

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 **Bachelor 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

Machine Learning | Predictive Protein Dynamics | Cryo-EM data processing | Molecular Dynamics Simulations.

Membrane Protein Function-Dynamics | Drug-Protein Interactions.

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 20)

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 AlphaFold3-like model and molecular dynamics" *PLOS Computational Biology*, 21(8): e1013367
- 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. Vasanth*, **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. Vasanth*, 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*, 21(7): e1013187.

Co-author (11)

- 2025 A. Schahl, **N. Haloi**, M. Carroni, S. Zhang, Q. J. Sattentau, E. Sezgin, L. Delemotte, R. Howard, "Lipid-facilitated opening of the ADAM10 sheddase revealed by enhanced sampling simulations" *bioRxiv*, doi: <https://doi.org/10.1101/2025.08.17.670722>
- 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 $\alpha 7$ nAChR 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**, 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 European Biophysical Societies' Association**, 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 newsletter.*
- 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
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- **Prof. Emad Tajkhorshid** - PhD Supervisor
Professor of Chemistry, Biophysics, Bioengineering, and Biophysics and Quantitative Biology
Directory of NIH Center for Macromolecular Modeling and Bioinformatics
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