Nandan Haloi

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

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 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 months)).

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

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

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.

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

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 Revision*.

2024 **N. Haloi**, R. J. Howard, E. Lindahl, "Adaptive sampling-based structural prediction reveals opening of a GABAA receptor through the $\alpha\beta$ interface" *bioRxiv*, doi: https://doi.org/10.1101/2024.05.03.592340, *Science Advances, Under 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. 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" *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.

Teaching

2024 **Co-Instructor**, Molecular Biophysics | Engineering Physics, KTH | Graduate.

2023 **Teaching Assistant**, 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 **Teaching Assistant**, Cells, Tissues & Development | Department of Biochemistry, UIUC | Undergraduate.

2018 **Teaching Assistant**, 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.

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 (NAISS) in Sweden

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.

2022-2023 **Reviewed articles**, Nat. Commun., JCTC, and PLOS Comput. Biol..

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

2017–2024 **Member of Biophysical Society**.

2019 **Judge for Undergraduate Poster Competition**, 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**
  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**
  Professor of Chemistry, Biophysics, Bioengineering, and Biophysics and Quantitative Biology
  Directory of NIH Center for Macromolecular Modeling and Bioinformatics
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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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