# Gachibowli Research Cluster Lecture Series

## Identifying Collective Displacements in Apo-proteins that Reveal Eventual Binding Pathways

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**Abstract:** Designing drugs which target specific proteins involved in diseases consumes a lot of time and effort in the pharmaceutical industry. In recent times, in silico design of drugs using all-atom molecular modelling has started to provide crucial inputs. Even so, discovery of binding pathways of small molecules both at the primary binding site, as well as sites for allosteric control, is time consuming and often fortuitous. We provide here a framework within which critical conformational changes likely to occur during binding are quantified from statistical analysis of configurations of proteins in their apo, or inactive form, greatly simplifying identification of target residues. We illustrate this idea by analyzing ligand binding pathways for three proteins T4- Lysozyme, P450 and Src kinase, which are active respectively in the immune system, metabolism and cancer.