



# COMPUTATIONAL BIOLOGY WEBINAR @ IMSc

## CONFORMATIONAL SELECTION IN A PROTEIN- PROTEIN INTERACTION

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Molecular recognition plays a central role in biology and protein dynamics has been acknowledged to be important in this process. However, it has been intensely debated for the last 50 years whether conformational changes happen before ligand binding to produce a binding-competent state (conformational selection) or are caused in response to ligand binding (induced fit) [1]. Proposals for both mechanisms in protein-protein interaction have been primarily based on structural arguments. However, the distinction between them is a question of the probabilities of going via these two opposing pathways. In this seminar I will discuss a direct demonstration of exclusive conformational selection in protein-protein recognition by measuring the flux for rhodopsin kinase binding to its regulator recoverin, an important molecular recognition in the vision system [2]. The combined use of nuclear magnetic resonance (NMR) spectroscopy, stopped-flow kinetics and isothermal calorimetry establishes that protein dynamics in free recoverin limits the overall rate of binding.

1. Changeux & Edelstein (2011) F1000 Biol. Rep. 3 19.
2. Chakrabarti et al. (2016) Cell Rep. 14 32-42.

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