Conclusions

- Path sampling methods are a powerful tool for sampling rare events, and interfacing with OpenPathSampling might be of interest to MD engine developers.
- Alchemical free energy methods provide vital tools for the drug discovery pipeline, and Open Free Energy is a new toolkit facilitating these simulations.
- Both of these methods are "campaign-scale," and clear APIs and good serialization mechanisms in underlying tools make our lives easier.

http://openpathsampling.org

https://openfree.energy