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FKBP binding free energies obtained via non-equilibrium simulation F. MARTY YTREBERG, University of Idaho — We discuss the advantages and disadvantages of estimating binding free energies (i.e., absolute binding affinities) via non-equilibrium unbinding simulations. The study utilizes the FKBP protein bound to two different ligands as a model system. The non-equilibrium methodology utilized is straight-forward, requiring little or no modification to modern molecular simulation packages, and is trivially parallelizable. The approach makes use of a physical pathway, eliminating the need for complicated alchemical decoupling schemes.

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