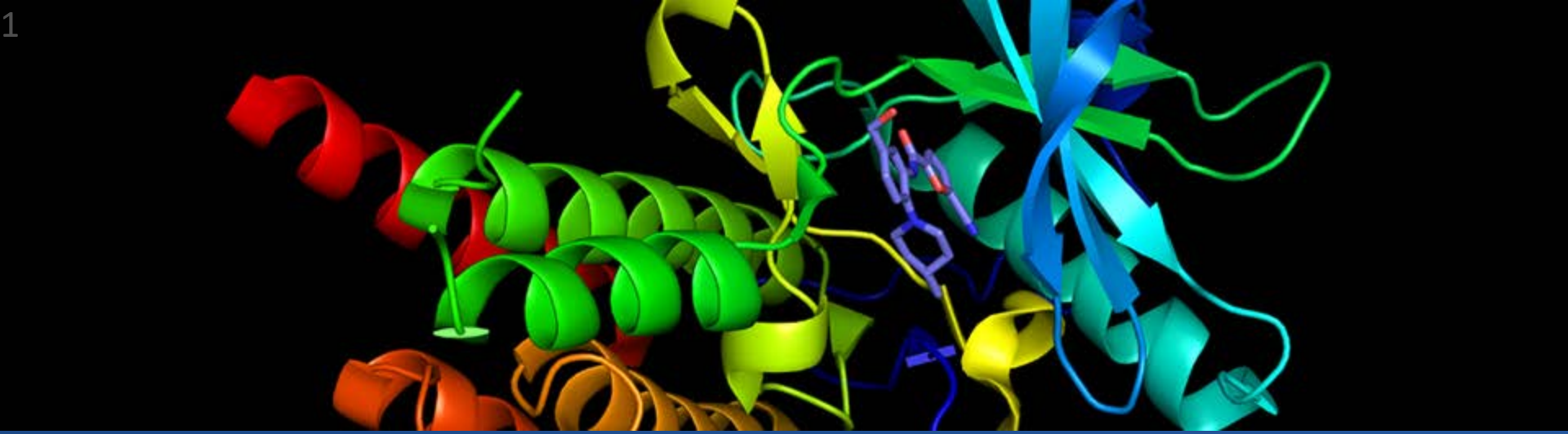

Protein Ligand Benchmark Update

David Hahn

OFF Advisory Board Meeting

2020/01/15

janssen | PHARMACEUTICAL COMPANIES OF Johnson&Johnson

Set up a repository for storing and presenting Protein-Ligand Benchmark Data

- Store only primary data. Derived data (e.g. dG instead of IC50; PDB format instead of SDF for ligands) is converted on the fly
- Easy-to-use (notebook examples)
- Clean presentation of data
- Link: https://github.com/openforcefield/PLBenchmarks
- Feedback welcome (what data is missing, which targets should be added, …)

Calculation of Free Energy Differences with a non-equilibrium approach

- Creation of OFF parameters of ligands and conversion to Gromacs format
- Calculation done with Gromacs-PMX workflow by the De Groot group at MPI Göttingen. Adaption to OFF topologies and to the repository.
- Issue: Very limited on compute resources. Now mainly run at UC Irvine (D. Mobley group), but also on AWS. In the future maybe at Janssen (local cluster) and at MSKCC (J. Chodera group).

Comparison between OPLS3e and QM optimized structured of OFF Release 1 Benchmark (vs. comparison of OFF Parsley FF and QM structures)

- Still pending