

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

Molecular Dynamics Simulations | Machine Learning | Experimental Data Integrations.
Protein-ligand Interactions | Membrane Protein Dynamics.

Honors and Awards

- 2023 **Marie Skłodowska-Curie Actions (MSCA) Postdoctoral Fellowships**, PI: Erik Lindahl.
- 2023 **PRACE Travel Grant**, International HPC Summer School.
- 2023 **EuroHPC Regular Access Super-computing Grant - Main-PI (EHPC-REG-2023R01103)**, Investigating conformational modulation of neuronal receptors by brain neurosteroids (24 million CPU/GPU core hours).
- 2023 **EuroHPC Regular Access Super-computing Grant - Co-PI (EHPC-REG-2022R03219)**, AlphaFold2-guided Markov state modeling the conformational landscape of inflammasome activation (55 million CPU core hours).
- 2022 **Berzelius AI/ML Super-computing Grant - Co-PI**, Improving flexible structure fitting into cryo-EM maps using multiple conformers generated by AlphaFold (20 k GPU hours).
- 2022 **EuroHPC Regular Access Super-computing Grant - Main-PI (EHPC-REG-2021R0074)**, Characterizing conformational landscape of neuronal receptors (23 million CPU core hours).
- 2022 **EMBO Postdoctoral Fellowships Acknowledge of Excellence**, PI: Erik Lindahl.
- 2021 **Poster Competition Winner**, Biophysical Society Meeting.
- 2021 **Illinois Blue Waters Super-computing Grant - Co-PI**, Mechanism of Antibiotic Resistance in Gram-negative Bacteria (estimated value of \$480K).
- 2021 **Illinois Blue Waters Super-computing Grant - Co-PI**, 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.

Publications (6 First authors, 1 Corresponding author, 16 Total)

- 2025 **N. Haloi**, S. E. Lidbrink, R. J. Howard, E. Lindahl, "Adaptive sampling-based structural prediction reveals opening of a GABAA receptor through the $\alpha\beta$ interface" *Science Advances*, 11, eadq3788.
- 2024 **N. Haloi**, E. Karlsson, M. Delarue, 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>, *Science Advances*, *Under Minor Revision*.
- 2024 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" *bioRxiv*, doi: <https://doi.org/10.1101/2024.09.05.611464> (Corresponding author)
- 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" *Chem. Commun.*, 60, 8419.
- 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.
- 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. Oehlich, 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" *J. Med. Chem.*, 66, 16, 11078–11093. (Cover Article)
- 2022 A. K. Vasani*, **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. Vasani*, 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.

Teaching

- 2024 **Co-Instructor**, Molecular Biophysics | Engineering Physics, KTH | Graduate.
- 2023 **Assistant Teacher**, Molecular Biophysics | Engineering Physics, KTH | Graduate.
- 2023 **Outreach Teacher**, Brain Awareness Week | High School, Stockholm.
- 2022 **Outreach Teacher**, Demonstrating the Power of Simulations | High School, Stockholm.
- 2021 **Assistant Teacher**, Cells, Tissues & Development | Department of Biochemistry, UIUC | Undergraduate.
- 2018 **Assistant Teacher**, Physical Biochemistry | Department of Biochemistry, UIUC | Undergraduate.

Student Supervision

- 2024 **Summer Internship Student**, Beatrice Pavesi.
- 2023-current **PhD Student**, Samuel Eriksson Lidbrink, KTH.
- 2022-current **PhD Student**, Tatjana Shugaeva, KTH.

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.

International Networks

- 2023-current **Prof. Marc Delarue**, Institut Pasteur, France.
- 2023-current **Dr. Maxwell Zimmerman**, Washington University in St. Louis, USA.
- 2023-current **Dr. Vytautas Gapsys**, Janssen Pharmaceuticals, Belgium.
- 2022-current **Dr. Laura Perez Benito**, Janssen Pharmaceuticals, Belgium.
- 2020-current **Prof. Debasis Manna**, Indian Institute of Technology Guwahati, India.
- 2022-2024 **Prof. Henry Lester**, California Institute of Technology, USA.
- 2022-2023 **Dr. Xiaodi YU**, Janssen Pharmaceuticals, USA.
- 2022-2023 **Prof. Pei Tang**, University of Pittsburg, USA.
- 2017-2021 **Prof. Wai-meng Kwok**, Medical College of Wisconsin, USA.
- 2017-2021 **Prof. Paul Hergenrother**, University of Illinois Urbana-Champaign, USA.
- 2019-2020 **Prof. Beth Stadtmueller**, University of Illinois Urbana-Champaign, USA.
- 2015 **Prof. Ryan McCulla**, Saint Louis University, USA.

Scientific Services

- 2024-current **Board Member of User Support Advisory Committee**, National Academic Infrastructure for Supercomputers, Sweden
- 2023-current **Organizer of MD/AI Biweekly Seminar**, Molecular Biophysics Stockholm, Sweden.
- 2023 **Assistant Organizer of EBSA**, Stockholm, Sweden.
- 2022-2023 **Scientific Article Reviewer**, Nat. Commun., JCTC, and PLOS Comput. Biol..
- 2017–2024 **Member of Scientific Community**, *Biophysical Society Meeting*.
- 2019 **Poster Competition Judge**, Biophysical Society Meeting.

Conferences

Structural and Energetic Characterizations of the Conformational Landscapes in 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)

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)

On the news

- 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**

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