Using Selectively Applied Accelerated Molecular Dynamics to Enhance Free Energy Calculations

Supplemental Material

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Figure S1: Free energies for individual BAR runs using cMD simulations for short (a), medium (b), and long (c) equilibration periods.

Figure S2: Free energies for individual BAR runs using selective aMD simulations for short (a), medium (b), and long (c) equilibration periods.
Figure S3: A comparison of average free energies for BAR runs between cMD and selective aMD simulations for short (a), medium (b), and long (c) equilibration periods. Note the different time scales (lower for cMD, upper for aMD).

Figure S4: Free energy values calculated from all-dihedral aMD show inaccurate results due to the high weights resulting from aMD simulations.