



Input molecular information

1D-3D format



Results with no errors / imag freq

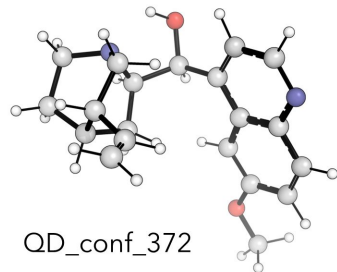
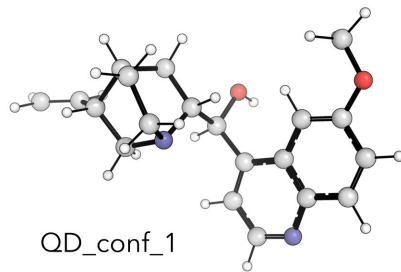


Further inputs (NMR, TDDFT, ...)

New input

PY AQ
ME =

Multiple conformers in input files ready to run



Process output

Boltzmann-weighted

- **Spectra**
 - UV-Vis
 - NMR
 - IR
 - VCD
- **Molecular descriptors**

