Nandan Haloi

Curriculum Vitae

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Education

2021 **Doctor of Philosophy in Biophysics and Quantitative Biology**, *University of Illinois at Urbana-Champaign*, Illinois, USA.

2016 **Bachelors of Technology in Chemical Science and Technology**, *Indian Institute of Technology Guwahati*, Assam, India.

Positions

2021–current **Postdoctoral Scholar**, *KTH Royal Institute of Technology*, Stockholm, Sweden.

Research Experience

2021, Nov –current **Postdoctoral Scholar at SciLifeLab**, *KTH Royal Institute of Technology*, Stockholm, Sweden.
Supervisor: Prof. Erik Lindahl

Marie-Curie Postdoctoral Fellow (2023-current):

- Characterizing ligand-protein interactions with a cryo-EM data-driven modeling approach.
- Investigating structural and energetic landscape of human neuronal receptors using adaptive sampling and Markov state modeling.
- Accurate flexible protein fitting into cryo-EM maps by combining MD simulations and machine learning.
- Determining Protein Conformational Ensembles by Combining Machine Learning and SAXS (Supervising a Master's student, Samuel Lidbrink).
- Designing intensity-based drug sensing proteins (collaboration Lester group, Caltech)

Industrial collaboration with Janssen Pharmaceuticals, Belgium (2021-2023):

- Refining protein-protein complex interfaces using Cryo-EM density-guided MD simulations.
- Investigating conformational landscape of NLRP3 activation using Markov state modeling.

2016–2021 **Graduate Research Assistant at Beckman Institute of Science and Technology**, *University of Illinois at Urbana-Champaign*, IL, USA.
Supervisor: Prof. Emad Tajkhorshid

- Developing a multiscale molecular/Brownian dynamics simulations approach to derive an atomic structural model for a key protein complex within the explicit context of mitochondrial membrane (collaboration with Kwok group, Medical College of Wisconsin).
- Investigating the gating kinetics of bacterial outer membrane porins using Markov state model (collaboration with Shukla group, UIUC).
- Developing a Monte Carlo based Pathway Search (MCPS) algorithm, combined with bias exchange umbrella sampling, for exploring molecular processes while considering multiple slow degrees of freedom (collaboration with Hergenrother group, UIUC).
- Combining computational modeling with cryo-EM to investigate host recognition of a key dimeric antibody (collaboration with Stadtmueller group, UIUC).

2019 **Visiting Research Assistant at École Polytechnique Fédérale de Lausanne**.
Supervisor: Prof. Matteo Dal Peraro

- Fitting protein structures into cryo-EM maps of low to high resolutions.

2015 **Visiting Research Assistant at Saint Louis University**.
Supervisor: Prof. Ryan D. Mcculla

- Computational investigation of the reactions of sulfenic acids with biologically relevant nucleophiles using QM calculations.

2012-2016 **Undergraduate Research Assistant at Indian Institute of Technolody Guwahati**.
Supervisor: Prof. Debasis Manna

- Docking of PIP2 to the PH Domain of Lamellipodin followed by MD simulation.

Publications

2023 **N. Haloi**, R. J. Howard, E. Lindahl, "Structural prediction of an open heteromeric GABAA receptor" *In Preparation*

2023 **N. Haloi**, E. Karlsson, R. J. Howard, E. Lindahl, "Discovering cryptic pocket opening and ligand binding in a vestibular site of the 5-HT$_{3A}$ receptor" *bioRxiv*, doi: https://doi.org/10.1101/2023.11.13.566806

2023 **N. Haloi***, S. Huang*, A. N. Nichols, E. J. Fine, C. B. Marotta, D. A. Dougherty, E. Lindahl, R. J. Howard, S. L. Mayo, H. A. Lester "Interactive computational and experimental approaches improve the sensitivity of periplasmic binding protein-based nicotine biosensors for measurements in biofluids" *bioRxiv*, Doi: https://doi.org/10.1101/2023.01.16.524298

2023 J. Cowgill*, C. Fan*, **N. Haloi**, V. Tobiasson, Y. Zhuang, R. J. Howard, and E. Lindahl "Structure and dynamics of differential ligand binding in the human ρ-type GABAA receptor" *Neuron*, 111,1–15.

2023 X. Yu*, R. E. Matico*, R. Miller, B. V. Schoubroeck, K. Grauwen, J. Suarez, B. Pietrak, **N. Haloi,** Y. Yin, G. Tresadern, L. Perez benito, E. Lindahl, A. Bottelbergs, D. Oehlrich, N. V. Opdenbosch, S. Sharma "Cryo-EM structures of NLRP3 reveal its self-activation mechanism" *Nature Communications*, Accepted.

2023 V. Bondarenko, Q. Chen, K. Singewald, **N. Haloi**, T. Tillman, R. Howard, E. Lindahl, Y. Xu, P. Tang "Structural Elucidation of Ivermectin Binding to α7nAChR and the Induced Channel Desensitization" *ACS Chemical Neuroscience* 14, 6, 1156–1165

2023 S. Dey, A. Patel, **N. Haloi**, S. Srimayee, S. Paul, G. K. Barik, N. Akhtar, D. Shaw, G. Hazarika, B. M. Prusty, M. Kumar, M. K. Santra, E. Tajkhorshid, S. Bhattacharjee, D. Manna "Quinoline-based Zinc Ionophores with Antimicrobial Activity" *J. Med. Chem.*, 66, 16, 11078–11093 (Cover Article)

2022 A. K. Vasan*, **N. Haloi***, P. C. Wen, R. J. Ulrich, M. E. Metcalf, W. W. Metcalf, P. Hergenrother, D. Shukla, and E. Tajkhorshid "Role of internal loop dynamics in antibiotic permeability of outer membrane porins" *PNAS*, 119(8):e2117009119

2021 **N. Haloi***, A. K. Vasan*, E. Geddes, A. Prasanna, P. C. Wen, W. W. Metcalf, P. Hergenrother, and E. Tajkhorshid "Rationalizing generation of broad spectrum antibiotics with the addition of a positive charge" *Chemical Science*, 12:15028-15044 (2021) (Cover Article) (Featured at Illinois News Bureau and TCBG highlight)

2021 **N. Haloi**, P. C. Wen, Q. Cheng, M. Yang, G. Natarajan, A. K. S. Camara, W. M. Kwok, and E. Tajkhorshid "Structural basis of complex formation between mitochondrial anion channel VDAC1 and Hexokinase-II" *Communications Biology*, 4:667. (Featured at TACC's Stampede2 HPC Supercomputers, HPCwire newsletters and TCBG highlight)

2020 S. K. Bharathkar, B. W. Parker, A. Malyutin, **N. Haloi**, E. Tajkhorshid, and B. M. Stadtmueller "The structures of secretory and dimeric Immunoglobulin A" *eLife*, 9:e56098.

2020 J. T. Petroff, S. M. Omlid, **N. Haloi**, L. Sith, S. Johnson, and R. D. McCulla "Reactions of sulfenic acids with amines, thiols, and thiolates studied by quantum chemical calculations" *Computational and Theoretical Chemistry*, 1189: 112979.

2018 S. Gorai, D. Paul, R. Borah, **N. Haloi**, M. K. Santra, and D. Manna "Role of cationic groove and hydrophobic residues in Phosphatidylinositol-dependent membrane-binding properties of Tks5-Phox homology domain" *ChemistrySelect*, 3:1205-1214.

2016 S. Gorai, D. Paul, **N. Haloi**, R. Borah, M. K. Santra, and D. Manna "Mechanistic insights into the phosphatidylinositols binding properties of pleckstrin homology domain of lamellipodin" *Molecular BioSystems*, 12:747-57.

Honors and Awards

2023 **Marie Skłodowska-Curie Actions (MSCA) Postdoctoral Fellowships**, *PI: Erik Lindhal*.

2023 **PRACE Travel Grant**, International HPC Summer School.

2023 **PI at EuroHPC Regular Access (EHPC-REG-2023R01103)**, Investigating conformational modulation of neuronal receptors by brain neurosteroids (24 million CPU/GPU core hours).

2023 **Co-PI at EuroHPC Regular Access (EHPC-REG-2022R03219)**, AlphaFold2-guided Markov state modeling the conformational landscape of inflammasome activation (55 million CPU core hours).

2022 **Co-PI at Berzelius AI/ML Cluster**, Improving flexible structure fitting into cryo-EM maps using multiple conformers generated by AlphaFold (3.3 k GPU hours per month for 6 monhts)).

2022 **PI at EuroHPC Regular Access (EHPC-REG-2021R0074)**, Characterizing conformational landscape of neuronal receptors (23 million CPU core hours)).

2022 **Acknowledge of Excellence**, European Molecular Biology Organization Postdoctoral Fellowships.

2021 **Poster Competition Winner**, Biophysical Society Meeting.

2021 **Co-PI at Illinois Blue Waters allocation**, Mechanism of Antibiotic Resistance in Gram-negative Bacteria (estimated value of $480K).

2021 **Co-PI at Illinois Blue Waters allocation**, Antibiotic Resistance Mechanism in Pseudomonas aeruginosa (estimated value of $465K).

2019 **Biochemistry Travel Award**, UIUC.

2019 **Biophysics Travel Award**, UIUC.

2019 **Honorarium from Prof. Peraro**, École Polytechnique Fédérale de Lausanne, Switzerland.

2015 **Honorarium from Prof. McCulla**, Saint Louis University, USA.

2013 **State Government Fellowship**, Assam, India.

Leadership and Management

2023 **Supervising Master's Student**, Samuel Eriksson Lidbrink, KTH.

2022-2024 **Supervising PhD Student**, Tatjana Shugaeva, KTH.

2023-current **Organizing MD/AI Biweekly Seminar**, Molecular Biophysics Stockholm, Sweden.

2023 **Assisting the Organization of EBSA**, Stockholm, Sweden.

2023 **Organizing "Culture Map" Workshop**, Departmental Retreat, Stockholm, Sweden.

2023 **Tutoring at High School Student Training Event**, Brain Awareness Week, SciLifeLab, Sweden.

2022 **Tutoring at High School Student Training Event**, Demonstrating the Power of Simulations, SciLifeLab, Sweden.

2021 **Career Counselling**, Gargaon College, Assam, India.

2021 **Seminar Moderator**, Black in International Physics of Living Systems Seminar, Virtual.

2019 **Judge for Undergraduate Poster Competition**, Biophysical Society Meeting.

Media Coverages

2021 **Scientists Discover how Antibiotics Penetrate Gram-negative Bacterial Cell Walls**, *Featured at research news of Illinois News Bureau, UIUC.*

2021 **TACC Supercomputer Delves into Protein Interactions**, *Featured at HPC Wire news letter.*

2021 **Cell's Energy Secrets Revealed with Supercomputers**, *Press release at Texas Advanced Computing Center (TACC) news letter.*

Presentations

Structural and Energetic Characterizations of the Conformational Landscapes in Ligand-gated Ion Channels using Adaptive Sampling and Markov State Modeling

2023 European Biophysical Societies Association, Stockholm, Sweden. (Talk)

2023 International HPC Summer School, Atlanta, USA. (Poster)

Investigating Antibiotic Permeation Mechanisms through Outer Membrane Porins in High-Dimensional Conformational Space

2022 1st Nordic Conference on Computational Chemistry, Gothenburg, Sweden. (Poster)

2022 Physical and Quantitative Approaches to Overcome Antibiotic Resistance - BPS Thematic meeting, Stockholm, Sweden. (Talk)

2022 Protein Dynamics Conference, Aussios, French. (Poster)

2022 Molecular Graphics and Modelling Society, United Kingdom, Virtual. (Talk)

2021 Recent Advances in Modelling Rare Events (RARE2021), India, Virtual. (Poster)

2021 European Molecular Biology Organization, Virtual. (Talk)

Gating Mechanism of Outer Membrane Porins of Gram-negative Bacteria:

2020 International Physics of Living Systems, Virtual. (Talk)

Structural Basis of Complex Formation between VDAC and Hexokinase:

2020 Biophysical Society Meeting, San Diego, California, USA. (Poster)

2019 Biophysical Society Meeting, Baltimore, Maryland, USA. (Poster)

Antibiotic Permeation Across the Bacterial Outer Membrane Porins:

2018 Biophysical Society Meeting, San Francisco, California, USA. (Poster)

2018 Gordon Research Seminar, Ventura Beach, California, USA. (Talk)

Teaching Experiences

2023 **Teaching Assistant**, *Molecular Biophysics*, Engineering Physics, KTH.

2021 **Teaching Assistant**, *Cells, Tissues & Development*, Department of Biochemistry, UIUC.

2018 **Teaching Assistant**, *Physical Biochemistry*, Department of Biochemistry, UIUC.

Scientific Services

2022-2023 Reviewed articles at Nature Communications and Journal of Chemical Theory and Computation.

2017–2020 Member of Biophysical Society.

Skills

Computational Techniques: Molecular Dynamics Simulations, Machine Learning, Brownian Dynamics Simulations, Monte Carlo Simulations, Quantum Mechanical Calculations, Bias Exchange Umbrella Sampling, Markov State Modeling, Force field development, Transition Path Theory, Docking, Integrative modeling

Software: VMD, NAMD, GROAMCS, ARBD, Gaussian09, AutoDock, HADDOCK, MDFF, pyEmma

Programming Languages	Python, Tcl, Fortran, Bash

References

- **Prof. Erik Lindahl**
  Professor of Biophysics, KTH Royal Institute of Technology
  Professor of Biophysics, Stockholm University
  Vice dean, Chemistry, Stockholm University
  co-Director, Swedish e-Science Research Center
  Chair, Chapter VII Royal Engineering Academy of Sciences
  Email: erik@kth.se
  Phone: +46-734618050
- **Prof. Emad Tajkhorshid**
  Professor of Chemistry, Biophysics, Bioengineering, and Biophysics and Quantitative Biology
  Directory of NIH Center for Macromolecular Modeling and Bioinformatics
  Beckman Institute for Advanced Science and Technology
  University of Illinois at Urbana Champaign, IL, USA
  Email: emad@illinois.edu
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- **Prof. Wai-Meng Kwok**
  Professor of Anesthesiology, Pharmacology & Toxicology
  Cancer Center and Cardiovascular Center
  Medical College of Wisconsin, Milwaukee, WI, USA
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- **Prof. Debasis Manna**
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  Indian Institute of Technology Guwahati, Assam, India
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