Abstract Submitted
for the TSF16 Meeting of
The American Physical Society

Simulating conformational transitions of the transmembrane symporter[1] TAYLOR COLBURN, SEAN SEYLER, OLIVER BECKSTEIN, Arizona State University, BECKSTEIN LAB TEAM — The function of many proteins depends on large-scale conformational changes. Because these conformational transitions are rare events, it is very difficult to investigate them with equilibrium molecular dynamics (MD) simulations, which have otherwise become an important tool to study the molecular mechanisms of macromolecular systems. A variety of techniques — such as the Dynamic IMportance Sampling (DIMS) method and various elastic network-based approaches — have been developed to overcome timescale limitations and produce physically plausible trajectories between putative metastable states. We sought to characterize a number of different path generating and sampling methods, including DIMS with and without an implicit membrane model, by producing multidirectional trajectories of the transmembrane nucleobase symporter Mhp1[1]. All trajectories were compared to one another using Root-Mean-Square Distances (RMSDs), structural order-parameters and Path Similarity Analysis (PSA)[2]. In particular, PSA showed that while trajectory generating methods were broadly similar, paths from each method were also clearly distinguishable.
1. Shimamura, T. et al. Science 328, 470473 (2010). 2. Seyler SL, Kumar A, Thorpe MF, Beckstein O (2015) PLoS Comput Biol 11(10)

[1]This work was supported by the College of Liberal Arts and Sciences at Arizona State University

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Date submitted: 23 Sep 2016 Electronic form version 1.4