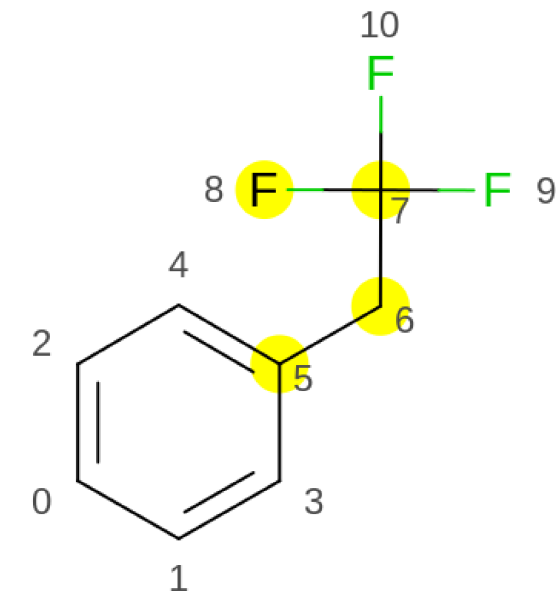
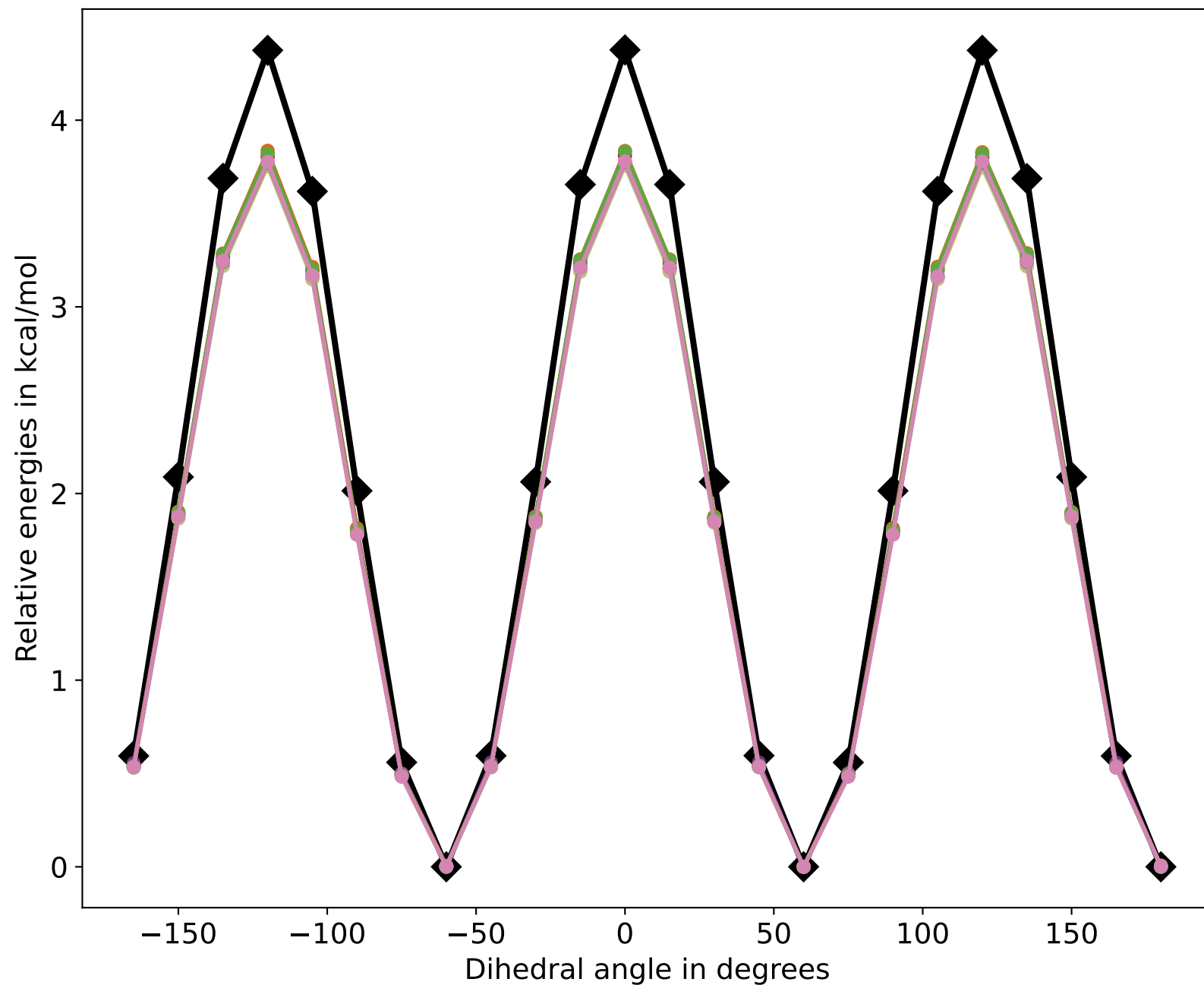
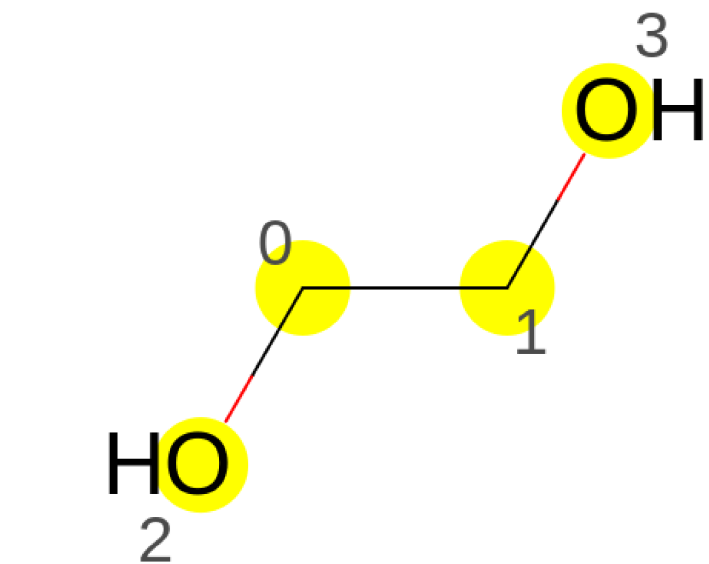
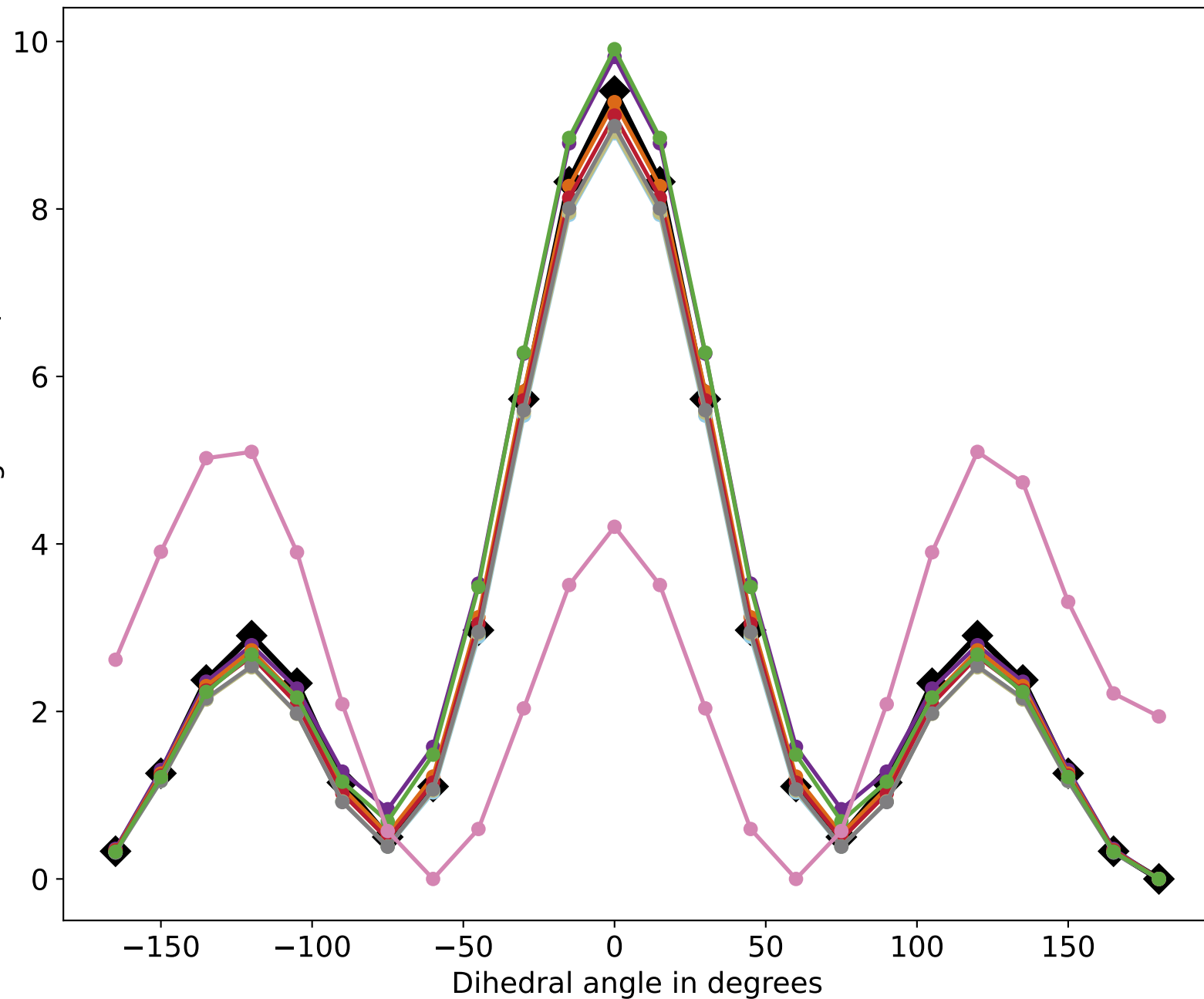
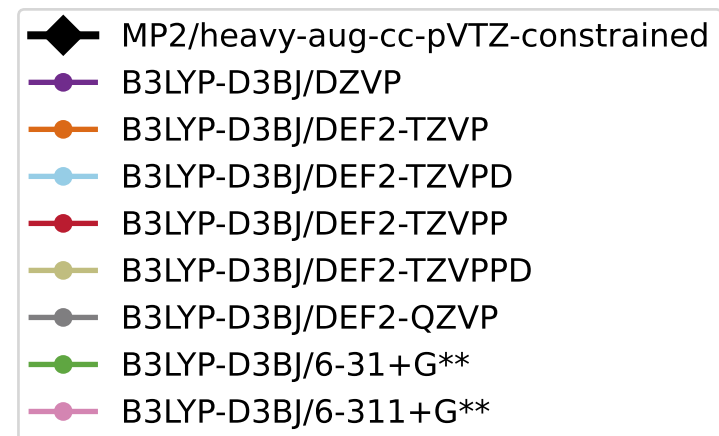
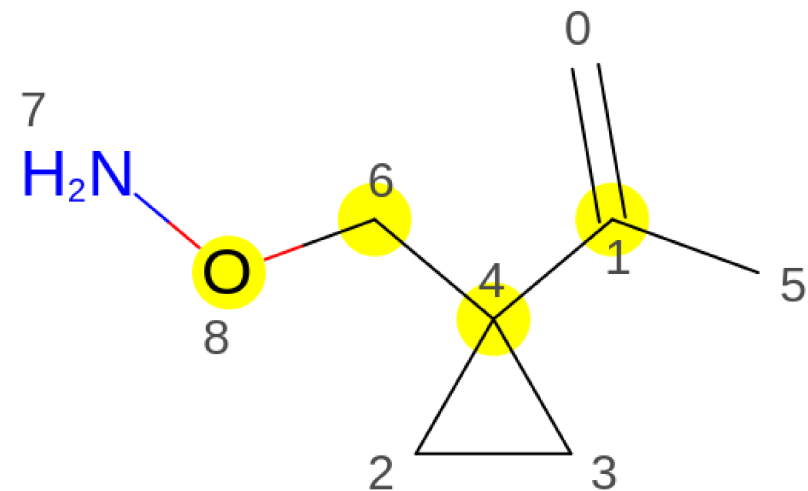
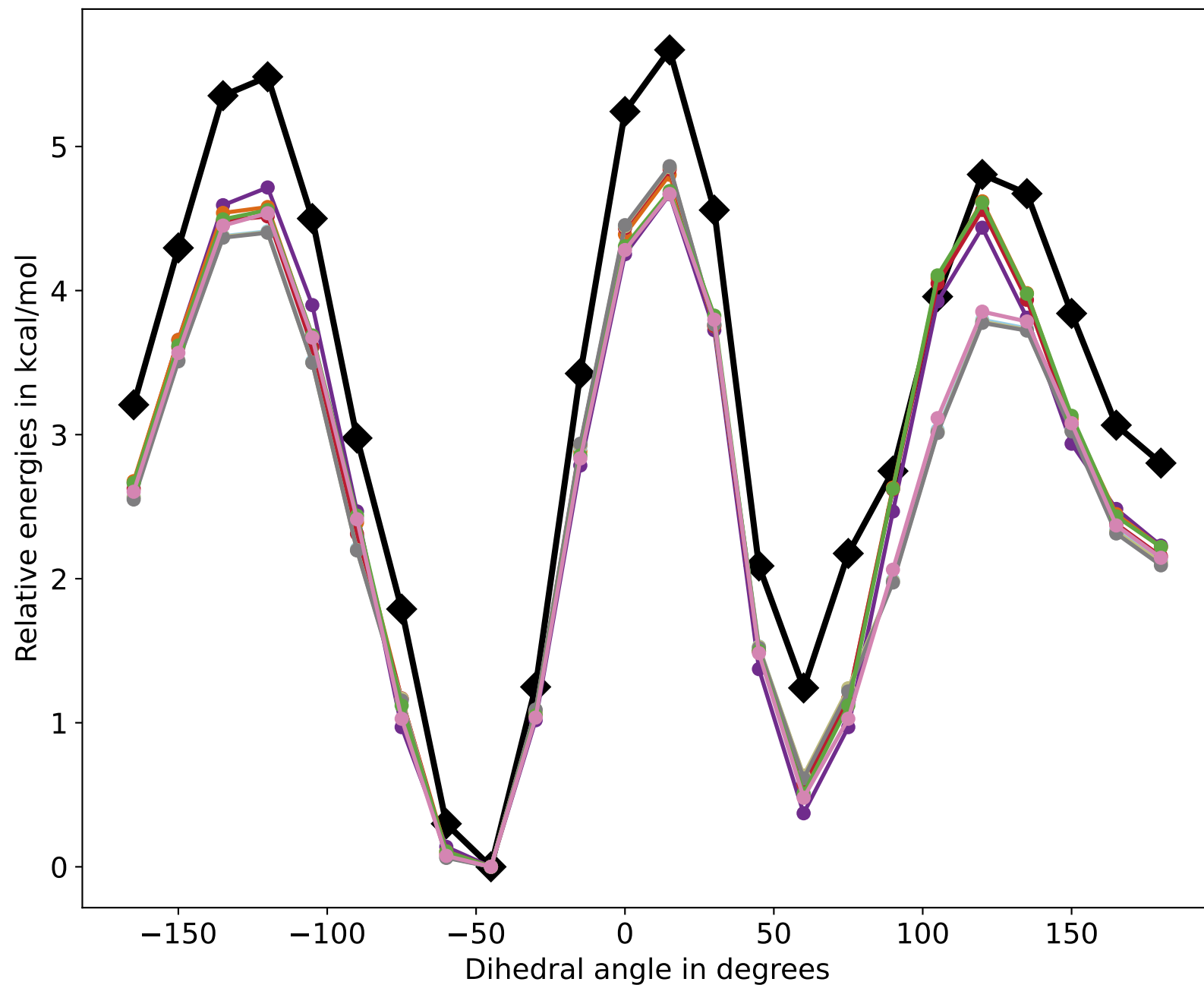


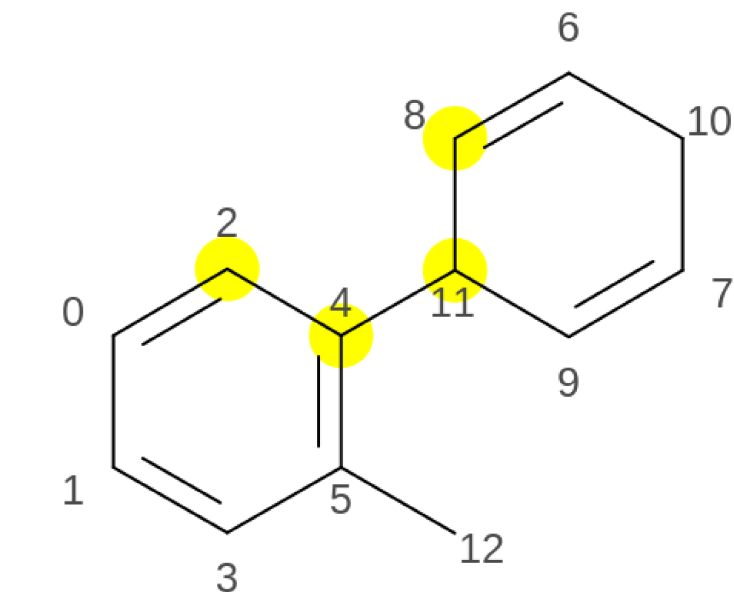
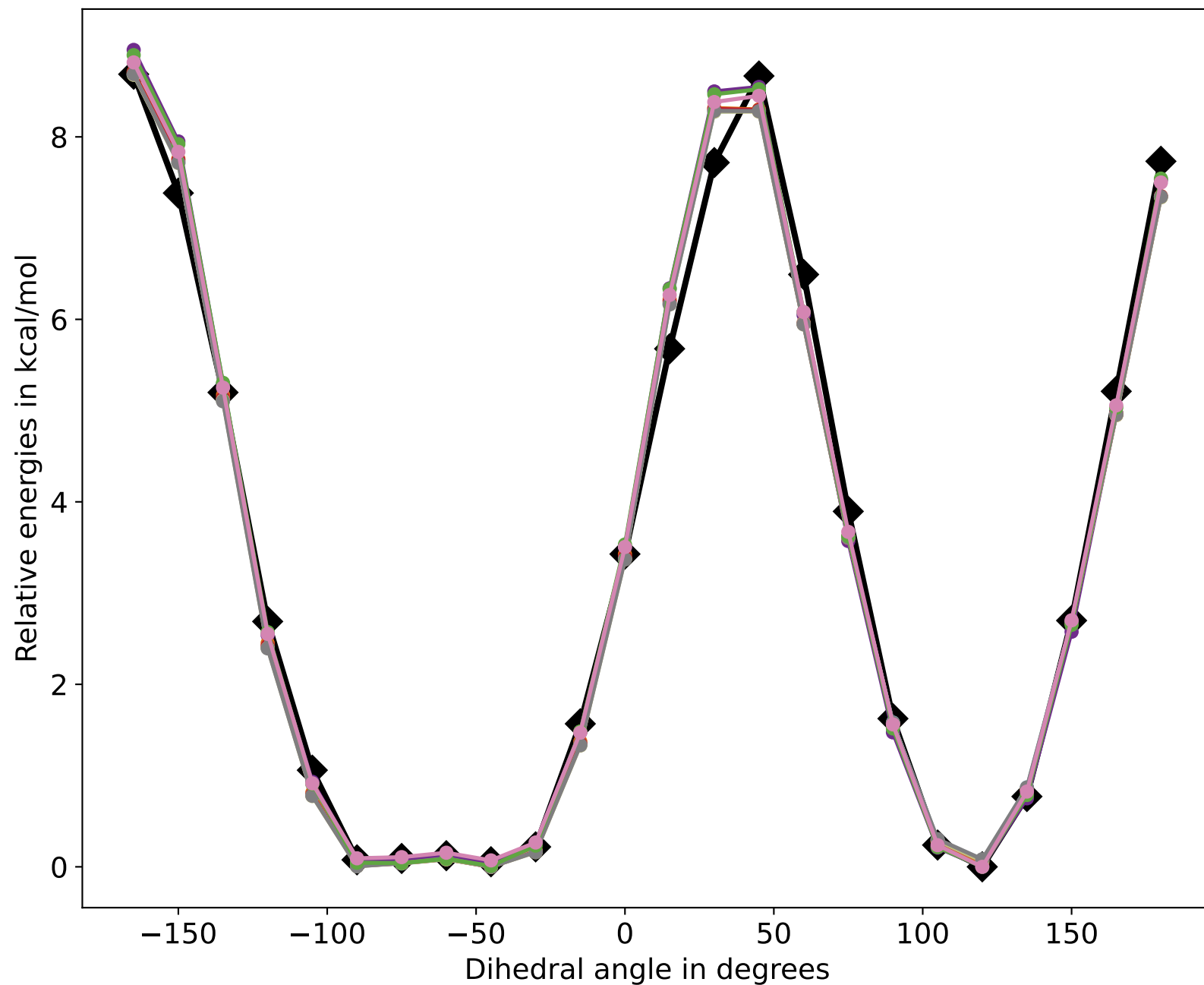
- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*

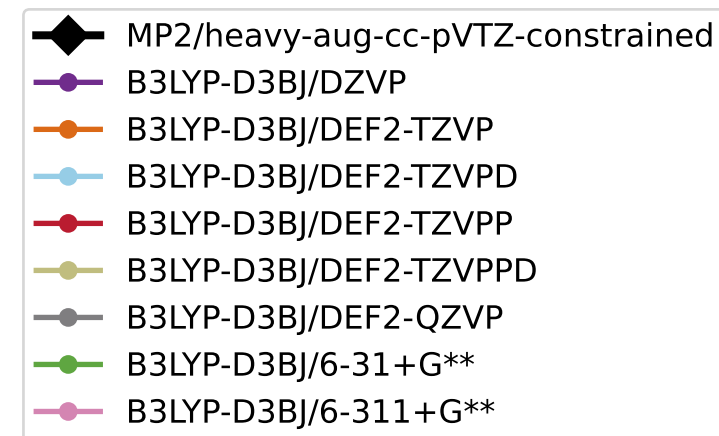
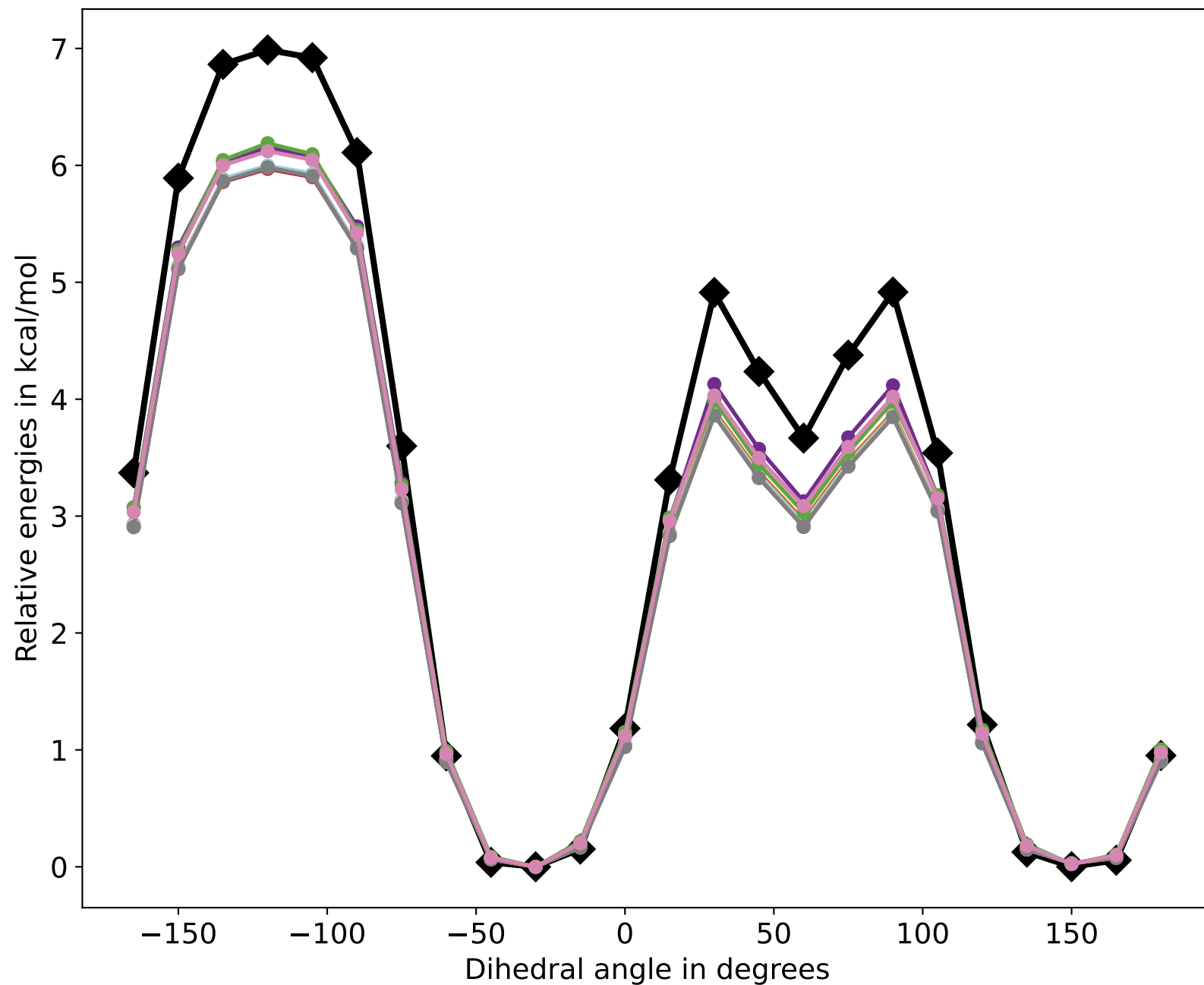


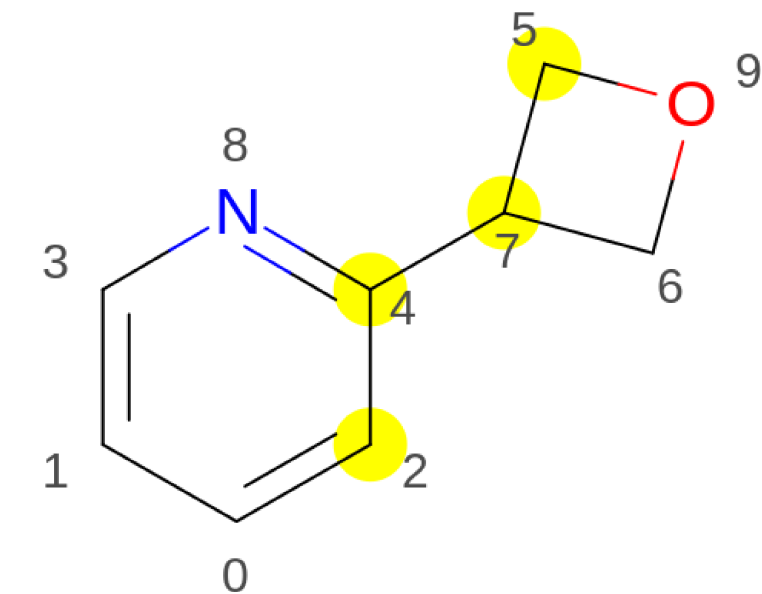
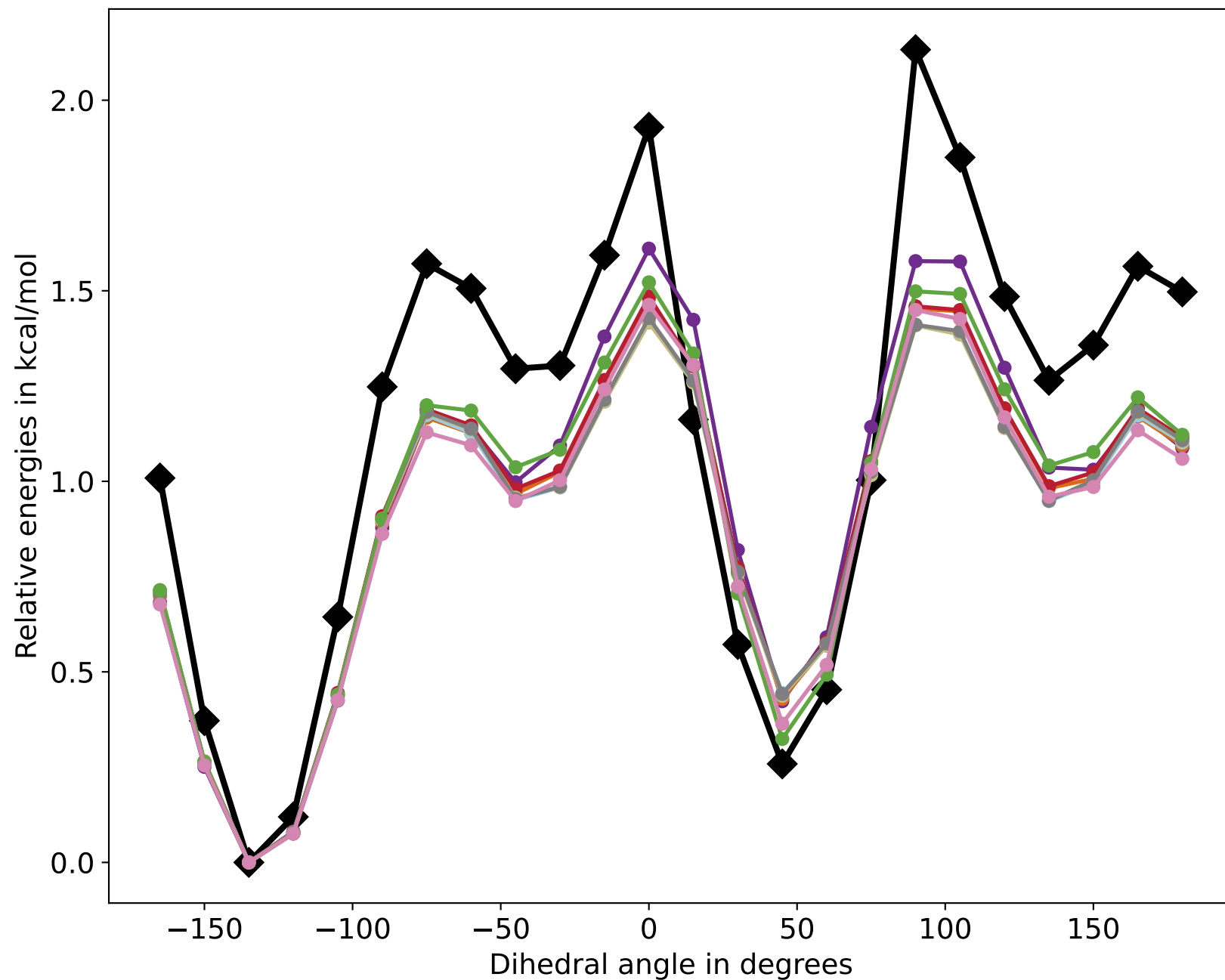
Relative energies in kcal/mol

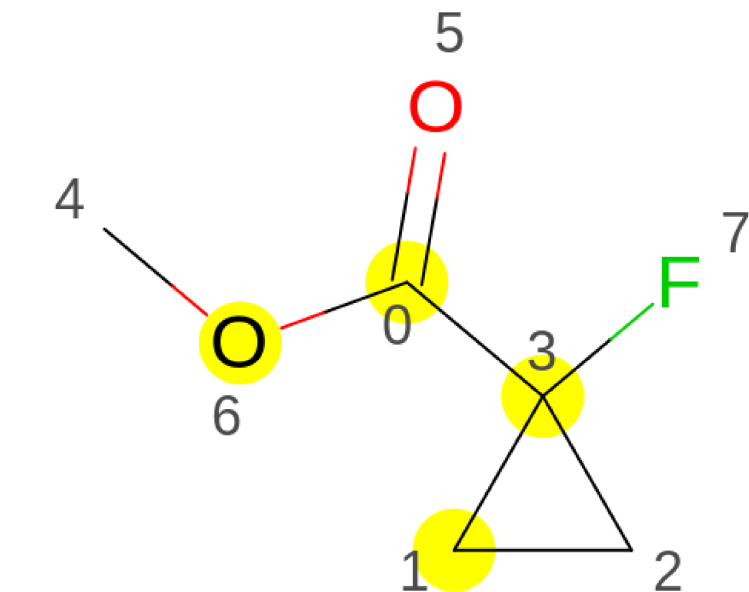
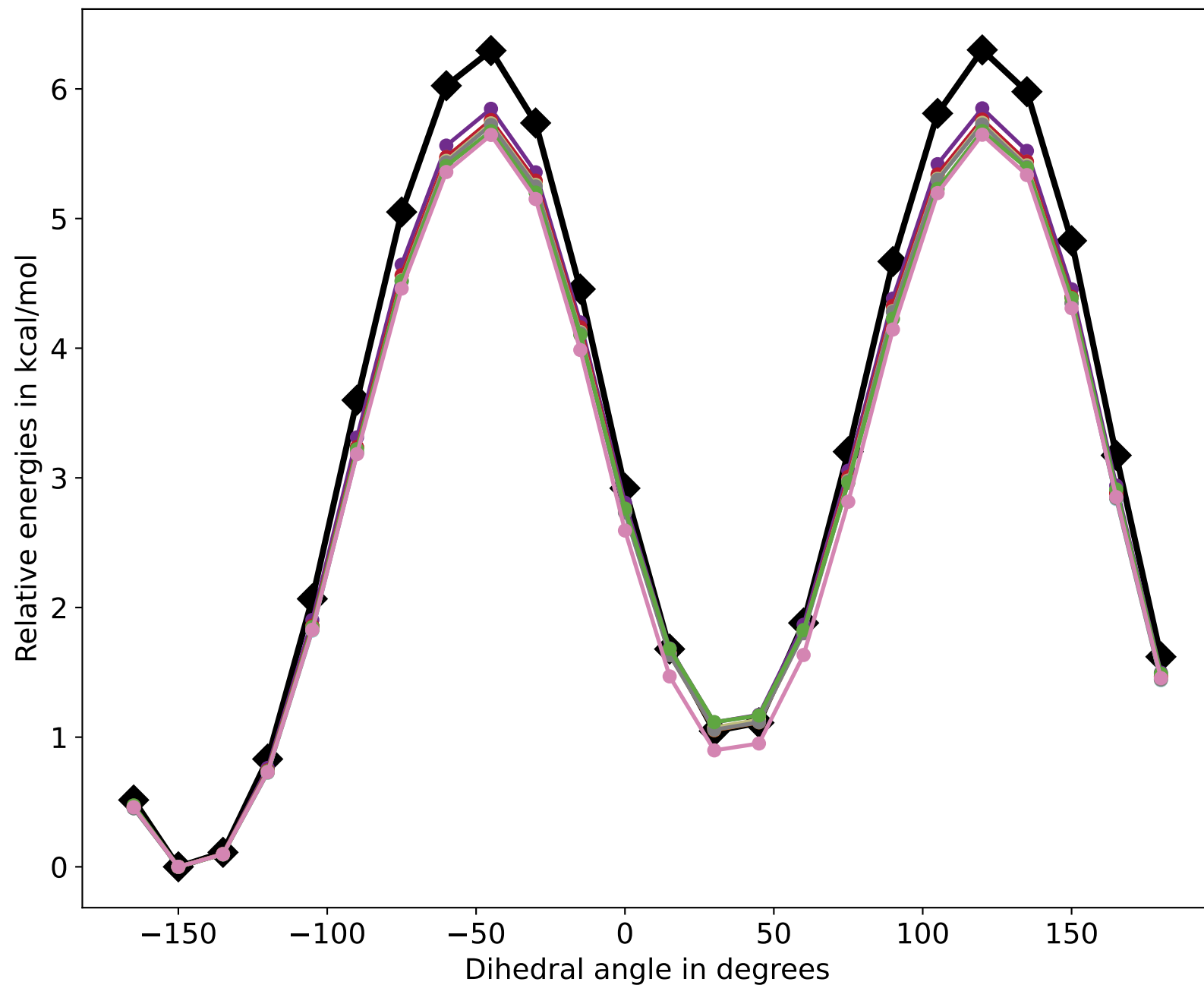




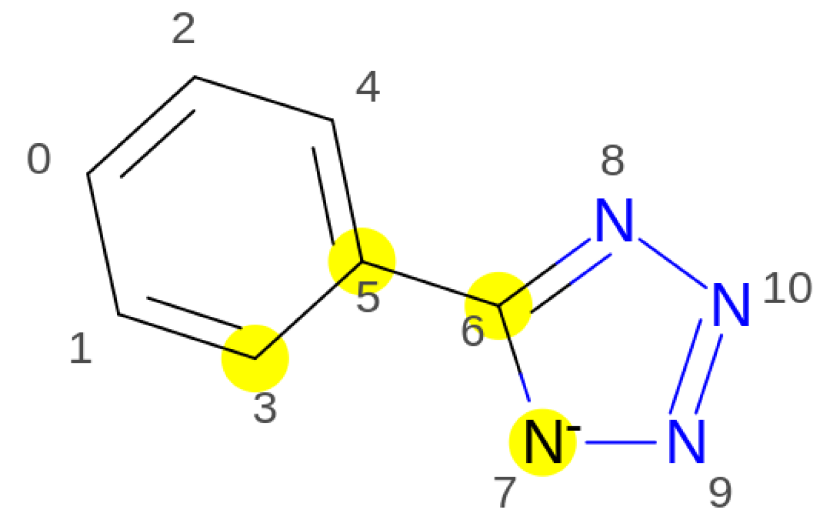
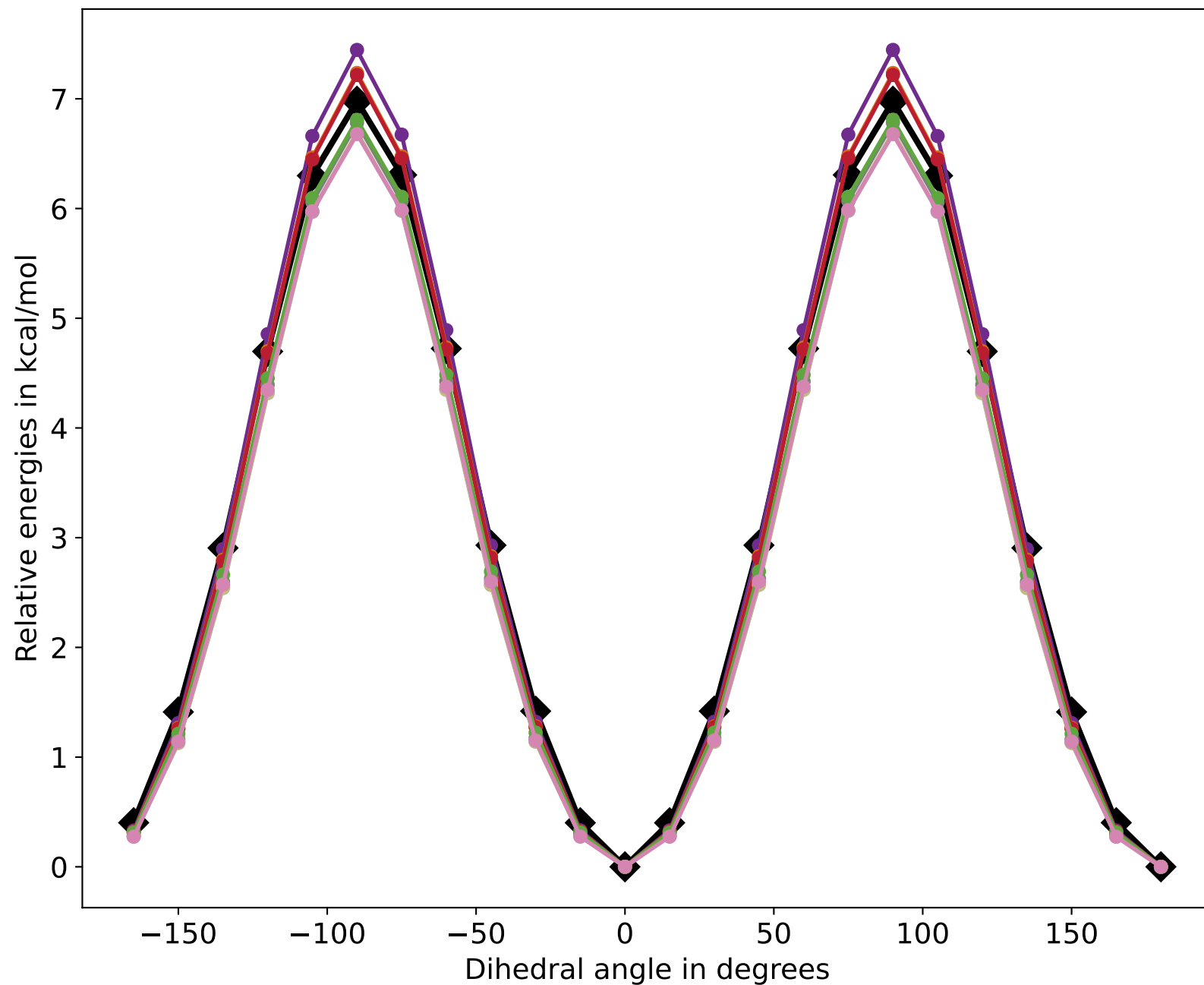






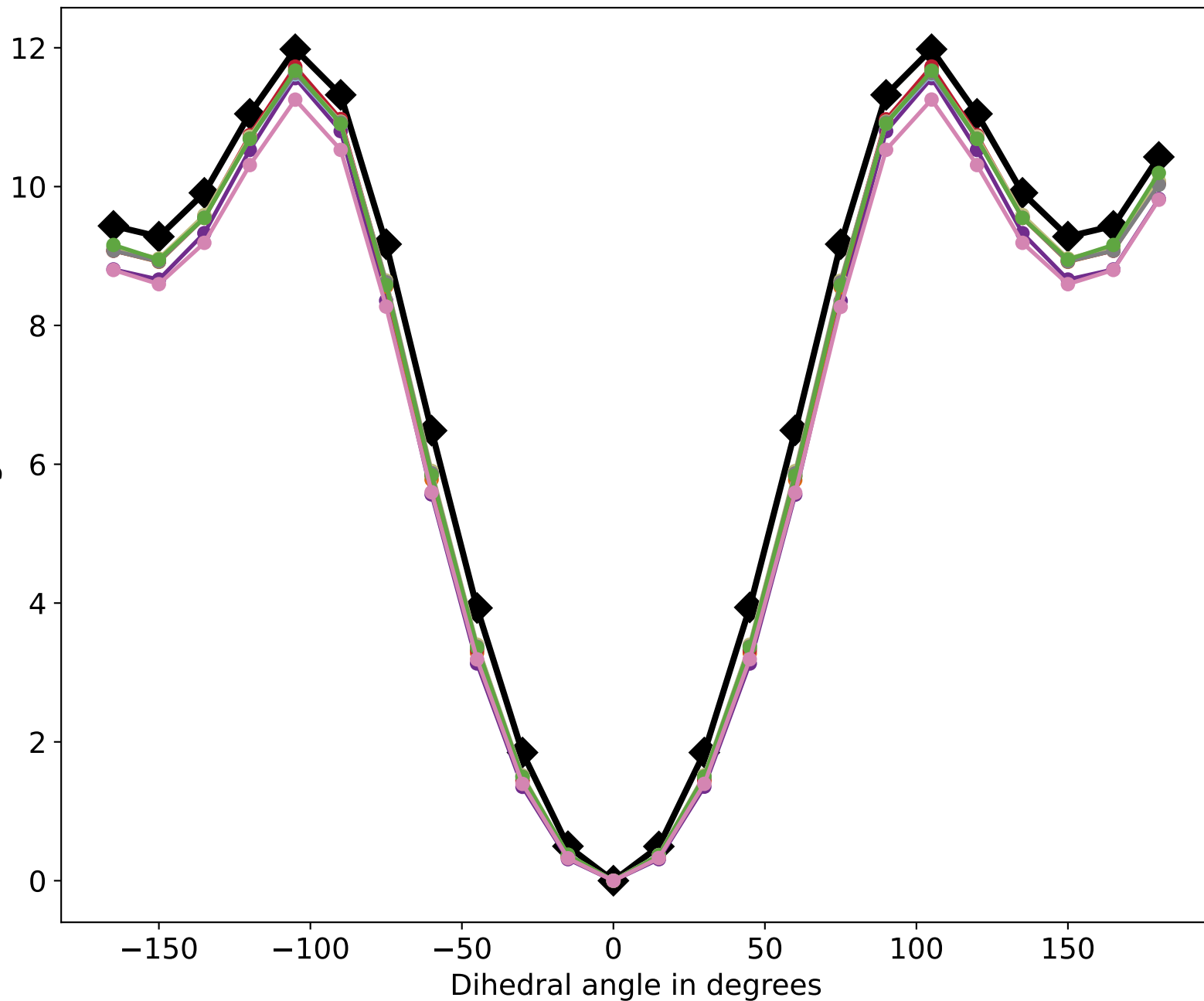




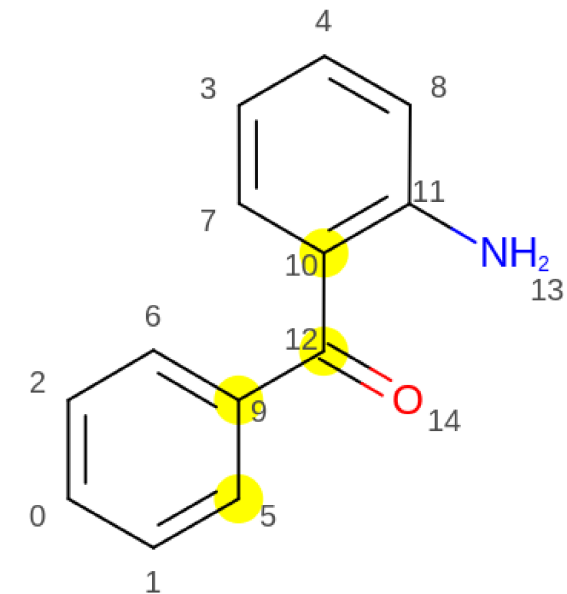
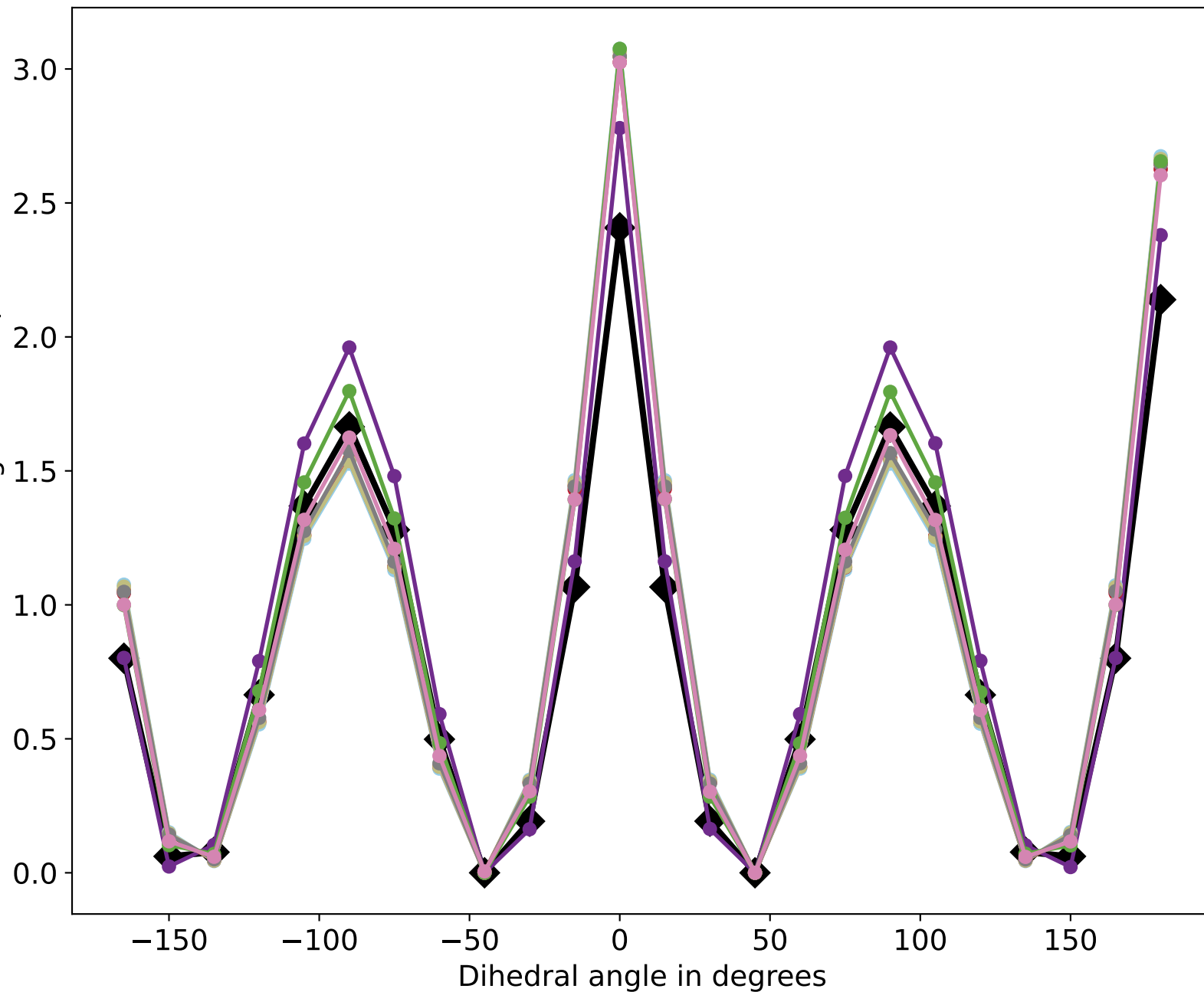


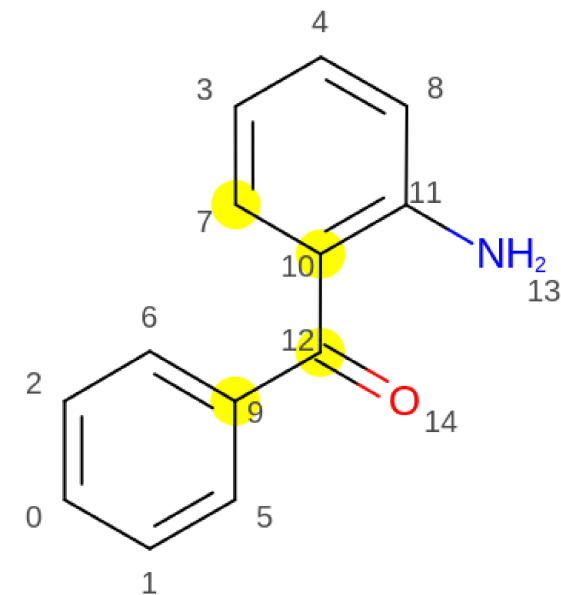
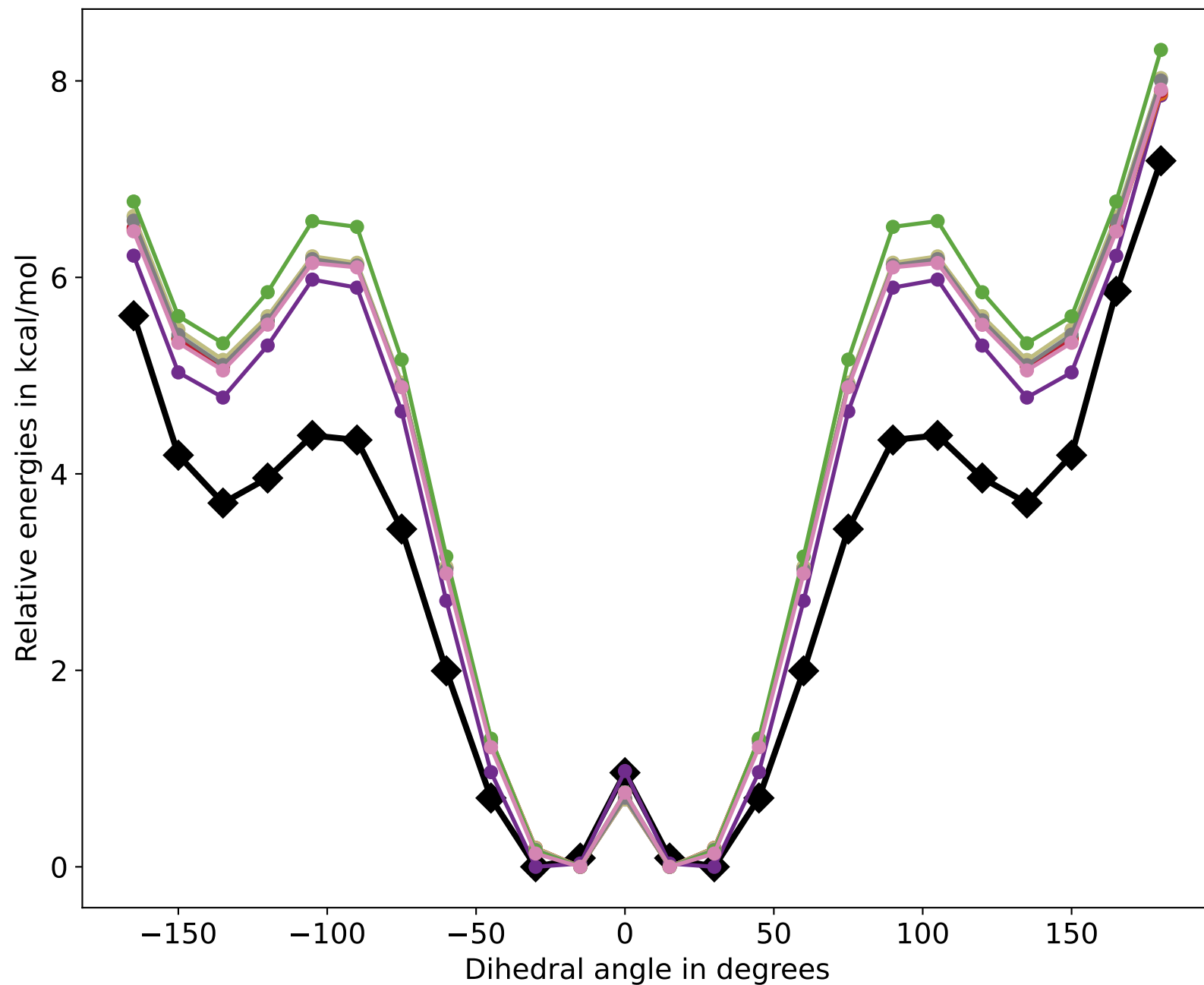
- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*

Relative energies in kcal/mol

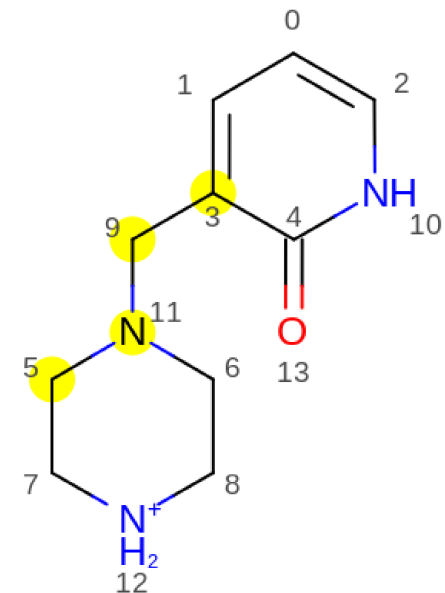
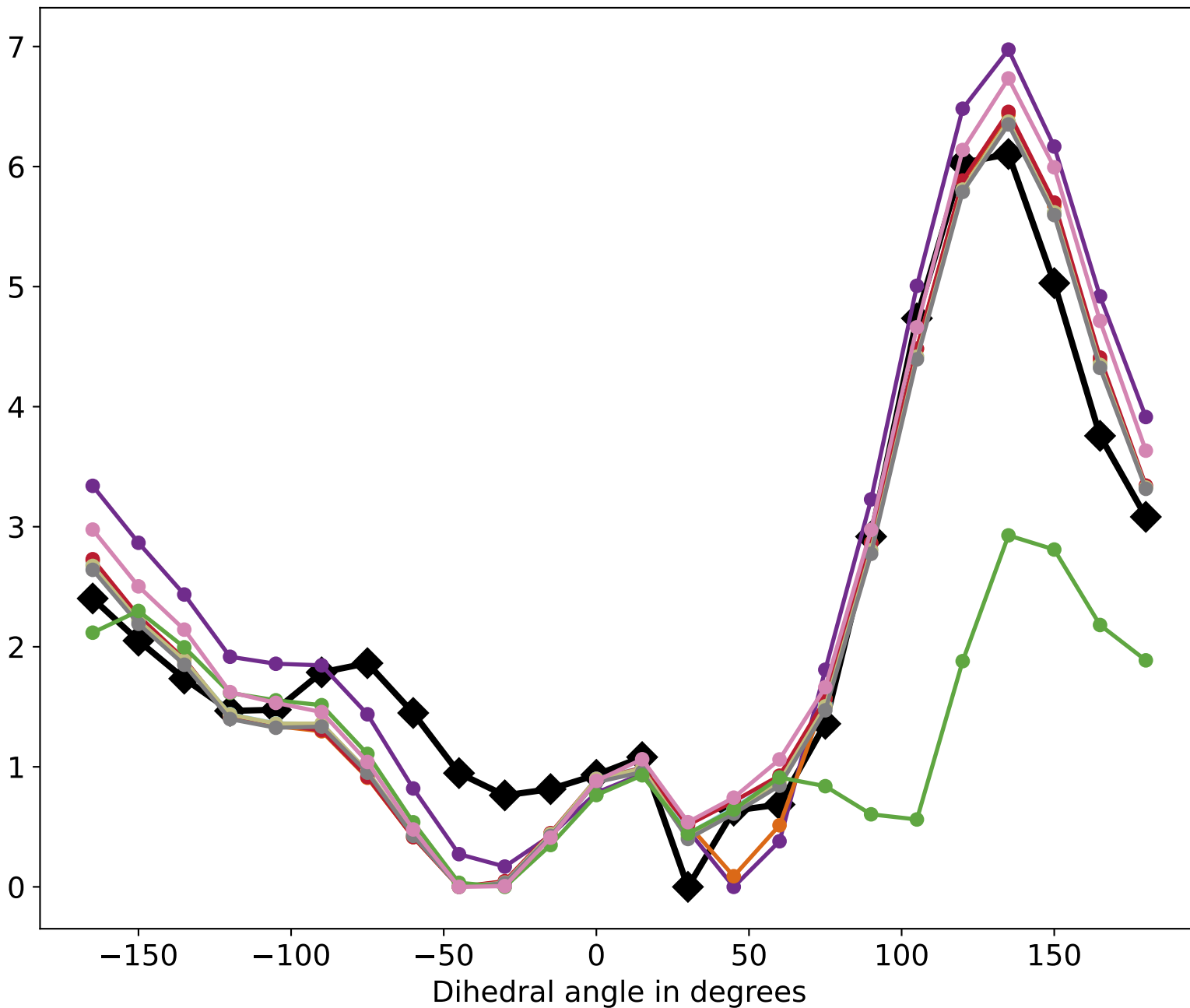


Relative energies in kcal/mol

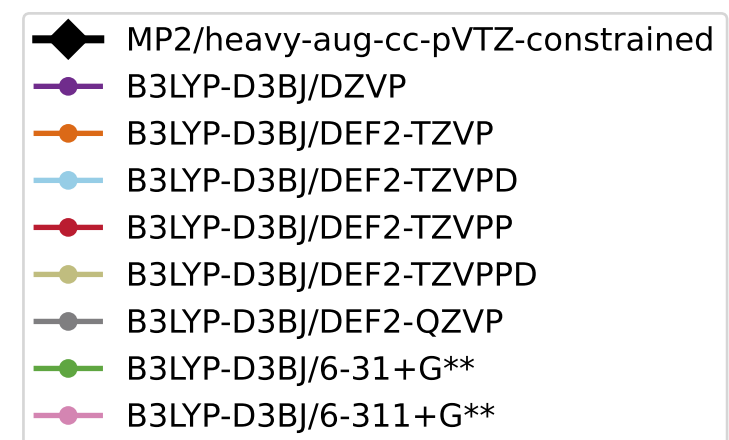
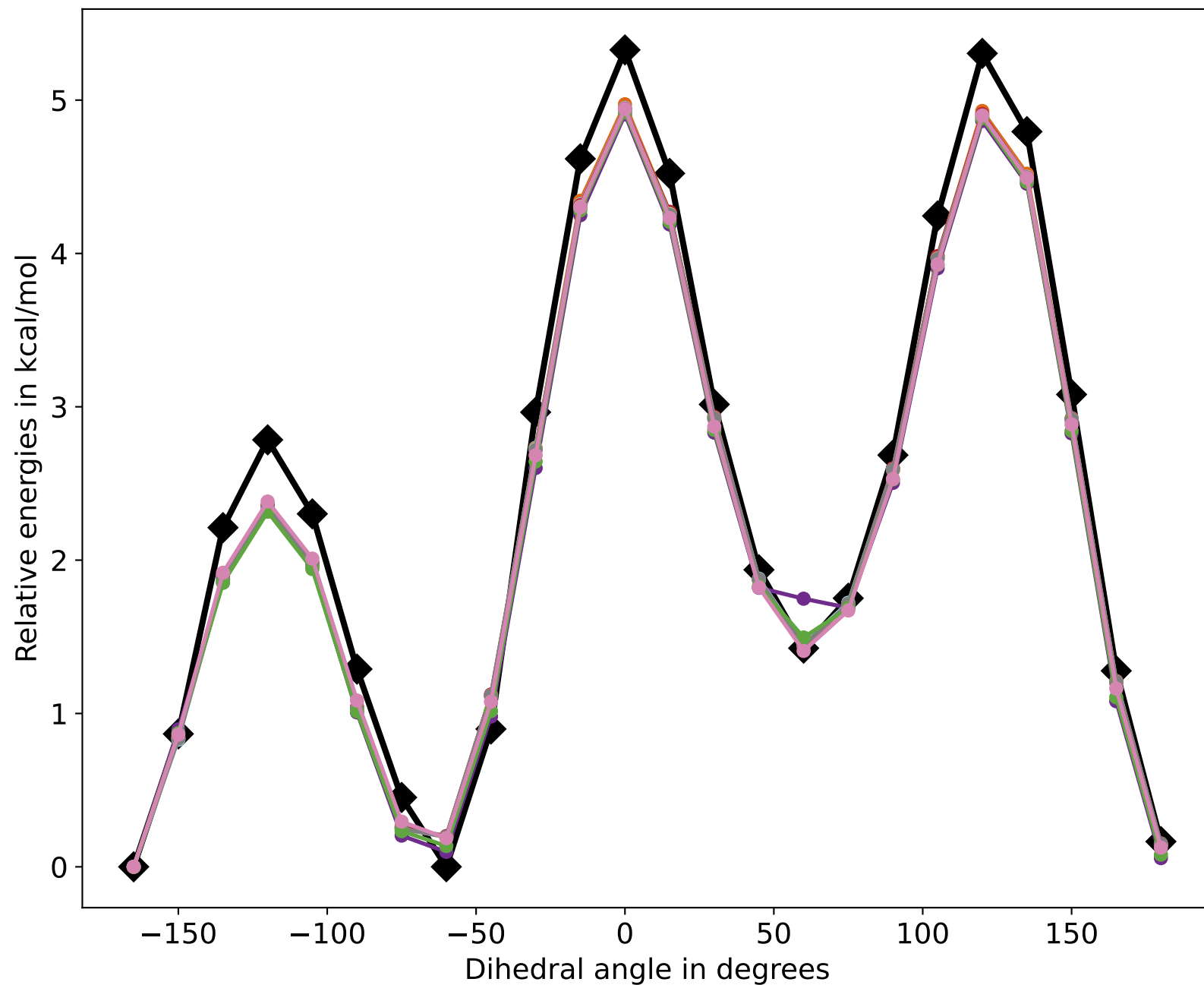




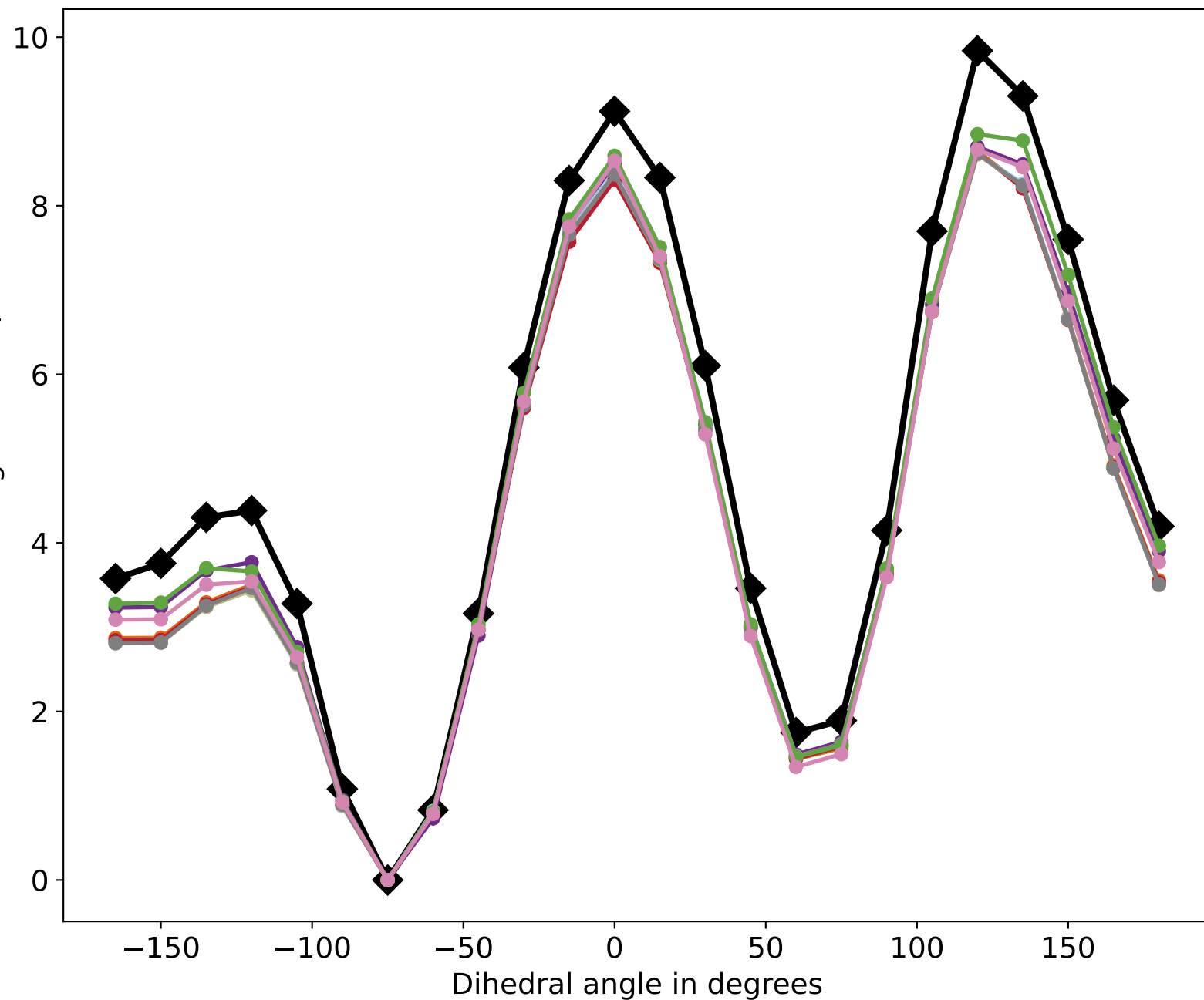
Relative energies in kcal/mol

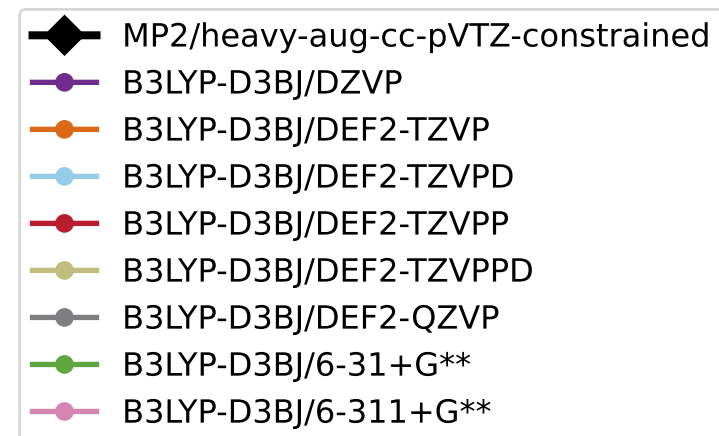
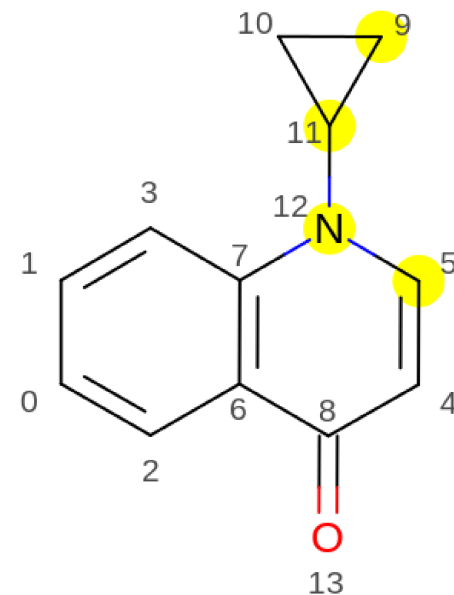
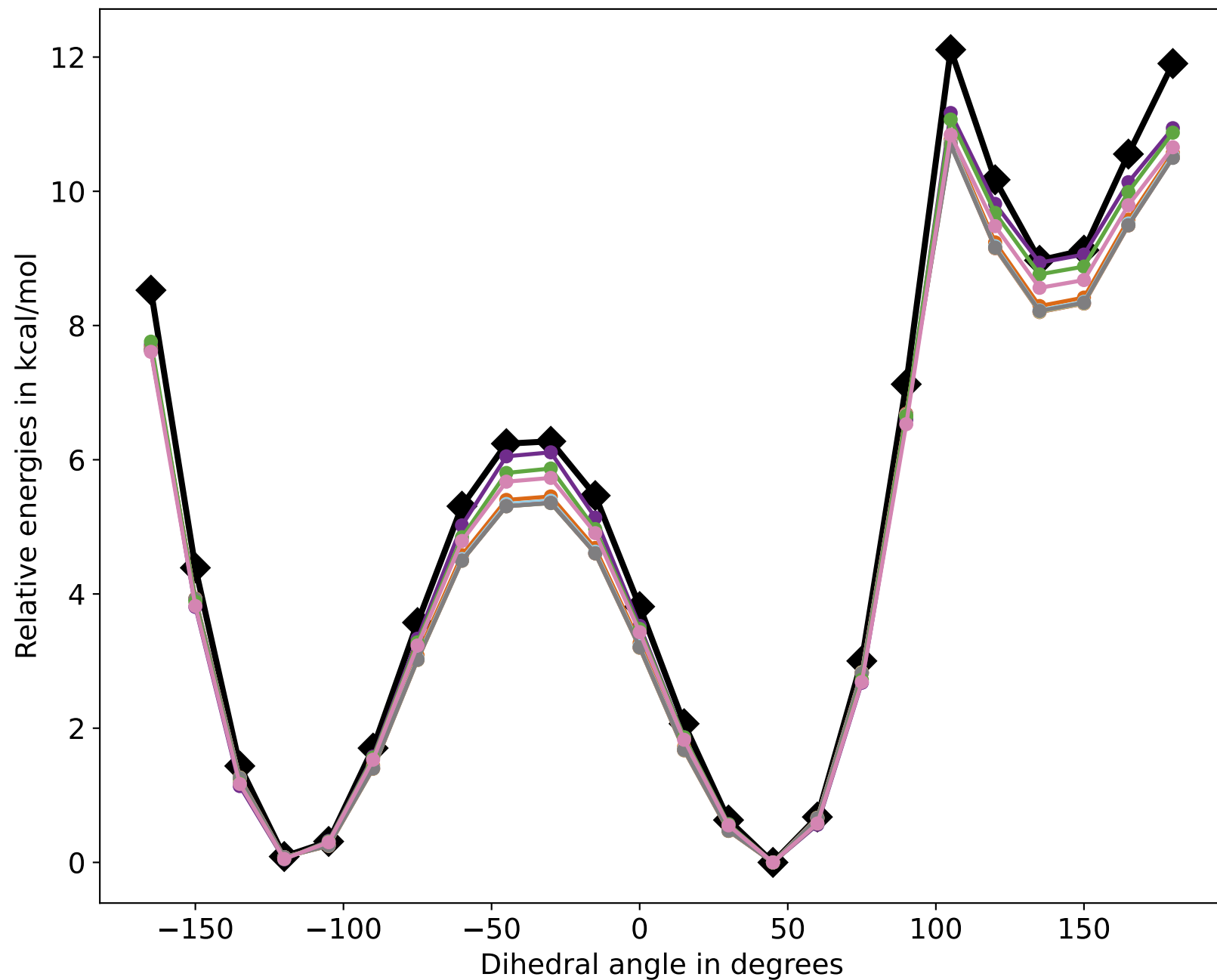


- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*

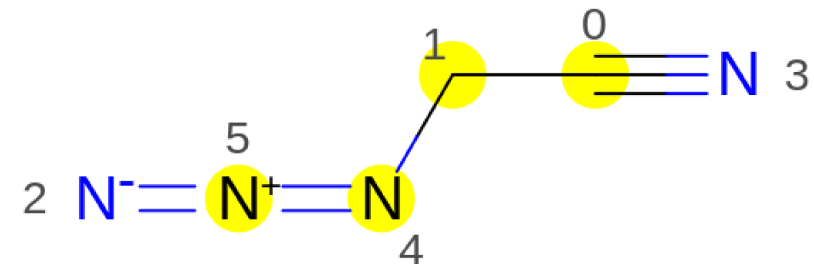
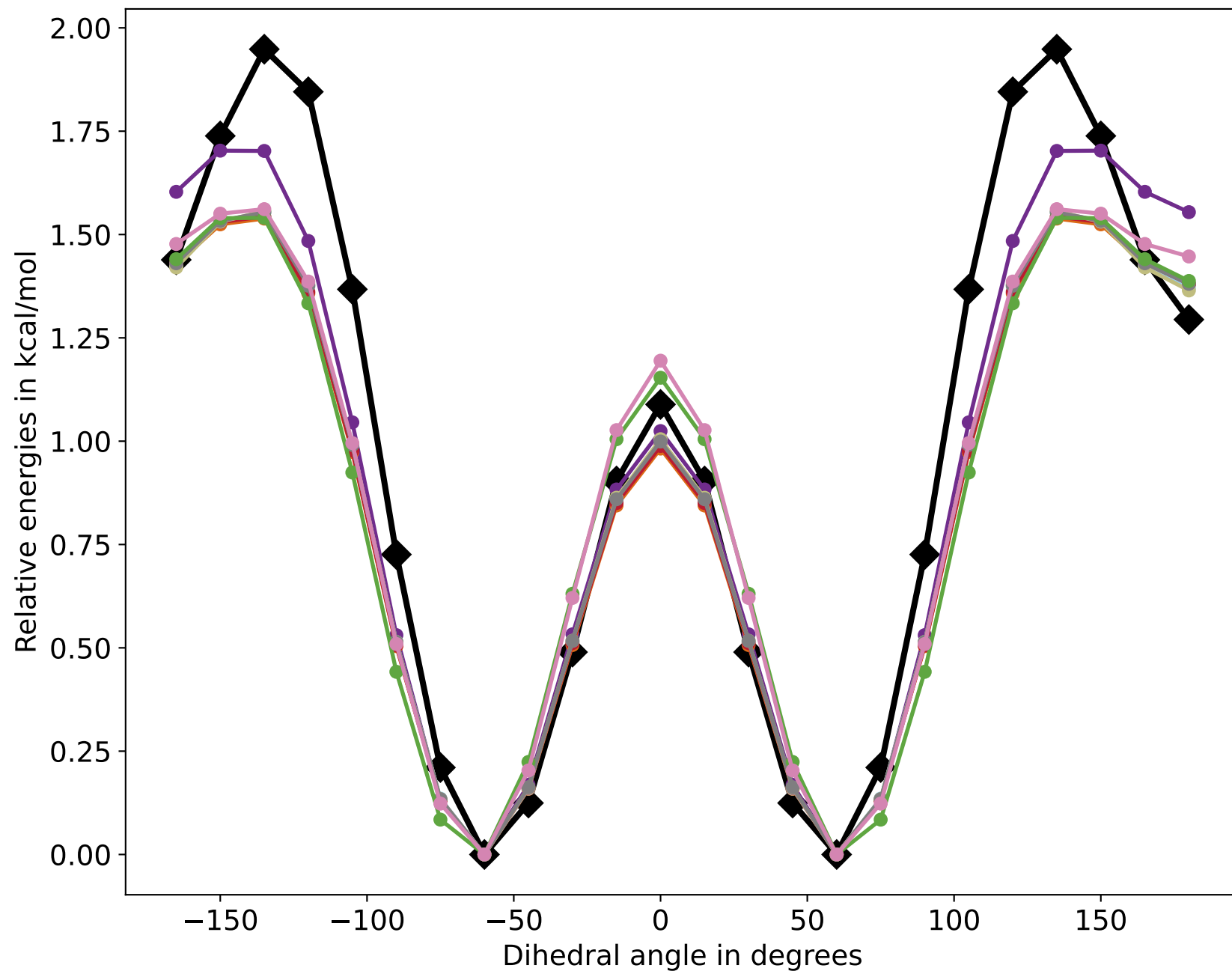


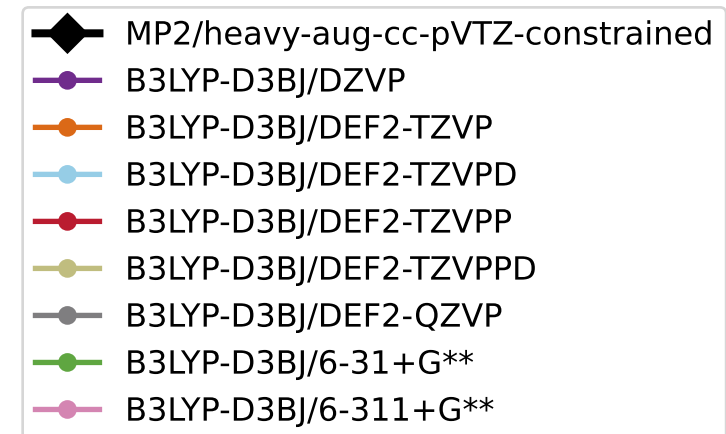
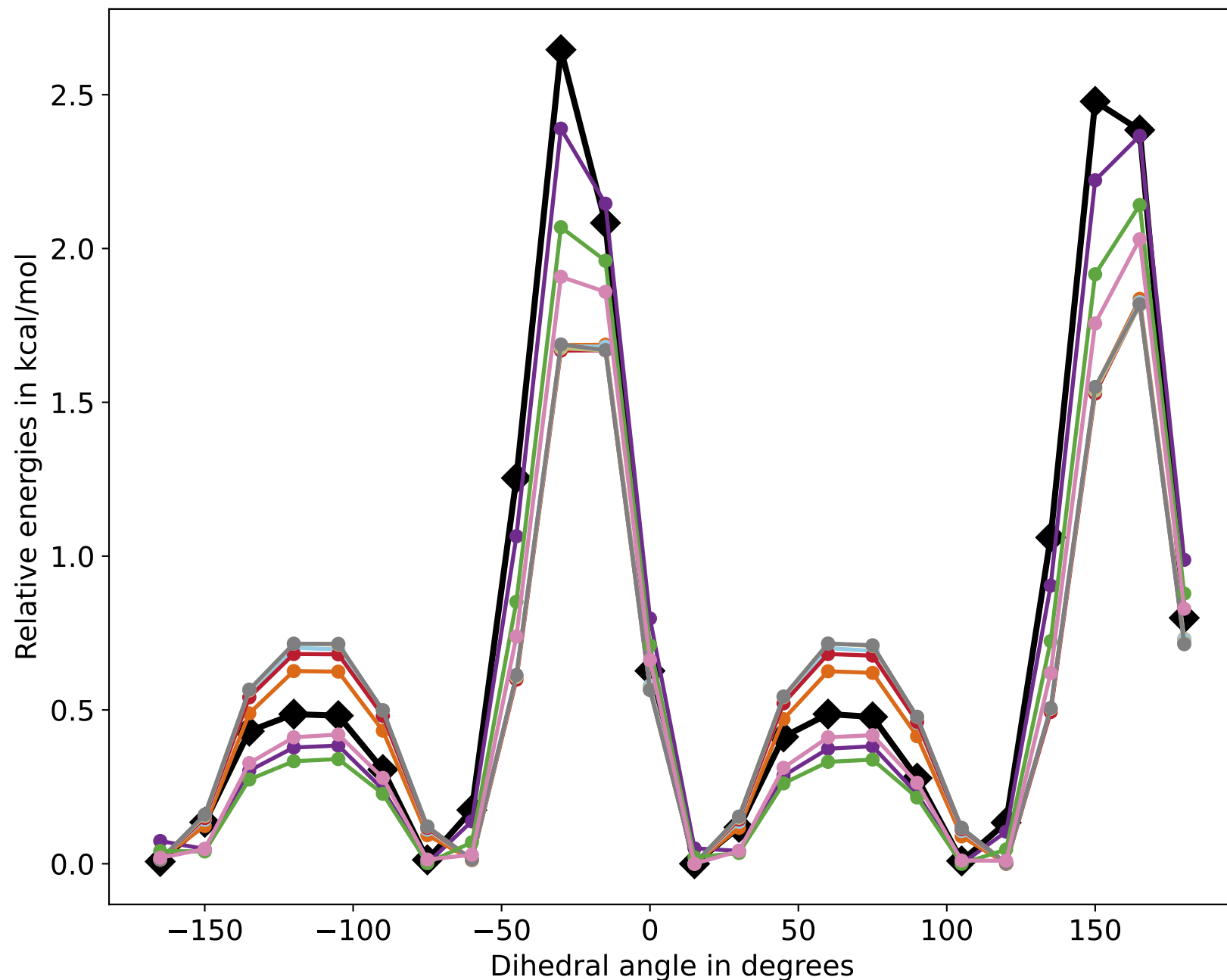
Relative energies in kcal/mol



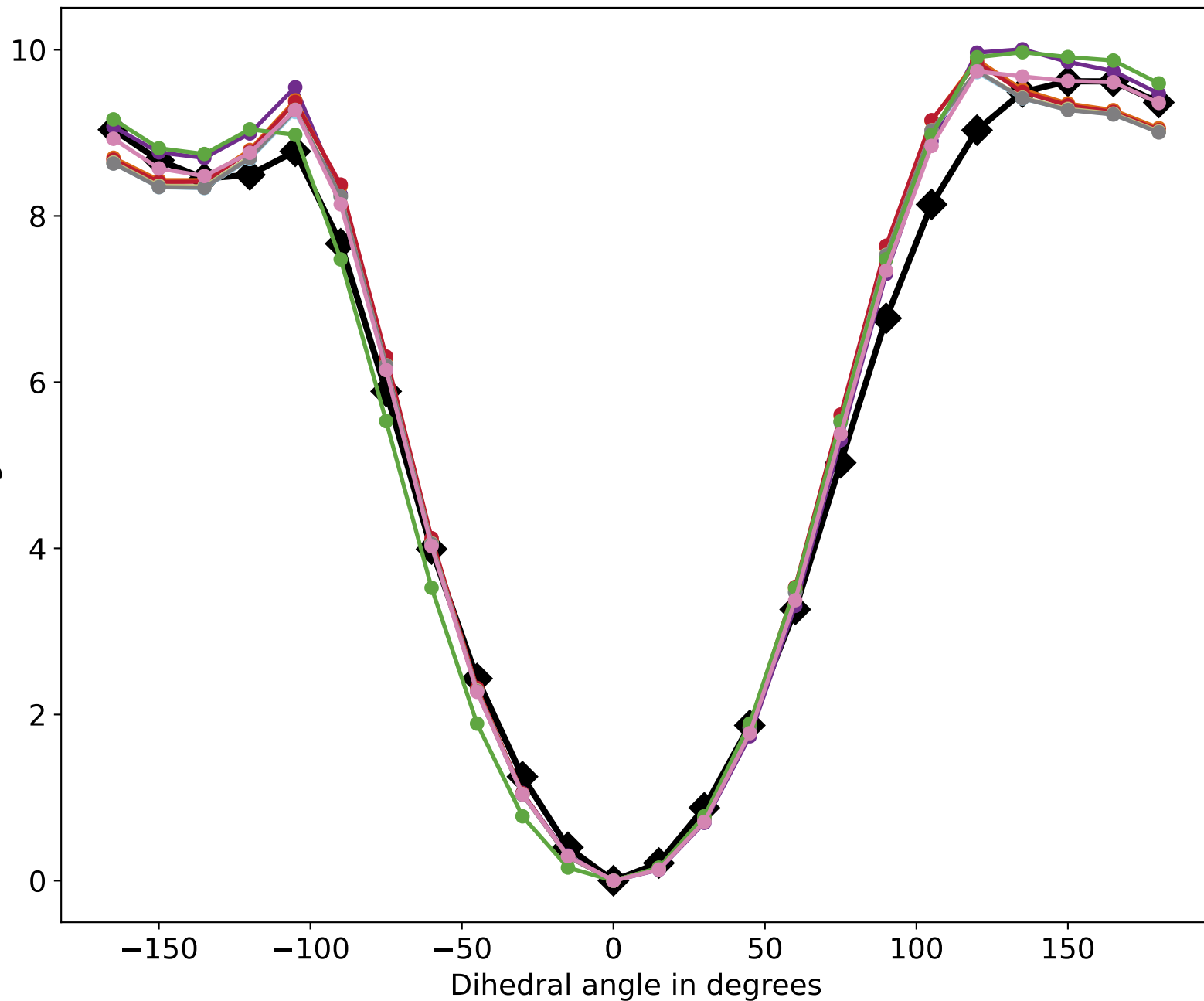




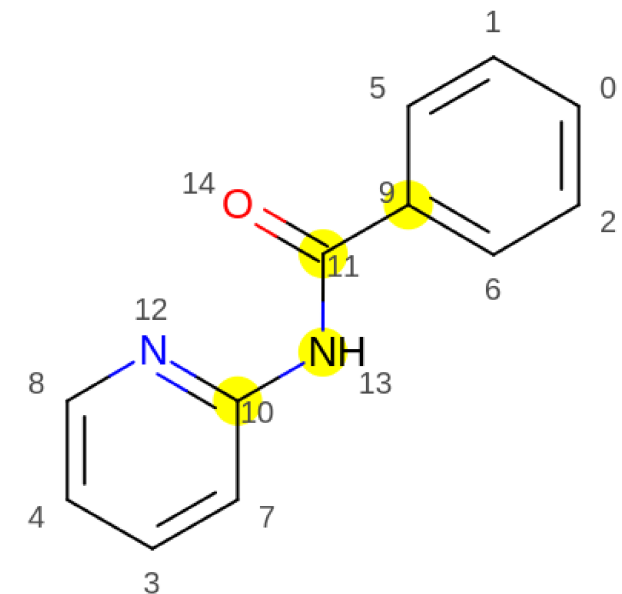
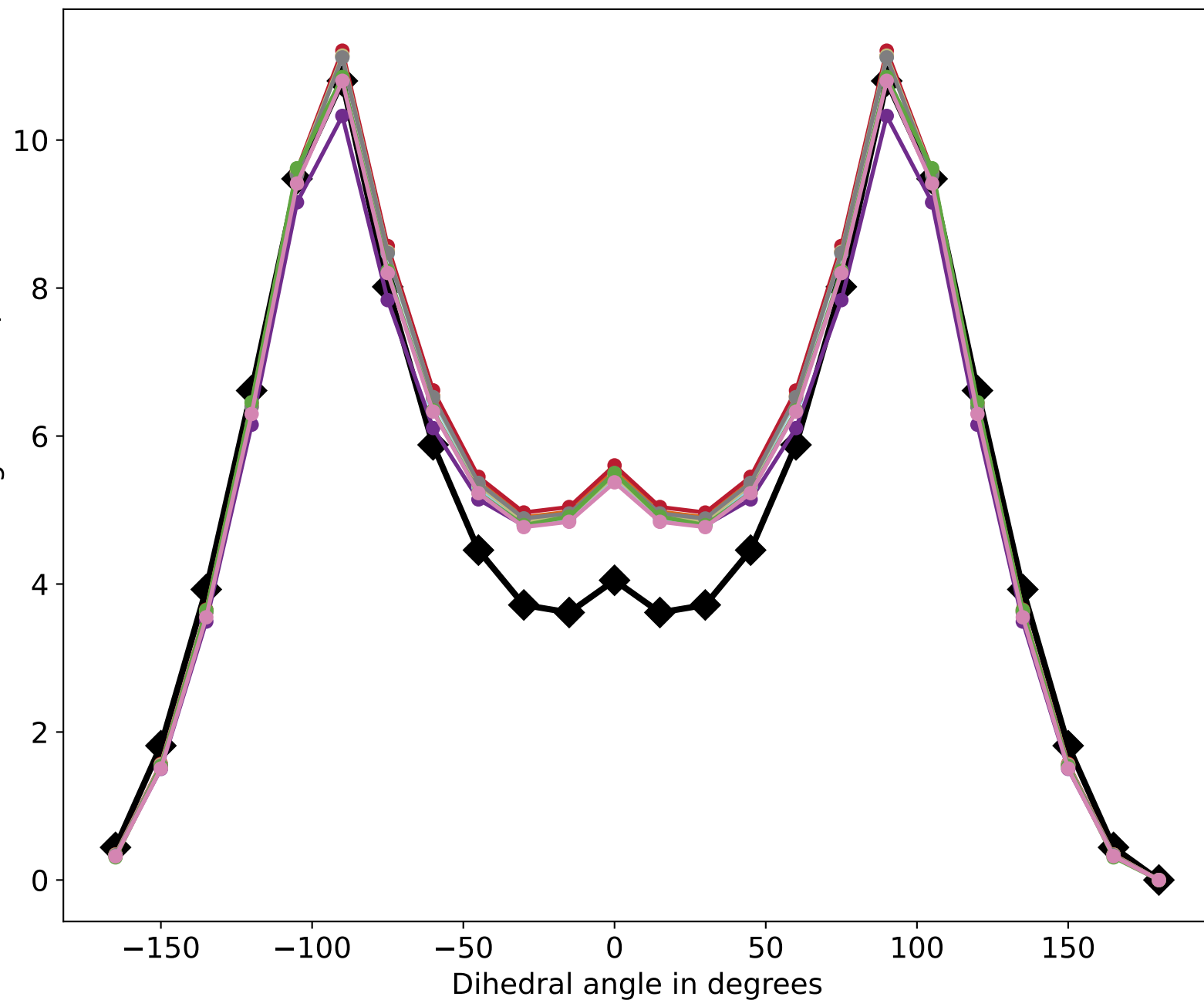


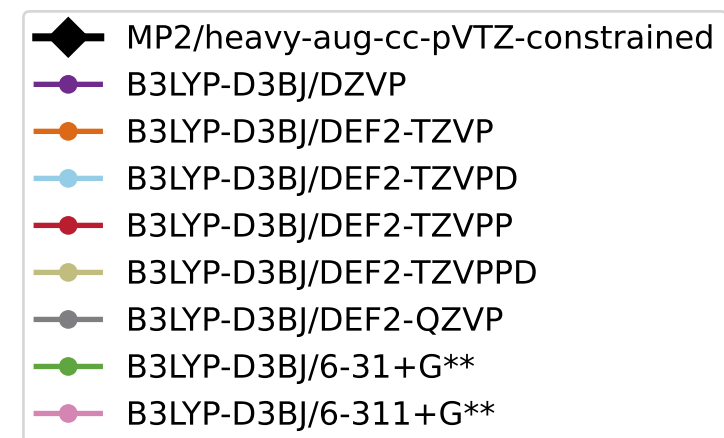
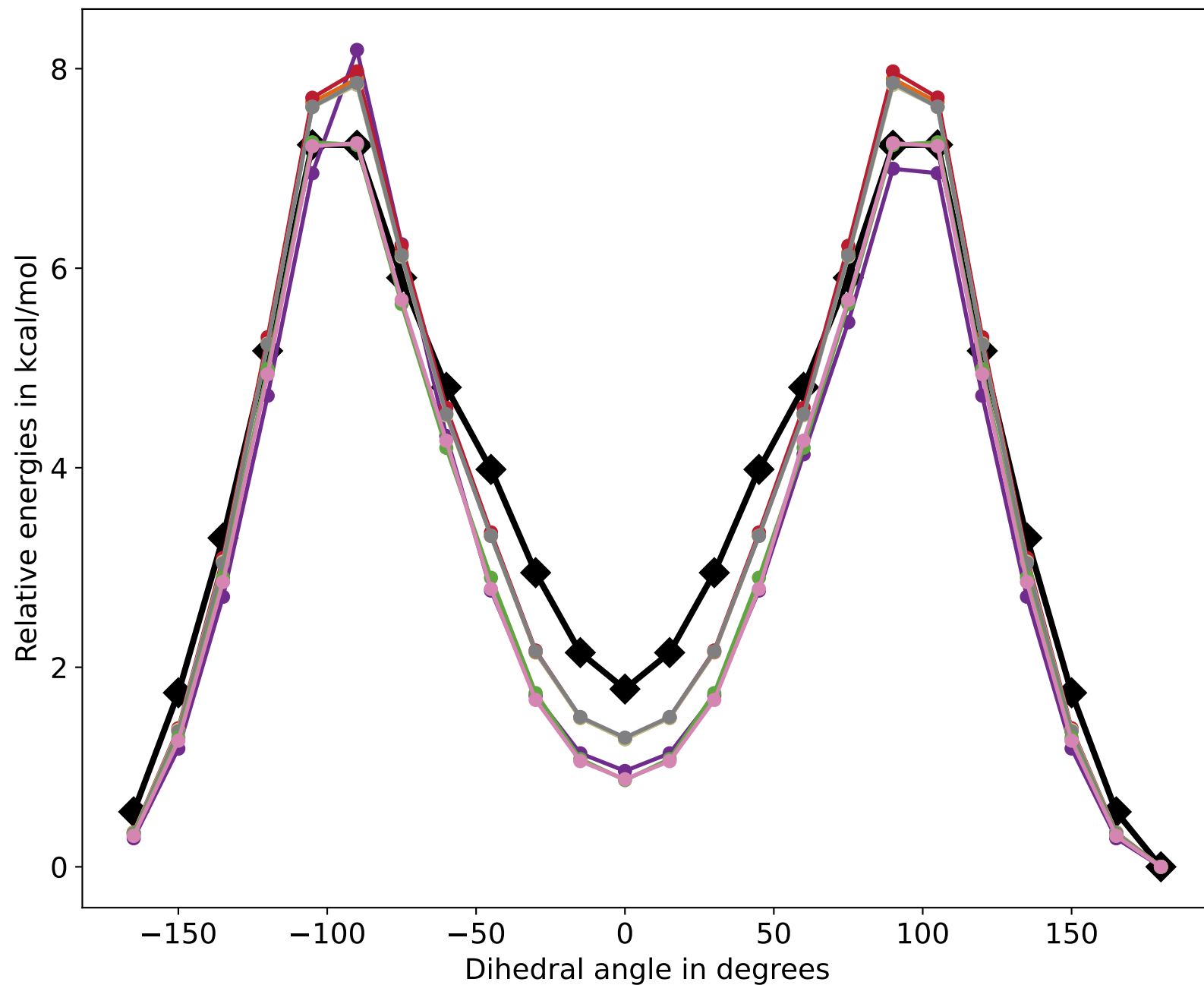


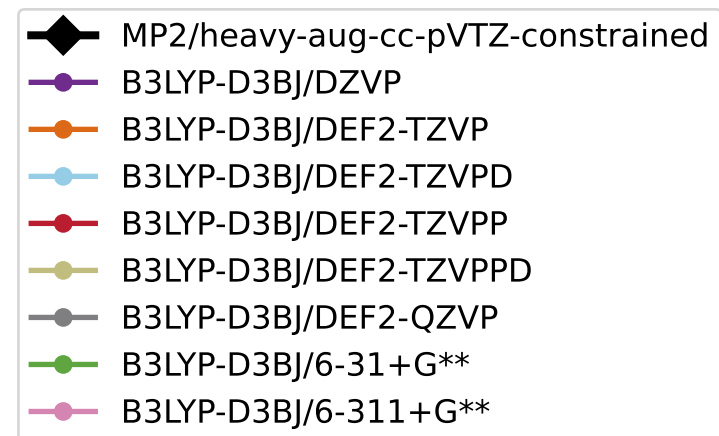
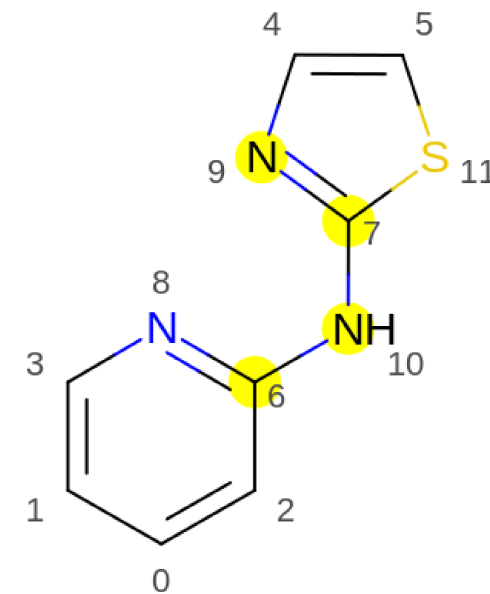
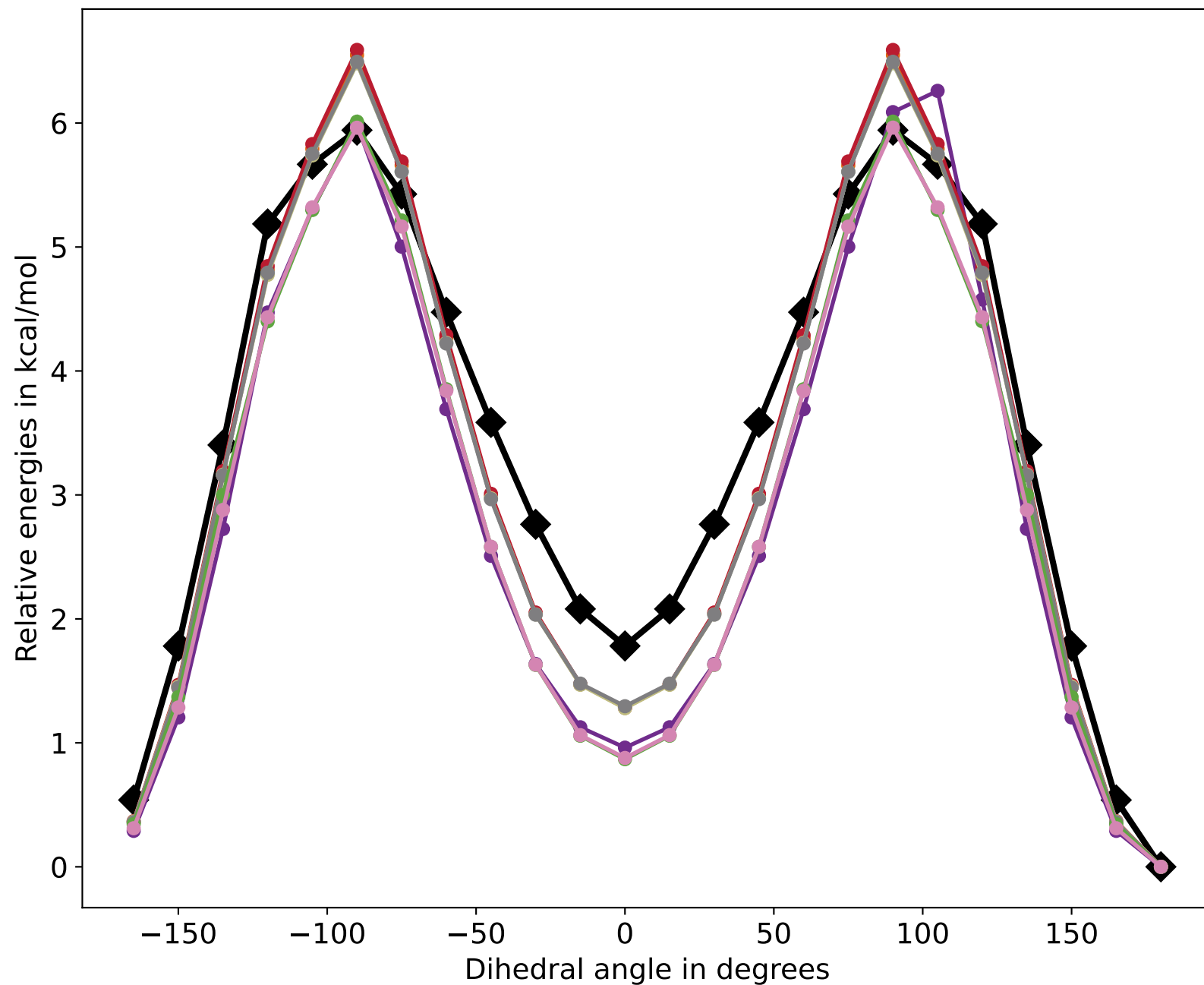
Relative energies in kcal/mol



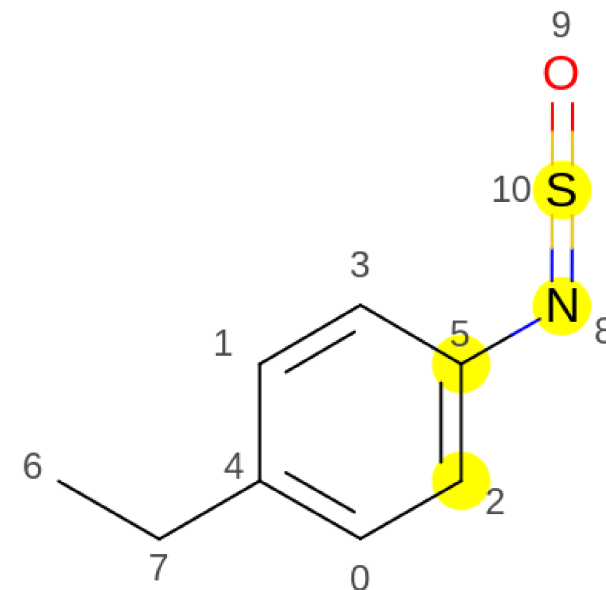
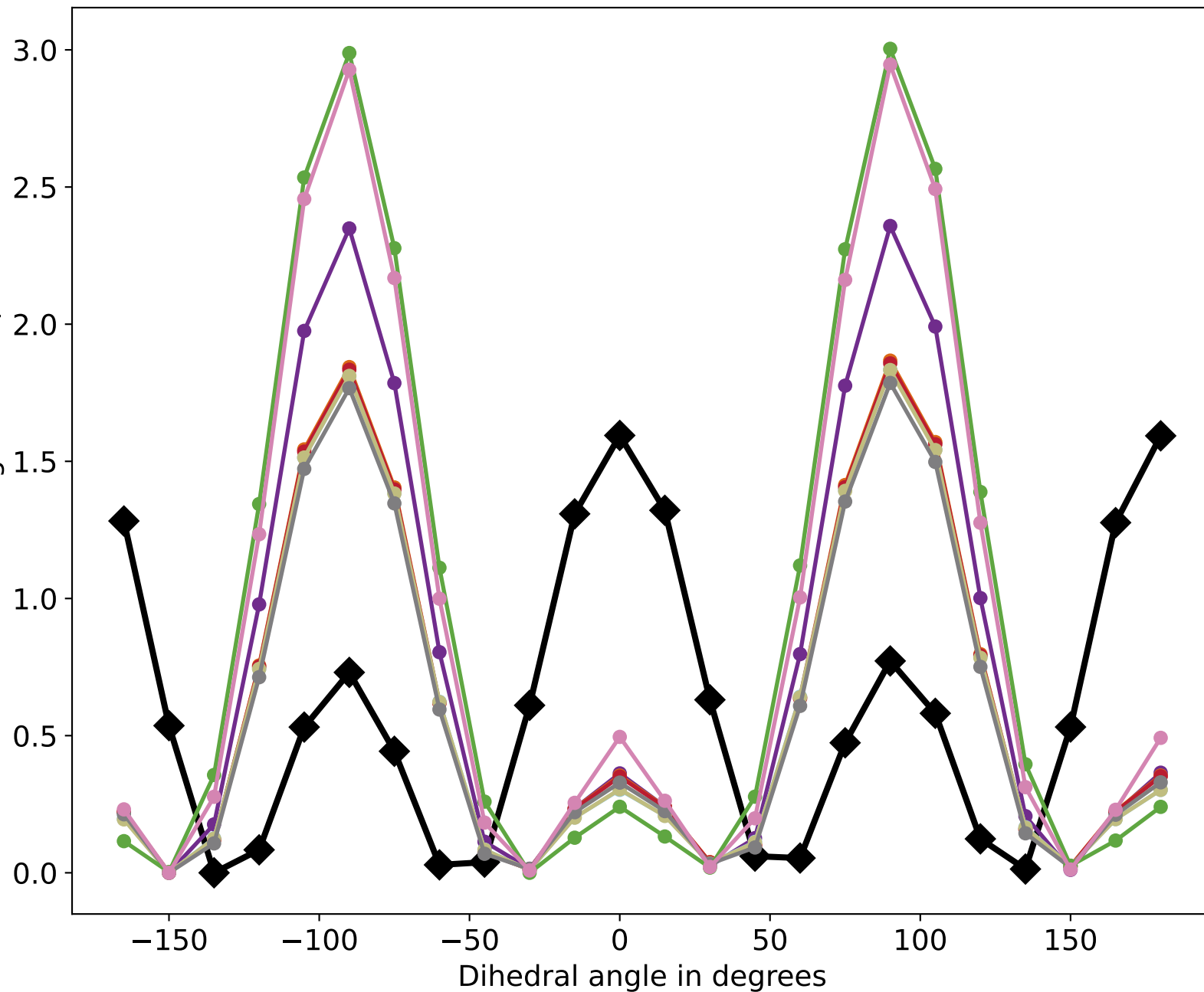
Relative energies in kcal/mol

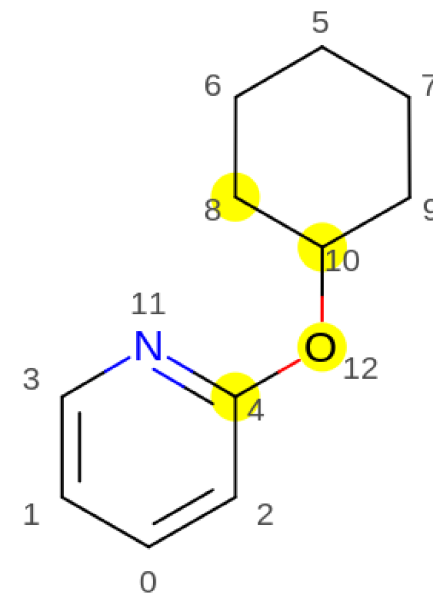
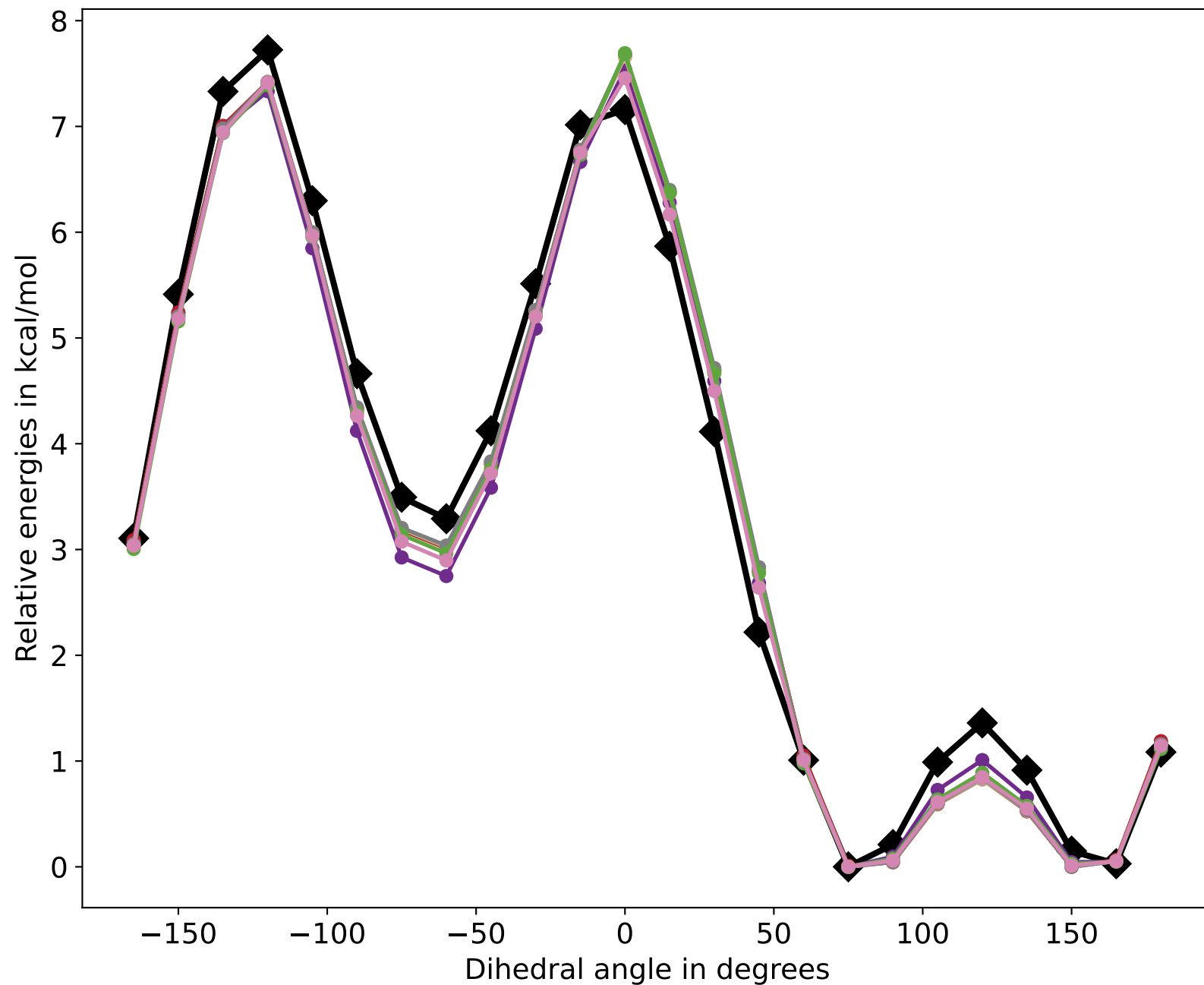






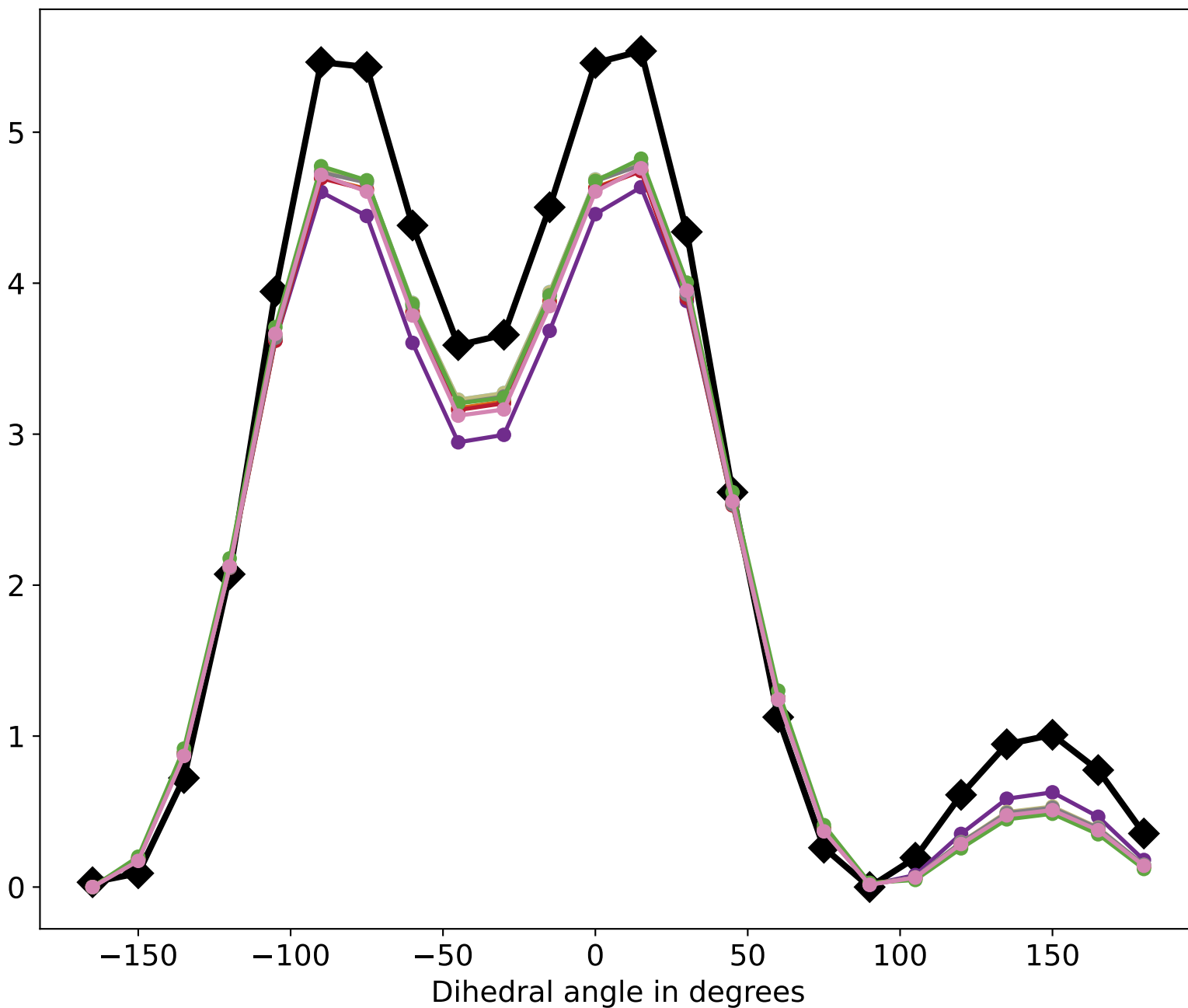
Relative energies in kcal/mol



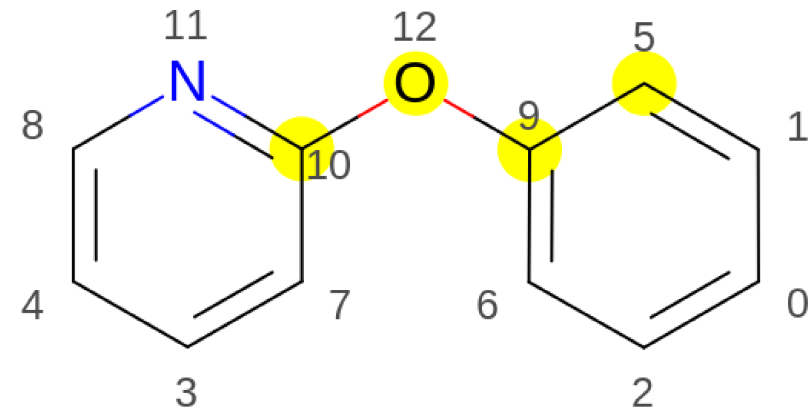
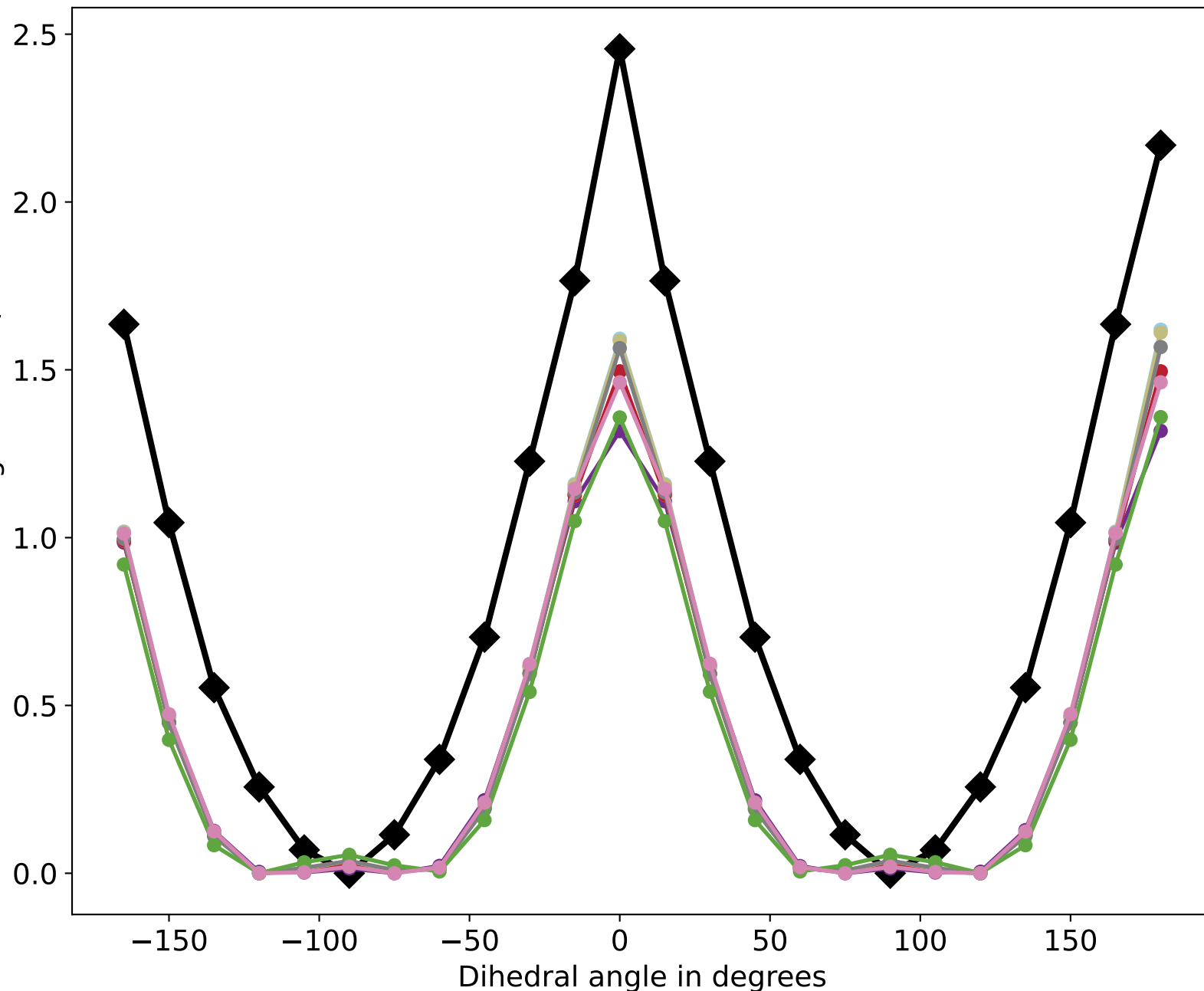


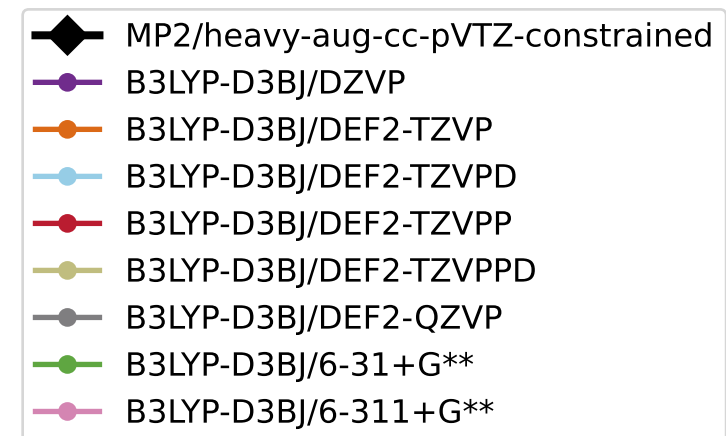
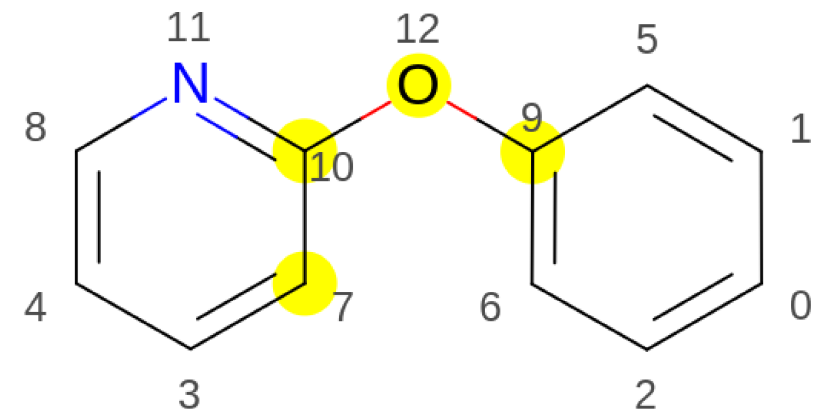
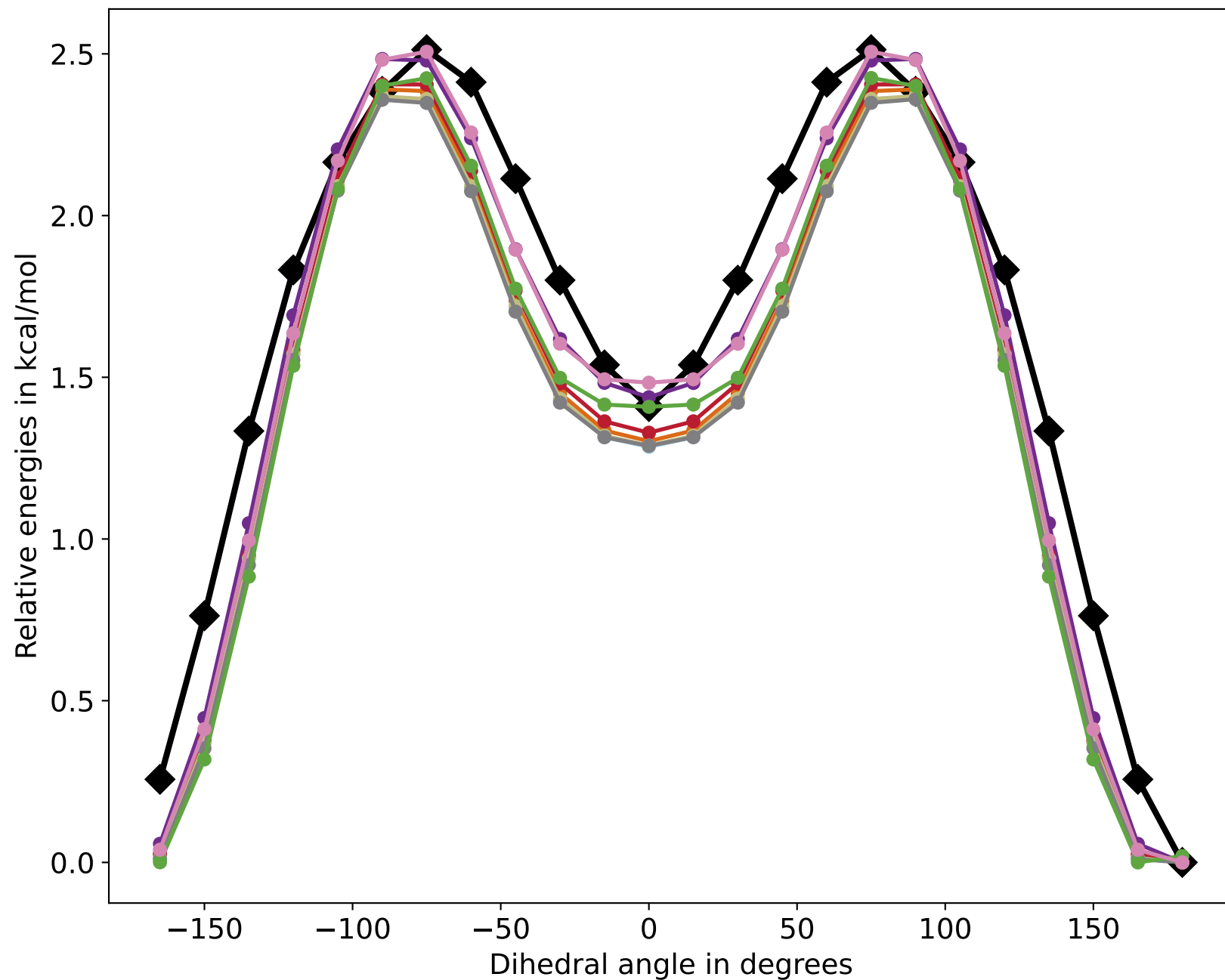


Relative energies in kcal/mol

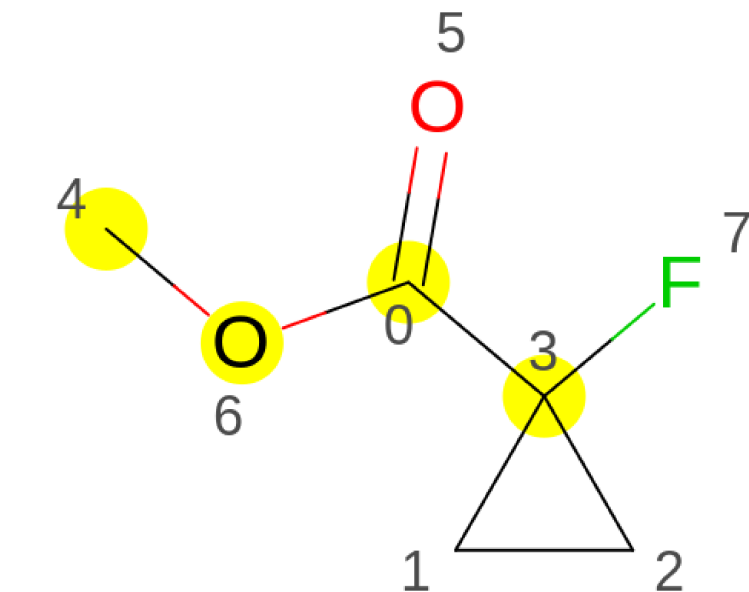
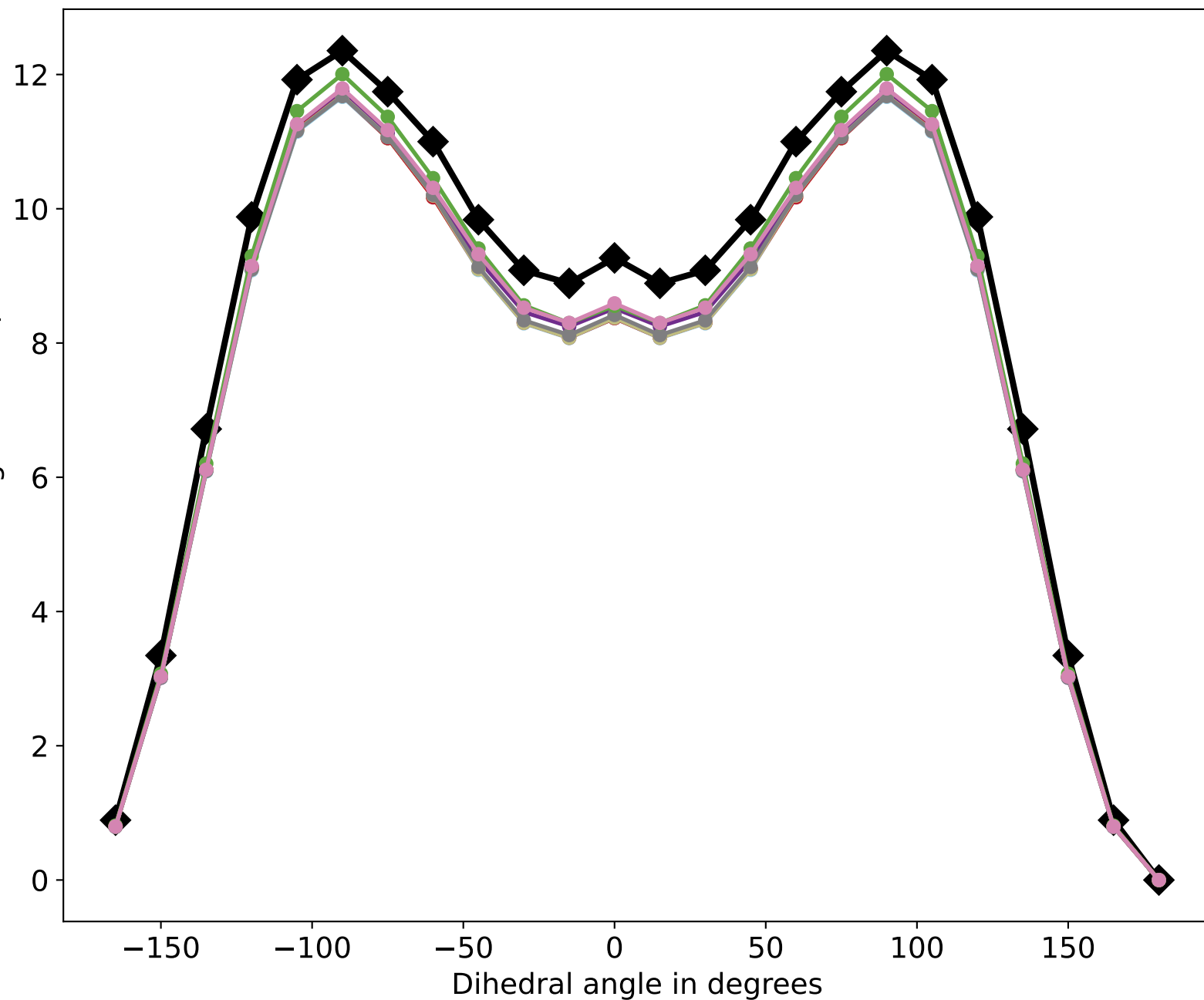


Relative energies in kcal/mol



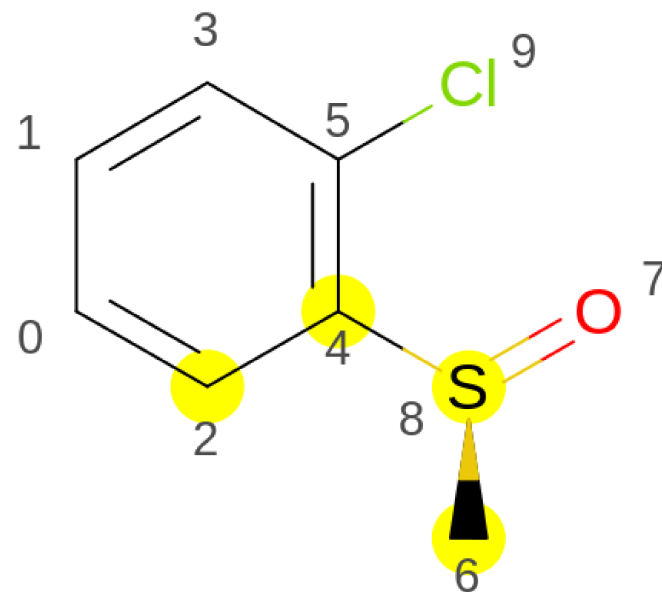
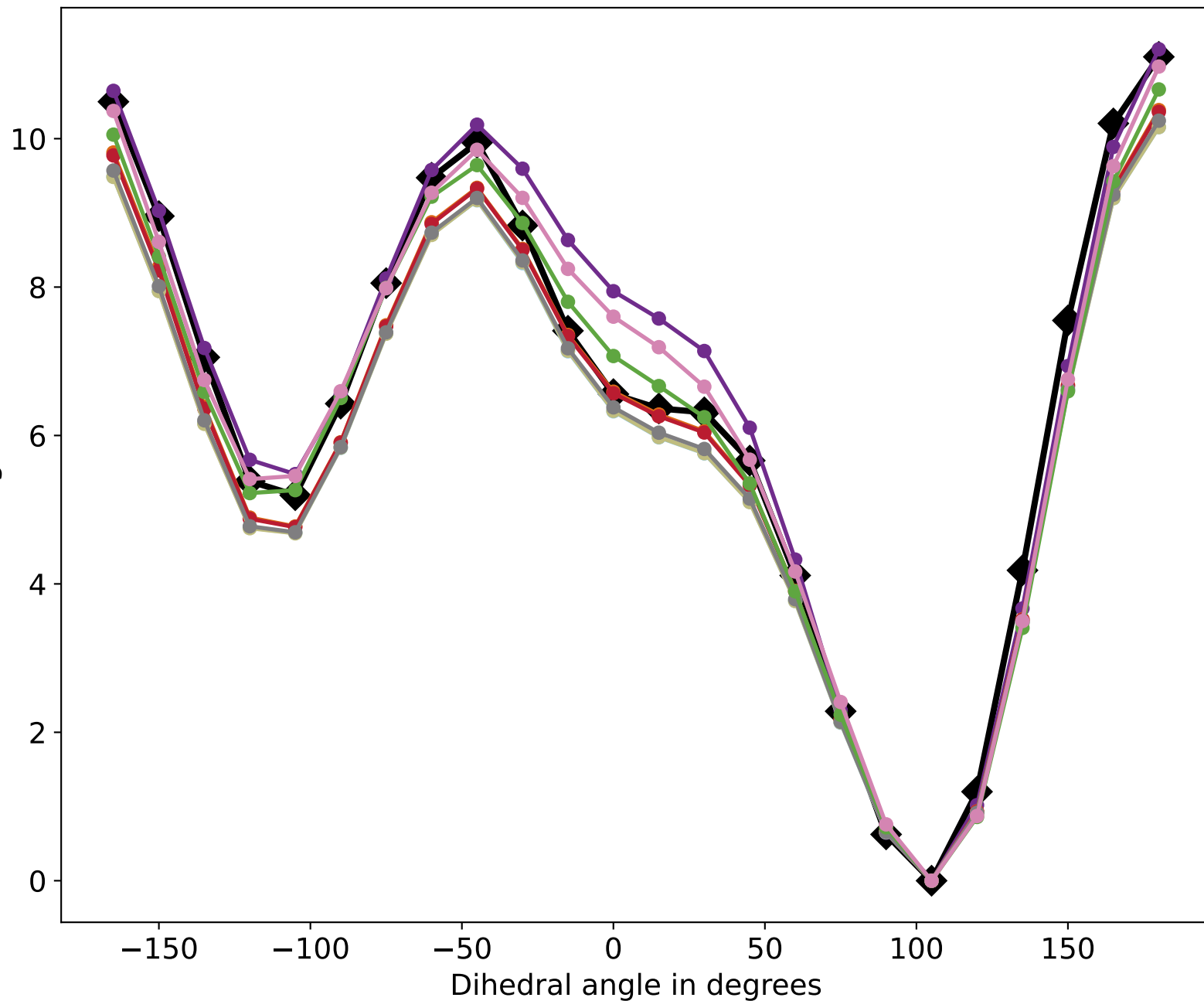


Relative energies in kcal/mol

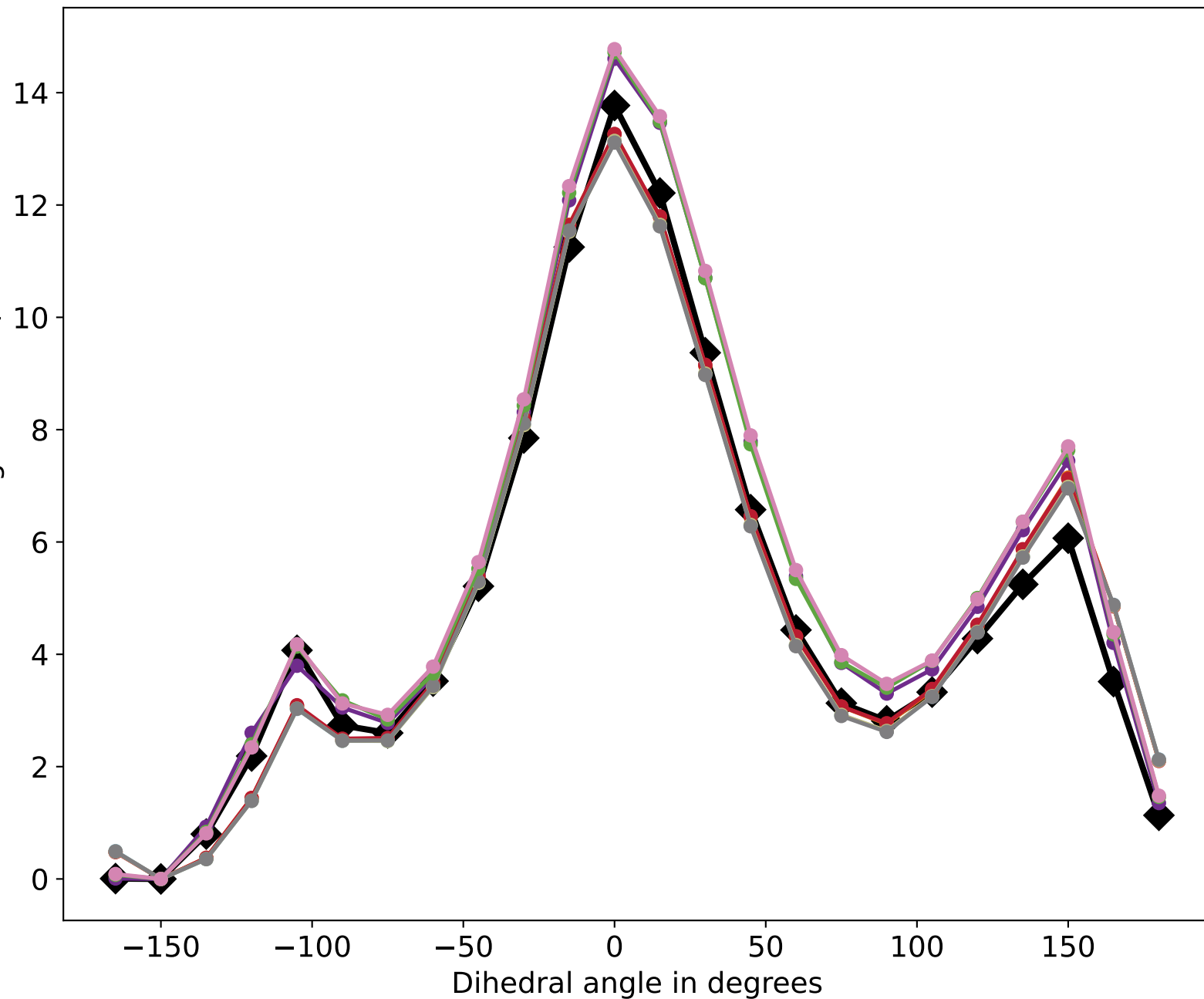


- MP2/heavy-aug-cc-pVTZ-constrained
- B3LYP-D3BJ/DZVP
- B3LYP-D3BJ/DEF2-TZVP
- B3LYP-D3BJ/DEF2-TZVPD
- B3LYP-D3BJ/DEF2-TZVPP
- B3LYP-D3BJ/DEF2-TZVPPD
- B3LYP-D3BJ/DEF2-QZVP
- B3LYP-D3BJ/6-31+G\*\*
- B3LYP-D3BJ/6-311+G\*\*

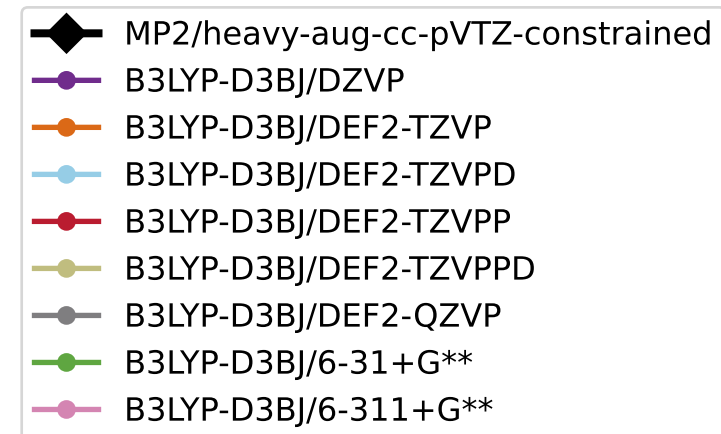
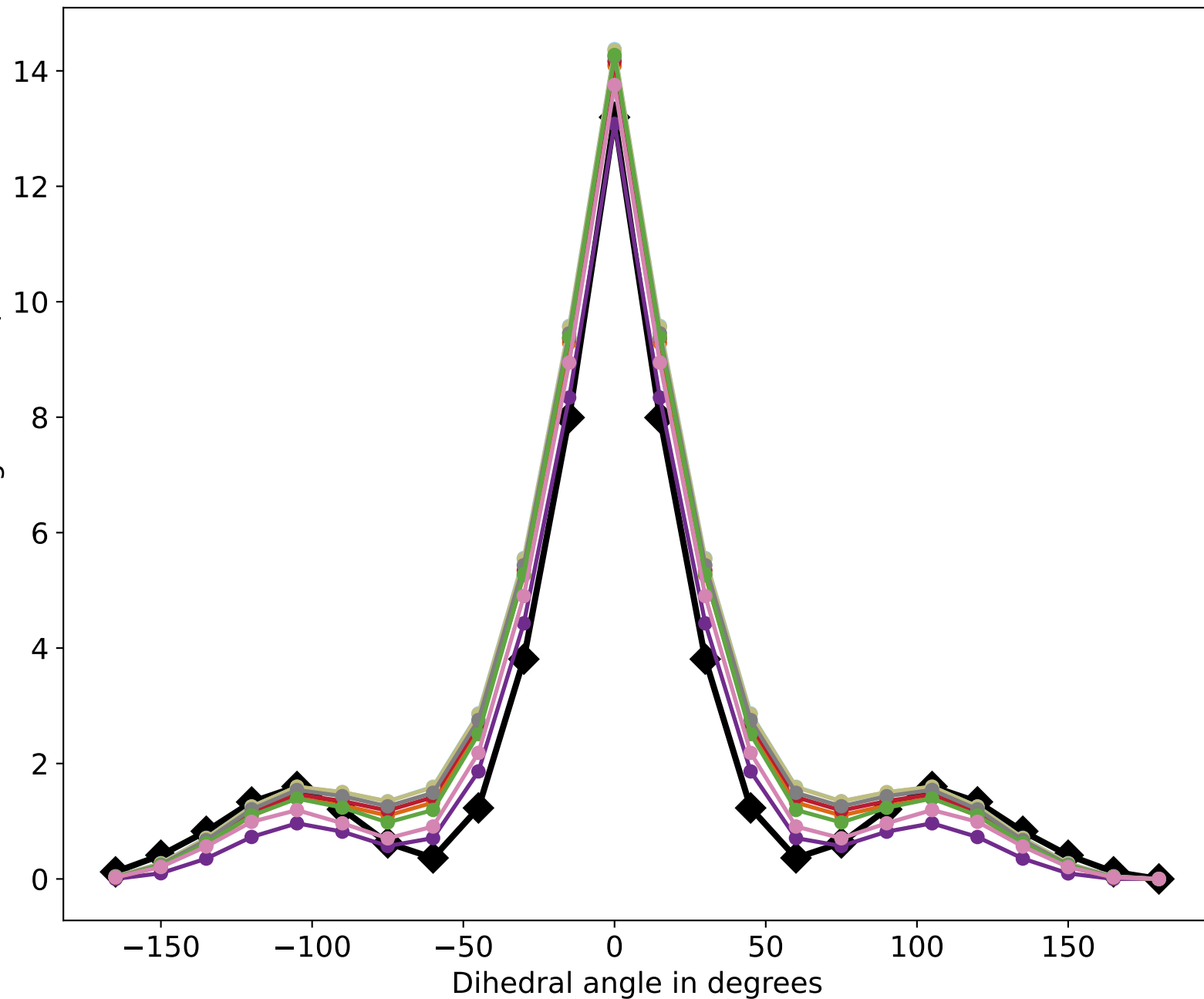
Relative energies in kcal/mol

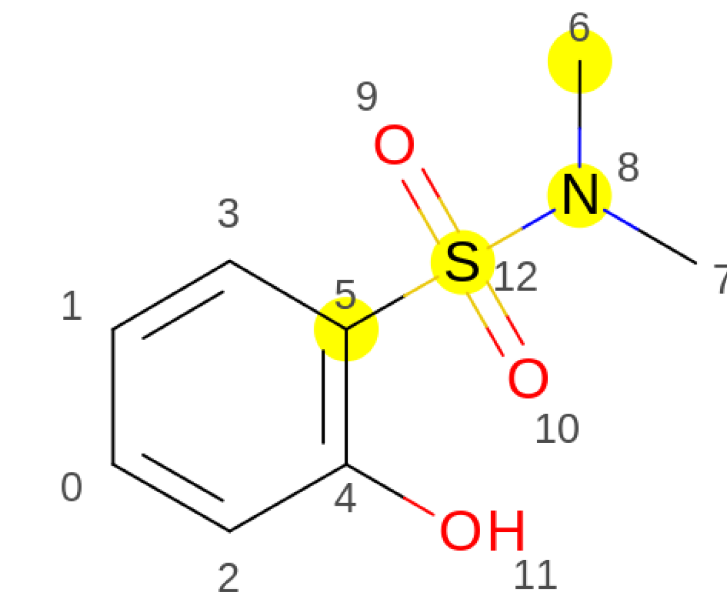
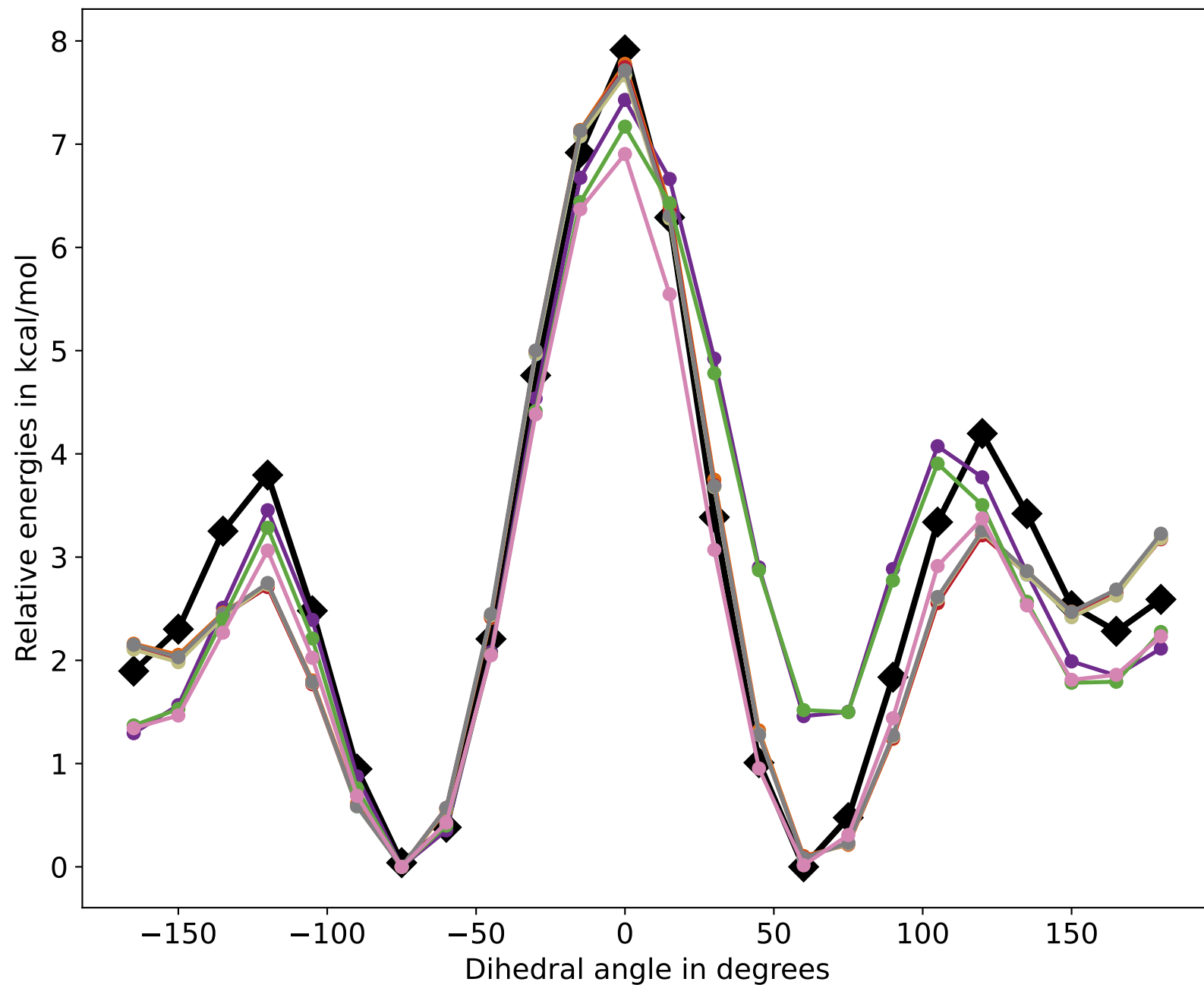


Relative energies in kcal/mol



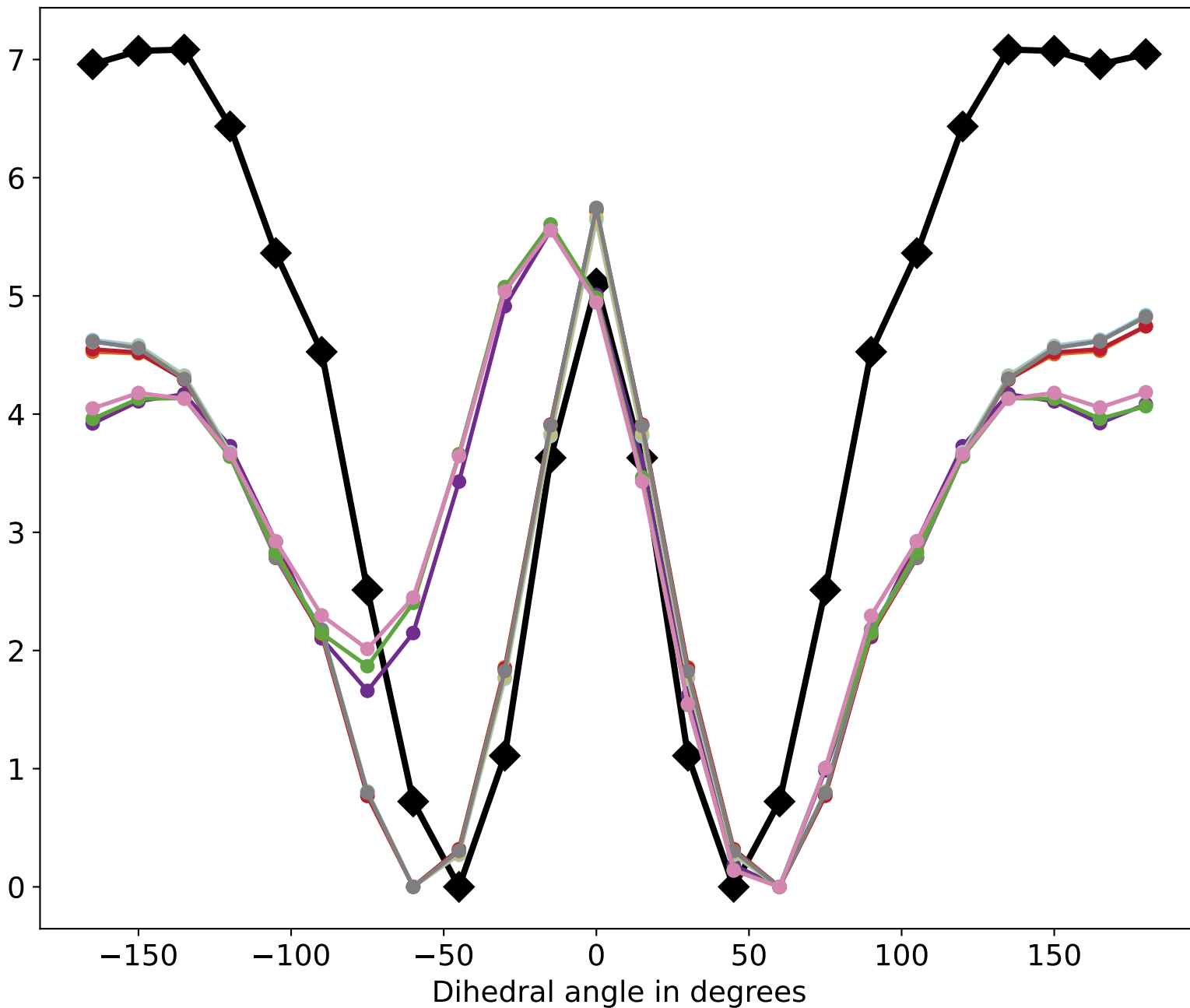
Relative energies in kcal/mol







Relative energies in kcal/mol



Relative energies in kcal/mol

