Open
Molecular
Software
Foundation

omsf.io
info@omsf.io
@openmsf

Join OpenFF to Ensure the Continuous Improvement in the Accuracy of Molecular Modeling for Drug Design

Molecular modeling and simulations in drug design are only as good as the energy models, or force fields, used in computation. Leading proprietary force fields are expensive and their ongoing improvement is uncertain, creating considerable interest in industry towards building open, pre-competitive alternatives with high and improving accuracy and domain of applicability which can be used without licensing fees.

To that end, the Open Force Field (OpenFF) Initiative is a network of academic and industry researchers working together to advance science and infrastructure for building next-generation small molecule and biomolecular force fields for drug discovery. These researchers seek to develop automated, systematic, data-driven techniques to parameterize and assess new generations of more accurate force fields. Software, data, and force fields are released under open licensing agreements to enable rapid application, validation, extension and any kind of modification by our users and contributors. In addition, the Initiative aims to grow a strong community of users and contributors from industry and academia. Currently, OpenFF focuses on small molecule and protein force fields, with longer-term goals of extending to nucleic acids and beyond, eventually likely including solvents, organic excipients, and polymers.

OpenFF already has produced arguably the best permissively licensed force field, Sage, judging by recent industry benchmarking efforts, based on public and proprietary datasets. OpenFF also produces tools like BespokeFit which can be used to improve force field accuracy on proprietary chemistries. Yet there is a great deal more science to be done and accuracy to be gained, including for prediction of protein-ligand binding. Ongoing efforts are numerous and far-reaching, including:

- Off-site charges for improved electrostatics (e.g. sigma holes for halogens, nitrogens, …)
- Protein FF fitted consistently with the Sage small molecule FF
- Improving starting points for fits, resulting in higher accuracy
- New fitting objective functions which produce higher accuracy force fields
- Automated chemical perception for better discrimination of new chemistries
- Benchmarking on protein-ligand binding free energies

OpenFF is supported in part by an industry Consortium, open to any interested industry partners. Industry partners play a key role in setting priorities to maximize the impact of our activities in the drug discovery setting. Partners can join at one of three financial levels, with increasing benefits, though all can use OpenFF under the MIT license:

- Facilitating Partner: $20K/yr, with involvement in the advisory board and public credit
- Supporting Partner: $50K/yr, with ability to prioritize regions of chemical space and receive technical consultation and support
- Sustaining Partner: $100K/yr, adding priority technical support and at least one partner at this level serving on the Governing Board, voting on OpenFF decisions.

Additional benefits of becoming a member include the participation in regular meetings that will enable you to benefit from the combined knowledge of this enthusiastic consortium. For information on joining please contact info@openforcefield.org, or see our how to join page.