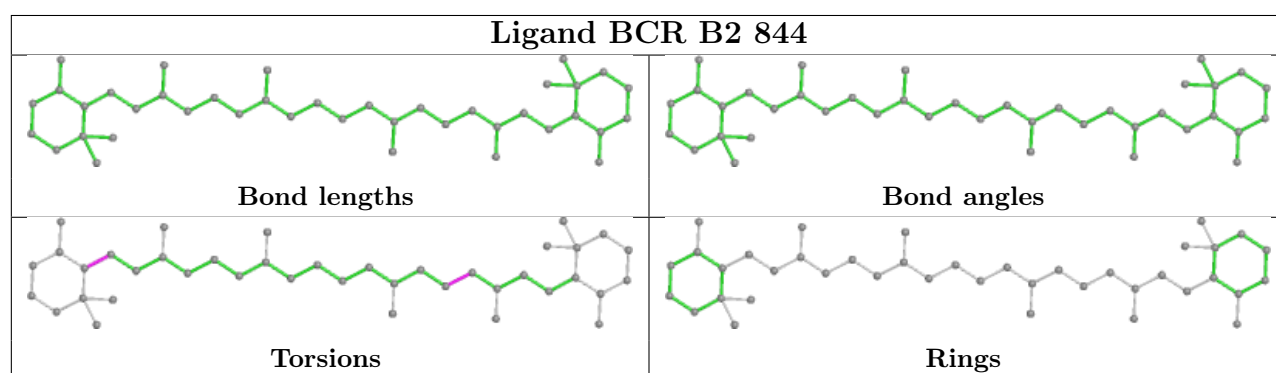
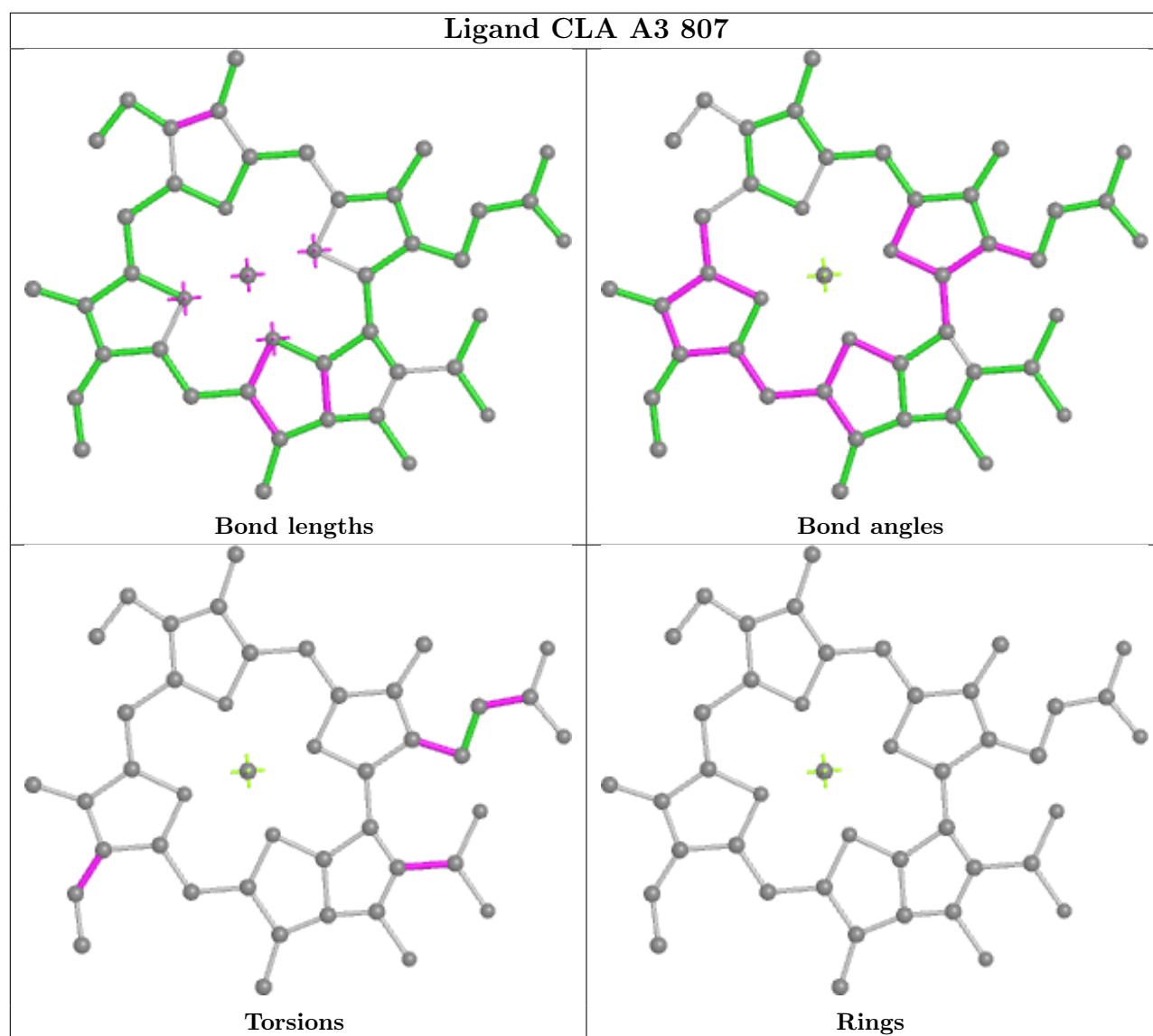




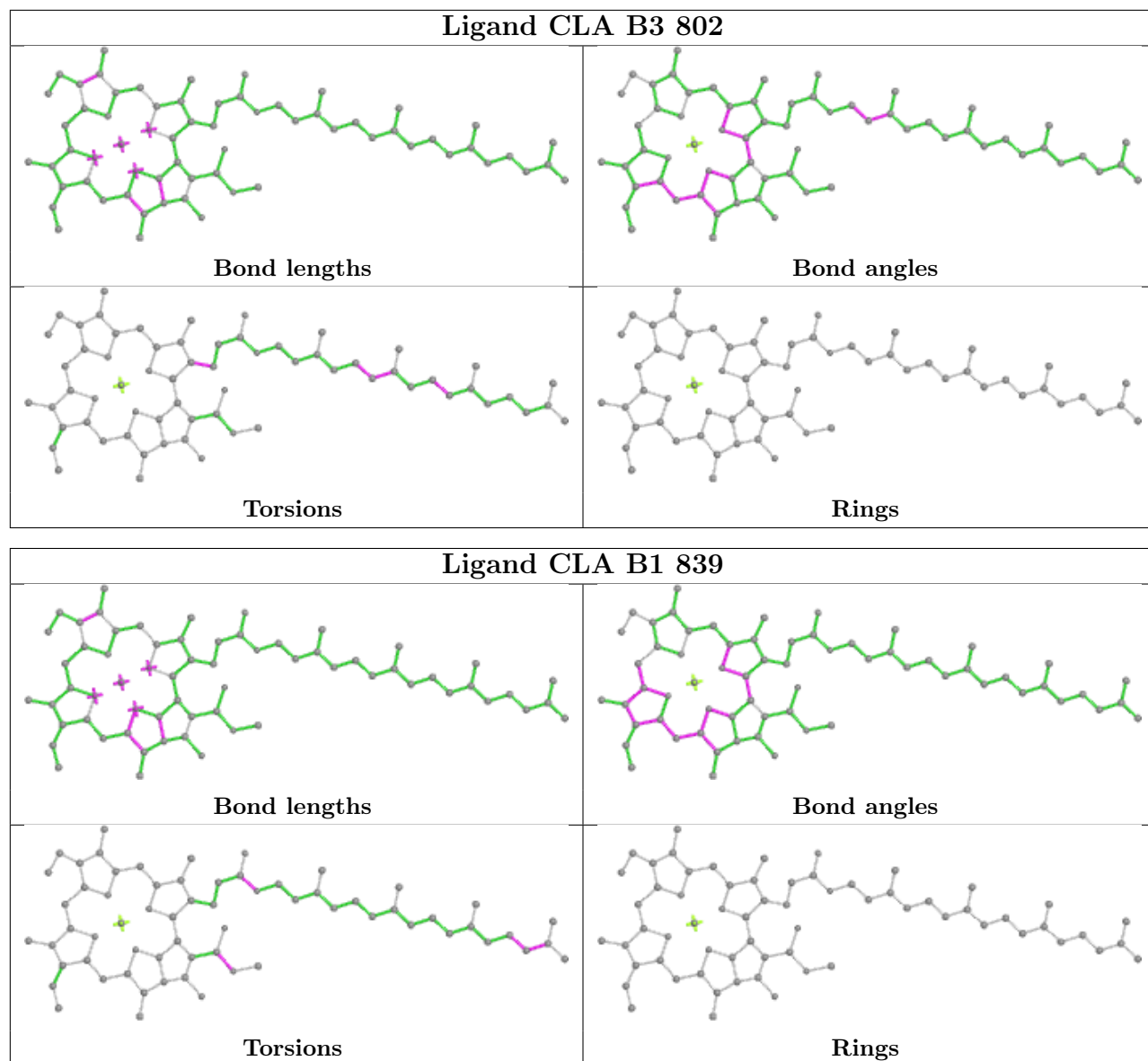


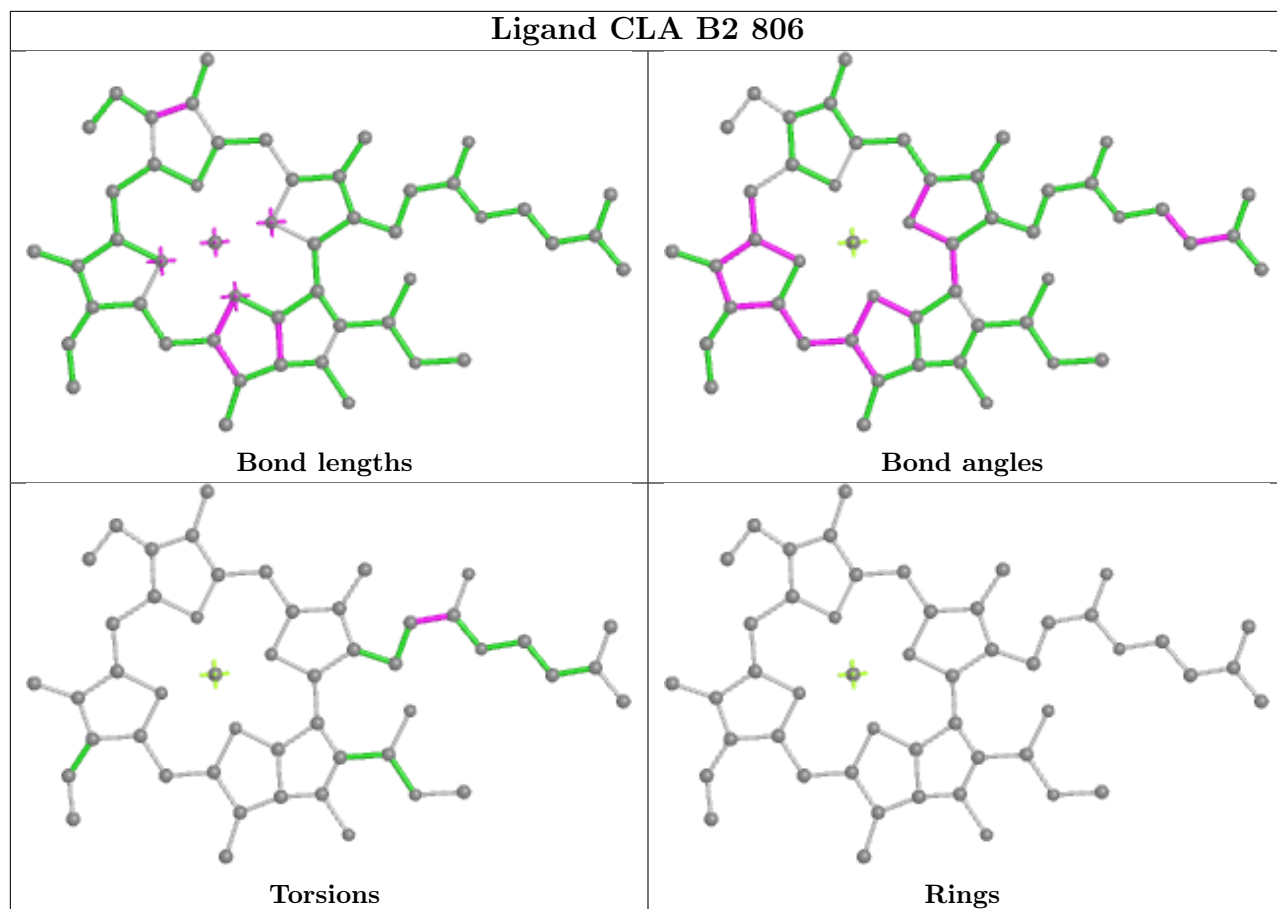


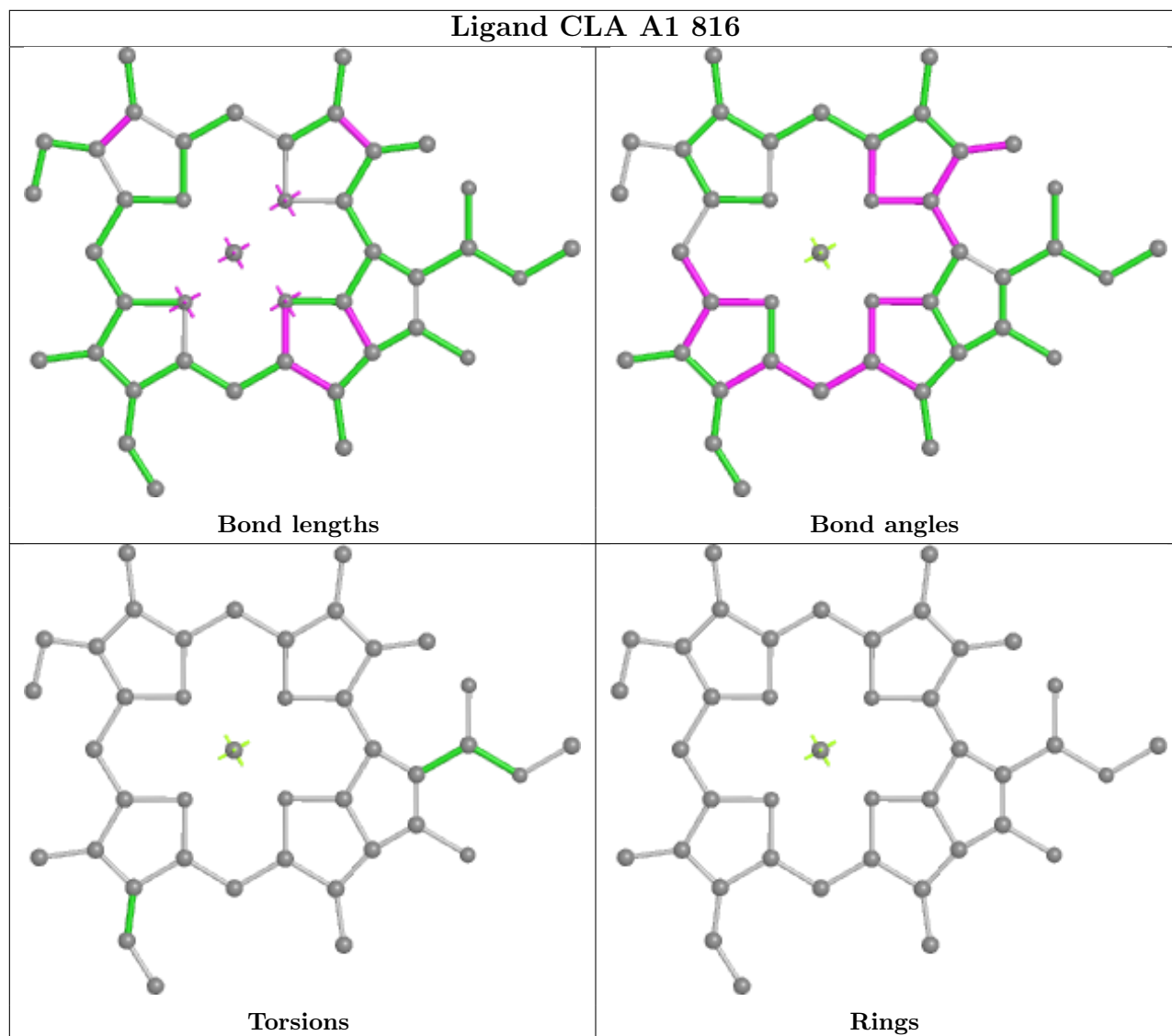


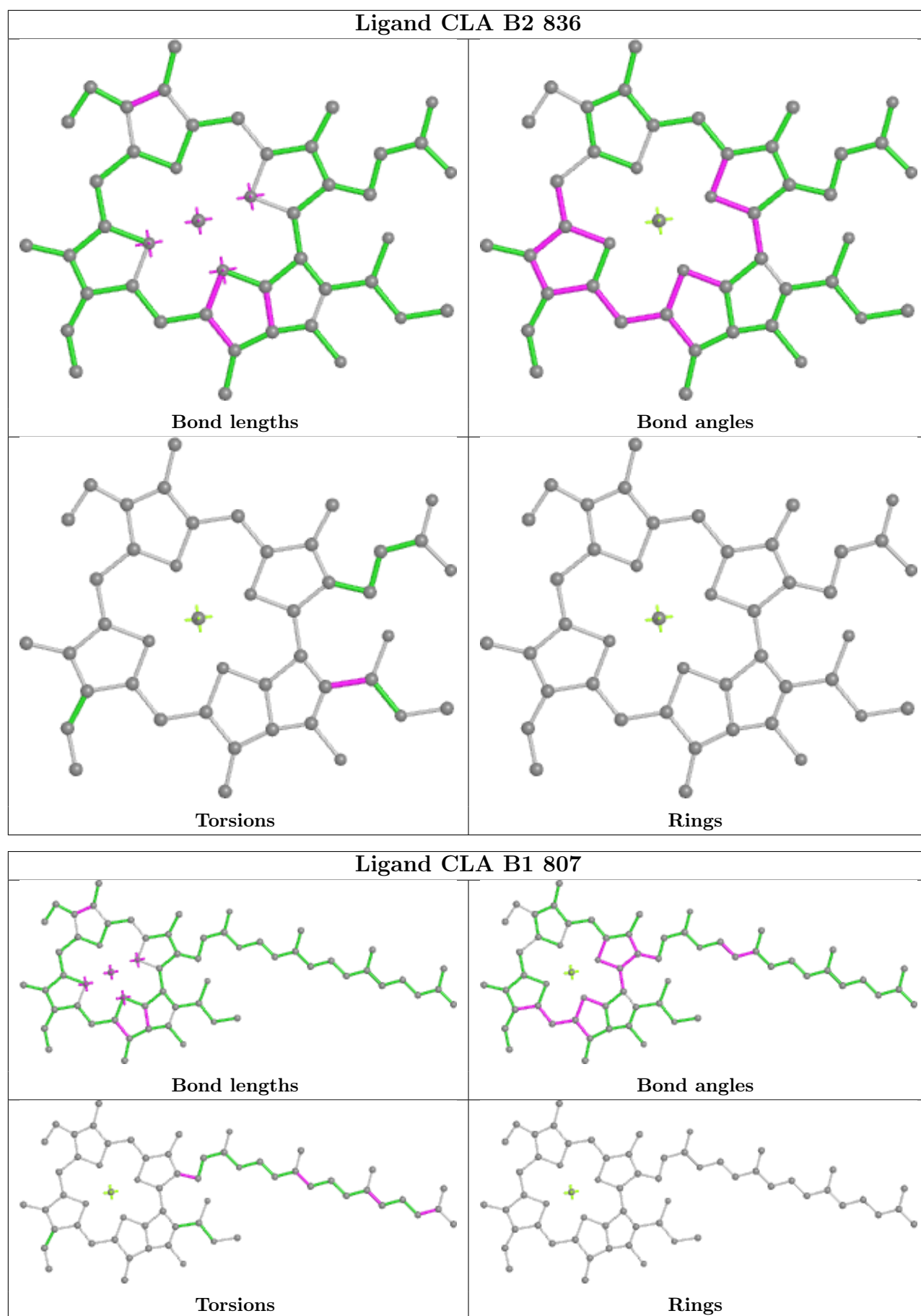


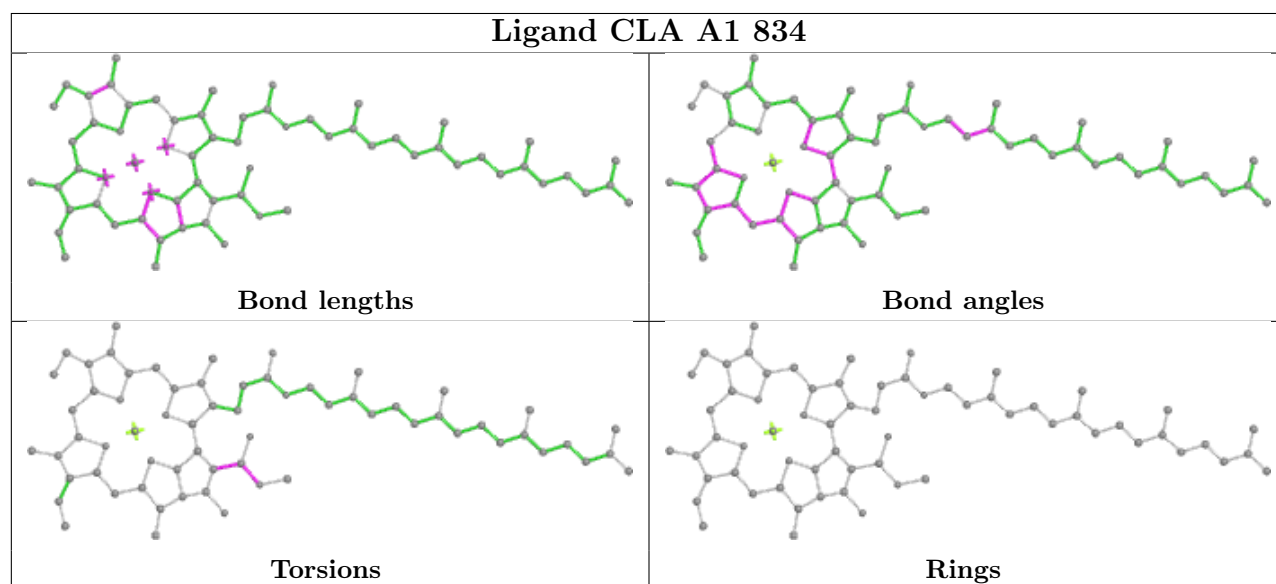
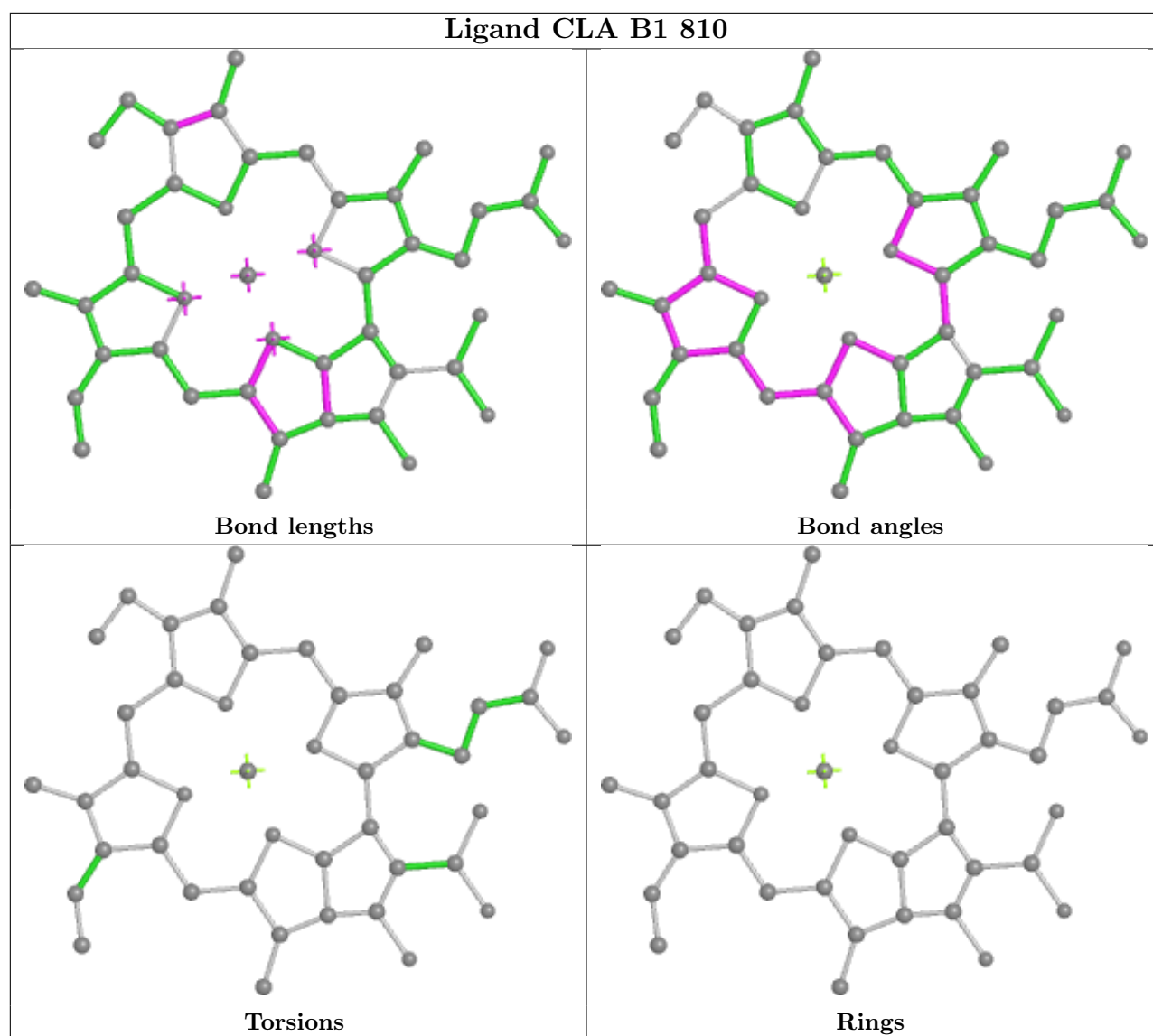


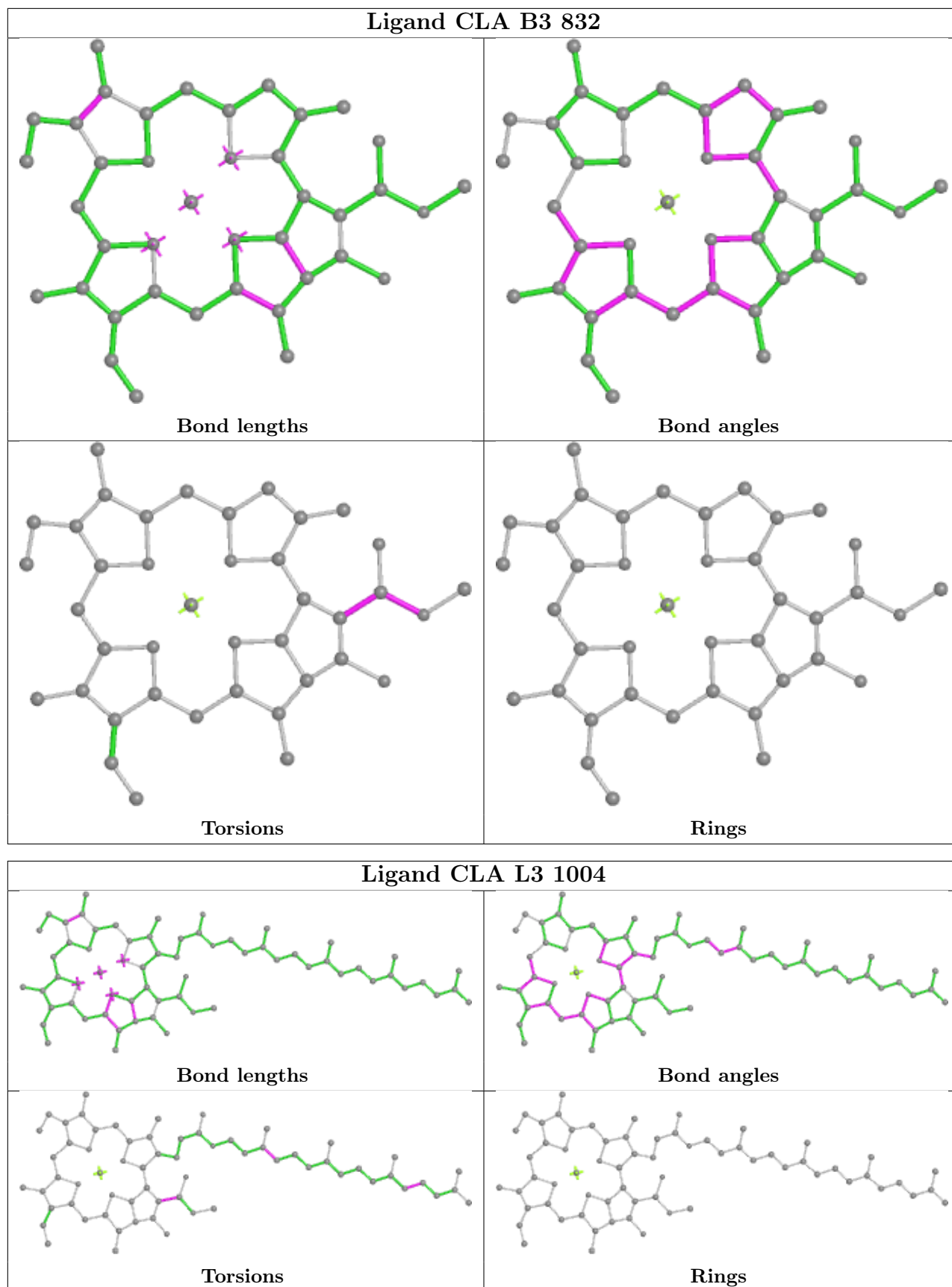


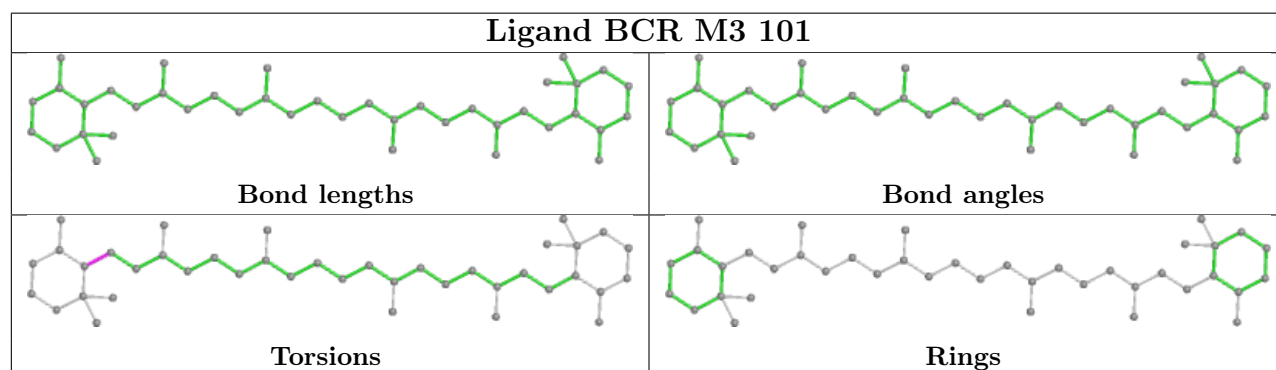
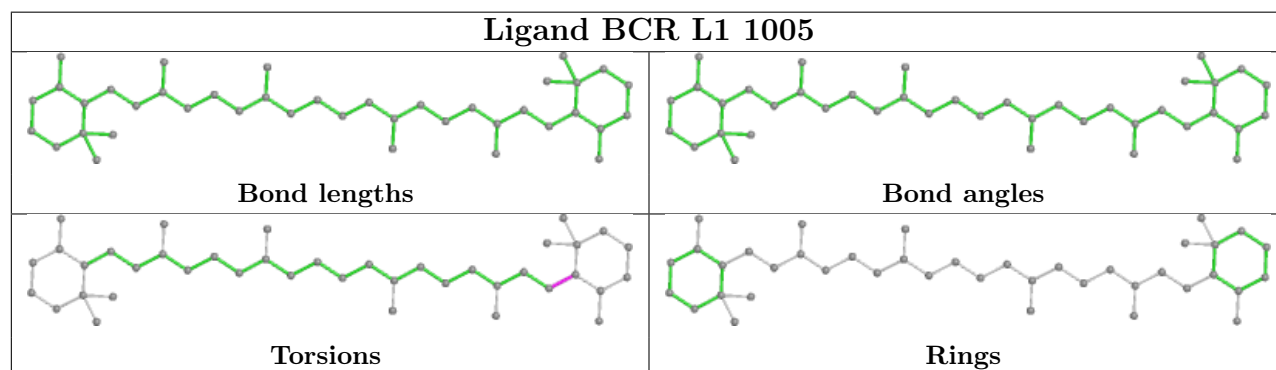
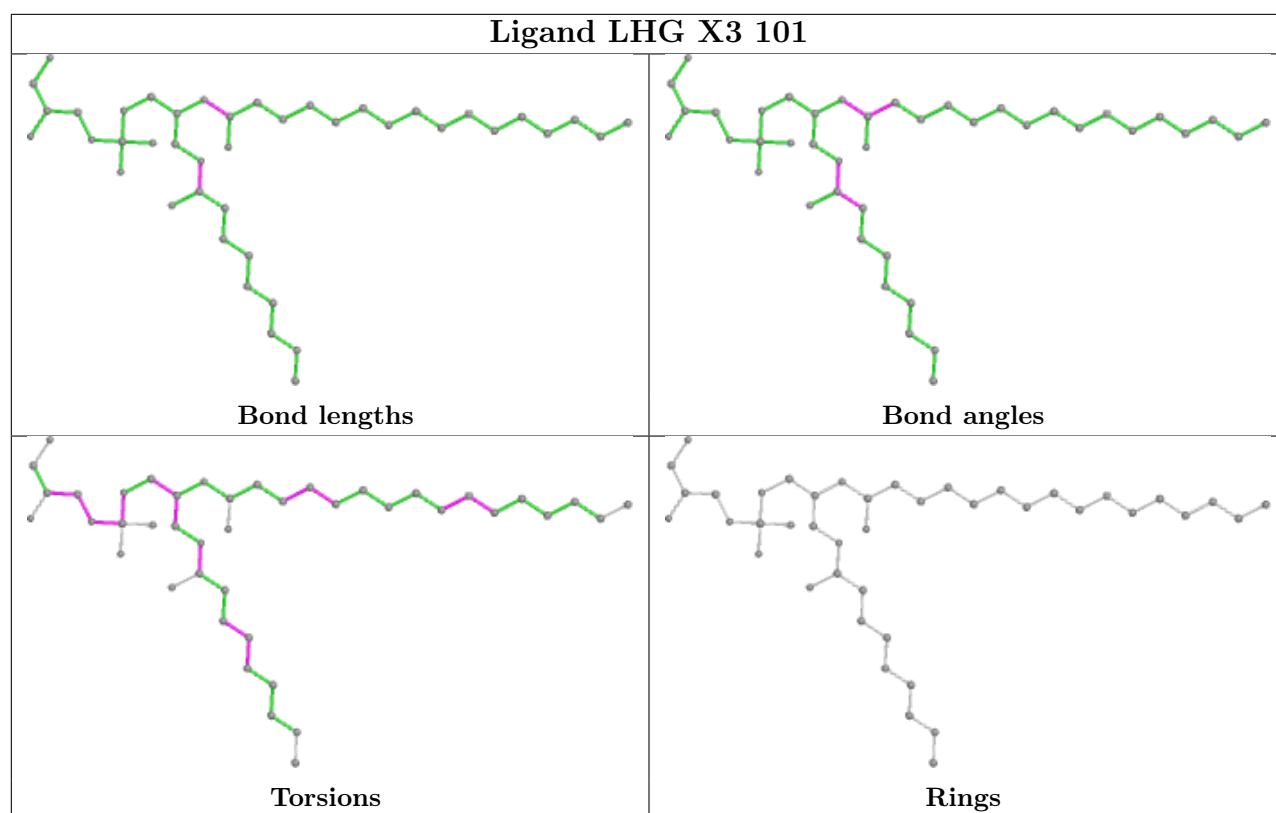


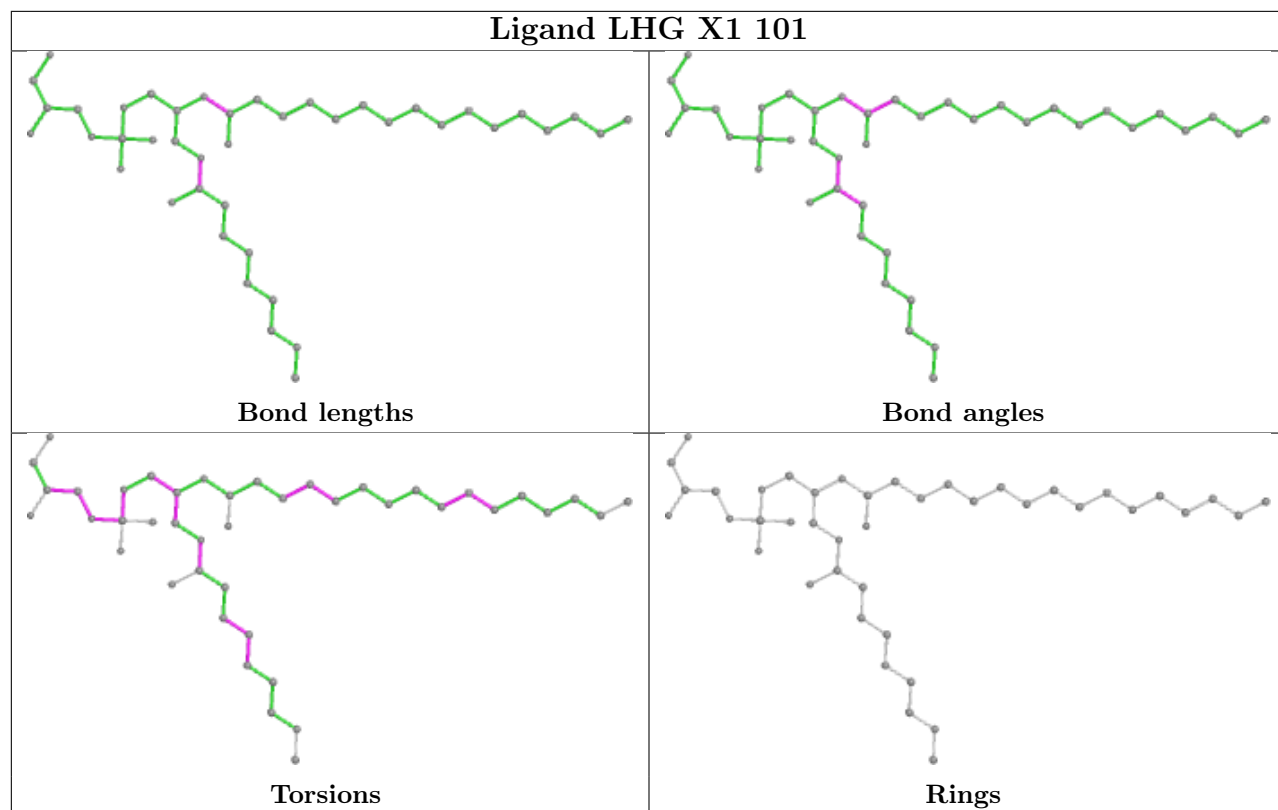




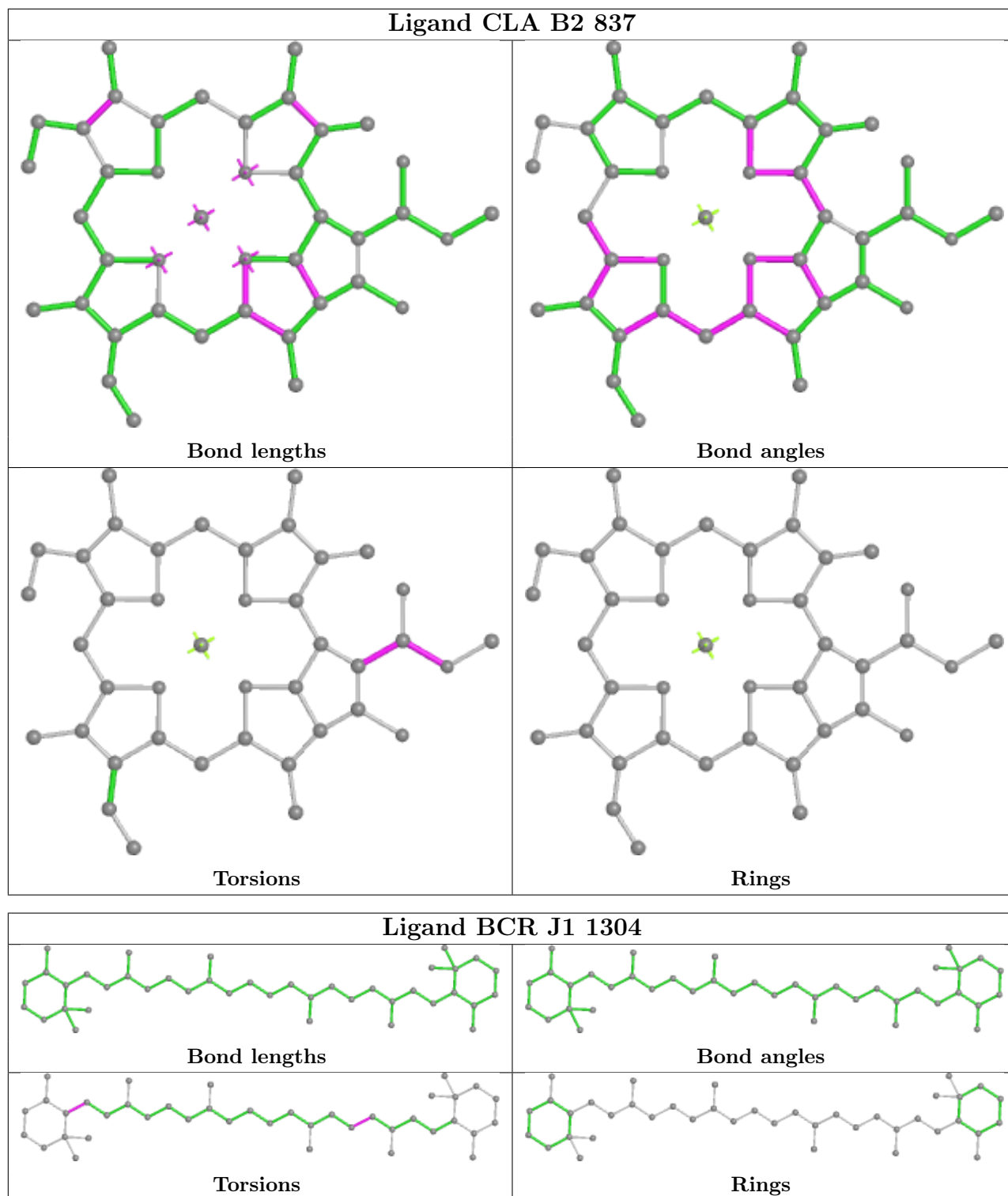


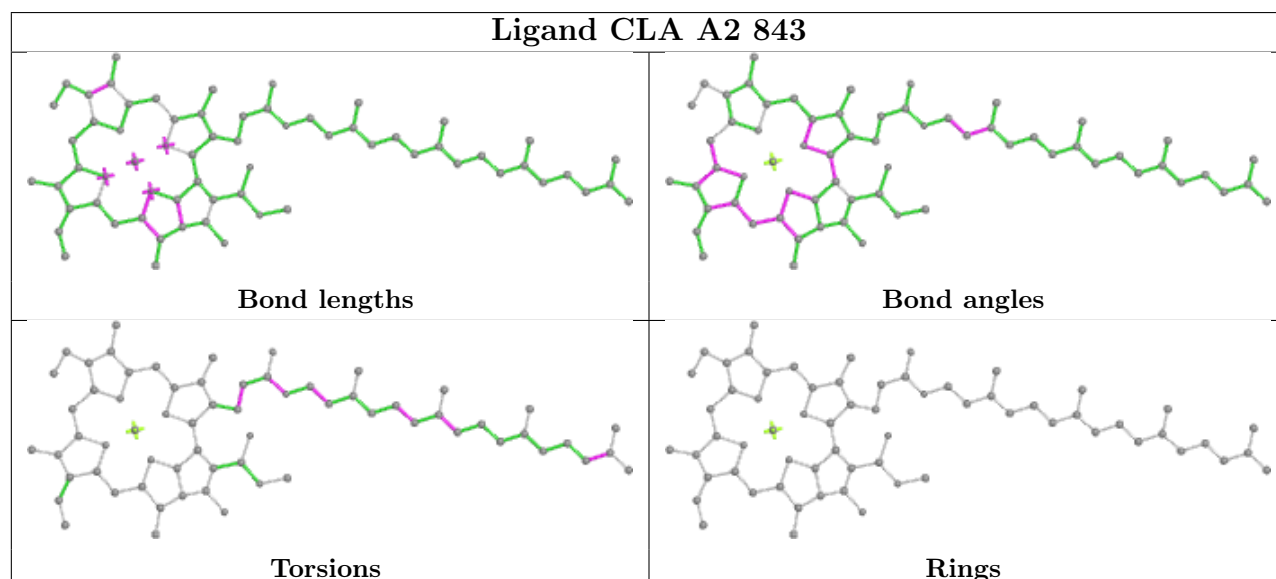
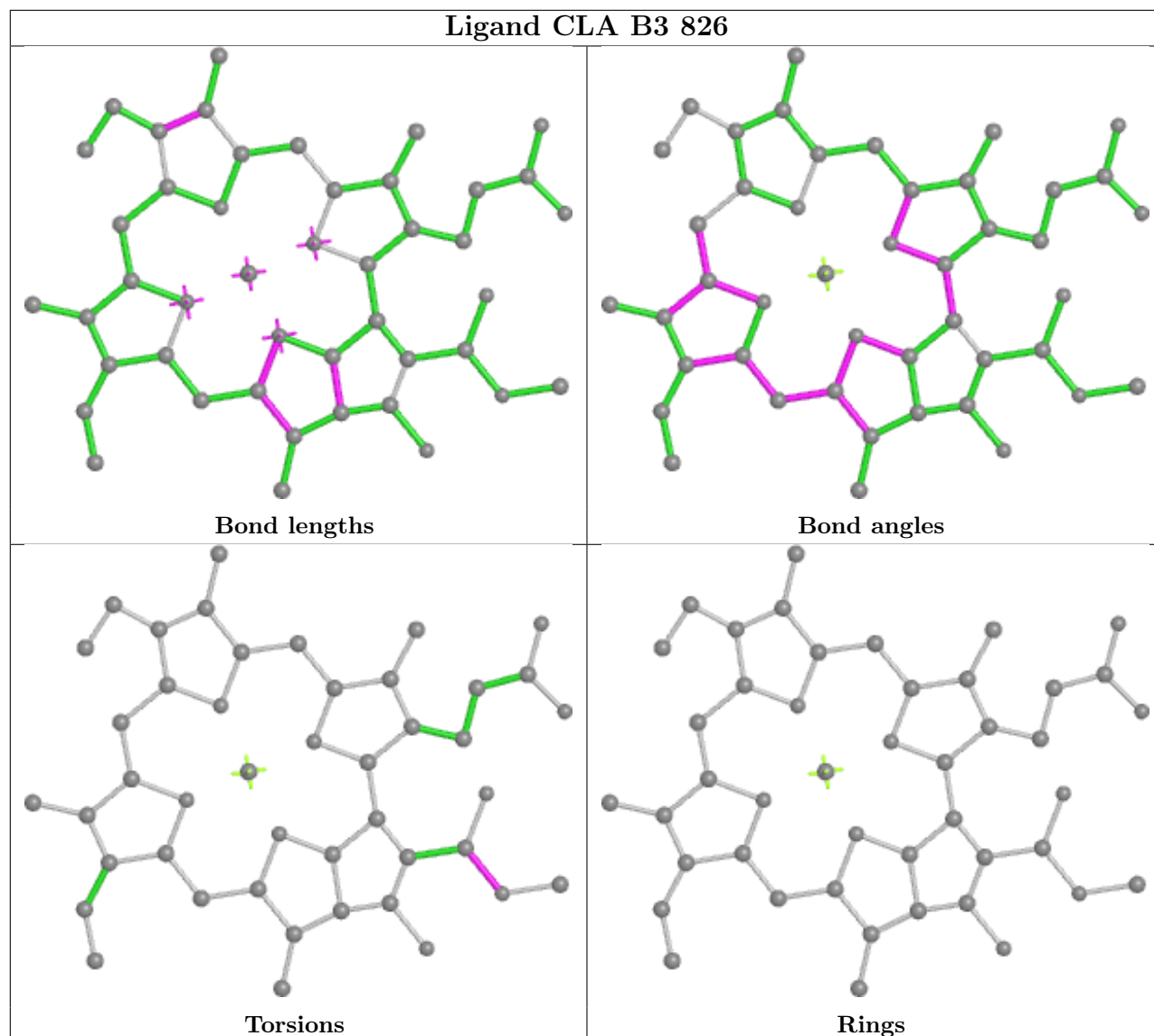


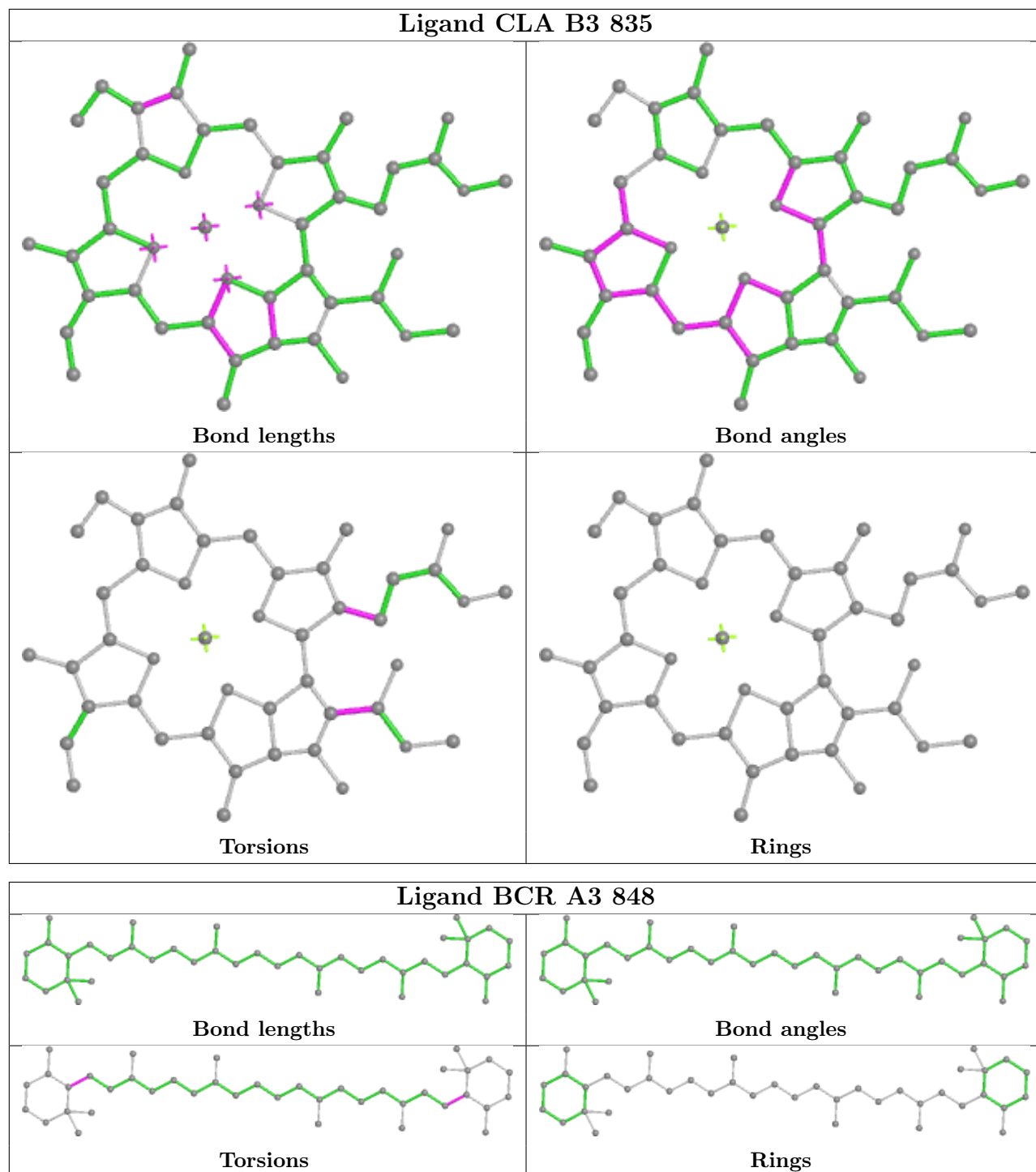


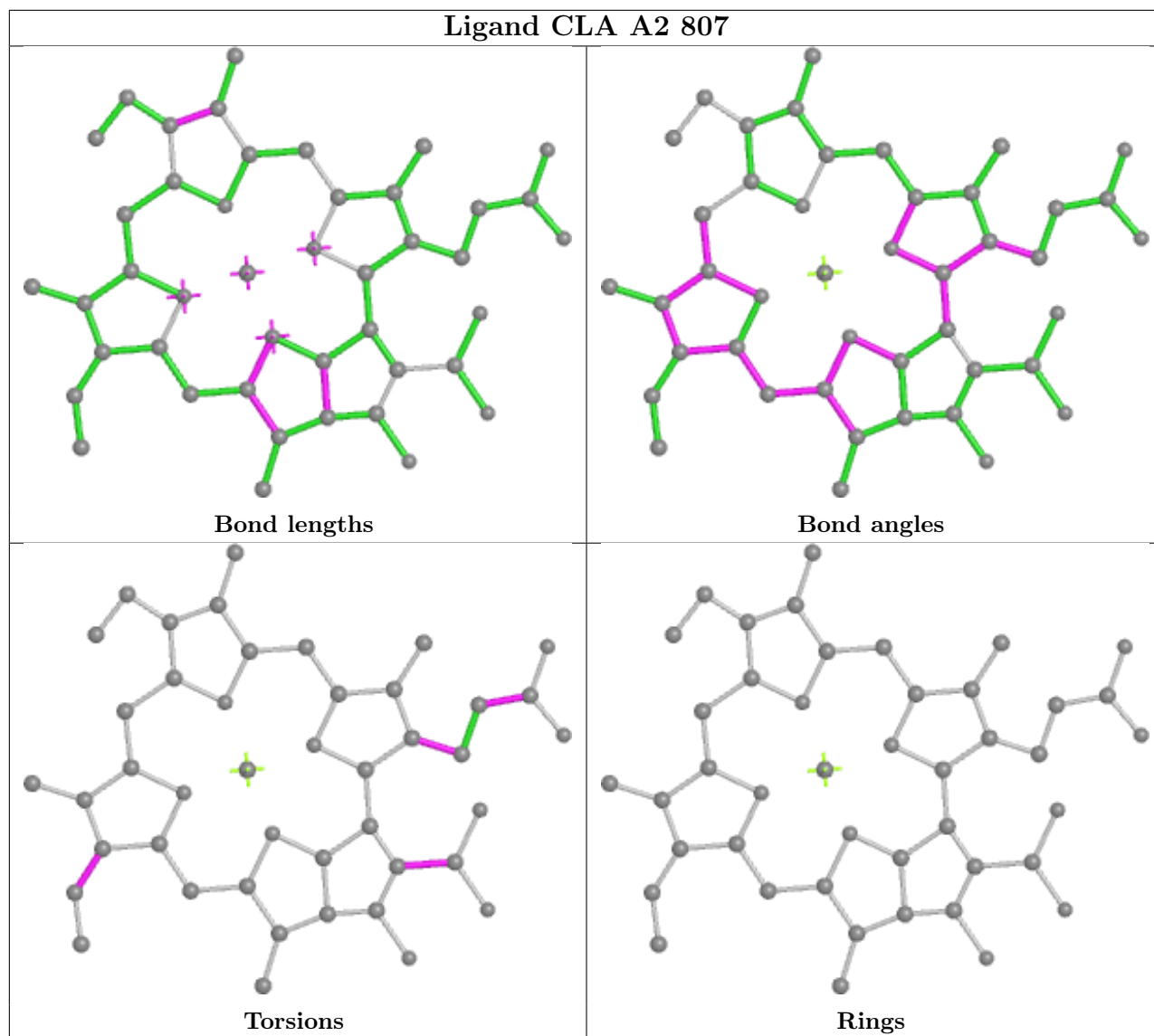
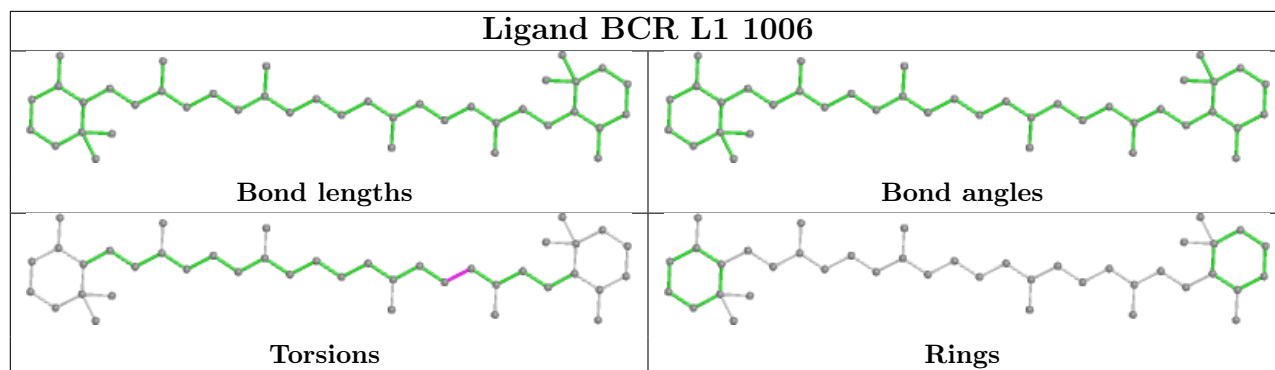


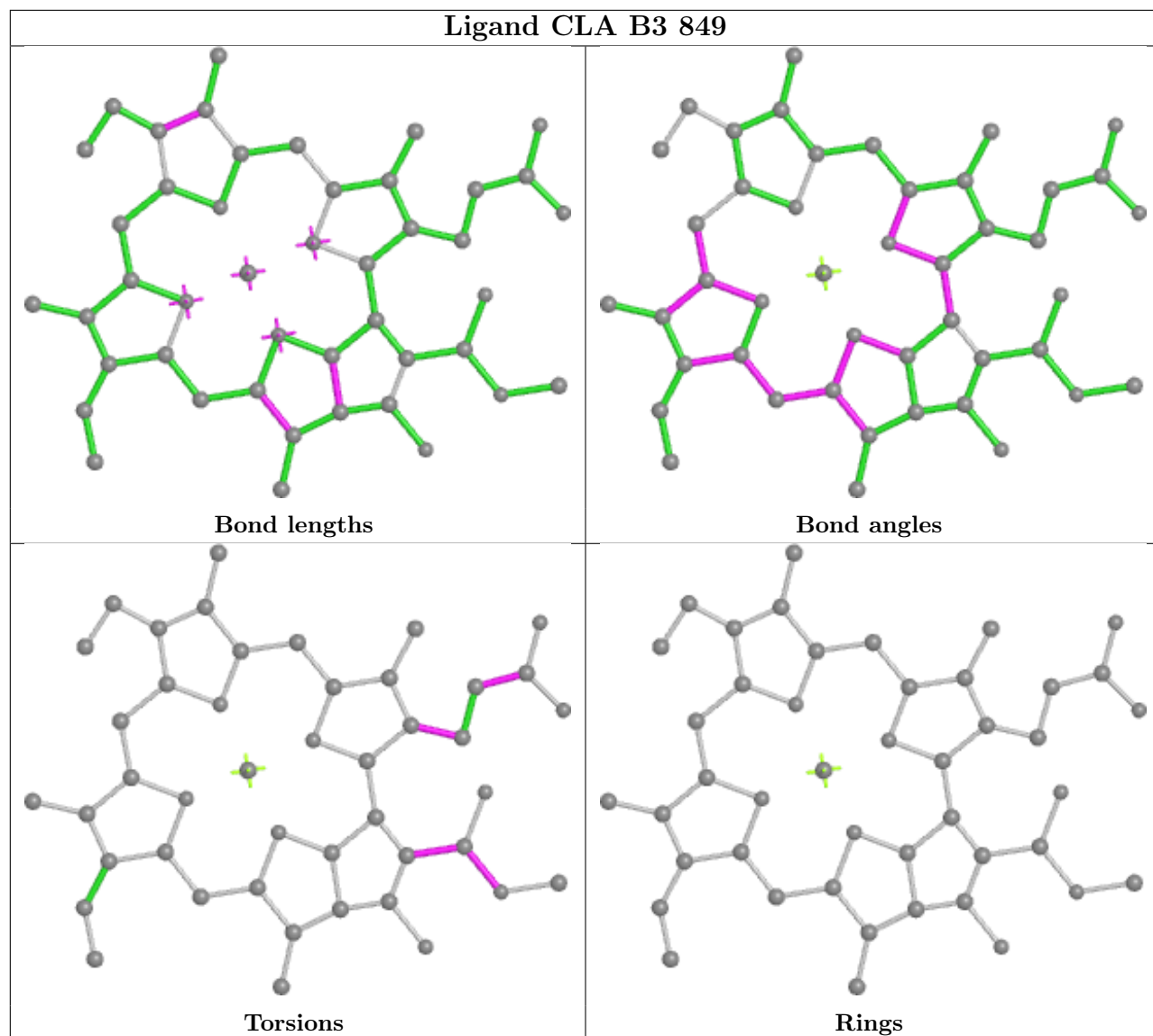


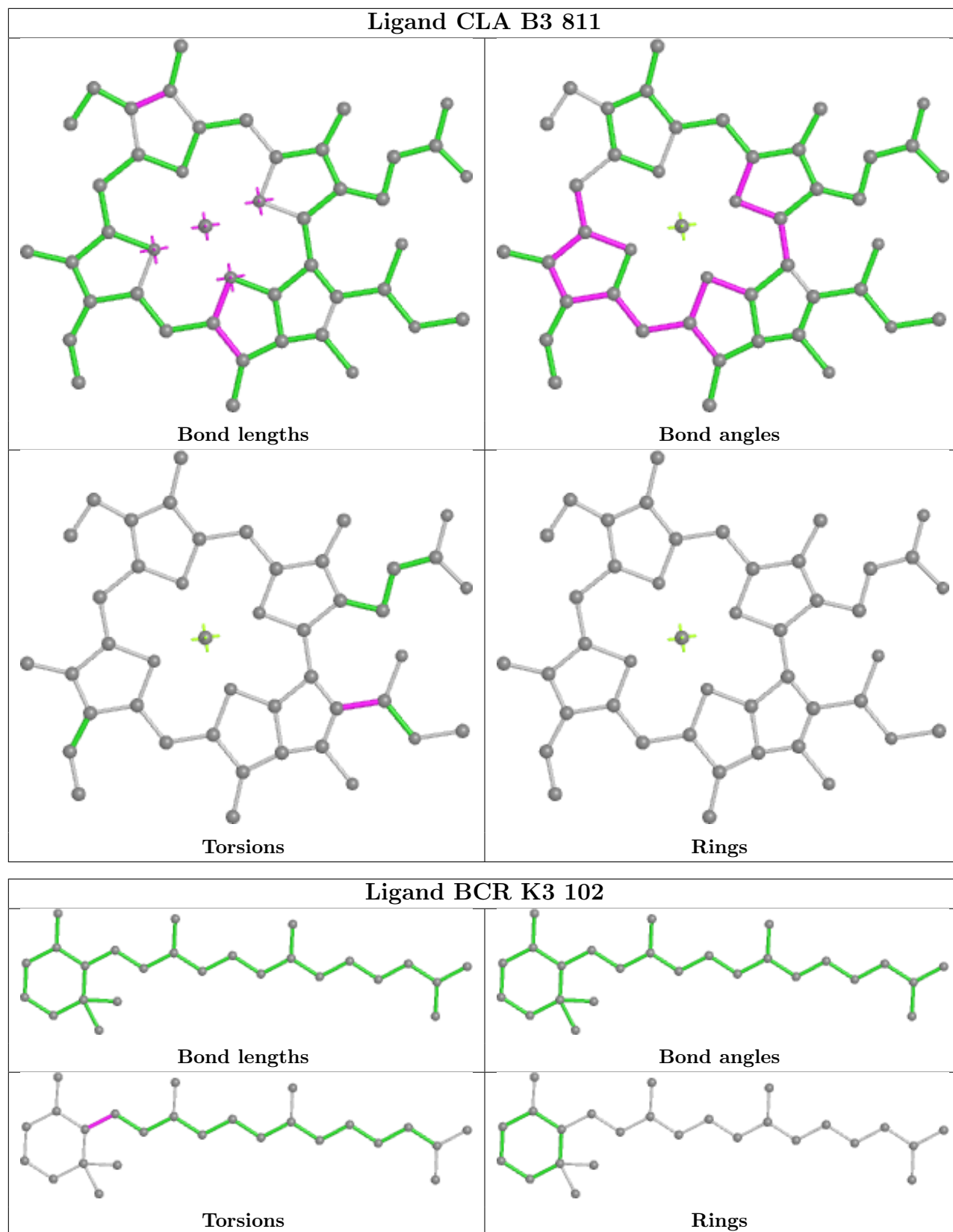


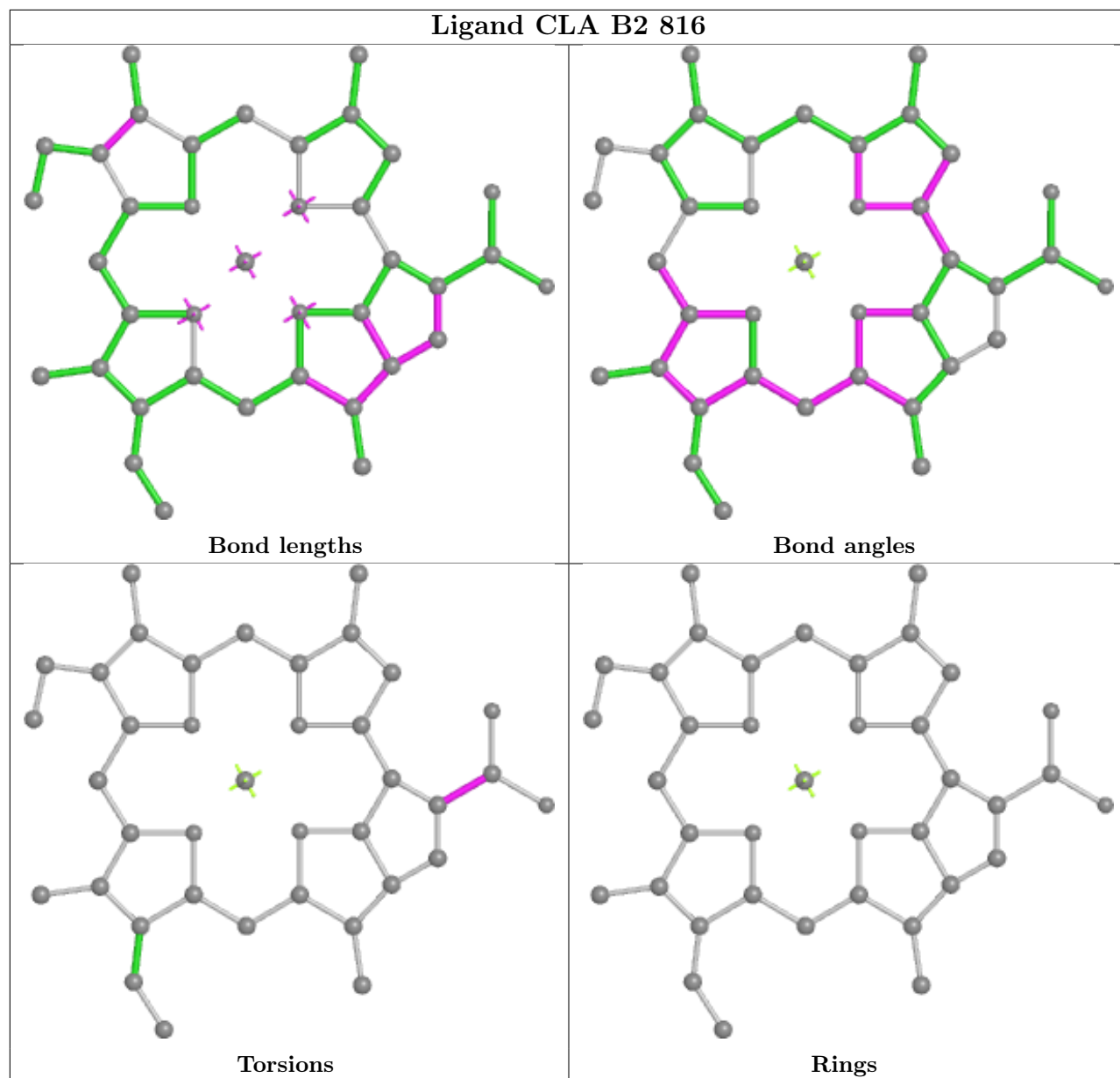


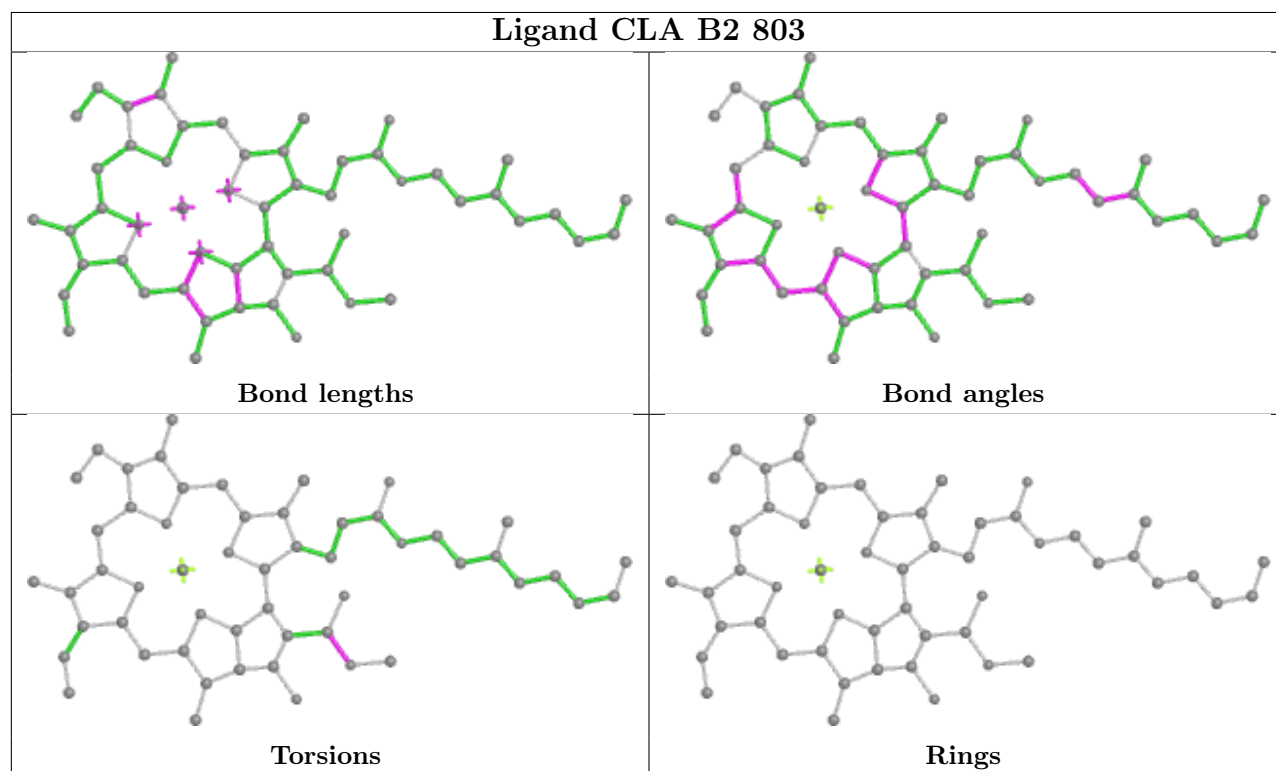
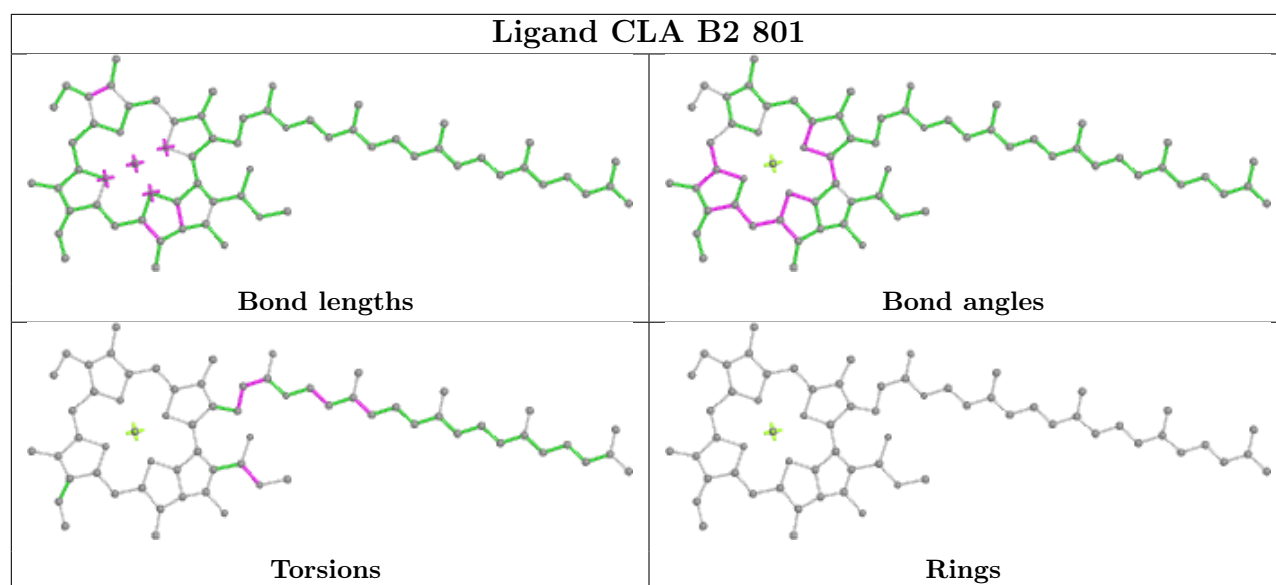




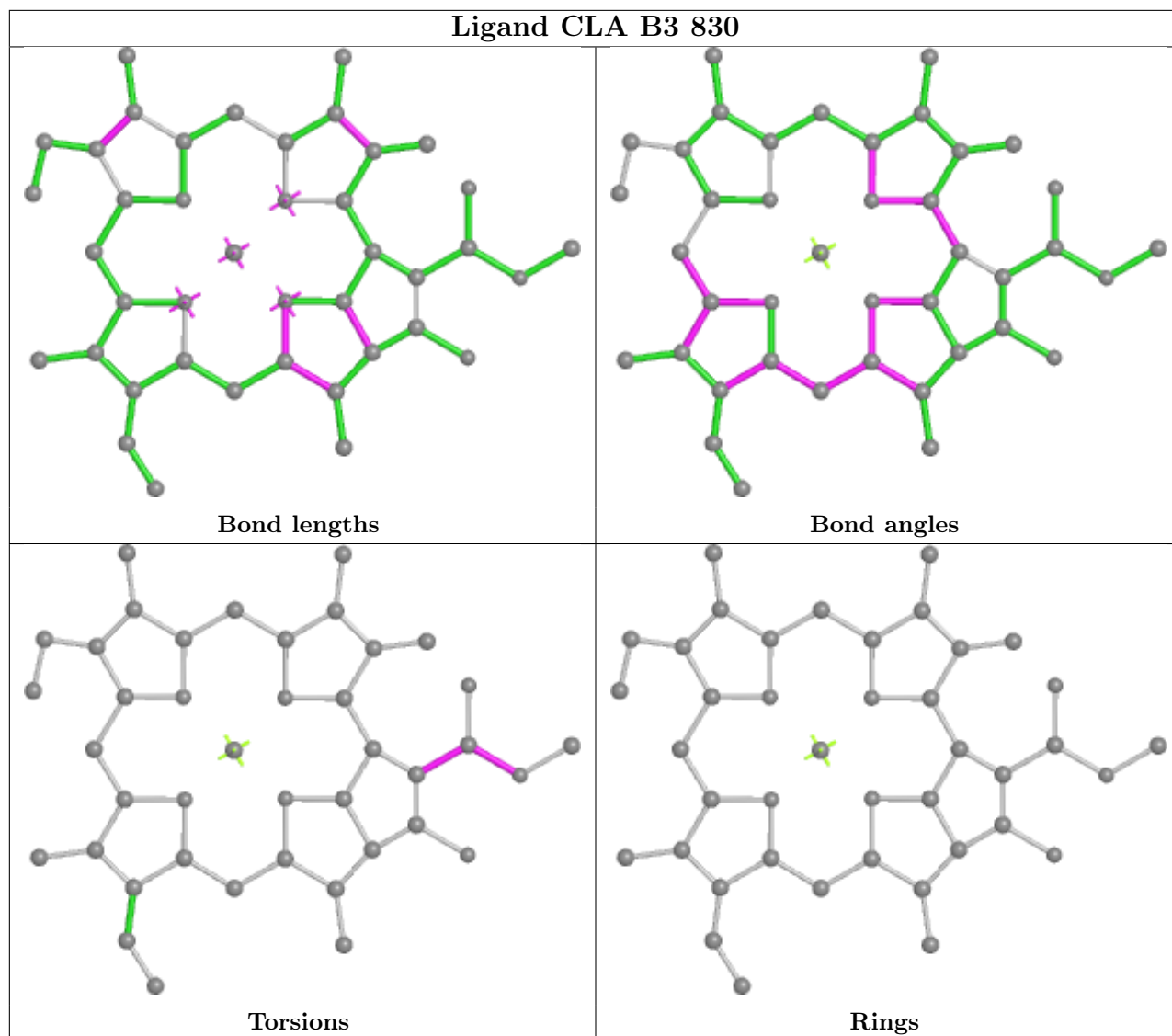


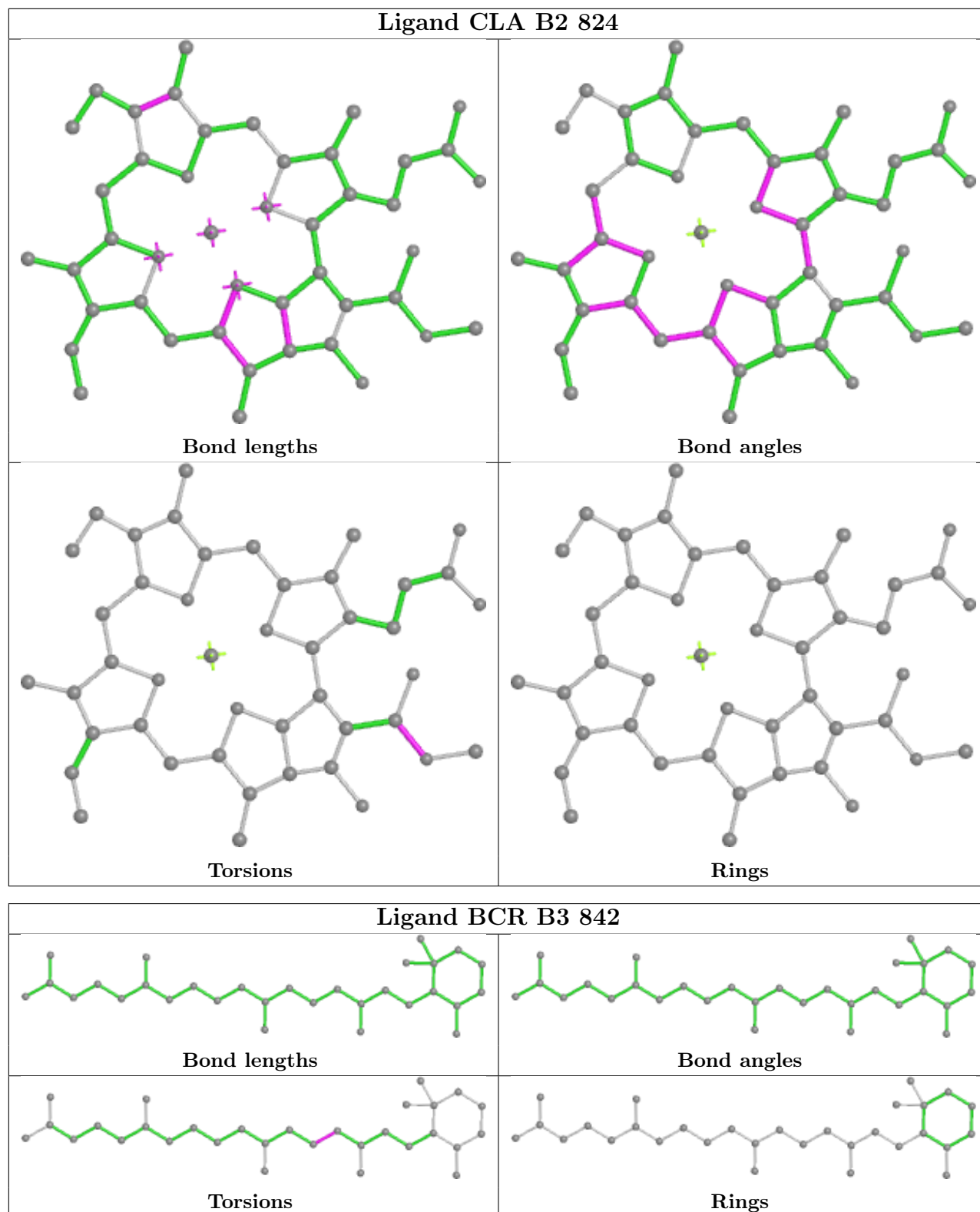


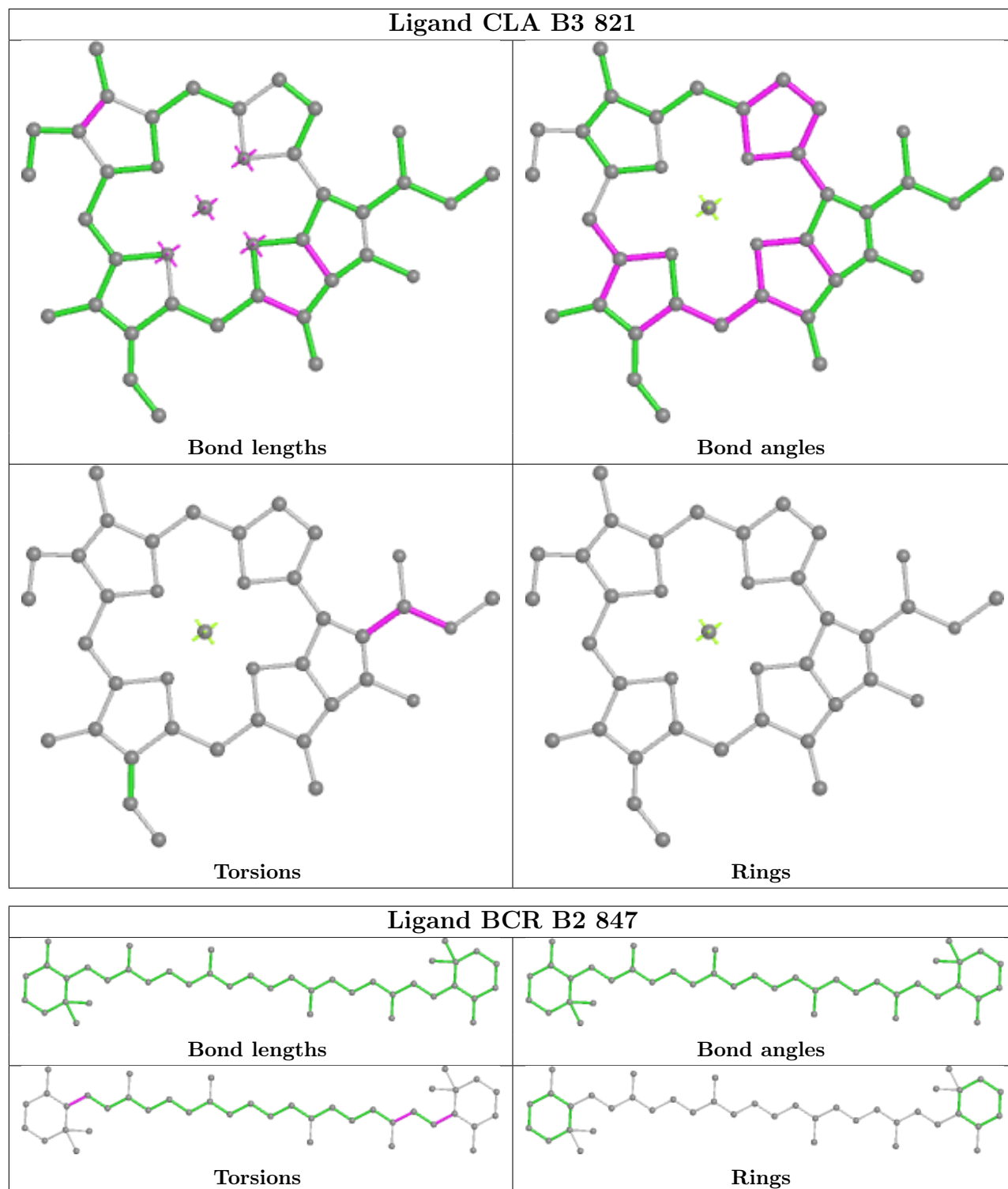


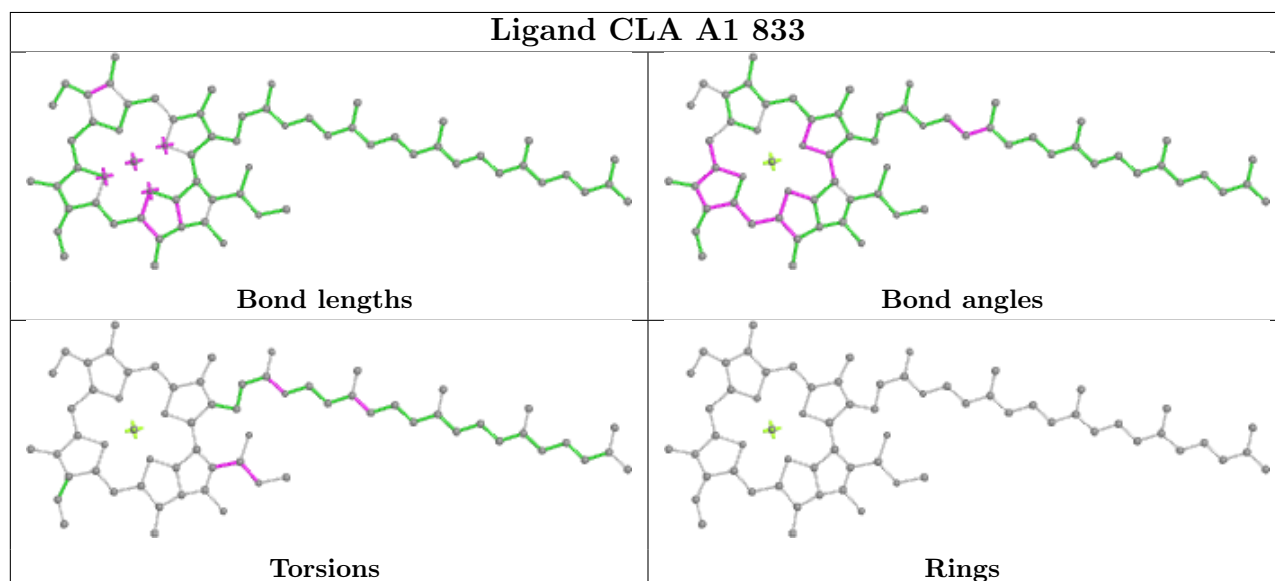
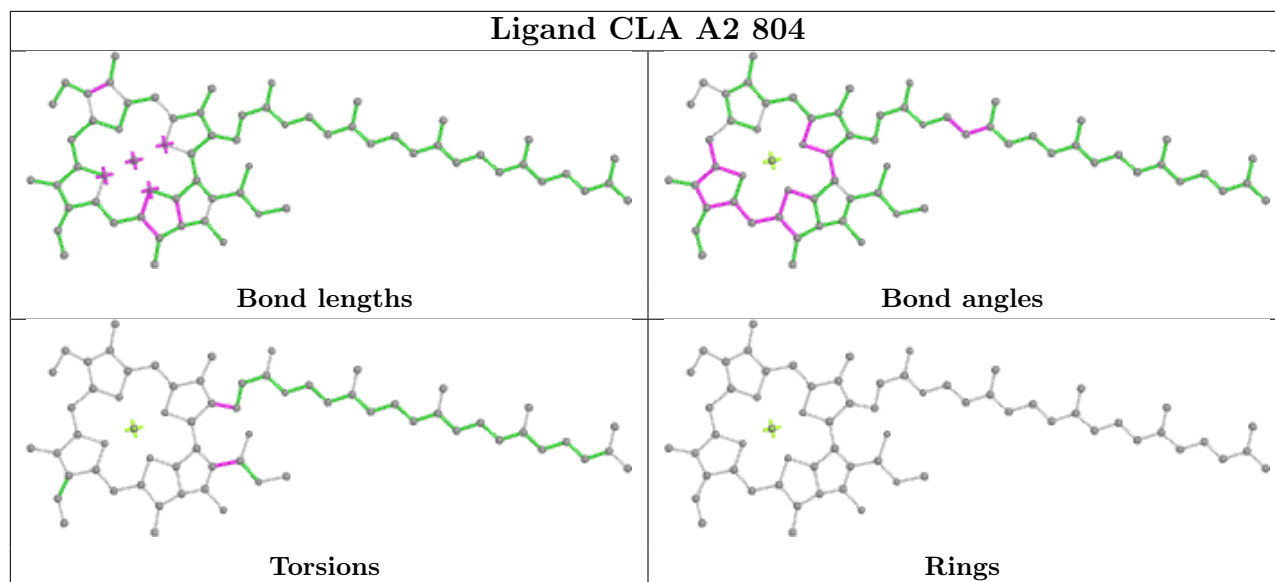


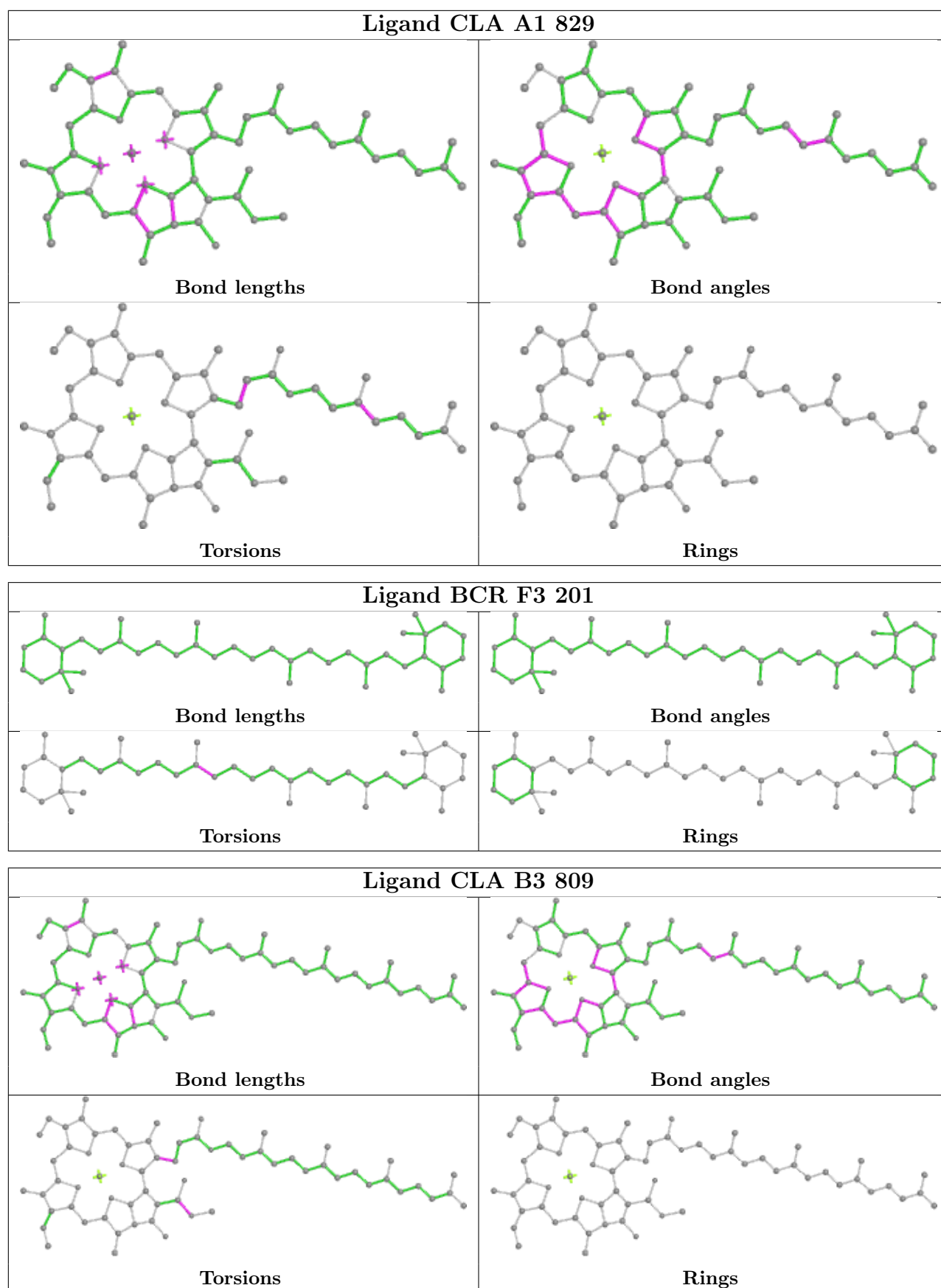


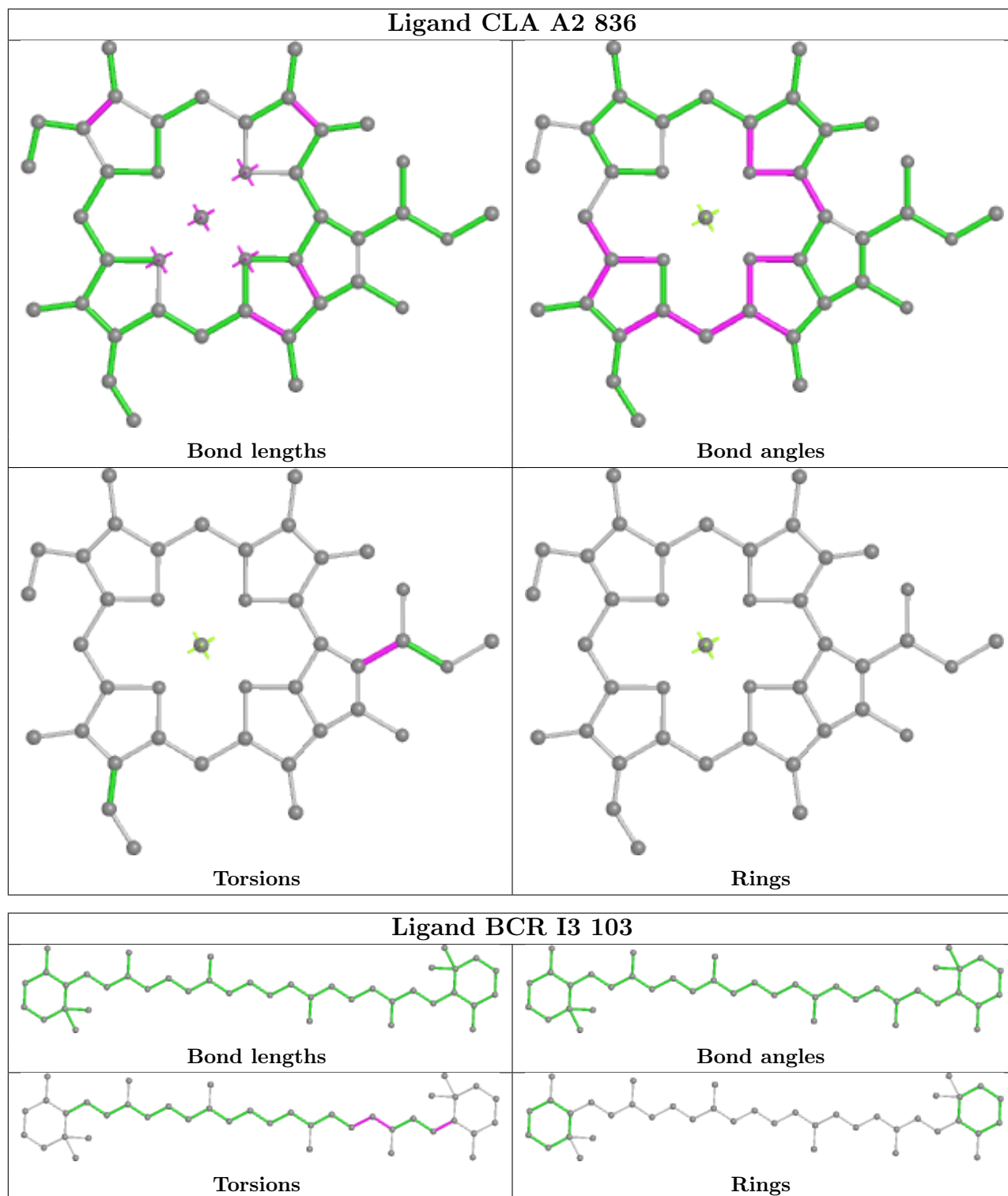


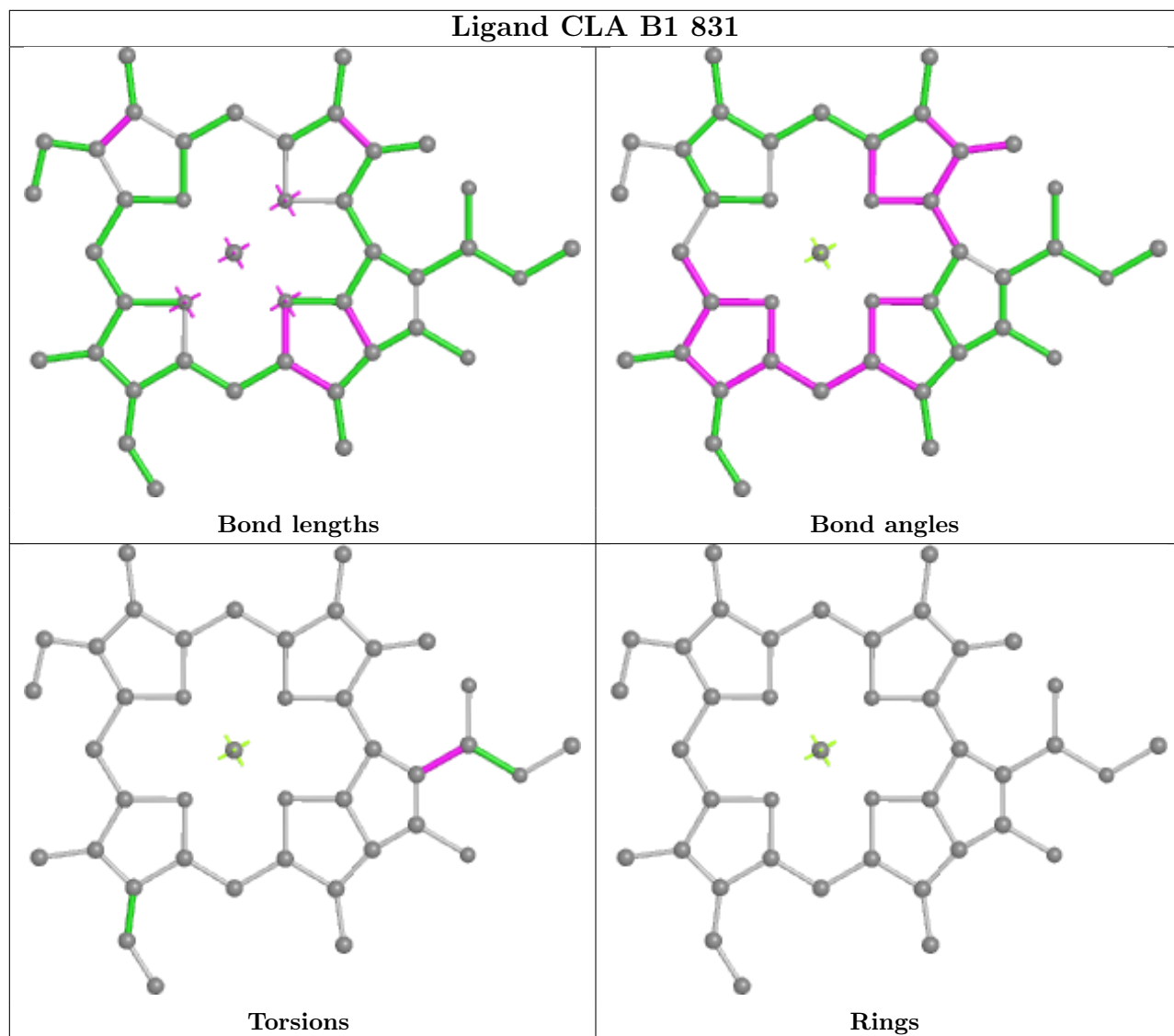


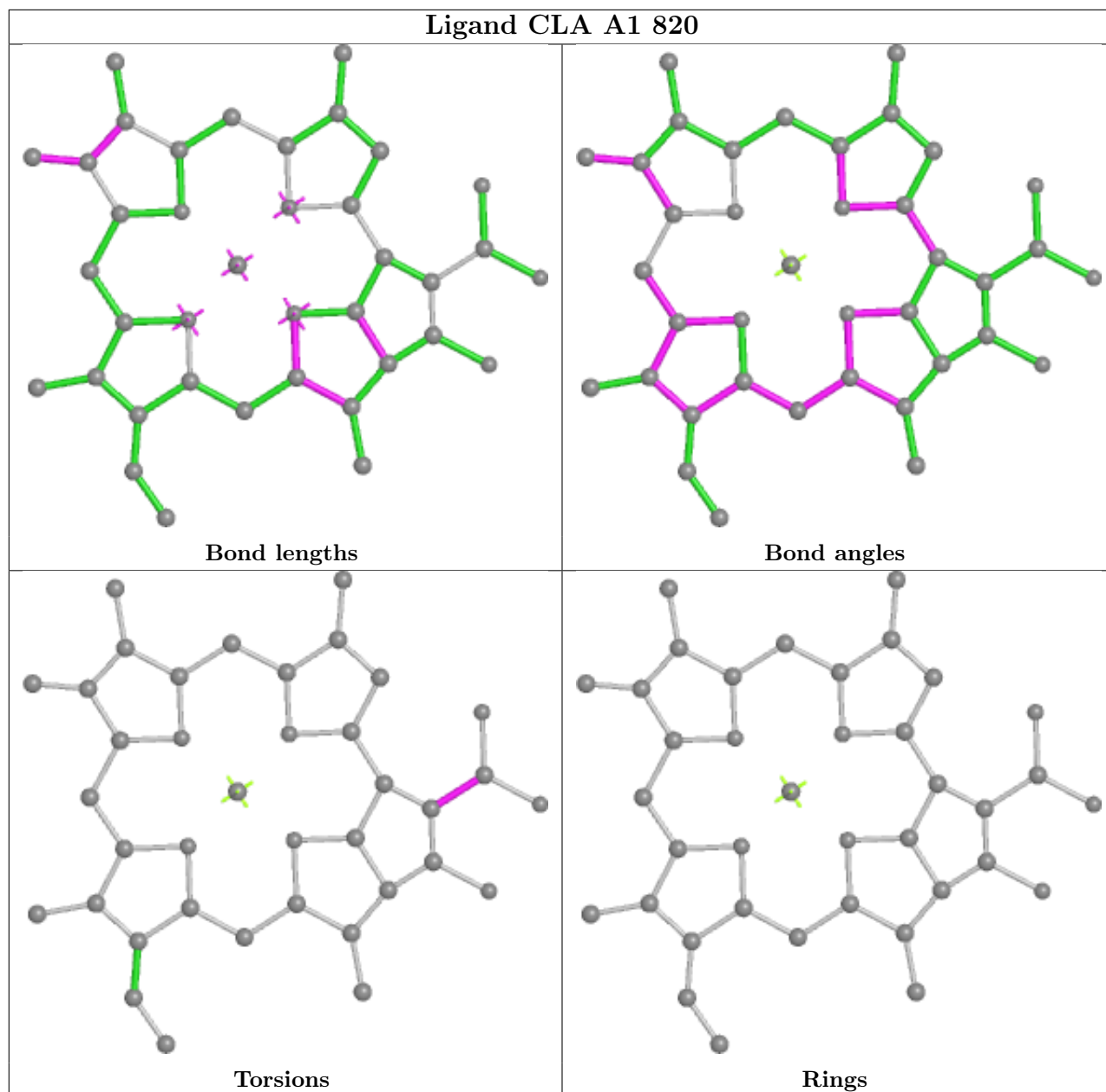




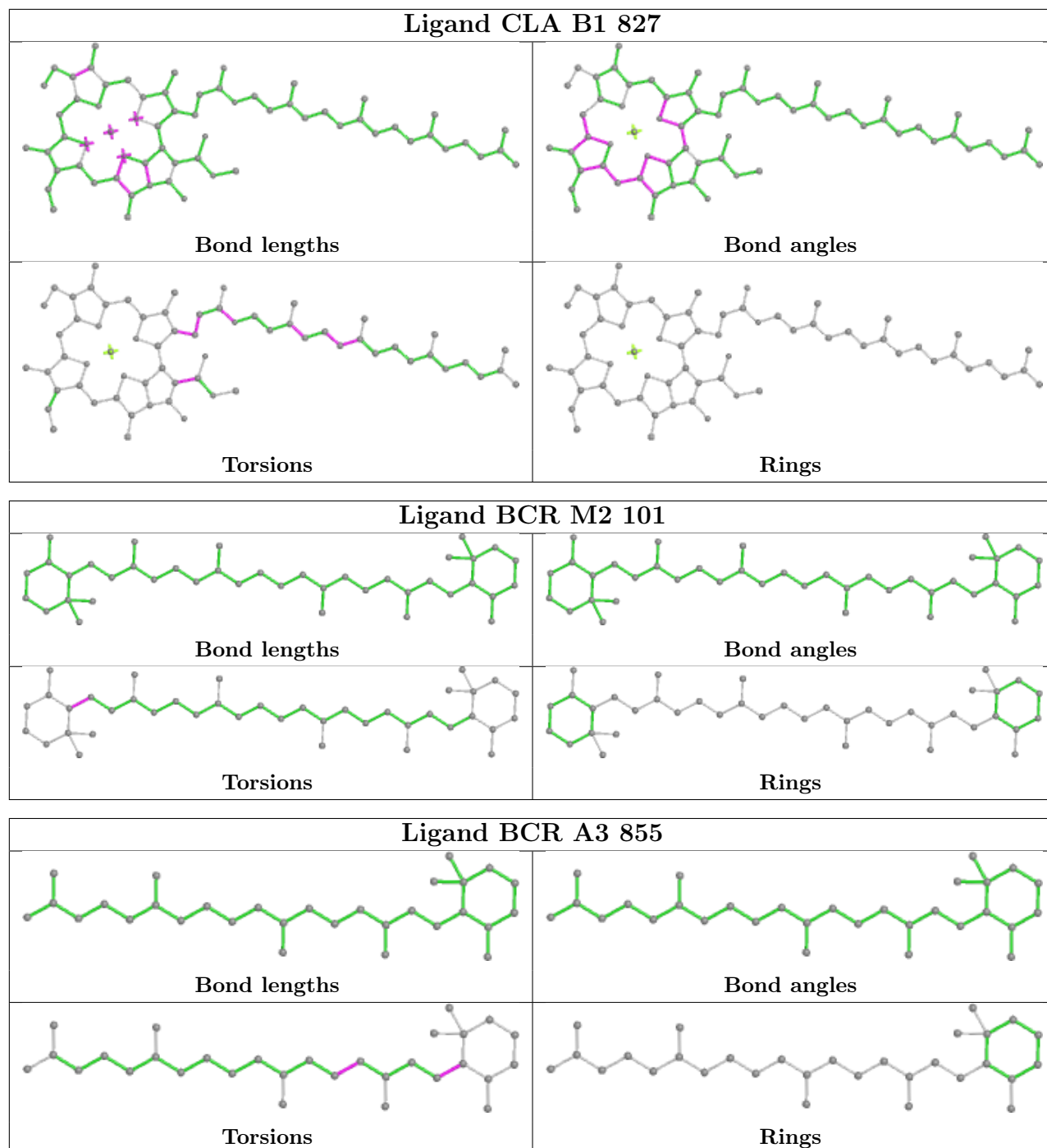


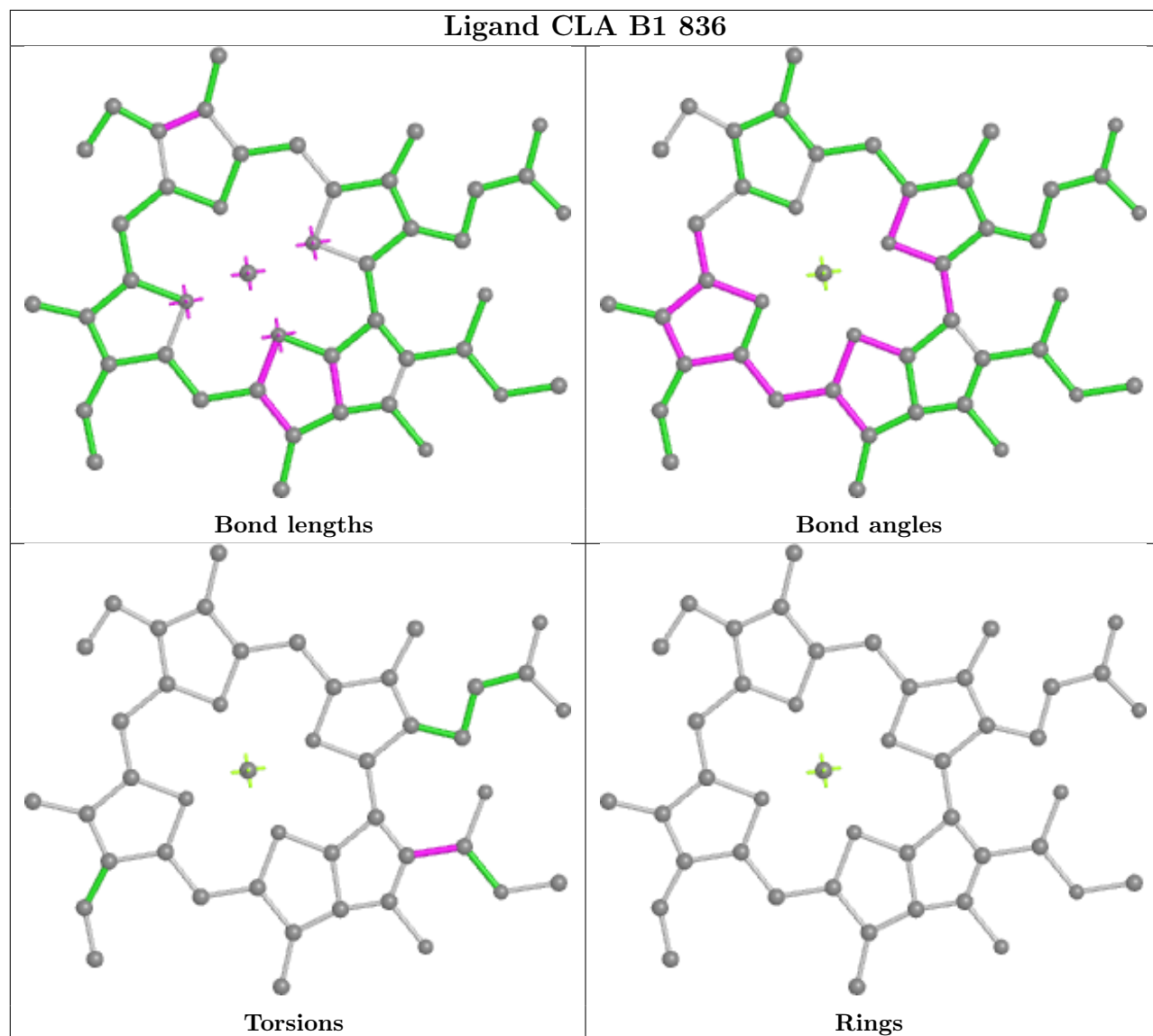


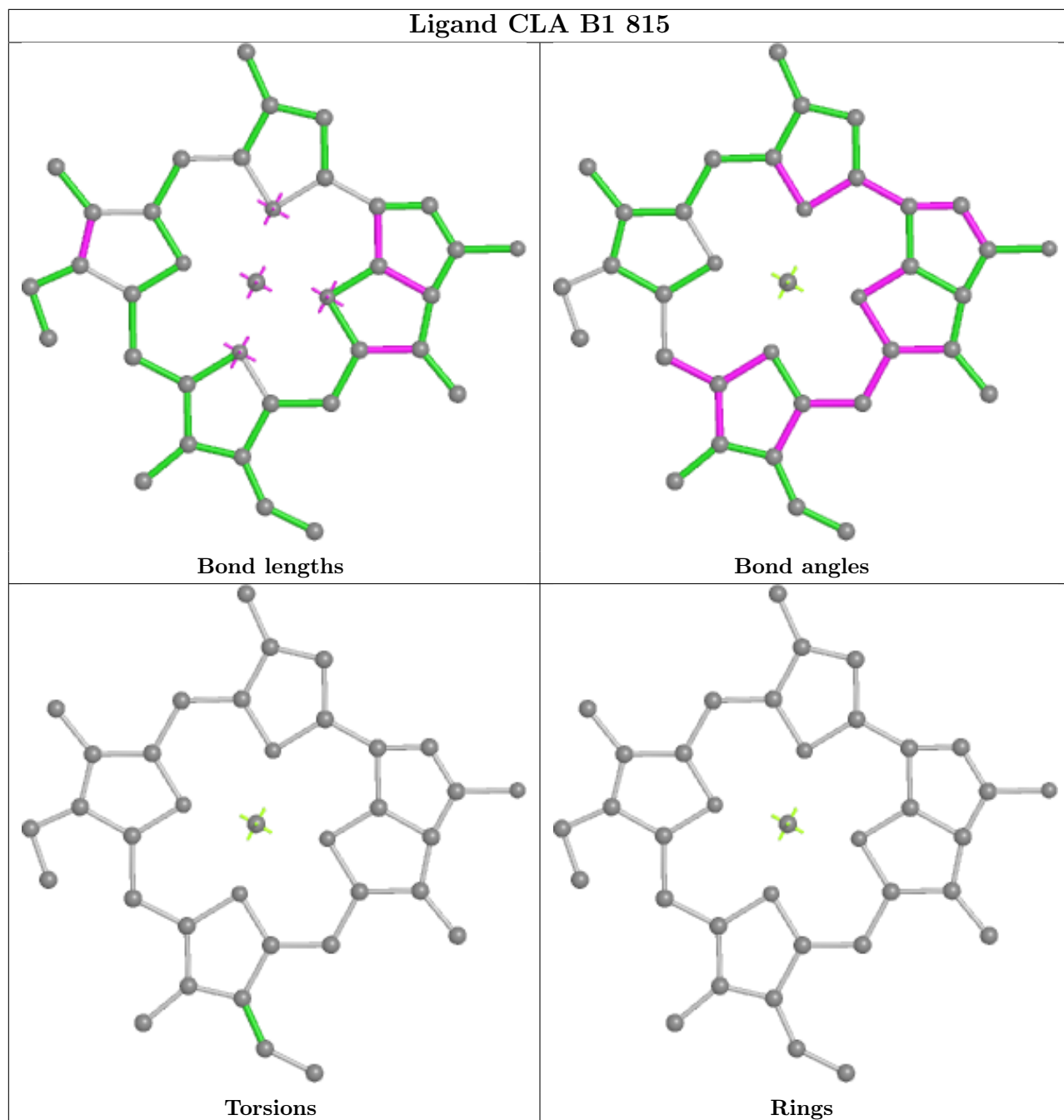


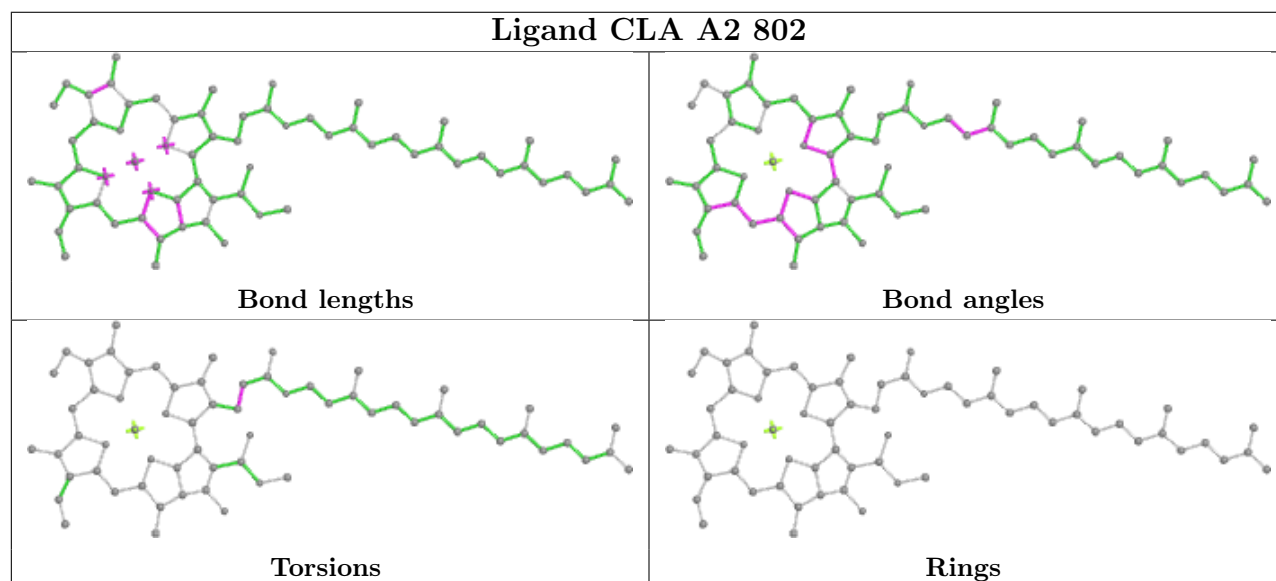
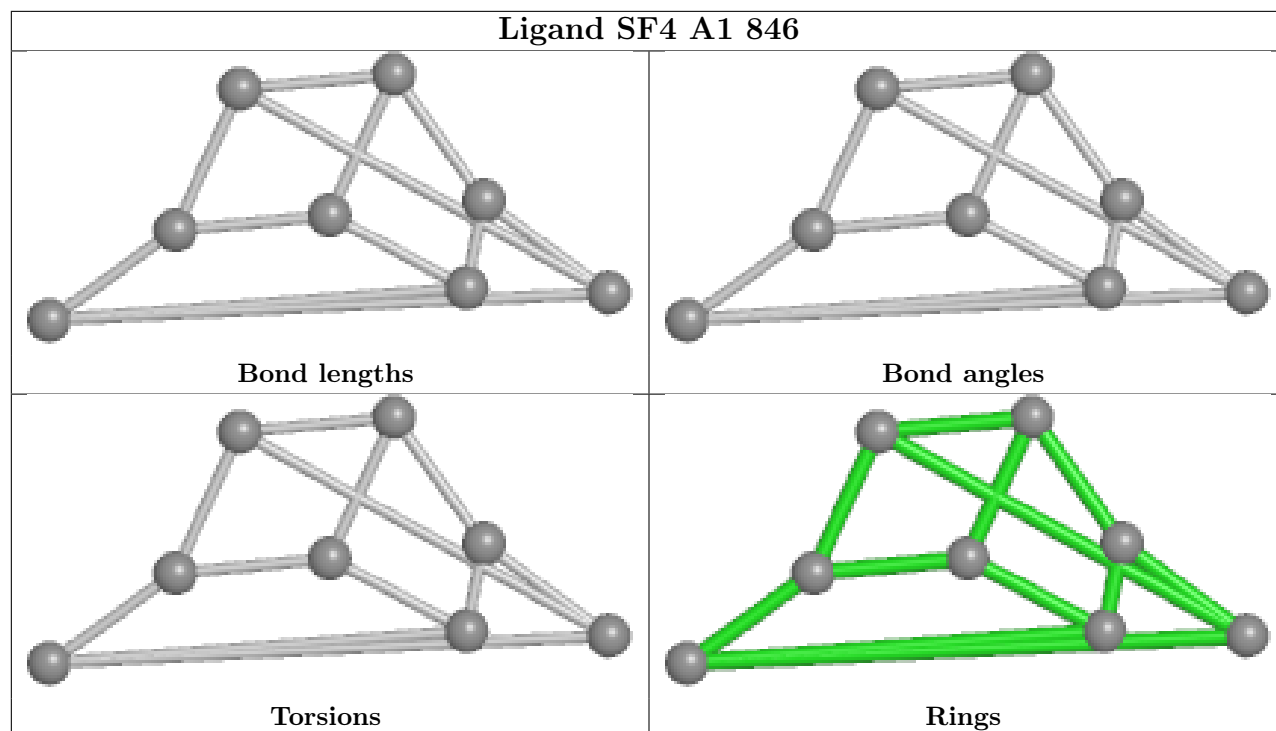


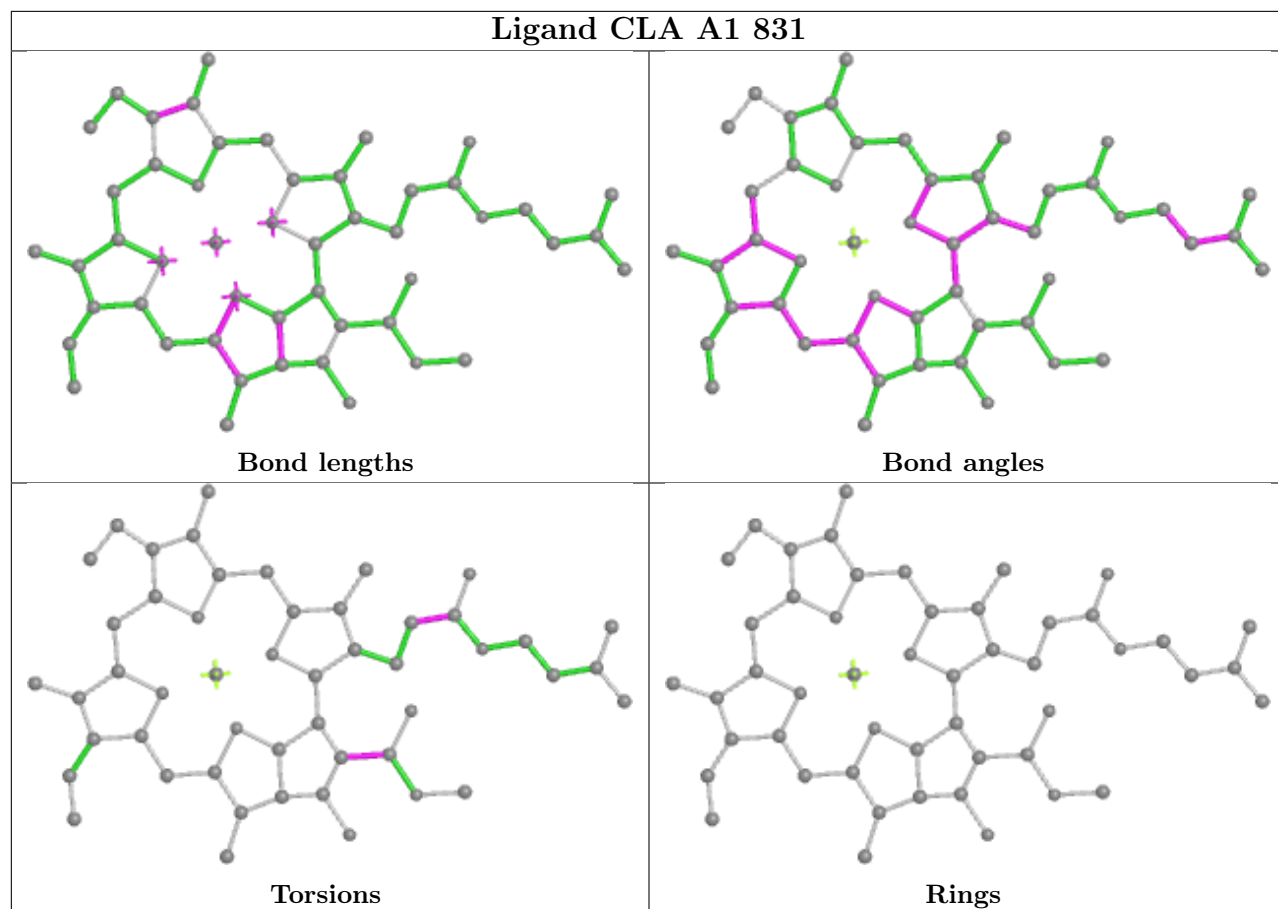


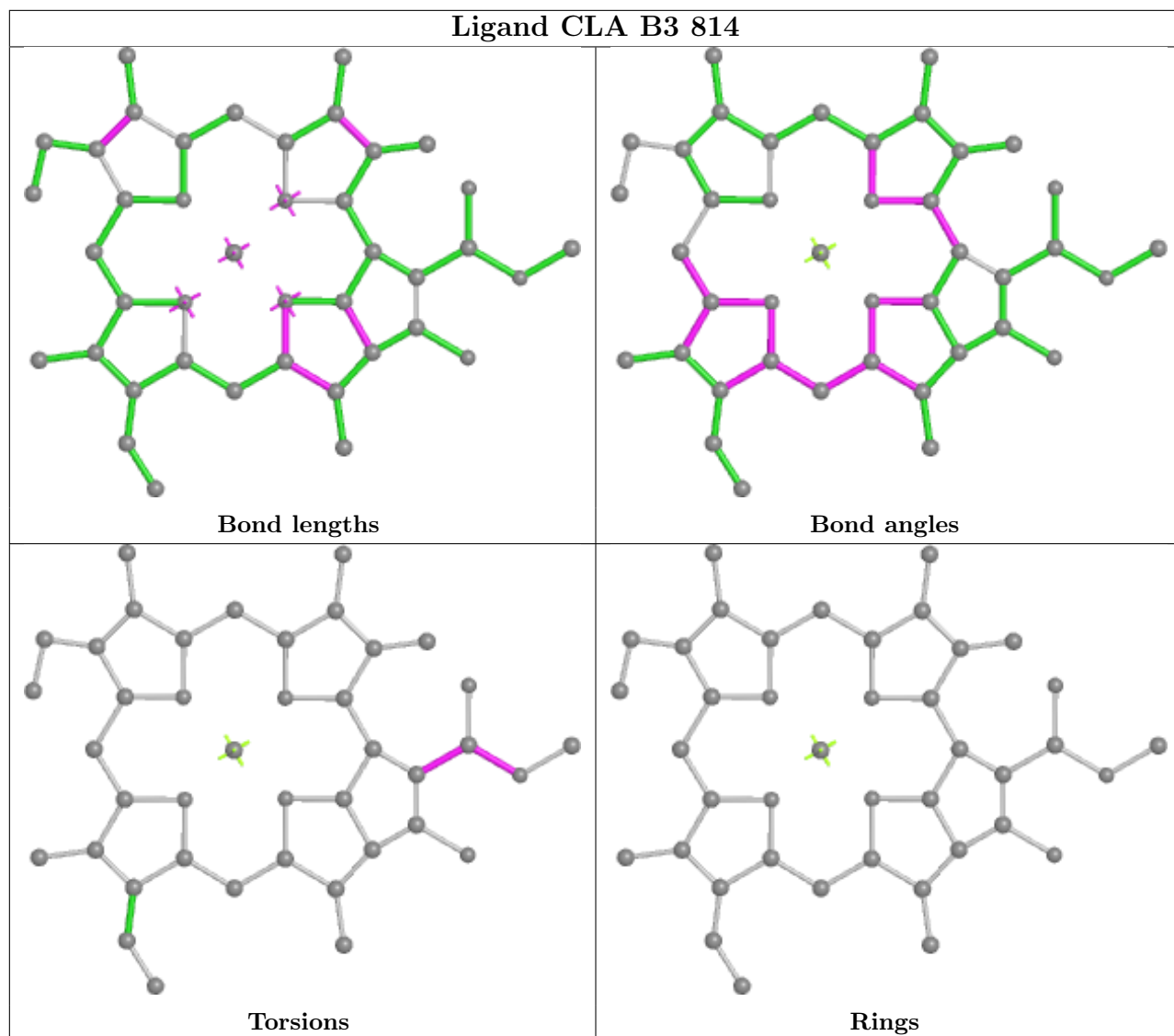


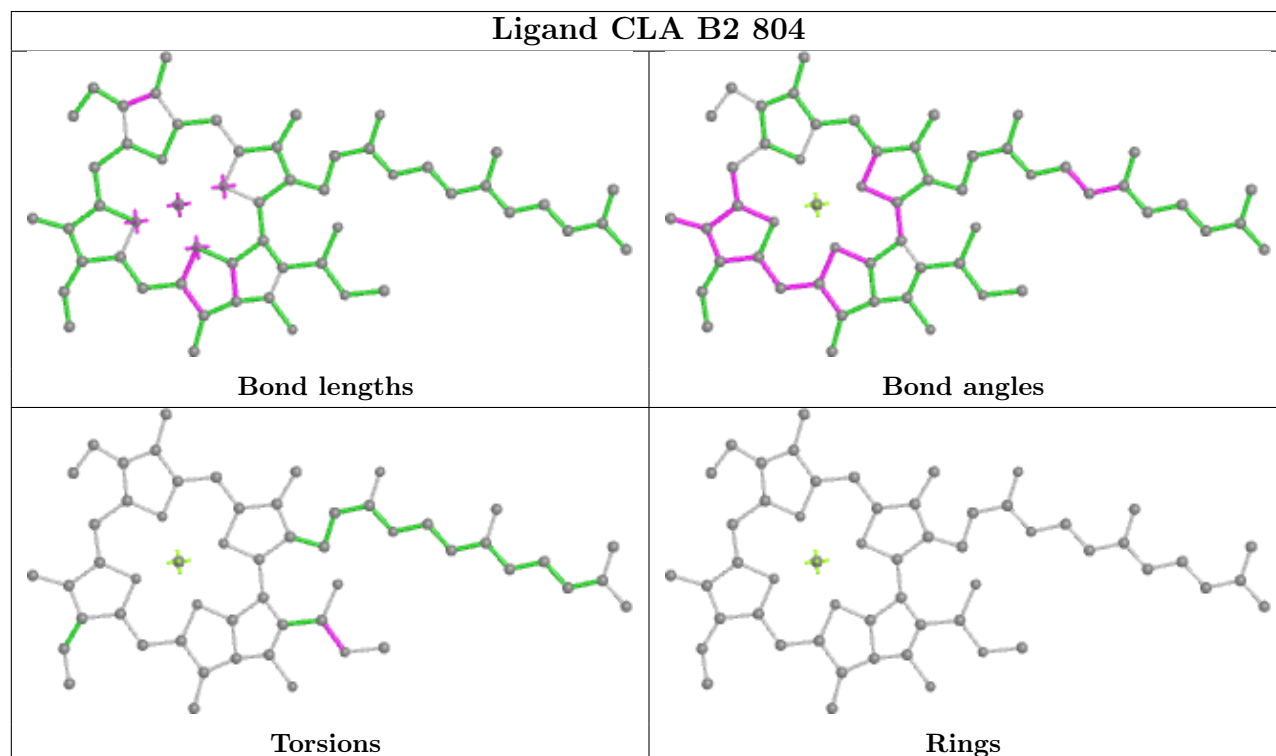
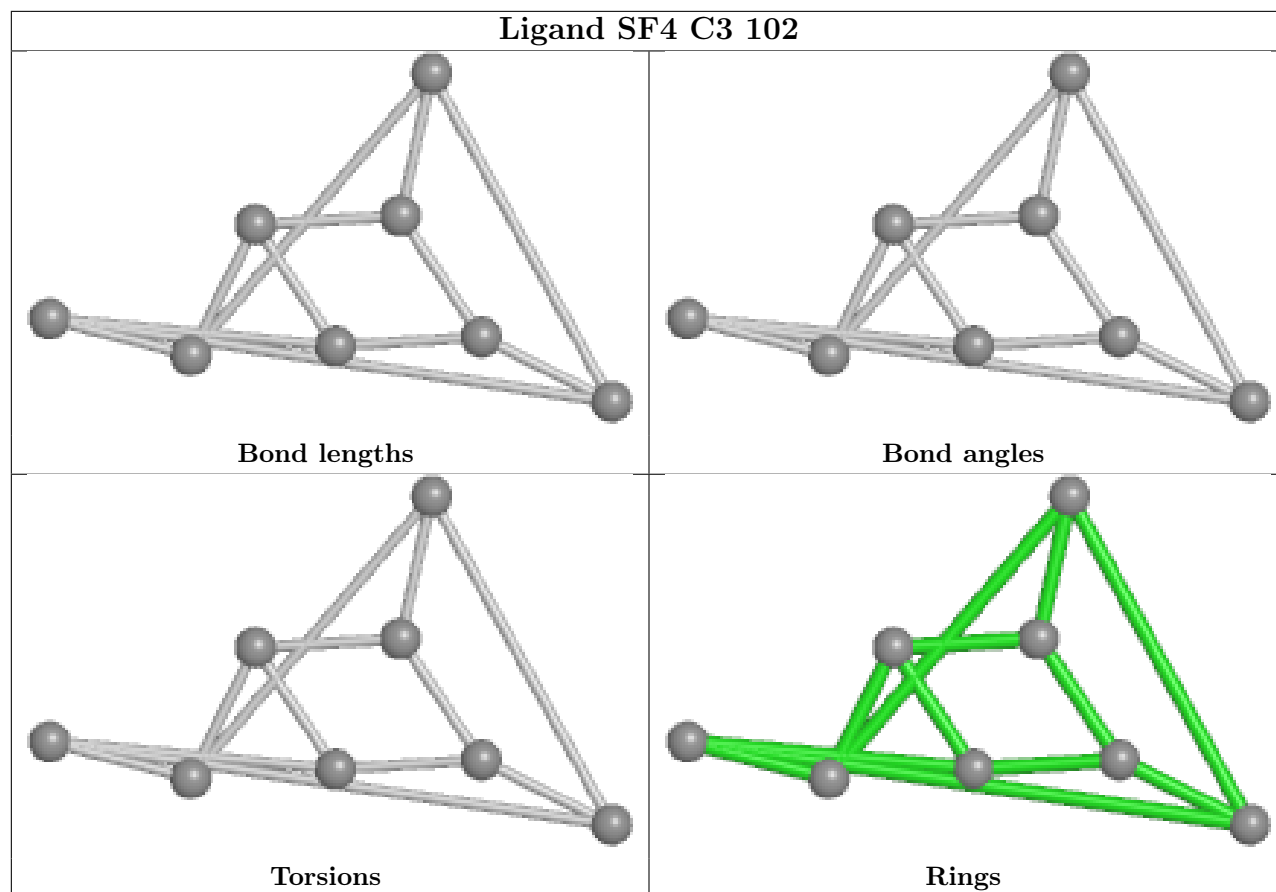


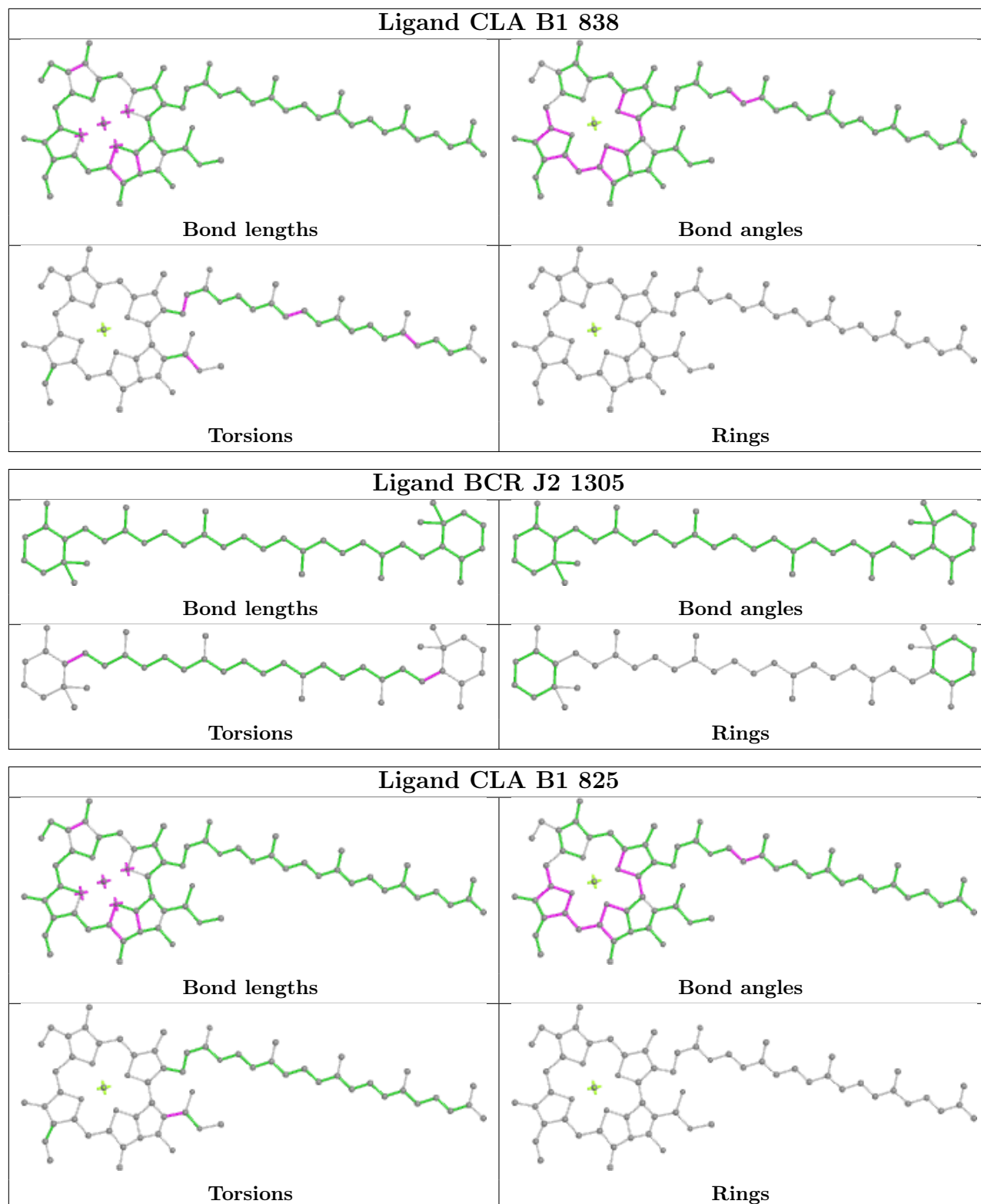




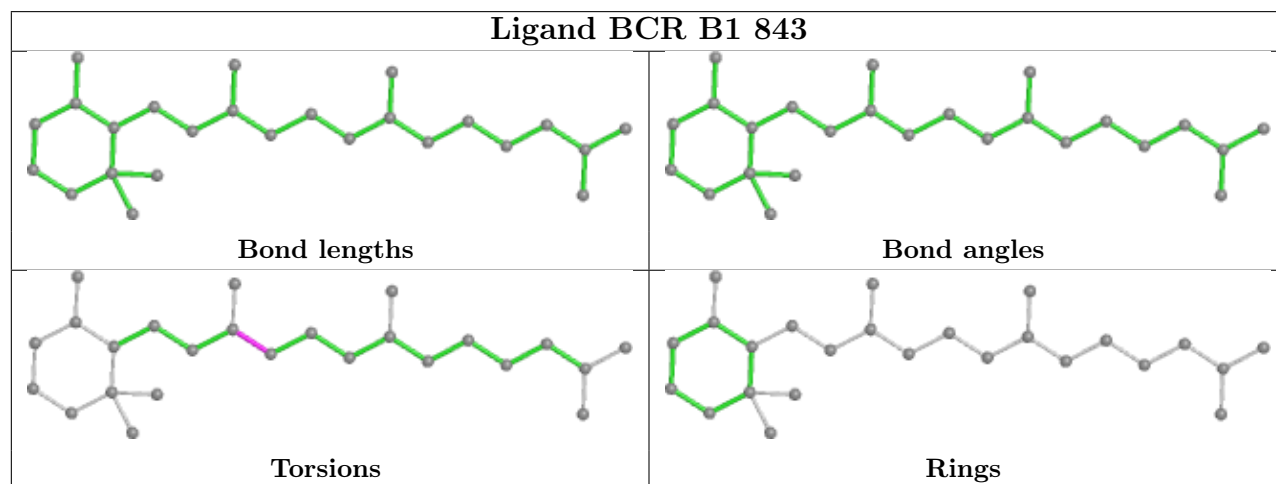
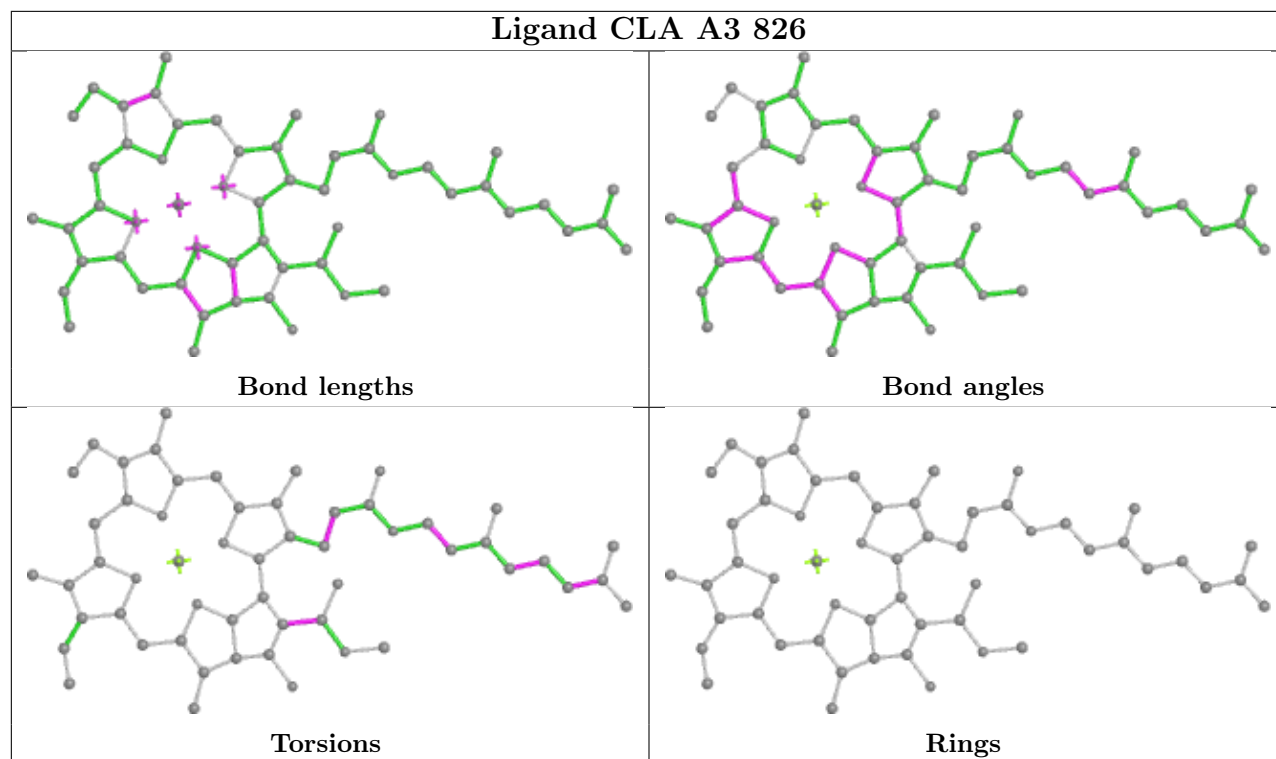


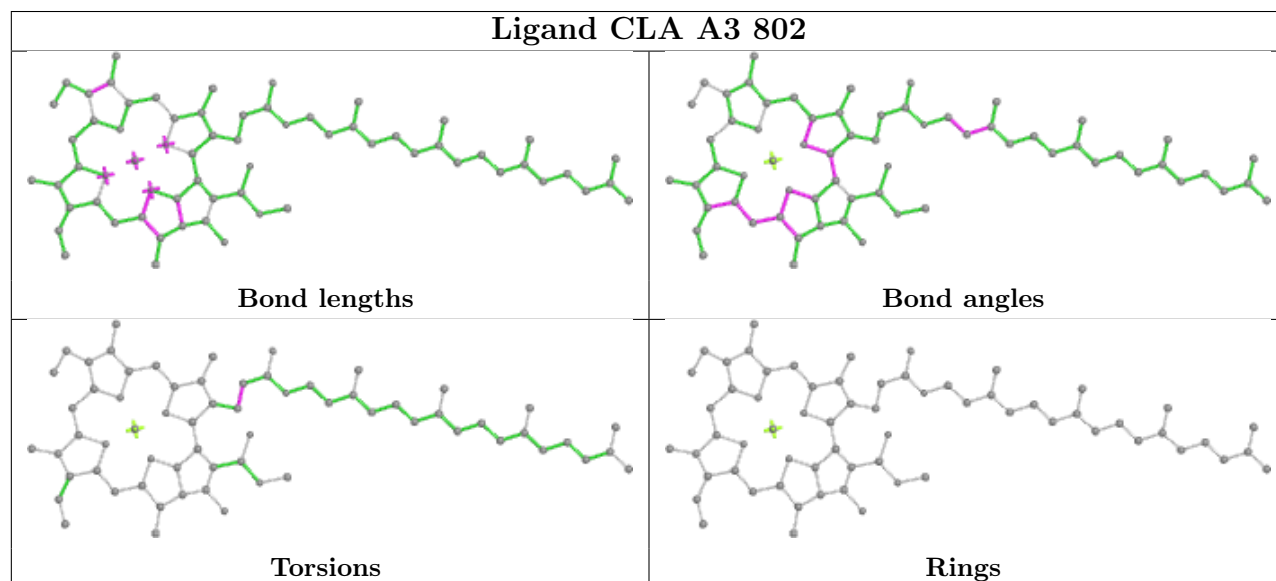
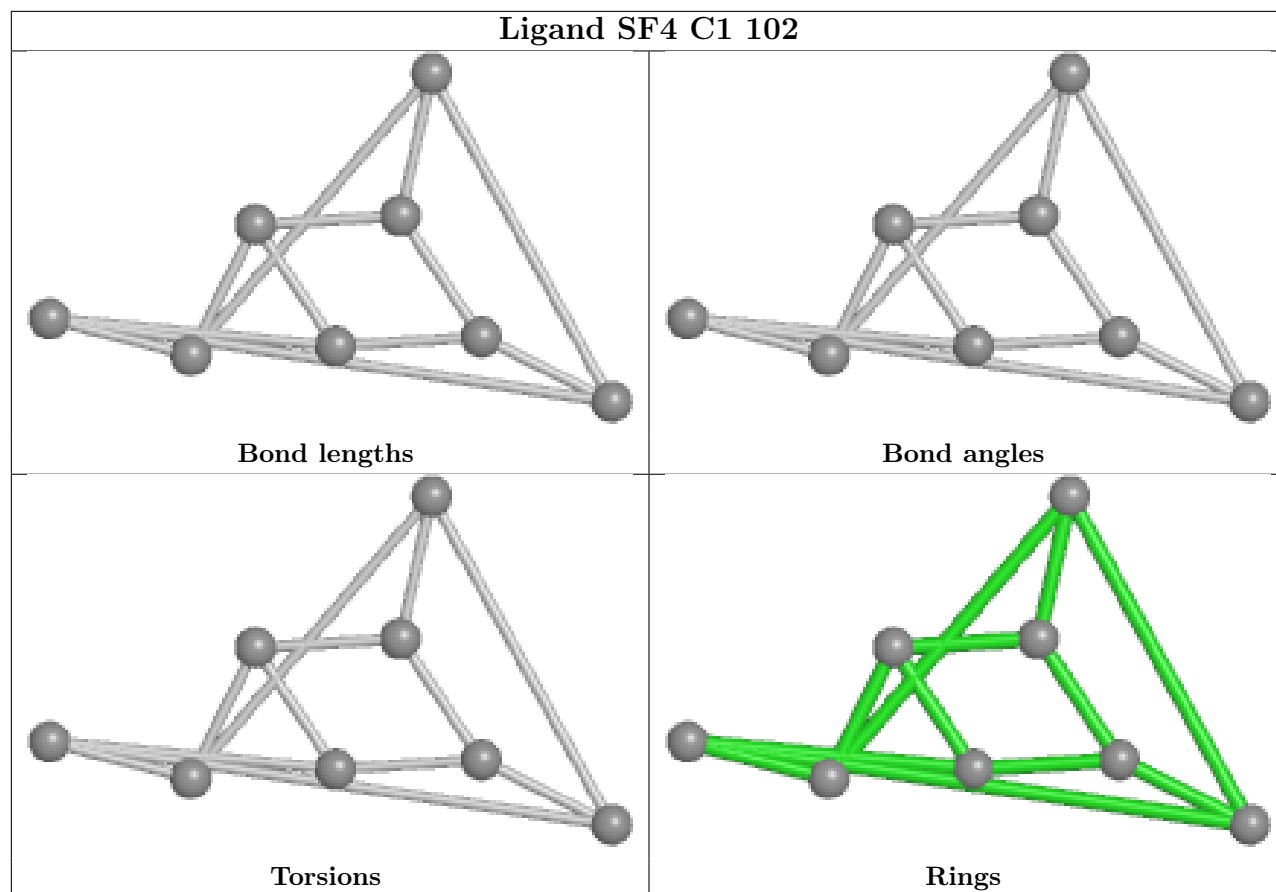


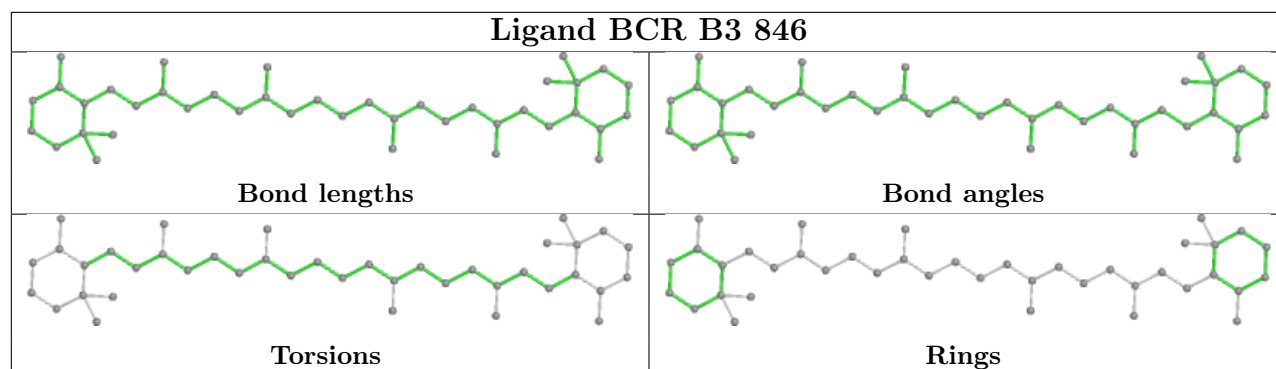
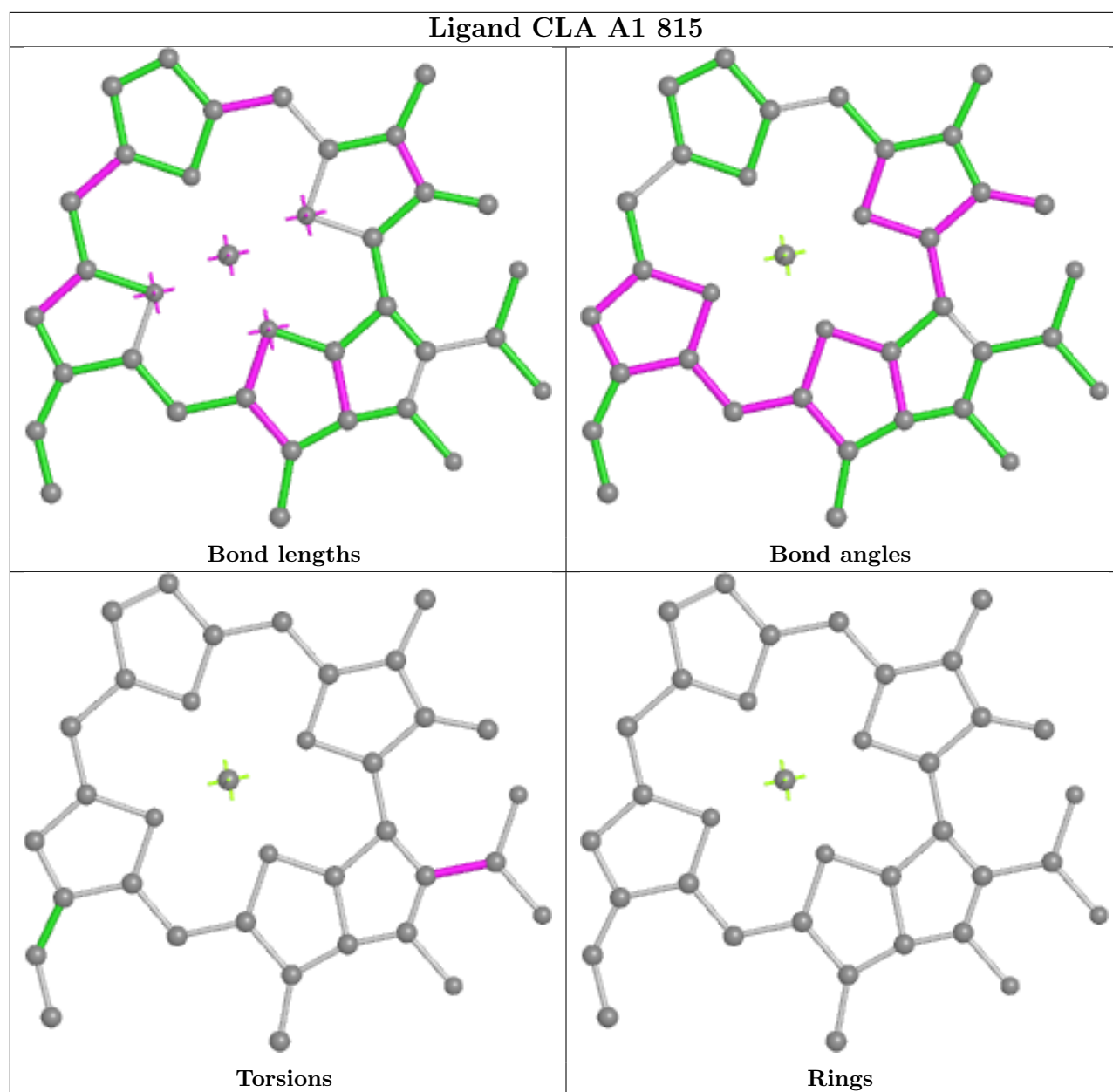


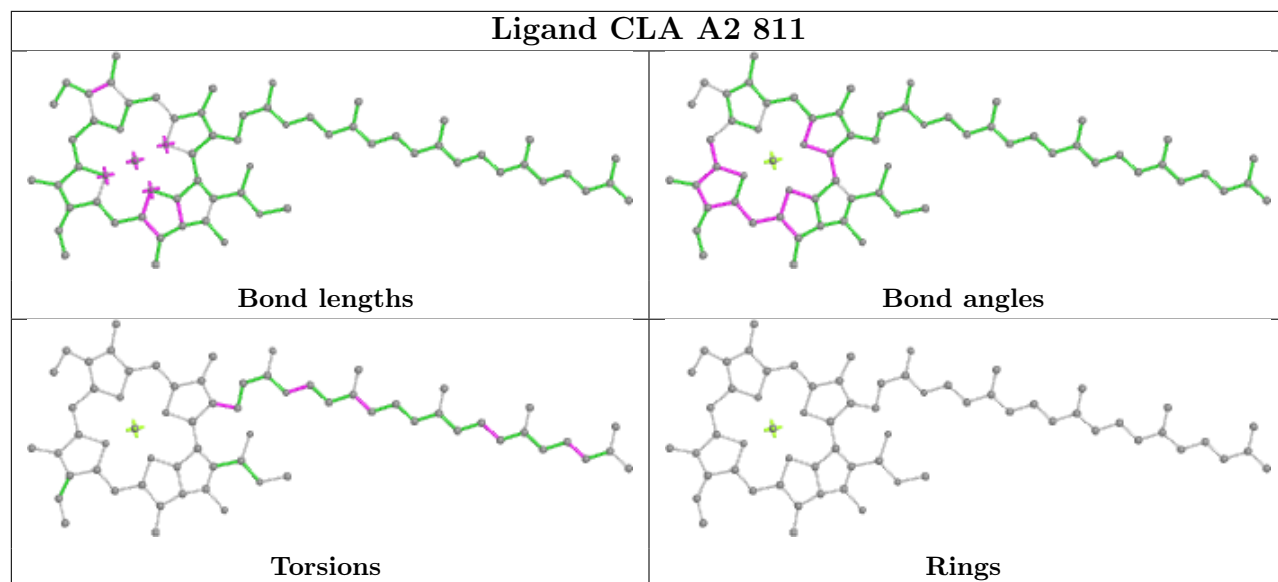


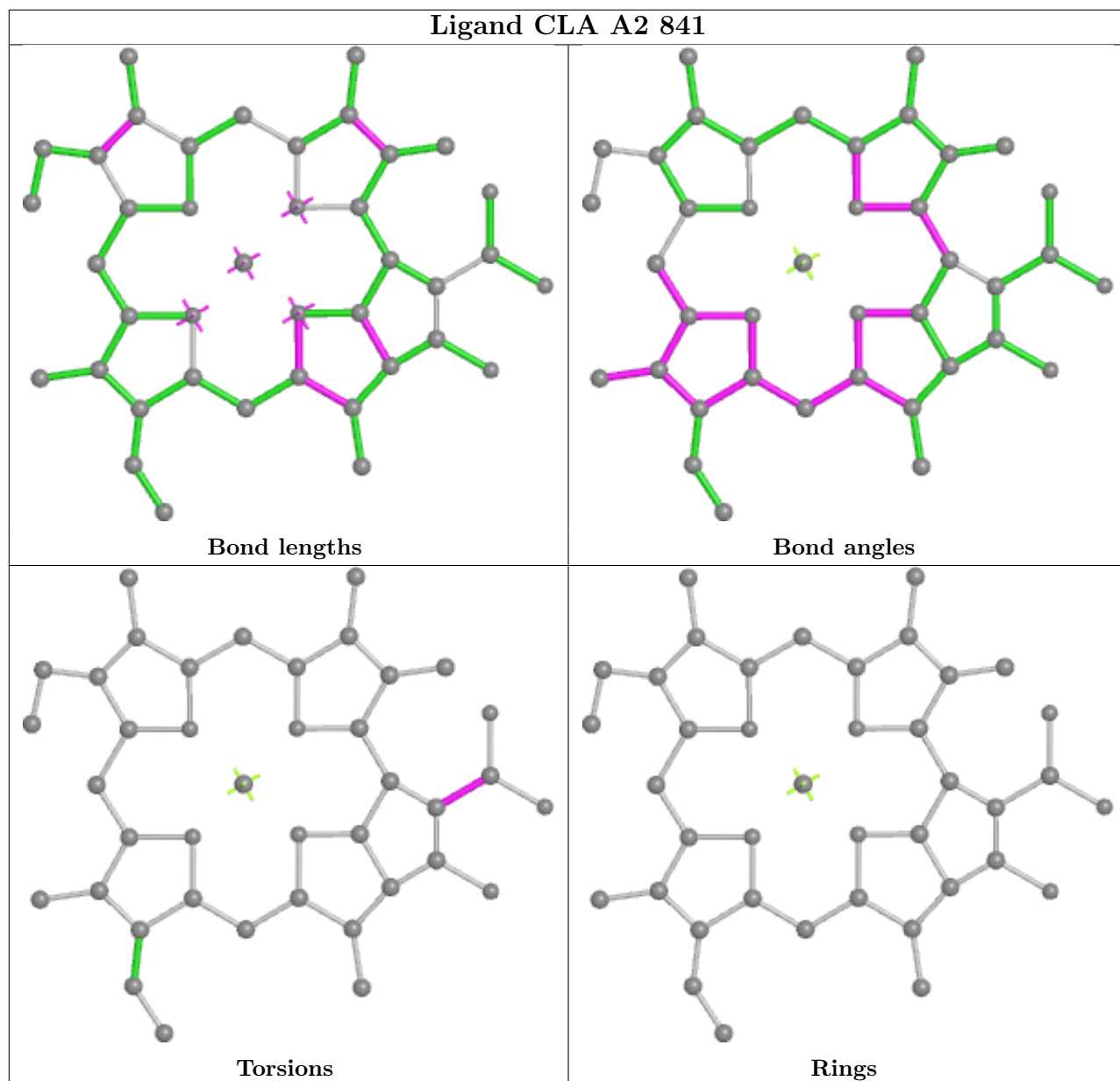


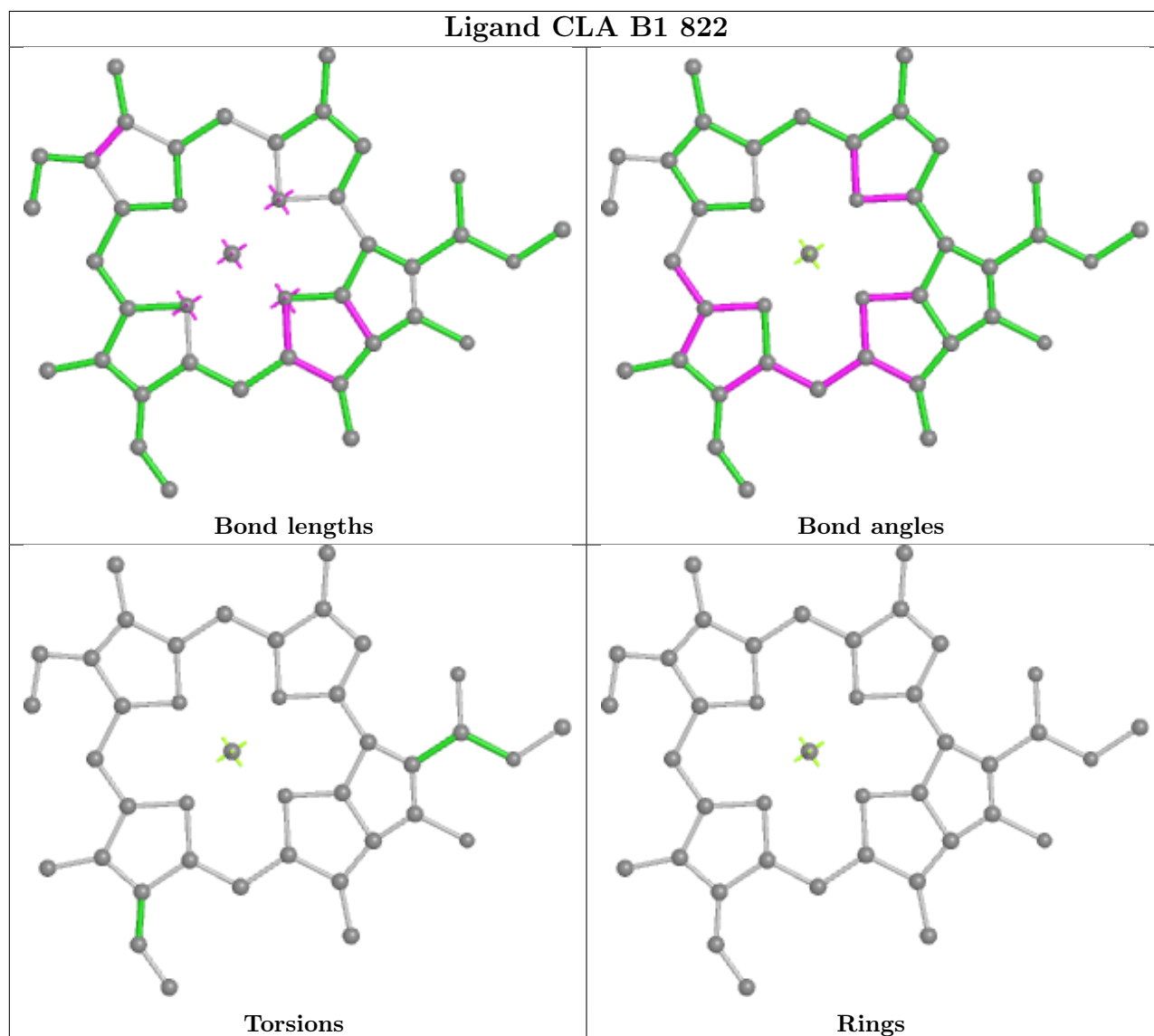
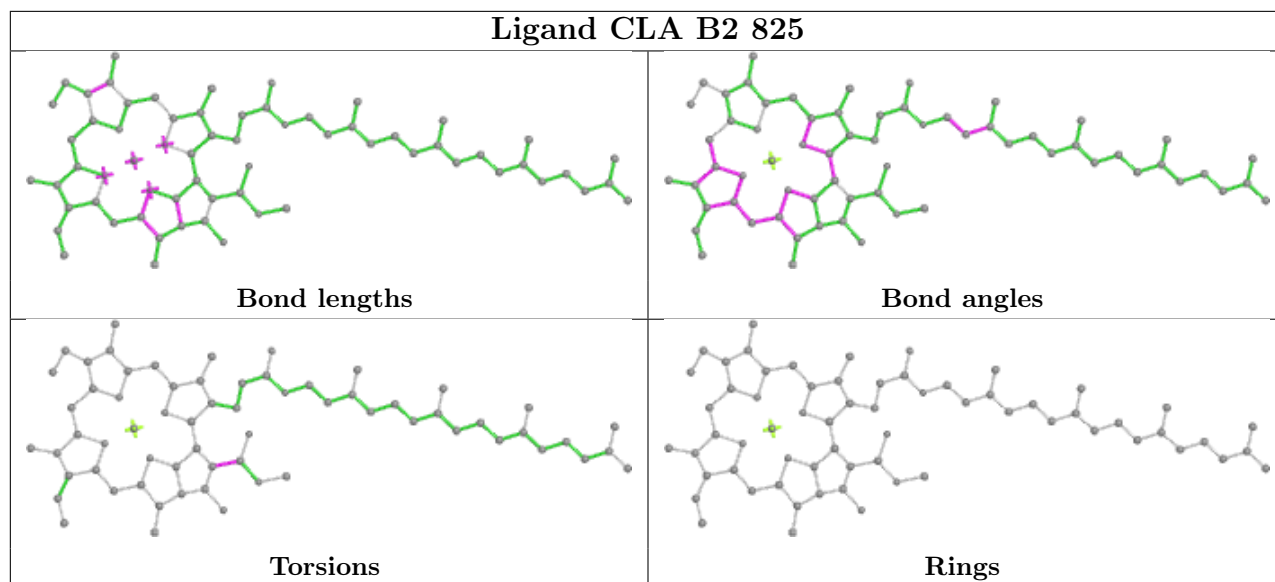


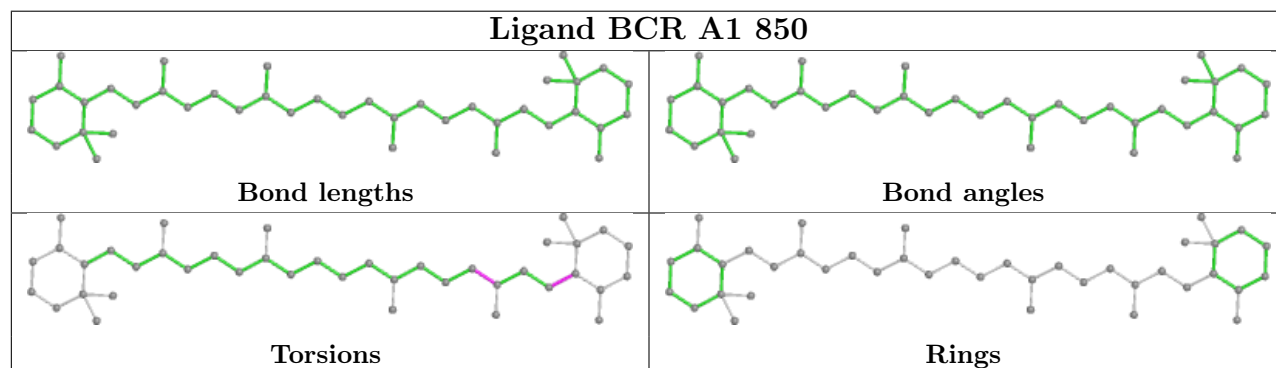
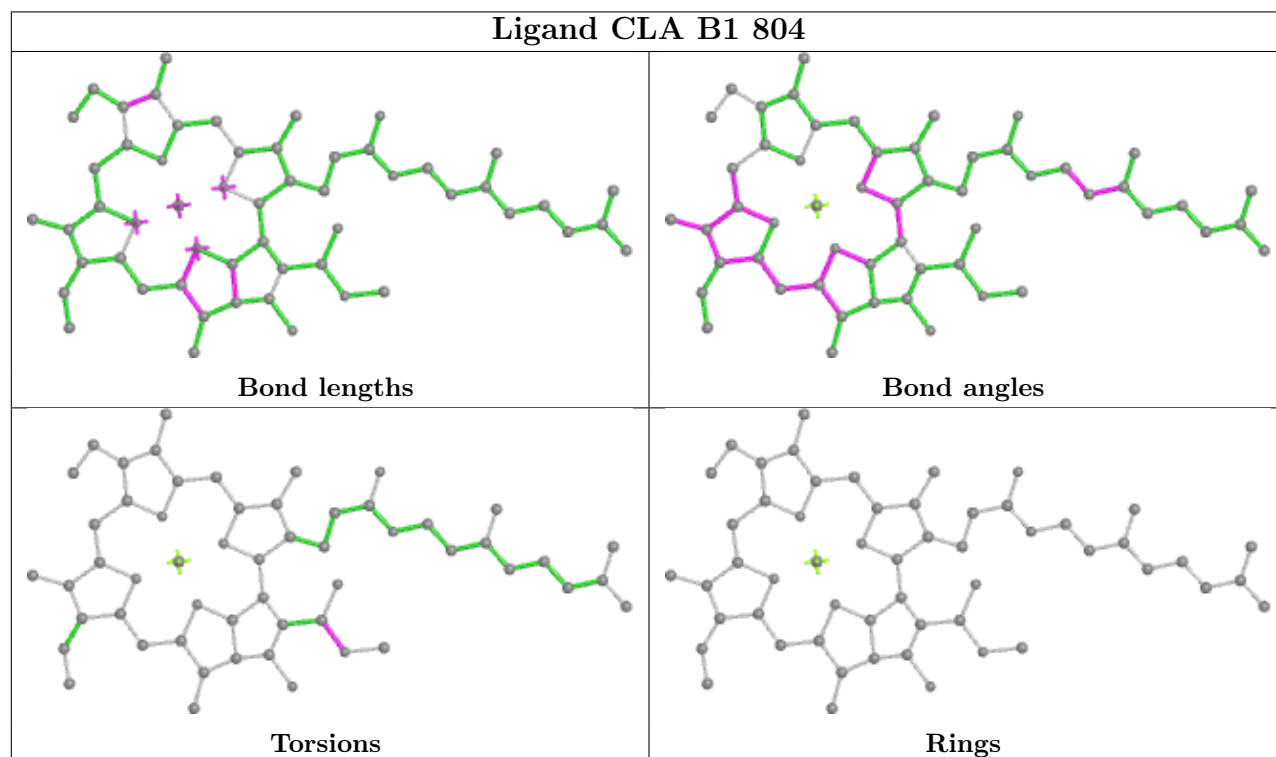
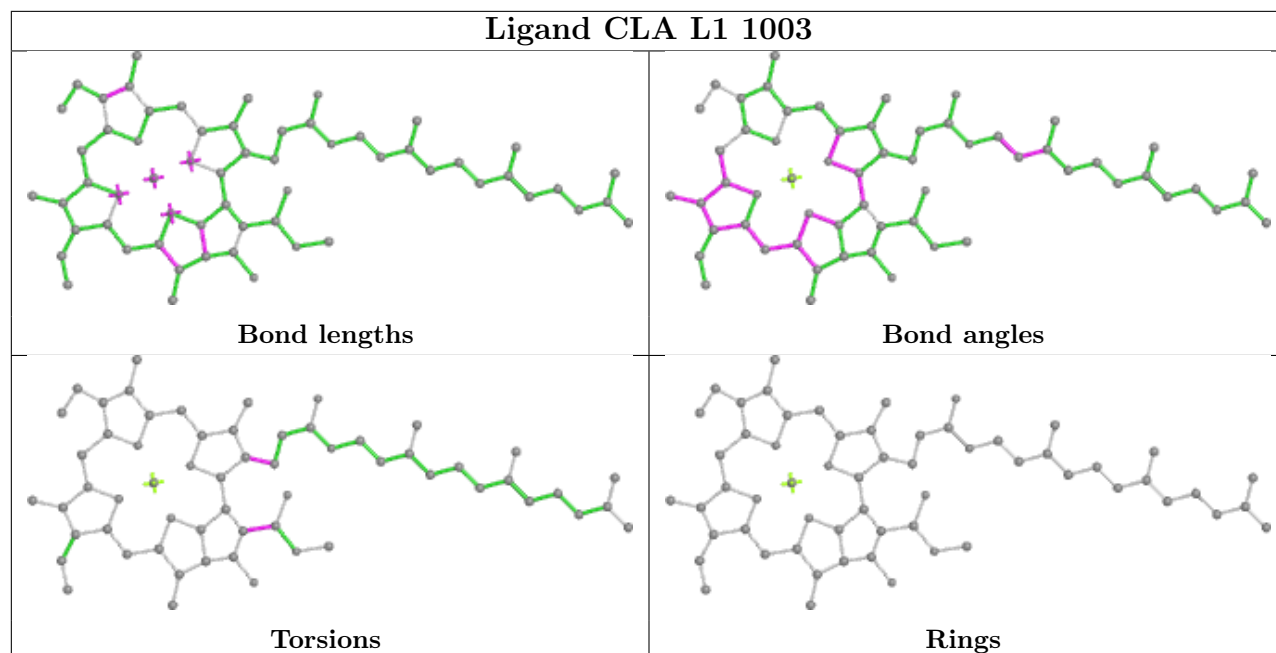


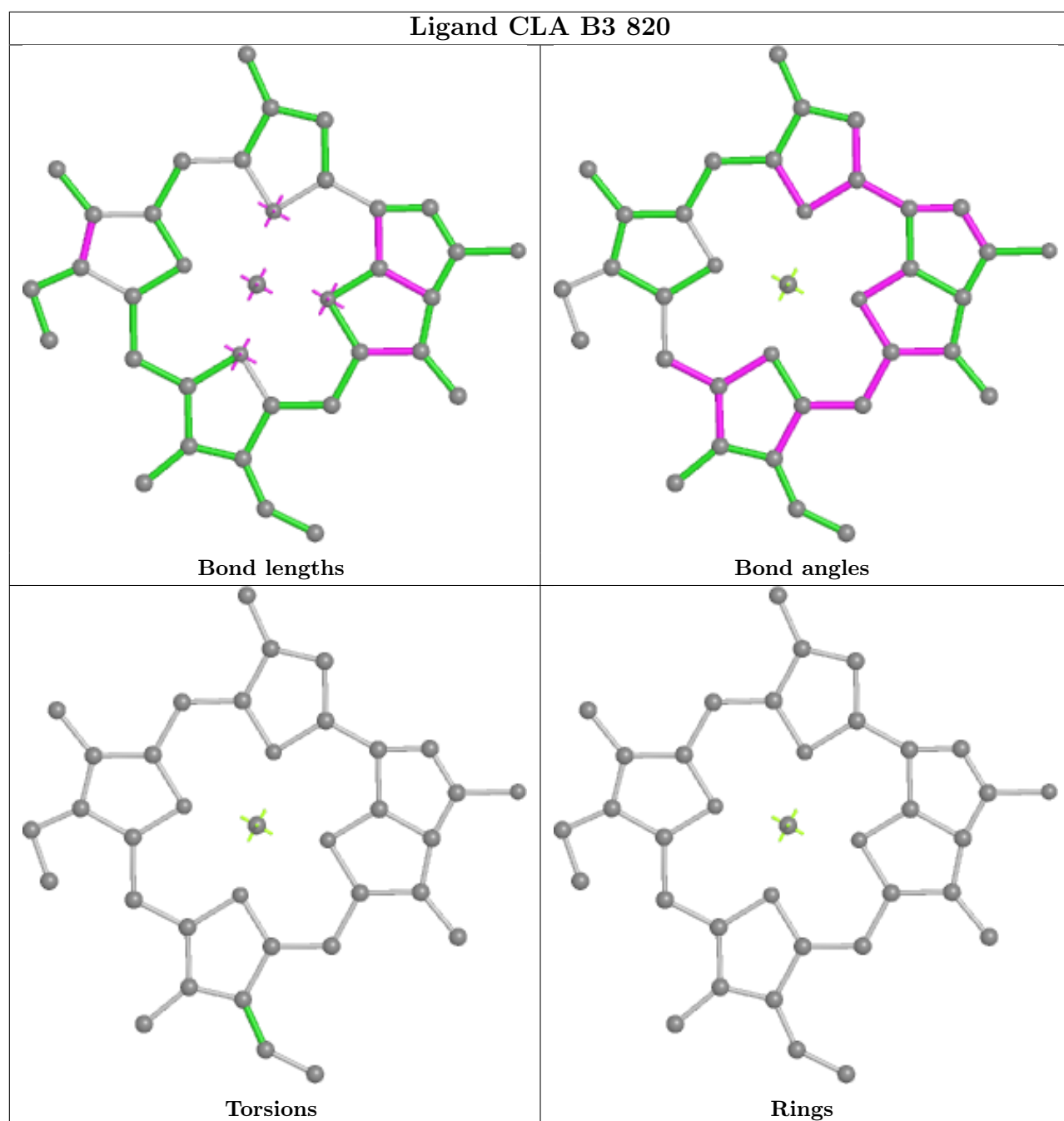




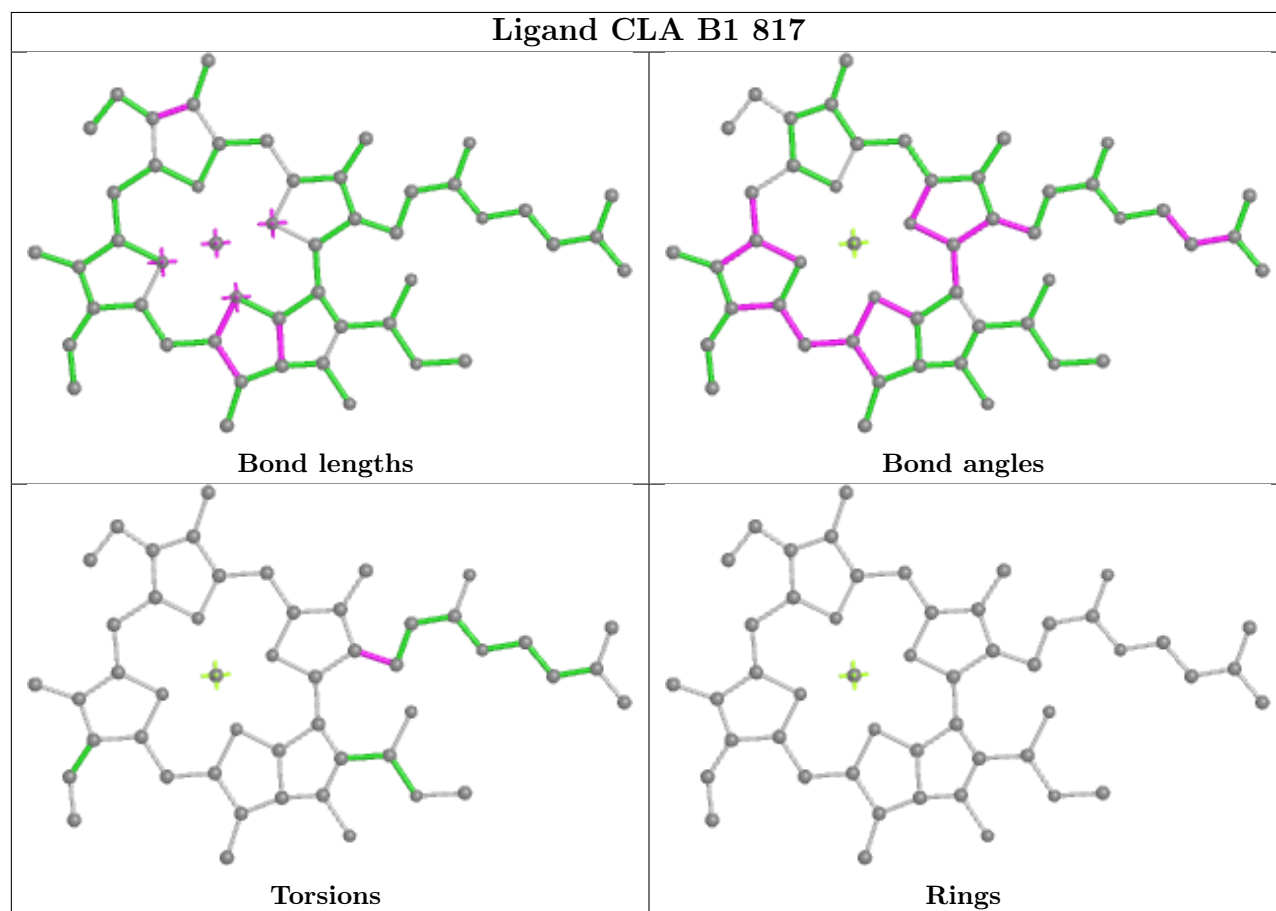
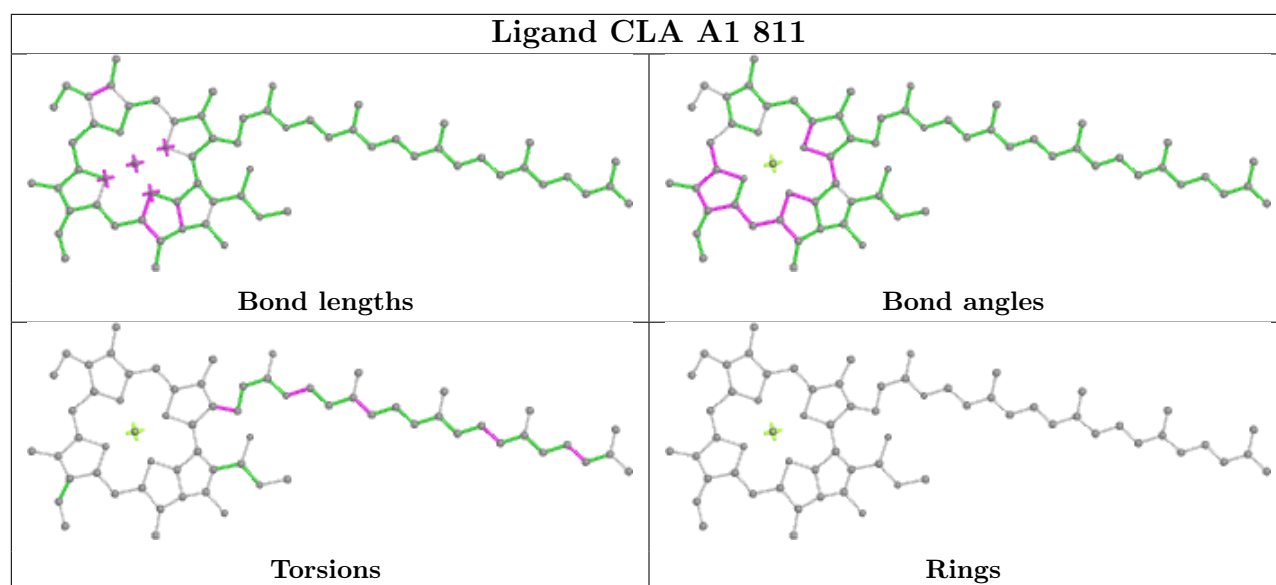


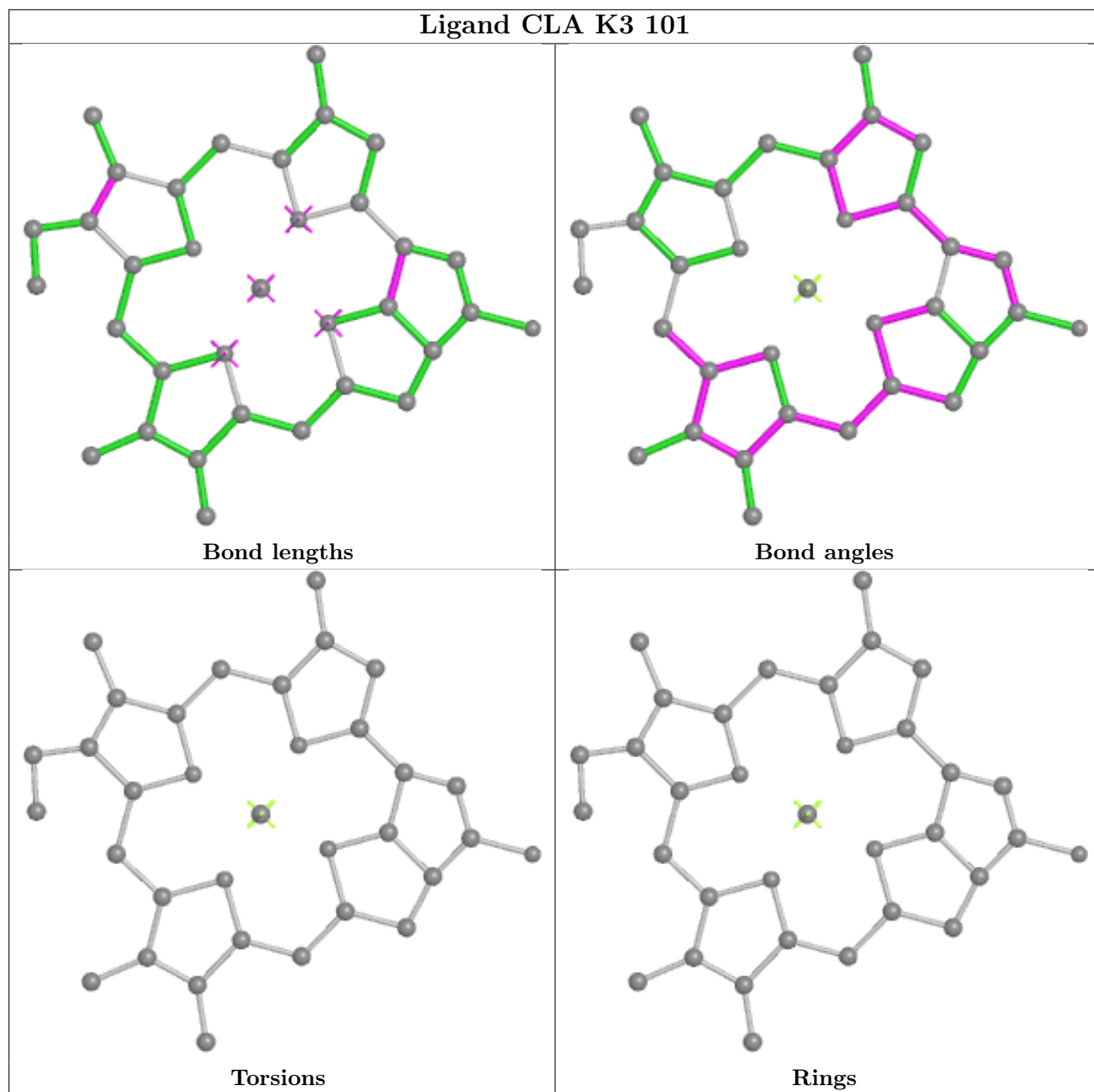


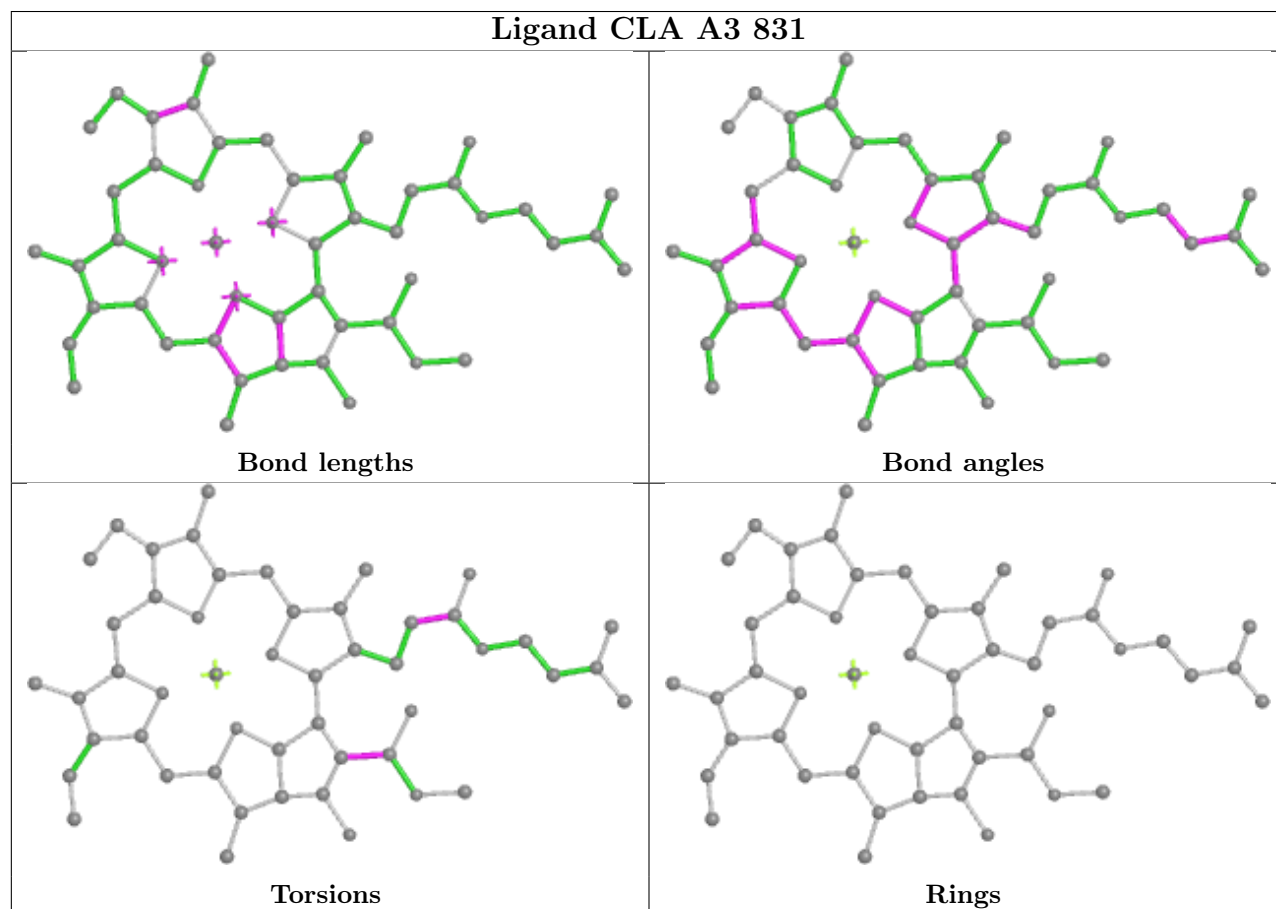
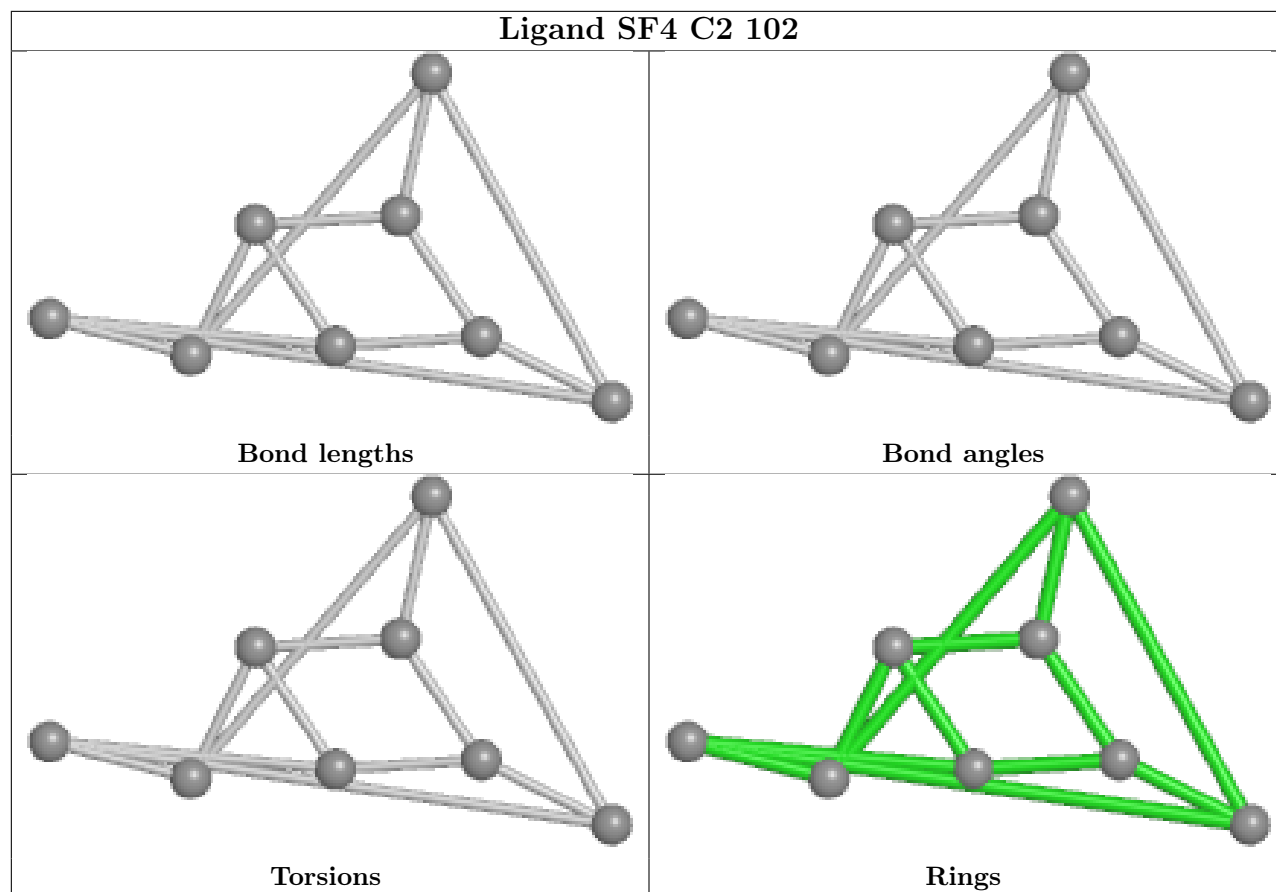


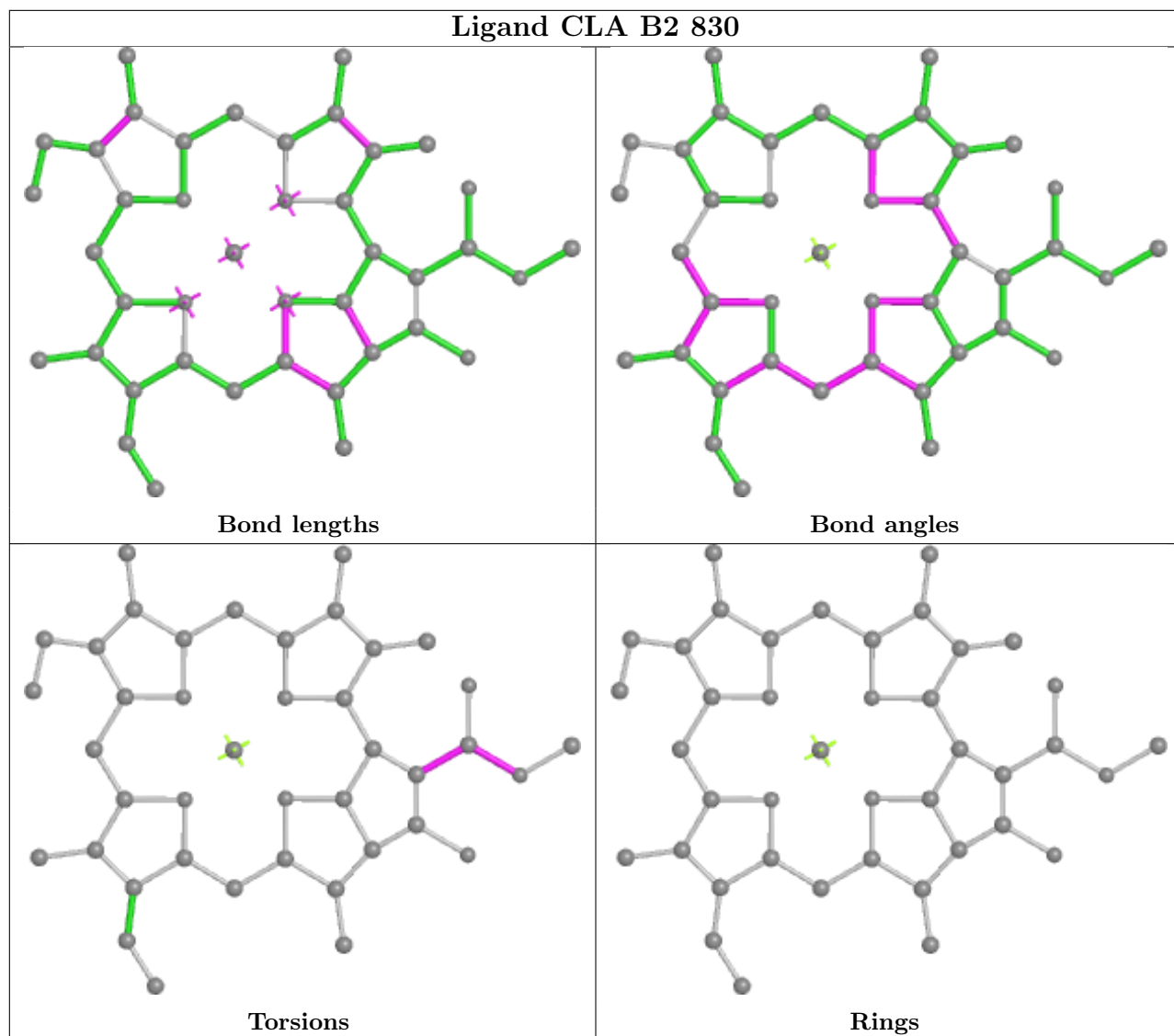


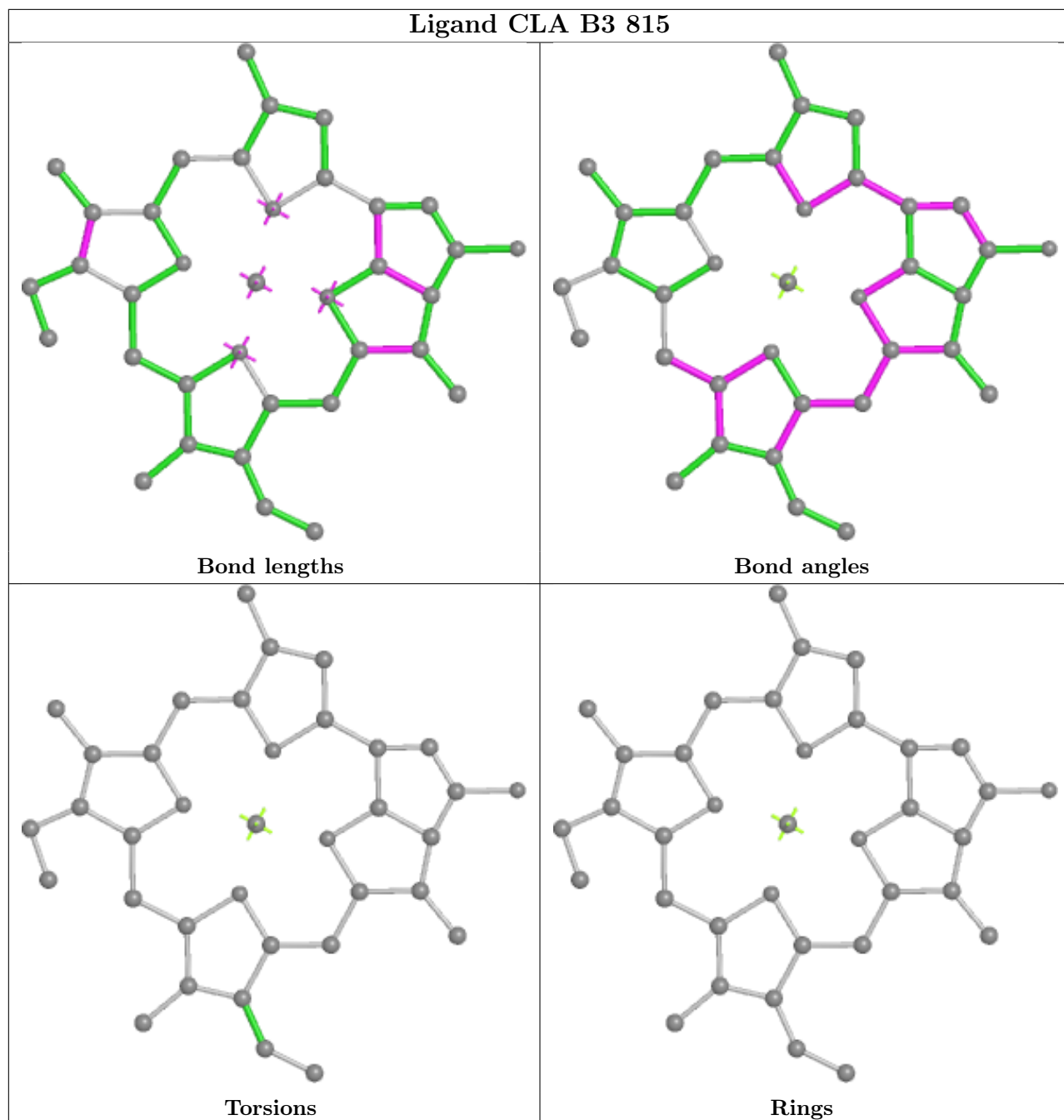


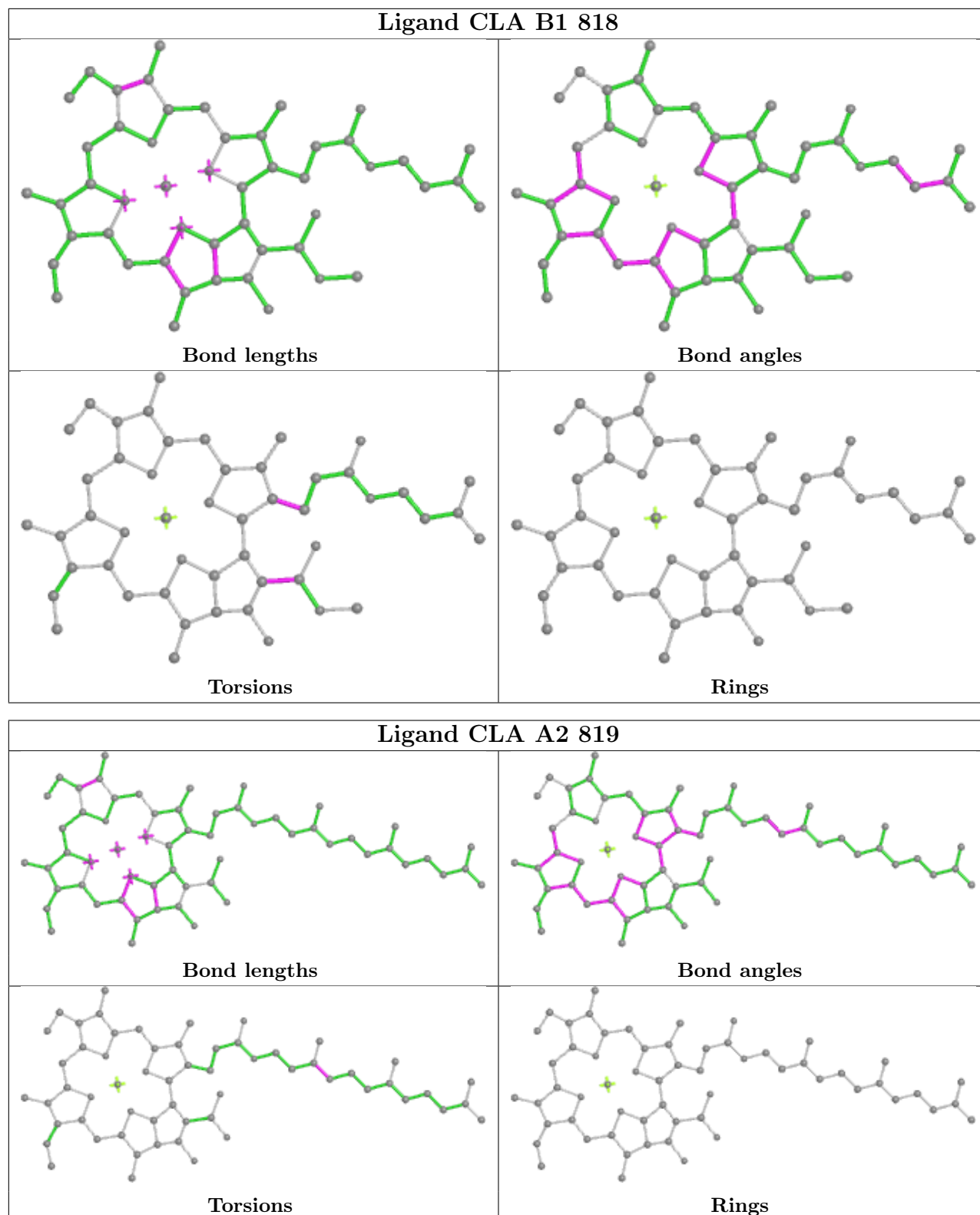


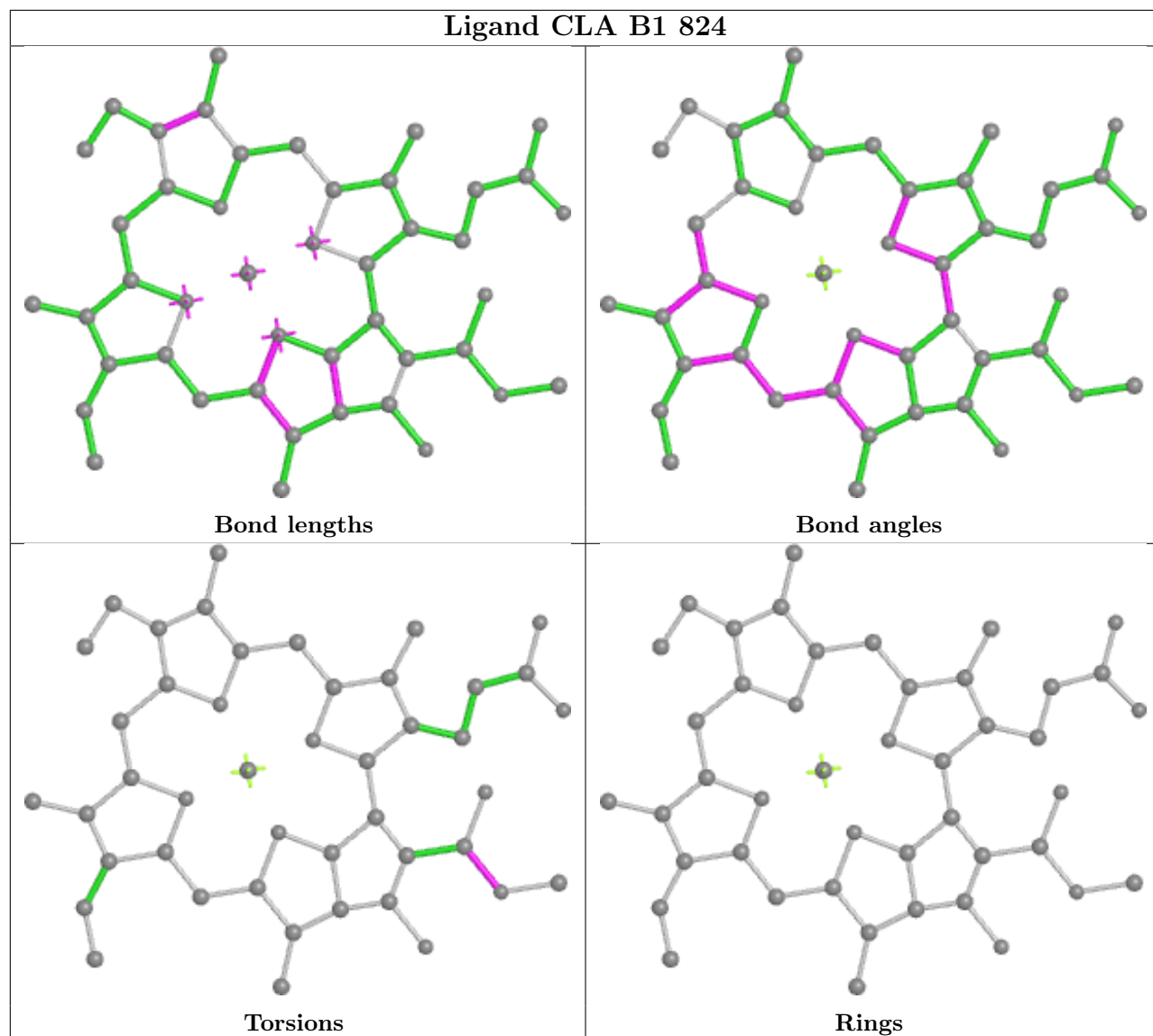


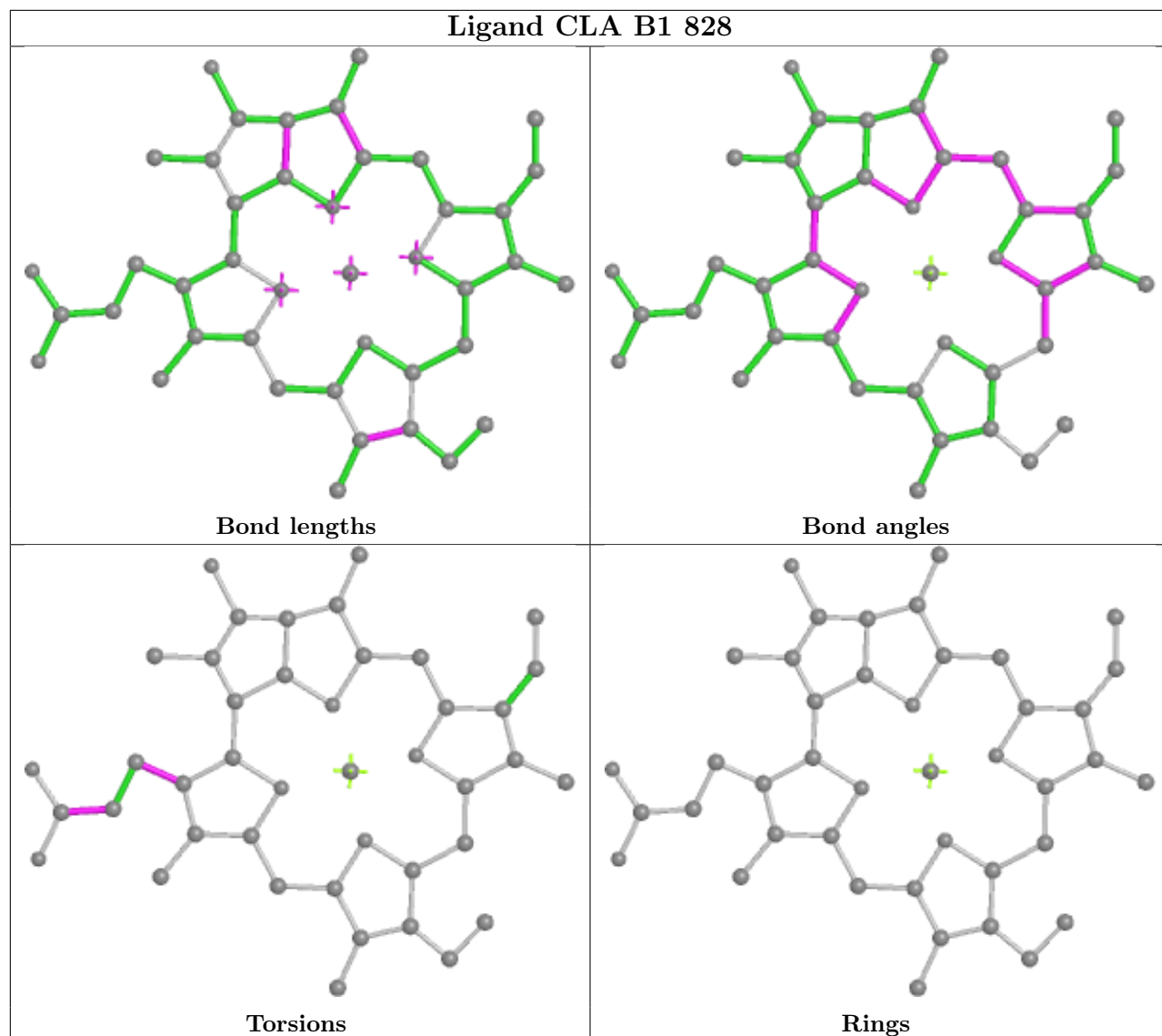




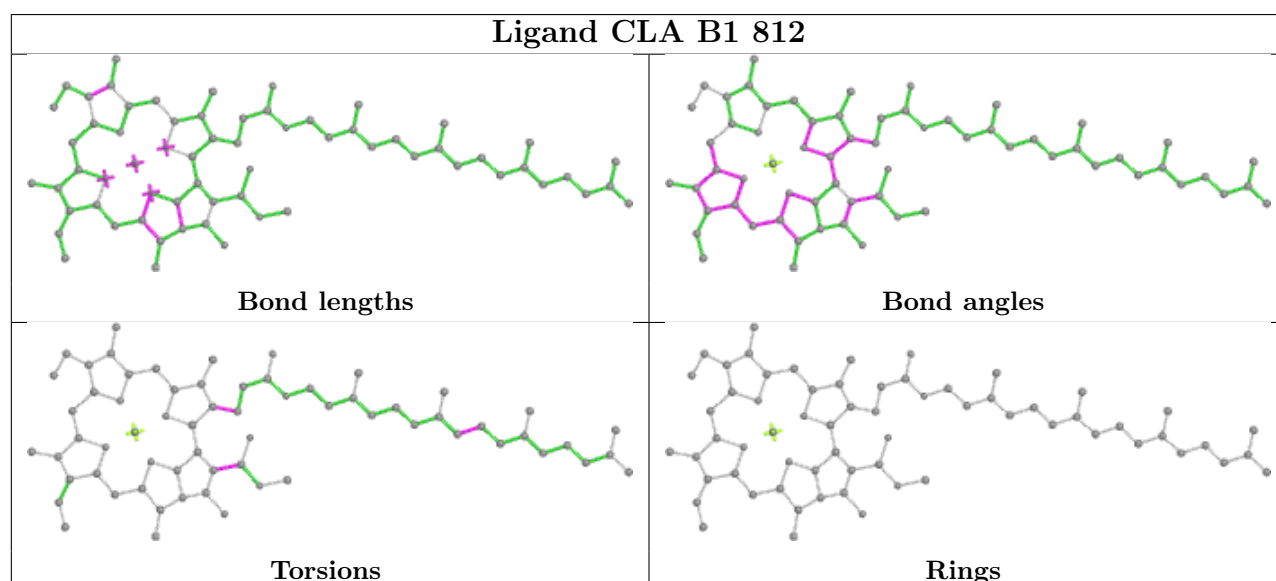
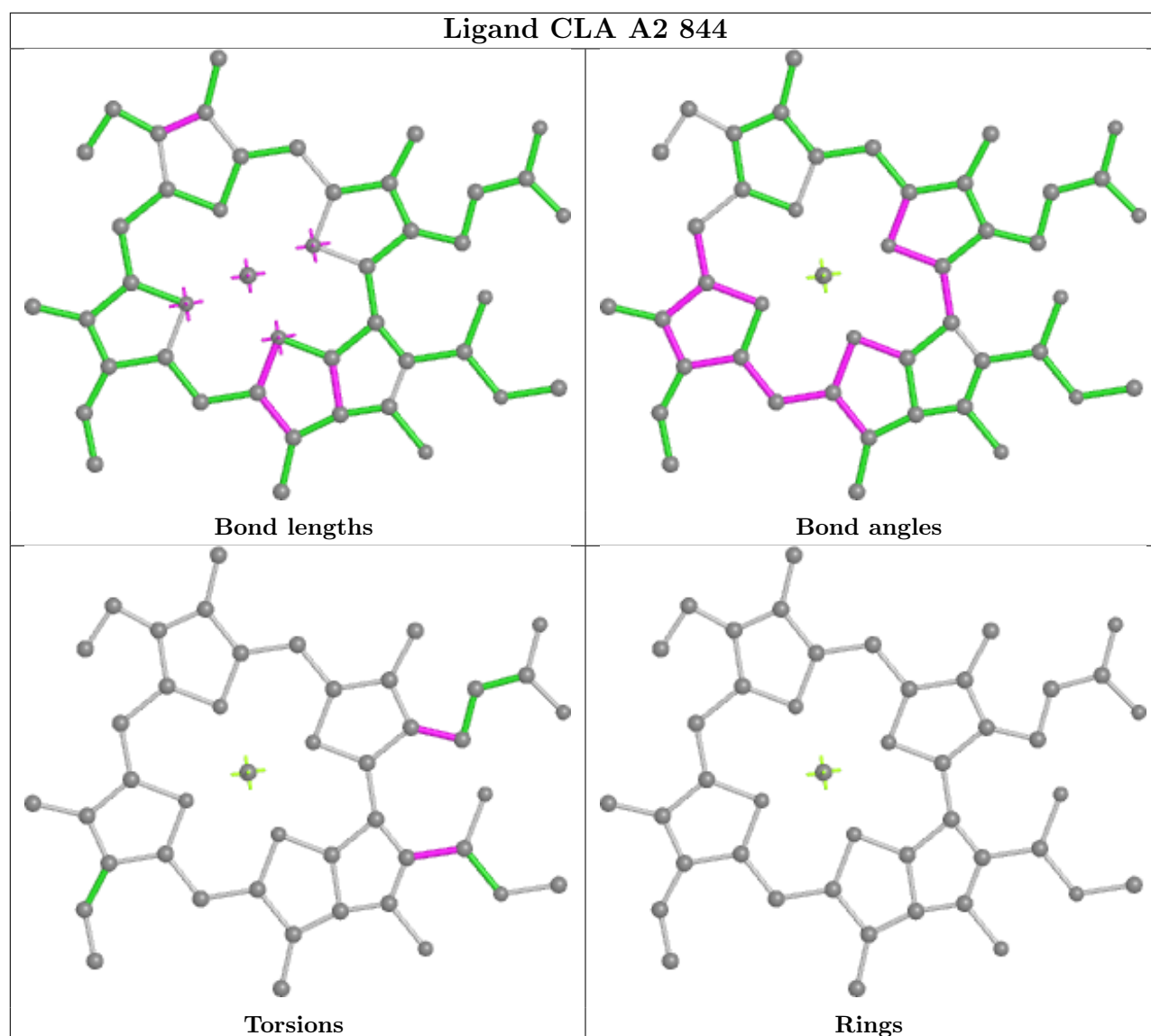


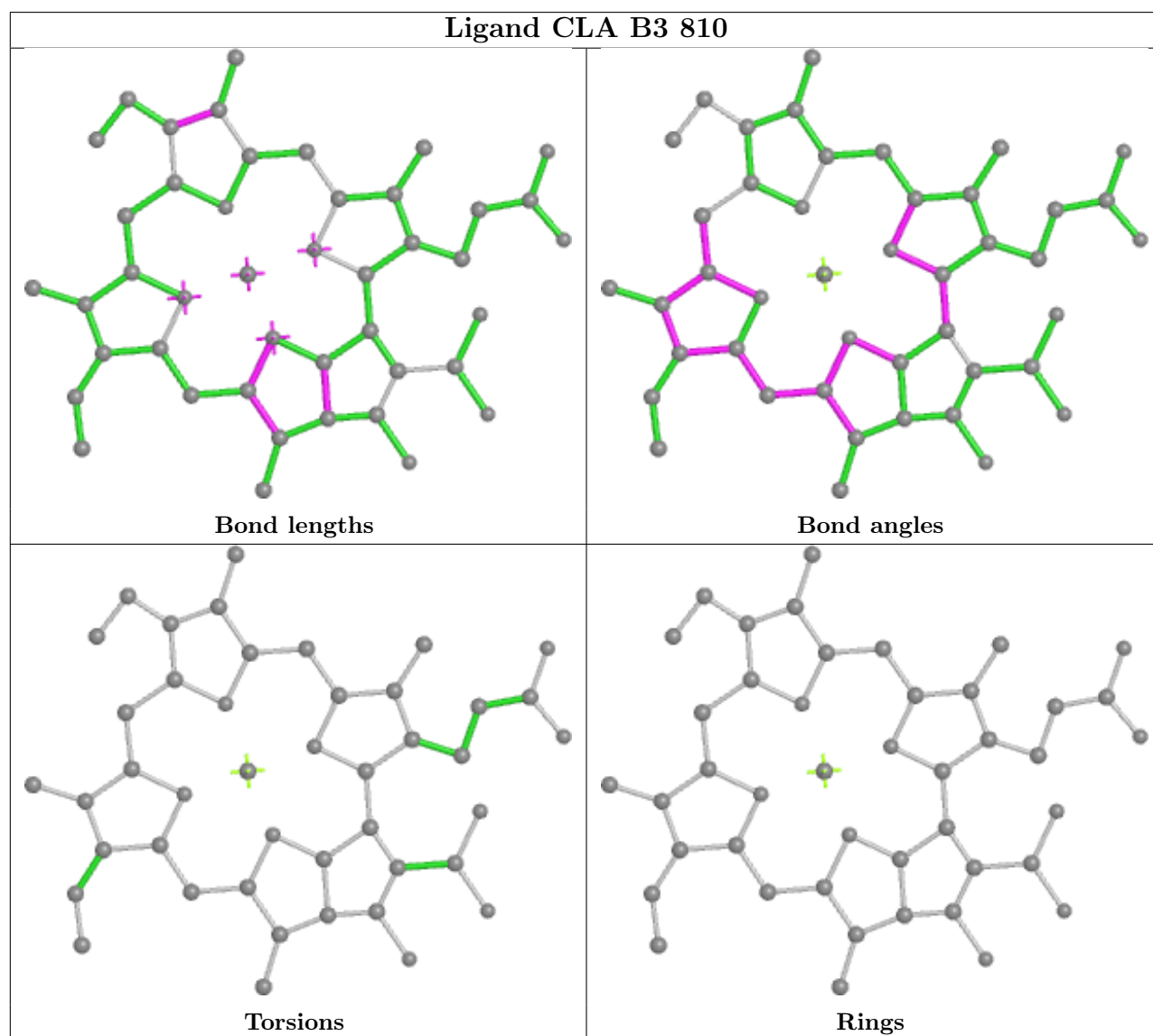
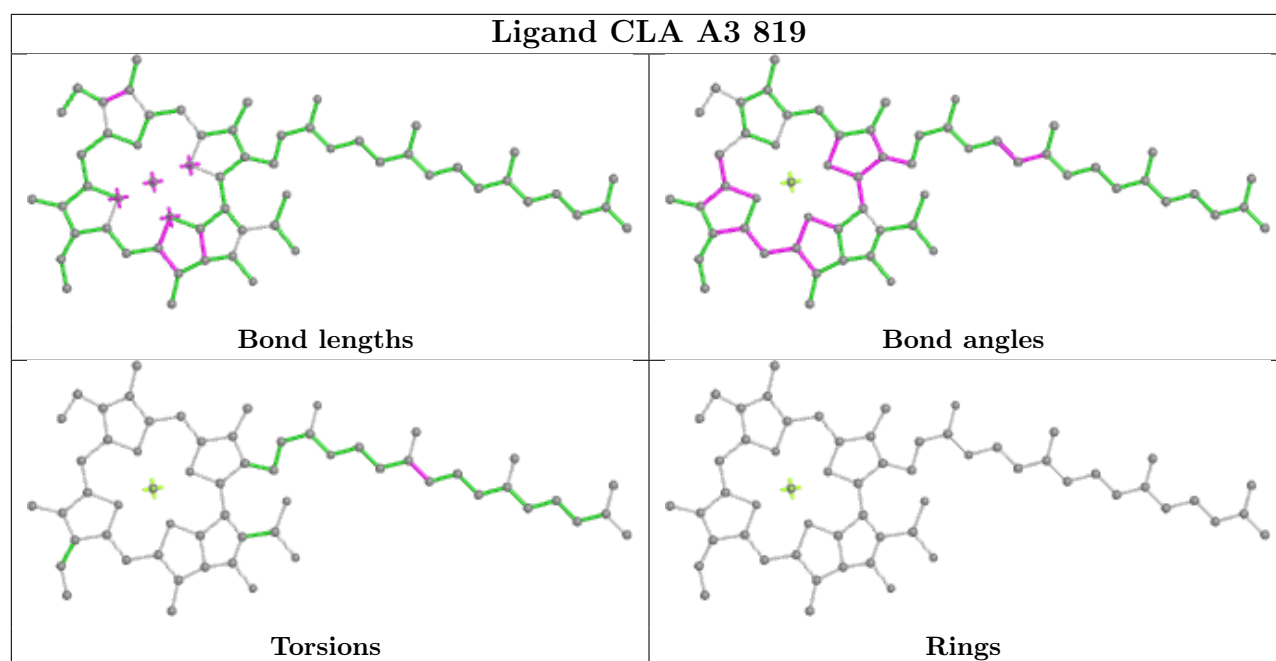


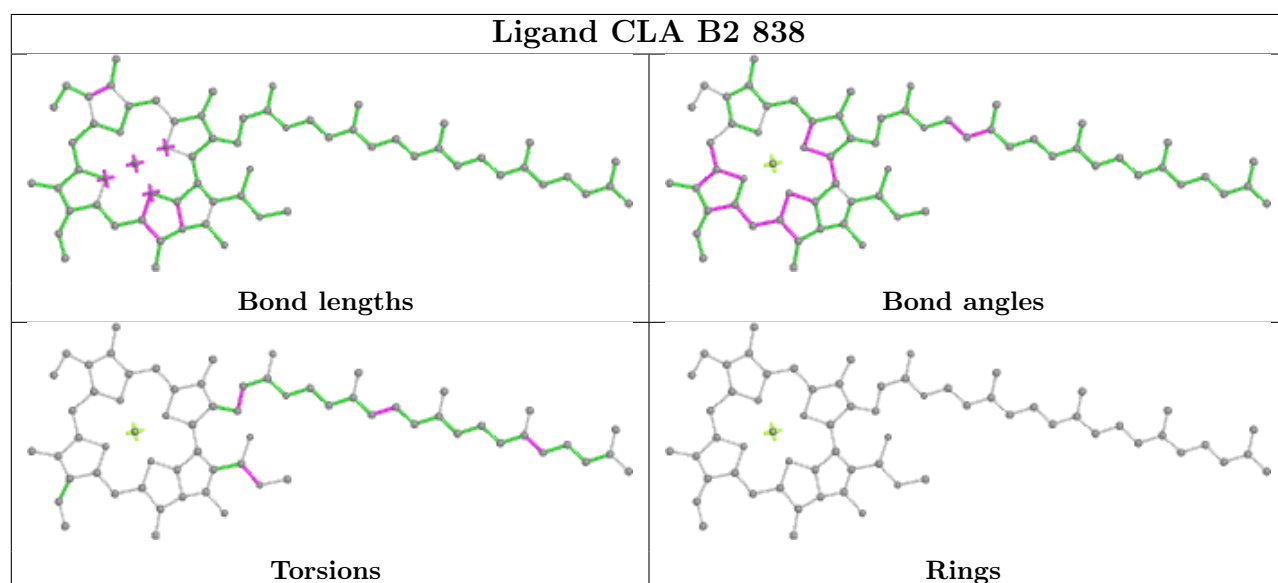
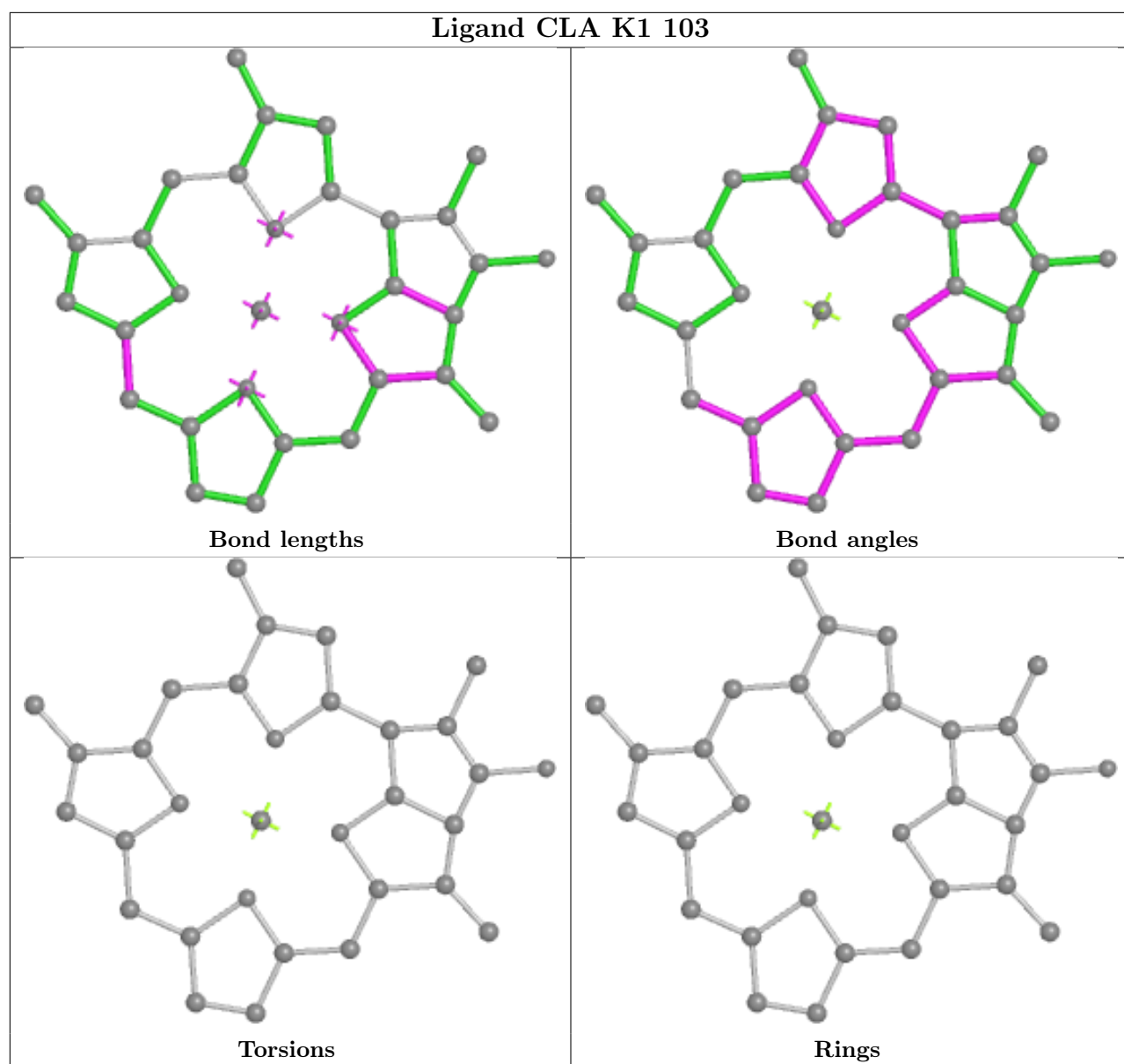


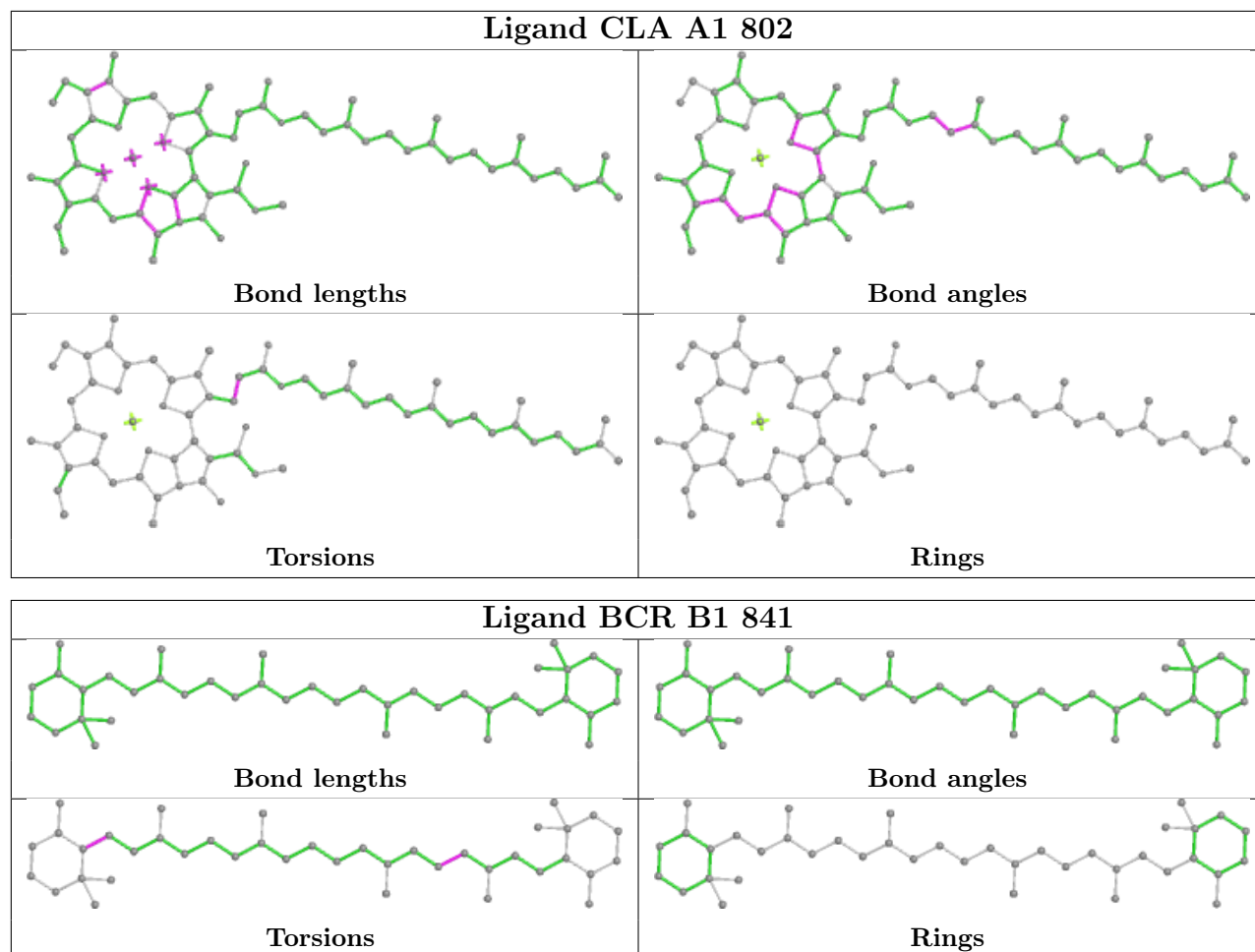


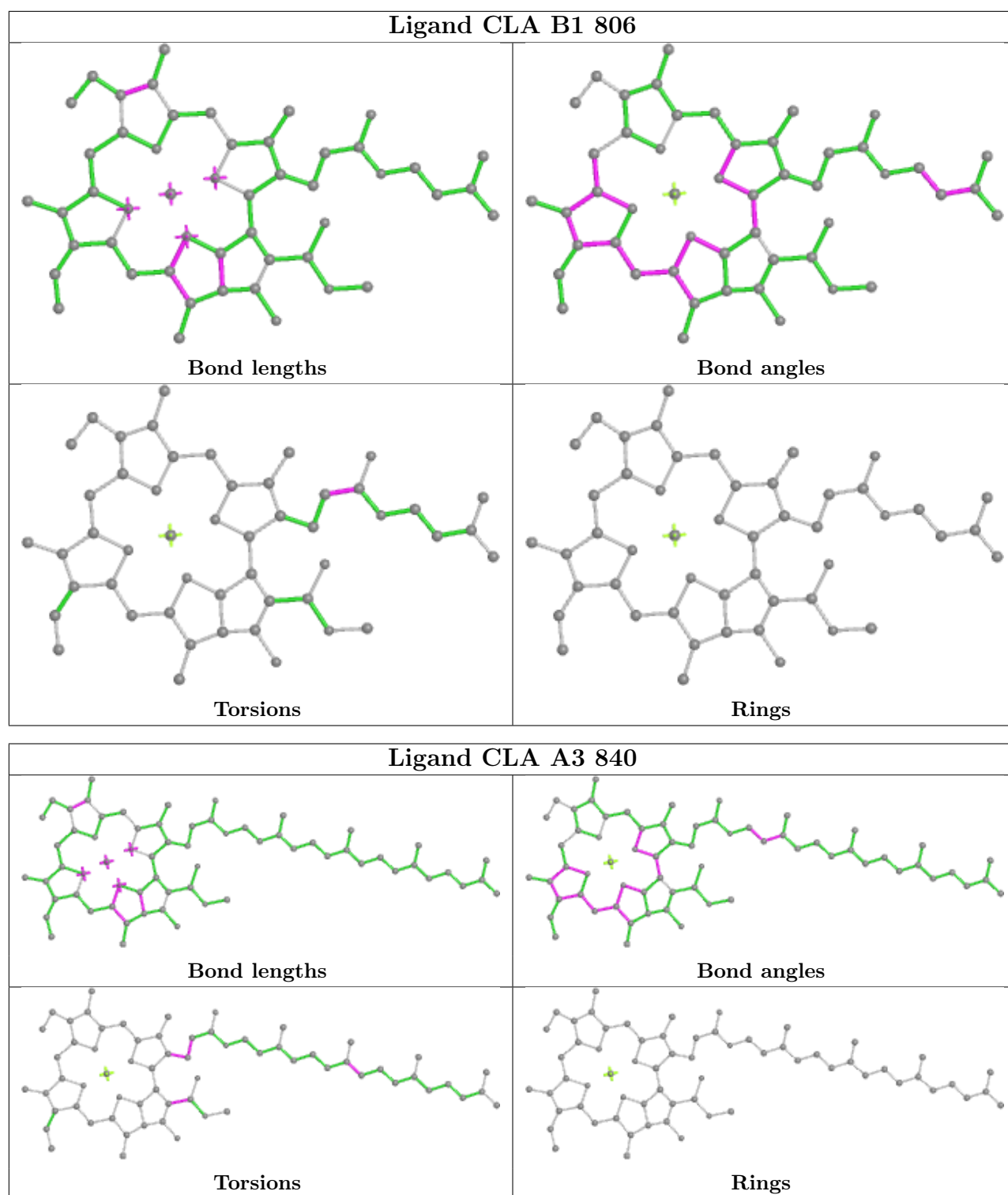


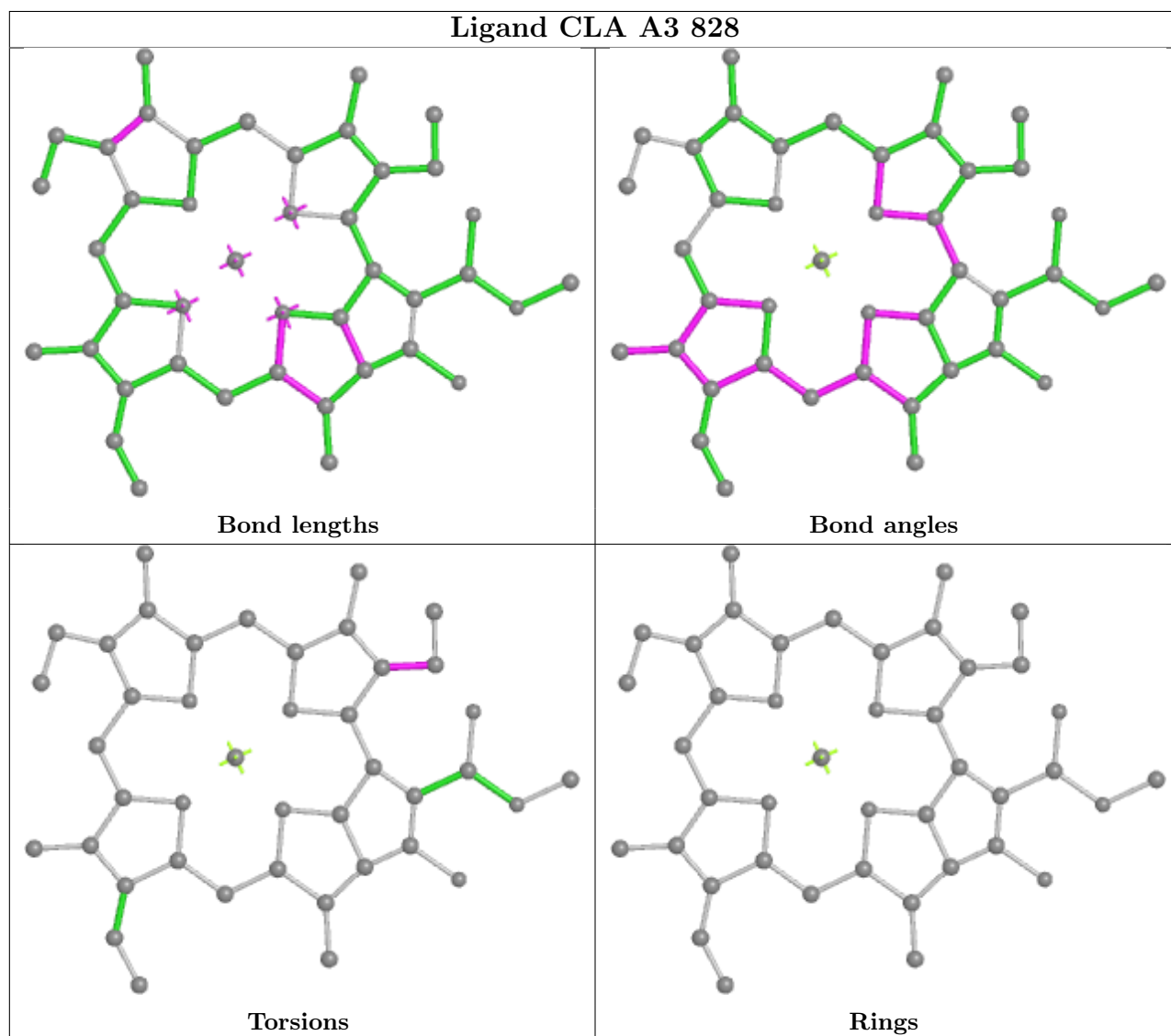
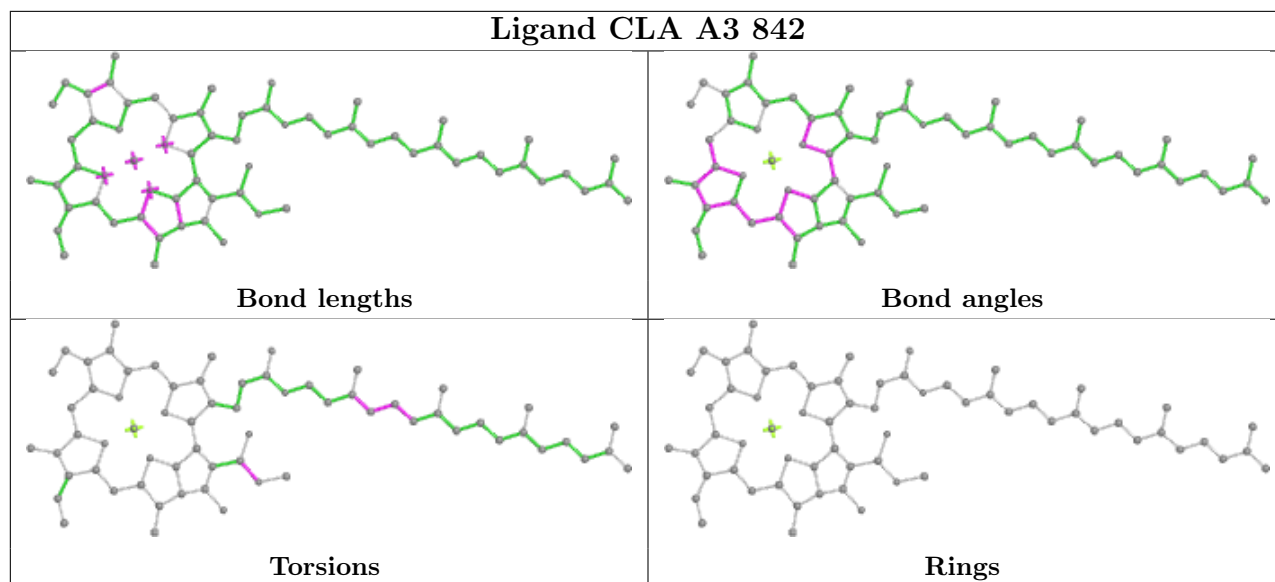


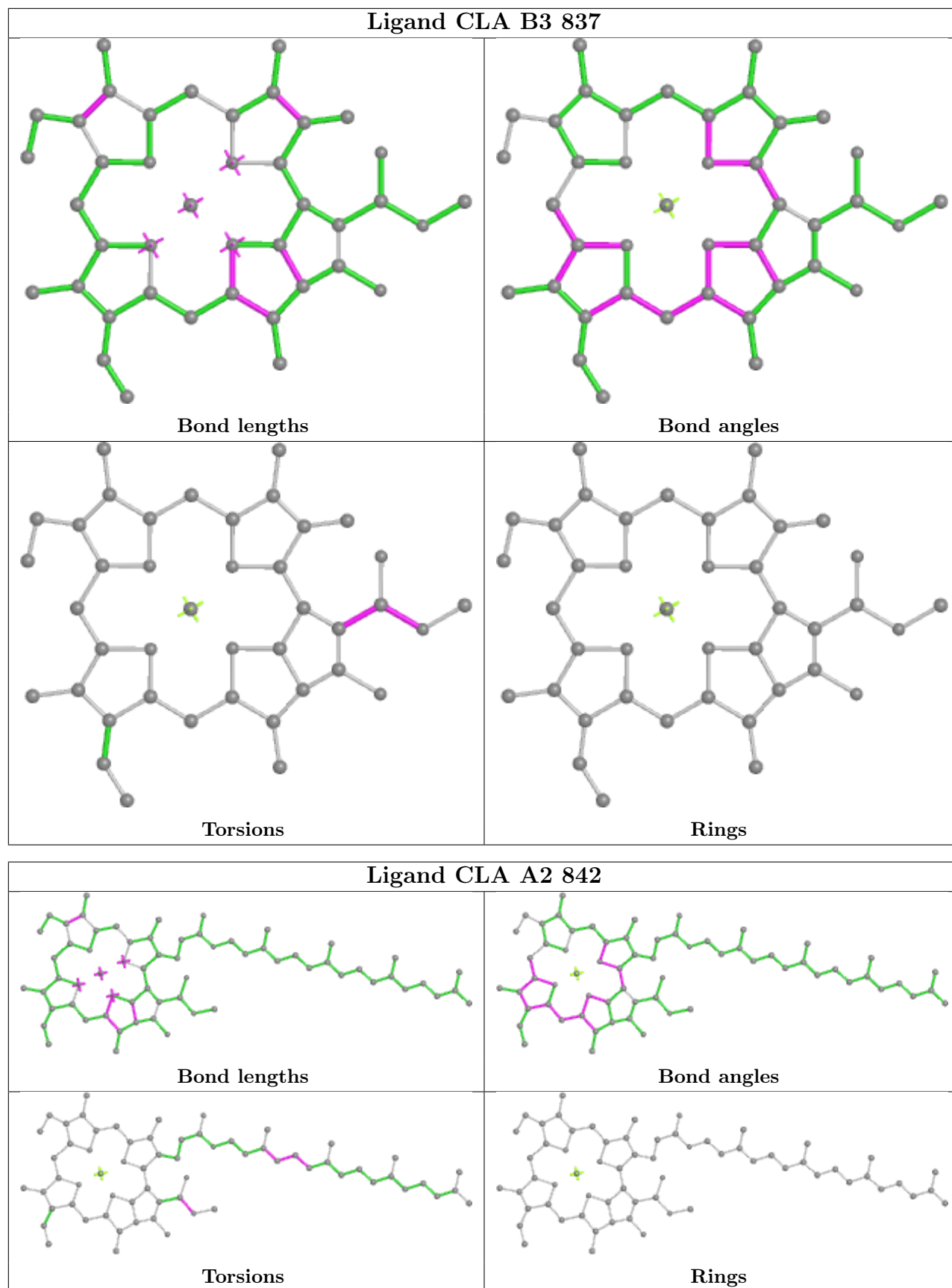


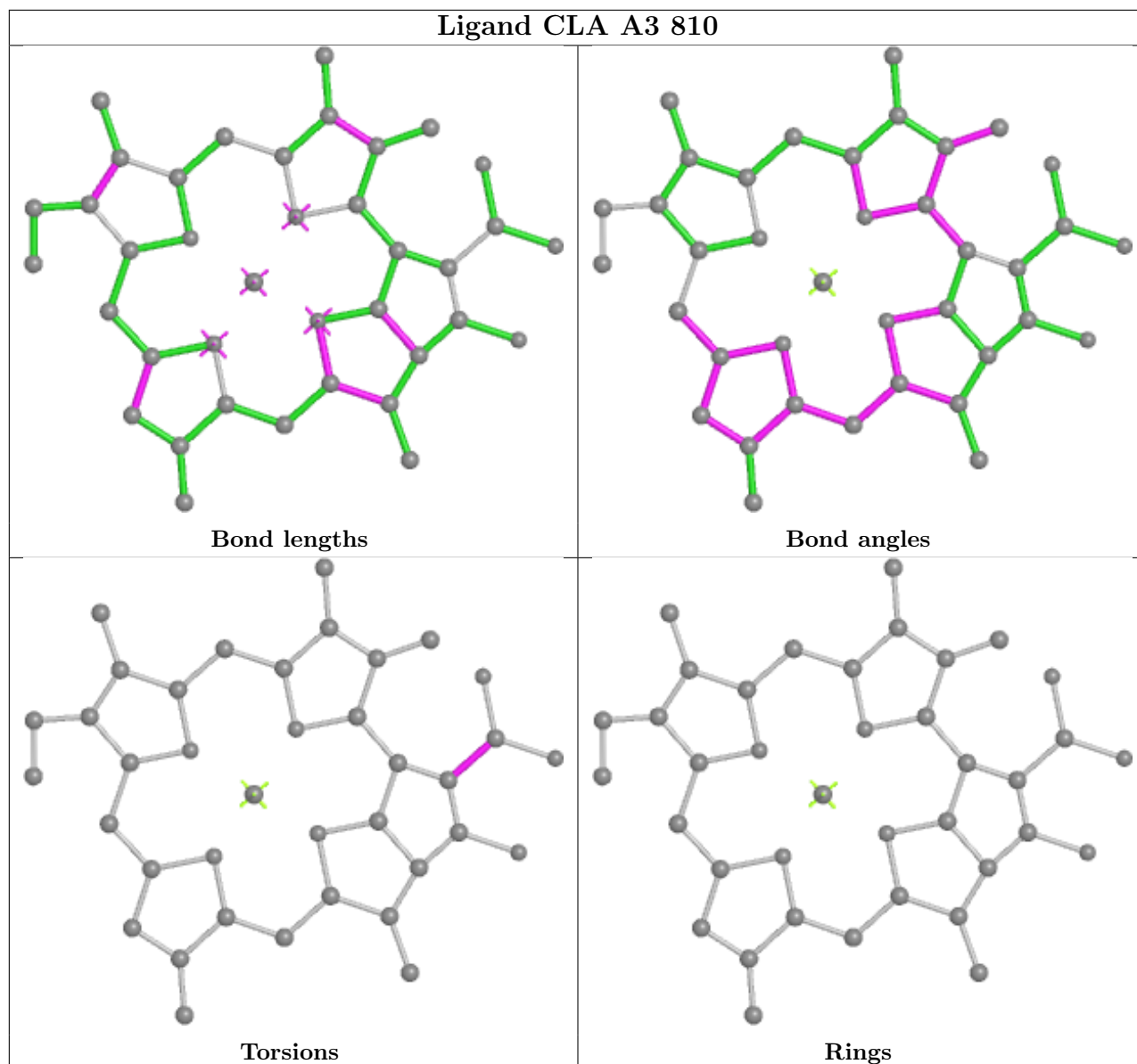
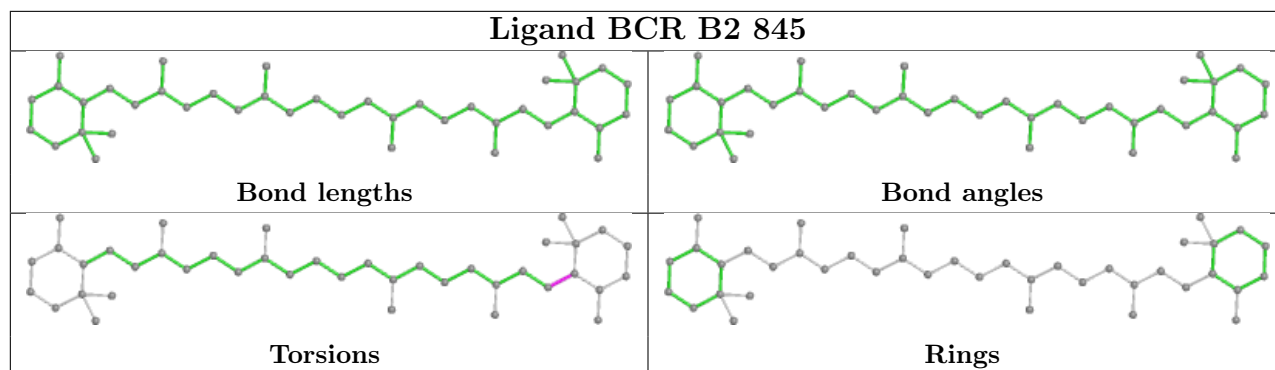




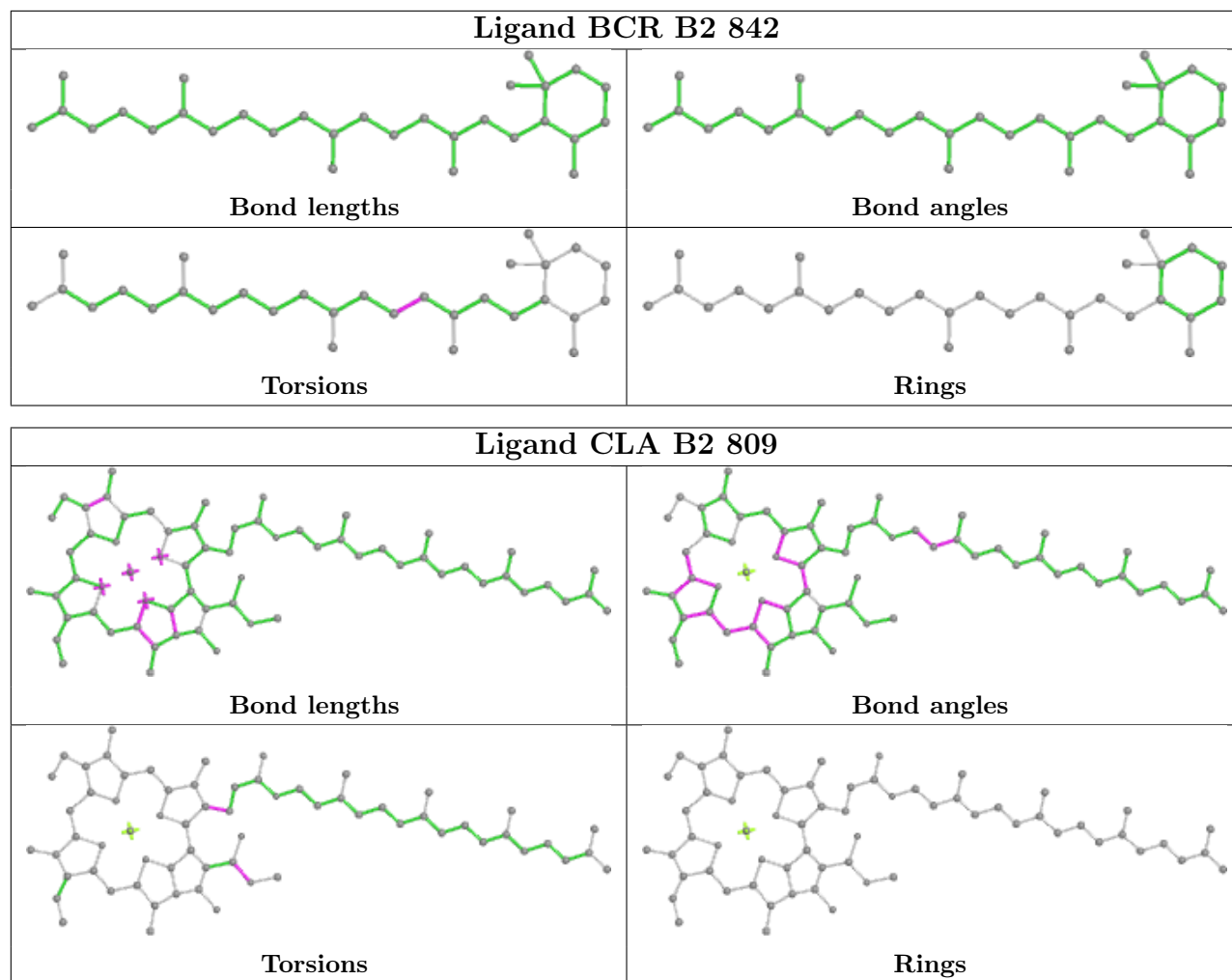


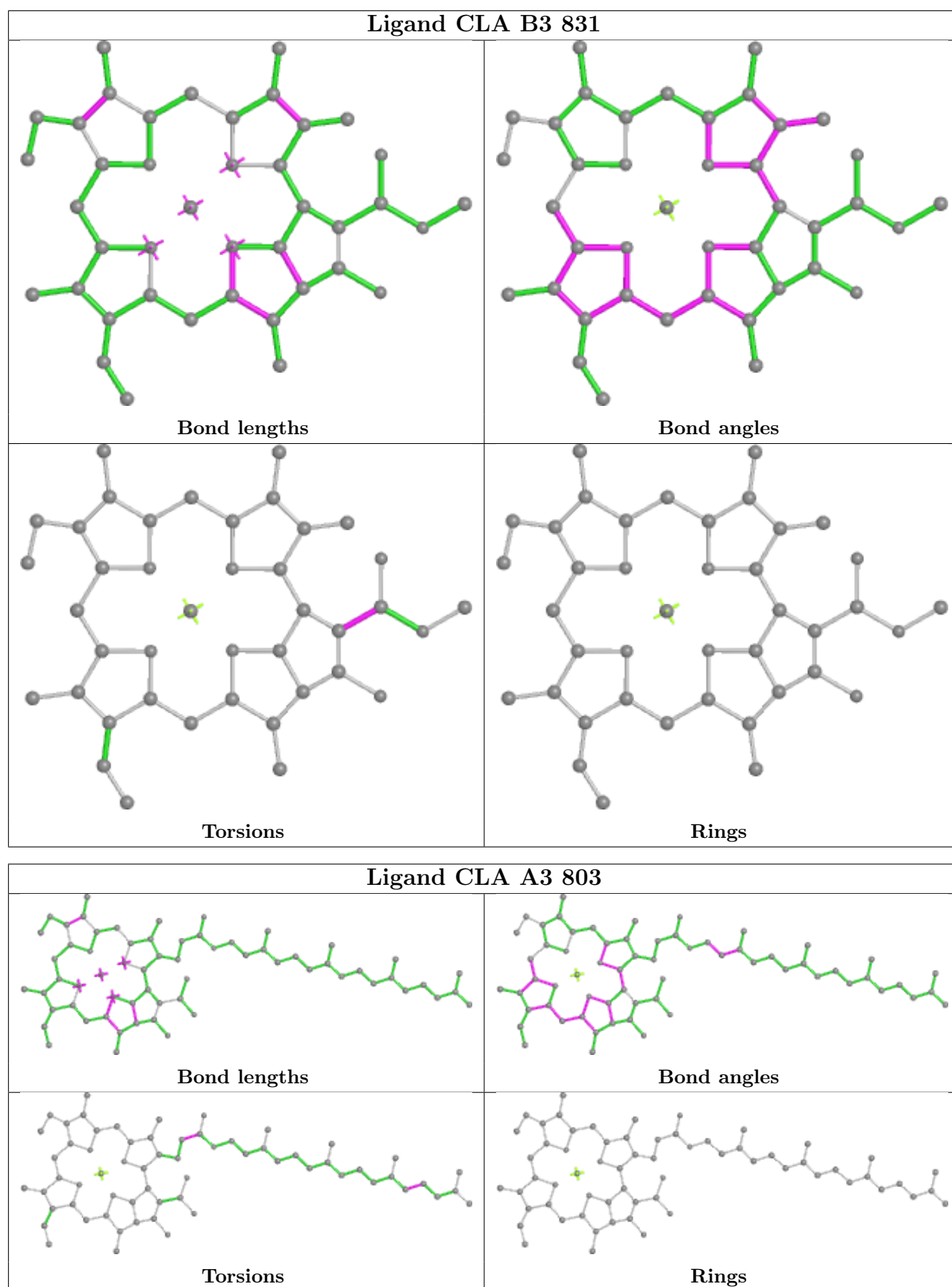


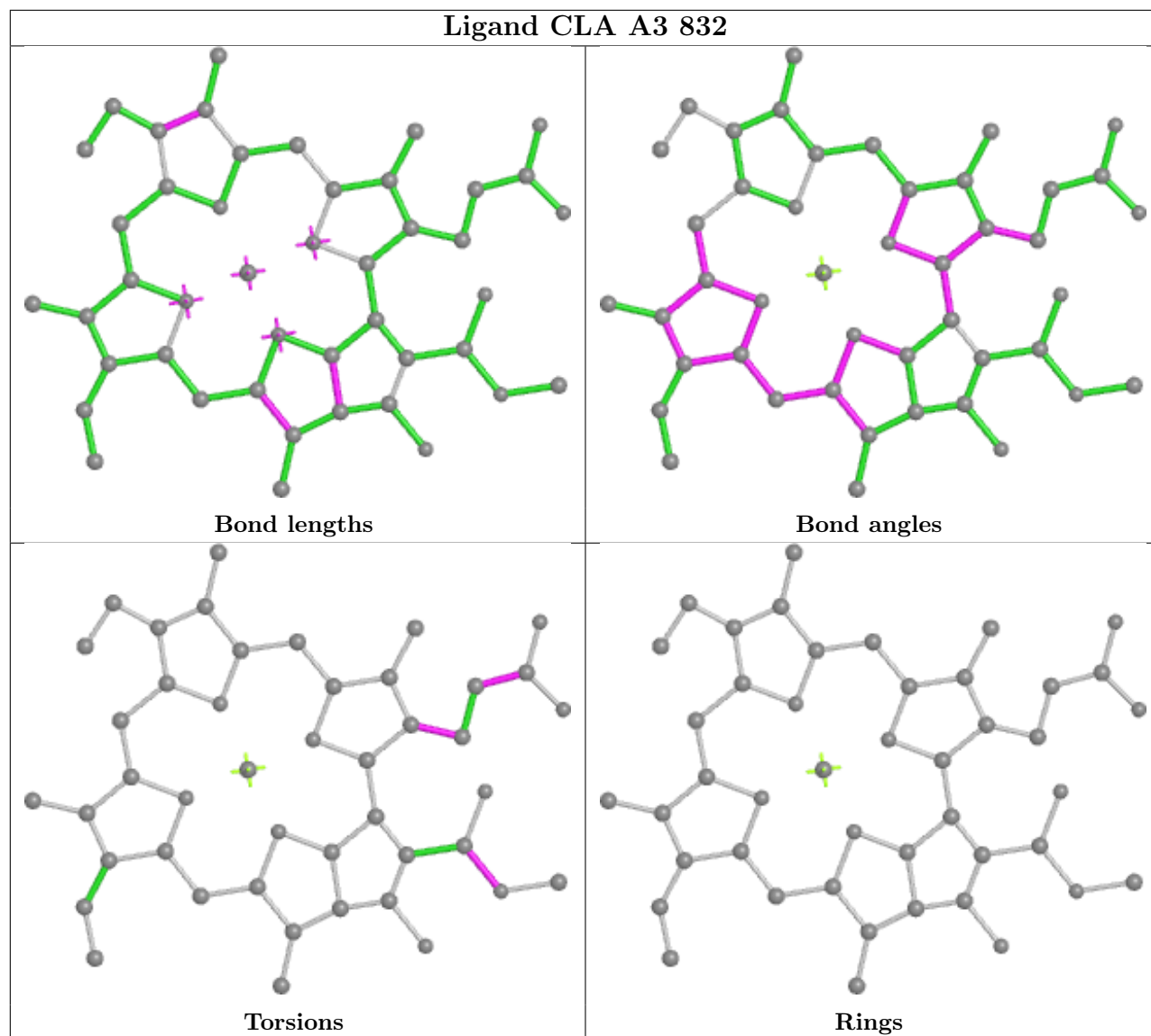
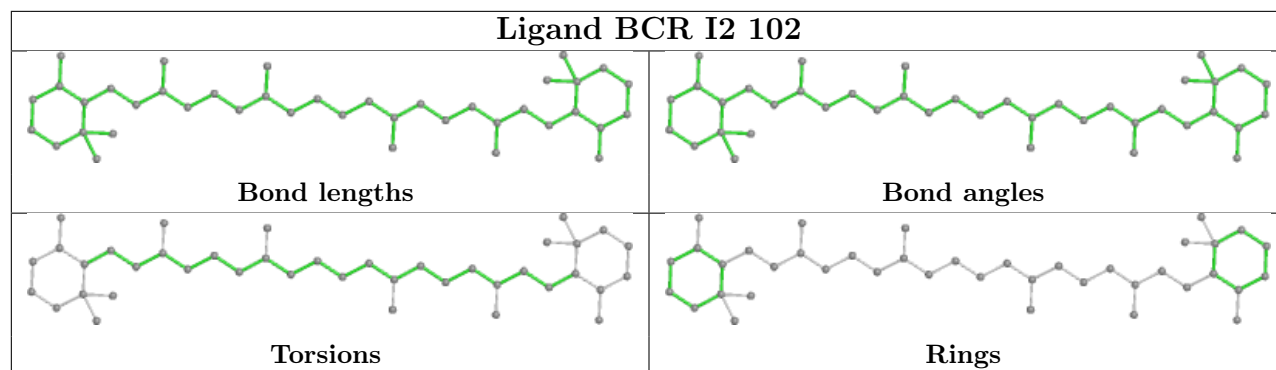


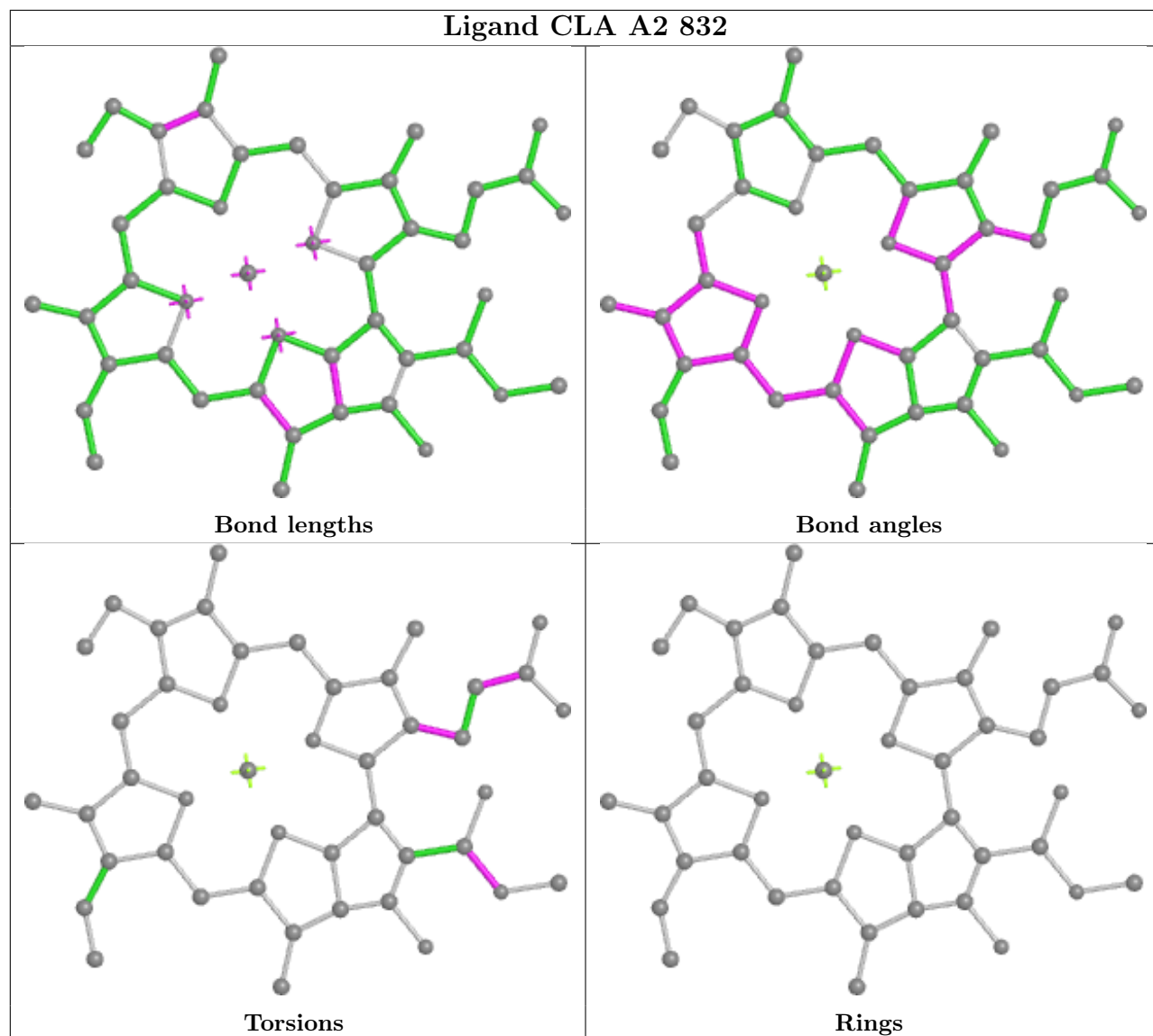


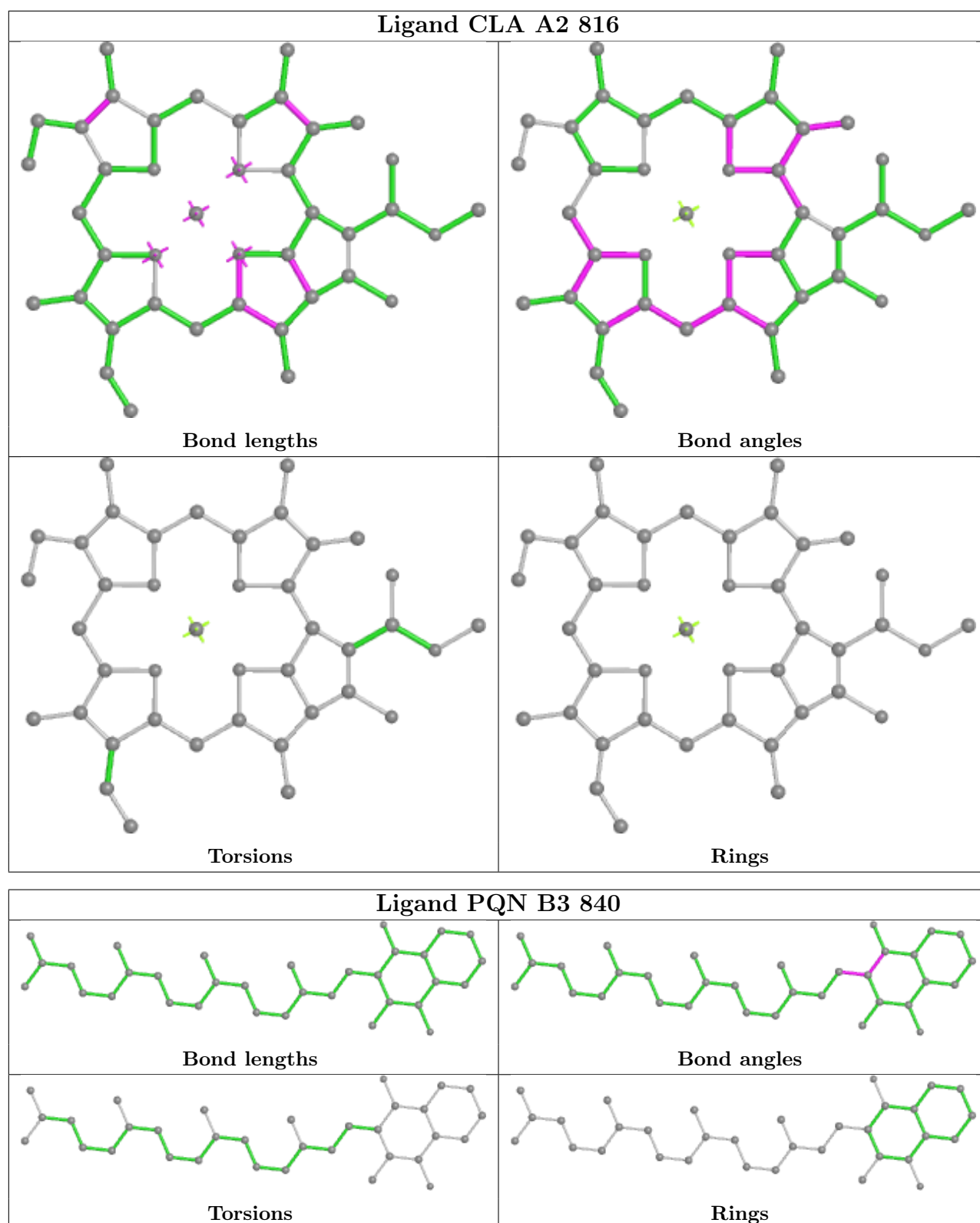


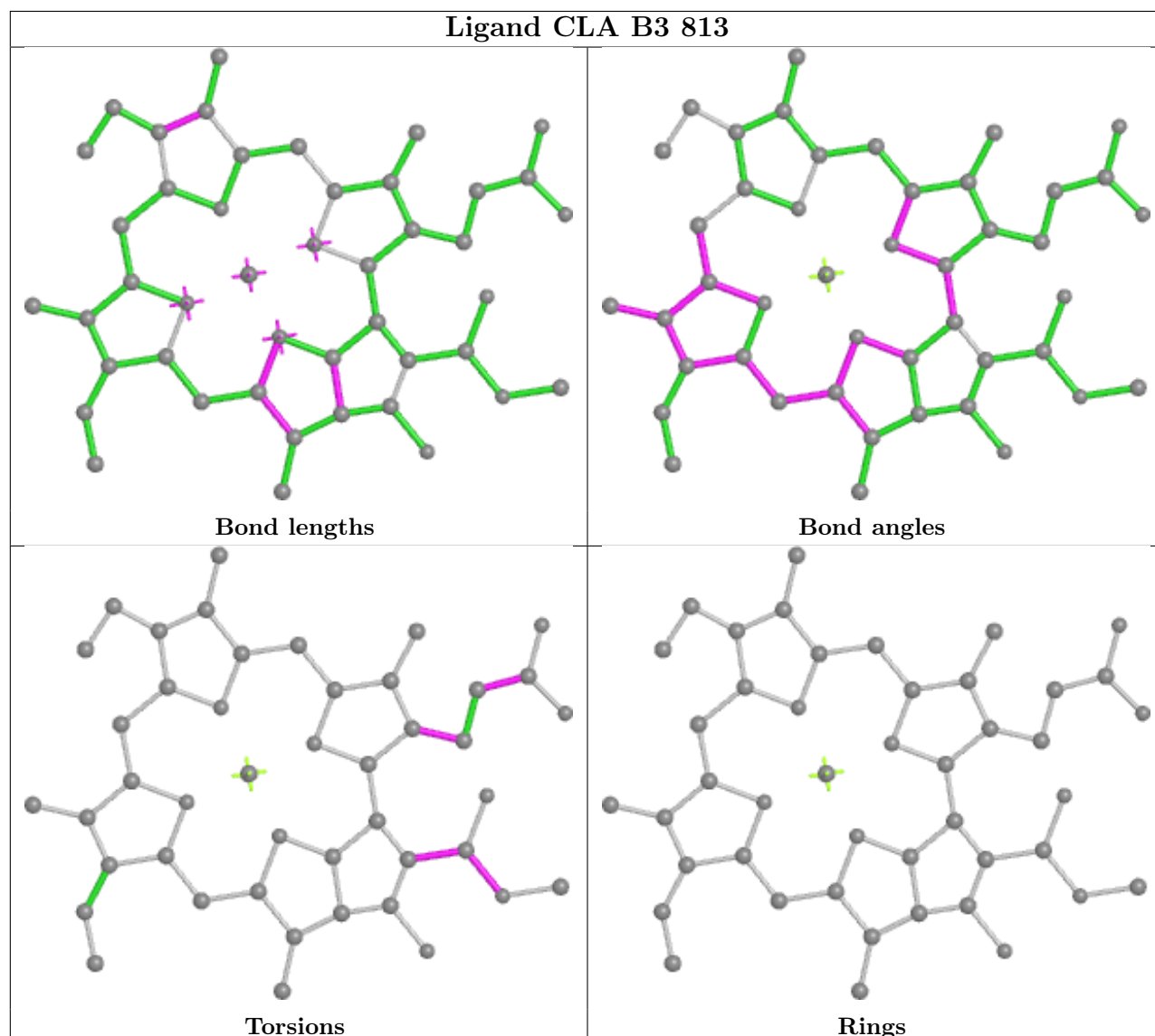
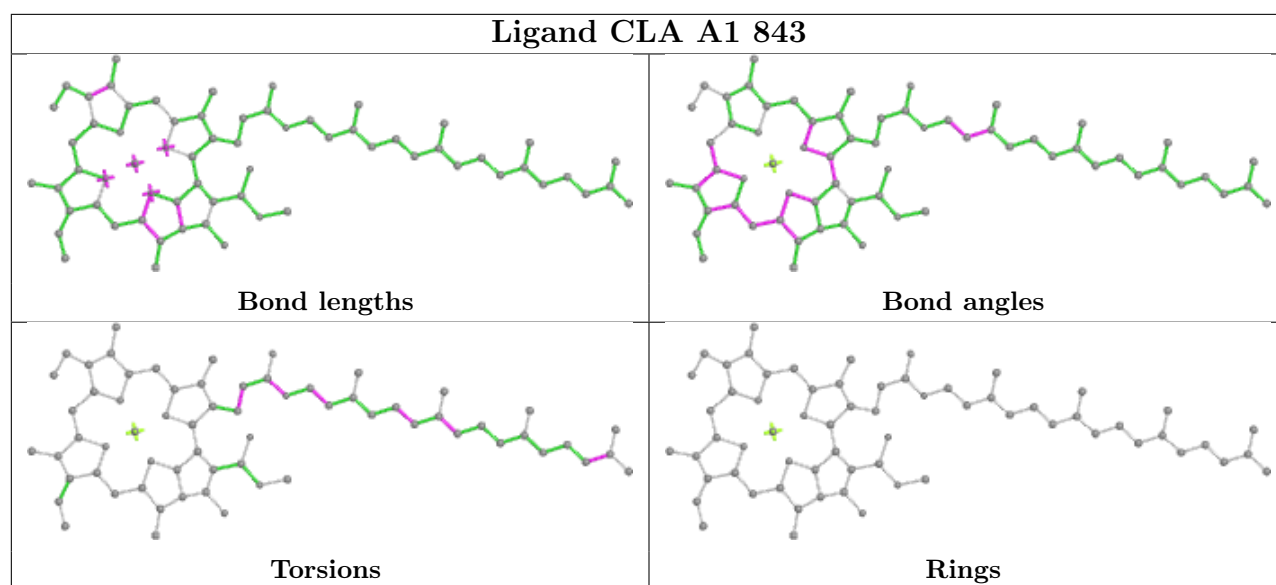


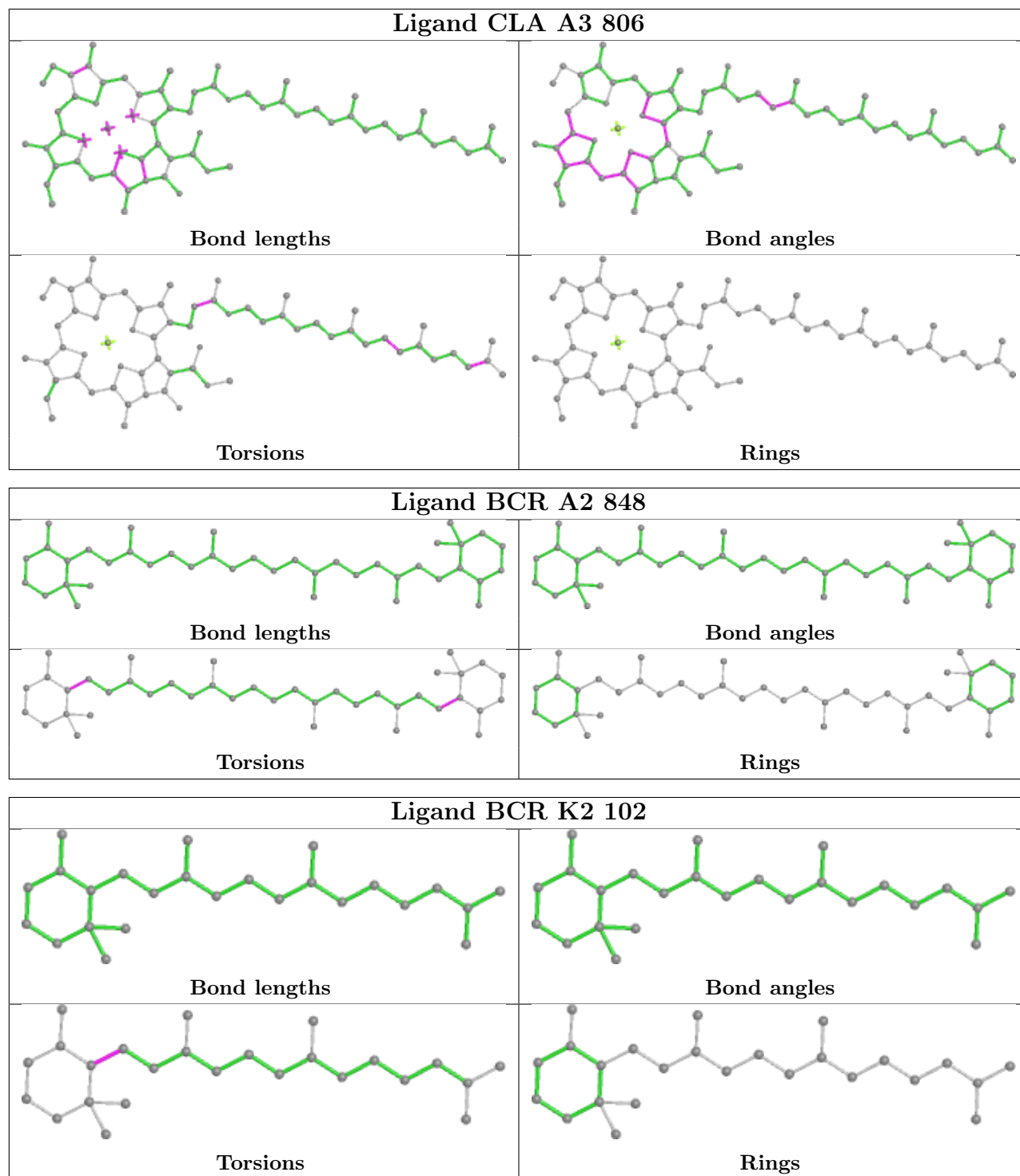


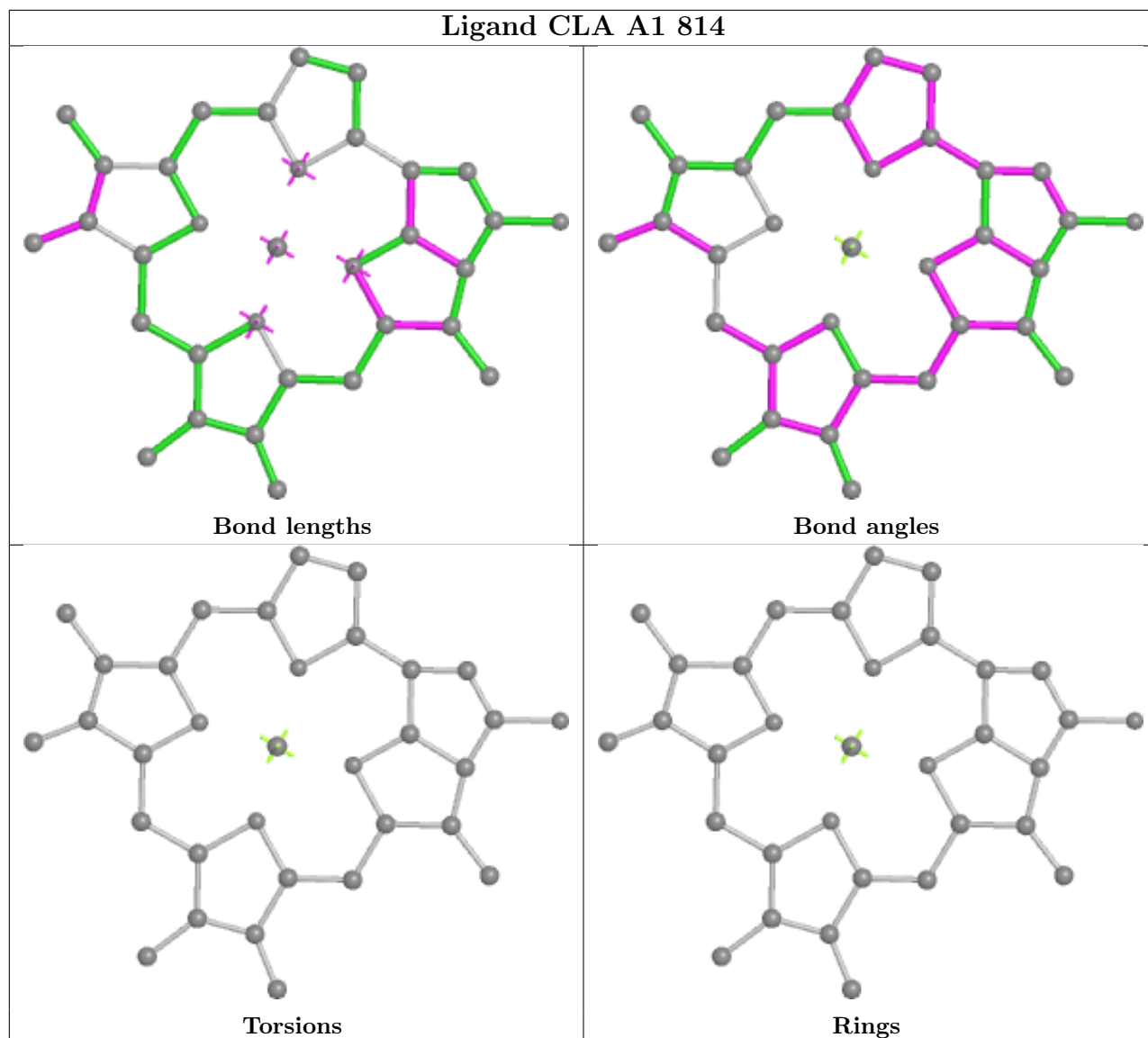
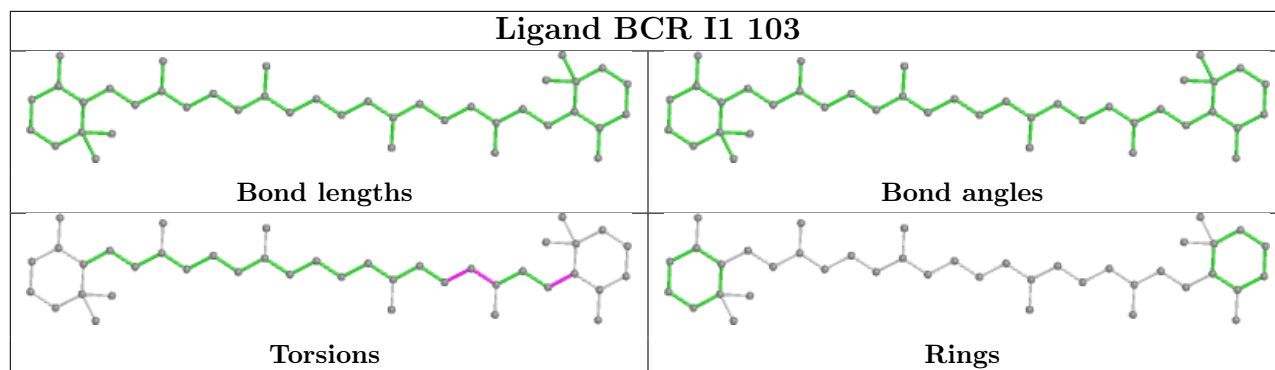




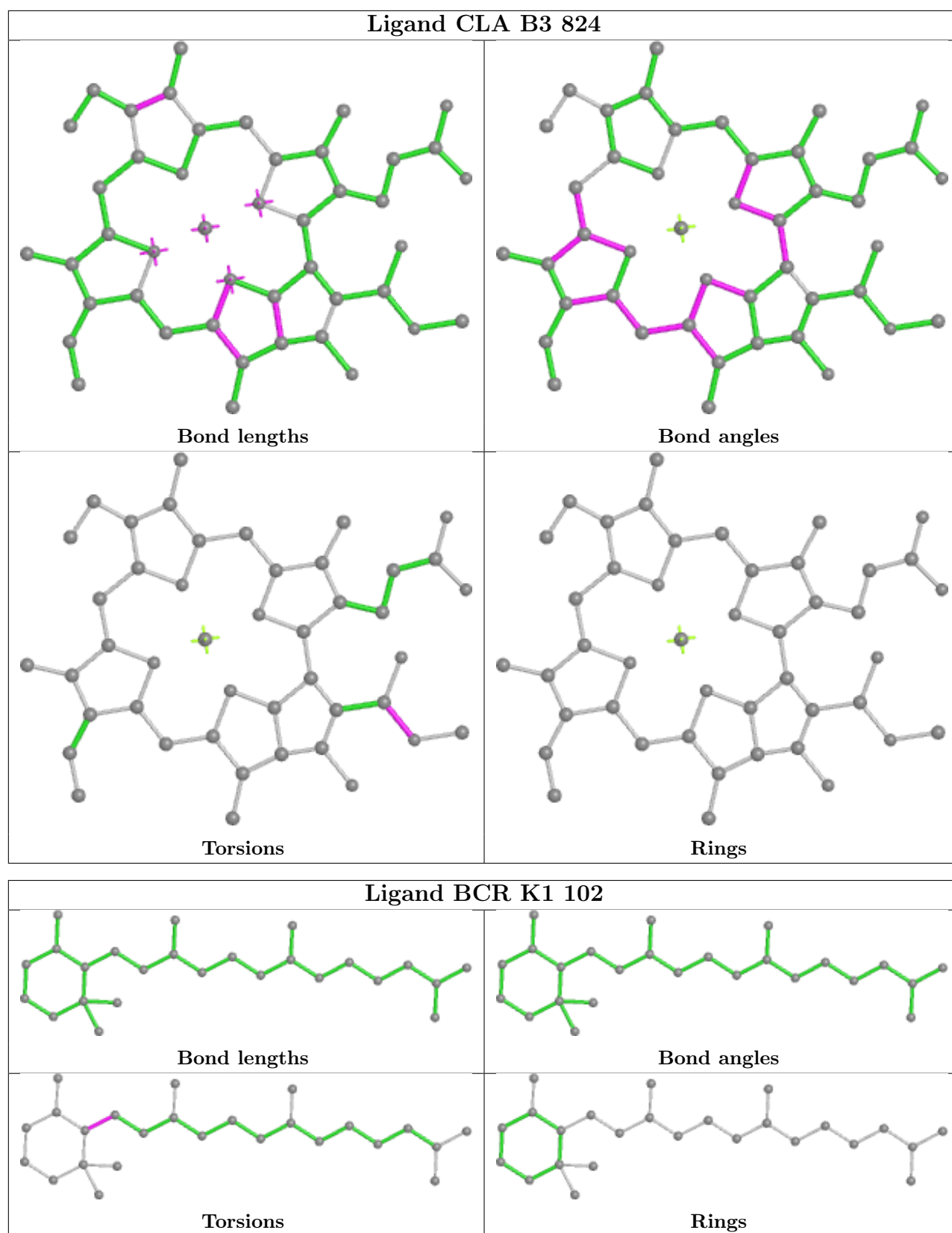


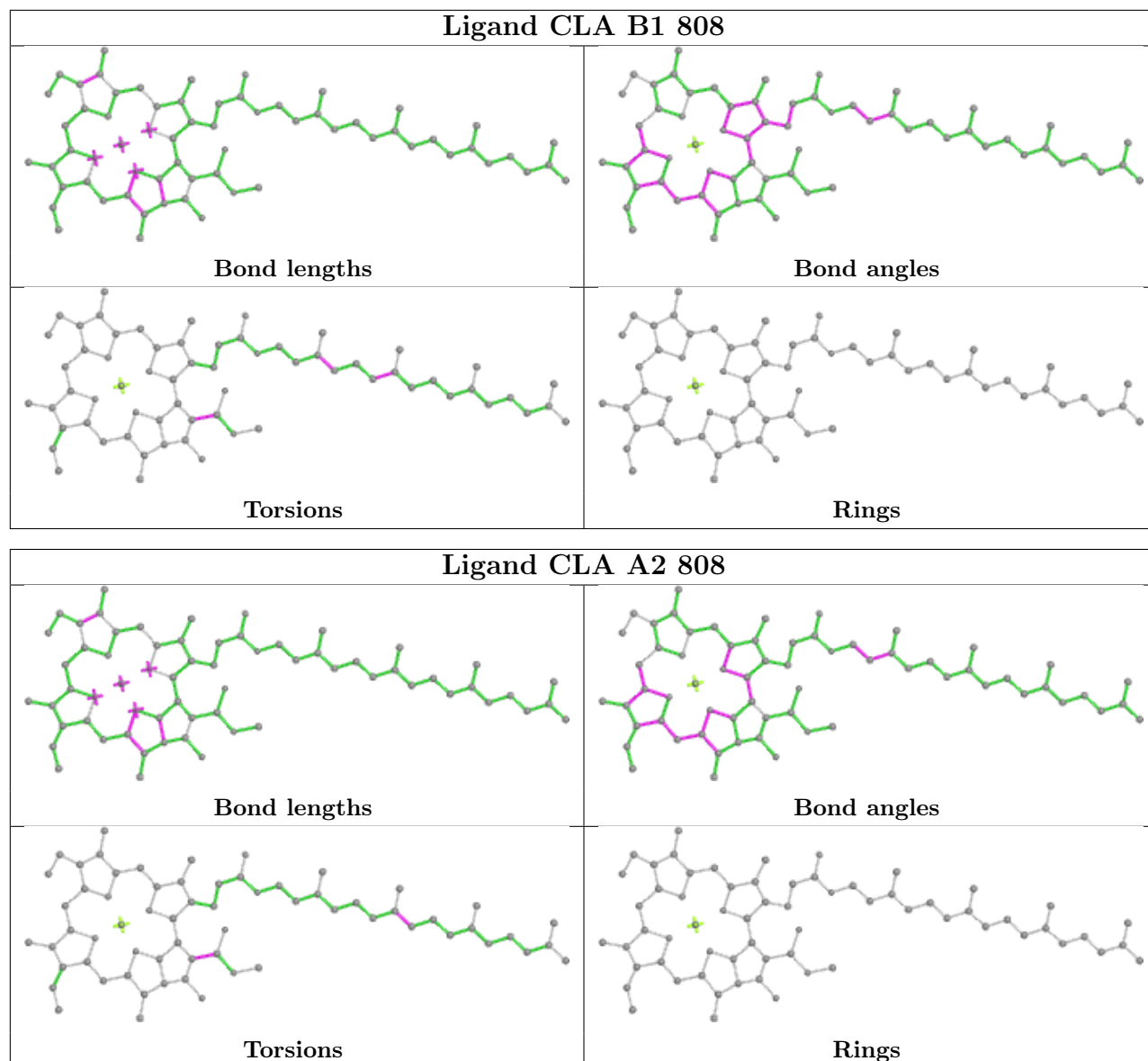


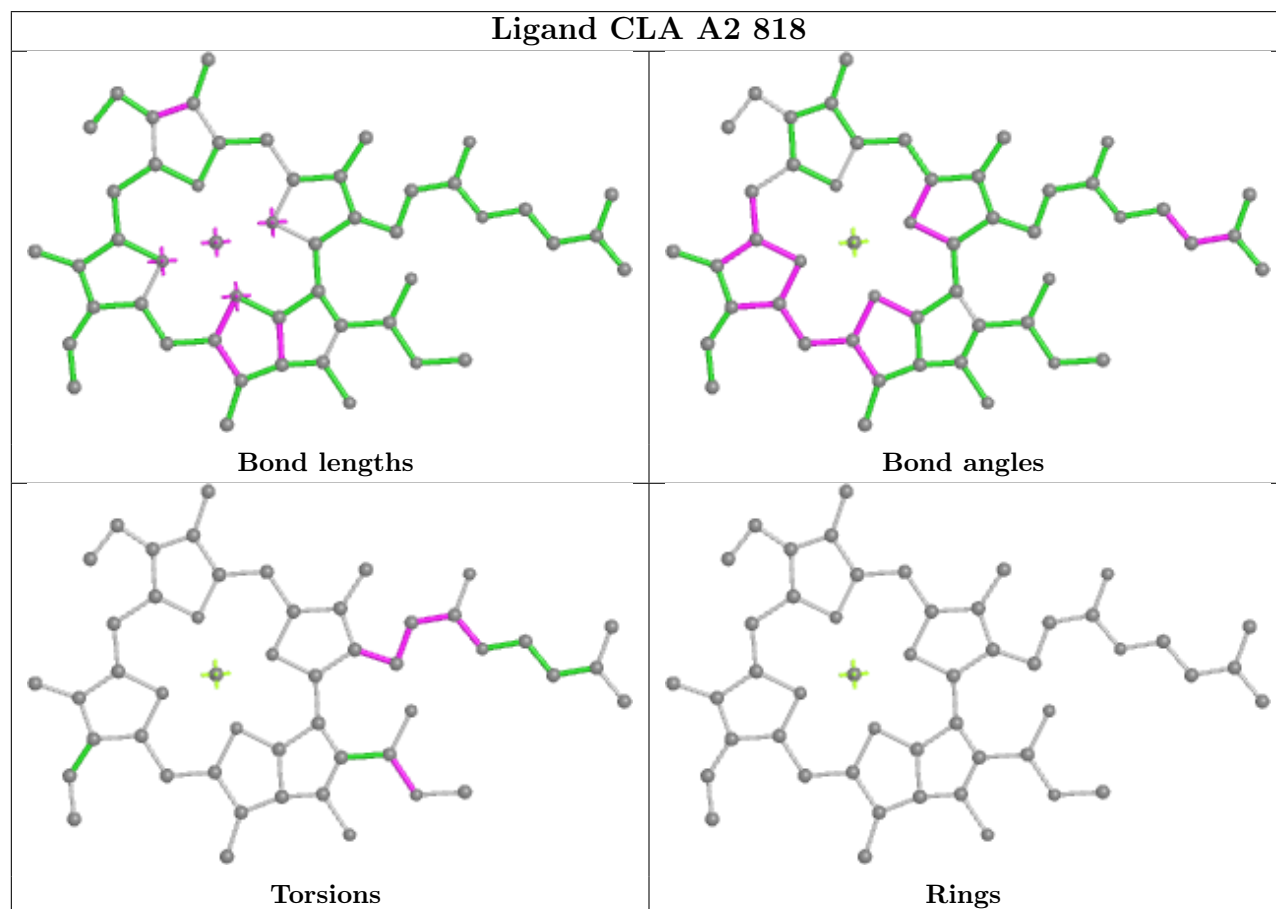
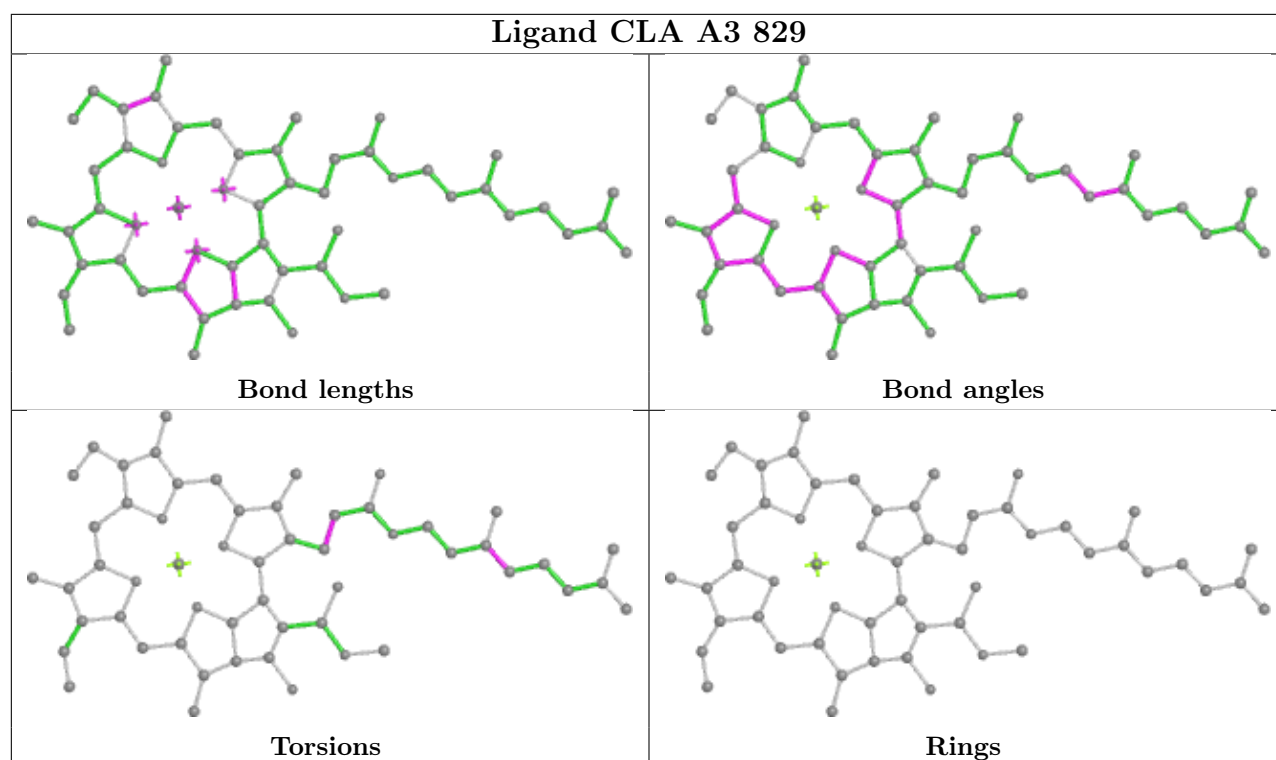


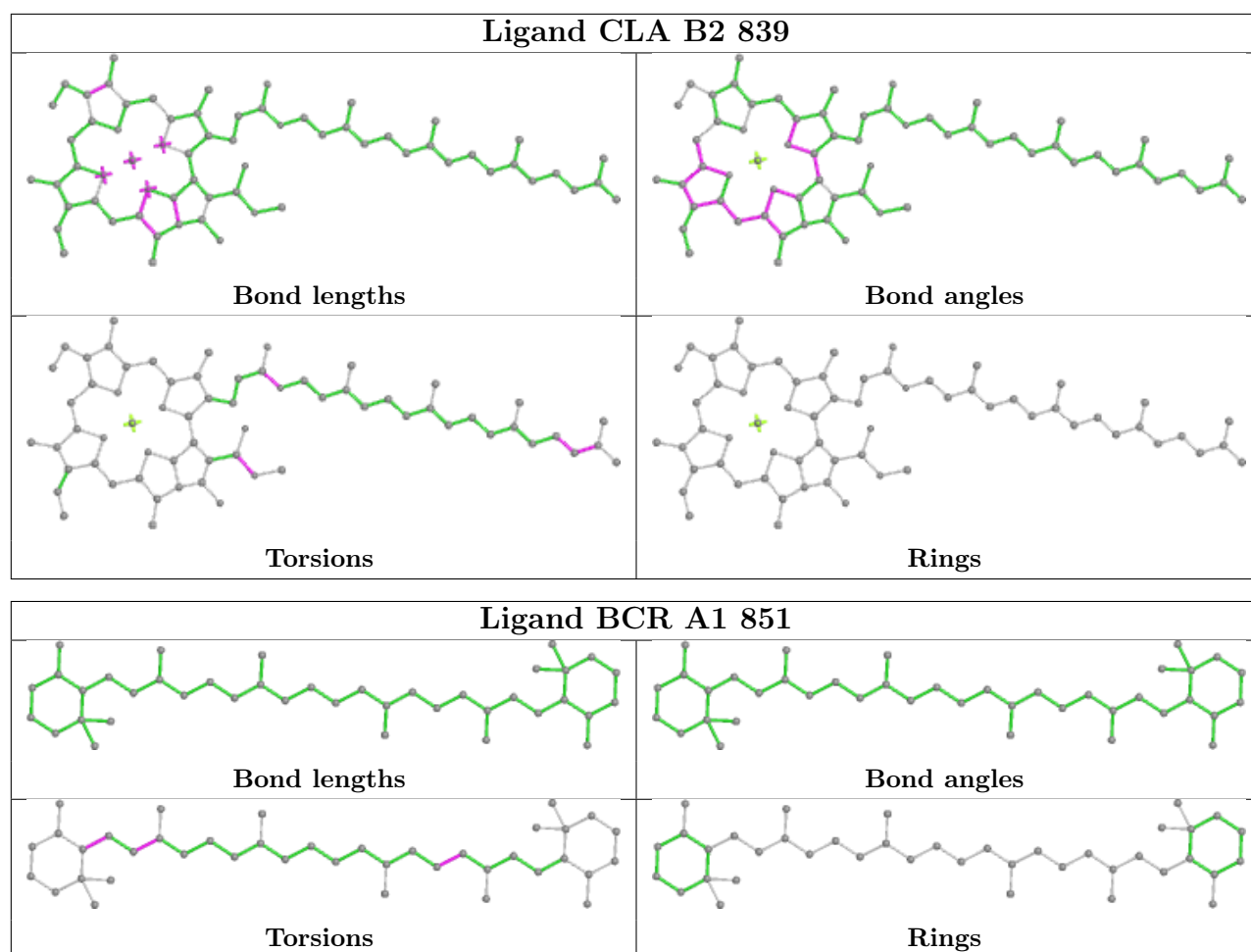


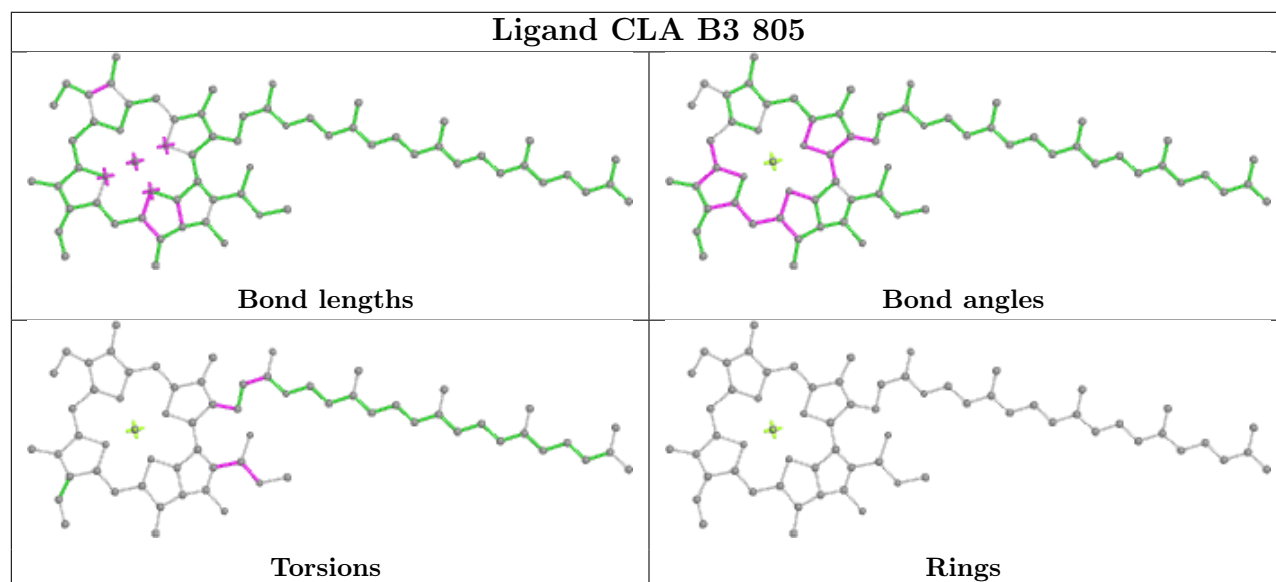
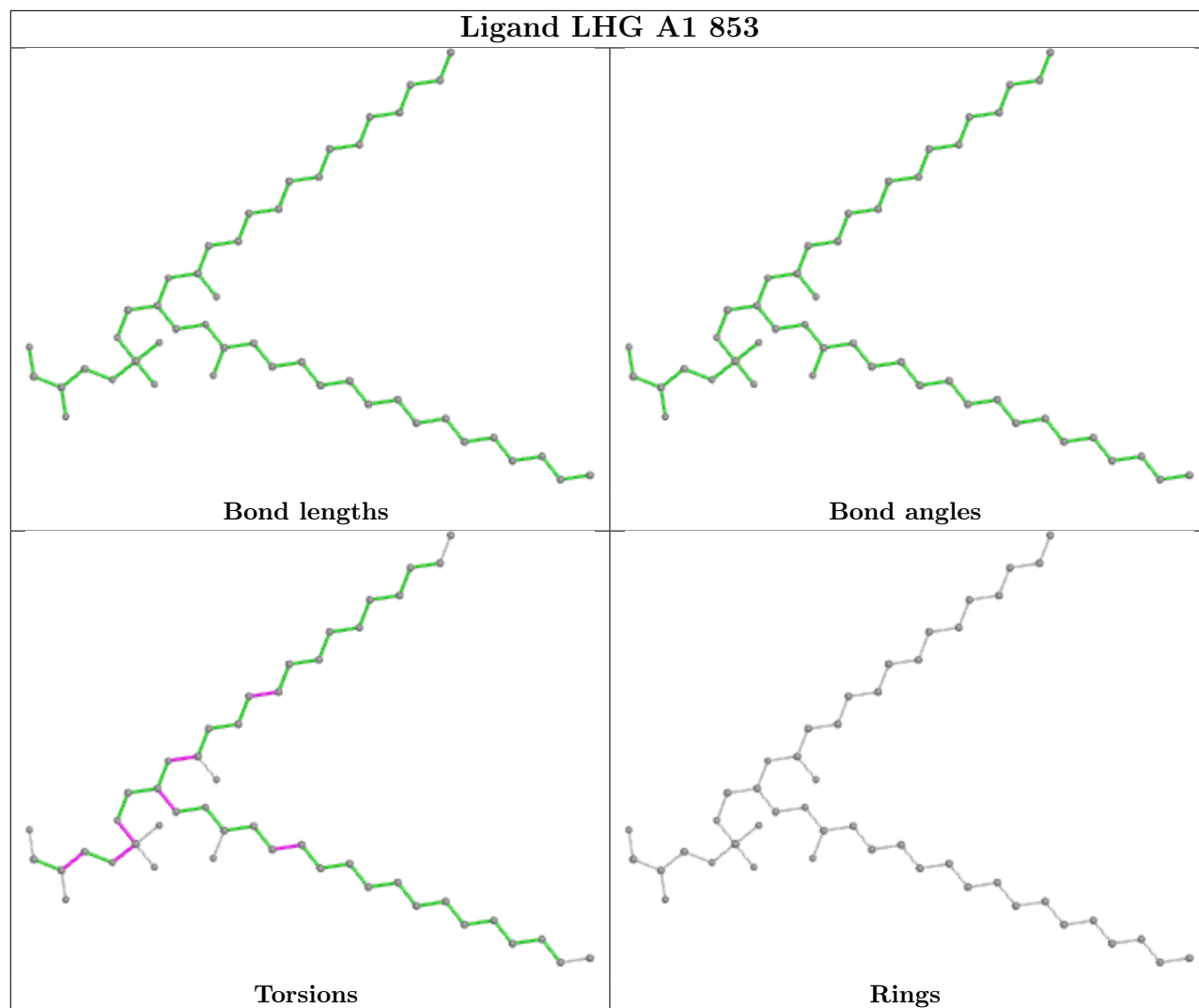


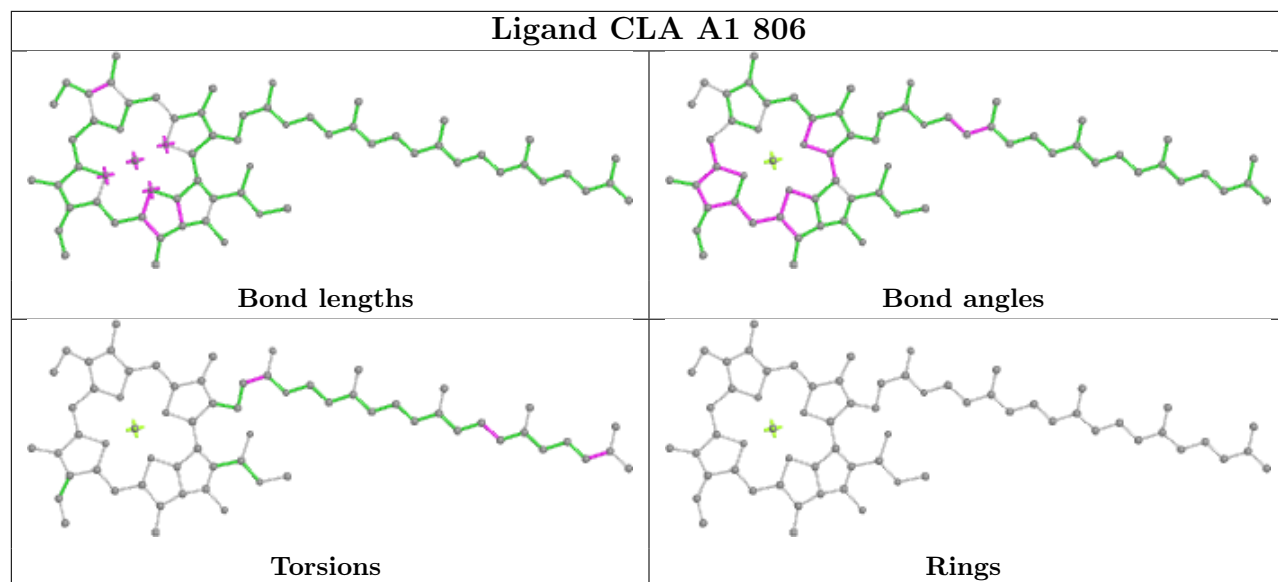


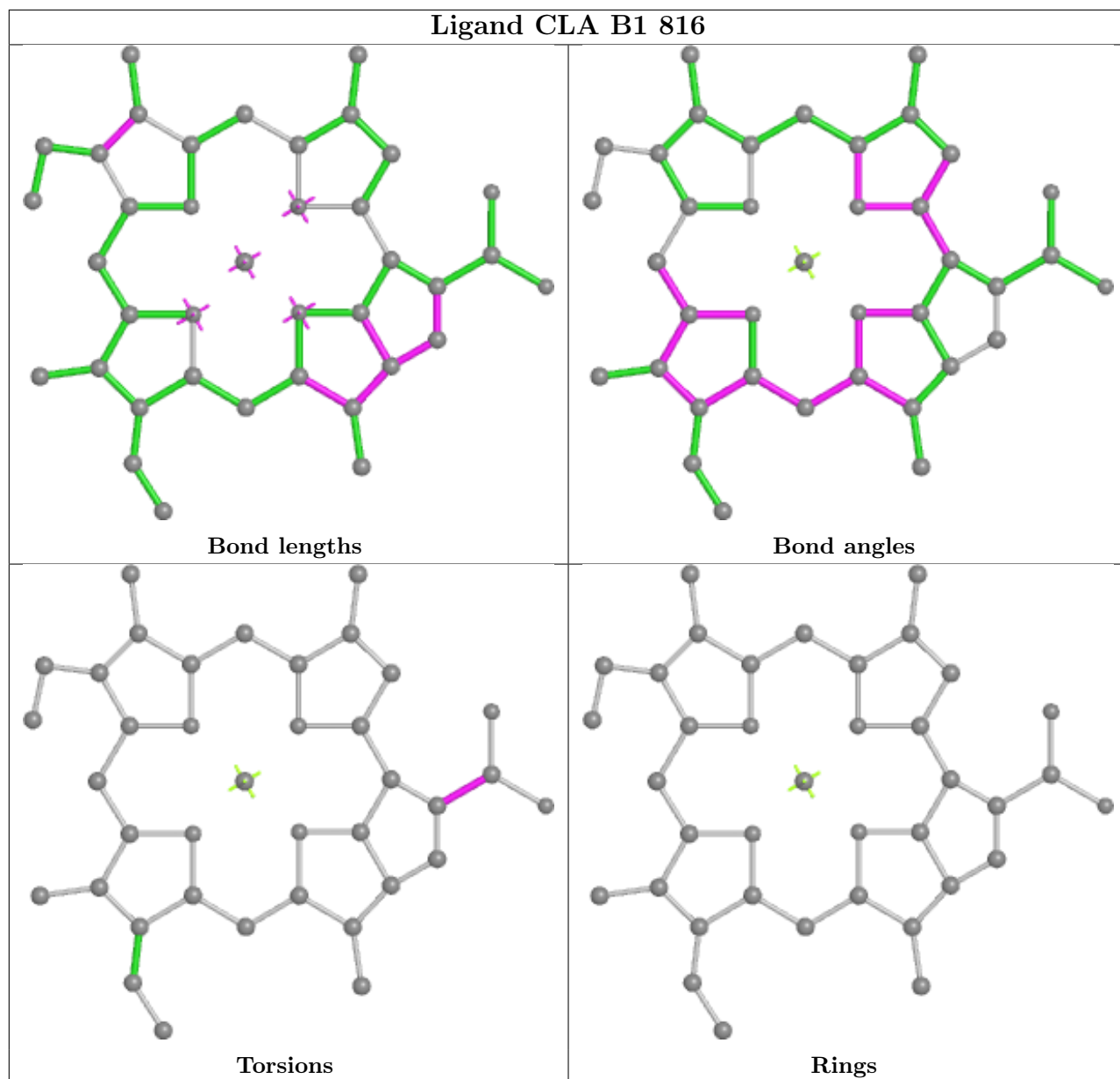


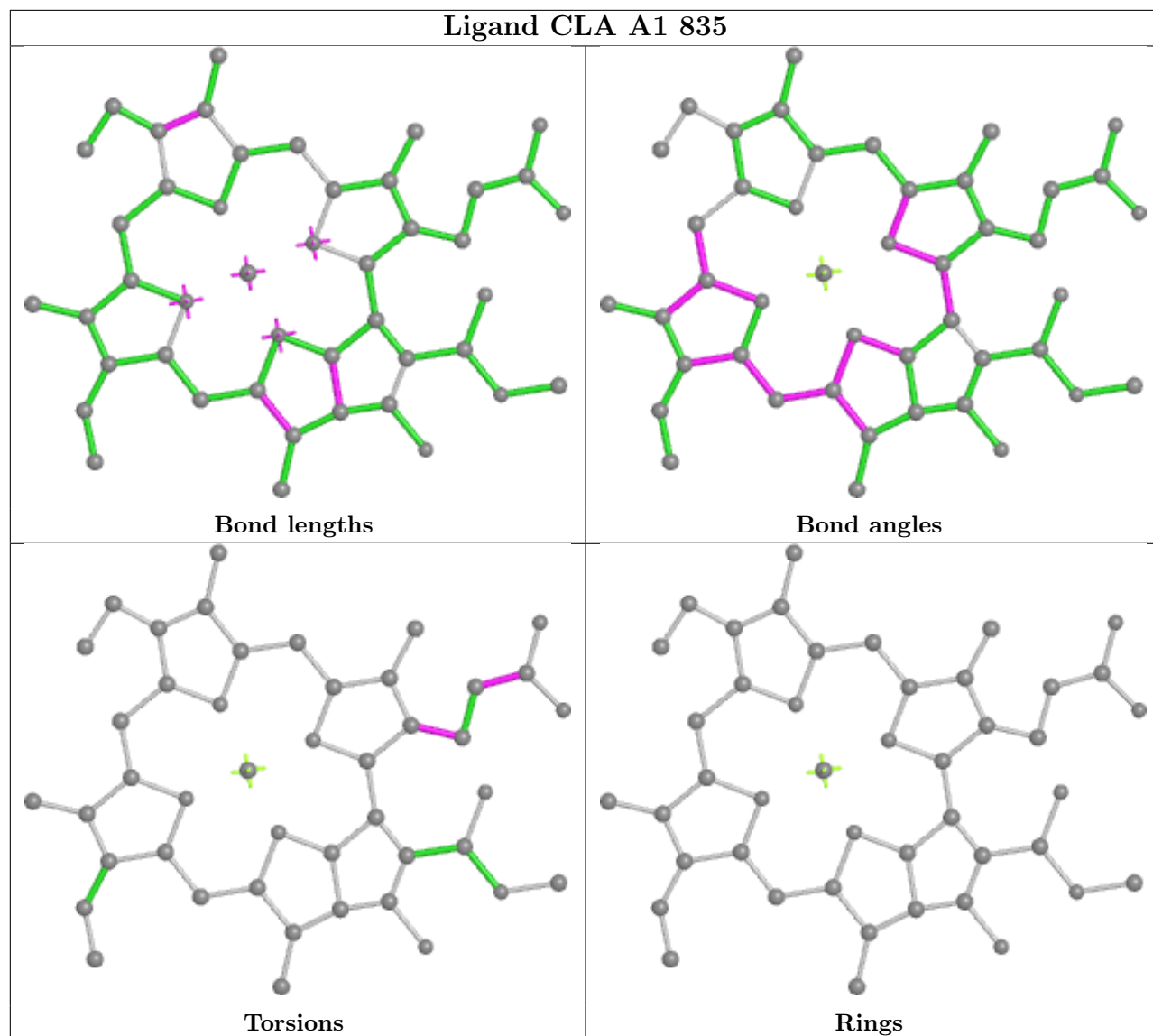




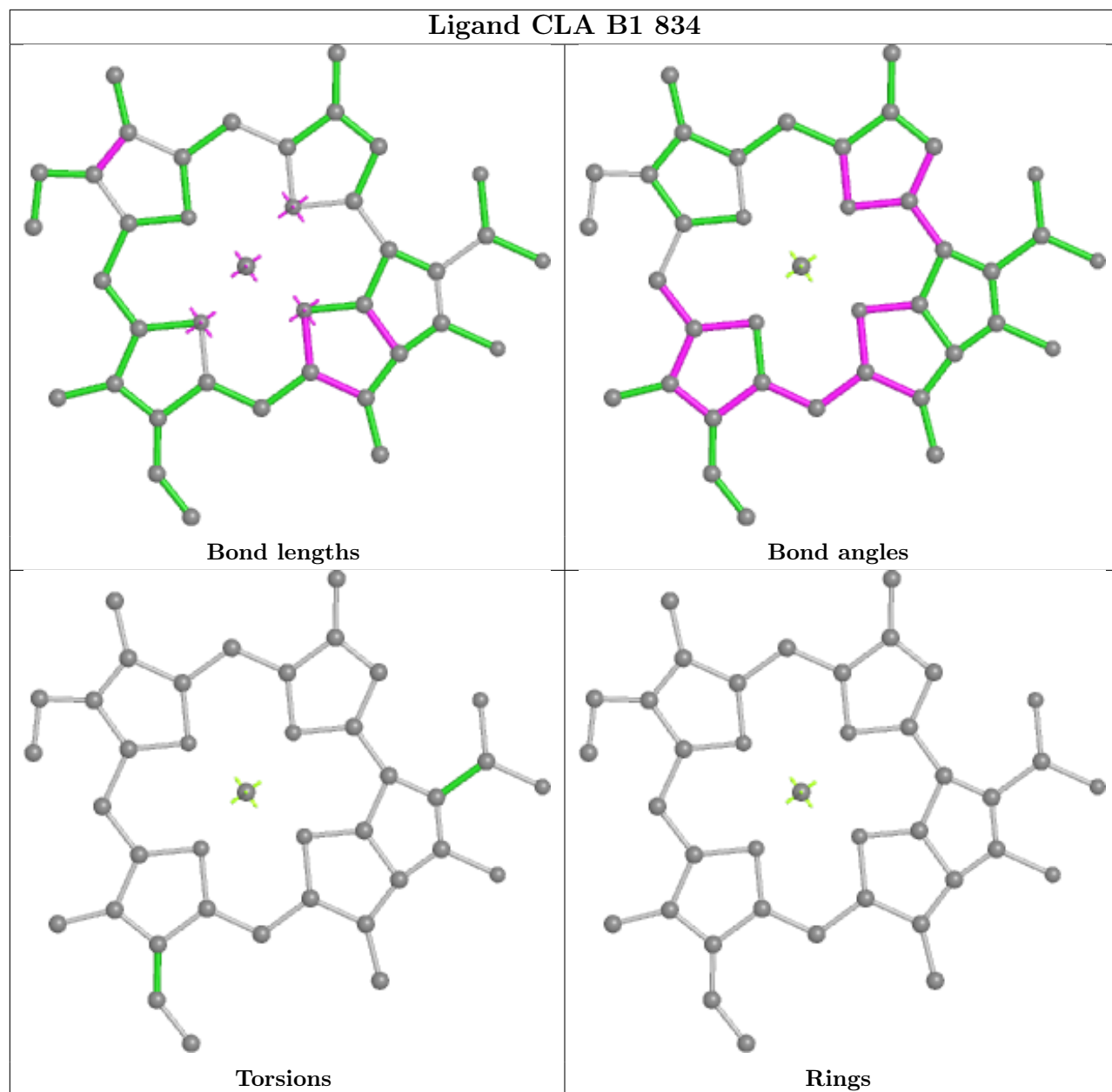


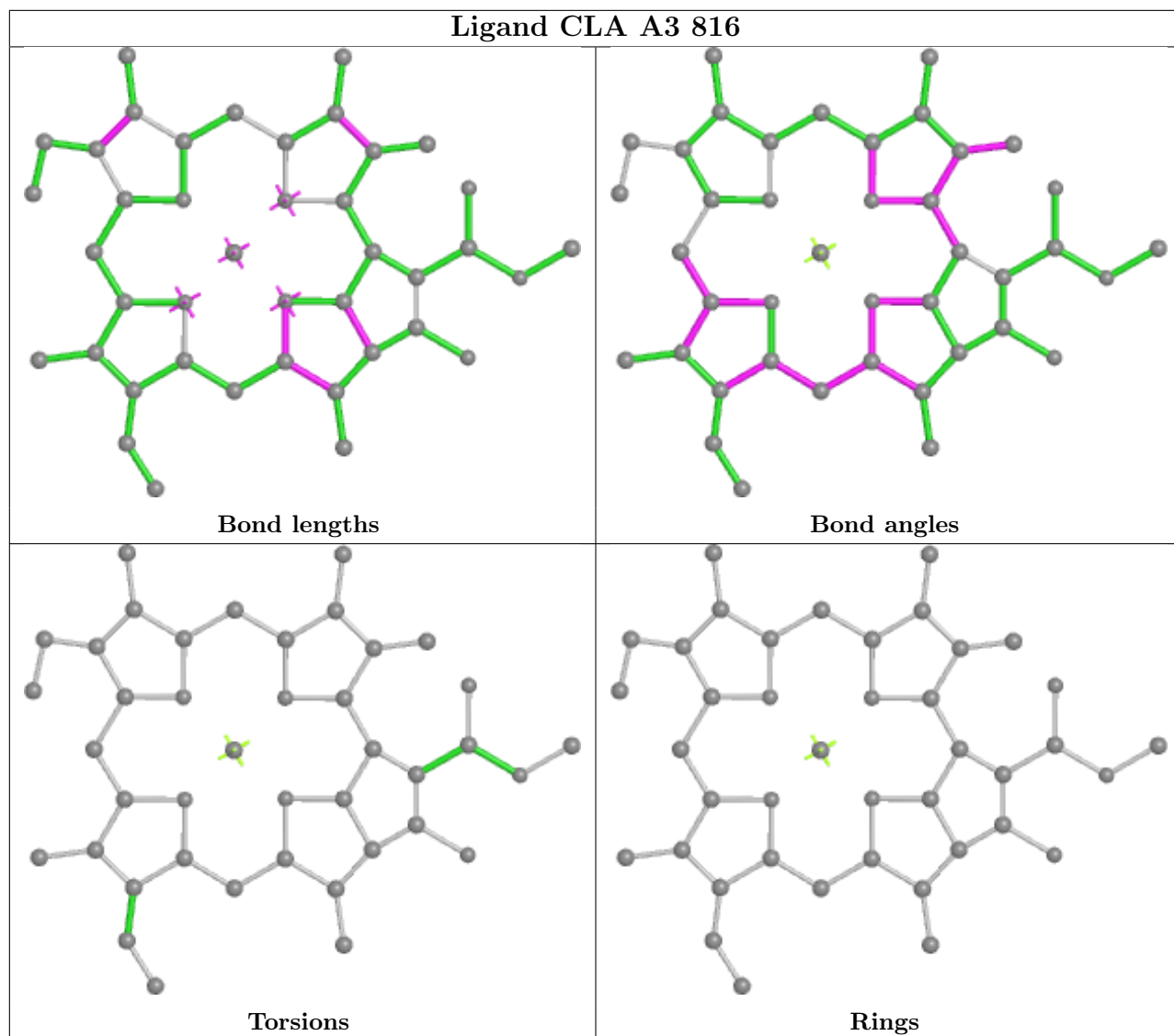


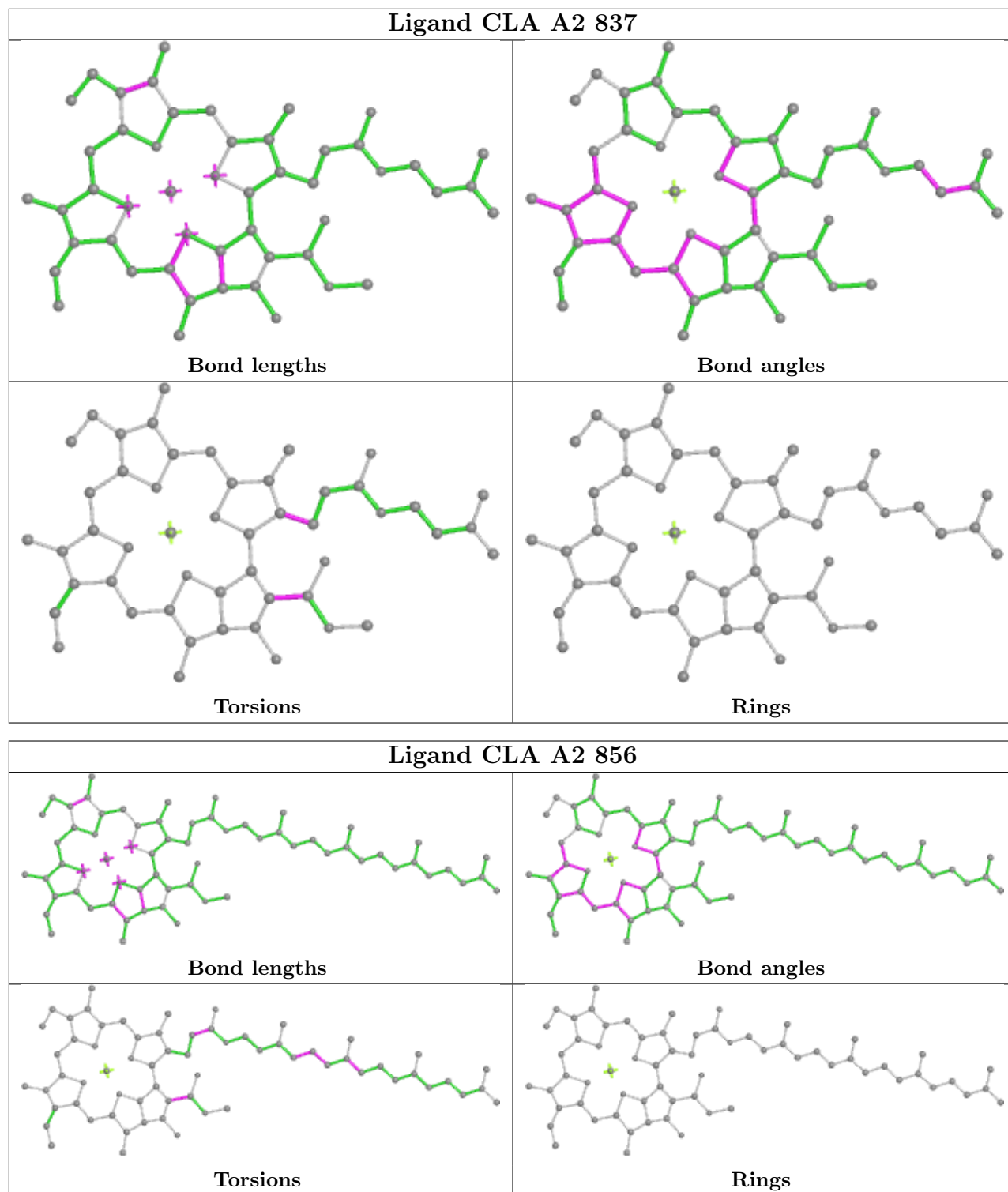


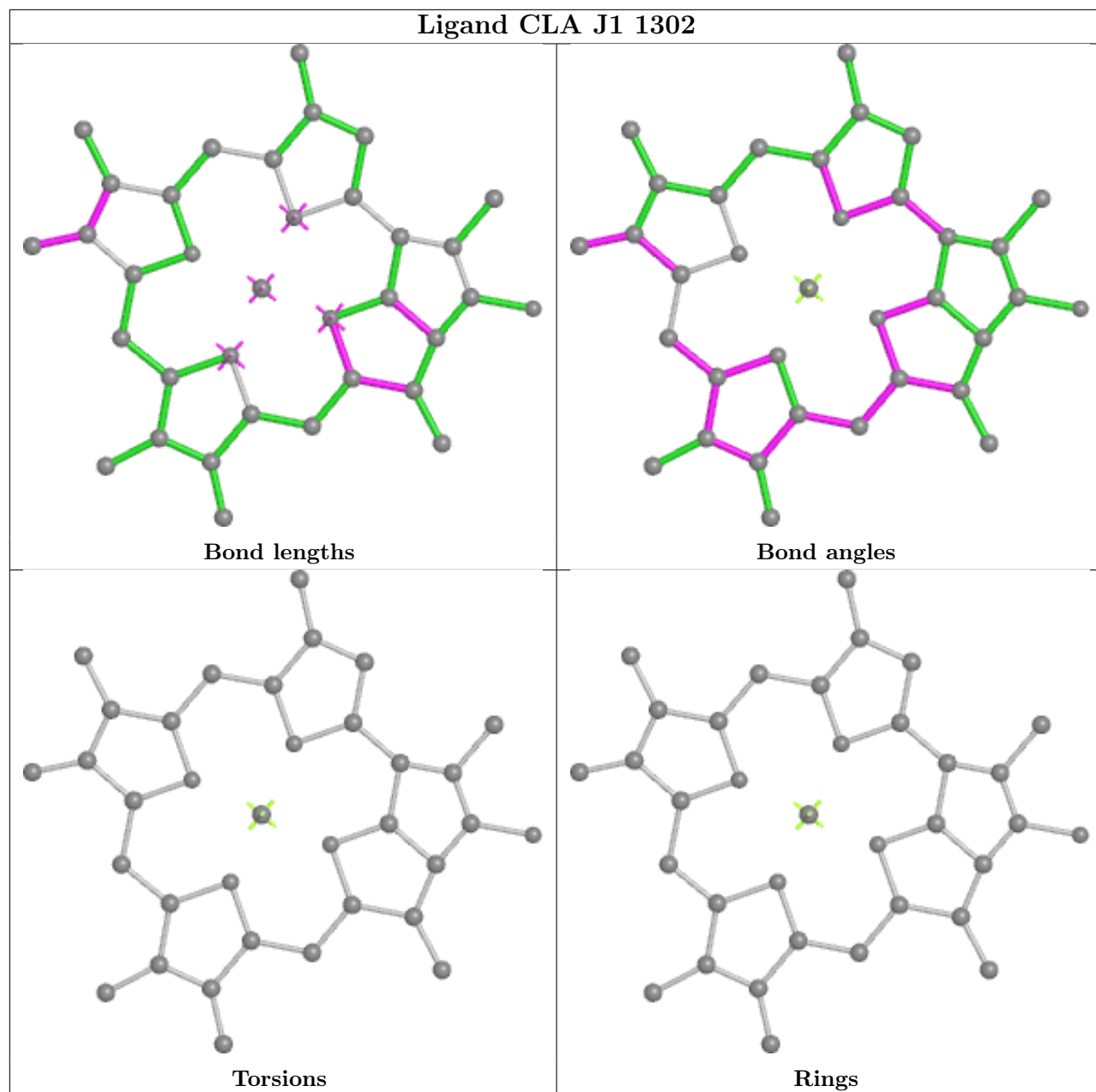


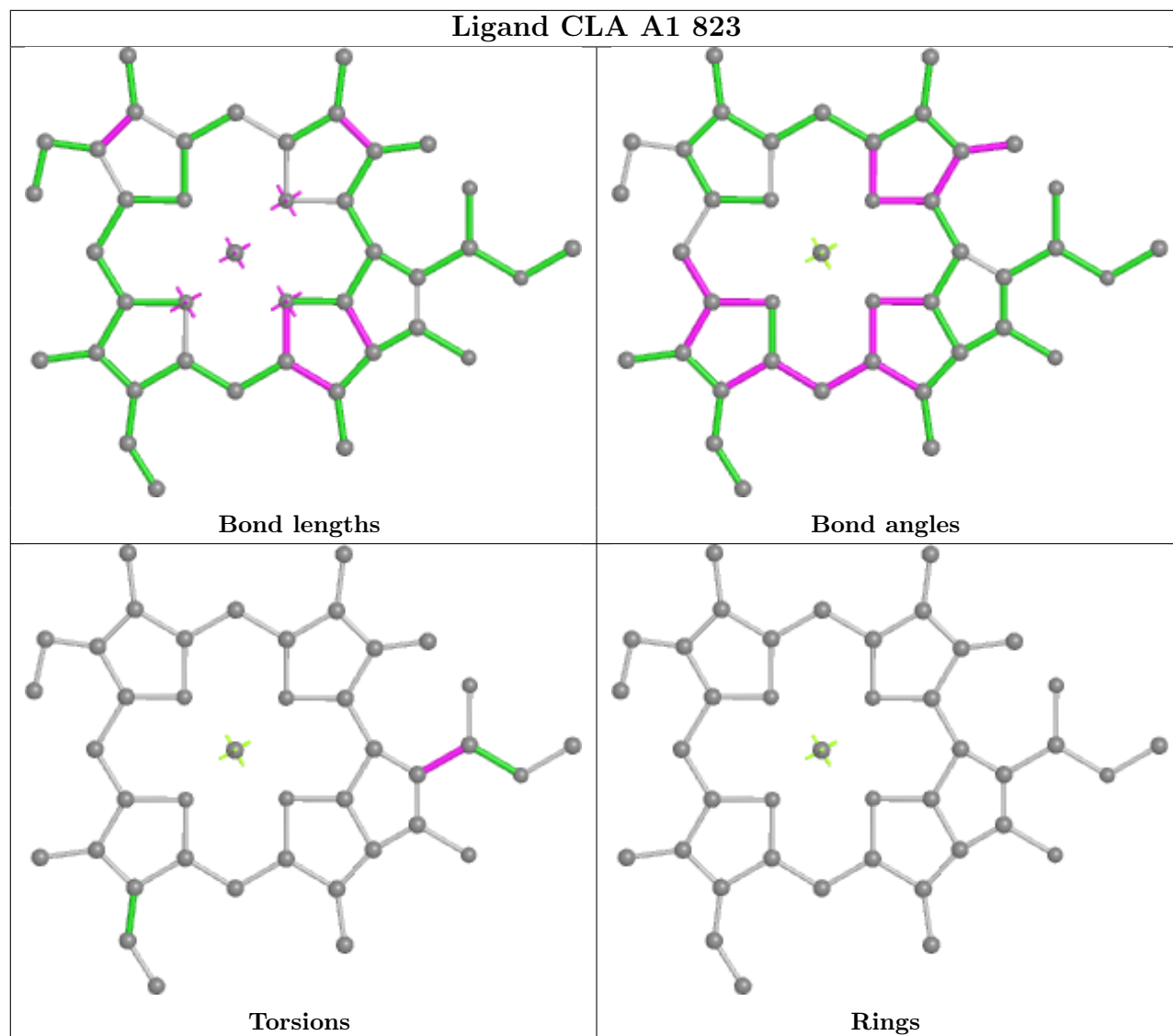


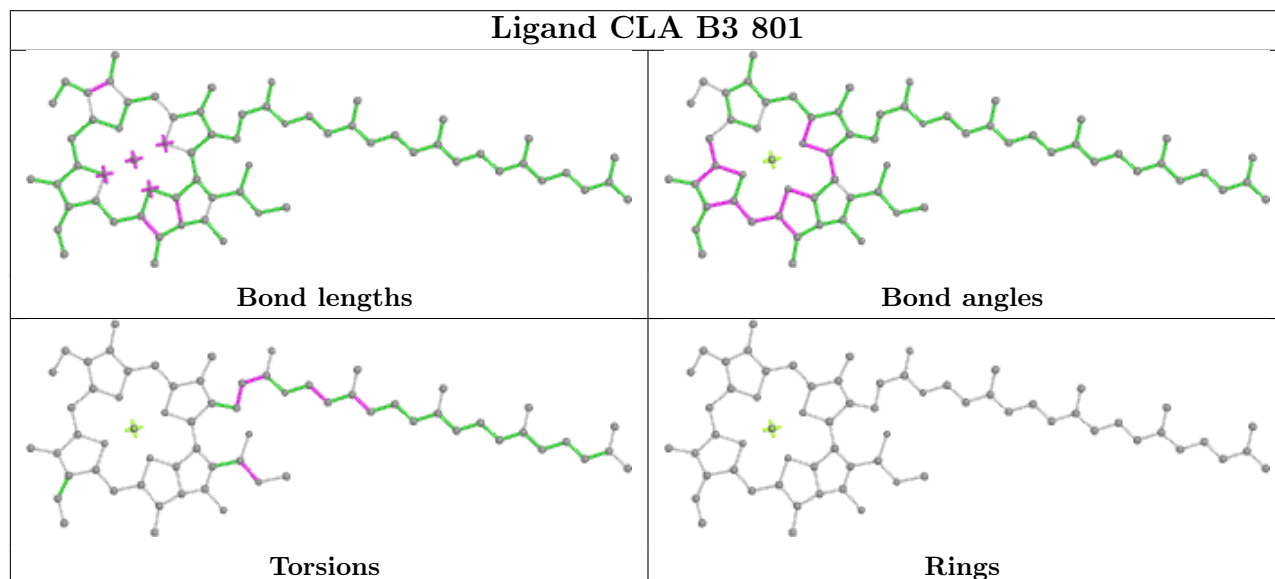
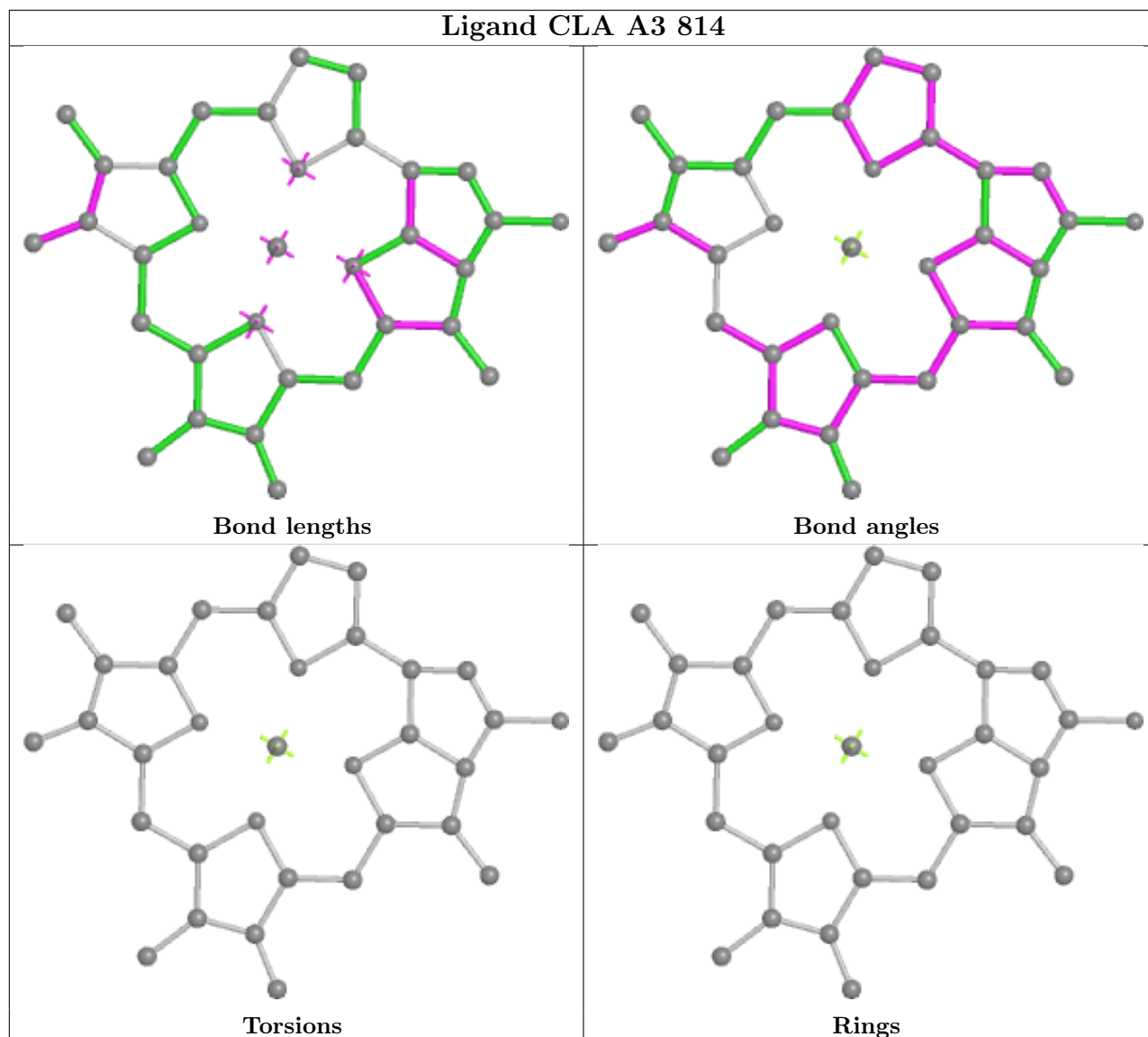


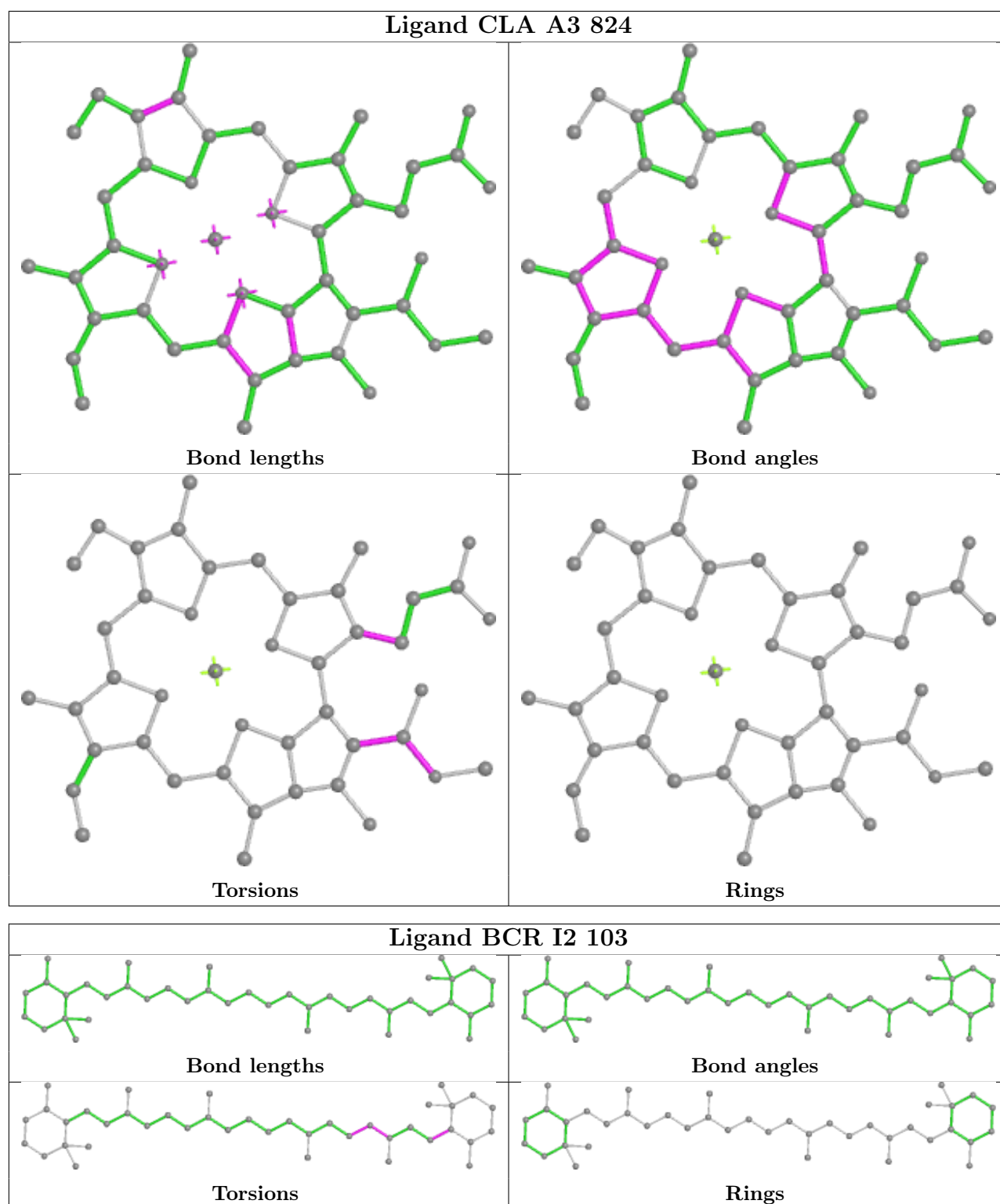


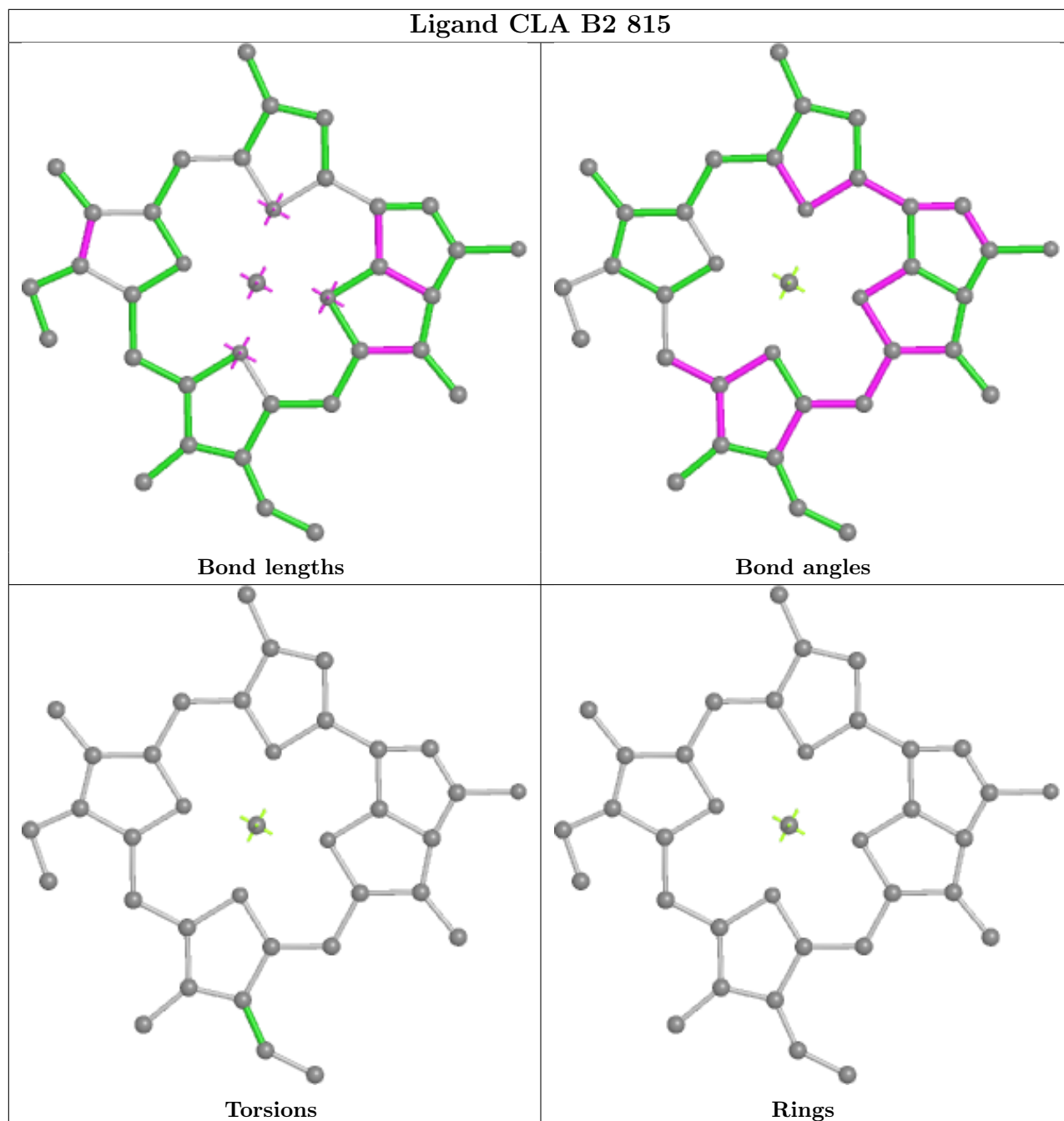
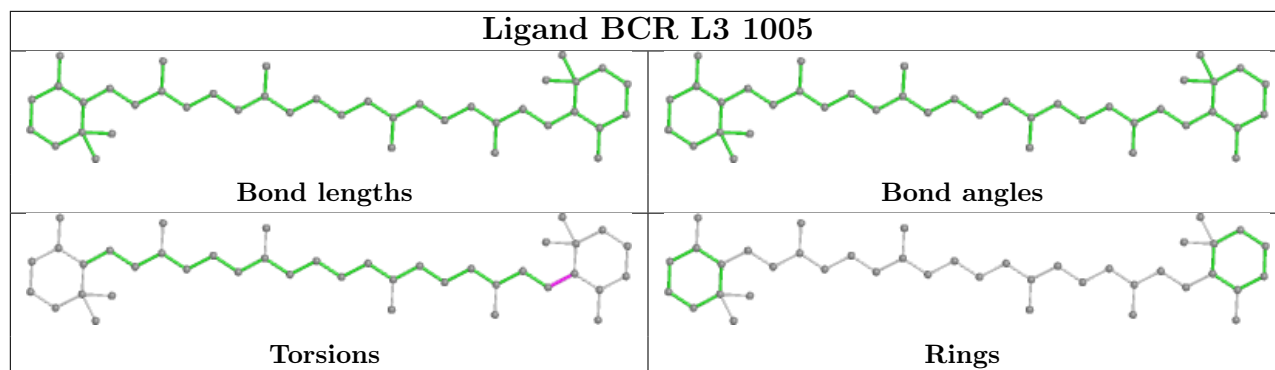




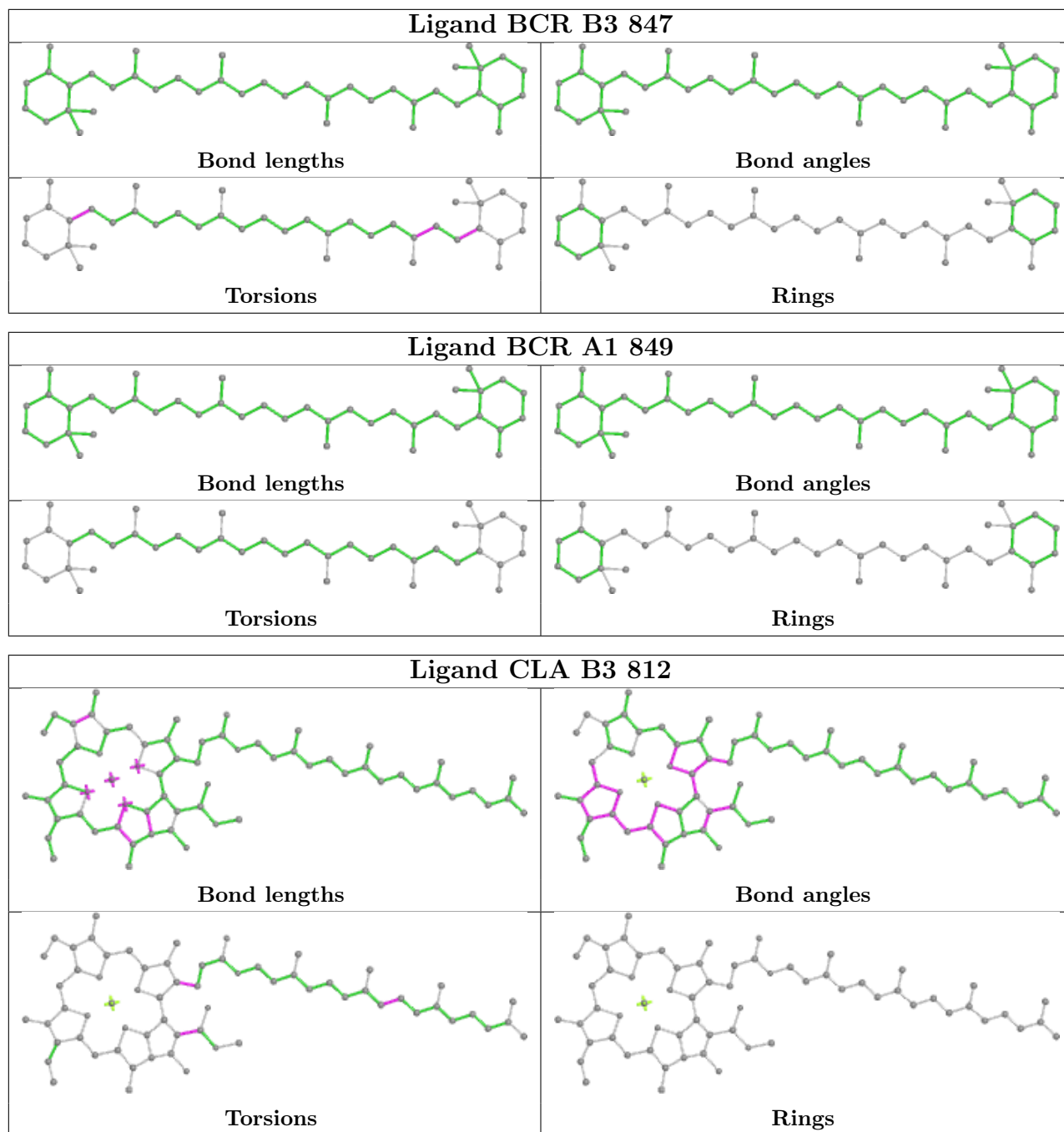


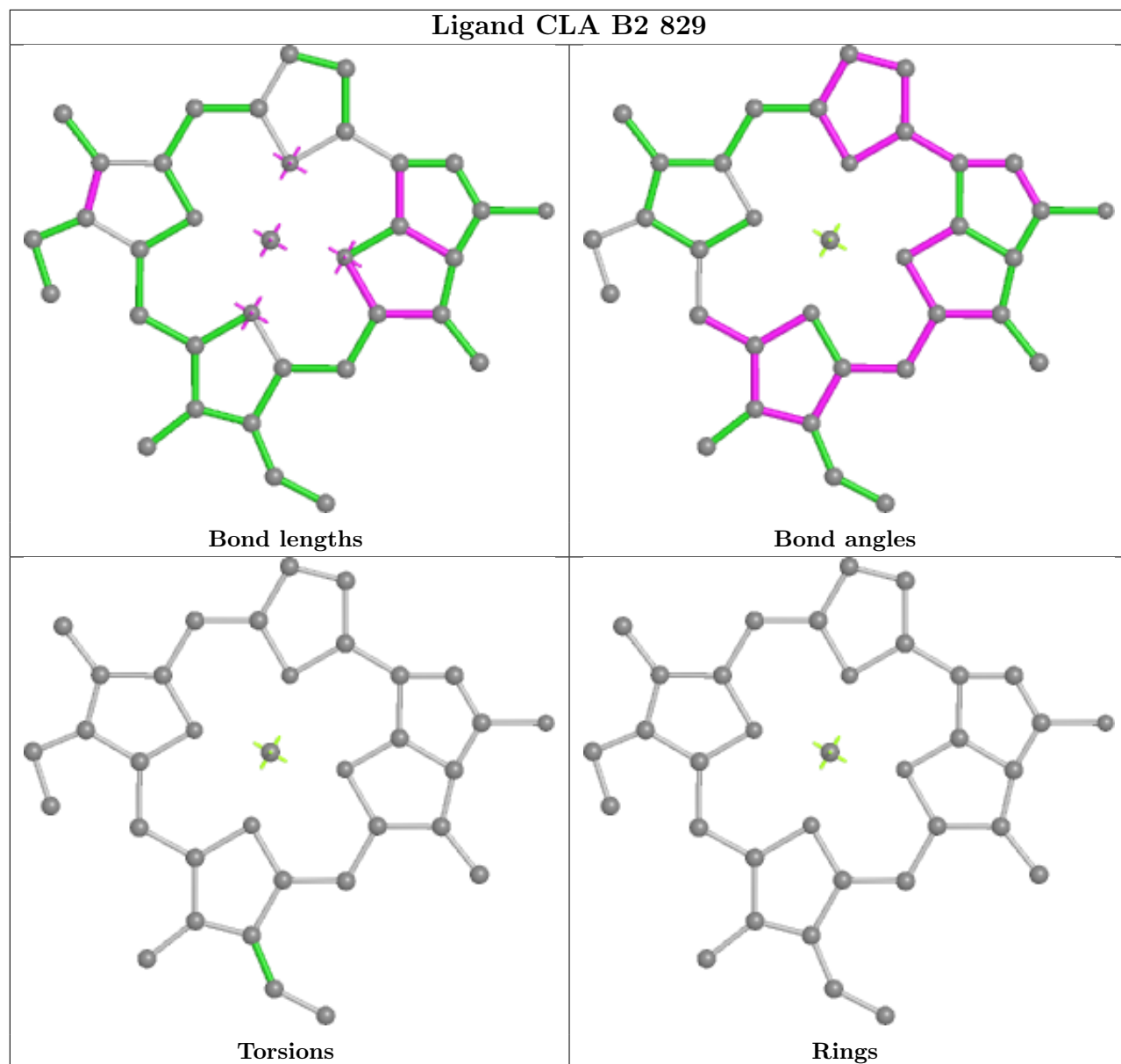


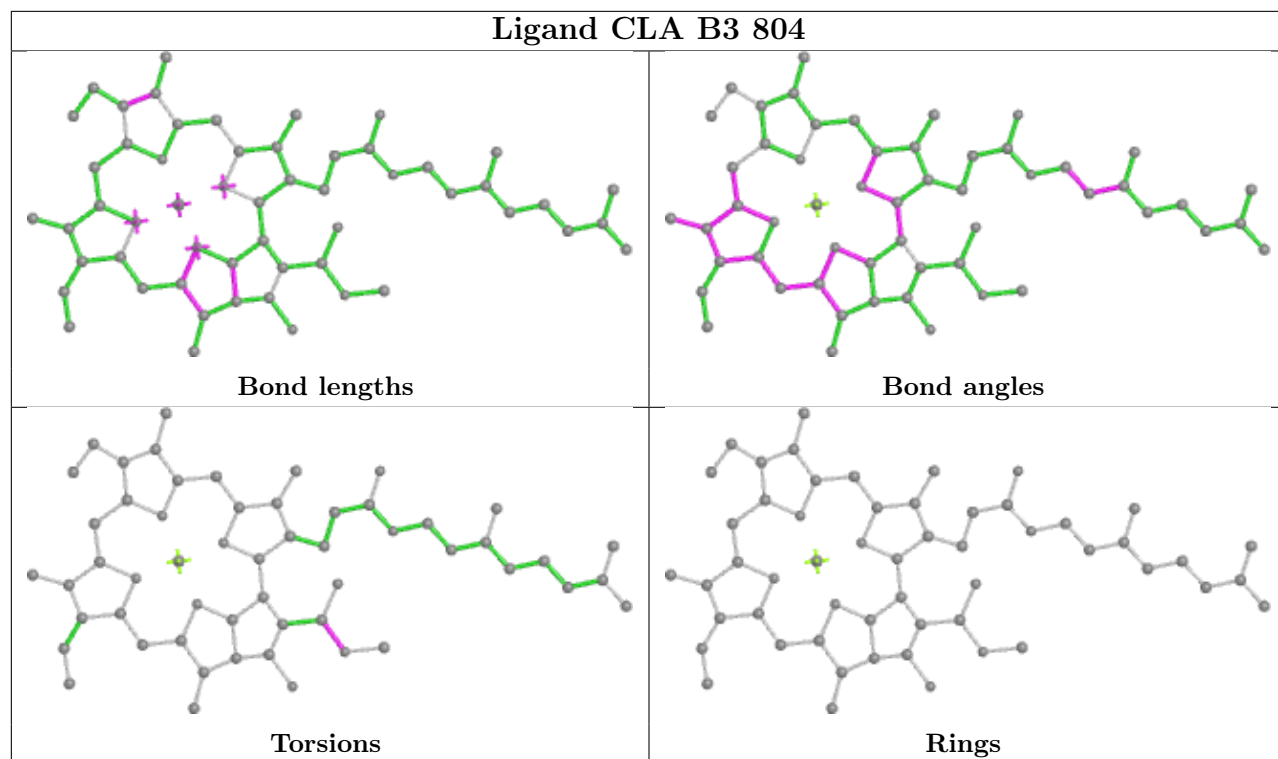


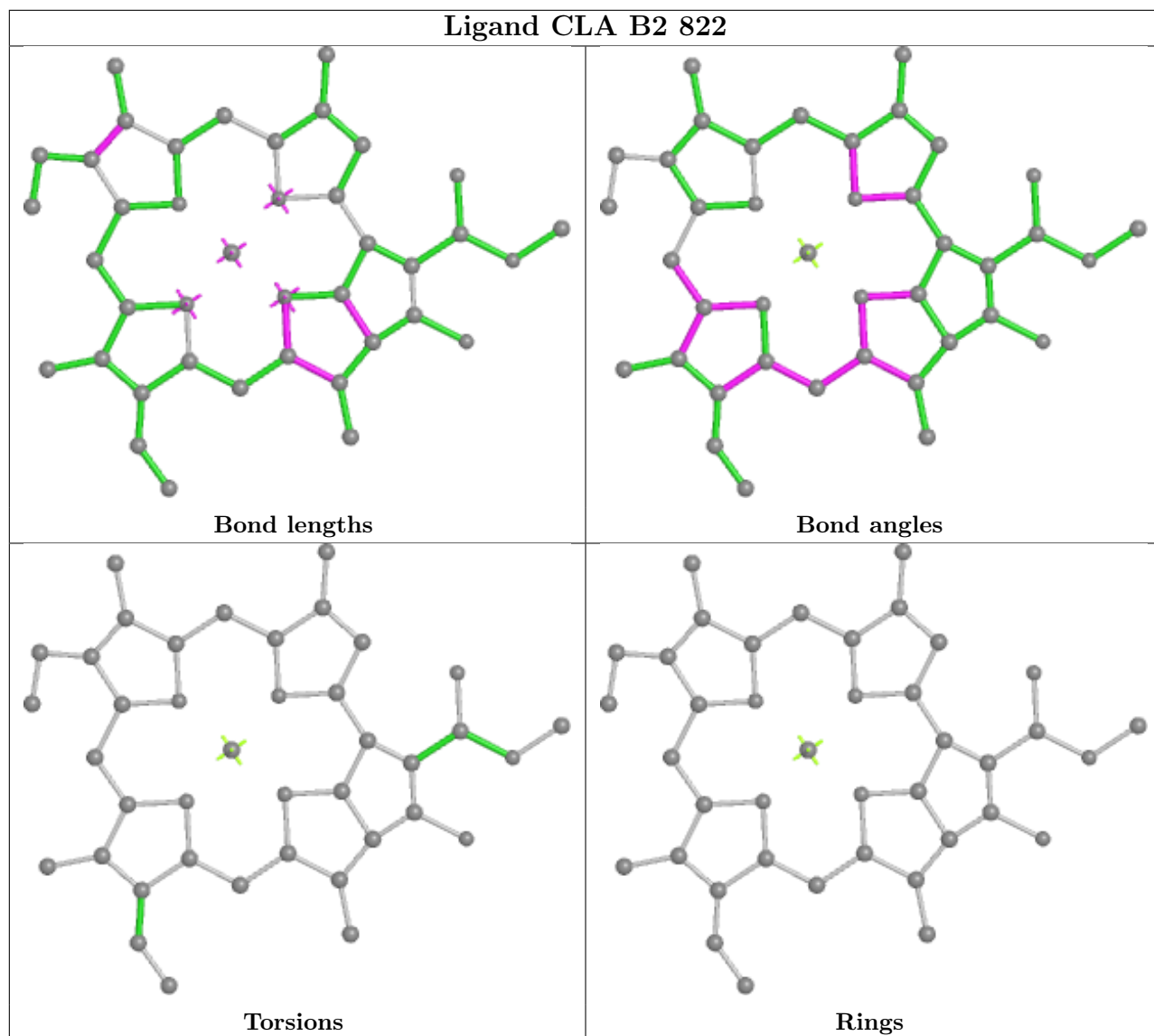


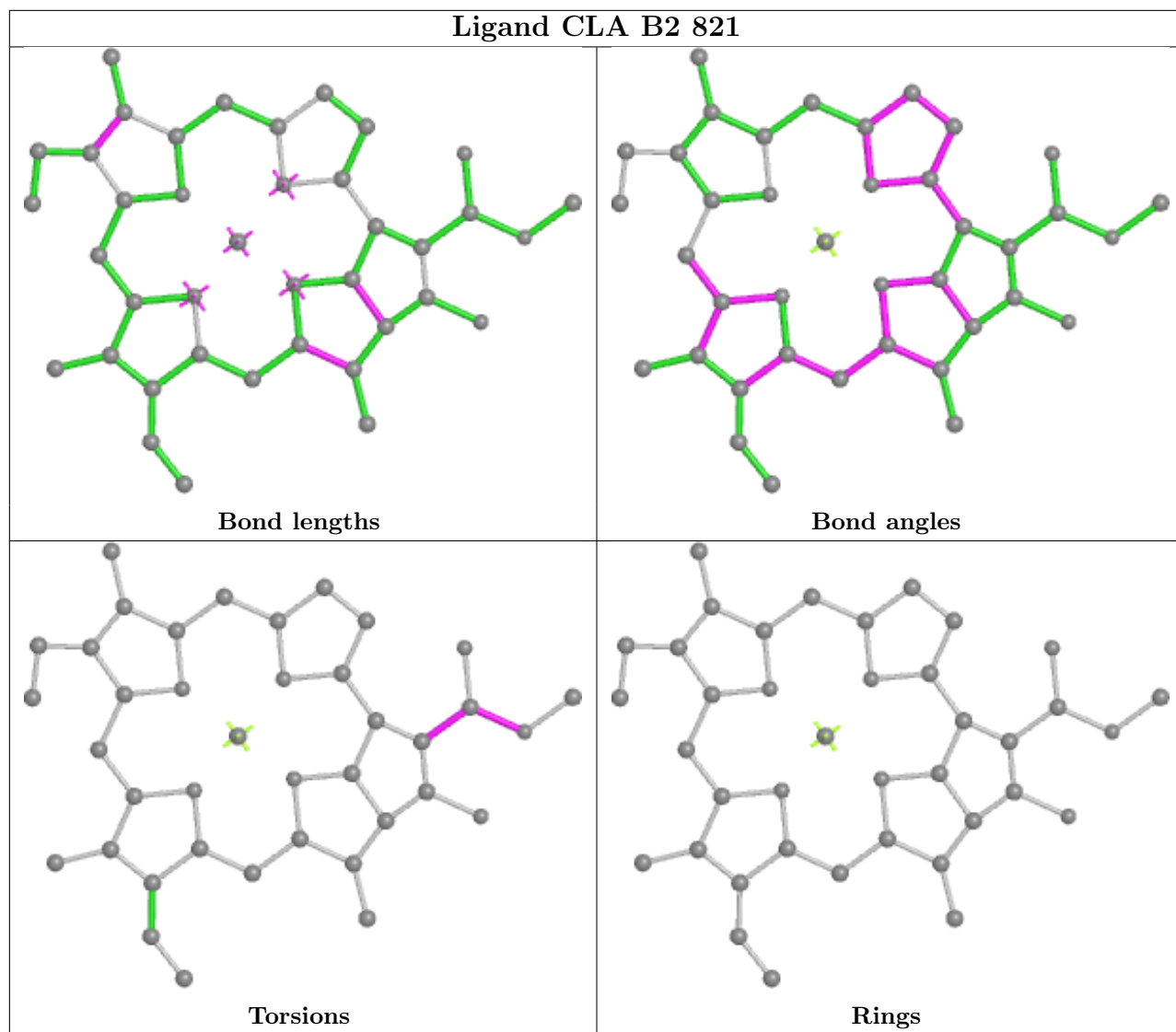


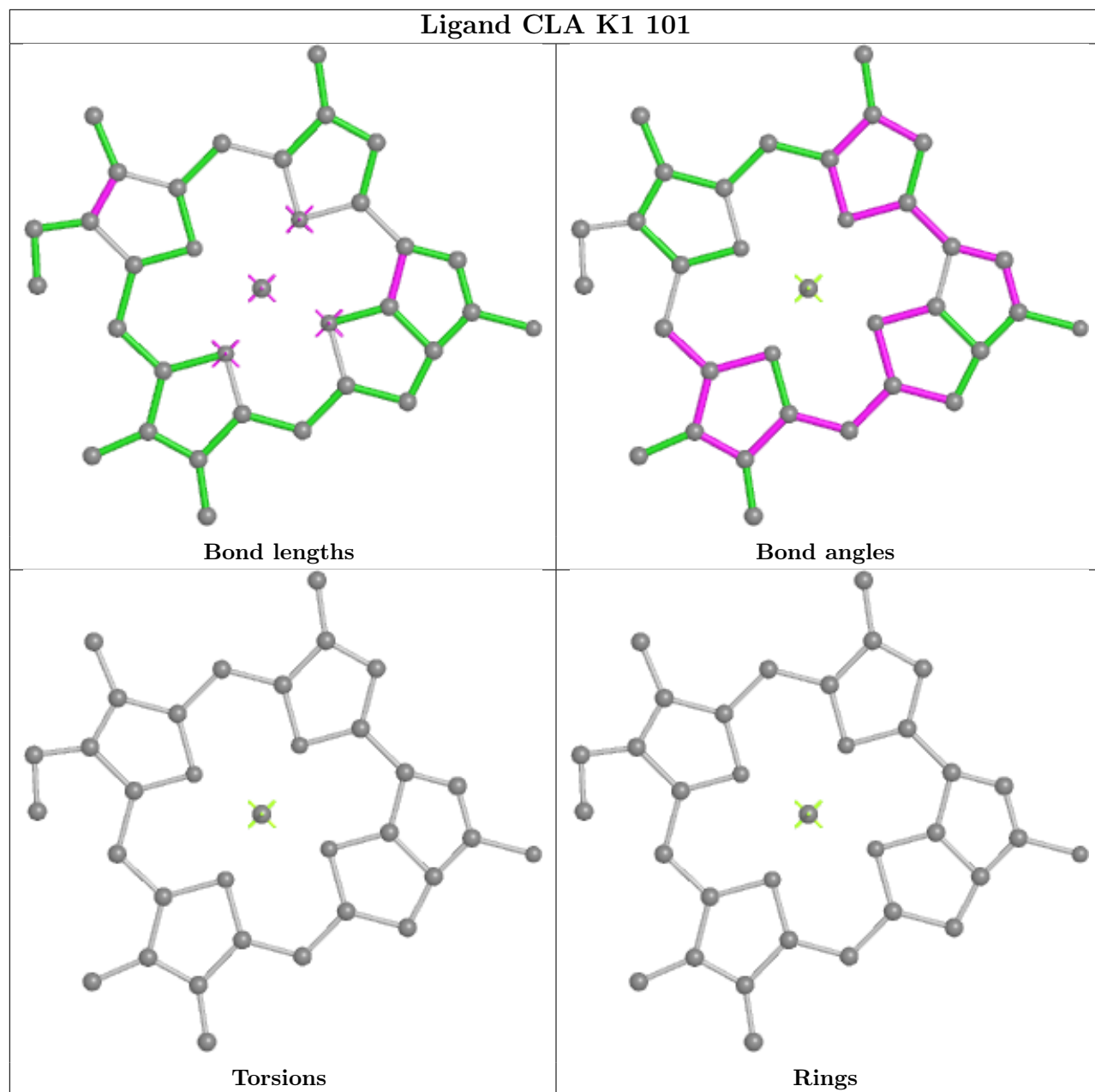


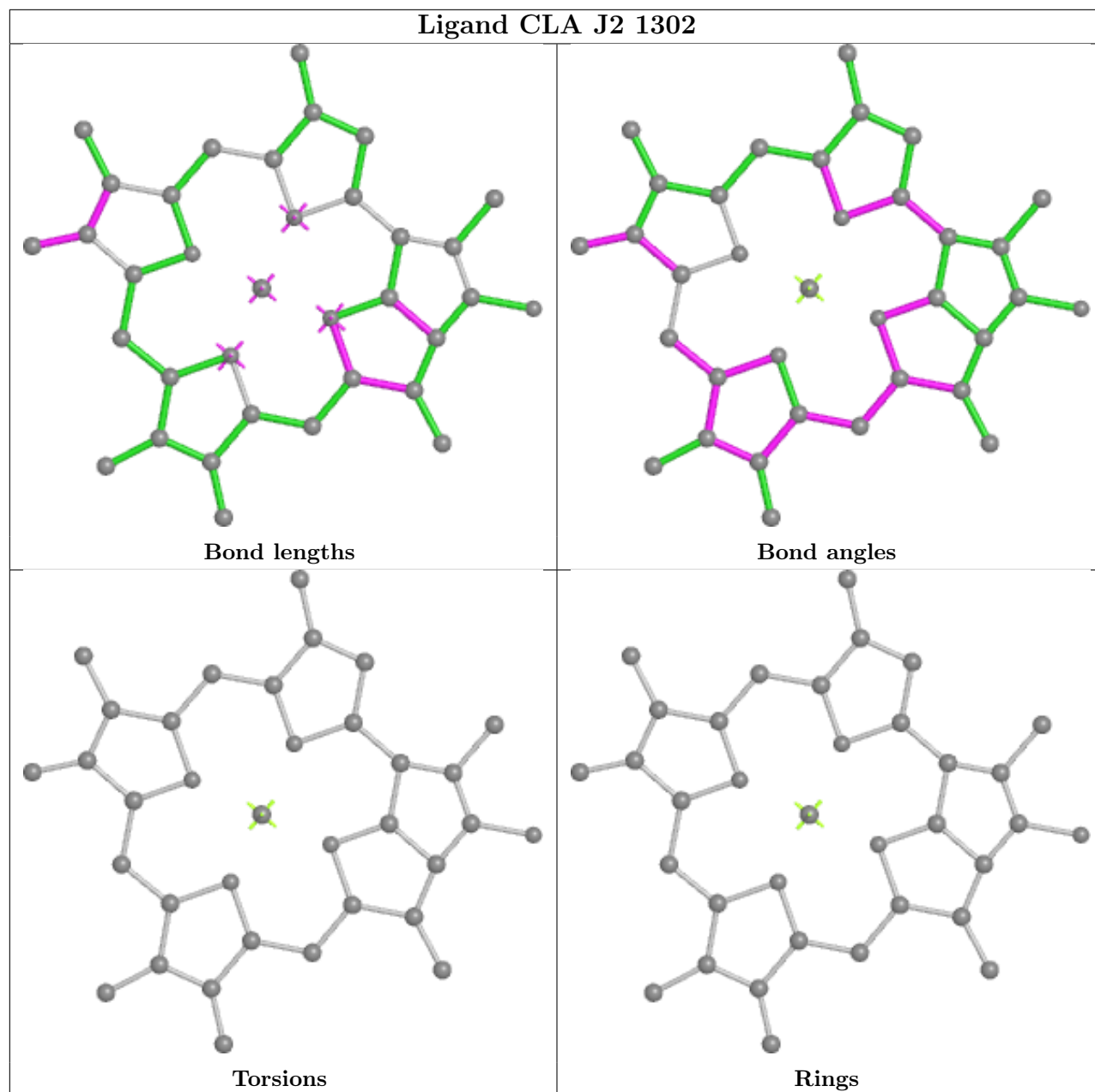


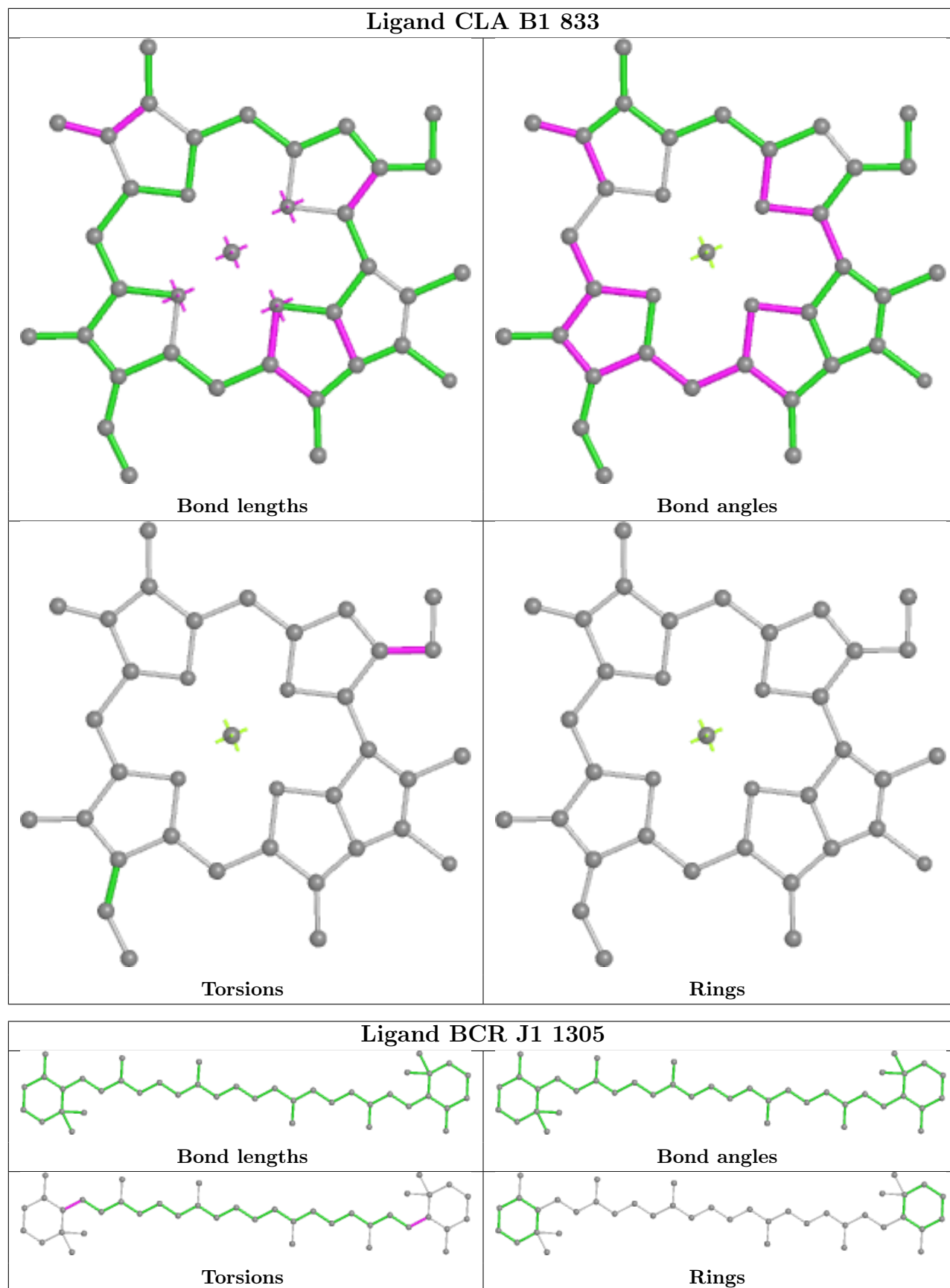




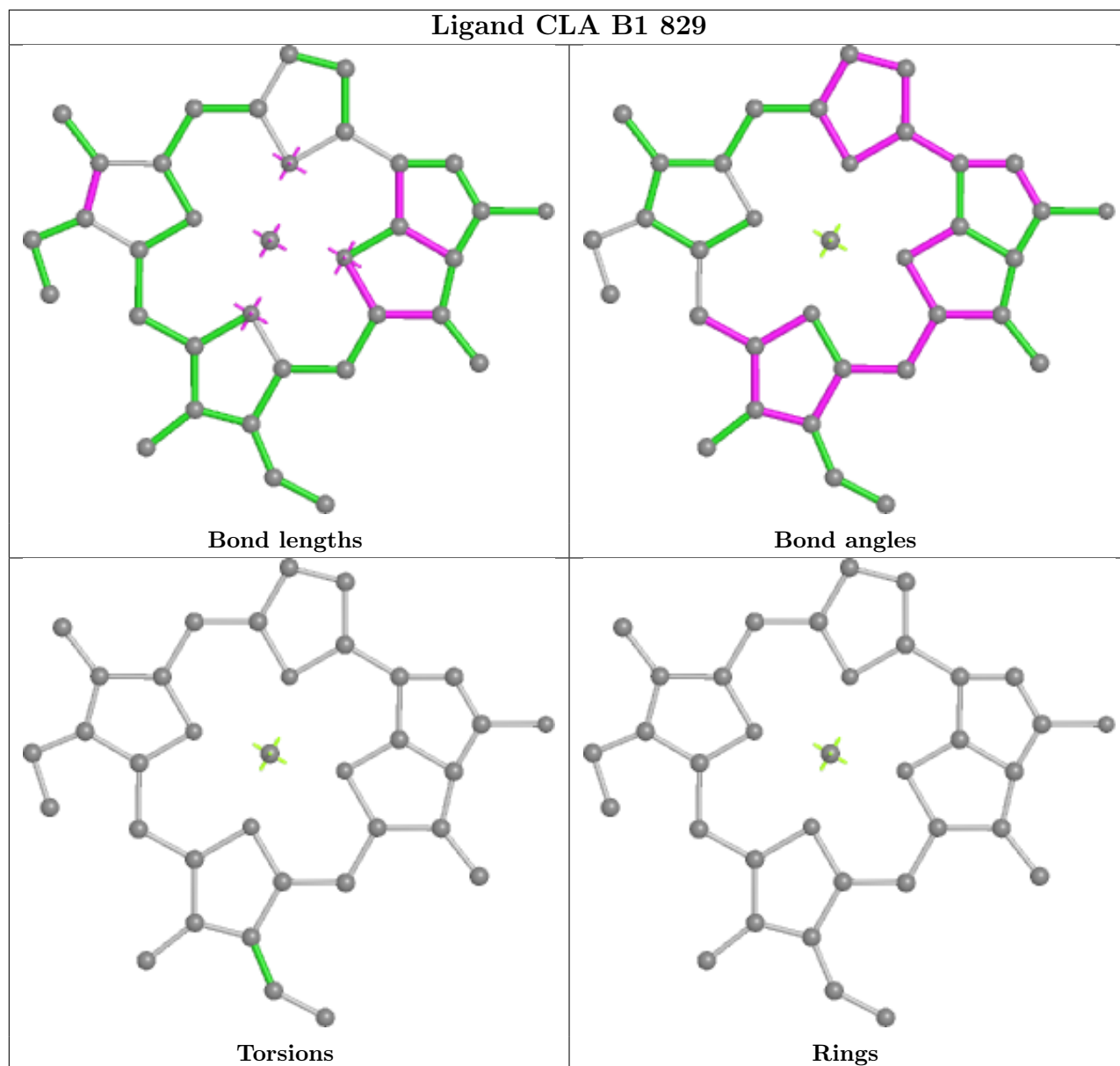


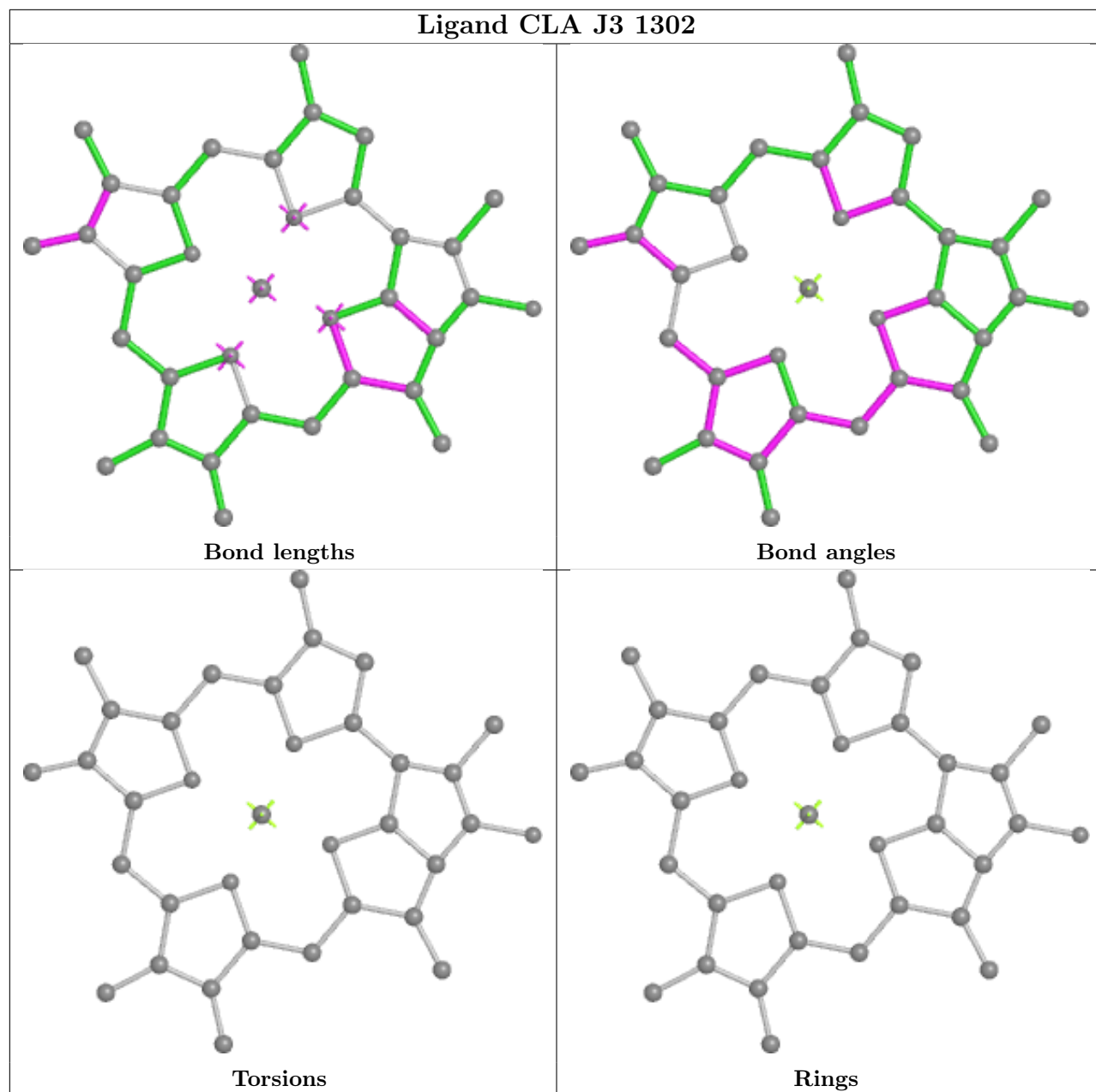


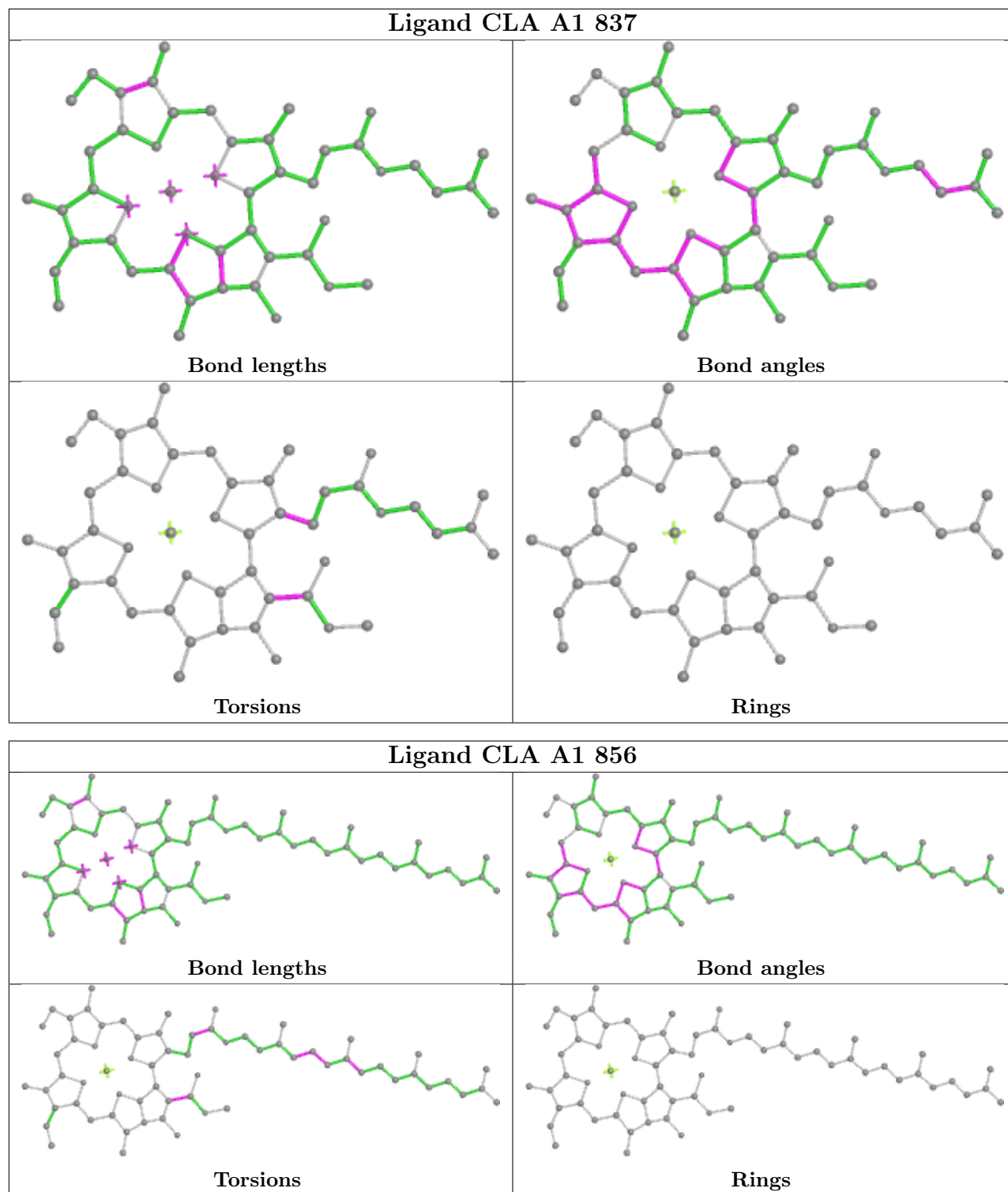


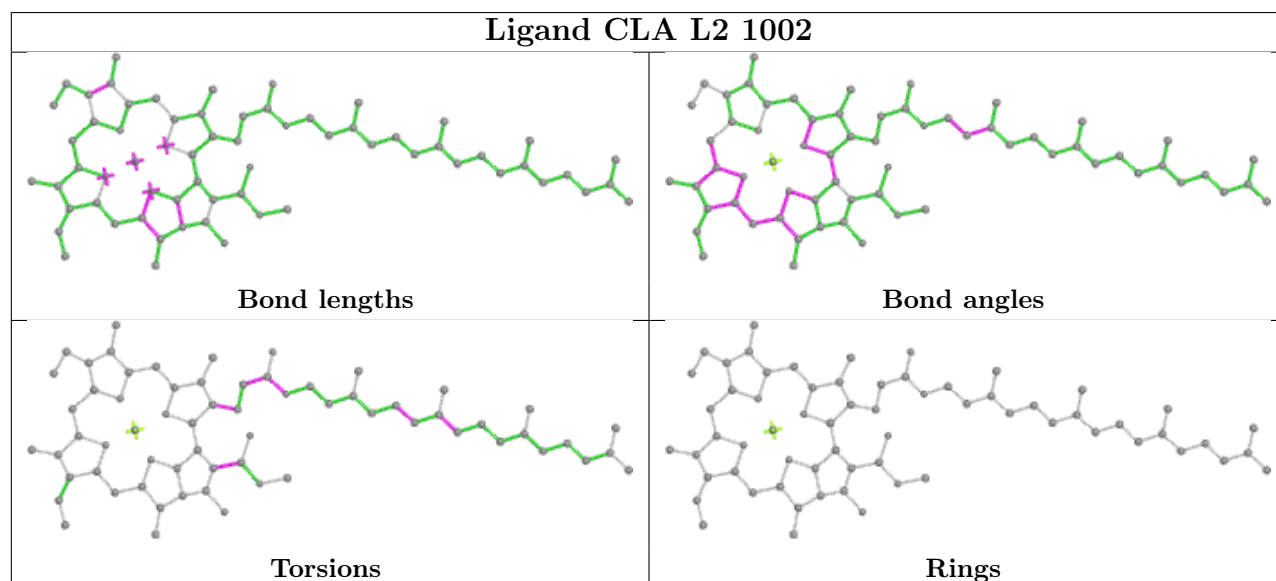
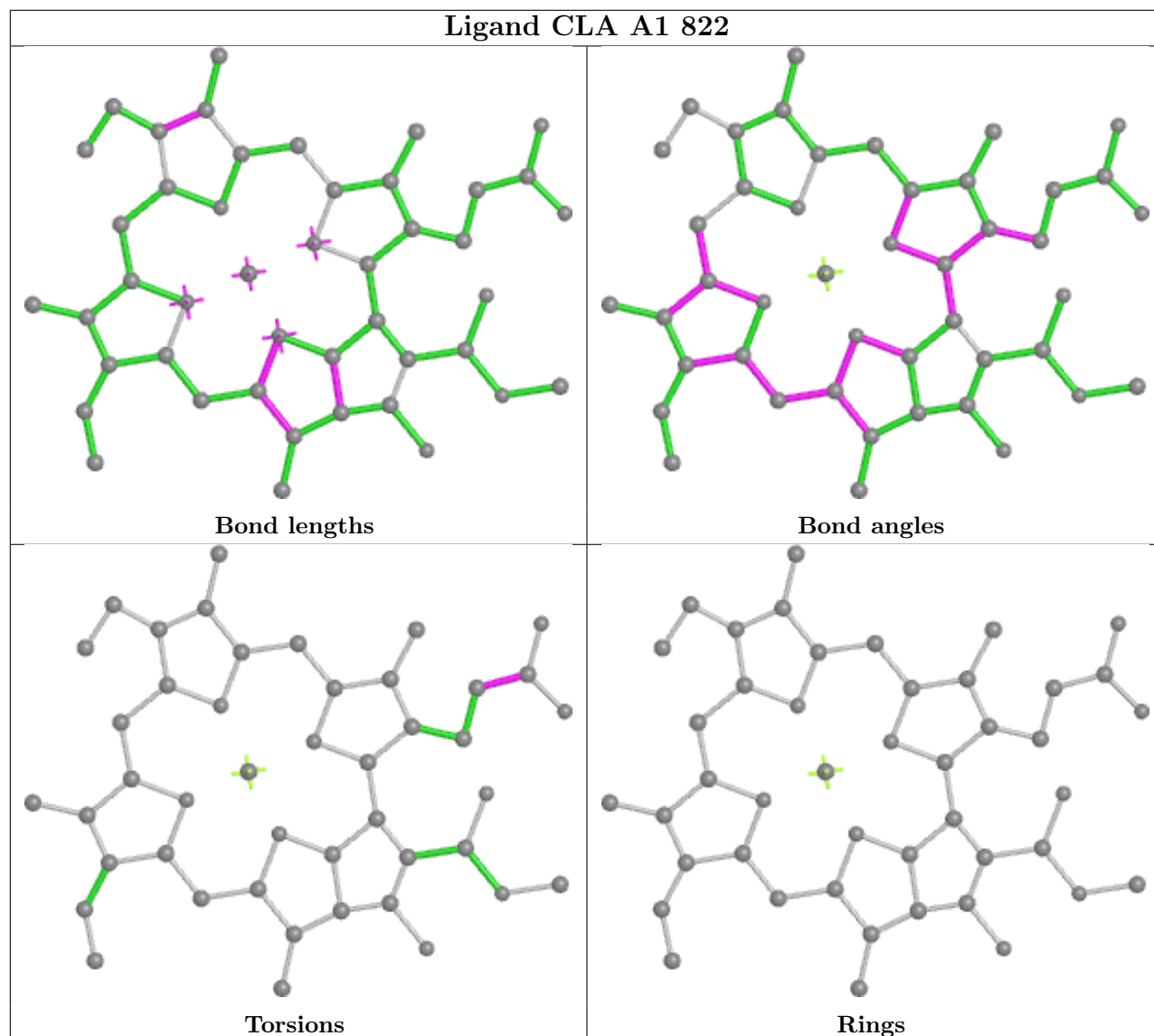


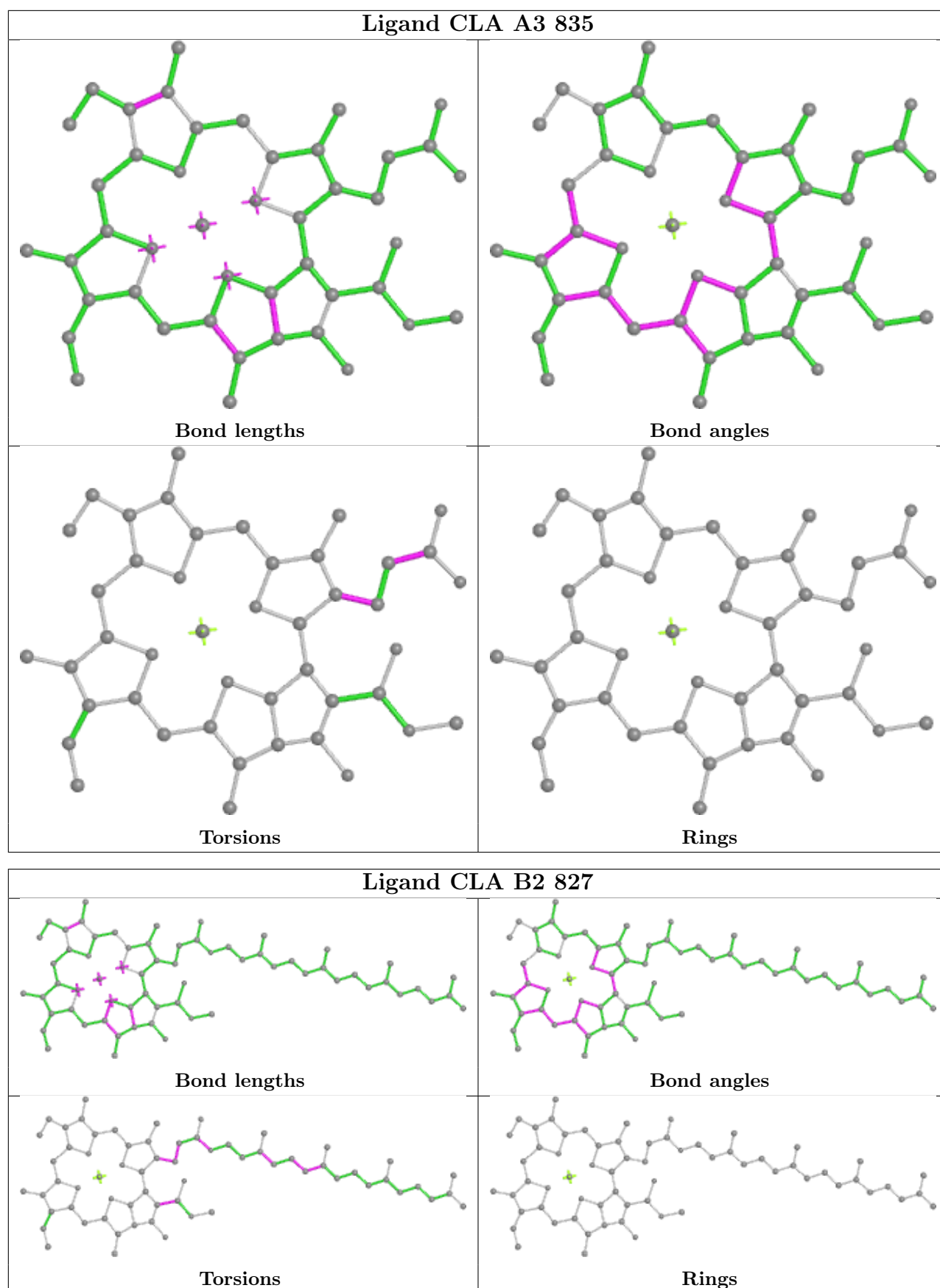


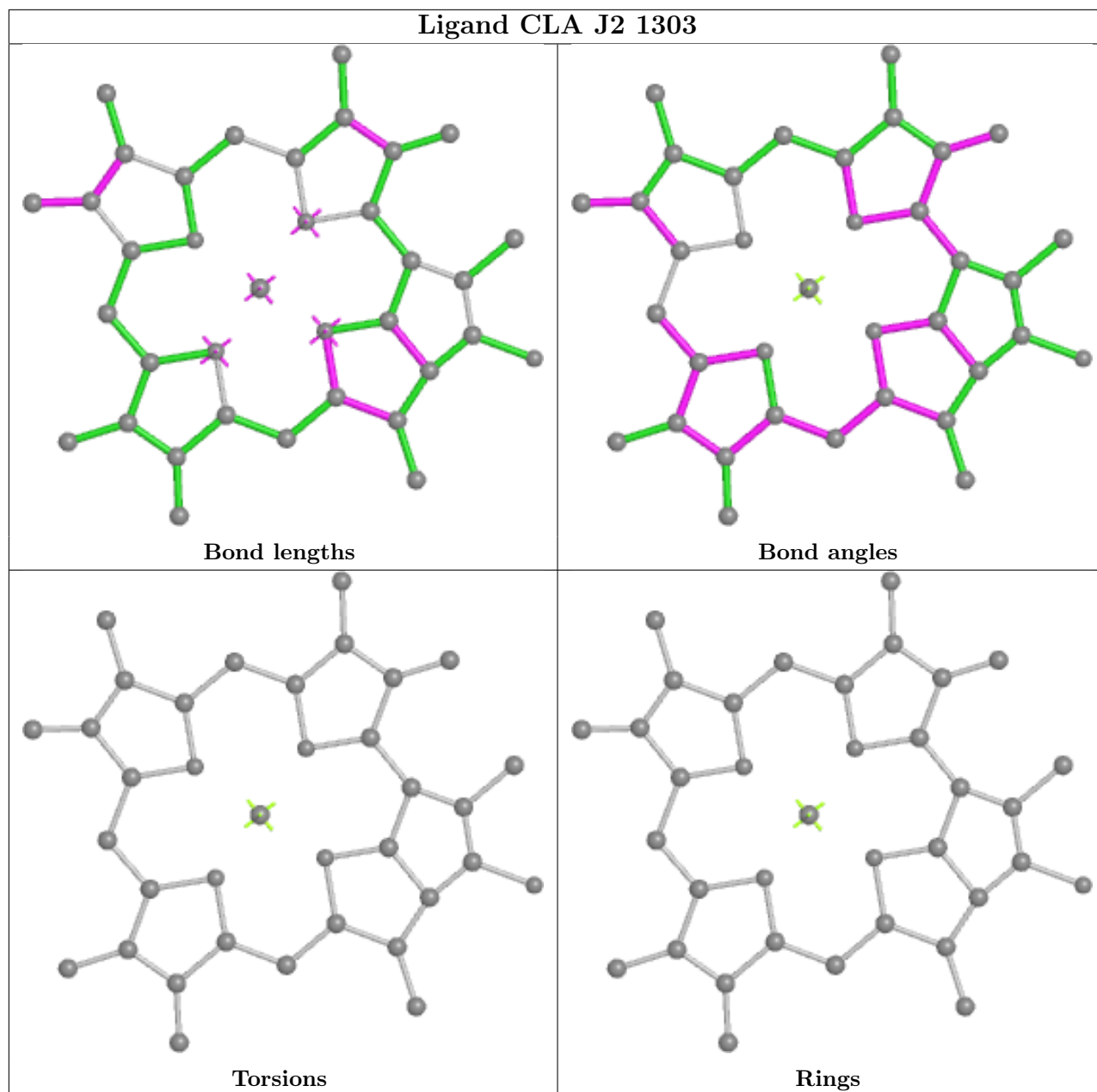


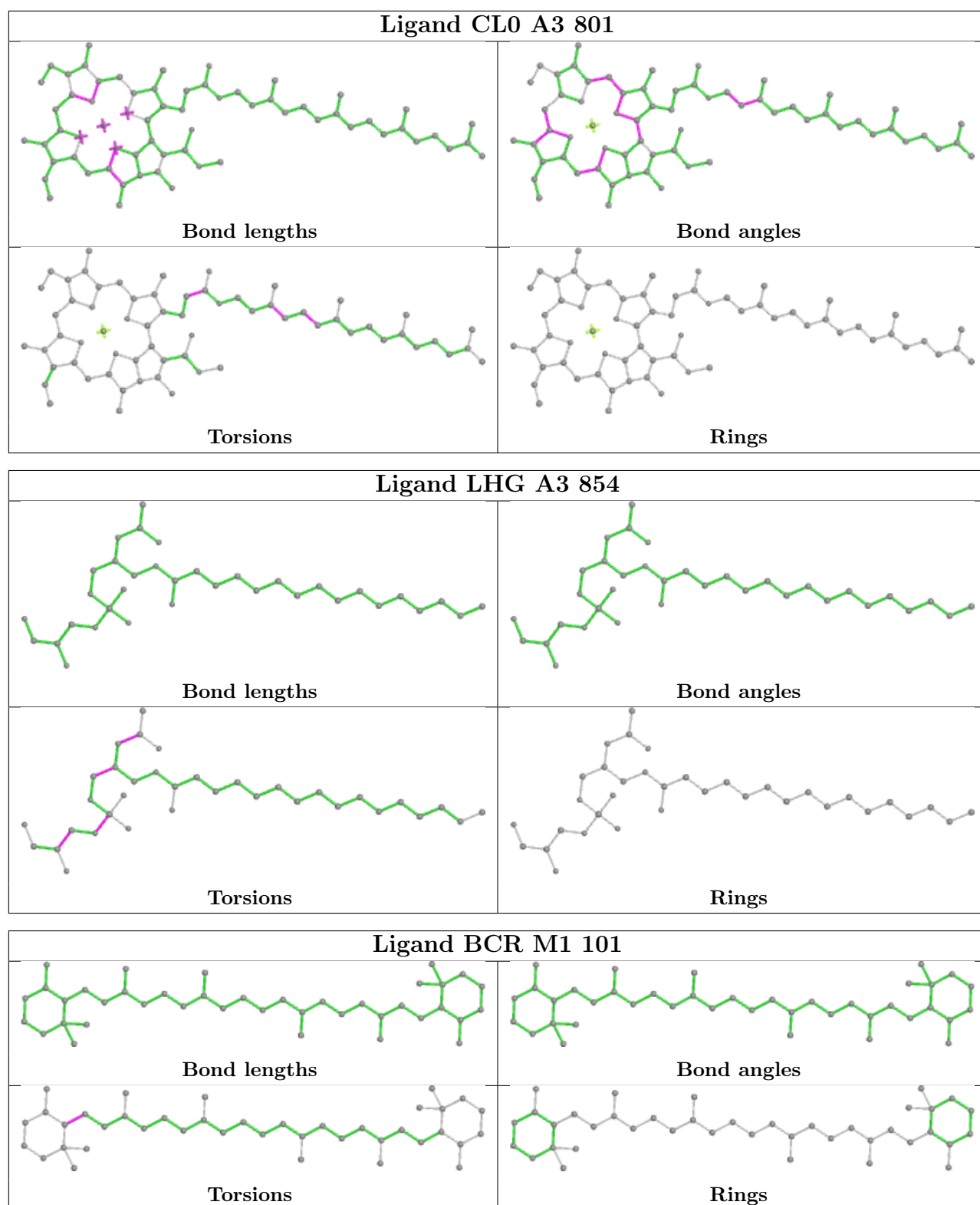


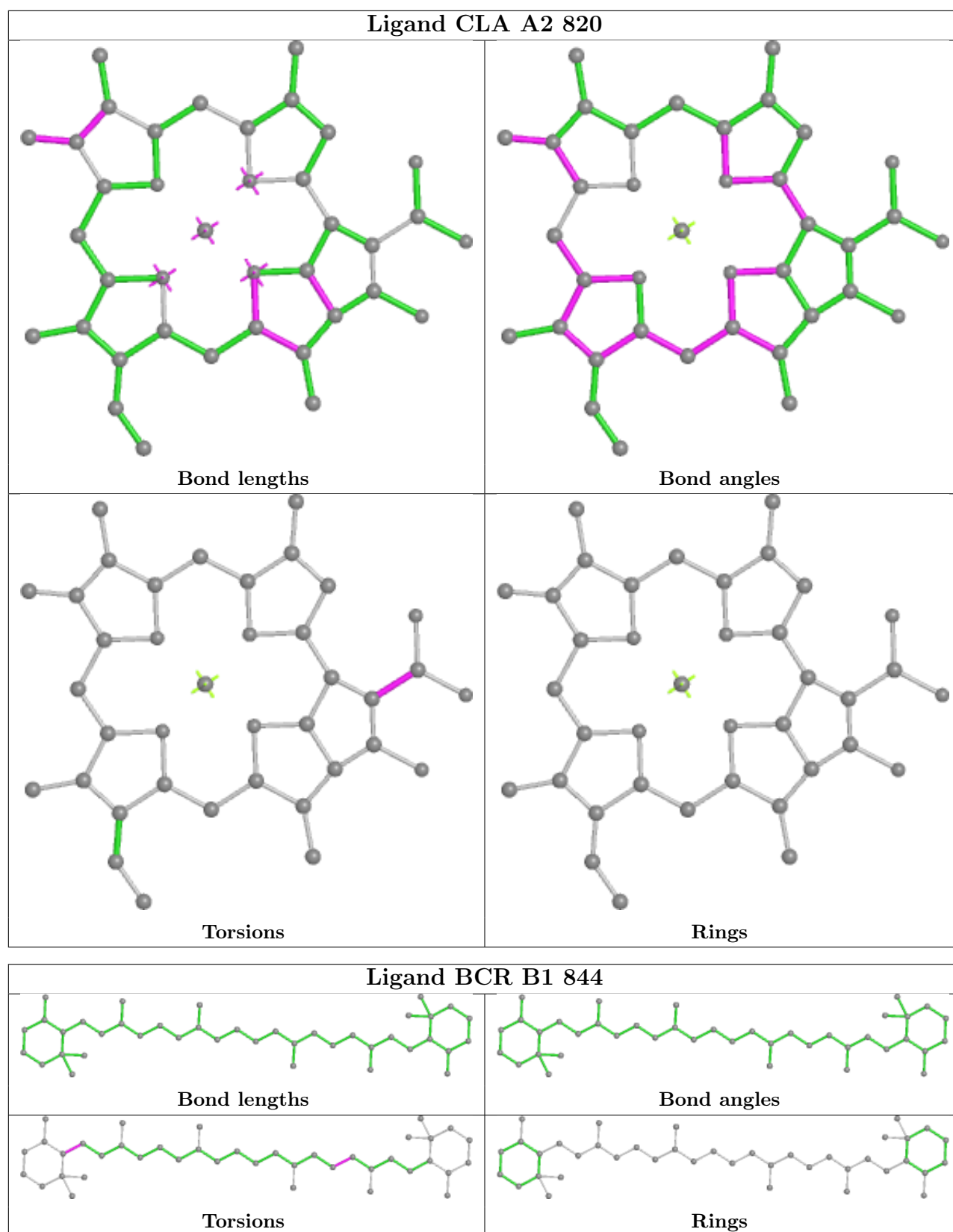




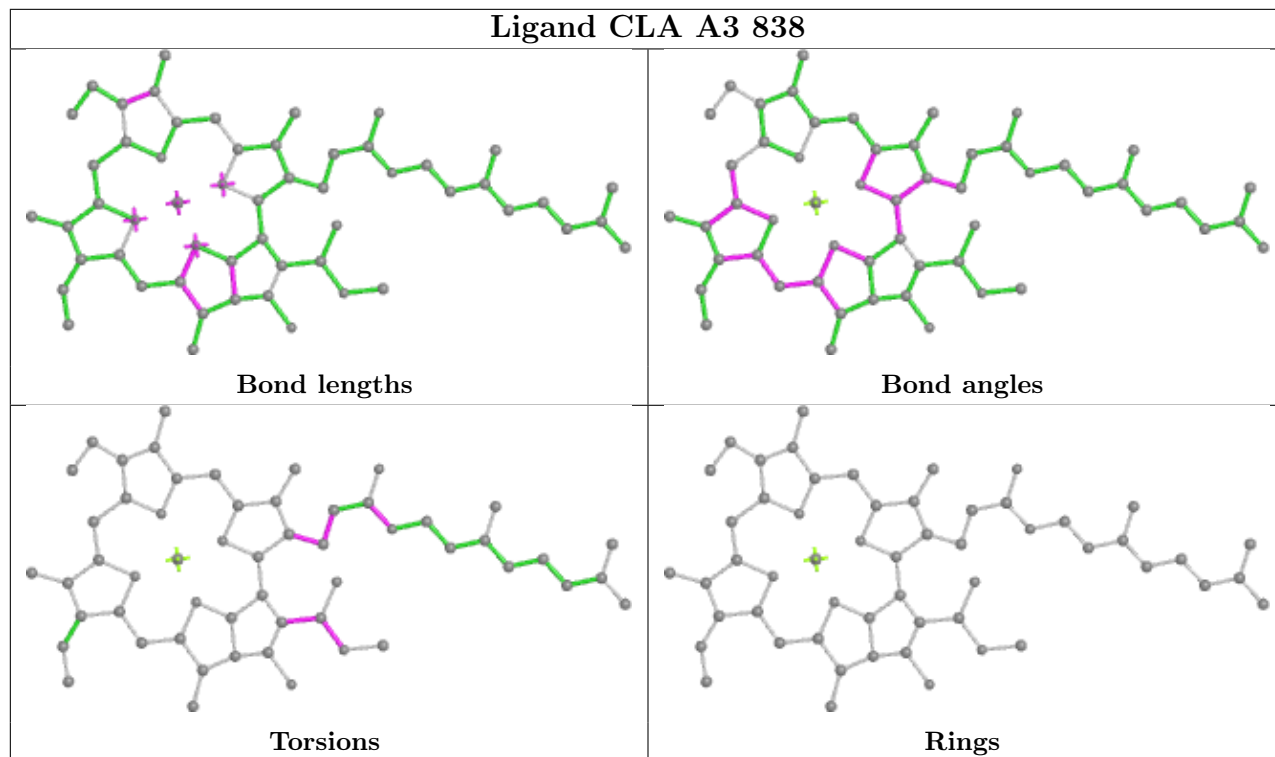
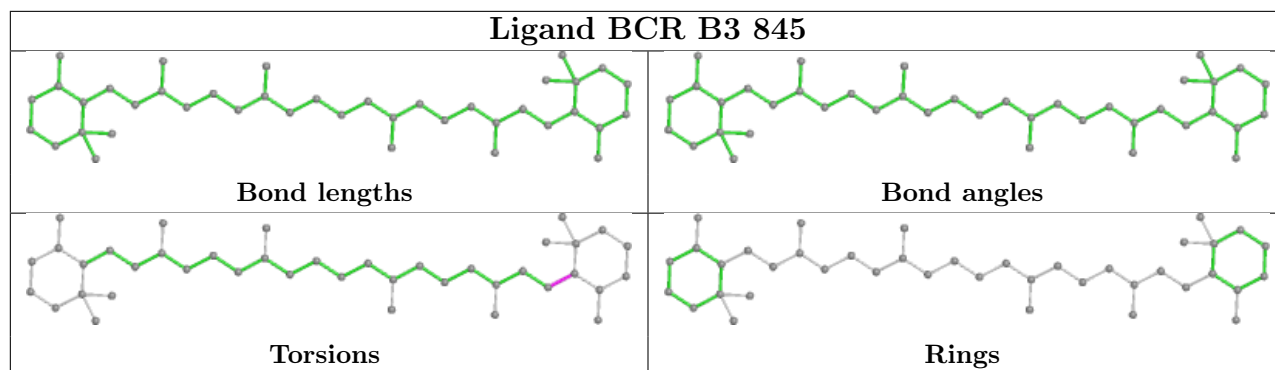


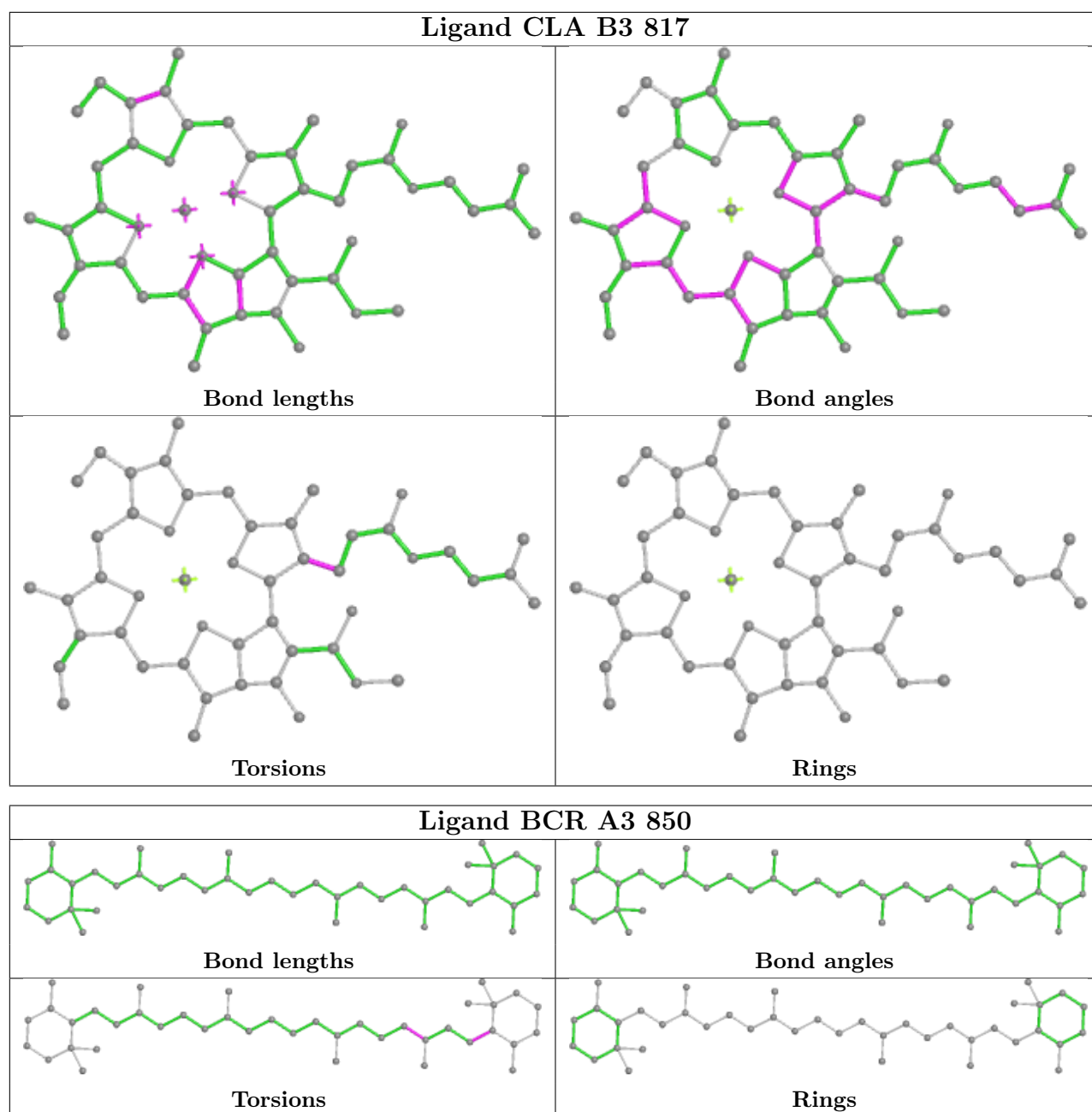


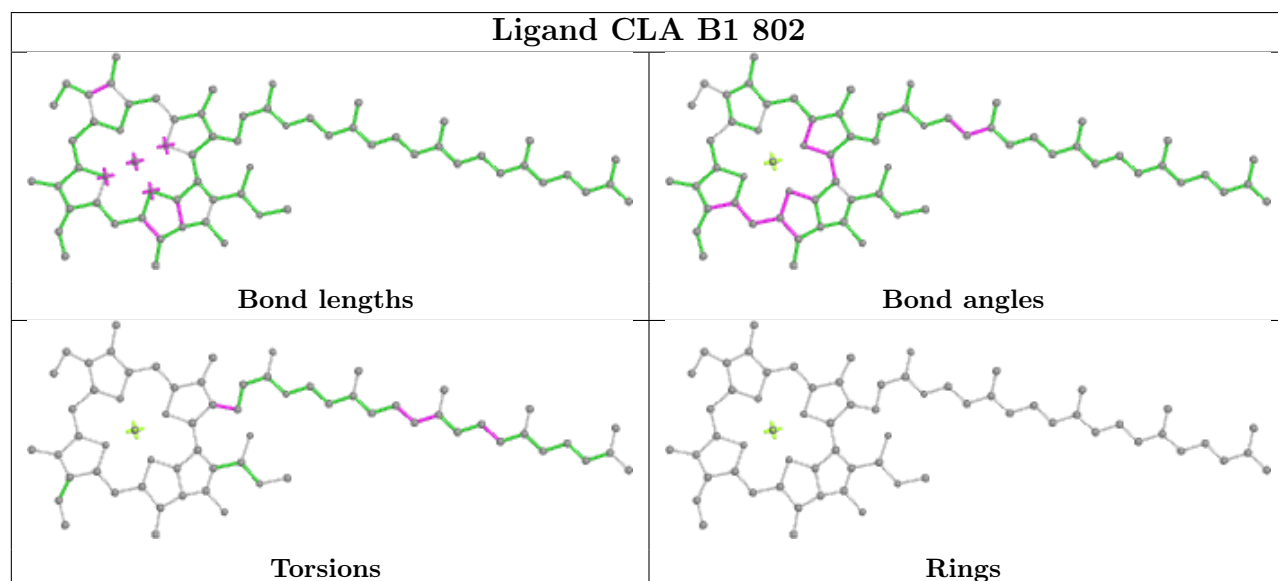
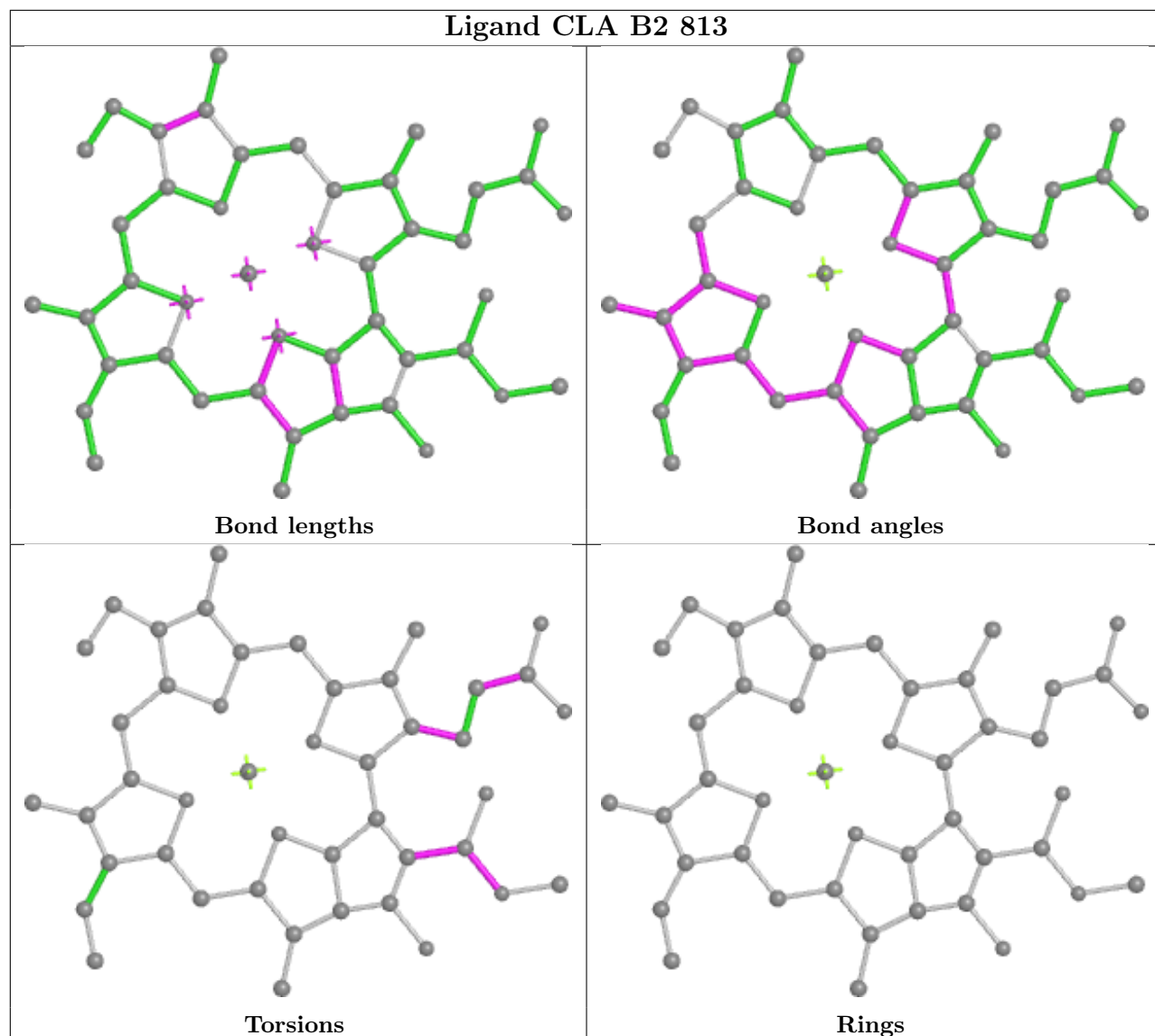


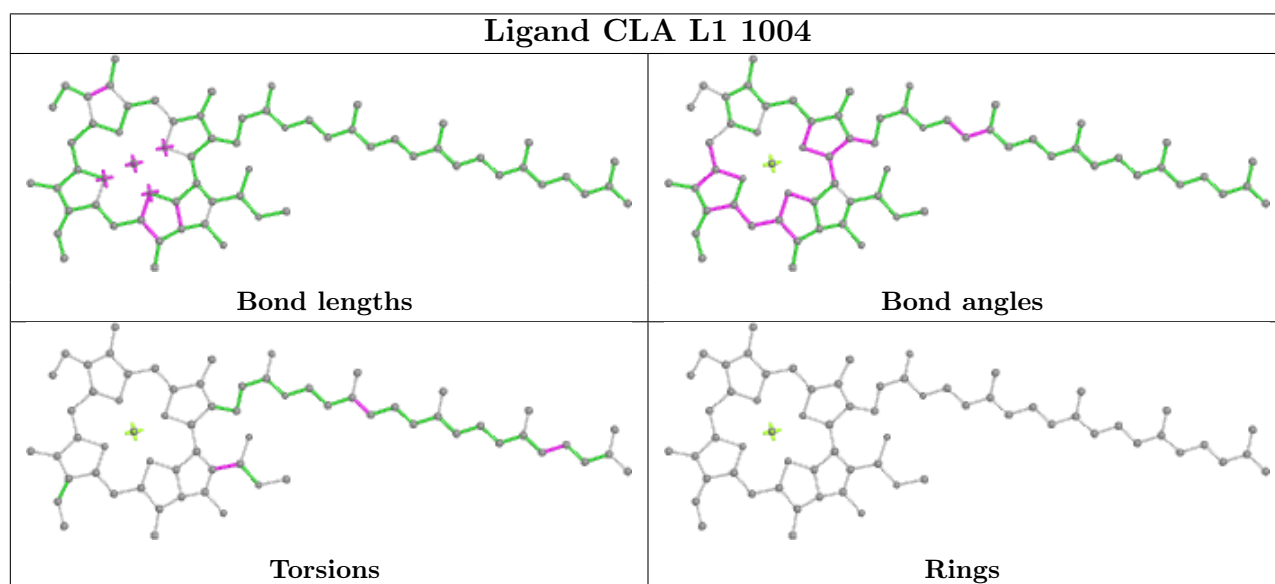
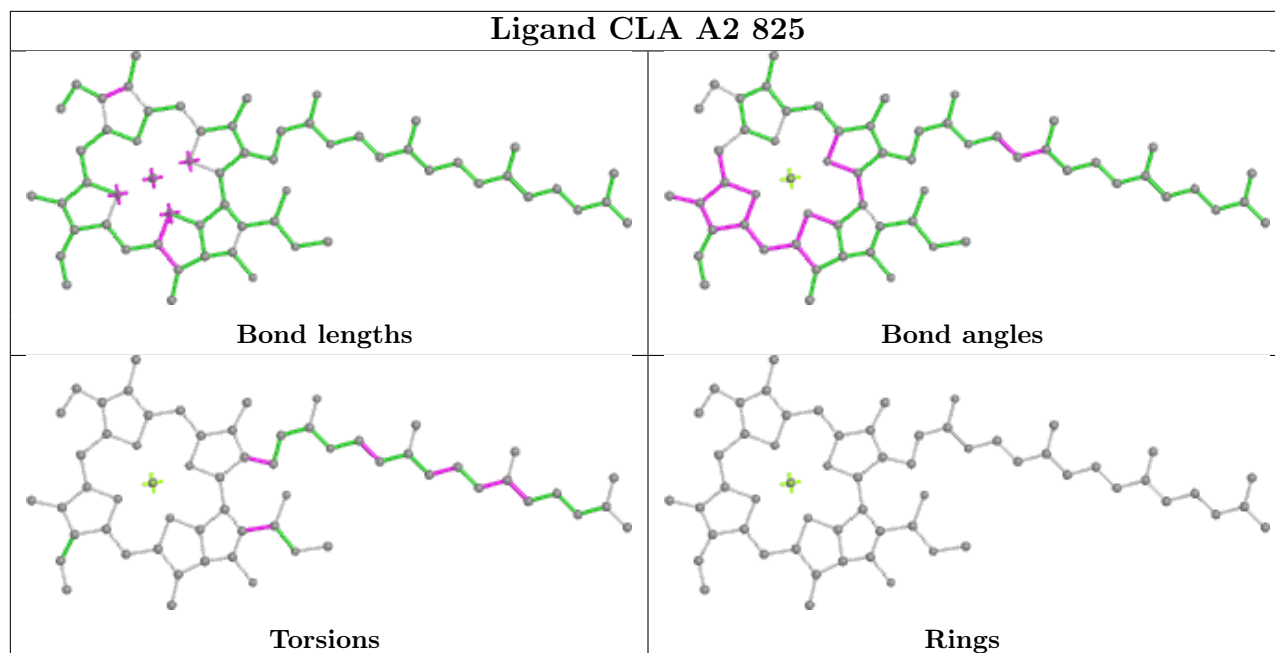
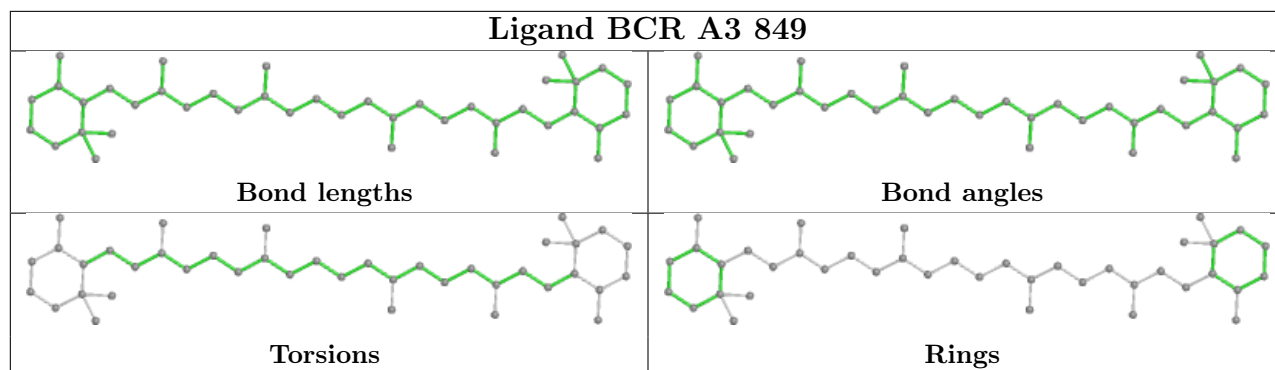


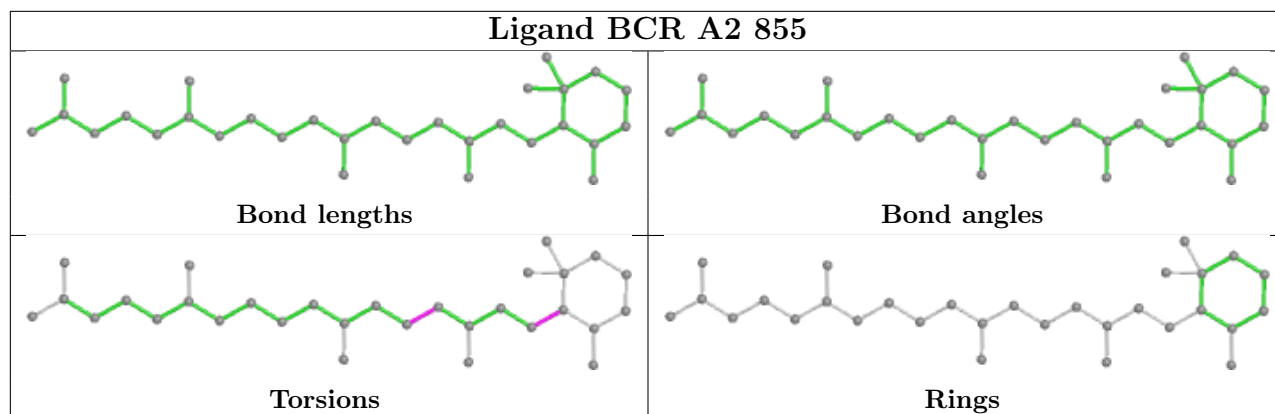
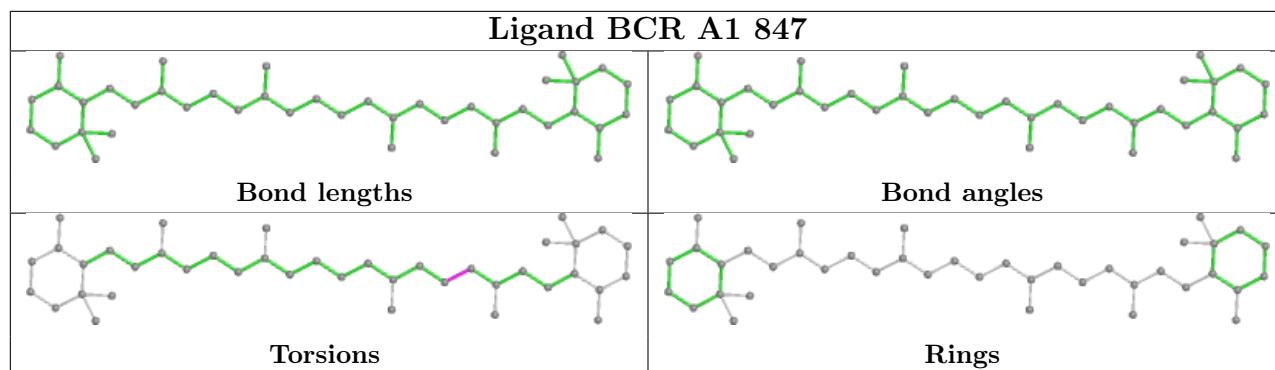


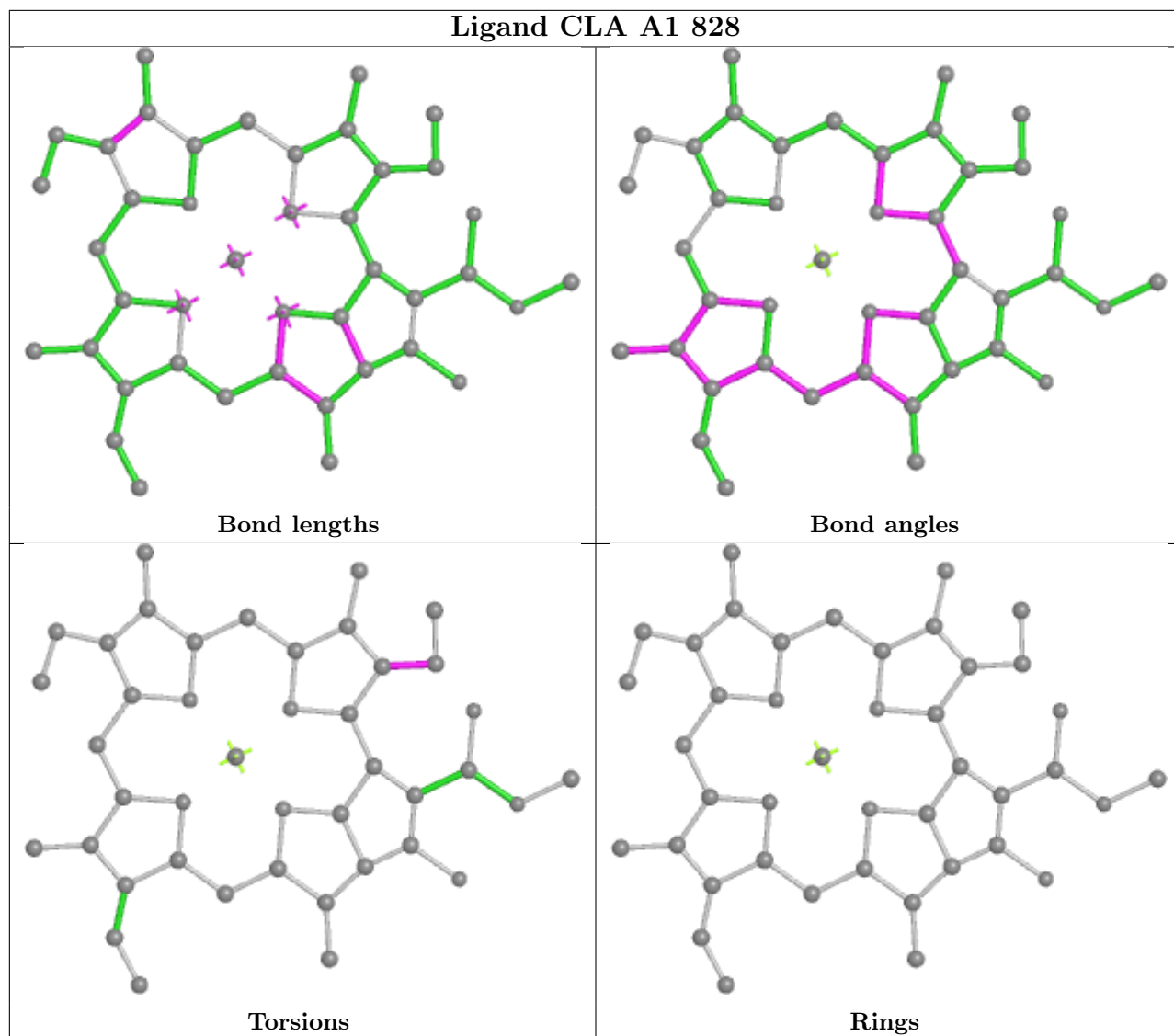


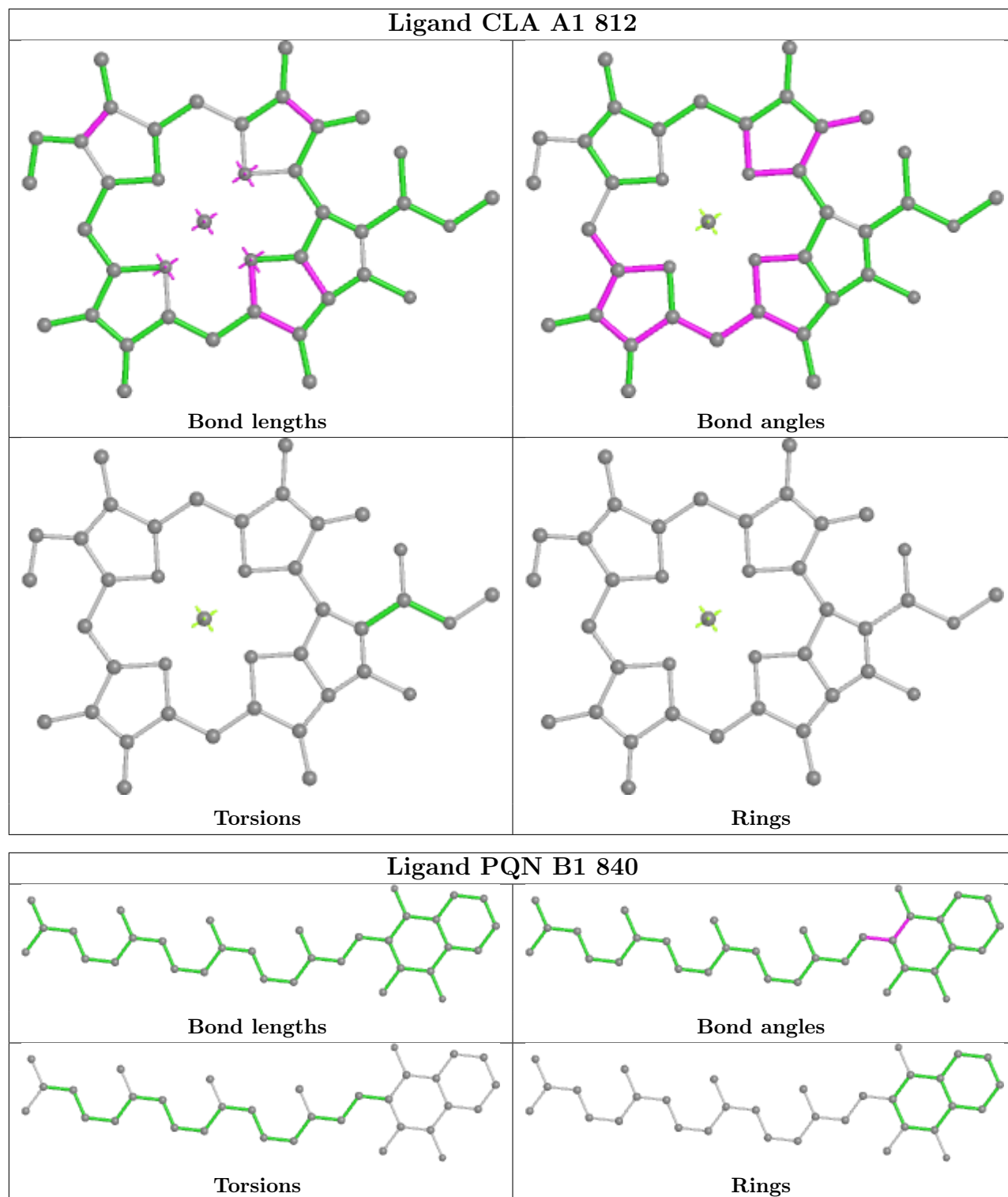


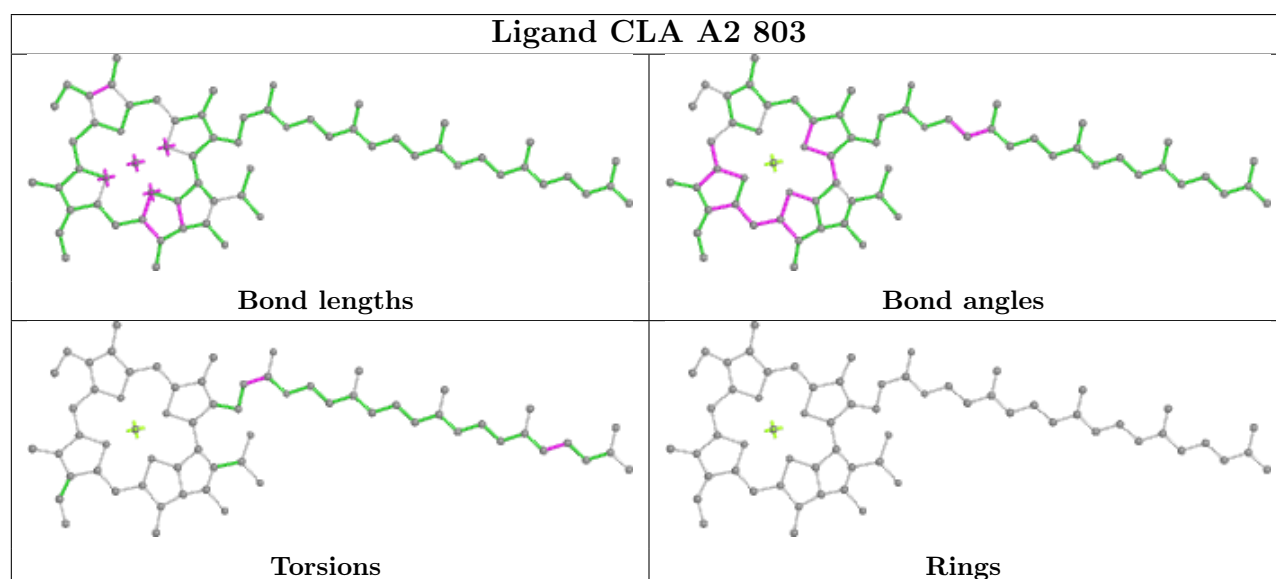
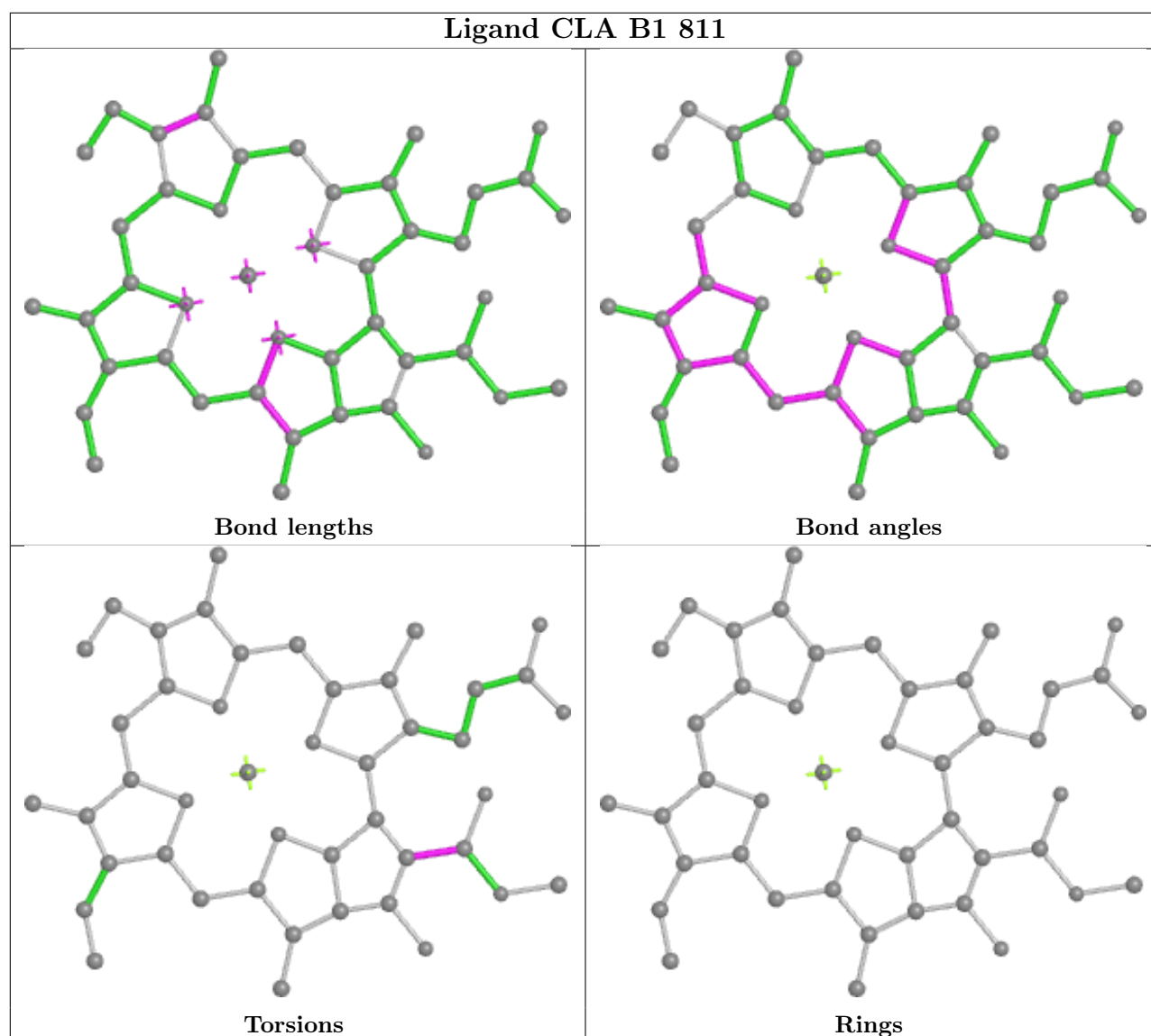




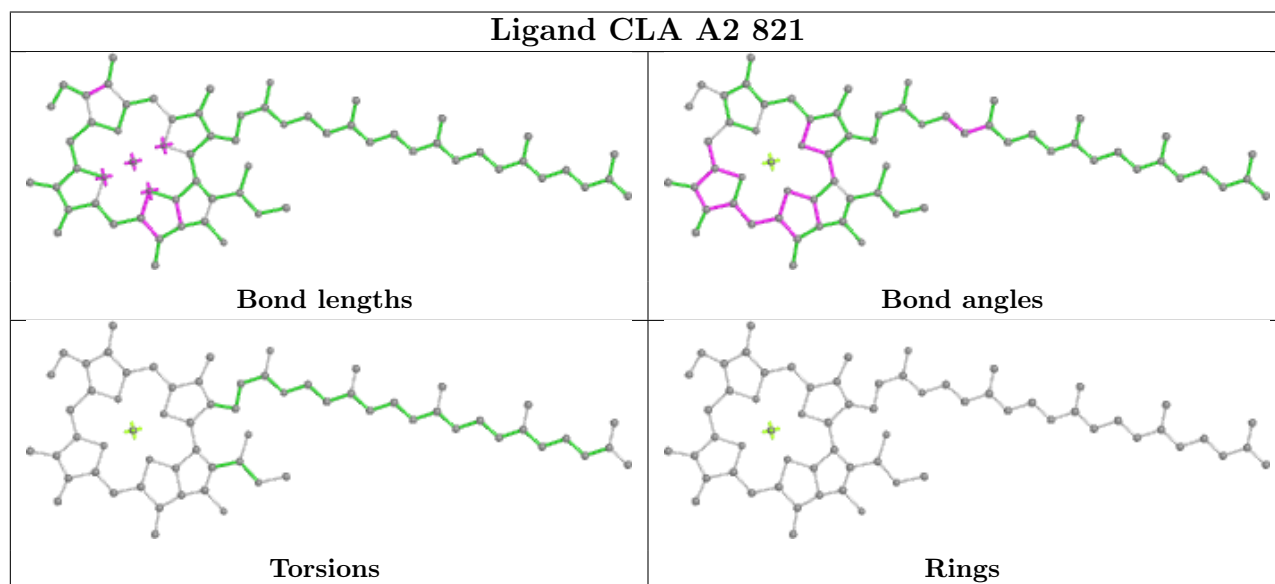
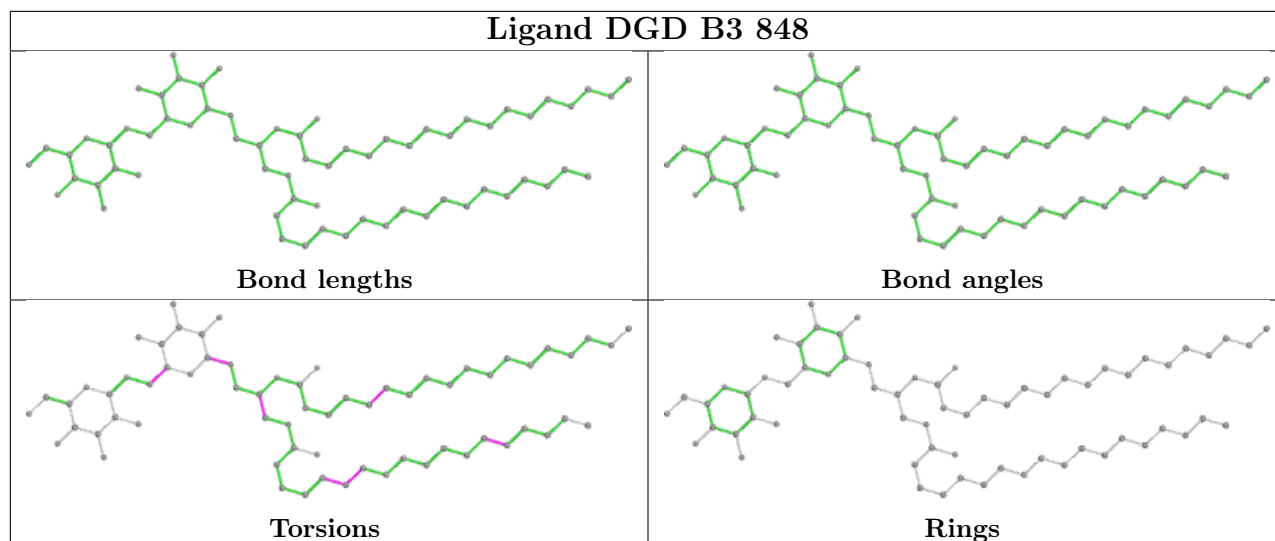


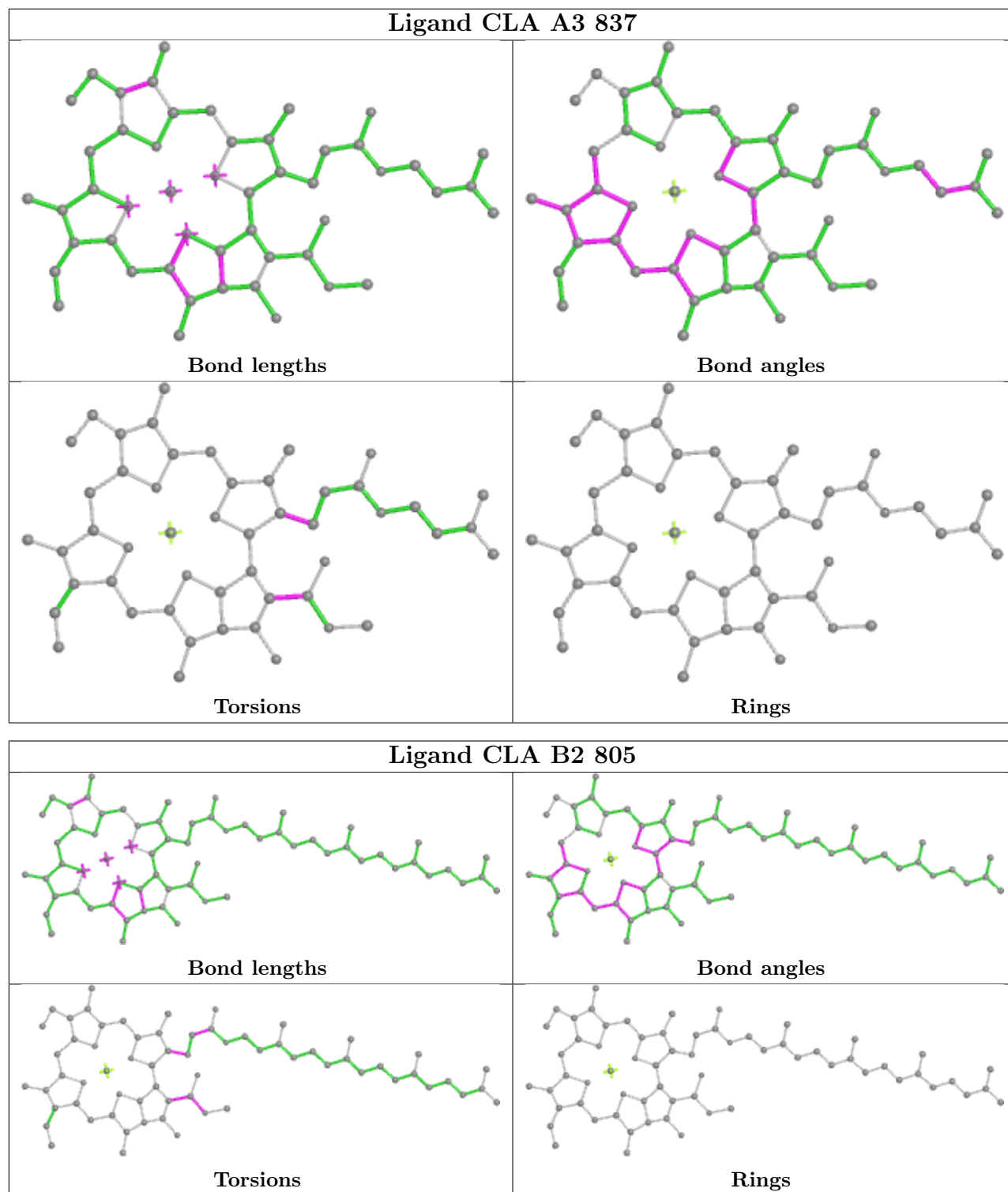


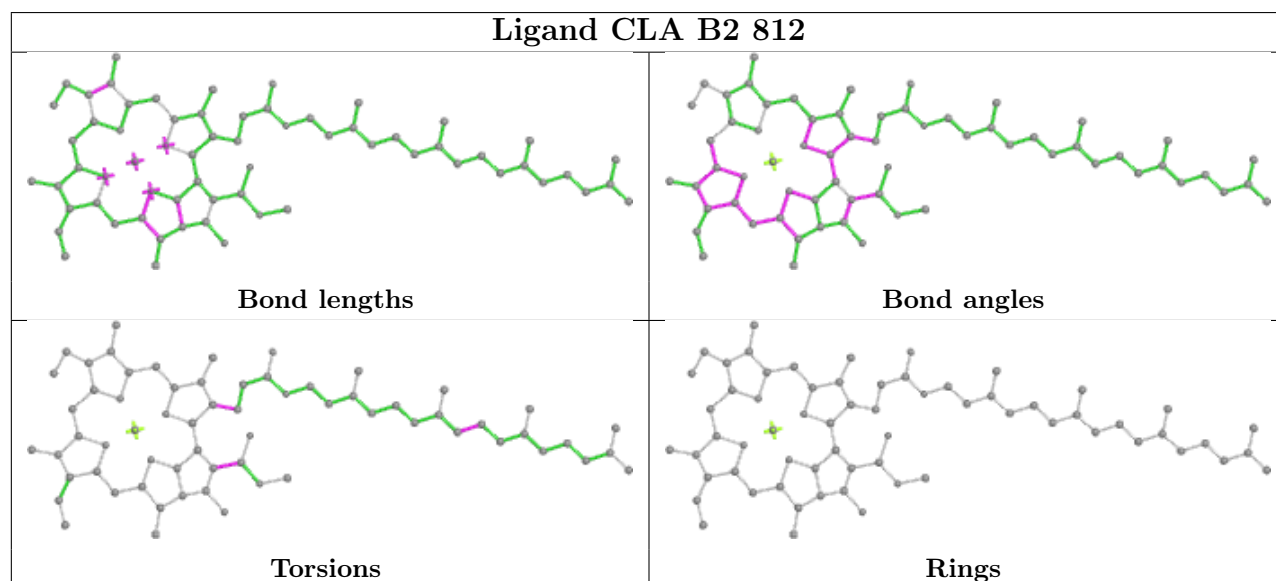
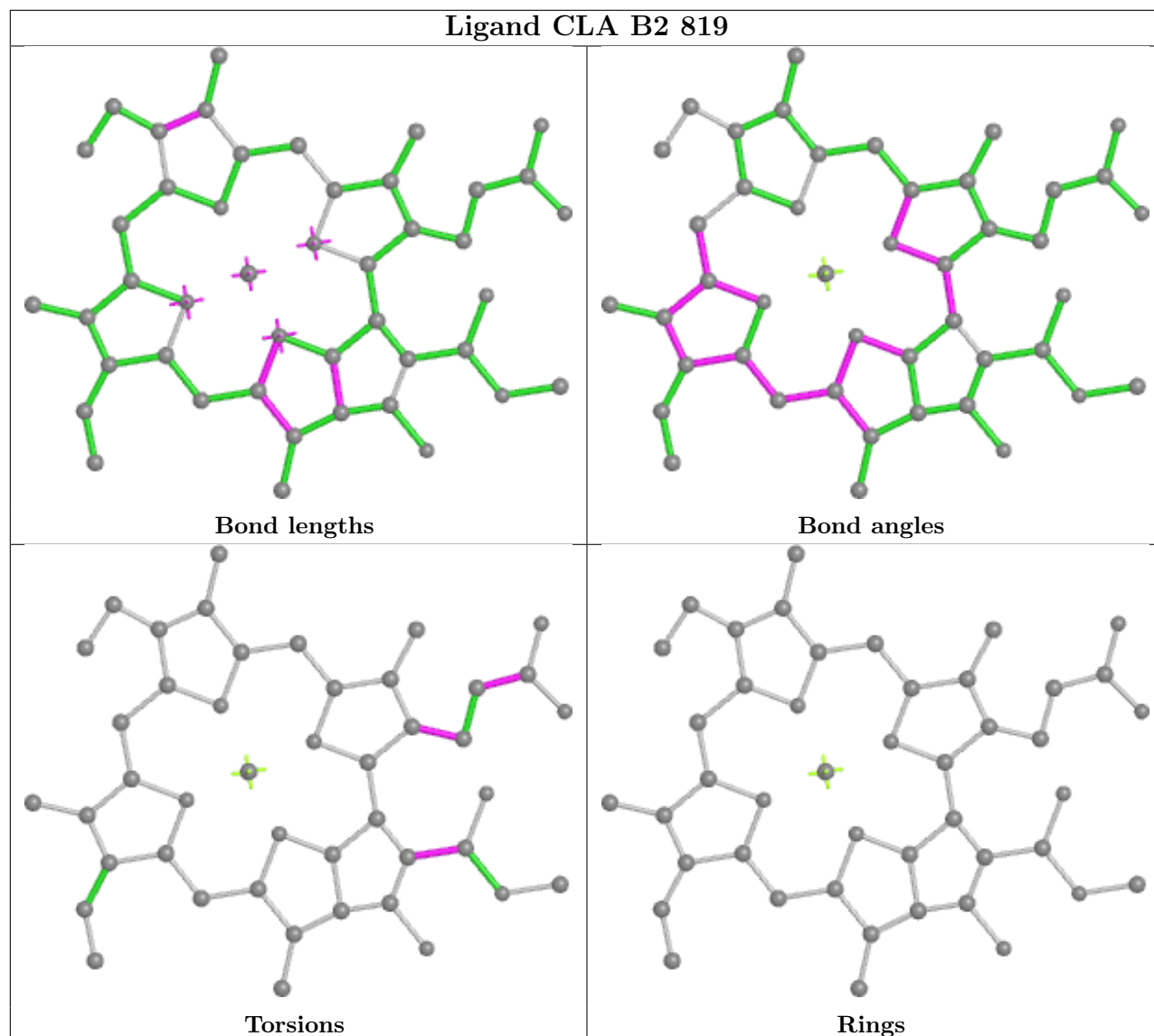


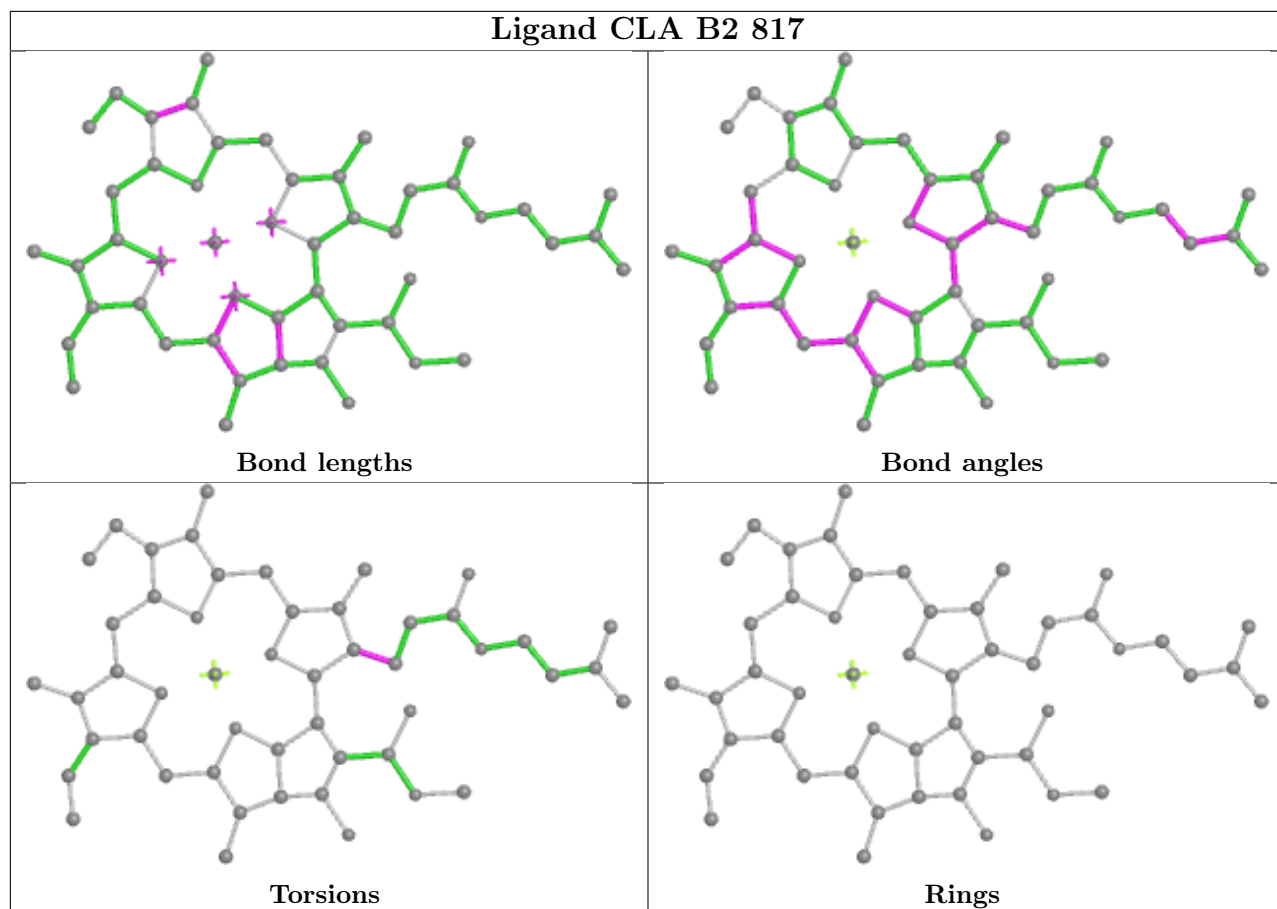


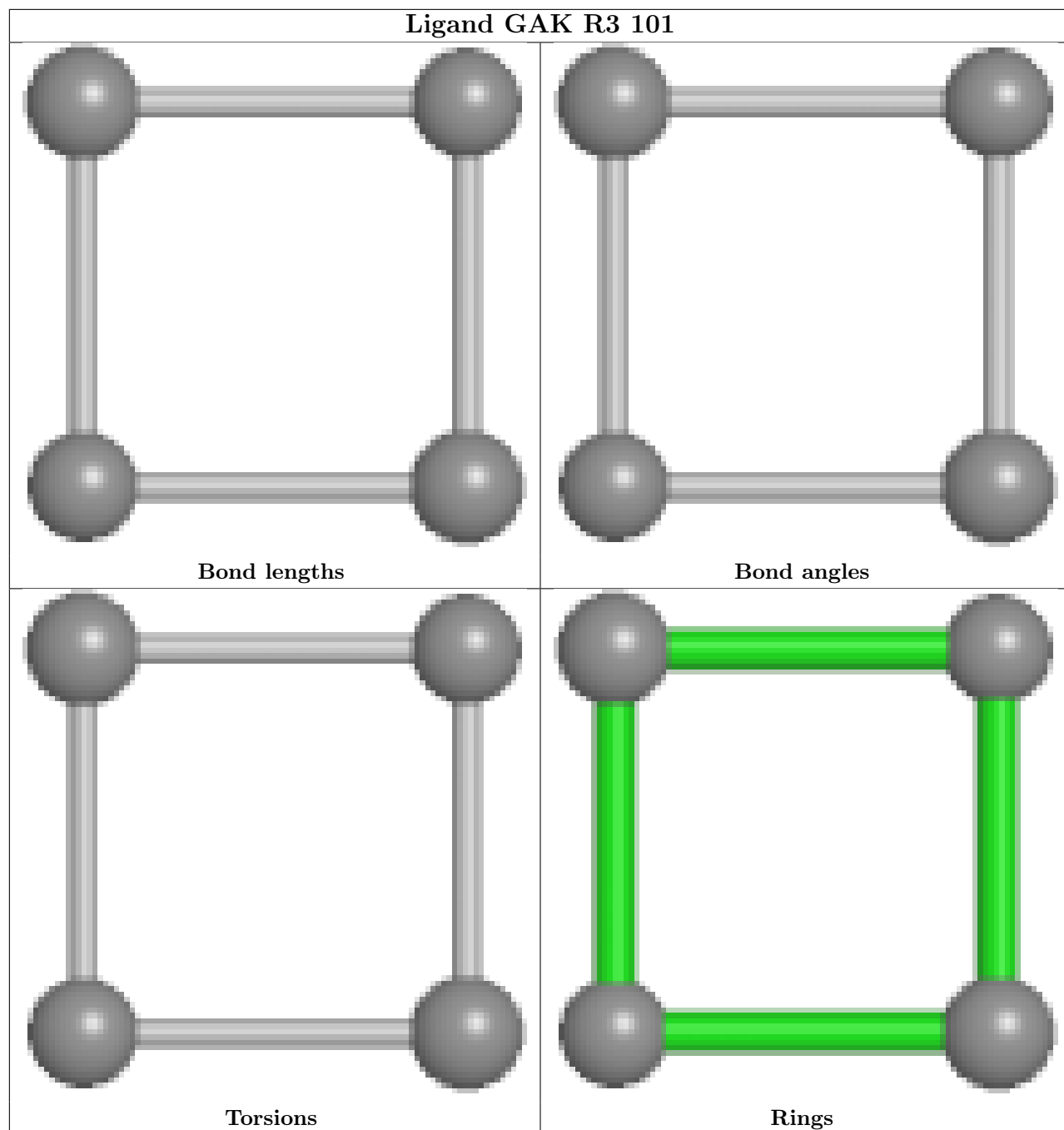


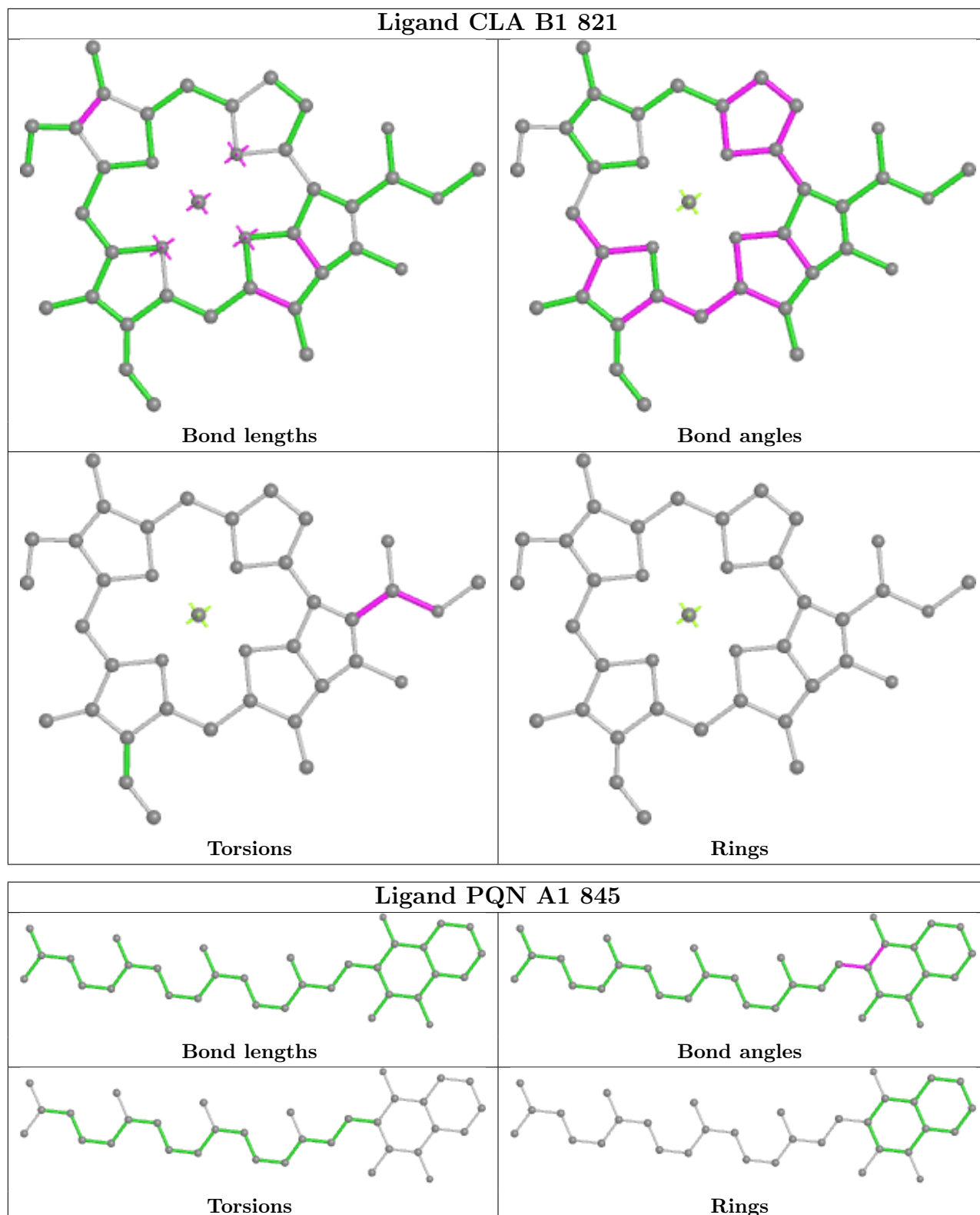


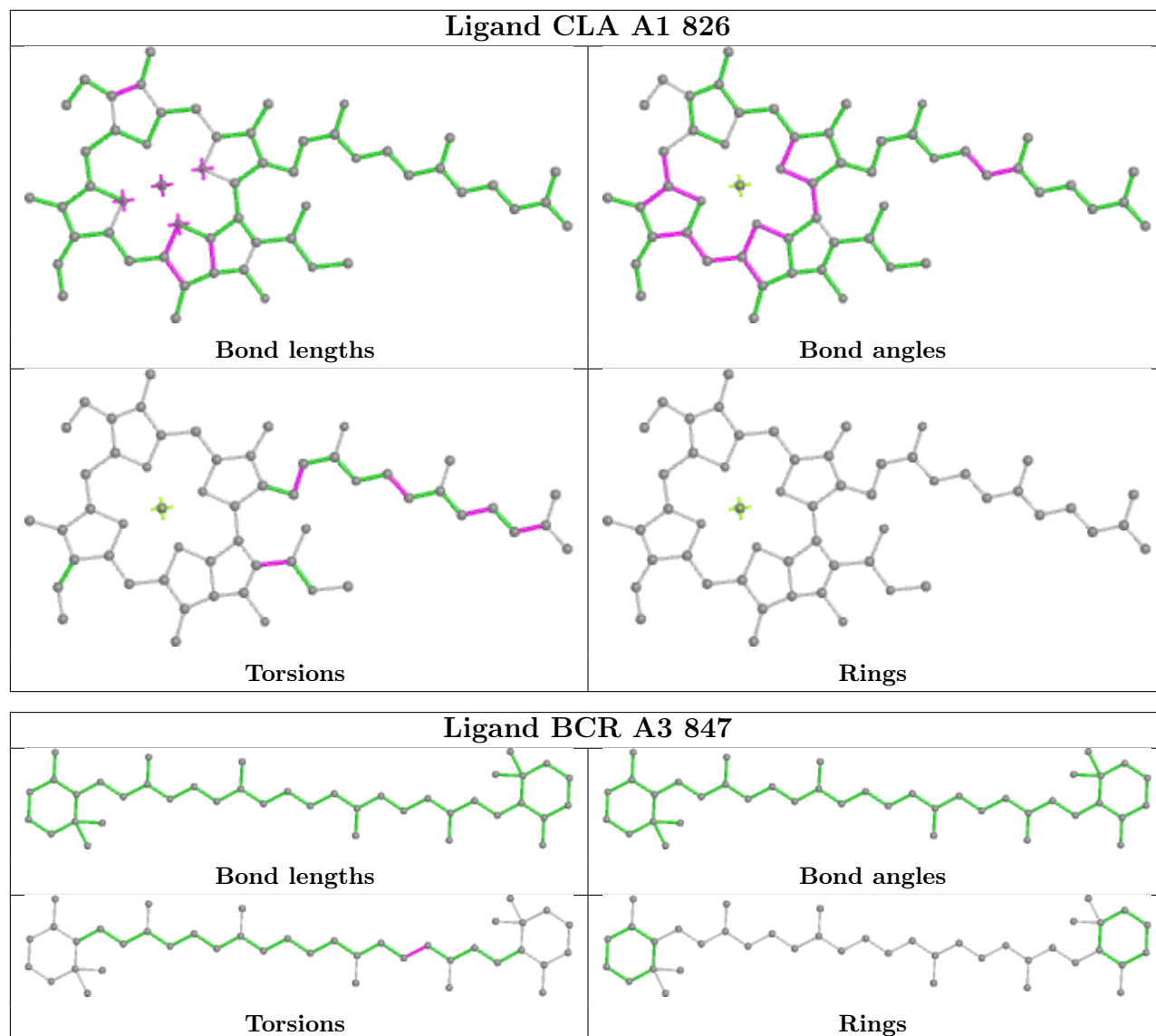


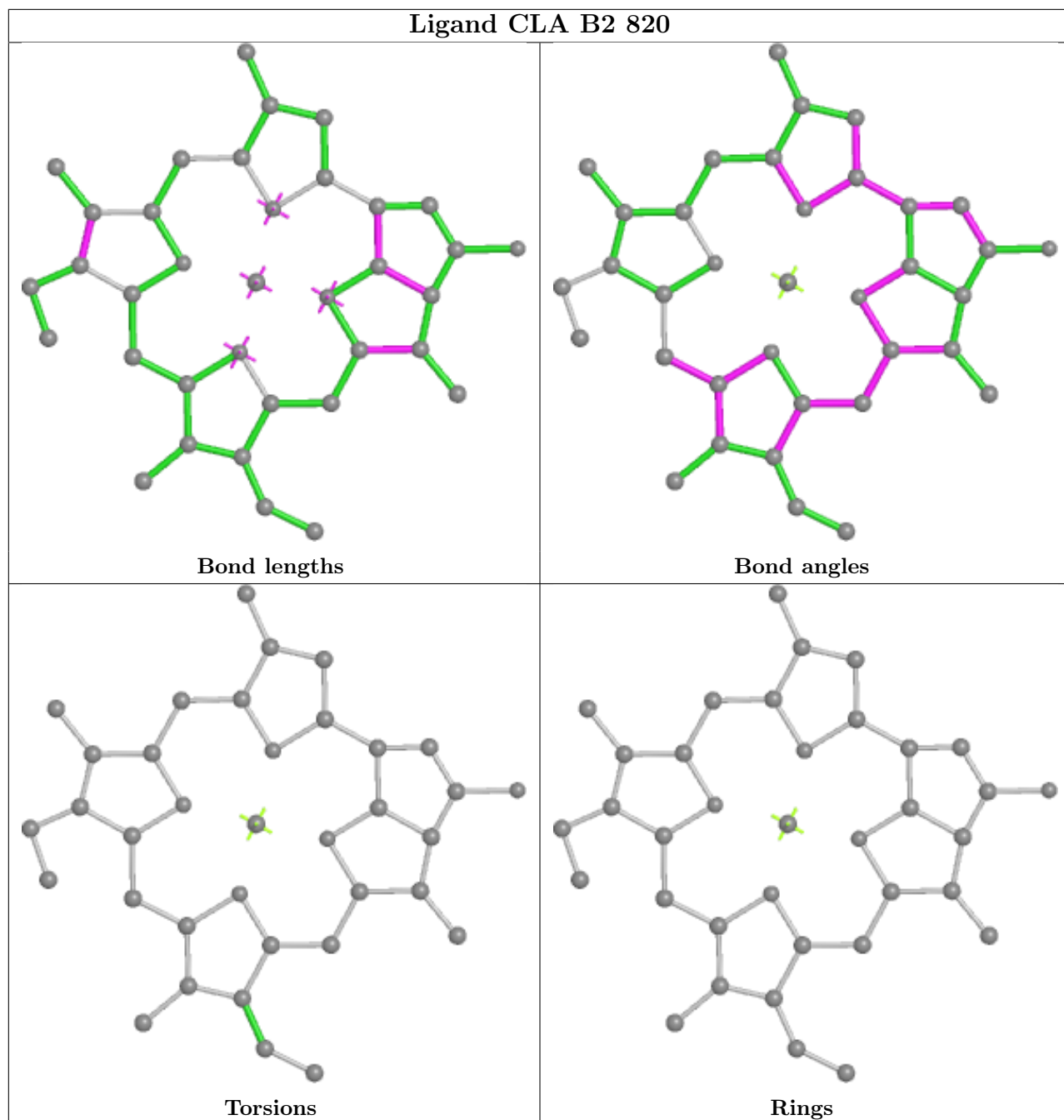




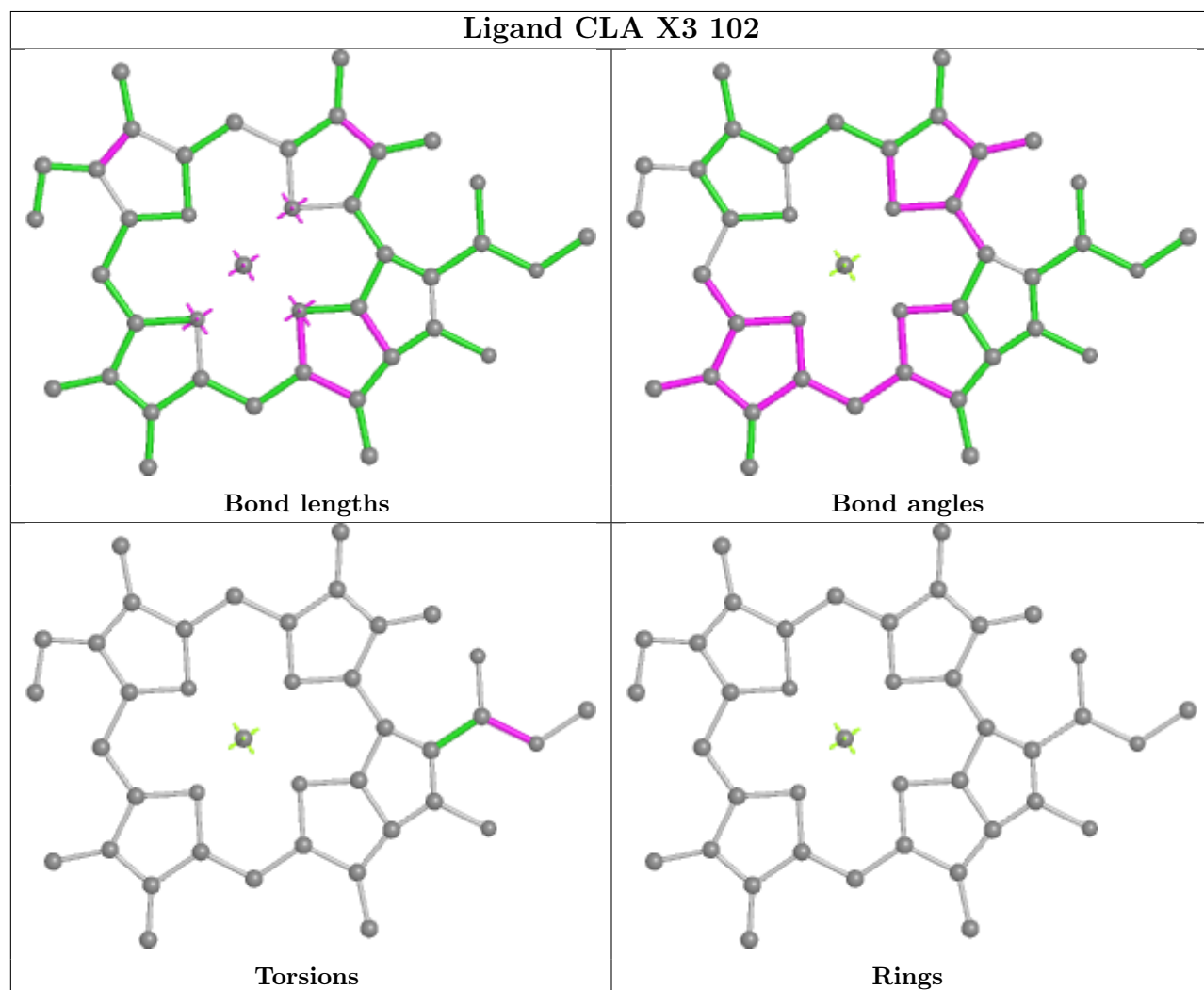
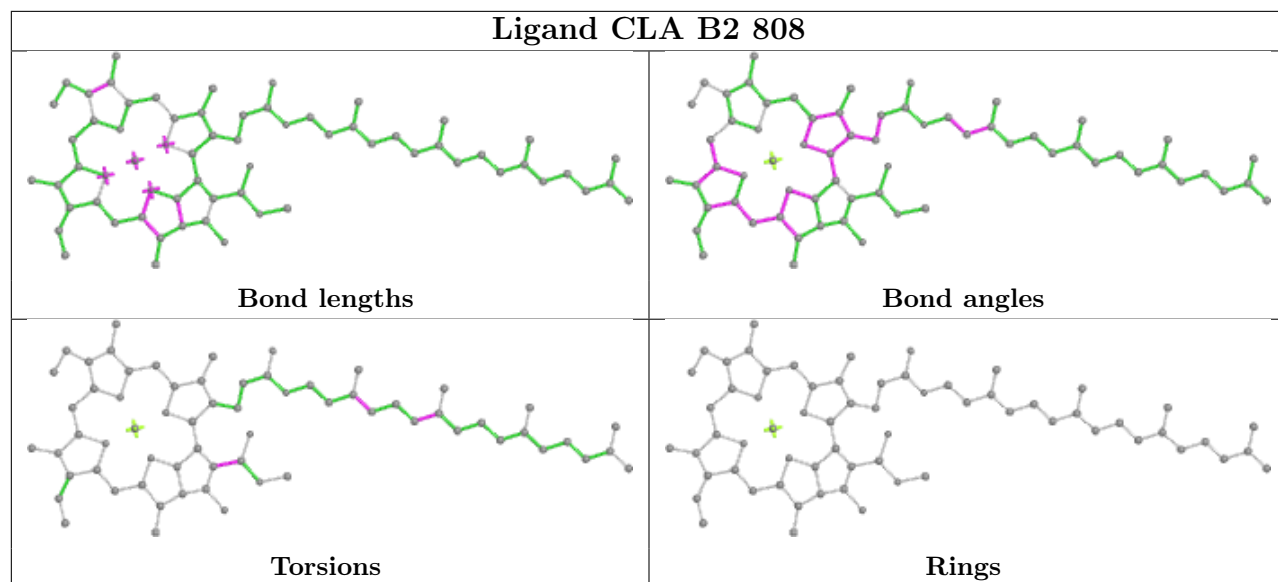


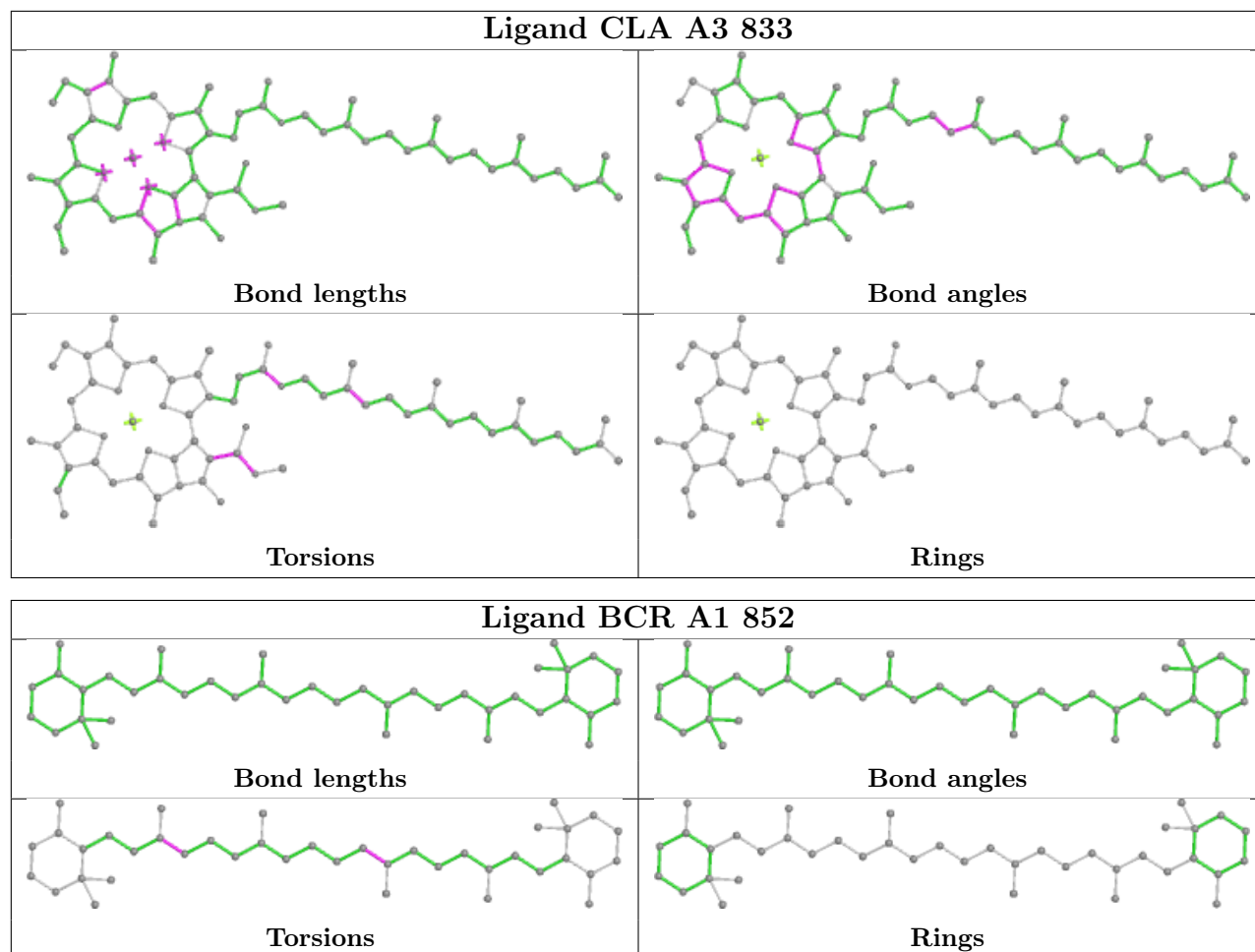


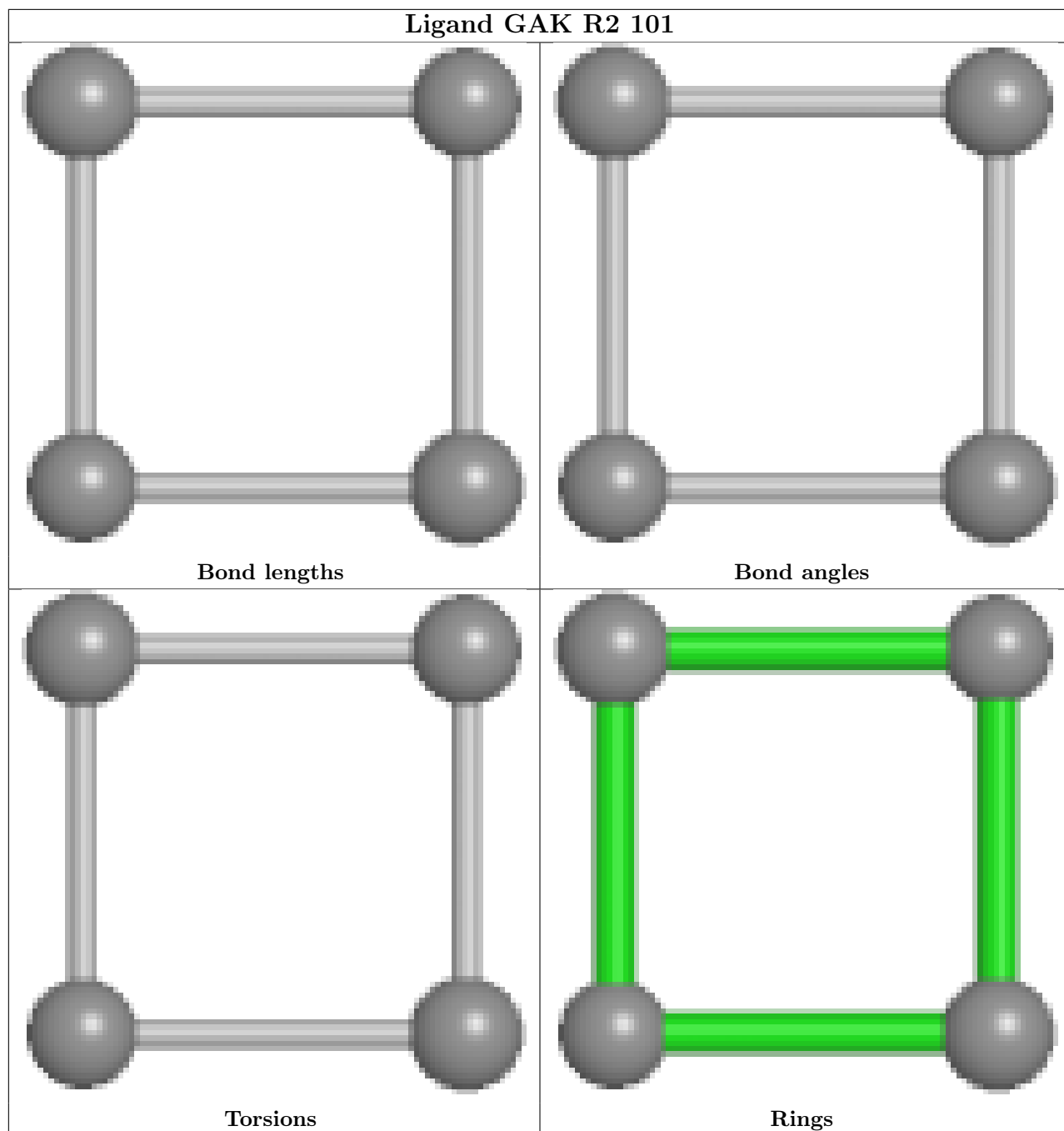


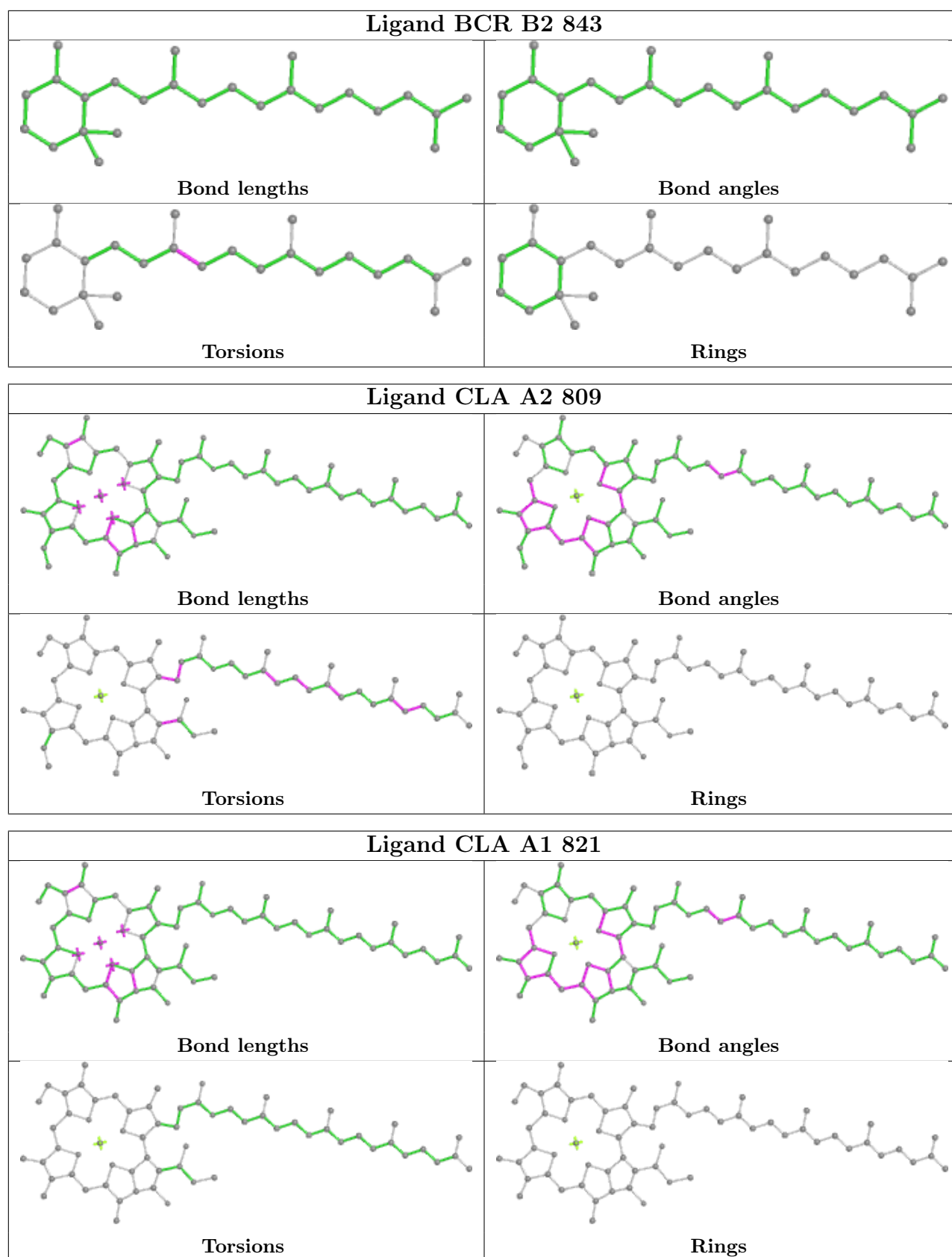


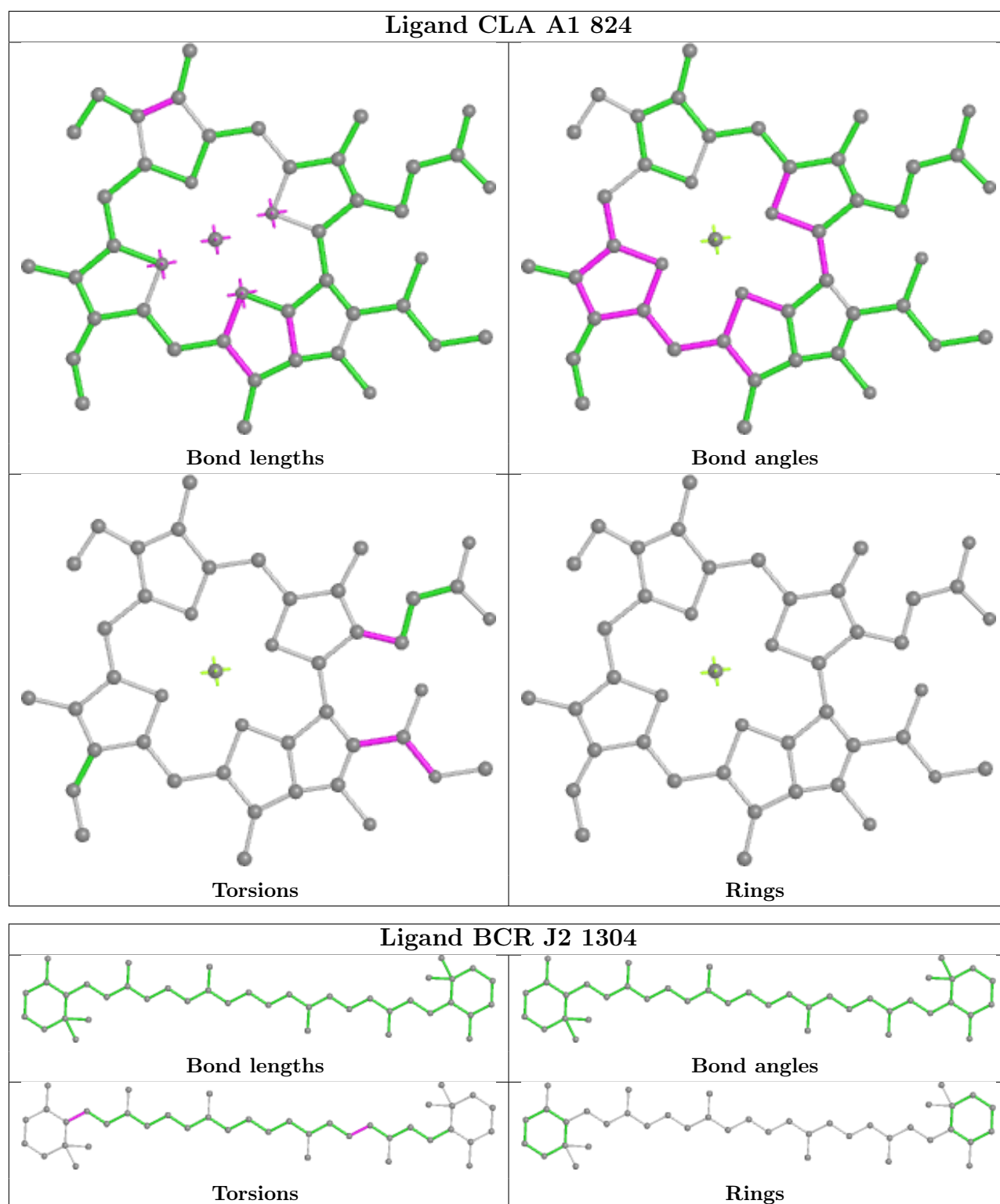


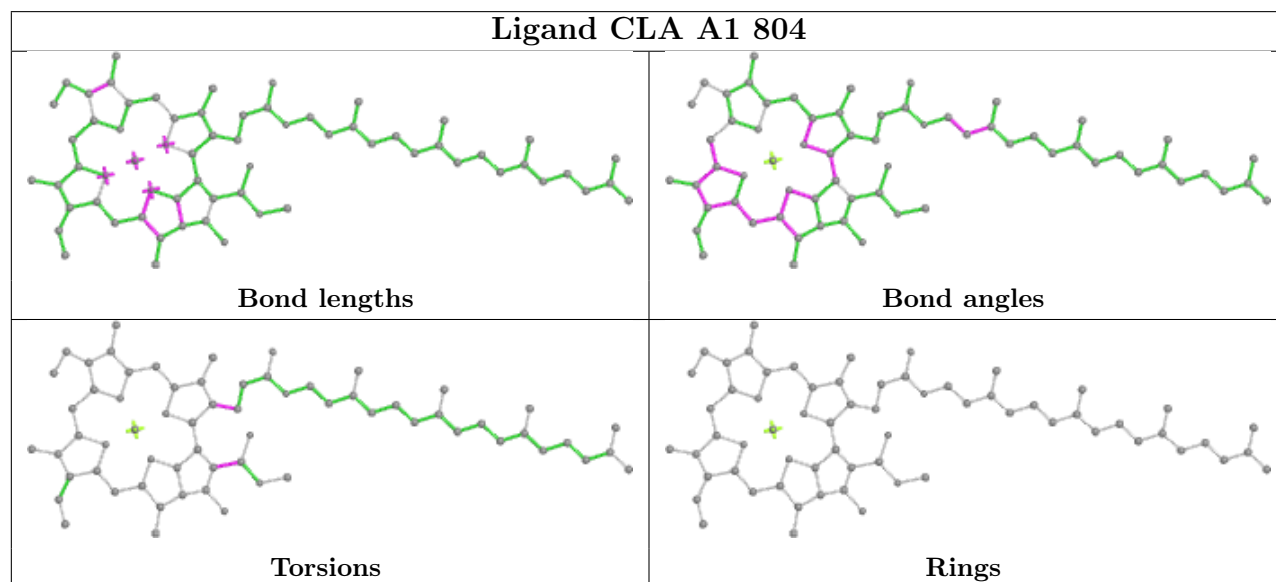
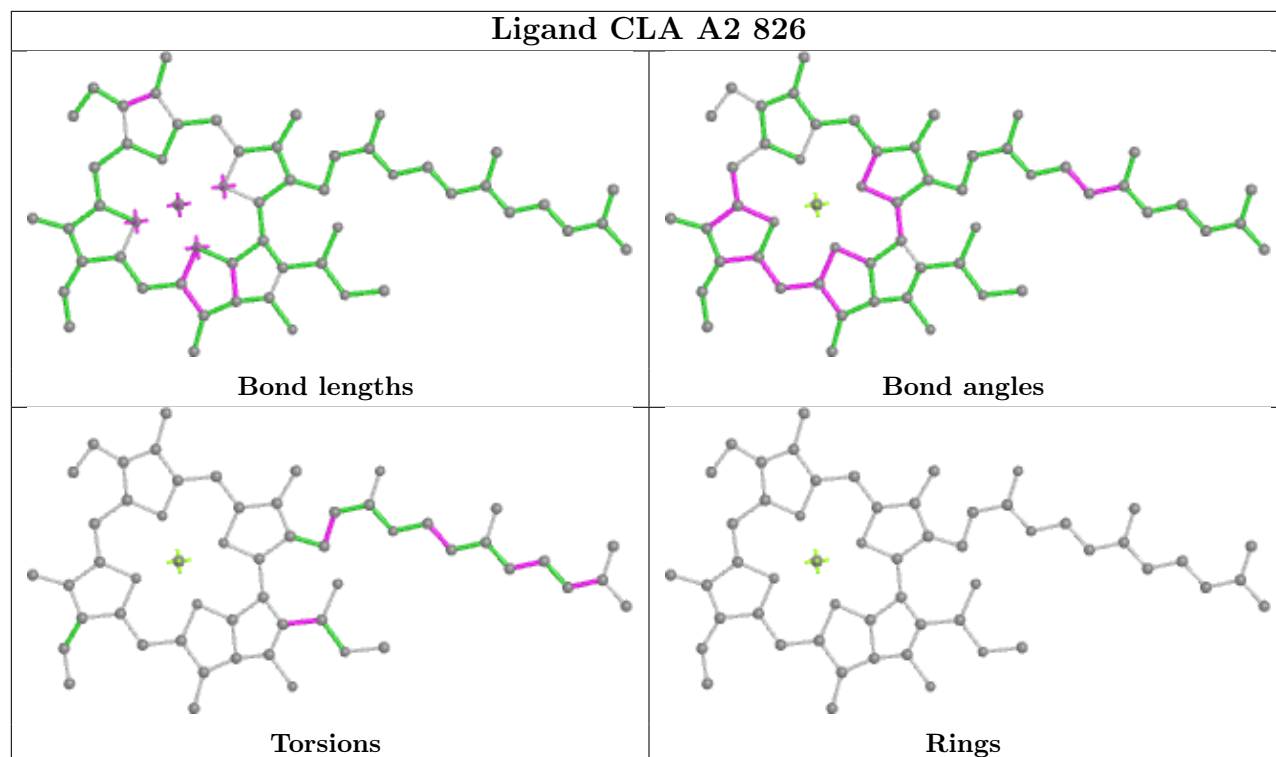


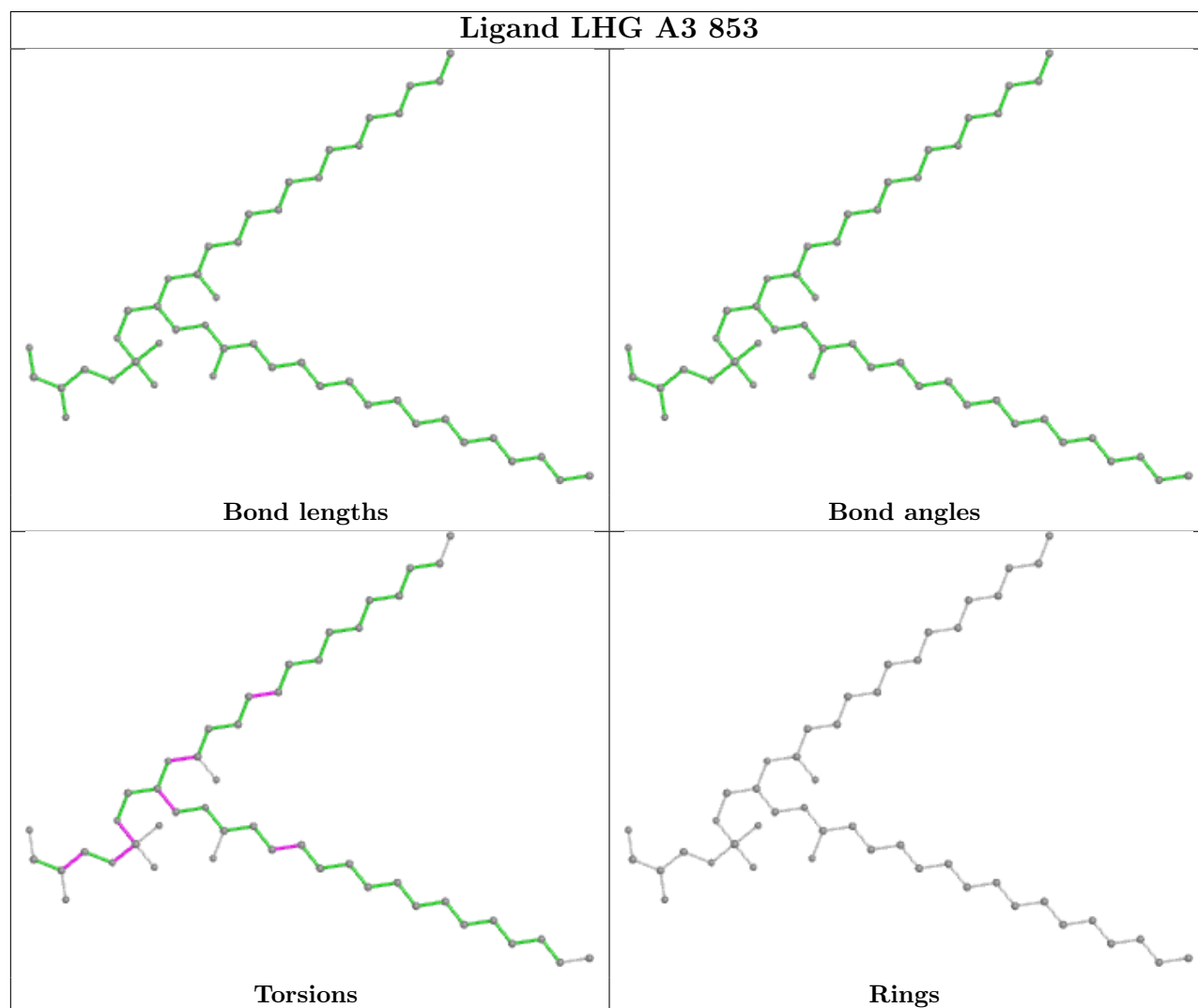
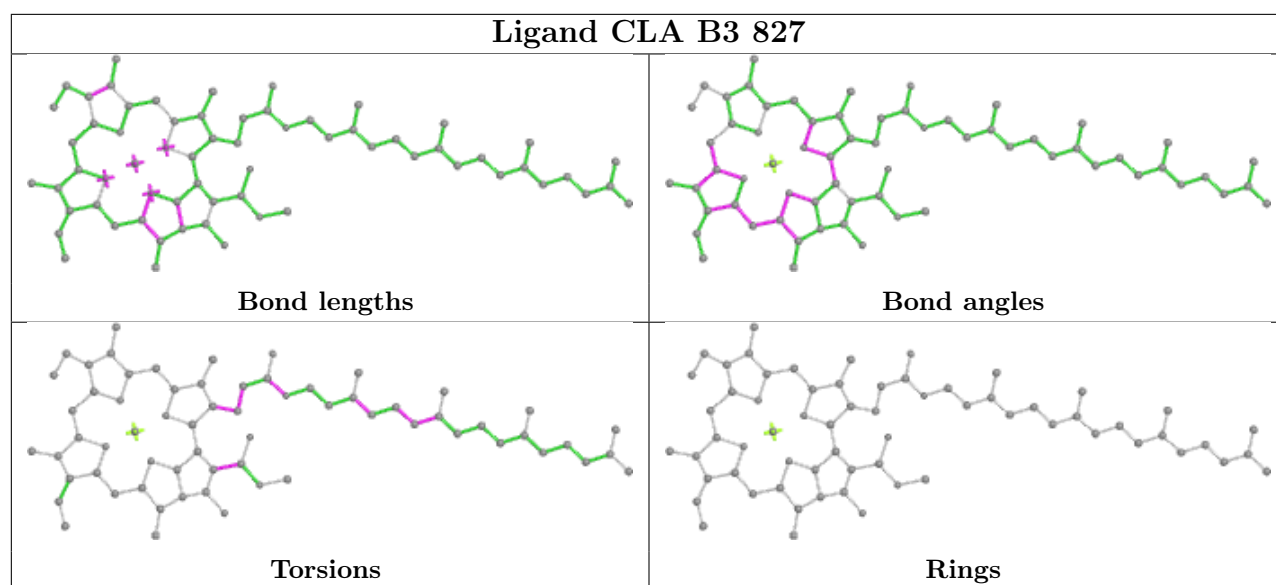


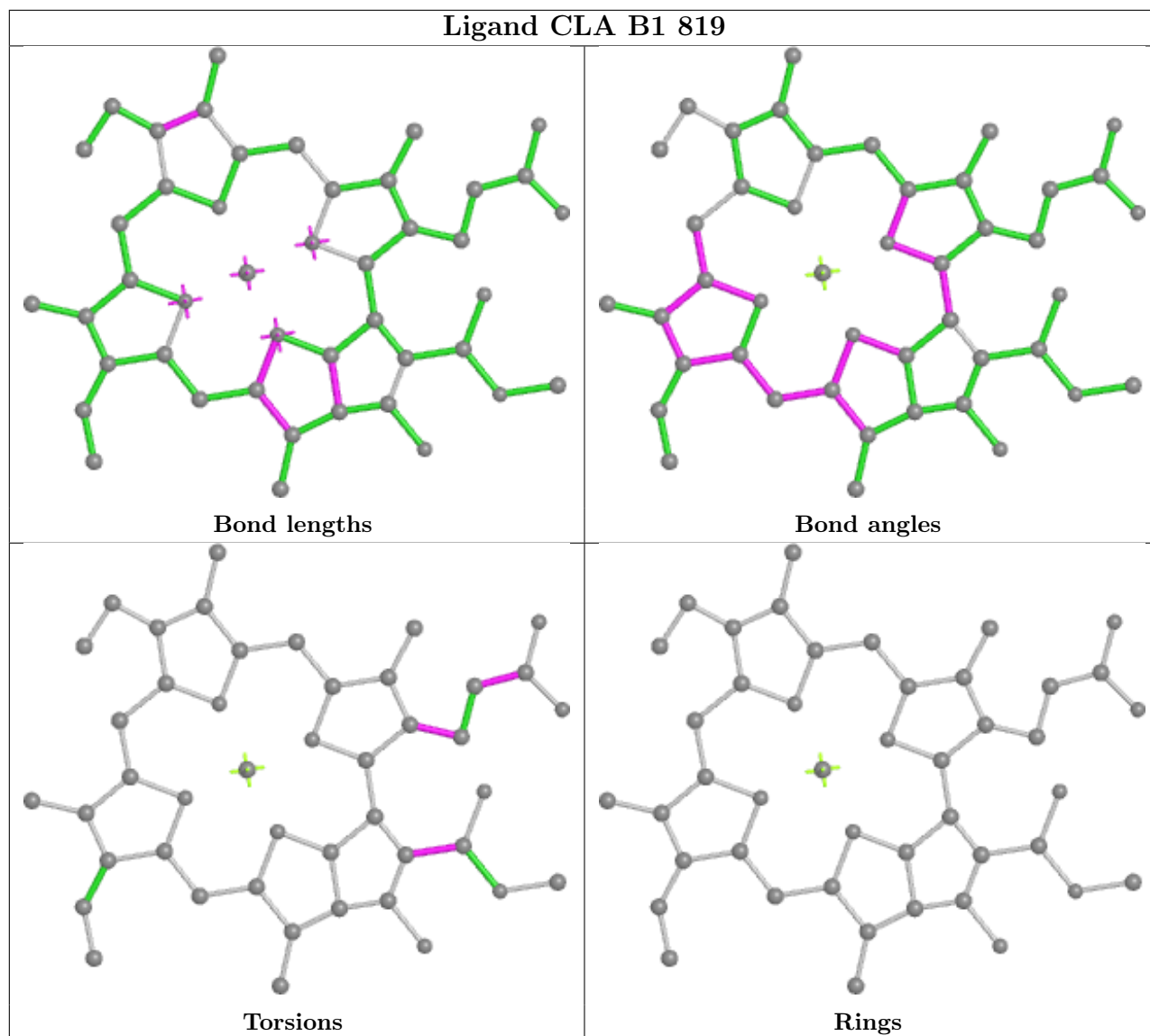
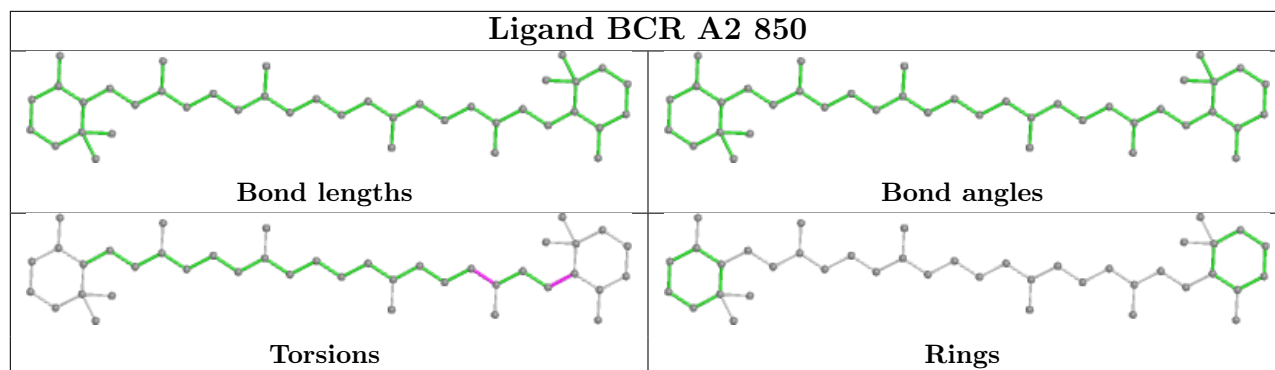




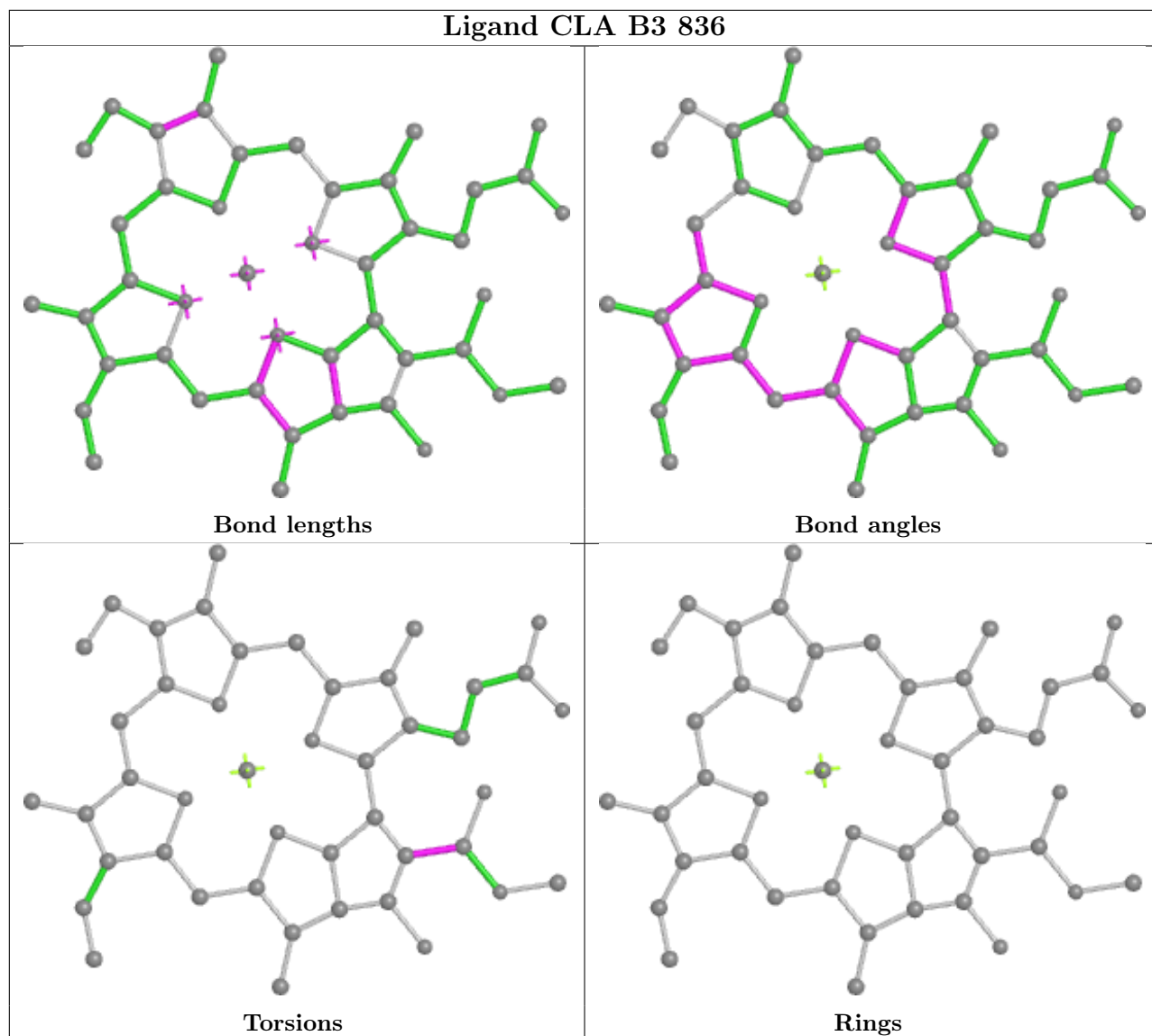


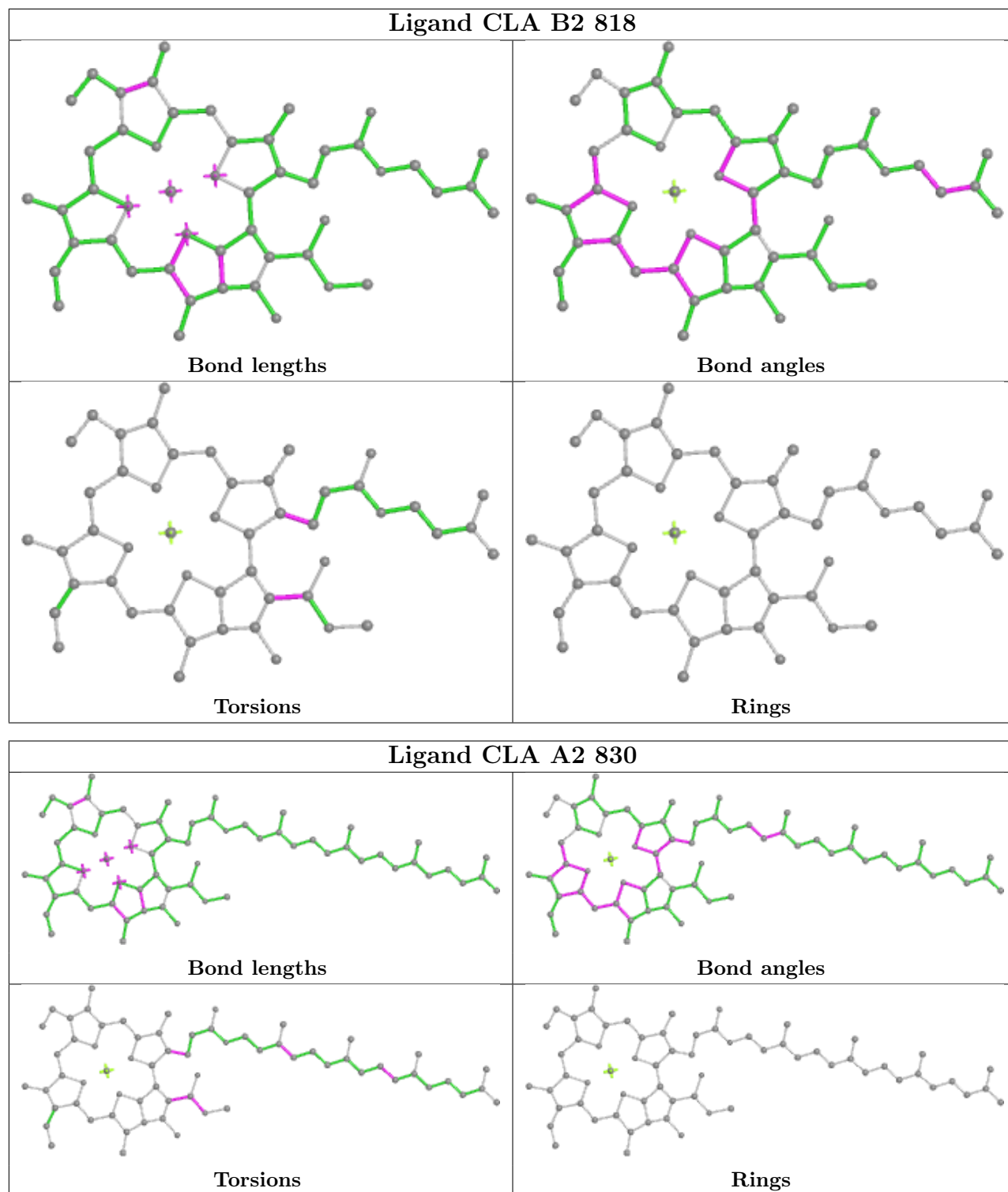


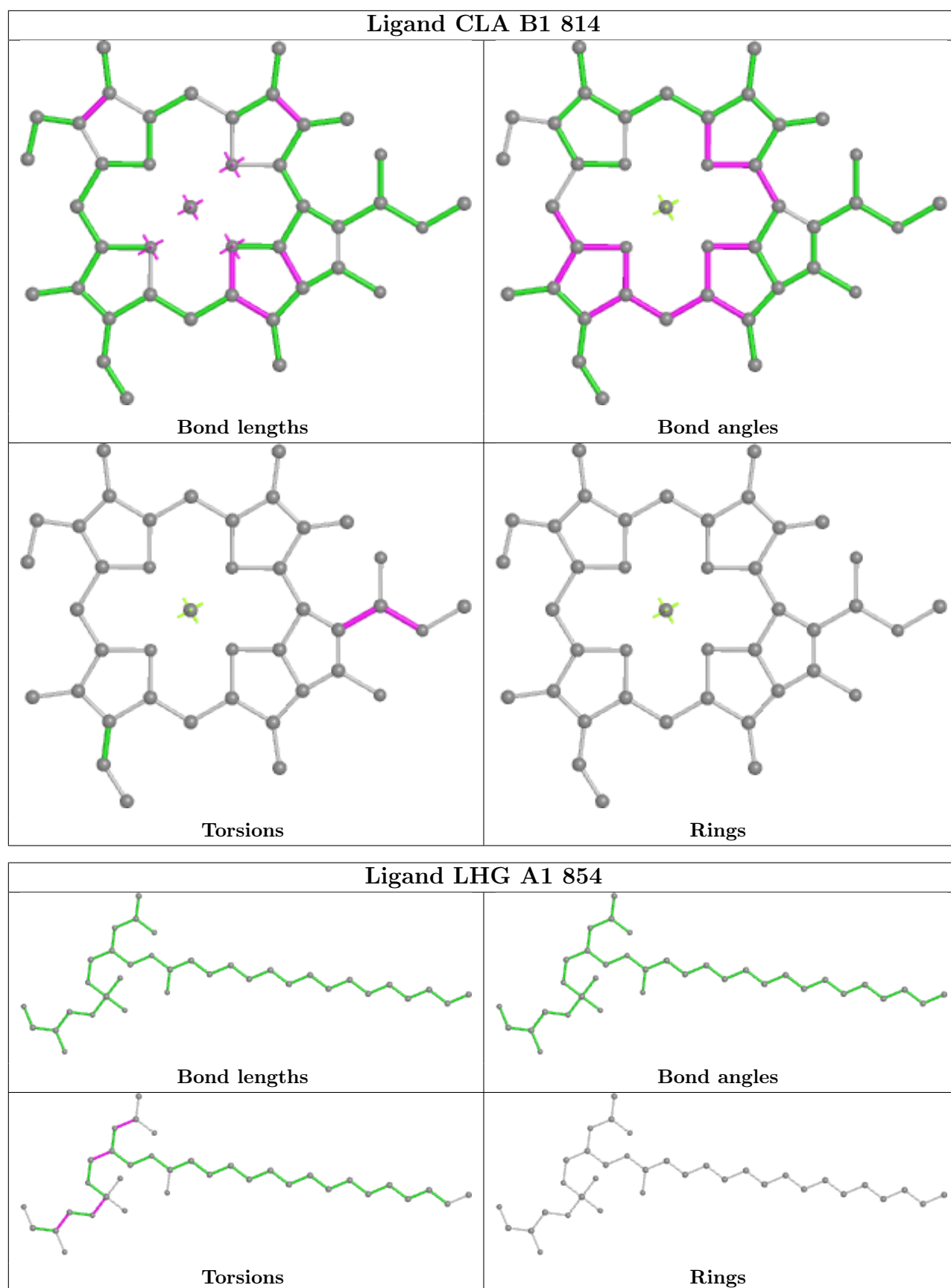


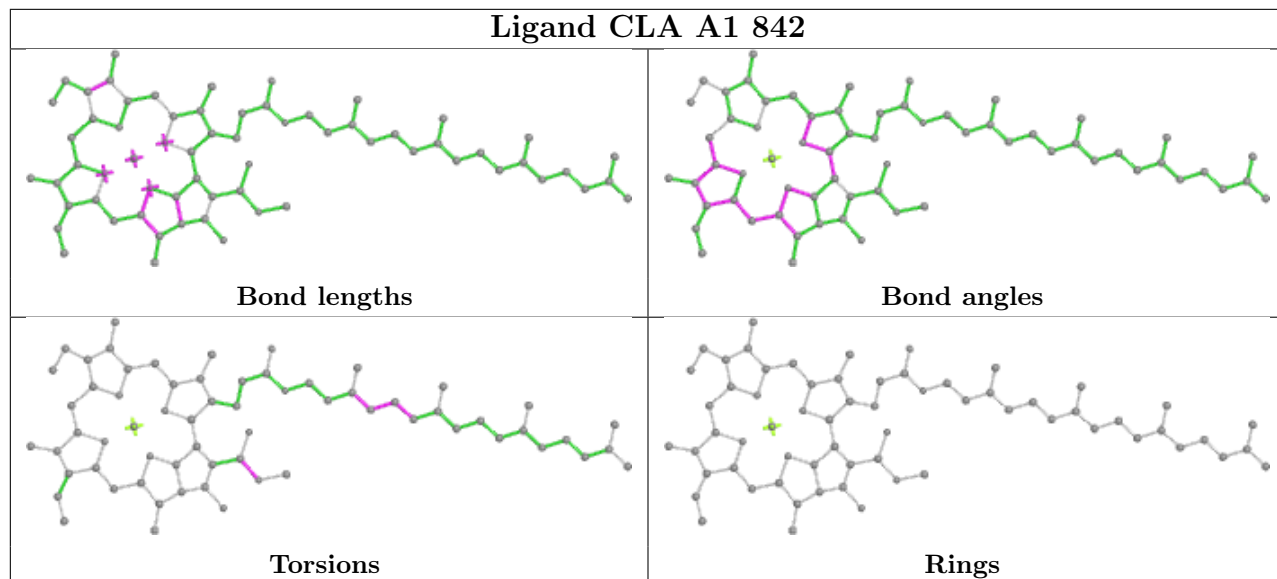
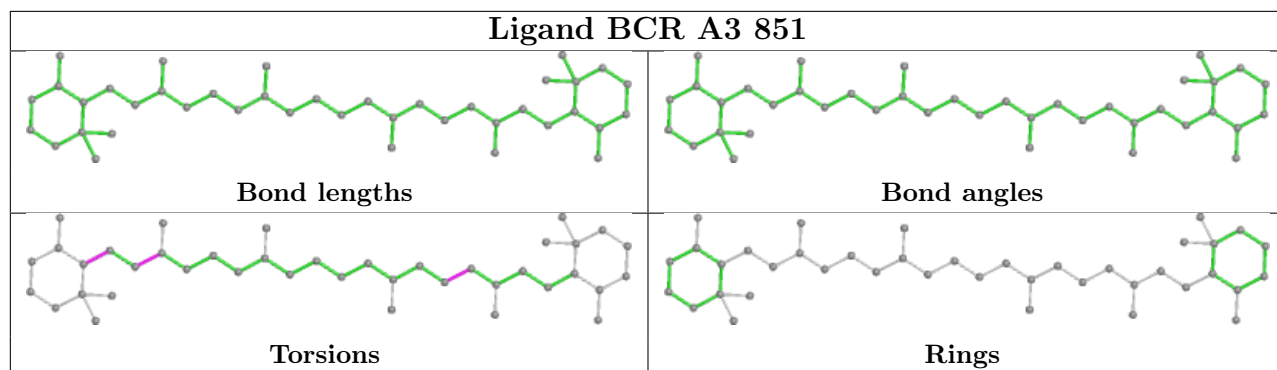


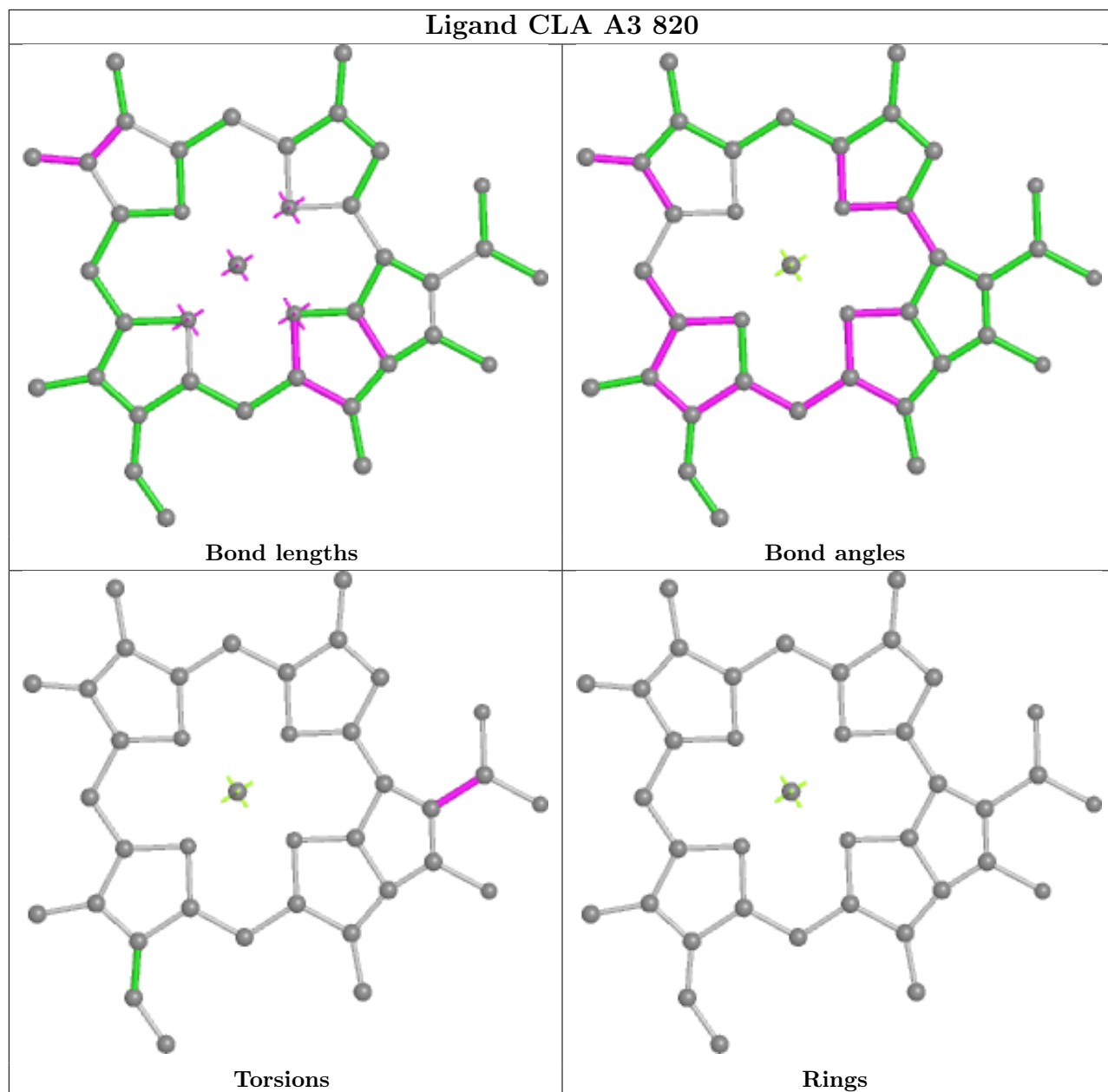


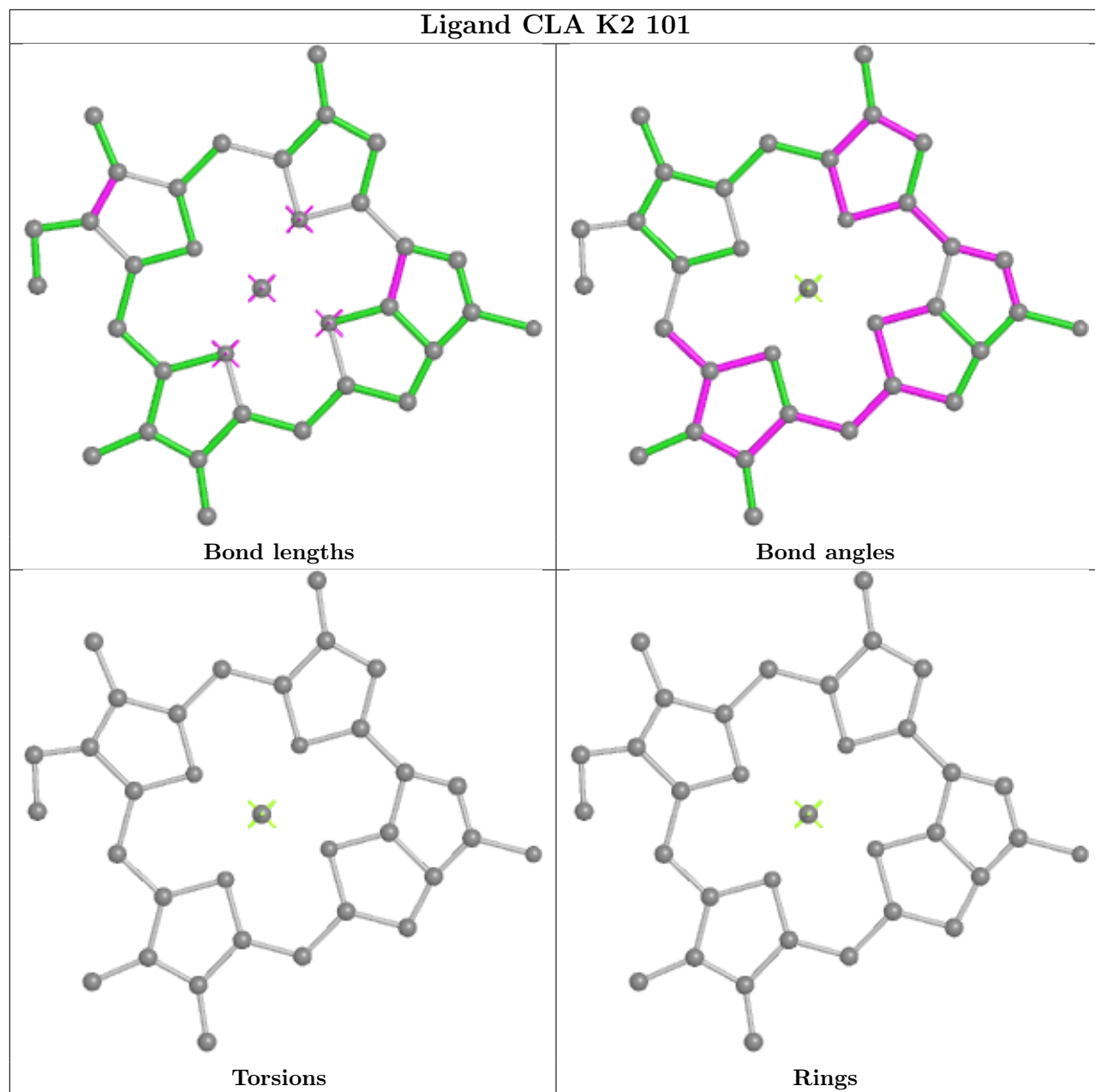


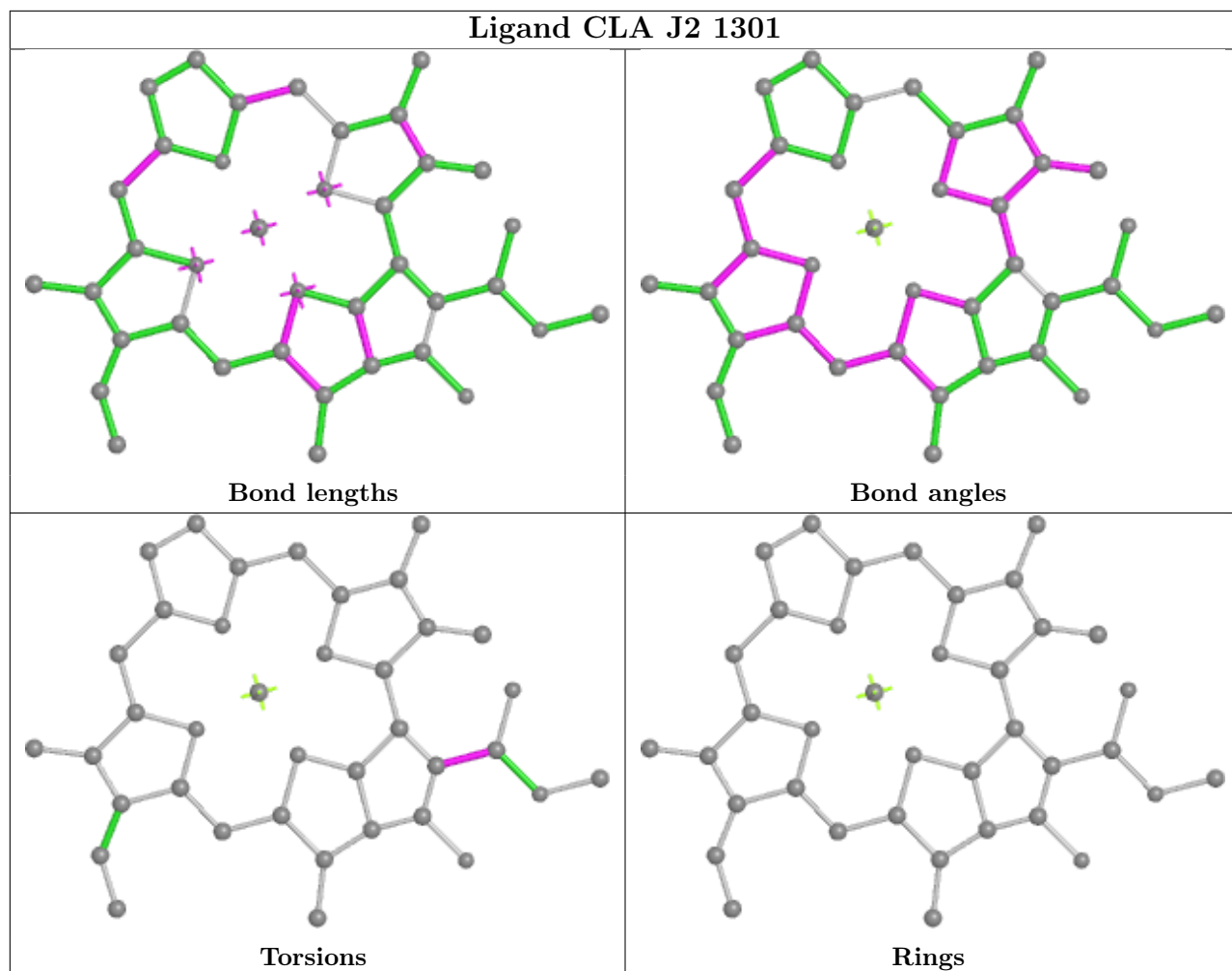


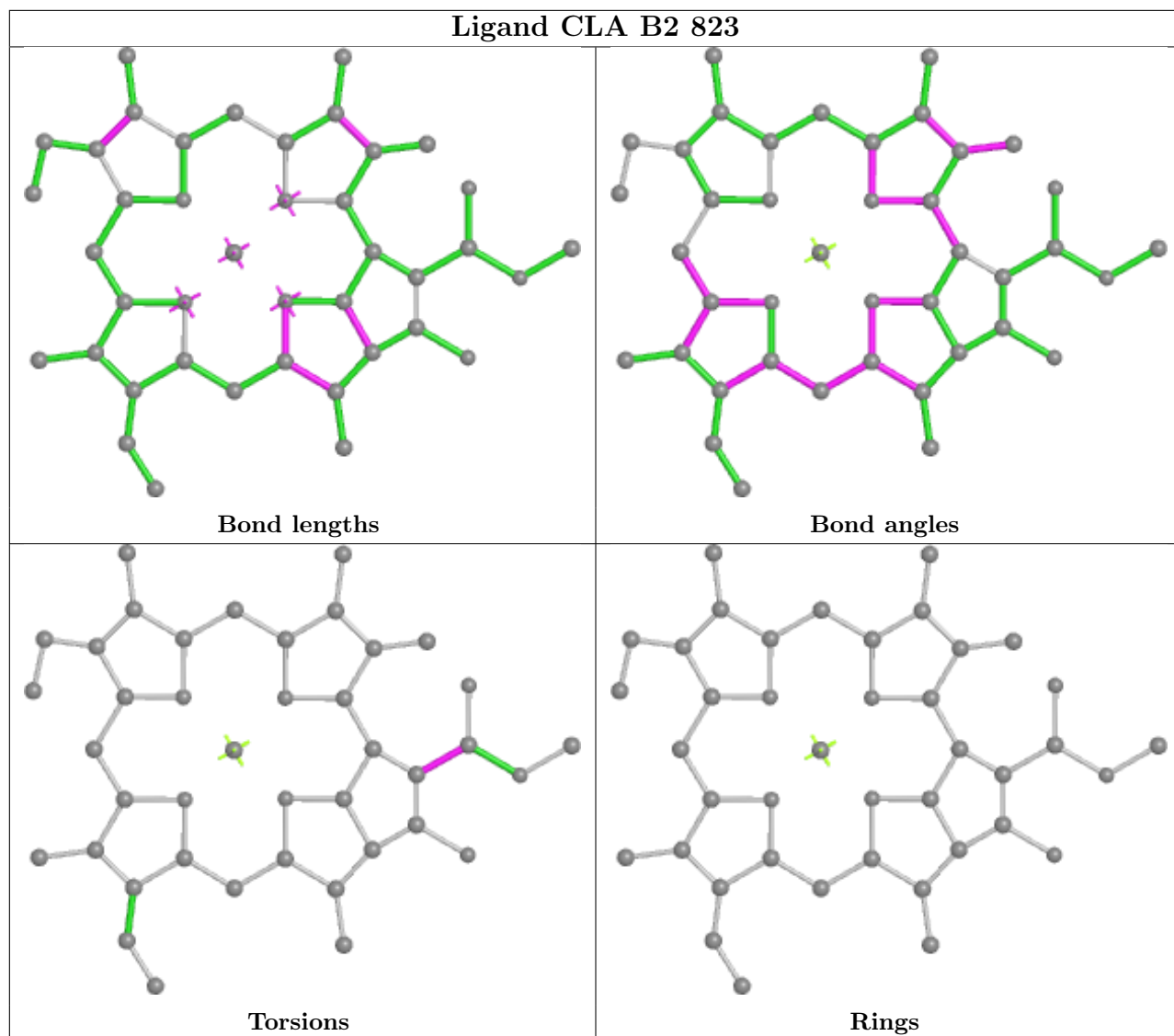




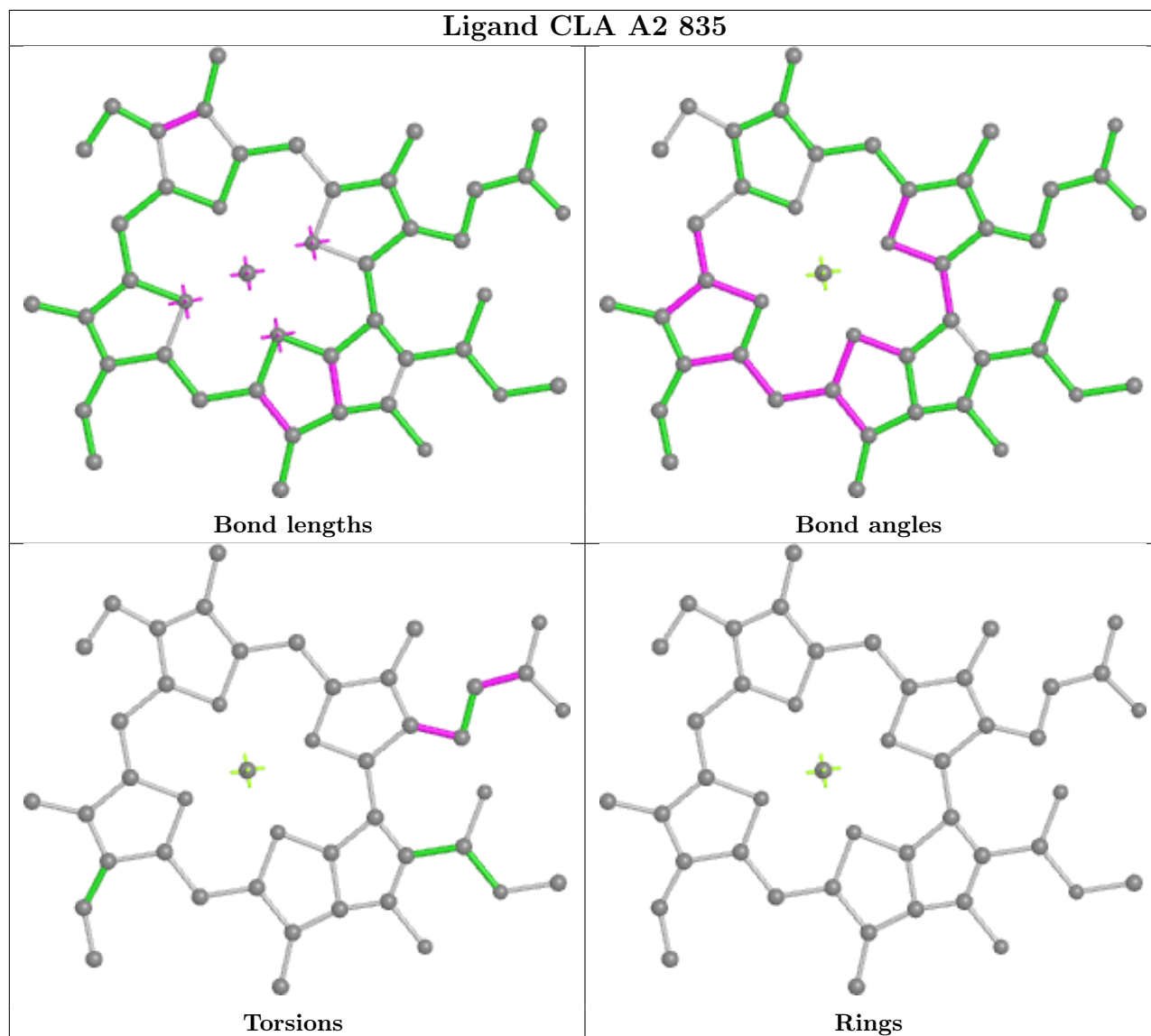


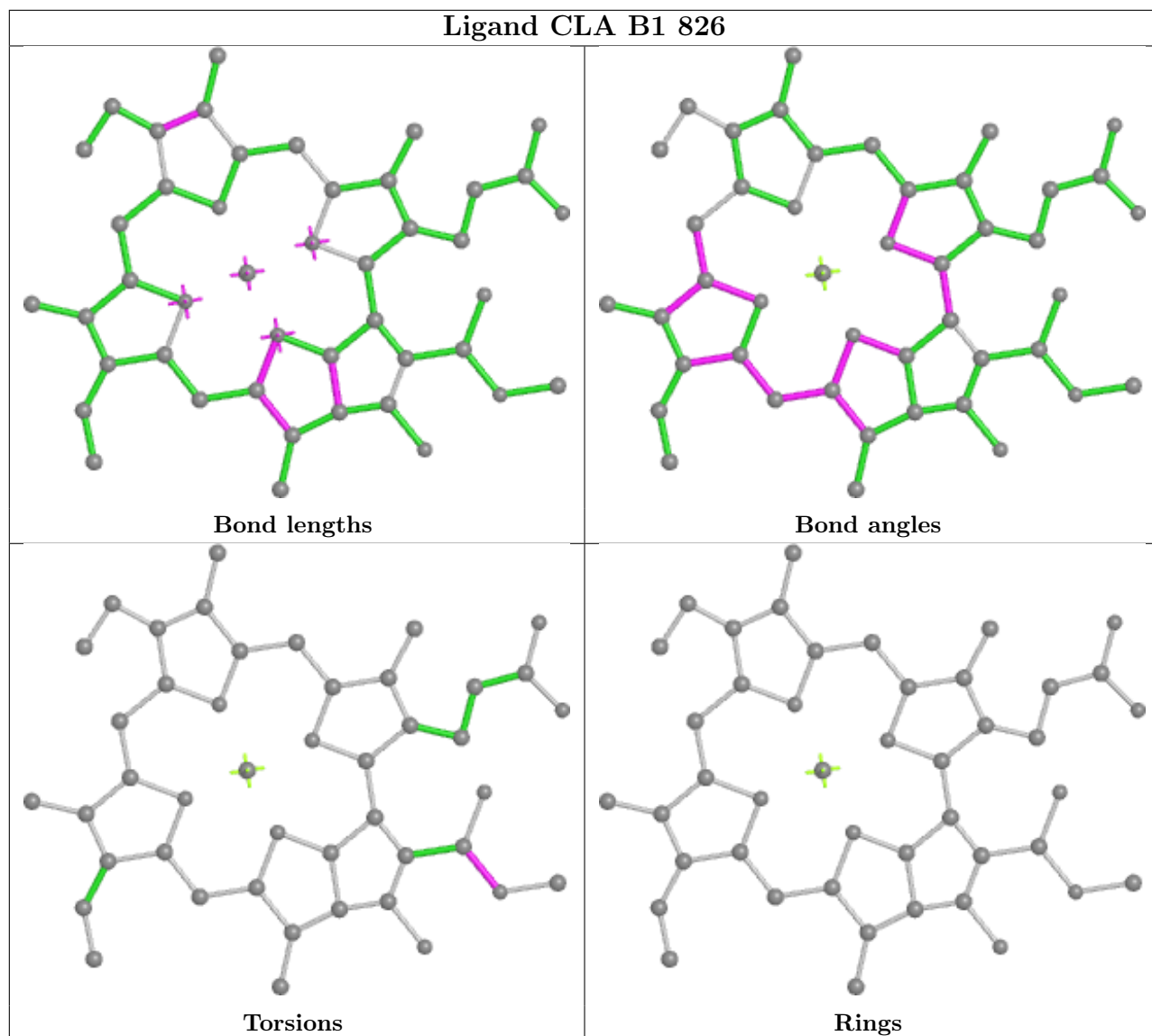


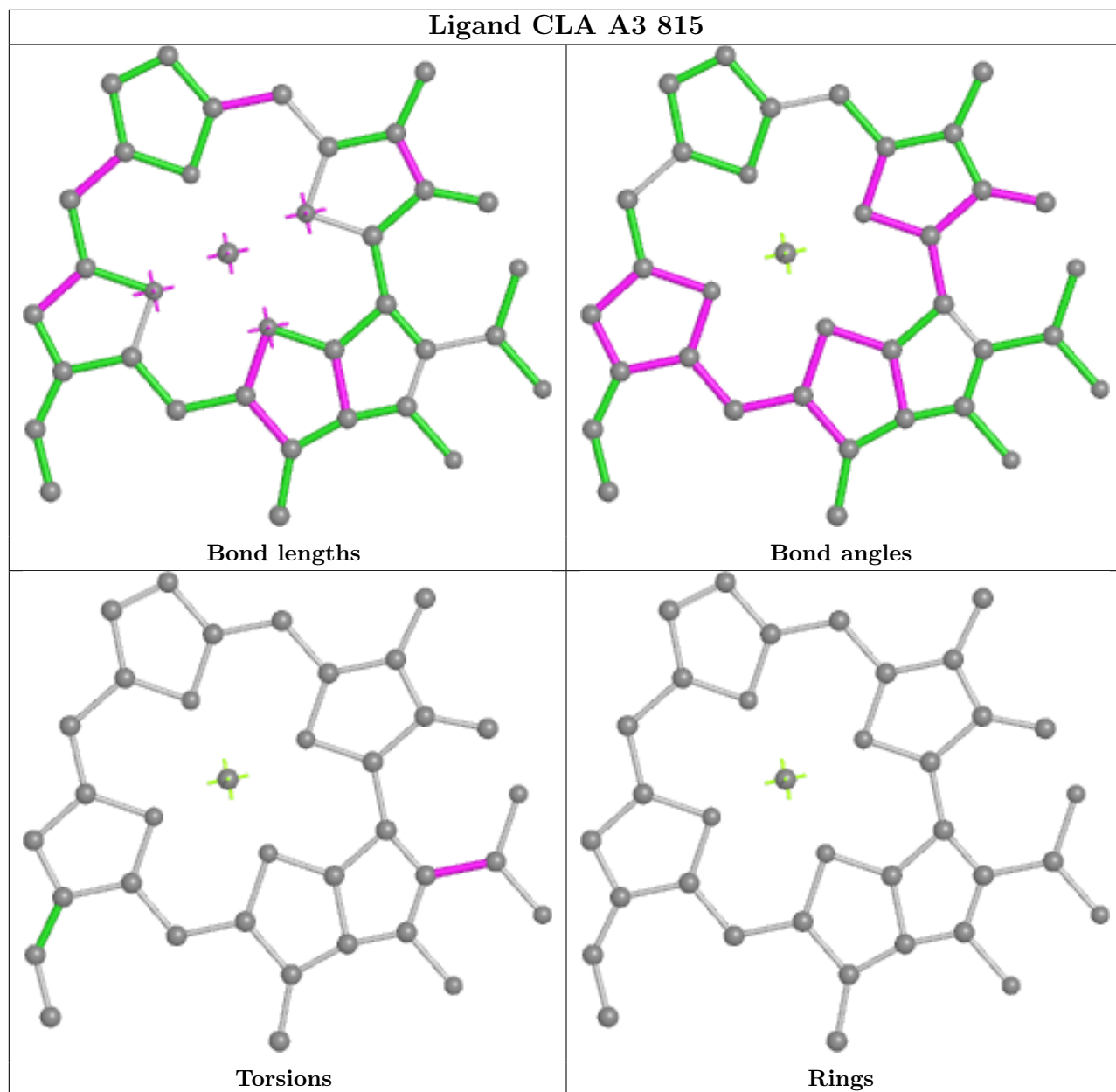


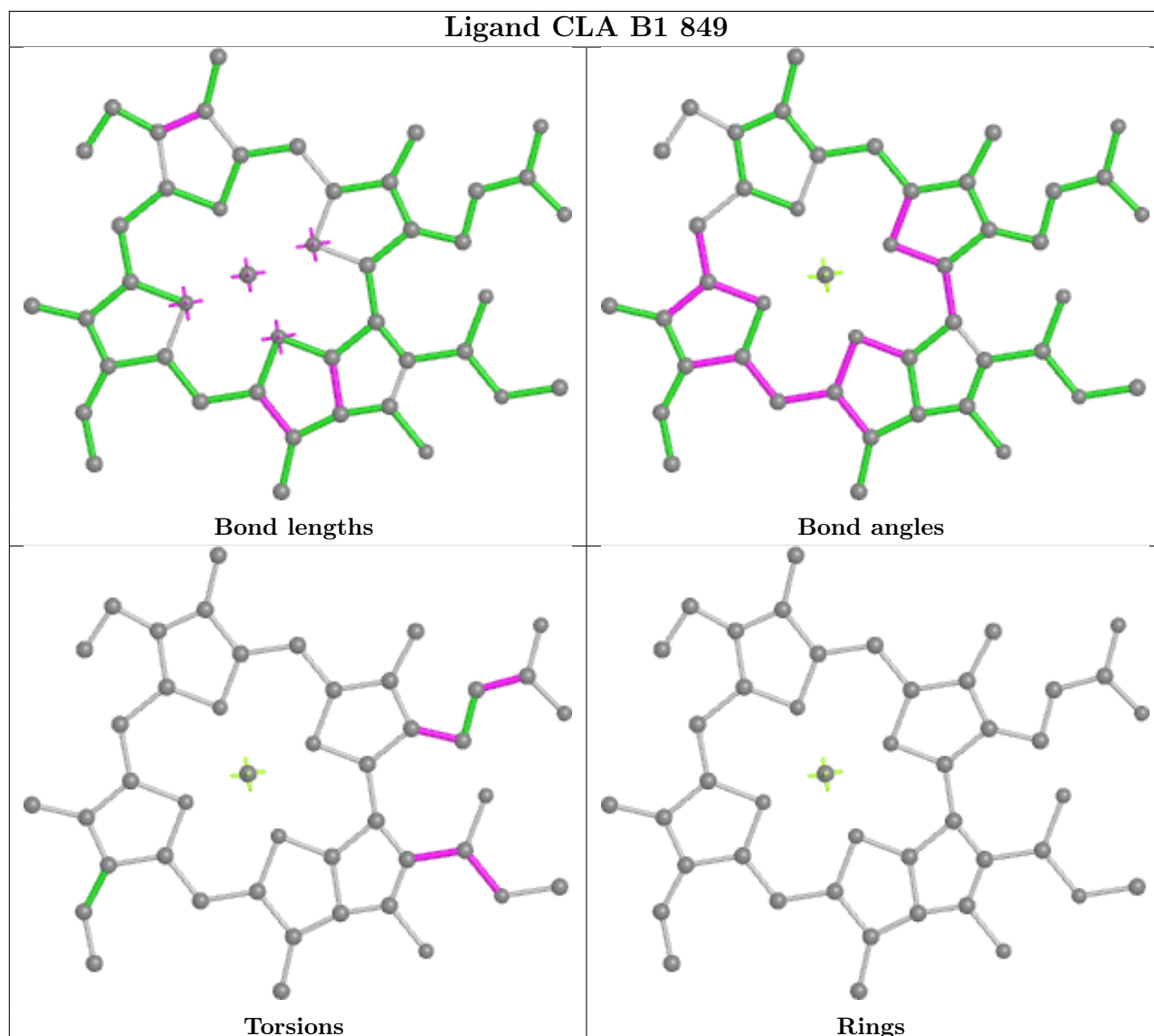
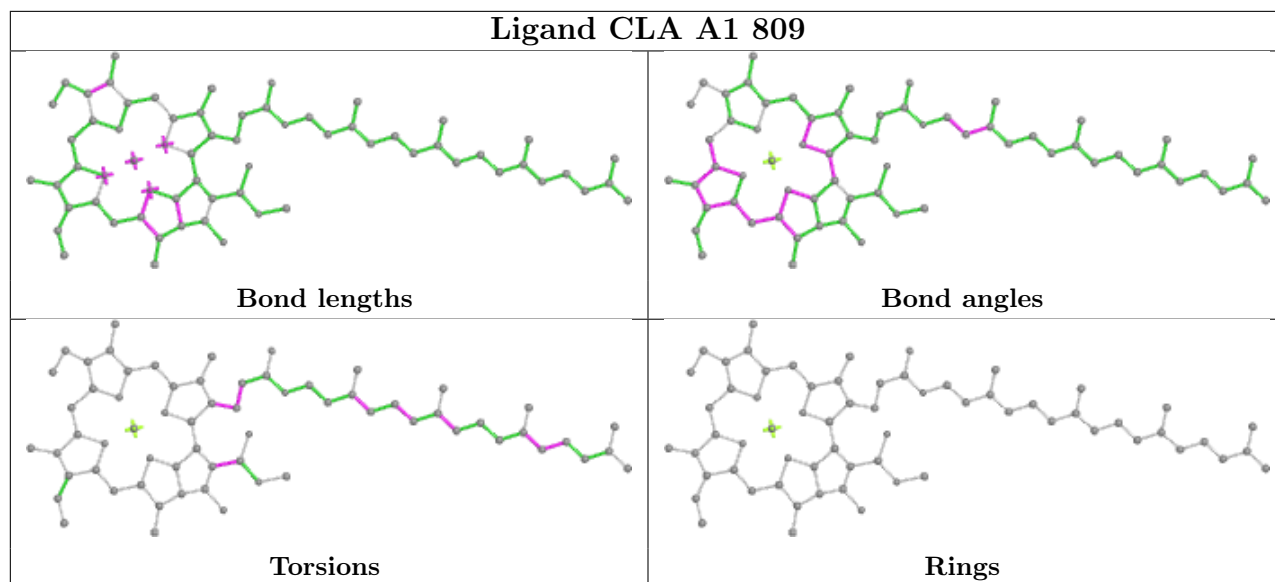


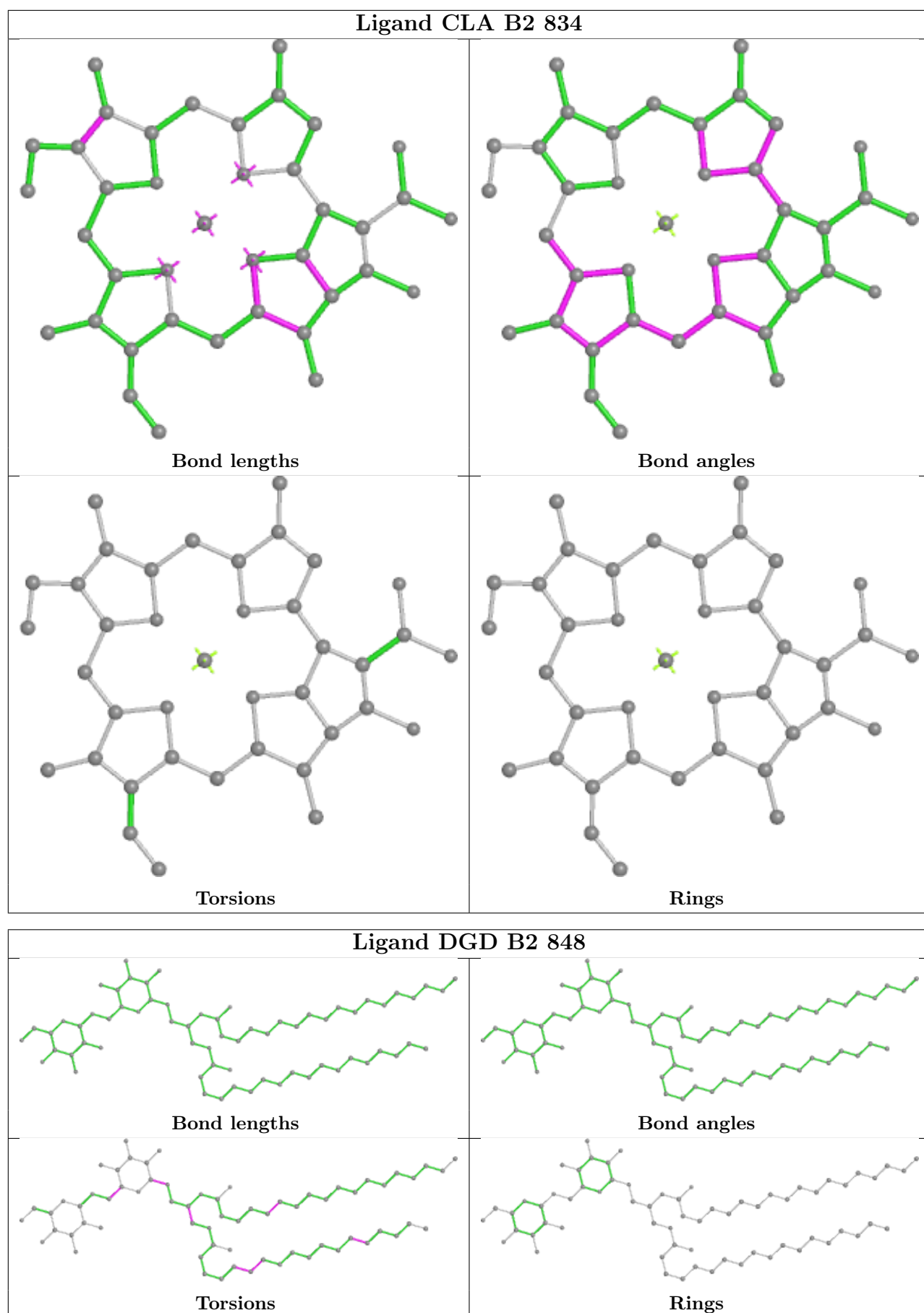


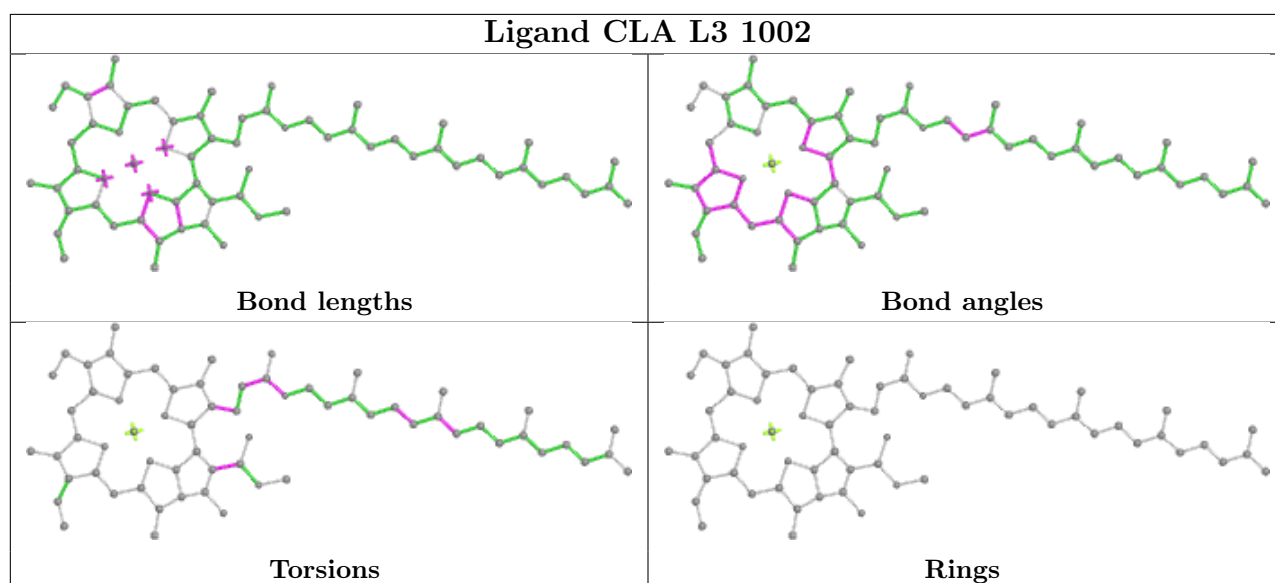
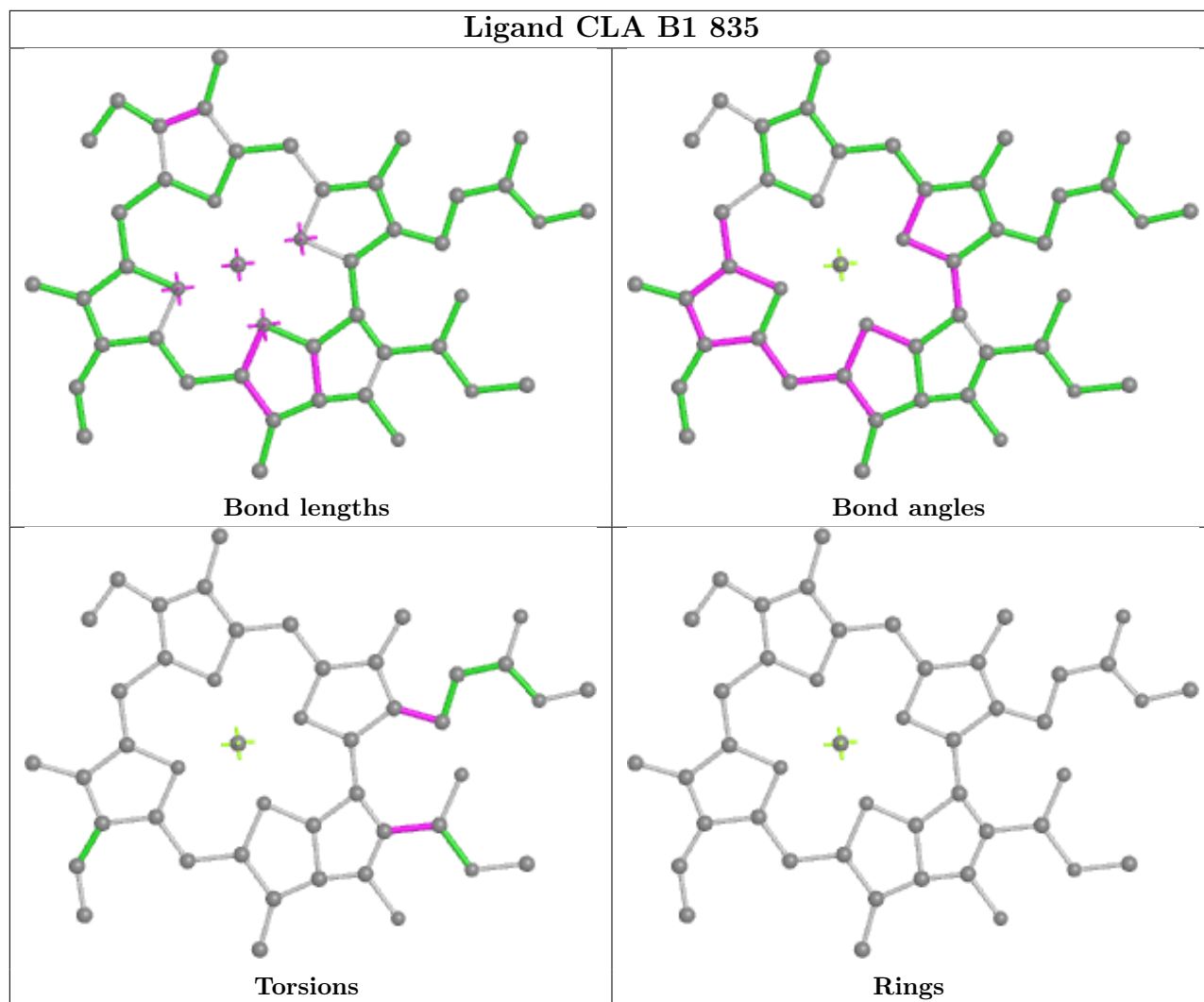


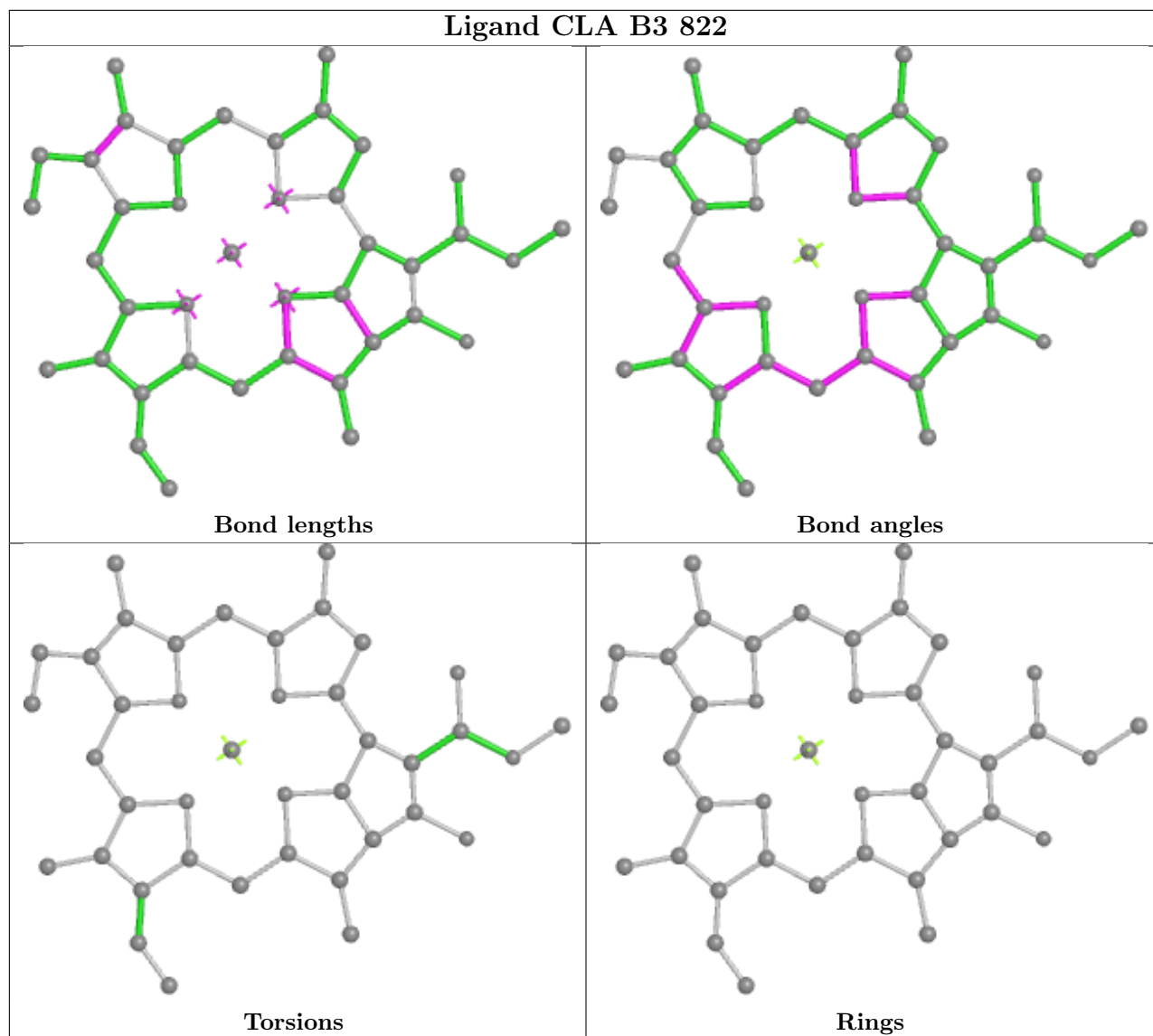


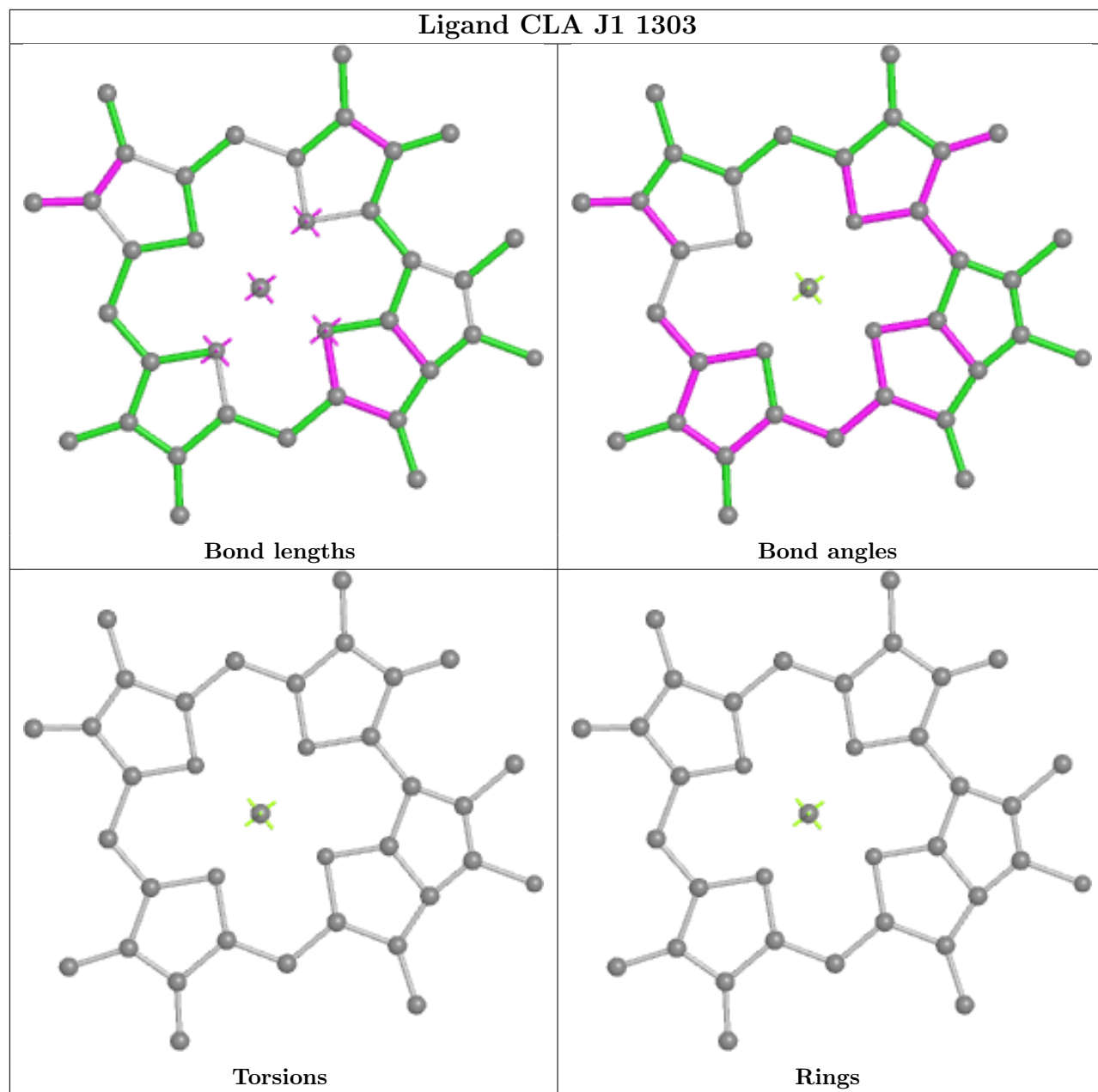






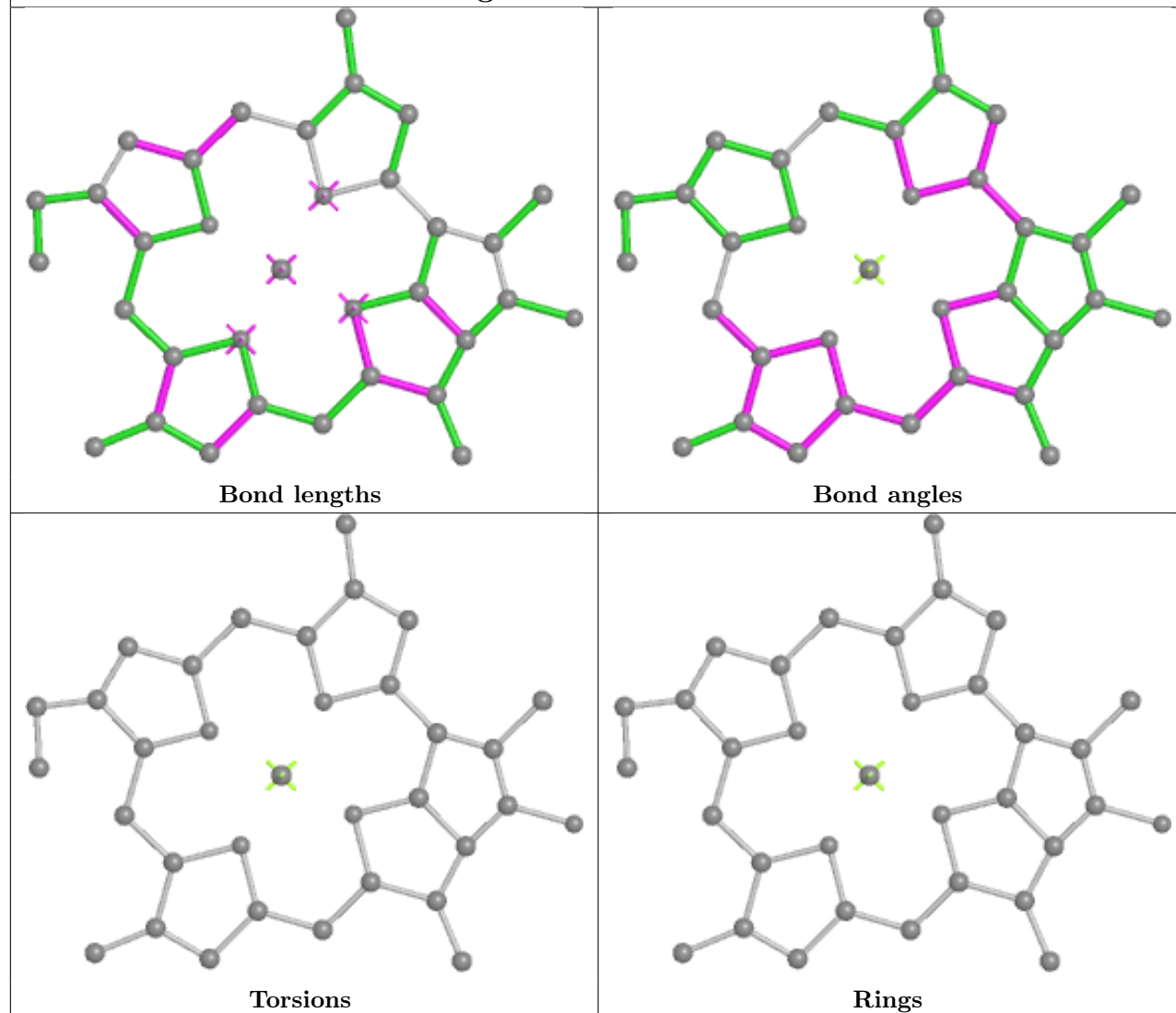




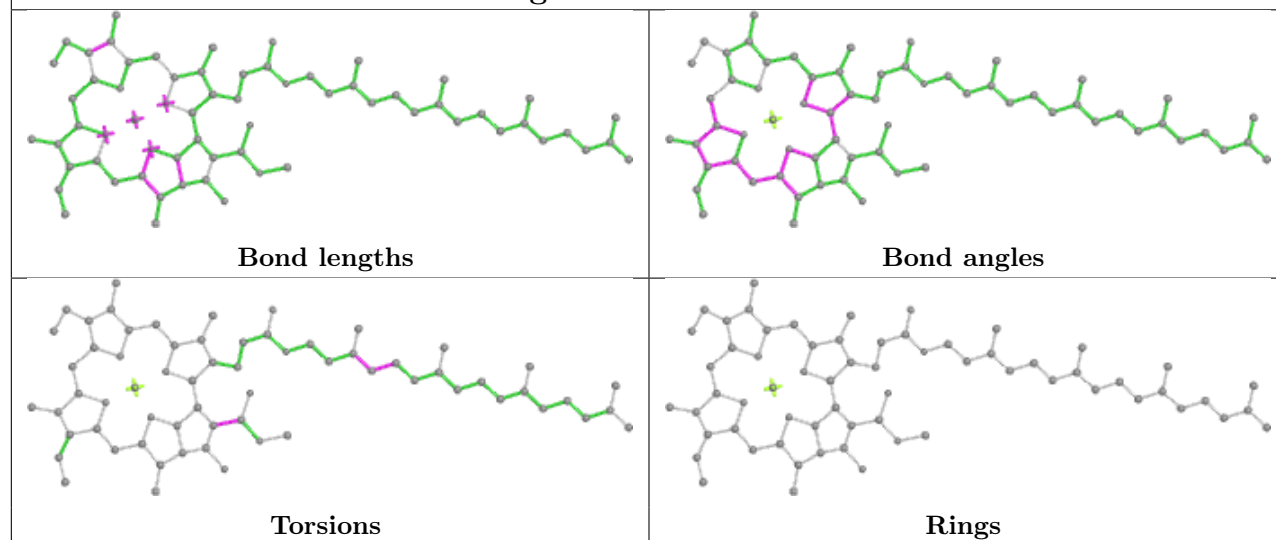


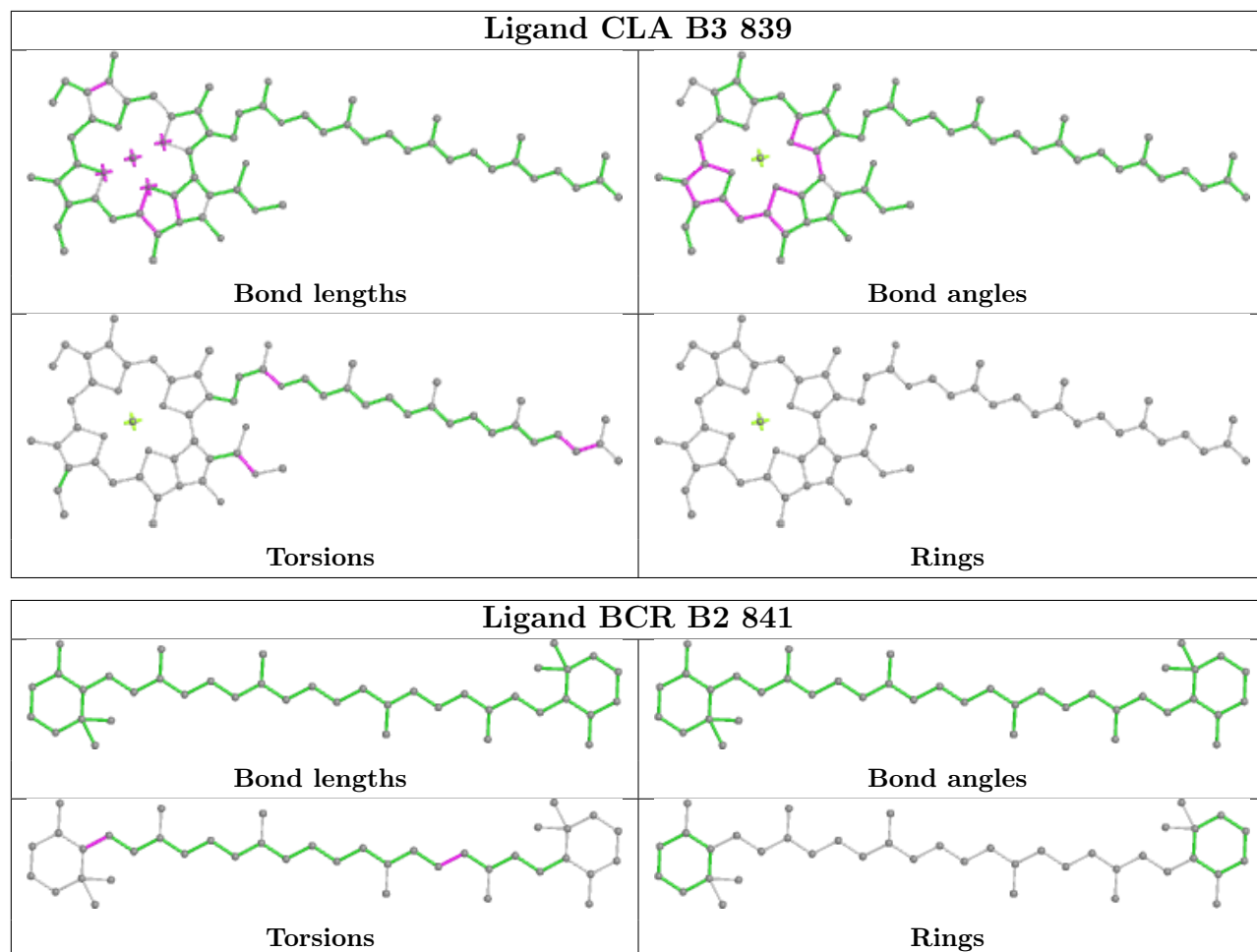


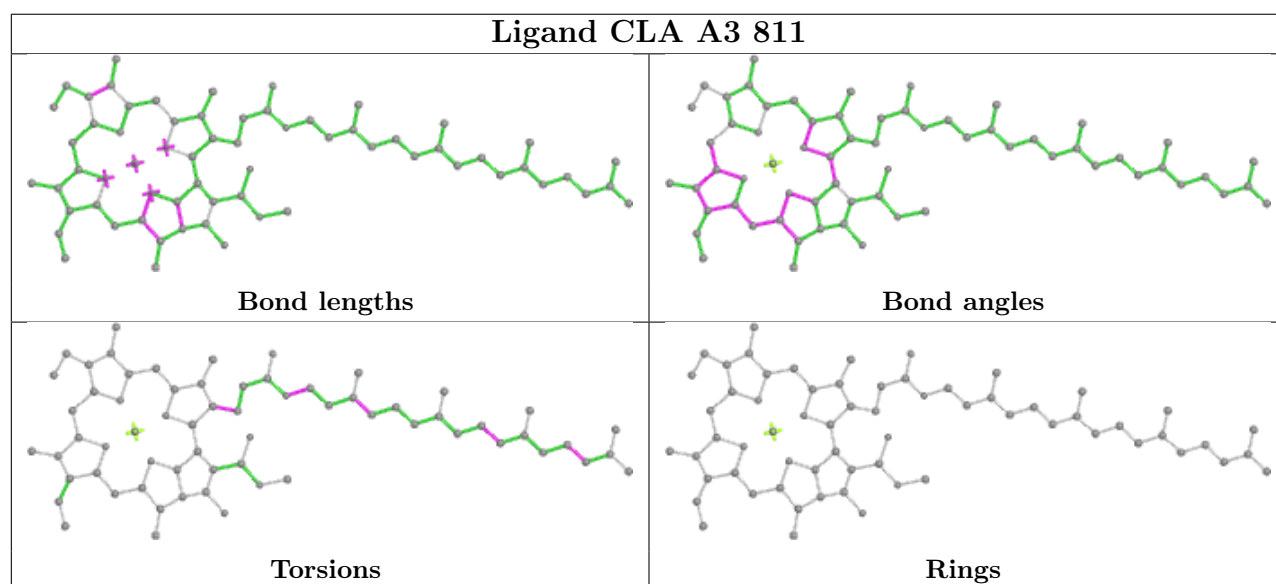
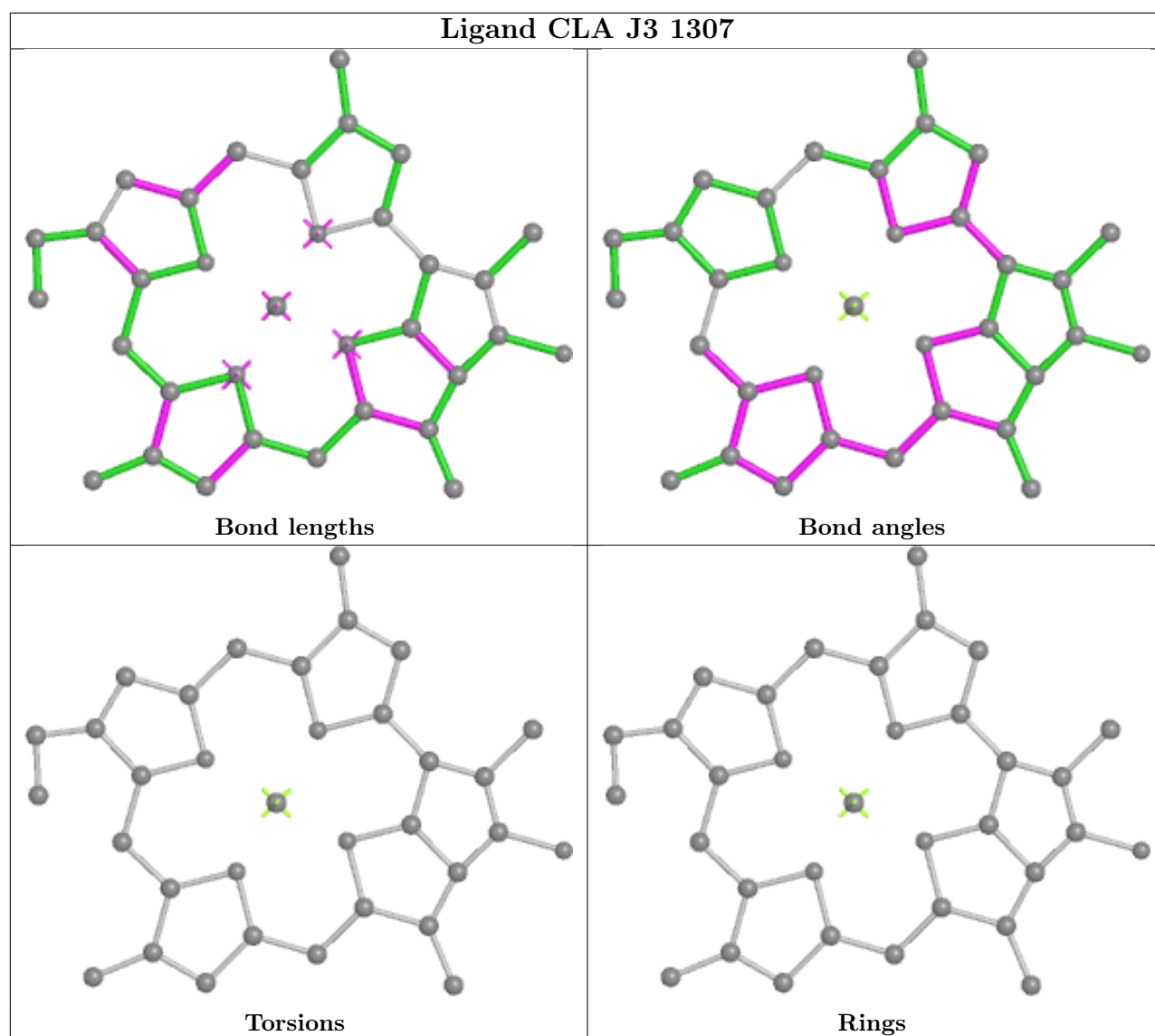
## Ligand CLA J2 1307

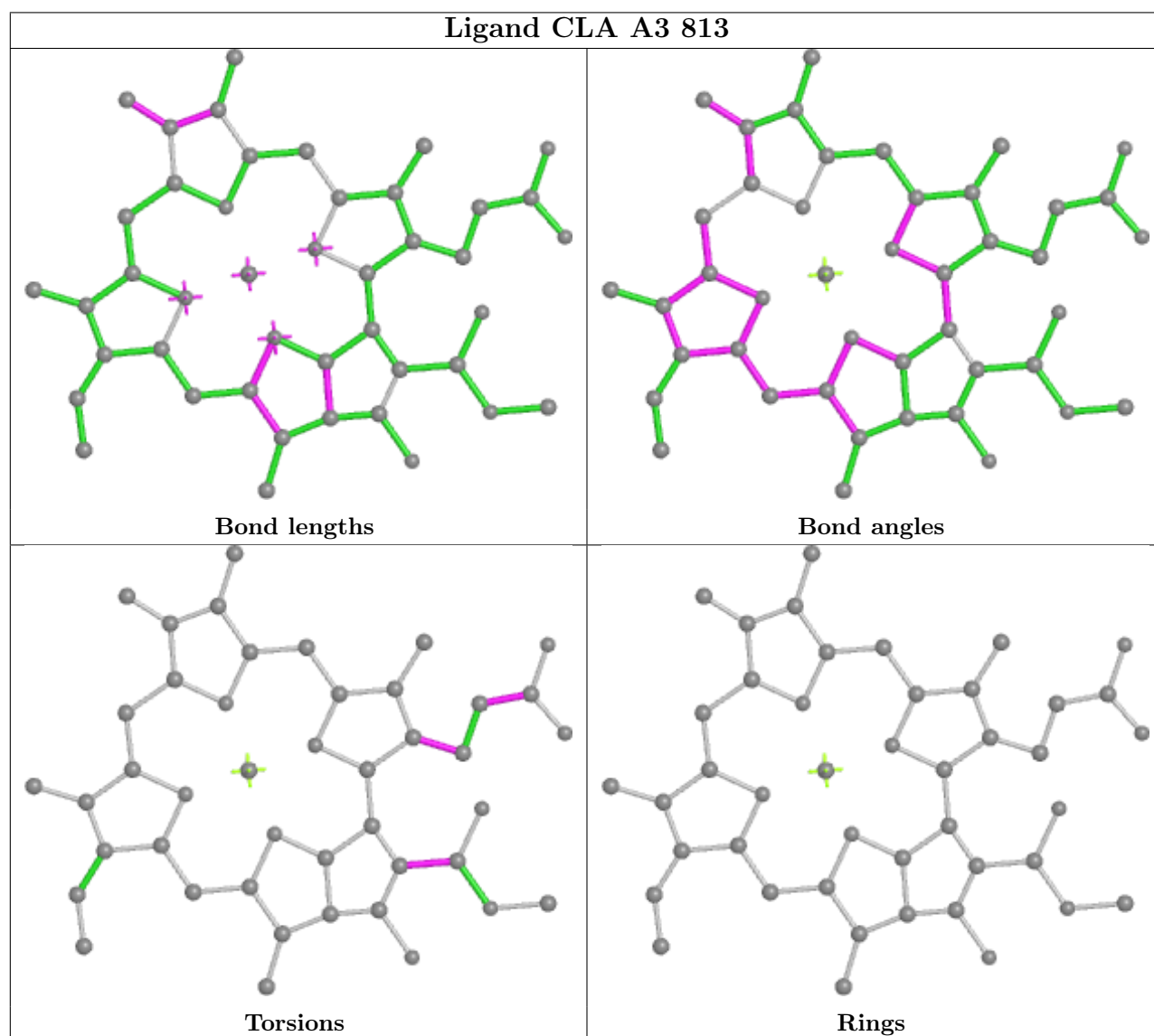
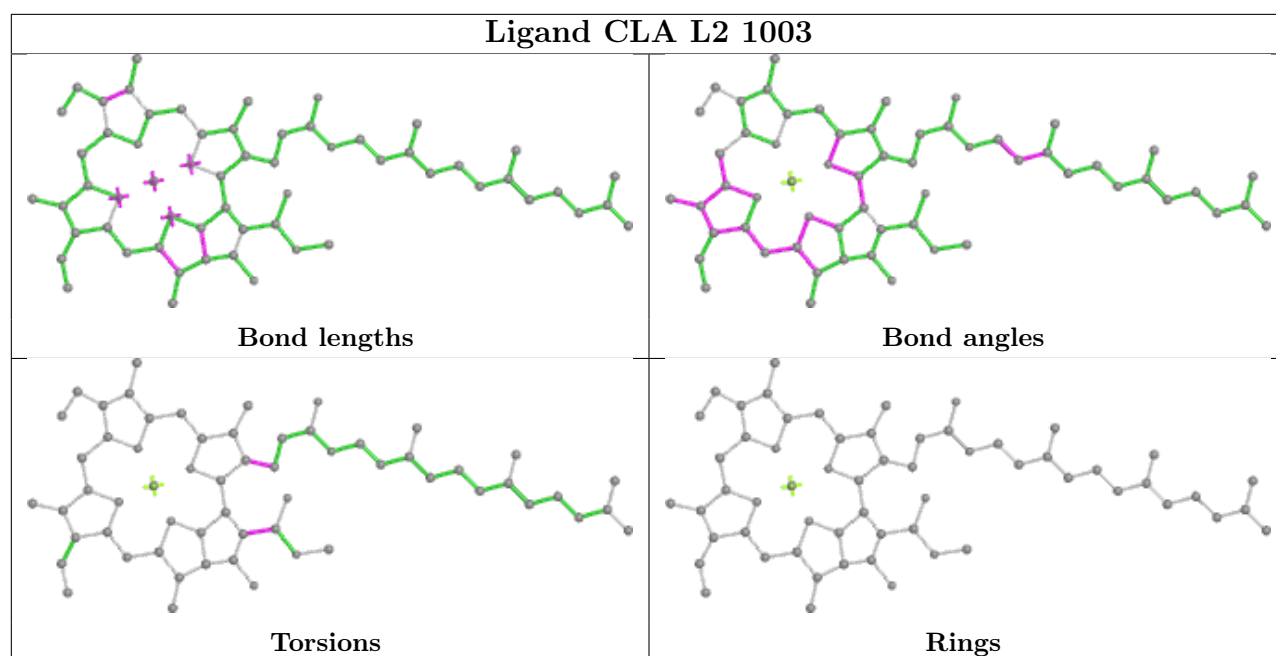


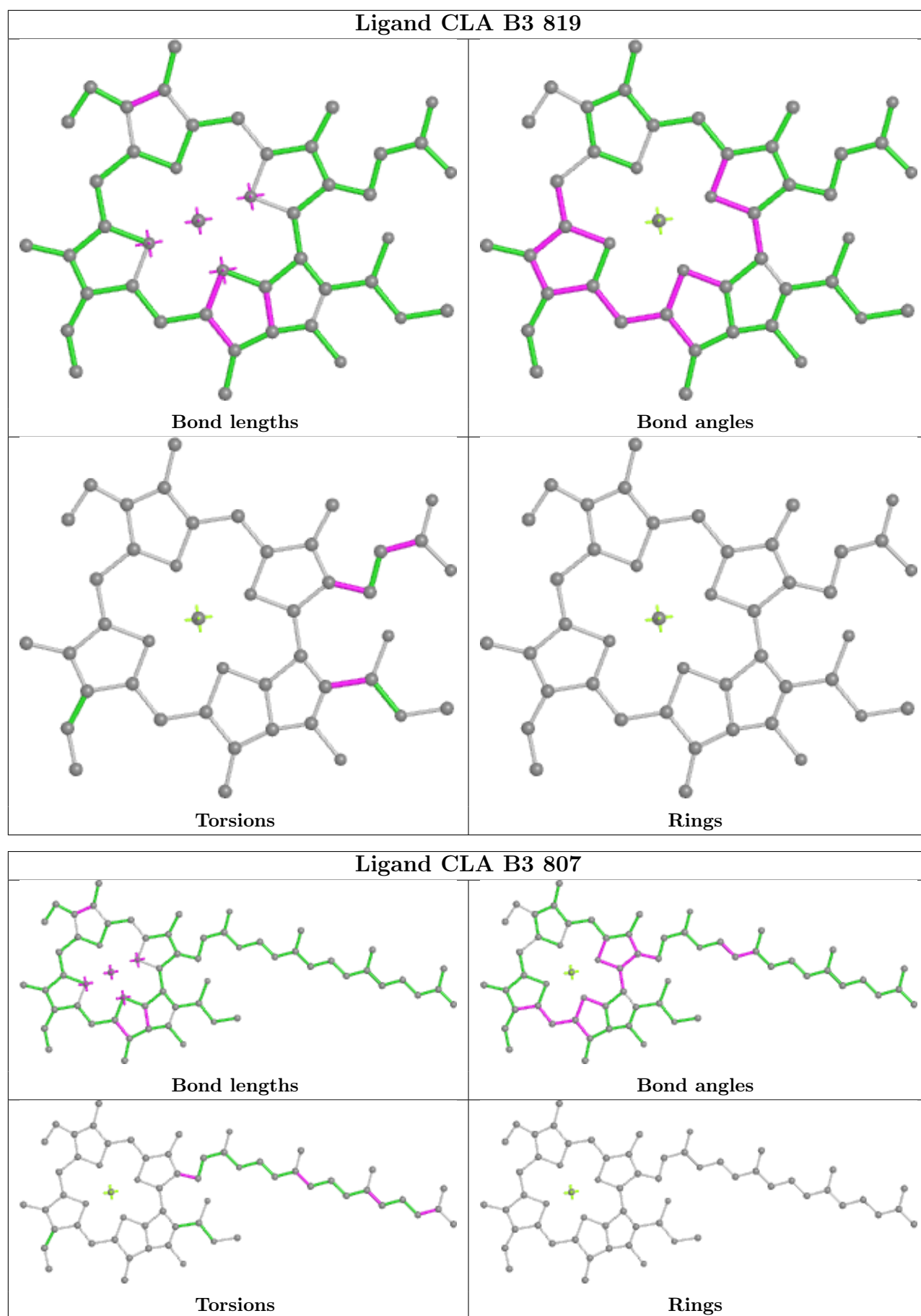
## Ligand CLA I1 101

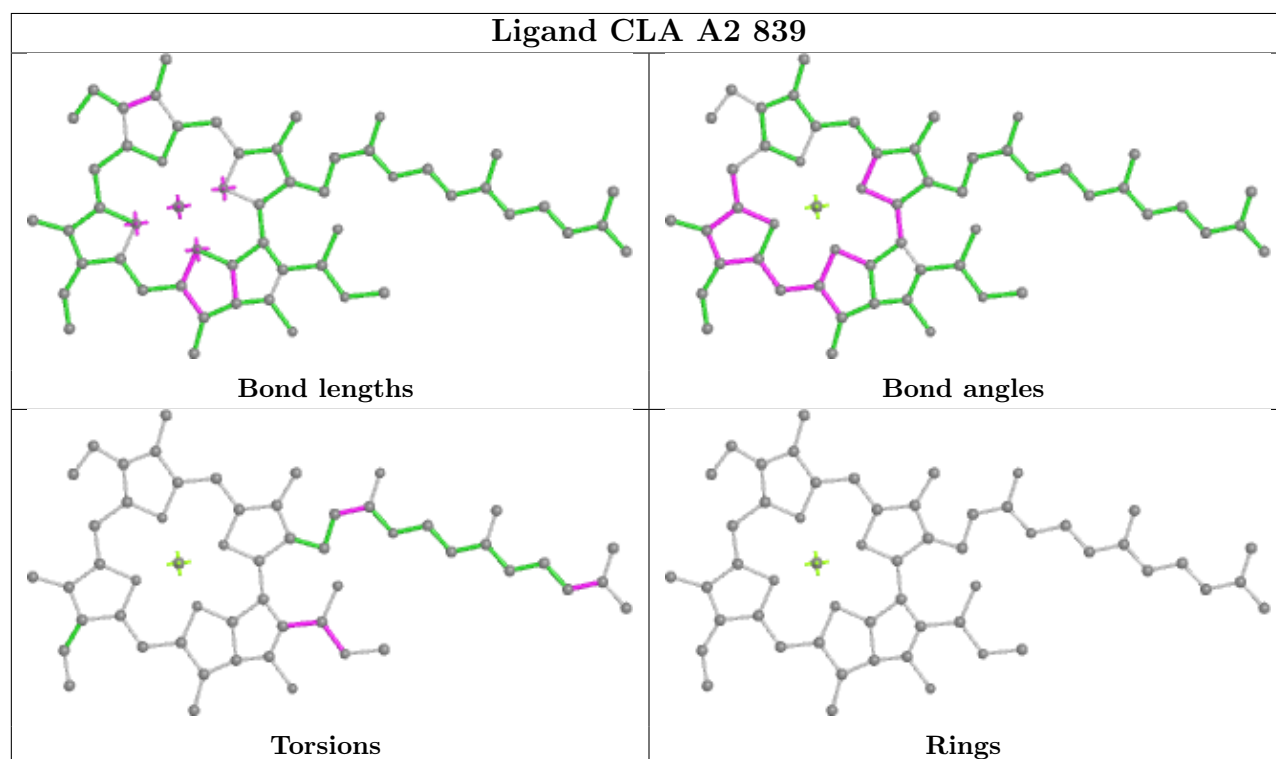
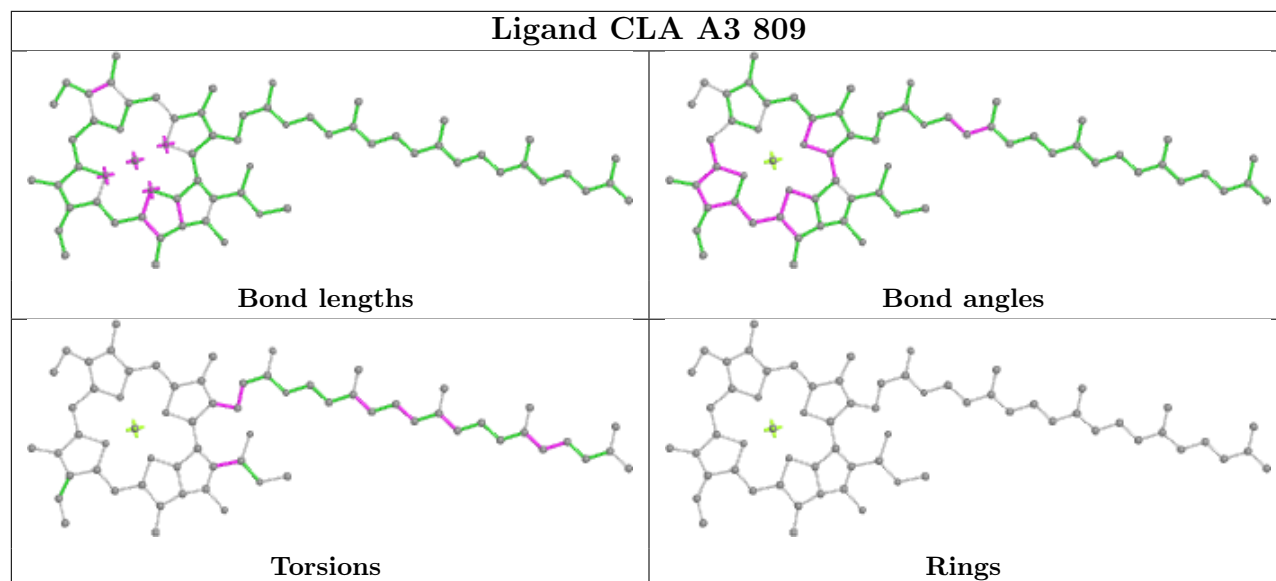
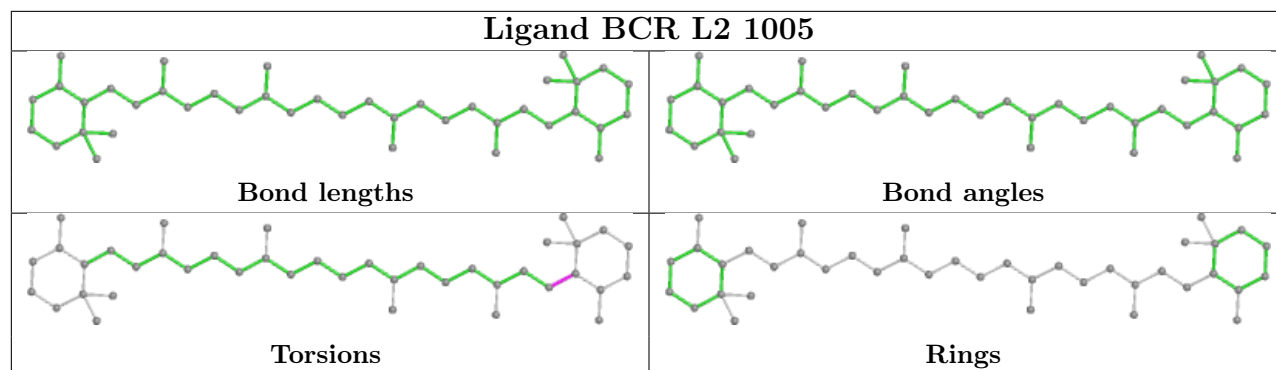


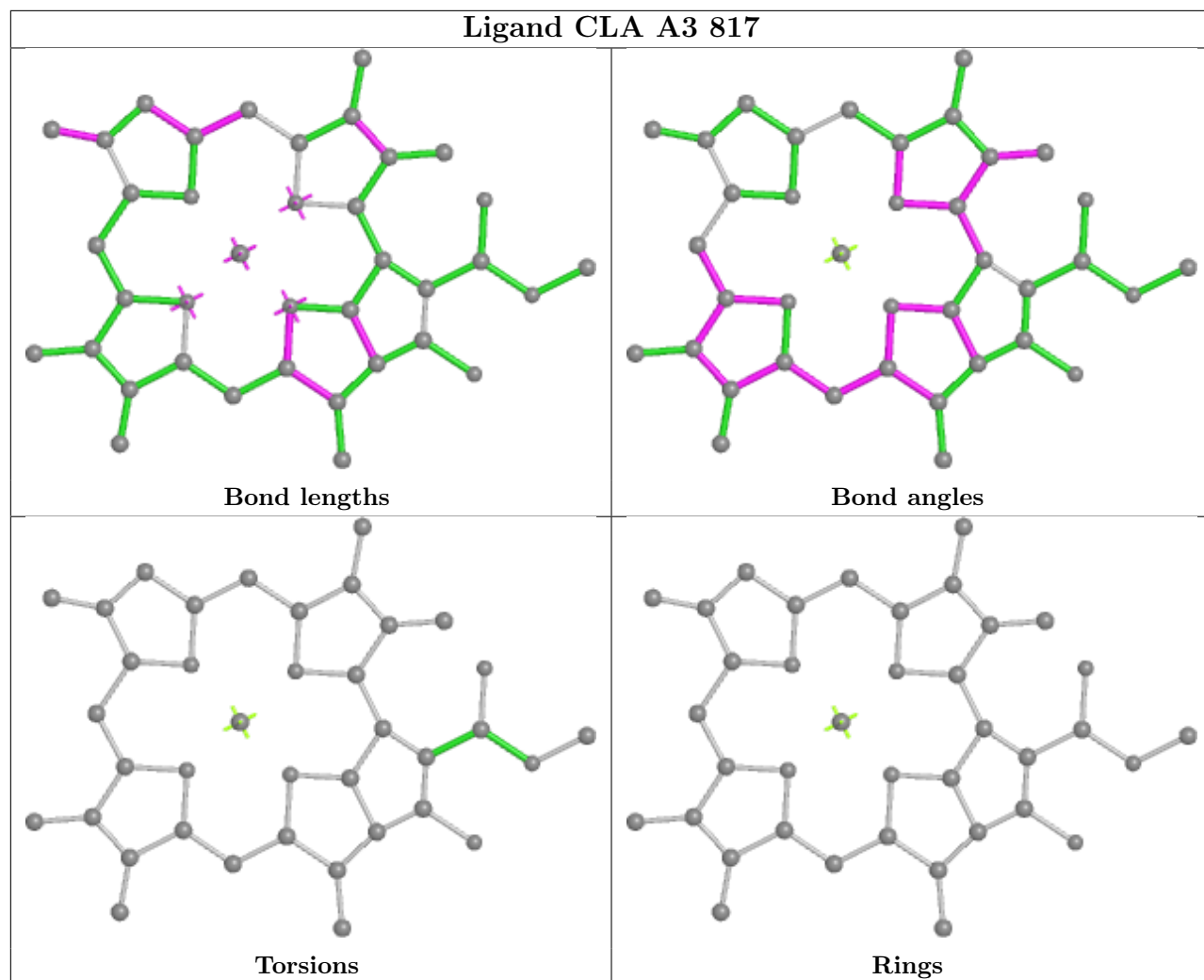


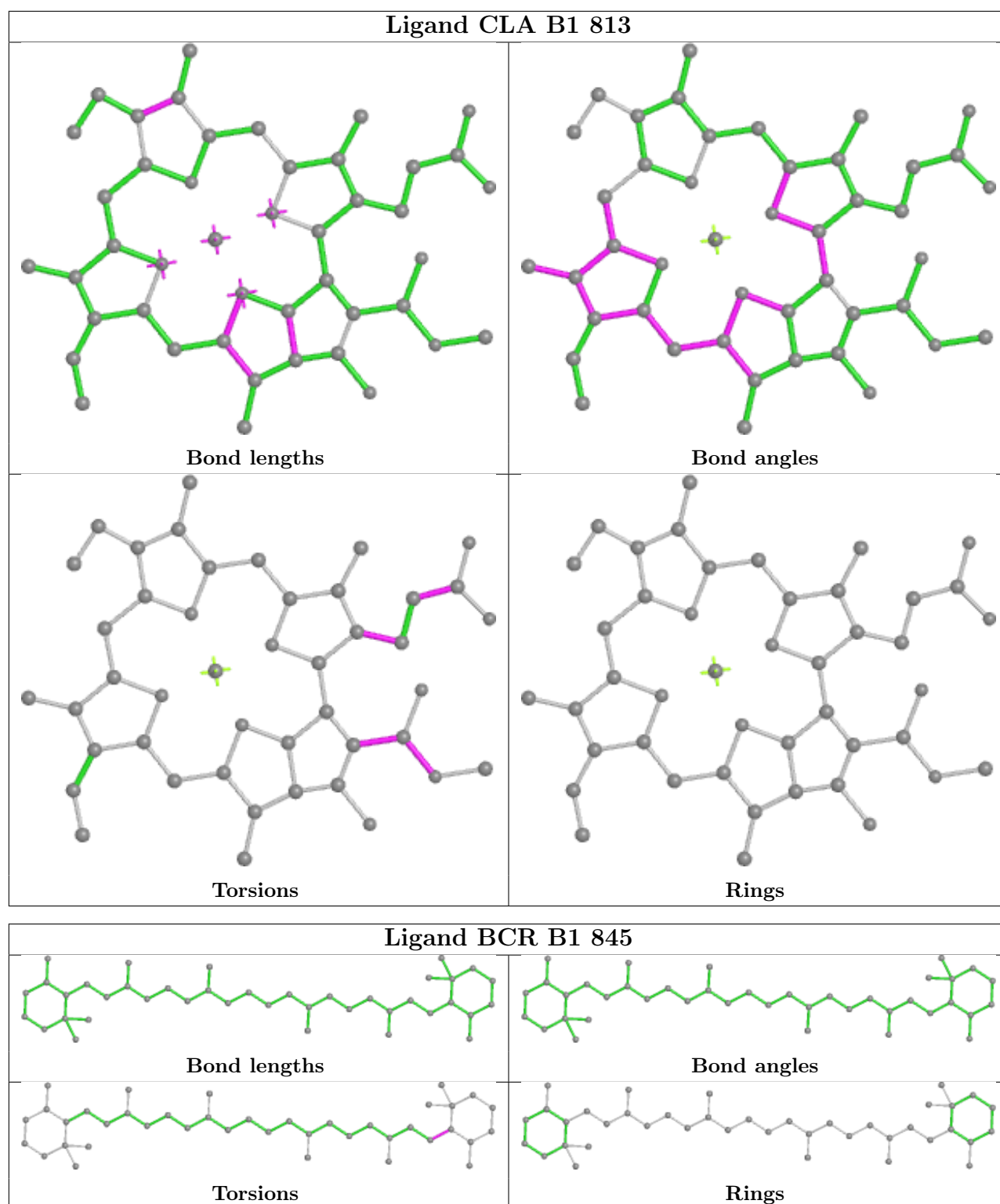




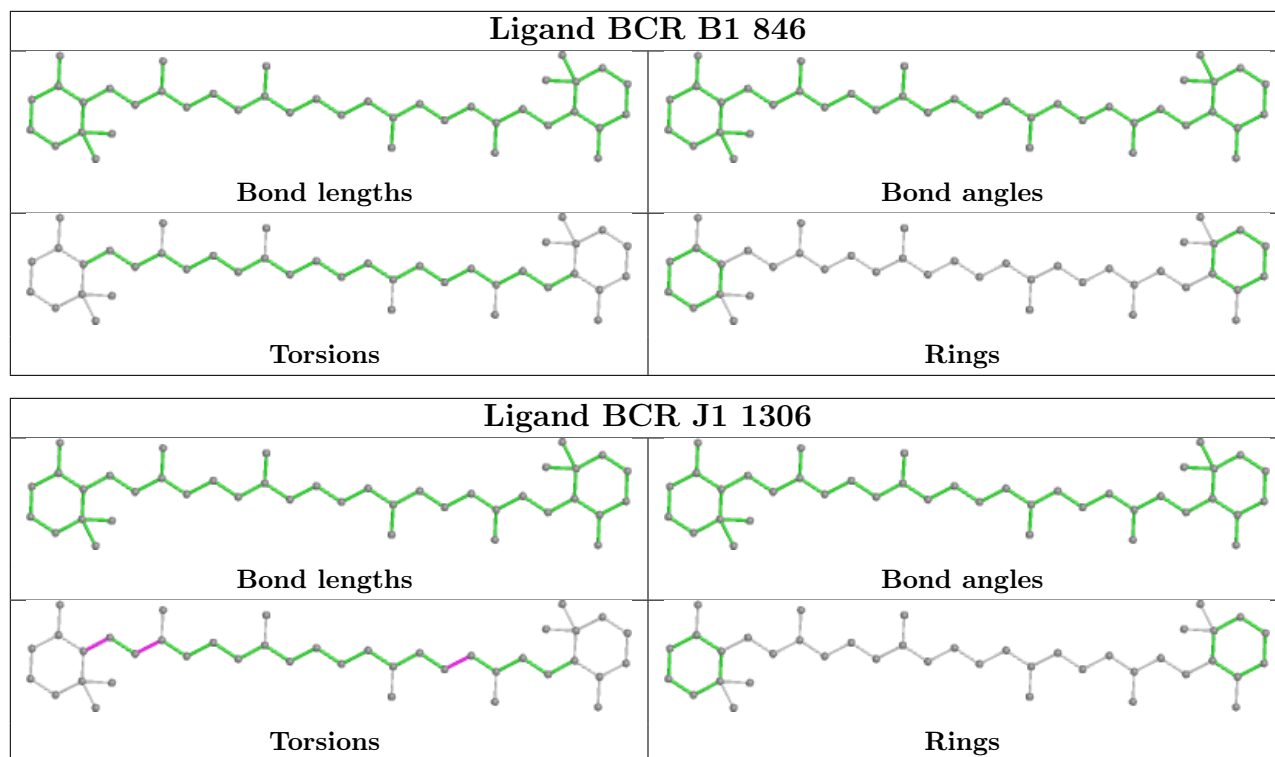


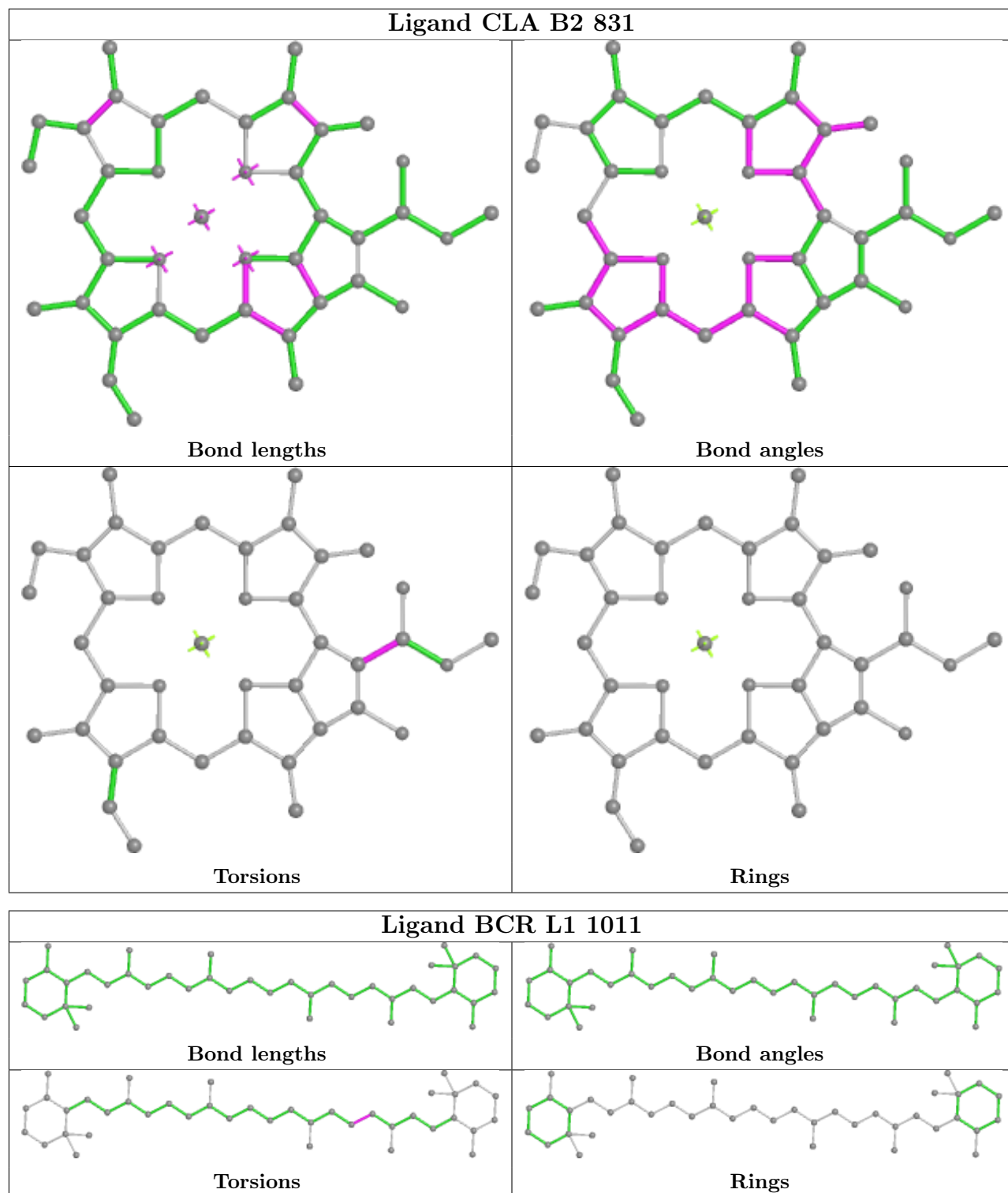


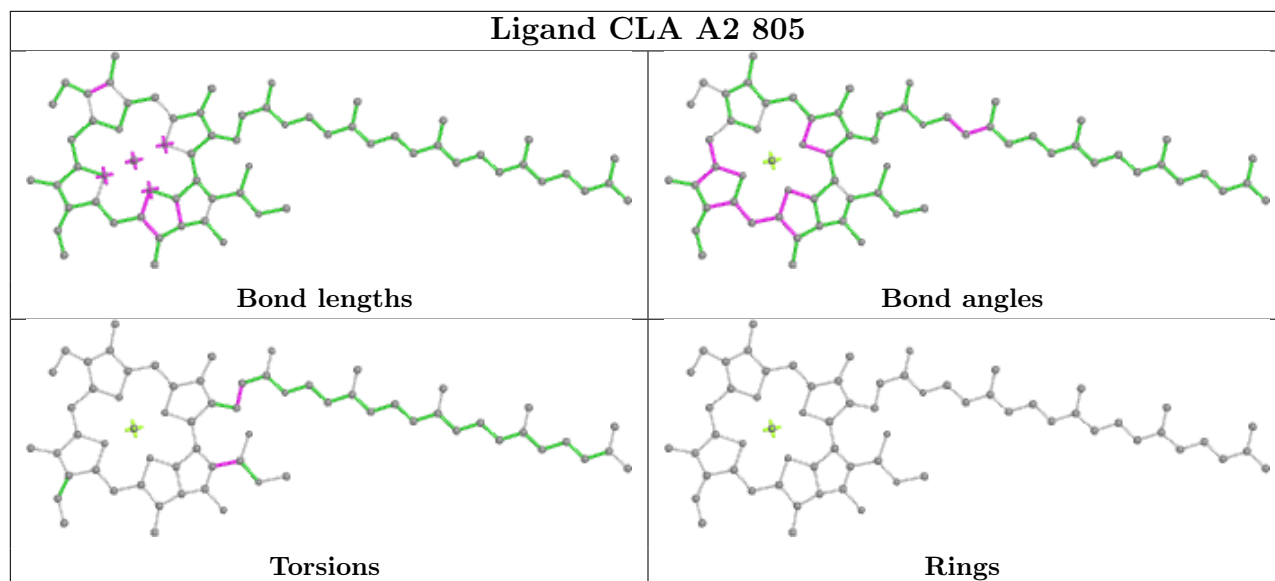
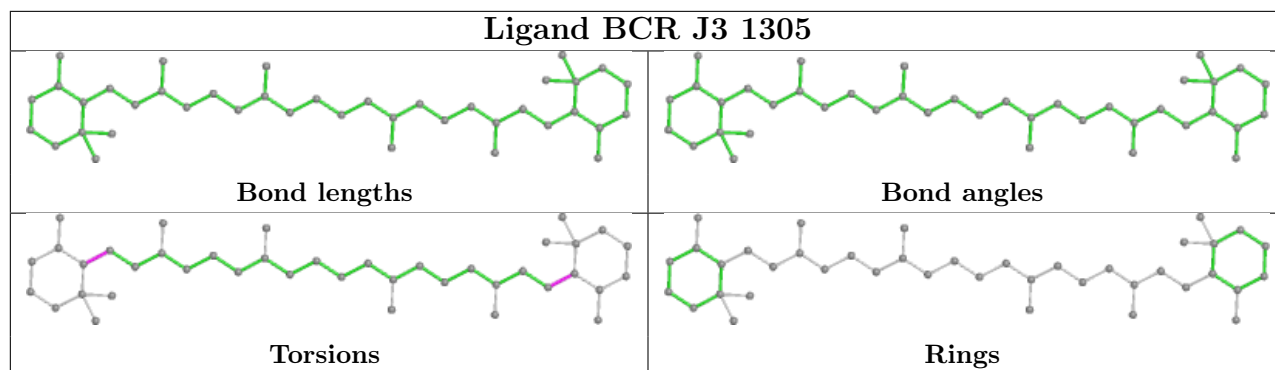


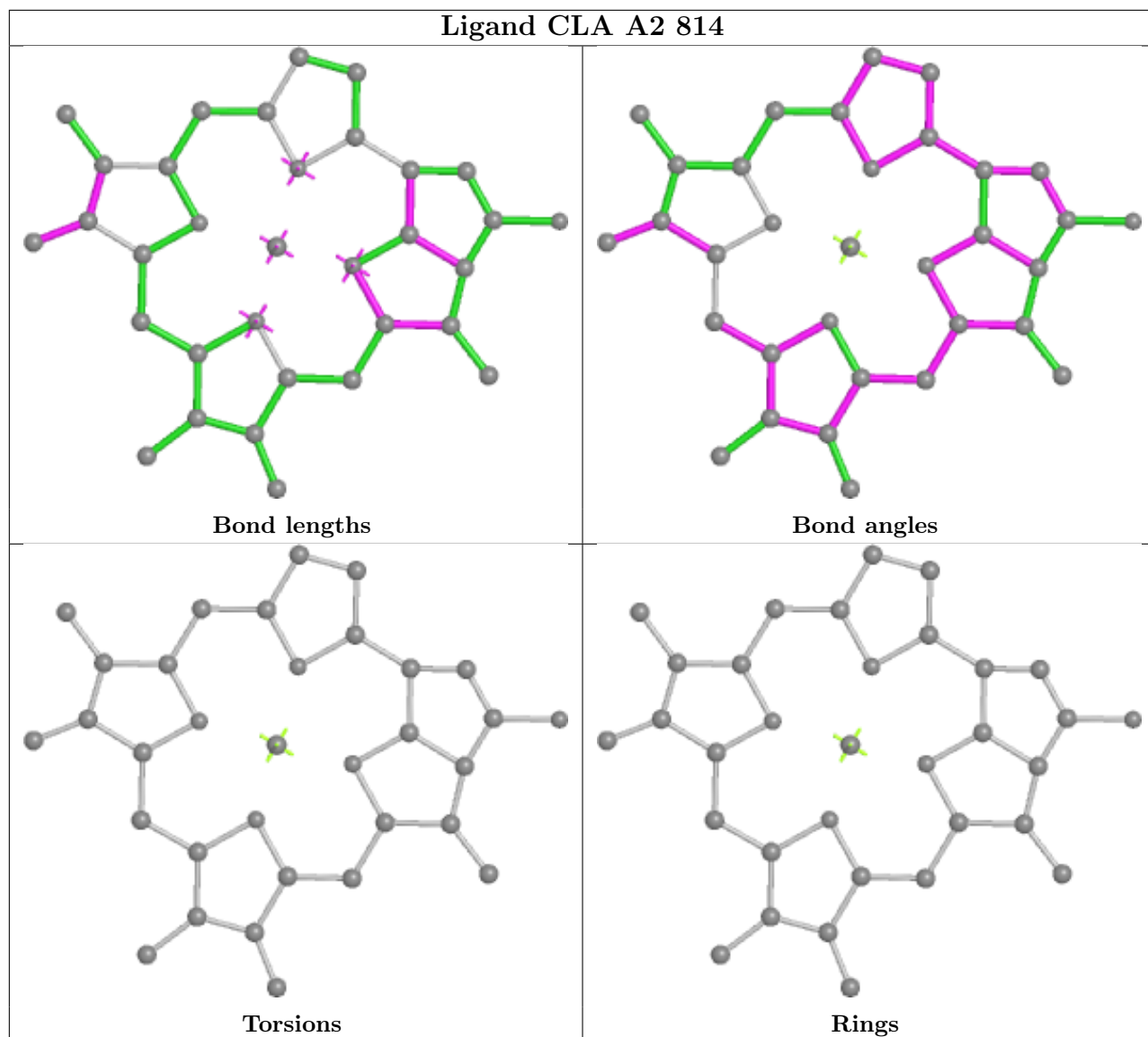


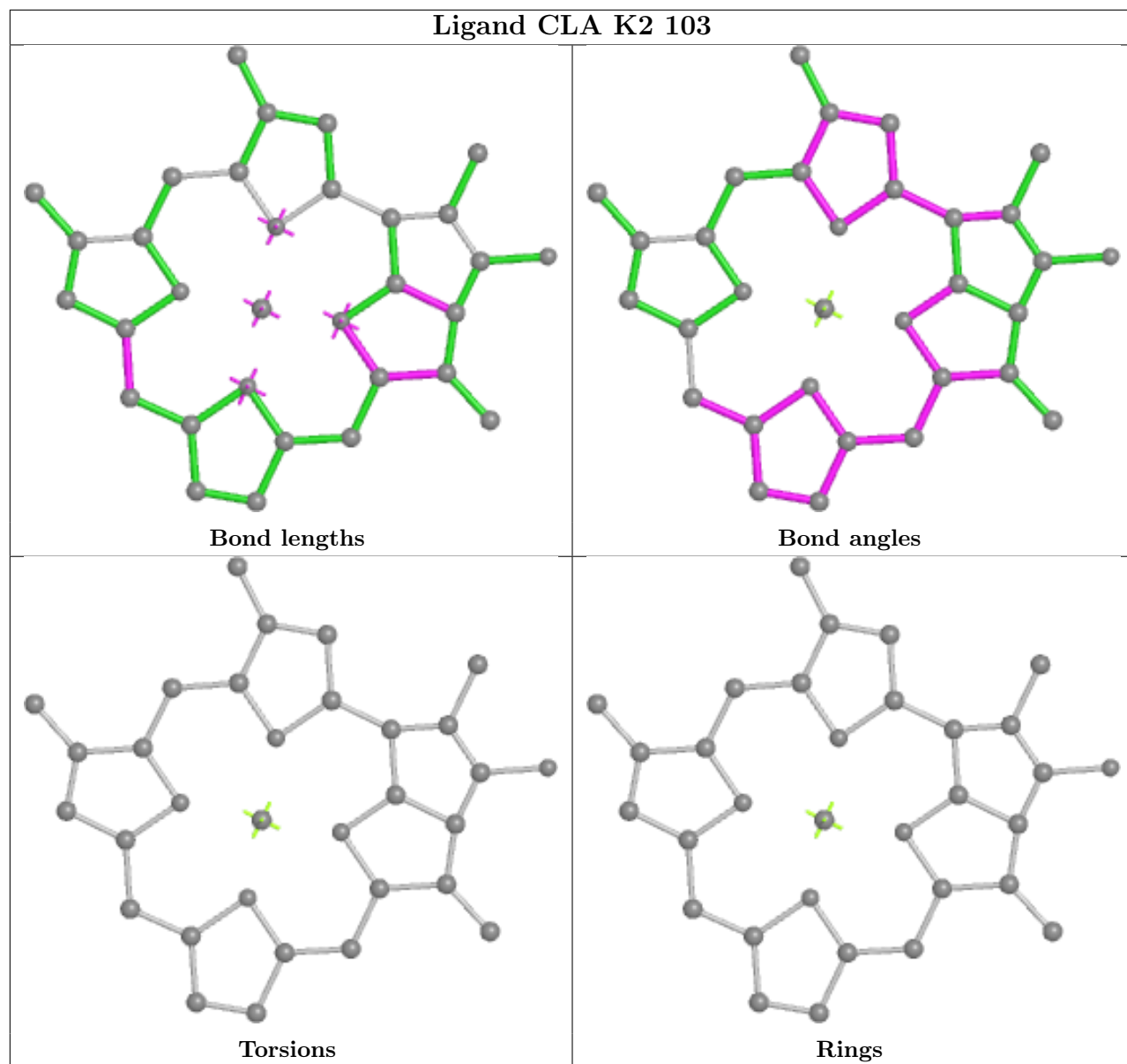


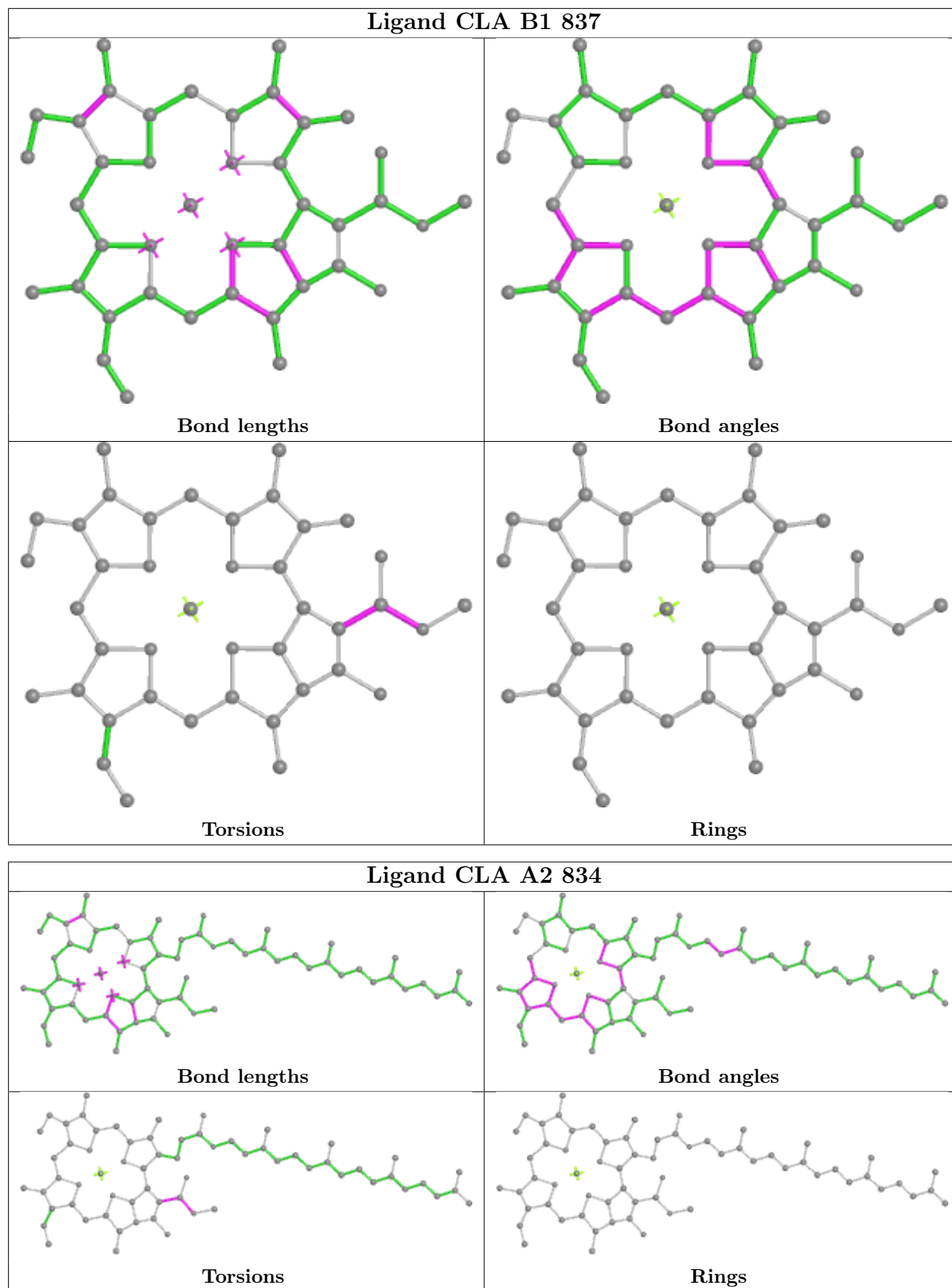


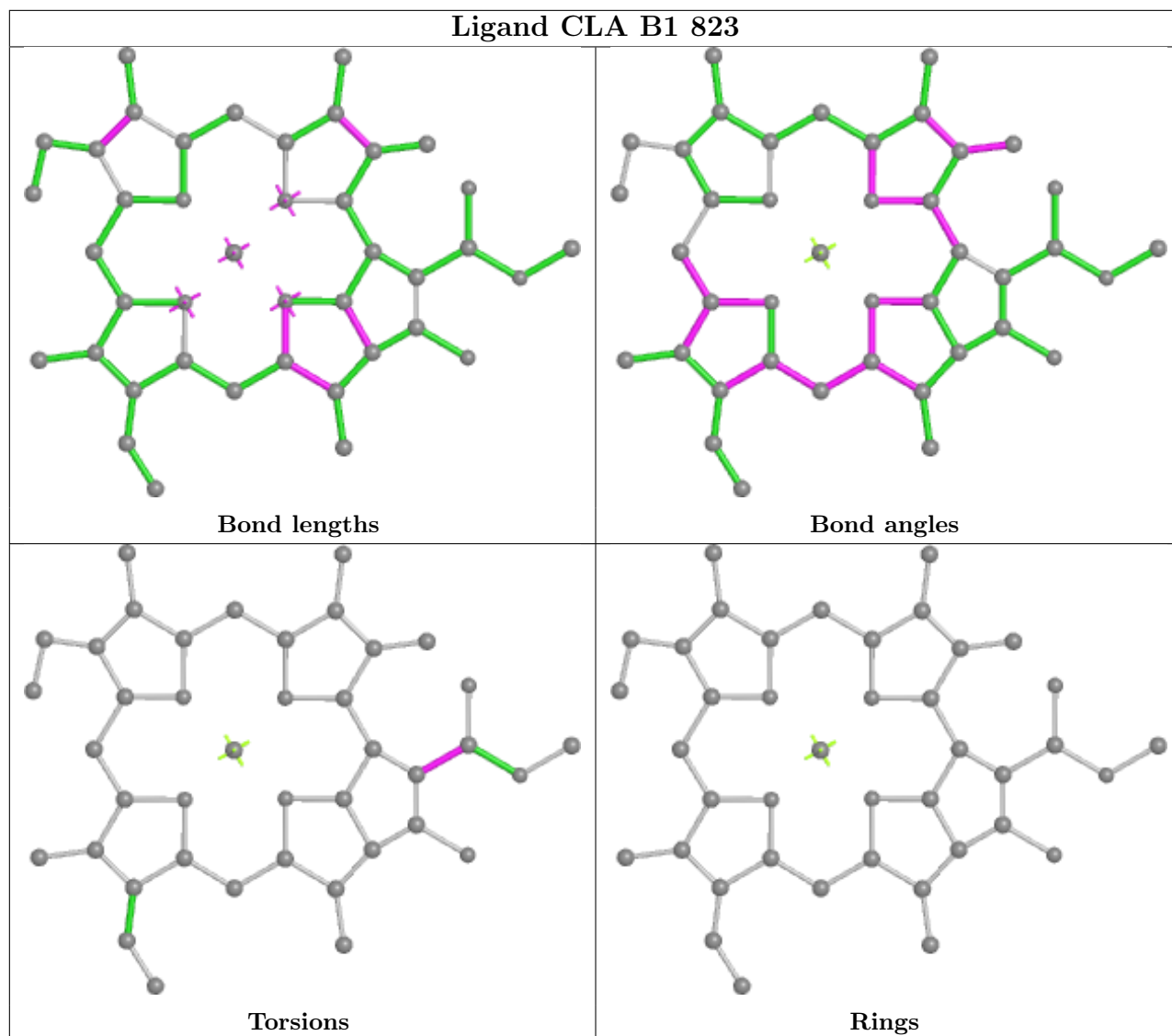


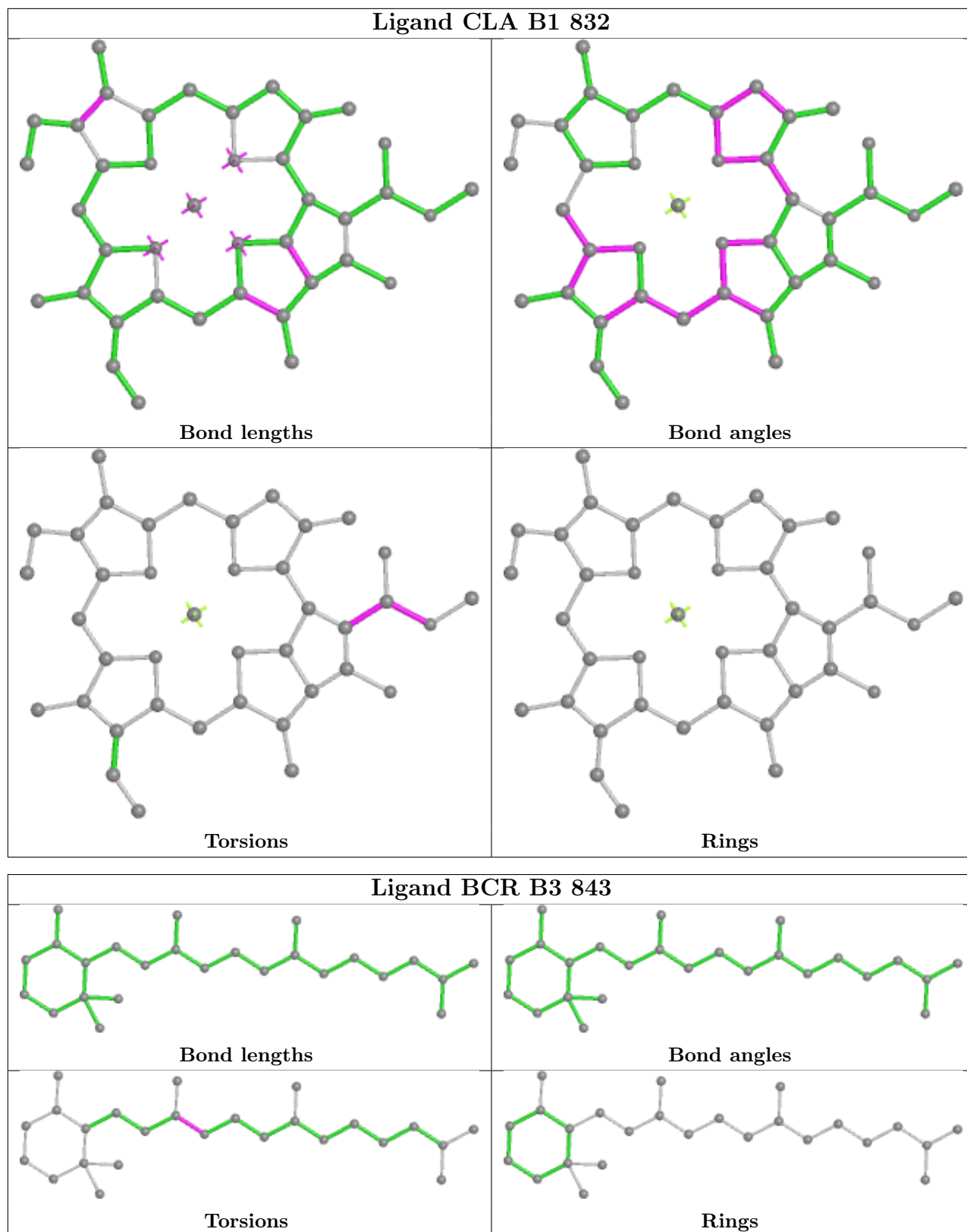




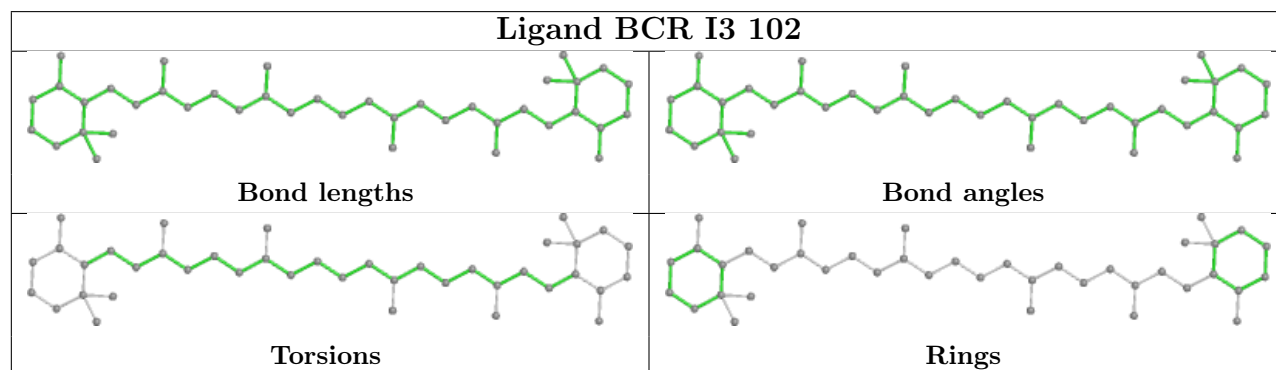
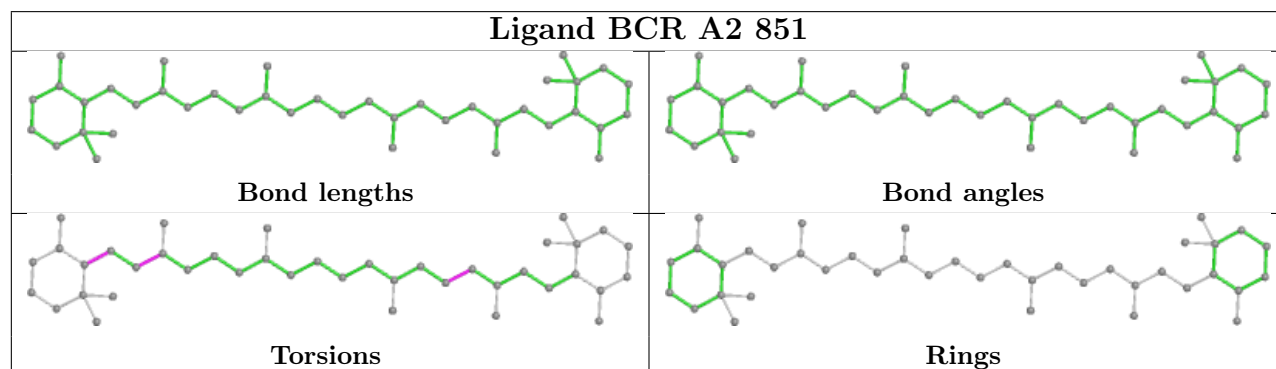
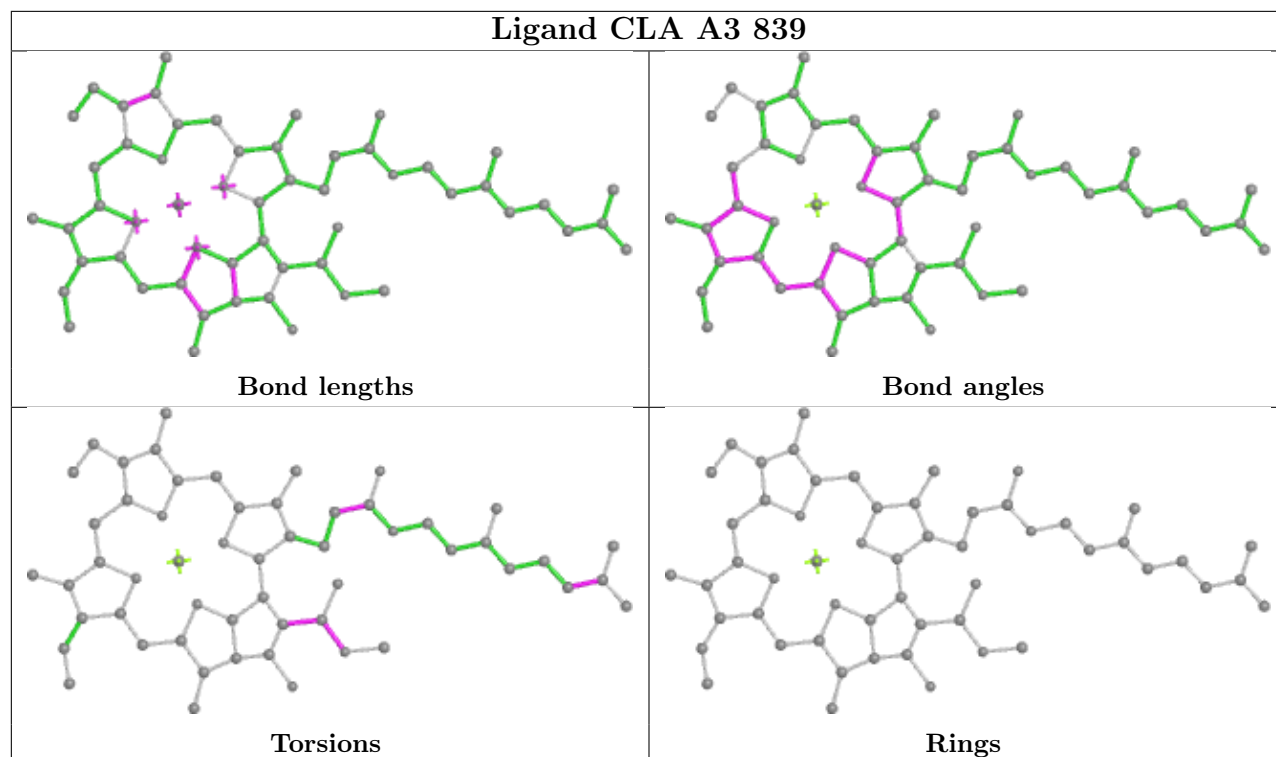


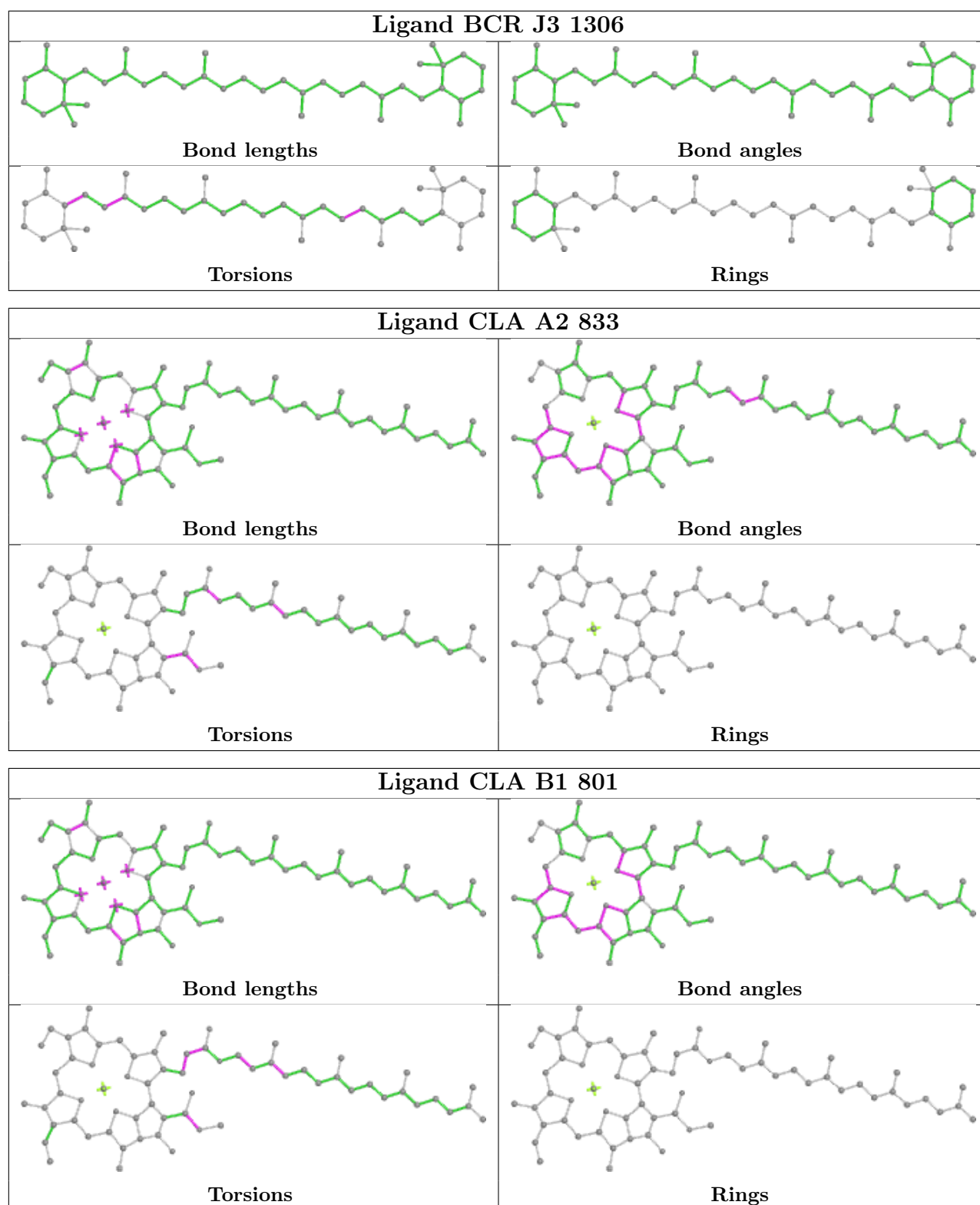


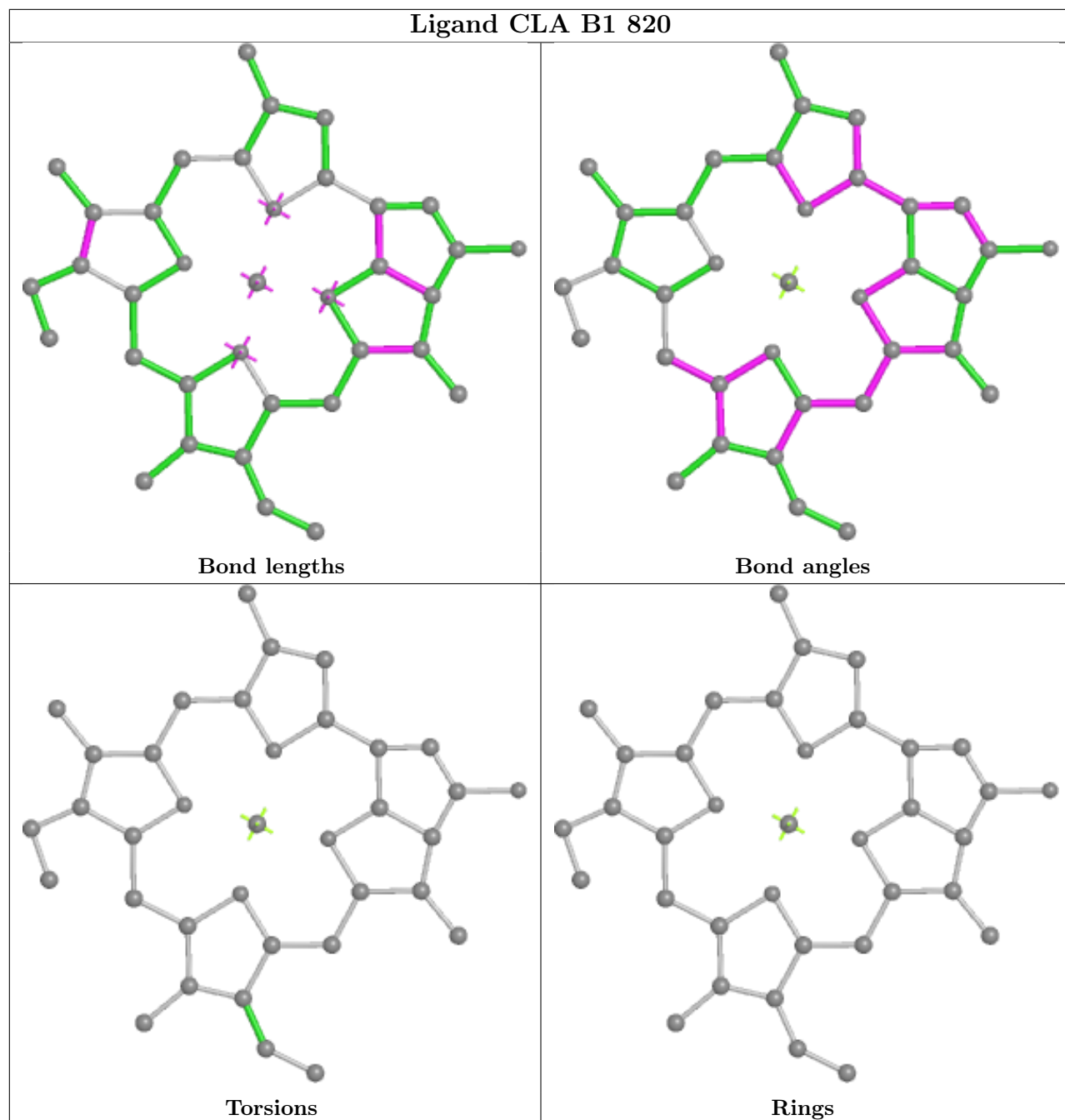


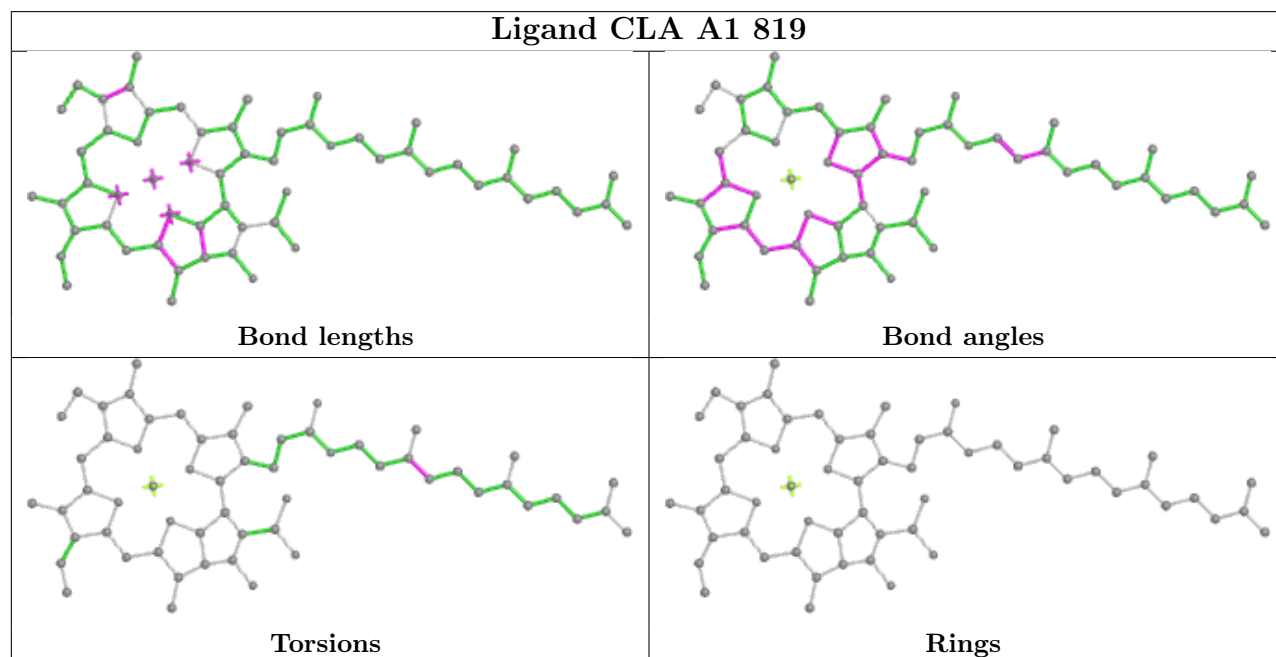
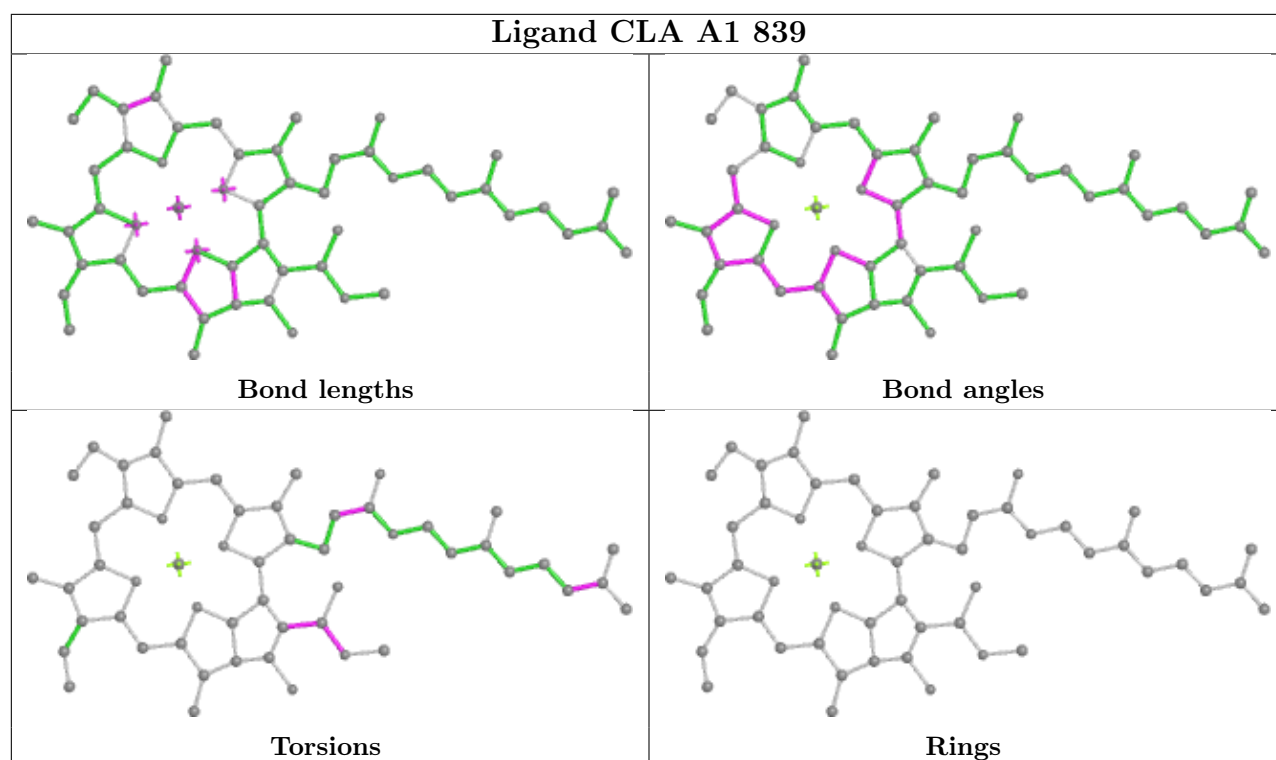


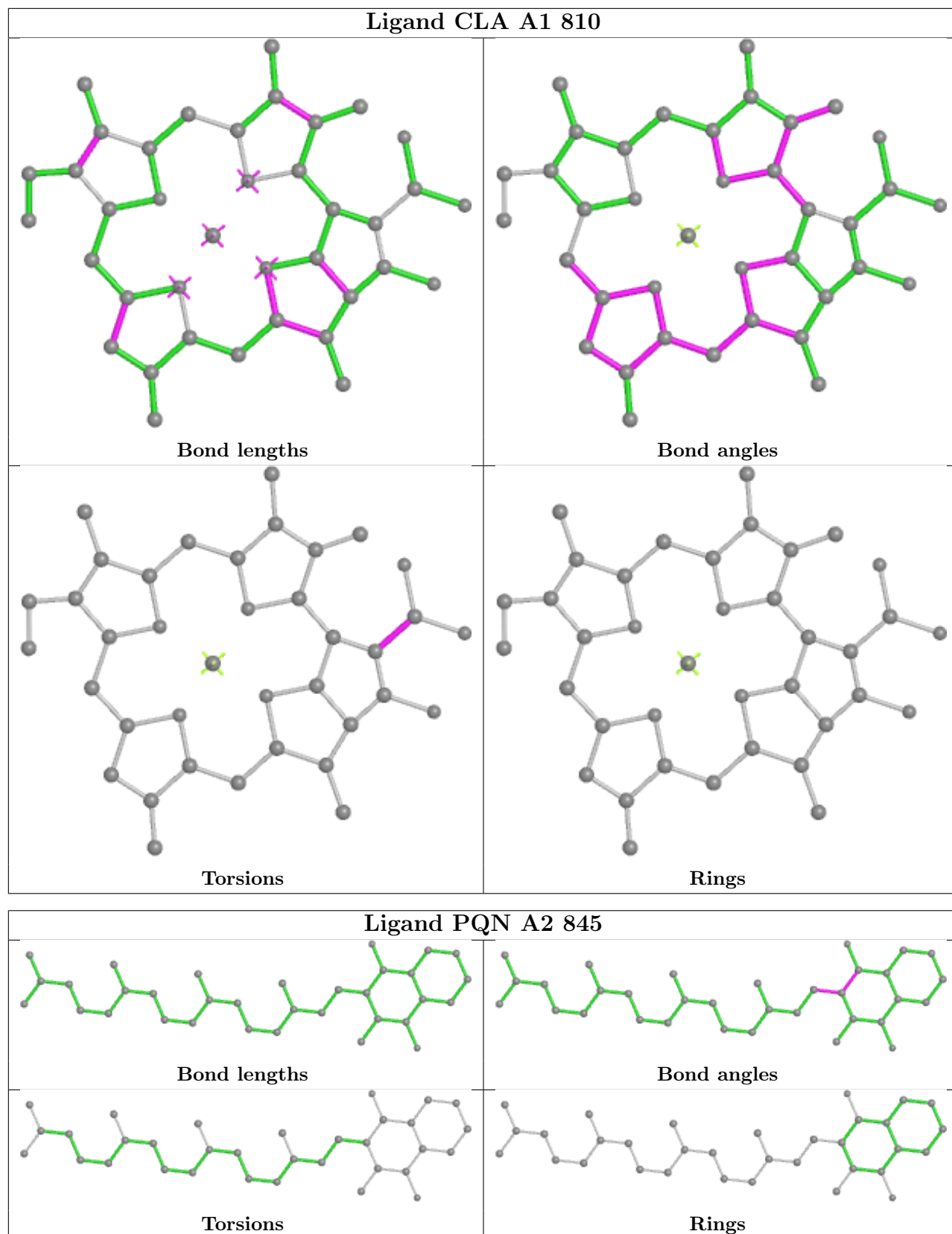


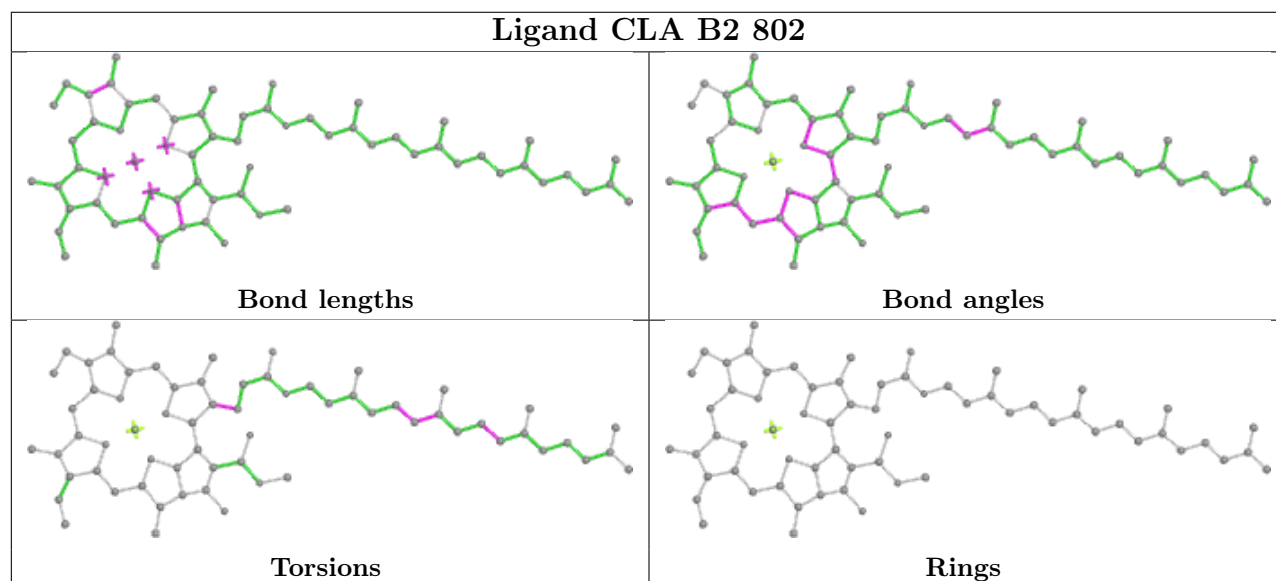
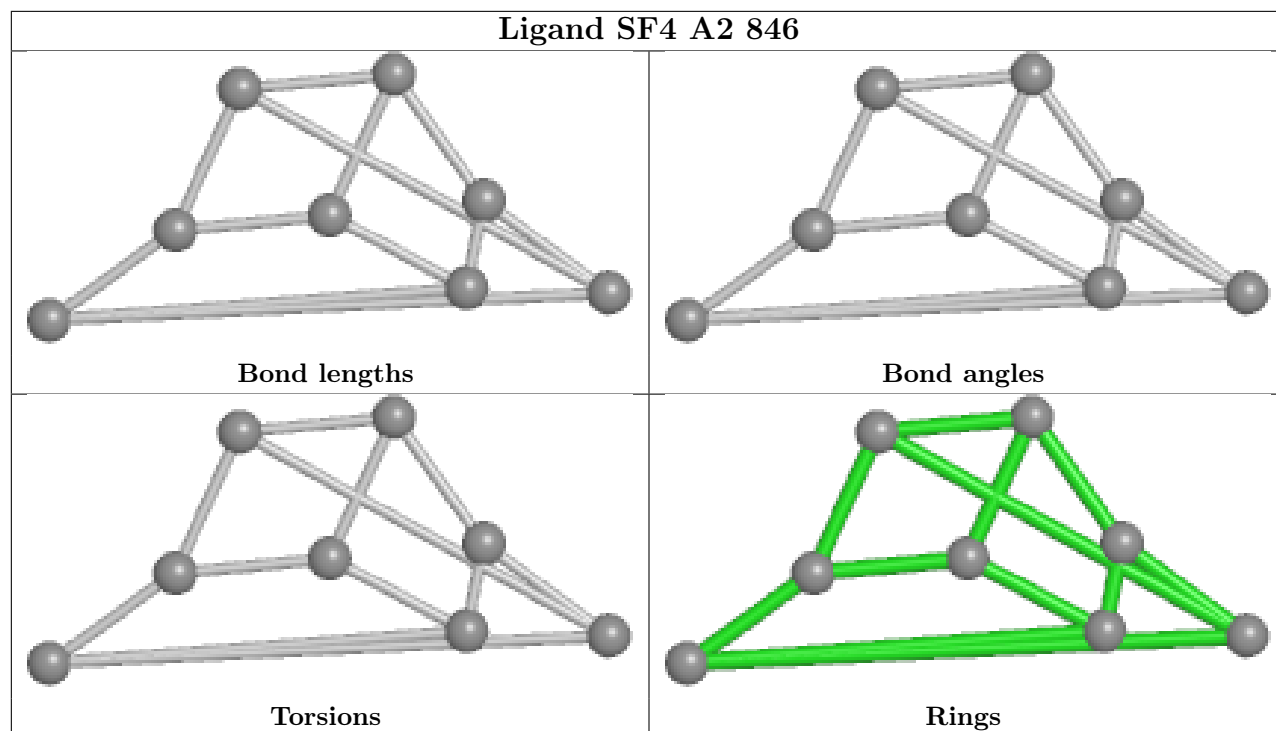


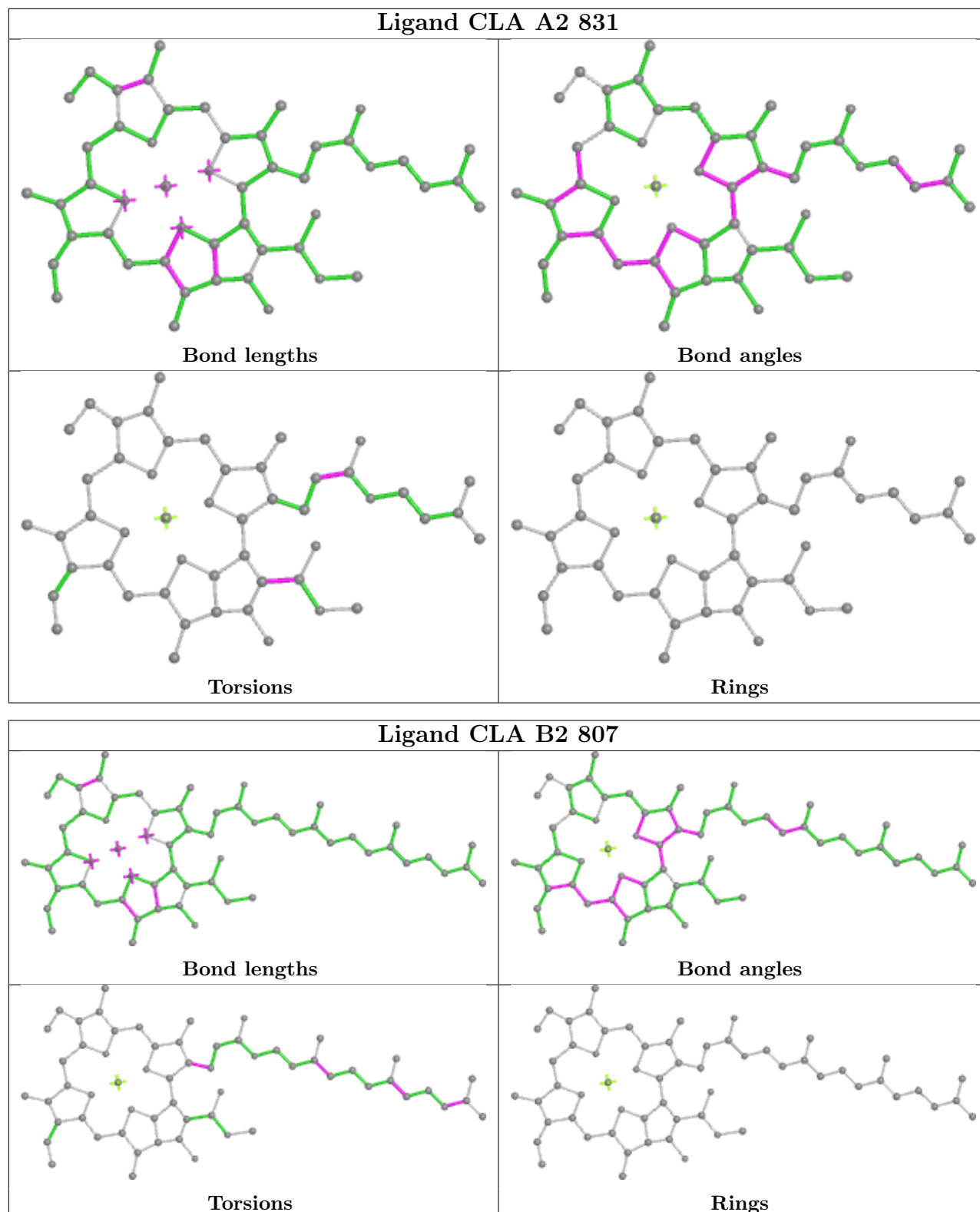


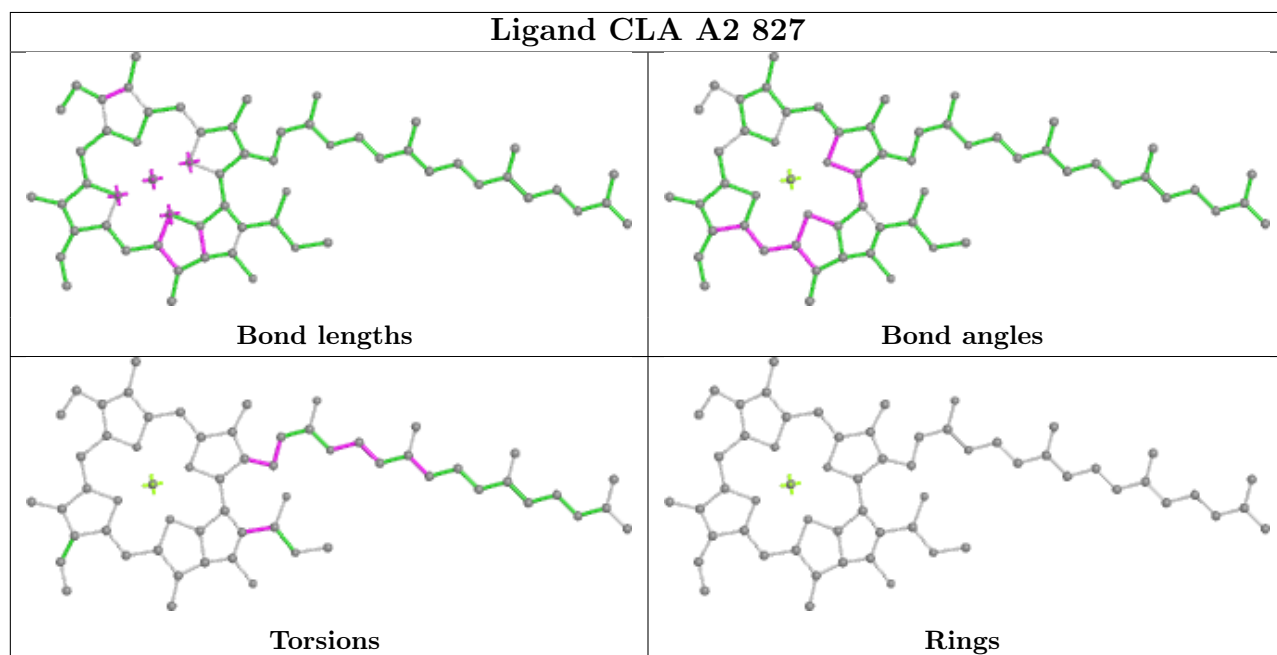
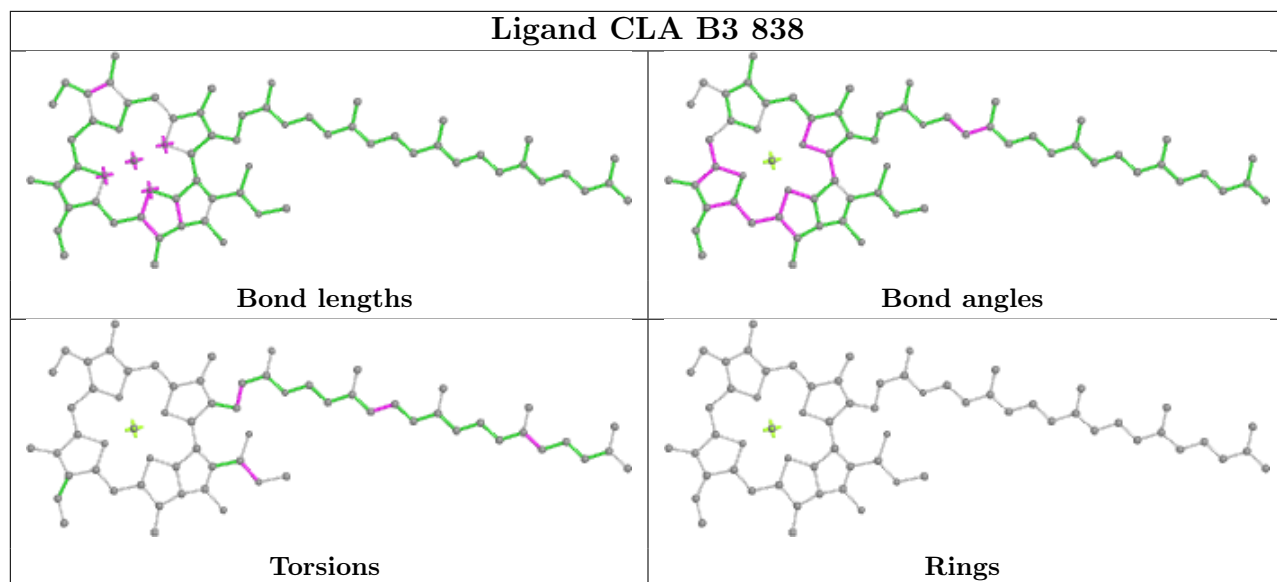




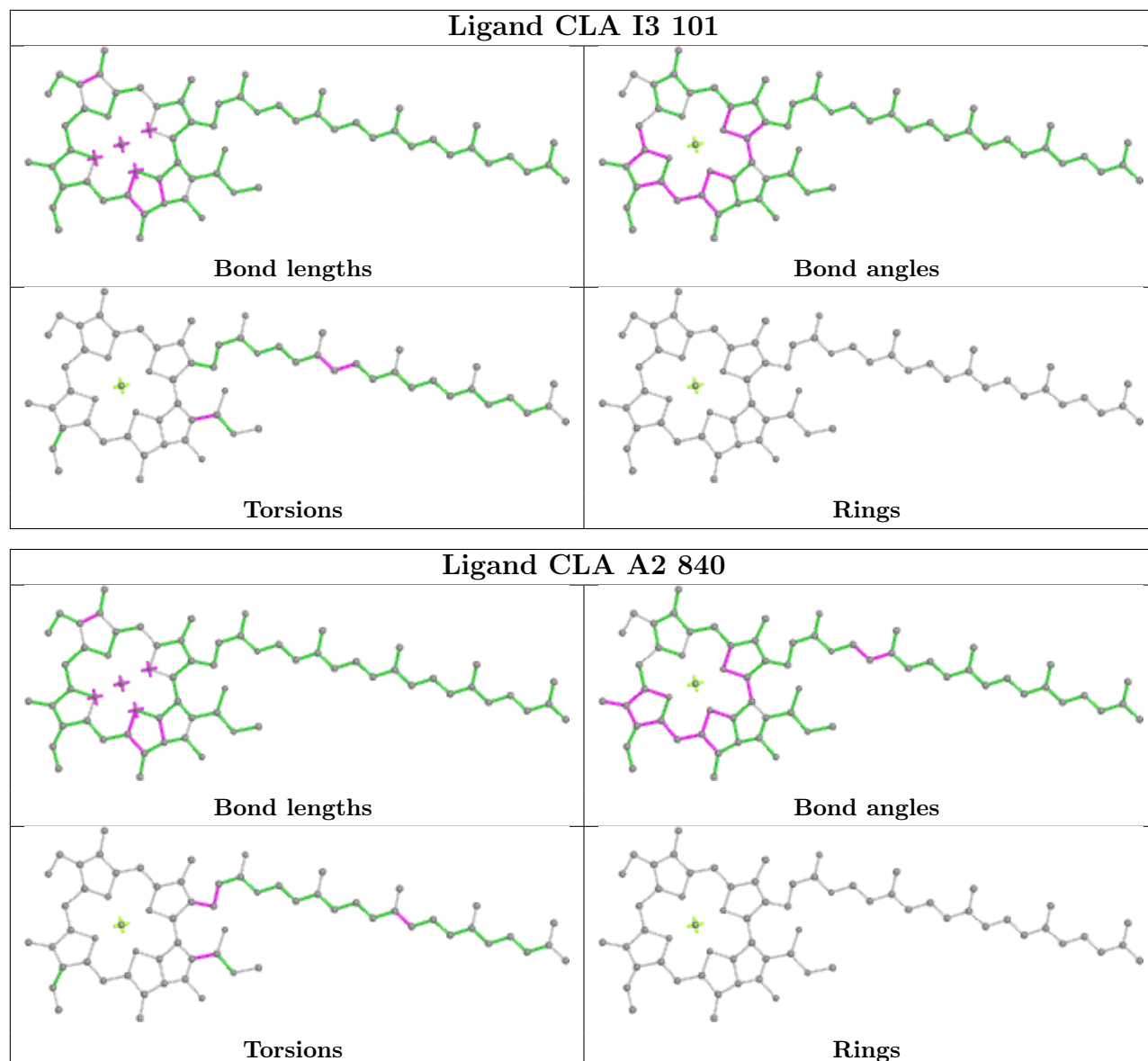


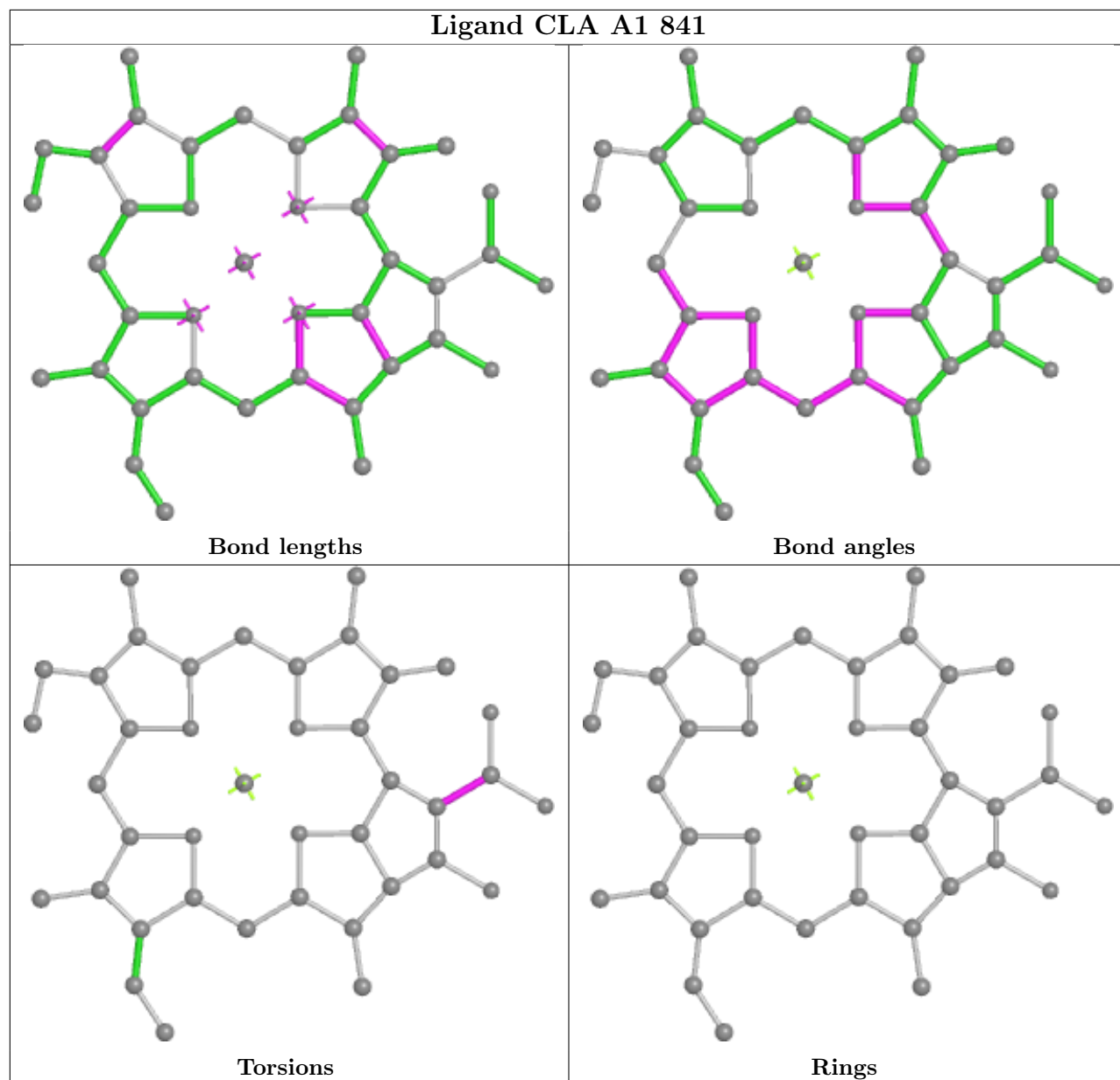


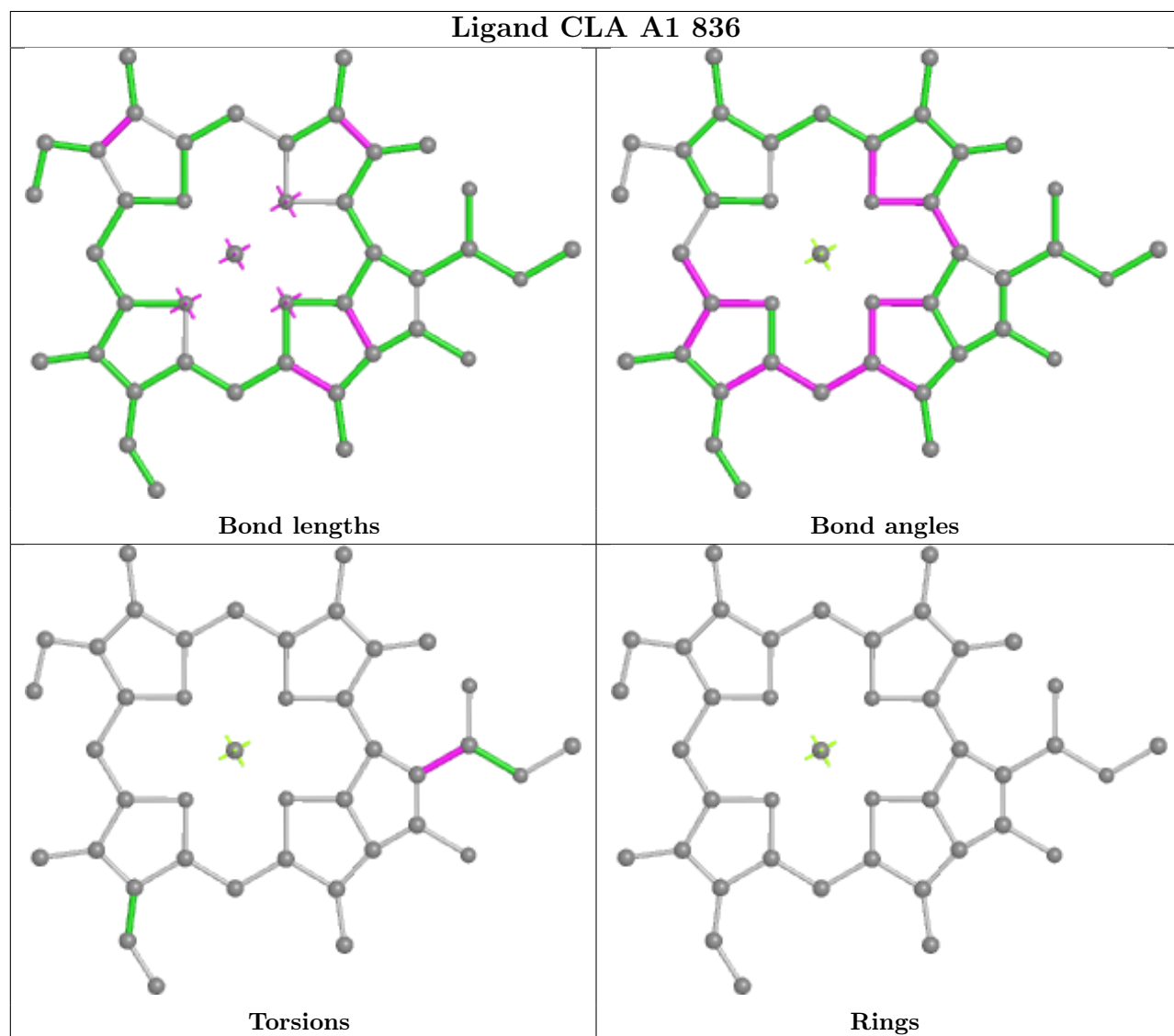
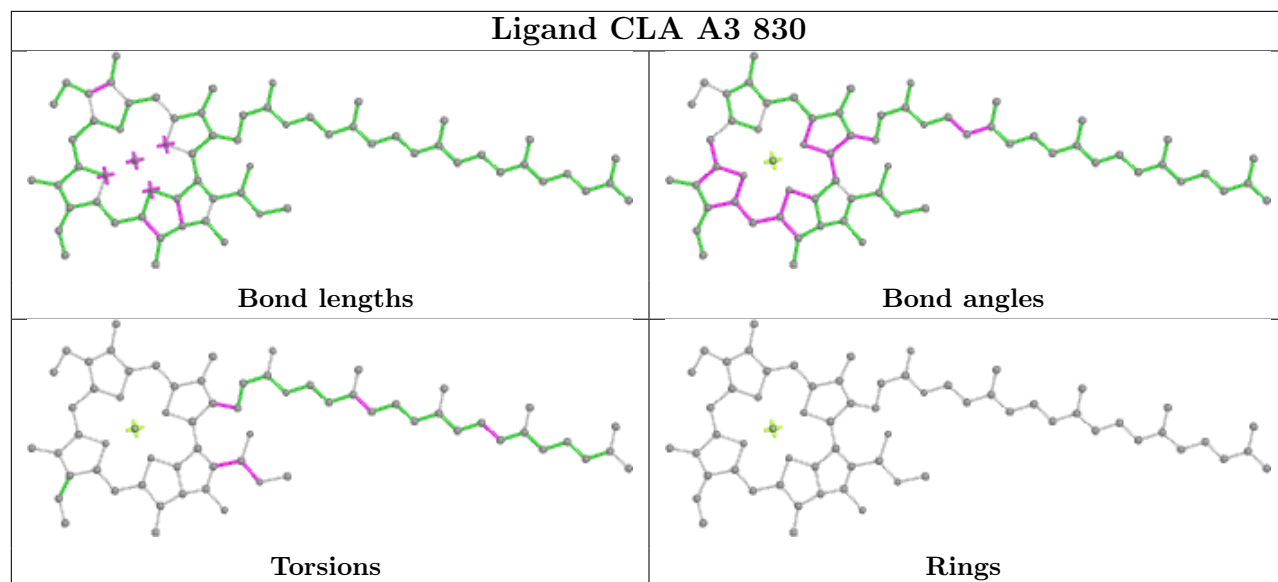


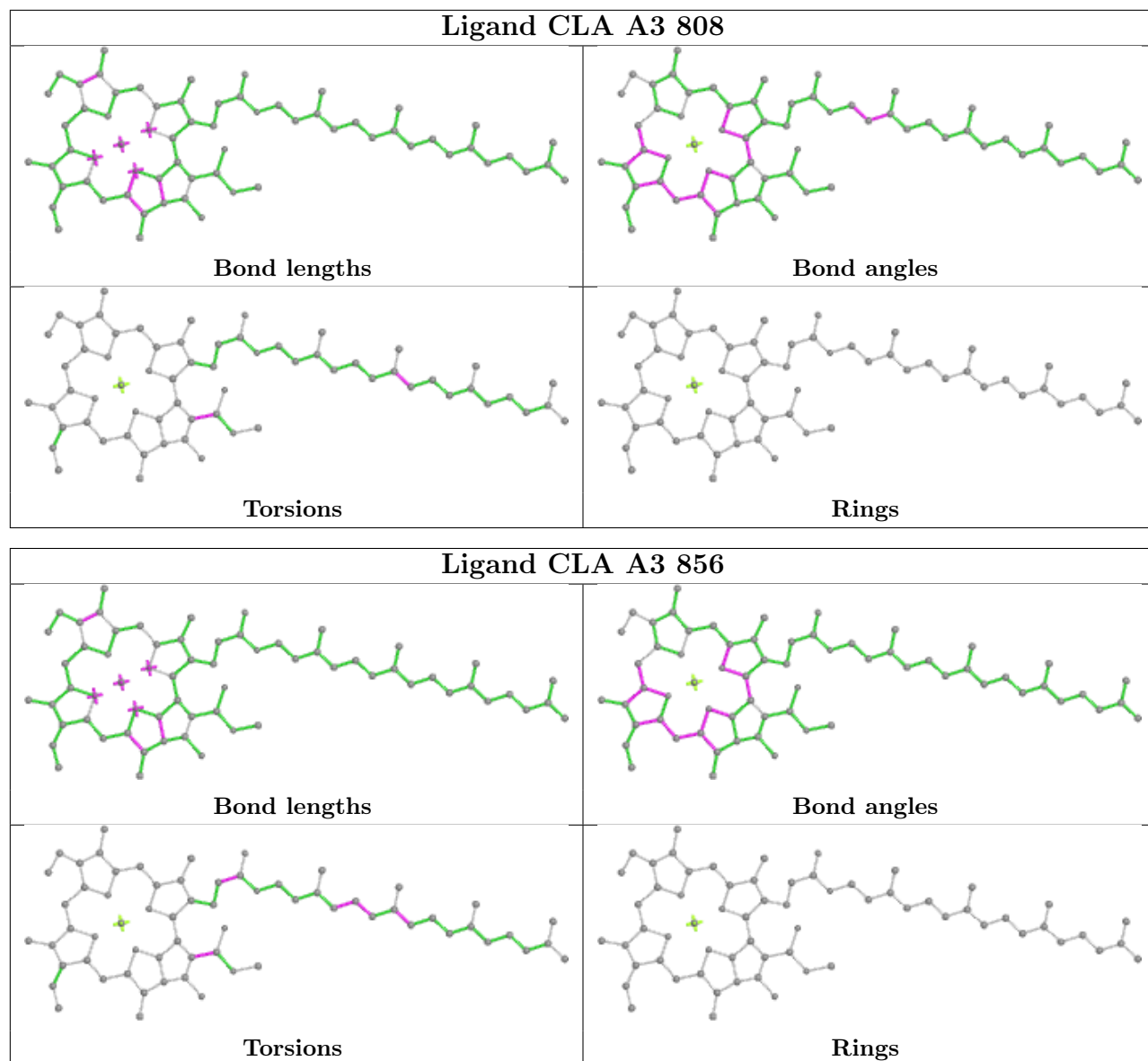


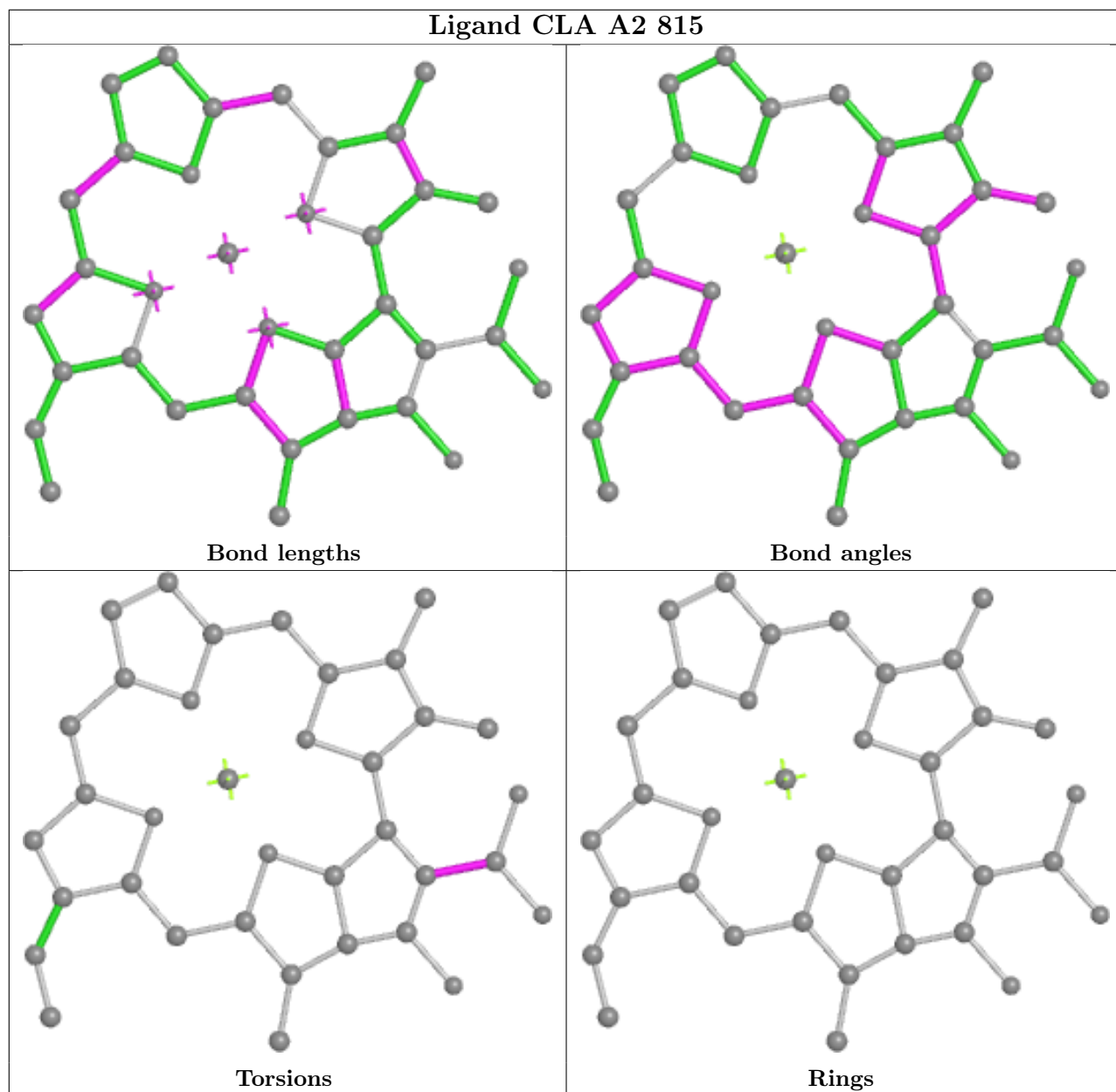


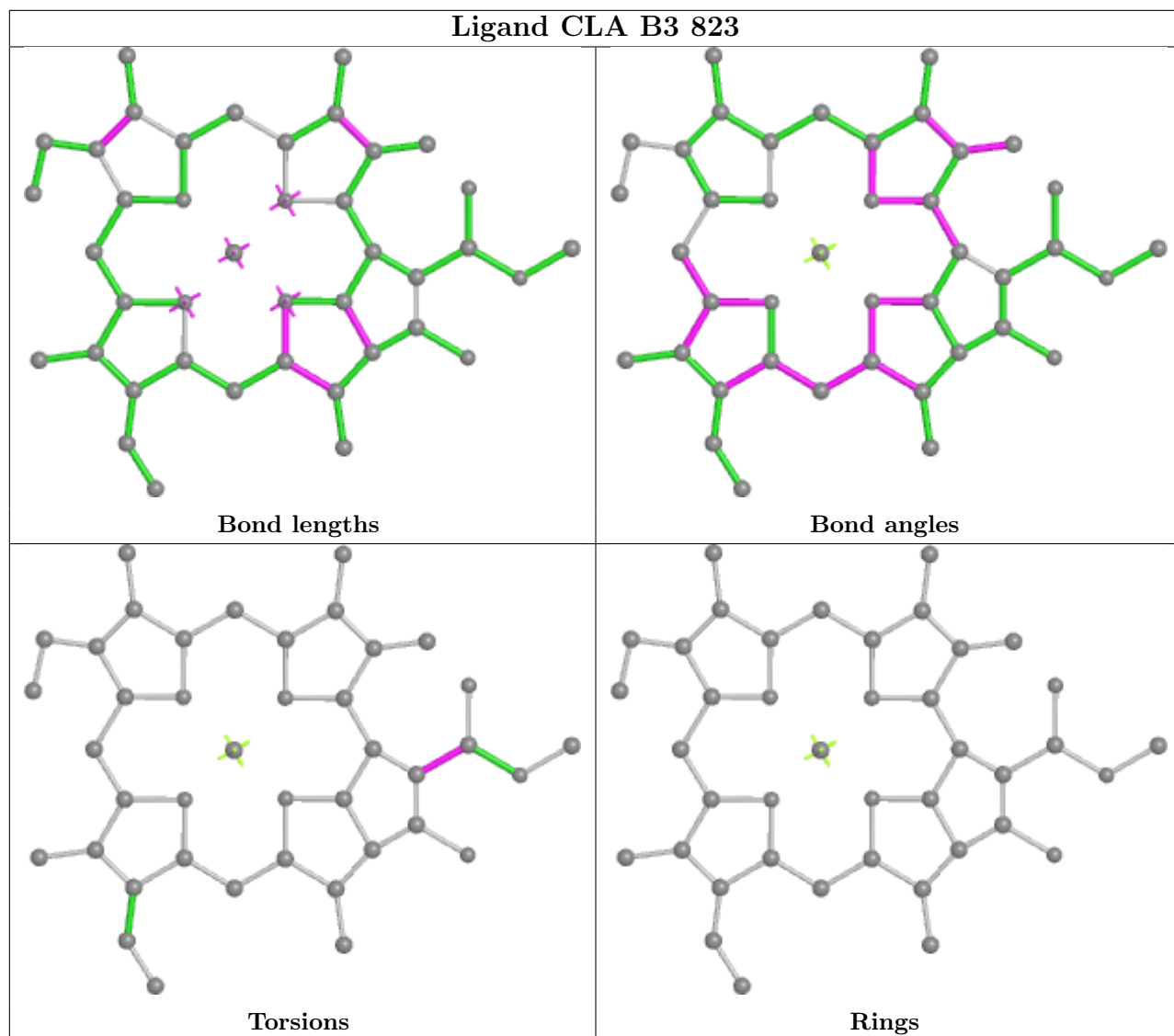


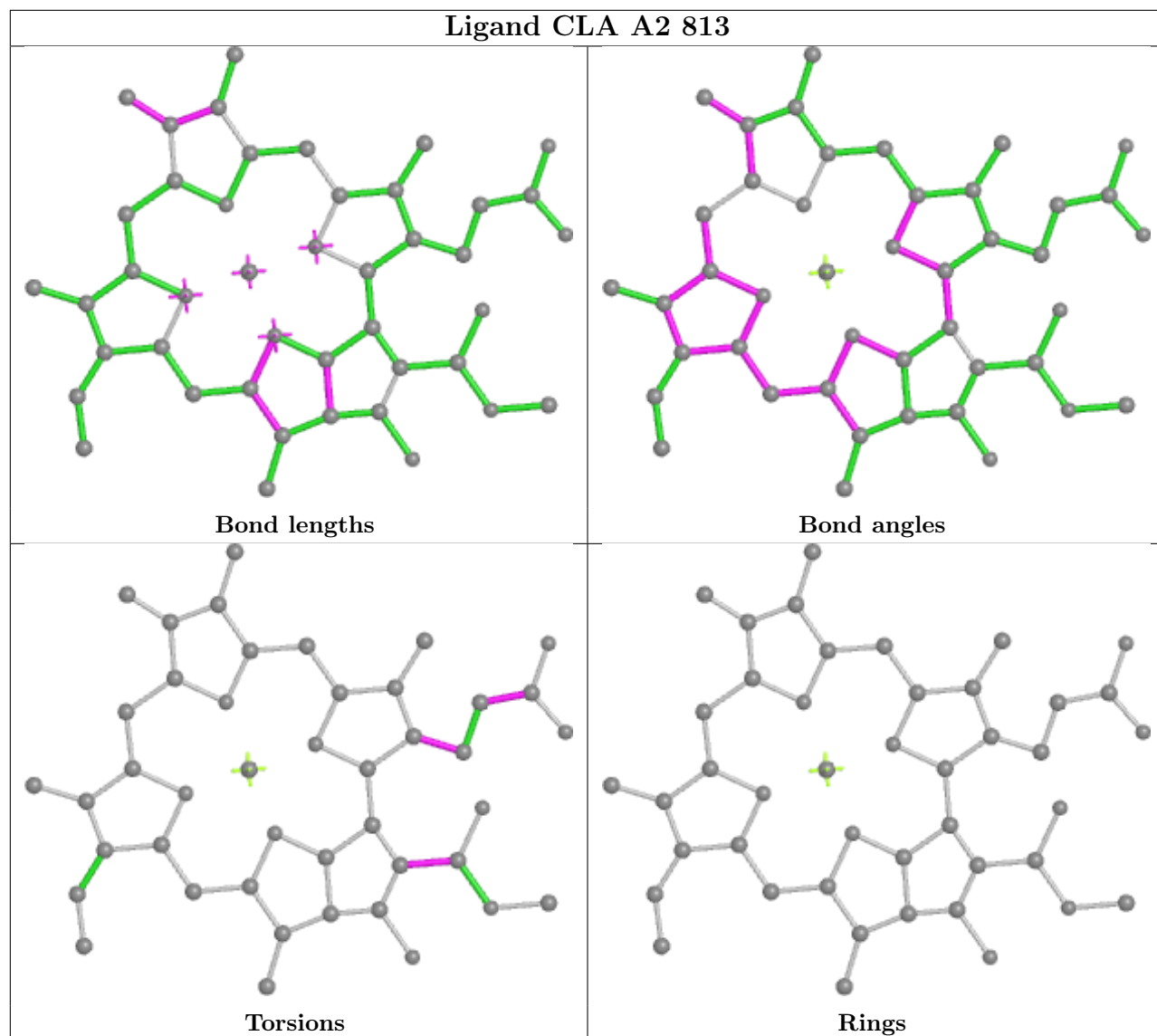


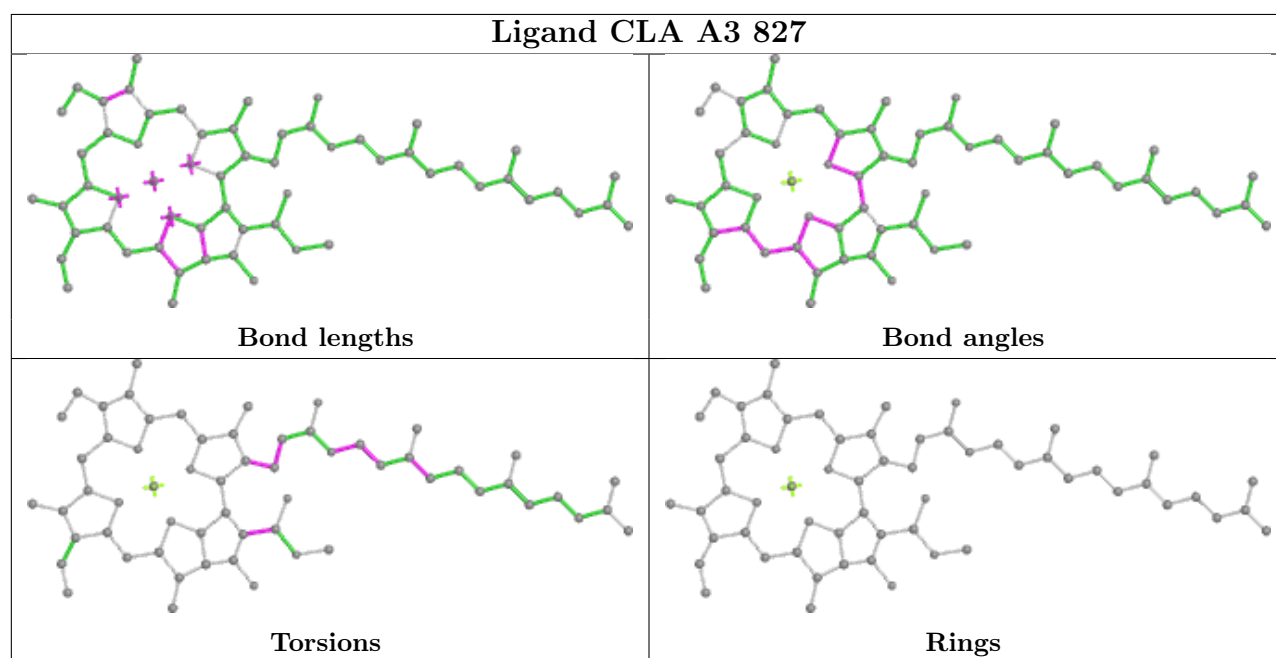
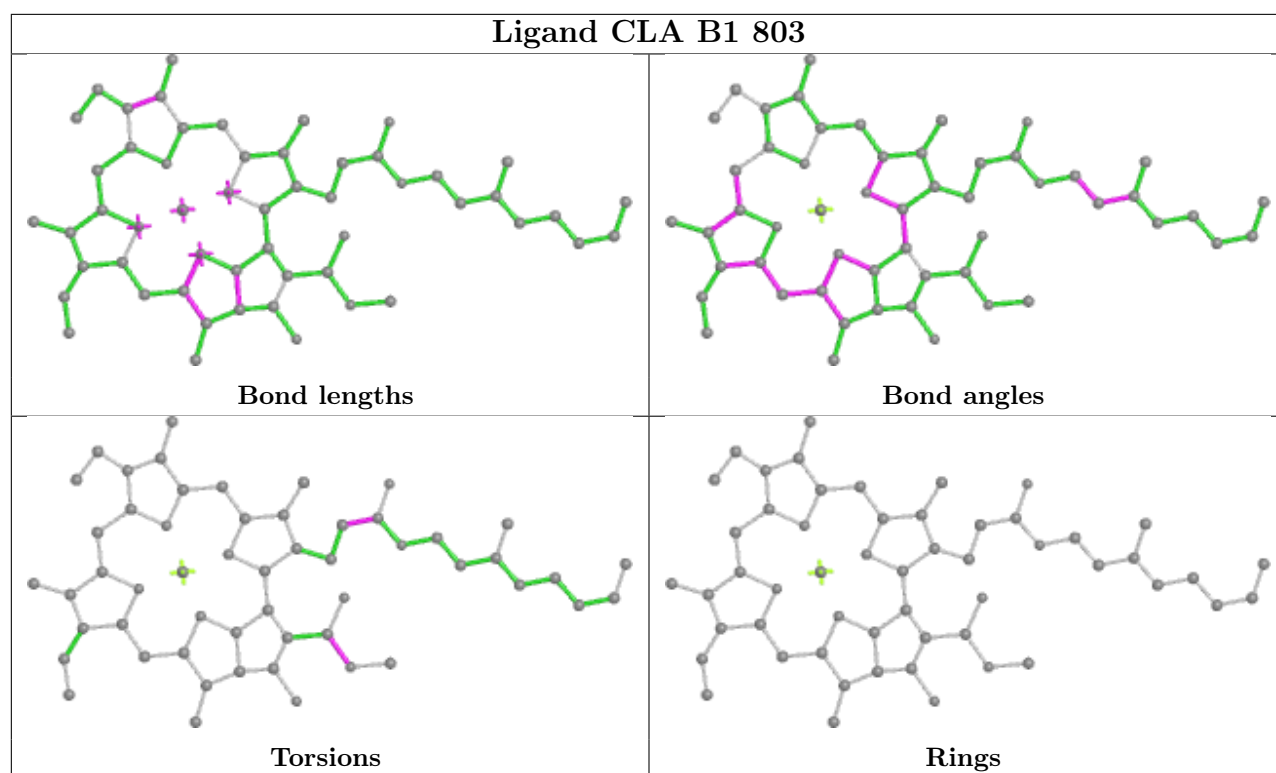




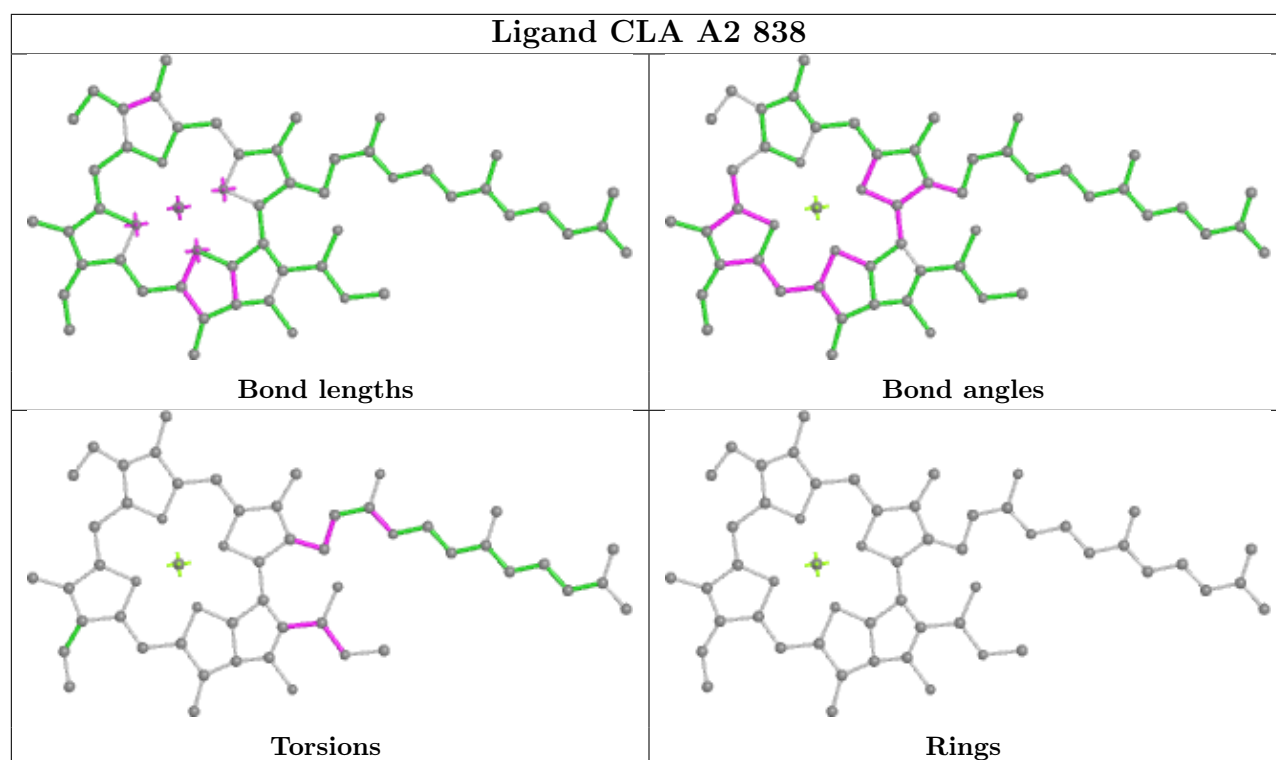












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

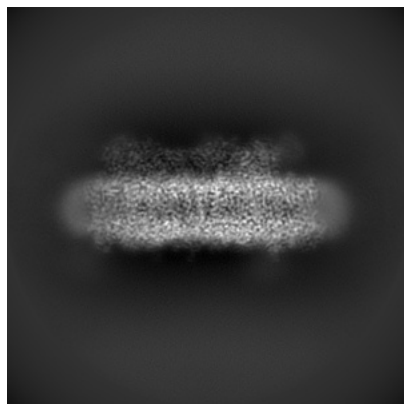
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31605. These allow visual inspection of the internal detail of the map and identification of artifacts.

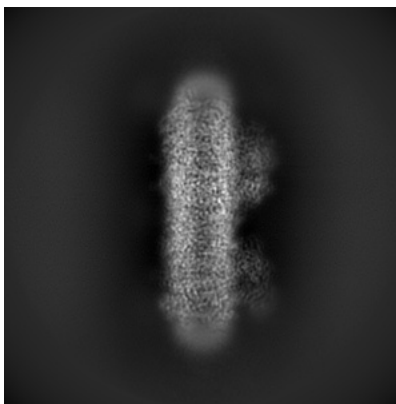
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

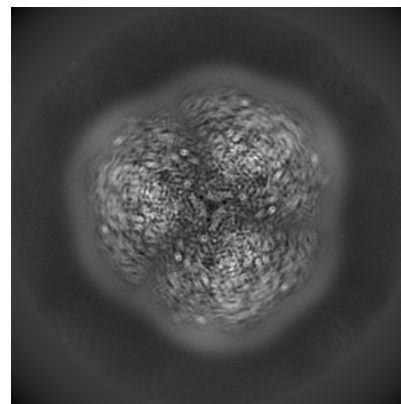
#### 6.1.1 Primary map



X

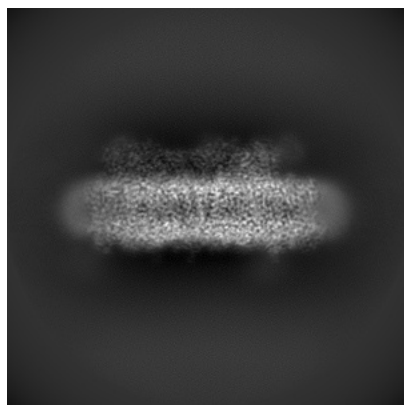


Y

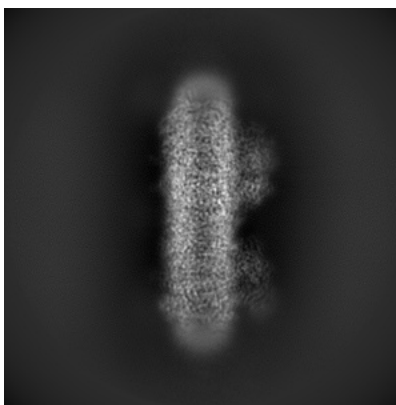


Z

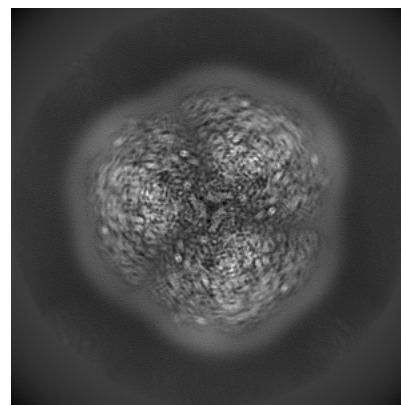
#### 6.1.2 Raw map



X



Y

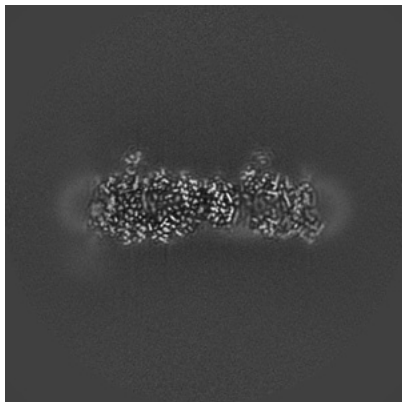


Z

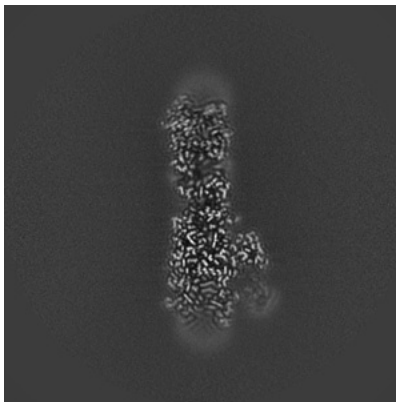
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

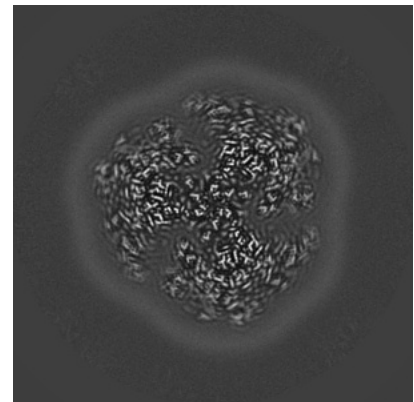
### 6.2.1 Primary map



X Index: 200

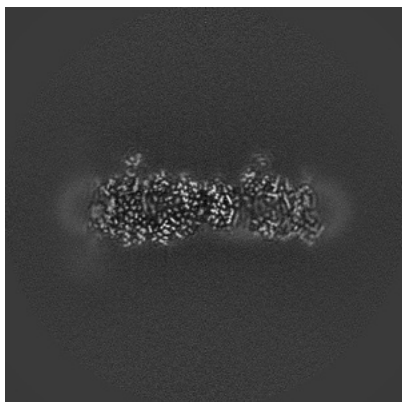


Y Index: 200

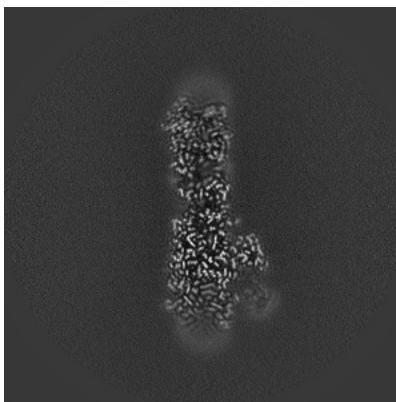


Z Index: 200

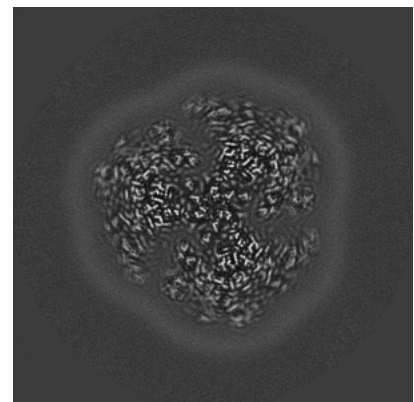
### 6.2.2 Raw map



X Index: 200



Y Index: 200

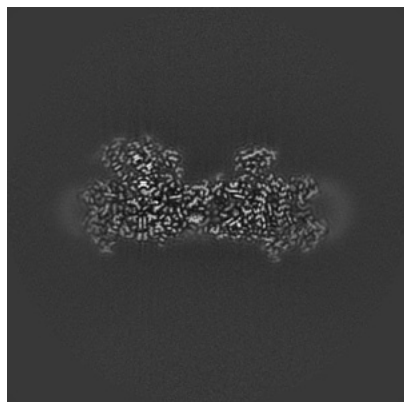


Z Index: 200

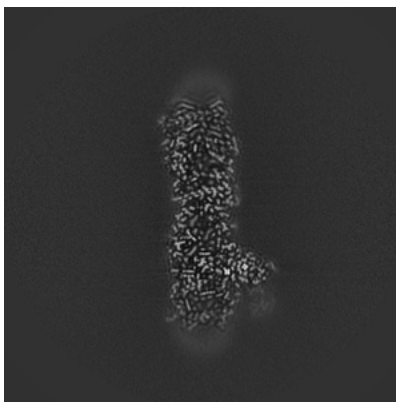
The images above show central slices of the map in three orthogonal directions.

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

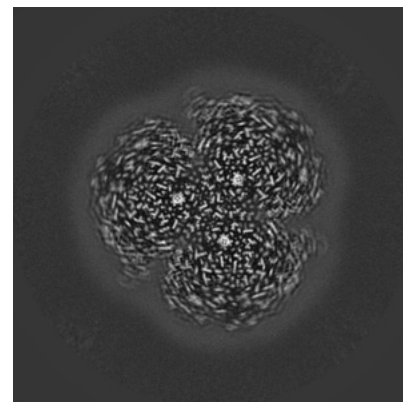
### 6.3.1 Primary map



X Index: 221

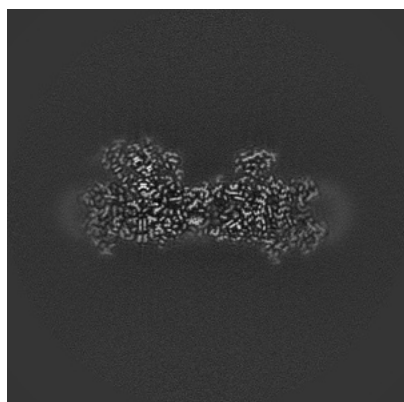


Y Index: 213

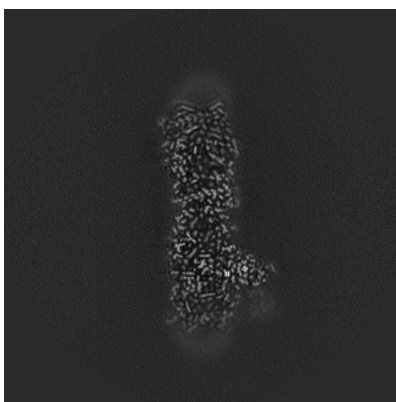


Z Index: 215

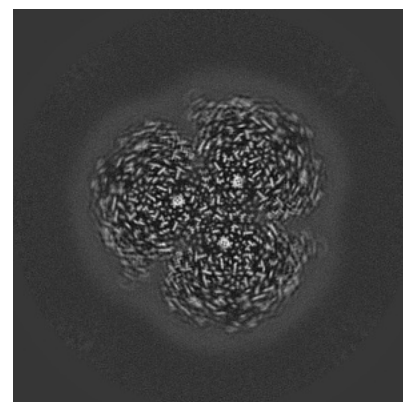
### 6.3.2 Raw map



X Index: 221



Y Index: 213

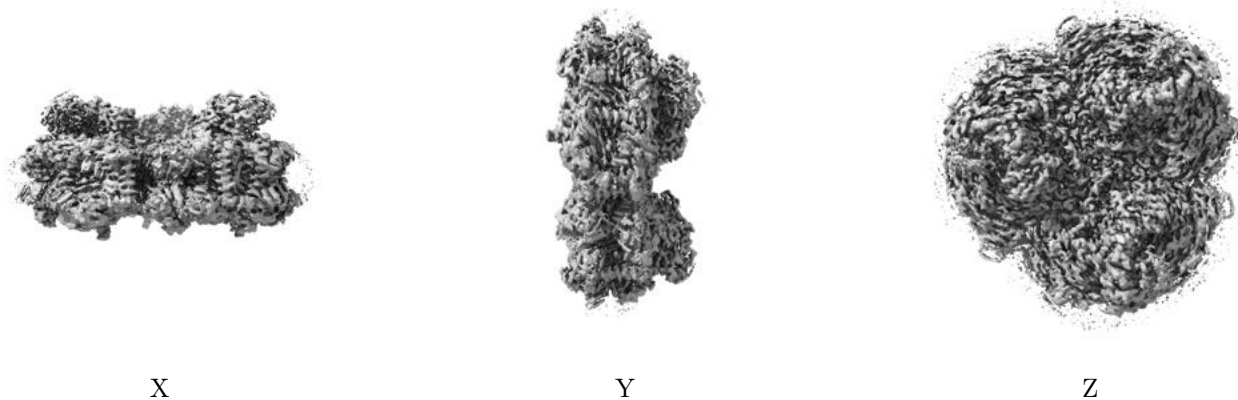


Z Index: 215

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

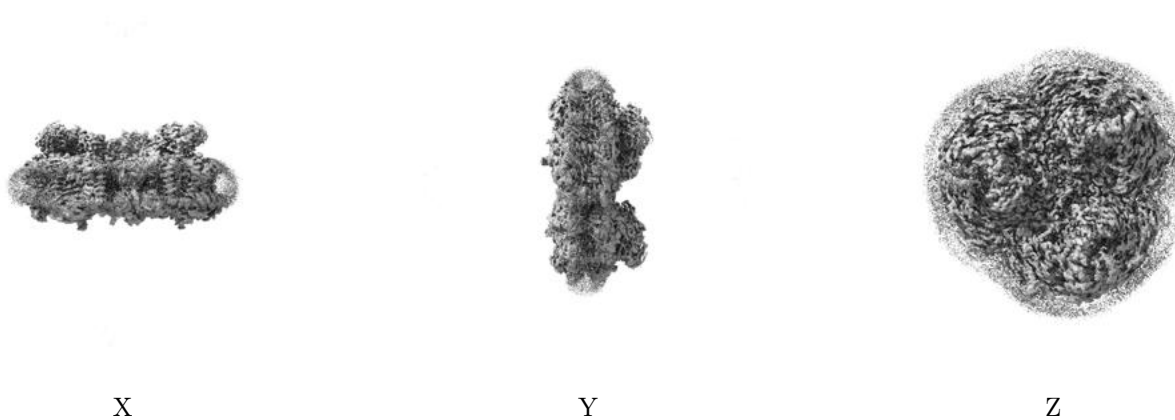
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

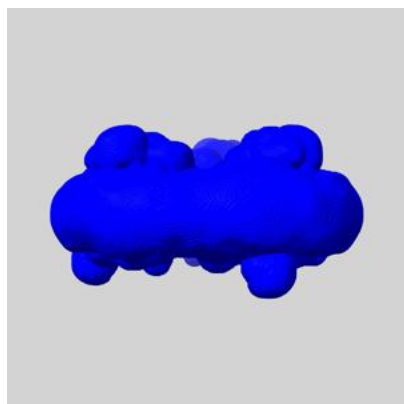
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

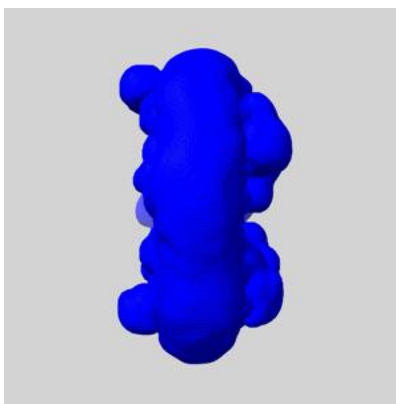
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

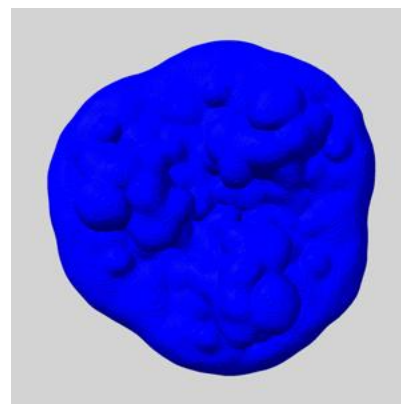
### 6.5.1 emd\_31605\_msk\_1.map [i](#)



X



Y

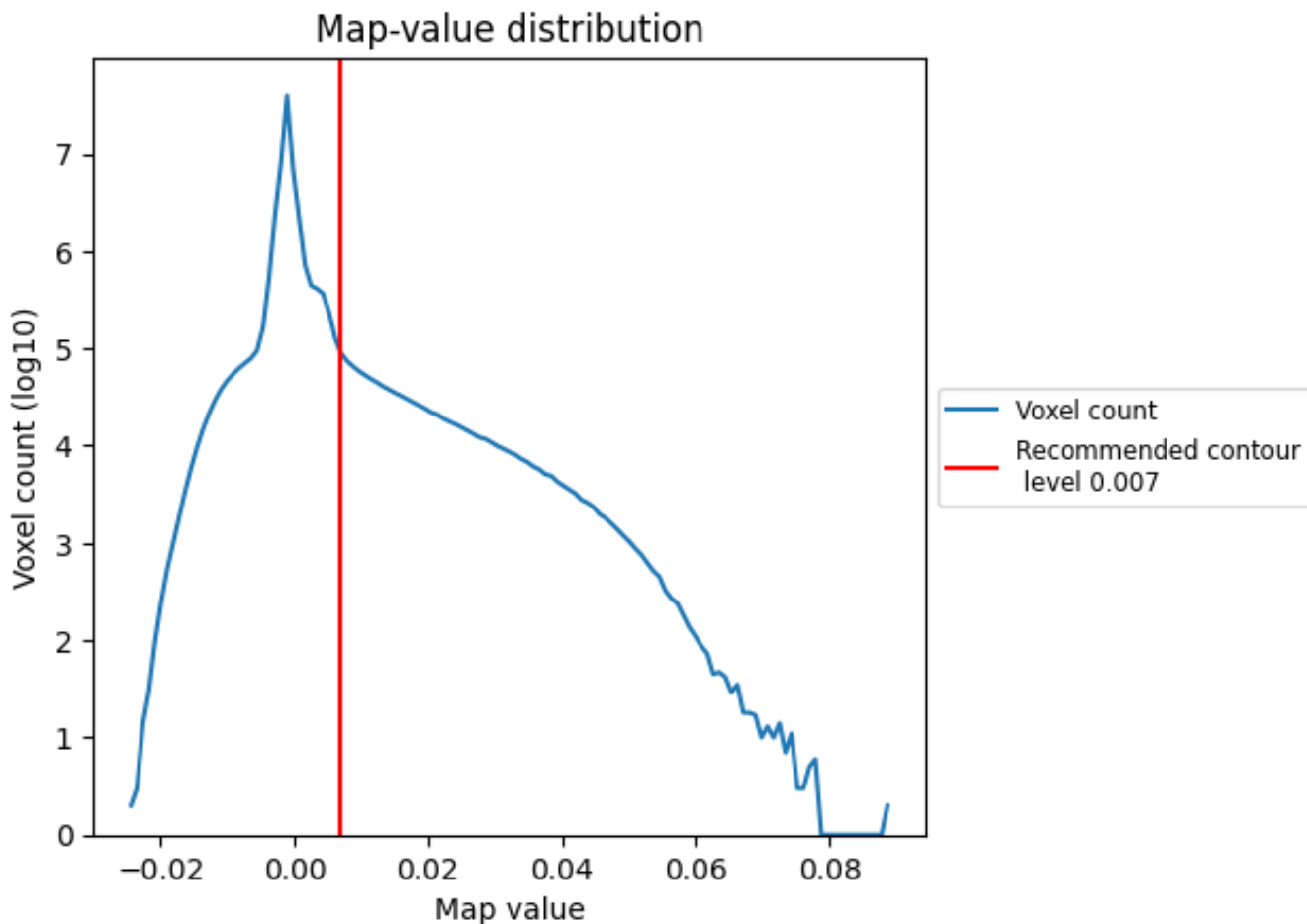


Z

## 7 Map analysis [i](#)

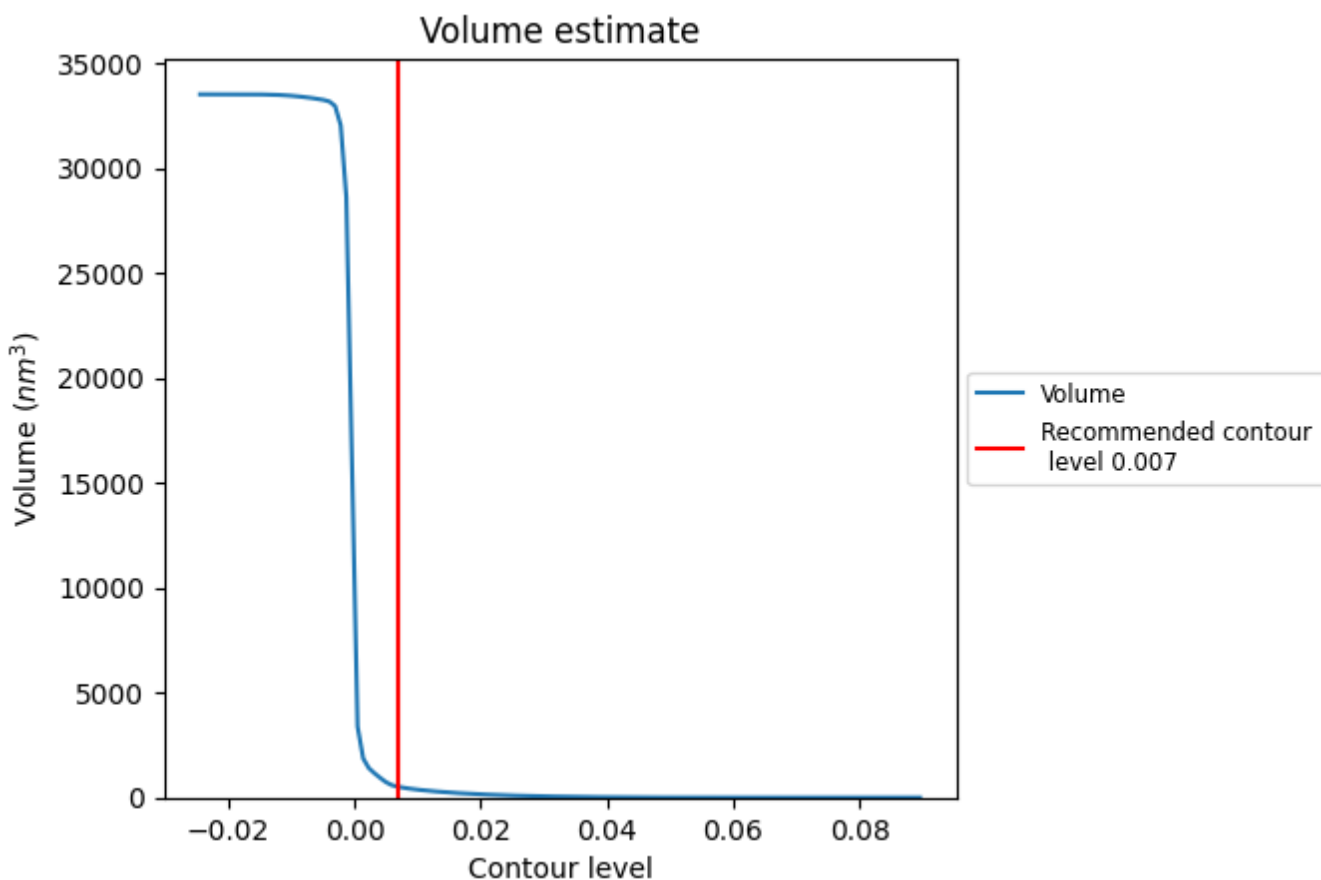
This section contains the results of statistical analysis of the map.

### 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](#)

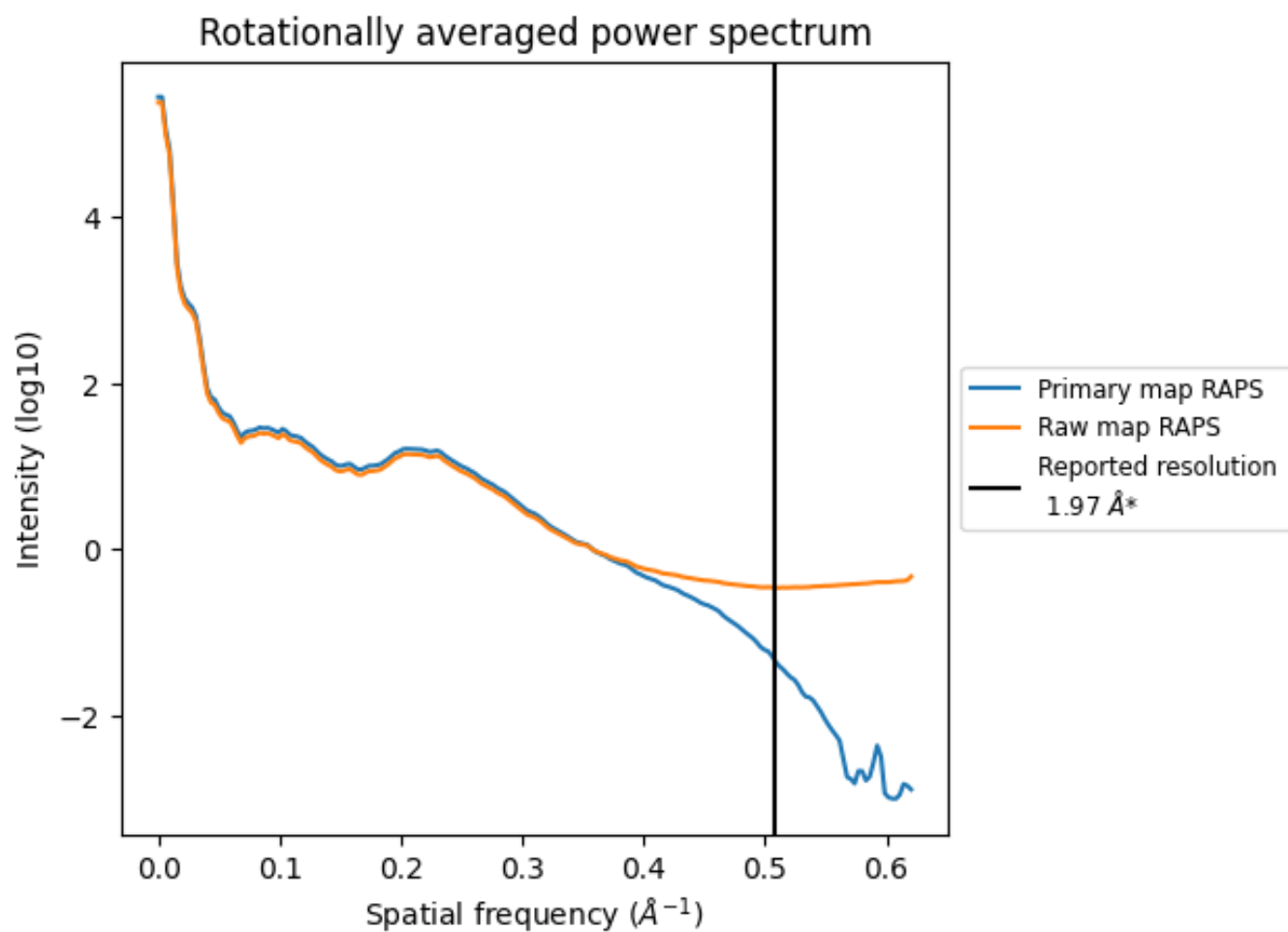


The volume at the recommended contour level is 511 nm<sup>3</sup>; this corresponds to an approximate mass of 461 kDa.

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](#)

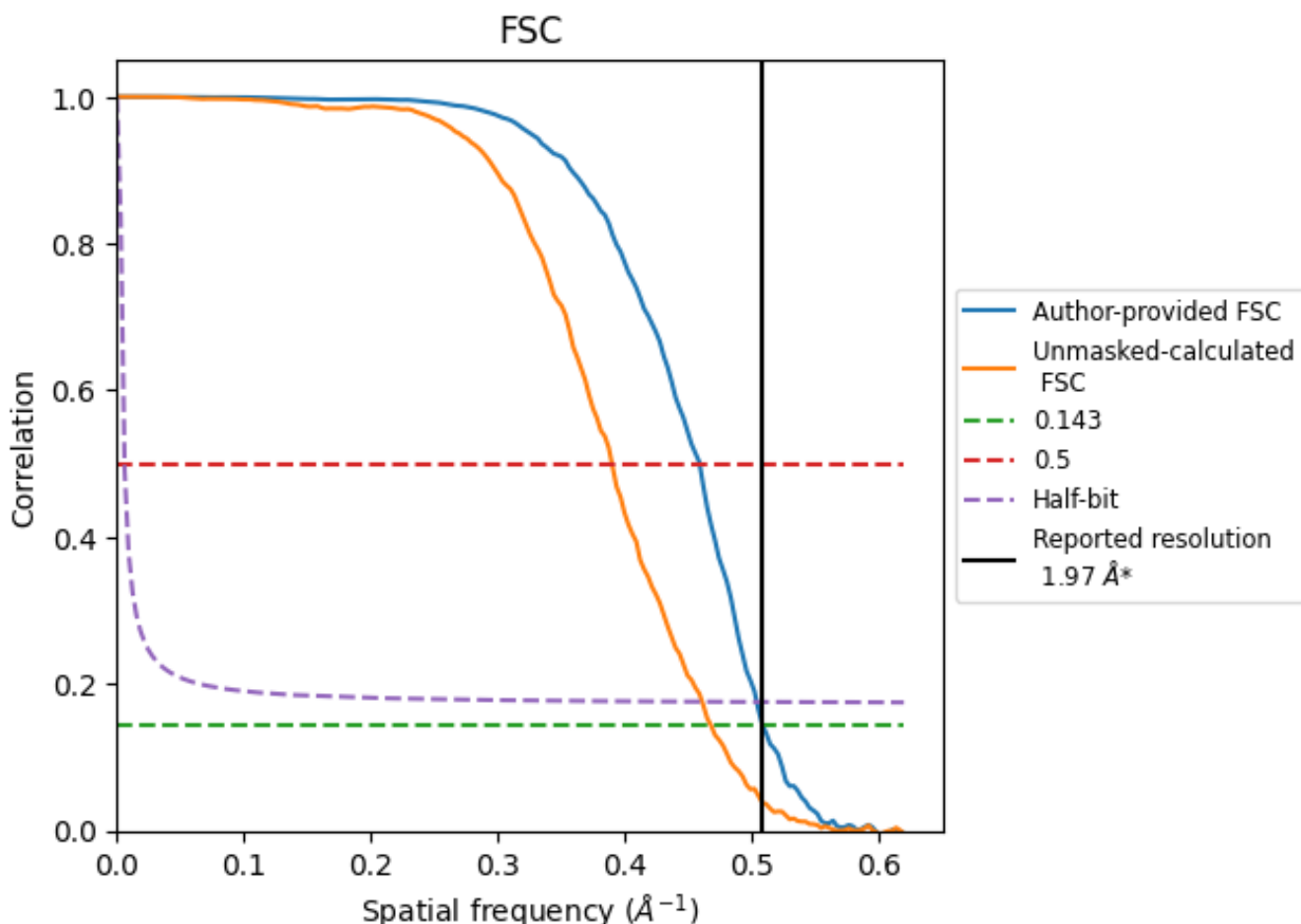


\*Reported resolution corresponds to spatial frequency of 0.508 Å<sup>-1</sup>

## 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 0.508 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

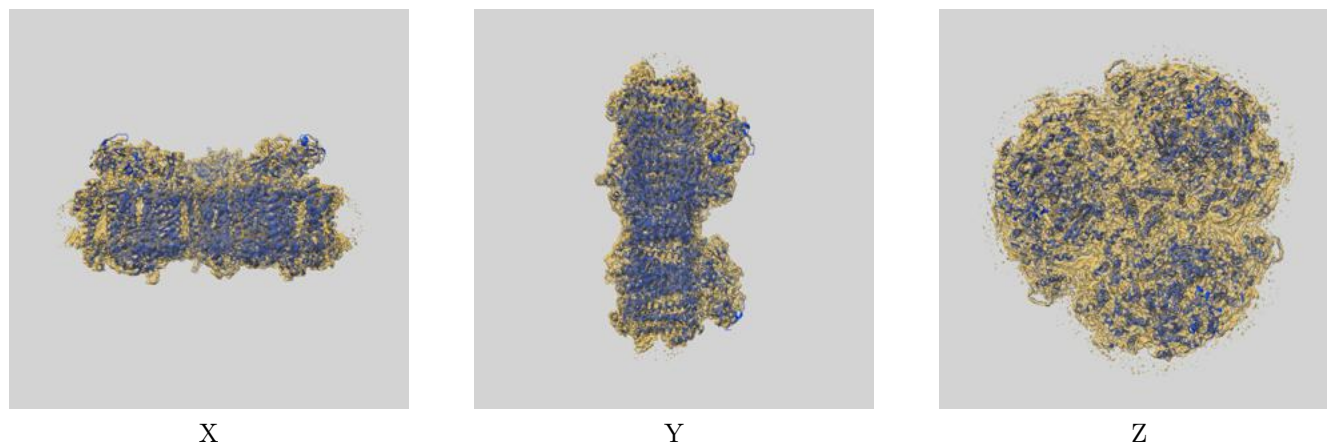
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 1.97                               | -    | -        |
| Author-provided FSC curve | 1.96                               | 2.18 | 1.98     |
| Unmasked-calculated*      | 2.14                               | 2.56 | 2.17     |

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

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

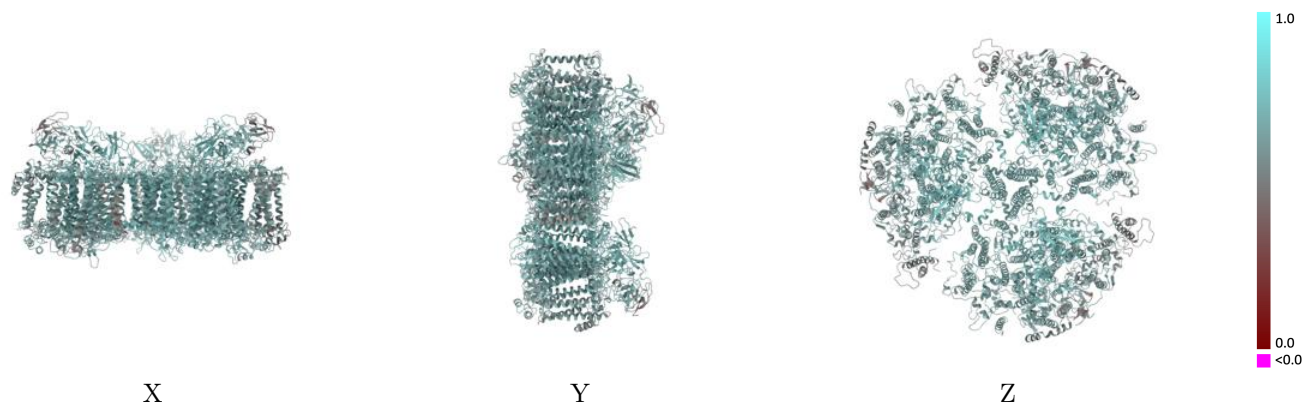
This section contains information regarding the fit between EMDB map EMD-31605 and PDB model 7FIX. Per-residue inclusion information can be found in section 3 on page 42.

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



The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



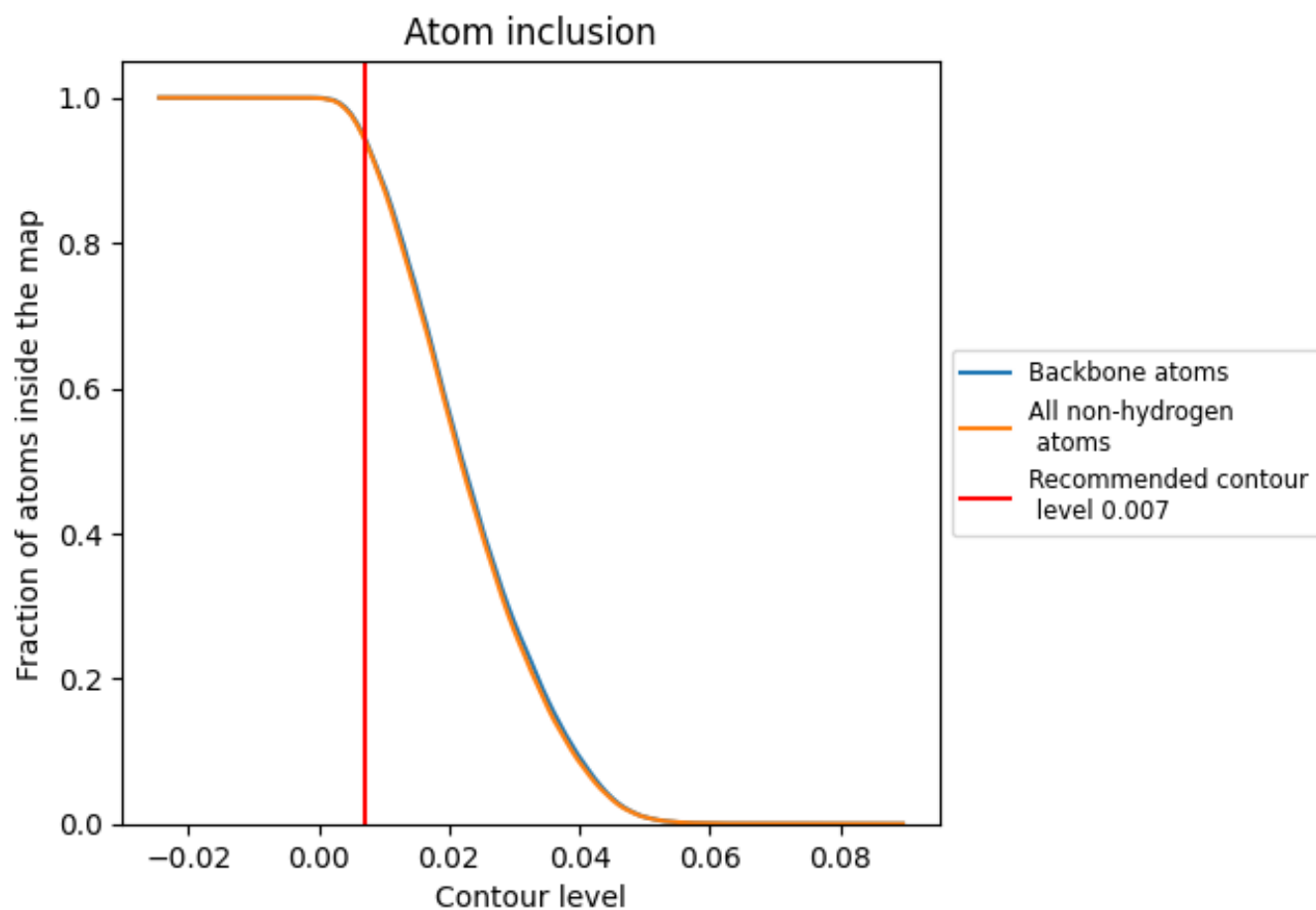
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.007) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9433   |  0.6510   |
| A1    |  0.9626   |  0.6500   |
| A2    |  0.9633   |  0.6500   |
| A3    |  0.9629   |  0.6480   |
| B1    |  0.9765   |  0.6710   |
| B2    |  0.9769   |  0.6700   |
| B3    |  0.9764   |  0.6690   |
| C1    |  0.9883   |  0.7040   |
| C2    |  0.9867   |  0.7030   |
| C3    |  0.9867   |  0.7030   |
| D1    |  0.9551   |  0.6810   |
| D2    |  0.9532   |  0.6810   |
| D3    |  0.9532   |  0.6800   |
| E1    |  0.9519   |  0.6450   |
| E2    |  0.9558  |  0.6500  |
| E3    |  0.9596 |  0.6450 |
| F1    |  0.9015 |  0.5810 |
| F2    |  0.8930 |  0.5760 |
| F3    |  0.9006 |  0.5770 |
| I1    |  0.9820 |  0.7090 |
| I2    |  0.9880 |  0.7080 |
| I3    |  0.9880 |  0.7050 |
| J1    |  0.9119 |  0.5770 |
| J2    |  0.9188 |  0.5750 |
| J3    |  0.9102 |  0.5750 |
| K1    |  0.8387 |  0.4810 |
| K2    |  0.8404 |  0.4870 |
| K3    |  0.8316 |  0.4860 |
| L1    |  0.9769 |  0.7110 |
| L2    |  0.9784 |  0.7100 |
| L3    |  0.9799 |  0.7100 |
| M1    |  0.9676 |  0.6650 |
| M2    |  0.9676 |  0.6660 |
| M3    |  0.9676 |  0.6620 |
| R1    |  0.3868 |  0.5300 |



*Continued on next page...*

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| R2    |  0.4016 |  0.5250 |
| R3    |  0.4016 |  0.5250 |
| X1    |  0.9259 |  0.5940 |
| X2    |  0.9125 |  0.5900 |
| X3    |  0.9293 |  0.5910 |