Supporting Information for

Transfer Learning from Markov models leads to efficient sampling of related systems

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Parameter	Value
Gaussian Height	0.5 kj/mol
Gaussian width	0.1
Bias Factor	6
Gaussian Drop rate	6ps
Swap rate	20ps
Number of tics	2
Feature Space	Dihedrals
Normalized Features	False

Table S1: Set of parameters used for the Bias-exchange tICA-Metadynamics simulations of Alanine dipeptide across 3 different FFs. For the amoeba calculation, we limited our sampling to only the dominant leading tIC.

Parameter	Value
Gaussian Height	0.5 kj/mol
Gaussian width	0.045,0.08 (25% of the standard deviation from the unbiased WW-FIP Anton simulation).
Bias Factor	6
Gaussian Drop rate	5ps
Swap rate	2ns
Number of tics	2
Simulation Temp	395 K
Number of walkers	25/tIC
Interval	#Based upon the WW-FIP Anton dataset tic_1: -1.07,1.95 tic_2: -12.11,1.83
Feature Space	Dihedrals + Closest Heavy atom contacts (Beta =10)
Normalized Features	True

Table S2: Set of parameters used for the Bias-exchange tICA-Metadynamics simulations of FIP and GTT mutants of WW domain. Each pair of tIC walkers is connected via MPI but the walkers themselves are only sharing the biases via a shared folder. For the closest heavy atom contacts, we used Plumed's definition of closest heavy atoms to make the contacts differentiable.

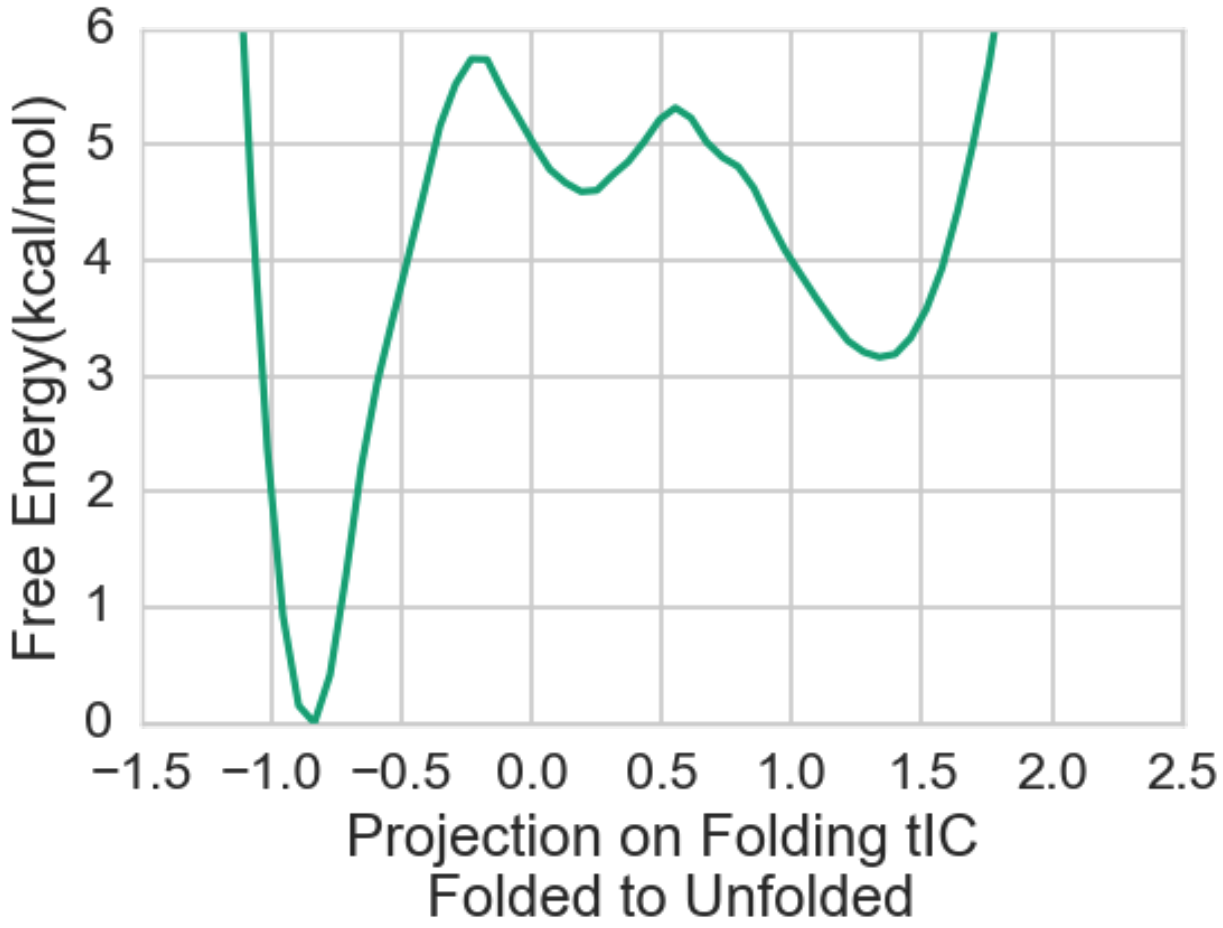

Figure S1: Anton - MSM solution to the FIP's free energy projection along the dominant tIC coordinate.

SI Note 1:

To reweight the FIP/GTT mutant multiple walkers Metadynamics simulation on to full phase space via MBAR, we used two different techniques though we found the results to be very similar. In the first instance, we used the last reported bias as input for MBAR. In the second, we corrected this bias using the time-independent free energy estimator of Tiwary et al[1]. To calculate the reversible work correction factor (c(t)) across multiple walkers, we used the methodology from a recent paper[2]. For both methods, the reported MBAR-weighted populations (with or without the correction) were highly similar. We also removed the first 40ns from each walker to account for equilibration.

(1) Tiwary, P.; Parrinello, M. A Time-Independent Free Energy Estimator for Metadynamics. *J. Phys. Chem. B* **2015**, *119* (3), 736–742.

(2) Prajapati, J. D.; Fernández Solano, C. J.; Winterhalter, M.; Kleinekathöfer, U. Characterization of Ciprofloxacin Permeation Pathways across the Porin OmpC Using

Metadynamics and a String Method. *J. Chem. Theory Comput.* **2017**, acs.jctc.7b00467.