Abstract Submitted
for the 4CF15 Meeting of
The American Physical Society

Towards an automated pipeline for solvation free energy calculations IAN KENNEY, OLIVER BECKSTEIN, Arizona State Univ, BOGDAN IORGA, Institut de Chimie des Substances Naturelles — Solvation free energies are used to determine solvent effects on molecules of interest, such as the log P_{ow} of drug-like molecules. We developed MDPOW, an automated pipeline to compute solvation free energies with molecular dynamics simulations using Python and Gromacs. In order to optimize the simulation protocol, we examined the effects of varying parameters on these free energy calculations. We employed benzene as a simple test case with an known experimental hydration free energy. We varied the parameters of the MD free energy perturbation (FEP) calculations, such as temperature and pressure coupling algorithms, sampling time of the FEP windows, dispersion correction, initial conditions. We also employed two different schemes to calculate the free energy, thermodynamic integration (TI) and the Bennett acceptance ratio (BAR) method. The Coulomb component of the hydration free energy was generally insensitive to variations in parameters. The Lennard-Jones component, however, can vary by many kJ/mol and is sensitive to the temperature coupling algorithm and inconsistent initial conditions when simulations are performed in the NVT ensemble.

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Date submitted: 10 Sep 2015 Electronic form version 1.4