Nandan Haloi, PhD

Curriculum Vitae

KTH Royal Institute of Technology
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Education

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

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

Positions

2023–current **Marie-Curie Postdoctoral Fellow**, *KTH Royal Institute of Technology*, Stockholm, Sweden.
PI: Erik Lindahl

2021–2023 **Postdoctoral Scholar**, *In Collaboration with Janssen Pharmaceutical*, Stockholm, Sweden.
PI: Erik Lindahl

Research Expertise

Membrane Protein Function-Dynamics | **Drug-Protein Interactions**.

Molecular Dynamics Simulations | **Machine Learning** | **Integrative Modeling**.

Grants and Awards

Research

2023 **Marie Skłodowska-Curie Actions (MSCA) Postdoctoral Fellowships (101107036)**.
Characterizing ligand-protein interactions with a cryo-EM data-driven modeling approach

2022 **EMBO Postdoctoral Fellowships Acknowledge of Excellence**.
Characterizing ligand-protein interactions with a cryo-EM data-driven modeling approach

Supercomputing

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

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

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

Travel and Others

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

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

2019 **Biochemistry Travel Award**, UIUC.

2019 **Biophysics Travel Award**, UIUC.

Publications (Total 19)

First-author (7)

2025 **N. Haloi**, E. Karlsson, M. Delarue, R. J. Howard, E. Lindahl, "Discovering cryptic pocket opening and binding of a stimulant derivative in a vestibular site of the 5-HT_{3A} receptor" ***Science Advances***, 11, eadr0797.

2025 **N. Haloi**, S. E. Lidbrink, R. J. Howard, E. Lindahl, "Adaptive sampling-based structural prediction reveals opening of a $GABA_A$ receptor through the $\alpha\beta$ interface" ***Science Advances***, 11, eadq3788.

2025 **N. Haloi,** R. J. Howard, and E. Lindahl, "Cryo-EM ligand building using generative AI and molecular dynamics "*bioRxiv*, doi: https://doi.org/10.1101/2025.02.10.637508

2024 **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" ***Protein Engineering, Design and Selection***, 37, gzae003.

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)

Corresponding-author (2)

2025 T. Shugaeva, R. J. Howard, **N. Haloi†**, and E. Lindahl†, "Modeling cryo-EM structures in alternative states with generative AI and density-guided simulations" *bioRxiv*, doi: https://doi.org/10.1101/2025.02.06.636862

2025 S. E. Lidbrink, R. J. Howard, **N. Haloi†**, and E. Lindahl†, "Resolving the conformational ensemble of a membrane protein by integrating small-angle scattering with AlphaFold" ***PLOS Computational Biology***, In Press.

Co-author (10)

2025 B. M. Prusty, S. Srimayee, R. Karn, **N. Haloi**, S. K. Singh, M. Winterhalter, D. Manna, "Supramolecular Nanochannels: Suprasome-Mediated Delivery of Ionophore To Regulate Transmembrane Zn2+ Ion Transport" ***Chemistry - A European Journal***, e202501013.

2024 M. K. Kar, R. Mahata, S. Srimayee, **N. Haloi**, R. Kumar, E. Lindahl, M. Santra, and D. Manna, "β-Carboline-based light and pH dual stimuli-responsive ion transporters induce cancer cell death" ***Chemical Communications***, 60, 8419.

2024 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***, 15, 1164.

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 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" ***Journal of Medicinal Chemistry*** , 66, 16, 11078–11093. (Cover Article)

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.

Teaching

2025 **Outreach Teaching**, Exploring Biomolecular Modeling and Simulations | Sabancı University, Istanbul.

2024 **Course Teaching**, Molecular Biophysics | Engineering Physics, KTH | Graduate.

2023 **Course Teaching**, Molecular Biophysics | Engineering Physics, KTH | Graduate.

2023 **Outreach Teaching**, Brain Awareness Week | High School, Stockholm.

2022 **Outreach Teaching**, Demonstrating the Power of Simulations | High School, Stockholm.

2021 **Course Teaching**, Cells, Tissues & Development | Department of Biochemistry, UIUC | Undergraduate.

2018 **Course Teaching**, Physical Biochemistry | Department of Biochemistry, UIUC | Undergraduate.

Student Supervision

2024-2025 **Master's Student**, Elisei Mankov, *Stockholm University*.
Improving cryo-EM resolution of ligands in protein-ligand complexes using deep learning

2024 **Summer Internship Student**, Beatrice Pavesi, *University of Pavia*.
Cryo-EM-guided machine learning to calculate free energy underlying protein conformational landscapes

2023-current **PhD Student**, Samuel Eriksson Lidbrink, *KTH Royal Institute of Technology*.
Resolving the conformational ensemble of a membrane protein by integrating small-angle scattering with AlphaFold

2022-current **PhD Student**, Tatjana Shugaeva, *KTH Royal Institute of Technology*.
Refining cryo-EM structures in alternative states through generative models and density-guided simulations

Diversity, Equity, and Inclusion Activities

2024 **Newcomer Mentor**, Nema Problema, Sweden.

2023 **Workshop Organizer**, Understanding Cultural Differences, Campus Solna Biophysics Environment, Stockholm, Sweden.

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

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

2019 **Refugee Mentor**, Foundation for International Medical Relief of Children, UIUC, USA.

Scientific Services

Board Member

2024-current **Board Member of User Support Advisory Committee**, National Academic Infrastructure for Supercomputers, Sweden

2017–2024 **Member of Scientific Community**, *Biophysical Society Meeting*.

Reviewer

2025 **Grant Reviewer**, IT4Innovations, HPC Center Czech Republic.

2022-current **Scientific Article Reviewer**, Nat. Commun., JCTC, and PLOS Comput. Biol..

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

Organizer/Host

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

2023 **Assistant Organizer of EBSA**, Stockholm, Sweden.

Conferences

Atomistic Model Refinement using Artificial Intelligence and Cryo-EM

2025 Machine Learning Applied to Macromolecular Structure and Function, USA. (Poster)

2024 Emerging Theoretical Approaches to Complement Single-Particle Cryo-Electron Microscopy, Italy. (Poster)

Conformational Dynamics of Ligand-gated Ion Channels using Adaptive Sampling and Markov State Modeling

2024 Computational Chemistry Seminar at Technische Universität Berlin, Germany. (Talk)

2024 Structural Bioinformatics Seminar at Linköping University, Sweden. (Talk)

2024 Biophysical Society Meeting, Philadelphia, USA. (Poster)

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

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

Antibiotic Permeations through Porins in Gram-negative Bacteria using Enhanced Sampling Simulations

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, France. (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)

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

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

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

Complex Formation between VDAC and Hexokinase using Multi-scale Modeling

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

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

On the news

2025 **New findings on how stimulant-like compounds modulate receptor activity**, *Featured at SciLifeLab news, Sweden*.

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*.

References

- **Prof. Erik Lindahl** - Postdoc Mentor
  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** - PhD Supervisor
  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`
  Phone: +1 217-244-6914
- **Prof. Wai-Meng Kwok** - Collaborator
  Professor of Anesthesiology, Pharmacology & Toxicology
  Cancer Center and Cardiovascular Center
  Medical College of Wisconsin, Milwaukee, WI, USA
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