Nandan Haloi, PhD

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Education

2016–2021 **PhD, Biophysics and Quantitative Biology** · University of Illinois at Urbana-Champaign, USA.
Advisor: Prof. Emad Tajkhorshid.

2012–2016 **BTech, Chemical Science and Technology** · Indian Institute of Technology Guwahati, India.

Appointments

Oct 2026– **Förste forskningsingenjör (First Research Engineer)** · IFM, Linköping University. Cryo-EM and machine-learning projects with Dr. Björn Forsberg (DDLS Fellow).

2021–2026 **Postdoctoral researcher** · Erik Lindahl group, SciLifeLab.
KTH Royal Institute of Technology (2021–2025) and Stockholm University (2025–2026).
Marie Skłodowska-Curie Postdoctoral Fellow · 2023–2025. Sole applicant; European Commission grant 101107036.
Earlier phase in collaboration with Janssen Pharmaceutica (Johnson & Johnson), 2021–2023.

Competitive funding and awards

Research fellowships

2023–2025 **Marie Skłodowska-Curie Actions Postdoctoral Fellowship** (101107036). Sole applicant; European Commission.

2022 **EMBO Postdoctoral Fellowship, Acknowledgement of Excellence.**

Computational resources (as Principal Investigator)

2023–2024 **EuroHPC Regular Access Grant** (EHPC-REG-2023R01103). PI, 24 million CPU/GPU core hours.

2022–2023 **EuroHPC Regular Access Grant** (EHPC-REG-2021R0074). PI, 23 million CPU core hours.

2021–2022 **Blue Waters Supercomputing Grant** · Co-PI; NCSA, University of Illinois (est. value USD 480,000).

Prizes and travel awards

2023 / 2021 / 2019 PRACE Travel Grant, International HPC Summer School; Poster Competition Winner, Biophysical Society Meeting; Biochemistry & Biophysics Travel Award, UIUC.

Software

2026 **CryoLigATE** · deep-learning enhancement of cryo-EM map resolvability in protein–ligand complexes.
github.com/nandanhaloi123/CryoLigate

2022 **MCPS** · Monte Carlo pathway search and free-energy calculation for small-molecule permeation.
github.com/nandanhaloi123/MonteCarloPathwaySearch

Supervision and mentoring

2022–2025 **PhD student: Tatjana Shugaeva**, KTH. Refining cryo-EM structures in alternative states with generative models and density-guided simulations. First-author paper *Commun. Chem.* 8:317 (2025), me co-corresponding.

2023–2025 **PhD student: Samuel Eriksson Lidbrink**, KTH. Conformational ensembles from small-angle scattering and AlphaFold. First-author paper *PLOS Comput. Biol.* 21(7) (2025), me co-corresponding.

2024–2025 **MSc student: Elisei Mankov**, Stockholm University. Deep learning for ligand resolvability in cryo-EM maps.

2024 **Summer intern: Beatrice Pavesi**, University of Pavia. Cryo-EM-guided machine learning for conformational free energies.

2026– **Project supervision at LiU (IFM)** · cryo-EM heterogeneity and machine-learning projects.

Teaching

2023, 2024 **Course teaching: Molecular Biophysics**, graduate level, Engineering Physics, KTH.

2025 **Outreach teaching: Biomolecular Modeling and Simulations**, Sabancı University, Istanbul.

2018, 2021 **Course teaching** · Physical Biochemistry; Cells, Tissues & Development, Dept. of Biochemistry, UIUC (undergraduate).

2022, 2023 **Outreach** · Brain Awareness Week and “Demonstrating the Power of Simulations”, high schools, Stockholm.

Academic service

2024–2025 **Board member**, User Support Advisory Committee, NAISS, Sweden.

2025 **Grant reviewer**, IT4Innovations National Supercomputing Center, Czech Republic.

2022– **Reviewer**, *Nature Communications*, *J. Chem. Theory Comput.*, *PLOS Computational Biology*.

2023–2026 **Founder and organiser**, MD/AI biweekly seminar series, Molecular Biophysics Stockholm.

2023 **Assistant organiser**, European Biophysical Societies' Association congress, Stockholm.

Equal opportunity and inclusion

2026– **Committee member**, Equality and Equal Treatment Committee, Stockholm University.

2025– **Committee member**, Diversity, Equity and Inclusion Committee, SciLifeLab.

2024 **Newcomer mentor**, Nema Problema, Sweden (mentoring of newly arrived academics).

2019–2021 **Refugee mentor** (FIMRC, UIUC); moderator, Black in International Physics of Living Systems; career counsellor, Gargaon College, India.

Invited talks (9 of 28 presentations)

2026 **Department of Pharmacology**, University of Cambridge, United Kingdom.

2026 **Department of Biochemistry**, University of Oxford, United Kingdom.

2026 **electron Bio-Imaging Centre (eBIC)**, Diamond Light Source national synchrotron, United Kingdom.

2026 **Giersch International Conference & SCALE Kick-Off**, Frankfurt, Germany.

2026 **Dept. of Biomedical and Clinical Sciences (BKV)**, Linköping University, Sweden.

2025 **Dept. of Neuroscience, Physiology and Pharmacology**, University College London, United Kingdom.

2025 **Centre for Structural Systems Biology (CSSB)**, Hamburg, Germany.

2024 **Department of Chemistry**, Technische Universität Berlin, Germany.

2024 **Dept. of Physics, Chemistry and Biology (IFM)**, Linköping University, Sweden.

Media coverage and special recognition

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

2021 **Scientists discover how antibiotics penetrate Gram-negative bacterial cell walls** · Illinois News Bureau, University of Illinois.

2021 **TACC supercomputer delves into protein interactions** · HPCwire, and a Texas Advanced Computing Center press release.

2023 / 2021 **Journal cover articles** · *Journal of Medicinal Chemistry* 66(16); *Chemical Science* 12(45).

Principal research collaborations

Sweden Mikael Akke (Lund University); Björn Wallner and Björn Forsberg (Linköping University).

USA Ryan Hibbs (UC San Diego); Henry Lester and Dennis Dougherty (Caltech); Emad Tajkhorshid and Paul Hergenrother (UIUC); Wai-Meng Kwok (Medical College of Wisconsin); Pei Tang (University of Pittsburgh).

Europe, Asia Marc Delarue (Institut Pasteur, France); Erdinc Sezgin (University of Oxford, UK); Debasis Manna (IIT Guwahati, India); Joel Yeo (National University of Singapore).

Industry Janssen Pharmaceutica / Johnson & Johnson, Belgium.

References

Prof. Erik Lindahl, Professor of Biophysics, KTH & Stockholm University; Co-Director, Swedish e-Science Research Centre. erik@kth.se

Prof. Emad Tajkhorshid, Professor of Biochemistry and Biophysics; Director, NIH Center for Macromolecular Modeling, UIUC, USA. emad@illinois.edu

Prof. Wai-Meng Kwok, Professor of Anesthesiology and Pharmacology, Medical College of Wisconsin, USA. wmkwok@mcw.edu

Publications and bibliometric summary

Nandan Haloi, PhD · ORCID 0000-0003-3542-333X · † corresponding author * co-first author

Bibliometric summary

Total publications	**23**	Total citations	**578**
Publications since PhD (2021–)	**15**	h-index	**12**
First-author publications	**8**	Invited talks	**9**
Corresponding-author publications	**3**	Contributed talks and posters	**19**

Publications since PhD (15)

2026 **N. Haloi**†, R. J. Howard, E. Lindahl. "CryoLigATE: enhancing the resolvability of cryo-EM maps in protein–ligand complexes using deep learning." *bioRxiv*. *Software released openly.*

2026 M. P. Dalton, J. Teng, B. Bhattacharjee, **N. Haloi**, R. J. Howard, B. T. Worrell, E. Lindahl, M. H. B. Stowell, R. E. Hibbs. "Visualizing activation of the muscle acetylcholine receptor." *Nature Structural & Molecular Biology*, in press.

2026 C. M. Borghese, N. G. Desai, P. Garlapati, S. K. Shah, J. D. Galpin, L. Segura, **N. Haloi**, H. H. Zakon, R. J. Howard, C. A. Ahern, M. P. Goldschen-Ohm. "An atomic interaction conserved for over 600 million years gates inhibitory neurotransmission." *bioRxiv*.

2026 A. Schahl, **N. Haloi**, M. Carroni, S. Zhang, Q. J. Sattentau, E. Sezgin, L. Delemotte, R. J. Howard. "Lipid-facilitated opening of the ADAM10 sheddase revealed by enhanced sampling simulations." *Advanced Science* e15713.

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 αβ interface." *Science Advances* 11, eadq3788.

2025 **N. Haloi**, R. J. Howard, E. Lindahl. "Cryo-EM ligand building using AlphaFold3-like model and molecular dynamics." *PLOS Computational Biology* 21(8): e1013367.

2025 T. Shugaeva, R. J. Howard, **N. Haloi**†, E. Lindahl†. "Modeling cryo-EM structures in alternative states with AlphaFold2-based models and density-guided simulations." *Communications Chemistry* 8:317.

2025 S. E. Lidbrink, R. J. Howard, **N. Haloi**†, E. Lindahl†. "Resolving the conformational ensemble of a membrane protein by integrating small-angle scattering with AlphaFold." *PLOS Computational Biology* 21(7): e1013187.

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 Zn^{2+} ion transport." *Chemistry – A European Journal* e202501013.

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 M. K. Kar, R. Mahata, S. Srimayee, **N. Haloi**, R. Kumar, E. Lindahl, M. Santra, 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, E. Lindahl. "Structure and dynamics of differential ligand binding in the human ρ-type $GABA_A$ 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.

Publications during and before PhD (8)

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)*

2022 A. K. Vasan*, **N. Haloi***, P. C. Wen, R. J. Ulrich, M. E. Metcalf, W. W. Metcalf, P. Hergenrother, D. Shukla, 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, E. Tajkhorshid. "Rationalizing the generation of broad spectrum antibiotics with the addition of a positive charge." *Chemical Science* 12, 15028–15044. *(Cover article; featured by Illinois News Bureau)*

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

2020 S. K. Bharathkar, B. W. Parker, A. Malyutin, **N. Haloi**, E. Tajkhorshid, 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, 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, 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, D. Manna. "Mechanistic insights into the phosphatidylinositols binding properties of pleckstrin homology domain of lamellipodin." *Molecular BioSystems* 12, 747–757.