

# Erik Nordquist

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## Education

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2023 **Ph.D.** Chemistry, University of Massachusetts Amherst.

2018 **B.S.** Chemistry and Physics, The College of Idaho.

## Work Experience

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2018–23 **Graduate Research Assistant**, University of Massachusetts, Amherst, Department of Chemistry.

- **Advisor:** Jianhan Chen, Ph.D.
  - **Thesis:** Understanding Protein Structure-Function Relationships Using Simulations and Machine Learning
  - Focus: Computational biophysics, Molecular dynamics, Machine learning
- 2023– **Postdoctoral Fellow**, University of Maryland Baltimore, Department of Pharmaceutical Sciences.
- **Advisor:** Alexander D. MacKerell, Jr., Ph.D.
  - Focus: Computer-aided drug design (CADD), Computational methods development, Molecular dynamics

## Appointments

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2023– **Postdoctoral Fellow**, University of Maryland, Baltimore, Department of Pharmaceutical Sciences.

2025– **Adjunct Professor**, Stevenson University, Department of Chemistry.

## Fellowships and Awards

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2025 **Excellence in Service Award**, University of Maryland, Baltimore.

2024 **Best of Biophysical Journal 2023**, publication titled “Inner pore hydration free energy...”  
**Talk award**, Research Symposium, UM Greenebaum Comprehensive Cancer Center.

2023– **NIH T32 Postdoctoral Fellowship**, University of Maryland, Baltimore.

2022 **Paul H. Terry Endowment Award**, Chemistry Dept., University of Massachusetts Amherst.  
**Teaching Fellowship**, College of Natural Sciences, University of Massachusetts Amherst.

2020–22 **NIH T32 Predoctoral Fellowship**, University of Massachusetts Amherst.

2020 **William E. McEwen Poster Award**, Chemistry Dept., University of Massachusetts Amherst.

## Peer-Reviewed Publications

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- **Nordquist E**, Zhao M, Yu W, MacKerell A. Computational Modeling of PROTAC Ternary Complexes as Ensembles Using SILCS-xTAC. **J. Chem. Inf. Model.** 2025. DOI: [10.1021/acs.jcim.5c02045](https://doi.org/10.1021/acs.jcim.5c02045)
- Patel R, **Nordquist E**, Polli J. Prediction of surfactant-mediated dissolution of poorly soluble drugs from drug particles. **Eur. J. Pharm. Sci.** 2025. DOI: [10.1016/j.ejps.2025.107052](https://doi.org/10.1016/j.ejps.2025.107052)
- **Nordquist E<sup>#</sup>**, Zhao M<sup>#</sup>, Kumar A, MacKerell A. Physics- and Machine-Learning Based Method to Identify Druggable Binding Sites Using SILCS-Hotspots. **J. Chem. Inf. Model.** 2024. DOI: [10.1021/acs.jcim.4c01189](https://doi.org/10.1021/acs.jcim.4c01189)
- **Nordquist E**, Jia Z, Chen J. Small Molecule NS11021 Promotes BK Channel Activation by Increasing Inner Pore Hydration. **J. Chem. Inf. Model.** 2024. DOI: [10.1021/acs.jcim.4c01012](https://doi.org/10.1021/acs.jcim.4c01012)

- **Nordquist E<sup>#</sup>**, Zhang G<sup>#</sup>, Barehiya S, Ji N, White K, Han L, Jia Z, Shi J, Cui J, and Chen J. Incorporating physics to overcome data scarcity in predictive modeling of protein function: a case study of BK channels. **PLOS Comput. Biol.** 2023. DOI: [10.1371/journal.pcbi.1011460](https://doi.org/10.1371/journal.pcbi.1011460)
- Zhang L, Barehiya S, **Nordquist E**, Chen J. Machine Learning Generation of Dynamic Protein Conformational Ensembles. **Molecules** 2023. DOI: [10.3390/molecules28104047](https://doi.org/10.3390/molecules28104047)
- **Nordquist E**, Zhiguang J, Chen J. Inner pore hydration free energy controls activations of the big potassium channel and its mutants. **Biophys. J.** 2023. DOI: [10.1016/j.bpj.2023.02.005](https://doi.org/10.1016/j.bpj.2023.02.005)
- **Nordquist E<sup>#</sup>**, Schultz S<sup>\*#</sup>, and Chen J. Using Metadynamics To Explore the Free Energy of Dewetting in Biologically Relevant Nanopores. **J. Phys. Chem. B** 2022 DOI: [10.1021/acs.jpcb.2c04157](https://doi.org/10.1021/acs.jpcb.2c04157)
- **Nordquist E**, Clerico E, Chen J, Giersch L. Computational Modeling of Hsp70-Client Interactions: Past, Present, and Future. **J. Phys. Chem. B** 2022. DOI: [10.1021/acs.jpcb.2c03806](https://doi.org/10.1021/acs.jpcb.2c03806)
- **Nordquist E**, English C, Clerico E, Sherman W, Giersch L, Chen J. Physics-based modeling provides predictive understanding of selectively promiscuous substrate binding by Hsp70 chaperones. **PLOS Comput. Biol.** 2021. DOI: [10.1371/journal.pcbi.1009567](https://doi.org/10.1371/journal.pcbi.1009567)
- Gong X, Chiricotto M, Liu X, **Nordquist E**, Feig M, Brooks C, Chen J. Accelerating the generalized born with molecular volume and solvent accessible surface area implicit solvent model using graphics processing units. **J. Comput. Chem.** 2020. DOI: [10.1002/jcc.26133](https://doi.org/10.1002/jcc.26133)

<sup>#</sup>: Contributed equally. <sup>\*</sup>: Mentored undergraduate student.

## Teaching and Mentoring

2025	<b>Instructor of record</b> , General Chemistry Lab, Stevenson University. Full teaching responsibility for one section of the lab class, including grading and office hours.
2022	<b>Instructor of record</b> , First-Year Seminar, University of Massachusetts Amherst. Title: “Reconciling Atomic Chaos and Human Order”. I designed this course through the College of Natural Science Teaching Fellowship, including a two-day “teaching bootcamp.” ( <a href="#">link</a> ) <b>Course goals:</b> develop skills in scientific communication, and a perform 4-week mini research project. Assessments were primarily formative, with self-feedback to foster growth mindsets.
2020–25	<b>Guest lectures:</b> Computer-aided Drug Design in a graduate Cancer Biology course, UMB (3x); Discussion seminar moderator on AlphaFold2 in an undergrad Biophysics course, Amherst College; Lecture on molecular mechanics and additive force fields in a graduate Stat. Mech. Course, UMass.
2018–19	<b>Lab TA</b> , General Chemistry I Lab, University of Massachusetts Amherst.

## Mentoring Experience:

Dami Showunmi (undergrad., UMBC, 2025–); Anthony O’Donnell (grad., JHU, 2024–); Samantha Schultz (undergrad., UMass, 2020–2021, **resulted in publication**); Callie Jillson (undergrad., UMass, 2019–2020)

## Presentations

2025	<b>Talk</b> , Frontiers at the Chemistry-Biology Interface Symposium, Johns Hopkins University, “Computational modeling of ternary complexes as ensembles using SILCS-PROTAC,” Baltimore, MD. <b>Talk</b> , Chemistry Department Seminar, George Washington University, “Computational design of PROTACs”, Washington D.C.
2024	<b>Talk</b> , Institute for Bioscience and Biotechnology Research, University of Maryland Baltimore, Early-Career Research Symposium, “Computational design of PROTACs”, Rockville, MD.

- Talk**, University of Maryland Greenbaum Comprehensive Cancer Center Research Symposium, "Physics- and machine-learning-based method for identifying druggable binding sites with SILCS-Hotspots." (Talk award) Baltimore, MD.
- Talk**, The College of Idaho Natural Science Symposium, "Computer simulations of proteins help understand their function." Caldwell, ID.
- Poster**, Biophysical Society Annual Meeting, "Computational mapping of allosteric modulators of the BK channel." Philadelphia, PA.
- 2023 **Poster**, Biophysical Society Annual Meeting, "A predictive model of voltage gating of BK channels via physical modeling and machine learning." San Diego, CA.
- 2022 **Talk**, University of Massachusetts Amherst ResearchFest (PH Terry award): "Predicting protein function with physics, experiments and machine learning." Amherst, MA.
- Poster**, Biophysical Society Annual Meeting, "Free energy of hydrophobic dewetting in gating of BK channels." San Francisco, CA.
- 2020 **Talk**, Northeastern Structural Symposium, "Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling." Virtual.
- Poster**, University of Massachusetts Amherst ResearchFest (WE McEwen Award): "Physical origins of selective promiscuity to Hsp70s revealed through physics-based modeling." Amherst, MA.
- 2019 **Talk**, Biophysics at University of Massachusetts Amherst, "Understanding the origins of DnaK's selective promiscuity with physics-based modeling"
- Poster**, Molecular Biophysics in the Northeast, "Understanding the origins of DnaK's selective promiscuity with physics-based modeling." Boston, MA.

## Service

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- 2025 **Facilitator**, Skills for Faculty Positions panel, University of Maryland Office of Postdoctoral Scholars  
**Moderator**, Career Panel Discussion, University of Maryland, Baltimore Cancer Retreat  
**Poster judge**, Frontiers at the Chemistry-Biology Interface Symposium, Johns Hopkins University
- 2023–24 **Facilitator**, Responsible Conduct of Research NIH training, University of Maryland, Baltimore
- 2024– **Organization committee, Annual Cancer Research Retreat**, University of Maryland, Baltimore (2x)
- 2020–20 **Organization committee, Alumni Networking Symposium**, Chemistry-Biology Interface program, University of Massachusetts Amherst (2x)
- 2020 **Search committee**, Grad. Program Manager, Chemistry Dept. University of Massachusetts Amherst
- 2019–21 **ResearchFest committee** for Chemistry Dept., University of Massachusetts Amherst (3x)

## Journals Refereed for:

Biophys. J., J. Phys. Chem., ACS Omega, J. Chem. Theory Comput., J. Chem. Inf. Model., Comm. Chem., Drug Discov. Today, ACS Chemical Biology

## Outreach

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- 2023–26 **Volunteer instructor**, Baltimore Underground Science Space (BUGSS) ([link](#)), STEM outreach for Baltimore community members in community-accessible lab space  
**Volunteer instructor**, RAMP Program for STEM activity for high-schoolers in Baltimore ([link](#)) (2x)  
**Poster judge**, Mount Royal Middle School Science Fair, Baltimore (2x)  
**Volunteer instructor**, CURE Program University of Maryland, Baltimore, STEM outreach for middle- and high-schoolers in Baltimore ([link](#)) (3x)  
**Volunteer**, Halloween STEM outreach event at Community Engagement Center, University of Maryland, Baltimore (2x)
- 2020–23 **Reviewer for Journal of Emerging Investigators**, 25 articles by middle- / high-school students ([link](#))

2022      **Lab for girls summer science camp**, Eureka! at University of Massachusetts Amherst ([link](#))

## Professional Development

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### Professional Society Memberships:

Biophysical Society (2022–), American Chemical Society (2025–)

2024      **Writing an Effective Teaching Philosophy Statement**, online CIRTL workshop

**Teaching Biophysics at a PUI workshop**, Biophysical Society Annual Meeting

2024      **Safety preparedness trainings**, CPR/AED, Stop the Bleed, Civilian Active Shooter Events, Fire Extinguishers, and Naloxone Training, University of Maryland, Baltimore ([certificates](#))

2022      **CIRTL associate certification**, University of Massachusetts Amherst, achieved through training on evidence-based and inclusive teaching practices ([link](#))

2021      **Evidence-based Undergraduate STEM Teaching**, online course ([link](#))

**Inclusive STEM Teaching**, online course ([link](#))

## Book Chapters

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- Nordquist E, Horrigan F, MacKerell A. Computational ligand binding site prediction. **Springer Nature**. (accepted) 2025.