open
forcefield

@openforcefield

www.openforcefield.org

OPEN FORCE FIELD CONSORTIUM

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Goals

Physics based molecular modeling can only be as good as the underlying energy model

OpenFF Goals:

- Develop best open source Force Field for small and large molecules
- Implement workflows to apply and benchmark OpenFF force field
- Continuously improve and maintain OpenFF by incorporating new cutting edge science and data
- Bring together scientist form academia and industry to advance the most impactful challenges

D'Amore; Hahn; Dotson; Horton; Anwar; Craig; Fox; Gobbi; Lakkaraju; Lucas; Meier; Mobley; Narayanan; Schindler; Swope; Veld; Wagner; Xue; Tresadern; Collaborative Assessment of Molecular Geometries and Energies from the Open Force Field. *J. Chem. Inf. Model.* **2022**.

The Open Force Field Consortium

INDUSTRY

AbbVie
AstraZeneca
Bayer
Cresset
Eli Lilly
Janssen
GlaxoSmithKline
Genentech
Merck KGaA
OpenEye
Pfizer
Roche
Vertex
Ventus
... and others

Open Molecular Software Foundation

PROJECT STAFF


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ACADEMIC


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Plus affiliates:

- Danny Cole (Newcastle)
- Lee-Ping Wang (UCD)
- Dennis Della Corte (BYU)
- MolSSI (Virginia Tech)

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Achievments

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Today

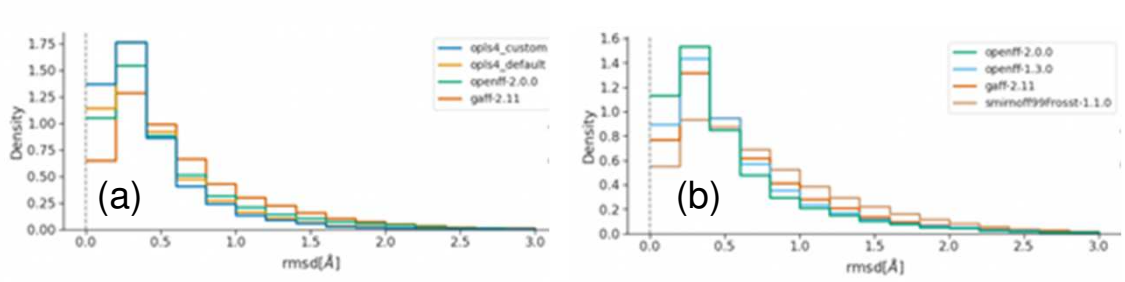
You can run OpenFF today!

Download from github: https://github.com/openforcefield/openff-toolkit/tree/master/examples#examples-using-smirnoff-with-the-toolkit
Tutorials are excellent and get you up and running in minutes

Modules include:

- Parametrization for widely used MD platforms: OpenMM, AMBER, GROMACS
- Bespoke force field parametrization

Results are comparable to some of the worlds best force fields and improving quickly:



Histograms of the RMSD values between force field structures as compared to QM structures. Values closer to zero indicate higher geometric similarity for both RMSD and TFD. Panels (a) compares the families of force fields over a **public** dataset. Panels (b) compares non-proprietary force fields over a **proprietary** set.

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The Future

OpenFF is continuously improving

Upcoming features include:

- Off-site charges
- AI based charge assignment
- Polymer support
- Protein Force Field
- Improved functional form

- Your specific need?

Become a member!

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The Future

OpenFF Needs You!

https://openforcefield.org/

You can also become a member of this consortium and:

- Contribute to the advancement of our science
- Help directing the direction of the OpenFF efforts
- Network with some of the best scientist in the field
- Varying level of commitment and influence:

Sustaining Partner (Tier 1):
Contributes a **minimum** of **$100,000** annually or equivalent in-kind support.

Supporting Partner (Tier 2):
Contributes a **minimum** of **$50,000** annually or equivalent in-kind support.

Facilitating Partner (Tier 3):
Contributes a **minimum** of **$20,000** annually or equivalent in-kind support

https://openforcefield.org/

Open Free Energy

OpenFE: Our vision

We are building an ecosystem of **tools for free energy calculations** which are:

- ➔ Permissive open source
  - Free to commercially use and extend
- ➔ Interoperable
  - Compatible with existing workflows
  - No lock in to any ecosystem
- ➔ Robust
  - Built and maintained to industry standards
- ➔ Automated and scalable
  - Designed for simple large scale deployment
- ➔ Modular and extensible
  - Clear API to allow reuse and adaptation of components

- AbbVie
- AstraZeneca
- Bayer
- Boehringer Ingelheim
- Bristol Myers Squibb
- Confo Therapeutics
- Eli Lilly
- Exscientia
- Genentech, a member of the Roche Group
- GSK
- Interline Therapeutics
- Janssen Pharmaceutica NV
- Merck KGaA
- Nurix Therapeutics
- Redesign Science Inc
- And others...

Our team

Richard Gowers
Project Lead

David W.H. Swenson
Infrastructure Lead

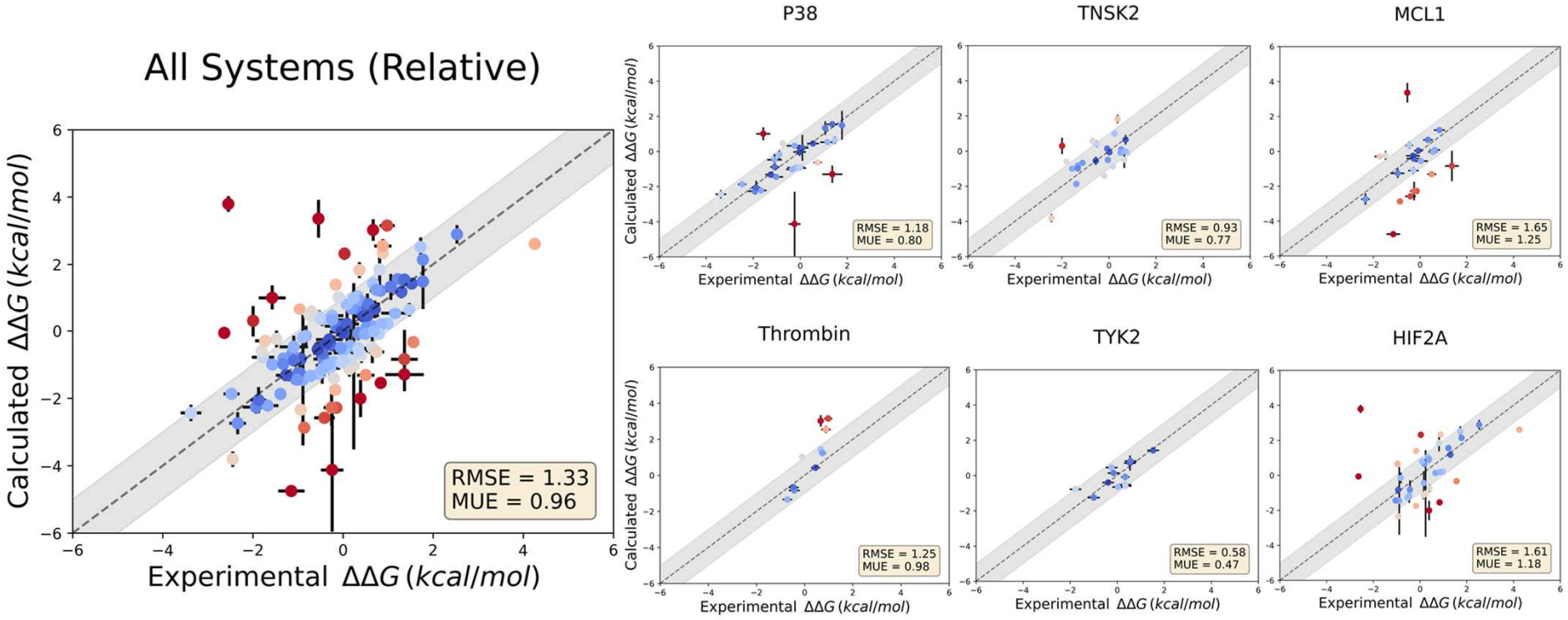
Irfan Alibay
Scientific Lead

Diego Nolasco
Project Manager

Benjamin Ries
Scientific Software Developer

Mike Henry
Software Scientist

RBFE benchmarking results - relative results



OpenFE: Our vision

OpenFE Needs You too!

You can also become a member of this consortium and:

- Contribute to the advancement of our science
- Help directing the direction of the OpenFE efforts
- Network with some of the best scientist in the field
- Varying level of commitment and influence:

- **Sustaining Partner (Tier 1):**
  Contributes a **minimum** of **$100,000** annually or equivalent in-kind support.
- **Supporting Partner (Tier 2):**
  Contributes a **minimum** of **$50,000** annually or equivalent in-kind support.
- **Facilitating Partner (Tier 3):**
  Contributes a **minimum** of **$20,000** annually or equivalent in-kind support

https://openfree.energy/