Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Students' Annual Seminar

Do non-affine atomic displacements in apo-proteins reveal eventual binding pathways?

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Observing and pinpointing these rare events in large scale, all-atom, computations of specific protein-ligand complexes, is expensive and to a great extent serendipitous. Further, relevant collective variables which characterise specific binding or un-binding scenarios are still difficult to identify despite the large body of work on the subject. We use a projection formalism, introduced earlier to study deformation in solids, to analyse local atomic displacements into two mutually orthogonal subspaces — those which are "affine" i.e. expressible as a homogeneous deformation of the native structure, and those which are not. We validate our observation with all-atom computations of two proteins, T4-Lysozyme and Src kinase. In each case, fluctuations of displacements in their apo forms, once analysed using the above strategy, correctly predict their ligand binding behaviour.

Monday, Feb 26th 2018

03:00 PM (Tea/Coffee at 02:00 PM)

Seminar Hall, TIFR-H