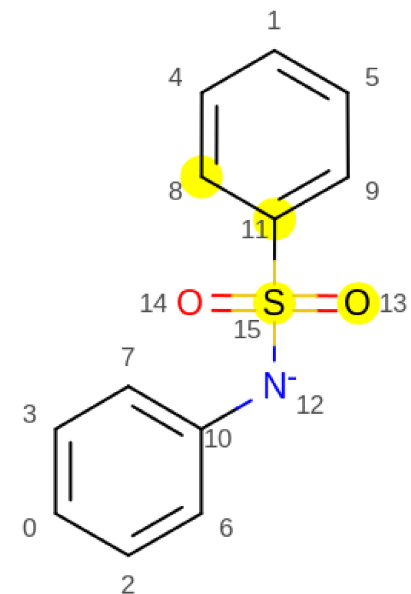
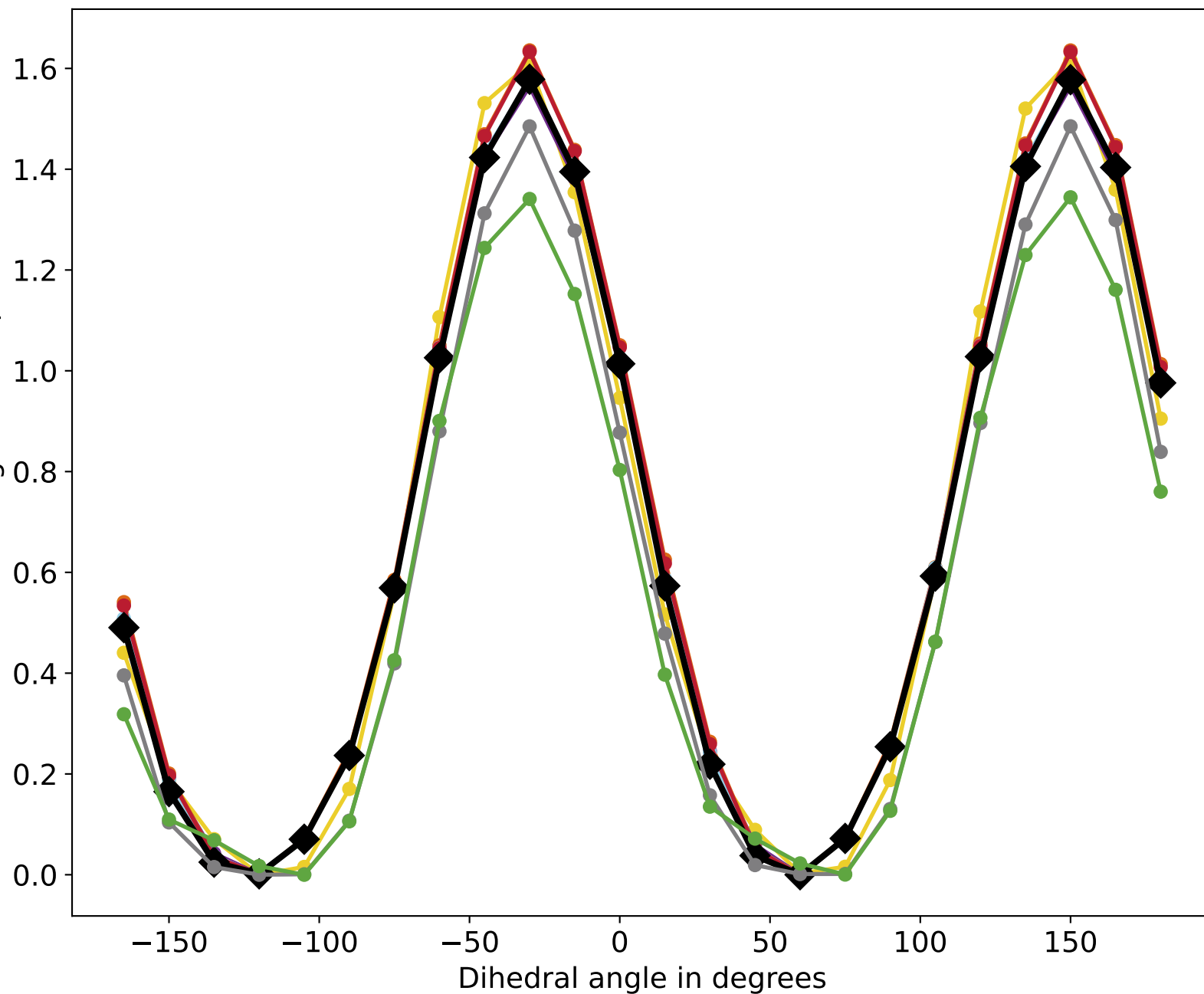
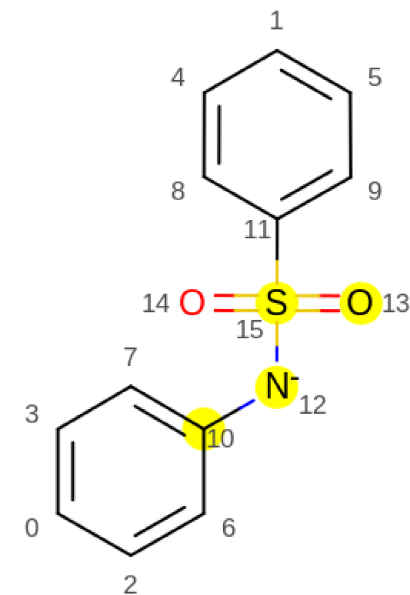
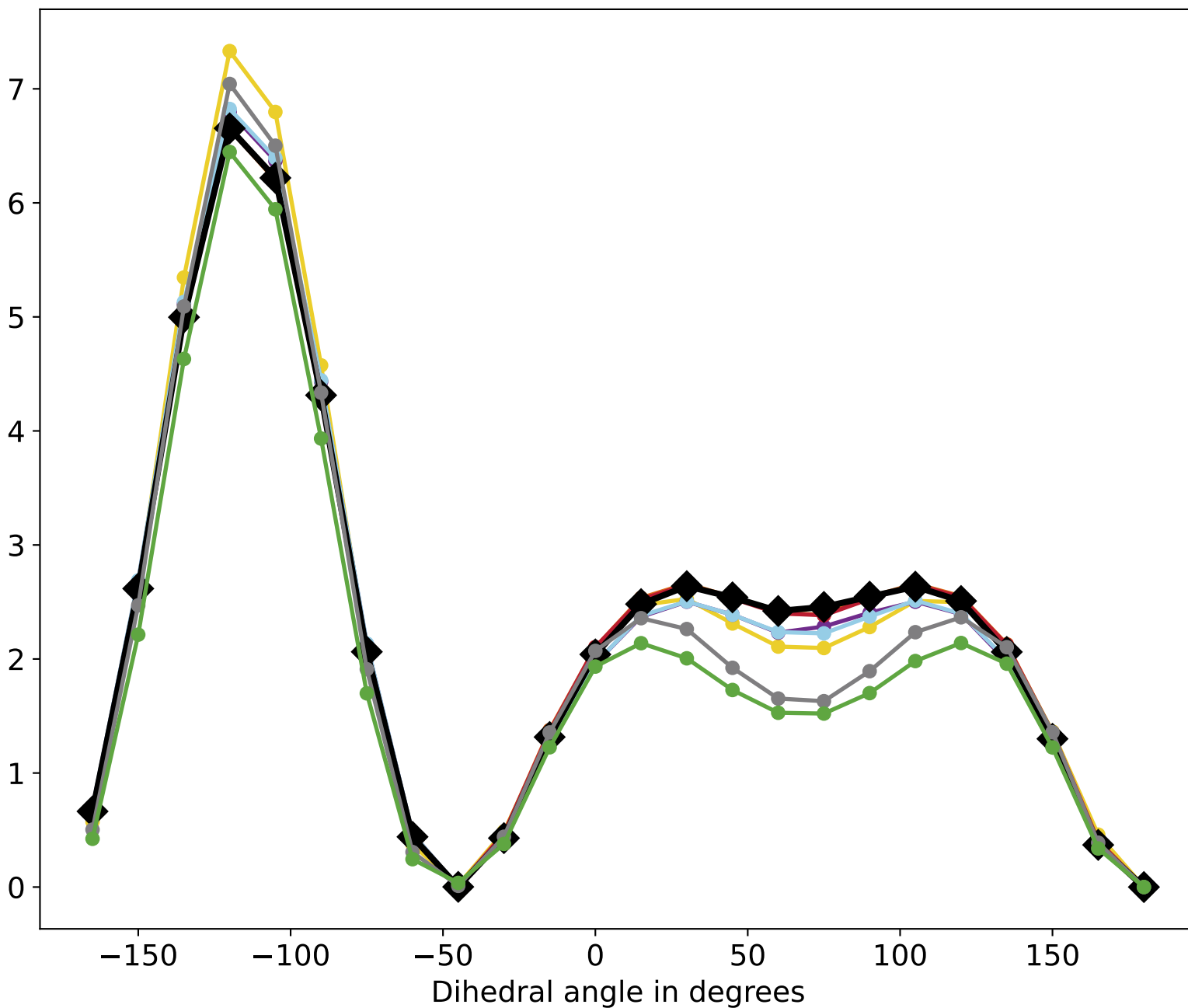


Relative energies in kcal/mol



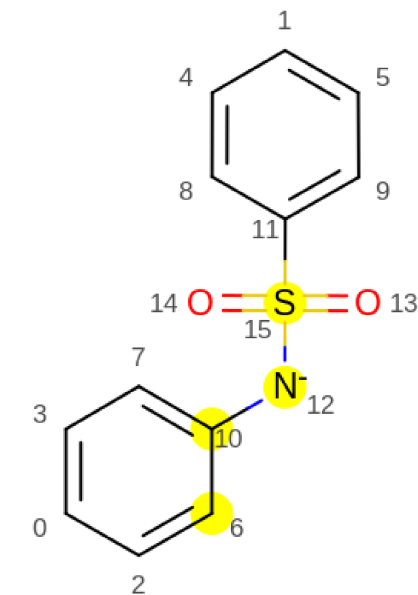
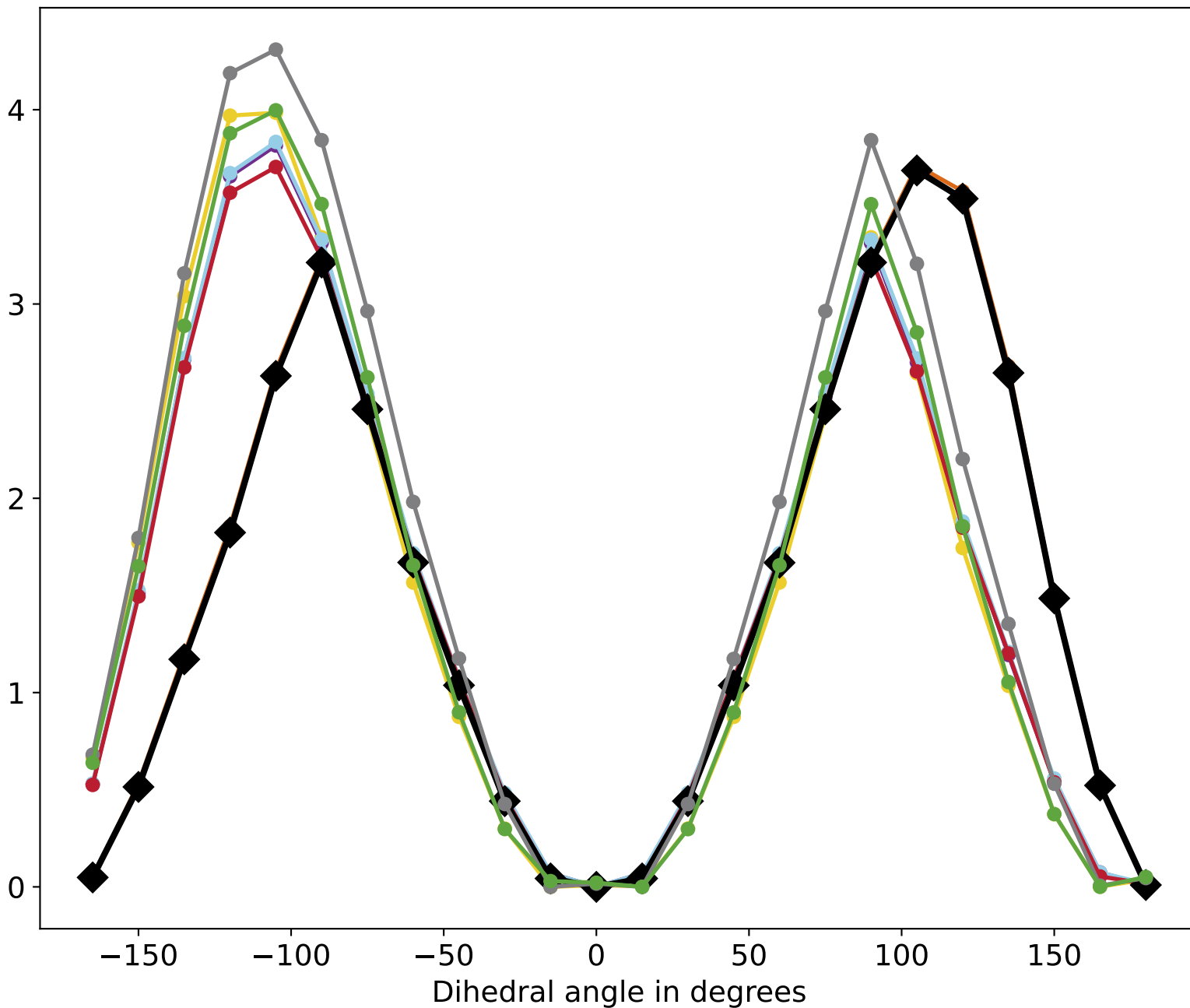
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



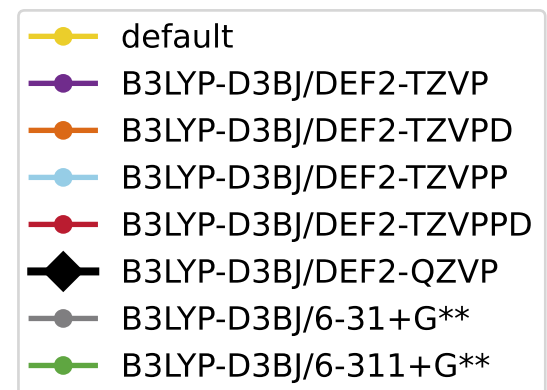
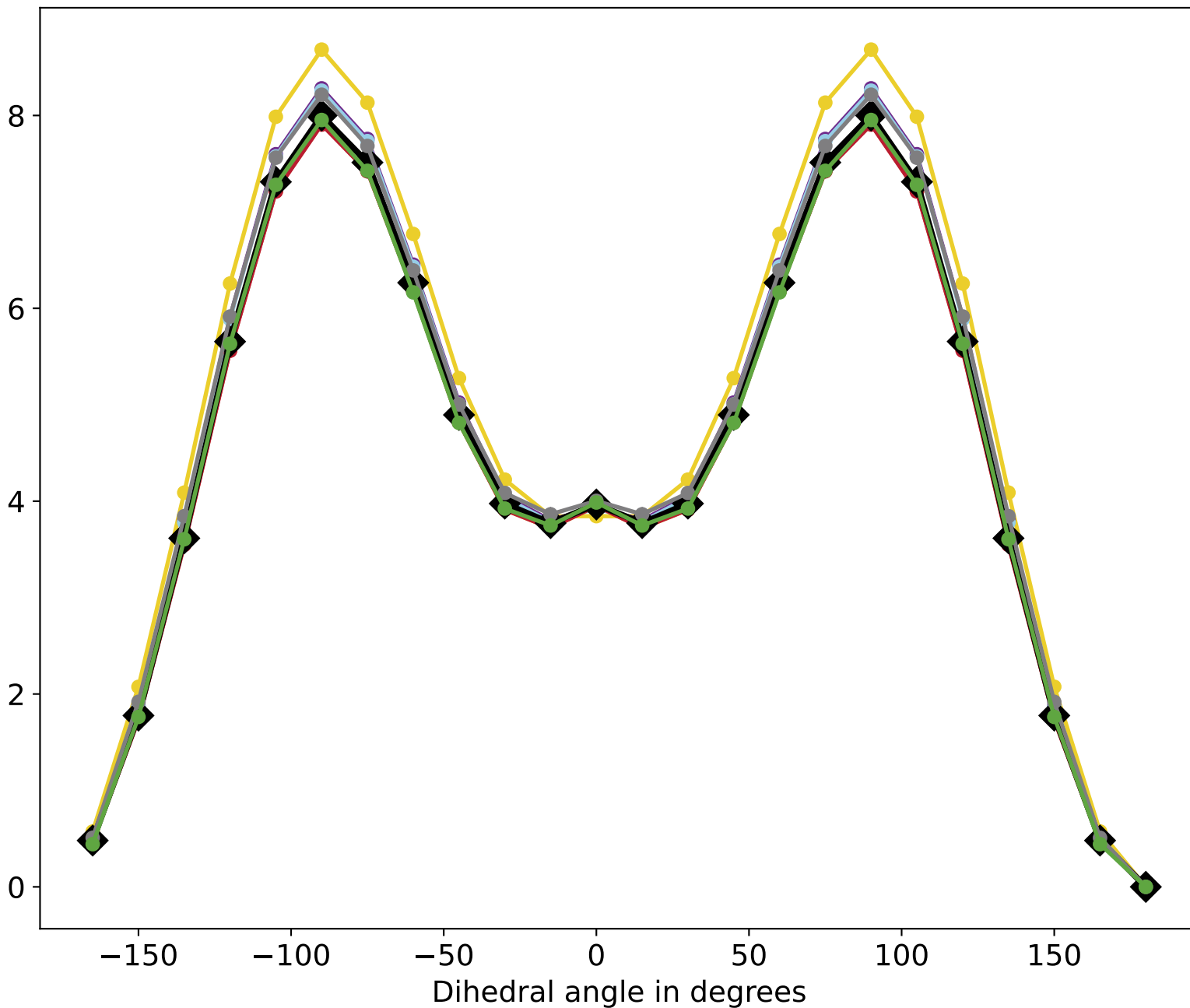
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

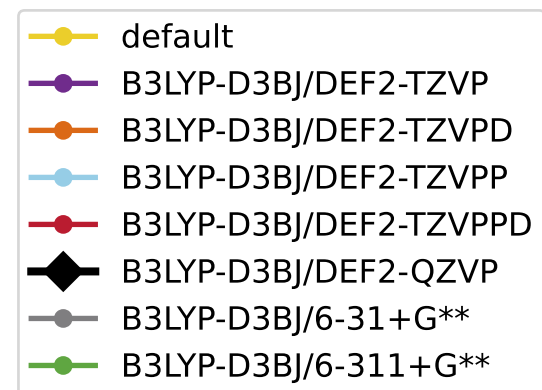
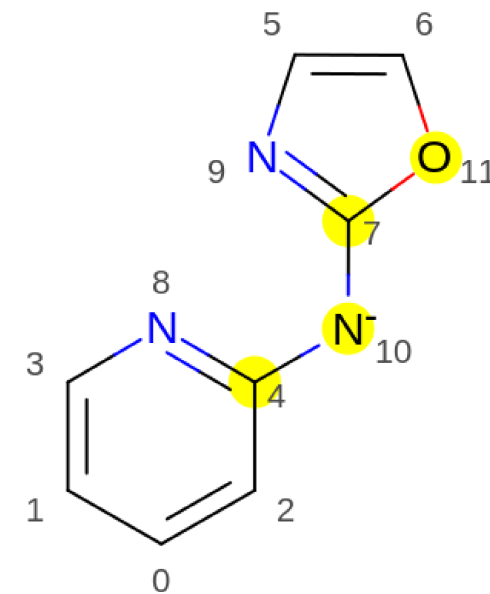
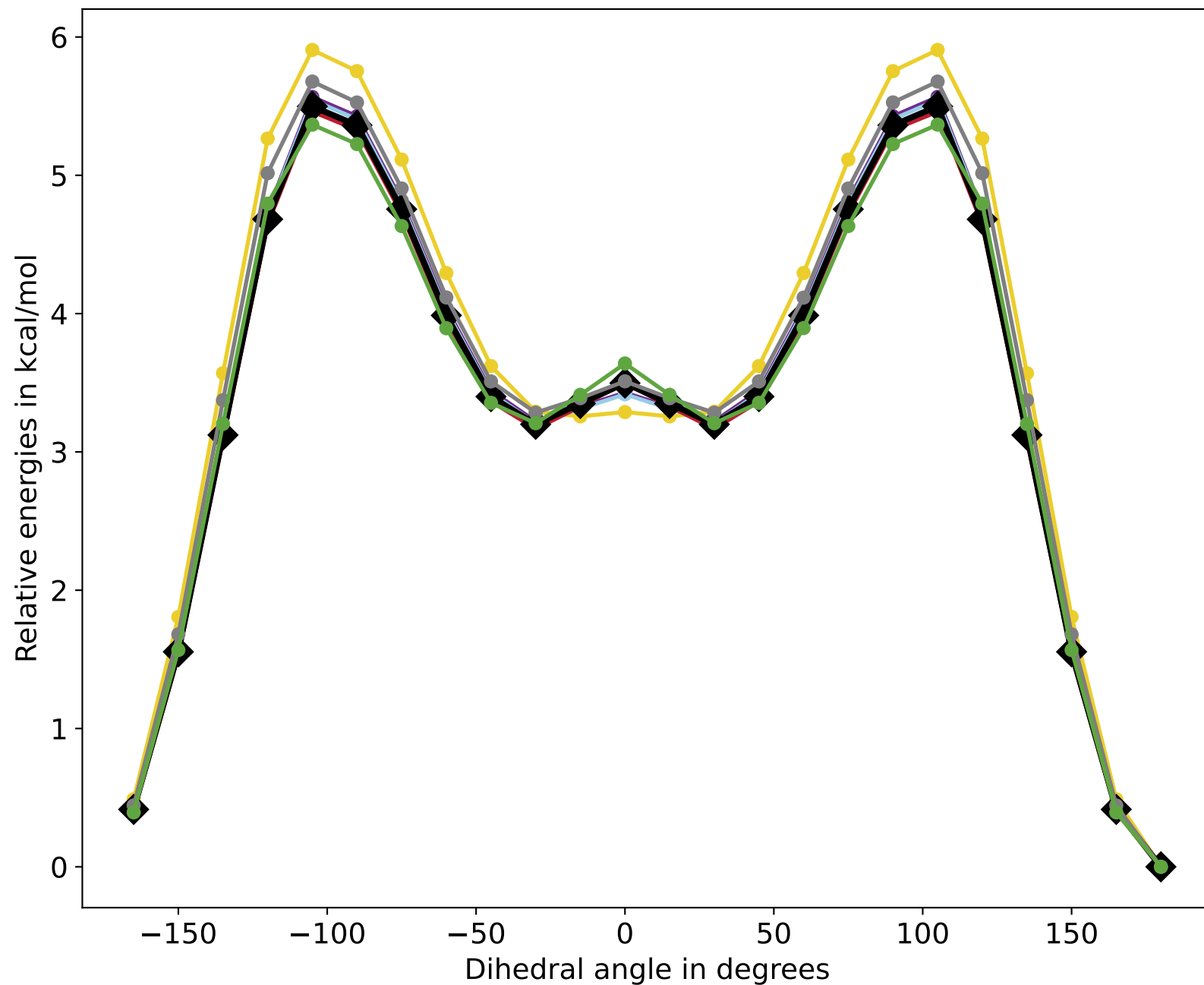
Relative energies in kcal/mol

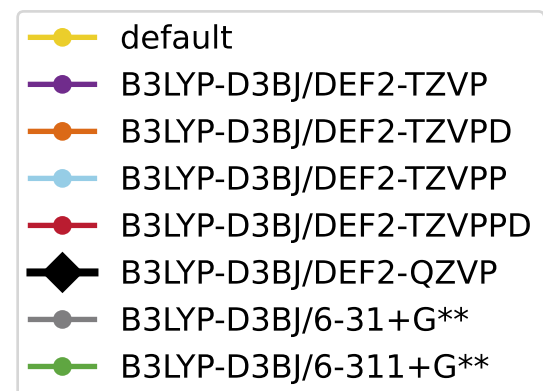
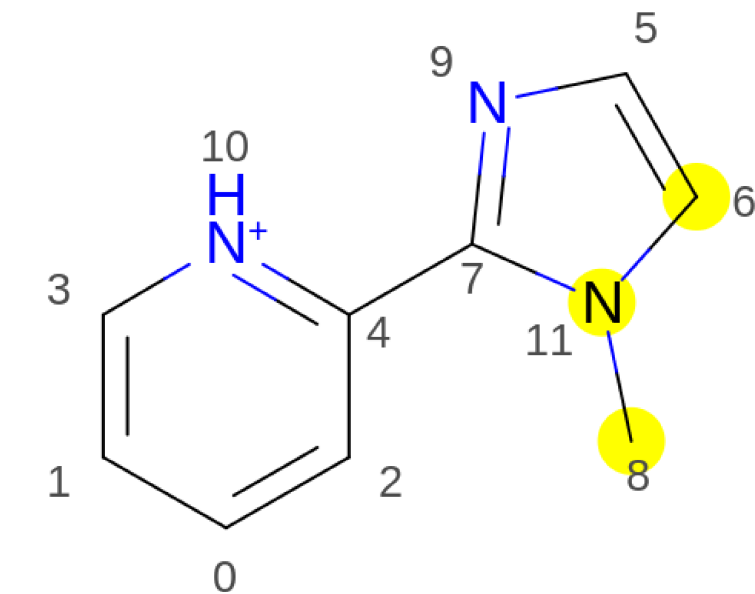
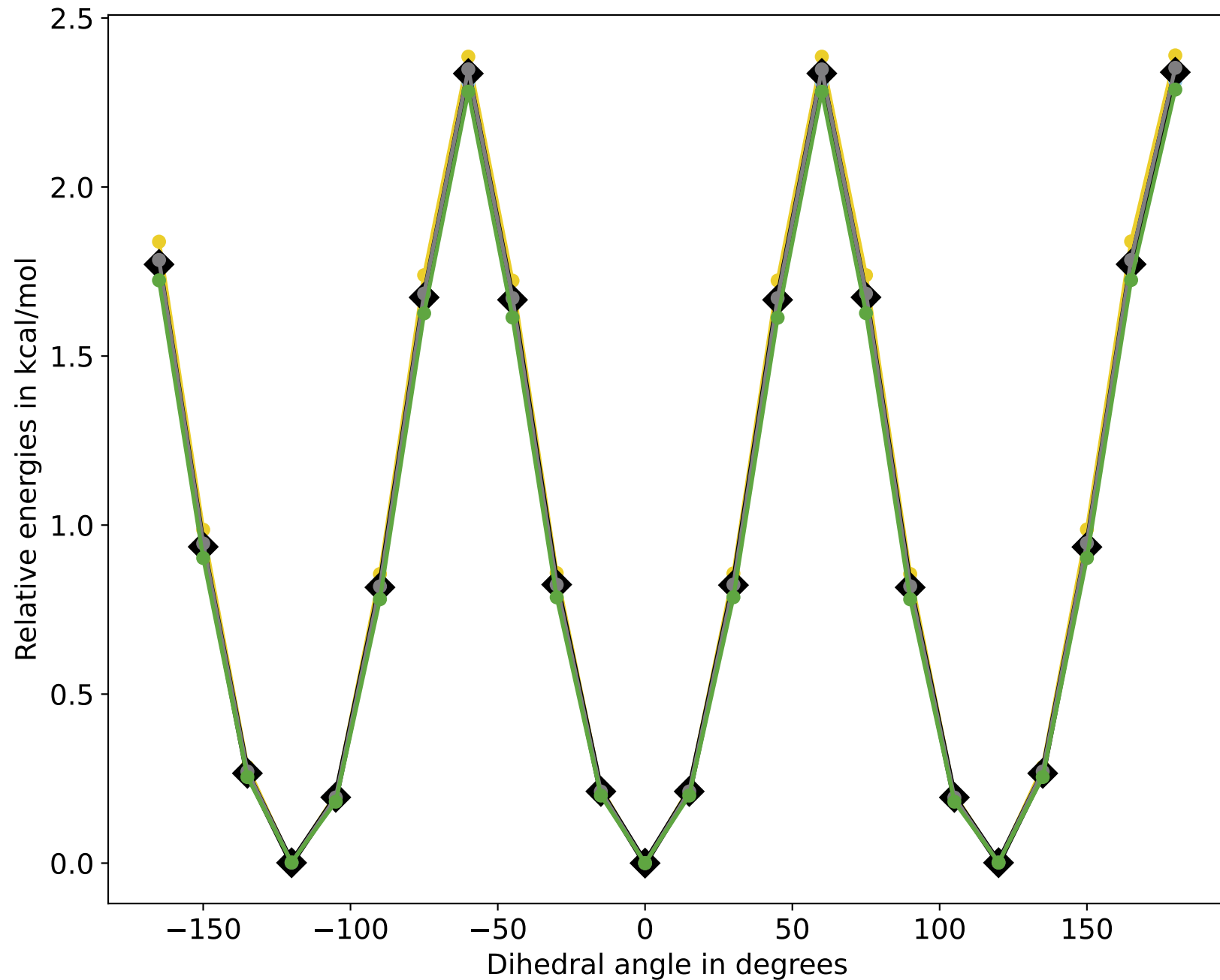


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

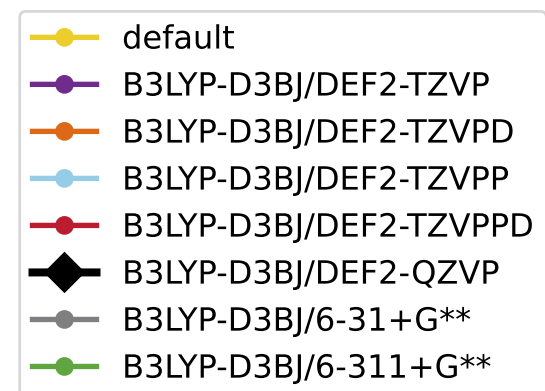
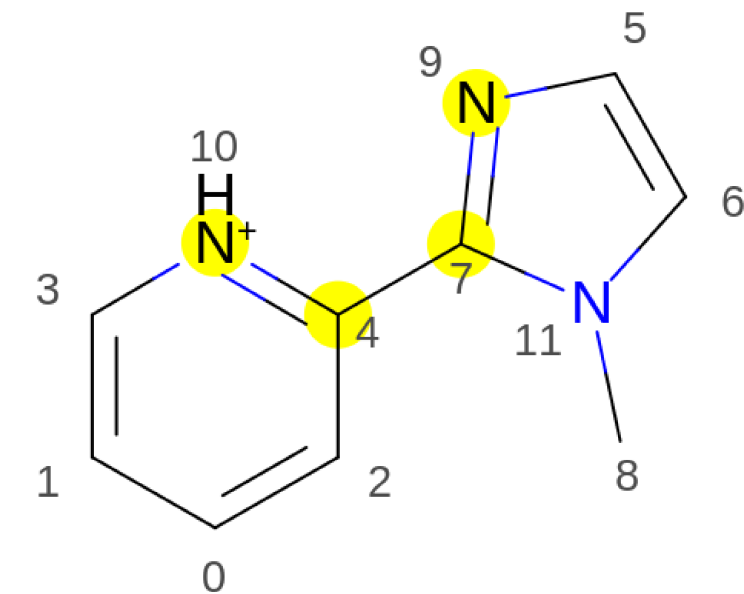
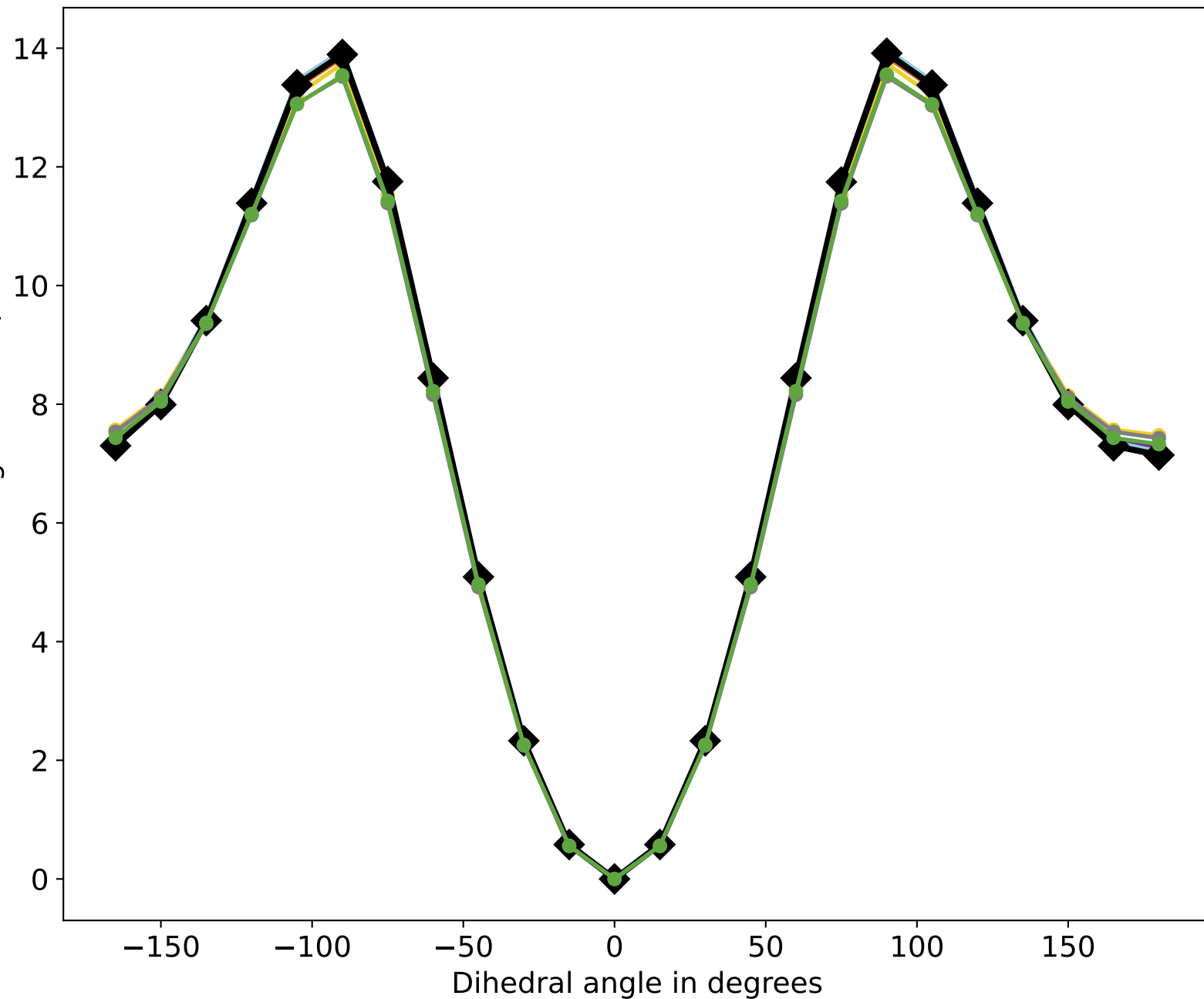
Relative energies in kcal/mol

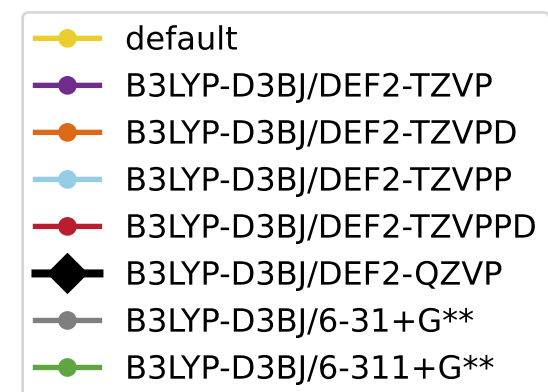
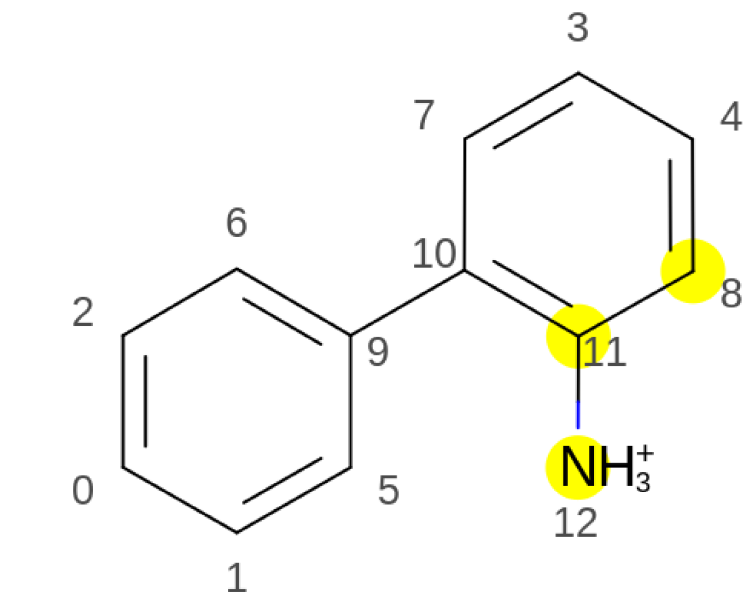
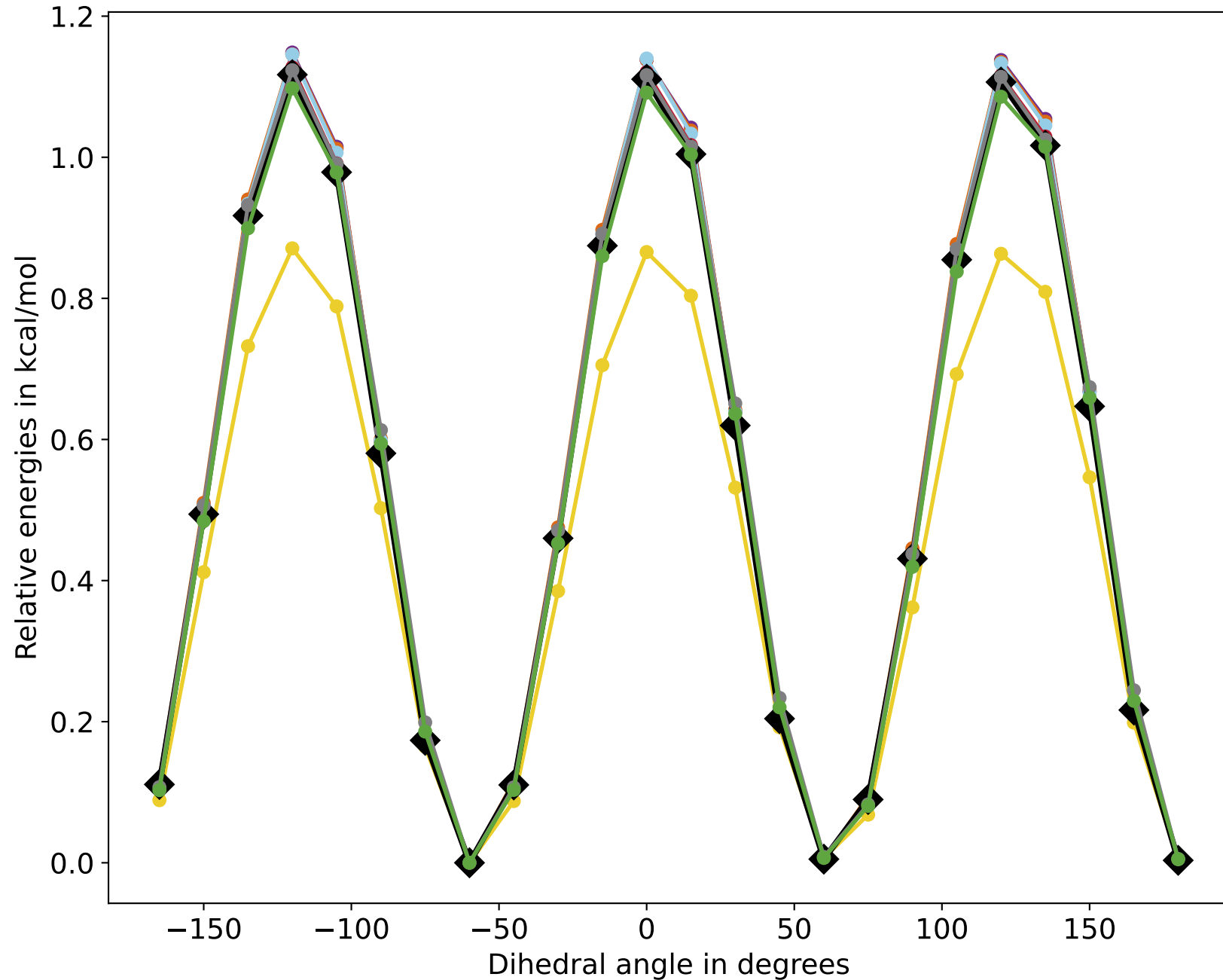


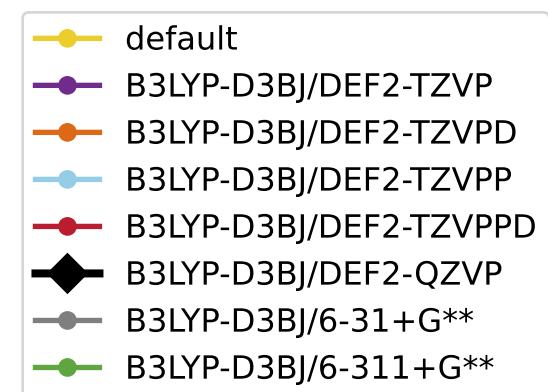
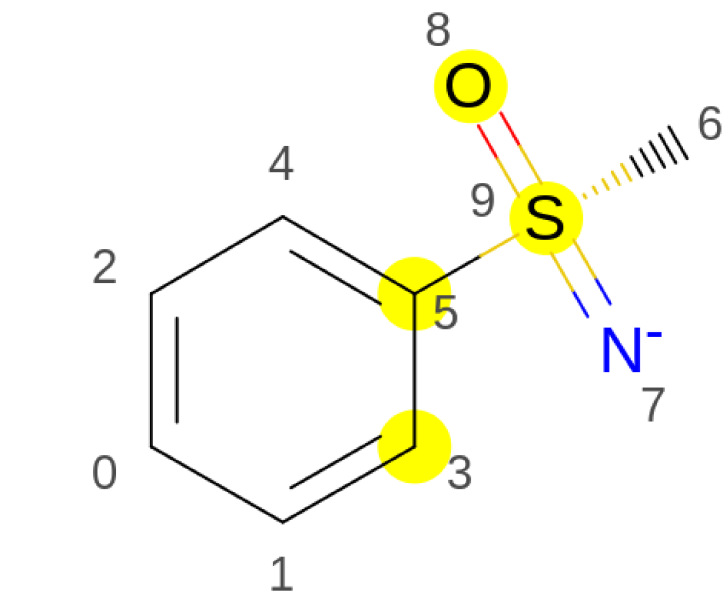
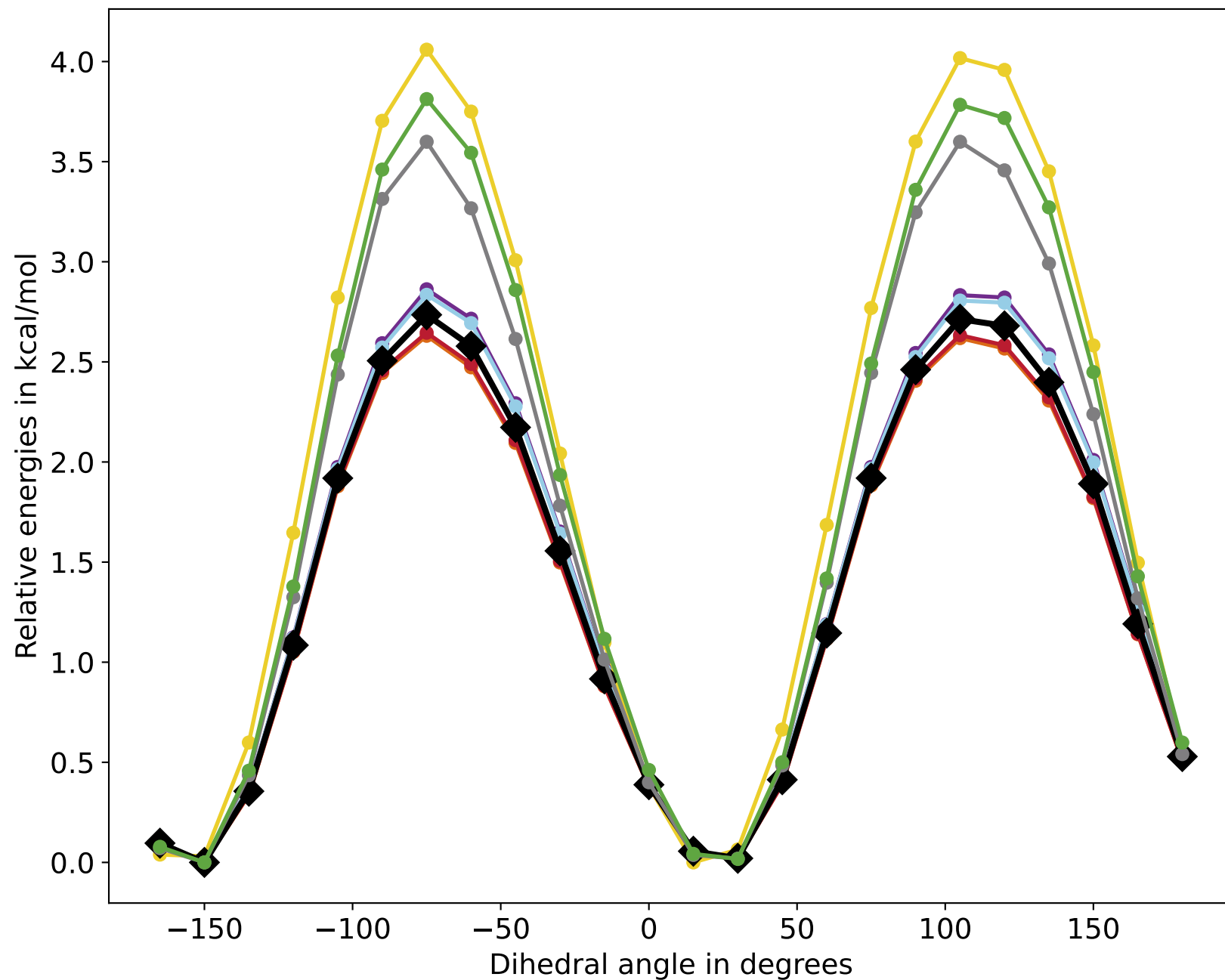


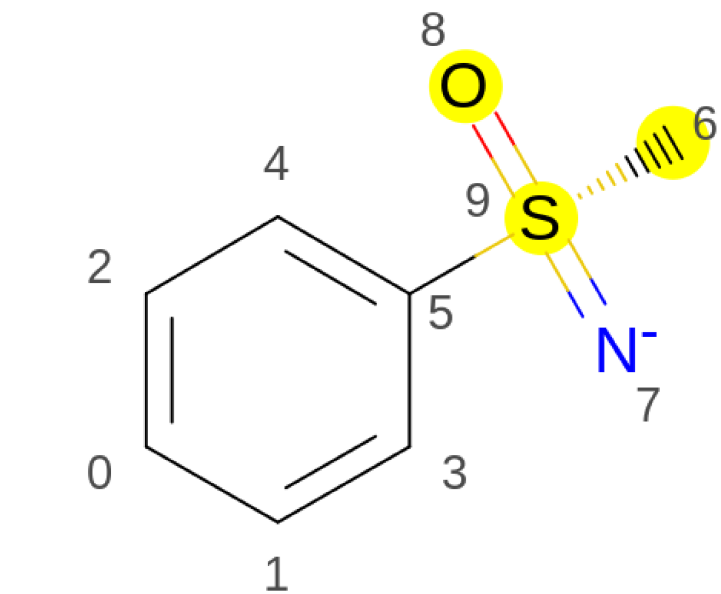
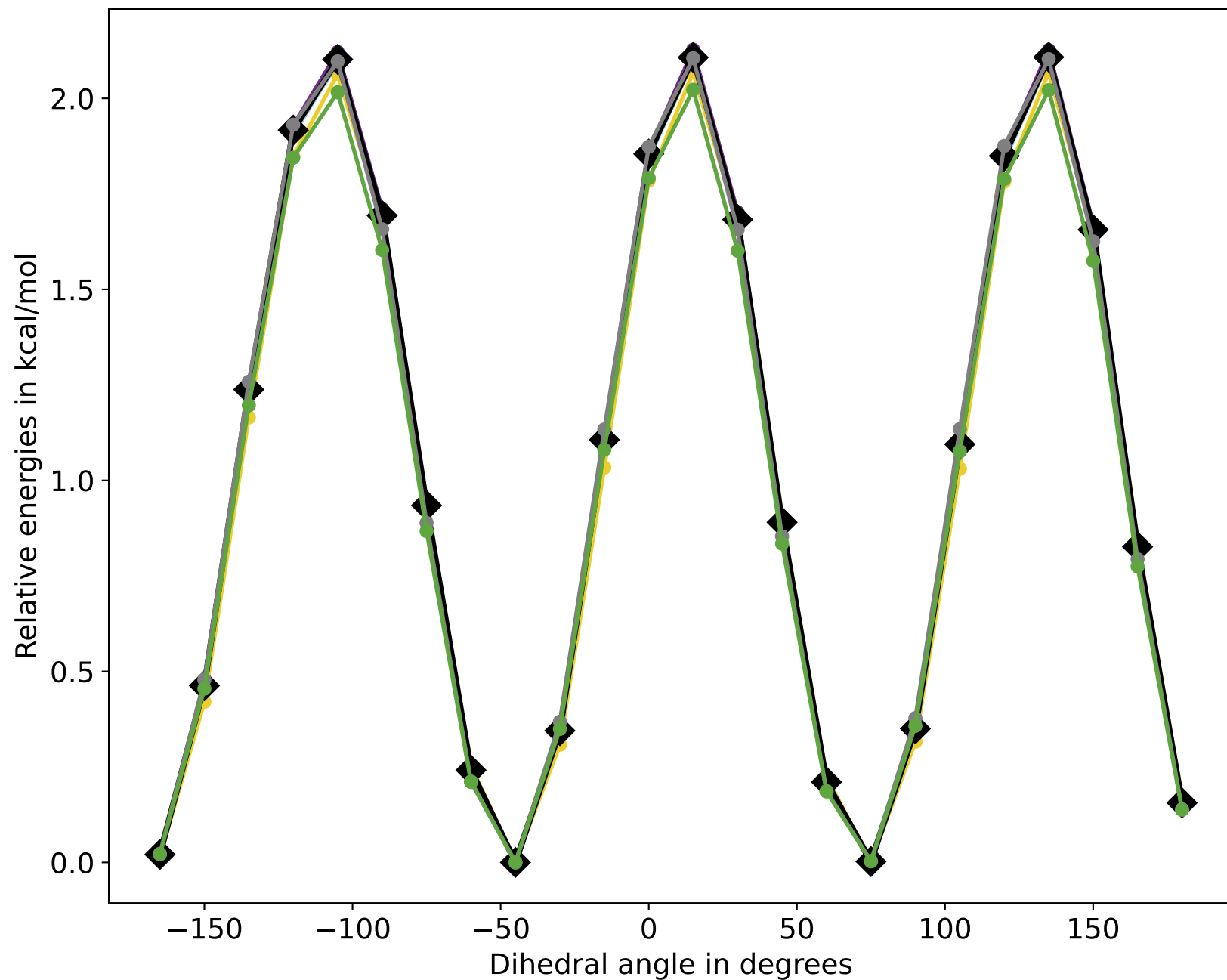


Relative energies in kcal/mol



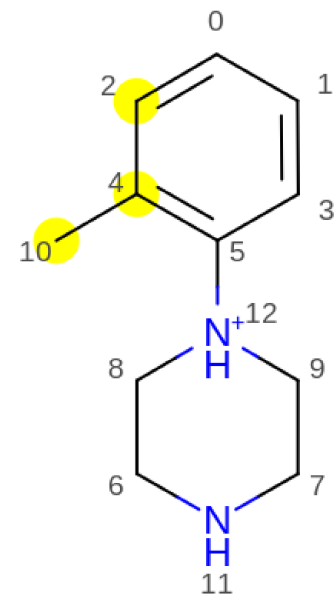
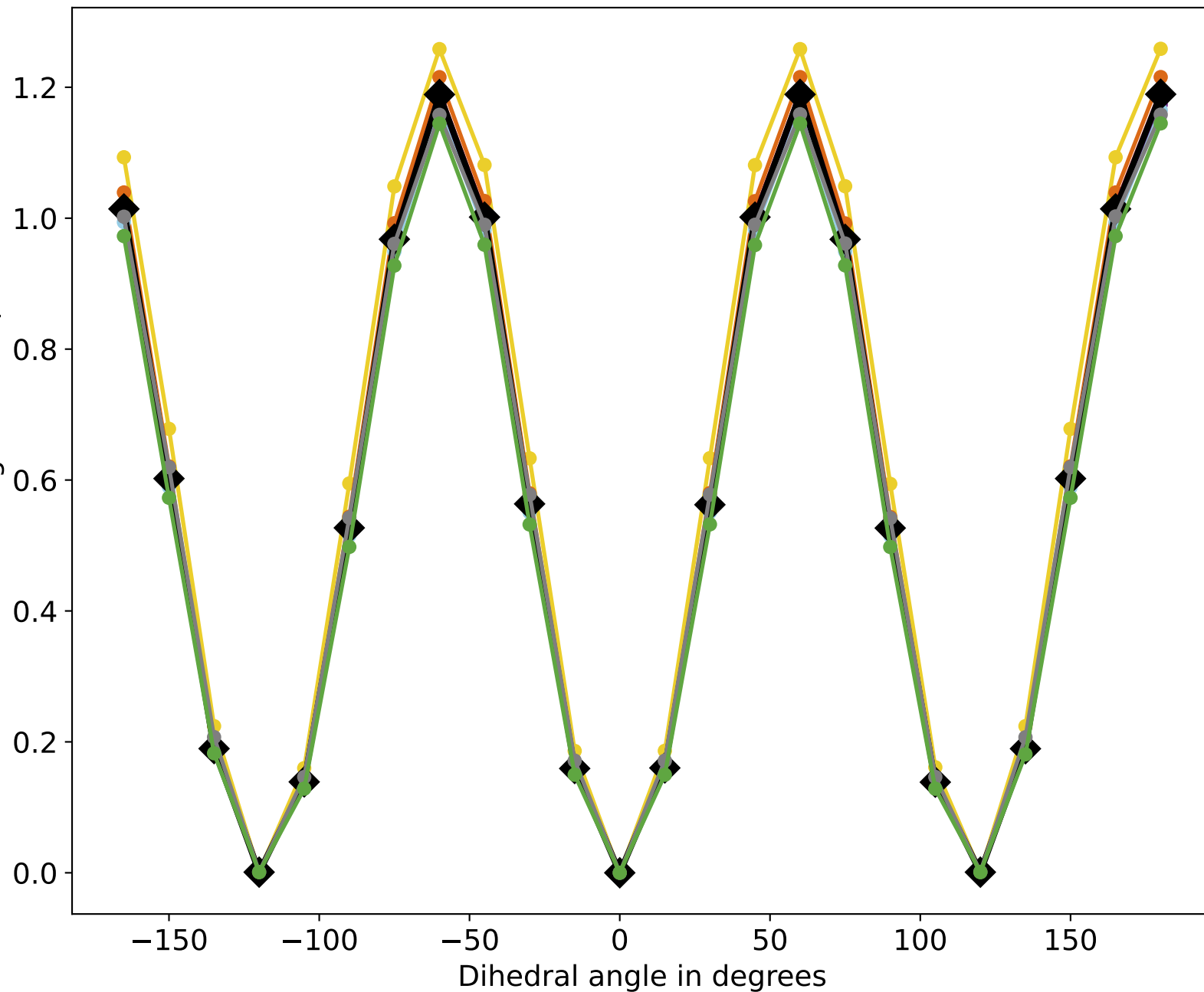




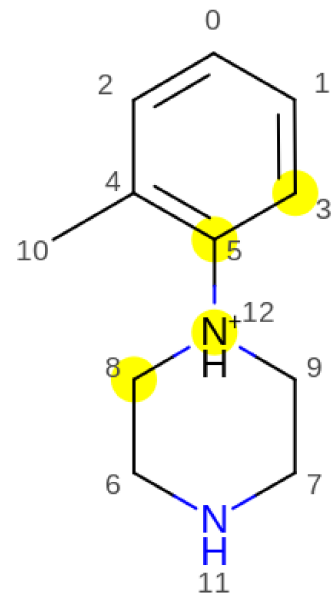
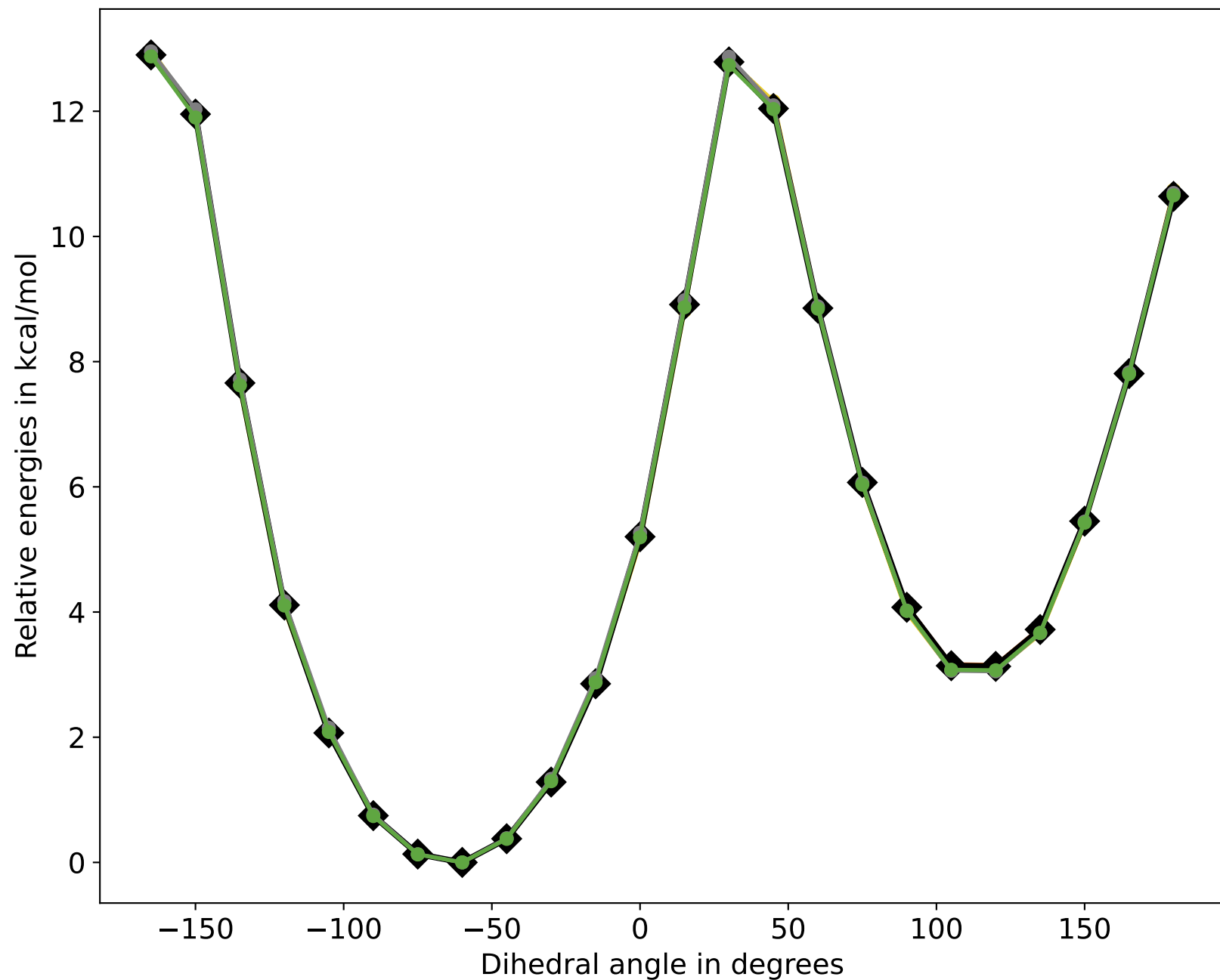


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

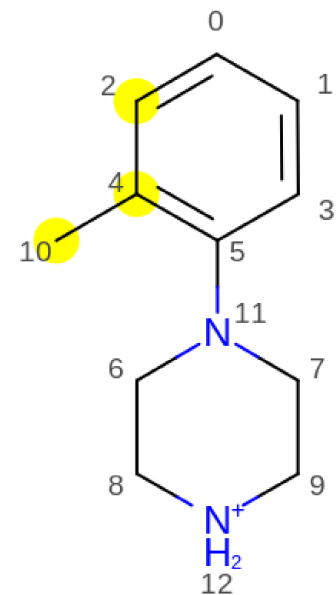
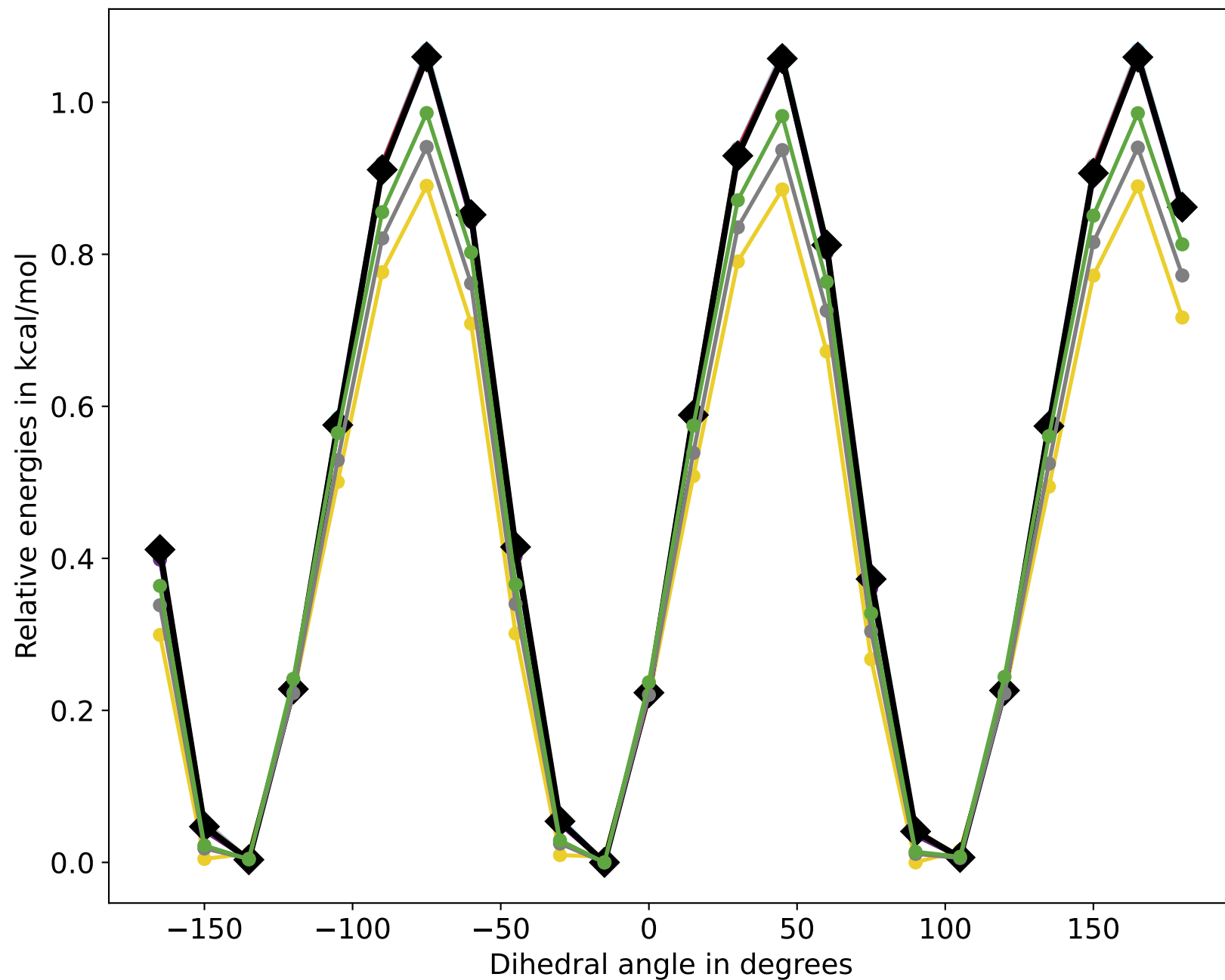
Relative energies in kcal/mol



- default
- 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**

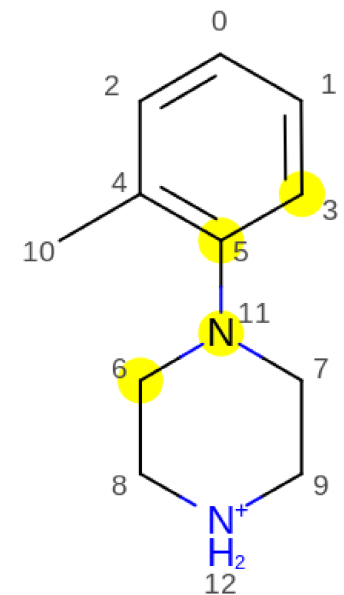
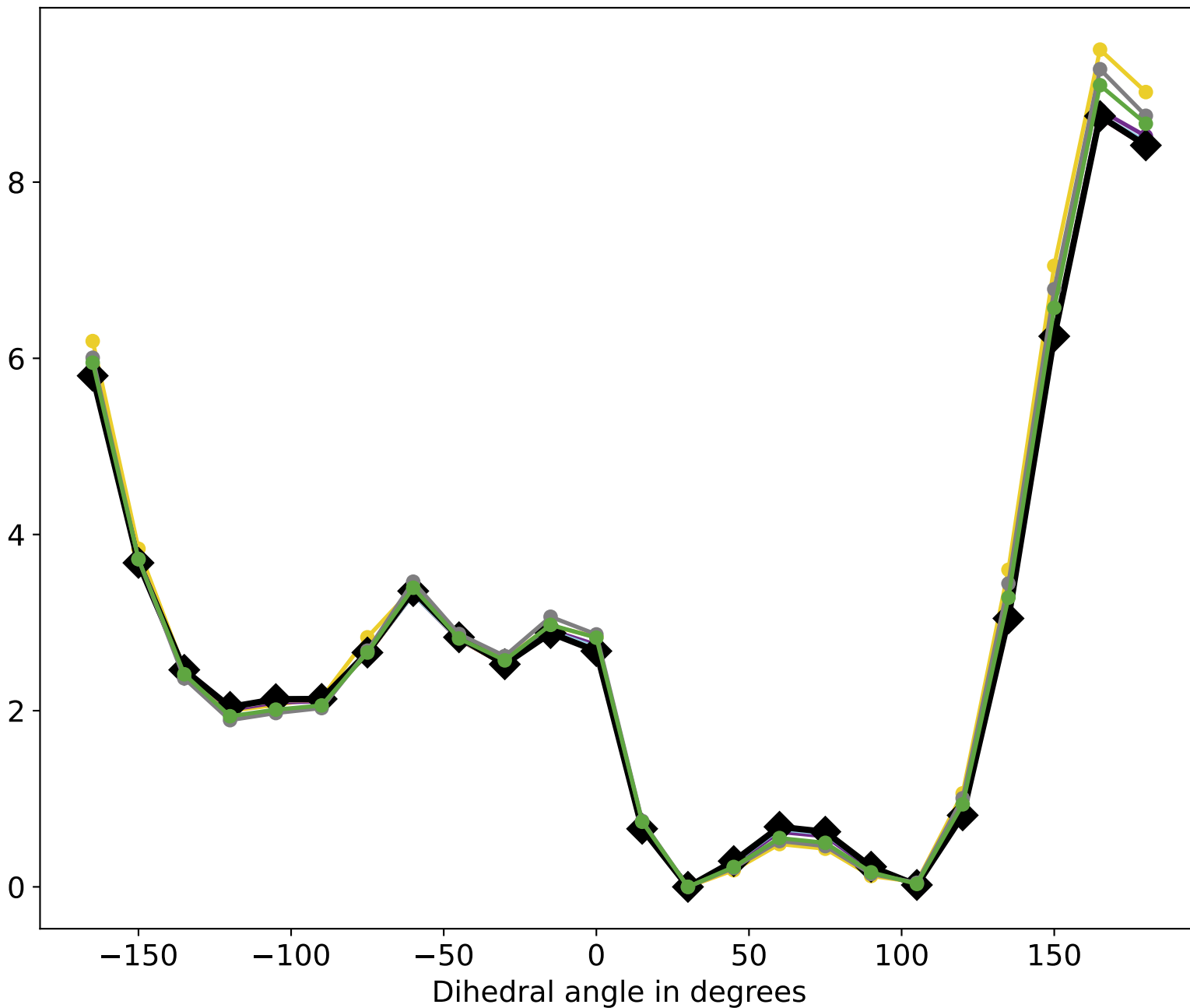


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

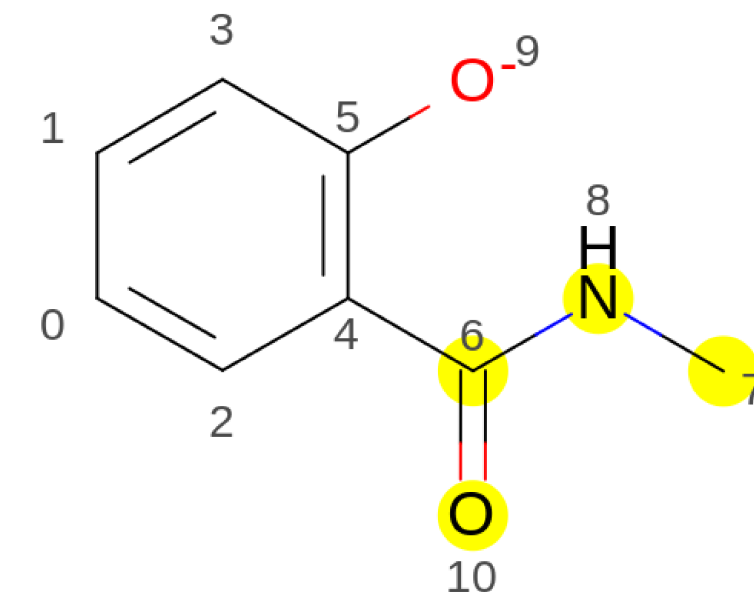
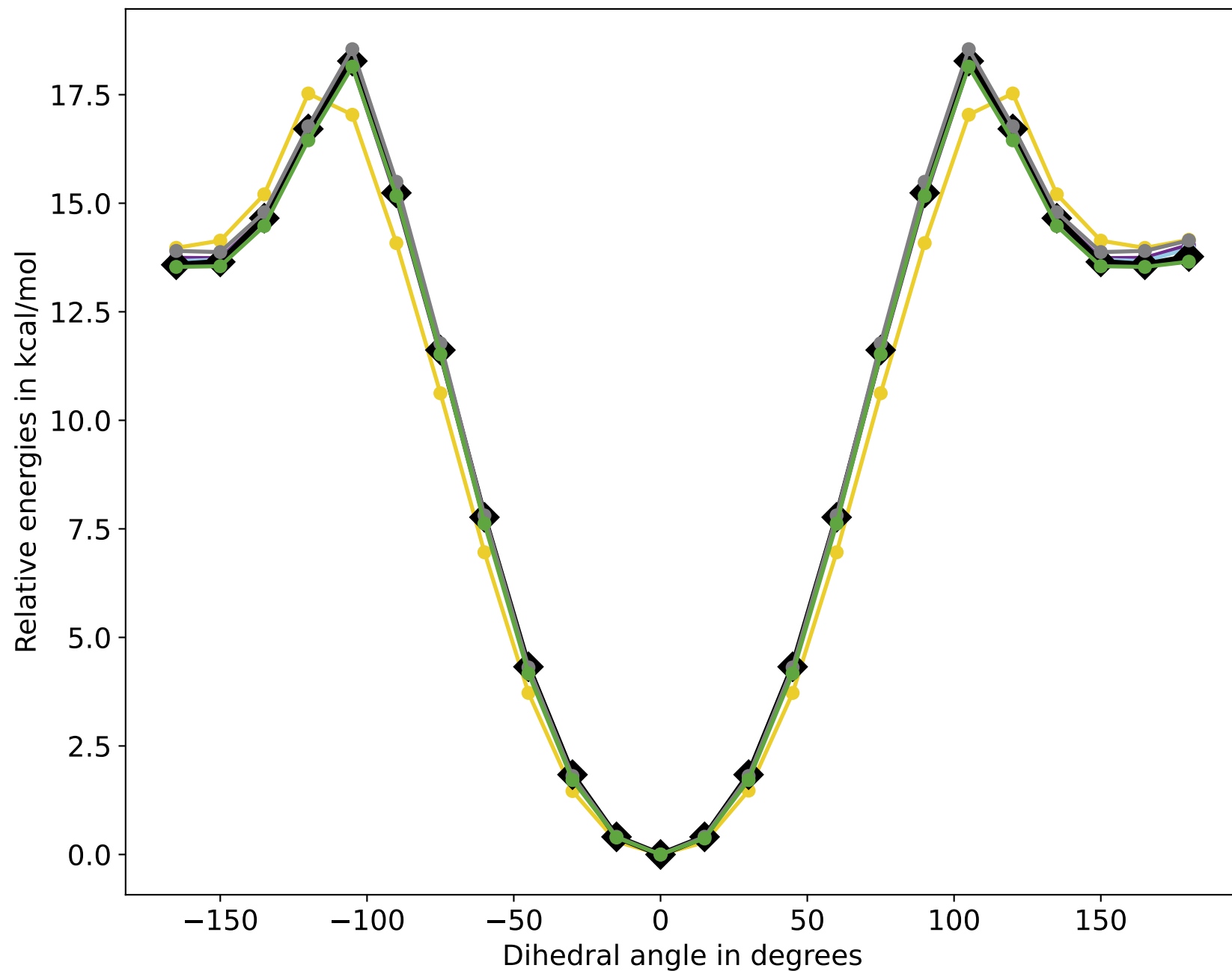


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

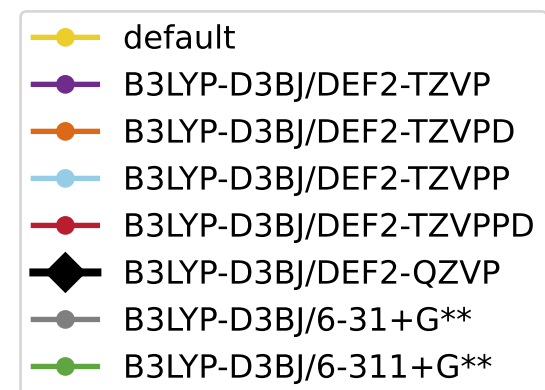
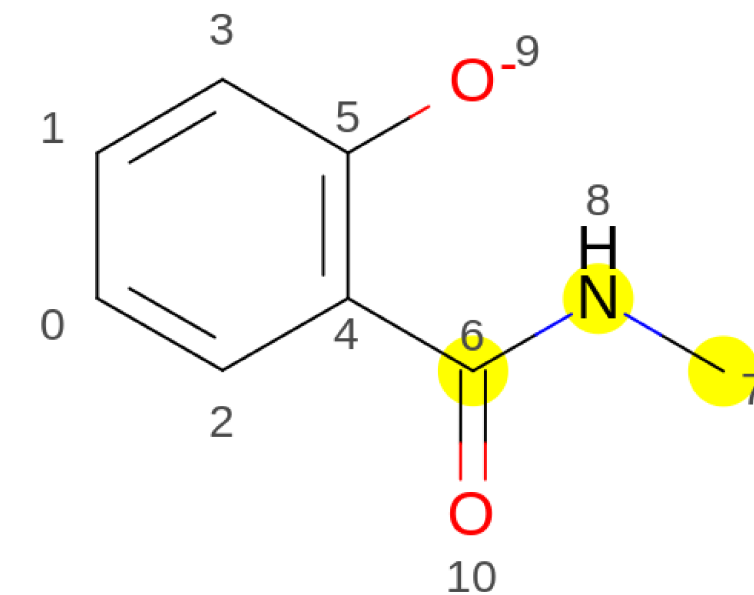
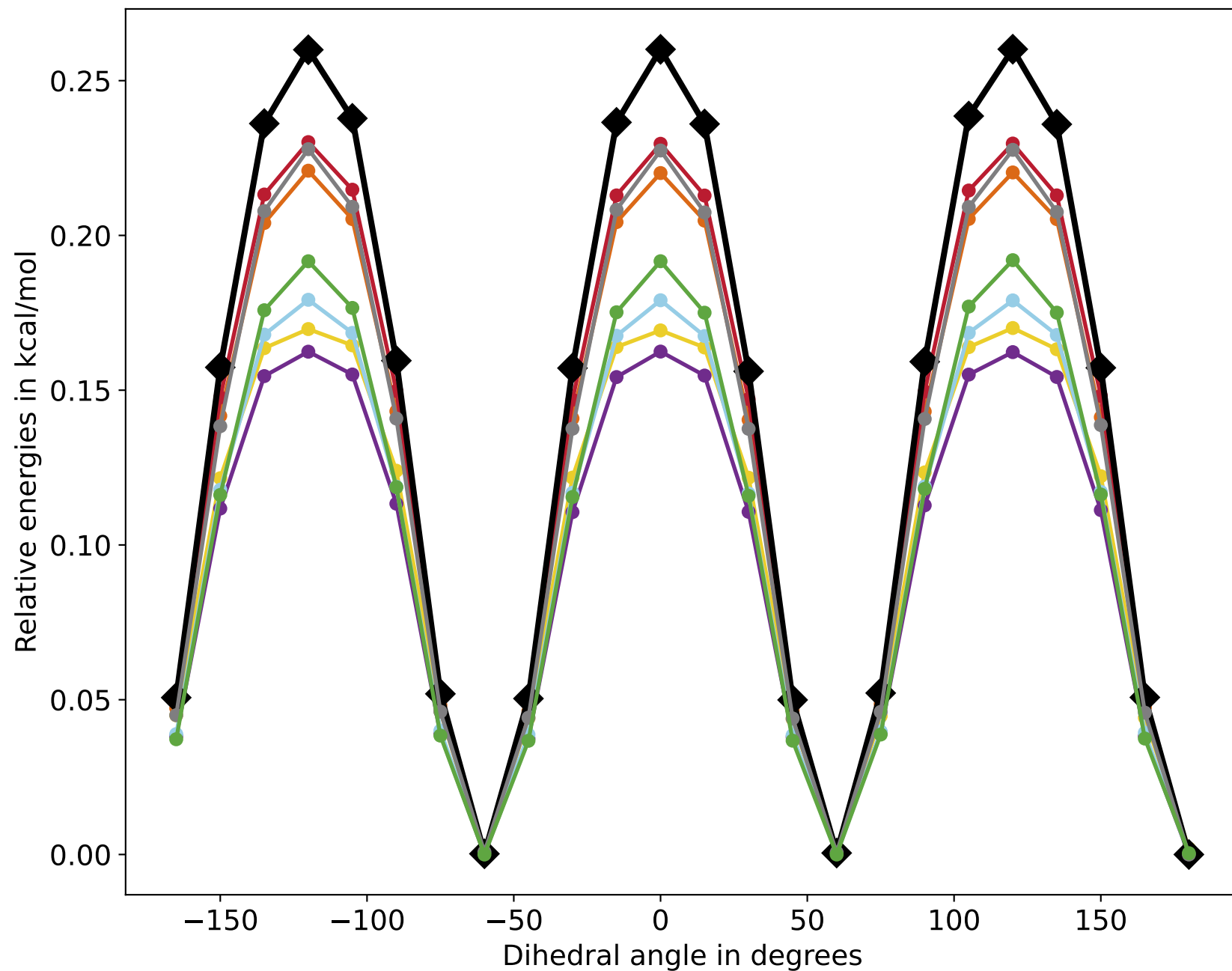
Relative energies in kcal/mol



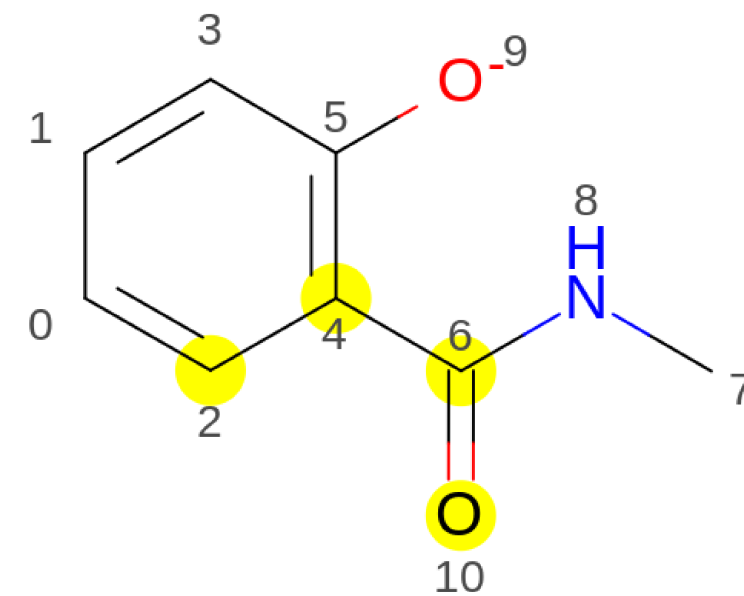
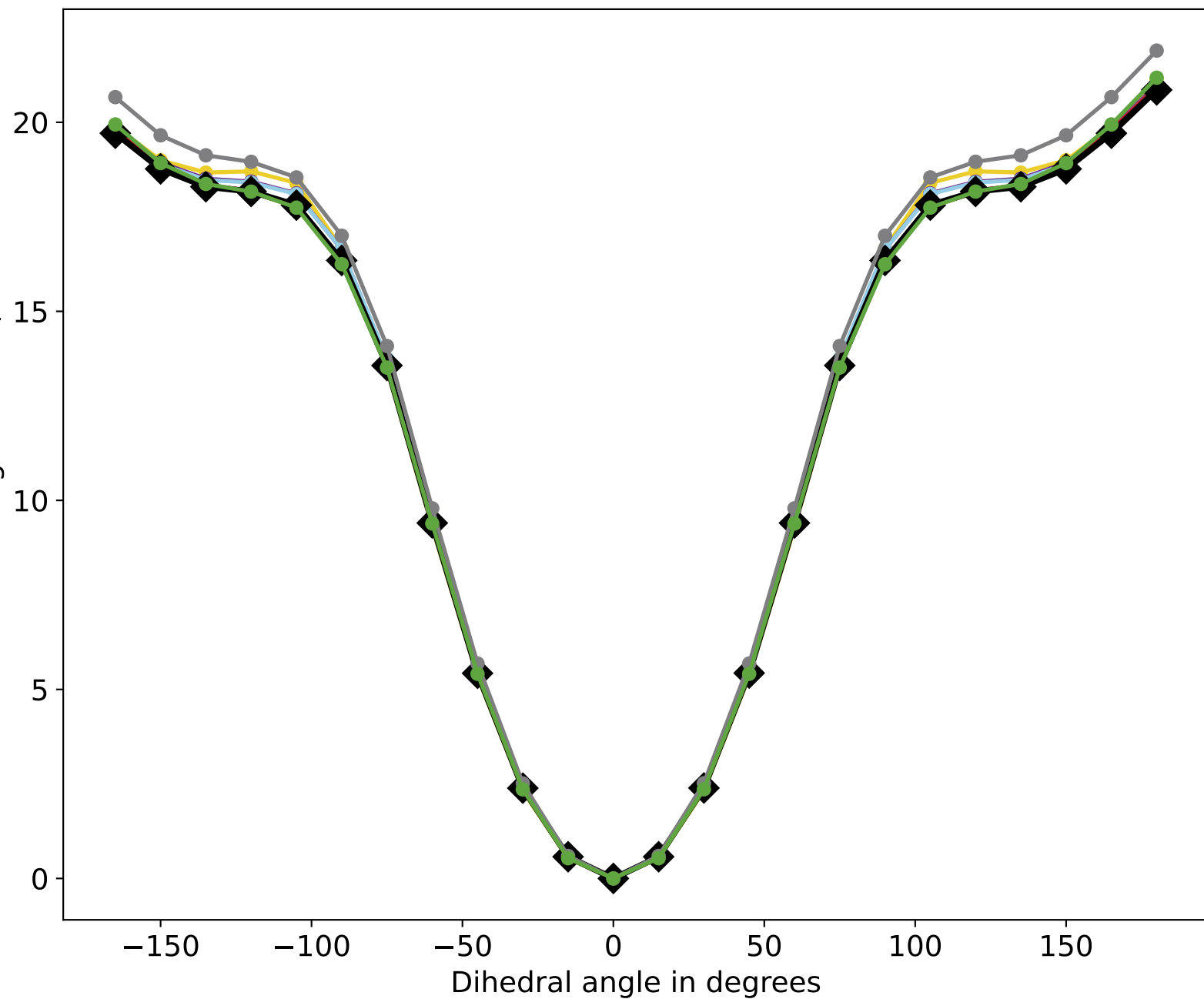
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



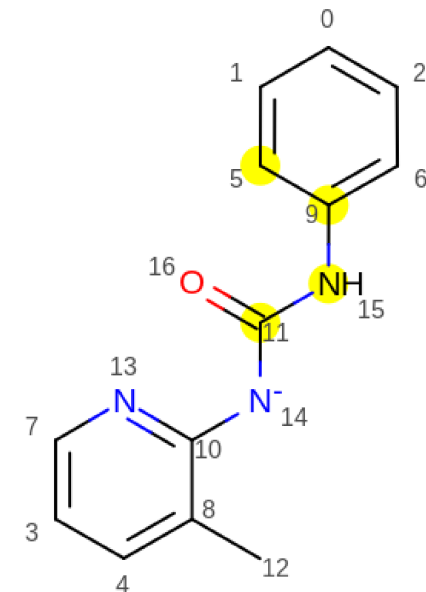
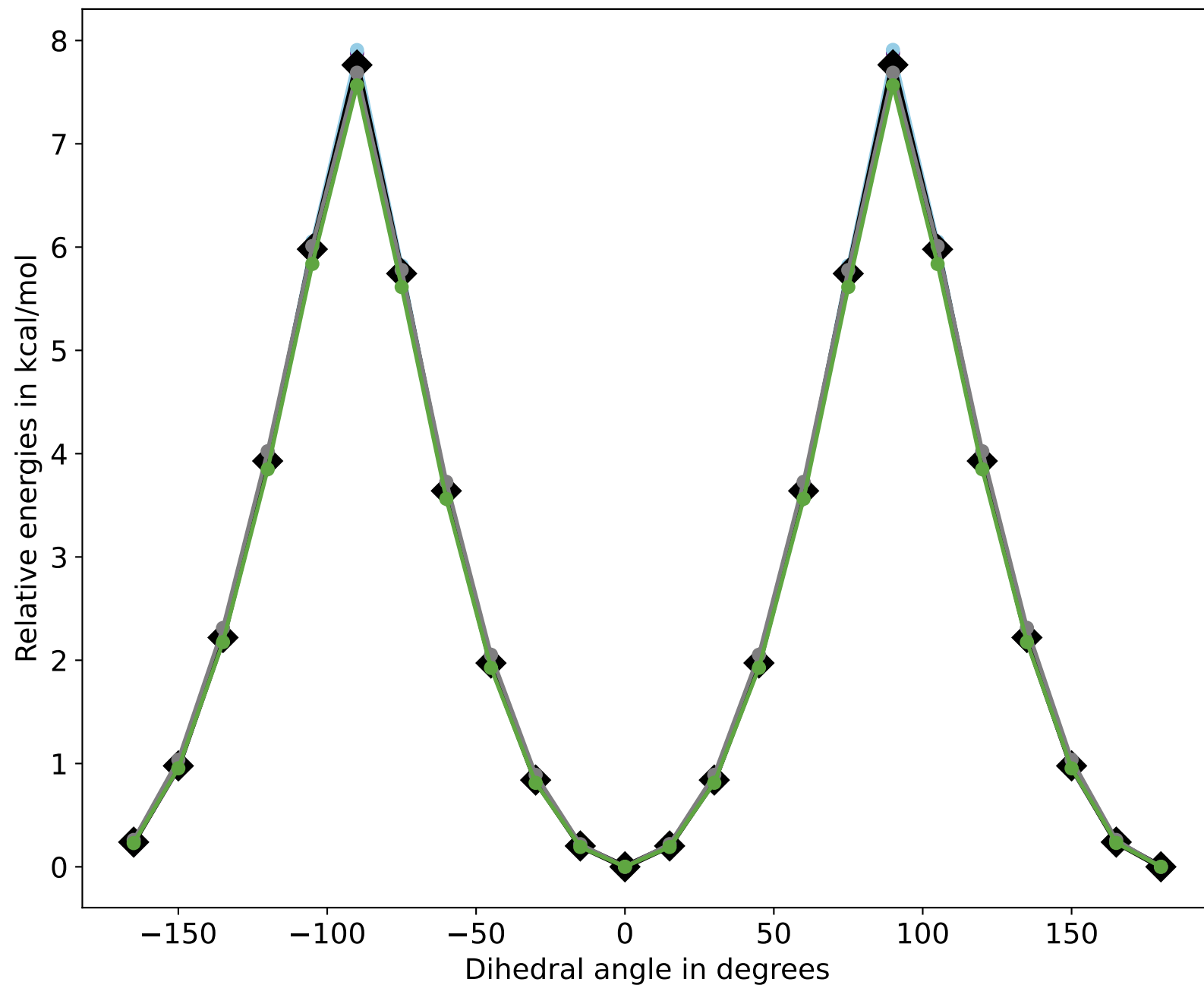
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

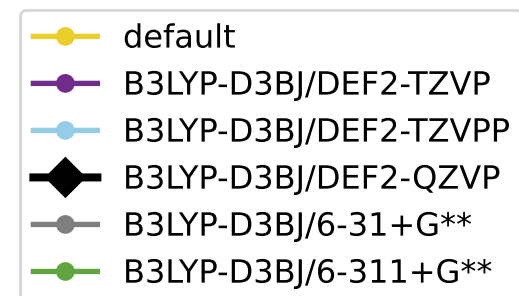
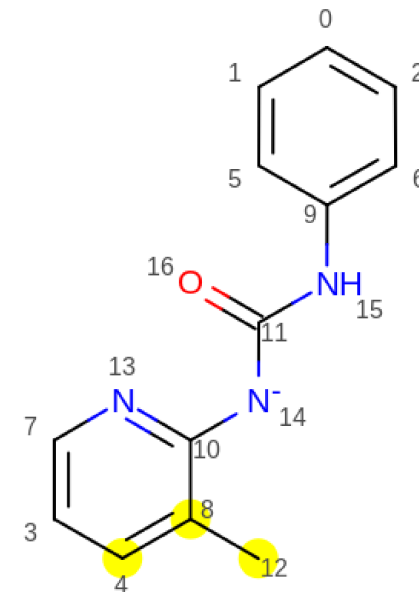
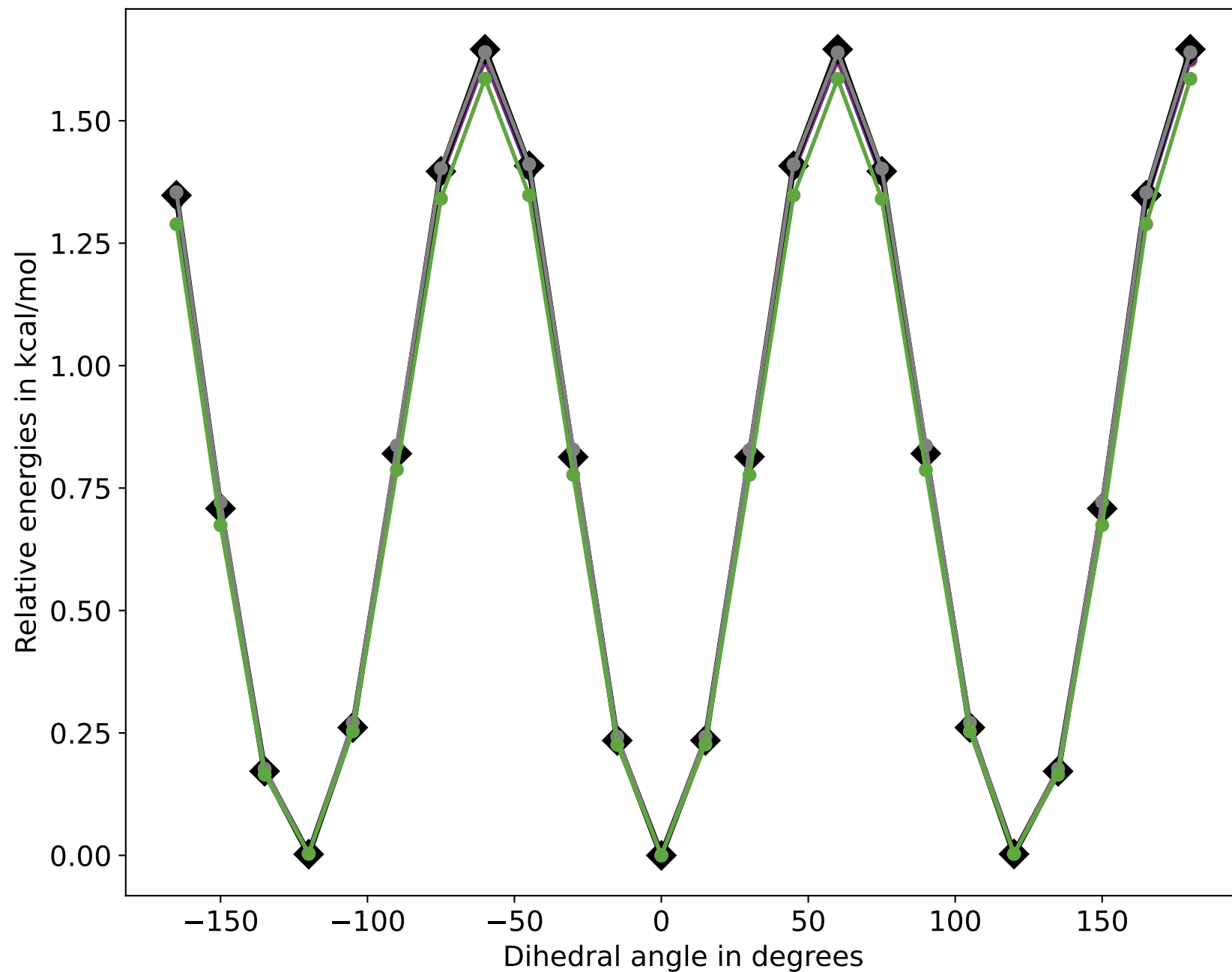


Relative energies in kcal/mol



- default
- 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**



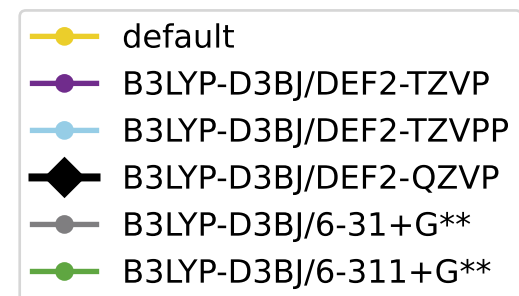
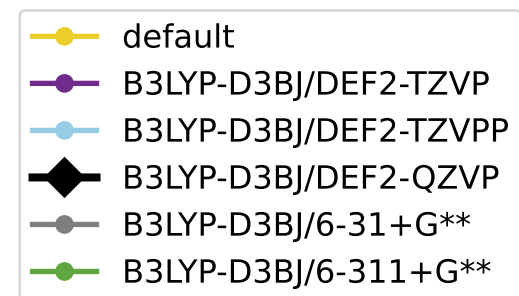


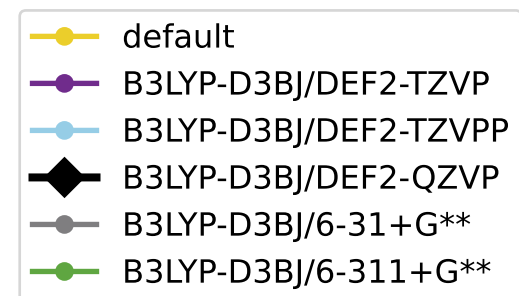
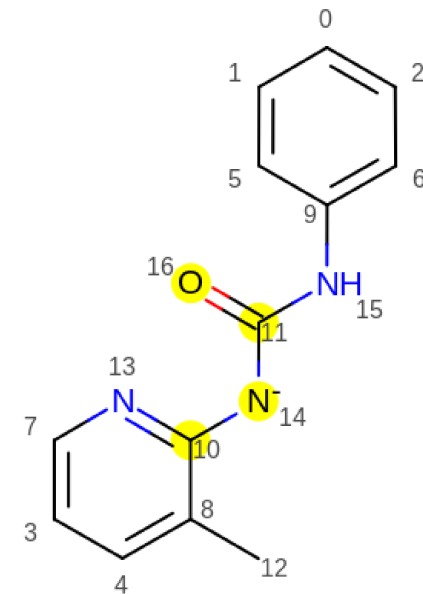
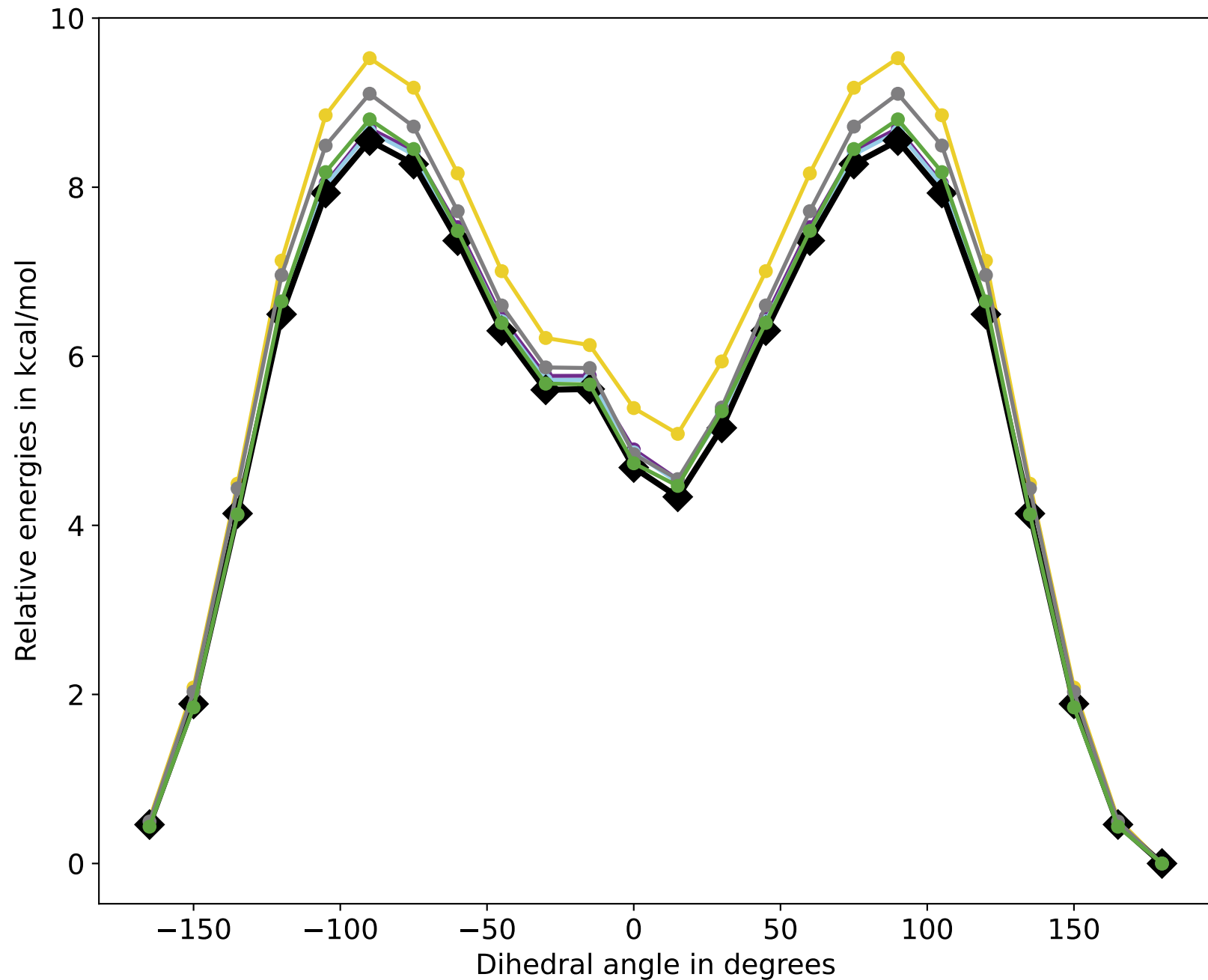
Relative energies in kcal/mol

10
8
6
4
2
0

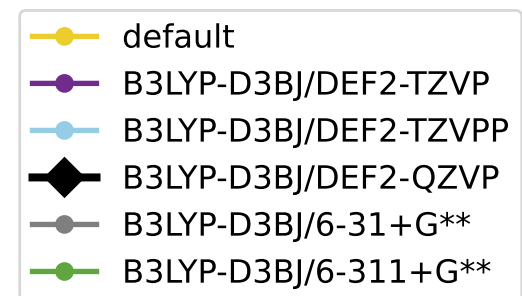
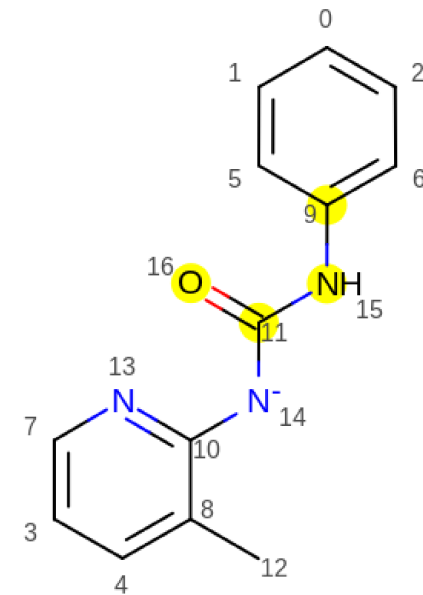
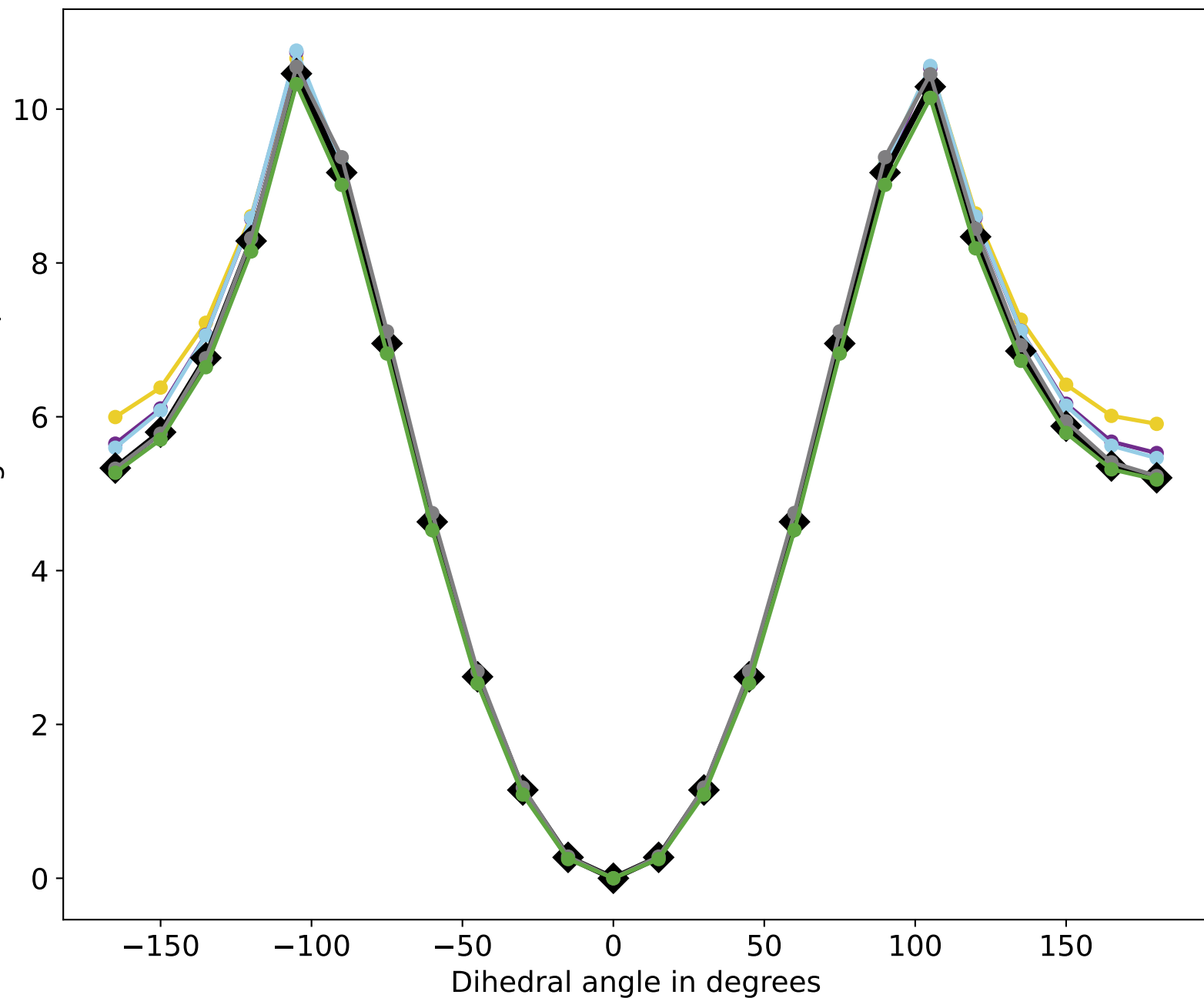
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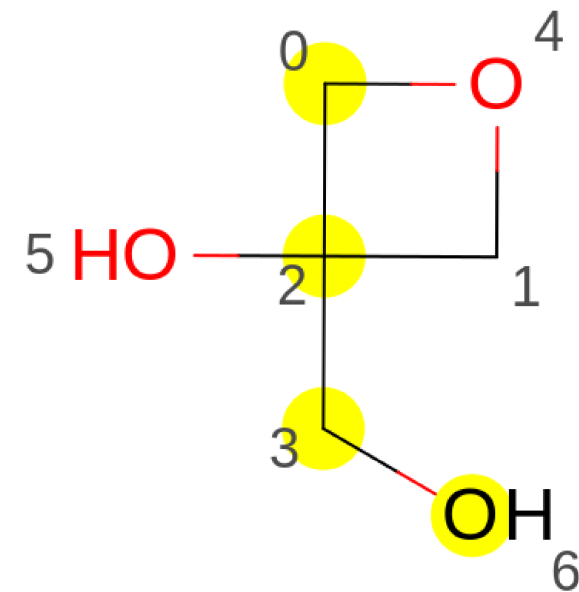
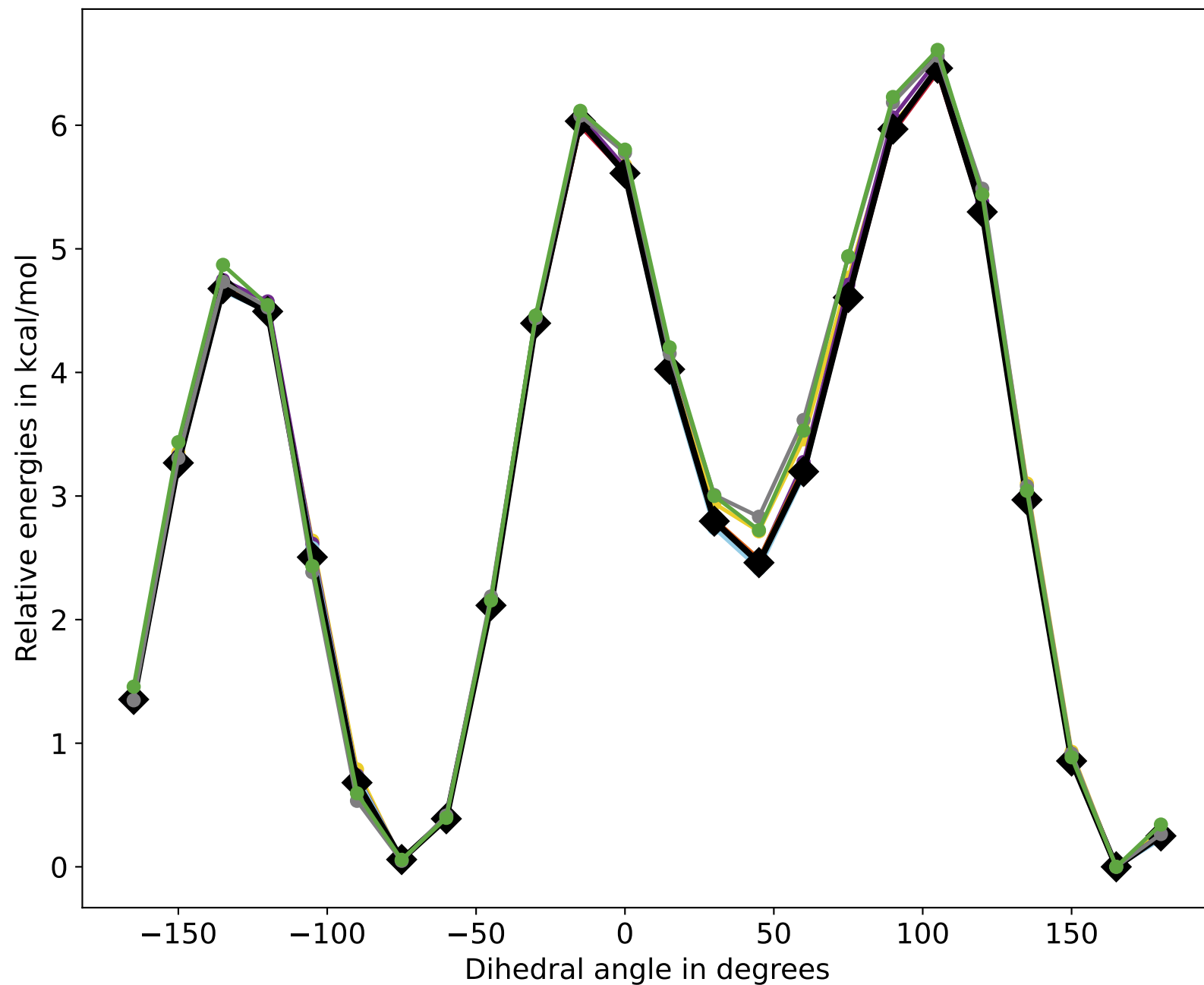
Dihedral angle in degrees



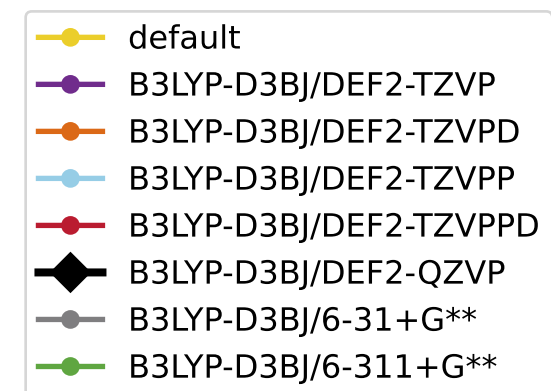
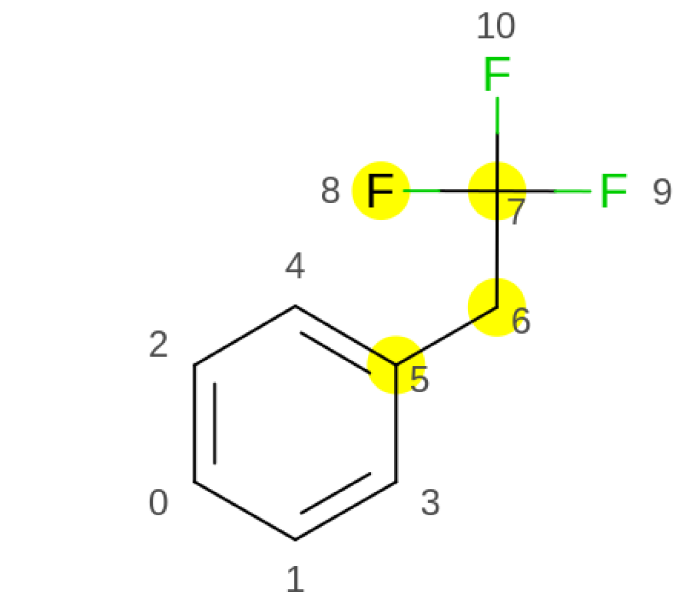
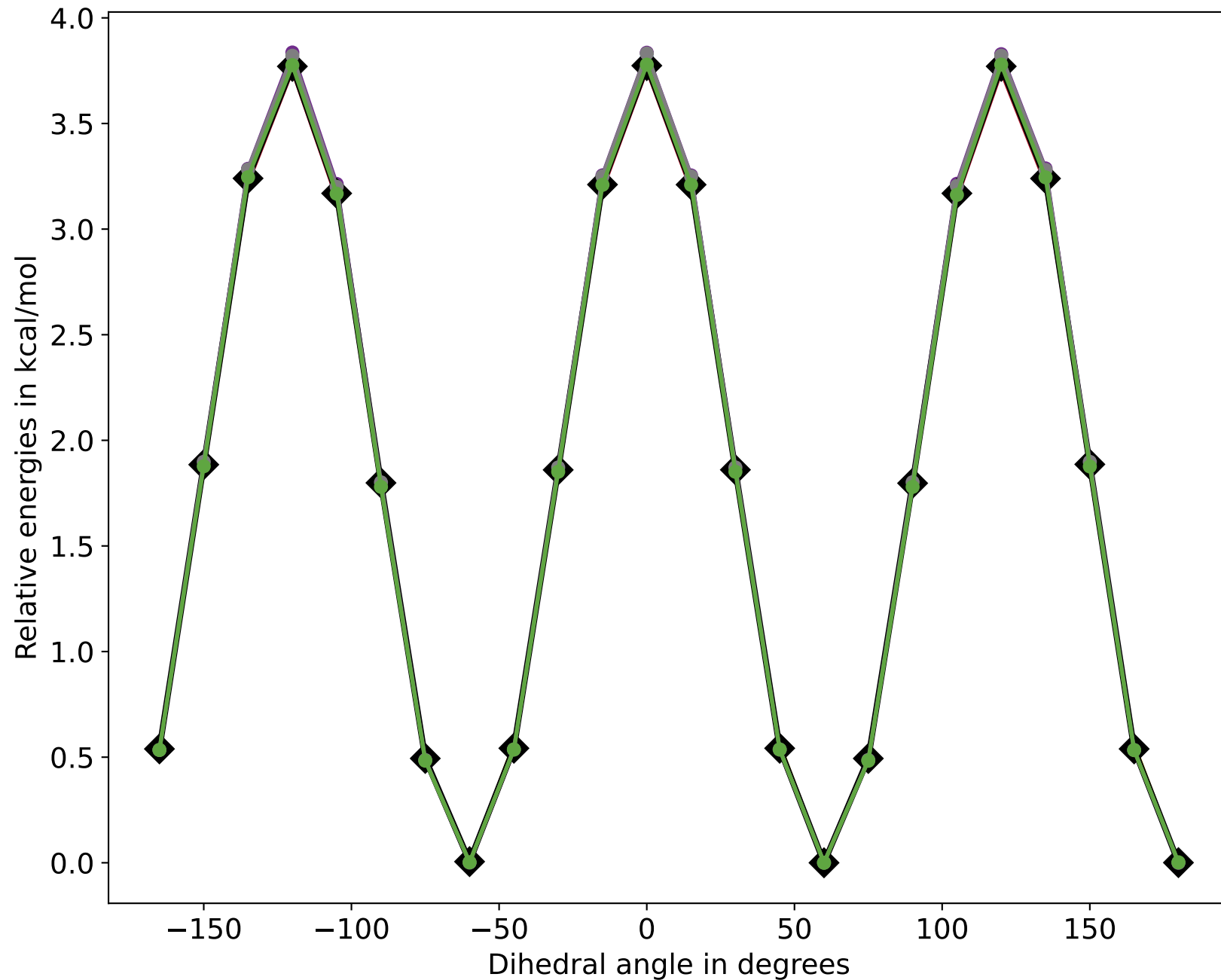


Relative energies in kcal/mol

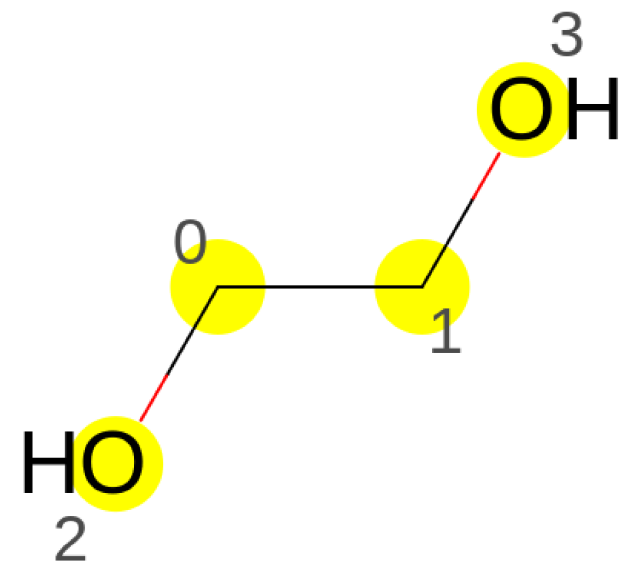
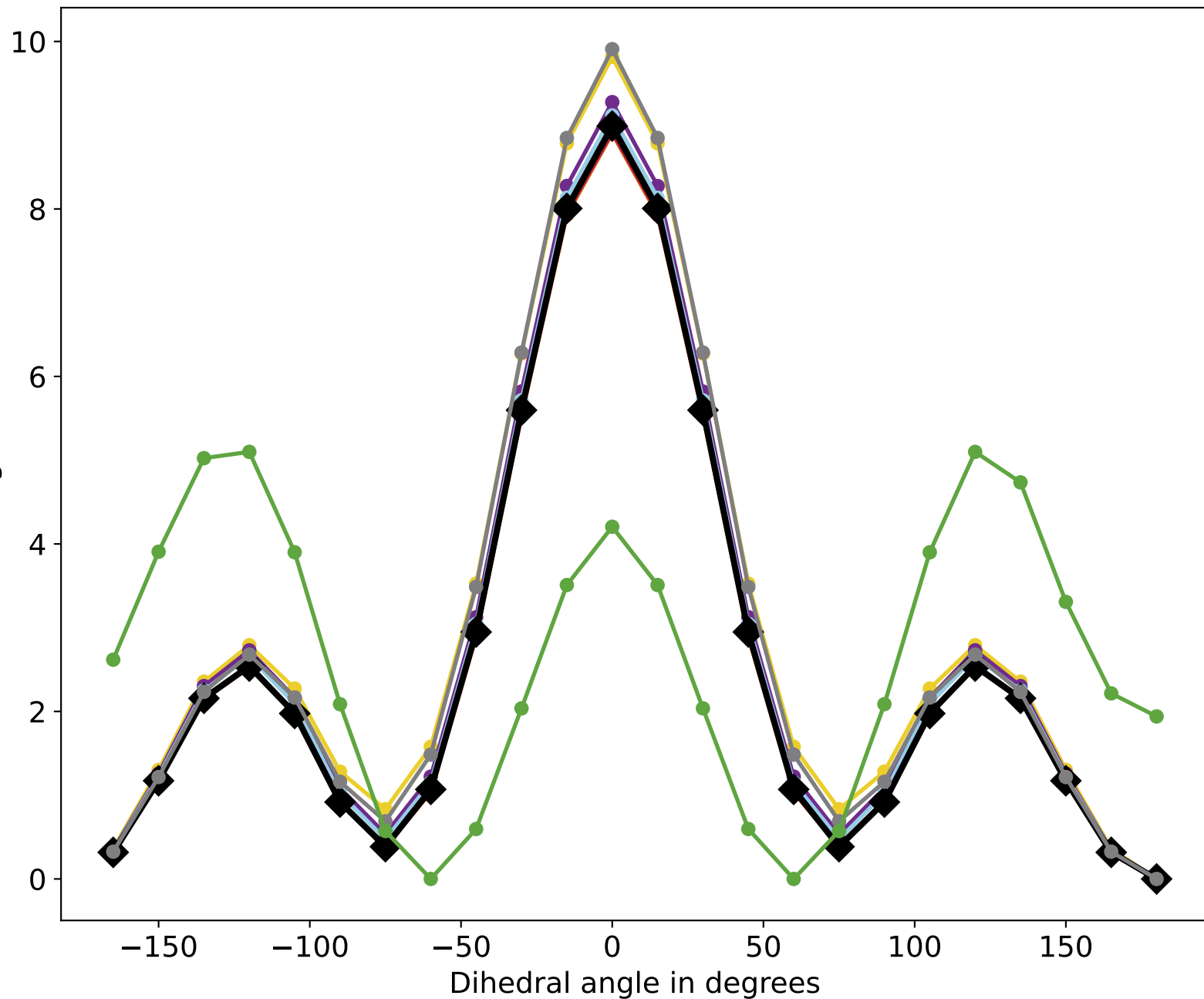




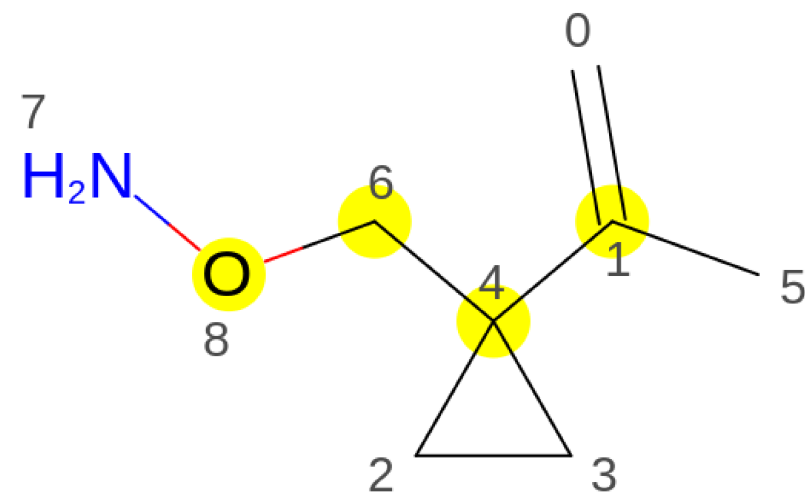
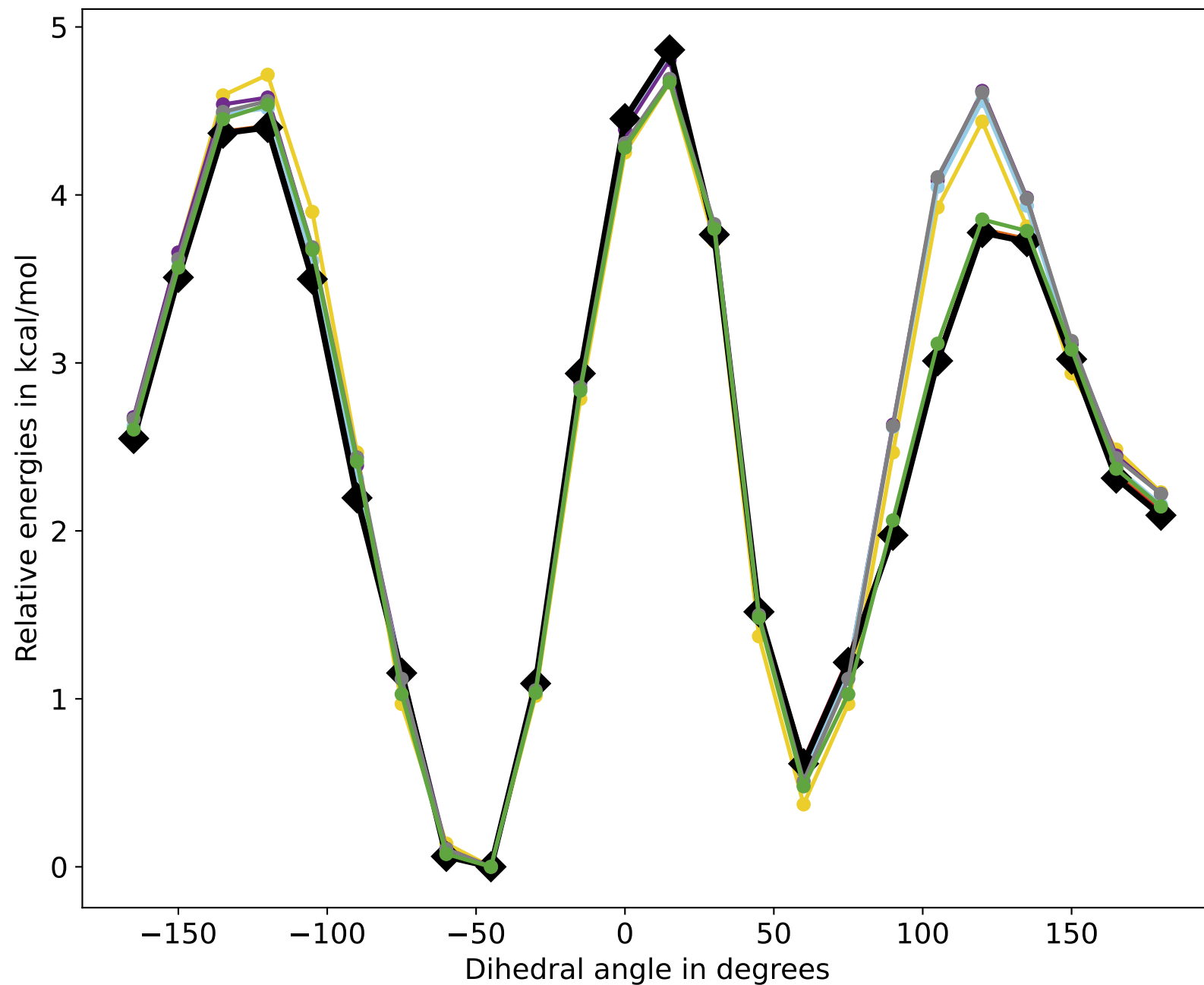
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



Relative energies in kcal/mol

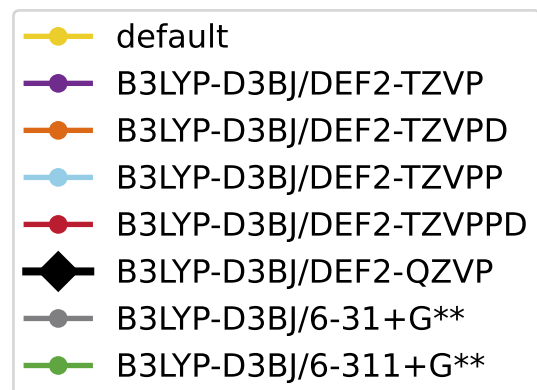
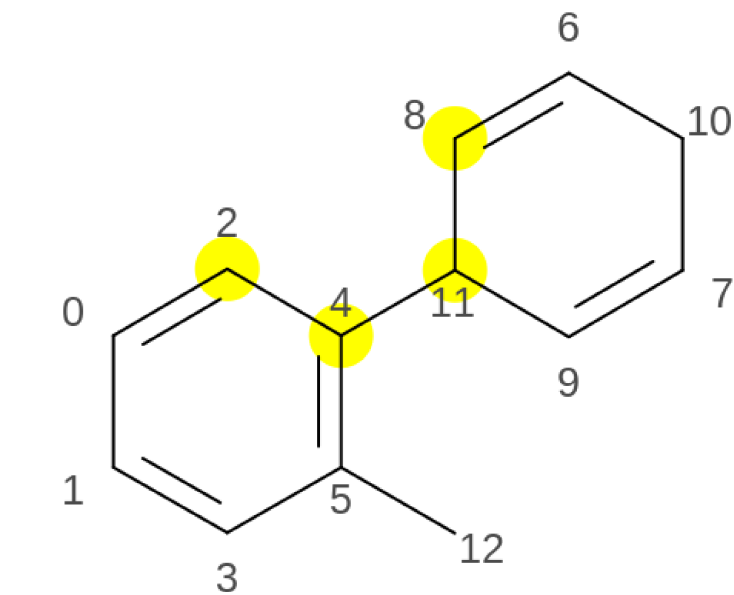
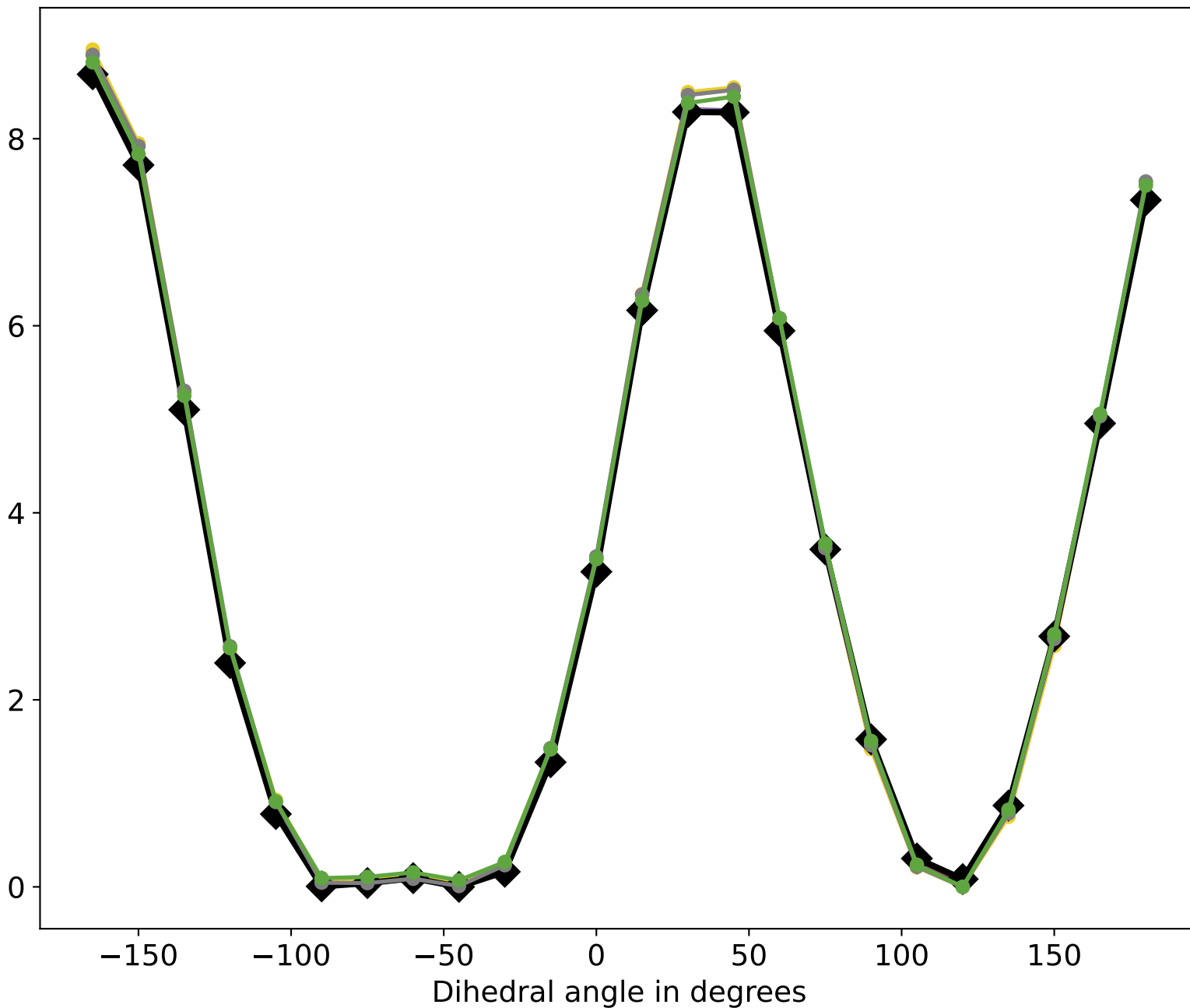


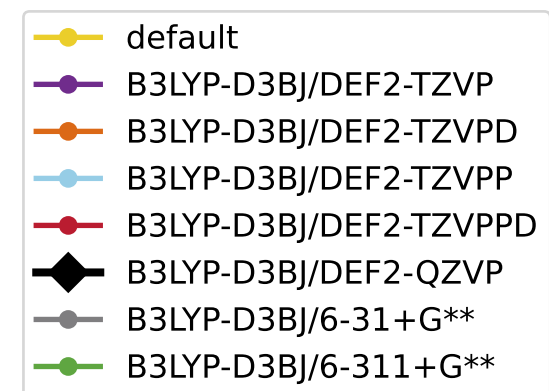
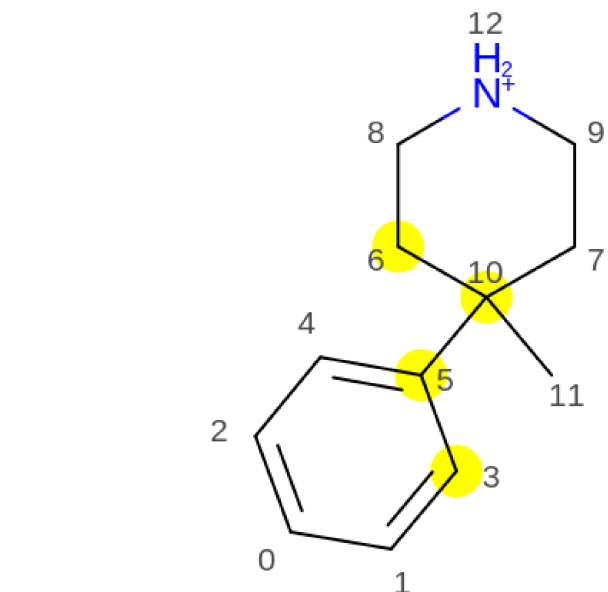
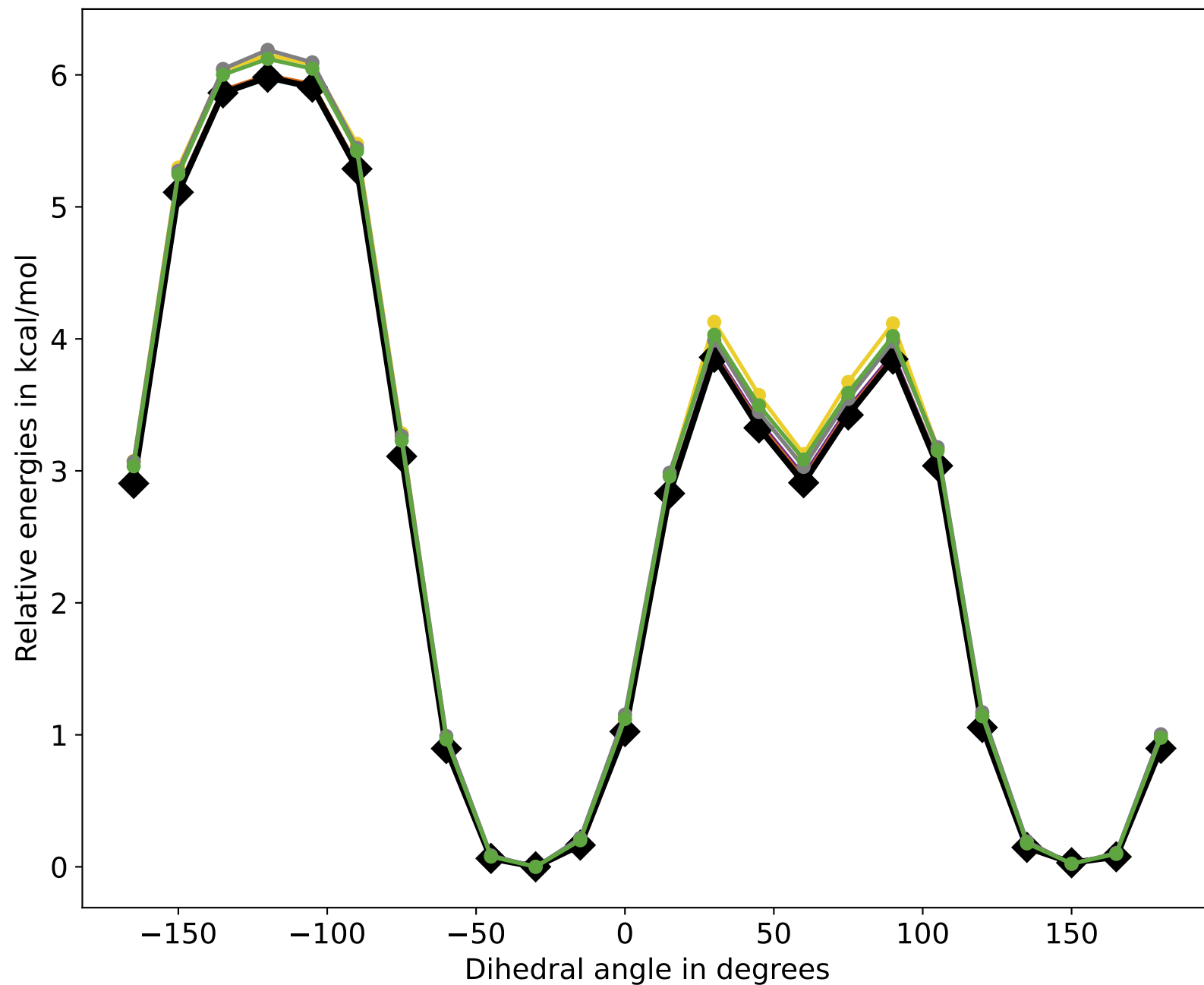
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

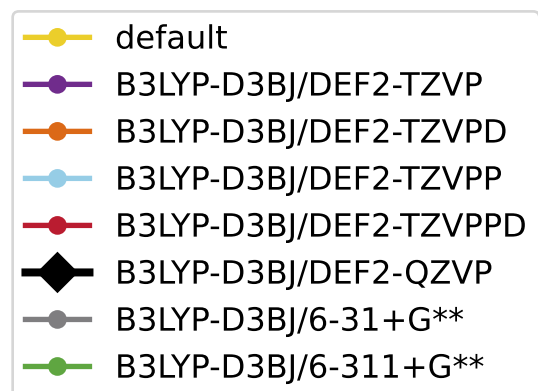
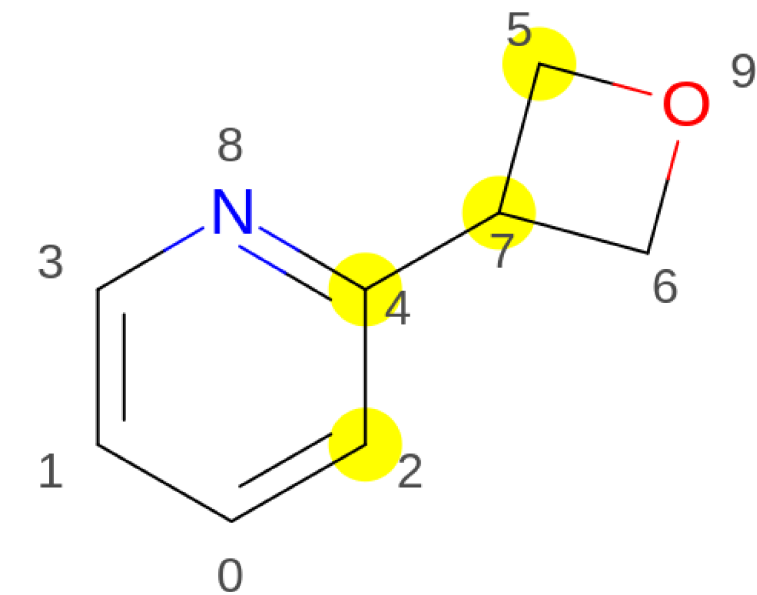
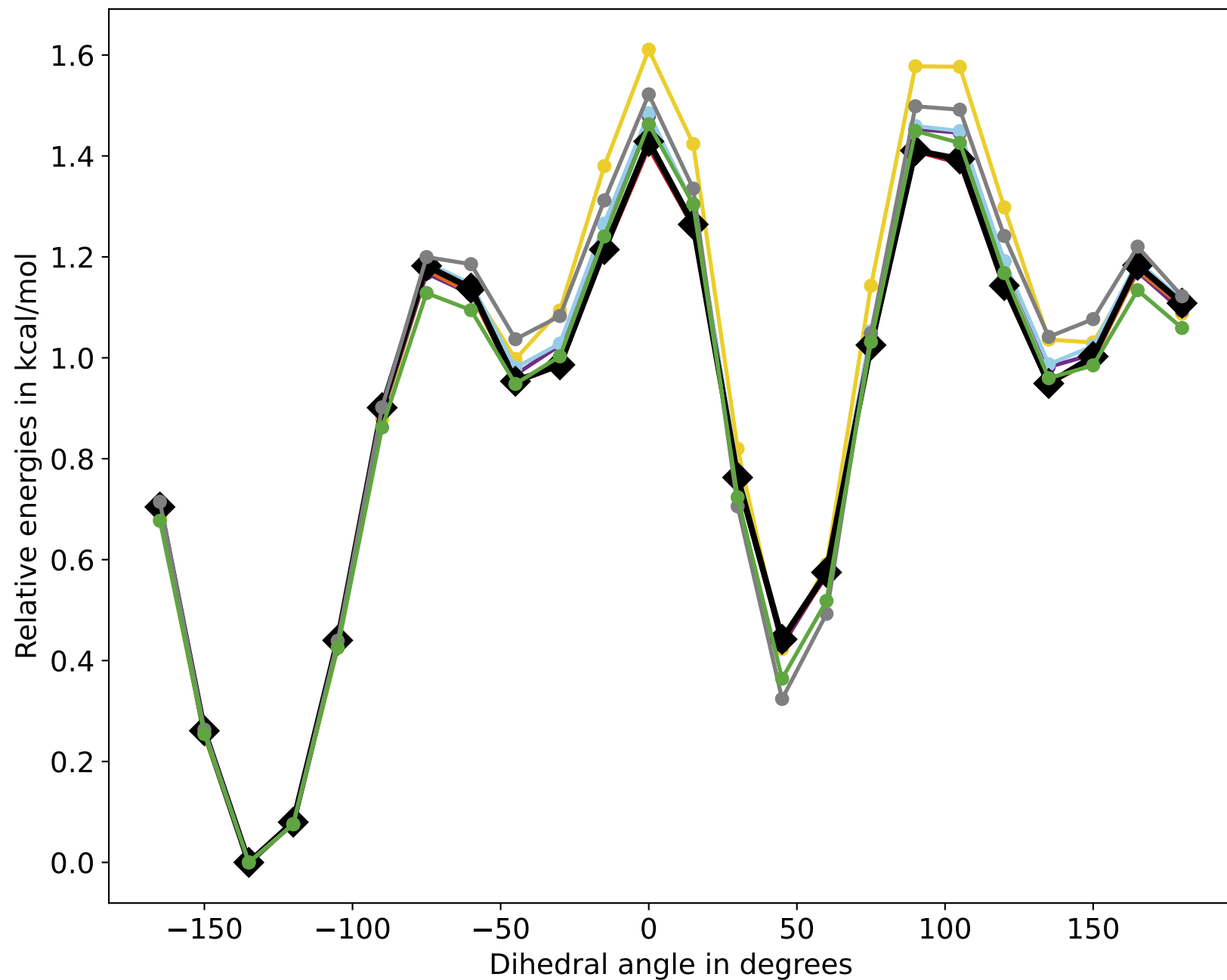


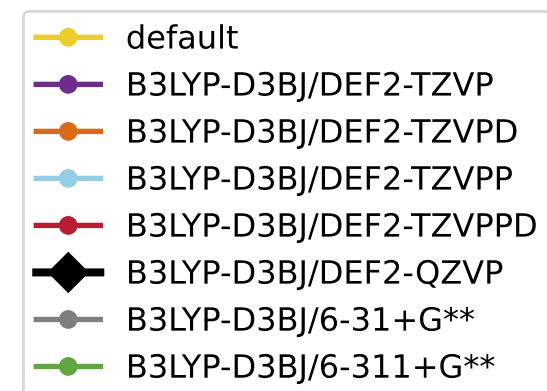
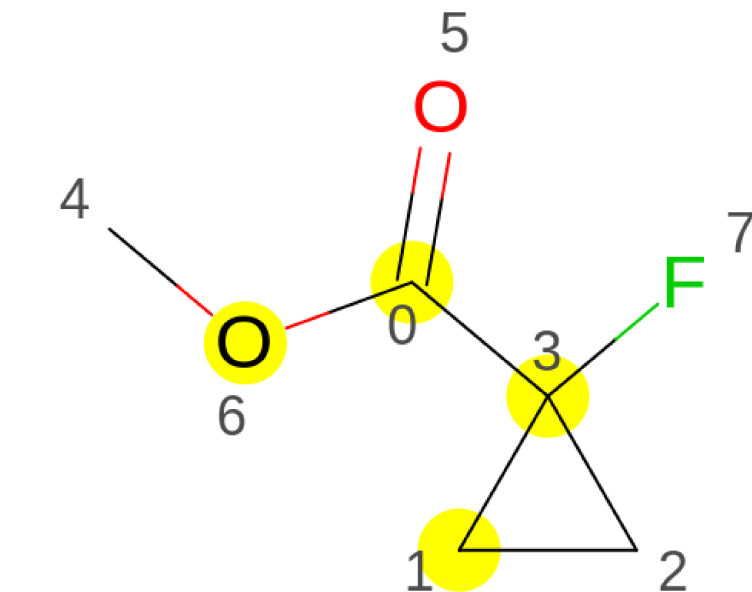
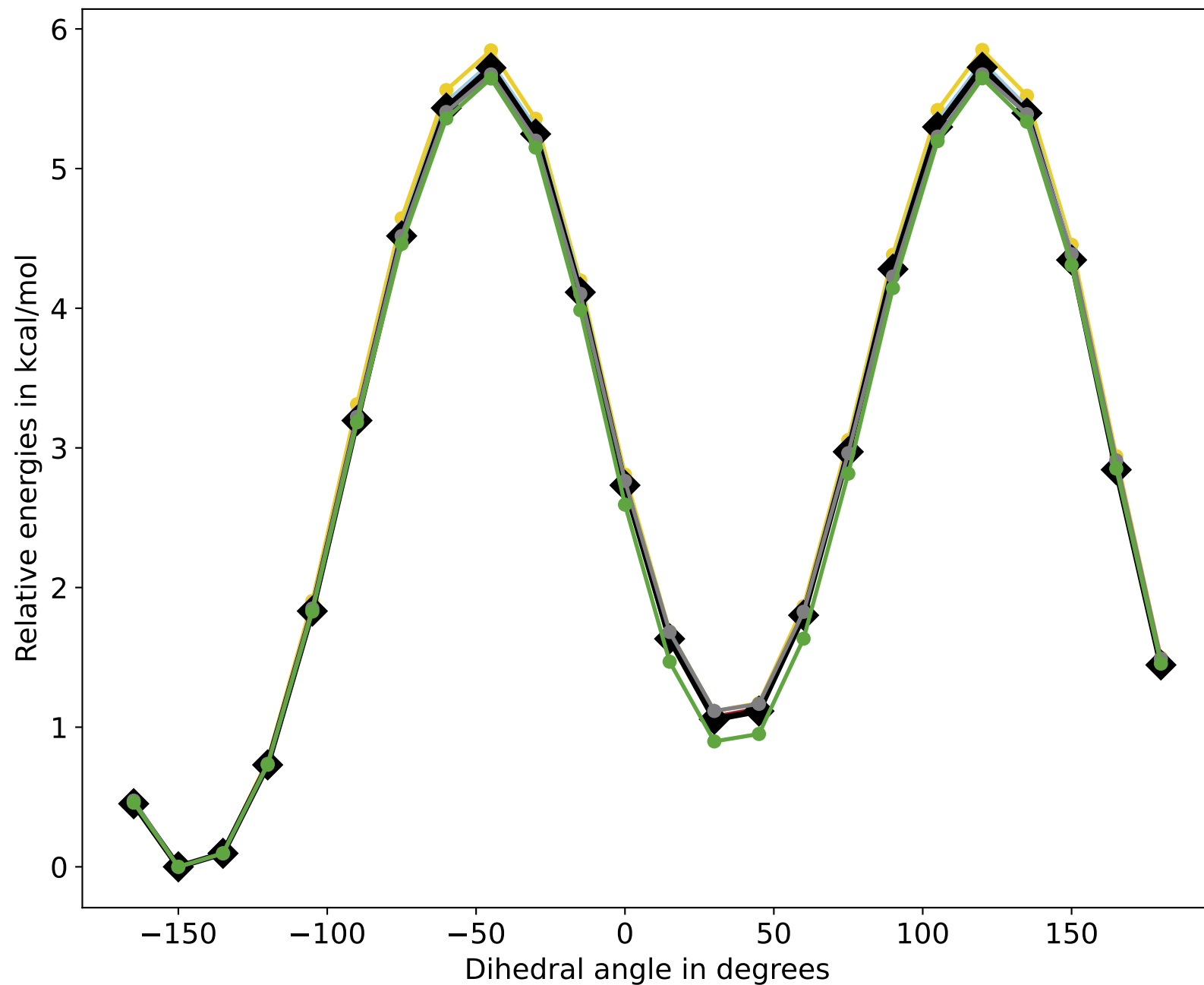
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

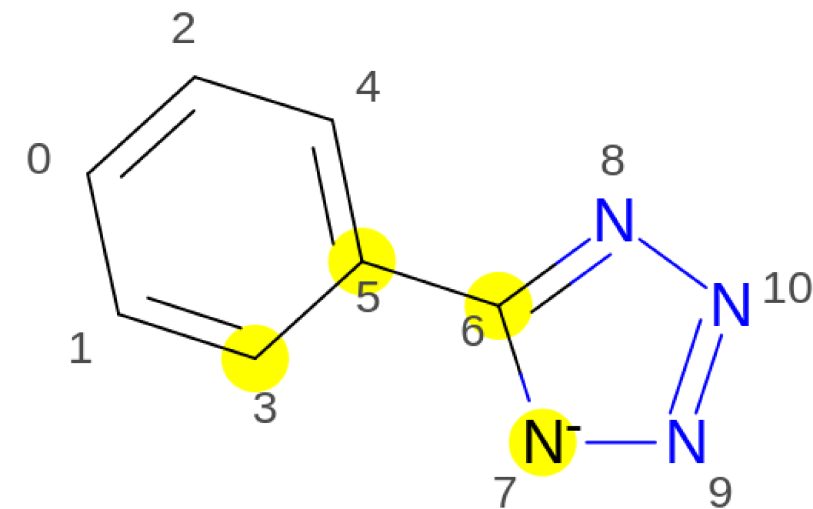
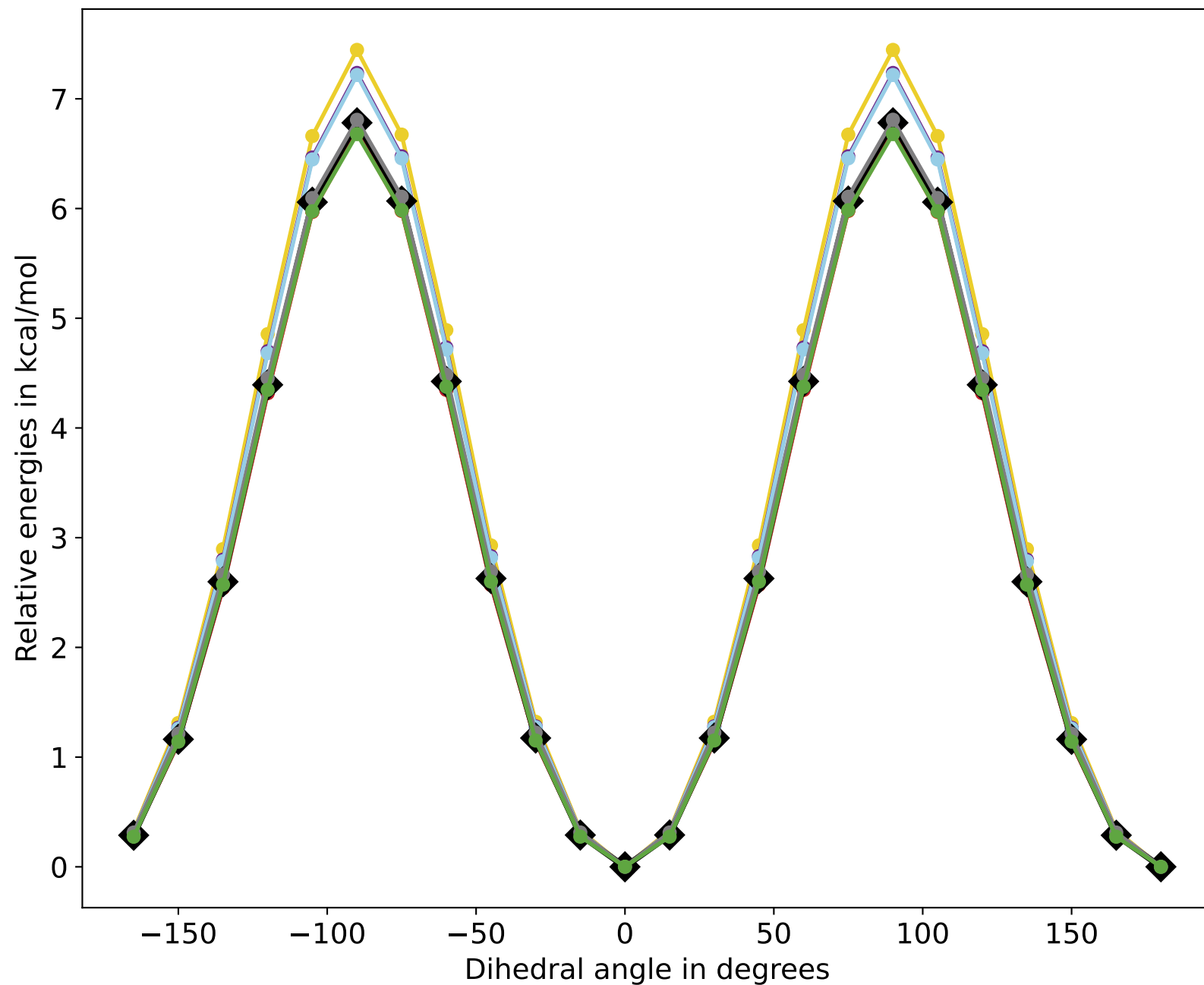
Relative energies in kcal/mol





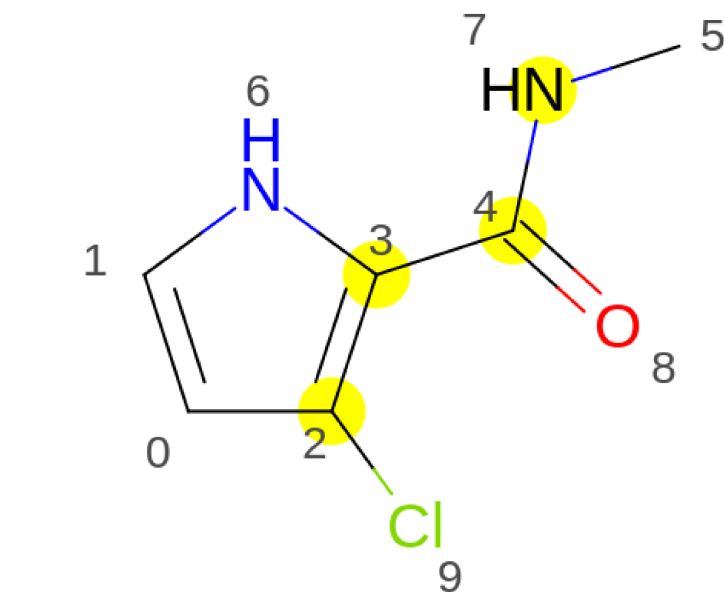
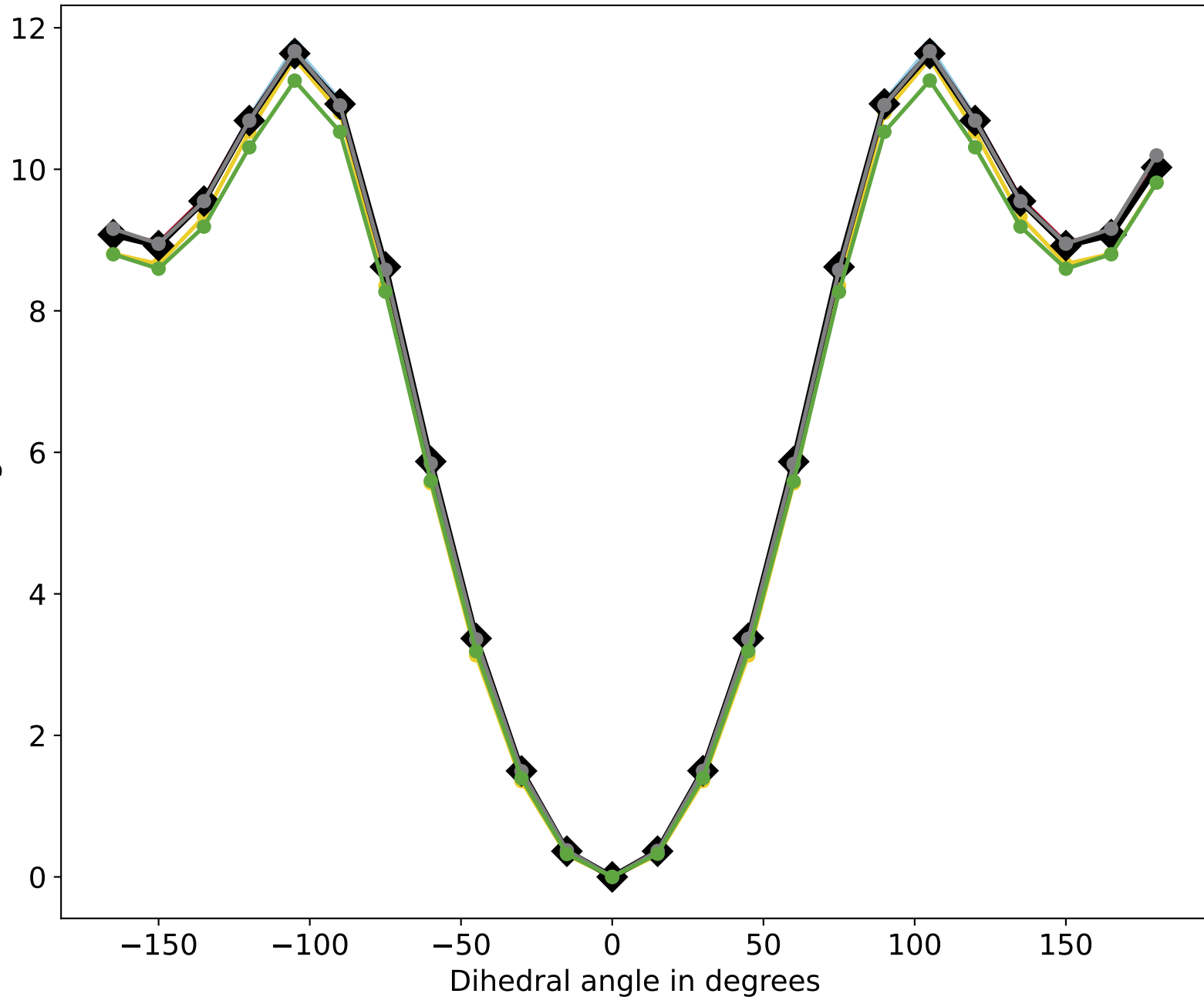






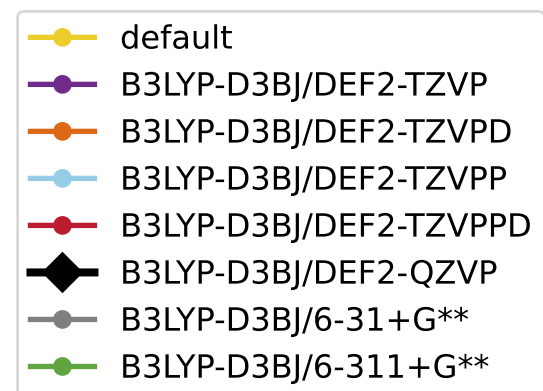
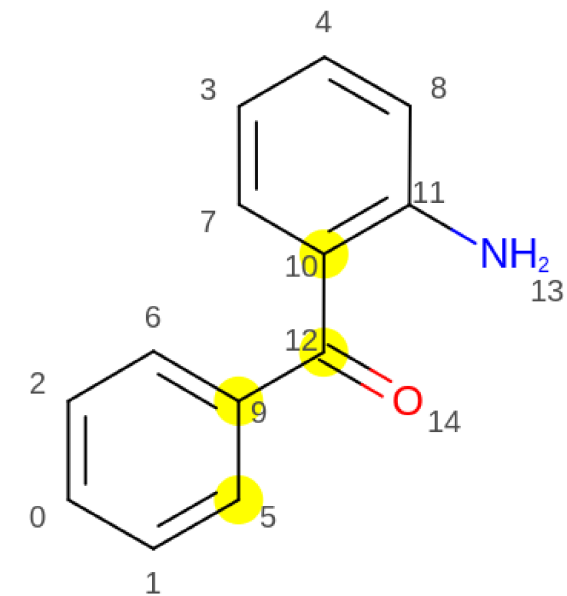
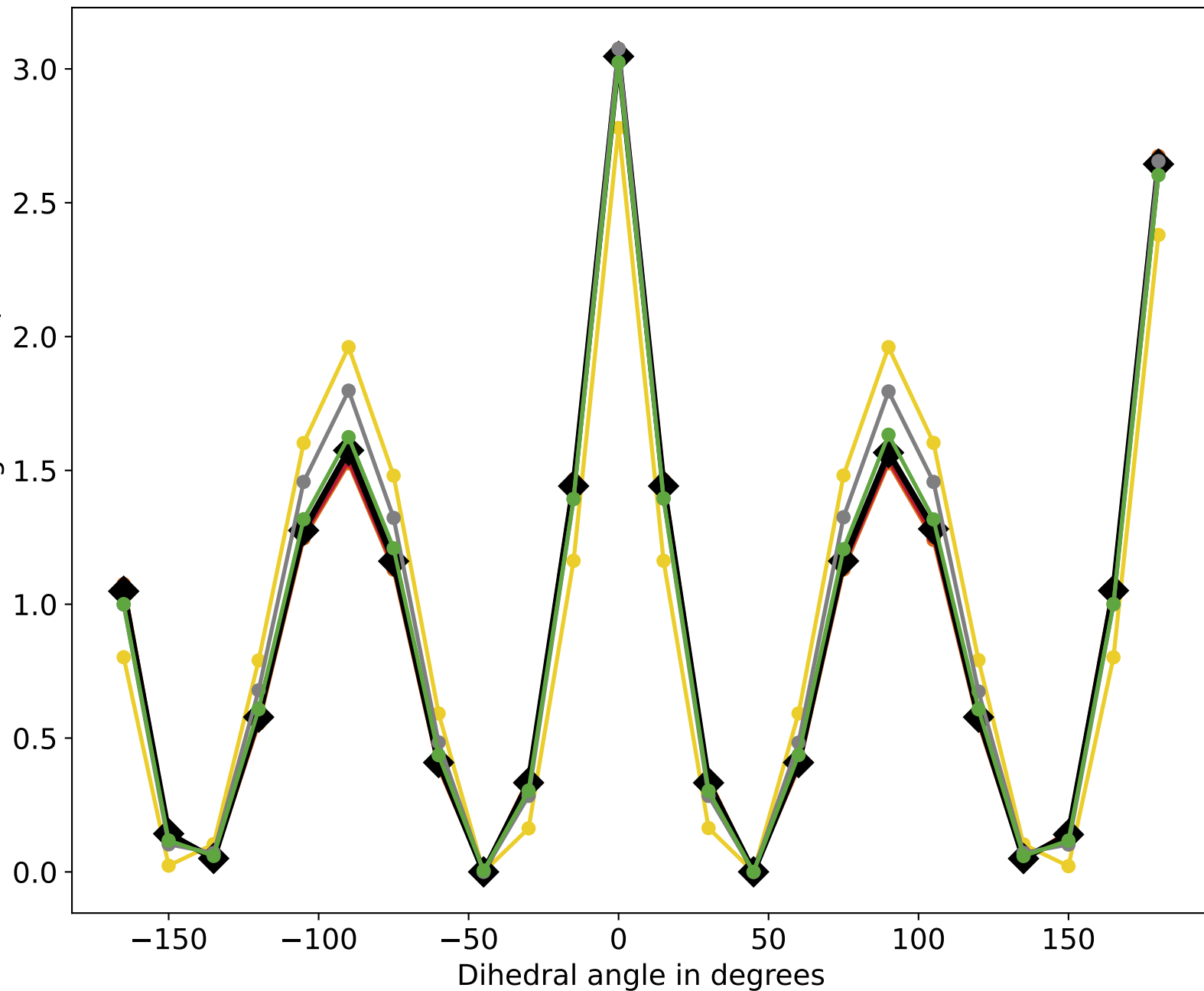
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

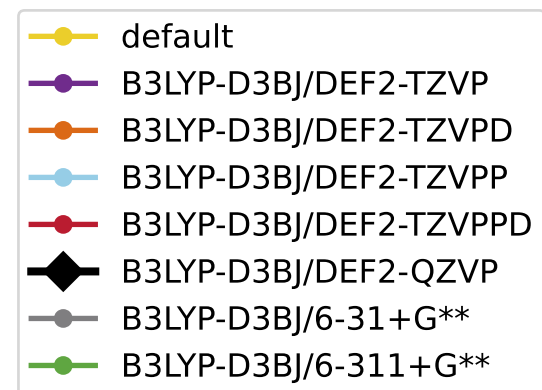
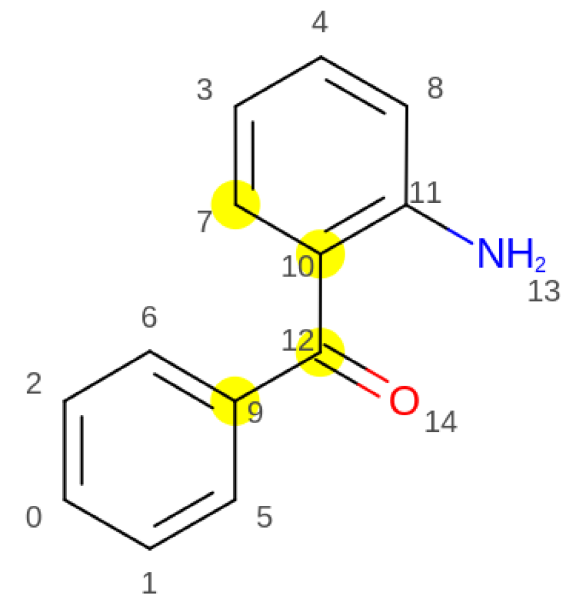
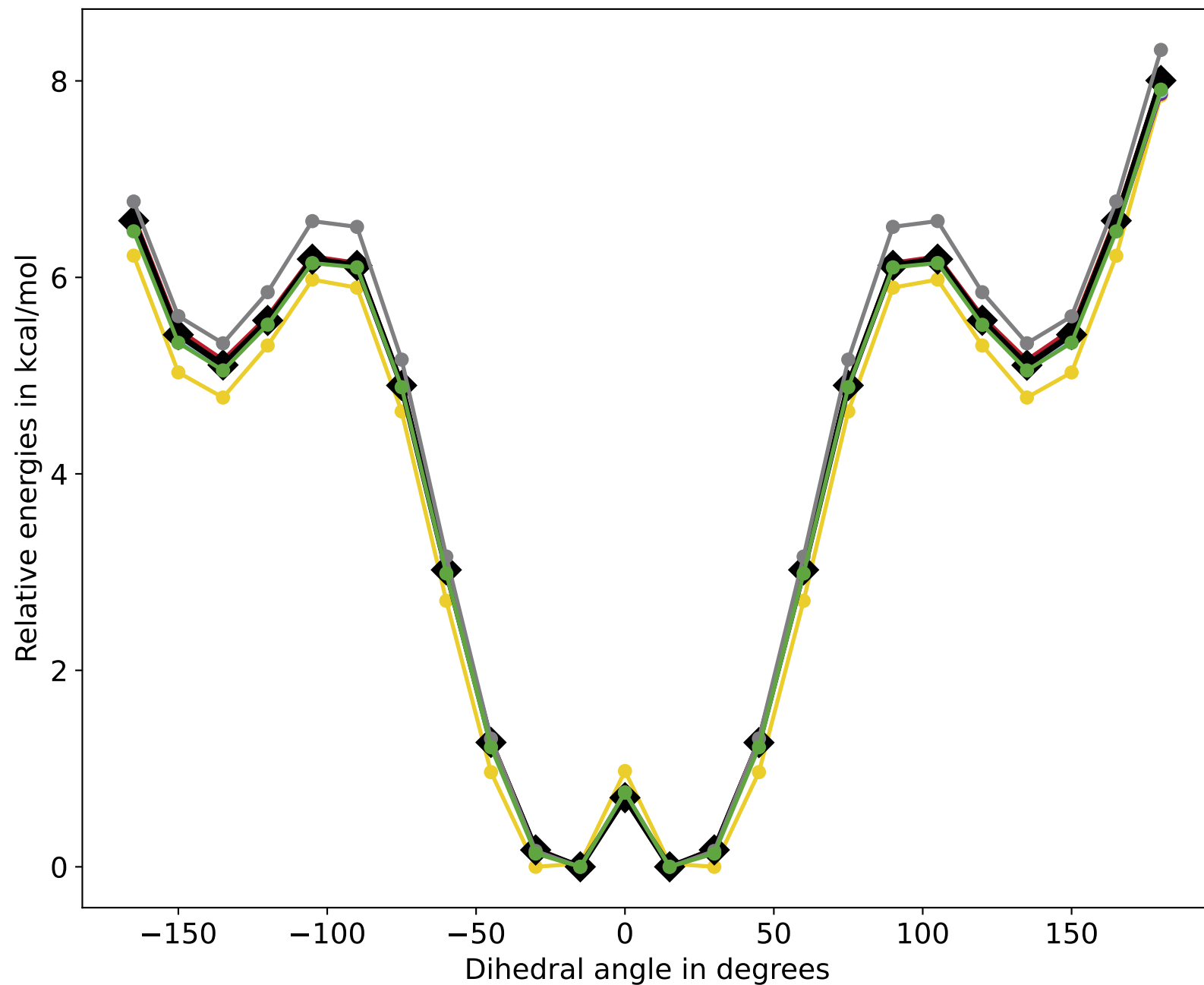
Relative energies in kcal/mol



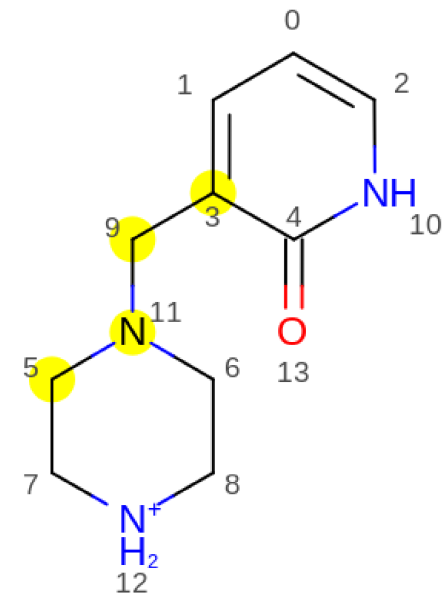
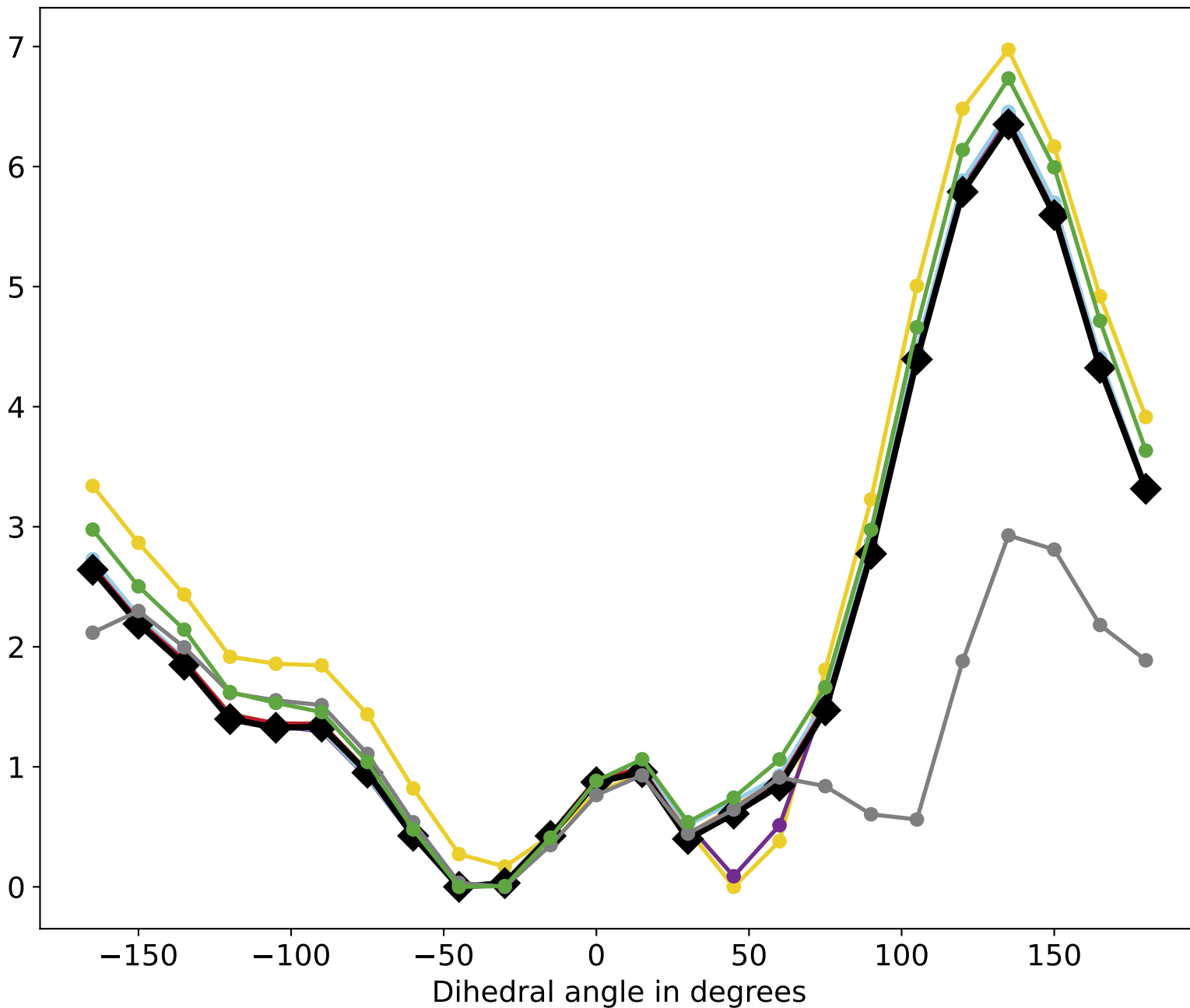
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



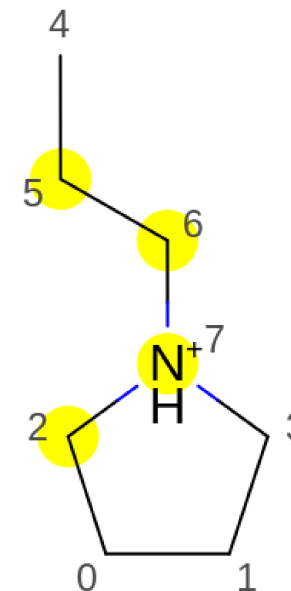
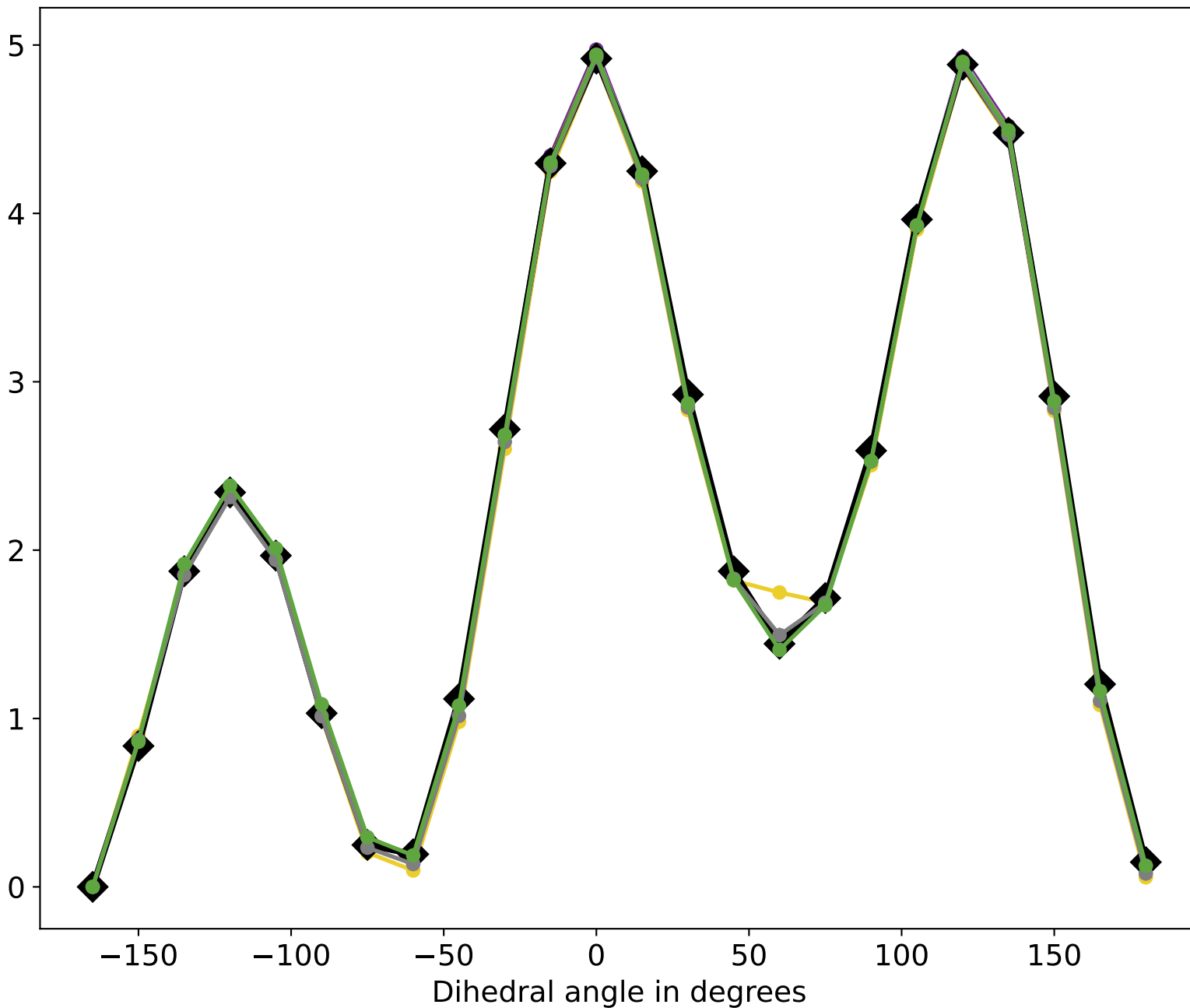


Relative energies in kcal/mol



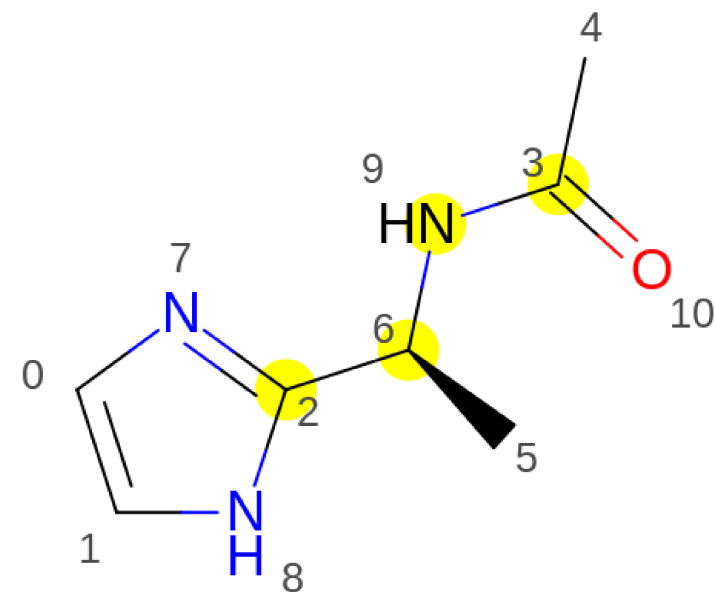
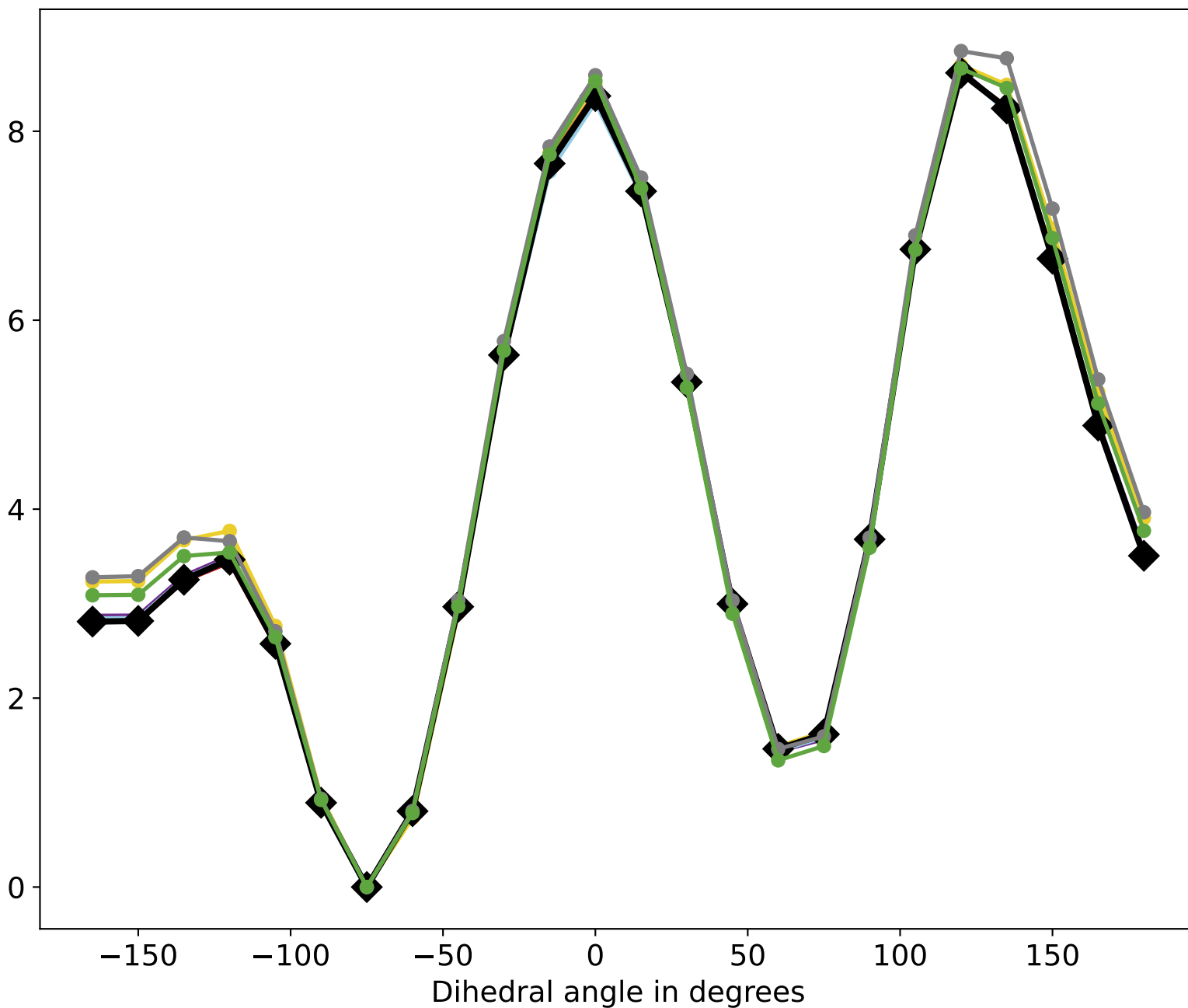
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



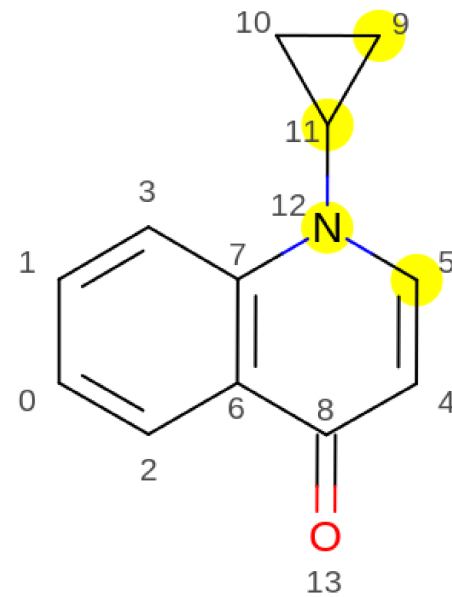
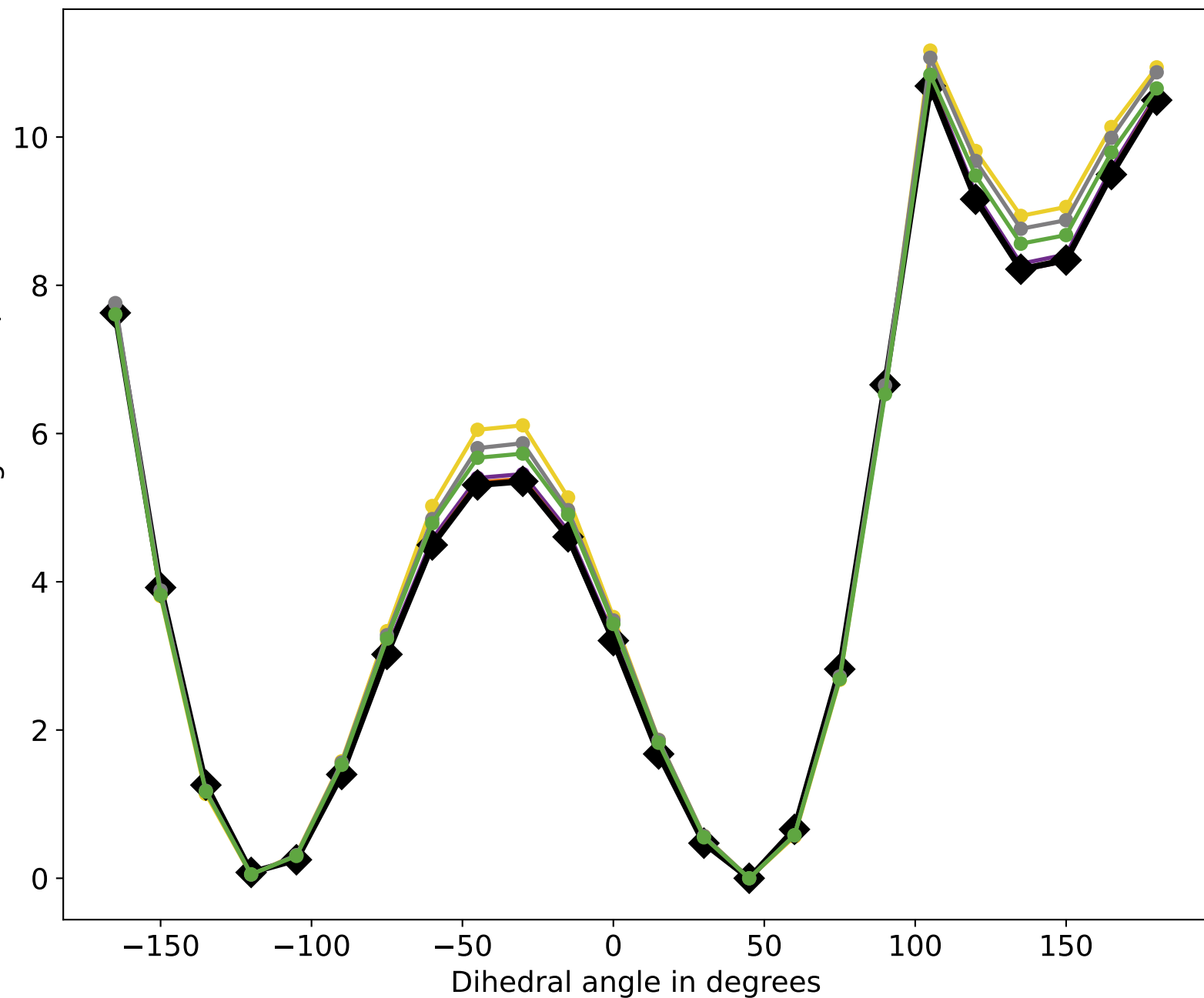
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol



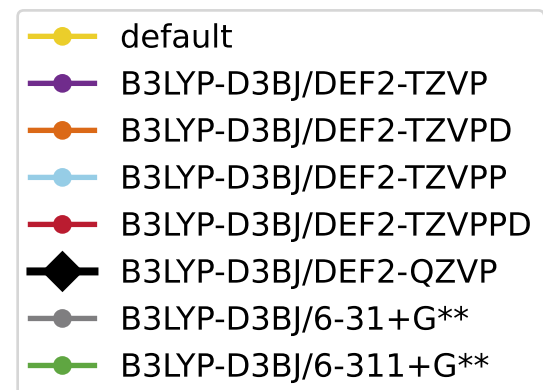
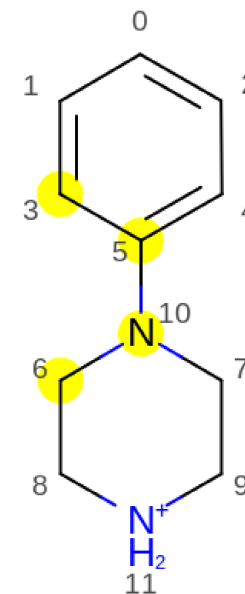
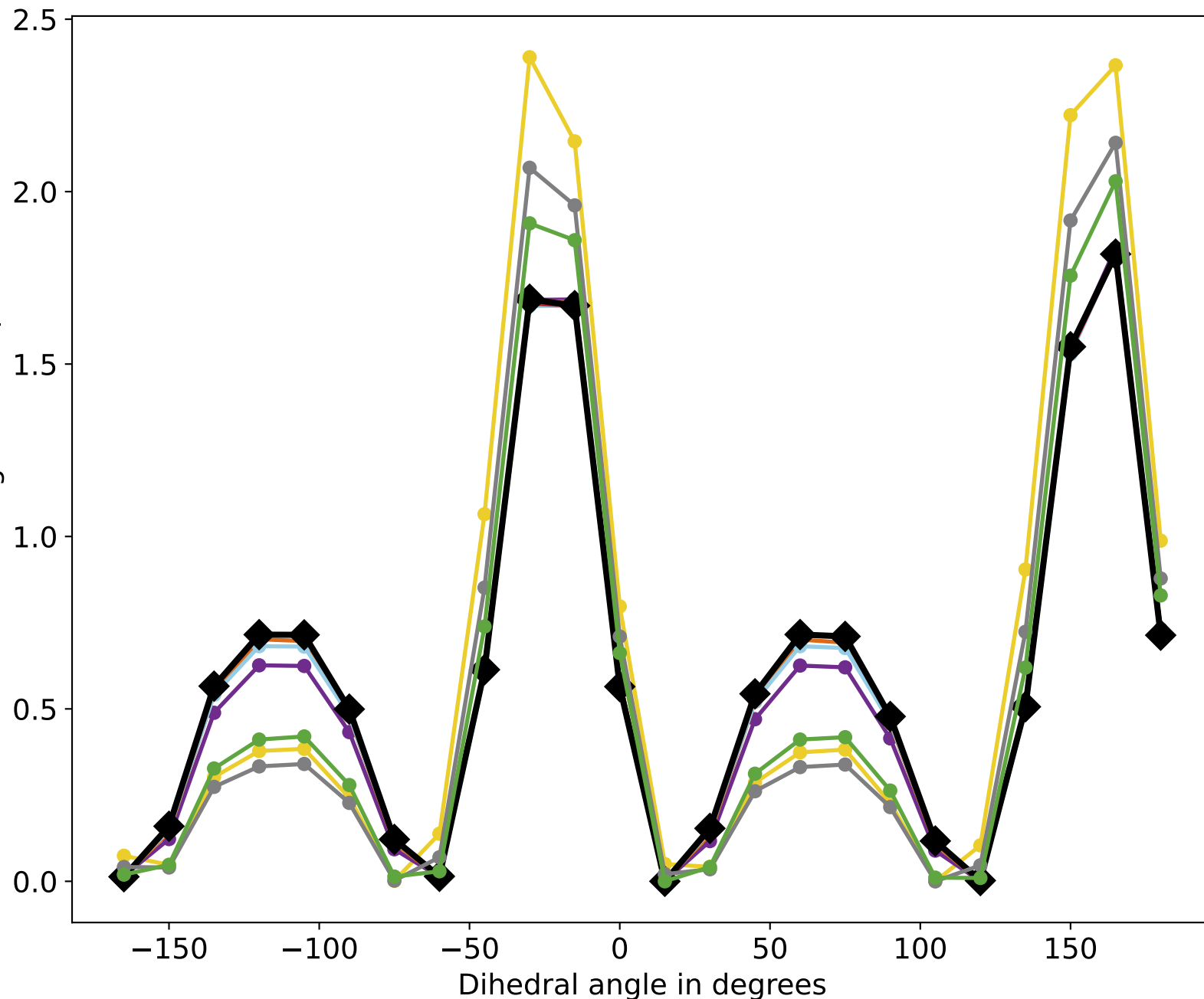
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

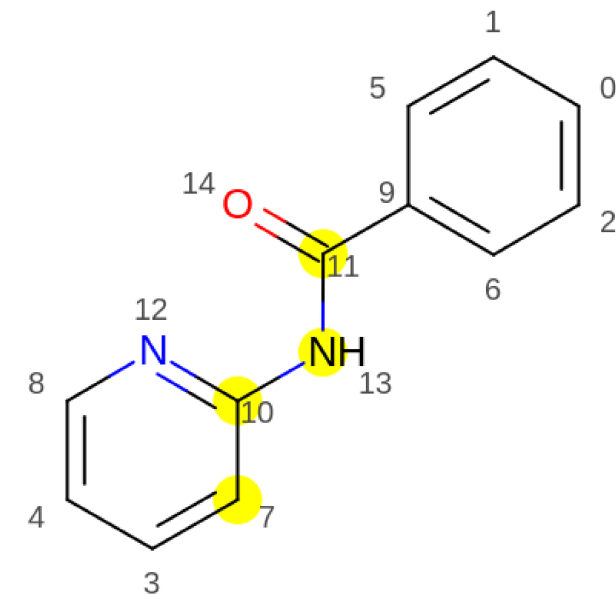
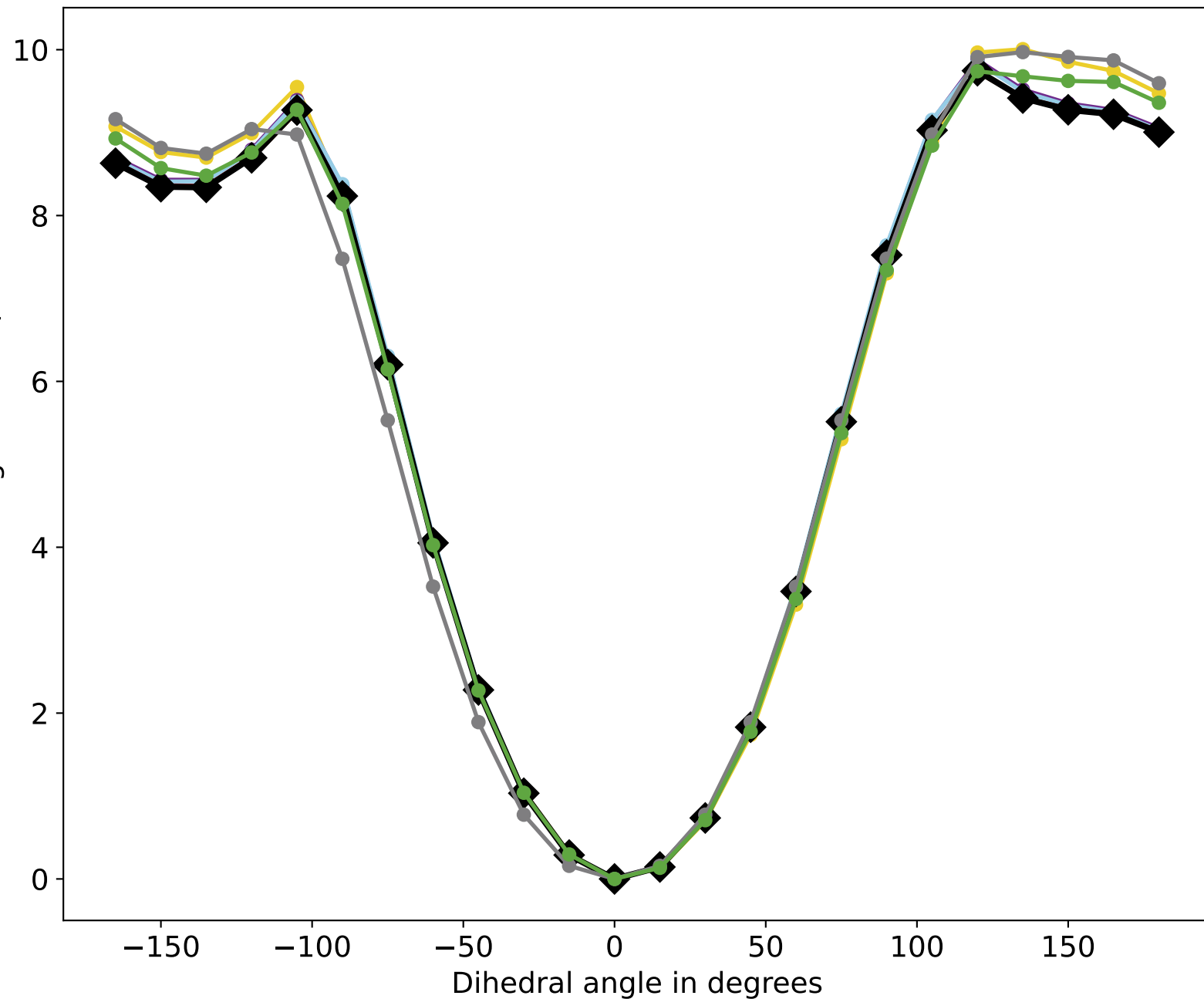


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

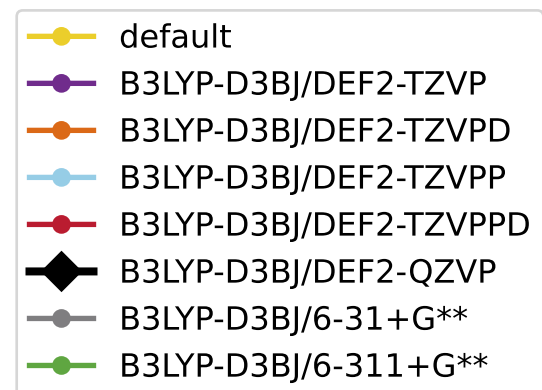
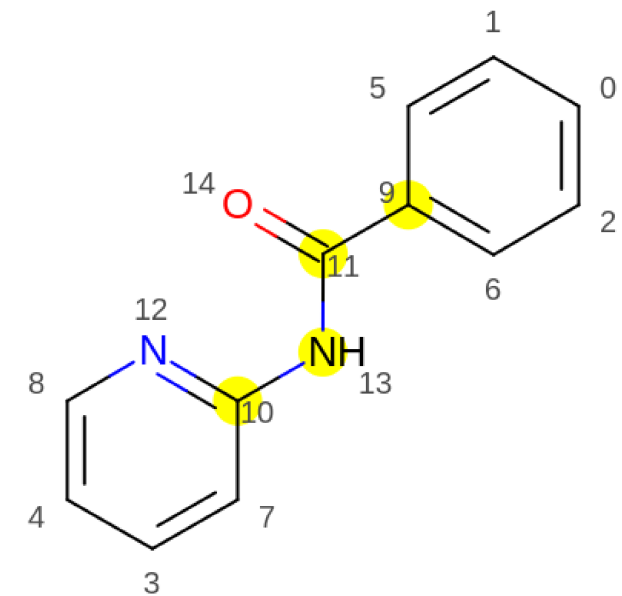
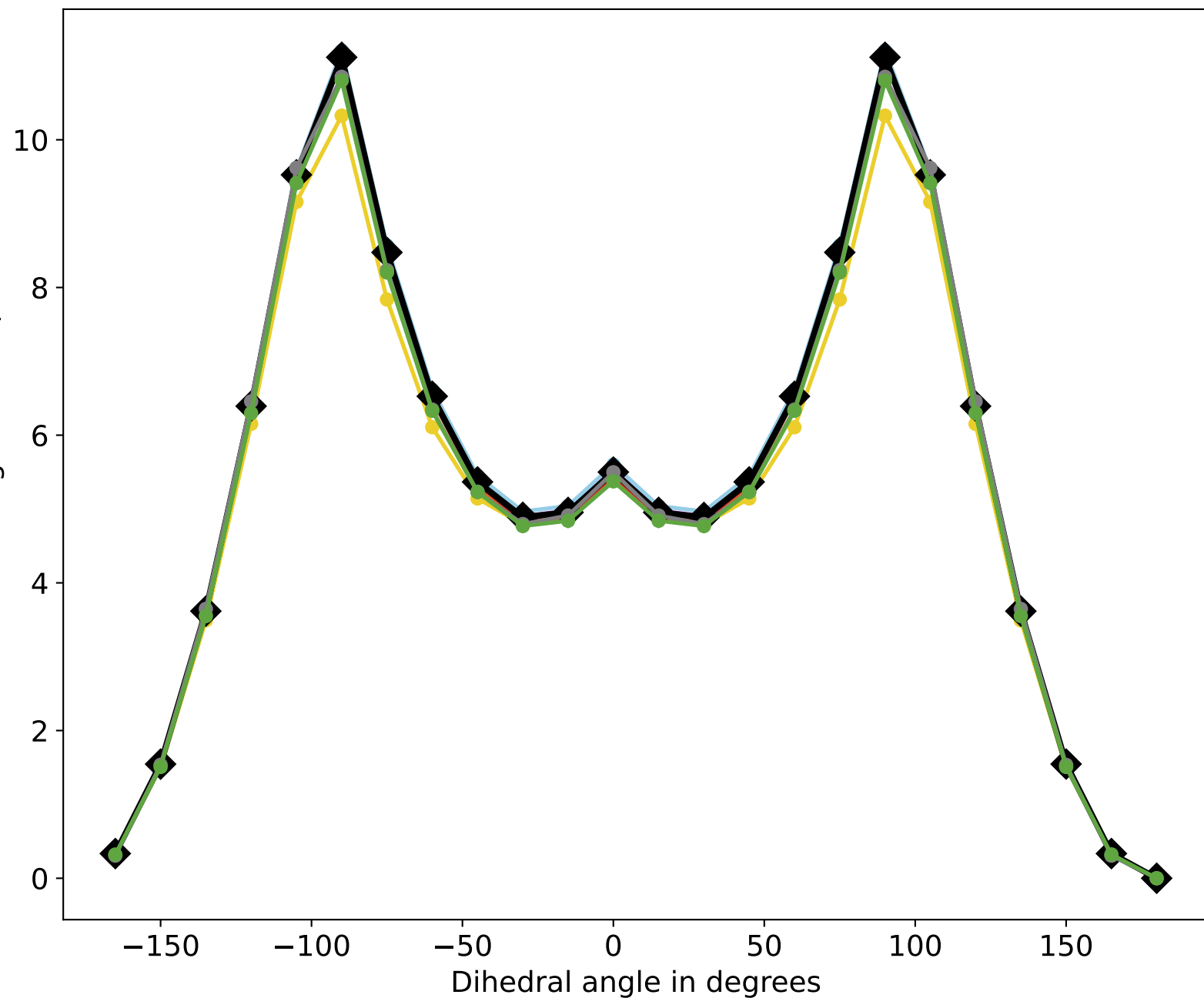


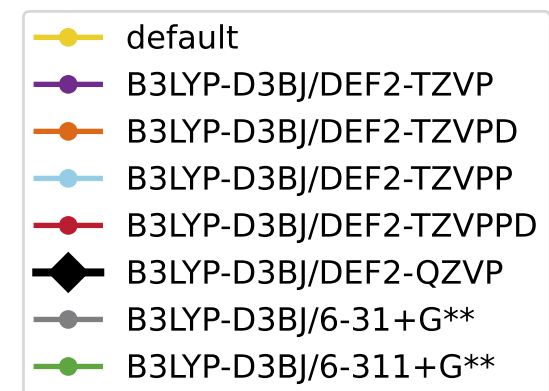
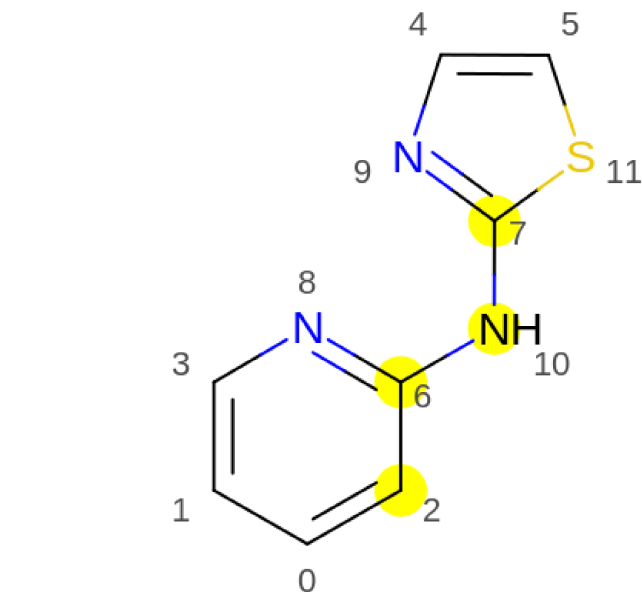
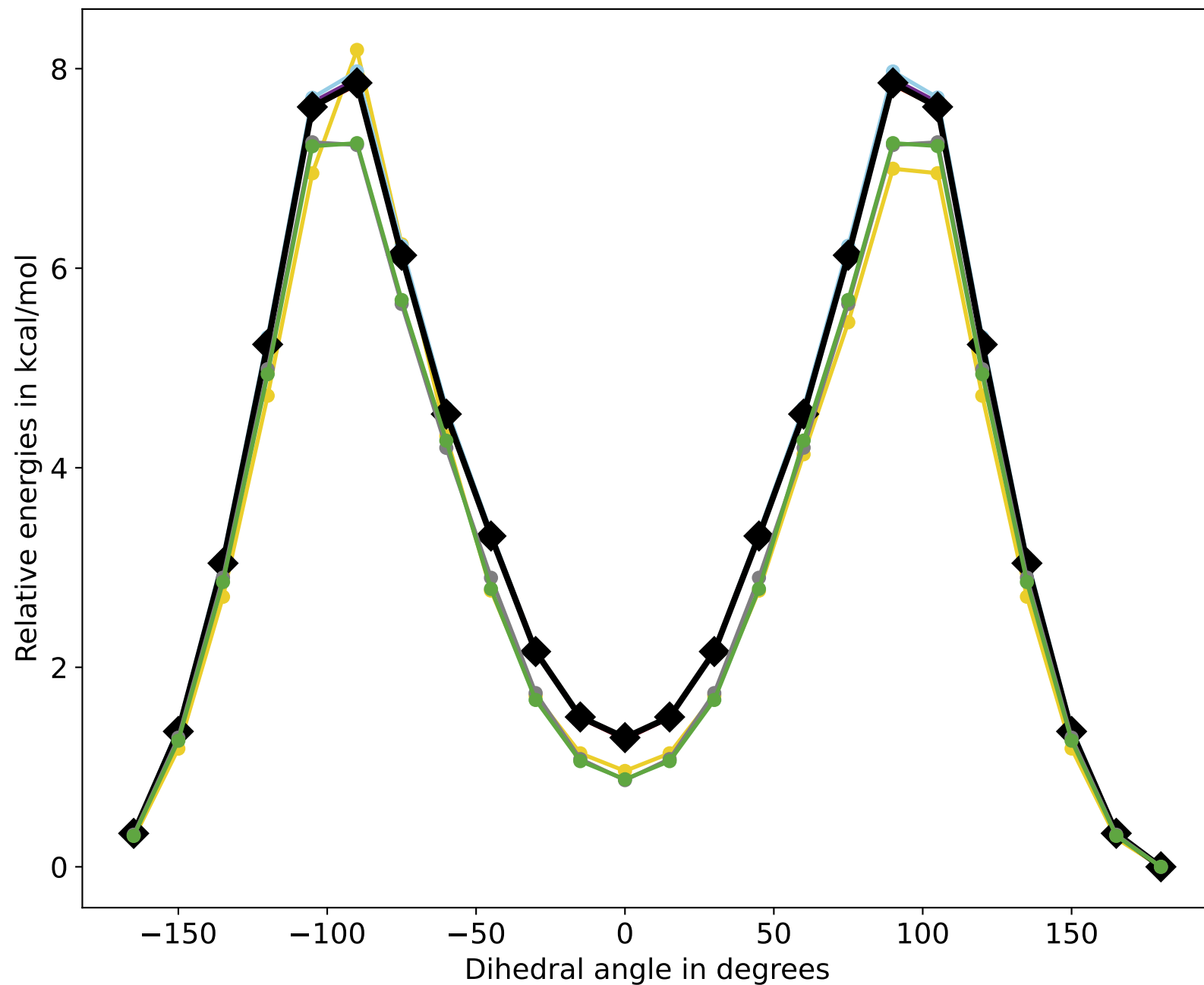
Relative energies in kcal/mol

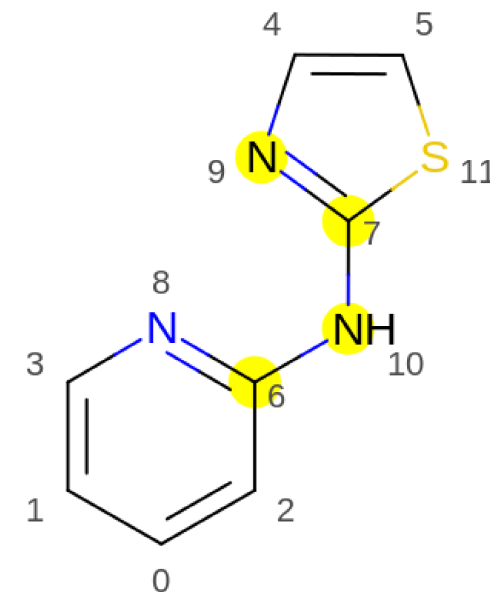
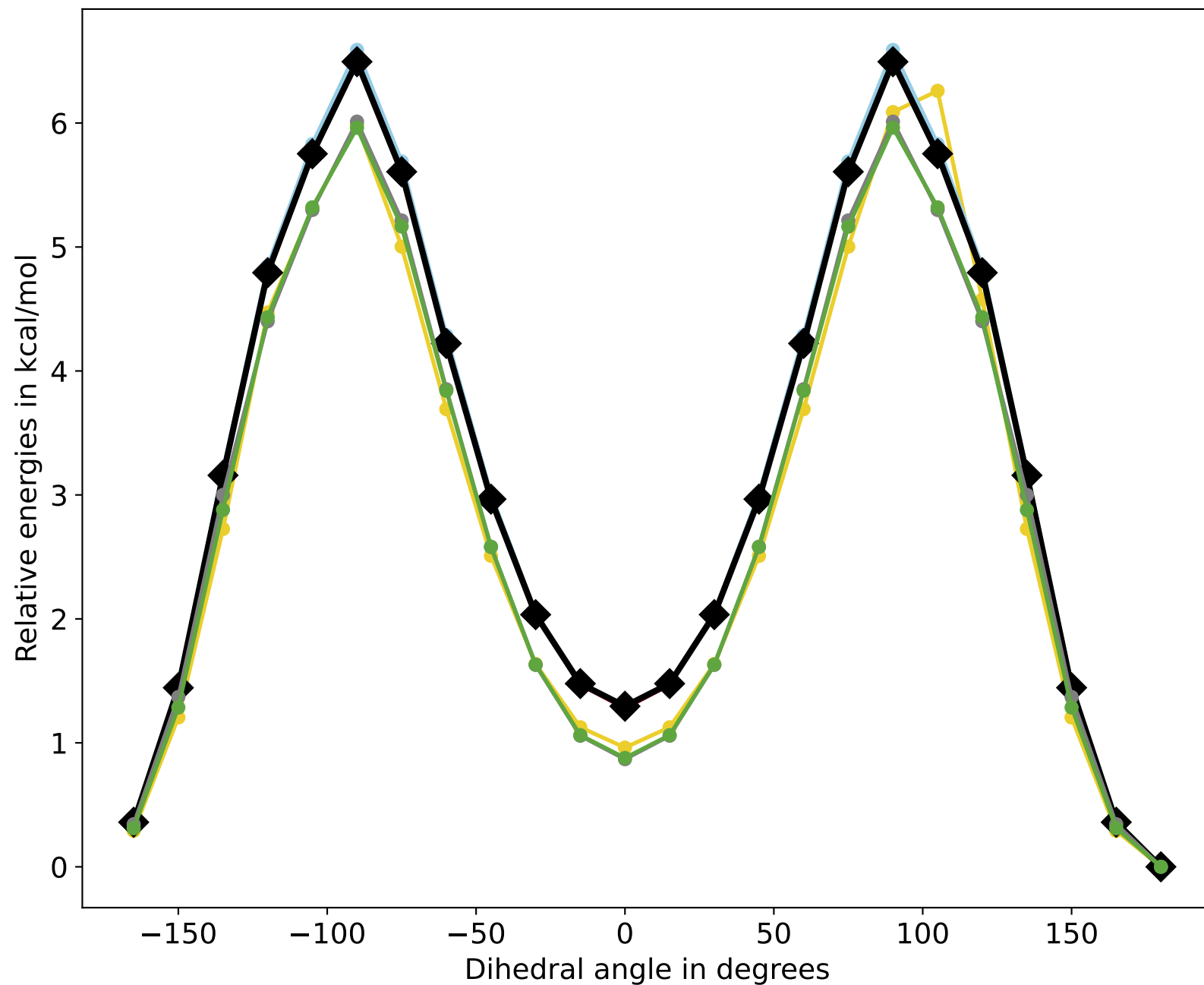


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

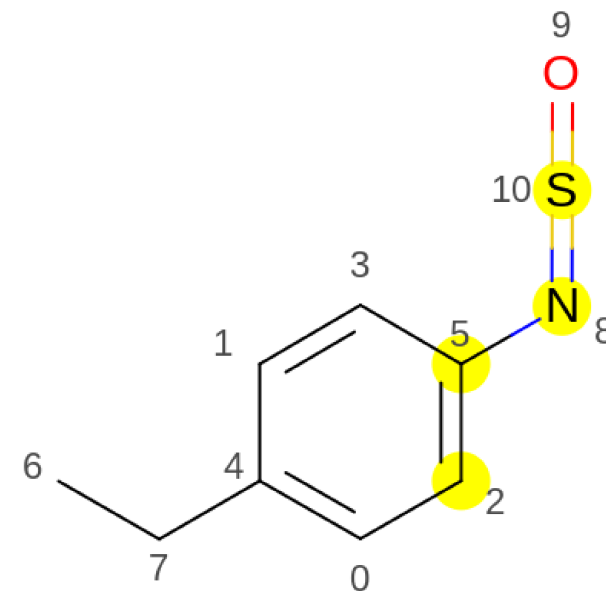
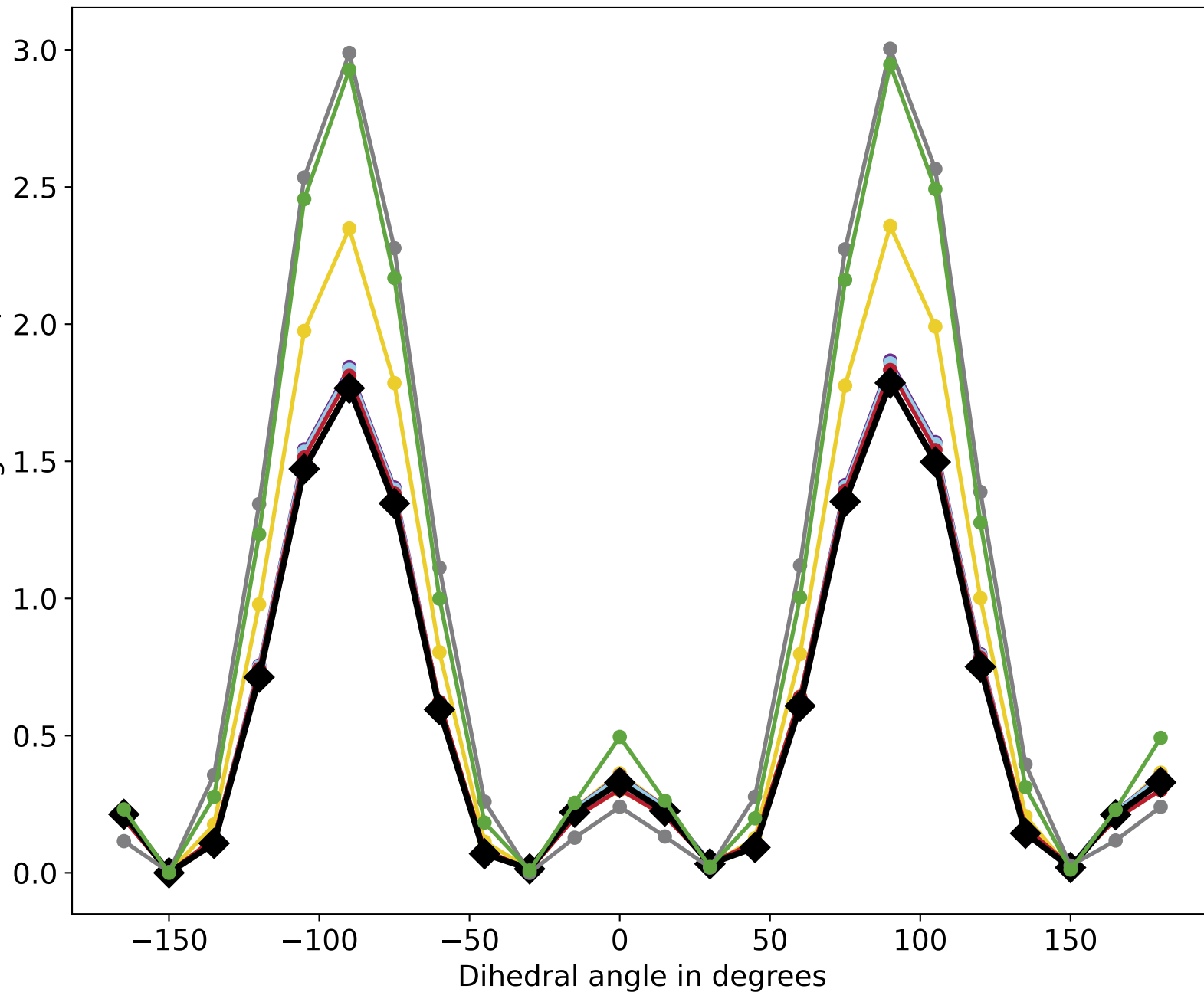




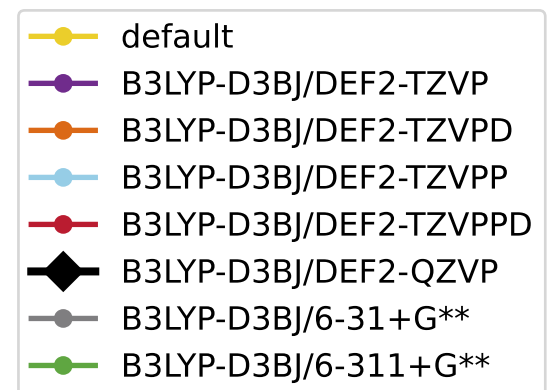
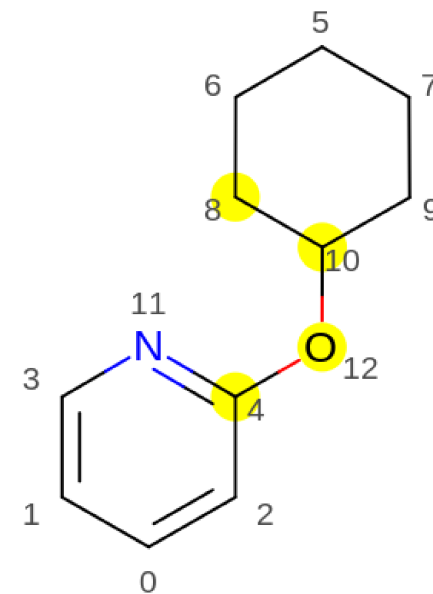
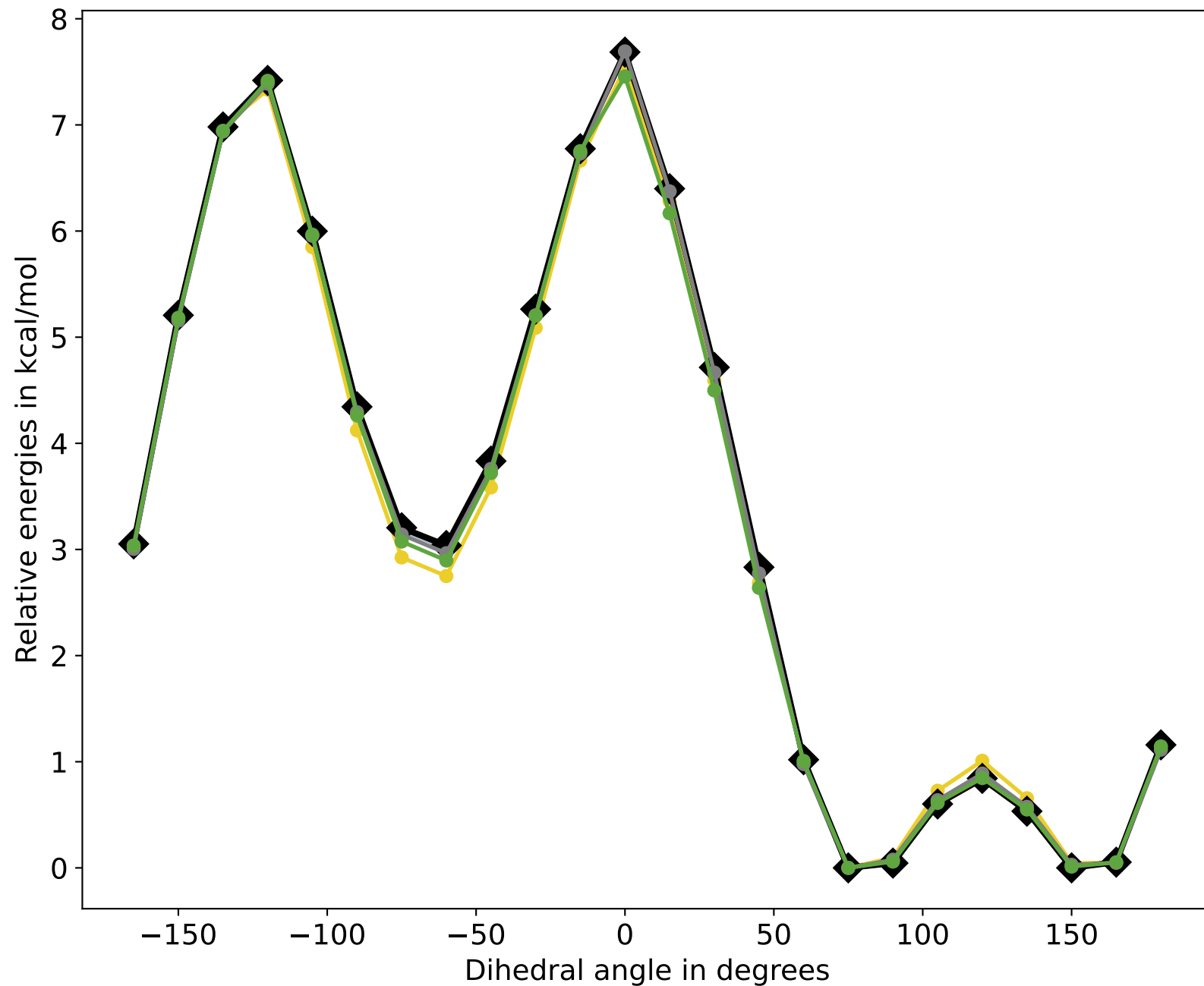


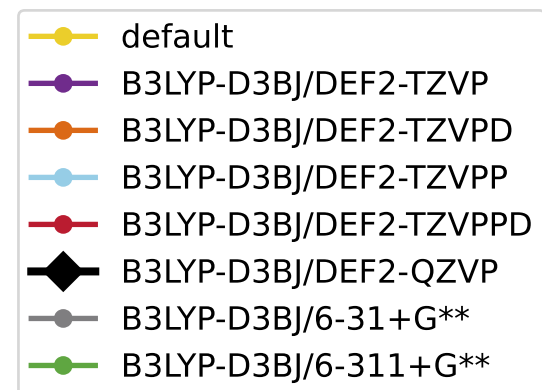
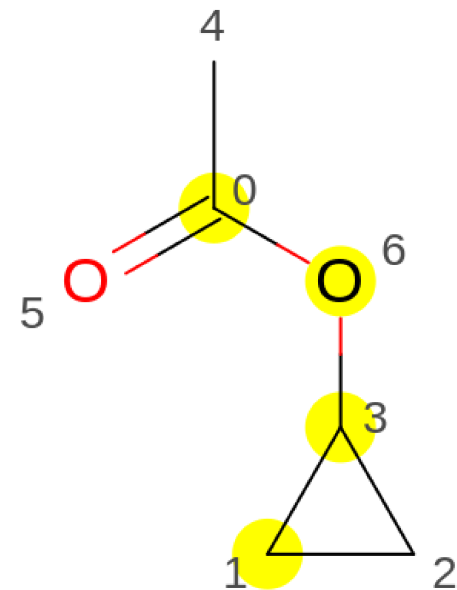
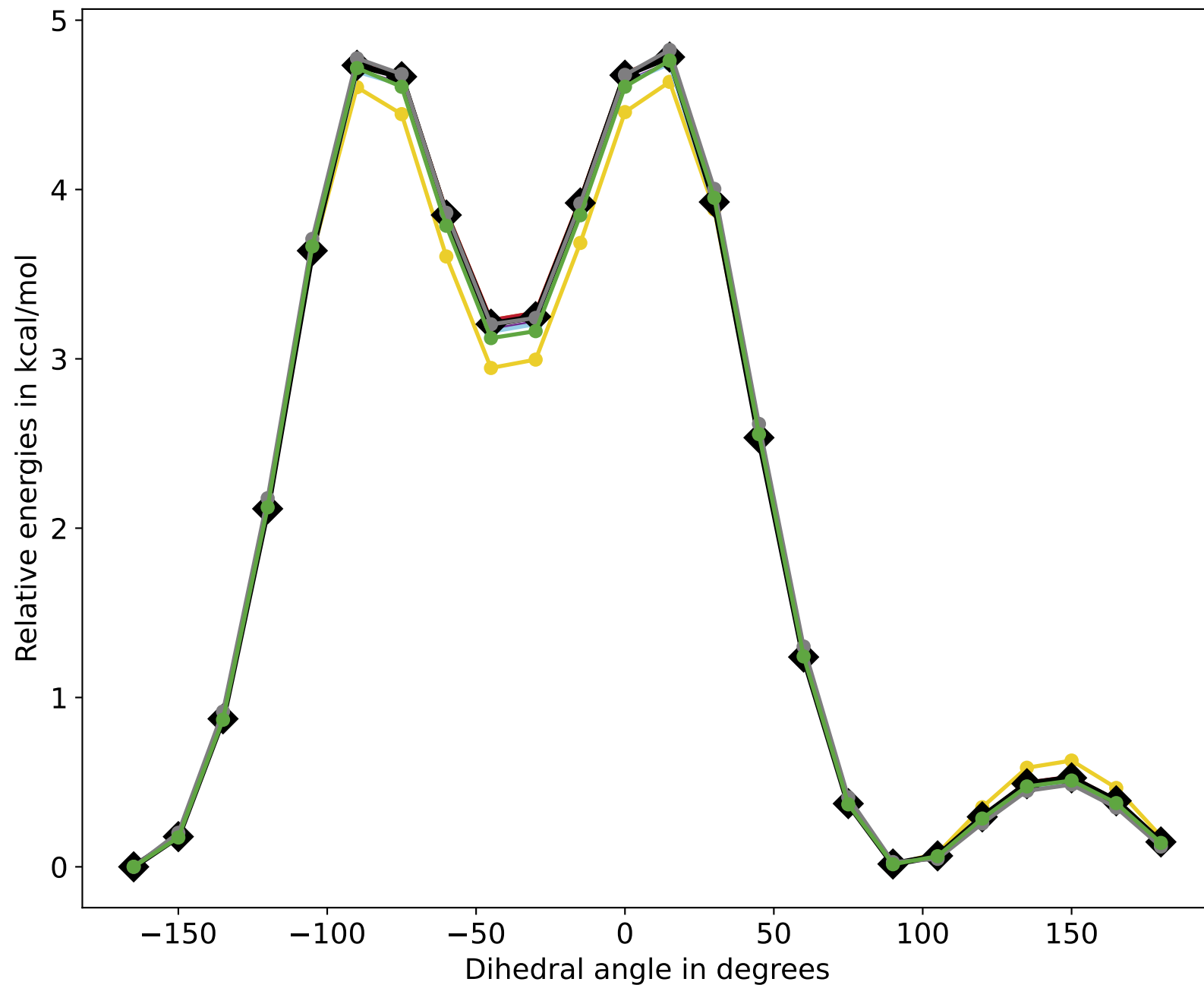
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

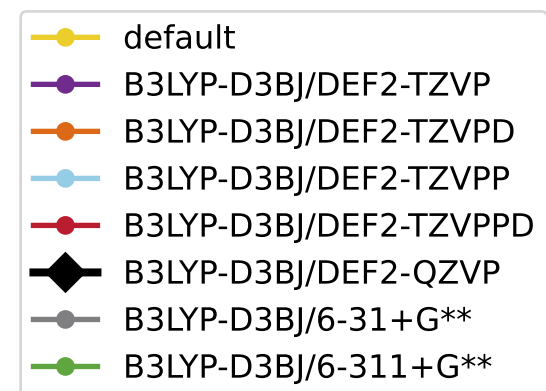
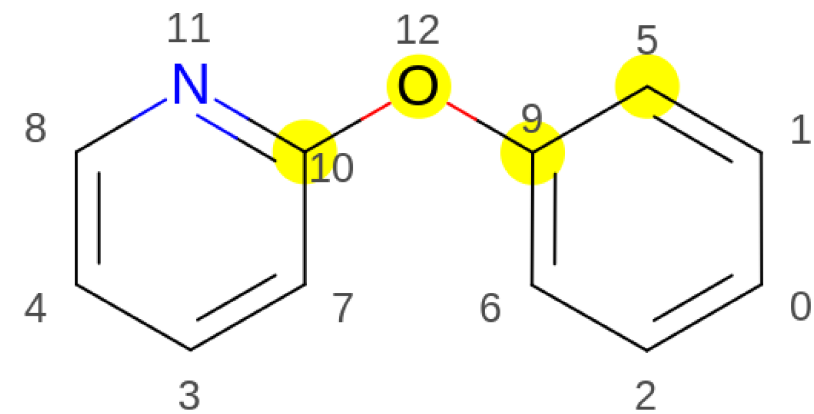
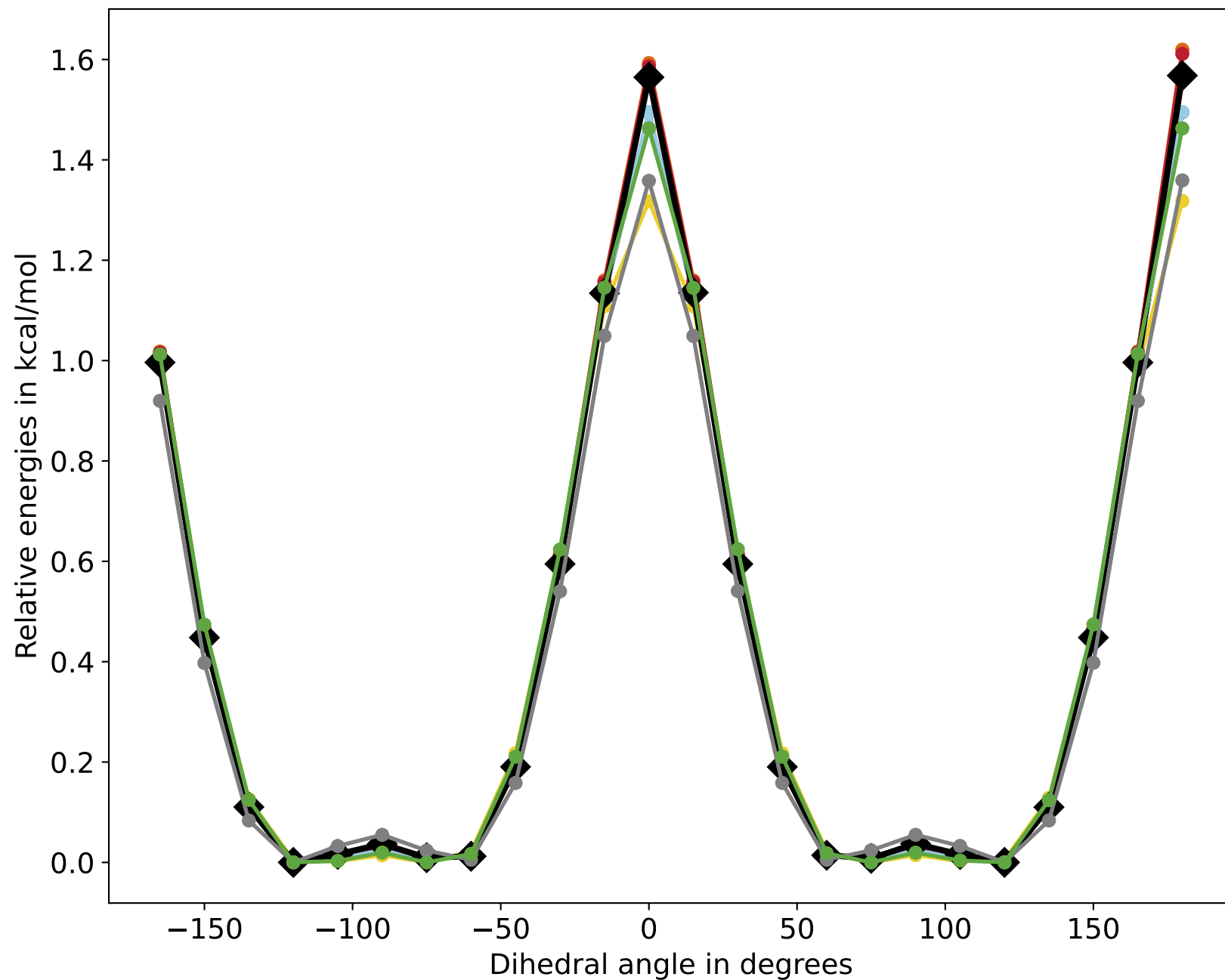
Relative energies in kcal/mol

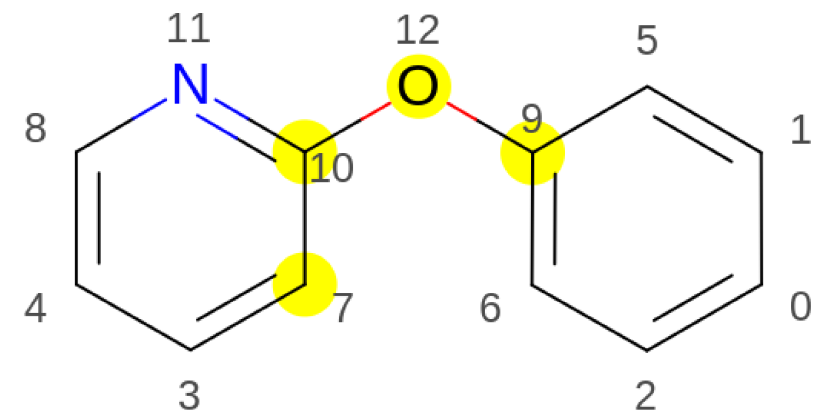
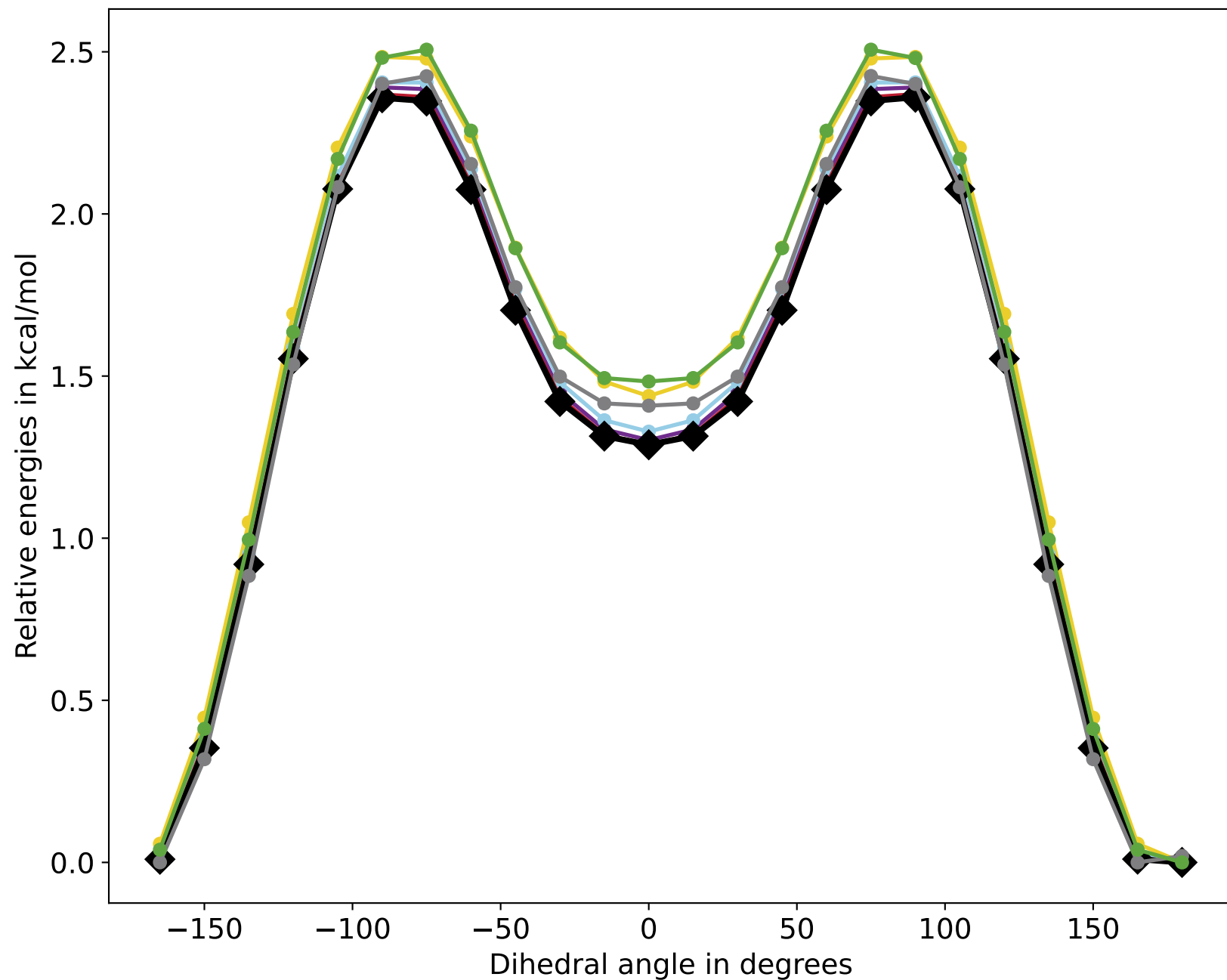


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



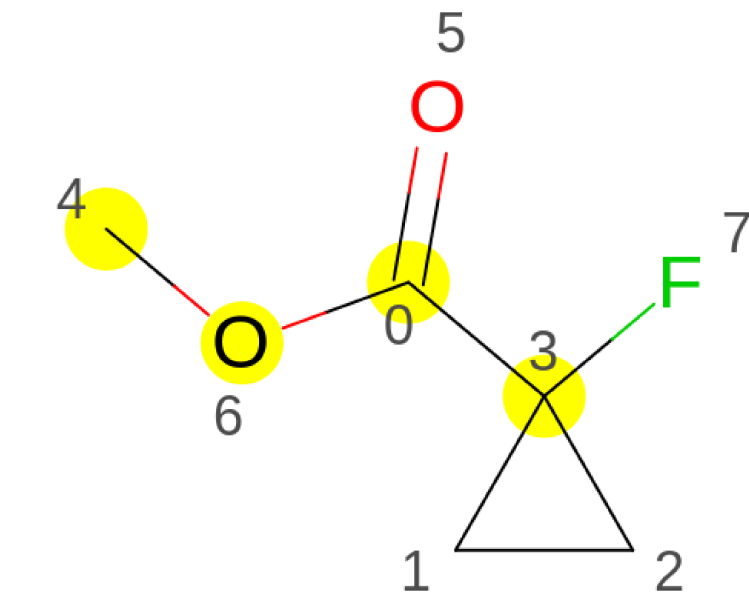
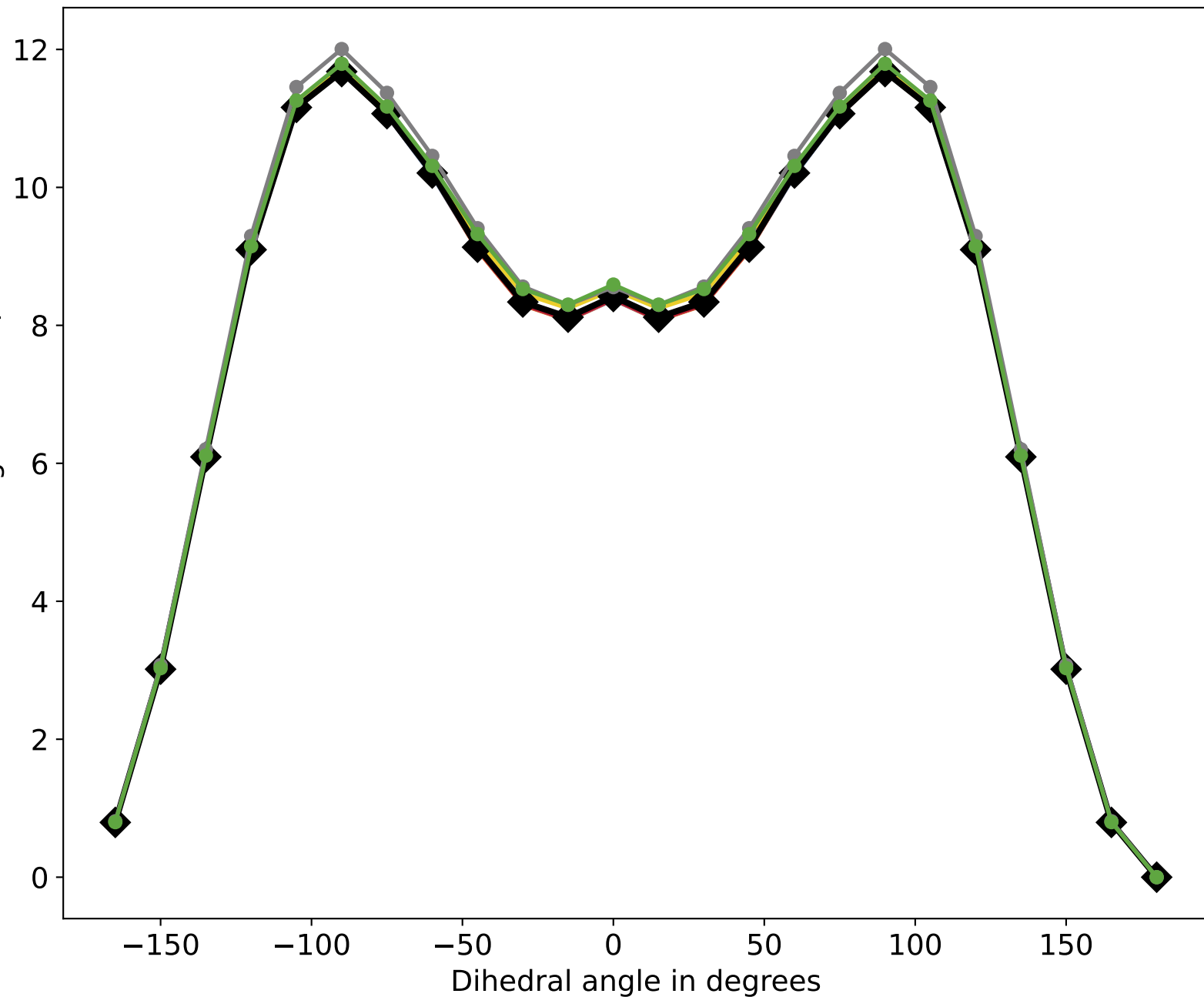






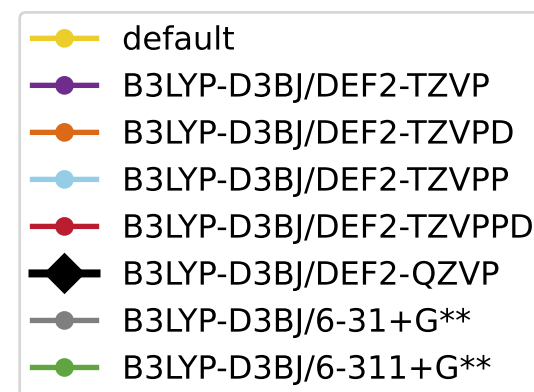
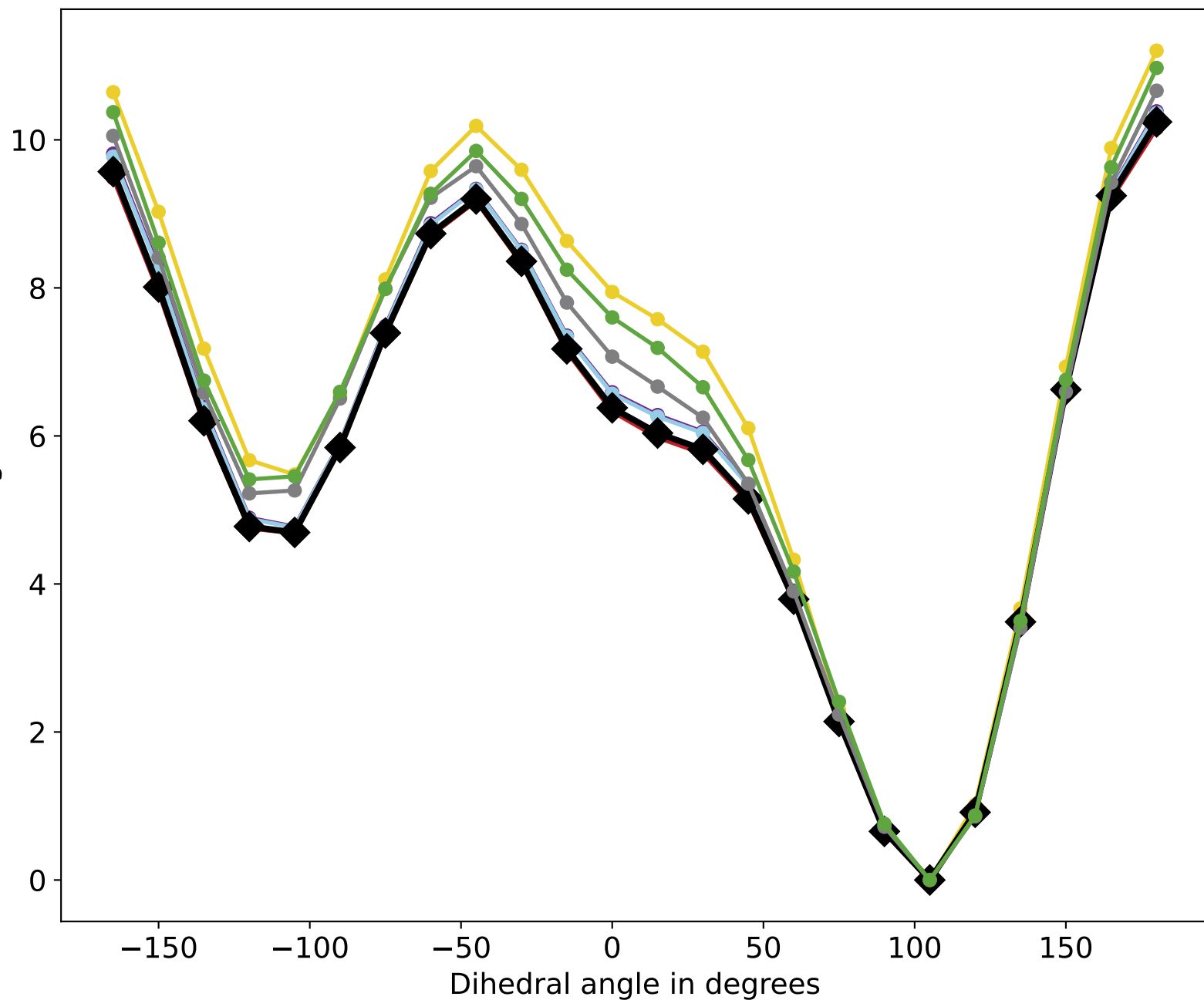
- default
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- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

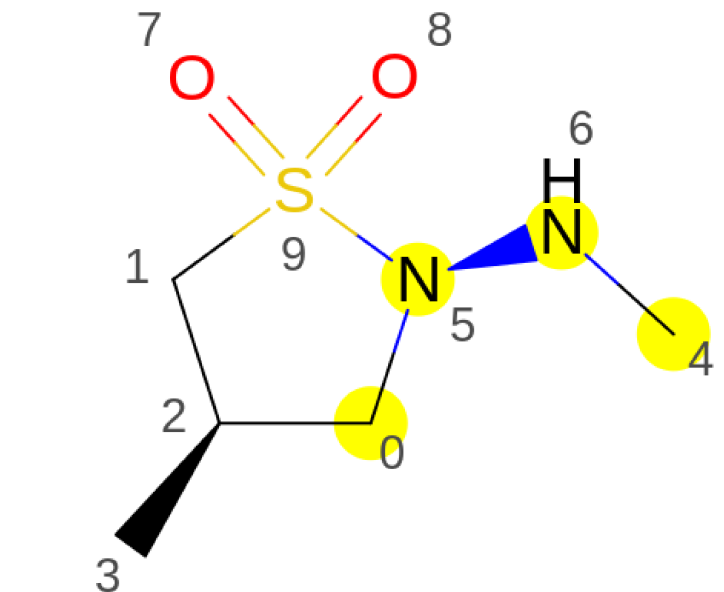
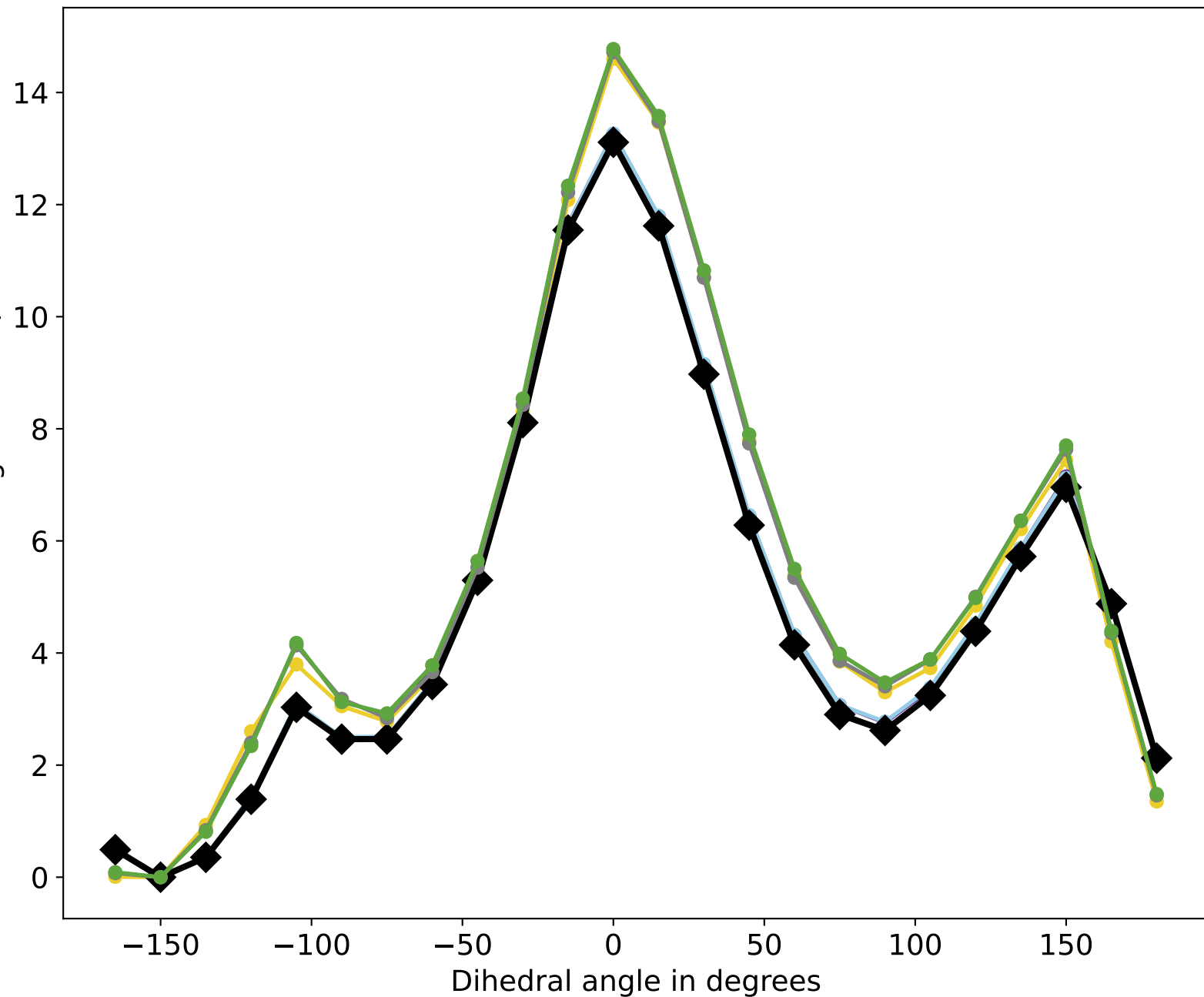


- default
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- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

Relative energies in kcal/mol

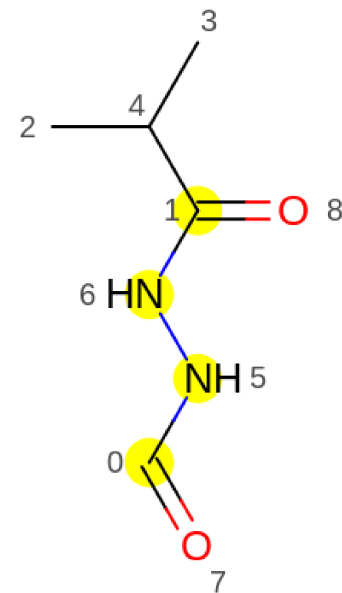
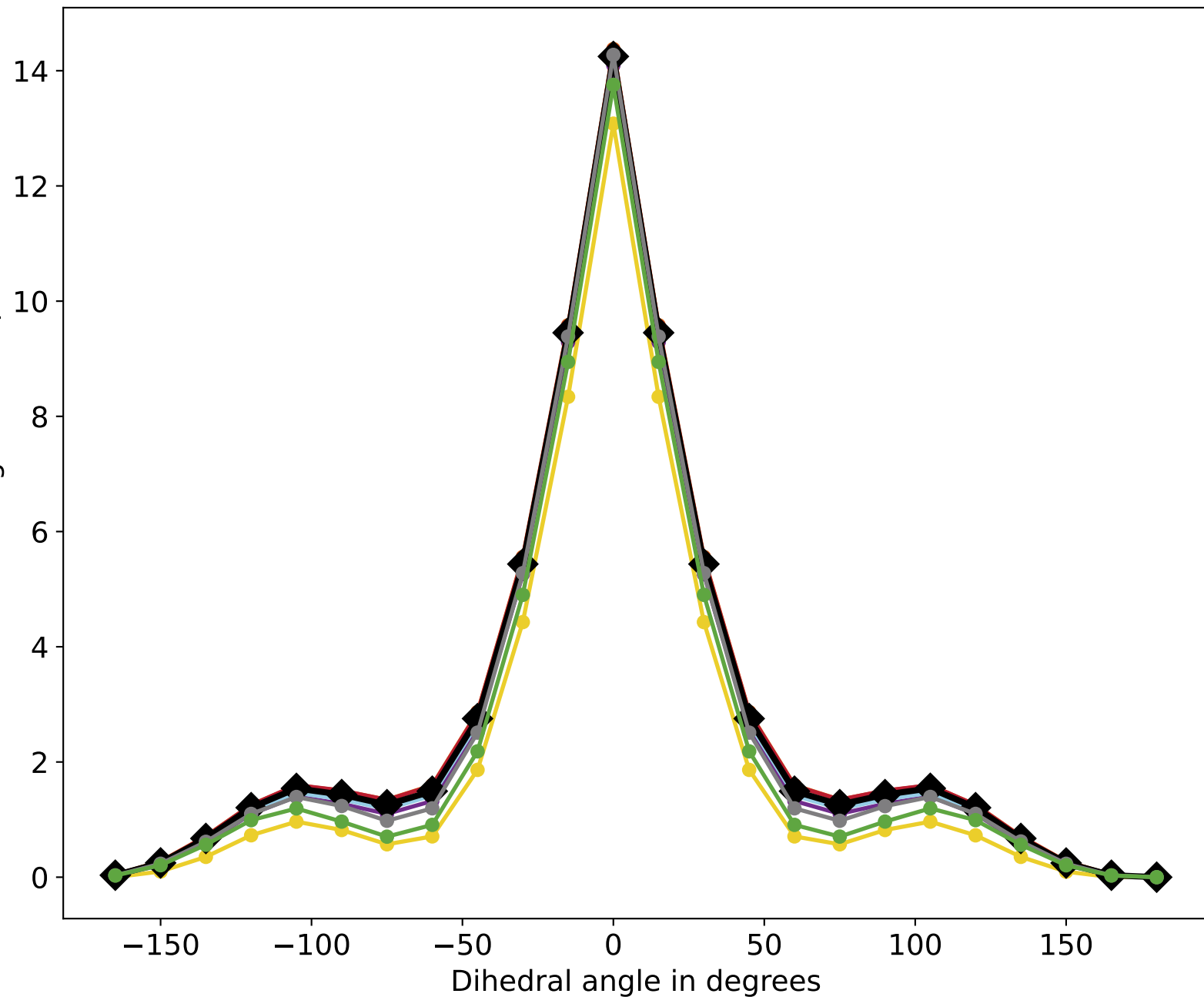


Relative energies in kcal/mol

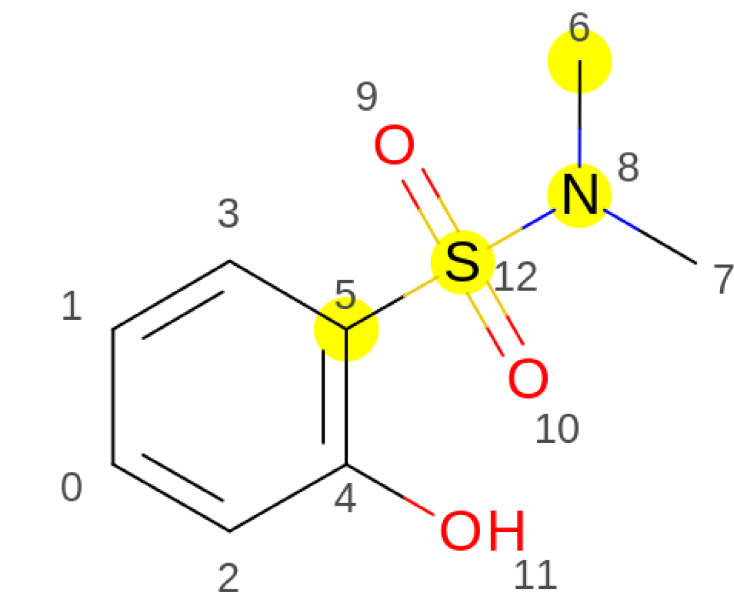
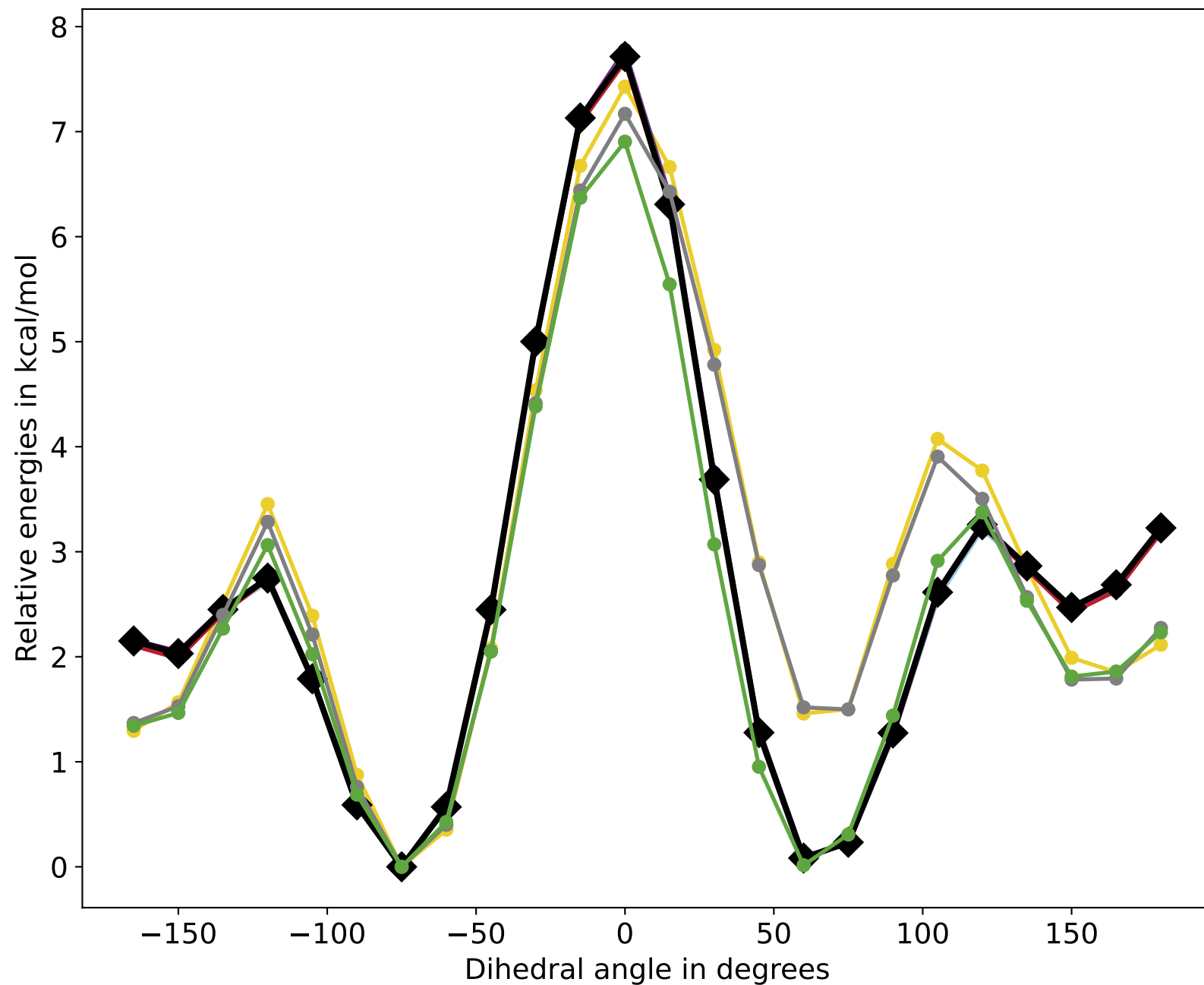


- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**

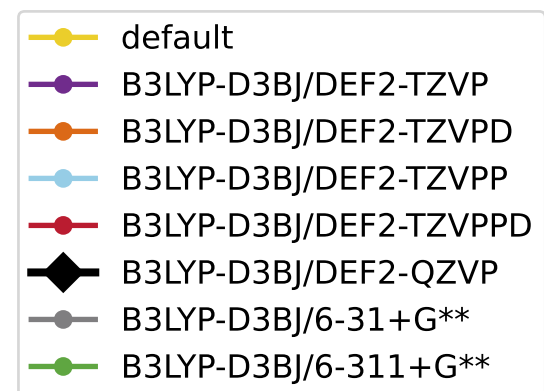
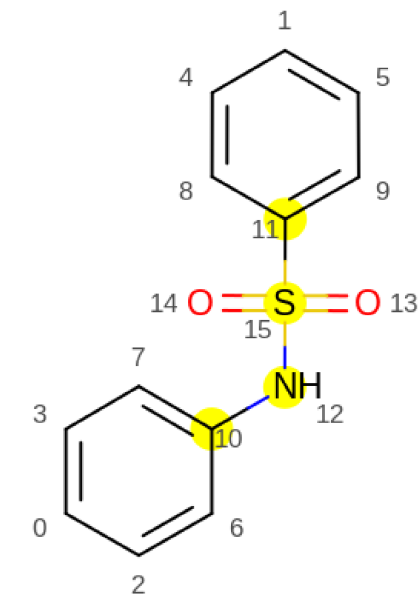
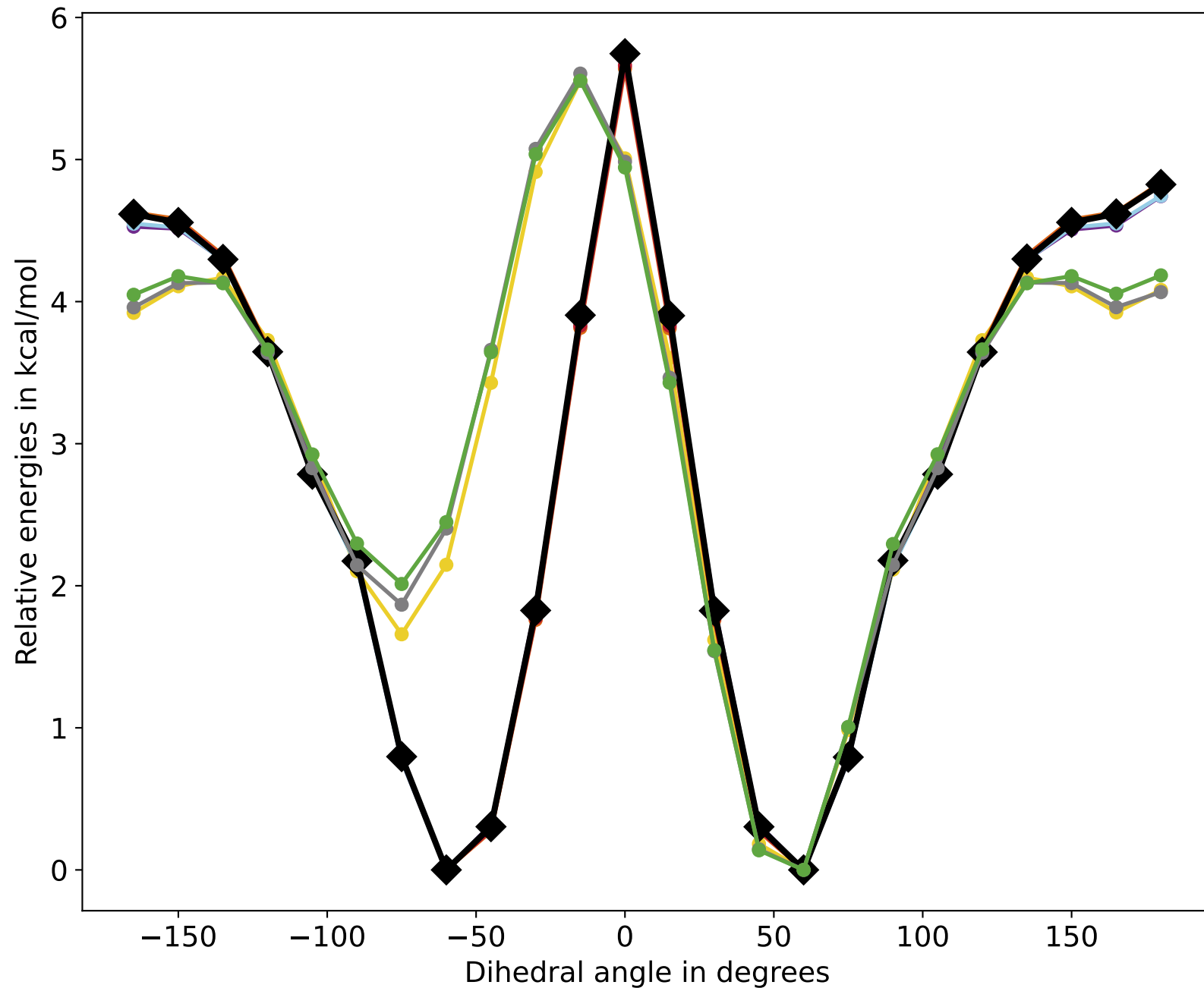
Relative energies in kcal/mol

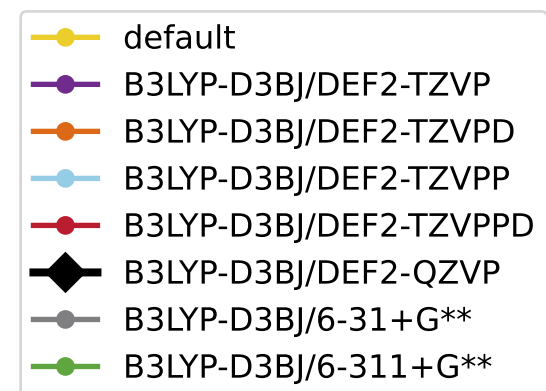
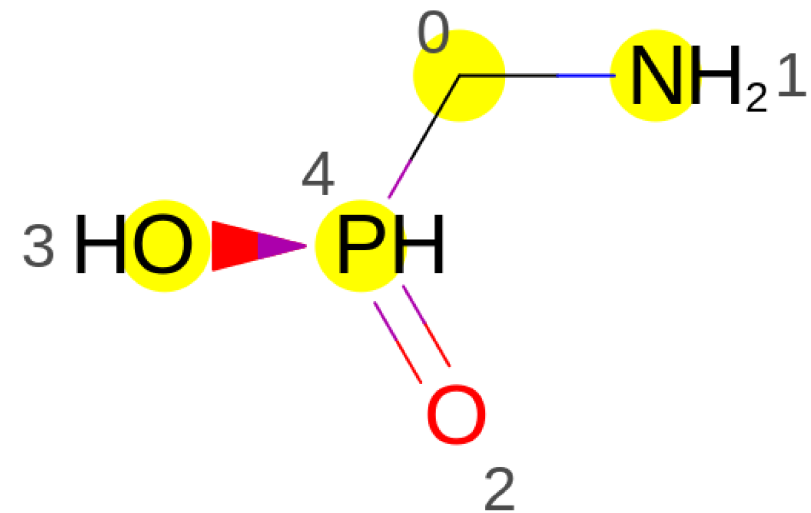
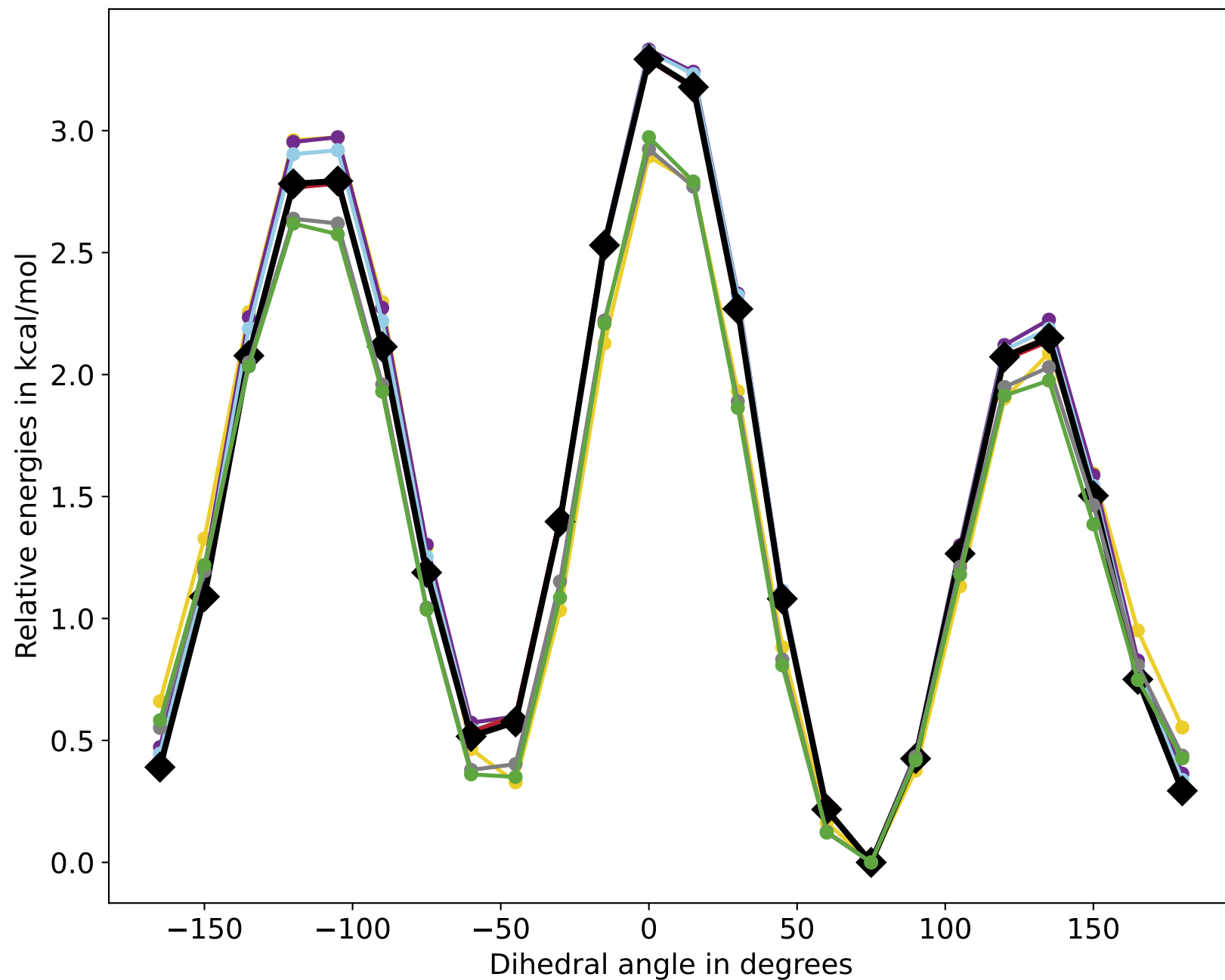


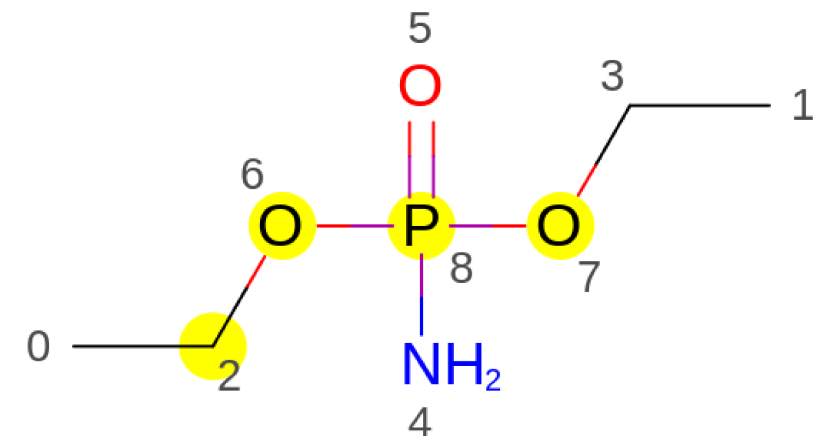
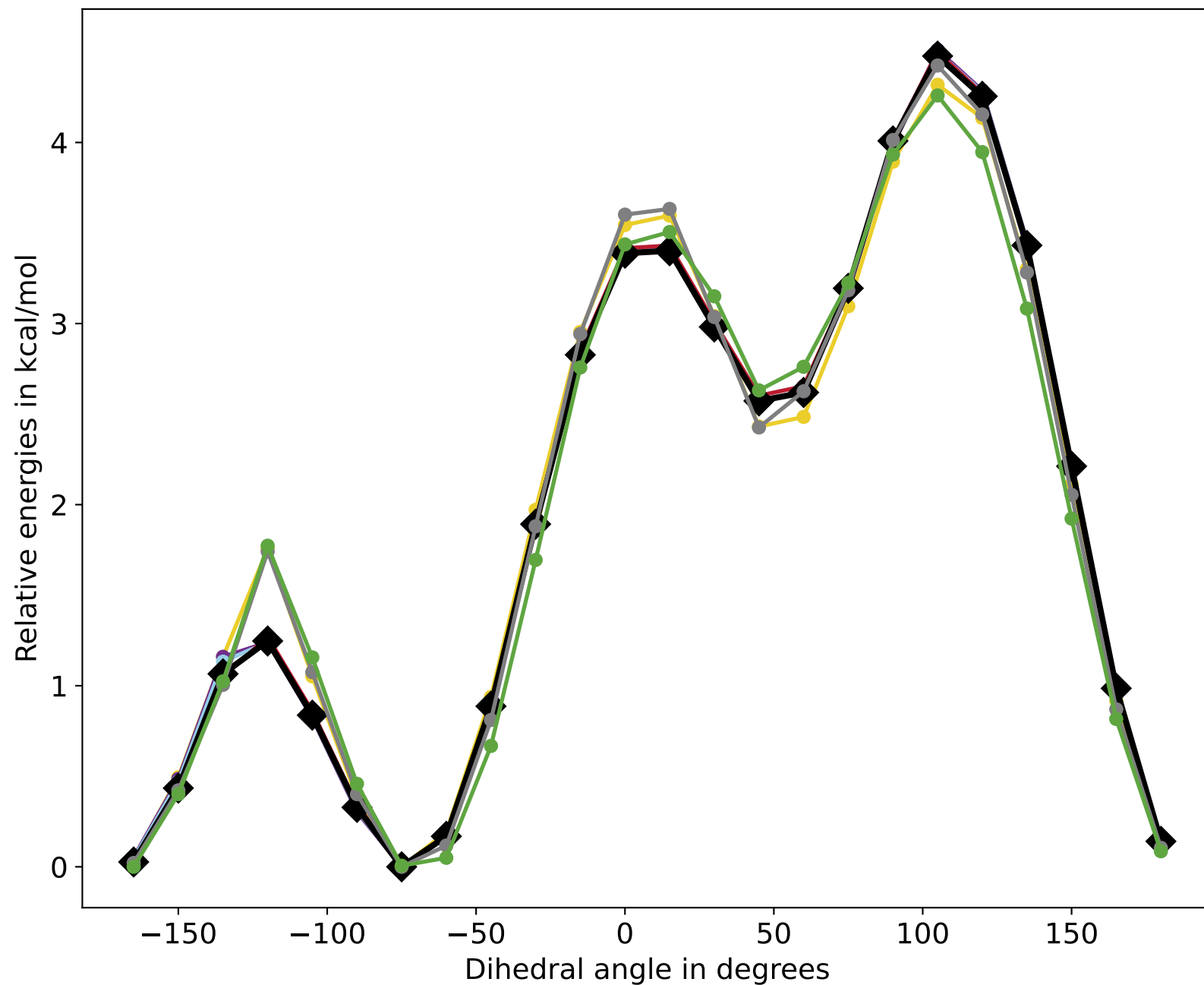
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**



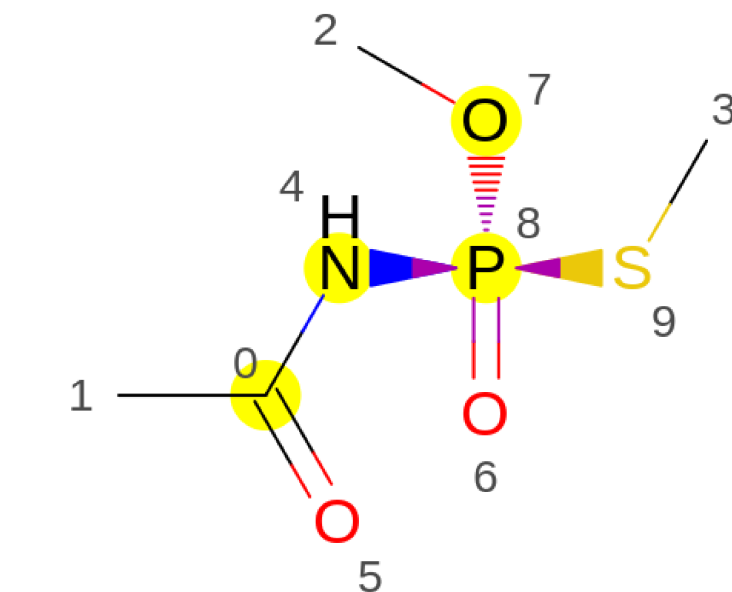
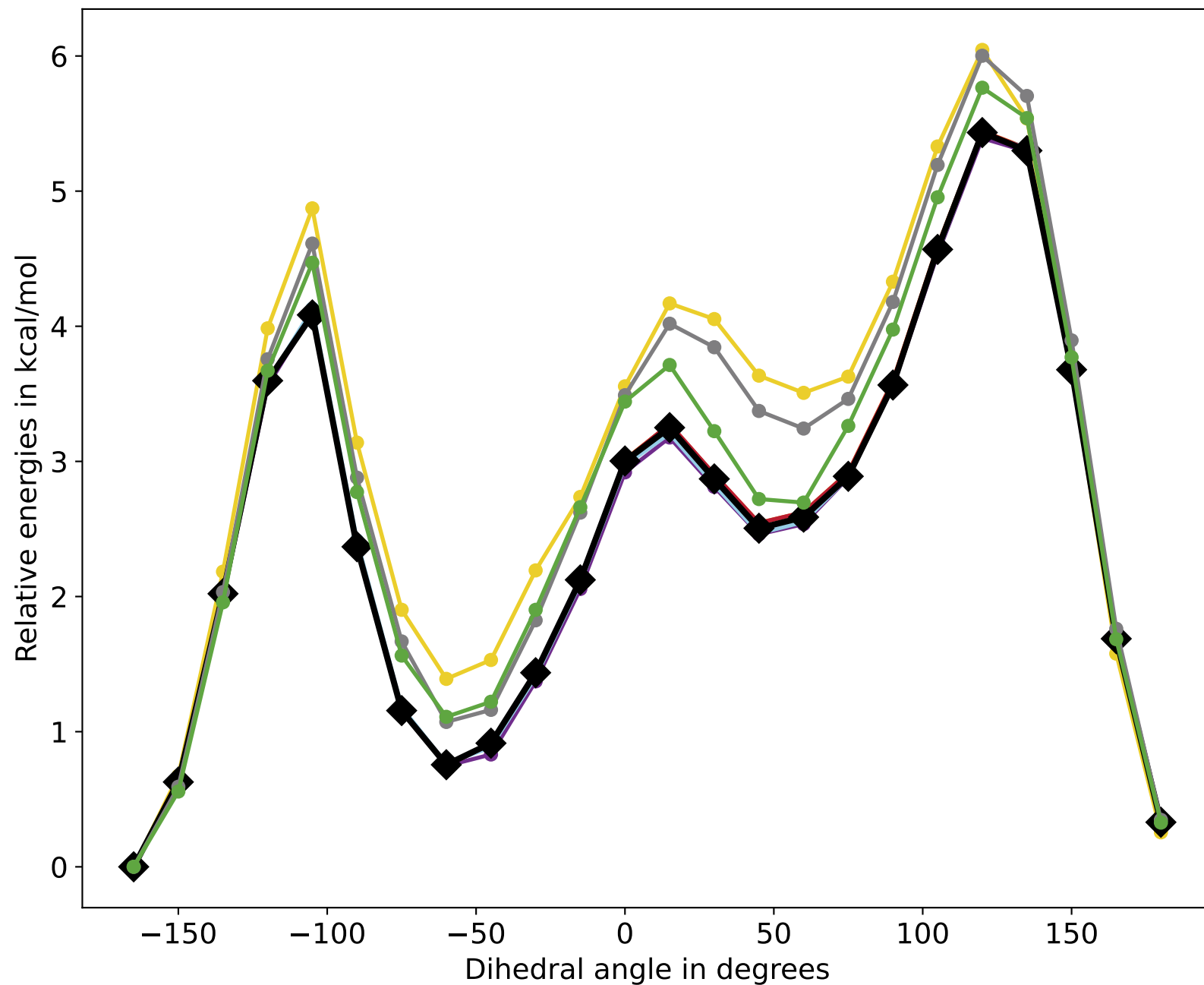
- default
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G**
- B3LYP-D3BJ/6-311+G**







- default
- 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**



- default
- 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**