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Native dynamics from diversity in NMR structures HEIKO LAMMERT, JOSE ONUCHIC, Rice Univ — Protein function relies on the characteristic dynamics that arise in the protein's unique native structure, controlled by the smooth, funneled energy landscape evolved to enable fast and reliable folding. Structure-based models draw on energy landscape theory to build an ideally funneled energy landscape only from a protein's native structure. Simplified interactions of homogeneous strength are used to eliminate energetic frustration. The dynamics of the model are controlled by geometric constraints imposed by the native fold. The energy landscapes of many actual proteins are smooth enough to let such unfrustrated models describe their folding mechanisms. But conflicting functional demands upon the sequence may introduce sufficient frustration into the energetics to affect the dynamics. For such cases heterogeneous interactions can be optimized based on additional data. We use the diversity among the conformations deposited in a set of NMR structures to estimate the extent of fluctuations in the native state to build an improved model of protein S6. Qualitative modifications bring the observed mechanism into agreement with experiment, and matching of the entire fluctuation profile leads to similar contact maps as optimization based on either phi-values of sequence data.

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