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BespokeFit

Automated bespoke parameters for OpenFF

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Force Fields

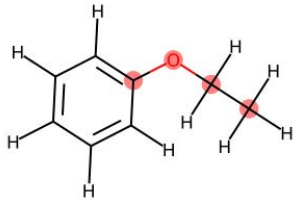
Allow us to parametrise vast amounts of chemical space quickly via:

- a large number of atom type specific parameters eg OPLS or GAFF
- or smart typing a smaller collection of parameters using chemical perception (OpenFF)

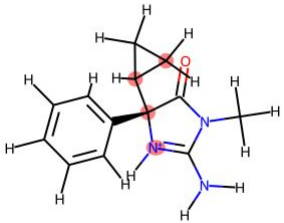
Force Field	Number of unique torsion parameters
OpenFF-1.0.0	157
OpenFF-1.2.0	163
OpenFF-1.3.0	167
OPLS3	48,142
OPLS3e	146,669

J. Chem. Theory Comput. 2019, 15, 1863–1874 Article

Torsion Parameters

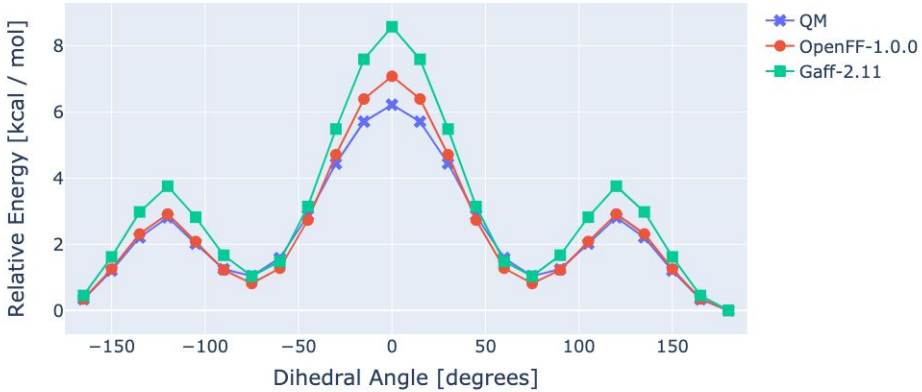


Openff-1.0.0 works well with no modifications on simple molecules.

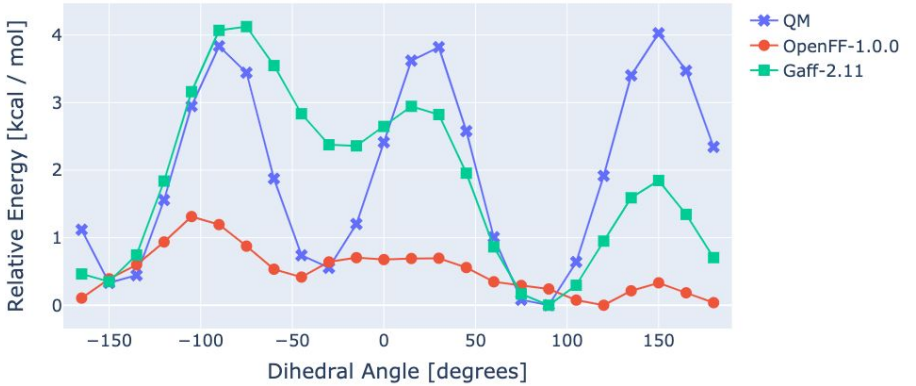


However it can struggle in some more complex cases seen in the Schrödinger benchmark systems. (BACE)

TorsionDriveDataset 1-D Plot

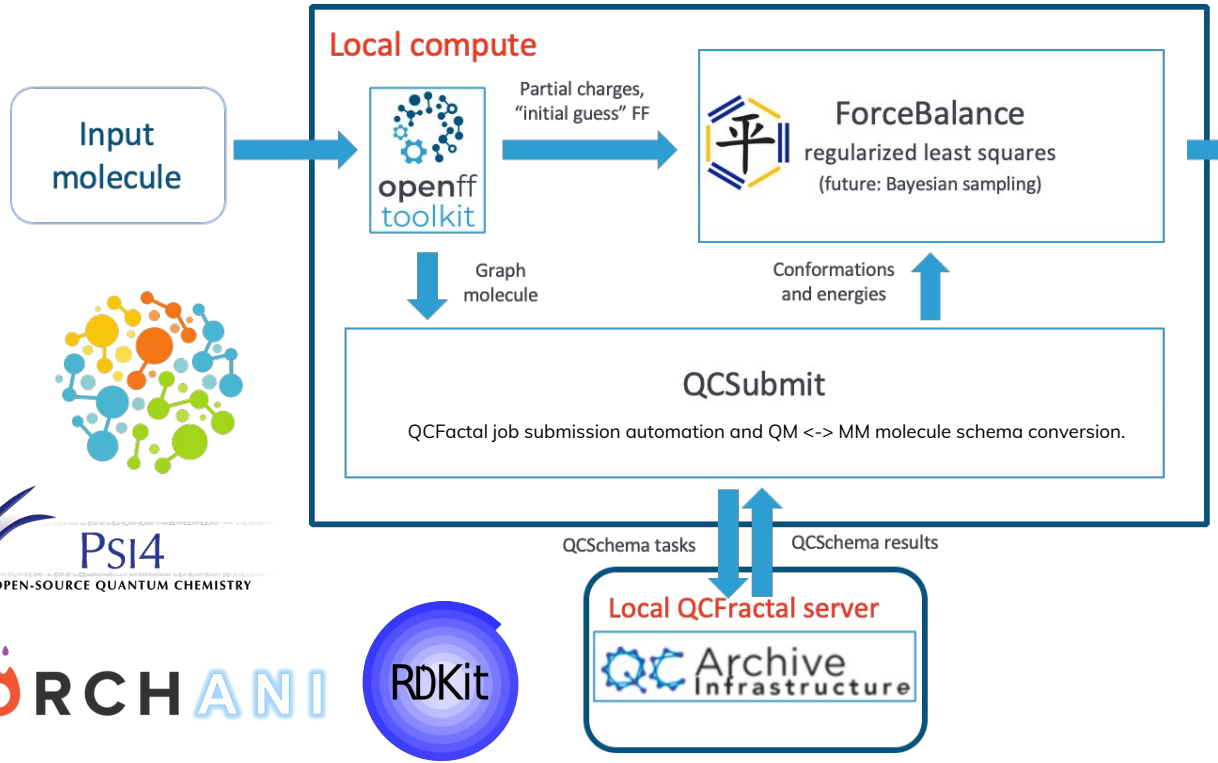


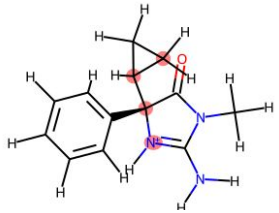
TorsionDriveDataset 1-D Plot



Bespoke framework

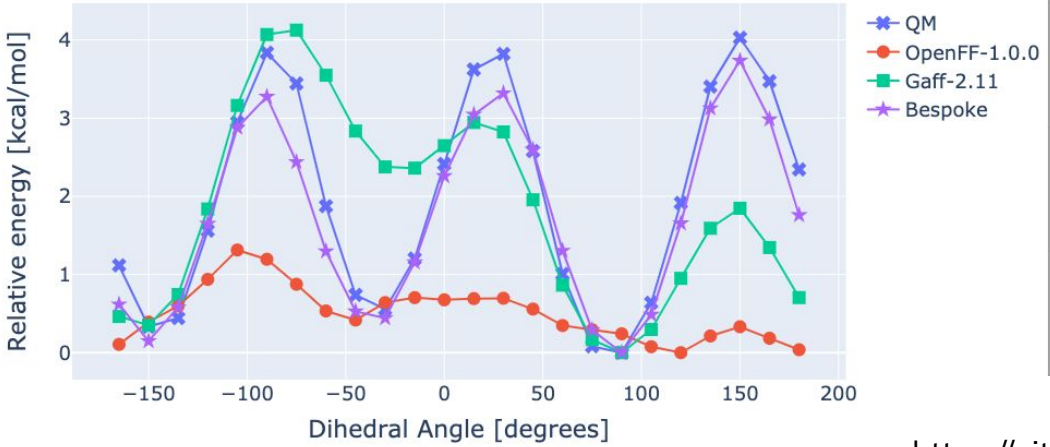
A typical bespoke pipeline powered with QCSubmit allowing for a direct interface with the QC ecosystem. One interface for many programs





TorsionDrive 1-D Plot

Clear improvement of the PES after fitting bespoke parameters.



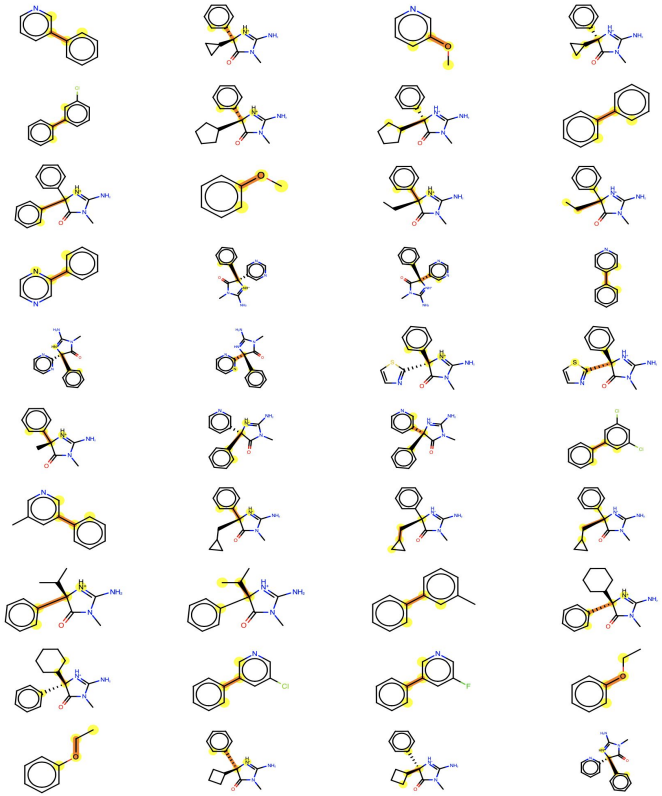
Force Field	RMSE (kcal/mol)
Openff-1.0.0	1.93
Gaff-2.11	1.14
Bespoke	0.39

https://github.com/openforcefield/bespoke-fit

BACE Fragments

Fitting results for the full set of fragments from the BACE Schrödinger set.

Force Field	Average RMSE (kcal/mol)	Average RMSD (angstrom)
OpenFF-1.3.0	0.97	0.17
OpenFF-1.3.0 + Bespoke	0.18	0.13



FAQ

- Can I use BespokeFit?
  - Yes, you can install BespokeFit using the environment file in the workshop repo. We aim to have a conda-forge package soon.
- Should I use BespokeFit?
  - While we have shown BespokeFit to be successful, the package is still pre-alpha and could change a lot while we make improvements. Testers are welcome, however, we recommend avoiding production work for now.

BespokeFit

Future features

- Bonds
- Angles
- Improper torsions?
- Charges?
- Predicting when to refit parameters?

Validation

- Free energy calculations starting with the TYK2 Schrödinger system.
- Expanding the Lim optimization benchmark to include a bespoke-fit force field.

Demonstration

Now a quick demonstration of how easy it is to construct a BespokeFit workflow.

Acknowledgement

- Jamshed Anwar
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UK Research and Innovation