

Population Based Reweighting of Scaled Molecular Dynamics

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Supporting Information

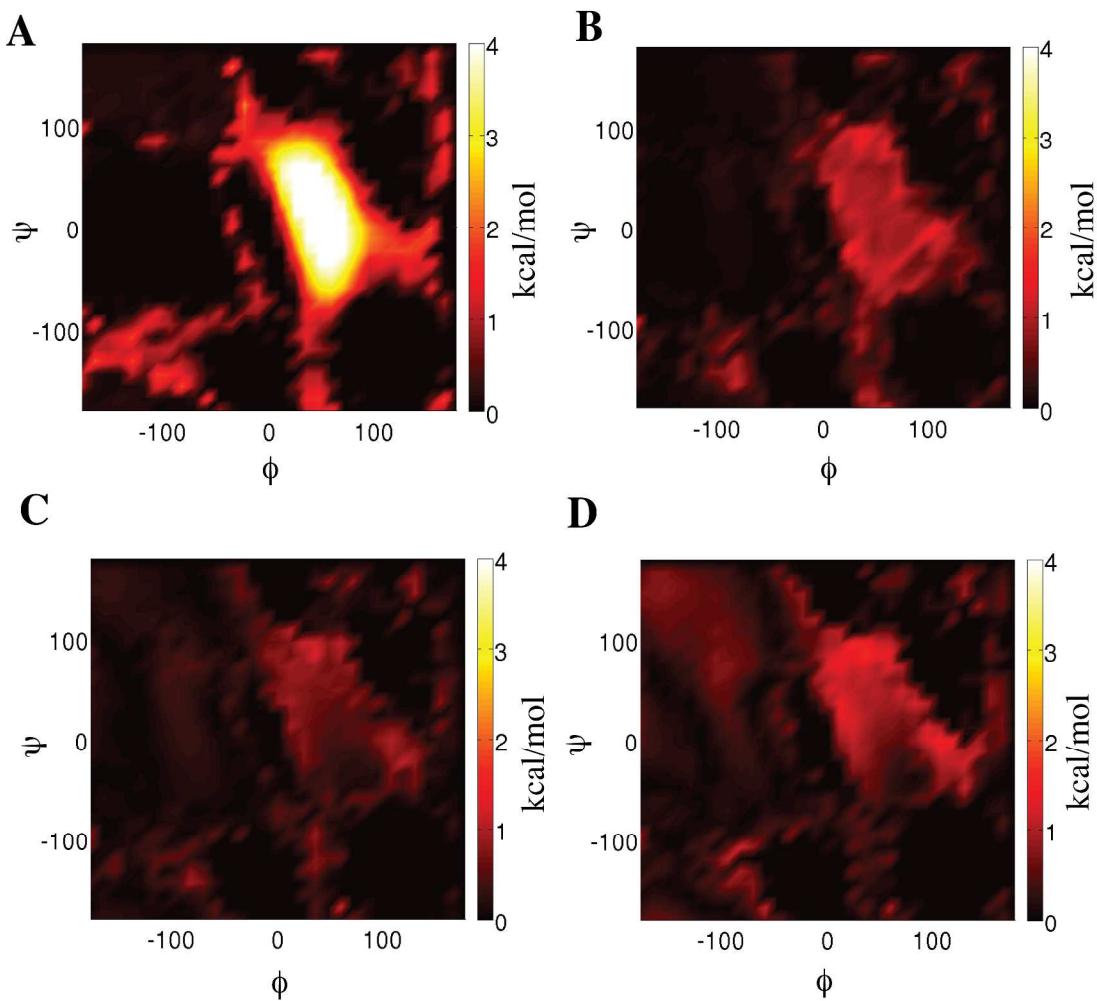


Figure S1: The differences between free energy profiles generated from five 20ns replica sMD simulations and one 1000ns MD simulation: A) $\lambda=1$ (equivalent to cMD), B) $\lambda=0.7$, C) $\lambda=0.5$ and D) $\lambda=0.3$.

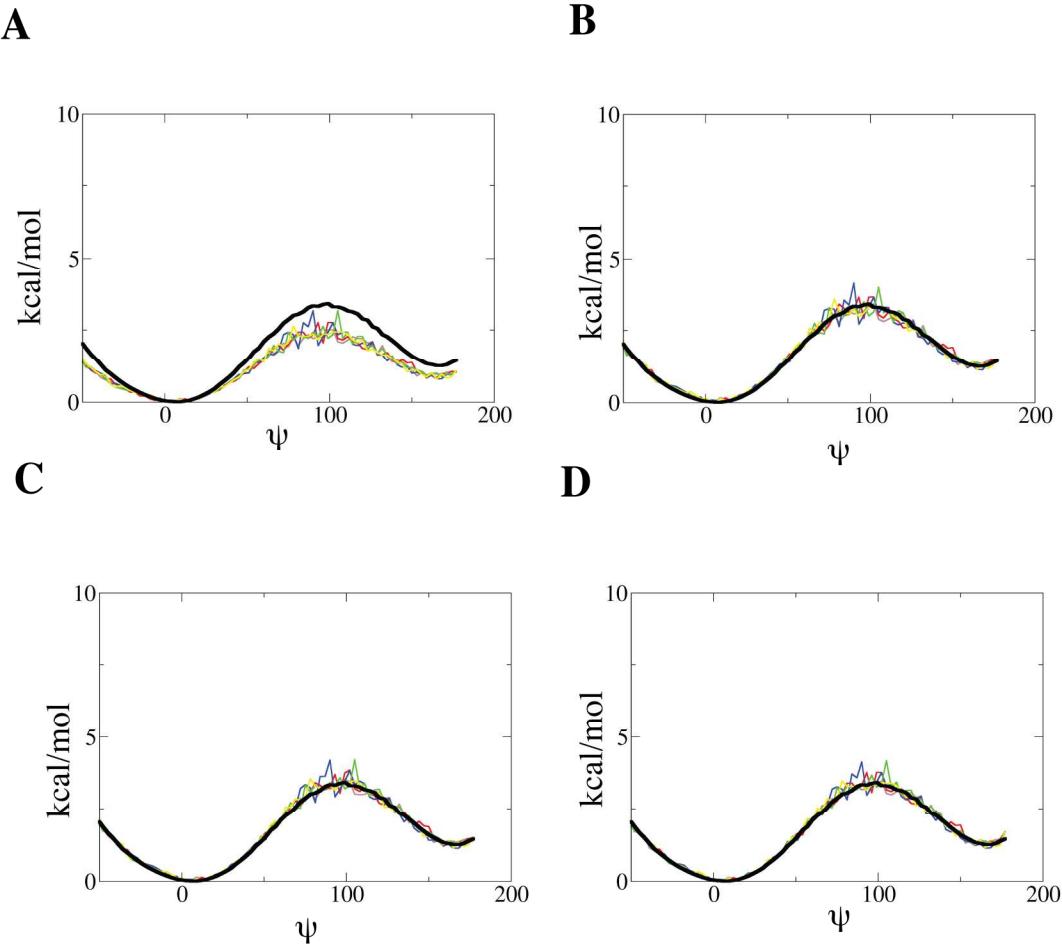


Figure S2: The differences between free energy profiles along Phi using different bin sizes to reweight as in Figure 4A generated from five 20ns replica sMD simulations and one 1000ns MD simulation (thick Black line) $\lambda=0.7$. A. unweighted sMD PMF. B. reweighting with a bin size of 1 degree C. 3 degree D. 12 degree. Note that the bin size used in reweighting was altered in A-D, but the plotted bin size is always 3 degrees.

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- (34) Case, D. A.; Darden, T. A.; Cheatham, T. E.; III; Simmerling, C. L.; Wang, J.; Duke, R. E.; Luo, R.; Walker, R. C.; Zhang, W.; Merz, K. M.; Roberts, B.; Wang, B.; Hayik, S.; Roitberg, A.; Seabra, G.; Kolossváry, I.; Wong, K. F.; Paesani, F.; Vanicek, J.; Liu, J.; Wu, X.; Brozell, S. R.; Steinbrecher, T.; Gohlke, H.; Cai, Q.; Ye, X.; Wang, J.; Hsieh, M. J.; Cui, G.; Roe, D. R.; Mathews, D. H.; Seetin, M. G.; Sagui, C.; Babin, V.; Luchko, T.; Gusarov, S.; Kovalenko, A.; Kollman, P. A.
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