Computationally Enhanced Dynamics Analysis of Protein NMR Data

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NMR spectroscopy provides unique insight into the amplitudes and time scales of biomolecular dynamics with high spatial and, in the case of nuclear spin relaxation, also temporal resolution. Due to the short range of dominant NMR spin interactions, such as the magnetic dipole-dipole coupling, the motional information that can be directly extracted is local in nature. By combining experimental data with analytical models and computational methods, including Gaussian axial fluctuation models, molecular dynamics simulations, normal mode analysis, and elastic network models, a more comprehensive collective interpretation of a growing body of experimental NMR data can be achieved. The concepts will be illustrated for several different protein systems.