TIFR Centre for Interdisciplinary Sciences, Narsingi, Hyderabad 500075

Seminar

Denaturant dependent folding of Green Fluorescent Protein

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Abstract: The folding landscape of Green Fluorescent Protein (GFP), which is extensively used as a marker in cell biology is mapped using molecular simulations and a coarse-grained model. Thermal and Guanidinium chloride (GdmCl) induced unfolding of a variant of GFP, without the chromophore, occurs in an apparent two-state manner. The calculated midpoint of the equilibrium folding in GdmCl, taken into account using the Molecular Transfer Model (MTM), is in excellent agreement with the experiments. The structural features of rarely populated equilibrium intermediates, visible only in free energy profiles projected along a few order parameters, are remarkably similar to those identified in a number of ensemble experiments in GFP with the chromophore. Despite the seeming simplicity of the equilibrium folding, flux to the native state flows through multiple channels and can be described by the kinetic partitioning mechanism. Interestingly, the intermediates characterized in the simulations coincide with those identified in single molecule pulling experiments. Our predictions, amenable to experimental tests, show that MTM is a practical way to simulate the effect of denaturants on
the folding of large proteins.

***Date*: Monday, March 11th 2013**
***Time*: 11:30AM (Tea/Coffee at 11:15AM)**
***Venue*: Conference Hall, TCIS**

All are cordially invited