



#### I. SMIRNOFF / Toolkit

SMIRNOFF v01 format specification / SMIRNOFF99Frosst implementation [10.1021/acs.jctc.8b00640]

SMIRNOFF v02 format specification.

Assessment: densities, dielectric constants, hydration free energies, host-guest thermodynamics.

Toolkit support for RDKit [v0.2] and AM1-BCC.

Torsion drive pipeline.

QCArchive

#### II. Datasets / Curation

Select representative small molecules for torsion generation.

Generate QM torsion profiles for selected molecules.

Curate dataset of densities, dielectrics, and enthalpies of mixing.

Implement property estimation parameter gradients for Lennard-Jones and test property estimation framework.

Continuous release of OFF toolkit updates including new features and API improvement.

#### 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 Assesment

Densities (neat and mixture)

Dielectric constants

Enthalpies of mixing

Host-guest thermodynamics

Limited protein-ligand benchmark set

Possible relative conformer energies