



I. SMIRNOFF / Toolkit

- Publish SMIRNOFF99Frosst 1.0 assessment paper: densities, dielectric constants, hydration free energies, host-guest thermodynamics
- Publish direct chemical perception paper
- Define SMIRNOFF 0.2 spec
- Add RDKit support for toolkit
- Create automated torsion drive pipeline
- Develop QCArchive

II. Datasets / Curation

- Generate QM torsion profiles for Roche fragment set
- Curate larger representative small molecule set for subsequent torsion drives
- Curate physical property dataset of densities, dielectrics, and enthalpies of mixing for fitting
- Implement property estimation parameter gradients for use in parameter fitting
- Release new OFF toolkit updates including new features, API improvement, and bugfixes

III. First Optimization Sprint

- Initiate torsion/valence fitting procedure for the selected molecules
- Expand dataset to include wider range of molecules and fragments
- L-J parameterization for selected organic liquid dataset
- Curate an initial host-guest (HG) dataset for assessment in Phase IV
- Curate a limited protein-ligand (PL) dataset for preliminary assessment in Phase IV [full assessment expected in Year 2]

IV. Automated Assessment

- Densities (neat and mixture)
- Dielectric constants
- Enthalpies of mixing
- Host-guest thermodynamics
- Limited protein-ligand benchmark set
- Possible relative conformer energies