Protein energy landscapes, solvent α-slaving and hydration β-coupling

P. W. Fenimore
T-10, Los Alamos National Laboratory, Los Alamos, NM USA

Protein function depends critically on both protein dynamics and structure. It is widely recognized that protein dynamics occur on a high-dimensional energy landscape, where distinct conformations are separated by free energy barriers. Yet the way in which a partition between protein, hydration shell and bulk solvent might be made has not always been fully considered in the context of the energy landscape. It is possible to include solvent α and hydration shell β processes explicitly in the protein energy landscape as temperature-dependent rates determined by the solvent and hydration shell respectively. Three classes of protein dynamics on the energy landscape are evident from a wide range of data: (1) α-slaved protein dynamics, (2) β-coupled protein dynamics and (3) unslaved (vibrational) protein dynamics. One cannot rule out additional classes of protein motion. The rate of α-slaved protein dynamics follow the temperature dependence of the solvent α process, slowed by an entropic contribution from the protein and hydration shell. Similarly to α-slaving, the β-coupled protein dynamics follow the hydration shell β process, but because all β-coupled data we have analyzed depend at least partly on amplitude, there are too few constraints to compute the slowing entropy (although we can bound it). In no case do we require a dynamic protein transition to explain existing β-coupled amplitude data. The empirical decomposition of protein dynamics into different categories suggests a corresponding decomposition of protein dynamical models that may assist in computing protein function.