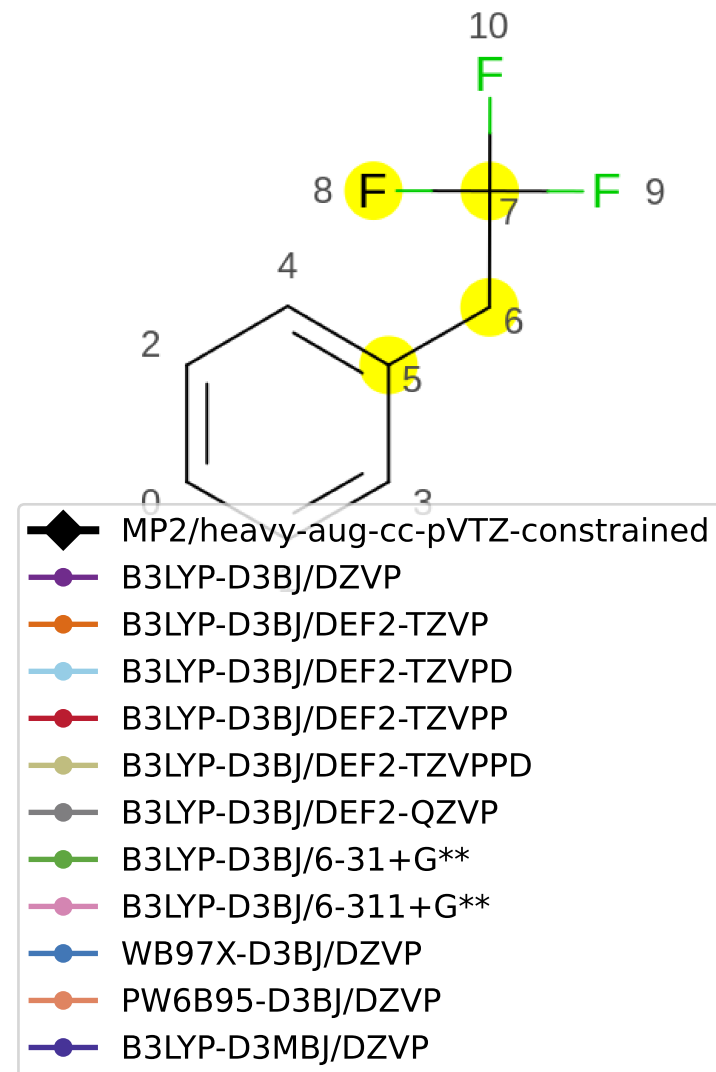
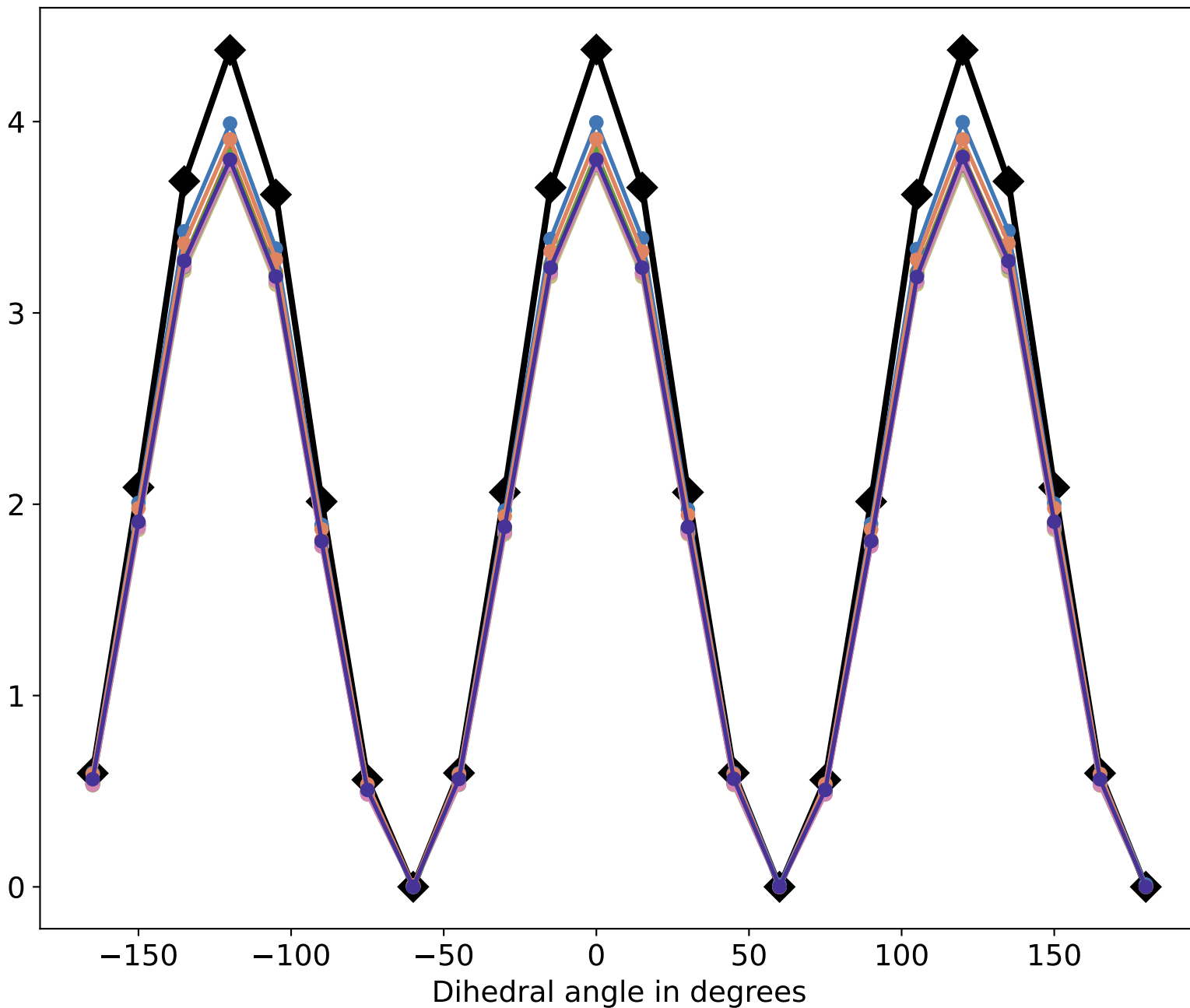
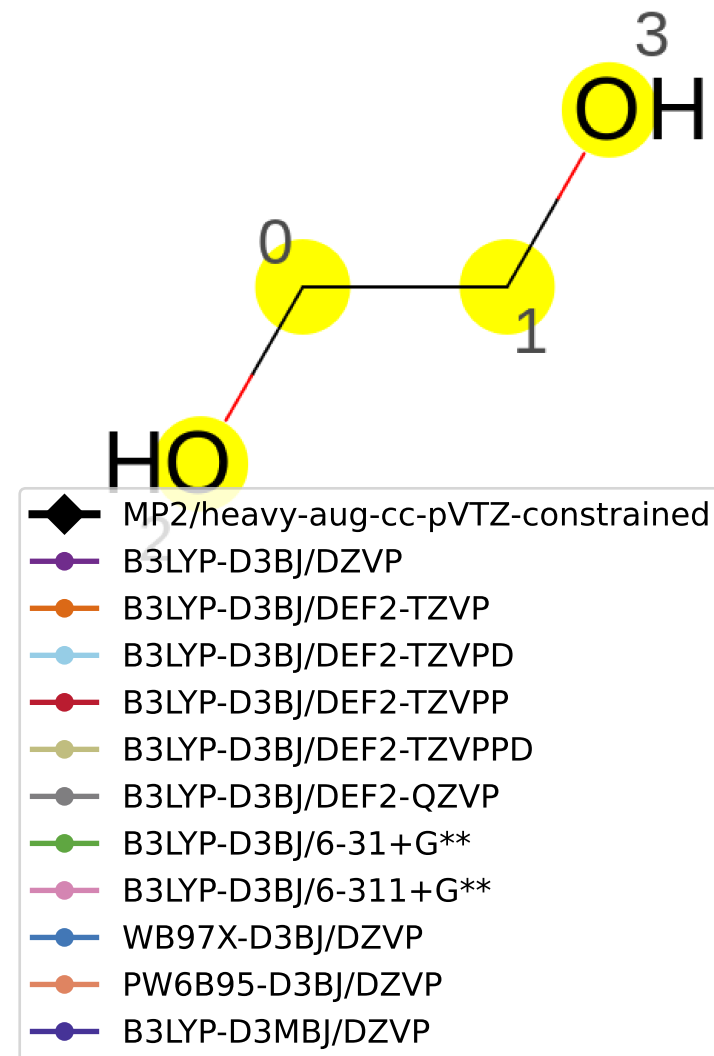
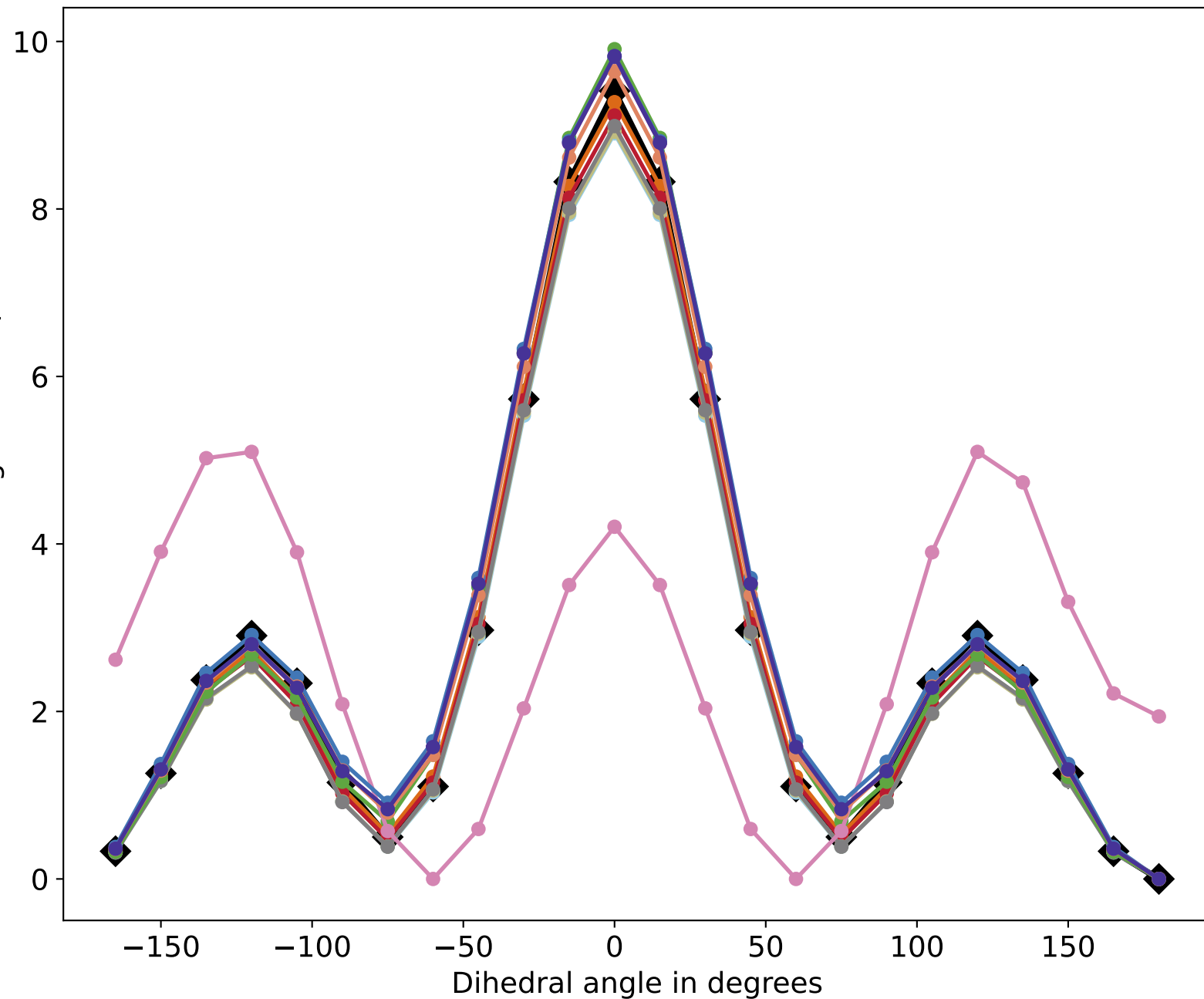
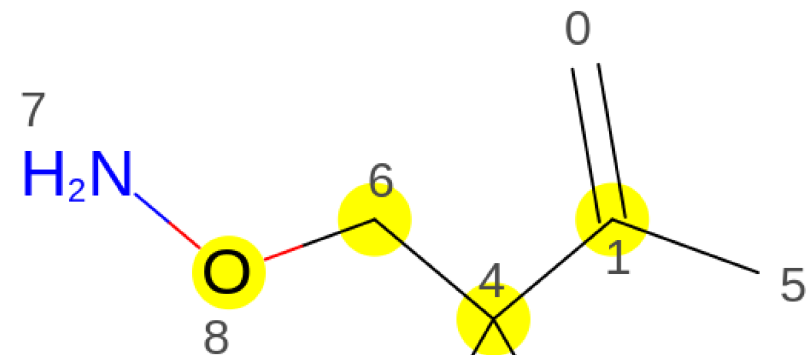
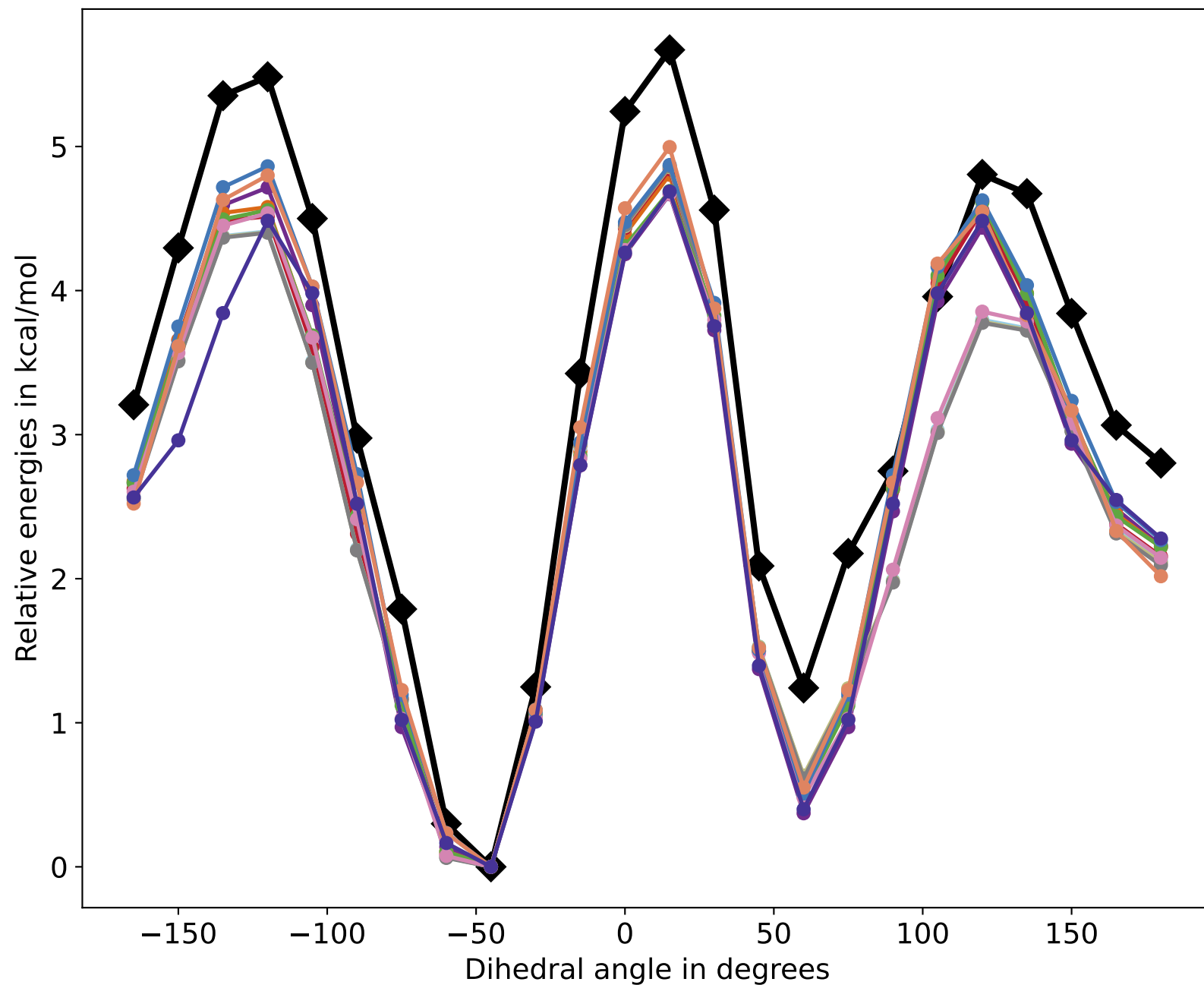


Relative energies in kcal/mol



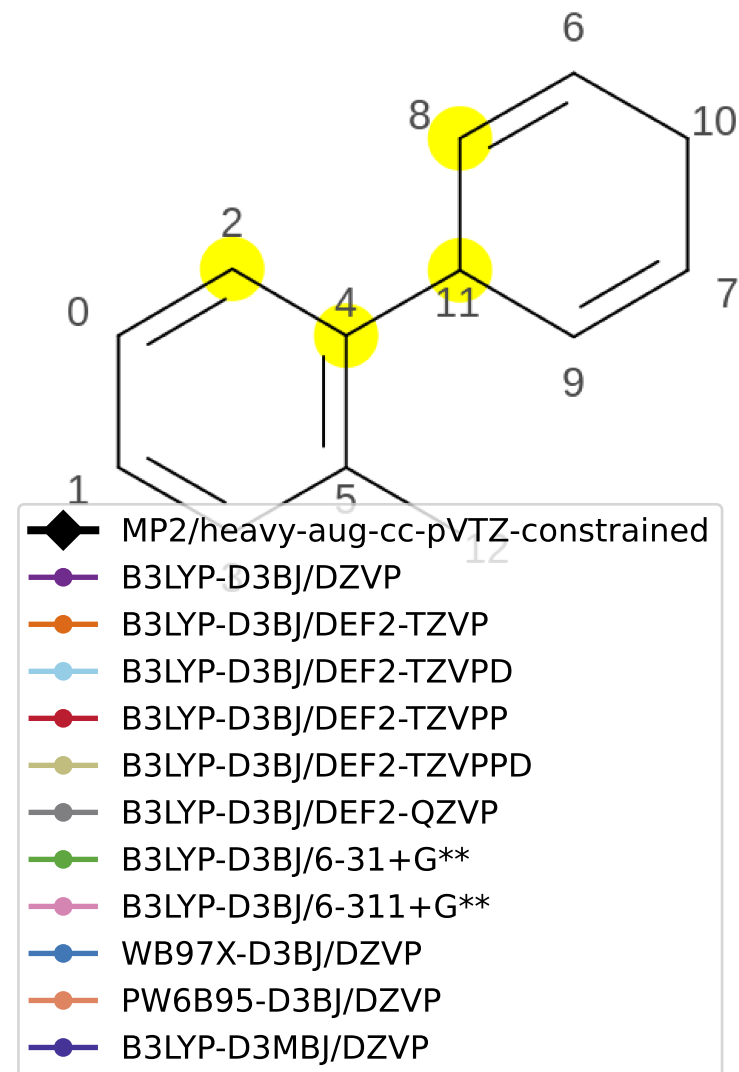
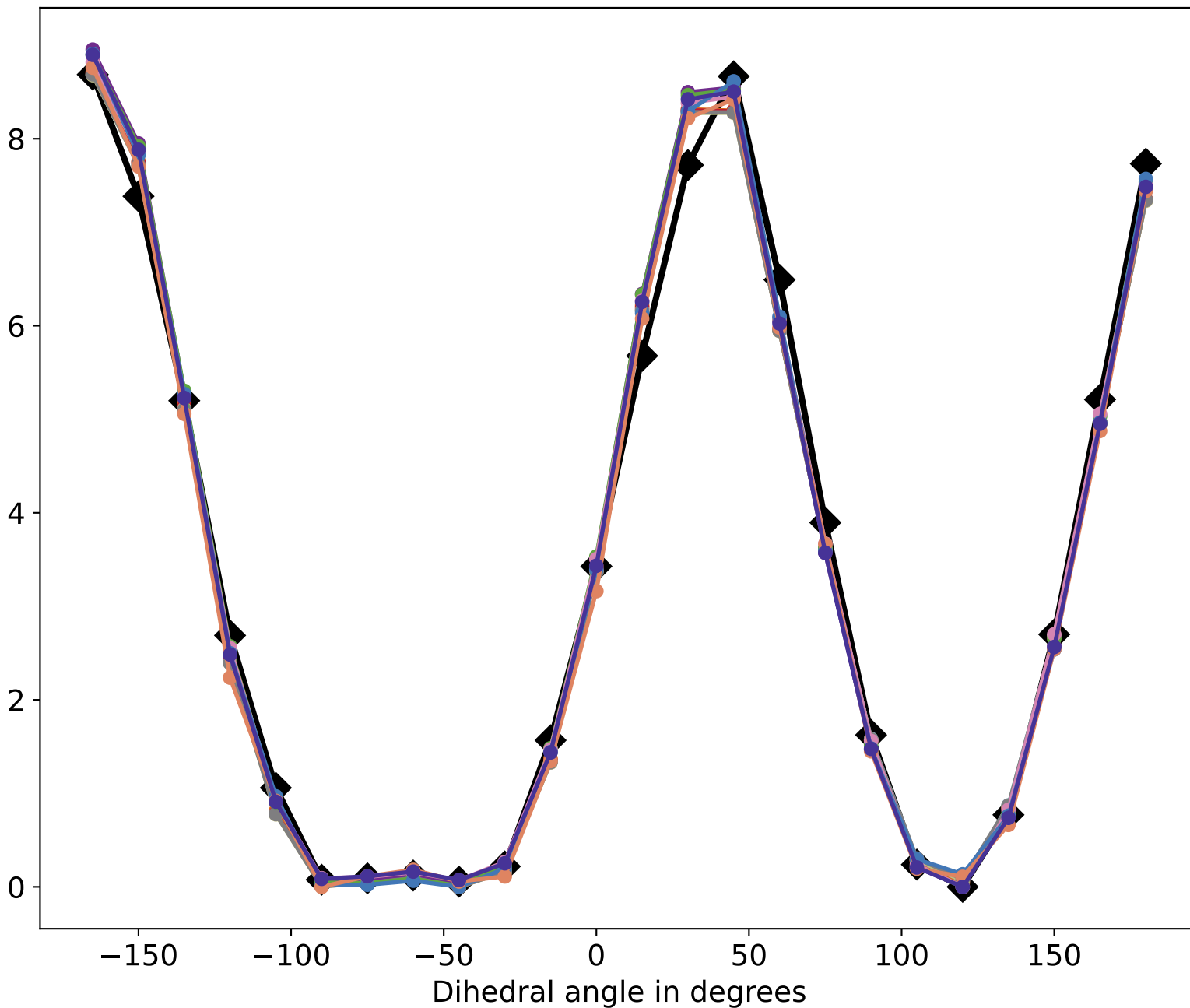
Relative energies in kcal/mol

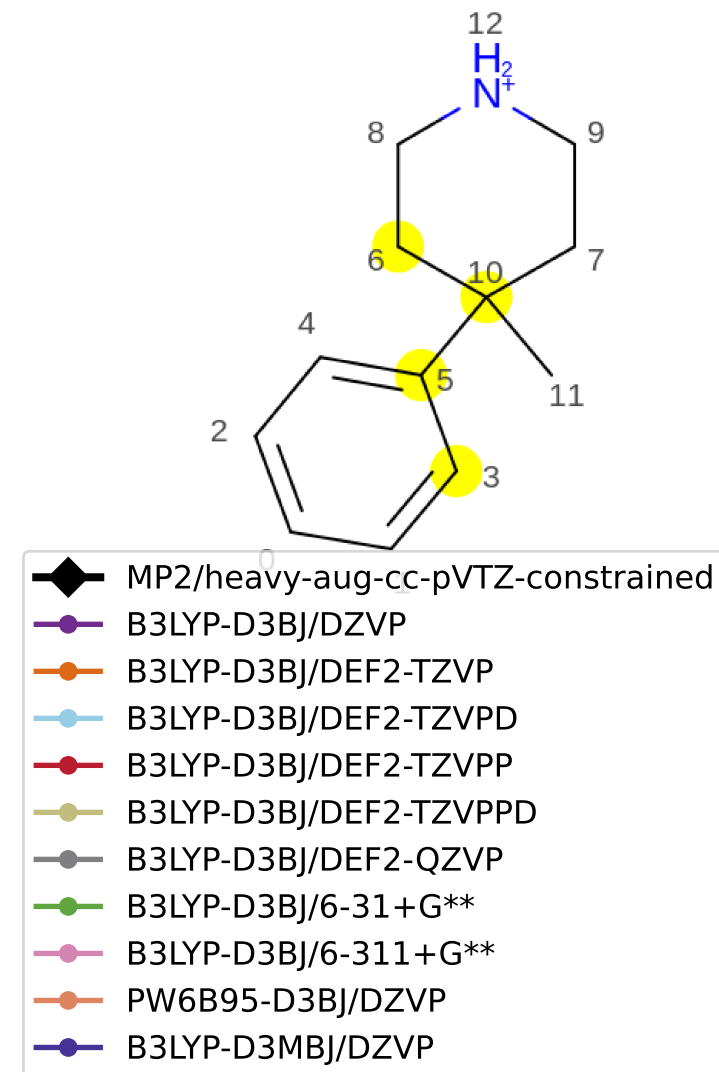
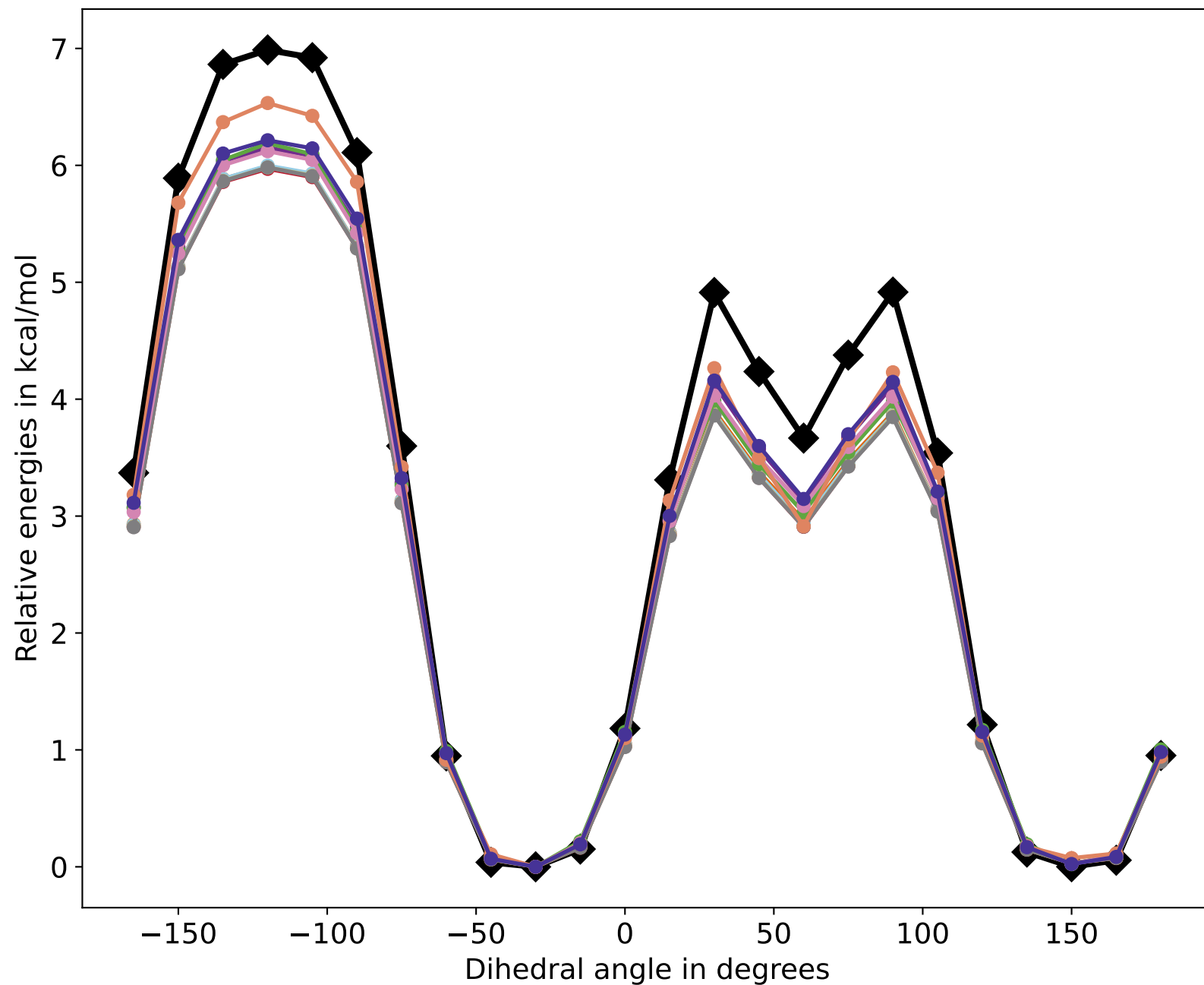


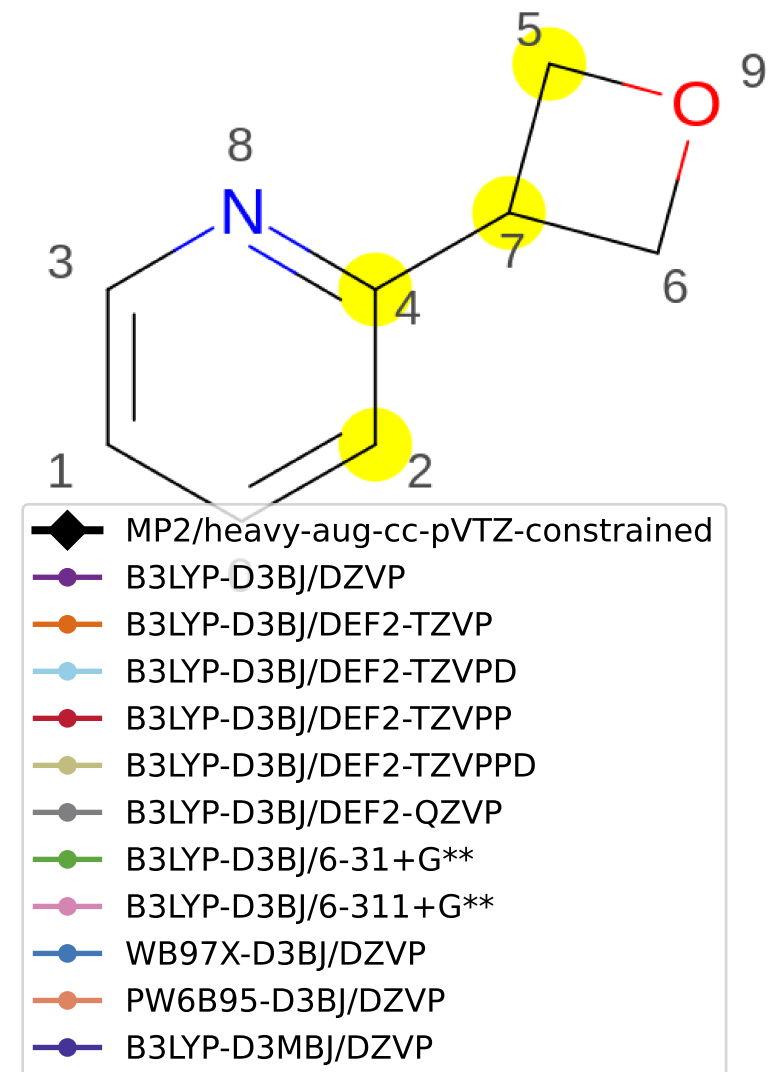
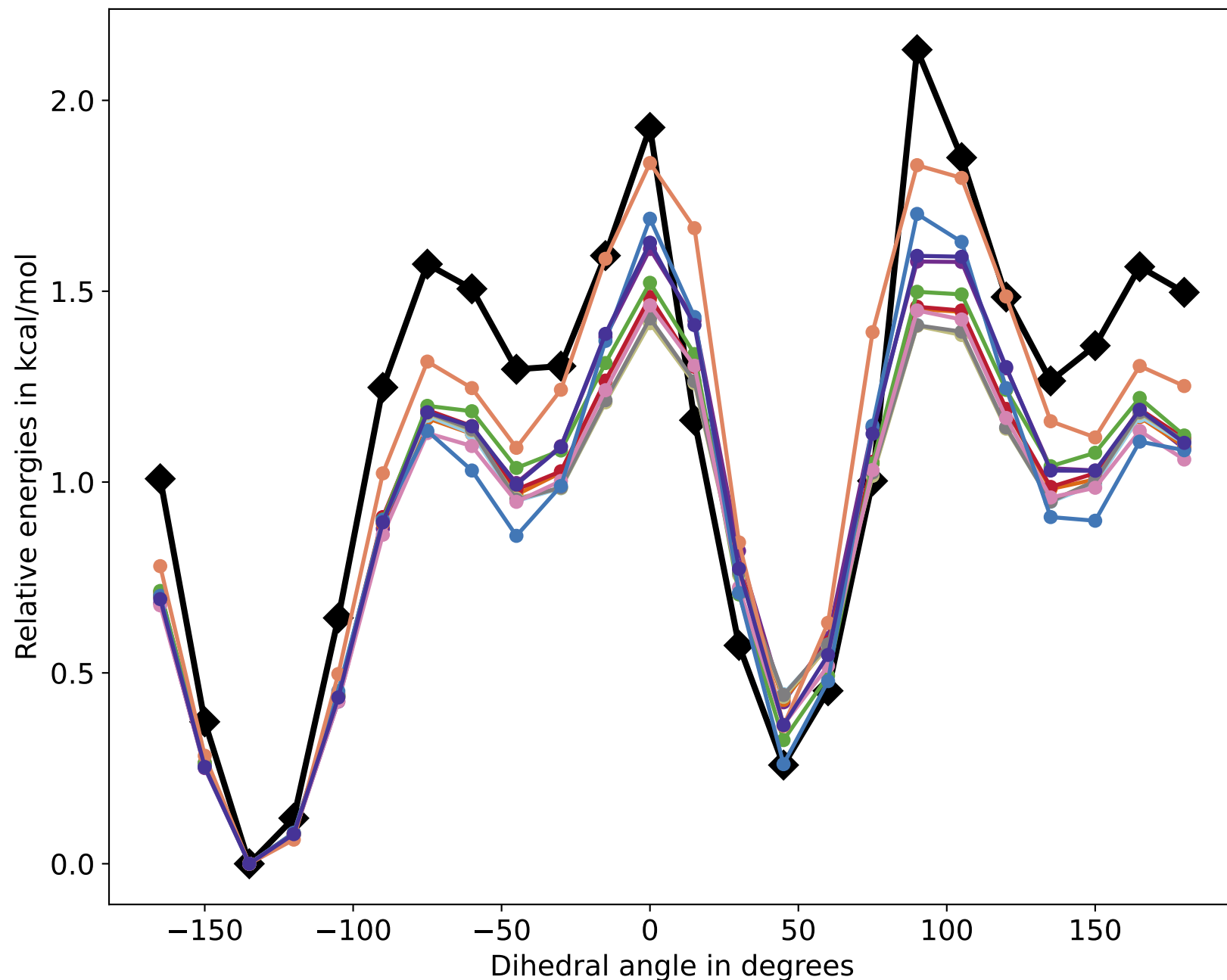


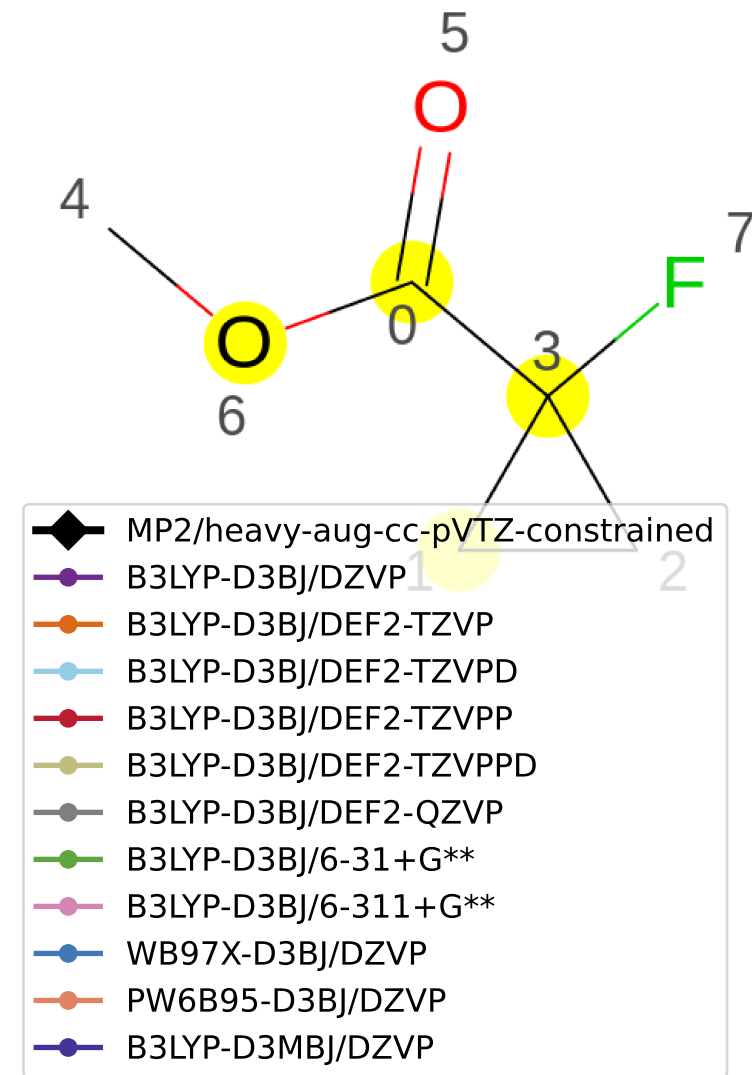
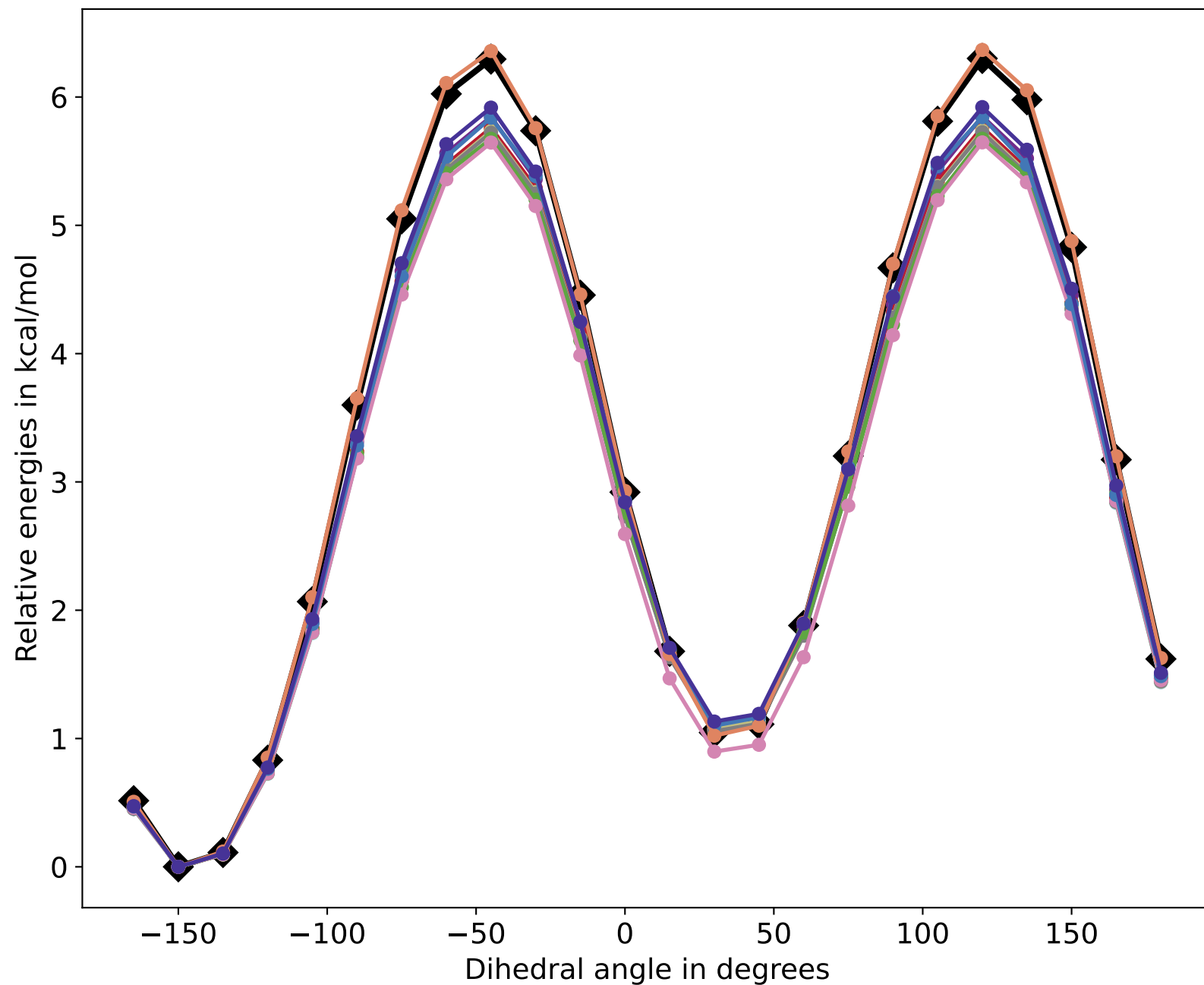
- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP

Relative energies in kcal/mol

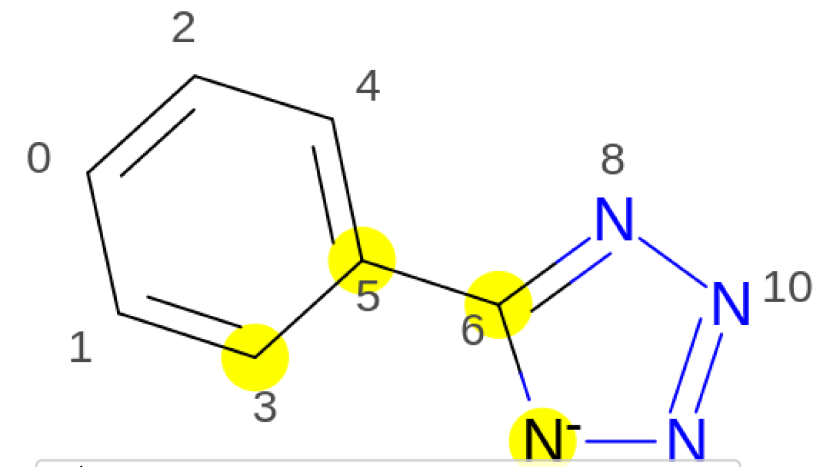
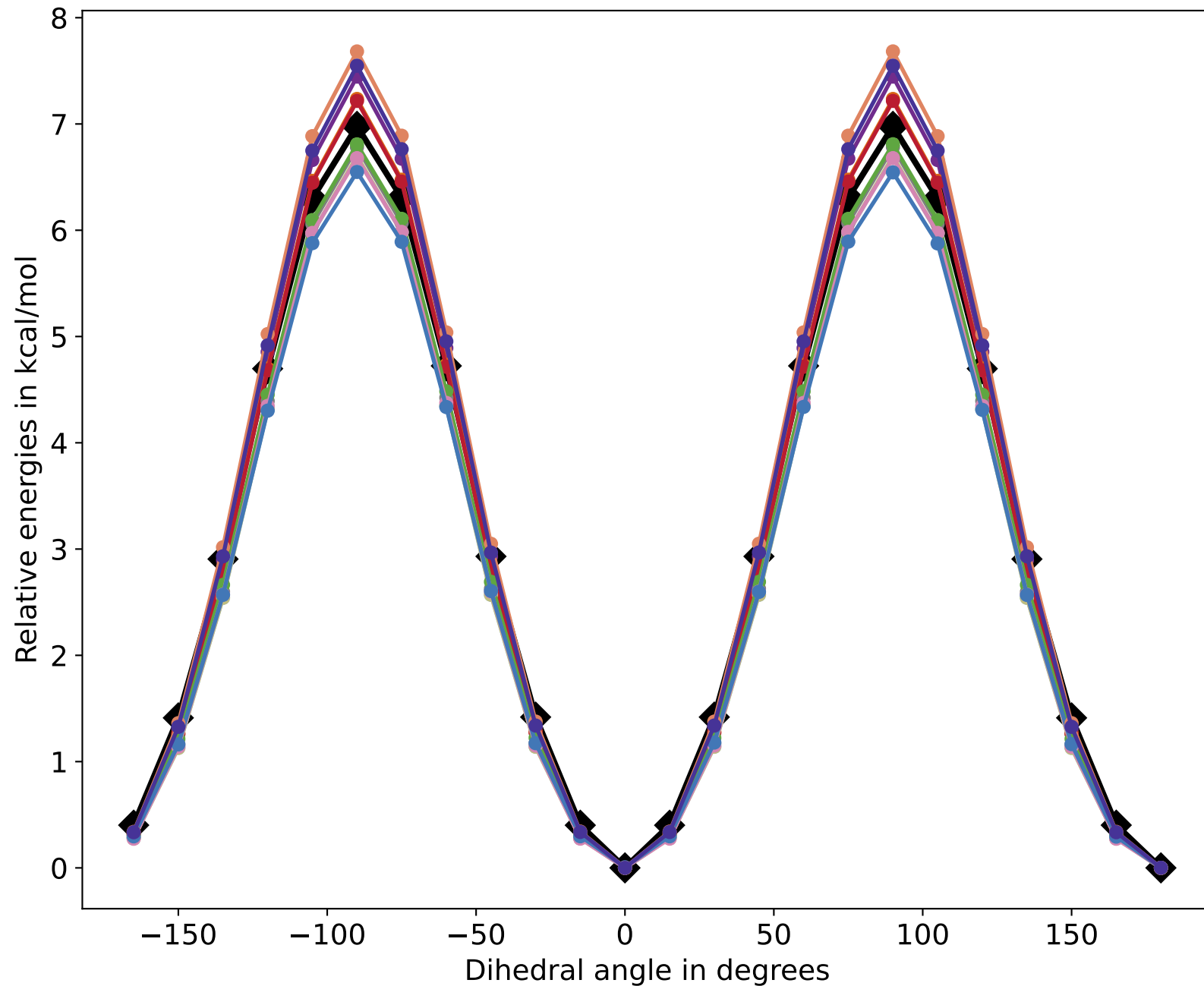






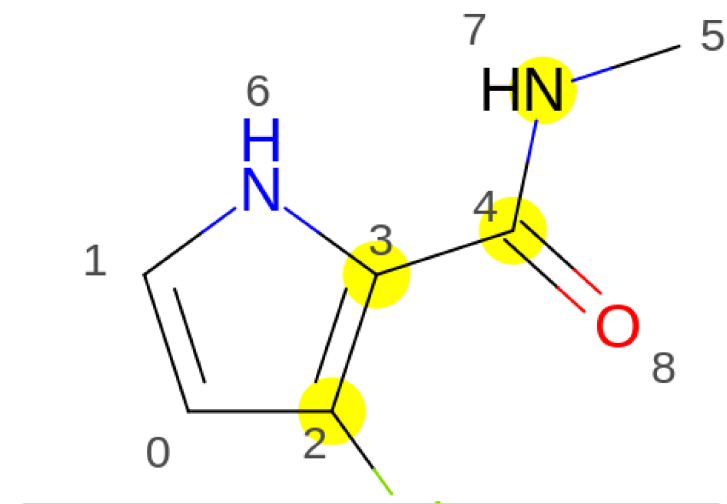
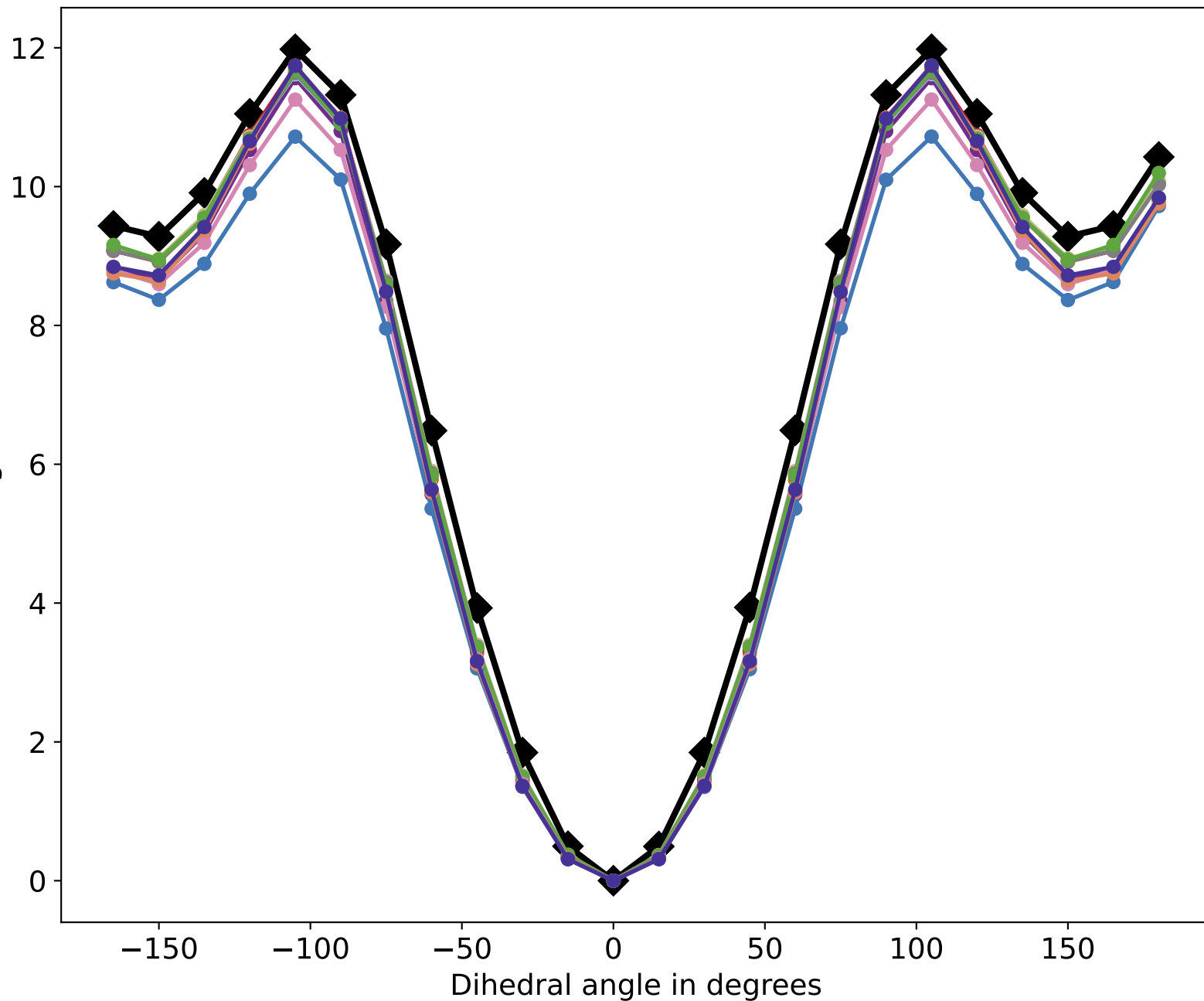






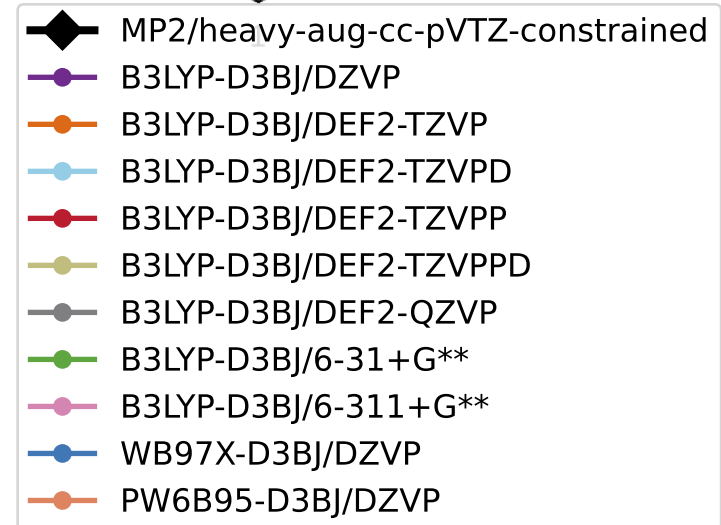
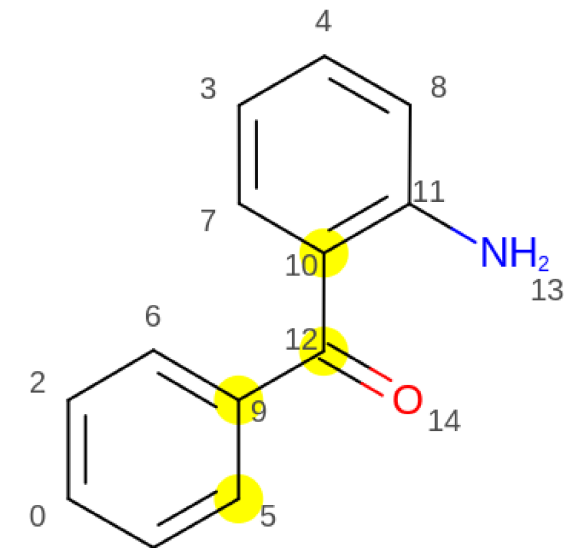
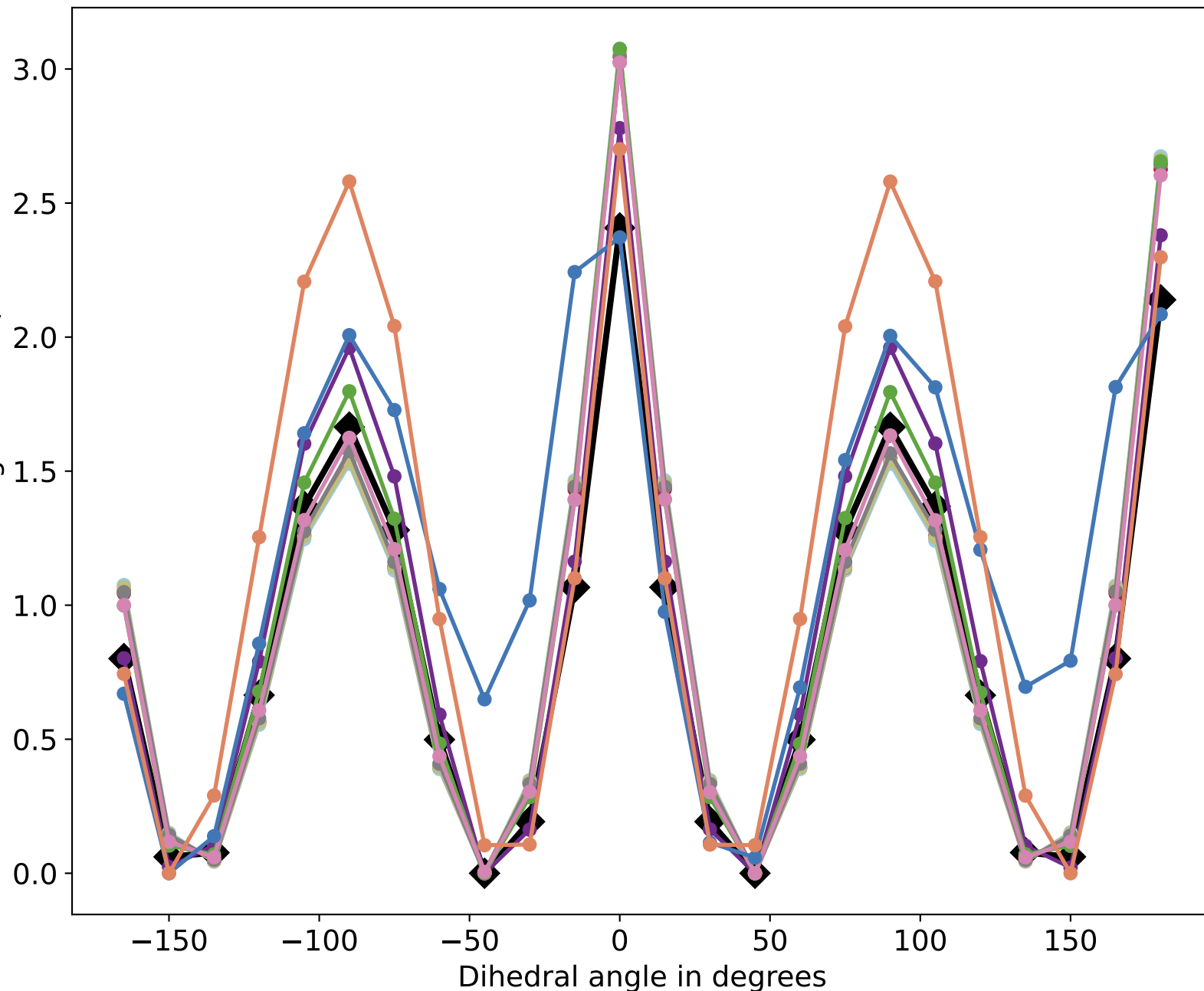
- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP

Relative energies in kcal/mol



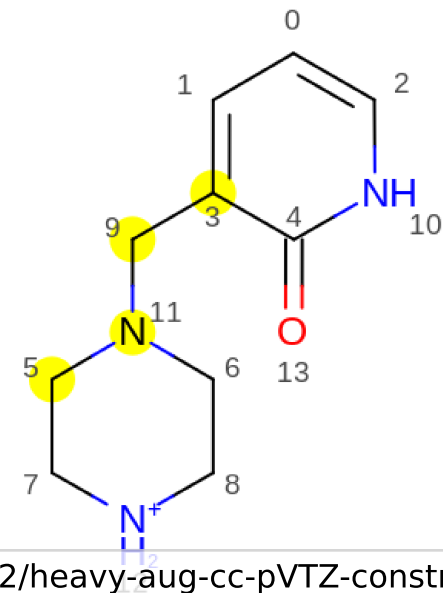
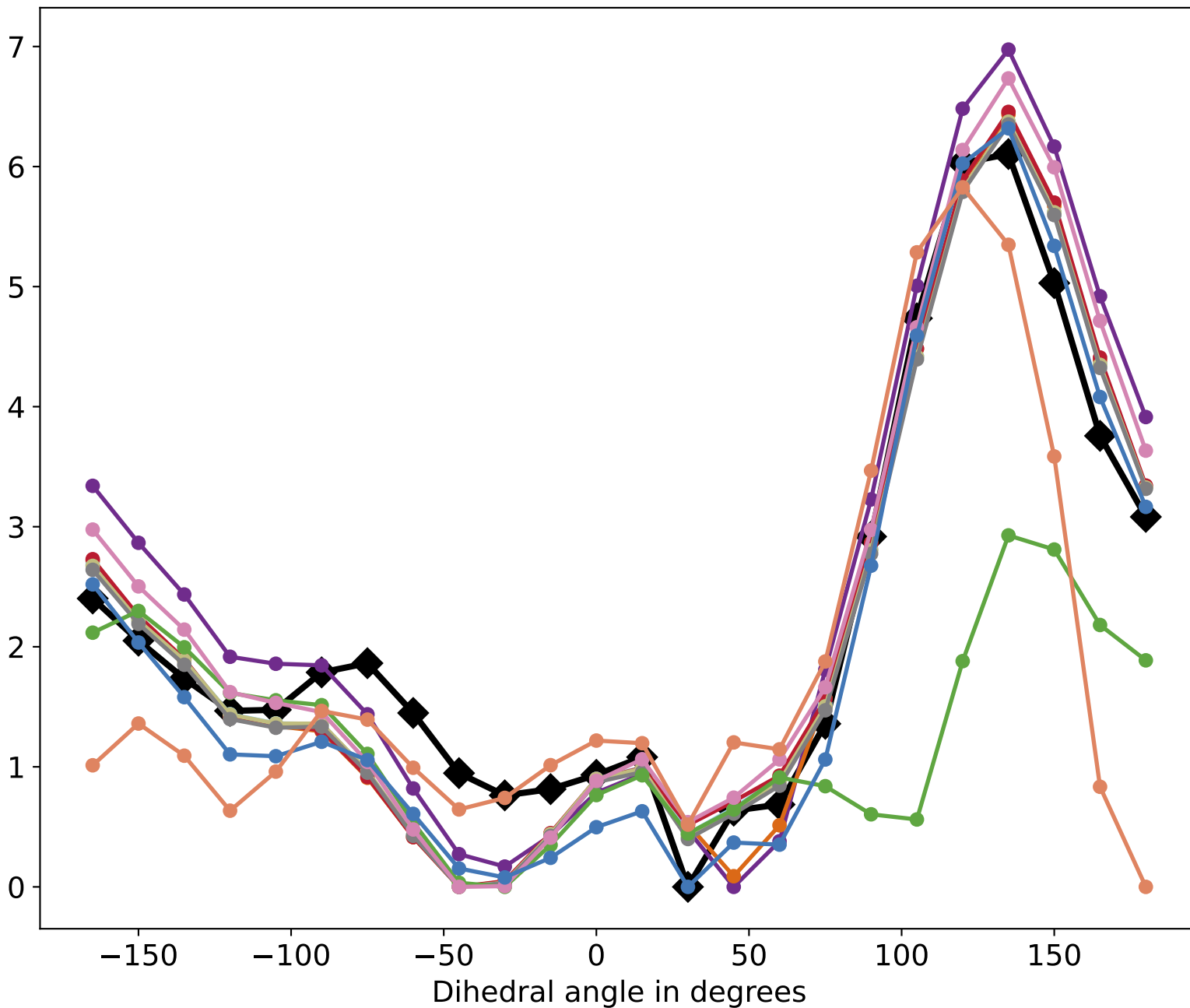
- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
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- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP

Relative energies in kcal/mol

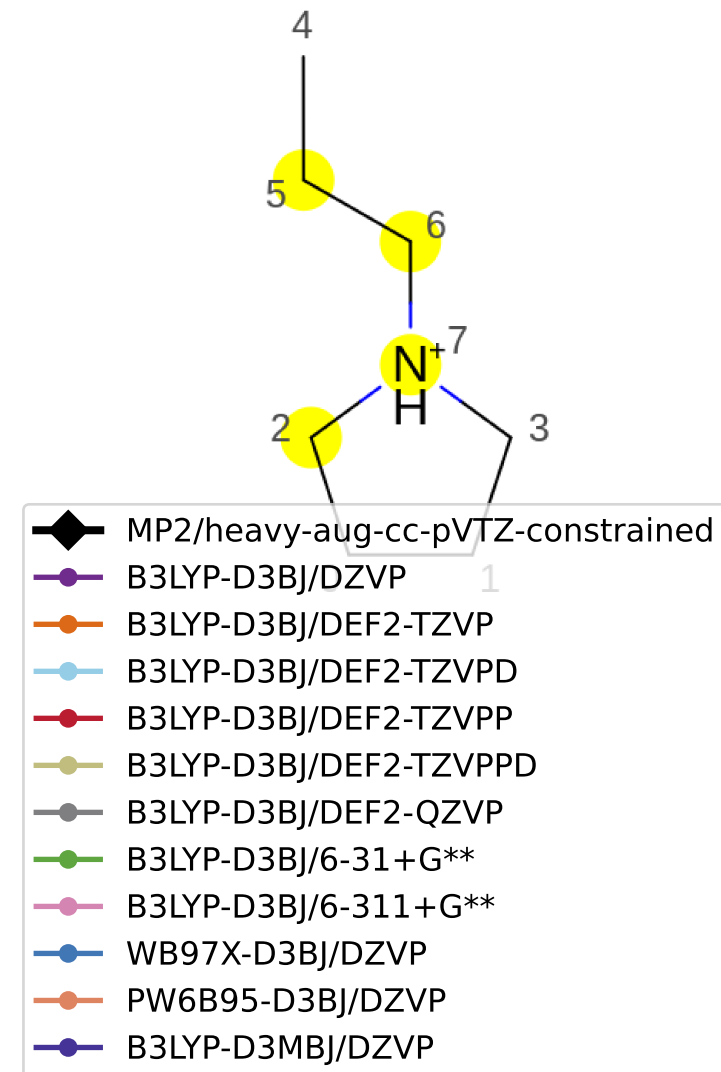
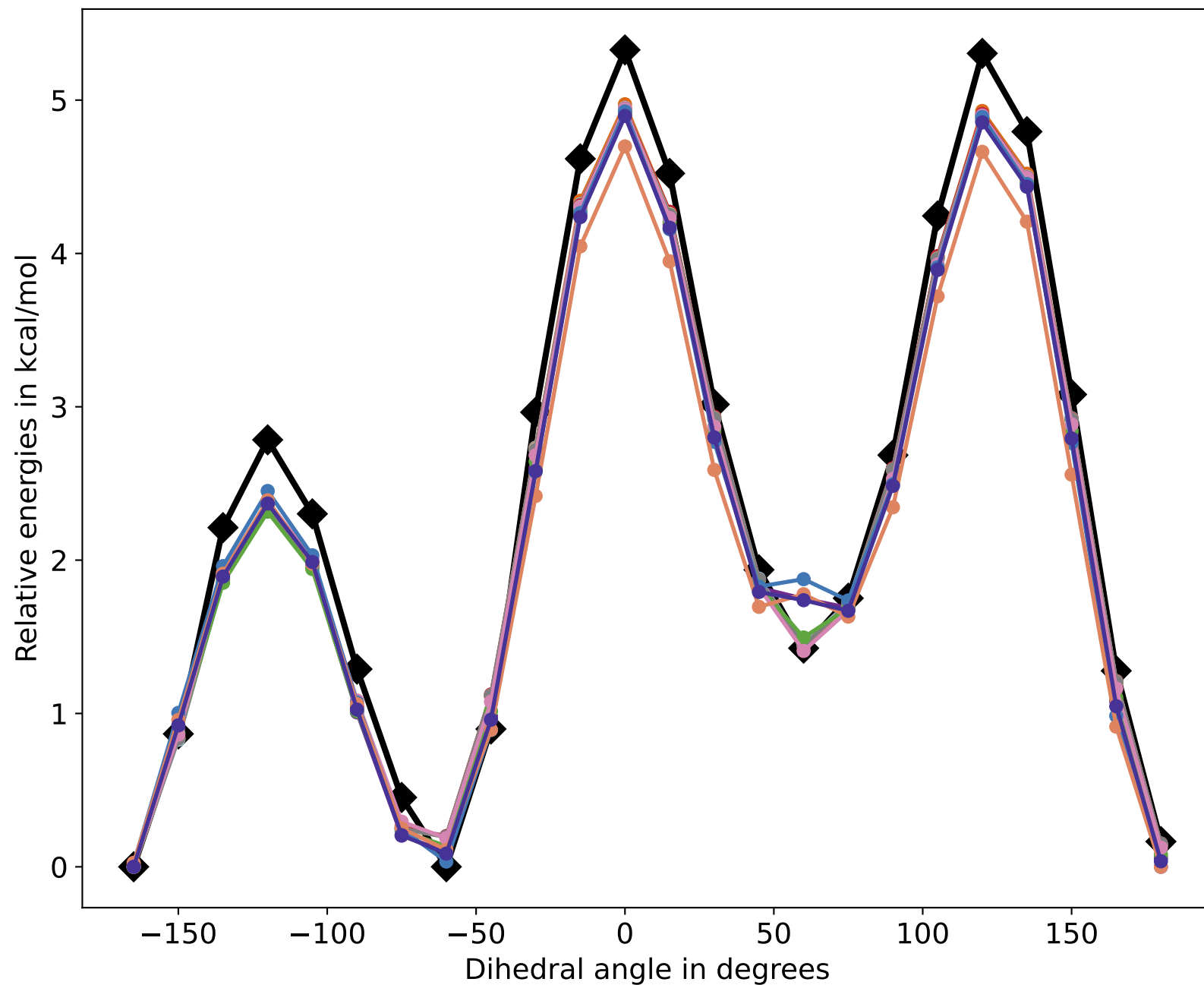




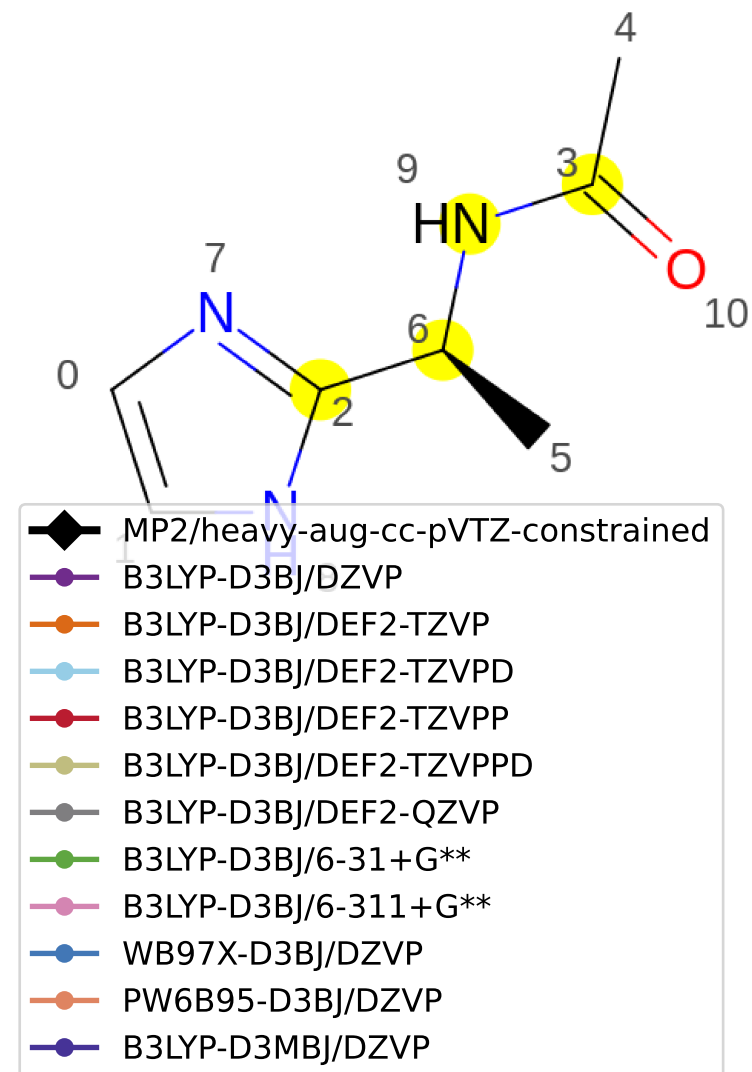
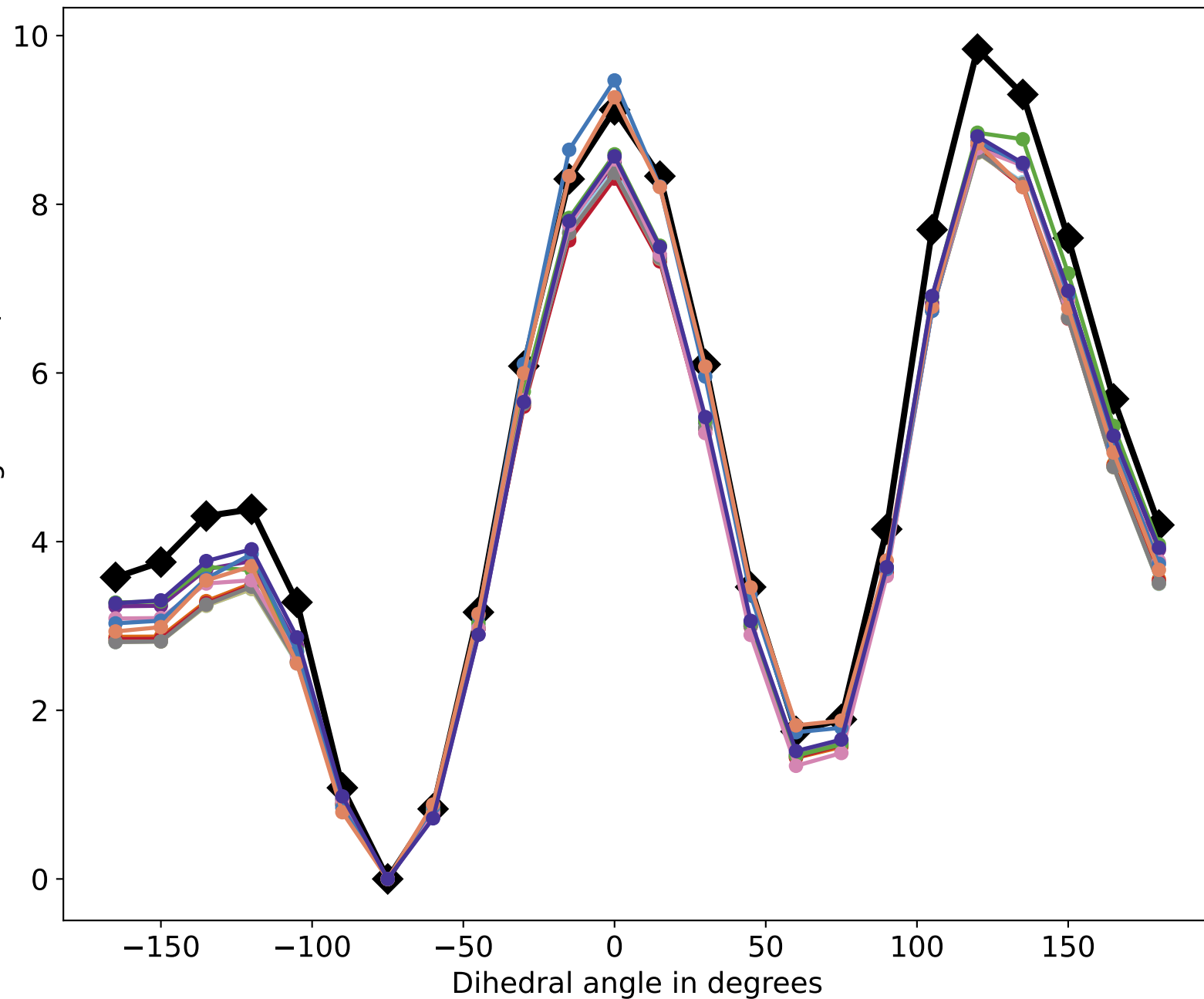
Relative energies in kcal/mol



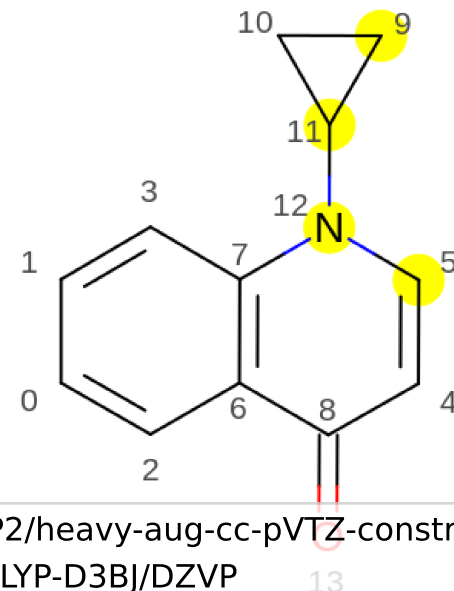
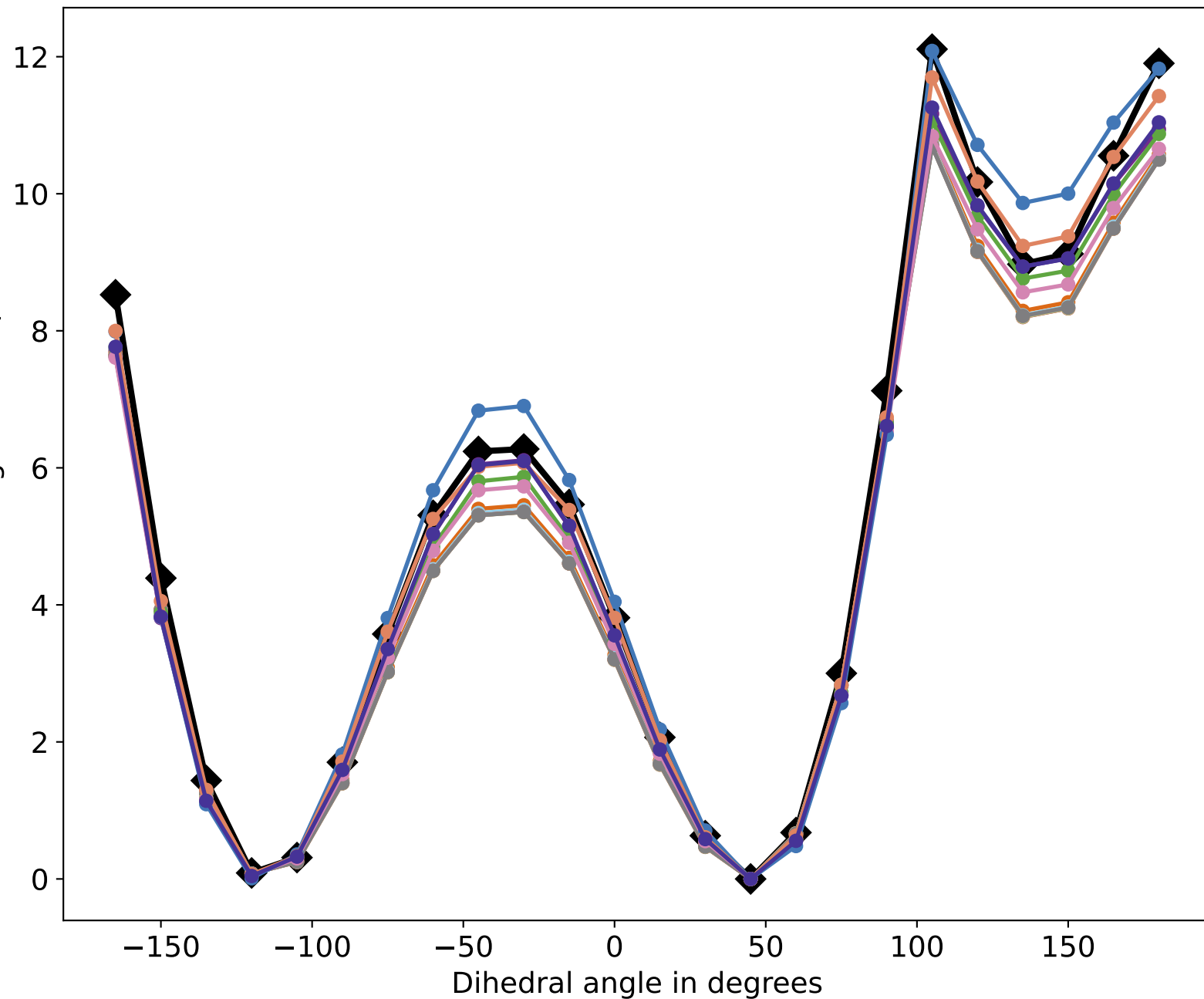
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- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP



Relative energies in kcal/mol

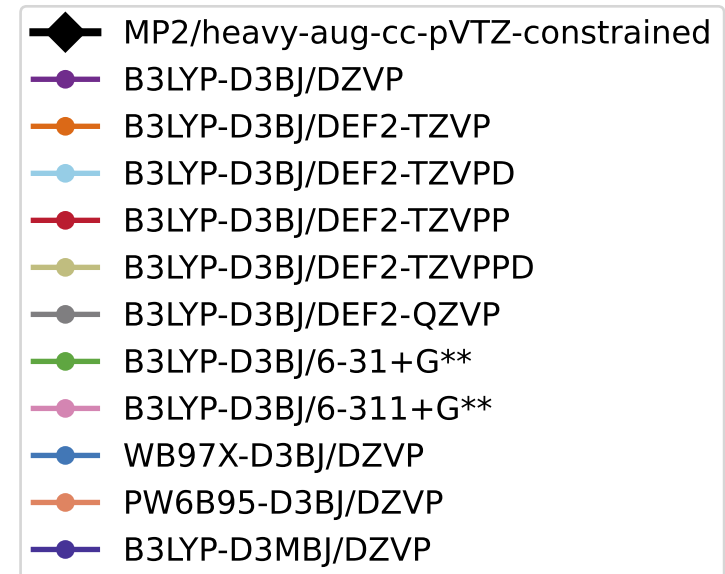
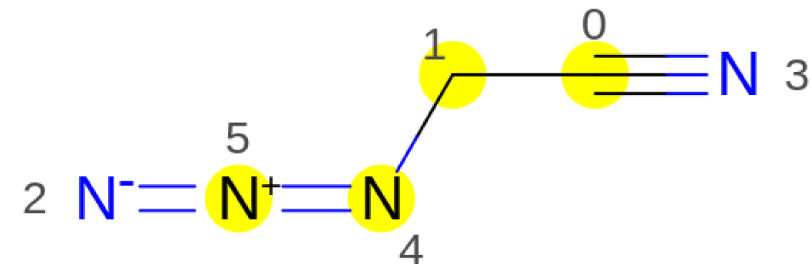
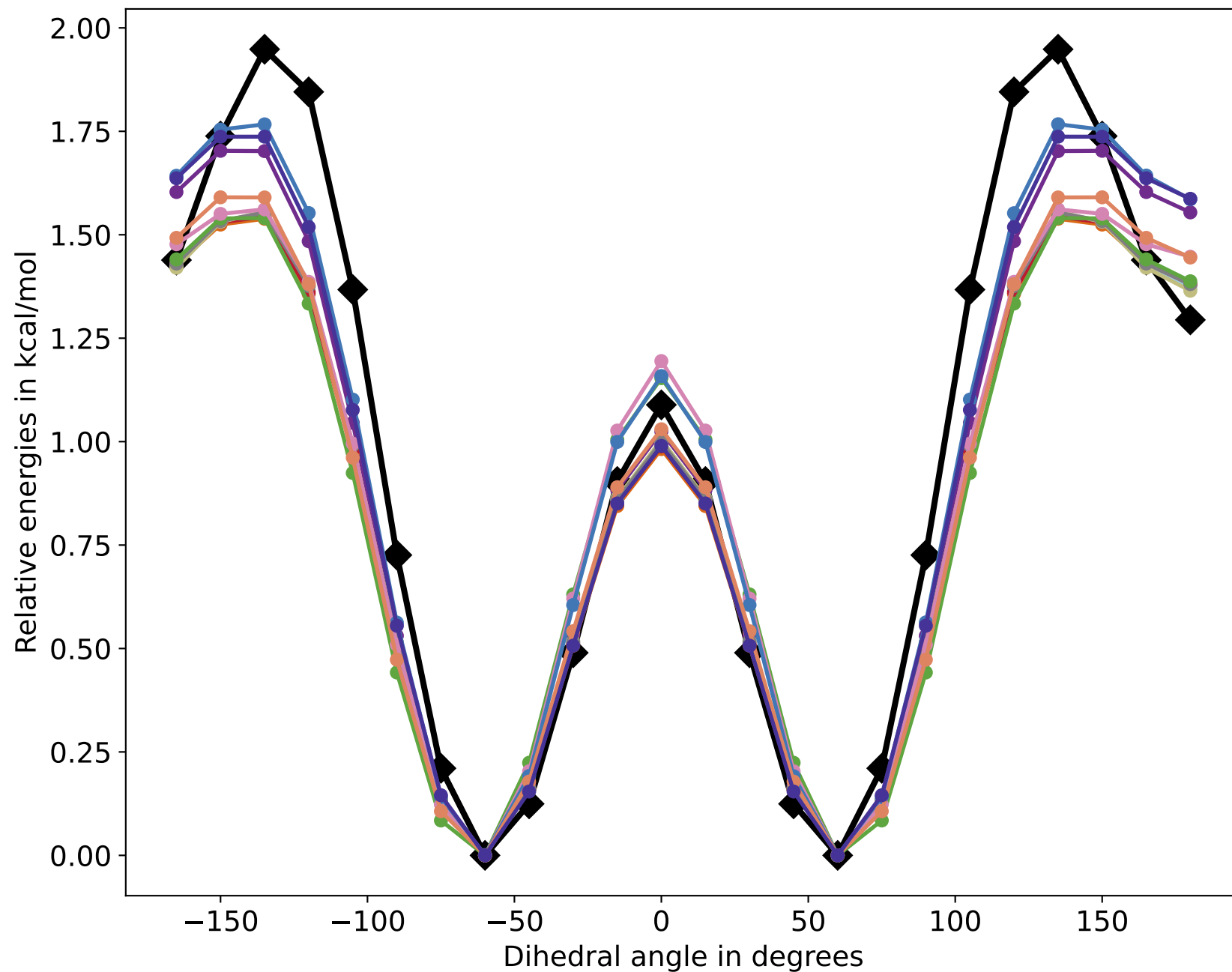


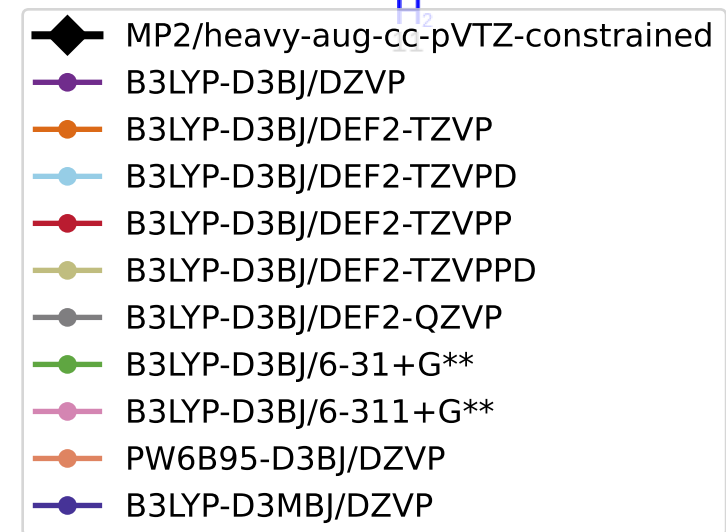
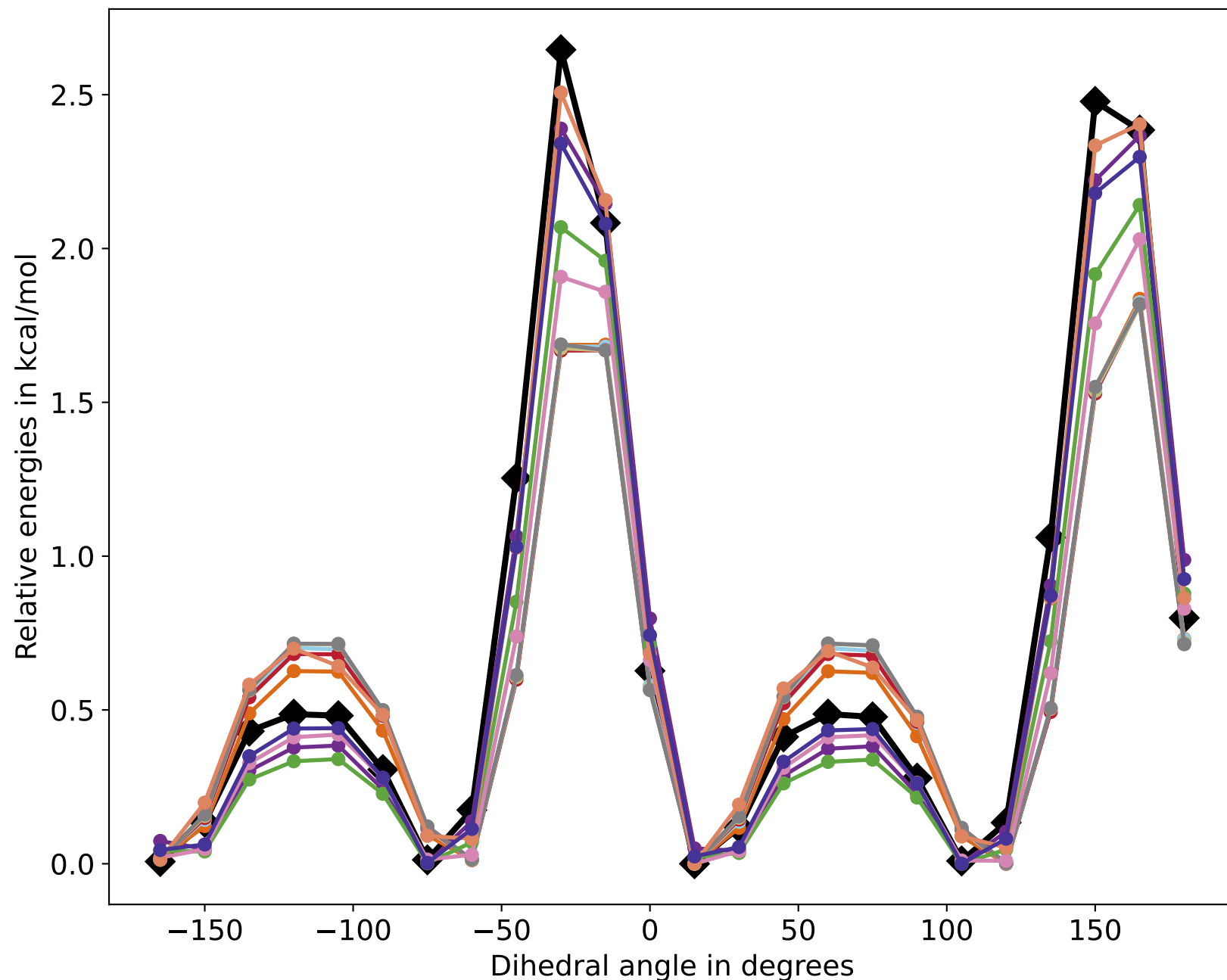
Relative energies in kcal/mol



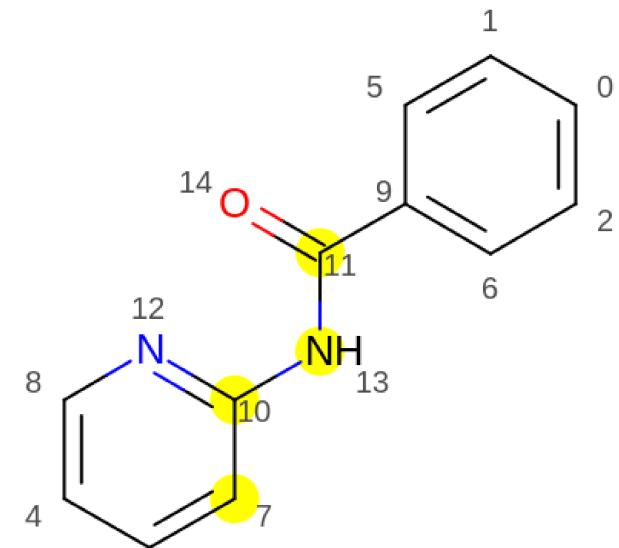
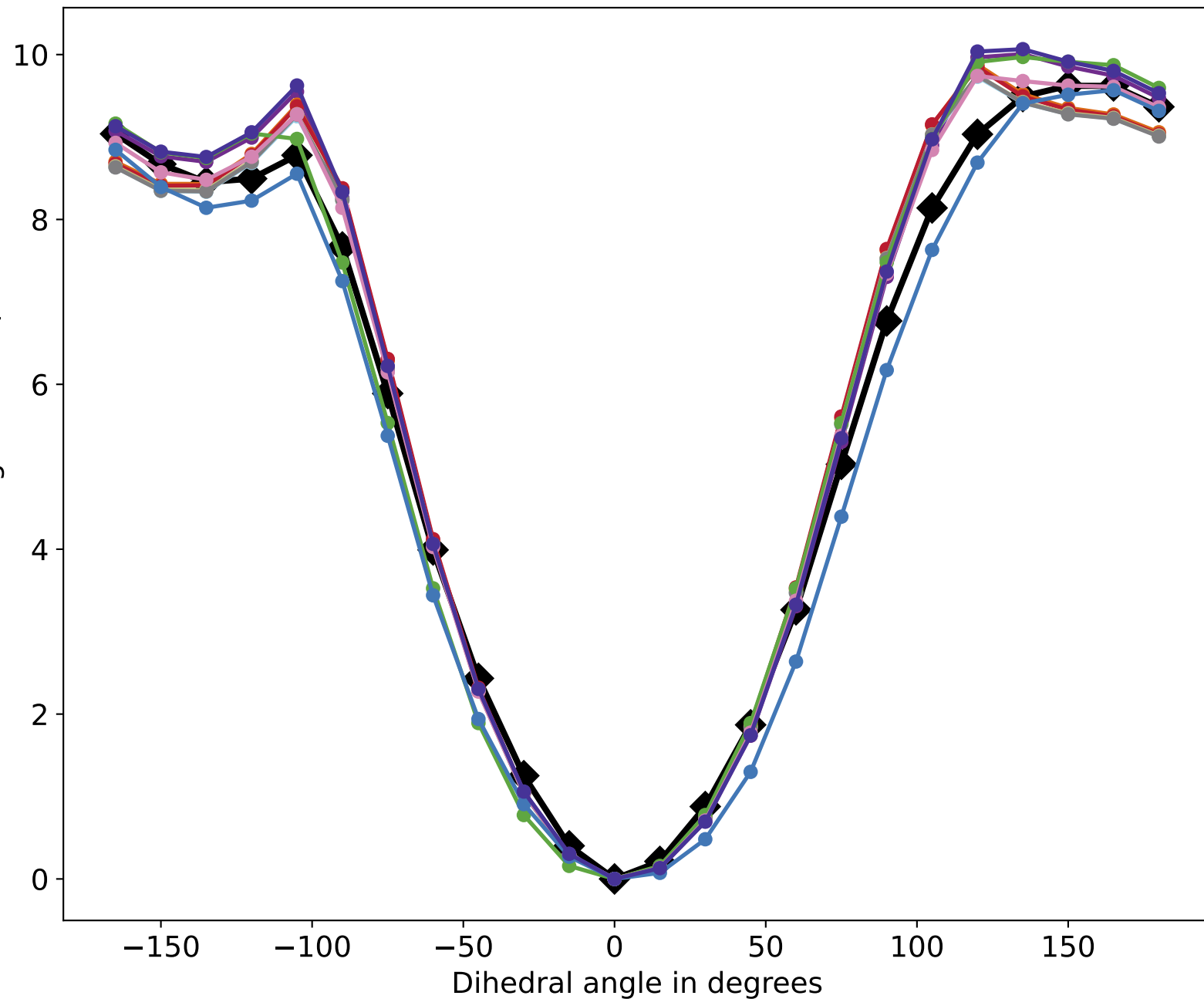
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- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP





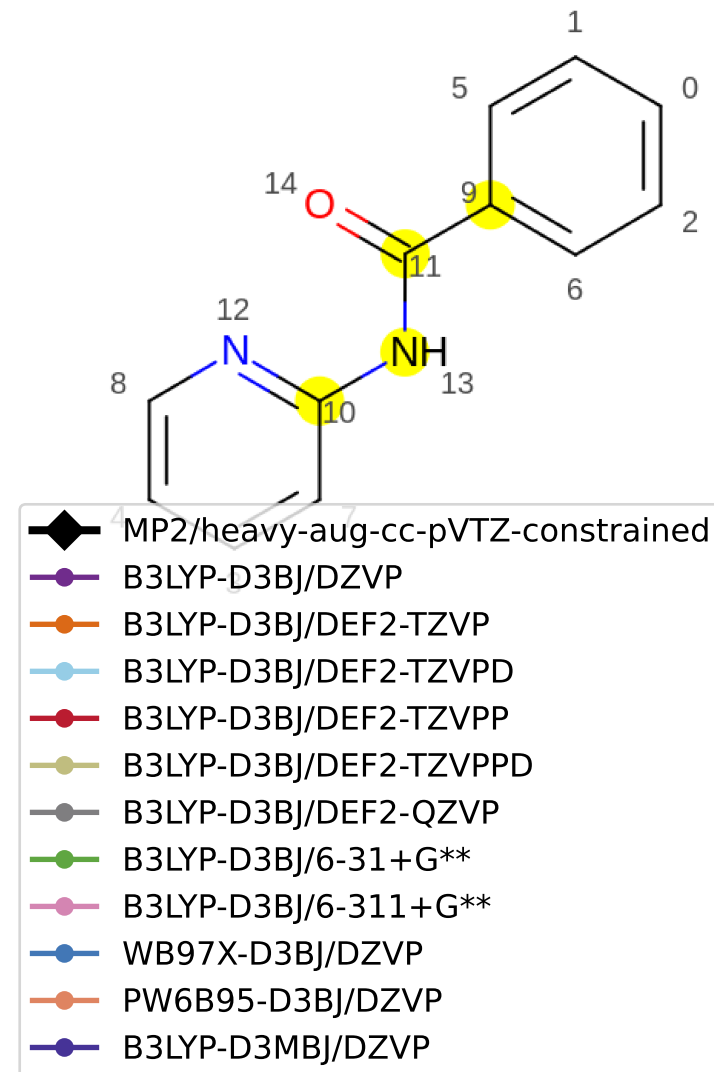
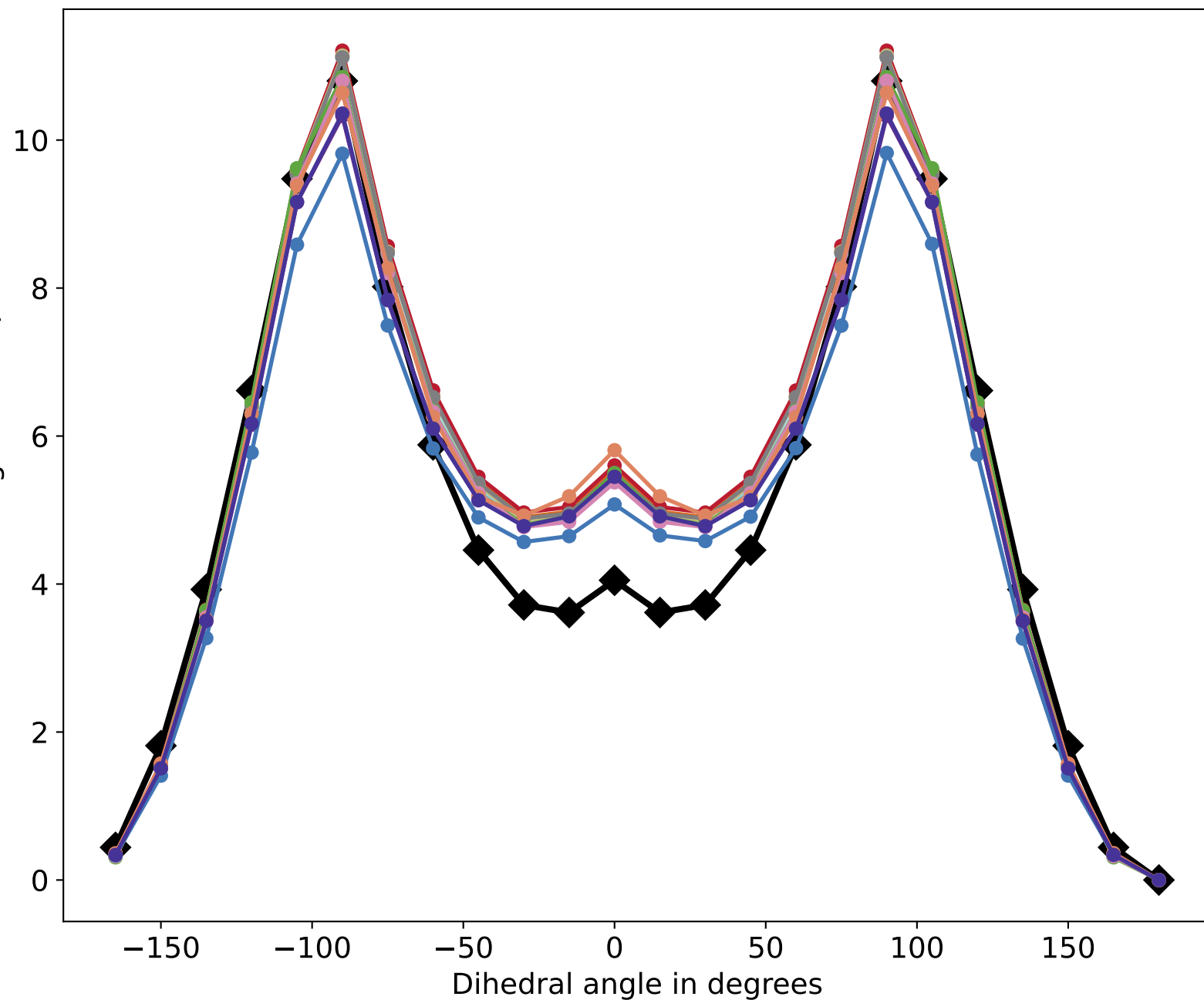


Relative energies in kcal/mol

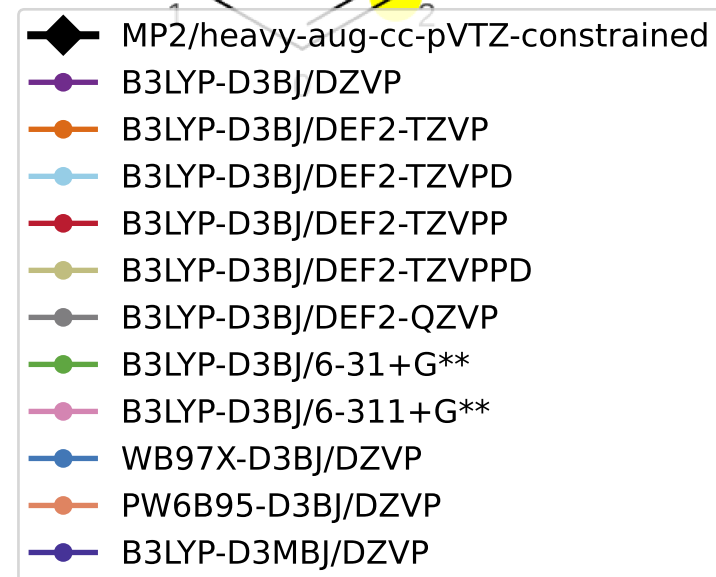
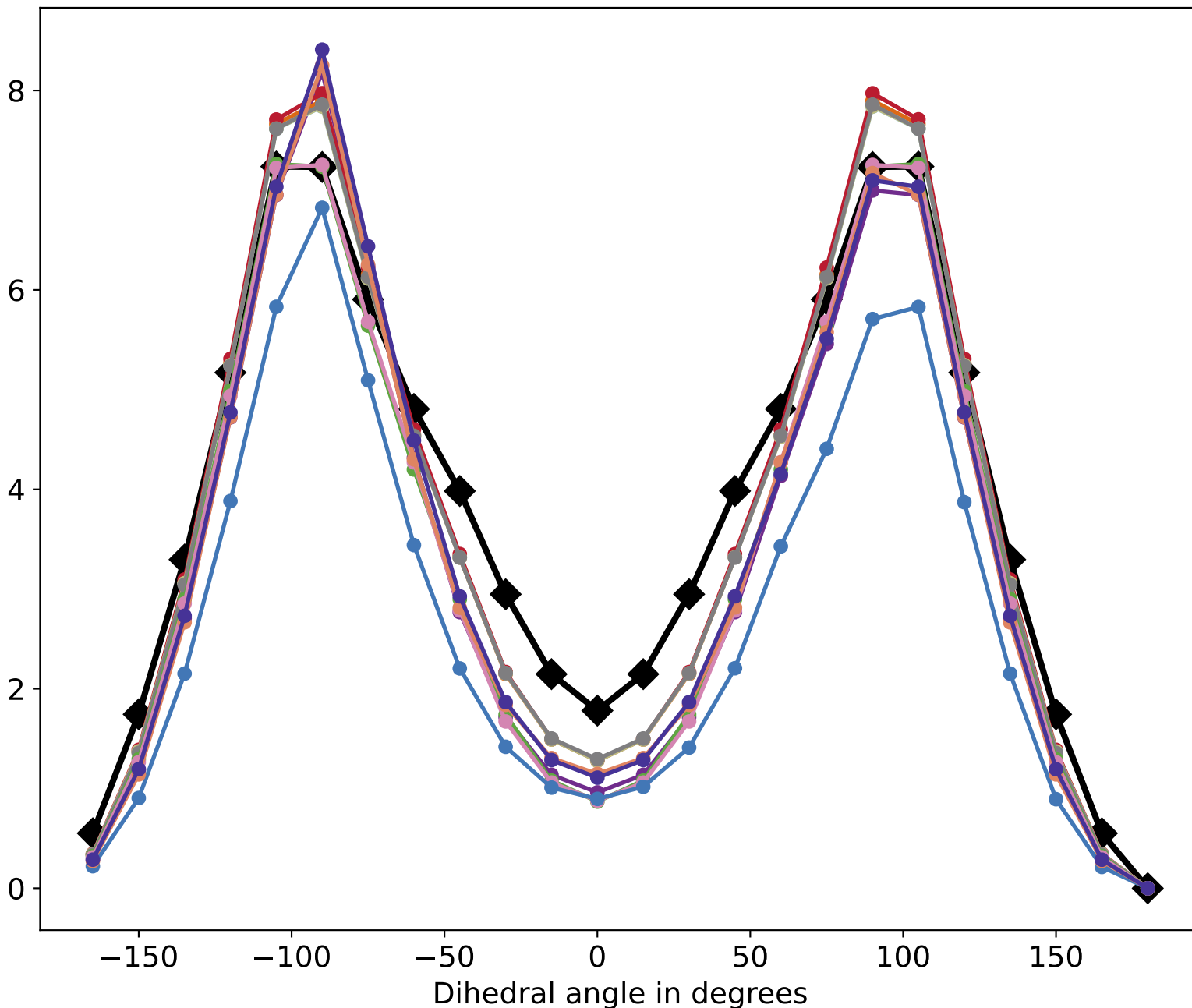


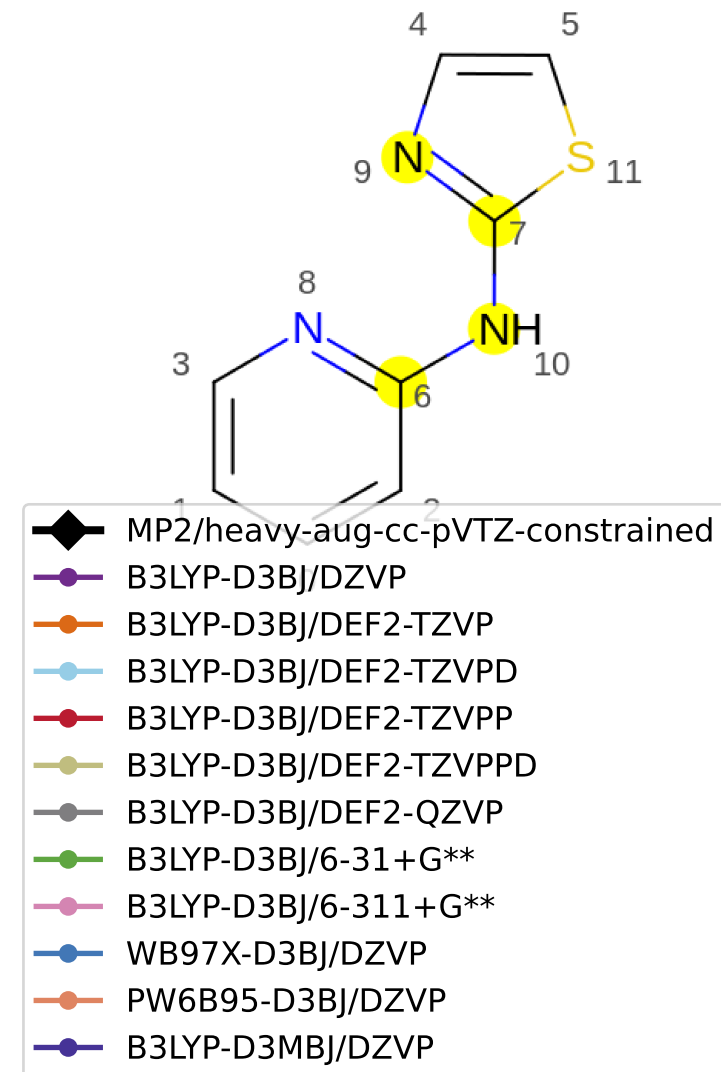
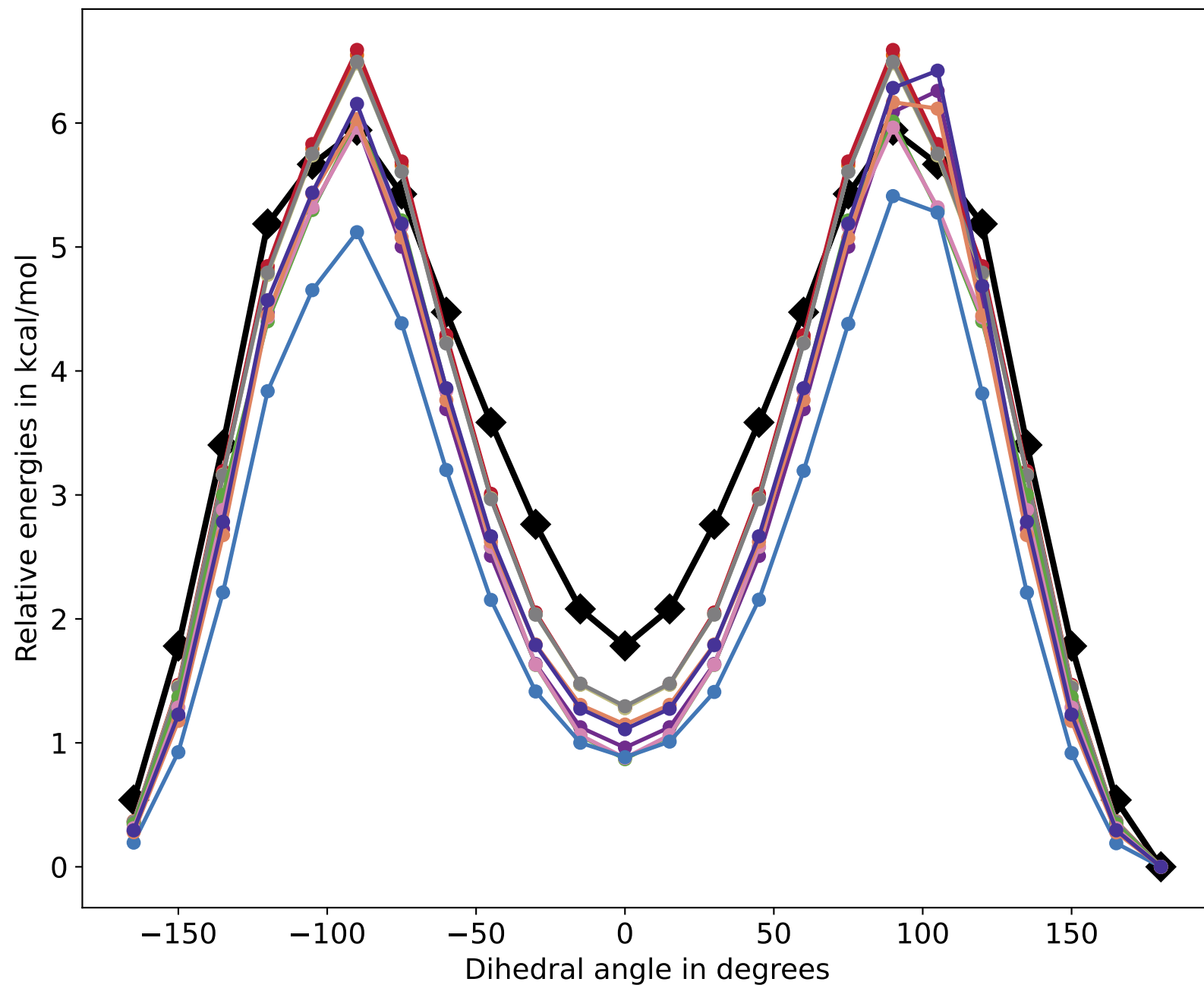
- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP

Relative energies in kcal/mol

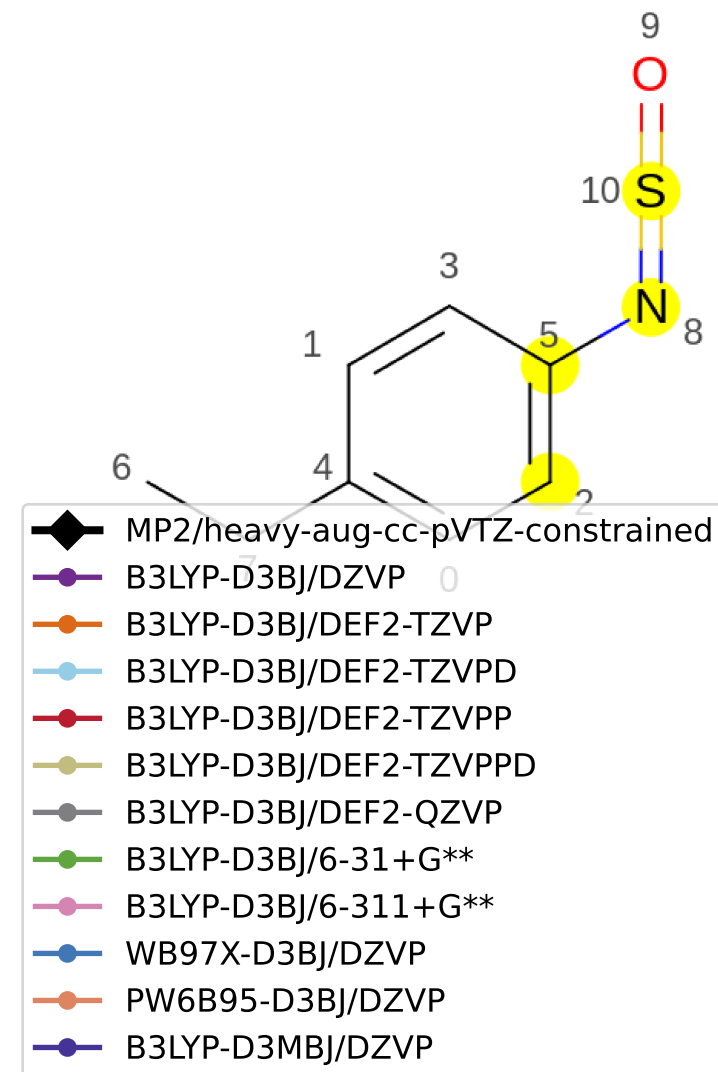
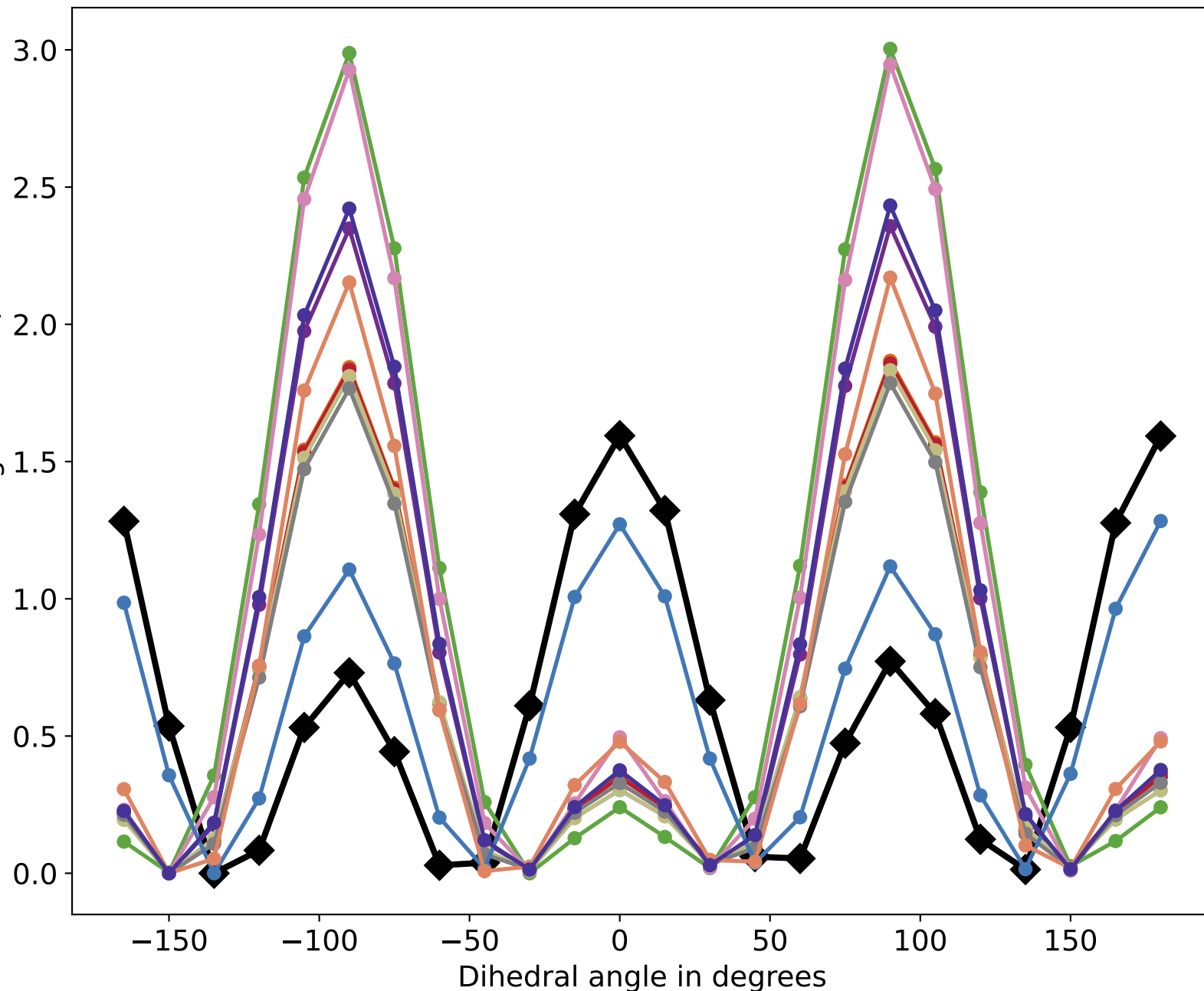


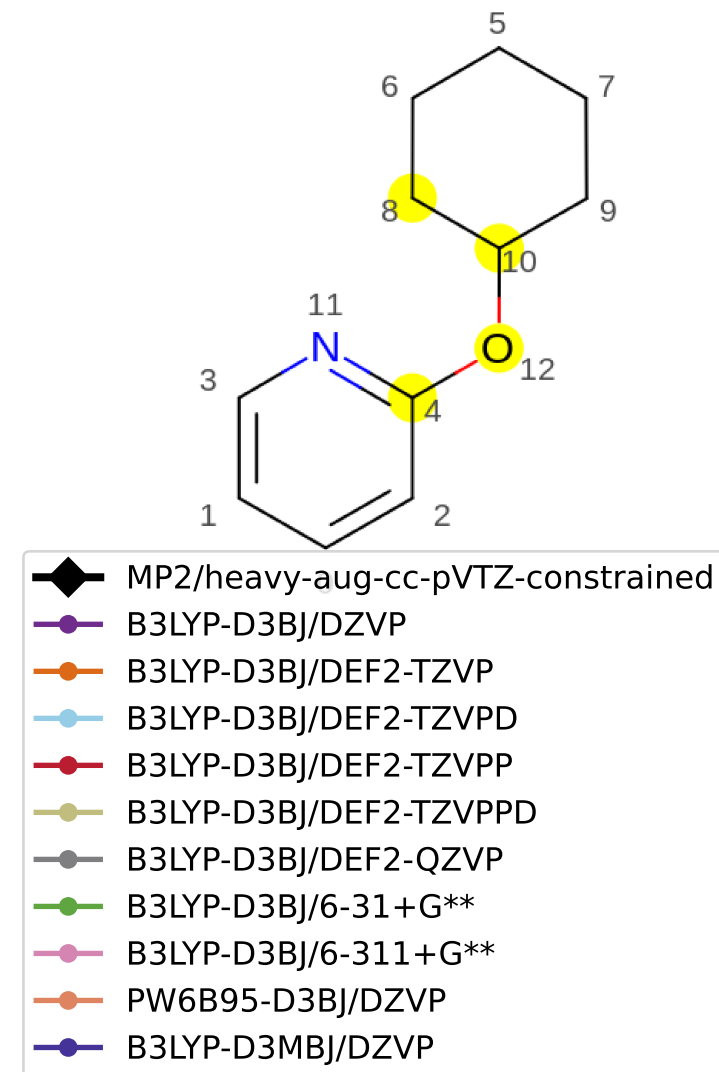
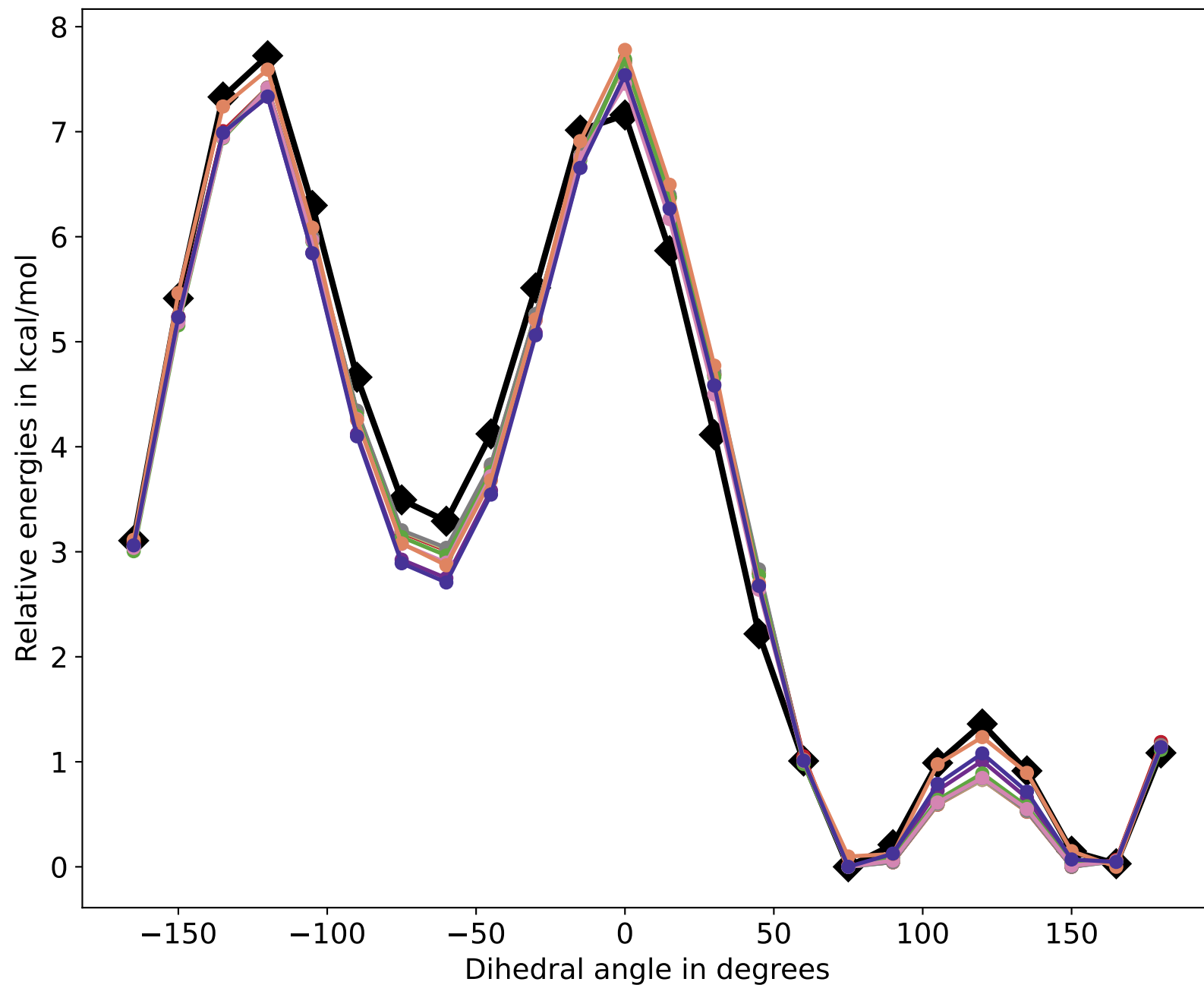
Relative energies in kcal/mol





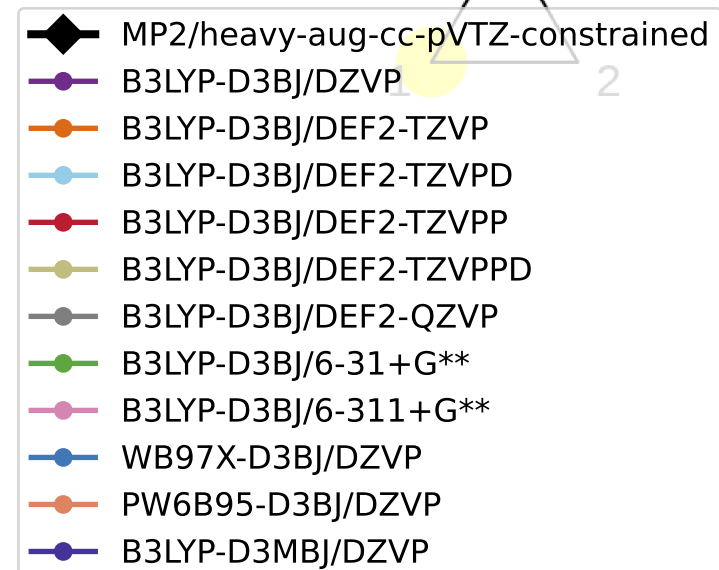
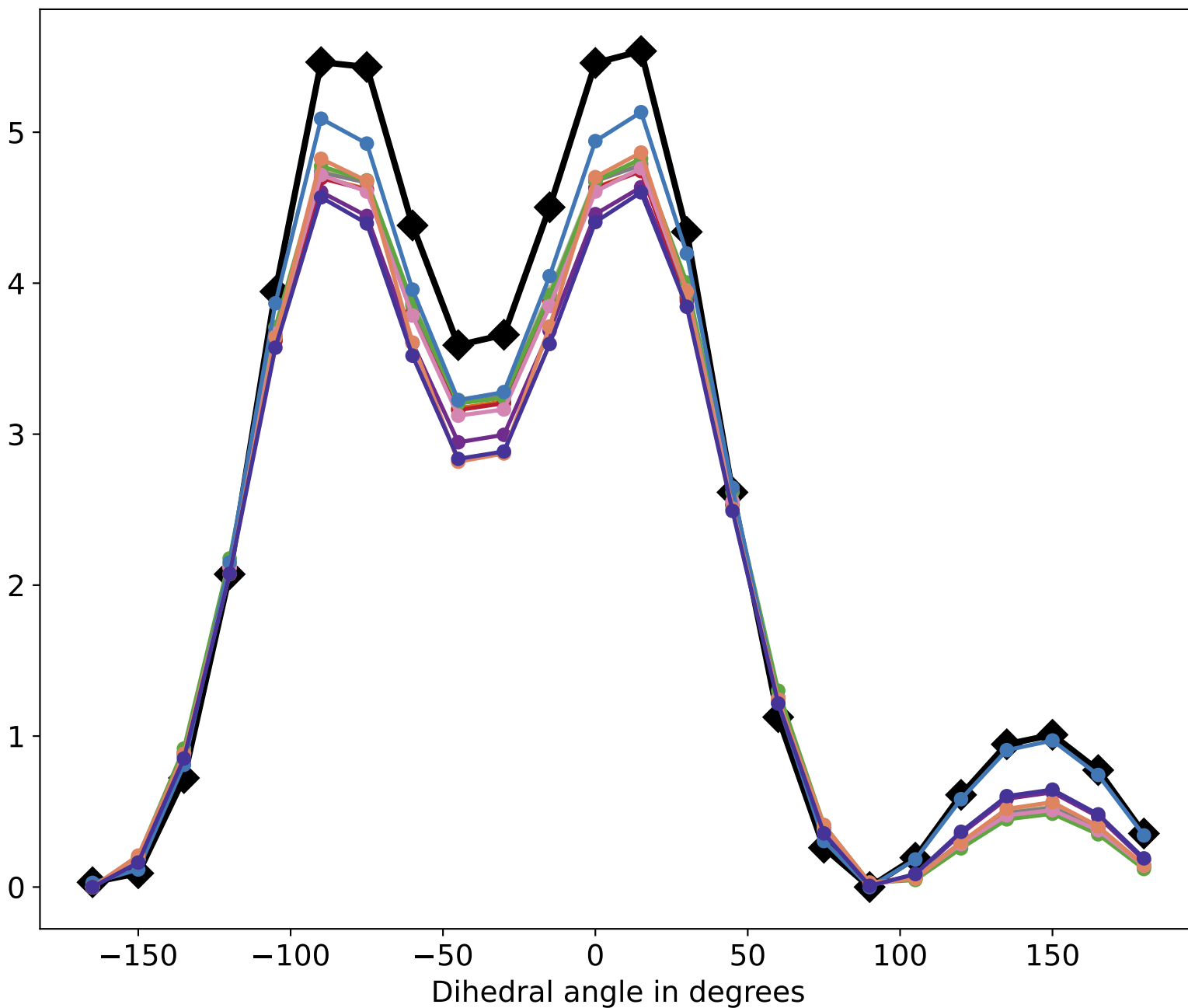
Relative energies in kcal/mol

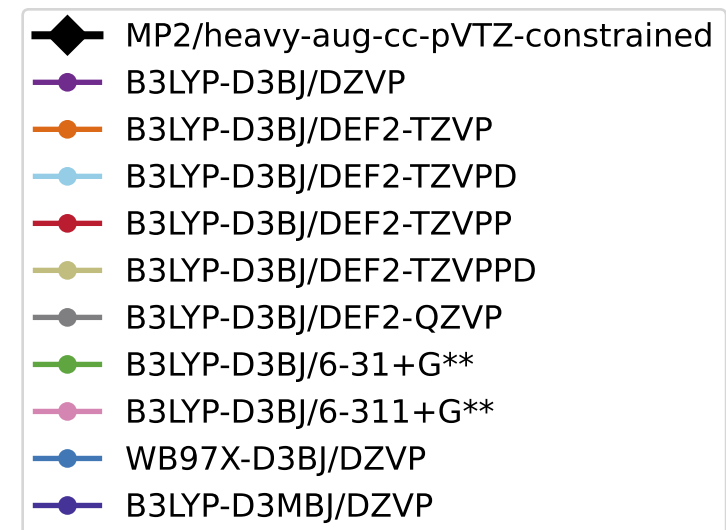
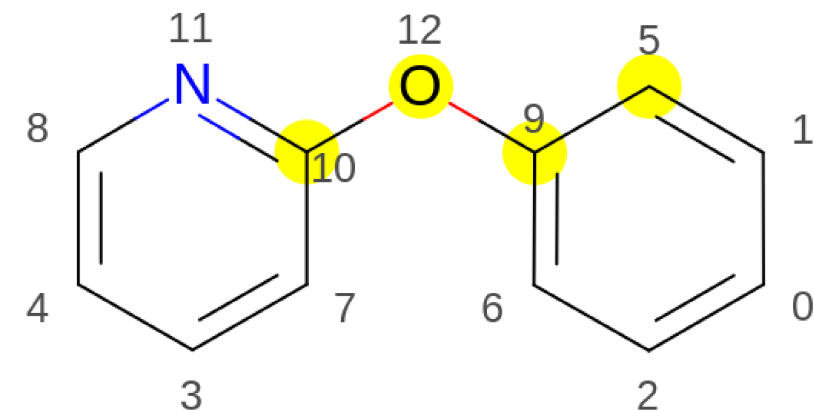
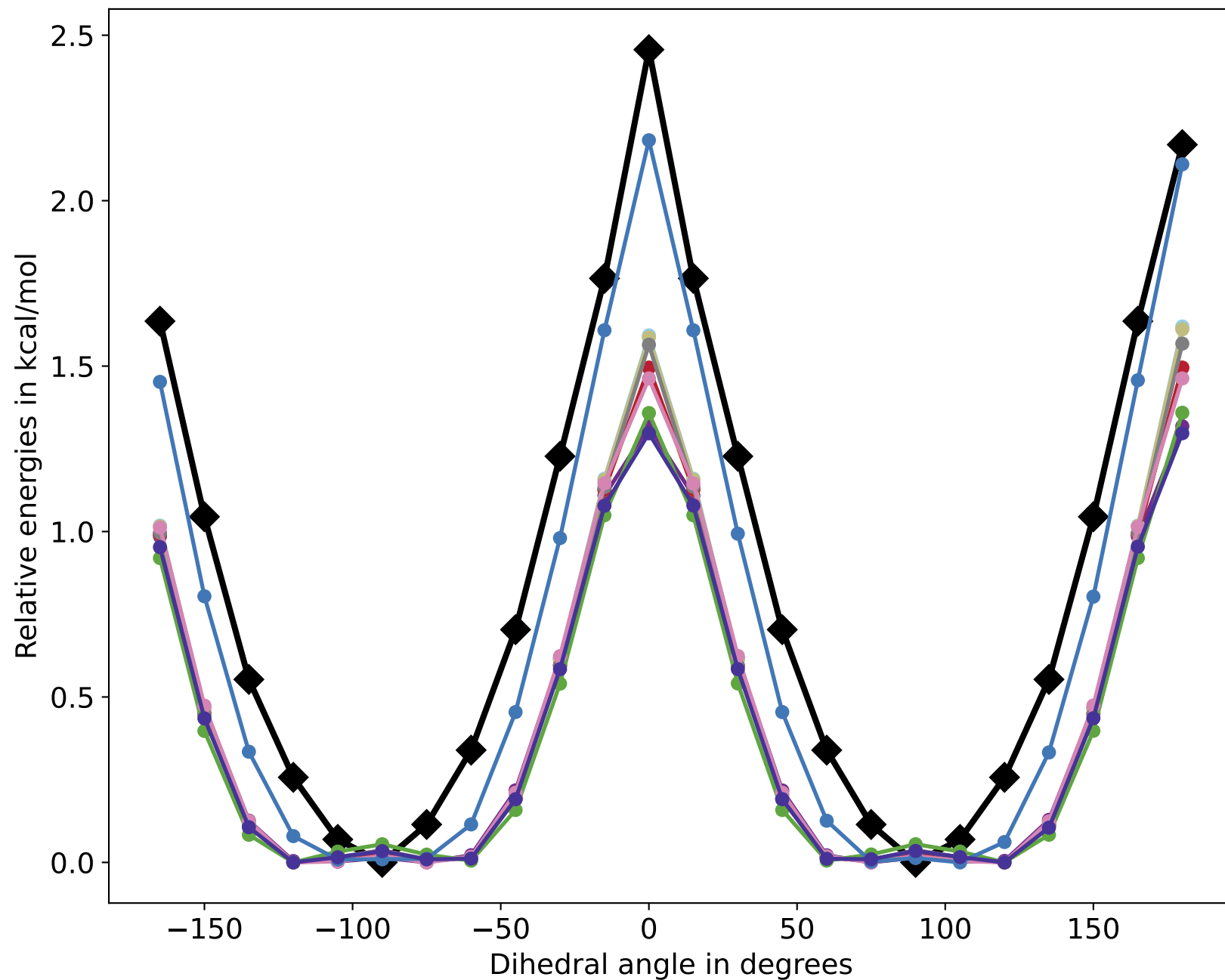


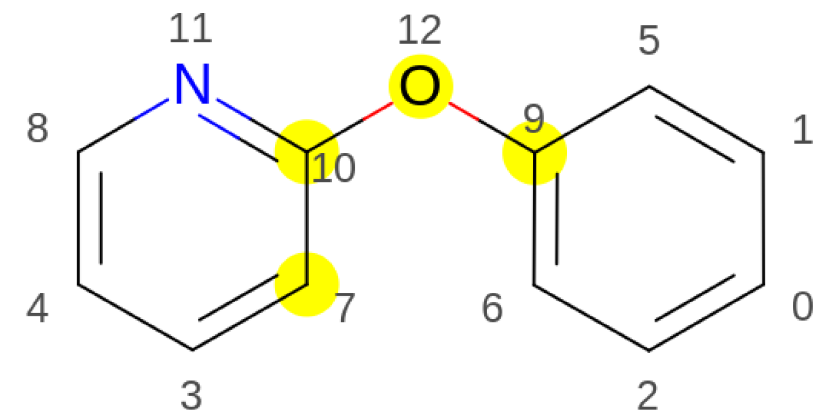
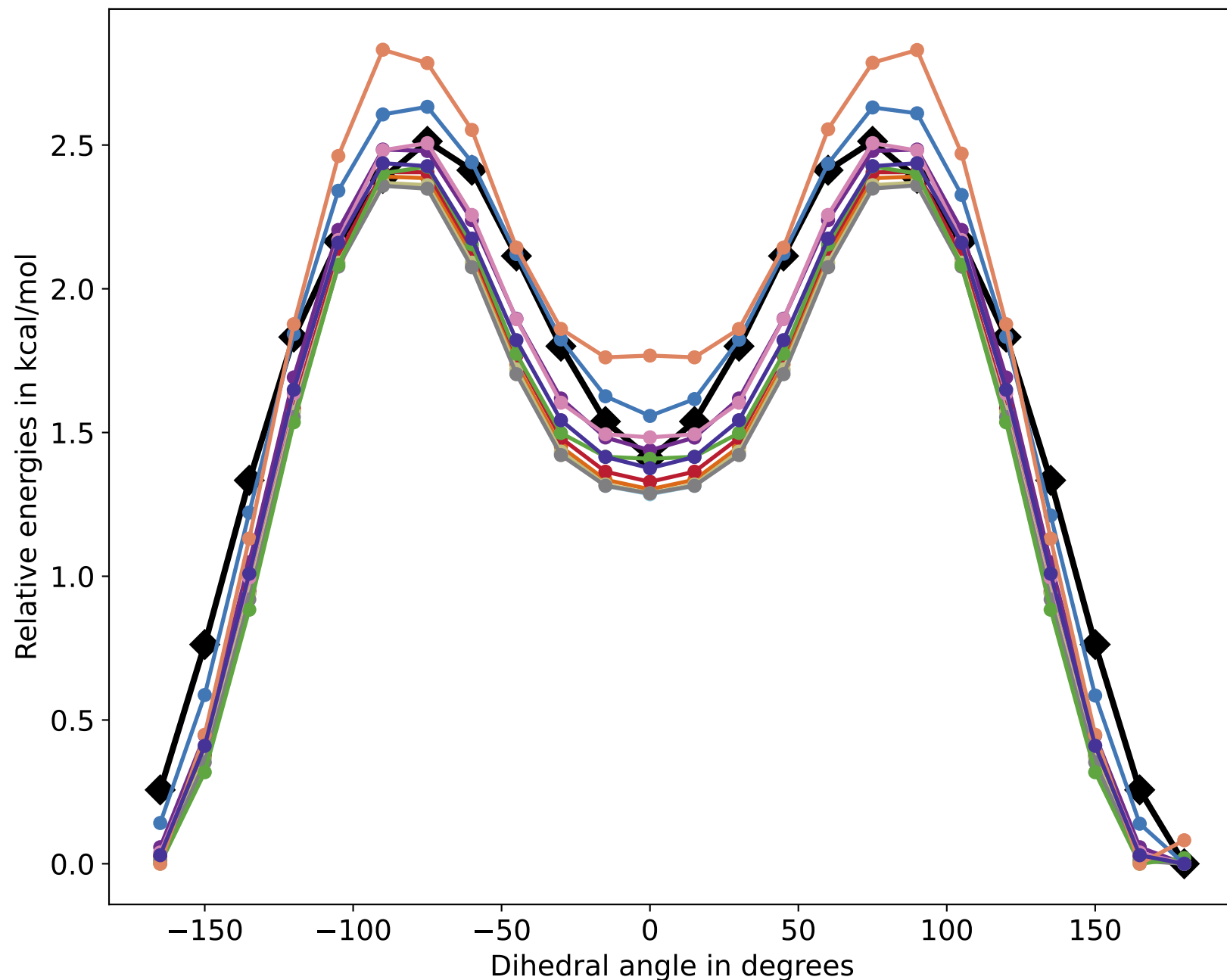




Relative energies in kcal/mol

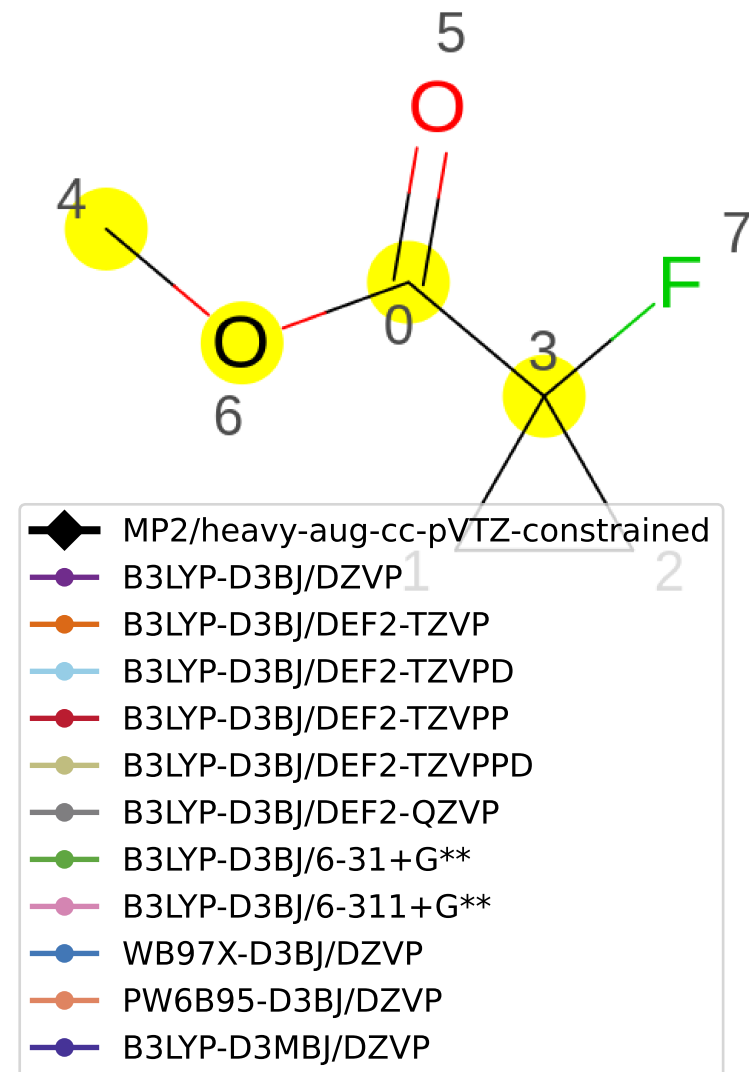
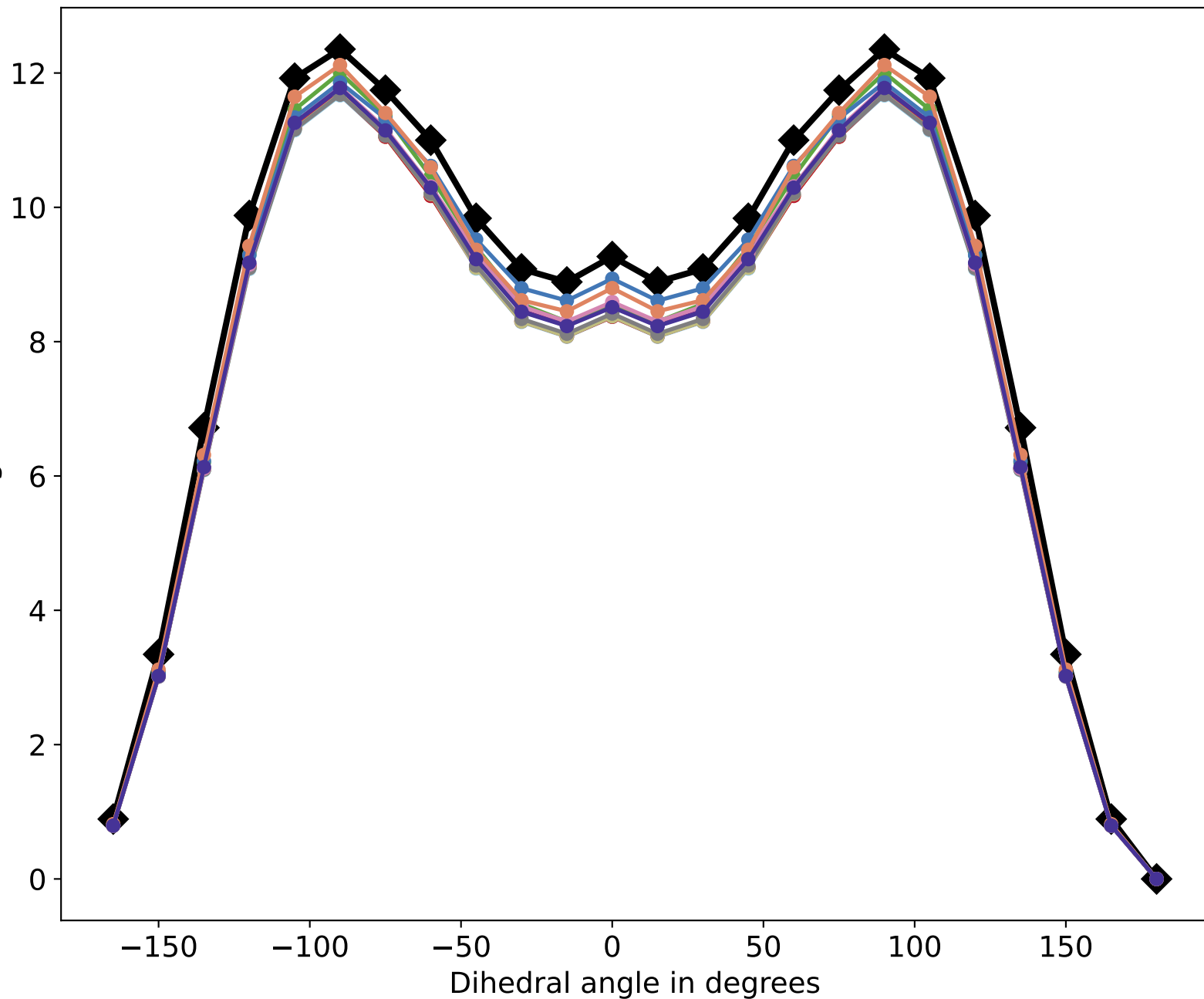




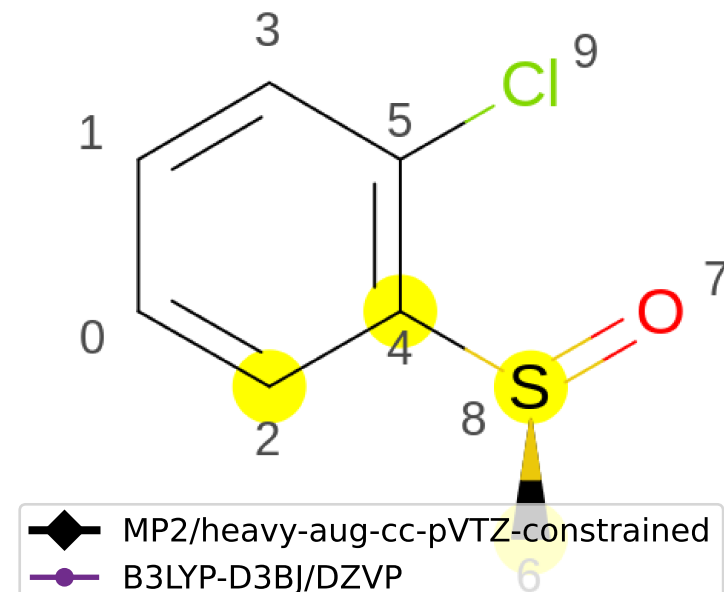
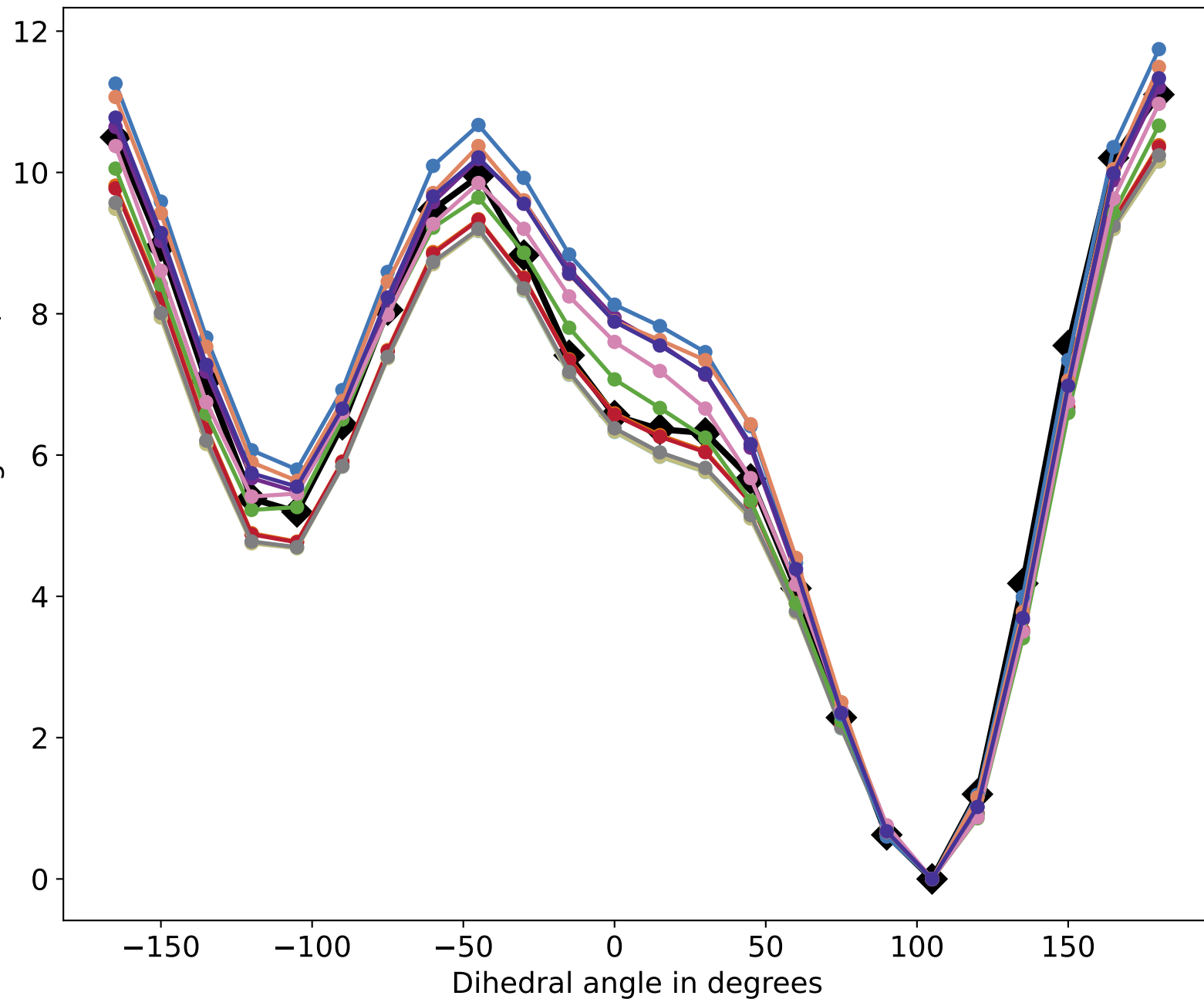


- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP

Relative energies in kcal/mol

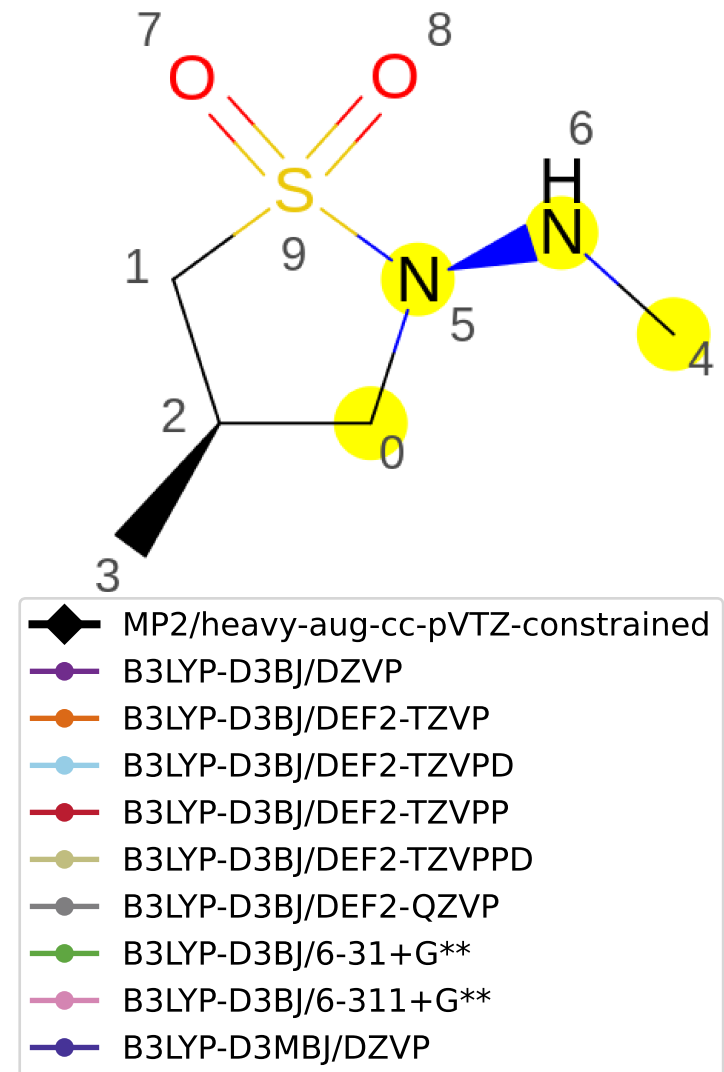
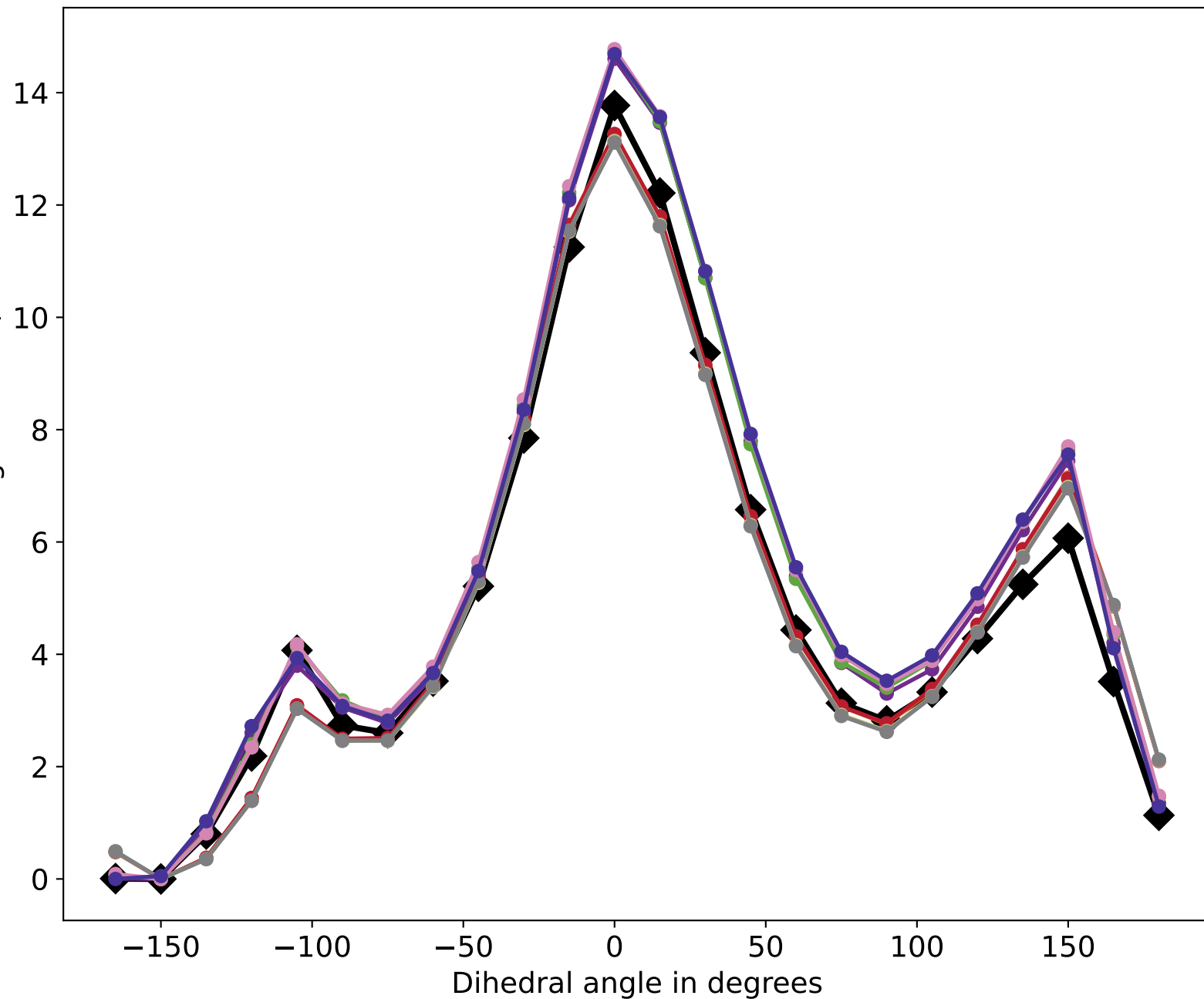


Relative energies in kcal/mol

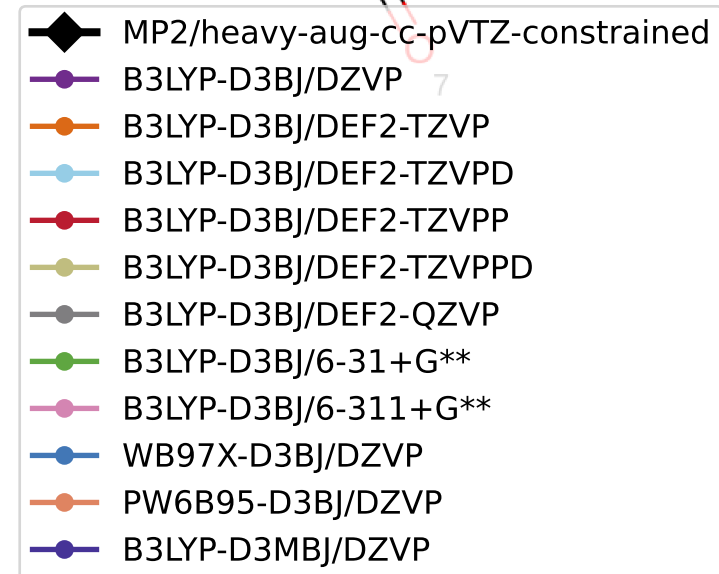
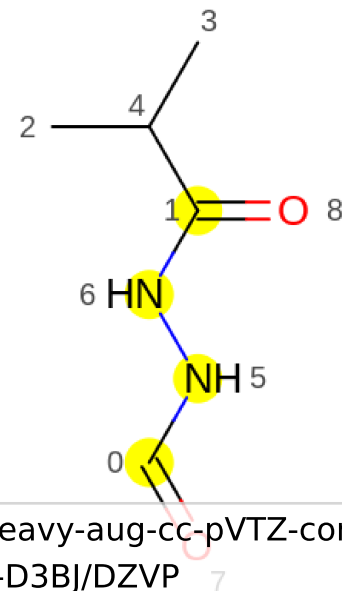
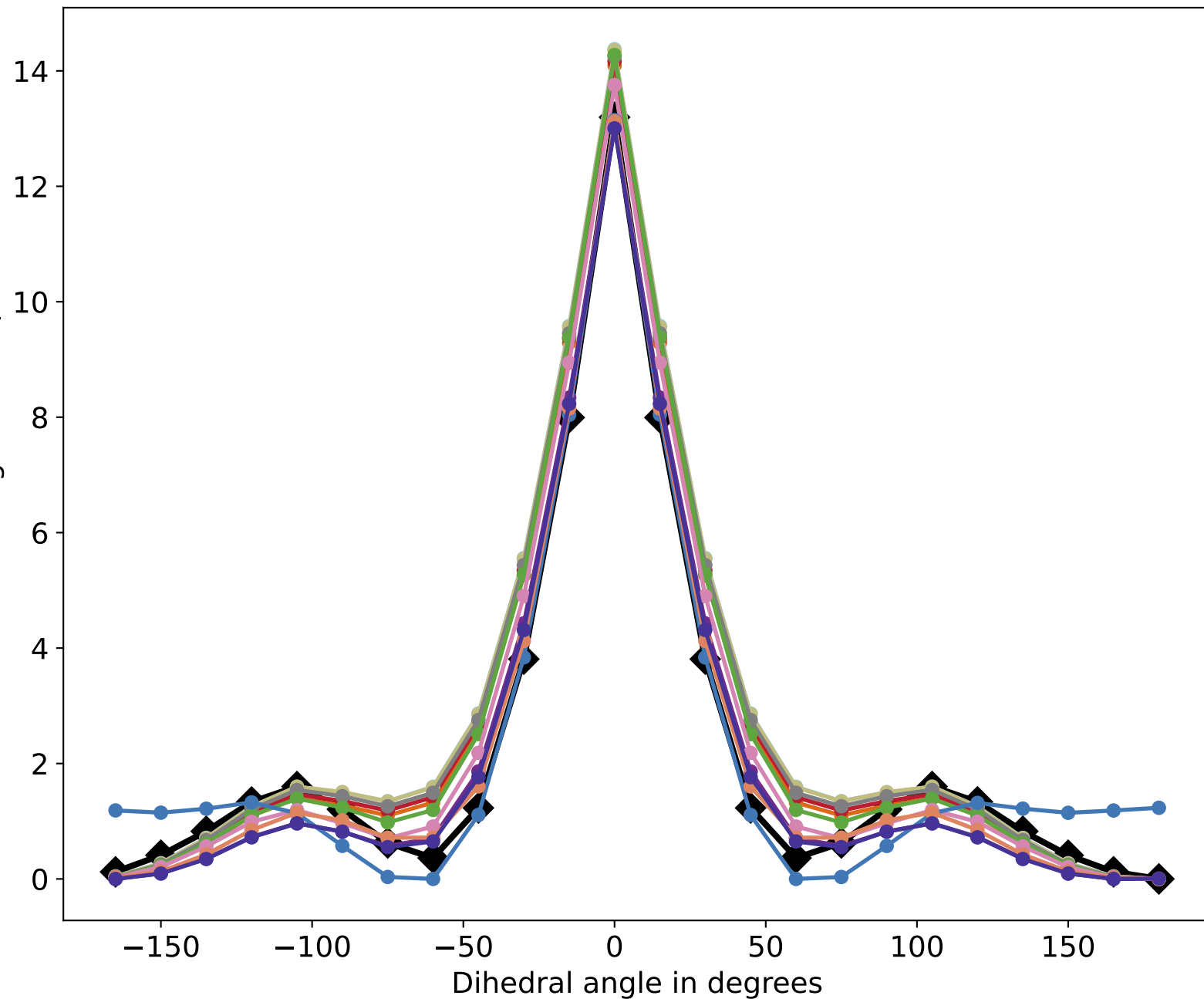


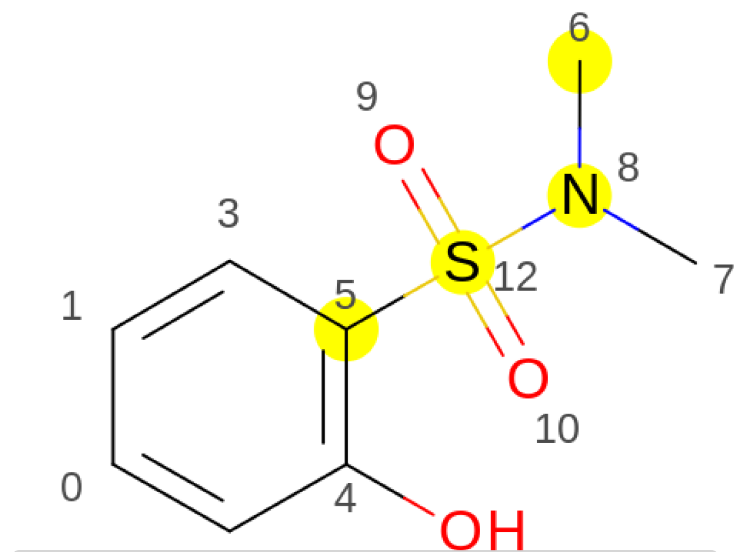
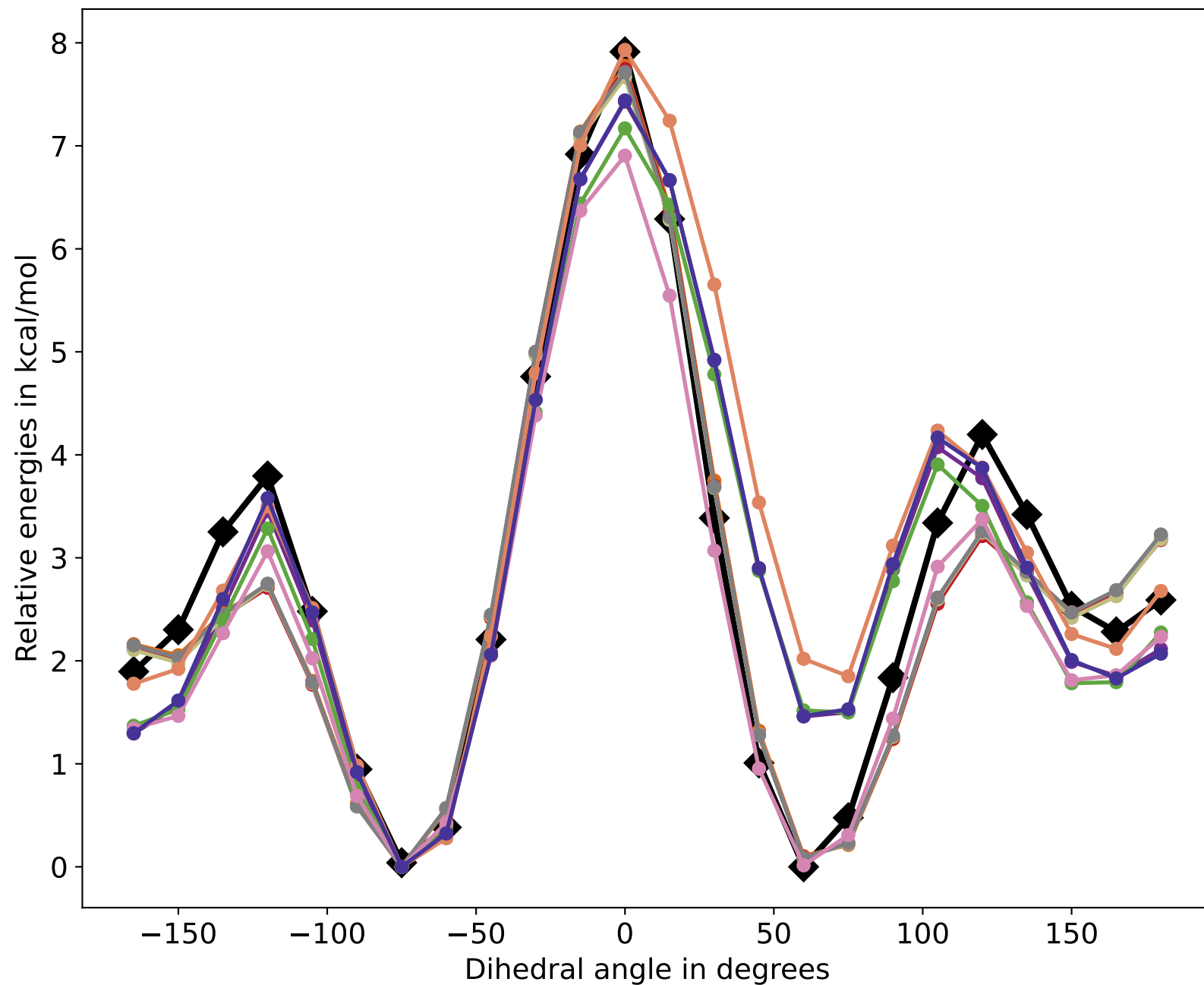
- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP

Relative energies in kcal/mol



Relative energies in kcal/mol

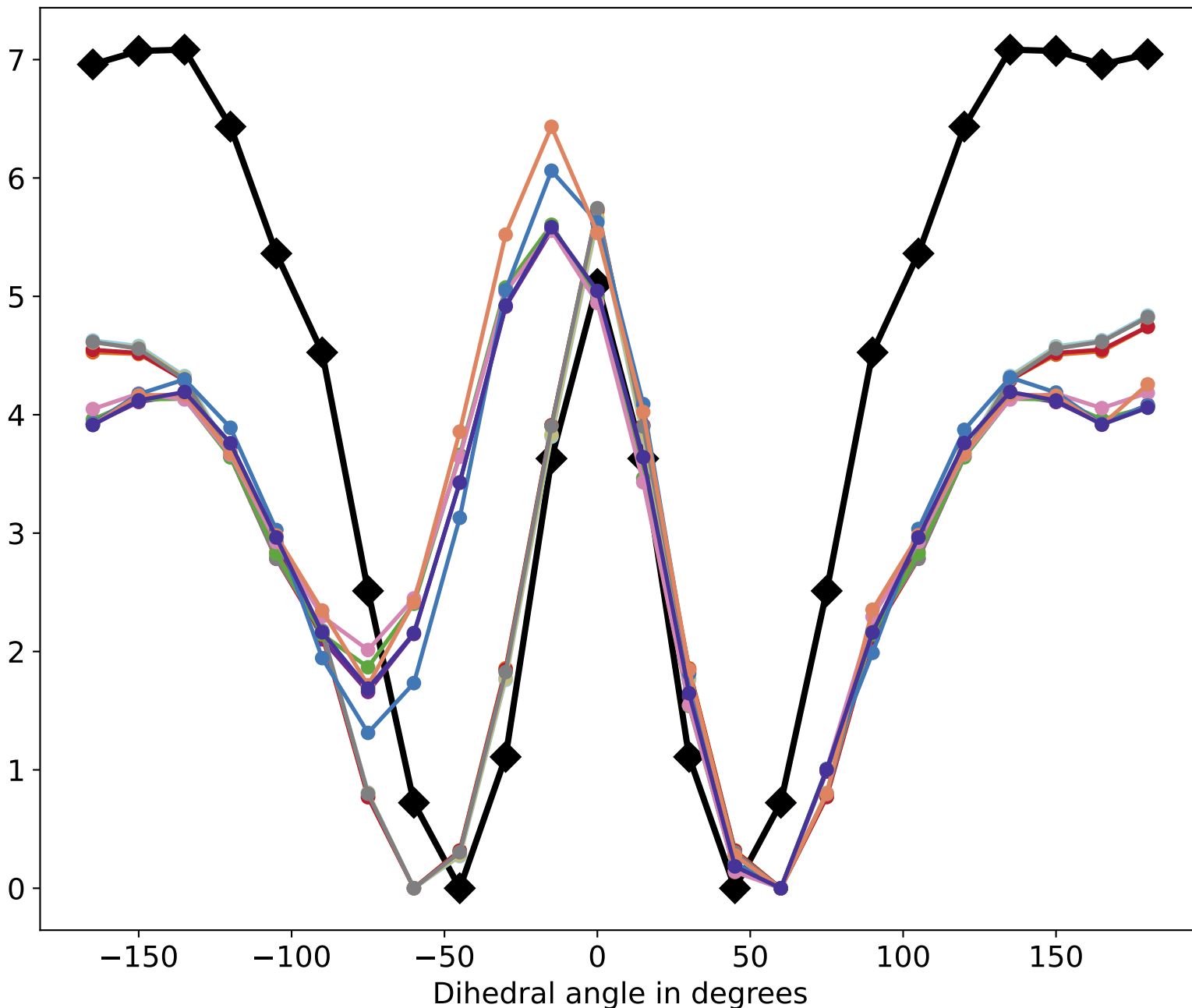




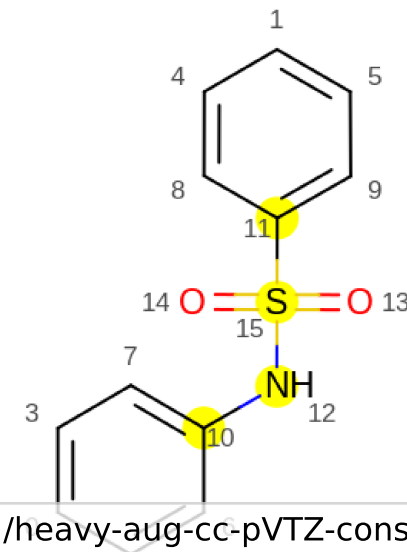
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- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- PW6B95-D3BJ/DZVP
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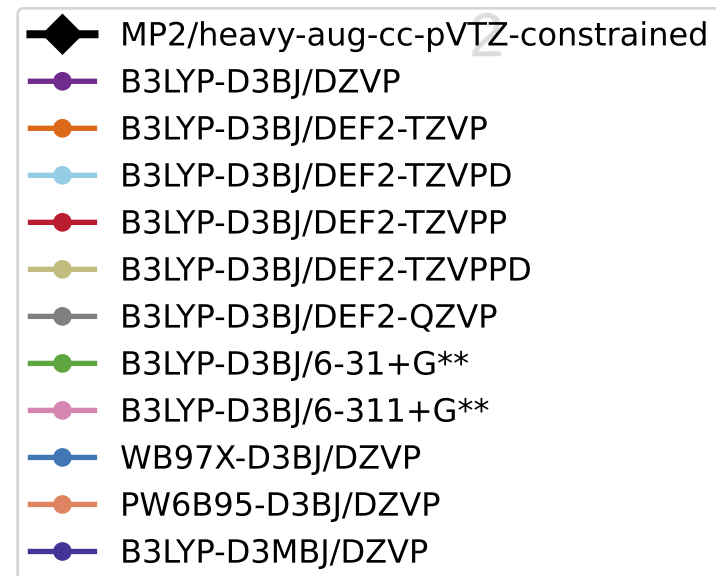
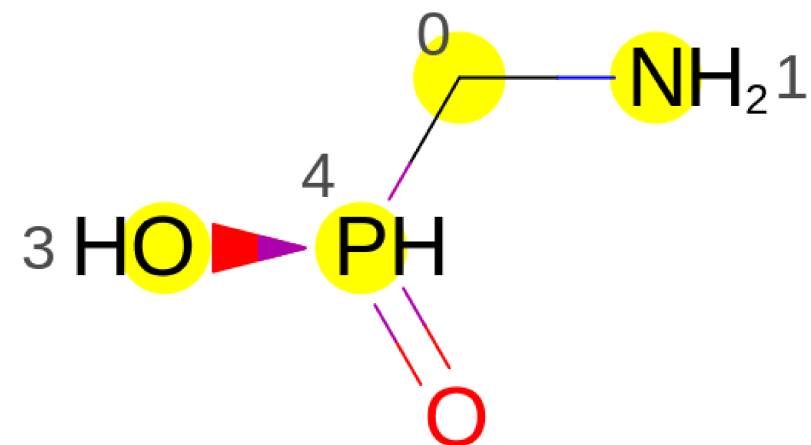
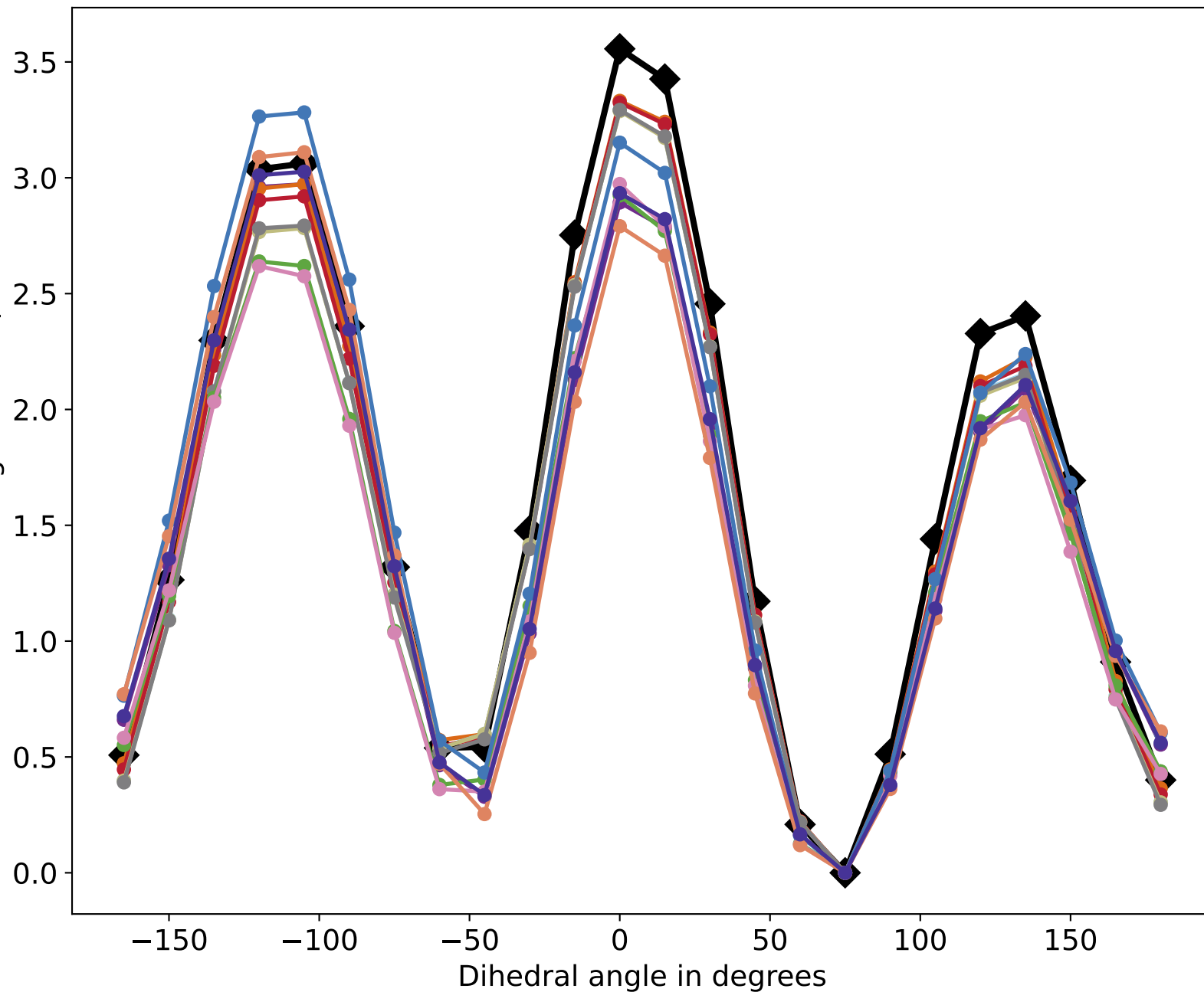
Relative energies in kcal/mol



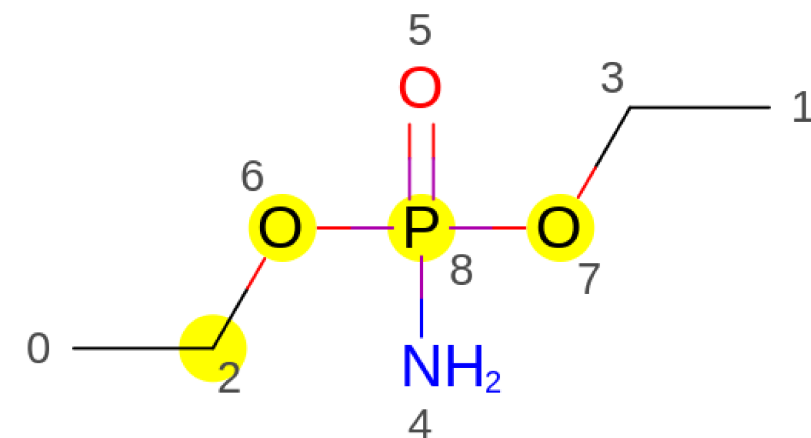
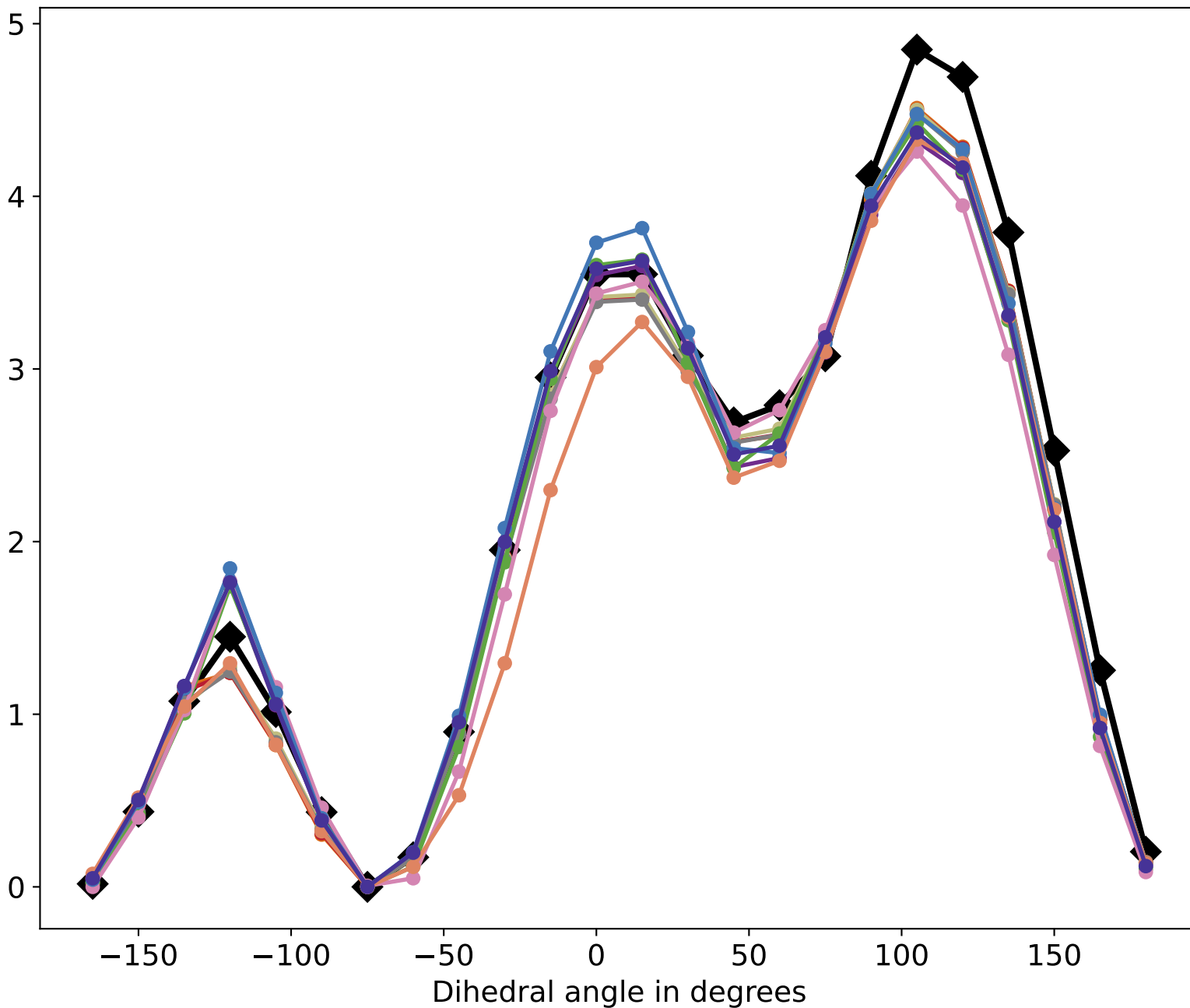
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- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*
- WB97X-D3BJ/DZVP
- PW6B95-D3BJ/DZVP
- B3LYP-D3MBJ/DZVP



Relative energies in kcal/mol



Relative energies in kcal/mol



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

