# Energy Landscape and Fast Side Chain Dynamics of Proteins

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## Abstract:

Fast side chain conformational dynamics play an important role in the biological function of proteins. High-resolution solution NMR spectroscopy uses side chain methyl spin probes to determine the amplitudes and rates of site-specific fast internal motions of proteins. In particular, the methyl axial order parameter (O2), which quantifies the spatial restriction of side chain motion, is commonly used to establish a molecular-level connection between the atomistic dynamics and thermodynamics of proteins.

We have examined the connection between the topography of the underlying energy landscape and the fast side chain conformational dynamics of proteins using molecular dynamics simulations and enhanced sampling free energy methods. The side chain conformational free energy surfaces obtained using the adaptive biasing force (ABF) method for a set of eight proteins with different molecular weights and secondary structures reveal universal features of fast side chain motions in proteins.