

Souvik Dey, Ph.D.

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Summary

Computational Chemist with 7+ years of experience applying AI, cheminformatics, and molecular modeling to study protein dynamics, drug discovery, and toxicity prediction. Specialized in transformers, VAEs, and multi-task learning applied to chemical/omics data. Proven success in interdisciplinary collaborations and tool development across academia and government, with a strong publication record in generative modeling, structural biophysics, and protein-ligand interactions. Passionate about fostering innovation and driving translational research through deep learning, generative AI, and biophysics.

Work Experience

Research Scientist II

Jan 2025 - Present

Research Scientist I

Oct 2023 - Dec 2024

DoD Biotechnology High Performance Computing Software Applications Institute

- Designed transformer-based dataset-balancing methods and improved balanced accuracy on imbalanced datasets by 30%
- Designing multi-task learning models for predicting blood-brain barrier permeability and neurotoxicity of small molecules
- Led the creation of a large-scale curated omics repository to support foundation model pretraining
- Provided cheminformatics expertise for building toxicology web tools used by academic and government researchers
- Wrote a DoD proposal on AI-driven GPCR drug discovery, securing \$1.1M in funding

Graduate Research Assistant

Aug 2018 - Sep 2023

University of Illinois Chicago

- Developed generative models (VAE) to explore conformations of intrinsically disordered proteins (IDPs)
- Integrated MD simulations and deep learning to model aggregation-linked dynamics in neurodegeneration
- Conducted free energy simulations to explore signal transduction in autoinhibited proteins
- Validated computational predictions via collaborations with NMR scientists
- Managed the group's high-performance computing (HPC) and software infrastructure

Computational Chemistry Intern

May 2022 - Aug 2022

NeuroX1

- Performed virtual screening using pharmacophore modeling, MM-GBSA, and FEP for CNS targets in Schrödinger
- Developed multi-objective scoring and prioritization strategies for large compound libraries

Undergraduate Internships

Indian Association for the Cultivation of Science

Aug 2017 - May 2018

- Uncovered the mechanisms of ATP hydrolysis in kinesin motor proteins using hybrid QM/MM simulations

University of Groningen

May 2017 - July 2017

- Investigated the role of a photolyase in repairing UV-induced DNA damage using MD simulations

Indian Institute of Technology Bombay

May 2016 - July 2016

- Identified the mechanism of urea-induced peptide unfolding and its attenuation by an ionic liquid using MD simulations

Bhabha Atomic Research Centre

May 2014 - July 2015

- Examined the preferential adsorption of DNA nucleobases on 2D nanosheets using density functional theory (DFT)

Computational Skills

- *AI/ML and Generative Modeling*:: Transformers (BioBERT, ChemBERTa), REINVENT, VAEs, RNNs, Transfer Learning
- *Cheminformatics and Docking*: RDKit, DeepChem, Chemprop, OpenBabel, Schrödinger Suite
- *Programming*: Python (PyTorch, TensorFlow, scikit-learn, Pandas, NumPy, SciPy), C, bash, Tcl/Tk
- *Molecular Dynamics simulations*: Amber, NAMD, GROMACS

Education

University of Illinois Chicago

Aug 2018 - Sep 2023

Ph.D. in Chemistry

Visva Bharati University, India

Aug 2013 - May 2018

BS+MS in Chemistry

Publications

- **Souvik Dey**, Mohamed Diwan M. AbdulHameed, and Anders Wallqvist (2025). Developing muscarinic receptor M1 classification models utilizing transfer learning and generative AI techniques. (*Scientific Reports (in press)*) ([GitHub](#))
- Mohamed Diwan M. AbdulHameed, **Souvik Dey**, Zhen Xu, Ben Clancy, Valmik Desai, and Anders Wallqvist (2025). [MONSTROUS: a web-based chemical-transporter interaction profiler](#). *Frontiers in Pharmacology* 16, 1498945 ([GitHub](#)) ([Web server](#))
- Matt MacAinsh, **Souvik Dey**, and Huan-Xiang Zhou (2024). [Direct and indirect salt effects on homotypic phase separation](#). *eLife* 13, RP100282 ([GitHub](#))
- **Souvik Dey**, and Huan-Xiang Zhou (2023). [N-WASP is competent for downstream signaling before full release from autoinhibition](#). *Journal of Chemical Physics* 158, 091105
- **Souvik Dey**, and Huan-Xiang Zhou (2023). [Why does synergistic activation of WASP, but not N-WASP, by Cdc42 and PIP2 require Cdc42 prenylation?](#) *Journal of Molecular Biology* 435, 168035
- Sean T. Smrt, Cristian A. Escobar, **Souvik Dey**, Timothy A. Cross, and Huan-Xiang Zhou (2023). [An Arg/Ala-rich helix in the N-terminal region of M. tuberculosis FtsQ anchors FtsZ to membranes](#). *Communications Biology* 6, 311
- **Souvik Dey**, and Huan-Xiang Zhou (2022). [Membrane tethering of SepF, a membrane anchor for the Mycobacterium tuberculosis Z-ring](#). *Journal of Molecular Biology* 434, 167817
- **Souvik Dey**, Matt MacAinsh, and Huan-Xiang Zhou (2022). [Sequence-dependent backbone dynamics of intrinsically disordered proteins](#). *Journal Chemical Theory and Computation* 18, 10 ([GitHub](#))
- Sanbo Qin, Alan Hicks, **Souvik Dey**, Ramesh Prasad, and Huan-Xiang Zhou (2022). [ReSMAP: Web server for predicting residue-specific membrane-association propensities of intrinsically disordered proteins](#). *Membranes* 12, 773
- Aayush Gupta, **Souvik Dey**, Alan Hicks, and Huan-Xiang Zhou (2022). [Artificial intelligence guided conformational mining of intrinsically disordered proteins](#). *Communications Biology* 5, 610 ([GitHub](#))
- Soumadwip Ghosh, **Souvik Dey**, Mahendra Patel, and Rajarshi Chakrabarti (2017). [Can ammonium-based room temperature ionic liquid counteract the urea induced denaturation of a small peptide?](#) *Physical Chemistry Chemical Physics* 19, 7772

Awards and Outreach

- \$1.1M DoD (CDMRP) Research Award for AI-driven GPCR screening (2024)
- UIC Graduate Student Council Travel Award for presenting at Biophysical Society Annual Meeting, San Diego, USA (2023)
- UIC Department of Chemistry Travel Award for presenting at Les Houches-TSRC Protein Dynamics Workshop, Aussois, France (2022)
- Awarded INSPIRE Fellowship by Department of Science and Technology, Government of India (2013-2018)
- Mentor at [Midtown Achievement Center for Boys](#) for tutoring 6th – 8th grade students (2021-2023)
- Mentor at [Science Club](#) organized by Northwestern University for helping 4th – 6th grade students carry out real-world science experiments (2019-2020)