

BIOGRAPHICAL SKETCH

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NAME: Raskar, Tushar Bhim

eRA COMMONS USER NAME (credential, e.g., agency login):

POSITION TITLE: Postdoctoral fellow

EDUCATION/TRAINING (*Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.*)

INSTITUTION AND LOCATION	DEGREE (if applicable)	Start Date MM/YYYY	Completion Date MM/YYYY	FIELD OF STUDY
University of Mumbai, Mumbai	BSc	06/2008	06/2011	Microbiology
University of Mumbai, Mumbai	MSc	07/2011	07/2013	Biophysics
ACTREC, Mumbai	Research fellow	08/2013	02/2015	Structural biology
NCBS, Bangalore	Graduate trainee	03/2015	06/2015	Structural biology
IITB, Mumbai	Junior Research Fellow	06/2015	11/2016	Structural biology
Universitaet Hamburg, Hamburg	PHD	01/2017	02/2021	Chemistry (Biophysics)

A. Personal Statement**B. Positions, Scientific Appointments and Honors**

2021-Present Postdoctoral fellow, Department of Bioengineering, University of California San Francisco, San Francisco, CA

C. Contributions to Science

- I investigated into the structural mechanism of urea induced denaturation of Lysozyme. Crystal structures of HEWL were solved in complex with urea by soaking native crystals in 9M urea for increasing time intervals to observe the dynamics and to get atomistic snapshots during the onset of urea denaturation and also to explore the mode of interaction of urea with protein. We could observe a consistent breakage of a few intraprotein hydrogen bonds (indicative of the onset of urea denaturation) and mmpbsa calculations gave an insight into the structural mechanism of urea induced denaturation.

a) **Raskar, T.**, Khavnekar, S., & Hosur, M. (2016). Time-dependent X-ray diffraction studies on urea/hen egg white lysozyme complexes reveal structural changes that indicate onset of denaturation. *Scientific reports*, 6, 32277.

b) **Raskar, T.**, Koh, C. Y., Niebling, S., Kini, R. M., & Hosur, M. V. (2019). X-ray crystallographic analysis of time-dependent binding of guanidine hydrochloride to HEWL: First steps during protein unfolding. *International journal of biological macromolecules*, 122, 903-913.

2. I worked on outer membrane porin of *Pseudomonas putida* CSV86 in order to investigate into the mechanism of glucose transport across the porin. For this purpose, steered molecular dynamics simulation was used and was coupled with C14 glucose binding studies. We could identify distinct regions of oprB where Glucose molecule stalled. This indicates distinct energy barriers for glucose transport. These energies were calculated by using weighted histogram analysis (WHAM) which enables the calculation of Potential of mean force (PMF).
3. During my PhD, I worked on two enzyme systems: E.coli copper amine oxidase (ECAO) and Aspartate α -decarboxylase (ADC). In case of ECAO, we have investigated into the basis of the effect of two mutations which are $\sim 20\text{-}30\text{\AA}$ away from the active site on enzyme activity. We have mainly used quasi elastic neutron scattering (QENS) to understand the influence of these mutations on the dynamics of ECAO while neutron diffraction was used to understand the influence on long range electrostatic interactions.
In case of ADC, we used QENS and inelastic neutron scattering to understand the timescales and changes in the intra and intermolecular conformational dynamics upon binding of a substrate analogue.
We have also collected neutron data over a broad energy range in order to capture diverse dynamical modes (from \AA to nm lengthscales) of ADC in its apo and ligand complexed states. These data will be complemented by THz spectroscopy datasets in order to study concerted protein and solvation dynamics as THz radiation is extremely sensitive to changes in collective modes of ordered and bulk water.

a) **Raskar, T.**, Niebling, S., Devos, J. M., Yorke, B. A., Härtlein, M., Forsyth, T.V., Seydel, T. & Pearson, A.R. (2020). Diffusive dynamics of Aspartate α -decarboxylase (ADC) liganded with D-serine in aqueous solution. *BioRxiv*.

D. List of publications

Raskar, T., Das, A., & Hosur, M. V. (2015) . 187 Drug resistance: crystallography of drug-resistant HIV-1 protease mutant. *Journal of Biomolecular Structure and Dynamics*, 33(sup1), 124-124. (Conference proceedings)

Raskar, T., Khavnekar, S., & Hosur, M. (2016). Time-dependent X-ray diffraction studies on urea/hen egg white lysozyme complexes reveal structural changes that indicate onset of denaturation. *Scientific reports*, 6, 32277.

Raskar, T., Koh, C. Y., Niebling, S., Kini, R. M., & Hosur, M. V. (2019). X-ray crystallographic analysis of time-dependent binding of guanidine hydrochloride to HEWL: First steps during protein unfolding. *International journal of biological macromolecules*, 122, 903-913.

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