Abstract Submitted
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Computing absolute binding affinities via non-equilibrium unbinding simulations F. MARTY YTREBERG, University of Idaho — We demonstrate that non-equilibrium unbinding simulations can be used to accurately estimate equilibrium absolute binding affinities (ΔG). Utilizing the FKBP protein bound to two different ligands we estimate ΔG within less than 1.0 kcal/mol of experimental values. The methodology is straight-forward, requiring no modification to many modern molecular simulation packages. The approach makes use of a physical pathway, eliminating the need for complicated alchemical decoupling schemes. These results suggest that non-equilibrium simulation could provide a viable means to accurately estimate protein-ligand binding affinities.

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