

Students' Annual Seminar

Global Non-Affinity Parameter: From local-to-Global picture

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In our group's work till now, we have proposed a method, which is extremely well suited to be adapted for high throughput searches of possible protein ligand pairs and allosteric control. The NAP formulation allows us to define a global parameter called global non affinity parameter using which, as a Collective variable, we try to explore the folding mechanism of protein systems. We perform the analysis for two model systems 1) GB1 and 2)32 bead neutral-charged polymer and see that the GNAP calculation equipped with proper protocol is indeed effective in clustering various important confirmations.

Friday, Feb 15th 2019

10:30 AM (Tea/Coffee at 10:15 AM)

Seminar Hall, TIFR-H