BIOGRAPHICAL SKETCH

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NAME	POSITION TITLE
Abhijeet Kapoor	Postdoctoral Research Associate
eRA COMMONS USER NAME (credential, e.g., agency login) NA	

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	YEAR(s)	FIELD OF STUDY
Jaypee University of Information Technology, India	B.Tech.	2004-2008	Bioinformatics
Iowa State University, USA	Ph.D.	2009-2014	Bioinformatics and Computational Biology
Icahn School of Medicine at Mount Sinai, USA	Post-Doc	2015-	Computational Structural Biology

A. Personal Statement

My PhD studies focused on using computational techniques such as coarse-grained and all-atom simulations to understand functional motions in Ras proteins, an oncology target of exceptional importance. The primary focus of the work was to develop a generic coarse-grained model of proteins, use it to study conformational transitions in Ras proteins with the goal to identify specific structural features controlling the intrinsic conformational transitions, and complement the results using all-atom simulations. First, I developed the coarse-grained model that successfully folded nineteen proteins to their native state starting from completely random conformations. Next, using the coarse-grained simulations in combination with all-atom simulations, I identified the structural features that regulate the intrinsic nucleotide (GDP) exchange reaction based on which a model for regulatory protein assisted exchange process was presented. Finally, I provided a comprehensive comparison of the dynamics of all the three Ras isoforms using extensive all-atom molecular dynamics simulations. Such an understanding is critical for the design of inhibitors that can selectively target a particular malfunctioning isoform.

I joined the Filizola lab to conduct simulation studies of important protein targets, such as G protein coupled receptors and integrins, with the aim of using the mechanistic insights obtained from simulations for drug designing.

B. Positions and Honors.

Positions and Employment

2008-2009 Research Assistant, Department of Biochemistry, University of Delhi South Campus, New Delhi, India
2009-2014 Research Assistant / Ph.D., Bioinformatics and Computational Biology, Iowa State University, USA
2014 Teaching Assistant / Ph.D., Bioinformatics and Computational Biology, Iowa State University, USA
2015- Postdoctoral Research Associate, Department of Chemical and Structural Biology, Icahn School of Medicine at Mount Sinai, USA

Other Experience, Professional Memberships, and Awards

2012-2014 Member, Biophysical Society
2012 Bioinformatics and Computational Biology Travel Fellowship Award, Iowa State University
2012 Best Oral Presentation Award at International Interdisciplinary Science Conference on Protein Folding and Diseases, Jamia Millia Islamia, New Delhi, India
2014 James Cornette Research Fellowship in Bioinformatics and Computational Biology, Iowa State University

2014 Research Excellence Award, Iowa State University

C. Selected Peer-Reviewed Publications (in chronological order)

1. Kapoor A, Shandilya M, Kundu S. Structural insight of dopamine β-hydroxylase, a drug target for complex traits, and functional significance of exonic single nucleotide polymorphisms. PLoS One. 2011;6(10):e26509.
2. Kapoor A, Travesset A. Folding and stability of helical bundle proteins from coarse-grained models. Proteins. 2013 Jul;81(7):1200-11.
3. Kapoor A, Travesset A. Folding 19 proteins to their native state and stability of large proteins from a coarse-grained model. Proteins. 2014 Mar;82(3):505-16.
4. Kapoor A, Travesset A. Mechanism of the exchange reaction in HRAS from multiscale modeling. PLoS One 2014;9(10):e108846.

D. Research Support

None