
DISCO
Distributing **C**omputed **O**utputs
(molecular feature parser)

Let’s go to the DISCO-tech

- What does it do?
  Python script that extracts NBO and NMR features and organizes into csv file.

- Features:
  - Atom charges
  - Frontier molecular orbitals energy: HOMO, LUMO
  - NMR shielding tensor values
  - Bond distances

- Files:
  - Gaussian NBO and NMR output files

- Runs in the terminal with commands:
  - --distance (atom)
  - --nmr (atom)
  - --charge (atom)
  - --fmo (homo, lumo, or both)
  - --csv (nmr, charge, fmo, nbo, all)
  - * (multiple files)