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Protein free energy landscapes from long equilibrium simulations

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Many computational techniques based on molecular dynamics (MD) simulation can be used to generate data to aid in the construction of protein free energy landscapes with atomistic detail. Unbiased, long, equilibrium MD simulations—although computationally very expensive—are particularly appealing, as they can provide direct kinetic and thermodynamic information on the transitions between the states that populate a protein free energy surface. It can be challenging to know how to analyze and interpret even results generated by this direct technique, however. I will discuss approaches we have employed, using equilibrium MD simulation data, to obtain descriptions of the free energy landscapes of proteins ranging in size from tens to thousands of amino acids.