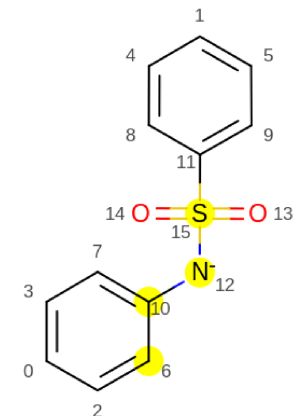
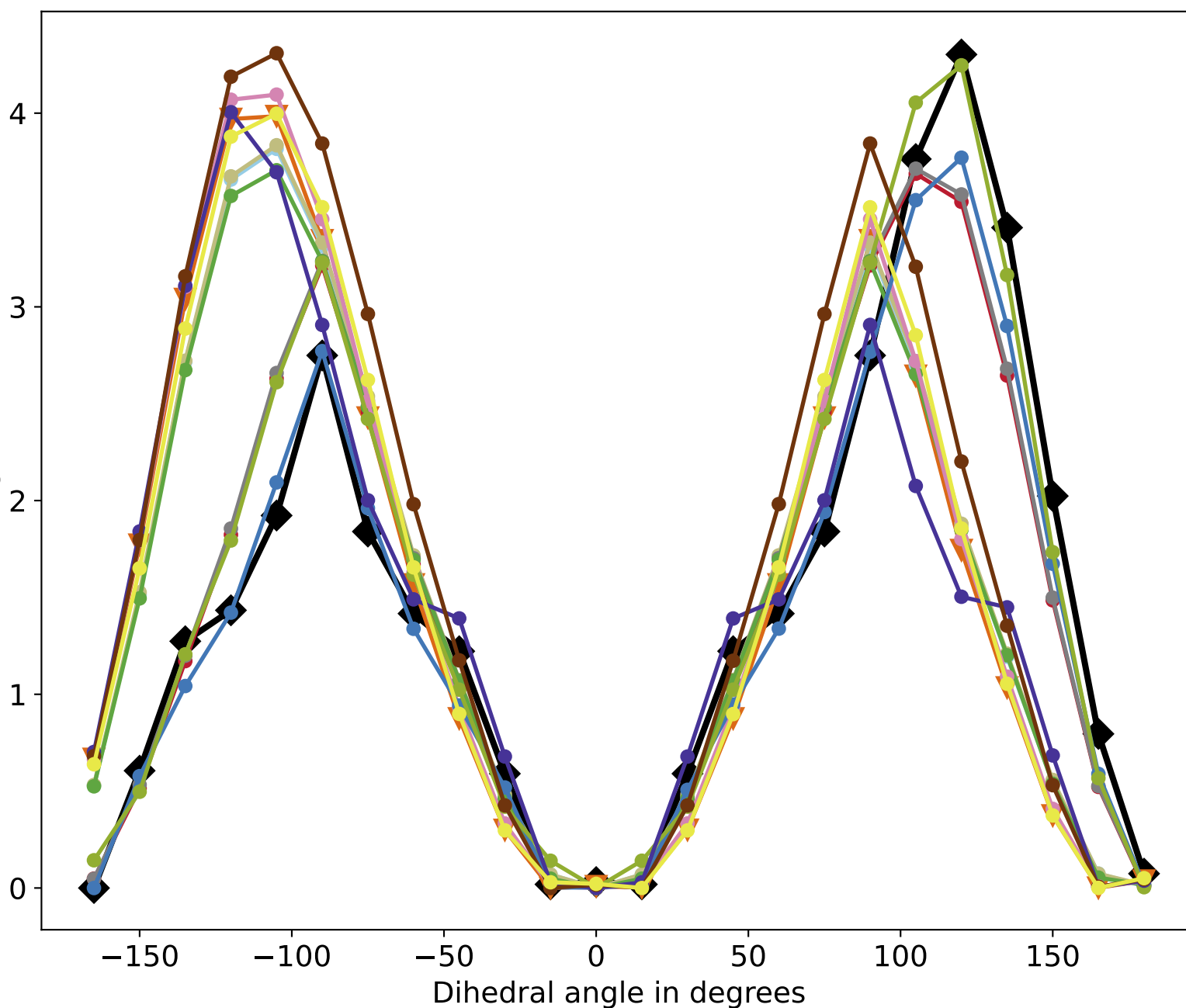
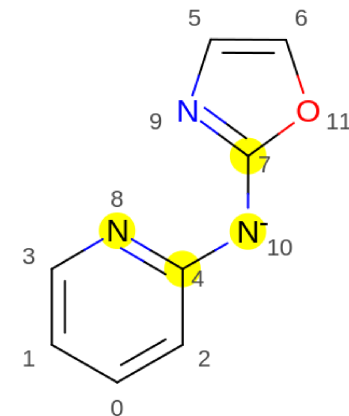
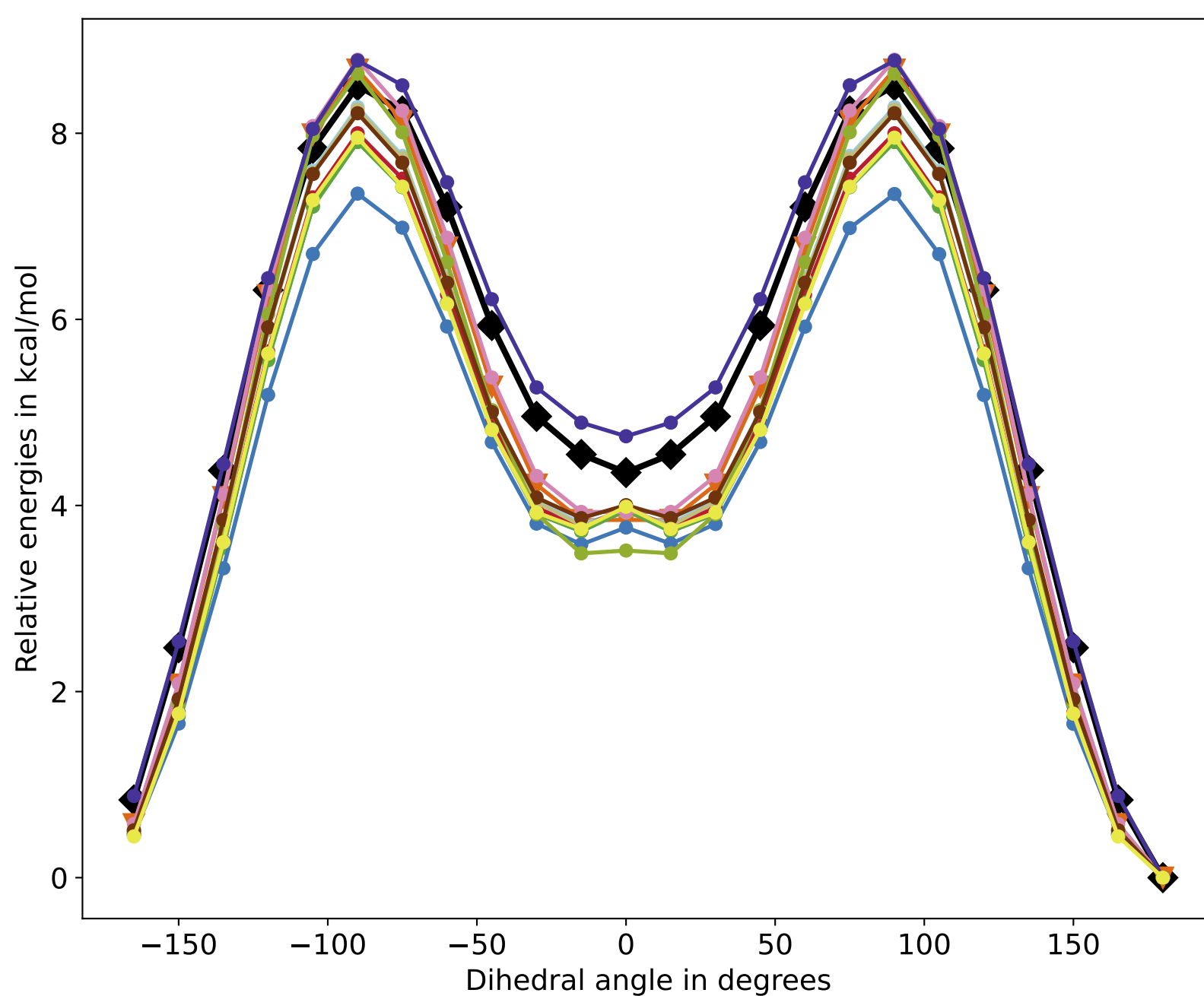


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

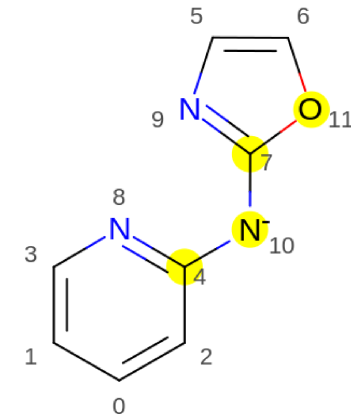
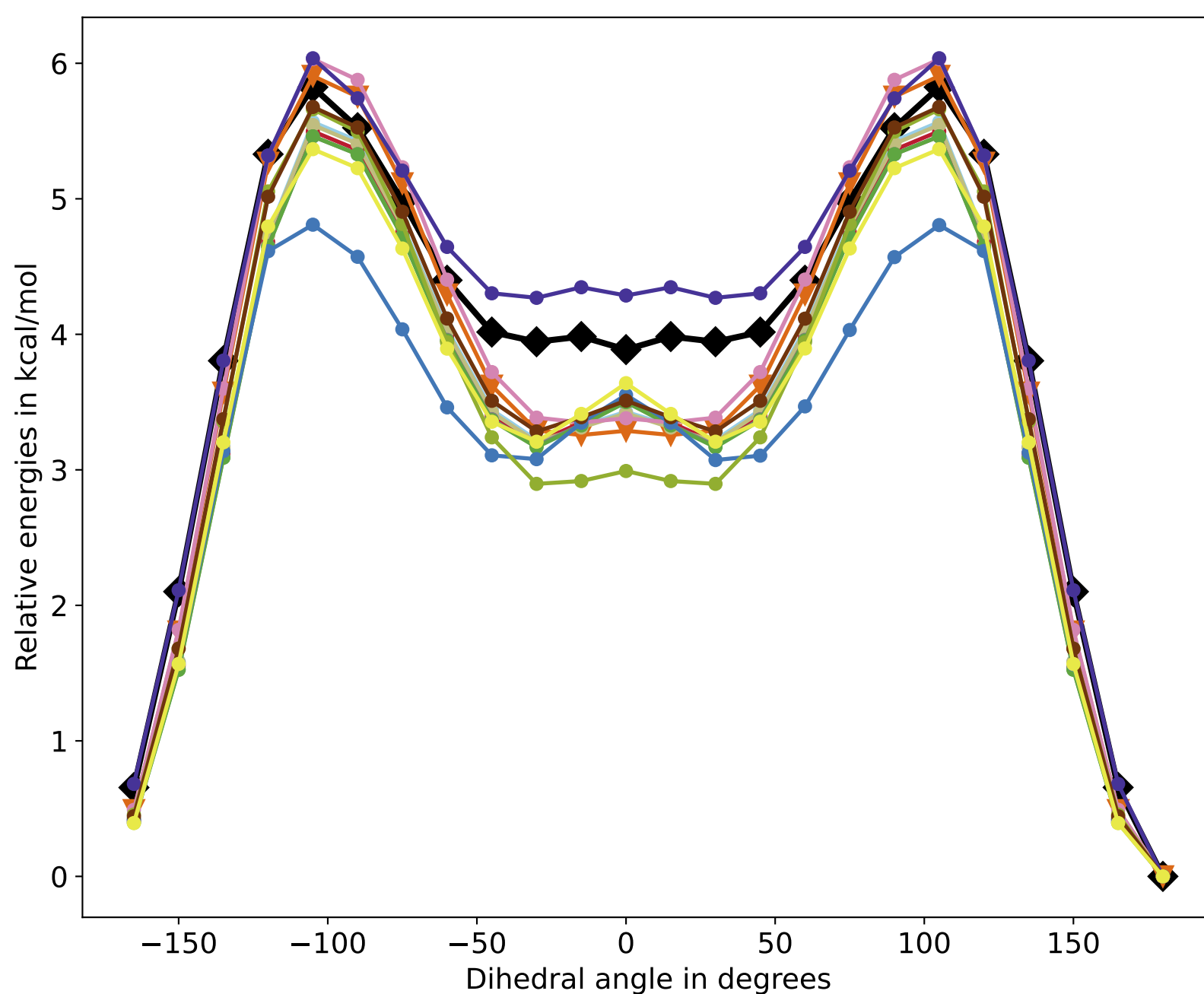
Relative energies in kcal/mol



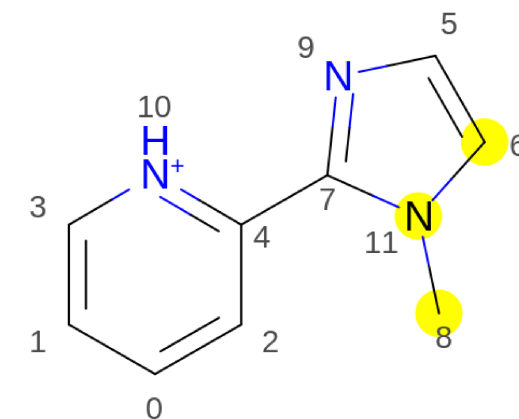
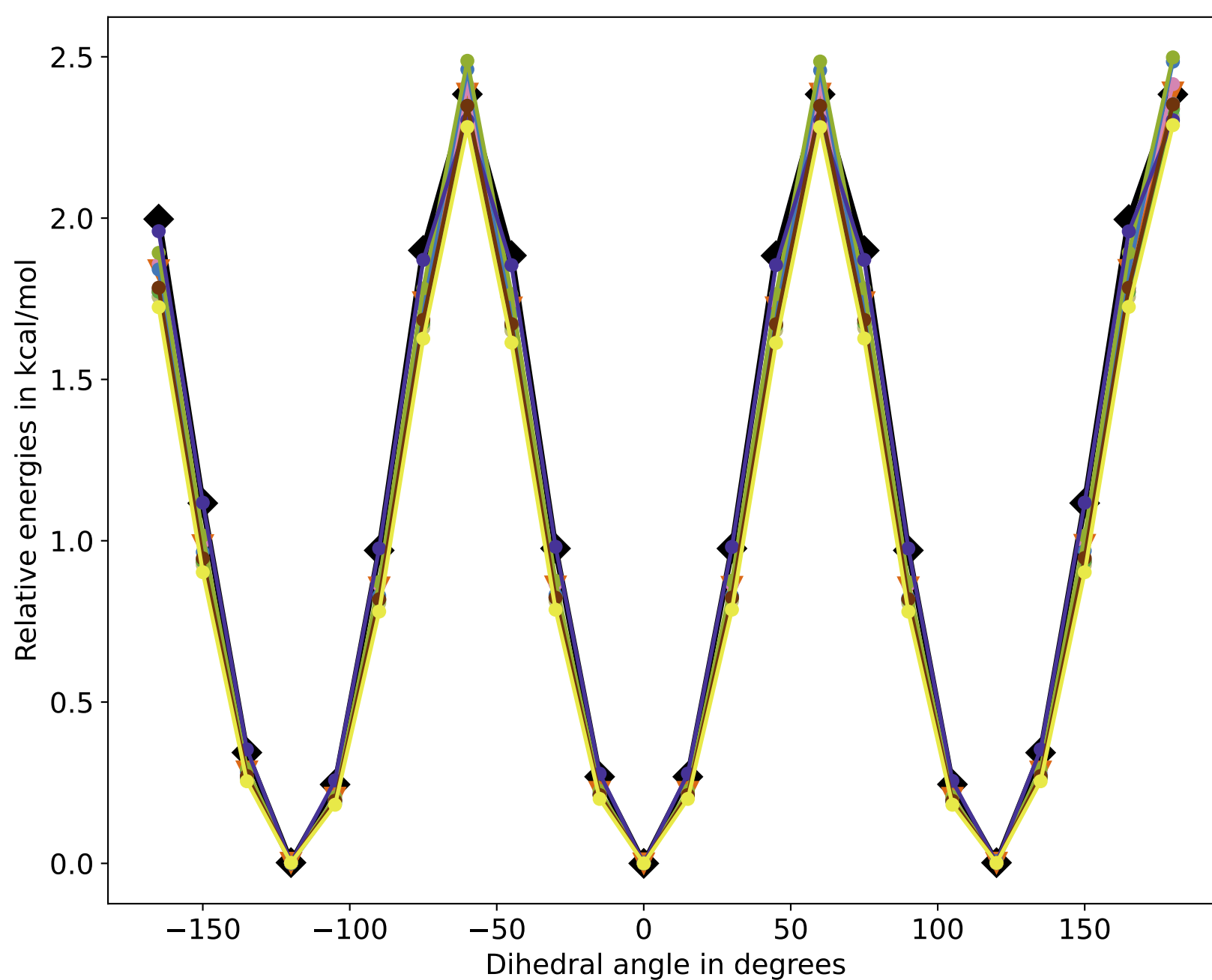
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

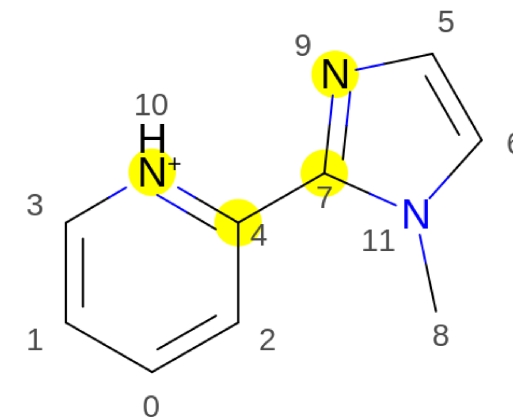
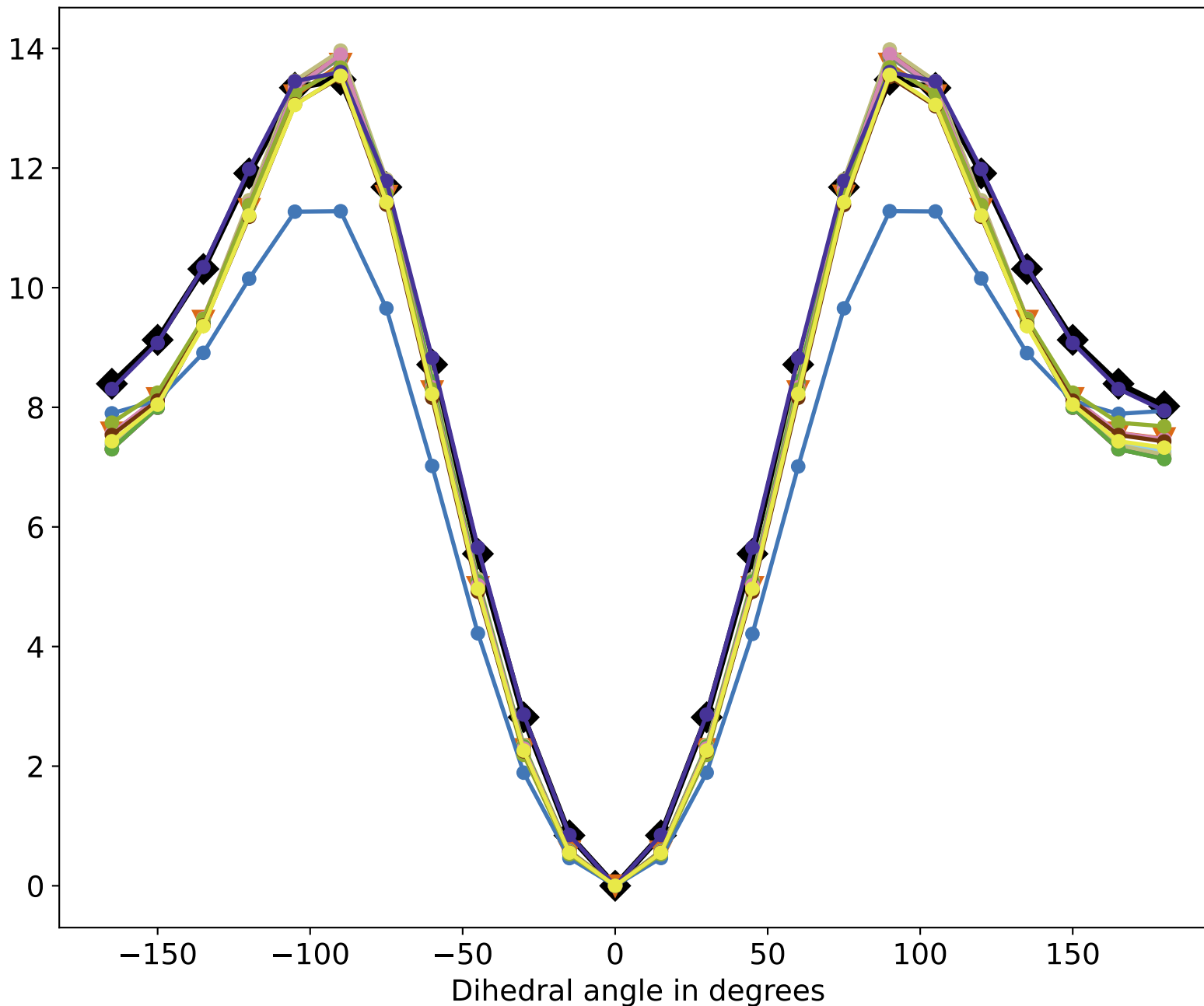


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



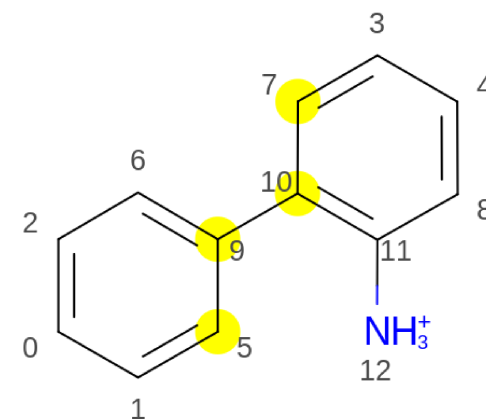
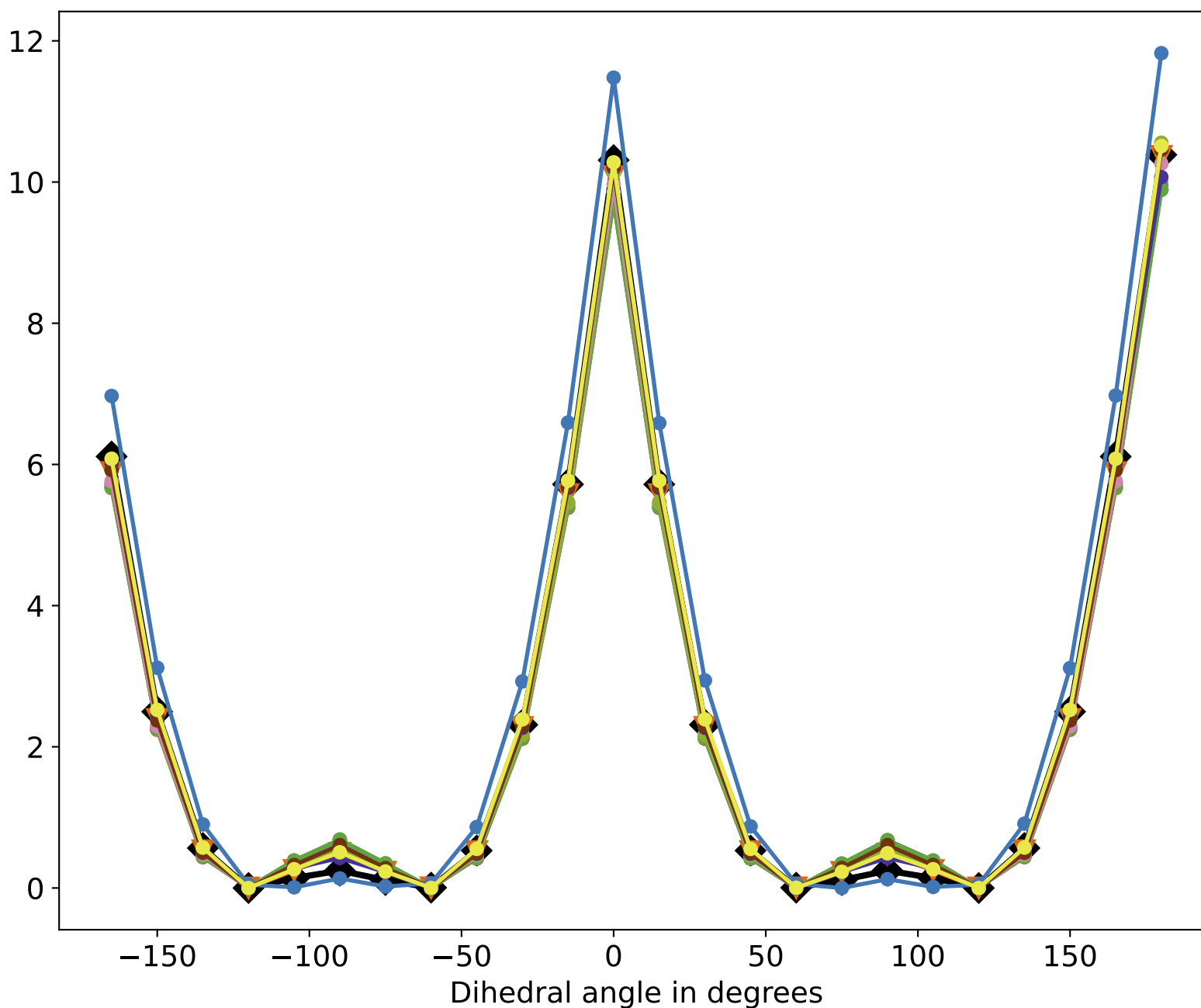
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

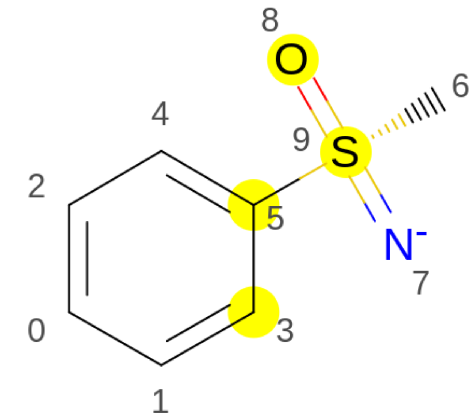
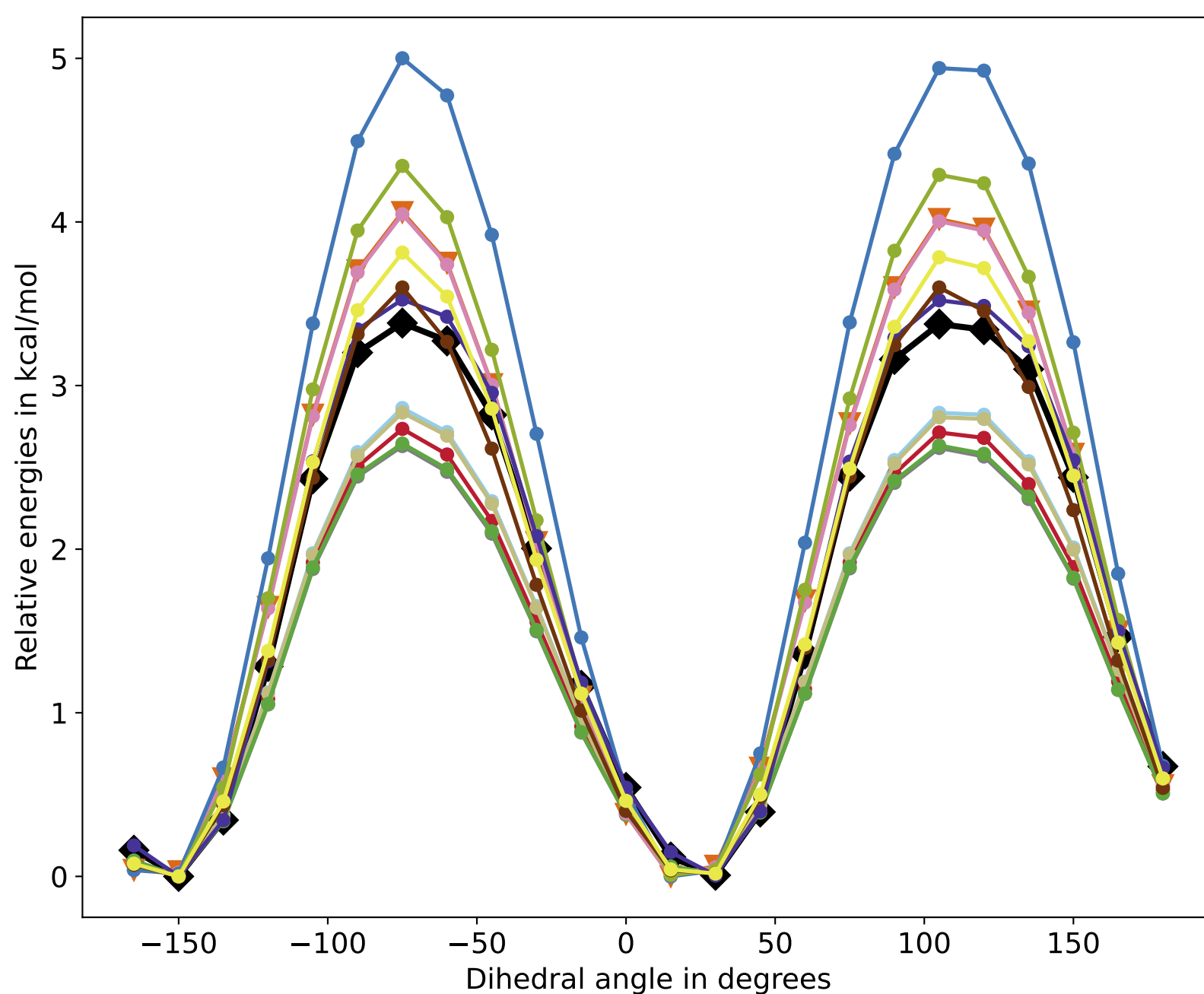


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

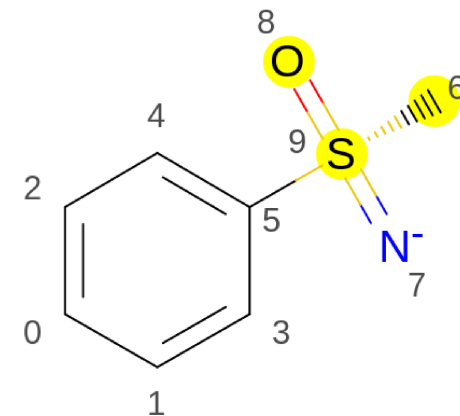
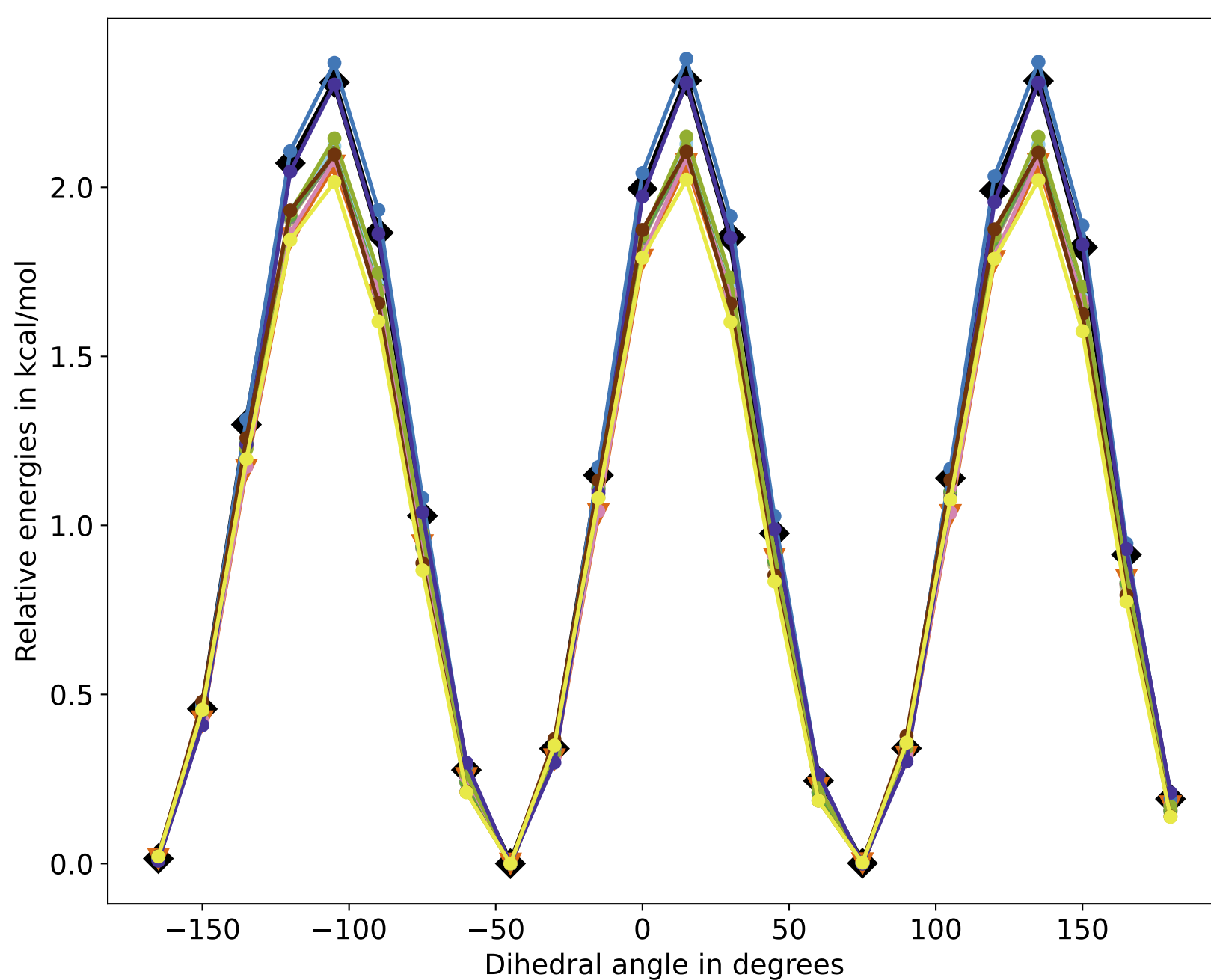
Relative energies in kcal/mol



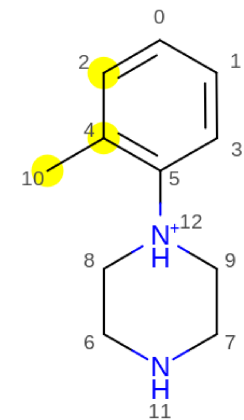
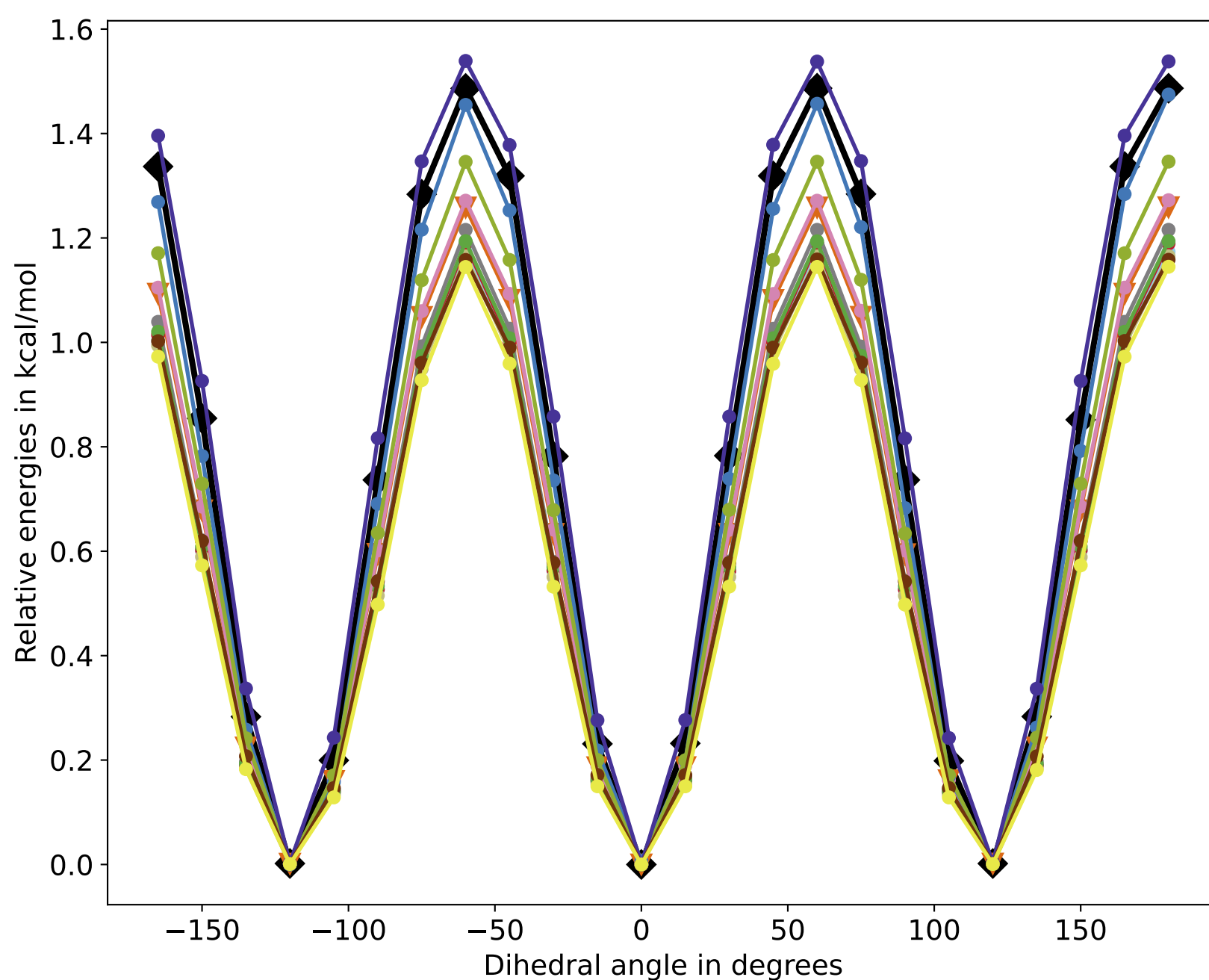
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



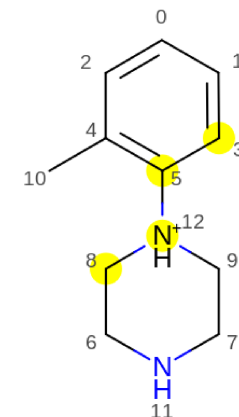
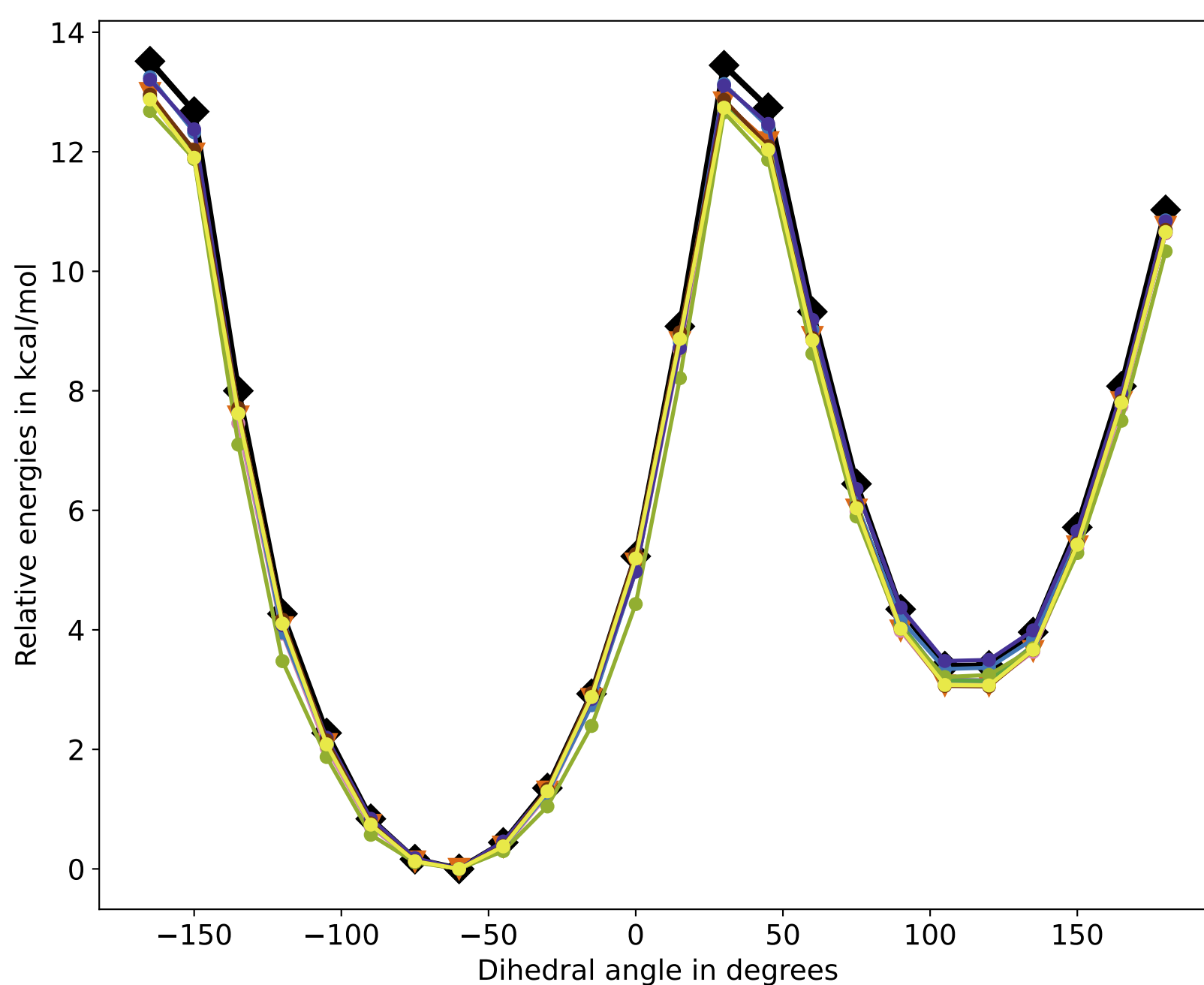
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- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



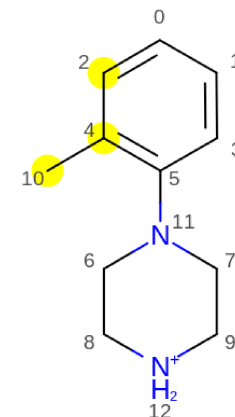
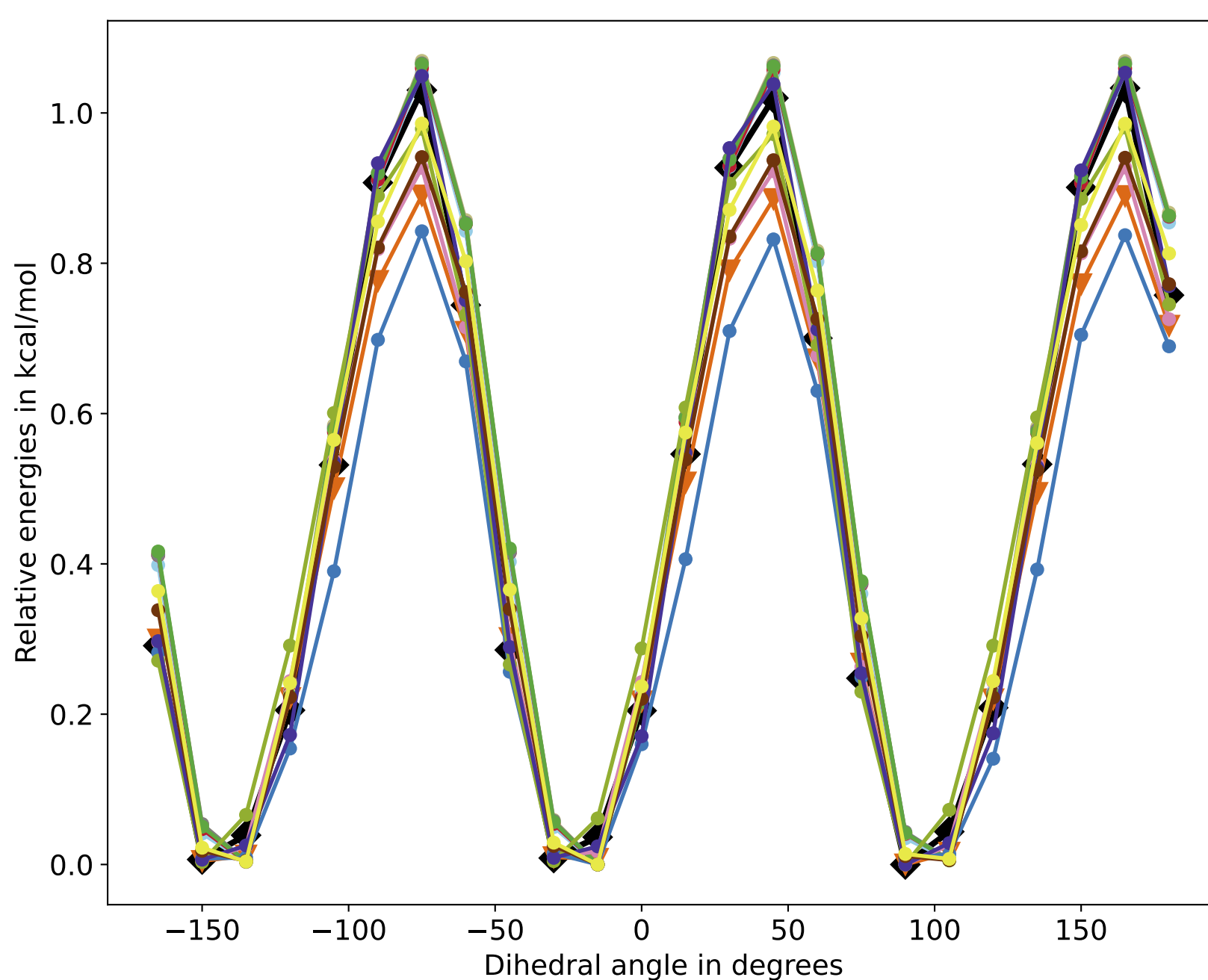
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

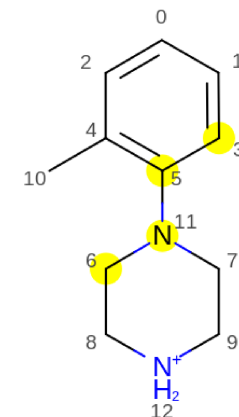
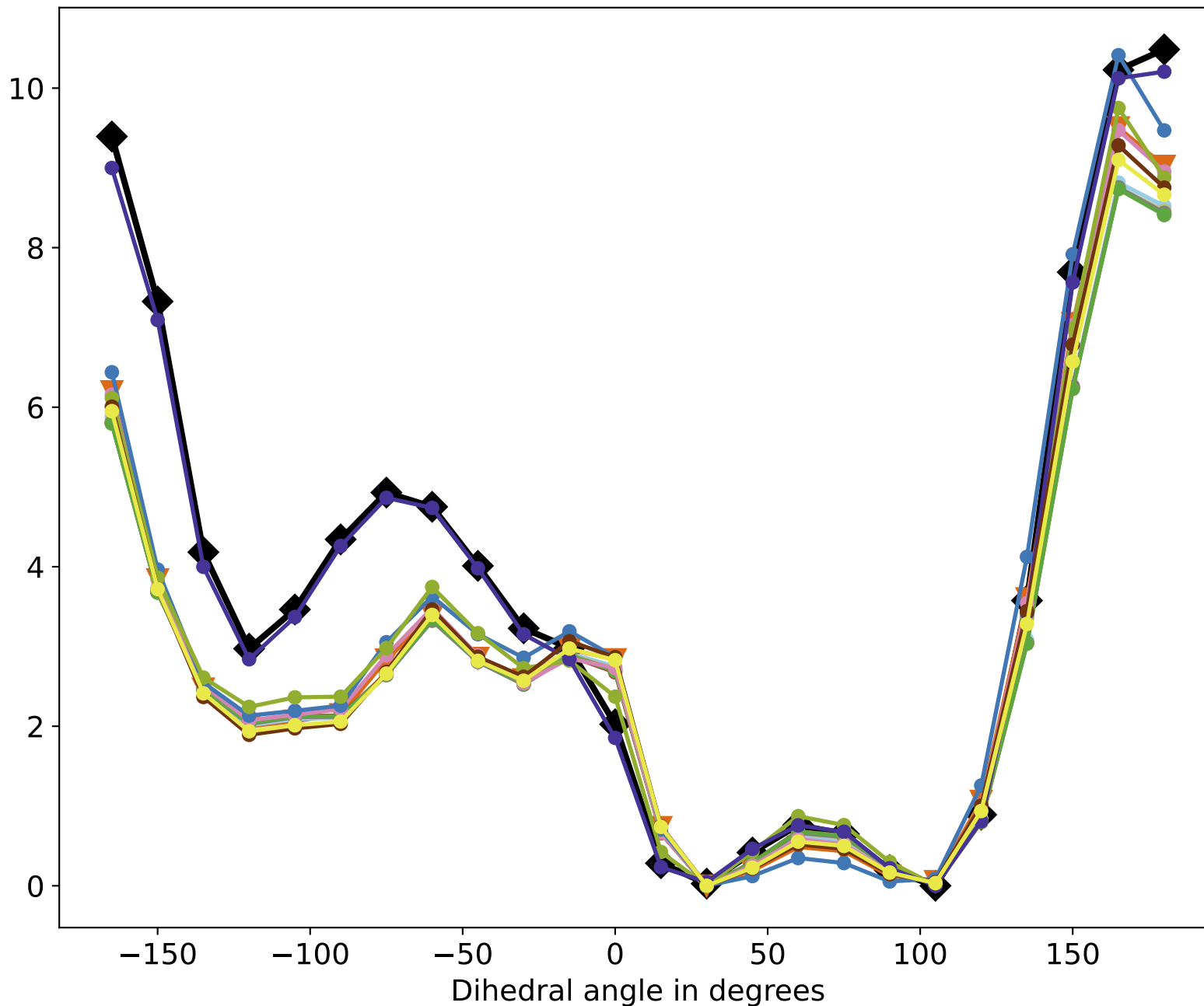


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

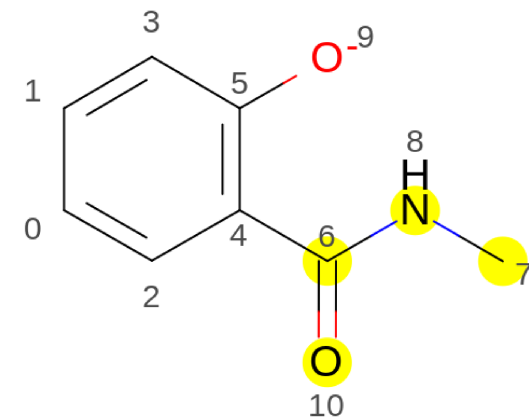
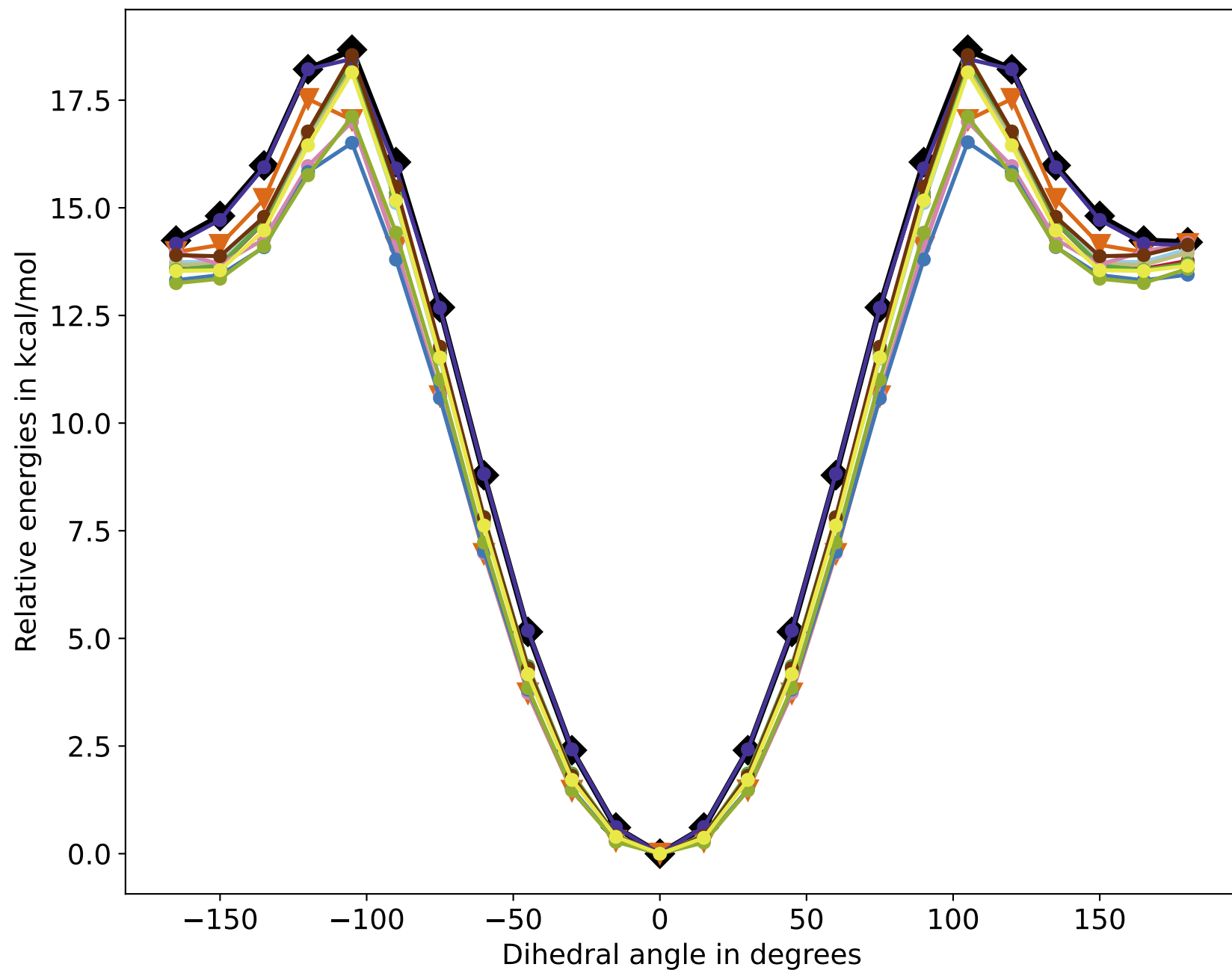


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

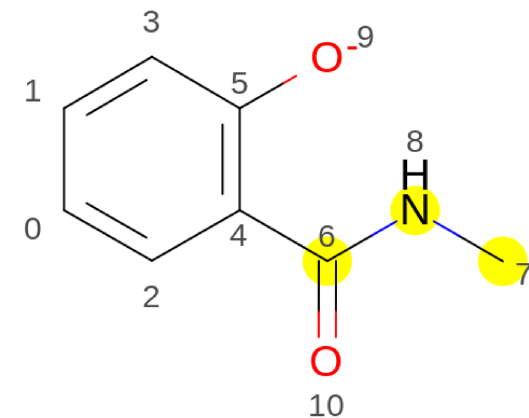
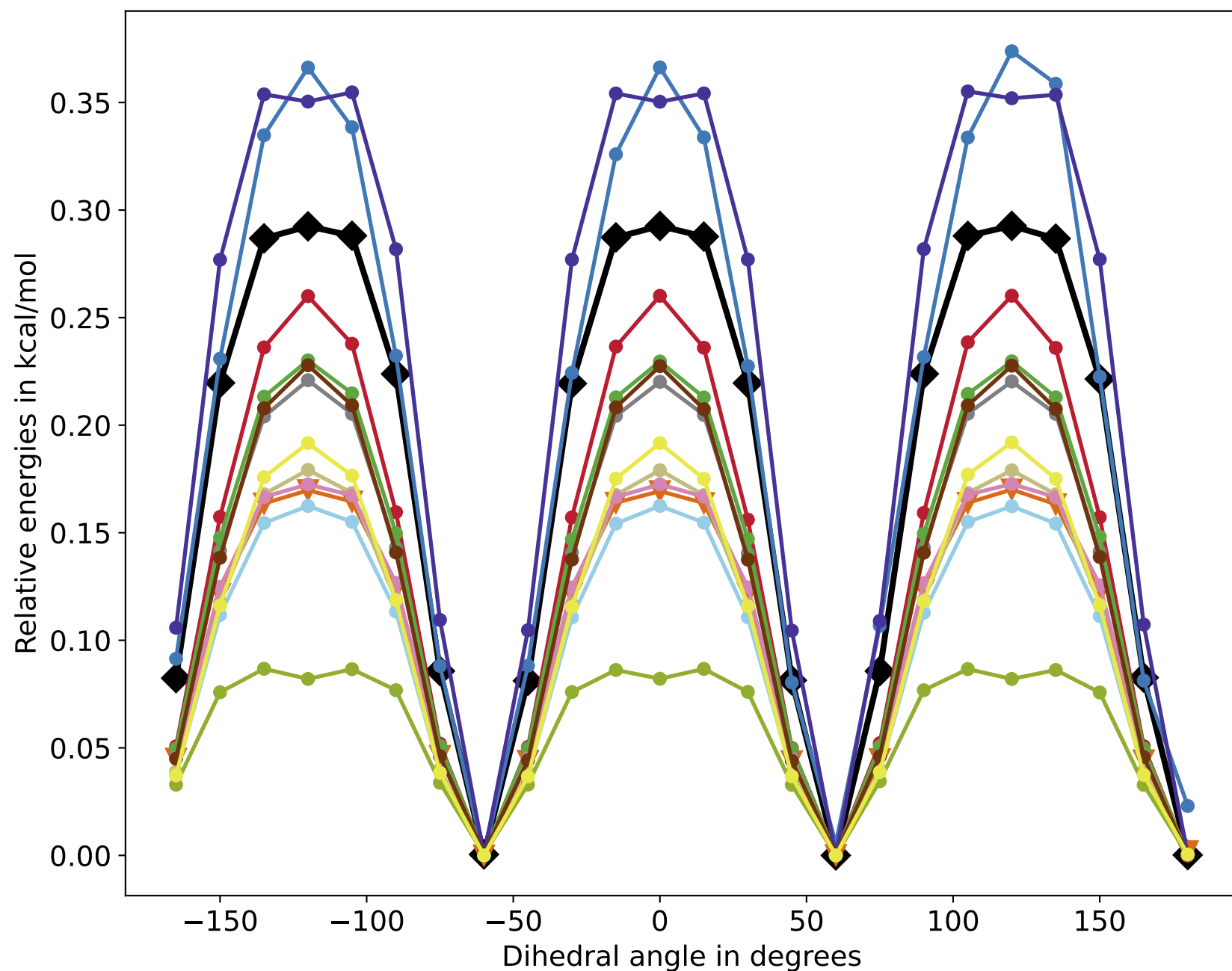
Relative energies in kcal/mol



- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

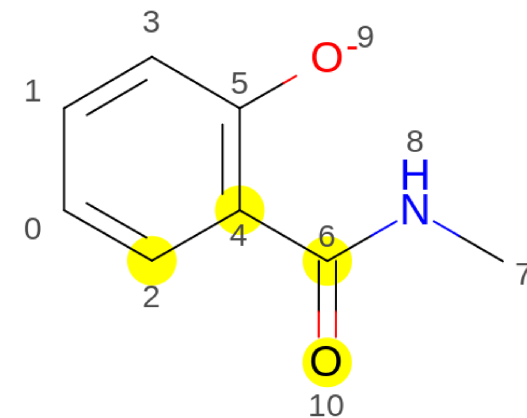
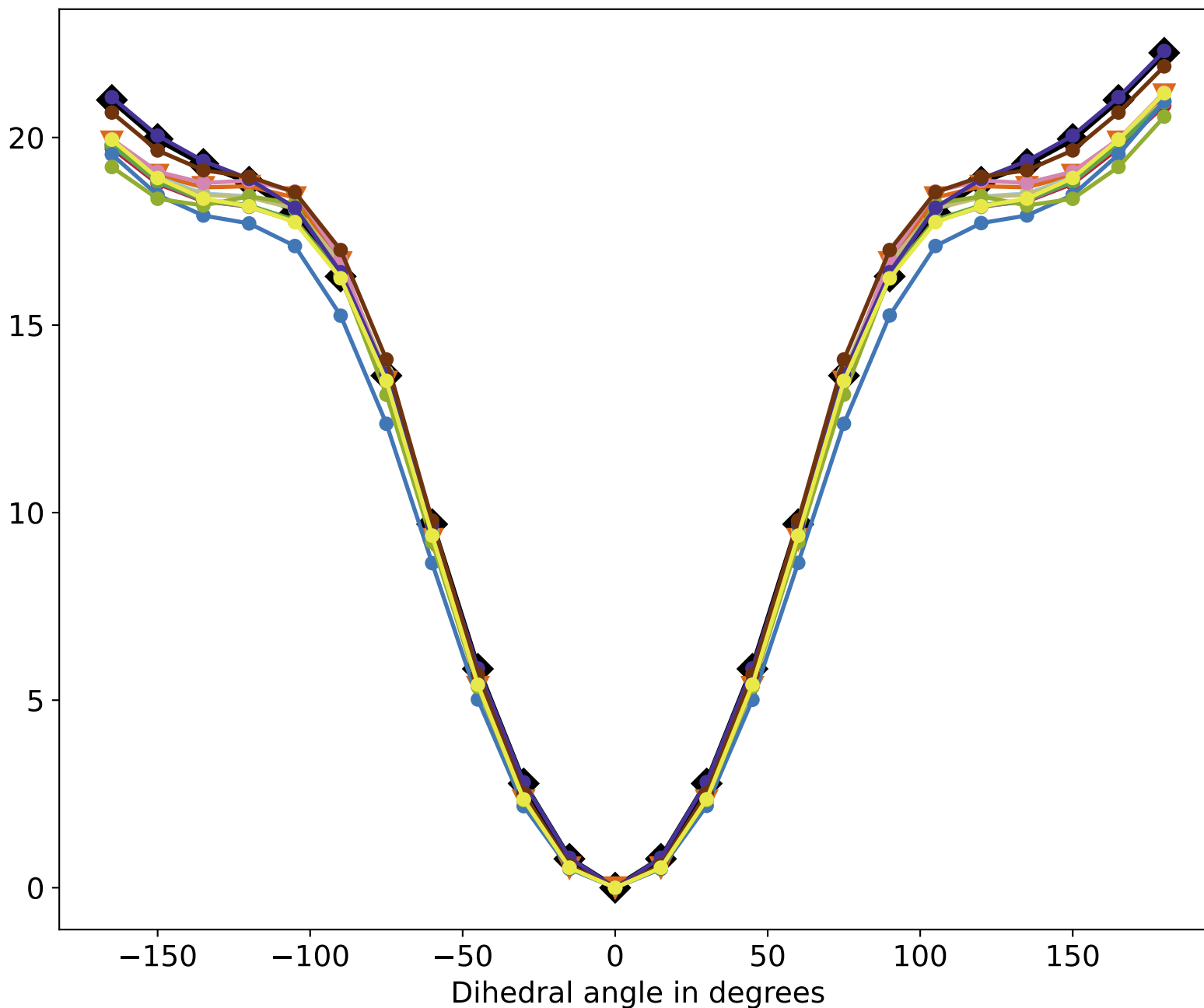


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

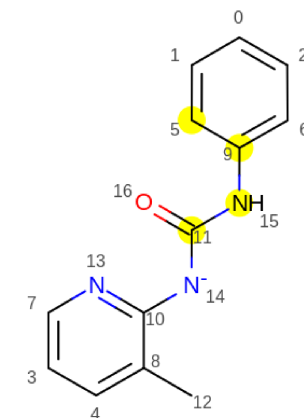
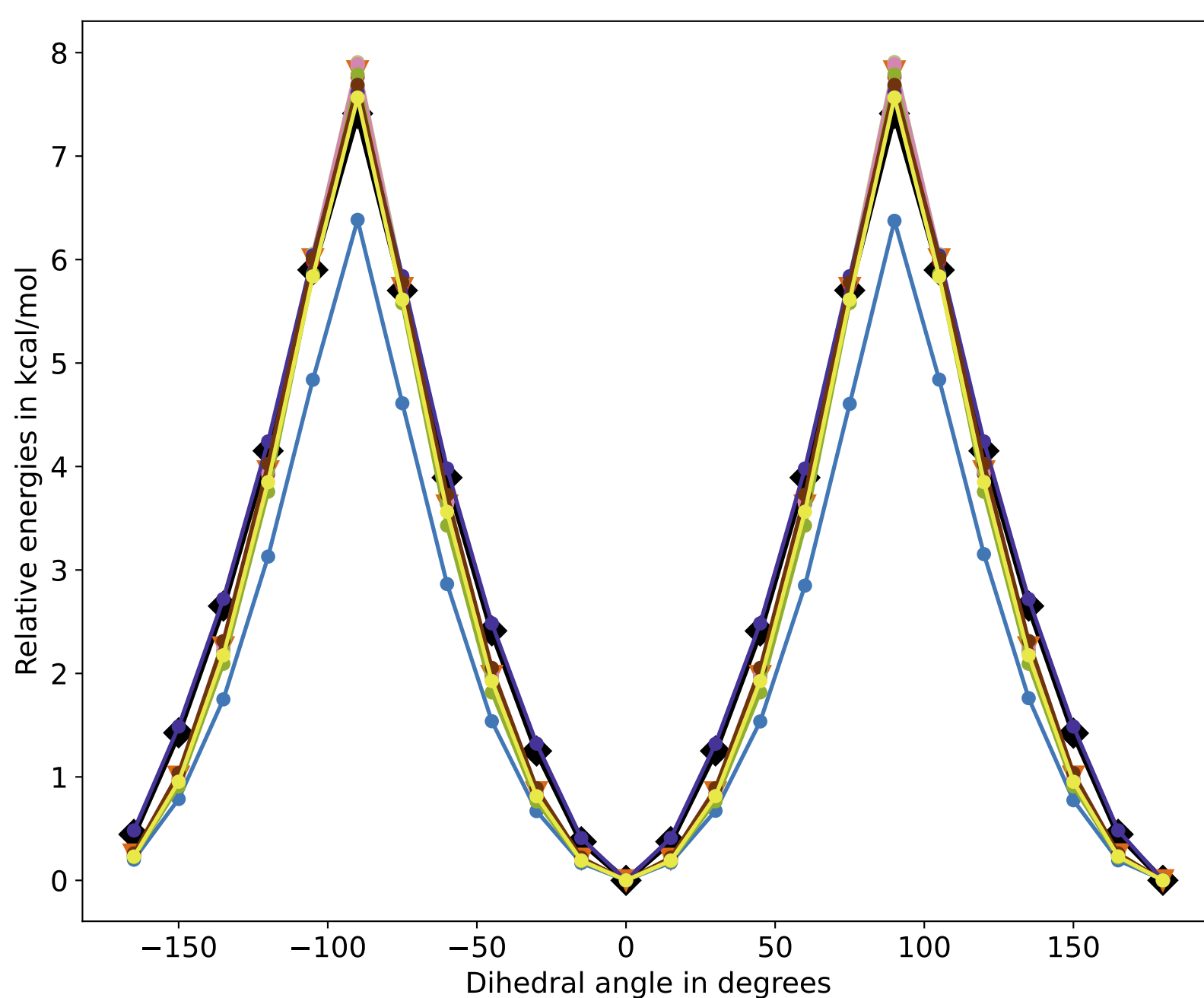


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

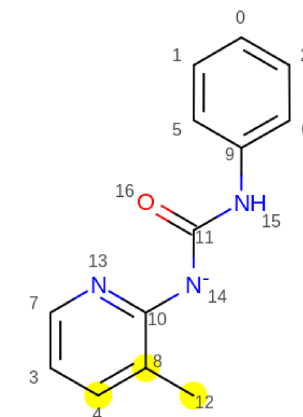
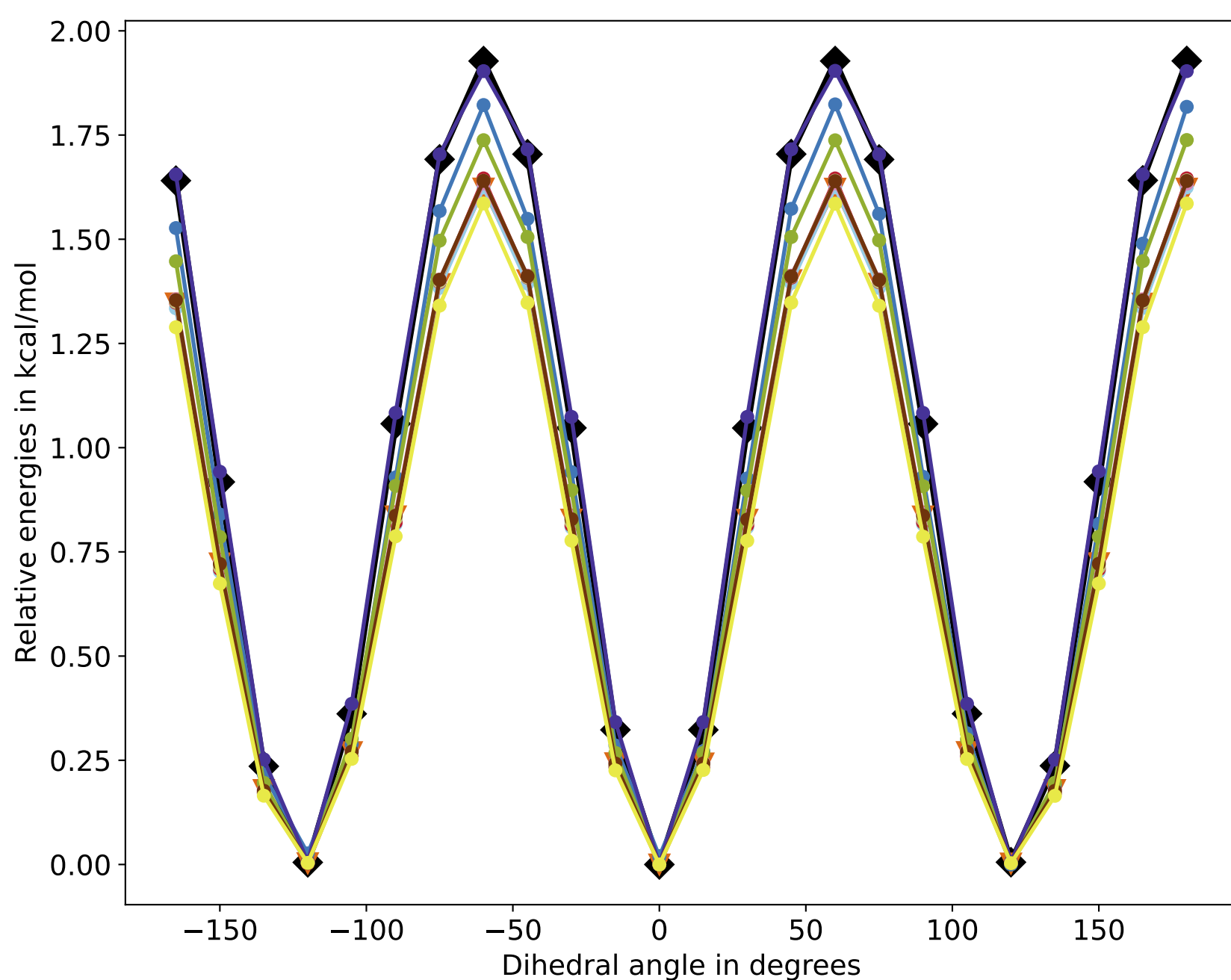
Relative energies in kcal/mol



- MP2/heavy-aug-cc-pVTZ
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- B3LYP-D3BJ/DEF2-TZVP
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- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

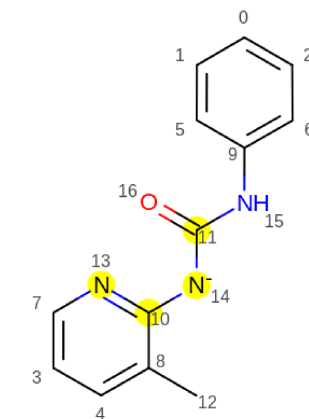
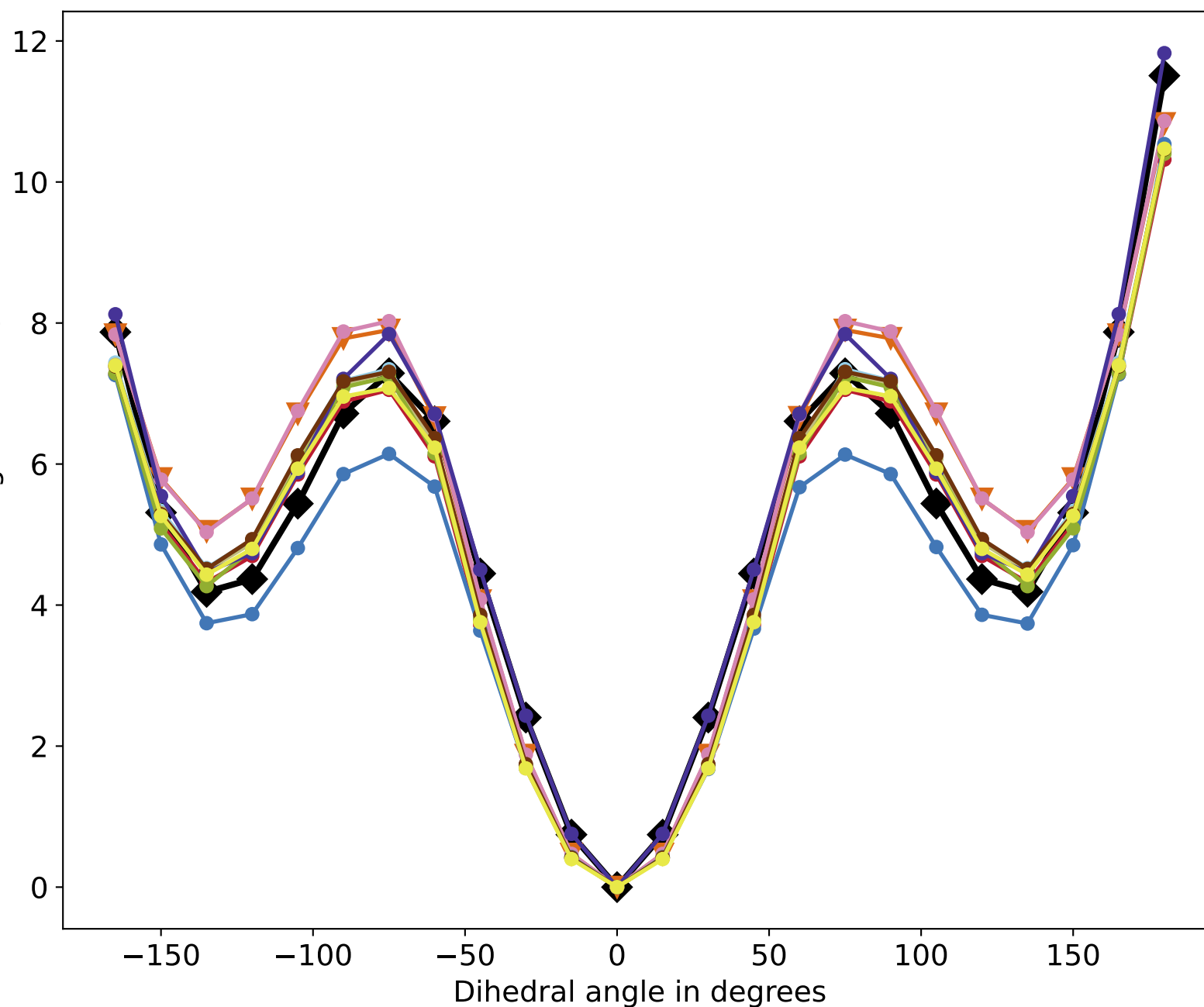


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



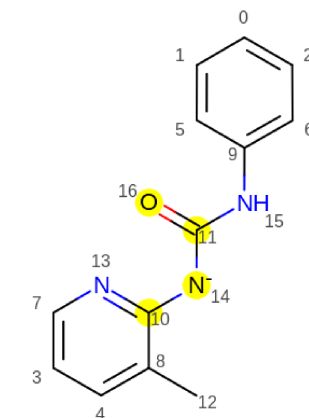
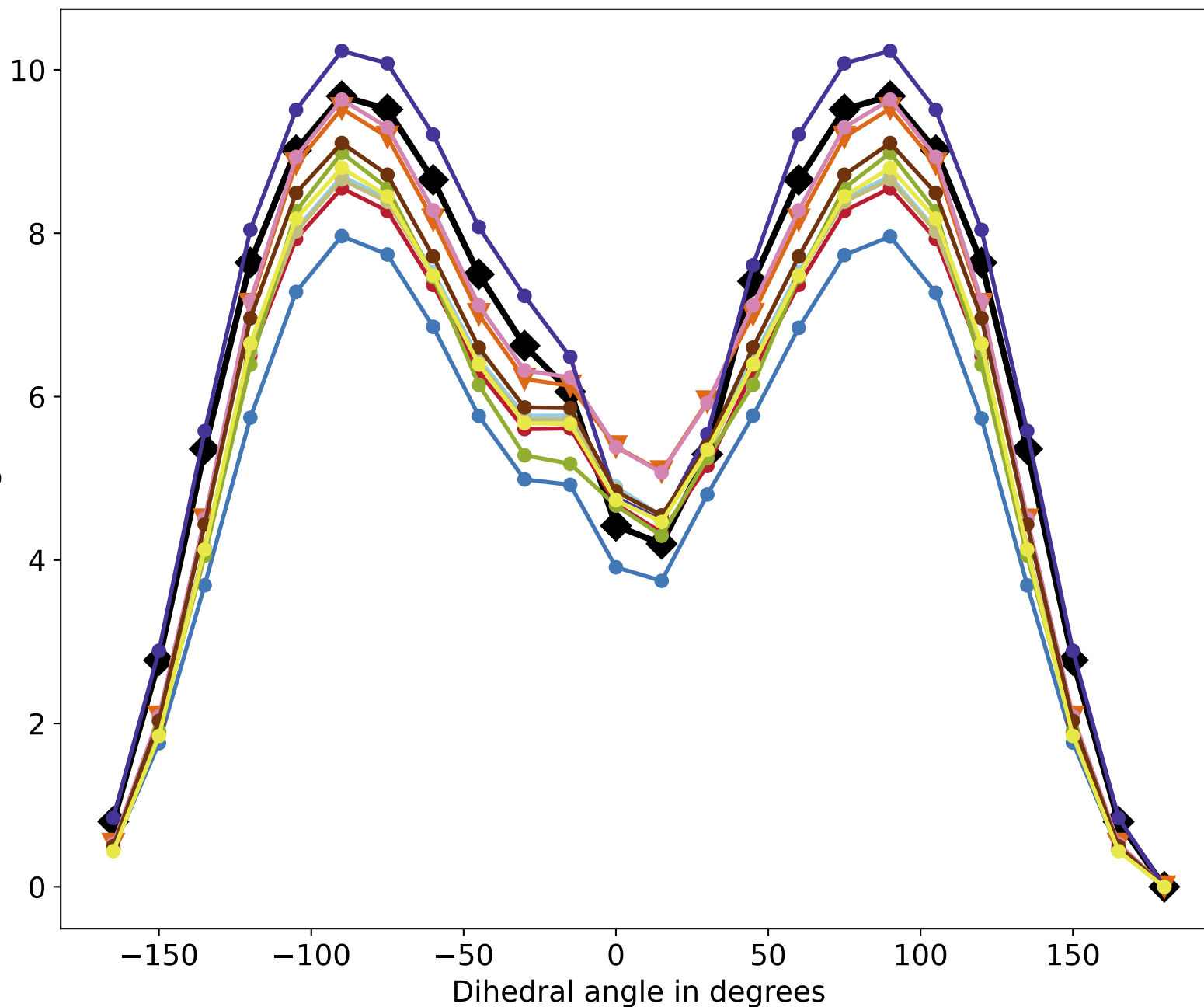
- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



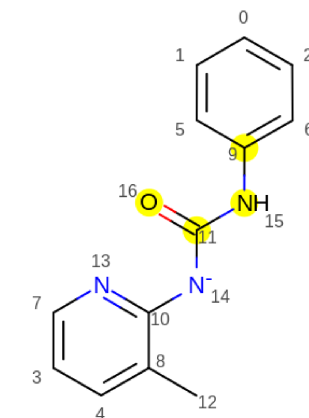
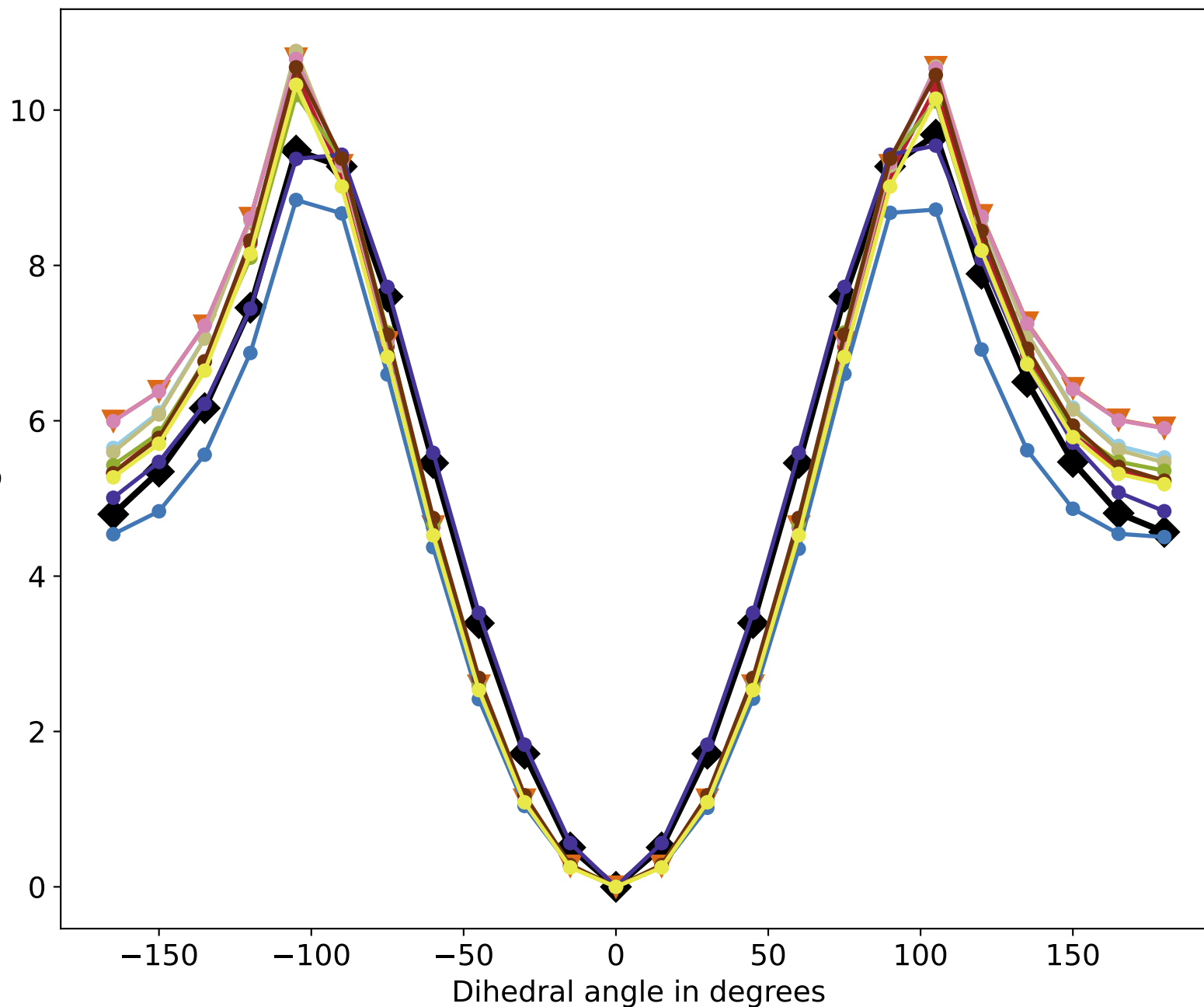
- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

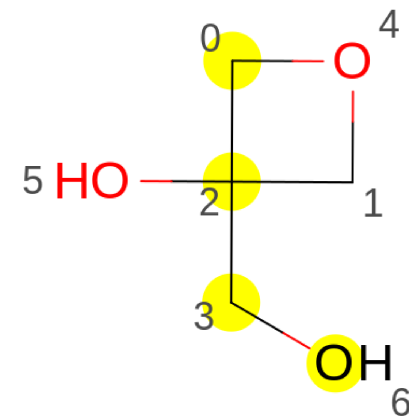
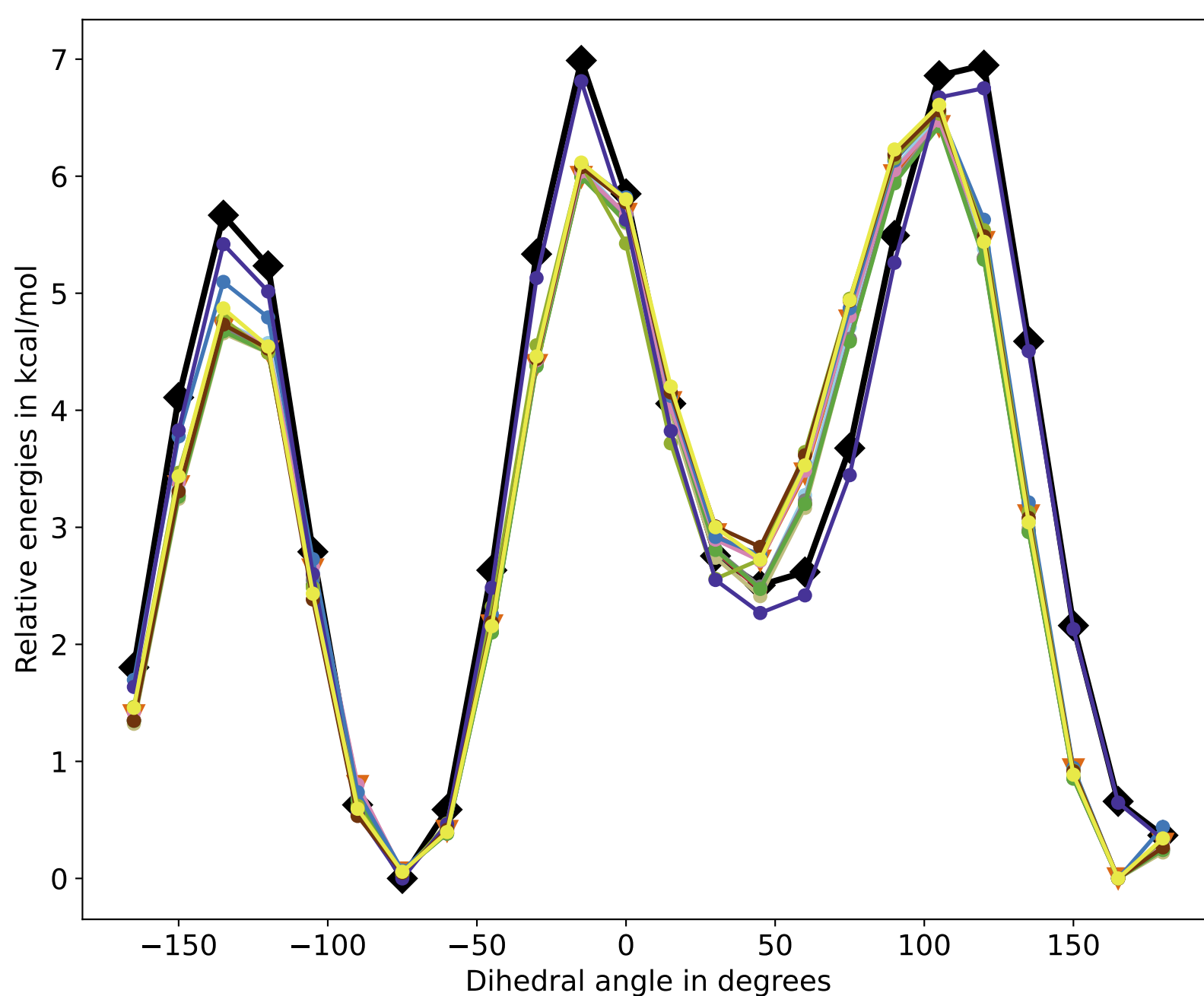


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

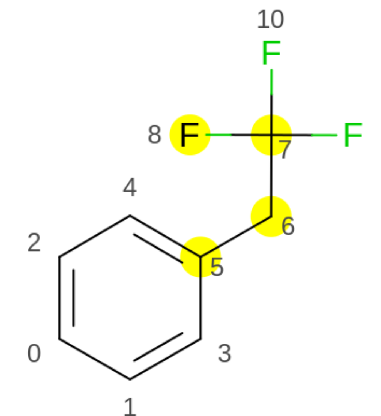
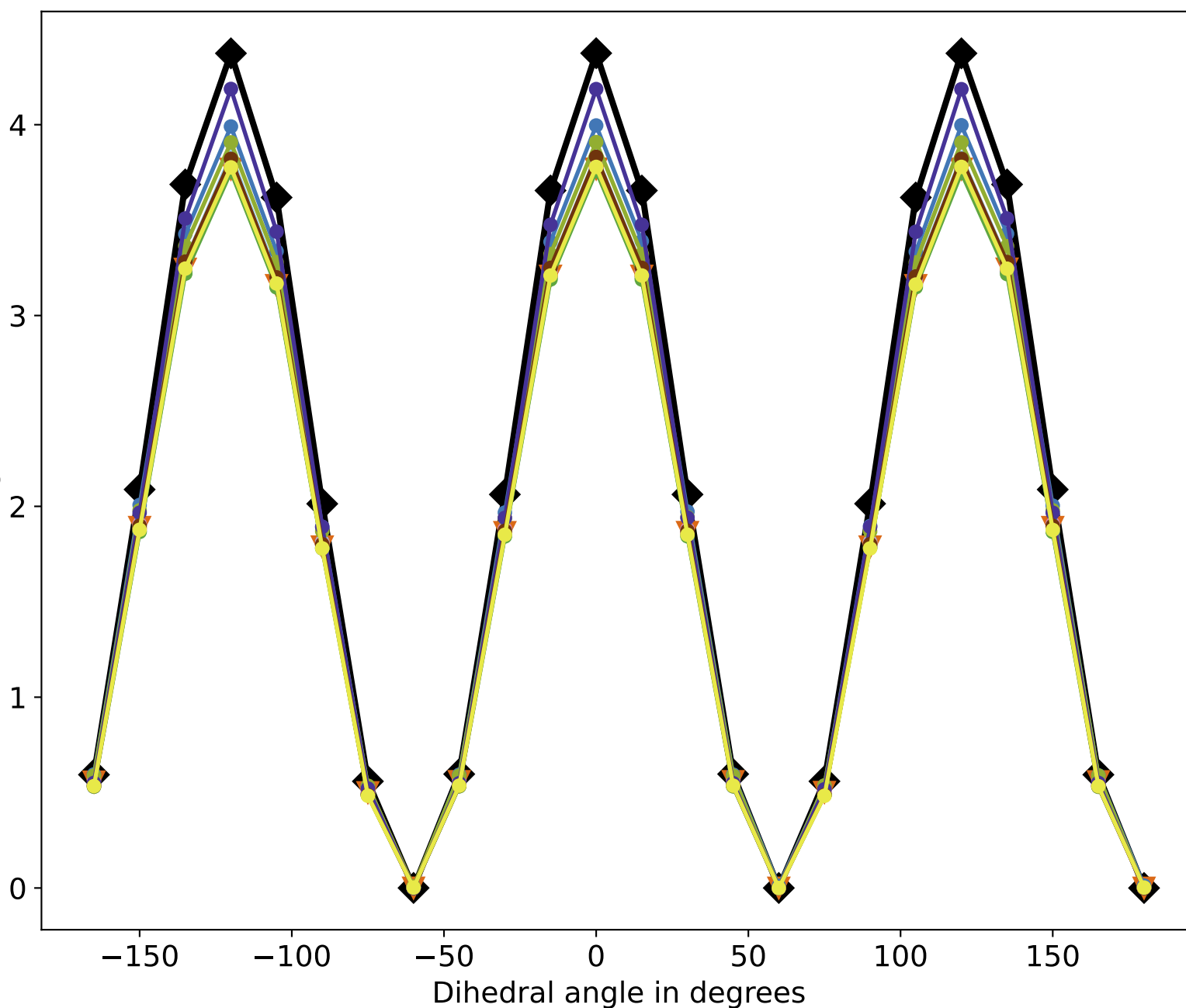


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



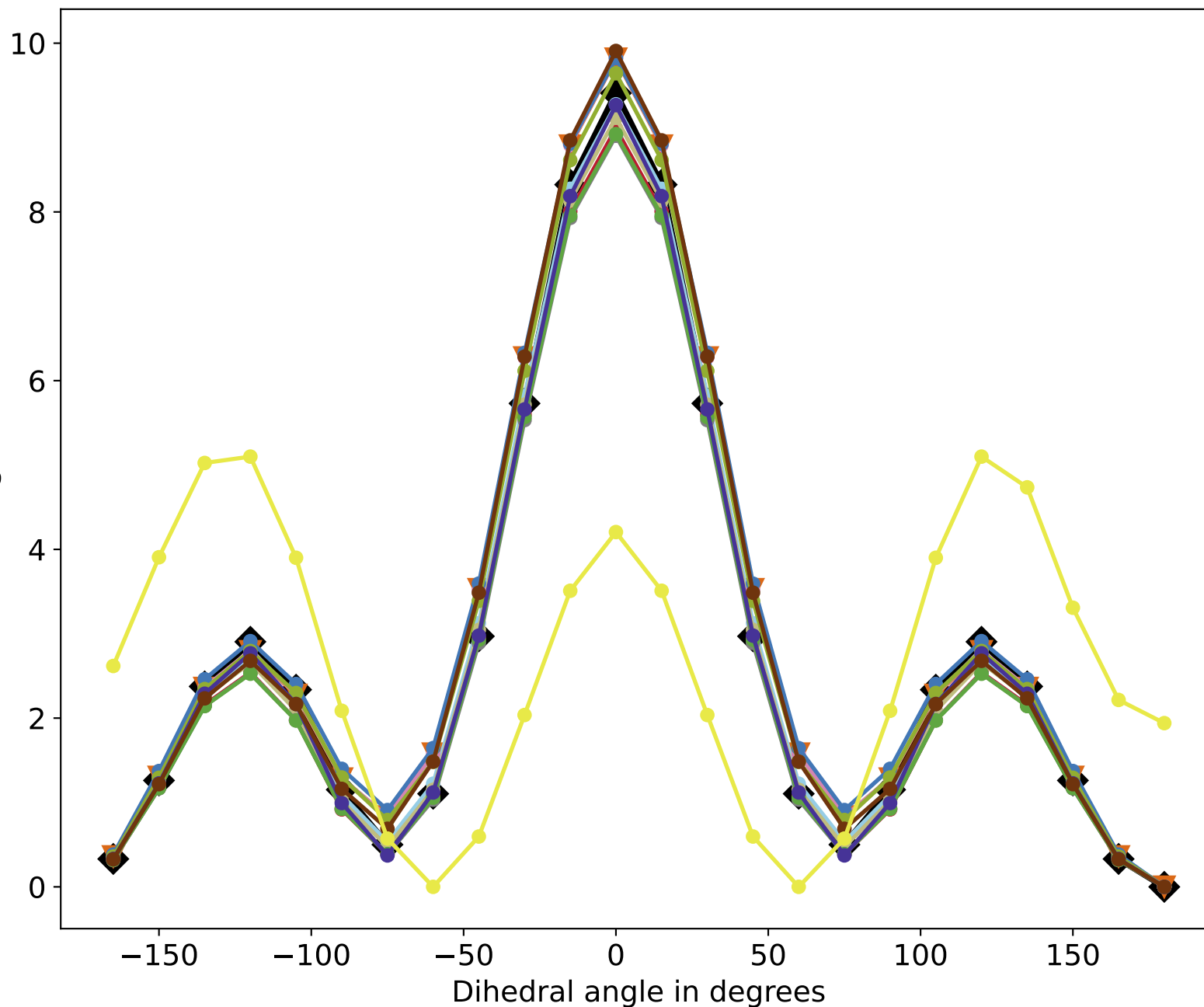
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

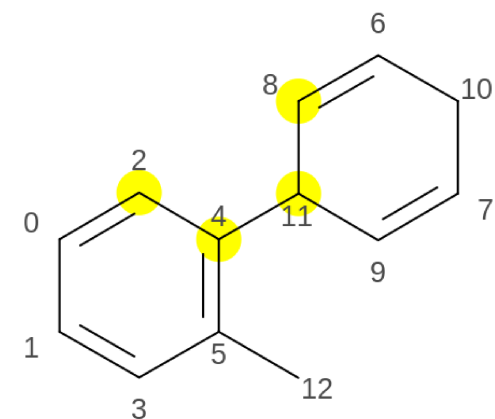
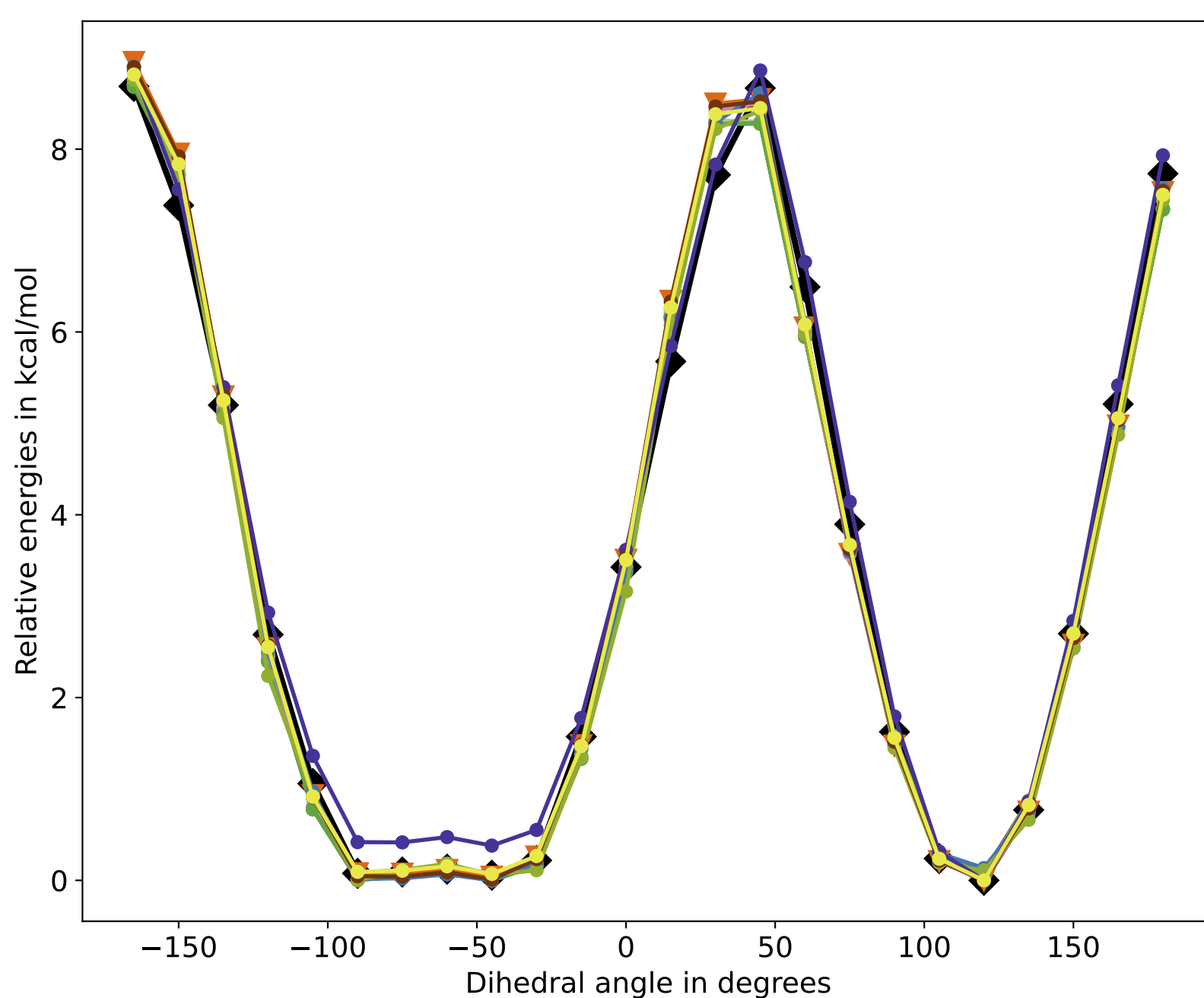
Relative energies in kcal/mol



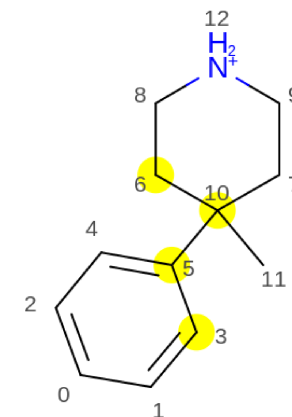
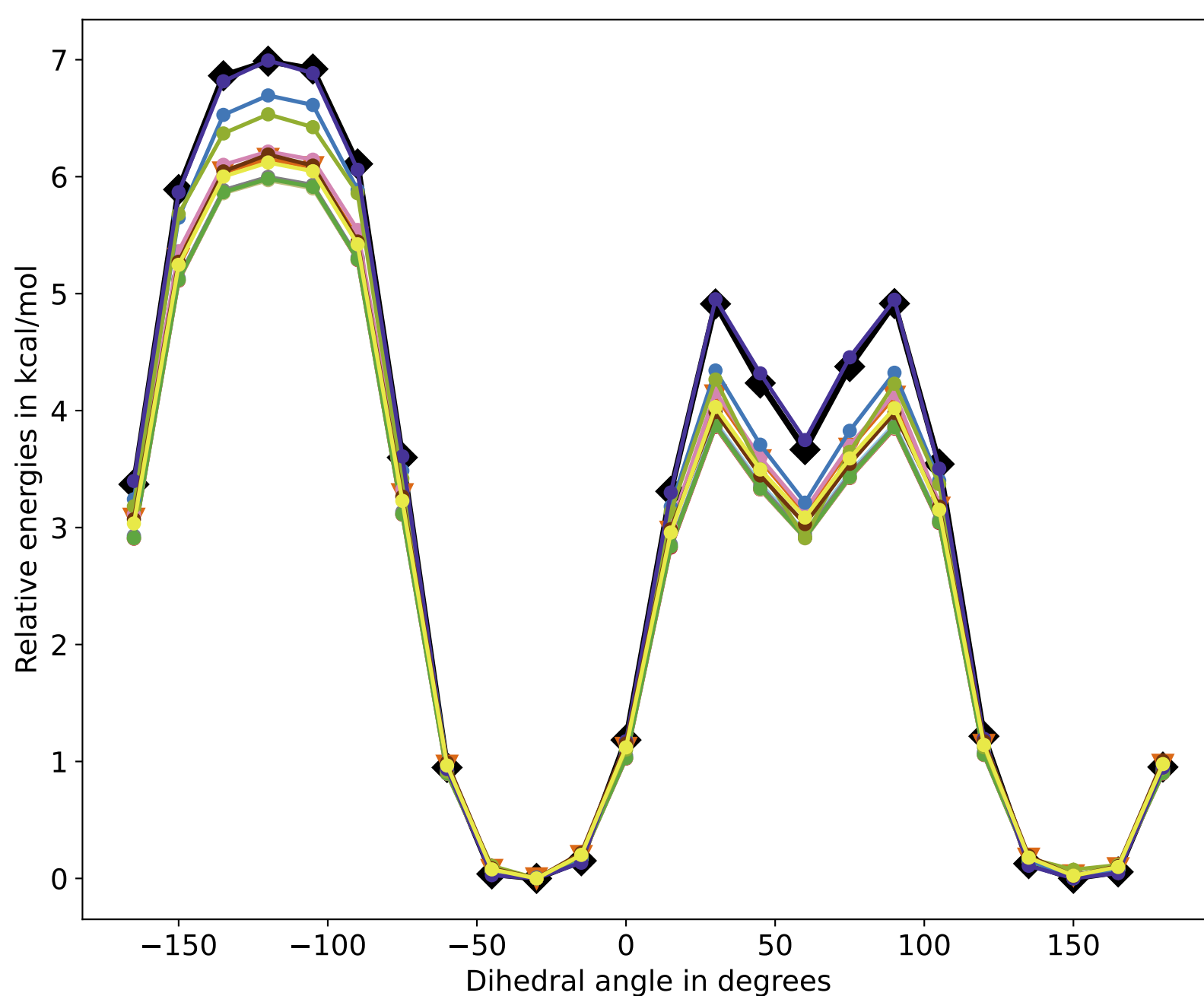
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

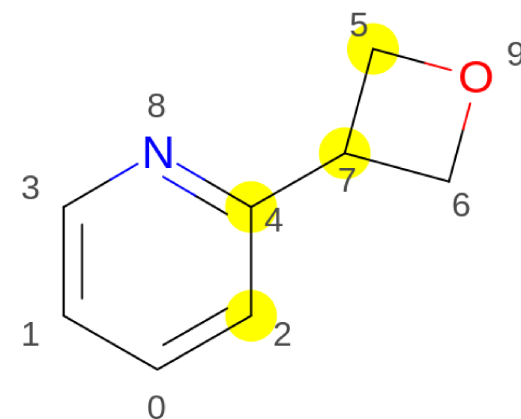
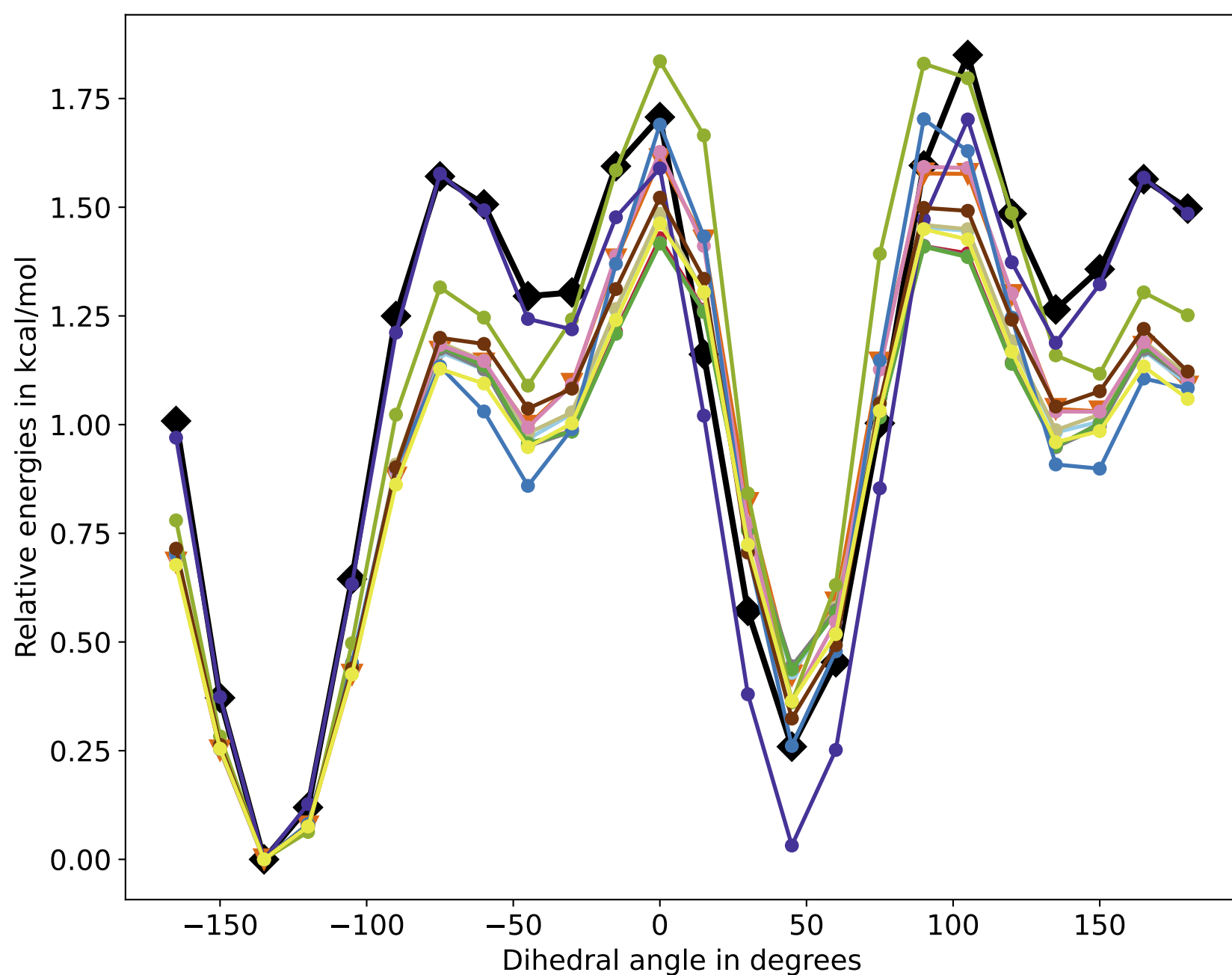


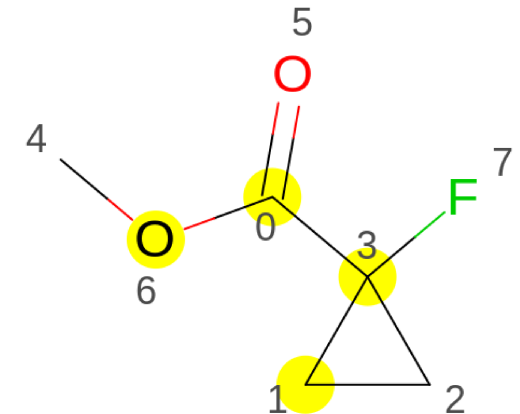
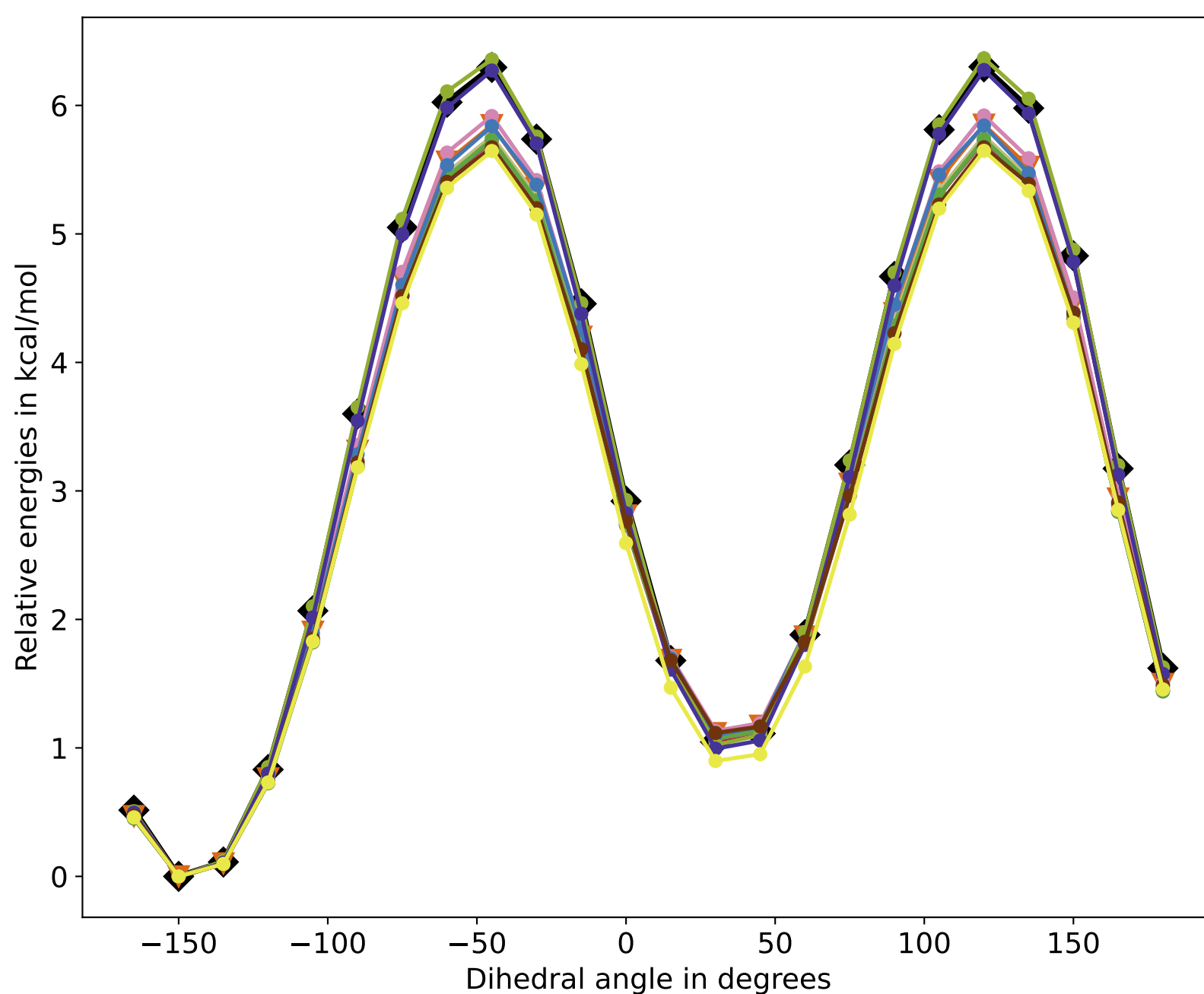


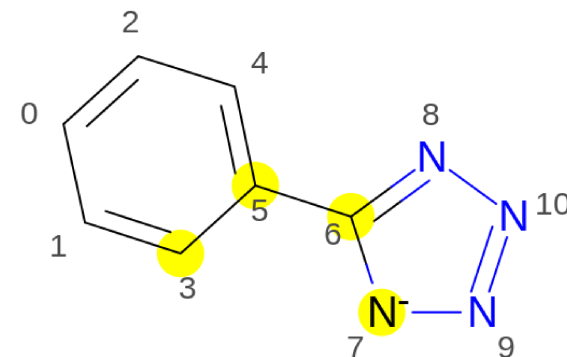
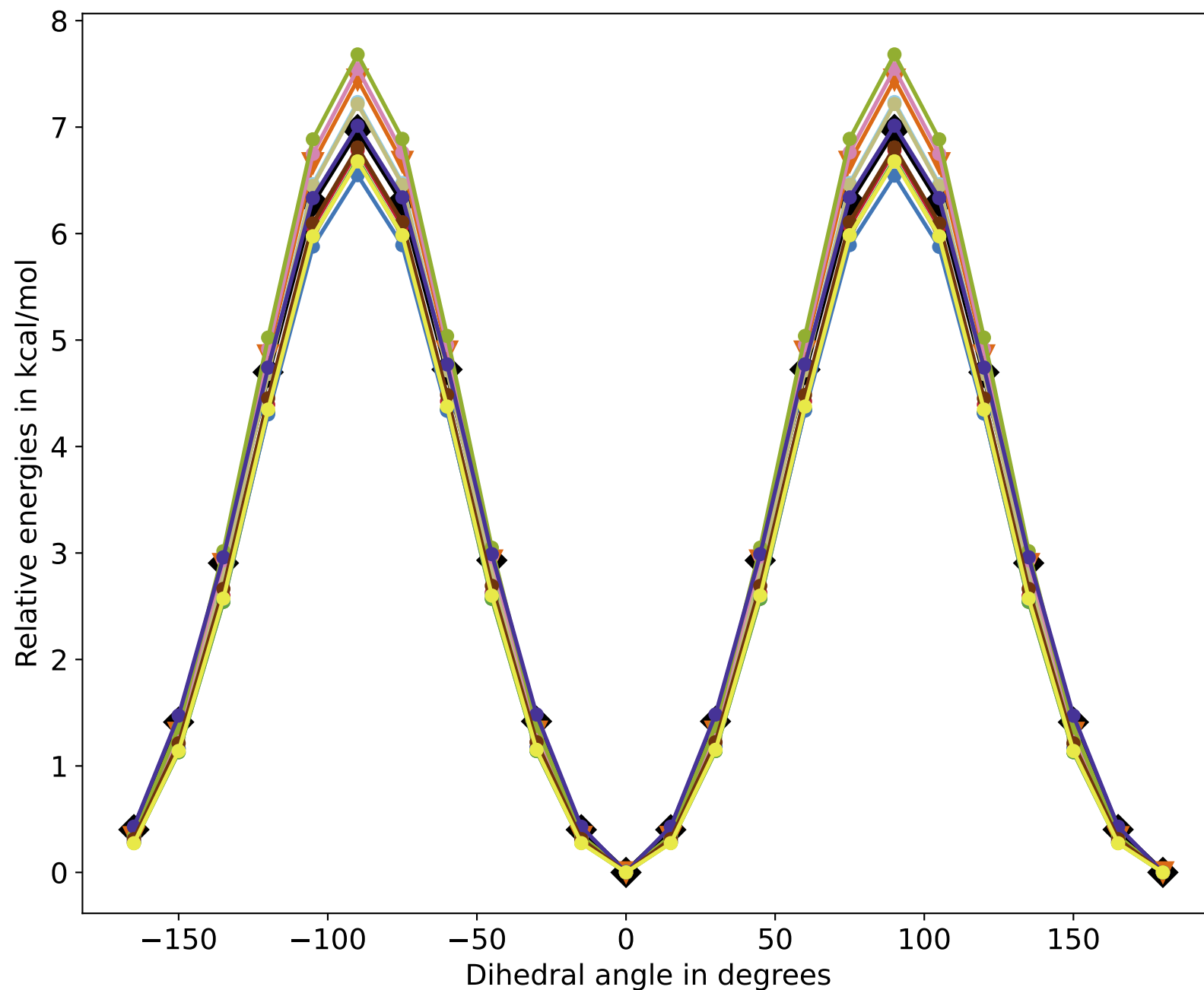
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- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

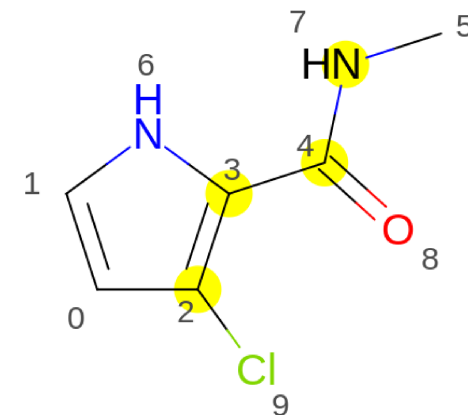
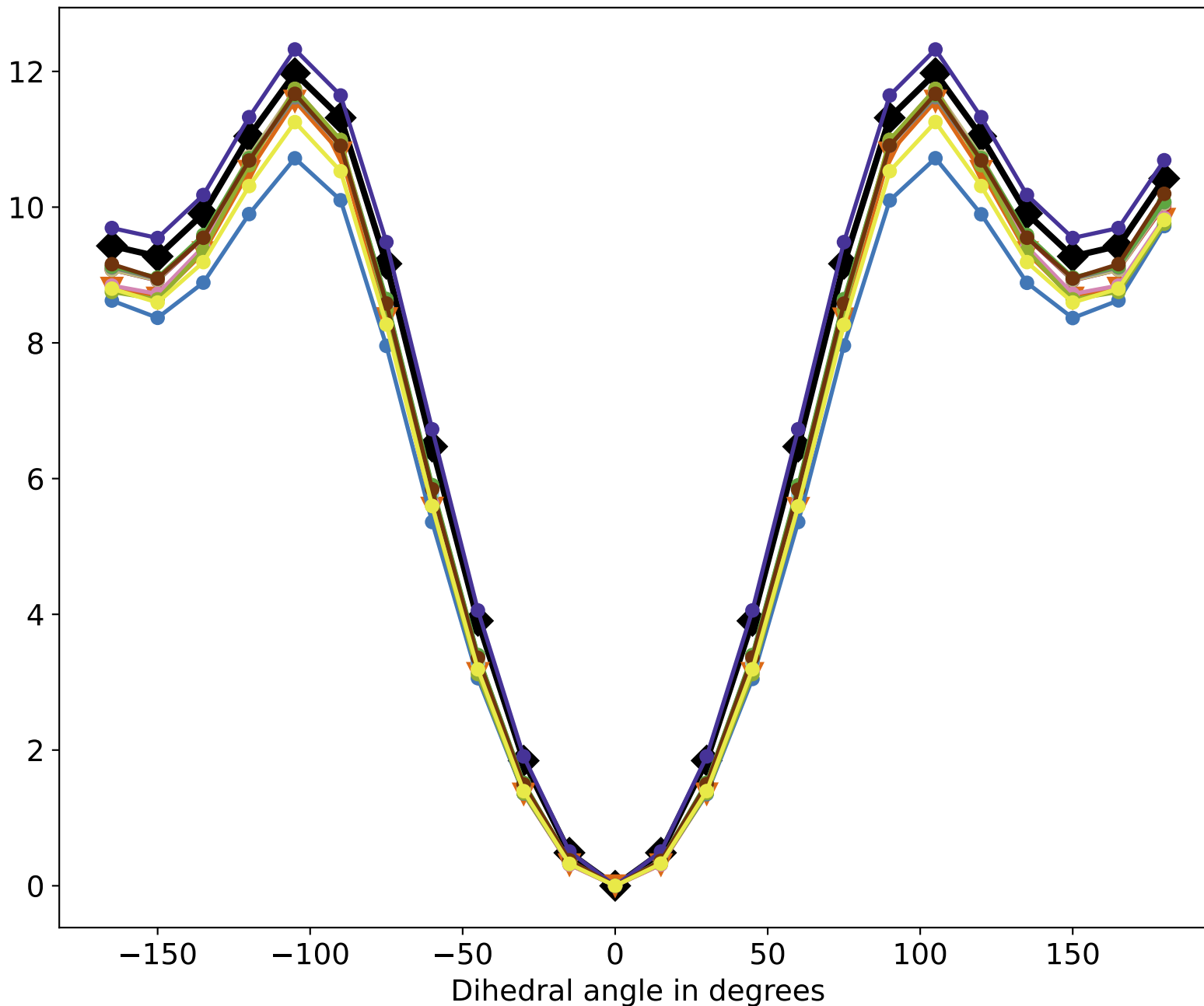




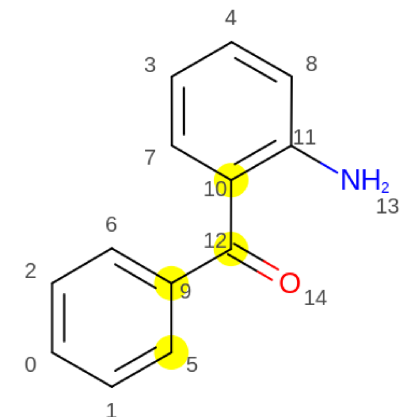
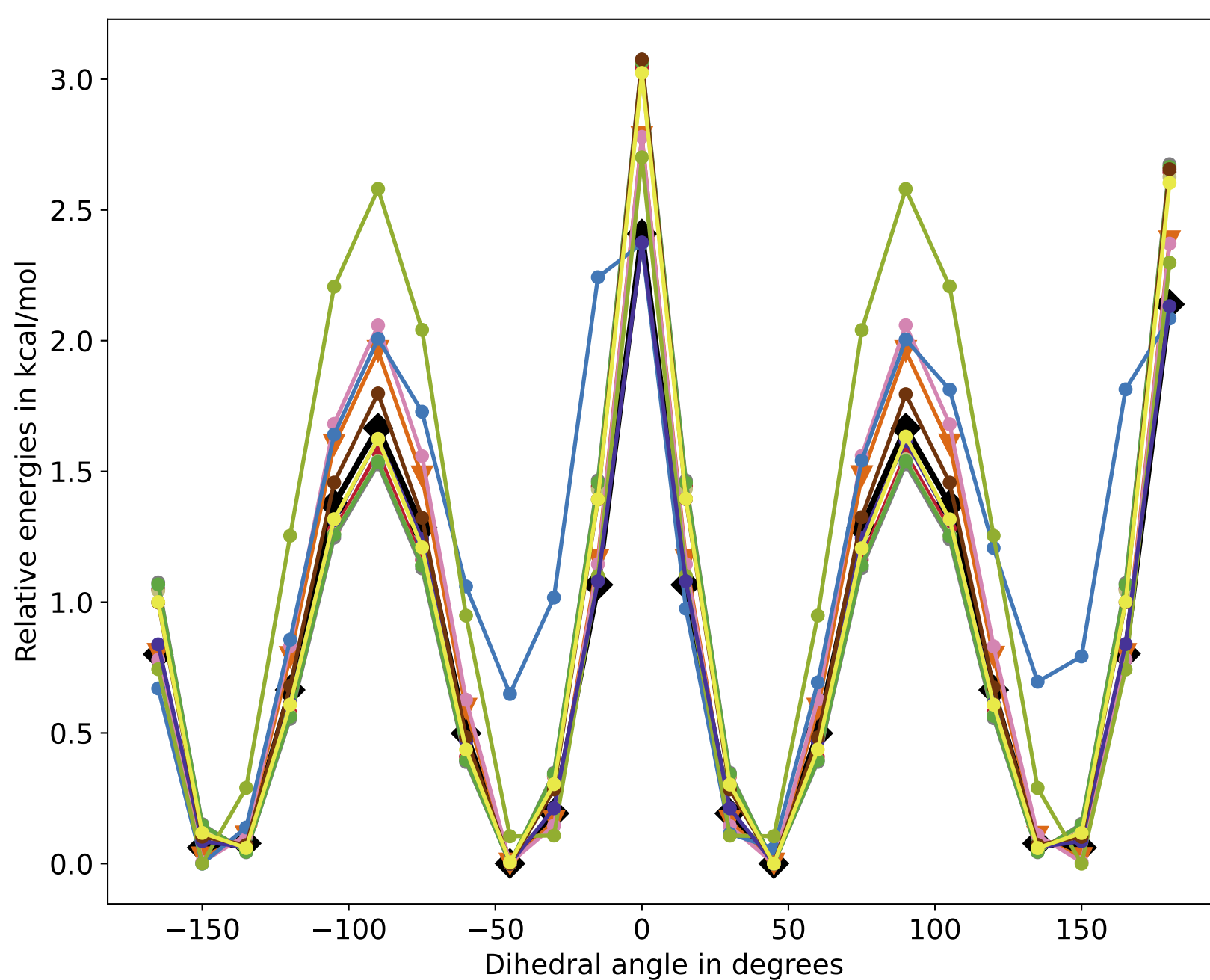


- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

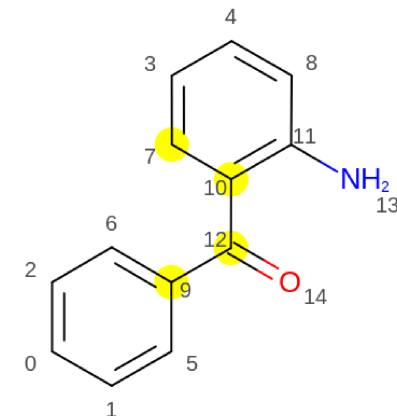
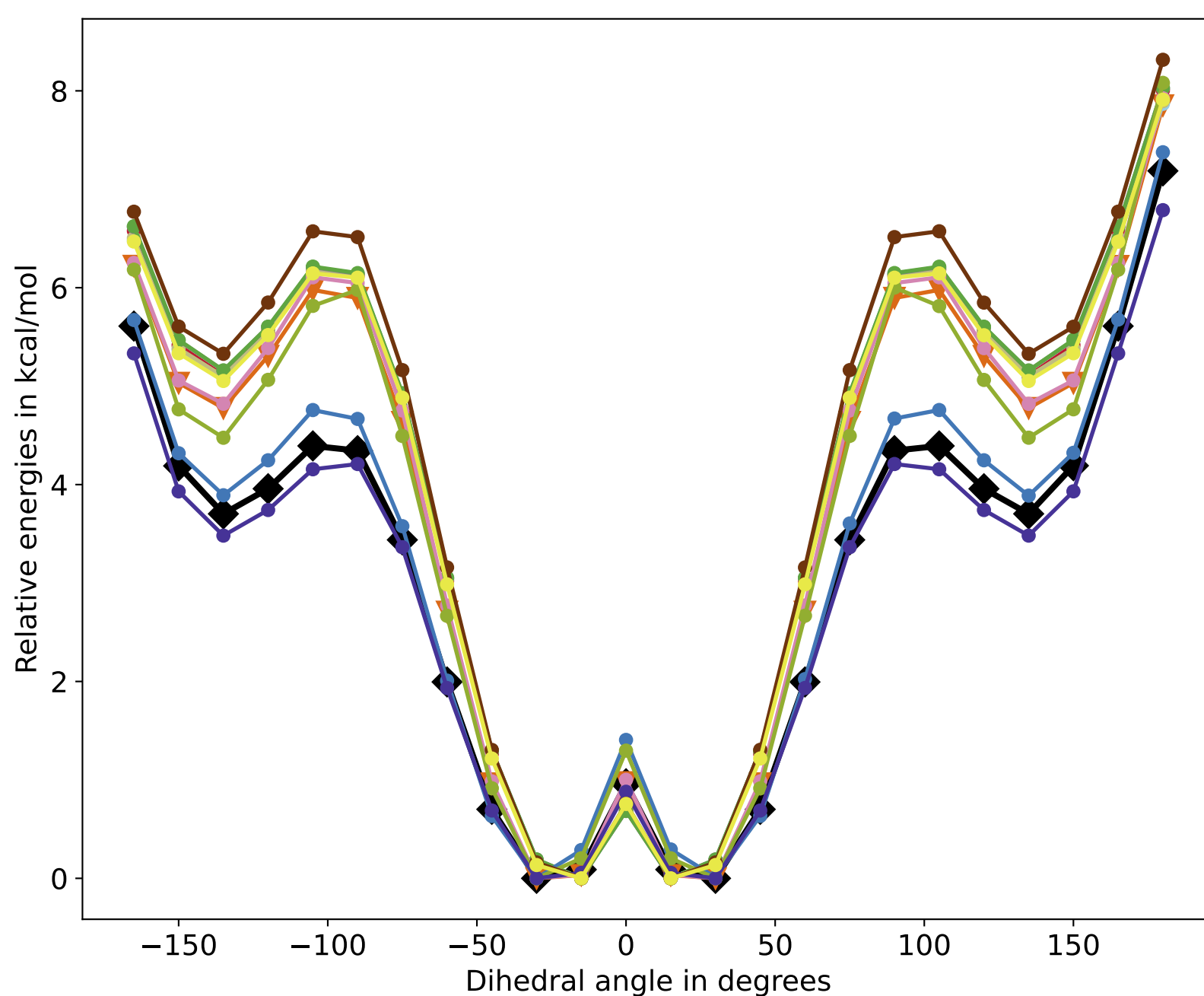
Relative energies in kcal/mol



- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
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- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



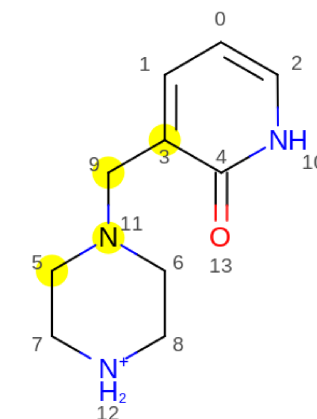
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



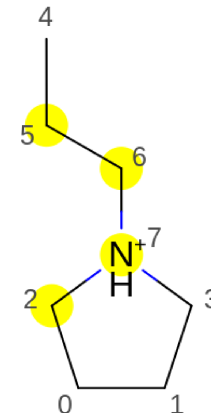
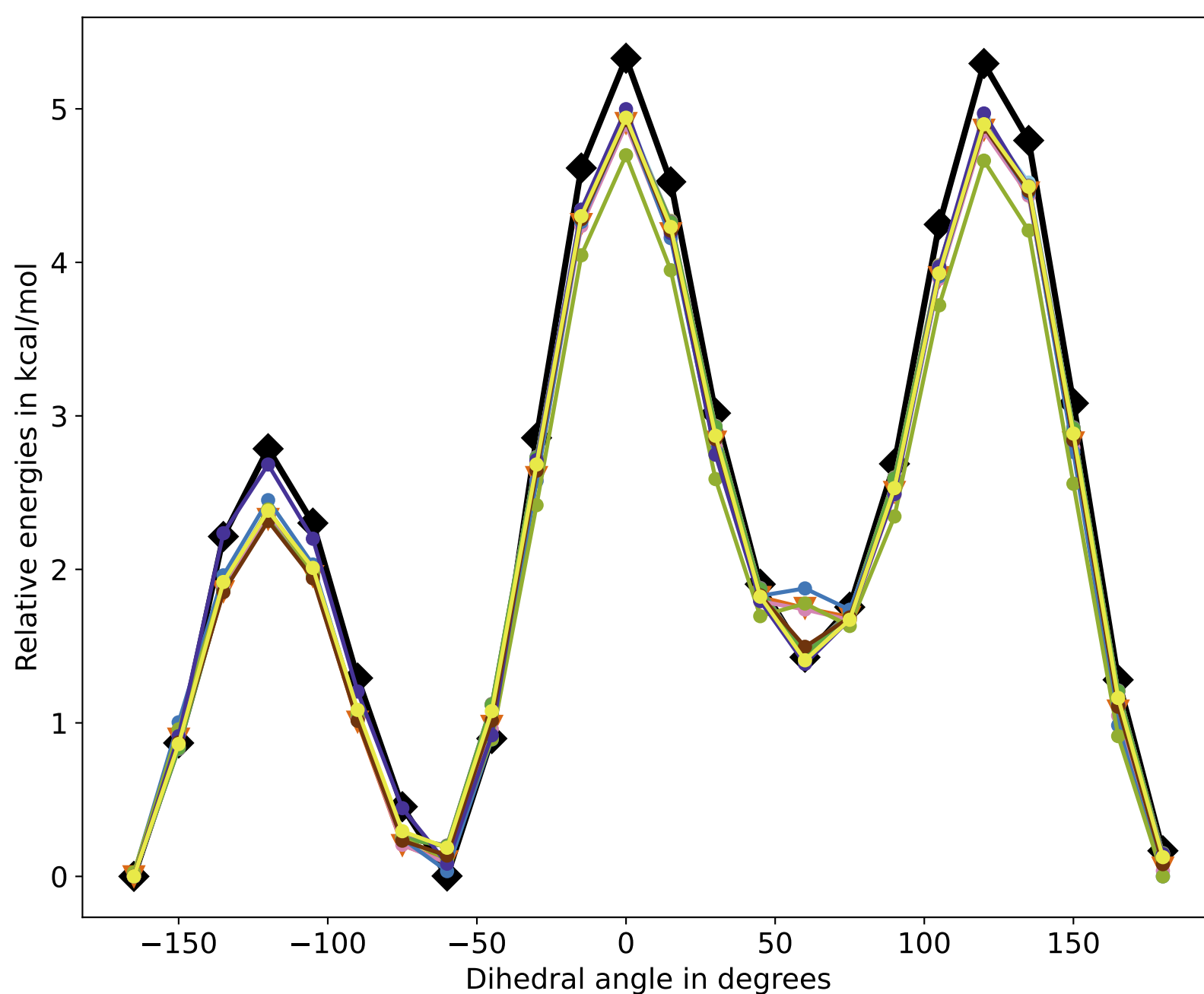
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

Dihedral angle in degrees

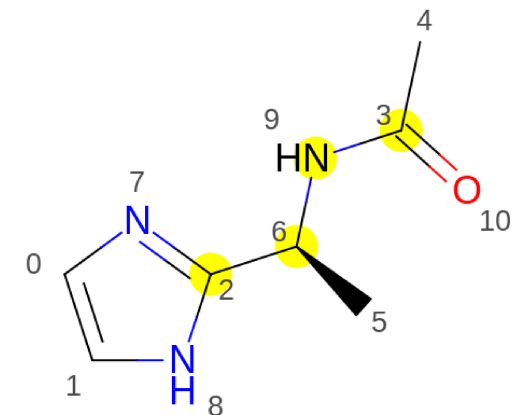
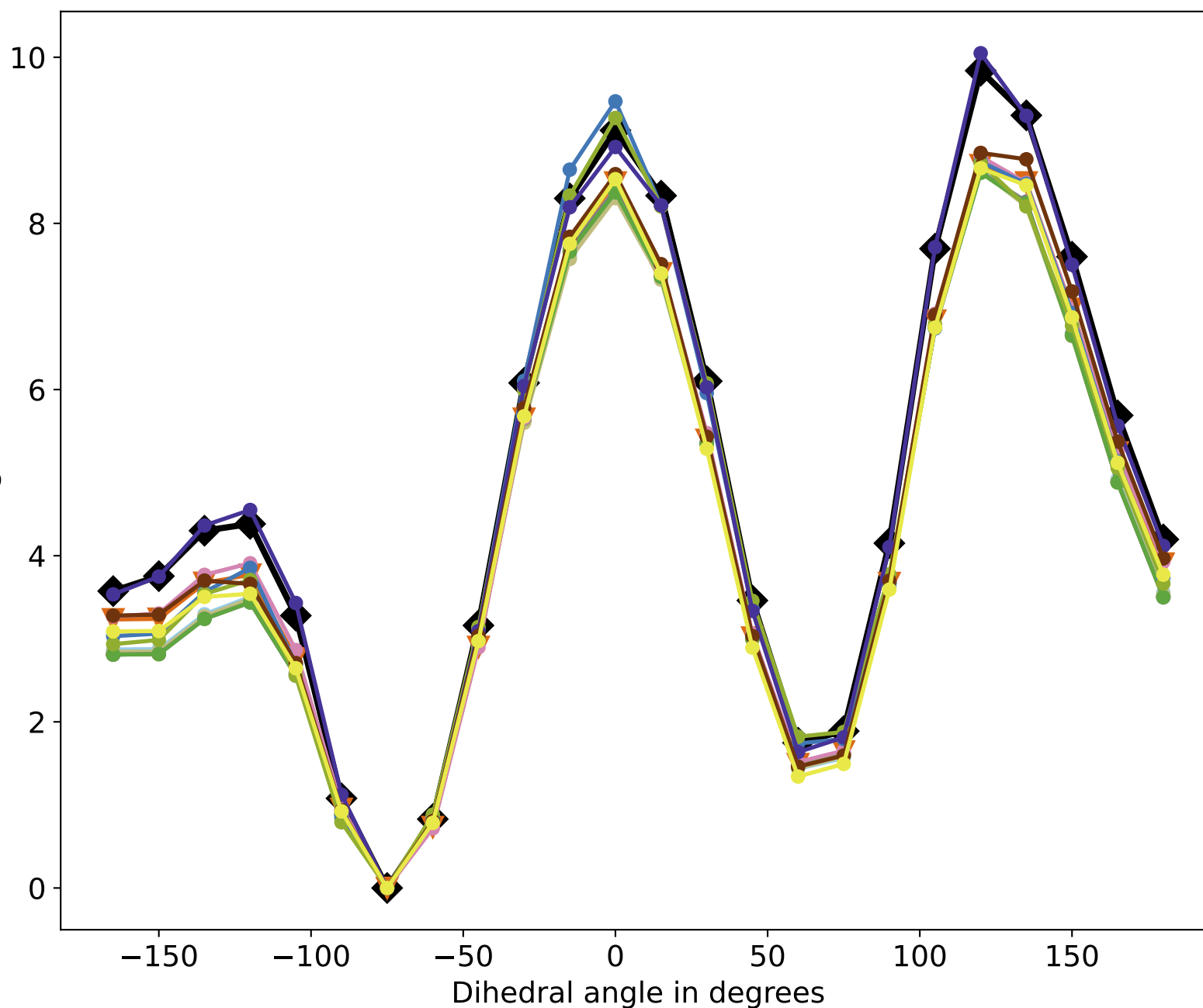


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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



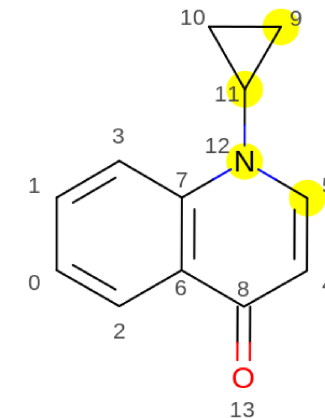
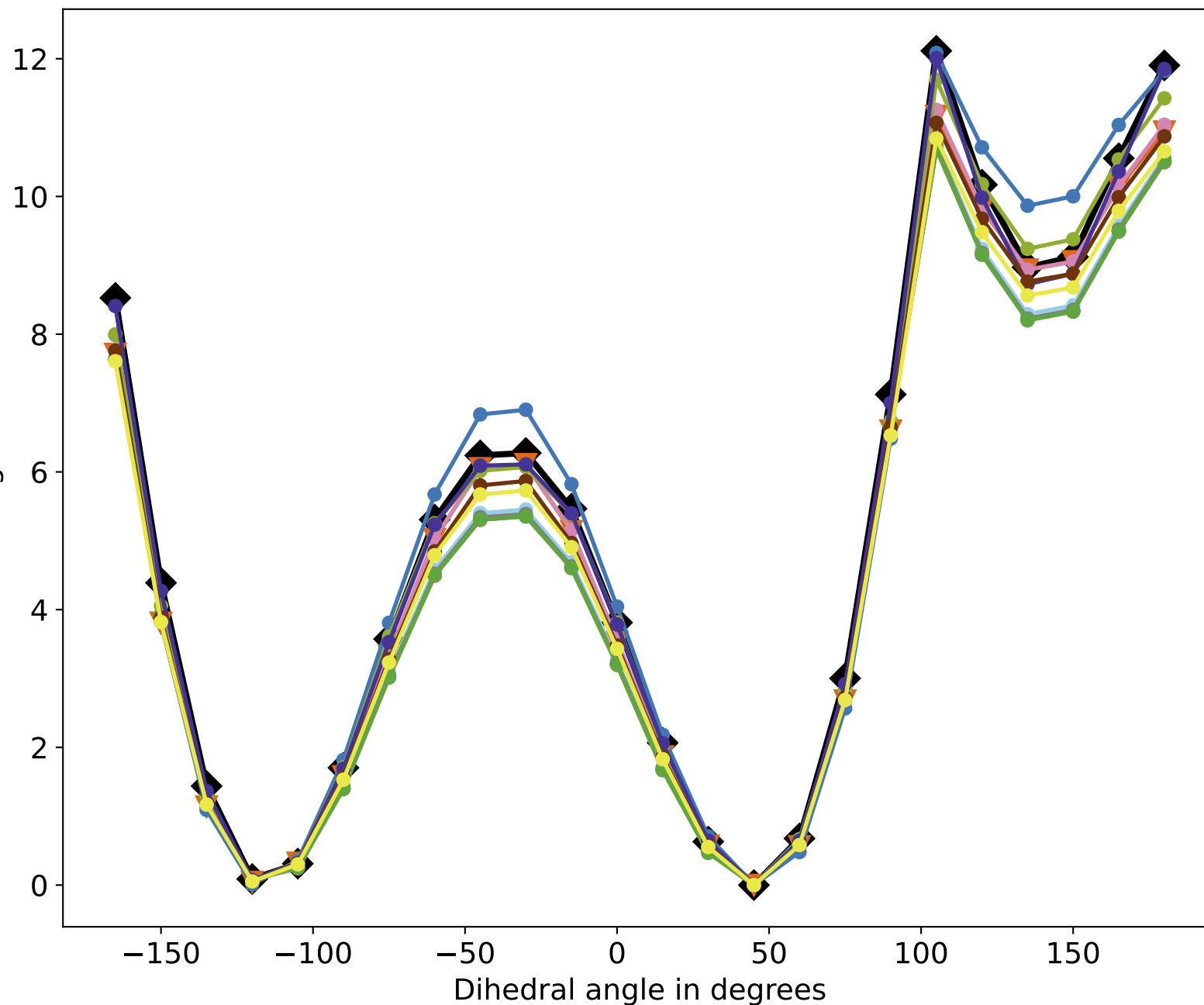
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

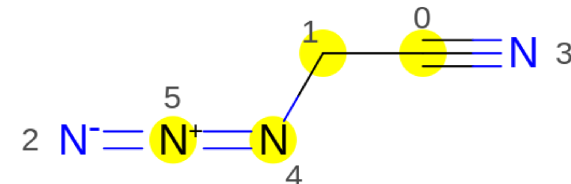
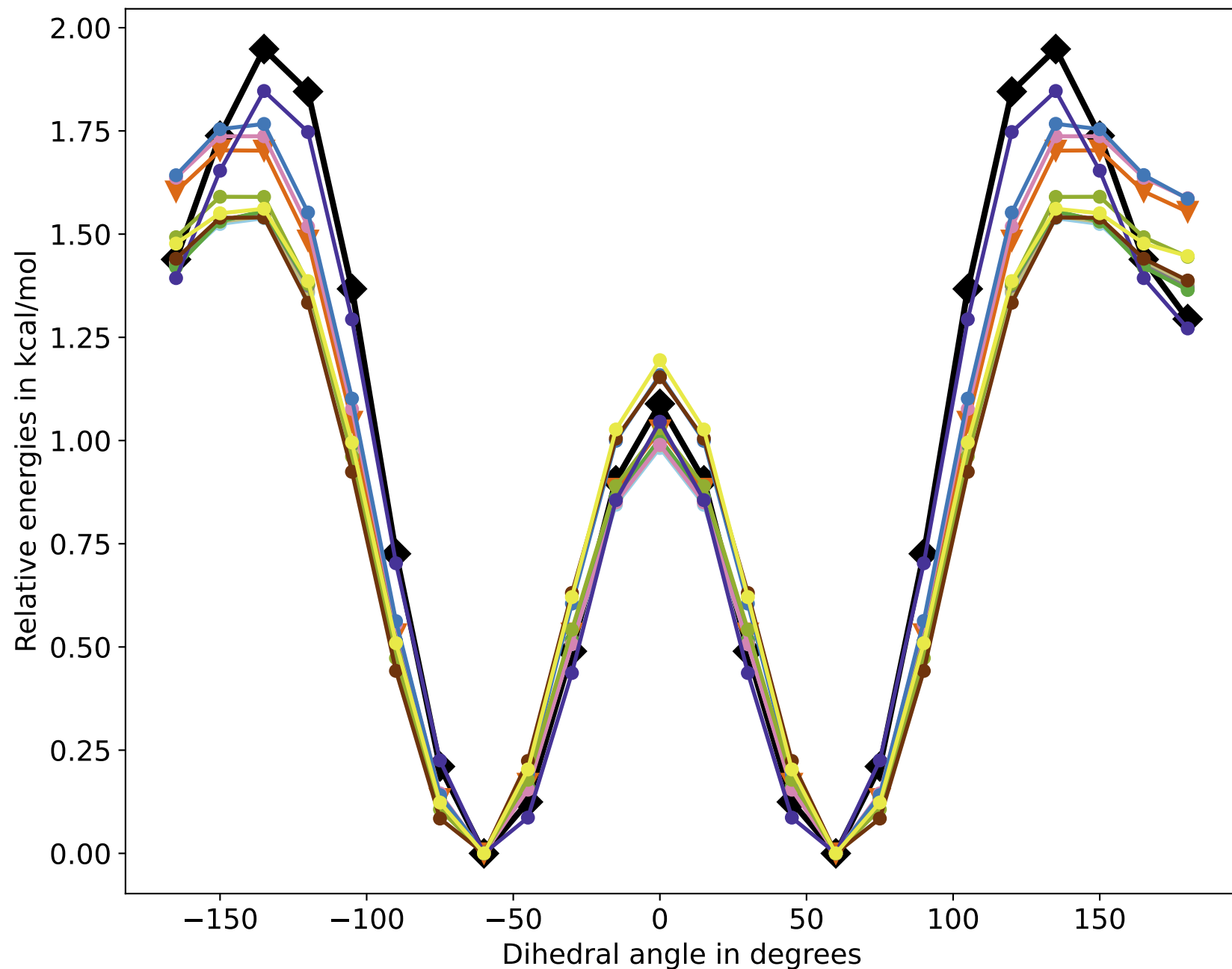


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- B3LYP-D3BJ/DEF2-QZVP
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

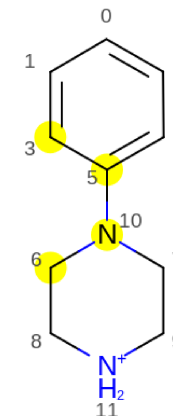
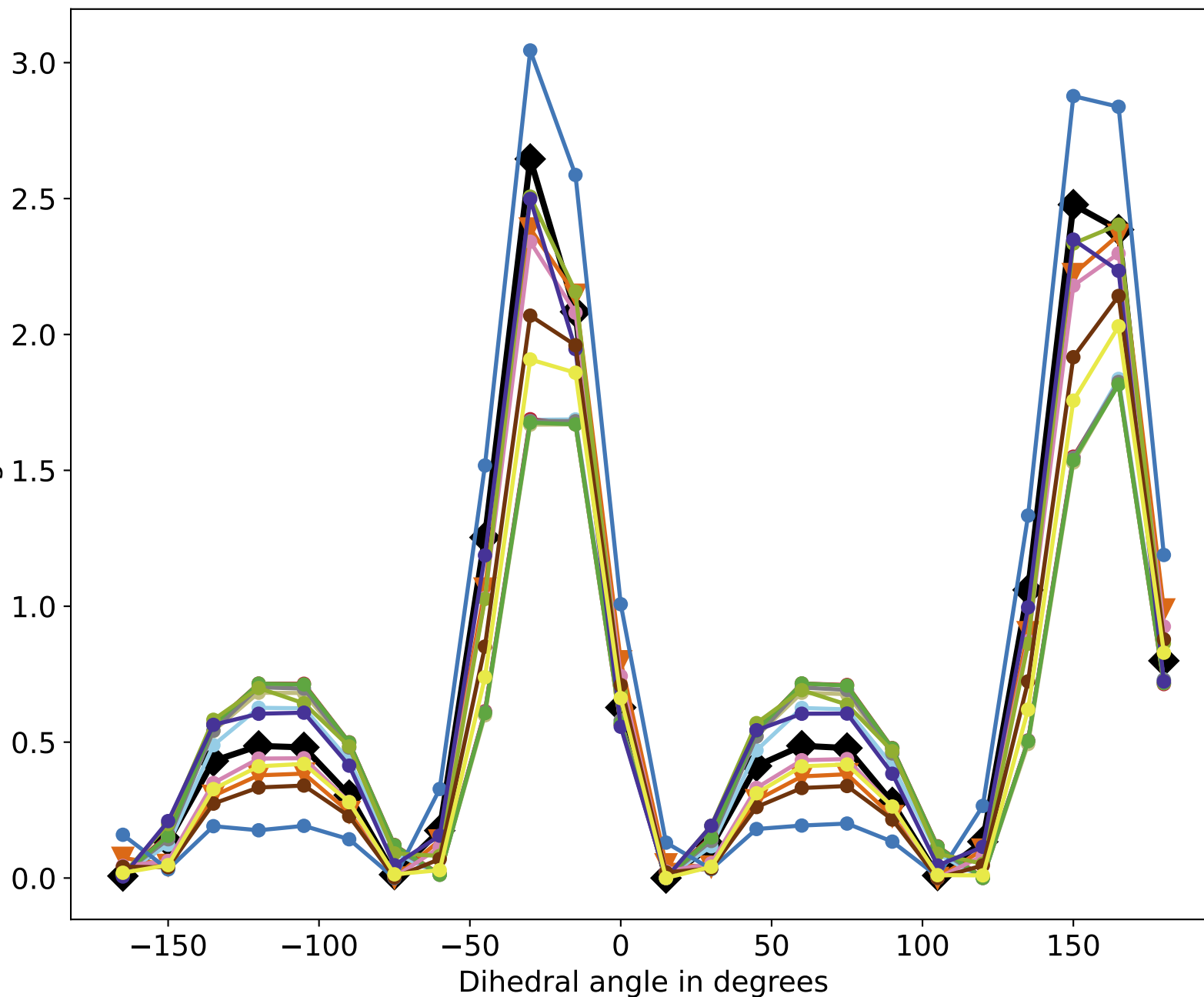


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- B3LYP-D3BJ/DEF2-QZVP
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



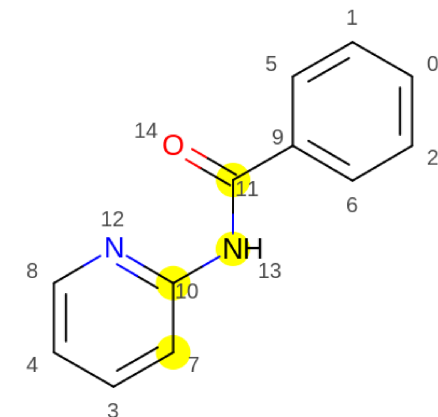
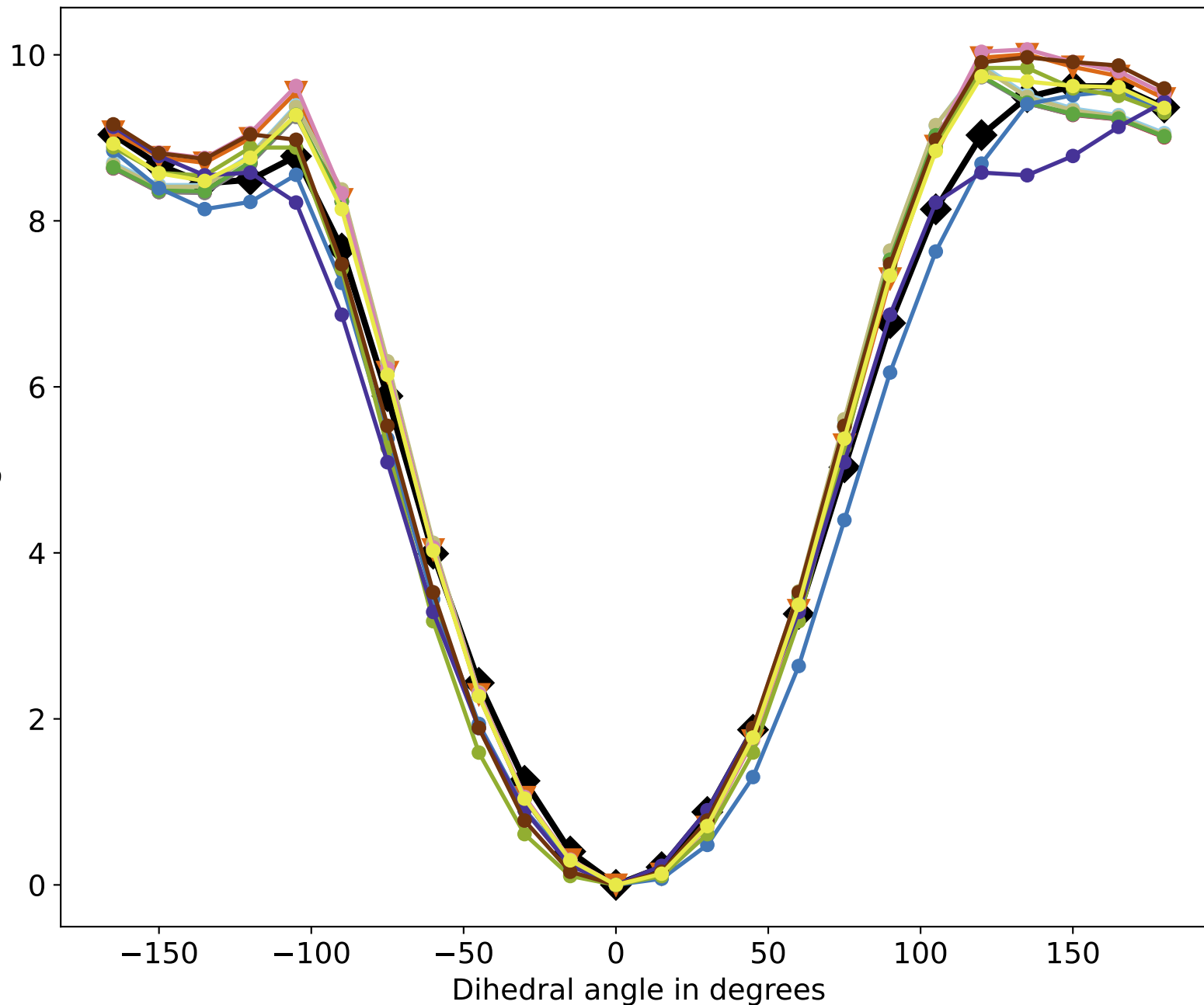
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



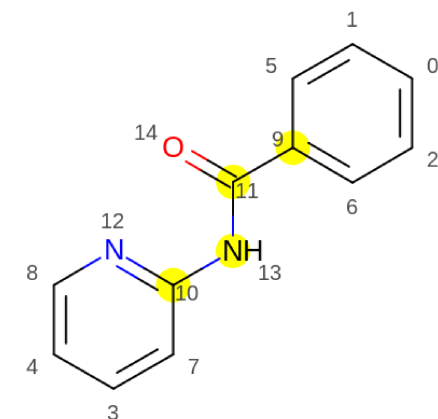
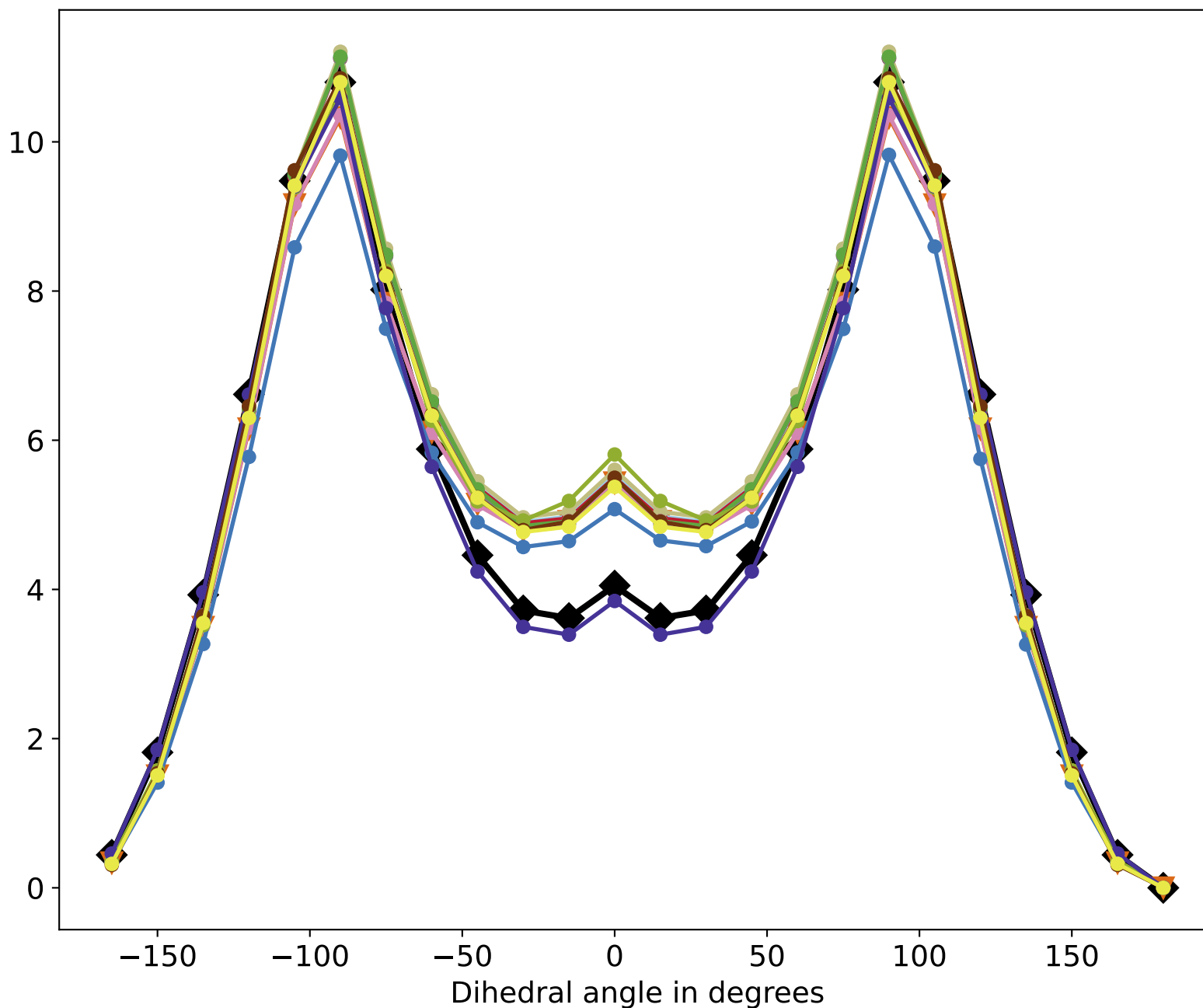
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



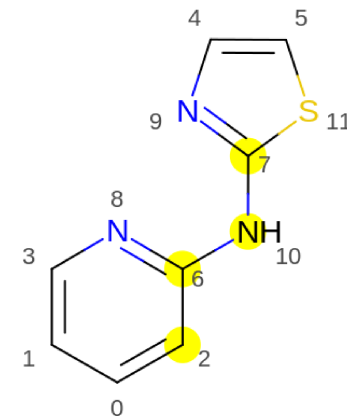
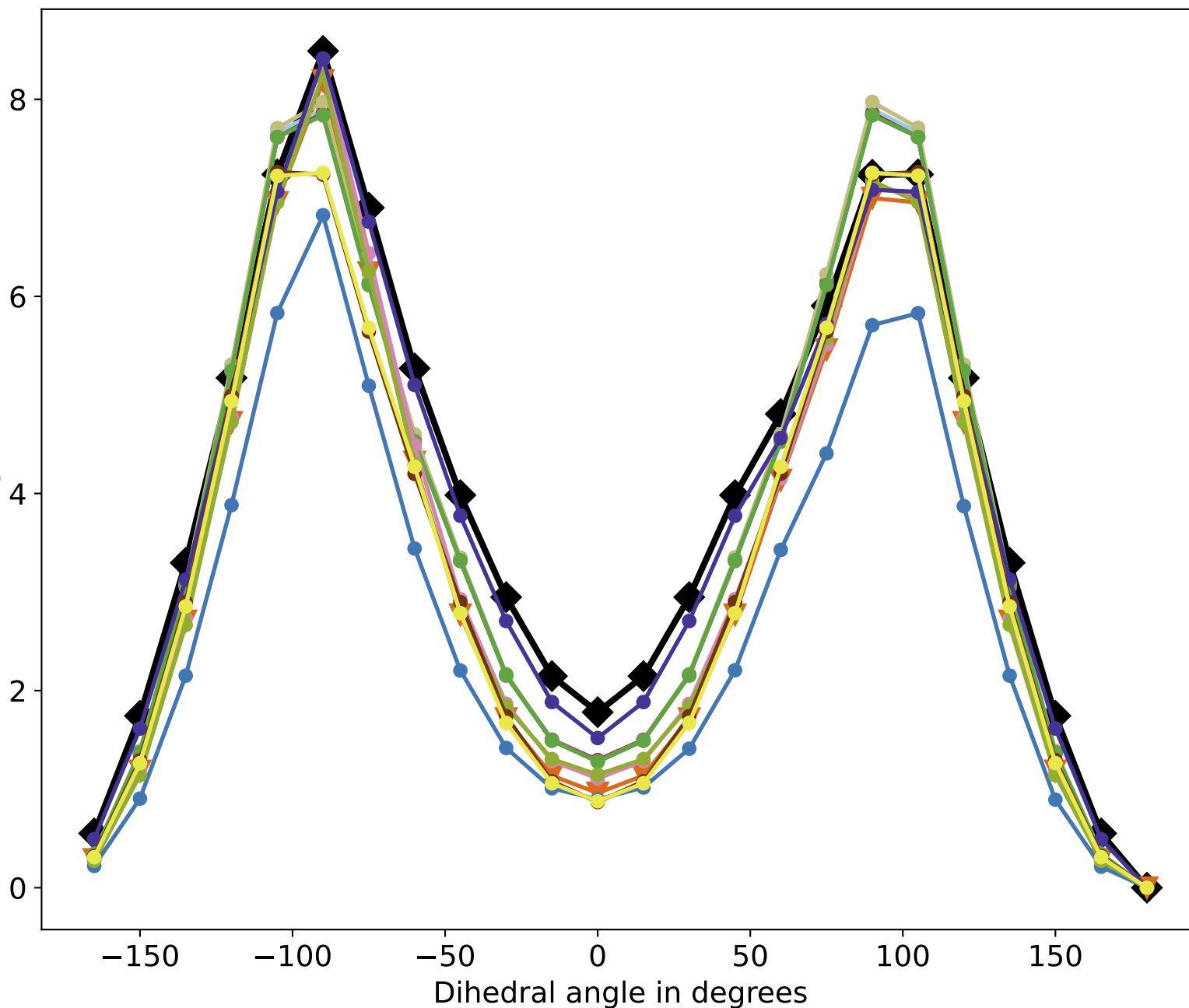
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- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

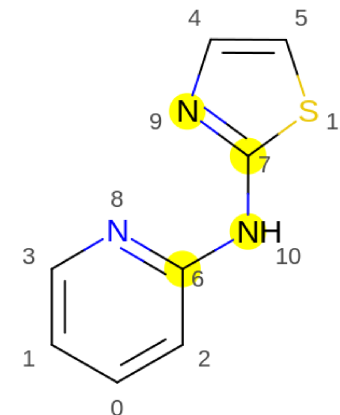
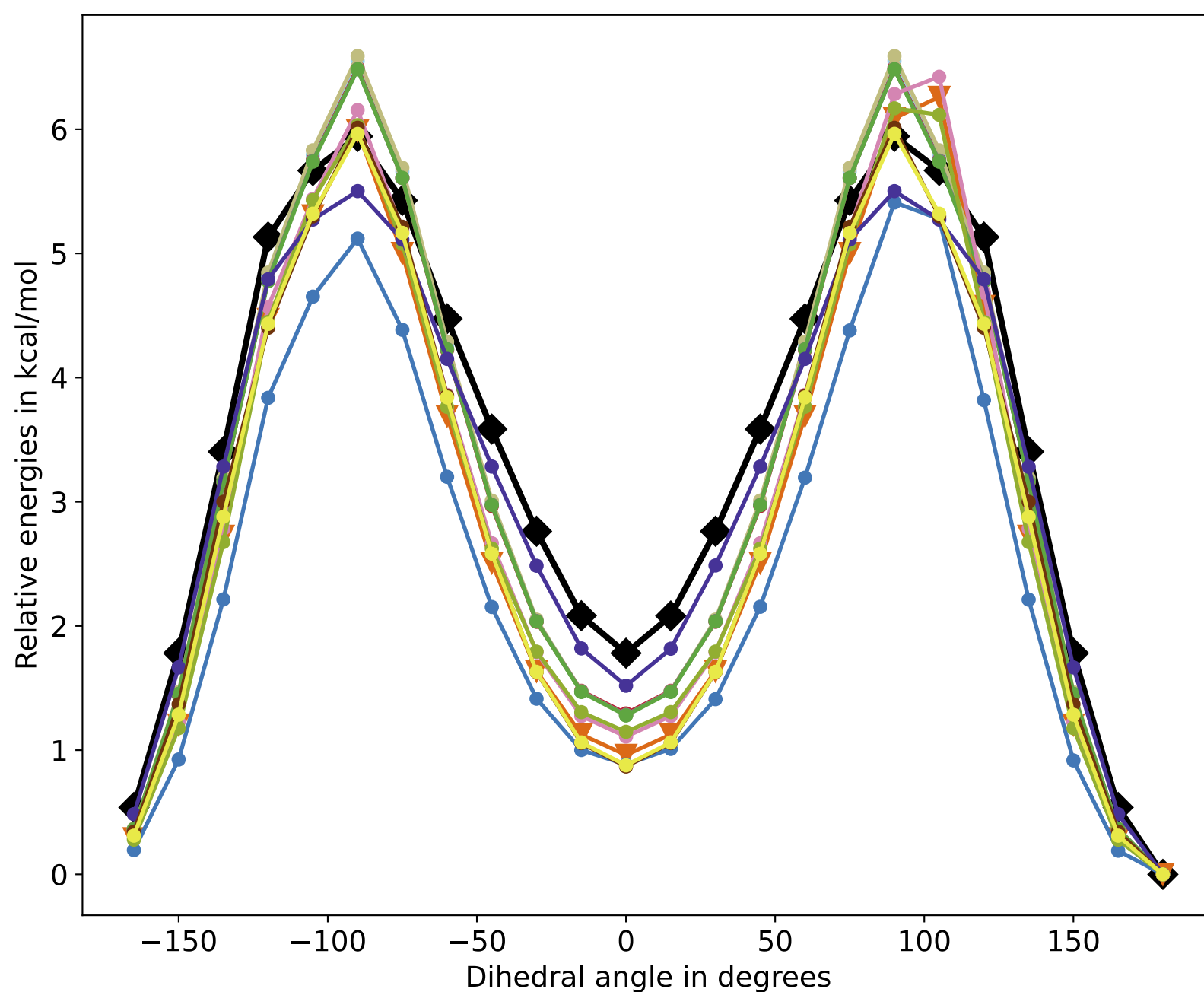


- MP2/heavy-aug-cc-pVTZ
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- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

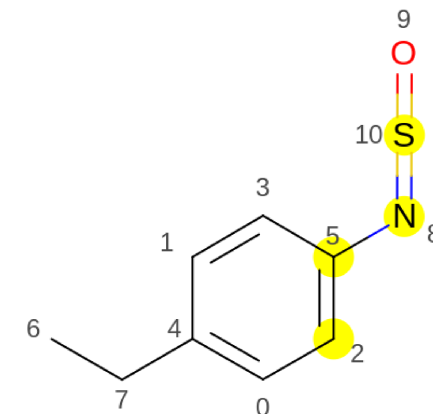
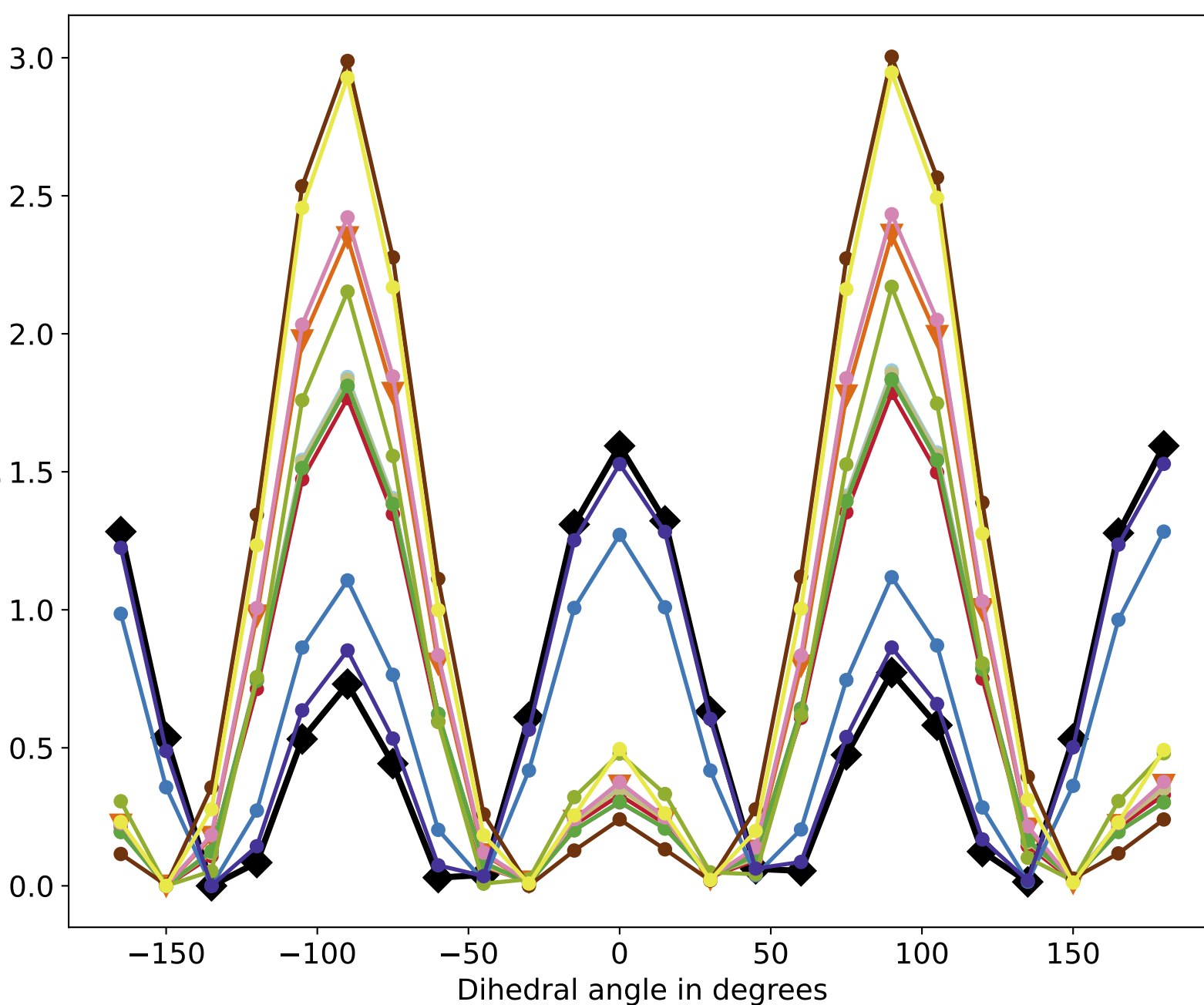


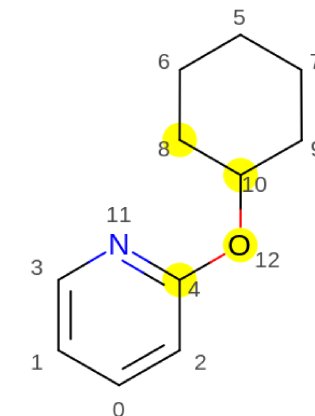
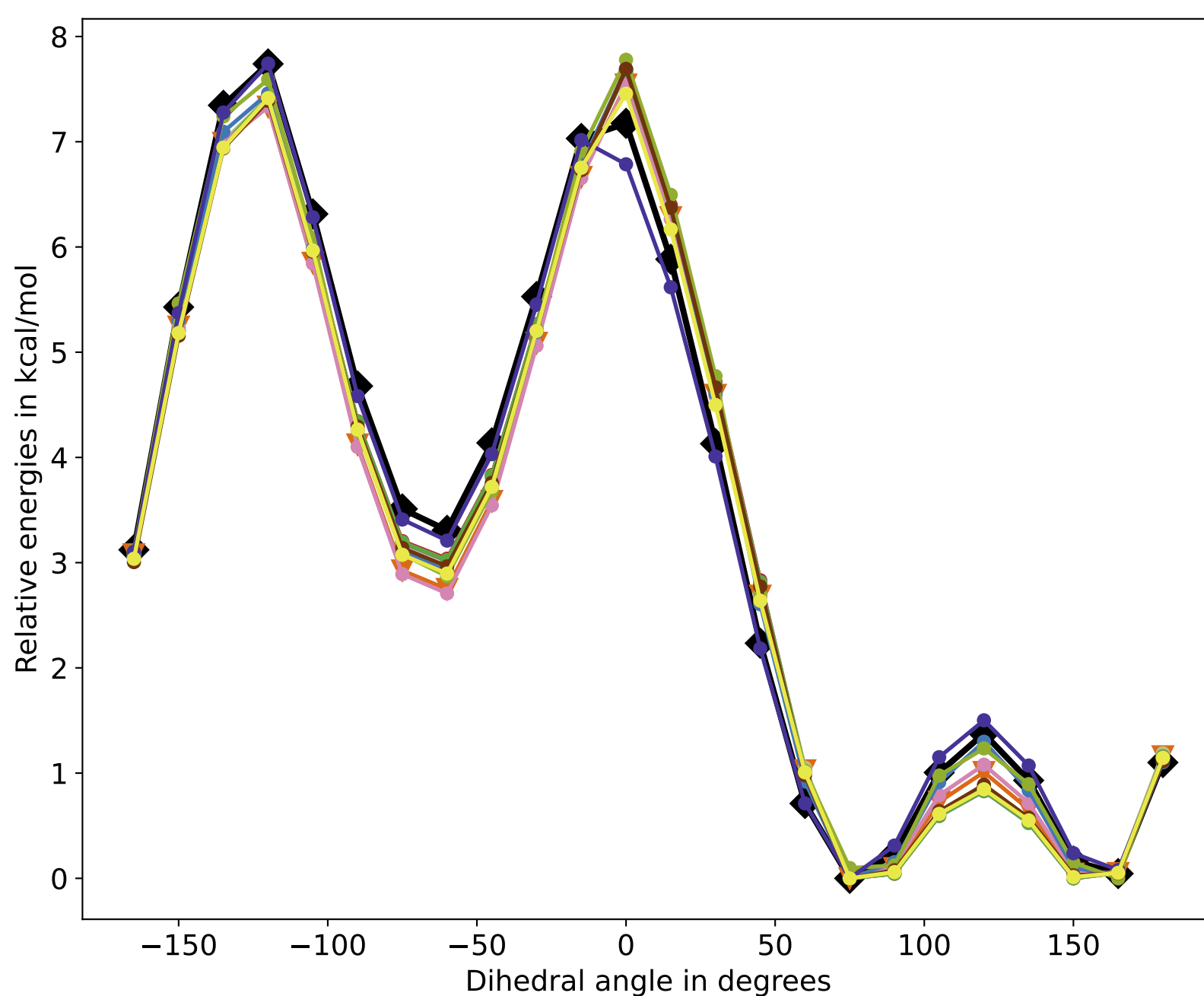
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



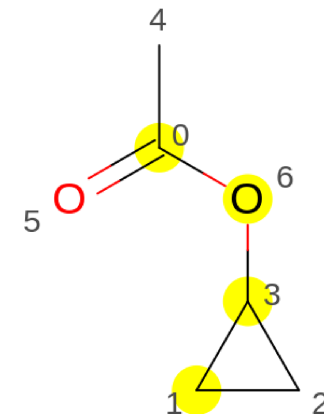
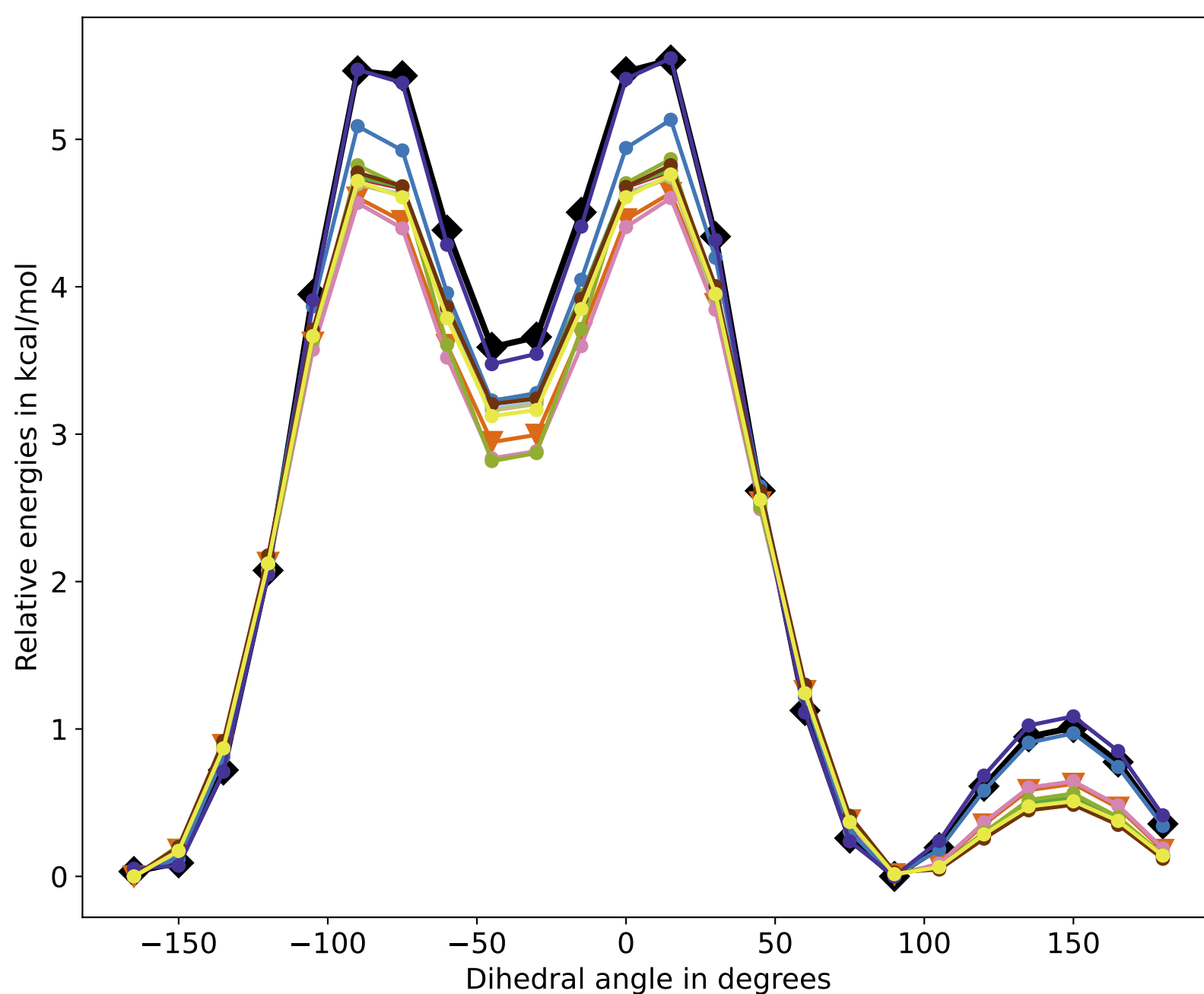
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

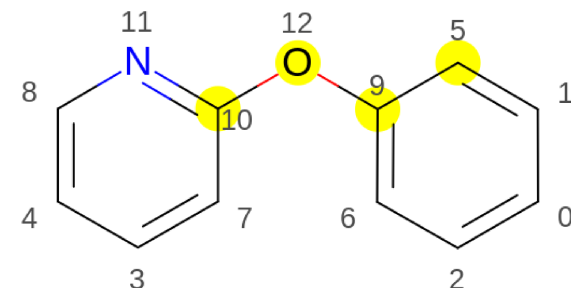
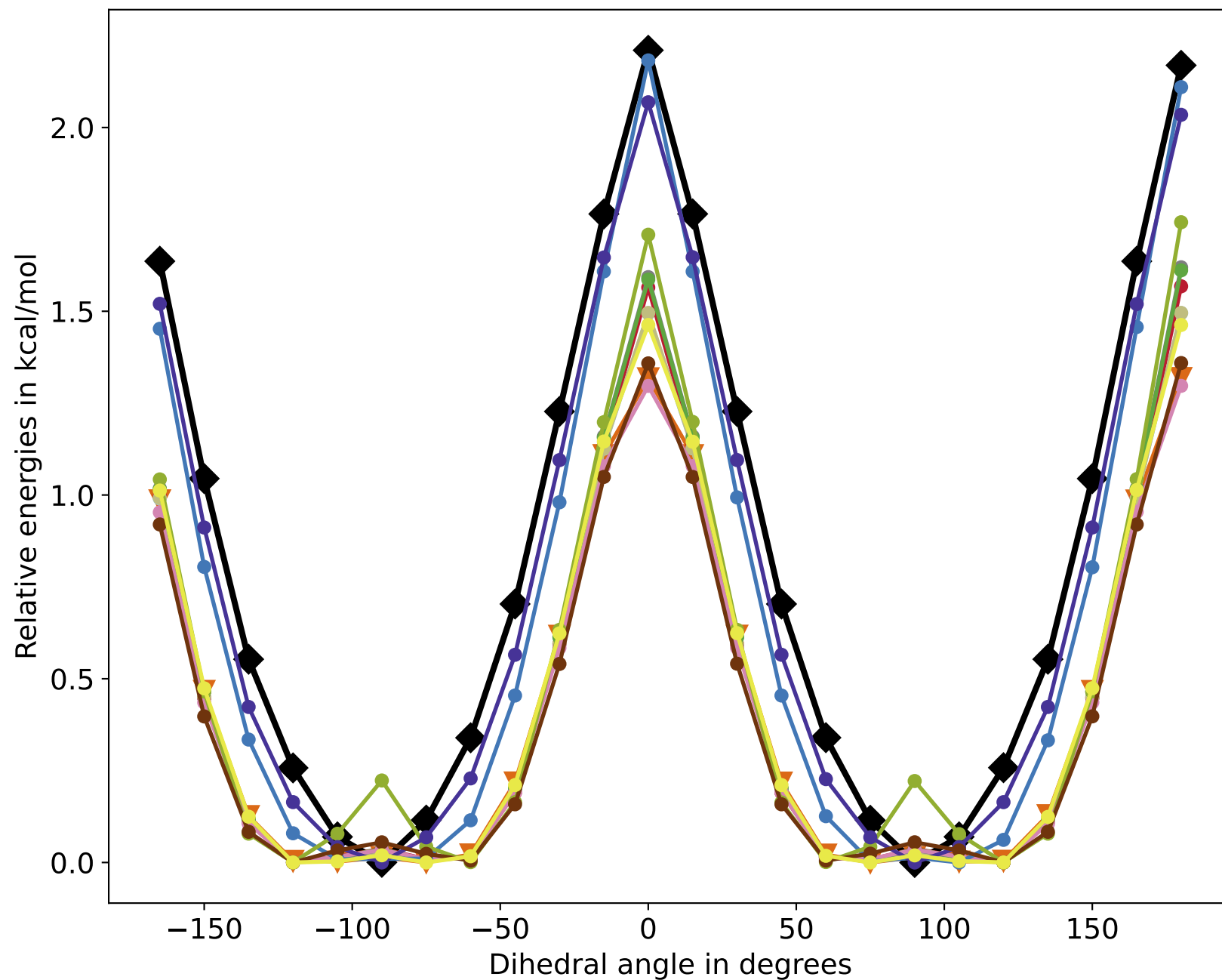




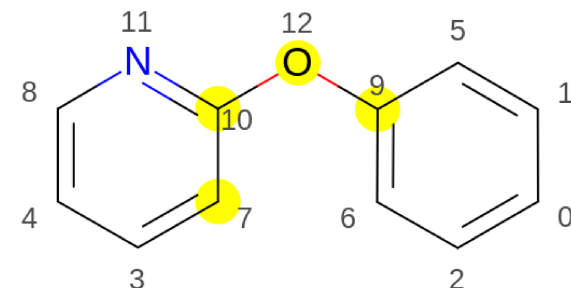
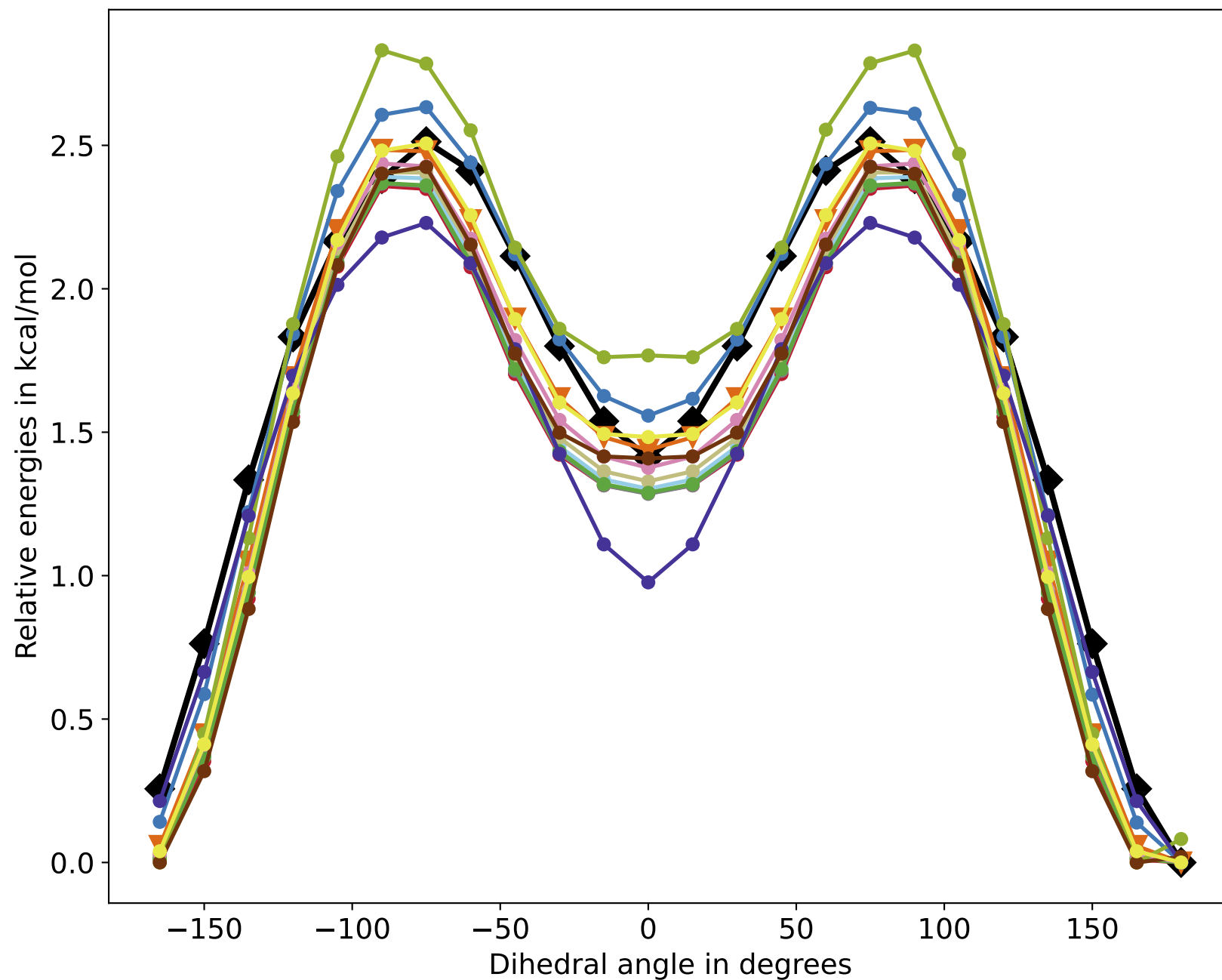
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- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



- MP2/heavy-aug-cc-pVTZ
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

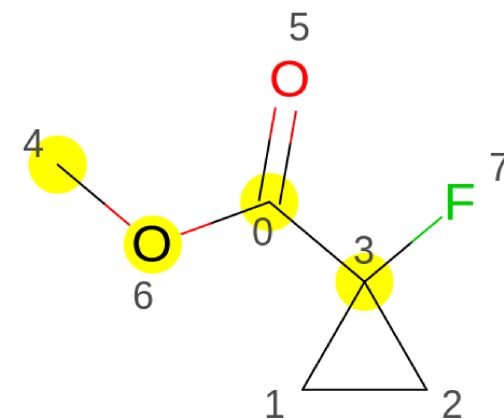
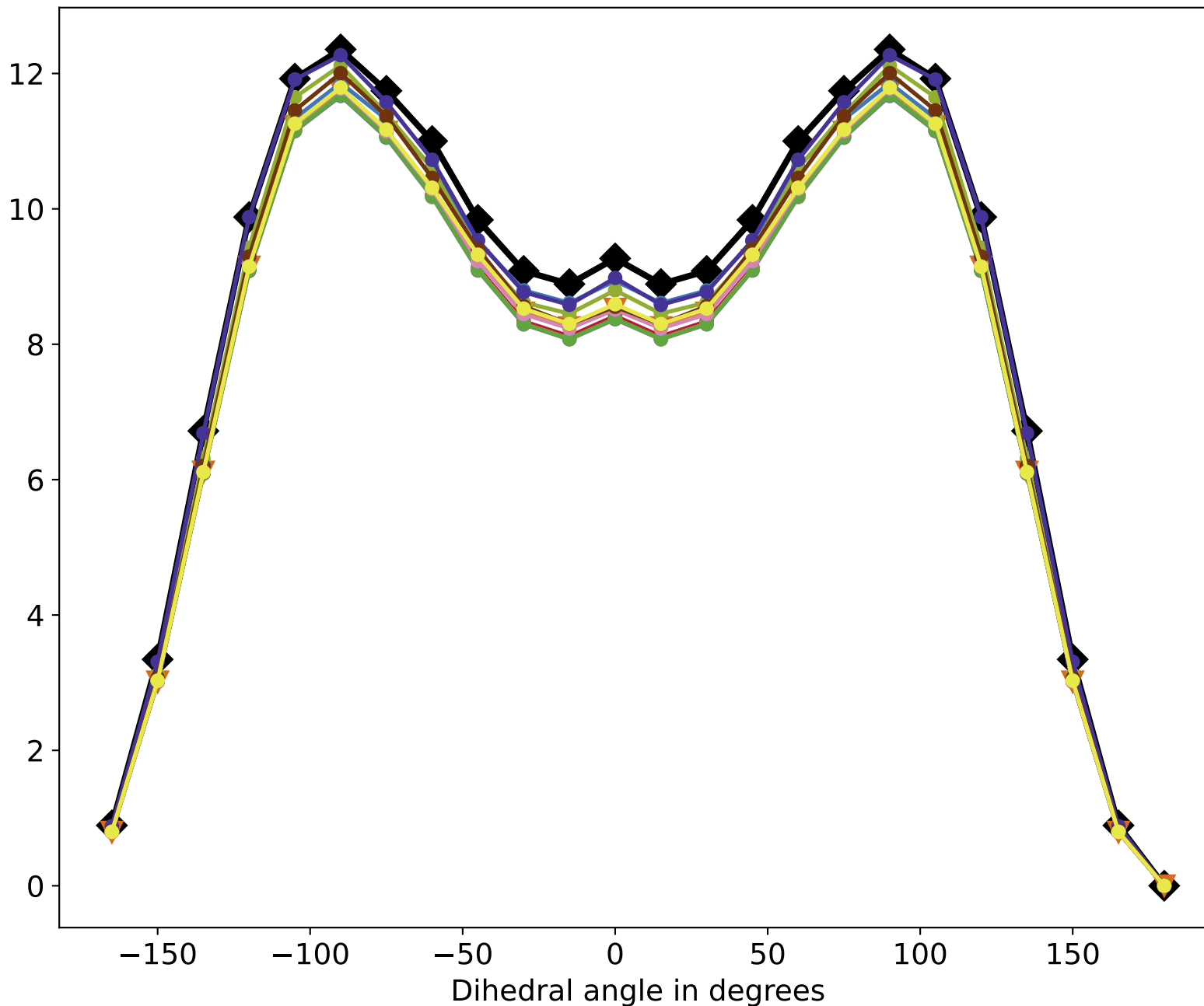


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- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



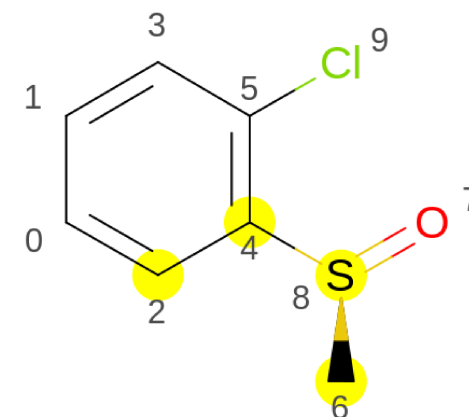
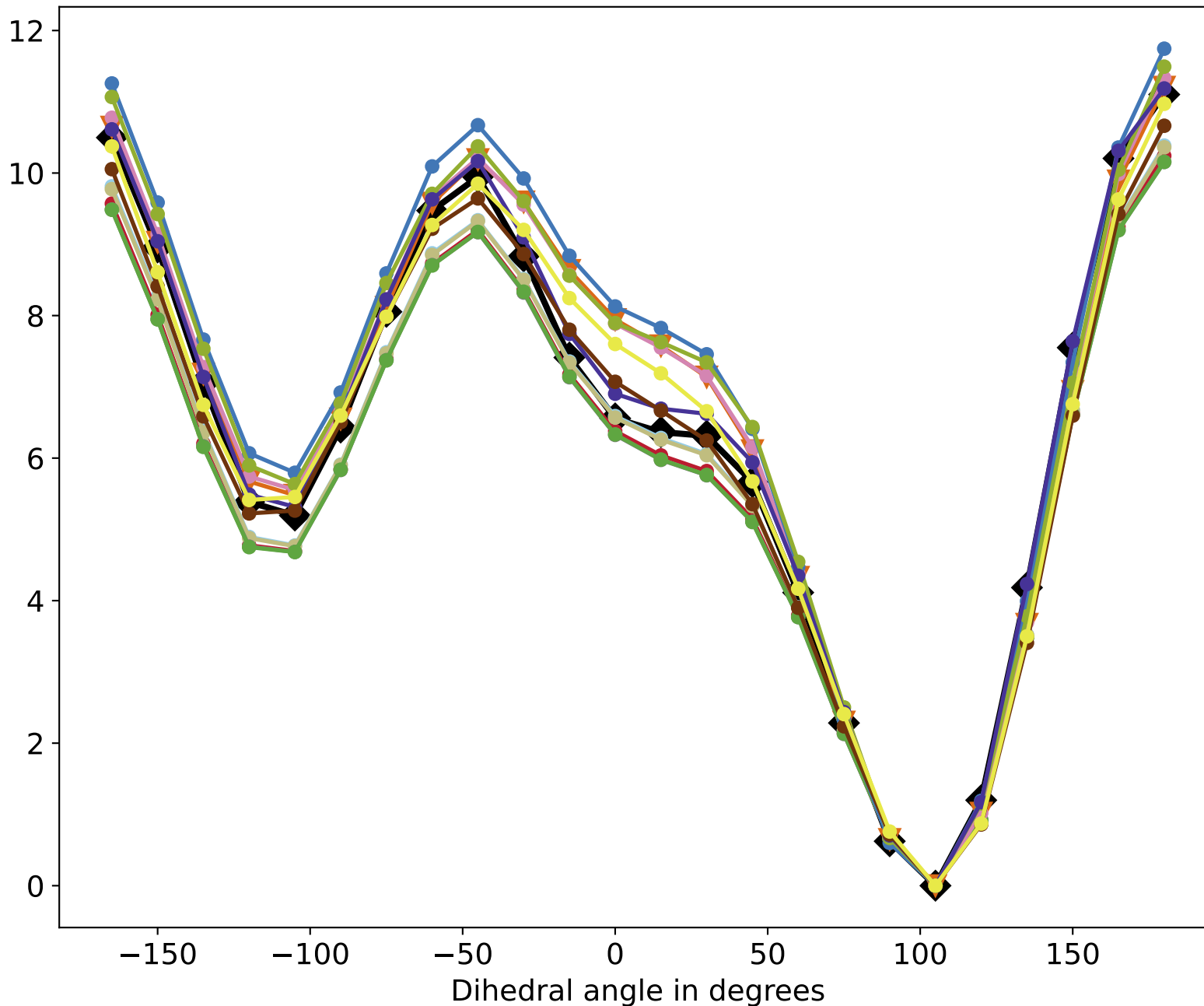
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- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



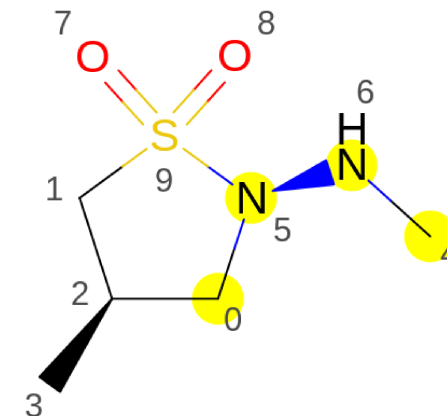
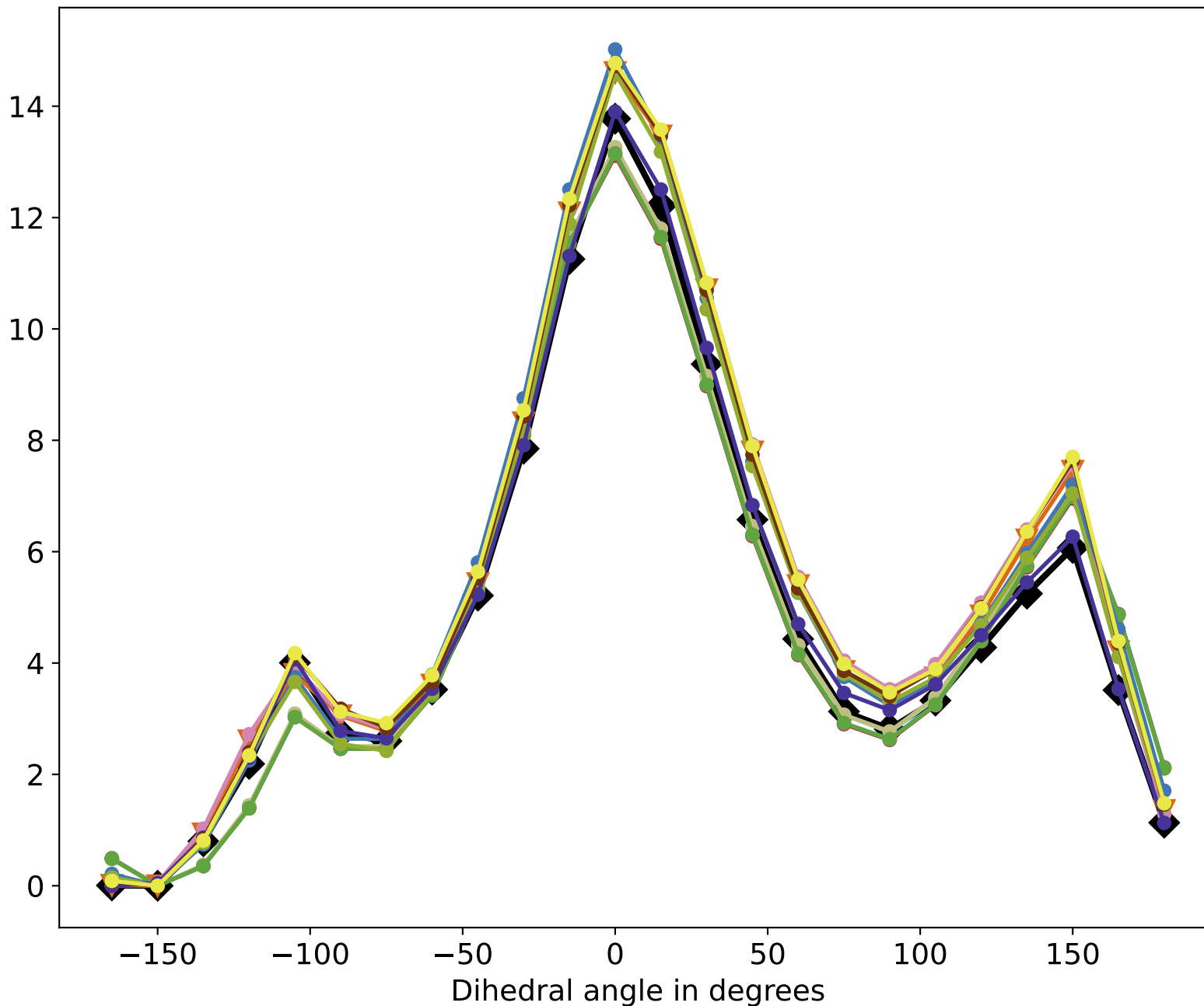
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- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



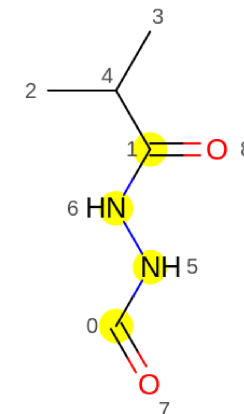
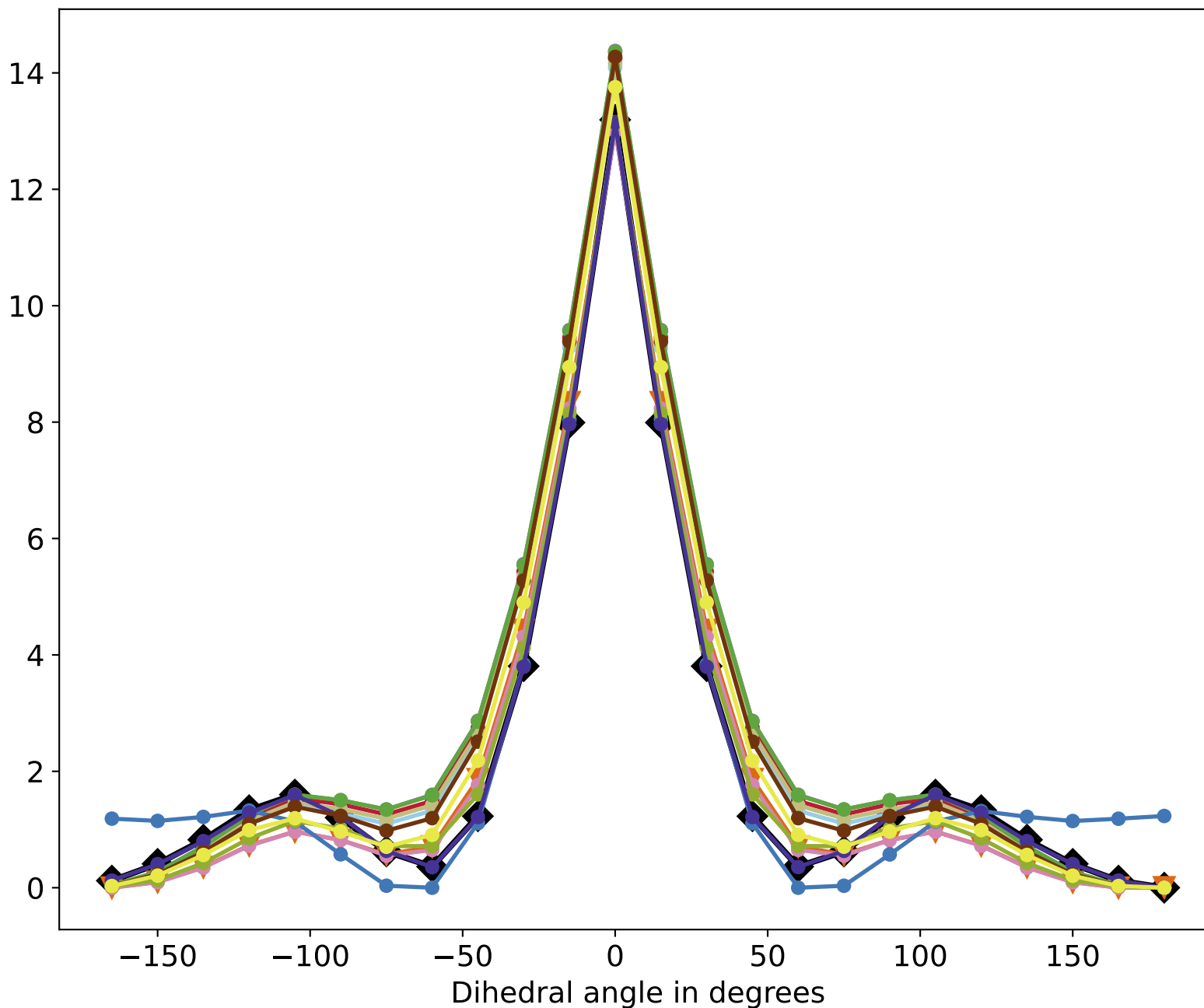
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- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
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- B3LYP-D3BJ/DEF2-TZVPPD
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- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

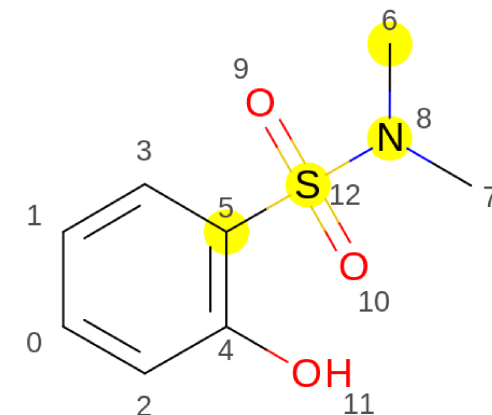
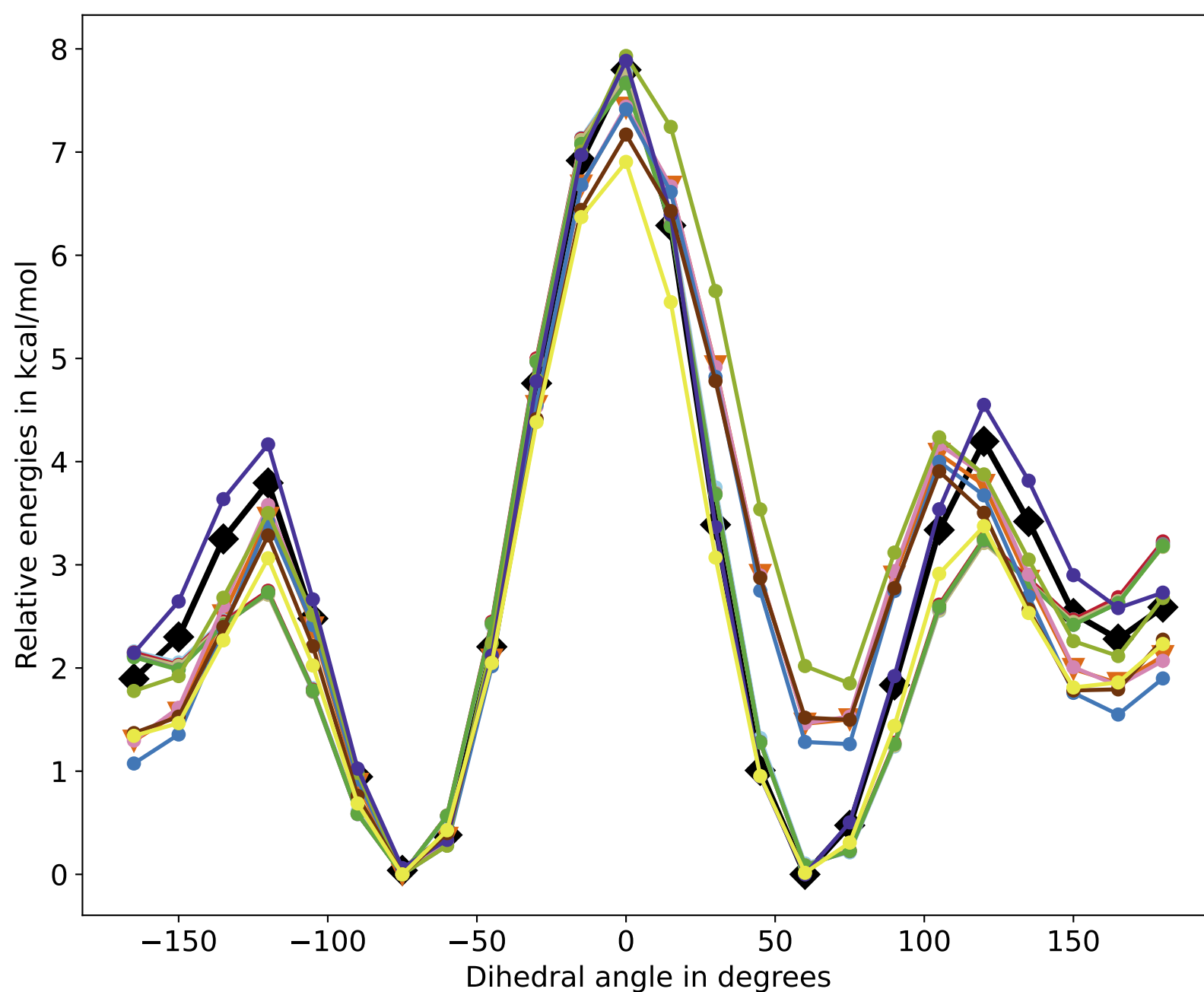


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- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

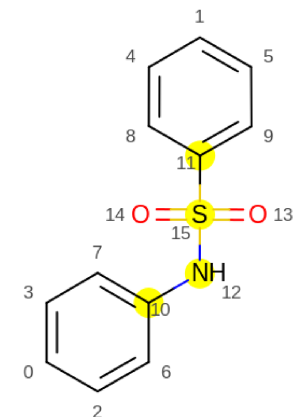
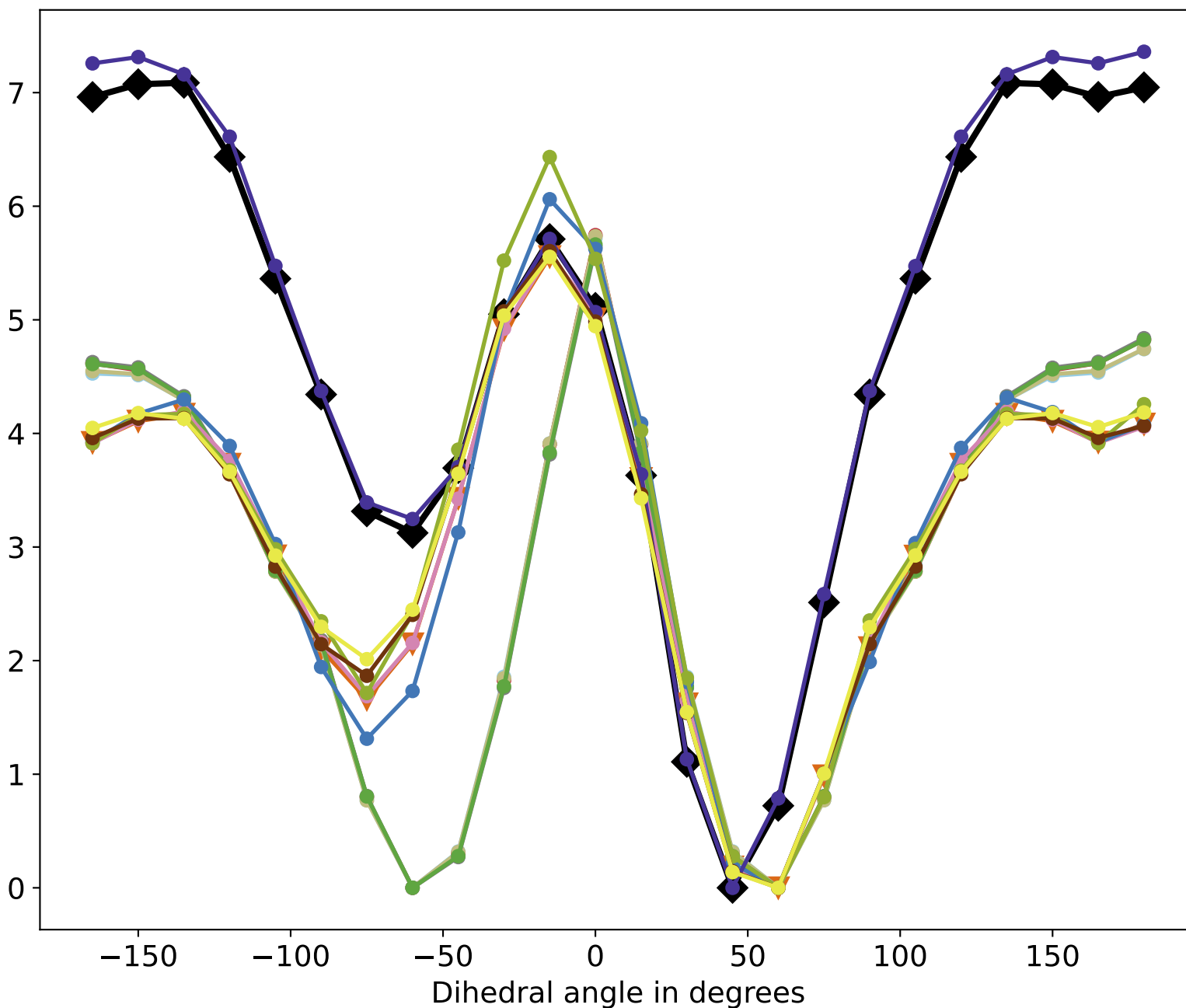


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- B3LYP-D3BJ/DEF2-QZVP
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- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

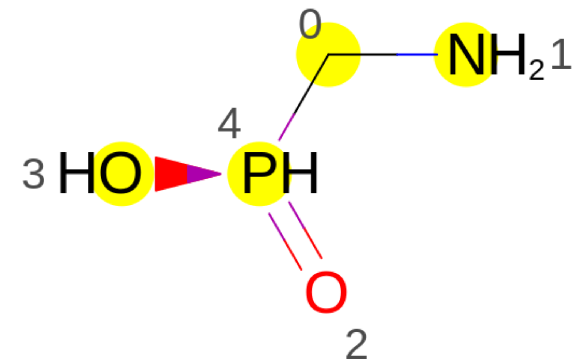
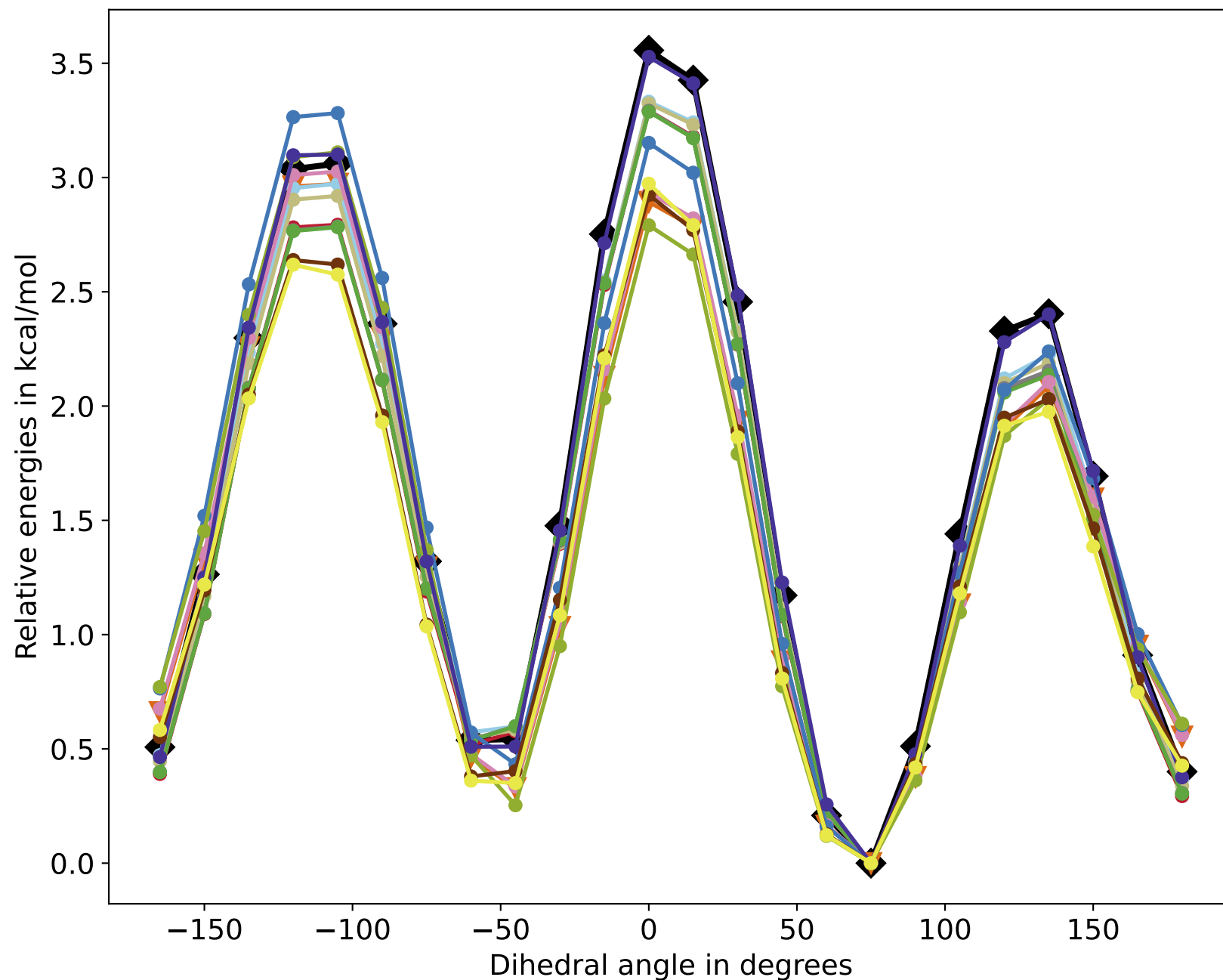


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- B3LYP-D3BJ/DEF2-QZVP
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- B3LYP-D3MBJ/DZVP
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
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- B3LYP-D3BJ/6-311+G**

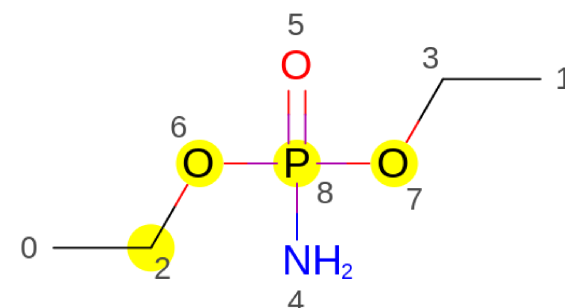
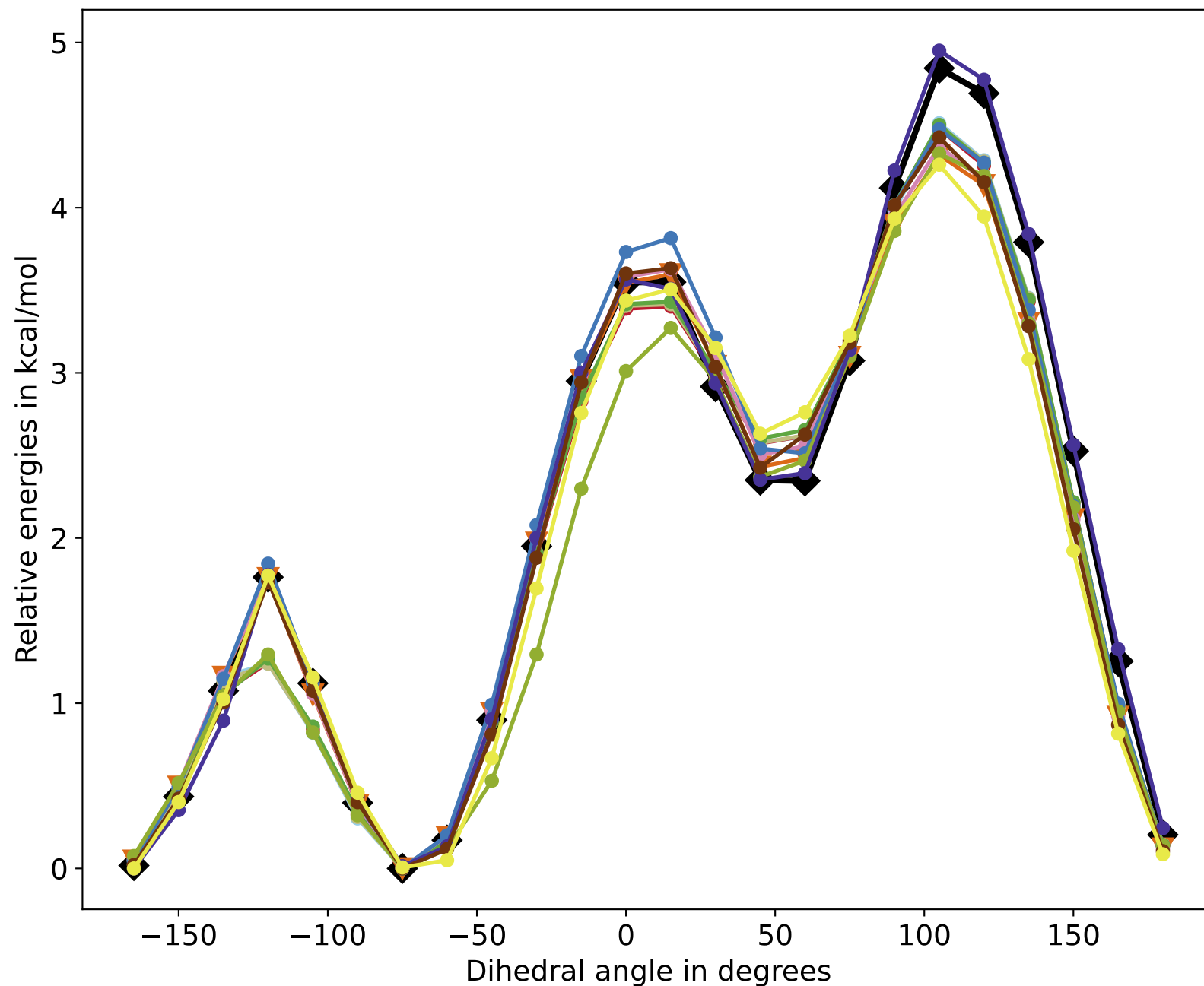
Relative energies in kcal/mol



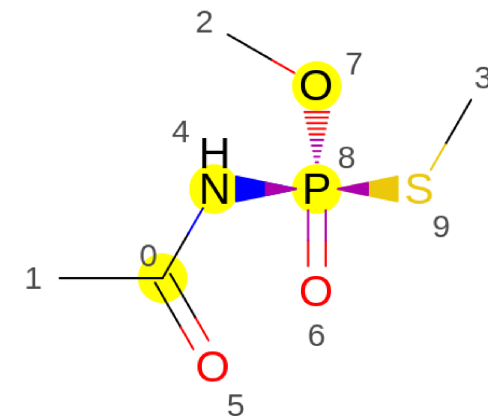
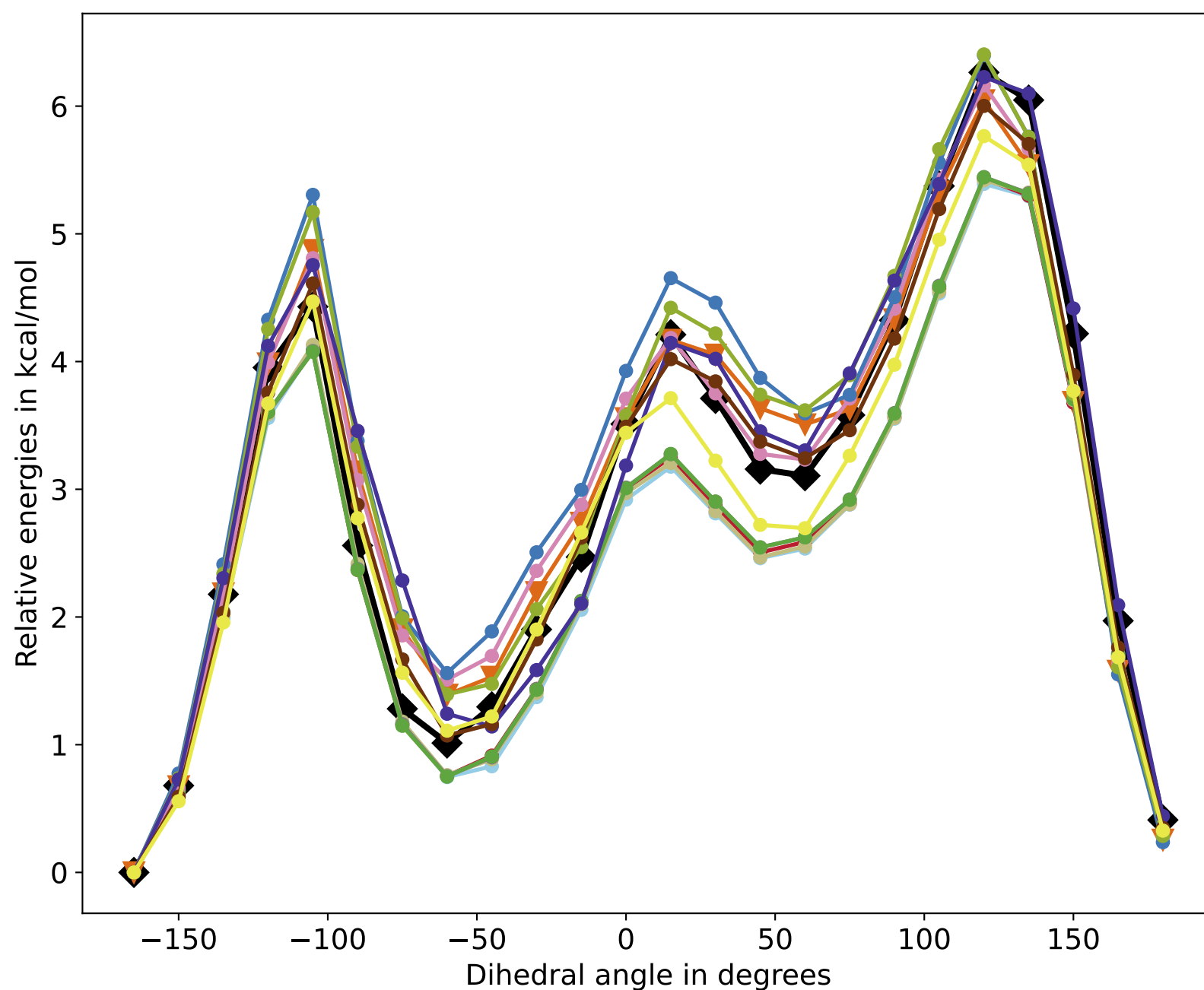
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- WB97X-D3BJ/DZVP
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- PW6B95-D3BJ/DZVP
- MP2/aug-cc-pVTZ
- B3LYP-D3BJ/6-31+G**
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