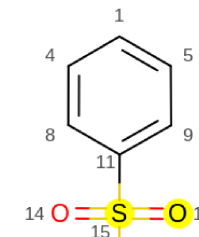
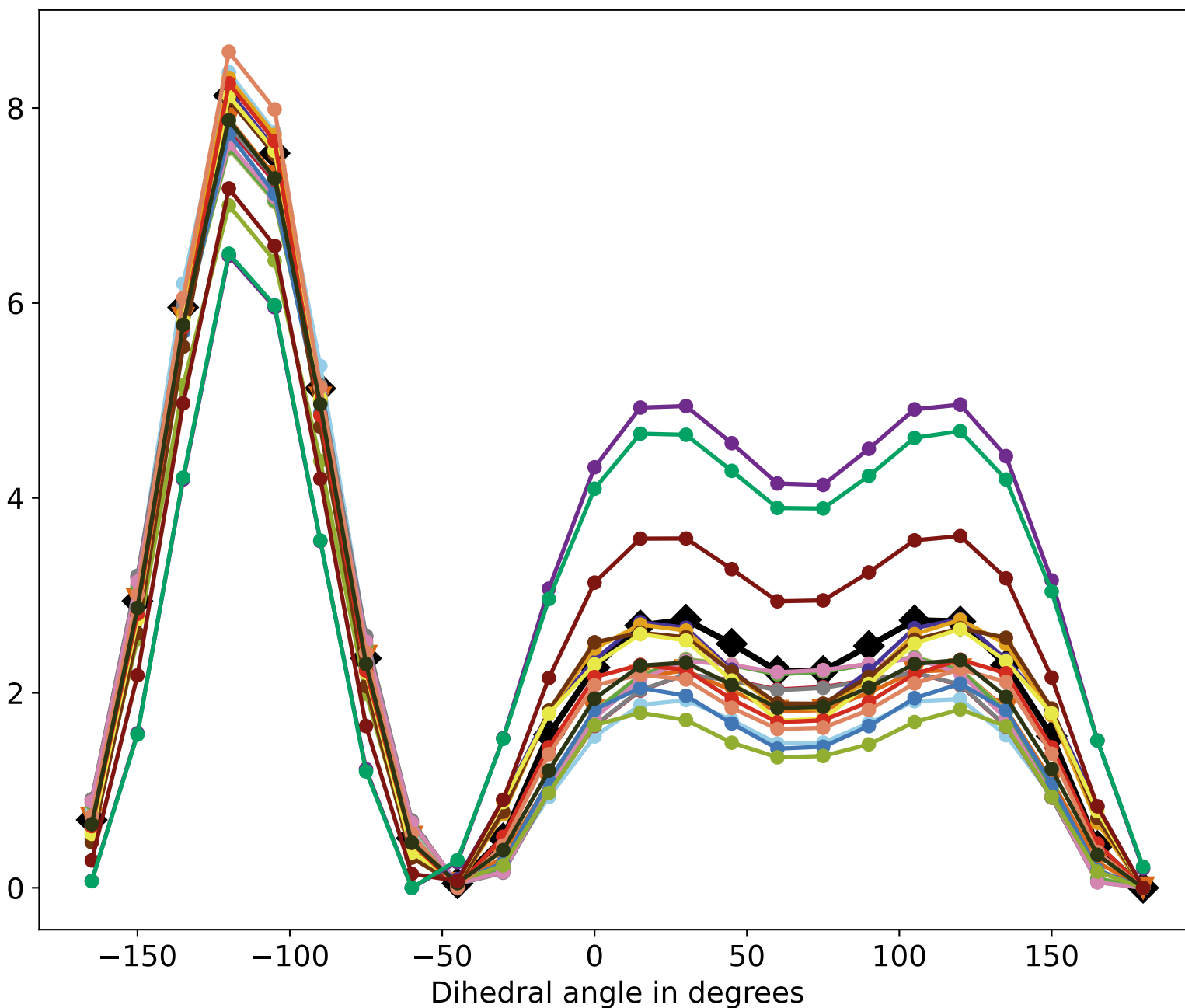


- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ

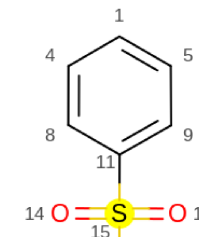
Relative energies in kcal/mol



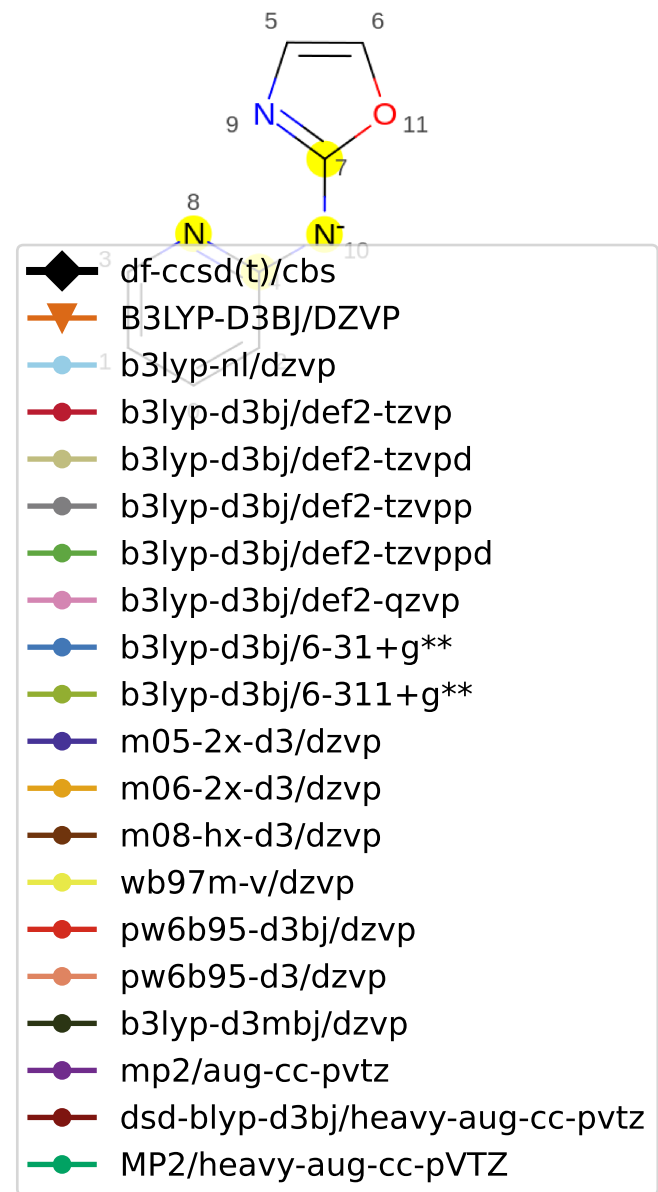
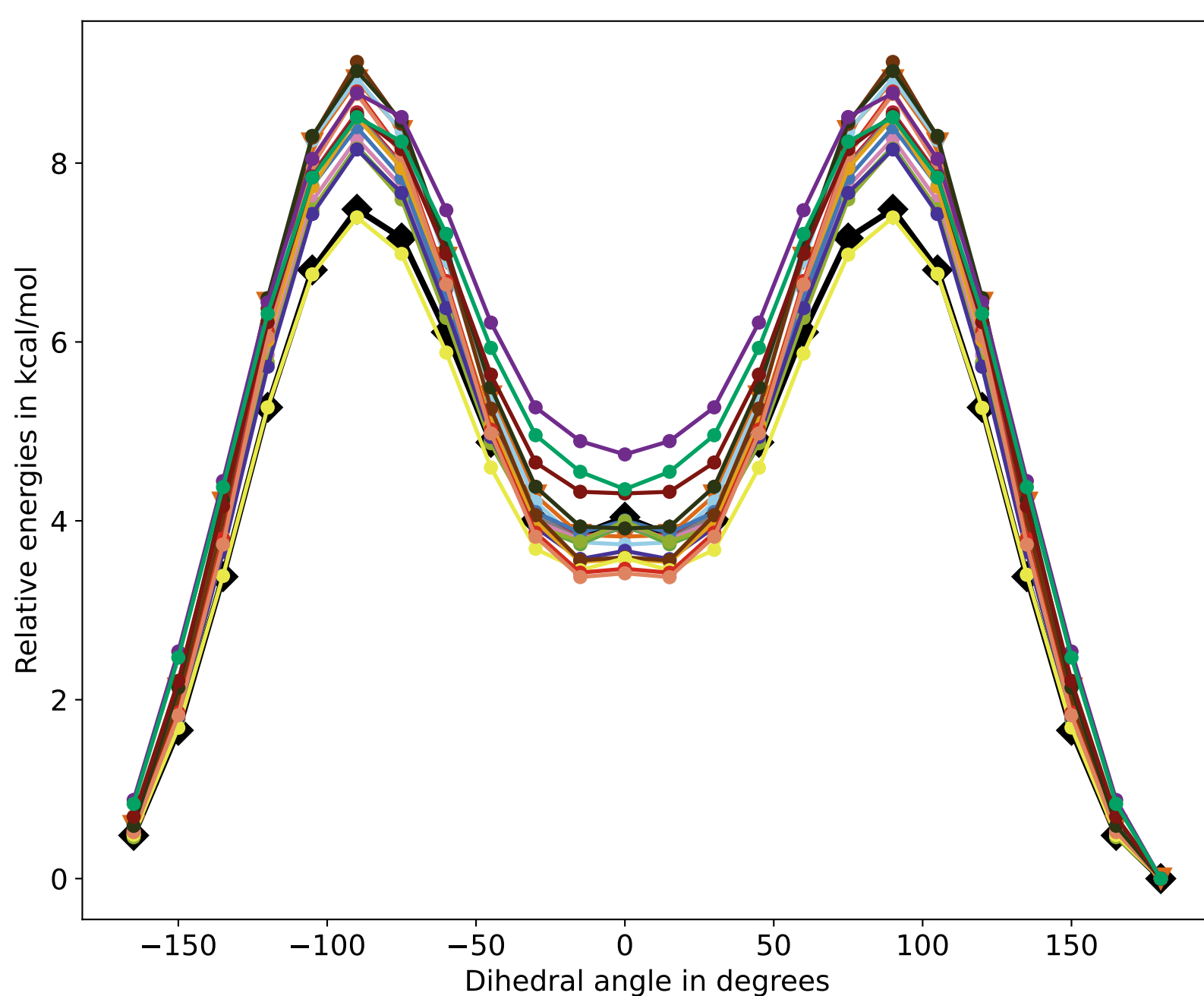
- df-ccsd(t)/cbs
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- b3lyp-nl/dzvp
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- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
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- MP2/heavy-aug-cc-pVTZ

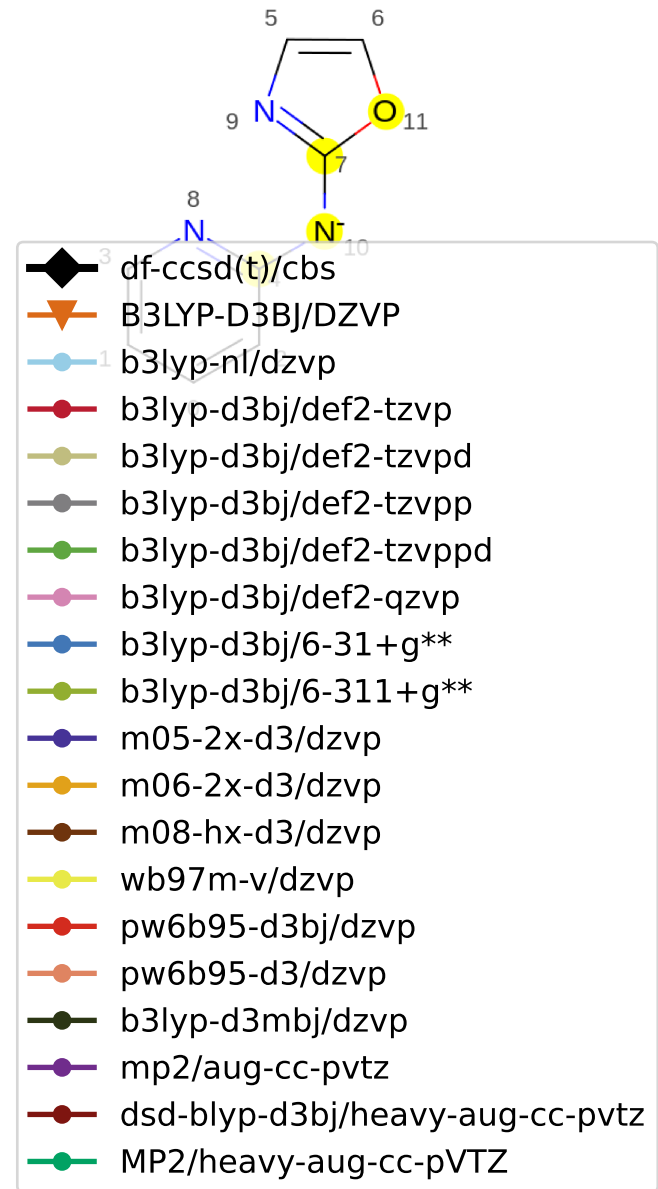
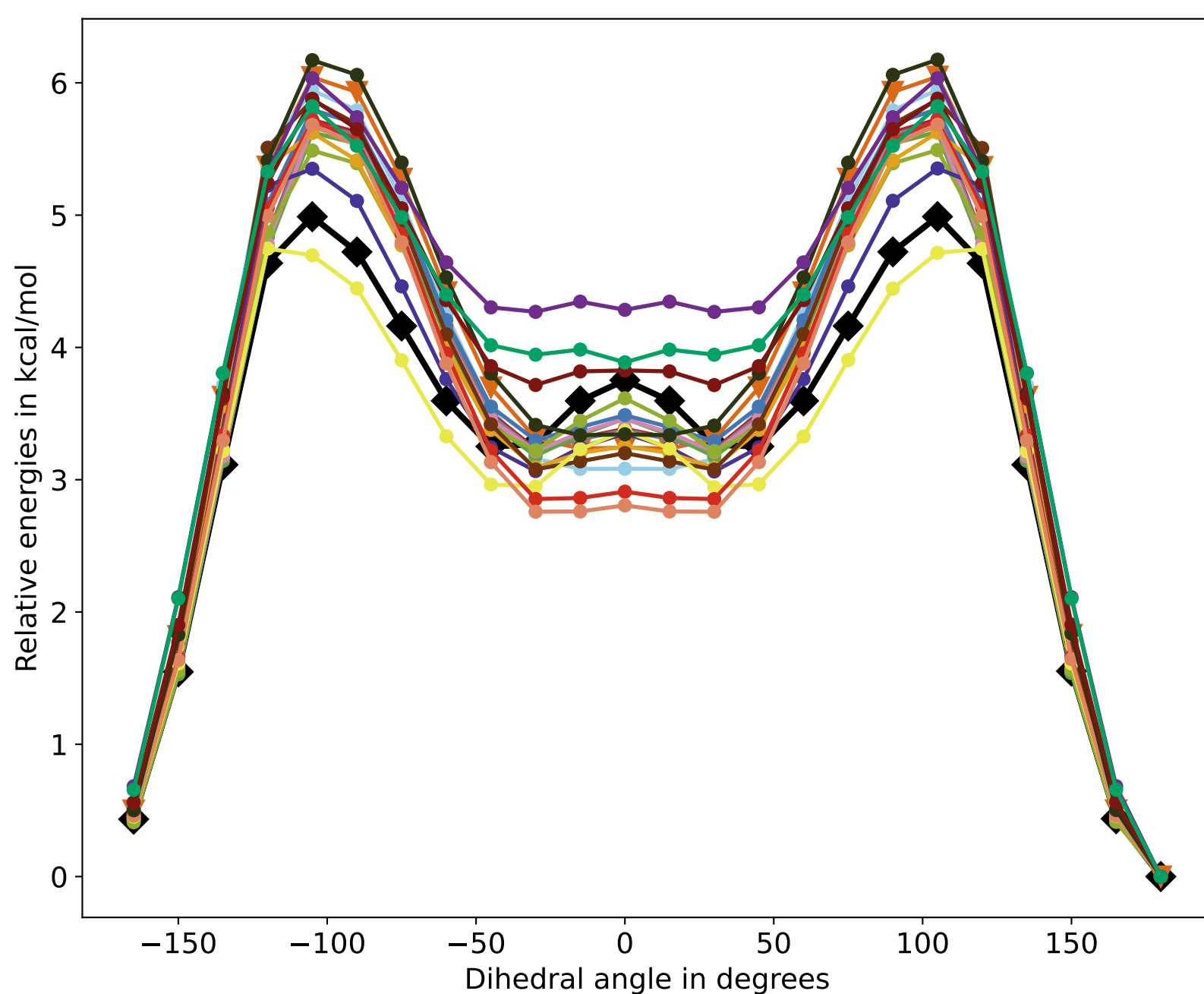
Relative energies in kcal/mol

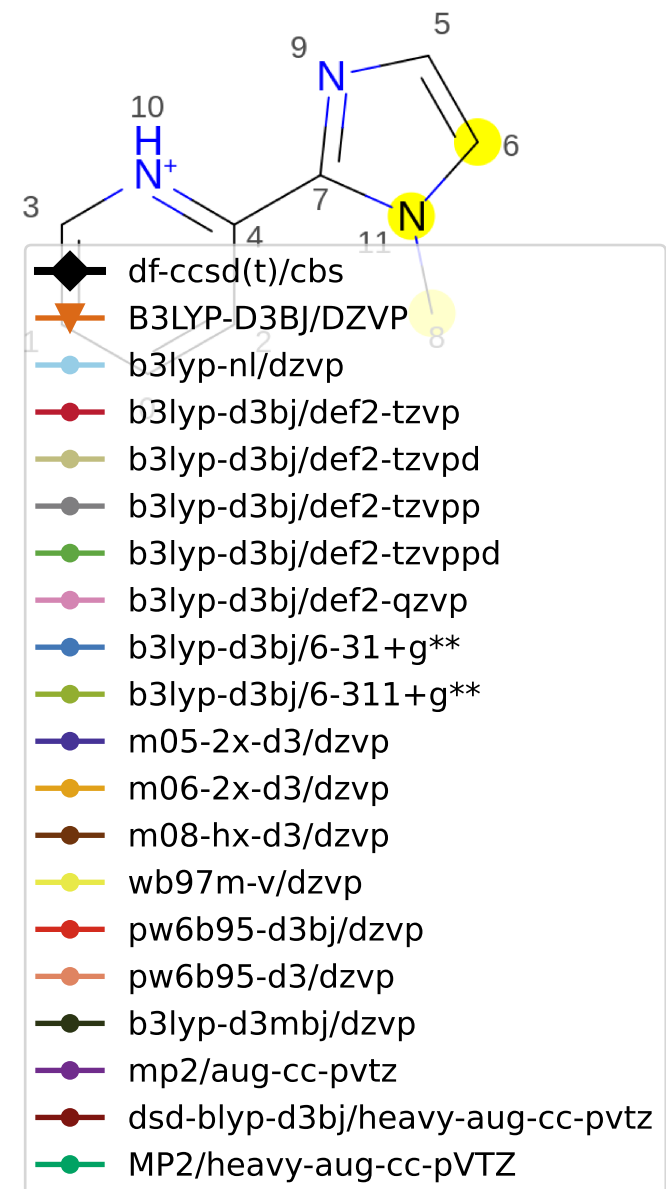
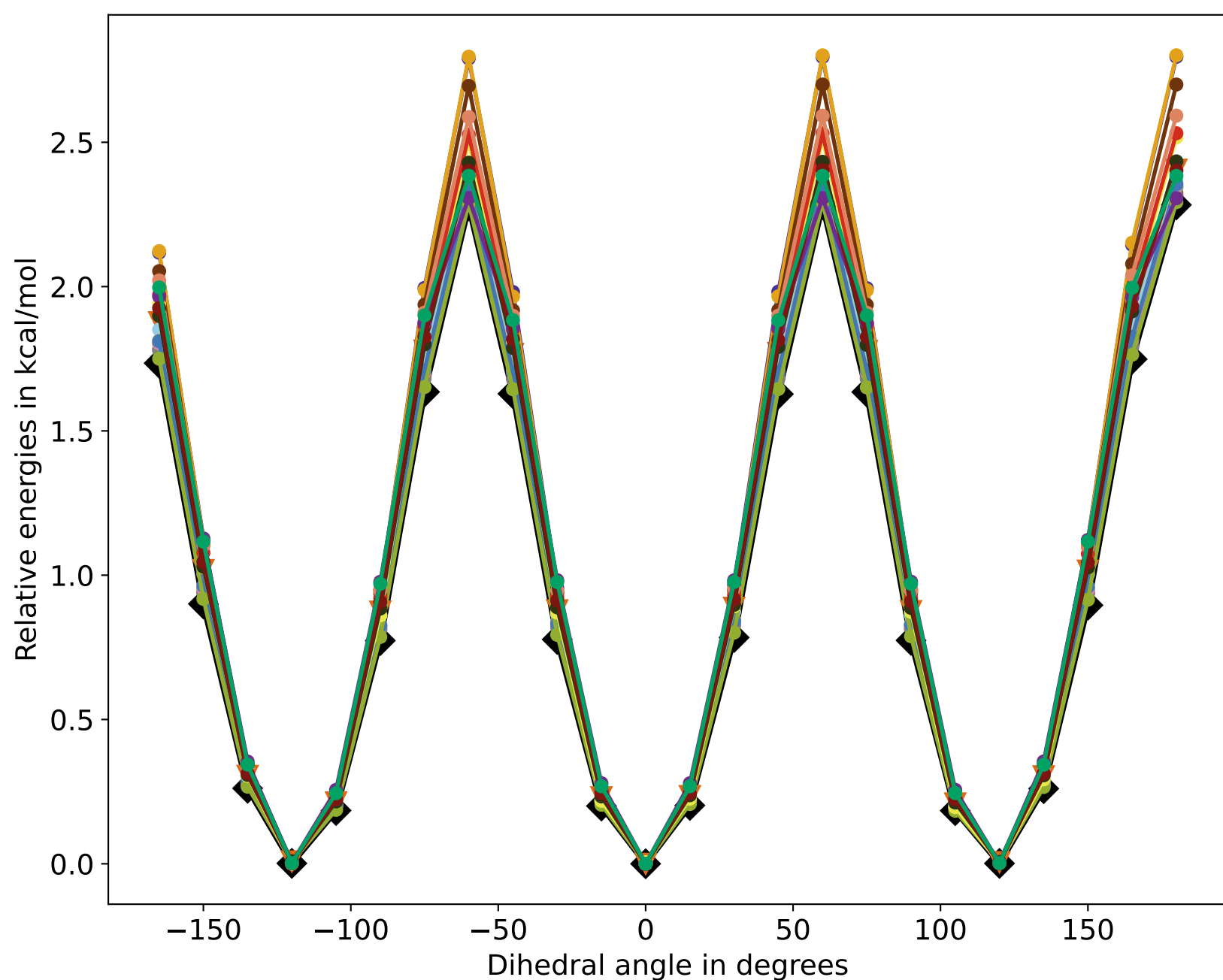
Dihedral angle in degrees

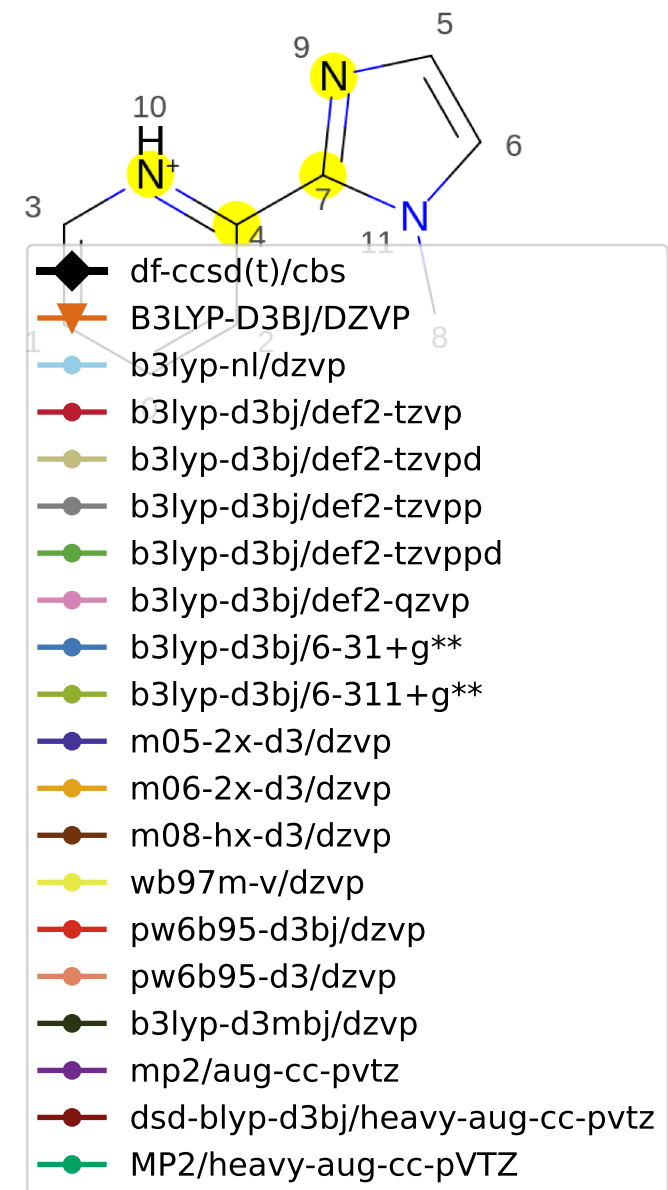
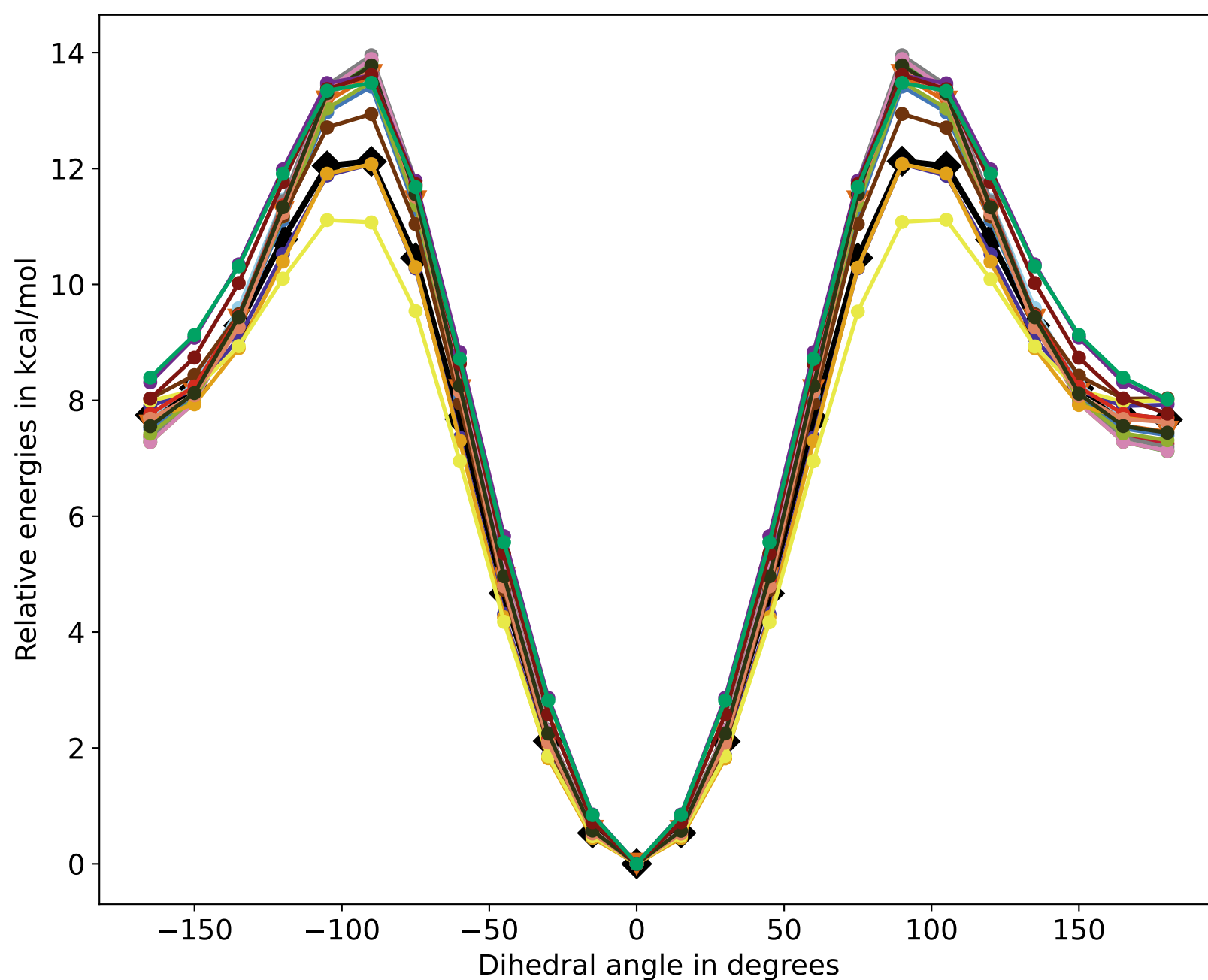


- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ

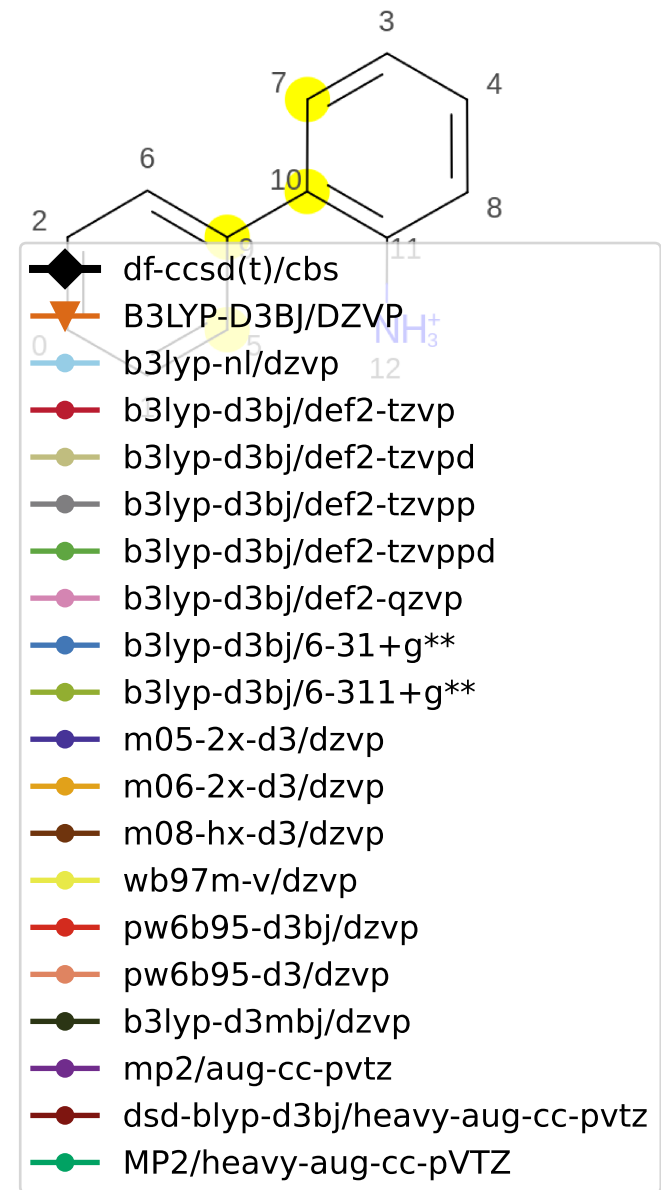
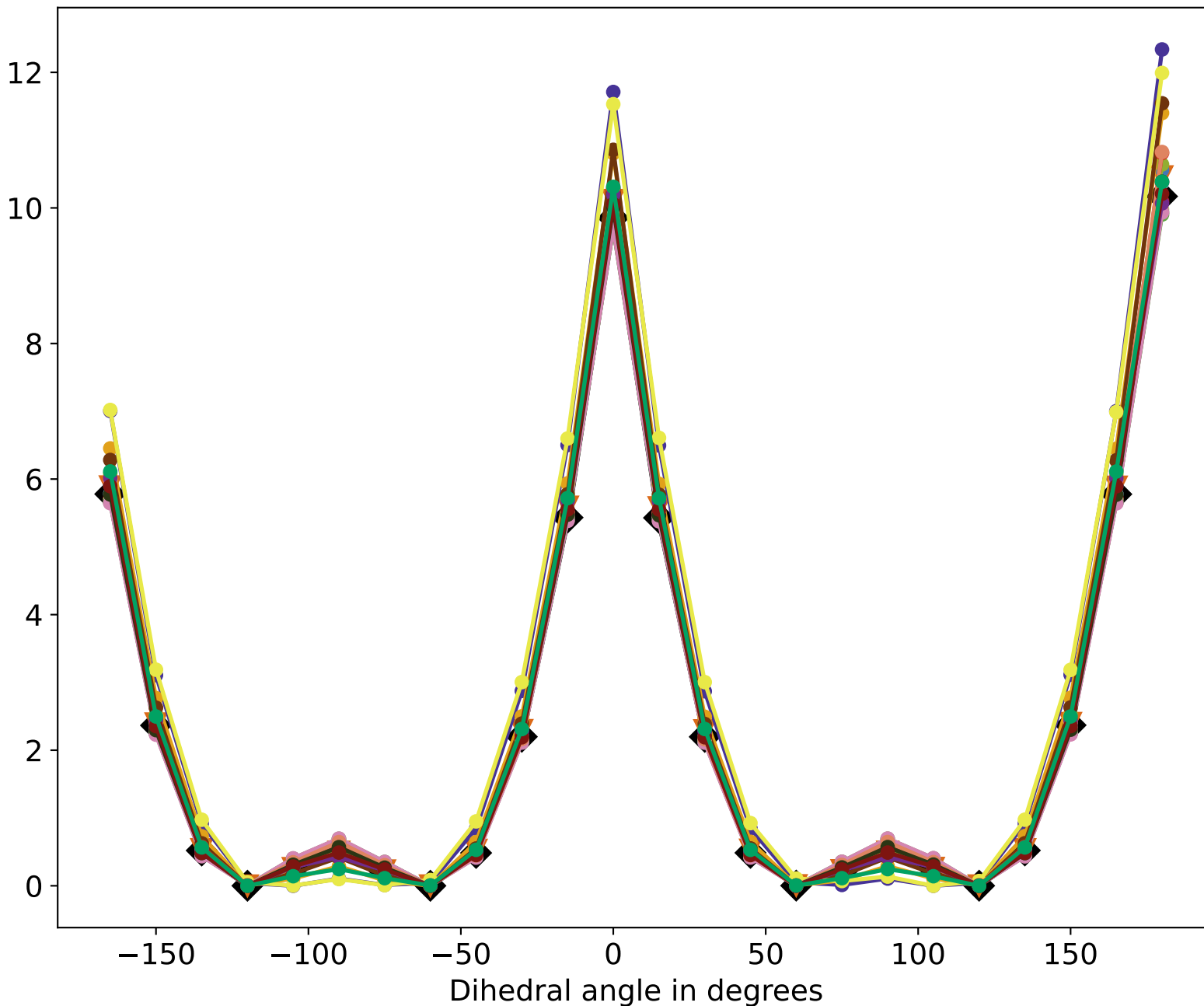


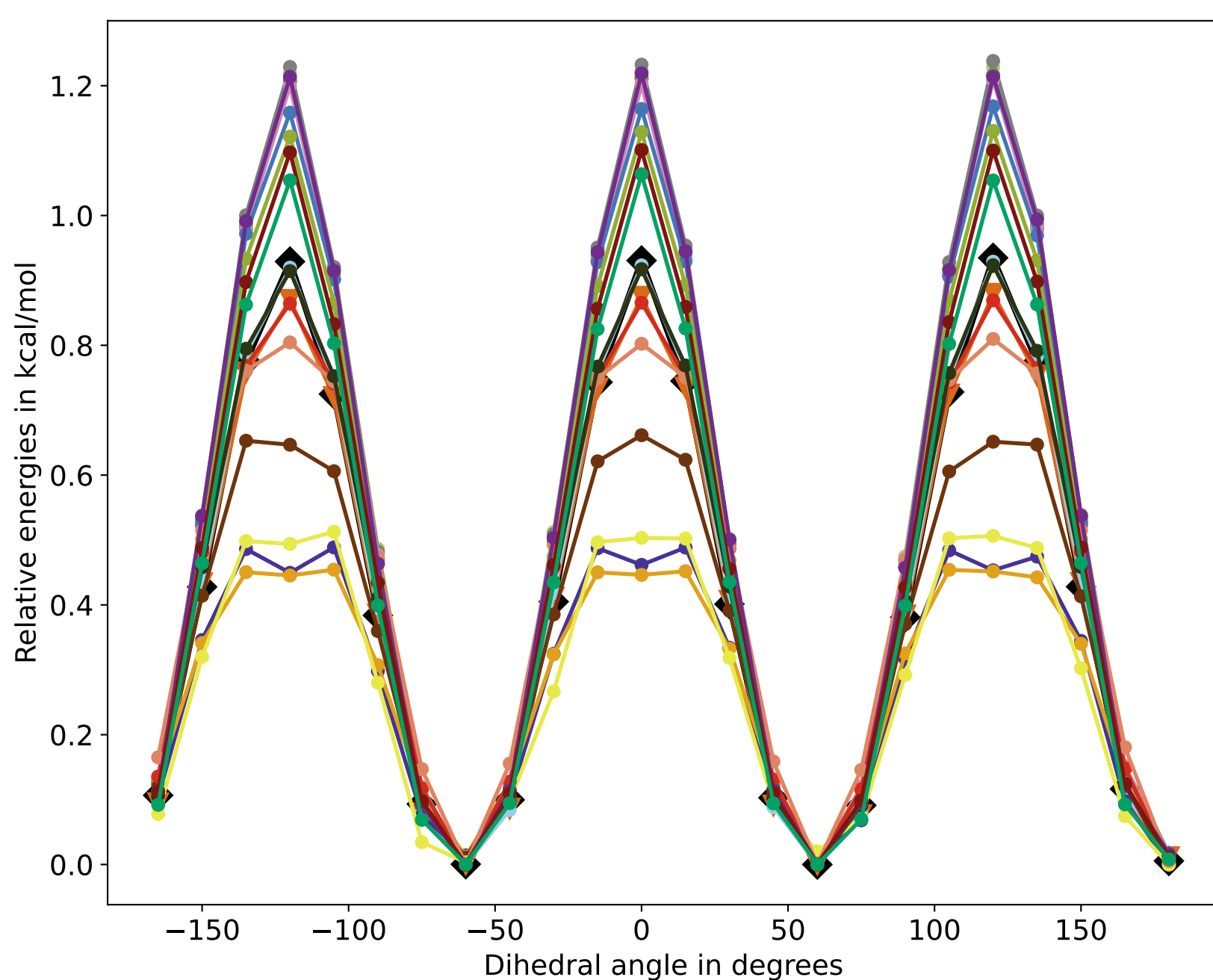


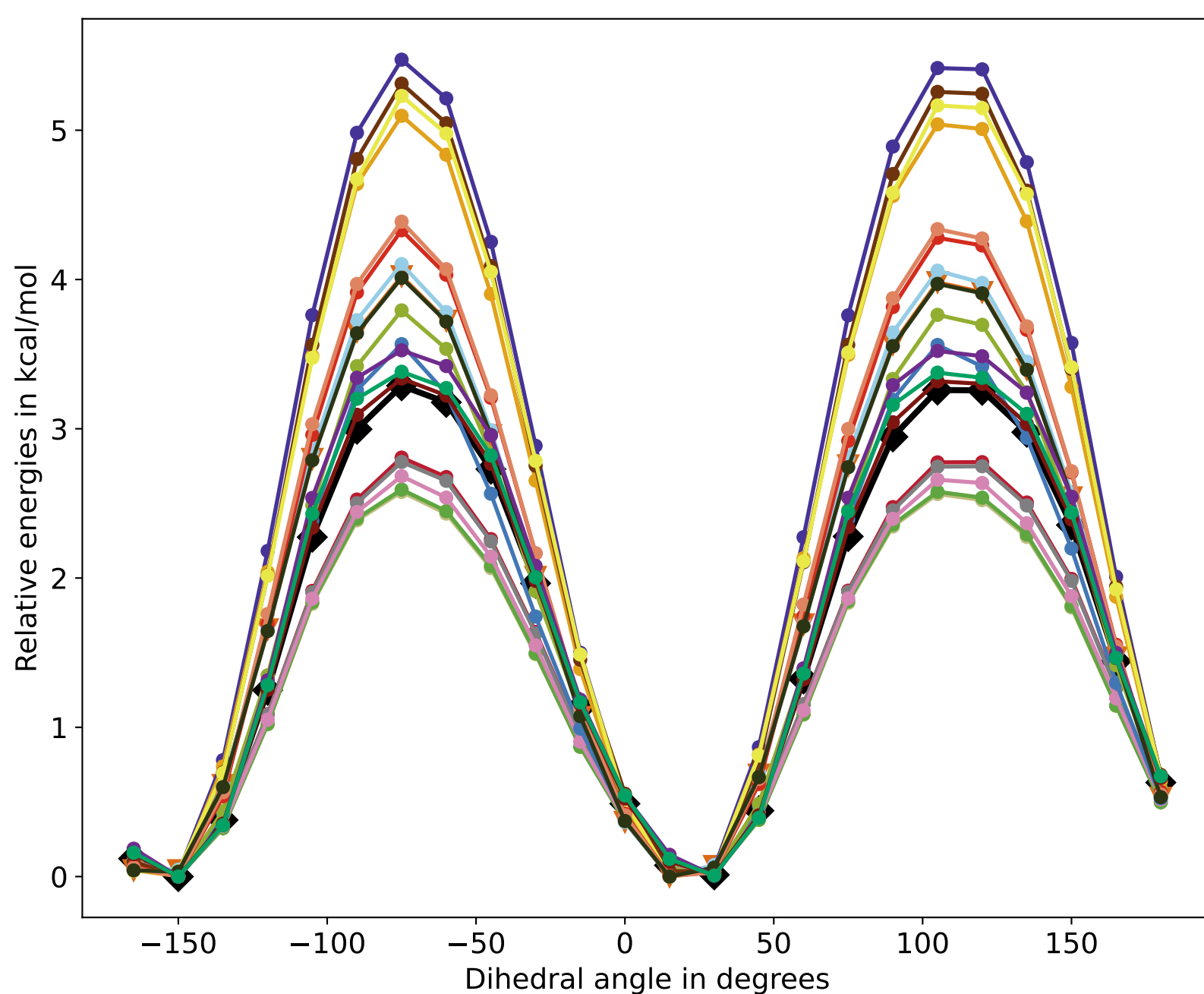


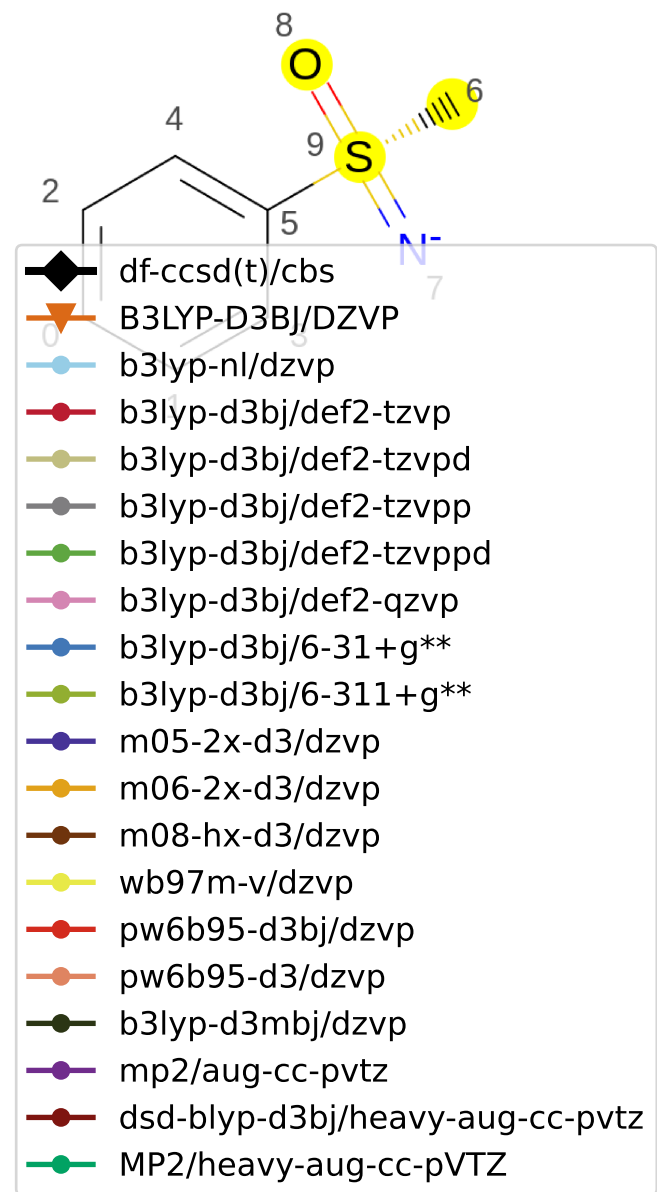
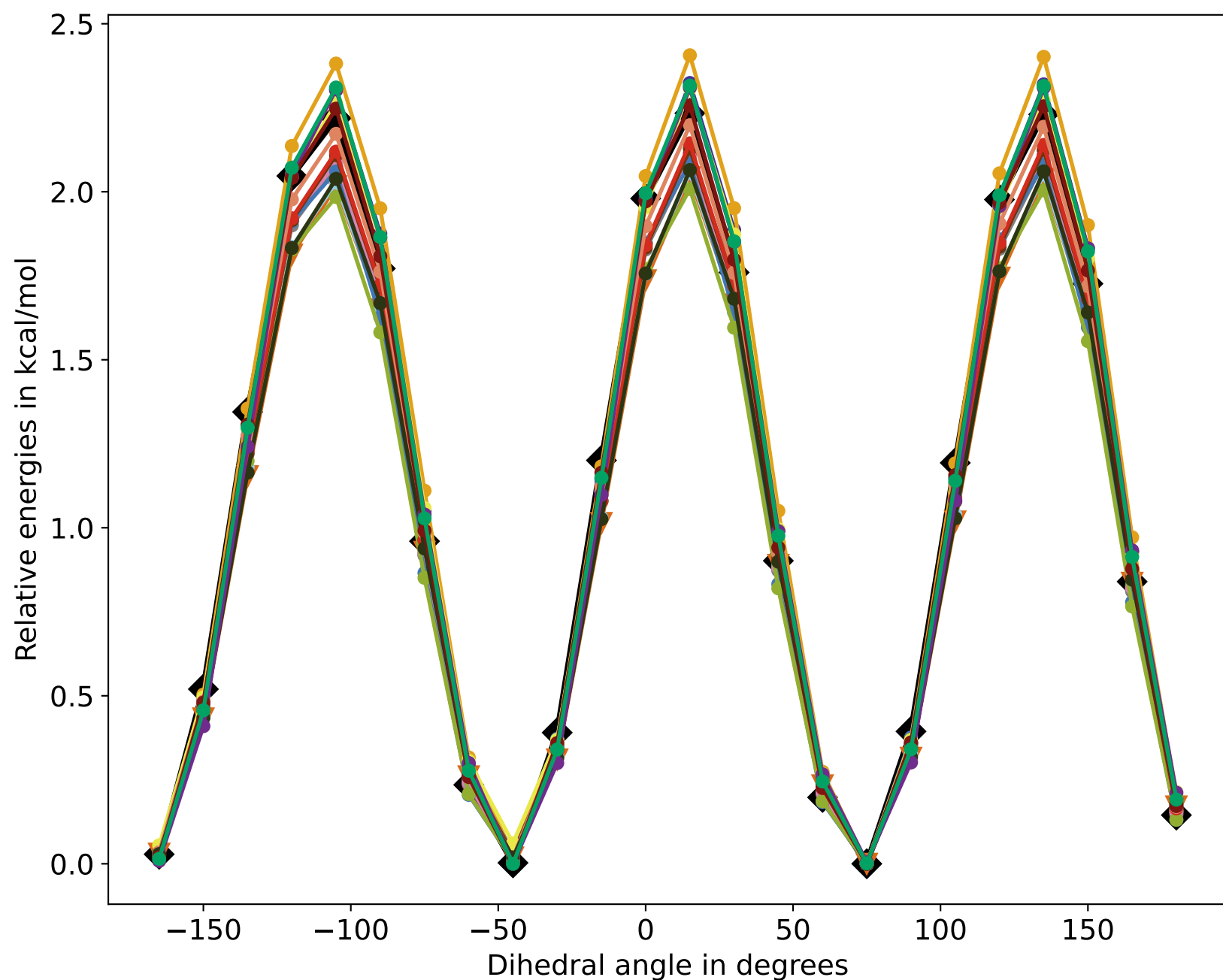


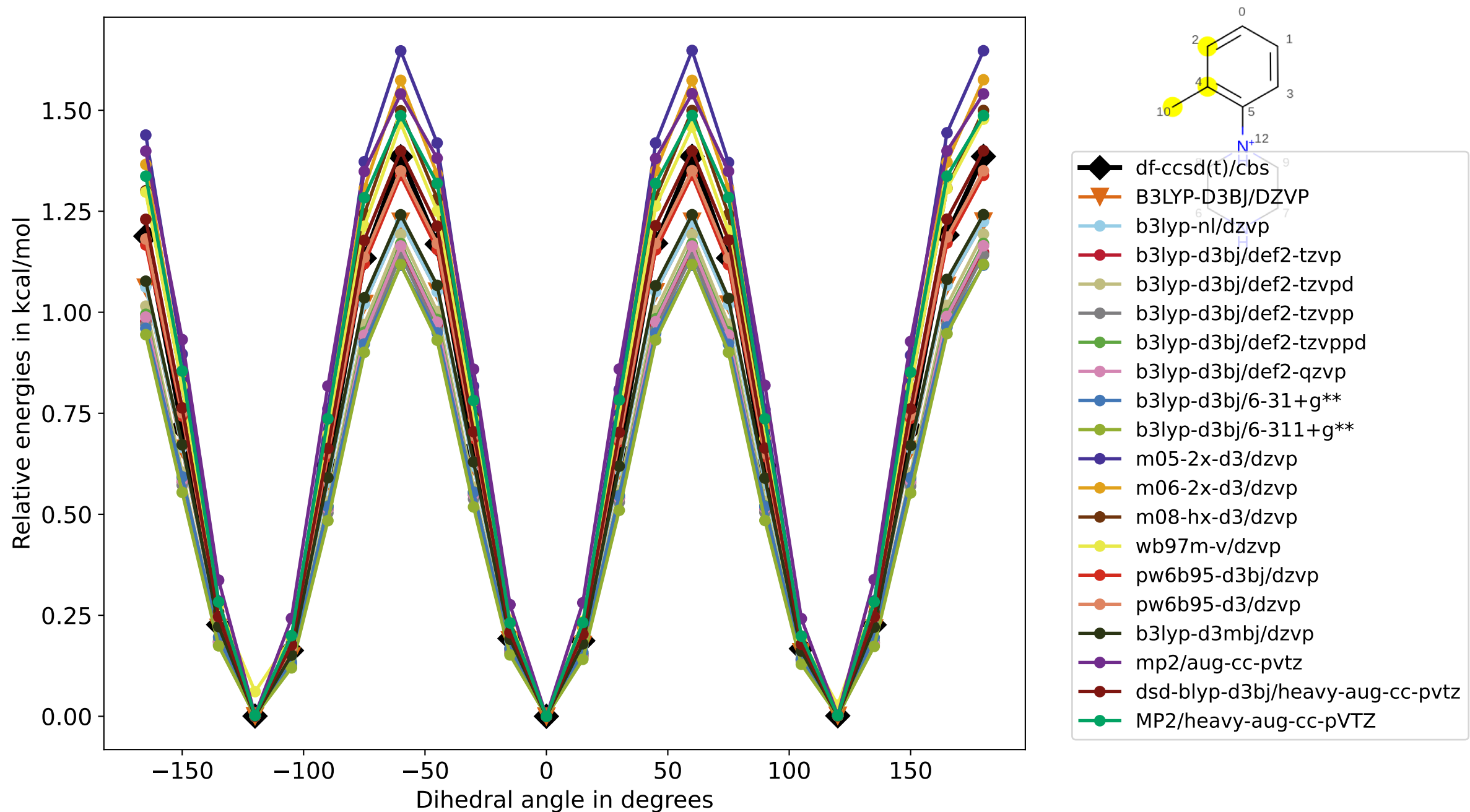
Relative energies in kcal/mol

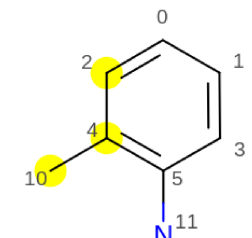
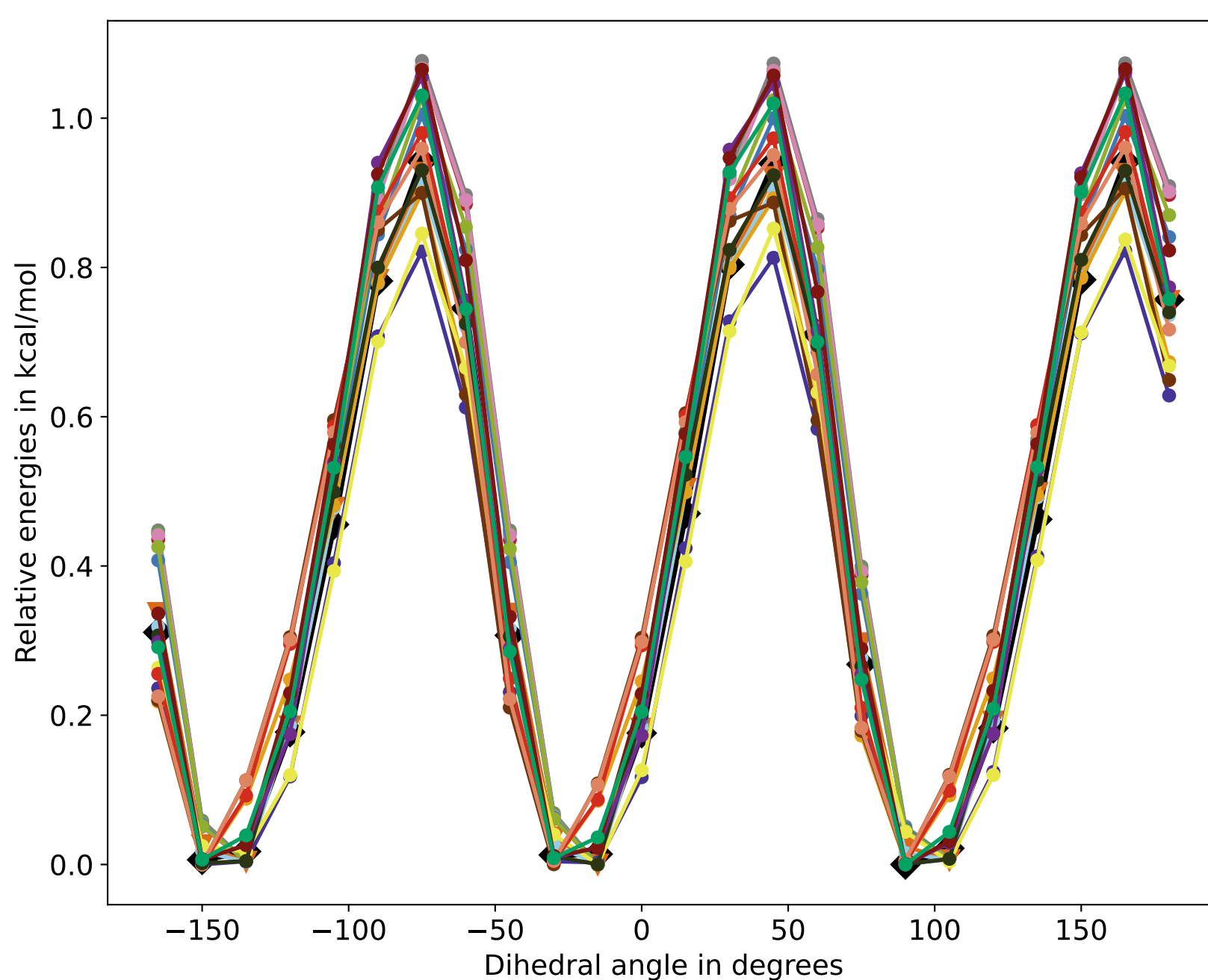




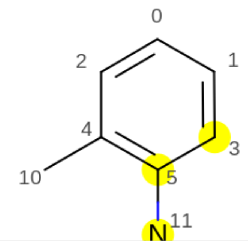
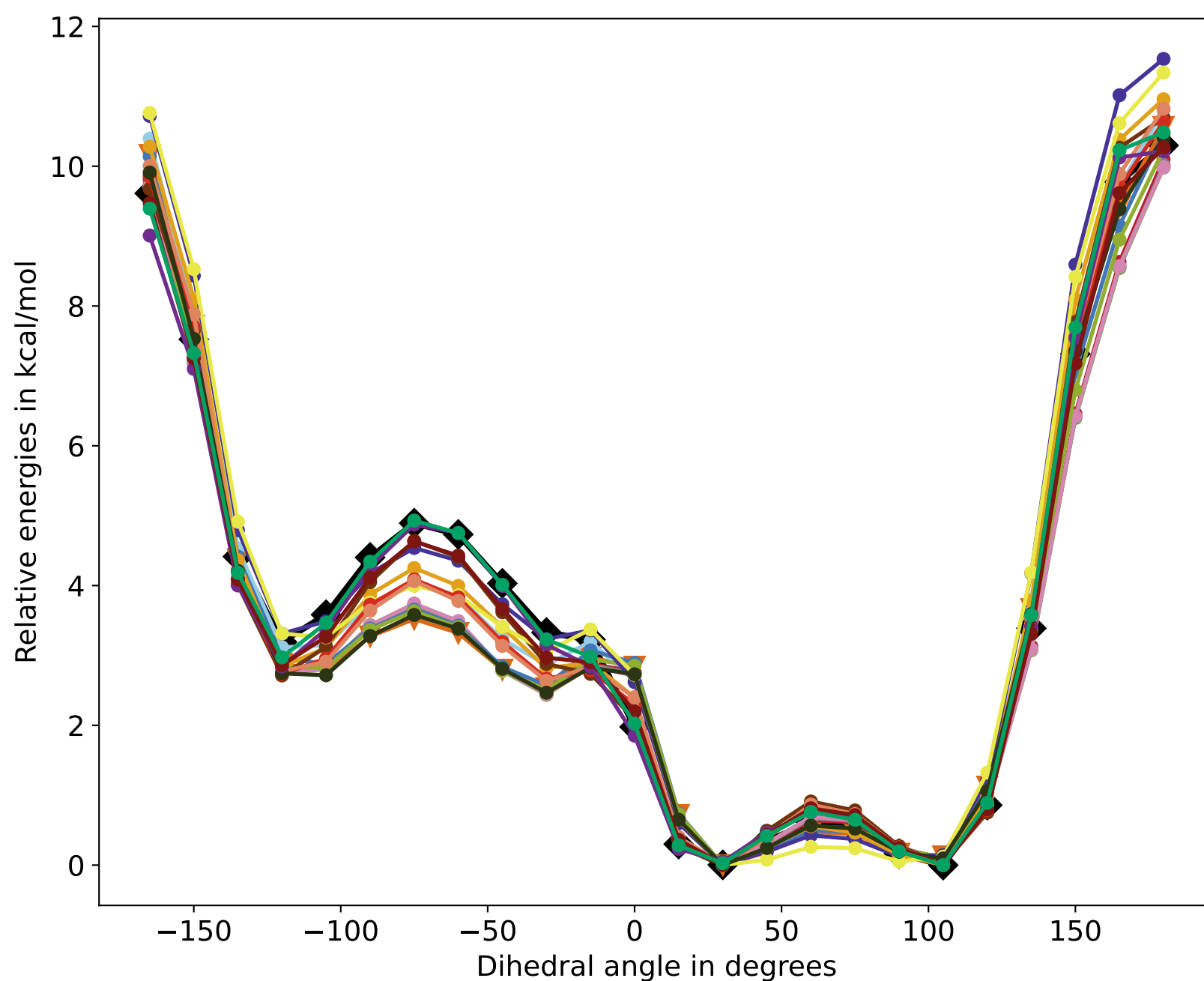




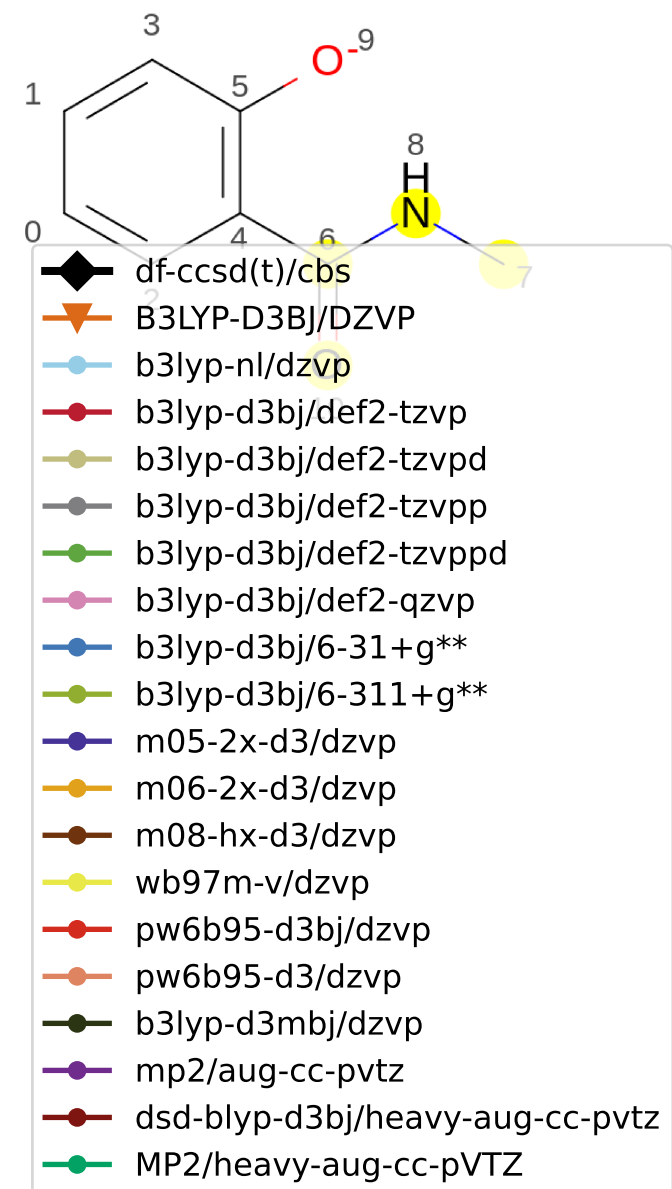
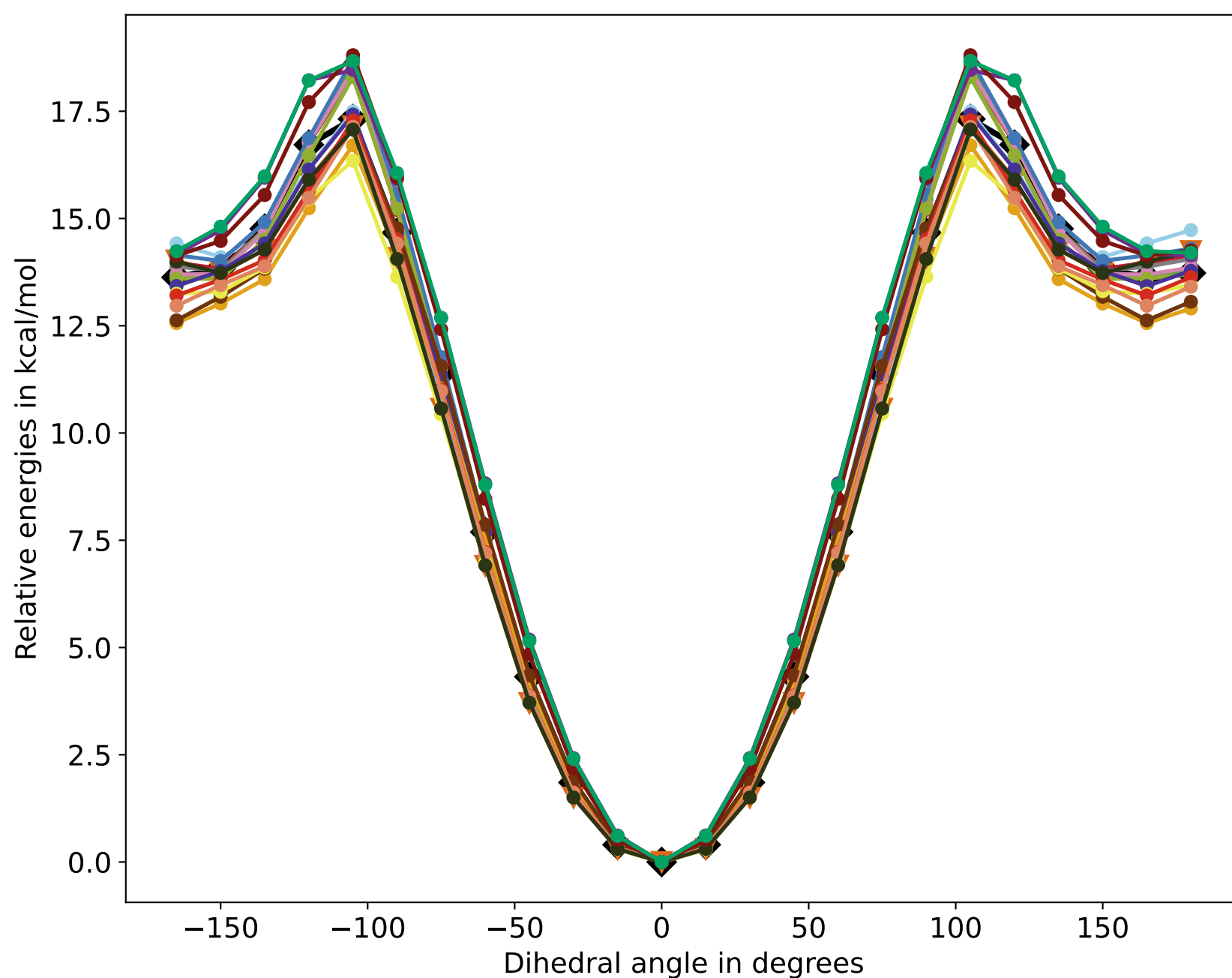


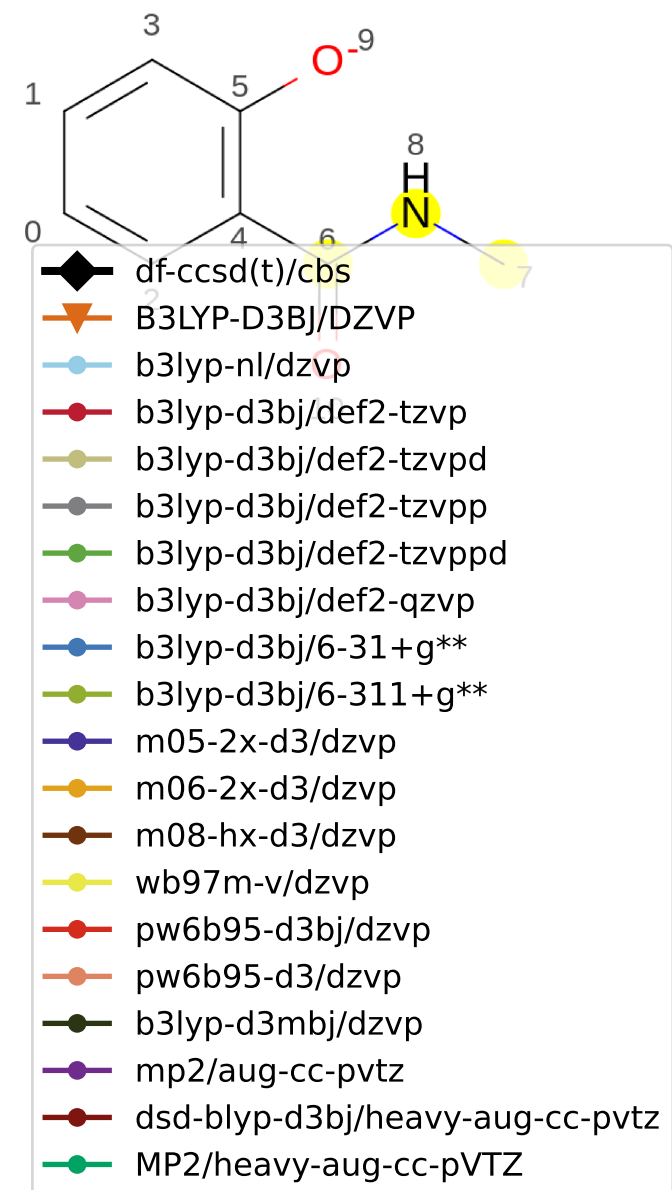
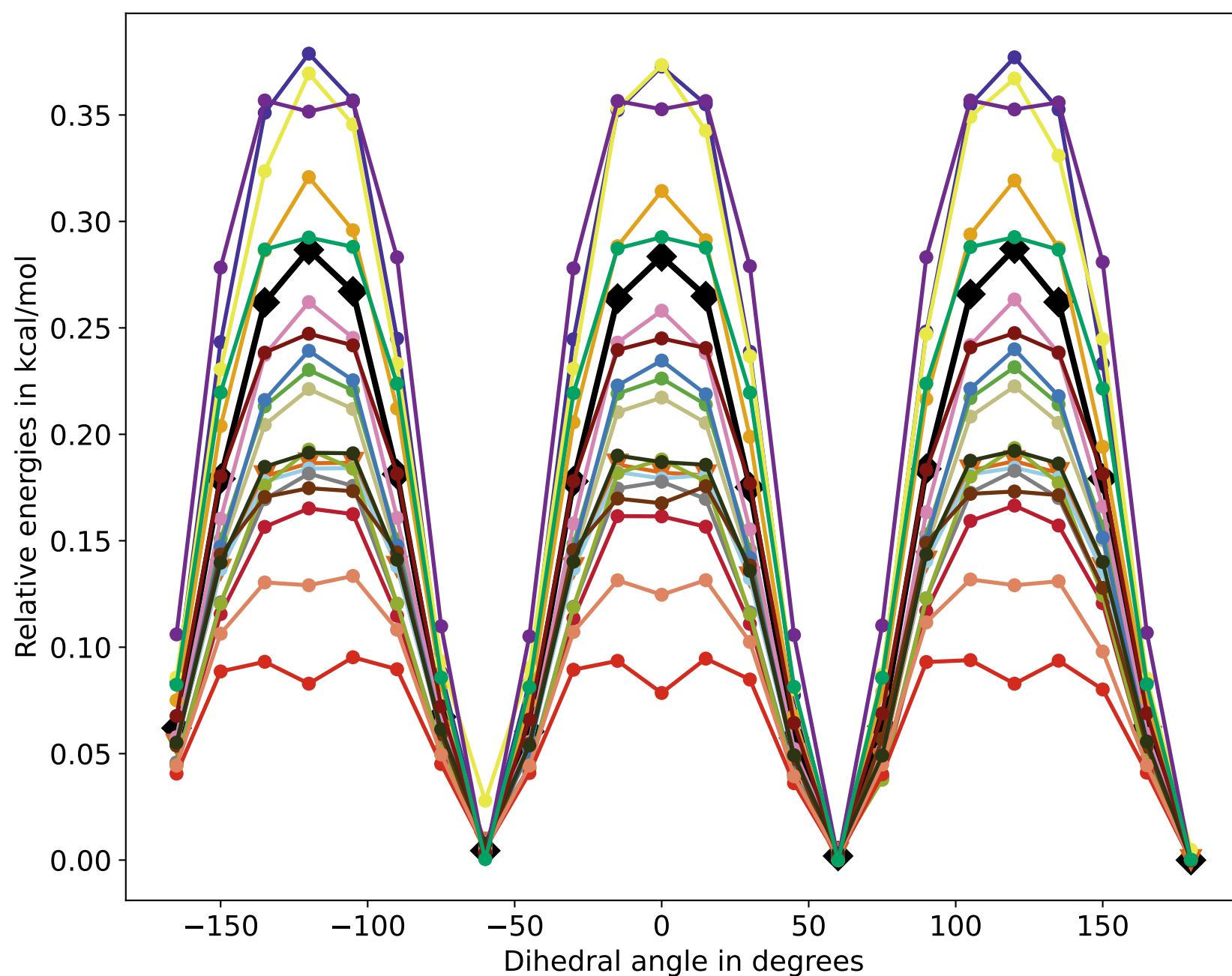


- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ

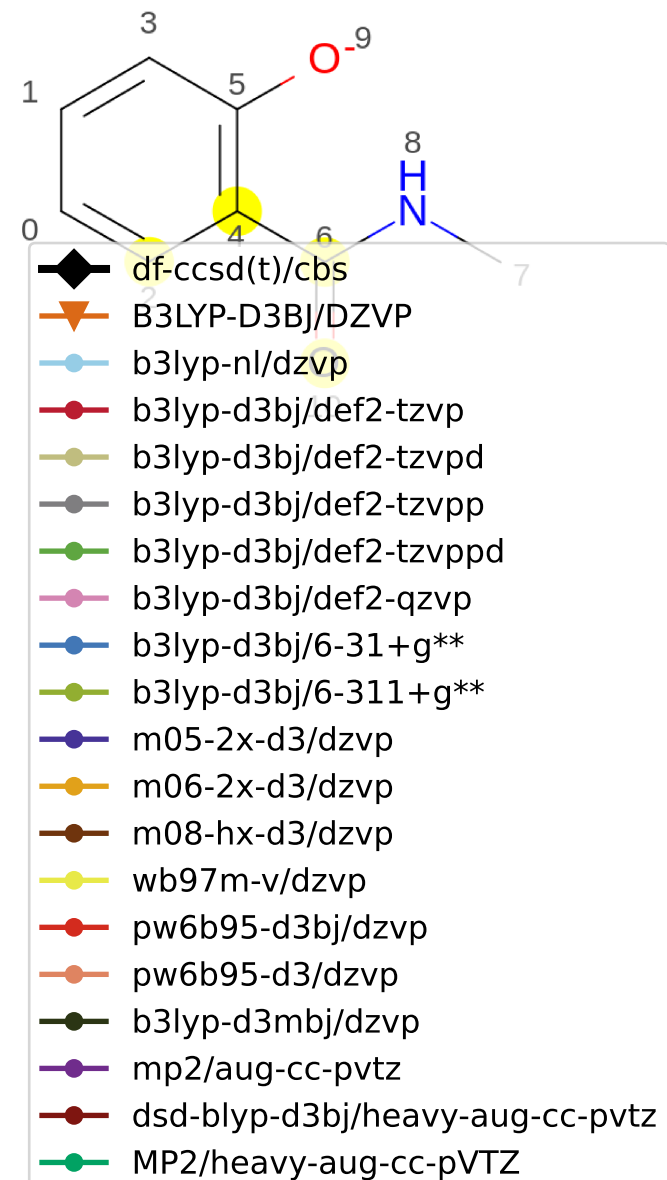
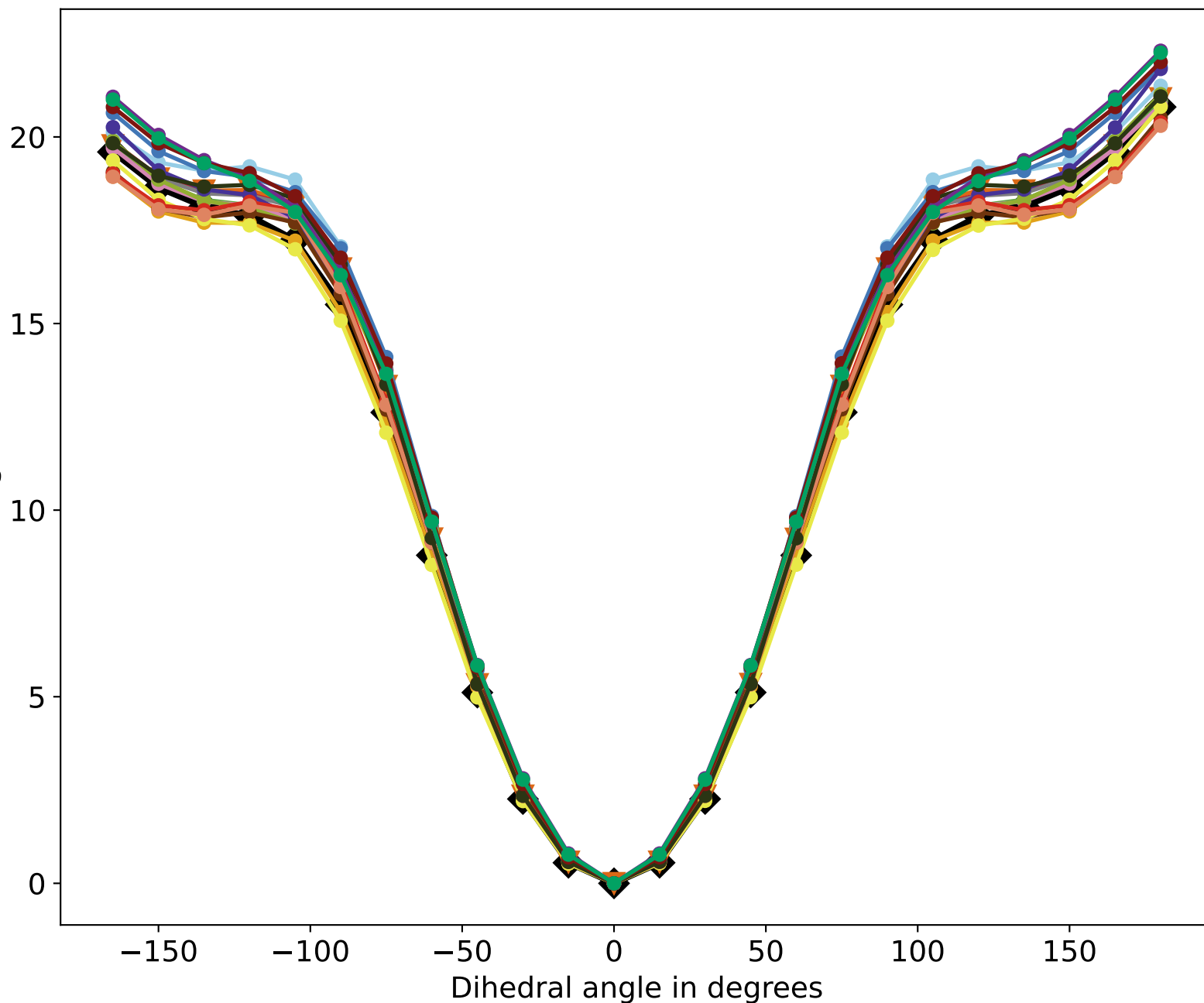


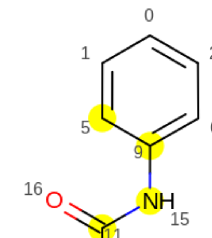
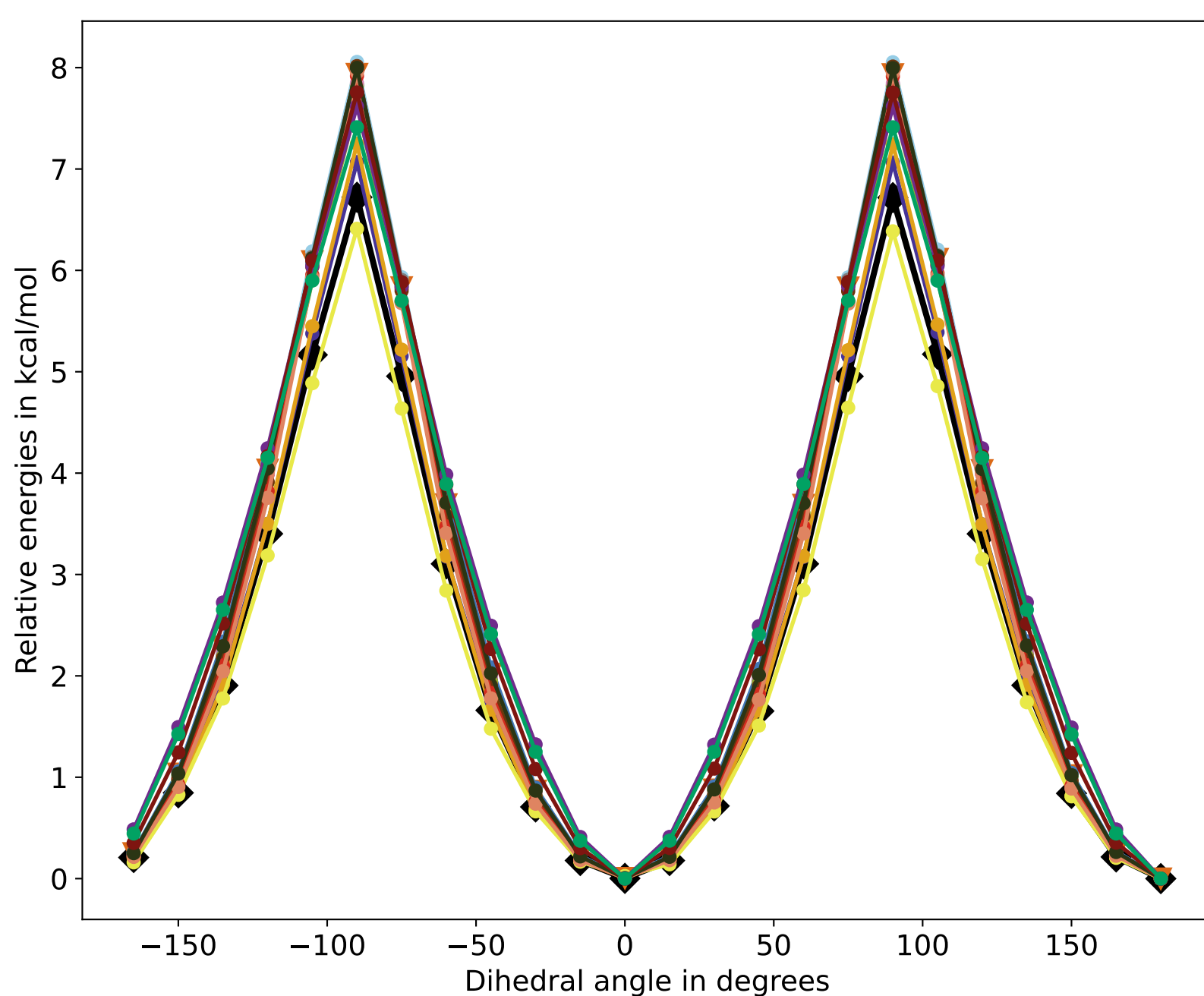
- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
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- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
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- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ



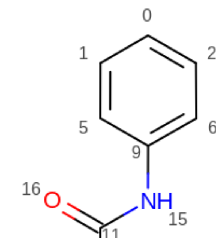
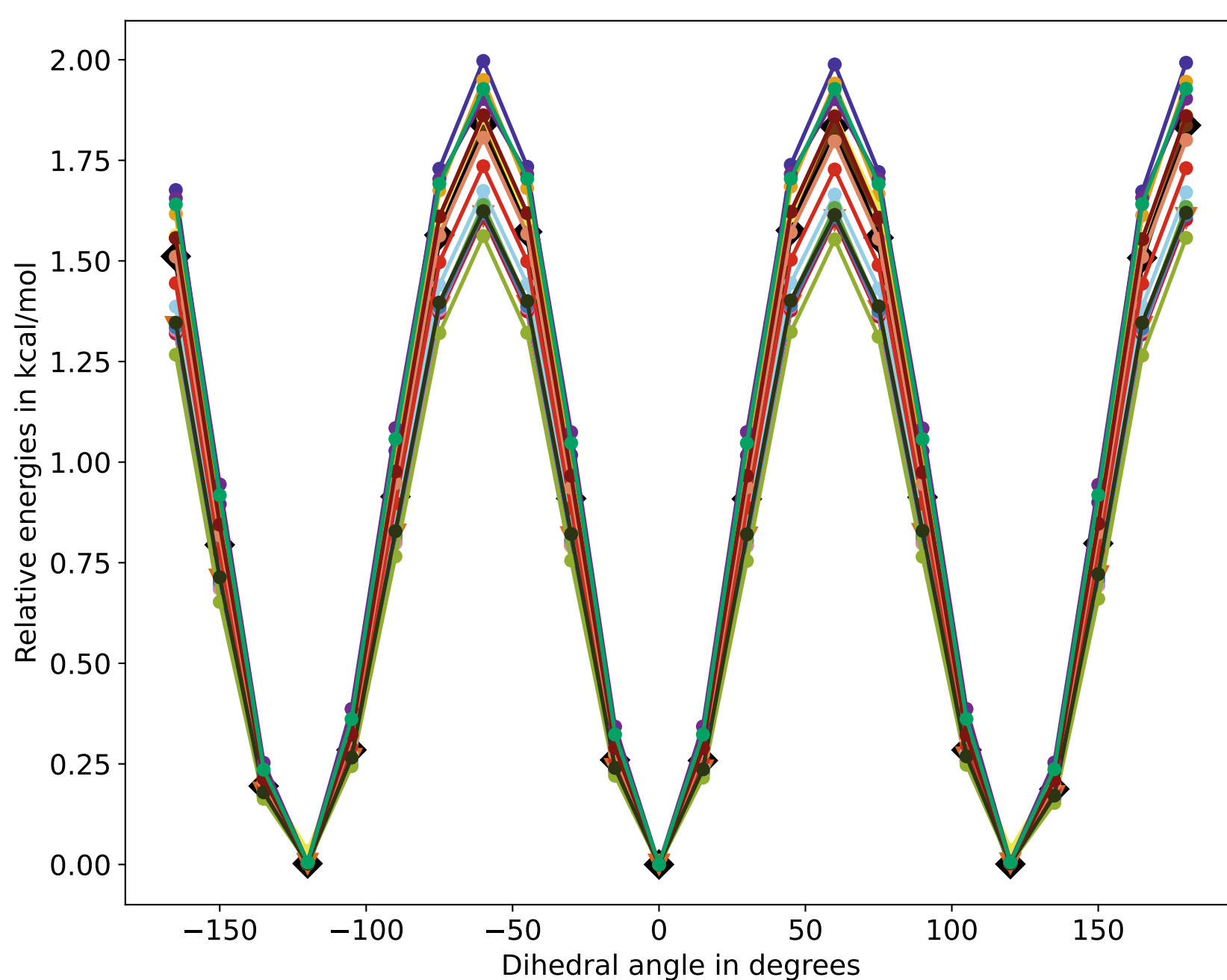


Relative energies in kcal/mol



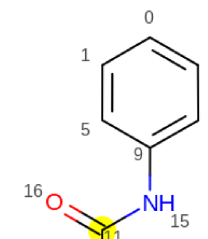
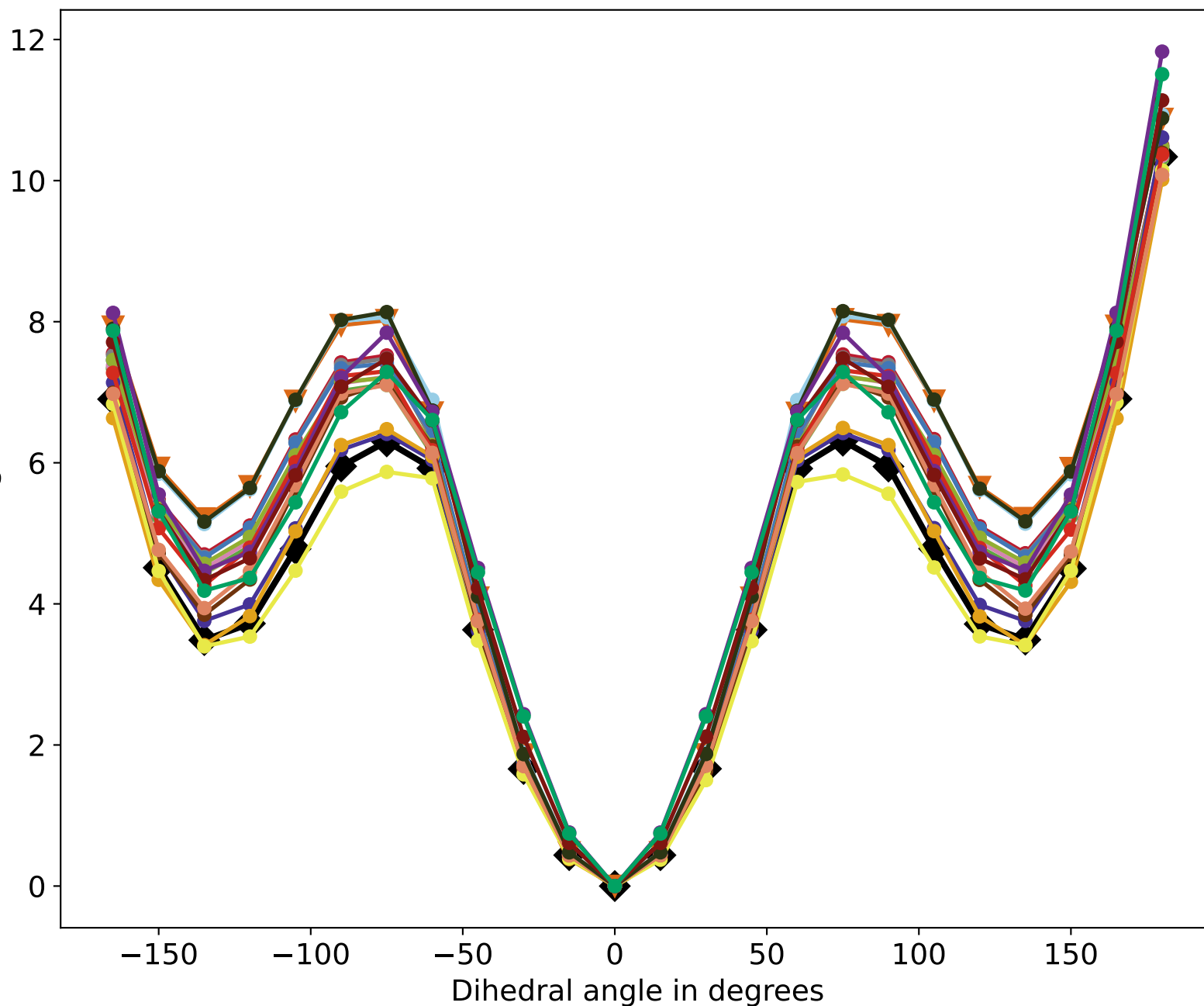


- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
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- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ



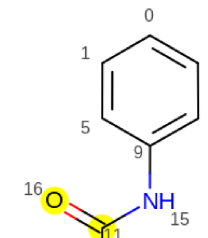
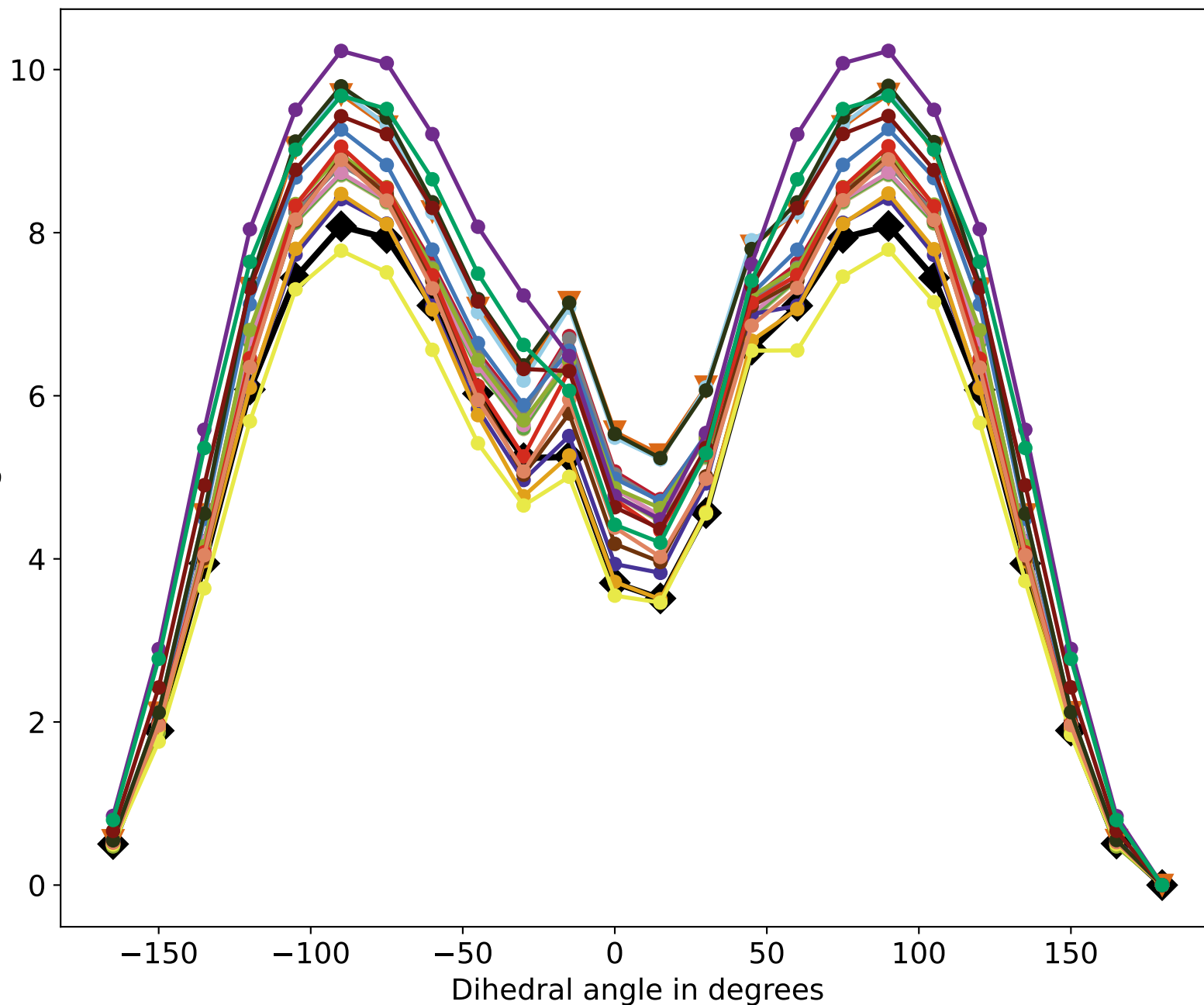
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- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
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- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
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- MP2/heavy-aug-cc-pVTZ

Relative energies in kcal/mol



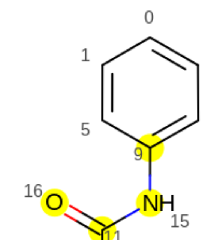
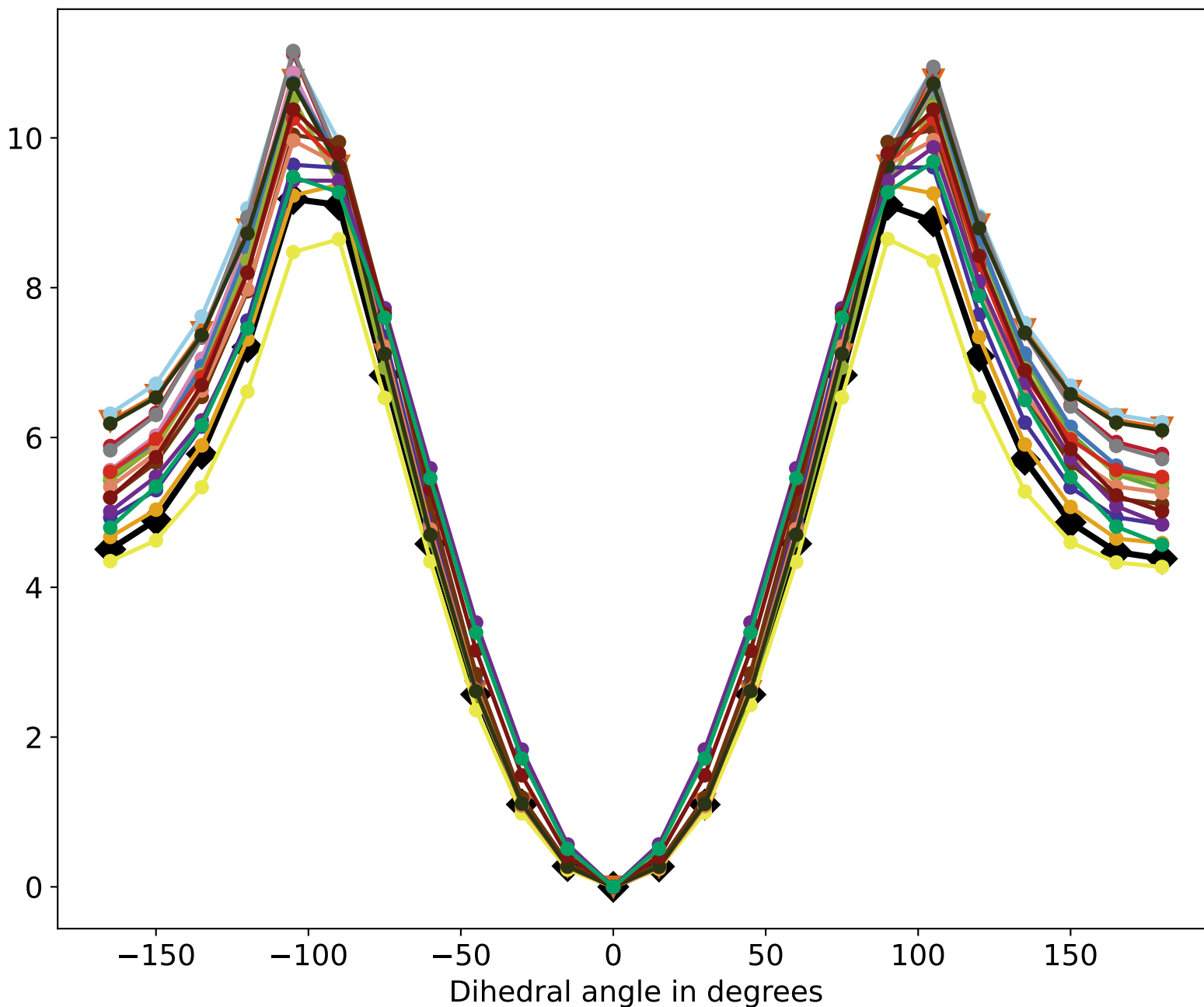
- df-ccsd(t)/cbs
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- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
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- MP2/heavy-aug-cc-pVTZ

Relative energies in kcal/mol

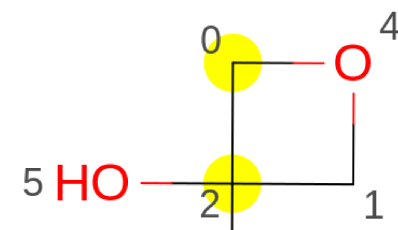
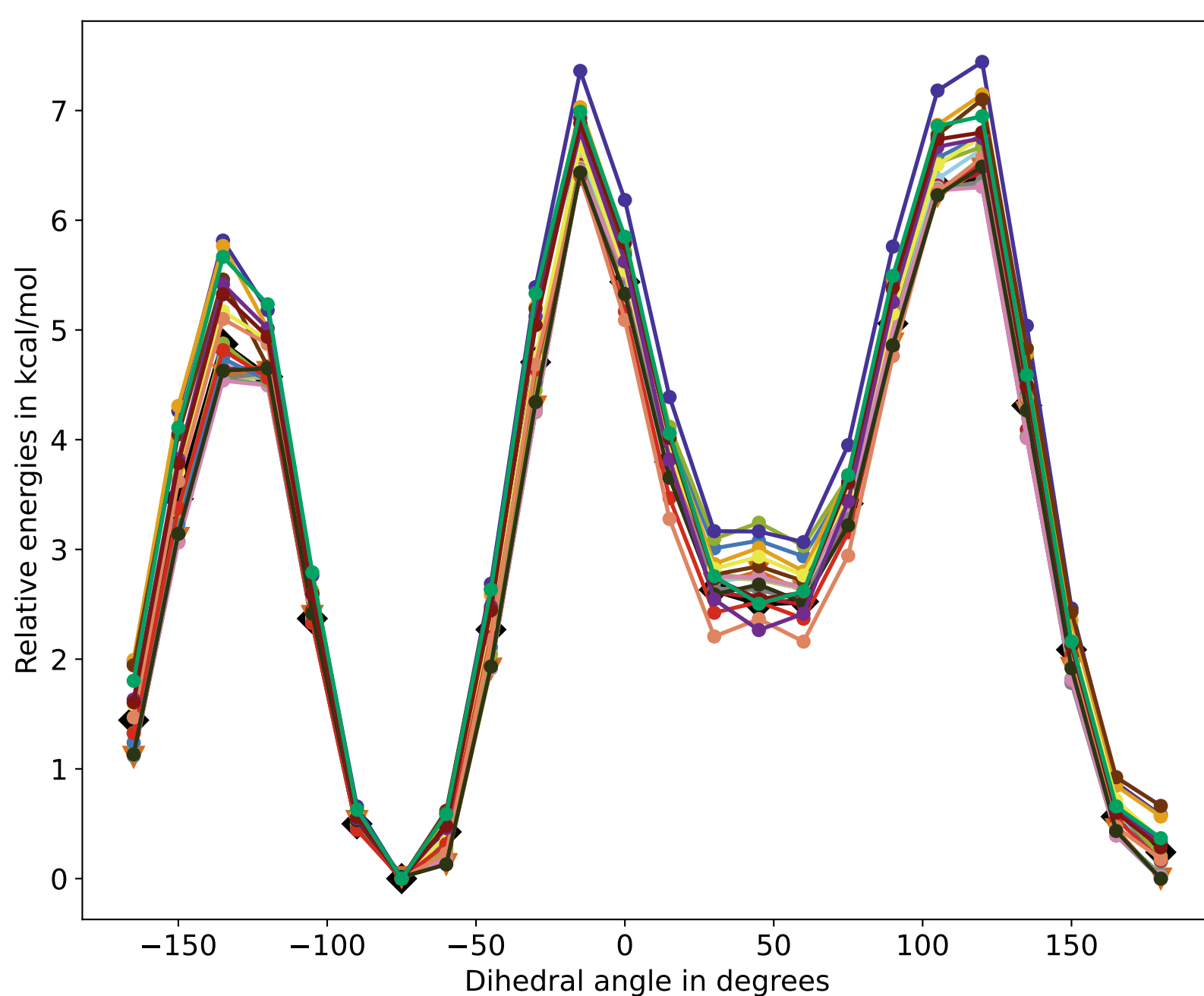


- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
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- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
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- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
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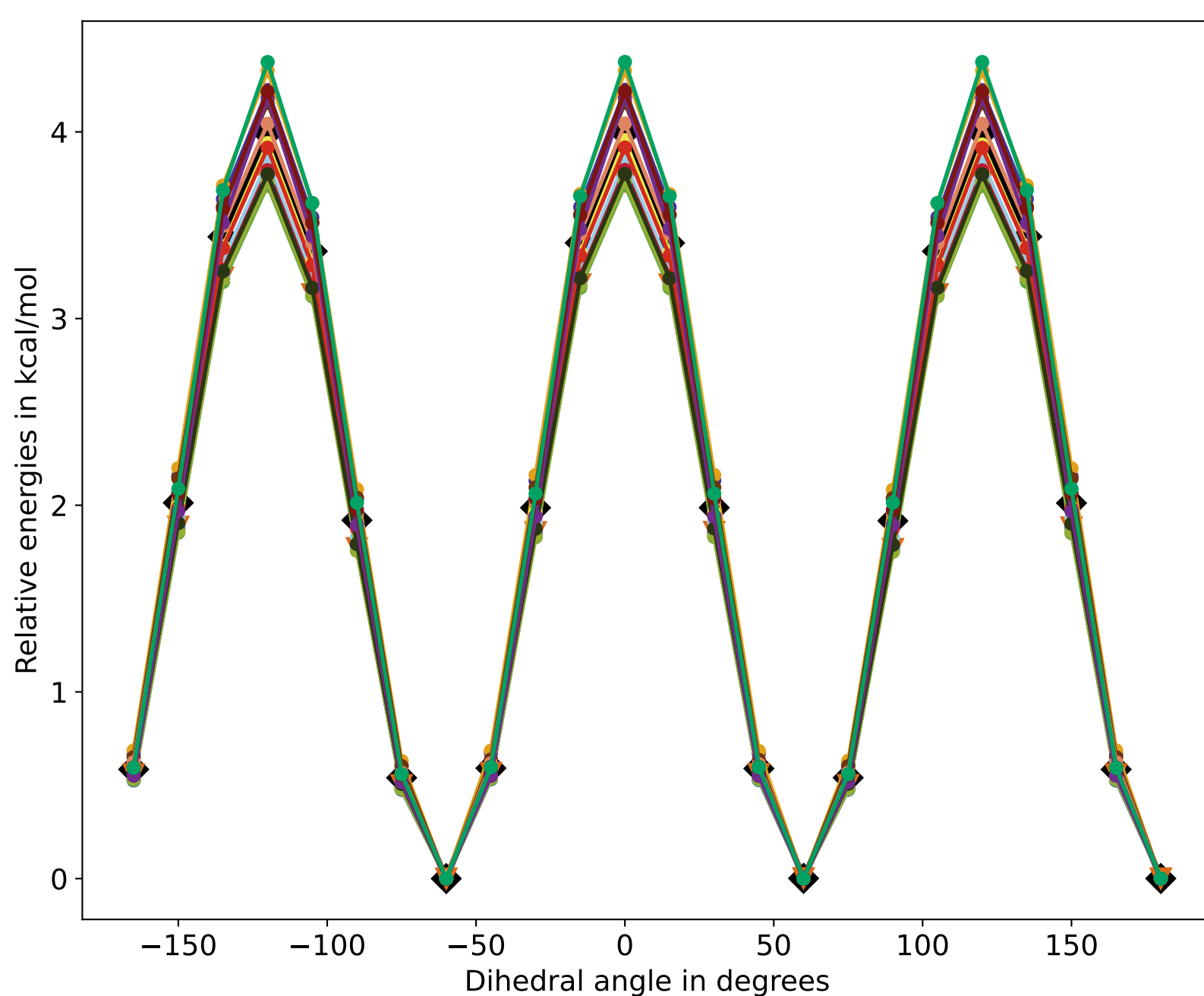
Relative energies in kcal/mol



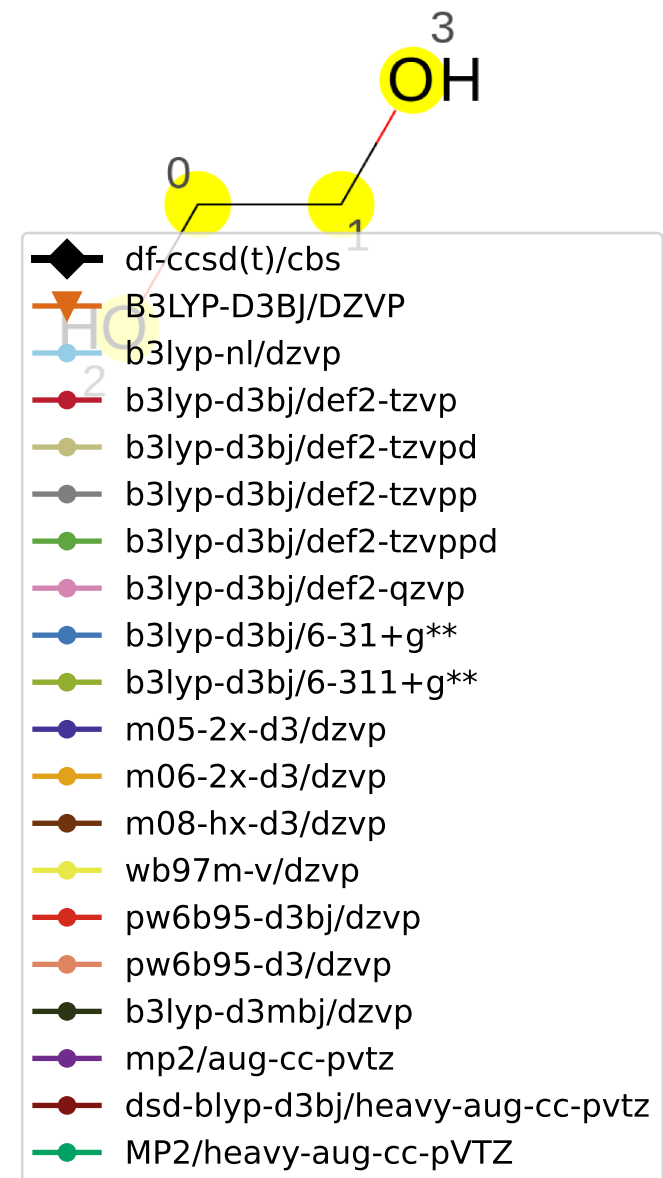
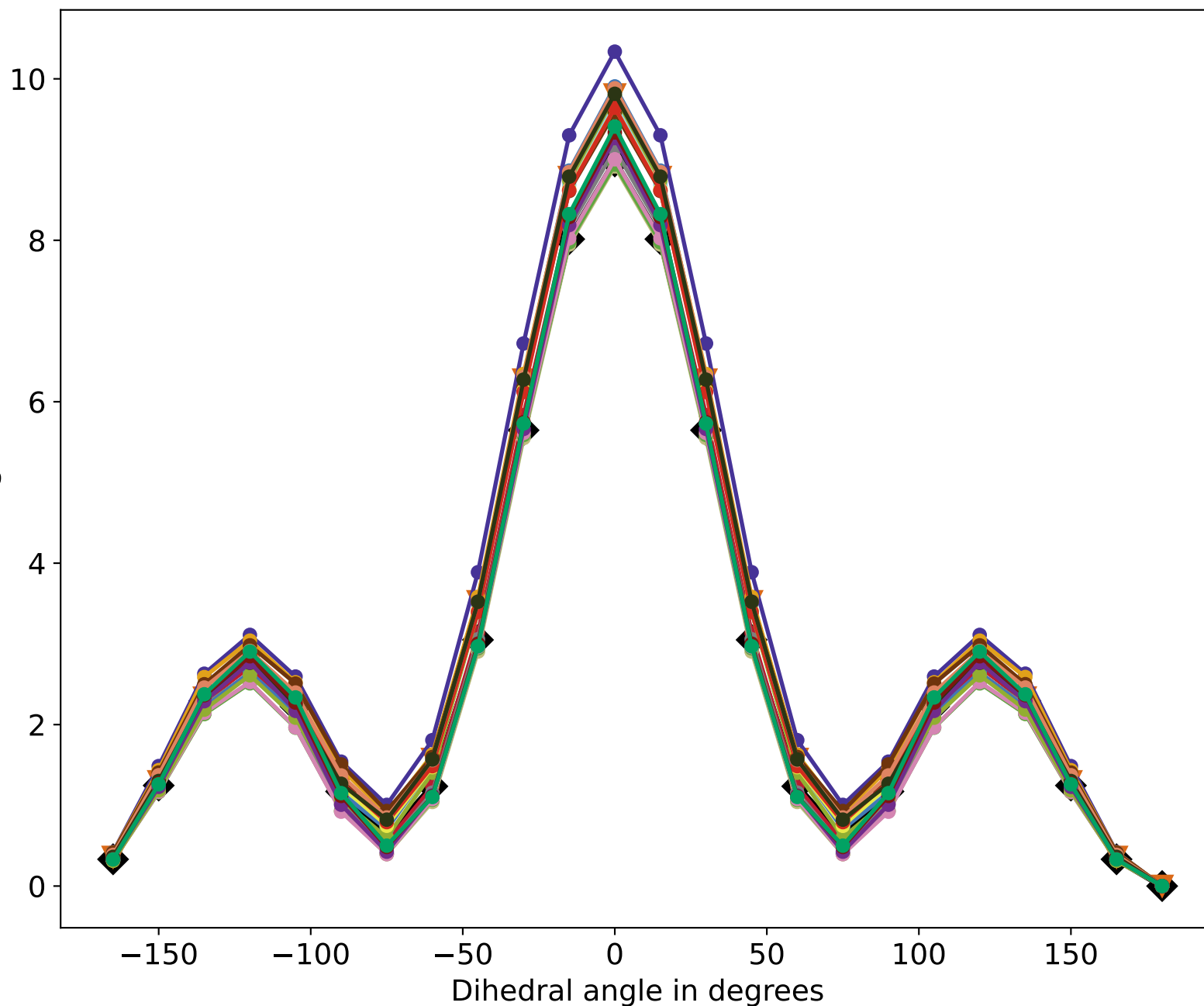
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- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
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- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
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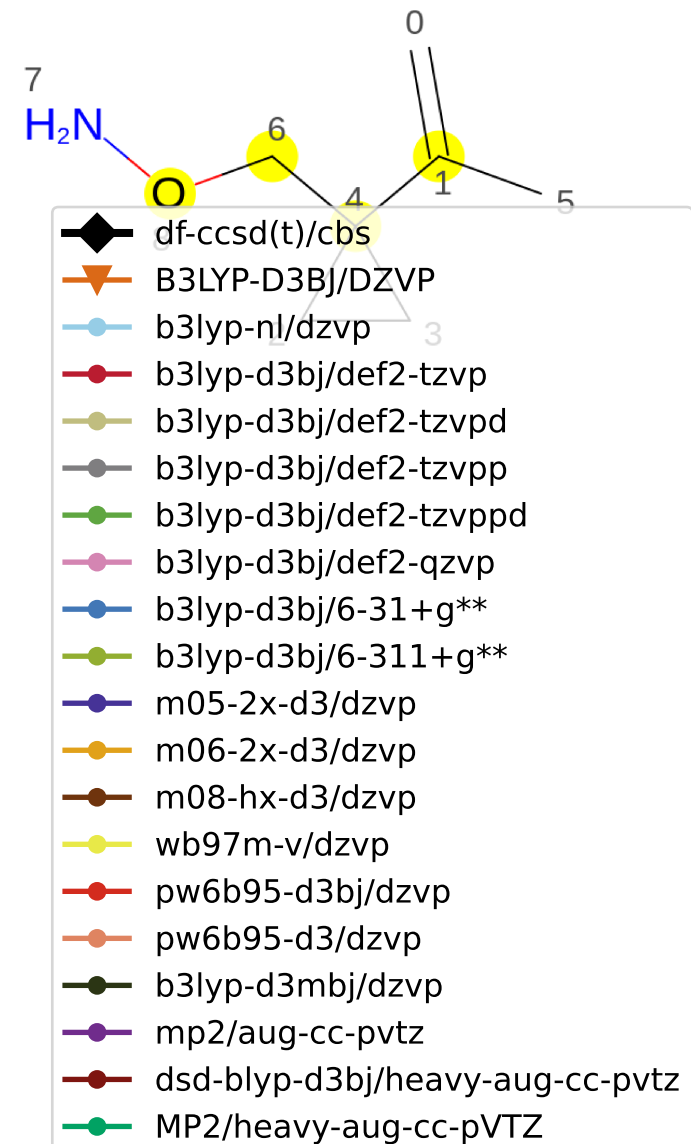
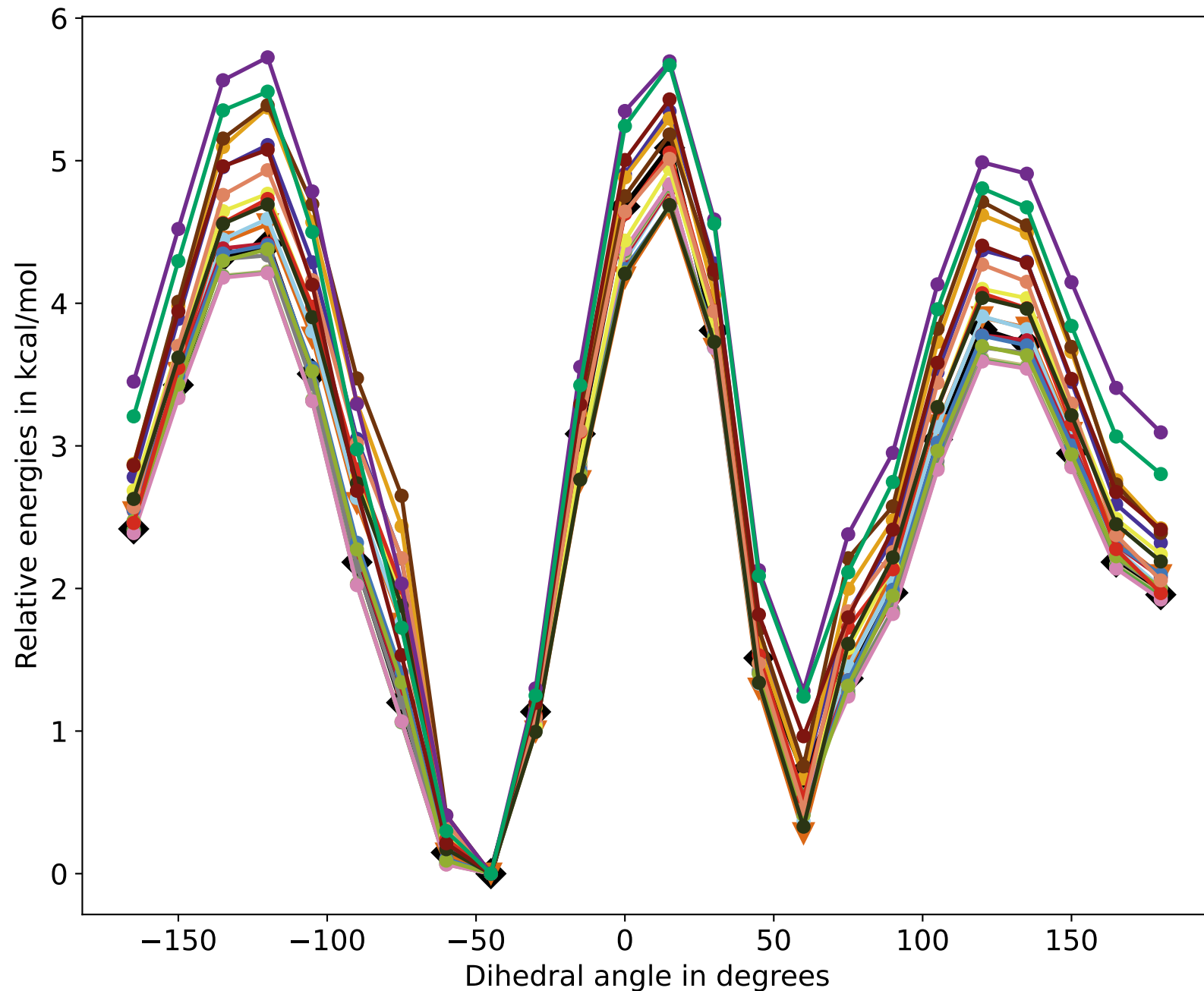


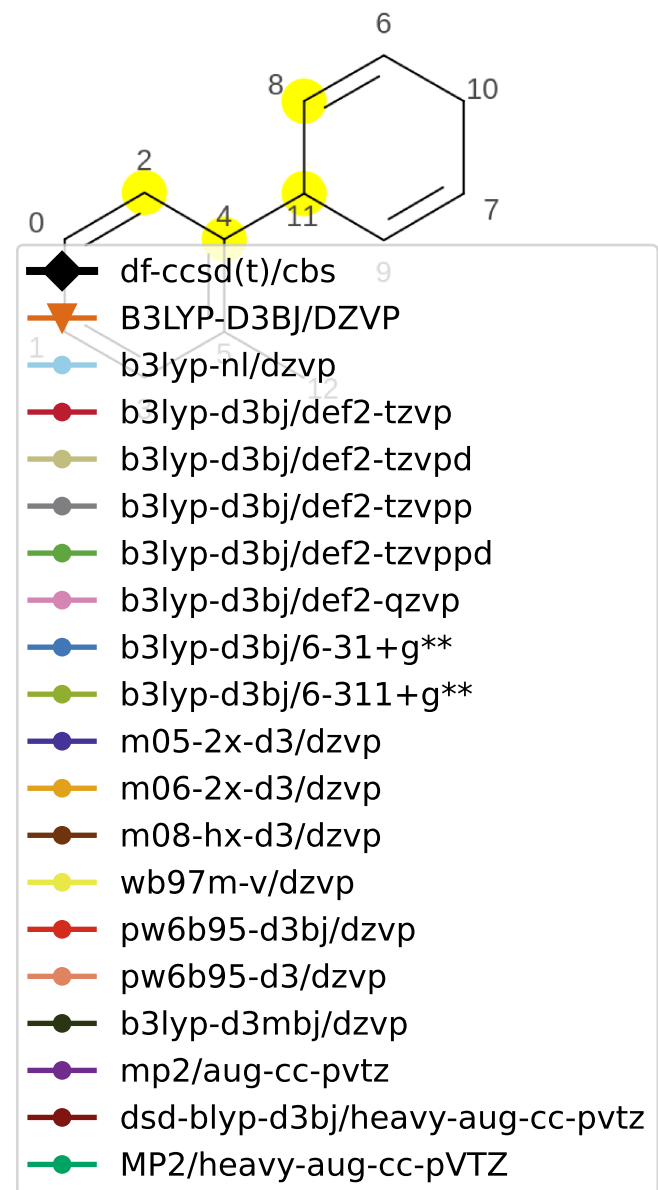
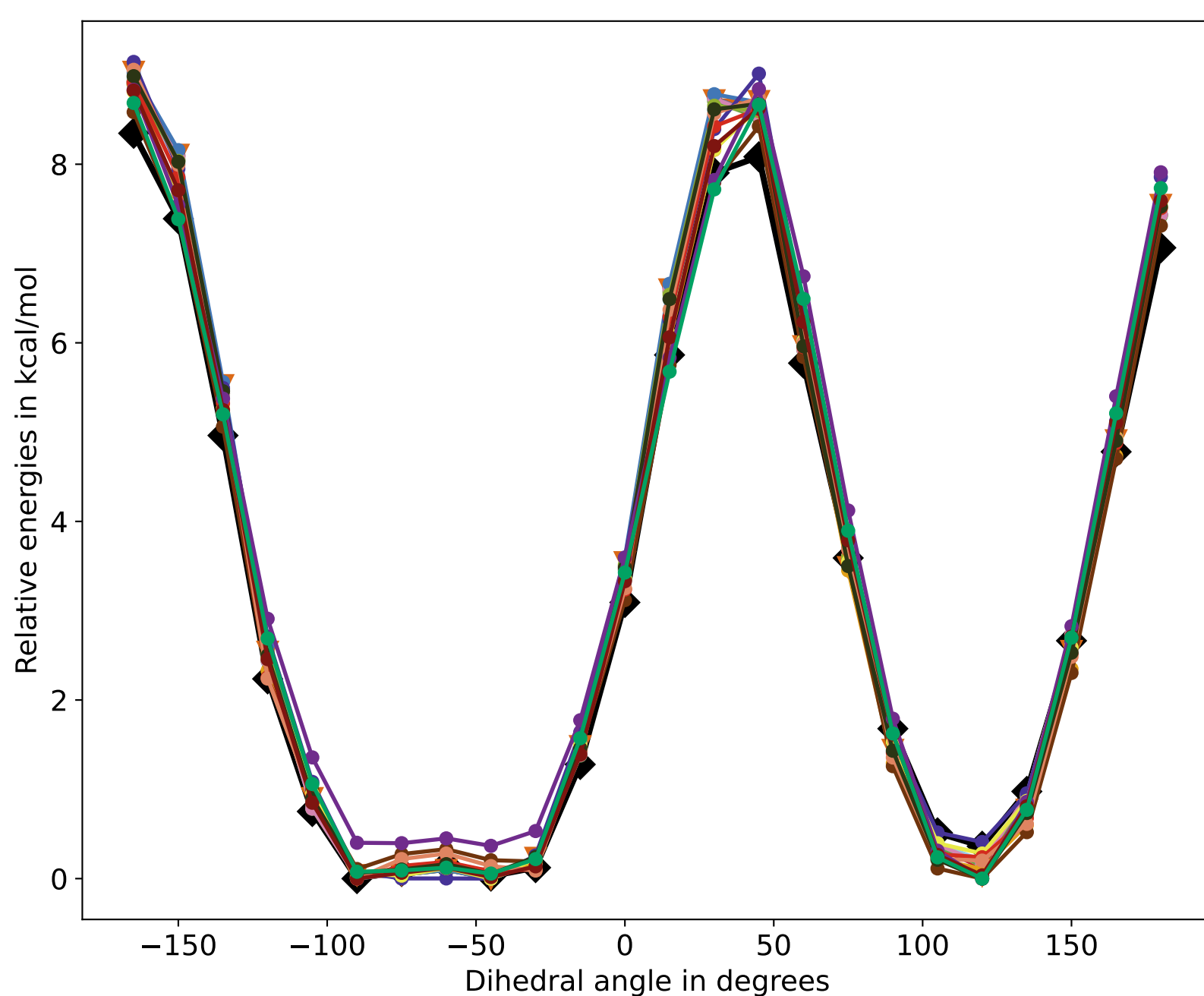
- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
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- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvppp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ

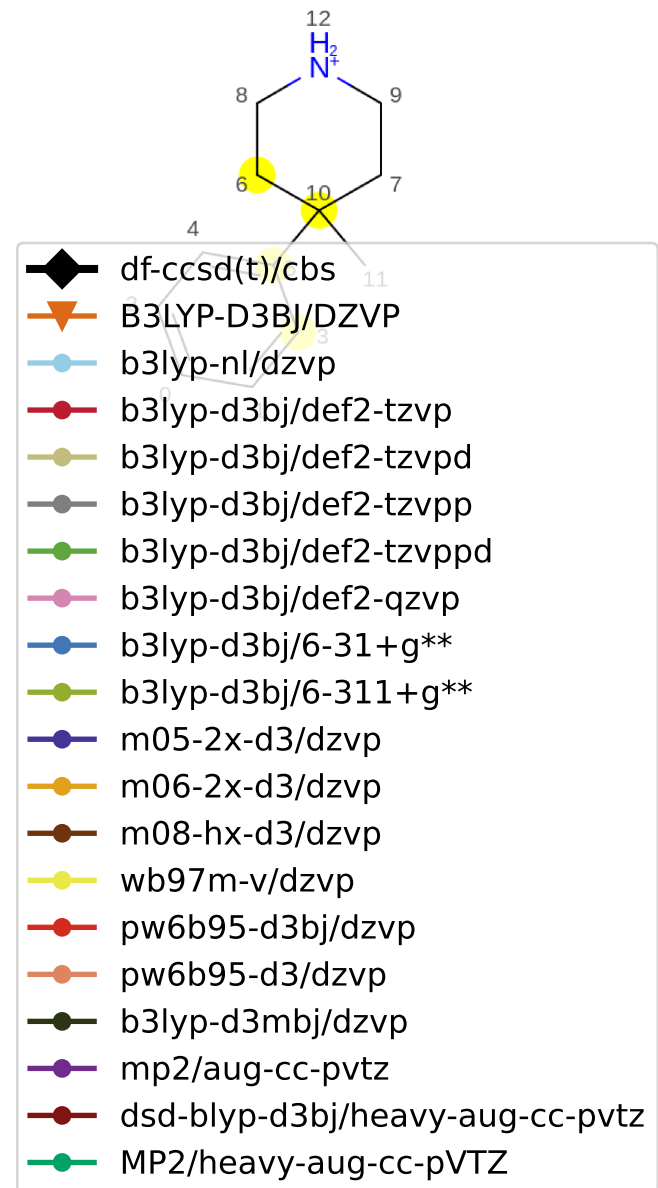
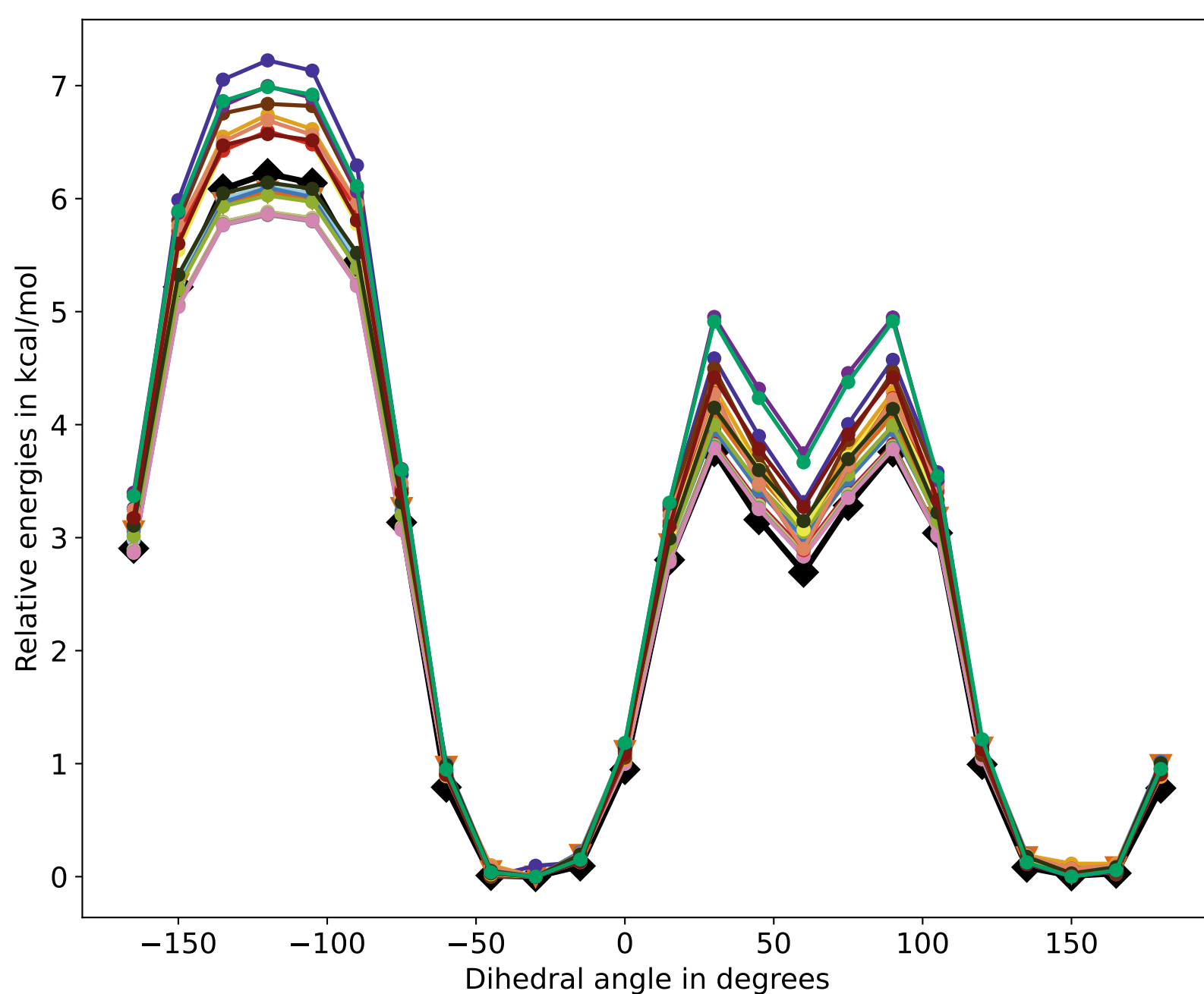


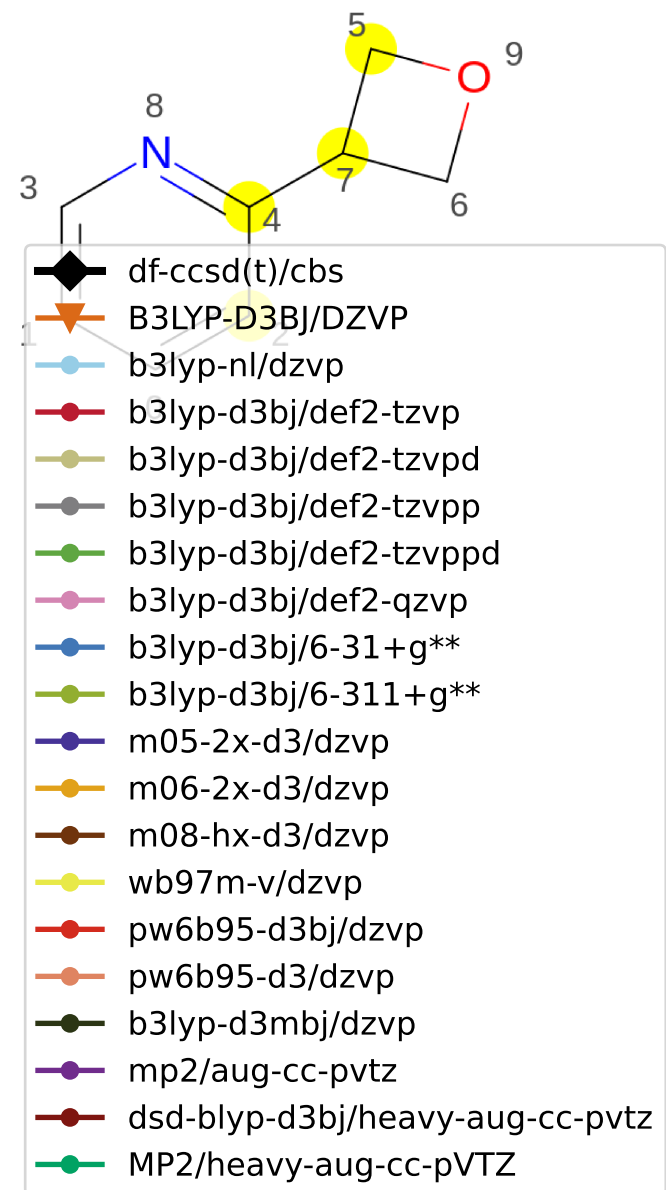
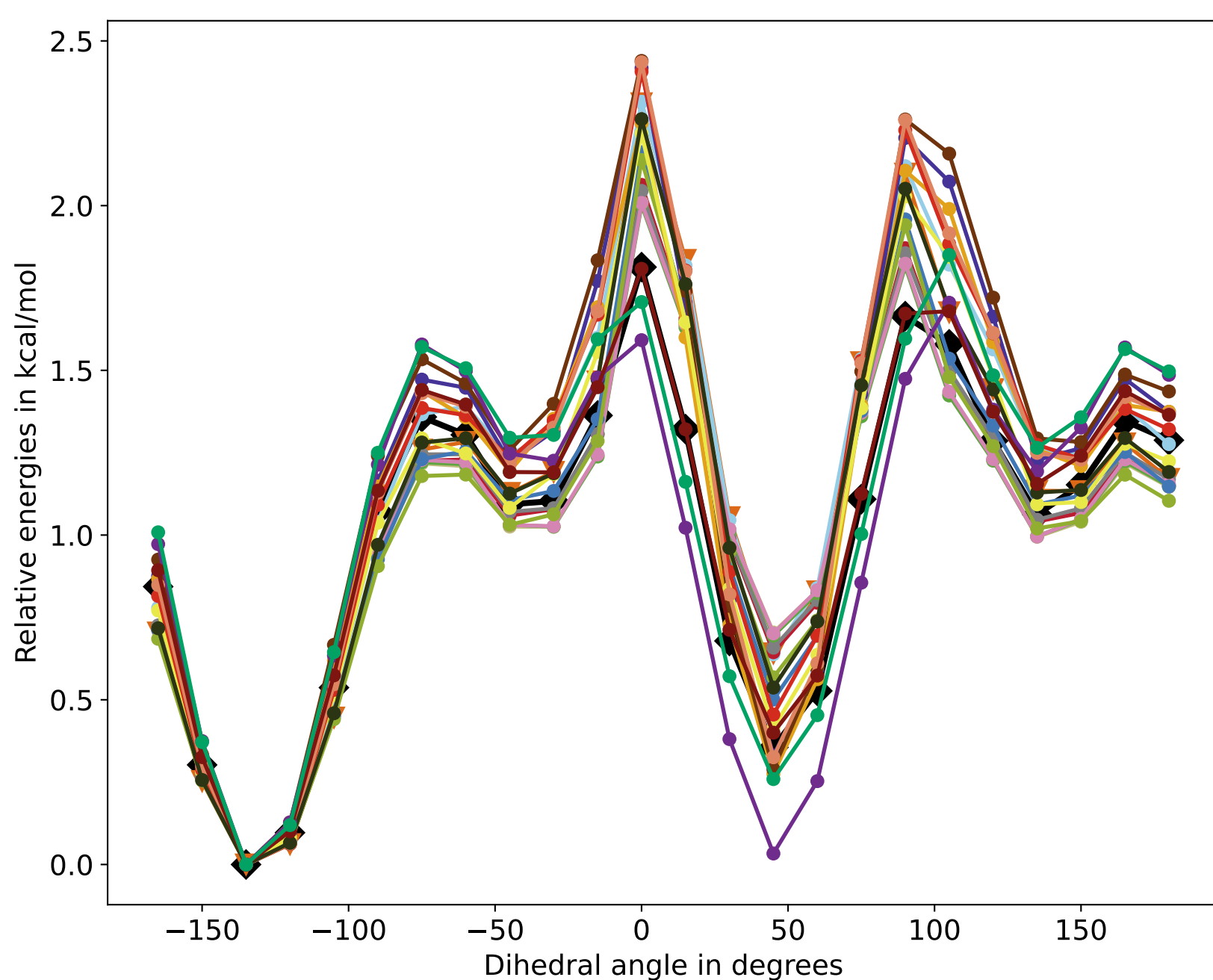
Relative energies in kcal/mol

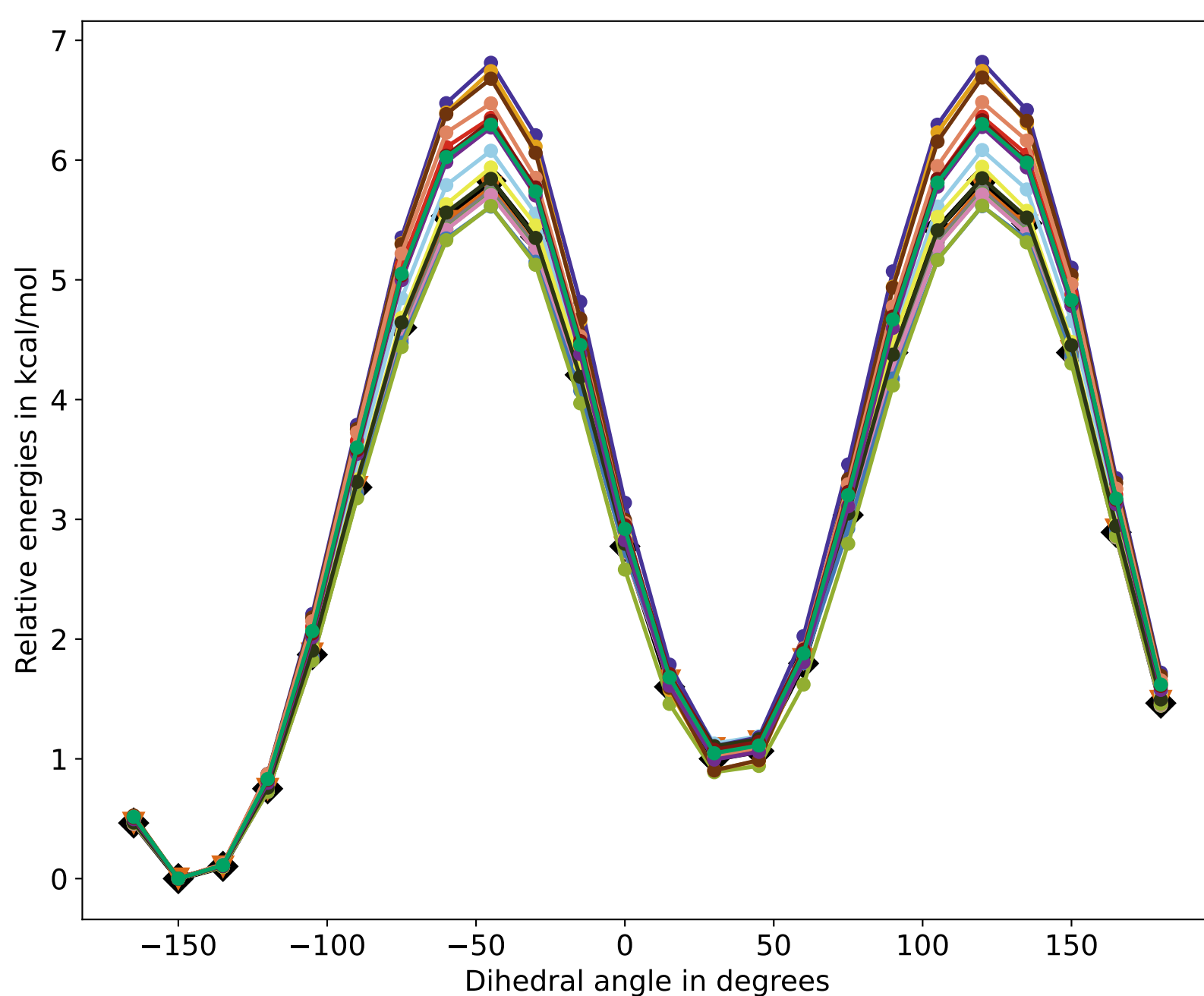


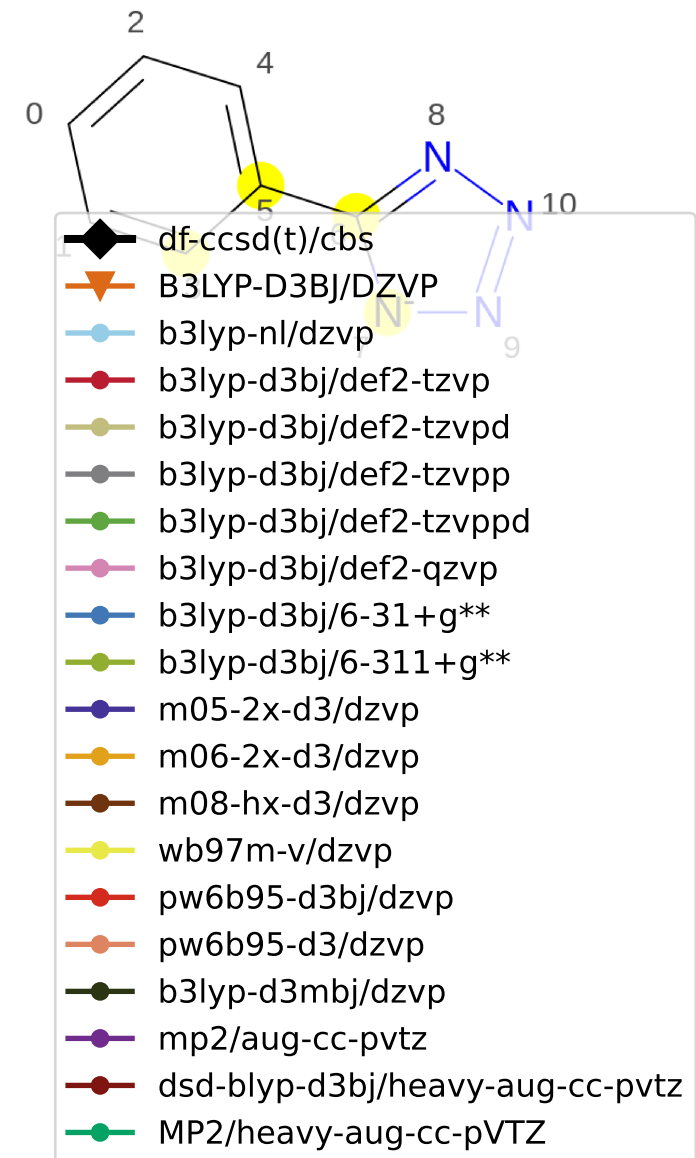
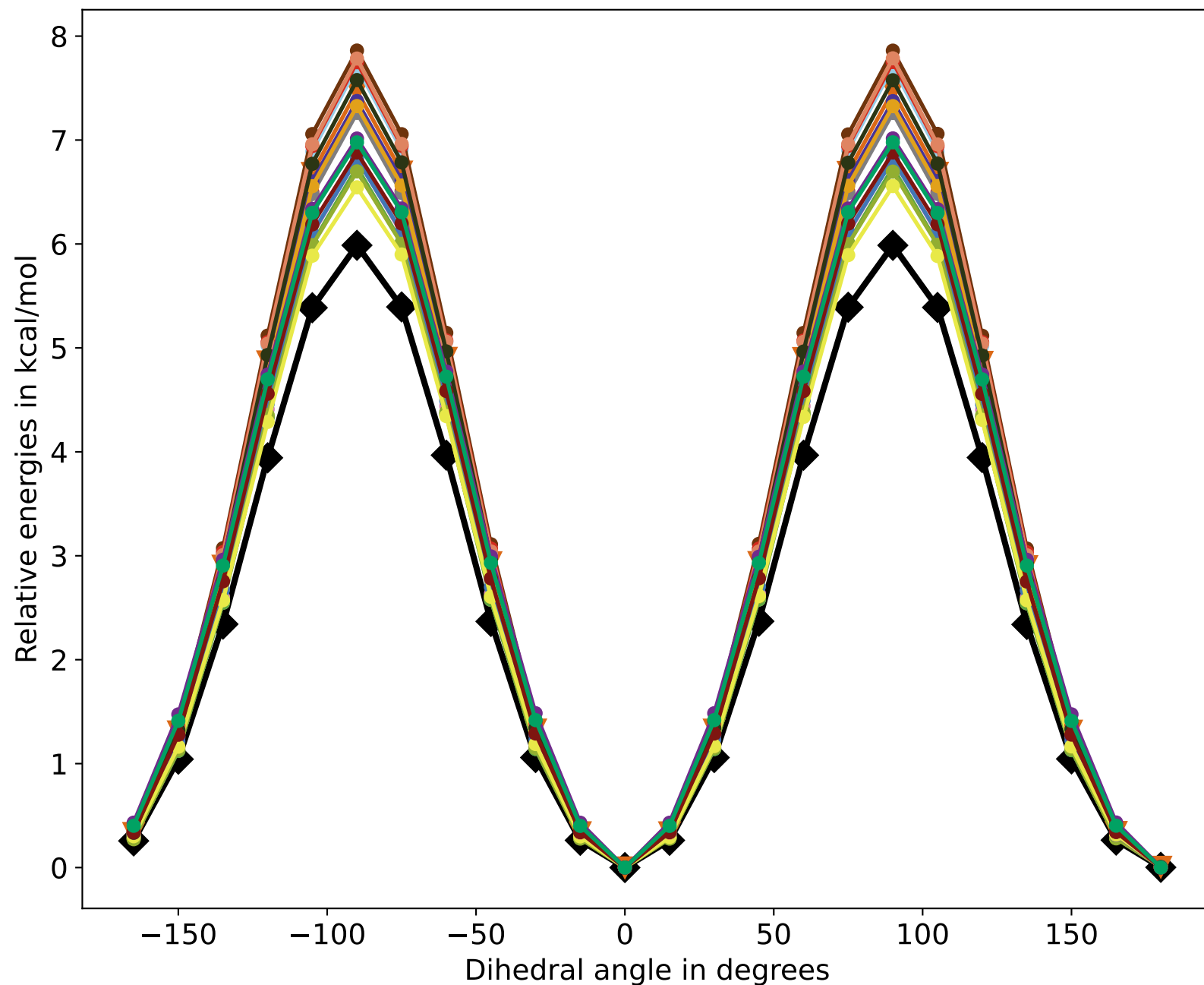




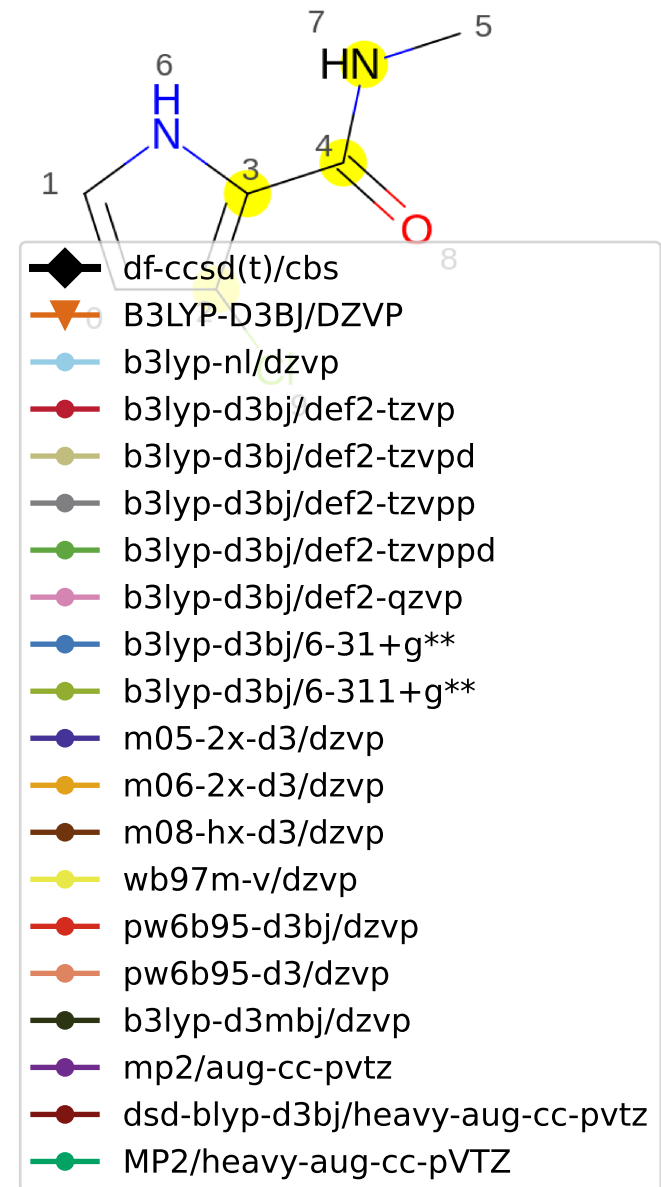
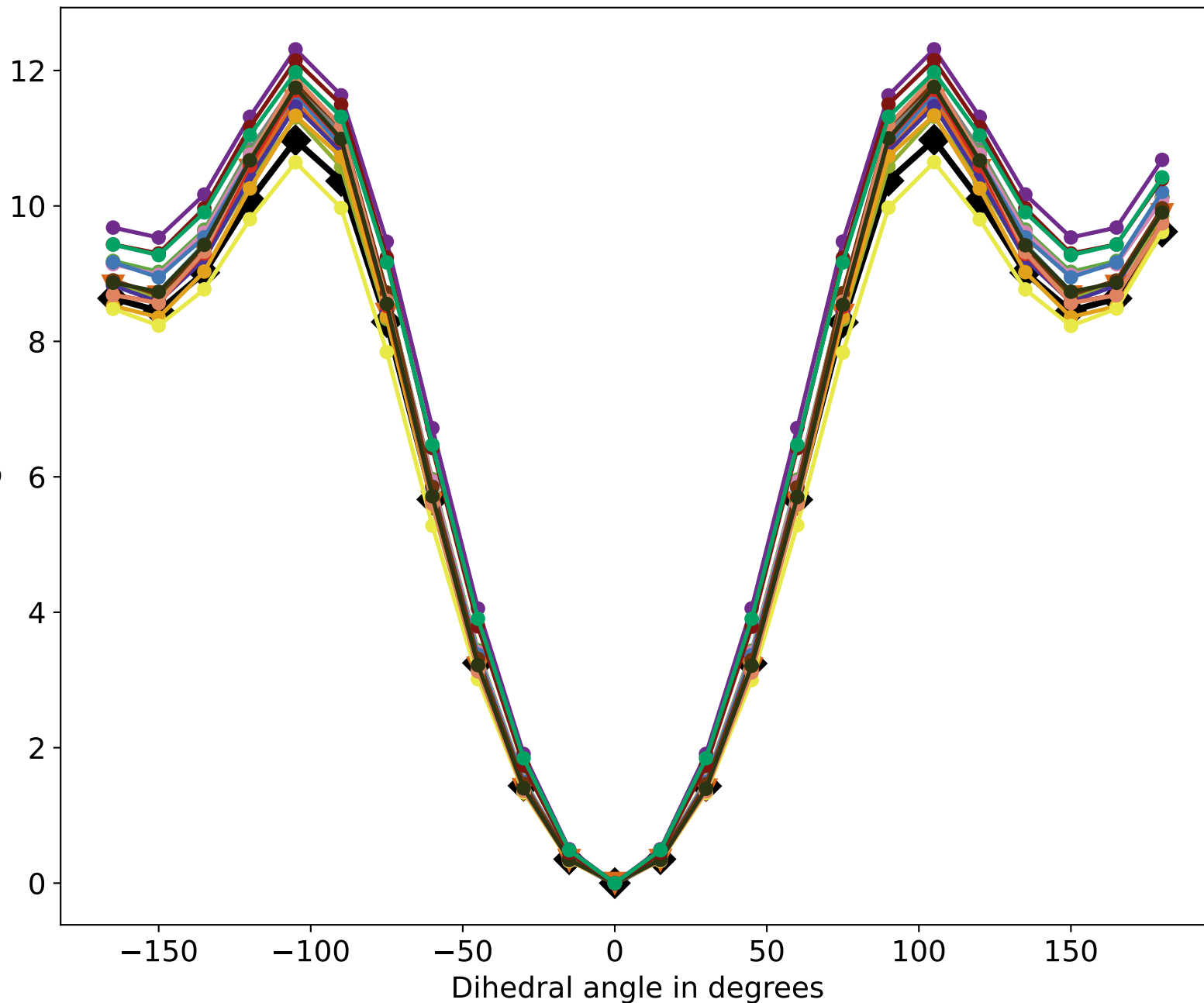


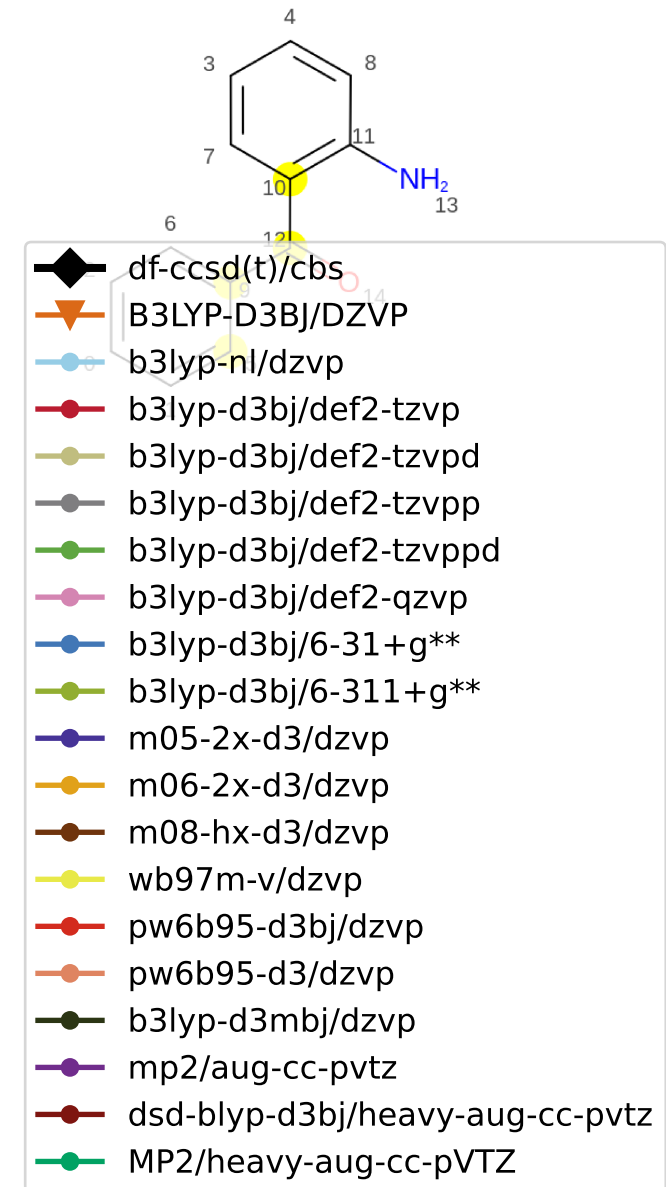
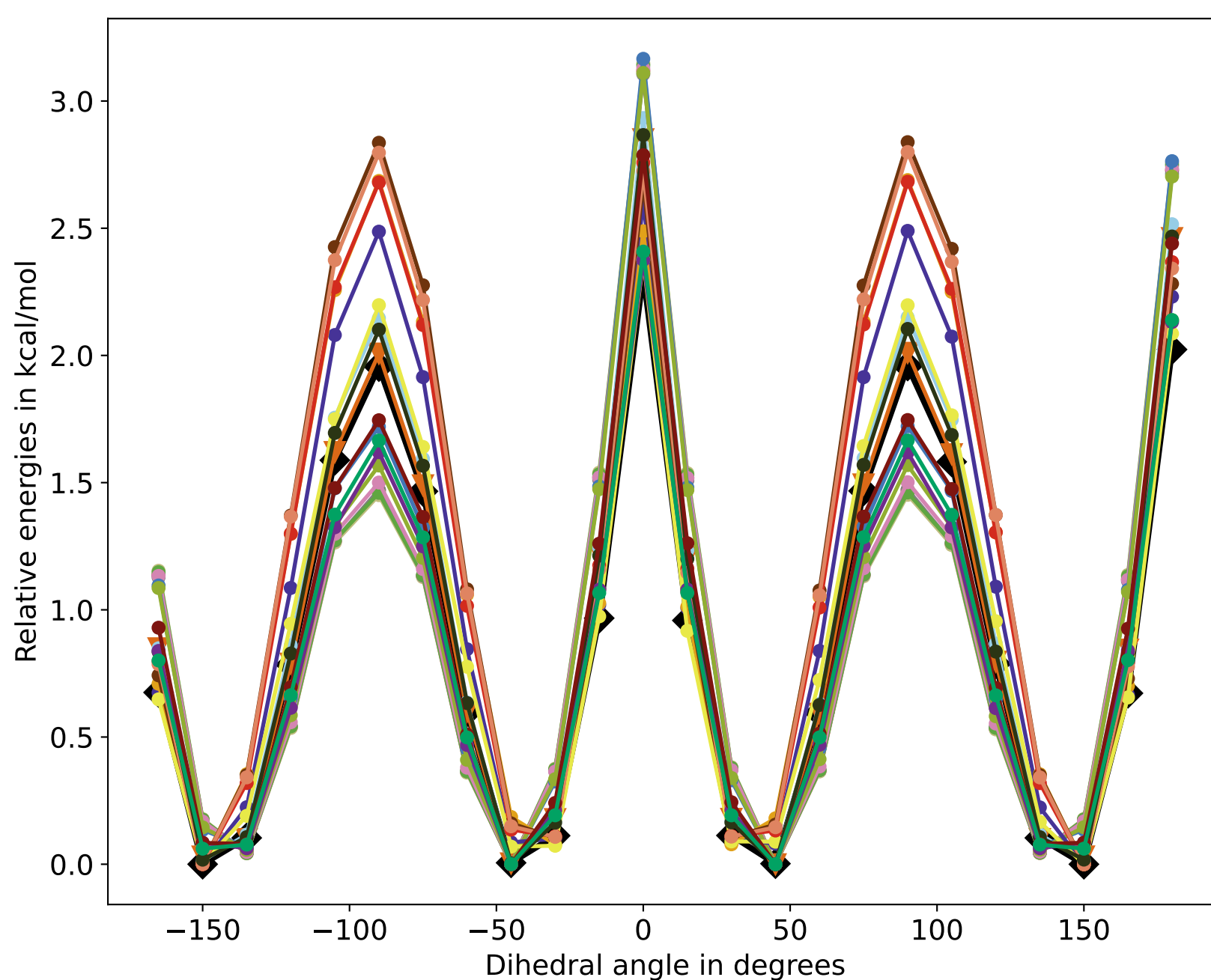


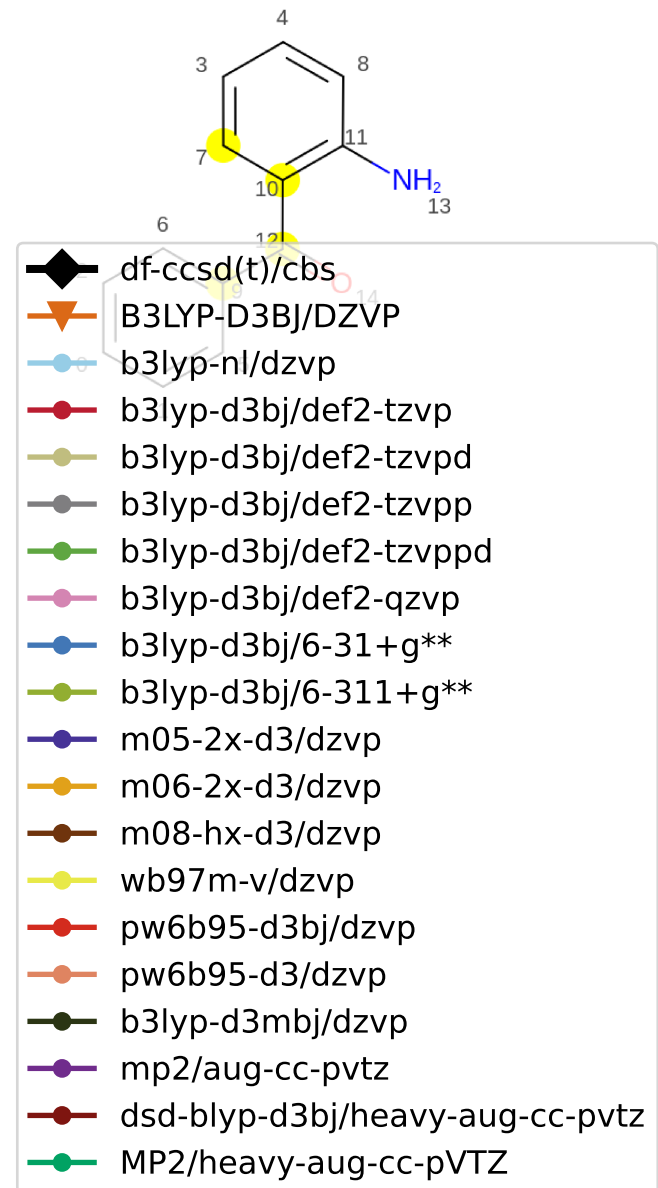
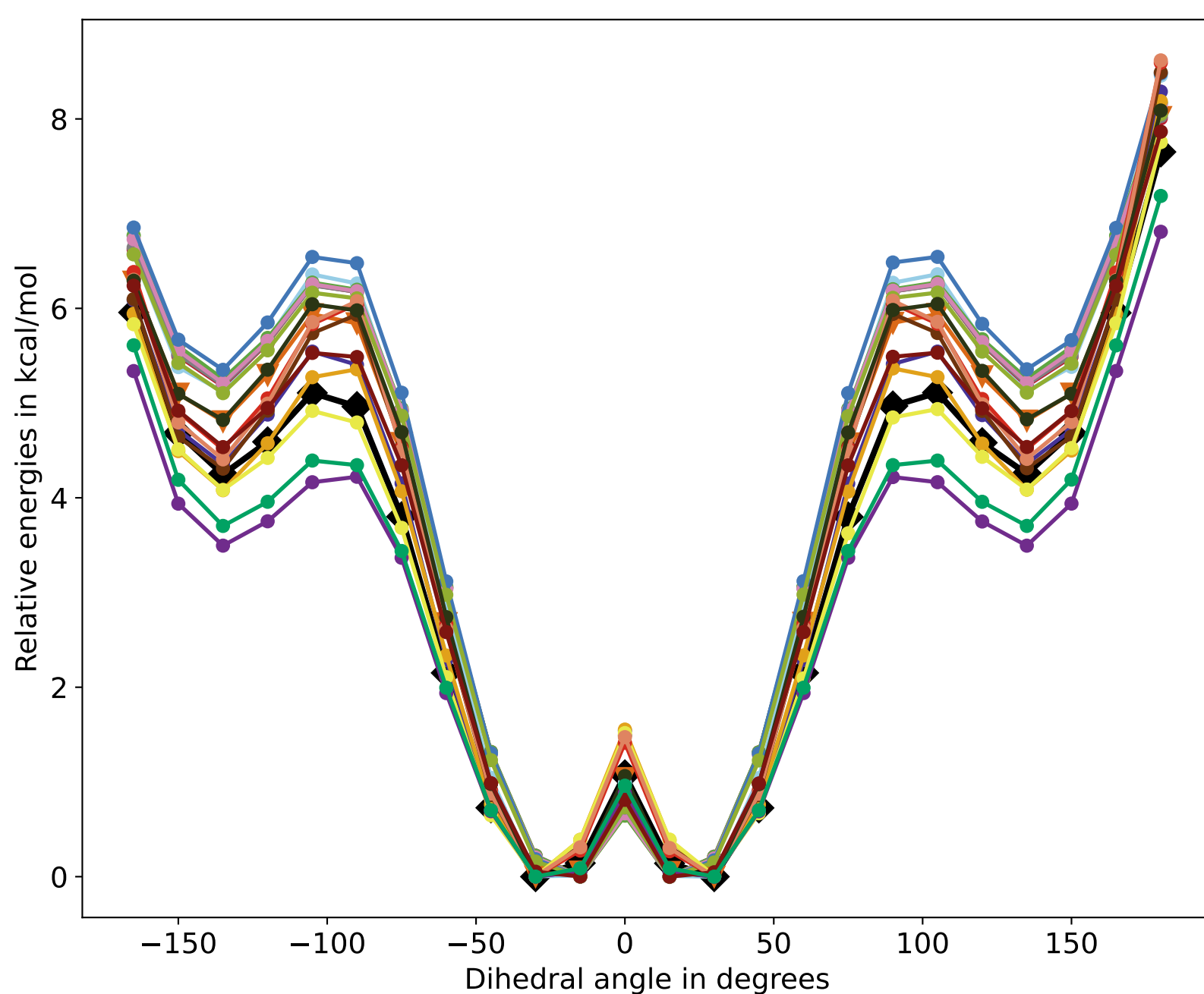




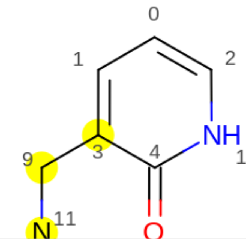
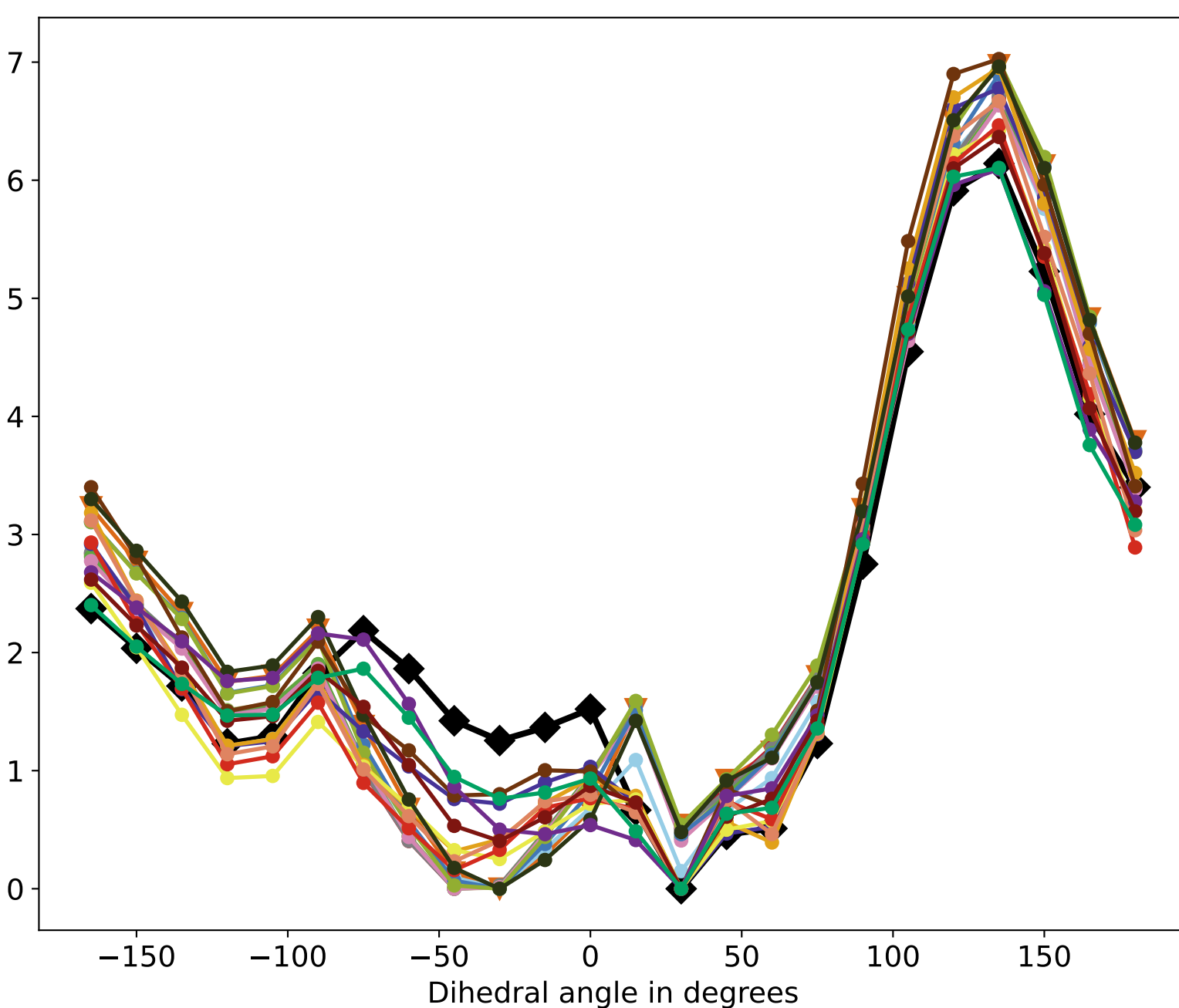
Relative energies in kcal/mol



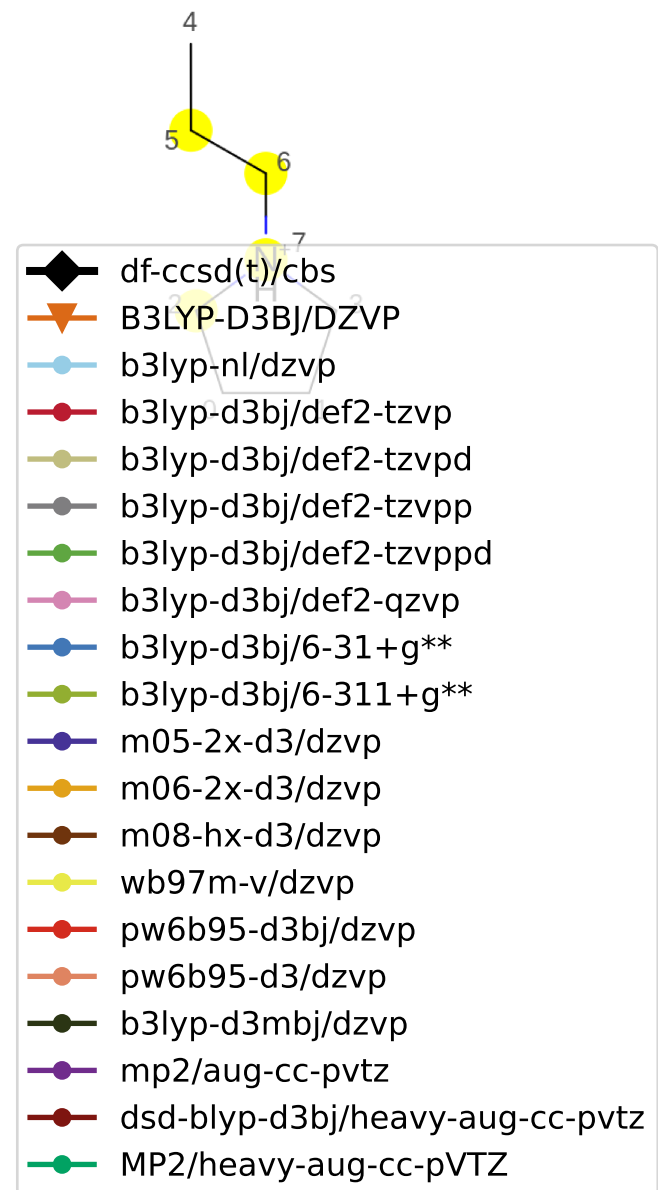
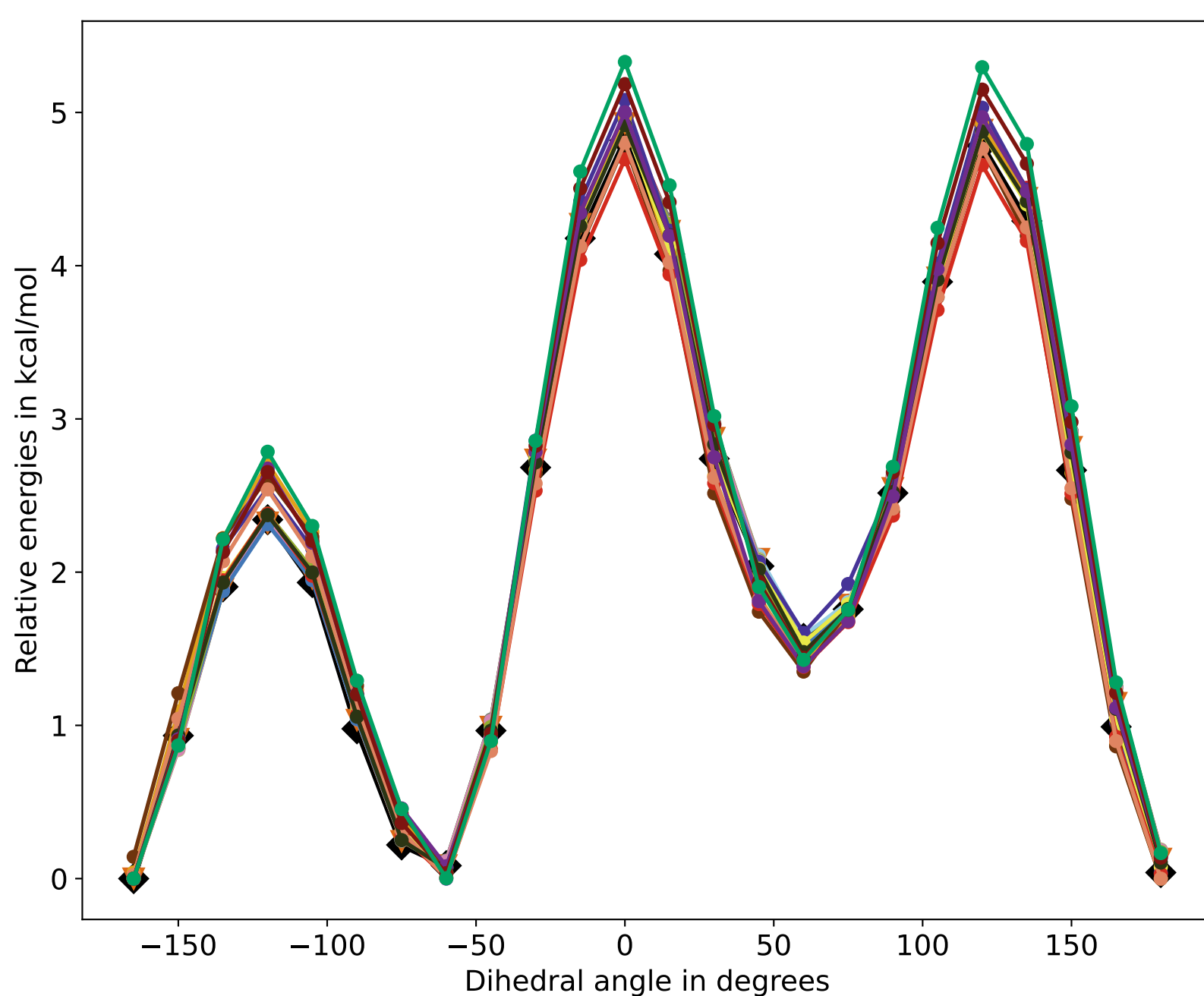


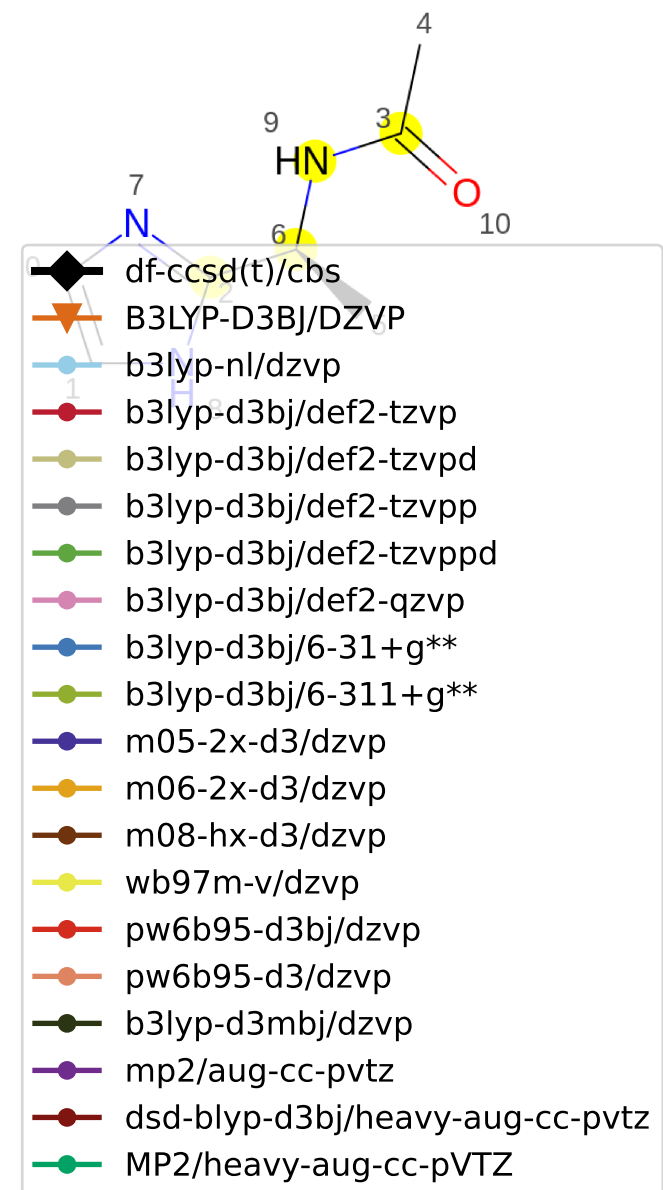
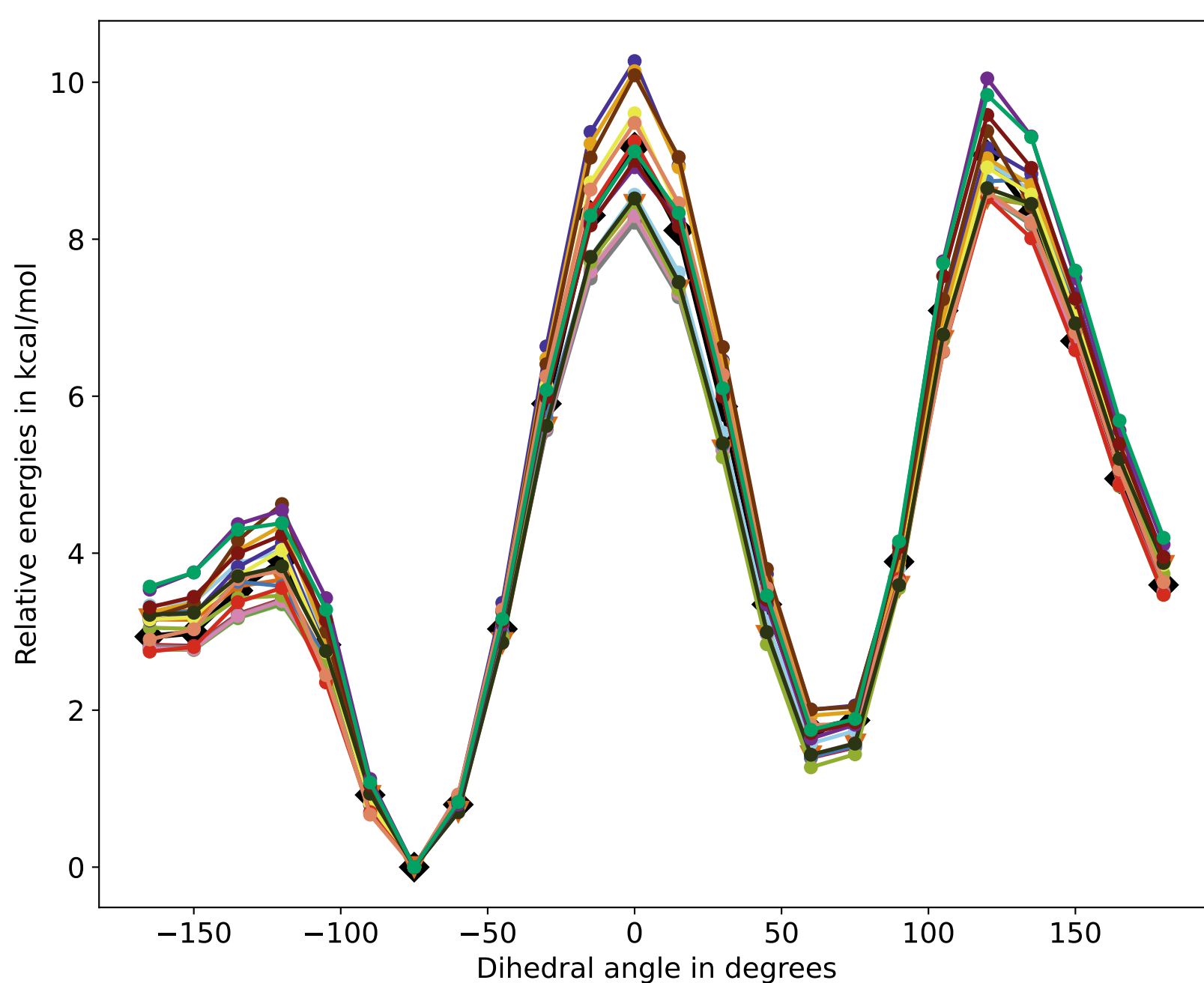


Relative energies in kcal/mol

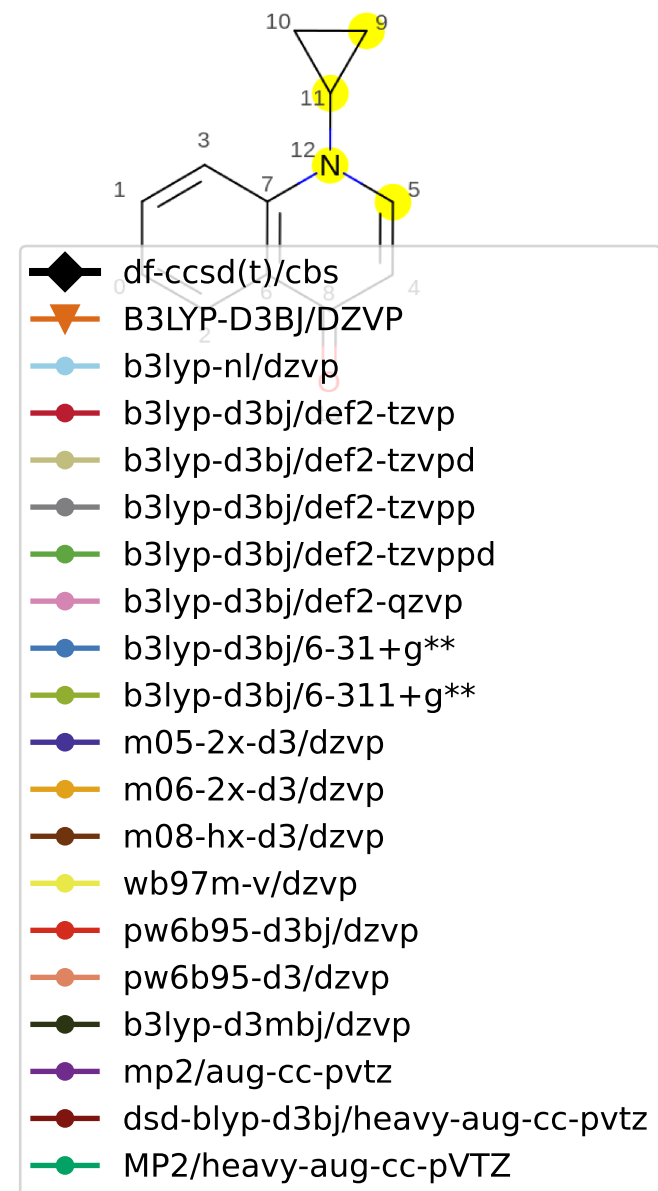
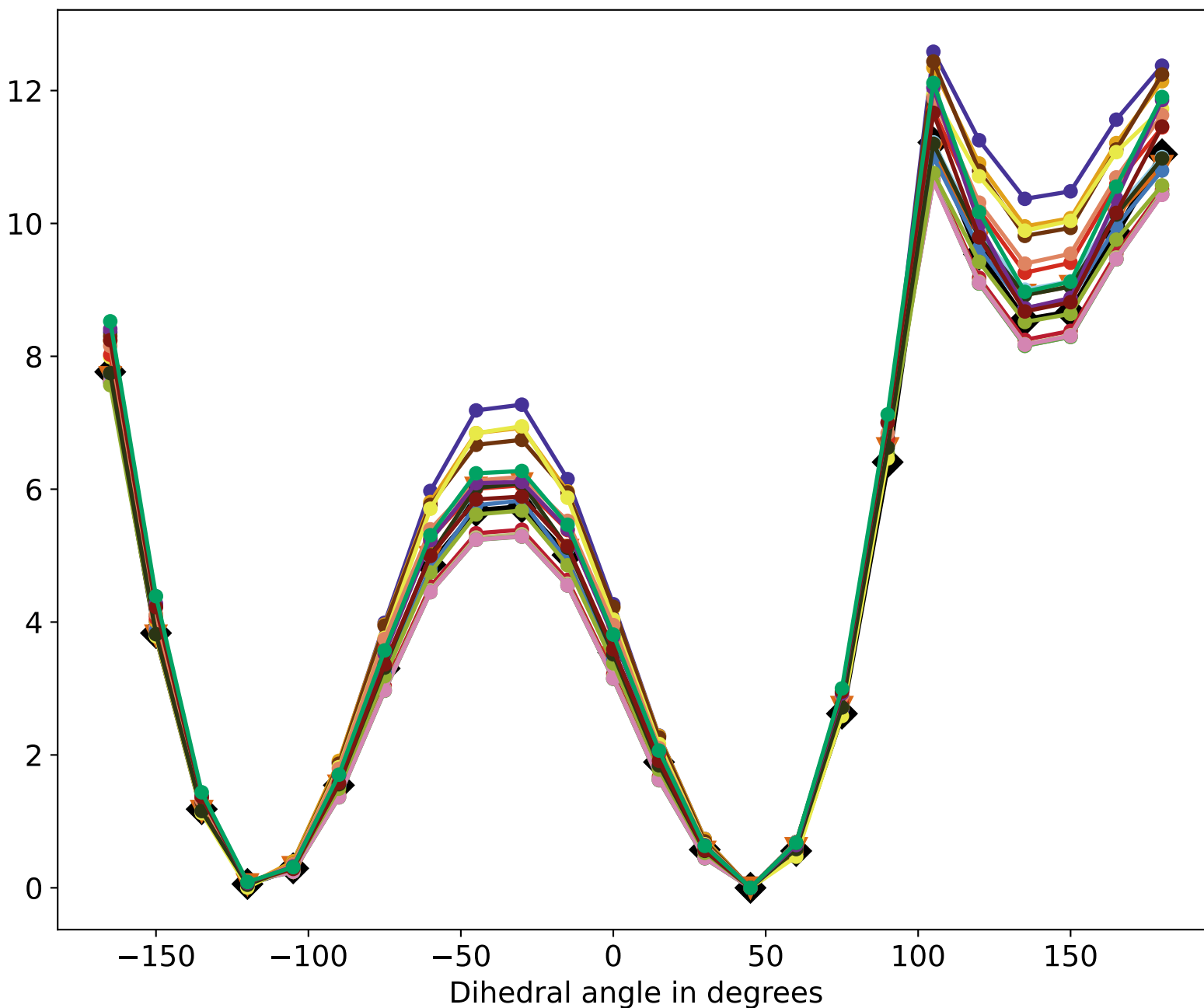


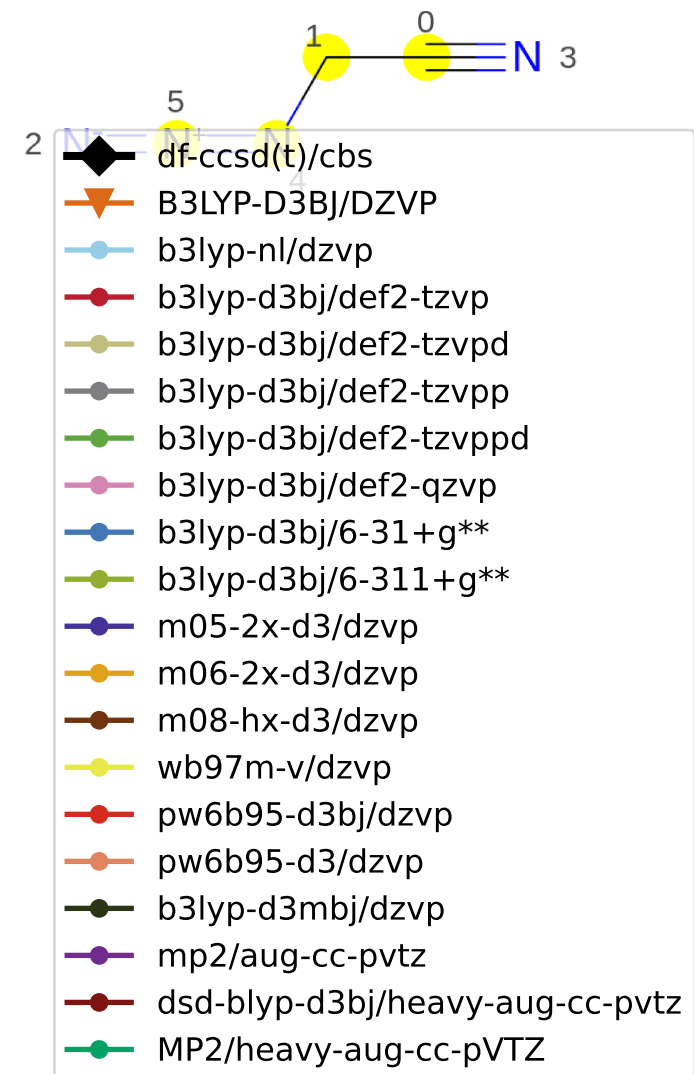
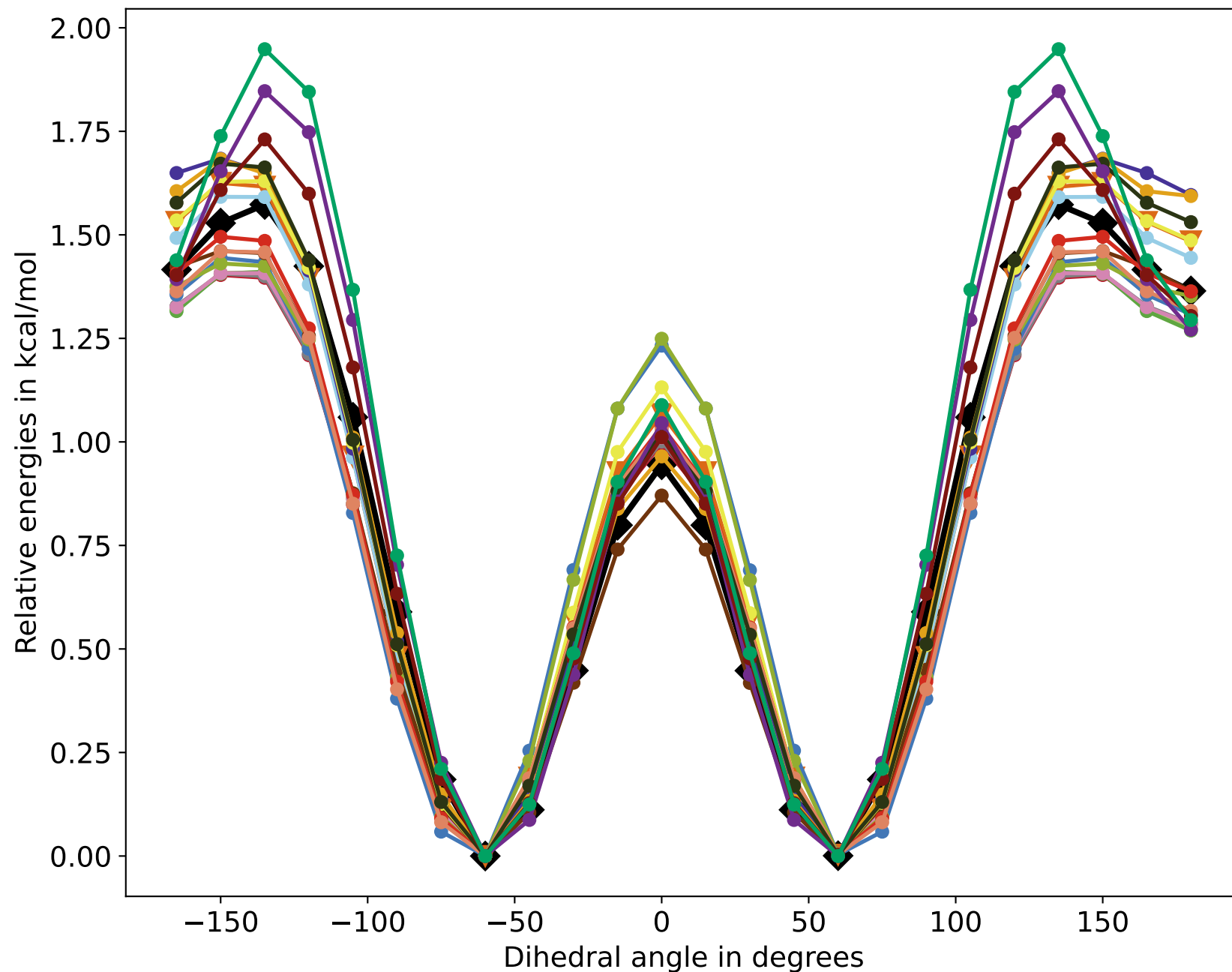
- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ

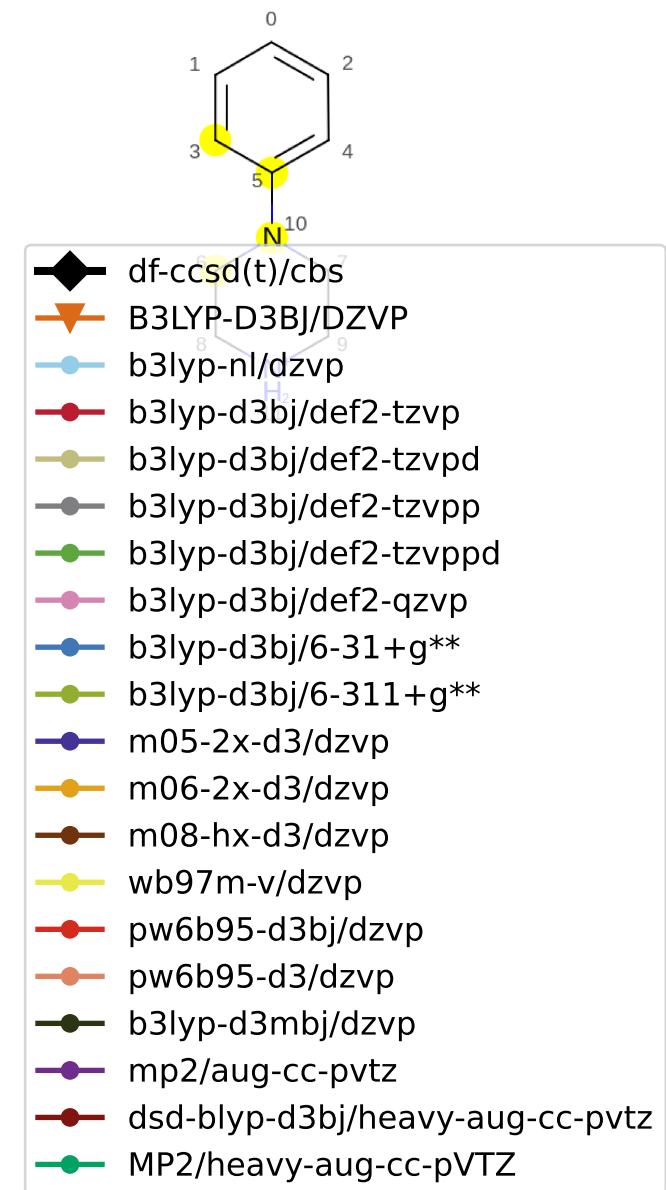
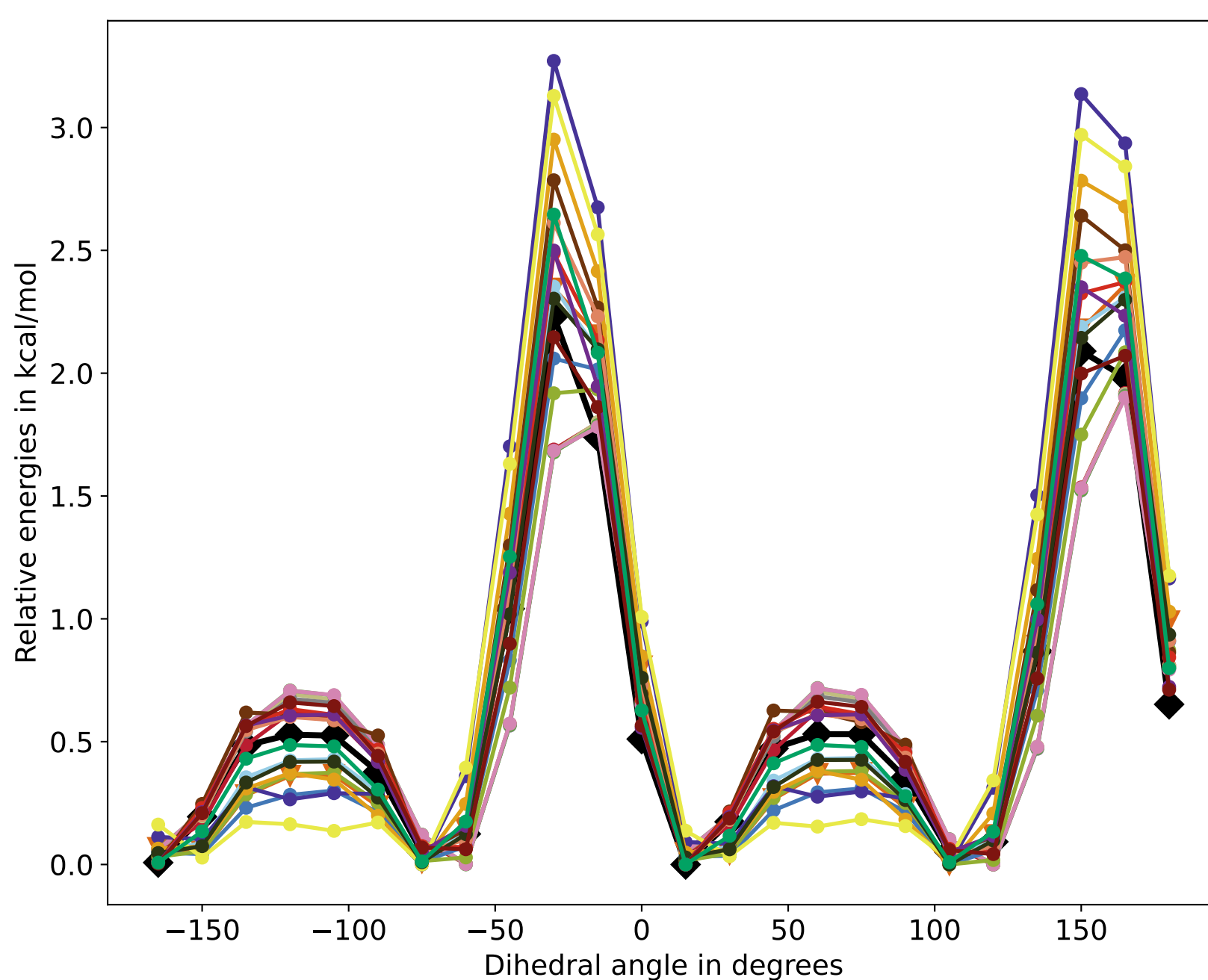




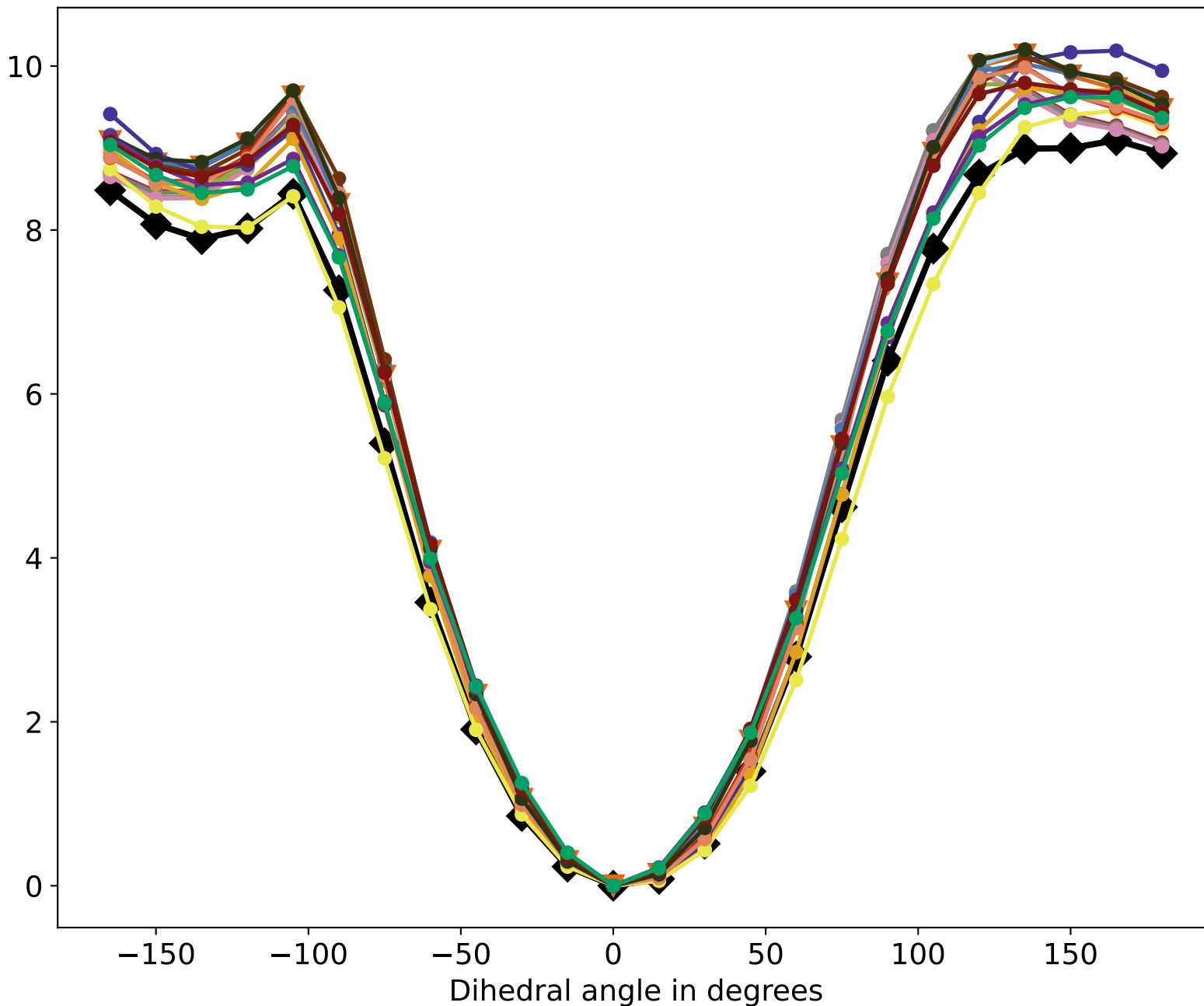
Relative energies in kcal/mol

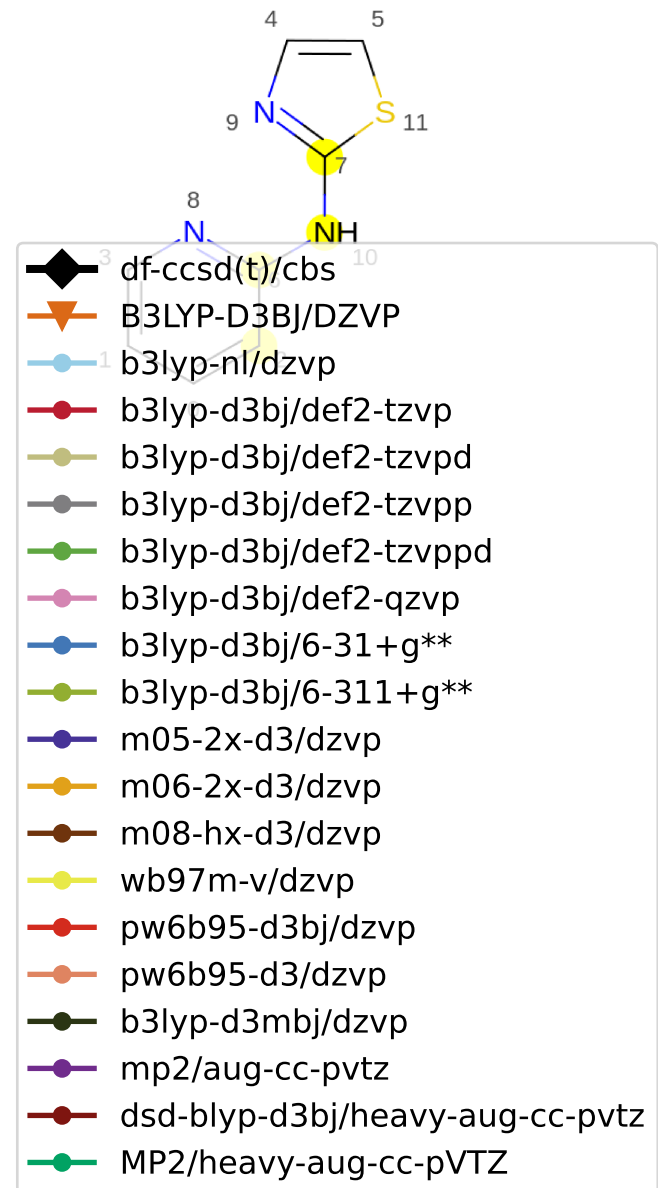
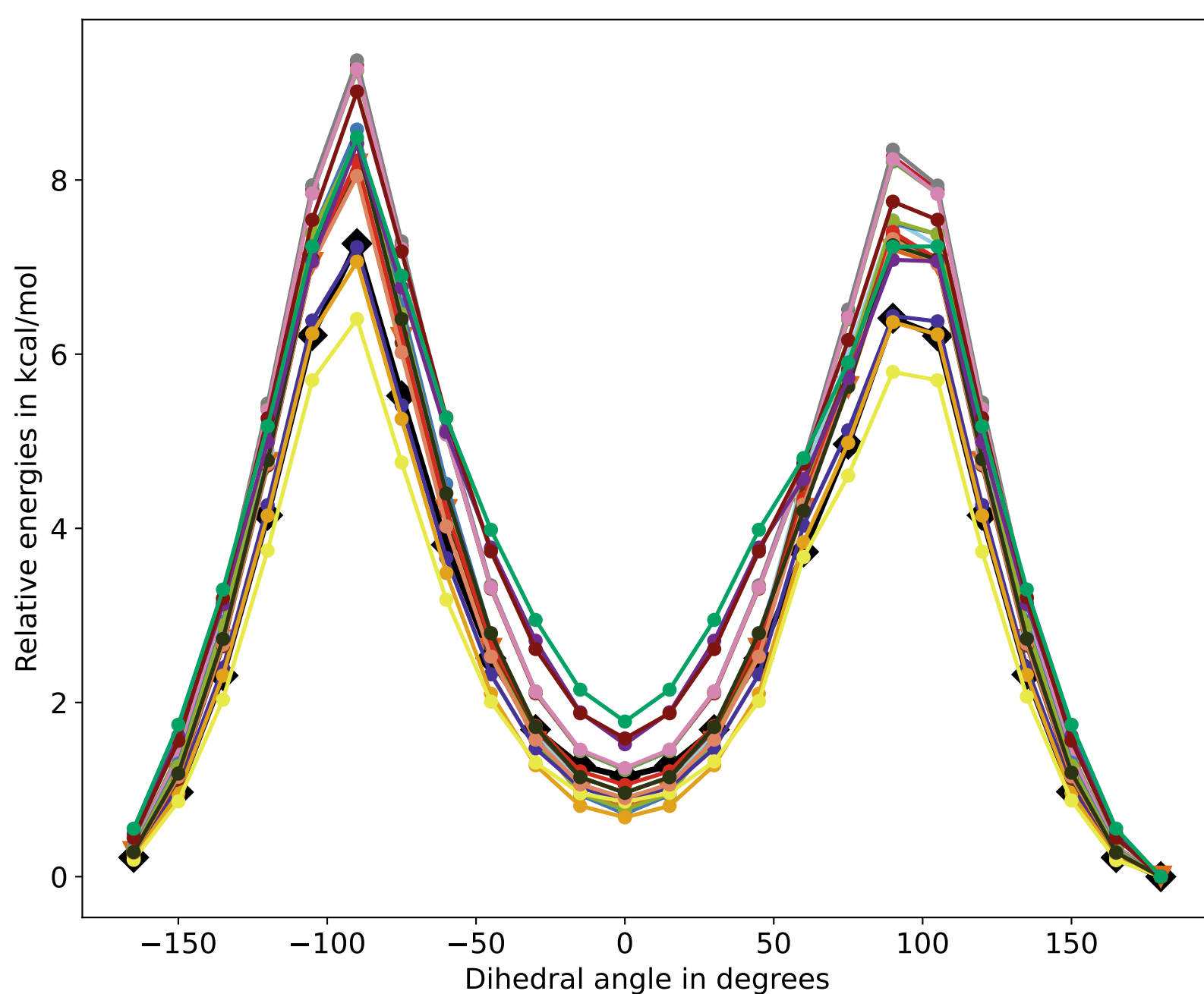


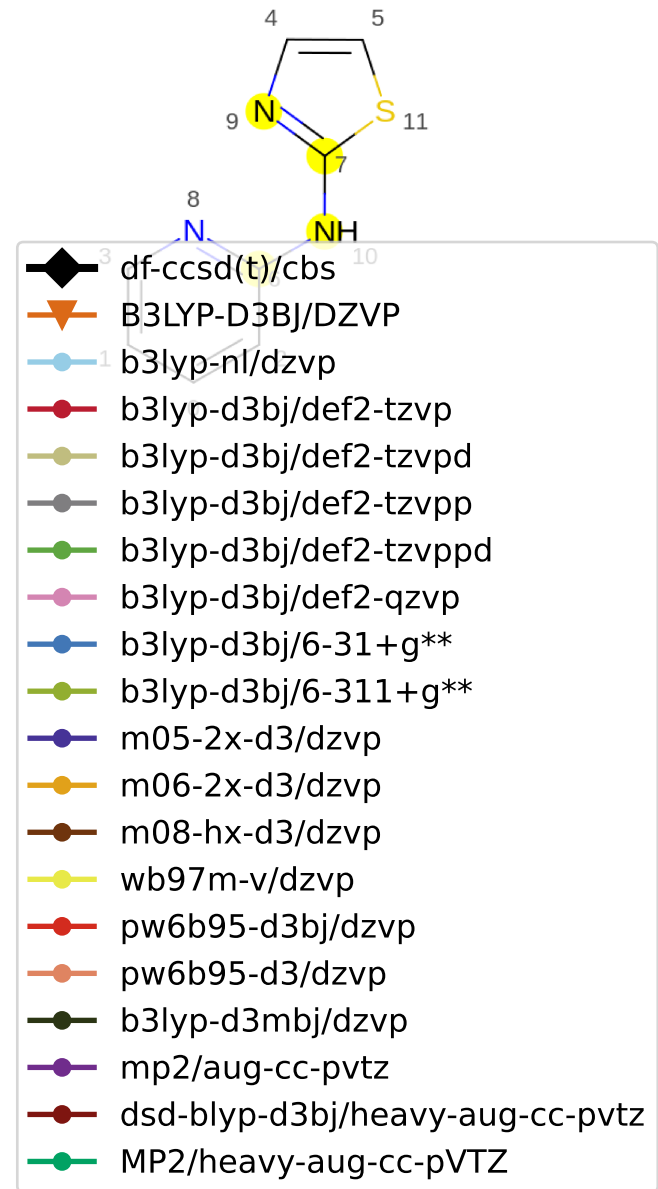
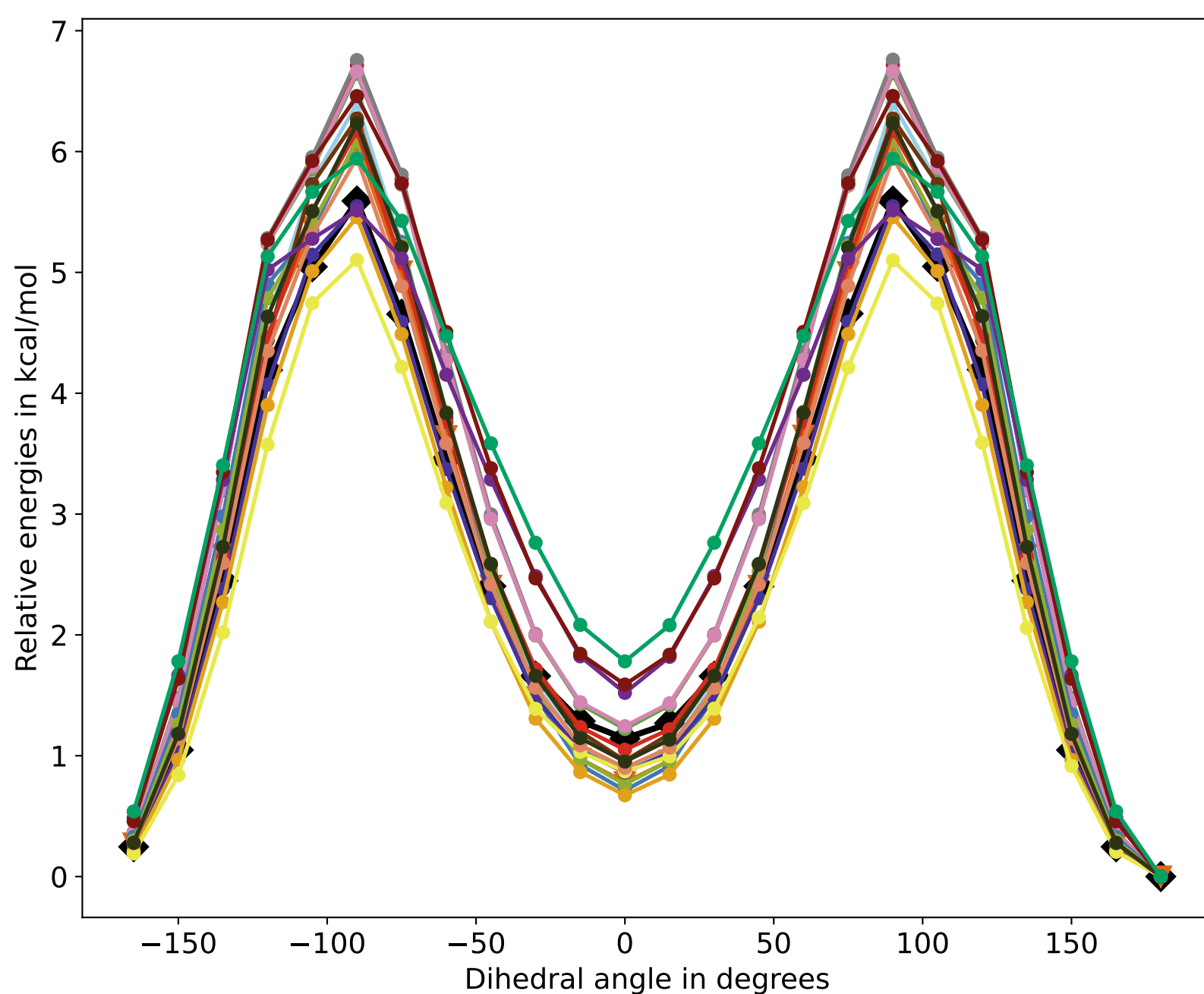




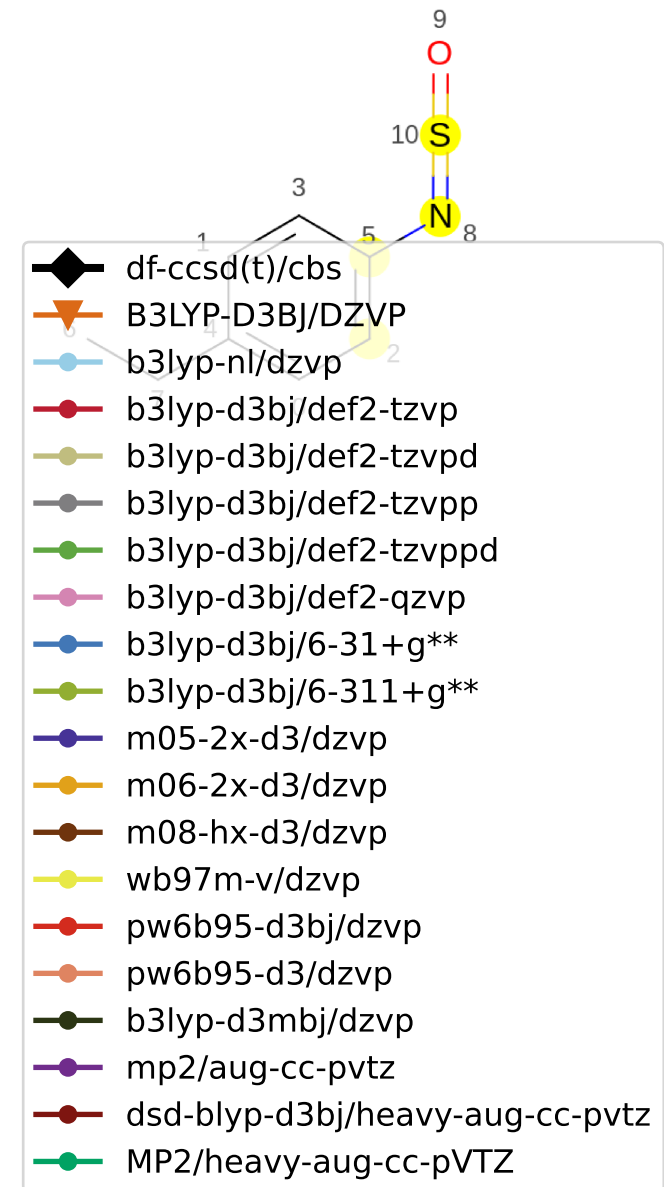
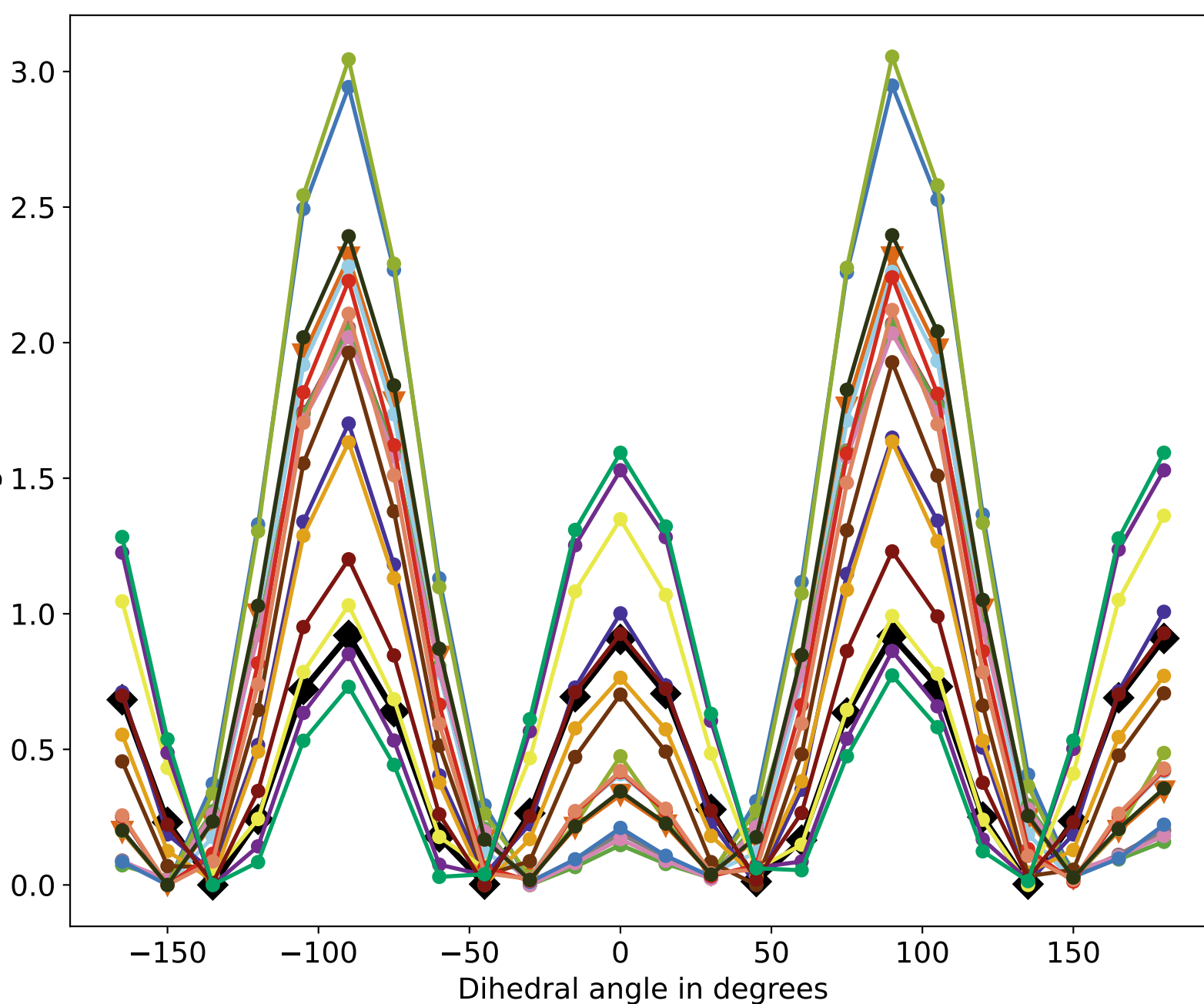
Relative energies in kcal/mol

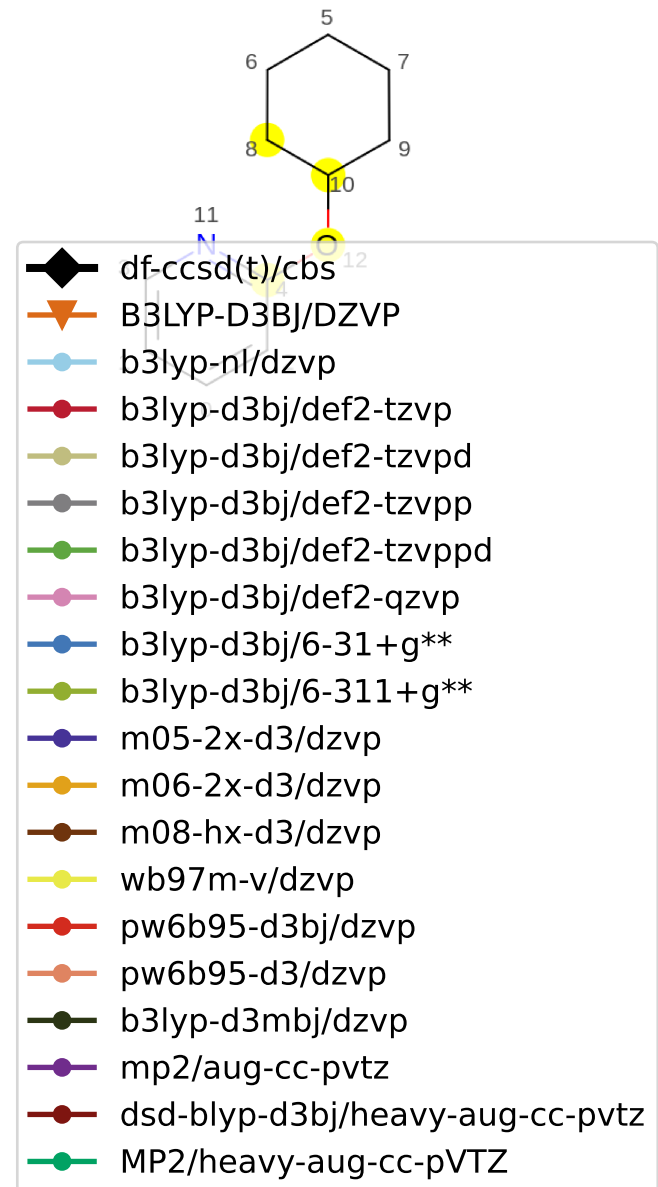
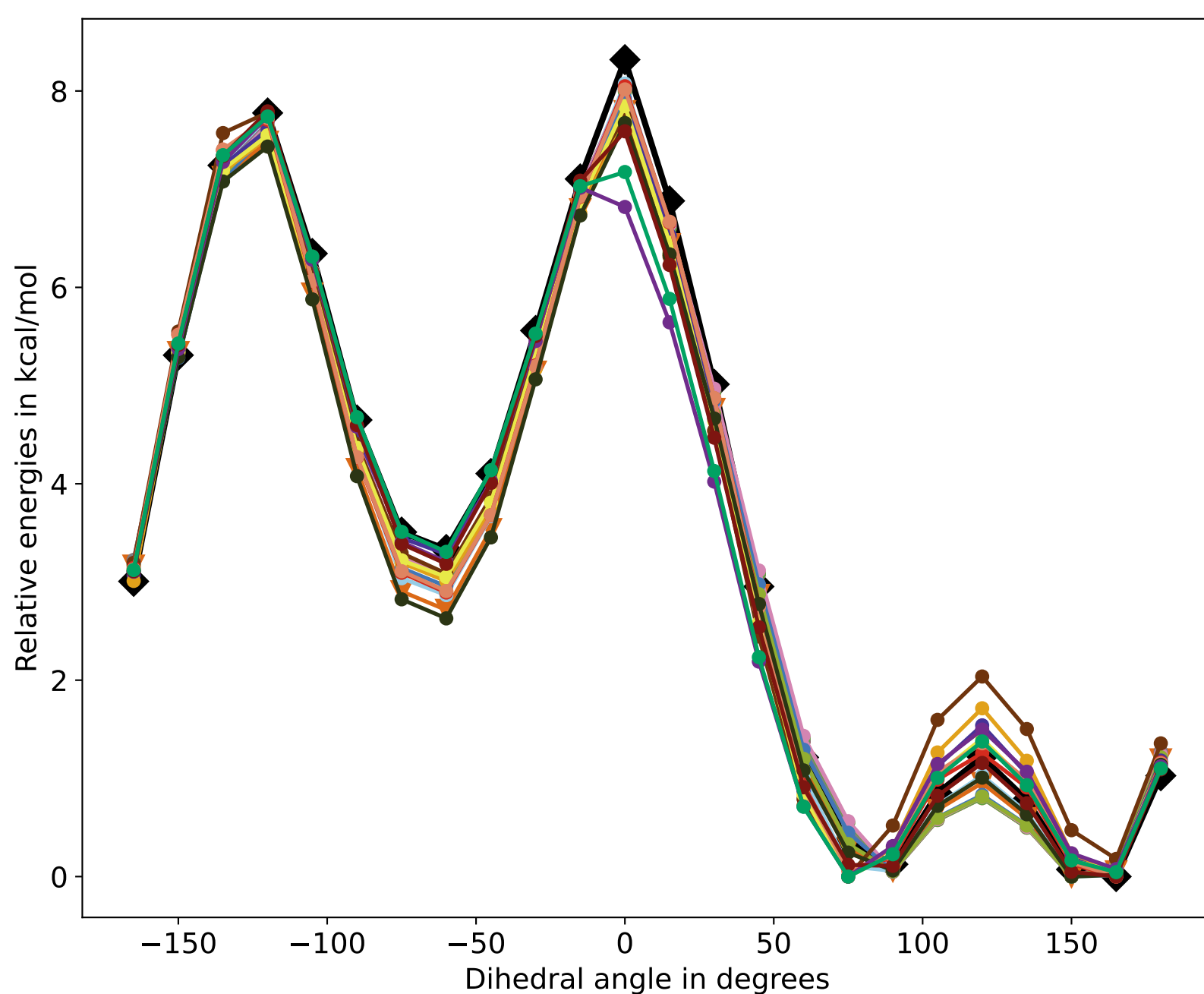


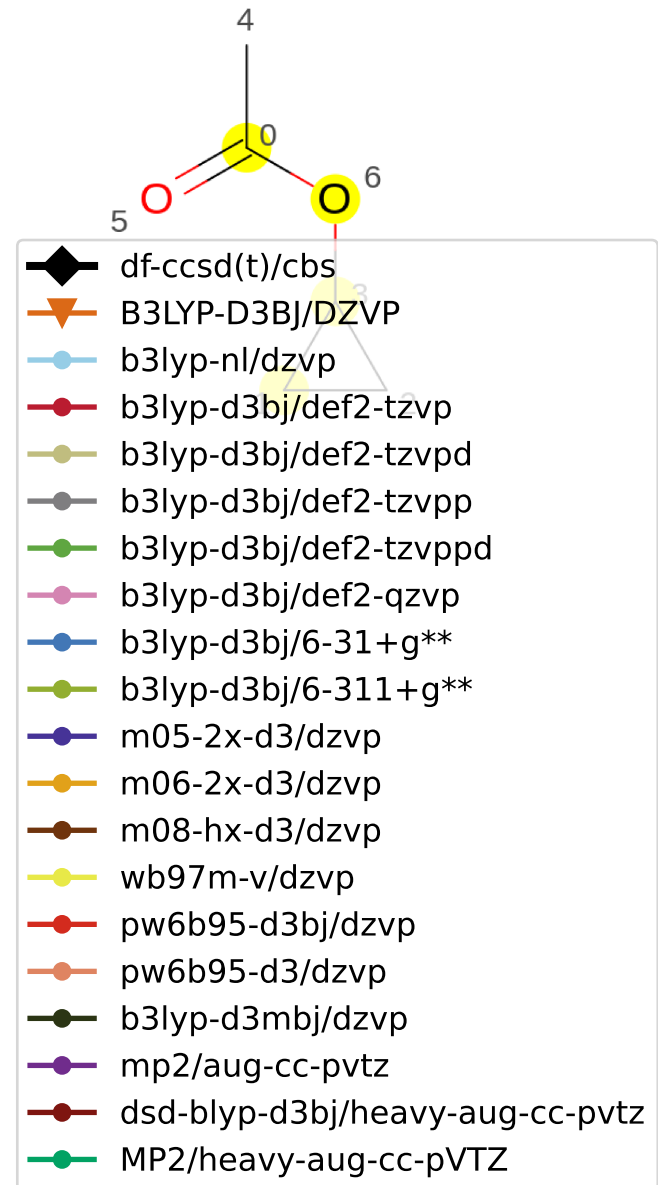
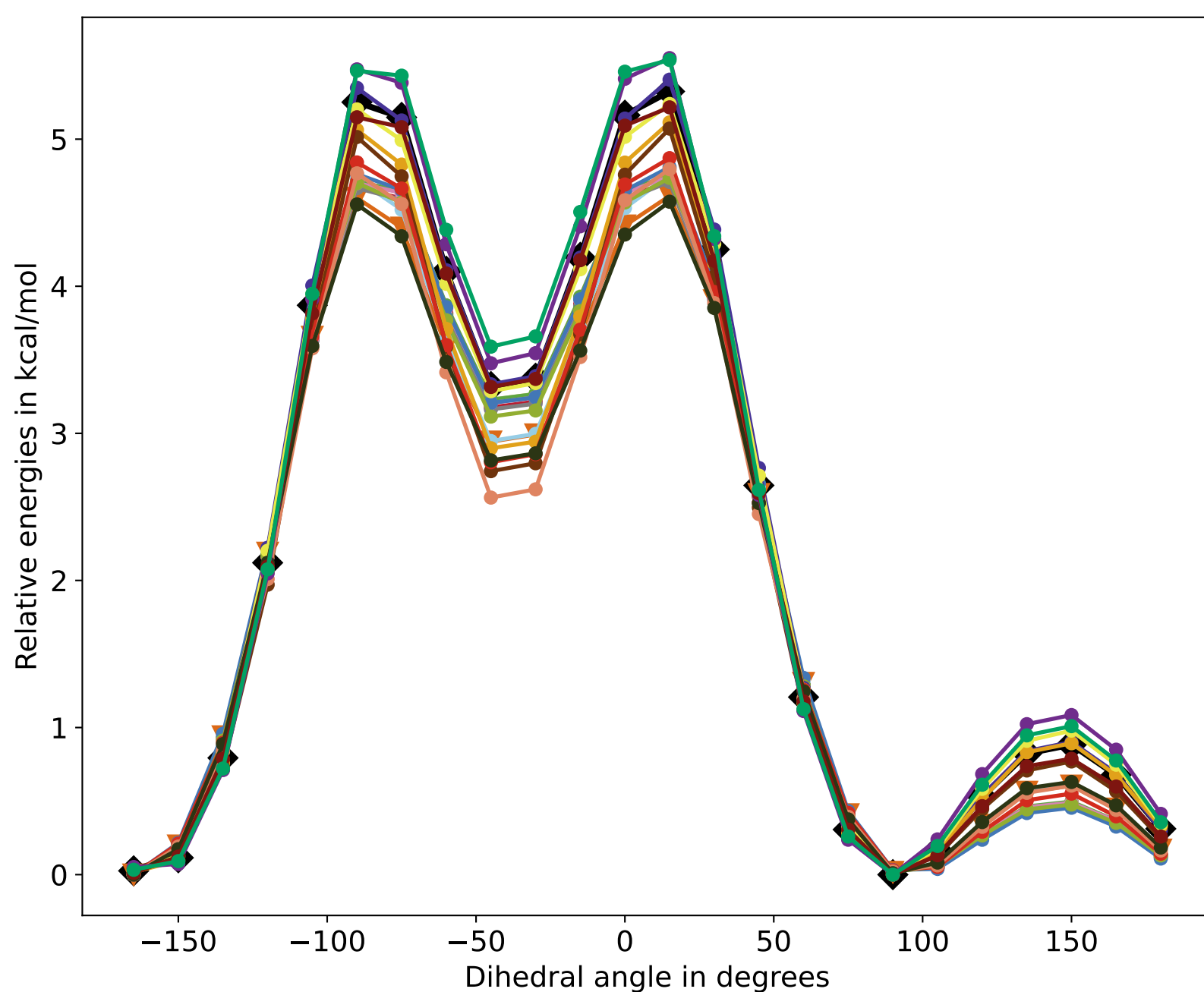


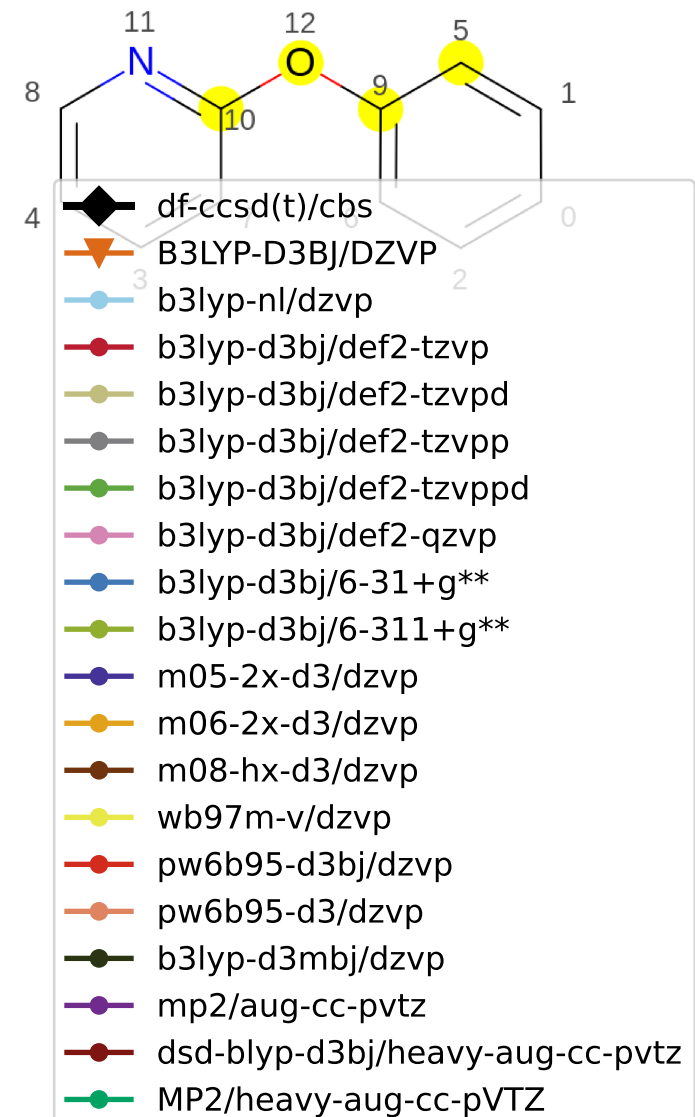
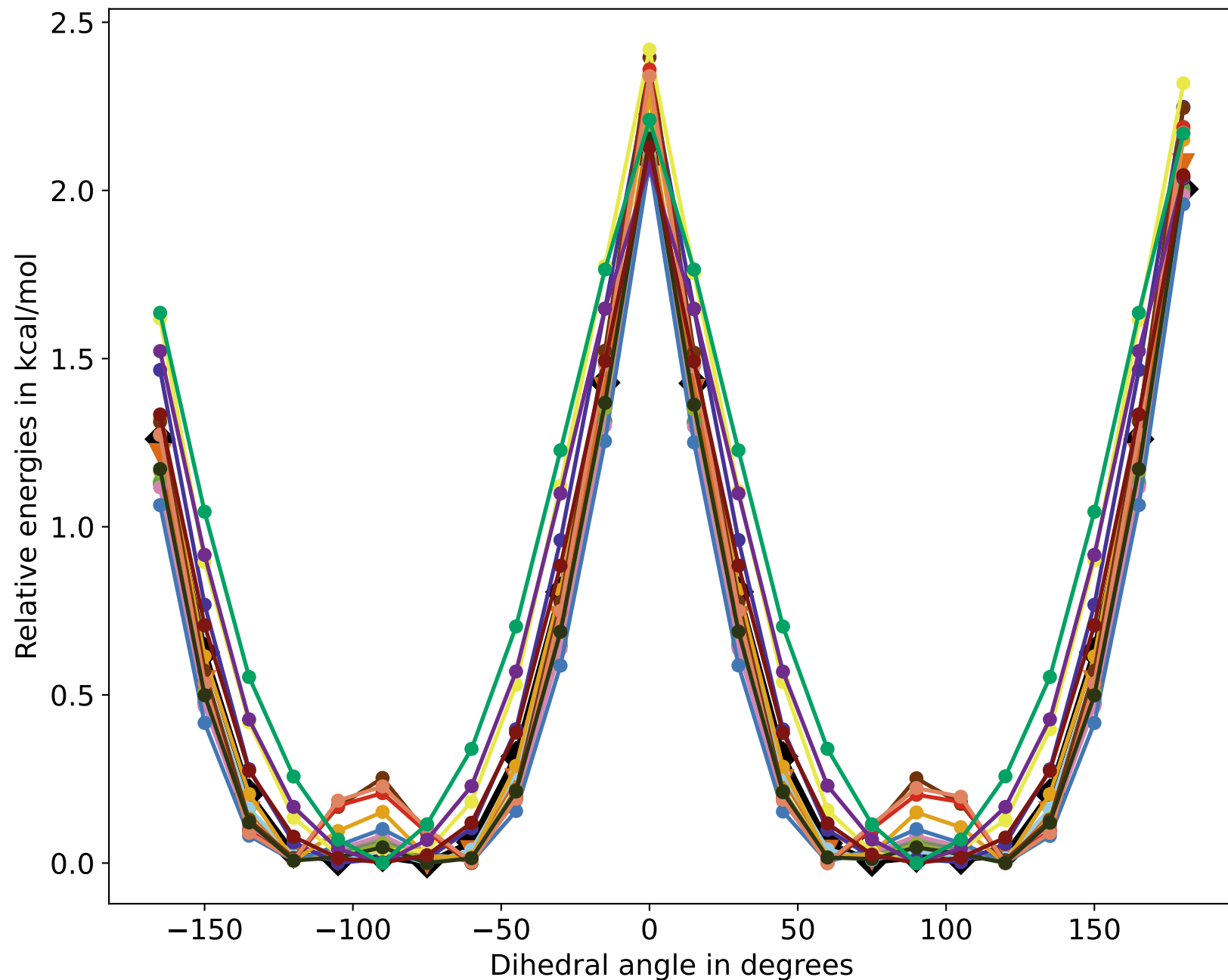


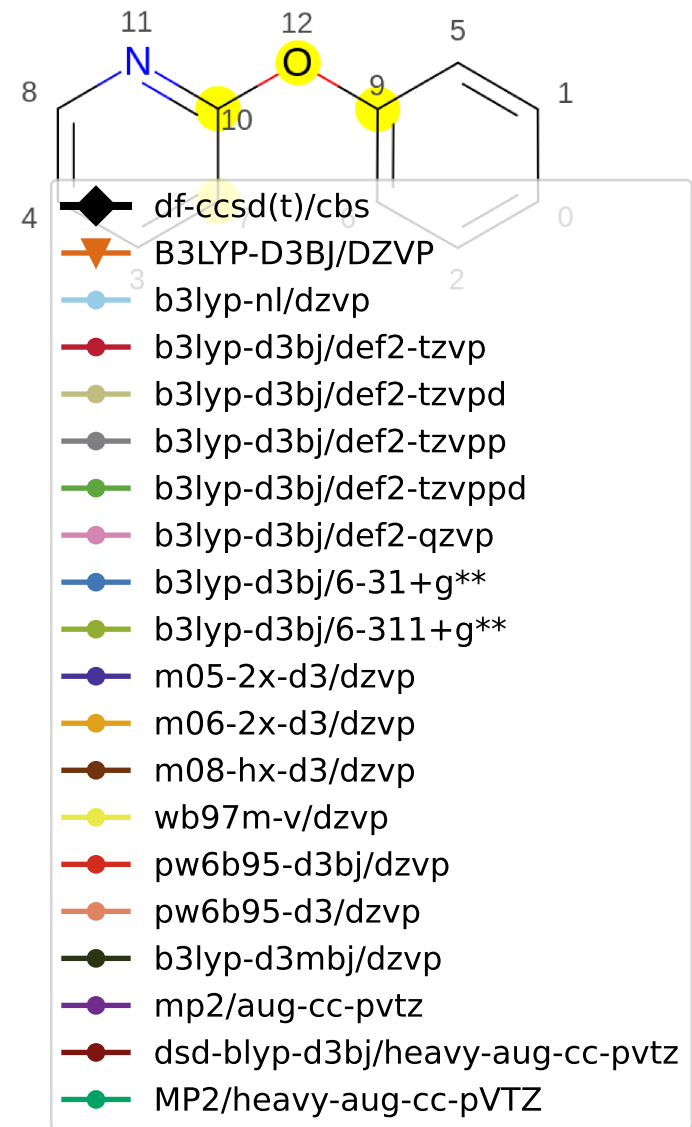
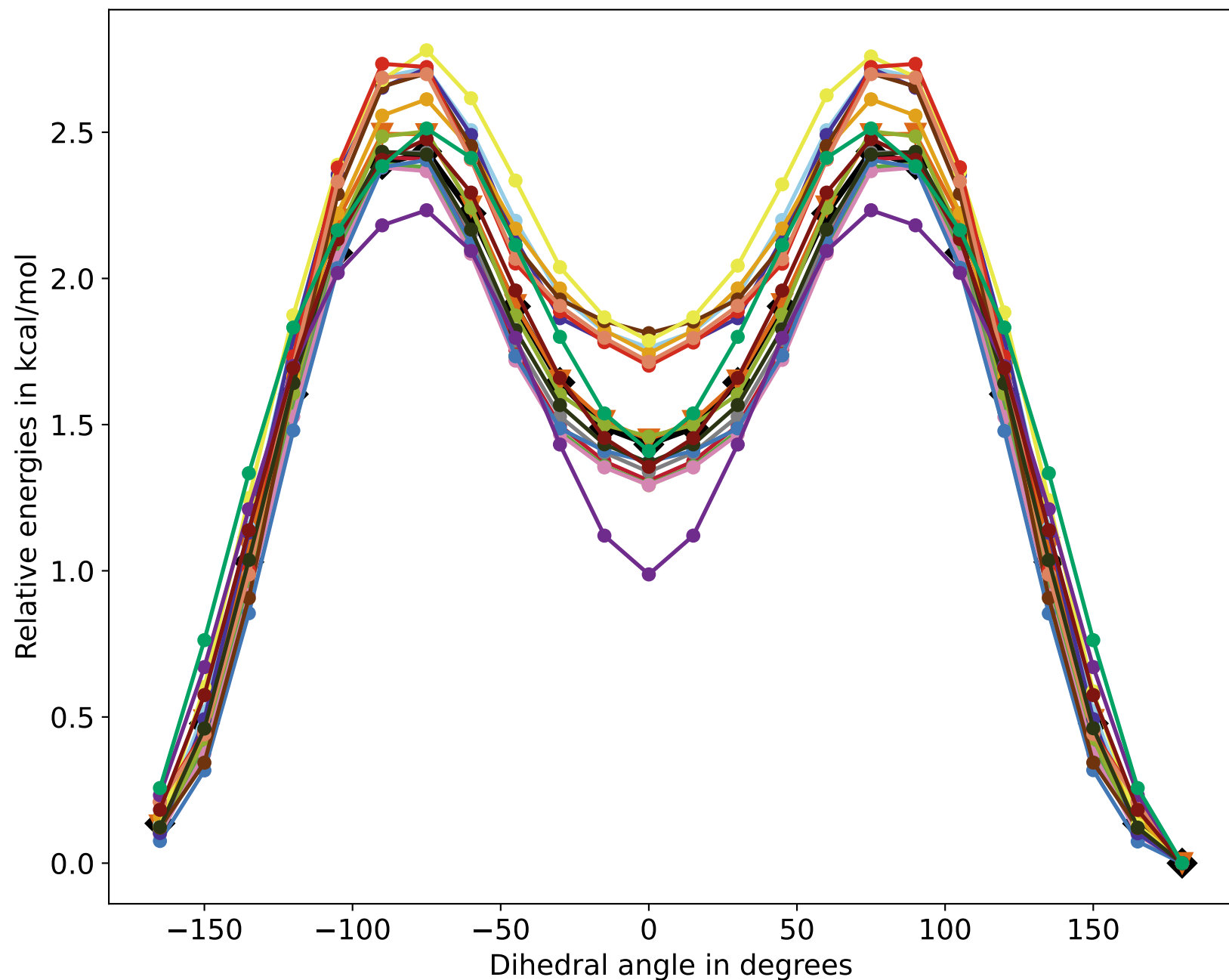
Relative energies in kcal/mol

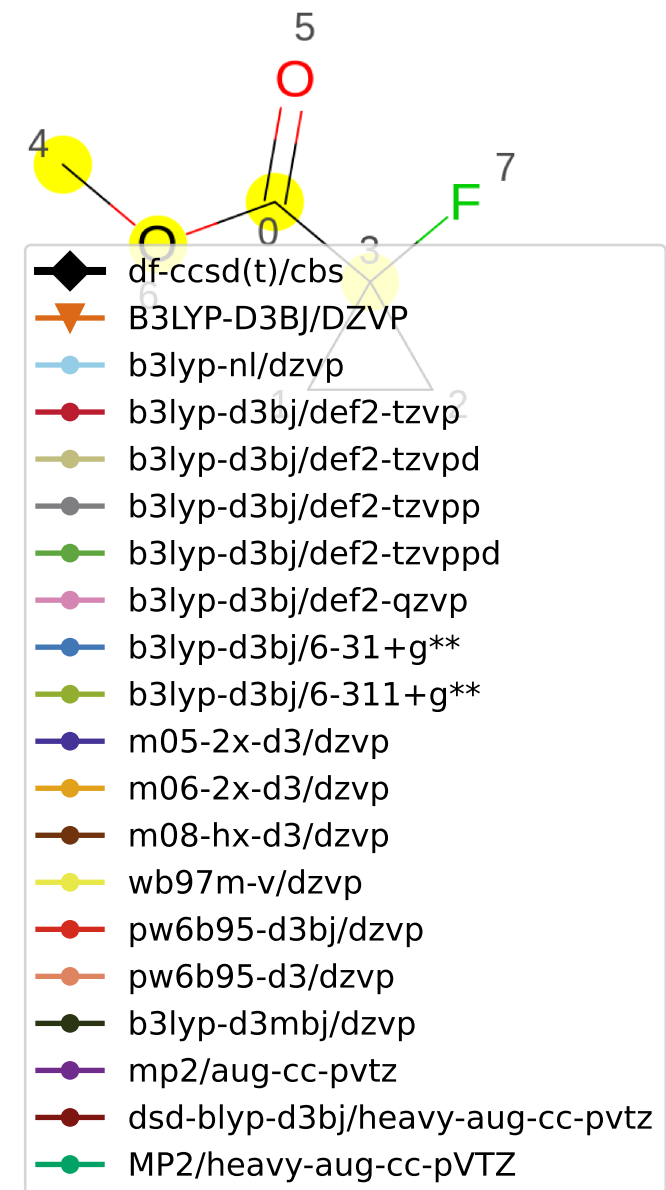
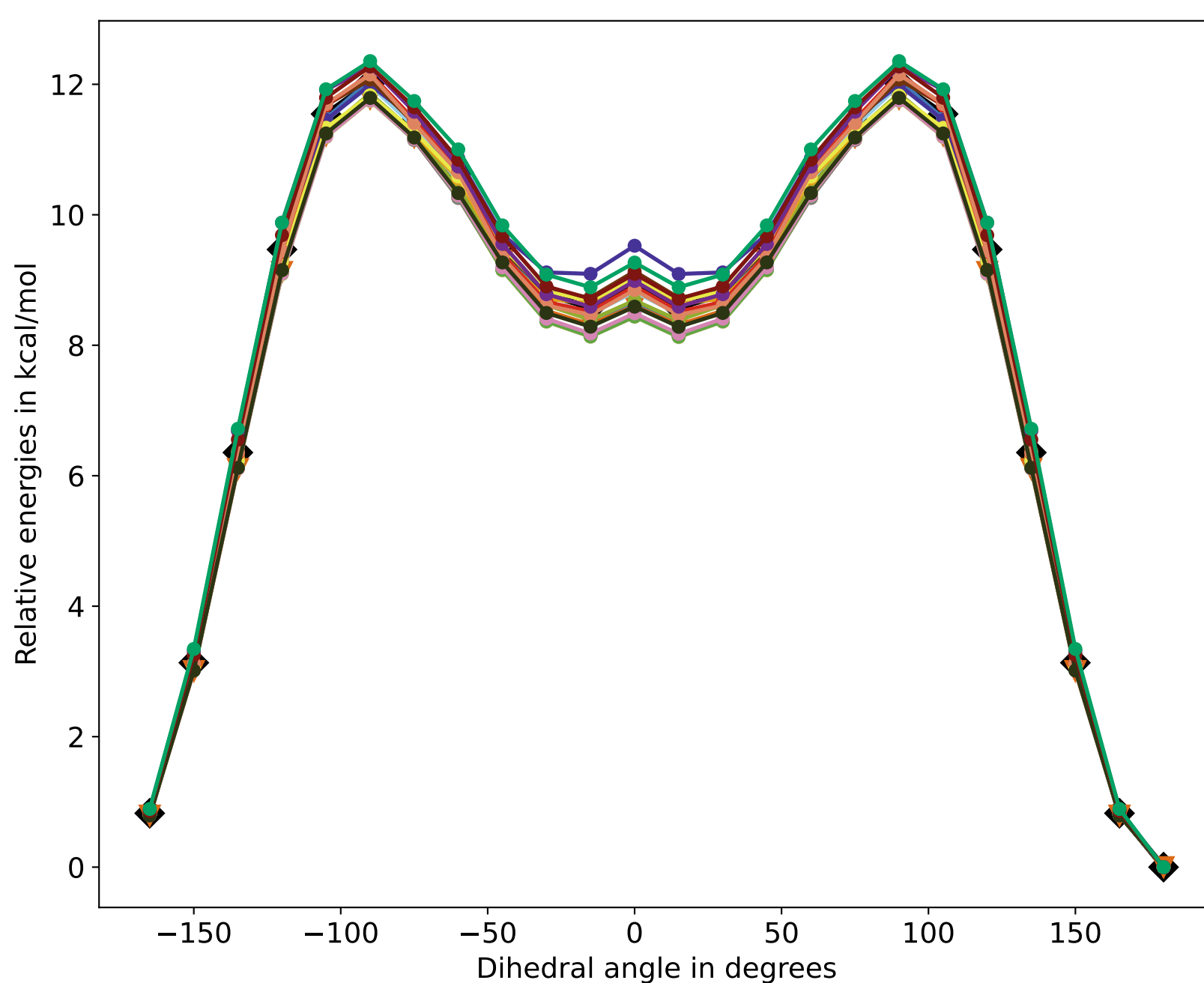


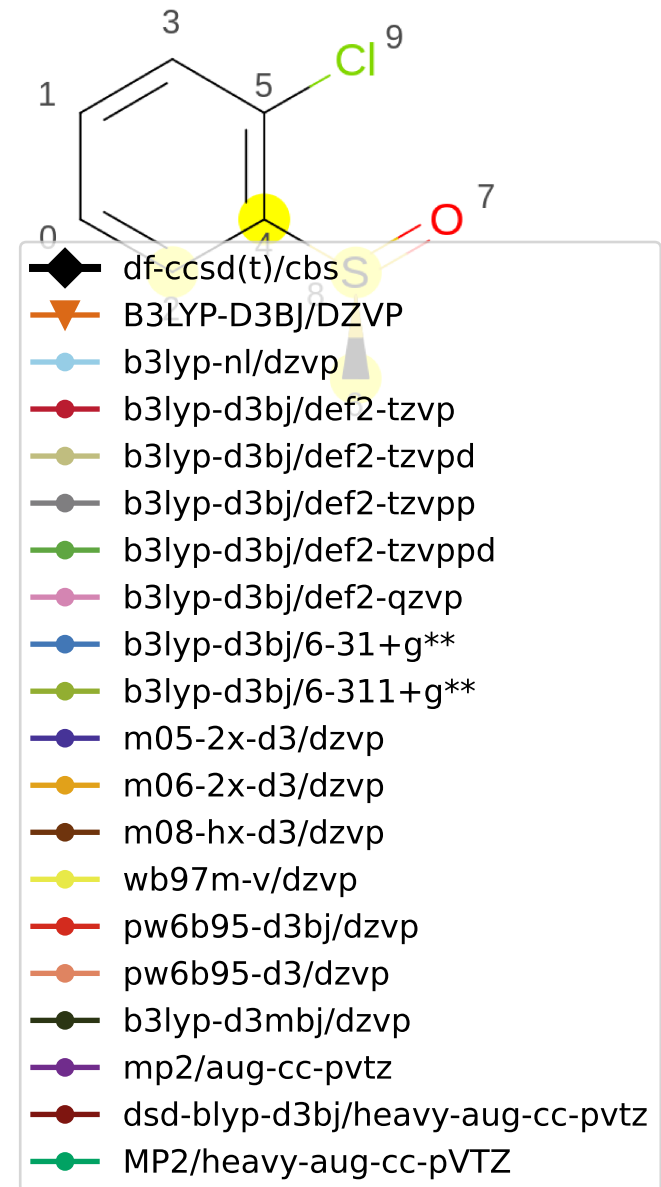
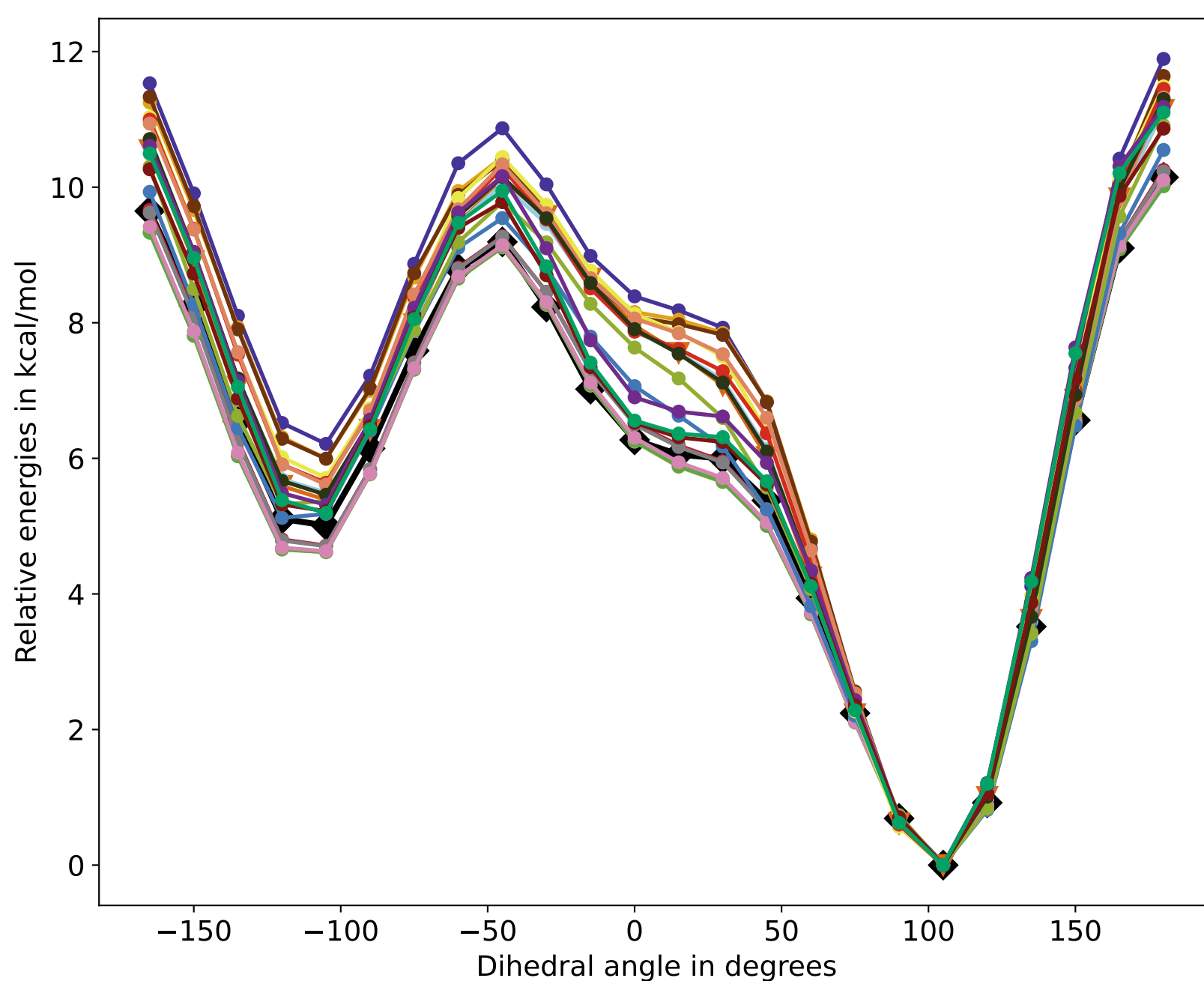


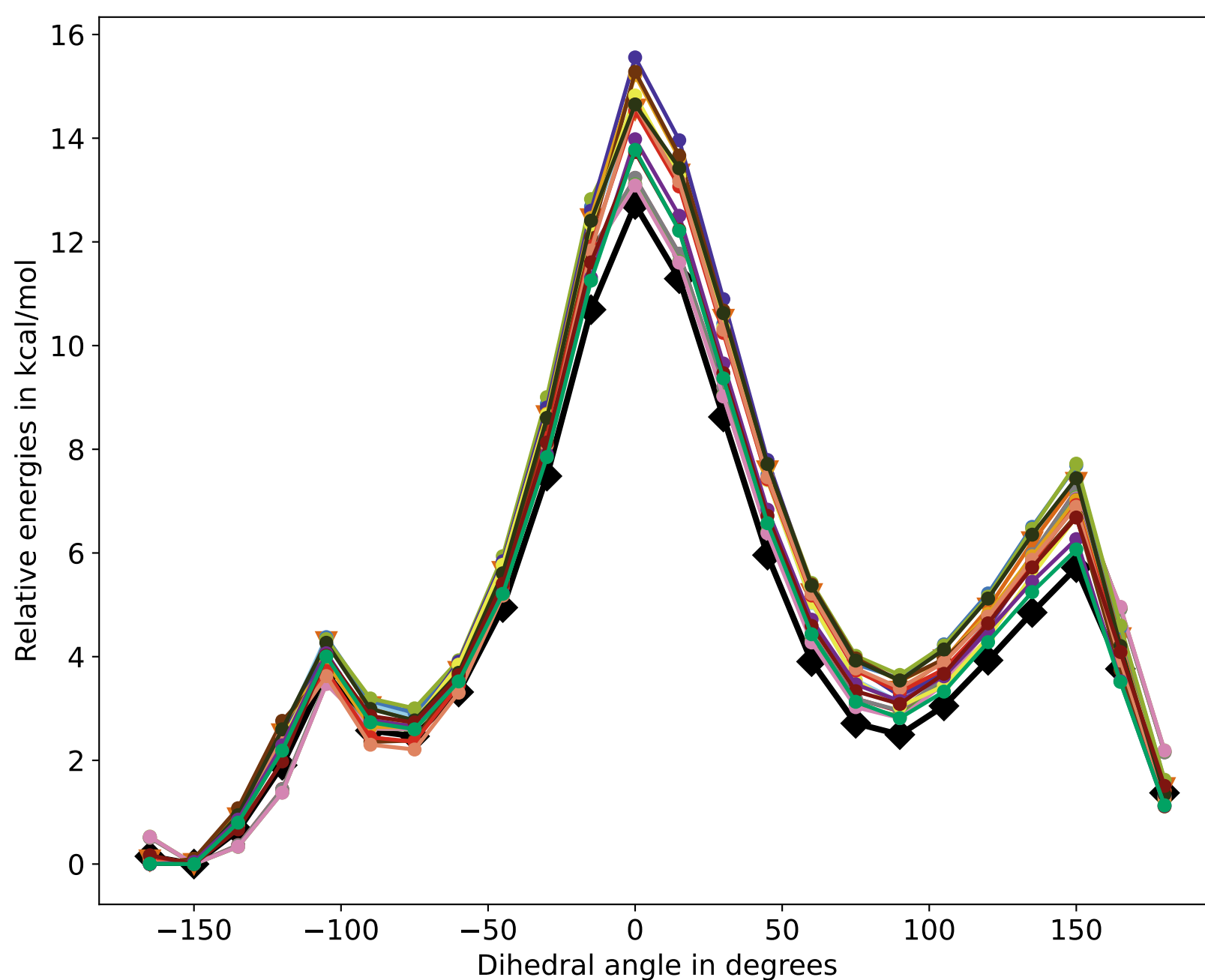




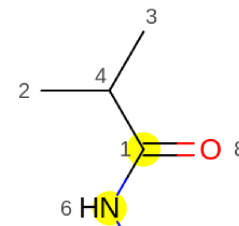
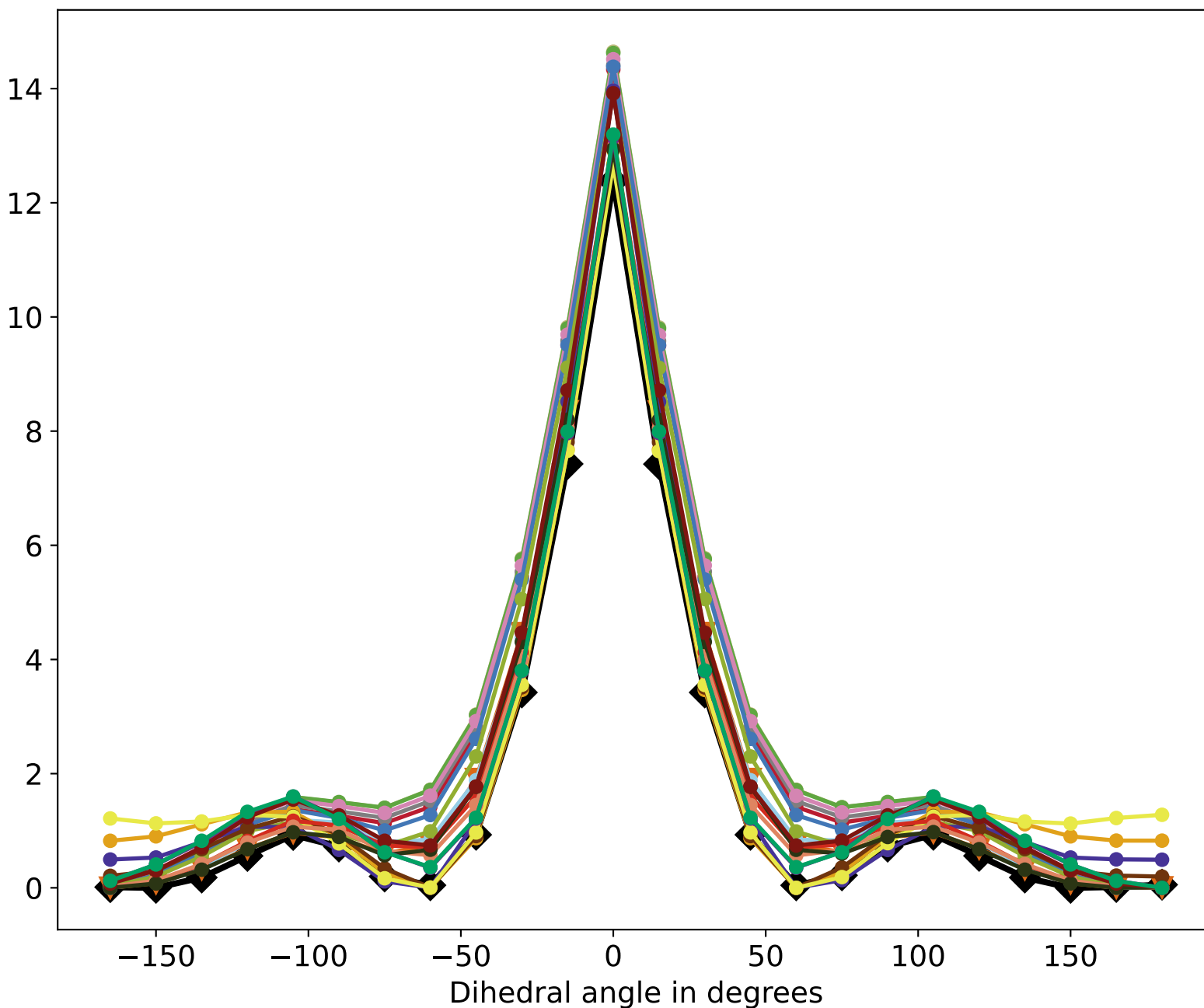




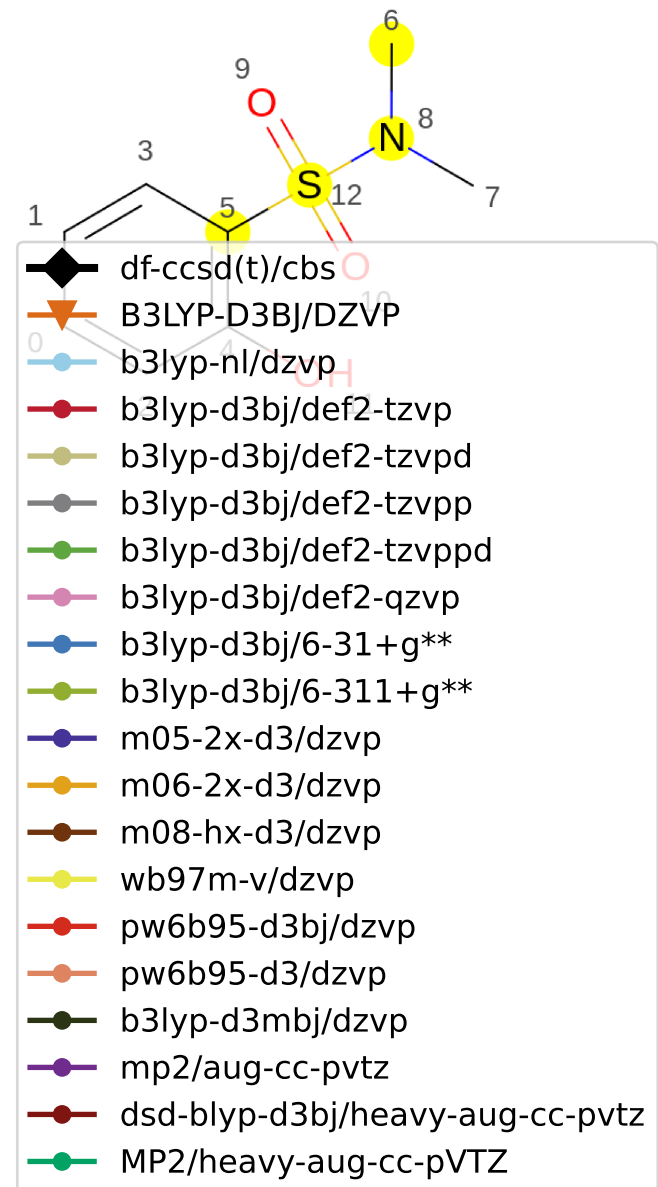
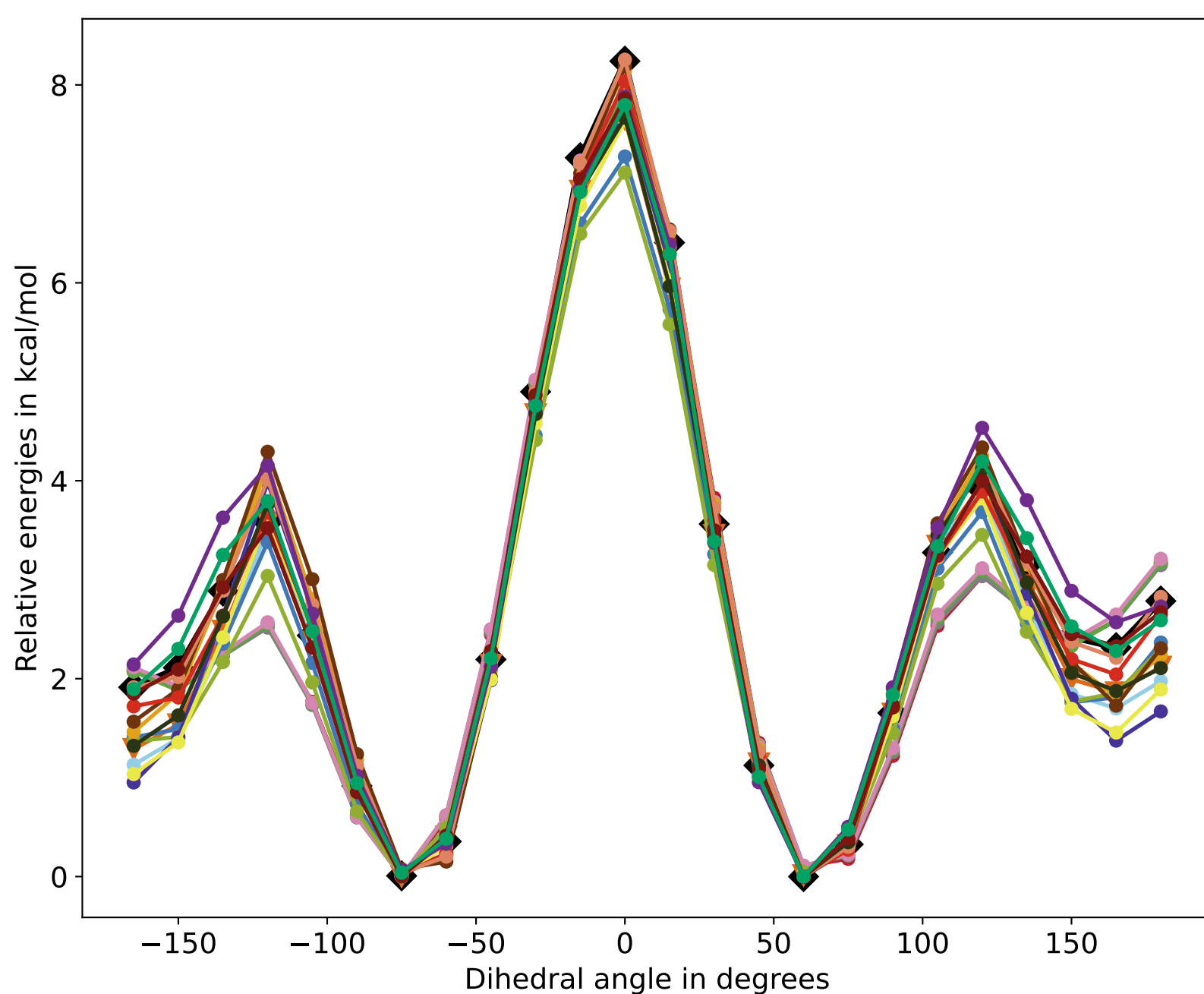


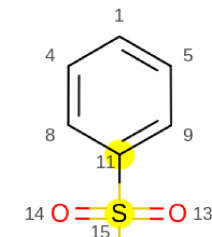
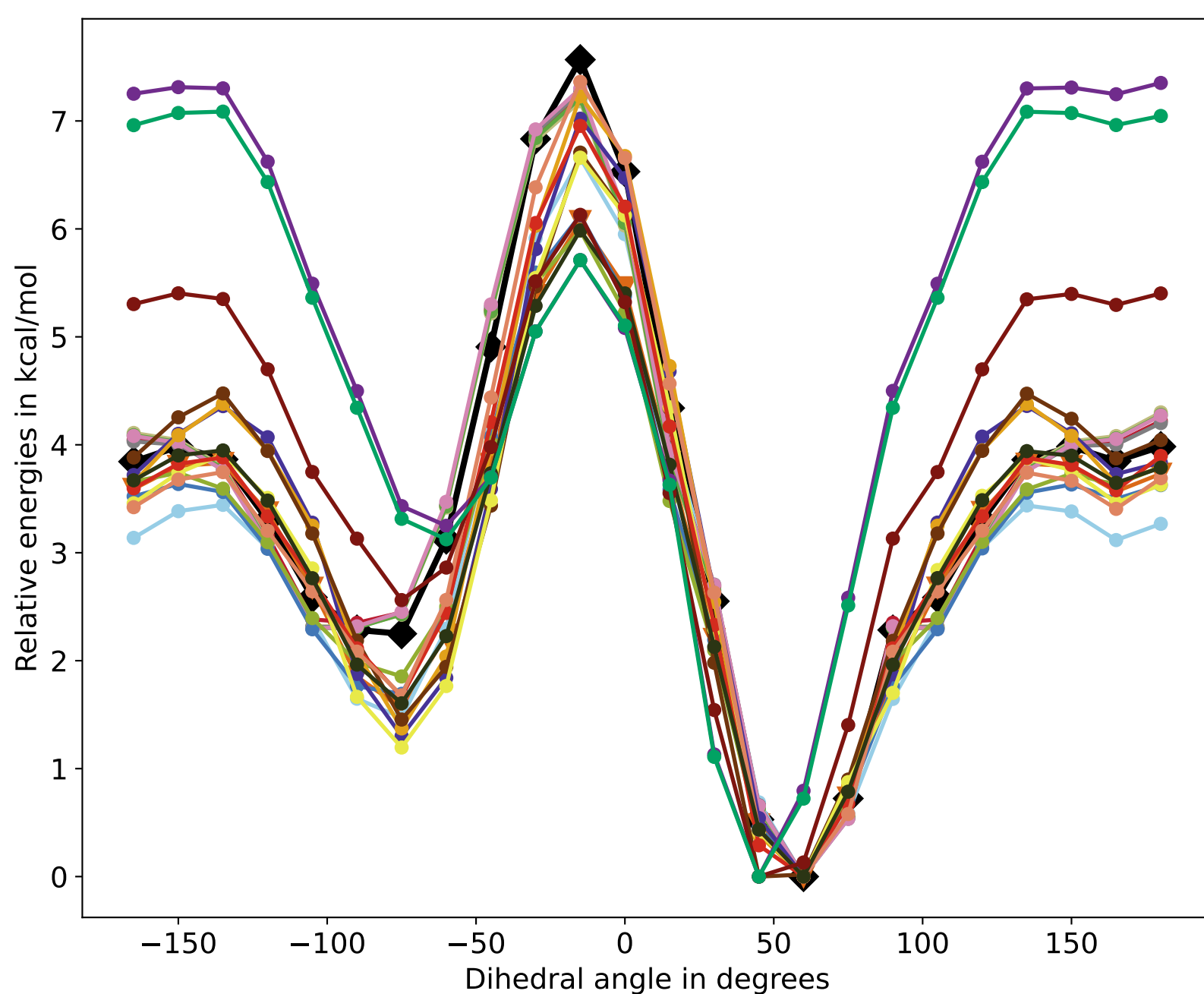


Relative energies in kcal/mol

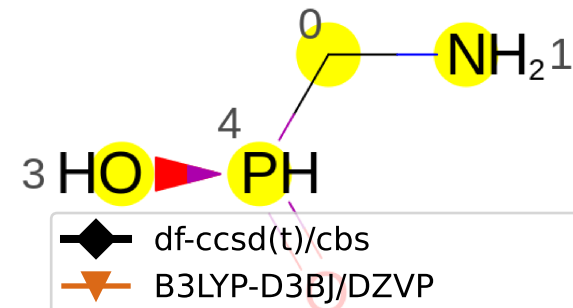
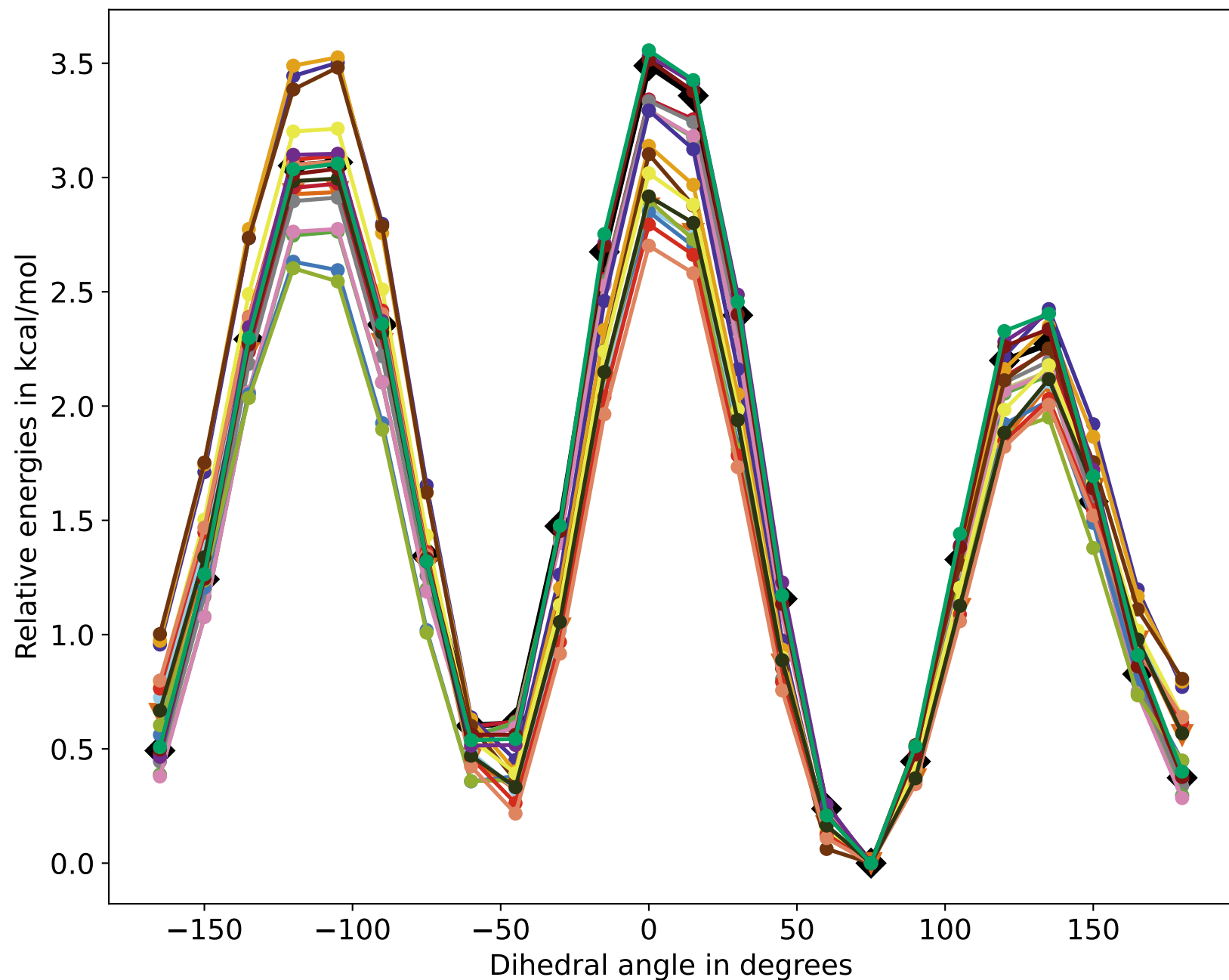


- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
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- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ





- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
- pw6b95-d3bj/dzvp
- pw6b95-d3/dzvp
- b3lyp-d3mbj/dzvp
- mp2/aug-cc-pvtz
- dsd-blyp-d3bj/heavy-aug-cc-pvtz
- MP2/heavy-aug-cc-pVTZ



- df-ccsd(t)/cbs
- B3LYP-D3BJ/DZVP
- b3lyp-nl/dzvp
- b3lyp-d3bj/def2-tzvp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-tzvpp
- b3lyp-d3bj/def2-tzvppd
- b3lyp-d3bj/def2-qzvp
- b3lyp-d3bj/6-31+g**
- b3lyp-d3bj/6-311+g**
- m05-2x-d3/dzvp
- m06-2x-d3/dzvp
- m08-hx-d3/dzvp
- wb97m-v/dzvp
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- mp2/aug-cc-pvtz
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