# Souvik Dey, Ph.D.

Frederick, MD souvik.dey29@gmail.com 312-774-8210 LinkedIn GitHub

## Summary

Computational Chemist with 7+ years of experience leveraging AI/ML (including transformers, VAEs, RNNs, and transfer learning) to accelerate drug discovery and toxicity prediction. Proven leader in developing novel computational tools and translating complex chemical/omics data into actionable insights. Expertise in small-molecule property prediction, protein dynamics, and structural biophysics. Passionate about pioneering translational research and fostering innovation at the intersection of AI and pharmaceutical sciences. Strong record of interdisciplinary collaboration, publication, and driving strategic research initiatives.

## Work Experience

**Research Scientist** *Oct 2023 - Present*
DoD Biotechnology High Performance Computing Software Applications Institute

- Designed a multi-modal transformer architecture for CNS neurotoxicity prediction of small molecules, applying both protein and chemical language models to proteomics, chemical potency, and multielectrode array data
- Implemented the use of generative AI and transfer learning to augment imbalanced public datasets, significantly improving protein-ligand binding predictions
- Led the curation of a multi-omics (transcriptomics and metabolomics) repository to enable foundation model pretraining
- Provided cheminformatics expertise for building toxicology web tools utilized by academic and government researchers

**Graduate Research Assistant** *Aug 2018 – Sep 2023*
University of Illinois Chicago

- Developed variational autoencoder models to explore conformations of intrinsically disordered proteins (IDPs)
- Integrated MD simulations and deep learning to explain the role of IDP dynamics in disease pathways
- Conducted free energy simulations to explore signal transduction mechanism in autoinhibited proteins
- Validated computational predictions through close collaborations with NMR experimentalists
- Managed the group's high-performance computing (HPC) and software infrastructure

**Computational Chemistry Intern** *May 2022 – Aug 2022*
NeuroX1

- Developed virtual screening campaigns for CNS drug targets using pharmacophore modeling, MM-GBSA, and FEP in Schrödinger, contributing to lead identification efforts

**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 (ESM, ChemBERTa), REINVENT, VAEs, RNNs, Transfer Learning
- *Cheminformatics and Docking*: RDKit, DeepChem, Chemprop, Schrödinger (for virtual screening, FEP, MM-GBSA)
- *Programming*: Python (PyTorch, TensorFlow, scikit-learn, Pandas, NumPy, SciPy), C, bash, Tcl/Tk
- *Molecular Modeling and Simulation*: Amber, NAMD, GROMACS, QM/MM, Free Energy Calculations

## 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* 15, 16486 (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

- Contributed to securing $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 $6^{th} - 8^{th}$ grade students (2021-2023)
- Mentor at Science Club organized by Northwestern University for helping $4^{th} - 6^{th}$ grade students carry our real-world science experiments (2019-2020)