

**Aquitaine –Karnataka collaboration
Scientific Project for Pre-PhD student exchange**

Scientific Proposal

Project Title	Computational Study of Peptide-Membrane Interactions at Nanoscale: Effects on Amyloid Diseases	
Scientific domain	Biophysics, Chemistry, Computational Biology	
Summary (ca. 10 lines)	Alzheimer's disease (AD) and type II diabetes (T2D) are associated with the aggregation of amyloid polypeptides into fibrillar β -sheet structures where toxicity results from amyloid-membrane interactions. These effects have been characterized experimentally to some extent, but structural and causal details are lacking. We intend to use molecular dynamics (MD) simulations to investigate the behavior of $A\beta$ peptide in AD and of human islet amyloid polypeptide (hIAPP) in T2D on lipid bilayers. The pathways and kinetics for $A\beta$ insertion and permeation, structure and dynamics on lipids and lipid associated molecules will be investigated using umbrella sampling and replica exchange MD simulations (REMD).	
Student profile wished	Chemist or Biophysicist or Molecular Biologist with knowledge of MD Simulations	
Supervisor Name	Dr. M. S. Santosh	
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Institute/laboratory/industry (full address)	Centre for Emerging Technologies, Jain University, Jain Global Campus, NH-209, 45th km, Jakkasandra Post, Kanakapura Taluk, Ramanagara District - 562112.	
Director Name Institute/laboratory/industry	Dr. M. S. Santosh	
Director Institute/laboratory/industry @ & phone	@: santoshgulwadi@gmail.com	Tel: +91-9480793007
Timing & duration for project (give approximate ranges)	3-6 months	
Selected Publications	M. S. Santosh et al. J. Phys. Chem. B 2010; M.S. Santosh et al. J. Solution Chem. 2010.	

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