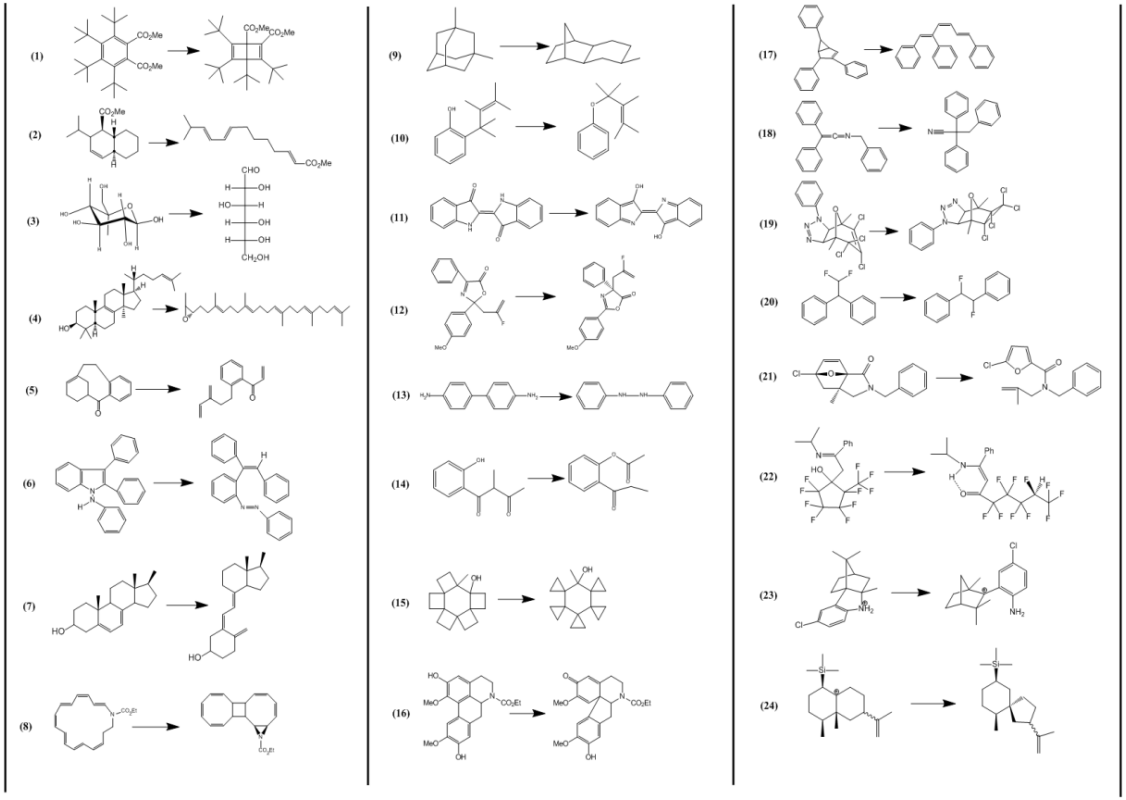
DFT for Isomerization Reactions of Large Organic Molecules

- Accurate Isomerization energies of large organic molecules are difficult to obtain in experiments.
- Benchmarks for a database of 24 reactions with 24-81 atoms were obtained by highly accurate calculations.
- Tests of various DFT methods show the best single-component functionals with and without MM corrections to be ωB97X-D and M08-SO, and the best local functional to be M06-L, where M0*x* functionals are from Minnesota.
- The database is recommended for future development of methods aimed at treatment of chemical reactions of large size.



Luo, Zhao, and Truhlar (Univ. of Minnesota), Phys. Chem. Chem. Phys. 13, 13683 (2011)